

**동북아시아 전통의학 비식물 약재
구성성분 (PubMed 문헌 조사)**

Second Edition



한국한의학연구원
KOREA INSTITUTE OF ORIENTAL MEDICINE

동북아시아 전통의학 비식물 약재 구성성분 (PubMed 문헌 조사)

Chemical constituents of non-botanical medicinal
materials in Northeast Asian traditional medicine:
A PubMed literature survey

2018년 4월 20일

초판 발행

2023년 11월 20일

개정 2판 발행



발행처 : 한국한의학연구원

저자 : 김상균

ISBN : 978-89-5970-538-2 (비매품)

비매품/무료

95510



9 788959 705382

ISBN 978-89-5970-538-2 (PDF)

- Citation : Sang-Kyun Kim. Chemical constituents of non-botanical medicinal materials in Northeast Asian traditional medicine: A PubMed literature survey. Second edition, Korea Institute of Oriental Medicine, Daejeon, 2023. (Korean)
- 본 도서는 미래창조과학부의 재원으로 한국연구재단의 지원을 받아 수행한 “빅데이터 기반 약재 조합 예측 AI 시스템 개발” 과제의 연구결과임 (No. 2022R1F1A1063342)

머리말

TCM(traditional Chinese medicine)을 포함한 동북아시아 전통의학(Northeast Asian traditional medicine)에서는 오래 전부터 질병을 치료하기 위해 자연에서 구할 수 있는 다양한 약재(medicinal material)들을 사용해 왔다. 대부분 이러한 약재들은 식물의 꽃, 잎, 가지, 뿌리 등을 이용하는 식물 약재(botanical drug 또는 herbal drug)들이지만 동물, 조개, 광물 등과 같은 비식물 약재(non-botanical drug)들도 사용해 왔다. 현대 의학에서는 전통 문헌에서 언급된 이러한 약재들이 실제 유의미한 효능을 보이는지에 대한 evidence 를 과학 기술을 이용해서 밝히는 연구들이 많이 수행되고 있다. 또한, 이와 같은 약재 효능의 evidence 에 대한 연구들이 많이 축적됨에 따라, 최근에는 약재의 phytochemistry 나 pharmacology 에 대한 systematic review 가 증가하고 있으나, 이러한 연구들은 주로 식물 약재들만 다루고 있으며, 상대적으로 비식물 약재들에 대한 연구는 많이 없는 상황이다.

최근 저자는 2018 년에 PubMed 데이터베이스에서 한국, 중국, 일본의 약전에 수재된 비식물 약재의 구성성분 정보를 조사하여 초판을 발행하였다. 하지만, 이후에 비식물 약재들의 구성성분에 대한 논문들이 지속적으로 발표됨에 따라 구성성분 정보에 대한 업데이트가 필요하여 개정 2 판을 발행하게 되었다. 이번 개정판에서는 섬피 약재가 추가되어 30 개의 약재가 수록되었으며, 성분은 432 개에서 600 개로 증가하였다. 도서의 구성 측면에서 가장 많이 바뀐 부분은 기존에는 구성성분의 구조식만 수록하였으나 구조식뿐만 아니라 성분에 대한 물리화학적 성질, Drug likeness, Oral bioavailability 들을 계산하여 추가로 제공함으로써, 네트워크 약리학 등 다양한 연구분야에서 활용이 될 수 있도록 정보들이 추가된 점이다. 또한, 일부 성분의 화학구조식에서 stereochemistry 를 포함한 일부 오류를 수정하였다.

일러두기

1. 각 약재들은 개별 장으로 나누어 기술하였다. 하지만, 동물의 담즙에 대한 약재들의 경우 약재들의 구성성분들이 유사하여 하나의 장에 포함하였으며, 진주모와 진주는 하나의 생물종일 뿐만 아니라 추출된 성분도 동일하여 하나의 장에서 기술하였다.
2. 각 약재의 이름은 한글, 한자, 중국 약전에 나오는 라틴명을 같이 기술하였으며, 영문명이 있는 경우 영문명도 언급하였고, 각 장에서 한국, 중국, 일본 약전에 나오는 학명들과 과명(Family name)도 기술하였다.
3. 약재의 구성 성분들은 각각의 장마다 하나의 테이블에 리스트 하였다. 테이블은 번호, 성분명, 클래스의 정보를 가지는데 번호는 본 서적 내에서 성분을 식별하는 유일한 번호이다. 또한, 번호는 부록의 구성성분 상세 정보의 번호와 일치한다. 번호가 같더라도 성분명이 동의어들이기 때문에 일치하지 않을 수 있으며 동의어 정보도 부록의 구성성분 상세 정보의 "TM-MC 성분 동의어"에서 확인이 가능하다.
4. 개별 약재의 구성성분이 추출된 참고문헌은 부록의 구성성분 상세 정보의 "PubMed ID"에서 확인이 가능하다.
5. 본 도서에서 제공하는 구성성분 정보는 <https://tm-mc.kr> 에서도 확인이 가능하다.

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1. 섬수(蟾酥), Bufonis Venenum

섬수(蟾酥, Bufonis Venenum, Toad Venom)는 Bufonidae 과에 속하는 두꺼비(*Bufo bufo gargarizans* Cantor, *Bufo melanostictus* Schneider)의 auricular gland 에서 분비된 흰색의 분비물을 건조한 것이다. 섬수의 유효 성분은 C-17 위치에 α -2-pyrone ring 을 가지는 C-24 steroid 의 한 종류인 bufadienolide 이며, bufadienolide 는 일반적으로 C-3 위치의 esterification 에 따라서 conjugated 타입인 bufotoxin 과 free 타입인 bufogenin 으로 나뉘어진다. 또한, C-14 위치의 형태에 따라서 14,15-epoxy group 과 14-hydroxy group 으로 나뉘어지는데, 섬수에서는 52 개의 14,15-epoxy bufadienolide 와 68 개의 14-hydroxy bufadienolide 가 식별되었다. 이러한 bufadienolide 들 중에서도 섬수에서는 bufogenin 들이 많은 것으로 알려져 있으며, 특히 resibufogenin (**1**), cinobufagin (**13**), bufalin (**53**), bufotalin (**67**)은 전체 bufadienolide 의 80% 이상을 차지하고 있다.

이외에도 섬수에는 serotonin (**134**)을 포함한 alkaloid 와 amino acid, nucleobase, nucleoside 등도 포함하고 있다. 아래 표는 섬수에서 포함되어 있다고 알려진 189 개의 성분 리스트이며, 이 중에서 163 개의 성분들에 대한 구조가 식별되었다.

번호	성분명	클래스
1	resibufogenin	14,15-epoxy bufadienolide
2	3-epi-resibufogenin	14,15-epoxy bufadienolide
3	resibufagin	14,15-epoxy bufadienolide
4	deacetylcinobufagin	14,15-epoxy bufadienolide
5	marinobufagin	14,15-epoxy bufadienolide
6	bufotalinin	14,15-epoxy bufadienolide
7	desacetylcinobufotalin	14,15-epoxy bufadienolide
8	11-hydroxyresibufogenin	14,15-epoxy bufadienolide
9	12 β -hydroxyresibufogenin	14,15-epoxy bufadienolide
10	19-oxo-desacetylcinobufagin	14,15-epoxy bufadienolide
11	22,23-epoxyresibufogenin	14,15-epoxy bufadienolide
12	resibufaginol	14,15-epoxy bufadienolide

번호	성분명	클래스
13	cinobufagin	14,15-epoxy bufadienolide
14	cinobufaginol	14,15-epoxy bufadienolide
15	cinobufotalin	14,15-epoxy bufadienolide
16	22,23-epoxycinobufotalin	14,15-epoxy bufadienolide
17	3-oxo-cinobufagin	14,15-epoxy bufadienolide
18	3-oxo-cinobufotalin	14,15-epoxy bufadienolide
19	12 β -hydroxycinobufagin	14,15-epoxy bufadienolide
20	5,12 β -dihydroxycinobufagin	14,15-epoxy bufadienolide
21	19-oxo-cinobufagin	14,15-epoxy bufadienolide
22	19-oxo-cinobufotalin	14,15-epoxy bufadienolide
23	resibufogenin-3-O-succinate-arginine	14,15-epoxy bufadienolide
24	resibufaginol-3-O-succinate-arginine	14,15-epoxy bufadienolide
25	cinobufagin-3-O-succinate-arginine	14,15-epoxy bufadienolide
26	cinobufaginol-3-O-succinate-arginine	14,15-epoxy bufadienolide
27	resibufogenin-3-O-glutarate-arginine	14,15-epoxy bufadienolide
28	cinobufagin-3-O-glutarate-arginine	14,15-epoxy bufadienolide
29	marinobufotoxin	14,15-epoxy bufadienolide
30	cinobufagin-3-O-adipate-arginine	14,15-epoxy bufadienolide
31	19-oxo-cinobufotalin-3-O-adipate-arginine	14,15-epoxy bufadienolide
32	resibufogenin-3-O-pimelate-arginine	14,15-epoxy bufadienolide
33	cinobufagin-3-O-pimelate-arginine	14,15-epoxy bufadienolide
34	cinobufaginol-3-O-pimelate-arginine	14,15-epoxy bufadienolide
35	cinobufotalitoxin	14,15-epoxy bufadienolide
36	resibufogenin-3-O-suberoyl ester	14,15-epoxy bufadienolide
37	cinobufagin-3-O-suberoyl ester	14,15-epoxy bufadienolide
38	resibufotoxin	14,15-epoxy bufadienolide
39	cinobufotoxin	14,15-epoxy bufadienolide
40	cinobufaginol-3-O-suberate-arginine	14,15-epoxy bufadienolide

번호	성분명	클래스
41	19-oxo-cinobufotalin-3-O-suberate-arginine	14,15-epoxy bufadienolide
42	19-oxo-cinobufotalin-3-O-suberate-methylhistidine	14,15-epoxy bufadienolide
43	cinobufagin-3-O-nonanedioic-arginine	14,15-epoxy bufadienolide
44	bufotalinin-3-O-sebacate-arginine	14,15-epoxy bufadienolide
45	methylated-cinobufagin	14,15-epoxy bufadienolide
46	16-desacetyl-19-oxocinobufotalin	14,15-epoxy bufadienolide
47	3-(N-adipoyl argininyl)marinobufagin	14,15-epoxy bufadienolide
48	3-(N-azelayl argininyl)resibufogenin	14,15-epoxy bufadienolide
49	3-(N-suberoyl argininyl)bufotalinin	14,15-epoxy bufadienolide
50	3-(N-suberoyl argininyl)resibufagin	14,15-epoxy bufadienolide
51	methylatedhydroxylcinobufagin	14,15-epoxy bufadienolide
52	3-epi-cinobufagin	14,15-epoxy bufadienolide
53	bufalin	14-hydroxy bufadienolide
54	1 β -hydroxybufalin	14-hydroxy bufadienolide
55	19-oxo-bufalin	14-hydroxy bufadienolide
56	19-hydroxybufalin	14-hydroxy bufadienolide
57	gamabufotalin	14-hydroxy bufadienolide
58	telocinobufagin	14-hydroxy bufadienolide
59	11 α -hydroxytelocinobufagin	14-hydroxy bufadienolide
60	hellebrigenin	14-hydroxy bufadienolide
61	hellebrigenol	14-hydroxy bufadienolide
62	arenobufagin	14-hydroxy bufadienolide
63	bufarenogin	14-hydroxy bufadienolide
64	φ -bufarenogin	14-hydroxy bufadienolide
65	bufalone	14-hydroxy bufadienolide
66	desacetylbufotalin	14-hydroxy bufadienolide
67	bufotalin	14-hydroxy bufadienolide
68	5-hydroxybufotalin	14-hydroxy bufadienolide

번호	성분명	클래스
69	16-O-acetylarenobufagin	14-hydroxy bufadienolide
70	16-acetoxybufarenogin	14-hydroxy bufadienolide
71	gamabufotalin-3-O-sulfate	14-hydroxy bufadienolide
72	arenobufagin-3-O-sulfate	14-hydroxy bufadienolide
73	bufotalin-3-O-sulfate	14-hydroxy bufadienolide
74	19-hydroxybufalin-3-O-sulfate	14-hydroxy bufadienolide
75	telocinobufagin-3-O-sulfate	14-hydroxy bufadienolide
76	desacetylbufotalin-3-O-sulfate	14-hydroxy bufadienolide
77	hellebrigenin-3-O-sulfate	14-hydroxy bufadienolide
78	hellebrigenol-3-O-sulfate	14-hydroxy bufadienolide
79	gamabufotalin-3-oxalate	14-hydroxy bufadienolide
80	bufalin-3-O-suberoyl ester	14-hydroxy bufadienolide
81	gamabufotalin-3-O-suberate	14-hydroxy bufadienolide
82	bufalin-3-O-succinate-arginine	14-hydroxy bufadienolide
83	gamabufotalin-3-O-succinate-arginine	14-hydroxy bufadienolide
84	bufotalin-3-O-succinate-arginine	14-hydroxy bufadienolide
85	bufotalin-3-O-glutarate-arginine	14-hydroxy bufadienolide
86	bufalin-3-O-glutarate-arginine	14-hydroxy bufadienolide
87	bufalin-3-O-adipate-arginine	14-hydroxy bufadienolide
88	gamabufotalin-3-O-adipate-arginine	14-hydroxy bufadienolide
89	gamabufotalin-3-O-pimelate-arginine	14-hydroxy bufadienolide
90	bufalin-3-O-pimelate-arginine	14-hydroxy bufadienolide
91	bufotalin-3-O-pimelate-arginine	14-hydroxy bufadienolide
92	gamabufotalitoxin	14-hydroxy bufadienolide
93	arenobufotoxin	14-hydroxy bufadienolide
94	bufotalin-3-O-suberate-histidine	14-hydroxy bufadienolide
95	bufalin-3-O-suberate-methylhistidine	14-hydroxy bufadienolide
96	bufalitoxin	14-hydroxy bufadienolide

번호	성분명	클래스
97	telocinobufatoxin	14-hydroxy bufadienolide
98	hellebritoxin	14-hydroxy bufadienolide
99	bufotoxin	14-hydroxy bufadienolide
100	3 β ,14 β ,19 β -trihydroxybufa-20,22-dienolide, 3-O-suberate-L-histidine	14-hydroxy bufadienolide
101	gamabufotalin-3-O-pelargonate-arginine	14-hydroxy bufadienolide
102	bufalin-3-O-sebacate-arginine	14-hydroxy bufadienolide
103	12-oxobufalin	14-hydroxy bufadienolide
104	12-oxobufotaline	14-hydroxy bufadienolide
105	monohydroxylbufotalin	14-hydroxy bufadienolide
106	3-(N-succinyl argininy)bufarenogin	14-hydroxy bufadienolide
107	12 β -hydroxylbufalin	14-hydroxy bufadienolide
108	3-(N-adipoyl argininy)arenobufagin	14-hydroxy bufadienolide
109	3-(N-adipoyl argininy)hellebrigenin	14-hydroxy bufadienolide
110	3-(N-adipoyl argininy)telocinobufagin	14-hydroxy bufadienolide
111	3-(N-glutaryl argininy)arenobufagin	14-hydroxy bufadienolide
112	3-(N-glutaryl argininy)hellebrigenin	14-hydroxy bufadienolide
113	3-(N-pimeloyl argininy)arenobufagin	14-hydroxy bufadienolide
114	3-(N-pimeloyl argininy)hellebrigenin	14-hydroxy bufadienolide
115	3-(N-pimeloyl argininy)telocinobufagin	14-hydroxy bufadienolide
116	3-(N-suberoyl argininy)hellebrigenol	14-hydroxy bufadienolide
117	3-(N-succinyl argininy)arenobufagin	14-hydroxy bufadienolide
118	3-(N-succinyl argininy)hellebrigenin	14-hydroxy bufadienolide
119	3-keto-arenobufagin	14-hydroxy bufadienolide
120	3-epi-bufalin	14-hydroxy bufadienolide
121	argentinogenin	other bufadienolide
122	argentinogenin-3-O-adipate-arginine	other bufadienolide
123	hellebrigenol-9,11-ene	other bufadienolide
124	3-dehydroscillarenin	other bufadienolide

번호	성분명	클래스
125	scillarenin-3-pimelate-arginine	other bufadienolide
126	scillarenin-3-suberate-arginine	other bufadienolide
127	3 β ,16 β -dihydroxybufa-8(14),20,22-trienolide	other bufadienolide
128	14,16-dihydroxybufa-5,20,22-trienolide, (14 β ,16 β)-form, 16-Ac	other bufadienolide
129	dehydrated cinobufagin	other bufadienolide
130	dehydro-dehydrated-cinobufagin	other bufadienolide
131	3-(N-adipoyl argininyl)scillarenin	other bufadienolide
132	scillaridin A	other bufadienolide
133	algestone acetonide	steroid
134	serotonin	alkaloid
135	N'-methyl serotonin	alkaloid
136	nicotinic acid	alkaloid
137	(5-hydroxy-1H-indol-3-yl)acetic acid	alkaloid
138	caffeine	alkaloid
139	adrenaline	alkaloid
140	N'-formylserotonin	alkaloid
141	indole-3-acetic acid	alkaloid
142	1-methyl-2,9-dihydro-1H-pyrido [3-b]indol-6-ol	alkaloid
143	5-hydroxy tryptophol	alkaloid
144	bufotenidine	alkaloid
145	bufotenine	alkaloid
146	bufothionine	alkaloid
147	dehydrobufotenine	alkaloid
148	arginine	amino acid
149	valine	amino acid
150	leucine	amino acid
151	undecanedioyl arginine	amino acid
152	azelayl arginine	amino acid

번호	성분명	클래스
153	sebacyl arginine	amino acid
154	glutaryl arginine	amino acid
155	suberoyl arginine	amino acid
156	adipyl arginine	amino acid
157	pimeloyl arginine	amino acid
158	5-hydroxy tryptophan	amino acid
159	succinyl arginine	amino acid
160	adenine	nucleobase
161	xanthine	nucleobase
162	hypoxanthine	nucleobase
163	adenosine	nucleoside
	3-(N-adipoyl argininyl)gamabufotalin isomer	14-hydroxy bufadienolide
	3-(N-azelayl argininyl)resibufogenin isomer	14,15-epoxy bufadienolide
	3-(N-pimeloyl argininyl)arenobufagin isomer	14-hydroxy bufadienolide
	3-(N-pimeloyl argininyl)gamabufotalin isomer	14-hydroxy bufadienolide
	3-(N-suberoyl argininyl)bufotalinin isomer	14,15-epoxy bufadienolide
	3-(N-suberoyl argininyl)cinobufaginol isomer	14,15-epoxy bufadienolide
	adipyl arginine isomer	amino acid
	arenobufotoxin isomer	14-hydroxy bufadienolide
	azelayl arginine isomer	amino acid
	bufotalinin isomer	14,15-epoxy bufadienolide
	cinobufagin isomer	14,15-epoxy bufadienolide
	cinobufagin-3-semi-succinate	14,15-epoxy bufadienolide
	cinobufotalin isomer	14,15-epoxy bufadienolide
	dihydroxybufotalin	14-hydroxy bufadienolide
	gamabufotalitoxin isomer	14-hydroxy bufadienolide
	hellebrigenol isomer	14-hydroxy bufadienolide
	hellebrigenol stereoisomer	14-hydroxy bufadienolide

번호	성분명	클래스
	hydroxybufalin	14-hydroxy bufadienolide
	hydroxytelocinobufagin	14-hydroxy bufadienolide
	marinobufotoxin isomer	14,15-epoxy bufadienolide
	resibufagin isomer	14,15-epoxy bufadienolide
	resibufagin stereoisomer	14,15-epoxy bufadienolide
	resibufogenin-3-suberate-arginine ester stereoisomer	14,15-epoxy bufadienolide
	scillaridin A stereoisomer	other bufadienolide
	sebacyl arginine isomer	amino acid
	undecanedioyl arginine isomer	amino acid

2. 섬피(蟾皮), Bufonis Cutis

섬피(蟾皮, Bufonis Cutis)는 Bufonidae 과에 속하는 두꺼비(*Bufo bufo gargarizans* Cantor, *Bufo melanostictus* Schneider)의 껍질을 건조한 것이다. 섬피의 주요 성분은 섬수와 마찬가지로 bufadienolide 들인데, 특히 섬피는 섬수보다 bufotoxin 성분들을 많이 포함하고 있는 것으로 알려져 있다.

또한, 섬피에도 serotonin (**134**)을 포함한 alkaloid 와 amino acid, nucleobase 등도 포함하고 있다. 아래 표는 섬피에서 포함되어 있다고 알려진 121 개의 성분 리스트이며, 이 중에서 110 개의 성분들에 대한 구조가 식별되었다.

번호	성분명	클래스
1	resibufogenin	14,15-epoxy bufadienolide
2	3-epi-resibufogenin	14,15-epoxy bufadienolide
4	desacetylcinobufagin	14,15-epoxy bufadienolide
5	marinobufagin	14,15-epoxy bufadienolide
6	bufotalinin	14,15-epoxy bufadienolide
7	desacetylcinobufotalin	14,15-epoxy bufadienolide
8	11-hydroxyl resibufogenin	14,15-epoxy bufadienolide
10	19-oxo-desacetylcinobufagin	14,15-epoxy bufadienolide
11	22,23-epoxyresibufogenin	14,15-epoxy bufadienolide
12	resibufaginol	14,15-epoxy bufadienolide
13	cinobufagin	14,15-epoxy bufadienolide
14	cinobufaginol	14,15-epoxy bufadienolide
15	cinobufotalin	14,15-epoxy bufadienolide
17	3-keto-cinobufagin	14,15-epoxy bufadienolide
21	19-oxo-cinobufagin	14,15-epoxy bufadienolide
22	19-oxo-cinobufotalin	14,15-epoxy bufadienolide
23	resibufogenin-3-O-succinate-arginine	14,15-epoxy bufadienolide
25	cinobufagin-3-O-succinate-arginine	14,15-epoxy bufadienolide
28	cinobufagin-3-O-glutarate-arginine	14,15-epoxy bufadienolide

번호	성분명	클래스
29	marinobufotoxin	14,15-epoxy bufadienolide
30	cinobufagin-3-O-adipate-arginine	14,15-epoxy bufadienolide
31	19-oxo-cinobufotalin-3-O-adipate-arginine	14,15-epoxy bufadienolide
32	resibufogenin-3-O-pimelate-arginine	14,15-epoxy bufadienolide
33	cinobufagin-3-O-pimelate-arginine	14,15-epoxy bufadienolide
35	cinobufotalitoxin	14,15-epoxy bufadienolide
38	resibufotoxin	14,15-epoxy bufadienolide
39	cinobufotoxin	14,15-epoxy bufadienolide
42	19-oxo-cinobufotalin-3-O-suberate-methylhistidine	14,15-epoxy bufadienolide
43	cinobufagin-3-O-nonanedioic-arginine	14,15-epoxy bufadienolide
164	3-keto-resibufagin	14,15-epoxy bufadienolide
165	3-keto-deacetylcinobufagin	14,15-epoxy bufadienolide
52	3-epi-cinobufagin	14,15-epoxy bufadienolide
53	bufalin	14-hydroxy bufadienolide
54	1 β -hydroxybufalin	14-hydroxy bufadienolide
55	19-oxo-bufalin	14-hydroxy bufadienolide
57	gamabufotalin	14-hydroxy bufadienolide
58	telocinobufagin	14-hydroxy bufadienolide
60	hellebrigenin	14-hydroxy bufadienolide
61	hellebrigenol	14-hydroxy bufadienolide
62	arenobufagin	14-hydroxy bufadienolide
63	bufarenogin	14-hydroxy bufadienolide
64	ψ -bufarenogin	14-hydroxy bufadienolide
65	3-keto-bufalin	14-hydroxy bufadienolide
66	desacetylbufotalin	14-hydroxy bufadienolide
67	bufotalin	14-hydroxy bufadienolide
71	gamabufotalin-3-O-sulfate	14-hydroxy bufadienolide
72	arenobufagin-3-O-sulfate	14-hydroxy bufadienolide

번호	성분명	클래스
73	bufotalin-3-O-sulfate	14-hydroxy bufadienolide
82	bufalin-3-O-succinate-arginine	14-hydroxy bufadienolide
83	gamabufotalin-3-O-succinate-arginine	14-hydroxy bufadienolide
84	bufotalin-3-O-succinate-arginine	14-hydroxy bufadienolide
87	bufalin-3-O-adipate-arginine	14-hydroxy bufadienolide
88	gamabufotalin-3-O-adipate-arginine	14-hydroxy bufadienolide
89	gamabufotalin-3-O-pimelate-arginine	14-hydroxy bufadienolide
91	bufotalin-3-O-pimelate-arginine	14-hydroxy bufadienolide
92	gamabufotalitoxin	14-hydroxy bufadienolide
93	arenobufotoxin	14-hydroxy bufadienolide
94	bufotalin-3-O-suberate-histidine	14-hydroxy bufadienolide
95	bufalin-3-O-suberate-methylhistidine	14-hydroxy bufadienolide
96	bufalitoxin	14-hydroxy bufadienolide
97	telocinobufotoxin	14-hydroxy bufadienolide
98	hellebritoxin	14-hydroxy bufadienolide
99	bufotoxin	14-hydroxy bufadienolide
100	3 β ,14 β ,19 β -trihydroxybufa-20,22-dienolide, 3-O-suberate-L-histidine	14-hydroxy bufadienolide
105	monohydroxybufotalin	14-hydroxy bufadienolide
107	12 β -hydroxyl-bufalin	14-hydroxy bufadienolide
119	3-keto-arenobufagin	14-hydroxy bufadienolide
120	3-epi bufalin	14-hydroxy bufadienolide
166	3-keto-bufotalin	14-hydroxy bufadienolide
121	argentinogenin	other bufadienolide
123	hellebrigenol-9,11-ene	other bufadienolide
124	3-dehydrobufagin	other bufadienolide
167	3-dehydrocinobufagin	other bufadienolide
168	Δ -3-oxo-resibufogenin	other bufadienolide
134	serotonin	alkaloid

번호	성분명	클래스
135	N-methyl serotonin	alkaloid
136	nicotinic acid	alkaloid
169	nicotinamide	alkaloid
137	(5-hydroxy-1H-indol-3-yl)acetic acid	alkaloid
138	caffeine	alkaloid
170	N-(2-(5-hydroxy-1H-indol-3-yl)ethyl)-N-methylformamide	alkaloid
140	N'-formylserotonin	alkaloid
171	5-methoxy bufotenine	alkaloid
172	cyclo(pro-gly)dipeptide	alkaloid
173	1,2,3,4-tetrahydro-6-hydroxy- β -carboline	alkaloid
174	2-methyl-6-hydroxy-1,2,3,4-tetrahydro- β -carboline	alkaloid
142	1-methyl-2,9-dihydro-1H-pyrido [3-b]indol-6-ol	alkaloid
144	bufotenidine	alkaloid
145	bufotenine	alkaloid
146	bufothionine	alkaloid
175	cyclotufotenine	alkaloid
147	dehydrobufotenine	alkaloid
176	eritadenine	alkaloid
177	O-methyl serotonin	alkaloid
178	shepherdine	alkaloid
149	valine	amino acid
150	leucine	amino acid
152	azelayl arginine	amino acid
153	sebacyl arginine	amino acid
155	suberoyl arginine	amino acid
156	adipyl arginine	amino acid
157	pimeloyl arginine	amino acid
179	bufobutarginine	amino acid

번호	성분명	클래스
159	succinyl arginine	amino acid
160	adenine	nucleobase
180	guanine	nucleobase
181	thymine	nucleobase
182	uracil	nucleobase
161	xanthine	nucleobase
162	hypoxanthine	nucleobase
	3-keto-bufalin stereoisomer	14-hydroxy bufadienolide
	9-19 resibufagin	14,15-epoxy bufadienolide
	BN4	14-hydroxy bufadienolide
	bufalin stereoisomer	14-hydroxy bufadienolide
	bufarenogin stereoisomer	14-hydroxy bufadienolide
	bufotalin stereoisomer	14-hydroxy bufadienolide
	bufotalinin stereoisomer	14,15-epoxy bufadienolide
	cinobufagin isomer	14,15-epoxy bufadienolide
	cinobufotalin stereoisomer	14,15-epoxy bufadienolide
	hellebrigenol-9,11-ene stereoisomer	14-hydroxy bufadienolide
	telocinobufagin stereoisomer	14-hydroxy bufadienolide

3. 봉교(蜂胶), Propolis

봉교(蜂胶, Propolis)는 Apidae 과에 속하는 꿀벌(*Apis mellifera* L.)이 식물에서 채취한 천연 수지에 자신의 분비물을 혼합하여 만든 물질이다. 봉교는 고대부터 약재료 이용되어 왔는데, 주요 성분은 phenolic, flavonoid, glycerol ester 로 알려져 왔다. 봉교의 성분은 수집된 지역의 특정 flora 에 의해서 영향을 받는다. 이러한 이유로 여기에서는 중국, 한국, 일본 지역에서 *A. mellifera* 에 의해서 만들어진 봉교의 성분들만 조사하였다.

봉교의 flavonoid 성분은 flavone, flavonol, flavanol, flavanone, flavanonol, isoflavone 들이 있다. Flavonol 은 flavone 에서 4H-chromene 의 C-3 position 에 hydroxy group 을 가진다. Flavanone 은 flavone 에서 C-2 와 C-3 위치에 수소가 추가된 구조이며, flavanonol 은 flavanone 에서 C-3 위치에 hydroxy 그룹을 가진다. 봉교에 있는 phenolic 들은 phenyl group 의 C-3 과 C-4 위치에 hydroxy 나 methoxy 그룹이 연결되어 있으며 카르복실 그룹에는 여러 esterification 들이 존재한다. 특히, chrysin (**183**), galangin (**192**), pinocembrin (**211**)의 flavonoid 들과 caffeic acid phenethyl ester (CAPE) (**238**)의 phenolic 은 봉교의 지표 성분 들로 알려져 있다.

이 외에도 봉교에는 cinnamic acid 와 같은 phenylalkyl acid 들과 esculetin, nicotinic acid 그리고 여러 형태의 glycerol ester 들도 존재한다. 아래 표는 봉교에 포함되어 있다고 알려진 86 개의 성분 리스트이며, 이 중에서 80 개의 성분들에 대한 구조가 식별되었다.

번호	성분명	클래스
183	chrysin	flavone
184	tectochrysin	flavone
185	apigenin	flavone
186	luteolin	flavone
187	luteolin 5-methyl ether	flavone
188	acacetin	flavone
189	baicalin	flavone
190	chrysin 5-methyl ether	flavone
191	apigenin-7-O-β-D-glucopyranoside	flavone

번호	성분명	클래스
192	galangin	flavonol
193	galangin-5-methyl ether	flavonol
194	fisetin	flavonol
195	quercetin	flavonol
196	quercetin-3-methyl ether	flavonol
197	quercetin 5,7-dimethyl ether	flavonol
198	rutin	flavonol
199	kaempferol	flavonol
200	isorhamnetin	flavonol
201	kaempferide	flavonol
202	izalpinin	flavonol
203	morin	flavonol
204	myricetin	flavonol
205	quercetin-7-methyl ether	flavonol
206	kaempferol-7-methyl ether	flavonol
207	kaempferol-3-methyl ether	flavonol
208	catechin	flavanol
209	α -catechin	flavanol
210	epicatechin	flavanol
211	pinocembrin	flavanone
212	pinocembrin 5-methyl ether	flavanone
213	pinocembrin 7-methyl ether	flavanone
214	naringenin	flavanone
215	hesperetin	flavanone
216	pinobanksin	flavanonol
217	pinobanksin 5-methyl ether	flavanonol
218	pinobanksin 7-methyl ether	flavanonol
219	pinobanksin-3-O-acetate	flavanonol

번호	성분명	클래스
220	pinobanksin-3-O-propionate	flavanonol
221	pinobanksin-3-O-butyrate	flavanonol
222	pinobanksin 3-O-isobutyrate	flavanonol
223	pinobanksin-3-O-pentanoate	flavanonol
224	pinobanksin 3-O-2-methylbutyrate	flavanonol
225	pinobanksin-3-O-hexanoate	flavanonol
226	pinobanksin-3-O-phenylpropionate	flavanonol
227	pinobanksin-5-methyl ether-3-O-acetate	flavanonol
228	pinobanksin-methyl ether	flavanonol
229	pinobanksin-3-O-acetate-5-O-phydroxyphenylpropionate	flavanonol
230	genistein	isoflavone
231	3,4-dimethoxycinnamic acid	phenolic
232	ferulic acid	phenolic
233	isoferulic acid	phenolic
234	p-coumaric acid	phenolic
235	p-coumaric acid benzyl ester	phenolic
236	caffeic acid	phenolic
237	caffeic acid benzyl ester	phenolic
238	caffeic acid phenethyl ester	phenolic
239	caffeic acid isoprenyl ester	phenolic
240	caffeic acid cinnamyl ester	phenolic
241	p-methoxycinnamic acid cinnamyl ester	phenolic
242	gallic acid	phenolic
243	resveratrol	phenolic
244	protocatechuic acid	phenolic
245	p-hydroxybenzoic acid	phenolic
246	hydroxy-cinnamic acid benzyl ester	phenolic
247	coumaric acid methyl ester	phenolic

번호	성분명	클래스
248	vanillic acid	phenolic
249	cinnamic acid	phenylalkyl acid
250	cinnamylidene acetic acid	phenylalkyl acid
251	esculetin	coumarin
136	nicotinic acid	alkaloid
252	(-)-2-acetyl-1-(E)-feruloyl-3-(3''(ζ),16'')-dihydroxy-palmitoylglycerol	glycerol ester
253	2-acetyl-1,3-dicaffeoylglycerol	glycerol ester
254	2-acetyl-1-caffeoyl-3-coumaroylglycerol	glycerol ester
255	2-acetyl-1-feruloyl-3-caffeoylglycerol	glycerol ester
256	2-acetyl-1-feruloyl-3-coumaroylglycerol	glycerol ester
257	2-acetyl-1,3-diferuloylglycerol	glycerol ester
258	(+)-2-acetyl-1-caffeoyl-3-cinnamoylglycerol	glycerol ester
259	2-acetyl-1-coumaroyl-3-cinnamoylglycerol	glycerol ester
260	(+)-2-acetyl-1-feruloyl-3-cinnamoylglycerol	glycerol ester
261	2-acetyl-1,3-dicinnamoylglycerol	glycerol ester
	caffeic acid isoprenyl ester isomer	phenolic
	kaempferol-methyl ether	flavonol
	pinobanksin-methyl ether isomer	flavanonol
	pinobanksin-O-hexenoate	flavanonol
	pinobanksin-O-hexenoate	flavanonol
	quercetin-dimethyl ether isomer	flavonol

4. 봉밀(蜂蜜), Mel

봉밀(蜂蜜, Mel, Honey)은 Apidae 과에 속하는 꿀벌(*Apis mellifera* L., *Apis cerana* Fabricus)이 식물의 nectar 와 honeydew 로부터 모은 sugary food substance 이다. 봉밀의 주요 성분은 carbohydrate 로서 monosaccharide (glucose and fructose), disaccharide, trisaccharide, tetrasaccharide 등의 oligosaccharide 들로 구성된다. 또한, 봉밀은 phenolic, flavonoid, amino acid, phytohormone, mineral 들을 포함하는 것으로 알려져 있다. 봉교의 경우와 마찬가지로 봉밀의 구성 성분은 중국, 한국, 일본에서 *A. mellifera* 와 *A. cerana* 에 의해서 만들어진 봉밀에 대해서만 조사하였다. PubMed 에서 검색된 대부분의 봉밀에 대한 연구들은 유럽이나 오스트레일리아 지역의 봉밀에 대한 연구들이었으며, 몇몇 연구들에서만 중국 봉밀에 대한 성분이 검색되었다. 아래 표는 봉밀의 126 개의 구성성분들의 리스트이며 이중에서 125 개의 성분 구조식이 식별되었다.

번호	성분명	클래스
262	glucose	carbohydrate
263	fructose	carbohydrate
264	turanose	carbohydrate
265	sucrose	carbohydrate
266	maltose	carbohydrate
267	isomaltose	carbohydrate
268	kojibiose	carbohydrate
269	cellobiose	carbohydrate
270	palatinose	carbohydrate
271	gentiobiose	carbohydrate
272	laminaribiose	carbohydrate
273	neotrehalose	carbohydrate
274	nigerose	carbohydrate
275	erlose	carbohydrate
276	panose	carbohydrate
277	isopanose	carbohydrate

번호	성분명	클래스
278	maltotriose	carbohydrate
279	theandrose	carbohydrate
280	melezitose	carbohydrate
281	isomaltotriose	carbohydrate
282	raffinose	carbohydrate
283	kestose	carbohydrate
284	isomelezitose	carbohydrate
285	isomaltotetraose	carbohydrate
286	maltotetraose	carbohydrate
287	stachyose	carbohydrate
288	nystose	carbohydrate
289	α -4'-glucosyl-erlose	carbohydrate
290	α -6'-glucosyl-erlose	carbohydrate
183	chrysin	flavone
185	apigenin	flavone
186	luteolin	flavone
189	baicalin	flavone
291	vitexin	flavone
192	galangin	flavonol
195	quercetin	flavonol
198	rutin	flavonol
199	kaempferol	flavonol
200	isorhamnetin	flavonol
203	morin	flavonol
204	myricetin	flavonol
292	quercetrin	flavonol
293	(-)-epigallocatechin	flavanol
211	pinocembrin	flavanone

번호	성분명	클래스
214	naringenin	flavanone
215	hesperetin	flavanone
294	hesperedin	flavanone
230	genistein	isoflavone
295	calycosin	isoflavone
296	calycosin-7-O-β-D-glucoside	isoflavone
297	formononetin	isoflavone
298	genistin	isoflavone
299	ononin	isoflavone
231	3,4-dimethoxycinnamic acid	phenolic
232	ferulic acid	phenolic
233	isoferulic acid	phenolic
234	p-coumaric acid	phenolic
236	caffeic acid	phenolic
238	CAPE	phenolic
242	gallic acid	phenolic
244	protocatechuic acid	phenolic
245	p-hydroxybenzoic acid	phenolic
300	syringic acid	phenolic
301	chlorogenic acid	phenolic
302	sinapic acid	phenolic
303	3-hydroxybenzoic acid	phenolic
304	rosmarinic acid	phenolic
248	vanillic acid	phenolic
305	salicylic acid	phenolic
306	(+)-abscisic acid	phenolic
307	(-)-abscisic acid	phenolic
308	Asp	amino acid

번호	성분명	클래스
309	Glu	amino acid
310	Ser	amino acid
311	Gln	amino acid
312	His	amino acid
313	Gly	amino acid
314	Thr	amino acid
148	Arg	amino acid
315	Ala	amino acid
316	Tyr	amino acid
149	Val	amino acid
317	Met	amino acid
318	Trp	amino acid
319	Phe	amino acid
320	Ile	amino acid
150	Leu	amino acid
321	Lys	amino acid
322	Pro	amino acid
323	2-methylthio-cis-zeatin	phytohormone
324	2-methylthio-cis-zeatin roboside	phytohormone
325	2-methylthio-N6-isopentenyladenine	phytohormone
326	2-methylthio-N6-isopentenyladenosine	phytohormone
327	2-methylthio-trans-zeatin	phytohormone
328	2-methylthio-trans-zeatin roboside	phytohormone
329	28-homobrassinolide	phytohormone
330	28-norbrassinolide	phytohormone
331	28-norcastasterone	phytohormone
332	brassinolide	phytohormone
333	castasterone	phytohormone

번호	성분명	클래스
334	cis-zeatin	phytohormone
335	cis-zeatin roboside	phytohormone
336	dihydrozeatin	phytohormone
337	dihydrozeatin riboside	phytohormone
338	gibberellin A1	phytohormone
339	gibberellin A15	phytohormone
340	gibberellin A24	phytohormone
341	gibberellin A34	phytohormone
342	gibberellin A4	phytohormone
343	gibberellin A51	phytohormone
344	gibberellin A6	phytohormone
345	gibberellin A8	phytohormone
141	indole-3-acetic acid	phytohormone
346	indole-3-butyric acid	phytohormone
347	jasmonic acid	phytohormone
348	jasmonoyl-leucine	phytohormone
349	jasmonoyl-phenylalanine	phytohormone
350	N6-isopentenyladenine	phytohormone
351	N6-isopentenyladenosine	phytohormone
352	trans-zeatin	phytohormone
353	trans-zeatin roboside	phytohormone
354	Ca	inorganic element
355	Mg	inorganic element
356	K	inorganic element
357	P	inorganic element

5. 해삼(海蔘), Stichopus

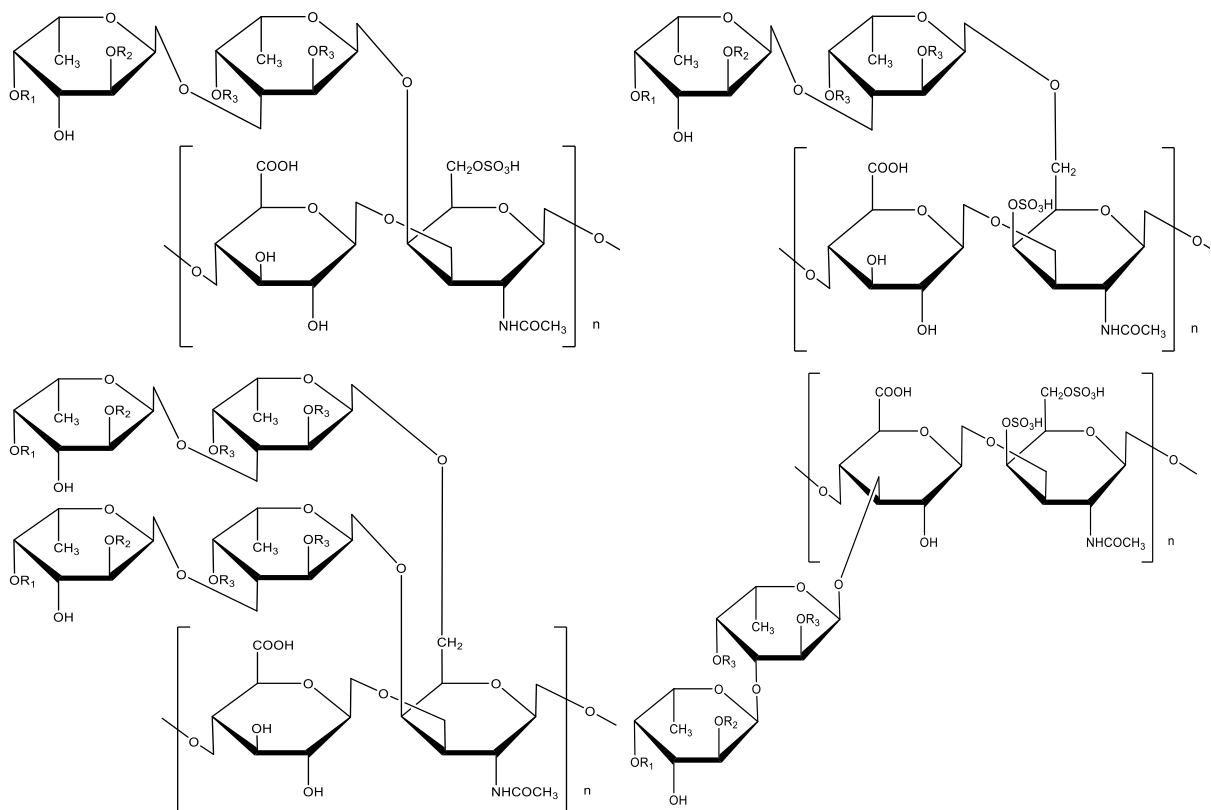
해삼(海蔘, Stichopus, Sea cucumber)은 Stichopodidae 과의 극피 동물이다. 한국 약전에서 해삼은 *Apostichopus japonicus* Selenka (*Stichopus japonicus* Selenka)의 몸체 벽이 약으로 이용된다고 기술되어 있으며, 중국을 포함한 아시아 지역에서는 수 천년 동안 몸에 좋은 음식으로 섭취되어 왔다. 해삼의 체벽에는 triterpene glycoside, glycosaminoglycan, cerebroside 와 같은 다양한 종류의 유효 성분들을 포함하고 있다.

이 성분들 중에서 triterpene glycoside 는 해삼에서 가장 중요한 secondary metabolite 이다. 그 동안 Aspidochirotida 목의 Stichopodidae 과와 Dendrochirotida 목의 Cucumariidae 과에 속해 있는 여러 종의 해삼들에 대해서 수 백 개의 triterpene glycoside 들이 발견되었는데, *A. japonicus* 는 17 개의 triterpene glycoside 들이 존재하는 것으로 알려져 있다. 모든 triterpene glycoside 들은 C18(20) lactone 그룹과 $\Delta 7(8)$ 또는 $\Delta 9(11)$ 이중 연결이 있는 holostane-type aglycone 을 가지며, aglycone 의 C-3 위치에 최대 6 개의 monosaccharide 가 공유 결합되어 있다. 아래 표는 해삼에서 포함되어 있다고 알려진 32 개의 성분 리스트이며, 이 중에서 30 개의 성분들은 성분 구조가 명확히 식별되었다.

번호	성분명	클래스
358	holothurin A1	triterpene glycoside
359	holothurin A	triterpene glycoside
360	echinoside A	triterpene glycoside
361	24-dehydroechinoside A	triterpene glycoside
362	pervicoside C	triterpene glycoside
363	holothurinoside A	triterpene glycoside
364	17-dehydroxyholothurinoside A	triterpene glycoside
365	cladoloside B	triterpene glycoside
366	holothurin B2	triterpene glycoside
367	holothurin B	triterpene glycoside
368	holotoxin A	triterpene glycoside
369	holotoxin B	triterpene glycoside

번호	성분명	클래스
370	holotoxin A1	triterpene glycoside
371	holotoxin B1	triterpene glycoside
372	bivittoside C	triterpene glycoside
373	frondoside A2	triterpene glycoside
374	frondoside A	triterpene glycoside
163	adenosine	amino acid
375	ethyl- α -D-glucopyranoside	carbohydrate
376	5,6-dihydro-3-methylthymidine	nucleoside
377	3-methy-2'-deoxyuridine	nucleoside
378	N-(1''-amino-3''-hexadecene)-2'-deoxyuridine	nucleoside
379	N-(2''-amino-1''-hydroxy-4''-hexadecene)-2'-deoxyuridine	nucleoside
380	N-(2''-amino-1'',3''-dihydroxy-4''-eicosene)-dihydroribothymidine	nucleoside
381	N-(2''-amino-1'',3''-dihydroxy-4''-eicosene)-thymidine	nucleoside
382	N-(2''-amino-1'',3''-dihydroxy-4'',8''-heptadecadiene)-dihydroribothymidine	nucleoside
383	N-(2''-amino-1'',3''-dihydroxy-4''-nonadecene)-thymidine	nucleoside
384	N-(2''-amino-1'',3''-dihydroxy-4'',8''-heptadecadiene)-ribothymidine	nucleoside
385	N-(2''-amino-1'',3''-dihydroxy-4'',8''-octadecadiene)-dihydroribothymidine	nucleoside
386	N-(2''-amino-1'',3''-dihydroxy-octodecane)-thymidine	nucleoside
	fucosylated chondroitin sulfate	glycosaminoglycan
	cerebroside	glycosaminoglycan

해삼의 glycosaminoglycan 클래스 성분인 fucosylated chondroitin sulfate 는 chondroitin sulfate 의 disaccharide unit 이 반복되어 구성되는 linear polysaccharide 구조를 가진다. Chondroitin sulfate 는 glucuronic acid (GlcA)와 C-4 과 C-6 위치에 sulfate 가 있는 N-acetylgalactosamine (GalNAc)들로 구성되며, GlcA 의 C-3 위치나 GalNAc 의 C-4 and/or C-6 위치에서 sulfated fucose branch 들과 글리코시드 결합이 존재한다. 이러한 chondroitin sulfate 의 fucosylation 의 형태는 holothurian 종마다 다른데, *A. japonicus* 은 아래 그림과 같이 fucose 가지에서 6 개 타입의 sulfate 패턴을 보인다. [R₁, R₂, R₃] = [SO₃H, SO₃H, H], [SO₃H, H, H], [H, SO₃H, H], [SO₃H, SO₃H, SO₃H], [SO₃H, H, SO₃H], and [H, SO₃H, SO₃H]



또 다른 해삼의 glycosaminoglycan 클래스 성분인 cerebroside 는 식물, 동물, 해양생물들에서 발견되는 glycosphingolipid 들이다. Cerebroside 는 sphingoid base, fatty acid, monosaccharide 들로 구성되어 있다. 여기에서 fatty acid 는 amide bond 를 통해 sphingoid base 에 연결되며, sphingoid base 의 1-hydroxyl moiety 에 glucose 나 galactose 중 하나의 monosaccharide 가 연결된다. Cerebroside 는 sphingoid base 와 fatty acid 의 chain length, saturation, hydroxylation 의 차이에 따라서 종류가 다양하다. 해삼에서 발견된 sphingoid base 와 fatty base 들의 종류는 아래 표와 같다.

Sphingoid base	Fatty acid
2-amino-1,3,4-trihydroxy-4-hexadecene (t16:0)	C24:1
2-amino-1,3-dihydroxy-4-hexadecene (d16:1)	C23:1, C24:0, C24:1, C25:0
2-amino-1,3-dihydroxy-4,8-hexadecadiene (d16:2)	C25:0
2-amino-1,3-dihydroxy-4-heptadecene (d17:1)	C18:0, C20:0, C22:0, C22:1, C23:0, C23:1, C24:0, C24:1, C25:0
sphingosine (4-sphingenine, d18:1)	C18:0, C21:0, C22:0, C24:0, C24:1, C25:0
4,8-sphingadienine (d18:2)	C18:0, C23:0, C24:0, C24:1, C25:0
2-amino-1,3-dihydroxy-4,8,10-octadecatriene (d18:3)	C18:0, C20:0, C22:0, C22:1, C23:1, C24:1
2-amino-1,3-dihydroxy-4-nonanedecene (d19:1)	C18:0, C22:0, C23:0, C24:0, C24:1, C25:0

9-methyl-4,8-sphingadienine (d19:2)	C18:0, C24:1, C25:0
2-amino-1,3-dihydroxy-9-methyl-4,8,10-octadecatriene (d19:3)	C18:0, C22:0, C22:1, C23:1, C24:1
2-amino-1,3-dihydroxy-4,8,10-icosadecatriene (d20:3)	C18:0

6. 우황(牛黃, Bovis Calculus), 인공우황(人工牛黃, Bovis Calculus Artifactus), 체외배육우황(体外培育牛黃, Bovis Calculus Sativus), 우담(牛膽, Bovis Fel), 웅담(熊膽, Ursi Fel), 저담(豬膽, Suis Fellis Pulvis), 사담(蛇膽, Serpentis Fel)

전통 의학에서는 오래 전부터 소, 돼지, 곰, 뱀과 같은 동물의 담석이나 담즙을 약재로 이용해왔다. 이 약재들에서 유효 성분은 bile acid 인데, 최근 약재별로 어떤 bile acid 들을 얼마나 가지고 있는지에 대한 연구가 수행되어 왔다.

우황(牛黃, Bovis Calculus, cow bezoar, natural Calculus Bovis)은 Bovidae 과에 속하는 소 *Bos taurus domesticus* Gmelin 의 담석을 건조한 것이다. 하지만 우황은 채취되는 양이 적고 가격도 비싸기 때문에 최근에는 우황의 대체제로 인공우황(人工牛黃, Bovis Calculus Artifactus, artificial Calculus Bovis)이 개발되었다. 인공우황은 cattle bile, cholic acid (387), hyodeoxycholic acid (390), taurine (400), bilirubin (401), cholesterol (407)을 섞어 만든 것으로 우황에 비해 가격은 훨씬 싸지만 우황과 비슷한 효능을 보이는 것으로 알려져 있다. 또한 체외배육우황(体外培育牛黃, Bovis Calculus Sativus)도 개발되었는데, 시장에서는 인공우황이 더 많이 거래되고 있다. 아래 표는 우황의 구성성분들로서, 22 개의 성분들 중 21 개 성분의 화학구조가 식별되었다. 우황의 주요 성분은 bild acid 로써, bile acid 는 스테로이드의 한 종류로써 C-17 위치에 있는 side chain 에 카르복실 그룹을 가지는 특징이 있다. 이외에도 우황에는 taurine, bilirubin 과 여러 종류의 steroid 들을 포함하고 있다.

번호	성분명	클래스
387	cholic acid	bile acid
388	deoxycholic acid	bile acid
389	chenodeoxycholic acid	bile acid
390	hyodeoxycholic acid	bile acid
391	ursodeoxycholic acid	bile acid
392	lithocholic acid	bile acid

번호	성분명	클래스
393	glycocholic acid	bile acid
394	glycodeoxycholic acid	bile acid
395	glycochenodeoxycholic acid	bile acid
396	taurocholic acid	bile acid
397	taurodeoxycholic acid	bile acid
398	taurochenodeoxycholic acid	bile acid
399	taurocholate sodium	bile acid
400	taurine	amino sulfonic acid
401	bilirubin	tetrapyrrole
402	7 β -hydroxycholesterol	steroid
403	25-hydroxycholesterol	steroid
404	5,6 α -epoxycholesterol	steroid
405	5,6 β -epoxycholesterol	steroid
406	cholestane-3 β ,5 α ,6 β -triol	steroid
407	cholesterol	steroid
	cholic acid isomer	bile acid

아래 표는 인공우황의 구성성분들로서, 25 개의 성분들 중 24 개 성분의 화학구조가 식별되었다. 이 중에서 glycolithocholic acid (**408**), tauroolithocholic acid (**409**), tauroursodeoxycholic acid (**410**)의 세 개의 성분은 우황에는 없지만 인공우황에서 발견된 성분들이다.

번호	성분명	클래스
387	cholic acid	bile acid
388	deoxycholic acid	bile acid
389	chenodeoxycholic acid	bile acid
390	hyodeoxycholic acid	bile acid
391	ursodeoxycholic acid	bile acid
392	lithocholic acid	bile acid

번호	성분명	클래스
393	glycocholic acid	bile acid
394	glycodeoxycholic acid	bile acid
395	glycochenodeoxycholic acid	bile acid
408	glycolithocholic acid	bile acid
396	taurocholic acid	bile acid
397	taurodeoxycholic acid	bile acid
398	taurochenodeoxycholic acid	bile acid
409	taurolithocholic acid	bile acid
410	tauroursodeoxycholic acid	bile acid
399	taurocholate sodium	bile acid
400	taurine	amino sulfonic acid
401	bilirubin	tetrapyrrole
402	7 β -hydroxycholesterol	steroid
403	25-hydroxycholesterol	steroid
404	5,6 α -epoxycholesterol	steroid
405	5,6 β -epoxycholesterol	steroid
406	cholestane-3 β ,5 α ,6 β -triol	steroid
407	cholesterol	steroid
	cholic acid isomer	bile acid

아래 표는 체외배육우황의 구성성분들로서, 18 개의 성분들 중 17 개 성분의 화학구조가 식별되었다. 이 중에서 3 α ,12 α -dihydroxy-7-oxo-5 β -cholanic acid (**411**)의 성분은 다른 약재에는 없는 성분이며 나머지 16 개의 성분은 모두 우황에도 존재하는 성분이다.

번호	성분명	클래스
387	cholic acid	bile acid
388	deoxycholic acid	bile acid
389	chenodeoxycholic acid	bile acid

번호	성분명	클래스
390	hyodeoxycholic acid	bile acid
391	ursodeoxycholic acid	bile acid
392	lithocholic acid	bile acid
411	3 α ,12 α -dihydroxy-7-oxo-5 β -cholanic acid	bile acid
393	glycocholic acid	bile acid
394	glycodeoxycholic acid	bile acid
395	glycochenodeoxycholic acid	bile acid
396	taurocholic acid	bile acid
397	taurodeoxycholic acid	bile acid
398	taurochenodeoxycholic acid	bile acid
399	taurocholate sodium	bile acid
400	taurine	amino sulfonic acid
401	bilirubin	tetrapyrrole
407	cholesterol	steroid
	cholic acid isomer	bile acid

우담(牛膽, Bovis Fel)은 Bovidae 과에 속하는 소(*Bos taurus domesticus* Gmelin) 또는 물소(*Bubalus bubalis* Linne)의 쓸개를 말린 것이다. 아래 표는 우담의 구성성분들로서, 17 개의 성분들 중 16 개 성분의 화학구조가 식별되었다. 이 중에서 glycohyodeoxycholic acid (**412**)과 taurohyodeoxycholic acid (**413**)의 두 개의 성분은 우황이나 인공우황에는 없지만 우담에서 발견된 성분들이다.

번호	성분명	클래스
387	cholic acid	bile acid
388	deoxycholic acid	bile acid
389	chenodeoxycholic acid	bile acid
391	ursodeoxycholic acid	bile acid
393	glycocholic acid	bile acid
394	glycodeoxycholic acid	bile acid

번호	성분명	클래스
395	glycochenodeoxycholic acid	bile acid
412	glycohyodeoxycholic acid	bile acid
396	taurocholic acid	bile acid
397	taurodeoxycholic acid	bile acid
398	taurochenodeoxycholic acid	bile acid
413	taurohyodeoxycholic acid	bile acid
409	taurolithocholic acid	bile acid
410	tauroursodeoxycholic acid	bile acid
399	taurocholate sodium	bile acid
407	cholesterol	steroid
	phosphatidylcholine	phospholipid

웅담(熊膽, Ursi Fel)은 Ursidae 과에 속하는 곰(*Ursus arctos* Linne, *Selenaretos thibetanus* Cuvier)의 담즙을 말린 것이다. 아래 표는 웅담의 구성성분들로서, 16 개의 성분들 중 13 개 성분의 화학구조가 식별되었다. 이 중에서 7-keto-taurochenodeoxycholic acid (**414**)는 웅담에서만 발견된 성분이다.

번호	성분명	클래스
387	cholic acid	bile acid
389	chenodeoxycholic acid	bile acid
391	ursodeoxycholic acid	bile acid
392	lithocholic acid	bile acid
394	glycodeoxycholic acid	bile acid
395	glycochenodeoxycholic acid	bile acid
408	glycolithocholic acid	bile acid
396	taurocholic acid	bile acid
397	taurodeoxycholic acid	bile acid
398	taurochenodeoxycholic acid	bile acid
409	taurolithocholic acid	bile acid

번호	성분명	클래스
410	tauroursodeoxycholic acid	bile acid
414	7-keto-taurochenodeoxycholic acid	bile acid
	phosphatidylcholine	phospholipid
	phosphatidylethanolamine	phospholipid
	phosphatidylinositol	phospholipid

저담(猪膽, Suis Fellis Pulvis)은 Suidae 과에 속하는 돼지(*Sus scrofa* Linne, *Sus scrofa domestica* Brisson)의 담즙을 말린 것이다. 아래 표는 저담의 구성성분들로서, 17 개의 성분들의 화학구조가 식별되었다. 이 중에서 glycohyodeoxycholic acid (**412**)과 taurohyodeoxycholic acid (**413**)의 두 개의 성분은 우황이나 인공우황에는 없으며 우담에서도 발견된 성분들이고, glycohyocholic acid (**415**)와 taurohyocholic acid (**416**)는 저담에서만 발견된 성분들이다.

번호	성분명	클래스
387	cholic acid	bile acid
388	deoxycholic acid	bile acid
389	chenodeoxycholic acid	bile acid
390	hyodeoxycholic acid	bile acid
391	ursodeoxycholic acid	bile acid
393	glycocholic acid	bile acid
394	glycodeoxycholic acid	bile acid
395	glycochenodeoxycholic acid	bile acid
415	glycohyocholic acid	bile acid
412	glycohyodeoxycholic acid	bile acid
408	glycolithocholic acid	bile acid
398	taurochenodeoxycholic acid	bile acid
416	taurohyocholic acid	bile acid
413	taurohyodeoxycholic acid	bile acid
409	taurolithocholic acid	bile acid

번호	성분명	클래스
399	taurocholate sodium	bile acid
407	cholesterol	steroid

사담(蛇膽, Serpentin Fel)은 Elapidae 과에 속하는 뱀(*Naja naja* Cantor, *Bungarus fasciatus* Schneider) 또는 Colubridae 과에 속하는 뱀(*Elaphe radiata* Schlegel, *Ptyas korros* Schlegel, *Zaocys dhumnades* Cantor)의 쓸개를 말린 것이다. 아래 표는 사담의 구성성분들로서, 5 개 성분들의 화학구조가 식별되었으며, 이 성분들은 전부 우황에서도 발견된 성분들이다.

번호	성분명	클래스
392	lithocholic acid	bile acid
394	glycodeoxycholic acid	bile acid
396	taurocholic acid	bile acid
397	taurodeoxycholic acid	bile acid
398	taurochenodeoxycholic acid	bile acid

7. 담낭성(膽南星), *Arisaema cum Bile*

담낭성(膽南星, *Arisaema cum Bile*)은 Araceae 과에 속하는 천남성(*Arisaema amurense* Maximowicz, *Arisaema erubescens* Schott, *Arisaema heterophyllum* Blume) 가루와 소, 양 또는 돼지의 담즙을 섞어 발효 가공한 약재이다. 담낭성은 전통의학에서 많이 사용되었으며, 고문헌에는 그 효능이 알려져 있으나 현대 의학에서는 담낭성에 대한 성분 분석과 같은 연구가 거의 없는 상황이다. PubMed 에는 담낭성에서 phenolic 과 bile acid 들을 추출한 연구들이 존재한다. 아래 표는 이러한 11 개의 성분들에 대한 리스트이다.

번호	성분명	클래스
232	ferulic acid	phenolic
242	gallic acid	phenolic
195	quercetin	phenolic
208	catechin	phenolic
300	syringic acid	phenolic
301	chlorogenic acid	phenolic
302	sinapic acid	phenolic
417	neohesperidin	phenolic
389	chenodeoxycholic acid	bile acid
390	porcine deoxycholic acid	bile acid
418	porcine cholic acid	bile acid

8. 사향(麝香, Moschus)

사향(麝香, Moschus, Musk)은 Moschidae 과에 속하는 사향쥐(*Moschus berezovskii* Flerove, *M. chrysogaster* Hodgson, *M. moschiferus* Linne, *M. sifanicus* Przewalski) 수컷의 사향선 분비물이다. 사향은 전세계적으로 향수 제조에 이용되는 중요한 재료일 뿐만 아니라, 전통의학 분야에서 가장 유명하고 비싼 약재들 중에 하나이다. 사향의 성분에 대해서는 많은 연구가 수행되어 왔는데 사향은 muscone (419)과 여러 steroid 들을 포함한다고 알려져 있다. 특히, muscone 은 사향의 독특한 향기를 내는 성분으로써 사향의 품질을 평가하는데 가장 중요하게 이용되는 지표 성분이다. 또한, muscone 과 비슷한 구조를 가지는 성분으로 normuscone (420) 과 muscopyridine (421)이 존재한다. 이외에도 사향에는 alkane, alcohol, aldehyde, carboxylic acid 들도 발견되었다. 사향의 구성성분은 38 개가 식별되었으며 아래 표에 리스트되어 있다.

번호	성분명	클래스
419	muscone	macrocyclic ketone
420	normuscone	macrocyclic ketone
421	muscopyridine	alkaloid
422	androsterone	steroid
423	etiocholanolone	steroid
424	5 α -androstane-3 α ,17 β -diol	steroid
425	5 β -androstane-3 α ,17 β -diol	steroid
426	epiandrosterone	steroid
427	androsterone, trifluoroacetate	steroid
428	dehydroandrosterone	steroid
429	3-ethyl-3-hydroxy-5 α -androstan-17-one	steroid
430	cholestan-3-ol	steroid
431	testosterone	steroid
432	epitestosterone	steroid
433	androst-4-ene-3,17-dione	steroid
407	cholesterol	steroid

번호	성분명	클래스
434	dehydroepiandrosterone	steroid
435	prasterone-3-sulfate	steroid
436	cholest-7-en-3 β -ol	steroid
437	4 α -methyl-5 α -cholest-8(14)-en-3 β -ol	steroid
438	androstan-17-one	steroid
1	resibufogenin	14,15-epoxy bufadienolide
439	acetal	acetal
440	6-methylheptane-1,6-diol	alcohol
441	1,2,6-hexanetriol	alcohol
442	12-methyl-E,E-2,13-octadecadien-1-ol	alcohol
443	olealdehyde	aldehyde
444	14-methyl-8-hexadecenal Z	aldehyde
445	13-tetradecenal	aldehyde
446	cis-9-hexadecenal	aldehyde
447	8-n-hexylpentadecane	alkane
448	2,6,10,15-tetramethylheptadecane	alkane
449	benzeneacetic acid	carboxylic acid
450	doconexent	carboxylic acid
451	1,2-benzenedicarboxylic acid	carboxylic acid
452	m-cresol	phenolic
453	2-tert-butyl-4,6-bis(3,5-di-tert-butyl-4-hydroxybenzyl)phenol	phenolic
454	antioxidant 2264	phenolic

9. 녹용(鹿茸), *Cervi Cornu Pantotrichum*

녹용(鹿茸, Deer antler)은 Cervidae 과에 속하는 사슴(*Cervus nippon* Temminck, *C. elaphus* Linne, *C. canadensis* Erxleben)의 골질화되지 않은 뿔을 말린 것이다. 녹용의 성분은 phospholipid, ganglioside, glycoprotein, nucleoside 등인 것으로 알려져 있다.

녹용은 C14:0, C16:0, C18:0, C18:1, C18:2, C20:4 타입의 fatty acid 를 가지는 phosphatidylcholine 들을 포함하고 있으며, 아래 표와 같은 5 가지 ganglioside 들도 가지고 있다.

Ganglioside	Sphingoid base	Fatty acid	Sialic acid
GM ₃	eicosasphingosine (C20)	C22:0	Neu5Ac
GM ₃	sphingosine (C18)	C16:0	Neu5Ac
GM ₃	sphingosine (C18)	C16:0	Neu5Gc
GD ₃	eicosasphingosine (C20)	C22:0	Neu5Ac
GD ₃	sphingosine (C18)	C16:0	Neu5Ac

또한, 녹용은 glycosaminoglycan 성분들을 가지고 있는데 chondroitin sulfate 는 녹용의 주요 glycosaminoglycan 성분이며, heparan sulfate 와 DWA-2 와 같은 성분들도 포함하는 것으로 알려져 있다. 이 외에도 녹용에는 아래 표와 같이 17 개의 nucleoside 와 nucleobase 들이 존재한다.

번호	성분명	클래스
160	adenine	nucleobase
180	guanine	nucleobase
181	thymine	nucleobase
182	uracil	nucleobase
455	cytidine	nucleobase
161	xanthine	nucleobase
162	hypoxanthine	nucleobase
163	adenosine	nucleoside
456	2'-deoxyadenosine	nucleoside
457	2'-deoxyguanosine	nucleoside
458	guanosine	nucleoside

번호	성분명	클래스
459	thymidine	nucleoside
460	2'-deoxyuridine	nucleoside
461	uridine	nucleoside
462	2'-deoxycytidine	nucleoside
463	2'-deoxyinosine	nucleoside
464	inosine	nucleoside
	ganglioside	ganglioside
	chondroitin sulfate	glycosaminoglycan
	heparan sulfate	glycosaminoglycan
	phosphatidylcholine	phospholipid
	DWA-2	polysaccharide

10. 수우각(水牛角), Bubali Cornu

수우각(水牛角, Bubali Cornu, water buffalo horn)은 Bovidae 과에 속하는 *Bubalus bubalis* Linnaeus 의 뿔이다. 수우각의 구성 성분은 amino acid, peptide 들을 포함하는 것으로 알려져 있다. 최근 Liu et al.의 연구¹에서는 수우각으로부터 WBH-1, WBH-2, WBH-3 의 세 종류의 peptide 들을 추출하였다. WBH-1, WBH-2, WBH-3 의 아미노산 시퀀스는 각각 Gln-Tyr-Asp-Gln-Gly-Val (708 Da), Tyr-Glu-Asp-Cys-Thr-Asp-Cys-Gly-Asn (1018 Da), Ala-Ala-Asp-Asn-Ala-Asn-Glu-Leu-Phe-Pro-Pro-Asn (1271 Da)이다.

번호	성분명	클래스
	WBH-1	peptide
	WBH-2	peptide
	WBH-3	peptide

¹ Liu R, Wang M, Duan JA, Guo JM, Tang YP: Purification and identification of three novel antioxidant peptides from Cornu Bubali (water buffalo horn). *Peptides* 2010, 31(5):786-793.

11. 수질(水蛭), Hirudo

수질(水蛭, Hirudo)은 거머리(Hirudinidae 과)에 속하는 *Hirudo nipponica* Whitman, Haemopidae 과)에 속하는 *Whitmania pigra* Whitman 나 *W. acranulata* Whitman)의 몸체를 말린 것이다. 수질에 포함된 성분은 nucleobase, amino acid, peptide 들로 알려져 있는데, 특히 수질의 anticoagulant peptide 들에 대해서 많은 약리학적 연구가 수행되어 왔다. Thrombin inhibitor 로 작용하는 대표적인 anticoagulant 인 hirudin 은 *Hirudo medicinalis* 에서 추출된 성분인데 오래 전부터 임상에서 많이 사용되어 왔다. 이러한 hirudin 과 유사한 anticoagulant peptide 들로써, 최근 whitmanin (8608 Da)², whitide (1997.1 Da)³, WP-30 (3140.63 Da)⁴, H1 (14998 Da), H2 (15988 Da), H3 (15956 Da)⁵, WA3-1 (1422 Da)⁶ 등이 수질에서 추출되었다. 이 peptide 들 중에서 whitide, WP-30, WA3-1 의 아미노산 시퀀스는 GPAGPVGAPGGPGVRGLPGDRG, VISRTQSNVQAAWGQVGGHA ADYSAVAIER, HDLNNKLEYE 로 알려져 있다. 또한, HF2 (<874 Da)⁷라는 high Fischer's ratio peptide 도 수질에서 추출되었다. Peptide 이외에도 아래 표와 같이 14 개 amino acid 와 uracil, xanthine, hypoxanthine 의 3 개의 nucleobase 도 수질에서 추출되었다.

번호	성분명	클래스
310	Ser	amino acid
312	His	amino acid
313	Gly	amino acid
314	Thr	amino acid

² Zhong S, Cui Z, Sakura N, Wang D, Li J, Zhai Y: A rapid method for isolation and purification of an anticoagulant from *Whitmania pigra*. Biomed Chromatogr 2007, 21(5):439-445.

³ Zheng X, Li J, Chen Z, Liu Y, Chen K: Purification and characterization of an anticoagulant oligopeptide from *Whitmania pigra* Whitman. Pharmacogn Mag 2015, 11(43):444-448.

⁴ Liu X, Wang C, Ding X, Liu X, Li Q, Kong Y: A novel selective inhibitor to thrombin-induced platelet aggregation purified from the leech *Whitmania pigra*. Biochem Biophys Res Commun 2016, 473(1):349-354.

⁵ Xiao L, Nie J, Li D, Chen K: Peptides from two sanguinivorous leeches analyzed by ultra-performance liquid chromatography coupled with electrospray ionization quadrupole time-of-flight mass spectrometric detector. Pharmacogn Mag 2015, 11(41):32-37

⁶ Ren Y, Yang Y, Wu W, Zhang M, Wu H, Li X: Identification and characterization of novel anticoagulant peptide with thrombolytic effect and nutrient oligopeptides with high branched chain amino acid from *Whitmania pigra* protein. Amino Acids 2016, 48(11):2657-2670.

⁷ Ren Y, Yang Y, Wu W, Zhang M, Wu H, Li X: Identification and characterization of novel anticoagulant peptide with thrombolytic effect and nutrient oligopeptides with high branched chain amino acid from *Whitmania pigra* protein. Amino Acids 2016, 48(11):2657-2670

번호	성분명	클래스
148	Arg	amino acid
315	Ala	amino acid
316	Tyr	amino acid
149	Val	amino acid
317	Met	amino acid
318	Trp	amino acid
319	Phe	amino acid
320	Ile	amino acid
150	Leu	amino acid
321	Lys	amino acid
182	uracil	nucleobase
161	xanthine	nucleobase
162	hypoxanthine	nucleobase
	H1	peptide
	H2	peptide
	H3	peptide
	HF2	peptide
	WA3-1	peptide
	whitide	peptide
	whitmanin	peptide
	WP-30	peptide

12. 영와(鈴蛙), Bombina

영와(鈴蛙, Bombina)는 Bombinatoridae 과에 속하는 무당개구리(*Bombina orientalis* Boulenger)의 몸체를 말린 것이다. 영와의 성분에 대한 연구들은 주로 영와의 피부에서 추출한 peptide 에 대해서 이루어졌다. Bombesin (**465**)은 영와에서 추출된 14-amino acid peptide (1619.9 Da)이다. Bombesin 의 아미노산 시퀀스는 Pyr-Gln-Arg-Leu-Gly-Asn-Gln-Trp-Ala-Val-Gly-His-Leu-Met 이며, N-terminal 에 pyroglutamic acid 가 있고 C-terminal 에 NH₂ 가 존재한다. 최근에는 DV-28 (3198.5 Da)라는 peptide⁸가 영와의 피부 분비물에서 발견되었는데, 이 peptide 의 아미노산 시퀀스는 DMYEIKGFKSAHGRPRVCPGECPIWV 이며, Cys18 과 Cys24 사이에 disulfide bridge 가 있고 amidated C-terminal Val residue 를 가지고 있다

번호	성분명	클래스
465	bombesin	peptide
	DV-28	peptide

⁸ Wang L, Chen Y, Yang M, Zhou M, Chen T, Sui DY, Shaw C: Peptide DV-28 amide: An inhibitor of bradykinin-induced arterial smooth muscle relaxation encoded by *Bombina orientalis* skin kininogen-2. *Peptides* 2010, 31(5):979-982

13. 오공(蜈蚣), Scolopendra

오공(蜈蚣, Scolopendra)은 Scolopendridae 과에 속하는 지네(*Scolopendra subspinipes mutilans* L. Koch)의 몸체를 말린 것이다. 오공에서는 antithrombotic activity 를 가지는 Ser-Gln-Leu (466)의 peptide⁹가 발견되었으며, Asp, Arg, Ala, Leu, Lys 의 5 개 아미노산을 포함하고 있다. 이외에도 최근 오공의 haemolymph 에서 12 개의 다양한 성분들이 추출되었다.

번호	성분명	클래스
308	aspartic acid	amino acid
148	arginine	amino acid
315	alanine	amino acid
150	leucine	amino acid
321	lysine	amino acid
466	Ser-Gln-Leu	peptide
467	2-dodecylbenzenesulfonic acid	sulfonic acid
468	3-butylidene-7-hydroxyphthalide	phthalide
469	3H-1,2-dithiole-3-thione	thione
470	8-acetoxy-4-acoren-3-one	cyclohexenone
471	acetylenedicarboxylate	carboxylic acid
472	albuterol	phenolic
473	curcumenol	sesquiterpene
474	docosanedioic acid	carboxylic acid
475	L-homotyrosine	carboxylic acid
476	N-undecylbenzenesulfonic acid	sulfonic acid
477	oleoyl ethanolamide	ethanolamine
478	tetradecylamine	alkylamine

⁹ Kong Y, Huang SL, Shao Y, Li S, Wei JF: Purification and characterization of a novel antithrombotic peptide from *Scolopendra subspinipes mutilans*. J Ethnopharmacol 2013, 145(1):182-186

14. 자충(蠊蟲), Eupolyphaga

자충(蠊蟲, Eupolyphaga)은 Corydiidae 과에 속하는 암컷바퀴(*Eupolyphaga sinensis* Walker, *Steleophaga plancyi* (Boleny))의 몸체를 말린 것으로, *Steleophaga* 또는 *Cockroach* 로도 알려져 있다. 자충에서는 antimicrobial peptide 인 Es-termicin¹⁰이 추출되었다. Es-termicin 의 아미노산 시퀀스는 ACDFQQCWVTCQRQYSINFISARCNQDSCVCTFRT 인데, filamentous fungi 를 억제하는 것으로 알려진 termicin 의 시퀀스와 매우 유사하다.

번호	성분명	클래스
	es-termicin	peptide

¹⁰ Liu Z, Yuan K, Zhang R, Ren X, Liu X, Zhao S, Wang D: Cloning and purification of the first termicin-like peptide from the cockroach *Eupolyphaga sinensis*. *J Venom Anim Toxins Incl Trop Dis* 2016, 22:5

15. 맹충(虻蟲), Tabanus

맹충(虻蟲, Tabanus)은 Tabanidae 과에 속하는 *Tabanus mandarinus* Schiner, *T. bivittatus* Matsumura 의 암컷 성충의 몸체를 말린 것이다. 맹충에서는 anticoagulant activity 를 가지는 tabanus anticoagulant protein (65k Da)¹¹이 추출되었다. Ding et al.의 연구¹²에서는 맹충에서 21 가지의 fatty acid 들을 추출하였는데, 이 중에서 palmitoleic acid, palmitic acid, linoleic acid, oleic acid, stearic acid 가 주요 성분이라는 것을 보였다.

번호	성분명	클래스
479	palmitic acid	fatty acid
480	linoleic acid	fatty acid
481	oleic acid	fatty acid
482	stearic acid	fatty acid
483	palmitoleic acid	fatty acid
	tabanus anticoagulant protein	protein

¹¹ Ahn MY, Hahn BS, Lee PJ, Wu SJ, Kim YS: Purification and characterization of anticoagulant protein from the tabanus, *Tabanus bivittatus*. Arch Pharm Res 2006, 29(5):418-423.

¹² Ding CH, Cao FP, Wang YH, Yang ML: [Extraction of fatty constituents from *Tabanus bivittatus* and their analysis by GC-MS]. Zhong Yao Cai 2013, 36(2):188-190

16. 반묘(斑猫), Mylabris

반묘(斑猫, Mylabris)는 Meloidae 과에 속하는 *Mylabris cichorii* Linne, *M. phalerata* Pallas, *Epicauta gorhami* Marseul 의 몸체를 말린 것이다. 한국 약전과 중국 약전에서는 반묘의 지표 성분은 cantharidin (342)이라고 기술되어 있다. 최근 연구들에서는 cantharidin 뿐만 아니라 아래 표와 같이 cantharimide, canthaminomide, palasoninimide, dicantharimide 타입의 다양한 cantharidin analog 들이 추출되었다.

번호	성분명	클래스
484	cantharidin	monoterpenoid
485	cantharidic acid	carboxylic acid
486	2'-(1-hydroxymethyl-2-methyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-1'-hydroxyethyl	canthaminomide
487	2'-(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-propanone	canthaminomide
488	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-3'-hydroxy propionic acid	canthaminomide
489	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-3'-hydroxy-butyric acid	canthaminomide
490	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-3'-methyl-butyric acid	canthaminomide
491	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-4'-methyl-pentanoic acid	canthaminomide
492	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-acetic acid	canthaminomide
493	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-propionic acid	canthaminomide
494	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-succinic acid	canthaminomide
495	5'-[(1R,2R,3S,6R)-1-hydroxymethyl-2-methyl-3,6-epoxycyclohexane-1,2-dicarboximide]-ethyl-2'-methyl-2'-butenoate	canthaminomide
496	8-(1-hydroxymethyl-2-methyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-methyl	canthaminomide
497	8-(1'-hydroxyethyl)-1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide	canthaminomide
498	8-(1'-hydroxypropyl)-1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide	canthaminomide
499	8-[(4'-hydroxyphenyl)-ethyl]-1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide	canthaminomide
500	cantharimide B	canthaminomide

번호	성분명	클래스
501	2'-(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-acetamide	cantharimide
502	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-3'-indol-propionic acid	cantharimide
503	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-5'-guanidino-pentanoic acid	cantharimide
504	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-pentanedioic acid	cantharimide
505	2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-succinamic acid	cantharimide
506	2'-[2''-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-4''-methyl-pentanoylamino]-4'-methyl-pentanoic acid	cantharimide
507	2'-[4''-carboxy-4''-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-butyrylamino]-4'-methyl-pentanoic acid	cantharimide
508	3'-(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-propionamide	cantharimide
509	6'-amino-2-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-hexanoic acid	cantharimide
510	8-(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-N-methyl-butylamide	cantharimide
511	cantharimide	cantharimide
512	bis-(1-methyl-2-hydroxymethyl-3,6-epoxycyclohexane-10,20-dimethyl-1,2-dicarboximido)-trimethylene	dicantharimide
513	bis-(1,2-dimethyl-3,6-epoxycyclohexane-20-methyl-1,2-dicarboximido)-ethyl butyrate	dicantharimide
514	bis(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximido)-tetramethylene	dicantharimide
515	bis(1,2-dimethyl-3,6-epoxycyclohexane-20-methyl-1,2-dicarboximido)-trimethylene	dicantharimide
516	dicantharimide A	dicantharimide
517	8-(acetamide) palasoninimide	palasoninimide
518	8-(N-methyl-butylamide) palasoninimide	palasoninimide
519	palasoninimide	palasoninimide
520	cyclo-(D-Pro-L-Tyr)	pyrazine
521	cyclo-(L-Pro-L-Ala)	pyrazine
522	cyclo-(R-Pro-R-Leu)	pyrazine
523	cyclo-(S-Pro-R-Leu)	pyrazine

번호	성분명	클래스
524	indole-3-aldehyde	aldehyde
525	valerolactam	alkaloid
526	4-hydroxyphthalid	benzofuran
141	3-indoleacetic acid	carboxylic acid

17. 전갈(全蝎), Scorpio

전갈(全蝎, Scorpio)은 Buthidae 과의 전갈(*Buthus martensii* Karsch) 몸체를 말린 것이다. 전갈 약재의 주요 성분은 전갈이 만든 독에 집중되어 있다고 알려져 있으며, 전갈 독은 analgesic peptide 또는 antitumor peptide 들을 포함하고 있다. 현재까지 전갈에서 추출된 대표적인 analgesic peptide 들은 BmK AngM1¹³, BmK AGP-SYPU2¹⁴, BmK I1, BmK I4, BmK I6, BmK AngP1, BmK dITAP3, BmK ANEP, BmK AS, BmK AS-1, BmK AGAP, BmK AGP-SYPU1, BmK AGAP-SYPU2¹⁵ 등이 있다. 전갈의 antitumor peptide 들은 BmK CT와 BmK CT-13¹⁶가 있는데, 이들의 아미노산 시퀀스는 항암제로 사용되고 있는 chlorotoxin 의 아미노산 시퀀스와 유사하다. 특히, analgesic peptide 들 중에서 BmK AGAP 와 BmK AGAP-SYPU2 는 analgesic activity 와 antitumor activity 를 가지는 것으로 알려져 있다. 이외에도 전갈에서는 3 β -acetoxyl,2,14,22-trihydroxy,19-hydroxymethyl,9 α ,5 β ,14 β -card-20(22)enolide (**528**)와 1,2,3,4-tetrahydro-6-hydroxy1-5-pyrimidinecarbox-aldehyde (**529**)의 성분이 있는데 이 성분들은 antibacterial activity 를 가진다고 알려져 있다. 이외에도 전갈에는 17 개의 아미노산이 포함되어 있다.

번호	성분명	클래스
308	aspartic acid	amino acid
309	glutamic acid	amino acid
310	serine	amino acid
312	histidine	amino acid
313	glycine	amino acid
314	threonine	amino acid
148	arginine	amino acid
315	alanine	amino acid

¹³ Cao Z, Wang W, Xiao X, Chen K, Liang X, Yu D: High-level expression and purification of an analgesic peptide from *Buthus martensii* Karsch. *Protein Pept Lett* 2007, 14(3):247-251.

¹⁴ Zhang R, Yang Z, Liu YF, Cui Y, Zhang JH: Purification, characterization and cDNA cloning of an analgesic peptide from the Chinese scorpion *Buthus martensii* Karsch (BmK AGP-SYPU2). *Mol Biol (Mosk)* 2011, 45(6):956-962

¹⁵ Shao JH, Cui Y, Zhao MY, Wu CF, Liu YF, Zhang JH: Purification, characterization, and bioactivity of a new analgesic-antitumor peptide from Chinese scorpion *Buthus martensii* Karsch. *Peptides* 2014, 53:89-96.

¹⁶ Zang M, Liu X, Chen L, Xiao Q, Yuan L, Yang J: Determination of BmKCT-13, a chlorotoxin-like peptide, in rat plasma by LC-MS/MS: application to a preclinical pharmacokinetic study. *J Chromatogr B Analyt Technol Biomed Life Sci* 2014, 947-948:125-131.

번호	성분명	클래스
316	tyrosine	amino acid
149	valine	amino acid
317	methionine	amino acid
319	phenylalanine	amino acid
320	isoleucine	amino acid
150	leucine	amino acid
321	lysine	amino acid
322	proline	amino acid
527	cysteine	amino acid
528	3 β -acetoxy,2,14,22-trihydroxy,19-hydroxymethyl,9 α ,5 β ,14 β -card-20(22)enolide	steroid
529	1,2,3,4-tetrahydro-6-hydroxy-5-pyrimidinecarbox-aldehyde	aldehyde
	BmK AGAP	peptide
	BmK AGAP-SYPU2	peptide
	BmK AGP-SYPU1	peptide
	BmK AGP-SYPU2	peptide
	BmK ANEP	peptide
	BmK AngM1	peptide
	BmK AngP1	peptide
	BmK AS	peptide
	BmK AS-1	peptide
	BmK CT	peptide
	BmK CT-13	peptide
	BmK dITAP3	peptide
	BmK I1	peptide
	BmK I4	peptide
	BmK I6	peptide

18. 제조(蟻螞), Holotrichia

제조(蟻螞, Holotrichia)는 Melolonthidae 과에 속하는 풍뎅이(*Holotrichia diomphalia* Bates) 또는 기타 근연곤충의 유충이다. 제조의 hemolymph 에서는 곤충의 방어 작용과 상처 치료에 관여하는 prophenoloxidase¹⁷가 추출되었다. 또한 제조에 함유되어 있는 oleic acid (**481**), palmitic acid (**479**), palmitoleic acid (**483**)는 anti-inflammatory 와 analgesic activity 를 보인다고 알려져 있다¹⁸. 최근에는 제조 유충에서 inosine (**464**)과 guanosine (**458**)의 성분을 추출하는 연구도 수행되었다.

번호	성분명	클래스
479	palmitic acid	fatty acid
481	oleic acid	fatty acid
483	palmitoleic acid	fatty acid
458	guanosine	nucleoside
464	inosine	nucleoside
	prophenoloxidase	protein

¹⁷ Kwon TH, Lee SY, Lee JH, Choi JS, Kawabata S, Iwanaga S, Lee BL: Purification and characterization of prophenoloxidase from the hemolymph of coleopteran insect, *Holotrichia diomphalia* larvae. *Mol Cells* 1997, 7(1):90-97

¹⁸ Pei K, Cao W, Guo QQ, Xie YH, He ZM, Wang SW: [Analysis of liposoluble constituents in *Holotrichia diomphalia* by GC-MS and investigation their anti-inflammatory and analgesic activities]. *Zhong Yao Cai* 2012, 35(3):357-360.

19. 지룡(地龍), *Pheretima*

지룡(地龍, *Pheretima*)은 지렁이(Megascolecidae 과에 속하는 *Pericaeta communisma* Gate et Hatai, *Pheretima aspergillum* E. Perrier, *P. vulgaris* Chen, *P. guillelmi* (Michaelsen), *P. pectinifera* Michaelsen. 또는, Lumbricidae 과에 속하는 *Allolobophora caliginosa* var. *trapezoides* Anton)의 몸체를 말린 것이다. Lumbricin-PG 는 antimicrobial peptide 로써 *P. guillelmi* (Michaelsen)의 피부에서 추출되었다¹⁹.

Lumbricin-PG 는 59 개의 amino acid 를 가지며 6908.7 Da 의 분자량을 가지는데, 이는 *Lumbricus rubellus* 에서 추출된 antimicrobial peptide 인 lumbricin 과 유사하다. 이외에도 oleic acid (**481**), linoleic acid (**480**), arachidonic acid (**530**), eicosatrienoic acid (**531**)과 같은 unsaturated fatty acid 들도 *P. aspergillum* 에서 추출되었으며, hypoxanthine 을 포함한 6 개의 nucleobase 와 nucleoside 들도 추출되었다.

번호	성분명	클래스
480	linoleic acid	fatty acid
481	oleic acid	fatty acid
530	arachidonic acid	fatty acid
531	eicosatrienoic acid	fatty acid
161	xanthine	nucleobase
162	hypoxanthine	nucleobase
163	adenosine	nucleoside
458	guanosine	nucleoside
461	uridine	nucleoside
464	inosine	nucleoside
	lumbricin-PG	peptide

¹⁹ Li W, Li S, Zhong J, Zhu Z, Liu J, Wang W: A novel antimicrobial peptide from skin secretions of the earthworm, *Pheretima guillelmi* (Michaelsen). *Peptides* 2011, 32(6):1146-1150.

20. 합마유(哈蟆油), Ranae Oviductus

합마유(哈蟆油, Ranae Oviductus)는 Ranidae 과에 속하는 *Rana temporaria chensinensis* David 의 수란관을 말린 것이다. 아래 표는 합마유에서 추출된 9 개의 cholesteryl ester 들과 steroid 들을 보인 것이다.

번호	성분명	클래스
402	cholest-5-en-3 β ,7 β -diol	steroid
532	cholesteryl palmitate	steroid
533	3 β -hydroxy-cholest-5-en-7-one	steroid
530	arachidonic acid	fatty acid
450	docosahexaenoic acid	fatty acid
534	eicosapentaenoic acid	fatty acid
480	linoleic acid	fatty acid
481	oleic acid	fatty acid
535	α -linolenic acid	fatty acid

21. 해룡(海龍), Syngnathus

해룡(海龍, Syngnathus)은 Syngnathidae 과에 속하는 실고기(*Solenognathus hardwickii* (Gray), *Syngnathoides biaculeatus* (Bloch), *Syngnathus acus* Linnaeus)의 몸체를 말린 것이다. 최근, 해룡에서 translation-inhibiting activity 를 가지는 protein 인 solenin²⁰이 추출되었다. 이 protein 은 18 kD 의 분자량을 보이고 있으며 AHDAEVNEVKAQVAA 의 N-terminal sequence 를 가지고 있다. 또한, 해룡에서는 antioxidant 성분인 hypoxanthine (**162**)도 추출되었다.

번호	성분명	클래스
162	hypoxanthine	nucleobase
	solenin	protein

²⁰ Ng TB, Lam YW: Solenin, a novel protein with translation-inhibiting activity from the traditional Chinese medicinal fish, the sea dragon *Solenognathus hardwickii*. Int J Biochem Cell Biol 2002, 34(6):625-631.

22. 해마(海馬), Hippocampus

해마(海馬, Hippocampus)는 Syngnathidae 과에 속하는 해마(*Hippocampus coronatus* Temminck et Schlegel, *H. kelloggi* Jordan et Snyder, *H. histrix* Kaup, *H. kuda* Bleeker, *H. trimaculatus* Leach, *H. japonicus* Kaup)의 몸체를 말린 것이다. 해마의 구성 성분은 amino acid, peptide, glycoprotein, lipid, steroid 등을 포함하는 것으로 알려져 있다. Su et al.²¹은 *H. kuda* Bleeker 에서 두 개의 glycoprotein 인 HG-11 과 HG-21 를 추출하였다. 이 두 glycoprotein 에서 saccharide 함유량은 56.7975%와 39.479%였으며, protein 함유량은 30.5475%와 51.747%였다. Chen et al.²²은 *H. trimaculatus* Leach 에서 anti-inflammatory activity 를 가지는 lipid 들을 분리하였다. 이 lipid 들은 neutral lipid, glycolipid, phospholipid 들을 포함하며, 다양한 fatty acid 조합을 가지고 있다. 이 외에도 해마에는 hypoxanthine (**162**)과 xanthine (**161**)이 포함된 것으로 알려져 있다.

번호	성분명	클래스
161	xanthine	nucleobase
162	hypoxanthine	nucleobase
	HG-11	protein
	HG-11	protein

²¹ Su Y, Xu Y: Study on the extraction and purification of glycoprotein from the yellow seahorse, *Hippocampus kuda* Bleeker. Food Sci Nutr 2015, 3(4):302-312.

²² Chen L, Shen X, Chen G, Cao X, Yang J: A Comparative Study of the Effects upon LPS Induced Macrophage RAW264.7 Inflammation in vitro of the Lipids of *Hippocampus trimaculatus* Leach. J Oleo Sci 2015, 64(12):1273-1281.

23. 백강잠(白殭蠶), *Bombyx Batryticatus*

백강잠(白殭蠶, *Bombyx Batryticatus*)은 Bombycoidea 과에 속하는 누에(*Bombyx mori* L.) 유충이 *Beauveria bassiana* (Bals.) Vuillant 에 감염되어 경직사한 몸체이다. 백강잠의 성분은 alkaloid, steroid, flavonoid, nucleoside 등을 포함하는 것으로 알려져 있다. 아래 표는 백강잠에서 식별된 21 개의 성분의 리스트이다.

번호	성분명	클래스
536	1-deoxynojirimycin	alkaloid
537	betaine	alkaloid
538	6-hydroxynicotinic acid	alkaloid
539	L-carnitine	alkaloid
540	choline	alkaloid
195	quercetin	flavonol
198	rutin	flavonol
199	kaempferol	flavonol
541	kaempferol-7-O-β-D-4-O-methylglucoside	flavonol
542	quercetin-7-O-β-D-4-O-methylglucoside	flavonol
182	uracil	nucleobase
312	L-histidine	nucleoside
163	adenosine	nucleoside
543	cordycepin	nucleoside
544	ergost-6,22-dien-3β,5α,8α-triol	steroid
545	β-sitosterol	steroid
546	daucosterol	steroid
547	meso-erythritol	sugar alcohol
548	mannitol	sugar alcohol
549	2-pyrrolidone-5-carboxylic acid	carboxylic acid
479	palmitic acid	fatty acid

24. 잠사(蠶沙), *Bombycis Faeces*

잠사(蠶沙, *Bombycis Faeces*)는 Bombycoidea 과에 속하는 누에(*Bombyx mori* L.) 유충의 분변을 말린 것이다. 잠사의 성분은 megastigmane sesquiterpene, megastigmane glycoside, carotenoid, alkaloid, amino acid 들을 포함하는 것으로 알려져 있다. 아래 표는 잠사에서 식별된 22 개의 성분 리스트이다.

번호	성분명	클래스
550	3S,5R-dihydroxy-6R,7-megstigmadien-9-one	megastigmane sesquiterpene
551	(S)-dehydrovomifoliol	megastigmane sesquiterpene
552	(6R,7E,9R)-9-hydroxy-4,7-megastigmadien-3-one	megastigmane sesquiterpene
553	(3S,5R,6S,7E)-3,5,6-trihydroxy-7-megastigmen-9-one	megastigmane sesquiterpene
554	(6R,9R)-9-hydroxy-4-megastigmen-3-one	megastigmane sesquiterpene
555	3S,5R-dihydroxy-6S,7-megstigmadien-9-one	megastigmane sesquiterpene
556	alangionoside L	megastigmane sesquiterpene glycoside
557	(6R,9R)-3-oxo- α -ionol- β -D-glucopyranoside	megastigmane sesquiterpene glycoside
558	(6R,9S)-3-oxo- α -ionol- β -D-glucopyranoside	megastigmane sesquiterpene glycoside
559	byzantionoside B	megastigmane sesquiterpene glycoside
560	blumenol C glucoside	megastigmane sesquiterpene glycoside
561	lutein	carotenoid
536	1-deoxynojirimycin	alkaloid
562	fagomine	alkaloid
563	3-epi-fagomine	alkaloid
537	betaine	alkaloid
564	pipecolic acid	alkaloid
309	glutamic acid	amino acid
315	alanine	amino acid
319	phenylalanine	amino acid
320	isoleucine	amino acid
150	leucine	amino acid

25. 노봉방(露蜂房), *Vespae Nidus*

노봉방(露蜂房, *Vespae Nidus*)은 Vespidae 과의 말벌(*Polistes mandarinus* Saussure et Geer, *P. olivaceous* (DeGeer), *P. japonicus* Saussure, *Parapolybia varia* Fabricius)이 만든 집이다. 최근 노봉방에서는 두 개의 sesquiterpenoid 과 여섯 개의 diarylheptanoid 가 추출되었다.

번호	성분명	클래스
565	fengfangin A	sesquiterpenoid
566	tutin	sesquiterpenoid
567	alnusone	diarylheptanoid
568	centrololol	diarylheptanoid
569	muricarpone B	diarylheptanoid
570	1-(3,4-dihydroxyphenyl)-7-(4-hydroxyphenyl)heptan-3-one	diarylheptanoid
571	(3S)-1-(3,4-dihydroxyphenyl)-7-(4-hydroxyphenyl)heptan-3-ol	diarylheptanoid
572	(3S)-1-(4-hydroxyphenyl)-7-(3,4-dihydroxyphenyl)heptan-3-ol	diarylheptanoid

26. 상표초(桑螵蛸), *Mantidis Oötheca*

상표초(桑螵蛸, *Mantidis Oötheca*)는 Mantidae 과에 속하는 사마귀(*Tenodera angustipennis* Saussure, *T. sinensis* Saussure, *Statilia maculata* (Thunberg), *Hierodula patellifera* (Serville))의 알집을 찢 다음 말린 것이다. 상표초는 fibrinolytic activity 를 가지는 protease 를 가지고 있다. 32.8k Da 의 분자량을 가지는 mantis-egg fibrolase (MEF)²³가 발견된 이후로 유사한 fibrinolytic protease 인 MEF-2 (32.9k Da)와 MEF-3 (35.6k Da)²⁴ 가 상표초에서 추출되었다. 아래 표는 상표초의 19 개의 성분 리스트이며, 16 개의 lipid 의 성분 구조식이 식별되었다.

번호	성분명	클래스
573	2,3,4,5,6-pentamethylbenzyl alcohol	lipid
480	9,12-octadecadienoic acid	lipid
574	9,12-octadecadienoic acid, ethyl ester	lipid
535	9,12,15-octadecatrienoic acid	lipid
575	9,12,15-octadecatrienoic acid ethyl ester	lipid
576	ethyl oleate	lipid
577	ethyl-9-hexadecenoate	lipid
578	hentriacontane	lipid
579	heptacosane	lipid
580	hexadecanoic acid ethyl ester	lipid
479	n-hexadecanoic acid	lipid
581	octacosane	lipid
481	oleic acid	lipid
582	tetratetracontane	lipid
583	Z-11-hexadecenoic acid	lipid
584	Z-9-octadecenoic acid methyl ester	lipid

²³ Hahn BS, Cho SY, Wu SJ, Chang IM, Baek K, Kim YC, Kim YS: Purification and characterization of a serine protease with fibrinolytic activity from *Tenodera sinensis* (praying mantis). *Biochim Biophys Acta* 1999, 1430(2):376-386

²⁴ Hahn BS, Cho SY, Ahn MY, Kim YS: Purification and characterization of a plasmin-like protease from *Tenodera sinensis* (Chinese mantis). *Insect Biochem Mol Biol* 2001, 31(6- 7):573-581

번호	성분명	클래스
	MEF	protein
	MEF-2	protein
	MEF-3	protein

27. 석결명(石決明), *Haliotidis Concha*

석결명(石決明, *Haliotidis Concha*)은 Haliotidae 과에 속하는 *Nardotis gigantea* (Gmelin), *Sulculus diversicolor supertexta* (Lischke), *Haliotis diversicolor* Reeve, *H. discus hannai* Ino, *H. ovina* Gmelin, *H. ruber* (Leach), *H. asinina* Linnaeus, *H. laevigata* (Donovan)의 조개껍질이다. 석결명을 구성하는 성분의 90% 이상은 calcium carbonate 이며, 이외에 유기 또는 비유기 물질들도 포함되어 있다. 최근, *H. laevigata* 의 껍질에서 perlucin (17k Da)과 perlustrin (13k Da)의 두 개의 protein²⁵이 추출되었으며, *H. discus hannai* Ino 의 껍질에서는 polyenic 화합물인 aquamarine blue pigment²⁶가 추출되었다.

번호	성분명	클래스
	perlucin	protein
	perlustrin	protein
	aquamarine blue pigment	pigment

²⁵ Weiss IM, Kaufmann S, Mann K, Fritz M: Purification and characterization of perlucin and perlustrin, two new proteins from the shell of the mollusc *Haliotis laevigata*. *Biochem Biophys Res Commun* 2000, 267(1):17-21

²⁶ Cai Z, Wu J, Chen L, Guo W, Li J, Wang J, Zhang Q: Purification and characterisation of aquamarine blue pigment from the shells of abalone (*Haliotis discus hannai* Ino). *Food Chem* 2011, 128(1):129-133.

28. 와릉자(瓦楞子), Arcae Concha

와릉자(瓦楞子, Arcae Concha)는 Arcidae 과에 속하는 *Scapharca subcrenata* (Lischke), *S. broughtonii* Schrenck, *Tegillarca granosa* (Linne), *Arca subcrenata* Lischke, *A. granosa* Linnaeus, *A. inflata* Reeve 의 조개껍질이다. 와릉자의 주요 성분은 calcium carbonate 이며, 최근 *S. subcrenata* 의 alcalase hydrolysate 에서 A-Bg1 과 A-Bh 의 두 antioxidant peptide²⁷가 추출되었다.

번호	성분명	클래스
	A-Bg1	peptide
	A-Bh	peptide

²⁷ Li TF, Ye B, Song LY, Yu RM: Isolation and purification of two antioxidant peptides from alcalase hydrolysate of *Arca subcrenata*. *Zhong Yao Cai* 2014, 37(7):1140-1144

29. 진주모(珍珠母, Margaritifera Concha), 진주(珍珠, Margarita)

진주모(珍珠母, Margaritifera Concha, mother of pearl or nacre)는 Unionidae 과에 속하는 *Hyriopsis cumingii* (Lea), *Cristaria plicata* (Leach)의 조개껍질, 또는 Pteriidae 과에 속하는 *Pteria martensii* (Dunker), *Pinctada fucata martensii* (Dunker)의 조개껍질이다. 그리고, 진주(珍珠, Margarita, pearl)는 이 조개들이 자극을 받아 생성한 구슬이다. 진주모와 진주의 주요 성분은 석결명과 와릉자와 같이 calcium carbonate 이며, 이외에 organic compound 로써 여러 protein^{28,29}들이 진주모와 진주에서 추출되었다.

번호	성분명	클래스
	acid soluble matrix	protein
	acid insoluble matrix	protein
	water soluble matrix	protein
	acid-soluble protein	protein
	acid-soluble protein	protein
	conchiolin protein	protein

²⁸ Ma Y, Berland S, Andrieu JP, Feng Q, Bedouet L: What is the difference in organic matrix of aragonite vs. vaterite polymorph in natural shell and pearl? Study of the pearl-forming freshwater bivalve mollusc *Hyriopsis cumingii*. Mater Sci Eng C Mater Biol Appl 2013, 33(3):1521-1529

²⁹ Zhang JX, Li SR, Yao S, Bi QR, Hou JJ, Cai LY, Han SM, Wu WY, Guo DA: Anticonvulsant and sedative-hypnotic activity screening of pearl and nacre (mother of pearl). J Ethnopharmacol 2016, 181:229-235

30. 용골(龍骨), Fossilia Ossis Mastodi

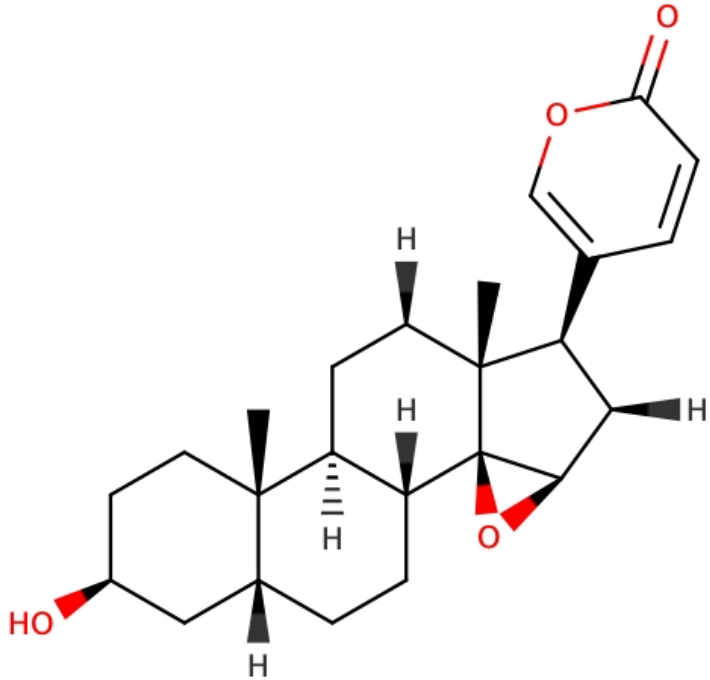
용골(龍骨, Fossilia Ossis Mastodi, Longgu)은 커다란 포유동물의 화석화된 뼈이다. 용골은 생산할 수 있는 것이 아니어서 양이 매우 제한적이지만, 전통의학에서는 수 천년 넘게 약재로 이용되어 왔다. 용골의 주요 성분은 aragonite 타입의 calcium carbonate (**585**)와 hydroxyapatite (**586**)이며, Al, Ba, Bi, Ca, Ge, I, Ir, K, Mn, Mo, Na, Ni, Si, V, Zn, Zr의 16 개의 원소들도 포함하는 것으로 알려져 있다³⁰.

번호	성분명	클래스
585	calcium carbonate	inorganic element
586	hydroxyapatite	inorganic element
587	Al	inorganic element
588	Ba	inorganic element
589	Bi	inorganic element
354	Ca	inorganic element
590	Ge	inorganic element
591	I	inorganic element
592	Ir	inorganic element
356	K	inorganic element
593	Mn	inorganic element
594	Mo	inorganic element
595	Na	inorganic element
596	Ni	inorganic element
597	Si	inorganic element
598	V	inorganic element
599	Zn	inorganic element
600	Zr	inorganic element

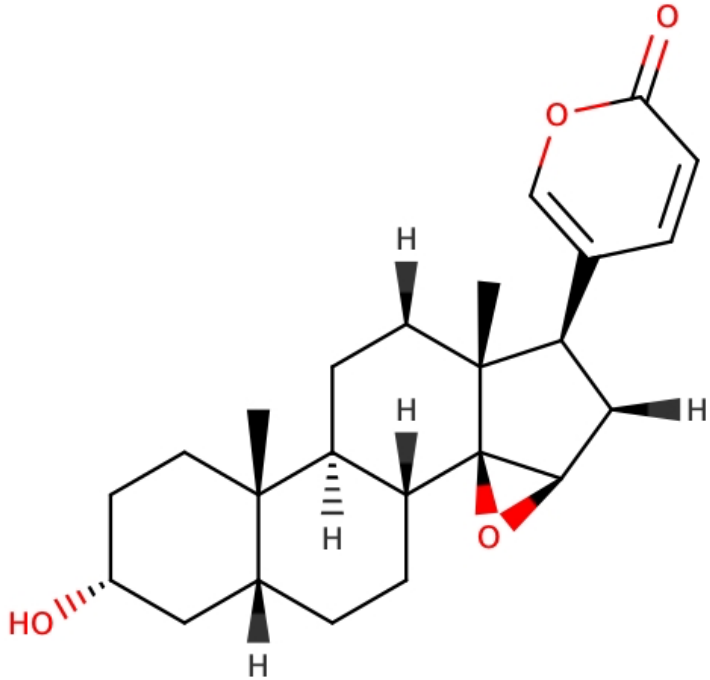
³⁰ Oguri K, Kawase M, Harada K, Shimada-Takaura K, Takahashi T, Takahashi K: Longgu (Fossilia Ossis Mastodi) alters the profiles of organic and inorganic components in Keishikaryukotsuboreito. J Nat Med 2016, 70(3):483-491

부록 1. 약재의 구성성분 상세정보

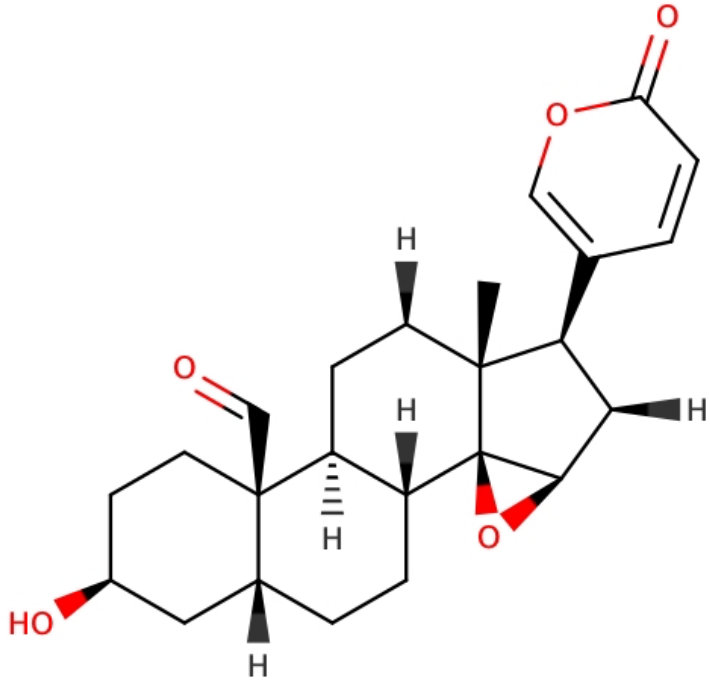
1. resibufogenin

화학 구조		PubMed ID	
		16723285, 20637273 21696903, 23311159 24484689, 25780654 26186722, 26621782 26744067, 27013094 27063985, 27328884 27790826, 29704033 30111043, 31178234 31342712, 31590467 31884035	
TM-MC 성분 ID	1		
TM-MC 성분 동의어	N/A		
PubChem ID	6917974		
InChI Key	ATLJNLYIJOCWJE-CWMZOUAVSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₄		
Molecular Weight	384.516	Exact Molecular Weight	384.23005951
LogP	3.364	Topological Polar Surface Area	59.06 Å ²
Atom Count	60	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.76	Oral Bioavailability	Y

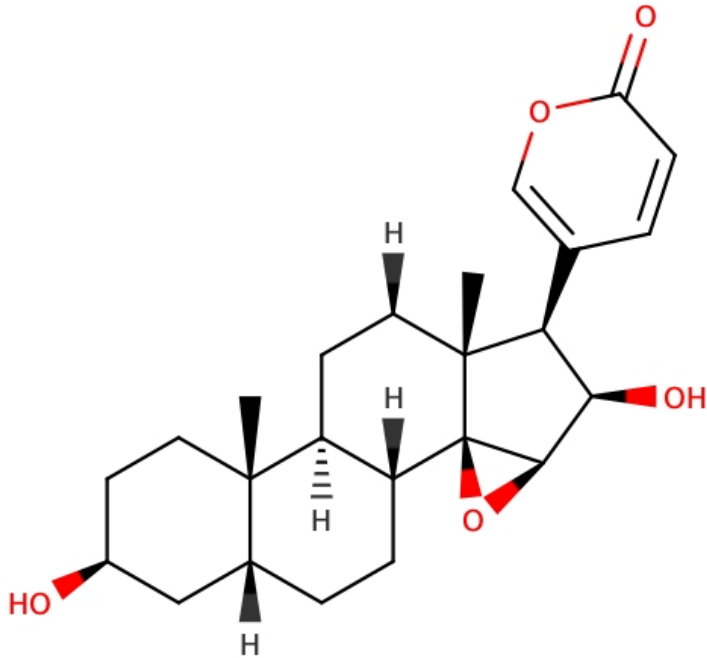
2. 3-epi-resibufogenin

화학 구조		PubMed ID	
		26621782, 27790826	
TM-MC 성분 ID	2		
TM-MC 성분 동의어	N/A		
PubChem ID	70684536		
InChI Key	ATLJNLYIJOCWJE-GBXHWQOESA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](O)CC[C@]34C)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₄		
Molecular Weight	384.516	Exact Molecular Weight	384.23005951
LogP	3.364	Topological Polar Surface Area	59.06 Å ²
Atom Count	60	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.76	Oral Bioavailability	Y

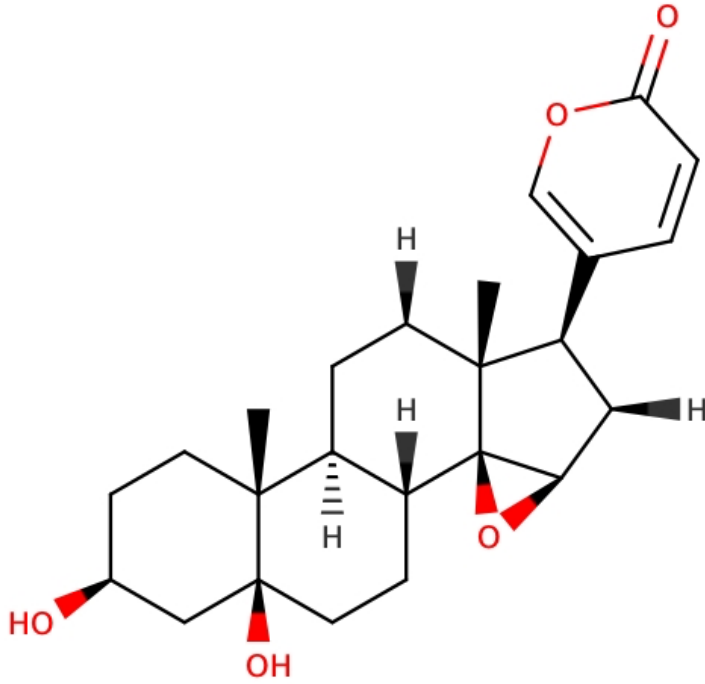
3. resibufagin

화학 구조		PubMed ID	
		<p>20637273, 21696903 26186722, 27328884 27790826, 29704033 31590467, 31884035</p>	
TM-MC 성분 ID	3		
TM-MC 성분 동의어	N/A		
PubChem ID	12314890		
InChI Key	LFLJTMIVTFTLOA-RLKKFORUSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₅		
Molecular Weight	398.499	Exact Molecular Weight	398.209324066
LogP	2.397	Topological Polar Surface Area	76.13 Å ²
Atom Count	59	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.61	Oral Bioavailability	Y

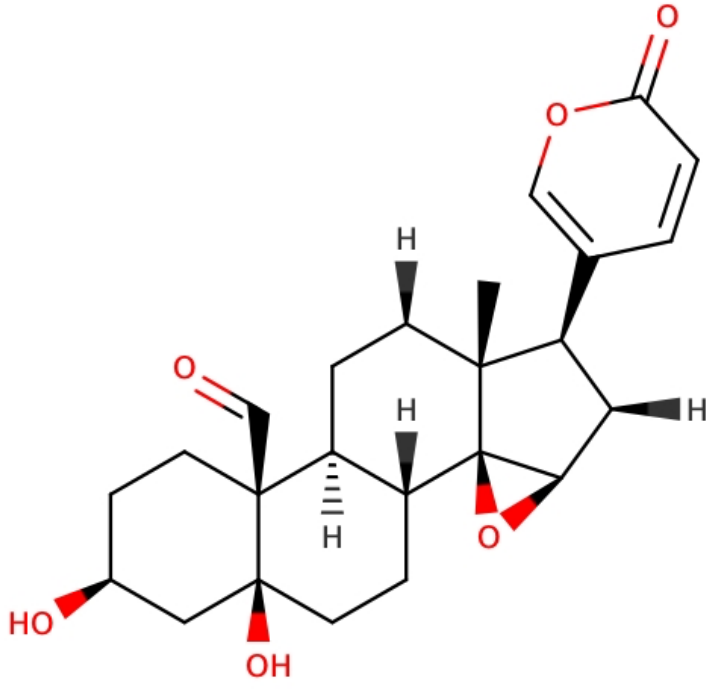
4. desacetylcinobufagin

화학 구조		PubMed ID	
		20637273, 21696903 24484689, 26186722 26621782, 27063985 27328884, 27790826 29704033, 31590467 31884035	
TM-MC 성분 ID	4		
TM-MC 성분 동의어	deacetylcinobufagin		
PubChem ID	11877495		
InChI Key	IXZHDDUFQVXHIL-UOAIQHMYSY-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](O)CC[C@]34C)[C@]11O[C@@H]1[C@H](O)[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₅		
Molecular Weight	400.515	Exact Molecular Weight	400.22497413
LogP	2.367	Topological Polar Surface Area	79.29 Å ²
Atom Count	61	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.71	Oral Bioavailability	Y

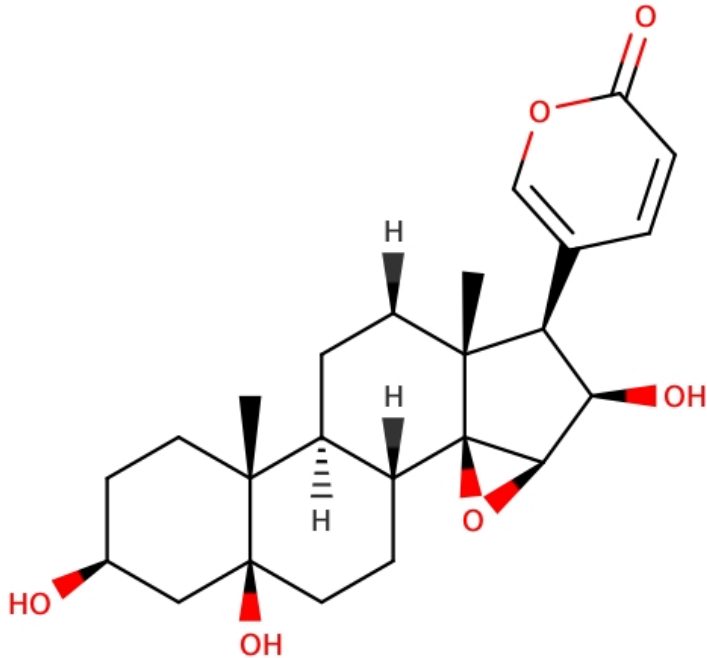
5. marinobufagin

화학 구조		PubMed ID	
		20637273, 21696903 26186722, 26621782 27063985, 27328884 29704033, 31590467	
TM-MC 성분 ID	5		
TM-MC 성분 동의어	N/A		
PubChem ID	11969465		
InChI Key	JMNQTHQLNRILMH-OBBGIPBRSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@@H](O)CC[C@]34C)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₅		
Molecular Weight	400.515	Exact Molecular Weight	400.22497413
LogP	2.131	Topological Polar Surface Area	79.29 Å ²
Atom Count	61	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.71	Oral Bioavailability	Y

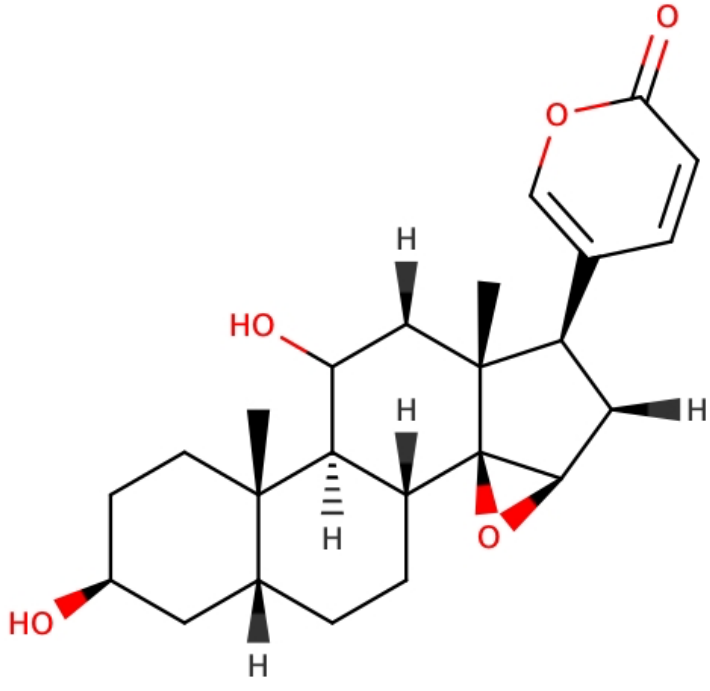
6. bufotalinin

화학 구조		PubMed ID	
		<p>16723285, 26186722 26621782, 27328884 29704033, 31590467</p>	
TM-MC 성분 ID	6		
TM-MC 성분 동의어	N/A		
PubChem ID	101286213		
InChI Key	TYFUTHRVUVOENP-JDDPQDQSSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)[C@@H](O)CC[C@]34C=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₆		
Molecular Weight	414.498	Exact Molecular Weight	414.204238686
LogP	1.165	Topological Polar Surface Area	96.36 Å ²
Atom Count	60	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.56	Oral Bioavailability	Y

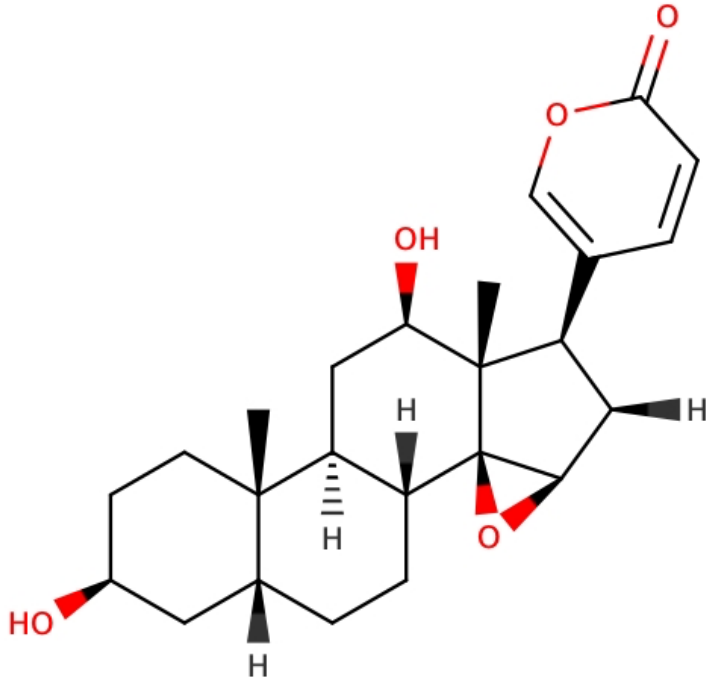
7. desacetylcinobufotalin

화학 구조		PubMed ID	
		20637273, 24484689 26186722, 26621782 27328884, 29704033 31590467	
TM-MC 성분 ID	7		
TM-MC 성분 동의어	de-O-acetylcinobufotalin		
PubChem ID	15513544		
InChI Key	FRYICJTUIXEEGK-NNWVIVGYSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@@H](O)CC[C@]34C)[C@]11O[C@@H]1[C@H](O)[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₆		
Molecular Weight	416.514	Exact Molecular Weight	416.21988875
LogP	1.135	Topological Polar Surface Area	99.52 Å ²
Atom Count	62	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.60	Oral Bioavailability	Y

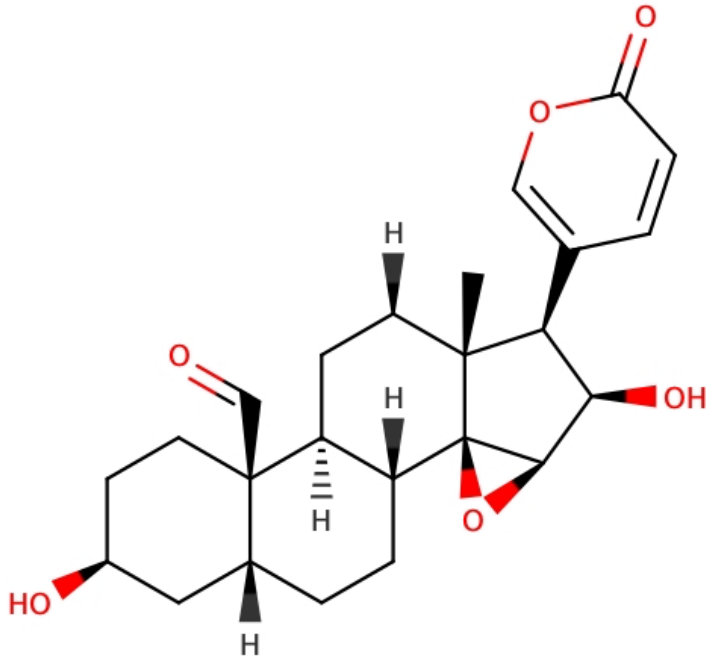
8. 11-hydroxyresibufogenin

화학 구조		PubMed ID	
		21696903, 26621782	
TM-MC 성분 ID	8		
TM-MC 성분 동의어	11-hydroxyl resibufogenin		
PubChem ID	N/A		
InChI Key	DKXGJUGMTLSEAZ-BBTRCNIKSA-N		
SMILES	<chem>C[C@]12CC(O)[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₅		
Molecular Weight	400.515	Exact Molecular Weight	400.22497413
LogP	2.055	Topological Polar Surface Area	79.29 Å ²
Atom Count	61	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.71	Oral Bioavailability	Y

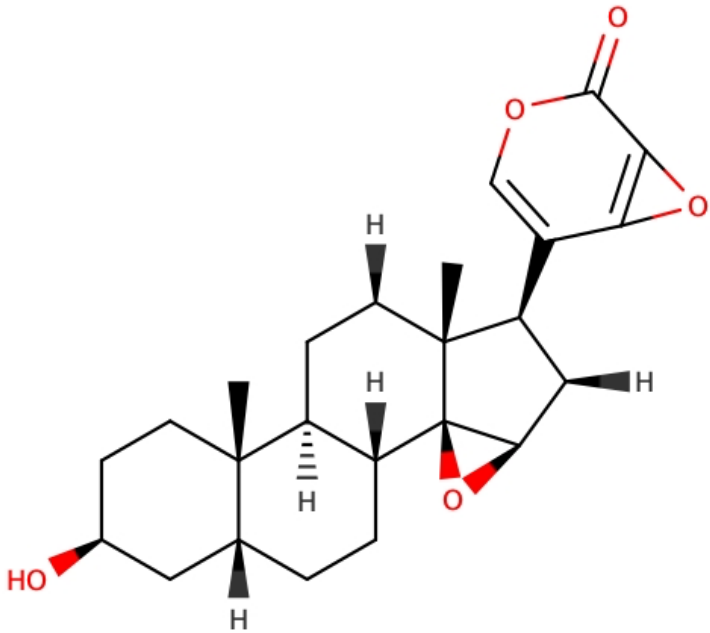
9. hydroxyl-resibufogenin

화학 구조		PubMed ID	
		26186722, 27328884 31590467	
TM-MC 성분 ID	9		
TM-MC 성분 동의어	12β-hydroxyresibufogenin; 12β-hydroxylresibufogenin		
PubChem ID	15513541		
InChI Key	DUDKFSOZKFNNCE-FEHGIAQLSA-N		
SMILES	<chem>C[C@@]12[C@H](C[C@H]3O[C@@]13[C@@H]1CC[C@@H]3C[C@@H](O)CC[C@]3(C)[C@H]1C[C@H]2O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₅		
Molecular Weight	400.515	Exact Molecular Weight	400.22497413
LogP	2.133	Topological Polar Surface Area	79.29 Å ²
Atom Count	61	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.71	Oral Bioavailability	Y

10. 19-oxo-desacetylcinobufagin

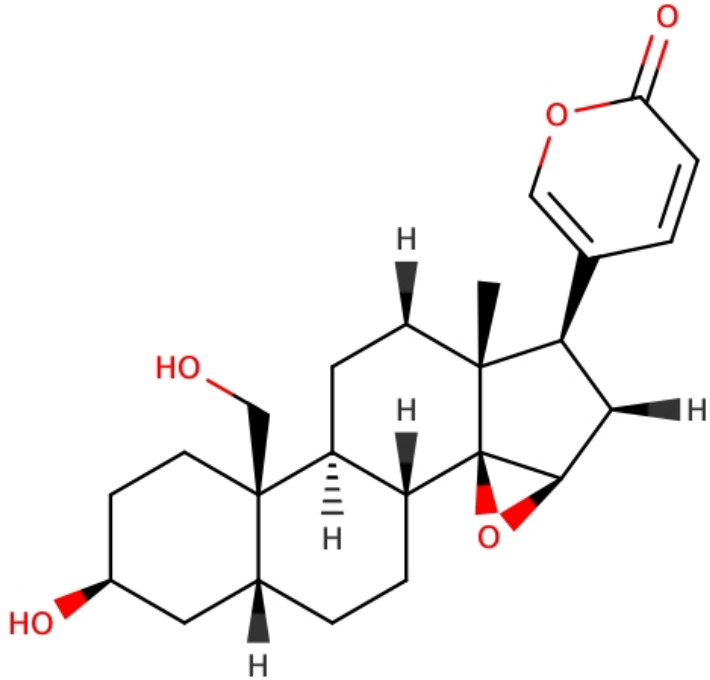
화학 구조		PubMed ID	
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TM-MC 성분 ID	10		
TM-MC 성분 동의어	N/A		
PubChem ID	11144140		
InChI Key	JNBBHUNHDKWCIR-DFJCLZAPSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C=O)[C@]11O[C@@H]1[C@H](O)[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₆		
Molecular Weight	414.498	Exact Molecular Weight	414.204238686
LogP	1.4	Topological Polar Surface Area	96.36 Å ²
Atom Count	60	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.56	Oral Bioavailability	Y

11. 22,23-epoxyresibufogenin

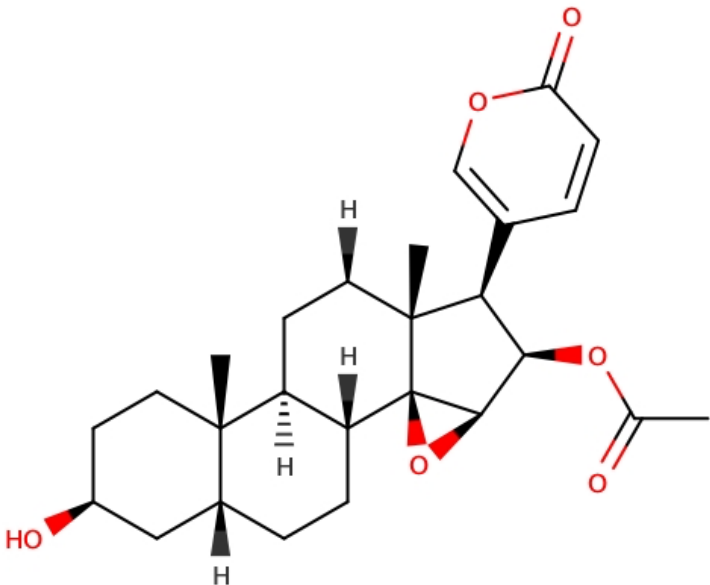
화학 구조	PubMed ID
	21696903, 26621782

TM-MC 성분 ID	11		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	HJTAGTBTFBNXLC-DZTRBTFBSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C)[C@]11O[C@@H]1C[C@@H]2c1coc(=O)c2Oc12</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₅		
Molecular Weight	398.499	Exact Molecular Weight	398.209324066
LogP	2.819	Topological Polar Surface Area	71.59 Å ²
Atom Count	59	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.74	Oral Bioavailability	Y

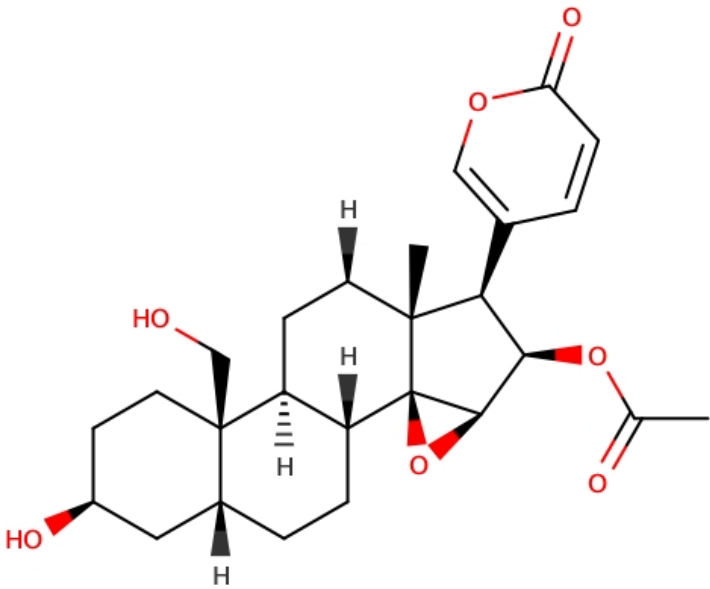
12. resibufaginol

화학 구조		PubMed ID	
		20637273, 26621782 29704033, 31590467	
TM-MC 성분 ID	12		
TM-MC 성분 동의어	monohydroxyl resibufogenin		
PubChem ID	12314891		
InChI Key	XTGMXQCGCNTMEI-RLKKFORUSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34CO)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₅		
Molecular Weight	400.515	Exact Molecular Weight	400.22497413
LogP	2.083	Topological Polar Surface Area	79.29 Å ²
Atom Count	61	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.75	Oral Bioavailability	Y

13. cinobufagin

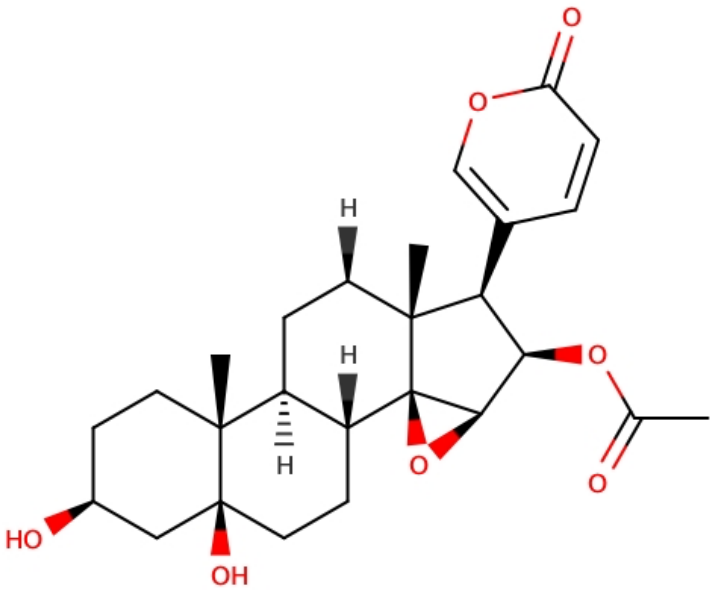
화학 구조		PubMed ID	
		16723285, 20637273 21696903, 23311159 24484689, 25780654 26186722, 26621782 27013094, 27063985 27328884, 27790826 29704033, 30111043 31342712, 31590467 31884035	
TM-MC 성분 ID	13		
TM-MC 성분 동의어	N/A		
PubChem ID	11969542		
InChI Key	SCULJPGYOQQXTK-OLRINKBESA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₄ O ₆		
Molecular Weight	442.552	Exact Molecular Weight	442.235538815
LogP	2.808	Topological Polar Surface Area	85.36 Å ²
Atom Count	66	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.58	Oral Bioavailability	Y

14. cinobufaginol

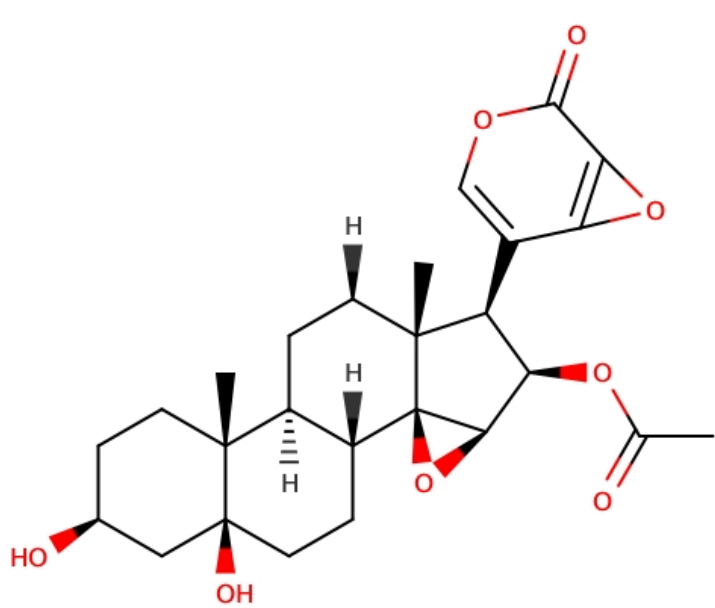
화학 구조	PubMed ID
	<p>26186722, 26621782 27328884, 29704033 31590467</p>

