

G1676AA Agilent Fiehn 2013 GC/MS Metabolomics RTL Library

CAS #	PubChem	Compound
20549-47-7	443163	(-)-dihydrocarveol 1
20549-47-7	443163	(-)-dihydrocarveol 2
35323-91-2	72276	(-)-epicatechin
35323-91-2	72276	(-)-epicatechin
51028-73-0	5816	(-)-epinephrine 1
51028-73-0	5816	(-)-epinephrine 2
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)-cis-1,2-dihydro-1,2-naphthalenediol
	1597617	(4-Hydroxy-2-oxo-1,2-dihydro-quinolin-3-yl)-acetic acid k
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 1
504-02-9	10434	1,3 cyclohexanedione 2
504-02-9	10434	1,3 cyclohexanedione 3
0-00-0	440168	1,3,5(10)-estratrien-3,6- beta-17-beta-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
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

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CAS #	PubChem	Compound
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 Aci
	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 F2alpha
35850-13-6	5280887	15-keto-prostaglandin F-2-alpha
	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'-diphosphat
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
	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

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CAS #	PubChem	Compound
	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
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

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CAS #	PubChem	Compound
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 2
653-63-4	621	2'-deoxyadenosine 5'-monophosphate
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
149-57-5	8697	2-ethylhexanoic acid
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
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
600-18-0	58	2-ketobutyric acid
13022-85-0	159664	2-ketocaproic acid
4502-00-5	70	2-ketoisocaproic acid 1
4502-00-5	70	2-ketoisocaproic acid 2

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CAS #	PubChem	Compound
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-
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
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
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'-Ethoxyscleroin
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 2
146255-66-5	443586	3,5-dihydroxyphenylglycine 1
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-tert-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

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CAS #	PubChem	Compound
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	3beta-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
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-methoxyindole 1
1504-06-9	150923	3-methoxyindole 2
1504-06-9	150923	3-methoxyindole 3
1504-06-9	150923	3-methoxyindole 4
621-44-3	65124	3-nitro-L-tyrosine 1
621-44-3	65124	3-nitro-L-tyrosine 2

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CAS #	PubChem	Compound
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 ac
3025-96-5	18189	4-acetamidobutyric acid 1
3025-96-5	18189	4-acetamidobutyric acid 2
3233-32-7	96009	4-Acetoxyphenol
3233-32-7	96009	4-Acetoxyphenol 1
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-beta-ol-3,17-dione 1
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 2
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 3
382-44-5	94141	4-androsten-11-beta-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-alpha-ol-3,17-dione 1
62-84-0	65542	4-androsten-7-alpha-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 2
123-08-0	126	4-hydroxybenzaldehyde 1
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

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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)
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
959-23-9	641818	4'-Methoxychalcone 1
959-23-9	641818	4'-Methoxychalcone 2
137-00-8	1136	4-methyl-5-thiazoleethanol
452-86-8	9958	4-methylcatechol
2107-77-9	5355836	4-Methyl-daphnetin
90-33-5	5280567	4-methylumbelliferone
90-33-5	5280567	4-methylumbelliferone
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

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CAS #	PubChem	Compound
504-07-4	649	5,6-dihydrouracil 1
504-07-4	649	5,6-dihydrouracil 2
846-46-8	439289	5alpha-Androstan-3, 17-Dione 1
846-46-8	439289	5alpha-Androstan-3, 17-Dione 2
42366-37-0	242332	5-alpha-androstane-3 beta,17 beta-diol
0	242332	5alpha-androstane-3beta,17beta-diol
80-97-7	3240	5alpha-Cholestan-3-beta-ol
1175-06-0	16219541	5alpha-Cholestan-3beta-OI-6-One 1
1175-06-0	16219541	5alpha-Cholestan-3beta-OI-6-One 2
566-88-1	92128	5alpha-cholestan-3-one 1
566-88-1	92128	5alpha-cholestan-3-one 2
80-97-7	6665	5alpha-Cholestanol
566-65-4	92810	5-alpha-pregnan-3,20-dione 1
566-65-4	92810	5-alpha-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	5beta-androstane-3,17-dione
547-96-6	160520	5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol 1
547-96-6	160520	5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol 2
566-26-7	107722	5-cholesten-3-beta-7-alpha-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 caproic acid
1191-25-9	14490	6-hydroxyhexanoic acid
5006-66-6	72924	6-hydroxynicotinic acid

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CAS #	PubChem	Compound
5006-66-6	72924	6-hydroxynicotinic acid
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
480-44-4	5280442	Acacetin 1
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	acetoacetic acid
116-09-6	8299	acetol 2
116-09-6	8299	acetol 1
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
58-61-7	60961	adenosine
130-49-4	94136	adenosine 2'-monophosphate

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CAS #	PubChem	Compound
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	alpha ketoglutaric acid
10191-41-0	2116	alpha tocophereol
2152-75-2	740	alpha-D-glucosamine 1-phosphate
2152-75-2	740	alpha-D-glucosamine phosphate
2152-75-2	740	alpha-glucosamine 1-phosphate
481-06-1	221071	alpha-santonin 1
481-06-1	221071	alpha-santonin 2
57-43-2	2164	Amobarbital
57-43-2	2164	Amobarbital 1
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
	4303260	Anhydrobrazilic Acid 1
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

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CAS #	PubChem	Compound
481-05-0	65030	Artemisin
481-05-0	65030	Artemisin 1
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	azelaic 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
3012-37-1	18170	benzyl thiocyanate
100-46-9	7504	benzylamine
884-33-3	3858	benzylsuccinic acid
107-95-9	239	Beta- alanine 1
107-95-9	239	Beta- alanine 2
45159-34-0	439742	beta-cyano-L-alanine
5996-00-9	441422	beta-gentiobiose 1
5996-00-9	441422	beta-gentiobiose 2
56-86-0	73064	beta-glutamic acid
819-83-0	2526	beta-glycerolphosphate

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CAS #	PubChem	Compound
625-08-1	69362	beta-hydroxyisovalerate
14901-07-6	638014	beta-ionone 1
14901-07-6	638014	beta-ionone 2
123-35-3	31253	beta-myrcene
83-46-5	5321342	beta-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
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

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CAS #	PubChem	Compound
140-10-3	444539	cinnamic acid
1792-81-0	92903	cis-1,2-cyclohexanediol
51268-88-3	440294	cis-1,2-dihydro-1,2-naphthalenediol
629-98-1	5354168	cis-13-Docosanol
3685-22-1	151138	cis-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
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

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CAS #	PubChem	Compound
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-Ala2
923-16-0	601	D-Ala-D-Ala3
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 1
3646-68-2	73563	D-glucosaminic acid 2
3646-68-2	73563	D-glucosaminic acid 2
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

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CAS #	PubChem	Compound
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
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

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CAS #	PubChem	Compound
0	443239	DL-threo-beta-hydroxyaspartic acid
1114-34-7	65550	D-lyxose 1
1114-34-7	439240	D-lyxose 1
1114-34-7	65550	D-lyxose 2
1114-34-7	439240	D-lyxose 2
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
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

