



G166766A Agilent Fiehn GC/MS Metabolomics RTL Library: List of Compounds

Data Sheet

800 Metabolite library for more compound identification

The Agilent Fiehn GC/MS metabolomics RTL Library is the most comprehensive commercially available GC/MS library of metabolite spectra. This expanding library currently contains over 1,400 entries for approximately 800 common metabolites, including spectra corresponding to partial derivatization of metabolites under the recommended conditions.

In this list, each entry includes the name, CAS, and PubChem numbers of the native molecule for easier compound recognition and subsequent literature, software, and pathway searching.



CAS #	PubChem	Compound
20549-47-7	443163	(-)-dihydrocarveol
20549-47-7	443163	(-)-dihydrocarveol
35323-91-2	72276	(-)-epicatechin 1
35323-91-2	72276	(-)-epicatechin 2
51028-73-0	5816	(-)-epinephrine
51028-73-0	5816	(-)-epinephrine
18457-55-1	369312	(-)-perillyl alcohol
601-57-0	91477	(+) -4-cholesten-3-one 1
601-57-0	91477	(+) -4-cholesten-3-one 2
551-16-6	11082	(+)-6-aminopenicillanic acid 1
551-16-6	11082	(+)-6-aminopenicillanic acid 2
551-16-6	11082	(+)-6-aminopenicillanic acid 3
551-16-6	11082	(+)-6-aminopenicillanic acid 4
64280-14-4	107885	(±)-11-nor-9-carboxy-delta-9-THC Standard
51268-88-3	440294	(1R,2S)- <i>cis</i> -1,2-dihydro-1,2-naphthalenediol
	1597617	(4-Hydroxy-2-oxo-1,2-dihydro-quinolin-3-yl)-acetic acid butyl ester
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic acid
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic acid
161886-59-5	11058264	(S)-Carnitine Mesylate Isobutylester
111-03-5	5283468	1 monoolein
123-94-4	24699	1 monostearin
95-93-2	7269	1,2,4,5-tetramethylbenzene
765-87-7	13006	1,2-cyclohexanedione 1
765-87-7	13006	1,2-cyclohexanedione 2
765-87-7	13006	1,2-cyclohexanedione 3
82950-64-9	1321	1,2-didecanoylglyceride
504-02-9	10434	1,3 cyclohexanedione
504-02-9	10434	1,3 cyclohexanedione
504-02-9	10434	1,3 cyclohexanedione
0-00-0	440168	1,3,5(10)-estratrien-3,6- <i>beta</i> -17- <i>beta</i> -triol
53-16-7	5870	1,3,5(10)-estratrien-3-ol-17-one 1
53-16-7	5870	1,3,5(10)-estratrien-3-ol-17-one 2
109-76-2	428	1,3-diaminopropane 1
109-76-2	428	1,3-diaminopropane 2
96-26-4	4180364	1,3-dihydroxyacetone
504-63-2	10442	1,3-propanediol
637-88-7	12511	1,4-cyclohexanedione 1
637-88-7	12511	1,4-cyclohexanedione 2
100937-52-8	451991	1,4-dideoxy-1,4-imino-D-arabinitol 1
100937-52-8	451991	1,4-dideoxy-1,4-imino-D-arabinitol 2

CAS #	PubChem	Compound
31519-22-9	671	1,4-dihydroxy-2-naphthoic acid
6892-68-8	439352	1,4-dithioerythritol
154-58-5	219984	1,5-anhydro-D-sorbitol
154-58-5	64960	1,5-anhydroglucitol
498-07-7	2724705	1,6-anhydro-glucose
1679-53-4	74300	10-hydroxydecanoic acid
2268-98-6	519975	11a-Acetoxyprogesterone 1
2268-98-6	519975	11a-Acetoxyprogesterone 2
	4620898	12a-Hydroxy-6-Deoxydehydromunduserone
	4646739	12a-Hydroxy-9-Demethylmunduserone-8-Carboxylic acid
	6708561	13-Methyl-4, 4-Bisnor-8,11,13-Podocarpatrien-3-One 1
	6708561	13-Methyl-4, 4-Bisnor-8,11,13-Podocarpatrien-3-One 2
35850-13-6	5280887	15-keto-prostaglandin F-2- <i>alpha</i>
35850-13-6	5280887	15-keto-prostaglandin F-2- <i>alpha</i>
0	122281	16-glucuronide-estriol
561-63-7	6453303	19-hydroxycholesterol
22059-21-8	535	1-aminocyclopropane-1-carboxylic acid
112-30-1	8174	1-decanol (decyl alcohol)
36653-82-4	2682	1-hexadecanol
36653-82-4	2682	1-hexadecanol, (cetyl alcohol)
86-48-6	6844	1-hydroxy-2-naphthoic acid
129-43-1	8512	1-hydroxyanthraquinone
6351-10-6	22819	1-indanol
3106-60-3	457	1-methyl nicotinamide 1
3106-60-3	457	1-methyl nicotinamide 2
15763-06-1	16219662	1-methyladenosine 1
15763-06-1	16219662	1-methyladenosine 2
616-04-6	69217	1-methylhydantoin 1
616-04-6	69217	1-methylhydantoin 2
21339-55-9	676159	1-methyl-L-tryptophan 1
21339-55-9	676159	1-methyl-L-tryptophan 2
21339-55-9	676159	1-methyl-L-tryptophan 3
143-08-8	8914	1-nonanol
112-88-9	8217	1-octadecene
111-87-5	957	1-octanol
3391-86-4	2724898	1-octen-3-ol
14838-15-4	26934	1R, 2S-Phenylpropylamine
123-94-4	24699	1-stearoyl-rac-glycerol
72003-83-9	188966	2' Deoxyadenosine 5'-diphosphate
102-32-9	547	2-(3,4-dihydroxyphenyl)acetic acid

CAS #	PubChem	Compound
501-94-0	10393	2-(4-hydroxyphenyl)ethanol
6698-26-6	65166	2', 5'-Dideoxyadenosine
	6708739	2,3,4-Trihydroxy-4'-Ethoxybenzophenone
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 1
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 2
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 3
513-85-9	262	2,3-butanediol 1
513-85-9	262	2,3-butanediol 2
	65161	2',3'-dideoxyuridine
38186-71-9	5379071	2',3-Dihydroxy-4,4',6'-Trimethoxychalcone
	6728940	2,3-Dihydroxy-4-Methoxy-4'-Ethoxybenzophenone
99-50-3	19	2,3-dihydroxybenzoic acid
1133-63-7	254	2,3-dihydroxybiphenyl
16867-04-2	28115	2,3-dihydroxypyridine
13545-04-5	11848	2,3-dimethylsuccinic acid
138-81-8	61	2,3-diphosphoglycerate
615-58-7	12005	2,4-dibromophenol
69616-74-6	5955473	2',4-Dihydroxy-3,4',6'-Trimethoxychalcone
23945-44-0	90301	2,4-dihydroxypyrimidine-5-carboxylic acid
6342-92-3	5355888	2',5'-Dihydroxy-4-Methoxychalcone
1194-98-5	70949	2,5-dihydroxybenzaldehyde
583-93-7	865	2,6-diaminopimelic acid 1
583-93-7	865	2,6-diaminopimelic acid 2
615-58-7	11847	2,6-dibromophenol
6307-89-7	238769	2,6-Dihydroxy-4-Methoxytoluene
128-37-0	31404	2,6-ditert-butyl-4-methylphenol 1
128-37-0	31404	2,6-ditert-butyl-4-methylphenol 2
15450-76-7	97250	2,8-quinolinediol
516-72-3	121935	20-hydroxycholesterol 1
516-72-3	121935	20-hydroxycholesterol 2
566-78-9	11276	21-Acetoxypregnenolone
17954-98-2	167685	22-hydroxycholesterol
2140-46-7	65094	25-hydroxycholesterol
7568-93-6	1000	2-amino-1-phenylethanol
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 1
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 2
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 1
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 2
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 3
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 4

CAS #	PubChem	Compound
3177-80-8	255720	2-amino-3-methoxybenzoic acid 1
3177-80-8	255720	2-amino-3-methoxybenzoic acid 2
60-23-1	6058	2-aminoethanethiol 1
60-23-1	6058	2-aminoethanethiol 2
644-90-6	69522	2-aminooctanoic acid 1
644-90-6	69522	2-aminooctanoic acid 2
95-55-6	5801	2-aminophenol 1
95-55-6	5801	2-aminophenol 2
95-55-6	5801	2-aminophenol 3
110-65-6	8066	2-butyne-1,4-diol
119-67-5	8406	2-carboxybenzaldehyde 1
119-67-5	8406	2-carboxybenzaldehyde 2
958-09-8	13730	2'-deoxyadenosine
93839-95-3	188955	2'-Deoxyadenosine 3':5'-cyclic monophosphate
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 1
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 2
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 3
652157-52-3	637	2'-deoxycytidine
1032-65-1	13945	2'-deoxycytidine 5'-monophosphoric acid
533-67-5	5460005	2-deoxy-D-ribose 1
533-67-5	5460005	2-deoxy-D-ribose 2
961-07-9	187790	2'-deoxyguanosine
102916-66-5	25245723	2-deoxyribose 5-phosphate
951-78-0	13712	2-deoxyuridine 1
951-78-0	13712	2-deoxyuridine 2
42155-08-8	18601100	2'-Deoxyuridine 5'-monophosphate 1
42155-08-8	18601100	2'-Deoxyuridine 5'-monophosphate 2
104-76-7	7720	2-ethyl-1-hexanol
149-57-5	8697	2-ethylcaproic acid
149-57-5	8697	2-ethylhexanoic acid 1
149-57-5	8697	2-ethylhexanoic acid 2
611-14-3	11903	2-ethyltoluene
88-14-2	6919	2-furoic acid
928-94-9	5318042	2-hexen 1-ol
13419-69-7	5282707	2-hexenoic acid
	5024745	2-Hydroxy-5 (6)Epoxy-Tetrahydrocaryophyllene
582-24-1	68490	2-hydroxyacetophenone 1
582-24-1	68490	2-hydroxyacetophenone 2
90-01-7	5146	2-hydroxybenzyl alcohol
90-43-7	7017	2-hydroxybiphenyl