TM-MC 성분 ID	14		
TM-MC 성분 동의어	N/A		
PubChem ID	12303266		
InChI Key	KDRVIPFIZZDLGB-CDIOGTMDSA-N		
SMILES	CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(CO)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1		
Molecular Formula	C ₂₆ H ₃₄ O ₇		
Molecular Weight	458.551	Exact Molecular Weight	458.230453435
LogP	1.527	Topological Polar Surface Area	105.59 Å ²
Atom Count	67	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.53	Oral Bioavailability	Y

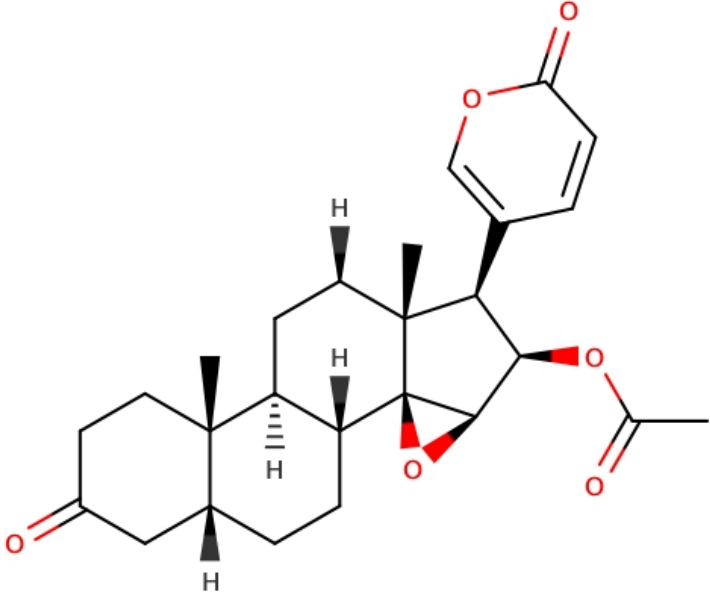
15. cinobufotalin

화학 구조		PubMed ID	
		16723285, 20637273 24484689, 25780654 26186722, 26621782 27013094, 27063985 27328884, 27790826 29704033, 30111043 31156437, 31342712 31590467, 31884035	
TM-MC 성분 ID	15		
TM-MC 성분 동의어	N/A		
PubChem ID	259776		
InChI Key	KBKUJFDSHBPPA-ZNCGZLKOSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@]4(O)C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₄ O ₇		
Molecular Weight	458.551	Exact Molecular Weight	458.230453435
LogP	1.576	Topological Polar Surface Area	105.59 Å ²
Atom Count	67	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.53	Oral Bioavailability	Y

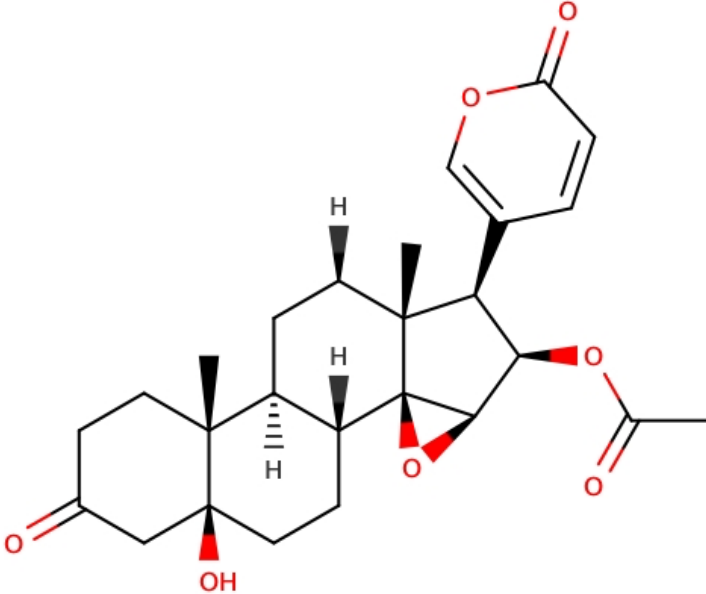
16. 22,23-epoxycinobufotalin

화학 구조		PubMed ID	
		21696903	
TM-MC 성분 ID	16		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	MJNJLVKCZIIAQE-FKAJFBFRSA-N		
SMILES	CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@]4(O)C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1coc(=O)c2Oc12		
Molecular Formula	C ₂₆ H ₃₂ O ₈		
Molecular Weight	472.534	Exact Molecular Weight	472.20971799
LogP	1.031	Topological Polar Surface Area	118.12 Å ²
Atom Count	66	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.50	Oral Bioavailability	Y

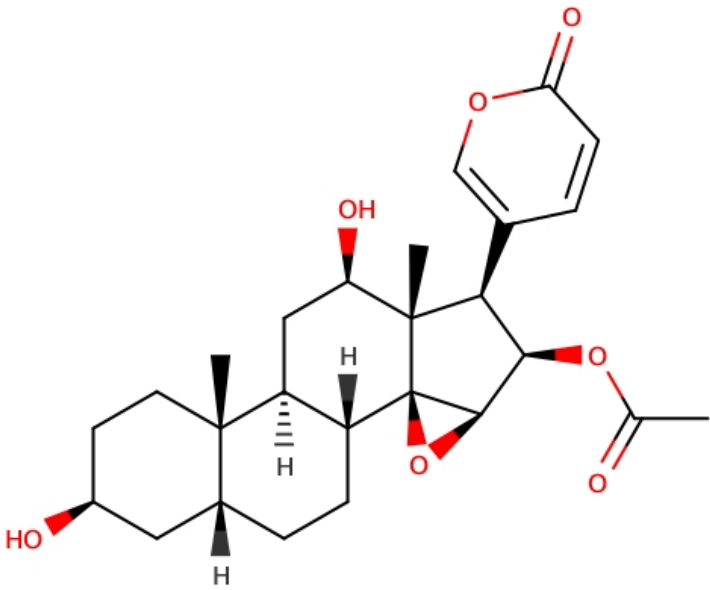
17. 3-oxo-cinobufagin

화학 구조		PubMed ID	
		26621782, 27790826	
TM-MC 성분 ID	17		
TM-MC 성분 동의어	3-keto-cinobufagin		
PubChem ID	22296647		
InChI Key	AOBHQOYFBDNLMA-BAEBVKMLSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4CC(=O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₂ O ₆		
Molecular Weight	440.536	Exact Molecular Weight	440.21988875
LogP	3.015	Topological Polar Surface Area	82.2 Å ²
Atom Count	64	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	0
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.53	Oral Bioavailability	Y

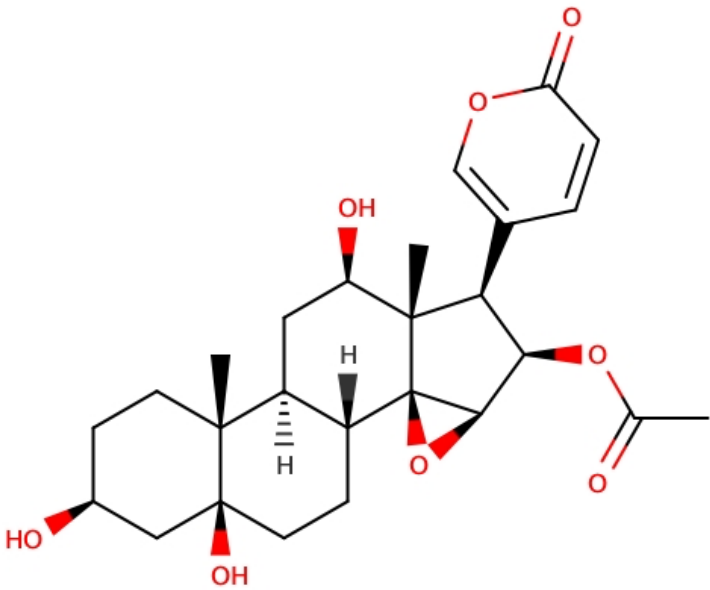
18. 3-oxo-cinobufotalin

화학 구조		PubMed ID	
		16723285	
TM-MC 성분 ID	18		
TM-MC 성분 동의어	N/A		
PubChem ID	102253150		
InChI Key	GLJGPLLAYVBZNS-AXVZYAHOSA-N		
SMILES	CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@]4(O)CC(=O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1		
Molecular Formula	C ₂₆ H ₃₂ O ₇		
Molecular Weight	456.535	Exact Molecular Weight	456.21480337
LogP	2.012	Topological Polar Surface Area	102.43 Å ²
Atom Count	65	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.55	Oral Bioavailability	Y

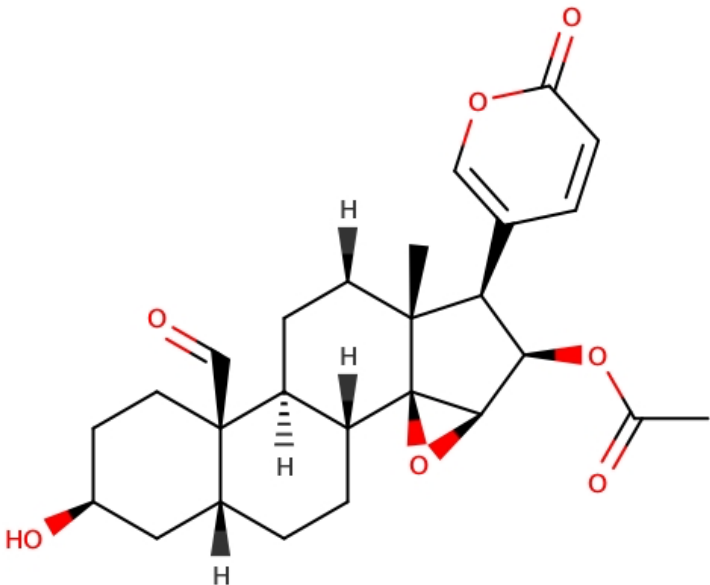
19. 12 β -hydroxycinobufagin

화학 구조		PubMed ID	
		26186722, 27063985 27790826, 29704033 31590467	
TM-MC 성분 ID	19		
TM-MC 성분 동의어	12 β -hydroxycinobufagin		
PubChem ID	15513542		
InChI Key	GZNLDYHFCFJOU-QLKRLITRSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(C)[C@H]3C[C@@H](O)[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₄ O ₇		
Molecular Weight	458.551	Exact Molecular Weight	458.230453435
LogP	1.577	Topological Polar Surface Area	105.59 Å ²
Atom Count	67	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.53	Oral Bioavailability	Y

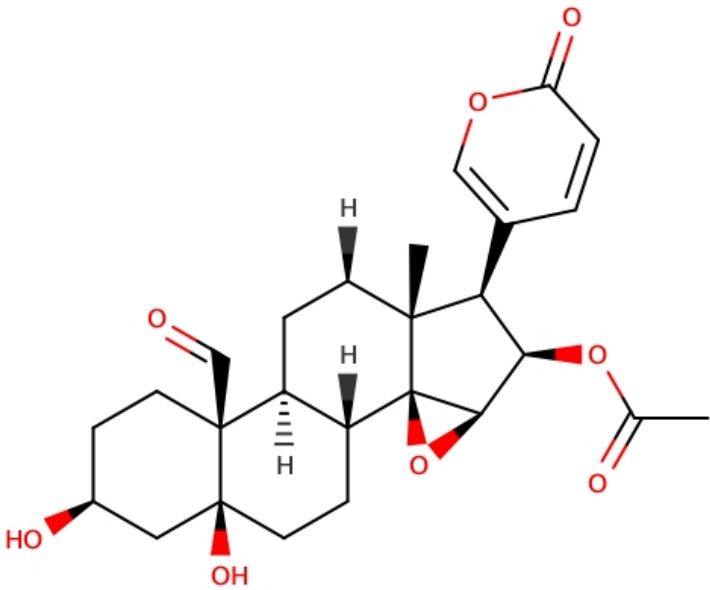
20. 5,12 β -dihydroxycinobufagin

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	20		
TM-MC 성분 동의어	N/A		
PubChem ID	24970584		
InChI Key	MJGBQRFJIZZZFQ-CIXQQPKYSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@]4(O)C[C@@H](O)CC[C@]4(C)[C@H]3C[C@@H](O)[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₄ O ₈		
Molecular Weight	474.55	Exact Molecular Weight	474.225368055
LogP	0.345	Topological Polar Surface Area	125.82 Å ²
Atom Count	68	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.43	Oral Bioavailability	Y

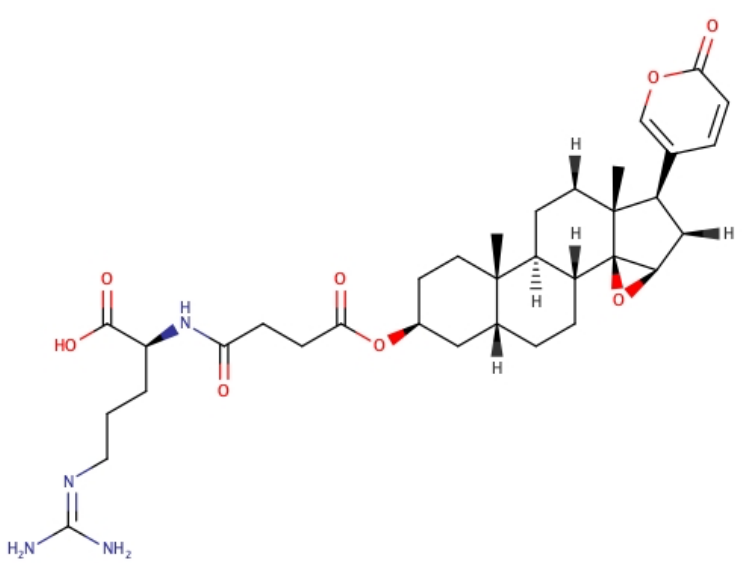
21. 19-oxo-cinobufagin

화학 구조		PubMed ID	
		<p>16723285, 20637273 26186722, 26621782 27063985, 27790826 29704033, 31590467 31884035</p>	
TM-MC 성분 ID	21		
TM-MC 성분 동의어	N/A		
PubChem ID	102093791		
InChI Key	FRUGXBQKMCOIBP-CDIOGTMDSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(C=O)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₂ O ₇		
Molecular Weight	456.535	Exact Molecular Weight	456.21480337
LogP	1.841	Topological Polar Surface Area	102.43 Å ²
Atom Count	65	Structural Alert Count	3
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.42	Oral Bioavailability	Y

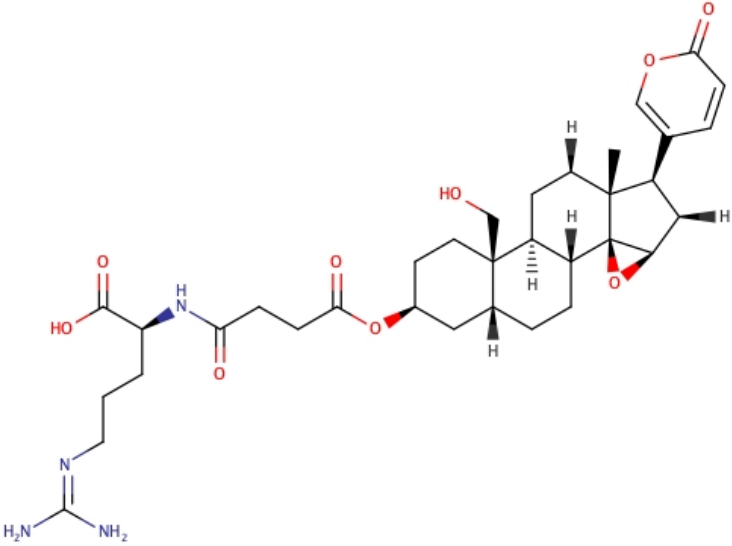
22. 19-oxo-cinobufotalin

화학 구조		PubMed ID	
		20637273, 21696903 26186722, 26621782 27063985, 27328884 29704033, 31590467 31884035	
TM-MC 성분 ID	22		
TM-MC 성분 동의어	N/A		
PubChem ID	102093790		
InChI Key	RDQNOOHJEOAAIW-FSVQXUKKSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@]4(O)C[C@@H](O)CC[C@]4(C=O)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₂ O ₈		
Molecular Weight	472.534	Exact Molecular Weight	472.20971799
LogP	0.609	Topological Polar Surface Area	122.66 Å ²
Atom Count	66	Structural Alert Count	3
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.38	Oral Bioavailability	Y

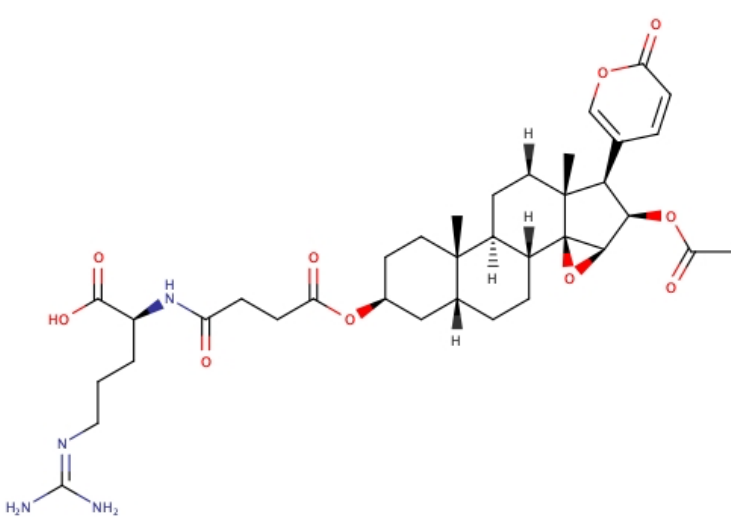
23. resibufogenin-3-O-succinate-arginine

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	23		
TM-MC 성분 동의어	3-(N-succinyl argininyl)resibufogenin		
PubChem ID	102574724		
InChI Key	QAJWYASXXLGROG-LLZTUUJGSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCC(=O)N[C@@H](CCCNC(=N)N)C(O)=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₄ H ₄₈ N ₄ O ₈		
Molecular Weight	640.778	Exact Molecular Weight	640.347214522
LogP	0.484	Topological Polar Surface Area	195.93 Å ²
Atom Count	94	Structural Alert Count	5
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	4
Rotatable Bond Count	12	Aromatic Ring Count	1
Drug Likeness	0.08	Oral Bioavailability	N

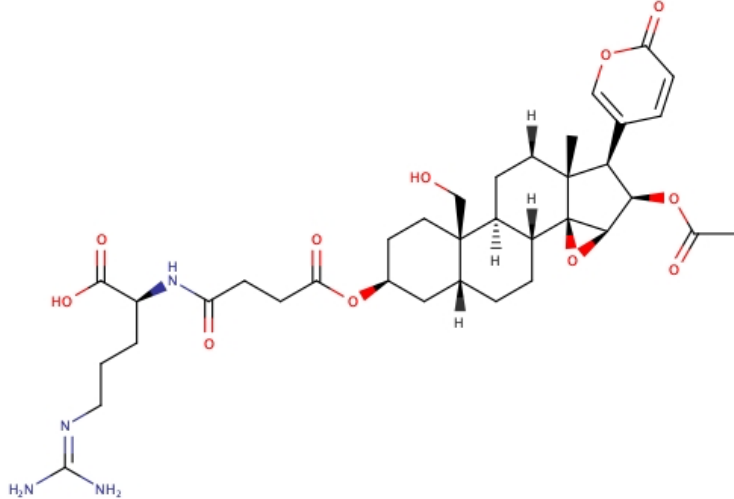
24. resibufaginol-3-O-succinate-arginine

화학 구조		PubMed ID	
		27790826	
TM-MC 성분 ID	24		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	BLWJSJPWNAEDFE-OMINFMMUSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34CO)OC(=O)CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₄ H ₄₈ N ₄ O ₉		
Molecular Weight	656.777	Exact Molecular Weight	656.342129142
LogP	-0.797	Topological Polar Surface Area	216.16 Å ²
Atom Count	95	Structural Alert Count	5
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	5
Rotatable Bond Count	13	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

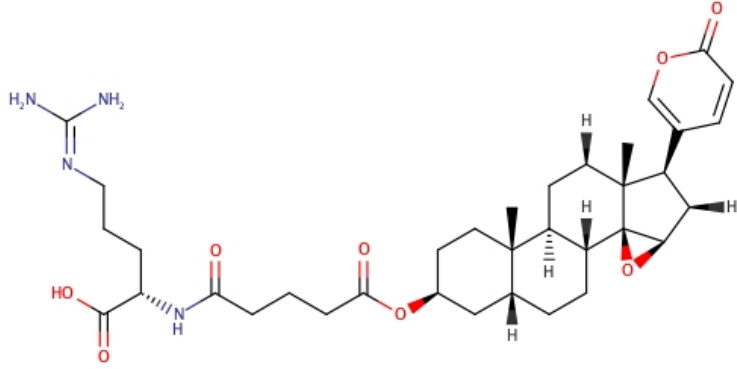
25. cinobufagin-3-O-succinate-arginine

화학 구조		PubMed ID	
		26186722, 27063985 27790826, 29704033 31590467	
TM-MC 성분 ID	25		
TM-MC 성분 동의어	3-(N-succinyl argininy)cinobufagin		
PubChem ID	163189854		
InChI Key	LQKLZDXEYGROGO-WWYNDBRESA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@H]22[C@@H]3CC[C@H]4C[C@H](CC[C@H]4(C)[C@H]3CC[C@H]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₆ H ₅₀ N ₄ O ₁₀		
Molecular Weight	698.814	Exact Molecular Weight	698.352693826
LogP	-0.072	Topological Polar Surface Area	222.23 Å ²
Atom Count	100	Structural Alert Count	5
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	4
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

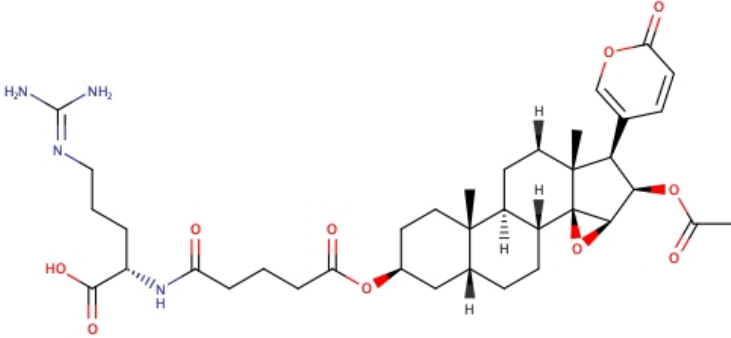
26. cinobufaginol-3-O-succinate-arginine

화학 구조		PubMed ID	
		26186722, 31590467	
TM-MC 성분 ID	26		
TM-MC 성분 동의어	3-(N-succinyl argininyl)cinobufaginol		
PubChem ID	N/A		
InChI Key	GRTCZURAMYWPBA-BDOOACQSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@H]22[C@@H]3CC[C@@H]4C[C@H](CC[C@H]4(CO)[C@H]3CC[C@H]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₆ H ₅₀ N ₄ O ₁₁		
Molecular Weight	714.813	Exact Molecular Weight	714.347608446
LogP	-1.353	Topological Polar Surface Area	242.46 Å ²
Atom Count	101	Structural Alert Count	5
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	5
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.05	Oral Bioavailability	N

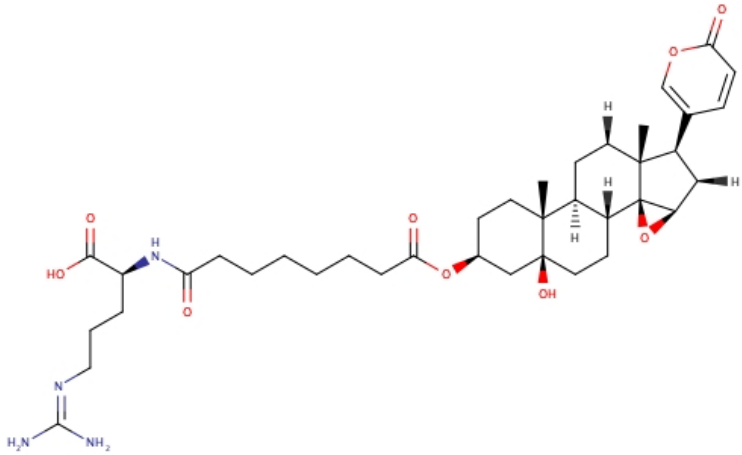
27. 3-(N-glutaryl argininy)resibufogenin

화학 구조		PubMed ID	
		27790826, 29704033 31590467	
TM-MC 성분 ID	27		
TM-MC 성분 동의어	resibufogenin-3-O-glutarate-arginine		
PubChem ID	N/A		
InChI Key	CXPTVPNHAIZTJG-OQPLOWK TSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)o</chem>		
Molecular Formula	C ₃₅ H ₅₀ N ₄ O ₈		
Molecular Weight	654.805	Exact Molecular Weight	654.362864586
LogP	0.928	Topological Polar Surface Area	195.93 Å ²
Atom Count	97	Structural Alert Count	5
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	4
Rotatable Bond Count	13	Aromatic Ring Count	1
Drug Likeness	0.08	Oral Bioavailability	N

28. cinobufagin-3-O-glutarate-arginine

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	28		
TM-MC 성분 동의어	N/A		
PubChem ID	163044499		
InChI Key	BHBXSEJUUXUOLE-OYOWPSGPSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₇ H ₅₂ N ₄ O ₁₀		
Molecular Weight	712.841	Exact Molecular Weight	712.36834389
LogP	0.373	Topological Polar Surface Area	222.23 Å ²
Atom Count	103	Structural Alert Count	5
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	4
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

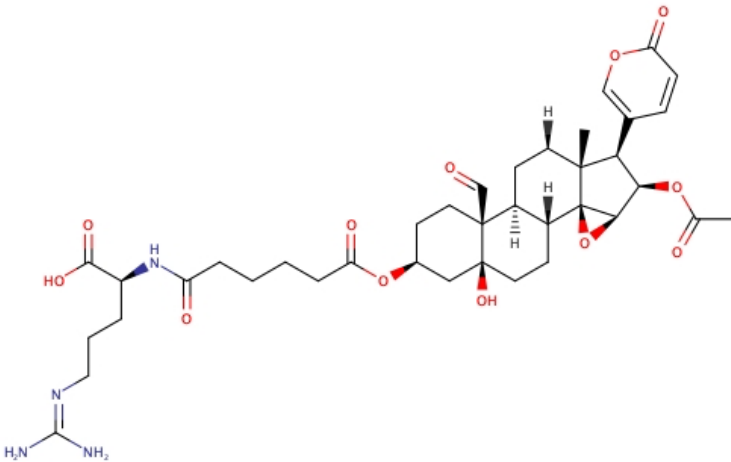
29. marinobufotoxin

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	29		
TM-MC 성분 동의어	3-(N-suberoyl argininy)marinobufagin		
PubChem ID	101996079		
InChI Key	SRSJNASBFYXJMJ-OQARAGJZSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C)OC(=O)CCCCC CC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₈ H ₅₆ N ₄ O ₉		
Molecular Weight	712.885	Exact Molecular Weight	712.404729399
LogP	1.03	Topological Polar Surface Area	216.16 Å ²
Atom Count	107	Structural Alert Count	5
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	5
Rotatable Bond Count	16	Aromatic Ring Count	1
Drug Likeness	0.05	Oral Bioavailability	N

30. cinobufagin-3-O-adipate-arginine

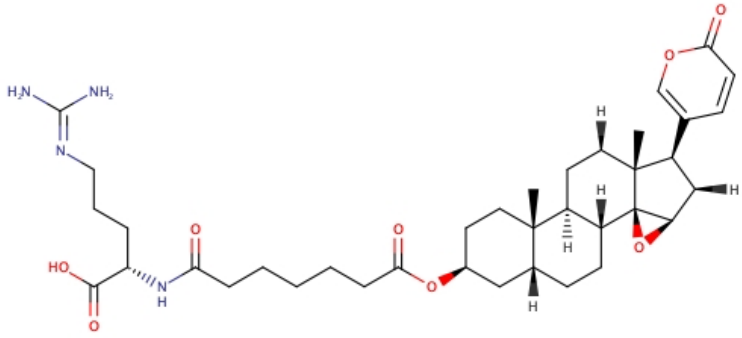
화학 구조		PubMed ID	
		26186722, 27063985 27790826, 29704033 31590467	
TM-MC 성분 ID	30		
TM-MC 성분 동의어	3-(N-adipoyl argininy)cinobufagin		
PubChem ID	162909124		
InChI Key	WJEWHSHTBPLSNS-BWBFKJLBSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@H]22[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₈ H ₅₄ N ₄ O ₁₀		
Molecular Weight	726.868	Exact Molecular Weight	726.383993955
LogP	0.817	Topological Polar Surface Area	222.23 Å ²
Atom Count	106	Structural Alert Count	5
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	4
Rotatable Bond Count	16	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

31. 19-oxo-cinobufotalin-3-O-adipate-arginine

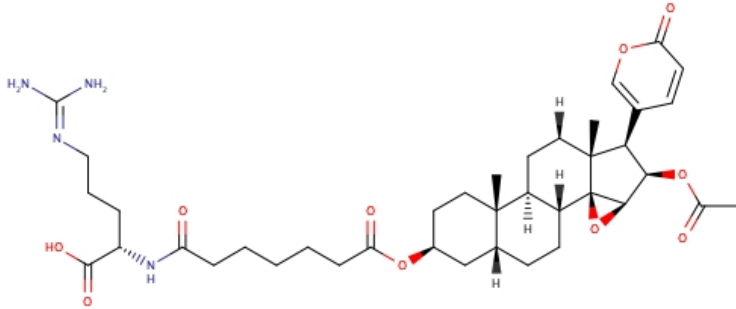
화학 구조	PubMed ID
	27063985

TM-MC 성분 ID	31		
TM-MC 성분 동의어	N/A		
PubChem ID	53253803		
InChI Key	DDJDJUKVEYFKHB-OQZPXGHPSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@]4(O)C[C@H](CC[C@]4(C=O)[C@H]3CC[C@]2(O)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₈ H ₅₂ N ₄ O ₁₂		
Molecular Weight	756.85	Exact Molecular Weight	756.35817313
LogP	-1.382	Topological Polar Surface Area	259.53 Å ²
Atom Count	106	Structural Alert Count	6
Hydrogen Bond Acceptor Count	12	Hydrogen Bond Donor Count	5
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.03	Oral Bioavailability	N

32. resibufogenin-3-O-pimelate-arginine

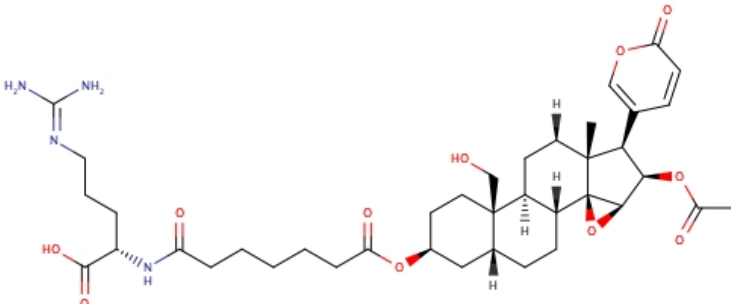
화학 구조		PubMed ID	
		26186722, 27063985 29704033, 31590467	
TM-MC 성분 ID	32		
TM-MC 성분 동의어	3-(N-pimeloyl argininy)resibufogenin		
PubChem ID	N/A		
InChI Key	XXRIZPQLYSQXAJ-ALZBOWOWSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₇ H ₅₄ N ₄ O ₈		
Molecular Weight	682.859	Exact Molecular Weight	682.394164715
LogP	1.817	Topological Polar Surface Area	195.93 Å ²
Atom Count	103	Structural Alert Count	5
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	4
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

33. cinobufagin-3-O-pimelate-arginine

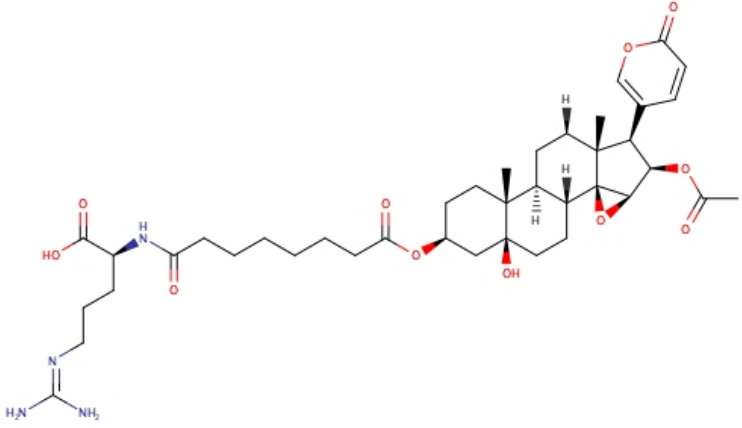
화학 구조	PubMed ID
	<p>27063985, 27790826 29704033, 31590467</p>

TM-MC 성분 ID	33		
TM-MC 성분 동의어	3-(N-pimeloyl argininy)cinobufagin		
PubChem ID	162895547		
InChI Key	HJVHZZPUOWTUMD-ARZJAYRVSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₉ H ₅₆ N ₄ O ₁₀		
Molecular Weight	740.895	Exact Molecular Weight	740.399644019
LogP	1.262	Topological Polar Surface Area	222.23 Å ²
Atom Count	109	Structural Alert Count	5
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	4
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

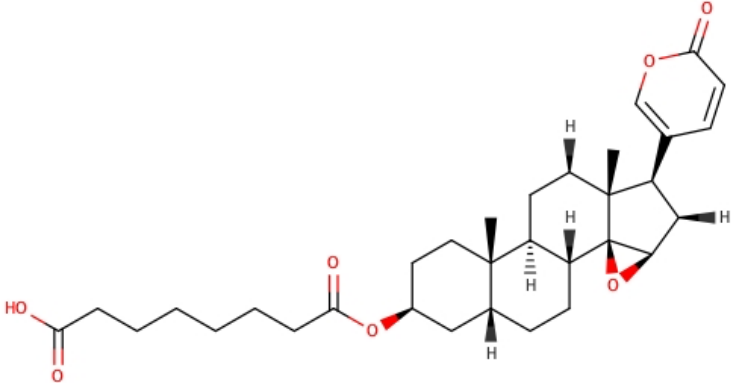
34. cinobufaginol-3-O-pimelate-arginine

화학 구조		PubMed ID	
		27790826	
TM-MC 성분 ID	34		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	JQGFYWYWGQSVDO-MHDRLEORSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(CO)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](CCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₉ H ₅₆ N ₄ O ₁₁		
Molecular Weight	756.894	Exact Molecular Weight	756.394558639
LogP	-0.019	Topological Polar Surface Area	242.46 Å ²
Atom Count	110	Structural Alert Count	5
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	5
Rotatable Bond Count	18	Aromatic Ring Count	1
Drug Likeness	0.04	Oral Bioavailability	N

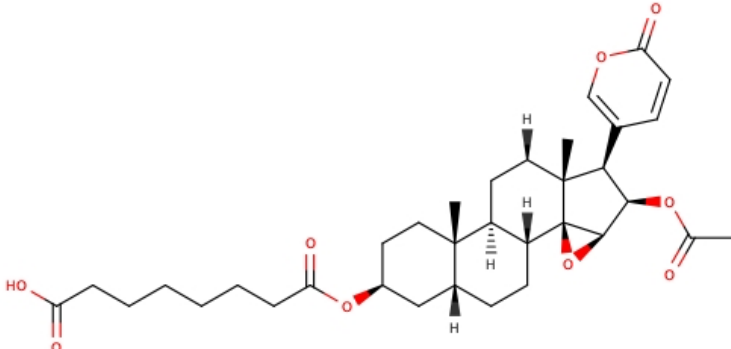
35. cinobufotalitoxin

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	35		
TM-MC 성분 동의어	3-(N-suberoyl argininy)cinobufotalin		
PubChem ID	163055984		
InChI Key	MBWKRBFITOTZCF-FHQRUICKSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@]4(O)C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₄₀ H ₅₈ N ₄ O ₁₁		
Molecular Weight	770.921	Exact Molecular Weight	770.410208704
LogP	0.474	Topological Polar Surface Area	242.46 Å ²
Atom Count	113	Structural Alert Count	5
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	5
Rotatable Bond Count	18	Aromatic Ring Count	1
Drug Likeness	0.05	Oral Bioavailability	N

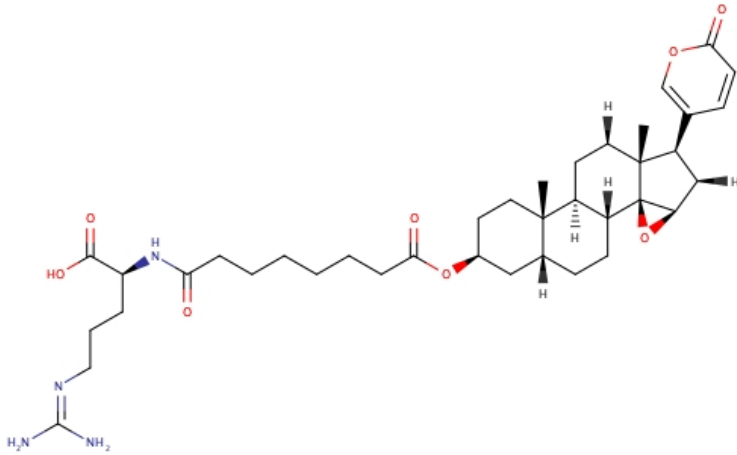
36. resibufogenin-3-O-suberoyl ester

화학 구조		PubMed ID	
		20637273	
TM-MC 성분 ID	36		
TM-MC 성분 동의어	N/A		
PubChem ID	102093784		
InChI Key	QNBHVXPSPWGVSA-VQRFTYGJSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCCC(O)=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₂ H ₄₄ O ₇		
Molecular Weight	540.697	Exact Molecular Weight	540.308703757
LogP	5.408	Topological Polar Surface Area	102.43 Å ²
Atom Count	83	Structural Alert Count	3
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	10	Aromatic Ring Count	1
Drug Likeness	0.24	Oral Bioavailability	Y

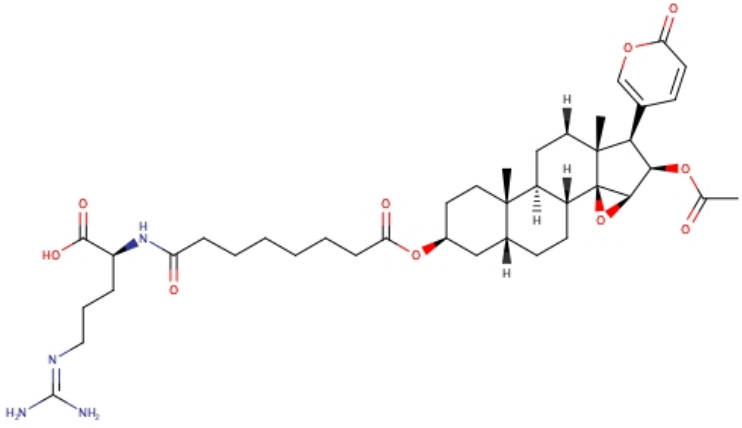
37. cinobufagin-3-O-suberoyl ester

화학 구조		PubMed ID	
		20637273	
TM-MC 성분 ID	37		
TM-MC 성분 동의어	N/A		
PubChem ID	70697081		
InChI Key	WNMNOTRKSZQFML-NDESRDLBSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)=O</chem>		
Molecular Formula	C ₃₄ H ₄₆ O ₉		
Molecular Weight	598.733	Exact Molecular Weight	598.314183061
LogP	4.852	Topological Polar Surface Area	128.73 Å ²
Atom Count	89	Structural Alert Count	3
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	1
Rotatable Bond Count	12	Aromatic Ring Count	1
Drug Likeness	0.21	Oral Bioavailability	N

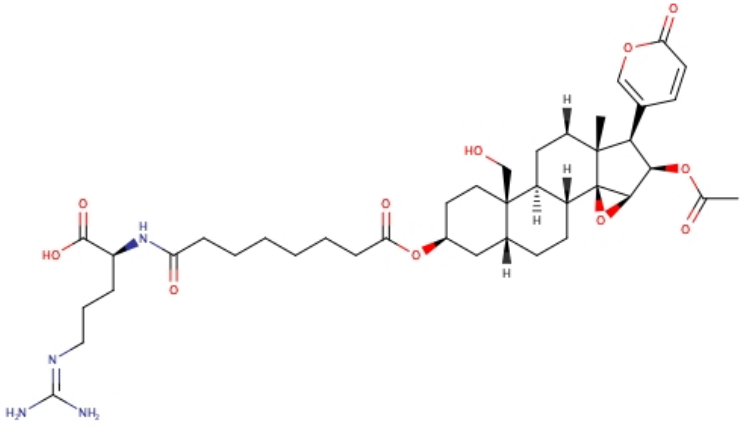
38. resibufotoxin

화학 구조		PubMed ID	
		26186722, 27063985 27790826, 29704033 31590467	
TM-MC 성분 ID	38		
TM-MC 성분 동의어	3-(N-suberoyl arginanyl)resibufogenin; resibufogenin-3-suberate-arginine; resibufogenin-3-O-suberate-arginine		
PubChem ID	101307888		
InChI Key	PRMSQQRXAFMHG-JUFMYRFISA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC C(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₈ H ₅₆ N ₄ O ₈		
Molecular Weight	696.886	Exact Molecular Weight	696.409814779
LogP	2.262	Topological Polar Surface Area	195.93 Å ²
Atom Count	106	Structural Alert Count	5
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	4
Rotatable Bond Count	16	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

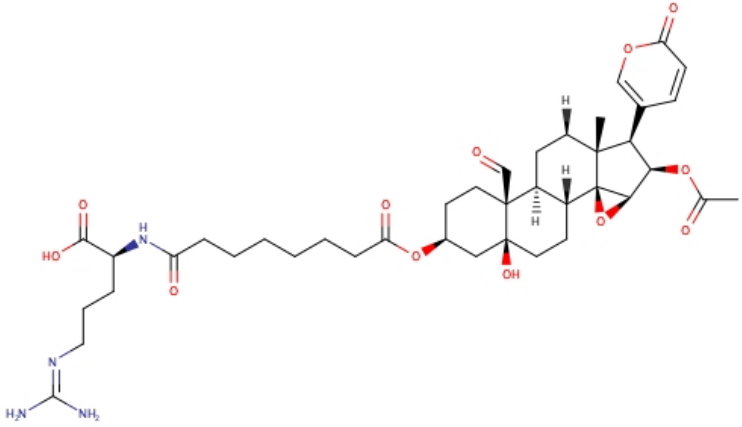
39. cinobufotoxin

화학 구조		PubMed ID	
		26186722, 27063985 29704033, 31590467	
TM-MC 성분 ID	39		
TM-MC 성분 동의어	3-(N-suberoyl argininy)cinobufagin; cinobufagin-3-O-suberate-arginine		
PubChem ID	102003563		
InChI Key	VBCVEPKUYJXQNV-IPAVRDLMSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@H]22[C@@H]3CC[C@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](CCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₄₀ H ₅₈ N ₄ O ₁₀		
Molecular Weight	754.922	Exact Molecular Weight	754.415294084
LogP	1.706	Topological Polar Surface Area	222.23 Å ²
Atom Count	112	Structural Alert Count	5
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	4
Rotatable Bond Count	18	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

40. 3-(N-suberoyl argininy)cinobufaginol

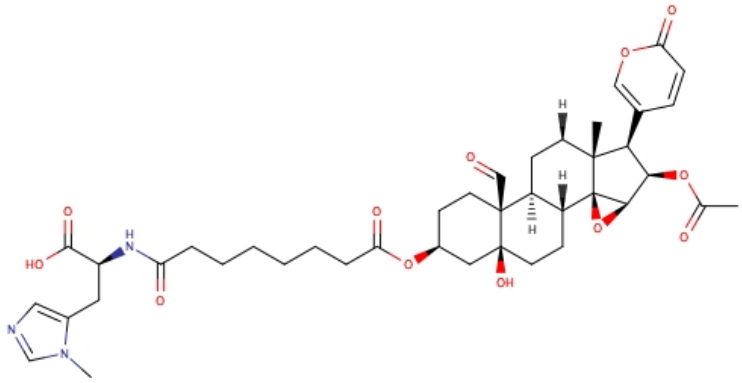
화학 구조		PubMed ID	
		27790826, 29704033 31590467	
TM-MC 성분 ID	40		
TM-MC 성분 동의어	cinobufaginol-3-O-suberate-arginine		
PubChem ID	N/A		
InChI Key	MPUSWPUYXLIZNQ-AUEPTBPSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(CO)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₄₀ H ₅₈ N ₄ O ₁₁		
Molecular Weight	770.921	Exact Molecular Weight	770.410208704
LogP	0.425	Topological Polar Surface Area	242.46 Å ²
Atom Count	113	Structural Alert Count	5
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	5
Rotatable Bond Count	19	Aromatic Ring Count	1
Drug Likeness	0.04	Oral Bioavailability	N

41. 19-oxo-cinobufotalin-3-O-suberate-arginine

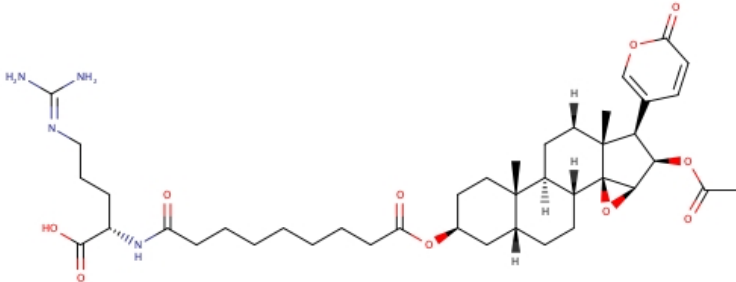
화학 구조	PubMed ID
	<p>27790826, 29704033 31590467</p>

TM-MC 성분 ID	41		
TM-MC 성분 동의어	3-(N-suberoyl argininy)19-oxocinobufotalin; 3-(N-suberoyl argininy)19-oxo-cinobufotalin		
PubChem ID	N/A		
InChI Key	GFIYACJTMPDWBI-QKUVUXRSA-N		
SMILES	CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@]4(O)C[C@H](CC[C@]4(C=O)[C@H]3CC[C@]2(O)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O		
Molecular Formula	C ₄₀ H ₅₆ N ₄ O ₁₂		
Molecular Weight	784.904	Exact Molecular Weight	784.389473259
LogP	-0.493	Topological Polar Surface Area	259.53 Å ²
Atom Count	112	Structural Alert Count	6
Hydrogen Bond Acceptor Count	12	Hydrogen Bond Donor Count	5
Rotatable Bond Count	19	Aromatic Ring Count	1
Drug Likeness	0.03	Oral Bioavailability	N

42. 19-oxocinobufotalin-3-suberate methylhistidine

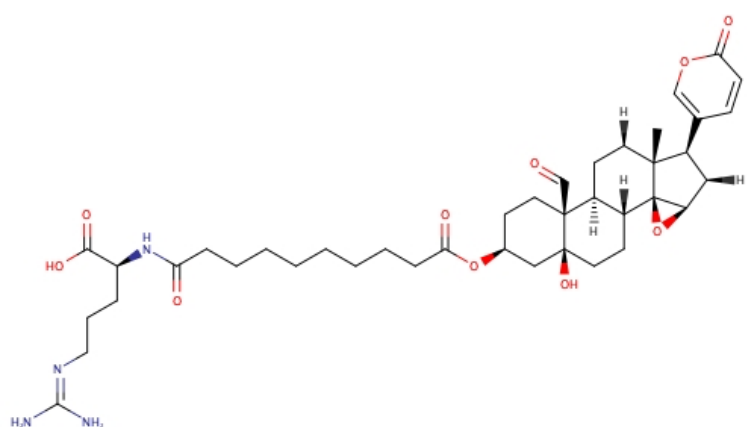
화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	42		
TM-MC 성분 동의어	19-oxo-cinobufotalin-3-O-suberate-methylhistidine		
PubChem ID	N/A		
InChI Key	GVKWWHOSBKEDHH-LLWQMYBFSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@]4(O)C[C@H](CC[C@]4(C=O)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](Cc1cncn1C)C(O)=O</chem>		
Molecular Formula	C ₄₁ H ₅₃ N ₃ O ₁₂		
Molecular Weight	779.884	Exact Molecular Weight	779.362924159
LogP	0.756	Topological Polar Surface Area	212.95 Å ²
Atom Count	109	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	3
Rotatable Bond Count	17	Aromatic Ring Count	2
Drug Likeness	0.09	Oral Bioavailability	N

43. cinobufagin-3-O-nonanedioic-arginine

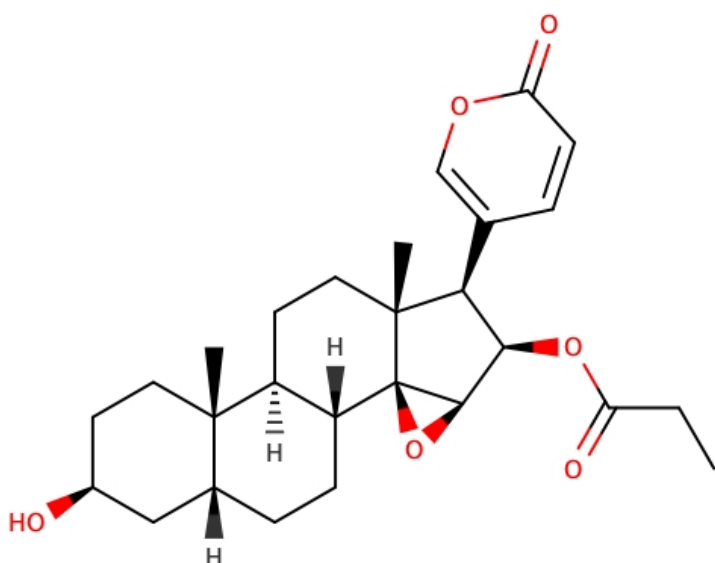
화학 구조	PubMed ID
	27063985, 31590467

TM-MC 성분 ID	43		
TM-MC 성분 동의어	3-(N-azelayl argininy)cinobufagin		
PubChem ID	N/A		
InChI Key	ABUPJLCWEDMOCY-FXHKPIBQSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₄₁ H ₆₀ N ₄ O ₁₀		
Molecular Weight	768.949	Exact Molecular Weight	768.430944148
LogP	2.151	Topological Polar Surface Area	222.23 Å ²
Atom Count	115	Structural Alert Count	5
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	4
Rotatable Bond Count	19	Aromatic Ring Count	1
Drug Likeness	0.05	Oral Bioavailability	N

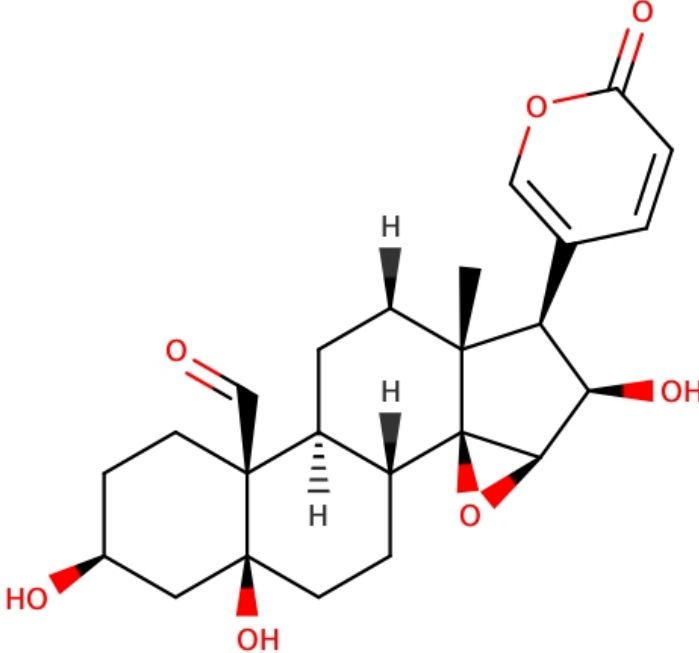
44. bufotalinin-3-O-sebacate-arginine

화학 구조		PubMed ID	
		21696903	
TM-MC 성분 ID	44		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	ACTKOJZNTNPGBW-KVUBNDDBSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C=O)OC(=O)CCCCCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₄₀ H ₅₈ N ₄ O ₁₀		
Molecular Weight	754.922	Exact Molecular Weight	754.415294084
LogP	0.952	Topological Polar Surface Area	233.23 Å ²
Atom Count	112	Structural Alert Count	6
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	5
Rotatable Bond Count	19	Aromatic Ring Count	1
Drug Likeness	0.03	Oral Bioavailability	N

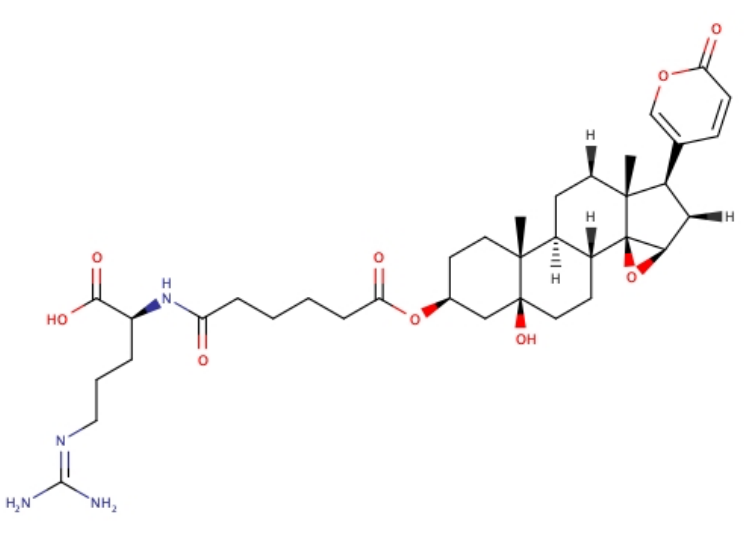
45. methylated-cinobufagin

화학 구조		PubMed ID	
		29704033	
TM-MC 성분 ID	93871		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	YKXQSHGPHCIODJ-KVGKDYBMSA-N		
SMILES	<chem>CCC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₇ H ₃₆ O ₆		
Molecular Weight	456.579	Exact Molecular Weight	456.251188879
LogP	3.508	Topological Polar Surface Area	85.36 Å ²
Atom Count	69	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.56	Oral Bioavailability	Y

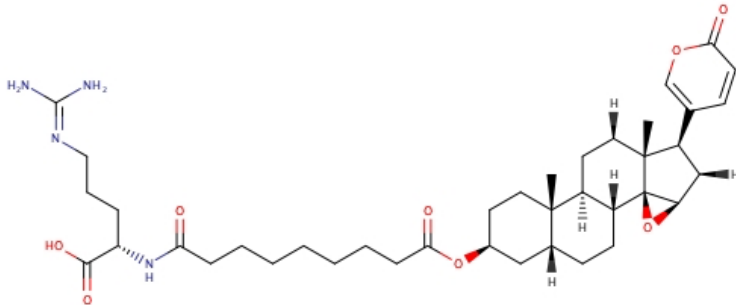
46. 16-desacetyl-19-oxocinobufotalin

화학 구조		PubMed ID	
		29704033	
TM-MC 성분 ID	93902		
TM-MC 성분 동의어	N/A		
PubChem ID	163044399		
InChI Key	OKUGDIFBWYYPKT-XFIALOPGSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@@H](O)CC[C@]34C=O)[C@]11O[C@@H]1[C@H](O)[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₇		
Molecular Weight	430.497	Exact Molecular Weight	430.199153306
LogP	0.168	Topological Polar Surface Area	116.59 Å ²
Atom Count	61	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.45	Oral Bioavailability	Y

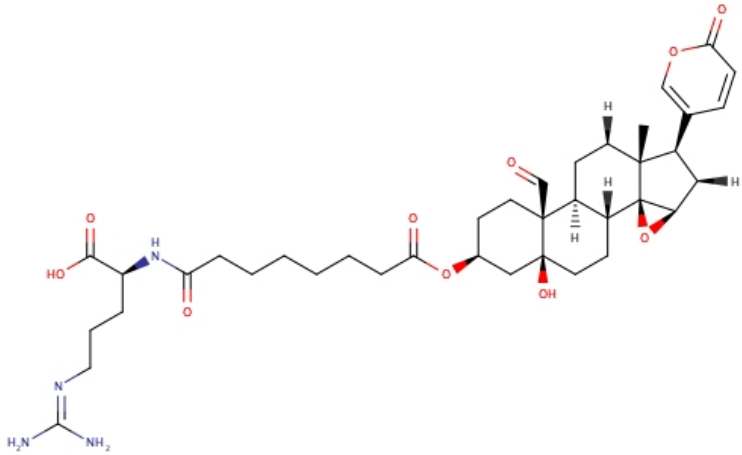
47. 3-(N-adipoyl argininy)marinobufagin

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	94393		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	LGIKUKRTFLNCSX-MTJSNBRWSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₆ H ₅₂ N ₄ O ₉		
Molecular Weight	684.831	Exact Molecular Weight	684.37342927
LogP	0.141	Topological Polar Surface Area	216.16 Å ²
Atom Count	101	Structural Alert Count	5
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	5
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

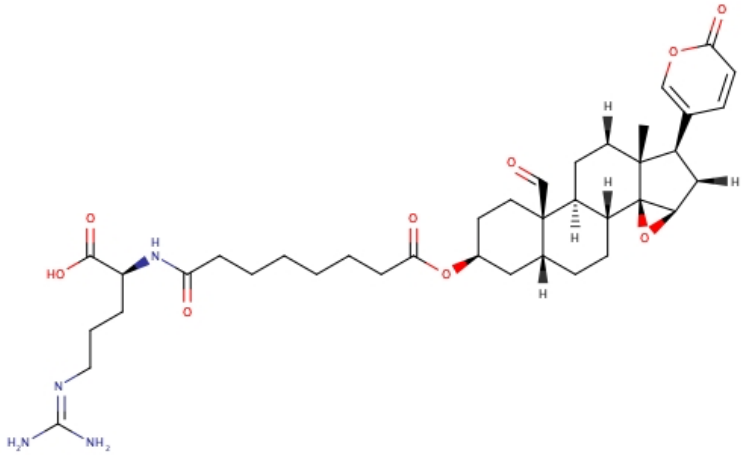
48. 3-(N-azelayl argininy)resibufogenin

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	94396		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	WHZJFHZGAFQLQD-GQAVFVPFSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC CC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₉ H ₅₈ N ₄ O ₈		
Molecular Weight	710.913	Exact Molecular Weight	710.425464844
LogP	2.707	Topological Polar Surface Area	195.93 Å ²
Atom Count	109	Structural Alert Count	5
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	4
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

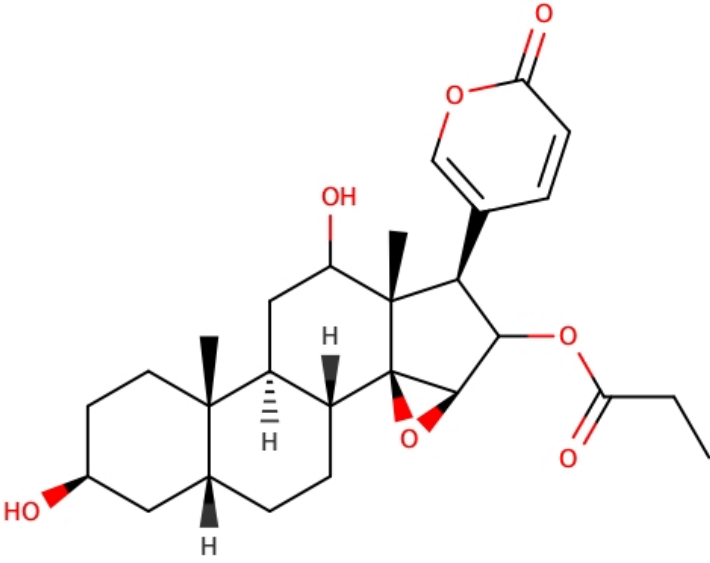
49. 3-(N-suberoyl argininy)bufotalinin

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	94411		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	WZTJLMRKAGCCJB-NTQLEGDYSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C=O)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@]11O[C@@H]1C[C@@H]2c1cc(=O)oc1</chem>		
Molecular Formula	C ₃₈ H ₅₄ N ₄ O ₁₀		
Molecular Weight	726.868	Exact Molecular Weight	726.383993955
LogP	0.063	Topological Polar Surface Area	233.23 Å ²
Atom Count	106	Structural Alert Count	6
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	5
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.04	Oral Bioavailability	N

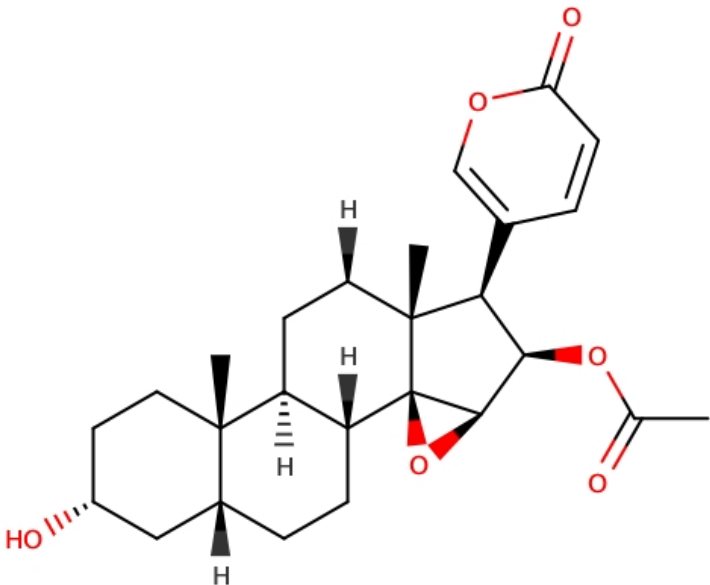
50. 3-(N-suberoyl argininy)resibufagin

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	94419		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	FLGAOLAIHFDJOI-FAWFDSHJSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C=O)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₈ H ₅₄ N ₄ O ₉		
Molecular Weight	710.869	Exact Molecular Weight	710.389079335
LogP	1.295	Topological Polar Surface Area	213 Å ²
Atom Count	105	Structural Alert Count	6
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	4
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.05	Oral Bioavailability	N

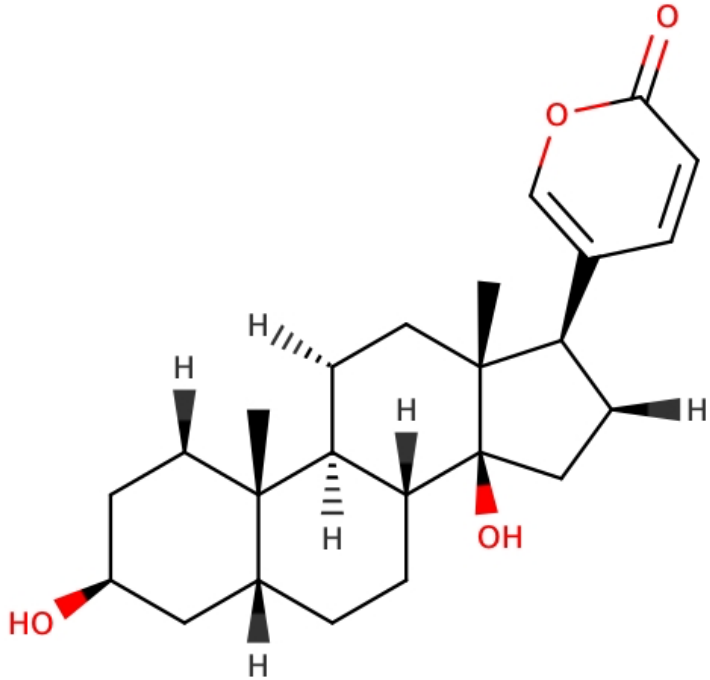
51. methylatedhydroxylcinobufagin

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	94433		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	OYNMZEQBFTDTF-RJZZVILLSA-N		
SMILES	<chem>CCC(=O)OC1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(C)[C@H]3CC(O)[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₇ H ₃₆ O ₇		
Molecular Weight	472.578	Exact Molecular Weight	472.246103499
LogP	2.277	Topological Polar Surface Area	105.59 Å ²
Atom Count	70	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.52	Oral Bioavailability	Y

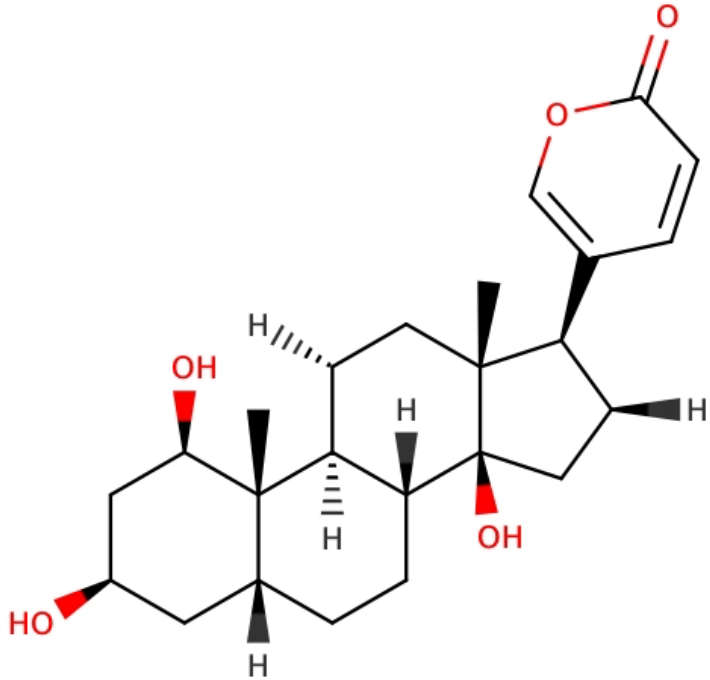
52. 3-epi-cinobufagin

화학 구조		PubMed ID	
		26621782, 31590467	
TM-MC 성분 ID	300406		
TM-MC 성분 동의어	N/A		
PubChem ID	70686663		
InChI Key	SCULJPGYOQQXTK-NPYRLWOYSA-N		
SMILES	CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1		
Molecular Formula	C ₂₆ H ₃₄ O ₆		
Molecular Weight	442.552	Exact Molecular Weight	442.235538815
LogP	2.808	Topological Polar Surface Area	85.36 Å ²
Atom Count	66	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.58	Oral Bioavailability	Y

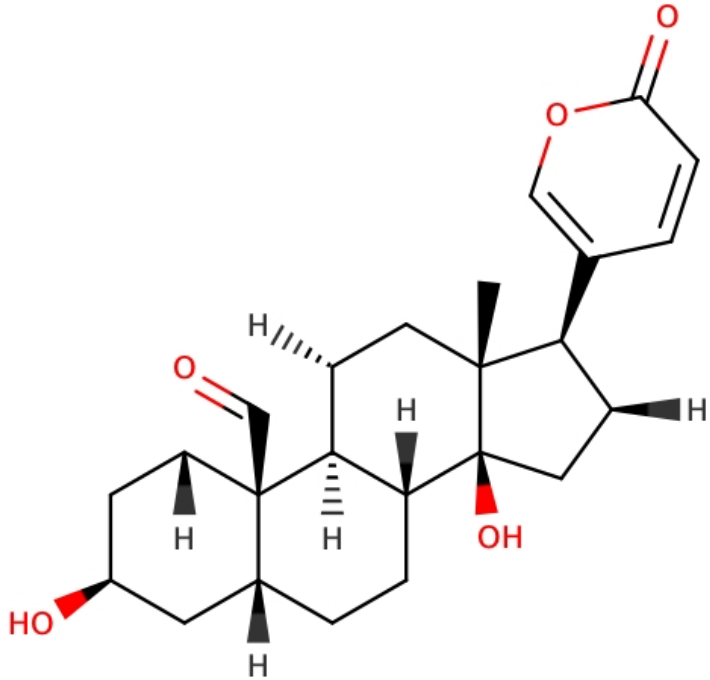
53. bufalin

화학 구조		PubMed ID	
		16723285, 20637273 21696903, 23311159 24484689, 25780654 26186722, 26621782 27013094, 27063985 27328884, 27790826 29704033, 30111043 31342712, 31590467 31884035	
TM-MC 성분 ID	45		
TM-MC 성분 동의어	N/A		
PubChem ID	9547215		
InChI Key	QEEBRPGZBVVINN-BMPKRDENSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₄		
Molecular Weight	386.532	Exact Molecular Weight	386.245709575
LogP	3.277	Topological Polar Surface Area	66.76 Å ²
Atom Count	62	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.78	Oral Bioavailability	Y

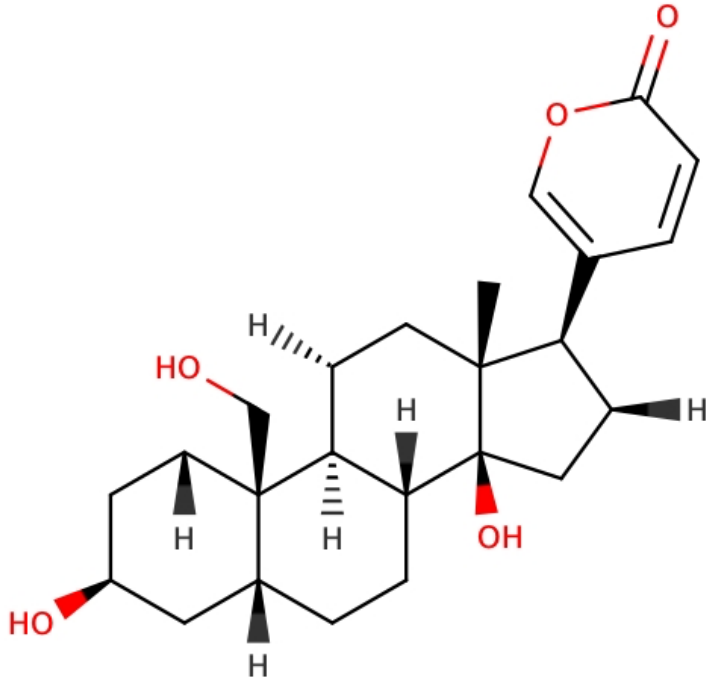
54. 1 β -hydroxybufalin

화학 구조		PubMed ID	
		26186722, 26621782 31590467	
TM-MC 성분 ID	46		
TM-MC 성분 동의어	1 β -hydroxybufalin		
PubChem ID	10993111		
InChI Key	IMWIOPJWKFUYSV-YXVUHCDSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)C[C@@H](O)[C@]34C)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₅		
Molecular Weight	402.531	Exact Molecular Weight	402.240624195
LogP	1.973	Topological Polar Surface Area	86.99 Å ²
Atom Count	63	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.67	Oral Bioavailability	Y

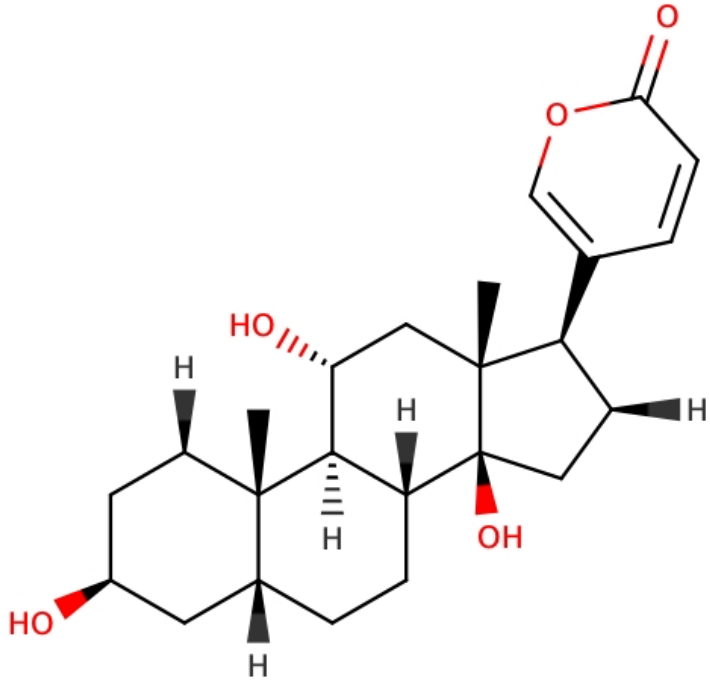
55. 19-oxo-bufalin

화학 구조		PubMed ID	
		<p>20637273, 26186722 26621782, 27328884 29704033, 31590467</p>	
TM-MC 성분 ID	47		
TM-MC 성분 동의어	N/A		
PubChem ID	10883889		
InChI Key	STSJQAAJJHGCMJ-KLAFWMLLSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₅		
Molecular Weight	400.515	Exact Molecular Weight	400.22497413
LogP	2.31	Topological Polar Surface Area	83.83 Å ²
Atom Count	61	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.75	Oral Bioavailability	Y

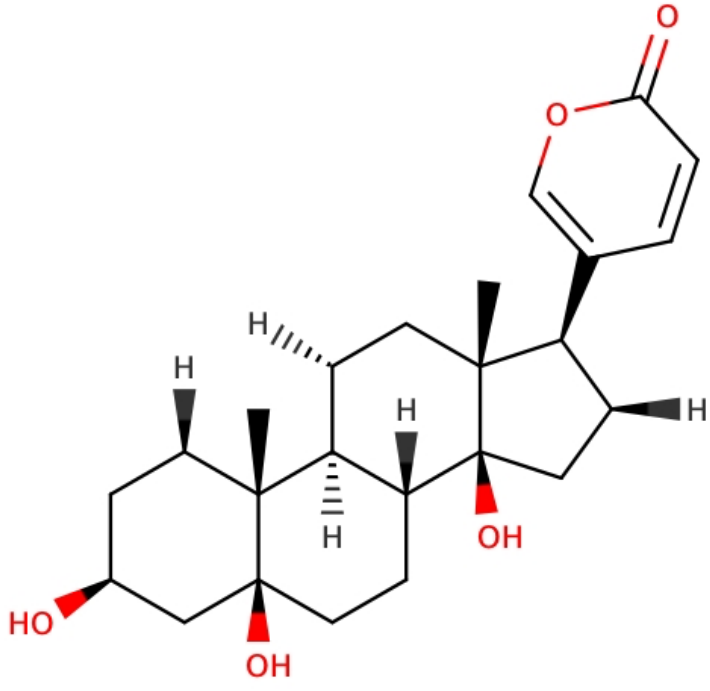
56. 19-hydroxybufalin

화학 구조		PubMed ID	
		20637273, 21696903 26186722, 29704033 31590467	
TM-MC 성분 ID	48		
TM-MC 성분 동의어	19-hydroxylbufalin		
PubChem ID	101375811		
InChI Key	AXTYMYOHGWVSQN-KLAFWMLLSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34CO)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₅		
Molecular Weight	402.531	Exact Molecular Weight	402.240624195
LogP	1.996	Topological Polar Surface Area	86.99 Å ²
Atom Count	63	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.71	Oral Bioavailability	Y

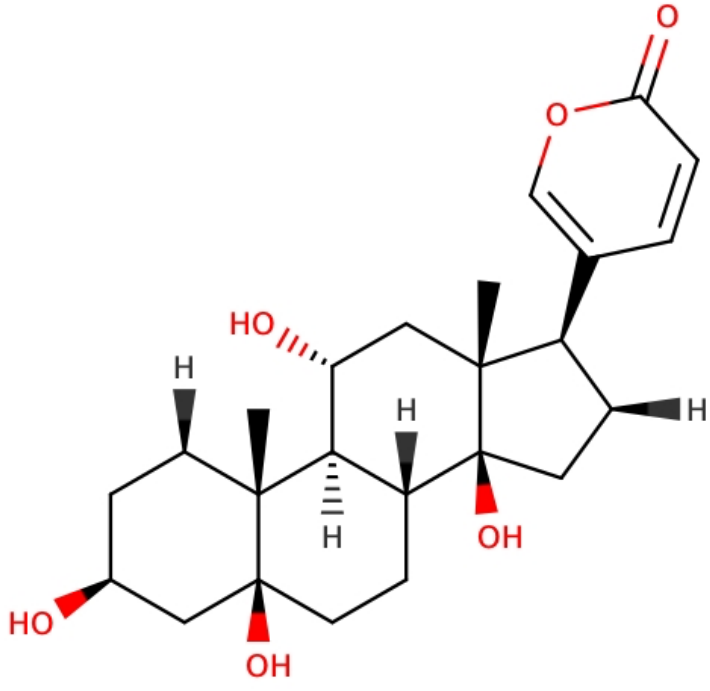
57. gamabufotalin

화학 구조		PubMed ID	
		<p>16723285, 20637273 21696903, 23311159 24484689, 26186722 26621782, 27063985 27328884, 27790826 29704033, 30111043 31590467, 31884035</p>	
TM-MC 성분 ID	49		
TM-MC 성분 동의어	N/A		
PubChem ID	259803		
InChI Key	FMTLOAVOGWSPEF-KJRPADTMSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₅		
Molecular Weight	402.531	Exact Molecular Weight	402.240624195
LogP	1.968	Topological Polar Surface Area	86.99 Å ²
Atom Count	63	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.67	Oral Bioavailability	Y

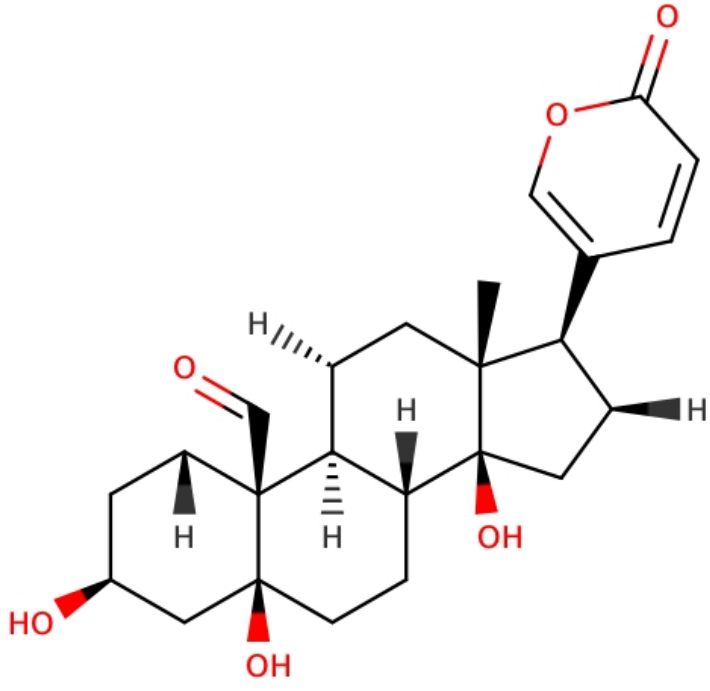
58. telocinobufagin

화학 구조		PubMed ID	
		<p>16723285, 20637273 21696903, 24484689 26186722, 26621782 27013094, 27063985 27328884, 29704033 30111043, 31342712 31590467, 31884035</p>	
TM-MC 성분 ID	50		
TM-MC 성분 동의어	N/A		
PubChem ID	259991		
InChI Key	PBSOJKPTQWWJJD-ZBDZJSKLSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@@H](O)CC[C@]34C)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₅		
Molecular Weight	402.531	Exact Molecular Weight	402.240624195
LogP	2.045	Topological Polar Surface Area	86.99 Å ²
Atom Count	63	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.67	Oral Bioavailability	Y

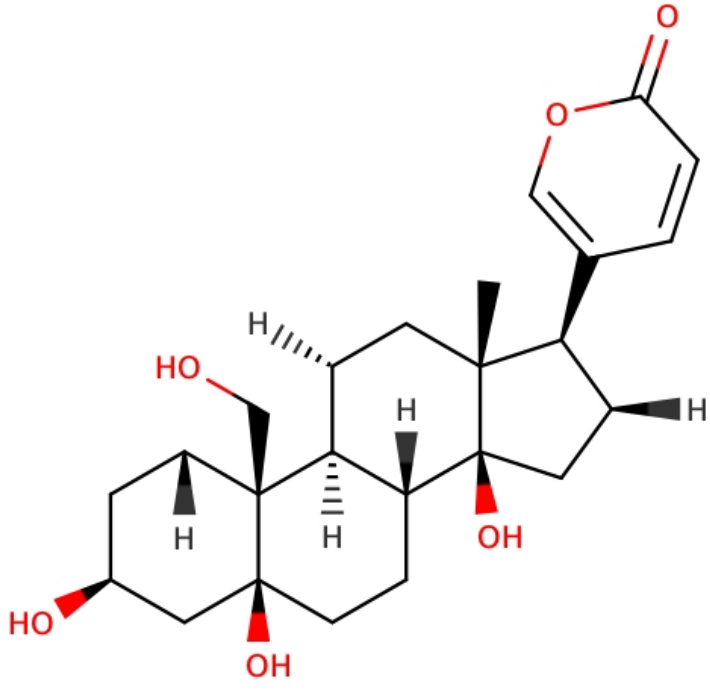
59. 11 α -hydroxytelocinobufagin

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	51		
TM-MC 성분 동의어	N/A		
PubChem ID	15789042		
InChI Key	DHZAUUHFNLOXIY-BZLDVOFMSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@]4(O)C[C@@H](O)CC[C@]34C)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₆		
Molecular Weight	418.53	Exact Molecular Weight	418.235538815
LogP	0.736	Topological Polar Surface Area	107.22 Å ²
Atom Count	64	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.54	Oral Bioavailability	Y

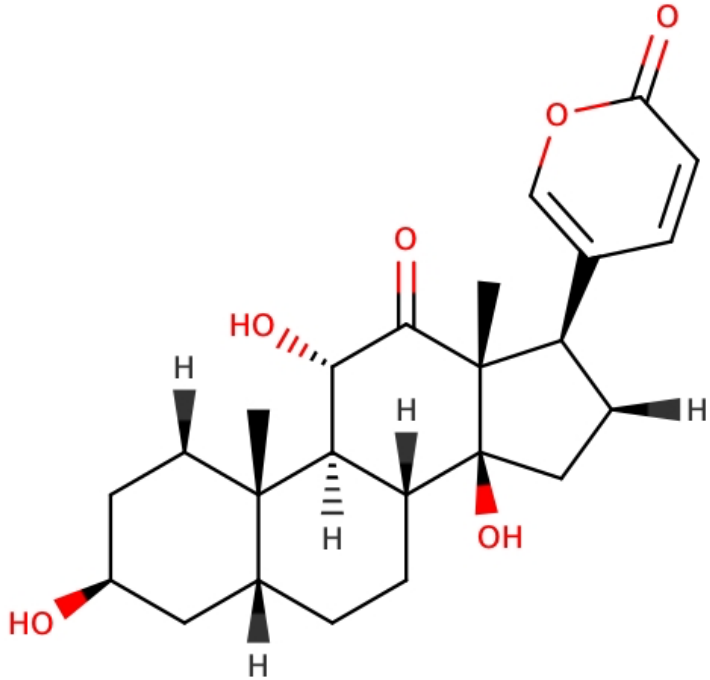
60. hellebrigenin

화학 구조		PubMed ID	
		<p>20637273, 26186722 26621782, 27013094 29704033, 30111043 31590467, 31884035</p>	
TM-MC 성분 ID	52		
TM-MC 성분 동의어	N/A		
PubChem ID	259577		
InChI Key	TVKPTWJPKVSGJB-XHCIOXAKSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@@H](O)CC[C@]34C=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₆		
Molecular Weight	416.514	Exact Molecular Weight	416.21988875
LogP	1.078	Topological Polar Surface Area	104.06 Å ²
Atom Count	62	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.63	Oral Bioavailability	Y

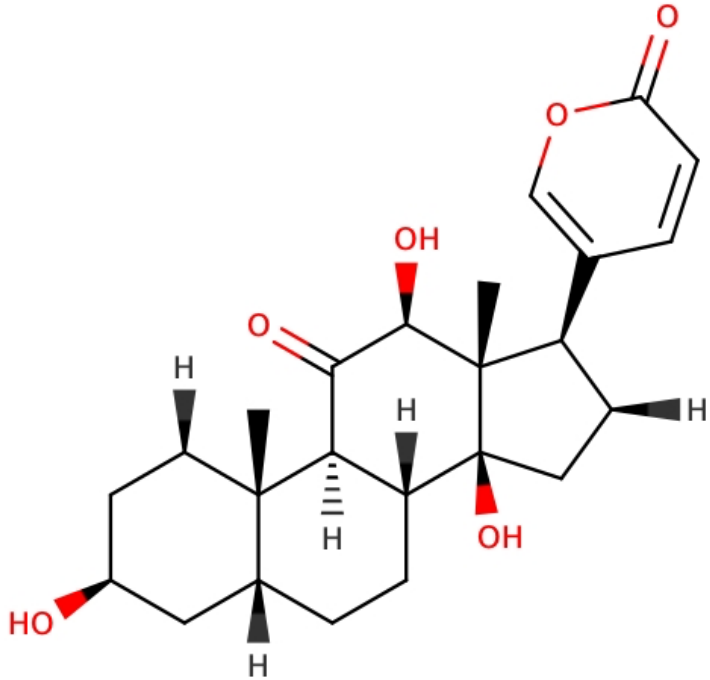
61. hellebrigenol

화학 구조		PubMed ID	
		20637273, 26621782 29704033, 31590467	
TM-MC 성분 ID	53		
TM-MC 성분 동의어	19-hydroxytelocinobufagin		
PubChem ID	10432170		
InChI Key	ABVKNZHLRVHZSO-XHCIOXAKSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@@H](O)CC[C@]34CO)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₆		
Molecular Weight	418.53	Exact Molecular Weight	418.235538815
LogP	0.764	Topological Polar Surface Area	107.22 Å ²
Atom Count	64	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.57	Oral Bioavailability	Y

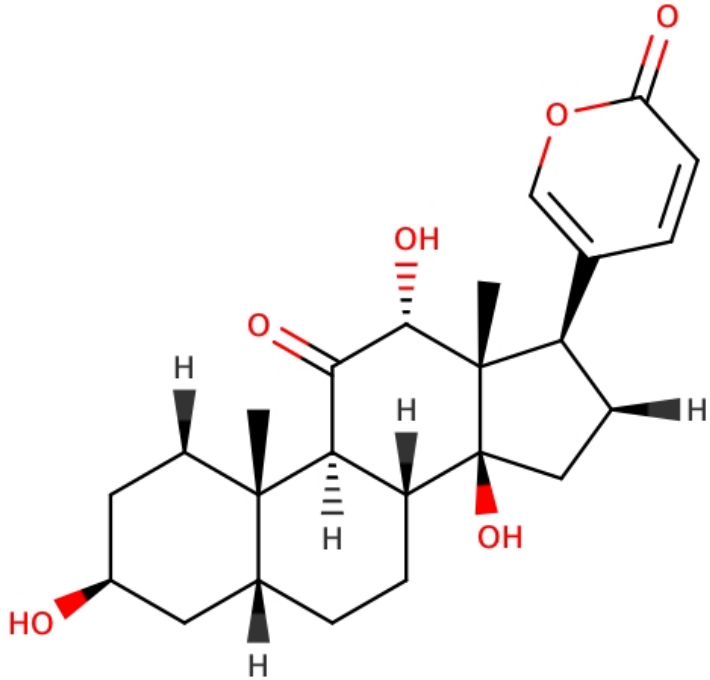
62. arenobufagin

화학 구조		PubMed ID	
		16723285, 20637273 21696903, 24484689 26186722, 26621782 27013094, 27063985 27328884, 29704033 30111043, 31590467 31866511, 31884035	
TM-MC 성분 ID	54		
TM-MC 성분 동의어	N/A		
PubChem ID	12305198		
InChI Key	JGDCRWYOMWSTFC-AZGSIFHYSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@@H](O)CC[C@]3(C)[C@H]1[C@H](O)C2=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₆		
Molecular Weight	416.514	Exact Molecular Weight	416.21988875
LogP	1.816	Topological Polar Surface Area	104.06 Å ²
Atom Count	62	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.65	Oral Bioavailability	Y

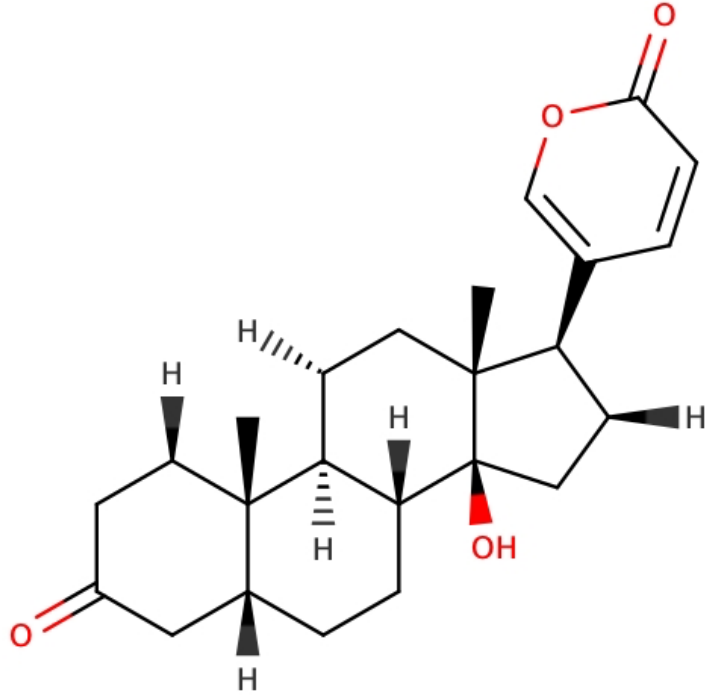
63. bufarenogin

화학 구조		PubMed ID	
		<p>20637273, 26621782 27063985, 27328884 27790826, 29704033 31590467</p>	
TM-MC 성분 ID	55		
TM-MC 성분 동의어	N/A		
PubChem ID	167607		
InChI Key	SOGONHOGEFLVPE-PUVOGLICSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@@H](O)CC[C@]3(C)[C@H]1C(=O)[C@H]2O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₆		
Molecular Weight	416.514	Exact Molecular Weight	416.21988875
LogP	1.638	Topological Polar Surface Area	104.06 Å ²
Atom Count	62	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.65	Oral Bioavailability	Y

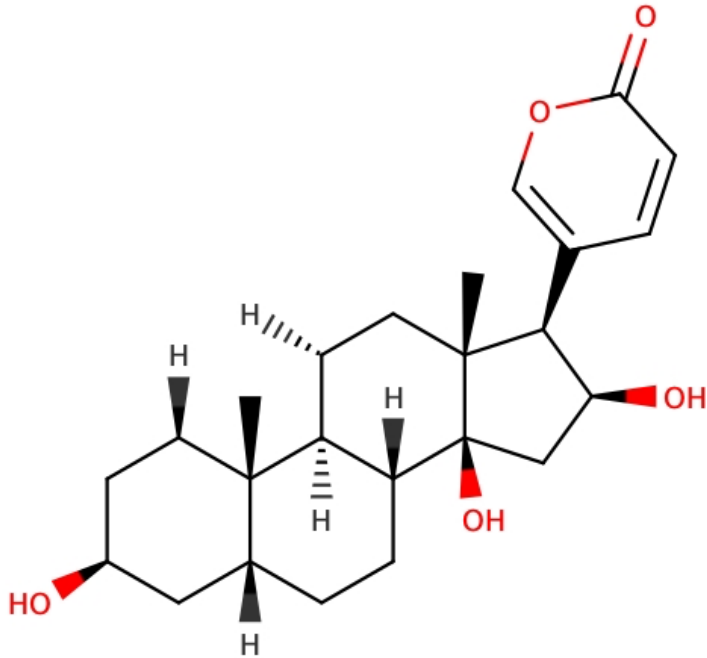
64. ψ -bufarenogin

화학 구조		PubMed ID	
		16723285, 20637273 21696903, 26621782 27328884, 29704033 31590467, 31884035	
TM-MC 성분 ID	56		
TM-MC 성분 동의어	ψ -bufarenogin		
PubChem ID	204810		
InChI Key	SOGONHOGFLVPE-BHZHDSHXSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@@H](O)CC[C@]3(C)[C@H]1C(=O)[C@@H]2O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₆		
Molecular Weight	416.514	Exact Molecular Weight	416.21988875
LogP	1.638	Topological Polar Surface Area	104.06 Å ²
Atom Count	62	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.65	Oral Bioavailability	Y

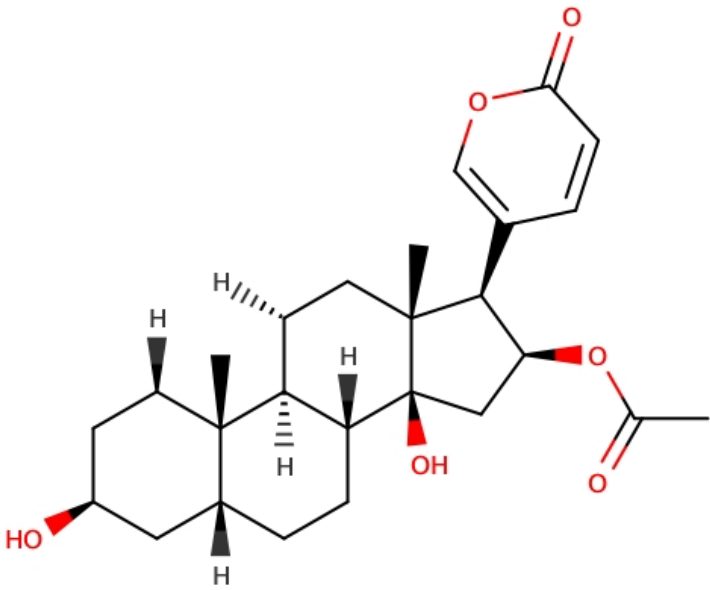
65. bufalone

화학 구조		PubMed ID	
		26621782, 27063985	
TM-MC 성분 ID	57		
TM-MC 성분 동의어	3-keto-bufalin		
PubChem ID	99606		
InChI Key	YHPFWEDUGHFFTA-PNERCMSUSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4CC(=O)CC[C@]34C)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₄		
Molecular Weight	384.516	Exact Molecular Weight	384.23005951
LogP	3.484	Topological Polar Surface Area	63.6 Å ²
Atom Count	60	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.81	Oral Bioavailability	Y

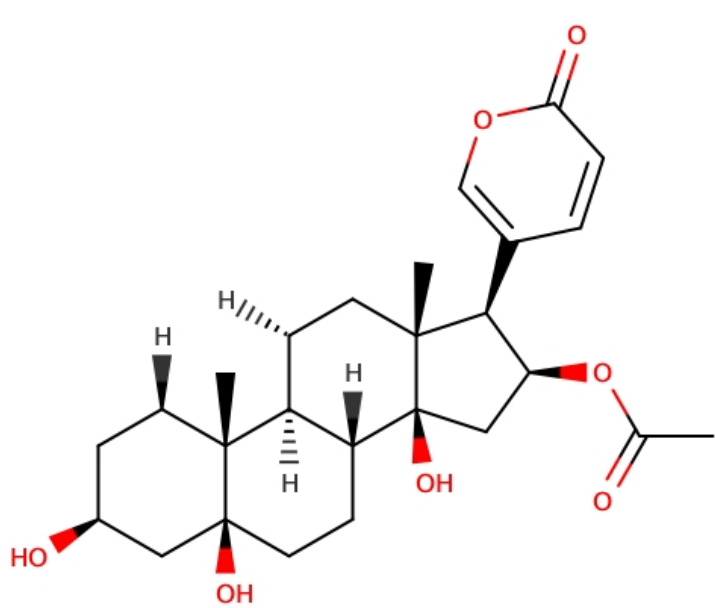
66. desacetylbufotalin

화학 구조		PubMed ID	
		20637273, 24484689 26186722, 26621782 27013094, 29704033 31590467	
TM-MC 성분 ID	58		
TM-MC 성분 동의어	N/A		
PubChem ID	12358889		
InChI Key	MWFCMSURKYLINK-QDLCSEJESA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@@H](O)CC[C@]34C)[C@@]1(O)C[C@H](O)[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₅		
Molecular Weight	402.531	Exact Molecular Weight	402.240624195
LogP	1.895	Topological Polar Surface Area	86.99 Å ²
Atom Count	63	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.67	Oral Bioavailability	Y

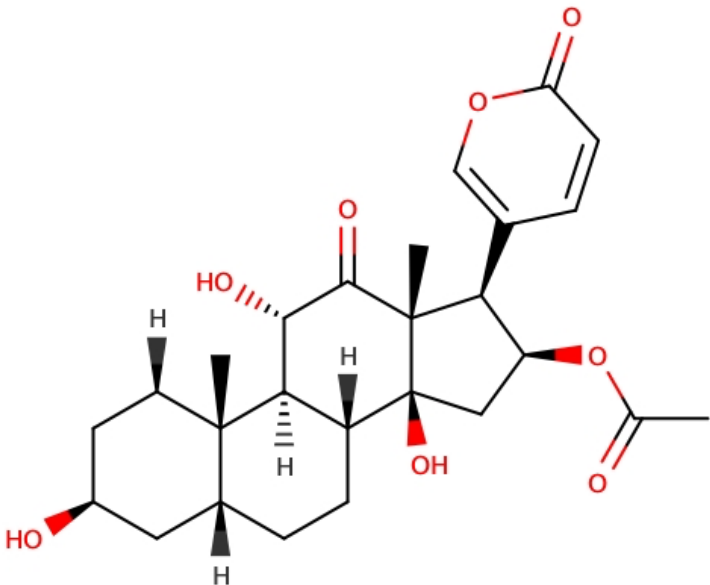
67. bufotalin

화학 구조		PubMed ID	
		16723285, 20637273 21696903, 23311159 24484689, 26186722 26621782, 27013094 27063985, 27328884 27790826, 29704033 30111043, 31590467 31884035	
TM-MC 성분 ID	59		
TM-MC 성분 동의어	N/A		
PubChem ID	12302120		
InChI Key	VOZHMAYHYHEWBW-NVOOAVKYSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₆ O ₆		
Molecular Weight	444.568	Exact Molecular Weight	444.251188879
LogP	2.336	Topological Polar Surface Area	93.06 Å ²
Atom Count	68	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.70	Oral Bioavailability	Y

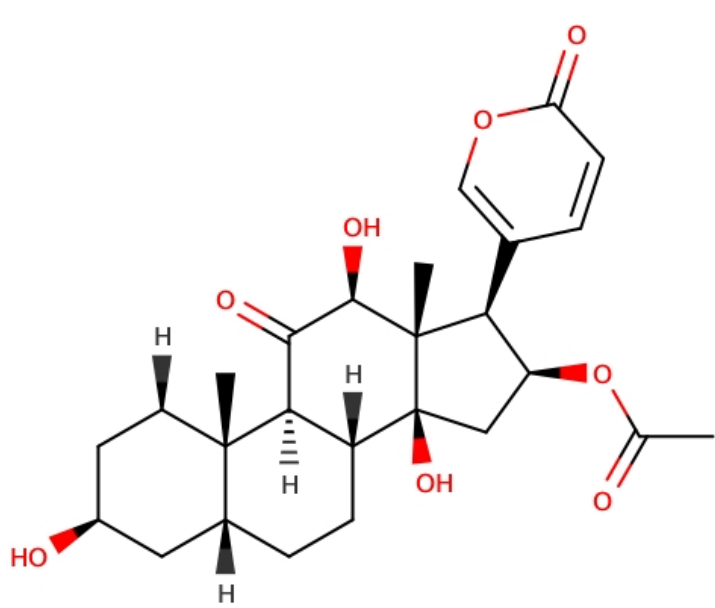
68. 5-hydroxybufotalin

화학 구조		PubMed ID	
		20637273	
TM-MC 성분 ID	60		
TM-MC 성분 동의어	N/A		
PubChem ID	15513540		
InChI Key	XXFFZCKSFHQEMN-JPDWBOAPSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@]4(O)C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₆ O ₇		
Molecular Weight	460.567	Exact Molecular Weight	460.246103499
LogP	1.104	Topological Polar Surface Area	113.29 Å ²
Atom Count	69	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.59	Oral Bioavailability	Y

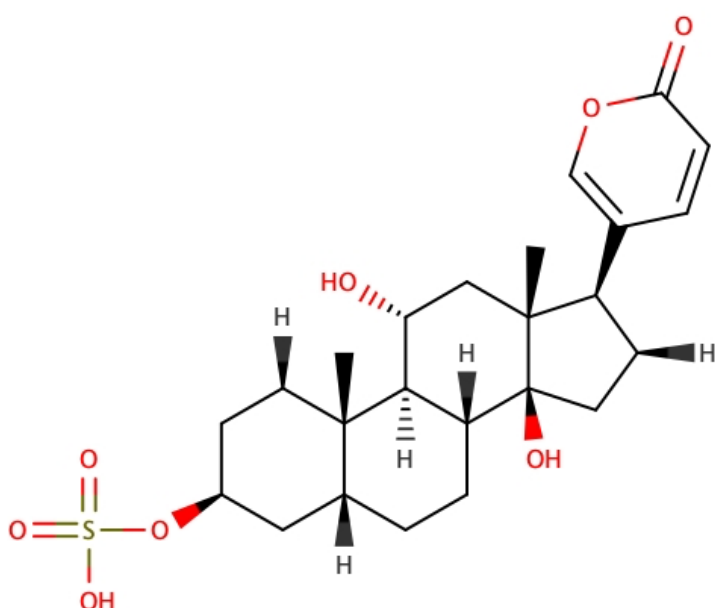
69. 16-O-acetylaerenobufagin

화학 구조		PubMed ID	
		20361780, 20637273	
TM-MC 성분 ID	61		
TM-MC 성분 동의어	N/A		
PubChem ID	46210730		
InChI Key	AKMUMYGVUCYWMD-XNHPCSCASA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(C)[C@H]3[C@H](O)C(=O)[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₄ O ₈		
Molecular Weight	474.55	Exact Molecular Weight	474.225368055
LogP	0.876	Topological Polar Surface Area	130.36 Å ²
Atom Count	68	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.56	Oral Bioavailability	Y

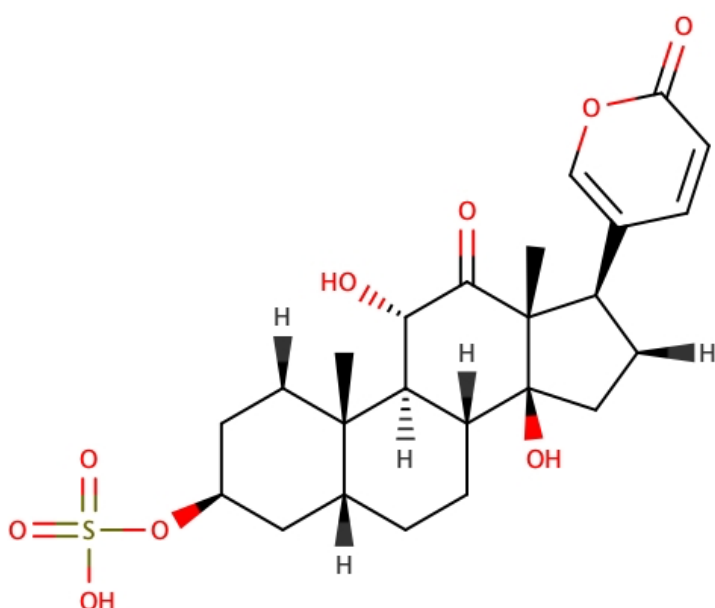
70. 16-acetoxybufarenogin

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	62		
TM-MC 성분 동의어	N/A		
PubChem ID	24809382		
InChI Key	NTPVNLXPPGBVAV-IDSXRIHJSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C(=O)[C@@H](O)[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₄ O ₈		
Molecular Weight	474.55	Exact Molecular Weight	474.225368055
LogP	0.698	Topological Polar Surface Area	130.36 Å ²
Atom Count	68	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.55	Oral Bioavailability	Y

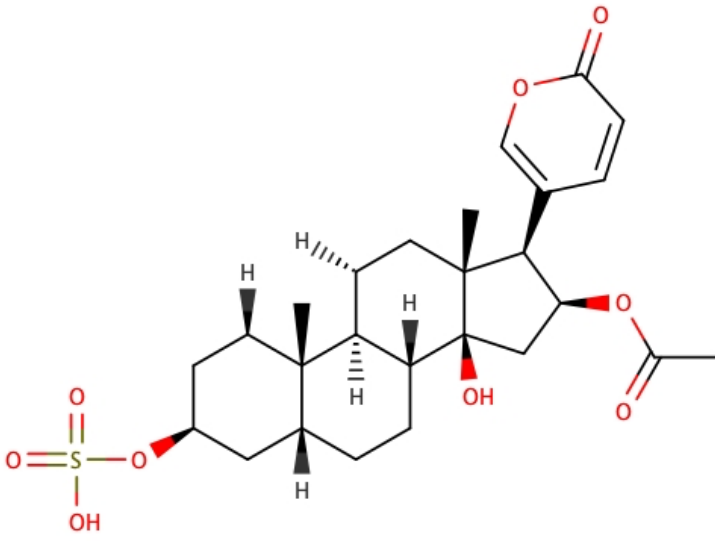
71. gamabufotalin-3-O-sulfate

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	63		
TM-MC 성분 동의어	N/A		
PubChem ID	163133527		
InChI Key	HAXKWAFMTWSKKD-KJRPADTMSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OS(=O)(=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₈ S		
Molecular Weight	482.59	Exact Molecular Weight	482.197439229
LogP	0.551	Topological Polar Surface Area	130.36 Å ²
Atom Count	67	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.54	Oral Bioavailability	Y

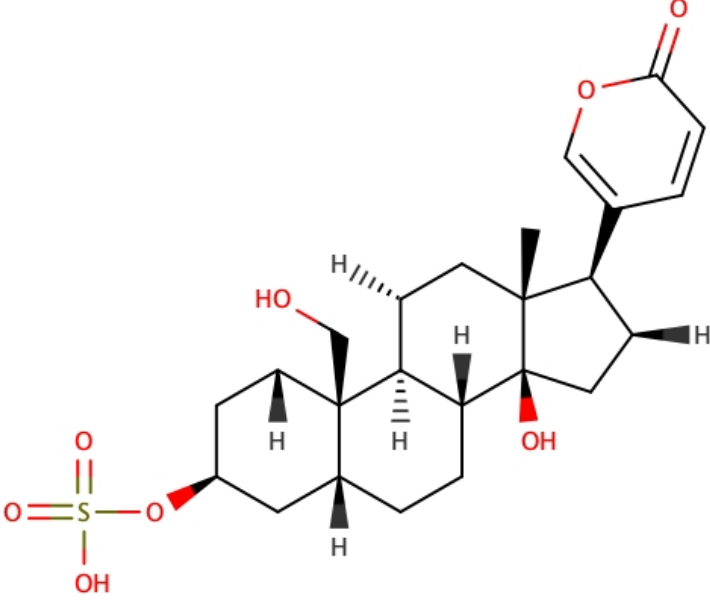
72. arenobufagin-3-O-sulfate

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	64		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	FUPUDTUQKOBQF-AZGSIFHYSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@H](CC[C@]3(C)[C@H]1[C@H](O)C2=O)OS(O)(=O)=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₉ S		
Molecular Weight	496.57	Exact Molecular Weight	496.176703784
LogP	0.294	Topological Polar Surface Area	147.43 Å ²
Atom Count	66	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.51	Oral Bioavailability	Y

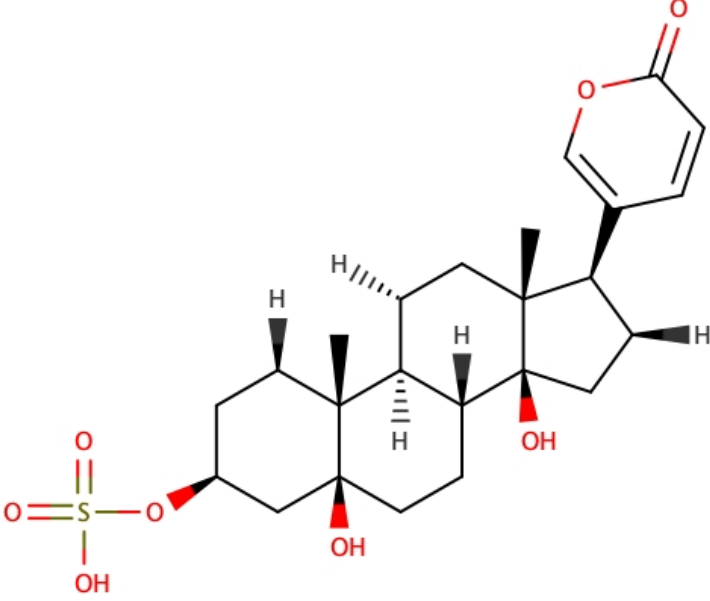
73. bufotalin-3-O-sulfate

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	65		
TM-MC 성분 동의어	N/A		
PubChem ID	163159580		
InChI Key	QMJOECXNDJGSM-NVOOAVKYSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OS(O)(=O)=O</chem>		
Molecular Formula	C ₂₆ H ₃₆ O ₉ S		
Molecular Weight	524.63	Exact Molecular Weight	524.208003913
LogP	0.976	Topological Polar Surface Area	136.43 Å ²
Atom Count	72	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	5	Aromatic Ring Count	1
Drug Likeness	0.44	Oral Bioavailability	Y

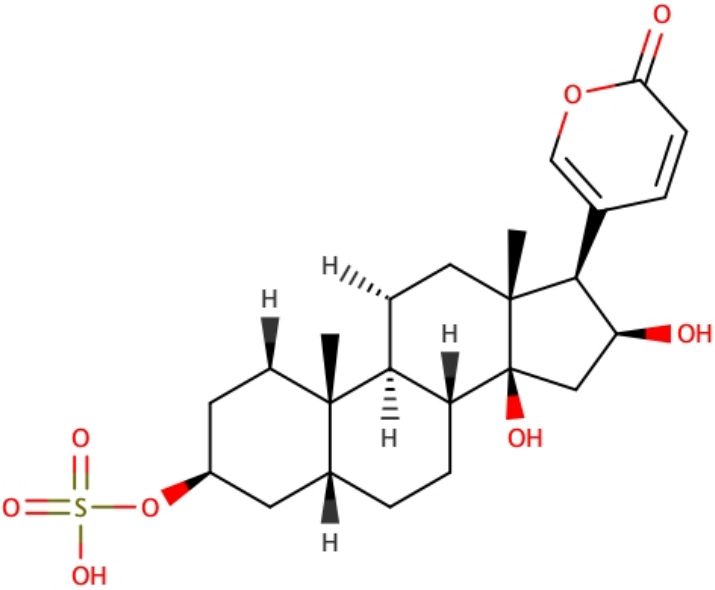
74. 19-hydroxybufalin-3-O-sulfate

화학 구조		PubMed ID	
		20361780, 20637273	
TM-MC 성분 ID	66		
TM-MC 성분 동의어	N/A		
PubChem ID	46210590		
InChI Key	ARJYDXCDFJGCS-KLAFWMLLSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34CO)OS(O)(=O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₈ S		
Molecular Weight	482.59	Exact Molecular Weight	482.197439229
LogP	0.268	Topological Polar Surface Area	130.36 Å ²
Atom Count	67	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.53	Oral Bioavailability	Y

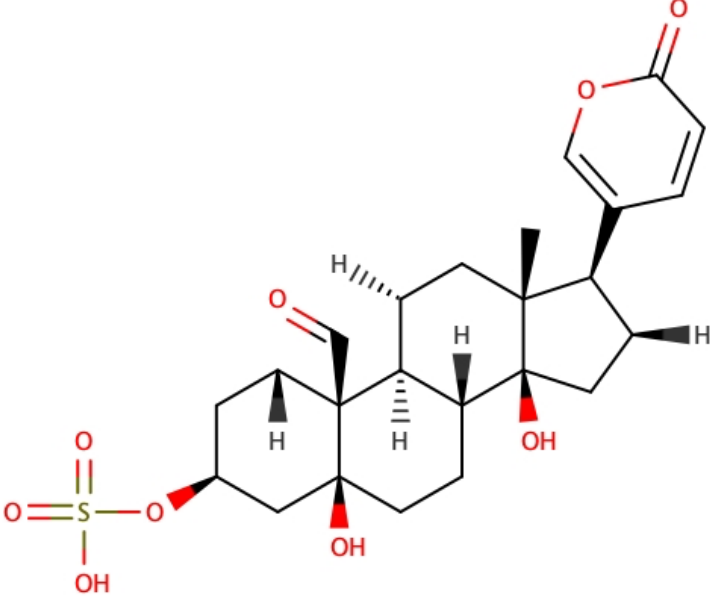
75. telocinobufagin-3-O-sulfate

화학 구조		PubMed ID	
		20361780, 20637273	
TM-MC 성분 ID	67		
TM-MC 성분 동의어	N/A		
PubChem ID	46210729		
InChI Key	RNRSYDQILACYBK-ZBDZJSLSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C)OS(O)(=O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₈ S		
Molecular Weight	482.59	Exact Molecular Weight	482.197439229
LogP	0.292	Topological Polar Surface Area	130.36 Å ²
Atom Count	67	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.53	Oral Bioavailability	Y

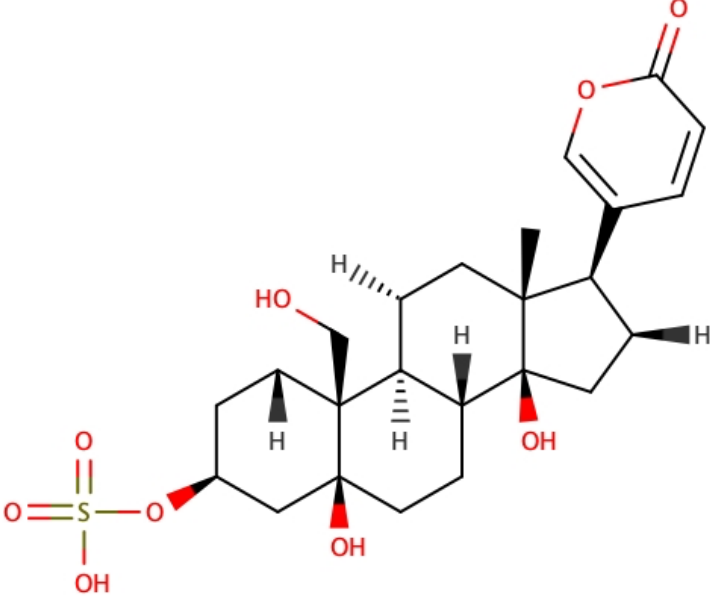
76. desacetylbufotalin-3-O-sulfate

화학 구조		PubMed ID	
		20361780, 20637273	
TM-MC 성분 ID	68		
TM-MC 성분 동의어	N/A		
PubChem ID	46210591		
InChI Key	AKBDSCBYBRPAMM-QDLCSJEJSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OS(O)(=O)=O)[C@@]1(O)C[C@H](O)[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₈ S		
Molecular Weight	482.59	Exact Molecular Weight	482.197439229
LogP	0.534	Topological Polar Surface Area	130.36 Å ²
Atom Count	67	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.54	Oral Bioavailability	Y

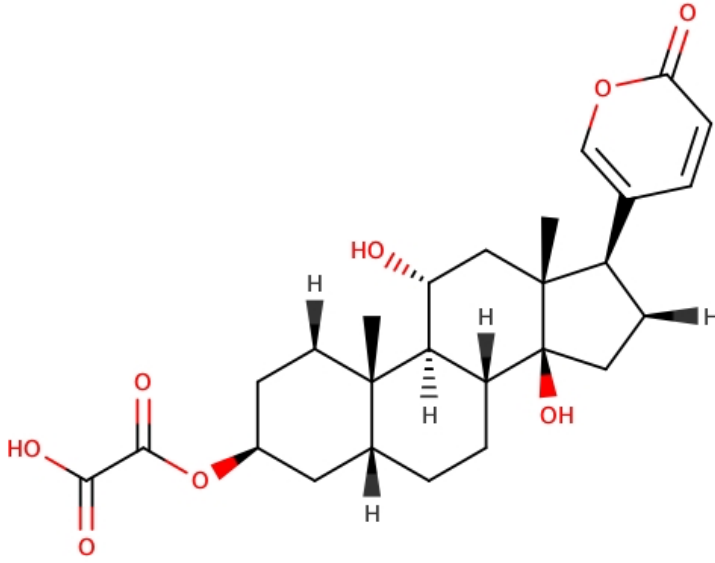
77. hellebrigenin-3-O-sulfate

화학 구조		PubMed ID	
		20361780, 20637273	
TM-MC 성분 ID	69		
TM-MC 성분 동의어	N/A		
PubChem ID	46210589		
InChI Key	DYORMTARWWEOFF-XHCIOXAKSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)[C@H](CC[C@]34C=O)OS(O)(=O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₉ S		
Molecular Weight	496.57	Exact Molecular Weight	496.176703784
LogP	-0.836	Topological Polar Surface Area	147.43 Å ²
Atom Count	66	Structural Alert Count	2
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.36	Oral Bioavailability	Y

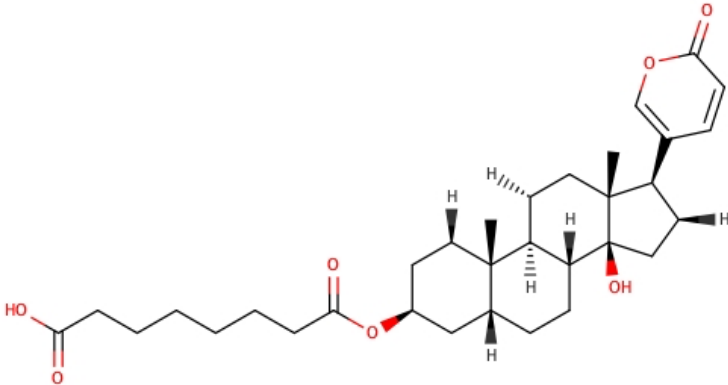
78. hellebrigenol-3-O-sulfate

화학 구조		PubMed ID	
		20361780, 20637273	
TM-MC 성분 ID	70		
TM-MC 성분 동의어	N/A		
PubChem ID	46210588		
InChI Key	MGPOGNBMLAFGGK-XHCIOXAKSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34CO)OS(O)(=O)=O)[C@@]1(O)CC[C@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₉ S		
Molecular Weight	498.59	Exact Molecular Weight	498.192353849
LogP	-1.044	Topological Polar Surface Area	150.59 Å ²
Atom Count	68	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.39	Oral Bioavailability	Y

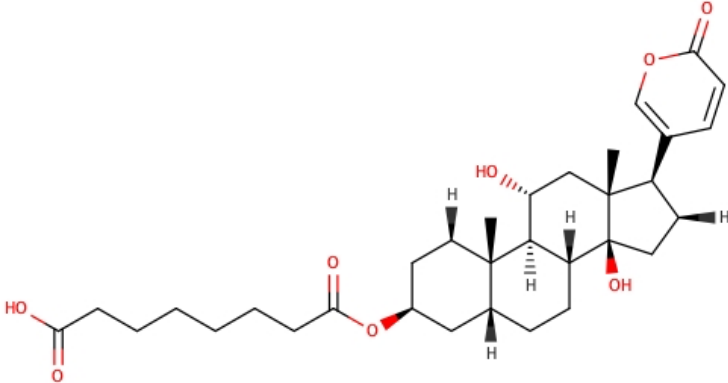
79. gamabufotalin-3-oxalate

화학 구조		PubMed ID	
		21696903, 29704033 31590467	
TM-MC 성분 ID	71		
TM-MC 성분 동의어	gamabufotalin 3-oxalate		
PubChem ID	N/A		
InChI Key	WJXKSRKDBRSBKB-RUPWZGJLSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₄ O ₈		
Molecular Weight	474.55	Exact Molecular Weight	474.225368055
LogP	2.602	Topological Polar Surface Area	130.36 Å ²
Atom Count	68	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.45	Oral Bioavailability	Y

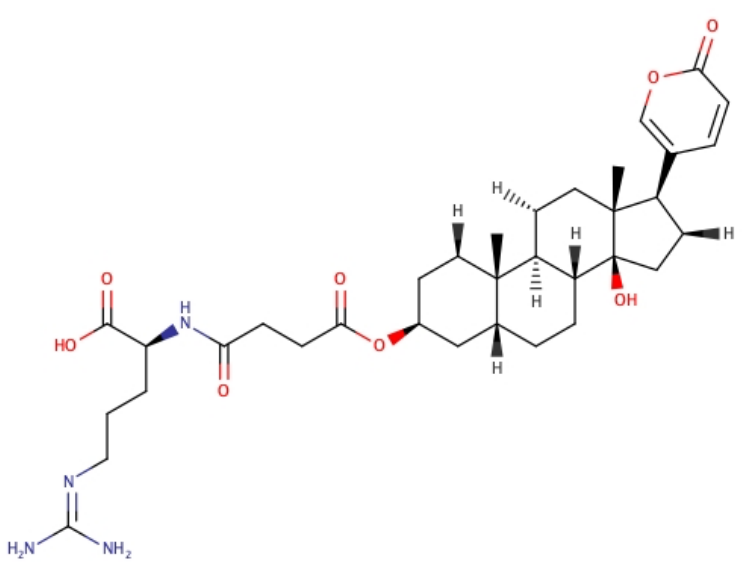
80. bufalin-3-O-suberoyl ester

화학 구조		PubMed ID	
		20637273	
TM-MC 성분 ID	72		
TM-MC 성분 동의어	N/A		
PubChem ID	67050194		
InChI Key	RMMRFKRTCRCMYRY-IHSZOXLFSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₂ H ₄₆ O ₇		
Molecular Weight	542.713	Exact Molecular Weight	542.324353821
LogP	5.321	Topological Polar Surface Area	110.13 Å ²
Atom Count	85	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	10	Aromatic Ring Count	1
Drug Likeness	0.31	Oral Bioavailability	Y

81. gamabufotalin-3-O-suberate

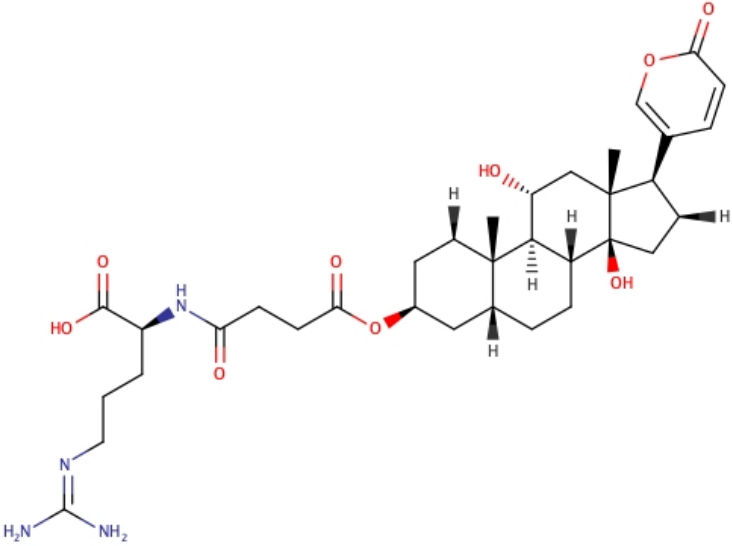
화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	73		
TM-MC 성분 동의어	N/A		
PubChem ID	162952112		
InChI Key	PIZLMBYRGJZNDF-NMFYPETMSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₂ H ₄₆ O ₈		
Molecular Weight	558.712	Exact Molecular Weight	558.319268441
LogP	4.012	Topological Polar Surface Area	130.36 Å ²
Atom Count	86	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	10	Aromatic Ring Count	1
Drug Likeness	0.29	Oral Bioavailability	Y

82. bufalin-3-O-succinate-arginine

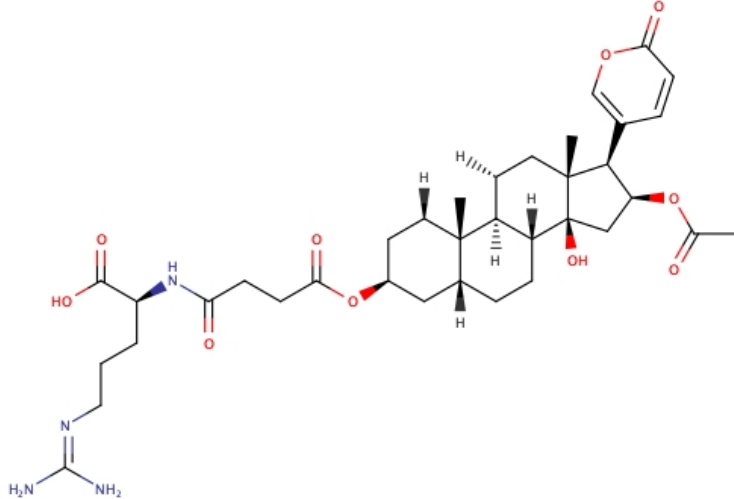
화학 구조	PubMed ID
	<p>21696903, 26186722 27063985, 29704033 31590467</p>

TM-MC 성분 ID	74		
TM-MC 성분 동의어	bufalone-3-O-succinate-arginine; 3-(N-succinyl argininy)bufalin; 3-(N-succinyl-argininy)bufalin		
PubChem ID	102595428		
InChI Key	VSYAVGJIENUTGR-LKWJOGBFSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₄ H ₅₀ N ₄ O ₈		
Molecular Weight	642.794	Exact Molecular Weight	642.362864586
LogP	0.397	Topological Polar Surface Area	203.63 Å ²
Atom Count	96	Structural Alert Count	4
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	12	Aromatic Ring Count	1
Drug Likeness	0.09	Oral Bioavailability	N

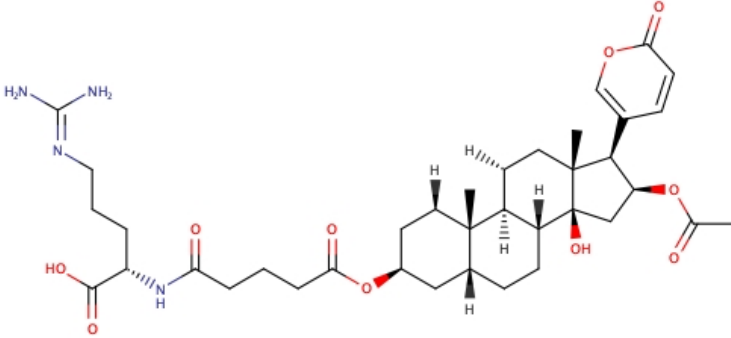
83. gamabufotalin-3-O-succinate-arginine

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	75		
TM-MC 성분 동의어	N/A		
PubChem ID	163193221		
InChI Key	PEDUWTJUACTTDA-XDXHQNGOSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₄ H ₅₀ N ₄ O ₉		
Molecular Weight	658.793	Exact Molecular Weight	658.357779206
LogP	-0.912	Topological Polar Surface Area	223.86 Å ²
Atom Count	97	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	12	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

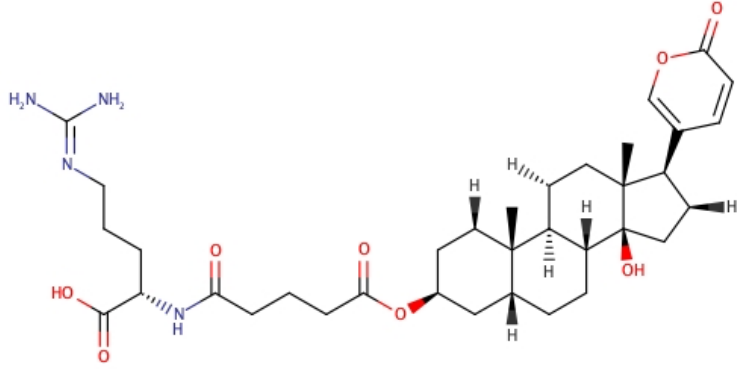
84. bufotalin-3-O-succinate-arginine

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	77		
TM-MC 성분 동의어	3-(N-succinyl argininy)bufotalin		
PubChem ID	162925488		
InChI Key	ZHIFTHYTXVBJCZ-FJRGKVFBSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₆ H ₅₂ N ₄ O ₁₀		
Molecular Weight	700.83	Exact Molecular Weight	700.36834389
LogP	-0.543	Topological Polar Surface Area	229.93 Å ²
Atom Count	102	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	5
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

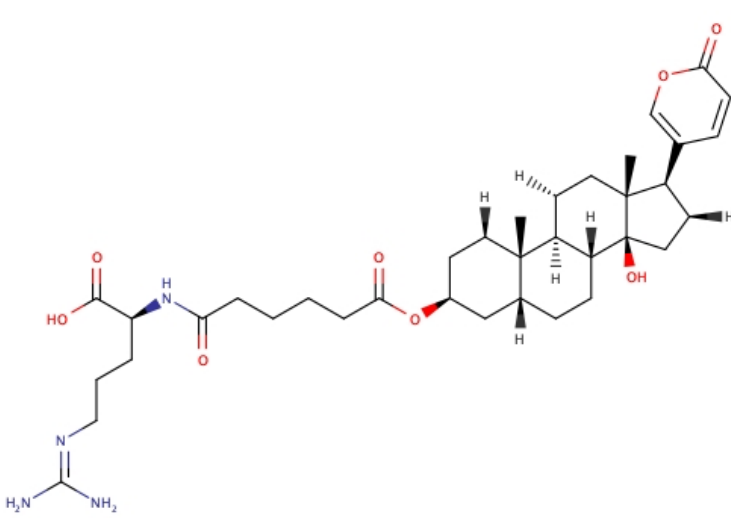
85. bufotalin-3-O-glutarate-arginine

화학 구조		PubMed ID	
		21696903	
TM-MC 성분 ID	78		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	OPCSUCPTRKEHQK-RRGWOQLESA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₇ H ₅₄ N ₄ O ₁₀		
Molecular Weight	714.857	Exact Molecular Weight	714.383993955
LogP	-0.099	Topological Polar Surface Area	229.93 Å ²
Atom Count	105	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	5
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

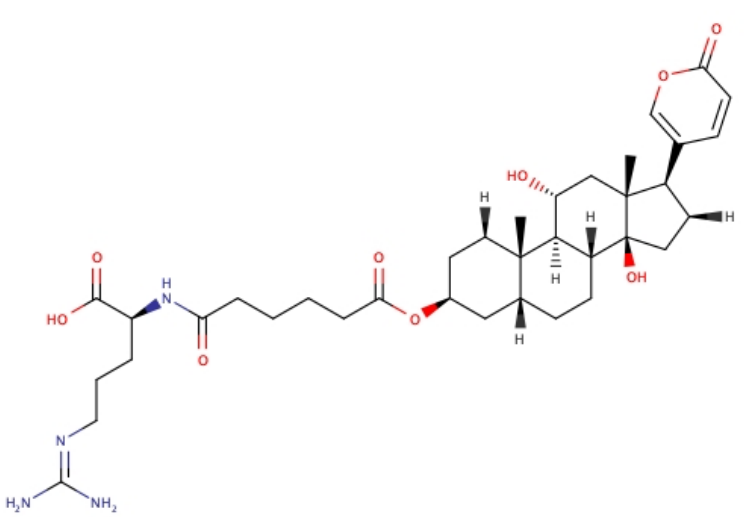
86. bufalin-3-O-glutarate-arginine

화학 구조		PubMed ID	
		27790826, 29704033	
TM-MC 성분 ID	79		
TM-MC 성분 동의어	3-(N-glutaryl argininy)bufalin		
PubChem ID	N/A		
InChI Key	BTNNVWJBPQLVPZ-RCJCPRHOSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₅ H ₅₂ N ₄ O ₈		
Molecular Weight	656.821	Exact Molecular Weight	656.37851465
LogP	0.842	Topological Polar Surface Area	203.63 Å ²
Atom Count	99	Structural Alert Count	4
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	13	Aromatic Ring Count	1
Drug Likeness	0.09	Oral Bioavailability	N

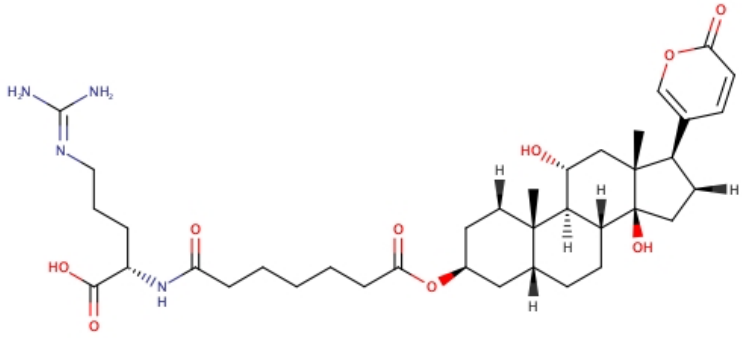
87. bufalin-3-O-adipate-arginine

화학 구조		PubMed ID	
		21696903, 26186722 27063985, 29704033 31590467	
TM-MC 성분 ID	80		
TM-MC 성분 동의어	3-(N-adipoyl arginanyl)bufalin		
PubChem ID	N/A		
InChI Key	FRCBECZEIYEAJI-MROFYLGOSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₆ H ₅₄ N ₄ O ₈		
Molecular Weight	670.848	Exact Molecular Weight	670.394164715
LogP	1.286	Topological Polar Surface Area	203.63 Å ²
Atom Count	102	Structural Alert Count	4
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.08	Oral Bioavailability	N

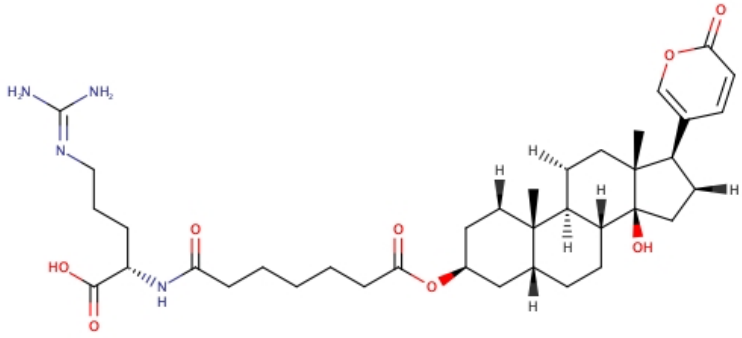
88. gamabufotalin-3-O-adipate-arginine

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	81		
TM-MC 성분 동의어	3-(N-adipoyl arginyl)gamabufotalin		
PubChem ID	162884054		
InChI Key	IHCHSKWJBBWPMX-APXSGGFZSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₆ H ₅₄ N ₄ O ₉		
Molecular Weight	686.847	Exact Molecular Weight	686.389079335
LogP	-0.023	Topological Polar Surface Area	223.86 Å ²
Atom Count	103	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

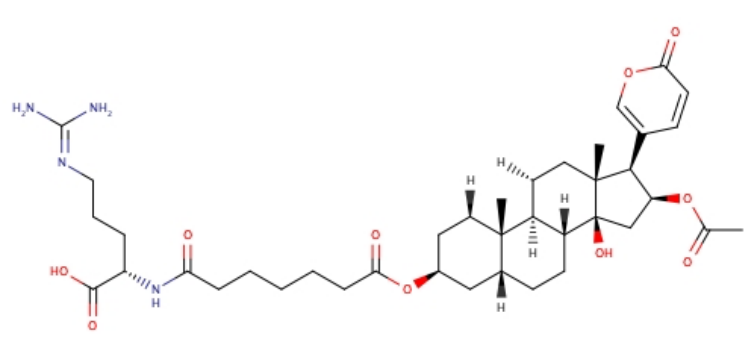
89. gamabufotalin-3-O-pimelate-arginine

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	82		
TM-MC 성분 동의어	3-(N-pimeloyl argininy)gamabufotalin		
PubChem ID	N/A		
InChI Key	GPZJDEMLEYEUGF-RSRSXCHRSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC(=O)N[C@@H](CCC=C(N)N)C(O)=O)[C@]1(O)CC[C@@H]2c1cc(=O)oc1</chem>		
Molecular Formula	C ₃₇ H ₅₆ N ₄ O ₉		
Molecular Weight	700.874	Exact Molecular Weight	700.404729399
LogP	0.422	Topological Polar Surface Area	223.86 Å ²
Atom Count	106	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

