



G1676AA Agilent Fiehn GC/MS メタボロミクス RTL ライブラリ： 化合物リスト

データシート

多くの代謝物が同定できる 800 種類 1400 エントリーの代謝物ライブラリ

Agilent Fiehn GC/MS メタボロミクス RTL ライブラリは、最も包括的な市販の代謝物 GC/MS スペクトルライブラリです。このライブラリには、推奨メソッドで測定した代謝物の部分誘導体化スペクトルを含む、一般的な約 800 種類の代謝物の 1400 種類を超えるエントリーが収録されています。

このリストの各エントリーには、誘導体化前の化合物名、CAS 番号、PubChem 番号が含まれているため、化合物の同定、関連文献検索、ソフトウェア検索、パスイ解析が容易になります。



Agilent Technologies

CAS #	PubChem	化合物名
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
31519-22-9	671	1,4-dihydroxy-2-naphthoic acid

CAS #	PubChem	化合物名
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
501-94-0	10393	2-(4-hydroxyphenyl)ethanol
6698-26-6	65166	2', 5'-Dideoxyadenosine

CAS #	PubChem	化合物名
	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
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

CAS #	PubChem	化合物名
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
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

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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
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

CAS #	PubChem	化合物名
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-Epoxyaryophyllan-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
	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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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)

CAS #	PubChem	化合物名
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-Methylaphnetin
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
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

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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-methoxypsoralen
7084-29-9	13845047	5-methyl-3'-deoxyuridine 1
7084-29-9	13845047	5-methyl-3'-deoxyuridine 2
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

CAS #	PubChem	化合物名
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-Oxcholesterol
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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-Docosenol
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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-fluorenylacetamide 1
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
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

CAS #	PubChem	化合物名
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
50-06-6	4763	Phenobarbital
122-09-8	4771	Pentermine 1
122-09-8	4771	Pentermine 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

CAS #	PubChem	化合物名
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
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

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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
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

CAS #	PubChem	化合物名
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
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

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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-aconitic acid
1460-57-7	92886	trans-cyclohexane-1,2-diol
53-43-0	5881	trans-dehydroandrosterone 1
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

CAS #	PubChem	化合物名
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
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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