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CAS #	PubChem	Compound
19317-11-4	5280598	farnesal 3
19317-11-4	5280598	farnesal 4
458-24-2	3337	Fenfluramine
458-24-2	3337	Fenfluramine 1
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
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
106-24-1	637566	geraniol
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

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CAS #	PubChem	Compound
90-80-2	736	gluconic acid lactone 2
90-80-2	736	gluconic acid lactone 3
6556-12-3	16213610	glucuronic acid 2
6556-12-3	16213610	glucuronic acid 1
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
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

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CAS #	PubChem	Compound
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
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
771-50-6	69867	indole-3-carboxylic acid
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 beta-D-1-thiogalactopyranoside
21637-25-2	5280804	isoquercitrin 1
21637-25-2	5280804	isoquercitrin 2

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CAS #	PubChem	Compound
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
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

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CAS #	PubChem	Compound
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
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

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CAS #	PubChem	Compound
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
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

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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
532-28-5	10758	mandelonitrile
108-39-4	342	m-cresol
306-08-1	896	melatonin 1
306-08-1	896	melatonin 3
306-08-1	896	melatonin2
306-08-1	896	melatonin4
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
99-24-1	7428	methyl gallate
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

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CAS #	PubChem	Compound
112-62-9	5364509	methyl oleate
112-39-0		Methyl Palmitate
1120-25-8	643801	methyl palmitoleate
1731-84-6		Methyl Pelargonate
112-61-8		Methyl Stearate
629-83-4		Methyl Triacontanoate
60-11-7	6053	methyl yellow
1824-94-8	94214	methyl-beta-D-galactopyranoside
1211-29-6	62388	methyljasmonate 1
1211-29-6	62388	methyljasmonate 1
1211-29-6	62388	methyljasmonate 2
1211-29-6	62388	methyljasmonate 2
1211-29-6	62388	methyljasmonate 3
1211-29-6	62388	methyljasmonate 4
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-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

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CAS #	PubChem	Compound
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
2018-61-3	74839	N-acetyl-L-phenylalanine 2
131-48-6	445063	n-acetylneuraminic acid 1
131-48-6	445063	n-acetylneuraminic acid 2
0	439232	N-acetyl-ornithine 1
0	439232	N-acetyl-ornithine 2
1946-82-3	92907	N-alpha-acetyl-L-lysine 1
1946-82-3	92907	N-alpha-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
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

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CAS #	PubChem	Compound
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 1
407-41-0	68841	O-phospho-L-serine 2
407-41-0	68841	O-phospho-L-serine 2
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
50887-69-9	967	orotic acid
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
604-75-1	4616	Oxazepam 1
76-41-5	5284604	Oxymorphone
76-41-5	5284604	Oxymorphone 1
79-57-2	5280972	oxytetracycline
585-88-6	3034828	palatinitol 1
64519-82-0	3034828	palatinitol 2

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CAS #	PubChem	Compound
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
6906-39-4	443654	peonidin-3-glucoside 2
6988-81-4	443651	petunidin-3-glucoside
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
21784-30-5	12460	Phendimetrazine 1
64-04-0	1001	phenethylamine
134-49-6	4762	Phenmetrazine
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 1
1464-44-4	65080	phenyl-beta-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

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CAS #	PubChem	Compound
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
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

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CAS #	PubChem	Compound
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
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

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CAS #	PubChem	Compound
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
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
50-89-5	5789	thymidine
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 1

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CAS #	PubChem	Compound
8/2/4298	440575	trans-3-hydroxy-L-proline 2
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
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

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CAS #	PubChem	Compound
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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CAS #	PubChem	Compound
611-14-3	11903	2-ethyltoluene
123-35-3	31253	beta-myrcene
928-94-9	5318042	2-hexen 1-ol
1118-68-9	673	N,N-dimethylglycine
51-79-6	5641	carbamic acid ethyl ester (urethane)
105-60-2	7768	epsilon-caprolactam
513-85-9	262	2,3-butanediol 1
627-01-0	316542	N-ethylglycine 1
151-18-8	1647	3-aminopropionitrile 1
142-08-5	8871	2-hydroxypyridine
99-87-6	7463	p-cymene
513-85-9	262	2,3-butanediol 2
5989-27-5	440917	limonene
127-17-3	1060	pyruvic acid
504-63-2	10442	1,3-propanediol
79-33-4	107689	L-(+) lactic acid
108-91-8	7965	cyclohexanamine
104-51-8	7705	butylbenzene
626-97-1	12298	valeramide 1
79-14-1	757	glycolic acid
142-62-1	8892	hexanoic acid
626-97-1	12298	valeramide 2
3391-86-4	2724898	1-octen-3-ol
72-18-4	6287	L-valine 1
110-93-0	9862	6-methyl-5-hepten-2-one
600-18-0	58	2-ketobutyric acid
225101-69-9	12205373	L-alanine-2,3,3,3-d4
56-41-7	5950	L-alanine 1
600-18-0	58	2-ketobutyric acid
589-98-0	11527	3-octanol
104-76-7	7720	2-ethyl-1-hexanol
3715-29-5	49	3-methyl-2-oxobutanoic acid 1
6600-40-4	65098	norvaline 1
1569-60-4	20745	6-methyl-5-hepten-2-ol
141-97-9	96	acetoacetate 1
100-52-7	240	benzaldehyde
546-88-3	1990	acetohydroxamic acid
13419-69-7	5282707	2-hexenoic acid
95-93-2	7269	1,2,4,5-tetramethylbenzene
111-11-5		Methyl Caprylate
565-70-8	11266	2-hydroxybutyric acid
141-97-9	96	acetoacetate 2
144-62-7	971	oxalic acid
3715-29-5	49	3-methyl-2-oxobutanoic acid 2
2043-43-8	94220	lactamide 1