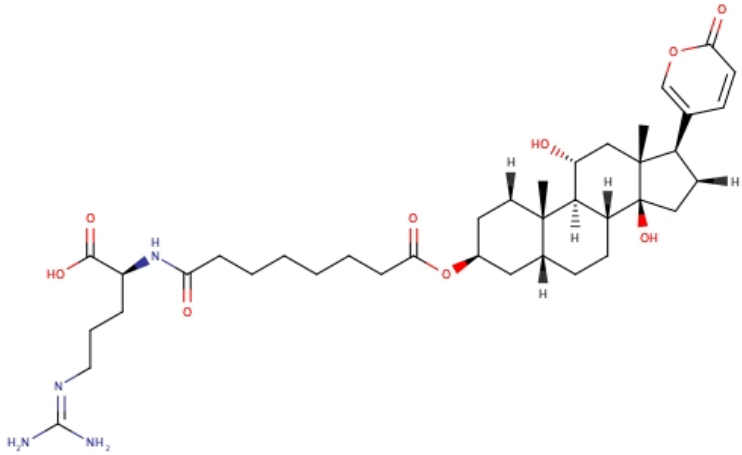
90. 3-(N-pimeloyl argininy)bufalin

화학 구조		PubMed ID	
		27790826, 29704033 31590467	
TM-MC 성분 ID	83		
TM-MC 성분 동의어	bufalin-3-O-pimelate-arginine		
PubChem ID	N/A		
InChI Key	JHHGGXQGJLIRBM-QZOZFHEESA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₇ H ₅₆ N ₄ O ₈		
Molecular Weight	684.875	Exact Molecular Weight	684.409814779
LogP	1.731	Topological Polar Surface Area	203.63 Å ²
Atom Count	105	Structural Alert Count	4
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.08	Oral Bioavailability	N

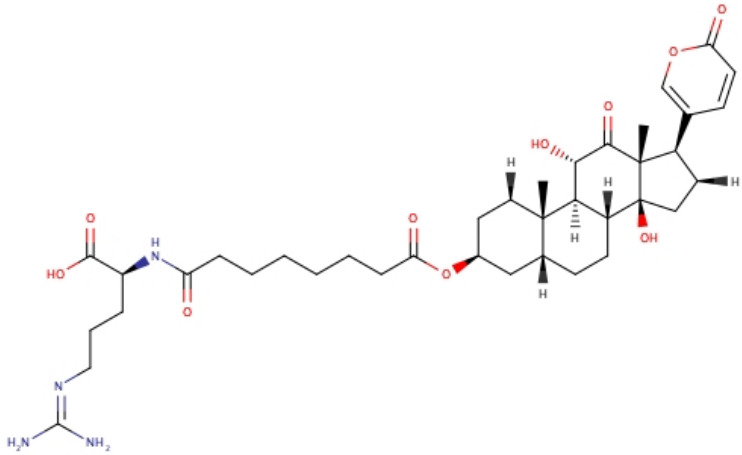
91. bufotalin-3-O-pimelate-arginine

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	84		
TM-MC 성분 동의어	N/A		
PubChem ID	46930230		
InChI Key	KMRRYJGABZCSGL-DFBJEOCLSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₃₉ H ₅₈ N ₄ O ₁₀		
Molecular Weight	742.911	Exact Molecular Weight	742.415294084
LogP	0.79	Topological Polar Surface Area	229.93 Å ²
Atom Count	111	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	5
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

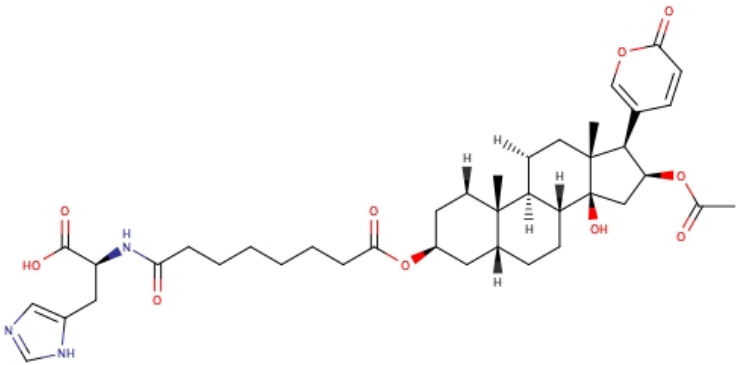
92. gamabufotalitoxin

화학 구조		PubMed ID	
		<p>21696903, 26186722 27063985, 27790826 29704033, 31590467</p>	
TM-MC 성분 ID	85		
TM-MC 성분 동의어	gamabufotalin-3-O-suberate-arginine; 3-(N-suberoyl argininyl)gamabufotalin; gamabufotalin-3-suberate-arginine ester		
PubChem ID	86341923		
InChI Key	UQWIHDZMOYEOHL-YXAZDFSTSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1c cc(=O)oc1</chem>		
Molecular Formula	C ₃₈ H ₅₈ N ₄ O ₉		
Molecular Weight	714.901	Exact Molecular Weight	714.420379464
LogP	0.866	Topological Polar Surface Area	223.86 Å ²
Atom Count	109	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	16	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

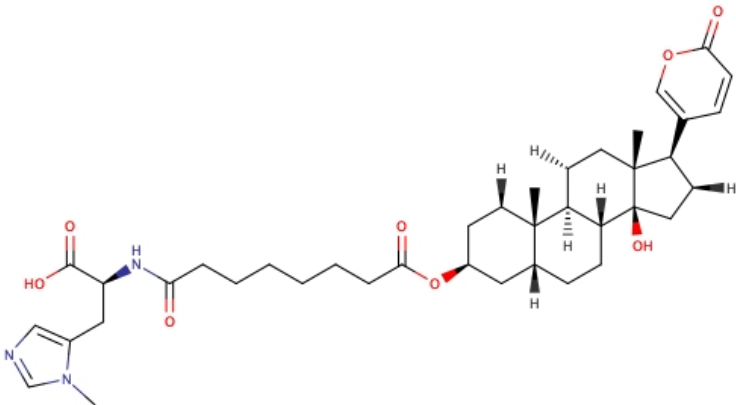
93. arenobufotoxin

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	86		
TM-MC 성분 동의어	3-(N-suberoyl argininy)arenobufagin		
PubChem ID	86341924		
InChI Key	DVTUBVYKYQYNDH-NZJARFEFSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@H](CC[C@]3(C)[C@H]1[C@H](O)C2=O)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₈ H ₅₆ N ₄ O ₁₀		
Molecular Weight	728.884	Exact Molecular Weight	728.399644019
LogP	0.715	Topological Polar Surface Area	240.93 Å ²
Atom Count	108	Structural Alert Count	4
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	16	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

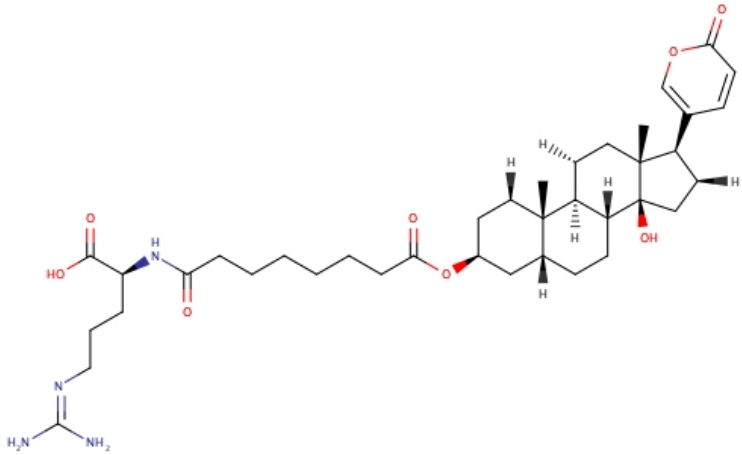
94. bufotalin-3-O-suberate-histidine

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	88		
TM-MC 성분 동의어	N/A		
PubChem ID	163186953		
InChI Key	WANWQPCJXGSVEB-YGBAFLPYSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](Cc1cnc[nH]1)C(O)=O</chem>		
Molecular Formula	C ₄₀ H ₅₅ N ₃ O ₁₀		
Molecular Weight	737.891	Exact Molecular Weight	737.388744983
LogP	2.265	Topological Polar Surface Area	194.21 Å ²
Atom Count	108	Structural Alert Count	2
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	4
Rotatable Bond Count	16	Aromatic Ring Count	2
Drug Likeness	0.15	Oral Bioavailability	N

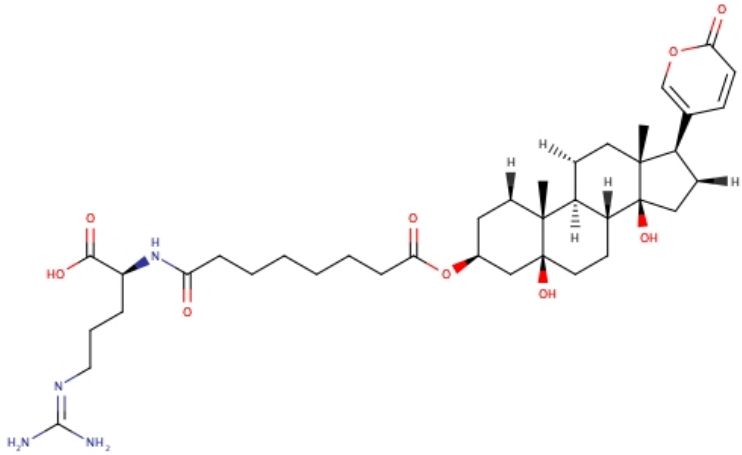
95. bufalin-3-O-suberate-methylhistidine

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	89		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	PZLGHZGYLCCDSV-WSSFCGRPSA-N		
SMILES	<chem>Cn1cncc1C[C@H](NC(=O)CCCCCCC(=O)O[C@H]1CC[C@@]2(C)[C@H](CC[C@@H]3[C@@H]2CC[C@]2(C)[C@H](CC[C@]32O)c2ccc(=O)oc2)C1)C(O)=O</chem>		
Molecular Formula	C ₃₉ H ₅₅ N ₃ O ₈		
Molecular Weight	693.882	Exact Molecular Weight	693.398915743
LogP	3.424	Topological Polar Surface Area	157.05 Å ²
Atom Count	105	Structural Alert Count	2
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	3
Rotatable Bond Count	14	Aromatic Ring Count	2
Drug Likeness	0.20	Oral Bioavailability	N

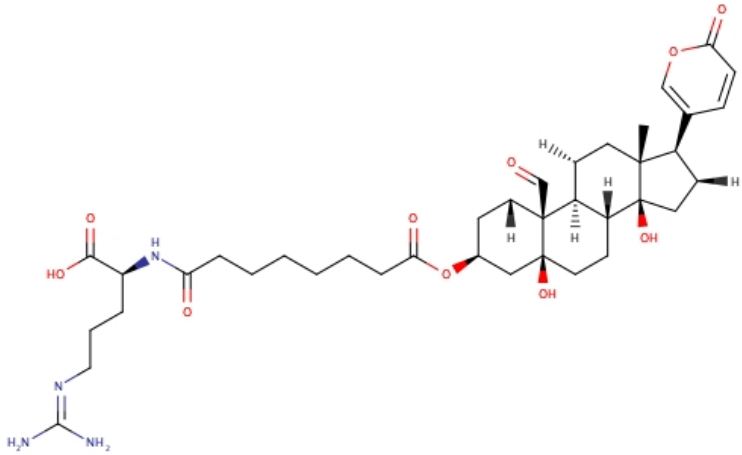
96. bufalitoxin

화학 구조		PubMed ID	
		27063985, 29704033 31590467	
TM-MC 성분 ID	90		
TM-MC 성분 동의어	3-(N-suberoyl argininy)bufalin		
PubChem ID	99882		
InChI Key	DIWIHIOEFFEDHN-BOLOFZJXSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4[C@H](CC[C@]34C)OC(=O)CCCCC C(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc 1</chem>		
Molecular Formula	C ₃₈ H ₅₈ N ₄ O ₈		
Molecular Weight	698.902	Exact Molecular Weight	698.425464844
LogP	2.175	Topological Polar Surface Area	203.63 Å ²
Atom Count	108	Structural Alert Count	4
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	16	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

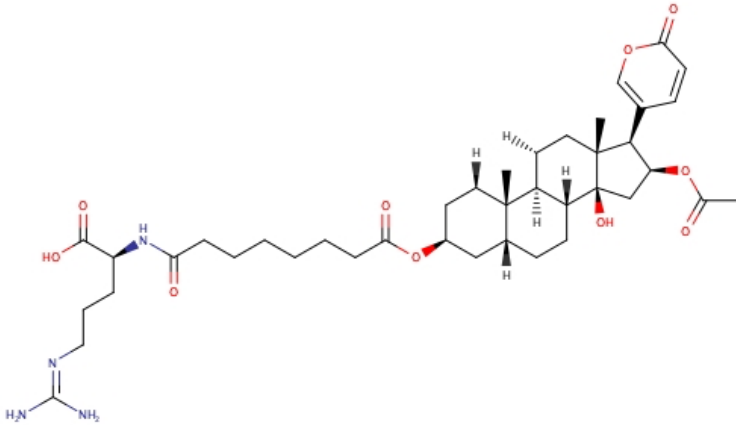
97. telocinobufatoxin

화학 구조		PubMed ID	
		<p>21696903, 26186722 27063985, 27790826 29704033, 31590467</p>	
TM-MC 성분 ID	91		
TM-MC 성분 동의어	telocinobufagin-3-O-suberate-arginine; 3-(N-suberoyl argininy)telocinobufagin; telocinobufagin-3-suberate-arginine ester		
PubChem ID	156077		
InChI Key	NVQQTFUNFWUIQD-KAQRSFMSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C)OC(=O)CCCCC CC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)o c1</chem>		
Molecular Formula	C ₃₈ H ₅₈ N ₄ O ₉		
Molecular Weight	714.901	Exact Molecular Weight	714.420379464
LogP	0.943	Topological Polar Surface Area	223.86 Å ²
Atom Count	109	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	16	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

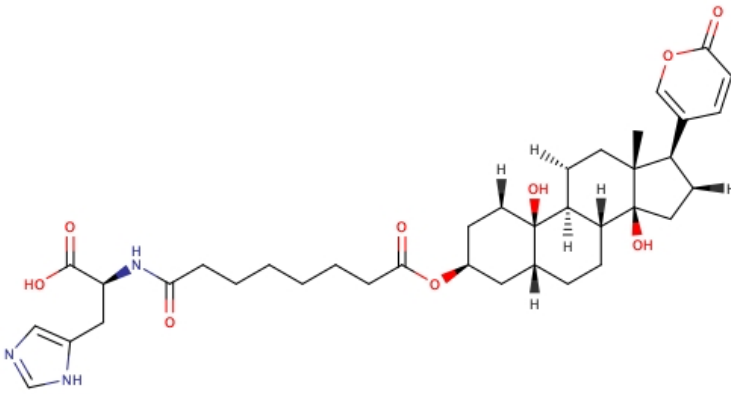
98. hellebritoxin

화학 구조		PubMed ID	
		26186722, 27063985 27790826, 29704033 31590467	
TM-MC 성분 ID	92		
TM-MC 성분 동의어	3-(N-suberoyl argininy)hellebrigenin; hellebrigenin-3-O-suberate-arginine; hellebrigenin-3-suberate-arginine ester		
PubChem ID	163070148		
InChI Key	AXMBOTQXJGDRS-QGBSCAKCSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C=O)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₈ H ₅₆ N ₄ O ₁₀		
Molecular Weight	728.884	Exact Molecular Weight	728.399644019
LogP	-0.024	Topological Polar Surface Area	240.93 Å ²
Atom Count	108	Structural Alert Count	5
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.04	Oral Bioavailability	N

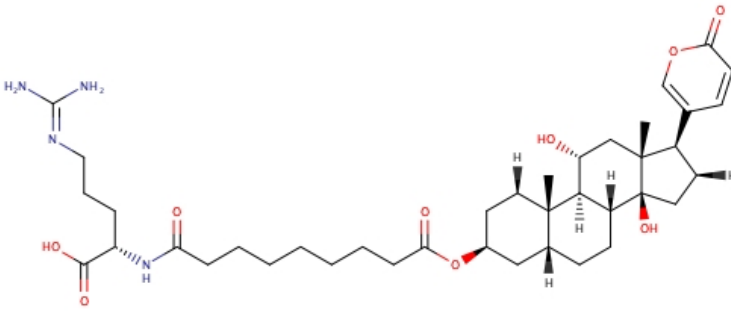
99. bufotoxin

화학 구조		PubMed ID	
		27063985, 27790826 29704033, 31590467	
TM-MC 성분 ID	93		
TM-MC 성분 동의어	3-(N-suberoyl argininy)bufotalin; bufotalin-3-O-suberate-arginine		
PubChem ID	20054854		
InChI Key	HDTHCLKLBSPBIS-JBXNKDOXSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O</chem>		
Molecular Formula	C ₄₀ H ₆₀ N ₄ O ₁₀		
Molecular Weight	756.938	Exact Molecular Weight	756.430944148
LogP	1.235	Topological Polar Surface Area	229.93 Å ²
Atom Count	114	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	5
Rotatable Bond Count	18	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

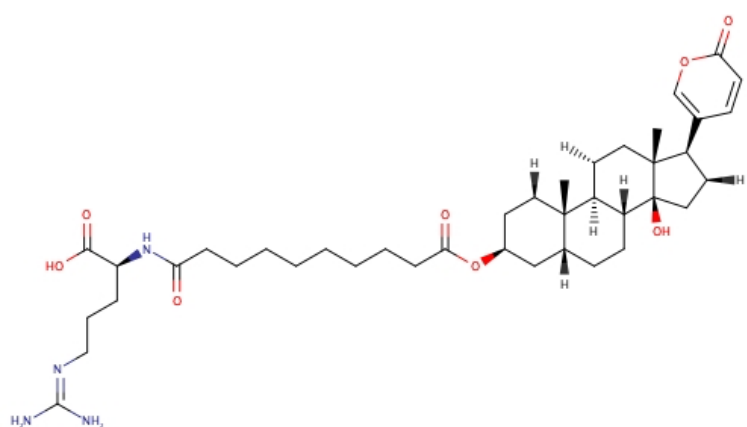
100. 3 β ,14 β ,19 β -trihydroxybufa-20,22-dienolide, 3-O-suberate-L-histidine

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	94		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	BDMXJXCJEZYEOI-MCMYDIIBSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34O)OC(=O)CCCCC C(=O)N[C@@H](Cc3cnc[nH]3)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)o c1</chem>		
Molecular Formula	C ₃₇ H ₅₁ N ₃ O ₉		
Molecular Weight	681.827	Exact Molecular Weight	681.362530234
LogP	1.746	Topological Polar Surface Area	188.14 Å ²
Atom Count	100	Structural Alert Count	2
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	14	Aromatic Ring Count	2
Drug Likeness	0.15	Oral Bioavailability	N

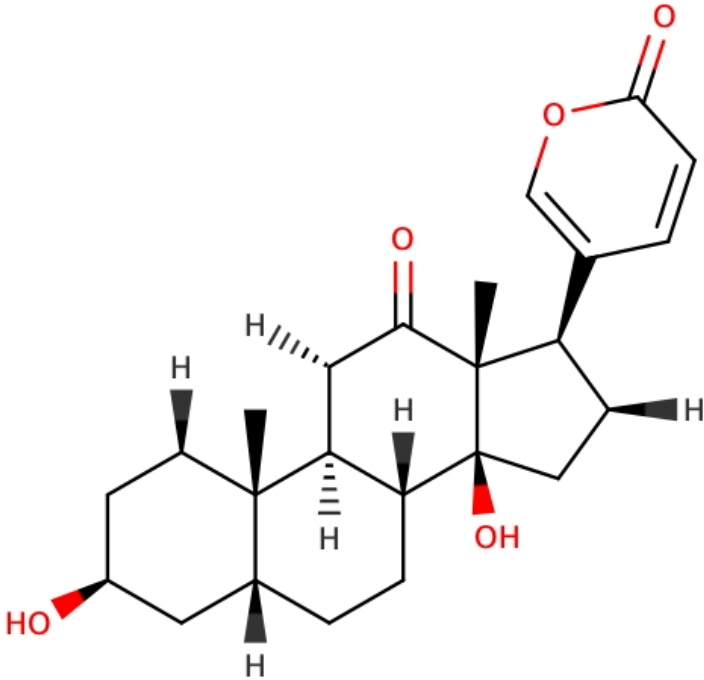
101. gamabufotalin-3-O-pelargonate-arginine

화학 구조		PubMed ID	
		21696903	
TM-MC 성분 ID	95		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	MCJWVLWPWHESDF-YVNBDBQBTSA-N		
SMILES	<chem>C[C@]12C[C@@H](O)[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₉ H ₆₀ N ₄ O ₉		
Molecular Weight	728.928	Exact Molecular Weight	728.436029528
LogP	1.311	Topological Polar Surface Area	223.86 Å ²
Atom Count	112	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

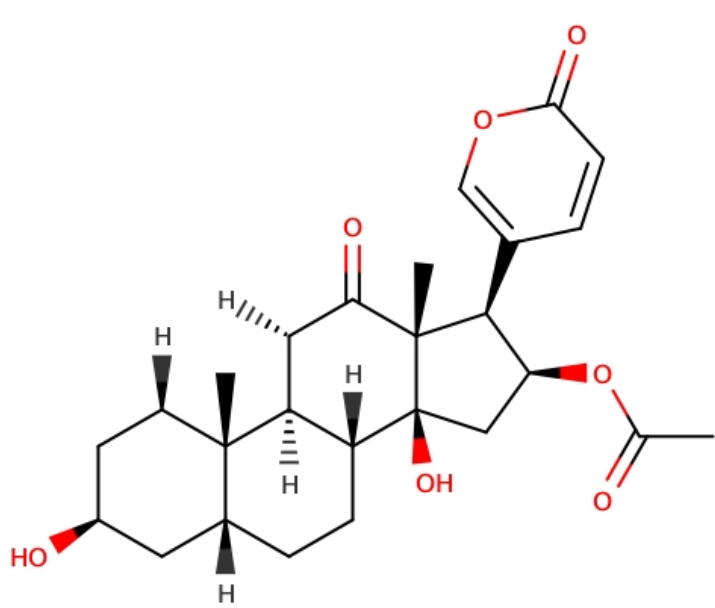
102. bufalin-3-O-sebacate-arginine

화학 구조		PubMed ID	
		21696903	
TM-MC 성분 ID	96		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	BVTDINMKHRPWND-CTYAYSGMSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](CC[C@]34C)OC(=O)CCCCC CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O) oc1</chem>		
Molecular Formula	C ₄₀ H ₆₂ N ₄ O ₈		
Molecular Weight	726.956	Exact Molecular Weight	726.456764972
LogP	3.064	Topological Polar Surface Area	203.63 Å ²
Atom Count	114	Structural Alert Count	4
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	18	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

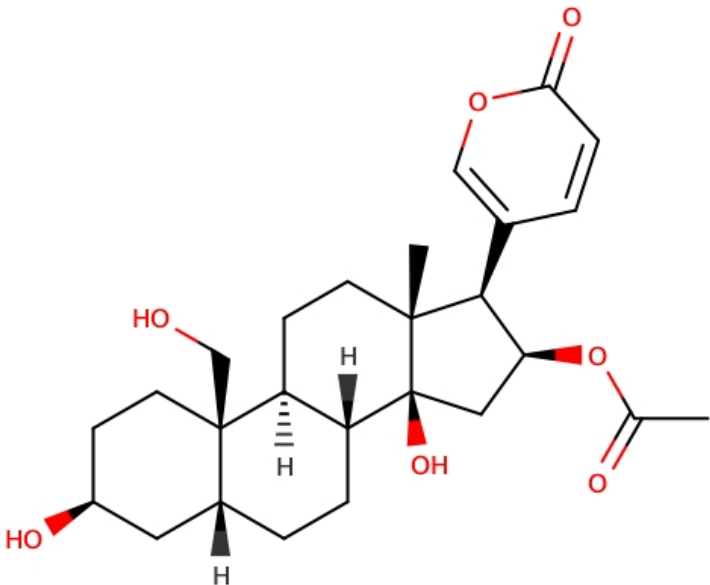
103. 12-oxobufalin

화학 구조		PubMed ID	
		31255247	
TM-MC 성분 ID	37682		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	FZPHETWLUFHBCS-XLWHJTIQSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@@H](O)CC[C@]3(C)[C@H]1CC2=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₅		
Molecular Weight	400.515	Exact Molecular Weight	400.22497413
LogP	2.609	Topological Polar Surface Area	83.83 Å ²
Atom Count	61	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.76	Oral Bioavailability	Y

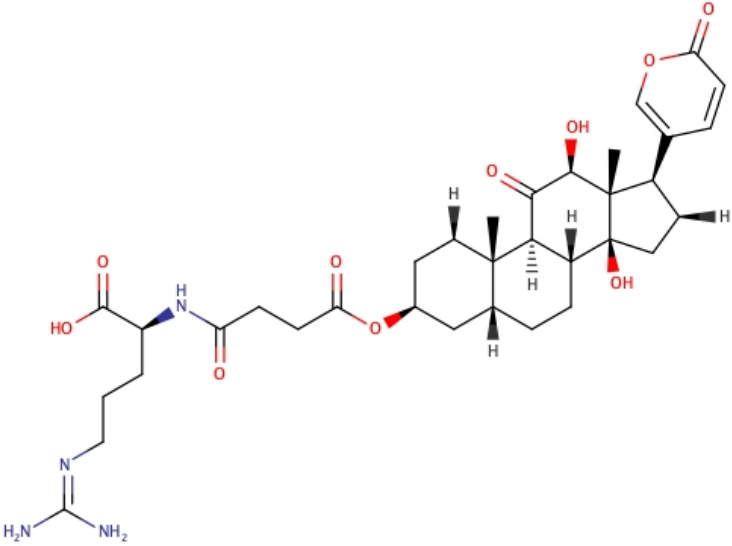
104. 12-oxobufotaline

화학 구조		PubMed ID	
		31255247	
TM-MC 성분 ID	37683		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	FGKMCNLSQUETG-KVGIRYJESA-N		
SMILES	CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(C)[C@H]3CC(=O)[C@]2(C)[C@H]1c1ccc(=O)oc1		
Molecular Formula	C ₂₆ H ₃₄ O ₇		
Molecular Weight	458.551	Exact Molecular Weight	458.230453435
LogP	1.669	Topological Polar Surface Area	110.13 Å ²
Atom Count	67	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.67	Oral Bioavailability	Y

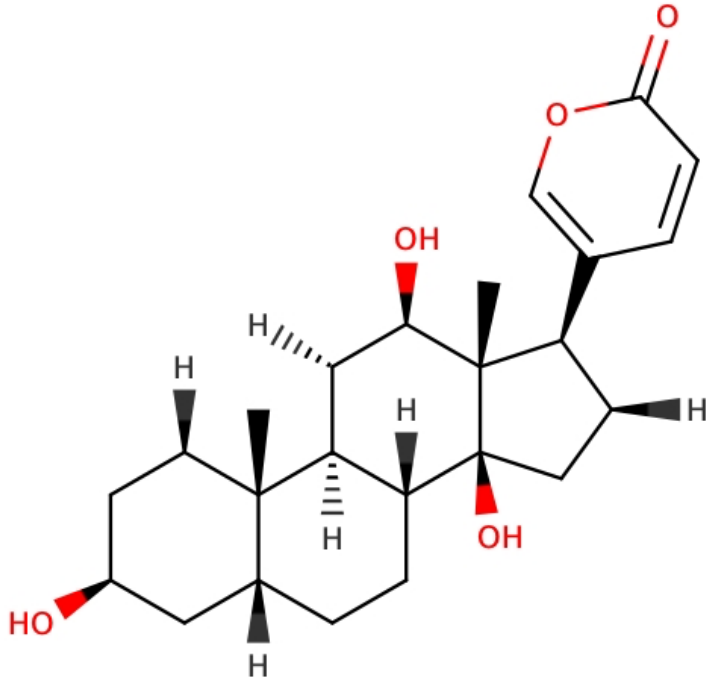
105. monohydroxybufotalin

화학 구조		PubMed ID	
		26621782, 29704033 31590467	
TM-MC 성분 ID	93906		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	DLGBUZMSMMAQKL-PWYQDPSTSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(CO)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₆ O ₇		
Molecular Weight	460.567	Exact Molecular Weight	460.246103499
LogP	1.056	Topological Polar Surface Area	113.29 Å ²
Atom Count	69	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.58	Oral Bioavailability	Y

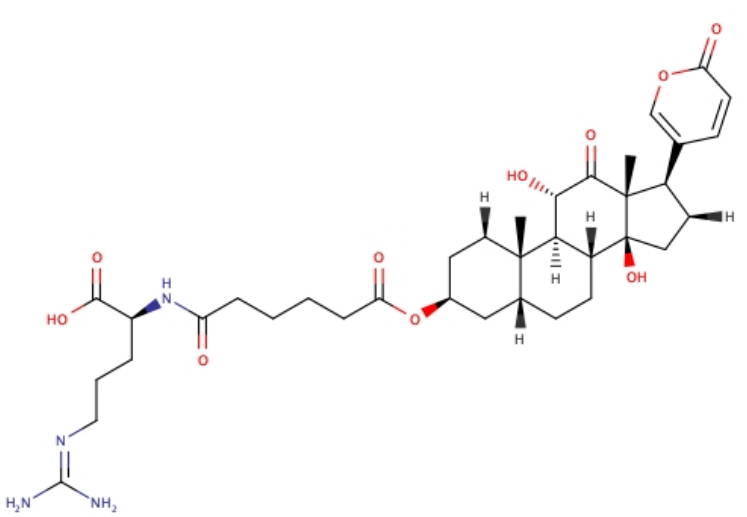
106. 3-(N-succinyl argininy)bufarenogin

화학 구조		PubMed ID	
		29704033	
TM-MC 성분 ID	94369		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	KCEHXRDNJAVTRH-INLIDPNJSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@H](CC[C@]3(C)[C@H]1C(=O)[C@H]2O)OC(=O)CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₄ H ₄₈ N ₄ O ₁₀		
Molecular Weight	672.776	Exact Molecular Weight	672.337043762
LogP	-1.241	Topological Polar Surface Area	240.93 Å ²
Atom Count	96	Structural Alert Count	4
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	12	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

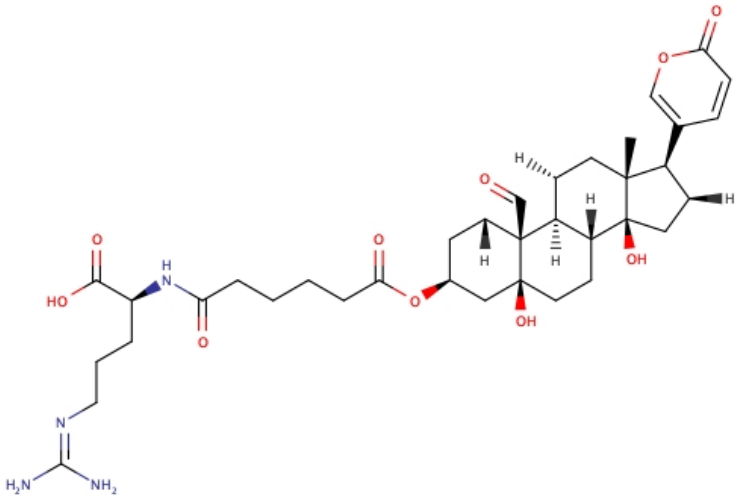
107. 12 β -hydroxylbufalin

화학 구조		PubMed ID	
		26621782, 31590467	
TM-MC 성분 ID	94383		
TM-MC 성분 동의어	12 β -hydroxyl-bufalin		
PubChem ID	23618129		
InChI Key	MDAMKPSXKUKLHO-UPISWOGTSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@@H](O)CC[C@]3(C)[C@H]1[C[C@H]2O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₅		
Molecular Weight	402.531	Exact Molecular Weight	402.240624195
LogP	2.046	Topological Polar Surface Area	86.99 Å ²
Atom Count	63	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.67	Oral Bioavailability	Y

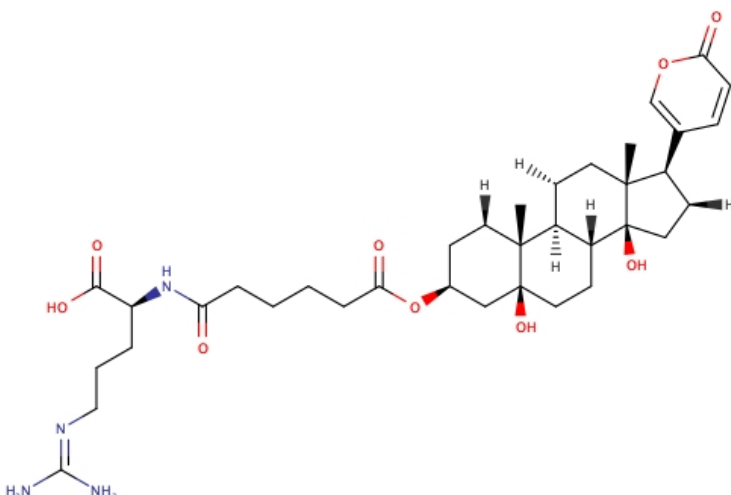
108. 3-(N-adipoyl argininy)arenobufagin

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	94387		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	PDZILWVQZHEEIIY-PEWZWXIBSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@H](CC[C@]3(C)[C@H]1[C@H](O)C2=O)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)c1cc(=O)oc1</chem>		
Molecular Formula	C ₃₆ H ₅₂ N ₄ O ₁₀		
Molecular Weight	700.83	Exact Molecular Weight	700.36834389
LogP	-0.174	Topological Polar Surface Area	240.93 Å ²
Atom Count	102	Structural Alert Count	4
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

109. 3-(N-adipoyl argininy)hellebrigenin

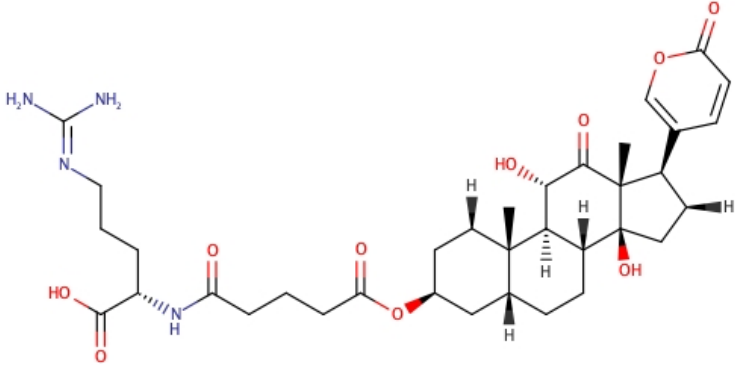
화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	94392		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	NFLLOWOFCWAGHU-JAPHDFRXSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C=O)OC(=O)CCC(CC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₆ H ₅₂ N ₄ O ₁₀		
Molecular Weight	700.83	Exact Molecular Weight	700.36834389
LogP	-0.913	Topological Polar Surface Area	240.93 Å ²
Atom Count	102	Structural Alert Count	5
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.04	Oral Bioavailability	N

110. 3-(N-adipoyl argininy)telocinobufagin

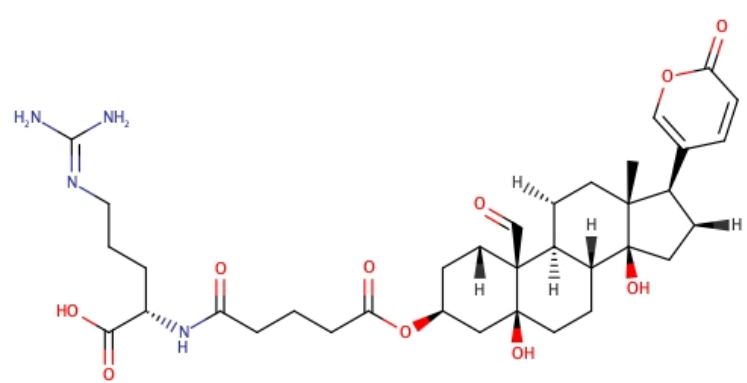
화학 구조	PubMed ID
	29704033, 31590467

TM-MC 성분 ID	94394		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	DUHMBLRBFFFMSZ-VZVWBWNYSY-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₆ H ₅₄ N ₄ O ₉		
Molecular Weight	686.847	Exact Molecular Weight	686.389079335
LogP	0.054	Topological Polar Surface Area	223.86 Å ²
Atom Count	103	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

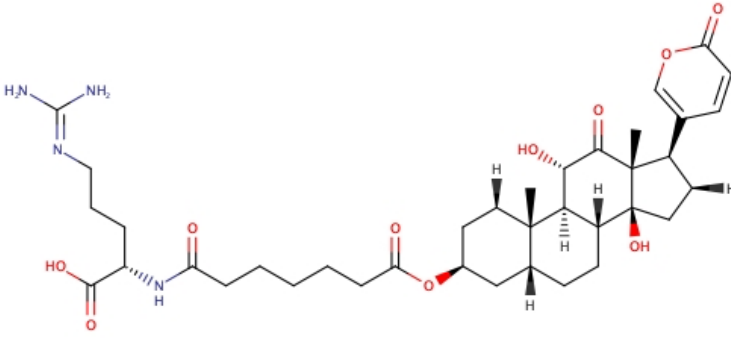
111. 3-(N-glutaryl argininy)arenobufagin

화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	94397		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	FINPGTZVEDMJPM-QTGZFHNSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@H](CC[C@]3(C)[C@H]1[C@H](O)C2=O)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)c1cc(=O)oc1</chem>		
Molecular Formula	C ₃₅ H ₅₀ N ₄ O ₁₀		
Molecular Weight	686.803	Exact Molecular Weight	686.352693826
LogP	-0.619	Topological Polar Surface Area	240.93 Å ²
Atom Count	99	Structural Alert Count	4
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	13	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

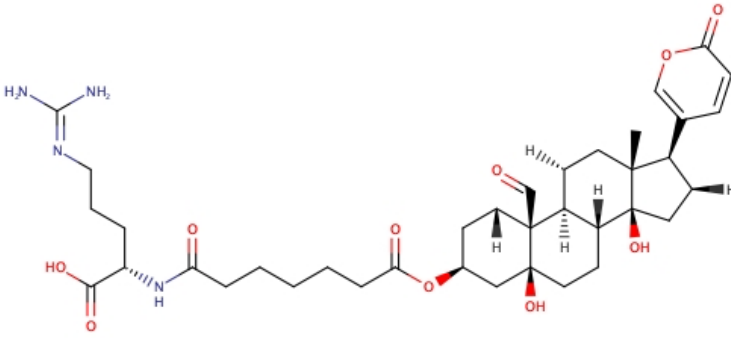
112. 3-(N-glutaryl argininy)hellebrigenin

화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	94398		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	RXMHNZOVBOQCC-DCMQSXMHSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C=O)OC(=O)CCC(=O)N[C@@H](CCCNC(=N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₅ H ₅₀ N ₄ O ₁₀		
Molecular Weight	686.803	Exact Molecular Weight	686.352693826
LogP	-1.357	Topological Polar Surface Area	240.93 Å ²
Atom Count	99	Structural Alert Count	5
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.04	Oral Bioavailability	N

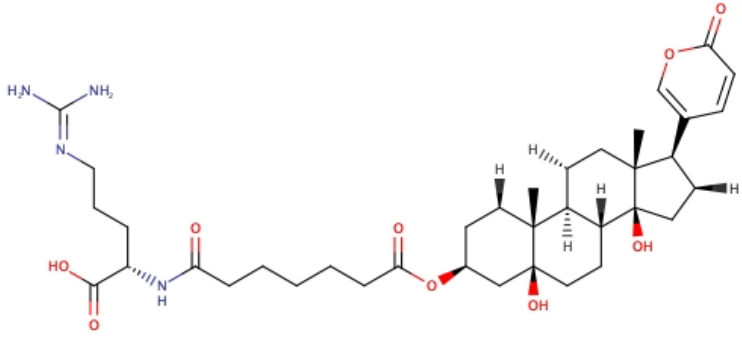
113. 3-(N-pimeloyl argininy)arenobufagin

화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	94400		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	CIDSJMLKGRLFFL-BSYCEGBGSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@H](CC[C@]3(C)[C@H]1[C@H](O)C2=O)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₇ H ₅₄ N ₄ O ₁₀		
Molecular Weight	714.857	Exact Molecular Weight	714.383993955
LogP	0.27	Topological Polar Surface Area	240.93 Å ²
Atom Count	105	Structural Alert Count	4
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

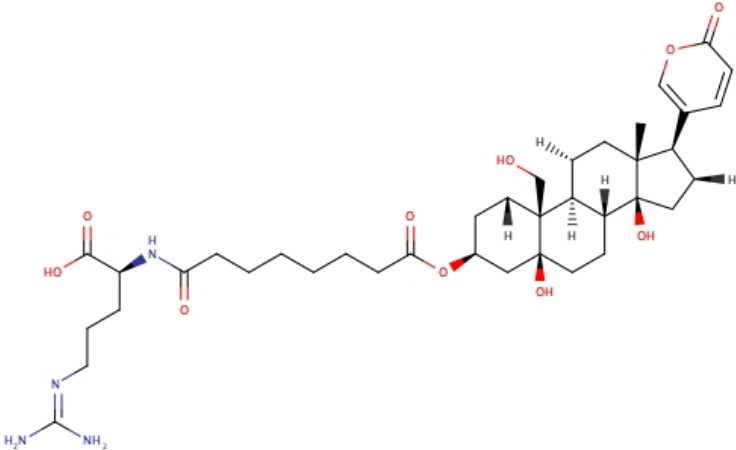
114. 3-(N-pimeloyl argininyloxy)hellebrigenin

화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	94404		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	LVZXBOPAQFPAEC-QPYUPLQNSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C=O)OC(=O)CCCCC(=O)N[C@@H](CCCNC(=N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₇ H ₅₄ N ₄ O ₁₀		
Molecular Weight	714.857	Exact Molecular Weight	714.383993955
LogP	-0.468	Topological Polar Surface Area	240.93 Å ²
Atom Count	105	Structural Alert Count	5
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	16	Aromatic Ring Count	1
Drug Likeness	0.04	Oral Bioavailability	N

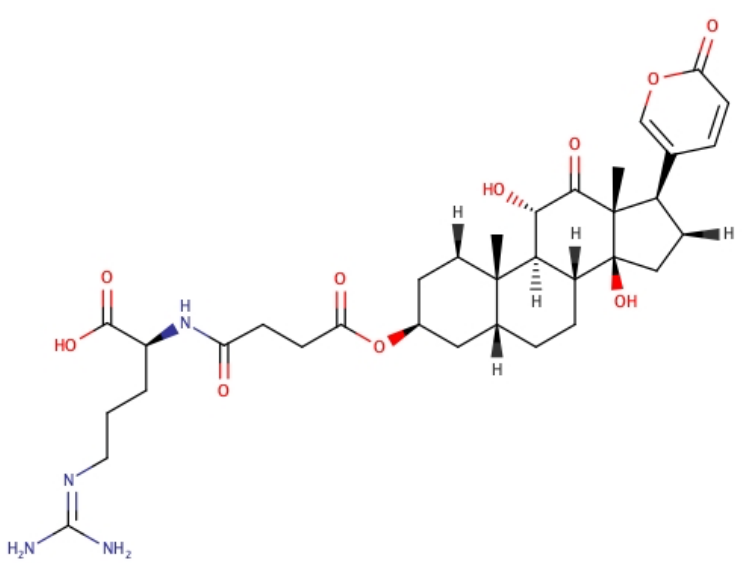
115. 3-(N-pimeloyl argininyl)telocinobufagin

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	94406		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	ZOGGZRDVDQYGLT-ZLZFRFJWSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C)OC(=O)CCCCC C(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc 1</chem>		
Molecular Formula	C ₃₇ H ₅₆ N ₄ O ₉		
Molecular Weight	700.874	Exact Molecular Weight	700.404729399
LogP	0.499	Topological Polar Surface Area	223.86 Å ²
Atom Count	106	Structural Alert Count	4
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

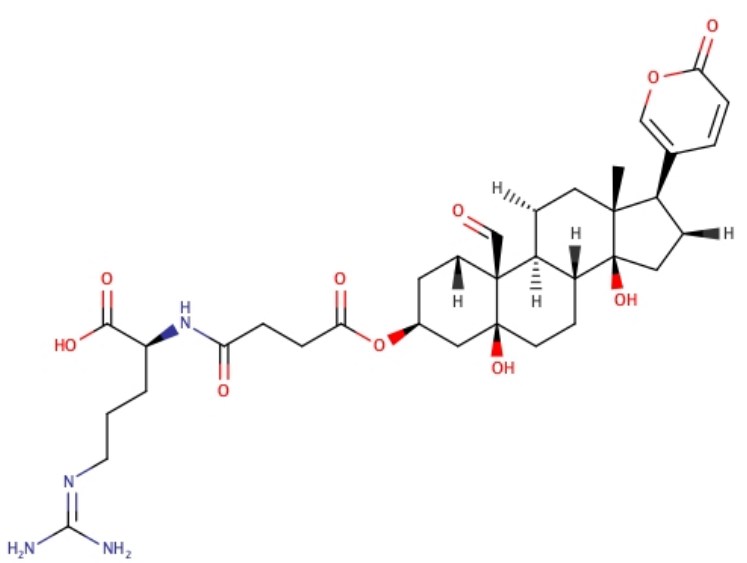
116. 3-(N-suberoyl argininyl)hellebrigenol

화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	94417		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	RVZQUZZVNI GLP-QGBSCAKCSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34CO)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₈ H ₅₈ N ₄ O ₁₀		
Molecular Weight	730.9	Exact Molecular Weight	730.415294084
LogP	-0.338	Topological Polar Surface Area	244.09 Å ²
Atom Count	110	Structural Alert Count	4
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	7
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.05	Oral Bioavailability	N

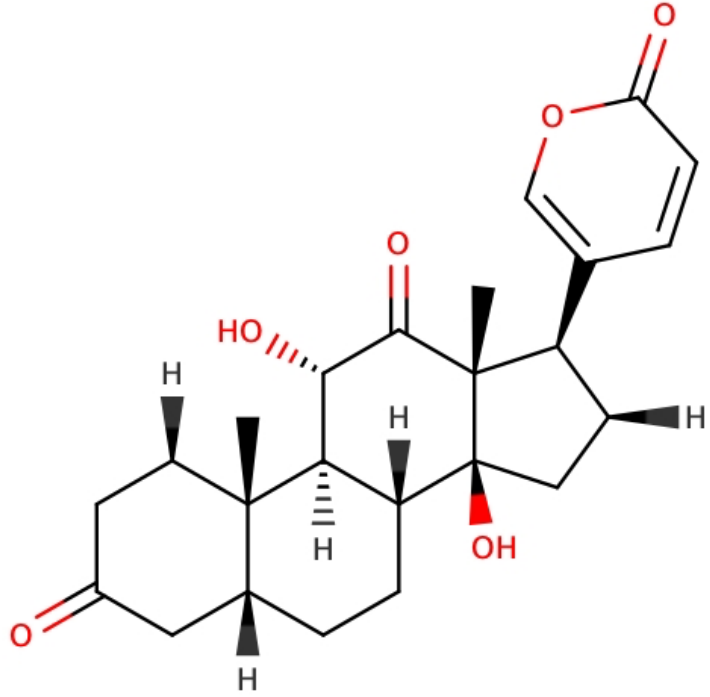
117. 3-(N-succinyl argininy)arenobufagin

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	94422		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	NJBKELZRVTJPR-AZYYEHFZSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@H](CC[C@]3(C)[C@H]1[C@H](O)C2=O)OC(=O)CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₄ H ₄₈ N ₄ O ₁₀		
Molecular Weight	672.776	Exact Molecular Weight	672.337043762
LogP	-1.063	Topological Polar Surface Area	240.93 Å ²
Atom Count	96	Structural Alert Count	4
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	12	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

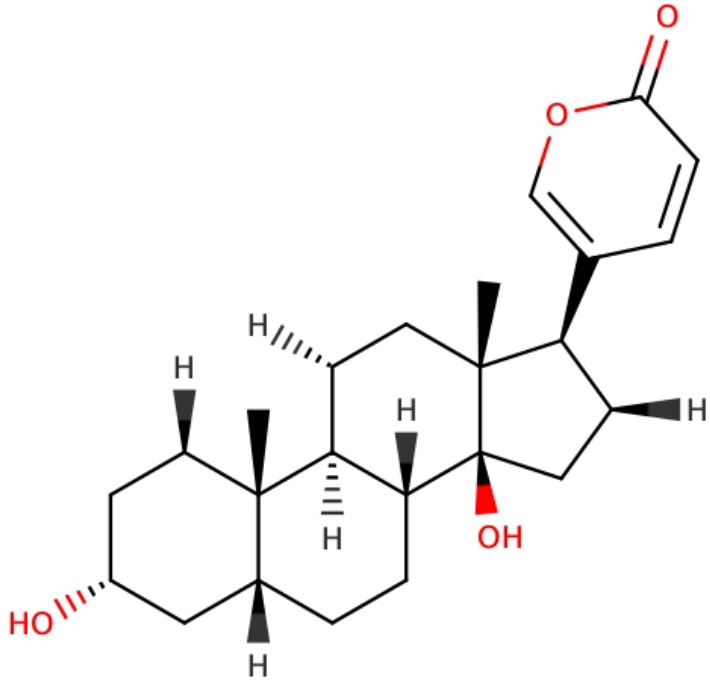
118. 3-(N-succinyl argininy)hellebrigenin

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	94426		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	GEJIVQYZDDAVIM-GJDQYMGSSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@]4(O)C[C@H](CC[C@]34C=O)OC(=O)CCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₄ H ₄₈ N ₄ O ₁₀		
Molecular Weight	672.776	Exact Molecular Weight	672.337043762
LogP	-1.802	Topological Polar Surface Area	240.93 Å ²
Atom Count	96	Structural Alert Count	5
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	13	Aromatic Ring Count	1
Drug Likeness	0.04	Oral Bioavailability	N

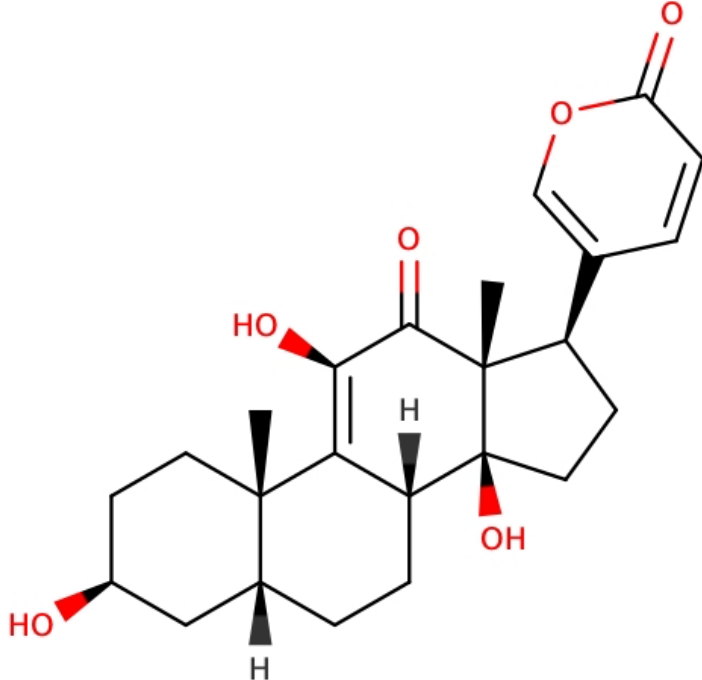
119. 3-keto-arenobufagin

화학 구조		PubMed ID	
		26621782, 31590467	
TM-MC 성분 ID	94429		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	DQXPIJIVTJHSJK-CELYVLGRSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3CC(=O)CC[C@]3(C)[C@H]1[C@H](O)C2=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₆		
Molecular Weight	414.498	Exact Molecular Weight	414.204238686
LogP	2.024	Topological Polar Surface Area	100.9 Å ²
Atom Count	60	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.73	Oral Bioavailability	Y

120. 3-epi bufalin

화학 구조		PubMed ID	
		26621782, 31590467	
TM-MC 성분 ID	300405		
TM-MC 성분 동의어	3-epi-bufalin		
PubChem ID	56844122		
InChI Key	QEEBRPGZBVVINN-SIBWXOBNSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](O)CC[C@]34C)[C@@]1(O)C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₄ O ₄		
Molecular Weight	386.532	Exact Molecular Weight	386.245709575
LogP	3.277	Topological Polar Surface Area	66.76 Å ²
Atom Count	62	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.78	Oral Bioavailability	Y

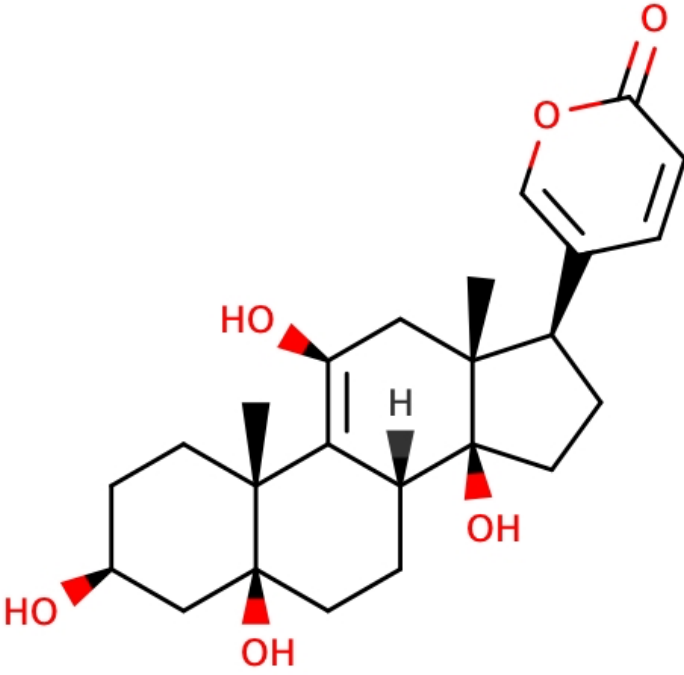
121. argentinogenin

화학 구조		PubMed ID	
		26621782, 27063985 29704033, 31590467	
TM-MC 성분 ID	97		
TM-MC 성분 동의어	N/A		
PubChem ID	12305202		
InChI Key	UJNYXLCWBDUNMH-UQPKIQGCSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@@H](O)CC[C@]3(C)C1=C(O)C2=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₆		
Molecular Weight	414.498	Exact Molecular Weight	414.204238686
LogP	2.045	Topological Polar Surface Area	104.06 Å ²
Atom Count	60	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.65	Oral Bioavailability	Y

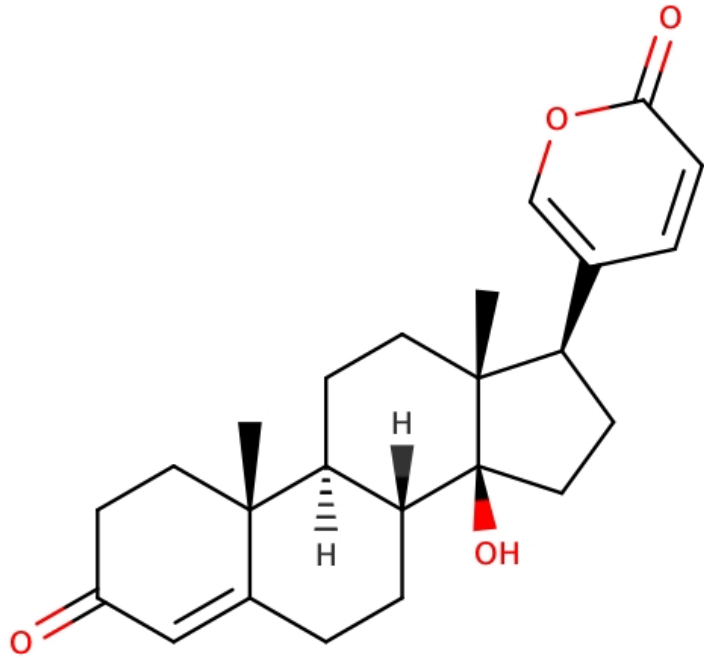
122. argentinogenin-3-O-adipate-arginine

화학 구조		PubMed ID	
		21696903	
TM-MC 성분 ID	98		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	ZNUWNMQTRKCZDS-LMURPIKZSA-N		
SMILES	<chem>C[C@@]12[C@H](CC[C@]1(O)[C@@H]1CC[C@@H]3C[C@H](CC[C@]3(C)C1=C(O)C2=O)OC(=O)CCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₆ H ₅₀ N ₄ O ₁₀		
Molecular Weight	698.814	Exact Molecular Weight	698.352693826
LogP	0.052	Topological Polar Surface Area	240.93 Å ²
Atom Count	100	Structural Alert Count	4
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.07	Oral Bioavailability	N

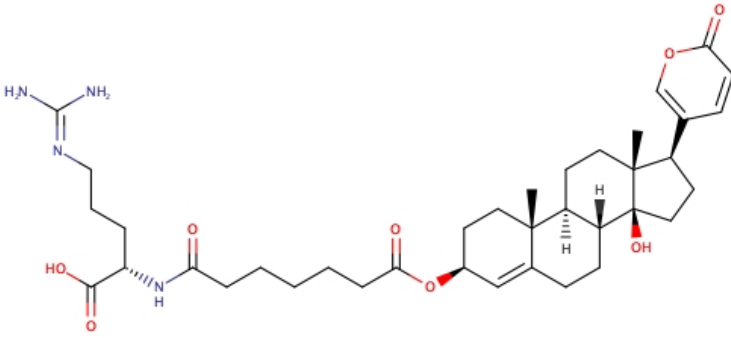
123. hellebrigenol-9,11-ene

화학 구조		PubMed ID	
		21696903, 26621782 31590467	
TM-MC 성분 ID	99		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	ZXBIKZDFPXLYKU-HUJXABIYSA-N		
SMILES	<chem>C[C@]12CC(O)=C3[C@@H](CC[C@]4(O)C[C@@H](O)CC[C@]34C)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₆		
Molecular Weight	416.514	Exact Molecular Weight	416.21988875
LogP	0.812	Topological Polar Surface Area	107.22 Å ²
Atom Count	62	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.54	Oral Bioavailability	Y

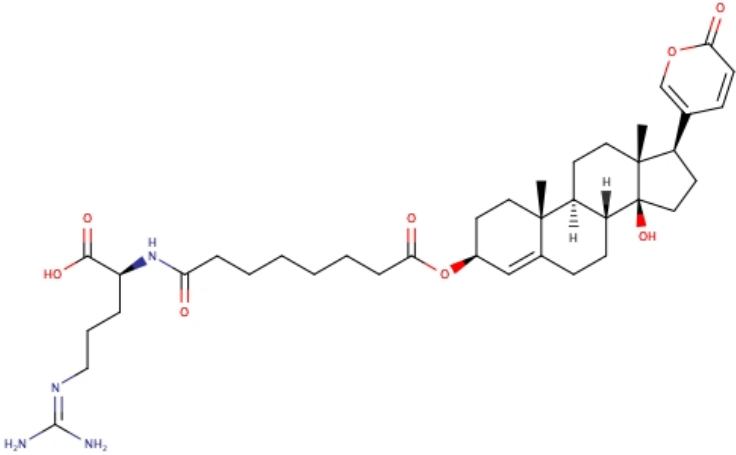
124. 3-dehydrobufagin

화학 구조		PubMed ID	
		26621782, 27790826	
TM-MC 성분 ID	100		
TM-MC 성분 동의어	3-dehydroscillarenin		
PubChem ID	12315395		
InChI Key	XJJBIDDTIZKCAO-FIJLXMTKSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₄		
Molecular Weight	382.5	Exact Molecular Weight	382.214409446
LogP	3.438	Topological Polar Surface Area	63.6 Å ²
Atom Count	58	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.81	Oral Bioavailability	Y

125. scillarenin-3-pimelate-arginine

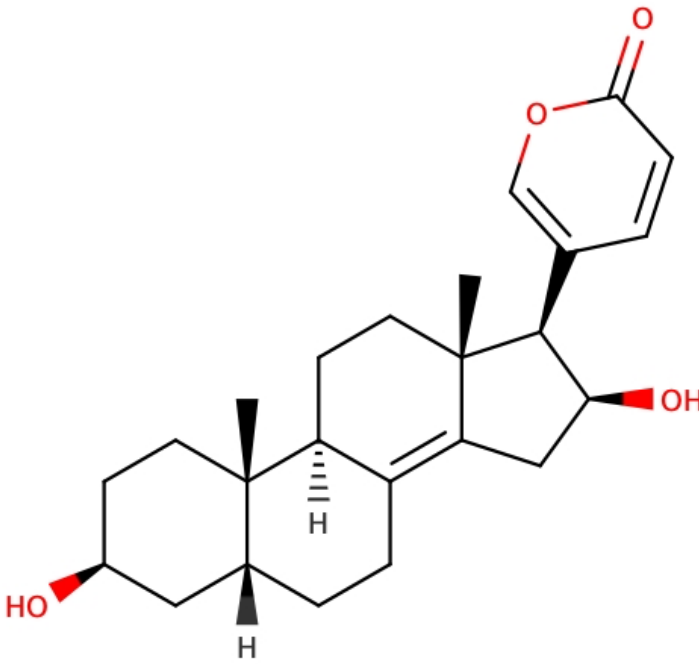
화학 구조		PubMed ID	
		21696903	
TM-MC 성분 ID	101		
TM-MC 성분 동의어	N/A		
PubChem ID	10484713		
InChI Key	OXEUZDFYLGPMV-ISMAOOLGSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=C[C@H](CC[C@]34C)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₇ H ₅₄ N ₄ O ₈		
Molecular Weight	682.859	Exact Molecular Weight	682.394164715
LogP	1.481	Topological Polar Surface Area	203.63 Å ²
Atom Count	103	Structural Alert Count	5
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	15	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

126. scillarenin-3-suberate-arginine

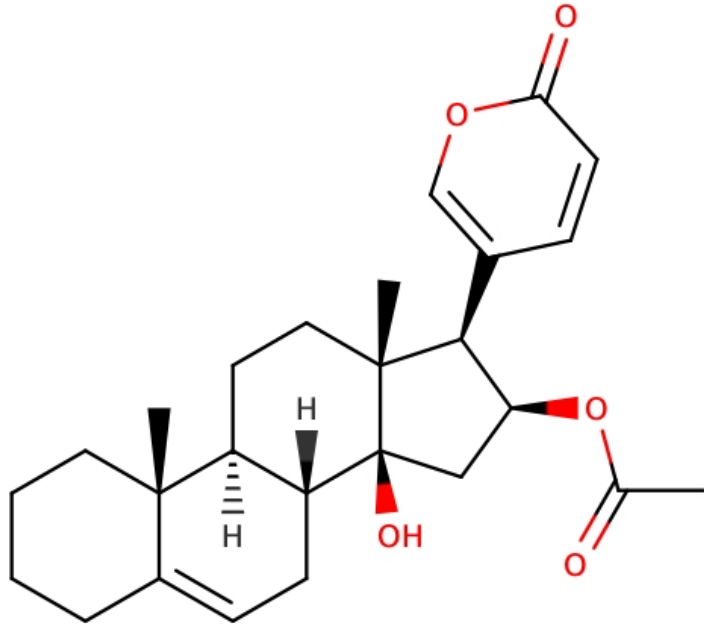
화학 구조	PubMed ID
	21696903

TM-MC 성분 ID	102		
TM-MC 성분 동의어	N/A		
PubChem ID	10078419		
InChI Key	NDTPUHWKNUAQV-KEVZCLCYSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=C[C@H](CC[C@]34C)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₈ H ₅₆ N ₄ O ₈		
Molecular Weight	696.886	Exact Molecular Weight	696.409814779
LogP	1.926	Topological Polar Surface Area	203.63 Å ²
Atom Count	106	Structural Alert Count	5
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	16	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

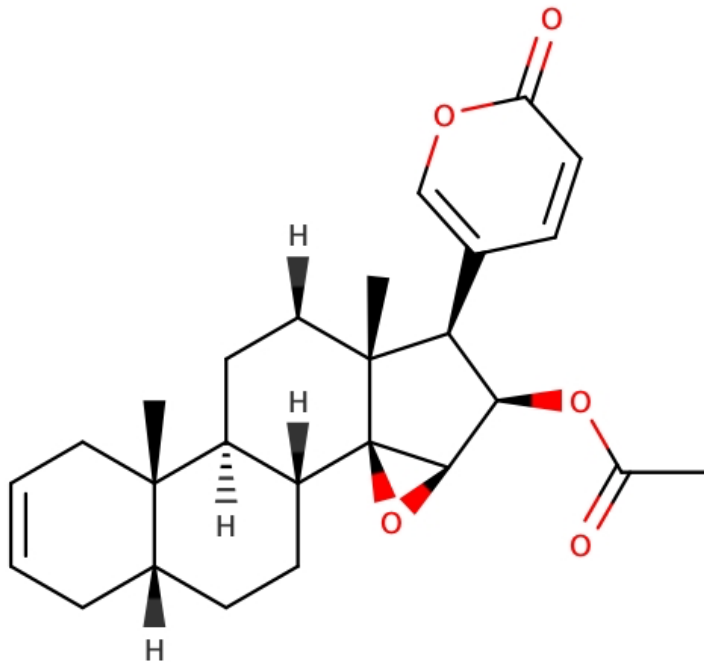
127. 3β,16β-dihydroxybufa-8(14),20,22-trienolide

화학 구조		PubMed ID	
		27063985	
TM-MC 성분 ID	103		
TM-MC 성분 동의어	N/A		
PubChem ID	46938954		
InChI Key	GJXJCPZVJOLKQN-DXAYDWCFS-A-N		
SMILES	<chem>C[C@]12CC[C@H]3C(CC[C@@H]4C[C@@H](O)CC[C@]34C)=C1C[C@H](O)[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₂ O ₄		
Molecular Weight	384.516	Exact Molecular Weight	384.23005951
LogP	2.6	Topological Polar Surface Area	66.76 Å ²
Atom Count	60	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.73	Oral Bioavailability	Y

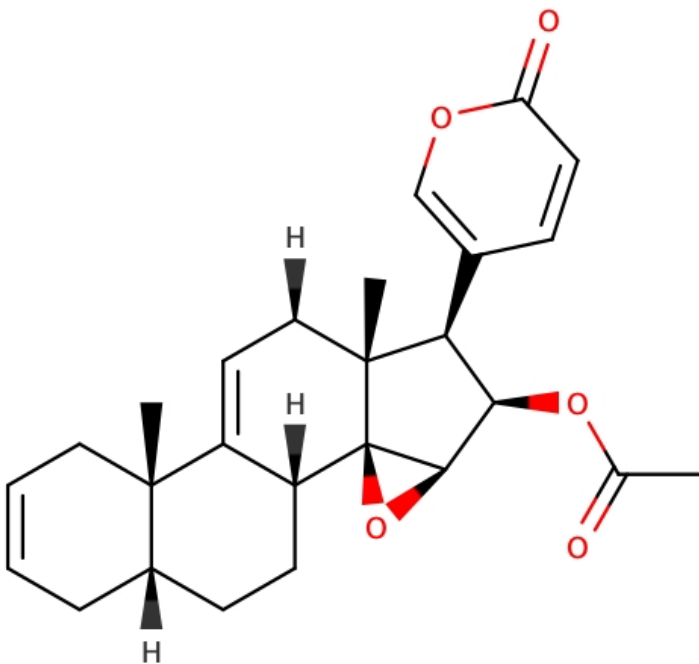
128. 14,16-dihydroxybufa-5,20,22-trienolide, (14 β ,16 β)-form, 16-Ac

화학 구조		PubMed ID	
		27063985, 29704033	
TM-MC 성분 ID	104		
TM-MC 성분 동의어	N/A		
PubChem ID	46938953		
InChi Key	OLHBYIOPPJESPH-CLKKNRCP5A-N		
SMILES	CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC=C4CCCC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1		
Molecular Formula	C ₂₆ H ₃₄ O ₅		
Molecular Weight	426.553	Exact Molecular Weight	426.240624195
LogP	3.317	Topological Polar Surface Area	72.83 Å ²
Atom Count	65	Structural Alert Count	2
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.60	Oral Bioavailability	Y

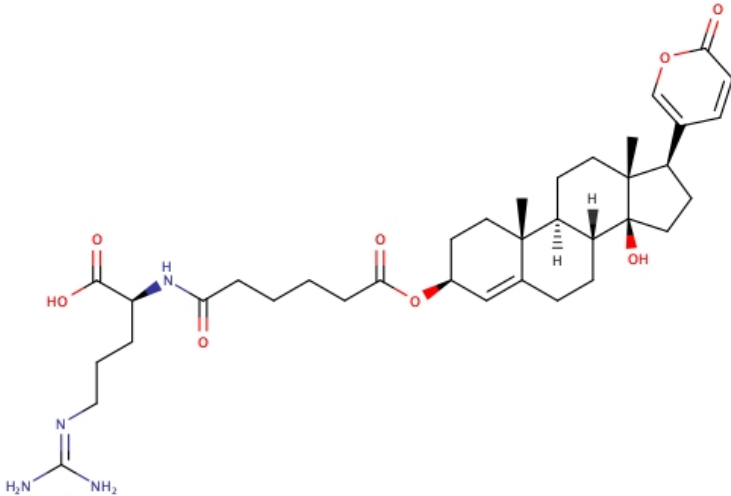
129. dehydrated-cinobufagin

화학 구조		PubMed ID	
		26186722, 29704033	
TM-MC 성분 ID	93907		
TM-MC 성분 동의어	dehydrated cinobufagin		
PubChem ID	N/A		
InChI Key	PYKGGWXWUQTLLH-SLMNAJOPSA-N		
SMILES	<chem>CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4CC=CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₂ O ₅		
Molecular Weight	424.537	Exact Molecular Weight	424.22497413
LogP	3.833	Topological Polar Surface Area	65.13 Å ²
Atom Count	63	Structural Alert Count	3
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	0
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.42	Oral Bioavailability	Y

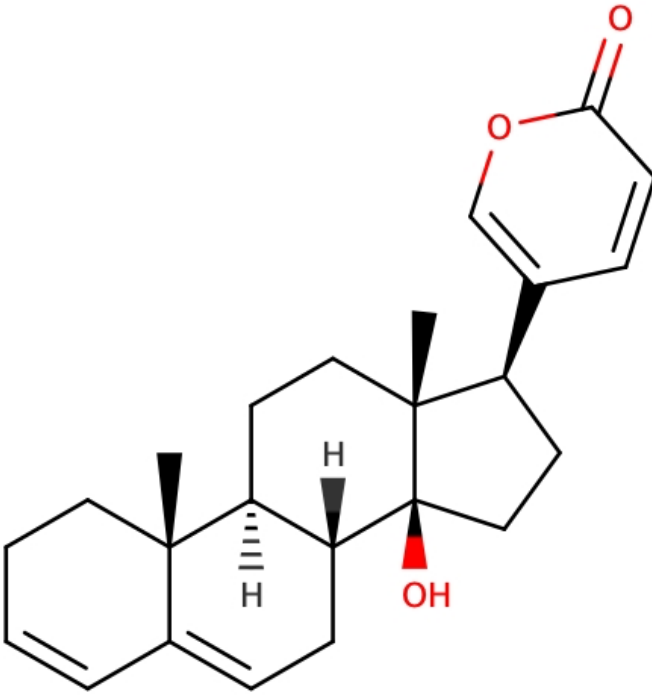
130. dehydro-dehydrated-cinobufagin

화학 구조		PubMed ID	
		29704033	
TM-MC 성분 ID	94304		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	LGFWJUIQHTUOFE-OCWSTYCFSA-N		
SMILES	CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@@H]4CC=CC[C@]4(C)C3=CC[C@]2(C)[C@H]1c1ccc(=O)oc1		
Molecular Formula	C ₂₆ H ₃₀ O ₅		
Molecular Weight	422.521	Exact Molecular Weight	422.209324066
LogP	3.427	Topological Polar Surface Area	65.13 Å ²
Atom Count	61	Structural Alert Count	3
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	0
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.43	Oral Bioavailability	Y

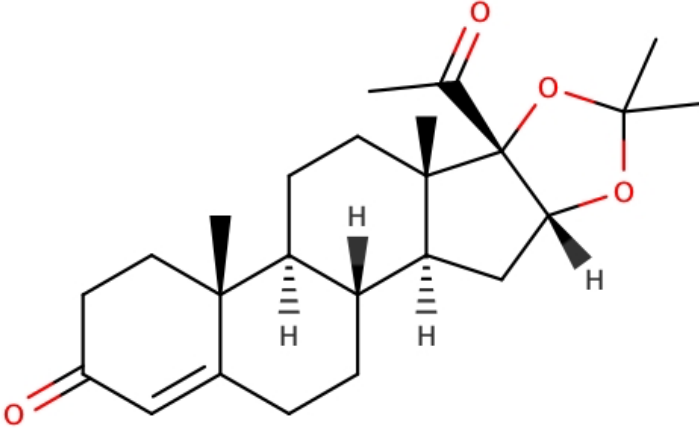
131. 3-(N-adipoyl argininy)scillarenin

화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	98018		
TM-MC 성분 동의어	N/A		
PubChem ID	10484582		
InChI Key	OFOFWUPAXXVNHW-HXVHQHHUSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=C[C@H](CC[C@]34C)OC(=O)CCCCC(=O)N[C@@H](CCCN=C(N)N)C(O)=O)[C@@]1(O)CC[C@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₃₆ H ₅₂ N ₄ O ₈		
Molecular Weight	668.832	Exact Molecular Weight	668.37851465
LogP	1.036	Topological Polar Surface Area	203.63 Å ²
Atom Count	100	Structural Alert Count	5
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	14	Aromatic Ring Count	1
Drug Likeness	0.06	Oral Bioavailability	N

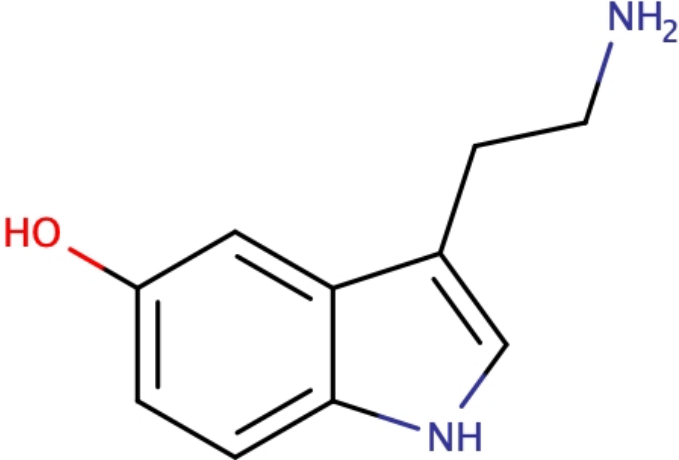
132. scillaridin A

화학 구조		PubMed ID	
		29704033, 31590467	
TM-MC 성분 ID	302393		
TM-MC 성분 동의어	N/A		
PubChem ID	12315396		
InChI Key	KBOQXVVZFSWICE-FIJLXMTKSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC=C4C=CCC[C@]34C)[C@@]1(O)CC[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₃		
Molecular Weight	366.501	Exact Molecular Weight	366.219494826
LogP	3.896	Topological Polar Surface Area	46.53 Å ²
Atom Count	57	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.82	Oral Bioavailability	Y

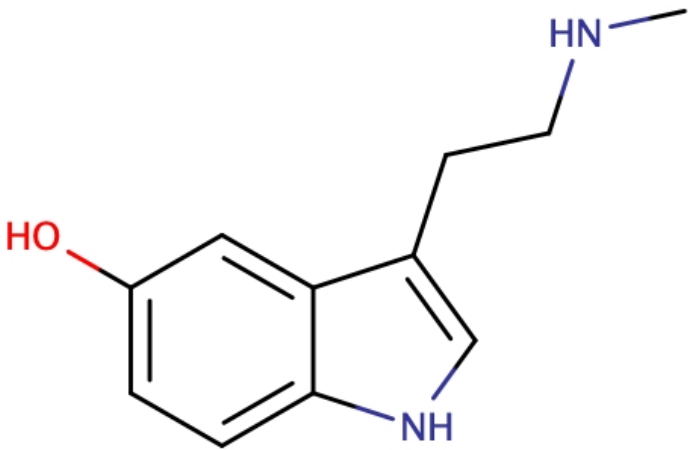
133. algestone acetonide

화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	300668		
TM-MC 성분 동의어	N/A		
PubChem ID	11740874		
InChI Key	LSWBQIAZNGURQV-WTBIUSKOSA-N		
SMILES	CC(=O)[C@@]12OC(C)O[C@@H]1C[C@H]1[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]21C		
Molecular Formula	C ₂₄ H ₃₄ O ₄		
Molecular Weight	386.532	Exact Molecular Weight	386.245709575
LogP	4.029	Topological Polar Surface Area	52.6 Å ²
Atom Count	62	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	0
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.68	Oral Bioavailability	Y

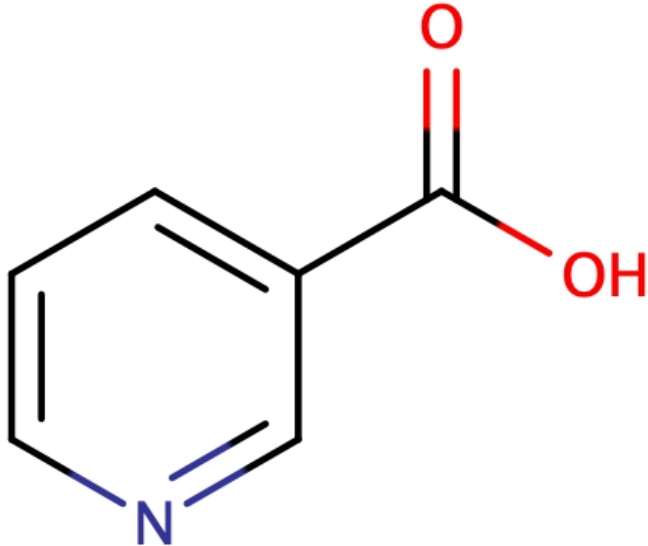
134. serotonin

화학 구조		PubMed ID	
		<p>23311159, 25780654 29680742, 29704033 30111043, 30591646 31590467</p>	
TM-MC 성분 ID	105		
TM-MC 성분 동의어	N/A		
PubChem ID	5202		
InChI Key	QZAYGJVTTNCVMB-UHFFFAOYSA-N		
SMILES	NCCc1c[nH]c2ccc(O)cc12		
Molecular Formula	C ₁₀ H ₁₂ N ₂ O		
Molecular Weight	176.219	Exact Molecular Weight	176.094963014
LogP	0.482	Topological Polar Surface Area	62.04 Å ²
Atom Count	25	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.62	Oral Bioavailability	Y

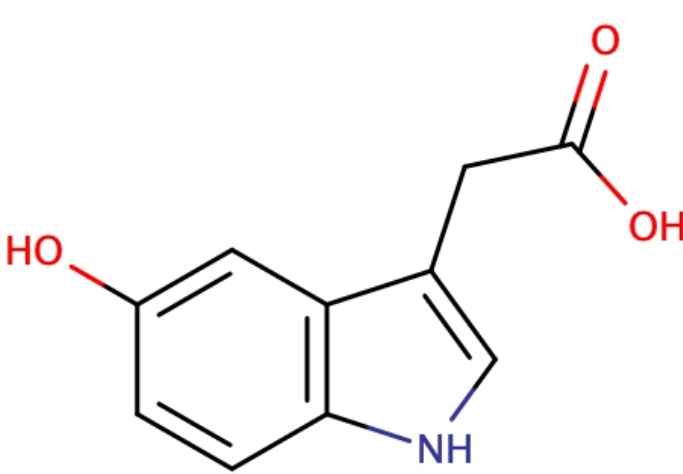
135. N-methyl serotonin

화학 구조		PubMed ID	
		23311159, 29680742 29704033, 30591646 31590467	
TM-MC 성분 ID	106		
TM-MC 성분 동의어	N-methylserotonin; N'-methyl-serotonin; N'-methyl serotonin; 5-hydroxy-N'-methyl tryptamine		
PubChem ID	150885		
InChI Key	ASUSBMNYRHGZIG-UHFFFAOYSA-N		
SMILES	CNCCc1c[nH]c2ccc(O)cc12		
Molecular Formula	C ₁₁ H ₁₄ N ₂ O		
Molecular Weight	190.246	Exact Molecular Weight	190.110613079
LogP	0.688	Topological Polar Surface Area	48.05 Å ²
Atom Count	28	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.67	Oral Bioavailability	Y

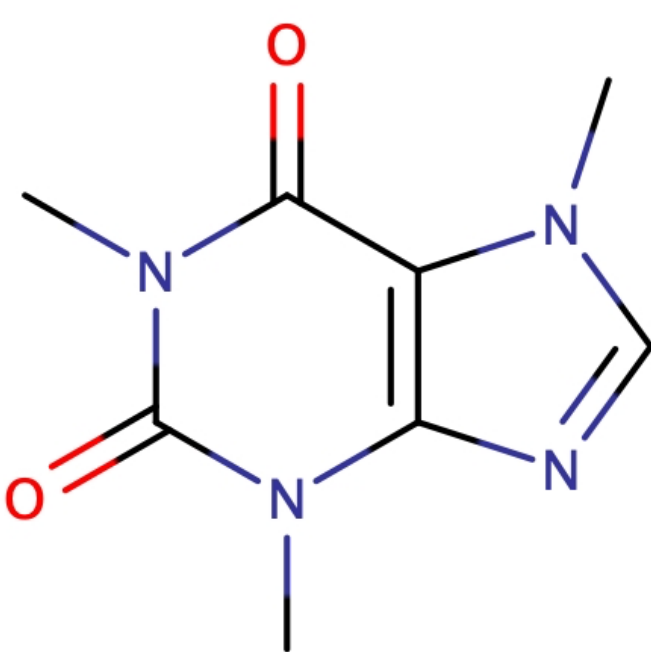
136. nicotinic acid

화학 구조		PubMed ID	
		15158983, 30591646 31590467	
TM-MC 성분 ID	158		
TM-MC 성분 동의어	niacin		
PubChem ID	938, 117629482		
InChI Key	PVNIIMVLHYAWGP-UHFFFAOYSA-N		
SMILES	OC(=O)c1cccnc1		
Molecular Formula	C ₆ H ₅ NO ₂		
Molecular Weight	123.111	Exact Molecular Weight	123.032028405
LogP	-0.166	Topological Polar Surface Area	50.19 Å ²
Atom Count	14	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.56	Oral Bioavailability	Y

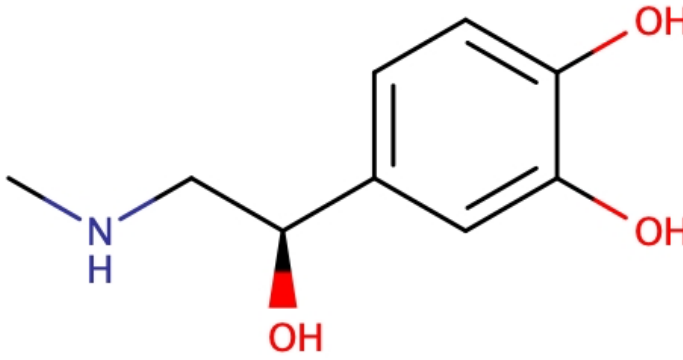
137. (5-hydroxy-1H-indol-3-yl)acetic acid

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	1826		
TM-MC 성분 동의어	5-hydroxyindole-3-acetate		
PubChem ID	1826		
InChI Key	DUUGKQCEGZLZNO-UHFFFAOYSA-N		
SMILES	<chem>OC(=O)Cc1c[nH]c2ccc(O)cc12</chem>		
Molecular Formula	C ₁₀ H ₉ NO ₃		
Molecular Weight	191.186	Exact Molecular Weight	191.058243154
LogP	1.406	Topological Polar Surface Area	73.32 Å ²
Atom Count	23	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.67	Oral Bioavailability	Y

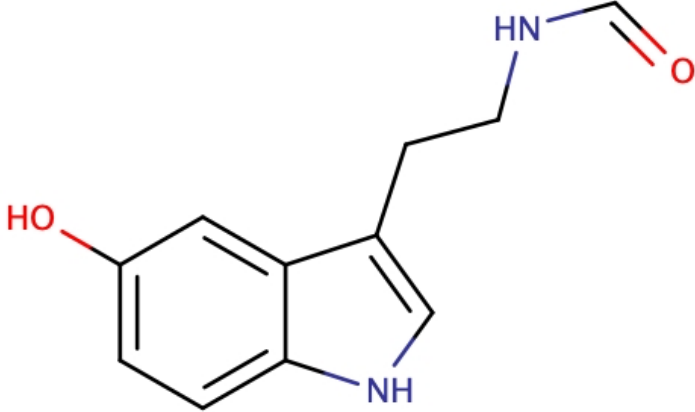
138. caffeine

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	2519		
TM-MC 성분 동의어	1,3,7-trimethyl-3,7-dihydro-1H-purine-2,6-dione		
PubChem ID	2519		
InChI Key	RYYVLZVUVIJVGH-UHFFFAOYSA-N		
SMILES	<chem>Cn1cnc2n(C)c(=O)n(C)c(=O)c12</chem>		
Molecular Formula	C ₈ H ₁₀ N ₄ O ₂		
Molecular Weight	194.194	Exact Molecular Weight	194.080375578
LogP	-0.546	Topological Polar Surface Area	58.44 Å ²
Atom Count	24	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.57	Oral Bioavailability	Y

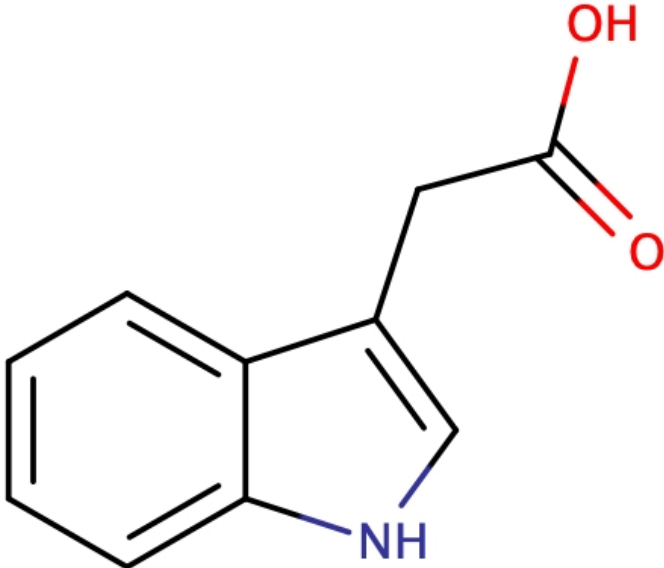
139. adrenaline

화학 구조		PubMed ID	
		29704033	
TM-MC 성분 ID	5816		
TM-MC 성분 동의어	epinephrine		
PubChem ID	5816, 139148732		
InChI Key	UCTWMZQNUQWSLP-VIFPVBQESA-N		
SMILES	CNC[C@H](O)c1ccc(O)c(O)c1		
Molecular Formula	C ₉ H ₁₃ NO ₃		
Molecular Weight	183.207	Exact Molecular Weight	183.089543283
LogP	-0.43	Topological Polar Surface Area	72.72 Å ²
Atom Count	26	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	4
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.48	Oral Bioavailability	Y

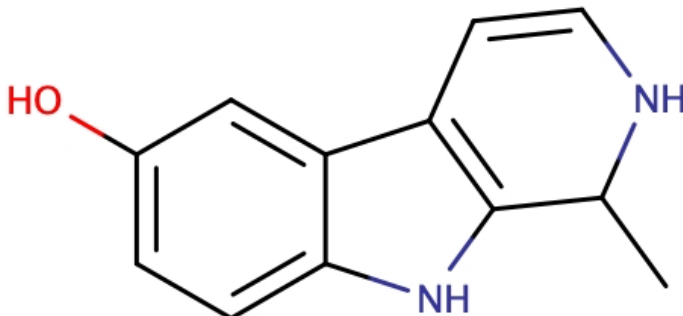
140. N'-formylserotonin

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	39378		
TM-MC 성분 동의어	N/A		
PubChem ID	53705553		
InChI Key	BWXYSRMTUMVGEA-UHFFFAOYSA-N		
SMILES	<chem>Oc1ccc2[nH]cc(CCNC=O)c2c1</chem>		
Molecular Formula	C ₁₁ H ₁₂ N ₂ O ₂		
Molecular Weight	204.229	Exact Molecular Weight	204.089877634
LogP	0.953	Topological Polar Surface Area	65.12 Å ²
Atom Count	27	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.51	Oral Bioavailability	Y

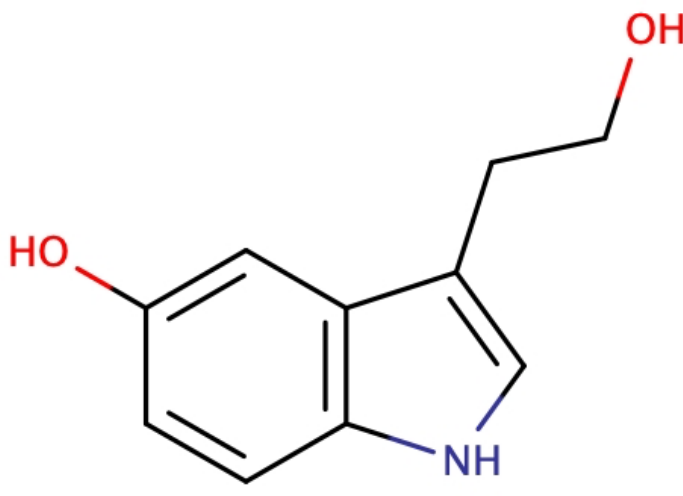
141. indole-3-acetic acid

화학 구조		PubMed ID	
		28032995, 28875639 31590467	
TM-MC 성분 ID	92082		
TM-MC 성분 동의어	3-indoleacetic acid; 1H-indole-3-acetic acid		
PubChem ID	802		
InChI Key	SEOVTRFCIGRIMH-UHFFFAOYSA-N		
SMILES	<chem>OC(=O)Cc1c[nH]c2ccccc12</chem>		
Molecular Formula	C ₁₀ H ₉ NO ₂		
Molecular Weight	175.187	Exact Molecular Weight	175.063328534
LogP	1.71	Topological Polar Surface Area	53.09 Å ²
Atom Count	22	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.73	Oral Bioavailability	Y

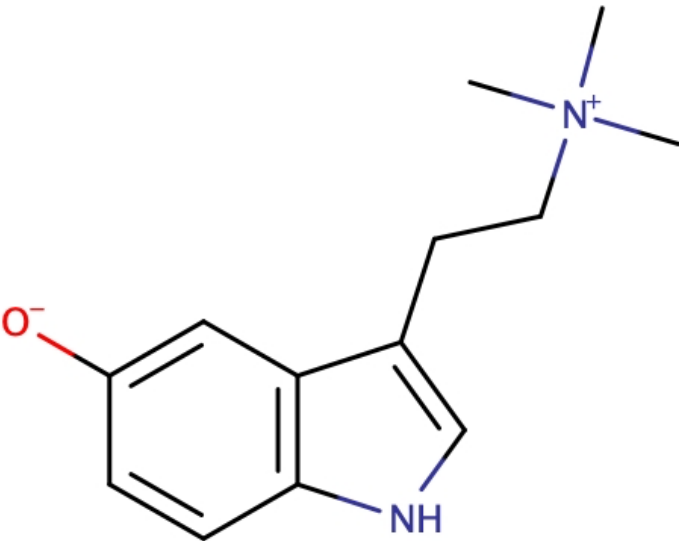
142. 1-methyl-2,9-dihydro-1H-pyrido [3-b]indol-6-ol

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	99580		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	GSMLBFQYBSKKAI-UHFFFAOYSA-N		
SMILES	<chem>CC1NC=Cc2c1[nH]c1ccc(O)cc21</chem>		
Molecular Formula	C ₁₂ H ₁₂ N ₂ O		
Molecular Weight	200.241	Exact Molecular Weight	200.094963014
LogP	1.798	Topological Polar Surface Area	48.05 Å ²
Atom Count	27	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	3
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.61	Oral Bioavailability	Y

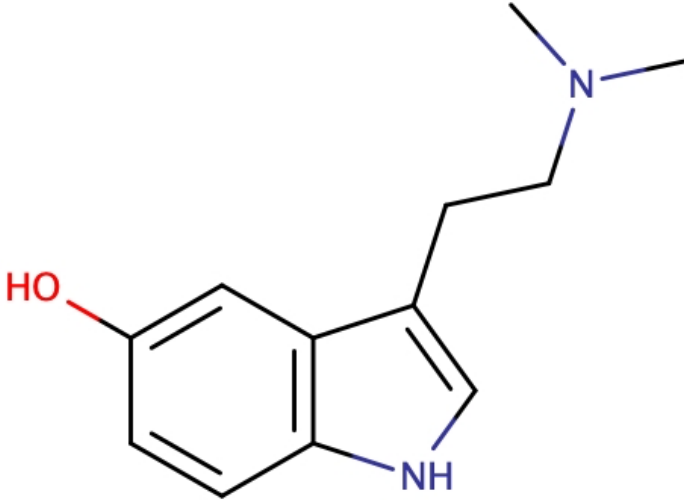
143. 5-hydroxy tryptophol

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	300530		
TM-MC 성분 동의어	N/A		
PubChem ID	9061		
InChI Key	KQROHCSYOGBQJ-UHFFFAOYSA-N		
SMILES	OCCc1c[nH]c2ccc(O)cc12		
Molecular Formula	C ₁₀ H ₁₁ NO ₂		
Molecular Weight	177.203	Exact Molecular Weight	177.078978598
LogP	1.29	Topological Polar Surface Area	56.25 Å ²
Atom Count	24	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.65	Oral Bioavailability	Y

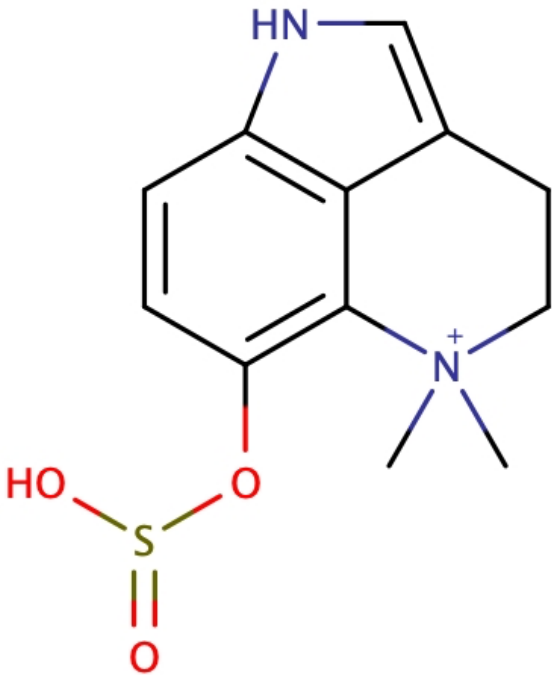
144. bufotenidine

화학 구조		PubMed ID	
		28421441, 29704033 30591646, 31590467	
TM-MC 성분 ID	300835		
TM-MC 성분 동의어	N/A		
PubChem ID	3083591		
InChI Key	HIYGARYIJZXGW-UHFFFAOYSA-N		
SMILES	C[N+](C)(C)CCc1c[nH]c2ccc([O-])cc12		
Molecular Formula	C ₁₃ H ₁₈ N ₂ O		
Molecular Weight	218.3	Exact Molecular Weight	218.141913208
LogP	-2.164	Topological Polar Surface Area	38.85 Å ²
Atom Count	34	Structural Alert Count	1
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.59	Oral Bioavailability	Y

145. bufotenine

화학 구조		PubMed ID	
		28421441, 29680742 29704033, 30591646 31590467	
TM-MC 성분 ID	300840		
TM-MC 성분 동의어	N/A		
PubChem ID	10257		
InChI Key	VTTONGPRPXSTJ-UHFFFAOYSA-N		
SMILES	<chem>CN(C)CCc1c[nH]c2ccc(O)cc12</chem>		
Molecular Formula	C ₁₂ H ₁₆ N ₂ O		
Molecular Weight	204.273	Exact Molecular Weight	204.126263143
LogP	1.292	Topological Polar Surface Area	39.26 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.79	Oral Bioavailability	Y

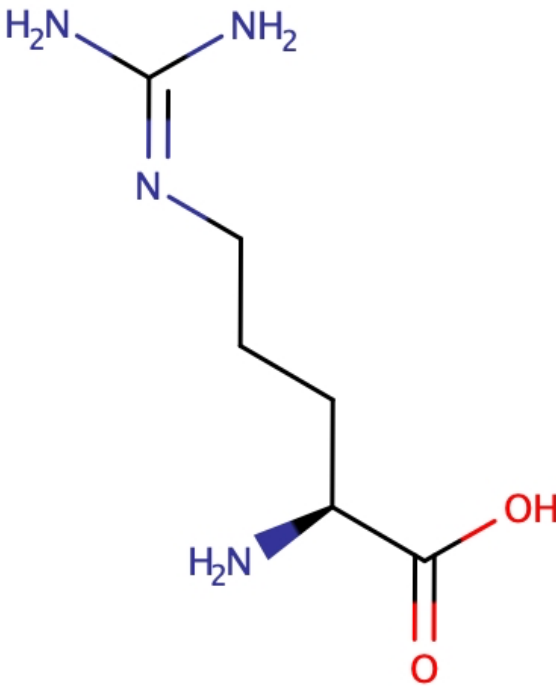
146. bufothionine

화학 구조		PubMed ID	
		29704033, 30591646 31590467	
TM-MC 성분 ID	300846		
TM-MC 성분 동의어	N/A		
PubChem ID	5315536		
InChI Key	XFIMEMVNMWDPRW-UHFFFAOYSA-O		
SMILES	C[N+](C)CCc2c[nH]c3ccc(OS(O)=O)c1c23		
Molecular Formula	C ₁₂ H ₁₅ N ₂ O ₃ S		
Molecular Weight	267.32	Exact Molecular Weight	267.079789945
LogP	-3.223	Topological Polar Surface Area	62.32 Å ²
Atom Count	33	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.44	Oral Bioavailability	Y

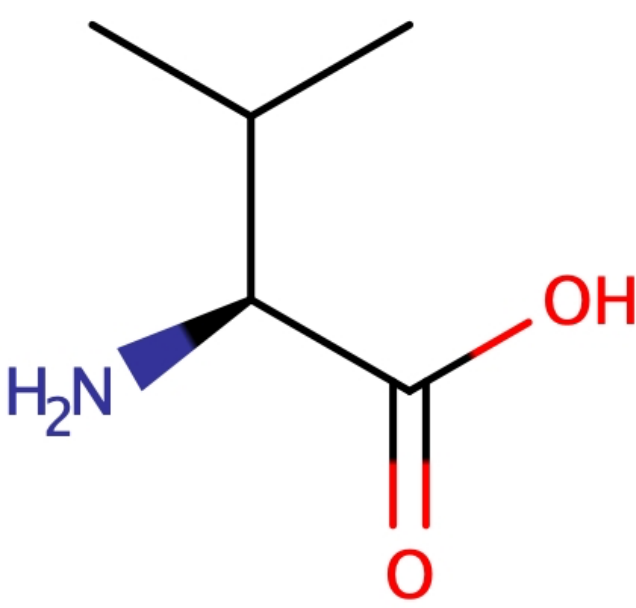
147. dehydrobufotenine

화학 구조		PubMed ID	
		29704033, 30591646 31590467	
TM-MC 성분 ID	301115		
TM-MC 성분 동의어	N/A		
PubChem ID	205042		
InChI Key	XRZDSPVDZKCARG-UHFFFAOYSA-O		
SMILES	C[N+]1(C)CCc2c[nH]c3ccc(O)c1c23		
Molecular Formula	C ₁₂ H ₁₅ N ₂ O		
Molecular Weight	203.264	Exact Molecular Weight	203.117889531
LogP	-2.132	Topological Polar Surface Area	36.02 Å ²
Atom Count	30	Structural Alert Count	1
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.47	Oral Bioavailability	Y

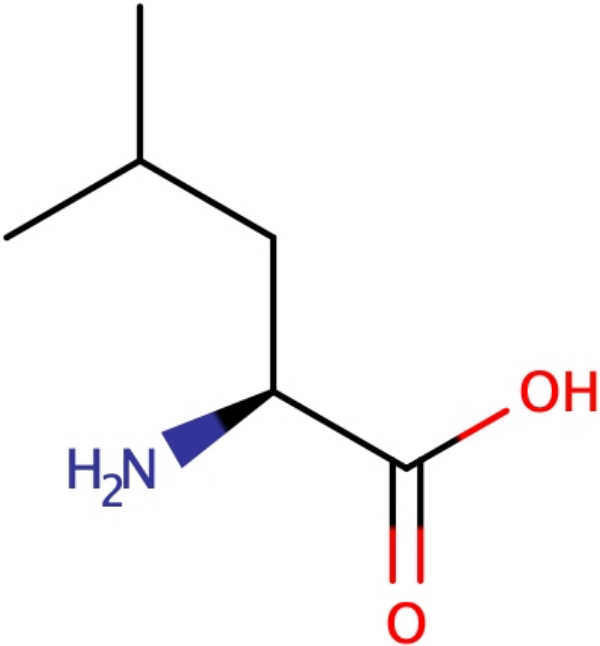
148. arginine

화학 구조		PubMed ID	
		17134710, 25780666 27558519, 29704033 31590467	
TM-MC 성분 ID	183		
TM-MC 성분 동의어	Arg; L-arginine		
PubChem ID	6322, 28782		
InChI Key	ODKSFYDXXFIFQN-BYPYZUCNSA-N		
SMILES	N[C@@H](CCCN=C(N)N)C(O)=O		
Molecular Formula	C ₆ H ₁₄ N ₄ O ₂		
Molecular Weight	174.204	Exact Molecular Weight	174.111675707
LogP	-3.24	Topological Polar Surface Area	127.72 Å ²
Atom Count	26	Structural Alert Count	3
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.20	Oral Bioavailability	Y

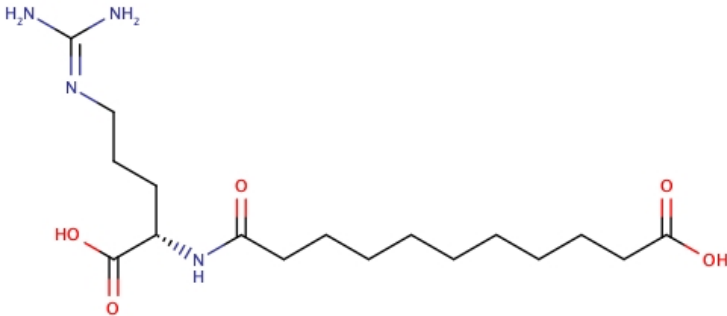
149. valine

화학 구조		PubMed ID	
		17134710, 25780666 27558519, 30591646	
TM-MC 성분 ID	186		
TM-MC 성분 동의어	Val; L-valine		
PubChem ID	6287, 6971018, 88733505		
InChI Key	KZSNJWFQEVHDMF-BYPYZUCNSA-N		
SMILES	CC(C)[C@H](N)C(O)=O		
Molecular Formula	C ₅ H ₁₁ NO ₂		
Molecular Weight	117.148	Exact Molecular Weight	117.078978598
LogP	-1.953	Topological Polar Surface Area	63.32 Å ²
Atom Count	19	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.44	Oral Bioavailability	Y

150. leucine

화학 구조		PubMed ID	
		17134710, 19149256 25780666, 27558519 30591646, 31590467	
TM-MC 성분 ID	191		
TM-MC 성분 동의어	Leu; L-leucine; 2-amino-4-methyl-pentanoic acid		
PubChem ID	6106, 7045798		
InChI Key	ROHFNLRQFUQHCH-YFKPBYRVSA-N		
SMILES	<chem>CC(C)C[C@H](N)C(O)=O</chem>		
Molecular Formula	C ₆ H ₁₃ NO ₂		
Molecular Weight	131.175	Exact Molecular Weight	131.094628663
LogP	-1.586	Topological Polar Surface Area	63.32 Å ²
Atom Count	22	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.49	Oral Bioavailability	Y

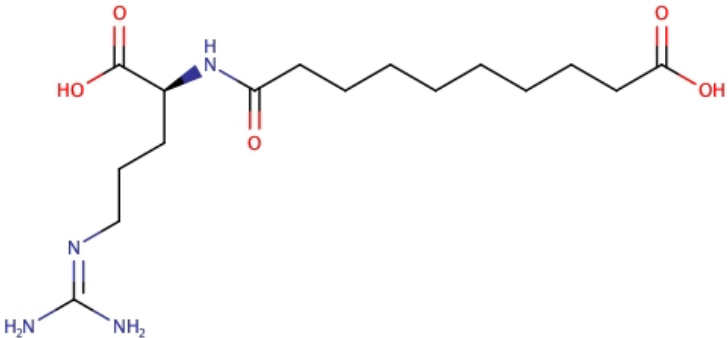
151. undecanedioyl arginine

화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	93424		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	WLXHOQCUWXYCII-ZDUSSCGKSA-N		
SMILES	NC(N)=NCCC[C@H](NC(=O)CCCCCCCCC(O)=O)C(O)=O		
Molecular Formula	C ₁₇ H ₃₂ N ₄ O ₅		
Molecular Weight	372.466	Exact Molecular Weight	372.237270146
LogP	-0.633	Topological Polar Surface Area	168.1 Å ²
Atom Count	58	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	16	Aromatic Ring Count	0
Drug Likeness	0.14	Oral Bioavailability	N

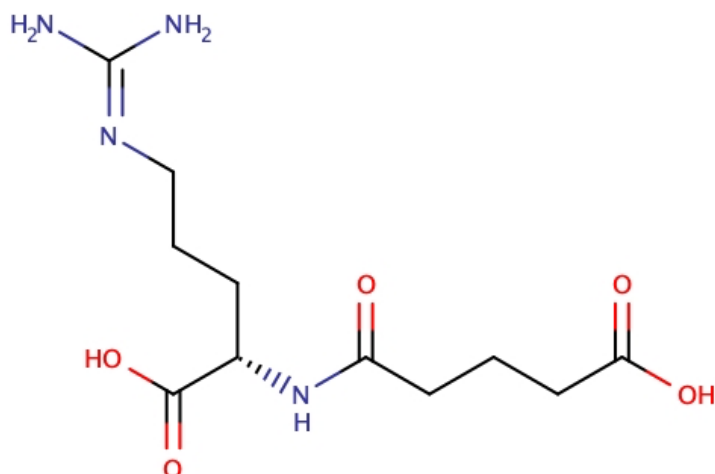
152. azelayl arginine

화학 구조		PubMed ID	
		29704033, 30591646 31590467	
TM-MC 성분 ID	93869		
TM-MC 성분 동의어	N/A		
PubChem ID	118550145		
InChI Key	HNRUJVNDUQRJOX-NSHDSACASA-N		
SMILES	NC(N)=NCCC[C@H](NC(=O)CCCCCCC(O)=O)C(O)=O		
Molecular Formula	C ₁₅ H ₂₈ N ₄ O ₅		
Molecular Weight	344.412	Exact Molecular Weight	344.205970018
LogP	-1.56	Topological Polar Surface Area	168.1 Å ²
Atom Count	52	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	14	Aromatic Ring Count	0
Drug Likeness	0.14	Oral Bioavailability	N

153. sebacyl arginine

화학 구조		PubMed ID	
		29704033, 30591646 31590467	
TM-MC 성분 ID	93903		
TM-MC 성분 동의어	N/A		
PubChem ID	118550146		
InChI Key	WZZNTJZCUWNFKQ-LBPRGKRZSA-N		
SMILES	NC(N)=NCCC[C@H](NC(=O)CCCCCCCCC(O)=O)C(O)=O		
Molecular Formula	C ₁₆ H ₃₀ N ₄ O ₅		
Molecular Weight	358.439	Exact Molecular Weight	358.221620082
LogP	-1.073	Topological Polar Surface Area	168.1 Å ²
Atom Count	55	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	15	Aromatic Ring Count	0
Drug Likeness	0.14	Oral Bioavailability	N

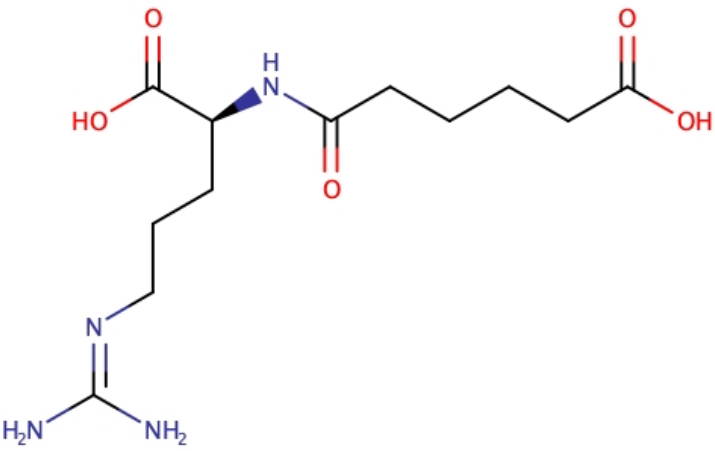
154. glutaryl arginine

화학 구조		PubMed ID	
		31590467	
TM-MC 성분 ID	94432		
TM-MC 성분 동의어	N/A		
PubChem ID	150676701		
InChI Key	JHAQFUPXUUKCMI-ZETCQYMHSA-N		
SMILES	NC(N)=NCCC[C@H](NC(=O)CCCC(O)=O)C(O)=O		
Molecular Formula	C ₁₁ H ₂₀ N ₄ O ₅		
Molecular Weight	288.304	Exact Molecular Weight	288.14336976
LogP	-3.391	Topological Polar Surface Area	168.1 Å ²
Atom Count	40	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	10	Aromatic Ring Count	0
Drug Likeness	0.16	Oral Bioavailability	N

155. suberoyl arginine

화학 구조		PubMed ID	
		20637273, 28726106 29704033, 30591646 31590467	
TM-MC 성분 ID	99925		
TM-MC 성분 동의어	suberoyl-arginine; N-suberylarginine		
PubChem ID	118550139		
InChI Key	ITNUIUFXPZKAHH-JTQLQIEISA-N		
SMILES	NC(N)=NCCC[C@H](NC(=O)CCCCCCC(=O)O)C(=O)O		
Molecular Formula	C ₁₄ H ₂₆ N ₄ O ₅		
Molecular Weight	330.385	Exact Molecular Weight	330.190319953
LogP	-2.016	Topological Polar Surface Area	168.1 Å ²
Atom Count	49	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	13	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

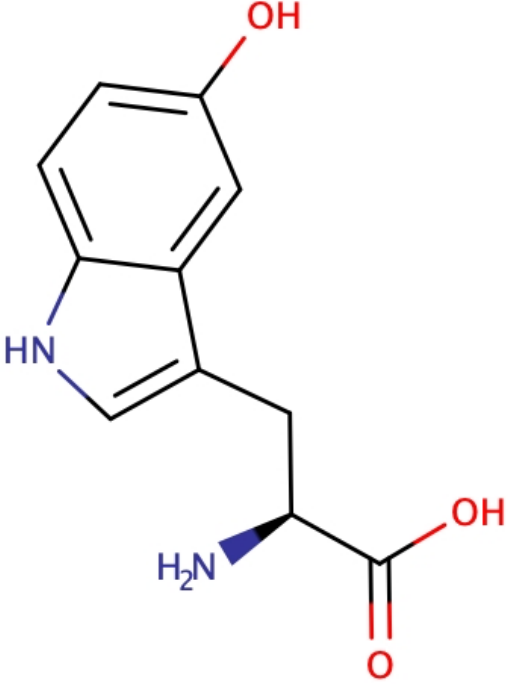
156. adipyl arginine

화학 구조		PubMed ID	
		28726106, 29704033 30591646, 31590467	
TM-MC 성분 ID	200167		
TM-MC 성분 동의어	N-adipoylarginine		
PubChem ID	118550147		
InChI Key	AFEUONDHTCGAPM-QMMMGPBSA-N		
SMILES	<chem>NC(N)=NCCC[C@H](NC(=O)CCCCC(O)=O)C(O)=O</chem>		
Molecular Formula	C ₁₂ H ₂₂ N ₄ O ₅		
Molecular Weight	302.331	Exact Molecular Weight	302.159019824
LogP	-2.934	Topological Polar Surface Area	168.1 Å ²
Atom Count	43	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	11	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

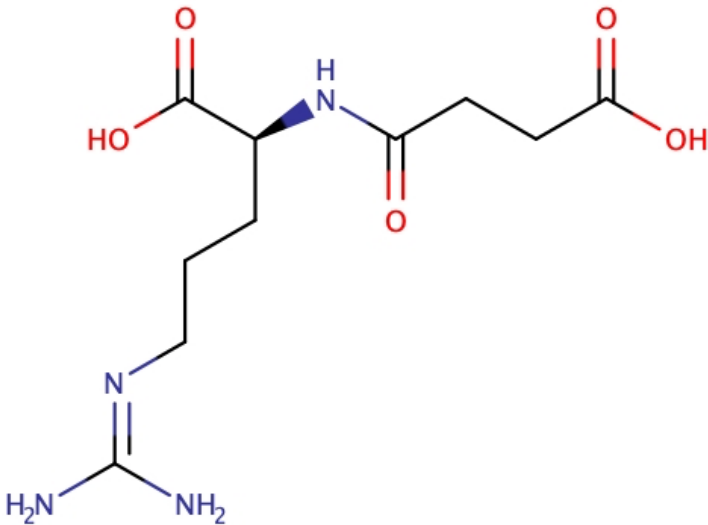
157. pimeloyl arginine

화학 구조		PubMed ID	
		28726106, 29704033 30591646, 31590467	
TM-MC 성분 ID	200168		
TM-MC 성분 동의어	pitneloyl arginine; N-pimeloylarginine		
PubChem ID	118550144		
InChI Key	FNMNVPPVRGSVLI-VIFPVBQESA-N		
SMILES	NC(N)=NCCC[C@H](NC(=O)CCCCC(O)=O)C(O)=O		
Molecular Formula	C ₁₃ H ₂₄ N ₄ O ₅		
Molecular Weight	316.358	Exact Molecular Weight	316.174669889
LogP	-2.476	Topological Polar Surface Area	168.1 Å ²
Atom Count	46	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	12	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

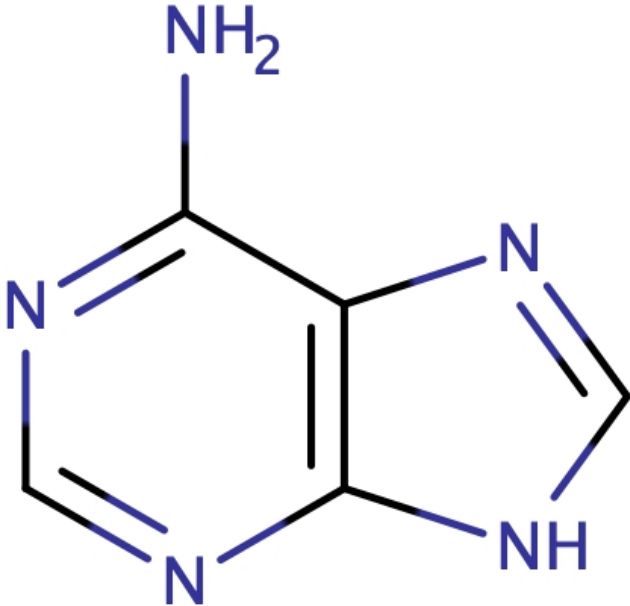
158. 5-hydroxy tryptophan

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	300529		
TM-MC 성분 동의어	N/A		
PubChem ID	439280, 6971044		
InChI Key	LDCYZAJDBXYCGN-VIFPVBQESA-N		
SMILES	N[C@@H](Cc1c[nH]c2ccc(O)cc12)C(O)=O		
Molecular Formula	C ₁₁ H ₁₂ N ₂ O ₃		
Molecular Weight	220.228	Exact Molecular Weight	220.084792254
LogP	-1.39	Topological Polar Surface Area	99.34 Å ²
Atom Count	28	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	4
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.51	Oral Bioavailability	Y

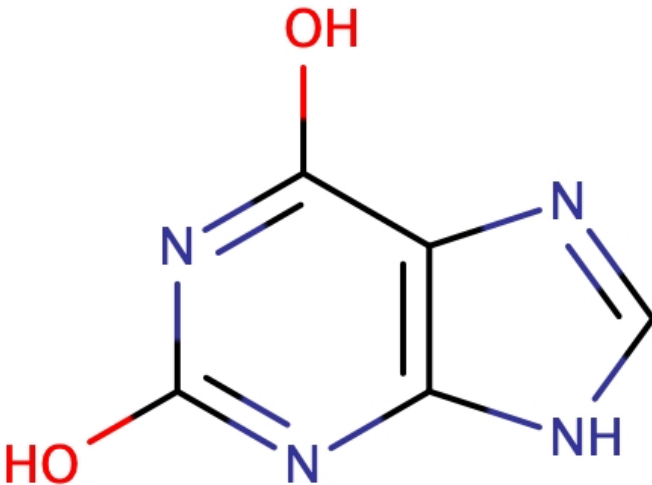
159. succinyl arginine

화학 구조		PubMed ID	
		29704033, 30591646 31590467	
TM-MC 성분 ID	302512		
TM-MC 성분 동의어	N/A		
PubChem ID	439968		
InChI Key	UMOXFSXIFQOWTD-LURJTMIESA-N		
SMILES	NC(N)=NCCC[C@H](NC(=O)CCC(O)=O)C(O)=O		
Molecular Formula	C ₁₀ H ₁₈ N ₄ O ₅		
Molecular Weight	274.277	Exact Molecular Weight	274.127719696
LogP	-3.857	Topological Polar Surface Area	168.1 Å ²
Atom Count	37	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	9	Aromatic Ring Count	0
Drug Likeness	0.16	Oral Bioavailability	N

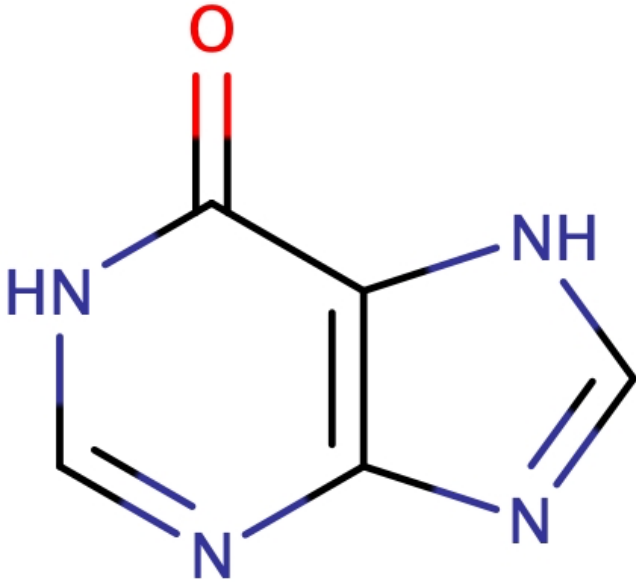
160. adenine

화학 구조		PubMed ID	
		23689025, 30591646	
TM-MC 성분 ID	305		
TM-MC 성분 동의어	pedatisectine B		
PubChem ID	190		
InChI Key	GFFGJBXGBJISGV-UHFFFAOYSA-N		
SMILES	<chem>Nc1ncnc2[nH]cnc12</chem>		
Molecular Formula	C ₅ H ₅ N ₅		
Molecular Weight	135.13	Exact Molecular Weight	135.054495181
LogP	-0.531	Topological Polar Surface Area	80.48 Å ²
Atom Count	15	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.51	Oral Bioavailability	Y

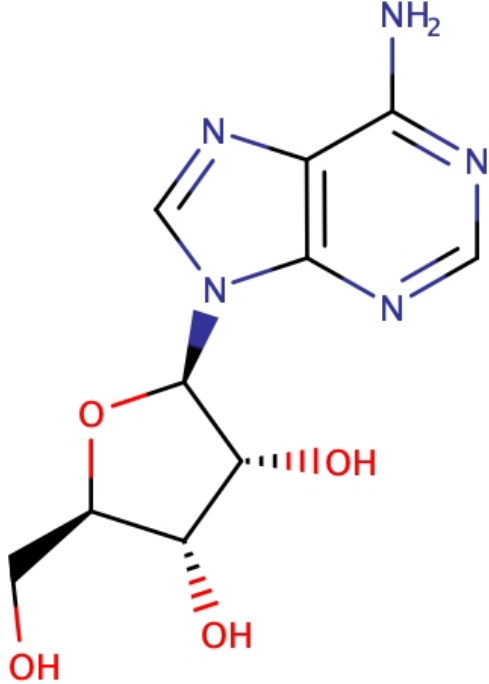
161. xanthine

화학 구조		PubMed ID	
		12575054, 15562718 23689025, 30591646 30728838, 31590467	
TM-MC 성분 ID	317		
TM-MC 성분 동의어	N/A		
PubChem ID	1188		
InChI Key	LRFVTYWOQMYALW-UHFFFAOYSA-N		
SMILES	<chem>Oc1nc(O)c2nc[nH]c2n1</chem>		
Molecular Formula	C ₅ H ₄ N ₄ O ₂		
Molecular Weight	152.113	Exact Molecular Weight	152.033425385
LogP	0.37	Topological Polar Surface Area	94.92 Å ²
Atom Count	15	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.51	Oral Bioavailability	Y

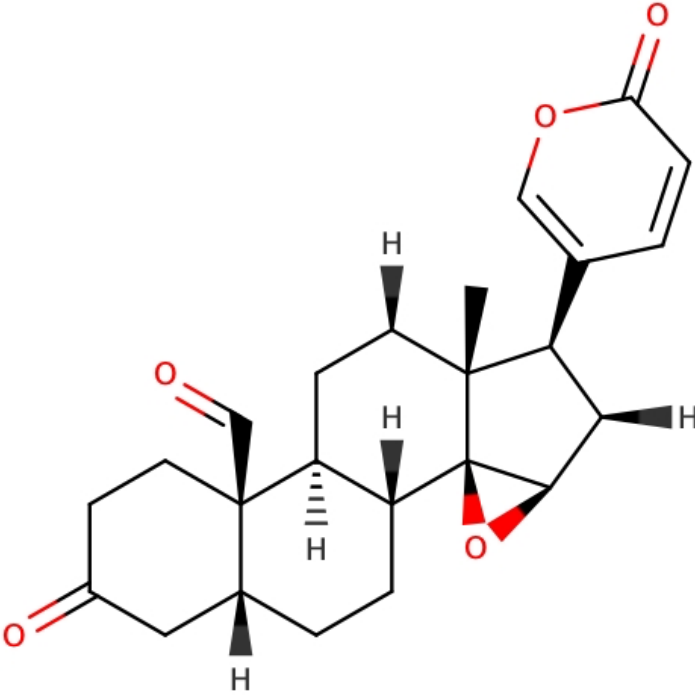
162. hypoxanthine

화학 구조		PubMed ID	
		11943593, 12575054 15562718, 16981455 18589774, 21995368 23689025, 25335278 25422536, 30591646 30728838, 31590467	
TM-MC 성분 ID	318		
TM-MC 성분 동의어	N/A		
PubChem ID	790, 135398638		
InChI Key	FDGQSTZJBFJUBT-UHFFFAOYSA-N		
SMILES	O=c1[nH]cnc2nc[nH]c12		
Molecular Formula	C ₅ H ₄ N ₄ O		
Molecular Weight	136.114	Exact Molecular Weight	136.038510765
LogP	-0.879	Topological Polar Surface Area	70.14 Å ²
Atom Count	14	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.49	Oral Bioavailability	Y

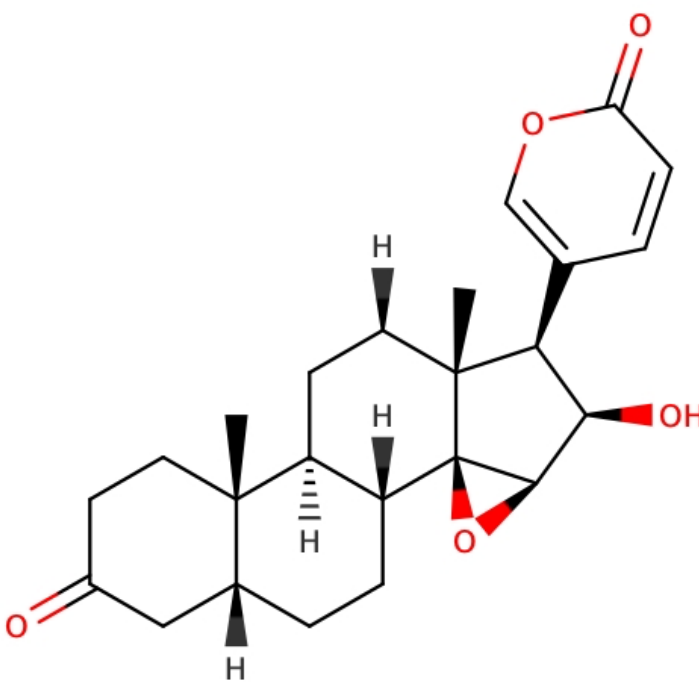
163. adenosine

화학 구조		PubMed ID	
		<p>21384380, 23689025 25335278, 25422536 30728838, 31590467 31800596</p>	
TM-MC 성분 ID	232		
TM-MC 성분 동의어	N/A		
PubChem ID	60961		
InChI Key	OIRDYFTABQOQ-KQYNXXCUSA-N		
SMILES	<chem>Nc1ncnc2n(cnc12)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₁₀ H ₁₃ N ₅ O ₄		
Molecular Weight	267.245	Exact Molecular Weight	267.096753919
LogP	-2.091	Topological Polar Surface Area	139.54 Å ²
Atom Count	32	Structural Alert Count	0
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	4
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.49	Oral Bioavailability	Y

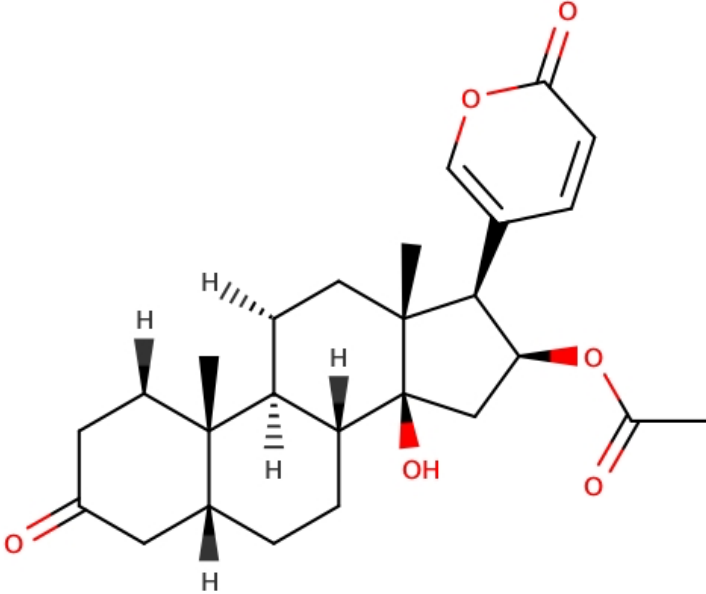
164. 3-keto-resibufagin

화학 구조		PubMed ID	
		26621782	
TM-MC 성분 ID	1334		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	LIGYLZ FAGDVYKK-CNYXOANESA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4CC(=O)CC[C@]34C=O)[C@]11O[C@@H]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₂₈ O ₅		
Molecular Weight	396.483	Exact Molecular Weight	396.193674002
LogP	2.604	Topological Polar Surface Area	72.97 Å ²
Atom Count	57	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	0
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.57	Oral Bioavailability	Y

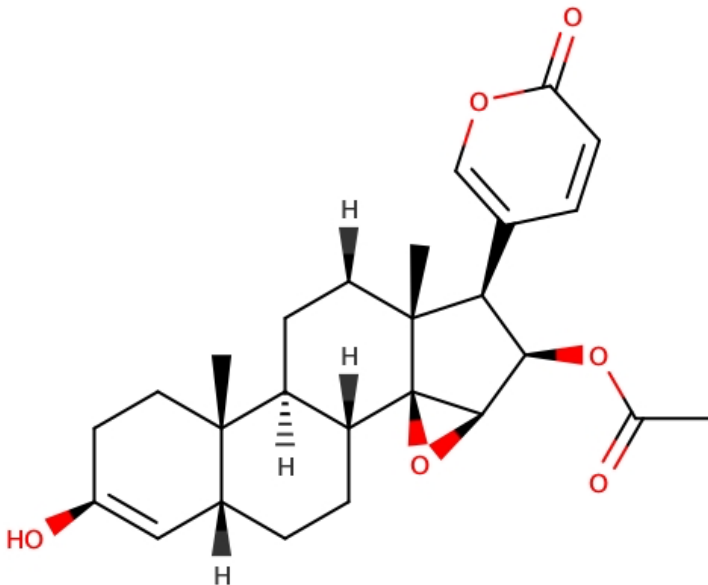
165. 3-keto-deacetylcinobufagin

화학 구조		PubMed ID	
		26621782	
TM-MC 성분 ID	92085		
TM-MC 성분 동의어	N/A		
PubChem ID	101590551		
InChI Key	JCCYKKRYWIVNQE-OGCGCHONSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4CC(=O)CC[C@]34C)[C@]11O[C@@H]1[C@H](O)[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₃₀ O ₅		
Molecular Weight	398.499	Exact Molecular Weight	398.209324066
LogP	2.574	Topological Polar Surface Area	76.13 Å ²
Atom Count	59	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.74	Oral Bioavailability	Y

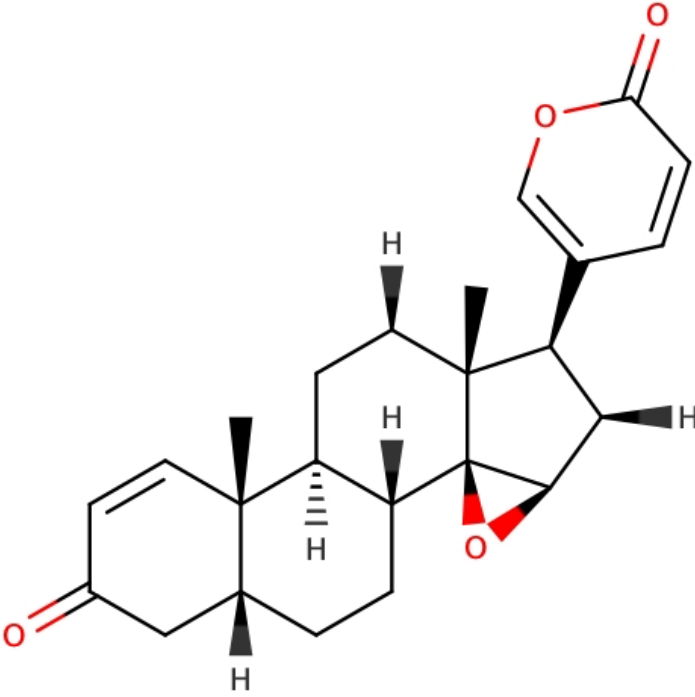
166. 3-keto-bufotalin

화학 구조		PubMed ID	
		26621782	
TM-MC 성분 ID	300409		
TM-MC 성분 동의어	N/A		
PubChem ID	101286226		
InChI Key	QEMXBVZVZSPAEA-KMUQWSQCSA-N		
SMILES	<chem>CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4CC(=O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₆ H ₃₄ O ₆		
Molecular Weight	442.552	Exact Molecular Weight	442.235538815
LogP	2.544	Topological Polar Surface Area	89.9 Å ²
Atom Count	66	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.73	Oral Bioavailability	Y

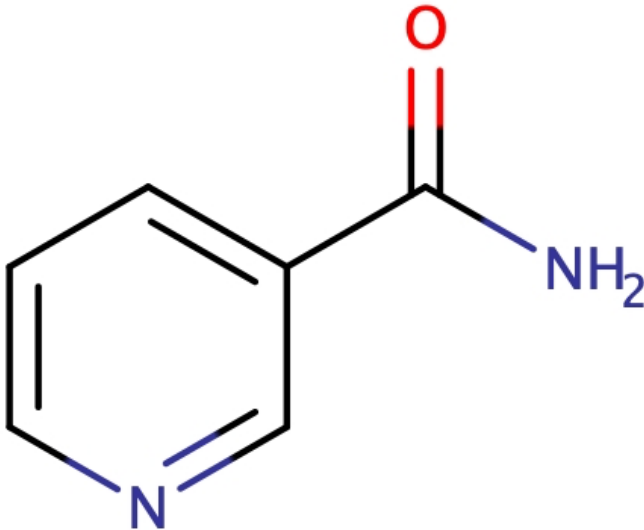
167. 3-dehydrocinobufagin

화학 구조		PubMed ID	
		26621782	
TM-MC 성분 ID	1333		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	NAMKIAKEINIZOG-BAEBVKMLSA-N		
SMILES	CC(=O)O[C@H]1[C@H]2O[C@]22[C@@H]3CC[C@H]4C=C(O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1c1ccc(=O)oc1		
Molecular Formula	C ₂₆ H ₃₂ O ₆		
Molecular Weight	440.536	Exact Molecular Weight	440.21988875
LogP	3.006	Topological Polar Surface Area	85.36 Å ²
Atom Count	64	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.58	Oral Bioavailability	Y

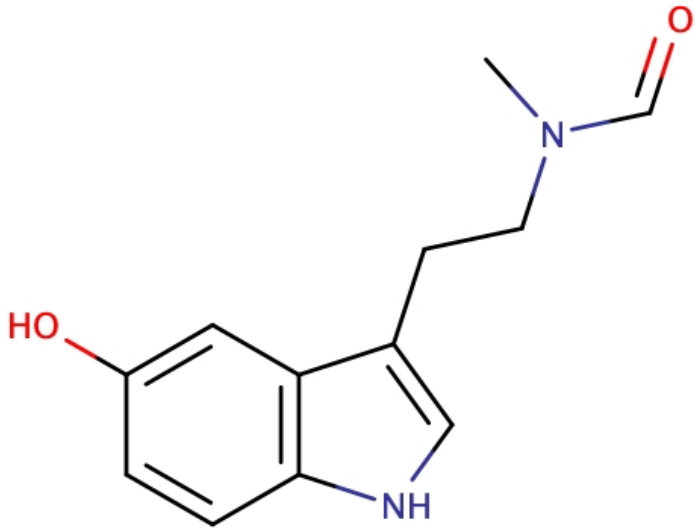
168. Δ-3-oxo-resibufogenin

화학 구조		PubMed ID	
		26621782	
TM-MC 성분 ID	1335		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	WVVRDXVBWQZBIM-LPPFXQTFSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4CC(=O)C=C[C@]34C)[C@]11O[C@@H]]1C[C@@H]2c1ccc(=O)oc1</chem>		
Molecular Formula	C ₂₄ H ₂₈ O ₄		
Molecular Weight	380.484	Exact Molecular Weight	380.198759382
LogP	3.569	Topological Polar Surface Area	55.9 Å ²
Atom Count	56	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	0
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.70	Oral Bioavailability	Y

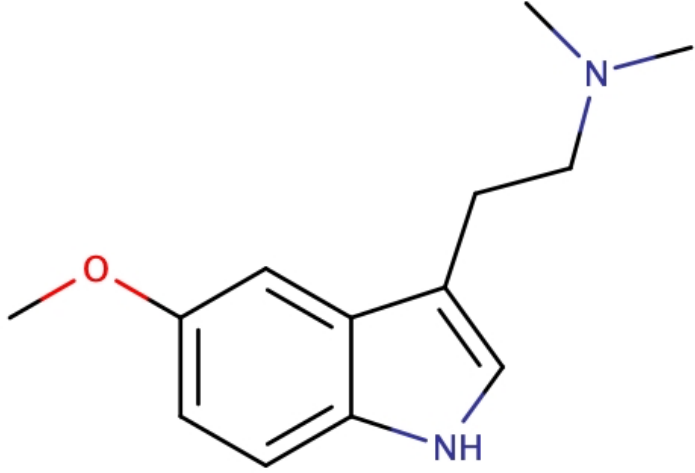
169. nicotinamide

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	936		
TM-MC 성분 동의어	vitamin B; niacinamide		
PubChem ID	936		
InChI Key	DFPAKSUCGFBDDF-UHFFFAOYSA-N		
SMILES	NC(=O)c1cccnc1		
Molecular Formula	C ₆ H ₆ N ₂ O		
Molecular Weight	122.127	Exact Molecular Weight	122.048012821
LogP	-0.394	Topological Polar Surface Area	55.98 Å ²
Atom Count	15	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.55	Oral Bioavailability	Y