CAS #	PubChem	Compound
565-70-8	11266	2-hydroxybutyric acid
1214-47-7	5367146	2-hydroxychalcone 1
1214-47-7	5367146	2-hydroxychalcone 2
614-60-8	637540	2-hydroxycinnamic acid
362-06-1	440623	2-hydroxyestrone 1
362-06-1	440623	2-hydroxyestrone 2
609-71-2	69114	2-hydroxynicotinic acid
614-75-5	11970	2-hydroxyphenylacetic acid
142-08-5	8871	2-hydroxypyridine
59-31-4	6038	2-hydroxyquinoline 1
59-31-4	6038	2-hydroxyquinoline 2
615-13-4	11983	2-indanone
3237-44-3	36	2-isopropylmalic acid
689-31-6	71	2-ketoadipic acid 1
689-31-6	71	2-ketoadipic acid 2
600-18-0	58	2-ketobutyric acid 1
600-18-0	58	2-ketobutyric acid 2
13022-85-0	159664	2-ketocaproic acid
4502-00-5	70	2-ketoisocaproic acid 1
4502-00-5	70	2-ketoisocaproic acid 2
342385-52-8	159793	2-keto-L-gulonic acid 1
342385-52-8	159793	2-keto-L-gulonic acid 2
	5781145	2'-Methoxyformonetin
29267-67-2	121805	2-Methoxyresorcinol
1214-20-6	71034	2-Methoxyxanthone
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO--10, 10-Dimethylbicyclo[7:2:0]Undeca 1
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO--10, 10-Dimethylbicyclo[7:2:0]Undeca 2
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO--10, 10-Dimethylbicyclo[7:2:0]Undeca 3
3443-84-3	5319879	2-oleoylglycerol
2140-79-6	317398	2-O-Methyladenosine
103-81-1	7680	2-phenylacetamide 1
103-81-1	7680	2-phenylacetamide 2
103-81-1	7680	2-phenylacetamide 3
675-20-7	12665	2-piperidone 1
675-20-7	12665	2-piperidone 2
112-12-9	8163	2-undecanone 1
112-12-9	8163	2-undecanone 2

CAS #	PubChem	Compound
2734-48-7	151491	3-(1-pyrazolyl)-L-alanine
495-78-3	873	3-(2-hydroxyphenyl)propanoic acid
621-54-5	91	3-(3-hydroxyphenyl)propionic acid
306-23-0	9378	3-(4-hydroxyphenyl)lactic acid
501-97-3	10394	3-(4-hydroxyphenyl)propionic acid
4104-45-4	77743	3-(methylthio)-propylamine
59-92-2	836	3,4 dihydroxyphenylalanine (DOPA) 1
59-92-2	836	3,4 dihydroxyphenylalanine (DOPA) 2
4472-73-5	521171	3,4',5,6,7-Pentamethoxyflavone
	4000243	3,4-Didesmethyl-5-Deshydroxy-3'-Ethoxyscleroiin
99-50-3	72	3,4-dihydroxybenzoic acid
14883-87-5	85782	3,4-dihydroxymandelic acid
102-32-9	547	3,4-dihydroxyphenylacetic acid
120-14-9	8419	3,4-dimethoxybenzaldehyde
2316-26-9	717531	3,4-Dimethoxycinnamic acid 1
2316-26-9	717531	3,4-Dimethoxycinnamic acid 2
82801-81-8	105039	3,4-MDEA
42542-10-9	1615	3,4-MDMA
146255-66-5	443586	3,5-dihydroxyphenylglycine 1
146255-66-5	443586	3,5-dihydroxyphenylglycine 2
530-59-6	637775	3,5-dimethoxy-4-hydroxycinnamic acid 1
530-59-6	637775	3,5-dimethoxy-4-hydroxycinnamic acid 2
128-37-0	31404	3,5-Di- <i>tert</i> -butyl-4-hydroxytoluene
492-00-2	5393152	3,7-Dihydroxyflavone
	688664	3,7-Dimethoxyflavone
	5176389	3,7-Epoxycaryophyllan-6-Ol
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 1
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 2
23279-22-3	160450	3-amino-L-tyrosine 1
23279-22-3	160450	3-amino-L-tyrosine 2
23279-22-3	160450	3-amino-L-tyrosine 3
151-18-8	1647	3-aminopropionitrile 1
151-18-8	1647	3-aminopropionitrile 2
	6728949	3- <i>beta</i> -Hydroxy-23, 24-Bisnorchol-5-Enic acid
35608-63-0	110992	3-chloro-L-tyrosine 1
35608-63-0	110992	3-chloro-L-tyrosine 2
2922-42-1	80	3-dehydroshikimic acid 1
2922-42-1	80	3-dehydroshikimic acid 2
7057-27-4	4085802	3'-deoxyuridine 1
7057-27-4	4085802	3'-deoxyuridine 2

CAS #	PubChem	Compound
	6708683	3-Deshydroxysappanol Trimethyl Ether
6889-80-1	97143	3-Hydroxy-3',4'-Dimethoxyflavone
503-49-1	1662	3-hydroxy-3-methylglutaric acid (dicrotalic acid)
548-93-6	86	3-hydroxyanthranilic acid 1
548-93-6	86	3-hydroxyanthranilic acid 2
100-83-4	101	3-hydroxybenzaldehyde
620-24-6	102	3-hydroxybenzyl alcohol
588-30-7	637541	3-hydroxycinnamic acid
577-85-5	11349	3-hydroxyflavone
621-37-4	12122	3-hydroxyphenylacetic acid
503-66-2	68152	3-hydroxypropanoic acid 1
503-66-2	68152	3-hydroxypropanoic acid 2
503-66-2	68152	3-hydroxypropanoic acid 3
109-00-2	7971	3-hydroxypyridine
87-51-4	802	3-indoleacetic acid
771-51-7	351795	3-indoleacetonitrile
1821-52-9	92904	3-indolelactic acid 1
1821-52-9	92904	3-indolelactic acid 2
4385-35-7	78092	3-isochromanone
	808242	3-methoxy-N-3-quinolinylbenzamide 1
	808242	3-methoxy-N-3-quinolinylbenzamide 2
3715-29-5	49	3-methyl-2-oxobutanoic acid 1
3715-29-5	49	3-methyl-2-oxobutanoic acid 2
488-17-5	340	3-methylcatechol
368-16-1	64969	3-methyl-L-histidine
4707-46-4	736228	3-Methylorsellinic acid 1
4707-46-4	736228	3-Methylorsellinic acid 2
1504-06-9	150923	3-methyloxyindole 1
1504-06-9	150923	3-methyloxyindole 2
1504-06-9	150923	3-methyloxyindole 3
1504-06-9	150923	3-methyloxyindole 4
621-44-3	65124	3-nitro-L-tyrosine 1
621-44-3	65124	3-nitro-L-tyrosine 2
589-98-0	11527	3-octanol
828-01-3	3848	3-phenyllactic acid
820-11-1	439183	3-phosphoglycerate
80731-10-8	439183	3-phosphoglyceric acid
462-88-4	111	3-ureidopropionate 1
462-88-4	111	3-ureidopropionate 2
462-88-4	111	3-ureidopropionate 3

CAS #	PubChem	Compound
501-94-0	10393	4-(2-hydroxyethyl)phenol (tyrosol)
	364106	4,4'-Dimethoxydalbergione 1
	364106	4,4'-Dimethoxydalbergione 2
446-72-0	5280961	4',5,7-trihydroxyisoflavone
59-00-7	5699	4,8-dihydroxyquinoline-2-carboxylic acid (xanthurenic acid)
3025-96-5	18189	4-acetamidobutyric acid 1
3025-96-5	18189	4-acetamidobutyric acid 2
3233-32-7	96009	4-Acetoxyphenol 1
3233-32-7	96009	4-Acetoxyphenol 2
13022-85-0	18407	4-acetylbutyric acid 1
13022-85-0	18407	4-acetylbutyric acid 2
150-13-0	978	4-aminobenzoic acid
123-30-8	403	4-aminophenol 1
123-30-8	403	4-aminophenol 2
123-30-8	403	4-aminophenol 3
382-44-5	94141	4-androsten-11- <i>beta</i> -ol-3,17-dione 1
382-44-5	94141	4-androsten-11- <i>beta</i> -ol-3,17-dione 2
382-44-5	94141	4-androsten-11- <i>beta</i> -ol-3,17-dione 3
382-44-5	94141	4-androsten-11- <i>beta</i> -ol-3,17-dione 4
63-05-8	6128	4-androsten-3,17-dione 1
63-05-8	6128	4-androsten-3,17-dione 2
62-84-0	65542	4-androsten-7- <i>alpha</i> -ol-3,17-dione 1
62-84-0	65542	4-androsten-7- <i>alpha</i> -ol-3,17-dione 2
463-00-3	500	4-guanidinobutyric acid 1
463-00-3	500	4-guanidinobutyric acid 2
121-34-6	8468	4-hydroxy-3-methoxybenzoic acid
498-00-0	62348	4-hydroxy-3-methoxybenzyl alcohol
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 1
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 2
675-10-5	12663	4-hydroxy-6-methyl-2-pyrone
675-10-5	12663	4-Hydroxy-6-Methylpyran-2-One
4637-56-3	5460367	4-Hydroxyaminoquinoline-N-oxide
123-08-0	126	4-hydroxybenzaldehyde 1
123-08-0	126	4-hydroxybenzaldehyde 2
114-63-6	135	4-hydroxybenzoic acid
14191-95-8	26548	4-hydroxybenzyl cyanide
608-07-1	637542	4-hydroxycinnamic acid
6851-36-1	166768	4-hydroxymandelonitrile 1
6851-36-1	166768	4-hydroxymandelonitrile 2
156-38-7	127	4-hydroxyphenylacetic acid

