



Supplementary Fig. 1. Schematic representation of the deep neural network architecture for predicting antioxidant activity. The network architecture comprises an input layer receiving a vector of 2,048 structural features, followed by four sequential fully connected layers with rectified linear unit (ReLU) activation functions. The final output layer consists of a single neuron employing a sigmoid activation function to produce a continuous output value between 0 and 1, signifying the predicted probability of antioxidant activity.

Supplementary Table 1. Predicted activity scores for natural product compounds

Compound	Inchikey	PubChem_CID	SVM	RF	Mean
Quercetin hydrate	OKXFBEYCRMINR-UHFFFAOYSA-N	16212154	1.00	1.00	1.00
Cyanidin chloride	COAWNPIQKJEHPG-UHFFFAOYSA-N	68247	0.99	1.00	1.00
Quercetagenin	ZVOLCUVKHLEPEV-UHFFFAOYSA-N	5281680	1.00	0.99	0.99
2-(3,4-Dihydroxy-phenyl)-5,7-dihydroxy-3-(3,4,5-trihydroxy-6-methyl-tetrahydro-pyran-2-yloxy)-chromen-4-one	OXGUCUVFOIWWQJ-UHFFFAOYSA-N	5353915	0.99	1.00	0.99
Hispolon	QDVIEIMMEUCFMW-QXYPORFMSA-N	10082188	0.99	1.00	0.99
Avicularin	BDCDNTVZSILEOY-UXYSNRGZSA-N	5490064	0.99	1.00	0.99
2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-3-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxochromen-4-one	OVSQVDMCBVZWGM-LVWULRLVSA-N	51402807	0.99	1.00	0.99
3,3',4',5,5',7-Hexahydroxyflavylium	JKHRCGUTYDNCLE-UHFFFAOYSA-O	128853	1.00	0.99	0.99
Delphinidin	FFNDMZIBVDSQFI-UHFFFAOYSA-N	68245	1.00	0.99	0.99
Ellagic acid dihydrate	ZEPCRIPMALGRJR-UHFFFAOYSA-N	16760409	1.00	0.99	0.99
(2R)-3-(3,4-dihydroxyphenyl)-2-[3-(3,4-dihydroxyphenyl)-1-oxoprop-2-enoyl]propanoic acid	DOUMFZQKYFQNTF-MRXNPFEDSA-N	65035	0.98	1.00	0.99
Epicatechin	PFTAWBLQPZVEMU-UKRRQHHSQA-N	72276	0.98	1.00	0.99
Piceatannol	CDRPUGZCRXLFL-OWOJBTEDSA-N	667639	1.00	0.98	0.99
Chicoric acid	YDDGKXBLOXEEMN-IABMMNSOSA-N	5281764	0.99	0.99	0.99
(1S,3R,4R,5R)-3-[3-(3,4-dihydroxyphenyl)prop-2-enoyloxy]-1,4,5-trihydroxy-cyclohexanecarboxylic acid	CWVRJTMFETXNAD-NCZKRNLISA-N	9476	0.98	1.00	0.99
Chlorogensaure	CWVRJTMFETXNAD-KJOPMHRFSA-N	12310830	0.98	1.00	0.99
Isorhapontigenin	ANNNBEZJTNXCHY-NSCUHMNNSA-N	5318650	1.00	0.98	0.99
Vanillin	MWOOGOJBHARFG-UHFFFAOYSA-N	1183	0.99	0.98	0.99
Nordihydroguaiaretic acid	HCZKYJDFEPMADG-UHFFFAOYSA-N	4534	0.98	0.99	0.98
Sulfuretin	RGNXWPVNPFAADO-NSIKDUERSA-N	5281295	1.00	0.97	0.98
Butein	AYMYWHCQALZEGT-ORCRQEGFSA-N	5281222	1.00	0.97	0.98
Ethyl vanillin	CBOQJANXLMLOSS-UHFFFAOYSA-N	8467	0.99	0.98	0.98
(1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione)	VFLDPWHFBUODDF-UHFFFAOYSA-N	2889	0.97	0.99	0.98
(+/-)-Taxifolin	CXQWRCVTCMQVQX-UHFFFAOYSA-N	471	0.99	0.97	0.98
cyclic 3,6-[(1R)-4,4',5,5',6,6'-hexahydroxy[1,1'-biphenyl]-2,2'-dicarboxylate] 1-(3,4,5-trihydroxybenzoate)-beta-D-glucopyranose	TUSDEZXZIRFGC-DMGSCOEISA-N	134692185	0.97	0.99	0.98
(1R,19R,21S,22R,23R)-6,7,8,11,12,13,22,23-octahydroxy-3,16-dioxo-2,17,20-trioxatetracyclo[17.3.1.0 ^{4,9} .0 ^{10,15}]tricosan-4(9),5,7,10,12,14-hexaen-21-yl 3,4,5-trihydroxybenzoate	TUSDEZXZIRFGC-ORQNFANSA-N	12303949	0.97	0.99	0.98
Dihydromyricetin	KJXSIXMJHKAJOD-LSDHHAUSA-N	161557	0.99	0.96	0.98
Strictinin	FYIJLTSMNUNLT-CXQFPWCTSA-N	73330	0.97	0.98	0.98
Oxyresveratrol	PDHAOJSHSJQANO-OWOJBTEDSA-N	5281717	0.99	0.96	0.98

2-(3,4-Dihydroxyphenyl)-2-hydroxypropanoic acid	NDGMYGNFKSMYBB-UHFFFAOYSA-N	152463	0.98	0.97	0.98
2-[(5R,7R)-13,14,15,18,19,20,31,35,36-nonahydroxy-2,10,23,28,32-pentaoxo-5-(3,4,5-trihydroxybenzoyl)oxy-3,6,9,24,27,33-hexaoxaheptacyclo[28.7.1.04,25.07,26.011,16.017,22.034,38]octatriaconta-1(37),11,13,15,17,19,21,34(38),35-nonaen-29-yl]acetic acid	HGXAVROWQLCTP-CATNJDLSA-N	134694193	0.97	0.98	0.98
quercetin 3-O-beta-D-glucuronide	DUBCCGAQYVUYEU-MBIBTLSJSA-N	13258914	0.98	0.97	0.98
Sappanchalcone	JVGNTXGHBHMJDO-QHHAJSJGSA-N	5319493	0.99	0.96	0.98
Cynarine	YDDUMTOHNYZQPO-RVXRWRWFUSA-N	5281769	0.96	0.99	0.97
(1E,4Z,6E)-5-hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,4,6-trien-3-one	ZIUSSTSXXLLKKK-KOBPDPAASA-N	5281767	0.97	0.98	0.97
4-Hydroxy-3-methoxycinnamaldehyde	DKZBBWMURDFHNE-NSCUHMNNSA-N	5280536	0.98	0.97	0.97
4-Nerolidylcatechol	ZBZZDHDWRSLAY-GZTJUNOSA-N	5352089	0.99	0.96	0.97
5-[(2S,3S)-4-[(E)-2-[(2R,3R)-3-[(2S,3S)-3-(3,5-dihydroxyphenyl)-6-hydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-1-benzofuran-4-yl]-2-(4-hydroxyphenyl)-2,3-dihydro-1-benzofuran-5-yl]ethenyl]-6-hydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-1-benzofuran-3-yl]benzene-1,3-diol	WZKKRZSJTLGPHH-QGYUWUKLSA-N	16138152	0.97	0.98	0.97
Hispidin	SGJNQVTUYXCBKH-HNQUOIGGSA-N	54685921	0.99	0.95	0.97
Petunidin	AFOLOMGWVXKIQI-UHFFFAOYSA-O	441774	0.99	0.95	0.97
Herbacetin	ZDOTZEDNGNPOEW-UHFFFAOYSA-N	5280544	0.98	0.96	0.97
Salvianolic acid A	YMGFTDKNIWPMGF-UCPJVGPRSA-N	5281793	0.99	0.95	0.97
Methyl rosmarinate	XHALVRQBZGZHF-BBOMDTFKSA-N	6479915	0.95	0.98	0.97
N-Caffeoyltyramine	VSHUQLRHTJOKTA-XBXARRHUSA-N	9994897	0.97	0.96	0.97
(1S)-3,4-bis[3-(3,4-dihydroxyphenyl)prop-2-enoyloxy]-1,5-dihydroxycyclohexane-1-carboxylic acid	UFCLZKMFXSILNL-VCFKWBLOSA-N	129316855	0.96	0.97	0.97
3,4-Dicaffeoylquinic acid	UFCLZKMFXSILNL-RVXRWRWFUSA-N	6474309	0.96	0.97	0.97
Eugenol	RRAFCDWBNXTKKO-UHFFFAOYSA-N	3314	0.98	0.95	0.97
Demethoxycurcumin	HJTVQHVGMGKONQ-LUZURFALSA-N	5469424	0.98	0.95	0.96
Forsythiaside	DTOUWTJYUCZJQD-UJERWXFOSA-N	5281773	0.96	0.97	0.96
Agrimoniin	BZAFROBDXRJYTQ-JVEQELPQSA-N	16129621	0.96	0.97	0.96
(2R,3R,4S,5R,6R)-6-(((3,4,5-Trihydroxybenzoyl)oxy)methyl)tetrahydro-2H-pyran-2,3,4,5-tetraol tetrakis(3,4,5-trihydroxybenzoate)	QJYNZEYHSMRWBK-HXSHIISNSA-N	9876301	0.97	0.96	0.96
Galangin	VCCRNZQBSJXYJD-UHFFFAOYSA-N	5281616	0.98	0.94	0.96
Quinalizarin	VBHKTXLJZIDJF-UHFFFAOYSA-N	5004	0.99	0.92	0.96
2-(3,5-Dihydroxyphenyl)-3,6,8-trihydroxychromen-4-one	TWOPRMPXDUALK-UHFFFAOYSA-N	467484	0.99	0.92	0.96
Morin	YXOLAZRVSSWPPT-UHFFFAOYSA-N	5281670	0.98	0.93	0.96
Eckol	PCZZRBGISTUIOA-UHFFFAOYSA-N	145937	0.96	0.95	0.96
Gallocatechin	XMOCLSLCDHWDHP-SWLSCSKDSA-N	65084	0.99	0.92	0.96
Epigallocatechin	XMOCLSLCDHWDHP-IUODEOHRSA-N	72277	0.99	0.92	0.96

(+/-)-Eriodictyol	SBHXYTNGIZCORC-UHFFFAOYSA-N	11095	0.99	0.92	0.95
(1R)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1R)-4-hydroxy-2,6,6-trimethylcyclohex-2-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaenyl]-3,5,5-trimethylcyclohex-3-en-1-ol	KBPHJBAIARWVSC-RTIVXWJOSA-N	6433159	0.97	0.94	0.95
Lutein	KBPHJBAIARWVSC-RGZFRNHPSA-N	5281243	0.97	0.94	0.95
Procyanidin B2, (+)-	XFZJEEAOWLFHDH-NFJBMHMQSA-N	122738	0.95	0.95	0.95
Procyanidin B1	XFZJEEAOWLFHDH-UKWJTHFESA-N	11250133	0.95	0.95	0.95
Xanthoangelol	LRMBOSQWGHYCW-MDGZPELGSA-N	643007	0.99	0.92	0.95
Dendrophenol	YTRAYUIKLRABOQ-UHFFFAOYSA-N	176096	1.00	0.90	0.95
Catechol	YCIMNLLNPGFGHC-UHFFFAOYSA-N	289	0.96	0.93	0.95
2-[11-(Carboxymethyl)-6,7,8-trihydroxy-3,12-dioxo-18-(2,3,4-trihydroxybenzoyl)oxy-17-(3,4,5-trihydroxybenzoyl)oxy-15-[(3,4,5-trihydroxybenzoyl)oxymethyl]-2,13,16-trioxatricyclo[12.3.1.04,9]octadeca-4,6,8-trien-10-yl]-2-hydroxyacetic acid	YTWADAOWDYGTCE-UHFFFAOYSA-N	5315810	0.94	0.95	0.94
10-Dehydrogingerdione	NILVTWAPVHQVPS-UINJHVQLSA-N	22608831	0.95	0.94	0.94
3',4'-Dihydroxyacetophenone	UCQUAMAQHEXGD-UHFFFAOYSA-N	14530	0.98	0.91	0.94
Daphnetin	ATEFPOUAMCWAQS-UHFFFAOYSA-N	5280569	0.99	0.89	0.94
Grifolin	PZHKNRPLTZPO-VZRGJMDUSA-N	5372312	0.98	0.90	0.94
Rhamnetin	JGUZGNYPMHHYRK-UHFFFAOYSA-N	5281691	0.96	0.92	0.94
Etilevodopa	NULMGOSOSZBEQL-QMMMGPBSA-N	170345	0.98	0.90	0.94
Lycopene	OAIJSZIZWZSQBC-GYZMGTAESA-N	446925	0.97	0.91	0.94
Silicristin	BMLIIPXVWESJG-LMBCONBSSA-N	441764	0.96	0.92	0.94
Magnolol	VVOAZFWZEDHOOU-UHFFFAOYSA-N	72300	0.98	0.89	0.93
Methylodopa	CJCSPKMFHVPWAR-JTQLQIEISA-N	38853	0.98	0.89	0.93
Levodopa	WTDRDQBEARUVNC-LURJTMIESA-N	6047	1.00	0.87	0.93
DL-Dopa	WTDRDQBEARUVNC-UHFFFAOYSA-N	836	1.00	0.87	0.93
2-[2R,3R-Dihydro-3-(4-hydroxy-3-methoxyphenyl)-2-(hydroxymethyl)-1,4-benzodioxin-6-yl]-2R,3R-dihydro-3,5,7-trihydroxy-4H-1-benzopyran-4-one	SEBFKMXJBCUCAI-HHXGKTILSA-N	24832061	0.97	0.90	0.93
Silymarin	SEBFKMXJBCUCAI-UHFFFAOYSA-N	5213	0.97	0.90	0.93
Silibinin B	SEBFKMXJBCUCAI-WAABAYLZSA-N	1548994	0.97	0.90	0.93
Rhapontigenin	PHMHDRYFAYWEG-NSCUHMNNSA-N	5320954	0.98	0.88	0.93
Phloroglucinol	QCDYQQDYXPDABM-UHFFFAOYSA-N	359	0.98	0.88	0.93
2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-3-methyl-2,3-dihydrochromen-4-one	NDKNYUFZUFHDFQ-UHFFFAOYSA-N	5321695	0.97	0.88	0.93
Bavachin	OAUREGNZECGNQS-IBGZPJMESA-N	14236566	0.98	0.87	0.92
Caffeic acid phenethyl ester	SWUARLUWKZWEBQ-VQHVLOKHSAN	5281787	0.94	0.91	0.92
Acetovanillone	DFYRUELUNQRZTB-UHFFFAOYSA-N	2214	0.94	0.91	0.92
5,8-Dihydroxy-1,4-naphthoquinone	RQNVIKXOOKXAJQ-UHFFFAOYSA-N	10141	0.97	0.88	0.92

[5-acetyloxy-6-[2-(3,4-dihydroxyphenyl)ethoxy]-3-hydroxy-4-(3,4,5-trihydroxy-6-methyloxan-2-yl)oxyoxan-2-yl]methyl (E)-3-(3,4-dihydroxyphenyl)prop-2-enoate	HFJIGXAMJFDVFR-VMPITWQZSA-N	5322171	0.93	0.91	0.92
Sylvatesmin	CPJKKWDCUOOTEW-YJPXFSGGSA-N	3083590	0.93	0.91	0.92
Gossypin	SJRXLVUZMMDCNG-KKPBLLMSA-N	5281621	0.96	0.88	0.92
Isoeugenol	BJIOGJUNALELMI-ONEGZZNKSA-N	853433	0.97	0.87	0.92
Centaureidin	BZXULYMZYPRZOG-UHFFFAOYSA-N	5315773	0.95	0.89	0.92
Pyridoxamine	NHZMQXZHNVTQA-UHFFFAOYSA-N	1052	0.96	0.87	0.92
Purpurin	BBNQADTFFCFGB-UHFFFAOYSA-N	6683	0.93	0.90	0.92
Eupafolin	FHHSEFRSDKWJK-UHFFFAOYSA-N	5317284	0.97	0.86	0.92
Morusin	XFFOMNJDRLDLQ-UHFFFAOYSA-N	5281671	0.97	0.86	0.92
Cannabigerol	QXACEHWTBCFNSA-SFQUDFHCSA-N	5315659	0.97	0.86	0.91
Pyridoxine	LXNHXLLTXMVWPM-UHFFFAOYSA-N	1054	0.96	0.86	0.91
Ethyl ferulate	ATJVZXXHKSVELS-FNORWQNLSA-N	736681	0.94	0.88	0.91
Punicalagin	ZJVUMAFASBFBUG-UYMKNUMKSA-N	44584733	0.96	0.86	0.91
(1R,35R,37R,38R,55S)-6,7,8,11,12,23,24,27,28,29,37,43,44,45,48,49,50-heptadecahydroxy-2,14,21,33,36,39,54-heptaaxaundecacyclo[33.20.0.04,9.010,19.013,18.016,25.017,22.026,31.038,55.041,46.047,52]pentapentaconta-4,6,8,10,12,16,18,22,24,26,28,30,41,43,45,47,49,51-octadecaene-3,15,20,32,40,53-hexone	ZJVUMAFASBFBUG-RILGRMFESA-N	16148440	0.96	0.86	0.91
Danshensu	PAFLSMZLRSPALU-MRVPVSSYSA-N	11600642	0.99	0.83	0.91
Glabridin	LBQIJVLKGVZRIW-ZDUSSCGKSA-N	124052	0.97	0.84	0.91
Fraxetin	HAVWRBANWNTJX-UHFFFAOYSA-N	5273569	0.97	0.84	0.91
	TYQCGQRIZGCHNB-UHFFFAOYSA-N	5785	0.93	0.88	0.91
7,8-Dihydroxyflavone	COCYGNDWFKTMF-UHFFFAOYSA-N	1880	1.00	0.81	0.90
Mulberrin	UWQYBLOHTQWSQD-UHFFFAOYSA-N	5481958	0.94	0.87	0.90
Honokiol	FVYXIJYOAGAUQK-UHFFFAOYSA-N	72303	0.96	0.85	0.90
Artepillin C	KABCFARPAMXCC-JXMROGBWSA-N	5472440	0.97	0.84	0.90
Boldine	LZJRNLRASBVRRX-ZDUSSCGKSA-N	10154	0.98	0.82	0.90
Scutellarein	JVXZRQGOXCEC-UHFFFAOYSA-N	5281697	0.95	0.85	0.90
Zeaxanthin	JKQXZKUSFCQOG-QAYBQHTQSA-N	5280899	0.92	0.88	0.90
5-Allyl-3-(3-allylphenoxy)benzene-1,2-diol	RVIUPPNYFNZVFG-UHFFFAOYSA-N	45270574	0.96	0.84	0.90
2,3,5,4'-tetrahydroxystilbene-2-O-beta-D-glucoside	JAYVHSBYKLLDJC-DSNJPTTOSA-N	5321884	0.95	0.85	0.90
(2R)-2-methyl-2-(4-methylpent-3-enyl)-7-pentylchromen-5-ol	UVOLYTDXHDXWJU-OAQYLSRUSA-N	76971722	0.96	0.83	0.90
Cannabichromene	UVOLYTDXHDXWJU-UHFFFAOYSA-N	30219	0.96	0.83	0.90
Methyl 4-hydroxy-3,5-dimethoxybenzoate	ZMXJAEJWHJMGX-UHFFFAOYSA-N	70164	0.95	0.84	0.90
Licochalcone D	RETRVWFVEFCGOK-RMKNXTFCSA-N	10473311	0.96	0.83	0.90
8-Prenylnaringenin	LPEZZAVFJPLNZ-SFHVURJKSA-N	480764	0.95	0.84	0.89
Cinnamtannin D1	BYSRPHRKESMCPO-HMQYECKYSA-N	46173958	0.91	0.88	0.89
Bavachinin	VOCGSQHKPZSIKB-FQEVSTJZSA-N	10337211	0.94	0.85	0.89
Arctigenin	NQWVSMVXKMHKTF-JKSUJKDBSA-N	64981	0.93	0.86	0.89
Isovanillin	JVTZYFYHCGSXJV-UHFFFAOYSA-N	12127	0.97	0.82	0.89
Octahydrocurcumin	OELMAFBLFOKZJD-UHFFFAOYSA-N	11068834	0.95	0.84	0.89

Isoorientin	ODBRNZZJSYPIDI-VJXVFPJBSA-N	114776	0.94	0.84	0.89
Astilbin	ZROGCCBNZBKLEL-MPRHSVQHSA-N	119258	0.87	0.91	0.89
Hypericin	YDOIFHVUBCIUHF-UHFFFAOYSA-N	3663	0.93	0.85	0.89
Salsolinol	IBRKLUSXDYATLG-LURJTMIESA-N	91588	0.97	0.81	0.89
1-Methyl-1,2,3,4-tetrahydroisoquinoline-6,7-diol	IBRKLUSXDYATLG-UHFFFAOYSA-N	54456	0.97	0.81	0.89
Casticin	PJQLSMYMOKWUJG-UHFFFAOYSA-N	5315263	0.92	0.85	0.89
Liothyronine	AUYCJSJGJYCDS-LBPRGKRZSA-N	5920	0.95	0.82	0.89
(1S,5R)-3-[(3,4-dihydroxyphenyl)-hydroxymethylidene]-6,6-dimethyl-5,7-bis(3-methylbut-2-enyl)-1-(5-methyl-2-prop-1-en-2-yl)hex-4-enyl)bicyclo[3.3.1]nonane-2,4,9-trione	DTTONLKLWRTCAB-AXXSNSRJSAN	138111558	0.90	0.87	0.88
(2S)-6-[(1S,5R,6S)-6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-(4-methylpent-3-enyl)cyclohex-2-en-1-yl]-2-(2,5-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydrochromen-4-one	ZXTQHAMOONDJY-YTAXAHCSSAN	44408701	0.94	0.83	0.88
1-(4-Hydroxy-3-methoxyphenyl)dodecan-3-one	TYQRTQZWHUXDLG-UHFFFAOYSA-N	213821	0.90	0.87	0.88
(S)-adrenaline	UCTWMZQNUQWSLP-SECBINFHSAN	247704	0.96	0.81	0.88
Epinephrine	UCTWMZQNUQWSLP-VIFPVBQESAN	5816	0.96	0.81	0.88
alpha-Viniferin	KUTVNHOAKHJFL-ZSIJVUTGSAN	196402	0.93	0.83	0.88
Guanidine	ZRALSGWFCBTJO-UHFFFAOYSA-N	3520	0.89	0.87	0.88
Dithioerythritol	VHJLVAABSRFDPM-ZXZARUISSAN	439352	0.91	0.85	0.88
Osthenol	RAKJVIPCCGXHHS-UHFFFAOYSA-N	5320318	0.96	0.80	0.88
C.I. Natural Red 20	NEZONWMXZKDMKF-UHFFFAOYSA-N	5208	0.94	0.83	0.88
Shikonin	NEZONWMXZKDMKF-SNVBAGLBSAN	479503	0.94	0.83	0.88
Alkannin	NEZONWMXZKDMKF-JTQLQIEISAN	72521	0.94	0.83	0.88
Hydroxytyrosol	JUUBCHWRXWPFHF-UHFFFAOYSA-N	82755	0.99	0.77	0.88
Warfarin	PJVWTKQMONHTI-UHFFFAOYSA-N	54678486	0.92	0.84	0.88
Kushenol X	ZJRPDIPXWGIHRB-SBCNVUAESAN	10599228	0.95	0.81	0.88
Idronoxil	ZZUBHVMHNVYXRR-UHFFFAOYSA-N	219100	0.96	0.80	0.88
Hydroquinone	QIGBRXMKCJVMJ-UHFFFAOYSA-N	785	0.92	0.83	0.88
Resorcinol	GHMLBKRAJXXBS-UHFFFAOYSA-N	5054	0.91	0.84	0.88
(E)-N-[(2S)-2-hydroxy-2-(4-hydroxyphenyl)ethyl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide	VJSCHQMOTSXAKB-UOWSJYKBSAN	10042201	0.96	0.79	0.88
nectandrin-B	GMXMKSFJQLFOSO-JARDSOJUSAN	156517	0.87	0.88	0.88
Cryptoxanthin	DMASLKHVQRHNES-FKKUPVFPSAN	5281235	0.89	0.86	0.87
Icaritin	TUUXBSASAQJECY-UHFFFAOYSA-N	5318980	0.90	0.85	0.87
Zingerone	OJYLAHXKWMRDGS-UHFFFAOYSA-N	31211	0.91	0.84	0.87
Rhapontin	GKAJCVFOJGXVIA-DXKBKAGUSAN	637213	0.94	0.80	0.87
Levothyroxine	XUIIKFGFIJCVMT-LBPRGKRZSAN	5819	0.94	0.80	0.87
Dextrothyroxine	XUIIKFGFIJCVMT-GFCCVEGCSAN	8730	0.94	0.80	0.87
l-Stepholidine	JKPISQIIWUONPB-HNNXBMFYSAN	6917970	0.97	0.77	0.87
(6aS)-7,11b-dihydro-6H-indeno[2,1-c]chromene-3,6a,9,10-tetrol	UWHUTZOCTZJUKC-OEMAIJDKSAN	44135406	0.97	0.77	0.87
Brazilin	UWHUTZOCTZJUKC-JKSUJKDBSAN	73384	0.97	0.77	0.87
Pinosylvin	YCVPRTHEGLPYPB-VOTSOKGWSAN	5280457	0.91	0.83	0.87
Guaiacol	LHGVFZTFXWLCP-UHFFFAOYSA-N	460	0.90	0.83	0.87
Norepinephrine	SFLSHLFXELFNJZ-QMMMGOBSAN	439260	0.99	0.74	0.87
Tetrahydrocurcumin	LBTVHXHERHESKG-UHFFFAOYSA-N	124072	0.90	0.83	0.87

(2S)-6-[(1S,5R,6S)-6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-(4-methylpent-3-enyl)cyclohex-2-en-1-yl]-2-(2,4-dihydroxyphenyl)-5,7-dihydroxy-2,3-dihydrochromen-4-one	VYCKCQBOVSSJSK-PYQWHEAPSA-N	101420350	0.92	0.81	0.87
Wtjiazwbwjbwfy-uhfffaoyasa-	WTJIAZWBWJBWJFEY-UHFFFAOYSA-N	13855598	0.96	0.77	0.87
Hispaglabridin B	CJUFYKORDZSOLF-INIZCTEOSA-N	15228661	0.93	0.80	0.87
Epinephrine Hydrochloride	ATADHKWKHYVBTJ-FVGYRXGTSA-N	441411	0.95	0.78	0.86
Thymol	MGSRCZKZVOBKFT-UHFFFAOYSA-N	6989	0.88	0.85	0.86
Sinapine	HUJXHFRXWWGYQH-UHFFFAOYSA-O	5280385	0.91	0.81	0.86
Psoralidin	YABIJLLNNFURIJ-UHFFFAOYSA-N	5281806	0.94	0.78	0.86
Liensinine	XCUCMLUTCAKSOZ-FIRIVFDPSA-N	160644	0.90	0.82	0.86
(1,2,2,14,15,16,19,20,21,35,36-Undecahydroxy-3,6,11,24,32-pentaoxo-7,10,25,28,31,40-hexaoxaoctacyclo[35.2.1.05,39.08,27.09,30.012,17.018,23.033,38]tetraconta-4,12,14,16,18,20,22,33,35,37-decaen-29-yl) 3,4,5-trihydroxybenzoate	WTKZYPVTAXZSEM-UHFFFAOYSA-N	158193	0.89	0.83	0.86
Salvianic acid B	SNKFFCBZYFGCQN-UHFFFAOYSA-N	119177	0.87	0.85	0.86
2-((2S,3S)-4-((E)-3-((R)-1-carboxy-2-(3,4-dihydroxyphenyl)ethoxy)-3-oxoprop-1-enyl)-2-(3,4-dihydroxyphenyl)-7-hydroxy-2,3-dihydrobenzo[b]furan-3-carbonyloxy)-3-(3,4-dihydroxyphenyl)propanoic acid	SNKFFCBZYFGCQN-ARBMFGAVSA-N	6449855	0.87	0.85	0.86
(2R)-2-[3-[(2R,3R)-3-[(1R)-1-carboxy-2-(3,4-dihydroxyphenyl)ethoxy]carbonyl-2-(3,4-dihydroxyphenyl)-7-hydroxy-2,3-dihydro-1-benzofuran-4-yl]prop-2-enoyloxy]-3-(3,4-dihydroxyphenyl)propanoic acid	SNKFFCBZYFGCQN-HIIQBPGSA-N	92132738	0.87	0.85	0.86
Isoxanthohumol	YKGCBLWILMDSAV-UHFFFAOYSA-N	513197	0.96	0.76	0.86
(2S)-Isoxanthohumol	YKGCBLWILMDSAV-SFHVURJKSA-N	9928523	0.96	0.76	0.86
4-Aminosalicylic acid	WUBBRNOQWQTFEX-UHFFFAOYSA-N	4649	0.96	0.75	0.86
Oxidopamine	DIVDFZHCJEHGG-UHFFFAOYSA-N	4624	0.99	0.72	0.85
(2r,3s)-1,4-Bis(4-hydroxy-3-methoxyphenyl)-2,3-dimethylbutan-1-one	FPJCOLPRFZWPHM-QWHCGFSZSA-N	169883	0.84	0.86	0.85
(5-Hydroxy-4,6-dimethylpyridin-3-yl)methyl phosphate	RBCOYOYDYNXafa-UHFFFAOYSA-L	104817	0.86	0.84	0.85
Morphine	BQJCRHHNABKAKU-KBQPJGBKSA-N	5288826	0.94	0.76	0.85
Bismuth	JCXGWMGpzLAOME-UHFFFAOYSA-N	5359367	0.76	0.94	0.85
Isobavachin	KYFBXCHUXFKMGQ-IBGZPJMESA-N	193679	0.97	0.73	0.85
S-nitrosoglutathione	HYHSBSXUHZOYLX-WDSKDSINSA-N	104858	0.93	0.77	0.85
Diallyl trisulfide	UBAXRAHSPKWNCX-UHFFFAOYSA-N	16315	0.83	0.87	0.85
Flopropione	PTHLEKANMPKYDB-UHFFFAOYSA-N	3362	0.92	0.78	0.85
Maackiain	HUKSJTUUSUGIDC-ZBEGNZNMSA-N	91510	0.92	0.77	0.85
Squalene	YYGNTYWPHWGJRM-AAJYLUCBSA-N	638072	0.92	0.77	0.85
Carvacrol	RECUKUPTGUEGMW-UHFFFAOYSA-N	10364	0.86	0.83	0.84
Beta-Carotene	OENHQHLEOONYIE-JLTXRGRSLA-N	5280489	0.83	0.86	0.84
Glycyrol	LWESBHWAQZORCQ-UHFFFAOYSA-N	5320083	0.93	0.76	0.84
Astragalin	JPUKWEQWGBDDQB-QSOFNFLRSA-N	5282102	0.91	0.78	0.84