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CAS #	PubChem	Compound
626-97-1	12298	valeramide 4
108-39-4	342	m-cresol
107-97-1	1088	sarcosine
109-00-2	7971	3-hydroxypyridine
675-20-7	12665	2-piperidone 1
88-14-2	6919	2-furoic acid
626-64-2	12290	4-hydroxypyridine
95-48-7	2879	p-cresol
100-51-6	244	benzyl alcohol
61-90-5	6106	L-leucine 1
122-09-8	4771	Phentermine 1
2043-43-8	94220	lactamide 2
149-57-5	8697	2-ethylhexanoic acid
149-57-5	8697	2-ethylhexanoic acid
100-61-8	5288725	N-methylalanine
626-97-1	12298	valeramide 3
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 1
111-14-8	8094	heptanoic acid
149-57-5	8697	2-ethylcaproic acid
4502-00-5	70	2-ketoisocaproic acid 1
147-85-3	145742	L-proline 1
443-79-8	791	DL-isoleucine 1
147-85-3	614	L-proline 1
122-78-1	998	phenylacetaldehyde 1
537-46-2	10836	Methamphetamine 1
5680-79-5	69221	glycine methyl ester
111-87-5	957	1-octanol
122-78-1	998	phenylacetaldehyde 2
675-20-7	12665	2-piperidone 2
627-01-0	316542	N-ethylglycine 2
52-52-8	2901	cycloleucine 1
106-32-1	7799	ethyl octanoate
500-44-7	440473	L-mimosine 1
91-20-3	931	naphthalene
141-82-2	867	malonic acid 1
98-89-5	7413	cyclohexanecarboxylic acid
327-57-1	21236	L-norleucine 1
13031-04-4	39	dihydro-4,4-dimethyl-2,3-furandione 1
56-82-6	751	DL-glyceraldehyde 1
22059-21-8	535	1-aminocyclopropane-1-carboxylic acid
4502-00-5	70	2-ketoisocaproic acid 2
599-04-2	989	pantolactone
10569-71-9	64956	DL-3-aminoisobutyric acid 1
625-08-1	69362	beta-hydroxyisovalerate
516-05-2	487	methylmalonic acid

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CAS #	PubChem	Compound
72-18-4	6287	L-valine 2
56-82-6	751	DL-glyceraldehyde 2
543-38-4	275	L-canavanine 1
1731-84-6		Methyl Pelargonate
90-05-1	460	guaiacol
60-12-8	6054	phenylethyl alcohol
458-24-2	3337	Fenfluramine
127-07-1	3657	hydroxyurea
110-65-6	8066	2-butyne-1,4-diol
3128-06-1	26447	L-menthone
6600-40-4	65098	norvaline 2
95-16-9	7222	benzothiazole
65-85-0	243	benzoic acid
57-13-6	1176	urea
96-26-4	4180364	1,3-dihydroxyacetone
1460-57-7	92886	trans-cyclohexane-1,2-diol
13031-04-4	39	dihydro-4,4-dimethyl-2,3-furandione 2
1792-81-0	92903	cis-1,2-cyclohexanediol
56-45-1	5951	L-serine 1
13022-85-0	159664	2-ketocaproic acid
68-11-1	1133	thioglycolic acid
124-07-2	379	caprylic acid
766-93-8	13017	N-cyclohexylformamide
535-75-1	439227	pipecolic acid 1
141-43-5	700	ethanolamine
151-18-8	1647	3-aminopropionitrile 2
56-81-5	753	glycerol
61-90-5	6106	L-leucine 2
20549-47-7	443163	(-)-dihydrocarveol 1
7664-38-2	1004	phosphoric acid
103-84-4	904	acetanilide 1
5147-00-2	189	acetyl-L-serine 1
143-08-8	8914	1-nonanol
652157-52-3	637	2'-deoxycytidine
363-24-6	62453	4-vinylphenol 1
95-55-6	5801	2-aminophenol 1
20549-47-7	443163	(-)-dihydrocarveol 2
637-88-7	12511	1,4-cyclohexanedione 1
28954-12-3	99289	L-allothreonine 1
72-19-5	6288	L-threonine 1
443-79-8	791	DL-isoleucine 2
504-02-9	10434	1,3 cyclohexanedione 1
51-64-9	5826	d-Amphetamine
59-67-6	938	nicotinic acid
147-85-3	145742	L-proline 2

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CAS #	PubChem	Compound
110-16-7	444266	maleic acid
147-85-3	614	L-proline 2
637-88-7	12511	1,4-cyclohexanedione 2
504-02-9	10434	1,3 cyclohexanedione 2
4896-77-9	2723970	glycine-d5 deuterated
56-40-6	750	glycine
16867-04-2	28115	2,3-dihydroxypyridine
89-83-8	6989	thymol
29915-38-6	1110	succinic acid
120-80-9	289	catechol
67-47-0	237332	5-(hydroxymethylfurfural) 1
5391-40-5	638011	citral 1
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 2
504-02-9	10434	1,3 cyclohexanedione 3
616-04-6	69217	1-methylhydantoin 1
106-51-4	4650	p-benzoquinone
98-98-6	1018	picolonic acid
327-57-1	21236	L-norleucine 2
13022-85-0	18407	4-acetylbutyric acid 1
110-42-9		Methyl Caprate
10482-56-1	17100	terpineol
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
473-81-4	439194	glyceric acid
16834-13-2	86073	5,10,15,20-tetra(4-pyridyl)-21H,23H-porphine
681295-24-9	66868	porphine 1
66-22-8	1174	uracil
498-23-7	638129	citraconic acid
13022-85-0	18407	4-acetylbutyric acid 2
298-12-4	760	glyoxylic acid
765-87-7	13006	1,2-cyclohexanedione 1
97-65-4	811	itaconic acid
5391-40-5	638011	citral 2
17013-01-3	444972	fumaric acid
634-97-9	12473	pyrrole -2-carboxylic acid
498-23-7	643798	citraconic acid 1
99-04-7	7418	m-toluic acid
595-98-2	136386	methyltartronic acid
532-28-5	10758	mandelonitrile
6351-10-6	22819	1-indanol
532-28-5	10758	mandelonitrile
123-30-8	403	4-aminophenol 1
3012-37-1	18170	benzyl thiocyanate
26016-99-9	3417	phosphonomycin
5391-40-5	638011	citral 3
112-05-0	8158	pelargonic acid (nonanoic acid)

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CAS #	PubChem	Compound
5965-53-7	97750	diethyl oxalpropionate 1
13545-04-5	11848	2,3-dimethylsuccinic acid
672-15-1	12647	L-homoserine 1
616-04-6	69217	1-methylhydantoin 2
106-24-1	637566	geraniol
5391-40-5	638011	citral 4
56-45-1	5951	L-serine 2
3068-00-6	18302	butantriol
106-24-1	637566	geraniol
56-41-7	5950	L-alanine 2
141-12-8	1549026	neryl acetate 1
6589-55-5	913	halostachine 1
99-98-9	7472	N,N-dimethyl-1,4-phenylenediamine 1
535-75-1	439227	pipecolic acid 2
137-00-8	1136	4-methyl-5-thiazoleethanol
52-52-8	2901	cycloleucine 2
122-09-8	4771	Phentermine 2
45159-34-0	439742	beta-cyano-L-alanine
112-12-9	8163	2-undecanone 1
112-30-1	8174	1-decanol (decyl alcohol)
103-84-4	904	acetanilide 2
622-78-6	2346	benzyl isothiocyanate
108-46-3	5054	resorcinol
537-46-2	10836	Methamphetamine 2
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 1
498-23-7	643798	citraconic acid 2
122-03-2	326	4-isopropylbenzaldehyde
141-12-8	1549026	neryl acetate 2
72-19-5	6288	L-threonine 2
112-12-9	8163	2-undecanone 2
92-52-4	7095	biphenyl
452-86-8	9958	4-methylcatechol
80-69-3	45	tartronic acid
644-90-6	69522	2-aminooctanoic acid 1
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 2
3233-32-7	96009	4-Acetoxyphenol
5147-00-2	189	acetyl-L-serine 2
103-26-4	637520	methyl cinnamate
103-81-1	7680	2-phenylacetamide 1
65-71-4	1135	thymine
5965-53-7	97750	diethyl oxalpropionate 2
108-13-4	7911	malonamide 1
696-04-8	93556	5,6-dihydro-5-methyluracil 1
2078-54-8	4943	propofol
488-17-5	340	3-methylcatechol