CAS #	PubChem	Compound
22818-40-2	36143	4-hydroxyphenylglycine 1
22818-40-2	36143	4-hydroxyphenylglycine 2
156-39-8	979	4-hydroxyphenylpyruvic acid 1
156-39-8	979	4-hydroxyphenylpyruvic acid 2
626-64-2	12290	4-hydroxypyridine
611-36-9	69141	4-hydroxyquinoline 1
611-36-9	69141	4-hydroxyquinoline 2
492-27-3	3845	4-hydroxyquinoline-2-carboxylic acid(kynurenic acid)
122-03-2	326	4-isopropylbenzaldehyde
536-66-3	10820	4-isopropylbenzoic acid
536-60-7	325	4-isopropylbenzyl alcohol
959-23-9	641818	4'-Methoxychalcone 1
959-23-9	641818	4'-Methoxychalcone 2
959-23-9	641818	4'-Methoxychalcone 3
137-00-8	1136	4-methyl-5-thiazoleethanol
452-86-8	9958	4-methylcatechol
2107-77-9	5355836	4-Methyldaphnetin
90-33-5	5280567	4-methylumbelliferone 1
90-33-5	5280567	4-methylumbelliferone 2
14528-64-4	3505109	4-nitrocatechol
100-02-7	980	4-nitrophenol
4264-83-9	378	4-nitrophenyl phosphate
56-57-5	77341	4-nitroquinoline
56-57-5	5955	4-nitroquinoline N-oxide
7507-89-3	24135	4-O-Methylphloracetophenone 1
7507-89-3	24135	4-O-Methylphloracetophenone 2
7507-89-3	24135	4-O-Methylphloracetophenone 3
82-82-6	6723	4-pyridoxic acid 1
82-82-6	6723	4-pyridoxic acid 2
486-74-8	10243	4-quinolinecarboxylic acid
363-24-6	62453	4-vinylphenol 1
363-24-6	62453	4-vinylphenol 2
67-47-0	237332	5-(hydroxymethylfurfural) 1
67-47-0	237332	5-(hydroxymethylfurfural) 2
16834-13-2	86073	5,10,15,20-tetra(4-pyridyl)-21H,23H-porphine
582-60-5	675	5,6-dimethylbenzimidazole 1
582-60-5	675	5,6-dimethylbenzimidazole 2
5626-99-3	3605363	5,6-dihydro-2'-deoxyuridine 1
5626-99-3	3605363	5,6-dihydro-2'-deoxyuridine 2
5626-99-3	3605363	5,6-dihydro-2'-deoxyuridine 3

CAS #	PubChem	Compound
696-04-8	93556	5,6-dihydro-5-methyluracil 1
696-04-8	93556	5,6-dihydro-5-methyluracil 2
696-04-8	93556	5,6-dihydro-5-methyluracil 3
504-07-4	649	5,6-dihydrouracil 1
504-07-4	649	5,6-dihydrouracil 2
846-46-8	439289	5- <i>alpha</i> -Androstan-3,17-Dione 1
846-46-8	439289	5- <i>alpha</i> -Androstan-3,17-Dione 2
42366-37-0	242332	5- <i>alpha</i> -androstane-3- <i>beta</i> ,17- <i>beta</i> -diol
0	242332	5- <i>alpha</i> -androstane-3- <i>beta</i> ,17- <i>beta</i> -diol
80-97-7	3240	5- <i>alpha</i> -Cholestan-3- <i>beta</i> -ol
1175-06-0	16219541	5- <i>alpha</i> -Cholestan-3- <i>beta</i> -Ol-6-One 1
1175-06-0	16219541	5- <i>alpha</i> -Cholestan-3- <i>beta</i> -Ol-6-One 2
566-88-1	92128	5- <i>alpha</i> -Cholestan-3-one 1
566-88-1	92128	5- <i>alpha</i> -Cholestan-3-one 2
80-97-7	6665	5- <i>alpha</i> -Cholestanol
566-65-4	92810	5- <i>alpha</i> -pregnan-3,20-dione 1
566-65-4	92810	5- <i>alpha</i> -pregnan-3,20-dione 2
360-97-4	9679	5-aminoimidazole-4-carboxamide 1
360-97-4	9679	5-aminoimidazole-4-carboxamide 2
360-97-4	9679	5-aminoimidazole-4-carboxamide 3
660-88-8	138	5-aminovaleric acid 1
660-88-8	138	5-aminovaleric acid 2
660-88-8	138	5-aminovaleric acid 3
1229-12-5	440114	5- <i>beta</i> -androstane-3,17-dione
547-96-6	160520	5- <i>beta</i> -cholestan-3- <i>alpha</i> -7- <i>alpha</i> -12- <i>alpha</i> -triol 1
547-96-6	160520	5- <i>beta</i> -cholestan-3- <i>alpha</i> -7- <i>alpha</i> -12- <i>alpha</i> -triol 2
566-26-7	107722	5-cholesten-3- <i>beta</i> -7- <i>alpha</i> -diol
2457-80-9	439176	5'-deoxy-5'-(methylthio)adenosine 1
2457-80-9	439176	5'-deoxy-5'-(methylthio)adenosine 2
123316-61-0		5-Hydroxy-2',4',7,8-Tetramethoxyflavone
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 1
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 2
54-16-0	1826	5-hydroxyindole-3-acetic acid
9/8/4350	439280	5-hydroxy-L-tryptophan 1
9/8/4350	439280	5-hydroxy-L-tryptophan 2
3471-31-6	18986	5-methoxy-3-indoleacetic acid 1
3471-31-6	18986	5-methoxy-3-indoleacetic acid 2
484-20-8	2355	5-methoxy psoralen
7084-29-9	13845047	5-methyl-3'-deoxyuridine 1
7084-29-9	13845047	5-methyl-3'-deoxyuridine 2

CAS #	PubChem	Compound
79786-40-6	676293	6,3'-Dimethoxyflavone
63046-09-3	182362	6,4'-Dihydroxyflavone
60-32-2	564	6-aminocaproic acid
7568-08-4	439746	6-deoxy-D-glucose 1
7568-08-4	439746	6-deoxy-D-glucose 2
1191-25-9	14490	6-hydroxy caporic acid
1191-25-9	14490	6-hydroxy hexanoic acid
5006-66-6	72924	6-hydroxynicotinic acid 1
5006-66-6	72924	6-hydroxynicotinic acid 2
1569-60-4	20745	6-methyl-5-hepten-2-ol
110-93-0	9862	6-methyl-5-hepten-2-one
50-66-8	5778	6-methylmercaptapurine 1
50-66-8	5778	6-methylmercaptapurine 2
53411-70-4	91493	6-phosphogluconic acid
2196-14-7	5282073	7,4'-Dihydroxyflavone
38183-03-8	1880	7,8-Dihydroxyflavone
1086-80-2	5326566	7,8-dimethylalloxazine
566-28-9	91474	7-Oxocholesterol
1002-57-9	66085	8-aminocaprylic acid
62471-63-0	124925	8-oxo-2'-deoxyadenosine
486-25-9	10241	9-fluorenone
73-24-5	190	9H-purine-6-amine
1689-64-1	74318	9-hydroxyfluorene
484-17-3	10229	9-phenanthrenol
514-10-3	10569	abietic acid
480-44-4	5280442	Acacetin 1
480-44-4	5280442	Acacetin 2
82-86-0	6724	acenaphthenequinone 1
82-86-0	6724	acenaphthenequinone 2
82-86-0	6724	acenaphthenequinone 3
103-84-4	904	acetanilide 1
103-84-4	904	acetanilide 2
141-97-9	96	acetoacetate 1
141-97-9	96	acetoacetate 2
546-88-3	1990	acetohydroxamic acid
116-09-6	8299	acetol 1
116-09-6	8299	acetol 2
116-09-6	8299	acetol 3
116-09-6	8299	acetol 4
2478-38-8	17198	Acetosyringone 1