3,4-Dihydroxybenzoate	YQUVCSBJEUQKSH-UHFFFAOYSA-M	54675866	0.91	0.78	0.84
Brazilein	PGERTGWKXFAEFR-UHFFFAOYSA-N	6453902	0.95	0.74	0.84
Berberrubine	GLYPKDKODVRYGP-UHFFFAOYSA-O	72704	0.96	0.73	0.84
Xylitol	HEBKCHPVOIAQTA-NGQZWWQHPA-N	6912	0.90	0.79	0.84
Nonivamide	RGOVYLWUIBMPGK-UHFFFAOYSA-N	2998	0.86	0.82	0.84
Licochalcone C	WBDNTJSRHDSPSR-KPKJPENVSA-N	9840805	0.90	0.78	0.84
Glycoumarin	NZYSZZDSYBYLC-UHFFFAOYSA-N	5317756	0.93	0.75	0.84
Manganous cation	WAEMQWOKJMHJLA-UHFFFAOYSA-N	27854	0.78	0.90	0.84
Swertiajaponin	DLVLXOYLQKCAMED-DGHBBABESA-N	442659	0.90	0.78	0.84
(E,Z)-farnesol	CRDAMVZIKSXFV-GNESMGCMSA-N	1549109	0.92	0.76	0.84
Geranylgeraniol	OJISWRZIEWCUBN-QIRCYJPOSA-N	5281365	0.92	0.76	0.84
trans,trans-Farnesol	CRDAMVZIKSXFV-YFVJMOTDSA-N	445070	0.92	0.76	0.84
Isogarcinol	KXTNVBQRLRYVCO-LPSZMIQCSA-N	11135781	0.89	0.79	0.84
16,17-Dimethoxytricyclo[12.3.1.1.2,6]nonadeca-1(17),2,4,6(19),14(18),15-hexaene-3,9,15-triol	SBGBAZQAEOWGFT-UHFFFAOYSA-N	5319978	0.94	0.73	0.84
Geraniol	GLZPCOQZEFWAFX-JXMROGBWSA-N	637566	0.92	0.75	0.84
Geraniin	JQQBXPJFAKSPG-SVYIMCMUSA-N	3001497	0.86	0.81	0.84
Dauricine	AQASRZOCERRGBL-ROJLCIKYSA-N	73400	0.89	0.78	0.84
Nalorphine	UIQMVEYFGZJHCZ-SSTWWWIQSA-N	5284595	0.91	0.76	0.83
Terbutaline	XWTYSIMOBUGWOL-UHFFFAOYSA-N	5403	0.93	0.74	0.83
Higenamine	WZRCQWQRFZITDX-UHFFFAOYSA-N	114840	0.90	0.76	0.83
Dicumarol	DOBMPNYZJYQDQZ-UHFFFAOYSA-N	54676038	0.86	0.80	0.83
Jatrorrhizine	MXTLAHSTUOXGQF-UHFFFAOYSA-O	72323	0.95	0.71	0.83
Oxitriptan	LDCYZAJDBXYCGN-VIFPVQESA-N	439280	0.94	0.72	0.83
Bakuchiol	LFYJSSARVMHQJB-QIXNEVBVSA-N	5468522	0.89	0.77	0.83
Mangiferin	AEDDIBAIWPIIBD-ZJKJAXBQSA-N	5281647	0.91	0.75	0.83
(10)-Gingerol	AIULWNKTYPYAN-SFHURJKSA-N	168115	0.84	0.82	0.83
3-(2-Hydroxyphenyl)prop-2-enal	BSDNZCQPDVDET-UHFFFAOYSA-N	98373	0.83	0.83	0.83
(1E)-1-(4-Hydroxy-3-methoxyphenyl)-7-phenyl-1-hepten-3-one	OKVCTOBWIAGOMR-ACCUITESSA-N	6440365	0.85	0.80	0.83
Glutamic Acid	WHUUTDBJXRKMK-VKHYHEASA-N	33032	0.94	0.71	0.83
Pentachlorophenol	IZUPBVBPLAPZRR-UHFFFAOYSA-N	992	0.95	0.70	0.83
Gingerol	NLDDIKRKFEXWBK-AWEZLNQCLSA-N	442793	0.83	0.82	0.82
Phellodendrine	RBBVNPQTBKHQEQ-KKSFZXQISA-O	3081405	0.93	0.72	0.82
Columbamine	YYFODHQVODIOQ-UHFFFAOYSA-O	72310	0.95	0.70	0.82
4-Hydroxycoumarin	VXIXUWQIVKSKSA-UHFFFAOYSA-N	54682930	0.92	0.72	0.82
Aspartic Acid	CKLJMWTZIZHCS-REOHCLBHTSA-N	5960	0.92	0.72	0.82
Cyclanoline	LKLWVKCEYSPQHL-KKSFZXQISA-O	3082134	0.93	0.71	0.82
Erianin	UXDFUVFNIAJEGM-UHFFFAOYSA-N	356759	0.85	0.79	0.82
Galactitol	FBPFZTCFMRRESA-GUCUJZISA-N	11850	0.87	0.77	0.82
Sorbitol	FBPFZTCFMRRESA-JGWLITMVSA-N	5780	0.87	0.77	0.82
Mannitol	FBPFZTCFMRRESA-KVTDHHQDSA-N	6251	0.87	0.77	0.82
Osajin	DCTLJGWMHPGCOS-UHFFFAOYSA-N	95168	0.85	0.79	0.82
Glycybenzofuran	OEIIVGQLDAYZNT-UHFFFAOYSA-N	46934435	0.88	0.76	0.82
Lecanoric acid	HEMSJKZDHNSSEW-UHFFFAOYSA-N	99613	0.91	0.73	0.82
Phenol	ISWSIDIOOBQZ-UHFFFAOYSA-N	996	0.85	0.78	0.82
Bisphenol A	IISBACLAFKSPIT-UHFFFAOYSA-N	6623	0.89	0.74	0.82
4-Allylphenol	RGBXDHONMXTLI-UHFFFAOYSA-N	68148	0.86	0.77	0.82
3,5-Dihydroxybenzoic acid	UYEMGAFJOZZIFP-UHFFFAOYSA-N	7424	0.90	0.74	0.82
Diphyllin	VMEJANRODATDOF-UHFFFAOYSA-N	100492	0.90	0.73	0.81
Octopamine	QHGUCRYDKWKLGM-UHFFFAOYSA-N	4581	0.90	0.73	0.81
Obtusifolin	NYRXUBDGDSTRBG-UHFFFAOYSA-N	3083575	0.90	0.73	0.81

Iodine	PNDPGZBMCMPRI-UHFFFAOYSA-N	807	0.73	0.89	0.81
o-Cresol	QWVGKYWNOKOFNN-UHFFFAOYSA-N	335	0.81	0.81	0.81
alpha-Peltatin	JGGWNGRBXJWAOC-HKJPBSJPSA-N	92129	0.93	0.69	0.81
Hydrogen Sulfide	RWSOTUBLDIXVET-UHFFFAOYSA-N	402	0.72	0.90	0.81
Isoliensinine	AJPXZTKPPINUKN-FIRIVFDPSA-N	5274591	0.87	0.75	0.81
5,7,2',3'-Tetrahydroxyflavone	STAGATUVRDVEAT-UHFFFAOYSA-N	5321864	0.89	0.73	0.81
Hexahydrocurcumin	RSAHICAPUYTWHW-UHFFFAOYSA-N	5318039	0.84	0.78	0.81
Potassium Chloride	WCUXLLCKKVVCTQ-UHFFFAOYSA-M	4873	0.74	0.88	0.81
Aluminum	XAGFODPZIPBFFR-UHFFFAOYSA-N	5359268	0.73	0.88	0.81
Cystine	LEVWYRKDKASIDU-IMJSIDKUSA-N	67678	0.92	0.69	0.81
Iron	XEEYBQQBJWHFJM-UHFFFAOYSA-N	23925	0.71	0.90	0.81
Ethylene Glycol	LYCAIKOWRPUZTN-UHFFFAOYSA-N	174	0.80	0.81	0.81
Chromium	VYZAMTAEIAYCRO-UHFFFAOYSA-N	23976	0.72	0.89	0.81
Irigenin	TUGWPJTTQNLKCL-UHFFFAOYSA-N	5464170	0.86	0.75	0.81
Silver	BQCADISMDOOEFD-UHFFFAOYSA-N	23954	0.71	0.90	0.81
Kurarinol	XMUPAAIHKAIUSU-QRQCRPRQSA-N	44563198	0.89	0.72	0.81
Copper	RYGMFSIKBFXOCR-UHFFFAOYSA-N	23978	0.72	0.89	0.81
Gossypol	QBKSWRVVCFDDOT-UHFFFAOYSA-N	3503	0.87	0.74	0.80
Juglone	KQPYUDDGWXQXHS-UHFFFAOYSA-N	3806	0.82	0.79	0.80
Potassium	ZLMJMSJWJFRBEC-UHFFFAOYSA-N	5462222	0.71	0.90	0.80
Vitamin e succinate	IELOKBJPULMYRW-NJQVLOCASA-N	20353	0.91	0.70	0.80
Qacsyxcuewlgne-morslucnsa-	QACSYXCUEWLGNE-MORSLUCNSA-N	14211700	0.87	0.73	0.80
(1R,3R,6R,7R,10R)-3-hydroxy-10-(4-hydroxy-3-methoxyphenyl)-8-[(2R)-3,5,7-trihydroxy-4-oxo-2,3-dihydrochromen-2-yl]-4-oxatricyclo[4.3.1.0 ^{3,7}]dec-8-en-2-one	CYGIJEJDYJOUAN-FAWCACSUSA-N	3033957	0.84	0.76	0.80
CID 3033858	OEXAKCYEHKMI-UHFFFAOYSA-N	3033858	0.70	0.90	0.80
(2S)-2-azaniumyl-5-[[[(2R)-3-[[[(2R)-2-[[[(4S)-4-azaniumyl-4-carboxylatobutanoyl]amino]-3-(carboxymethylamino)-3-oxopropyl]disulfanyl]-1-(carboxymethylamino)-1-oxopropan-2-yl]amino]-5-oxopentanoate	YPZRWBKMTBYPTK-BJDJZHNGSA-N	11215652	0.91	0.69	0.80
alpha-Carotene	ANVAOWXLWRTKGA-NTXLUARGSA-N	6419725	0.76	0.84	0.80
(-)-Neferine	MIBATSHDJRIUJK-IADGFXSZA-N	134693217	0.86	0.74	0.80
Neferine	MIBATSHDJRIUJK-ROJLCIKYSA-N	159654	0.86	0.74	0.80
Isoferulic acid	QURCVMIKCOAJU-HWKANZROSA-N	736186	0.88	0.72	0.80
	BTXNYTINYBABQR-UHFFFAOYSA-N	5281051	0.75	0.84	0.80
3,4-Methylenedioxyphenol	LUSZGTFNYDARNI-UHFFFAOYSA-N	68289	0.89	0.70	0.80
(3R,6E)-nerolidol	FQTLCLSUCAZDY-GOFCXVBSSA-N	11241545	0.85	0.74	0.79
Capillarisin	NTKNGUAZSFAKEE-UHFFFAOYSA-N	5281342	0.85	0.74	0.79
Cystathionine	ILRYPWNYFXEMH-UHFFFAOYSA-N	834	0.91	0.67	0.79
3-Hydroxyflavone	HVQAJTFOCKOKIN-UHFFFAOYSA-N	11349	0.93	0.65	0.79
Pyridoxal	RADKZDMFGJYCBB-UHFFFAOYSA-N	1050	0.84	0.75	0.79
Pamoic acid	WLJNZVDCPSBLRP-UHFFFAOYSA-N	8546	0.87	0.71	0.79
Boron	ZOXJGFHDHILPTG-UHFFFAOYSA-N	5462311	0.68	0.90	0.79
Icariin	TZJALUIVHRYQQB-XLRXWWTNSA-N	5318997	0.85	0.73	0.79
Plaunotol	SUWYPNNPLSRNPS-UNTSEYQFSA-N	5282197	0.85	0.73	0.79
Moracin G	PRQYZCKJWCQXNM-UHFFFAOYSA-N	5319890	0.86	0.71	0.78
D-serine	MTCFGRXMJLQNBG-UWTATZPHSA-N	71077	0.89	0.68	0.78

5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one	AIONOLUJZLIMTK-UHFFFAOYSA-N	3593	0.90	0.67	0.78
Hesperetin	AIONOLUJZLIMTK-AWEZLNQCLSA-N	72281	0.90	0.67	0.78
Leonurine	WNGSUWLDMMZFYNZ-UHFFFAOYSA-N	161464	0.84	0.72	0.78
(R)-1-(5,8-Dihydroxy-1,4-dioxo-1,4-dihydronaphthalen-2-yl)-4-methylpent-3-en-1-yl acetate	WNFXUXZJJKTOZ-OAHLLOKOSA-N	479501	0.86	0.71	0.78
Norathyriol	ZHTQCPCDXKMMLU-UHFFFAOYSA-N	5281656	0.94	0.62	0.78
Danthron	QBPFULOKWLNW-UHFFFAOYSA-N	2950	0.84	0.72	0.78
Asparagine	DCXYFEDJOCDAF-REOHCLBNSA-N	6267	0.87	0.69	0.78
Cysteamine	UFULAYFCSOUIOV-UHFFFAOYSA-N	6058	0.81	0.75	0.78
5-Hydroxyindole-3-acetic acid	DUUGKQCEGZLNO-UHFFFAOYSA-N	1826	0.90	0.66	0.78
Dihydrocapsaicin	XJQPQKLURWNAAH-UHFFFAOYSA-N	107982	0.85	0.70	0.78
Acetaminophen	RZVAJINKPMORJF-UHFFFAOYSA-N	1983	0.88	0.67	0.78
(2r)-7-Hydroxy-5-methoxy-2-phenylchroman-4-one	QQQCWVDPMPFUGF-CYBMUJFWSA-N	821279	0.86	0.68	0.77
7-Hydroxy-5-methoxy-2-phenylchroman-4-one	QQQCWVDPMPFUGF-UHFFFAOYSA-N	4053302	0.86	0.68	0.77
Selenocystine	JULROCUWKLNSBN-UHFFFAOYSA-N	15104	0.86	0.69	0.77
Tromethamine	LENZDBCJOHFCAS-UHFFFAOYSA-N	6503	0.77	0.78	0.77
Capsaicin	YKPUWZUDDOIDPM-SOFGYWHQSA-N	1548943	0.83	0.71	0.77
L-ornithine	AHLPHDHHMVZTML-BYPYZUCNSA-N	6262	0.83	0.71	0.77
Glutamine	ZDXPYRJPNDTMRX-VKHMHEASA-N	5961	0.88	0.66	0.77
P-Cresol	IWDCLRJOBRRNH-UHFFFAOYSA-N	2879	0.83	0.71	0.77
Cardamonin	NYSZJNUIVBQMM-BQYQJAHWSA-N	641785	0.81	0.73	0.77
Retinol	FPIPGXGPPQFEQ-OVSJKPMPSA-N	445354	0.75	0.78	0.77
Metformin	XZWYZLIPXDOLR-UHFFFAOYSA-N	4091	0.82	0.71	0.77
Phytol	BOTWFXYSPFMFN-RPYDDKJGSSA-N	5280435	0.86	0.67	0.77
(E,7R,11R)-15-methyl-3,7,11-tri((13C)methyl)(1,5,9,13,16-13C5)hexadec-2-en-1-ol	BOTWFXYSPFMFN-WGBUPJQTSAN	11301173	0.86	0.67	0.77
Pinocembrin	URFCJEUYNNAHFI-ZDUSSCGKSA-N	68071	0.94	0.59	0.77
Polydatin	HSTZMXCBWJGKHG-CUYWLFDKSA-N	5281718	0.82	0.71	0.76
Narciclasine	LZAZURSABQIKGB-AEKRLRDSA-N	72376	0.79	0.74	0.76
Tubocurarine	JFJZZMVDLULRGK-URLMMPGGSA-O	6000	0.92	0.61	0.76
Yakuchinone-A	TXELARZTKDBEKS-UHFFFAOYSA-N	133145	0.77	0.75	0.76
Lysine	KDXKERNBIXSRK-YFKPBYRVSAN	5962	0.82	0.70	0.76
Tyrosine	OUYCCASQSFEME-QMMMGPBSAN	6057	0.85	0.67	0.76
Isofangchinoline	IIQSIHUEZBTSAT-UHFFFAOYSA-N	321937	0.86	0.66	0.76
(1R,14S)-9,20,25-Trimethoxy-15,30-dimethyl-7,23-dioxo-15,30-diazaheptacyclo[22.6.2.23.6.18,12.114,18.027,31.022,33]hexatriaconta-3(36),4,6(35),8,10,12(34),18,20,22(33),24,26,31-dodecaen-21-ol	IIQSIHUEZBTSAT-WDYNHAJCSAN	5458555	0.86	0.66	0.76
Fangchinoline	IIQSIHUEZBTSAT-VMPREFPWSAN	73481	0.86	0.66	0.76
Dehydrocorybulbine	XWCVASCMTXXRY-UHFFFAOYSA-O	5316439	0.84	0.67	0.76
Plumbagin	VCMMXZQDRFWYSE-UHFFFAOYSA-N	10205	0.79	0.72	0.75
Berbamine	DFOCUWZXBASUQ-URLMMPGGSA-N	275182	0.89	0.62	0.75
Alizarin 1-methyl ether	VRGZEPNGEFVIZ-UHFFFAOYSA-N	80309	0.80	0.71	0.75
Pyridoxal phosphate	NGVDGCNFYWLIFO-UHFFFAOYSA-N	1051	0.79	0.72	0.75
Alkannin-beta-hydroxyisovalerate	MXANJRGHSFELEJ-UHFFFAOYSA-N	100203	0.86	0.65	0.75
Methylophiopogonanone A	BXTNNJQILYHJB-GFCCVEGCSAN	53466984	0.75	0.75	0.75

Methanol	OKKJLVBELUTLKV-UHFFFAOYSA-N	887	0.77	0.73	0.75
(2S)-7-[(2S,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-2,3-dihydrochromen-4-one	ARGKVCXINMKCAZ-QGFYHPQASA-N	73395	0.86	0.63	0.75
4-Hydroxybenzyl alcohol	BVJSUAQZOZWCKN-UHFFFAOYSA-N	125	0.77	0.73	0.75
Theanine	DATAGRPVKZEWAH-YFKPBYRVSA-N	439378	0.83	0.66	0.74
Salsalate	WVYADZUPLLSGPU-UHFFFAOYSA-N	5161	0.71	0.77	0.74
Vigabatrin	PJDFLNIOAUIZSL-UHFFFAOYSA-N	5665	0.88	0.60	0.74
Icariside II	NGMYNFJANBHLKA-XAPMVYOVSAN	44587252	0.78	0.70	0.74
Dimethyl sulfide	QMMFVYPAHWMCMS-UHFFFAOYSA-N	1068	0.74	0.74	0.74
Picroside II	AKNILCMFRRDTEY-NUGKWEESA-N	11944602	0.76	0.72	0.74
4-Nitrophenol	BTJIUGUIPKRLHP-UHFFFAOYSA-N	980	0.78	0.70	0.74
Gentisein	JJUNZBRHHGLJQW-UHFFFAOYSA-N	5281635	0.85	0.62	0.74
(+)-Pentazocine	VOKSWYLNZZRQPF-CCKFTAQKSA-N	12259685	0.77	0.69	0.73
Pentazocine	VOKSWYLNZZRQPF-GDIGMMSISA-N	441278	0.77	0.69	0.73
Isoindigotin	VBMISAYWIMDRCV-UHFFFAOYSA-N	164610	0.77	0.69	0.73
Folic Acid	OVBPIULPVIDEAO-LBPRGKRZSA-N	135398658	0.80	0.66	0.73
Liquiritin	DEMKZLAVQYISIA-ZRWXNEIDSA-N	503737	0.80	0.66	0.73
Pinostrobin	ORDDOBAOGKRJV-AWEZLNQCLSA-N	73201	0.83	0.63	0.73
Kojic acid	BEJNERDRQOWKJM-UHFFFAOYSA-N	3840	0.83	0.61	0.72
(+)-Tubocurarine chloride hydrochloride	GXFZCDMWGMFGFL-KKXMJGKMSA-N	64645	0.87	0.57	0.72
Oroxilin A	LKOJGSWUMISDOF-UHFFFAOYSA-N	5320315	0.81	0.63	0.72
Eupatorin	KLAOKWJLUQKWIF-UHFFFAOYSA-N	97214	0.80	0.64	0.72
Salicylamide	SKZKZFZAGNVIMN-UHFFFAOYSA-N	5147	0.68	0.76	0.72
Coumestrol	ZZIALNLLNHEQPJ-UHFFFAOYSA-N	5281707	0.85	0.58	0.72
Triclosan	XEFQLINVKFYRCS-UHFFFAOYSA-N	5564	0.84	0.59	0.72
Farrerol	DYHOLQACRGJEHX-ZDUSSCGKSA-N	442396	0.78	0.65	0.72
Glycerin	PEDCQBHIVMGVHV-UHFFFAOYSA-N	753	0.67	0.76	0.71
Jaceosidin	GLAAQZFBFGEBPS-UHFFFAOYSA-N	5379096	0.86	0.57	0.71
1,3-dimethyl-1H-pyrazol-4-amine	AXLKRXWNAFFPDB-UHFFFAOYSA-N	4431056	0.79	0.64	0.71
2-Methoxyestradiol	CQOQDQWUFQDJMK-SSTWWWIQSA-N	66414	0.80	0.62	0.71
Aloe emodin	YDQWDHRMZQUTBA-UHFFFAOYSA-N	10207	0.72	0.70	0.71
Tectorigenin	OBBCRPUNCUPUOS-UHFFFAOYSA-N	5281811	0.69	0.72	0.71
Rhein	FCDLCPWAQCPTKC-UHFFFAOYSA-N	10168	0.80	0.61	0.71
Gambogic acid	GEZHEQNLKAOMCA-RRZNCOCZSA-N	9852185	0.79	0.62	0.71
(Z)-4-[(1R,8R,17R,19R)-12-hydroxy-8,21,21-trimethyl-5-(3-methylbut-2-enyl)-8-(4-methylpent-3-enyl)-14,18-dioxo-3,7,20-trioxahexacyclo[15.4.1.02,15.02,19.04,13.06,11]docosa-4(13),5,9,11,15-pentaen-19-yl]-2-methylbut-2-enoic acid	GEZHEQNLKAOMCA-WUSASQBISA-N	6444190	0.79	0.62	0.71
Choline	OEYIOHPDSNJKLS-UHFFFAOYSA-N	305	0.70	0.71	0.70
Thiram	KUAZQDVKQLNFPE-UHFFFAOYSA-N	5455	0.76	0.65	0.70
Naloxone	UZHSEJADLWPNLE-GRGSLBFTSA-N	5284596	0.75	0.65	0.70
Choline hydroxide	KIZQNNOULOCVDM-UHFFFAOYSA-M	31255	0.70	0.70	0.70
Novobiocin	YJQPYGGHQPGBLI-KGSXXDOSSA-N	54675769	0.77	0.63	0.70
Hispidulin	IHFBPDAQLQOCBX-UHFFFAOYSA-N	5281628	0.78	0.62	0.70
Rottlerin	DEZFNHCVIZBHBI-ZHACJKMWSA-N	5281847	0.67	0.73	0.70
Licoflavone C	MEHHCBCRXIDGKZ-UHFFFAOYSA-N	10246505	0.73	0.66	0.70

Licochalcone a	KAZSKMJFUPEHHW-DHZHZOJOSA-N	5318998	0.68	0.71	0.70
Choline Chloride	SGMZJAMFUVOLNK-UHFFFAOYSA-M	6209	0.70	0.69	0.70
Allyl isothiocyanate	ZOJBYZNEUISWFT-UHFFFAOYSA-N	5971	0.59	0.80	0.70
Hesperidin	QUQPHWDTPGMPEX-QJBIFVCTSA-N	10621	0.83	0.56	0.69
(2S)-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[[[(2R,3R,4S,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxymethyl]oxan-2-yl]oxy-2,3-dihydrochromen-4-one	QUQPHWDTPGMPEX-REDIAKJPSA-N	129010007	0.83	0.56	0.69
Thiazole	FZWLAABWBMGSTSO-UHFFFAOYSA-N	9256	0.67	0.71	0.69
Inositol	CDAISMWEOUEBRE-UHFFFAOYSA-N	892	0.67	0.71	0.69
Indolo[2,1-b]quinazoline-6,12-dione	VQQVWGVXDIPORV-UHFFFAOYSA-N	73549	0.81	0.58	0.69
Fastigenin	VKOSQMWSWLZQPA-UHFFFAOYSA-N	162464	0.81	0.57	0.69
CID 15479638	XETHJOZXBVWLLM-HUKCQOFTSA-N	15479638	0.70	0.68	0.69
Tyrosol	YCCILVSKPBXVIP-UHFFFAOYSA-N	10393	0.75	0.62	0.68
Carnosine	CQOVNPNJLQNMDG-ZETCQYMHSA-N	439224	0.73	0.64	0.68
Dronabinol	CYQFCXCEBYINGO-IAGOWNOFSAN	16078	0.72	0.65	0.68
Pyridine	JUJWROOIHQBZHMGM-UHFFFAOYSA-N	1049	0.73	0.64	0.68
Linalool, (+/-)-	CDOSHBSSFJOMGT-UHFFFAOYSA-N	6549	0.69	0.67	0.68
Chloroform	HEDRZPFGACZZDS-UHFFFAOYSA-N	6212	0.61	0.75	0.68
2-Hydroxy-6-(8,11,14-pentadecatrienyl)benzoic acid	QUVGEKPNSCFQIR-AOSYACOCOSA-N	5388781	0.76	0.61	0.68
2-hydroxy-6-[(8Z,11Z)-pentadeca-8,11,14-trienyl]benzoic acid	QUVGEKPNSCFQIR-UTOQUPLUSA-N	9875131	0.76	0.61	0.68
Dyphylline	KSCFJBIXMNOVSH-UHFFFAOYSA-N	3182	0.73	0.63	0.68
Amantadine	DKNWSYNQZKUICI-UHFFFAOYSA-N	2130	0.70	0.66	0.68
Cupric Chloride	ORTQZVOHEJQUHG-UHFFFAOYSA-L	24014	0.61	0.74	0.68
Tocoretinate	RIQIXOWVAHQES-UNAKLNRMSA-N	5282180	0.67	0.68	0.68
Scopoletin	RODXRVNMMDRFIK-UHFFFAOYSA-N	5280460	0.72	0.63	0.68
Citral	WTEVQBCEXWBHNA-JXMROGBWSA-N	638011	0.81	0.54	0.68
Sakuranetin	DJOJDHGQRNZXQQ-AWEZLNQLSA-N	73571	0.83	0.52	0.68
Knipholone	DUENHQWYLVQDQK-UHFFFAOYSA-N	442753	0.74	0.61	0.67
Diosmin	GZSOSUNBTXMUFQ-YFAPSIMESA-N	5281613	0.74	0.61	0.67
Wedelolactone	XQDCKJKKMFWXGB-UHFFFAOYSA-N	5281813	0.78	0.56	0.67
Ethanol	LFQSCWFLJHTTHZ-UHFFFAOYSA-N	702	0.70	0.64	0.67
2-Hydroxy-6-(pentadec-8-en-1-yl)benzoic acid	YXHVCZZLWZYHSA-BQYQJAHWSA-N	5317600	0.69	0.66	0.67
Lupulone	LSDULPZJLTZEFD-UHFFFAOYSA-N	68051	0.78	0.56	0.67
Isosorbide	KLDXJTOISGUMSJ-JGWLITMVSA-N	12597	0.70	0.64	0.67
Methionine	FFEARJCKVFRZRR-BYPYZUCNSA-N	6137	0.84	0.50	0.67
D-Methionine	FFEARJCKVFRZRR-SCSAIBSYSAN	84815	0.84	0.50	0.67
Licarin A	ITDOFWOJEDZPCF-FNINDUDTSA-N	5281836	0.71	0.63	0.67
Orientin	PLAPMLGJVGLZOV-VPRICQMDSA-N	5281675	0.66	0.67	0.67
Berbinium, 7,8,13,13a-tetrahydro-9,10-dimethoxy-2,3-(methylenedioxy)-, chloride	VKJGBAJNNALVAV-UHFFFAOYSA-M	6426334	0.77	0.56	0.67
Carbon Tetrachloride	VZGDMQKNWNREIO-UHFFFAOYSA-N	5943	0.58	0.75	0.66
Amentoflavone	YUSWMAULDZXHPY-UHFFFAOYSA-N	5281600	0.65	0.68	0.66
Tetraethylammonium chloride	YMB CJWGV CUEGHA-UHFFFAOYSA-M	5946	0.66	0.67	0.66
trans-Dihydro-3R,4R-bis[(3-hydroxyphenyl)methyl]-2(3H)-furanone	HVDGDHBAMCBBLR-XPCCGILXSA-N	71684354	0.74	0.58	0.66
Caffeine	RYYVLZVUVIIVGH-UHFFFAOYSA-N	2519	0.73	0.59	0.66