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CAS #	PubChem	Compound
98-92-0	936	nicotinamide 1
536-60-7	325	4-isopropylbenzyl alcohol
123-31-9	785	hydroquinone
104-55-2	637511	cinnamaldehyde 1
67-47-0	237332	5-(hydroxymethylfurfural) 2
103-81-1	7680	2-phenylacetamide 2
18457-55-1	369312	(-)-perillyl alcohol
123-31-9	785	benzoquinone
765-87-7	13006	1,2-cyclohexanedione 2
104-55-2	637511	cinnamaldehyde 2
63-68-3	6137	L-methionine 1
628-48-8	5280498	glutaconic acid 1
353-09-3	67701	guanidinopropionic acid 1
4104-45-4	77743	3-(methylthio)-propylamine
501-52-0	107	hydrocinnamic acid
29267-67-2	121805	2-Methoxyresorcinol
141-82-2	867	malonic acid 2
8/2/4298	440575	trans-3-hydroxy-L-proline 1
3233-32-7	96009	4-Acetoxyphenol 1
91-22-5	6998	salicylaldehyde
56-84-8	5960	aspartic acid 1
8/2/4298	440575	trans-3-hydroxy-L-proline 1
95-55-6	5801	2-aminophenol 2
1191-25-9	14490	6-hydroxyhexanoic acid
107-95-9	239	Beta- alanine 1
1191-25-9	14490	6-hydroxy caproic acid
90-01-7	5146	2-hydroxybenzyl alcohol
582-24-1	68490	2-hydroxyacetophenone 1
108-13-4	7911	malonamide 2
55-21-0	2331	benzamide
100-46-9	7504	benzylamine
1188-21-2	1995	N-acetyl-L-leucine
557-24-4	5280451	maleamic acid 1
500-44-7	440473	L-mimosine 2
498-23-7	643798	citraconic acid 3
458-24-2	3337	Fenfluramine 1
125-64-4	4162	Methyprylon
95-43-2	439665	threose 1
498-23-7	643798	citraconic acid 4
504-15-4	10436	orcinol
100-83-4	101	3-hydroxybenzaldehyde
504-07-4	649	5,6-dihydrouracil 1
628-48-8	5280498	glutaconic acid 2
459-80-3	5275520	geranic acid
672-15-1	12647	L-homoserine 2

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CAS #	PubChem	Compound
95-43-2	439665	threose 2
334-48-5	2969	capric acid
6753-62-4	268779	N-methylglutamic acid 1
582-24-1	68490	2-hydroxyacetophenone 2
328-42-7	970	oxalacetic acid
765-87-7	13006	1,2-cyclohexanedione 3
71-30-7	597	cytosine 1
10569-71-9	64956	DL-3-aminoisobutyric acid 2
142-73-4	8897	iminodiacetic acid 1
103-81-1	7680	2-phenylacetamide 3
498-23-7	643798	citraconic acid 5
696-04-8	93556	5,6-dihydro-5-methyluracil 2
8/2/4298	440575	trans-3-hydroxy-L-proline 2
154-41-6	441457	Phenylpropanolamine
52-90-4	594	L-cysteine 1
14838-15-4	26934	1R, 2S-Phenylpropylamine
21784-30-5	12460	Phendimetrazine
17199-29-0	439616	mandelic acid
620-24-6	102	3-hydroxybenzyl alcohol
8/2/4298	440575	trans-3-hydroxy-L-proline 2
51-35-4	5810	trans-4-hydroxy-L-proline 1
6263-10-8	439766	citramalic acid
5965-53-7	97750	diethyl oxalpropionate 3
675-10-5	12663	4-Hydroxy-6-Methylpyran-2-One
611-73-4	11915	benzoylformic acid 1
3106-60-3	457	1-methyl nicotinamide 1
98-92-0	936	nicotinamide 2
696-04-8	93556	5,6-dihydro-5-methyluracil 3
504-07-4	649	5,6-dihydouracil 2
3685-22-1	151138	cis-4-hydroxycyclohexanecarboxylic acid
617-48-1	92824	D-malic acid
675-10-5	12663	4-hydroxy-6-methyl-2-pyrone
6851-36-1	166768	4-hydroxymandelonitrile 1
644-90-6	69522	2-aminooctanoic acid 2
123-08-0	126	4-hydroxybenzaldehyde 1
3025-96-5	18189	4-acetamidobutyric acid 1
59-31-4	6038	2-hydroxyquinoline 1
609-71-2	69114	2-hydroxynicotinic acid
4707-46-4	736228	3-Methylorsellinic Acid 1
1504-06-9	150923	3-methoxyindole 1
6968-16-7	169019	D-threitol
108-13-4	7911	malonamide 3
124-04-9	196	adipic acid
123-08-0	126	4-hydroxybenzaldehyde 2
154-58-5	64960	1,5-anhydroglucitol

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CAS #	PubChem	Compound
535-83-1	5570	trigonelline
50-78-2	2244	O-acetylsalicylic acid
128-37-0	31404	2,6-ditert-butyl-4-methylphenol 1
3025-96-5	18189	4-acetamidobutyric acid 2
1188-37-0	70914	N-acetyl-L-glutamic acid 1
119-84-6	660	dihydrocoumarin 1
100-02-7	980	4-nitrophenol
69-72-7	338	salicylic acid
4436-74-2	5351896	trans-3-hexenedioic acid
463-00-3	500	4-guanidinobutyric acid 1
480-44-4	5280442	Acacetin
14191-95-8	26548	4-hydroxybenzyl cyanide
63-68-3	6137	L-methionine 2
6589-55-5	913	halostachine 2
56-84-8	5960	aspartic acid 2
0		L-glutamic acid-2,3,3,4,4-d5 3 (dehydrated)
98-79-3	7405	L-pyroglutamic acid
100-09-4	7478	p-anisic acid
56-86-0	33032	L-glutamic acid 3 (dehydrated)
536-66-3	10820	4-isopropylbenzoic acid
111-82-0		Methyl Laurate
71-30-7	597	cytosine 2
5746-86-1	412	nornicotine
4385-35-7	78092	3-isochromanone
51-35-4	5810	trans-4-hydroxy-L-proline 2
56-86-0	73064	beta-glutamic acid
142-73-4	8897	iminodiacetic acid 2
116-09-6	8299	acetol 1
123-30-8	403	4-aminophenol 2
56-12-2	119	gamma-aminobutyric acid (GABA)
0		L-glutamic acid-2,3,3,4,4-d5 1
56-86-0	33032	L-glutamic acid 1
557-24-4	5280451	maleamic acid 2
6753-62-4	268779	N-methyl-DL-glutamic acid 1
463-00-3	500	4-guanidinobutyric acid 2
1504-06-9	150923	3-methoxyindole 2
923-16-0	601	D-Ala-D-Ala 1
6753-62-4	268779	N-methylglutamic acid 2
611-73-4	11915	benzoylformic acid 2
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 3
615-58-7	11847	2,6-dibromophenol
132-64-9	568	dibenzofuran
56-85-9	738	L-glutamine 1
87-66-1	1057	pyrogallol
95-55-6	5801	2-aminophenol 3