CAS #	PubChem	Compound
2478-38-8	17198	Acetosyringone 2
574-17-4	11321	acetylisatin 1
574-17-4	11321	acetylisatin 2
574-17-4	11321	acetylisatin 3
574-17-4	11321	acetylisatin 4
574-17-4	11321	acetylisatin 5
574-17-4	11321	acetylisatin 6
5147-00-2	189	acetyl-L-serine 1
5147-00-2	189	acetyl-L-serine 2
73-24-5	190	adenine 1
73-24-5	190	adenine 2
58-61-7	60961	adenosine
130-49-4	94136	adenosine 2'-monophosphate
60-92-4	6076	adenosine 3',5'-cyclic monophosphate
20398-34-9	6022	adenosine 5'-diphosphate
56-65-5	5957	adenosine 5'-triphosphate
699012-36-7	41211	adenosine-3'-monophosphate
84-21-9	224	adenosine-5-monophosphate 1
84-21-9	224	adenosine-5-monophosphate 2
628-94-4	12364	adipamide 1
628-94-4	12364	adipamide 2
628-94-4	12364	adipamide 3
628-94-4	12364	adipamide 4
124-04-9	196	adipic acid
51-43-4	5816	adrenaline 1
51-43-4	5816	adrenaline 2
382-45-6	223997	adrenosterone 1
382-45-6	223997	adrenosterone 2
54965-21-8	2082	albendazole
72-48-0	6293	alizarin
97-59-6	204	allantoin 1
97-59-6	204	allantoin 2
97-59-6	204	allantoin 3
87-89-8	892	allo-inositol
328-50-7	51	<i>alpha</i> ketoglutaric acid
10191-41-0	2116	<i>alpha</i> tocophereol
2152-75-2	740	<i>alpha</i> -D-glucosamine 1-phosphate
2152-75-2	740	<i>alpha</i> -D-glucosamine phosphate
2152-75-2	740	<i>alpha</i> -glucosamine 1-phosphate
481-06-1	221071	<i>alpha</i> -santonin 1

CAS #	PubChem	Compound
481-06-1	221071	<i>alpha</i> -santonin 2
57-43-2	2164	Amobarbital 1
57-43-2	2164	Amobarbital 2
897-06-3	6710699	Androsta-1, 4-Dien-3, 17-Dione 1
897-06-3	6710699	Androsta-1, 4-Dien-3, 17-Dione 2
53-41-8	5879	androsterone
	4303260	Anhydrobrazilic acid 1
	4303260	Anhydrobrazilic acid 2
88-21-1	6926	aniline-o-sulfonic acid
22862-76-6	31549	Anisomycin
10410-83-0	99980	Anthothecol
642-71-7	69505	Antiarol
520-36-5	5280443	Apigenin
77-02-1	6464	Aprobarbital
10323-20-3	66308	arabinose
488-82-4	94154	arabitol
506-30-9	10467	arachidic acid
497-76-7	440936	arbutin
481-05-0	65030	Artemisin 1
481-05-0	65030	Artemisin 2
133-05-1	101612	Asarinin (-)
4460-86-0	20525	Asarylaldehyde 1
4460-86-0	20525	Asarylaldehyde 2
56-84-8	5960	aspartic acid 1
56-84-8	5960	aspartic acid 2
0	4130574	asp-glu 1
0	4130574	asp-glu 2
0	4130574	asp-glu 3
0	4130574	asp-glu 4
0	4130574	asp-glu 5
2163-68-0	16553	atrazin-2-hydroxy 1
2163-68-0	16553	atrazin-2-hydroxy 2
2163-68-0	16553	atrazin-2-hydroxy 3
2163-68-0	16553	atrazin-2-hydroxy 4
2163-68-0	16553	atrazin-2-hydroxy 5
24607-05-4	3015189	Avocadyne
123-99-9	2266	azaleic acid
57-44-3	2294	barbital
112-85-6	8215	behenic acid
100-52-7	240	benzaldehyde

CAS #	PubChem	Compound
55-21-0	2331	benzamide
533-73-3	10787	benzene-1,2,4-triol
65-85-0	243	benzoic acid
119-53-9	8400	benzoin 1
119-53-9	8400	benzoin 2
123-31-9	785	benzoquinone
95-16-9	7222	benzothiazole
519-09-5	448223	Benzoyllecgonine
611-73-4	11915	benzoylformic acid 1
611-73-4	11915	benzoylformic acid 2
156-08-1	2341	Benzphetamine
100-51-6	244	benzyl alcohol
622-78-6	2346	benzyl isothiocyanate
3012-37-1	18170	benzyl thiocyanate
100-46-9	7504	benzylamine
884-33-3	3858	benzylsuccinic acid
107-95-9	239	<i>Beta</i> - alanine 1
107-95-9	239	<i>Beta</i> - alanine 2
45159-34-0	439742	<i>beta</i> -cyano-L-alanine
5996-00-9	441422	<i>beta</i> -gentiobiose 1
5996-00-9	441422	<i>beta</i> -gentiobiose 2
56-86-0	73064	<i>beta</i> -glutamic acid
819-83-0	2526	<i>beta</i> -glycerolphosphate
625-08-1	69362	<i>beta</i> -hydroxyisovalerate
14901-07-6	638014	<i>beta</i> -ionone 1
14901-07-6	638014	<i>beta</i> -ionone 2
123-35-3	31253	<i>beta</i> -myrcene
83-46-5	5321342	<i>beta</i> -sitosterol
22879-79-4	171548	biotin
92-52-4	7095	biphenyl
108-19-0	7913	biuret 1
108-19-0	7913	biuret 2
1812-30-2	2441	Bromazepam
97164-73-3	2479	Butabarbital
77-26-9	2481	Butalbital
3068-00-6	18302	butantriol
104-51-8	7705	butylbenzene
331-39-5	1549111	caffeic acid
58-08-2	2519	caffeine
13956-29-1	644019	Cannabidiol

CAS #	PubChem	Compound
521-35-7	2543	Cannabinol
334-48-5	2969	capric acid
124-07-2	379	caprylic acid
404-86-4	1548943	capsaicin
51-79-6	5641	carbamic acid ethyl ester (urethane)
86-74-8	6854	carbazole 1
86-74-8	6854	carbazole 2
305-84-0	9369	carnosine 1
305-84-0	9369	carnosine 2
154-23-4	9064	catechin
18829-70-4	73160	catechin
130405-40-2	6419835	catechin gallate
120-80-9	289	catechol
528-50-7	10712	cellobiose 1
528-50-7	10712	cellobiose 2
38819-01-1	439626	cellotetraose
56-75-7	5959	chloramphenicol 1
56-75-7	5959	chloramphenicol 2
327-97-9	6537496	chlorogenic acid 1
327-97-9	6537496	chlorogenic acid 2
67-97-0	5280795	cholecalciferol 1
67-97-0	5280795	cholecalciferol 2
57-88-5	304	cholesterol
1731-84-6	16213400	Cholestrol D6
480-40-0	5281607	chrysin
2041-14-7	339	ciliatine
104-55-2	637511	cinnamaldehyde 1
104-55-2	637511	cinnamaldehyde 2
140-10-3	444539	cinnamic acid
1792-81-0	92903	<i>cis</i> -1,2-cyclohexanediol
51268-88-3	440294	<i>cis</i> -1,2-dihydro-1,2-naphthalenediol
629-98-1	5354168	<i>cis</i> -13-Docosanol
3685-22-1	151138	<i>cis</i> -4-hydroxycyclohexanecarboxylic acid
498-23-7	638129	citraconic acid
498-23-7	643798	citraconic acid 1
498-23-7	643798	citraconic acid 2
498-23-7	643798	citraconic acid 3
498-23-7	643798	citraconic acid 4
498-23-7	643798	citraconic acid 5
5391-40-5	638011	citral 1

CAS #	PubChem	Compound
5391-40-5	638011	citral 2
5391-40-5	638011	citral 3
5391-40-5	638011	citral 4
6263-10-8	439766	citramalic acid
5949-29-1	311	citric acid
372-75-8	9750	citrulline 1
372-75-8	9750	citrulline 2
372-75-8	9750	citrulline 3
22316-47-8	2789	Clobazam
303-49-1	2801	clomipramine
1622-61-3	2802	Clonazepam
529-38-4	644006	Cocaethylene
50-36-2	446220	Cocaine
76-57-3	5284371	Codeine
6090-95-5	119054	conduritol epoxide 1
6090-95-5	119054	conduritol epoxide 2
458-35-5	1549095	coniferyl alcohol
601-53-6	85881	coprostan-3-one
53-06-5	222786	cortisone
60-27-5	588	Creatinine
60-92-4	6076	cyclic AMP
7665-99-8	295	cyclic GMP
108-91-8	7965	cyclohexanamine
98-89-5	7413	cyclohexanecarboxylic acid
52-52-8	2901	cycloleucine 1
52-52-8	2901	cycloleucine 2
19246-18-5	65270	cysteinylglycine 1
19246-18-5	65270	cysteinylglycine 2
19246-18-5	65270	cysteinylglycine 3
65-46-3	596	cytidine 1
65-46-3	596	cytidine 2
63-37-6	6131	cytidine-5'-monophosphate 1
63-37-6	6131	cytidine-5'-monophosphate 2
71-30-7	597	cytosine 1
71-30-7	597	cytosine 2
71-30-7	597	cytosine 3
59-23-4	206	D (+) galactose 1
59-23-4	206	D (+) galactose 2
1990-29-0	441032	D (+)altrose 1
1990-29-0	441032	D (+)altrose 2