Nanaomycin A	ZCJHPTKRISJQTN-JGVFFNPUSA-N	442757	0.67	0.65	0.66
Lapachol	CWPGNVFCJOPXFB-UHFFFAOYSA-N	3884	0.65	0.66	0.66
Potassium Nitrate	FGIUAXJPYTZDNR-UHFFFAOYSA-N	24434	0.67	0.64	0.65
(Z)-methyl 4-(2-(3,4-dihydroxyphenethoxy)-2-oxoethyl)-3-ethylidene-2-((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yloxy)-3,4-dihydro-2H-pyran-5-carboxylate	RFWGABANNQMHMZ-DAYOUXAKSA-N	134688908	0.61	0.70	0.65
Oleuropein	RFWGABANNQMHMZ-ZCHJGGQASA-N	5281544	0.61	0.70	0.65
(4S,5Z,6R)-4-[2-[2-(3,4-dihydroxyphenyl)ethoxy]-2-oxoethyl]-5-ethylidene-6-(((2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)-2-oxanyl]oxy)-4H-pyran-3-carboxylic acid methyl ester	RFWGABANNQMHMZ-WLFYAOHHSAN	6325757	0.61	0.70	0.65
Propylene Glycol	DNIAPMSPWPWGF-UHFFFAOYSA-N	1030	0.68	0.63	0.65
Tiliroside	DVGGLGXQSFURLP-VWMSDXGPSA-N	5320686	0.65	0.65	0.65
Bergaptol	GIJHDGJRTUSBJR-UHFFFAOYSA-N	5280371	0.70	0.61	0.65
Dalfampridine	NUKYPUAOHBNCYP-UHFFFAOYSA-N	1727	0.69	0.61	0.65
1-Propanol	BDERNNFJNOAEC-UHFFFAOYSA-N	1031	0.67	0.63	0.65
Isopropyl Alcohol	KFZMGEQAYNKOFK-UHFFFAOYSA-N	3776	0.63	0.67	0.65
Daminozide	NOQGZXFHARMLW-UHFFFAOYSA-N	15331	0.79	0.51	0.65
Famotidine	XUFQPHANEPEMJ-UHFFFAOYSA-N	5702160	0.74	0.56	0.65
Adenine	GFFGJBXGBJISGV-UHFFFAOYSA-N	190	0.73	0.56	0.65
Coumarin, 6-(2,3-dihydroxy-3-methylbutyl)-7-hydroxy-	WRTWKAQFZYXAEJ-LBPRGKRZSA-N	11149722	0.64	0.65	0.65
Usnic acid	CUCUKJLRRAKFN-UHFFFAOYSA-N	5646	0.64	0.65	0.65
3-Hydroxybenzoic acid	IJFXRHURBJZNAO-UHFFFAOYSA-N	7420	0.66	0.63	0.65
Ferruginol	QXNWVJJOHUAQHLM-AZUAARDMSA-N	442027	0.69	0.60	0.65
Allicin	JDLKFOPOAOFWQN-UHFFFAOYSA-N	65036	0.61	0.68	0.64
3-[(S)-prop-2-enylsulfanyl]sulfanylprop-1-ene	JDLKFOPOAOFWQN-VIFPVBQESA-N	51380898	0.61	0.68	0.64
Berberine	YBHILYKTIRIUTE-UHFFFAOYSA-N	2353	0.74	0.55	0.64
Phytonadione	MBWXNTAXLNYFJB-NKFFZRIASA-N	5284607	0.59	0.70	0.64
(2S)-2-hydroxypentanedioic acid	HWXBTNAVRSUOJR-VKHMHEASA-N	439939	0.75	0.53	0.64
Damnacanthal	IPDMWUNUULAXLU-UHFFFAOYSA-N	2948	0.66	0.62	0.64
Ajoene	IXELFRANAOWSF-FNORWQNLSA-N	5386591	0.63	0.65	0.64
(E)-1-(prop-2-enylsulfanyl)-3-[(S)-prop-2-enylsulfanyl]prop-1-ene	IXELFRANAOWSF-IYNGYCSASA-N	76962525	0.63	0.65	0.64
(Z)-Ajoene	IXELFRANAOWSF-ALCCZGGFSA-N	9881148	0.63	0.65	0.64
trans-Zeatin	UZKQTCBAMSWPJD-FARCUNLSSA-N	449093	0.70	0.58	0.64
Carnosol	XUSYGBPHQBWGAD-PJSUUKDQSA-N	442009	0.73	0.55	0.64
Tetrahydrocoptisine	UXYJCYXWJGAKQY-UHFFFAOYSA-N	6770	0.72	0.56	0.64
Tyramine	DZGWFCGJZKUFP-UHFFFAOYSA-N	5610	0.71	0.57	0.64
Dimethyl Sulfoxide	IAZDPXIOMUYVGZ-UHFFFAOYSA-N	679	0.69	0.58	0.64
Titanium Dioxide	GWEVSGVZZGPLCZ-UHFFFAOYSA-N	26042	0.59	0.68	0.64
D-Glucosamine	MSWZFWKMSRAUBD-IVMDWMLBSA-N	439213	0.63	0.64	0.63
Gamma-Aminobutyric Acid	BTCSSZJGUNDROE-UHFFFAOYSA-N	119	0.76	0.51	0.63

1-[(2Z)-2-(2,6-dicarboxy-2,3-dihydro-1H-pyridin-4-ylidene)ethylidene]-6-hydroxy-5-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-2,3-dihydroindol-1-ium-2-carboxylate	DHHFDKNIEVKVKS-UHFFFAOYSA-N	54600918	0.66	0.61	0.63
Hexachlorocyclohexane	JLYXXMFPNIAWKQ-UHFFFAOYSA-N	727	0.58	0.69	0.63
4-Hydroxybutanoic acid	SJZRECIVHVDYJC-UHFFFAOYSA-N	10413	0.76	0.50	0.63
Ikiizlytispeni-yridssqksa-	IKIIZLYTISPENI-YRIDSSQKSA-N	1549028	0.62	0.64	0.63
Baicalin	IKIIZLYTISPENI-ZFORQUDYSA-N	64982	0.62	0.64	0.63
Esculin	XHCADAYNFUFHF-TVKJYDDYSA-N	5281417	0.59	0.67	0.63
Cannabidiolic acid	WVOLTBSCXRRQFR-DLBZAZTESA-N	160570	0.65	0.61	0.63
3-[7,12-Bis[1-[2-amino-3-(methylamino)-3-oxopropyl]sulfanylethyl]-18-(2-carboxyethyl)-3,8,13,17-tetramethylporphyrin-21,23-diid-2-yl]propanoic acid;iron(2+)	WFBVWSTZNVJEAY-UHFFFAOYSA-L	439171	0.73	0.52	0.63
Prunin	DLIKSSGEMUFQOK-SFTVRKLSSA-N	92794	0.79	0.46	0.63
Cannabinol	VBGLYOIFKLUMQG-UHFFFAOYSA-N	2543	0.61	0.64	0.63
Isotrifoliol	OVLUQDOJWGTPHA-UHFFFAOYSA-N	5318679	0.77	0.48	0.63
Canthaxanthin	FDSDTBUPSURDBL-DKLMTRRASA-N	5281227	0.66	0.59	0.62
5,7-Dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	FTWIRXFELQLPI-UHFFFAOYSA-N	932	0.95	0.30	0.62
(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-4H-chromen-4-one	FTWIRXFELQLPI-CYBMUJFWSA-N	667495	0.95	0.30	0.62
Sphingosine	WWUZIQUQRGPMGP-KRWOKUGFSA-N	5280335	0.66	0.58	0.62
Theophylline	ZFXYFBGIUFBOJW-UHFFFAOYSA-N	2153	0.73	0.51	0.62
Benzene	UHOVQNZJYSORNB-UHFFFAOYSA-N	241	0.56	0.68	0.62
Hyperforin	KGSZHKRKHXOAMG-HQKKAZOISA-N	441298	0.67	0.57	0.62
Naringin	DFPMSGMNTNDNHN-ZPHOTFPESA-N	442428	0.72	0.51	0.62
Succinic Acid	KDYFGRWQOYBRFD-UHFFFAOYSA-N	1110	0.72	0.51	0.62
Eupatilin	DRRWBCNQOKKOL-UHFFFAOYSA-N	5273755	0.66	0.57	0.62
Humulone	VMSLCPKYRPDLN-OAQYLSRUSA-N	442911	0.65	0.58	0.61
Orcinol glucoside	YTXIGTCAQNODGD-UJPOAAIUSA-N	12315192	0.66	0.57	0.61
beta-D-Ribofuranose	HMFHBZSHGGEWLO-TXICZTDVSA-N	447347	0.56	0.67	0.61
Acetylcysteine	PWKSIMOEOPYIA-BYPYZUCNSA-N	12035	0.67	0.55	0.61
Creatine	CVSVTCORWBXHQV-UHFFFAOYSA-N	586	0.76	0.46	0.61
Aminophylline	FQFPAHBPWDRTLU-UHFFFAOYSA-N	9433	0.71	0.51	0.61
Astaxanthin	MQZIGYBFDPAKN-UWFIBFSHSA-N	5281224	0.69	0.53	0.61
beta-CITRONELLOL, (+/-)-	QMVPMAAFGQKVCJ-UHFFFAOYSA-N	8842	0.65	0.57	0.61
beta-CITRONELLOL, (R)-	QMVPMAAFGQKVCJ-SNVBAGLBSA-N	101977	0.65	0.57	0.61
iron;(2R,3R,4S,5S)-2,3,4,5,6-pentahydroxyhexanoic acid	QDUZQOIJXPPTLY-GMBKLUGCSA-N	9291	0.75	0.47	0.61
Echinatin	QJKMIJNRNLQSS-WEVVVXLNSA-N	6442675	0.59	0.63	0.61
Thiamine	JZRWCGZRTZMZEH-UHFFFAOYSA-N	1130	0.71	0.50	0.61
1,4-Diaminobutane	KIDHWZJUCRJVML-UHFFFAOYSA-N	1045	0.59	0.62	0.61
S-adenosyl-L-homocysteine	ZJUKTBDGOFHSH-WFMPWKQPSA-N	439155	0.66	0.55	0.60
Coptisine	XYHOBCEMEDLZUMP-UHFFFAOYSA-N	72322	0.65	0.56	0.60
Xanthoxylin	FBUBVLUPUDBFME-UHFFFAOYSA-N	66654	0.67	0.54	0.60
Anacardic acid	ADFWQBGTDIJESE-UHFFFAOYSA-N	167551	0.54	0.66	0.60
Bisdemethoxycurcumin	PREBVFJICNPEKM-YDWXAUTNSA-N	5315472	0.67	0.53	0.60
Lycorine	XGVJWXAYKUHD00-DANLNKNASA-N	72378	0.66	0.54	0.60
Pyrene-d10	BBEAQIROQSPTKN-LHNTUAQVSA-N	6912026	0.53	0.66	0.60

5-Hydroxy-1-(3-hydroxy-4-methoxyphenyl)decan-3-one	LPRPIMHDDACJHT-UHFFFAOYSA-N	90942	0.58	0.61	0.59
Glyceraldehyde	MNQZXJOMYWMBOU-UHFFFAOYSA-N	751	0.62	0.57	0.59
3-Iodothyronamine	XIINYOJWNGOUPF-UHFFFAOYSA-N	9950514	0.64	0.54	0.59
Raloxifene	GZUITABIKMVPG-UHFFFAOYSA-N	5035	0.64	0.53	0.59
Flavone	VHBFFQKBGNRLFZ-UHFFFAOYSA-N	10680	0.62	0.56	0.59
beta-L-Arabinopyranose	SRBFZHDQGSBBOR-KLVWXMOSA-N	439764	0.56	0.62	0.59
(2R)-3-(2-hydroxy-3-methoxyphenyl)-2-[2-methoxy-4-(3-sulfopropyl)phenoxy]propane-1-sulfonic acid	FOGYNLXERPKEGN-MRXNPFEDSA-N	25113471	0.59	0.58	0.59
Aniline	PAYRUJLWNCNPSJ-UHFFFAOYSA-N	6115	0.54	0.63	0.59
Adenosine	OIRDTQYFTABQOQ-KQYNXXCUSA-N	60961	0.59	0.58	0.58
Vidarabine	OIRDTQYFTABQOQ-UHTZMRCNSA-N	21704	0.59	0.58	0.58
Artemetin	RIGYMJVFEJNCKD-UHFFFAOYSA-N	5320351	0.58	0.58	0.58
N,N-Dimethylarginine	YDGMGEXADBMOMJ-LURJTMIESA-N	123831	0.62	0.54	0.58
Moracin F	MQRQKQBOYQLFAI-UHFFFAOYSA-N	5319889	0.70	0.46	0.58
Leucine enkephalin	URLZCHNOLZSCCA-VABKMULXSA-N	461776	0.65	0.51	0.58
3-Chloro-1,2-propanediol	SSZWWUDQMAHNAQ-UHFFFAOYSA-N	7290	0.51	0.64	0.58
Senna	IPQVTOJGNYVQEO-KGFNBKMBSA-N	73111	0.53	0.62	0.58
(7R,11R)-3,7,11,15-tetramethylhexadecanoic acid	RLCKHJSFHOZMDR-PWCWUJKSA-N	468706	0.67	0.48	0.58
Sulfur Dioxide	RAHZWNYVWXNFOC-UHFFFAOYSA-N	1119	0.50	0.65	0.58
angiotensin II	CZGUSIXMZVURDU-JZXHSEFVSA-N	172198	0.59	0.56	0.57
Pterisin B	SJNCSXMTBXDZQA-SECBINFHSA-N	115049	0.57	0.58	0.57
Triptobenzene H	NZQIHCWNAMEWEW-KKSFZXQISA-N	53363843	0.53	0.62	0.57
Sinomenine	INYYVPSBIVGPH-QHRIQVBSA-N	5459308	0.59	0.55	0.57
(1S,9R,10S)-3-hydroxy-4,12-dimethoxy-17-methyl-17-azatetracyclo[7.5.3.0.1,10.02,7]heptadeca-2(7),3,5,11-tetraen-13-one	INYYVPSBIVGPH-VPZZIHKRSA-N	1403661	0.59	0.55	0.57
D-Galactose	WQZGKKKJIFFOK-SVZMEOIVSA-N	6036	0.51	0.63	0.57
alpha-D-Mannopyranose	WQZGKKKJIFFOK-PQMKYFCFSA-N	185698	0.51	0.63	0.57
alpha-D-GALACTOSE	WQZGKKKJIFFOK-PHYPRDBBSA-N	439357	0.51	0.63	0.57
Estrone	DNXHEGUUPJUMQT-CBZIJGRNSA-N	5870	0.61	0.53	0.57
(8R,9R,13R,14S)-3-hydroxy-13-methyl-7,8,9,11,12,14,15,16-octahydro-6H-cyclopenta[a]phenanthren-17-one	DNXHEGUUPJUMQT-UIBILWFHSA-N	6918970	0.61	0.53	0.57
Scutellarin	DJSISFGPUUYILV-ZFORQUDYSA-N	185617	0.56	0.58	0.57
1-Butanol	LRHPLDYGVMQRHN-UHFFFAOYSA-N	263	0.54	0.60	0.57
Chelidonine	GHKISGDRQRSCII-ZOCIIQOWSA-N	197810	0.52	0.62	0.57
L-Fucose	SHZGCJCMOBCMKK-DHVFOXMCSA-N	17106	0.59	0.54	0.57
5-Azaniumyl-4-oxopentanoate	ZGXJTSGNIOSYLO-UHFFFAOYSA-N	7048523	0.65	0.48	0.56
leukotriene D4	YEESKJGWJFYOOK-IJHYULJSSA-N	5280878	0.65	0.48	0.56
Retinal	NCYCYZXNIZJOKI-OVSJKPMPSA-N	638015	0.59	0.53	0.56
Piperidine	NQRYJNQNLNOLGT-UHFFFAOYSA-N	8082	0.52	0.60	0.56
4-Chlorophenol	WXNZTHHGJRFKXQ-UHFFFAOYSA-N	4684	0.69	0.43	0.56
1-Tetradecanol	HLZKNKRTKFSKGZ-UHFFFAOYSA-N	8209	0.51	0.61	0.56
1-Octanol	KBPLFHHGFOOTCA-UHFFFAOYSA-N	957	0.51	0.61	0.56
Mesoridazine	SLVMESMUMVCIQY-UHFFFAOYSA-N	4078	0.53	0.59	0.56
Embelin	IRSFLDGTQHBADP-UHFFFAOYSA-N	3218	0.54	0.58	0.56
Imidazole	RAXXELZNTBOGNW-UHFFFAOYSA-N	795	0.60	0.52	0.56
D-(-)-Fructose	BJHIKXHVCFQLS-UYFOZJQFSA-N	5984	0.63	0.48	0.56
Isovitexin	MYXNWGACZJSMBT-VJXVFPJBSA-N	162350	0.57	0.54	0.56

Falcarinol	UGJAEDFOKNAMQD-QXPKXGMISA-N	5281149	0.56	0.55	0.56
Panaxynol	UGJAEDFOKNAMQD-MQNTZWLQSA-N	5469789	0.56	0.55	0.56
Valine	KZSNJWFQEVHDMF-BYPYZUCNSA-N	6287	0.66	0.44	0.55
Amarogentin	DBOVHQOUSDWAPQ-WTONXPSSSA-N	115149	0.50	0.59	0.55
Urea	XSQUKJJFZCRTK-UHFFFAOYSA-N	1176	0.57	0.51	0.54
Rhododendrol	SFUCGABQOMYVJW-MRVPVSSYSA-N	919205	0.54	0.54	0.54
Worenine	LCXREBMNASQAOC-UHFFFAOYSA-N	20055073	0.53	0.55	0.54
Threonine	AYFVYJQAPQTCCC-GBXIUSLDSA-N	6288	0.67	0.41	0.54
2-Azaniumylacetate	DHMQDGOQFOQNFH-UHFFFAOYSA-N	5257127	0.57	0.51	0.54
Calycosin	ZZAJQOPSWWVMBI-UHFFFAOYSA-N	5280448	0.54	0.54	0.54
5'-Deoxy-5'-methylthioadenosine	WUUGFSXJNOTRMR-IOSLPCCCSA-N	439176	0.59	0.49	0.54
Benzo[a]pyrene	FMMWHPNWAFZXNH-UHFFFAOYSA-N	2336	0.60	0.47	0.53
Acrolein	HGINCPLSRVDWNT-UHFFFAOYSA-N	7847	0.46	0.60	0.53
Bradykinin	QXZGBUJJYSZLT-FDISYFBSA-N	439201	0.49	0.57	0.53
	UGQMRVRMYASKQ-UHFFFAOYSA-N	6021	0.50	0.56	0.53
Carnosic acid	QRYRORQUOLYVBU-VBKZILBWSA-N	65126	0.65	0.41	0.53
Pectolarigenin	GPQLHGCIUEJQK-UHFFFAOYSA-N	5320438	0.62	0.44	0.53
Alanine	QNAYBMKLOCPYJG-REOHCLBHSA-N	5950	0.65	0.41	0.53
Hydroxysafflor Yellow A	IAVUBSCVWHLRGE-UXEKTNMQSA-N	6443665	0.51	0.54	0.53
Diosmetin	MBNGWHIJMBWFHU-UHFFFAOYSA-N	5281612	0.51	0.55	0.53
7-[(2Z)-3,7-dimethylocta-2,6-dienoxy]chromen-2-one	RSDDHGSKLOSQFK-PTNGSMBKSA-N	1795390	0.49	0.56	0.53
Auraptene	RSDDHGSKLOSQFK-RVDMUPIBSA-N	1550607	0.49	0.56	0.53
Chrysophanic acid	LQGUBLBATBMXHT-UHFFFAOYSA-N	10208	0.59	0.46	0.52
Phenylephrine	SONNWWYBIRXJNDC-VIFPVQESA-N	6041	0.52	0.53	0.52
Corynoline	IQUGPRHKZLNCHGC-TYPHKJRSA-N	177014	0.46	0.59	0.52
Triptophenolide	KPXIBWGPZSPABK-FXAWDEMLSA-N	173273	0.51	0.53	0.52
Rhoifolin	RPMNUQRUHXIGHK-PYXJVEZSA-N	5282150	0.54	0.50	0.52
Bamipine	VZSXTYKGYWISGQ-UHFFFAOYSA-N	72075	0.50	0.54	0.52
Histamine	NTYJOPFIAHURM-UHFFFAOYSA-N	774	0.51	0.53	0.52
L-Tartaric acid	FEWJPZIEWOKRBE-JCYAYHJZSA-N	444305	0.62	0.42	0.52
Epiberberine	FPJQGFLUORYYPE-UHFFFAOYSA-N	160876	0.53	0.51	0.52
Asparaginyl-glycyl-aspartyl-phenylalanyl-glutamyl-glutamyl-isoleucyl-prolyl-glutamyl-glutamyl-O-sulfotyrosyl-leucine	MGVRBUNKWISLAM-DQWUKECYSA-N	16130959	0.60	0.44	0.52
Glycitein	DXYUAIFZCFRPTH-UHFFFAOYSA-N	5317750	0.49	0.55	0.52
Pentosalen	OLOOJGVNMBJLLR-UHFFFAOYSA-N	10212	0.53	0.50	0.52
Oxalic Acid	MUBZPKHOEPUJKR-UHFFFAOYSA-N	971	0.59	0.44	0.52
Imatinib	KTUFNOKKBVMGRW-UHFFFAOYSA-N	5291	0.53	0.50	0.52
Codeine	OROGSEYTTFOCAN-DNJOTXNNSA-N	5284371	0.57	0.46	0.51
Nonane	BKIMMITUMNQMOS-UHFFFAOYSA-N	8141	0.41	0.62	0.51
Tetradecane	BGHCVCJXZWKCC-UHFFFAOYSA-N	12389	0.41	0.62	0.51
Heptadecane	NDJXXXCMXVBJW-UHFFFAOYSA-N	12398	0.41	0.62	0.51
Agmatine	QYPPJABKJHAVHS-UHFFFAOYSA-N	199	0.46	0.57	0.51
Estriol	PROQIPRRNZUXQM-ZXXIGWHRSA-N	5756	0.58	0.44	0.51
Quetiapine	URKOMYMAXPYINW-UHFFFAOYSA-N	5002	0.50	0.52	0.51
Ethinyl Estradiol	BFPYWIDHMRZLRN-SLHNCBLASA-N	5991	0.62	0.40	0.51
1-Butene, 4-isothiocyanato-1-(methylsulfinyl)-	KQGJFQMGPDOVOE-RXNUUUNCSA-N	90479303	0.46	0.56	0.51
Phenanthrene	YNPNZTXNASCQKK-UHFFFAOYSA-N	995	0.53	0.49	0.51
Calcium Phosphate	QORWJWZARLRLPR-UHFFFAOYSA-H	24456	0.43	0.58	0.51
Phenylephrine Hydrochloride	OCYSGIYOXAGKQ-FVGYRXG TSA-N	5284443	0.48	0.53	0.50
Ubidecarenone	ACTIUHUUMQJHFO-UPTCCGCD SA-N	5281915	0.58	0.43	0.50

Abacavir	MCGSCOLBFJQGHM-SCZZXKLOSA-N	441300	0.51	0.50	0.50
(2S,3S,4S,5R)-2,3,4,5-tetrahydroxy-6-oxohexanoic acid	IAJILQKETJEXLJ-QTBDDELSSA-N	65041	0.59	0.42	0.50
Piperazine	GLUUGHFHGXJENI-UHFFFAOYSA-N	4837	0.40	0.61	0.50
N,N''''-Hexane-1,6-diylbis[N'-(4-chlorophenyl)triimidodicarbonic diamide]	GHXZTYHSJHQHIJ-UHFFFAOYSA-N	88536661	0.55	0.45	0.50
Glycolic Acid	AEMRFAOFKBGASW-UHFFFAOYSA-N	757	0.54	0.46	0.50
Carbonic Acid	BVKZGUZCCUSVTD-UHFFFAOYSA-N	767	0.57	0.43	0.50
Croctin	PANKHBYNKQNAHN-MQQNZMFNSA-N	5281232	0.59	0.41	0.50
	IRSCQMHWQWYFCW-UHFFFAOYSA-N	3454	0.56	0.43	0.50
(1R,5R,6R,7R,9S,11S,13S,14R)-3-amino-14-(hydroxymethyl)-8,10-dioxo-2,4-diazatetracyclo[7.3.1.1.7,11.01,6]tetradec-3-ene-5,9,12,13,14-pentol	CFMYXEVWODSLAX-DSCPYQGSSA-N	139251219	0.49	0.50	0.50
Tetrodotoxin	CFMYXEVWODSLAX-QOZOJKKESA-N	11174599	0.49	0.50	0.50
Cepharanthine	YVPVXANRNDGTA-WDYNHAJCSA-N	10206	0.50	0.49	0.50
Propionic Acid	XBDQKXXYIPTUBI-UHFFFAOYSA-N	1032	0.62	0.37	0.49
Cearoin	NFJVELXCUBWAFL-UHFFFAOYSA-N	3938139	0.43	0.56	0.49
Sulforaphane	SUVMJBTUFCVSAD-UHFFFAOYSA-N	5350	0.43	0.55	0.49
Tacedinaline	VAZAPHZUAVEOMC-UHFFFAOYSA-N	2746	0.44	0.54	0.49
Tetrandrine	WVTKBKWTSCRNU-KYJUHHHDHSA-N	73078	0.50	0.48	0.49
Hanfangchin A	WVTKBKWTSCRNU-ZSXSBBPPSA-N	5321894	0.50	0.48	0.49
Norephedrine	DLNKOYKMWOXYQA-VXNVDRBHSA-N	26934	0.46	0.52	0.49
Cathine	DLNKOYKMWOXYQA-IONNQARKSA-N	441457	0.46	0.52	0.49
Phenylpropanolamine	DLNKOYKMWOXYQA-CBAPKCEASA-N	10297	0.46	0.52	0.49
1-Deoxynojirimycin	LXBIFEVIBLOUGU-JGWLITMVSA-N	29435	0.48	0.49	0.49
Isosorbide Dinitrate	MOYKHGMNXAOIAT-JGWLITMVSA-N	6883	0.45	0.52	0.49
Corylin	PWAACAMQKVIIPZ-UHFFFAOYSA-N	5316097	0.58	0.39	0.49
Palmitoleic Acid	SECPZKHBENQXJG-FPLPWBNSLA-N	445638	0.62	0.35	0.49
Elaidic Acid	ZQPPMHVWEC SIRJ-MDZDMXLPSA-N	637517	0.62	0.35	0.49
Erucic Acid	DPUOLQHDNGRHBS-KTKRTIGZSA-N	5281116	0.62	0.35	0.49
Oleic Acid	ZQPPMHVWEC SIRJ-KTKRTIGZSA-N	445639	0.62	0.35	0.49
Tryptamine	APJYDQYYACXCRM-UHFFFAOYSA-N	1150	0.39	0.58	0.49
Chryseriol	SCZVLDHREVKTSH-UHFFFAOYSA-N	5280666	0.50	0.47	0.49
Valproic Acid	NIJJYAXOARWZEE-UHFFFAOYSA-N	3121	0.62	0.35	0.48
Panduratin A	LYDZCXVWCFJAKQ-ZFGGDYGUSA-N	6483648	0.38	0.58	0.48
Alfatradiol	VOXZDWNVPJITMN-SFFUCWETSA-N	68570	0.51	0.46	0.48
Estradiol	VOXZDWNVPJITMN-ZBRFXRBCSA-N	5757	0.51	0.46	0.48
Acrylamide	HRPVXLWXLDXGHG-UHFFFAOYSA-N	6579	0.49	0.48	0.48
Tryptophan	QIVBCDIJAJPQS-VIFPVBQESA-N	6305	0.49	0.47	0.48
Trihexyphenidyl	HWHLPGVTGWGOCJO-UHFFFAOYSA-N	5572	0.44	0.52	0.48
Crotonoside	MIKUYHYGGJMLM-UUOKFMHZSA-N	65085	0.55	0.41	0.48
Linolenic Acid	DTOSIQBPPRVQHS-PDBXOOCHSA-N	5280934	0.56	0.40	0.48
Cannabidiol	QHMBSVQNZTUGM-ZWKOTPCHSA-N	644019	0.45	0.51	0.48
1,3-Benzenediol, 2-[3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-, (1R-trans)-	QHMBSVQNZTUGM-MSOLQXFVSA-N	36688143	0.45	0.51	0.48
Malonic acid	OFOBLEOULBTSOW-UHFFFAOYSA-N	867	0.55	0.41	0.48
Solifenacin Succinate	RXZMMZZRUPYENV-VROPFNGYSA-N	216457	0.53	0.42	0.47
Flavin adenine dinucleotide	VWWQXMAJ TJZDQX-UYBVJOGSSA-N	643975	0.46	0.48	0.47
Daidzein	ZQSIURDFPHDXIC-UHFFFAOYSA-N	5281708	0.51	0.43	0.47
Ifenprodil	UYNVMODNBIQB MV-UHFFFAOYSA-N	3689	0.46	0.48	0.47
Swainsonine	FXUAIOAOAVCGD-WCTZXXKLSA-N	51683	0.40	0.54	0.47