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CAS #	PubChem	Compound
63585-09-1	13000987	L-phenylalanine-phenyl-d5-2,3,3-d3 1
2734-48-7	151491	3-(1-pyrazolyl)-L-alanine
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 4
106-57-0	7817	glycine anhydride 1
119-68-6	67069	N-methylantranilic acid 1
14901-07-6	638014	beta-ionone 1
63-91-2	994	Phenylalanine 1
63-91-2	994	Phenylalanine 1
140-10-3	444539	cinnamic acid
615-58-7	12005	2,4-dibromophenol
52-90-4	594	L-cysteine 2
60-27-5	588	Creatinine
56-57-5	77341	4-nitroquinoline
7306-96-9	5460407	threonic acid
119-84-6	660	dihydrocoumarin 2
557-24-4	5280451	maleamic acid 3
6753-62-4	268779	N-methyl-DL-glutamic acid 2
100937-52-8	451991	1,4-dideoxy-1,4-imino-D-arabinitol 1
14901-07-6	638014	beta-ionone 2
106-57-0	7817	glycine anhydride 2
64-04-0	1001	phenethylamine
6753-62-4	268779	N-methylglutamic acid 3
503-66-2	68152	3-hydroxypropanoic acid 1
64-04-0	1001	phenylethylamine
614-75-5	11970	2-hydroxyphenylacetic acid
533-67-5	5460005	2-deoxy-D-ribose 1
119-67-5	8406	2-carboxybenzaldehyde 1
5006-66-6	72924	6-hydroxynicotinic acid
3237-44-3	36	2-isopropylmalic acid
110-94-1	743	glutaric acid
533-67-5	5460005	2-deoxy-D-ribose 2
501-94-0	10393	2-(4-hydroxyphenyl)ethanol
5006-66-6	72924	6-hydroxynicotinic acid
503-66-2	68152	3-hydroxypropanoic acid 2
352-97-6	763	guanidinoacetic acid 1
328-50-7	51	alpha ketoglutaric acid
501-94-0	10393	4-(2-hydroxyethyl)phenol (tyrosol)
353-09-3	67701	guanidinopropionic acid 2
120-14-9	8419	3,4-dimethoxybenzaldehyde
100937-52-8	451991	1,4-dideoxy-1,4-imino-D-arabinitol 2
156-06-9	997	phenylpyruvate
828-01-3	3848	3-phenyllactic acid
19253-88-4	159660	trimethyllysine
123-30-8	403	4-aminophenol 3
84-66-2	6781	diethyl phthalate

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CAS #	PubChem	Compound
529-64-6	10726	tropic acid
16096-97-2	439196	L-dithiothreitol 1
56-85-9	738	L-glutamine 2
462-88-4	111	3-ureidopropionate 1
701-64-4	12793	phenylphosphoric acid
923-16-0	601	D-Ala-D-Ala2
300-84-5	107812	hypotaurine
95648-83-2	529	phosphoglycolic acid
106-33-2	7800	ethyl dodecanoate
642-71-7	69505	Antiarol
533-73-3	10787	benzene-1,2,4-triol
138-08-9	1005	phosphoenolpyruvic acid
86-73-7	6853	fluorene
111-16-0	385	pimelic acid
90-43-7	7017	2-hydroxybiphenyl
629-73-2	12395	hexadecene
70-47-3	16217724	L-asparagine-15N2,d8 1
57-44-3	2294	Barbital
527-52-6	258531	digitoxose 1
503-49-1	1662	3-hydroxy-3-methylglutaric acid (dicrotalic acid)
527-52-6	258531	digitoxose 2
621-37-4	12122	3-hydroxyphenylacetic acid
6192-52-5	6101	p-toluenesulfonic acid
119-67-5	8406	2-carboxybenzaldehyde 2
119-68-6	67069	N-methylantranilic acid 2
70-26-8	6262	L-ornithine 1
21784-30-5	12460	Phendimetrazine 1
0		L-glutamic acid-2,3,3,4,4-d5 2
56-86-0	33032	L-glutamic acid 2
3588-17-8	5356793	trans,trans-muconic acid
63585-09-1	13000987	L-phenylalanine-phenyl-d5-2,3,3-d3 2
660-88-8	138	5-aminovaleric acid 1
102-71-6	7618	triethanolamine
6307-89-7	238769	2,6-Dihydroxy-4-Methoxytoluene
70-47-3	236	L-asparagine 1
70-47-3	16217724	L-asparagine-15N2,d8 2
114-63-6	135	4-hydroxybenzoic acid
71-30-7	597	cytosine 3
611-36-9	69141	4-hydroxyquinoline 1
107-95-9	239	Beta- alanine 2
498-00-0	62348	4-hydroxy-3-methoxybenzyl alcohol
133-37-9	444305	tartaric acid
156-38-7	127	4-hydroxyphenylacetic acid
360-97-4	9679	5-aminoimidazole-4-carboxamide 1
108-73-6	359	phloroglucinol

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CAS #	PubChem	Compound
99-98-9	7472	N,N-dimethyl-1,4-phenylenediamine 2
	5176389	3,7-Epoxycaryophyllan-6-Ol
	5024745	2-Hydroxy-5 (6)Epoxy-Tetrahydrocaryophyllene
481-37-8	91460	Ecgonine
58-86-6	6027	xylose 1
121-33-5	1183	vanillin
109-76-2	428	1,3-diaminopropane 1
1114-34-7	65550	D-lyxose 1
3943-74-6	19844	methyl 4-hydroxy-3-methoxybenzoate
352-97-6	763	guanidinoacetic acid 2
1114-34-7	439240	D-lyxose 1
134-49-6	4762	Phenmetrazine
689-31-6	71	2-ketoadipic acid 1
143-07-7	3893	lauric acid
58-86-6	6027	xylose 2
7298-99-9	443239	threo-3-hydroxy-L-aspartate
997-55-7	65065	N-acetyl-L-aspartic acid 1
1114-34-7	65550	D-lyxose 2
51268-88-3	440294	cis-1,2-dihydro-1,2-naphthalenediol
689-31-6	71	2-ketoadipic acid 2
0	443239	DL-threo-beta-hydroxyaspartic acid
1114-34-7	439240	D-lyxose 2
10323-20-3	66308	arabinose
462-88-4	111	3-ureidopropionate 2
51268-88-3	440294	(1R,2S)-cis-1,2-dihydro-1,2-naphthalenediol
107-35-7	1123	taurine
660-88-8	138	5-aminovaleric acid 2
997-55-7	65065	N-acetyl-L-aspartic acid 2
70-47-3	16217724	L-asparagine-15N2,d8 3
70-47-3	236	L-asparagine 2
9/3/2466	1023	pyrophosphate
1504-06-9	150923	3-methoxyindole 3
5336-08-3	111064	ribonic acid-gamma-lactone 1
462-88-4	111	3-ureidopropionate 3
551-84-8	439204	xylulose
672-15-1	12647	L-homoserine 3
495-78-3	873	3-(2-hydroxyphenyl)propanoic acid
119-84-6	660	dihydrocoumarin 3
4289-98-9	911	N-formyl-L-methionine 1
24259-59-4	993	ribose
6753-62-4	268779	N-methyl-DL-glutamic acid 3
94-07-5	7172	synephrine 1
3177-80-8	255720	2-amino-3-methoxybenzoic acid 1
5336-08-3	111064	ribonic acid-gamma-lactone 2
1211-29-6	62388	methyljasmonate 1