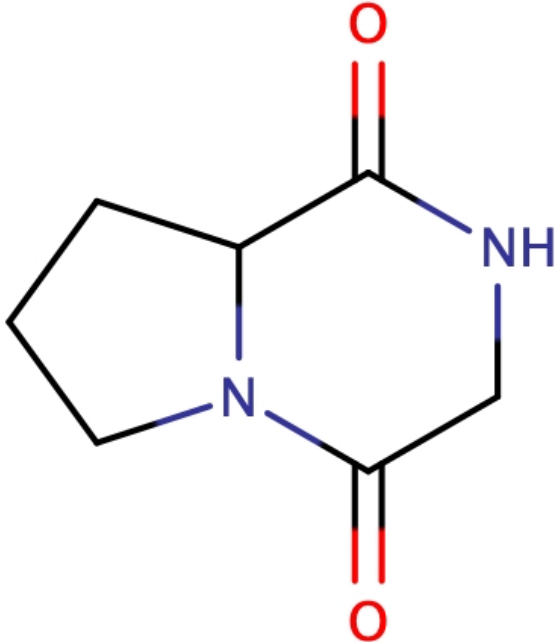
170. N-(2-(5-hydroxy-1H-indol-3-yl)ethyl)-N-methylformamide

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	39335		
TM-MC 성분 동의어	N/A		
PubChem ID	155770255		
InChI Key	QZUPLIRYTSWBFV-UHFFFAOYSA-N		
SMILES	CN(CCC1c[nH]c2ccc(O)cc12)C=O		
Molecular Formula	C ₁₂ H ₁₄ N ₂ O ₂		
Molecular Weight	218.256	Exact Molecular Weight	218.105527699
LogP	1.177	Topological Polar Surface Area	56.33 Å ²
Atom Count	30	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.76	Oral Bioavailability	Y

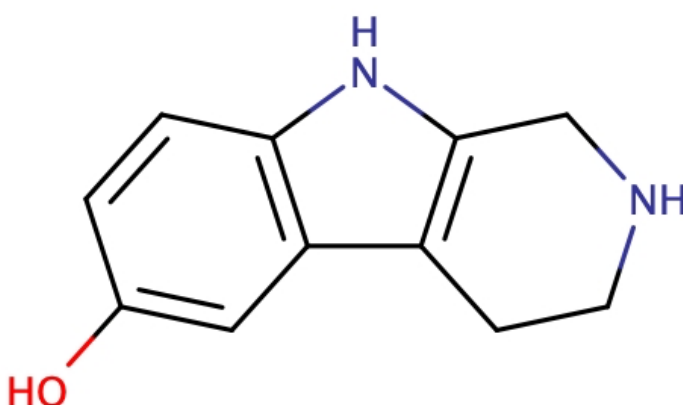
171. 5-methoxy bufotenine

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	90764		
TM-MC 성분 동의어	5-methoxy-N,N-dimethyltryptamine		
PubChem ID	1832		
InChI Key	ZSTKHSQDNIGFLM-UHFFFAOYSA-N		
SMILES	<chem>COC1ccc2[nH]cc(CCN(C)C)c2c1</chem>		
Molecular Formula	C ₁₃ H ₁₈ N ₂ O		
Molecular Weight	218.3	Exact Molecular Weight	218.141913208
LogP	2.144	Topological Polar Surface Area	28.26 Å ²
Atom Count	34	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.85	Oral Bioavailability	Y

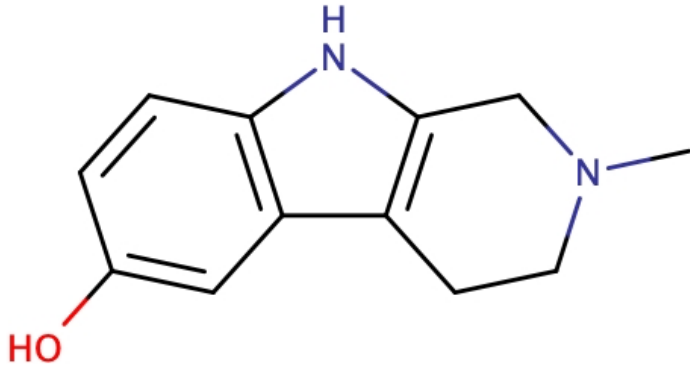
172. cyclo (Gly-Pro)

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	90891		
TM-MC 성분 동의어	cyclo(pro-gly)dipeptide; pyrrolo[1,2,a]pyrazine-1,4-dione, hexahydro-		
PubChem ID	193540		
InChI Key	OWOHLURDBZHNGG-UHFFFAOYSA-N		
SMILES	O=C1CNC(=O)C2CCCN12		
Molecular Formula	C ₇ H ₁₀ N ₂ O ₂		
Molecular Weight	154.169	Exact Molecular Weight	154.07422757
LogP	-1.369	Topological Polar Surface Area	49.41 Å ²
Atom Count	21	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.47	Oral Bioavailability	Y

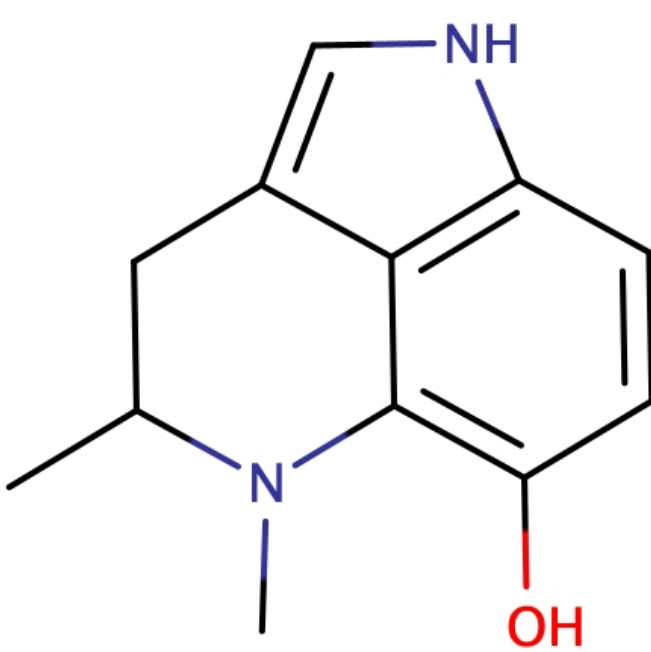
173. 1,2,3,4-tetrahydro-6-hydroxy-β-carboline

화학 구조		PubMed ID
		30591646
TM-MC 성분 ID	93177	
TM-MC 성분 동의어	N/A	
PubChem ID	159959	
InChI Key	HASNCBJLQYTILW-UHFFFAOYSA-N	
SMILES	<chem>Oc1ccc2[nH]c3CNCCc3c2c1</chem>	
Molecular Formula	C ₁₁ H ₁₂ N ₂ O	
Molecular Weight	188.23	Exact Molecular Weight 188.094963014
LogP	0.838	Topological Polar Surface Area 48.05 Å ²
Atom Count	26	Structural Alert Count 0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count 3
Rotatable Bond Count	0	Aromatic Ring Count 2
Drug Likeness	0.57	Oral Bioavailability Y

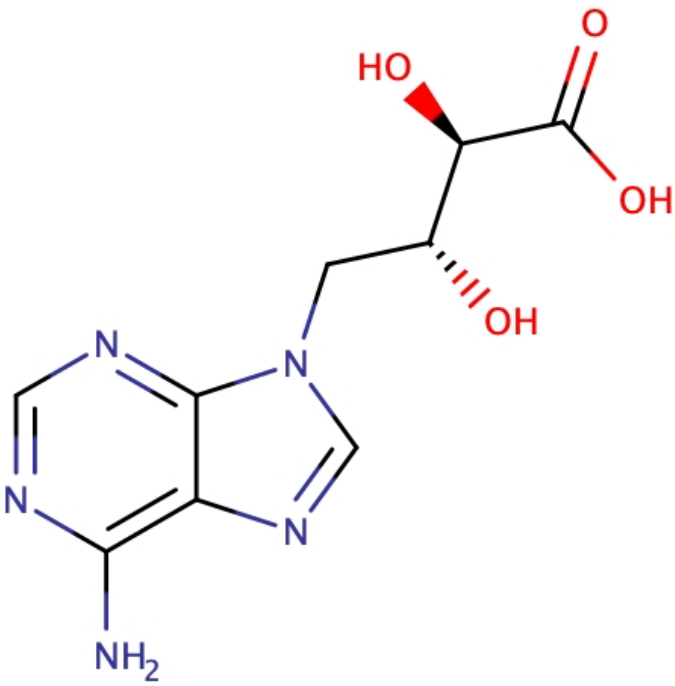
174. 2-methyl-6-hydroxy-1,2,3,4-tetrahydro-β-carboline

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	98129		
TM-MC 성분 동의어	N/A		
PubChem ID	71371962		
InChI Key	SWZIYPSCWPVCAO-UHFFFAOYSA-N		
SMILES	CN1CCc2c(C1)[nH]c1ccc(O)cc21		
Molecular Formula	C ₁₂ H ₁₄ N ₂ O		
Molecular Weight	202.257	Exact Molecular Weight	202.110613079
LogP	1.67	Topological Polar Surface Area	39.26 Å ²
Atom Count	29	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.68	Oral Bioavailability	Y

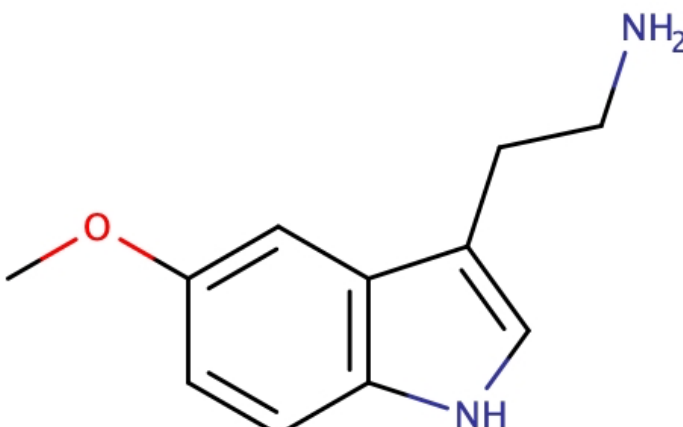
175. cyclotufotenine

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	300859		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	CQRCGOWYZRCIJO-UHFFFAOYSA-N		
SMILES	<chem>CC1Cc2c[nH]c3ccc(O)c(N1C)c23</chem>		
Molecular Formula	C ₁₂ H ₁₄ N ₂ O		
Molecular Weight	202.257	Exact Molecular Weight	202.110613079
LogP	2.333	Topological Polar Surface Area	39.26 Å ²
Atom Count	29	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.69	Oral Bioavailability	Y

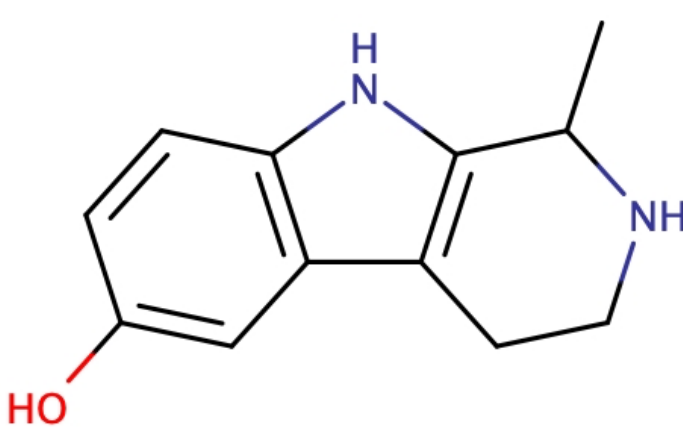
176. eritadenine

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	301246		
TM-MC 성분 동의어	N/A		
PubChem ID	159961		
InChI Key	LIEMBEWXEZJEEZ-INEUFUBQSA-N		
SMILES	<chem>Nc1ncnc2n(C[C@@H](O)[C@@H](O)C(O)=O)cnc12</chem>		
Molecular Formula	C ₉ H ₁₁ N ₅ O ₄		
Molecular Weight	253.218	Exact Molecular Weight	253.081103854
LogP	-3.098	Topological Polar Surface Area	147.38 Å ²
Atom Count	29	Structural Alert Count	0
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	4
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.45	Oral Bioavailability	Y

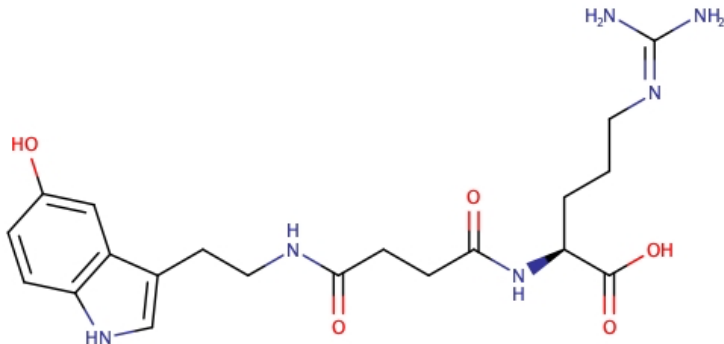
177. O-methyl serotonin

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	301919		
TM-MC 성분 동의어	N/A		
PubChem ID	1833		
InChI Key	JTEJPPKMYBDEMY-UHFFFAOYSA-N		
SMILES	<chem>COc1ccc2[nH]cc(CCN)c2c1</chem>		
Molecular Formula	C ₁₁ H ₁₄ N ₂ O		
Molecular Weight	190.246	Exact Molecular Weight	190.110613079
LogP	1.329	Topological Polar Surface Area	51.04 Å ²
Atom Count	28	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.77	Oral Bioavailability	Y

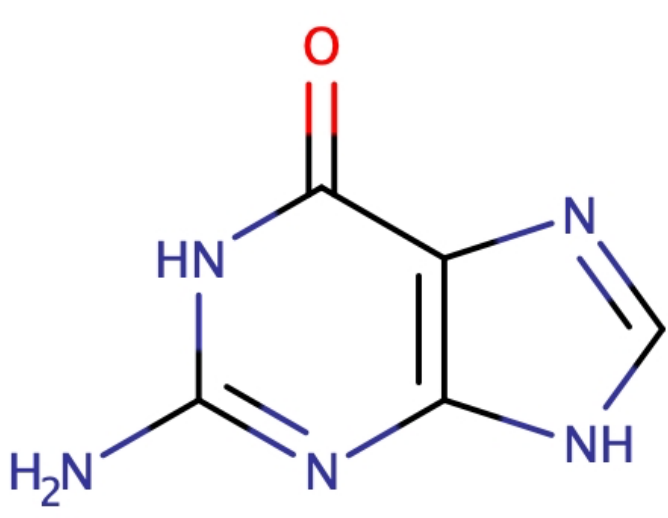
178. shepherdine

화학 구조		PubMed ID	
		30591646	
TM-MC 성분 ID	302444		
TM-MC 성분 동의어	N/A		
PubChem ID	98248		
InChI Key	GHKJDZJAHHVUTD-UHFFFAOYSA-N		
SMILES	CC1NCCc2c1[nH]c1ccc(O)cc21		
Molecular Formula	C ₁₂ H ₁₄ N ₂ O		
Molecular Weight	202.257	Exact Molecular Weight	202.110613079
LogP	1.206	Topological Polar Surface Area	48.05 Å ²
Atom Count	29	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	3
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.60	Oral Bioavailability	Y

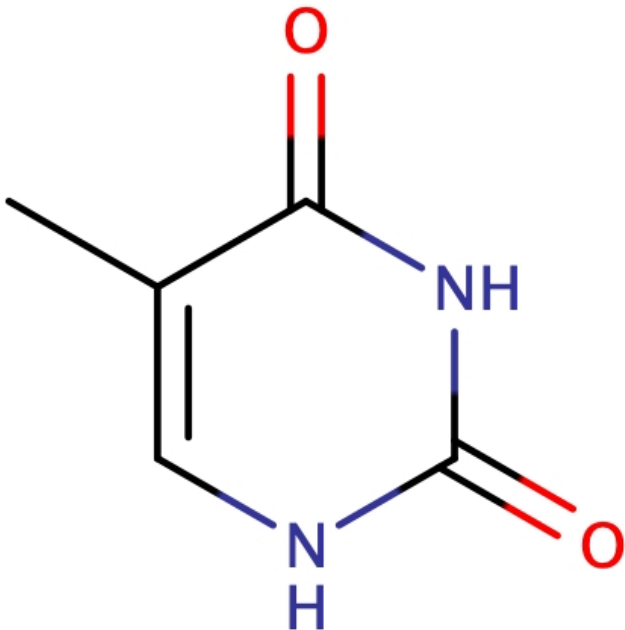
179. bufobutarginine

화학 구조		PubMed ID	
 <p>The chemical structure of bufobutarginine is shown. It features a 5-hydroxytryptamine (5-HT) core (indole ring with a hydroxyl group at the 5-position) connected via a propyl chain to a primary amine. This amine is part of a butyramide chain, which is further connected to a secondary amine. This secondary amine is attached to a chiral carbon atom (marked with a wedge bond) that also bears a hydroxyl group and a propyl chain. The terminal carbon of this propyl chain is part of a guanidino group (C(=NH2)NH2).</p>		30591646	
TM-MC 성분 ID	300834		
TM-MC 성분 동의어	N/A		
PubChem ID	132581143		
InChI Key	QFRQWDIAHCXRJU-INIZCTEOSA-N		
SMILES	NC(N)=NCCC[C@H](NC(=O)CCC(=O)NCCc1c[nH]c2ccc(O)cc12)C(O)=O		
Molecular Formula	C ₂₀ H ₂₈ N ₆ O ₅		
Molecular Weight	432.481	Exact Molecular Weight	432.212118026
LogP	-2.32	Topological Polar Surface Area	195.92 Å ²
Atom Count	59	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	7
Rotatable Bond Count	12	Aromatic Ring Count	2
Drug Likeness	0.11	Oral Bioavailability	N

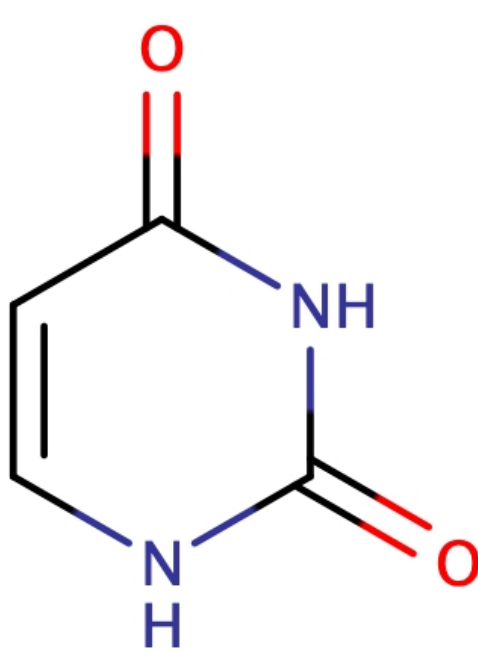
180. guanine

화학 구조		PubMed ID	
		23689025, 25335278 25422536, 30591646	
TM-MC 성분 ID	307		
TM-MC 성분 동의어	N/A		
PubChem ID	135398634		
InChI Key	UYTPUPDQBNUYGX-UHFFFAOYSA-N		
SMILES	<chem>Nc1nc2[nH]cnc2c(=O)[nH]1</chem>		
Molecular Formula	C ₅ H ₅ N ₅ O		
Molecular Weight	151.129	Exact Molecular Weight	151.049409801
LogP	-1.146	Topological Polar Surface Area	96.16 Å ²
Atom Count	16	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.44	Oral Bioavailability	Y

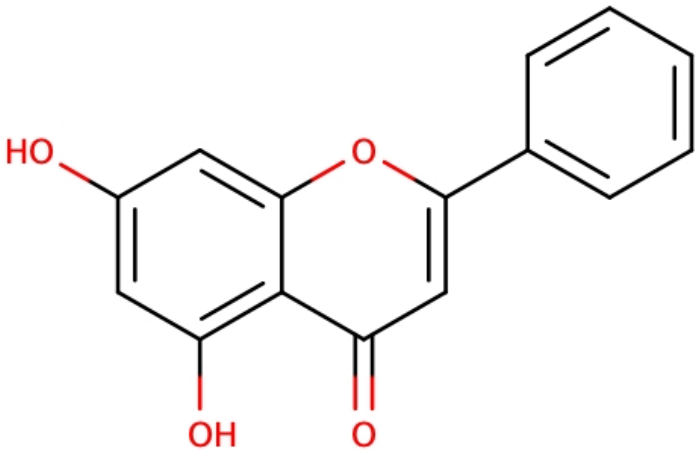
181. thymine

화학 구조		PubMed ID	
		23689025, 25335278 30591646	
TM-MC 성분 ID	310		
TM-MC 성분 동의어	5-methyluracil; 5-methyl uracil		
PubChem ID	1135		
InChI Key	RWQNBRDOKXIBIV-UHFFFAOYSA-N		
SMILES	<chem>Cc1c[nH]c(=O)[nH]c1=O</chem>		
Molecular Formula	C ₅ H ₆ N ₂ O ₂		
Molecular Weight	126.115	Exact Molecular Weight	126.042927441
LogP	-0.46	Topological Polar Surface Area	58.2 Å ²
Atom Count	15	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	1
Drug Likeness	0.49	Oral Bioavailability	Y

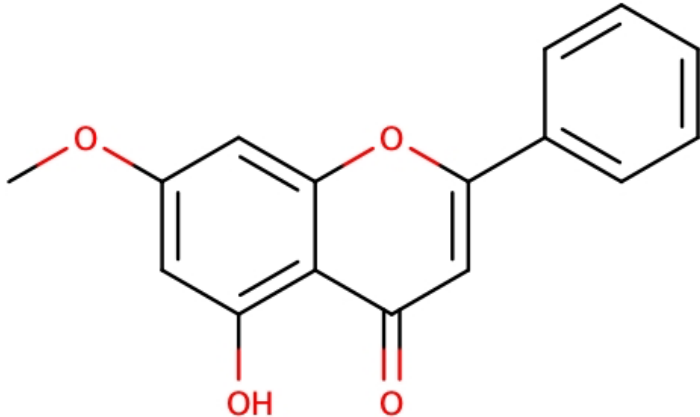
182. uracil

화학 구조		PubMed ID	
		<p>12575054, 15709383 23689025, 25335278 25422536, 30591646</p>	
TM-MC 성분 ID	312		
TM-MC 성분 동의어	2,4-dihydroxypyrimidine		
PubChem ID	1174		
InChI Key	ISAKRJDGNUQOIC-UHFFFAOYSA-N		
SMILES	<chem>O=c1cc[nH]c(=O)[nH]1</chem>		
Molecular Formula	C ₄ H ₄ N ₂ O ₂		
Molecular Weight	112.088	Exact Molecular Weight	112.027277377
LogP	-0.855	Topological Polar Surface Area	58.2 Å ²
Atom Count	12	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	1
Drug Likeness	0.46	Oral Bioavailability	Y

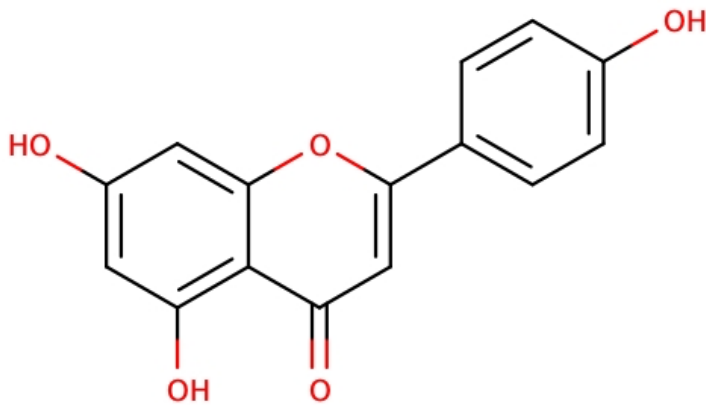
183. chrysin

화학 구조		PubMed ID	
		10898155, 12242799 15563208, 16621403 18257304, 18485465 19634328, 22026502 23176258, 23401705 23945741, 24128567 24882729, 24894633 25190186, 25802536 26059157, 26807704 27049854, 27123037 27329777, 28335972 28899513, 29724195 29738446, 29889351 30356413, 30965600 31227360, 31590214	
TM-MC 성분 ID	122		
TM-MC 성분 동의어	5,7-dihydroxy flavone; 5,7-flavonone		
PubChem ID	5281607		
InChI Key	RTIXKCRFFJGDFG-UHFFFAOYSA-N		
SMILES	<chem>Oc1cc(O)c2c(c1)oc(cc2=O)-c1cccc1</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₄		
Molecular Weight	254.241	Exact Molecular Weight	254.057908802
LogP	3.01	Topological Polar Surface Area	66.76 Å ²
Atom Count	29	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.70	Oral Bioavailability	Y

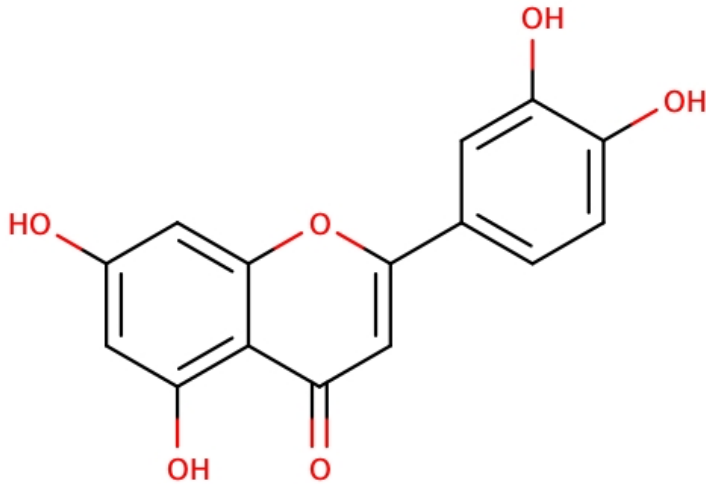
184. tectochrysin

화학 구조		PubMed ID	
		12242799, 15563208 16621403, 23176258	
TM-MC 성분 ID	123		
TM-MC 성분 동의어	chrysin-7-methyl ether; 5-hydroxy-7-methoxyflavone		
PubChem ID	5281954		
InChI Key	IRZVHDLBAYNPCT-UHFFFAOYSA-N		
SMILES	COc1cc(O)c2c(c1)oc(cc2=O)-c1ccccc1		
Molecular Formula	C ₁₆ H ₁₂ O ₄		
Molecular Weight	268.268	Exact Molecular Weight	268.073558866
LogP	3.156	Topological Polar Surface Area	55.76 Å ²
Atom Count	32	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.78	Oral Bioavailability	Y

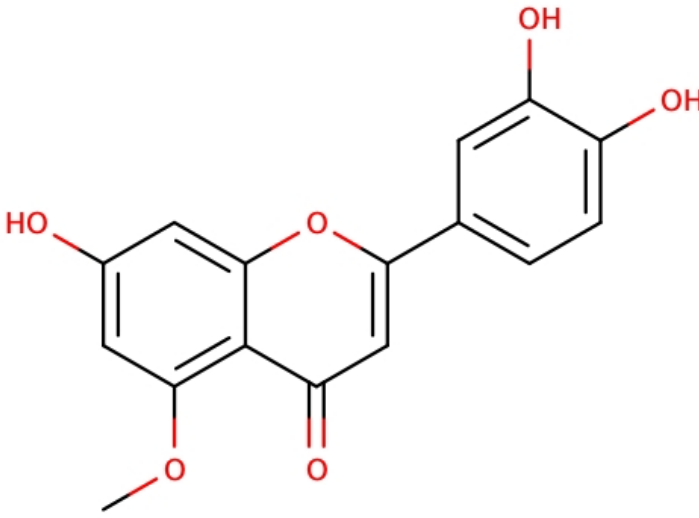
185. apigenin

화학 구조		PubMed ID	
		10898155, 15563208 16621403, 18257304 18485465, 22026502 23176258, 23401705 24128567, 24882729 24894633, 25190186 25802536, 26059157 26807704, 27049854 27123037, 28335972 28899513, 29724195 29738446, 29889351 30356413, 30965600 31227360	
TM-MC 성분 ID	124		
TM-MC 성분 동의어	5,7,4'-trihydroxyflavone		
PubChem ID	5280443		
InChI Key	KZNIFHPLKGYRTM-UHFFFAOYSA-N		
SMILES	<chem>Oc1ccc(cc1)-c1cc(=O)c2c(O)cc(O)cc2o1</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₅		
Molecular Weight	270.24	Exact Molecular Weight	270.052823422
LogP	2.707	Topological Polar Surface Area	86.99 Å ²
Atom Count	30	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.63	Oral Bioavailability	Y

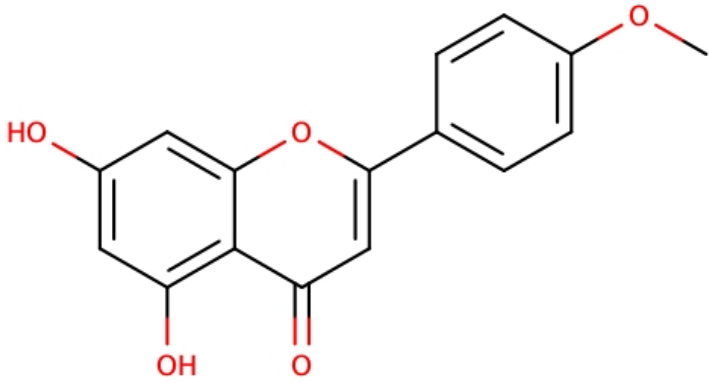
186. luteolin

화학 구조		PubMed ID	
		18485465, 22026502 25190186, 27049854 28899513, 29724195 29738446, 29889351 30356413, 31227360 31590214	
TM-MC 성분 ID	125		
TM-MC 성분 동의어	3',4',5,7-tetrahydroxyflavone; luteoline; 5,7,3',4'-tetrahydroxyflavone		
PubChem ID	5280445		
InChI Key	IQPNAANSBPBGFQ-UHFFFAOYSA-N		
SMILES	<chem>Oc1cc(O)c2c(c1)oc(cc2=O)-c1ccc(O)c(O)c1</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₆		
Molecular Weight	286.239	Exact Molecular Weight	286.047738042
LogP	2.403	Topological Polar Surface Area	107.22 Å ²
Atom Count	31	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.51	Oral Bioavailability	Y

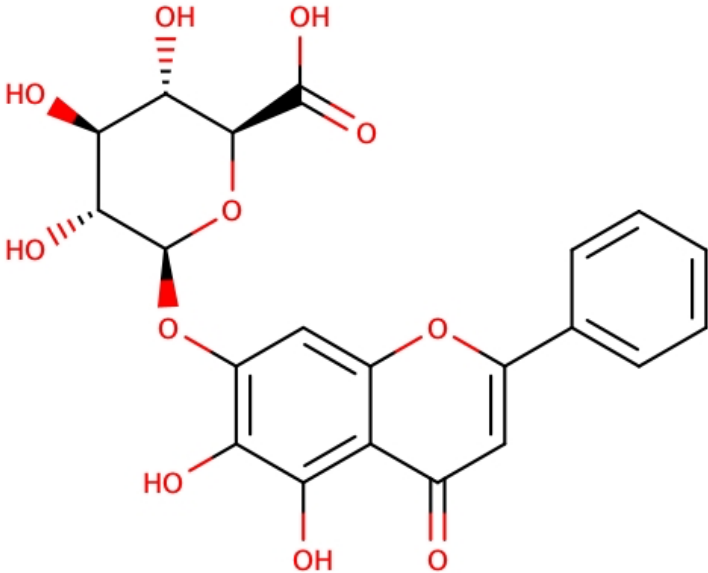
187. luteolin 5-methyl ether

화학 구조		PubMed ID	
		23176258	
TM-MC 성분 ID	126		
TM-MC 성분 동의어	N/A		
PubChem ID	13964550		
InChI Key	OZPMKAZMPNDLKX-UHFFFAOYSA-N		
SMILES	<chem>COc1cc(O)cc2oc(cc(=O)c12)-c1ccc(O)c(O)c1</chem>		
Molecular Formula	C ₁₆ H ₁₂ O ₆		
Molecular Weight	300.266	Exact Molecular Weight	300.063388106
LogP	1.899	Topological Polar Surface Area	96.22 Å ²
Atom Count	34	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.63	Oral Bioavailability	Y

188. acacetin

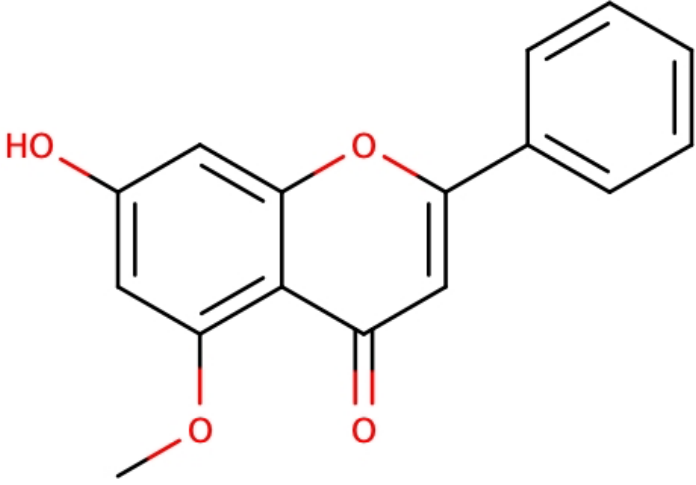
화학 구조		PubMed ID	
		18257304, 18485465 31590214	
TM-MC 성분 ID	127		
TM-MC 성분 동의어	4'-O-methyl-apigenin; 4'-O-methyl apigenin		
PubChem ID	5280442		
InChI Key	DANYIYRPLHHOCZ-UHFFFAOYSA-N		
SMILES	<chem>COc1ccc(cc1)-c1cc(=O)c2c(O)cc(O)cc2o1</chem>		
Molecular Formula	C ₁₆ H ₁₂ O ₅		
Molecular Weight	284.267	Exact Molecular Weight	284.068473486
LogP	2.853	Topological Polar Surface Area	75.99 Å ²
Atom Count	33	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.76	Oral Bioavailability	Y

189. baicalin

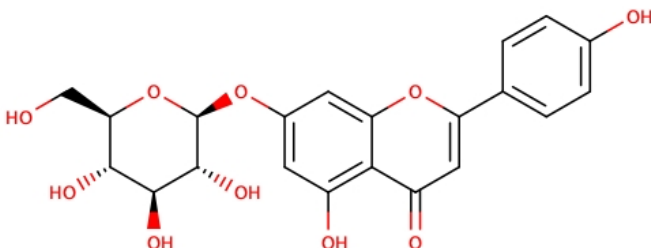
화학 구조	PubMed ID
	22026502, 29738446

TM-MC 성분 ID	128		
TM-MC 성분 동의어	baicalein-7-O-glucuronide; baicalein-7-glucuronide; baicalein 7-O-glucuronide; baicalein-7-O-glucuronic acid; 5,6,7-trihydroxyflavone-7-β-D-glucuronide		
PubChem ID	64982		
InChI Key	IKIIZLYTISPENI-ZFORQUDYSA-N		
SMILES	O[C@H]1[C@H](Oc2cc3oc(cc(=O)c3c(O)c2O)-c2ccccc2)O[C@@H]([C@@H](O)[C@H]1O)C(O)=O		
Molecular Formula	C ₂₁ H ₁₈ O ₁₁		
Molecular Weight	446.364	Exact Molecular Weight	446.0849114
LogP	0.759	Topological Polar Surface Area	183.21 Å ²
Atom Count	50	Structural Alert Count	1
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	4	Aromatic Ring Count	3
Drug Likeness	0.31	Oral Bioavailability	N

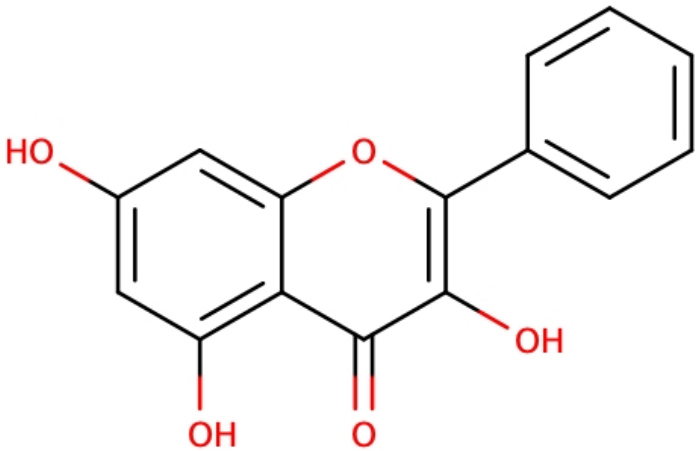
190. chrysin 5-methyl ether

화학 구조		PubMed ID	
		28335972, 31590214	
TM-MC 성분 ID	92464		
TM-MC 성분 동의어	chrysin-5-methyl-ether		
PubChem ID	5490127		
InChI Key	JVEMWXSMSUNXSD-UHFFFAOYSA-N		
SMILES	COc1cc(O)cc2oc(cc(=O)c12)-c1ccccc1		
Molecular Formula	C ₁₆ H ₁₂ O ₄		
Molecular Weight	268.268	Exact Molecular Weight	268.073558866
LogP	2.506	Topological Polar Surface Area	55.76 Å ²
Atom Count	32	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.78	Oral Bioavailability	Y

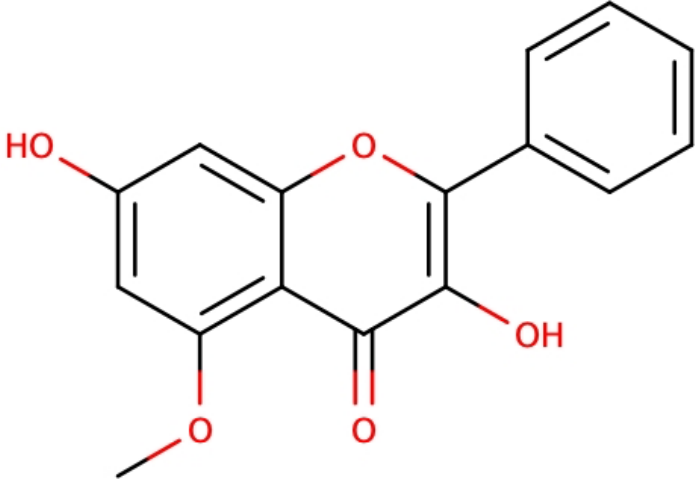
191. apigenin-7-O-glucoside

화학 구조		PubMed ID	
		31590214	
TM-MC 성분 ID	94465		
TM-MC 성분 동의어	apigenin-7-O-β-D-glucoside; apigenin-7-O-β-D-glucopyranoside; cosmosiin; apigenin 7-O-glucoside; apigenin-7-glucoside; apigetrin; apigenin-7-O-glycoside; apigenin-7-O-β-glucoside; apigenin 7-O-β-D-glucopyranoside; cyranoside; apigenin-7-O-glc; cosmos glycoside; apigenin 7-glucoside; apigenin 7-O-β-glucoside; apigenin-7-O-glucopyranoside		
PubChem ID	5280704		
InChI Key	KMOUJOKENFFTPU-QNDFHXLGSA-N		
SMILES	<chem>OC[C@H]1O[C@@H](Oc2cc(O)c3c(c2)oc(cc3=O)-c2ccc(O)cc2)[C@H](O)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₂₁ H ₂₀ O ₁₀		
Molecular Weight	432.381	Exact Molecular Weight	432.105646844
LogP	0.439	Topological Polar Surface Area	166.14 Å ²
Atom Count	51	Structural Alert Count	0
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	4	Aromatic Ring Count	3
Drug Likeness	0.34	Oral Bioavailability	N

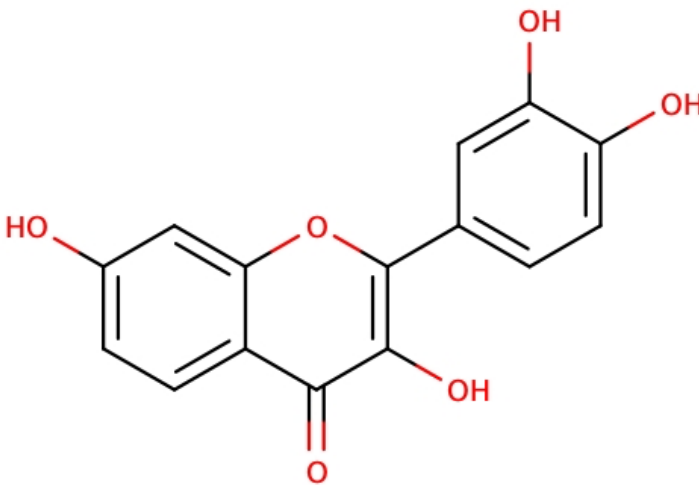
192. galangin

화학 구조		PubMed ID	
		10898155, 12242799 15563208, 16621403 17727062, 18257304 19634328, 23176258 23401705, 23945741 24128567, 24882729 24894633, 25802536 26059157, 26807704 27049854, 27123037 27329777, 28335972 28899513, 29337369 29724195, 29889351 30356413, 30965600 31227360, 31590214	
TM-MC 성분 ID	129		
TM-MC 성분 동의어	3,5,7-trihydroxyflavone		
PubChem ID	5281616		
InChI Key	VCCRNZQBSJXYJD-UHFFFAOYSA-N		
SMILES	<chem>Oc1cc(O)c2c(c1)oc(-c1cccc1)c(O)c2=O</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₅		
Molecular Weight	270.24	Exact Molecular Weight	270.052823422
LogP	2.763	Topological Polar Surface Area	86.99 Å ²
Atom Count	30	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.63	Oral Bioavailability	Y

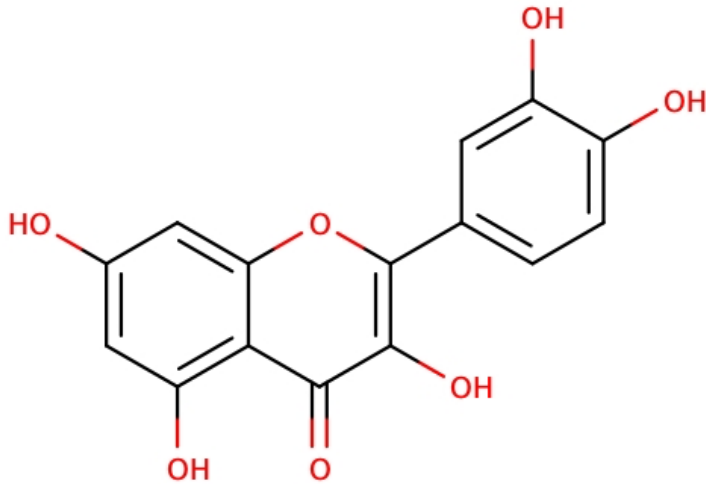
193. galangin-5-methyl ether

화학 구조		PubMed ID	
		23176258, 28335972 31590214	
TM-MC 성분 ID	130		
TM-MC 성분 동의어	galangin 5-methyl ether		
PubChem ID	5488105		
InChI Key	LDRJANCOJOKOPS-UHFFFAOYSA-N		
SMILES	COc1cc(O)cc2oc(-c3ccccc3)c(O)c(=O)c12		
Molecular Formula	C ₁₆ H ₁₂ O ₅		
Molecular Weight	284.267	Exact Molecular Weight	284.068473486
LogP	2.259	Topological Polar Surface Area	75.99 Å ²
Atom Count	33	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.75	Oral Bioavailability	Y

194. fisetin

화학 구조		PubMed ID	
		22026502	
TM-MC 성분 ID	131		
TM-MC 성분 동의어	N/A		
PubChem ID	5281614		
InChI Key	XHEFDIBZLXQHF-UHFFFAOYSA-N		
SMILES	<chem>Oc1ccc2c(c1)oc(-c1ccc(O)c(O)c1)c(O)c2=O</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₆		
Molecular Weight	286.239	Exact Molecular Weight	286.047738042
LogP	1.81	Topological Polar Surface Area	107.22 Å ²
Atom Count	31	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.51	Oral Bioavailability	Y

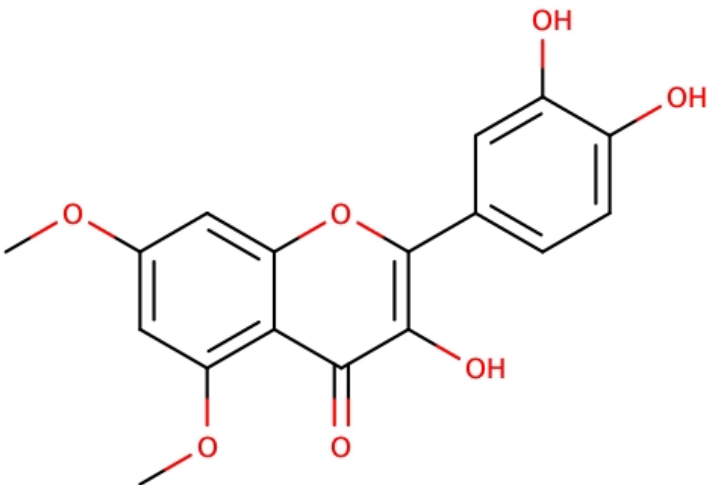
195. quercetin

화학 구조		PubMed ID	
		18257304, 22026502 22239430, 23176258 23401705, 24128567 24882729, 24894633 25190186, 26059157 27049854, 28335972 28899513, 29337369 29724195, 29738446 29880742, 29889351 30356413, 30965600 31227360, 31590214	
TM-MC 성분 ID	132		
TM-MC 성분 동의어	quercitin; quercetol; quceritin; meletin		
PubChem ID	5280343		
InChI Key	REFJWTPEDVJJIY-UHFFFAOYSA-N		
SMILES	<chem>Oc1cc(O)c2c(c1)oc(-c1ccc(O)c(O)c1)c(O)c2=O</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₇		
Molecular Weight	302.238	Exact Molecular Weight	302.042652662
LogP	2.156	Topological Polar Surface Area	127.45 Å ²
Atom Count	32	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	5
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.44	Oral Bioavailability	Y

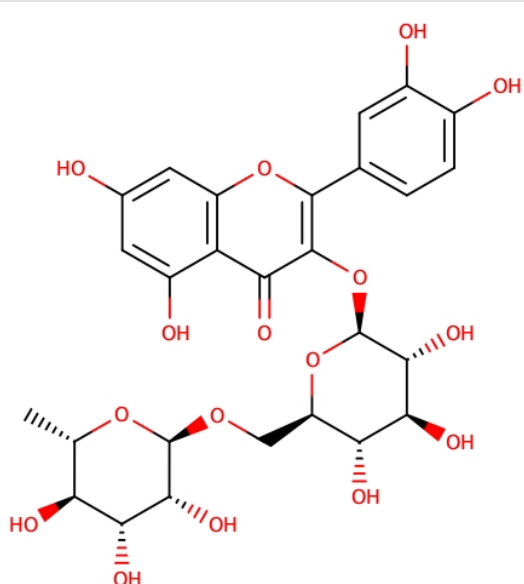
196. quercetin-3-methyl ether

화학 구조		PubMed ID	
		23176258, 28335972 31590214	
TM-MC 성분 ID	133		
TM-MC 성분 동의어	3-O-methylquercetin; quercetin-3-O-methyl; quercetin 3-methyl ether; quercetin-3-O-methyl ether		
PubChem ID	5280681		
InChI Key	WEPBGSIWZTEJR-UHFFFAOYSA-N		
SMILES	<chem>COc1c(oc2cc(O)cc(O)c2c1=O)-c1ccc(O)c(O)c1</chem>		
Molecular Formula	C ₁₆ H ₁₂ O ₇		
Molecular Weight	316.265	Exact Molecular Weight	316.058302726
LogP	2.269	Topological Polar Surface Area	116.45 Å ²
Atom Count	35	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.54	Oral Bioavailability	Y

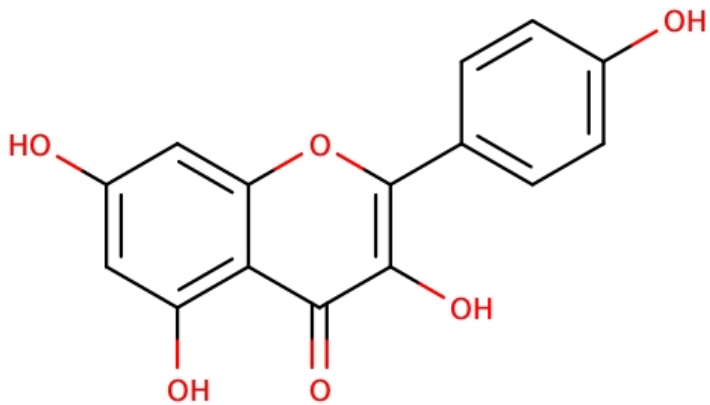
197. quercetin 5,7-dimethyl ether

화학 구조		PubMed ID	
		23176258	
TM-MC 성분 ID	134		
TM-MC 성분 동의어	N/A		
PubChem ID	26034		
InChI Key	FXGCMNIMMTVBFZ-UHFFFAOYSA-N		
SMILES	<chem>COc1cc(OC)c2c(c1)oc(-c1ccc(O)c(O)c1)c(O)c2=O</chem>		
Molecular Formula	C ₁₇ H ₁₄ O ₇		
Molecular Weight	330.292	Exact Molecular Weight	330.073952791
LogP	1.798	Topological Polar Surface Area	105.45 Å ²
Atom Count	38	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	3
Drug Likeness	0.63	Oral Bioavailability	Y

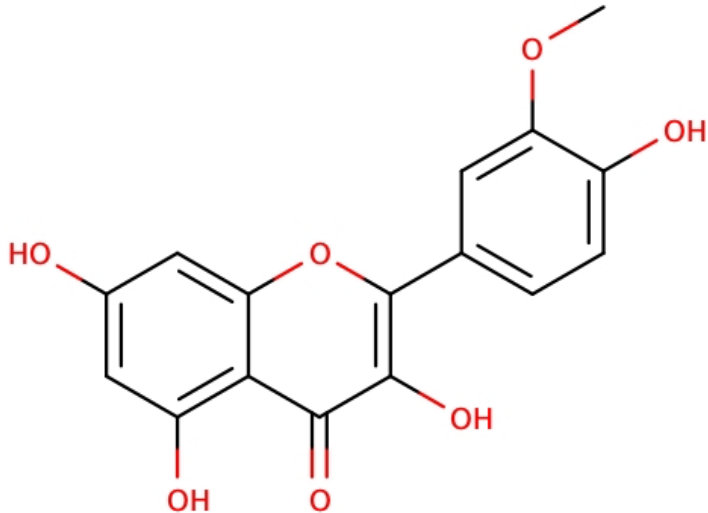
198. rutin

화학 구조		PubMed ID	
		<p>18257304, 22026502 23265456, 23401705 24128567, 26059157 28899513, 29337369 29738446, 29880742 31227360</p>	
TM-MC 성분 ID	135		
TM-MC 성분 동의어	<p>quercetin-3-O-rutinoside; quercetin 3-O-rutinoside; quercetin rutinoside; quercetin 3-rutinoside; quercetin 3-O-[6-O-(α-L-rhamnosyl)-β-D-glucoside]; quercetin 3-O-rhamnopyranosyl-(1->6)-glucopyranoside; quercetin-3-rutinoside; rutinoside; 3-O-[6-O-(α-L-rhamnosyl)-β-D-glucosyl]quercetin; 3-O-[6-O-(α-L-rhamnosyl)-β-D-glucosyl] quercetin; 3-O-(6''-O-(α-L-rhamnosyl)-β-D-glucosyl)quercetin; rutinum; quercetin-O-rutinoside; quercetin-3-O-rutinoside; quercetin-3-rhamnoglucoside; quercetin 3-O-β-D-rutinoside; quercetin-3-O-glucorhamnoside; quercetin-3-O-rhamnosylglucoside; quercetin-3-O-[α-L-rhamnosyl(1->6)]-β-D-glucoside; 3-O-β-D-glucopyranosyl (6->1)-α-L-rhamnosyl quercetin; quercetin 3-O-α-L-rhamnopyranosyl(1->6)-β-D-glucopyranoside</p>		
PubChem ID	5280805		
InChI Key	IKGXIBQEMLURG-NVPNHPEKSA-N		
SMILES	<chem>C[C@@H]1O[C@@H](OC[C@H]2O[C@@H](Oc3c(oc4cc(O)cc(O)c4c3=O)-c3ccc(O)c(O)c3)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O</chem>		
Molecular Formula	C ₂₇ H ₃₀ O ₁₆		
Molecular Weight	610.521	Exact Molecular Weight	610.153384886
LogP	-0.869	Topological Polar Surface Area	265.52 Å ²
Atom Count	73	Structural Alert Count	1
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	10
Rotatable Bond Count	6	Aromatic Ring Count	3
Drug Likeness	0.15	Oral Bioavailability	N

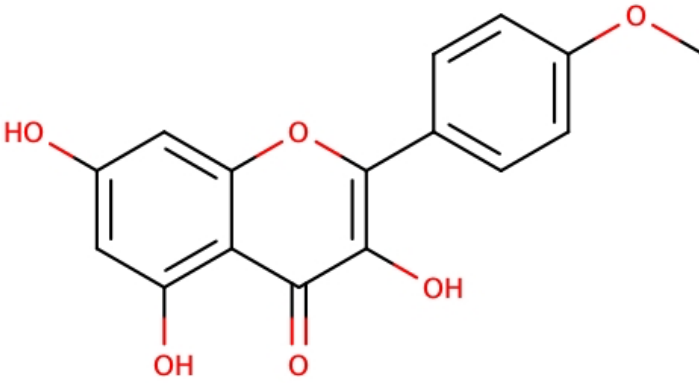
199. kaempferol

화학 구조		PubMed ID	
		15563208, 16621403 18257304, 18485465 22026502, 23401705 24128567, 24882729 24894633, 26059157 27049854, 28335972 28899513, 29337369 29724195, 29738446 29880742, 29889351 30356413, 30691151 30965600, 31227360 31590214	
TM-MC 성분 ID	136		
TM-MC 성분 동의어	kaemferol; kampferol; isotein; campherol; kaempherol; kaempferal		
PubChem ID	5280863		
InChI Key	IYRMWMYZSQPKC-UHFFFAOYSA-N		
SMILES	<chem>Oc1ccc(cc1)-c1oc2cc(O)cc(O)c2c(=O)c1O</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₆		
Molecular Weight	286.239	Exact Molecular Weight	286.047738042
LogP	2.46	Topological Polar Surface Area	107.22 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.55	Oral Bioavailability	Y

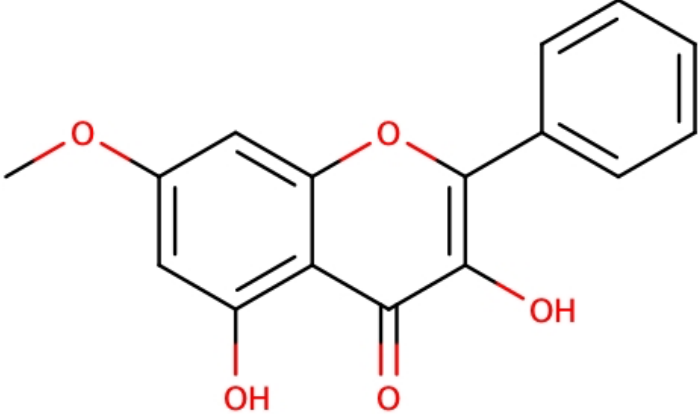
200. isorhamnetin

화학 구조		PubMed ID	
		22026502, 23176258 29738446, 31590214	
TM-MC 성분 ID	137		
TM-MC 성분 동의어	isorhamntin; isorhmnetin; isorhamnetine; 3-methoxyquercetin; 3',5,7,4-tetrahydroxy-3-methoxyflavon		
PubChem ID	5281654		
InChI Key	IZQSVBPOUDKVDZ-UHFFFAOYSA-N		
SMILES	<chem>COc1cc(ccc1O)-c1oc2cc(O)cc(O)c2c(=O)c1O</chem>		
Molecular Formula	C ₁₆ H ₁₂ O ₇		
Molecular Weight	316.265	Exact Molecular Weight	316.058302726
LogP	2.302	Topological Polar Surface Area	116.45 Å ²
Atom Count	35	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.57	Oral Bioavailability	Y

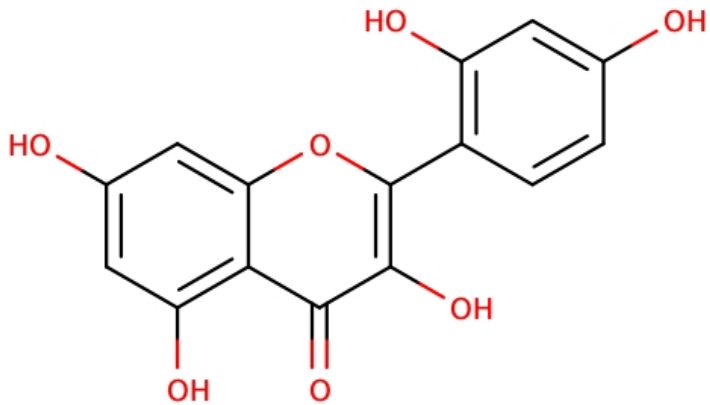
201. kaempferide

화학 구조		PubMed ID	
		25190186	
TM-MC 성분 ID	138		
TM-MC 성분 동의어	dihydroxymethoxyflavone; kampferide; 4'-methylkaempferol; 3,5,7-trihydroxy-4'-methoxyflavone; 5,7,3-trihydroxy-4'-methoxy flavone		
PubChem ID	5281666		
InChI Key	SQFSKOYWJBQGKQ-UHFFFAOYSA-N		
SMILES	COc1ccc(cc1)-c1oc2cc(O)cc(O)c2c(=O)c1O		
Molecular Formula	C ₁₆ H ₁₂ O ₆		
Molecular Weight	300.266	Exact Molecular Weight	300.063388106
LogP	2.606	Topological Polar Surface Area	96.22 Å ²
Atom Count	34	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.67	Oral Bioavailability	Y

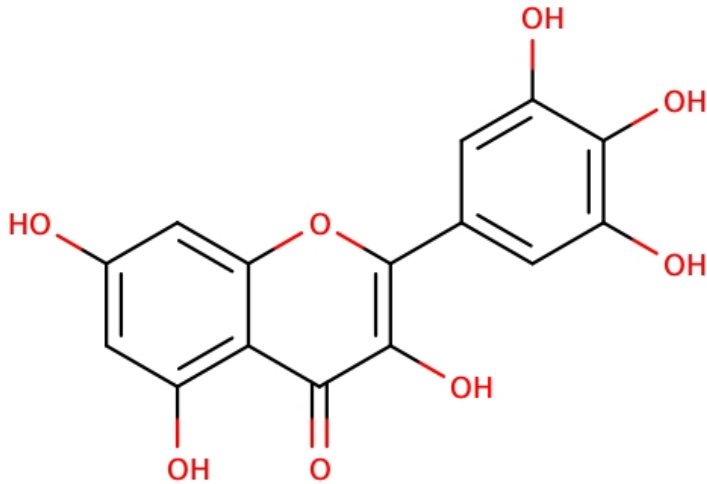
202. izalpinin

화학 구조		PubMed ID	
		12242799	
TM-MC 성분 ID	139		
TM-MC 성분 동의어	3,5-dihydroxy-7-methoxyflavone		
PubChem ID	5318691		
InChI Key	PVJNLMXWZXXHSZ-UHFFFAOYSA-N		
SMILES	<chem>COc1cc(O)c2c(c1)oc(-c1ccccc1)c(O)c2=O</chem>		
Molecular Formula	C ₁₆ H ₁₂ O ₅		
Molecular Weight	284.267	Exact Molecular Weight	284.068473486
LogP	2.909	Topological Polar Surface Area	75.99 Å ²
Atom Count	33	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.76	Oral Bioavailability	Y

203. morin

화학 구조		PubMed ID	
		18257304, 22026502 24128567, 25190186	
TM-MC 성분 ID	140		
TM-MC 성분 동의어	moric acid		
PubChem ID	5281670		
InChI Key	YXOLAZRVSSWPPT-UHFFFAOYSA-N		
SMILES	<chem>Oc1ccc(c(O)c1)-c1oc2cc(O)cc(O)c2c(=O)c1O</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₇		
Molecular Weight	302.238	Exact Molecular Weight	302.042652662
LogP	2.156	Topological Polar Surface Area	127.45 Å ²
Atom Count	32	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	5
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.47	Oral Bioavailability	Y

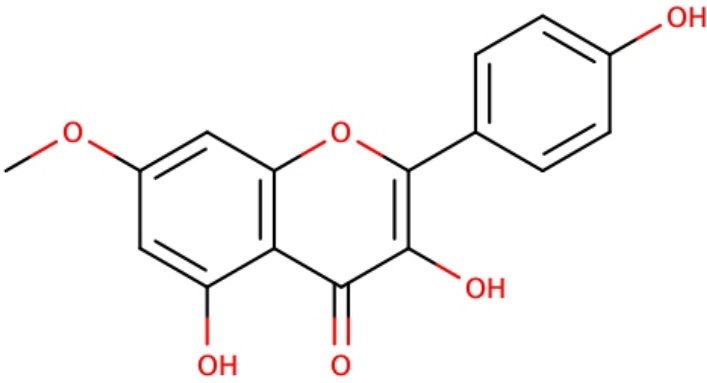
204. myricetin

화학 구조		PubMed ID	
		18257304, 22026502 23401705, 24128567 26059157, 28899513 29738446, 31227360	
TM-MC 성분 ID	141		
TM-MC 성분 동의어	N/A		
PubChem ID	5281672		
InChI Key	IKMDFBPHZJCSN-UHFFFAOYSA-N		
SMILES	<chem>Oc1cc(O)c2c(c1)oc(-c1cc(O)c(O)c(O)c1)c(O)c2=O</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₈		
Molecular Weight	318.237	Exact Molecular Weight	318.037567282
LogP	1.853	Topological Polar Surface Area	147.68 Å ²
Atom Count	33	Structural Alert Count	1
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	6
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.37	Oral Bioavailability	N

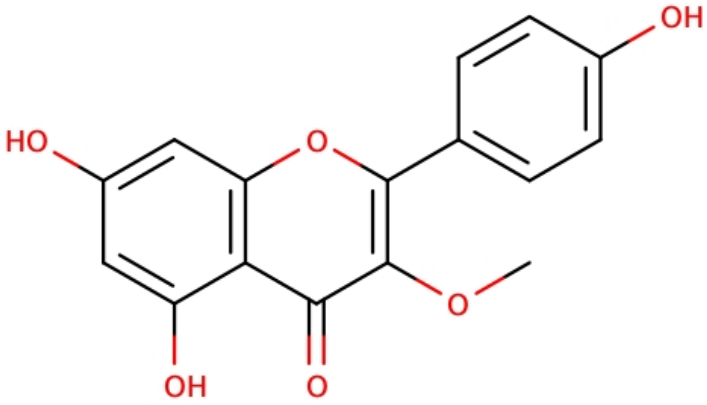
205. rhamnetin

화학 구조		PubMed ID	
		28335972	
TM-MC 성분 ID	91995		
TM-MC 성분 동의어	3',3,4',5-tetrahydroxy-7-methoxyflavone; quercetin-7-methyl ether		
PubChem ID	5281691		
InChI Key	JGUZGNYPMHHRK-UHFFFAOYSA-N		
SMILES	<chem>COc1cc(O)c2c(c1)oc(-c1ccc(O)c(O)c1)c(O)c2=O</chem>		
Molecular Formula	C ₁₆ H ₁₂ O ₇		
Molecular Weight	316.265	Exact Molecular Weight	316.058302726
LogP	2.302	Topological Polar Surface Area	116.45 Å ²
Atom Count	35	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.54	Oral Bioavailability	Y

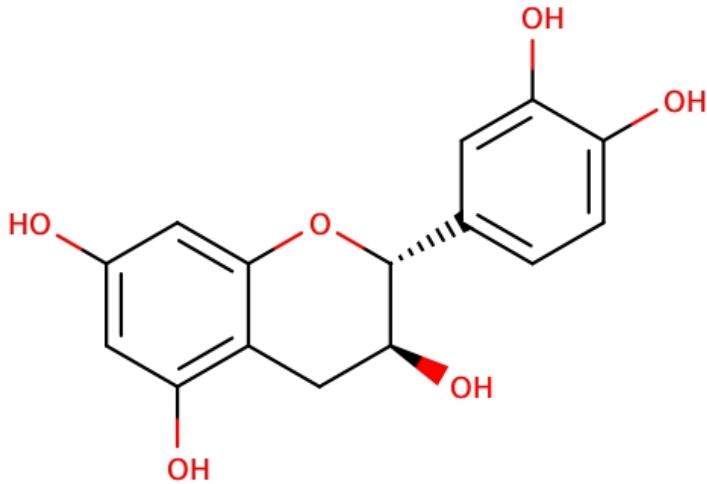
206. rhamnocitrin

화학 구조		PubMed ID	
		31590214	
TM-MC 성분 ID	94382		
TM-MC 성분 동의어	3-hydroxyl-genkwanin; kaempferol-7-methyl ether		
PubChem ID	5320946		
InChI Key	MQSZRBPYXNEFHF-UHFFFAOYSA-N		
SMILES	COc1cc(O)c2c(c1)oc(-c1ccc(O)cc1)c(O)c2=O		
Molecular Formula	C ₁₆ H ₁₂ O ₆		
Molecular Weight	300.266	Exact Molecular Weight	300.063388106
LogP	2.606	Topological Polar Surface Area	96.22 Å ²
Atom Count	34	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.67	Oral Bioavailability	Y

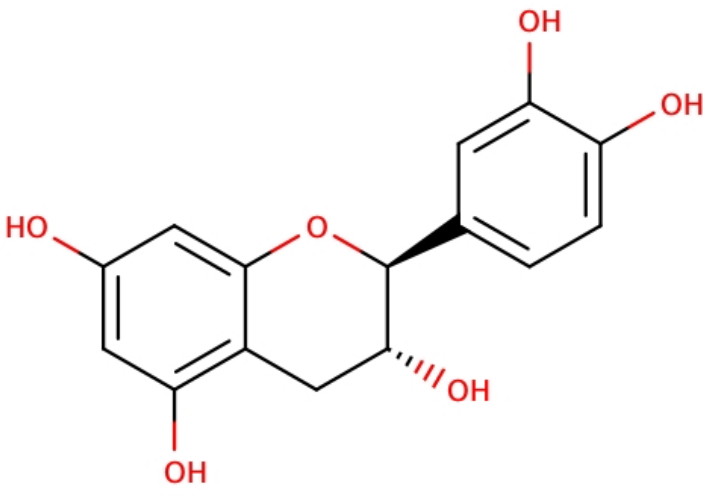
207. 3-methylkaempferol

화학 구조		PubMed ID	
		31590214	
TM-MC 성분 ID	280862		
TM-MC 성분 동의어	isokaempferide; kaempferol 3-methyl ether; kaempferol-3-methyl ether; kaempferol-3-O-methyl ether; kaempferol 3-O-methyl ether		
PubChem ID	5280862		
InChI Key	VJJZBUCDWKPLC-UHFFFAOYSA-N		
SMILES	COc1c(oc2cc(O)cc(O)c2c1=O)-c1ccc(O)cc1		
Molecular Formula	C ₁₆ H ₁₂ O ₆		
Molecular Weight	300.266	Exact Molecular Weight	300.063388106
LogP	2.573	Topological Polar Surface Area	96.22 Å ²
Atom Count	34	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.67	Oral Bioavailability	Y

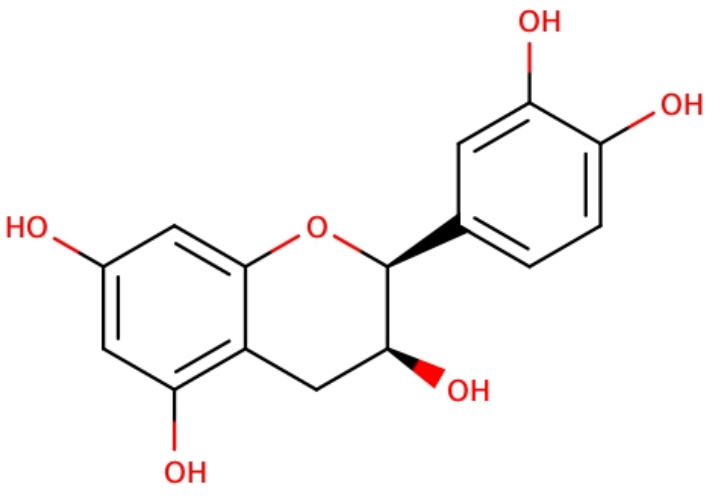
208. catechin

화학 구조		PubMed ID	
		22026502, 22239430	
TM-MC 성분 ID	156		
TM-MC 성분 동의어	(+)-catechin; D-catechin; cianidanol; (+/-)-catechin		
PubChem ID	9064		
InChI Key	PFTAWBLQPZVEMU-DZGCQCFKSA-N		
SMILES	O[C@H]1Cc2c(O)cc(O)cc2O[C@@H]1c1ccc(O)c(O)c1		
Molecular Formula	C ₁₅ H ₁₄ O ₆		
Molecular Weight	290.271	Exact Molecular Weight	290.079038171
LogP	1.795	Topological Polar Surface Area	110.38 Å ²
Atom Count	35	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	5
Rotatable Bond Count	1	Aromatic Ring Count	2
Drug Likeness	0.51	Oral Bioavailability	Y

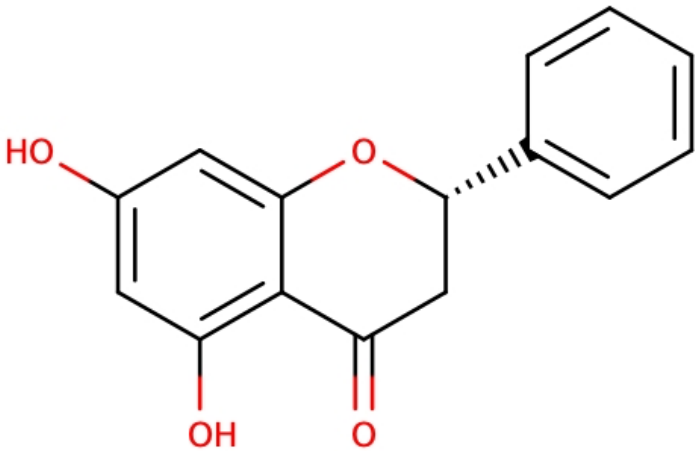
209. α -catechin

화학 구조		PubMed ID	
		22026502	
TM-MC 성분 ID	15611		
TM-MC 성분 동의어	(-)-catechin		
PubChem ID	73160		
InChI Key	PFTAWBLQPZVEMU-HIFRSBDPSA-N		
SMILES	<chem>O[C@@H]1Cc2c(O)cc(O)cc2O[C@H]1c1ccc(O)c(O)c1</chem>		
Molecular Formula	C ₁₅ H ₁₄ O ₆		
Molecular Weight	290.271	Exact Molecular Weight	290.079038171
LogP	1.795	Topological Polar Surface Area	110.38 Å ²
Atom Count	35	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	5
Rotatable Bond Count	1	Aromatic Ring Count	2
Drug Likeness	0.51	Oral Bioavailability	Y

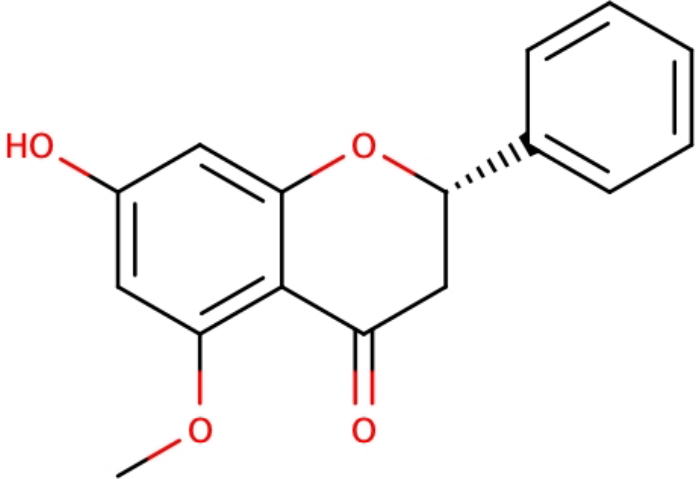
210. epicatechin

화학 구조		PubMed ID	
		22026502	
TM-MC 성분 ID	15620		
TM-MC 성분 동의어	(+)-epicatechin; (epi)catechin		
PubChem ID	182232		
InChI Key	PFTAWBLQPZVEMU-ZFWWWQNUSA-N		
SMILES	<chem>O[C@H]1Cc2c(O)cc(O)cc2O[C@H]1c1ccc(O)c(O)c1</chem>		
Molecular Formula	C ₁₅ H ₁₄ O ₆		
Molecular Weight	290.271	Exact Molecular Weight	290.079038171
LogP	1.795	Topological Polar Surface Area	110.38 Å ²
Atom Count	35	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	5
Rotatable Bond Count	1	Aromatic Ring Count	2
Drug Likeness	0.51	Oral Bioavailability	Y

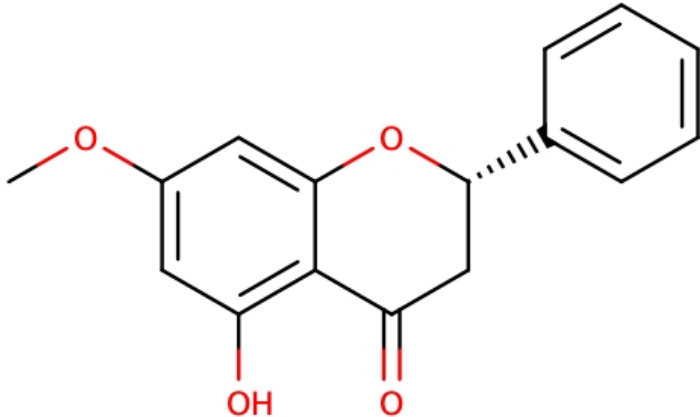
211. pinocembrin

화학 구조		PubMed ID	
		10898155, 12242799 15563208, 16621403 18257304, 19634328 22026502, 22978445 23176258, 23401705 24128567, 24882729 24894633, 25802536 26059157, 26807704 27049854, 27123037 27329777, 28335972 28899513, 29724195 29738446, 29889351 30356413, 30965600 31227360, 31590214	
TM-MC 성분 ID	142		
TM-MC 성분 동의어	(2S)-5,7-dihydroxy-dihydroflavone; pinocembrine; pinocernbrin; (2S)-pinocembrin		
PubChem ID	68071		
InChI Key	URFCJEUYNNAHFI-ZDUSSCGKSA-N		
SMILES	<chem>Oc1cc(O)c2C(=O)C[C@H](Oc2c1)c1cccc1</chem>		
Molecular Formula	C ₁₅ H ₁₂ O ₄		
Molecular Weight	256.257	Exact Molecular Weight	256.073558866
LogP	3.139	Topological Polar Surface Area	66.76 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	2
Drug Likeness	0.82	Oral Bioavailability	Y

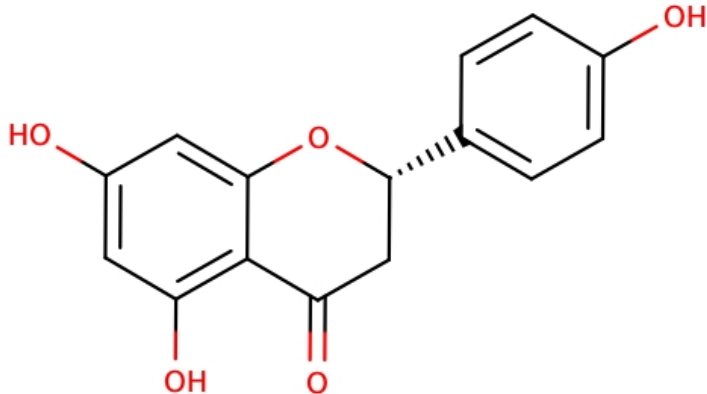
212. alpinetin

화학 구조		PubMed ID	
		23176258, 31590214	
TM-MC 성분 ID	143		
TM-MC 성분 동의어	pinocembrin 5-methyl ether; 7-hydroxy-5-methoxyflavanone; 7-hydroxy-5-methoxyflavanone		
PubChem ID	154279		
InChI Key	QQQCWVDPMPFUGF-ZDUSSCGKSA-N		
SMILES	COc1cc(O)cc2O[C@@H](CC(=O)c12)c1ccccc1		
Molecular Formula	C ₁₆ H ₁₄ O ₄		
Molecular Weight	270.284	Exact Molecular Weight	270.089208931
LogP	2.635	Topological Polar Surface Area	55.76 Å ²
Atom Count	34	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.91	Oral Bioavailability	Y

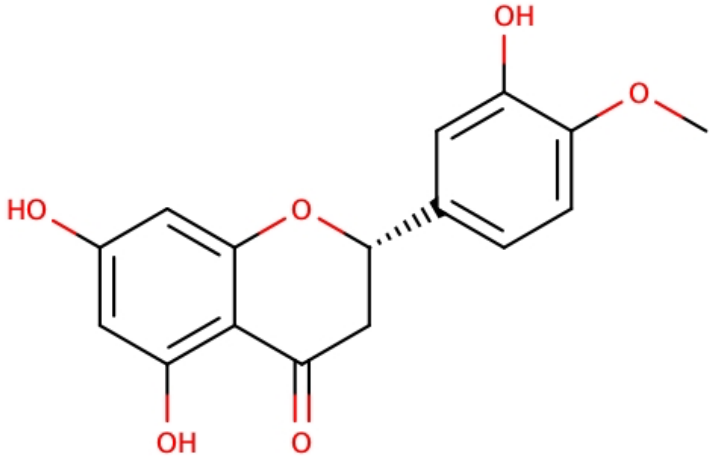
213. pinostrobin

화학 구조		PubMed ID	
		12242799, 23176258	
TM-MC 성분 ID	144		
TM-MC 성분 동의어	pinocembrin 7-methyl ether; (S)-2,3-dihydro-5-hydroxy-7-methoxy-2-phenyl-4H-1-benzopyran-4-one		
PubChem ID	73201		
InChI Key	ORJDDOBAOGKRJV-AWEZLNQCLSA-N		
SMILES	<chem>COc1cc(O)c2C(=O)C[C@H](Oc2c1)c1ccccc1</chem>		
Molecular Formula	C ₁₆ H ₁₄ O ₄		
Molecular Weight	270.284	Exact Molecular Weight	270.089208931
LogP	3.285	Topological Polar Surface Area	55.76 Å ²
Atom Count	34	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.91	Oral Bioavailability	Y

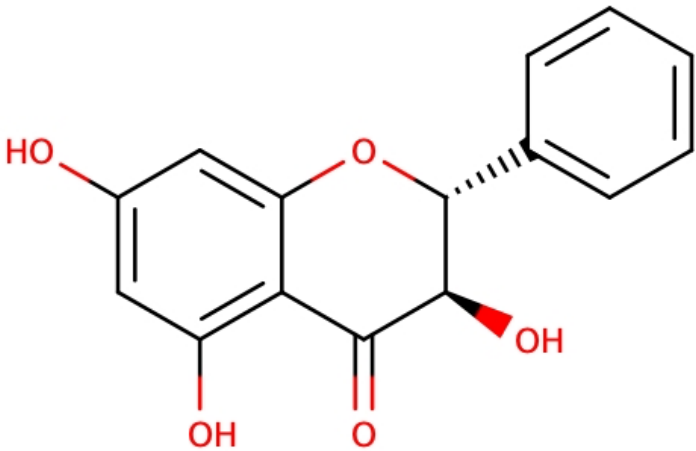
214. naringenin

화학 구조		PubMed ID	
		10898155, 22026502 24128567, 24894633 27049854, 28899513 29738446, 30965600	
TM-MC 성분 ID	154		
TM-MC 성분 동의어	5,7,4'-trihydroxy flavanone; narigenin; (2S)-naringenin		
PubChem ID	439246		
InChI Key	FTVWIRXFELQLPI-ZDUSSCGKSA-N		
SMILES	<chem>Oc1ccc(cc1)[C@@H]1CC(=O)c2c(O)cc(O)cc2O1</chem>		
Molecular Formula	C ₁₅ H ₁₂ O ₅		
Molecular Weight	272.256	Exact Molecular Weight	272.068473486
LogP	2.835	Topological Polar Surface Area	86.99 Å ²
Atom Count	32	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	2
Drug Likeness	0.74	Oral Bioavailability	Y

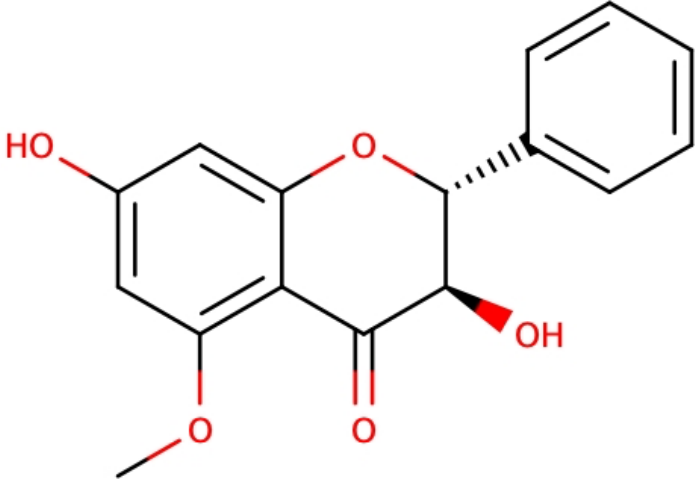
215. hesperetin

화학 구조		PubMed ID	
		15158983, 29738446 29889351	
TM-MC 성분 ID	155		
TM-MC 성분 동의어	hesperetin		
PubChem ID	72281		
InChI Key	AIONOLUJZLIMTK-AWEZNLQCLSA-N		
SMILES	<chem>COc1ccc(cc1O)[C@@H]1CC(=O)c2c(O)cc(O)cc2O1</chem>		
Molecular Formula	C ₁₆ H ₁₄ O ₆		
Molecular Weight	302.282	Exact Molecular Weight	302.079038171
LogP	2.677	Topological Polar Surface Area	96.22 Å ²
Atom Count	36	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.79	Oral Bioavailability	Y

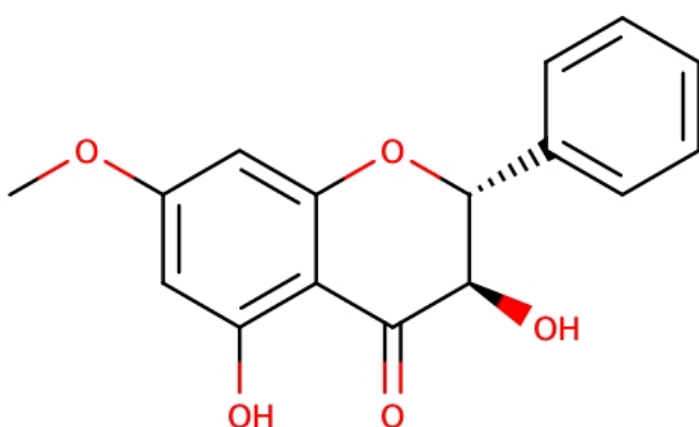
216. pinobanksin

화학 구조		PubMed ID	
		15563208, 16621403 23176258, 24894633 26807704, 27049854 27123037, 27329777 28335972, 28899513 29724195, 29889351 30356413, 30965600 31590214	
TM-MC 성분 ID	145		
TM-MC 성분 동의어	N/A		
PubChem ID	73202		
InChI Key	SUYJZKRQHBQNCA-LSDHAIUSA-N		
SMILES	O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1cccc1		
Molecular Formula	C ₁₅ H ₁₂ O ₅		
Molecular Weight	272.256	Exact Molecular Weight	272.068473486
LogP	2.424	Topological Polar Surface Area	86.99 Å ²
Atom Count	32	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	2
Drug Likeness	0.74	Oral Bioavailability	Y

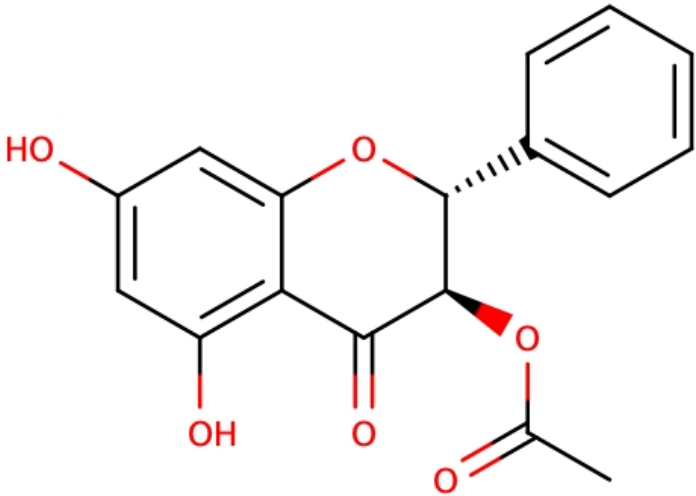
217. pinobanksin 5-methyl ether

화학 구조		PubMed ID	
		15563208, 16621403 19634328, 23176258 28335972, 31590214	
TM-MC 성분 ID	146		
TM-MC 성분 동의어	pinobanksin-5-methyl ether		
PubChem ID	147459		
InChI Key	NIMIDMFTGGTHOH-JKSUJKDBSA-N		
SMILES	<chem>COc1cc(O)cc2O[C@@H]([C@@H](O)C(=O)c12)c1cccc1</chem>		
Molecular Formula	C ₁₆ H ₁₄ O ₅		
Molecular Weight	286.283	Exact Molecular Weight	286.084123551
LogP	1.919	Topological Polar Surface Area	75.99 Å ²
Atom Count	35	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.88	Oral Bioavailability	Y

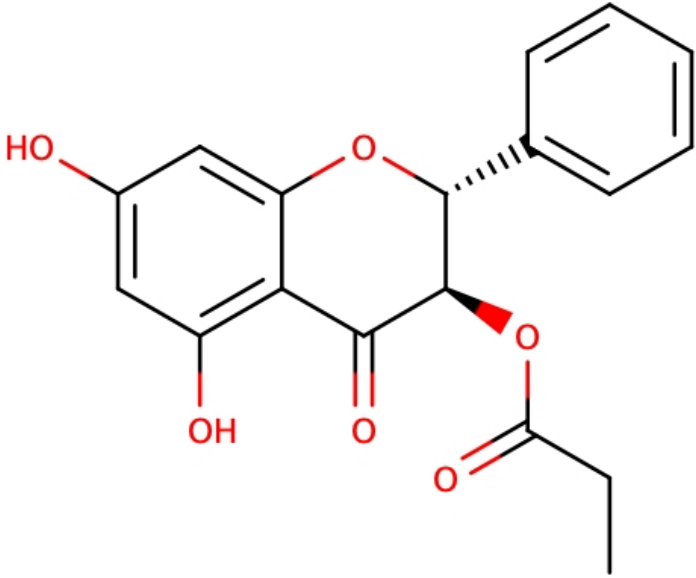
218. pinobanksin 7-methyl ether

화학 구조		PubMed ID	
		22978445, 23176258	
TM-MC 성분 ID	147		
TM-MC 성분 동의어	N/A		
PubChem ID	46883390		
InChI Key	QPOCKDYXXFOBCM-JKSUJKDBSA-N		
SMILES	COc1cc(O)c2C(=O)[C@H](O)[C@H](Oc2c1)c1cccc1		
Molecular Formula	C ₁₆ H ₁₄ O ₅		
Molecular Weight	286.283	Exact Molecular Weight	286.084123551
LogP	2.569	Topological Polar Surface Area	75.99 Å ²
Atom Count	35	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.89	Oral Bioavailability	Y

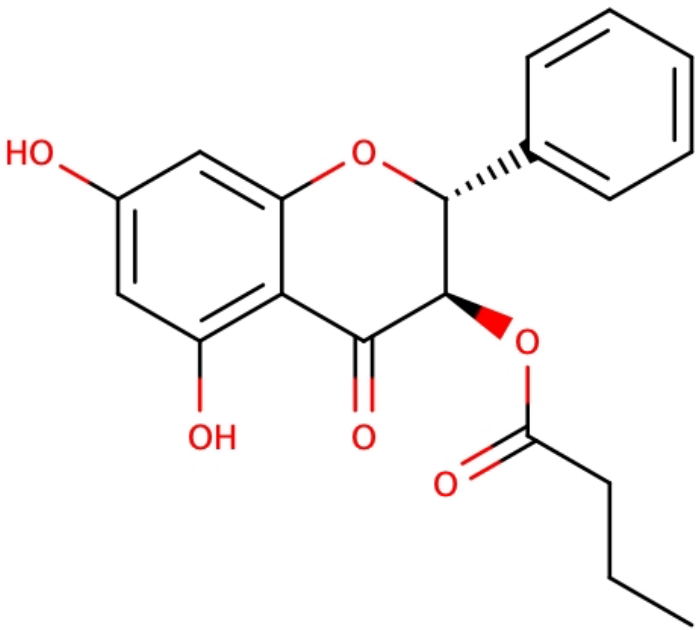
219. 3-O-acetylpinobanksin

화학 구조		PubMed ID	
		15563208, 16621403 18485465, 23176258 24894633, 27049854 27329777, 28335972 28899513, 29889351 30965600, 31590214	
TM-MC 성분 ID	148		
TM-MC 성분 동의어	pinobanksin 3-O-acetate; pinobanksin-3-O-acetate; 3-O-acetyl pinobanksin		
PubChem ID	148556		
InChI Key	BJYHZSNSMVEQEH-SJORKVTESA-N		
SMILES	<chem>CC(=O)O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1cccc1</chem>		
Molecular Formula	C ₁₇ H ₁₄ O ₆		
Molecular Weight	314.293	Exact Molecular Weight	314.079038171
LogP	2.865	Topological Polar Surface Area	93.06 Å ²
Atom Count	37	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.85	Oral Bioavailability	Y

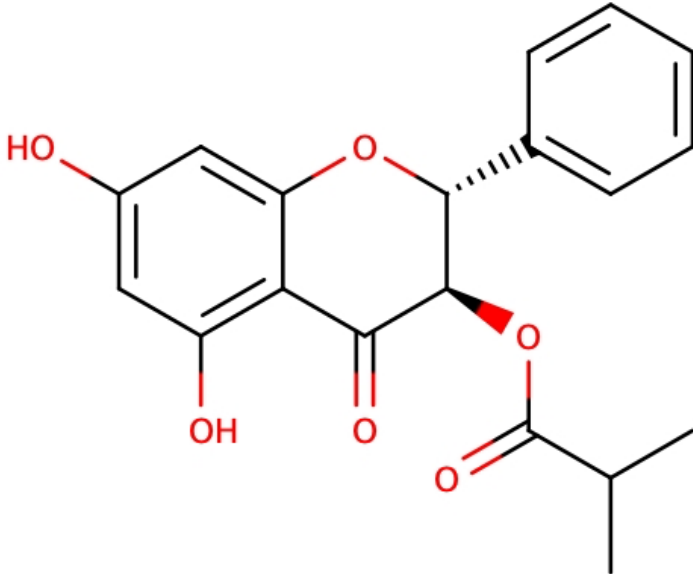
220. pinobanksin-3-O-propionate

화학 구조		PubMed ID	
		23176258, 31590214	
TM-MC 성분 ID	149		
TM-MC 성분 동의어	pinobanksin 3-O-propionate		
PubChem ID	46886755		
InChI Key	LIVRDRUFOJECRK-MSOLQXFVSA-N		
SMILES	CCC(=O)O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1cccc1		
Molecular Formula	C ₁₈ H ₁₆ O ₆		
Molecular Weight	328.32	Exact Molecular Weight	328.094688235
LogP	3.565	Topological Polar Surface Area	93.06 Å ²
Atom Count	40	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.84	Oral Bioavailability	Y

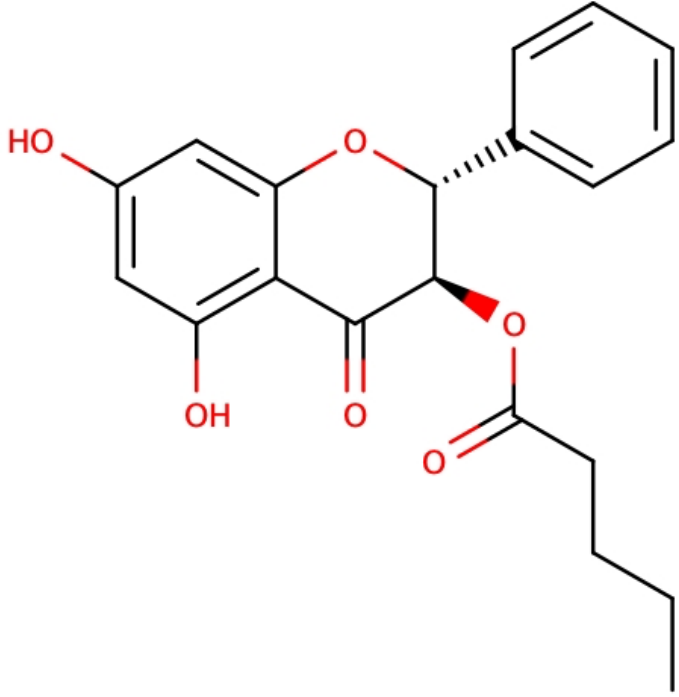
221. pinobanksin-3-O-butyrate

화학 구조		PubMed ID	
		23176258, 31590214	
TM-MC 성분 ID	150		
TM-MC 성분 동의어	pinobanksin 3-O-butyrate		
PubChem ID	163043808		
InChI Key	VOPFBLHVYNHXHX-MOPGFXCFS-A-N		
SMILES	CCCC(=O)O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1cccc1		
Molecular Formula	C ₁₉ H ₁₈ O ₆		
Molecular Weight	342.347	Exact Molecular Weight	342.1103383
LogP	4.01	Topological Polar Surface Area	93.06 Å ²
Atom Count	43	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	5	Aromatic Ring Count	2
Drug Likeness	0.80	Oral Bioavailability	Y

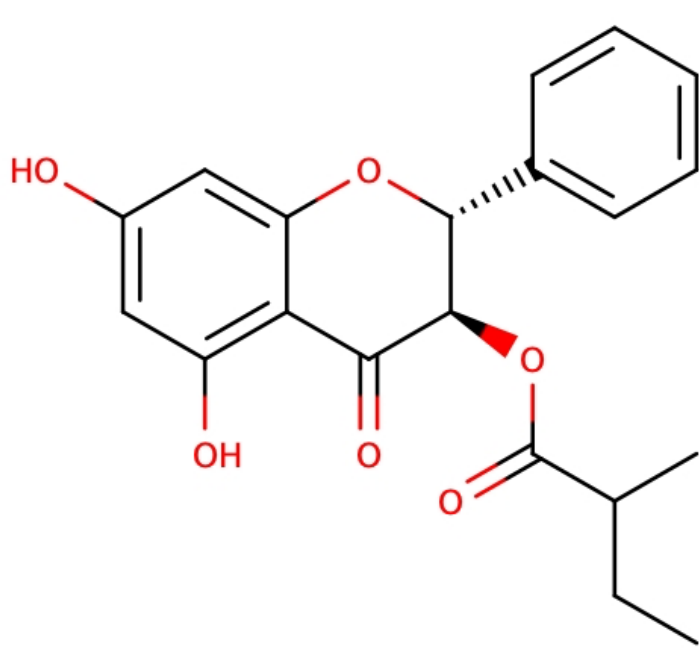
222. pinobanksin 3-O-isobutyrate

화학 구조		PubMed ID	
		23176258	
TM-MC 성분 ID	151		
TM-MC 성분 동의어	N/A		
PubChem ID	46886756		
InChI Key	JNCYKKGPRMPXLQ-MSOLQXFVSA-N		
SMILES	CC(C)C(=O)O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1cccc1		
Molecular Formula	C ₁₉ H ₁₈ O ₆		
Molecular Weight	342.347	Exact Molecular Weight	342.1103383
LogP	4.108	Topological Polar Surface Area	93.06 Å ²
Atom Count	43	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.82	Oral Bioavailability	Y

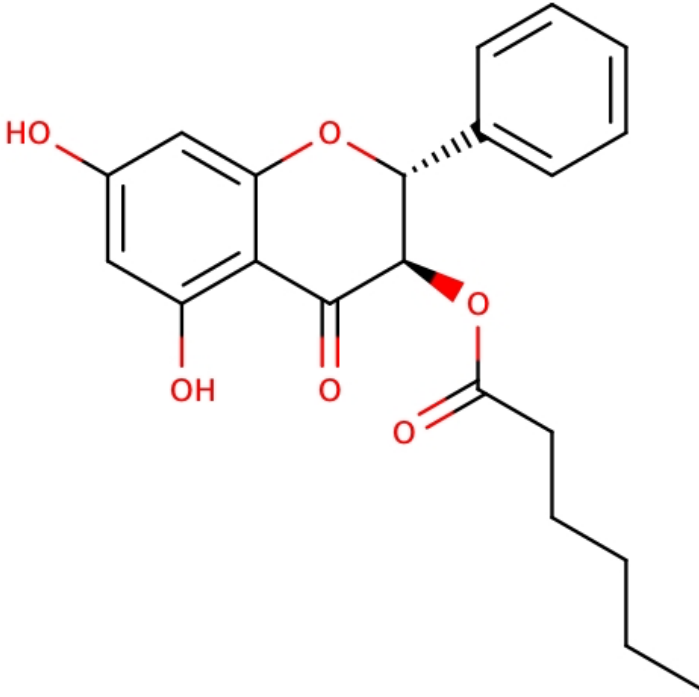
223. pinobanksin-3-O-pentanoate

화학 구조		PubMed ID	
		23176258, 31590214	
TM-MC 성분 ID	152		
TM-MC 성분 동의어	pinobanksin 3-O-pentanoate		
PubChem ID	N/A		
InChI Key	LZGYHOWKKQVGCM-UXHICEINSA-N		
SMILES	<chem>CCCCC(=O)O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1cccc1</chem>		
Molecular Formula	C ₂₀ H ₂₀ O ₆		
Molecular Weight	356.374	Exact Molecular Weight	356.125988364
LogP	4.454	Topological Polar Surface Area	93.06 Å ²
Atom Count	46	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	6	Aromatic Ring Count	2
Drug Likeness	0.75	Oral Bioavailability	Y

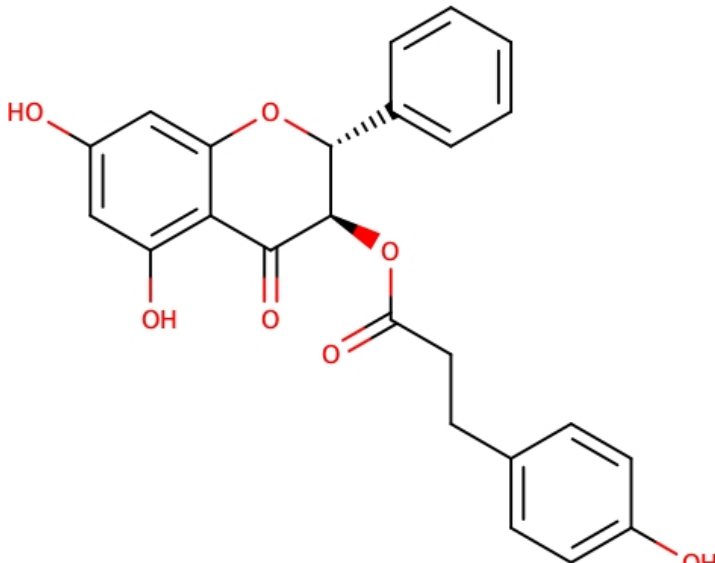
224. pinobanksin 3-O-2-methylbutyrate

화학 구조		PubMed ID	
		23176258, 31590214	
TM-MC 성분 ID	153		
TM-MC 성분 동의어	pinobanksin 3-O-(2-methyl)butyrate		
PubChem ID	101190335		
InChI Key	ZDDSHWOLTYMTJG-VEQZCADJSA-N		
SMILES	CCC(C)C(=O)O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1cccc1		
Molecular Formula	C ₂₀ H ₂₀ O ₆		
Molecular Weight	356.374	Exact Molecular Weight	356.125988364
LogP	4.553	Topological Polar Surface Area	93.06 Å ²
Atom Count	46	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	5	Aromatic Ring Count	2
Drug Likeness	0.77	Oral Bioavailability	Y

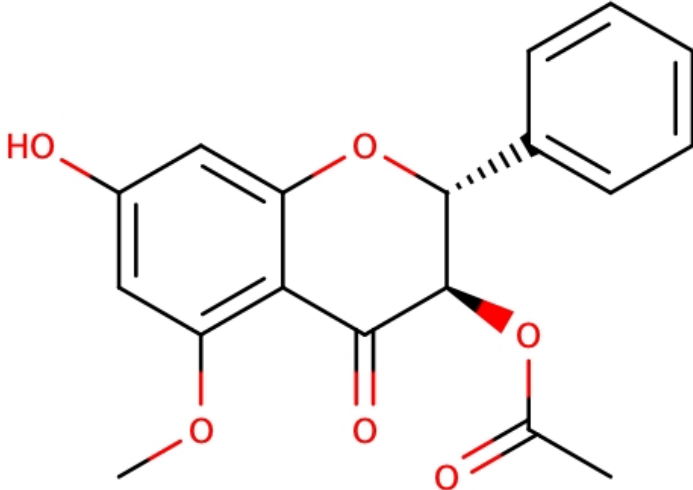
225. pinobanksin-3-O-hexanoate

화학 구조		PubMed ID	
		31590214	
TM-MC 성분 ID	93254		
TM-MC 성분 동의어	N/A		
PubChem ID	162913708		
InChI Key	HHDYLMGNZOFWPD-RTWAWAEBSA-N		
SMILES	CCCCCC(=O)O[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1cccc1		
Molecular Formula	C ₂₁ H ₂₂ O ₆		
Molecular Weight	370.401	Exact Molecular Weight	370.141638428
LogP	4.899	Topological Polar Surface Area	93.06 Å ²
Atom Count	49	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	7	Aromatic Ring Count	2
Drug Likeness	0.53	Oral Bioavailability	Y

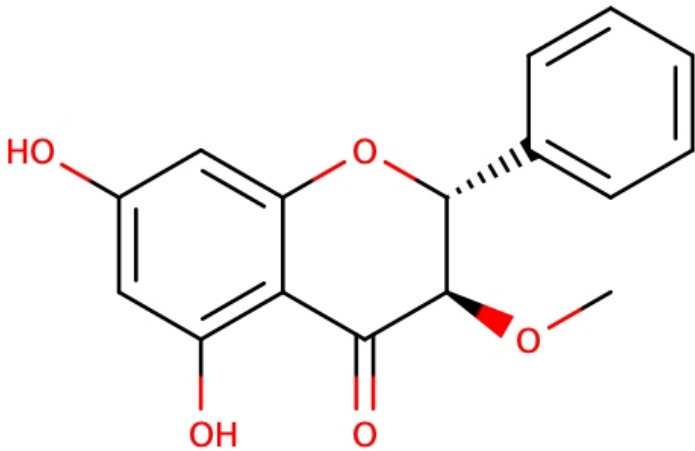
226. pinobanksin-3-O-phenylpropionate

화학 구조		PubMed ID	
		31590214	
TM-MC 성분 ID	93255		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	IKJASTUTPHTBIW-RPWUZVMVSA-N		
SMILES	<chem>Oc1ccc(CCC(=O)O[C@@H]2[C@H](Oc3cc(O)cc(O)c3C2=O)c2ccccc2)cc1</chem>		
Molecular Formula	C ₂₄ H ₂₀ O ₇		
Molecular Weight	420.417	Exact Molecular Weight	420.120902984
LogP	4.84	Topological Polar Surface Area	113.29 Å ²
Atom Count	51	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	6	Aromatic Ring Count	3
Drug Likeness	0.49	Oral Bioavailability	Y

227. pinobanksin-5-methyl ether-3-O-acetate

화학 구조		PubMed ID	
		31590214	
TM-MC 성분 ID	93256		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	MPLPYSFHZOEYIZ-MSOLQXFVSA-N		
SMILES	COc1cc(O)cc2O[C@@H]([C@@H](OC(=O)C(=O)c12)c1cccc1		
Molecular Formula	C ₁₈ H ₁₆ O ₆		
Molecular Weight	328.32	Exact Molecular Weight	328.094688235
LogP	2.361	Topological Polar Surface Area	82.06 Å ²
Atom Count	40	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.87	Oral Bioavailability	Y

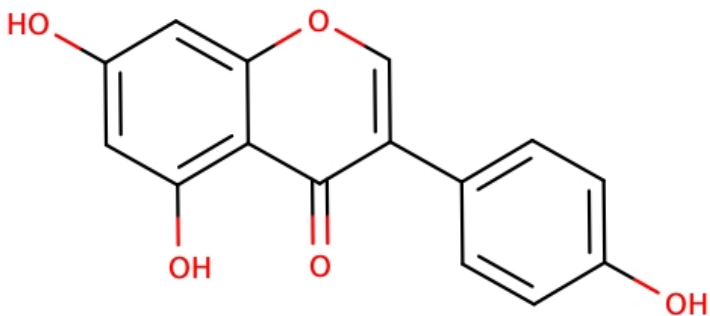
228. pinobanksin-methyl ether

화학 구조		PubMed ID	
		31590214	
TM-MC 성분 ID	93257		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	NWNHVJMRRDSFHQ-CVEARBPZSA-N		
SMILES	<chem>CO[C@@H]1[C@H](Oc2cc(O)cc(O)c2C1=O)c1ccccc1</chem>		
Molecular Formula	C ₁₆ H ₁₄ O ₅		
Molecular Weight	286.283	Exact Molecular Weight	286.084123551
LogP	3.067	Topological Polar Surface Area	75.99 Å ²
Atom Count	35	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.89	Oral Bioavailability	Y

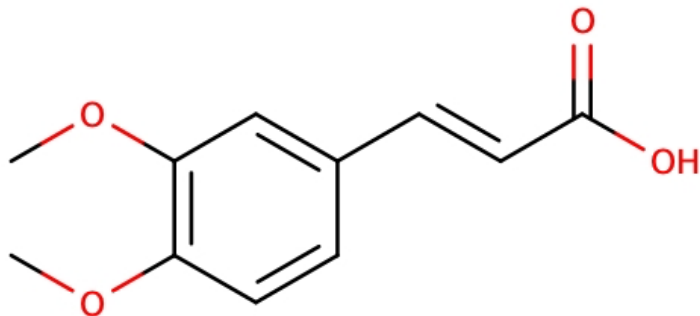
229. pinobanksin-3-O-acetate-5-O-phydroxyphenylpropionate

화학 구조		PubMed ID	
		31590214	
TM-MC 성분 ID	93738		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	PKASHTFHPDWLCJ-FTJBHMTQSA-N		
SMILES	CC(=O)O[C@@H]1[C@H](Oc2cc(O)cc(OC(=O)CCc3ccc(O)cc3)c2C1=O)c1cccc1		
Molecular Formula	C ₂₆ H ₂₂ O ₈		
Molecular Weight	462.454	Exact Molecular Weight	462.131467668
LogP	4.101	Topological Polar Surface Area	119.36 Å ²
Atom Count	56	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	8	Aromatic Ring Count	3
Drug Likeness	0.38	Oral Bioavailability	Y

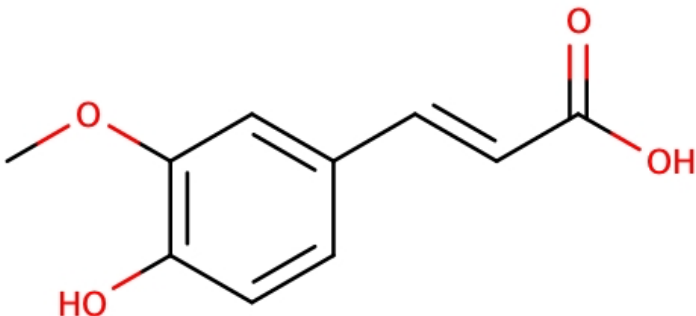
230. genistein

화학 구조		PubMed ID	
		18485465, 22026502 29738446	
TM-MC 성분 ID	157		
TM-MC 성분 동의어	4',5,7-trihydroxy isoflavone; 5,7,4'-trihydroxy dihydroisoflavone		
PubChem ID	5280961		
InChI Key	TZBJGXHYKVUXJN-UHFFFAOYSA-N		
SMILES	<chem>Oc1ccc(cc1)-c1coc2cc(O)cc(O)c2c1=O</chem>		
Molecular Formula	C ₁₅ H ₁₀ O ₅		
Molecular Weight	270.24	Exact Molecular Weight	270.052823422
LogP	3.077	Topological Polar Surface Area	86.99 Å ²
Atom Count	30	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	3
Drug Likeness	0.63	Oral Bioavailability	Y

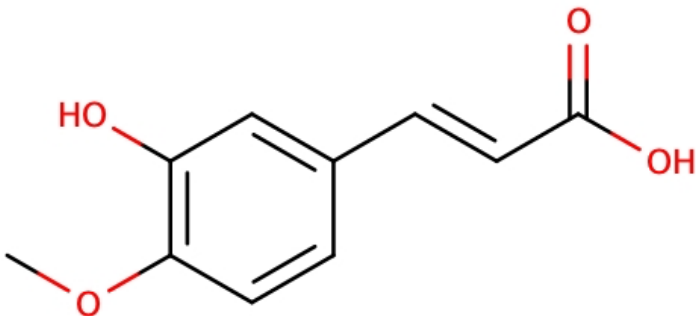
231. 3,4-dimethoxycinnamic acid

화학 구조		PubMed ID	
		15563208, 16621403 18485465, 19634328 22026502, 23176258 24894633, 26807704 27049854, 27123037 28899513, 29889351 30356413, 30691151 30965600, 31227360	
TM-MC 성분 ID	108		
TM-MC 성분 동의어	dimethyl caffeic acid; dimethoxycinnamic acid; dimethoxy-cinnamic acid; 3,4-dimethylcaffeic acid		
PubChem ID	717531		
InChI Key	HJBWJAPEBGSQPR-GQCTYLIASA-N		
SMILES	COc1ccc(\C=C\C(O)=O)cc1OC		
Molecular Formula	C ₁₁ H ₁₂ O ₄		
Molecular Weight	208.213	Exact Molecular Weight	208.073558866
LogP	1.821	Topological Polar Surface Area	55.76 Å ²
Atom Count	27	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.77	Oral Bioavailability	Y

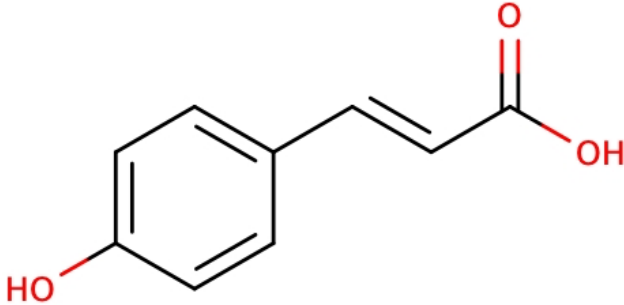
232. ferulic acid

화학 구조		PubMed ID	
		18257304, 18485465 22026502, 22239430 22978445, 23176258 23265456, 24128567 24882729, 24894633 25190186, 25802536 26807704, 27049854 27123037, 28335972 28899513, 29724195 29738446, 29889351 30356413, 30965600 31227360	
TM-MC 성분 ID	109		
TM-MC 성분 동의어	trans-ferulic acid; (E)-ferulic acid; E-ferulic acid; fumalic acid; ferulaic acid; t-ferulic acid		
PubChem ID	445858		
InChI Key	KSEBMYQBYZTDHS-HWKANZROSA-N		
SMILES	<chem>COc1cc(\C=C\C(O)=O)ccc1O</chem>		
Molecular Formula	C ₁₀ H ₁₀ O ₄		
Molecular Weight	194.186	Exact Molecular Weight	194.057908802
LogP	1.675	Topological Polar Surface Area	66.76 Å ²
Atom Count	24	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.72	Oral Bioavailability	Y

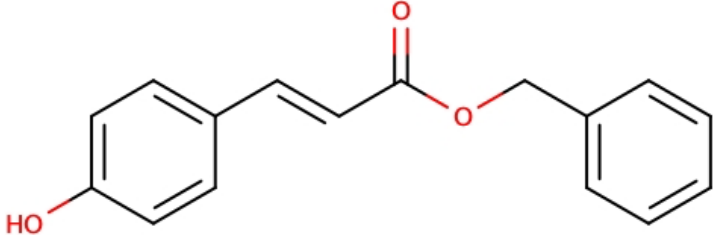
233. isoferulic acid

화학 구조		PubMed ID	
		19634328, 23176258 24894633, 26807704 27049854, 27123037 28899513, 29724195 29738446, 29889351 30356413, 30691151 30965600, 31590214	
TM-MC 성분 ID	110		
TM-MC 성분 동의어	trans-isoferulic acid; isoferulic acid ; iso-ferulic acid; 3-hydroxy-4-methoxycinnamic acid		
PubChem ID	736186		
InChI Key	QURCVMIEKCOAJU-HWKANZROSA-N		
SMILES	<chem>COc1ccc(\C=C\C(O)=O)cc1O</chem>		
Molecular Formula	C ₁₀ H ₁₀ O ₄		
Molecular Weight	194.186	Exact Molecular Weight	194.057908802
LogP	1.675	Topological Polar Surface Area	66.76 Å ²
Atom Count	24	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.72	Oral Bioavailability	Y

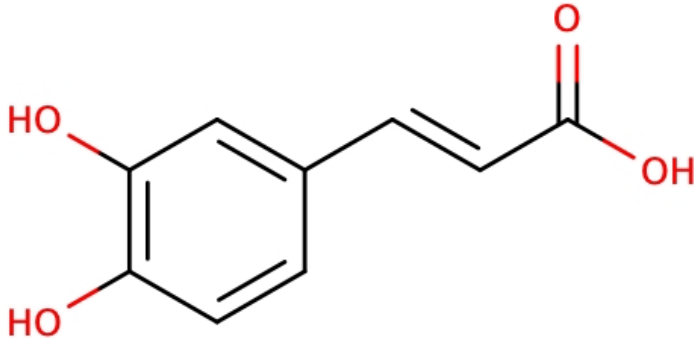
234. p-coumaric acid

화학 구조		PubMed ID	
		15563208, 16621403 18485465, 22026502 22978445, 23176258 23265456, 24882729 24894633, 25802536 27049854, 28335972 28899513, 29337369 29724195, 29738446 29889351, 30356413 30691151, 30965600 31590214	
TM-MC 성분 ID	111		
TM-MC 성분 동의어	coumaric acid; p-hydroxycinnamic acid; 4-hydroxycinnamic acid; 4-coumaric acid; trans-p-coumaric acid; 4-hydroxy cinnamic acid; p-coumaric acid; E-p-hydroxy-cinnamic acid; trans-p-hydroxycinnamic acid; (E)-p-coumaric acid; hydroxycinnamic acid; p-hydroxy-cinnamic acid; p-hydroxylcinnamic acid; E-coumaric acid; trans-coumaric acid; trans-p-coumaric acid; p-hydroxy cinnamic acid; (E)-p-hydroxycinnamic acid; trans-4-hydroxycinnamic acid		
PubChem ID	637542		
InChI Key	NGSWKAQJWESNS-ZZXKWWIFSA-N		
SMILES	<chem>OC(=O)C=Cc1ccc(O)cc1</chem>		
Molecular Formula	C ₉ H ₈ O ₃		
Molecular Weight	164.16	Exact Molecular Weight	164.047344118
LogP	1.833	Topological Polar Surface Area	57.53 Å ²
Atom Count	20	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.66	Oral Bioavailability	Y

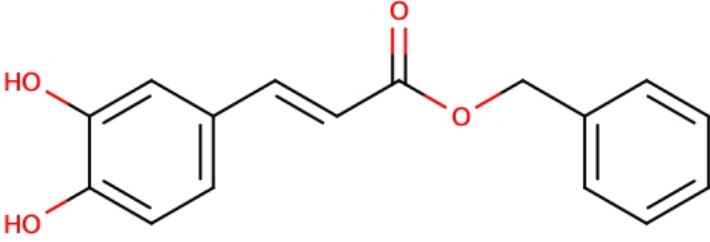
235. p-coumaric acid benzyl ester

화학 구조		PubMed ID	
		23176258	
TM-MC 성분 ID	112		
TM-MC 성분 동의어	N/A		
PubChem ID	10083644		
InChI Key	RGZZCZQP NJCPO-DHZHZOJOSA-N		
SMILES	<chem>Oc1ccc(\C=C\C(=O)OCc2ccccc2)cc1</chem>		
Molecular Formula	C ₁₆ H ₁₄ O ₃		
Molecular Weight	254.285	Exact Molecular Weight	254.094294311
LogP	3.936	Topological Polar Surface Area	46.53 Å ²
Atom Count	33	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	2
Drug Likeness	0.65	Oral Bioavailability	Y

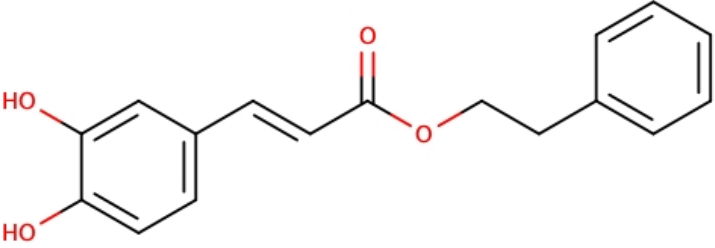
236. caffeic acid

화학 구조		PubMed ID	
		15563208, 16621403 18485465, 19634328 22026502, 22978445 23176258, 23265456 24882729, 24894633 25190186, 25802536 26807704, 27049854 27123037, 28335972 28899513, 29337369 29724195, 29738446 29889351, 30356413 30691151, 30965600 31227360, 31590214	
TM-MC 성분 ID	113		
TM-MC 성분 동의어	trans-caffeic acid; (E)-caffeic acid; 3,4-dihydroxycinnamic acid; caffeic acid ; E-caffeic acid; E-3,4-dihydroxy cinnamic acid		
PubChem ID	689043		
InChI Key	QAIPRVGONGVQAS-DUXPYHPUSA-N		
SMILES	OC(=O)WC=Cc1ccc(O)c(O)c1		
Molecular Formula	C ₉ H ₈ O ₄		
Molecular Weight	180.159	Exact Molecular Weight	180.042258738
LogP	1.529	Topological Polar Surface Area	77.76 Å ²
Atom Count	21	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.48	Oral Bioavailability	Y

237. caffeic acid benzyl ester

화학 구조		PubMed ID	
		19634328, 26807704 27123037, 30965600 31590214	
TM-MC 성분 ID	114		
TM-MC 성분 동의어	benzyl caffeate		
PubChem ID	5919576		
InChI Key	WWVKQTNONPWVEL-VQHVLOKHSA-N		
SMILES	<chem>Oc1ccc(\C=C\C(=O)OCc2ccccc2)cc1O</chem>		
Molecular Formula	C ₁₆ H ₁₄ O ₄		
Molecular Weight	270.284	Exact Molecular Weight	270.089208931
LogP	3.633	Topological Polar Surface Area	66.76 Å ²
Atom Count	34	Structural Alert Count	3
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	5	Aromatic Ring Count	2
Drug Likeness	0.49	Oral Bioavailability	Y

238. CAPE

화학 구조		PubMed ID	
		15563208, 16004979 16621403, 18257304 23176258, 24128567 24882729, 24894633 25802536, 26807704 27049854, 27123037 28335972, 28899513 29724195, 29889351 30356413, 30691151 30965600, 31590214	
TM-MC 성분 ID	115		
TM-MC 성분 동의어	caffeic acid phenethyl ester; phenethyl caffeate; phenylethylcaffeate; caffeic acid phenylethyl ester		
PubChem ID	5281787		
InChI Key	SWUARLUWKZWEBQ-VQHVLOKHSA-N		
SMILES	Oc1ccc(\C=C\C(=O)OCCc2ccccc2)cc1O		
Molecular Formula	C ₁₇ H ₁₆ O ₄		
Molecular Weight	284.311	Exact Molecular Weight	284.104858995
LogP	3.921	Topological Polar Surface Area	66.76 Å ²
Atom Count	37	Structural Alert Count	3
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	6	Aromatic Ring Count	2
Drug Likeness	0.48	Oral Bioavailability	Y

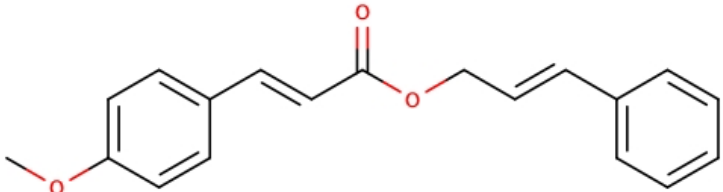
239. caffeic acid isoprenyl ester

화학 구조		PubMed ID	
		23176258, 31590214	
TM-MC 성분 ID	116		
TM-MC 성분 동의어	dimethylallylcaffeate		
PubChem ID	5281790		
InChI Key	TTYOHMFLCXENHR-GQCTYLIASA-N		
SMILES	<chem>CC(C)=CCOC(=O)WC=CWc1ccc(O)c(O)c1</chem>		
Molecular Formula	C ₁₄ H ₁₆ O ₄		
Molecular Weight	248.278	Exact Molecular Weight	248.104858995
LogP	3.269	Topological Polar Surface Area	66.76 Å ²
Atom Count	34	Structural Alert Count	4
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	5	Aromatic Ring Count	1
Drug Likeness	0.36	Oral Bioavailability	Y

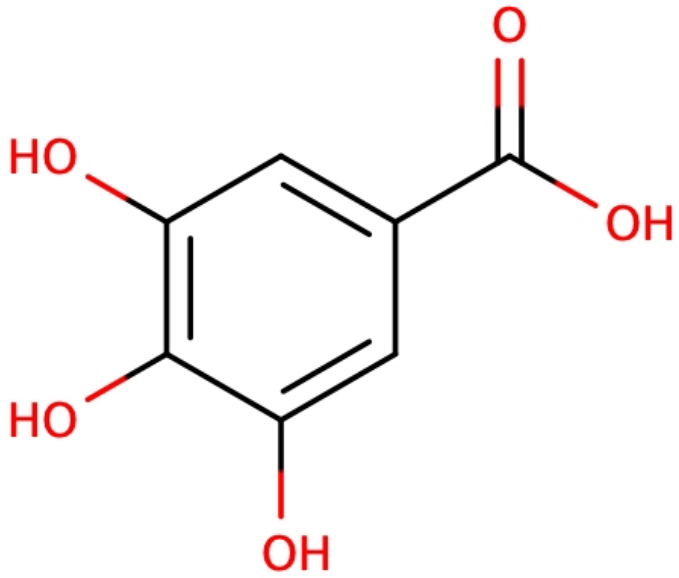
240. cinnamyl caffeate

화학 구조		PubMed ID	
		15563208, 16621403 23176258, 31590214	
TM-MC 성분 ID	117		
TM-MC 성분 동의어	caffeic acid cinnamyl ester		
PubChem ID	11380911		
InChI Key	GRZQNEYQRVFNRY-WUZDHUPESA-N		
SMILES	<chem>Oc1ccc(OC(=O)C=Cc2ccccc2)cc1O</chem>		
Molecular Formula	C ₁₈ H ₁₆ O ₄		
Molecular Weight	296.322	Exact Molecular Weight	296.104858995
LogP	4.243	Topological Polar Surface Area	66.76 Å ²
Atom Count	38	Structural Alert Count	3
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	6	Aromatic Ring Count	2
Drug Likeness	0.48	Oral Bioavailability	Y

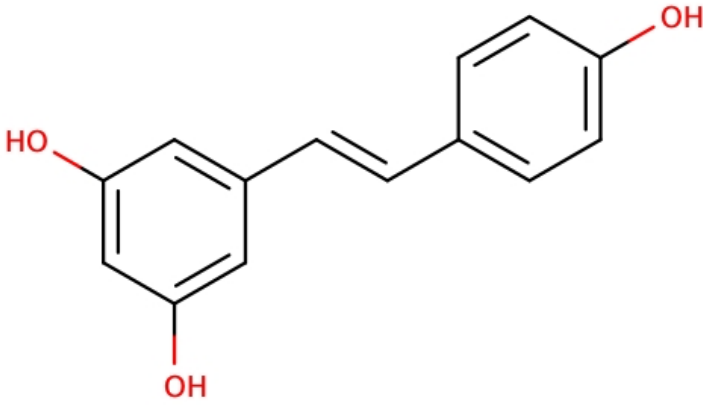
241. p-methoxycinnamic acid cinnamyl ester

화학 구조		PubMed ID	
		23176258	
TM-MC 성분 ID	118		
TM-MC 성분 동의어	N/A		
PubChem ID	129865763		
InChI Key	FSUPHWQVIFYWBEW-HLSRHWEPSA-N		
SMILES	COc1ccc(WC=CWC(=O)OCWC=CWc2ccccc2)cc1		
Molecular Formula	C ₁₉ H ₁₈ O ₃		
Molecular Weight	294.35	Exact Molecular Weight	294.12559444
LogP	4.692	Topological Polar Surface Area	35.53 Å ²
Atom Count	40	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	0
Rotatable Bond Count	7	Aromatic Ring Count	2
Drug Likeness	0.55	Oral Bioavailability	Y

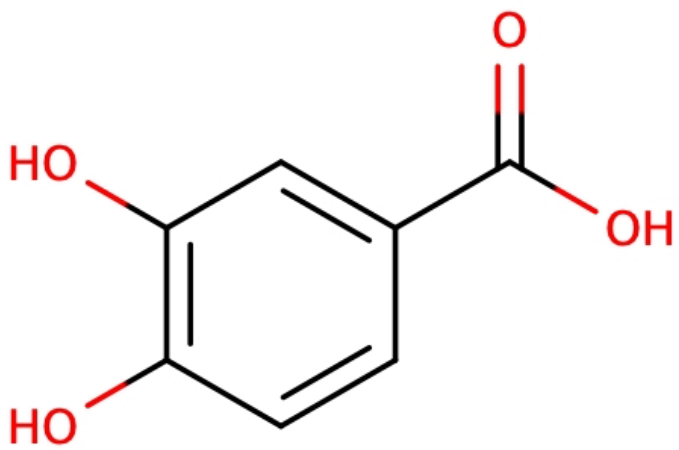
242. gallic acid

화학 구조		PubMed ID	
		22026502, 22239430 23265456, 29337369 29738446, 29889351 31227360	
TM-MC 성분 ID	119		
TM-MC 성분 동의어	gallate; 3,4,5-trihydroxybenzoate; 3,4,5-trihydroxybenzoic acid		
PubChem ID	370		
InChI Key	LNTHITQWFMADLM-UHFFFAOYSA-N		
SMILES	<chem>OC(=O)c1cc(O)c(O)c(O)c1</chem>		
Molecular Formula	C ₇ H ₆ O ₅		
Molecular Weight	170.12	Exact Molecular Weight	170.021523293
LogP	0.72	Topological Polar Surface Area	97.99 Å ²
Atom Count	18	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.47	Oral Bioavailability	Y

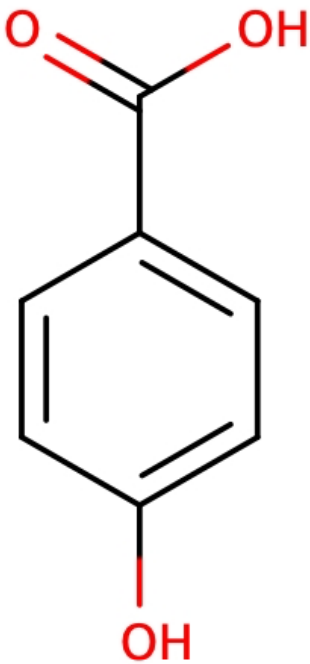
243. resveratrol

화학 구조		PubMed ID	
		24882729	
TM-MC 성분 ID	120		
TM-MC 성분 동의어	trans-resveratrol; trans-3,5,4'-trihydroxystilbene; 3,5,4'-trihydroxystilbene; 3,5,4'-trihydroxy-trans-stilbene; stilbenoid; t-resveratrol; cis-resveratrol; (E)-resveratrol; 3,4',5-trihydroxystilbene; 3,4',5-trihydrohydroxystilbene; (E)-diastereomer of resveratrol; 5-[(E)-2-(4-hydroxyphenyl)-ethenyl]benzene-1,3-diol		
PubChem ID	445154		
InChI Key	LUKBXSAWLPMMSZ-OWOJBTEDSA-N		
SMILES	<chem>Oc1ccc(WC=CWc2cc(O)cc(O)c2)cc1</chem>		
Molecular Formula	C ₁₄ H ₁₂ O ₃		
Molecular Weight	228.247	Exact Molecular Weight	228.078644246
LogP	3.402	Topological Polar Surface Area	60.69 Å ²
Atom Count	29	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.69	Oral Bioavailability	Y

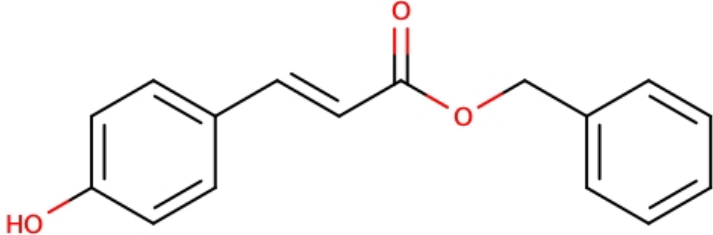
244. protocatechuic acid

화학 구조		PubMed ID	
		23265456, 29337369 29724195, 29738446 29889351, 31227360	
TM-MC 성분 ID	171		
TM-MC 성분 동의어	3,4-dihydroxybenzoic acid; protocatechuate; procatechuic acid; 3,4-dihydroxy benzoic acid; protocatechulic acid; 3,4-dihydroxybenzoate; 3,4-dihydrobenzoic acid; 3,4-dihydroxy benzoic acid; 3,4-dihydroxybenzoic acid; 3,4-dihydroxy-benzoic acid		
PubChem ID	72		
InChI Key	YQUVCSBJEUQKSH-UHFFFAOYSA-N		
SMILES	<chem>OC(=O)c1ccc(O)c(O)c1</chem>		
Molecular Formula	C ₇ H ₆ O ₄		
Molecular Weight	154.121	Exact Molecular Weight	154.026608673
LogP	1.024	Topological Polar Surface Area	77.76 Å ²
Atom Count	17	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.53	Oral Bioavailability	Y

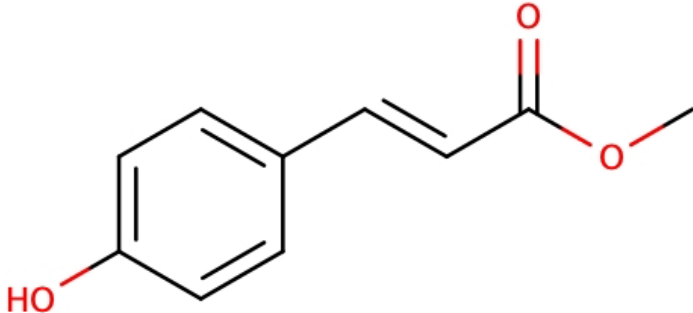
245. p-hydroxybenzoic acid

화학 구조		PubMed ID	
		23265456, 29337369 29738446, 31590214	
TM-MC 성분 ID	172		
TM-MC 성분 동의어	4-hydroxybenzoic acid; hydroxybenzoic acid; 4-hydroxy benzoic acid; p-hydroxy benzoic acid; p-salicylic acid; para-hydroxybenzoic acid; p-hydroxybenzoate; 4-hydroxybenzoate; p-hydroxy-bezoic acid; 4-hydroxybenzene carboxylic acid		
PubChem ID	135, 3702506		
InChI Key	FJKROLUGYXJWQN-UHFFFAOYSA-N		
SMILES	OC(=O)c1ccc(O)cc1		
Molecular Formula	C ₇ H ₆ O ₃		
Molecular Weight	138.122	Exact Molecular Weight	138.031694053
LogP	1.327	Topological Polar Surface Area	57.53 Å ²
Atom Count	16	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.61	Oral Bioavailability	Y

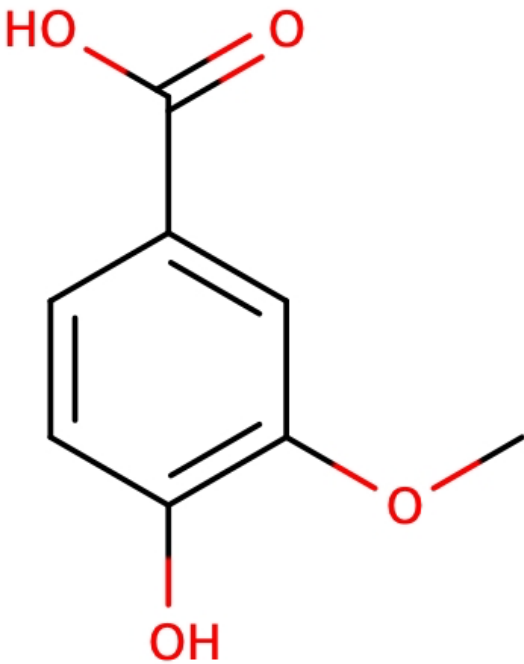
246. hydroxy-cinnamic acid benzyl ester

화학 구조		PubMed ID	
		23176258	
TM-MC 성분 ID	1123		
TM-MC 성분 동의어	N/A		
PubChem ID	10083644		
InChI Key	RGZZCZQP NJCPO-DHZHZOJOSA-N		
SMILES	<chem>Oc1ccc(\C=C\C(=O)OCc2ccccc2)cc1</chem>		
Molecular Formula	C ₁₆ H ₁₄ O ₃		
Molecular Weight	254.285	Exact Molecular Weight	254.094294311
LogP	3.936	Topological Polar Surface Area	46.53 Å ²
Atom Count	33	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	2
Drug Likeness	0.65	Oral Bioavailability	Y

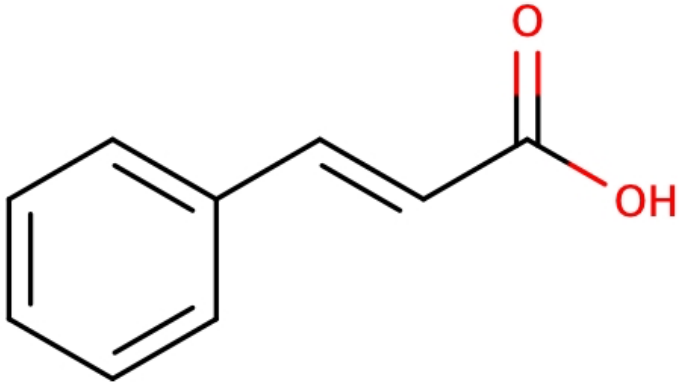
247. 2-propenoic acid, 3-(4-hydroxyphenyl)-, methyl ester

화학 구조		PubMed ID	
		28335972	
TM-MC 성분 ID	60053		
TM-MC 성분 동의어	methyl coumarate; methyl 4-hydroxycinnamate; coumaric acid methyl ester; p-hydroxy methyl cinnamate; 4-hydroxycinnamic acid methylester; trans-p-coumaric acid methyl ester		
PubChem ID	5319562		
InChI Key	NITWSHWHQAQBAW-QPJJXVBHSA-N		
SMILES	COC(=O)WC=Cc1ccc(O)cc1		
Molecular Formula	C ₁₀ H ₁₀ O ₃		
Molecular Weight	178.187	Exact Molecular Weight	178.062994182
LogP	2.212	Topological Polar Surface Area	46.53 Å ²
Atom Count	23	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.57	Oral Bioavailability	Y