CAS #	PubChem	Compound
6138-23-4	7427	D-(+) trehalose
10030-67-8	92817	D-(+)-melezitose
486-66-8	5281708	daidzein
923-16-0	601	D-Ala-D-Ala 1
923-16-0	601	D-Ala-D-Ala 2
923-16-0	601	D-Ala-D-Ala 3
579-36-2	448388	D-allose 1
579-36-2	448388	D-allose 2
51-64-9	5826	d-Amphetamine
490-83-5	835	dehydroascorbic acid 1
490-83-5	835	dehydroascorbic acid 2
490-83-5	835	dehydroascorbic acid 3
490-83-5	835	dehydroascorbic acid 4
490-83-5	835	dehydroascorbic acid 5
490-83-5	835	dehydroascorbic acid 6
6906-38-3	443650	delphinidin 3-glucoside
6906-38-3	443650	delphinidin 3-glucoside 2
6906-38-3	443650	delphinidin 3-glucoside 3
154-17-6	439268	deoxyglucose 1
154-17-6	439268	deoxyglucose 2
0	5459862	D-erythrose-4-phosphate 1
0	5459862	D-erythrose-4-phosphate 2
3646-68-2	73563	D-glucosaminic acid 1
3646-68-2	73563	D-glucosaminic acid 2
3646-68-2	73563	D-glucosaminic acid 3
3646-68-2	73563	D-glucosaminic acid 4
59-23-4	24749	D-glucose 1
59-23-4	24749	D-glucose 2
56-73-5	439958	D-glucose-6-phosphate 1
56-73-5	439958	D-glucose-6-phosphate 2
0	16217112	D-glucose-C-d7 1
0	16217112	D-glucose-C-d7 2
439-14-5	3016	Diazepam
132-64-9	568	dibenzofuran
5965-53-7	97750	diethyl oxalpropionate 1
5965-53-7	97750	diethyl oxalpropionate 2
5965-53-7	97750	diethyl oxalpropionate 3
84-66-2	6781	diethyl phthalate
5894-59-7	3294434	digalacturonic acid 1
5894-59-7	3294434	digalacturonic acid 2

CAS #	PubChem	Compound
5894-59-7	3294434	digalacturonic acid 3
5894-59-7	3294434	digalacturonic acid 4
527-52-6	258531	digitoxose 1
527-52-6	258531	digitoxose 2
627-82-7	42953	diglycerol 1
627-82-7	42953	diglycerol 2
627-82-7	42953	diglycerol 3
13031-04-4	39	dihydro-4,4-dimethyl-2,3-furandione 1
13031-04-4	39	dihydro-4,4-dimethyl-2,3-furandione 2
19408-84-5	107982	dihydrocapsaicin
119-84-6	660	dihydrocoumarin 1
119-84-6	660	dihydrocoumarin 2
119-84-6	660	dihydrocoumarin 3
119-84-6	660	dihydrocoumarin 4
119-84-6	660	dihydrocoumarin 5
79-36-0	440560	dihydrolanosterol
462-20-4	421	dihydrolipoic acid
6202-10-4	439216	dihydroorotic acid 1
6202-10-4	439216	dihydroorotic acid 2
6202-10-4	439216	dihydroorotic acid 3
521-18-6	10635	dihydrotestosterone 1
521-18-6	10635	dihydrotestosterone 2
62147-49-3	668	dihydroxyacetone phosphate 1
62147-49-3	668	dihydroxyacetone phosphate 2
117-81-7	8343	dioctyl phthalate
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 1
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 2
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 3
28822-73-3	91528	DL-3,4-dihydroxyphenyl glycol
10569-71-9	64956	DL-3-aminoisobutyric acid 1
10569-71-9	64956	DL-3-aminoisobutyric acid 2
55-10-7	1245	DL-4-hydroxy-3-methoxymandelic acid
7198-10-9	328	DL-4-hydroxymandelic acid
13552-09-5	3126	DL-dihydrosphingosine 1
13552-09-5	3126	DL-dihydrosphingosine 2
13552-09-5	3126	DL-dihydrosphingosine 3
56-82-6	751	DL-glyceraldehyde 1
56-82-6	751	DL-glyceraldehyde 2
93965-35-6	729	DL-glyceraldehyde 3-phosphate 1
93965-35-6	729	DL-glyceraldehyde 3-phosphate 2

CAS #	PubChem	Compound
443-79-8	791	DL-isoleucine 1
443-79-8	791	DL-isoleucine 2
6482-98-0	9378	DL-p-hydroxyphenyllactic acid
0	443239	DL-threo- <i>beta</i> -hydroxyaspartic acid
1114-34-7	65550	D-lyxose 1
1114-34-7	439240	D-lyxose 2
1114-34-7	65550	D-lyxose 3
1114-34-7	439240	D-lyxose 4
617-48-1	92824	D-malic acid
87-78-5	6251	D-mannitol
87-78-5	18950	D-mannose 1
87-78-5	18950	D-mannose 2
51-61-6	681	dopamine (hydroxytyramine)
81-13-0	131204	D-panthenol 1
81-13-0	131204	D-panthenol 2
469-62-5	10100	d-Propoxyphene
15673-79-7	439167	D-ribose-5-phosphate 1
15673-79-7	439167	D-ribose-5-phosphate 2
87-73-0	5460673	D-saccharic acid
50-70-4	5780	D-sorbitol
123-78-4	5280335	D-sphingosine 2
123-78-4	5280335	D-sphingosine 3
123-78-4	5280335	D-sphingosine 1
6968-16-7	169019	D-threitol
479-18-5	3182	dyphylline
481-37-8	91460	Ecgonine
2091-39-6	5282805	eicosa-11,14-dienoic acid
112-95-8	8222	eicosane
10417-94-4	446284	eicosapentaenoic acid
112-79-8	637517	elaidic acid
476-66-4	5281855	ellagic acid
35323-91-2	72276	epicatechin 1
35323-91-2	72276	epicatechin 2
970-74-1	72277	epigallocatechin
989-51-5	1287	epigallocatechin gallate
105-60-2	7768	epsilon-caprolactam
57-87-4	444679	ergosterol
585-18-2	697	erythrose 4-phosphate 1
585-18-2	697	erythrose 4-phosphate 2
50-28-2	5757	estradiol

CAS #	PubChem	Compound
50-27-1	5756	estriol
53-16-7	5870	estrone 1
53-16-7	5870	estrone 2
141-43-5	700	ethanolamine
106-33-2	7800	ethyl dodecanoate
106-32-1	7799	ethyl octanoate
19317-11-4	5280598	farnesal 1
19317-11-4	5280598	farnesal 2
19317-11-4	5280598	farnesal 3
19317-11-4	5280598	farnesal 4
458-24-2	3337	Fenfluramine 1
458-24-2	3337	Fenfluramine 2
1135-24-6	445858	ferulic acid
487-26-3	10251	flavanone 1
487-26-3	10251	flavanone 2
525-82-6	10680	flavone
487-26-3	10251	flavonone 1
487-26-3	10251	flavonone 2
1622-62-4	3380	Flunitrazepam
86-73-7	6853	fluorene
17617-23-1	3393	Flurazepam
57-48-7	5984	fructose 1
57-48-7	5984	fructose 2
488-69-7	10267	fructose-1,6-diphosphate 1
488-69-7	10267	fructose-1,6-diphosphate 2
17013-01-3	444972	fumaric acid
3687-64-7	439451	galactinol 1
3687-64-7	439451	galactinol 2
608-66-2	11850	galactitol
13382-27-9	128869	galactonic acid 1
13382-27-9	128869	galactonic acid 2
1772-03-8	24154	galactosamine 1
1772-03-8	24154	galactosamine 2
1772-03-8	24154	galactosamine 3
1772-03-8	24154	galactosamine 4
1772-03-8	24154	galactosamine 5
14982-50-4	439215	galacturonic acid 1
14982-50-4	445929	galacturonic acid 1
14982-50-4	439215	galacturonic acid 2
14982-50-4	445929	galacturonic acid 2

CAS #	PubChem	Compound
149-91-7	370	gallic acid
3371-27-5	9882981	gallocatechin
56-12-2	119	gamma-aminobutyric acid (GABA)
490-79-9	3469	gentisic acid
459-80-3	5275520	geranic acid
106-24-1	637566	geraniol 1
106-24-1	637566	geraniol 2
10094-62-9	101713	glucoheptonic acid 1
10094-62-9	101713	glucoheptonic acid 2
10094-62-9	101713	glucoheptonic acid 3
526-95-4	604	gluconic acid 1
526-95-4	604	gluconic acid 2
90-80-2	736	gluconic acid lactone 1
90-80-2	736	gluconic acid lactone 2
90-80-2	736	gluconic acid lactone 3
6556-12-3	16213610	glucuronic acid 1
6556-12-3	16213610	glucuronic acid 2
6556-12-3	16213610	glucuronic acid 3
6556-12-3	16213610	glucuronic acid 4
32449-92-6	439782	glucuronolactone 1
32449-92-6	439782	glucuronolactone 2
32449-92-6	439782	glucuronolactone 3
628-48-8	5280498	glutaconic acid 1
628-48-8	5280498	glutaconic acid 2
110-94-1	743	glutaric acid
473-81-4	439194	glyceric acid
56-81-5	753	glycerol
34363-28-5	754	glycerol 1-phosphate
56-40-6	750	glycine
106-57-0	7817	glycine anhydride 1
106-57-0	7817	glycine anhydride 2
5680-79-5	69221	glycine methyl ester
4896-77-9	2723970	glycine-d5 deuterated
79-14-1	757	glycolic acid
658-79-7	92829	glycyl-L-tyrosine 1
658-79-7	92829	glycyl-L-tyrosine 2
704-15-4	79101	glycylproline
0	194988	glycyl-tyrosyl-alanine 1
0	194988	glycyl-tyrosyl-alanine 2