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CAS #	PubChem	Compound
1211-29-6	62388	methyljasmonate 1
6753-62-4	268779	N-methylglutamic acid 4
128-37-0	31404	2,6-ditert-butyl-4-methylphenol 2
3106-60-3	457	1-methyl nicotinamide 2
88-99-3	1017	phthalic acid
128-37-0	31404	3,5-Di-tert-butyl-4-hydroxytoluene
616-91-1	12035	N-acetyl-L-cysteine 1
4289-98-9	911	N-formyl-L-methionine 2
6851-36-1	166768	4-hydroxymandelonitrile 2
116-09-6	8299	acetol 2
505-48-6	10457	suberic acid
498-07-7	2724705	1,6-anhydro-glucose
660-88-8	138	5-aminovaleric acid 3
88-21-1	6926	aniline-o-sulfonic acid
87-99-0	6912	xylitol
116-09-6	8299	acetol 3
1211-29-6	62388	methyljasmonate 2
1194-98-5	70949	2,5-dihydroxybenzaldehyde
541-15-1	10918	L-carnitine 1
77-02-1	6464	Aprobarbital
42542-10-9	1615	3,4-MDMA
108-19-0	7913	biuret 1
93965-35-6	729	DL-glyceraldehyde 3-phosphate 1
616-91-1	12035	N-acetyl-L-cysteine 2
116-09-6	8299	acetol 4
118-74-1	8370	hexachlorobenzene
59-31-4	6038	2-hydroxyquinoline 2
77-93-0	6506	triethyl citrate
3615-41-6	220001	rhamnose 1
60-32-2	564	6-aminocaproic acid
7507-89-3	24135	4-O-Methylphloracetophenone 1
93965-35-6	729	DL-glyceraldehyde 3-phosphate 2
621-54-5	91	3-(3-hydroxyphenyl)propionic acid
124-10-7		Methyl Myristate
7568-08-4	439746	6-deoxy-D-glucose 1
488-82-4	94154	arabitol
2438-80-4	17106	L-(-)-fucose 1
89-00-9	1066	quinolinic acid
1211-29-6	62388	methyljasmonate 3
1211-29-6	62388	methyljasmonate 2
582-60-5	675	5,6 - dimethylbenzimidazole 1
819-83-0	2526	beta-glycerolphosphate
3615-41-6	220001	rhamnose 2
488-81-3	827	ribitol
119-84-6	660	dihydrocoumarin 4

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CAS #	PubChem	Compound
7568-93-6	1000	2-amino-1-phenylethanol
97164-73-3	2479	Butabarbital
99-50-3	19	2,3-dihydroxybenzoic acid
110-60-1	1045	putrescine
77-26-9	2481	Butalbital
6202-10-4	439216	dihydroorotic acid 1
161886-59-5	11058264	(S)-Carnitine Mesylate Isobutylester
541-15-1	10918	L-carnitine 2
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 1
7568-08-4	439746	6-deoxy-D-glucose 2
2438-80-4	17106	L-(-)-fucose 2
627-82-7	42953	diglycerol 1
50887-69-9	967	orotic acid
50887-69-9	967	orotic acid
62147-49-3	668	dihydroxyacetone phosphate 1
14528-64-4	3505109	4-nitrocatechol
372-75-8	9750	citrulline 1
6202-10-4	439216	dihydroorotic acid 2
585-84-2	444212	trans-aconic acid
2041-14-7	339	ciliatine
3226-65-1	158980	L-methionine sulfoxide 1
1211-29-6	62388	methyljasmonate 4
4460-86-0	20525	Asarylaldehyde 1
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 1
499-83-2	10367	pyridine-2,6-dicarboxylic acid
62147-49-3	668	dihydroxyacetone phosphate 2
548-93-6	86	3-hydroxyanthranilic acid 1
627-82-7	42953	diglycerol 2
57-43-2	2164	Amobarbital
1188-37-0	70914	N-acetyl-L-glutamic acid 2
628-94-4	12364	adipamide 1
501-97-3	10394	3-(4-hydroxyphenyl)propionic acid
186537-58-6	193653	S-carboxymethylcysteine 1
121-34-6	8468	4-hydroxy-3-methoxybenzoic acid
627-82-7	42953	diglycerol 3
57-43-2	2164	Amobarbital 1
3081-61-6	228398	L-theanine 1
6202-10-4	439216	dihydroorotic acid 3
2478-38-8	17198	Acetosyringone 1
5704-04-1	79784	tricine 1
34363-28-5	754	glycerol 1-phosphate
4460-86-0	20525	Asarylaldehyde 2
23945-44-0	90301	2,4-dihydroxypyrimidine-5-carboxylic acid
306-08-1	1738	homovanillic acid (HVA)
486-74-8	10243	4-quinolinecarboxylic acid