Schisandrin B	RTZKSTLPRTWFEV-UHFFFAOYSA-N	108130	0.51	0.42	0.47
(2S,3R,4S,5R,6S)-3,4,5-trihydroxy-6-(5-hydroxy-6-methoxy-4-oxo-2-phenylchromen-7-yl)oxyoxane-2-carboxylic acid	QXIPXNZUEQYPLZ-ICTYFKLBSA-N	636815	0.43	0.50	0.47
Ademetionine	MEFKEPWMEQBKI-AIRLBKTGSA-N	34755	0.46	0.46	0.46
Isosorbide Mononitrate	YWXYYSYQOXTPL-SLPGGIOYSA-N	27661	0.42	0.50	0.46
Riboflavin	AUNGANRZJHBGPY-SCRDCRAPSA-N	493570	0.52	0.40	0.46
Sarcosine	FSYKLYZXJSPZ-UHFFFAOYSA-N	1088	0.50	0.42	0.46
Episesamin	PEYUIKBAABKQKQ-UHFFFAOYSA-N	5204	0.35	0.57	0.46
Sesamin	PEYUIKBAABKQKQ-AFHBHXEDSA-N	72307	0.35	0.57	0.46
Bicuculline	IYGYMKDQCDDOMRE-ZWKOTPCHSA-N	10237	0.38	0.54	0.46
4'-Hydroxyacetophenone	TXFPEBPIARQUIG-UHFFFAOYSA-N	7469	0.40	0.51	0.46
Succinate	KDYFGRWQOYBRFD-UHFFFAOYSA-L	160419	0.47	0.45	0.46
Thebaine	FQXXSQDCDRQNQE-VMDGZTHMSA-N	5324289	0.45	0.46	0.46
Citric Acid	KRKNYBCHXNGOX-UHFFFAOYSA-N	311	0.46	0.45	0.45
(3R,8S,9E)-heptadeca-1,9-dien-4,6-diyne-3,8-diol	QWCNQXNAFCBLV-KPJXMDVSA-N	56935895	0.39	0.52	0.45
Irisolidone	VOOFPOMXNLNEOF-UHFFFAOYSA-N	5281781	0.39	0.52	0.45
Eucalyptol	WEEGYLXZBRQIMU-UHFFFAOYSA-N	2758	0.41	0.49	0.45
Secalonic acid D	NFZJAYYORNVZNI-OCHURCMPSA-N	73431	0.30	0.60	0.45
(2S)-2-ammonio-4-(carbamimidamidooxy)butanoate	FSBIGDSBMBYOPN-VKHMHEASA-N	46224610	0.42	0.48	0.45
Palmitine	QUCQEUCGKTEBI-UHFFFAOYSA-N	19009	0.45	0.44	0.45
Paroxypropione	RARSHUDCJQSEFJ-UHFFFAOYSA-N	6271	0.41	0.47	0.44
Anonaine	VZTUKBKUWSDHFM-CYBMUJFWSA-N	160597	0.34	0.55	0.44
Ascaridole	MGYMHQJELJYRQS-UHFFFAOYSA-N	10545	0.34	0.54	0.44
Biperiden	YSXKPIUOCJLQIE-UHFFFAOYSA-N	2381	0.38	0.50	0.44
Alvolidib	BIIVYFLTOXDAOV-YVEFUNNKSA-N	5287969	0.38	0.50	0.44
Theobromine	YAPQBXYLJRXSA-UHFFFAOYSA-N	5429	0.49	0.39	0.44
Deoxydopphyllotoxin	ZGLXUQQMLLIKAN-SVIJTADQSA-N	345501	0.49	0.39	0.44
Gymnasterkoreayne B	HEYJULODWUSFKN-VVNDQVNCSA-N	10264498	0.40	0.48	0.44
1,2,3,4-Cyclobutanetetracarboxylic dianhydride	YGYCECQIOXZODZ-UHFFFAOYSA-N	107280	0.38	0.49	0.44
Sodium Sulfate	PMZURENOXWZQFD-UHFFFAOYSA-L	24436	0.31	0.55	0.43
Besigomsin	ZWRRJEICIPUPHZ-MYODQAERSA-N	3001662	0.46	0.40	0.43
(9S,10S)-3,4,5,19-tetramethoxy-9,10-dimethyl-15,17-dioxatetracyclo[10.7.0.0.2,7.0.14,18]nonadeca-1(19),2,4,6,12,14(18)-hexaen-10-ol	YBZZAVZIVCBPDJ-MYODQAERSA-N	59203477	0.46	0.40	0.43
Schizandrol B	ZWRRJEICIPUPHZ-SFDCACGMSA-N	68781	0.46	0.40	0.43
Topiramate	KJADKKWYZYXHBB-XBWDGYHZA-N	5284627	0.43	0.43	0.43
Humulene	FAMPSKZZVDUYOS-HRGUGZIWSA-N	5281520	0.31	0.55	0.43
Magnesium Carbonate	ZLNQXNFFQJAIU-UHFFFAOYSA-L	11029	0.40	0.45	0.43
	UYTPUPDQBNUYGX-UHFFFAOYSA-N	764	0.50	0.35	0.43
Noscapine	AKNNEGZIBPJZG-MSOLQXFVSA-N	275196	0.35	0.50	0.42
Gefitinib	XGALLCVXEZPNRQ-UHFFFAOYSA-N	123631	0.36	0.49	0.42
	ZOOGRGPOEVQDDX-UHFFFAOYSA-N	24316	0.45	0.40	0.42
Daunorubicin	STQGQHZAVUOBTE-VGBVRHCVSA-N	30323	0.39	0.46	0.42
Galantamine	ASUTZQLVASHGKV-JDFRZJQESA-N	9651	0.44	0.41	0.42
4-Aminobenzoic acid	ALYNCZNDIQEVRV-UHFFFAOYSA-N	978	0.39	0.45	0.42
Sesamol	ZZMNWJVJUKMZJY-AFHBHXEDSA-N	101746	0.37	0.47	0.42
4-Flavanol	YTMFRMLVZQOBDR-UHFFFAOYSA-N	253959	0.41	0.43	0.42

3,4,5-Trihydroxy-6-(5-hydroxy-8-methoxy-4-oxo-2-phenylchromen-7-yl)oxyoxane-2-carboxylic acid	LNOHXHDWGC MVCO-UHFFFAOYSA-N	12004622	0.37	0.48	0.42
Oroxindin	LNOHXHDWGC MVCO-NTKSAMNMSA-N	3084961	0.37	0.48	0.42
Ferrous sulfate heptahydrate	SURQXAFEQWPFV-UHFFFAOYSA-L	62662	0.29	0.55	0.42
Ergotamine	XCGSFFUVFURLIX-VFGNJEKYSA-N	8223	0.29	0.55	0.42
Emetine	AUVVAXYIELKVAI-CKBKHPWSWA-N	10219	0.48	0.35	0.42
Atorvastatin	XUKUURHRXDUEBC-KAYWLYCHSA-N	60823	0.44	0.39	0.42
alpha-Santalol	PDEQKAVEYSOLJX-RQGDDBKYSA-N	11085337	0.37	0.46	0.42
(Z)-alpha-Santalol	PDEQKAVEYSOLJX-YHYXMXQVSA-N	5281531	0.37	0.46	0.42
Indirubin	JNLNPCNGMHKCKO-UHFFFAOYSA-N	10177	0.34	0.49	0.42
Hydron;nonanedioate	BDJRBEYXGGNYIS-UHFFFAOYSA-N	19347555	0.43	0.40	0.42
Peimine	IUKLSMSEHKDIIP-BZMYINFQSA-N	131900	0.37	0.46	0.42
Fumaric Acid	VZCYOOQTPOCHFL-OWOJBTEDSA-N	444972	0.44	0.39	0.41
Sodium Nitrite	LPXPTNMVRIOKMN-UHFFFAOYSA-M	23668193	0.31	0.52	0.41
Nuciferine	ORJVQPIHKOARKV-OAHLLOKOSA-N	10146	0.39	0.44	0.41
Liriodenine	MUMCCPUVOAUBAN-UHFFFAOYSA-N	10144	0.31	0.52	0.41
Oxytocin	XNOPRXBHLZRZKH-DSZYJQQASA-N	439302	0.41	0.42	0.41
Melanin	XUMBMVFBXHLACL-UHFFFAOYSA-N	6325610	0.31	0.52	0.41
Wogonin	XLTFNNCXVBYBSX-UHFFFAOYSA-N	5281703	0.39	0.44	0.41
5-(2-Oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl)pentanoic acid	YBJHBAHKTGYVGT-UHFFFAOYSA-N	253	0.42	0.41	0.41
Biotin	YBJHBAHKTGYVGT-ZKWXMUHSA-N	171548	0.42	0.41	0.41
Echothiophate Iodide	OVXQHPWHMXOFRD-UHFFFAOYSA-M	10547	0.43	0.39	0.41
CID 134688154	RAFQELQLHMBRHD-BLOCSRKMSA-N	134688154	0.49	0.33	0.41
Magnesium Sulfate	CSNNHWWHGAXBCP-UHFFFAOYSA-L	24083	0.29	0.52	0.41
Acrylic acid	NIXOWILDQLNWCW-UHFFFAOYSA-N	6581	0.44	0.37	0.41
Oxyphenbutazone	HFHZKZSRXITVMK-UHFFFAOYSA-N	4641	0.35	0.46	0.41
Dipyron	DJGAAPFSPWAYTJ-UHFFFAOYSA-M	522325	0.31	0.50	0.41
Tylophorine, (-)-	SSEUDFYBEOIWGF-CQSZACIVSA-N	10883727	0.45	0.36	0.40
Tylophorine	SSEUDFYBEOIWGF-AWEZLNQCLSA-N	92114	0.45	0.36	0.40
Icosapent	JAZBEHYOTPTENJ-JLNKQSITSA-N	446284	0.46	0.35	0.40
Propranolol	AQHHDHLLHXJYJD-UHFFFAOYSA-N	4946	0.33	0.48	0.40
Susdlzpsrusarc-uhfffaoyasa-	SUSDLZPSRUSARC-UHFFFAOYSA-N	11762232	0.41	0.40	0.40
cobalt(2+);[(2R,5S)-5-(5,6-dimethylbenzimidazol-1-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl] 1-[3-[(4Z,9Z,14Z)-2,13,18-tris(2-amino-2-oxoethyl)-7,12,17-tris(3-amino-3-oxopropyl)-3,5,8,8,13,15,18,19-octamethyl-2,7,12,17-tetrahydrocorrin-3-yl]propanoylamino]propan-2-yl phosphate;cyanide	OWLMJFLNVIKMTJ-AKMVRCBCSA-M	16686079	0.43	0.38	0.40
Protopine	GPTFURBXHJWNHR-UHFFFAOYSA-N	4970	0.35	0.46	0.40
1-O-[(2R,3S,6R)-4-methoxy-16,18-dioxo-10-azapentacyclo[11.7.0.0.2.6.0.6.10.0.15.19]icosa-1(20),4,13,15(19)-tetraen-3-yl] 4-O-methyl 2-hydroxy-2-(4-hydroxy-4-methylpentyl)butanedioate	HYFHYPWGAURHIV-ZEDNPHJLSA-N	72332	0.37	0.43	0.40
Omacetaxine Mepesuccinate	HYFHYPWGAURHIV-JFIAXGOJSA-N	285033	0.37	0.43	0.40
Cobalin	AGVAZMGAQJOSFJ-UHFFFAOYSA-M	54605677	0.44	0.36	0.40
Cordycepin	OFEZSBMBBKLLBJ-BAJZRUMYSA-N	6303	0.31	0.49	0.40

Adenosine cyclic phosphate	IVOMOUWHDPKRL-LKQYNXXCUSA-N	6076	0.37	0.43	0.40
(3r)-8-[(2r,3s)-3-Heptyloxiran-2-yl]oct-1-ene-4,6-diyne-3-ol	GVLDGSIQZAFIAN-IXDOHACOSA-N	126312	0.35	0.45	0.40
Glc(b1-3)[Glc(b1-6)]Glc(b1-3)Glc(b1-3)Glc(b1-3)[Glc(b1-6)]b-Glc	MAXBMUKIXLNXGX-DMWITZOWSA-N	37723	0.40	0.40	0.40
Arachidonic Acid	YZXBAPSDXZZRGB-DOFZRALJSA-N	444899	0.44	0.35	0.40
Ritonavir	NCDNCNXCDXHOMX-XGKFQTDJSA-N	392622	0.27	0.52	0.40
Taurine	XOAAWQZATWQOTB-UHFFFAOYSA-N	1123	0.30	0.49	0.40
Stearic Acid	QIQXTHQIDYTRH-UHFFFAOYSA-N	5281	0.48	0.31	0.40
Tetracosanoic acid	QZZGJDVWLFXDLK-UHFFFAOYSA-N	11197	0.48	0.31	0.40
Lauric Acid	POULHZVOKOAJMA-UHFFFAOYSA-N	3893	0.48	0.31	0.40
Octanoic Acid	WWZKQHOCKIZLMA-UHFFFAOYSA-N	379	0.48	0.31	0.40
Nonanoic acid	FBUKVWPVBMHYJY-UHFFFAOYSA-N	8158	0.48	0.31	0.40
Myristic Acid	TUNFSRHWOTWDNC-UHFFFAOYSA-N	11005	0.48	0.31	0.40
Palmitic Acid	IPCSVZSSVZIGE-UHFFFAOYSA-N	985	0.48	0.31	0.40
Eleutheroside B	QJVXKWHHAMZTBY-GCPOEHJPSA-N	5316860	0.41	0.39	0.40
Pramoxine	DQKXQSGTHWVTAD-UHFFFAOYSA-N	4886	0.33	0.46	0.40
Meglutol	NPOAOTPXWNWTSN-UHFFFAOYSA-N	1662	0.42	0.37	0.39
Hydroflumethiazide	DMDGGSIALPNSEE-UHFFFAOYSA-N	3647	0.43	0.36	0.39
Pulmatin	WMMOMSNMMDMSRB-JNHRPPPUSA-N	442731	0.28	0.51	0.39
Calcium citrate	FNAQSUUGMSOBHW-UHFFFAOYSA-H	13136	0.34	0.45	0.39
[(2R,4S)-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl]-quinolin-4-ylmethanol	KMPWYEUPVWOPIM-RUAQEJLXSA-N	92131260	0.43	0.35	0.39
(2R,4aS,6aS,6aS,14aS,14bR)-10-hydroxy-2,4a,6a,6a,14a-pentamethyl-11-oxo-1,3,4,5,6,13,14,14b-octahydronicene-2-carboxylic acid	FXLVCCDIUNLGKU-BRUCSKOJSA-N	5701992	0.39	0.39	0.39
Deoxyschizandrin	JEJFTTRHGBKKEI-UHFFFAOYSA-N	43595	0.40	0.38	0.39
schisandrin A	JEJFTTRHGBKKEI-OKILXGFUSA-N	155256	0.40	0.38	0.39
Levofloxacin	GSDSWSVVLHKDQ-JTQLQIEISA-N	149096	0.43	0.34	0.39
Ofloxacin	GSDSWSVVLHKDQ-UHFFFAOYSA-N	4583	0.43	0.34	0.39
Urapidil	ICMGLRUYEQNHPE-UHFFFAOYSA-N	5639	0.38	0.39	0.39
3-Aminobenzoic acid	XFDUHJPVQKIXHO-UHFFFAOYSA-N	7419	0.41	0.36	0.39
Flavin mononucleotide	FVTCRASFAZXNN-SCRDCRAPSA-N	643976	0.39	0.38	0.39
Spinosin	VGGSLWDCMWZPO-ODEMIOGVSA-N	155692	0.31	0.46	0.39
Emedastine	KBUZBQVCBVDWGX-UHFFFAOYSA-N	3219	0.27	0.50	0.39
Dihomo-gamma-linolenic acid	HOBALERKJCKHQD-QNEBEIHSSA-N	5280581	0.42	0.35	0.38
Linoleic Acid	OYHQOLUKZRVURQ-HZJYTTRNSA-N	5280450	0.42	0.35	0.38
Pyrene	BBEAQIROQSPTKN-UHFFFAOYSA-N	31423	0.28	0.49	0.38
Cystadane	KWIUHFFTVRNATP-UHFFFAOYSA-O	248	0.41	0.36	0.38
Amyl Nitrite	OWFXIOWLTKNBAP-UHFFFAOYSA-N	8053	0.37	0.40	0.38
Acetamide	DLFVBJFMPXGRIB-UHFFFAOYSA-N	178	0.41	0.35	0.38
gamma-Linolenic acid	VZCETWTMQHEPK-QNEBEIHSSA-N	5280933	0.41	0.35	0.38
Kynurenine	YGPSJZOEDVAXAB-UHFFFAOYSA-N	846	0.27	0.49	0.38
Pyrazine-2-carboxylic acid	NIPZZXUFJPQHNH-UHFFFAOYSA-N	1047	0.42	0.34	0.38
Podofilox	YJGVMLPVUAXIQN-XVVDYKMHSA-N	10607	0.42	0.34	0.38
Picropodophyllin	YJGVMLPVUAXIQN-HAEOHBJNSA-N	72435	0.42	0.34	0.38
Acetic Acid	QTBSBXVTEAMEQO-UHFFFAOYSA-N	176	0.49	0.27	0.38
	RQFCJASXJCIDSX-UHFFFAOYSA-N	6804	0.37	0.39	0.38
(2R,3S,4S,5S,6R)-2,6-bis(hydroxymethyl)oxane-2,3,4,5-tetrol	HAIWUXASLYEWLM-ULQPCXBYSA-N	9815697	0.28	0.47	0.38
N-Methyldeoxynojirimycin	AAKDPDFZMNYDLR-XZBKPIIISA-N	92381	0.36	0.39	0.38
Dihydroberberine	FZAGOOYMTGPGF-UHFFFAOYSA-N	10217	0.41	0.34	0.38

prostaglandin A2	MYHXHCUNDDAE0Z-FOSBLDSVSA-N	5280880	0.41	0.34	0.38
	QGWNDRXFNRZMB-UHFFFAOYSA-N	8977	0.36	0.39	0.38
Isotretinoin	SHGAZHPCJPHSC-XYFACQKRSA-N	5282379	0.33	0.42	0.37
Tretinoin	SHGAZHPCJPHSC-YCNIQYBTSA-N	444795	0.33	0.42	0.37
Alitretinoin	SHGAZHPCJPHSC-ZVICIMWCZSA-N	449171	0.33	0.42	0.37
4,6-Methano-6H,14H-indolo[3,2,1-ij]oxepino[2,3,4-de]pyrrolo[2,3-h]quinoline, strychnidin-10-one deriv.	QMGVPSVNSZLJIA-UHFFFAOYSA-N	5304	0.39	0.36	0.37
Strychnine	QMGVPSVNSZLJIA-FVWCLLPLSA-N	441071	0.39	0.36	0.37
Fucoxanthin	SJWWTRQNNRNTPU-ABBNZJFMSA-N	5281239	0.34	0.41	0.37
Somatostatin	NHXLMOGPVYXJNR-ATOGVRKGSAN	16129706	0.34	0.41	0.37
Triptolide	DFBIRQPKNDILPW-CIVMWXNOSA-N	107985	0.35	0.39	0.37
2-Nonenal	BSAIUMLZVGUGKX-BQYQJAHWSA-N	5283335	0.32	0.42	0.37
Emetine dication	AUVVAXYIELKVAI-CKBKHPSWSA-P	11865426	0.37	0.37	0.37
Phenylethyl Alcohol	WRMNZCZEMHIOCP-UHFFFAOYSA-N	6054	0.20	0.54	0.37
Safrole	ZMQAAUBTXCXRIC-UHFFFAOYSA-N	5144	0.24	0.50	0.37
Beta-Elemene	OPFTUNCRGUEPRZ-QLFBSQMISA-N	6918391	0.35	0.38	0.37
Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, (1R,2R,4S)-rel-	OPFTUNCRGUEPRZ-UHFFFAOYSA-N	10583	0.35	0.38	0.37
Pilocarpine	QCHFTSOMWOSFHM-WPRPVWTQSA-N	5910	0.46	0.27	0.37
Tetrahydropalmatine	AEQDJSRLRWYMAQI-KRWDZBQOSA-N	72301	0.42	0.31	0.37
DL-Tetrahydropalmatine	AEQDJSRLRWYMAQI-UHFFFAOYSA-N	5417	0.42	0.31	0.37
7-[(E)-5-[(1S,3R)-3-hydroxy-2,2-dimethyl-6-methylidenecyclohexyl]-3-methylpent-2-enoyl]chromen-2-one	XXKXCRGLMFAXTK-ZTKAZNOESA-N	6443023	0.24	0.49	0.37
Bilobetin	IWEIJEPIYMAGTH-UHFFFAOYSA-N	5315459	0.26	0.48	0.37
Laminaran	DBTMGCOVALSLOR-VPNXCSTESA-N	439306	0.32	0.41	0.36
Schisandrol A	YEFOAORQXAOVJQ-RKNYENMMSA-N	11102092	0.35	0.38	0.36
Schisandrin	YEFOAORQXAOVJQ-RZFZLAGVSA-N	3001664	0.35	0.38	0.36
2,4-Decadienal	JZQKTMZYLHNFPL-BLHCBFLLSA-N	5283349	0.31	0.42	0.36
Anemonin	JLUQTCXCAFSSLD-UHFFFAOYSA-N	10496	0.28	0.45	0.36
Arbutin	BJRNKVDLDYUGJ-RMPHYRLSA-N	440936	0.29	0.44	0.36
Physcione	FFWOKTFYGVYKIR-UHFFFAOYSA-N	10639	0.42	0.31	0.36
D-Pinitol	DSCFFEYQKRSRV-FEPQRWDDSA-N	164619	0.34	0.39	0.36
6-Methoxycyclohexane-1,2,3,4,5-pentol	DSCFFEYQKRSRV-UHFFFAOYSA-N	230881	0.34	0.39	0.36
Phenoxyethanol	QCDWFXQBSFUVSP-UHFFFAOYSA-N	31236	0.26	0.46	0.36
(1R,2S)-2-(dimethylamino)-1-phenylpropan-1-ol	FMCGSUUUBYTWNDP-ONGXEEELSA-N	64782	0.23	0.49	0.36
Monocrotaline	QVCMHGGNRFMRAD-XFGHUUIASA-N	9415	0.35	0.37	0.36
Testolactone	BPEWUONVYDABNZ-DZBHQSCQSA-N	13769	0.28	0.44	0.36
Chelerythrine	LLEJIEBFSOEYIV-UHFFFAOYSA-N	2703	0.39	0.33	0.36
Hydrastine	JZUTXVTYJDCMDU-MOPGFXCFSA-N	197835	0.25	0.47	0.36
Chelerythrine hydroxide	YZYNINHQZLUUAW-UHFFFAOYSA-M	5351594	0.40	0.32	0.36
Benzylamine	WGQKYBSKWIADBV-UHFFFAOYSA-N	7504	0.24	0.48	0.36
Guaiol	TWVJWDMOZJXUID-SDDRHMPMSA-N	227829	0.30	0.42	0.36
(+)-Pronuciferine	WUYQEGNOQLRQAQ-CQSZACIVSA-N	200480	0.38	0.34	0.36
Malathion	JXSJBGJIGXNWCJ-UHFFFAOYSA-N	4004	0.38	0.33	0.36
Ellipticine	CTSPAMFJBXKSOY-UHFFFAOYSA-N	3213	0.32	0.39	0.36
3,3'-Diindolylmethane	VFTRKSBEFQDZKX-UHFFFAOYSA-N	3071	0.20	0.51	0.36
Dimenhydrinate	NFLKCVHYJRNRH-UHFFFAOYSA-N	10660	0.27	0.44	0.36

(1R,3R,5S,8S,9R,12S,13R)-1-hydroxy-14-(2-hydroxypropan-2-yl)-13-methyl-4,7,10-trioxapentacyclo[6.4.1.19,12.03,5.05,13]te tradecane-6,11-dione;(1R,3R,5S,8S,9R,12S,13R)-1-hydroxy-13-methyl-14-prop-1-en-2-yl-4,7,10-trioxapentacyclo[6.4.1.19,12.03,5.05,13]te tradecane-6,11-dione	VJKUPQSHOVKBCO-ZYMHLGHZSA-N	131704481	0.34	0.37	0.36
Adenosine-5'-triphosphate	ZKHQWZAMYRWXGA-KQYNXXCUSA-N	5957	0.30	0.41	0.36
[[[(2S,3R,4S,5S)-5-(6-aminopurin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxyhydroxyphosphoryl] phosphono hydrogen phosphate	ZKHQWZAMYRWXGA-DEGSGYPDSA-N	14308007	0.30	0.41	0.36
Diazepam	AAOVKJBEBIDNHE-UHFFFAOYSA-N	3016	0.30	0.41	0.36
Ajmaline	CJDRUOGAGYHKKD-RQBLFBSQSA-N	6100671	0.33	0.38	0.35
(S)-[(2R,5R)-5-ethylquinuclidin-2-yl]-(6-methoxy-4-quinolyl)methanol	LJQQGZACKSYWCH-QPWZMSJCSA-N	76974754	0.32	0.39	0.35
Atrazine	MXWJVTOOROXGIU-UHFFFAOYSA-N	2256	0.28	0.43	0.35
Oleamide	FATBGEAMYMYZAF-KTKRTIGZSA-N	5283387	0.41	0.30	0.35
Adenosine Phosphate	UDMBCSSLTHHNCN-KQYNXXCUSA-N	6083	0.30	0.41	0.35
Undecanal	KMPQYAYAQWNLME-UHFFFAOYSA-N	8186	0.28	0.43	0.35
Chlorpromazine	ZPEIMTDSQAKGNT-UHFFFAOYSA-N	2726	0.35	0.35	0.35
Lovenox	HTTJABKRGRZYRN-UHFFFAOYSA-N	772	0.34	0.36	0.35
Hexanal	JARKCYVAAOWBJS-UHFFFAOYSA-N	6184	0.27	0.43	0.35
Nortriptyline Hydrochloride	SHAYBENGXDALFF-UHFFFAOYSA-N	441358	0.14	0.56	0.35
Mescaline	RHCSKNNOAZULRK-UHFFFAOYSA-N	4076	0.33	0.36	0.35
Sanguinarium	INVGWHRKADIJHF-UHFFFAOYSA-N	5154	0.29	0.40	0.35
Acepromazine	NOSIYYJFMPDDSA-UHFFFAOYSA-N	6077	0.30	0.39	0.35
beta-Bourbonene	YIRAHEODBQONHI-ZQNQSHIBSA-N	62566	0.32	0.37	0.35
Virosecurinine	SWZMSZQQJKFBP-UHFFFAOYSA-N	267769	0.21	0.48	0.35
Securinine	SWZMSZQQJKFBP-WZRBSPASSA-N	442872	0.21	0.48	0.35
CID 107770	BJDCWCLMFKKGEE-KWWHLHYHASA-N	107770	0.27	0.42	0.35
Dihydroartemisinin	BJDCWCLMFKKGEE-ISOSDAIHSA-N	3000518	0.27	0.42	0.35
Brimonidine	XYLJNLCSTIOKRM-UHFFFAOYSA-N	2435	0.27	0.42	0.35
(4S)-4-methyl-3,4-dihydro-2H-chromene	LPQYIGNYKIDLEY-QMMMGPBSA-N	15939502	0.21	0.48	0.35
1-hydroxy-2-[(2S)-1-hydroxypropan-2-yl]-8,8-dimethyl-6,7-dihydro-5H-phenanthrene-3,4-dione	LGZJHSHOBYVDLA-SNVBAGLBSA-N	44425165	0.24	0.45	0.34
Indole-3-acetic acid	SEOVTRFCIGRIMH-UHFFFAOYSA-N	802	0.29	0.40	0.34
Paeonol	UILPJVPSNHJFIK-UHFFFAOYSA-N	11092	0.21	0.48	0.34
Phenylalanine	COLNVLDHVKWLRT-QMMMGPBSA-N	6140	0.22	0.46	0.34
Deguelin	ORDAZKGHNSNRHTD-UXHICEINSA-N	107935	0.30	0.38	0.34