CAS #	PubChem	Compound
0	194988	glycyl-tyrosyl-alanine 3
0	194988	glycyl-tyrosyl-alanine 4
298-12-4	760	glyoxylic acid
704-15-4	79101	gly-pro
90-05-1	460	guaiacol
352-97-6	763	guanidinoacetic acid 1
352-97-6	763	guanidinoacetic acid 2
353-09-3	67701	guanidinopropionic acid 1
353-09-3	67701	guanidinopropionic acid 2
6133-30-8	97856	guanidinosuccinic acid 1
6133-30-8	97856	guanidinosuccinic acid 2
6133-30-8	97856	guanidinosuccinic acid 3
118-00-3	6802	guanosine 1
118-00-3	6802	guanosine 2
5550-12-9	6804	guanosine-5'-monophosphate
6589-55-5	913	halostachine 1
6589-55-5	913	halostachine 2
593-49-7	11636	heptacosane
506-12-7	10465	heptadecanoic acid
111-14-8	8094	heptanoic acid
41001-90-5	3593	hesperetin 1
41001-90-5	3593	hesperetin 2
41001-90-5	3593	hesperetin 3
118-74-1	8370	hexachlorobenzene
629-73-2	12395	hexadecene
142-62-1	8892	hexanoic acid
56-29-1	3608	Hexobarbital
495-69-2	464	hippuric acid 1
495-69-2	464	hippuric acid 2
451-13-8	780	homogentisic acid
306-08-1	1738	homovanillic acid (HVA)
501-52-0	107	hydrocinnamic acid
466-99-9	5284570	Hydromorphone 1
466-99-9	5284570	Hydromorphone 2
123-31-9	785	hydroquinone
127-07-1	3657	hydroxyurea
101-31-5	3661	hyoscyamine (atropine)
300-84-5	107812	hypotaurine
68-94-0	790	hypoxanthine

CAS #	PubChem	Compound
68-94-0	790	hypoxanthine 1
68-94-0	790	hypoxanthine 2
142-73-4	8897	iminodiacetic acid 1
142-73-4	8897	iminodiacetic acid 2
830-96-6	3744	indole 3-propionic acid 1
830-96-6	3744	indole 3-propionic acid 2
879-37-8	397	indole-3-acetamide 1
879-37-8	397	indole-3-acetamide 2
879-37-8	397	indole-3-acetamide 3
487-89-8	10256	indole-3-carbaldehyde 1
487-89-8	10256	indole-3-carbaldehyde 2
700-06-1	3712	indole-3-carbinol (3-indolemethanol)
700-06-1	3712	indole-3-carbinol 1
771-50-6	69867	indole-3-carboxylic acid 1
771-50-6	69867	indole-3-carboxylic acid 2
392-12-1	803	indole-3-pyruvic acid
830-96-6	3744	indolepropionic acid
58-63-9	6021	inosine
131-99-7	797	inosine 5'-monophosphate
1637-73-6	1198	isocitric acid
499-40-1	439193	isomaltose 1
499-40-1	439193	isomaltose 2
367-93-1	656894	isopropyl <i>beta</i> -D-1-thiogalactopyranoside
21637-25-2	5280804	isoquercitrin 1
21637-25-2	5280804	isoquercitrin 2
5041-82-7	5318644	isorhamnetin-3--glucoside
529-69-1	10729	isoxanthopterin
97-65-4	811	itaconic acid
481-39-0	3806	juglone
520-18-3	5280863	kaempferol 1
520-18-3	5280863	kaempferol 2
470-69-9	440080	kestose
3615-56-3	1101	L- sorbose 1
3615-56-3	1101	L- sorbose 2
2438-80-4	17106	L-(-)-fucose 1
2438-80-4	17106	L-(-)-fucose 2
79-33-4	107689	L-(+) lactic acid
2043-43-8	94220	lactamide 1
2043-43-8	94220	lactamide 2
96-82-2	91476	lactitol

CAS #	PubChem	Compound
96-82-2	16219560	lactobionic acid 1
96-82-2	16219560	lactobionic acid 2
96-82-2	16219560	lactobionic acid 3
63-42-3	84571	lactose 1
63-42-3	84571	lactose 2
4618-18-2	11333	lactulose 1
4618-18-2	11333	lactulose 2
4618-18-2	11333	lactulose 3
56-41-7	5950	L-alanine 1
56-41-7	5950	L-alanine 2
225101-69-9	12205373	L-alanine-2,3,3,3-d4
28954-12-3	99289	L-allothreonine 1
28954-12-3	99289	L-allothreonine 2
79-36-0	246983	lanosterol
53472-37-0	5282154	laricitrin
50-81-7	5785	L-ascorbic acid
		L-Ascorbic acid-13C6 1
		L-Ascorbic acid-13C6 2
		L-Ascorbic acid-13C6 3
		L-Ascorbic acid-13C6 4
		L-Ascorbic acid-13C6 5
70-47-3	236	L-asparagine 1
70-47-3	236	L-asparagine 2
70-47-3	16217724	L-asparagine-15N2,d8 1
70-47-3	16217724	L-asparagine-15N2,d8 2
70-47-3	16217724	L-asparagine-15N2,d8 3
143-07-7	3893	lauric acid
543-38-4	275	L-canavanine 1
543-38-4	275	L-canavanine 2
541-15-1	10918	L-carnitine 1
541-15-1	10918	L-carnitine 2
498-40-8	72886	L-cysteic acid
52-90-4	594	L-cysteine 1
52-90-4	594	L-cysteine 2
56-89-3	67678	L-cystine 1
56-89-3	67678	L-cystine 2
56-89-3	67678	L-cystine 3
16096-97-2	439196	L-dithiothreitol 1
16096-97-2	439196	L-dithiothreitol 2
57-92-7	6047	L-DOPA 1

CAS #	PubChem	Compound
57-92-7	6047	L-DOPA 2
7158-70-5	165577	leucrose
14769-73-4	26879	levamisole
1128-23-0	608	L-galactono-gamma-lactone 1
1128-23-0	608	L-galactono-gamma-lactone 2
56-86-0	33032	L-glutamic acid 1
56-86-0	33032	L-glutamic acid 2
56-86-0	33032	L-glutamic acid 3 (dehydrated)
0		L-glutamic acid-2,3,3,4,4-d5 1
0		L-glutamic acid-2,3,3,4,4-d5 2
0		L-glutamic acid-2,3,3,4,4-d5 3 (dehydrated)
56-85-9	738	L-glutamine 1
56-85-9	738	L-glutamine 2
56-85-9	738	L-glutamine 3
70-18-8	124886	L-glutathione reduced
1128-23-0	439373	L-gulonic acid gamma-lactone
5934-29-2	6274	L-histidine 1
5934-29-2	6274	L-histidine 2
5934-29-2	6274	L-histidine 3
626-72-2	439579	L-homocystine 1
626-72-2	439579	L-homocystine 2
626-72-2	439579	L-homocystine 3
672-15-1	12647	L-homoserine 1
672-15-1	12647	L-homoserine 2
672-15-1	12647	L-homoserine 3
101-31-5	154417	L-hyoscyamine
5989-27-5	440917	limonene
1180-71-8	16219587	limonin
60-33-3	5280450	linoleic acid
3206-73-3	863	lipoamide 1
3206-73-3	863	lipoamide 2
3206-73-3	863	lipoamide 3
578-86-9	1889	liquiritigenin 1
578-86-9	1889	liquiritigenin 2
578-86-9	1889	liquiritigenin 3
2922-83-0	161166	L-kynurenine 1
2922-83-0	161166	L-kynurenine 2
61-90-5	6106	L-leucine 1
61-90-5	6106	L-leucine 2
56-87-1	5962	L-lysine 1

CAS #	PubChem	Compound
56-87-1	5962	L-lysine 2
3128-06-1	26447	L-menthone
63-68-3	6137	L-methionine 1
63-68-3	6137	L-methionine 2
3226-65-1	158980	L-methionine sulfoxide 1
3226-65-1	158980	L-methionine sulfoxide 2
3226-65-1	158980	L-methionine sulfoxide 3
500-44-7	440473	L-mimosine 1
500-44-7	440473	L-mimosine 2
327-57-1	21236	L-norleucine 1
327-57-1	21236	L-norleucine 2
18524-94-2	16212335	loganin
846-49-1	3958	Lorazepam
70-26-8	6262	L-ornithine 1
70-26-8	6262	L-ornithine 2
63585-09-1	13000987	L-phenylalanine-phenyl-d5-2,3,3-d3 1
63585-09-1	13000987	L-phenylalanine-phenyl-d5-2,3,3-d3 2
147-85-3	614	L-proline 1
147-85-3	145742	L-proline 1
147-85-3	614	L-proline 2
147-85-3	145742	L-proline 2
98-79-3	7405	L-pyroglutamic acid
56-45-1	5951	L-serine 1
56-45-1	5951	L-serine 2
3081-61-6	228398	L-theanine 1
3081-61-6	228398	L-theanine 2
72-19-5	6288	L-threonine 1
72-19-5	6288	L-threonine 2
73-22-3	6305	L-tryptophan 1
73-22-3	6305	L-tryptophan 2
60-18-4	6057	L-tyrosine 1
60-18-4	6057	L-tyrosine 2
0	16213445	L-tyrosine-3,3-d2 1
0	16213445	L-tyrosine-3,3-d2 2
487-21-8	10250	lumazine
72-18-4	6287	L-valine 1
72-18-4	6287	L-valine 2
557-24-4	5280451	maleamic acid 1
557-24-4	5280451	maleamic acid 2
557-24-4	5280451	maleamic acid 3