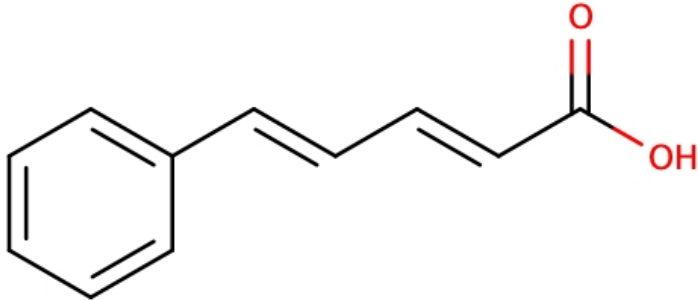
248. vanillic acid

화학 구조		PubMed ID	
		28899513, 29889351 31227360	
TM-MC 성분 ID	90767		
TM-MC 성분 동의어	4-hydroxy-3-methoxybenzoic acid; vanillinic acid; 3-methoxy-4-hydroxybenzoic acid; 3-methoxy-4-hydroxy-benzoic acid		
PubChem ID	8468		
InChI Key	WKOLLVMJNQIZCI-UHFFFAOYSA-N		
SMILES	<chem>COc1cc(ccc1O)C(O)=O</chem>		
Molecular Formula	$C_8H_8O_4$		
Molecular Weight	168.148	Exact Molecular Weight	168.042258738
LogP	1.17	Topological Polar Surface Area	66.76 Å ²
Atom Count	20	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.70	Oral Bioavailability	Y

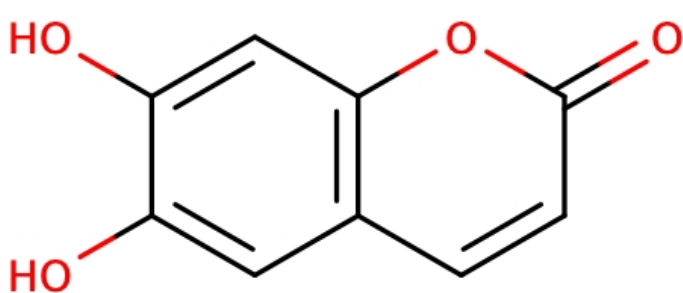
249. cinnamic acid

화학 구조		PubMed ID	
		15158983, 22026502 24894633, 27049854 28899513, 29724195 29889351, 30691151	
TM-MC 성분 ID	107		
TM-MC 성분 동의어	trans-cinnamic acid; t-cinnamic acid; E-cinnamic acid; 3-phenyl-2-propenoic acid; (E)-cinnamic acid		
PubChem ID	444539		
InChI Key	WBYWAXJHAXSJNI-VOTSOKGWSA-N		
SMILES	OC(=O)C=Cc1ccccc1		
Molecular Formula	C ₉ H ₈ O ₂		
Molecular Weight	148.161	Exact Molecular Weight	148.052429498
LogP	2.136	Topological Polar Surface Area	37.3 Å ²
Atom Count	19	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.65	Oral Bioavailability	Y

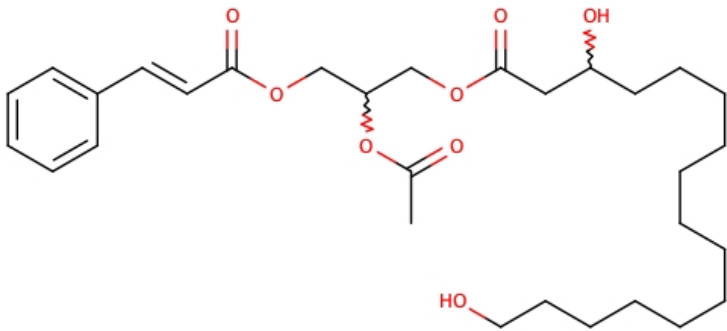
250. cinnamylidene acetic acid

화학 구조		PubMed ID	
		15563208, 16621403	
TM-MC 성분 ID	121		
TM-MC 성분 동의어	N/A		
PubChem ID	1549512		
InChI Key	FEIQOMCWGDNMHH-KBXRYBNXSA-N		
SMILES	OC(=O)WC=CWC=CWc1ccccc1		
Molecular Formula	C ₁₁ H ₁₀ O ₂		
Molecular Weight	174.199	Exact Molecular Weight	174.068079562
LogP	2.663	Topological Polar Surface Area	37.3 Å ²
Atom Count	23	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.56	Oral Bioavailability	Y

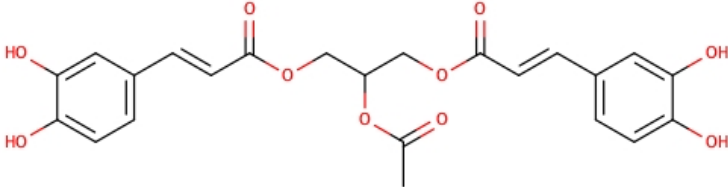
251. esculetin

화학 구조		PubMed ID	
		28335972	
TM-MC 성분 ID	301770		
TM-MC 성분 동의어	aesculetin; eculetin; 6,7-hydroxycoumarin; 6,7-dihydroxycoumarin		
PubChem ID	5281416		
InChI Key	ILEDWLMCKZNDJK-UHFFFAOYSA-N		
SMILES	<chem>Oc1cc2ccc(=O)oc2cc1O</chem>		
Molecular Formula	C ₉ H ₆ O ₄		
Molecular Weight	178.143	Exact Molecular Weight	178.026608673
LogP	1.176	Topological Polar Surface Area	66.76 Å ²
Atom Count	19	Structural Alert Count	2
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.47	Oral Bioavailability	Y

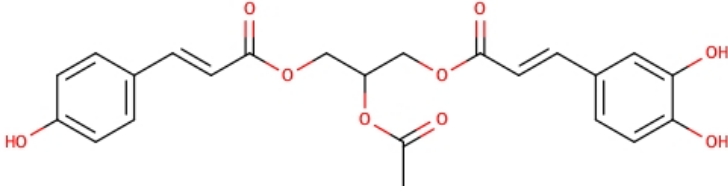
252. (-)-2-acetyl-1-(E)-feruloyl-3-(3''(ζ),16'')-dihydroxy-palmitoylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	159		
TM-MC 성분 동의어	N/A		
PubChem ID	71619030		
InChI Key	AQFCBNKUCUBVBK-FMQUCEESA-N		
SMILES	CC(=O)OC(COC(=O)CC(O)CCCCCCCCCCCCCO)COC(=O)C=CC=C1CCCC1		
Molecular Formula	C ₃₀ H ₄₆ O ₈		
Molecular Weight	534.69	Exact Molecular Weight	534.319268441
LogP	5.89	Topological Polar Surface Area	119.36 Å ²
Atom Count	84	Structural Alert Count	3
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	25	Aromatic Ring Count	1
Drug Likeness	0.09	Oral Bioavailability	N

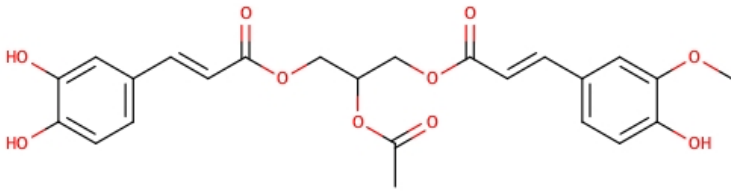
253. 2-acetyl-1,3-dicaffeoylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	160		
TM-MC 성분 동의어	N/A		
PubChem ID	101316991		
InChI Key	YDTIZZNTZGZHKT-KBXRYBNXSA-N		
SMILES	CC(=O)OC(COC(=O)WC=CWc1ccc(O)c(O)c1)COC(=O)WC=CWc1ccc(O)c(O)c1		
Molecular Formula	C ₂₃ H ₂₂ O ₁₀		
Molecular Weight	458.419	Exact Molecular Weight	458.121296908
LogP	3.456	Topological Polar Surface Area	159.82 Å ²
Atom Count	55	Structural Alert Count	3
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	12	Aromatic Ring Count	2
Drug Likeness	0.22	Oral Bioavailability	N

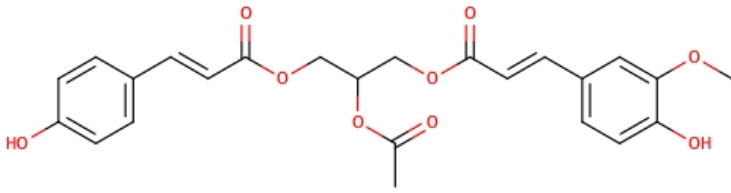
254. 2-acetyl-1-caffeoyl-3-coumaroylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	161		
TM-MC 성분 동의어	N/A		
PubChem ID	46886814		
InChI Key	GLVFLAONFKWEJN-YOYBCKCWSA-N		
SMILES	CC(=O)OC(COC(=O)WC=CWc1ccc(O)cc1)COC(=O)WC=CWc1ccc(O)c(O)c1		
Molecular Formula	C ₂₃ H ₂₂ O ₉		
Molecular Weight	442.42	Exact Molecular Weight	442.126382288
LogP	3.759	Topological Polar Surface Area	139.59 Å ²
Atom Count	54	Structural Alert Count	3
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	12	Aromatic Ring Count	2
Drug Likeness	0.26	Oral Bioavailability	N

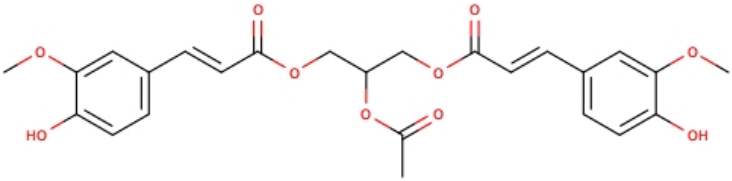
255. 2-acetyl-1-feruloyl-3-caffeoylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	162		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	OVCBATCZMRVHCC-NXZHAIsvsa-N		
SMILES	COc1cc(WC=CWC(=O)OCC(COC(=O)WC=CWc2ccc(O)c(O)c2)OC(C)=O)ccc1O		
Molecular Formula	C ₂₄ H ₂₄ O ₁₀		
Molecular Weight	472.446	Exact Molecular Weight	472.136946973
LogP	3.602	Topological Polar Surface Area	148.82 Å ²
Atom Count	58	Structural Alert Count	3
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	3
Rotatable Bond Count	13	Aromatic Ring Count	2
Drug Likeness	0.23	Oral Bioavailability	N

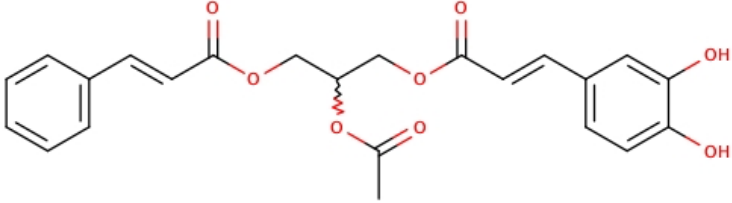
256. 2-acetyl-1-feruloyl-3-coumaroylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	163		
TM-MC 성분 동의어	N/A		
PubChem ID	46886812		
InChI Key	SSRYGMNKGHCFDE-GNXPCCSA-N		
SMILES	COc1cc(WC=CWC(=O)OCC(COC(=O)WC=CWc2ccc(O)cc2)OC(C)=O)ccc1O		
Molecular Formula	C ₂₄ H ₂₄ O ₉		
Molecular Weight	456.447	Exact Molecular Weight	456.142032353
LogP	3.905	Topological Polar Surface Area	128.59 Å ²
Atom Count	57	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	13	Aromatic Ring Count	2
Drug Likeness	0.35	Oral Bioavailability	N

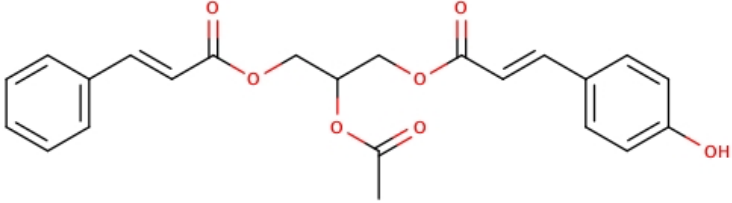
257. 2-acetyl-1,3-diferuloylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	164		
TM-MC 성분 동의어	N/A		
PubChem ID	46886777		
InChI Key	HVZMOVKKIOLLAD-JMQWPVDRSA-N		
SMILES	COc1cc(WC=CWC(=O)OCC(COC(=O)WC=CWc2ccc(O)c(OC)c2)OC(C)=O)ccc1O		
Molecular Formula	C ₂₅ H ₂₆ O ₁₀		
Molecular Weight	486.473	Exact Molecular Weight	486.152597037
LogP	3.747	Topological Polar Surface Area	137.82 Å ²
Atom Count	61	Structural Alert Count	2
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	2
Rotatable Bond Count	14	Aromatic Ring Count	2
Drug Likeness	0.31	Oral Bioavailability	N

258. (+)-2-acetyl-1-caffeoyl-3-cinnamoylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	165		
TM-MC 성분 동의어	(-)-2-acetyl-1-caffeoyl-3-cinnamoylglycerol		
PubChem ID	N/A		
InChI Key	OOBUWNALJLFBRF-HZOWPXDZSA-N		
SMILES	CC(=O)OC(COC(=O)WC=CWc1cccc1)COC(=O)WC=CWc1ccc(O)c(O)c1		
Molecular Formula	C ₂₃ H ₂₂ O ₈		
Molecular Weight	426.421	Exact Molecular Weight	426.131467668
LogP	4.063	Topological Polar Surface Area	119.36 Å ²
Atom Count	53	Structural Alert Count	3
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	12	Aromatic Ring Count	2
Drug Likeness	0.30	Oral Bioavailability	N

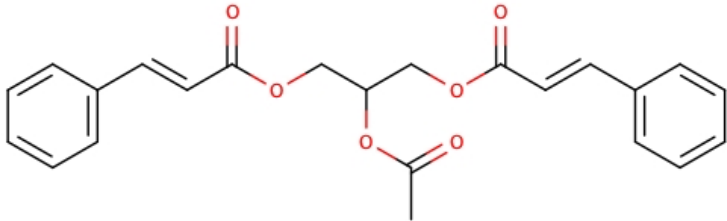
259. 2-acetyl-1-coumaroyl-3-cinnamoylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	167		
TM-MC 성분 동의어	N/A		
PubChem ID	71618935		
InChI Key	YYSVMGYBENFERR-UTLPMFLDSA-N		
SMILES	CC(=O)OC(COC(=O)C=Cc1ccccc1)COC(=O)C=Cc1ccc(O)cc1		
Molecular Formula	C ₂₃ H ₂₂ O ₇		
Molecular Weight	410.422	Exact Molecular Weight	410.136553048
LogP	4.366	Topological Polar Surface Area	99.13 Å ²
Atom Count	52	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	12	Aromatic Ring Count	2
Drug Likeness	0.41	Oral Bioavailability	N

260. (-)-2-acetyl-1-feruloyl-3-cinnamoylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	168		
TM-MC 성분 동의어	(+)-2-acetyl-1-feruloyl-3-cinnamoylglycerol		
PubChem ID	71619028		
InChI Key	MAKHMNPJGLCMJM-JOWSBRCASA-N		
SMILES	COc1cc(\C=C\C(=O)OCC(COC(=O)\C=C\c2ccccc2)OC(C)=O)ccc1O		
Molecular Formula	C ₂₄ H ₂₄ O ₈		
Molecular Weight	440.448	Exact Molecular Weight	440.147117733
LogP	4.209	Topological Polar Surface Area	108.36 Å ²
Atom Count	56	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	13	Aromatic Ring Count	2
Drug Likeness	0.37	Oral Bioavailability	N

261. 2-acetyl-1,3-dicinnamoylglycerol

화학 구조		PubMed ID	
		22978445	
TM-MC 성분 ID	170		
TM-MC 성분 동의어	N/A		
PubChem ID	71619029		
InChI Key	ANLOTVCSWUBHSM-QUMQEAAQSA-N		
SMILES	CC(=O)OC(COC(=O)WC=CWc1ccccc1)COC(=O)WC=CWc1ccccc1		
Molecular Formula	C ₂₃ H ₂₂ O ₆		
Molecular Weight	394.423	Exact Molecular Weight	394.141638428
LogP	4.67	Topological Polar Surface Area	78.9 Å ²
Atom Count	51	Structural Alert Count	2
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	0
Rotatable Bond Count	12	Aromatic Ring Count	2
Drug Likeness	0.39	Oral Bioavailability	N

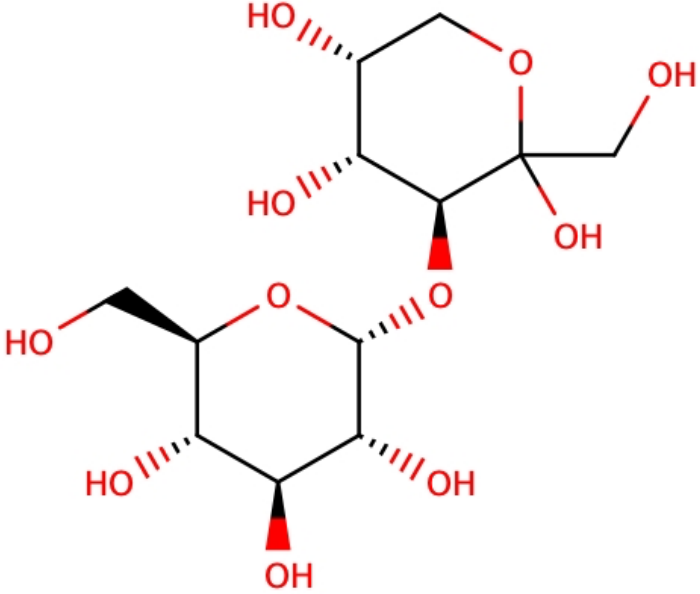
262. glucose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	5793		
TM-MC 성분 동의어	D-glucose		
PubChem ID	5793		
InChI Key	WQZGKKKIJFFOK-GASJEMHNSA-N		
SMILES	OC[C@H]1OC(O)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₆ H ₁₂ O ₆		
Molecular Weight	180.156	Exact Molecular Weight	180.063388106
LogP	-2.933	Topological Polar Surface Area	110.38 Å ²
Atom Count	24	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	5
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.30	Oral Bioavailability	Y

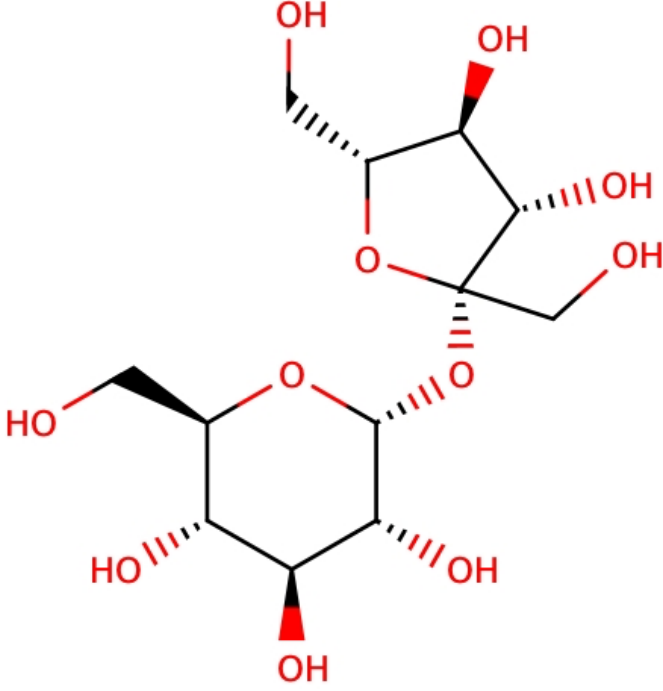
263. fructose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	723872		
TM-MC 성분 동의어	D-fructose; β-D-fructose		
PubChem ID	2723872		
InChI Key	LKDRXBCSQODPBY-VRPWFDPXSA-N		
SMILES	OCC1(O)OC[C@@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₆ H ₁₂ O ₆		
Molecular Weight	180.156	Exact Molecular Weight	180.063388106
LogP	-2.758	Topological Polar Surface Area	110.38 Å ²
Atom Count	24	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	5
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.30	Oral Bioavailability	Y

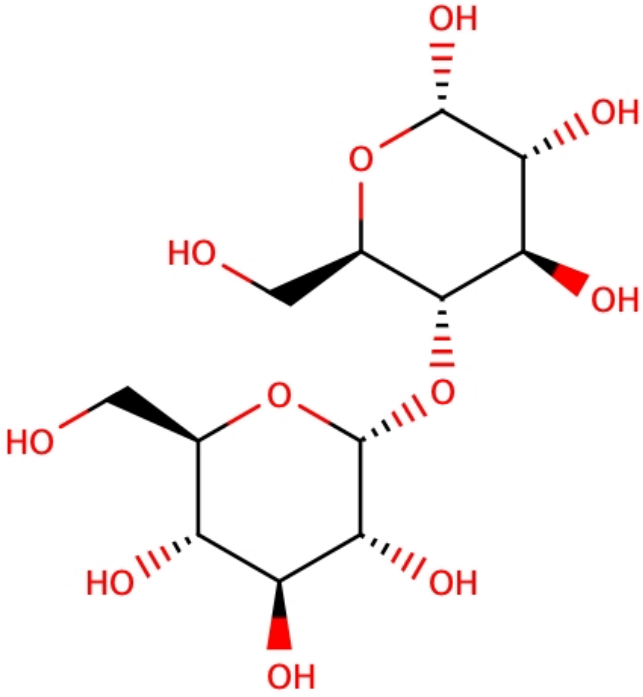
264. turanose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	460935		
TM-MC 성분 동의어	N/A		
PubChem ID	54301978		
InChI Key	SEWFWJUQVJHATO-PUVWEJBASA-N		
SMILES	OC[C@H]1O[C@H](O[C@H]2[C@H](O)[C@H](O)COC2(O)CO)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.529	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.25	Oral Bioavailability	N

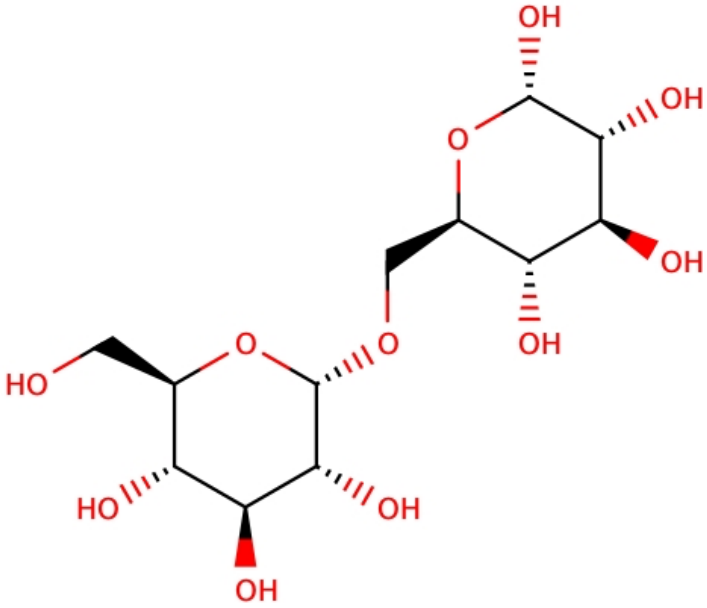
265. sucrose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	5988		
TM-MC 성분 동의어	saccharose; β-D-fructofuranosyl-α-D-glucopyranoside		
PubChem ID	5988		
InChI Key	CZMRCDWAGMRECN-UGDNZRGBSA-N		
SMILES	OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.529	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

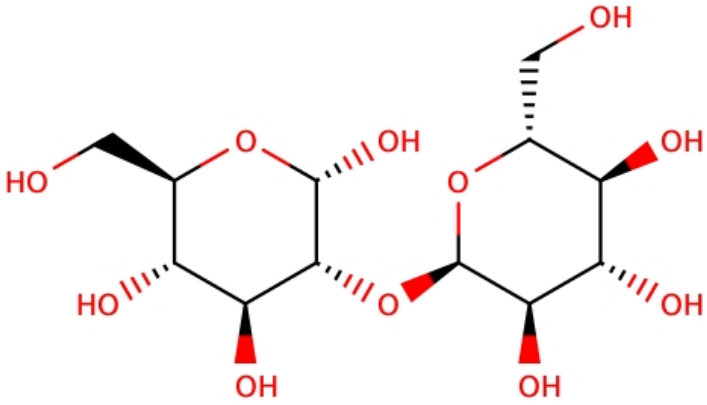
266. maltose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	439186		
TM-MC 성분 동의어	α-maltose		
PubChem ID	439341		
InChI Key	GUBGYTABKSRVRQ-ASMJPISFSA-N		
SMILES	OC[C@H]1O[C@H](O[C@H]2[C@H](O)[C@@H](O)[C@@H](O)O[C@@H]2CO)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.703	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

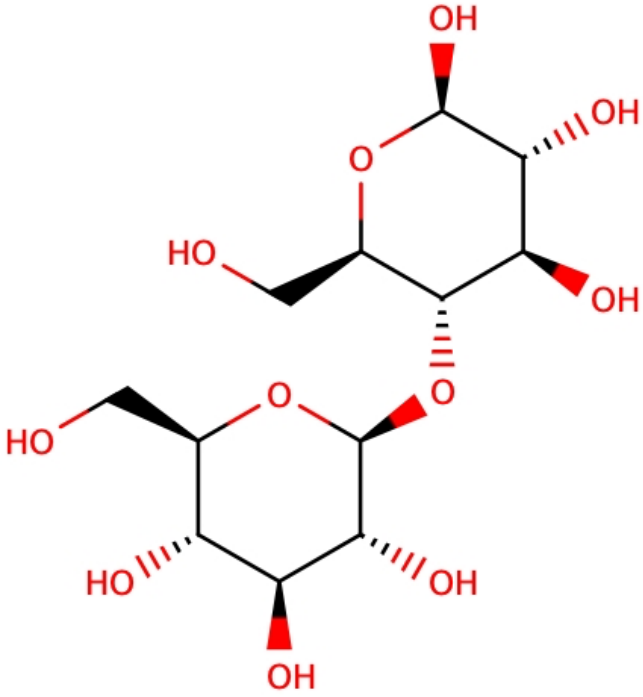
267. melibiose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	92507		
TM-MC 성분 동의어	isomaltose		
PubChem ID	11968638		
InChI Key	DLRVVLDZNNYCBX-NCFXGAEVSA-N		
SMILES	OC[C@H]1O[C@H](OC[C@H]2O[C@H](O)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.703	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

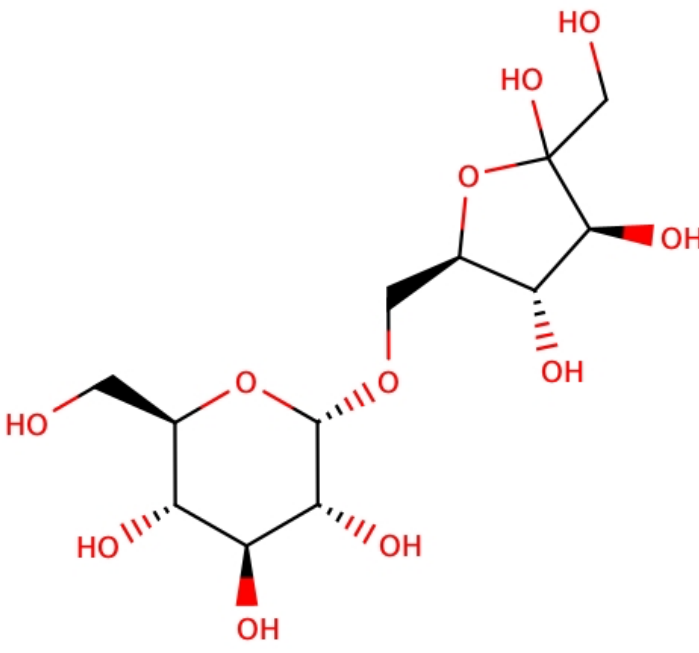
268. kojibiose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301607		
TM-MC 성분 동의어	α-kojibiose		
PubChem ID	12304907		
InChI Key	HIWPGCMGAMJNRG-LFWCVFAXSA-N		
SMILES	OC[C@H]1O[C@H](O)[C@H](O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.703	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

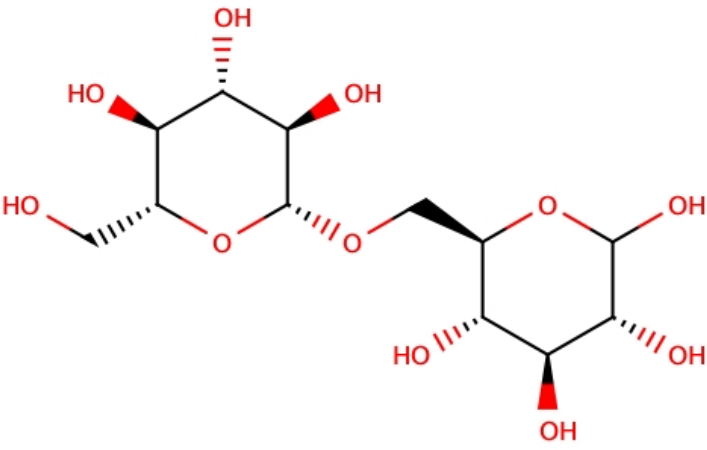
269. cellobiose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	10712		
TM-MC 성분 동의어	D-(+)-cellobiose		
PubChem ID	10712		
InChI Key	GUBGYTABKSRVRQ-QRZGKKJRSA-N		
SMILES	OC[C@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@H](O)O[C@@H]2CO)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.703	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

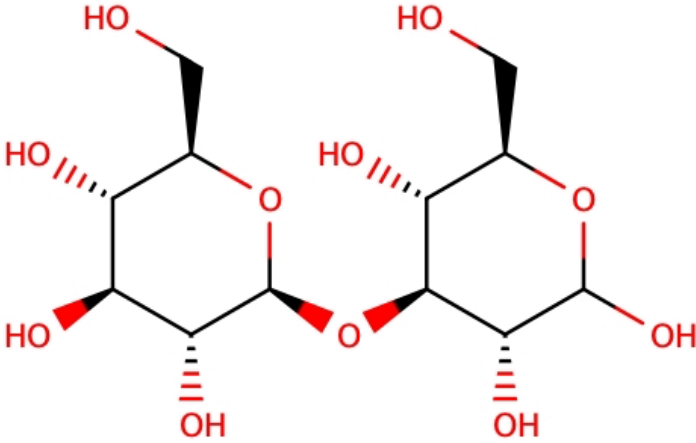
270. palatinose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	439559		
TM-MC 성분 동의어	N/A		
PubChem ID	439559		
InChI Key	PVXPPJIGRGXGCY-TZLCEDOOSA-N		
SMILES	OC[C@H]1O[C@H](OC[C@H]2OC(O)(CO)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.529	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

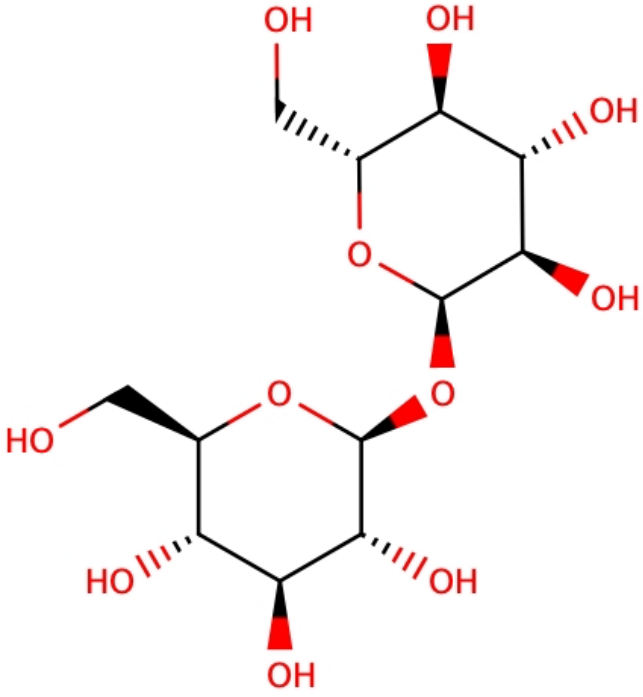
271. gentiobiose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	802156		
TM-MC 성분 동의어	N/A		
PubChem ID	5460026		
InChI Key	DLRVVLDZNNYCBX-CQUJWQHSSA-N		
SMILES	OC[C@H]1O[C@@H](OC[C@H]2OC(O)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.703	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

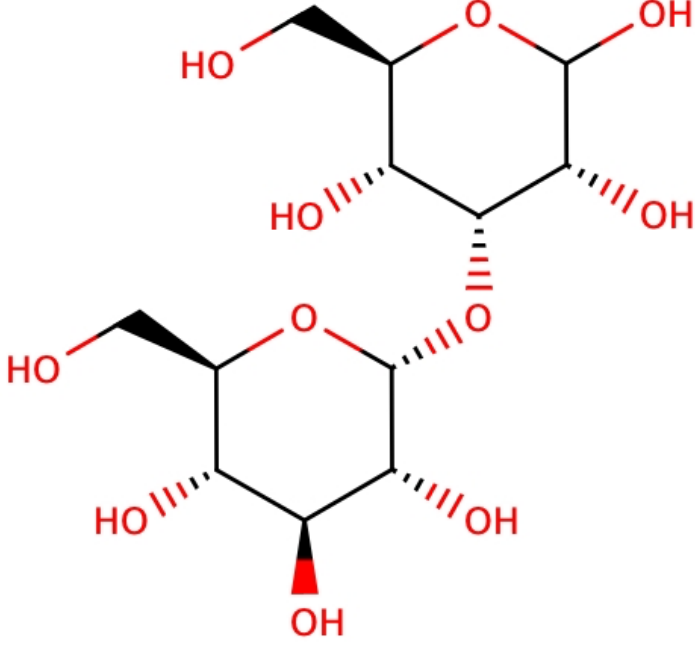
272. laminaribiose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301638		
TM-MC 성분 동의어	N/A		
PubChem ID	439637		
InChI Key	QIGJYVCQYDKYDW-LCOYTZNXSA-N		
SMILES	OC[C@H]1O[C@@H](O[C@@H]2[C@H](O)C(O)O[C@H](CO)[C@H]2O)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.703	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

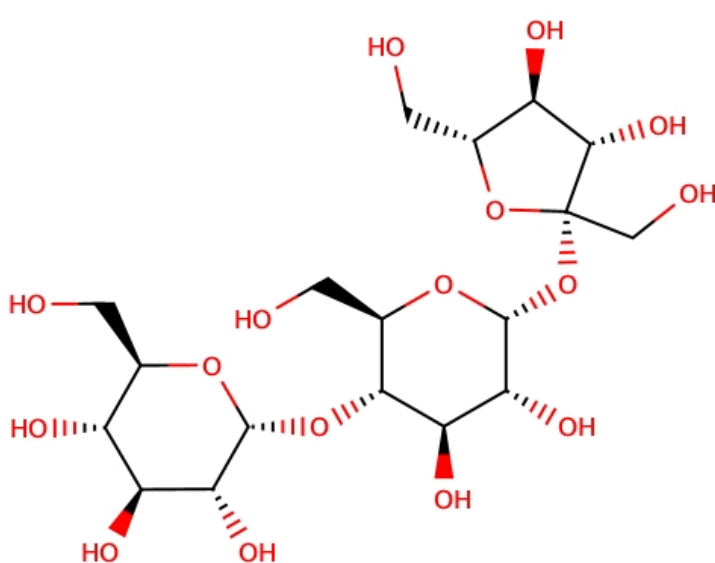
273. neotrehalose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301873		
TM-MC 성분 동의어	N/A		
PubChem ID	10871590		
InChI Key	HDTRYLNUVZCQOY-BTLHAWITSA-N		
SMILES	OC[C@H]1O[C@H](O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.703	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

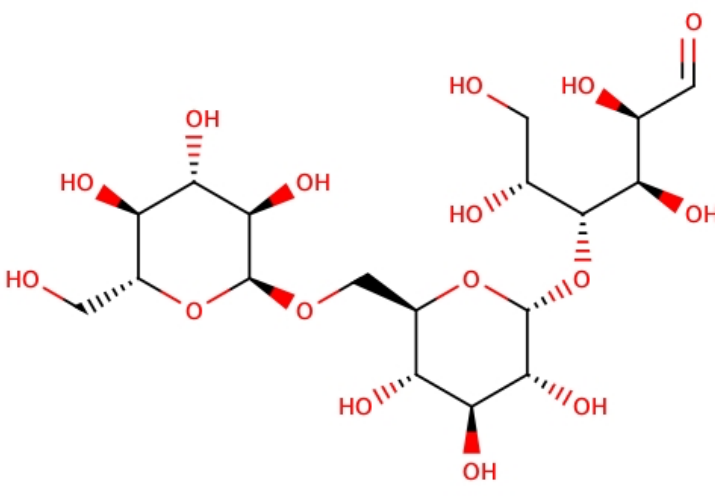
274. nigerose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301880		
TM-MC 성분 동의어	N/A		
PubChem ID	15560010		
InChI Key	QIGJYVCQYDKYDW-JWWQGTGASA-N		
SMILES	OC[C@H]1O[C@H](O[C@H]2[C@@H](O)C(O)O[C@H](CO)[C@H]2O)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₂ H ₂₂ O ₁₁		
Molecular Weight	342.297	Exact Molecular Weight	342.116211528
LogP	-4.703	Topological Polar Surface Area	189.53 Å ²
Atom Count	45	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	8
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.24	Oral Bioavailability	N

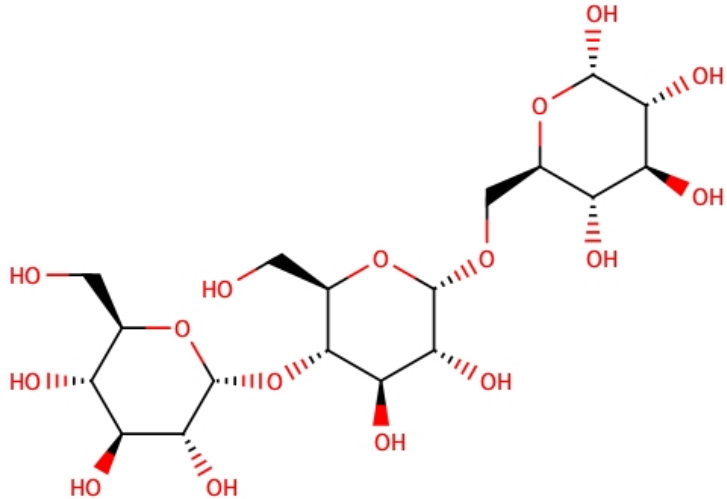
275. erlose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301247		
TM-MC 성분 동의어	N/A		
PubChem ID	193471		
InChI Key	FVVCFHXLWDDRHG-KKNDGLDKSA-N		
SMILES	<chem>OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO)[C@@H](O[C@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-6.3	Topological Polar Surface Area	268.68 Å ²
Atom Count	66	Structural Alert Count	0
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	8	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

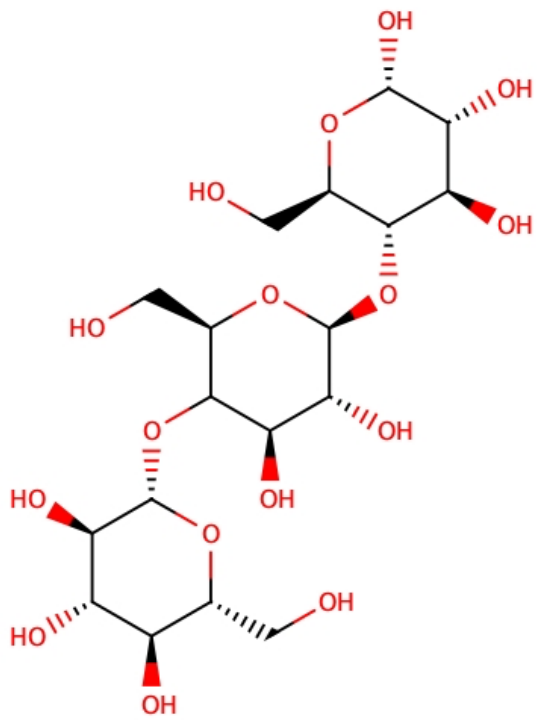
276. panose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	39091		
TM-MC 성분 동의어	N/A		
PubChem ID	94448		
InChI Key	ZCLAHGAZPPEVDX-MQHGYCBSA-N		
SMILES	OC[C@H](O)[C@H](O[C@H]1O[C@H](CO[C@H]2O[C@H](CO)[C@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@H]1O)[C@H](O)[C@H](O)C=O		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-7.11	Topological Polar Surface Area	276.52 Å ²
Atom Count	66	Structural Alert Count	1
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	11	Aromatic Ring Count	0
Drug Likeness	0.12	Oral Bioavailability	N

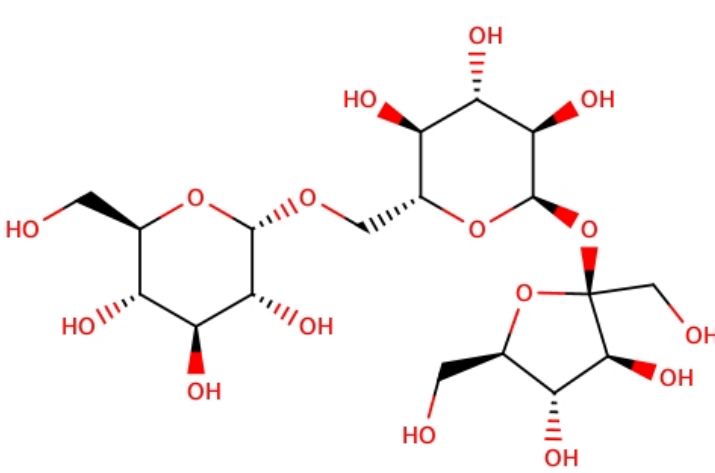
277. isopanose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	39095		
TM-MC 성분 동의어	N/A		
PubChem ID	5288413		
InChI Key	QSESWLKFTMBIPZ-QNHQVNOCSA-N		
SMILES	<chem>OC[C@H]1O[C@H](O[C@H]2[C@H](O)[C@@H](O)[C@@H](OC[C@H]3O[C@H](O)[C@H](O)[C@@H](O)[C@@H]3O)O[C@@H](O)[C@@H](O)[C@@H]2CO)[C@H](O)[C@@H](O)[C@@H]1O</chem>		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-6.474	Topological Polar Surface Area	268.68 Å ²
Atom Count	66	Structural Alert Count	0
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

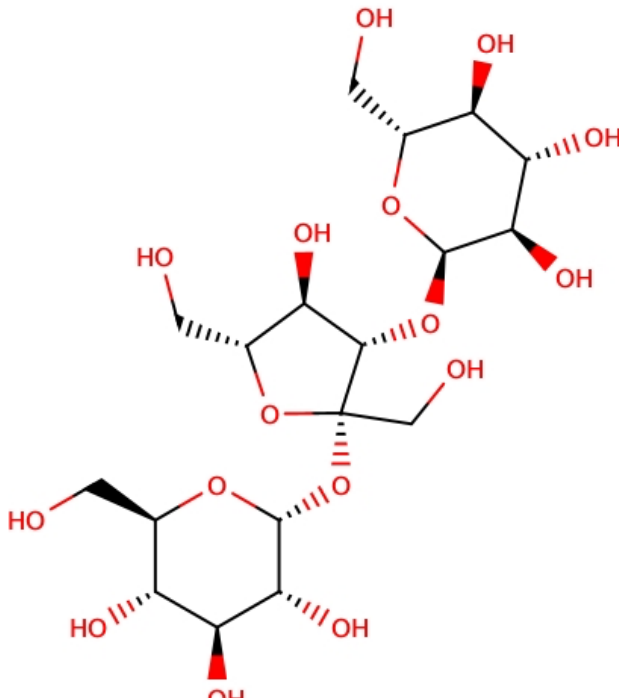
278. β-D-glucan

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	17313		
TM-MC 성분 동의어	maltotriose; β-glucan		
PubChem ID	46173706		
InChI Key	FYGDTMLNFKZSV-WFYNNLPOSA-N		
SMILES	OC[C@H]1O[C@@H](OC2[C@H](O)[C@@H](O)[C@H](O[C@H]3[C@H](O)[C@@H](O)[C@@H](O)O[C@H]3O)O[C@@H](O)O[C@@H](O)O[C@@H]2CO)O[C@@H](CO)[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-6.474	Topological Polar Surface Area	268.68 Å ²
Atom Count	66	Structural Alert Count	0
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

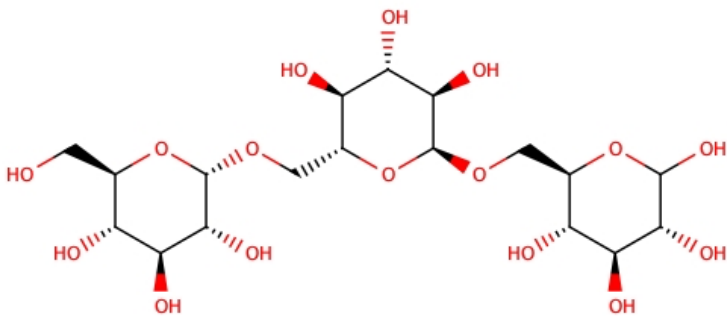
279. theanderose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	302584		
TM-MC 성분 동의어	N/A		
PubChem ID	91848658		
InChI Key	MUPFEKGTMRGPLJ-HRUWSWHBSA-N		
SMILES	<chem>OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO[C@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-6.3	Topological Polar Surface Area	268.68 Å ²
Atom Count	66	Structural Alert Count	0
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	8	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

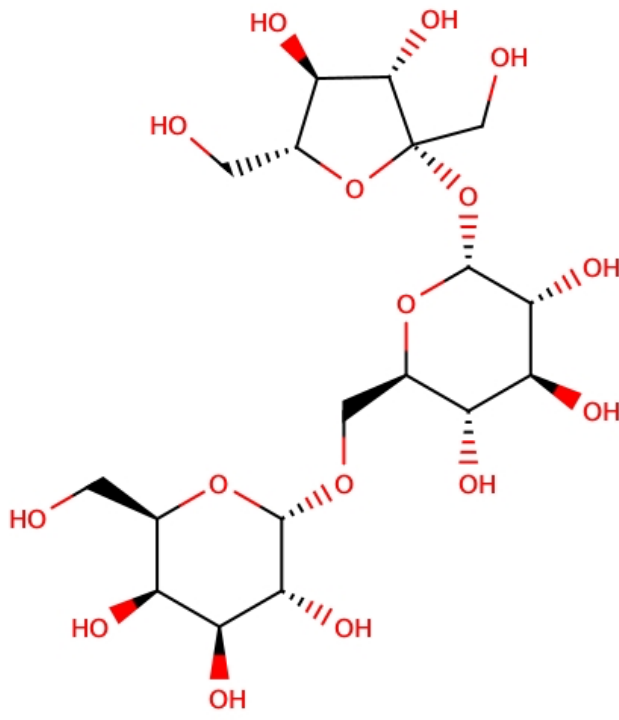
280. melezitose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	92817		
TM-MC 성분 동의어	N/A		
PubChem ID	92817		
InChI Key	QWIZNVHXZXRPRD-WSCXOGSTSA-N		
SMILES	OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H]1O		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-6.3	Topological Polar Surface Area	268.68 Å ²
Atom Count	66	Structural Alert Count	0
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	8	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

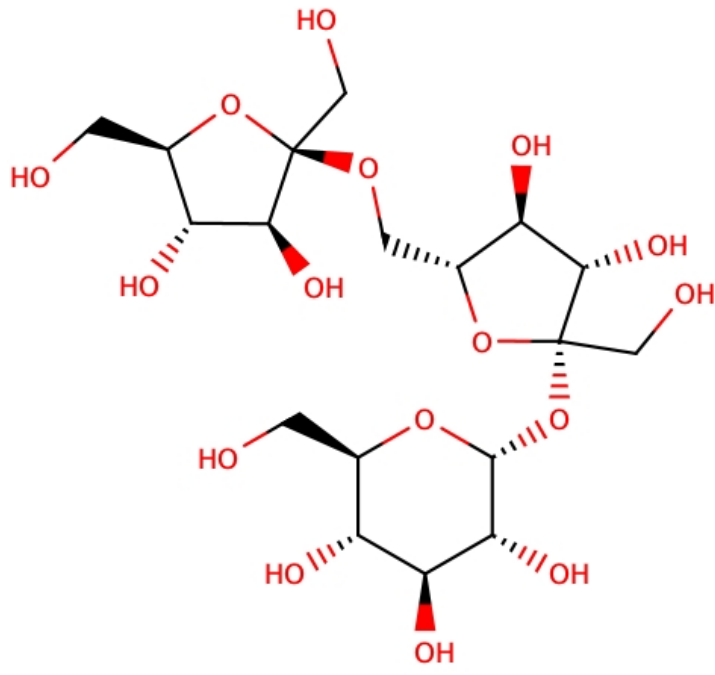
281. isomaltotriose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301522		
TM-MC 성분 동의어	N/A		
PubChem ID	439668		
InChI Key	FBJQEBRMDXPWNX-FYHZSNTMSA-N		
SMILES	<chem>OC[C@H]1O[C@H](OC[C@H]2O[C@H](OC[C@H]3OC(O)[C@H](O)[C@@H](O)[C@@H]3O)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@@H]1O</chem>		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-6.474	Topological Polar Surface Area	268.68 Å ²
Atom Count	66	Structural Alert Count	0
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

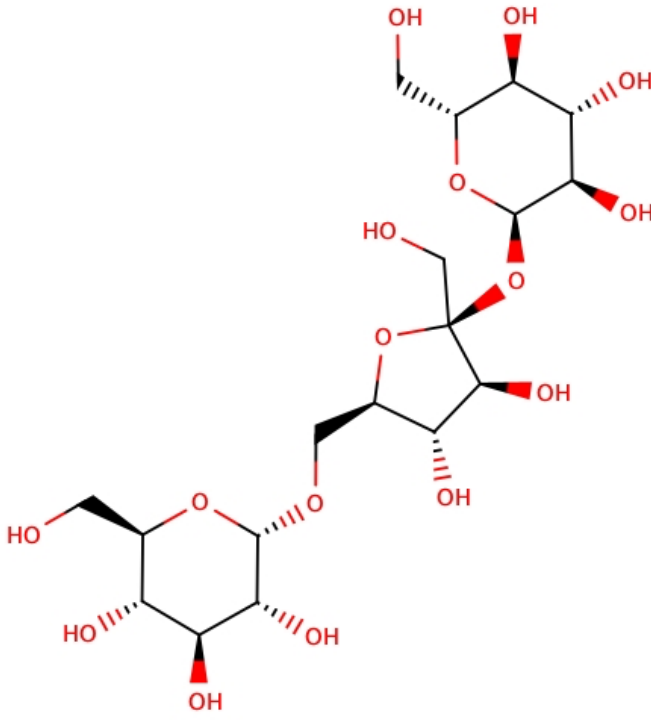
282. raffinose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	698388		
TM-MC 성분 동의어	N/A		
PubChem ID	439242		
InChI Key	MUPFEKGTMRGPLJ-ZQSKZDJDSA-N		
SMILES	OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO[C@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H]2O)[C@H](O)[C@H]1O		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-6.3	Topological Polar Surface Area	268.68 Å ²
Atom Count	66	Structural Alert Count	0
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	8	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

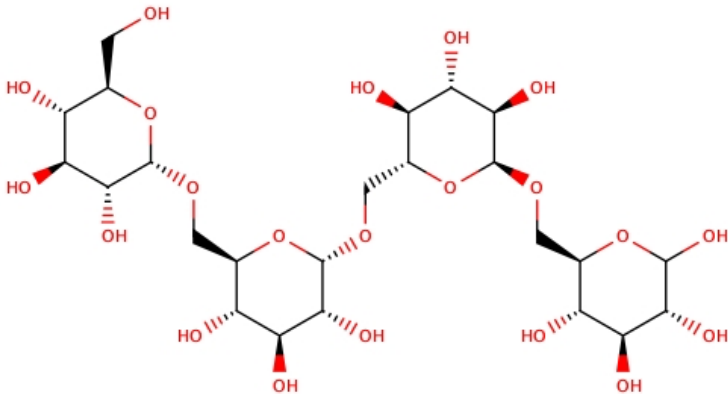
283. kestose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	304825		
TM-MC 성분 동의어	N/A		
PubChem ID	9914062		
InChI Key	ODEHMIGXGLNAKK-OESPXIITSA-N		
SMILES	OC[C@H]1O[C@@](CO)(OC[C@H]2O[C@@](CO)(O[C@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]3O)[C@@H](O)[C@H]2O)[C@@H](O)[C@H]1O		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-6.125	Topological Polar Surface Area	268.68 Å ²
Atom Count	66	Structural Alert Count	0
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	9	Aromatic Ring Count	0
Drug Likeness	0.14	Oral Bioavailability	N

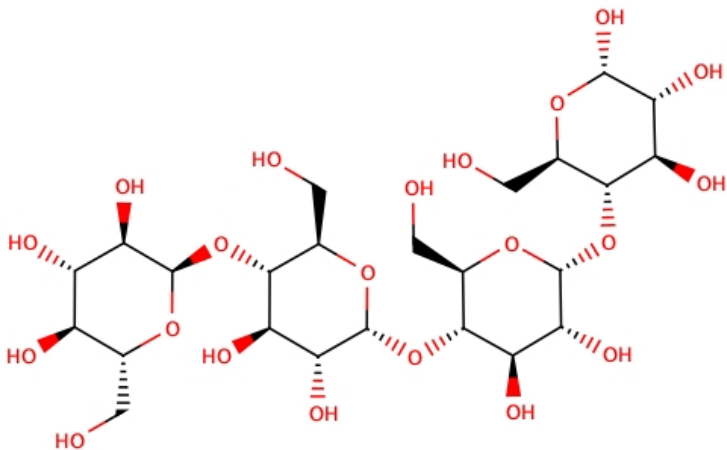
284. isomelezitose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301523		
TM-MC 성분 동의어	N/A		
PubChem ID	11306674		
InChI Key	NIBVDXPSJBYJFT-HRUWSWHBSA-N		
SMILES	OC[C@H]1O[C@H](OC[C@H]2O[C@@](CO)(O[C@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H]2O)[C@@H](O)[C@H]1O		
Molecular Formula	C ₁₈ H ₃₂ O ₁₆		
Molecular Weight	504.438	Exact Molecular Weight	504.16903495
LogP	-6.3	Topological Polar Surface Area	268.68 Å ²
Atom Count	66	Structural Alert Count	0
Hydrogen Bond Acceptor Count	16	Hydrogen Bond Donor Count	11
Rotatable Bond Count	8	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

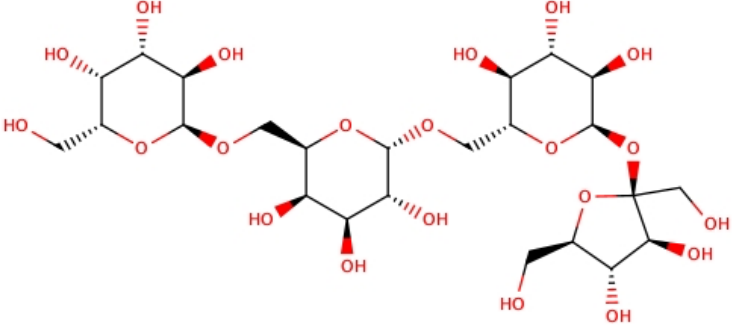
285. isomaltotetraose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	92380		
TM-MC 성분 동의어	N/A		
PubChem ID	13938912		
InChI Key	DFKPJBWUFOESDV-KGUZVYKUSA-N		
SMILES	<chem>OC[C@H]1O[C@H](OC[C@H]2O[C@H](OC[C@H]3O[C@H](OC[C@H]4OC(O)[C@H](O)[C@@H](O)[C@@H]4O)[C@H](O)[C@@H](O)[C@@H]3O)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@@H]1O</chem>		
Molecular Formula	C ₂₄ H ₄₂ O ₂₁		
Molecular Weight	666.579	Exact Molecular Weight	666.221858372
LogP	-8.245	Topological Polar Surface Area	347.83 Å ²
Atom Count	87	Structural Alert Count	0
Hydrogen Bond Acceptor Count	21	Hydrogen Bond Donor Count	14
Rotatable Bond Count	10	Aromatic Ring Count	0
Drug Likeness	0.10	Oral Bioavailability	N

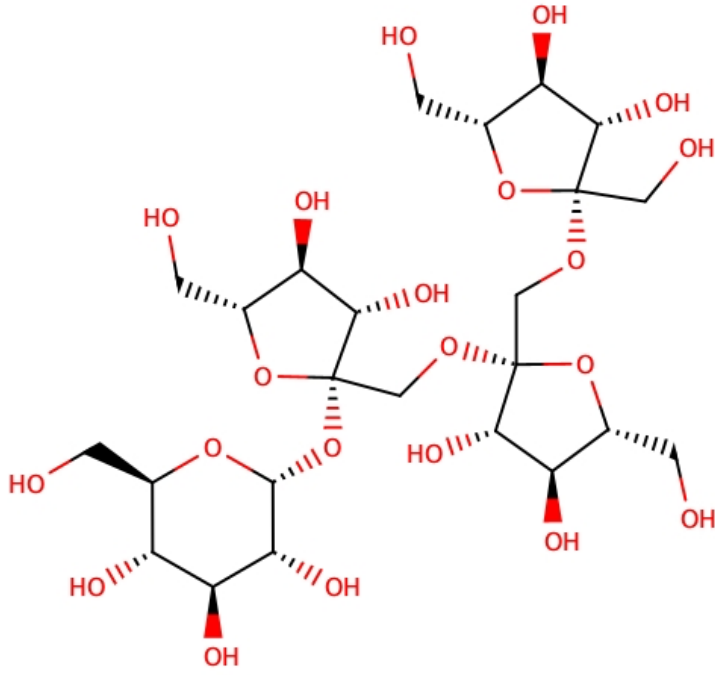
286. maltotetraose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301740		
TM-MC 성분 동의어	N/A		
PubChem ID	446495		
InChI Key	LUEWUZLMQUOBSB-ZLBHSGTGSA-N		
SMILES	<chem>OC[C@H]1O[C@H](O[C@H]2[C@H](O)[C@@H](O)[C@@H](O[C@H]3[C@H](O)[C@@H](O)[C@@H](O[C@H]4[C@H](O)[C@@H](O)[C@@H](O)O[C@@H]4CO)O[C@H]2CO)[C@H](O)[C@@H](O)[C@@H]1O</chem>		
Molecular Formula	C ₂₄ H ₄₂ O ₂₁		
Molecular Weight	666.579	Exact Molecular Weight	666.221858372
LogP	-8.245	Topological Polar Surface Area	347.83 Å ²
Atom Count	87	Structural Alert Count	0
Hydrogen Bond Acceptor Count	21	Hydrogen Bond Donor Count	14
Rotatable Bond Count	10	Aromatic Ring Count	0
Drug Likeness	0.10	Oral Bioavailability	N

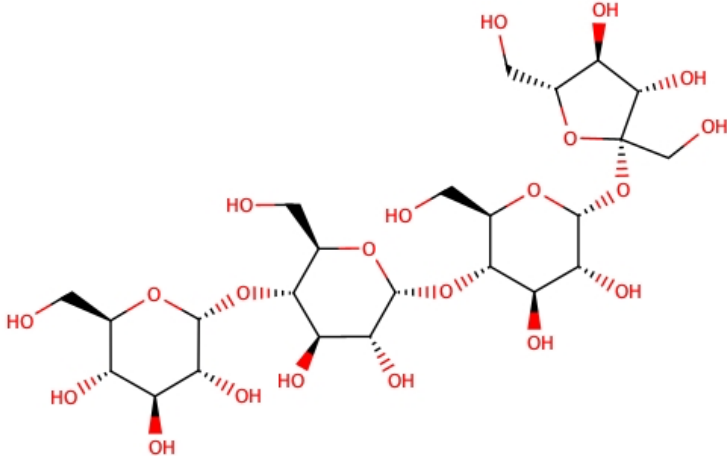
287. stachyose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	990894		
TM-MC 성분 동의어	N/A		
PubChem ID	439531		
InChI Key	UQZIYBXSHAGNOE-XNSRJBNMSA-N		
SMILES	<chem>OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO[C@H]3O[C@H](CO[C@H]4O[C@H](CO)[C@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₂₄ H ₄₂ O ₂₁		
Molecular Weight	666.579	Exact Molecular Weight	666.221858372
LogP	-8.071	Topological Polar Surface Area	347.83 Å ²
Atom Count	87	Structural Alert Count	0
Hydrogen Bond Acceptor Count	21	Hydrogen Bond Donor Count	14
Rotatable Bond Count	11	Aromatic Ring Count	0
Drug Likeness	0.10	Oral Bioavailability	N

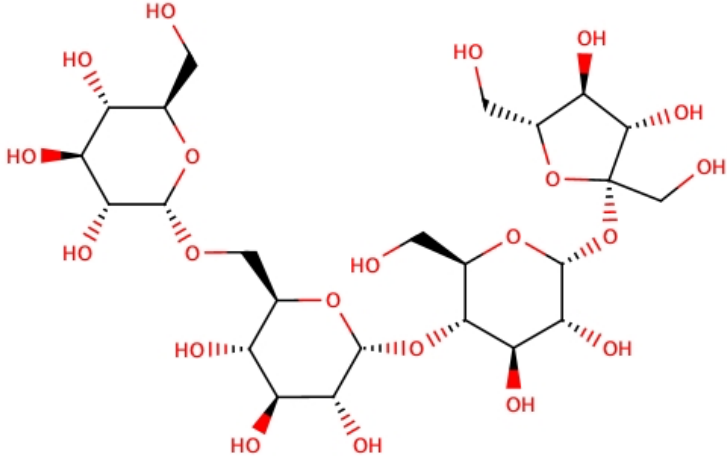
288. nystose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	166775		
TM-MC 성분 동의어	N/A		
PubChem ID	166775		
InChI Key	FLDFNEBHXLZRX-DLQNOBSRSA-N		
SMILES	<chem>OC[C@H]1O[C@@](CO)(OC[C@@]2(OC[C@@]3(O[C@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]4O)O[C@H](CO)[C@@H](O)[C@@H]3O)O[C@H](CO)[C@@H](O)[C@@H]2O)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₂₄ H ₄₂ O ₂₁		
Molecular Weight	666.579	Exact Molecular Weight	666.221858372
LogP	-7.721	Topological Polar Surface Area	347.83 Å ²
Atom Count	87	Structural Alert Count	0
Hydrogen Bond Acceptor Count	21	Hydrogen Bond Donor Count	14
Rotatable Bond Count	13	Aromatic Ring Count	0
Drug Likeness	0.09	Oral Bioavailability	N

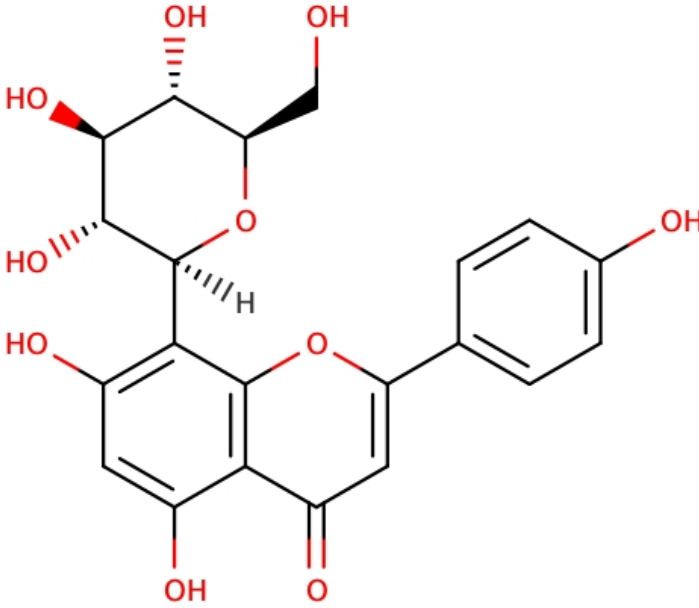
289. α-4'-glucosyl-erlose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301277		
TM-MC 성분 동의어	N/A		
PubChem ID	91850252		
InChI Key	JFISLVOULYSJEI-YZVYRDJSSA-N		
SMILES	<chem>OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO)[C@@H](O[C@H]3O[C@H](CO)[C@@H](O[C@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H]3O)[C@H](O)[C@H]2O)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₂₄ H ₄₂ O ₂₁		
Molecular Weight	666.579	Exact Molecular Weight	666.221858372
LogP	-8.071	Topological Polar Surface Area	347.83 Å ²
Atom Count	87	Structural Alert Count	0
Hydrogen Bond Acceptor Count	21	Hydrogen Bond Donor Count	14
Rotatable Bond Count	11	Aromatic Ring Count	0
Drug Likeness	0.10	Oral Bioavailability	N

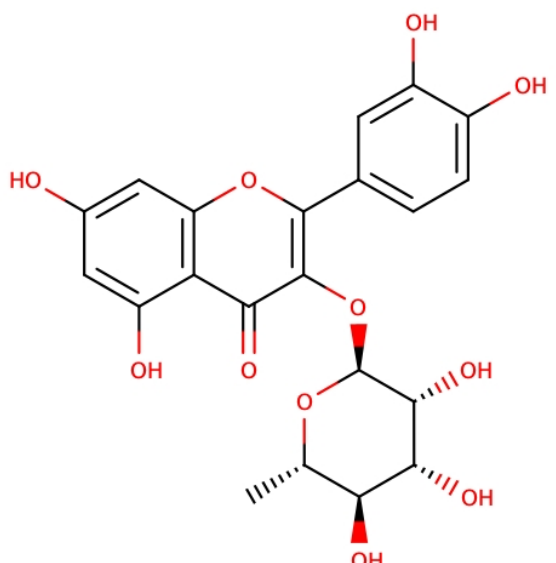
290. α-6'-glucosyl-erlose

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	301278		
TM-MC 성분 동의어	N/A		
PubChem ID	91855986		
InChI Key	GPNLTLFZLXKLIJ-BBYWSZLGSA-N		
SMILES	<chem>OC[C@H]1O[C@@](CO)(O[C@H]2O[C@H](CO)[C@@H](O[C@H]3O[C@H](CO[C@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H]2O)[C@@H](O)[C@@H]1O</chem>		
Molecular Formula	C ₂₄ H ₄₂ O ₂₁		
Molecular Weight	666.579	Exact Molecular Weight	666.221858372
LogP	-8.071	Topological Polar Surface Area	347.83 Å ²
Atom Count	87	Structural Alert Count	0
Hydrogen Bond Acceptor Count	21	Hydrogen Bond Donor Count	14
Rotatable Bond Count	11	Aromatic Ring Count	0
Drug Likeness	0.10	Oral Bioavailability	N

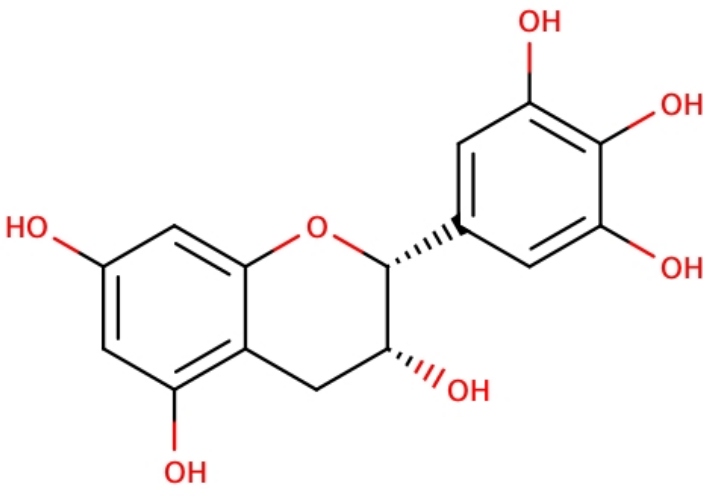
291. vitexin

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	6855		
TM-MC 성분 동의어	apigenin 8-C-glucoside; apigenin-8-C-glucoside; 8-C-glucosyl apigenin; 8-glycosyl apigenin		
PubChem ID	5280441		
InChI Key	SGEWCQFRYRRZDC-VPRICQMDSA-N		
SMILES	OC[C@H]1O[C@H]([C@H](O)[C@@H](O)[C@@H]1O)c1c(O)cc(O)c2c1oc(c2=O)-c1ccc(O)cc1		
Molecular Formula	C ₂₁ H ₂₀ O ₁₀		
Molecular Weight	432.381	Exact Molecular Weight	432.105646844
LogP	-0.051	Topological Polar Surface Area	177.14 Å ²
Atom Count	51	Structural Alert Count	0
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	7
Rotatable Bond Count	3	Aromatic Ring Count	3
Drug Likeness	0.30	Oral Bioavailability	N

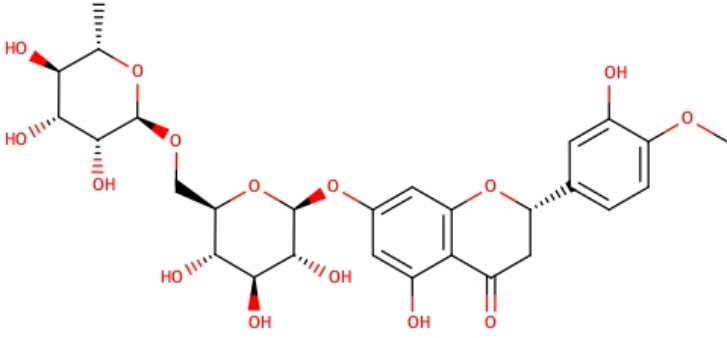
292. quercitrin

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	91599		
TM-MC 성분 동의어	quercetin-3-O-rhamnoside; quercetin 3-O-rhamnoside; quercetin-3-rhamnoside; quercetin 3-O- α -L-rhamnoside; quercetin-3-O- α -L-rhamnoside; quercetrin; quercetin 3-rhamnoside; quercetin-3-O-L-rhamnoside; quercetin 3-O- α -L-rhamnopyranoside; quercetin-3-O-rhamnose; quericitrin; quercitroside; quercetin 3-O-L-rhamnoside; 3-O-(α -L-rhamnosyl)quercetin; quercetin-3-O- β -D-rhamnoside; quercetin-3-O- α -L-rhamnoside; quercetin 3-O- α -L-rhamnopyranoside; quercetin-3- α -L-rhamnopyranoside; quercetin-3-O- α -L-rhamnopyranoside		
PubChem ID	5280459		
InChI Key	OXGUCUVFOIWWQJ-HQBVPOQASA-N		
SMILES	<chem>C[C@@H]1O[C@@H](Oc2c(oc3cc(O)cc(O)c3c2=O)-c2ccc(O)c(O)c2)[C@H](O)[C@H](O)[C@H]1O</chem>		
Molecular Formula	C ₂₁ H ₂₀ O ₁₁		
Molecular Weight	448.38	Exact Molecular Weight	448.100561464
LogP	0.902	Topological Polar Surface Area	186.37 Å ²
Atom Count	52	Structural Alert Count	1
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	7
Rotatable Bond Count	3	Aromatic Ring Count	3
Drug Likeness	0.28	Oral Bioavailability	N

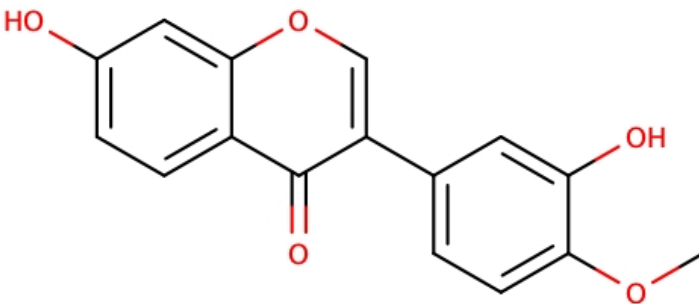
293. (-)-epigallocatechin

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	40003		
TM-MC 성분 동의어	N/A		
PubChem ID	72277		
InChI Key	XMOCLSLCDHWDHP-IUODEOHRSA-N		
SMILES	O[C@@H]1Cc2c(O)cc(O)cc2O[C@@H]1c1cc(O)c(O)c(O)c1		
Molecular Formula	C ₁₅ H ₁₄ O ₇		
Molecular Weight	306.27	Exact Molecular Weight	306.073952791
LogP	1.492	Topological Polar Surface Area	130.61 Å ²
Atom Count	36	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	6
Rotatable Bond Count	1	Aromatic Ring Count	2
Drug Likeness	0.44	Oral Bioavailability	Y

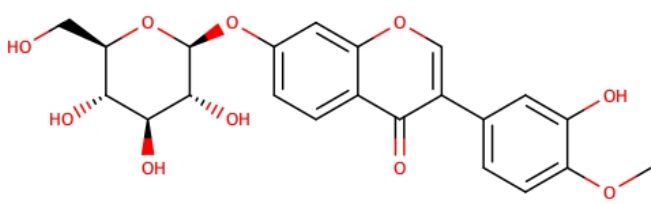
294. hesperidin

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	92314		
TM-MC 성분 동의어	hesperidoside; hesperedin; hespiridin; hesperetin-7-O-rutinoside		
PubChem ID	10621		
InChI Key	QUQPHWDTPGMPEX-QJBIFVCTSA-N		
SMILES	COc1ccc(cc1O)[C@@H]1CC(=O)c2c(O)cc(O[C@@H]3O[C@H](CO[C@@H]4O[C@@H](C)[C@H](O)[C@@H](O)[C@H]4O)[C@@H](O)[C@H](O)[C@H]3O)c2O1		
Molecular Formula	C ₂₈ H ₃₄ O ₁₅		
Molecular Weight	610.565	Exact Molecular Weight	610.189770395
LogP	-0.315	Topological Polar Surface Area	234.29 Å ²
Atom Count	77	Structural Alert Count	0
Hydrogen Bond Acceptor Count	15	Hydrogen Bond Donor Count	8
Rotatable Bond Count	7	Aromatic Ring Count	2
Drug Likeness	0.20	Oral Bioavailability	N

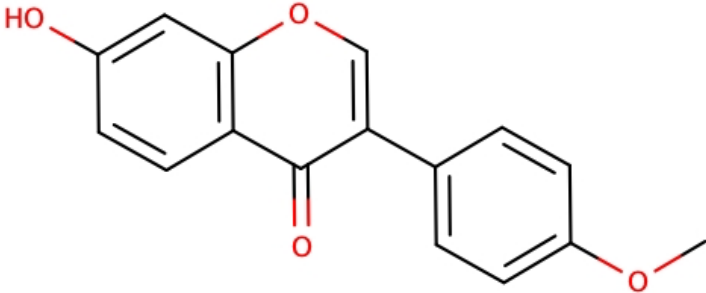
295. calycosin

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	4551		
TM-MC 성분 동의어	7,3'-dihydroxy-4'-methoxyisoflavone; 3',7-dihydroxy-4'-methoxy-isoflavone; calycosine; 3',7-dihydroxy-4'-methoxylisoflavone		
PubChem ID	5280448		
InChI Key	ZZAJQOPSWWVMBI-UHFFFAOYSA-N		
SMILES	<chem>COC1CCC(CC1O)-C1C(=O)C2=CC(O)=CC=C2O</chem>		
Molecular Formula	C ₁₆ H ₁₂ O ₅		
Molecular Weight	284.267	Exact Molecular Weight	284.068473486
LogP	2.573	Topological Polar Surface Area	75.99 Å ²
Atom Count	33	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.76	Oral Bioavailability	Y

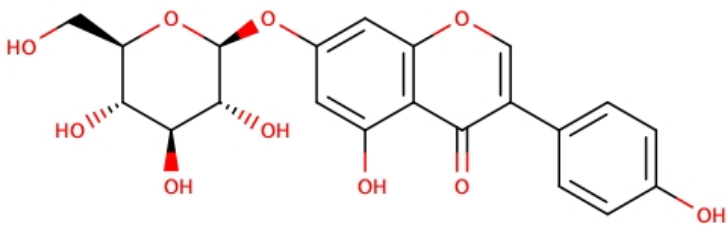
296. calycosin-7-O-β-D-glucoside

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	8493		
TM-MC 성분 동의어	calycosin-7-O-β-D-glucopyranoside; calycosin-7-glucoside; calycosin-7-O-β-D-glycoside; calycosin 7-O-glucoside; calycosin-7-O-glucoside; 5'-hydroxyononin; calycosin-7-O-glycoside; calycosine-O-β-D-glucoside; calycosine-7-O-β-D-glucoside; calycosin 7-β-D-glucopyranoside		
PubChem ID	5318267		
InChI Key	WACBUPFEGWUGPB-MIUGBVLSSA-N		
SMILES	COc1ccc(cc1O)-c1coc2cc(O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)ccc2c1=O		
Molecular Formula	C ₂₂ H ₂₂ O ₁₀		
Molecular Weight	446.408	Exact Molecular Weight	446.121296908
LogP	0.305	Topological Polar Surface Area	155.14 Å ²
Atom Count	54	Structural Alert Count	0
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	5
Rotatable Bond Count	5	Aromatic Ring Count	3
Drug Likeness	0.37	Oral Bioavailability	N

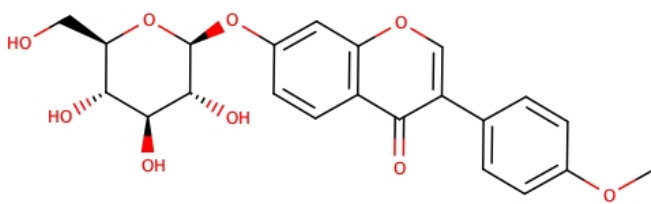
297. formononetin

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	10624		
TM-MC 성분 동의어	fermononetin; 7-hydroxy-4'-methoxyisoflavone		
PubChem ID	5280378		
InChI Key	HKQYGTCOHHOMP-UHFFFAOYSA-N		
SMILES	COc1ccc(cc1)-c1coc2cc(O)ccc2c1=O		
Molecular Formula	C ₁₆ H ₁₂ O ₄		
Molecular Weight	268.268	Exact Molecular Weight	268.073558866
LogP	2.876	Topological Polar Surface Area	55.76 Å ²
Atom Count	32	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	3
Drug Likeness	0.78	Oral Bioavailability	Y

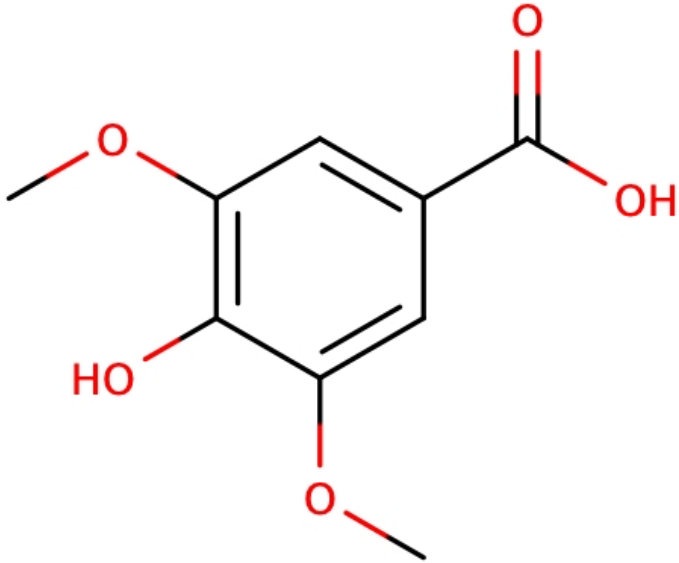
298. genistin

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	317062		
TM-MC 성분 동의어	genistein-7-O-glucoside; genistein-7-O-β-D-glucoside; genistein-7-O-β-glucopyranoside		
PubChem ID	5281377		
InChI Key	ZCOLJUOHXRHDI-CMWLGVBASA-N		
SMILES	<chem>OC[C@H]1O[C@@H](Oc2cc(O)c3c(c2)occ(-c2ccc(O)cc2)c3=O)[C@H](O)[C@@H](O)[C@@H]1O</chem>		
Molecular Formula	C ₂₁ H ₂₀ O ₁₀		
Molecular Weight	432.381	Exact Molecular Weight	432.105646844
LogP	0.809	Topological Polar Surface Area	166.14 Å ²
Atom Count	51	Structural Alert Count	0
Hydrogen Bond Acceptor Count	10	Hydrogen Bond Donor Count	6
Rotatable Bond Count	4	Aromatic Ring Count	3
Drug Likeness	0.35	Oral Bioavailability	N

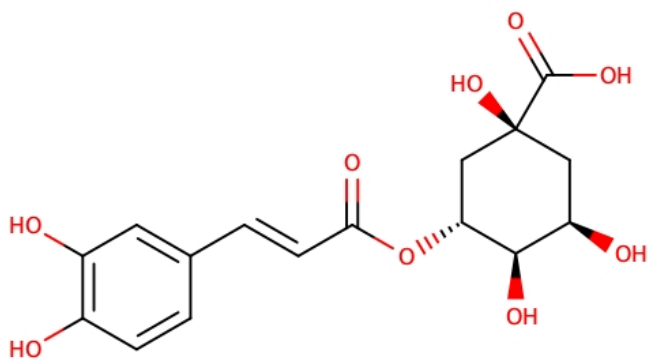
299. ononin

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	442813		
TM-MC 성분 동의어	formononetin 7-O-β-D-glucoside; formononetin 7-O-glucoside; formononetin-7-O-β-D-glucoside; formononetin 7-O-β-D-glycoside; formononetin 7-O-β-D-glucopyranoside; formononetin-7-O-glycoside; formononetin-7-O-β-D-glycoside		
PubChem ID	442813		
InChI Key	MGJLSBDCWOSMHL-MIUGBVLSSA-N		
SMILES	COc1ccc(cc1)-c1coc2cc(O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)ccc2c1=O		
Molecular Formula	C ₂₂ H ₂₂ O ₉		
Molecular Weight	430.409	Exact Molecular Weight	430.126382288
LogP	0.608	Topological Polar Surface Area	134.91 Å ²
Atom Count	53	Structural Alert Count	0
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	3
Drug Likeness	0.46	Oral Bioavailability	Y

300. syringic acid

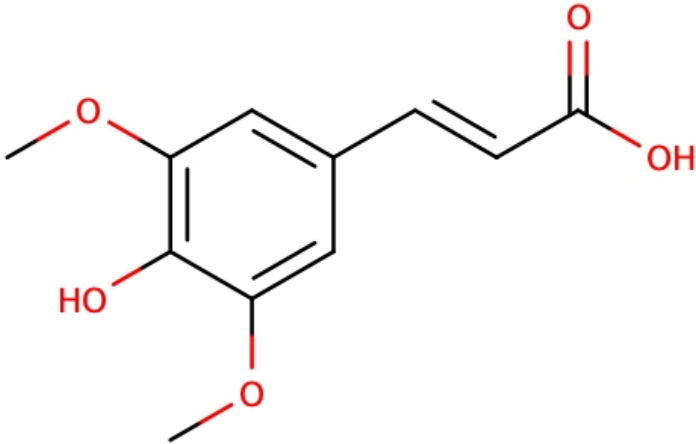
화학 구조		PubMed ID	
		22239430, 23265456 29738446	
TM-MC 성분 ID	173		
TM-MC 성분 동의어	3,5-dimethoxy-4-hydroxybenzoic acid		
PubChem ID	10742		
InChI Key	JMSVCTWVEWCHDZ-UHFFFAOYSA-N		
SMILES	<chem>COc1cc(cc(OC)c1O)C(O)=O</chem>		
Molecular Formula	C ₉ H ₁₀ O ₅		
Molecular Weight	198.174	Exact Molecular Weight	198.052823422
LogP	1.012	Topological Polar Surface Area	75.99 Å ²
Atom Count	24	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.70	Oral Bioavailability	Y

301. chlorogenic acid

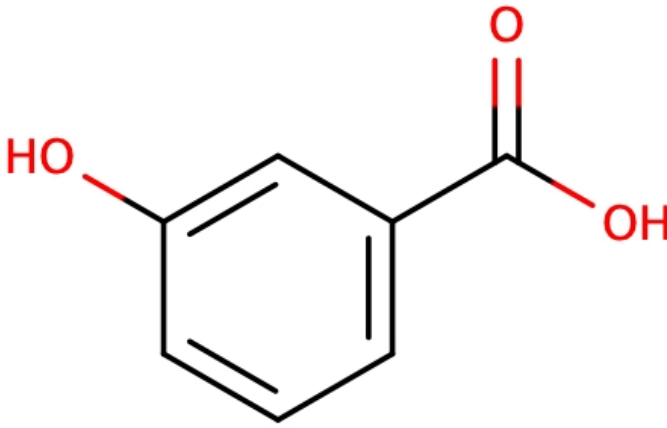
화학 구조	PubMed ID
	<p>22239430, 23265456 29337369, 29738446</p>

TM-MC 성분 ID	174		
TM-MC 성분 동의어	3-O-caffeoylquinic acid; 3-caffeoylquinic acid; caffeoylquinic acid; 3-O-caffeoylquinic acid; 3-O-caffeoyl-D-quinic acid; 3-chlorogenic acid; caffeoyl quinic acid; 3'-caffeolquinic acid; trans-chlorogenic acid; 3-O-caffeoyl-quinic acid; trans-3-caffeoylquinic acid; 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-cyclohexanecarboxylic acid		
PubChem ID	1794427		
InChI Key	CWVRJTMFETXNAD-JUHZACGLSA-N		
SMILES	O[C@@H]1C[C@](O)(C[C@@H](OC(=O)WC=CWc2ccc(O)c(O)c2)[C@@H]1O)C(=O)=O		
Molecular Formula	C ₁₆ H ₁₈ O ₉		
Molecular Weight	354.311	Exact Molecular Weight	354.09508216
LogP	-0.269	Topological Polar Surface Area	164.75 Å ²
Atom Count	43	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	6
Rotatable Bond Count	5	Aromatic Ring Count	1
Drug Likeness	0.24	Oral Bioavailability	N

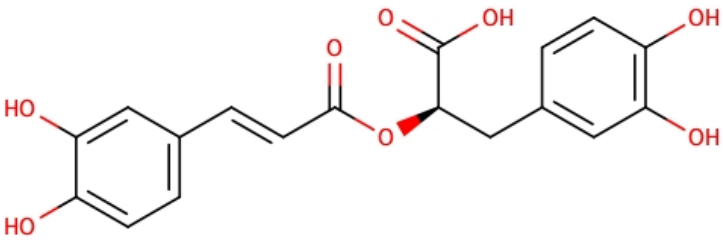
302. sinapic acid

화학 구조		PubMed ID	
		22239430, 29337369 29738446, 31227360	
TM-MC 성분 ID	265		
TM-MC 성분 동의어	sinapinic acid; 3,5-dimethoxy-4-hydroxycinnamic acid		
PubChem ID	637775		
InChI Key	PCMORTLOPMLFEB-ONEGZZNKSA-N		
SMILES	<chem>COC1cc(=C(C=C1)C(=O)O)C(OC)C1O</chem>		
Molecular Formula	C ₁₁ H ₁₂ O ₅		
Molecular Weight	224.212	Exact Molecular Weight	224.068473486
LogP	1.517	Topological Polar Surface Area	75.99 Å ²
Atom Count	28	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.76	Oral Bioavailability	Y

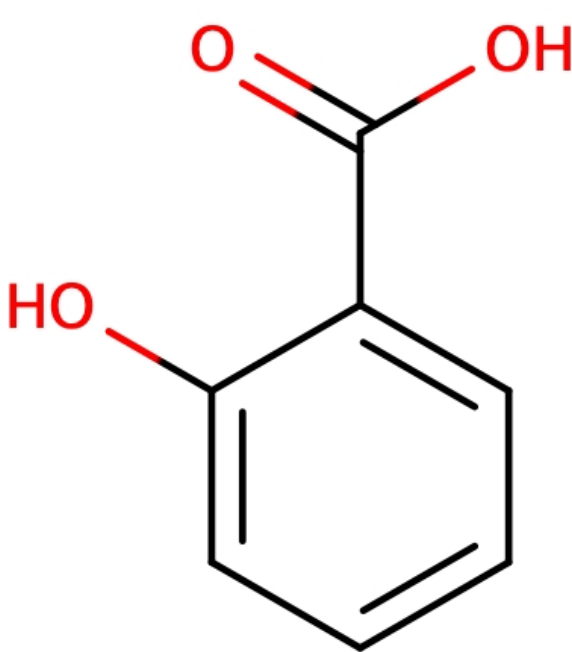
303. 3-hydroxybenzoic acid

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	7420		
TM-MC 성분 동의어	m-hydroxybenzoic acid; 3-OH benzoic acid; 3-hydroxy benzoic acid		
PubChem ID	7420		
InChI Key	IJFXRHURBJZNAO-UHFFFAOYSA-N		
SMILES	<chem>OC(=O)c1cccc(O)c1</chem>		
Molecular Formula	C ₇ H ₆ O ₃		
Molecular Weight	138.122	Exact Molecular Weight	138.031694053
LogP	1.327	Topological Polar Surface Area	57.53 Å ²
Atom Count	16	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.61	Oral Bioavailability	Y

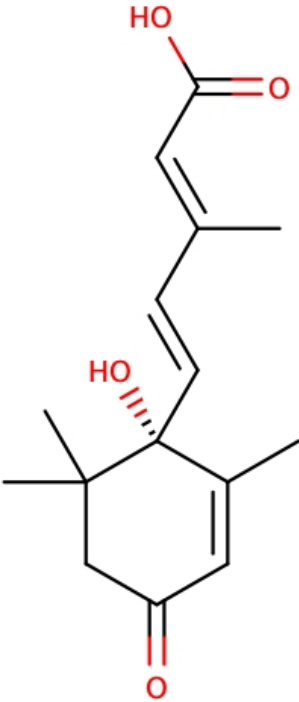
304. rosmarinic acid

화학 구조		PubMed ID	
		29337369, 31227360	
TM-MC 성분 ID	15454		
TM-MC 성분 동의어	rosmarimic acid; rosemarinic acid; rosemary acid		
PubChem ID	5281792		
InChI Key	DOUMFZQKYFQNTF-WUTVXBCWSA-N		
SMILES	<chem>OC(=O)[C@@H](Cc1ccc(O)c(O)c1)OC(=O)C=Cc2ccc(O)c(O)c2</chem>		
Molecular Formula	C ₁₈ H ₁₆ O ₈		
Molecular Weight	360.318	Exact Molecular Weight	360.084517475
LogP	3.004	Topological Polar Surface Area	144.52 Å ²
Atom Count	42	Structural Alert Count	3
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	5
Rotatable Bond Count	7	Aromatic Ring Count	2
Drug Likeness	0.29	Oral Bioavailability	Y

305. salicylic acid

화학 구조		PubMed ID	
		28032995, 29738446	
TM-MC 성분 ID	93273		
TM-MC 성분 동의어	2-hydroxyl benzoic acid; salicylic acid; 2-hydroxybenzoic acid; o-hydroxy-benzoic acid		
PubChem ID	338, 118212070		
InChI Key	YGSDEFMJJLZEOE-UHFFFAOYSA-N		
SMILES	OC(=O)c1ccccc1O		
Molecular Formula	C ₇ H ₆ O ₃		
Molecular Weight	138.122	Exact Molecular Weight	138.031694053
LogP	1.977	Topological Polar Surface Area	57.53 Å ²
Atom Count	16	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.62	Oral Bioavailability	Y

306. abscisic acid

화학 구조		PubMed ID	
		28032995, 29738446	
TM-MC 성분 ID	280896		
TM-MC 성분 동의어	(+)-abscisic acid; (S)-(+)-abscisic acid		
PubChem ID	5702609		
InChI Key	JLIDBLDQVAYHNE-IBPUIESWSA-N		
SMILES	<chem>C#C(=C=C[C@@]1(O)C(C)=CC(=O)CC1(C)C)=C/C(O)=O</chem>		
Molecular Formula	C ₁₅ H ₂₀ O ₄		
Molecular Weight	264.321	Exact Molecular Weight	264.136159124
LogP	2.093	Topological Polar Surface Area	74.6 Å ²
Atom Count	39	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.60	Oral Bioavailability	Y

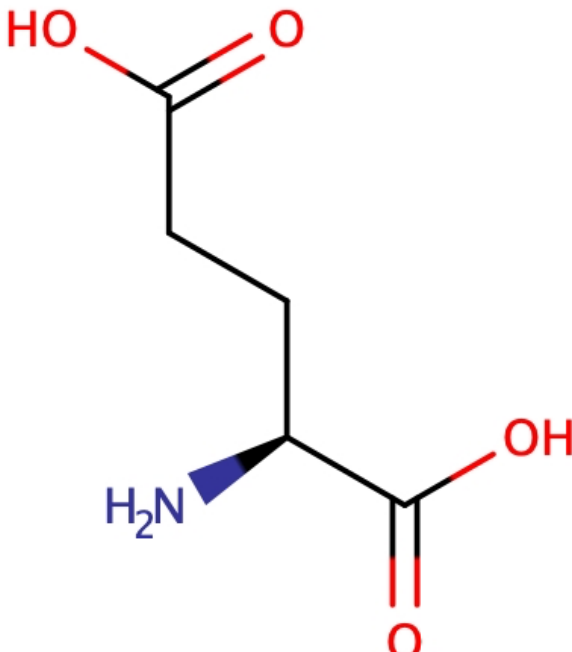
307. (-)-abscisic acid

화학 구조		PubMed ID	
		29738446	
TM-MC 성분 ID	280897		
TM-MC 성분 동의어	N/A		
PubChem ID	636693		
InChI Key	JLIDBLDQVAYHNE-XQFZKXHBSA-N		
SMILES	CWC(WC=CW[C@]1(O)C(C)=CC(=O)CC1(C)C)=C/C(O)=O		
Molecular Formula	C ₁₅ H ₂₀ O ₄		
Molecular Weight	264.321	Exact Molecular Weight	264.136159124
LogP	2.093	Topological Polar Surface Area	74.6 Å ²
Atom Count	39	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.60	Oral Bioavailability	Y

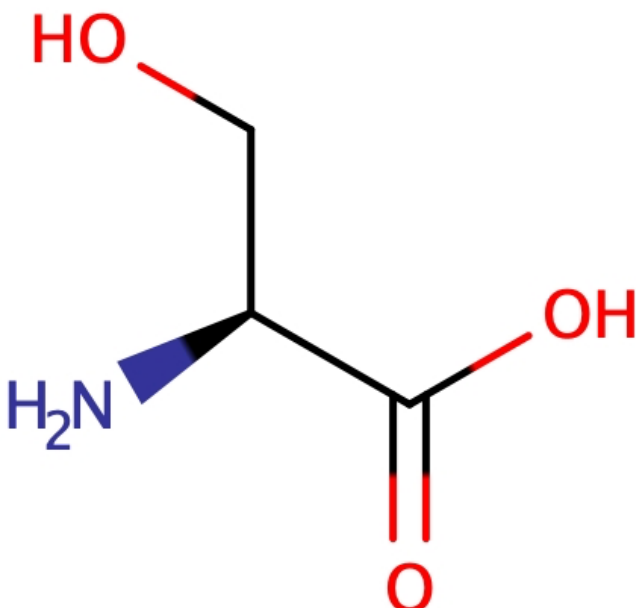
308. aspartic acid

화학 구조		PubMed ID	
		25780666, 25830058 27558519	
TM-MC 성분 ID	176		
TM-MC 성분 동의어	Asp; L-aspartic acid; asparaginic acid		
PubChem ID	5960, 44367445, 139060126		
InChI Key	CKLJMWZIZZHCS-REOHCLBHSA-N		
SMILES	N[C@@H](CC(O)=O)C(O)=O		
Molecular Formula	C ₄ H ₇ NO ₄		
Molecular Weight	133.103	Exact Molecular Weight	133.037507709
LogP	-3.504	Topological Polar Surface Area	100.62 Å ²
Atom Count	16	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.37	Oral Bioavailability	Y

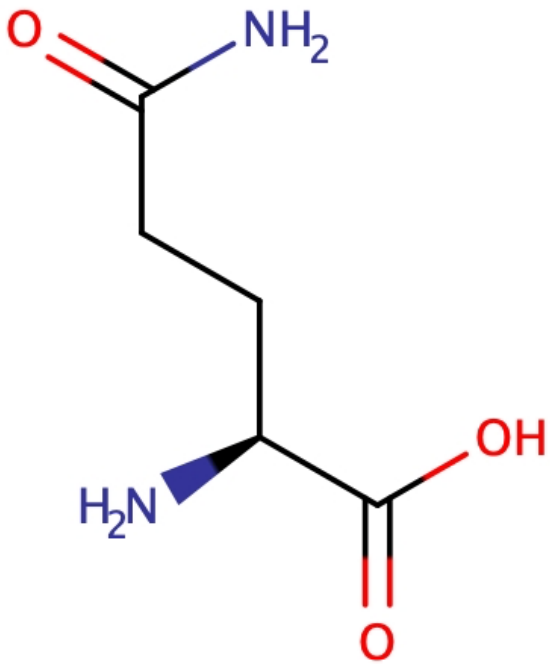
309. glutamic acid

화학 구조		PubMed ID	
		19149256, 25780666 27558519	
TM-MC 성분 ID	177		
TM-MC 성분 동의어	Glu; glutamate; L-glutamate; L-glutamic acid		
PubChem ID	33032, 44272391, 88747398		
InChI Key	WHUUTDBJXRKMK-VKHYHEASA-N		
SMILES	N[C@@H](CCC(O)=O)C(O)=O		
Molecular Formula	C ₅ H ₉ NO ₄		
Molecular Weight	147.13	Exact Molecular Weight	147.053157774
LogP	-3.241	Topological Polar Surface Area	100.62 Å ²
Atom Count	19	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.39	Oral Bioavailability	Y

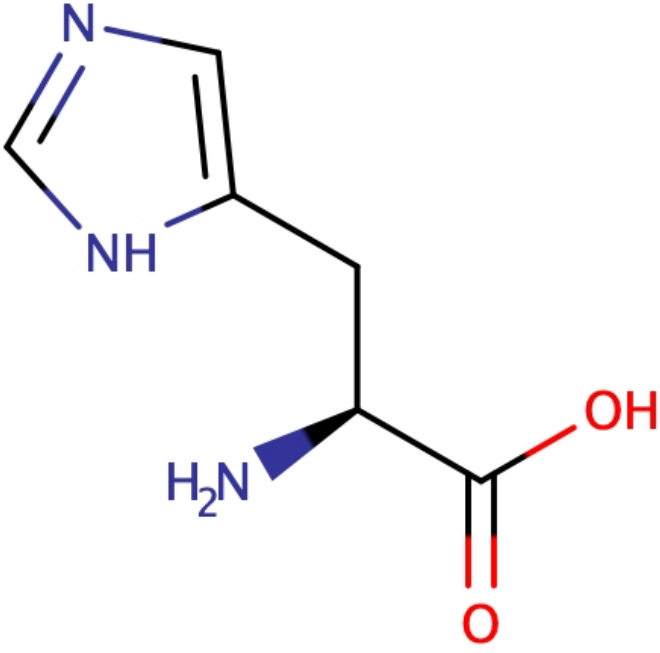
310. serine

화학 구조		PubMed ID	
		17134710, 25780666 27558519	
TM-MC 성분 ID	178		
TM-MC 성분 동의어	Ser; L-serine		
PubChem ID	5951, 6857581		
InChI Key	MTCFGRXMJLQNBG-REOHCLBHSA-N		
SMILES	N[C@@H](CO)C(O)=O		
Molecular Formula	C ₃ H ₇ NO ₃		
Molecular Weight	105.093	Exact Molecular Weight	105.042593089
LogP	-3.888	Topological Polar Surface Area	83.55 Å ²
Atom Count	14	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.34	Oral Bioavailability	Y

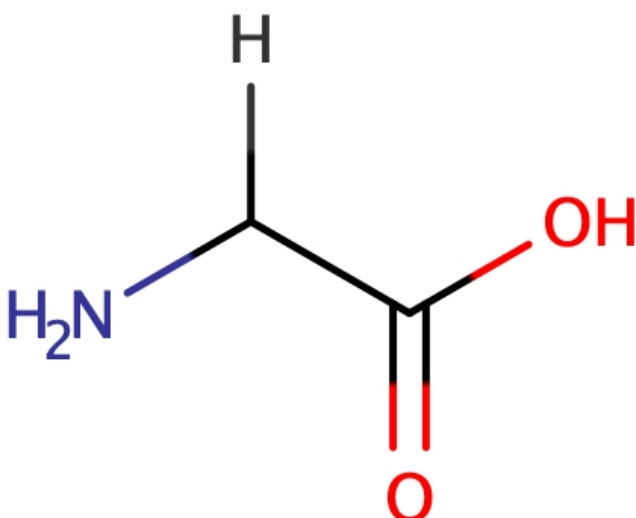
311. glutamine

화학 구조		PubMed ID	
		27558519	
TM-MC 성분 ID	179		
TM-MC 성분 동의어	Gln		
PubChem ID	5961, 6992086		
InChI Key	ZDXPYRJPNDTMRX-VKHMHEASA-N		
SMILES	N[C@@H](CCC(N)=O)C(O)=O		
Molecular Formula	C ₅ H ₁₀ N ₂ O ₃		
Molecular Weight	146.146	Exact Molecular Weight	146.06914219
LogP	-4.001	Topological Polar Surface Area	106.41 Å ²
Atom Count	20	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.38	Oral Bioavailability	Y

312. histidine

화학 구조		PubMed ID	
		<p>17134710, 25780666 27558519, 31640173</p>	
TM-MC 성분 ID	180		
TM-MC 성분 동의어	His; L-histidine		
PubChem ID	6274, 6971009		
InChI Key	HNDVDQJCIGZPNO-YFKPBYRVSA-N		
SMILES	N[C@@H](Cc1cnc[nH]1)C(O)=O		
Molecular Formula	C ₆ H ₉ N ₃ O ₂		
Molecular Weight	155.157	Exact Molecular Weight	155.069476542
LogP	-3.616	Topological Polar Surface Area	92 Å ²
Atom Count	20	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.42	Oral Bioavailability	Y

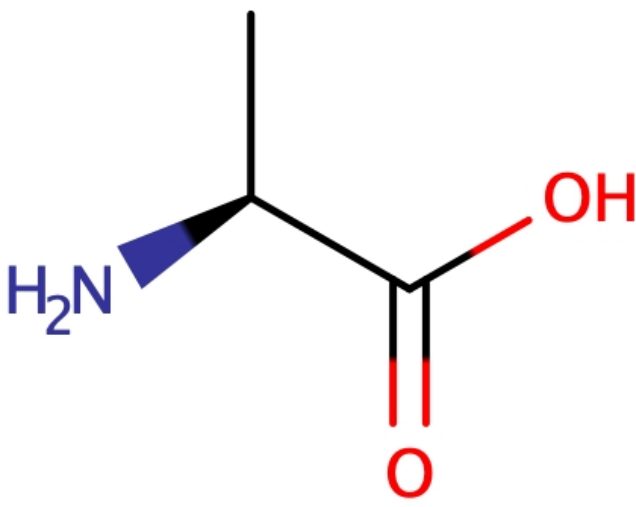
313. glycine

화학 구조		PubMed ID	
		17134710, 25780666 27558519	
TM-MC 성분 ID	181		
TM-MC 성분 동의어	Gly		
PubChem ID	750, 5257127		
InChI Key	DHMQDGOQFOQNFH-UHFFFAOYSA-N		
SMILES	NCC(O)=O		
Molecular Formula	C ₂ H ₅ NO ₂		
Molecular Weight	75.067	Exact Molecular Weight	75.032028405
LogP	-3.409	Topological Polar Surface Area	63.32 Å ²
Atom Count	10	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.34	Oral Bioavailability	Y

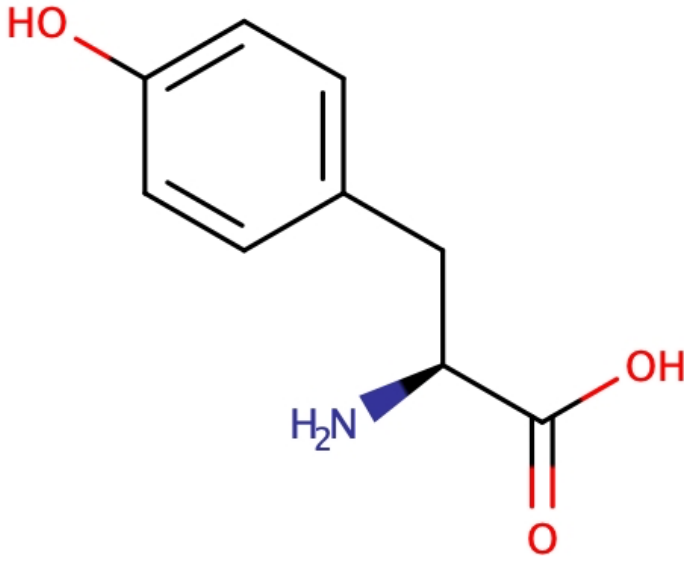
314. threonine

화학 구조		PubMed ID	
		17134710, 25780666 27558519	
TM-MC 성분 ID	182		
TM-MC 성분 동의어	Thr; L-threonine		
PubChem ID	6288, 6971019		
InChI Key	AYFVYJQAPQTCCC-GBXIJSLDSA-N		
SMILES	<chem>C[C@@H](O)[C@H](N)C(=O)O</chem>		
Molecular Formula	C ₄ H ₉ NO ₃		
Molecular Weight	119.12	Exact Molecular Weight	119.058243154
LogP	-3.471	Topological Polar Surface Area	83.55 Å ²
Atom Count	17	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.35	Oral Bioavailability	Y

315. alanine

화학 구조		PubMed ID	
		17134710, 19149256 25780666, 27558519	
TM-MC 성분 ID	184		
TM-MC 성분 동의어	Ala; L-alanine; D-alanine		
PubChem ID	5950, 7311724		
InChI Key	QNAYBMKLOCPYGJ-REOHCLBHSA-N		
SMILES	C[C@H](N)C(O)=O		
Molecular Formula	C ₃ H ₇ NO ₂		
Molecular Weight	89.094	Exact Molecular Weight	89.047678469
LogP	-2.841	Topological Polar Surface Area	63.32 Å ²
Atom Count	13	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.36	Oral Bioavailability	Y

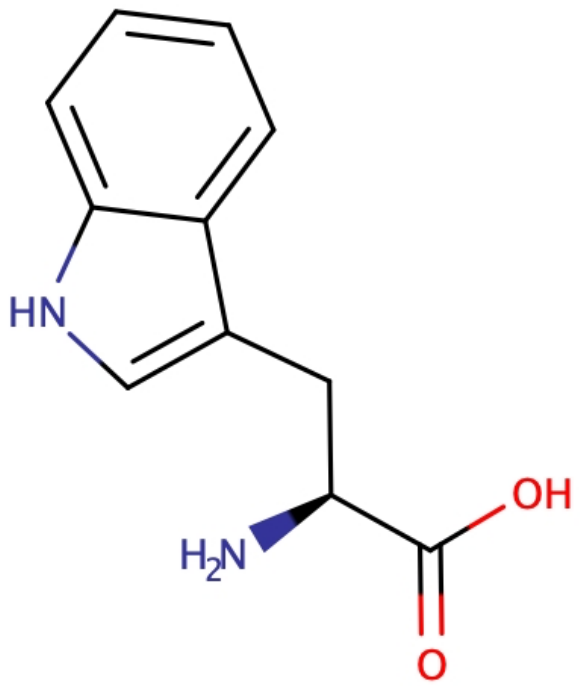
316. tyrosine

화학 구조		PubMed ID	
		17134710, 25780666 27558519	
TM-MC 성분 ID	185		
TM-MC 성분 동의어	Tyr; L-tyrosine		
PubChem ID	6057, 6942100		
InChI Key	OUYCCASQSFEME-QMMMGPBSA-N		
SMILES	N[C@@H](Cc1ccc(O)cc1)C(O)=O		
Molecular Formula	C ₉ H ₁₁ NO ₃		
Molecular Weight	181.191	Exact Molecular Weight	181.073893218
LogP	-1.489	Topological Polar Surface Area	83.55 Å ²
Atom Count	24	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.53	Oral Bioavailability	Y

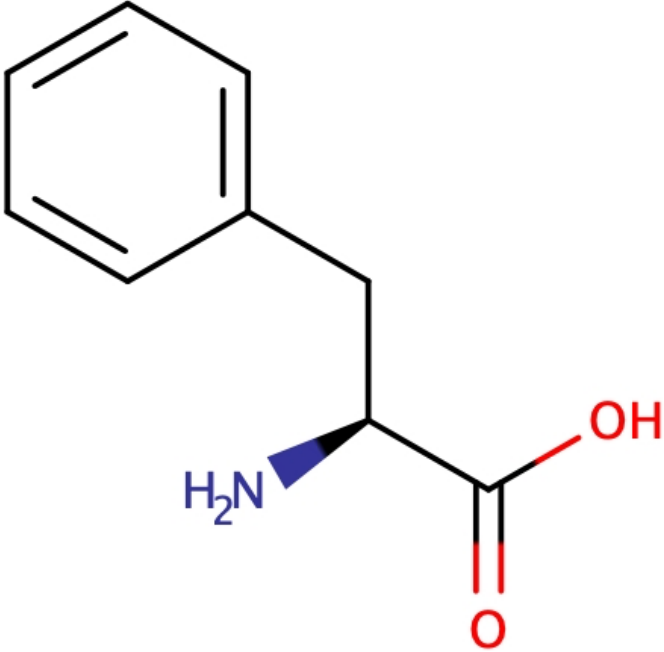
317. methionine

화학 구조		PubMed ID	
		17134710, 25780666 27558519	
TM-MC 성분 ID	187		
TM-MC 성분 동의어	Met		
PubChem ID	6137, 6992087		
InChI Key	FFEARJCKVFRZRR-BYPYZUCNSA-N		
SMILES	CSCC[C@H](N)C(O)=O		
Molecular Formula	C ₅ H ₁₁ NO ₂ S		
Molecular Weight	149.21	Exact Molecular Weight	149.051049772
LogP	-2.189	Topological Polar Surface Area	63.32 Å ²
Atom Count	20	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.48	Oral Bioavailability	Y

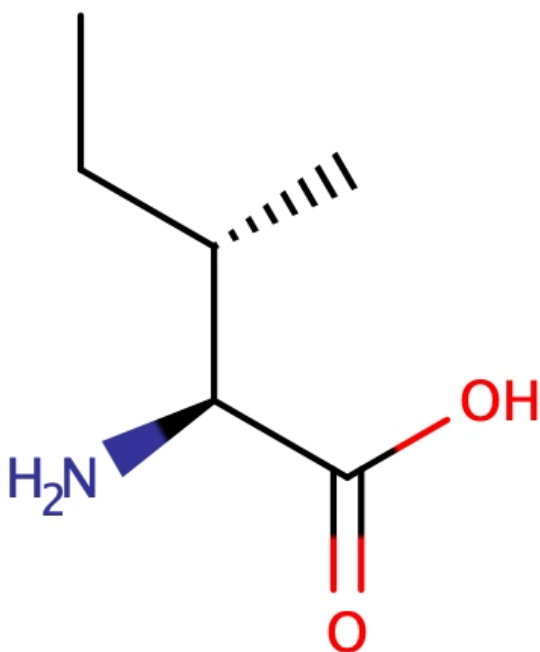
318. tryptophan

화학 구조		PubMed ID	
		17134710, 27558519	
TM-MC 성분 ID	188		
TM-MC 성분 동의어	L-tryptophan; Trp; L-(-)-tryptophan		
PubChem ID	6305, 6923516		
InChI Key	QIVBCDIJIAJPQS-VIFPVBQESA-N		
SMILES	N[C@@H](Cc1c[nH]c2ccccc12)C(O)=O		
Molecular Formula	C ₁₁ H ₁₂ N ₂ O ₂		
Molecular Weight	204.229	Exact Molecular Weight	204.089877634
LogP	-1.085	Topological Polar Surface Area	79.11 Å ²
Atom Count	27	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.59	Oral Bioavailability	Y

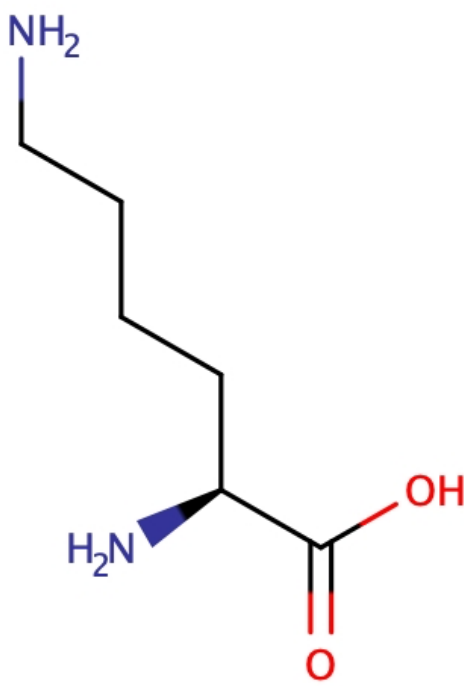
319. phenylalanine

화학 구조		PubMed ID	
		17134710, 19149256 25780666, 27558519	
TM-MC 성분 ID	189		
TM-MC 성분 동의어	L-phenylalanine; Phe; 2-amino-3-phenyl-propionic acid		
PubChem ID	6140, 6925665		
InChI Key	COLNVLDHVKWLRT-QMMMGPBSA-N		
SMILES	N[C@@H](Cc1ccccc1)C(O)=O		
Molecular Formula	C ₉ H ₁₁ NO ₂		
Molecular Weight	165.192	Exact Molecular Weight	165.078978598
LogP	-1.184	Topological Polar Surface Area	63.32 Å ²
Atom Count	23	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.59	Oral Bioavailability	Y

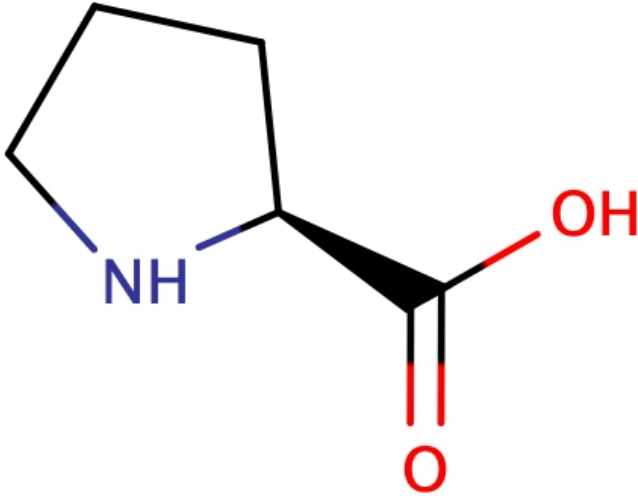
320. isoleucine

화학 구조		PubMed ID	
		17134710, 19149256 25780666, 27558519	
TM-MC 성분 ID	190		
TM-MC 성분 동의어	Ile; L-isoleucine; DL-isoleucine		
PubChem ID	6306, 7043901		
InChI Key	AGPKZVBTJJNPAG-WHFBIAKZSA-N		
SMILES	CC[C@H](C)[C@H](N)C(O)=O		
Molecular Formula	C ₆ H ₁₃ NO ₂		
Molecular Weight	131.175	Exact Molecular Weight	131.094628663
LogP	-1.508	Topological Polar Surface Area	63.32 Å ²
Atom Count	22	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.49	Oral Bioavailability	Y

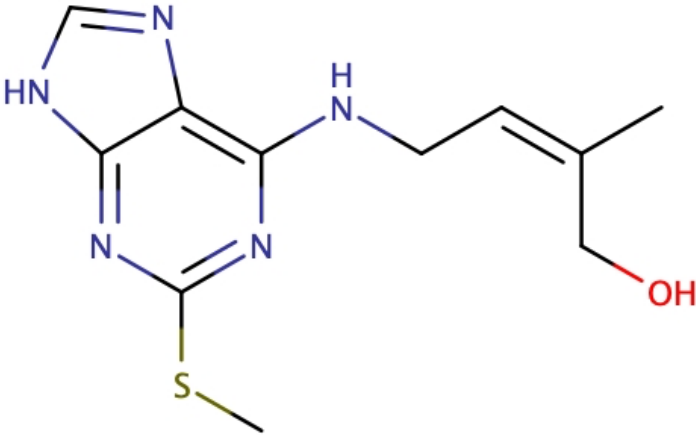
321. lysine

화학 구조		PubMed ID	
		17134710, 25780666 27558519	
TM-MC 성분 ID	192		
TM-MC 성분 동의어	Lys; L-lysine		
PubChem ID	5962, 71774817, 122198194, 168007633		
InChI Key	KDXKERNBIXSRK-YFKPBYRVSA-N		
SMILES	NCCCC[C@H](N)C(O)=O		
Molecular Formula	C ₆ H ₁₄ N ₂ O ₂		
Molecular Weight	146.19	Exact Molecular Weight	146.105527699
LogP	-3.215	Topological Polar Surface Area	89.34 Å ²
Atom Count	24	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.36	Oral Bioavailability	Y

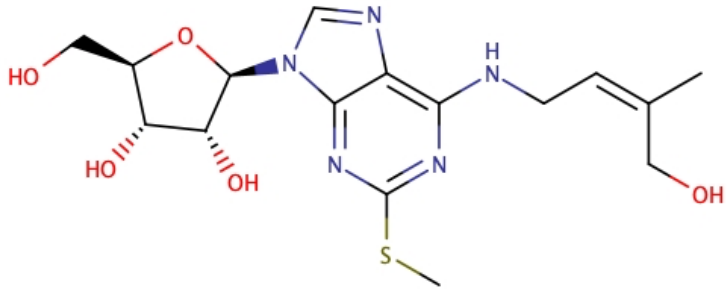
322. proline

화학 구조		PubMed ID	
		25780666, 27558519 28051308	
TM-MC 성분 ID	193		
TM-MC 성분 동의어	Pro; L-proline		
PubChem ID	145742, 6971047		
InChI Key	ONIBWKKTOPOVIA-BYPYZUCNSA-N		
SMILES	OC(=O)[C@@H]1CCCN1		
Molecular Formula	C ₅ H ₉ NO ₂		
Molecular Weight	115.132	Exact Molecular Weight	115.063328534
LogP	-2.569	Topological Polar Surface Area	49.33 Å ²
Atom Count	17	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.39	Oral Bioavailability	Y

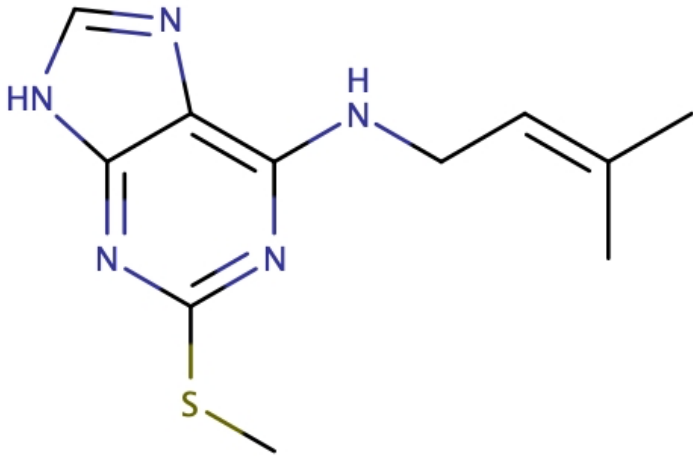
323. 2-methylthio-cis-zeatin

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440987		
TM-MC 성분 동의어	N/A		
PubChem ID	102258395		
InChI Key	OQCUYSWDVHSTFH-CLTKARDFSA-N		
SMILES	CSc1nc(NCWC=C(WC)CO)c2nc[nH]c2n1		
Molecular Formula	C ₁₁ H ₁₅ N ₅ OS		
Molecular Weight	265.34	Exact Molecular Weight	265.099731297
LogP	1.158	Topological Polar Surface Area	86.72 Å ²
Atom Count	33	Structural Alert Count	3
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	5	Aromatic Ring Count	2
Drug Likeness	0.43	Oral Bioavailability	Y

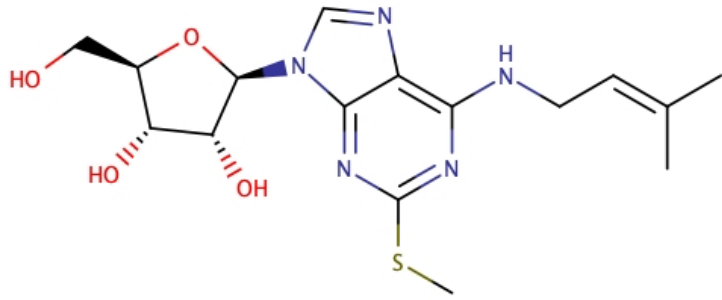
324. 2-methylthio-cis-zeatin roboside

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440988		
TM-MC 성분 동의어	N/A		
PubChem ID	53477660		
InChI Key	QEWSGVMSLPHELX-RFLXNSOUSA-N		
SMILES	CSc1nc(NCWC=C(WC)CO)c2ncn([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)c2n1		
Molecular Formula	C ₁₆ H ₂₃ N ₅ O ₅ S		
Molecular Weight	397.45	Exact Molecular Weight	397.141990035
LogP	-0.402	Topological Polar Surface Area	145.78 Å ²
Atom Count	50	Structural Alert Count	3
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	7	Aromatic Ring Count	2
Drug Likeness	0.24	Oral Bioavailability	N

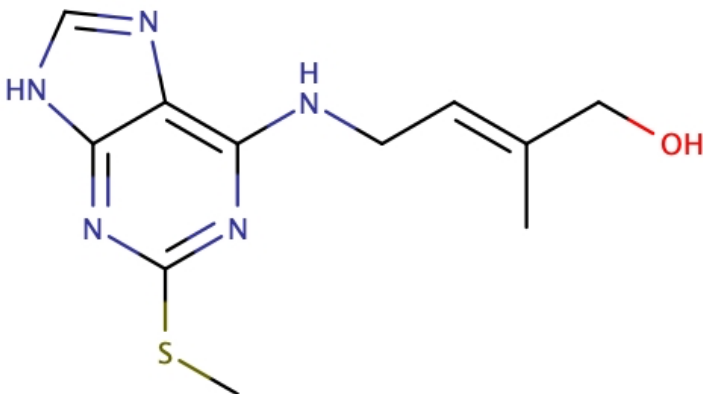
325. 2-methylthio-N6-isopentenyladenine

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440972		
TM-MC 성분 동의어	N/A		
PubChem ID	57375645		
InChI Key	VVJZYTNYVBSADL-UHFFFAOYSA-N		
SMILES	CSc1nc(NCC=C(C)C)c2nc[nH]c2n1		
Molecular Formula	C ₁₁ H ₁₅ N ₅ S		
Molecular Weight	249.34	Exact Molecular Weight	249.104816677
LogP	2.439	Topological Polar Surface Area	66.49 Å ²
Atom Count	32	Structural Alert Count	3
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.50	Oral Bioavailability	Y

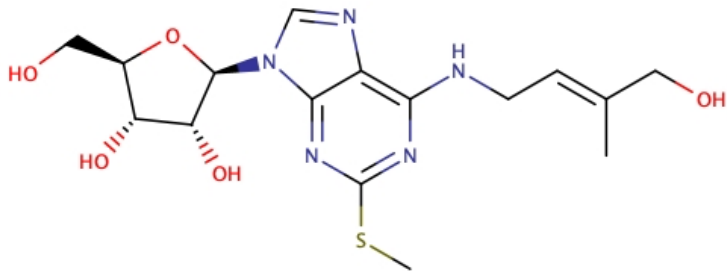
326. 2-methylthio-N6-isopentenyladenosine

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440973		
TM-MC 성분 동의어	N/A		
PubChem ID	161337		
InChI Key	VZQXUWKZDSEQRR-SDBHATRESA-N		
SMILES	CSc1nc(NCC=C(C)C)c2ncn([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)c2n1		
Molecular Formula	C ₁₆ H ₂₃ N ₅ O ₄ S		
Molecular Weight	381.45	Exact Molecular Weight	381.147075415
LogP	0.879	Topological Polar Surface Area	125.55 Å ²
Atom Count	49	Structural Alert Count	3
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	4
Rotatable Bond Count	6	Aromatic Ring Count	2
Drug Likeness	0.33	Oral Bioavailability	Y

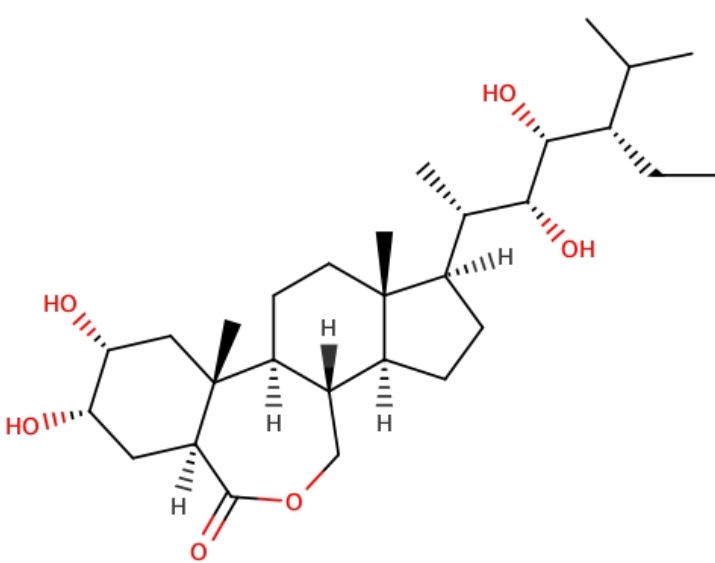
327. 2-methylthio-trans-zeatin

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440985		
TM-MC 성분 동의어	N/A		
PubChem ID	11666142		
InChI Key	OQCUYSWDVHSTFH-XVNBXDOJSA-N		
SMILES	CSc1nc(NC#C=C(/C)CO)c2nc[nH]c2n1		
Molecular Formula	C ₁₁ H ₁₅ N ₅ OS		
Molecular Weight	265.34	Exact Molecular Weight	265.099731297
LogP	1.158	Topological Polar Surface Area	86.72 Å ²
Atom Count	33	Structural Alert Count	3
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	5	Aromatic Ring Count	2
Drug Likeness	0.43	Oral Bioavailability	Y

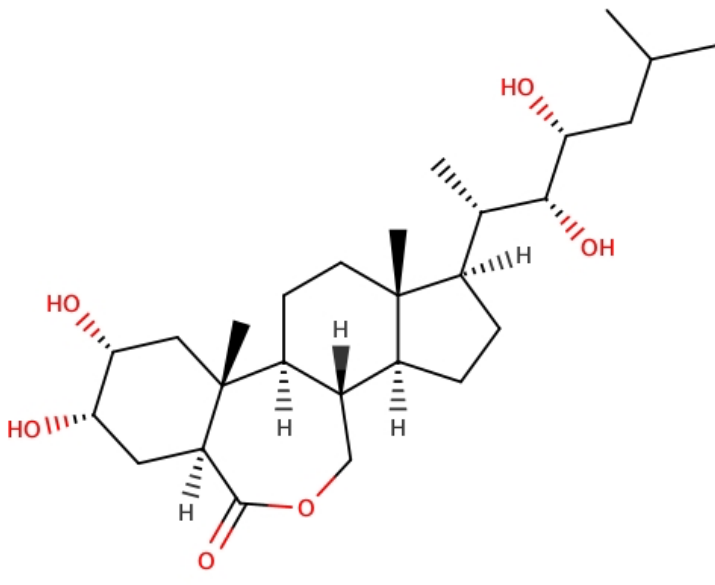
328. 2-methylthio-trans-zeatin roboside

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440986		
TM-MC 성분 동의어	N/A		
PubChem ID	6440977		
InChI Key	QEWSGVMSLPHELX-LECLTHIMSA-N		
SMILES	CSC1nc(NCWC=C(/C)CO)c2ncn([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)c2n1		
Molecular Formula	C ₁₆ H ₂₃ N ₅ O ₅ S		
Molecular Weight	397.45	Exact Molecular Weight	397.141990035
LogP	-0.402	Topological Polar Surface Area	145.78 Å ²
Atom Count	50	Structural Alert Count	3
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	7	Aromatic Ring Count	2
Drug Likeness	0.24	Oral Bioavailability	N

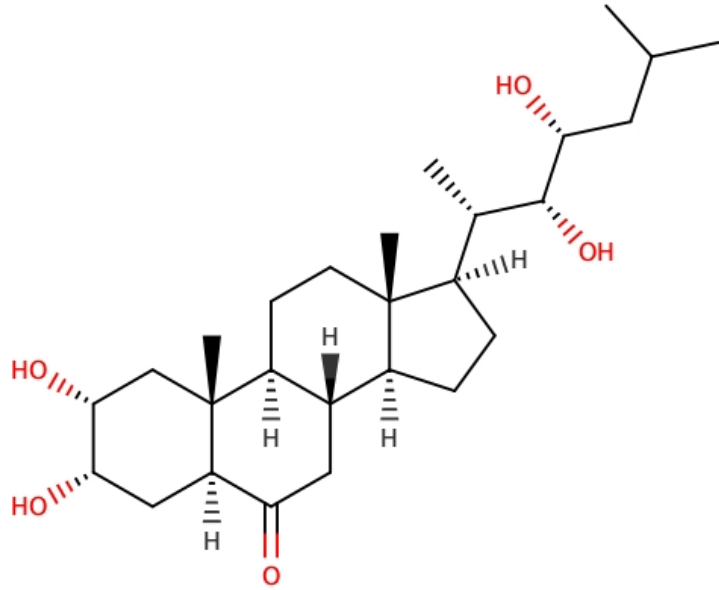
329. 28-homobrassinolide

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	133535		
TM-MC 성분 동의어	N/A		
PubChem ID	11038340		
InChI Key	HJIKODJJEORHMZ-NNPZUXBVSA-N		
SMILES	CC[C@@H](C(C)C)[C@@H](O)[C@H](O)[C@@H](C)[C@H]1CC[C@H]2[C@@H]3COC(=O)[C@H]4C[C@H](O)[C@H](O)C[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₉ H ₅₀ O ₆		
Molecular Weight	494.713	Exact Molecular Weight	494.36073933
LogP	3.575	Topological Polar Surface Area	107.22 Å ²
Atom Count	85	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.42	Oral Bioavailability	Y

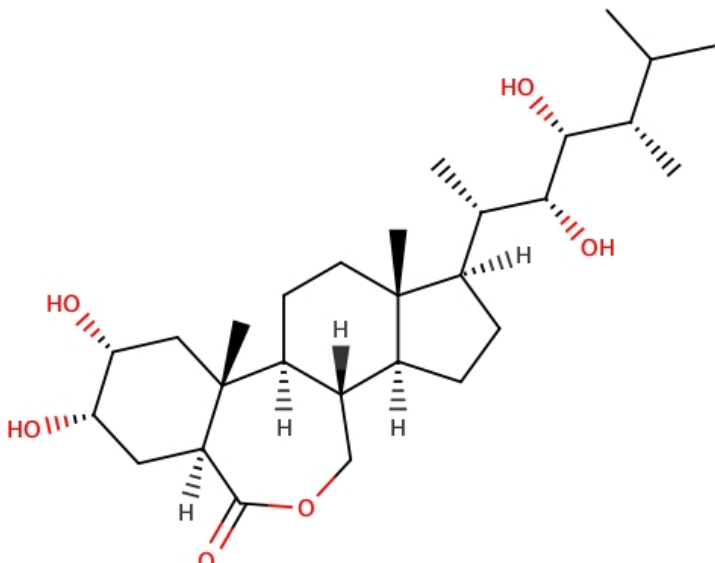
330. 28-norbrassinolide

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	133536		
TM-MC 성분 동의어	N/A		
PubChem ID	13845880		
InChI Key	CJNLSQRTIXIHW-BNYRCUELSA-N		
SMILES	<chem>CC(C)C[C@@H](O)[C@H](O)[C@@H](C)[C@H]1CC[C@H]2[C@@H]3COC(=O)[C@H]4C[C@H](O)[C@H](O)C[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₇ H ₄₆ O ₆		
Molecular Weight	466.659	Exact Molecular Weight	466.329439201
LogP	2.765	Topological Polar Surface Area	107.22 Å ²
Atom Count	79	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.47	Oral Bioavailability	Y

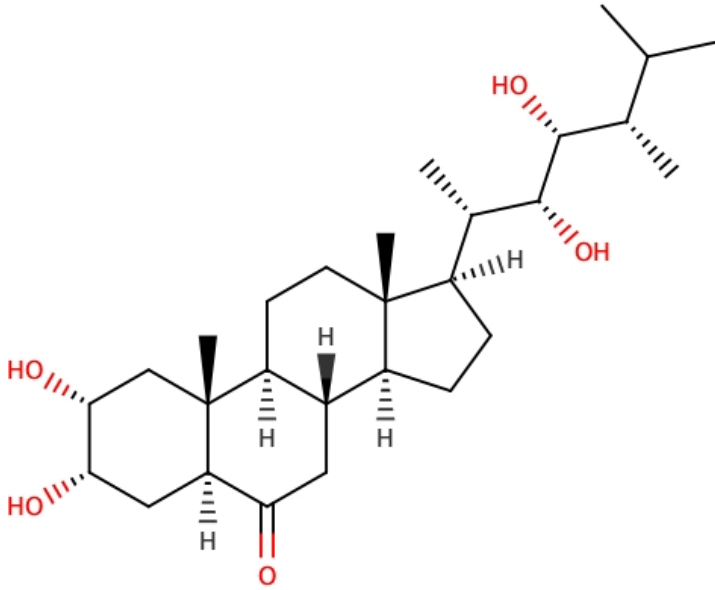
331. 28-norcastasterone

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	133537		
TM-MC 성분 동의어	N/A		
PubChem ID	13982110		
InChI Key	YNZRNENZMVIPBX-SCLBUMFYSA-N		
SMILES	CC(C)C[C@H](O)[C@H](O)[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC(=O)[C@H]4C[C@H](O)[C@H](O)C[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₇ H ₄₆ O ₅		
Molecular Weight	450.66	Exact Molecular Weight	450.334524581
LogP	3.137	Topological Polar Surface Area	97.99 Å ²
Atom Count	78	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.52	Oral Bioavailability	Y

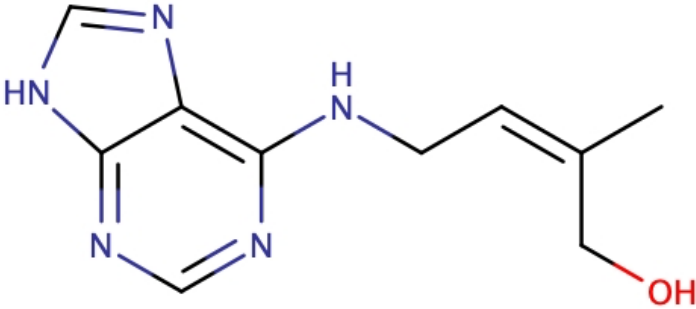
332. brassinolide

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	115196		
TM-MC 성분 동의어	epibrassinolide		
PubChem ID	115196		
InChI Key	IXVMHGVQKLDLDRKH-KNBKMWSGSA-N		
SMILES	CC(C)[C@H](C)[C@@H](O)[C@H](O)[C@@H](C)[C@H]1CC[C@H]2[C@@H]3COC(=O)[C@H]4C[C@H](O)[C@H](O)C[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₈ H ₄₈ O ₆		
Molecular Weight	480.686	Exact Molecular Weight	480.345089266
LogP	3.13	Topological Polar Surface Area	107.22 Å ²
Atom Count	82	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.45	Oral Bioavailability	Y