2-[tert-butyl(dimethyl)silyl]oxy-5-trimethylsilylpent-4-ynal;ethoxyethane;[(E,6R)-10-methoxy-6-methyl-10-oxodec-2-en-4-ynoxy]-oxophosphonium;methyl (5R,8E,10E,12R)-5,12-dihydropentadeca-8,10-dien-6,14-diynoate;methyl (5R,8E,10E,12R)-5,12-dimethyl-15-trimethylsilylpentadeca-8,10-dien-6,14-diynoate	KUHCOHZWZMPBSF-YTYCSIDQSA-N	123916661	0.35	0.33	0.34
Gaboxadol	ZXRVKCBLGJOCEE-UHFFFAOYSA-N	3448	0.25	0.43	0.34
Macimorelin	UJVDJAPJQWZRFR-DHIUTWEWSA-N	9804938	0.32	0.36	0.34
L-Ala-L-Pro	WPWUFUBLGADILS-WDSKDSINSA-N	11892823	0.37	0.31	0.34
Celastrol	KQJSQWZMSAGSHN-JJWQIEB TSA-N	122724	0.36	0.31	0.34
3,13,21-Triazapentacyclo[11.8.0.02,10.04,9.015,20]henicosa-1(21),4,6,8,15,17,19-heptaen-14-one	FRMGMPSSCBFTSV-UHFFFAOYSA-N	118603930	0.35	0.32	0.34
17-[(E)-2,6-dihydroxy-6-methyl-3-oxohept-4-en-2-yl]-2,16-dihydroxy-4,4,9,13,14-pentamethyl-8,10,12,15,16,17-hexahydro-7H-cyclopenta[a]phenanthrene-3,11-dione	NISPVUDLMHQFRQ-VAWYXSNFSA-N	5353548	0.33	0.34	0.34
Cucurbitacin I	NISPVUDLMHQFRQ-MKIKIEMVSA-N	5281321	0.33	0.34	0.34
Cucurbitacin E	NDYMQXYDSVBNLL-MUYMLXPFS A-N	5281319	0.32	0.35	0.33
ELATERIN, alpha	NDYMQXYDSVBNLL-OUKQBFOZSA-N	5353547	0.32	0.35	0.33
	BXZVICBKDXVGW-UHFFFAOYSA-N	50599	0.22	0.45	0.33
Nitrazepam	KJONHKAYOJNZEC-UHFFFAOYSA-N	4506	0.21	0.46	0.33
Escitalopram	WSEQXVZVJXJVFP-FQEVSTJZSA-N	146570	0.16	0.51	0.33
Rotenone	JUVIOZPCNVVQFO-HBGVWJBISA-N	6758	0.29	0.38	0.33
Triptonide	SWOVVKGLGOOUKI-ZHGGVEMFSA-N	65411	0.31	0.36	0.33
Pyruvic Acid	LCTONWCANYUPML-UHFFFAOYSA-N	1060	0.38	0.29	0.33
Dextroamphetamine	KWTSXDURSIMDCE-QMMMGPBSA-N	5826	0.22	0.44	0.33
3-[(2E,5Z)-2-[[3-(2-carboxyethyl)-5-[(Z)-(3-ethenyl-4-methyl-5-oxopyrrol-2-ylidene)methyl]-4-methyl-1H-pyrrol-2-yl]methylidene]-5-[(4-ethenyl-3-methyl-5-oxopyrrol-2-yl)methylidene]-4-methylpyrrol-3-yl]propanoic acid	RCNSAJSGRJSBKK-NSQVQWHSSA-L	25245769	0.34	0.32	0.33
methyl (1R,9R,10S,11R,12R,19R)-11-acetyloxy-12-ethyl-4-[(13S,15S,17S)-17-ethyl-17-hydroxy-13-methoxycarbonyl-1,11-diazatetracyclo[13.3.1.04,12.05,10]nonadeca-4(12),5,7,9-tetraen-13-yl]-10-hydroxy-5-methoxy-8-methyl-8,16-diazapentacyclo[10.6.1.01,9.02,7.016,19]nonadeca-2,4,6,13-tetraene-10-carboxylate	JXLYSJRDCGARV-XQKSVPLYS A-N	241903	0.33	0.33	0.33

methyl (1S,10R,11S,12S)-11-acetyloxy-12-ethyl-4-[(13R,15R,17R)-17-ethyl-17-hydroxy-13-methoxycarbonyl-1,11-diazatetracyclo[13.3.1.04,12.05,10]nonadeca-4(12),5,7,9-tetraen-13-yl]-10-hydroxy-5-methoxy-8-methyl-8,16-diazapentacyclo[10.6.1.01,9.02,7.016,19]nonadeca-2,4,6,13-tetraene-10-carboxylate	JXLYSJRDCGCGARV-PFZUDZJ TSA-N	133126830	0.33	0.33	0.33
Vinblastine	JXLYSJRDCGCGARV-CFWMRBGOSA-N	13342	0.33	0.33	0.33
N-Acetyl-L-tryptophan	DZTHIGRZJZPRDV-LBPRGKRZSA-N	700653	0.26	0.40	0.33
Crocin	SEBIKDIMAPSUBY-RTJKDTQDSA-N	5281233	0.30	0.36	0.33
Atractylenolide III	FBMORZZOJSDNRQ-GLQYFDAESA-N	155948	0.27	0.39	0.33
(8aR)-9a-hydroxy-3,8a-dimethyl-5-methylidene-4,4a,6,7,8,9-hexahydrobenzo[f][1]benzofuran-2-one	FBMORZZOJSDNRQ-XGTXGMFGSA-N	5321031	0.27	0.39	0.33
Phlorizin	IOUVKUPGCMWBWT-QNDFHXLGSA-N	6072	0.27	0.39	0.33
Isoniazid	QRXWMOHMRWLFY-UHFFFAOYSA-N	3767	0.26	0.40	0.33
Osthol	MBRLOUHOWLUMFF-UHFFFAOYSA-N	10228	0.29	0.37	0.33
Quinoline	SMWDFEZVXVKB-UHFFFAOYSA-N	7047	0.22	0.43	0.33
Styrene	PPBRXRYQALVLMV-UHFFFAOYSA-N	7501	0.28	0.37	0.32
2,4-Dioxaspiro[5.5]undec-8-ene, 3-(2-furanyl)-	ODVKSTFPQDVPJZ-UHFFFAOYSA-N	105102	0.24	0.41	0.32
(2R)-2-[[[(1R,2S,6S)-5-hydroxy-2-(hydroxymethyl)-3,9-dioxatricyclo[4.4.0.02,4]dec-7-en-10-yl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol	LHDWRKICQLTVDL-IONKOTTMSA-N	138107792	0.36	0.29	0.32
CID 24721256	LHDWRKICQLTVDL-CLLMHHLUSA-N	24721256	0.36	0.29	0.32
Catalpol	LHDWRKICQLTVDL-PZYDOOQISA-N	91520	0.36	0.29	0.32
Biphenyl	ZUOUZKKEUPVFJK-UHFFFAOYSA-N	7095	0.24	0.41	0.32
(25R)-5alpha-Spirostan-3beta-ol	GMBQZIIUCVWOC-UHFFFAOYSA-N	219836	0.27	0.37	0.32
alpha-Maltose	GUBGYTABKSRVRQ-ASMJPISFSA-N	439341	0.21	0.43	0.32
Maltose	GUBGYTABKSRVRQ-QUYVBRFLSA-N	6255	0.21	0.43	0.32
Furo[2,3-c]pyridine, 4,5,6,7-tetrahydro-6-methyl-	KFHOLYHZRZLBP-UHFFFAOYSA-N	5325719	0.24	0.40	0.32
Cinnamamide, p-hydroxy-N-(p-hydroxyphenethyl)-	RXGUTQNKCXHALN-UHFFFAOYSA-N	89322	0.36	0.28	0.32
Lactic Acid	JVTAAEKCFNVCJ-UHFFFAOYSA-N	612	0.36	0.28	0.32
Lactic Acid, L-	JVTAAEKCFNVCJ-REOHCLB HSA-N	107689	0.36	0.28	0.32
N,N-Dimethylformamide	ZMXDDKWLCZADIW-UHFFFAOYSA-N	6228	0.25	0.39	0.32
ganoderic acid F	BWCNWXLKMWWVBT-AIMUVTGPSA-N	23247895	0.29	0.35	0.32
Linalyl acetate	UWKAYLJWKGQEPM-UHFFFAOYSA-N	8294	0.32	0.32	0.32
Quinine	LOUPRKONTZGTKE-WZBLMQSHSA-N	3034034	0.31	0.33	0.32
Quinidine	LOUPRKONTZGTKE-LHHVKLHASA-N	441074	0.31	0.33	0.32
(R)-[(2S,5R)-5-ethenyl-1-azabicyclo[2.2.2]octan-2-yl]-(6-methoxyquinolin-4-yl)methanol	LOUPRKONTZGTKE-VOMFEXJBSA-N	8549	0.31	0.33	0.32
(5E,9Z)-3,6,10-Trimethyl-8,11-dihydro-7H-cyclodeca[b]furan-4-one	XVOHELPNOXGRBQ-SJUGDSPGSA-N	13559418	0.14	0.49	0.32
Muscimol	ZJQHPWUVQJPQT-UHFFFAOYSA-N	4266	0.19	0.44	0.32
Isocorynoxine	MUVGVMUWMAGNSY-VKCGGMIFSA-N	3037448	0.25	0.38	0.32
Corynoxine	MUVGVMUWMAGNSY-KAXDATADSA-N	44568160	0.25	0.38	0.32

Brucine	RRKTZKIUPZVBMF-IBTVXLQLSA-N	442021	0.37	0.26	0.32
7-[(1R,2R,3R)-3-hydroxy-2-[(3S)-3-hydroxyoct-1-enyl]-5-oxocyclopentyl]heptanoic acid	GMVPRGQOIOIIMI-DODZYUBVSA-N	149351	0.30	0.33	0.32
Alprostadiil	GMVPRGQOIOIIMI-DWKJAMRDSA-N	5280723	0.30	0.33	0.32
Isorhynchophylline	DAXYUDFNWXHGBE-VKCGGMIFSA-N	3037048	0.26	0.37	0.32
Rhynchophylline	DAXYUDFNWXHGBE-KAXDATADSA-N	5281408	0.26	0.37	0.32
methyl (Z)-2-[(3R,6'S,7'S,8'aS)-6'-ethyl-2-oxospiro[1H-indole-3,1'-3,5,6,7,8,8a-hexahydro-2H-indolizine]-7'-yl]-3-methoxyprop-2-enoate	DAXYUDFNWXHGBE-KFFVICKMSA-N	53326136	0.26	0.37	0.32
m-Xylene	IVSZLXZYQVIEFR-UHFFFAOYSA-N	7929	0.18	0.45	0.31
Fluoranthene	GVEPBHOBDDJJI-UHFFFAOYSA-N	9154	0.20	0.43	0.31
Dehydrocostus lactone, (-)-	NETSQGRTUNRXEO-XUXIUHFCSA-N	73174	0.28	0.35	0.31
1-[[3-(Hydroxymethyl)phenyl]methyl]-5-phenylsulfanylpyrimidine-2,4-dione	GYPZBQHYLJOEML-UHFFFAOYSA-N	406936	0.28	0.35	0.31
delta-Elementene	MXDMETWAEGIFOE-UHFFFAOYSA-N	89316	0.21	0.41	0.31
Phenmetrazine Hydrochloride	VJNXVAVKCZJOFQ-UHFFFAOYSA-N	92159	0.20	0.42	0.31
Tuberostemonine	GYOGHROCTSEKDY-JJDZUBOLSA-N	100781	0.27	0.35	0.31
Maytansine	WKPWGQKGSOKKOO-RSFHAFMBSA-N	5281828	0.27	0.35	0.31
Crotonaldehyde	MLUCVPSAIDOCQM-NSCUHMNNSA-N	447466	0.25	0.37	0.31
Caryophyllene	NPNUFJAVOONJE-GFUGXAQUSA-N	5281515	0.17	0.45	0.31
Isocaryophyllene	NPNUFJAVOONJE-FLDDASRSA-N	5281522	0.17	0.45	0.31
(E)-2-epi-beta-caryophyllene	NPNUFJAVOONJE-QWAJQTJBSA-N	6429274	0.17	0.45	0.31
Caryophyllene, alpha + beta mixt.	NPNUFJAVOONJE-IZZDOVSWSA-N	5354499	0.17	0.45	0.31
Bethanidine	NIVZHWNOUVJHKV-UHFFFAOYSA-N	2368	0.18	0.44	0.31
Serlopitant	FLNYCRJBCNNHRH-OIYLJQICSA-N	23653789	0.21	0.41	0.31
Nitidine chloride	QLDAACVSUMUMOR-UHFFFAOYSA-M	25659	0.32	0.29	0.31
Hirsutine	NMLUOJBSAYAYEM-AZQGJTAVSA-N	3037884	0.26	0.35	0.31
Betaine	KWIUHFFTVRNATP-UHFFFAOYSA-N	247	0.29	0.32	0.31
Acetaldehyde	IKHGUXGNIITLKF-UHFFFAOYSA-N	177	0.25	0.36	0.30
Tilianin	NLZCOTZRUYWYPTP-MIUGBVLSSA-N	5321954	0.32	0.29	0.30
Kainic acid	VLSMHEGGTFMBBZ-OOZYFLPDSA-N	10255	0.38	0.23	0.30
Patchouli alcohol	GGHMUJBYLPPWFD-CUZKYEQNSA-N	10955174	0.22	0.39	0.30
2-methyl-3-[(2Z,6E,10E)-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenyl]naphthalene-1,4-dione	DKHGMERMDICWU-IFQAVNAMSA-N	13728967	0.30	0.31	0.30
Menaquinone 6	PFRQBZFETXBLTP-RCIYGOBDSA-N	5283547	0.30	0.31	0.30
Jasmone	XMLSXPIVAXONDL-PLNGDYQASA-N	1549018	0.24	0.37	0.30
(13S)-13-oxido-7-aza-13-azoniatetracyclo[7.7.1.0.2,7.0.13,17]heptadecan-6-one	XVPBINOPNYFXID-MTDTVKPRSA-N	137705180	0.24	0.37	0.30
(4R,7aS,13aR,13bR)-10-oxododecahydro-1H,5H-dipyrido[2,1-f:3',2',1'-ij][1,6]naphthyridine 4(41H)-oxide	XVPBINOPNYFXID-KAHWEZKRSA-N	124708617	0.24	0.37	0.30
Aristolochic acid	BBFQZRXYNIEMAW-UHFFFAOYSA-N	2236	0.29	0.31	0.30
Germacrone	CAULGCQHVOVVRN-SWZPTJTJSA-N	6436348	0.25	0.35	0.30
Vincristine	OGWKCGZFUXNPDA-XQKSVPLYSAN	5978	0.30	0.30	0.30
Hydroxy-(1-hydroxy-1-phosphono-2-pyridin-1-ium-3-ylethyl)phosphinate	IIDJRNMFWDHID-UHFFFAOYSA-N	44400168	0.22	0.38	0.30
Methoxsalen	QXKHYNVANLEOEG-UHFFFAOYSA-N	4114	0.21	0.39	0.30
Nicotine	SNICXCGAKADSCV-JTQLQIEISA-N	89594	0.27	0.33	0.30
3-(1-Methylpyrrolidin-2-yl)pyridine	SNICXCGAKADSCV-UHFFFAOYSA-N	942	0.27	0.33	0.30

Obacunone	MAYJEFRPIKEYBL-OASIGRBWSA-N	119041	0.21	0.39	0.30
	VGONTNSXDCQUGY-UHFFFAOYSA-N	65058	0.20	0.40	0.30
(1S,3R,6S,8S,9S,11S,12S,14S,15R,16R)-15-[(2R,5S)-5-(2-hydroxypropan-2-yl)-2-methyloxolan-2-yl]-7,7,12,16-tetramethylpentacyclo[9.7.0.0.1,3.0.3,8.0.1 2,16]octadecane-6,9,14-triol	WENNORDXYGDTP-WULFDVMBSA-N	13943290	0.26	0.34	0.30
Doconexent	MBMBGCFOFBJSJT-KUBAVDMBSA-N	445580	0.28	0.31	0.30
Peperomin E	HSEIBOLBSKVJFP-CQSZACIVSA-N	10476763	0.26	0.33	0.30
Tamsulosin	DRHKJLXIJQTDTD-OAHLLOKOSA-N	129211	0.22	0.37	0.30
Vincristine Sulfate	AQTQHPDCURKLT-KJDPCLQSA-N	249332	0.28	0.31	0.30
Quindoline	QOAKRWLMTKEDDL-UHFFFAOYSA-N	98912	0.26	0.33	0.30
Laevuflex	LKDRXBCSQODPBY-UHFFFAOYSA-N	3426	0.15	0.44	0.29
beta-D-Fructopyranose	LKDRXBCSQODPBY-ARQDHWQXSA-N	24310	0.15	0.44	0.29
D-Fructose	LKDRXBCSQODPBY-VRPWFDXSA-N	2723872	0.15	0.44	0.29
rosthorin A	AOUAZUQTHDBROH-BAFGBBEMSA-N	44445757	0.28	0.31	0.29
(4S,6R)-6-[(2R,4R)-4,6-dihydroxy-5-(sulfonatoamino)-2-(sulfonatooxymethyl)oxan-3-yl]oxy-3,4-dihydroxy-5-sulfonatooxoxane-2-carboxylate	OHJKXVLJWUPWQG-IUYNYSKSA-J	25244225	0.20	0.39	0.29
Zingiberene	KKOXKNGSUHTUBV-LSDHHAUSA-N	92776	0.19	0.40	0.29
Kinetin	QANMHLXAZMSUEX-UHFFFAOYSA-N	3830	0.21	0.38	0.29
Naphthalene	UFWIBTONFRDIAS-UHFFFAOYSA-N	931	0.16	0.43	0.29
Cyclohexanone	JHIVVAPYMSGYDF-UHFFFAOYSA-N	7967	0.20	0.38	0.29
	YKBGVZYEHEMREMT-UHFFFAOYSA-N	187790	0.25	0.33	0.29
(4E,7S,8R,11S,16R,21S)-11-[(2R,4R,5S,6R)-4-hydroxy-5-[(2S,4S,5S,6R)-4-hydroxy-5-[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-6-methyloxan-2-yl]oxy-6-methyloxan-2-yl]oxy-6-methyloxan-2-yl]oxy-1,8-dimethyl-2,18,22-trioxapentacyclo[17.2.1.0.4,21.0.7,16.0.8,13]docosa-4,13-diene-3,17-dione	LLMKHWMZTMSLENL-GRWKKFABSA-N	101010462	0.21	0.38	0.29
Demecolcine	NNJPGOLRFBJNIW-HNNXBMFYSA-N	220401	0.17	0.41	0.29
(E)-3-[3-(3-methylbut-2-enyl)-4-(3-phenylpropanoyloxy)phenyl]prop-2-enoic acid	BJIVLGIZOMJQRT-GXDHUFHOSA-N	9947201	0.22	0.36	0.29
Matrine	ZSBXGIUJOOQZMP-JLNYLFASSA-N	91466	0.21	0.37	0.29
Sophoridine	ZSBXGIUJOOQZMP-BHPKHCPMSA-N	165549	0.21	0.37	0.29
(+)-Sophoridine	ZSBXGIUJOOQZMP-UHFFFAOYSA-N	285698	0.21	0.37	0.29
Fomepizole	RIKMMFOAQPJVMX-UHFFFAOYSA-N	3406	0.20	0.38	0.29
	HAAZLUGHYHWQIW-UHFFFAOYSA-N	65103	0.24	0.33	0.29
Nitidine	KKMPGJPCJYRV-UHFFFAOYSA-N	4501	0.29	0.28	0.29
CID 5311489	WGWZNYKOUXOZTC-NAGNLMCHSA-N	5311489	0.25	0.32	0.29
Peiminine	IQDIERHFZVCNRZ-YUYPDVIUSA-N	167691	0.24	0.33	0.28
Dihydratanshinone I	HARGZZNYNSYSGJ-JTQLQIEISA-N	11425923	0.17	0.39	0.28
l-Menthol	NOOLISFMXDJSKH-KXUCPTDWSA-N	16666	0.17	0.39	0.28
Menthol	NOOLISFMXDJSKH-UHFFFAOYSA-N	1254	0.17	0.39	0.28
(+)-Menthol	NOOLISFMXDJSKH-AEJSXWLSA-N	165675	0.17	0.39	0.28
Linamarin	QLTCHMYAEJEXBT-ZEBDFXRSSA-N	11128	0.22	0.34	0.28
beta-EUDESOMOL	BOPIMTNSYWYZOC-VNHYZAJKSA-N	91457	0.23	0.33	0.28
1,4-Benzoquinone	AZQWKYJCGOJGHM-UHFFFAOYSA-N	4650	0.19	0.37	0.28

Ginkgolide J	LMEHVEUFNRJAAV-UKWFQYJISA-N	11154476	0.25	0.31	0.28
Vitamin A Palmitate	VYGQUTWHTHXGQB-FFHKNEKCSA-N	5280531	0.23	0.33	0.28
Regaloside A	PADHSFRQMFRWLS-MUUVXHEGSA-N	5459131	0.17	0.39	0.28
Alvespimycin	KUFRQPKVAVMTJO-LMZWQJSESA-N	5288674	0.19	0.37	0.28
Seselin	QUVCQYQEIOLHFZ-UHFFFAOYSA-N	68229	0.21	0.35	0.28
Bruceantinol	SREUSBYRKOPNJK-AJPRWBMOSEA-N	5281305	0.28	0.28	0.28
Domoic acid	VZFRNCSOCOPNDB-AOKDLOFSSA-N	5282253	0.30	0.25	0.28
(6R,7R,9R,11S)-16,17-Didehydro-9-de-2-piperidinylormosanine	SKOLRLSBMUGVOY-QPSCCSFWSA-N	139055730	0.19	0.36	0.28
prostaglandin A1(1-)	BGKHLCLZFGPIKKU-LDDQNKHRSA-M	22796709	0.26	0.29	0.28
Oxycodone	BRUQQQPBMZOVGD-XFKAJCMBSA-N	5284603	0.21	0.34	0.28
Loliolide	XEVQXKKKAVVSMW-WRWORJQWSA-N	100332	0.14	0.41	0.27
CID 441295	AMOGMTLMADGEOQ-WXQWCWKOSA-N	441295	0.23	0.32	0.27
Ginkgolide C	AMOGMTLMADGEOQ-DTDWCABLSA-N	9867869	0.23	0.32	0.27
Rutaecarpine	ACVGWSKVRYFWRP-UHFFFAOYSA-N	65752	0.22	0.33	0.27
Glyceryl Trioleate	PHYFQTYBJUILEZ-IUPFWZBISA-N	5497163	0.33	0.22	0.27
Justicidin D	WOELDRZIQLRDQB-UHFFFAOYSA-N	5318737	0.21	0.34	0.27
Azelastine	MBUVEWMHONZEQD-UHFFFAOYSA-N	2267	0.17	0.38	0.27
3,6,9-trimethyloctahydro-3,12-epoxy[1,2]dioxepino[4,3- <i>i</i>]isochromen-10(3H)-one	BLUAFEHZUWYNDE-UHFFFAOYSA-N	2240	0.21	0.34	0.27
(1R,13R)-1,5,9-trimethyl-11,14,15,16-tetraoxatetracyclo[10.3.1.0.4,13.0.8,13]hexadecan-10-one	BLUAFEHZUWYNDE-WJRFXBBSA-N	137704955	0.21	0.34	0.27
Artemisinin	BLUAFEHZUWYNDE-NNWCWBAJSA-N	68827	0.21	0.34	0.27
N-Acetyl-D-Glucosamine	OVRNDRQMDRJTHS-RTRLRJTCISA-N	439174	0.22	0.32	0.27
2-Acetamido-2-deoxy-alpha-D-glucopyranose	OVRNDRQMDRJTHS-PVFLNQBWSA-N	82313	0.22	0.32	0.27
N-ACETYL-beta-D-GLUCOSAMINE	OVRNDRQMDRJTHS-FMDGEEDCSA-N	24139	0.22	0.32	0.27
Celecoxib	RZEKVGVFLEQIL-UHFFFAOYSA-N	2662	0.25	0.29	0.27
Levocarnitine	PHIQHXFUZVPYII-ZCFIWBBSA-N	10917	0.24	0.30	0.27
Nifedipine	HYIMSNHJOBUNT-UHFFFAOYSA-N	4485	0.13	0.41	0.27
cyclosporin A	PMATZTZNYRCHOR-CGLBZJNRSA-N	5284373	0.23	0.31	0.27
alpha-IONONE	UZFLPKAIBPNNCA-BQYQJAHWSA-N	5282108	0.15	0.39	0.27
[S-(E)]-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	UZFLPKAIBPNNCA-ABZNLVYFSA-N	638013	0.15	0.39	0.27
Hippuric Acid	QIAFMBKCNZACKA-UHFFFAOYSA-N	464	0.16	0.38	0.27
Verapamil	SGTNSNPWRIOYBX-UHFFFAOYSA-N	2520	0.18	0.36	0.27
Meperidine	XADCESSVHJOZHK-UHFFFAOYSA-N	4058	0.15	0.38	0.27
Linderalactone	LWCKQMHSRRAA-QGQQYVBWSA-N	6450191	0.16	0.37	0.27
Methyl Ethyl Ketone	ZWEHNKRNPVVGH-UHFFFAOYSA-N	6569	0.23	0.30	0.27
[(2R)-2-pentadecanoyloxy-3-tridecanoyloxypropyl] hydrogen phosphate	UOOPRMYAWVCCZ-GDLZYMKVSA-M	5287505	0.27	0.26	0.27
Tolazoline	JIVZKJQOZQXQB-UHFFFAOYSA-N	5504	0.12	0.41	0.27
6-[(2R,3R)-3-[(3,4-dimethoxyphenyl)methyl]-4-methoxy-2-(methoxymethyl)butyl]-4-methoxy-1,3-benzodioxole	RCFGIEPQSDGMJJ-OALUTQOASA-N	13989915	0.27	0.26	0.27
Bilirubin	BPYKTIZUTYGOLE-IFADSCNNSA-N	5280352	0.22	0.31	0.27
Zaluzanin C	XFVLNEYIZGZDHP-PEDHHIEDSA-N	72646	0.20	0.33	0.26
Elatol	HZKGRKICQBHSNA-KCQAQPDRSA-N	479931	0.20	0.33	0.26
Pteropodine	JMIAZDVHNCCPDM-QLMFUGSGSA-N	10429112	0.17	0.35	0.26
Isopteropodine	JMIAZDVHNCCPDM-PFDNRQJHSA-N	9885603	0.17	0.35	0.26

Mitraphylline	JMIAZDVHNCPPDM-DAFCLMLCSA-N	94160	0.17	0.35	0.26
Isomitraphylline	JMIAZDVHNCPPDM-NWQITLLVSA-N	11726520	0.17	0.35	0.26
Tomatidine	XYNPYHXGMWJBLV-VXPJTDKGSAN	65576	0.21	0.31	0.26
Vernodalin	ZSXNBLOPYIJLQV-WSVVRNJXSA-N	179375	0.25	0.27	0.26
Ephedrine	KWGRBVOPPLSCSI-WPRPVWTQSA-N	9294	0.14	0.38	0.26
Pseudoephedrine	KWGRBVOPPLSCSI-WCBMZHEXSA-N	7028	0.14	0.38	0.26
Pachymic acid	VDYCLYGKCVBHN-DRCQUEPLSA-N	5484385	0.15	0.37	0.26
Dichlorvos	OEBRKCOSUFCWJD-UHFFFAOYSA-N	3039	0.27	0.25	0.26
Ephedrine Hydrochloride	BALXUFOVQVENIU-GNAZCLTHSA-N	65326	0.13	0.39	0.26
Pseudoephedrine Hydrochloride	BALXUFOVQVENIU-KXNXZCPBSA-N	9581	0.13	0.39	0.26
Pristimerin	JFACETXYABVHFD-WXPPGMDDSA-N	159516	0.24	0.28	0.26
Bilobalide	MOLPUWBMSBJXER-YDGSQGCISA-N	73581	0.20	0.32	0.26
(1R,3R,6R,8S,10R,11S,13S,16S,17R)-8-tert-butyl-6,17-dihydroxy-16-methyl-2,4,14,19-tetraoxahexacyclo[8.7.2.0.1,11.0.3,7.0.7,11.0.13,17]nonadecane-5,15,18-trione	FPUXKXIZEIDQKW-XUYRAXNCSA-N	10431574	0.24	0.28	0.26
Phenethylamine	BHHGXPLMPWCGHP-UHFFFAOYSA-N	1001	0.12	0.40	0.26
N-[1,2,10-trimethoxy-9-oxo-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-6,7-dihydro-5H-benzo[a]heptalen-7-yl]acetamide	UXAFRQPVHYZDED-UHFFFAOYSA-N	233866	0.15	0.36	0.26
Deoxycholic Acid	KXGVEGMKQFWNSR-LLQZFEROSA-N	222528	0.21	0.31	0.26
4-[(3R,12S)-3,12-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoic acid	KXGVEGMKQFWNSR-GPTTVZJUSA-N	45358122	0.21	0.31	0.26
Miconazole	BYBLEWFAAKGYCD-UHFFFAOYSA-N	4189	0.24	0.28	0.26
Gentianine	DFNZYFAJQPLFI-UHFFFAOYSA-N	354616	0.21	0.31	0.26
Methyl 10,15,16-trihydroxy-9,13-dimethyl-3-(3-methylbut-2-enoyloxy)-4,11-dioxo-5,18-dioxapentacyclo[12.5.0.0.1,6.0.2,17.0.8,13]nonadec-9-ene-17-carboxylate	ZZZYHIMVKOHVIH-UHFFFAOYSA-N	299645	0.23	0.29	0.26
Brusatol	ZZZYHIMVKOHVIH-VILODJCFSA-N	73432	0.23	0.29	0.26
Methyl (1R,2S,3R,6R,8R,13S,14R,15R,16S,17R)-10,15,16-trihydroxy-9,13-dimethyl-3-(3-methylbut-2-enoyloxy)-4,11-dioxo-5,18-dioxapentacyclo[12.5.0.0.1,6.0.2,17.0.8,13]nonadec-9-ene-17-carboxylate	ZZZYHIMVKOHVIH-MWFXHRFLSA-N	12302104	0.23	0.29	0.26
methyl (1R,2R,6R,8S,13S,14S,17S)-10,15,16-trihydroxy-9,13-dimethyl-3-(3-methylbut-2-enoyloxy)-4,11-dioxo-5,18-dioxapentacyclo[12.5.0.0.1,6.0.2,17.0.8,13]nonadec-9-ene-17-carboxylate	ZZZYHIMVKOHVIH-ZDMPXFSSA-N	137704670	0.23	0.29	0.26
(+)-Terpinen-4-ol	WRYLYDPHFGVWKC-SNVBAGLBSA-N	2724161	0.12	0.39	0.26
4-Terpineol, (+/-)-	WRYLYDPHFGVWKC-UHFFFAOYSA-N	11230	0.12	0.39	0.26
Trimetaphan camsylate	HALWUDBBYKMPW-UHFFFAOYSA-M	441310	0.20	0.31	0.26
Cytochalasin B	GBOGMAARMMDZGR-TYHYBEHESA-N	5311281	0.19	0.32	0.26