CAS #	PubChem	Compound
110-16-7	444266	maleic acid
108-13-4	7911	malonamide 1
108-13-4	7911	malonamide 2
108-13-4	7911	malonamide 3
141-82-2	867	malonic acid 1
141-82-2	867	malonic acid 2
585-88-6	16217663	maltitol
69-79-4	6255	maltose 2
69-79-4	6255	maltose 1
32860-62-1	3625615	maltotriitol
1109-28-0	192826	maltotriose 1
1109-28-0	192826	maltotriose 2
7228-78-6	443652	malvidin-3-glucoside
17199-29-0	439616	mandelic acid
532-28-5	10758	mandelonitrile 1
532-28-5	10758	mandelonitrile 2
108-39-4	342	m-cresol
306-08-1	896	melatonin 1
306-08-1	896	melatonin 2
306-08-1	896	melatonin 3
306-08-1	896	melatonin 4
10030-67-8	92817	melezitose
66009-10-7	440658	melibiose 1
66009-10-7	440658	melibiose 2
115-38-8	8271	Mephobarbital
537-46-2	10836	Methamphetamine 1
537-46-2	10836	Methamphetamine 2
76-99-3	4095	Methaqualone
18652-93-2	9034	Methohexital
608-07-1	1833	methoxytryptamine
3943-74-6	19844	methyl 4-hydroxy-3-methoxybenzoate
110-42-9		Methyl Caprate
111-11-5		Methyl Caprylate
103-26-4	637520	methyl cinnamate
929-77-1		Methyl Docosanoate
1120-28-1		Methyl Eicosanoate
99-24-1	7428	methyl gallate 1
99-24-1	7428	methyl gallate 2
1731-92-6	15609	methyl heptadecanoate
5802-82-4		Methyl Hexacosanoate

CAS #	PubChem	Compound
111-82-0		Methyl Laurate
2442-49-1		Methyl Linocerate
301-00-8	9316	methyl linolenate
124-10-7		Methyl Myristate
55682-92-3		Methyl Octacosanoate
112-62-9	5364509	methyl oleate
112-39-0		Methyl Palmitate
1120-25-8	643801	methyl palmitoleate
60-11-7	6053	methyl yellow
1824-94-8	94214	methyl- <i>beta</i> -D-galactopyranoside
1211-29-6	62388	methyljasmonate 1
1211-29-6	62388	methyljasmonate 2
1211-29-6	62388	methyljasmonate 3
1211-29-6	62388	methyljasmonate 4
1211-29-6	62388	methyljasmonate 5
1211-29-6	62388	methyljasmonate 6
516-05-2	487	methylmalonic acid
595-98-2	136386	methyltartronic acid
125-64-4	4162	Methyprylon
4376-20-9	20393	mono(2-ethylhexyl)phthalate
57-27-2	5288826	Morphine
99-04-7	7418	m-toluic acid
526-99-8	3037582	mucic acid
87-89-8	892	myo-inositol
529-44-2	5281672	myricetin
544-63-8	11005	myristic acid
60658-41-5		Myristic acid d27
2018-66-8	74840	N- carbobenzoxy-L-leucine 1
2018-66-8	74840	N- carbobenzoxy-L-leucine 2
2018-66-8	74840	N- carbobenzoxy-L-leucine 3
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 1
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 2
2875-41-4	10034670	N-(3-Aminopropyl)glycine 1
2875-41-4	10034670	N-(3-Aminopropyl)glycine 2
99-98-9	7472	N,N-dimethyl-1,4-phenylenediamine 1
99-98-9	7472	N,N-dimethyl-1,4-phenylenediamine 2
65005-57-4	123831	N,N-dimethylarginine
1118-68-9	673	N,N-dimethylglycine
24940-57-6	440274	N,N-dimethyl-L-histidine
53-96-3	5897	N-2-fluorenylacетamide 1

CAS #	PubChem	Compound
53-96-3	5897	N-2-fluorenylacetamide 2
1210-83-9	903	N-acetyl-5-hydroxytryptamine 1
1210-83-9	903	N-acetyl-5-hydroxytryptamine 2
1210-83-9	903	N-acetyl-5-hydroxytryptamine 3
7512-17-6	16218892	N-acetyl-D-glucosamine 1
7512-17-6	16218892	N-acetyl-D-glucosamine 2
7772-94-3	899	N-acetyl-D-mannosamine 1
7772-94-3	899	N-acetyl-D-mannosamine 2
2280-01-5	439917	N-acetyl-D-tryptophan 1
2280-01-5	439917	N-acetyl-D-tryptophan 2
1/5/2280	439917	N-acetyl-D-tryptophan 3
997-55-7	65065	N-acetyl-L-aspartic acid 1
997-55-7	65065	N-acetyl-L-aspartic acid 2
616-91-1	12035	N-acetyl-L-cysteine 1
616-91-1	12035	N-acetyl-L-cysteine 2
1188-37-0	70914	N-acetyl-L-glutamic acid 1
1188-37-0	70914	N-acetyl-L-glutamic acid 2
1188-37-0	70914	N-acetyl-L-glutamic acid 3
2497-02-1	273260	N-acetyl-L-histidine 1
2497-02-1	273260	N-acetyl-L-histidine 2
1188-21-2	1995	N-acetyl-L-leucine
2018-61-3	74839	N-acetyl-L-phenylalanine 1
0	439232	N-acetyl-ornithine 1
0	439232	N-acetyl-ornithine 2
1946-82-3	92907	N- <i>alpha</i> -acetyl-L-lysine 1
1946-82-3	92907	N- <i>alpha</i> -acetyl-L-lysine 2
91-20-3	931	naphthalene
10236-47-2	25075	naringin
1138-80-3	14349	N-benzyloxycarbonylglycine
1188-38-1	3679006	N-carbamyl-L-glutamic acid 1
1188-38-1	3679006	N-carbamyl-L-glutamic acid 2
1188-38-1	3679006	N-carbamyl-L-glutamic acid 3
1188-38-1	3679006	N-carbamyl-L-glutamic acid 4
1188-38-1	3679006	N-carbamyl-L-glutamic acid 5
766-93-8	13017	N-cyclohexylformamide
13241-33-3	442439	neohesperidin
141-12-8	1549026	neryl acetate 1
141-12-8	1549026	neryl acetate 2
627-01-0	316542	N-ethylglycine 1
627-01-0	316542	N-ethylglycine 2

CAS #	PubChem	Compound
4289-98-9	911	N-formyl-L-methionine 1
4289-98-9	911	N-formyl-L-methionine 2
52450-38-1	171161	N-gamma-acetyl-N-2-formyl-5-methoxykynurenamine 1
52450-38-1	171161	N-gamma-acetyl-N-2-formyl-5-methoxykynurenamine 2
52450-38-1	171161	N-gamma-acetyl-N-2-formyl-5-methoxykynurenamine 3
98-92-0	936	nicotinamide 1
98-92-0	936	nicotinamide 2
59-67-6	938	nicotinic acid
583-08-4	68499	nicotinoylglycine
146-22-5	4506	Nitrazepam
100-61-8	5288725	N-methylalanine
119-68-6	67069	N-methylanthranilic acid 1
119-68-6	67069	N-methylanthranilic acid 2
6753-62-4	268779	N-methyl-DL-glutamic acid 1
6753-62-4	268779	N-methyl-DL-glutamic acid 2
6753-62-4	268779	N-methyl-DL-glutamic acid 3
6753-62-4	268779	N-methylglutamic acid 1
6753-62-4	268779	N-methylglutamic acid 2
6753-62-4	268779	N-methylglutamic acid 3
6753-62-4	268779	N-methylglutamic acid 4
673-49-4	69602	N-omega-acetylhistamine 1
673-49-4	69602	N-omega-acetylhistamine 2
630-03-5	12409	nonacosane
51-41-2	5814	norepinephrine (noradrenalin)
5746-86-1	412	nornicotine
6600-40-4	65098	norvaline 1
6600-40-4	65098	norvaline 2
50-78-2	2244	O-acetylsalicylic acid
16652-64-5	725701	O-benzyl-L-tyrosine 1
16652-64-5	725701	O-benzyl-L-tyrosine 2
34522-32-2	108172	octopine 1
34522-32-2	108172	octopine 2
112-80-1	445639	oleic acid
1071-23-4	1015	O-phosphocolamine
407-41-0	68841	O-phospho-L-serine 1
407-41-0	68841	O-phospho-L-serine 2
407-41-0	68841	O-phospho-L-serine 3
407-41-0	68841	O-phospho-L-serine 4
1114-81-4	3246323	O-phospho-L-threonine 1
1114-81-4	3246323	O-phospho-L-threonine 2

CAS #	PubChem	Compound
504-15-4	10436	orcinol
50887-69-9	967	orotic acid 1
50887-69-9	967	orotic acid 2
1492-23-5	954	O-succinylhomoserine 1
1492-23-5	954	O-succinylhomoserine 2
328-42-7	970	oxalacetic acid
144-62-7	971	oxalic acid
604-75-1	4616	Oxazepam 1
604-75-1	4616	Oxazepam 2
76-41-5	5284604	Oxymorphone 1
76-41-5	5284604	Oxymorphone 2
79-57-2	5280972	oxytetracycline
585-88-6	3034828	palatinitol 1
64519-82-0	3034828	palatinitol 2
13718-94-2	439559	palatinose
64519-82-0	985	palmitic acid
373-49-9	445638	palmitoleic acid
100-09-4	7478	p-anisic acid
599-04-2	989	pantolactone
137-08-6	6613	pantothenic acid 1
137-08-6	6613	pantothenic acid 2
311-45-5	9395	paraoxon
106-51-4	4650	p-benzoquinone
95-48-7	2879	p-cresol
99-87-6	7463	p-cymene
112-05-0	8158	pelargonic acid (nonanoic acid)
359-83-1	441278	Pentazocine
76-74-4	4737	Pentobarbital
6906-39-4	443654	peonidin-3-glucoside 1
6906-39-4	443654	peonidin-3-glucoside 2
6988-81-4	443651	petunidin-3-glucoside 1
6988-81-4	443651	petunidin-3-glucoside 2
500-98-1	68144	phenaceturic acid 1
500-98-1	68144	phenaceturic acid 2
85-01-8	995	phenanthrene
77-10-1	6468	Phencyclidine
21784-30-5	12460	Phendimetrazine 1
21784-30-5	12460	Phendimetrazine 2
64-04-0	1001	Phenethylamine
134-49-6	4762	Phenmetrazine