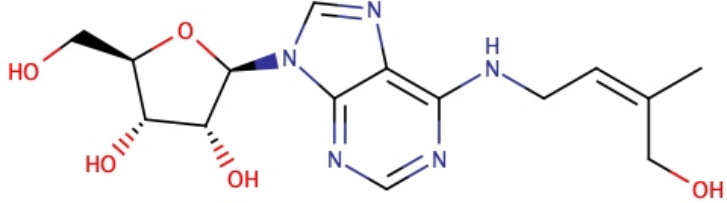
333. castasterone

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	133534		
TM-MC 성분 동의어	N/A		
PubChem ID	133534		
InChI Key	VYUIKSFYFRVQLF-YLNAYWRASA-N		
SMILES	CC(C)[C@H](C)[C@@H](O)[C@H](O)[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC(=O)[C@H]4C[C@H](O)[C@H](O)C[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₈ H ₄₈ O ₅		
Molecular Weight	464.687	Exact Molecular Weight	464.350174646
LogP	3.502	Topological Polar Surface Area	97.99 Å ²
Atom Count	81	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.50	Oral Bioavailability	Y

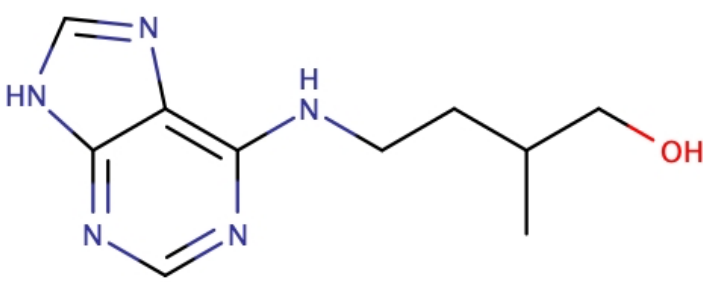
334. cis-zeatin

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440983		
TM-MC 성분 동의어	N/A		
PubChem ID	688597		
InChI Key	UZKQTCBAMSWPJD-UQCOIBPSSA-N		
SMILES	C=C(CO)=CNC1ncnc2[nH]cnc12		
Molecular Formula	C ₁₀ H ₁₃ N ₅ O		
Molecular Weight	219.248	Exact Molecular Weight	219.112010059
LogP	-0.149	Topological Polar Surface Area	86.72 Å ²
Atom Count	29	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.62	Oral Bioavailability	Y

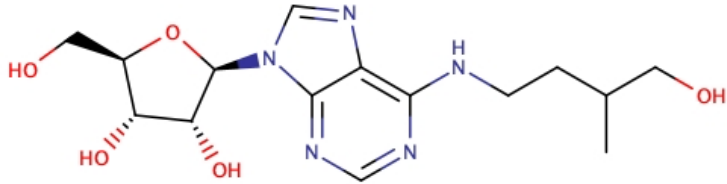
335. cis-zeatin roboside

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440984		
TM-MC 성분 동의어	N/A		
PubChem ID	13935024		
InChI Key	GOSWTRUMMSCNCW-BAJUWZQUSA-N		
SMILES	<chem>C#C(CO)=C#CNc1ncnc2n(cnc12)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₁₅ H ₂₁ N ₅ O ₅		
Molecular Weight	351.363	Exact Molecular Weight	351.154268796
LogP	-1.709	Topological Polar Surface Area	145.78 Å ²
Atom Count	46	Structural Alert Count	1
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	6	Aromatic Ring Count	2
Drug Likeness	0.38	Oral Bioavailability	N

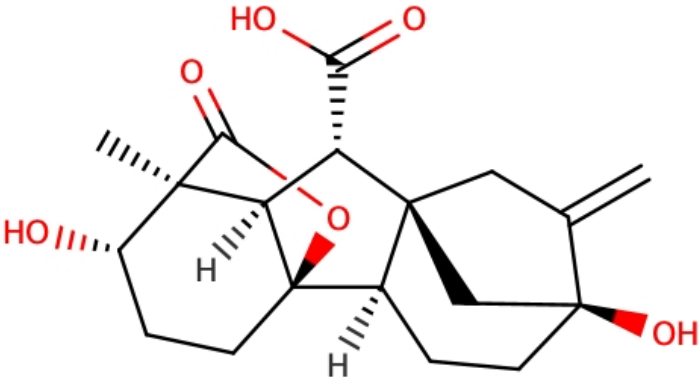
336. dihydrozeatin

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440989		
TM-MC 성분 동의어	N/A		
PubChem ID	32021		
InChI Key	XXFACTAYGKQOB-UHFFFAOYSA-N		
SMILES	CC(CO)CCNc1ncnc2[nH]cnc12		
Molecular Formula	C ₁₀ H ₁₅ N ₅ O		
Molecular Weight	221.264	Exact Molecular Weight	221.127660123
LogP	0.023	Topological Polar Surface Area	86.72 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	5	Aromatic Ring Count	2
Drug Likeness	0.66	Oral Bioavailability	Y

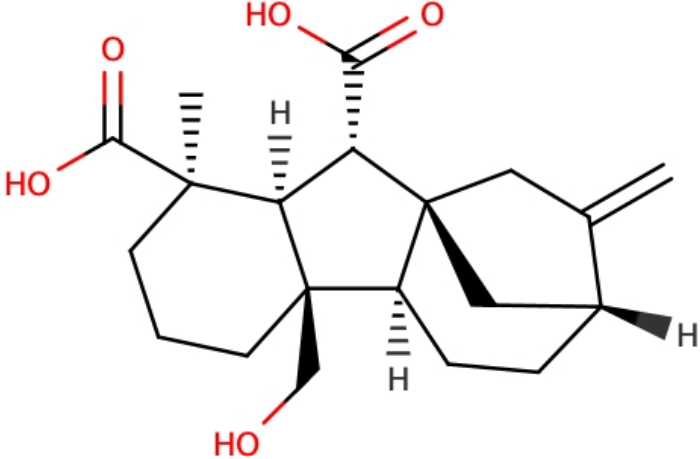
337. dihydrozeatin riboside

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440980		
TM-MC 성분 동의어	N/A		
PubChem ID	10522005		
InChI Key	DBVVQDGIJAEAZ-YXYADJKSSA-N		
SMILES	CC(CO)CCNc1ncnc2n(cnc12)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O		
Molecular Formula	C ₁₅ H ₂₃ N ₅ O ₅		
Molecular Weight	353.379	Exact Molecular Weight	353.169918861
LogP	-1.537	Topological Polar Surface Area	145.78 Å ²
Atom Count	48	Structural Alert Count	0
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	7	Aromatic Ring Count	2
Drug Likeness	0.40	Oral Bioavailability	N

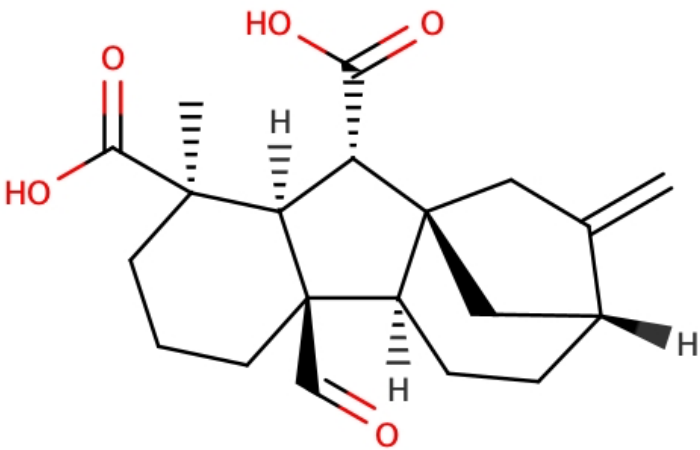
338. gibberellin A1

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	193311		
TM-MC 성분 동의어	N/A		
PubChem ID	5280379		
InChI Key	JLJLRLWOEMWYQK-OB DJNFEBSA-N		
SMILES	C[C@]12[C@H]3[C@H](C(O)=O)[C@@]45CC(=C)[C@@](O)(C4)CC[C@H]5[C@@]3(CC[C@@H]1O)OC2=O		
Molecular Formula	C ₁₉ H ₂₄ O ₆		
Molecular Weight	348.395	Exact Molecular Weight	348.157288493
LogP	0.401	Topological Polar Surface Area	104.06 Å ²
Atom Count	49	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.47	Oral Bioavailability	Y

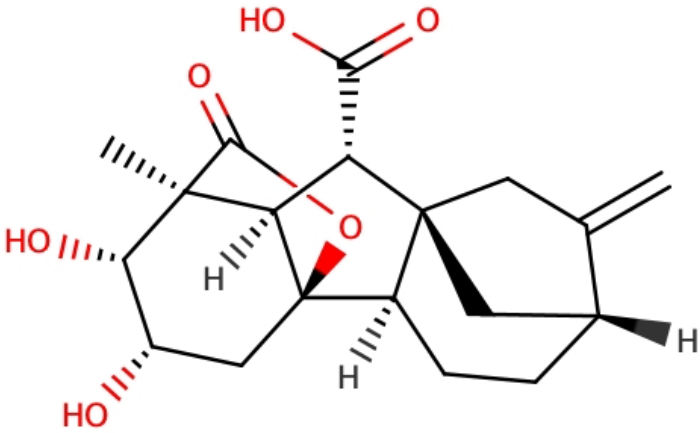
339. gibberellin A15

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	244529		
TM-MC 성분 동의어	N/A		
PubChem ID	443453		
InChI Key	TZGXVFYTKTWKCU-CXXOJBQZSA-N		
SMILES	C[C@]1(CCC[C@@]2(CO)[C@@H]3CC[C@@H]4C[C@]3(CC4=C)[C@H]([C@H]12)C(O)=O)C(O)=O		
Molecular Formula	C ₂₀ H ₂₈ O ₅		
Molecular Weight	348.439	Exact Molecular Weight	348.193674002
LogP	2.305	Topological Polar Surface Area	94.83 Å ²
Atom Count	53	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.68	Oral Bioavailability	Y

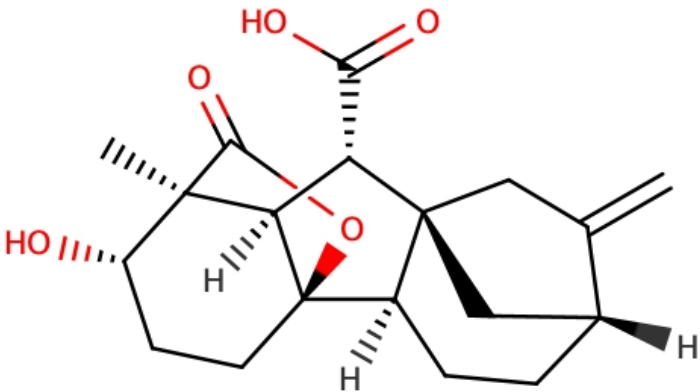
340. gibberellin A24

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	443454		
TM-MC 성분 동의어	N/A		
PubChem ID	443454		
InChI Key	QQRSSHFXYSOMF-CXXOJBQZSA-N		
SMILES	C[C@]1(CCC[C@@]2(C=O)[C@@H]3CC[C@@H]4C[C@]3(CC4=C)[C@H]([C@H]12)C(O)=O)C(O)=O		
Molecular Formula	C ₂₀ H ₂₆ O ₅		
Molecular Weight	346.423	Exact Molecular Weight	346.178023937
LogP	2.619	Topological Polar Surface Area	91.67 Å ²
Atom Count	51	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.61	Oral Bioavailability	Y

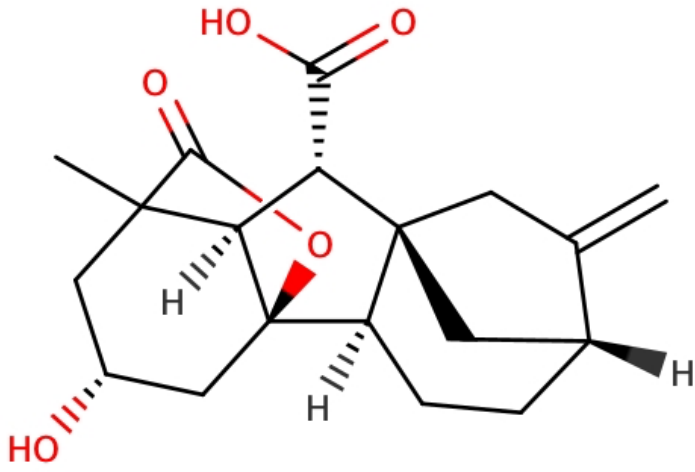
341. gibberellin A34

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	40044		
TM-MC 성분 동의어	N/A		
PubChem ID	5281987		
InChI Key	IGZIQAJXGRAJF-TXZPEUJSSA-N		
SMILES	C[C@]12[C@H]3[C@H](C(O)=O)[C@@]45C[C@@H](CC[C@H]4[C@@]3(C[C@H](O)[C@@H]1O)OC2=O)C(=C)C5		
Molecular Formula	C ₁₉ H ₂₄ O ₆		
Molecular Weight	348.395	Exact Molecular Weight	348.157288493
LogP	0.413	Topological Polar Surface Area	104.06 Å ²
Atom Count	49	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.47	Oral Bioavailability	Y

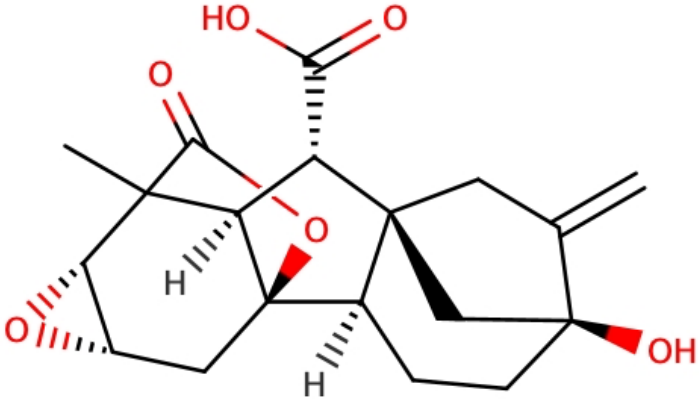
342. gibberellin A4

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	306853		
TM-MC 성분 동의어	N/A		
PubChem ID	92109		
InChI Key	RSQSQJNRHICNNH-NFMPGMCNSA-N		
SMILES	<chem>C[C@]12[C@H]3[C@H](C(O)=O)[C@@]45C[C@@H](CC[C@H]4[C@@]3(CC[C@@H]1O)OC2=O)C(=C)C5</chem>		
Molecular Formula	C ₁₉ H ₂₄ O ₅		
Molecular Weight	332.396	Exact Molecular Weight	332.162373873
LogP	1.56	Topological Polar Surface Area	83.83 Å ²
Atom Count	48	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.56	Oral Bioavailability	Y

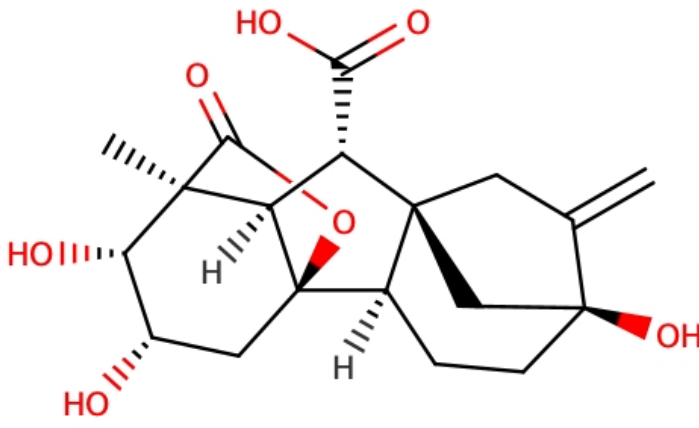
343. gibberellin A51

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	460373		
TM-MC 성분 동의어	N/A		
PubChem ID	443458		
InChI Key	HHDWSDSMWJQURA-NKHCVNPESA-N		
SMILES	CC12C[C@@H](O)C[C@@]3(OC1=O)[C@@H]1CC[C@@H]4C[C@]1(CC4=C)[C@H]([C@H]23)C(O)=O		
Molecular Formula	C ₁₉ H ₂₄ O ₅		
Molecular Weight	332.396	Exact Molecular Weight	332.162373873
LogP	1.332	Topological Polar Surface Area	83.83 Å ²
Atom Count	48	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.56	Oral Bioavailability	Y

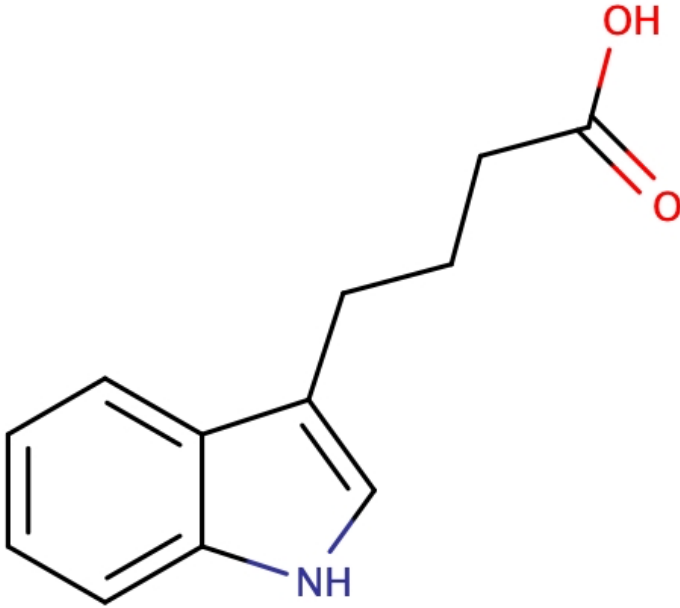
344. gibberellin A6

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	281989		
TM-MC 성분 동의어	N/A		
PubChem ID	443449		
InChI Key	XNBWKKYPKJHUKD-JXHFLFEZSA-N		
SMILES	CC12[C@H]3O[C@H]3C[C@@]3(OC1=O)[C@@H]1CC[C@]4(O)C[C@]1(CC4=C)[C@H]([C@H]23)C(O)=O		
Molecular Formula	C ₁₉ H ₂₂ O ₆		
Molecular Weight	346.379	Exact Molecular Weight	346.141638428
LogP	0.415	Topological Polar Surface Area	96.36 Å ²
Atom Count	47	Structural Alert Count	3
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.41	Oral Bioavailability	Y

345. gibberellin A8

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	281990		
TM-MC 성분 동의어	N/A		
PubChem ID	5280607		
InChI Key	WZRRJZYGOOHR-C-UQJXHNCSA-N		
SMILES	<chem>C[C@]12[C@H]3[C@H](C(O)=O)[C@@]45CC(=C)[C@@](O)(C4)CC[C@H]5[C@@]3(C[C@H](O)[C@@H]1O)OC2=O</chem>		
Molecular Formula	C ₁₉ H ₂₄ O ₇		
Molecular Weight	364.394	Exact Molecular Weight	364.152203113
LogP	-0.747	Topological Polar Surface Area	124.29 Å ²
Atom Count	50	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.36	Oral Bioavailability	Y

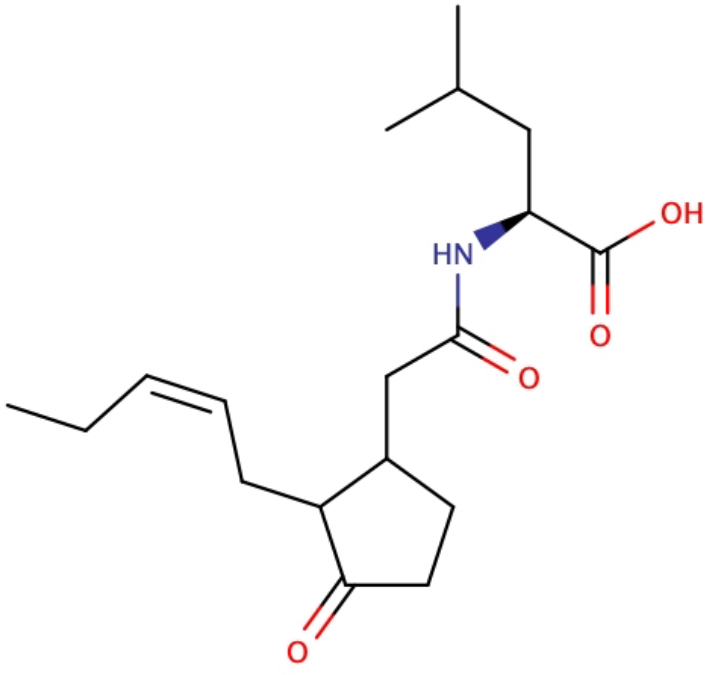
346. indole-3-butyric acid

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	92346		
TM-MC 성분 동의어	N/A		
PubChem ID	8617		
InChI Key	JTEDVYBZBROSJT-UHFFFAOYSA-N		
SMILES	OC(=O)CCCc1c[nH]c2ccccc12		
Molecular Formula	C ₁₂ H ₁₃ NO ₂		
Molecular Weight	203.241	Exact Molecular Weight	203.094628663
LogP	2.599	Topological Polar Surface Area	53.09 Å ²
Atom Count	28	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.80	Oral Bioavailability	Y

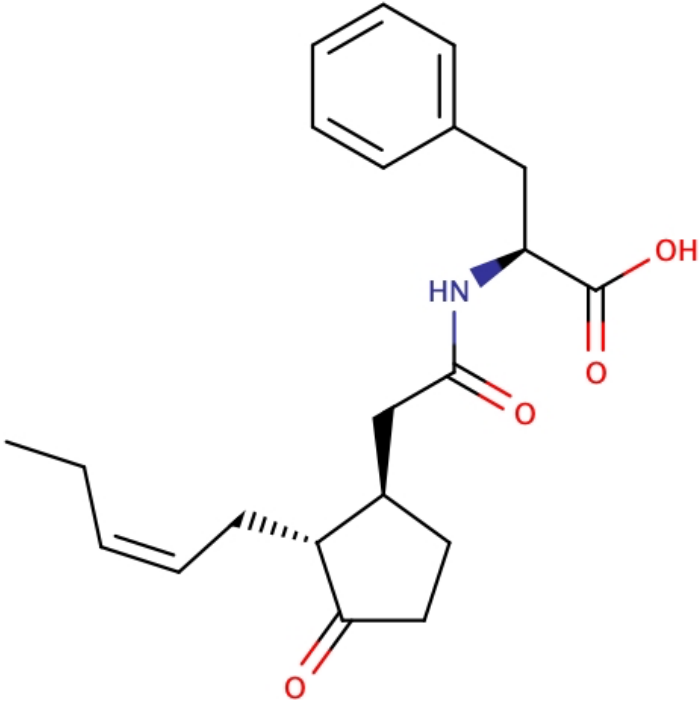
347. jasmonic acid

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	281166		
TM-MC 성분 동의어	N/A		
PubChem ID	12304694		
InChI Key	ZNJFBWYDHIGLCU-ARJAWSKDSA-N		
SMILES	CCWC=C/CC1C(CC(O)=O)CCC1=O		
Molecular Formula	C ₁₂ H ₁₈ O ₃		
Molecular Weight	210.273	Exact Molecular Weight	210.12559444
LogP	2.414	Topological Polar Surface Area	54.37 Å ²
Atom Count	33	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.71	Oral Bioavailability	Y

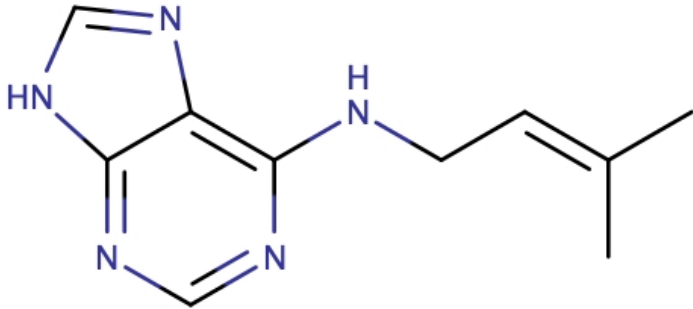
348. jasmonoyl-leucine

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	39137		
TM-MC 성분 동의어	N/A		
PubChem ID	146037204		
InChI Key	BDUIIOHQSYXRT-GJKCTVFGSA-N		
SMILES	<chem>CC=C/C/C1C(CC(=O)N[C@@H](CC(C)C)C(O)=O)CCC1=O</chem>		
Molecular Formula	C ₁₈ H ₂₉ NO ₄		
Molecular Weight	323.433	Exact Molecular Weight	323.209658418
LogP	3.132	Topological Polar Surface Area	83.47 Å ²
Atom Count	52	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	9	Aromatic Ring Count	0
Drug Likeness	0.64	Oral Bioavailability	Y

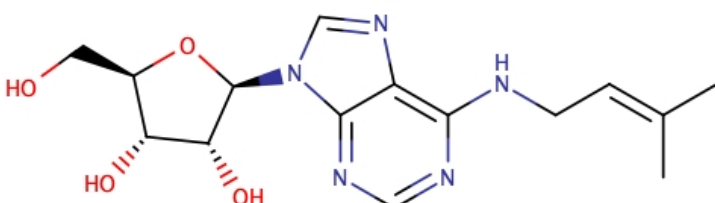
349. jasmonoyl-phenylalanine

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	1889		
TM-MC 성분 동의어	N/A		
PubChem ID	14455523		
InChI Key	BYYWRCJZFSTRMQ-WSKZCNLGSA-N		
SMILES	CC#C=C/C[C@@H]1[C@@H](CC(=O)N[C@@H](Cc2ccccc2)C(O)=O)CCC1=O		
Molecular Formula	C ₂₁ H ₂₇ NO ₄		
Molecular Weight	357.45	Exact Molecular Weight	357.194008353
LogP	3.534	Topological Polar Surface Area	83.47 Å ²
Atom Count	53	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	9	Aromatic Ring Count	1
Drug Likeness	0.66	Oral Bioavailability	Y

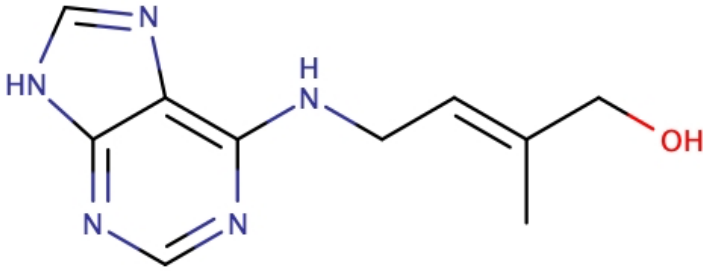
350. N6-isopentenyladenine

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440970		
TM-MC 성분 동의어	N/A		
PubChem ID	92180		
InChI Key	HYVABZIGRDEKCD-UHFFFAOYSA-N		
SMILES	CC(C)=CCNc1ncnc2[nH]cnc12		
Molecular Formula	C ₁₀ H ₁₃ N ₅		
Molecular Weight	203.249	Exact Molecular Weight	203.117095439
LogP	1.132	Topological Polar Surface Area	66.49 Å ²
Atom Count	28	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	2
Drug Likeness	0.73	Oral Bioavailability	Y

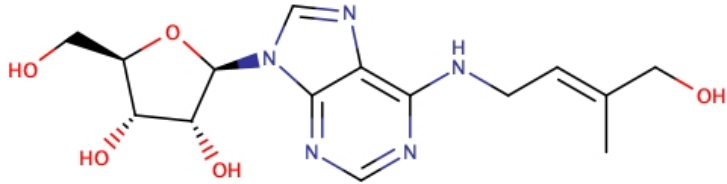
351. N6-isopentenyladenosine

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440971		
TM-MC 성분 동의어	N/A		
PubChem ID	24405		
InChI Key	USVMJSALORZVDV-SDBHATRESA-N		
SMILES	<chem>CC(C)=CCNc1ncnc2n(cnc12)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₁₅ H ₂₁ N ₅ O ₄		
Molecular Weight	335.364	Exact Molecular Weight	335.159354176
LogP	-0.428	Topological Polar Surface Area	125.55 Å ²
Atom Count	45	Structural Alert Count	1
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	2
Drug Likeness	0.54	Oral Bioavailability	Y

352. trans-zeatin

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440981		
TM-MC 성분 동의어	N/A		
PubChem ID	449093		
InChI Key	UZKQTCBAMSWPJD-FARCUNLSSA-N		
SMILES	C=C(C)C/C=C/C1=NC2=C(N1)N=CN=C2		
Molecular Formula	C ₁₀ H ₁₃ N ₅ O		
Molecular Weight	219.248	Exact Molecular Weight	219.112010059
LogP	-0.149	Topological Polar Surface Area	86.72 Å ²
Atom Count	29	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.62	Oral Bioavailability	Y

353. trans-zeatin riboside

화학 구조		PubMed ID	
		28032995	
TM-MC 성분 ID	440982		
TM-MC 성분 동의어	trans-zeatin riboside		
PubChem ID	6440982		
InChI Key	GOSWTRUMMSCNCW-HNNGNKQASA-N		
SMILES	<chem>C#C(CO)=C/CNc1ncnc2n(cnc12)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₁₅ H ₂₁ N ₅ O ₅		
Molecular Weight	351.363	Exact Molecular Weight	351.154268796
LogP	-1.709	Topological Polar Surface Area	145.78 Å ²
Atom Count	46	Structural Alert Count	1
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	5
Rotatable Bond Count	6	Aromatic Ring Count	2
Drug Likeness	0.38	Oral Bioavailability	N


354. Ca

화학 구조		PubMed ID	
		26841944, 28051308	
TM-MC 성분 ID	420		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	FAQLAUHZSGTTLN-UHFFFAOYSA-N		
SMILES	[Ca]		
Molecular Formula	Ca		
Molecular Weight	40.078	Exact Molecular Weight	39.9625909
LogP	-0.57	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.32	Oral Bioavailability	Y


355. Mg

화학 구조		PubMed ID
		28051308
TM-MC 성분 ID	433	
TM-MC 성분 동의어	N/A	
PubChem ID	N/A	
InChI Key	RSHAOIXHUHAZPM-UHFFFAOYSA-N	
SMILES	[Mg]	
Molecular Formula	Mg	
Molecular Weight	24.305	Exact Molecular Weight 23.9850417
LogP	-0.57	Topological Polar Surface Area 0 Å ²
Atom Count	1	Structural Alert Count 1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count 0
Rotatable Bond Count	0	Aromatic Ring Count 0
Drug Likeness	0.31	Oral Bioavailability Y

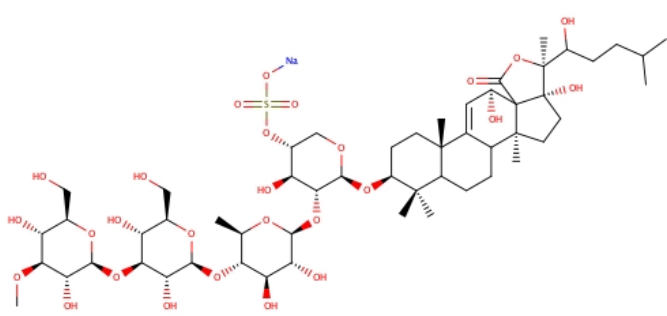
356. K

화학 구조		PubMed ID	
		26841944, 28051308	
TM-MC 성분 ID	424		
TM-MC 성분 동의어	potassium		
PubChem ID	N/A		
InChI Key	NTTOTNSKUYCDAV-UHFFFAOYSA-N		
SMILES	[K]		
Molecular Formula	K		
Molecular Weight	39.0983	Exact Molecular Weight	38.96370649
LogP	0.2	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.34	Oral Bioavailability	Y

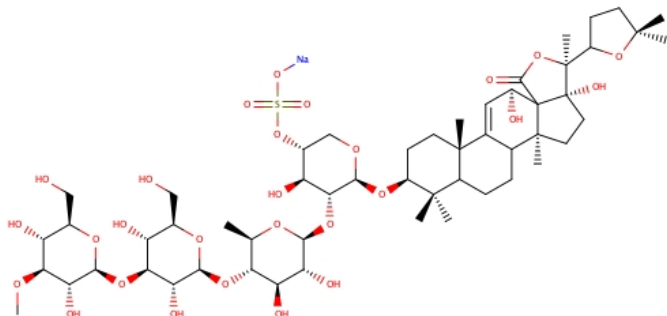
357. P

화학 구조		PubMed ID	
		28051308	
TM-MC 성분 ID	434		
TM-MC 성분 동의어	N/A		
PubChem ID	24404		
InChI Key	XYFCBTPGUUZFHI-UHFFFAOYSA-N		
SMILES	P		
Molecular Formula	H ₃ P		
Molecular Weight	33.998	Exact Molecular Weight	33.997237095
LogP	-0.678	Topological Polar Surface Area	0 Å ²
Atom Count	4	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.31	Oral Bioavailability	Y

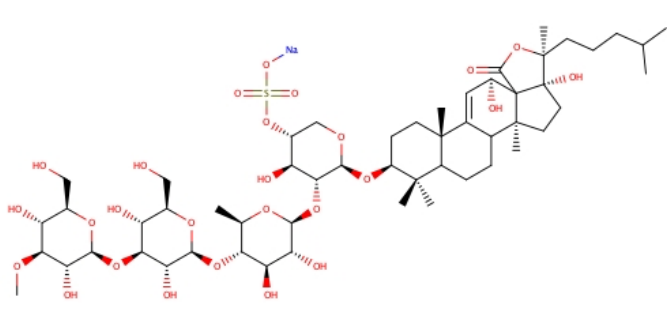
358. holothurin A1

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	194		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	BAAQJFWJJHQDPH-DNVGHQFKSA-M		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)[C@@H](O[C@@H]3[C@@H](C)O[C@@H](O[C@@H]4[C@@H](O)[C@@H](CO[C@H]4O[C@H]4CC[C@@]5(C)C(CCC6C5=C[C@H](O)C57C(=O)O[C@@](C)(C(O)CCC(C)C)[C@@]5(O)CC[C@@]67C)C4(C)C)OS(=O)(=O)O[Na])[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₅₄ H ₈₇ NaO ₂₇ S		
Molecular Weight	1223.31	Exact Molecular Weight	1222.505313
LogP	-2.041	Topological Polar Surface Area	404.73 Å ²
Atom Count	170	Structural Alert Count	4
Hydrogen Bond Acceptor Count	24	Hydrogen Bond Donor Count	12
Rotatable Bond Count	18	Aromatic Ring Count	0
Drug Likeness	0.03	Oral Bioavailability	N

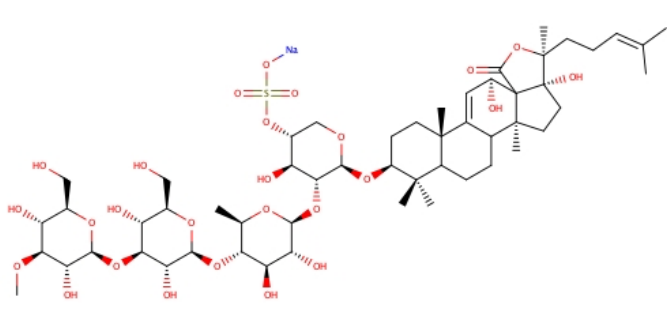
359. holothurin A

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	195		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	KXDQPKMJSMCBEY-CBULQOSWSA-M		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)O[C@@H](O[C@@H]3[C@@H](C)O[C@H](O[C@@H]4[C@@H](O)[C@@H](CO)[C@H]4O[C@H]4CC[C@@]5(C)C(CCC6C5=C[C@H](O)C57C(=O)O[C@@](C)(C8CCC(C)(C)O8)[C@@]5(O)CC[C@@]67C)C4(C)C)OS(=O)(=O)O[Na])[C@H](O)[C@H]3O)[C@@H]2O)[C@H]1O</chem>		
Molecular Formula	C ₅₄ H ₈₅ NaO ₂₇ S		
Molecular Weight	1221.3	Exact Molecular Weight	1220.48966293
LogP	-2.58	Topological Polar Surface Area	393.73 Å ²
Atom Count	168	Structural Alert Count	4
Hydrogen Bond Acceptor Count	24	Hydrogen Bond Donor Count	11
Rotatable Bond Count	15	Aromatic Ring Count	0
Drug Likeness	0.03	Oral Bioavailability	N

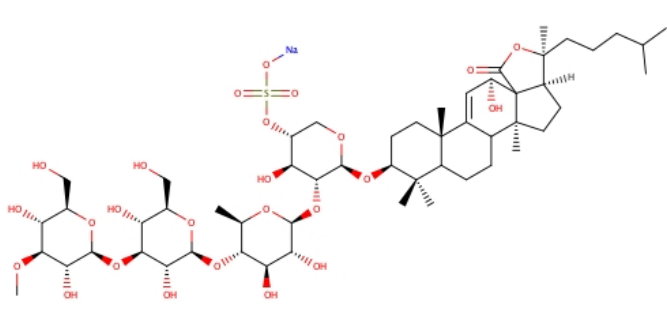
360. echinoside A

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	196		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	JEBRMYZXRSTSKU-DPLSTWQQSA-M		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)O[C@@H](O[C@H]3[C@@H](C)O[C@@H](O[C@@H]4[C@H](O)[C@@H](CO[C@H]4O)[C@H]4CC[C@@]5(C)C(CCC6C5=C[C@H](O)C57C(=O)O[C@@](C)(CCCC(C)C)[C@@]5(O)CC[C@@]67C)C4(C)C)OS(=O)(=O)O[Na])[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₅₄ H ₈₇ NaO ₂₆ S		
Molecular Weight	1207.31	Exact Molecular Weight	1206.51039838
LogP	-0.973	Topological Polar Surface Area	384.5 Å ²
Atom Count	169	Structural Alert Count	4
Hydrogen Bond Acceptor Count	23	Hydrogen Bond Donor Count	11
Rotatable Bond Count	18	Aromatic Ring Count	0
Drug Likeness	0.03	Oral Bioavailability	N

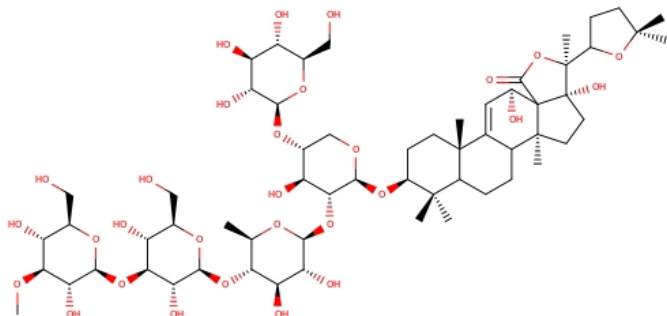
361. 24-dehydroechinoside A

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	197		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	GPYUOTNTUNCQBX-DPLSTWQQSA-M		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)O[C@@H](O[C@@H]3[C@@H](CO)O[C@@H](O[C@@H]4[C@H](O)[C@@H](CO)[C@H]4O[C@H]4CC[C@@]5(C)C(CCC6C5=C[C@H](O)C57C(=O)O[C@@](C)(CCC=C(C)C)[C@@]5(O)CC[C@@]67C)C4(C)C)OS(=O)(=O)O[Na])[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₅₄ H ₈₅ NaO ₂₆ S		
Molecular Weight	1205.3	Exact Molecular Weight	1204.49474831
LogP	-1.41	Topological Polar Surface Area	384.5 Å ²
Atom Count	167	Structural Alert Count	4
Hydrogen Bond Acceptor Count	23	Hydrogen Bond Donor Count	11
Rotatable Bond Count	17	Aromatic Ring Count	0
Drug Likeness	0.03	Oral Bioavailability	N

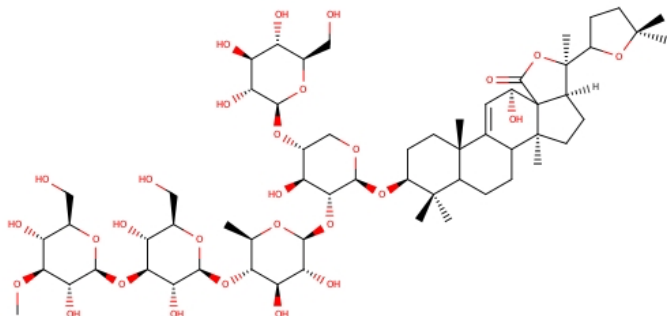
362. pervicoside C

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	198		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	DEHSMOLOWCNYJI-SVNOZUPNSA-M		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)[C@@H](O[C@@H]3[C@@H](CO)[C@@H](O[C@@H]4[C@H](O)[C@@H](CO)[C@H]4O[C@H]4CC[C@@]5(C)C(CCC6C5=C[C@H](O)C57[C@H](CC[C@@]65C)[C@@](C)(CCCC(C)OC7=O)C4(C)OS(=O)(=O)O[Na])[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₅₄ H ₈₇ NaO ₂₅ S		
Molecular Weight	1191.31	Exact Molecular Weight	1190.51548376
LogP	0.204	Topological Polar Surface Area	364.27 Å ²
Atom Count	168	Structural Alert Count	4
Hydrogen Bond Acceptor Count	22	Hydrogen Bond Donor Count	10
Rotatable Bond Count	18	Aromatic Ring Count	0
Drug Likeness	0.04	Oral Bioavailability	N

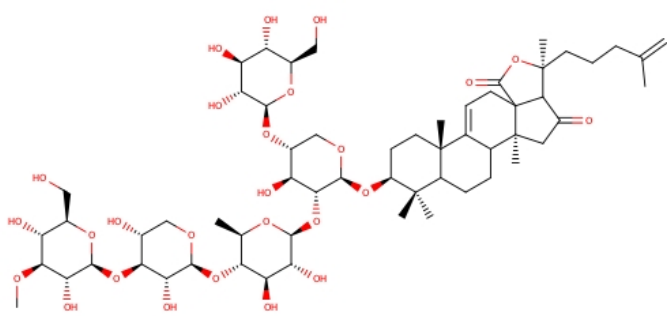
363. holothurinoside A

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	199		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	ANIOUAZKPOMNEP-CODFWGIPSA-N		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)O[C@@H](O[C@H]3[C@@H](C)O[C@@H](O[C@@H]4[C@H](O)[C@@H](CO[C@H]4O[C@H]4CC[C@@]5(C)C(CCC6C5=C[C@H](O)C57C(=O)O[C@@](C)(C8CCC(C)(C)O8)[C@@]5(O)CC[C@@]67C)C4(C)C)O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₆₀ H ₉₆ O ₂₉		
Molecular Weight	1281.399	Exact Molecular Weight	1280.603727071
LogP	-3.222	Topological Polar Surface Area	440.51 Å ²
Atom Count	185	Structural Alert Count	3
Hydrogen Bond Acceptor Count	28	Hydrogen Bond Donor Count	15
Rotatable Bond Count	15	Aromatic Ring Count	0
Drug Likeness	0.04	Oral Bioavailability	N

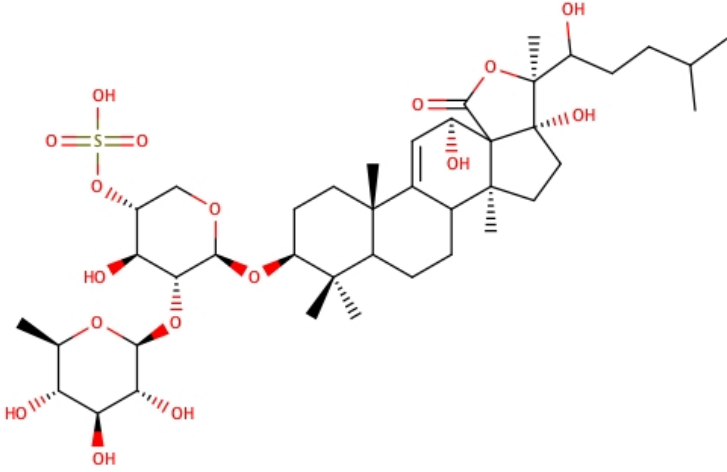
364. 17-dehydroxyholothurinoside A

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	200		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	QNJQNJVTLMPYQ-JUIAZNSSA-N		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)[C@@H](O[C@@H]3[C@@H](C)O[C@@H](O[C@@H]4[C@H](O)[C@@H](CO)[C@H]4O[C@H]4CC[C@@]5(C)C(CCC6C5=C[C@H](O)C57[C@H](CC[C@@]65C)[C@@](C)(OC7=O)C5CCC(C)(C)O5)C4(C)O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₆₀ H ₉₆ O ₂₈		
Molecular Weight	1265.4	Exact Molecular Weight	1264.608812451
LogP	-2.296	Topological Polar Surface Area	420.28 Å ²
Atom Count	184	Structural Alert Count	3
Hydrogen Bond Acceptor Count	27	Hydrogen Bond Donor Count	14
Rotatable Bond Count	15	Aromatic Ring Count	0
Drug Likeness	0.05	Oral Bioavailability	N

365. cladolose B

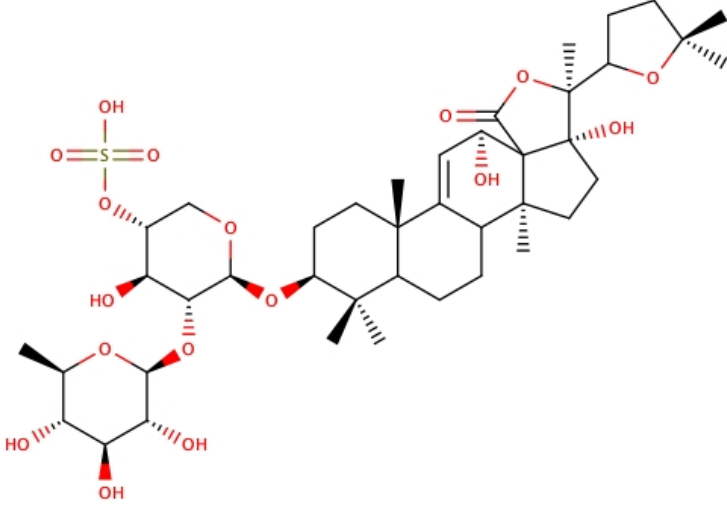
화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	201		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	KMSJITANQAAJDO-ZNJOLZFASA-N		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)CO[C@@H](O[C@@H]3[C@@H](CO)O[C@@H](O[C@@H]4[C@@H](O)[C@@H](CO[C@H]4O[C@H]4CC[C@@]5(C)C(CCC6C5=CCC57C(C(=O)C[C@@]65C)[C@](C)(CCCC(C)=C)OC7=O)C4(C)CO[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)[C@H](O)[C@H]3O)[C@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₅₉ H ₉₂ O ₂₆		
Molecular Weight	1217.359	Exact Molecular Weight	1216.587683082
LogP	-0.4	Topological Polar Surface Area	387.66 Å ²
Atom Count	177	Structural Alert Count	3
Hydrogen Bond Acceptor Count	25	Hydrogen Bond Donor Count	12
Rotatable Bond Count	17	Aromatic Ring Count	0
Drug Likeness	0.05	Oral Bioavailability	N

366. holothurin B2

화학 구조	PubMed ID
	25604752

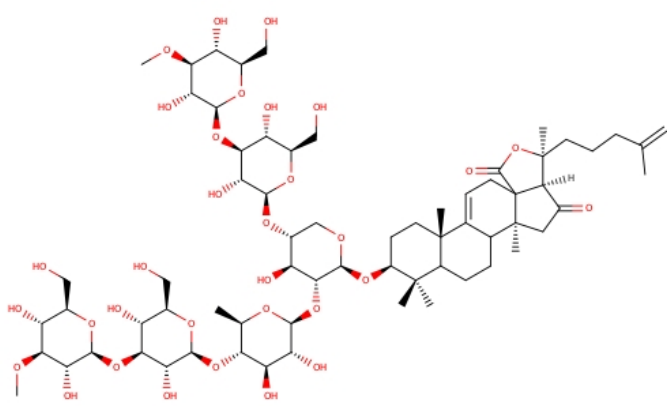
TM-MC 성분 ID	202		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	QKXKHWVDHNLJNC-IGWPHFCNSA-N		
SMILES	<chem>CC(C)CCC(O)[C@]1(C)OC(=O)C23[C@@H](O)C=C4C(CCC5C(C)(C)[C@H](CC[C@]45C)O[C@@H]4OC[C@@H](OS(O)(=O)=O)[C@H](O)[C@H]4O[C@@H]4O[C@H](C)[C@@H](O)[C@H](O)[C@H]4O)[C@]2(C)CC[C@]13O</chem>		
Molecular Formula	C ₄₁ H ₆₆ O ₁₇ S		
Molecular Weight	863.02	Exact Molecular Weight	862.402071839
LogP	-0.018	Topological Polar Surface Area	268.43 Å ²
Atom Count	125	Structural Alert Count	4
Hydrogen Bond Acceptor Count	15	Hydrogen Bond Donor Count	8
Rotatable Bond Count	10	Aromatic Ring Count	0
Drug Likeness	0.06	Oral Bioavailability	N

367. holothurin B

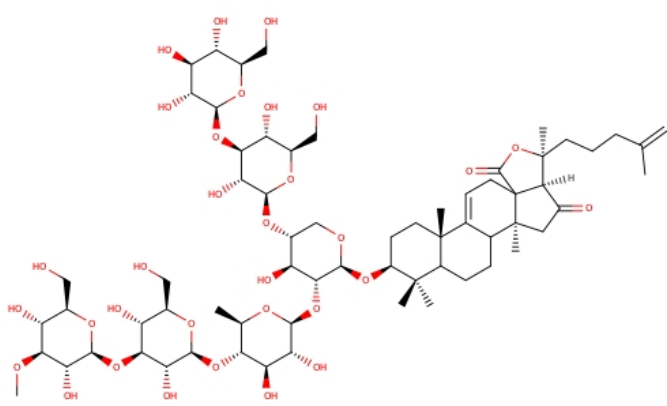
화학 구조	PubMed ID
	25604752

TM-MC 성분 ID	203		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	HZPAESJKJRHHK-IQWDHQOSSA-N		
SMILES	<chem>C[C@H]1O[C@@H](O[C@@H]2[C@@H](O)[C@@H](CO[C@H]2O[C@H]2CC[C@@]3(C)C(CCC4C3=C[C@H](O)C35C(=O)O[C@@](C)(C6CCC(C)(C)O6)[C@@]3(O)CC[C@@]45C)C2(C)OS(O)(=O)=O)[C@H](O)[C@@H](O)[C@@H]1O</chem>		
Molecular Formula	C ₄₁ H ₆₄ O ₁₇ S		
Molecular Weight	861.01	Exact Molecular Weight	860.386421775
LogP	-0.327	Topological Polar Surface Area	257.43 Å ²
Atom Count	123	Structural Alert Count	4
Hydrogen Bond Acceptor Count	15	Hydrogen Bond Donor Count	7
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.07	Oral Bioavailability	N

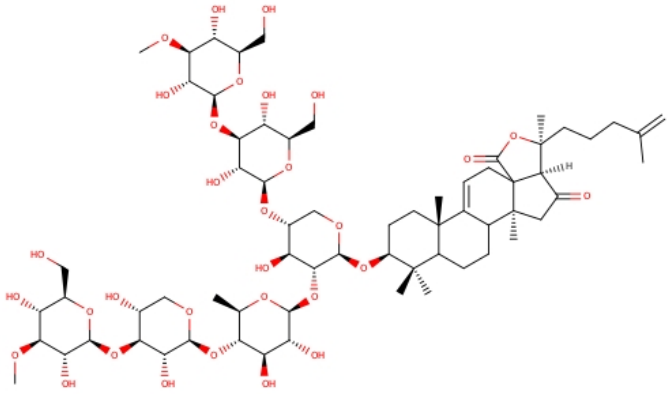
368. holotoxin A

화학 구조		PubMed ID	
		18557622	
TM-MC 성분 ID	204		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	BIHNZKYXOTXXSP-MQNQNXGMSA-N		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)O[C@@H](O[C@H]3CO[C@@H](O[C@H]4CC[C@@]5(C)C(CCC6C5=CCC57[C@H](C(=O)C[C@@]65C)[C@](C)(CCCC(C)=C)OC7=O)C4(C)C)[C@H](O[C@@H]4O[C@H](C)[C@@H](O[C@@H]5O[C@H](CO)[C@@H](O)[C@H](O[C@@H]6O[C@H](CO)[C@@H](O)[C@H](OC)[C@H]6O)[C@H]5O)[C@H](O)[C@H]4O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₆₇ H ₁₀₆ O ₃₂		
Molecular Weight	1423.553	Exact Molecular Weight	1422.666721253
LogP	-2.158	Topological Polar Surface Area	476.04 Å ²
Atom Count	205	Structural Alert Count	3
Hydrogen Bond Acceptor Count	31	Hydrogen Bond Donor Count	15
Rotatable Bond Count	22	Aromatic Ring Count	0
Drug Likeness	0.03	Oral Bioavailability	N

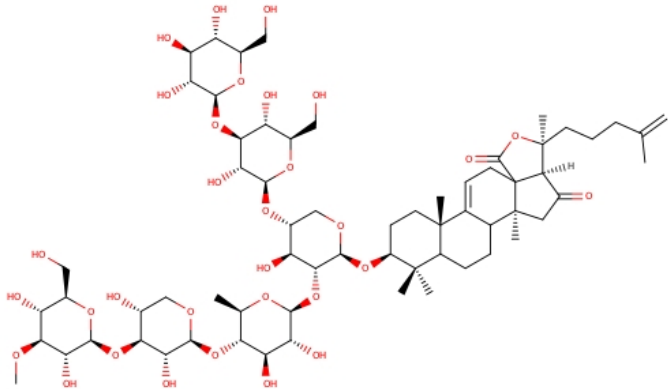
369. holotoxin B

화학 구조		PubMed ID	
		18557622	
TM-MC 성분 ID	205		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	GUALTKRMLRUEHJ-IPUIGULZSA-N		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)O[C@@H](O[C@@H]3[C@@H](C)O[C@@H](O[C@@H]4[C@@H](O)[C@@H](CO[C@H]4O[C@H]4CC[C@@]5(C)C(CCC6C5=CCC57[C@H](C(=O)C[C@@]65C)[C@](C)(CCCC(C)=C)OC7=O)C4(C)O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O[C@@H]5O[C@H](CO)[C@@H](O)[C@H](O)[C@H]5O)[C@H]4O)[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₆₆ H ₁₀₄ O ₃₂		
Molecular Weight	1409.526	Exact Molecular Weight	1408.651071189
LogP	-2.801	Topological Polar Surface Area	487.04 Å ²
Atom Count	202	Structural Alert Count	3
Hydrogen Bond Acceptor Count	31	Hydrogen Bond Donor Count	16
Rotatable Bond Count	21	Aromatic Ring Count	0
Drug Likeness	0.03	Oral Bioavailability	N

370. holotoxin A1

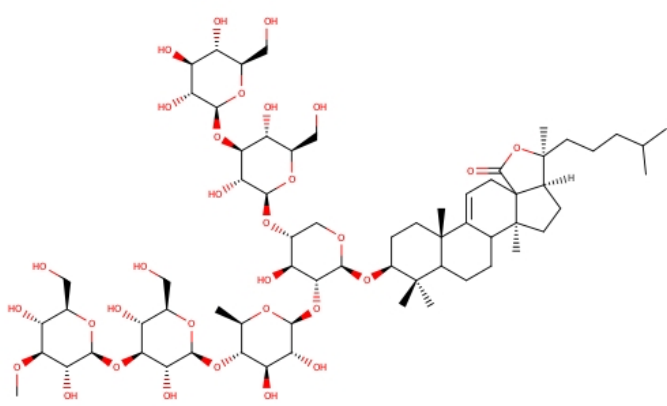
화학 구조		PubMed ID	
		18557622, 25604752 6467906	
TM-MC 성분 ID	206		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	QGOPAAXXSCRHID-MHCJNZEHSA-N		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)CO[C@@H](O[C@@H]3[C@@H](C)O[C@@H](O[C@@H]4[C@@H](O)[C@@H](CO[C@H]4O[C@H]5C(C)C(CCC6C5=CCC57[C@H](C(=O)C[C@]65C)[C@](C)(CCCC(C)=C)O C7=O)C4(C)C)O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O[C@@H]5O[C@H](CO)[C@@H](O)[C@H](OC[C@H]5O)[C@H]4O)[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₆₆ H ₁₀₄ O ₃₁		
Molecular Weight	1393.527	Exact Molecular Weight	1392.656156569
LogP	-1.527	Topological Polar Surface Area	455.81 Å ²
Atom Count	201	Structural Alert Count	3
Hydrogen Bond Acceptor Count	30	Hydrogen Bond Donor Count	14
Rotatable Bond Count	21	Aromatic Ring Count	0
Drug Likeness	0.04	Oral Bioavailability	N

371. holotoxin B1

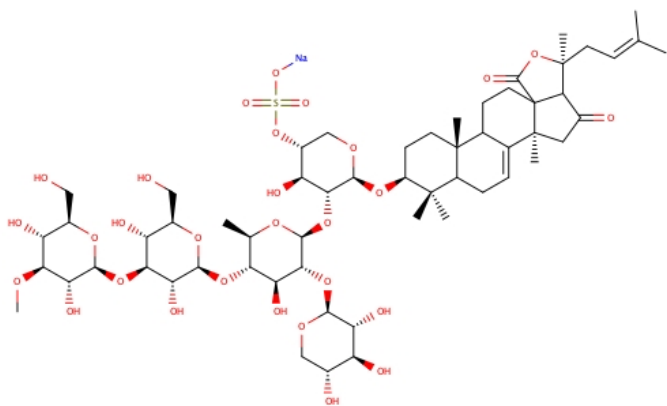
화학 구조	PubMed ID
	18557622, 6467906

TM-MC 성분 ID	207		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	OILUHBGADWOLFV-DWSVPGDISA-N		
SMILES	CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)CO[C@@H](O[C@@H]3[C@@H](C)O[C@@H](O[C@@H]4[C@@H](O)[C@@H](CO[C@H]4O[C@H]5C)C(CCC6C5=CCC57[C@H](C(=O)C[C@@]65O)[C@](C)(CCCC(C)=C)OC7=O)C4(C)C)O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O[C@@H]5O[C@H](CO)[C@@H](O)[C@H](O)[C@H]5O)[C@H]4O)[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O		
Molecular Formula	C ₆₅ H ₁₀₂ O ₃₁		
Molecular Weight	1379.5	Exact Molecular Weight	1378.640506504
LogP	-2.17	Topological Polar Surface Area	466.81 Å ²
Atom Count	198	Structural Alert Count	3
Hydrogen Bond Acceptor Count	30	Hydrogen Bond Donor Count	15
Rotatable Bond Count	20	Aromatic Ring Count	0
Drug Likeness	0.04	Oral Bioavailability	N

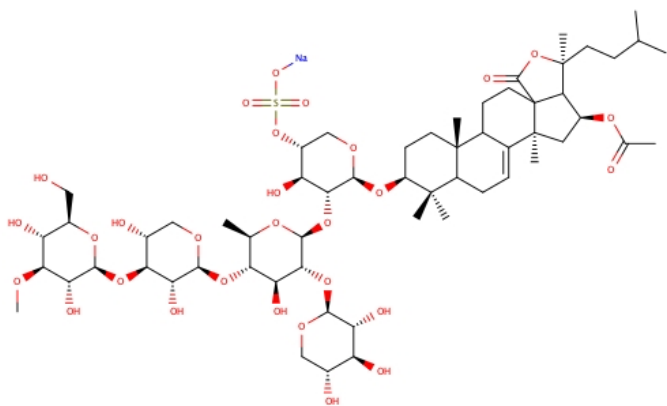
372. bivittoside C

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	208		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	SPXUDMDSBLAINQ-OTLKIFHWSA-N		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)O[C@@H](O[C@H]3[C@@H](C)O[C@@H](O[C@@H]4[C@H](O)[C@@H](CO)[C@H]4O[C@H]4CC[C@@]5(C)C(CCC6C5=CCC57[C@H](CC[C@@]65C)[C@](C)(CC(C)C)OC7=O)C4(C)O[C@@H]4O[C@H](CO)[C@@H](O)[C@H](O[C@@H]5O[C@H](CO)[C@@H](O)[C@H](O)[C@H]5O)[C@H]4O)[C@H](O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₆₆ H ₁₀₈ O ₃₁		
Molecular Weight	1397.559	Exact Molecular Weight	1396.687456698
LogP	-1.608	Topological Polar Surface Area	469.97 Å ²
Atom Count	205	Structural Alert Count	3
Hydrogen Bond Acceptor Count	30	Hydrogen Bond Donor Count	16
Rotatable Bond Count	21	Aromatic Ring Count	0
Drug Likeness	0.03	Oral Bioavailability	N

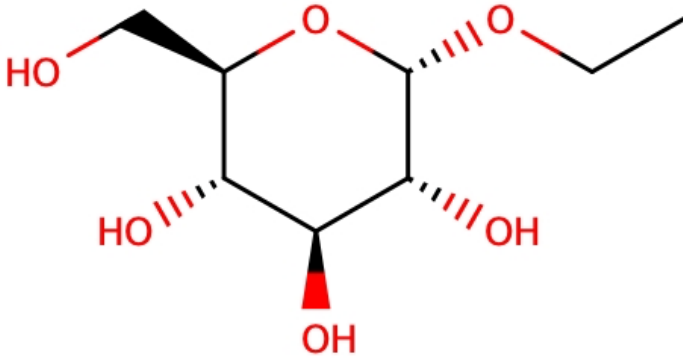
373. frondoside A2

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	209		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	XQBSWOKNEWDHSY-OCFIKCSHSA-M		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)[C@@H](CO)O[C@@H](O[C@H]3[C@@H](C)O[C@@H](O[C@H]4[C@H](O)[C@@H](CO)[C@H]4O[C@H]4CC[C@]5(C)C6CCC78C(C=O)C[C@@]7(C)C6=CCC5C4(C)C)[C@](C)(CC=C(C)C)OC8=O)OS(=O)(=O)O[Na])[C@H](O[C@@H]4OC[C@@H](O)[C@H](O)[C@H]4O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₅₈ H ₈₉ NaO ₂₉ S		
Molecular Weight	1305.37	Exact Molecular Weight	1304.5107923
LogP	-1.551	Topological Polar Surface Area	420.03 Å ²
Atom Count	178	Structural Alert Count	3
Hydrogen Bond Acceptor Count	26	Hydrogen Bond Donor Count	11
Rotatable Bond Count	18	Aromatic Ring Count	0
Drug Likeness	0.04	Oral Bioavailability	N

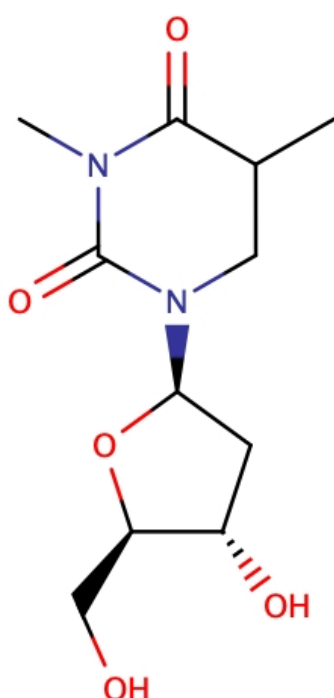
374. frondoside A

화학 구조		PubMed ID	
		25604752	
TM-MC 성분 ID	210		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	NDKBKIGKUZOHOP-WDOAVNQKSA-M		
SMILES	<chem>CO[C@H]1[C@H](O)[C@@H](CO)O[C@@H](O[C@H]2[C@H](O)CO[C@@H](O[C@@H]3[C@H](O)[C@@H](O[C@@H]4[C@@H](O)[C@@H](CO[C@H]4O[C@H]4CC[C@]5(C)C6CCC78C([C@H](C[C@@]7(C)C6=CCC5C4(C)C)OC(C)=O)[C@](C)(CCC(C)C)OC8=O)OS(=O)(=O)O[Na])[C@H](O[C@@H]4OC[C@@H](O)[C@H](O)[C@H]4O)[C@H]3O)[C@@H]2O)[C@@H]1O</chem>		
Molecular Formula	C ₅₉ H ₉₃ NaO ₂₉ S		
Molecular Weight	1321.41	Exact Molecular Weight	1320.54209243
LogP	-0.779	Topological Polar Surface Area	409.03 Å ²
Atom Count	183	Structural Alert Count	3
Hydrogen Bond Acceptor Count	25	Hydrogen Bond Donor Count	10
Rotatable Bond Count	20	Aromatic Ring Count	0
Drug Likeness	0.04	Oral Bioavailability	N

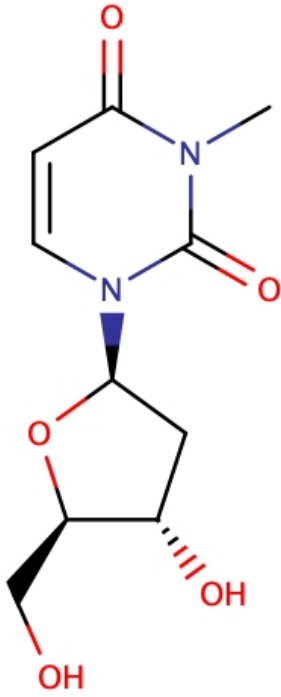
375. ethyl- α -D-glucopyranoside

화학 구조		PubMed ID	
		21384380	
TM-MC 성분 ID	233		
TM-MC 성분 동의어	N/A		
PubChem ID	9815668		
InChI Key	WYUFTYLVLQZQNH-CBQIKETKSA-N		
SMILES	CCO[C@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O		
Molecular Formula	C ₈ H ₁₆ O ₆		
Molecular Weight	208.21	Exact Molecular Weight	208.094688235
LogP	-1.933	Topological Polar Surface Area	99.38 Å ²
Atom Count	30	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.43	Oral Bioavailability	Y

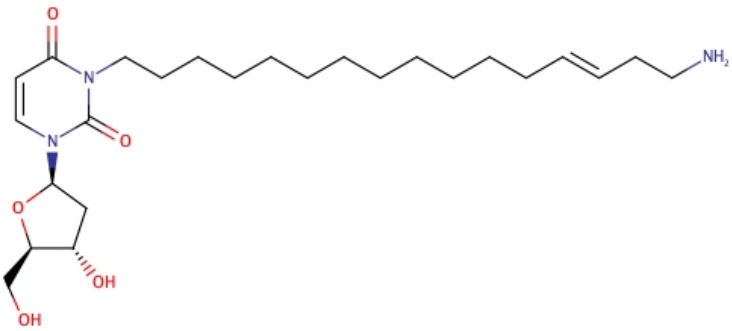
376. 5,6-dihydro-3-methylthymidine

화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	37873		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	NIBYECLYHAQASO-GSLILNRNSA-N		
SMILES	CC1CN([C@H]2C[C@H](O)[C@@H](CO)O2)C(=O)N(C)C1=O		
Molecular Formula	C ₁₁ H ₁₈ N ₂ O ₅		
Molecular Weight	258.274	Exact Molecular Weight	258.121571688
LogP	-1.106	Topological Polar Surface Area	90.31 Å ²
Atom Count	36	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.66	Oral Bioavailability	Y

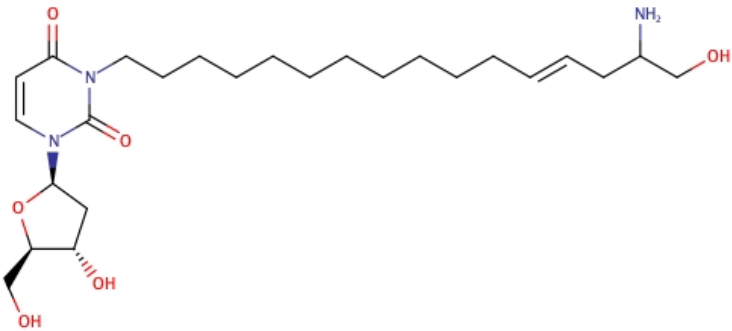
377. 3-methy-2'-deoxyuridine

화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	37892		
TM-MC 성분 동의어	N/A		
PubChem ID	13845047		
InChI Key	ZTSLWUGHMGGCM-LKEWCRSYSA-N		
SMILES	<chem>Cn1c(=O)ccn([C@H]2C[C@H](O)[C@@H](CO)O2)c1=O</chem>		
Molecular Formula	C ₁₀ H ₁₄ N ₂ O ₅		
Molecular Weight	242.231	Exact Molecular Weight	242.090271559
LogP	-1.291	Topological Polar Surface Area	90.31 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.67	Oral Bioavailability	Y

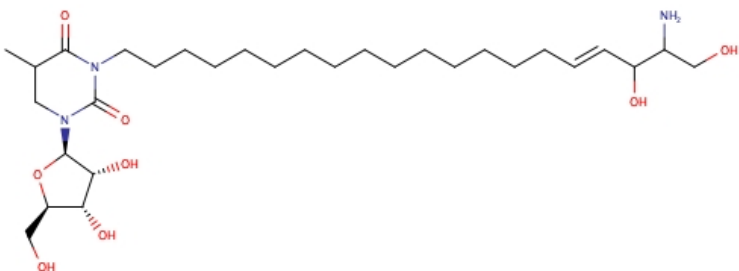
378. N-(1''-amino-3''-hexadecene)-2'-deoxyuridine

화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	39342		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	BLRKGJDDNWWZPU-RBAHGQGGSA-N		
SMILES	NCC#C=C#CCCCCCCCCCCCc1c(=O)ccn([C@H]2C[C@H](O)[C@@H](CO)O2)c1=O		
Molecular Formula	C ₂₅ H ₄₃ N ₃ O ₅		
Molecular Weight	465.635	Exact Molecular Weight	465.320271497
LogP	3.462	Topological Polar Surface Area	116.33 Å ²
Atom Count	76	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.24	Oral Bioavailability	N

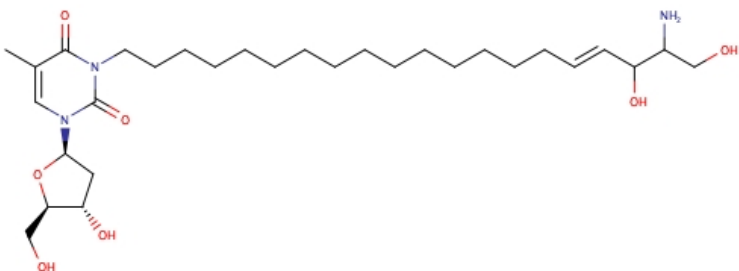
379. N-(2''-amino-1''-hydroxy-4''-hexadecene)-2'-deoxyuridine

화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	39343		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	ZFFPYWDEKQGTOI-FANIPHAFA-SA-N		
SMILES	NC(CO)C#C=C#CCCCCCCCCCCCn1c(=O)ccn([C@H]2C[C@H](O)[C@@H](CO)O2)c1=O		
Molecular Formula	C ₂₅ H ₄₃ N ₃ O ₆		
Molecular Weight	481.634	Exact Molecular Weight	481.315186117
LogP	2.387	Topological Polar Surface Area	136.56 Å ²
Atom Count	77	Structural Alert Count	2
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.20	Oral Bioavailability	N

380. N-(2''-amino-1'',3''-dihydroxy-4''-eicosene)-dihydroribothymidine

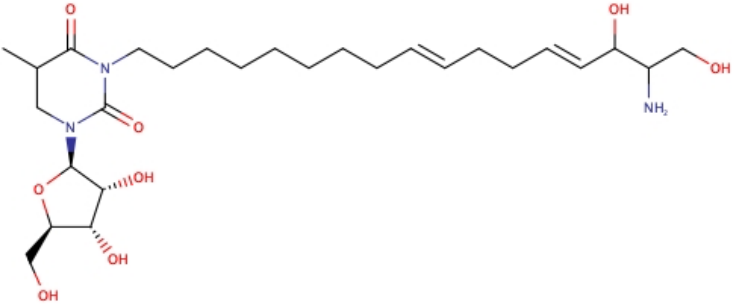
화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	39344		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	SMOGLZKBQVWUFZ-MTKHJTFRSA-N		
SMILES	CC1CN([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C(=O)N(CCCCCCCCCCCCCC=C[C@@H](O)[C@H](O)CO)C1=O		
Molecular Formula	C ₃₀ H ₅₅ N ₃ O ₈		
Molecular Weight	585.783	Exact Molecular Weight	585.398915743
LogP	2.531	Topological Polar Surface Area	177.02 Å ²
Atom Count	96	Structural Alert Count	2
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	6
Rotatable Bond Count	21	Aromatic Ring Count	0
Drug Likeness	0.09	Oral Bioavailability	N

381. N-(2''-amino-1'',3''-dihydroxy-4''-eicosene)-thymidine

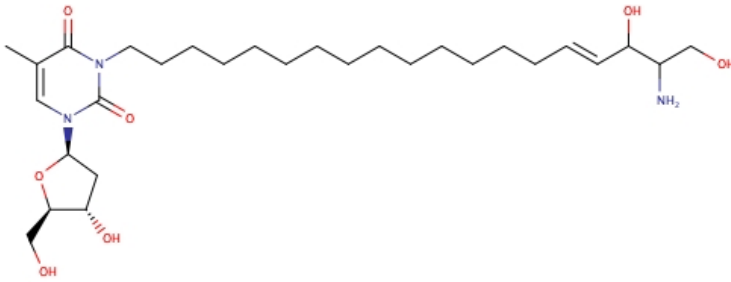
화학 구조	PubMed ID
	30588871

TM-MC 성분 ID	39345		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	RSAYKULRMOXPCS-NZYCKFKRSA-N		
SMILES	Cc1cn([C@H]2C[C@H](O)[C@@H](CO)O2)c(=O)n(CCCCCCCCCCCCCC=C\C(O)C(N)CO)c1=O		
Molecular Formula	C ₃₀ H ₅₃ N ₃ O ₇		
Molecular Weight	567.768	Exact Molecular Weight	567.388351059
LogP	3.642	Topological Polar Surface Area	156.79 Å ²
Atom Count	93	Structural Alert Count	2
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	21	Aromatic Ring Count	1
Drug Likeness	0.11	Oral Bioavailability	N

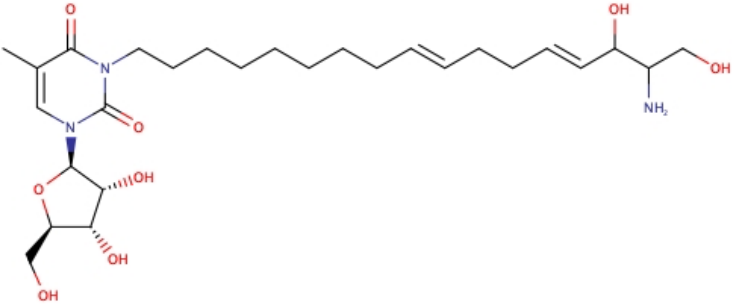
382. N-(2''-amino-1'',3''-dihydroxy-4'',8''-heptadecadiene)-dihydroribothymidine

화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	39346		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	USURRMITXQJHCS-NPVOKNTPSA-N		
SMILES	CC1CN([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C(=O)N(CCCCCCCCWC=CWCCWC=CWC(O)C(N)CO)C1=O		
Molecular Formula	C ₂₇ H ₄₇ N ₃ O ₈		
Molecular Weight	541.686	Exact Molecular Weight	541.336315485
LogP	0.835	Topological Polar Surface Area	177.02 Å ²
Atom Count	85	Structural Alert Count	2
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	6
Rotatable Bond Count	17	Aromatic Ring Count	0
Drug Likeness	0.11	Oral Bioavailability	N

383. N-(2''-amino-1'',3''-dihydroxy-4''-nonadecene)-thymidine

화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	39347		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	QPKSENDCEJZMOV-USLVZNHZSA-N		
SMILES	Cc1cn([C@H]2C[C@H](O)[C@@H](CO)O2)c(=O)n(CCCCCCCCCCCCCC=CWC=CW C(O)C(N)CO)c1=O		
Molecular Formula	C ₂₉ H ₅₁ N ₃ O ₇		
Molecular Weight	553.741	Exact Molecular Weight	553.372700994
LogP	3.198	Topological Polar Surface Area	156.79 Å ²
Atom Count	90	Structural Alert Count	2
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	20	Aromatic Ring Count	1
Drug Likeness	0.12	Oral Bioavailability	N

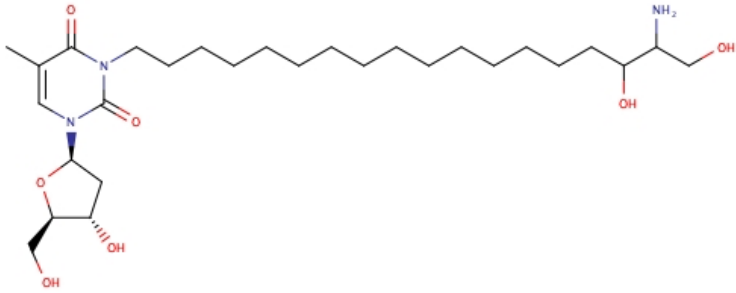
384. N-(2''-amino-1'',3''-dihydroxy-4'',8''-heptadecadiene)-ribothymidine

화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	39348		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	CHCHIDYLKOQCAQ-WMRDTEOUSA-N		
SMILES	Cc1cn([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)c(=O)n(CCCCCCCCWC=CWCCWC=CWC(O)C(N)CO)c1=O		
Molecular Formula	C ₂₇ H ₄₅ N ₃ O ₈		
Molecular Weight	539.67	Exact Molecular Weight	539.320665421
LogP	1.046	Topological Polar Surface Area	177.02 Å ²
Atom Count	83	Structural Alert Count	2
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	6
Rotatable Bond Count	17	Aromatic Ring Count	1
Drug Likeness	0.12	Oral Bioavailability	N

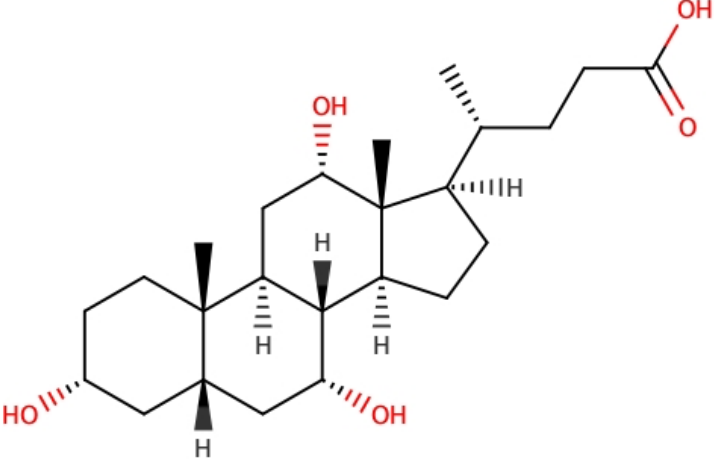
385. N-(2''-amino-1'',3''-dihydroxy-4'',8''-octadecadiene)-dihydroribothymidine

화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	39349		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	RIIJFEKUESJHQK-AASDUJRJA-N		
SMILES	CC1CN([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C(=O)N(CCCCCCCC=C\C=C\C=C(O)C(N)CO)C1=O		
Molecular Formula	C ₂₈ H ₄₉ N ₃ O ₈		
Molecular Weight	555.713	Exact Molecular Weight	555.35196555
LogP	1.28	Topological Polar Surface Area	177.02 Å ²
Atom Count	88	Structural Alert Count	2
Hydrogen Bond Acceptor Count	9	Hydrogen Bond Donor Count	6
Rotatable Bond Count	18	Aromatic Ring Count	0
Drug Likeness	0.11	Oral Bioavailability	N

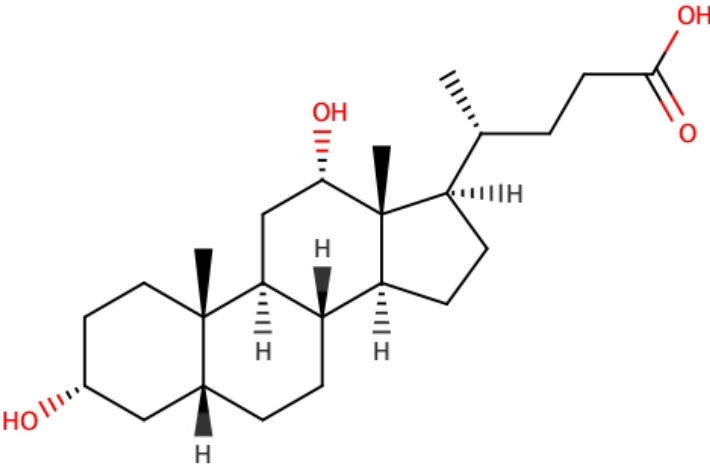
386. N-(2''-amino-1'',3''-dihydroxy-octodecane)-thymidine

화학 구조		PubMed ID	
		30588871	
TM-MC 성분 ID	39350		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	WTNXLASUOSVOAE-QFIOHLPESA-N		
SMILES	Cc1cn([C@H]2C[C@H](O)[C@@H](CO)O2)c(=O)n(CCCCCCCCCCCCCCCC(O)C(N)CO)c1=O		
Molecular Formula	C ₂₈ H ₅₁ N ₃ O ₇		
Molecular Weight	541.73	Exact Molecular Weight	541.372700994
LogP	2.959	Topological Polar Surface Area	156.79 Å ²
Atom Count	89	Structural Alert Count	1
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	20	Aromatic Ring Count	1
Drug Likeness	0.16	Oral Bioavailability	N

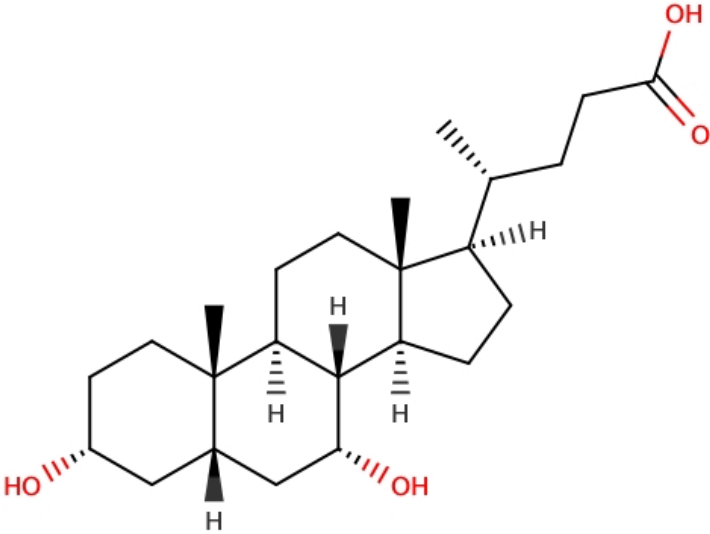
387. cholic acid

화학 구조		PubMed ID	
		16651035, 17202716 20155752, 21111425 22019293, 22058087 23099565, 23315150 25214136, 25829769 26016891, 27169647 31825798	
TM-MC 성분 ID	234		
TM-MC 성분 동의어	3 α ,7 α -dihydroxy-5 β -cholic acid		
PubChem ID	221493		
InChI Key	BHQCQFFYZLCCQO-OELDTZBJSA-N		
SMILES	<chem>C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@]12C</chem>		
Molecular Formula	C ₂₄ H ₄₀ O ₅		
Molecular Weight	408.579	Exact Molecular Weight	408.287574388
LogP	2.482	Topological Polar Surface Area	97.99 Å ²
Atom Count	69	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.57	Oral Bioavailability	Y

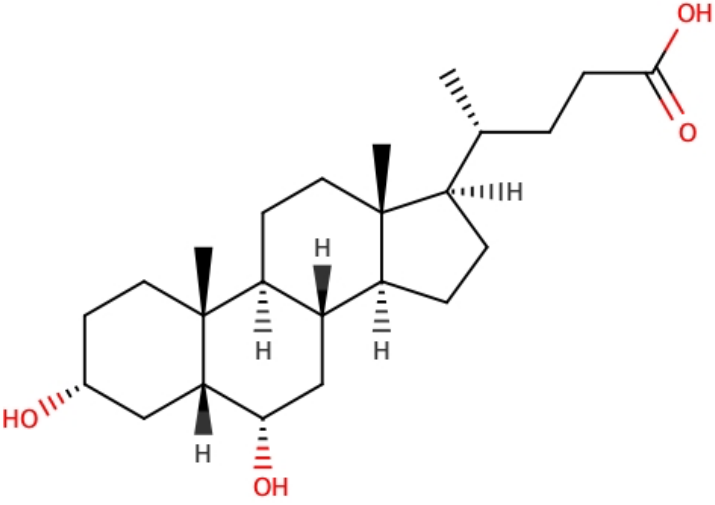
388. deoxycholic acid

화학 구조		PubMed ID	
		17202716, 20155752 21111425, 22019293 22058087, 23099565 23315150, 25214136 26016891, 27169647 31825798	
TM-MC 성분 ID	235		
TM-MC 성분 동의어	N/A		
PubChem ID	222528		
InChI Key	KXGVEGMKQFWNSR-LLQZFEROSA-N		
SMILES	<chem>C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3[C@H](O)[C@]12C</chem>		
Molecular Formula	C ₂₄ H ₄₀ O ₄		
Molecular Weight	392.58	Exact Molecular Weight	392.292659768
LogP	3.791	Topological Polar Surface Area	77.76 Å ²
Atom Count	68	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.68	Oral Bioavailability	Y

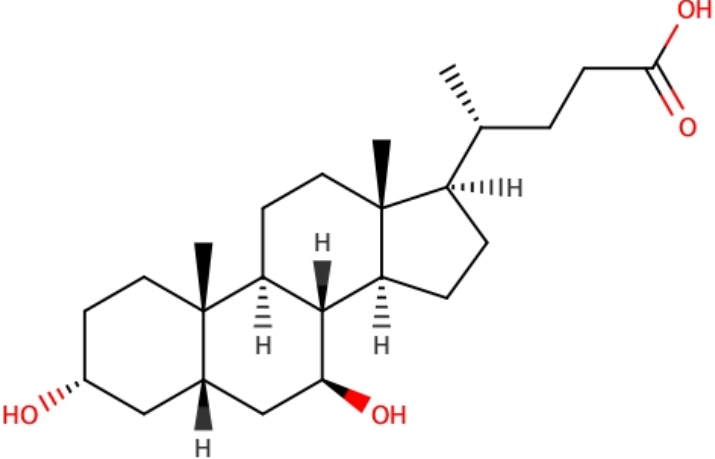
389. chenodeoxycholic acid

화학 구조		PubMed ID	
		<p>16651035, 17202716 20155752, 21111425 22058087, 23099565 23315150, 25214136 26016891, 27169647 30593238, 31825798</p>	
TM-MC 성분 ID	236		
TM-MC 성분 동의어	N/A		
PubChem ID	10133		
InChI Key	RUDATBOHQWOJDD-BSWAIDMHSA-N		
SMILES	<chem>C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₄ H ₄₀ O ₄		
Molecular Weight	392.58	Exact Molecular Weight	392.292659768
LogP	3.713	Topological Polar Surface Area	77.76 Å ²
Atom Count	68	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.68	Oral Bioavailability	Y

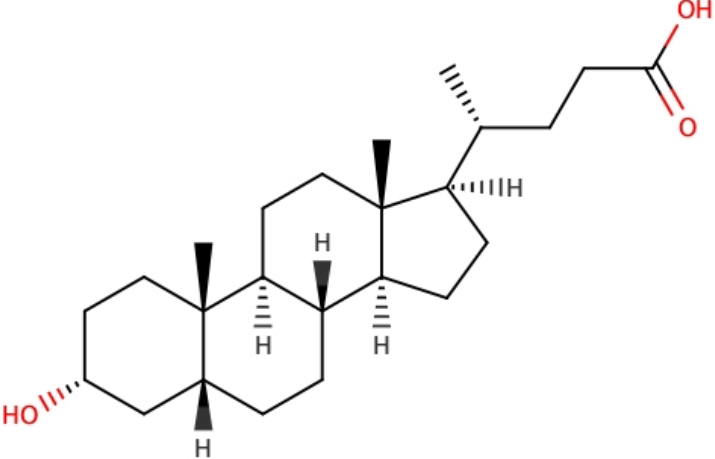
390. hyodeoxycholic acid

화학 구조		PubMed ID	
		<p>16651035, 17136860 17202716, 20155752 21111425, 22019293 23099565, 23315150 25214136, 26016891 30593238, 31825798</p>	
TM-MC 성분 ID	237		
TM-MC 성분 동의어	porcine deoxycholic acid		
PubChem ID	5283820		
InChI Key	DGABKXLVPYZII-SIBKNCMHSA-N		
SMILES	<chem>C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@@H]3C[C@H](O)[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₄ H ₄₀ O ₄		
Molecular Weight	392.58	Exact Molecular Weight	392.292659768
LogP	3.713	Topological Polar Surface Area	77.76 Å ²
Atom Count	68	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.68	Oral Bioavailability	Y

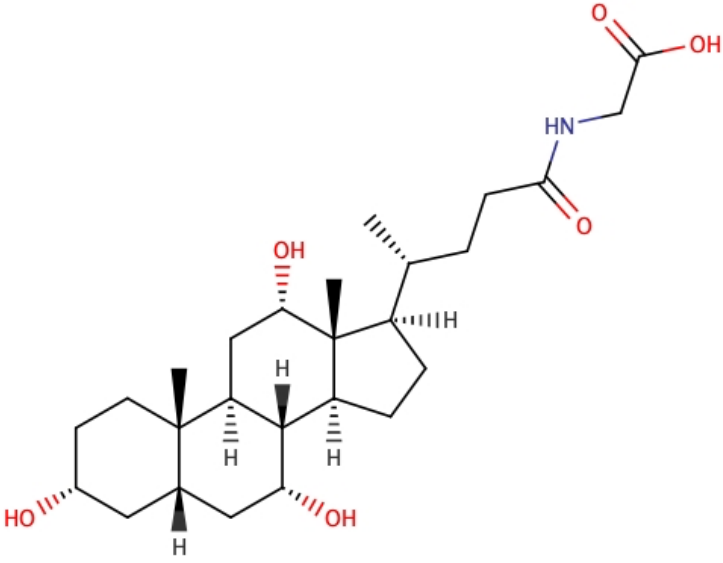
391. ursodeoxycholic acid

화학 구조		PubMed ID	
		17202716, 20155752 21111425, 22019293 22058087, 23099565 23315150, 25214136 27169647, 31825798	
TM-MC 성분 ID	238		
TM-MC 성분 동의어	N/A		
PubChem ID	31401		
InChI Key	RUDATBOHQWOJDD-UZVSRGJWSA-N		
SMILES	<chem>C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@@H]3[C@@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₄ H ₄₀ O ₄		
Molecular Weight	392.58	Exact Molecular Weight	392.292659768
LogP	3.713	Topological Polar Surface Area	77.76 Å ²
Atom Count	68	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.68	Oral Bioavailability	Y

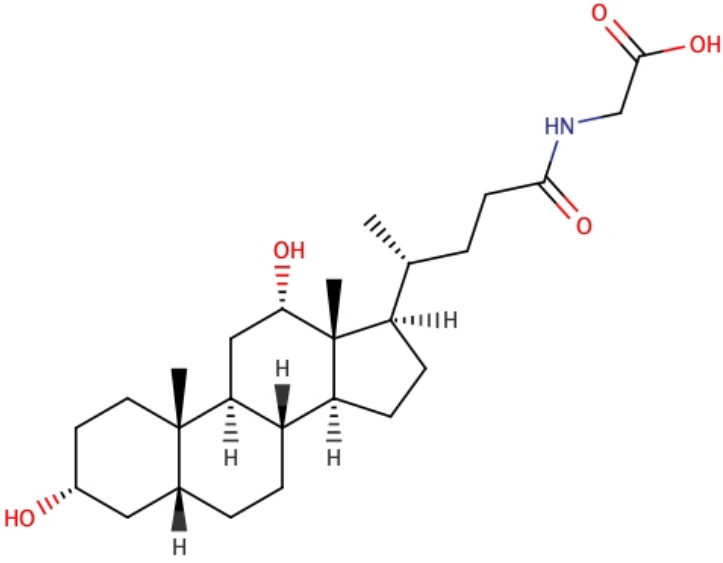
392. lithocholic acid

화학 구조		PubMed ID	
		21111425, 23315150 25829769, 27169647 31825798	
TM-MC 성분 ID	239		
TM-MC 성분 동의어	N/A		
PubChem ID	9903		
InChI Key	SMEROWZSTRWXGI-HVATVPOCSA-N		
SMILES	<chem>C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₄ H ₄₀ O ₃		
Molecular Weight	376.581	Exact Molecular Weight	376.297745148
LogP	5.022	Topological Polar Surface Area	57.53 Å ²
Atom Count	67	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.72	Oral Bioavailability	Y

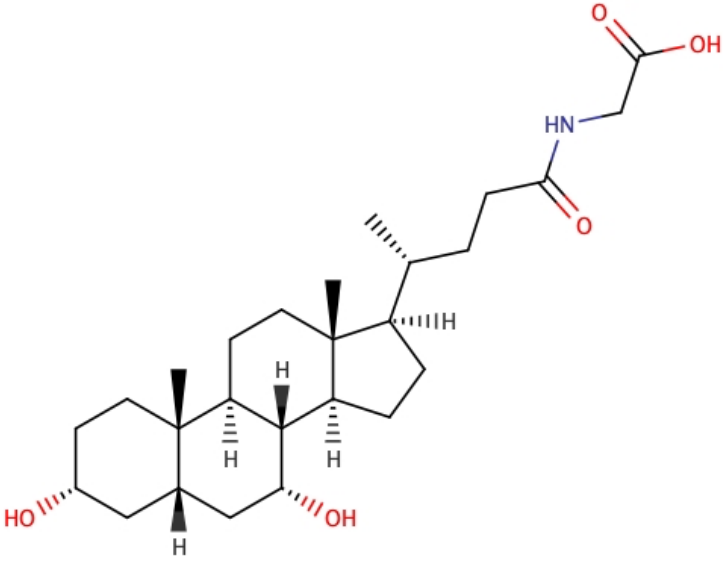
393. glycocholic acid

화학 구조		PubMed ID	
		<p>19619630, 21111425 23315150, 25829769 27169647, 29950079 31825798</p>	
TM-MC 성분 ID	241		
TM-MC 성분 동의어	N/A		
PubChem ID	10140		
InChI Key	RFDAIACWWDREDC-FRVQLJSFSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCC(O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@]12C</chem>		
Molecular Formula	C ₂₆ H ₄₃ NO ₆		
Molecular Weight	465.631	Exact Molecular Weight	465.309038109
LogP	1.377	Topological Polar Surface Area	127.09 Å ²
Atom Count	76	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	5
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.40	Oral Bioavailability	Y

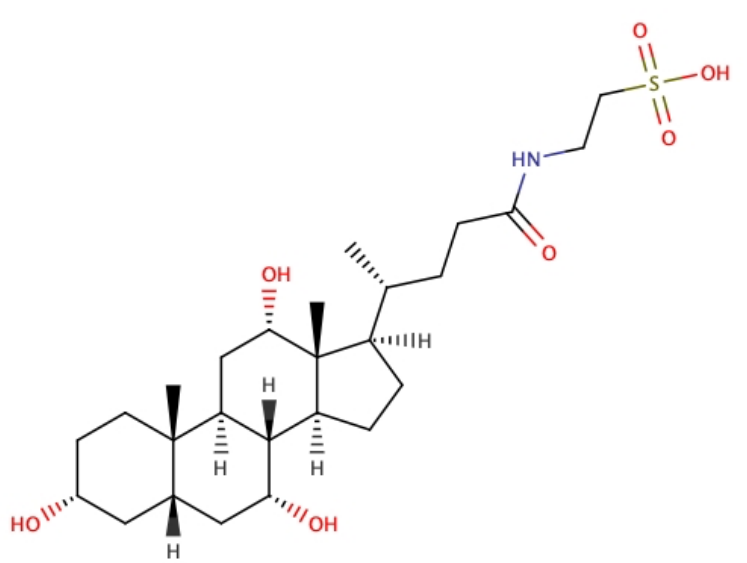
394. glycodeoxycholic acid

화학 구조		PubMed ID	
		<p>19619630, 21111425 25829769, 27169647 29950079, 31825798</p>	
TM-MC 성분 ID	242		
TM-MC 성분 동의어	N/A		
PubChem ID	3035026		
InChI Key	WVULKSPCQVQLCU-BUXLTGKBSA-N		
SMILES	C[C@H](CCC(=O)NCC(O)=O)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@]12C		
Molecular Formula	C ₂₆ H ₄₃ NO ₅		
Molecular Weight	449.632	Exact Molecular Weight	449.314123489
LogP	2.686	Topological Polar Surface Area	106.86 Å ²
Atom Count	75	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.50	Oral Bioavailability	Y

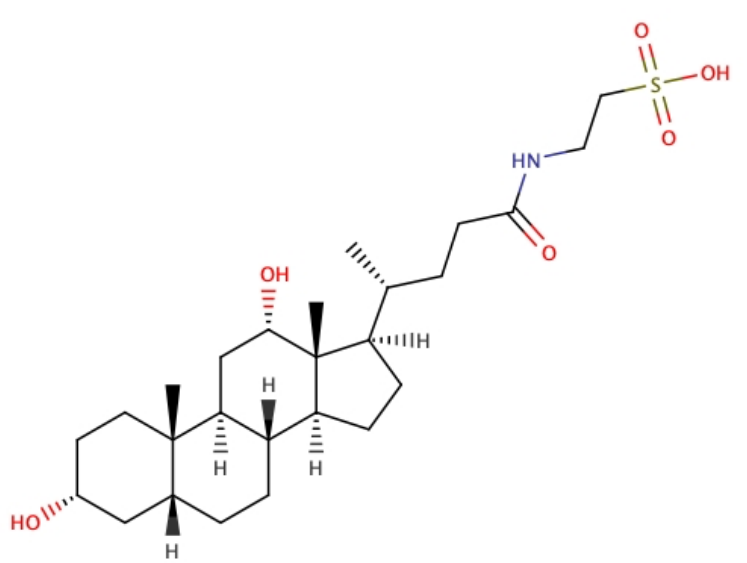
395. glycochenodeoxycholic acid

화학 구조		PubMed ID	
		<p>21111425, 23008527 23315150, 27169647 29950079, 31342711 31825798</p>	
TM-MC 성분 ID	243		
TM-MC 성분 동의어	glycochenodeoxycholate		
PubChem ID	12544		
InChI Key	GHCZAUBVMUEKKP-GYPHWSFCSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCC(O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₆ H ₄₃ NO ₅		
Molecular Weight	449.632	Exact Molecular Weight	449.314123489
LogP	2.608	Topological Polar Surface Area	106.86 Å ²
Atom Count	75	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.50	Oral Bioavailability	Y

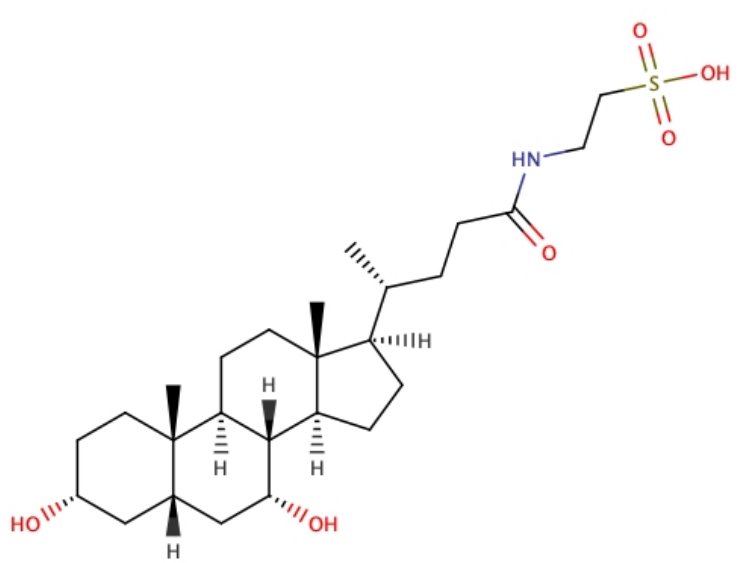
396. taurocholic acid

화학 구조		PubMed ID	
		19619630, 21111425 23315150, 25829769 27169647, 29950079 31825798	
TM-MC 성분 ID	247		
TM-MC 성분 동의어	taurocholate acid		
PubChem ID	6675		
InChI Key	WBWWGRHZICKQGZ-HZAMXZRMSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCCS(O)(=O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@]12C</chem>		
Molecular Formula	C ₂₆ H ₄₅ NO ₇ S		
Molecular Weight	515.71	Exact Molecular Weight	515.291673967
LogP	-0.244	Topological Polar Surface Area	144.16 Å ²
Atom Count	80	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	5
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.29	Oral Bioavailability	Y

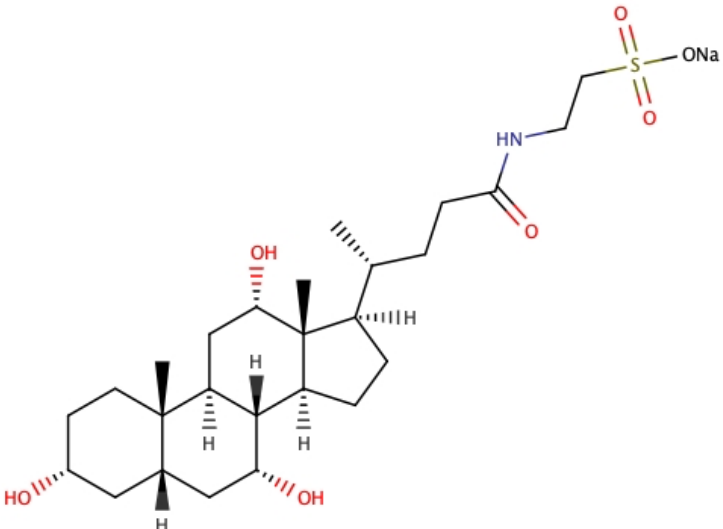
397. taurodeoxycholic acid

화학 구조		PubMed ID	
		<p>19619630, 21111425 23315150, 27169647 31825798</p>	
TM-MC 성분 ID	248		
TM-MC 성분 동의어	N/A		
PubChem ID	2733768		
InChI Key	AWDRATDZQPJFN-VAYUFCLWSA-N		
SMILES	C[C@H](CCC(=O)NCCS(O)(=O)=O)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3[C@H](O)[C@]12C		
Molecular Formula	C ₂₆ H ₄₅ NO ₆ S		
Molecular Weight	499.71	Exact Molecular Weight	499.296759347
LogP	1.136	Topological Polar Surface Area	123.93 Å ²
Atom Count	79	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.39	Oral Bioavailability	Y

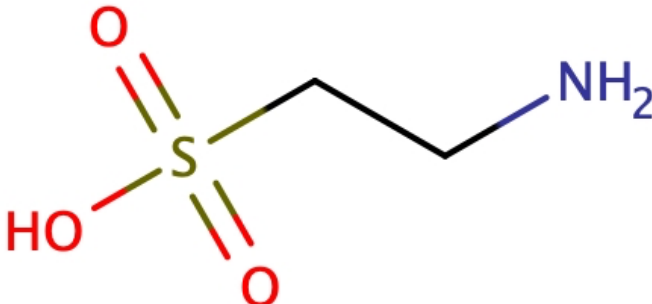
398. taurochenodeoxycholic acid

화학 구조		PubMed ID	
		<p>19619630, 21111425 21442029, 27169647 29950079, 31825798</p>	
TM-MC 성분 ID	249		
TM-MC 성분 동의어	N/A		
PubChem ID	387316		
InChI Key	BHTRKEVKTKCXOH-BJLOMENOSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCCS(O)(=O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₆ H ₄₅ NO ₆ S		
Molecular Weight	499.71	Exact Molecular Weight	499.296759347
LogP	1.097	Topological Polar Surface Area	123.93 Å ²
Atom Count	79	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.39	Oral Bioavailability	Y

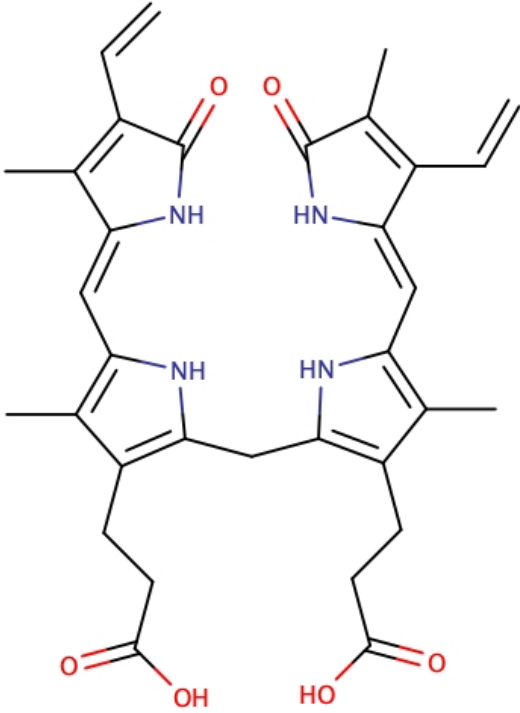
399. taurocholate sodium

화학 구조		PubMed ID	
		<p>20155752, 22019293 22058087, 23099565 25214136</p>	
TM-MC 성분 ID	2472		
TM-MC 성분 동의어	N/A		
PubChem ID	23666345, 101627506		
InChI Key	JAJWGBVLPIOOH-IZYKLYLVSA-M		
SMILES	C[C@H](CCC(=O)NCCS(=O)(=O)O[Na])[C@H]1CC[C@H]2[C@@H]3[C@H](O)C[C@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@]12C		
Molecular Formula	C ₂₆ H ₄₄ NNaO ₇ S		
Molecular Weight	537.69	Exact Molecular Weight	537.27361821
LogP	1.586	Topological Polar Surface Area	133.16 Å ²
Atom Count	80	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.36	Oral Bioavailability	Y

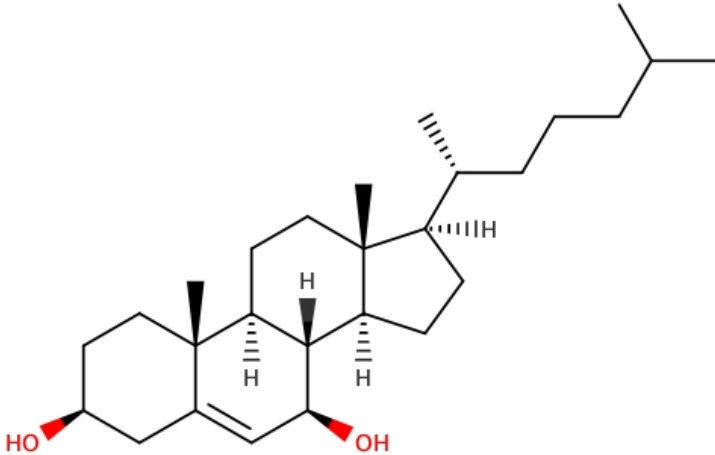
400. taurine

화학 구조		PubMed ID	
		23315150, 31825798	
TM-MC 성분 ID	255		
TM-MC 성분 동의어	N/A		
PubChem ID	1123, 4068592		
InChI Key	XOAAWQZATWQOTB-UHFFFAOYSA-N		
SMILES	NCCS(O)(=O)=O		
Molecular Formula	C ₂ H ₇ NO ₃ S		
Molecular Weight	125.14	Exact Molecular Weight	125.014664263
LogP	-2.615	Topological Polar Surface Area	80.39 Å ²
Atom Count	14	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.40	Oral Bioavailability	Y

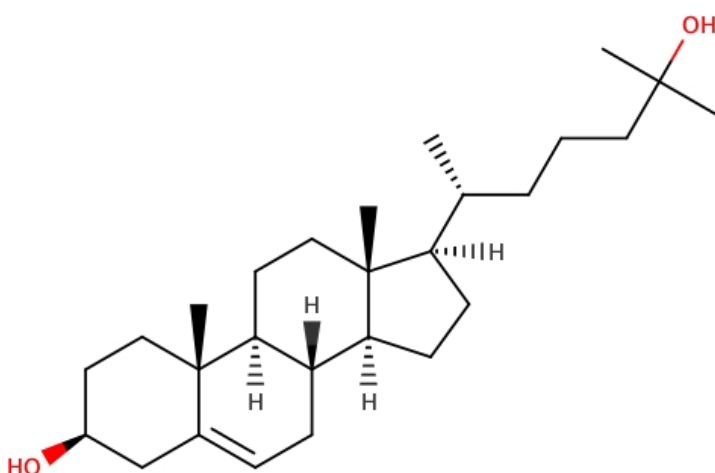
401. bilirubin

화학 구조		PubMed ID	
		17202716, 23315150	
TM-MC 성분 ID	256		
TM-MC 성분 동의어	N/A		
PubChem ID	5280352		
InChI Key	BPYKTIZUTYGOLE-IFADSCNNSA-N		
SMILES	<chem>CC1=C(C(=O)WC(NC1=O)=C)Wc1[nH]c(Cc2[nH]c(WC=C3/NC(=O)C(C=C)=C3C)c(C)c2CCC(O)=O)c(CCC(O)=O)c1C</chem>		
Molecular Formula	C ₃₃ H ₃₆ N ₄ O ₆		
Molecular Weight	584.673	Exact Molecular Weight	584.263484895
LogP	3.119	Topological Polar Surface Area	164.38 Å ²
Atom Count	79	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	6
Rotatable Bond Count	12	Aromatic Ring Count	2
Drug Likeness	0.22	Oral Bioavailability	N

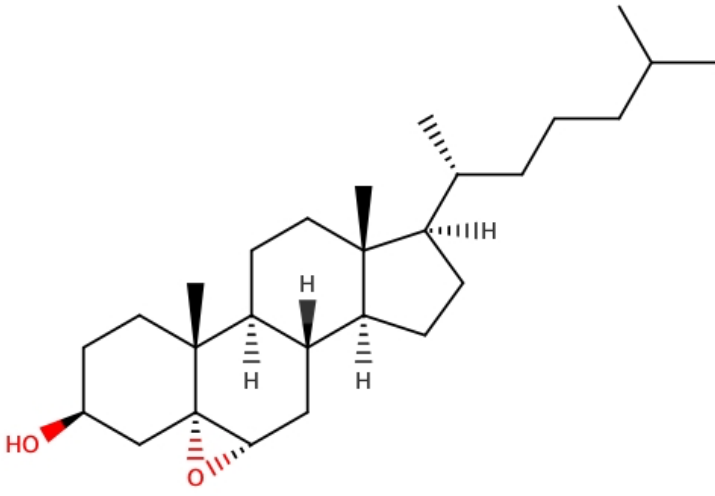
402. 7 β -hydroxycholesterol

화학 구조		PubMed ID	
		20835952, 25545614	
TM-MC 성분 ID	257		
TM-MC 성분 동의어	cholest-5-ene-3,7-diol; cholest-5-en-3 β ,7 β -diol		
PubChem ID	473141		
InChI Key	OYXZMSRRJOYLLO-KGZHIOMZSA-N		
SMILES	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3[C@@H](O)C=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₇ H ₄₆ O ₂		
Molecular Weight	402.663	Exact Molecular Weight	402.349780721
LogP	5.96	Topological Polar Surface Area	40.46 Å ²
Atom Count	75	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.56	Oral Bioavailability	Y

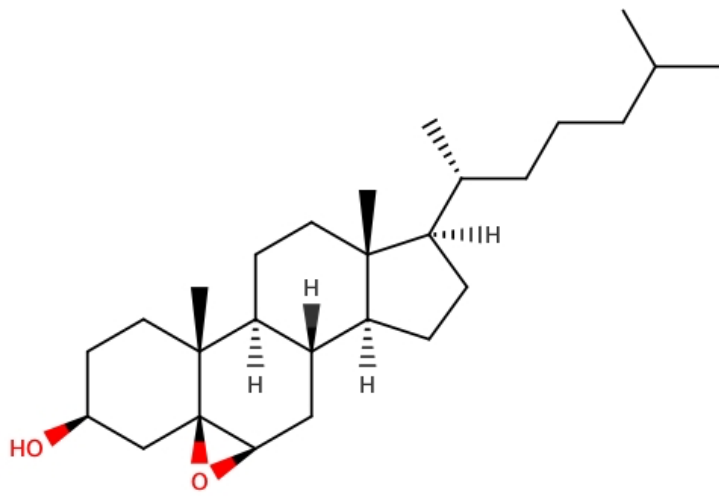
403. 25-hydroxycholesterol

화학 구조		PubMed ID	
		25545614	
TM-MC 성분 ID	258		
TM-MC 성분 동의어	N/A		
PubChem ID	65094		
InChI Key	INBG SXNNRGWLJU-ZHHJOTBYSA-N		
SMILES	C[C@H](CCCC(C)O)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₇ H ₄₆ O ₂		
Molecular Weight	402.663	Exact Molecular Weight	402.349780721
LogP	5.642	Topological Polar Surface Area	40.46 Å ²
Atom Count	75	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.58	Oral Bioavailability	Y

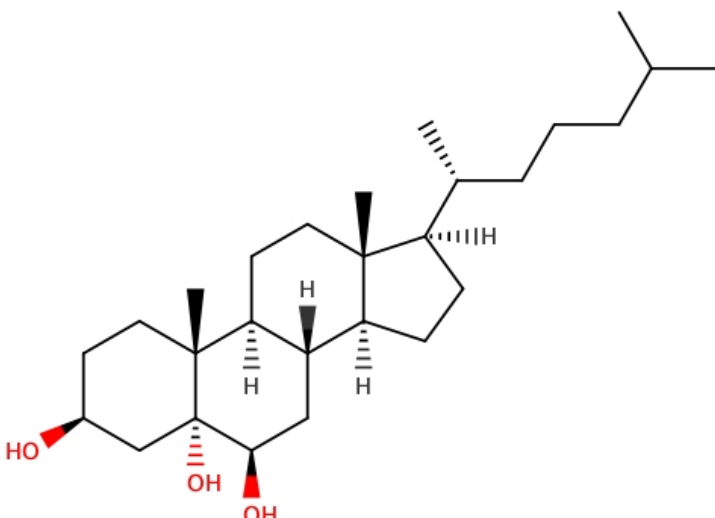
404. 5,6 α -epoxycholesterol

화학 구조		PubMed ID	
		25545614	
TM-MC 성분 ID	259		
TM-MC 성분 동의어	N/A		
PubChem ID	227037		
InChI Key	PRYIJAGAEJZDBO-ZEQHCUNVSA-N		
SMILES	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3C[C@@H]4O[C@@]44C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₇ H ₄₆ O ₂		
Molecular Weight	402.663	Exact Molecular Weight	402.349780721
LogP	6.373	Topological Polar Surface Area	32.76 Å ²
Atom Count	75	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.54	Oral Bioavailability	Y

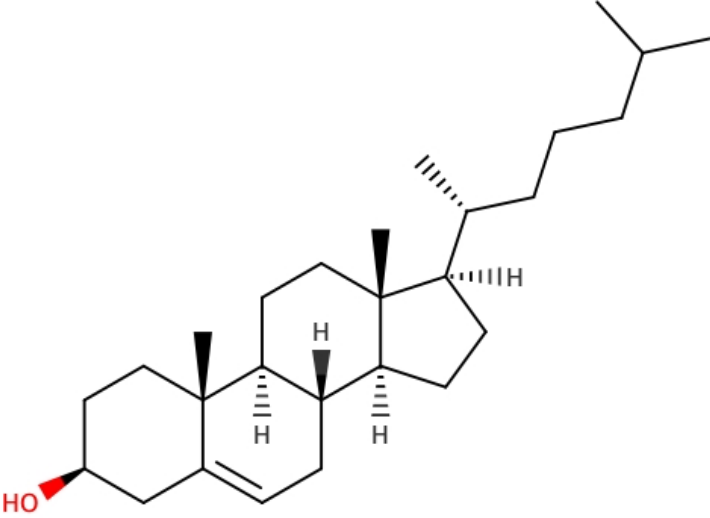
405. 5,6 β -epoxycholesterol

화학 구조		PubMed ID	
		25545614	
TM-MC 성분 ID	260		
TM-MC 성분 동의어	N/A		
PubChem ID	108109		
InChI Key	PRYIJAGAEJZDBO-DTLXENBRSA-N		
SMILES	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3C[C@H]4O[C@]44C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₇ H ₄₆ O ₂		
Molecular Weight	402.663	Exact Molecular Weight	402.349780721
LogP	6.373	Topological Polar Surface Area	32.76 Å ²
Atom Count	75	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.54	Oral Bioavailability	Y

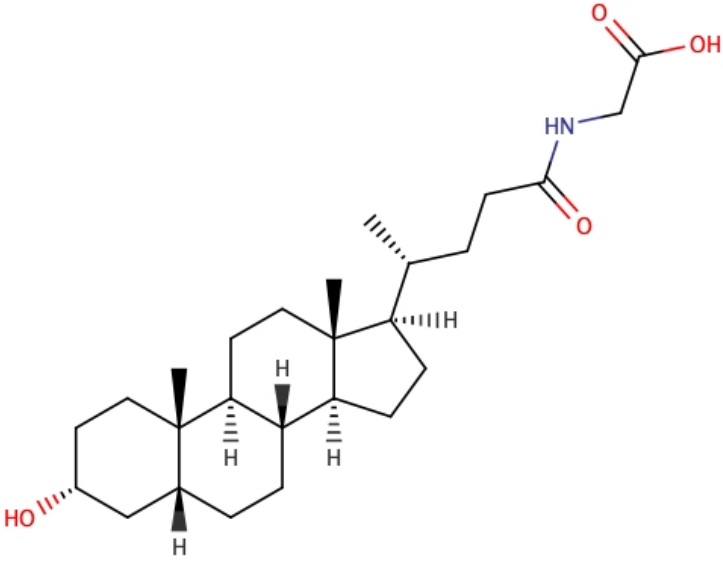
406. cholestane-3 β ,5 α ,6 β -triol

화학 구조		PubMed ID	
		25545614	
TM-MC 성분 ID	261		
TM-MC 성분 동의어	N/A		
PubChem ID	91498		
InChI Key	YMMFNKXZULYSOQ-RUXQDQFYSA-N		
SMILES	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3C[C@@H](O)[C@@]4(O)C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₇ H ₄₈ O ₃		
Molecular Weight	420.678	Exact Molecular Weight	420.360345406
LogP	5.211	Topological Polar Surface Area	60.69 Å ²
Atom Count	78	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	3
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.57	Oral Bioavailability	Y

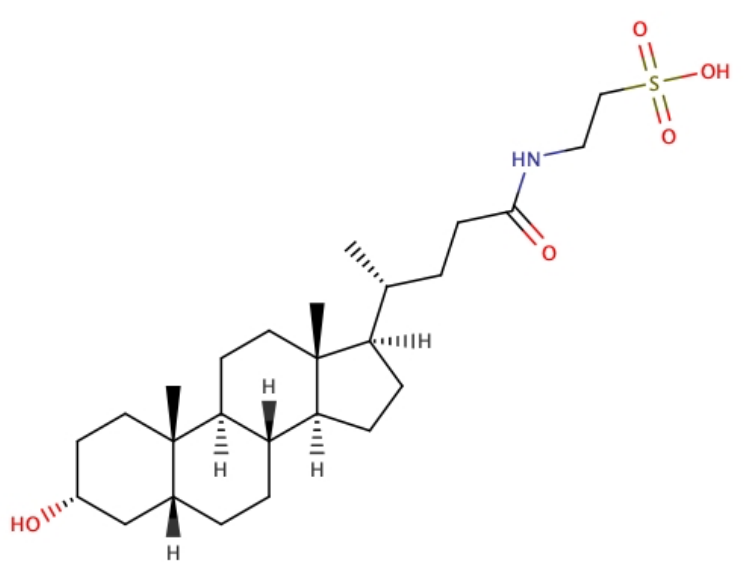
407. cholesterol

화학 구조		PubMed ID	
		20155752, 23891647 26744067	
TM-MC 성분 ID	283		
TM-MC 성분 동의어	N/A		
PubChem ID	5997		
InChI Key	HVYWMOMLDIMFJA-DPAQBDFISA-N		
SMILES	<chem>CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₇ H ₄₆ O		
Molecular Weight	386.664	Exact Molecular Weight	386.354866101
LogP	7.113	Topological Polar Surface Area	20.23 Å ²
Atom Count	74	Structural Alert Count	1
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.50	Oral Bioavailability	Y

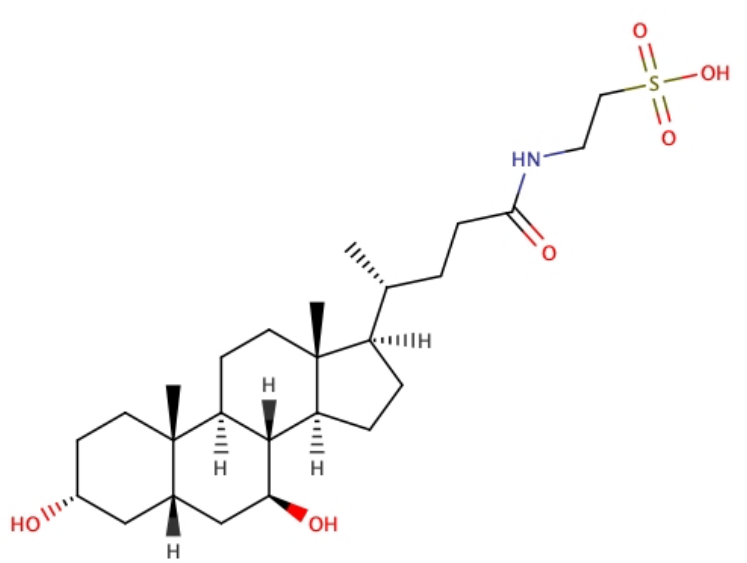
408. glycolithocholic acid

화학 구조		PubMed ID	
		21111425, 27169647	
TM-MC 성분 ID	246		
TM-MC 성분 동의어	N/A		
PubChem ID	115245		
InChI Key	XBSQTYHEGZTYJE-OETIFKL TSA-N		
SMILES	C[C@H](CCC(=O)NCC(O)=O)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₆ H ₄₃ NO ₄		
Molecular Weight	433.633	Exact Molecular Weight	433.319208869
LogP	3.917	Topological Polar Surface Area	86.63 Å ²
Atom Count	74	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.59	Oral Bioavailability	Y

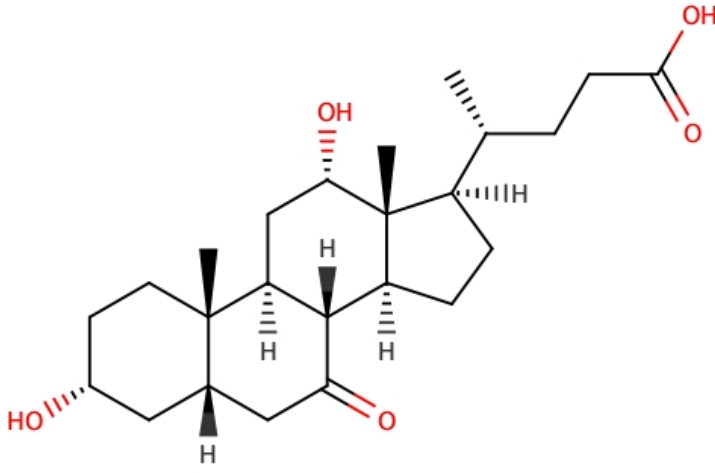
409. tauroolithocholic acid

화학 구조		PubMed ID	
		21111425, 23315150 27169647	
TM-MC 성분 ID	252		
TM-MC 성분 동의어	N/A		
PubChem ID	439763		
InChI Key	QBYUNVOYXHFKC-GBURMNQMSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCCS(O)(=O)=O)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₆ H ₄₅ NO ₅ S		
Molecular Weight	483.71	Exact Molecular Weight	483.301844727
LogP	2.481	Topological Polar Surface Area	103.7 Å ²
Atom Count	78	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.48	Oral Bioavailability	Y

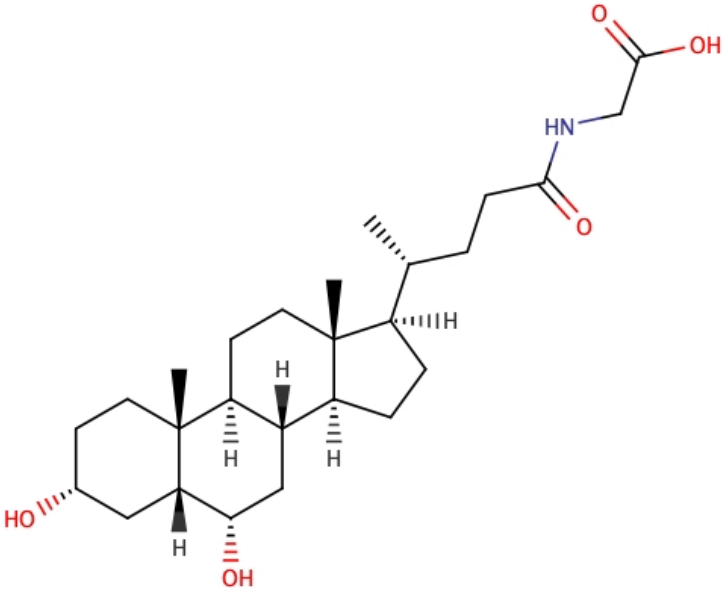
410. taoursodeoxycholic acid

화학 구조		PubMed ID	
		19619630, 21111425 27169647	
TM-MC 성분 ID	253		
TM-MC 성분 동의어	N/A		
PubChem ID	9848818		
InChI Key	BHTRKEVKTKCXOH-LBSADWJPSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCCS(O)(=O)=O)[C@H]1CC[C@H]2[C@@H]3[C@@H](O)C[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₆ H ₄₅ NO ₆ S		
Molecular Weight	499.71	Exact Molecular Weight	499.296759347
LogP	1.097	Topological Polar Surface Area	123.93 Å ²
Atom Count	79	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.39	Oral Bioavailability	Y

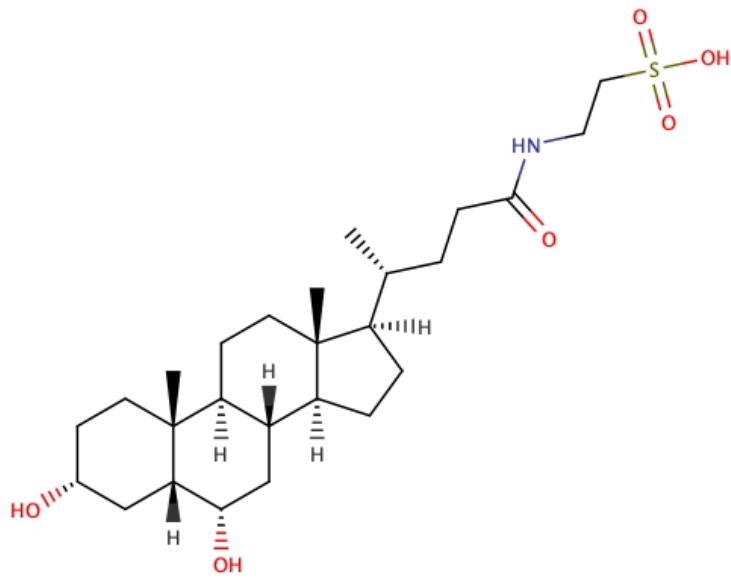
411. 3 α ,12 α -dihydroxy-7-oxo-5 β -cholanic acid

화학 구조		PubMed ID	
		25829769	
TM-MC 성분 ID	240		
TM-MC 성분 동의어	N/A		
PubChem ID	188292		
InChI Key	RHCPKKNRWFXMAT-RRWYKFPJSA-N		
SMILES	C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@H]3[C@H](C[C@H](O)[C@]12C)[C@@]1(C)CC[C@@H](O)C[C@H]1CC3=O		
Molecular Formula	C ₂₄ H ₃₈ O ₅		
Molecular Weight	406.563	Exact Molecular Weight	406.271924324
LogP	2.868	Topological Polar Surface Area	94.83 Å ²
Atom Count	67	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.67	Oral Bioavailability	Y

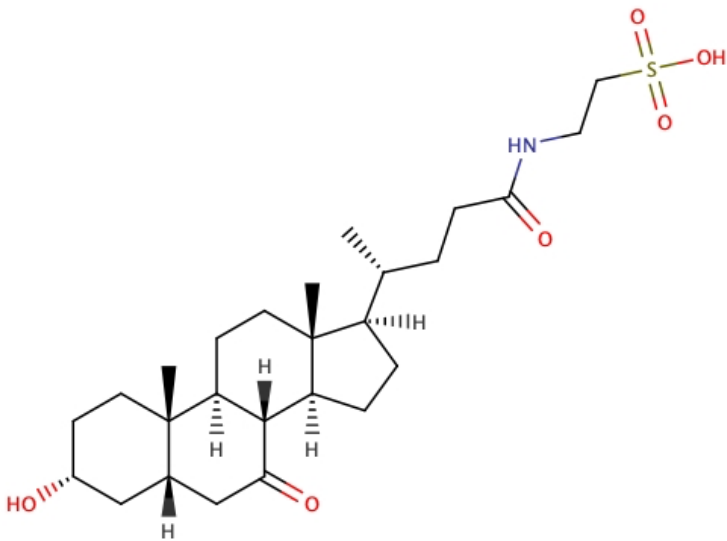
412. glycohyodeoxycholic acid

화학 구조		PubMed ID	
		21111425, 23008527 29950079, 31342711	
TM-MC 성분 ID	245		
TM-MC 성분 동의어	N/A		
PubChem ID	114611		
InChI Key	SPOIYSFQOFYOFZ-BRDORRHWSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCC(O)=O)[C@H]1CC[C@H]2[C@@H]3C[C@H](O)[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₆ H ₄₃ NO ₅		
Molecular Weight	449.632	Exact Molecular Weight	449.314123489
LogP	2.608	Topological Polar Surface Area	106.86 Å ²
Atom Count	75	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.50	Oral Bioavailability	Y

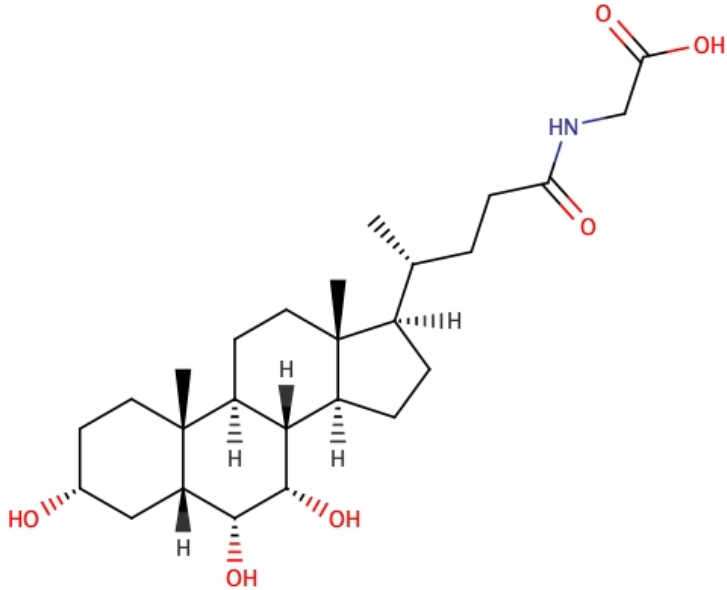
413. taurohyodeoxycholic acid

화학 구조		PubMed ID	
		21111425, 21442029 29950079	
TM-MC 성분 ID	251		
TM-MC 성분 동의어	N/A		
PubChem ID	119046		
InChI Key	HMXP0CDLAFANT-BHYUGXBJSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCCS(O)(=O)=O)[C@H]1CC[C@H]2[C@@H]3C[C@H](O)[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₆ H ₄₅ NO ₆ S		
Molecular Weight	499.71	Exact Molecular Weight	499.296759347
LogP	1.188	Topological Polar Surface Area	123.93 Å ²
Atom Count	79	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.39	Oral Bioavailability	Y

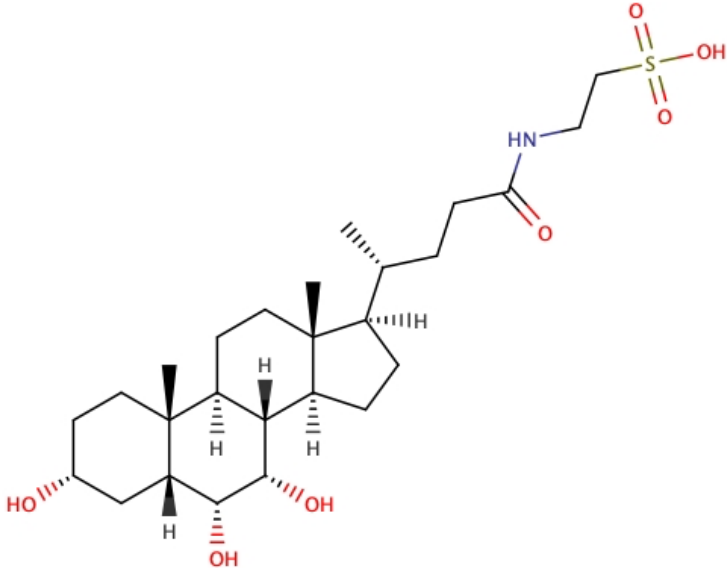
414. 7-keto-taurochenodeoxycholic acid

화학 구조		PubMed ID	
		27169647	
TM-MC 성분 ID	254		
TM-MC 성분 동의어	N/A		
PubChem ID	10323609		
InChI Key	QNRIYEYAHVEGQJ-SWQVIYSDSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCCS(O)(=O)=O)[C@H]1CC[C@H]2[C@H]3[C@H](CC[C@]12C)[C@@]1(C)CC[C@@H](O)C[C@H]1CC3=O</chem>		
Molecular Formula	C ₂₆ H ₄₃ NO ₆ S		
Molecular Weight	497.69	Exact Molecular Weight	497.281109283
LogP	1.561	Topological Polar Surface Area	120.77 Å ²
Atom Count	77	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.46	Oral Bioavailability	Y

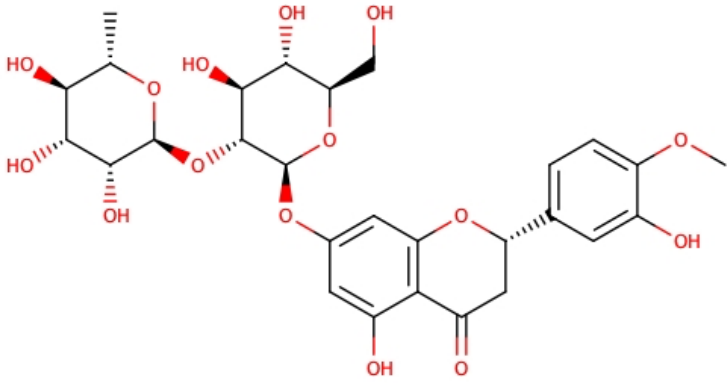
415. glycohyocholic acid

화학 구조		PubMed ID	
		23008527	
TM-MC 성분 ID	244		
TM-MC 성분 동의어	N/A		
PubChem ID	71361462		
InChI Key	ZQYUKJFJPJDMMR-ZDWCHQGWSA-N		
SMILES	<chem>C[C@H](CCC(=O)NCC(O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)[C@H](O)[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₆ H ₄₃ NO ₆		
Molecular Weight	465.631	Exact Molecular Weight	465.309038109
LogP	1.611	Topological Polar Surface Area	127.09 Å ²
Atom Count	76	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	5
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.41	Oral Bioavailability	Y

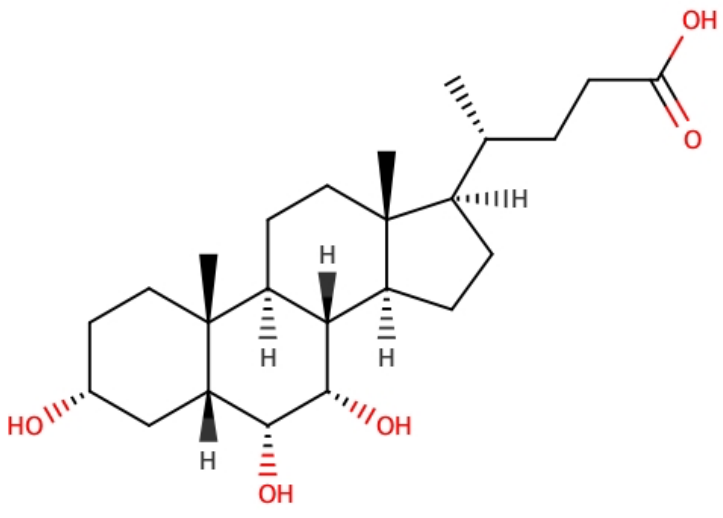
416. taurohyocholic acid

화학 구조		PubMed ID	
		21442029	
TM-MC 성분 ID	250		
TM-MC 성분 동의어	N/A		
PubChem ID	11954195		
InChI Key	XSOLDPYUICCHJX-QZEPYOAJSA-N		
SMILES	C[C@H](CCC(=O)NCCS(O)(=O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)[C@H](O)[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₆ H ₄₅ NO ₇ S		
Molecular Weight	515.71	Exact Molecular Weight	515.291673967
LogP	0.191	Topological Polar Surface Area	144.16 Å ²
Atom Count	80	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	5
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.30	Oral Bioavailability	Y