Macrostemonoside A	JWWCJQFYNBGCAX-UOUUDHCBSA-N	197480	0.22	0.29	0.26
Wilforine	ZOCKGJZEUVPPPI-UHFFFAOYSA-N	601100	0.22	0.29	0.26
beta-Ionone	PSQYTAPXSHCGMF-BQYQJAHWSA-N	638014	0.18	0.33	0.25
Oseltamivir	VSZGPKBBMSAYNT-RRFJBIMHSA-N	65028	0.23	0.28	0.25
Poricoic acid A	KVAQLXUMUVEKGR-SMFZDKLCSA-N	5471851	0.20	0.31	0.25
Nagilactone B	AEGWYWSJGKOLGB-ZLNDBNLZSA-N	3084329	0.14	0.37	0.25
Apicidin	JWOGUUIOCYMBPV-GMFLJSBRSA-N	6918328	0.16	0.34	0.25
Trifluridine	VSQQQLOSPVPAZ-RRKCRQDMSA-N	6256	0.12	0.38	0.25
Norethynodrel	ICTXHFFSOAJUMG-SLHNCBLASA-N	6231	0.17	0.33	0.25
Terephthalic acid	KKEYFWRCBNTPAC-UHFFFAOYSA-N	7489	0.11	0.39	0.25
Secobarbital	KQPKPCNLIDLUMF-UHFFFAOYSA-N	5193	0.16	0.34	0.25
Cholic Acid	BHQCQFFYRZLCCQ-OELDTZBJS-A-N	221493	0.20	0.30	0.25
Calcimycin	HIYAVKIYRIFSCZ-CYEMHPAKSA-N	11957499	0.14	0.35	0.25
Abietic acid	RSWGJHLUYNHMPX-ONCXSQPRSA-N	10569	0.14	0.35	0.25
Epidihydrocholesterin	QYIXCDOBOSTCEI-FBVYSKEZSA-N	66066	0.19	0.30	0.25
Paclitaxel	RCINICONZNJXQF-MZXODVADSA-N	36314	0.23	0.26	0.24
N-(1,2,3,10-Tetramethoxy-9-oxo-5,6,7,9-tetrahydrobenzo[a]heptalen-7-yl)acetamide	IAKHMKGGTNLSZ-UHFFFAOYSA-N	2833	0.16	0.33	0.24
Colchicine	IAKHMKGGTNLSZ-INIZCTEOSA-N	6167	0.16	0.33	0.24
Niacinamide	DFPAKSUCGFBDDF-UHFFFAOYSA-N	936	0.16	0.33	0.24
Piperlongumine	VABYUUZNAVQNPQ-BQYQJAHWSA-N	637858	0.19	0.30	0.24
Methylglyoxal	AIJULSRZWUXGPQ-UHFFFAOYSA-N	880	0.23	0.26	0.24
Curculigoside	SJRKHVKAXVFJQ-QKYBYQKWSA-N	158845	0.16	0.33	0.24
(1S,5S,6S,8S,13R,16S,17R)-11-ethyl-6-methoxy-13-(methoxymethyl)-11-azahexacyclo[7.7.2.12.5.01,10.03,8.013,17]nonadecane-4,8,16-triol	RBSZCNOWHDHRFZ-NKNRFIKZSA-N	138404392	0.19	0.30	0.24
Cytidine-5'-diphosphate	ZWIADYZPOWUWUW-XVFCMESISA-N	6132	0.18	0.30	0.24
	HXNFUBHNUDHIGC-UHFFFAOYSA-N	4644	0.20	0.28	0.24
2-Arachidonoylglycerol	RCRCTBLIHCHWDZ-DOFZRALJSA-N	5282280	0.25	0.23	0.24
(2S,3R,4S,5S,6R)-2-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-2-[[[(10R,12S,13R,14R,17R)-12-hydroxy-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,10,14-tetramethyl-1,2,3,5,6,7,8,9,11,12,13,15,16,17-tetradecahydrocyclopenta[a]phenanthren-3-yl]oxy]-6-(hydroxymethyl)oxan-3-yl]oxy-4,6-bis(hydroxymethyl)oxane-3,5-diol	VXIVCXOKABMNOW-MLLGVTEASA-N	159727	0.21	0.27	0.24
Phillyrin	KFFCKOBAMGMTMW-LGQRSHAYSA-N	101712	0.21	0.27	0.24
	FUWUEFKEXZQKKA-UHFFFAOYSA-N	71773484	0.14	0.34	0.24
(2S,4R,6S)-2-[[[(1R,3S,6R,8S,9R,11R,14R,15S,16S)-14-hydroxy-15-[(2S,5R)-5-(2-hydroxypropan-2-yl)-2-methyloxolan-2-yl]-7,7,12,16-tetramethyl-6-[[[(2R,3S,4R,5S)-3,4,5-trihydroxyoxan-2-yl]oxy-9-pentacyclo[9.7.0.01,3.03,8.012,16]octadecanyl]oxy]-6-(hydroxymethyl)oxane-3,4,5-triol	QMNWISYXSJWHRY-OVTNMLBFSA-N	122130767	0.22	0.26	0.24

(2R,3R,4S,5S,6R)-2- [[[(1S,3R,6S,8S,9S,11S,12S,14S,15R,16R)- 14-hydroxy-15-[(2R,5S)-5-(2- hydroxypropan-2-yl)-2-methyloxolan-2- yl]-7,7,12,16-tetramethyl-6- [(2S,3R,4S,5R)-3,4,5-trihydroxyoxan-2- yl]oxy-9- pentacyclo[9.7.0.01,3.03,8.012,16]octade canyl]oxy]-6-(hydroxymethyl)oxane- 3,4,5-triol	QMNWISYXSJWHRY-YFAFVBNPSA-N	124761776	0.22	0.26	0.24
Guaifenesin	HSRJKNPTNIJEKV-UHFFFAOYSA-N	3516	0.12	0.36	0.24
Ilanatoside C	JAYAGDXJIDEKI-PTGWOZRBSA-N	656630	0.14	0.34	0.24
5'-Cytidylic acid	IERHLVCPSMICTF-XVFCMESISA-N	6131	0.18	0.30	0.24
Miltirone	FEFAIBOZOKSLJR-UHFFFAOYSA-N	160142	0.07	0.41	0.24
1,3-Dicyclohexylurea	ADFXKUOMJKEIND-UHFFFAOYSA-N	4277	0.18	0.30	0.24
Nalidixic Acid	MHWLWQUZZRMNGJ-UHFFFAOYSA-N	4421	0.19	0.29	0.24
Calophyllolide	PMBLOLOJQZPEND-GIDUJCDVSA-N	5281392	0.19	0.29	0.24
Perilla alcohol	NDTYTMIUWGWIMO-SNVBAGLBSA-N	369312	0.13	0.34	0.24
Perillyl alcohol	NDTYTMIUWGWIMO-UHFFFAOYSA-N	10819	0.13	0.34	0.24
Fluoxetine	RTHCYVBBDHJXIQ-UHFFFAOYSA-N	3386	0.08	0.39	0.24
Pantoprazole	IQPSEEYGBUAQFF-UHFFFAOYSA-N	4679	0.13	0.34	0.24
Stemofoline	DTVYAHOUHQCSMS-VHEBQXMUSA-N	3005205	0.18	0.29	0.24
(+)-Stemofoline	DTVYAHOUHQCSMS-NPBMAUCESA-N	70697717	0.18	0.29	0.24
Nomilin	KPDOJFFZKAUIOE-WNGDLQANSA-N	72320	0.11	0.36	0.24
CID 12313416	KPDOJFFZKAUIOE-MFPNAYRGSAN	12313416	0.11	0.36	0.24
Estradiol dipropionate	JQIYNMYZKRGDFK-RUFWAXPRSA-N	8225	0.20	0.27	0.24
Borneol, (-)-	DTGKSKDOIYIVQL-QXFUBDJGSA-N	1201518	0.16	0.31	0.24
CID 44630107	DTGKSKDOIYIVQL-HHCGNCNQSA-N	44630107	0.16	0.31	0.24
Borneol	DTGKSKDOIYIVQL-WEDXCCLWSA-N	6552009	0.16	0.31	0.24
Bicyclo[2.2.1]heptan-2-ol, 1,7,7- trimethyl-, exo-	DTGKSKDOIYIVQL-CCNFQMFSA-N	439569	0.16	0.31	0.24
Rescinamine	SZLZWPPUNLXJEA-QEGASFHISA-N	5280954	0.21	0.26	0.24
Pseudolaricacidb	VDGOFNMYZYBUDT-JVPLZENUSA-N	129316864	0.13	0.34	0.24
2-(2-hydroxypropan-2-yl)-4-methoxy-7- [[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6- (hydroxymethyl)oxan-2-yl]oxymethyl]- 2,3-dihydrofuro[3,2-g]chromen-5-one	XIUHVHOSBDSYXRG-RZMKGNTASA-N	11968852	0.16	0.31	0.23
Salidroside	ILRCGYURZSFMEG-RKQHYHRCSA-N	159278	0.15	0.32	0.23
(2R,3R,4R,5R)-3,4-Dimethyl-2,5-bis(3,4,5- trimethoxyphenyl)tetrahydrofuran	ZPINJJOPURFFNV-LPINMEDASA-N	10048436	0.21	0.26	0.23
Grandisin	ZPINJJOPURFFNV-WJWAULOUSAN	442876	0.21	0.26	0.23
Isocryptotanshinone	VUIHARLRBGHPEA-UHFFFAOYSA-N	626608	0.09	0.38	0.23
5beta-Cholanic acid	RPKLZQLYODPWTM-LVVAJZGHSAN	92803	0.18	0.29	0.23
(-)-alpha-Terpineol	WUOACPNHFRMFNP-SECBINFHSA-N	443162	0.10	0.37	0.23
(S)-Auraptanol	SQSRYWNOKPJENY-UHFFFAOYSA-N	13343540	0.22	0.25	0.23

2-(hydroxymethyl)-6-[2-[6-[6-(hydroxymethyl)-3-methyl-4,5-bis(oxidanyl)oxan-2-yl]oxy-4,4,8,10,14-pentamethyl-3,12-bis(oxidanyl)-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-methyl-hept-5-en-2-yl]oxy-oxane-3,4,5-triol; oxa	ZBXDHDDTAIOMHK-UHFFFAOYSA-N	53399243	0.22	0.25	0.23
Proline	ONIBWKKTOPOVIA-BYPYZUCNSA-N	145742	0.19	0.28	0.23
Mestranol	IMSSROKUHAOUJS-MJCUULBUSA-N	6291	0.16	0.30	0.23
Decursinol	BGXFQDFSVDZUIW-LBPRGKRZSA-N	442127	0.10	0.36	0.23
Sauchinone	GMTJIWUFFXGFHH-WPAOEJHSSA-N	11725801	0.14	0.32	0.23
vibsanin B	GYXPHGPELZUVGI-QYGPLFBNBSA-N	15817377	0.16	0.30	0.23
Gallopamil	XQLWNAFCTODIRK-UHFFFAOYSA-N	1234	0.15	0.31	0.23
Hecogenin	QOLRLLFJMZYQJ-LOBDNJQFSA-N	91453	0.18	0.28	0.23
Isoalantolactone	CVUANYCQTOGILD-QVHKTLOISA-N	73285	0.15	0.31	0.23
Rocaglamide	DAPAQENNNINUPW-IDAMAFBJSAN	331783	0.18	0.28	0.23
Notoginsenoside R1	LLPWNQMSUYAGQI-OOSPGMBYSAN	441934	0.22	0.24	0.23
Chenodiol	RUDATBOHQWOJDD-BSWAIMHNSAN	10133	0.20	0.26	0.23
Ursodiol	RUDATBOHQWOJDD-UZVSRGJWSAN	31401	0.20	0.26	0.23
5beta-Chol-24-oic acid-3alpha,7beta-diol	RUDATBOHQWOJDD-HEGLNSLBSAN	388708	0.20	0.26	0.23
Notopterol	BKIACVAZUKISOR-MKMNVTDBSAN	5320227	0.19	0.27	0.23
Toluene	YXFVVABEGXRONW-UHFFFAOYSA-N	1140	0.12	0.34	0.23
n-Oleoyethanolamine	BOWVQLFMWHZBEF-KTKRTIGZSAN	5283454	0.21	0.25	0.23
Ginsenoside Rb3	NODILNFGTFIURN-USYOXQFSSAN	12912363	0.23	0.23	0.23
Ginsenoside C	NODILNFGTFIURN-GZPRDHCNSAN	6917976	0.23	0.23	0.23
4-((3S,5R,8R,9S,10S,12R,13S,14S,17R)-3-((2R,4S,5S,6R)-5-((2S,4S,5S,6R)-5-((2S,4S,5S,6R)-4,5-dihydroxy-6-methyltetrahydro-2H-pyran-2-yloxy)-4-hydroxy-6-methyltetrahydro-2H-pyran-2-yloxy)-4-hydroxy-6-methyltetrahydro-2H-pyran-2-yloxy)-12,14-dihydroxy-10,13-	LTMHDMANZUZIPE-YUICGFAKSAN	30322	0.12	0.34	0.23
Digoxin	LTMHDMANZUZIPE-PUGKRICDSAN	2724385	0.12	0.34	0.23
Piperine	MXXWOMGUGJBKIW-YPCICBESAN	638024	0.14	0.32	0.23
Metoprolol	IUBSYMUCCVWXPE-UHFFFAOYSA-N	4171	0.09	0.36	0.23
(R)-3-Amino-4-[(S)-2-((R)-1-[(S)-1-[(R)-1-(1H-indol-3-ylmethyl)-2-oxoethylcarbamoyl]-3-methyl-but-3-enylcarbamoyl]-2-methylpropylcarbamoyl)-pyrrolidin-1-yl]-4-oxo-butyric acid	VYCAAOURFJIHD-AOYLRCGGSAN	52943236	0.10	0.35	0.23
Ergothioneine	SSISHJTAXXQAX-ZETCQYMHNSAN	5351619	0.11	0.34	0.23
Octanoate	WWZKQHOCKIZLMA-UHFFFAOYSA-M	119389	0.24	0.21	0.23
Thapsigargin	IXFPJGBNCFXKPI-FSIHEZPISAN	446378	0.25	0.20	0.22
Tectoridin	CNOURESJATUGPN-UDEBZQQRSAN	5281810	0.06	0.39	0.22
Lithocholic acid	SMEROWZSTRWXGI-HVATVPOCSAN	9903	0.18	0.27	0.22
(-)-Rasfonin	OHRGHFXATDKGOV-FXYCKZMJNSAN	11259090	0.20	0.25	0.22
Cyclopamine	QASFUMOKHFSJGL-LAFRSMQTNSAN	442972	0.19	0.26	0.22

(1S,2S,4S,6R,8S,9S,12R,13R)-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0.2,9.0.4,8.0.13,18]icos-18-ene-6,2'-oxane]-16-ol	WQLVFSAGQJTQCK-FFRUGWTFSA-N	137704703	0.17	0.28	0.22
Diosgenin	WQLVFSAGQJTQCK-VKROHFNGSA-N	99474	0.17	0.28	0.22
Calcifediol	JWUBBDSIWDLEOM-DTOXIADCSEA-N	5283731	0.21	0.24	0.22
Ginsenoside F1	XNGXWSFSJIQMNC-FIYORUNESA-N	9809542	0.17	0.28	0.22
(1R)-1,6,6-trimethyl-1,2,6,7,8,9-hexahydrophenanthro[1,2-b]furan-10,11(3aH,11aH)-dione	IJSBKZLSTIFYIE-FPKDZHNTSA-N	25181389	0.09	0.36	0.22
Ergocalciferol	MECHNRXZTMCUDQ-RKHKHRCZSA-N	5280793	0.21	0.23	0.22
Chloramphenicol	WIIZWVCIJKGZOK-RKDXNWHRSA-N	5959	0.13	0.31	0.22
Hydrocortisone	JYGXADMDTFJGBT-VWUMJDOOSA-N	5754	0.07	0.37	0.22
Diphenhydramine	ZZVUWRFHKOJYTH-UHFFFAOYSA-N	3100	0.10	0.34	0.22
Andrographolide	BOJKULTULYSRAS-OTESTREVSA-N	5318517	0.16	0.28	0.22
methyl 4-[(1S)-4,6-dimethoxy-3-oxo-1H-2-benzofuran-1-yl]-3,5-dimethoxybenzoate	ZXUSFNWVWVJJOZ-SFHVURJKSA-N	5324642	0.20	0.24	0.22
3-Carene	BQOFWKZOCNGFEC-UHFFFAOYSA-N	26049	0.12	0.32	0.22
Benzamide	KXDAEFPNCMNJSK-UHFFFAOYSA-N	2331	0.14	0.30	0.22
(6Z,10Z)-4-hydroxy-6,10-dimethyl-3-methylidene-3a,4,5,8,9,11a-hexahydrocyclodeca[b]furan-2-one	PDEJECFRCJOMEN-UDRCNDPASA-N	6436794	0.16	0.28	0.22
CID 162355	QQUHMASGPODSIW-RPLHGOISSA-N	162355	0.07	0.37	0.22
[(1R,3R,4R,6S,9S)-4-hydroxy-6-methyl-8-oxo-1-[(2R,3S,4R,5R,6S)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-7-oxatricyclo[4.3.0.0.3,9]nonan-9-yl]methyl benzoate	QQUHMASGPODSIW-DRASSFSVSA-N	134761887	0.07	0.37	0.22
Albiflorin	QQUHMASGPODSIW-ICECTASOSA-N	24868421	0.07	0.37	0.22
Senkyunolide A	ZPIKVDODKJUKIN-NSHDSACASA-N	3085257	0.18	0.26	0.22
3-N-Butyl-4,5-dihydrophthalide	ZPIKVDODKJUKIN-UHFFFAOYSA-N	173843	0.18	0.26	0.22
Inulobiose	WOHYVFWWTVNXTPTWOHWVPZSA-N	439552	0.12	0.31	0.22
Diphenyl ether	USIUUVZYUHIAEV-UHFFFAOYSA-N	7583	0.09	0.34	0.22
Ophiopogonin D	FHKHGNFKBPFJCB-LYLKFOBISA-N	46173859	0.23	0.20	0.22
Ibrolipim	KPRTURMJVWXURQ-UHFFFAOYSA-N	131601	0.10	0.33	0.22
(1S,2S,8R,9S,11R)-9,10,15,18-tetrahydroxy-12,12-dimethyl-6-methylidene-17-oxapentacyclo[7.6.2.15,8.0.1,11.0.2,8]octadecan-7-one	SDHTXBWLVGWJFT-RPBPHXRPSA-N	138107787	0.19	0.24	0.22
Oridonin	SDHTXBWLVGWJFT-XKCURVIJSA-N	5321010	0.19	0.24	0.22
Ent-Oridonin	SDHTXBWLVGWJFT-BAFGBBEMSA-N	15923208	0.19	0.24	0.22
Tutin	CCAZWUJBLKKBAY-ULZPOIKGSA-N	75729	0.20	0.23	0.22
(2S,3R,4S,5S,6R)-2-[(2R,3R,4S,5S,6R)-2-[[[(6R,10R,12S,13S,14R,17S)-3,12-dihydroxy-17-[(E,2S)-2-hydroxy-6-methyloct-5-en-2-yl]-4,4,10,14-tetramethyl-1,2,3,5,6,7,8,9,11,12,13,15,16,17-tetradecahydrocyclopenta[a]phenanthren-6-yl]oxy]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol	HFAWXTRAHOUDSG-YZAFHMOOSA-N	6441008	0.18	0.25	0.22

Suberosin	RSZDAYHEZSRVHS-UHFFFAOYSA-N	68486	0.15	0.28	0.22
Aconitin	XFSBVAOIAHNAPC-NPVHKAFCSA-N	24832676	0.15	0.28	0.22
Aconitine	XFSBVAOIAHNAPC-XTHSEXKGSAN-N	245005	0.15	0.28	0.22
(R)-Methysticin	GTEXBOVBADJOQH-RQOWECAXSA-N	90125683	0.09	0.34	0.21
(1S,2R,4R,7E,11R)-4,8-dimethyl-12-methylidene-3,14-dioxatricyclo[9.3.0.0.2,4]tetradec-7-en-13-one	KTEXNACQROZXEV-CMFZEQLMSA-N	124463365	0.13	0.30	0.21
Parthenolide	KTEXNACQROZXEV-PVLRGYAZSA-N	7251185	0.13	0.30	0.21
Cryptotanshinone	GVKJJOMQCNPG-BJTQLQIEISA-N	160254	0.07	0.36	0.21
Muscarine	UQOFGTXDASPILL-XHNCKOQMSA-N	9308	0.13	0.30	0.21
(3R,8R,9R,10S,13R,14R,17R)-17-[(E,2R,5R)-5-ethyl-6-methylhept-3-en-2-yl]-3,10,13-trimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene	GYDIPQRLDOTECG-PYURGGNSA-N	50930798	0.11	0.32	0.21
Raffinose	MUPFEKGTMRGPIJ-ZQSKZDJDSA-N	439242	0.20	0.23	0.21
(1R)-21-methyl-3,13,21-triazapentacyclo[11.8.0.0.2,10.0.4,9.0.15,20]henicosane-2(10),4,6,8,15,17,19-heptaen-14-one	TXDUTHBFYKGSAN-GOSISDBHSA-N	6971167	0.09	0.34	0.21
Evodiamine	TXDUTHBFYKGSAN-SFHVURJKSA-N	442088	0.09	0.34	0.21
Isoevodiamine	TXDUTHBFYKGSAN-UHFFFAOYSA-N	151289	0.09	0.34	0.21
Nicotinic acid	PVNIIMVLHYAWGP-UHFFFAOYSA-N	938	0.13	0.30	0.21
Calcitriol	GMRQFYUWCNGIN-NKMMMHOESA-N	5280453	0.19	0.24	0.21
Stachydrine	CMUNUTVVOHQPW-LURJTMIESA-N	115244	0.23	0.20	0.21
Prednisolone	OIGNJSKLLXVSLV-VWUMJDOOSA-N	5755	0.09	0.34	0.21
Papaverine	XQYZDYMELSDRZ-UHFFFAOYSA-N	4680	0.17	0.26	0.21
Chlorpheniramine	SOYKEARSMXGVTM-UHFFFAOYSA-N	2725	0.12	0.30	0.21
Guggulsterone	WDXRGPWQVHZTQJ-OSJVMJFVSA-N	6450278	0.11	0.31	0.21
2-Mercaptobenzothiazole	YXIWHUQXZSMYRE-UHFFFAOYSA-N	697993	0.08	0.34	0.21
Isoguvacine	KRVDMAABKYMVBHG-UHFFFAOYSA-N	3765	0.15	0.27	0.21
Disopyramide	UVTNFZQICZKOEM-UHFFFAOYSA-N	3114	0.11	0.31	0.21
Uridine	DRTQHJPMGMBUCF-XVFCMESISA-N	6029	0.11	0.31	0.21
Arabinofuranosyluracil	DRTQHJPMGMBUCF-UHFFFAOYSA-N	1177	0.11	0.31	0.21
Endosulfan	RDYMFUSUJZBWLH-UHFFFAOYSA-N	3224	0.16	0.26	0.21
(2R)-2-[(2R)-4-[(2R)-4,5-dihydroxy-6-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]-3-[(2R)-3,4,5-trihydroxyoxan-2-yl]oxyoxan-2-yl]oxy-5-hydroxy-2-[[[(1S,2R,5R,10R,11R,14S,15R,16S,20S)-16-hydroxy-2,6,6,10,16-pentamethyl-18-(2-methylprop-1-enyl)-19,21-dioxahexacyclo[18.2.1.0.1,14.0.2,11.0.5,10.0.15,20]tricosan-7-yl]oxy]oxan-3-yl]oxy-6-methyloxane-3,4,5-triol	KVKRFLVYLIZFD-HEXGHNAPSA-N	138114261	0.27	0.15	0.21
Stigmasterol	HCVXJBMSMIARIN-PHZDYDNGSA-N	5280794	0.14	0.28	0.21
17-[(E)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol	HCVXJBMSMIARIN-CMDGGOBGSA-N	5364569	0.14	0.28	0.21

Poriferasterol	HCVXJBMSMIARIN-KEJCWXRGSAN	5281330	0.14	0.28	0.21
Deslanoside	OBATZBGFDVVCJD-LALPQLPRSA-N	28620	0.11	0.31	0.21
Aucubin	RJWJHRPNHHPHBRN-FKVJWERZSA-N	91458	0.15	0.27	0.21
Anemoside B4	OUIHKBZTUPLIIA-QEEGUAPESA-N	71307558	0.23	0.19	0.21
Ethosuximide	HAPOVYFOVWVWLRU-UHFFFAOYSA-N	3291	0.11	0.30	0.21
Cortodoxone	WHBHBVVOGNECLV-OBQKJFGGSA-N	440707	0.06	0.35	0.21
Cholecalciferol	QYSXJUF SXHHAJI-YRZJWOYSA-N	5280795	0.22	0.19	0.21
Nodakenin	HXCGUCZXPFBNRD-DNLMCPORSA-N	73191	0.07	0.34	0.21
26-Hydroxycholesterol	FYHRJWMENCALJY-CCDZVGGQSA-N	99470	0.15	0.26	0.21
(2S,3R,4S,5S,6R)-2-[(2R,3R,4S,5S,6R)-2-[[[(10R,12S,13S,14R,17S)-17-[(2S)-4,6-dimethyl-2-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhept-5-en-2-yl]-12-hydroxy-4,4,10,14-tetramethyl-1,2,3,5,6,7,8,9,11,12,13,15,16,17-tetradecahydrocyclopenta[a]phenanthren-3-yl]oxy]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol	IRBVCFDYIGGFFY-ADSMOORZSA-N	3036963	0.17	0.24	0.21
Gnidimacrin	SSXCVTWXHGTLK-VFZTJWSWSA-N	3085204	0.16	0.25	0.21
Vincamine	RXPRRQLKFXBCSJ-GIVPXCWWSA-N	15376	0.12	0.29	0.21
Ginkgetin	AIFCFBUSLAEIBR-UHFFFAOYSA-N	5271805	0.12	0.29	0.20
Papaverine Hydrochloride	UOTMYNBWXDUBNX-UHFFFAOYSA-N	6084	0.15	0.26	0.20
Esatenolol	METKIMKYRQLGS-LBPRGKRZSA-N	175540	0.11	0.30	0.20
Atenolol	METKIMKYRQLGS-UHFFFAOYSA-N	2249	0.11	0.30	0.20
[(3R)-2,2-dimethyl-8-oxo-3,4-dihydropyrano[3,2-g]chromen-3-yl] 3-methylbut-2-enoate	CUKSFECWKQBVED-MRXNPFEDSA-N	44144310	0.11	0.30	0.20
Decursin	CUKSFECWKQBVED-INIZCTEOSA-N	442126	0.11	0.30	0.20
Chuanliansu	NAHTXVIXCMUDLF-SLWGVJJJSA-N	115060	0.12	0.29	0.20
[(1S,2R,4R,5R,8R,10S,11S,12R,14R,15R,19S,21R)-4-acetyloxy-6-(furan-3-yl)-12,16,19-trihydroxy-5,11,15-trimethyl-3-oxo-9,17-dioxahexacyclo[13.3.3.0.1,14.0.2,11.0.5,10.0.8,10]henicosan-21-yl] acetate	NAHTXVIXCMUDLF-OLTMAMAMSA-N	139225400	0.12	0.29	0.20
[(1S,2R,4R,5R,6S,8R,10S,11S,12R,14R,15S,16S,19S,21R)-4-acetyloxy-6-(furan-3-yl)-12,16,19-trihydroxy-5,11,15-trimethyl-3-oxo-9,17-dioxahexacyclo[13.3.3.0.1,14.0.2,11.0.5,10.0.8,10]henicosan-21-yl] acetate	NAHTXVIXCMUDLF-CBRNTUCOSA-N	100950797	0.12	0.29	0.20
Reserpine	QEVHRUUCFGRFIF-MDEJGZGSSA-N	5770	0.17	0.24	0.20
Pinusolide	WTKBZJAWPZXKJU-NLEAXPPASA-N	161721	0.09	0.32	0.20
Camphor (synthetic)	DSSYKIVIOFKYAU-XCBNKYQSSA-N	159055	0.15	0.25	0.20
Camphor	DSSYKIVIOFKYAU-UHFFFAOYSA-N	2537	0.15	0.25	0.20
Mezerein	DLEDLHFNQDHEOJ-CSWXFLMBSA-N	6434191	0.09	0.31	0.20
4alpha-Phorbol	QGVLYPPODPLXMB-UHFFFAOYSA-N	290670	0.12	0.28	0.20
Phorbol	QGVLYPPODPLXMB-UBTYZVCOSA-N	442070	0.12	0.28	0.20
Hexafluorenum Bromide	WDEFPRUEZRUYNW-UHFFFAOYSA-L	9434	0.08	0.32	0.20
Yuanhuacin	CGSGRJNIBXQJQ-CAAOHEDASA-N	6440205	0.14	0.26	0.20
Nodakenetin	FWYSBEAFFPBAQU-GFCCVEGCSA-N	26305	0.07	0.33	0.20
Tanshinone IIA	HYXITZLLTYIPOF-UHFFFAOYSA-N	164676	0.02	0.38	0.20