CAS #	PubChem	Compound
50-06-6	4763	Phenobarbital
122-09-8	4771	Phentermine 1
122-09-8	4771	Phentermine 2
122-78-1	998	phenylacetaldehyde 1
122-78-1	998	phenylacetaldehyde 2
63-91-2	994	Phenylalanine 1
63-91-2	994	Phenylalanine 2
1464-44-4	65080	phenyl- <i>beta</i> -glucopyranoside
60-12-8	6054	phenylethyl alcohol
64-04-0	1001	phenylethylamine
701-64-4	12793	phenylphosphoric acid
154-41-6	441457	Phenylpropanolamine
156-06-9	997	phenylpyruvate
60-82-2	4788	phloretin
3555-86-0	77093	phlorobenzophenone 1
3555-86-0	77093	phlorobenzophenone 2
108-73-6	359	phloroglucinol
138-08-9	1005	phosphoenolpyruvic acid
95648-83-2	529	phosphoglycolic acid
26016-99-9	3417	phosphonomycin
7664-38-2	1004	phosphoric acid
88-99-3	1017	phthalic acid
14721-66-5	26840	phytanic acid
7541-49-3	5366244	phytol 1
7541-49-3	6430833	phytol 1
7541-49-3	5366244	phytol 2
7541-49-3	6430833	phytol 2
554-62-1	122121	phytosphingosine 1
554-62-1	122121	phytosphingosine 2
10083-24-6	667639	piceatannol
98-98-6	1018	picolonic acid
111-16-0	385	pimelic acid
535-75-1	439227	pipecolic acid 1
535-75-1	439227	pipecolic acid 2
94-62-2	638024	piperine 1
94-62-2	638024	piperine 2
681295-24-9	66868	porphine 1
681295-24-9	66868	porphine 2
487-90-1	1021	porphobilinogen
2955-38-6	4890	Prazepam

CAS #	PubChem	Compound
2078-54-8	4943	propofol
	9925625	propofol hemisuccinate
552-59-0	5281804	prunetin
551-68-8	90008	psicose 1
551-68-8	90008	psicose 2
6192-52-5	6101	p-toluenesulfonic acid
550-33-4	68368	purine riboside
110-60-1	1045	putrescine
499-83-2	10367	pyridine-2,6-dicarboxylic acid
41468-25-1	1051	pyridoxal 5'-phosphate 1
41468-25-1	1051	pyridoxal 5'-phosphate 2
41468-25-1	1051	pyridoxal 5'-phosphate 3
65-23-6	1054	pyridoxine
87-66-1	1057	pyrogallol
9/3/2466	1023	pyrophosphate
634-97-9	12473	pyrrole -2-carboxylic acid
127-17-3	1060	pyruvic acid
93-10-7	7124	quinaldinic acid
77-95-2	6508	quinic acid
89-00-9	1066	quinolinic acid
17629-30-0	439242	Raffinose
108-46-3	5054	resorcinol
501-36-0	445154	resveratrol
302-79-4	444795	retinoic acid
3615-41-6	220001	rhamnose 1
3615-41-6	220001	rhamnose 2
488-81-3	827	ribitol
5336-08-3	111064	ribonic acid-gamma-lactone 1
5336-08-3	111064	ribonic acid-gamma-lactone 2
24259-59-4	993	ribose
108321-99-9	439184	ribulose-5-phosphate 3
113573-73-2	440053	S(-)willardiine 1
113573-73-2	440053	S(-)willardiine 2
82385-42-0	5143	saccharin 1
82385-42-0	5143	saccharin 2
91-22-5	6998	salicylaldehyde
69-72-7	338	salicylic acid
487-54-7	10253	salicylurate 1
487-54-7	10253	salicylurate 2
107-97-1	1088	sarcosine

CAS #	PubChem	Compound
186537-58-6	193653	S-carboxymethylcysteine 2
186537-58-6	193653	S-carboxymethylcysteine 1
92-61-5	5280460	scopoletin
76-73-3	5193	Secobarbital
469-90-9	16219957	sedoheptulose anhydride monohydrate
50-67-9	5202	serotonin 1
50-67-9	5202	serotonin 2
138-59-0	8742	shikimic acid
537-33-7	5280507	sinapyl alcohol 1
537-33-7	5280507	sinapyl alcohol 2
534-46-3	4623424	sophorose 1
534-46-3	4623424	sophorose 2
124-20-9	1102	spermidine 1
124-20-9	1102	spermidine 2
71-44-3	1103	spermine 1
71-44-3	1103	spermine 2
111-02-4	5280370	squalene
57-11-4	5281	stearic acid
110-15-6	5321515	stigmasterol
505-48-6	10457	suberic acid
29915-38-6	1110	succinic acid
111-11-5	5988	Sucrose
585-18-2	439762	sucrose-6-phosphate 1
585-18-2	439762	sucrose-6-phosphate 2
94-07-5	7172	synephrine 1
94-07-5	7172	synephrine 2
4423-37-4	5281953	syringetin
530-57-4	10742	syringic acid
87-81-0	2724552	tagatose 1
87-81-0	2724552	tagatose 2
115-44-6	8275	Talbutal
2595-98-4	441035	talose 1
2595-98-4	441035	talose 2
1401-55-4	16133892	tannic acid
133-37-9	444305	tartaric acid
80-69-3	45	tartronic acid
107-35-7	1123	taurine
480-18-2	439533	taxifolin
846-50-4	5391	Temazepam
10482-56-1	17100	terpineol

CAS #	PubChem	Compound
7365-44-8	446188	TES
53-43-0	6013	testosterone 1
53-43-0	6013	testosterone 2
646-31-1	12592	tetracosane
68-42-8	65553	tetrahydrocorticosterone 1
68-42-8	65553	tetrahydrocorticosterone 2
68-42-8	65553	tetrahydrocorticosterone 3
68-42-8	65553	tetrahydrocorticosterone 4
14167-59-0	26519	tetratriacontane
115-37-7	5324289	Thebaine
68-11-1	1133	thioglycolic acid
7298-99-9	443239	threo-3-hydroxy-L-aspartate
7306-96-9	5460407	threonic acid
95-43-2	439665	threose 1
95-43-2	439665	threose 2
50-89-5	5789	thymidine 1
50-89-5	5789	thymidine 2
365-07-1	1139	thymidine 5'-phosphate 1
365-07-1	1139	thymidine 5'-phosphate 2
65-71-4	1135	thymine
89-83-8	6989	thymol
67879-58-7	642609	trans caftaric acid 1
67879-58-7	642609	trans caftaric acid 2
		trans coutaric acid
	641605	trans fertaric acid
27208-80-6	12314237	trans piceid
501-36-0	445154	trans- resveratrol
3588-17-8	5356793	trans,trans-muconic acid
693-71-0	6161490	trans-13-octadecenoic acid
4206-58-0	5280802	trans-3,5-dimethoxy-4-hydroxycinnamaldehyde
4436-74-2	5351896	trans-3-hexenedioic acid
8/2/4298	440575	trans-3-hydroxy-L-proline 1
8/2/4298	440575	trans-3-hydroxy-L-proline 2
8/2/4298	440575	trans-3-hydroxy-L-proline 3
8/2/4298	440575	trans-3-hydroxy-L-proline 4
51-35-4	5810	trans-4-hydroxy-L-proline 1
51-35-4	5810	trans-4-hydroxy-L-proline 2
585-84-2	444212	trans-aconic acid
1460-57-7	92886	trans-cyclohexane-1,2-diol
53-43-0	5881	trans-dehydroandrosterone 1

CAS #	PubChem	Compound
53-43-0	5881	trans-dehydroandrosterone 2
106-28-5	445070	trans-trans-farnesol
6025-53-2	6440982	trans-Zeatin-riboside
4484-88-2	122336	trehalose-6-phosphate
28911-01-5	5556	Triazolam
5704-04-1	79784	tricine 1
5704-04-1	79784	tricine 2
102-71-6	7618	triethanolamine
77-93-0	6506	triethyl citrate
535-83-1	5570	trigonelline
19253-88-4	159660	trimethyllysine
529-64-6	10726	tropic acid
547-25-1	5460935	turanose 1
547-25-1	5460935	turanose 2
51-67-2	5610	tyramine
60-18-4	6057	tyrosine 1
60-18-4	6057	tyrosine 2
1080-06-4	70652	tyrosine methyl ester 1
1080-06-4	70652	tyrosine methyl ester 2
66-22-8	1174	uracil
57-13-6	1176	urea
66-22-8	1175	uric acid 1
66-22-8	1175	uric acid 2
58-96-8	6029	uridine
3387-36-8	6030	uridine 5'-monophosphate 1
3387-36-8	6030	uridine 5'-monophosphate 2
104-98-3	1178	urocanic acid 1
104-98-3	1178	urocanic acid 2
626-97-1	12298	valeramide 1
626-97-1	12298	valeramide 2
626-97-1	12298	valeramide 3
626-97-1	12298	valeramide 4
121-33-5	1183	vanillin
3681-93-4	5280441	vitexin 1
3681-93-4	5280441	vitexin 2
69-89-6	1188	xanthine
146-80-5	1189	xanthosine
298-81-7	4114	xanthotoxin 1
298-81-7	4114	xanthotoxin 2
59-00-7	5699	xanthurenic acid

CAS #	PubChem	Compound
87-99-0	6912	xylitol
58-86-6	6027	xylose 1
58-86-6	6027	xylose 2
551-84-8	439204	xylulose
13114-27-7	449093	zeatin 1
13114-27-7	449093	zeatin 2

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