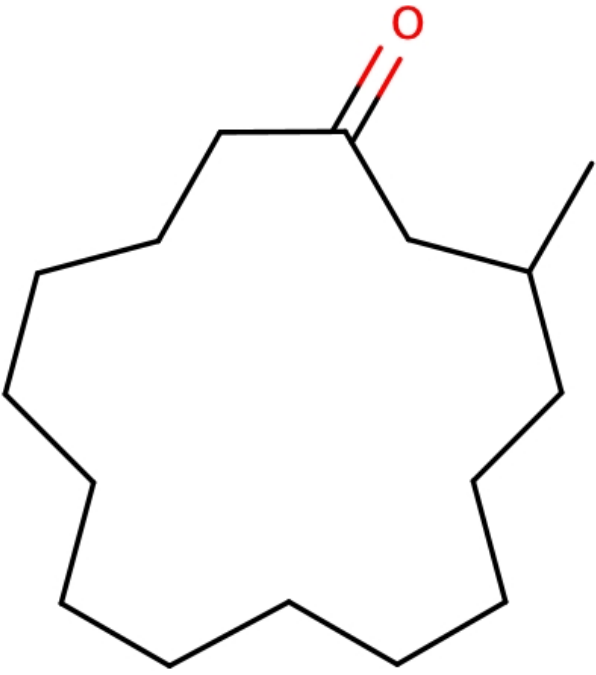
417. neohesperidin

화학 구조		PubMed ID	
		22239430	
TM-MC 성분 ID	266		
TM-MC 성분 동의어	hesperetin-7-O-neohesperidoside		
PubChem ID	442439		
InChI Key	ARGKVCXINMKCAZ-UZRWAPQLSA-N		
SMILES	<chem>COC1ccc(cc1O)[C@@H]1CC(=O)c2c(O)cc(O[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](C)[C@H](O)[C@@H](O)[C@H]3O)c2O1</chem>		
Molecular Formula	C ₂₈ H ₃₄ O ₁₅		
Molecular Weight	610.565	Exact Molecular Weight	610.189770395
LogP	-0.315	Topological Polar Surface Area	234.29 Å ²
Atom Count	77	Structural Alert Count	0
Hydrogen Bond Acceptor Count	15	Hydrogen Bond Donor Count	8
Rotatable Bond Count	7	Aromatic Ring Count	2
Drug Likeness	0.20	Oral Bioavailability	N

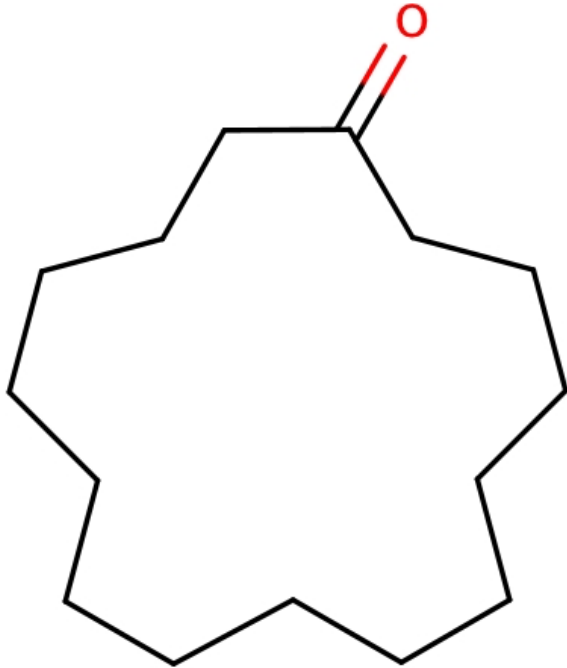
418. hyocholic acid

화학 구조		PubMed ID	
		30593238	
TM-MC 성분 ID	301455		
TM-MC 성분 동의어	porcine cholic acid		
PubChem ID	92805		
InChI Key	DKPMWHFRUGMUKF-KWXDGCAGSA-N		
SMILES	<chem>C[C@H](CCC(O)=O)[C@H]1CC[C@H]2[C@@H]3[C@H](O)[C@H](O)[C@@H]4[C@H](O)CC[C@]4(C)[C@H]3CC[C@]12C</chem>		
Molecular Formula	C ₂₄ H ₄₀ O ₅		
Molecular Weight	408.579	Exact Molecular Weight	408.287574388
LogP	2.716	Topological Polar Surface Area	97.99 Å ²
Atom Count	69	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.57	Oral Bioavailability	Y

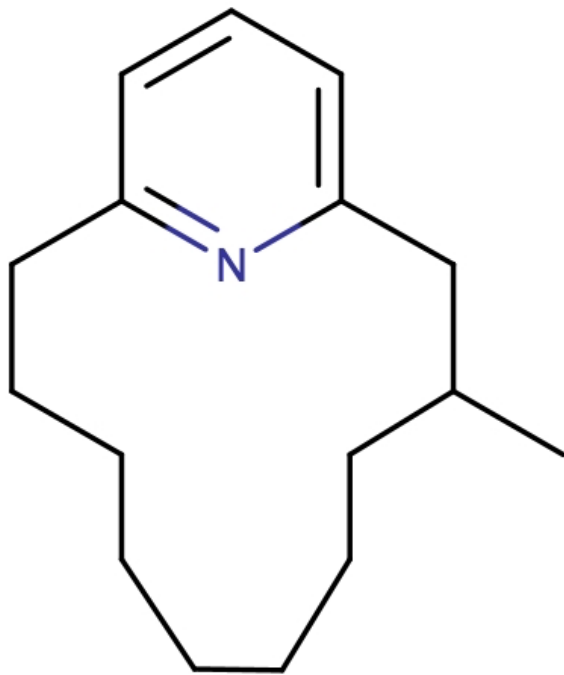
419. muscone

화학 구조		PubMed ID	
		15568689, 23520031 25976179, 26744067 29551642	
TM-MC 성분 ID	267		
TM-MC 성분 동의어	3-methylcyclopentadecanone		
PubChem ID	10947		
InChI Key	ALHUZKCOMYUFRB-UHFFFAOYSA-N		
SMILES	<chem>CC1CCCCCCCCCCCCC(=O)C1</chem>		
Molecular Formula	C ₁₆ H ₃₀ O		
Molecular Weight	238.415	Exact Molecular Weight	238.229665586
LogP	5.776	Topological Polar Surface Area	17.07 Å ²
Atom Count	47	Structural Alert Count	0
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.52	Oral Bioavailability	Y

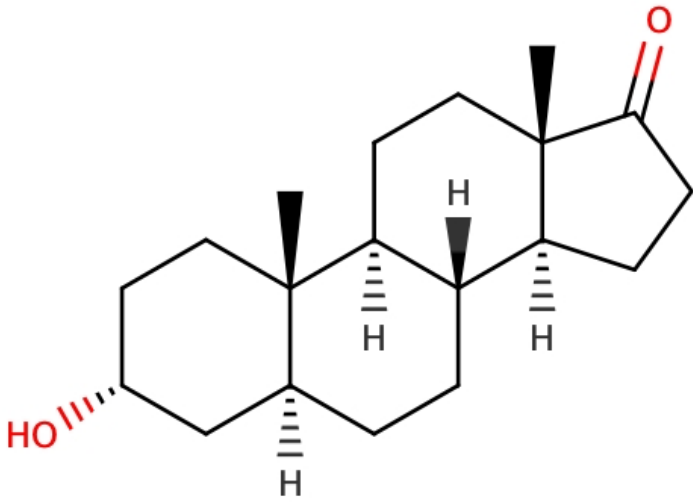
420. normuscone

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	268		
TM-MC 성분 동의어	cyclopentadecanone		
PubChem ID	10409		
InChI Key	OSOIQGOYGSIMF-UHFFFAOYSA-N		
SMILES	O=C1CCCCCCCCCCCCC1		
Molecular Formula	C ₁₅ H ₂₈ O		
Molecular Weight	224.388	Exact Molecular Weight	224.214015522
LogP	5.489	Topological Polar Surface Area	17.07 Å ²
Atom Count	44	Structural Alert Count	0
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.53	Oral Bioavailability	Y

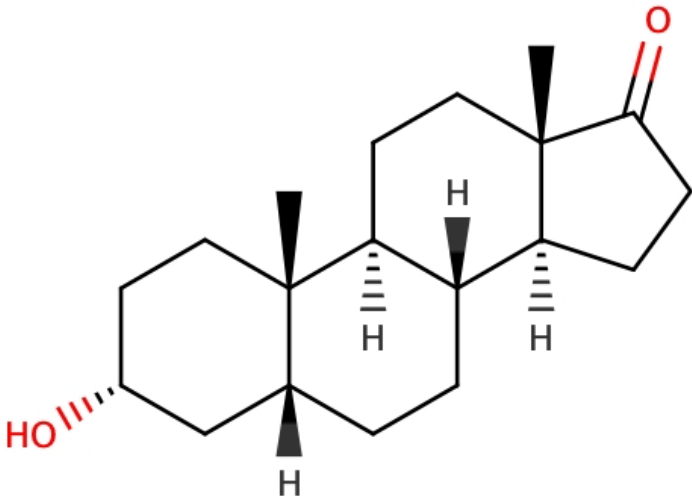
421. muscopyridine

화학 구조		PubMed ID	
		15568689	
TM-MC 성분 ID	269		
TM-MC 성분 동의어	N/A		
PubChem ID	5319970		
InChI Key	IMNKABOILQOFDL-UHFFFAOYSA-N		
SMILES	<chem>CC1CCCCCCCCc2cccc(C1)n2</chem>		
Molecular Formula	C ₁₆ H ₂₅ N		
Molecular Weight	231.383	Exact Molecular Weight	231.198699809
LogP	4.91	Topological Polar Surface Area	12.89 Å ²
Atom Count	42	Structural Alert Count	0
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	1
Drug Likeness	0.62	Oral Bioavailability	Y

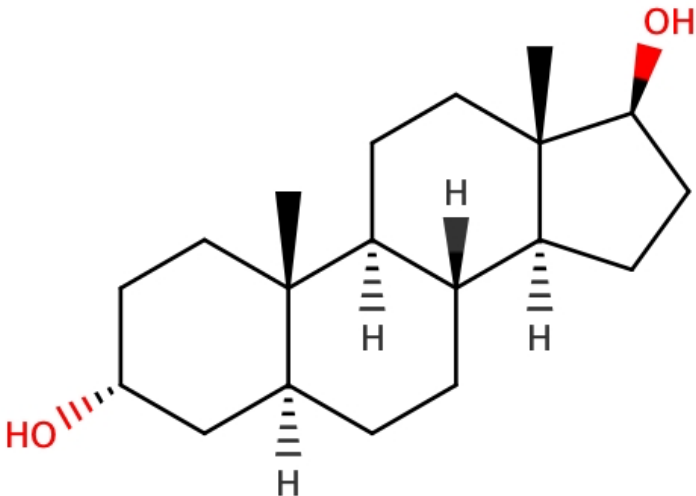
422. androsterone

화학 구조		PubMed ID	
		23891647	
TM-MC 성분 ID	270		
TM-MC 성분 동의어	N/A		
PubChem ID	5879		
InChI Key	QGXBDMJGAMFCBF-HLUDHZFRSA-N		
SMILES	C[C@]12CC[C@H]3[C@@H](CC[C@H]4C[C@H](O)CC[C@]34C)[C@@H]1CCC2=O		
Molecular Formula	C ₁₉ H ₃₀ O ₂		
Molecular Weight	290.447	Exact Molecular Weight	290.224580206
LogP	3.767	Topological Polar Surface Area	37.3 Å ²
Atom Count	51	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.74	Oral Bioavailability	Y

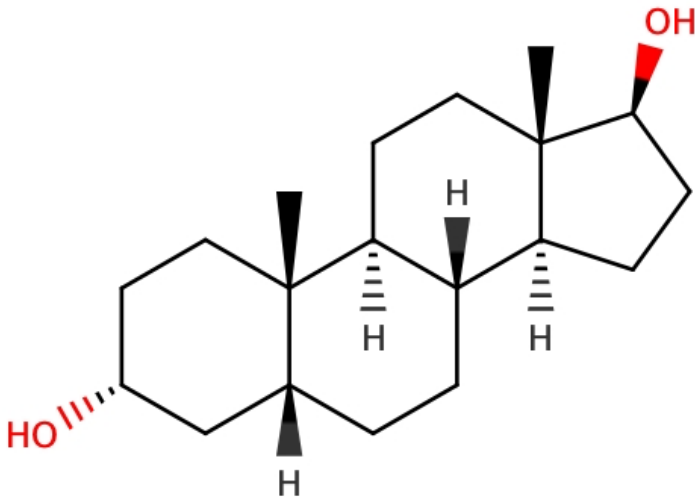
423. etiocholanolone

화학 구조		PubMed ID	
		23891647, 26744067	
TM-MC 성분 ID	271		
TM-MC 성분 동의어	3 α -hydroxy-5 β -androstan-17-one		
PubChem ID	5880		
InChI Key	QGXBDMJGAMFCBF-BNSUEQOYSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](O)CC[C@]34C)[C@@H]1CCC2=O</chem>		
Molecular Formula	C ₁₉ H ₃₀ O ₂		
Molecular Weight	290.447	Exact Molecular Weight	290.224580206
LogP	3.767	Topological Polar Surface Area	37.3 Å ²
Atom Count	51	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.74	Oral Bioavailability	Y

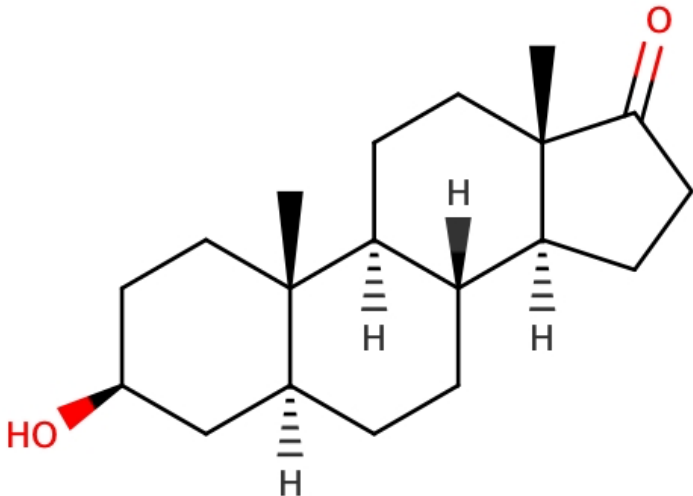
424. 5 α -androstane-3 α ,17 β -diol

화학 구조		PubMed ID	
		23891647, 26744067	
TM-MC 성분 ID	272		
TM-MC 성분 동의어	N/A		
PubChem ID	15818		
InChI Key	CBMYJHIOYJESB-KHOSGYARSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4C[C@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>		
Molecular Formula	C ₁₉ H ₃₂ O ₂		
Molecular Weight	292.463	Exact Molecular Weight	292.24023027
LogP	3.204	Topological Polar Surface Area	40.46 Å ²
Atom Count	53	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.72	Oral Bioavailability	Y

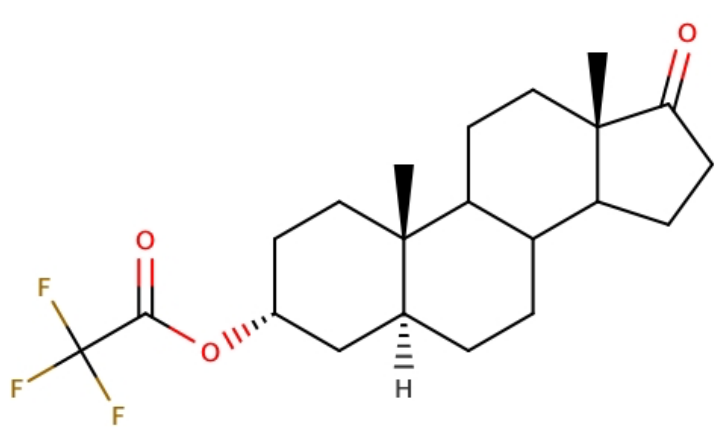
425. 5 β -androstane-3 α ,17 β -diol

화학 구조		PubMed ID	
		23891647	
TM-MC 성분 ID	273		
TM-MC 성분 동의어	N/A		
PubChem ID	134494		
InChI Key	CBMYJHIOYJEBSB-GCXXXECGSA-N		
SMILES	C[C@]12CC[C@H]3[C@@H](CC[C@@H]4C[C@H](O)CC[C@]34C)[C@@H]1CC[C@@H]2O		
Molecular Formula	C ₁₉ H ₃₂ O ₂		
Molecular Weight	292.463	Exact Molecular Weight	292.24023027
LogP	3.204	Topological Polar Surface Area	40.46 Å ²
Atom Count	53	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.72	Oral Bioavailability	Y

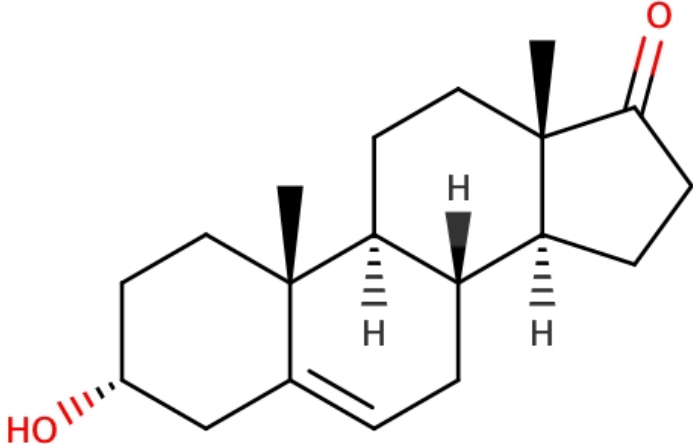
426. epiandrosterone

화학 구조		PubMed ID	
		23891647	
TM-MC 성분 ID	274		
TM-MC 성분 동의어	N/A		
PubChem ID	441302		
InChI Key	QGXBDMJGAMFCBF-LUJOEAJASA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC[C@H]4C[C@@H](O)CC[C@]34C)[C@@H]1CCC2=O</chem>		
Molecular Formula	C ₁₉ H ₃₀ O ₂		
Molecular Weight	290.447	Exact Molecular Weight	290.224580206
LogP	3.767	Topological Polar Surface Area	37.3 Å ²
Atom Count	51	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.74	Oral Bioavailability	Y

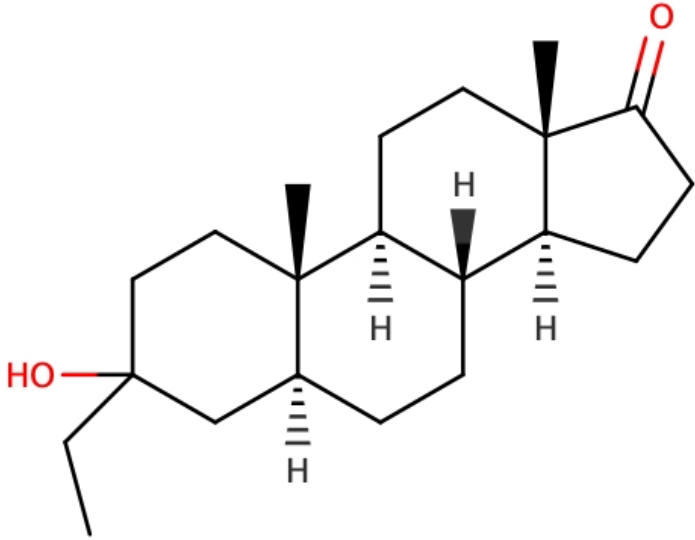
427. androsterone, trifluoroacetate

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	276		
TM-MC 성분 동의어	N/A		
PubChem ID	91748067		
InChI Key	NTPCFTHVUCOBOX-NIYLZHLASA-N		
SMILES	C[C@]12CCC3C(CC[C@H]4C[C@@H](CC[C@]34C)OC(=O)C(F)(F)F)C1CCC2=O		
Molecular Formula	C ₂₁ H ₂₉ F ₃ O ₃		
Molecular Weight	386.455	Exact Molecular Weight	386.206879283
LogP	5.341	Topological Polar Surface Area	43.37 Å ²
Atom Count	56	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	0
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.61	Oral Bioavailability	Y

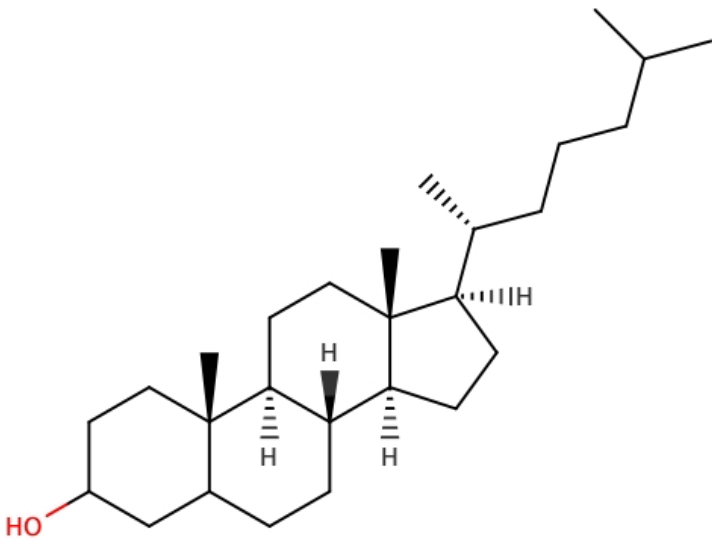
428. dehydroandrosterone

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	277		
TM-MC 성분 동의어	N/A		
PubChem ID	134506		
InChI Key	FMGSKLZLMKYGDP-HKQXQEGQSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC=C4C[C@H](O)CC[C@]34C)[C@@H]1CCCC2=O</chem>		
Molecular Formula	C ₁₉ H ₂₈ O ₂		
Molecular Weight	288.431	Exact Molecular Weight	288.208930142
LogP	3.362	Topological Polar Surface Area	37.3 Å ²
Atom Count	49	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.69	Oral Bioavailability	Y

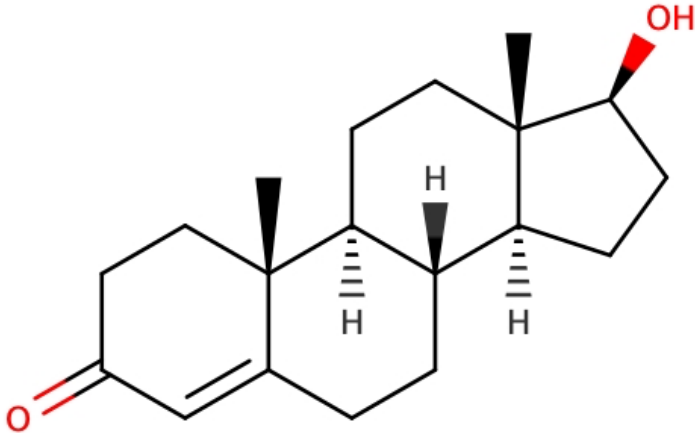
429. 3-ethyl-3-hydroxy-5 α -androst-17-one

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	278		
TM-MC 성분 동의어	androst-17-one, 3-ethyl 3-hydroxy-, (5- α)		
PubChem ID	14681481		
InChI Key	SPKGPDRGORWGNP-SISSWOJISA-N		
SMILES	<chem>CCC1(O)CC[C@@]2(C)[C@@H](CC[C@H]3[C@@H]4CCCC(=O)[C@@]4(C)CC[C@@H]23)C1</chem>		
Molecular Formula	C ₂₁ H ₃₄ O ₂		
Molecular Weight	318.501	Exact Molecular Weight	318.255880335
LogP	4.57	Topological Polar Surface Area	37.3 Å ²
Atom Count	57	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.77	Oral Bioavailability	Y

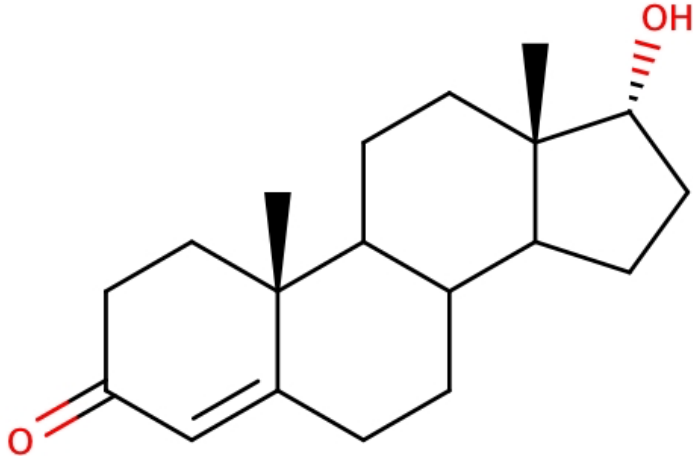
430. cholestan-3-ol

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	279		
TM-MC 성분 동의어	N/A		
PubChem ID	10992748		
InChI Key	QYIXCDOBOSTCEI-BPAAZKTESA-N		
SMILES	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CCC4CC(O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₇ H ₄₈ O		
Molecular Weight	388.68	Exact Molecular Weight	388.370516166
LogP	7.518	Topological Polar Surface Area	20.23 Å ²
Atom Count	76	Structural Alert Count	0
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.52	Oral Bioavailability	Y

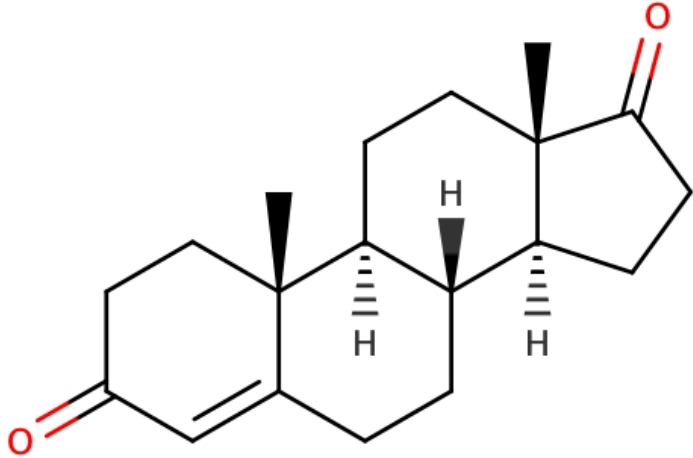
431. testosterone

화학 구조		PubMed ID	
		23891647	
TM-MC 성분 ID	280		
TM-MC 성분 동의어	N/A		
PubChem ID	6013		
InChI Key	MUMGGOZAMZWBJJ-DYKIIFRCSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CC[C@@H]2O</chem>		
Molecular Formula	C ₁₉ H ₂₈ O ₂		
Molecular Weight	288.431	Exact Molecular Weight	288.208930142
LogP	3.365	Topological Polar Surface Area	37.3 Å ²
Atom Count	49	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.74	Oral Bioavailability	Y

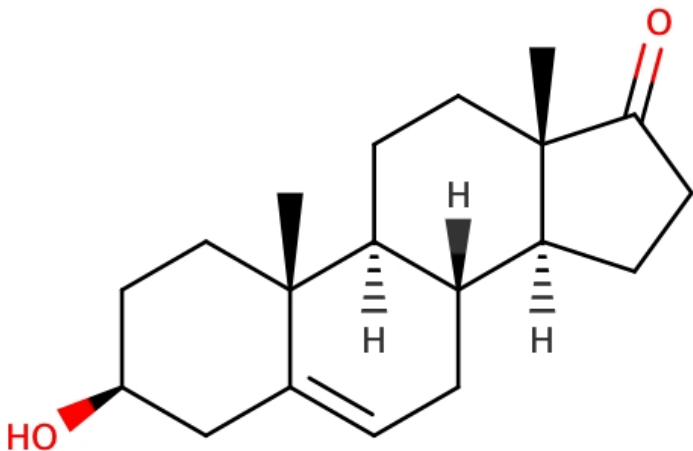
432. epitestosterone

화학 구조		PubMed ID	
		23891647	
TM-MC 성분 ID	281		
TM-MC 성분 동의어	N/A		
PubChem ID	10108190		
InChI Key	MUMGGOZAMZWBJJ-YKBUPIRMSA-N		
SMILES	C[C@]12CCC3C(CCC4=CC(=O)CC[C@]34C)C1CC[C@H]2O		
Molecular Formula	C ₁₉ H ₂₈ O ₂		
Molecular Weight	288.431	Exact Molecular Weight	288.208930142
LogP	3.365	Topological Polar Surface Area	37.3 Å ²
Atom Count	49	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.74	Oral Bioavailability	Y

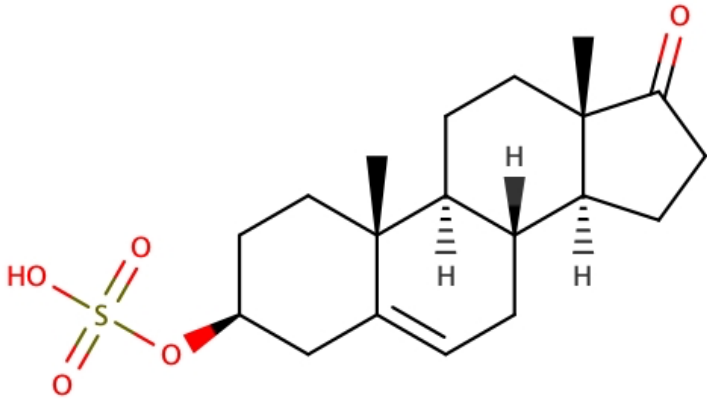
433. androstenedione

화학 구조		PubMed ID	
		23891647	
TM-MC 성분 ID	282		
TM-MC 성분 동의어	androst-4-ene-3,17-dione		
PubChem ID	6128		
InChI Key	AEMFNILZOJQLW-QAGGRKNESA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@]34C)[C@@H]1CCC2=O</chem>		
Molecular Formula	C ₁₉ H ₂₆ O ₂		
Molecular Weight	286.415	Exact Molecular Weight	286.193280077
LogP	3.929	Topological Polar Surface Area	34.14 Å ²
Atom Count	47	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.68	Oral Bioavailability	Y

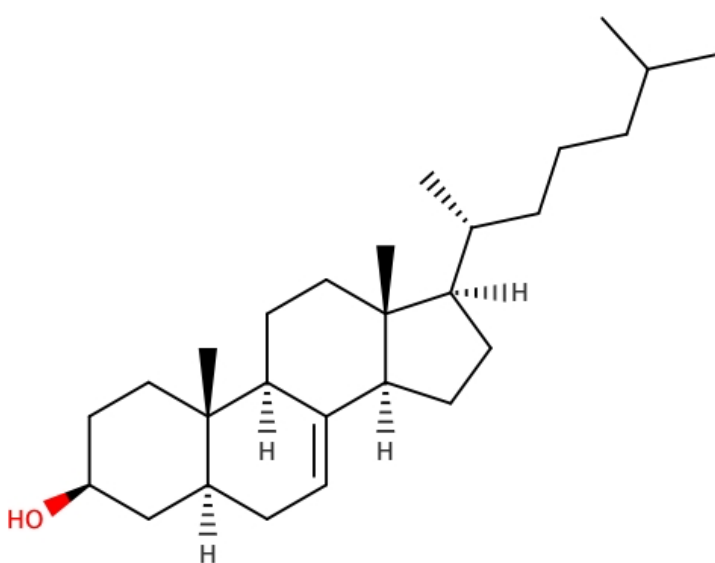
434. dehydroepiandrosterone

화학 구조		PubMed ID	
		23891647	
TM-MC 성분 ID	284		
TM-MC 성분 동의어	N/A		
PubChem ID	5881		
InChI Key	FMGSKLZLMKYGDP-USOAJAOKSA-N		
SMILES	<chem>C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@]34C)[C@@H]1CCC2=O</chem>		
Molecular Formula	C ₁₉ H ₂₈ O ₂		
Molecular Weight	288.431	Exact Molecular Weight	288.208930142
LogP	3.362	Topological Polar Surface Area	37.3 Å ²
Atom Count	49	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.69	Oral Bioavailability	Y

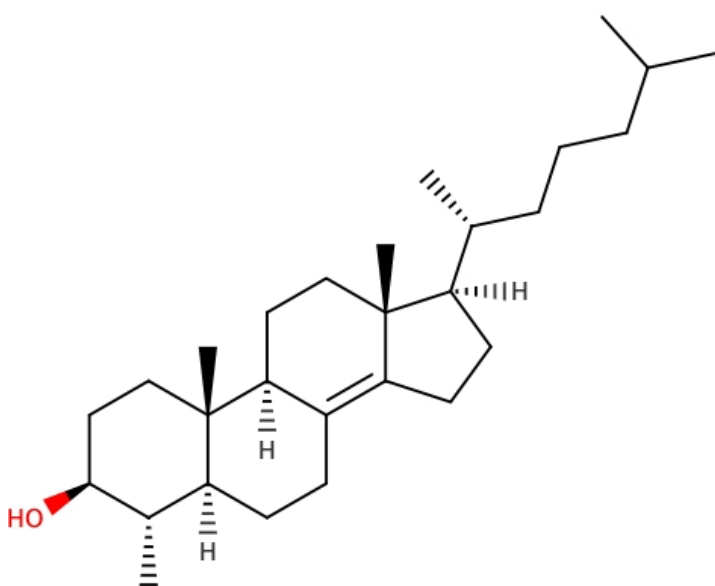
435. prasterone-3-sulfate

화학 구조		PubMed ID	
		26744067, 29551642	
TM-MC 성분 ID	285		
TM-MC 성분 동의어	N/A		
PubChem ID	12594		
InChI Key	CZWCKYRVOZZJNM-USOAJAOKSA-N		
SMILES	C[C@]12CC[C@H]3[C@@H](CC=C4C[C@H](CC[C@]34C)OS(O)(=O)=O)[C@@H]1CCC2=O		
Molecular Formula	C ₁₉ H ₂₈ O ₅ S		
Molecular Weight	368.49	Exact Molecular Weight	368.165745176
LogP	3.417	Topological Polar Surface Area	80.67 Å ²
Atom Count	53	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.60	Oral Bioavailability	Y

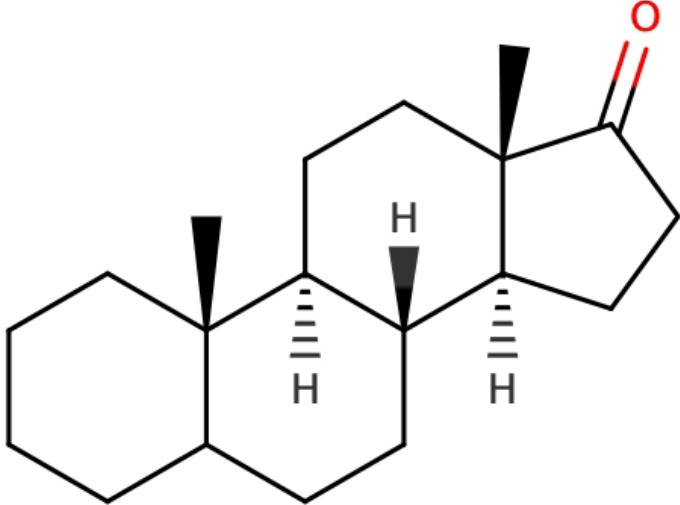
436. cholest-7-en-3 β -ol

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	286		
TM-MC 성분 동의어	N/A		
PubChem ID	65728		
InChI Key	IZVFFXVYBHFHY-SKCNUYALSA-N		
SMILES	CC(C)CCC[C@H](C)[C@H]1CC[C@H]2C3=CC[C@H]4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₇ H ₄₆ O		
Molecular Weight	386.664	Exact Molecular Weight	386.354866101
LogP	7.113	Topological Polar Surface Area	20.23 Å ²
Atom Count	74	Structural Alert Count	1
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.50	Oral Bioavailability	Y

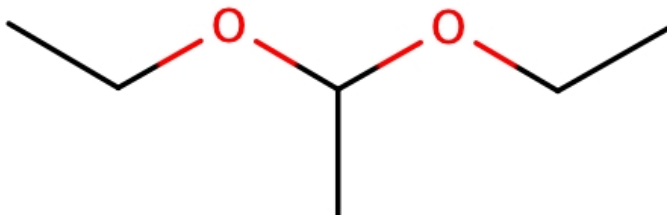
437. 4 α -methyl-5 α -cholest-8(14)-en-3 β -ol

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	287		
TM-MC 성분 동의어	N/A		
PubChem ID	23621393		
InChI Key	UIPYFONRKZTOIY-GQZGFCDBSA-N		
SMILES	CC(C)CCC[C@@H](C)[C@H]1CCC=C3CC[C@H]4[C@H](C)[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C		
Molecular Formula	C ₂₈ H ₄₈ O		
Molecular Weight	400.691	Exact Molecular Weight	400.370516166
LogP	7.434	Topological Polar Surface Area	20.23 Å ²
Atom Count	77	Structural Alert Count	1
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.48	Oral Bioavailability	Y

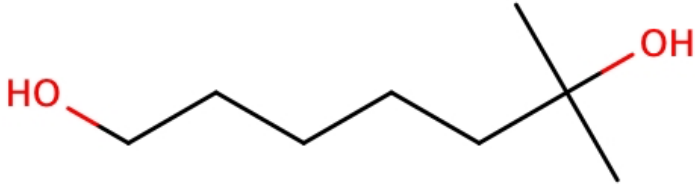
438. androstan-17-one

화학 구조		PubMed ID	
		29551642	
TM-MC 성분 ID	300693		
TM-MC 성분 동의어	N/A		
PubChem ID	10880319		
InChI Key	YJDYCVLVYZDESB-HQEMIIEJSA-N		
SMILES	C[C@]12CC[C@H]3[C@@H](CCC4CCCC[C@]34C)[C@@H]1CCC2=O		
Molecular Formula	C ₁₉ H ₃₀ O		
Molecular Weight	274.448	Exact Molecular Weight	274.229665586
LogP	5.154	Topological Polar Surface Area	17.07 Å ²
Atom Count	50	Structural Alert Count	0
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.60	Oral Bioavailability	Y

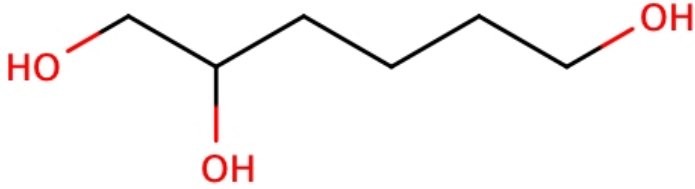
439. acetal

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	288		
TM-MC 성분 동의어	1,1-diethoxy-ethane; ethane, 1,1-diethoxy-		
PubChem ID	7765		
InChI Key	DHKHKXVYLBGOIT-UHFFFAOYSA-N		
SMILES	CCOC(C)OCC		
Molecular Formula	C ₆ H ₁₄ O ₂		
Molecular Weight	118.176	Exact Molecular Weight	118.099379691
LogP	1.131	Topological Polar Surface Area	18.46 Å ²
Atom Count	22	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	0
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.52	Oral Bioavailability	Y

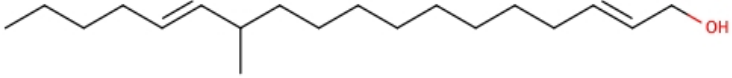
440. 6-methylheptane-1,6-diol

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	291		
TM-MC 성분 동의어	N/A		
PubChem ID	547731		
InChI Key	XICLOMYOBVKLTR-UHFFFAOYSA-N		
SMILES	<chem>CC(C)(O)CCCCCO</chem>		
Molecular Formula	C ₈ H ₁₈ O ₂		
Molecular Weight	146.23	Exact Molecular Weight	146.13067982
LogP	0.955	Topological Polar Surface Area	40.46 Å ²
Atom Count	28	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.57	Oral Bioavailability	Y

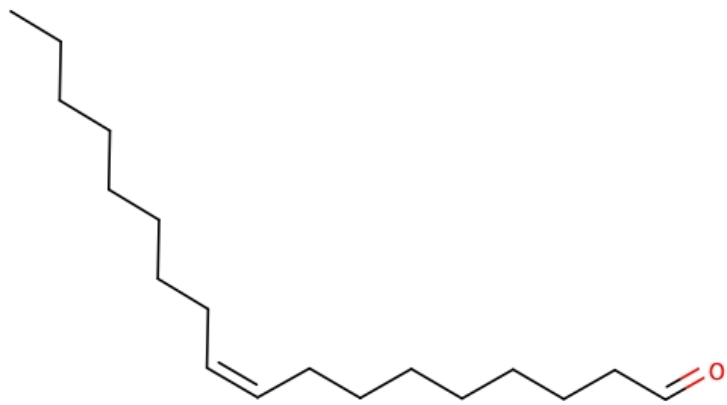
441. 1,2,6-hexanetriol

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	292		
TM-MC 성분 동의어	N/A		
PubChem ID	7823		
InChI Key	ZWVMLYRJXORSEP-UHFFFAOYSA-N		
SMILES	OCCCCC(O)CO		
Molecular Formula	C ₆ H ₁₄ O ₃		
Molecular Weight	134.175	Exact Molecular Weight	134.094294311
LogP	-0.817	Topological Polar Surface Area	60.69 Å ²
Atom Count	23	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	3
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.43	Oral Bioavailability	Y

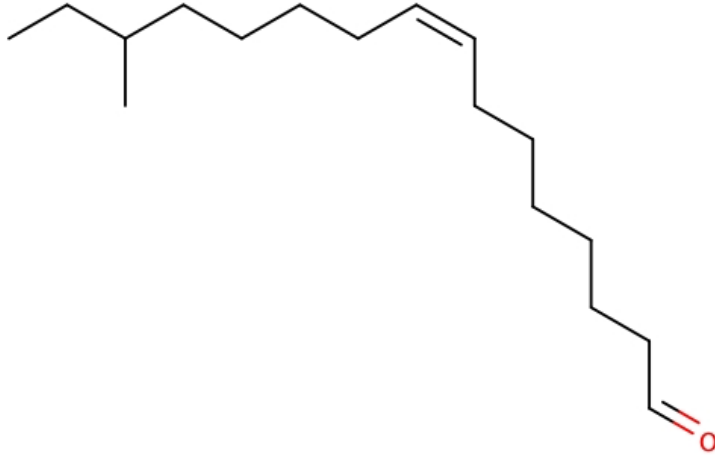
442. 12-methyl-E,E-2,13-octadecadien-1-ol

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	297		
TM-MC 성분 동의어	N/A		
PubChem ID	90107969		
InChI Key	QQRKGLQLQDQGQI-WSGPNKEYSA-N		
SMILES	CCCCWC=CWC(C)CCCCCCCCWC=CWCO		
Molecular Formula	C ₁₉ H ₃₆ O		
Molecular Weight	280.496	Exact Molecular Weight	280.276615779
LogP	6.748	Topological Polar Surface Area	20.23 Å ²
Atom Count	56	Structural Alert Count	2
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	14	Aromatic Ring Count	0
Drug Likeness	0.28	Oral Bioavailability	N

443. 9-octadecenal, (Z)

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	293		
TM-MC 성분 동의어	olealdehyde; (Z)-9-octadecenal; 9-octadecenal,(Z)-		
PubChem ID	5364492		
InChI Key	ZENZJGDPWWLORF-KTKRTIGZSA-N		
SMILES	<chem>CCCCCCCCC=C/CCCCCCCC=O</chem>		
Molecular Formula	C ₁₈ H ₃₄ O		
Molecular Weight	266.469	Exact Molecular Weight	266.260965715
LogP	6.625	Topological Polar Surface Area	17.07 Å ²
Atom Count	53	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	15	Aromatic Ring Count	0
Drug Likeness	0.18	Oral Bioavailability	N

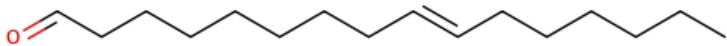
444. 14-methyl-8-hexadecenal Z

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	295		
TM-MC 성분 동의어	N/A		
PubChem ID	5364688		
InChI Key	HSGUJTMCFWXGAP-ALCCZGGFSA-N		
SMILES	<chem>CCC(C)CCCC=C/C=CCCCC=O</chem>		
Molecular Formula	C ₁₇ H ₃₂ O		
Molecular Weight	252.442	Exact Molecular Weight	252.24531565
LogP	6.023	Topological Polar Surface Area	17.07 Å ²
Atom Count	50	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	13	Aromatic Ring Count	0
Drug Likeness	0.22	Oral Bioavailability	N

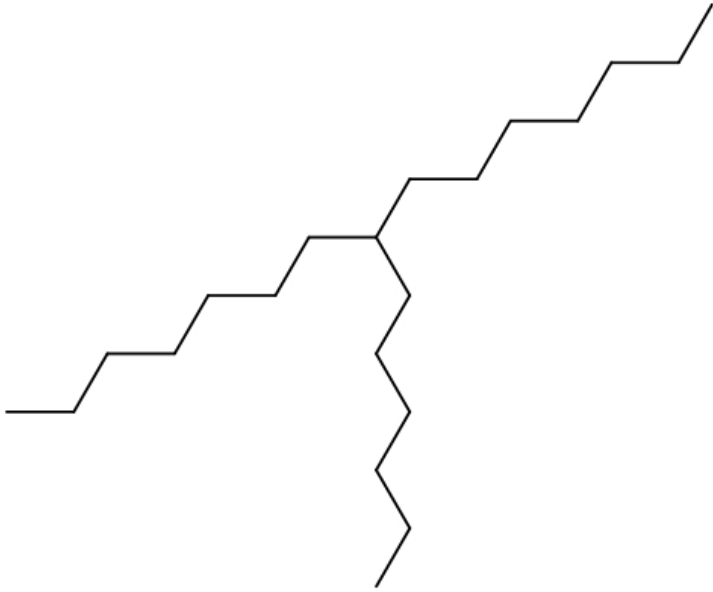
445. 13-tetradecenal

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	298		
TM-MC 성분 동의어	N/A		
PubChem ID	522841		
InChI Key	ZVJRAGVPKPPDKE-UHFFFAOYSA-N		
SMILES	C=CCCCCCCCCCCCC=O		
Molecular Formula	C ₁₄ H ₂₆ O		
Molecular Weight	210.361	Exact Molecular Weight	210.198365457
LogP	4.905	Topological Polar Surface Area	17.07 Å ²
Atom Count	41	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	12	Aromatic Ring Count	0
Drug Likeness	0.25	Oral Bioavailability	N

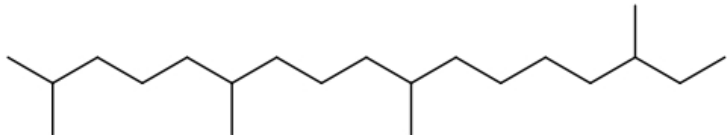
446. cis-9-hexadecenal

화학 구조		PubMed ID	
		29551642	
TM-MC 성분 ID	283375		
TM-MC 성분 동의어	9-hexadecenal, (Z)-		
PubChem ID	5283375		
InChI Key	QFPVVMKZTVQDTL-BQYQJAHWSA-N		
SMILES	CCCCCWC=CWCCCCCCC=O		
Molecular Formula	C ₁₆ H ₃₀ O		
Molecular Weight	238.415	Exact Molecular Weight	238.229665586
LogP	5.736	Topological Polar Surface Area	17.07 Å ²
Atom Count	47	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	13	Aromatic Ring Count	0
Drug Likeness	0.23	Oral Bioavailability	N

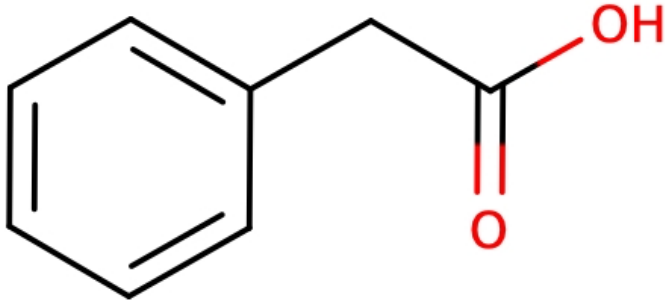
447. 8-n-hexylpentadecane

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	294		
TM-MC 성분 동의어	pentadecane, 8-hexyl-		
PubChem ID	300518		
InChI Key	FASYBMUJVAMAFB-UHFFFAOYSA-N		
SMILES	<chem>CCCCCCCC(CCCCC)CCCCCCC</chem>		
Molecular Formula	C ₂₁ H ₄₄		
Molecular Weight	296.583	Exact Molecular Weight	296.3443014168
LogP	9.642	Topological Polar Surface Area	0 Å ²
Atom Count	65	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	17	Aromatic Ring Count	0
Drug Likeness	0.23	Oral Bioavailability	N

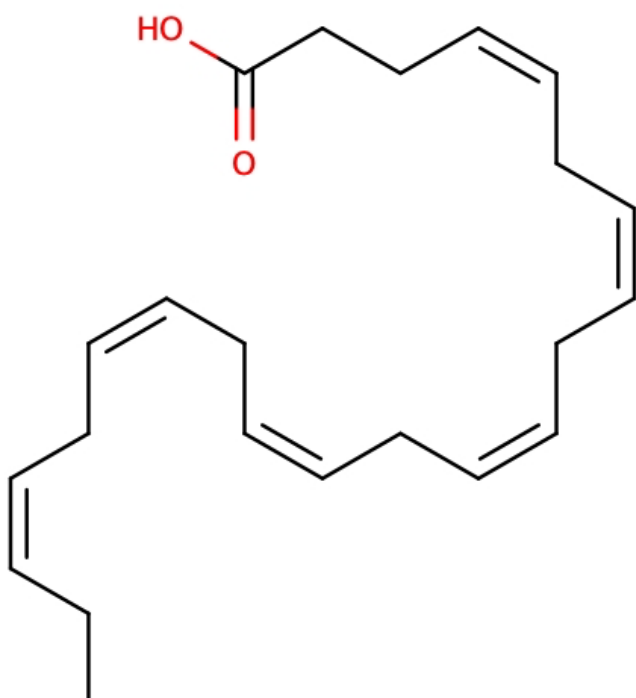
448. 2,6,10,15-tetramethylheptadecane

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	296		
TM-MC 성분 동의어	heptadecane,2,6,10,15-tetramethyl-		
PubChem ID	41209		
InChI Key	ZZEQNXPBKOFBKG-UHFFFAOYSA-N		
SMILES	<chem>CCC(C)CCCC(C)CCCC(C)CCCC(C)C</chem>		
Molecular Formula	C ₂₁ H ₄₄		
Molecular Weight	296.583	Exact Molecular Weight	296.3443014168
LogP	9.169	Topological Polar Surface Area	0 Å ²
Atom Count	65	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	14	Aromatic Ring Count	0
Drug Likeness	0.28	Oral Bioavailability	N

449. phenylacetic acid

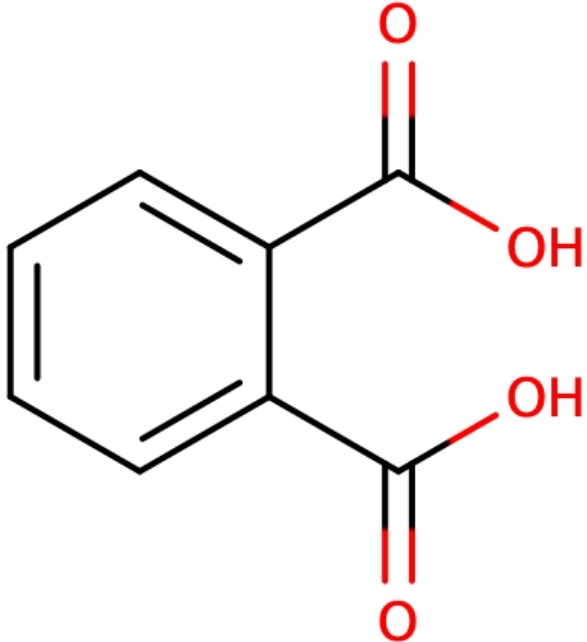
화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	290		
TM-MC 성분 동의어	benzeneacetic acid		
PubChem ID	999		
InChI Key	WLJVXDMOQOGPHL-UHFFFAOYSA-N		
SMILES	<chem>OC(=O)Cc1ccccc1</chem>		
Molecular Formula	C ₈ H ₈ O ₂		
Molecular Weight	136.15	Exact Molecular Weight	136.052429498
LogP	1.611	Topological Polar Surface Area	37.3 Å ²
Atom Count	18	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.67	Oral Bioavailability	Y

450. doconexent

화학 구조	PubMed ID
	26744067, 31394825

TM-MC 성분 ID	299		
TM-MC 성분 동의어	docosahexaenoic acid; 2,5,8,11,14,17-docosahexaenoic acid		
PubChem ID	445580		
InChI Key	MBMBGCFOFBJSJT-KUBAVDMBSA-N		
SMILES	<chem>CC=CC=CC=CC=CC=CC=CC=CC(=O)O</chem>		
Molecular Formula	C ₂₂ H ₃₂ O ₂		
Molecular Weight	328.496	Exact Molecular Weight	328.24023027
LogP	6.752	Topological Polar Surface Area	37.3 Å ²
Atom Count	56	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	14	Aromatic Ring Count	0
Drug Likeness	0.36	Oral Bioavailability	N

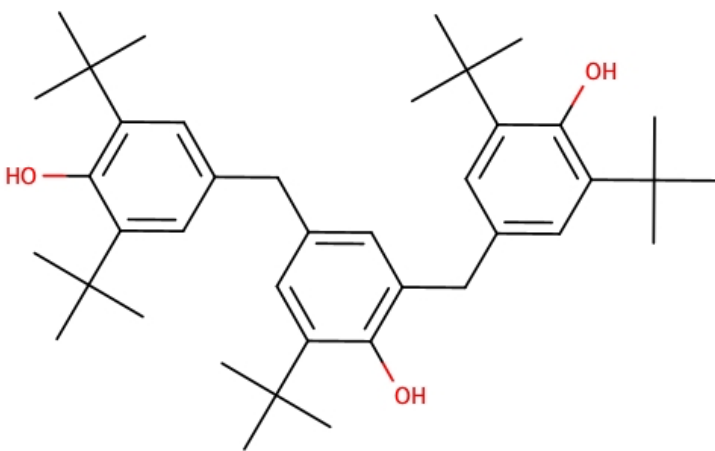
451. phthalic acid

화학 구조		PubMed ID	
		29551642	
TM-MC 성분 ID	1017		
TM-MC 성분 동의어	1,2-benzenedicarboxylic acid; O-phthalic acid		
PubChem ID	1017, 18183610		
InChI Key	XNGIFLGASWRNHJ-UHFFFAOYSA-N		
SMILES	OC(=O)c1ccccc1C(O)=O		
Molecular Formula	C ₈ H ₆ O ₄		
Molecular Weight	166.132	Exact Molecular Weight	166.026608673
LogP	1.288	Topological Polar Surface Area	74.6 Å ²
Atom Count	18	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.69	Oral Bioavailability	Y

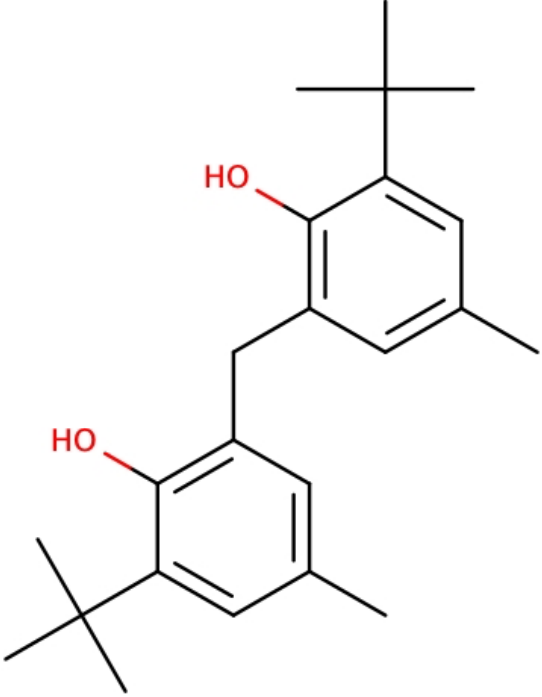
452. m-cresol

화학 구조		PubMed ID
		26744067
TM-MC 성분 ID	289	
TM-MC 성분 동의어	phenol, 3-methyl-	
PubChem ID	342	
InChI Key	RLSSMJSEOOYNOY-UHFFFAOYSA-N	
SMILES	<chem>Cc1cccc(O)c1</chem>	
Molecular Formula	C ₇ H ₈ O	
Molecular Weight	108.14	Exact Molecular Weight 108.057514878
LogP	2.183	Topological Polar Surface Area 20.23 Å ²
Atom Count	16	Structural Alert Count 0
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count 1
Rotatable Bond Count	0	Aromatic Ring Count 1
Drug Likeness	0.54	Oral Bioavailability Y

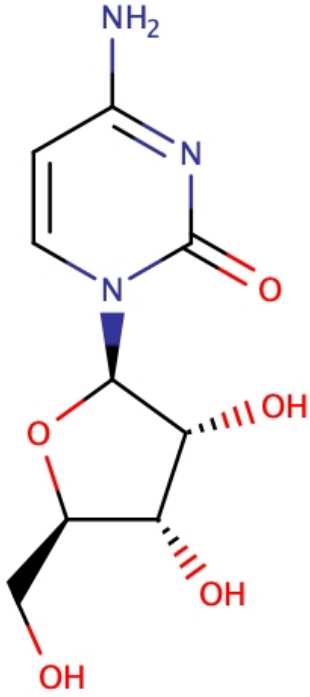
453. 2-tert-butyl-4,6-bis(3,5-di-tert-butyl-4-hydroxybenzyl)phenol

화학 구조		PubMed ID	
		26744067	
TM-MC 성분 ID	300		
TM-MC 성분 동의어	N/A		
PubChem ID	545456		
InChI Key	ZPKNRTASNRLDMM-UHFFFAOYSA-N		
SMILES	<chem>CC(C)(C)c1cc(Cc2cc(c(O)c(c2)C(C)(C)C(C)(C)C(C)(C)cc(Cc2cc(c(O)c(c2)C(C)(C)C(C)(C)C(C)(C)C1O</chem>		
Molecular Formula	C ₄₀ H ₅₈ O ₃		
Molecular Weight	586.901	Exact Molecular Weight	586.438595728
LogP	12.971	Topological Polar Surface Area	60.69 Å ²
Atom Count	101	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	3
Rotatable Bond Count	9	Aromatic Ring Count	3
Drug Likeness	0.23	Oral Bioavailability	Y

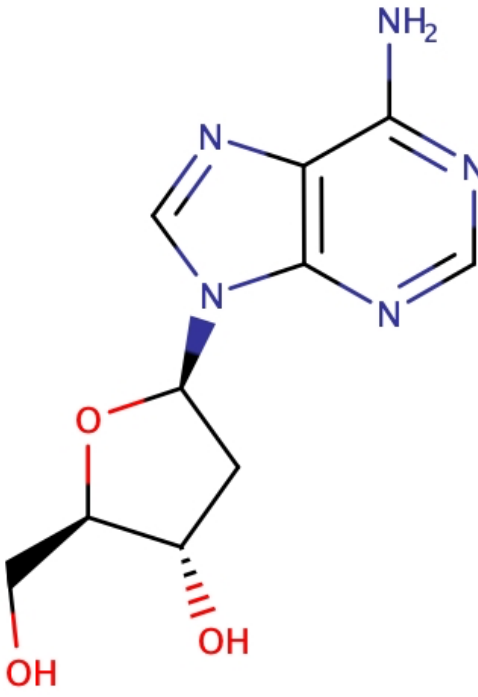
454. antioxidant 2264

화학 구조		PubMed ID	
		29551642	
TM-MC 성분 ID	30069		
TM-MC 성분 동의어	2,2'-methylenebis [6-(1,1-dimethylethyl)-4-methylphenol]		
PubChem ID	8398		
InChI Key	KGRVJHAUYBGFFP-UHFFFAOYSA-N		
SMILES	<chem>Cc1cc(Cc2cc(C)cc(c2O)C(C)(C)C)c(O)c(c1)C(C)(C)C</chem>		
Molecular Formula	C ₂₃ H ₃₂ O ₂		
Molecular Weight	340.507	Exact Molecular Weight	340.24023027
LogP	7.575	Topological Polar Surface Area	40.46 Å ²
Atom Count	57	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.60	Oral Bioavailability	Y

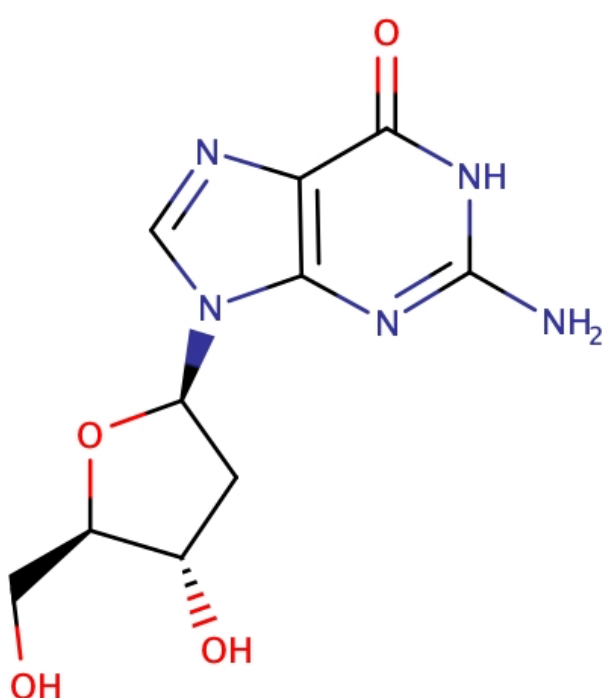
455. cytidine

화학 구조		PubMed ID	
		23689025, 25335278	
TM-MC 성분 ID	316		
TM-MC 성분 동의어	N/A		
PubChem ID	6175		
InChI Key	UHDGCWIWMRVCDJ-XVFCMESISA-N		
SMILES	<chem>Nc1ccn([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)c(=O)n1</chem>		
Molecular Formula	C ₉ H ₁₃ N ₃ O ₅		
Molecular Weight	243.219	Exact Molecular Weight	243.085520531
LogP	-2.798	Topological Polar Surface Area	128.61 Å ²
Atom Count	30	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.44	Oral Bioavailability	Y

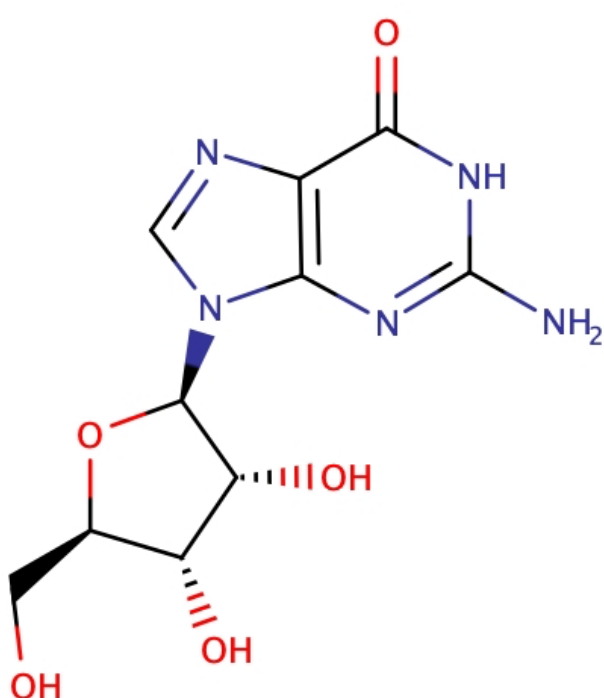
456. 2'-deoxyadenosine

화학 구조		PubMed ID	
		23689025	
TM-MC 성분 ID	306		
TM-MC 성분 동의어	2-deoxyadenosine; deoxyadenosine		
PubChem ID	13730		
InChI Key	OLXZPDWKRNYJJZ-RRKCRQDMSA-N		
SMILES	<chem>Nc1ncnc2n(cnc12)[C@H]1C[C@H](O)[C@@H](CO)O1</chem>		
Molecular Formula	C ₁₀ H ₁₃ N ₅ O ₃		
Molecular Weight	251.246	Exact Molecular Weight	251.101839299
LogP	-1.19	Topological Polar Surface Area	119.31 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.61	Oral Bioavailability	Y

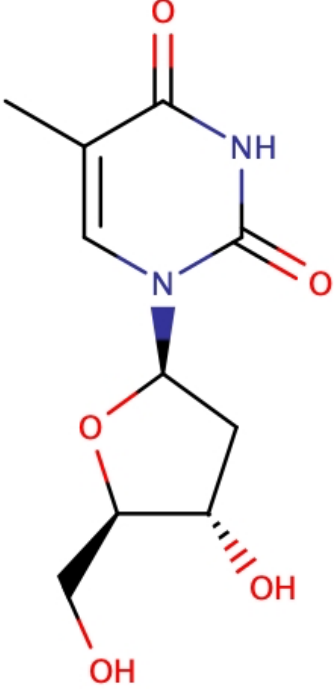
457. 2'-deoxyguanosine

화학 구조		PubMed ID	
		23689025, 25335278 25422536	
TM-MC 성분 ID	308		
TM-MC 성분 동의어	deoxyguanosine; 2'-deoxyguanosine		
PubChem ID	135398592		
InChI Key	YKBGVTZYEHREMT-KVQBGUIXSA-N		
SMILES	<chem>Nc1nc2n(cnc2c(=O)[nH]1)[C@H]1C[C@H](O)[C@@H](CO)O1</chem>		
Molecular Formula	C ₁₀ H ₁₃ N ₅ O ₄		
Molecular Weight	267.245	Exact Molecular Weight	267.096753919
LogP	-1.806	Topological Polar Surface Area	134.99 Å ²
Atom Count	32	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.50	Oral Bioavailability	Y

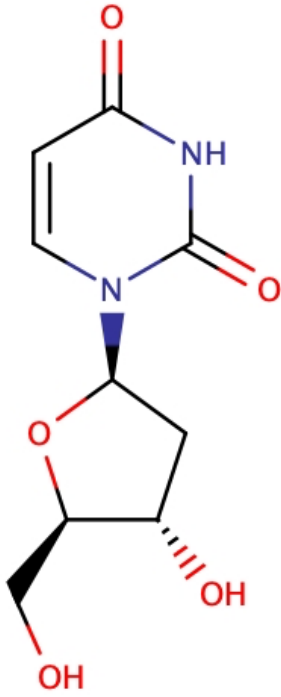
458. guanosine

화학 구조		PubMed ID	
		<p>23689025, 25335278 25422536, 29676127 30728838</p>	
TM-MC 성분 ID	309		
TM-MC 성분 동의어	vernine		
PubChem ID	135398635		
InChI Key	NYHBQMYGNKIUIF-UUOKFMHZSA-N		
SMILES	<chem>Nc1nc2n(cnc2c(=O)[nH]1)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O</chem>		
Molecular Formula	C ₁₀ H ₁₃ N ₅ O ₅		
Molecular Weight	283.244	Exact Molecular Weight	283.091668539
LogP	-2.706	Topological Polar Surface Area	155.22 Å ²
Atom Count	33	Structural Alert Count	0
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	5
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.40	Oral Bioavailability	N

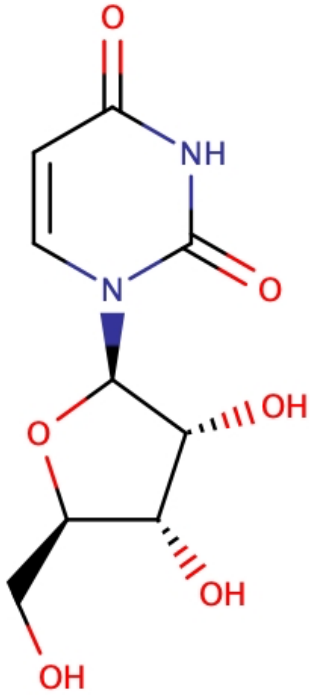
459. thymidine

화학 구조		PubMed ID	
		23689025, 25335278	
TM-MC 성분 ID	311		
TM-MC 성분 동의어	β-thymidine; 5-methyl-2'-deoxyuridine		
PubChem ID	5789		
InChI Key	IQFYKMMVGJFEH-XLPZGREQSA-N		
SMILES	<chem>Cc1cn([C@H]2C[C@H](O)[C@@H](CO)O2)c(=O)[nH]c1=O</chem>		
Molecular Formula	C ₁₀ H ₁₄ N ₂ O ₅		
Molecular Weight	242.231	Exact Molecular Weight	242.090271559
LogP	-1.119	Topological Polar Surface Area	99.1 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.61	Oral Bioavailability	Y

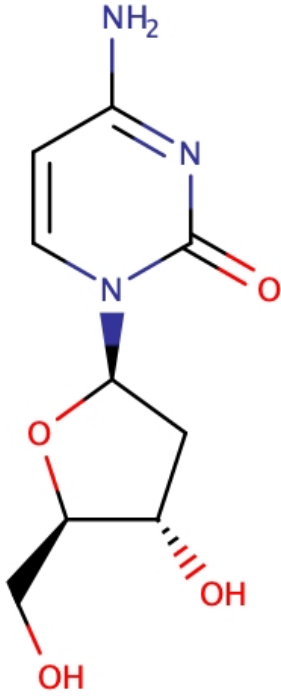
460. 2'-deoxyuridine

화학 구조		PubMed ID	
		23689025	
TM-MC 성분 ID	313		
TM-MC 성분 동의어	2-deoxyuridine		
PubChem ID	13712		
InChI Key	MXHRCPNRJAMMIM-SHYZEUOFS-A-N		
SMILES	OC[C@H]1O[C@H](C[C@@H]1O)n1ccc(=O)[nH]c1=O		
Molecular Formula	C ₉ H ₁₂ N ₂ O ₅		
Molecular Weight	228.204	Exact Molecular Weight	228.074621494
LogP	-1.515	Topological Polar Surface Area	99.1 Å ²
Atom Count	28	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.57	Oral Bioavailability	Y

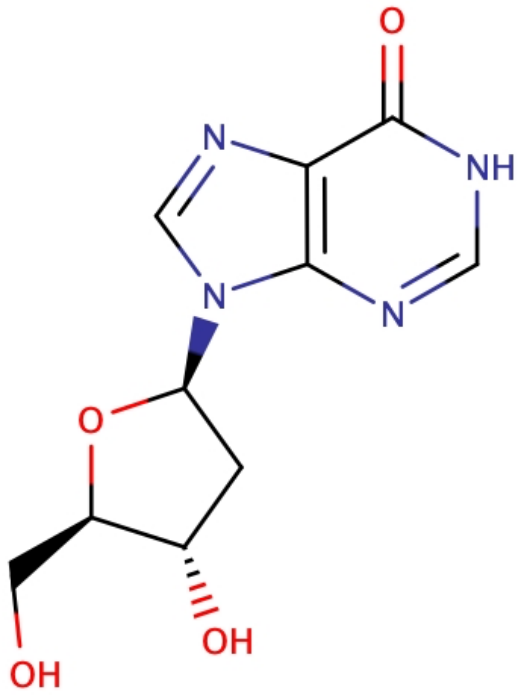
461. uridine

화학 구조		PubMed ID	
		23689025, 25335278 25422536, 30728838	
TM-MC 성분 ID	314		
TM-MC 성분 동의어	N/A		
PubChem ID	6029		
InChI Key	DRTQHJPVMGBUCF-XVFCMESISA-N		
SMILES	OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)n1ccc(=O)[nH]c1=O		
Molecular Formula	C ₉ H ₁₂ N ₂ O ₆		
Molecular Weight	244.203	Exact Molecular Weight	244.069536114
LogP	-2.415	Topological Polar Surface Area	119.33 Å ²
Atom Count	29	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.46	Oral Bioavailability	Y

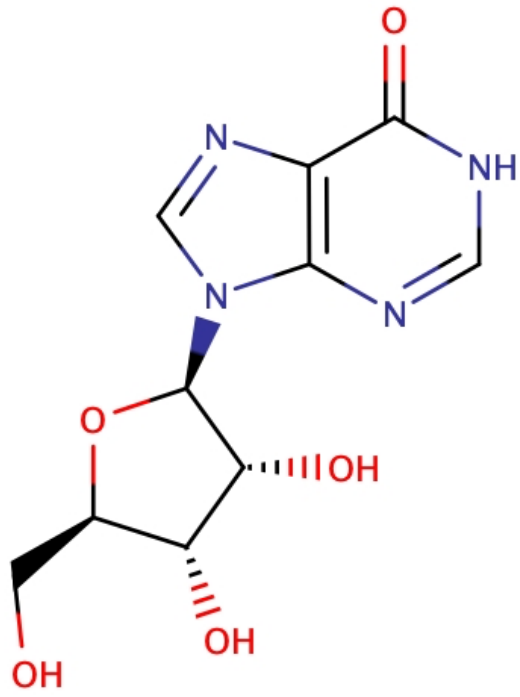
462. 2'-deoxycytidine

화학 구조		PubMed ID	
		23689025	
TM-MC 성분 ID	315		
TM-MC 성분 동의어	2-deoxycytidine		
PubChem ID	13711		
InChI Key	CKTSBUTUHBMZGZ-SHYZEUFSA-N		
SMILES	<chem>Nc1ccn([C@H]2C[C@H](O)[C@@H](CO)O2)c(=O)n1</chem>		
Molecular Formula	C ₉ H ₁₃ N ₃ O ₄		
Molecular Weight	227.22	Exact Molecular Weight	227.090605911
LogP	-1.897	Topological Polar Surface Area	108.38 Å ²
Atom Count	29	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.54	Oral Bioavailability	Y

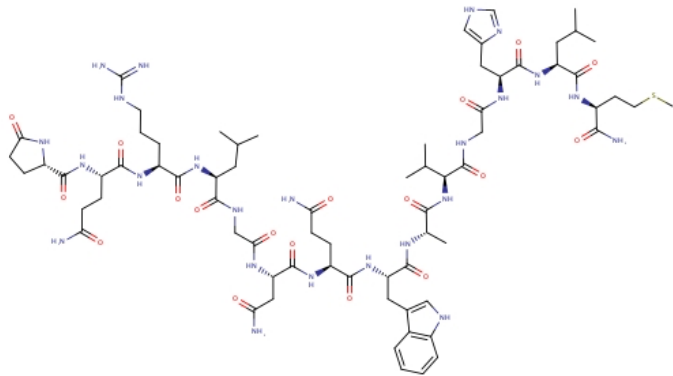
463. 2'-deoxyinosine

화학 구조		PubMed ID	
		23689025	
TM-MC 성분 ID	319		
TM-MC 성분 동의어	N/A		
PubChem ID	135398593		
InChI Key	VGONTNSXDCQUGY-RRKCRQDMSA-N		
SMILES	OC[C@H]1O[C@H](C[C@@H]1O)n1cnc2c1nc[nH]c2=O		
Molecular Formula	C ₁₀ H ₁₂ N ₄ O ₄		
Molecular Weight	252.23	Exact Molecular Weight	252.085854882
LogP	-1.578	Topological Polar Surface Area	108.97 Å ²
Atom Count	30	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.60	Oral Bioavailability	Y

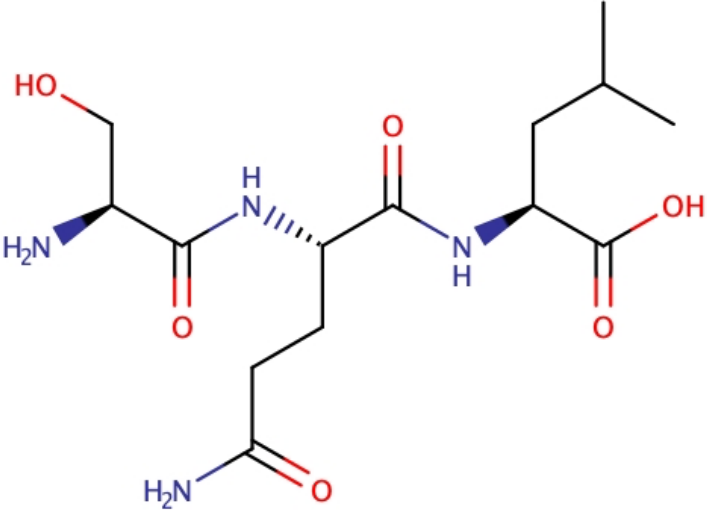
464. inosine

화학 구조		PubMed ID	
		<p>23689025, 25335278 25422536, 29676127 30728838</p>	
TM-MC 성분 ID	320		
TM-MC 성분 동의어	hypoxanthine-9-β-D-ribofuranoside		
PubChem ID	135398641		
InChI Key	UGQMRVRMYASKQ-KQYNXXCUSA-N		
SMILES	<chem>OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)n1cnc2c1nc[nH]c2=O</chem>		
Molecular Formula	C ₁₀ H ₁₂ N ₄ O ₅		
Molecular Weight	268.229	Exact Molecular Weight	268.080769502
LogP	-2.479	Topological Polar Surface Area	129.2 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.47	Oral Bioavailability	Y

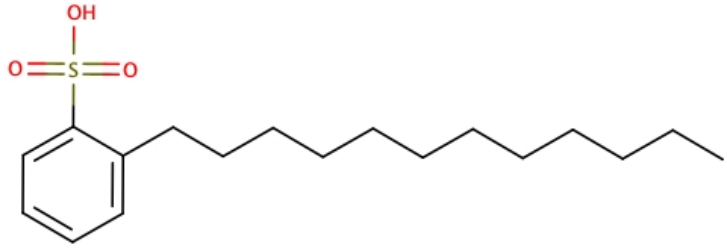
465. bombesin

화학 구조		PubMed ID	
		2263631	
TM-MC 성분 ID	332		
TM-MC 성분 동의어	N/A		
PubChem ID	16133800, 16201612, 91898967, 101835328		
InChI Key	QXZBMSIDSOZZHK-DOPDSADYSA-N		
SMILES	<chem>CSCC[C@H](NC(=O)[C@H](CC(C)C)NC(=O)[C@H](Cc1c[nH]cn1)NC(=O)CNC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)[C@H](Cc1c[nH]c2ccccc12)NC(=O)[C@H](CCC(N)=O)NC(=O)[C@H](CC(N)=O)NC(=O)CNC(=O)[C@H](CC(C)C)NC(=O)[C@H](CCCNC(N)=N)NC(=O)[C@H](CCC(N)=O)NC(=O)[C@@H]1CCCC(=O)N1)C(C)C(N)=O</chem>		
Molecular Formula	C ₇₁ H ₁₁₀ N ₂₄ O ₁₈ S		
Molecular Weight	1619.87	Exact Molecular Weight	1618.815063972
LogP	-9.681	Topological Polar Surface Area	686.13 Å ²
Atom Count	224	Structural Alert Count	3
Hydrogen Bond Acceptor Count	22	Hydrogen Bond Donor Count	23
Rotatable Bond Count	51	Aromatic Ring Count	3
Drug Likeness	0.01	Oral Bioavailability	N

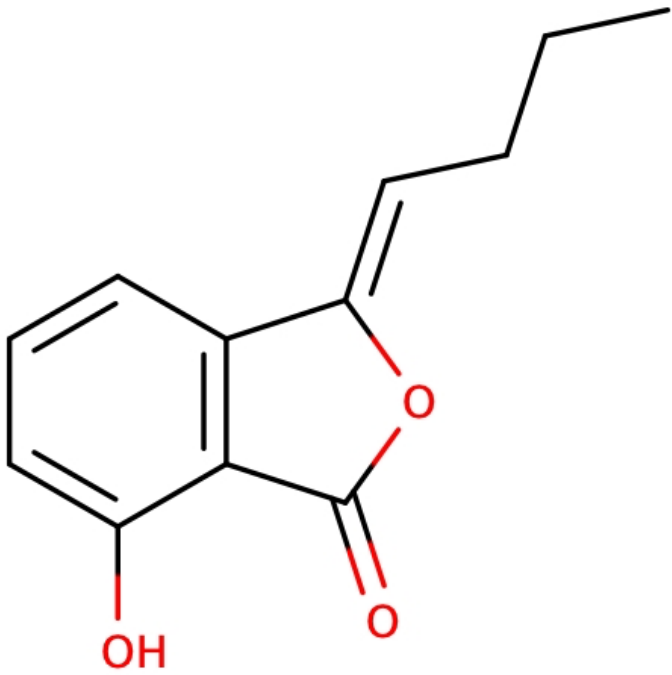
466. Ser-Gln-Leu

화학 구조		PubMed ID	
		23127646	
TM-MC 성분 ID	302437		
TM-MC 성분 동의어	N/A		
PubChem ID	46208561		
InChI Key	OJPHFSOMBZKQKQ-GUBZILKMSA-N		
SMILES	CC(C)[C@H](NC(=O)[C@H](CCC(N)=O)NC(=O)[C@@H](N)CO)C(O)=O		
Molecular Formula	C ₁₄ H ₂₆ N ₄ O ₆		
Molecular Weight	346.384	Exact Molecular Weight	346.185234573
LogP	-4.872	Topological Polar Surface Area	184.84 Å ²
Atom Count	50	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	6
Rotatable Bond Count	11	Aromatic Ring Count	0
Drug Likeness	0.22	Oral Bioavailability	N

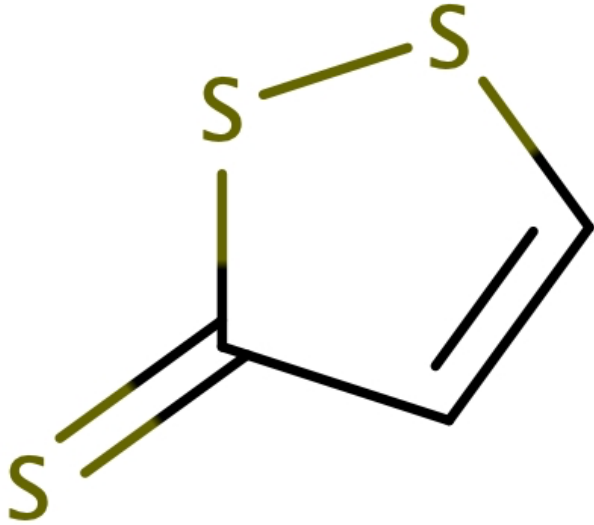
467. 2-dodecylbenzenesulfonic acid

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	300265		
TM-MC 성분 동의어	N/A		
PubChem ID	25457		
InChI Key	WBIQQQGBSDOWNP-UHFFFAOYSA-N		
SMILES	CCCCCCCCCCCCc1cccc1S(O)(=O)=O		
Molecular Formula	C ₁₈ H ₃₀ O ₃ S		
Molecular Weight	326.5	Exact Molecular Weight	326.191566
LogP	6.558	Topological Polar Surface Area	54.37 Å ²
Atom Count	52	Structural Alert Count	2
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	12	Aromatic Ring Count	1
Drug Likeness	0.35	Oral Bioavailability	N

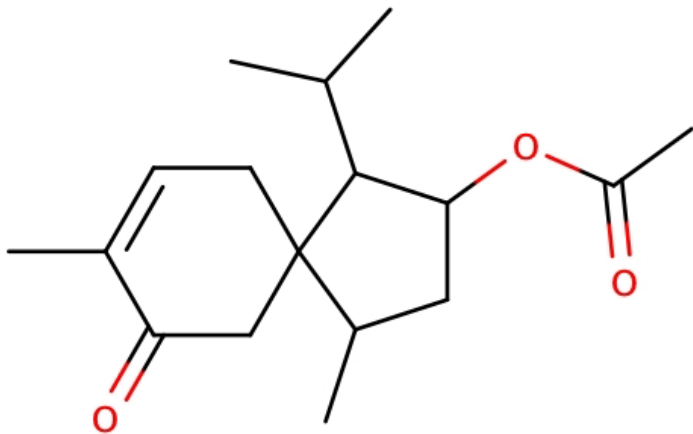
468. senkyunolide B

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	281559		
TM-MC 성분 동의어	3-butylidene-7-hydroxyphthalide; (Z)-3-butylidene-7-hydroxyphthalide		
PubChem ID	5281559		
InChI Key	XLFDJKJEYMKLIX-YFHOEESVSA-N		
SMILES	<chem>CCC=C1/OC(=O)c2c1cccc2O</chem>		
Molecular Formula	C ₁₂ H ₁₂ O ₃		
Molecular Weight	204.225	Exact Molecular Weight	204.078644246
LogP	3.37	Topological Polar Surface Area	46.53 Å ²
Atom Count	27	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.75	Oral Bioavailability	Y

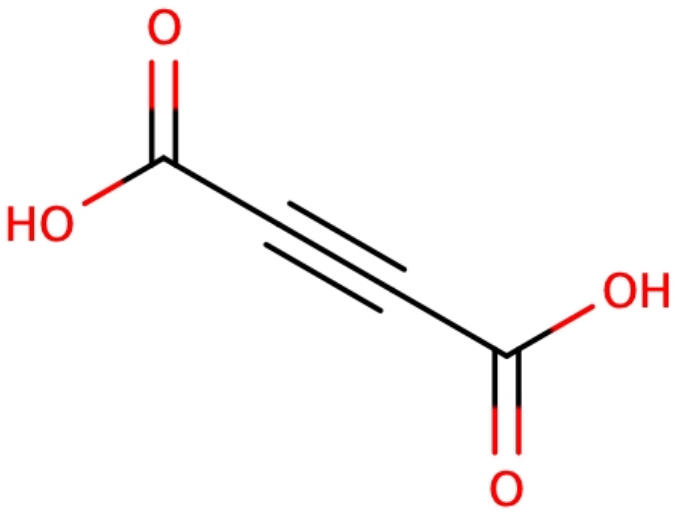
469. 3H-1,2-dithiole-3-thione

화학 구조		PubMed ID
		31254123
TM-MC 성분 ID	300472	
TM-MC 성분 동의어	N/A	
PubChem ID	68296	
InChI Key	LZENMJMJWQSSNJ-UHFFFAOYSA-N	
SMILES	S=c1ccss1	
Molecular Formula	C ₃ H ₂ S ₃	
Molecular Weight	134.23	Exact Molecular Weight 133.931863586
LogP	2.07	Topological Polar Surface Area 0 Å ²
Atom Count	8	Structural Alert Count 2
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count 0
Rotatable Bond Count	0	Aromatic Ring Count 1
Drug Likeness	0.38	Oral Bioavailability Y

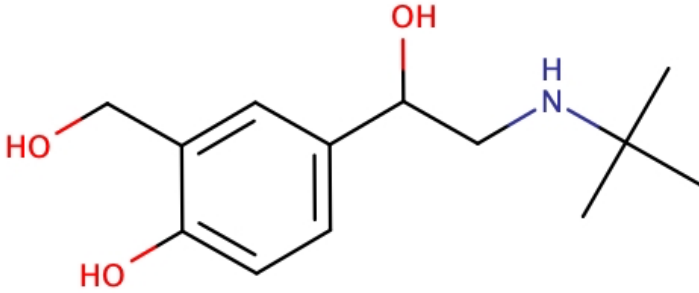
470. 8-acetoxy-4-acoren-3-one

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	300618		
TM-MC 성분 동의어	N/A		
PubChem ID	85288994		
InChI Key	LDEHIZSFHFOEKN-UHFFFAOYSA-N		
SMILES	<chem>CC(C)C1C(CC(C)C11CC=C(C)C(=O)C1)OC(C)=O</chem>		
Molecular Formula	C ₁₇ H ₂₆ O ₃		
Molecular Weight	278.392	Exact Molecular Weight	278.188194697
LogP	3.332	Topological Polar Surface Area	43.37 Å ²
Atom Count	46	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	0
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.74	Oral Bioavailability	Y

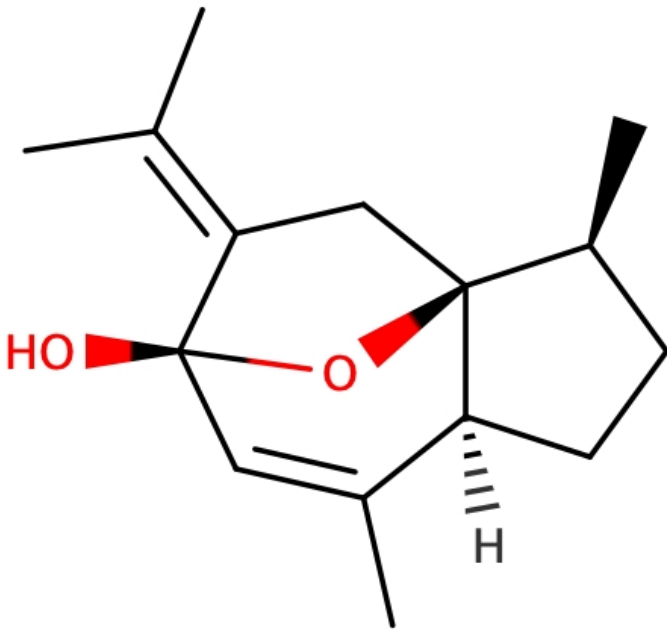
471. acetylenedicarboxylate

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	300651		
TM-MC 성분 동의어	N/A		
PubChem ID	371		
InChI Key	YTIVTFGABIZHHX-UHFFFAOYSA-N		
SMILES	<chem>OC(=O)C#CC(=O)O</chem>		
Molecular Formula	C ₄ H ₂ O ₄		
Molecular Weight	114.056	Exact Molecular Weight	113.995308544
LogP	0.21	Topological Polar Surface Area	74.6 Å ²
Atom Count	10	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.50	Oral Bioavailability	Y

472. albuterol

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	300666		
TM-MC 성분 동의어	N/A		
PubChem ID	2083		
InChI Key	NDAUXUAQIAJITI-UHFFFAOYSA-N		
SMILES	<chem>CC(C)(C)NCC(O)c1ccc(O)c(CO)c1</chem>		
Molecular Formula	C ₁₃ H ₂₁ NO ₃		
Molecular Weight	239.315	Exact Molecular Weight	239.15214354
LogP	0.344	Topological Polar Surface Area	72.72 Å ²
Atom Count	38	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	1
Drug Likeness	0.60	Oral Bioavailability	Y

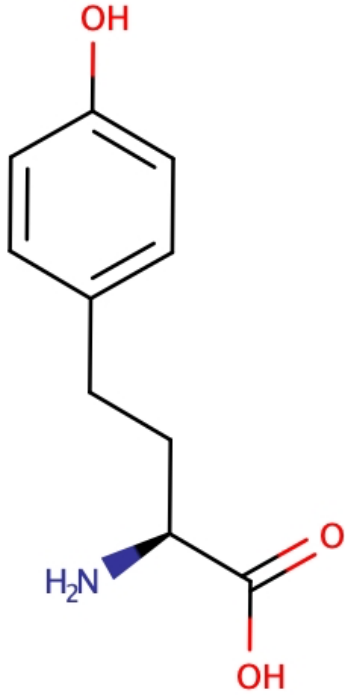
473. curcumenol

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	167812		
TM-MC 성분 동의어	N/A		
PubChem ID	167812		
InChI Key	ISFMXVMWEWLJGJ-NZBPQXDJSA-N		
SMILES	<chem>C[C@H]1CC[C@H]2C(C)=C[C@@]3(O)O[C@@]12CC3=C(C)C</chem>		
Molecular Formula	C ₁₅ H ₂₂ O ₂		
Molecular Weight	234.339	Exact Molecular Weight	234.161979948
LogP	3.143	Topological Polar Surface Area	29.46 Å ²
Atom Count	39	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.65	Oral Bioavailability	Y

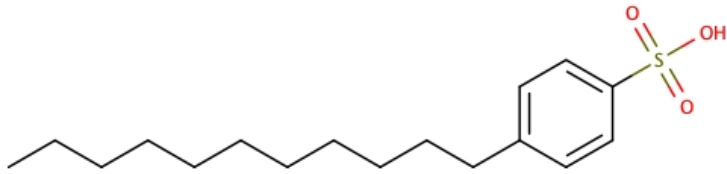
474. docosanedioic acid

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	301199		
TM-MC 성분 동의어	N/A		
PubChem ID	244872		
InChI Key	DGXRZJSPDXZJFG-UHFFFAOYSA-N		
SMILES	OC(=O)CCCCCCCCCCCCCCCCCCCCC(O)=O		
Molecular Formula	C ₂₂ H ₄₂ O ₄		
Molecular Weight	370.574	Exact Molecular Weight	370.308309832
LogP	7.604	Topological Polar Surface Area	74.6 Å ²
Atom Count	68	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	21	Aromatic Ring Count	0
Drug Likeness	0.20	Oral Bioavailability	N

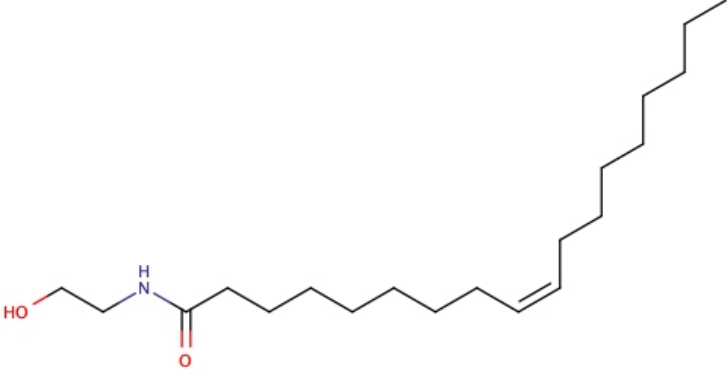
475. L-homotyrosine

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	301624		
TM-MC 성분 동의어	N/A		
PubChem ID	15160483, 40429050		
InChI Key	LOOZZTFGSTZNRX-VIFPVBQESA-N		
SMILES	N[C@@H](CCc1ccc(O)cc1)C(O)=O		
Molecular Formula	C ₁₀ H ₁₃ NO ₃		
Molecular Weight	195.218	Exact Molecular Weight	195.089543283
LogP	-1.044	Topological Polar Surface Area	83.55 Å ²
Atom Count	27	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	1
Drug Likeness	0.57	Oral Bioavailability	Y

476. N-undecylbenzenesulfonic acid

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	301846		
TM-MC 성분 동의어	N/A		
PubChem ID	38222		
InChI Key	UCDCOJNNUVYFKJ-UHFFFAOYSA-N		
SMILES	<chem>CCCCCCCCCCC1ccc(cc1)S(O)(=O)=O</chem>		
Molecular Formula	C ₁₇ H ₂₈ O ₃ S		
Molecular Weight	312.47	Exact Molecular Weight	312.175915936
LogP	6.113	Topological Polar Surface Area	54.37 Å ²
Atom Count	49	Structural Alert Count	2
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	11	Aromatic Ring Count	1
Drug Likeness	0.40	Oral Bioavailability	N

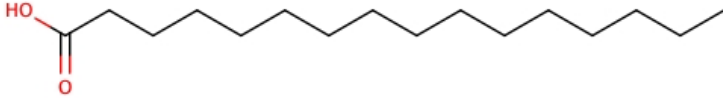
477. oleoyl ethanolamide

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	301941		
TM-MC 성분 동의어	N/A		
PubChem ID	5283454		
InChI Key	BOWVQLFMWHZBEF-KTKRTIGZSA-N		
SMILES	CCCCCCCCC=C/CCCCCCCC(=O)NCCO		
Molecular Formula	C ₂₀ H ₃₉ NO ₂		
Molecular Weight	325.537	Exact Molecular Weight	325.2980795
LogP	5.51	Topological Polar Surface Area	49.33 Å ²
Atom Count	62	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	17	Aromatic Ring Count	0
Drug Likeness	0.27	Oral Bioavailability	N

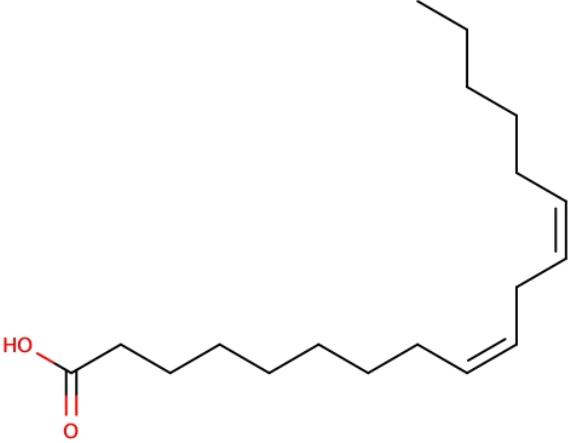
478. tetradecylamine

화학 구조		PubMed ID	
		31254123	
TM-MC 성분 ID	302559		
TM-MC 성분 동의어	N/A		
PubChem ID	16217		
InChI Key	PLZVEHJLHYMBBY-UHFFFAOYSA-N		
SMILES	CCCCCCCCCCCCCN		
Molecular Formula	C ₁₄ H ₃₁ N		
Molecular Weight	213.409	Exact Molecular Weight	213.245650002
LogP	5.144	Topological Polar Surface Area	26.02 Å ²
Atom Count	46	Structural Alert Count	1
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	12	Aromatic Ring Count	0
Drug Likeness	0.45	Oral Bioavailability	N

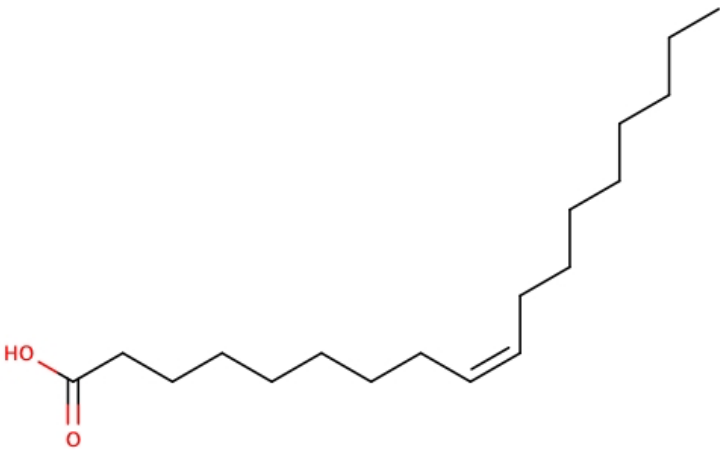
479. palmitic acid

화학 구조		PubMed ID	
		15709383, 22876670 23901639, 29732747	
TM-MC 성분 ID	338		
TM-MC 성분 동의어	hexadecanoic acid; n-hexadecanoic acid; palmitate; cetylic acid; palmitinic acid; n-hexadecoic acid		
PubChem ID	985, 135369651		
InChI Key	IPCSVZSSVZVIGE-UHFFFAOYSA-N		
SMILES	<chem>CCCCCCCCCCCCCCCC(O)=O</chem>		
Molecular Formula	C ₁₆ H ₃₂ O ₂		
Molecular Weight	256.43	Exact Molecular Weight	256.24023027
LogP	6.257	Topological Polar Surface Area	37.3 Å ²
Atom Count	50	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	14	Aromatic Ring Count	0
Drug Likeness	0.37	Oral Bioavailability	N

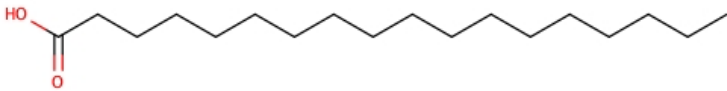
480. linoleic acid

화학 구조		PubMed ID	
		12575114, 23901639 29732747, 31394825	
TM-MC 성분 ID	339		
TM-MC 성분 동의어	9,12-octadecadienoic acid; 9,12-octadecadienoic acid (Z,Z)-; (Z,Z)-9,12-octadecadienoic acid; linoleate; linolic acid; [Z,Z]-9,12-octadecadienoic acid; 9,12-linoleic acid; cis,cis-linoleic acid; cis-9,12-octadecadienoic acid; telfairic acid; α-linoleic acid; octadeca-9,12-dienoic acid; 9Z,12Z-octadecadienoic acid; 9,12(Z,Z)-octadecadienoic acid; (Z,Z) 9,12-octadecadienoic acid; (Z,Z)-octadeca-9,12-dienoic acid; cis-9,cis-12-octadecadienoic acid; octadeca-9C,12C dienoic acid(Z,Z); (9Z,12Z)-9,12-octadecadienoic acid; 9,12-octadecadienoic acid (Z,Z)-(CAS,1)		
PubChem ID	5280450		
InChI Key	OYHQOLUKZRVURQ-HZJYTTRNSA-N		
SMILES	<chem>CCCCC=CC=CCCCCCCC(=O)O</chem>		
Molecular Formula	C ₁₈ H ₃₂ O ₂		
Molecular Weight	280.452	Exact Molecular Weight	280.24023027
LogP	6.422	Topological Polar Surface Area	37.3 Å ²
Atom Count	52	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	14	Aromatic Ring Count	0
Drug Likeness	0.29	Oral Bioavailability	N

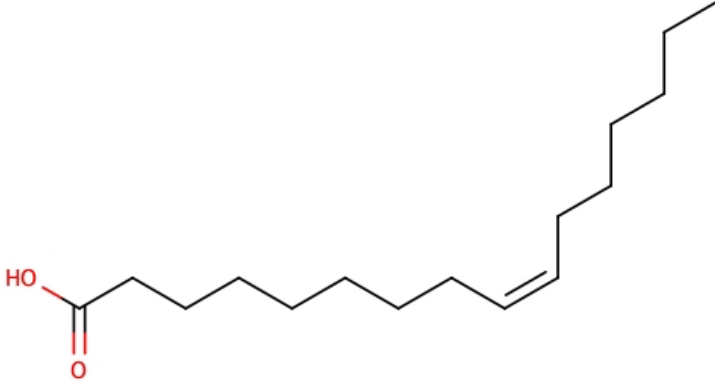
481. oleic acid

화학 구조		PubMed ID	
		12575114, 22876670 23901639, 29732747 31394825	
TM-MC 성분 ID	340		
TM-MC 성분 동의어	9-octadecenoic acid; octadec-9-enoic acid; oleate; 9-octadecanoic acid; cis-9-octadecenoic acid; oleinic acid; (Z)-9-octadecenoic acid; 9-(Z)-octadecenoic acid; (Z)-octadec-9-enoic acid; (9Z)-9-octadecenoic acid; (9Z)-octadec-9-enoic acid		
PubChem ID	445639		
InChI Key	ZQPPMHVWECSIRJ-KTKRTIGZSA-N		
SMILES	<chem>CCCCCCCC=C/CCCCCCC(O)=O</chem>		
Molecular Formula	C ₁₈ H ₃₄ O ₂		
Molecular Weight	282.468	Exact Molecular Weight	282.255880335
LogP	6.784	Topological Polar Surface Area	37.3 Å ²
Atom Count	54	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	15	Aromatic Ring Count	0
Drug Likeness	0.27	Oral Bioavailability	N

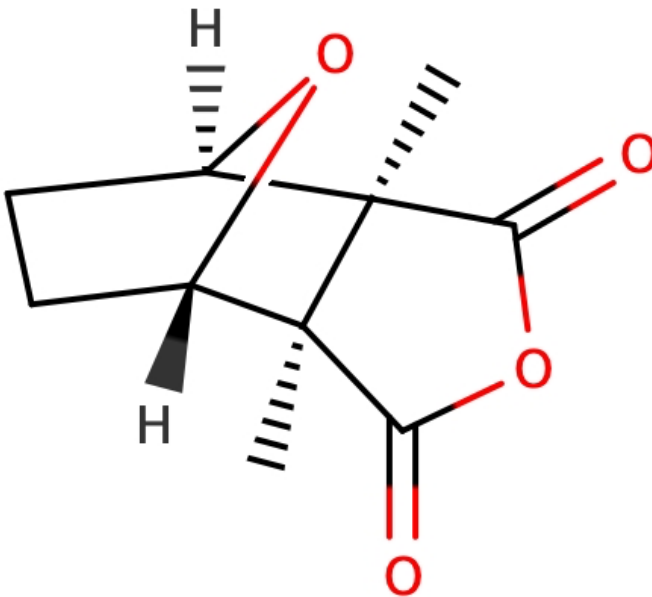
482. stearic acid

화학 구조		PubMed ID	
		23901639	
TM-MC 성분 ID	341		
TM-MC 성분 동의어	octadecanoic acid; stearate; steric acid; stearin acid; octadecaonic acid; n-octadecanoic acid; cis-9-octadecanoic acid		
PubChem ID	5281, 139057051		
InChI Key	QIQXTHQIDYTFRH-UHFFFAOYSA-N		
SMILES	<chem>CCCCCCCCCCCCCCCCCC(O)=O</chem>		
Molecular Formula	C ₁₈ H ₃₆ O ₂		
Molecular Weight	284.484	Exact Molecular Weight	284.271530399
LogP	7.146	Topological Polar Surface Area	37.3 Å ²
Atom Count	56	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	16	Aromatic Ring Count	0
Drug Likeness	0.31	Oral Bioavailability	N

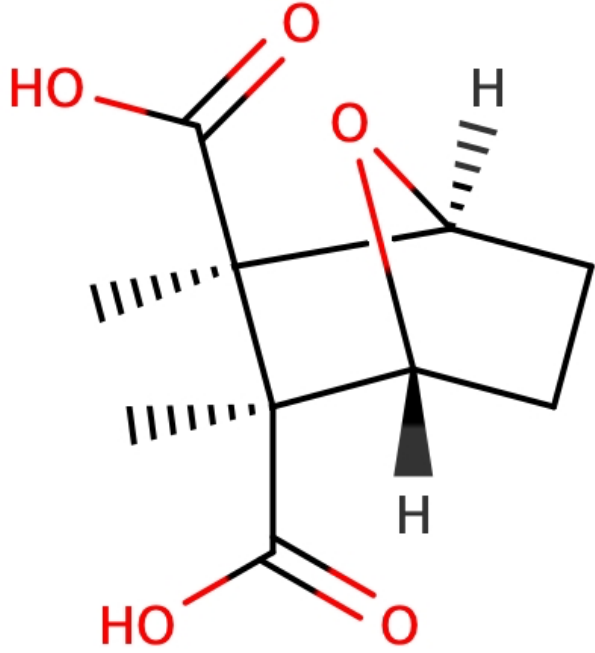
483. palmitoleic acid

화학 구조		PubMed ID	
		22876670, 23901639	
TM-MC 성분 ID	4668		
TM-MC 성분 동의어	9-hexadecenoic acid; palmitelaidic acid; hexadec-9-enoic acid		
PubChem ID	445638		
InChI Key	SECPZKHBENQXJG-FPLPWBNSA-N		
SMILES	<chem>CCCCC=C/C(=O)O</chem>		
Molecular Formula	C ₁₆ H ₃₀ O ₂		
Molecular Weight	254.414	Exact Molecular Weight	254.224580206
LogP	5.895	Topological Polar Surface Area	37.3 Å ²
Atom Count	48	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	13	Aromatic Ring Count	0
Drug Likeness	0.33	Oral Bioavailability	N

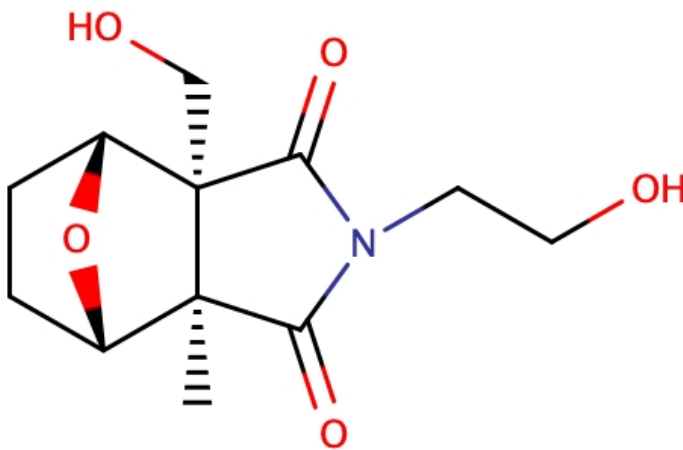
484. cantharidin

화학 구조		PubMed ID	
		22233030, 28875639 28914023, 30043217 31999361	
TM-MC 성분 ID	342		
TM-MC 성분 동의어	N/A		
PubChem ID	5944		
InChI Key	DHZBEENLJMYSHQ-XCVPVQRUSA-N		
SMILES	<chem>C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)OC2=O</chem>		
Molecular Formula	C ₁₀ H ₁₂ O ₄		
Molecular Weight	196.202	Exact Molecular Weight	196.073558866
LogP	1.059	Topological Polar Surface Area	52.6 Å ²
Atom Count	26	Structural Alert Count	2
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.43	Oral Bioavailability	Y

485. cantharidic acid

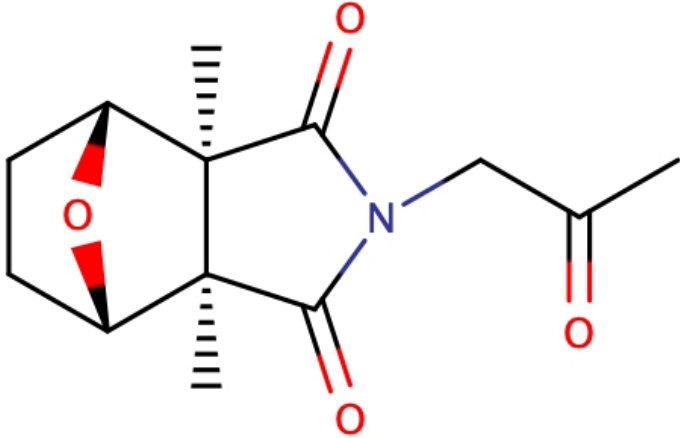
화학 구조		PubMed ID	
		28914023	
TM-MC 성분 ID	300889		
TM-MC 성분 동의어	N/A		
PubChem ID	121475		
InChI Key	NMTNUQBORQILRK-XCVPVQRUSA-N		
SMILES	<chem>C[C@@]1([C@@H]2CC[C@@H](O2)[C@@]1(C)C(O)=O)C(O)=O</chem>		
Molecular Formula	C ₁₀ H ₁₄ O ₅		
Molecular Weight	214.217	Exact Molecular Weight	214.084123551
LogP	0.925	Topological Polar Surface Area	83.83 Å ²
Atom Count	29	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.71	Oral Bioavailability	Y

486. 2'-(1-hydroxymethyl-2-methyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-1'-hydroxyethyl

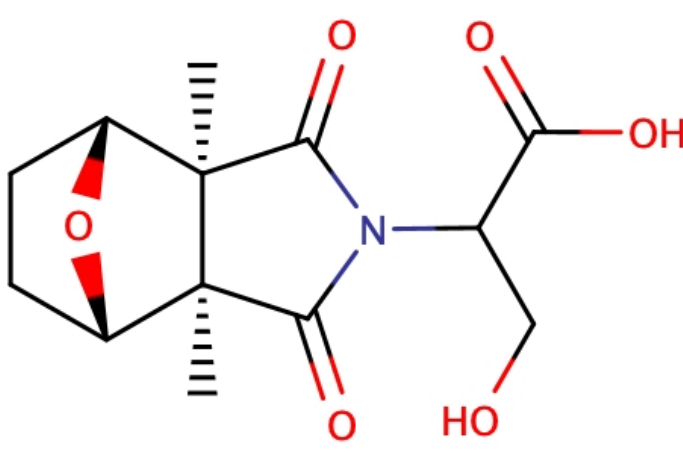
화학 구조	PubMed ID
	31999361

TM-MC 성분 ID	94226		
TM-MC 성분 동의어	N/A		
PubChem ID	134140818		
InChI Key	NDLFEGGUCLCOCE-MDSNHJATSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(CO)C(=O)N(CCO)C2=O		
Molecular Formula	C ₁₂ H ₁₇ NO ₅		
Molecular Weight	255.27	Exact Molecular Weight	255.110672651
LogP	-1.417	Topological Polar Surface Area	87.07 Å ²
Atom Count	35	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.60	Oral Bioavailability	Y

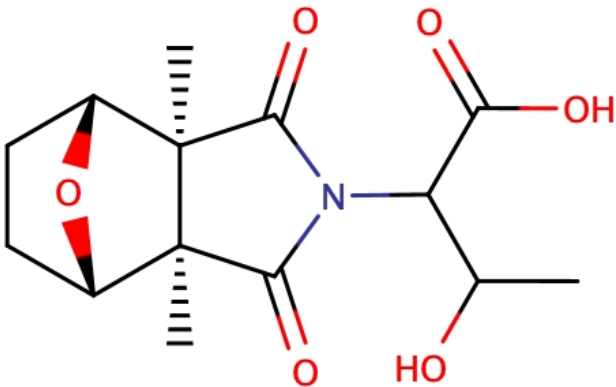
487. 2'-(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-propanone

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94227		
TM-MC 성분 동의어	N/A		
PubChem ID	134157694		
InChI Key	GIQHOYHNWFGMLL-JDNZLRHBSA-N		
SMILES	CC(=O)CN1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(C)C1=O		
Molecular Formula	C ₁₃ H ₁₇ NO ₄		
Molecular Weight	251.282	Exact Molecular Weight	251.115758031
LogP	0.361	Topological Polar Surface Area	63.68 Å ²
Atom Count	35	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	0
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.66	Oral Bioavailability	Y

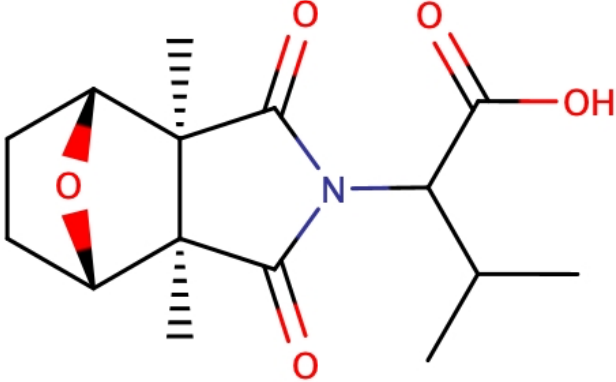
488. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-3'-hydroxy propionic acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94225		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	KFXOCYAKMXXNKW-NSKRIWLVSA-N		
SMILES	<chem>C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(C(CO)C(O)=O)C2=O</chem>		
Molecular Formula	C ₁₃ H ₁₇ NO ₆		
Molecular Weight	283.28	Exact Molecular Weight	283.105587271
LogP	-0.446	Topological Polar Surface Area	104.14 Å ²
Atom Count	37	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.68	Oral Bioavailability	Y

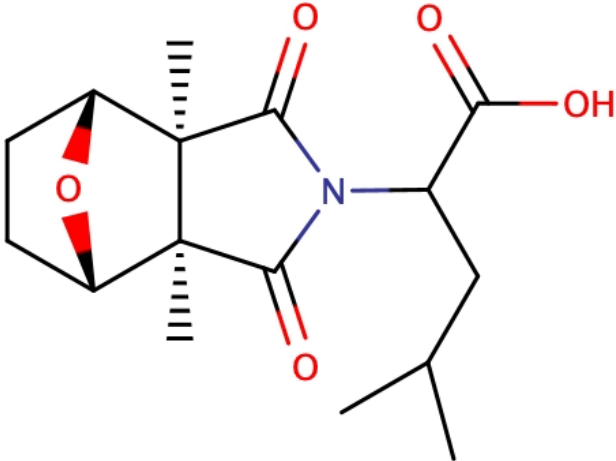
489. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-3'-hydroxybutyric acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94224		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	AXKYIPSGMVKMGY-CYUDTWSZSA-N		
SMILES	CC(O)C(N1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(C)C1=O)C(O)=O		
Molecular Formula	C ₁₄ H ₁₉ NO ₆		
Molecular Weight	297.307	Exact Molecular Weight	297.121237336
LogP	-0.03	Topological Polar Surface Area	104.14 Å ²
Atom Count	40	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.71	Oral Bioavailability	Y

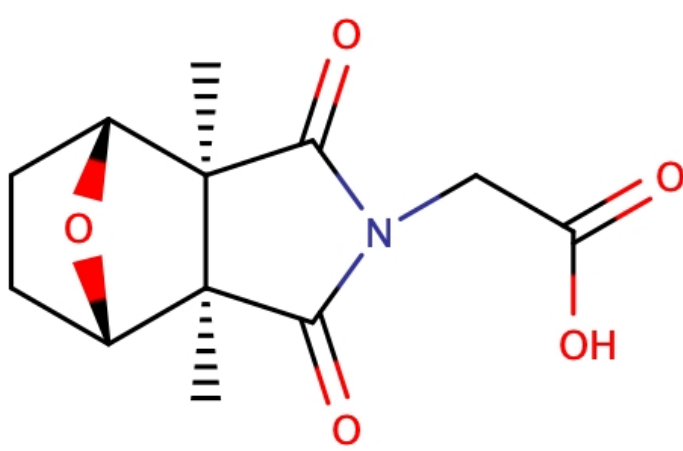
490. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-3'-methylbutyric acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94222		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	JZYGDDGGSVOESJJ-MTGKNFNGSA-N		
SMILES	CC(C)C(N1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(C)C1=O)C(O)=O		
Molecular Formula	C ₁₅ H ₂₁ NO ₅		
Molecular Weight	295.335	Exact Molecular Weight	295.14197278
LogP	1.488	Topological Polar Surface Area	83.91 Å ²
Atom Count	42	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.80	Oral Bioavailability	Y

491. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-4'-methylpentanoic acid

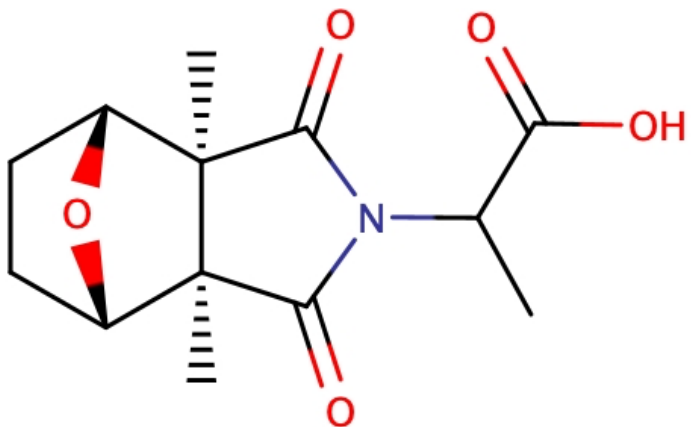
화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94220		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	VAABDRVJHPLZFY-CHCWFGPISA-N		
SMILES	<chem>CC(C)CC(N1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(C)C1=O)C(O)=O</chem>		
Molecular Formula	C ₁₆ H ₂₃ NO ₅		
Molecular Weight	309.362	Exact Molecular Weight	309.157622845
LogP	1.855	Topological Polar Surface Area	83.91 Å ²
Atom Count	45	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.80	Oral Bioavailability	Y

492. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-acetic acid

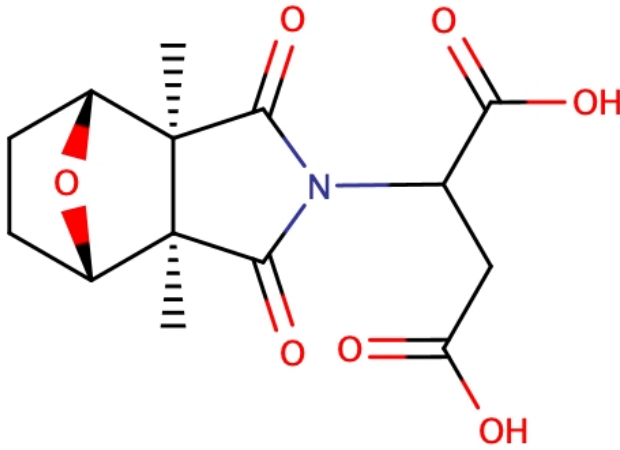
화학 구조	PubMed ID
	31999361

TM-MC 성분 ID	94218		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	INGIJXXPFXREQF-AIQZBZIUSA-N		
SMILES	<chem>C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(CC(O)=O)C2=O</chem>		
Molecular Formula	C ₁₂ H ₁₅ NO ₅		
Molecular Weight	253.254	Exact Molecular Weight	253.095022587
LogP	0.032	Topological Polar Surface Area	83.91 Å ²
Atom Count	33	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.70	Oral Bioavailability	Y

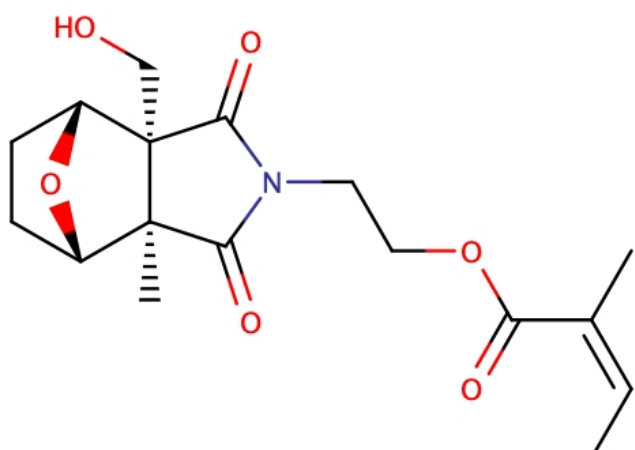
493. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-propionic acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94212		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	XVBOZUAVRDGLMU-NSKRIWLVSA-N		
SMILES	<chem>CC(N1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(C)C1=O)C(O)=O</chem>		
Molecular Formula	C ₁₃ H ₁₇ NO ₅		
Molecular Weight	267.281	Exact Molecular Weight	267.110672651
LogP	0.6	Topological Polar Surface Area	83.91 Å ²
Atom Count	36	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.74	Oral Bioavailability	Y

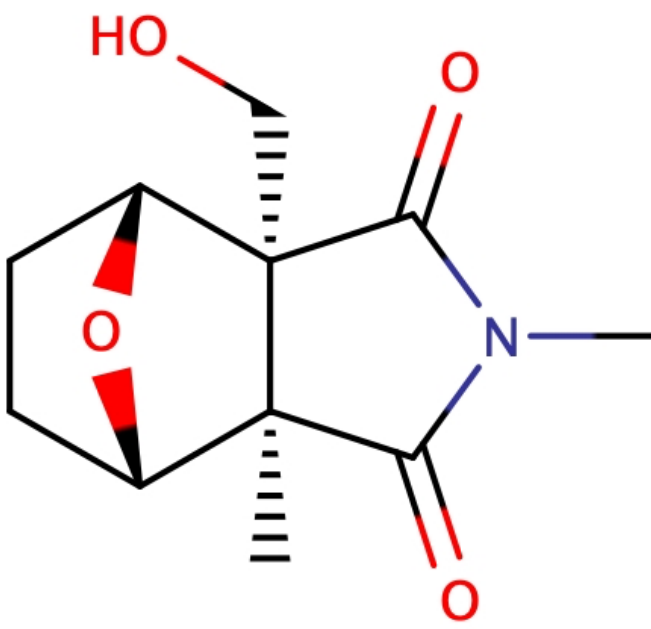
494. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-succinic acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94210		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	QFZHSYJFUKAAPL-USJRYORUSA-N		
SMILES	<chem>C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(C(CC(O)=O)C(O)=O)C2=O</chem>		
Molecular Formula	C ₁₄ H ₁₇ NO ₇		
Molecular Weight	311.29	Exact Molecular Weight	311.100501891
LogP	-0.041	Topological Polar Surface Area	121.21 Å ²
Atom Count	39	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.70	Oral Bioavailability	Y

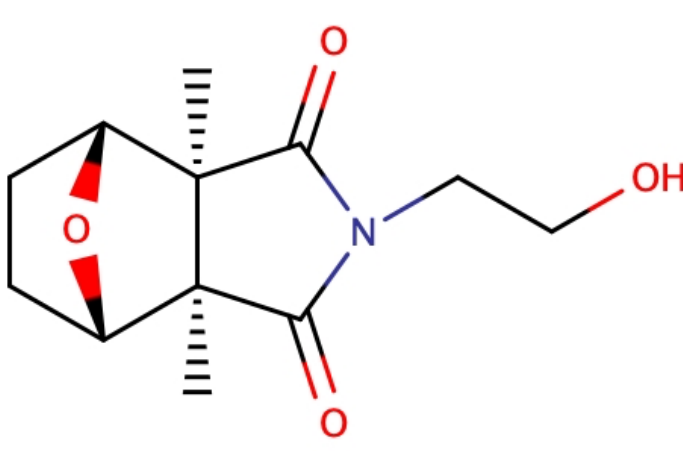
495. 5'-[(1R,2R,3S,6R)-1-hydroxymethyl-2-methyl-3,6-epoxycyclohexane-1,2-dicarboximide]-ethyl-2'-methyl-2'-butenoate

화학 구조		PubMed ID	
		28875639	
TM-MC 성분 ID	99435		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	DZYTXXBFMLFZLJ-RNQRQFJOSA-N		
SMILES	C#C=C(C)C(=O)OCCN1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(CO)C1=O		
Molecular Formula	C ₁₇ H ₂₃ NO ₆		
Molecular Weight	337.372	Exact Molecular Weight	337.152537465
LogP	0.796	Topological Polar Surface Area	93.14 Å ²
Atom Count	47	Structural Alert Count	3
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	1
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.44	Oral Bioavailability	Y

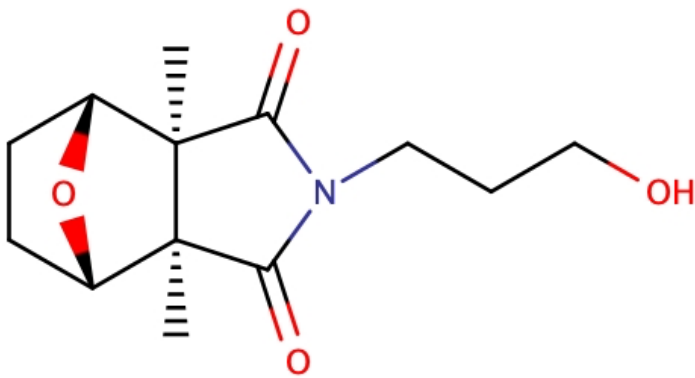
496. 8-(1-hydroxymethyl-2-methyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-methyl

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94202		
TM-MC 성분 동의어	N/A		
PubChem ID	134143387		
InChI Key	RHGKXQLPGZLOFU-HJGGDWJDSA-N		
SMILES	CN1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(CO)C1=O		
Molecular Formula	C ₁₁ H ₁₅ NO ₄		
Molecular Weight	225.244	Exact Molecular Weight	225.100107967
LogP	-0.727	Topological Polar Surface Area	66.84 Å ²
Atom Count	31	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.60	Oral Bioavailability	Y

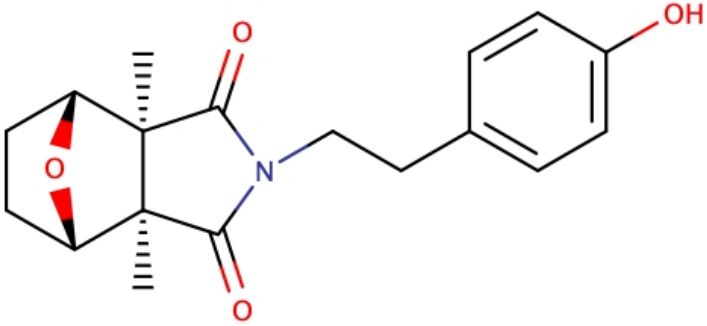
497. 8-(1'-hydroxyethyl)-1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94203		
TM-MC 성분 동의어	N/A		
PubChem ID	101077138		
InChI Key	HWRPFCLFXMQUPU-IVQVNHISA-N		
SMILES	<chem>C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(CCO)C2=O</chem>		
Molecular Formula	C ₁₂ H ₁₇ NO ₄		
Molecular Weight	239.271	Exact Molecular Weight	239.115758031
LogP	-0.136	Topological Polar Surface Area	66.84 Å ²
Atom Count	34	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.68	Oral Bioavailability	Y

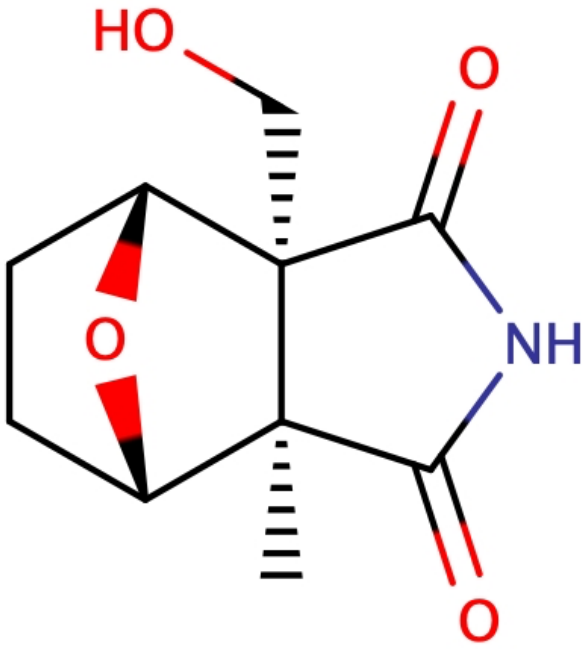
498. 8-(1'-hydroxypropyl)-1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94201		
TM-MC 성분 동의어	N/A		
PubChem ID	134148728		
InChI Key	COYZAYXESCUATO-JDNZLRHBSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(CCCO)C2=O		
Molecular Formula	C ₁₃ H ₁₉ NO ₄		
Molecular Weight	253.298	Exact Molecular Weight	253.131408096
LogP	-0.076	Topological Polar Surface Area	66.84 Å ²
Atom Count	37	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.71	Oral Bioavailability	Y

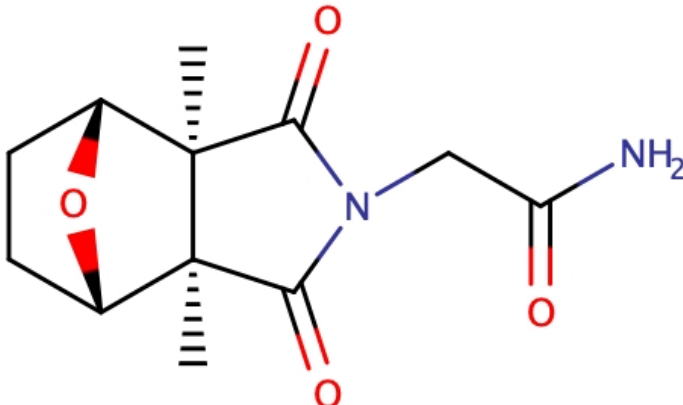
499. 8-[(4'-hydroxyphenyl)-ethyl]-1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94198		
TM-MC 성분 동의어	N/A		
PubChem ID	11336028		
InChI Key	HJLDVSLYLWZYQY-PURYLZLUSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(CCC1ccc(O)cc1)C2=O		
Molecular Formula	C ₁₈ H ₂₁ NO ₄		
Molecular Weight	315.369	Exact Molecular Weight	315.14705816
LogP	2.263	Topological Polar Surface Area	66.84 Å ²
Atom Count	44	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	1
Drug Likeness	0.87	Oral Bioavailability	Y

500. cantharimide B

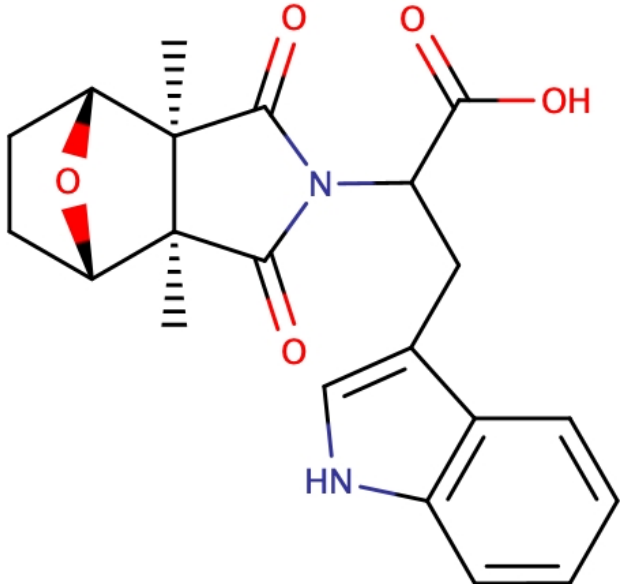
화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94229		
TM-MC 성분 동의어	1-hydroxymethyl-2-methyl-1,7-epoxycyclohexane-1,2-dicarboximide		
PubChem ID	16105341		
InChI Key	YFPSPJLMOAVHRT-ZRVLKLQWSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(CO)C(=O)NC2=O		
Molecular Formula	C ₁₀ H ₁₃ NO ₄		
Molecular Weight	211.217	Exact Molecular Weight	211.084457903
LogP	-0.951	Topological Polar Surface Area	75.63 Å ²
Atom Count	28	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.55	Oral Bioavailability	Y

501. 2'-(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-acetamide

화학 구조	PubMed ID
	31999361

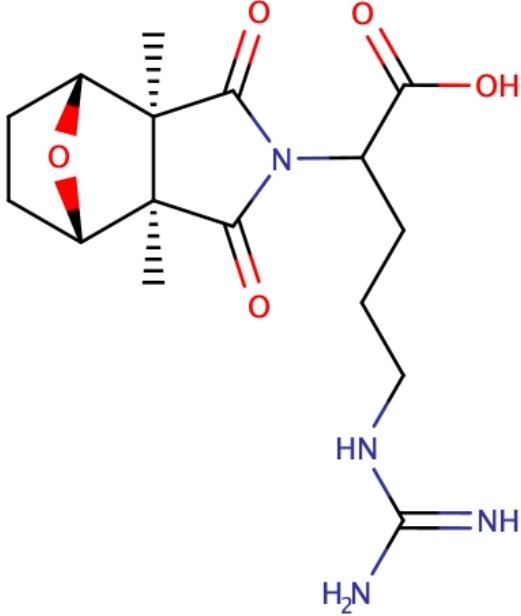
TM-MC 성분 ID	94228		
TM-MC 성분 동의어	N/A		
PubChem ID	134132514		
InChI Key	HPVIBMNHDQMPDD-AIQZBZIUSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(CC(N)=O)C2=O		
Molecular Formula	C ₁₂ H ₁₆ N ₂ O ₄		
Molecular Weight	252.27	Exact Molecular Weight	252.111007003
LogP	-0.775	Topological Polar Surface Area	89.7 Å ²
Atom Count	34	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.65	Oral Bioavailability	Y

502. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-3'-indol-propionic acid

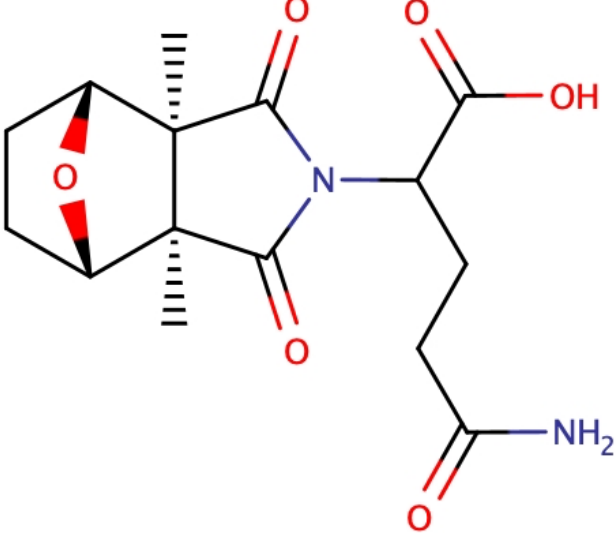
화학 구조	PubMed ID
	31999361

TM-MC 성분 ID	94223		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	GYDFKFRJOWAOX-NKIIOANBSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(C(Cc1c[nH]c3ccccc13)C(O)=O)C2=O		
Molecular Formula	C ₂₁ H ₂₂ N ₂ O ₅		
Molecular Weight	382.416	Exact Molecular Weight	382.152871816
LogP	2.356	Topological Polar Surface Area	99.7 Å ²
Atom Count	50	Structural Alert Count	1
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	2
Drug Likeness	0.79	Oral Bioavailability	Y