Ergometrine	WVVSZNPYNCNODU-XTQGRXLLSA-N	443884	0.12	0.28	0.20
ginkgolide-B	SQOJOAFXDQDRGF-MMQTXUMRSA-N	6324617	0.19	0.21	0.20
(1R,3R,8S,10R,13S,16S,17R)-8-tert-butyl-6,12,17-trihydroxy-16-methyl-2,4,14,19-tetraoxahexacyclo[8.7.2.01,11.03,7.07,11.013,17]nonadecane-5,15,18-trione	SQOJOAFXDQDRGF-OOHPMXMZSA-N	441294	0.19	0.21	0.20
Tumulosic acid	XADJANKGURNTIA-YEXRKOARSA-N	12314446	0.12	0.28	0.20
Amygdalin	XUCIJNAGGSZNQT-JHSLDZIXSA-N	656516	0.12	0.28	0.20
alpha-Cyperone	KUFXJZXMWHNCEH-DOMZBBRYSA-N	6452086	0.18	0.22	0.20
	OTBXOEAOVRKTNQ-UHFFFAOYSA-N	2182	0.06	0.34	0.20
(3R,4S,5S,6R)-2-[[[(2R,3S,4S,5R,6S)-6-[2-[[[(3S,5R,8R,9R,10R,12R,13R,14R,17S)-3-[[[(2R,3R,4S,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-methylhept-5-en-2-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	GZYPWOGIYAIIPV-NGBMAODDSA-N	73148	0.19	0.21	0.20
2-[[[6-[(2S)-2-[(14R)-3-[4,5-dihydroxy-6-(hydroxymethyl)-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyoxan-2-yl]oxy-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-methylhept-5-en-2-yl]oxy-3,4,5-trihydroxyoxan-2-yl]methoxy]-6-(hydroxymethyl)oxane-3,4,5-triol	GZYPWOGIYAIIPV-DFRIBHHNSA-N	59070837	0.19	0.21	0.20
2-[2-[[[17-[2-[6-[[[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl]oxy-6-methylhept-5-en-2-yl]-12-hydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-yl]oxy]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol	JDCPEKQWFDWQLI-UHFFFAOYSA-N	100018	0.19	0.21	0.20
Ginsenoside Rb1	GZYPWOGIYAIIPV-JBDTYSNRSA-N	9898279	0.19	0.21	0.20
Anandamide	LGEQQWQMCRITYG-DOFZRALJSA-N	5281969	0.14	0.26	0.20
Cynaropicrin	KHSCYOFDKADJDJ-NQLMQOPMSA-N	119093	0.12	0.28	0.20
(-)-Zuonin A	QFUXQRHAJWXPGP-YLYZPNOSA-N	12310041	0.06	0.34	0.20
Phellopterin	BMLZFLQMBMYVHG-UHFFFAOYSA-N	98608	0.11	0.28	0.20
Hispanolone	UVKYPKNCQJIGKV-PEFDPPMSA-N	5458747	0.08	0.31	0.20
Simvastatin	RYMZZMVNJRMUDD-HGQWONQESA-N	54454	0.13	0.26	0.20

Loperamide	RDOIQAHTMMDAJ-UHFFFAOYSA-N	3955	0.10	0.29	0.20
Sophocarpine	AAGFPTSOPGCENQ-JLNYLFASSA-N	115269	0.09	0.30	0.20
(1R,3aS,5aS,5bR,7aR,8R,11aR,11bR,13aR,13bR)-9-[(2S,3R,4S,5S)-4,5-dihydroxy-3-[[2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxy-8-(hydroxymethyl)-5a,5b,8,11a-tetramethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7a,9,10,11,11b,12,13,13a,13b-hexadecahydrocyclopenta[a]chrysene-3a-carboxylic acid	ISNDTNDJSXYNKT-ATMBFCKSSA-N	101778158	0.19	0.20	0.20
3,4-Methylenedioxymethamphetamine	SHXWCVYOXRDMCX-UHFFFAOYSA-N	1615	0.07	0.32	0.20
Abscisic acid	JLIDBLDQVAYHNE-YKALOCIXSA-N	5280896	0.10	0.29	0.20
Dormin	JLIDBLDQVAYHNE-LXGGSRJLSA-N	5375199	0.10	0.29	0.20
Diphacinone	JYGLAHS AISAEAL-UHFFFAOYSA-N	6719	0.07	0.32	0.20
Harmine	BXNJHAXVSOCGBA-UHFFFAOYSA-N	5280953	0.15	0.24	0.19
Zerumbone	GIHNTRQPEMKFKO-SKTNYSRSSA-N	5470187	0.14	0.25	0.19
Benzoylpaeoniflorin	LATYEZNGPQKAIK-HRCYFWENSA-N	21631106	0.08	0.31	0.19
Physostigmine	PIJVFDBKTWXHHD-HIFRSBDPSA-N	5983	0.08	0.31	0.19
2-(hydroxymethyl)-6-[6-(hydroxymethyl)-2-[[17-[2-[6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-3,12-bis(oxidanyl)-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-6-yl]oxy]-4,5-b	FBFMBWCLBGQEBU-UHFFFAOYSA-N	12855925	0.16	0.23	0.19
Limonin	KBDSLGBFQAGHBE-MSGMIQHVSA-N	179651	0.14	0.25	0.19
prostaglandin D2	BHMBVRSMPMRCCGG-OUTUXVNYSAN	448457	0.19	0.20	0.19
Telekin	LIDPBIULZNRIJE-QHSBEEBCSA-N	12443309	0.12	0.27	0.19
AICA ribonucleotide	NOTGFIUVDGNKRI-UUOKFMHZSAN	65110	0.18	0.20	0.19
O-Xylene	CTQNGGLPUBDAKN-UHFFFAOYSA-N	7237	0.05	0.33	0.19
Panaxatriol	QFJUJMMIBFBOJY-UXZRANASAN	73599	0.16	0.22	0.19
Arctiin	XOJVHLIYNZOZOO-SWOBOCGESAN	100528	0.16	0.22	0.19
(3aS,6aS)-3,6-bis(3,4-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[3,4-c]furan	PEUUVVGQIVMSAW-KILAXVPQSAN	137795855	0.16	0.22	0.19
Ajmalicine	GRTOGORTSDXSFK-XJZBENFASAN	441975	0.13	0.25	0.19
Periplocin	KWBPKUMWVXUSCA-AXQDKOMKSAN	14463159	0.10	0.28	0.19
Quinolinic acid	GJAWHXHKYXBSV-UHFFFAOYSA-N	1066	0.09	0.29	0.19
Hydroxyprogesterone Caproate	DOMWKUIIPQCAJU-LJHIYBGHSAN	169870	0.09	0.29	0.19

(2S,3R,4R,5R,6S)-2-[(2R,3R,4S,5S,6R)-2-[[[(3S,5R,6S,8R,10R,12R,13S,14R,17S)-3,12-dihydroxy-4,4,8,10,14-pentamethyl-17-[(2S)-6-methyl-2-[(2S,3R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyhept-5-en-2-yl]-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-6-yl]oxy]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy-6-methyloxane-3,4,5-triol	PWAOOJDMFUQOKB-QVPADXGFSA-N	73149	0.17	0.21	0.19
Ginsenoside B2	PWAOOJDMFUQOKB-WCZZMFLVSA-N	441921	0.17	0.21	0.19
Tanshinone I	AIGAZQPHXLWMOJ-UHFFFAOYSA-N	114917	0.06	0.32	0.19
Ergosterol peroxide	VXOZCESVZIRHCJ-KGHQQZOUSAN-N	5351516	0.13	0.25	0.19
(2S,4R)-4-[[[(1S,2S,5R,7S,8R,9R,10S,11S,14R,15R)-8-ethyl-5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.0.0 ^{2,7} .0 ^{11,15}]]heptadecan-14-yl]-2-methylpentanoic acid	HSINOMROUCMIEA-FGVHQWLLSA-N	17755104	0.16	0.21	0.19
Isoimperatorin	IGWDEVSBEKYORK-UHFFFAOYSA-N	68081	0.12	0.25	0.19
1-(Diphenylmethyl)-4-(3-phenylprop-2-enyl)piperazine	DERZBLKQOCDDZ-UHFFFAOYSA-N	2761	0.12	0.25	0.19
Sodium dodecyl sulfate	DBMJMQXJHONAFJ-UHFFFAOYSA-M	3423265	0.09	0.28	0.19
Uridine 5'-triphosphate	PGAVKCOVUIYSFO-XVFCMESISA-N	6133	0.11	0.26	0.19
Acetylcholine	OIPILFWXSMYKGL-UHFFFAOYSA-N	187	0.15	0.22	0.19
Floxuridine	ODKNJVUHOIMIIZ-RRKCRQDMSA-N	5790	0.07	0.30	0.19
(2S,3R,4S,5S,6R)-2-[(2R,3R,4S,5S,6R)-4,5-dihydroxy-2-[[[(10R,12S,13R,14R,17S)-12-hydroxy-17-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,10,13,14-pentamethyl-2,3,5,6,7,8,9,11,12,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-yl]oxy]-6-(hydroxymethyl)oxan-3-yl]oxy-6-(hydroxymethyl)oxane-3,4,5-triol	VOWJAFYNABYJKY-LXEJHJHAYSA-N	181573	0.16	0.21	0.19
Phytolaccoside E	YRHWKFMGEDDGJ-UHFFFAOYSA-N	125210	0.12	0.25	0.18
(4aS,8aS)-3,8a-dimethyl-5-methylene-4a,5,6,7,8,8a-hexahydronaphtho[2,3-b]furan-2(4H)-one	ZTVSGQPHMUYCRS-UHFFFAOYSA-N	14448072	0.13	0.24	0.18
Atractylenolide I	ZTVSGQPHMUYCRS-SWLSCSKDSA-N	5321018	0.13	0.24	0.18
Ginsenoside Rg1	YURJSTAIMNSZAE-HHNZYBFYSA-N	441923	0.14	0.23	0.18
Isoginkgetin	HUOOMAOYXQFIDQ-UHFFFAOYSA-N	5318569	0.13	0.24	0.18
7-Dehydrocholesterol	UCLRSWJYQTBZFZ-DDPQNLDTSA-N	439423	0.14	0.23	0.18
Gabapentin	UGJMXCAKCUNAIE-UHFFFAOYSA-N	3446	0.16	0.21	0.18
Taurocholic acid	WBWWGRHZICKQZ-HZAMXZRMSA-N	6675	0.12	0.25	0.18
Testosterone Enanthate	VOCBWIIFXDYGNZ-IXKNJLPQSA-N	9416	0.10	0.27	0.18
Testosterone Undecanoate	UDSFVOAUHKGBEK-CNQKSKJFSA-N	65157	0.10	0.27	0.18
Testosterone Propionate	PDMMFKSKQVNJMI-BLQWBTKSA-N	5995	0.09	0.27	0.18

[(6R)-6-[(2S,8S,9R,10R,13R,14S,16R,17R)-2,16-dihydroxy-4,4,9,13,14-pentamethyl-3,11-dioxo-2,7,8,10,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-hydroxy-2-methyl-5-oxohept-3-en-2-yl] acetate	IXQKXEUSCPEQRD-NRNCYQGDSA-N	180751	0.14	0.22	0.18
[(E,6R)-6-[(2S,9R,10R,13R,14S,16R)-2,16-dihydroxy-4,4,9,13,14-pentamethyl-3,11-dioxo-2,7,8,10,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-hydroxy-2-methyl-5-oxohept-3-en-2-yl] acetate	IXQKXEUSCPEQRD-KQONOONZSA-N	25245488	0.14	0.22	0.18
[(E,6R)-6-[(2S,8S,9R,10S,13R,14S,16R,17R)-2,16-dihydroxy-4,4,9,13,14-pentamethyl-3,11-dioxo-2,7,8,10,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-6-hydroxy-2-methyl-5-oxohept-3-en-2-yl] acetate	IXQKXEUSCPEQRD-QATBOUOLSA-N	15944763	0.14	0.22	0.18
Cucurbitacin B	IXQKXEUSCPEQRD-DKRGWESNSA-N	5281316	0.14	0.22	0.18
[(1R,2R,4S,7R,8S,12R,19S)-7-(furan-3-yl)-1,8,12,16,16-pentamethyl-5,15-dioxo-3,6-dioxapentacyclo[9.8.0.02,4.02,8.012,17]nonadec-13-en-19-yl] acetate	YJXDGWUNRYLINJ-UKZLNSFASA-N	134692703	0.08	0.28	0.18
Gedunin	YJXDGWUNRYLINJ-BHAPSIHVSA-N	12004512	0.08	0.28	0.18
Platycodin D	CYBWUNOAQPMRBA-NDTOZIJESA-N	162859	0.16	0.20	0.18
Ethyl palmitate	XIRNKXNNONJFQO-UHFFFAOYSA-N	12366	0.17	0.19	0.18
Nomegestrol	KZUIYQJTUIACIG-YBZCJVABSA-N	68783	0.08	0.28	0.18
Limonene, (-)-	XMGQYMWWDOXHJM-SNVBAGLBSA-N	439250	0.10	0.26	0.18
Limonene, (+)-	XMGQYMWWDOXHJM-JTQLQIEISA-N	440917	0.10	0.26	0.18
(2S,5S,6S,14R,15S,16R)-18-hydroxy-2-(2-hydroxyacetyl)-14-methyl-17-oxapentacyclo[14.2.1.01,5.06,15.09,14]nonadec-9-en-11-one	QUQBHBRVKLEOEI-JINKLZQFSA-N	201562	0.10	0.27	0.18
Ginsenoside Rd	RLDVZILFNVRJTL-IWFVLDDISA-N	11679800	0.15	0.21	0.18
2,15-Dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadec-7-en-5-ol	HVYWMOMLDIMFJA-UHFFFAOYSA-N	304	0.10	0.26	0.18
Cholesterol	HVYWMOMLDIMFJA-DPAQBDFISA-N	5997	0.10	0.26	0.18
Ethanesulfonic acid,2-[[[(3a,5b,7b)-3,7-dihydroxy-24-oxocholan-24-yl]amino]-	BHTRKEVKTKCXOH-AYSJQVDDSA-N	3034759	0.11	0.25	0.18
2-[4-[(3R,5S,7R,8R,9S,10S,13R,14S,17R)-3,7-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoylamino]ethanesulfonic acid	BHTRKEVKTKCXOH-XZWNVYQJSA-N	10591	0.11	0.25	0.18
Tauroursodeoxycholic acid	BHTRKEVKTKCXOH-LBSADWJPSA-N	9848818	0.11	0.25	0.18

Methyltestosterone	GCKMFJBGXUYNAG-HLXURNFRSA-N	6010	0.07	0.29	0.18
Coroglaucigenin	CDMVQQAHEQVSMF-AULARHRYSAN	12302399	0.14	0.22	0.18
7-Ketocholesterol	YIKKMWSQVKJOP-ABXCMAEBSAN	91474	0.12	0.24	0.18
Tadeonal	AZJUJOFIHHNCSV-KCQAQPDRSAN	72503	0.11	0.25	0.18
Kappadione	GZBACHSOZNEZOG-UHFFFAOYSA-J	8555	0.08	0.28	0.18
Uridine-5'-diphosphate-glucose	HSCJRCZDFQWRP-JZMIEXBBSAN	8629	0.12	0.24	0.18
Gracillin	YQEMAKEYNNOCBY-IEMDQPGHSA-N	159861	0.16	0.20	0.18
Flavanone	ZONYXWQDUYMKFB-UHFFFAOYSA-N	10251	0.14	0.22	0.18
Allantoin	POJWUDADGALRAB-UHFFFAOYSA-N	204	0.15	0.21	0.18
Carvone, (+/-)-	ULDHMXUKGWMISQ-UHFFFAOYSA-N	7439	0.13	0.23	0.18
Hex-2-ulofuranosyl hexopyranoside	CZMRCDWAGMRECEN-UHFFFAOYSA-N	1115	0.14	0.22	0.18
Sodium Benzoate	WXMKPNITSTVMEF-UHFFFAOYSA-M	517055	0.06	0.29	0.18
Ouabain	LPMXVESGRSUGHW-HBYQJFLCSAN	439501	0.10	0.25	0.18
Acetyldigitoxin	HPMZBILYSWLILX-UMDUKNJSSAN	5284512	0.09	0.26	0.18
ginsenoside F2	SWIROVJVGSGSPO-JBVRGBGGGSAN	9918692	0.13	0.22	0.18
Withaferin A	DBRXOUCRJQVYJQ-CKNDUULBSAN	265237	0.14	0.21	0.18
Parathion	LCCNCVORNKJIRZ-UHFFFAOYSA-N	991	0.07	0.28	0.18
(1S,3Z,5R,9S,12Z)-3,12-dimethyl-8-methylidene-6,18-dioxatricyclo[14.2.1.05,9]nonadeca-3,12,16(19)-triene-7,17-dione	KTYZKXFERQUCPX-AUJUDHDNSAN	101821136	0.07	0.28	0.18
Yohimbine	BLGXFZZNTVWLAY-SCYLSFHTSAN	8969	0.09	0.26	0.18
Safranal	SGAWOGXMMPSZPB-UHFFFAOYSA-N	61041	0.10	0.25	0.18
Sibutramine	UNAANXDKBXWMLN-UHFFFAOYSA-N	5210	0.07	0.28	0.18
Venlafaxine	PNVNVHUZROLTJ-UHFFFAOYSA-N	5656	0.08	0.27	0.18
Sophoramine	MMCQRJPAMIHLQX-ZOWXZIJZSAN	169014	0.12	0.23	0.17
Fraxinellone	XYAFLHHHZVPRN-GXTWGEPEZSAN	124039	0.07	0.28	0.17
4alpha-Phorbol 12-myristate 13-acetate	PHEDXBVPIONUQT-LQLWEASQSAN	122634	0.09	0.26	0.17
Phorbol 12-myristate 13-acetate	PHEDXBVPIONUQT-RGYGYFBISAN	27924	0.09	0.26	0.17
Yohimbine Hydrochloride	PIPZGJSEDRMUAW-VJDCAHTMSAN	6169	0.09	0.26	0.17
Cotinine	UIKROCXWUNQSPJ-VIFPVBQESAN	854019	0.13	0.22	0.17
Costunlide	HRYLQFBHBWLLLL-GRFSRWIASAN	5380858	0.07	0.28	0.17
Costunolide	HRYLQFBHBWLLLL-AHNJNIBGSAN	5281437	0.07	0.28	0.17
(3aS,6E,11aR)-6,10-dimethyl-3-methylidene-3a,4,5,8,9,11a-hexahydrocyclodeca[b]furan-2-one	HRYLQFBHBWLLLL-BOHUOVHSSAN	133640194	0.07	0.28	0.17
1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 1,2,3,4,5,6-hexahydro-, (1R)-	ANJTVLIZGCUXLD-UHFFFAOYSA-N	22407	0.11	0.24	0.17
Cytisine	ANJTVLIZGCUXLD-DTWKUNHWSAN	10235	0.11	0.24	0.17
Madecassoside	BNMGUJRJUUDLHW-HCZMHFOYSA-N	24825675	0.13	0.22	0.17

[(2S,3R,4S,5S,6R)-6-[[[(2R,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]oxymethyl]-3,4,5-trihydroxyoxan-2-yl](1S,2R,4aS,6aR,6aR,6bR,8R,8aS,9R,10R,11R,12aR,14bS)-8,10,11-trihydroxy-9-(hydroxymethyl)-1,2,6a,6b,9,12a-hexamethyl-2,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydro-1H-picene-4a-carboxylate	BNMGUJRJUUDLHW-VSVAVZEUSA-N	131801373	0.13	0.22	0.17
Cyasterone	NEFYSBQJYCICOG-YSEUJXISSA-N	119444	0.13	0.21	0.17
Prasterone	FMGSKLZLMKYGDP-USOAJAOKSA-N	5881	0.10	0.24	0.17
(E,5S,6S)-5-acetyloxy-6-[[[(3R,10S,13R,14R,15S,17R)-3,15-diacetyloxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-methylhept-2-enoic acid	OCLVBEOPEKEKNM-ABOXVQNFSAN	6443499	0.07	0.27	0.17
Cucurbitacin Q	LMJMTWXDWFVZHV-CWJYERATSA-N	5281323	0.12	0.22	0.17
Graveolone	WEDGVCZUPFZNDU-UHFFFAOYSA-N	177751	0.09	0.25	0.17
Methylprednisolone	VHRSUDSXCMTMA-PJHHCJLFSAN	6741	0.06	0.28	0.17
Butylphthalide	HJXMNVQARNZTEE-UHFFFAOYSA-N	61361	0.09	0.25	0.17
Prednicarbate	FNPXMHRZILFCKX-KAJVQRHHSAN	6714002	0.11	0.23	0.17
(24E)-24-N-Propylidenecholesterol	OSELKOCHBMDKEJ-JUGJNGJRSA-N	5281328	0.09	0.25	0.17
ar-Turmerone	NAAJVHWFAXWBOK-ZDUSSCGKSA-N	160512	0.04	0.30	0.17
Alantolactone	PXOYOCNNSUAQNS-AGNJHWRGSA-N	72724	0.10	0.24	0.17
Benzyl alcohol, o-chloro-alpha-((isopropylamino)methyl)-, hydrochloride, monohydrate	DBPRUZCKPFOVDV-UHFFFAOYSA-N	21784	0.06	0.28	0.17
Taurolithocholic acid	QBYUNVOYXHFVKC-GBURMNQMSAN	439763	0.10	0.24	0.17
Xanthatin	RBRPTFMVULVGIC-ZTIIIDENSA-N	5281511	0.11	0.23	0.17
Isolinderalactone	VXZIFOKTSURLNL-YDHLFZDLSAN	5318587	0.10	0.24	0.17
Alisol A	HNOSJVWYGXOFRP-UNPOXIGHSAN	15558616	0.15	0.19	0.17
alpha-Spinasterin	JZVFJDZBLUFKCA-FXIAWGAOSAN	5281331	0.13	0.20	0.17
Deserpidine	CVBMAZKCSYWQR-WCGOZPBSSAN	8550	0.16	0.17	0.17
Nobiletin	MRIAQLRQZPPODS-UHFFFAOYSA-N	72344	0.03	0.30	0.17
Arcoline	HJJPJSXJAXAIPN-UHFFFAOYSA-N	2230	0.13	0.21	0.17
Methyleugenol	ZYEMGPIYFIJGTP-UHFFFAOYSA-N	7127	0.14	0.19	0.16
[(1R,2S,3S,5S,6R,8S)-6-hydroxy-8-methyl-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-9,10-dioxatetracyclo[4.3.1.0.2,5.0.3,8]decan-2-yl]methyl benzoate	YKRGDOXKVOZESV-QYDSDWLYSAN	46882877	0.06	0.27	0.16
Peoniflorin	YKRGDOXKVOZESV-WRJNSLSBSAN	442534	0.06	0.27	0.16
Gentiopicrin	DUAGQYUORDTXOR-GPQRQXLASAN	88708	0.07	0.26	0.16
Lovastatin	PCZOHLXUXFIOCF-BXMDZJMSAN	53232	0.10	0.23	0.16
Androstenediol	QADHLRWLCPCEKT-LOVVWNRFSAN	10634	0.08	0.25	0.16
alpha-Solanine	ZGVSETXHNHBTBK-UDJLNFBSAN	9549171	0.17	0.16	0.16
L-Pyroglutamic acid	ODHCTXKNWHHXJC-VKHMHEASAN	7405	0.09	0.24	0.16
DL-Pyroglutamic acid	ODHCTXKNWHHXJC-UHFFFAOYSA-N	499	0.09	0.24	0.16

Propoxyphene	XMLALTXPSGQGBX-GCJJKVERSA-N	10100	0.07	0.25	0.16
Menthone	NFLGAXVYCFJBMK-BDAKNGLRSA-N	26447	0.09	0.23	0.16
Digitoxin	WDJUZGPOPHTGOT-XUDUSOBPSA-N	441207	0.08	0.24	0.16
(-)-alpha-Pinene	GRWFGVWFFZKLTII-UACAKERBSA-N	440968	0.07	0.25	0.16
Fucoxidant (Technical Grade)	WZPKXSSMRAQGAC-DWOU CZDBSA-N	129532628	0.09	0.23	0.16
Demethoxyyangonin	DKKJNZYHGRUXBS-BQYQJAHWSA-N	5273621	0.06	0.26	0.16
Gastrodin	PUQSUZTXKPLAPR-UJPOAAIJSAN	115067	0.06	0.26	0.16
Inflatine	MXYUKLILVYORSK-UHFFFAOYSA-N	3945	0.08	0.24	0.16
Lobeline	MXYUKLILVYORSK-HBMCJLEFSA-N	101616	0.08	0.24	0.16
Testosterone	MUMGGOZAMZWBII-DYKIIIFRCSA-N	6013	0.06	0.26	0.16
Indobufen	AYDXAULLCROVIT-UHFFFAOYSA-N	107641	0.09	0.23	0.16
Ethacrynic acid	AVOLMBLBETYQHXX-UHFFFAOYSA-N	3278	0.08	0.24	0.16
Tangeretin	ULSUXBXHSYSGDT-UHFFFAOYSA-N	68077	0.03	0.29	0.16
Lupeol	MQYXUWHLBZFQQO-QGTGJCAVSA-N	259846	0.13	0.19	0.16
Nootkatone	WTOYNNBCKUYIKC-JMSVASOKSA-N	1268142	0.11	0.21	0.16
3'-Uridylic acid	FOGRQMPFHUIGU-XVFCMESISA-N	101543	0.08	0.23	0.16
Cortisone	MFYSYFVPBJMHGN-ZPOLXVRWSA-N	222786	0.08	0.23	0.16
Cortisone-[2H7]	MFYSYFVPBJMHGN-UHFFFAOYSA-N	521440	0.08	0.23	0.16
(20S)-Protopanaxadiol	PYXFVCFISTUSOO-HKUCOEKDSA-N	11213350	0.10	0.21	0.16
(8R,10R,14R)-17-[(2R)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	PYXFVCFISTUSOO-ODWQXCPLSA-N	145706029	0.10	0.21	0.16
	COHYTHOBIJLSHDF-UHFFFAOYSA-N	5318432	0.04	0.27	0.16
T-Ome-byakangelicin	SCGNAXSXMFSZME-GFCCVEGCSA-N	15945069	0.07	0.24	0.16
Cafestol	DNJVYWXIDISQRD-HWUKTEKMSA-N	108052	0.09	0.22	0.16
Esculentoside A	ZMXXKPCQLHYTHY-OWRBLJEPSA-N	11657924	0.10	0.21	0.16
Ergosterol	DNVPPKQSNMYLRS-APGDWVJISA-N	444679	0.11	0.20	0.16
Hydron;benzoate	WPYMKLBDIGXBTP-UHFFFAOYSA-N	20144841	0.06	0.25	0.16
Palmitoylethanolamide	HXYVTAGFYLMHSSO-UHFFFAOYSA-N	4671	0.11	0.20	0.16
Genkwadaphnin	QKMXESBAFIKRAD-LPHDITAFSA-N	124210	0.08	0.23	0.15
Dimethyl Fumarate	LDCRTTIIJACKKU-ONEGZZNKSA-N	637568	0.15	0.16	0.15
Desoxycortone	ZESRJSZRDMNHYY-FWFAHHUSA-N	6166	0.08	0.23	0.15
Chalepentin	FYCCUNGXGKNJV-UHFFFAOYSA-N	128834	0.08	0.23	0.15
(1R,9S,13Z)-1-amino-13-ethylidene-11-methyl-6-azatricyclo[7.3.1.0 ^{2,7}]trideca-2(7),3,10-trien-5-one	ZRJBHWIHUMBLCN-HNWKQCISSA-N	71308731	0.08	0.23	0.15
Huperzine A	ZRJBHWIHUMBLCN-YQJEDHNSA-N	854026	0.08	0.23	0.15
Procaine	MFDFFERRIHVXMIY-UHFFFAOYSA-N	4914	0.11	0.19	0.15
Gniditricin	NEIGQRKMHFDLTK-JXXNAEBBSA-N	5369749	0.10	0.20	0.15
Dictamnine	WIONIXOBNMDFJF-UHFFFAOYSA-N	68085	0.10	0.20	0.15
	CRDNMYFJWFXXOCH-UHFFFAOYSA-N	5318433	0.06	0.24	0.15
Progesterone	RJKFOVLPORLFTN-LEKSSAKUSA-N	5994	0.08	0.22	0.15
Brexanolone	AURFZBICLPNKBZ-SYBPFIFISA-N	92786	0.11	0.19	0.15

2-[2-[[[3S,6S,8R,10R,12R,13R,14R,17S)-3,12-dihydroxy-17-[(2S,5R)-5-(1-hydroxy-1-methyl-ethyl)-2-methyl-tetrahydrofuran-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-6-yl]oxy]-4,5-dihydroxy-6-(hydroxyme	JBGYSAVRIDZKA-CXYZVIKQSA-N	137795541	0.13	0.17	0.15
neoechinulin A	MYRPIYZIAHOECW-SAIKJTDSA-N	9996305	0.05	0.25	0.15
Atractylodin	GRBKWAXRYITKG-QFMFGICSA-N	5321047	0.06	0.24	0.15
Prunetin	KQMVAGISDHMJJ-UHFFFAOYSA-N	5281804	0.05	0.25	0.15
Ligustilide	IQVQXVMNOFTMU-FLIBITNWSA-N	5319022	0.12	0.18	0.15
Ginsenoside Rf	UZIOUZHBUYLDHW-XUBRWZAZSA-N	441922	0.13	0.17	0.15
Dioscin	VNONINPVFQTJOC-ZGXDEBHDSA-N	119245	0.13	0.17	0.15
(3R,4R,5R,6S)-2-[(2R,3S,4S,5R,6R)-4-hydroxy-2-(hydroxymethyl)-6-[[[1S,2R,4S,5'R,6R,7S,8R,9S,12S,13R,16S)-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.02,9.04,8.013,18]icos-18-ene-6,2'-oxane]-16-yl]oxy-5-[[[2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-3-yl]oxy-6-methyloxane-3,4,5-triol	VNONINPVFQTJOC-RFYRBAQGSA-N	45358125	0.13	0.17	0.15
3-O-[alpha-L-ramnopyranosyl(1 to 2)]-O-[alpha-L-ramnopyranosyl(1 to 4)]-O-beta-D-galactopyranosid(1)]-(25S)-spirost-5-ene-3beta-ol	VNONINPVFQTJOC-OKXOJKZSA-N	10653210	0.13	0.17	0.15
alpha-Asarone	RKFAZBXYICVSKP-AATRIKPKSA-N	636822	0.09	0.21	0.15
beta-Asarone	RKFAZBXYICVSKP-WAYWQWQTSA-N	5281758	0.09	0.21	0.15
Psoralen	ZCCUUQDIBDJBTU-UHFFFAOYSA-N	6199	0.05	0.25	0.15
Antineoplaston A10	OQGRFQCUGLKS AV-JTQLQIEISA-N	56260	0.06	0.24	0.15
4,4,8,10,14-pentamethyl-17-(2,6,6-trimethyloxan-2-yl)-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthrene-3,12-diol	PVLHOJXLNBFHDX-UHFFFAOYSA-N	328778	0.09	0.21	0.15
[(1R,2S,6R,10R,11S,13S)-1,6-dihydroxy-8-(hydroxymethyl)-4,12,12,15-tetramethyl-5-oxo-13-tetracyclo[8.5.0.02,6.011,13]pentadeca-3,8-dienyl] acetate	BOJKFRKNLSCGHY-VTWCCFLYSA-N	138114131	0.08	0.21	0.15
Elatericin	QCIDDKUNTHOJBT-WPSTUIQMSA-N	44387852	0.12	0.17	0.15
Sinensetin	LKMNXDYDUQAUCZ-UHFFFAOYSA-N	145659	0.03	0.26	0.15
Dibenzoylmethane	NZZIMKJIVMHWJC-UHFFFAOYSA-N	8433	0.05	0.24	0.15
Tramadol Hydrochloride	PPKXEPBICJTCRU-XMZRRARIVSA-N	63013	0.08	0.21	0.15
Scopolamine	STECJAGHUSJQJN-USLFZFAMSA-N	3000322	0.08	0.21	0.15
Sciadopitysin	YCXRBCHEOFVYEN-UHFFFAOYSA-N	5281696	0.09	0.21	0.15
[9-[(Z)-but-2-enyl]-8,8-dimethyl-2-oxo-9,10-dihydropyrano[2,3-f]chromen-10-yl] acetate	LTSBAPIBOQOBOR-WAYWQWQTSA-N	5320690	0.08	0.21	0.15
Cantharidin	DHZBEENLJMYSHQ-XCVPVQRUSA-N	5944	0.06	0.23	0.15
Brefeldin A (BFA)	KQNZDYTLMIZCT-KFKPYADVSA-N	6436187	0.10	0.19	0.15