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CAS #	PubChem	Compound
56-85-9	738	L-glutamine 3
22818-40-2	36143	4-hydroxyphenylglycine 1
82385-42-0	5143	saccharin 2
7507-89-3	24135	4-O-Methylphloracetophenone 2
108-19-0	7913	biuret 2
490-79-9	3469	gentisic acid
115-44-6	8275	Talbutal
119-84-6	660	dihydrocoumarin 5
7198-10-9	328	DL-4-hydroxymandelic acid
19317-11-4	5280598	farnesal 1
2875-41-4	10034670	N-(3-Aminopropyl)glycine 1
1114-81-4	3246323	O-phospho-L-threonine 1
3081-61-6	228398	L-theanine 2
574-17-4	11321	acetylisatin 1
407-41-0	68841	O-phospho-L-serine 1
360-97-4	9679	5-aminoimidazole-4-carboxamide 2
1080-06-4	70652	tyrosine methyl ester 1
109-76-2	428	1,3-diaminopropane 2
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 2
1071-23-4	1015	O-phosphocolamine
1188-37-0	70914	N-acetyl-L-glutamic acid 3
3226-65-1	158980	L-methionine sulfoxide 2
407-41-0	68841	O-phospho-L-serine 1
5704-04-1	79784	tricine 2
2018-61-3	74839	N-acetyl-L-phenylalanine 1
2922-42-1	80	3-dehydroshikimic acid 1
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 3
154-17-6	439268	deoxyglucose 1
5934-29-2	6274	L-histidine 1
19317-11-4	5280598	farnesal 2
628-94-4	12364	adipamide 2
1032-65-1	13945	2'-deoxycytidine 5'-monophosphoric acid
154-17-6	439268	deoxyglucose 2
123-99-9	2266	azelaic acid
112-88-9	8217	1-octadecene
28954-12-3	99289	L-allothreonine 2
76-74-4	4737	Pentobarbital
3206-73-3	863	lipoamide 1
360-97-4	9679	5-aminoimidazole-4-carboxamide 3
2922-42-1	80	3-dehydroshikimic acid 2
495-69-2	464	hippuric acid 1
368-16-1	64969	3-methyl-L-histidine
106-28-5	445070	trans-trans-farnesol
138-59-0	8742	shikimic acid
93-10-7	7124	quinaldinic acid

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CAS #	PubChem	Compound
68-94-0	790	hypoxanthine 1
673-49-4	69602	N-omega-acetylhistamine 2
82801-81-8	105039	3,4-MDEA
700-06-1	3712	indole-3-carbinol (3-indolemethanol)
2018-61-3	74839	N-acetyl-L-phenylalanine 2
68-94-0	790	hypoxanthine
614-60-8	637540	2-hydroxycinnamic acid
574-17-4	11321	acetylisatin 2
820-11-1	439183	3-phosphoglycerate
3177-80-8	255720	2-amino-3-methoxybenzoic acid 2
80731-10-8	439183	3-phosphoglyceric acid
2163-68-0	16553	atrazin-2-hydroxy 1
1679-53-4	74300	10-hydroxydecanoic acid
628-94-4	12364	adipamide 3
700-06-1	3712	indole-3-carbinol 1
119-53-9	8400	benzoin 1
85-01-8	995	phenanthrene
22818-40-2	36143	4-hydroxyphenylglycine 2
1689-64-1	74318	9-hydroxyfluorene
19317-11-4	5280598	farnesal 3
1637-73-6	1198	isocitric acid
99-50-3	72	3,4-dihydroxybenzoic acid
19246-18-5	65270	cysteinylglycine 1
582-60-5	675	5,6 - dimethylbenzimidazole 2
15450-76-7	97250	2,8-quinolinediol
94-07-5	7172	synephrine 2
19317-11-4	5280598	farnesal 4
2152-75-2	740	alpha-D-glucosamine 1-phosphate
5949-29-1	311	citric acid
2152-75-2	740	alpha-D-glucosamine phosphate
2152-75-2	740	alpha-glucosamine 1-phosphate
70-26-8	6262	L-ornithine 2
1114-81-4	3246323	O-phospho-L-threonine 2
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 2
574-17-4	11321	acetylisatin 3
372-75-8	9750	citrulline 2
82385-42-0	5143	saccharin 1
102-32-9	547	2-(3,4-dihydroxyphenyl)acetic acid
186537-58-6	193653	S-carboxymethylcysteine 2
451-13-8	780	homogentisic acid
60658-41-5		Myristic Acid d27
102-32-9	547	3,4-dihydroxyphenylacetic acid
150-13-0	978	4-aminobenzoic acid
76-73-3	5193	Secobarbital
82-82-6	6723	4-pyridoxic acid 1

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CAS #	PubChem	Compound
407-41-0	68841	O-phospho-L-serine 2
2875-41-4	10034670	N-(3-Aminopropyl)glycine 2
673-49-4	69602	N-omega-acetylhistamine 1
1188-38-1	3679006	N-carbamyl-L-glutamic acid 1
2163-68-0	16553	atrazin-2-hydroxy 2
18652-93-2	9034	Methohexital
407-41-0	68841	O-phospho-L-serine 2
51-43-4	5816	adrenaline 1
		L-Ascorbic Acid-13C6 1
490-83-5	835	dehydroascorbic acid 1
495-69-2	464	hippuric acid 2
544-63-8	11005	myristic acid
1133-63-7	254	2,3-dihydroxybiphenyl
923-16-0	601	D-Ala-D-Ala3
51028-73-0	5816	(-)-epinephrine 1
2478-38-8	17198	Acetosyringone 2
1824-94-8	94214	methyl-beta-D-galactopyranoside
156-39-8	979	4-hydroxyphenylpyruvic acid 1
2163-68-0	16553	atrazin-2-hydroxy 3
58-08-2	2519	caffeine
154-58-5	219984	1,5-anhydro-D-sorbitol
32449-92-6	439782	glucuronolactone 1
2316-26-9	717531	3,4-Dimethoxycinnamic Acid 1
156-08-1	2341	Benzphetamine
583-93-7	865	2,6-diaminopimelic acid 1
56-87-1	5962	L-lysine 1
87-81-0	2724552	tagatose 1
1504-06-9	150923	3-methoxyindole 4
487-21-8	10250	lumazine
3226-65-1	158980	L-methionine sulfoxide 3
1080-06-4	70652	tyrosine methyl ester 2
86-74-8	6854	carbazole 1
551-68-8	90008	psicose 1
73-24-5	190	adenine 1
548-93-6	86	3-hydroxyanthranilic acid 2
628-94-4	12364	adipamide 4
73-24-5	190	9H-purine-6-amine
77-95-2	6508	quinic acid
7507-89-3	24135	4-O-Methylphloracetophenone 3
16096-97-2	439196	L-dithiothreitol 2
119-53-9	8400	benzoin 2
6133-30-8	97856	guanidinosuccinic acid 1
574-17-4	11321	acetylisatin 4
6892-68-8	439352	1,4-dithioerythritol
490-83-5	835	dehydroascorbic acid 2