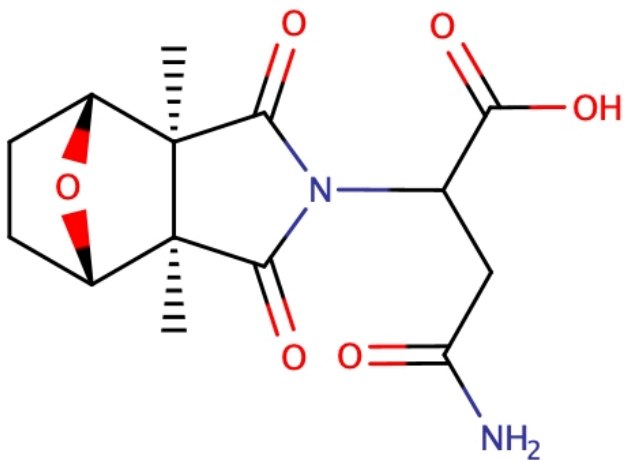
503. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-5'-guanidino-pentanoic acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94219		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	DYJXSJANLQKJAG-DBJGFWSUSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(C(CCCNC(N)=N)C(O)=O)C2=O		
Molecular Formula	C ₁₆ H ₂₄ N ₄ O ₅		
Molecular Weight	352.391	Exact Molecular Weight	352.174669889
LogP	-1.955	Topological Polar Surface Area	145.81 Å ²
Atom Count	49	Structural Alert Count	4
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	4
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.19	Oral Bioavailability	Y

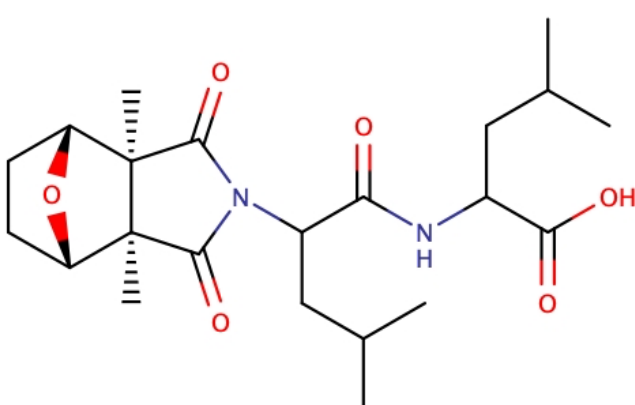
504. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-pentanedioic acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94215		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	WKOHFDRGRPIGQM-ACCMDAOCSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(C(CCC(N)=O)C(O)=O)C2=O		
Molecular Formula	C ₁₅ H ₂₀ N ₂ O ₆		
Molecular Weight	324.333	Exact Molecular Weight	324.132136372
LogP	-0.56	Topological Polar Surface Area	127 Å ²
Atom Count	43	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.65	Oral Bioavailability	Y

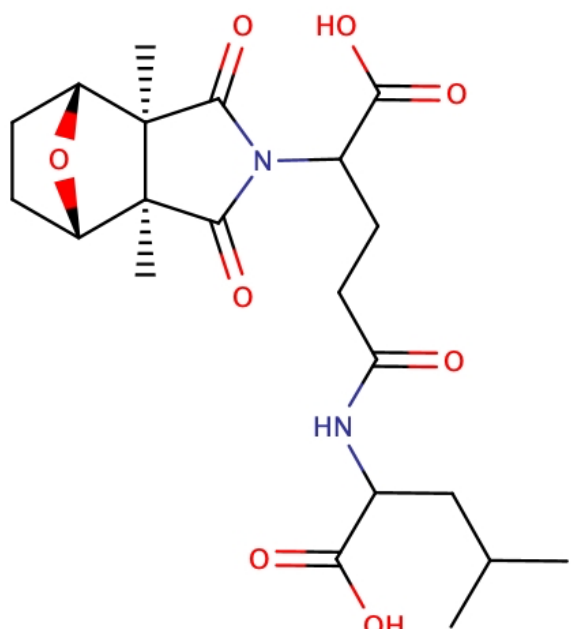
505. 2'-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-succinamic acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94211		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	RQKFORKFAGOPRP-USJRYORUSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(C(CC(N)=O)C(O)=O)C2=O		
Molecular Formula	C ₁₄ H ₁₈ N ₂ O ₆		
Molecular Weight	310.306	Exact Molecular Weight	310.116486308
LogP	-0.848	Topological Polar Surface Area	127 Å ²
Atom Count	40	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.65	Oral Bioavailability	Y

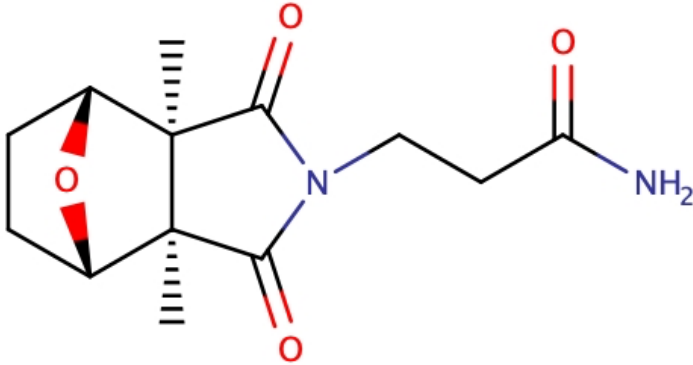
506. 2'-[2''-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-4''-methyl-pentanoylamino]-4'-methyl-pentanoic acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94209		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	PQMNVKZKLJZBKK-PRHJSFTQSA-N		
SMILES	CC(C)CC(NC(=O)C(CC(C)C)N1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(C)C1=O)C(O)=O		
Molecular Formula	C ₂₂ H ₃₄ N ₂ O ₆		
Molecular Weight	422.522	Exact Molecular Weight	422.241686823
LogP	2.572	Topological Polar Surface Area	113.01 Å ²
Atom Count	64	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	8	Aromatic Ring Count	0
Drug Likeness	0.58	Oral Bioavailability	Y

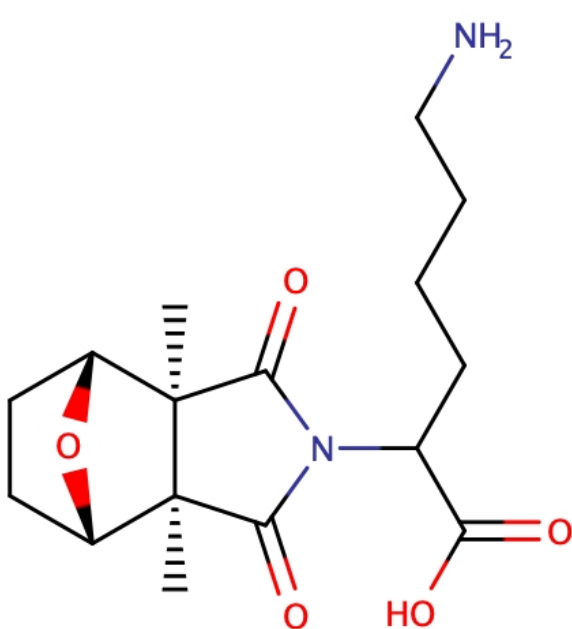
507. 2'-[4''-carboxy-4''-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-butyrylamino]-4'-methyl-pentanoic acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94208		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	YBYJPPFNALPDNX-GAQKAFIASA-N		
SMILES	CC(C)CC(NC(=O)CCC(N1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(C)C1=O)C(O)=O)C(O)=O		
Molecular Formula	C ₂₁ H ₃₀ N ₂ O ₈		
Molecular Weight	438.477	Exact Molecular Weight	438.200215934
LogP	0.965	Topological Polar Surface Area	150.31 Å ²
Atom Count	61	Structural Alert Count	1
Hydrogen Bond Acceptor Count	8	Hydrogen Bond Donor Count	3
Rotatable Bond Count	9	Aromatic Ring Count	0
Drug Likeness	0.45	Oral Bioavailability	Y

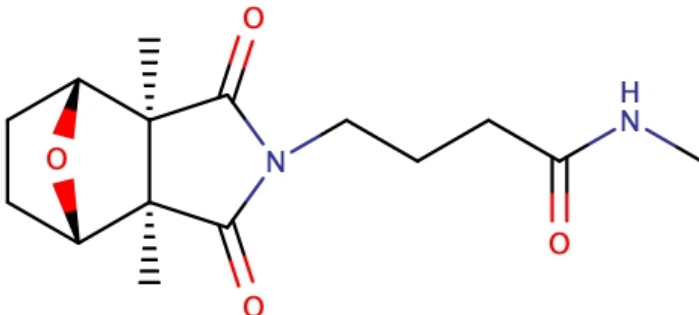
508. 3'-(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-propionamide

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94207		
TM-MC 성분 동의어	N/A		
PubChem ID	134156540		
InChI Key	NSWHASWNADBUKA-GRUGVGOFSAN		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(CCC(N)=O)C2=O		
Molecular Formula	C ₁₃ H ₁₈ N ₂ O ₄		
Molecular Weight	266.297	Exact Molecular Weight	266.126657068
LogP	-0.538	Topological Polar Surface Area	89.7 Å ²
Atom Count	37	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.69	Oral Bioavailability	Y

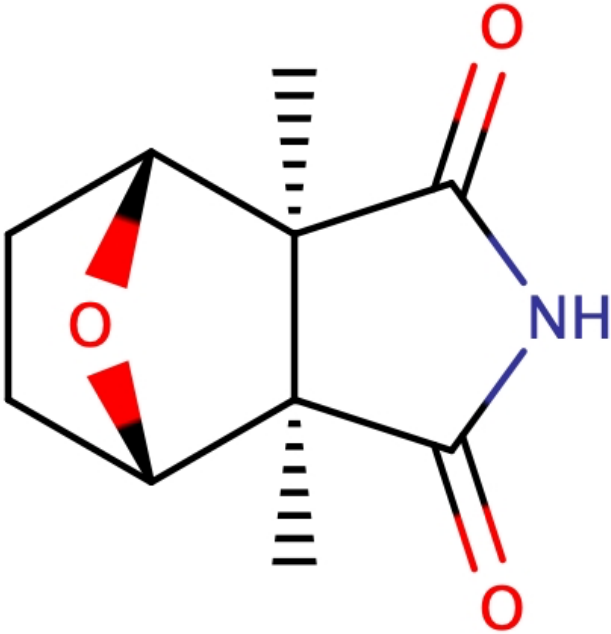
509. 6'-amino-2-(2,6-dimethyl-3,5-dioxo-1,7-epoxyoctahydroisoindol-4-yl)-hexanoic acid

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94206		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	ARYRWLFTNUTIFR-CHCWFGPISA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)N(C(CCCCN)C(O)=O)C2=O		
Molecular Formula	C ₁₆ H ₂₄ N ₂ O ₅		
Molecular Weight	324.377	Exact Molecular Weight	324.168521881
LogP	-1.794	Topological Polar Surface Area	109.93 Å ²
Atom Count	47	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	2
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.44	Oral Bioavailability	Y

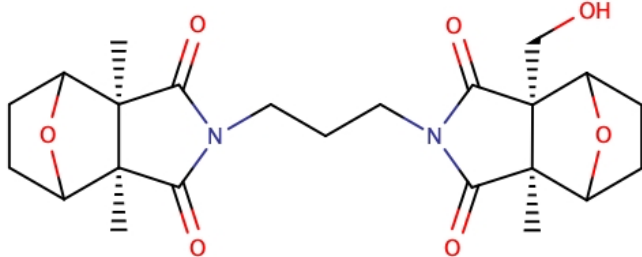
510. 8-(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximide-8-yl)-N-methyl-butylamide

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94205		
TM-MC 성분 동의어	N/A		
PubChem ID	134132157		
InChI Key	NCHHBHYIMZNCOH-FHYCKABGSA-N		
SMILES	<chem>CNC(=O)CCCN1C(=O)[C@@]2(C)[C@@H]3CC[C@@H](O3)[C@@]2(C)C1=O</chem>		
Molecular Formula	C ₁₅ H ₂₂ N ₂ O ₄		
Molecular Weight	294.351	Exact Molecular Weight	294.157957196
LogP	-0.026	Topological Polar Surface Area	75.71 Å ²
Atom Count	43	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.74	Oral Bioavailability	Y

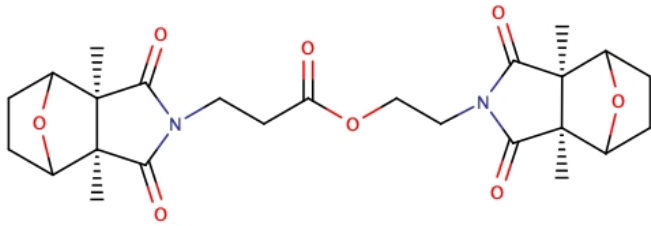
511. cantharimide

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	300890		
TM-MC 성분 동의어	N/A		
PubChem ID	10954464		
InChI Key	PHOUKBDDOYWEMY-XCVPVQRUSA-N		
SMILES	C[C@]12[C@@H]3CC[C@@H](O3)[C@@]1(C)C(=O)NC2=O		
Molecular Formula	C ₁₀ H ₁₃ NO ₃		
Molecular Weight	195.218	Exact Molecular Weight	195.089543283
LogP	0.33	Topological Polar Surface Area	55.4 Å ²
Atom Count	27	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.57	Oral Bioavailability	Y

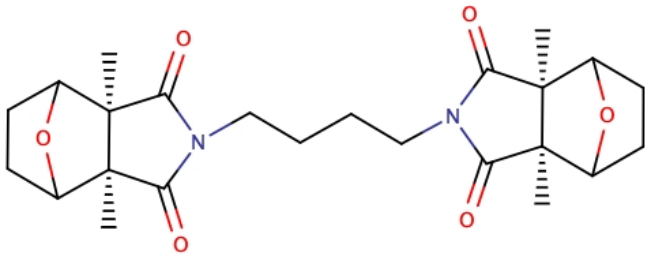
512. bis-(1-methyl-2-hydroxymethyl-3,6-epoxycyclohexane-10,20-dimethyl-1,2-dicarboximido)-trimethylene

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94193		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	YYLXEJQRZXNLBJ-VXPJYSSISA-N		
SMILES	C[C@]12C3CCC(O3)[C@@]1(C)C(=O)N(CCCN1C(=O)[C@]3(C)C4CCC(O4)[C@]3(CO)C1=O)C2=O		
Molecular Formula	C ₂₃ H ₃₀ N ₂ O ₇		
Molecular Weight	446.5	Exact Molecular Weight	446.205301314
LogP	-0.285	Topological Polar Surface Area	113.45 Å ²
Atom Count	62	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.58	Oral Bioavailability	Y

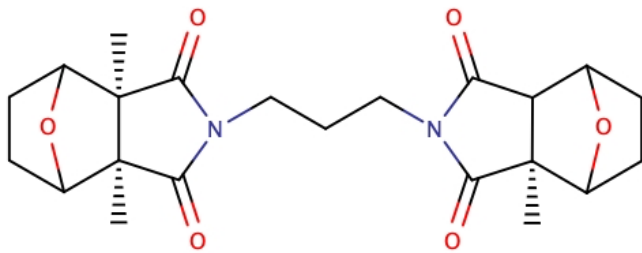
513. bis-(1,2-dimethyl-3,6-epoxycyclohexane-20-methyl-1,2-dicarboximido)-ethyl butyrate

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94195		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	LJTWXDAVMPDRKM-YYCCOVATSA-N		
SMILES	<chem>C[C@]12C3CCC(O3)[C@@]1(C)C(=O)N(CCOC(=O)CCN1C(=O)[C@@]3(C)C4CCC(O4)[C@@]3(C)C1=O)C2=O</chem>		
Molecular Formula	C ₂₅ H ₃₂ N ₂ O ₈		
Molecular Weight	488.537	Exact Molecular Weight	488.215865998
LogP	0.797	Topological Polar Surface Area	119.52 Å ²
Atom Count	67	Structural Alert Count	2
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	0
Rotatable Bond Count	7	Aromatic Ring Count	0
Drug Likeness	0.38	Oral Bioavailability	Y

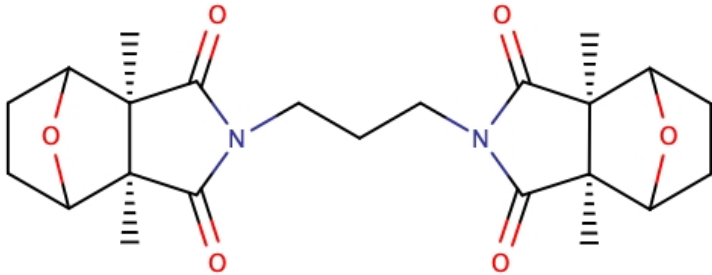
514. bis(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximido)-tetramethylene

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94197		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	ZBBCUJQKNYUHCN-BQWCGIQYSA-N		
SMILES	C[C@]12C3CCC(O3)[C@@]1(C)C(=O)N(CCCCN1C(=O)[C@@]3(C)C4CCC(O4)[C@@]3(C)C1=O)C2=O		
Molecular Formula	C ₂₄ H ₃₂ N ₂ O ₆		
Molecular Weight	444.528	Exact Molecular Weight	444.226036758
LogP	1.513	Topological Polar Surface Area	93.22 Å ²
Atom Count	64	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	0
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.47	Oral Bioavailability	Y

515. bis(1,2-dimethyl-3,6-epoxycyclohexane-20-methyl-1,2-dicarboximido)-trimethylene

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94194		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	JMBWOEIFCXZOCY-LGTKLAAESA-N		
SMILES	C[C@@]12C3CCC(O3)C1C(=O)N(CCCN1C(=O)[C@@]3(C)C4CCC(O4)[C@@]3(C)C1=O)C2=O		
Molecular Formula	C ₂₂ H ₂₈ N ₂ O ₆		
Molecular Weight	416.474	Exact Molecular Weight	416.19473663
LogP	0.44	Topological Polar Surface Area	93.22 Å ²
Atom Count	58	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	0
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.62	Oral Bioavailability	Y

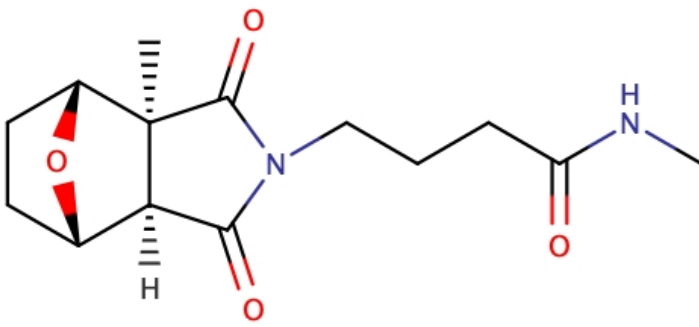
516. dicantharimide A

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94192		
TM-MC 성분 동의어	bis(1,2-dimethyl-3,6-epoxycyclohexane-1,2-dicarboximido)-trimethylene		
PubChem ID	N/A		
InChI Key	QAJLNPRUKGVGJK-XDZDJPAXSA-N		
SMILES	C[C@]12C3CCC(O3)[C@@]1(C)C(=O)N(CCCN1C(=O)[C@@]3(C)C4CCC(O4)[C@@]3(C)C1=O)C2=O		
Molecular Formula	C ₂₃ H ₃₀ N ₂ O ₆		
Molecular Weight	430.501	Exact Molecular Weight	430.210386694
LogP	0.996	Topological Polar Surface Area	93.22 Å ²
Atom Count	61	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	0
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.62	Oral Bioavailability	Y

517. 8-(acetamide) palasoninimide

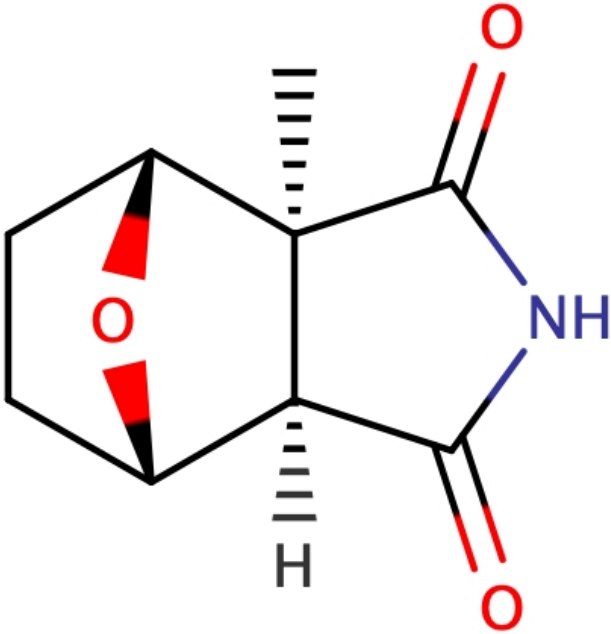
화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	94200		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	GPIWDPIJLMQYFB-YKNIRZD TSA-N		
SMILES	<chem>C[C@@]12[C@H]3CC[C@H](O3)[C@@H]1C(=O)N(CC(N)=O)C2=O</chem>		
Molecular Formula	C ₁₁ H ₁₄ N ₂ O ₄		
Molecular Weight	238.243	Exact Molecular Weight	238.095356939
LogP	-1.331	Topological Polar Surface Area	89.7 Å ²
Atom Count	31	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.60	Oral Bioavailability	Y

518. 8-(N-methyl-butylamide) palasoninimide

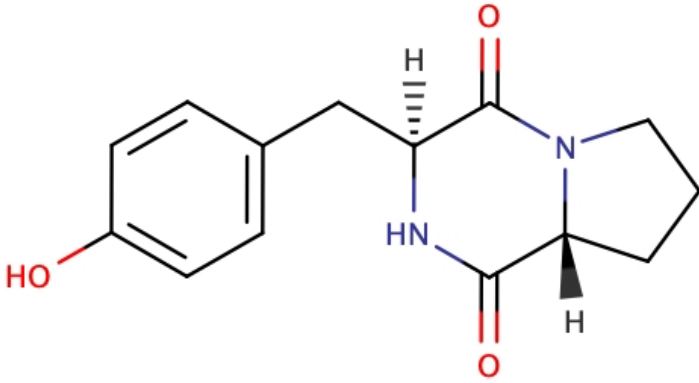
화학 구조	PubMed ID
	31999361

TM-MC 성분 ID	94199		
TM-MC 성분 동의어	N/A		
PubChem ID	134141537		
InChI Key	LSVRQRSDBPKME-AUDJIGTPSA-N		
SMILES	CNC(=O)CCCN1C(=O)[C@H]2[C@@H]3CC[C@@H](O3)[C@@]2(C)C1=O		
Molecular Formula	C ₁₄ H ₂₀ N ₂ O ₄		
Molecular Weight	280.324	Exact Molecular Weight	280.142307132
LogP	-0.582	Topological Polar Surface Area	75.71 Å ²
Atom Count	40	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.70	Oral Bioavailability	Y

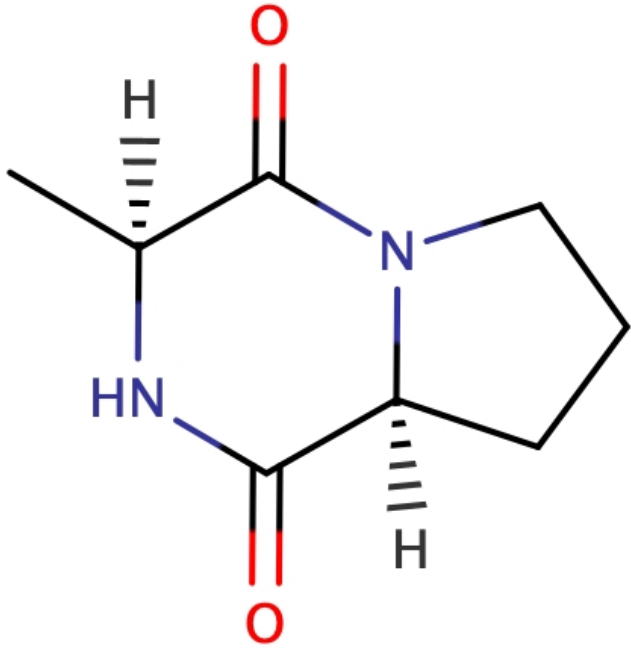
519. palasoninimide

화학 구조		PubMed ID	
		31999361	
TM-MC 성분 ID	93331		
TM-MC 성분 동의어	N/A		
PubChem ID	134145210		
InChI Key	MFTAIYCOICTLKW-BKIHBWCSSA-N		
SMILES	C[C@@]12[C@H]3CC[C@H](O3)[C@@H]1C(=O)NC2=O		
Molecular Formula	C ₉ H ₁₁ NO ₃		
Molecular Weight	181.191	Exact Molecular Weight	181.073893218
LogP	-0.226	Topological Polar Surface Area	55.4 Å ²
Atom Count	24	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.53	Oral Bioavailability	Y

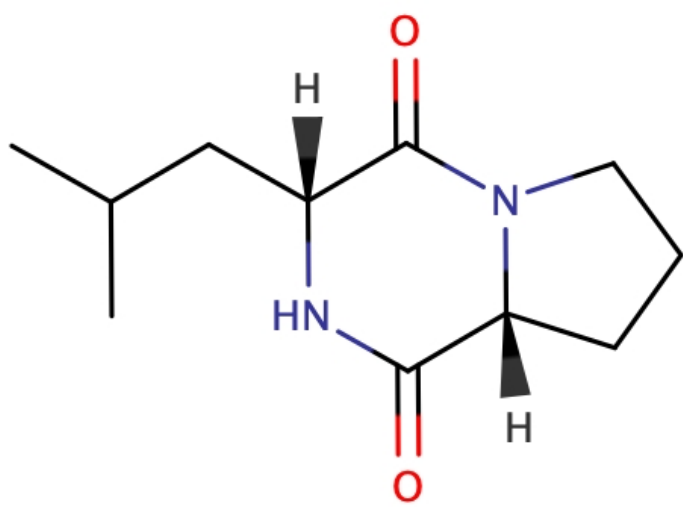
520. cyclo-(D-Pro-L-Tyr)

화학 구조		PubMed ID	
		28875639	
TM-MC 성분 ID	301060		
TM-MC 성분 동의어	N/A		
PubChem ID	6993323		
InChI Key	LSGOTAXPWMCUCK-NWDGAFQWSA-N		
SMILES	<chem>Oc1ccc(C[C@@H]2NC(=O)[C@H]3CCCN3C2=O)cc1</chem>		
Molecular Formula	C ₁₄ H ₁₆ N ₂ O ₃		
Molecular Weight	260.293	Exact Molecular Weight	260.116092383
LogP	0.552	Topological Polar Surface Area	69.64 Å ²
Atom Count	35	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	2	Aromatic Ring Count	1
Drug Likeness	0.82	Oral Bioavailability	Y

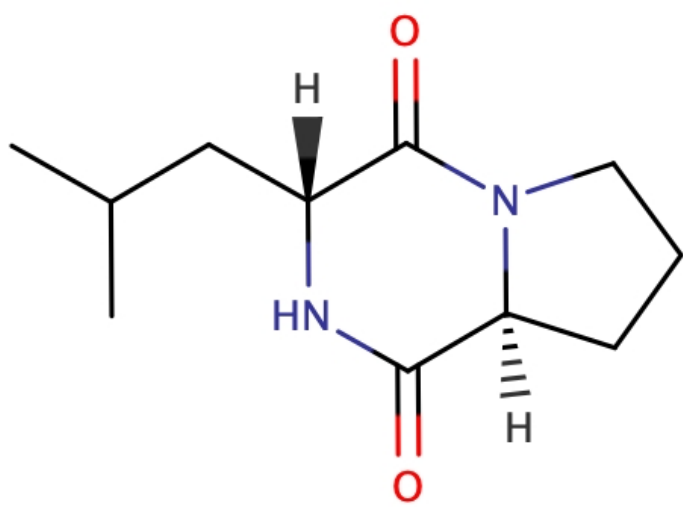
521. cyclo-(L-Pro-L-Ala)

화학 구조		PubMed ID	
		28875639	
TM-MC 성분 ID	98983		
TM-MC 성분 동의어	N/A		
PubChem ID	13879951		
InChI Key	WSLYCILIEOFQPK-WDSKDSINSA-N		
SMILES	C[C@@H]1NC(=O)[C@@H]2CCCN2C1=O		
Molecular Formula	C ₈ H ₁₂ N ₂ O ₂		
Molecular Weight	168.196	Exact Molecular Weight	168.089877634
LogP	-0.8	Topological Polar Surface Area	49.41 Å ²
Atom Count	24	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.51	Oral Bioavailability	Y

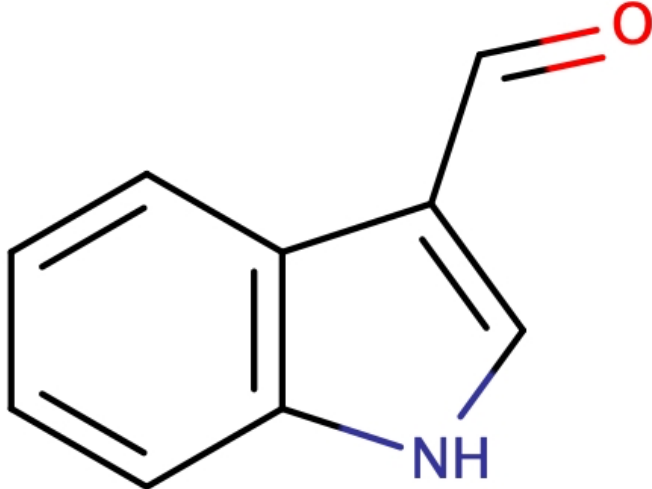
522. cyclo-(R-Pro-R-Leu)

화학 구조		PubMed ID	
		28875639	
TM-MC 성분 ID	99436		
TM-MC 성분 동의어	N/A		
PubChem ID	927566		
InChI Key	SZJNCZMRZAUNQT-RKDXNWHRSA-N		
SMILES	CC(C)C[C@H]1NC(=O)[C@H]2CCCN2C1=O		
Molecular Formula	C ₁₁ H ₁₈ N ₂ O ₂		
Molecular Weight	210.277	Exact Molecular Weight	210.136827828
LogP	0.454	Topological Polar Surface Area	49.41 Å ²
Atom Count	33	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.72	Oral Bioavailability	Y

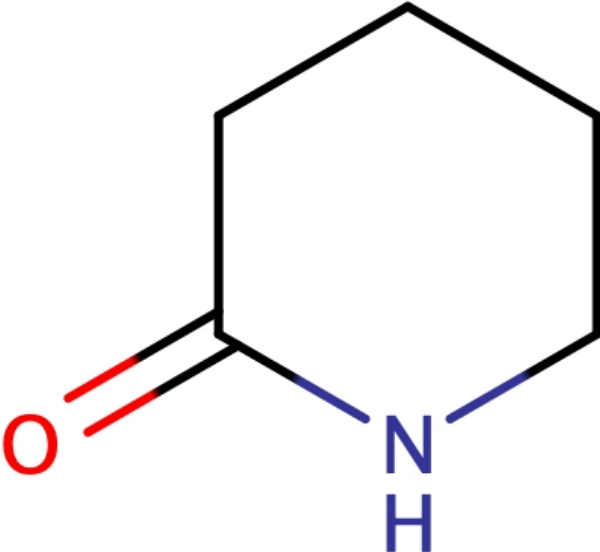
523. cyclo-(S-Pro-R-Leu)

화학 구조		PubMed ID	
		28875639	
TM-MC 성분 ID	38717		
TM-MC 성분 동의어	N/A		
PubChem ID	927565		
InChI Key	SZJNCZMRZAUNQT-BDAKNGLRSA-N		
SMILES	CC(C)C[C@H]1NC(=O)[C@@H]2CCCN2C1=O		
Molecular Formula	C ₁₁ H ₁₈ N ₂ O ₂		
Molecular Weight	210.277	Exact Molecular Weight	210.136827828
LogP	0.454	Topological Polar Surface Area	49.41 Å ²
Atom Count	33	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.72	Oral Bioavailability	Y

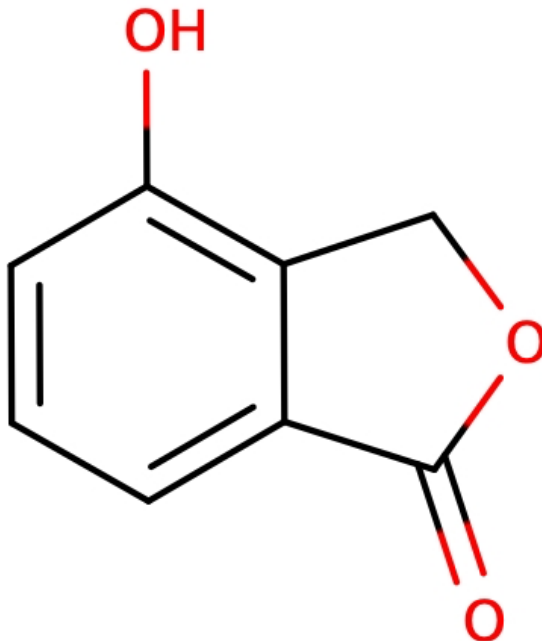
524. indole-3-carboxaldehyde

화학 구조		PubMed ID	
		28875639	
TM-MC 성분 ID	10256		
TM-MC 성분 동의어	indole-3-aldehyde; 3-formylindole; 1H-indole-3-aldehyde; 1H-indole-3-carbaldehyde		
PubChem ID	10256		
InChI Key	OLNJUISKUQQNIM-UHFFFAOYSA-N		
SMILES	<chem>O=Cc1c[nH]c2ccccc12</chem>		
Molecular Formula	C ₉ H ₇ NO		
Molecular Weight	145.161	Exact Molecular Weight	145.052763849
LogP	1.785	Topological Polar Surface Area	32.86 Å ²
Atom Count	18	Structural Alert Count	1
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	2
Drug Likeness	0.61	Oral Bioavailability	Y

525. valerolactam

화학 구조		PubMed ID	
		28875639	
TM-MC 성분 ID	10257		
TM-MC 성분 동의어	N/A		
PubChem ID	12665		
InChI Key	XUWHAWMETYGRKB-UHFFFAOYSA-N		
SMILES	O=C1CCCCN1		
Molecular Formula	C ₅ H ₉ NO		
Molecular Weight	99.133	Exact Molecular Weight	99.068413914
LogP	-0.135	Topological Polar Surface Area	29.1 Å ²
Atom Count	16	Structural Alert Count	0
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.45	Oral Bioavailability	Y

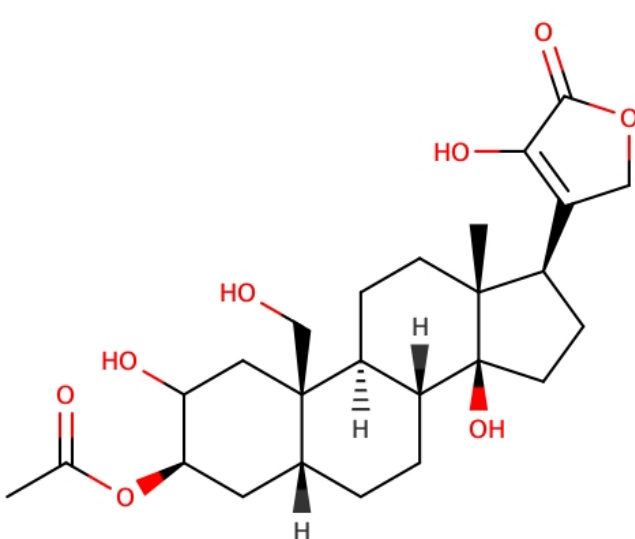
526. 4-hydroxyphthalid

화학 구조		PubMed ID	
		28875639	
TM-MC 성분 ID	99434		
TM-MC 성분 동의어	N/A		
PubChem ID	12662077		
InChI Key	ZSCIMKFWMUXNBS-UHFFFAOYSA-N		
SMILES	<chem>Oc1cccc2C(=O)OCc12</chem>		
Molecular Formula	C ₈ H ₆ O ₃		
Molecular Weight	150.133	Exact Molecular Weight	150.031694053
LogP	1.224	Topological Polar Surface Area	46.53 Å ²
Atom Count	17	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	0	Aromatic Ring Count	1
Drug Likeness	0.57	Oral Bioavailability	Y

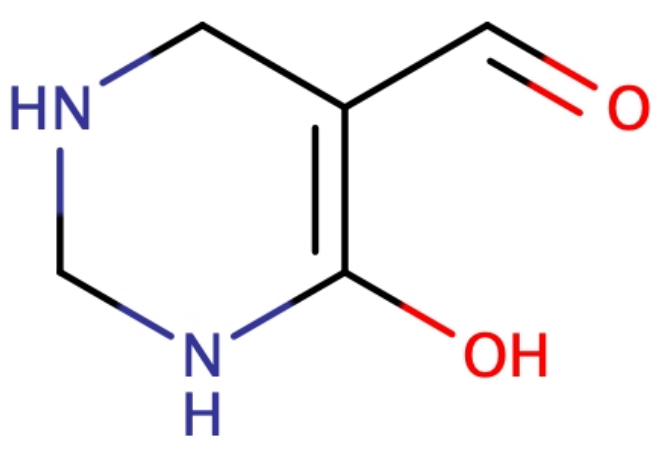
527. cysteine

화학 구조		PubMed ID	
		25780666	
TM-MC 성분 ID	362		
TM-MC 성분 동의어	Cys		
PubChem ID	5862, 6419722		
InChI Key	XUJNEKJLAYXESH-REOHCLBHSA-N		
SMILES	N[C@@H](CS)C(O)=O		
Molecular Formula	C ₃ H ₇ NO ₂ S		
Molecular Weight	121.15	Exact Molecular Weight	121.019749643
LogP	-2.792	Topological Polar Surface Area	63.32 Å ²
Atom Count	14	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.35	Oral Bioavailability	Y

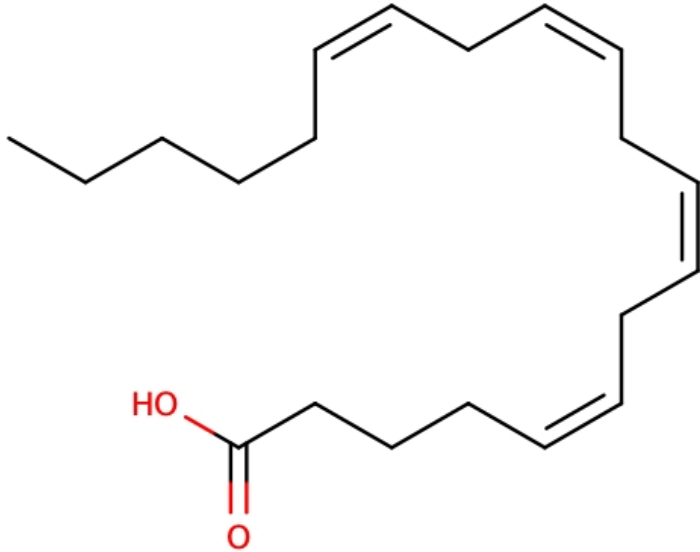
528. 3 β -acetoxy,2,14,22-trihydroxy,19-hydroxymethyl,9 α ,5 β ,14 β -card-20(22)enolide

화학 구조		PubMed ID	
		24456483	
TM-MC 성분 ID	358		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	HXJMBMYSFCHTLQ-BJGGBMFZSA-N		
SMILES	CC(=O)O[C@@H]1C[C@H]2CC[C@@H]3[C@H](CC[C@]4(C)[C@H](CC[C@]34O)C3=C(O)C(=O)OC3)[C@@]2(CO)CC1O		
Molecular Formula	C ₂₅ H ₃₆ O ₈		
Molecular Weight	464.555	Exact Molecular Weight	464.241018119
LogP	0.634	Topological Polar Surface Area	133.52 Å ²
Atom Count	69	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.45	Oral Bioavailability	Y

529. 1,2,3,4-tetrahydro-6-hydroxy-1-5-pyrimidinecarbox-aldehyde

화학 구조		PubMed ID	
		24456483	
TM-MC 성분 ID	359		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	CQROFWZEURPZRP-UHFFFAOYSA-N		
SMILES	<chem>OC1=C(CNCN1)C=O</chem>		
Molecular Formula	C ₅ H ₈ N ₂ O ₂		
Molecular Weight	128.131	Exact Molecular Weight	128.058577506
LogP	-0.764	Topological Polar Surface Area	61.36 Å ²
Atom Count	17	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.41	Oral Bioavailability	Y

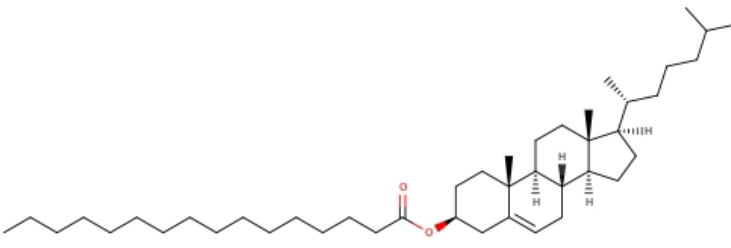
530. arachidonic acid

화학 구조		PubMed ID	
		12575114, 31394825	
TM-MC 성분 ID	365		
TM-MC 성분 동의어	6,9,12,15-arachidonic acid		
PubChem ID	444899		
InChI Key	YZXBAPSDXZZRGB-DOFZRALJSA-N		
SMILES	<chem>CCCCC=C/C=C/C=C/C=C/C(=O)O</chem>		
Molecular Formula	C ₂₀ H ₃₂ O ₂		
Molecular Weight	304.474	Exact Molecular Weight	304.24023027
LogP	6.587	Topological Polar Surface Area	37.3 Å ²
Atom Count	54	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	14	Aromatic Ring Count	0
Drug Likeness	0.29	Oral Bioavailability	N

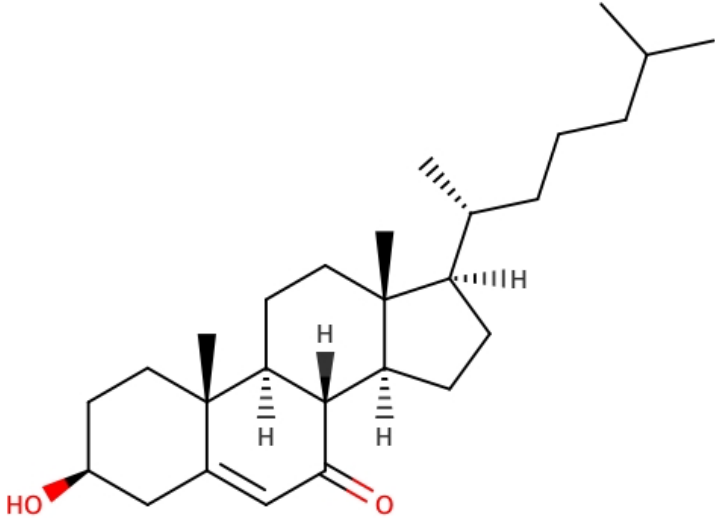
531. eicosatrienoic acid

화학 구조		PubMed ID	
		12575114	
TM-MC 성분 ID	366		
TM-MC 성분 동의어	N/A		
PubChem ID	5312529		
InChI Key	AHANXAKGNAKFSK-PDBXOOCHSA-N		
SMILES	<chem>CC=CC=CC=CCCCCCCC(O)=O</chem>		
Molecular Formula	C ₂₀ H ₃₄ O ₂		
Molecular Weight	306.49	Exact Molecular Weight	306.255880335
LogP	6.949	Topological Polar Surface Area	37.3 Å ²
Atom Count	56	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	15	Aromatic Ring Count	0
Drug Likeness	0.26	Oral Bioavailability	N

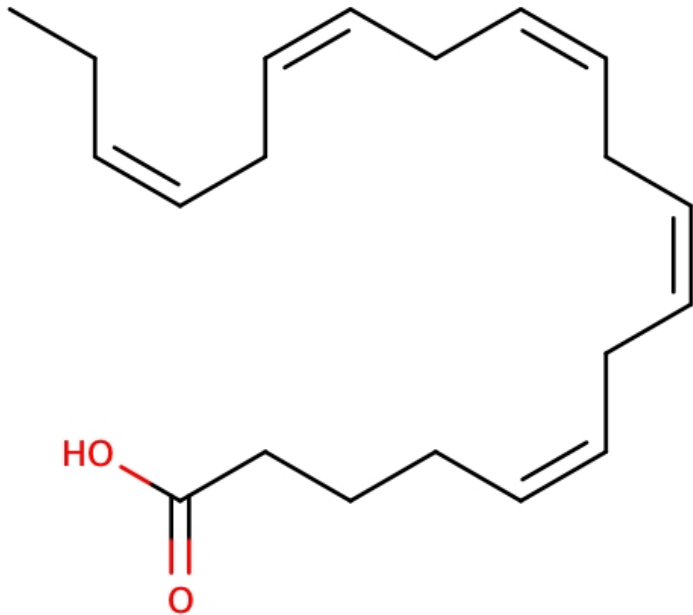
532. cholesteryl palmitate

화학 구조		PubMed ID	
		16161425	
TM-MC 성분 ID	367		
TM-MC 성분 동의어	N/A		
PubChem ID	246520		
InChI Key	BBJQPKLGPMQWBU-JADYGXMSA-N		
SMILES	CCCCCCCCCCCCCCCC(=O)O[C@H]1CC[C@]2(C)[C@H]3CC[C@]4(C)[C@H](C)[C@H]4[C@@H]3CC=C2C1)[C@H](C)CCCC(C)C		
Molecular Formula	C ₄₃ H ₇₆ O ₂		
Molecular Weight	625.079	Exact Molecular Weight	624.584531687
LogP	14.034	Topological Polar Surface Area	26.3 Å ²
Atom Count	121	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	21	Aromatic Ring Count	0
Drug Likeness	0.07	Oral Bioavailability	N

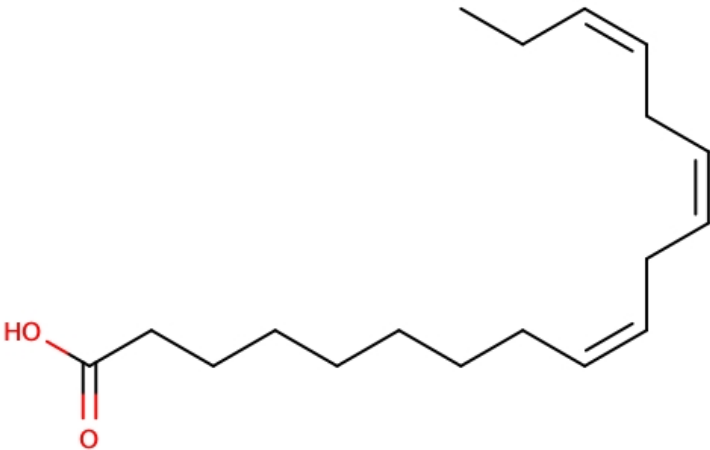
533. 3 β -hydroxy-cholest-5-en-7-one

화학 구조		PubMed ID	
		20835952	
TM-MC 성분 ID	369		
TM-MC 성분 동의어	N/A		
PubChem ID	91474		
InChI Key	YIKKMWSQVKJ COP-ABXCMAEBSA-N		
SMILES	CC(C)CCC[C@@H](C)[C@H]1CC[C@H]2[C@H]3[C@H](CC[C@]12C)[C@@]1(C)CC[C@H](O)CC1=CC3=O		
Molecular Formula	C ₂₇ H ₄₄ O ₂		
Molecular Weight	400.647	Exact Molecular Weight	400.334130657
LogP	6.549	Topological Polar Surface Area	37.3 Å ²
Atom Count	73	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.57	Oral Bioavailability	Y

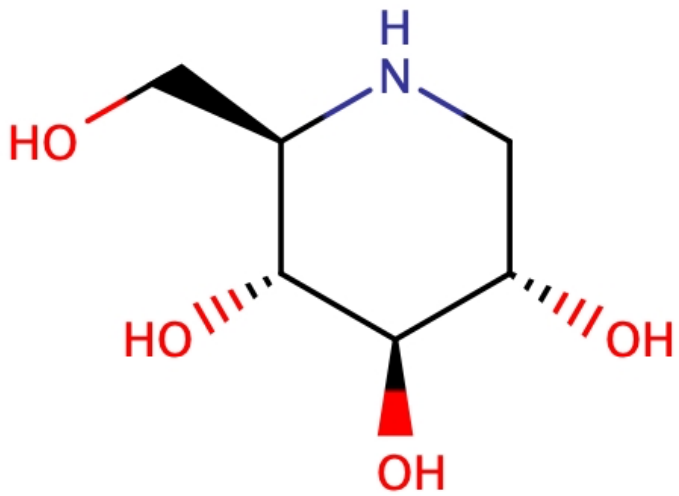
534. eicosapentaenoic acid

화학 구조		PubMed ID	
		31394825	
TM-MC 성분 ID	98015		
TM-MC 성분 동의어	timnodonic acid; cis-5,8,11,14,17-eicosapentanoic acid; cis-5,8,11,14,17-eicosapentaenoic acid		
PubChem ID	446284		
InChI Key	JAZBEHYOTPTENJ-JLNKQSITSA-N		
SMILES	CCWC=C/CWC=C/CWC=C/CWC=C/CWC=C/CCCC(O)=O		
Molecular Formula	C ₂₀ H ₃₀ O ₂		
Molecular Weight	302.458	Exact Molecular Weight	302.224580206
LogP	6.225	Topological Polar Surface Area	37.3 Å ²
Atom Count	52	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	13	Aromatic Ring Count	0
Drug Likeness	0.32	Oral Bioavailability	N

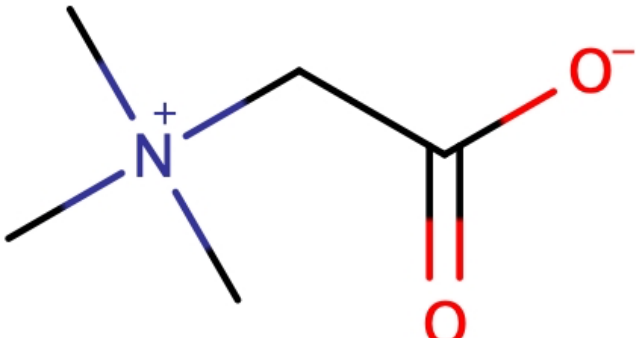
535. linolenic acid

화학 구조		PubMed ID	
		29732747, 31394825	
TM-MC 성분 ID	280934		
TM-MC 성분 동의어	α-linolenic acid; 9,12,15-octadecatrienoic acid; linolenate; (Z,Z,Z)-9,12,15-octadecatrienoic acid; cis-9,12,15-octadecatrienoic acid; (Z,Z,Z)-9,12-octadecatrienoic acid; 9,12,15-octadecatrienoic acid, (Z,Z,Z)-		
PubChem ID	5280934		
InChI Key	DTOSIQBPPRVQHS-PDBXOOCHSA-N		
SMILES	CCWC=C/CWC=C/CWC=C/CCCCCCCC(O)=O		
Molecular Formula	C ₁₈ H ₃₀ O ₂		
Molecular Weight	278.436	Exact Molecular Weight	278.224580206
LogP	6.06	Topological Polar Surface Area	37.3 Å ²
Atom Count	50	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	13	Aromatic Ring Count	0
Drug Likeness	0.33	Oral Bioavailability	N

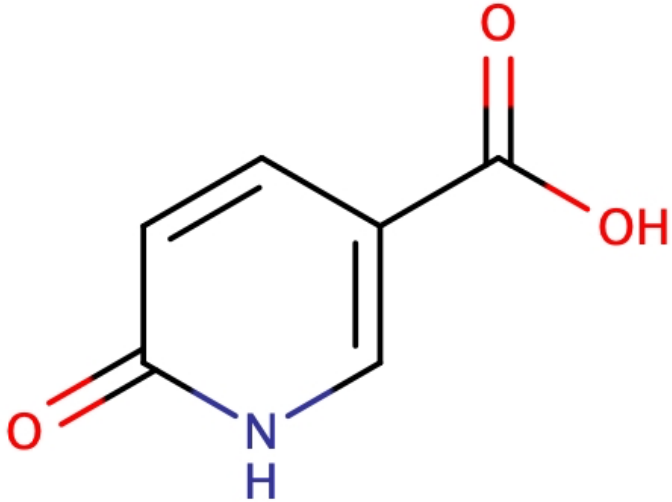
536. 1-deoxynojirimycin

화학 구조		PubMed ID	
		18323202, 29880742	
TM-MC 성분 ID	390		
TM-MC 성분 동의어	DNJ		
PubChem ID	29435		
InChI Key	LXBIFEVIBLOUGU-JGWLITMVSA-N		
SMILES	OC[C@H]1NC[C@H](O)[C@@H](O)[C@@H]1O		
Molecular Formula	C ₆ H ₁₃ NO ₄		
Molecular Weight	163.173	Exact Molecular Weight	163.084457903
LogP	-2.886	Topological Polar Surface Area	92.95 Å ²
Atom Count	24	Structural Alert Count	0
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	5
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.29	Oral Bioavailability	Y

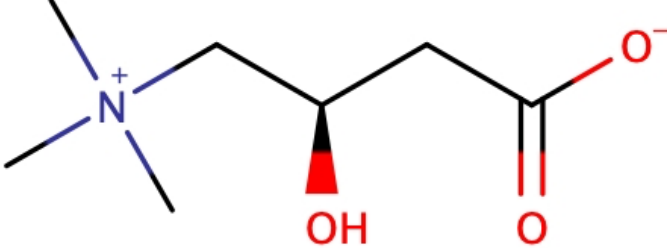
537. betaine

화학 구조		PubMed ID	
		19149256, 31640173	
TM-MC 성분 ID	393		
TM-MC 성분 동의어	glycine betaine		
PubChem ID	247		
InChI Key	KWIUHFFTVRNATP-UHFFFAOYSA-N		
SMILES	C[N+](C)(C)CC([O-])=O		
Molecular Formula	C ₅ H ₁₁ NO ₂		
Molecular Weight	117.148	Exact Molecular Weight	117.078978598
LogP	-4.494	Topological Polar Surface Area	40.13 Å ²
Atom Count	19	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	0
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.34	Oral Bioavailability	Y

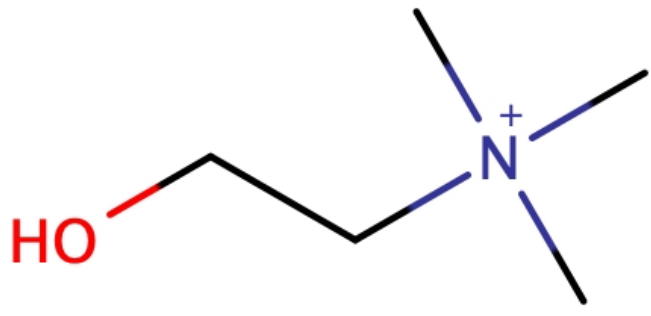
538. 6-hydroxynicotinic acid

화학 구조		PubMed ID	
		31640173	
TM-MC 성분 ID	300580		
TM-MC 성분 동의어	N/A		
PubChem ID	72924		
InChI Key	BLHCMGRVFXRYRN-UHFFFAOYSA-N		
SMILES	<chem>OC(=O)c1ccc(=O)[nH]c1</chem>		
Molecular Formula	C ₆ H ₅ NO ₃		
Molecular Weight	139.11	Exact Molecular Weight	139.026943025
LogP	-0.548	Topological Polar Surface Area	66.4 Å ²
Atom Count	15	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.55	Oral Bioavailability	Y

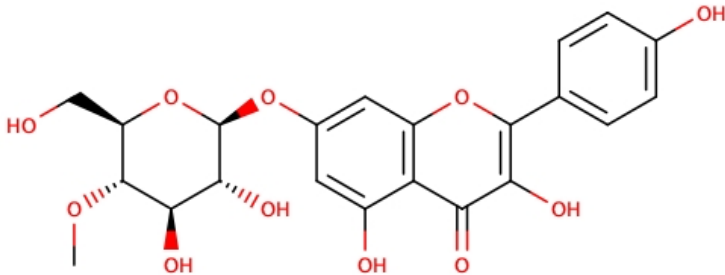
539. carnitine

화학 구조		PubMed ID	
		31640173	
TM-MC 성분 ID	900288		
TM-MC 성분 동의어	L-carnitine		
PubChem ID	10917		
InChI Key	PHIQHXFUZVPYII-ZCFIWIBFSA-N		
SMILES	C[N+](C)(C)C[C@H](O)CC([O-])=O		
Molecular Formula	C ₇ H ₁₅ NO ₃		
Molecular Weight	161.201	Exact Molecular Weight	161.105193347
LogP	-4.888	Topological Polar Surface Area	60.36 Å ²
Atom Count	26	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.42	Oral Bioavailability	Y

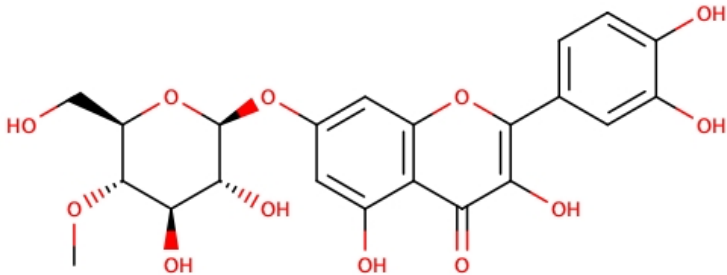
540. choline

화학 구조		PubMed ID	
		31640173	
TM-MC 성분 ID	900305		
TM-MC 성분 동의어	N/A		
PubChem ID	305		
InChI Key	OEYIOHPDSNJKLS-UHFFFAOYSA-N		
SMILES	C[N+](C)(C)CCO		
Molecular Formula	C ₅ H ₁₄ NO		
Molecular Weight	104.172	Exact Molecular Weight	104.106990495
LogP	-4.662	Topological Polar Surface Area	20.23 Å ²
Atom Count	21	Structural Alert Count	1
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.35	Oral Bioavailability	Y

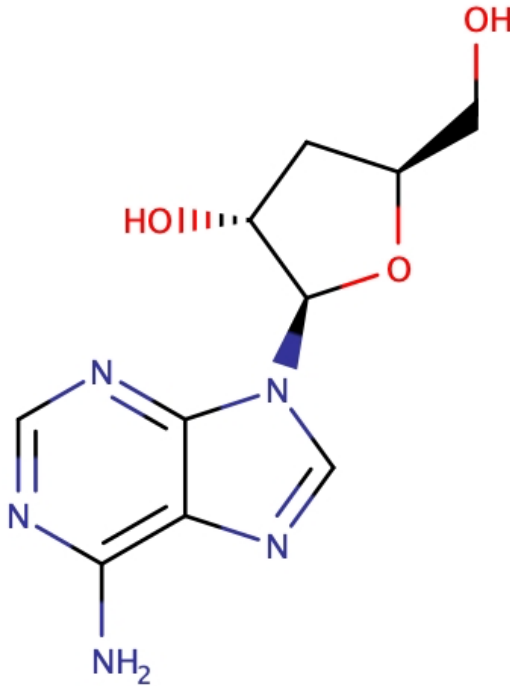
541. kaempferol-7-O-β-D-4-O-methylglucoside

화학 구조		PubMed ID	
		31640173	
TM-MC 성분 ID	95135		
TM-MC 성분 동의어	N/A		
PubChem ID	25111340		
InChI Key	ISZVIPCAULDCLG-SPJAQXOISA-N		
SMILES	CO[C@@H]1[C@@H](CO)O[C@@H](Oc2cc(O)c3c(c2)oc(c(O)c3=O)-c2ccc(O)cc2)[C@H](O)[C@H]1O		
Molecular Formula	C ₂₂ H ₂₂ O ₁₁		
Molecular Weight	462.407	Exact Molecular Weight	462.116211528
LogP	0.835	Topological Polar Surface Area	175.37 Å ²
Atom Count	55	Structural Alert Count	0
Hydrogen Bond Acceptor Count	11	Hydrogen Bond Donor Count	6
Rotatable Bond Count	5	Aromatic Ring Count	3
Drug Likeness	0.32	Oral Bioavailability	N

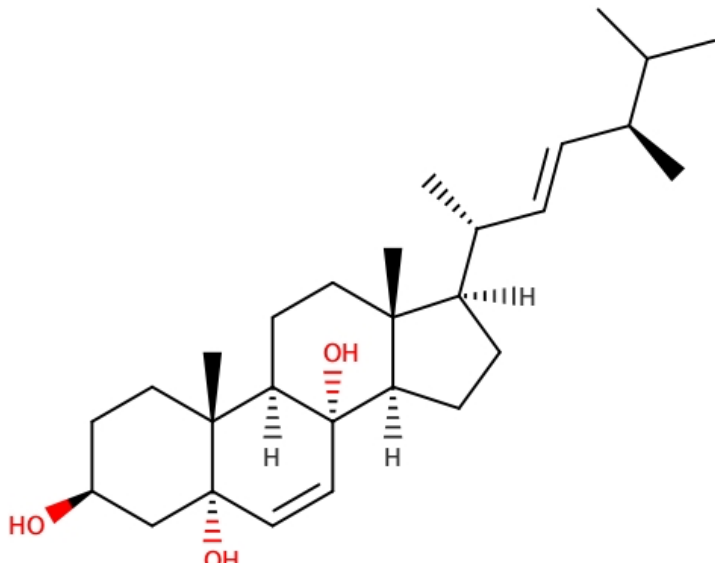
542. quercetin-7-O-β-D-4-O-methylglucoside

화학 구조		PubMed ID	
		31640173	
TM-MC 성분 ID	95136		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	YFIAQFOPVRDZEZ-SPJAQXOISA-N		
SMILES	<chem>CO[C@H]1[C@@H](CO)O[C@H](Oc2cc(O)c3c(c2)oc(c(O)c3=O)-c2ccc(O)c(O)c2)[C@H](O)[C@H]1O</chem>		
Molecular Formula	C ₂₂ H ₂₂ O ₁₂		
Molecular Weight	478.406	Exact Molecular Weight	478.111126148
LogP	0.531	Topological Polar Surface Area	195.6 Å ²
Atom Count	56	Structural Alert Count	1
Hydrogen Bond Acceptor Count	12	Hydrogen Bond Donor Count	7
Rotatable Bond Count	5	Aromatic Ring Count	3
Drug Likeness	0.25	Oral Bioavailability	N

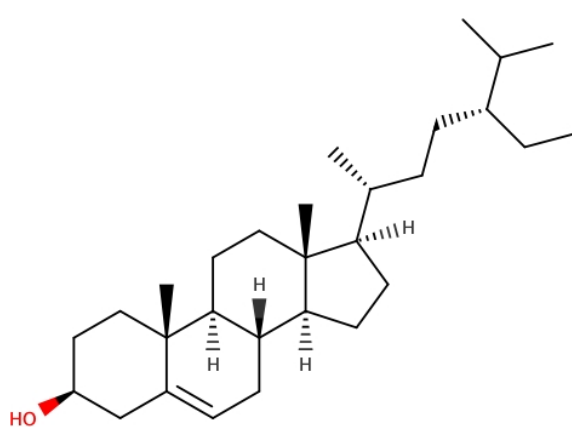
543. cordycepin

화학 구조		PubMed ID	
		31800596	
TM-MC 성분 ID	6303		
TM-MC 성분 동의어	3'-deoxyadenosine		
PubChem ID	6303		
InChI Key	OFEZSBMBBKLBJ-BAJZRUMYSA-N		
SMILES	<chem>Nc1ncnc2n(cnc12)[C@@H]1O[C@H](CO)C[C@H]1O</chem>		
Molecular Formula	C ₁₀ H ₁₃ N ₅ O ₃		
Molecular Weight	251.246	Exact Molecular Weight	251.101839299
LogP	-1.401	Topological Polar Surface Area	119.31 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	2
Drug Likeness	0.60	Oral Bioavailability	Y

544. ergost-6,22-dien-3 β ,5 α ,8 α -triol

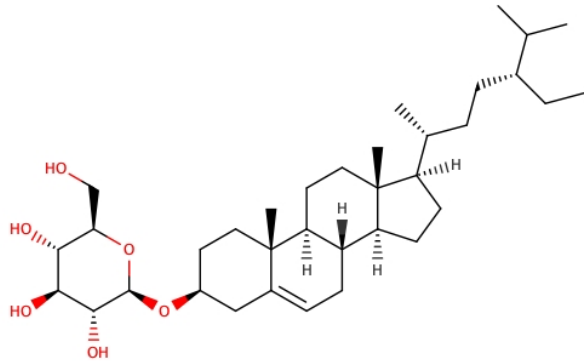
화학 구조		PubMed ID	
		15709383	
TM-MC 성분 ID	374		
TM-MC 성분 동의어	N/A		
PubChem ID	15251535		
InChI Key	UPJVQRZPXLZUET-KGHQQZOUSI-N		
SMILES	CC(C)[C@@H](C)WC=CW[C@@H](C)[C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@]2(O)C=C[C@@]2(O)C[C@H](O)CC[C@]12C		
Molecular Formula	C ₂₈ H ₄₆ O ₃		
Molecular Weight	430.673	Exact Molecular Weight	430.344695341
LogP	5.002	Topological Polar Surface Area	60.69 Å ²
Atom Count	77	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	3
Rotatable Bond Count	4	Aromatic Ring Count	0
Drug Likeness	0.55	Oral Bioavailability	Y

545. β -sitosterol

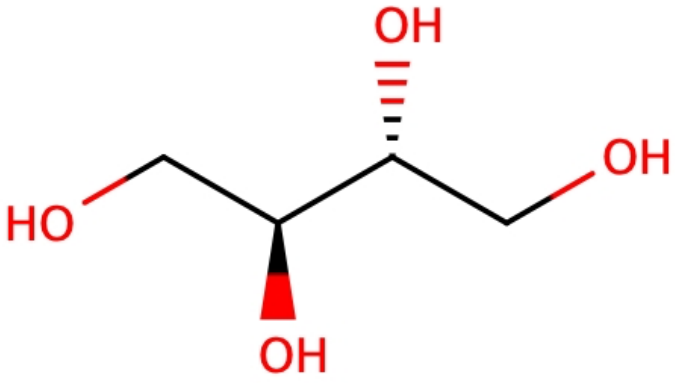
화학 구조	PubMed ID
	15709383

TM-MC 성분 ID	375		
TM-MC 성분 동의어	sitosterol; clionasterol; (-)- β -sitosterol; stigmast-5-en-3-ol; stigmast-5-en-3 β -ol; 22,23-dihydrostigmasterol; 17-(5-ethyl-6-methylheptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol; (3S,8S,9S,10R,13R,14S,17R)-17-[(2R,5R)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol; (3S,8S,9S,10R,13R,14S,17R)17[(2R,5R)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl 2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol		
PubChem ID	222284		
InChI Key	KZJWDPNRJALLNS-VJSFXXLFSAN		
SMILES	<chem>CC[C@H](CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]12C)C(C)C</chem>		
Molecular Formula	C ₂₉ H ₅₀ O		
Molecular Weight	414.718	Exact Molecular Weight	414.38616623
LogP	7.844	Topological Polar Surface Area	20.23 Å ²
Atom Count	80	Structural Alert Count	1
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.44	Oral Bioavailability	Y

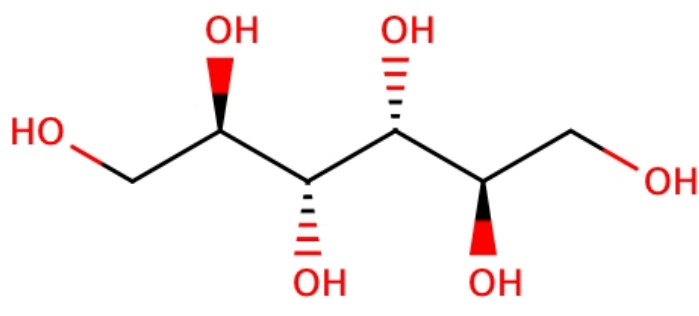
546. daucosterol

화학 구조		PubMed ID	
		15709383	
TM-MC 성분 ID	376		
TM-MC 성분 동의어	β-sitosterol glucopyranoside; β-daucosterol; daucosterin; β-sitosteryl-D-glucoside; sitogluside; eleutheroside A; β-sitosterol glucoside; β-sitosterol-3-O-glucoside; β-sitosterin-3-O-glucoside; β-sitosterol-3-O-β-D-glucoside; sitosterol 3-O-β-D-glucopyranoside; β-sitosterol-3-O-β-glucopyranoside; β-sitosterol-3-O-β-D-glucopyranoside		
PubChem ID	5742590		
InChI Key	NPJICTMALKLTFW-OFUAXYCQSA-N		
SMILES	<chem>CC[C@H](CC[C@@H](C)[C@H]1CC[C@H]2[C@@H]3CC=C4C[C@H](CC[C@]4(C)[C@H]3CC[C@]12C)O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)C(C)C</chem>		
Molecular Formula	C ₃₅ H ₆₀ O ₆		
Molecular Weight	576.859	Exact Molecular Weight	576.438989652
LogP	6.074	Topological Polar Surface Area	99.38 Å ²
Atom Count	101	Structural Alert Count	1
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	4
Rotatable Bond Count	9	Aromatic Ring Count	0
Drug Likeness	0.25	Oral Bioavailability	Y

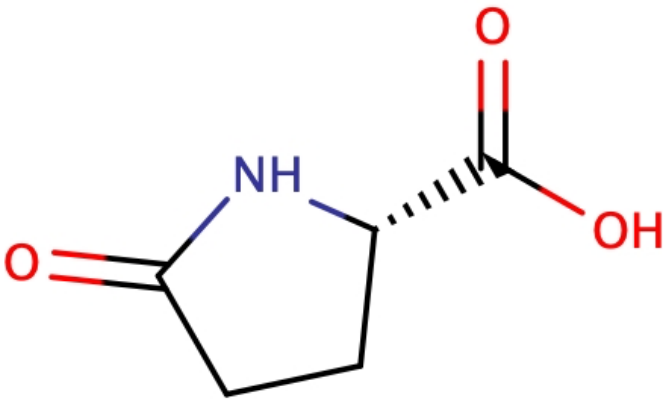
547. meso-erythritol

화학 구조		PubMed ID
		15709383
TM-MC 성분 ID	377	
TM-MC 성분 동의어	erythritol; 1,2,3,4-butanetetrol	
PubChem ID	222285	
InChI Key	UNXHWFMMPAWVPI-ZXZARUISSA-N	
SMILES	<chem>OC[C@H](O)[C@H](O)CO</chem>	
Molecular Formula	C ₄ H ₁₀ O ₄	
Molecular Weight	122.12	Exact Molecular Weight 122.057908802
LogP	-2.469	Topological Polar Surface Area 80.92 Å ²
Atom Count	18	Structural Alert Count 0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count 4
Rotatable Bond Count	3	Aromatic Ring Count 0
Drug Likeness	0.33	Oral Bioavailability Y

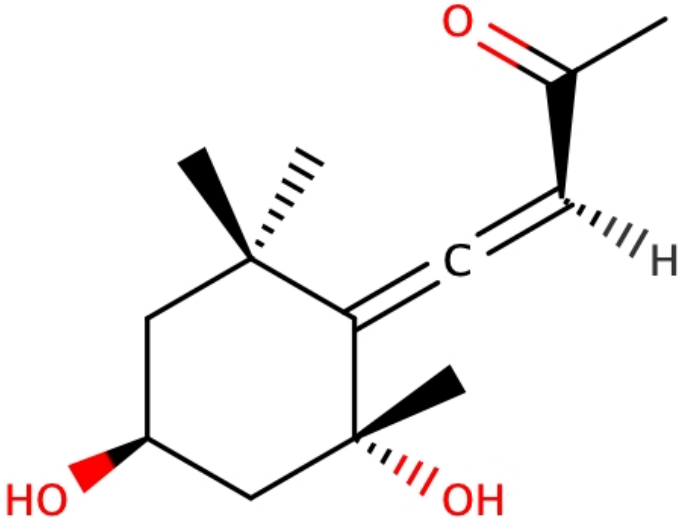
548. mannitol

화학 구조		PubMed ID	
		15709383, 31800596	
TM-MC 성분 ID	378		
TM-MC 성분 동의어	D-mannitol; D-(-)-mannitol		
PubChem ID	6251		
InChI Key	FBPFZTCFMRRESA-KVTDHHQDSA-N		
SMILES	OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO		
Molecular Formula	C ₆ H ₁₄ O ₆		
Molecular Weight	182.172	Exact Molecular Weight	182.079038171
LogP	-3.73	Topological Polar Surface Area	121.38 Å ²
Atom Count	26	Structural Alert Count	0
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	6
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.26	Oral Bioavailability	Y

549. L-pyroglutamic acid

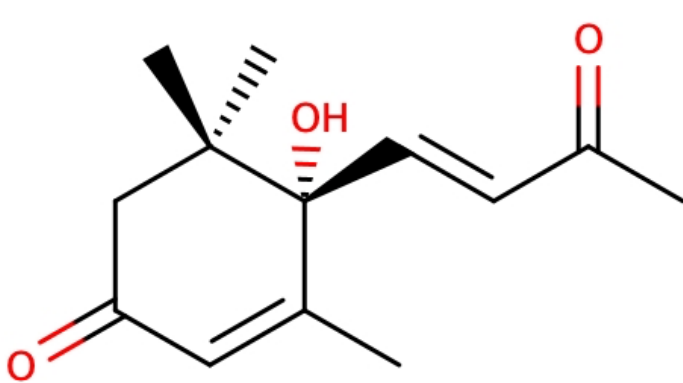
화학 구조		PubMed ID	
		31640173	
TM-MC 성분 ID	7405		
TM-MC 성분 동의어	pyroglutamic acid; 2-pyrrolidone-5-carboxylic acid		
PubChem ID	7405		
InChI Key	ODHCTXKNWHXJC-VKHMYYEASA-N		
SMILES	<chem>OC(=O)[C@@H]1CCC(=O)N1</chem>		
Molecular Formula	C ₅ H ₇ NO ₃		
Molecular Weight	129.115	Exact Molecular Weight	129.042593089
LogP	-0.89	Topological Polar Surface Area	66.4 Å ²
Atom Count	16	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.48	Oral Bioavailability	Y

550. 3S,5R-dihydroxy-6R,7-megstigmadien-9-one

화학 구조	PubMed ID
	19149256, 21544718

TM-MC 성분 ID	379		
TM-MC 성분 동의어	(3S,5R,8R)-3,5-dihydroxymegastigma-6,7-dien-9-one		
PubChem ID	N/A		
InChI Key	QMXLZUOHZGYGDY-ANSXDHORSA-N		
SMILES	CC(=O)C=[C@]=C1C(C)(C)C[C@H](O)C[C@@]1(C)O		
Molecular Formula	C ₁₃ H ₂₀ O ₃		
Molecular Weight	224.3	Exact Molecular Weight	224.141244504
LogP	0.777	Topological Polar Surface Area	57.53 Å ²
Atom Count	36	Structural Alert Count	2
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.51	Oral Bioavailability	Y

551. (+)-dehydrovomifoliol

화학 구조		PubMed ID	
		21544718	
TM-MC 성분 ID	380		
TM-MC 성분 동의어	dihydrovomifoliol; (S)-dehydrovomifoliol; S-(+)-dehydrovomifoliol		
PubChem ID	688492		
InChI Key	JJRYPZMXNLLZFH-URWSZGRFSA-N		
SMILES	CC(=O)WC=CW[C@@]1(O)C(C)=CC(=O)CC1(C)C		
Molecular Formula	C ₁₃ H ₁₈ O ₃		
Molecular Weight	222.284	Exact Molecular Weight	222.12559444
LogP	1.652	Topological Polar Surface Area	54.37 Å ²
Atom Count	34	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.72	Oral Bioavailability	Y

552. (6R,7E,9R)-9-hydroxy-4,7-megastigmadien-3-one

화학 구조		PubMed ID	
		21544718	
TM-MC 성분 ID	381		
TM-MC 성분 동의어	6R,9R-3-oxo- α -ionol		
PubChem ID	13857510		
InChI Key	MDCGEAGEQVMWPE-SXGMEYSMSA-N		
SMILES	<chem>C[C@@H](O)WC=CW[C@H]1C(C)=CC(=O)CC1(C)C</chem>		
Molecular Formula	C ₁₃ H ₂₀ O ₂		
Molecular Weight	208.301	Exact Molecular Weight	208.146329884
LogP	2.266	Topological Polar Surface Area	37.3 Å ²
Atom Count	35	Structural Alert Count	1
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.71	Oral Bioavailability	Y

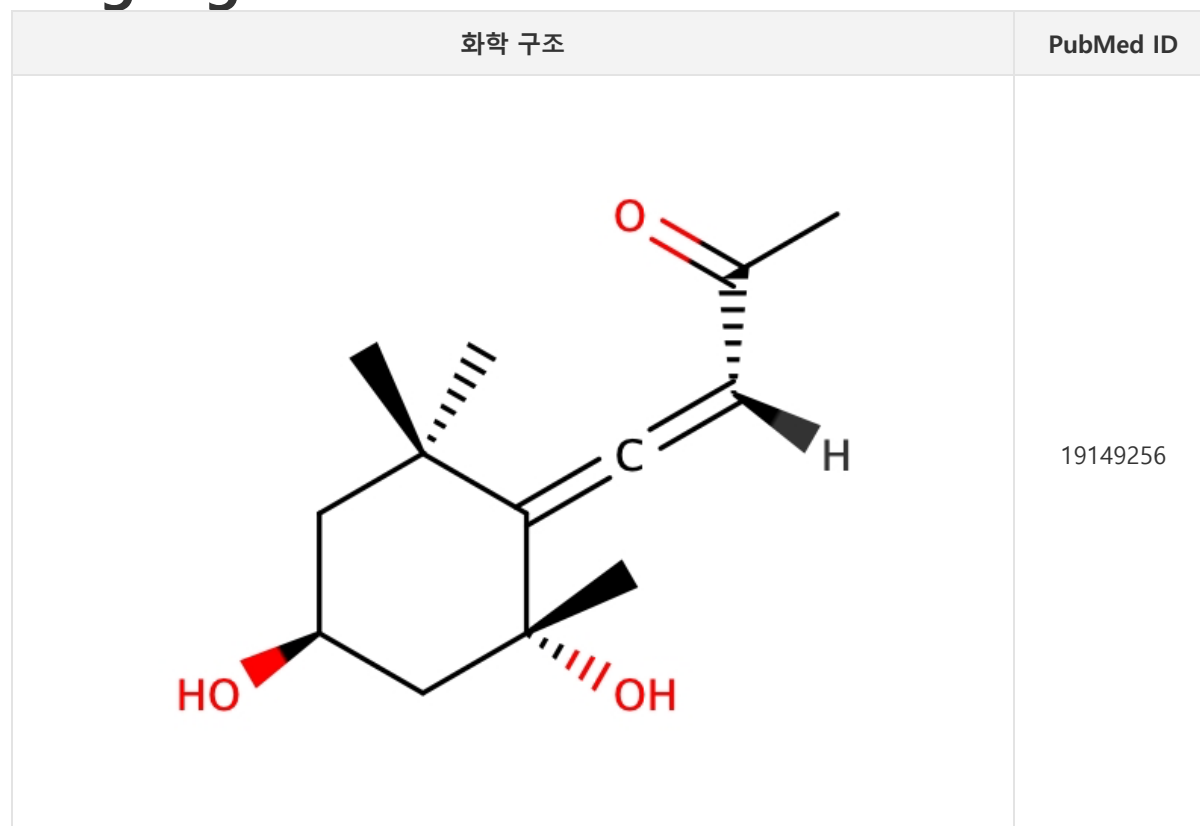
553. (3S,5R,6S,7E)-3,5,6-trihydroxy-7-megastigmen-9-one

화학 구조		PubMed ID	
		21544718	
TM-MC 성분 ID	382		
TM-MC 성분 동의어	N/A		
PubChem ID	51537163		
InChI Key	QASOACWK TAXFSE-IRIVYCKASA-N		
SMILES	CC(=O)WC=CW[C@]1(O)C(C)(C)C[C@H](O)C[C@@]1(C)O		
Molecular Formula	C ₁₃ H ₂₂ O ₄		
Molecular Weight	242.315	Exact Molecular Weight	242.151809188
LogP	0.181	Topological Polar Surface Area	77.76 Å ²
Atom Count	39	Structural Alert Count	1
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.60	Oral Bioavailability	Y

554. (6R,9R)-9-hydroxy-4-megastigmen-3-one

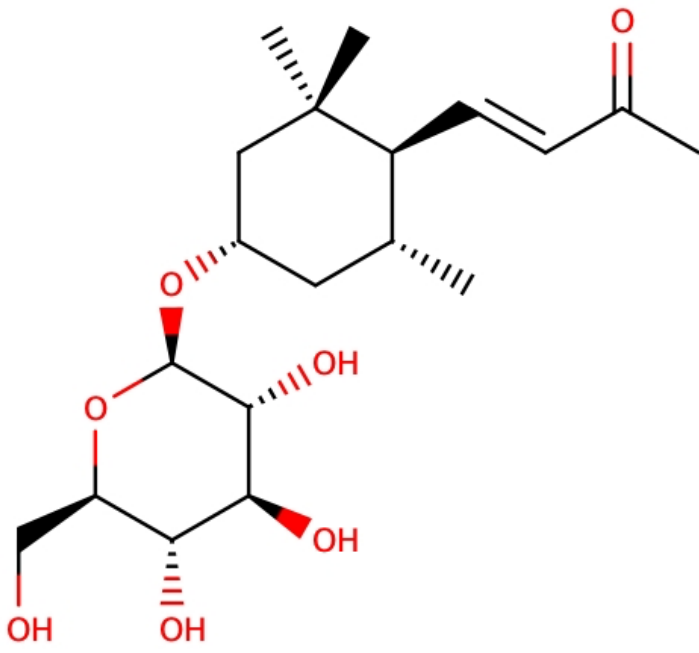
화학 구조		PubMed ID	
		21544718	
TM-MC 성분 ID	383		
TM-MC 성분 동의어	N/A		
PubChem ID	14135400		
InChI Key	UEEJDIUOCUCVHN-PWSUYJOCSA-N		
SMILES	C[C@@H](O)CC[C@H]1C(C)=CC(=O)CC1(C)C		
Molecular Formula	C ₁₃ H ₂₂ O ₂		
Molecular Weight	210.317	Exact Molecular Weight	210.161979948
LogP	2.472	Topological Polar Surface Area	37.3 Å ²
Atom Count	37	Structural Alert Count	0
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	3	Aromatic Ring Count	0
Drug Likeness	0.78	Oral Bioavailability	Y

555. 3S,5R-dihydroxy-6S,7-megstigmadien-9-one

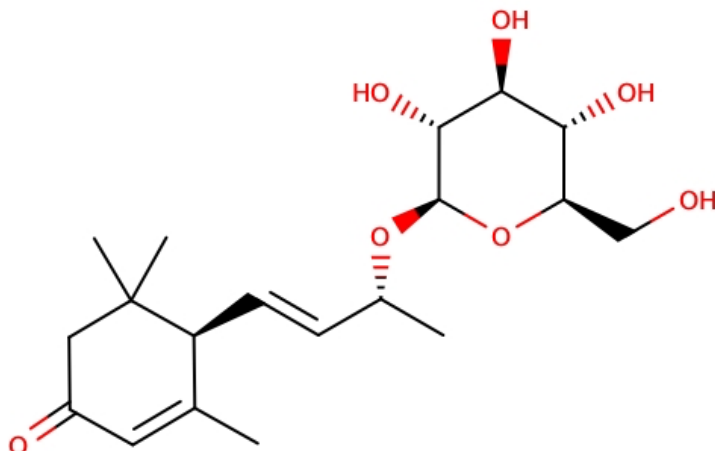


TM-MC 성분 ID	3790		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	QMXLZUOHZGYGDY-JPRWIHHQSA-N		
SMILES	CC(=O)C=[C@@]=C1C(C)(C)C[C@H](O)C[C@@]1(C)O		
Molecular Formula	C ₁₃ H ₂₀ O ₃		
Molecular Weight	224.3	Exact Molecular Weight	224.141244504
LogP	0.777	Topological Polar Surface Area	57.53 Å ²
Atom Count	36	Structural Alert Count	2
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.51	Oral Bioavailability	Y

556. alangionoside L

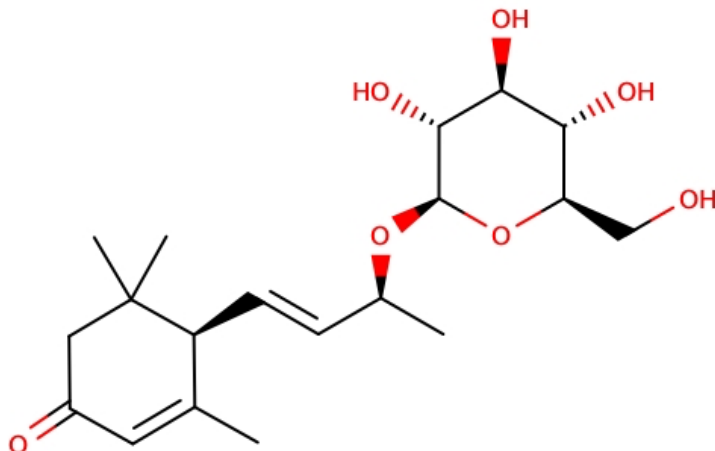
화학 구조		PubMed ID	
		19149256	
TM-MC 성분 ID	384		
TM-MC 성분 동의어	N/A		
PubChem ID	10339245		
InChI Key	NSDJVCFZKFOLGV-ZOSSRMHFSA-N		
SMILES	<chem>C[C@@H]1C[C@@H](CC(C)(C)[C@H]1#C=C#C(C)=O)O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O</chem>		
Molecular Formula	C ₁₉ H ₃₂ O ₇		
Molecular Weight	372.458	Exact Molecular Weight	372.21480337
LogP	0.567	Topological Polar Surface Area	116.45 Å ²
Atom Count	58	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.52	Oral Bioavailability	Y

557. (6R,9R)-3-oxo- α -ionol- β -D-glucopyranoside

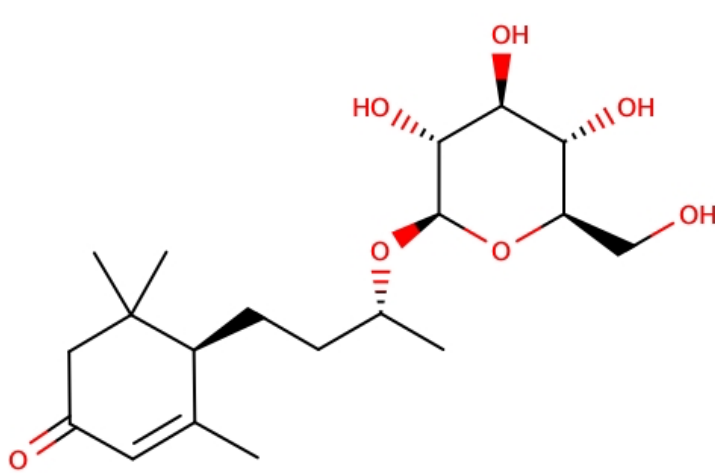
화학 구조	PubMed ID
	19149256

TM-MC 성분 ID	385		
TM-MC 성분 동의어	N/A		
PubChem ID	9820702		
InChI Key	SZOPSAFLRCYJCX-ITEOXOHJSA-N		
SMILES	<chem>C[C@@H](O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)C=C[C@H]1C(C)=CC(=O)CC1(C)C</chem>		
Molecular Formula	C ₁₉ H ₃₀ O ₇		
Molecular Weight	370.442	Exact Molecular Weight	370.199153306
LogP	0.496	Topological Polar Surface Area	116.45 Å ²
Atom Count	56	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.52	Oral Bioavailability	Y

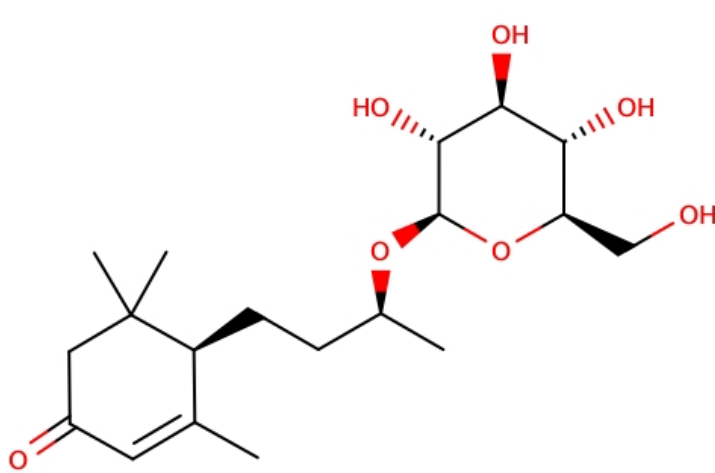
558. (6R,9S)-3-oxo- α -ionol- β -D-glucopyranoside

화학 구조		PubMed ID	
		19149256	
TM-MC 성분 ID	386		
TM-MC 성분 동의어	N/A		
PubChem ID	21630888		
InChI Key	SZOPSAFLRCYJCX-RBOSQNBPSA-N		
SMILES	<chem>C[C@H](O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)WC=CW[C@H]1C(C)=CC(=O)CC1(C)C</chem>		
Molecular Formula	C ₁₉ H ₃₀ O ₇		
Molecular Weight	370.442	Exact Molecular Weight	370.199153306
LogP	0.496	Topological Polar Surface Area	116.45 Å ²
Atom Count	56	Structural Alert Count	1
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	5	Aromatic Ring Count	0
Drug Likeness	0.52	Oral Bioavailability	Y

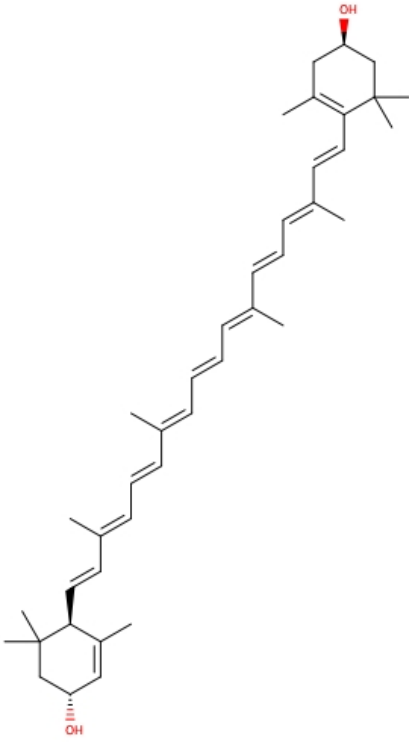
559. byzantionoside B

화학 구조		PubMed ID	
		19149256	
TM-MC 성분 ID	387		
TM-MC 성분 동의어	N/A		
PubChem ID	14135395		
InChI Key	NYLNHNDMNOPWAZ-ZLEFDVGRSA-N		
SMILES	C[C@H](CC[C@H]1C(C)=CC(=O)CC1(C)O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)[C@H](O)[C@H]1O		
Molecular Formula	C ₁₉ H ₃₂ O ₇		
Molecular Weight	372.458	Exact Molecular Weight	372.21480337
LogP	0.702	Topological Polar Surface Area	116.45 Å ²
Atom Count	58	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.54	Oral Bioavailability	Y

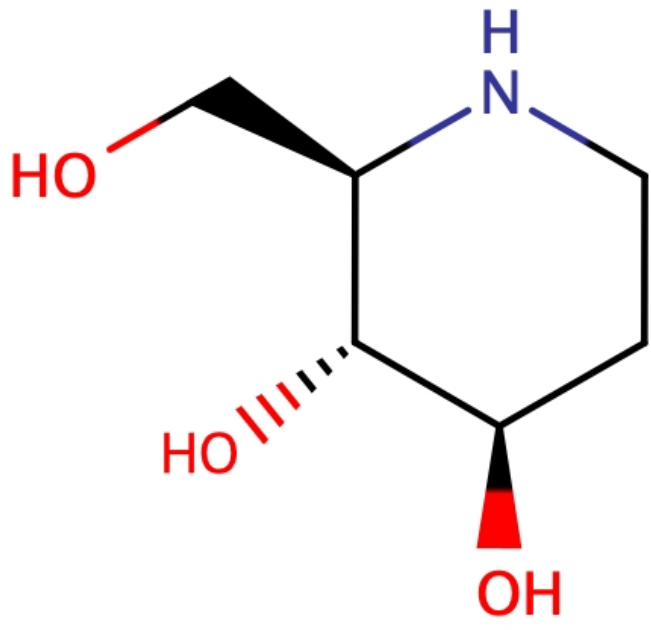
560. blumenol C glucoside

화학 구조		PubMed ID	
		19149256	
TM-MC 성분 ID	388		
TM-MC 성분 동의어	N/A		
PubChem ID	38346961		
InChI Key	NYLNHNDMNOPWAZ-CODAKJSOSA-N		
SMILES	C[C@@H](CC[C@H]1C(C)=CC(=O)CC1(C)C)O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O		
Molecular Formula	C ₁₉ H ₃₂ O ₇		
Molecular Weight	372.458	Exact Molecular Weight	372.21480337
LogP	0.702	Topological Polar Surface Area	116.45 Å ²
Atom Count	58	Structural Alert Count	0
Hydrogen Bond Acceptor Count	7	Hydrogen Bond Donor Count	4
Rotatable Bond Count	6	Aromatic Ring Count	0
Drug Likeness	0.54	Oral Bioavailability	Y

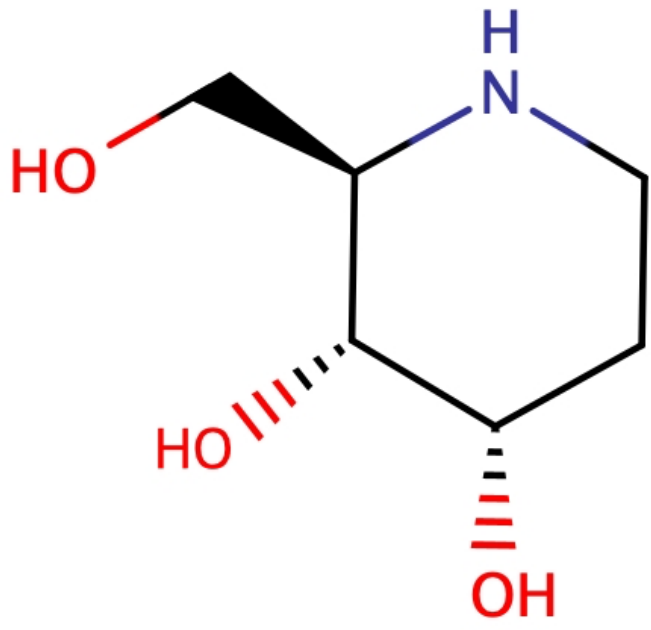
561. lutein

화학 구조		PubMed ID	
		19149256	
TM-MC 성분 ID	389		
TM-MC 성분 동의어	(all-E)-lutein		
PubChem ID	5281243		
InChI Key	KBPHJBAIARWVSC-RGZFRNHPSA-N		
SMILES	<chem>CWC(WC=CWC=C(/C)WC=CW[C@H]1C(C)=C[C@H](O)CC1(C)C)=C/C=C/C=C(WC)/C=C/C=C(WC)/C=C/C1=C(C)C[C@@H](O)CC1(C)C</chem>		
Molecular Formula	C ₄₀ H ₅₆ O ₂		
Molecular Weight	568.886	Exact Molecular Weight	568.428031043
LogP	8.55	Topological Polar Surface Area	40.46 Å ²
Atom Count	98	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	2
Rotatable Bond Count	10	Aromatic Ring Count	0
Drug Likeness	0.20	Oral Bioavailability	Y

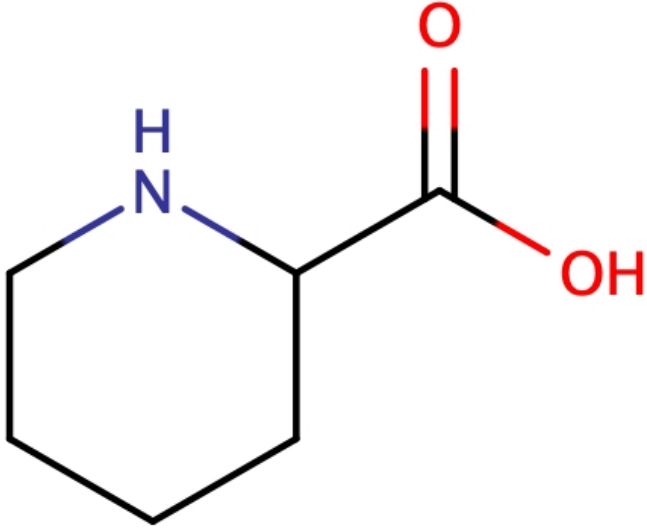
562. fagomine

화학 구조		PubMed ID	
		18323202	
TM-MC 성분 ID	391		
TM-MC 성분 동의어	D-fagomine		
PubChem ID	72259		
InChI Key	YZNNBIPIQWYLDM-HSUXUTPPSA-N		
SMILES	OC[C@H]1NCC[C@@H](O)[C@H]1O		
Molecular Formula	C ₆ H ₁₃ NO ₃		
Molecular Weight	147.174	Exact Molecular Weight	147.089543283
LogP	-2.195	Topological Polar Surface Area	72.72 Å ²
Atom Count	23	Structural Alert Count	0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	4
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.34	Oral Bioavailability	Y

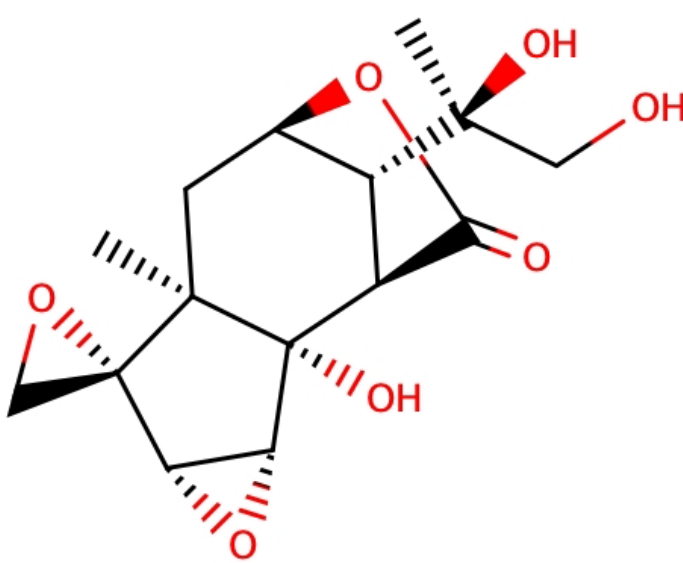
563. 3-epi-fagomine

화학 구조		PubMed ID
		18323202
TM-MC 성분 ID	392	
TM-MC 성분 동의어	N/A	
PubChem ID	10290867	
InChI Key	YZNNBIPIQWYLDM-NGJCXOISSA-N	
SMILES	OC[C@H]1NCC[C@H](O)[C@@H]1O	
Molecular Formula	C ₆ H ₁₃ NO ₃	
Molecular Weight	147.174	Exact Molecular Weight 147.089543283
LogP	-2.195	Topological Polar Surface Area 72.72 Å ²
Atom Count	23	Structural Alert Count 0
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count 4
Rotatable Bond Count	1	Aromatic Ring Count 0
Drug Likeness	0.34	Oral Bioavailability Y

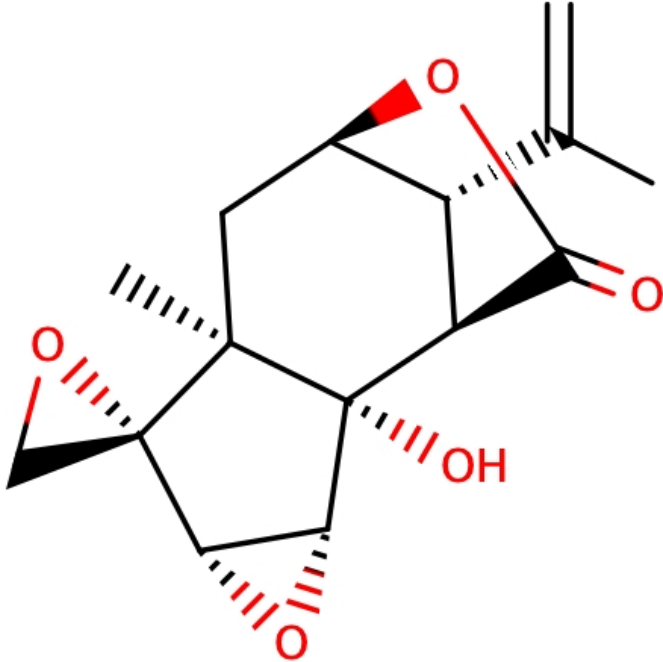
564. pipecolic acid

화학 구조		PubMed ID	
		19149256	
TM-MC 성분 ID	394		
TM-MC 성분 동의어	N/A		
PubChem ID	849, 25200477		
InChI Key	HXEACLLIILLPRG-UHFFFAOYSA-N		
SMILES	OC(=O)C1CCCCN1		
Molecular Formula	C ₆ H ₁₁ NO ₂		
Molecular Weight	129.159	Exact Molecular Weight	129.078978598
LogP	-2.124	Topological Polar Surface Area	49.33 Å ²
Atom Count	20	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.43	Oral Bioavailability	Y

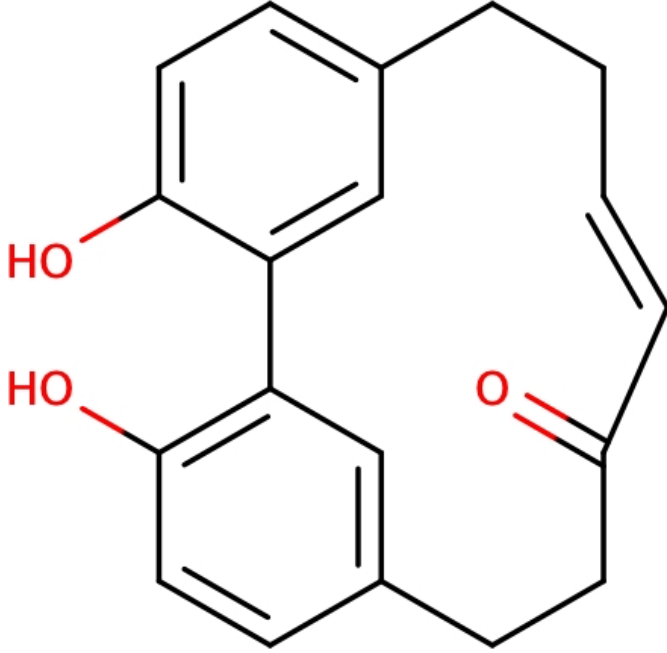
565. fengfangin A

화학 구조		PubMed ID	
		22162164	
TM-MC 성분 ID	395		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	VTGMXXCMIYRWIY-KFHVZYALSA-N		
SMILES	<chem>C[C@](O)(CO)[C@H]1[C@H]2C[C@]3(C)[C@]4(CO4)[C@H]4O[C@H]4[C@]3(O)[C@@H]1C(=O)O2</chem>		
Molecular Formula	C ₁₅ H ₂₀ O ₇		
Molecular Weight	312.318	Exact Molecular Weight	312.120902984
LogP	-1.872	Topological Polar Surface Area	112.05 Å ²
Atom Count	42	Structural Alert Count	2
Hydrogen Bond Acceptor Count	6	Hydrogen Bond Donor Count	3
Rotatable Bond Count	2	Aromatic Ring Count	0
Drug Likeness	0.41	Oral Bioavailability	Y

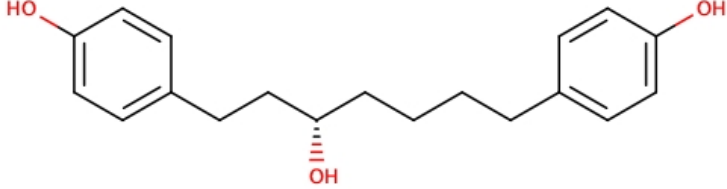
566. tutin

화학 구조		PubMed ID	
		22162164	
TM-MC 성분 ID	396		
TM-MC 성분 동의어	N/A		
PubChem ID	73060		
InChI Key	BWWDLKVKPVKBGJ-LHSZFNMKSA-N		
SMILES	CC(=C)[C@H]1[C@H]2C[C@]3(C)[C@]4(CO4)[C@H]4O[C@H]4[C@]3(O)[C@H]1C(=O)O2		
Molecular Formula	C ₁₅ H ₁₈ O ₅		
Molecular Weight	278.304	Exact Molecular Weight	278.11542368
LogP	0.257	Topological Polar Surface Area	71.59 Å ²
Atom Count	38	Structural Alert Count	3
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	0
Drug Likeness	0.42	Oral Bioavailability	Y

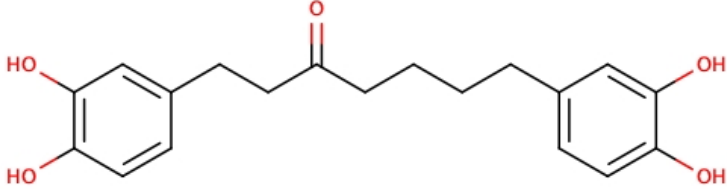
567. alnusone

화학 구조		PubMed ID	
		22162164	
TM-MC 성분 ID	397		
TM-MC 성분 동의어	N/A		
PubChem ID	12751128		
InChI Key	VWORGKSAVUQKSQ-DUXPYHPUSA-N		
SMILES	<chem>Oc1ccc2CC#C=C#C(=O)CCc3ccc(O)c(c3)-c1c2</chem>		
Molecular Formula	C ₁₉ H ₁₈ O ₃		
Molecular Weight	294.35	Exact Molecular Weight	294.12559444
LogP	4.618	Topological Polar Surface Area	57.53 Å ²
Atom Count	40	Structural Alert Count	0
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	2
Rotatable Bond Count	0	Aromatic Ring Count	2
Drug Likeness	0.75	Oral Bioavailability	Y

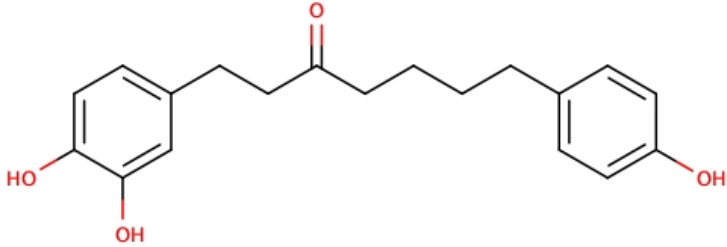
568. centrolobol

화학 구조		PubMed ID	
		22162164	
TM-MC 성분 ID	398		
TM-MC 성분 동의어	N/A		
PubChem ID	14427393		
InChI Key	UYJAYWZGEZOHURU-KRWDZBQOSA-N		
SMILES	O[C@@H](CCCCc1ccc(O)cc1)CCc1ccc(O)cc1		
Molecular Formula	C ₁₉ H ₂₄ O ₃		
Molecular Weight	300.398	Exact Molecular Weight	300.172544633
LogP	4.739	Topological Polar Surface Area	60.69 Å ²
Atom Count	46	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	3
Rotatable Bond Count	8	Aromatic Ring Count	2
Drug Likeness	0.62	Oral Bioavailability	Y

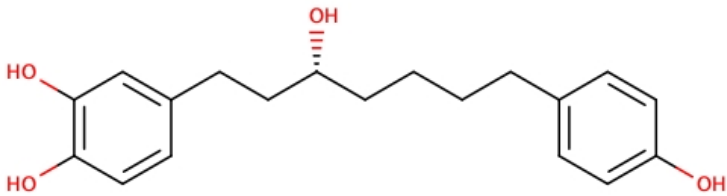
569. muricarpone B

화학 구조		PubMed ID	
		22162164	
TM-MC 성분 ID	399		
TM-MC 성분 동의어	N/A		
PubChem ID	11573476		
InChI Key	UHRUXUCWHIGENP-UHFFFAOYSA-N		
SMILES	<chem>Oc1ccc(CCCCC(=O)CCc2ccc(O)c(O)c2)cc1O</chem>		
Molecular Formula	C ₁₉ H ₂₂ O ₅		
Molecular Weight	330.38	Exact Molecular Weight	330.146723808
LogP	4.339	Topological Polar Surface Area	97.99 Å ²
Atom Count	46	Structural Alert Count	2
Hydrogen Bond Acceptor Count	5	Hydrogen Bond Donor Count	4
Rotatable Bond Count	8	Aromatic Ring Count	2
Drug Likeness	0.43	Oral Bioavailability	Y

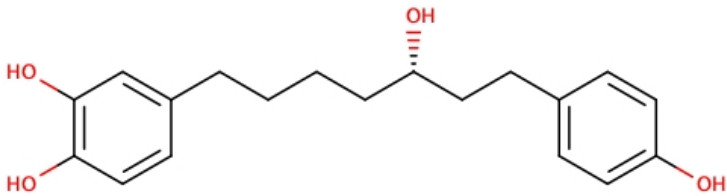
570. 1-(3,4-dihydroxyphenyl)-7-(4-hydroxyphenyl)heptan-3-one

화학 구조		PubMed ID	
		22162164	
TM-MC 성분 ID	400		
TM-MC 성분 동의어	N/A		
PubChem ID	38361380		
InChI Key	NORHBOUZICGKOK-UHFFFAOYSA-N		
SMILES	<chem>Oc1ccc(CCCCC(=O)CCc2ccc(O)c(O)c2)cc1</chem>		
Molecular Formula	C ₁₉ H ₂₂ O ₄		
Molecular Weight	314.381	Exact Molecular Weight	314.151809188
LogP	4.643	Topological Polar Surface Area	77.76 Å ²
Atom Count	45	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	3
Rotatable Bond Count	8	Aromatic Ring Count	2
Drug Likeness	0.49	Oral Bioavailability	Y

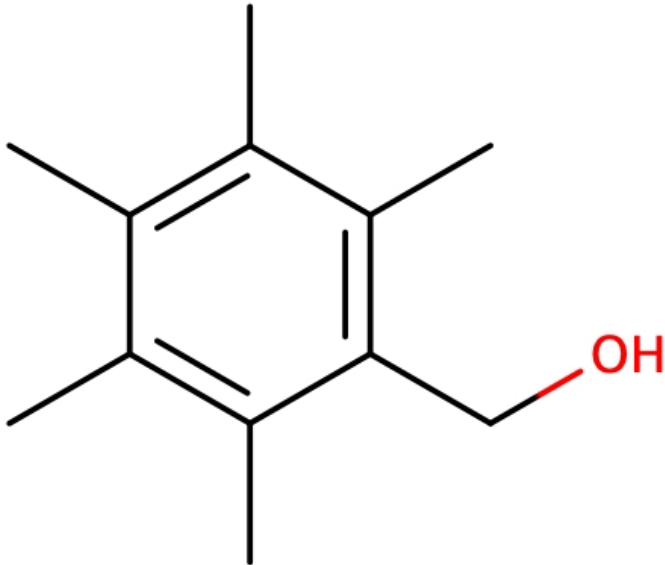
571. (3S)-1-(3,4-dihydroxyphenyl)-7-(4-hydroxyphenyl)heptan-3-ol

화학 구조		PubMed ID	
		22162164	
TM-MC 성분 ID	401		
TM-MC 성분 동의어	N/A		
PubChem ID	49831806		
InChI Key	SENGGJLGUFGNIH-MRXNPFEDSA-N		
SMILES	O[C@H](CCCCc1ccc(O)cc1)CCc1ccc(O)c(O)c1		
Molecular Formula	C ₁₉ H ₂₄ O ₄		
Molecular Weight	316.397	Exact Molecular Weight	316.167459253
LogP	4.435	Topological Polar Surface Area	80.92 Å ²
Atom Count	47	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	4
Rotatable Bond Count	8	Aromatic Ring Count	2
Drug Likeness	0.43	Oral Bioavailability	Y

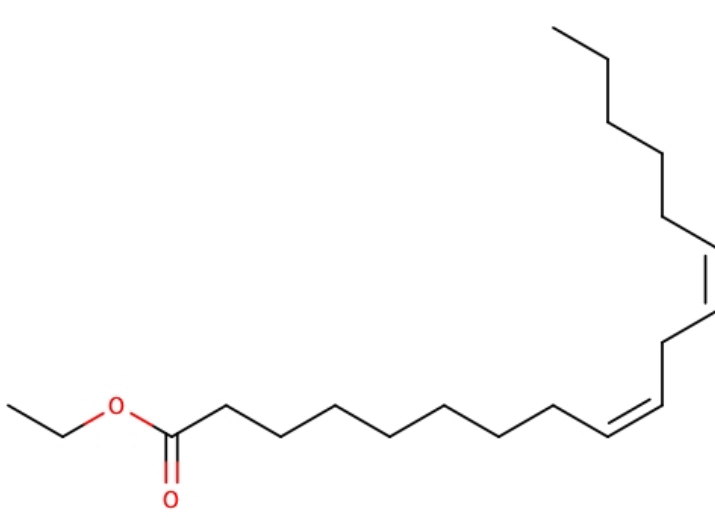
572. (3S)-1-(4-hydroxyphenyl)-7-(3,4-dihydroxyphenyl)heptan-3-ol

화학 구조		PubMed ID	
		22162164	
TM-MC 성분 ID	402		
TM-MC 성분 동의어	N/A		
PubChem ID	56593535		
InChI Key	WPEUAPAFZISHMD-INIZCTEOSA-N		
SMILES	O[C@@H](CCCCc1ccc(O)c(O)c1)CCc1ccc(O)cc1		
Molecular Formula	C ₁₉ H ₂₄ O ₄		
Molecular Weight	316.397	Exact Molecular Weight	316.167459253
LogP	4.435	Topological Polar Surface Area	80.92 Å ²
Atom Count	47	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	4
Rotatable Bond Count	8	Aromatic Ring Count	2
Drug Likeness	0.43	Oral Bioavailability	Y

573. 2,3,4,5,6-pentamethylbenzyl alcohol

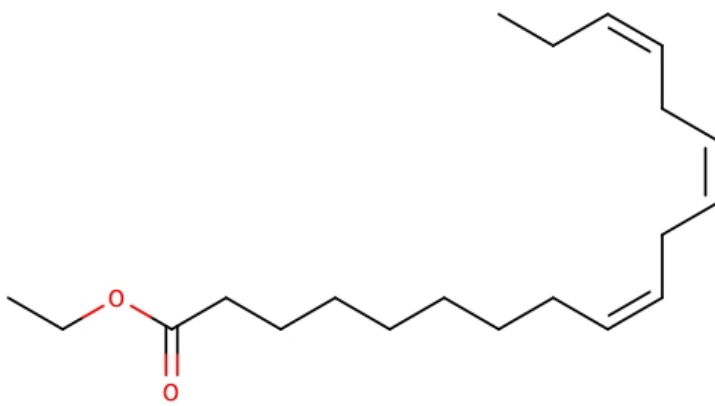
화학 구조		PubMed ID	
		29732747	
TM-MC 성분 ID	241629		
TM-MC 성분 동의어	2,3,4,5,6-pentamethyl benzyl alcohol		
PubChem ID	1241629		
InChI Key	CMBCAWNOBIGGTE-UHFFFAOYSA-N		
SMILES	<chem>Cc1c(C)c(C)c(CO)c(C)c1C</chem>		
Molecular Formula	C ₁₂ H ₁₈ O		
Molecular Weight	178.275	Exact Molecular Weight	178.1357652
LogP	3.773	Topological Polar Surface Area	20.23 Å ²
Atom Count	31	Structural Alert Count	0
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	1
Rotatable Bond Count	1	Aromatic Ring Count	1
Drug Likeness	0.69	Oral Bioavailability	Y

574. linoleic acid ethyl ester

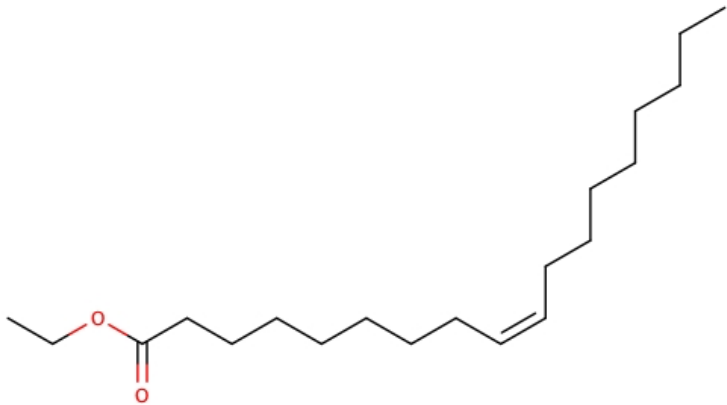
화학 구조	PubMed ID
	29732747

TM-MC 성분 ID	301993		
TM-MC 성분 동의어	ethyl linoleate; 9,12-octadecadienoic acid, ethyl ester; ethyl linolate; mandenol; ethyl linoleolate; linoleic acid, ethyl ester; ethyl octadec-9,12-dienoate		
PubChem ID	5282184		
InChI Key	FMMOOAYVCKXGMF-MURFETPASA-N		
SMILES	<chem>CCCCC=C/C=C/C/CCCCCCC(=O)OCC</chem>		
Molecular Formula	C ₂₀ H ₃₆ O ₂		
Molecular Weight	308.506	Exact Molecular Weight	308.271530399
LogP	6.925	Topological Polar Surface Area	26.3 Å ²
Atom Count	58	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	16	Aromatic Ring Count	0
Drug Likeness	0.17	Oral Bioavailability	N

575. 9,12,15-octadecatrienoic acid ethyl ester

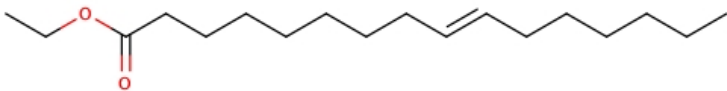
화학 구조		PubMed ID	
		29732747	
TM-MC 성분 ID	300641		
TM-MC 성분 동의어	N/A		
PubChem ID	5367460		
InChI Key	JYYFMIOPGOFNPK-AGRJPVHOSA-N		
SMILES	CCOC(=O)CCCCCCC=C/C=C/C=C/C=CC		
Molecular Formula	C ₂₀ H ₃₄ O ₂		
Molecular Weight	306.49	Exact Molecular Weight	306.255880335
LogP	6.563	Topological Polar Surface Area	26.3 Å ²
Atom Count	56	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	15	Aromatic Ring Count	0
Drug Likeness	0.19	Oral Bioavailability	N

576. ethyl oleate

화학 구조	PubMed ID
	29732747

TM-MC 성분 ID	92599		
TM-MC 성분 동의어	oleic acid, ethyl ester; ethyl-cis-9-octadecanoate; 9-octadecenoic acid ethyl ester; 9-octadecenoic acid, ethyl ester		
PubChem ID	5363269		
InChI Key	LVGKNOAMLMIIKO-QXMHVHEDSA-N		
SMILES	<chem>CCCCCCCC=C/C(=O)OCC</chem>		
Molecular Formula	C ₂₀ H ₃₈ O ₂		
Molecular Weight	310.522	Exact Molecular Weight	310.287180464
LogP	7.287	Topological Polar Surface Area	26.3 Å ²
Atom Count	60	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	17	Aromatic Ring Count	0
Drug Likeness	0.16	Oral Bioavailability	N

577. ethyl-9-hexadecenoate

화학 구조		PubMed ID	
		29732747	
TM-MC 성분 ID	364759		
TM-MC 성분 동의어	ethyl 9-hexadecenoate		
PubChem ID	5364759		
InChI Key	JELGPLUONQGOHF-MDZDMXLPSA-N		
SMILES	CCCCC=CWCCCCCCCC(=O)OCC		
Molecular Formula	C ₁₈ H ₃₄ O ₂		
Molecular Weight	282.468	Exact Molecular Weight	282.255880335
LogP	6.397	Topological Polar Surface Area	26.3 Å ²
Atom Count	54	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	15	Aromatic Ring Count	0
Drug Likeness	0.19	Oral Bioavailability	N

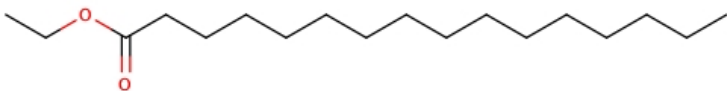
578. hentriacontane

화학 구조		PubMed ID	
		29732747	
TM-MC 성분 ID	12410		
TM-MC 성분 동의어	untriacontane; n-hentriacontane		
PubChem ID	12410		
InChI Key	IUJAMGNYPWYUPM-UHFFFAOYSA-N		
SMILES	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC		
Molecular Formula	C ₃₁ H ₆₄		
Molecular Weight	436.853	Exact Molecular Weight	436.5008020608
LogP	14.245	Topological Polar Surface Area	0 Å ²
Atom Count	95	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	28	Aromatic Ring Count	0
Drug Likeness	0.11	Oral Bioavailability	N

579. heptacosane


화학 구조		PubMed ID	
		29732747	
TM-MC 성분 ID	11636		
TM-MC 성분 동의어	n-heptacosane		
PubChem ID	11636		
InChI Key	BJQWYEJQWHSSCJ-UHFFFAOYSA-N		
SMILES	CCCCCCCCCCCCCCCCCCCCCCCCCC		
Molecular Formula	C ₂₇ H ₅₆		
Molecular Weight	380.745	Exact Molecular Weight	380.4382018032
LogP	12.467	Topological Polar Surface Area	0 Å ²
Atom Count	83	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	24	Aromatic Ring Count	0
Drug Likeness	0.15	Oral Bioavailability	N

580. hexadecanoic acid, ethyl ester

화학 구조	PubMed ID
	29732747

TM-MC 성분 ID	12366		
TM-MC 성분 동의어	ethyl palmitate; ethyl hexadecanoate; hexadecanoic acid ethyl ester; palmitic acid ethyl ester; palmitic acid, ethyl ester		
PubChem ID	12366		
InChI Key	XIRNKXNNONJFQO-UHFFFAOYSA-N		
SMILES	CCCCCCCCCCCCCCCC(=O)OCC		
Molecular Formula	C ₁₈ H ₃₆ O ₂		
Molecular Weight	284.484	Exact Molecular Weight	284.271530399
LogP	6.759	Topological Polar Surface Area	26.3 Å ²
Atom Count	56	Structural Alert Count	2
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	16	Aromatic Ring Count	0
Drug Likeness	0.23	Oral Bioavailability	N

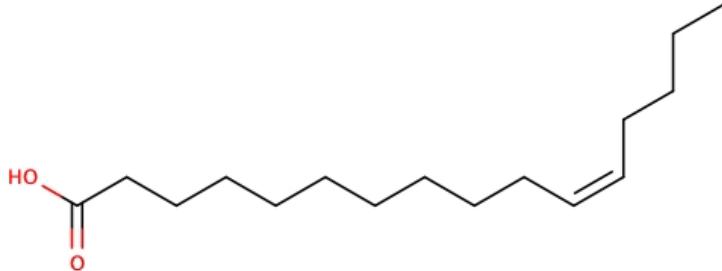
581. octacosane

화학 구조		PubMed ID	
		29732747	
TM-MC 성분 ID	12408		
TM-MC 성분 동의어	n-octacosane		
PubChem ID	12408		
InChI Key	ZYURHZPYMFLWSH-UHFFFAOYSA-N		
SMILES	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC		
Molecular Formula	C ₂₈ H ₅₈		
Molecular Weight	394.772	Exact Molecular Weight	394.4538518676
LogP	12.912	Topological Polar Surface Area	0 Å ²
Atom Count	86	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	25	Aromatic Ring Count	0
Drug Likeness	0.13	Oral Bioavailability	N

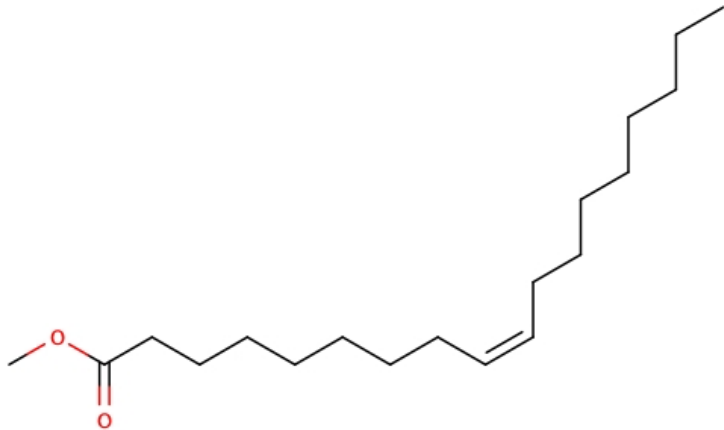
582. tetratetracontane

화학 구조		PubMed ID	
		29732747	
TM-MC 성분 ID	302574		
TM-MC 성분 동의어	N/A		
PubChem ID	23494		
InChI Key	KMXFZRSJMDYPPG-UHFFFAOYSA-N		
SMILES	CC		
Molecular Formula	C ₄₄ H ₉₀		
Molecular Weight	619.204	Exact Molecular Weight	618.704252898
LogP	20.025	Topological Polar Surface Area	0 Å ²
Atom Count	134	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	41	Aromatic Ring Count	0
Drug Likeness	0.06	Oral Bioavailability	N

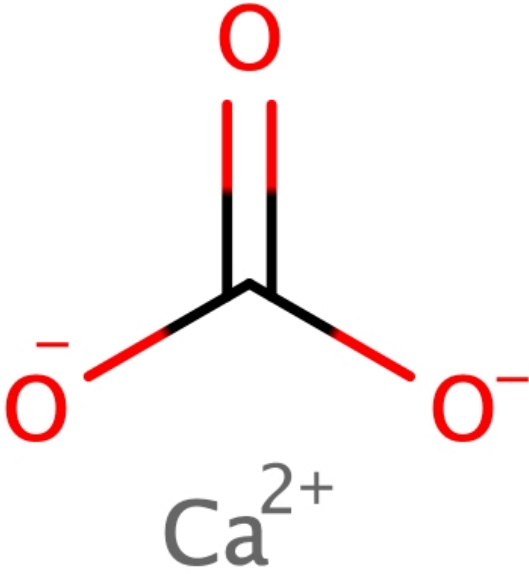
583. Z-11-hexadecenoic acid

화학 구조		PubMed ID	
		29732747	
TM-MC 성분 ID	312414		
TM-MC 성분 동의어	(Z)-11-hexadecenoic acid; neryl propionate; 11-hexadecenoic acid		
PubChem ID	5312414		
InChI Key	JGMYDQCXGIMHLL-WAYWQWQ TSA-N		
SMILES	<chem>CCCC=CCCCCCCCC(O)=O</chem>		
Molecular Formula	C ₁₆ H ₃₀ O ₂		
Molecular Weight	254.414	Exact Molecular Weight	254.224580206
LogP	5.895	Topological Polar Surface Area	37.3 Å ²
Atom Count	48	Structural Alert Count	2
Hydrogen Bond Acceptor Count	2	Hydrogen Bond Donor Count	1
Rotatable Bond Count	13	Aromatic Ring Count	0
Drug Likeness	0.33	Oral Bioavailability	N

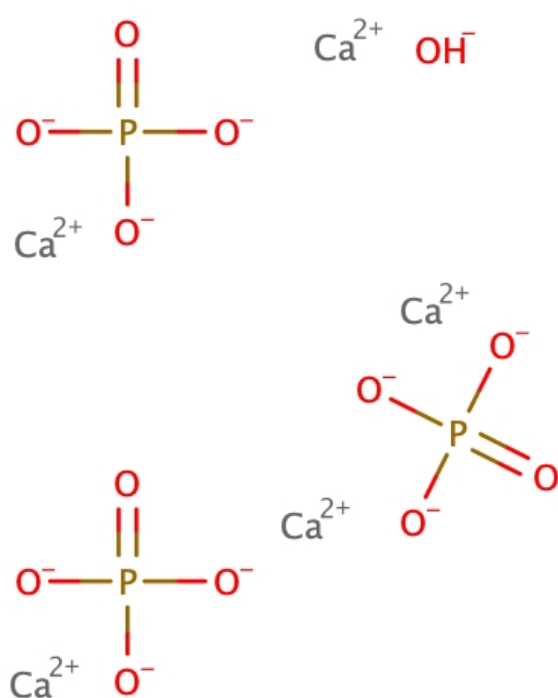
584. methyl oleate

화학 구조		PubMed ID	
		29732747	
TM-MC 성분 ID	280590		
TM-MC 성분 동의어	oleic acid, methyl ester; 9-octadecenoic acid, methyl ester; 9-octadecenoic acid (Z)-, methyl ester; methyl elaidate; methyl 9-octadecenoate; oleic acid methyl ester; 9-octadecenoic acid-methyl ester; Z-9-octadecenoic acid methyl ester; (Z)-9-octadecenoic acid, methyl ester		
PubChem ID	5364509		
InChI Key	QYDYPVFESGNLHU-KHPPLWFESA-N		
SMILES	CCCCCCCC=C/C(=O)OC		
Molecular Formula	C ₁₉ H ₃₆ O ₂		
Molecular Weight	296.495	Exact Molecular Weight	296.271530399
LogP	6.93	Topological Polar Surface Area	26.3 Å ²
Atom Count	57	Structural Alert Count	3
Hydrogen Bond Acceptor Count	1	Hydrogen Bond Donor Count	0
Rotatable Bond Count	16	Aromatic Ring Count	0
Drug Likeness	0.17	Oral Bioavailability	N

585. calcium carbonate

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	415		
TM-MC 성분 동의어	N/A		
PubChem ID	10112, 516889		
InChI Key	VTYYLEPIZMXCLO-UHFFFAOYSA-L		
SMILES	[Ca++].[O-]C([O-])=O		
Molecular Formula	CCaO ₃		
Molecular Weight	100.086	Exact Molecular Weight	99.9473348
LogP	0.25	Topological Polar Surface Area	63.19 Å ²
Atom Count	5	Structural Alert Count	1
Hydrogen Bond Acceptor Count	3	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.41	Oral Bioavailability	Y

586. hydroxyapatite

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	416		
TM-MC 성분 동의어	N/A		
PubChem ID	14781, 139036604		
InChI Key	XYJRXVWERLGGKC-UHFFFAOYSA-D		
SMILES	[OH-].[Ca++].[Ca++].[Ca++].[Ca++].[Ca++].[O-]P([O-])([O-])=O .[O-]P([O-])([O-])=O.[O-]P([O-])([O-])=O		
Molecular Formula	Ca ₅ HO ₁₃ P ₃		
Molecular Weight	502.306	Exact Molecular Weight	501.6759556
LogP	-1.02	Topological Polar Surface Area	86.25 Å ²
Atom Count	22	Structural Alert Count	2
Hydrogen Bond Acceptor Count	4	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.31	Oral Bioavailability	Y

587. Al

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	417		
TM-MC 성분 동의어	N/A		
PubChem ID	14488		
InChI Key	AZDRQVAHHNSJOQ-UHFFFAOYSA-N		
SMILES	[Al]		
Molecular Formula	Al		
Molecular Weight	26.9815384	Exact Molecular Weight	26.9815385
LogP	1.45	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.35	Oral Bioavailability	Y

588. Ba

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	418		
TM-MC 성분 동의어	N/A		
PubChem ID	N/A		
InChI Key	MUBOSUMMMUSVEO-UHFFFAOYSA-N		
SMILES	[Ba]		
Molecular Formula	Ba		
Molecular Weight	137.327	Exact Molecular Weight	137.905247
LogP	-0.2	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.41	Oral Bioavailability	Y


589. Bi

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	419		
TM-MC 성분 동의어	N/A		
PubChem ID	9242		
InChI Key	BPBOBPIKWGUSQG-UHFFFAOYSA-N		
SMILES	[Bi]		
Molecular Formula	Bi		
Molecular Weight	208.9804	Exact Molecular Weight	208.9804
LogP	0.15	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.50	Oral Bioavailability	Y


590. Ge

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	421		
TM-MC 성분 동의어	N/A		
PubChem ID	23984		
InChI Key	QUZPNFFHZPRKJD-UHFFFAOYSA-N		
SMILES	[GeH4]		
Molecular Formula	GeH ₄		
Molecular Weight	76.662	Exact Molecular Weight	77.95247789
LogP	-1.304	Topological Polar Surface Area	0 Å ²
Atom Count	5	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.31	Oral Bioavailability	Y

591. I

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	422		
TM-MC 성분 동의어	N/A		
PubChem ID	807		
InChI Key	PNDPGZBMCMUPRI-UHFFFAOYSA-N		
SMILES	I2		
Molecular Formula	I ₂		
Molecular Weight	253.80894	Exact Molecular Weight	253.80894
LogP	1.358	Topological Polar Surface Area	0 Å ²
Atom Count	2	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.57	Oral Bioavailability	Y

592. Ir

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	423		
TM-MC 성분 동의어	N/A		
PubChem ID	23924		
InChI Key	GKOZUEZYRPOHIO-UHFFFAOYSA-N		
SMILES	[Ir]		
Molecular Formula	Ir		
Molecular Weight	192.217	Exact Molecular Weight	192.9629216
LogP	0	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	0
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.51	Oral Bioavailability	Y


593. Mn

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	425		
TM-MC 성분 동의어	N/A		
PubChem ID	23930		
InChI Key	PWHULOQIROXLJO-UHFFFAOYSA-N		
SMILES	[Mn]		
Molecular Formula	Mn		
Molecular Weight	54.938043	Exact Molecular Weight	54.938044
LogP	-0.156	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.34	Oral Bioavailability	Y

594. Mo

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	426		
TM-MC 성분 동의어	N/A		
PubChem ID	23932		
InChI Key	ZOKXTWBITQBERF-UHFFFAOYSA-N		
SMILES	[Mo]		
Molecular Formula	Mo		
Molecular Weight	95.95	Exact Molecular Weight	97.905405
LogP	0	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.37	Oral Bioavailability	Y

595. Na

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	427		
TM-MC 성분 동의어	sodium		
PubChem ID	N/A		
InChI Key	MPPMYQQHEHYDOCL-UHFFFAOYSA-N		
SMILES	[Na]		
Molecular Formula	Na		
Molecular Weight	22.98976928	Exact Molecular Weight	22.98976928
LogP	-0.77	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.30	Oral Bioavailability	Y


596. Ni

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	428		
TM-MC 성분 동의어	N/A		
PubChem ID	935		
InChI Key	PXHVJJICTQNCMI-UHFFFAOYSA-N		
SMILES	[Ni]		
Molecular Formula	Ni		
Molecular Weight	58.6934	Exact Molecular Weight	57.935342
LogP	0.156	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.35	Oral Bioavailability	Y


597. silane

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	429		
TM-MC 성분 동의어	Si		
PubChem ID	23953		
InChI Key	BLRPTPMANUNPDV-UHFFFAOYSA-N		
SMILES	[SiH4]		
Molecular Formula	H ₄ Si		
Molecular Weight	32.117	Exact Molecular Weight	32.008226664
LogP	-1.259	Topological Polar Surface Area	0 Å ²
Atom Count	5	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.29	Oral Bioavailability	Y


598. V

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	430		
TM-MC 성분 동의어	N/A		
PubChem ID	23990		
InChI Key	LEONUFNNVUYDNQ-UHFFFAOYSA-N		
SMILES	[V]		
Molecular Formula	V		
Molecular Weight	50.9415	Exact Molecular Weight	50.943957
LogP	0	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	0
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.36	Oral Bioavailability	Y

599. Zn

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	431		
TM-MC 성분 동의어	N/A		
PubChem ID	23994		
InChI Key	HCHKCACWOHOZIP-UHFFFAOYSA-N		
SMILES	[Zn]		
Molecular Formula	Zn		
Molecular Weight	65.38	Exact Molecular Weight	63.929142
LogP	0.156	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	1
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.35	Oral Bioavailability	Y

600. Zr

화학 구조		PubMed ID	
		26841944	
TM-MC 성분 ID	432		
TM-MC 성분 동의어	N/A		
PubChem ID	23995		
InChI Key	QCWXUUIWCKQGHC-UHFFFAOYSA-N		
SMILES	[Zr]		
Molecular Formula	Zr		
Molecular Weight	91.224	Exact Molecular Weight	89.9047
LogP	0	Topological Polar Surface Area	0 Å ²
Atom Count	1	Structural Alert Count	0
Hydrogen Bond Acceptor Count	0	Hydrogen Bond Donor Count	0
Rotatable Bond Count	0	Aromatic Ring Count	0
Drug Likeness	0.39	Oral Bioavailability	Y