(1R,2E,7R,10E,12S,13S,15R)-12,15-dihydroxy-7-methyl-8-oxabicyclo[11.3.0]hexadeca-2,10-dien-9-one	KQNZDYYTLMIZCT-SWGFJCPHSA-N	5352004	0.10	0.19	0.15
Skatole	ZFRKQXVRDFCRJG-UHFFFAOYSA-N	6736	0.05	0.24	0.14
Medrogestone	HCFSGRMEEXUOSS-JXEXPEPMSA-N	9949848	0.07	0.22	0.14
Byakangelicin	PKRPFNXROFUNDE-LLVKDONJSA-N	10211	0.07	0.22	0.14
Ginsenoside RG2	AGBCLJAHARWNLA-DQUQINEDSA-N	21599924	0.14	0.15	0.14
(2S,3R,4R,5R,6S)-2-[(2R,3R,4S,5S,6R)-2-[[[(3S,5R,6S,8R,9R,10R,12R,13R,14R,17R)-3,12-dihydroxy-17-[(2S)-2-hydroxy-6-methylhept-5-en-2-yl]-4,4,8,10,14-pentamethyl-2,3,5,6,7,9,11,12,13,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-6-yl]oxy]-4,5-dihydroxy-6-(hydroxymethyl)oxan-3-yl]oxy-6-methyloxane-3,4,5-triol	AGBCLJAHARWNLA-VPKRQXCNSA-N	124893126	0.14	0.15	0.14
Solasonine	QCTMYNGDIBTNSK-XEAAVONHSA-N	119247	0.14	0.15	0.14
(+)-Bornyl acetate	KGEKLUUHTZCSIP-SCVCMIEPSA-N	6950274	0.09	0.20	0.14
Swertiamarin	HEYZWP RKKUGDCR-QBXMVCASA-N	442435	0.06	0.22	0.14
Betulin	FVWJYYTZTCVBKE-ROUWMTJPSA-N	72326	0.11	0.17	0.14
Tropone	QVWDCTQRORVHHT-UHFFFAOYSA-N	10881	0.05	0.23	0.14
Isradipine	HMJIYCCIJYRONP-UHFFFAOYSA-N	3784	0.05	0.23	0.14
Loratadine	JCCNYMKQOSZNPW-UHFFFAOYSA-N	3957	0.12	0.16	0.14
(Z,6R)-6-[(3R,5R,10S,13R,14R,15S,17R)-3,15-diacetyloxy-4,4,10,13,14-pentamethyl-2,3,5,6,12,15,16,17-octahydro-1H-cyclopenta[a]phenanthren-17-yl]-2-methylhept-2-enoic acid	OTUZGGS AOMCYNC-WQRGJCNTSA-N	5317517	0.05	0.23	0.14
(3R,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	KZJWDPNRJALLNS-ZFVHJZABSA-N	12303645	0.09	0.19	0.14
Beta-Sitosterol	KZJWDPNRJALLNS-VJSFXXLFS A-N	222284	0.09	0.19	0.14
3-(2-((4aS,5R,8aS)-5,8a-Dimethyl-2-methylene-5-(((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl)oxy)methyl)decahydronaphthalen-1-yl)ethyl)furan-2(5H)-one	YGCYRQKJYWQXHG-JXAGCRMJSA-N	160143	0.08	0.19	0.14
1'-Acetoxychavicol acetate	JAMQIUWGGBSIKZ-ZDUSSCGKSA-N	119104	0.06	0.21	0.14
Benzophenone	RWCCWEUUXYIKHB-UHFFFAOYSA-N	3102	0.05	0.22	0.14
Aldosterone	PQSUYGKTWSAVDQ-ZVIOFETBSA-N	5839	0.08	0.19	0.14
Benzaldehyde	HUMNYLRZRPPJDN-UHFFFAOYSA-N	240	0.10	0.17	0.14
CID 14021529	GKQMMZUXYRXFOH-QBLSGNHRSA-N	14021529	0.09	0.18	0.14
Hyoscyamine	RKUNBYITZUJHSG-VFSICIBPSA-N	154417	0.07	0.20	0.14
Atropine	RKUNBYITZUJHSG-PJPHBNEVSA-N	174174	0.07	0.20	0.14
Saponin	MAEBCGDGGATMSC-OSHGGGOQSA-N	198016	0.15	0.12	0.14
Curcumol	QRMPRVXWPCLVNI-YYFQZIEXSA-N	14240392	0.08	0.19	0.14

(1S,5R,8R)-2-methyl-6-methylidene-9-propan-2-yl-11-oxatricyclo[6.2.1.01,5]undecan-8-ol	QRMPRVXWPCLVNI-FJGURNMVSA-N	138107810	0.08	0.19	0.14
20-Hydroxyecdysone	NKDFYOWSKOHCCO-YPVLXUMRSA-N	5459840	0.10	0.17	0.13
Megestrol Acetate	RQZAXGRLVPAYTJ-GQFGMJRRSA-N	11683	0.05	0.22	0.13
Uracil	ISAKRJGNGUQOIC-UHFFFAOYSA-N	1174	0.06	0.21	0.13
Glucocalyxin A	UCDVIBNDYLUWFP-MJTHGBBVSA-N	10471963	0.10	0.17	0.13
Cinobufotalin	KBKUJFDSHBPPA-ZNCGZLKOSA-N	259776	0.08	0.19	0.13
[(1R,2S,7R,10S,11R,16S)-14,16-dihydroxy-7,11-dimethyl-6-(6-oxopyran-3-yl)-3-oxapentacyclo[8.8.0.02,4.02,7.011,16]octadecan-5-yl] acetate	KBKUJFDSHBPPA-PMULFBEUSA-N	137705737	0.08	0.19	0.13
Shionone	HXPXUNQUXCHJLL-LZQQOHPBSA-N	12315507	0.09	0.17	0.13
Ginsenoside Rh2	CKUVNOCSBYHIS-IRFFNABBSA-N	119307	0.10	0.16	0.13
(20R)-Ginsenoside Rh2	CKUVNOCSBYHIS-UHFFFAOYSA-N	14081290	0.10	0.16	0.13
Angelicin	XDROKJSWHURZGO-UHFFFAOYSA-N	10658	0.06	0.20	0.13
[(1S,4R,5R,6R,7S,8R,11R,13S,17S,18S,19R)-4,5,17-Trihydroxy-6,14,18-trimethyl-9,16-dioxo-3,10-dioxapentacyclo[9.8.0.01,7.04,19.013,18]nonadec-14-en-8-yl] 2-hydroxy-2-methylbutanoate	WRBGCYVAJRRQKP-KOMPIFHDSA-N	12310232	0.10	0.16	0.13
Cycloheximide	YPHMISFOHDHNIV-FSZOTQKASA-N	6197	0.11	0.15	0.13
	QMNUDYFKZYBWQX-UHFFFAOYSA-N	63112	0.05	0.21	0.13
Desoxycorticosterone Acetate	VPGRYOFKCNULNK-ACXQXYJUSA-N	5952	0.05	0.21	0.13
Corticosterone	OMFXVFTZEKFJZ-HJTSIMOOSA-N	5753	0.08	0.18	0.13
Betulonic acid	SLJTDWNVZKIDAU-SVAFSPIFSA-N	122844	0.13	0.13	0.13
biochanin A(1-)	WUADCCWRTIWANL-UHFFFAOYSA-M	25203224	0.07	0.19	0.13
Mexicanin-I	ZVLOPMNVFLSSAA-PYOYICEGSA-N	118701068	0.09	0.17	0.13
alpha-Sanshool	SBXYHCXVUCYYJT-UEOYEZOQSA-N	6440935	0.09	0.17	0.13
Isatin	JXDYKVIHCLTXOP-UHFFFAOYSA-N	7054	0.04	0.22	0.13
Proscillaridin	MYEFUXQJGHEQK-ALRJYLEOSA-N	5284613	0.06	0.20	0.13
5-((3S,8R,9S,10R,13R,14S,17R)-14-hydroxy-10,13-dimethyl-3-((2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyltetrahydro-2H-pyran-2-yloxy)-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl)-2H-pyran-2-one	MYEFUXQJGHEQK-XSSFRMRSAN	124328164	0.06	0.20	0.13
Caradrin	MYEFUXQJGHEQK-OWBILYANSA-N	222154	0.06	0.20	0.13
Manassantin A	ZGXXNVOBEIRACL-VOGCUZRYSA-N	15605952	0.08	0.18	0.13
6-Methoxy-7-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-2-one	SGTCGCCQZOOMJJ-UHFFFAOYSA-N	346340	0.05	0.21	0.13
Scopolin	SGTCGCCQZOOMJJ-YMILTQATSA-N	439514	0.05	0.21	0.13
Aristolone	UGVIZCBJCSXBCJ-JWFUOXDNSA-N	165536	0.05	0.20	0.13
Permethrin	RLLPVAHGXCWKJ-UHFFFAOYSA-N	40326	0.08	0.17	0.13
Sertraline	VGKDLMBJGBXTGI-SJCJKPOMSA-N	68617	0.04	0.21	0.13
6-Hydroxyhyoscyamine	WTQYWNWRJNXDEG-ABSNHQIMSA-N	442993	0.04	0.21	0.13

(1R,2R,5S,8S,9S,10R,12S)-5,12-dihydroxy-11-methyl-6-methylidene-16-oxo-15-oxapentacyclo[9.3.2.15,8.01,10.02,8]heptadec-13-ene-9-carboxylic acid	IXORZMNAPKEEDV-QTWFBFKQSA-N	439551	0.08	0.17	0.13
Plumericin	VFXXNAVZODKBIW-JKXVGBJFSA-N	5281545	0.04	0.21	0.12
Cocaine	ZPUCINDJVIVPJ-LJISPDSOSA-N	446220	0.06	0.19	0.12
Momordin Ic	HWYBGIDROCYPOE-WEAQAMGWSA-N	176596	0.11	0.14	0.12
Nandrolone Decanoate	JKWKMORAXJQQR-MOPIKTETSA-N	9677	0.08	0.16	0.12
Lidocaine	NNJVILVZKWQKPM-UHFFFAOYSA-N	3676	0.08	0.16	0.12
5,7-Dimethoxyflavone	JRFZSUMZAUHNSL-UHFFFAOYSA-N	88881	0.02	0.22	0.12
Asiaticoside	WYQVAPGDARQUBT-FGWHUUCPSA-N	11954171	0.09	0.15	0.12
Androstanolone	NVKAWKQGWIIWPM-ABEVXSGRSA-N	10635	0.05	0.19	0.12
Taraxasterol	XWMMEBCFHUKHEX-ZJJHUPNSA-N	115250	0.08	0.16	0.12
(3S,4aR,6aR,6bR,8aR,12S,12aS,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylidene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydricen-3-ol	XWMMEBCFHUKHEX-CWFQSGEHSAN	441686	0.08	0.16	0.12
[(3S,8R,9S,10S,13R,14S,16S,17R)-14-hydroxy-3-[(2R,4S,5S,6S)-5-hydroxy-4-methoxy-6-methyl-tetrahydropyran-2-yl]oxy-10,13-dimethyl-17-(5-oxo-2H-furan-3-yl)-1,2,3,4,5,6,7,8,9,11,12,15,16,17-tetradecahydrocyclopenta[a]phenanthren-16-yl] acetate	JLPDBLFVFSOCC-KYYHTQDCSA-N	6478017	0.08	0.16	0.12
Benzocaine	BLFLLBZGZJTVJG-UHFFFAOYSA-N	2337	0.07	0.17	0.12
Anisodine	JEJREKXHLFEVHN-QDXGGTILSA-N	11616712	0.05	0.19	0.12
Glyburide	ZNNLBTZKUZBEKO-UHFFFAOYSA-N	3488	0.03	0.21	0.12
Ponasterone A	PJYYBCXMCWUAZ-JJZTNILSA-N	115127	0.08	0.16	0.12
Pancuronium Bromide	NPIJXCQZLFKBMV-YTGGZJNLSA-L	27350	0.12	0.12	0.12
3-ACETYL-11-KETO-beta-BOSWELLIC ACID	HMMGKOVEOFBCAU-BCDBGHSCSA-N	11168203	0.09	0.15	0.12
Germacra-1(10),4,11(13)-triene-12,14-dioic acid, 2-beta,6-alpha,8-alpha-trihydroxy-, 12,6:14,2-dilactone, methacrylate, (E)-	JMUOPRSXUVOHFE-UXBLZVDNSA-N	6381428	0.10	0.13	0.12
Arnicolide D	NZESEVTYUVXOTC-APDQSUQKSA-N	182199	0.08	0.15	0.12
Ailanthone	WBBVXGHSWZIJST-RLQZCPESA-N	72965	0.08	0.15	0.12
Cinobufagin	SCULJPGYOQXQTK-OLRINKBESA-N	11969542	0.06	0.17	0.12
Anthraquinone	RZVHIXYEVGDQDX-UHFFFAOYSA-N	6780	0.02	0.21	0.12
Diethylpropion	XXEPPPIWZFCOJ-UHFFFAOYSA-N	7029	0.05	0.18	0.12
Solamargine	MBWUSSKCCUMJHO-ZGXDEBHDSA-N	73611	0.11	0.12	0.12
Solamarin, beta	MBWUSSKCCUMJHO-UHFFFAOYSA-N	437080	0.11	0.12	0.12
Ganodermanontriol	KASALCUNLBTNAA-LIPCCPSCSA-N	3001811	0.08	0.15	0.12
Khasianine	KRQDMAXNTWLTZ-UHFFFAOYSA-N	3479482	0.11	0.12	0.11
Hastatoside	PRZVXHGUJPSME-CZMSZWTGSA-N	92043450	0.04	0.19	0.11
Melatonin	DRLFMBDRBRZALE-UHFFFAOYSA-N	896	0.06	0.17	0.11
Aspirin	BSYNRYMUTXBXSQ-UHFFFAOYSA-N	2244	0.03	0.19	0.11
Betulinic Acid	QGJZLNKBHJESQX-FZFNOLFKSA-N	64971	0.08	0.14	0.11
Cyclandelate	WZHCOOQXZCIUNC-UHFFFAOYSA-N	2893	0.03	0.19	0.11
alpha-Amyrin acetate	UDXDFWBZZQHRO-UHFFFAOYSA-N	293754	0.04	0.17	0.11
Fotemustine	YAKWPXVTIGTRJH-UHFFFAOYSA-N	104799	0.08	0.13	0.11

Harpagoside	KVRQGMOSZKPBNS-FMHLWDFHSA-N	5281542	0.05	0.16	0.11
[(1R,8aR)-1,8a-dimethyl-6-oxo-7-prop-1-en-2-yl-1,2,3,4,7,8-hexahydronaphthalen-2-yl] (Z)-3-methylsulfanylprop-2-enoate	OHANKWLYDFHJOJ-ZRMWPANMSA-N	5320503	0.06	0.15	0.11
Dexamethasone acetate	AKUJBENLRBOFTD-RPRRAYFGSA-N	236702	0.06	0.15	0.11
Ketoprofen	DKYWVDODHFEZIM-UHFFFAOYSA-N	3825	0.07	0.14	0.11
Forskolin	OHCQJHSOBTURHG-KGGHGJDLA-N	47936	0.06	0.15	0.10
Nandrolone	NPAGDVCDWIYMMC-IZPLOLNSA-N	9904	0.05	0.16	0.10
Tetrahydrocortisone	SYGWGHVTLUBCEM-ZIZPXRJBSA-N	5866	0.06	0.15	0.10
Raddeanin A	VQQGPFHGWNGX-PPCHTBMASA-N	174742	0.08	0.12	0.10
Cinnamaldehyde	KJPRLNWUNMBNBZ-QPJXVBHSA-N	637511	0.07	0.13	0.10
Araloside A	KQSFNXMDCOFFGW-GNDIVNLPSA-N	10079497	0.07	0.13	0.10
(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl acetate	XHXUANMFYXWVNG-WCQGTBRESA-N	62335	0.06	0.14	0.10
Phenobarbital	DDBREPKUVSBGFI-UHFFFAOYSA-N	4763	0.06	0.14	0.10
1,4-Naphthoquinone	FRASJONUBLZVQX-UHFFFAOYSA-N	8530	0.02	0.18	0.10
Myrtenal	KMRMUZKLFIEVAO-UHFFFAOYSA-N	61130	0.08	0.12	0.10
Benzoyl Peroxide	OMPJBNCRMGITSC-UHFFFAOYSA-N	7187	0.04	0.16	0.10
Pregnenolone	ORNBQBICIOFOEO-QGVNFLTSA-N	8955	0.07	0.13	0.10
Trigonelline	WWNNZCOKKKDOPX-UHFFFAOYSA-N	5570	0.05	0.15	0.10
Methenolone acetate	PGAUJQOPTMSERF-QWQRBHLCSA-N	252372	0.04	0.15	0.10
Morroniside	YTZSBJLNMIQROD-SFBCHFHNLSA-N	11228693	0.03	0.16	0.10
methyl (4aS,8aS)-3-hydroxy-1-methyl-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,3,4,4a,8,8a-hexahydropyrano[3,4-c]pyran-5-carboxylate	YTZSBJLNMIQROD-RZYLQQLPSA-N	138107798	0.03	0.16	0.10
Methyl palmitate	FLIACVVOZYBSBS-UHFFFAOYSA-N	8181	0.05	0.14	0.10
Adenanthin	WQVYSFBBFDGRG-FYHXSELJSA-N	15011073	0.07	0.12	0.10
Triamcinolone	GFNANZIMVAIWHM-OBYCQNJPSA-N	31307	0.07	0.12	0.10
Ecdysone	UPEZCKBFRMILAV-JMZLNJERSA-N	19212	0.08	0.11	0.10
[(3aS,5R,5aS,6R,8S,8aS,9S,9aR)-9-acetyloxy-8-hydroxy-5,8a-dimethyl-1-methylidene-2-oxo-4,5,5a,6,7,8,9,9a-octahydro-3aH-azuleno[6,5-b]furan-6-yl] acetate	JXEGMONJOSAULB-NKNCCKRASA-N	5315501	0.06	0.13	0.10
Ethyl Acetate	XEKOWRVHYACXOJ-UHFFFAOYSA-N	8857	0.10	0.09	0.09
5,7-Dimethoxycoumarin	NXJCRELRQHQBQA-UHFFFAOYSA-N	2775	0.03	0.16	0.09
alpha-Amyrin	FSLPMRQHCOLESF-SFMCKYFRSA-N	73170	0.05	0.14	0.09
Propoxur	ISRUGXGCCGIOQO-UHFFFAOYSA-N	4944	0.03	0.16	0.09
Soyasaponin I	PTDAHAWQAGSZDD-IOVCITQVSA-N	122097	0.05	0.13	0.09
Benzyl Benzoate	SESFYSPDFLNCH-UHFFFAOYSA-N	2345	0.02	0.16	0.09
Brevelin A	KUPPVZXLWANEJJ-UXPPPGFSFA-N	12302076	0.05	0.13	0.09
Chalcone	DQFBYFPFKXHELB-VAWYXSNFSA-N	637760	0.05	0.14	0.09
6-[[4,4,6a,6b,11,11,14b-Heptamethyl-8a-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxycarbonyl-1,2,3,4a,5,6,7,8,9,10,12,12a,14,14a-tetradecahydricen-3-yl]oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	YOSRLTNUOCHBEA-UHFFFAOYSA-N	13909679	0.06	0.12	0.09
beta-Amyrine	JFSHUTJDVKUMTJ-QKAPCWNWSA-N	15942855	0.03	0.15	0.09
2-Hydroxyquinoline	LISFMEBWQUVKPJ-UHFFFAOYSA-N	6038	0.03	0.15	0.09

Gamabufotalin	FMTLOAVOGWSPEF-KJRPADTMSA-N	259803	0.05	0.13	0.09
Acetophenone	KWOLFJPFCHCOCG-UHFFFAOYSA-N	7410	0.05	0.12	0.08
Genipin	AZKVWQKMDGGDSV-BCMRRTOSA-N	442424	0.04	0.13	0.08
Gaillardin	UTPGJEROJZHISI-DFGCIRUSA-N	267247	0.05	0.11	0.08
Petasin	ISTBXSFGFOYLTM-NZEDGPFZSA-N	5281526	0.03	0.13	0.08
7-Hydroxy-3-(4-hydroxyphenyl)-8-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]chromen-4-one	HKEAFJYKMMKDOR-UHFFFAOYSA-N	5385074	0.04	0.12	0.08
7-hydroxy-3-(4-hydroxyphenyl)-8-[(2S,3S,5S)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]chromen-4-one	HKEAFJYKMMKDOR-DTYSYODJSA-N	53384442	0.04	0.12	0.08
Ganoderic acid DM	ZTKZZRIVAYGFSF-PIPDTRPPSA-N	11784642	0.04	0.11	0.08
Resibufogenin	ATLJNLJIJOCWJE-CWMZOUAVSA-N	6917974	0.04	0.11	0.08
Uralsaponin A	LPLVUJXQOOQHMX-MOGLOQIBSA-N	128229	0.05	0.10	0.07
Glycyrrhizin	LPLVUJXQOOQHMX-QWBHMCJMSA-N	14982	0.05	0.10	0.07
6-[2-[[[(6aR,6bS,8aS,11S,12aS,14aS,14bS)-11-carboxy-4,4,6a,6b,8a,11,14b-heptamethyl-14-oxo-2,3,4a,5,6,7,8,9,10,12,12a,14a-dodecahydro-1H-picen-3-yl]oxy]-6-carboxy-4,5-dihydroxyoxan-3-yl]oxy-3,4,5-trihydroxyoxane-2-carboxylic acid	LPLVUJXQOOQHMX-UHVJGROESA-N	137706400	0.05	0.10	0.07
Ammonium glycyrrhizate	ILRKKHJEINIICQ-OOFFSTKBASA-N	62074	0.05	0.10	0.07
rubiarbonone C	NKSVARYCVTXDAJ-DMDMSIRMSA-N	44566786	0.04	0.11	0.07
Ibuprofen	HEFNNWSXXWATRW-UHFFFAOYSA-N	3672	0.05	0.10	0.07
Saccharin	CVHZOJKTDOEJC-UHFFFAOYSA-N	5143	0.02	0.13	0.07
Erythrodiol	PSZDOEIIJFCFE-OSQDELBUSAN	101761	0.03	0.11	0.07
5-[(5R,8R,9R,10S,13R,14S)-3,14-dihydroxy-10,13-dimethyl-1,2,3,4,5,6,7,8,9,11,12,15,16,17-tetradecahydrocyclopenta[a]phenanthren-17-yl]pyran-2-one	QEEBRPGZBVVINN-FRXUBUBWSA-N	137705150	0.03	0.11	0.07
Bufalin	QEEBRPGZBVVINN-BMPKRDENSA-N	9547215	0.03	0.11	0.07
Visnagin	NZVQLVGOZRELTG-UHFFFAOYSA-N	6716	0.02	0.12	0.07
Geniposide	IBFYXTRXDNAPMM-BVTMAQQCSA-N	107848	0.03	0.11	0.07
methyl (4aR,7aS)-7-(hydroxymethyl)-1-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-1,4a,5,7a-tetrahydrocyclopenta[c]pyran-4-carboxylate	IBFYXTRXDNAPMM-VBNMSVSYSA-N	137706142	0.03	0.11	0.07
beta-Boswellic acid	NBGQZFQREPIKMG-PONOSELZSA-N	168928	0.06	0.08	0.07
3-Butylidenephthalide	WMBOCUXNNSOQHM-FLIBITNWSA-N	642376	0.03	0.10	0.07
Scoparone	GUAFOGOEJLSQBT-UHFFFAOYSA-N	8417	0.02	0.11	0.07
ziyuglycoside II	MFIXLWYJTVEVGO-YHGWSDCJSA-N	71773126	0.05	0.08	0.06
Loganin	AMBQHHVBBHTQBF-UOUCRYGSSA-N	87691	0.02	0.11	0.06
Naproxen	CMWTZPSULFXXJA-VIFVVBQESA-N	156391	0.05	0.07	0.06
Arjuginin	IFIQVSCCFRJSJV-NWCCWSSZSA-N	12444386	0.06	0.06	0.06
Menadione	MJVAVZPDRWSRRC-UHFFFAOYSA-N	4055	0.02	0.09	0.06
Bis(2-ethylhexyl) phthalate	BJQHLKABXJIVAM-UHFFFAOYSA-N	8343	0.01	0.10	0.05

Bergapten	BGEBZHIAGXMEMV-UHFFFAOYSA-N	2355	0.02	0.08	0.05
Asiatic Acid	JXSIVIRDWWRQRT-UYDOISQJSA-N	119034	0.06	0.04	0.05
beta-Ursolic acid	WCGUUGGRBIKTOS-GPOJBZKASA-M	7163175	0.02	0.07	0.05
Arjunolic acid	RWNHLTKFBKYDOJ-DDHMHSPCSA-N	73641	0.04	0.05	0.05
Esculentic acid (Phytolacca)	CLXOLTFMHAXJST-GOYMLYASSA-N	187898	0.02	0.06	0.04
Anethole	RUVINXPYWBROJD-ONEGZZNKSA-N	637563	0.02	0.06	0.04
Genisteol 7-monoglucoside	ZCOLJUOHXJRHDI-UHFFFAOYSA-N	5284639	0.03	0.05	0.04
Corosolic acid	HFGSQOYIOKBQOW-ZSDYHTTISA-N	6918774	0.04	0.04	0.04
Tormentic acid	OXVUXGFZHDKYLS-BLIWDXROSA-N	73193	0.02	0.04	0.03
Oleanolic Acid	MIJYXULNPSFWEK-GTOFXWBISA-N	10494	0.02	0.04	0.03
Dimethyl Phthalate	NIQCNGHVCWTJSM-UHFFFAOYSA-N	8554	0.01	0.05	0.03
18alpha-Glycyrrhetic acid	MPDGHEJMBKOTSU-PMTKVOBESA-N	73398	0.01	0.03	0.02
Glycyrrhetin	MPDGHEJMBKOTSU-UHFFFAOYSA-N	3230	0.01	0.03	0.02
Enoxolone	MPDGHEJMBKOTSU-YKLVYJNSSA-N	10114	0.01	0.03	0.02
beta-Glycyrrhetic acid	MPDGHEJMBKOTSU-WFJWYAKSA-N	18526330	0.01	0.03	0.02
Saikosaponin D	KYWSCMDFVARMPPN-LCSVLAELSA-N	107793	0.03	0.01	0.02
(2S)-2-[(2S)-3,5-dihydroxy-2- [[[(1S,4S,5R,8S,9R,13S,14R,17S,18S)-2- hydroxy-9-(hydroxymethyl)- 4,5,9,13,20,20-hexamethyl-24- oxahexacyclo[15.5.2.01,18.04,17.05,14.08, 13]tetracos-15-en-10-yl]oxy]-6- methyloxan-4-yl]oxy-6- (hydroxymethyl)oxane-3,4,5-triol	KYWSCMDFVARMPPN-SXLNWCAISA-N	137705034	0.03	0.01	0.02
(2S)-2-[(2R)-3,5-dihydroxy-2- [[[(1S,4S,5R,8R,9R,13S,14R,17S,18R)-2- hydroxy-9-(hydroxymethyl)- 4,5,9,13,20,20-hexamethyl-24- oxahexacyclo[15.5.2.01,18.04,17.05,14.08, 13]tetracos-15-en-10-yl]oxy]-6- methyloxan-4-yl]oxy-6- (hydroxymethyl)oxane-3,4,5-triol	KYWSCMDFVARMPPN-RPLIYQGKSA-N	138114182	0.03	0.01	0.02
Dibutyl Phthalate	DOIRQSBPFJWKBE-UHFFFAOYSA-N	3026	0.00	0.03	0.02

This table presents the predicted activity scores for 1,594 natural product compounds using Random Forest (RF) and Support Vector Machine (SVM) models. The structural information for these compounds was retrieved from the BATMAN Traditional Chinese Medicine (TCM) database (<http://bionet.ncpsb.org.cn/batman-tcm/>).