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CAS #	PubChem	Compound
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 1
		L-Ascorbic Acid-13C6 2
81-13-0	131204	D-panthenol 1
55-10-7	1245	DL-4-hydroxy-3-methoxymandelic acid
588-30-7	637541	3-hydroxycinnamic acid
57-48-7	5984	fructose 1
3615-56-3	1101	L- sorbose 1
551-68-8	90008	psicose 2
884-33-3	3858	benzylsuccinic acid
28822-73-3	91528	DL-3,4-dihydroxyphenyl glycol
87-81-0	2724552	tagatose 2
771-51-7	351795	3-indoleacetonitrile
487-89-8	10256	indole-3-carbaldehyde 1
500-98-1	68144	phenaceturic acid 1
5934-29-2	6274	L-histidine 2
3615-56-3	1101	L- sorbose 2
1772-03-8	24154	galactosamine 1
87-89-8	892	allo-inositol
99-24-1	7428	methyl gallate
99-24-1	7428	methyl gallate
579-36-2	448388	D-allose 1
87-78-5	18950	D-mannose 1
57-48-7	5984	fructose 2
500-98-1	68144	phenaceturic acid 2
97-59-6	204	allantoin 1
574-17-4	11321	acetylisatin 5
90-80-2	736	gluconic acid lactone 1
73-24-5	190	adenine 2
1128-23-0	608	L-galactono-gamma-lactone 1
60-18-4	6057	L-tyrosine 1
13382-27-9	128869	galactonic acid 1
1188-38-1	3679006	N-carbamyl-L-glutamic acid 2
583-08-4	68499	nicotinoylglycine
0	16213445	L-tyrosine-3,3-d2 1
60-18-4	6057	tyrosine 1
97-59-6	204	allantoin 2
530-57-4	10742	syringic acid
574-17-4	11321	acetylisatin 6
24940-57-6	440274	N,N-dimethyl-L-histidine
65-23-6	1054	pyridoxine
1772-03-8	24154	galactosamine 2
1990-29-0	441032	D (+)altrose 1
2595-98-4	441035	talose 1
59-23-4	206	D (+) galactose 1
0	16217112	D-glucose-C-d7 1

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CAS #	PubChem	Compound
32449-92-6	439782	glucuronolactone 2
6482-98-0	9378	DL-p-hydroxyphenyllactic acid
59-23-4	24749	D-glucose 1
1946-82-3	92907	N-alpha-acetyl-L-lysine 1
342385-52-8	159793	2-keto-L-gulonic acid 1
306-23-0	9378	3-(4-hydroxyphenyl)lactic acid
90-80-2	736	gluconic acid lactone 2
87-78-5	18950	D-mannose 2
1990-29-0	441032	D (+)altrose 2
1120-25-8	643801	methyl palmitoleate
104-98-3	1178	urocanic acid 1
6556-12-3	16213610	glucuronic acid 1
6556-12-3	16213610	glucuronic acid 3
		L-Ascorbic Acid-13C6 3
490-83-5	835	dehydroascorbic acid 3
585-18-2	697	erythrose 4-phosphate 1
156-39-8	979	4-hydroxyphenylpyruvic acid 2
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 2
0	5459862	D-erythrose-4-phosphate 1
579-36-2	448388	D-allose 2
56-29-1	3608	Hexobarbital
1772-03-8	24154	galactosamine 3
51-67-2	5610	tyramine
486-25-9	10241	9-fluorenone
2595-98-4	441035	talose 2
2163-68-0	16553	atrazin-2-hydroxy 4
585-18-2	697	erythrose 4-phosphate 2
0	5459862	D-erythrose-4-phosphate 2
0	16217112	D-glucose-C-d7 2
59-23-4	24749	D-glucose 2
487-89-8	10256	indole-3-carbaldehyde 2
4637-56-3	5460367	4-Hydroxyaminoquinoline-N-oxide
14883-87-5	85782	3,4-dihydroxymandelic acid
77-10-1	6468	Phencyclidine
56-87-1	5962	L-lysine 2
1128-23-0	439373	L-gulonic acid gamma-lactone
5934-29-2	6274	L-histidine 3
4707-46-4	736228	3-Methylorsellinic Acid 2
59-23-4	206	D (+) galactose 2
526-95-4	604	gluconic acid 1
1002-57-9	66085	8-aminocaprylic acid
32449-92-6	439782	glucuronolactone 3
311-45-5	9395	paraoxon
90-80-2	736	gluconic acid lactone 3
112-39-0		Methyl Palmitate

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CAS #	PubChem	Compound
		L-Ascorbic Acid-13C6 4
490-83-5	835	dehydroascorbic acid 4
50-66-8	5778	6-methylmercaptapurine 1
6090-95-5	119054	conduritol epoxide 1
1128-23-0	608	L-galactono-gamma-lactone 2
6556-12-3	16213610	glucuronic acid 2
6556-12-3	16213610	glucuronic acid 4
469-90-9	16219957	sedoheptulose anhydride monohydrate
2163-68-0	16553	atrazin-2-hydroxy 5
0	16213445	L-tyrosine-3,3-d2 2
115-38-8	8271	Mephobarbital
1772-03-8	24154	galactosamine 4
87-78-5	6251	D-mannitol
1946-82-3	92907	N-alpha-acetyl-L-lysine 2
1188-38-1	3679006	N-carbamyl-L-glutamic acid 3
458-35-5	1549095	coniferyl alcohol
82-82-6	6723	4-pyridoxic acid 2
608-07-1	637542	4-hydroxycinnamic acid
60-18-4	6057	L-tyrosine 2
81-13-0	131204	D-panthenol 2
60-18-4	6057	tyrosine 2
50-66-8	5778	6-methylmercaptapurine 2
490-83-5	835	dehydroascorbic acid 5
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 1
1138-80-3	14349	N-benzyloxycarbonylglycine
1772-03-8	24154	galactosamine 5
50-70-4	5780	D-sorbitol
137-08-6	6613	pantothenic acid 1
14982-50-4	445929	galacturonic acid 1
372-75-8	9750	citrulline 3
1188-38-1	3679006	N-carbamyl-L-glutamic acid 4
14982-50-4	439215	galacturonic acid 1
487-54-7	10253	salicylurate 1
50-81-7	5785	L-ascorbic acid
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic acid
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 2
498-40-8	72886	L-cysteic acid
537-33-7	5280507	sinapyl alcohol 1
608-66-2	11850	galactitol
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic acid
342385-52-8	159793	2-keto-L-gulonic acid 2
6090-95-5	119054	conduritol epoxide 2
		L-Ascorbic Acid-13C6 5
490-83-5	835	dehydroascorbic acid 6
149-91-7	370	gallic acid

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CAS #	PubChem	Compound
1401-55-4	16133892	tannic acid
51-43-4	5816	adrenaline 2
36653-82-4	2682	1-hexadecanol
551-16-6	11082	(+)-6-aminopenicillanic acid 1
146255-66-5	443586	3,5-dihydroxyphenylglycine 1
51028-73-0	5816	(-)-epinephrine 2
87-51-4	802	3-indoleacetic acid
14982-50-4	445929	galacturonic acid 2
36653-82-4	2682	1-hexadecanol, (cetyl alcohol)
14982-50-4	439215	galacturonic acid 2
879-37-8	397	indole-3-acetamide 1
146255-66-5	443586	3,5-dihydroxyphenylglycine 2
50-06-6	4763	Phenobarbital
0	439232	N-acetyl-ornithine 1
1492-23-5	954	O-succinylhomoserine 1
704-15-4	79101	gly-pro
611-36-9	69141	4-hydroxyquinoline 2
	9925625	propofol hemisuccinate
4264-83-9	378	4-nitrophenyl phosphate
526-95-4	604	gluconic acid 2
583-93-7	865	2,6-diaminopimelic acid 2
704-15-4	79101	glycylproline
543-38-4	275	L-canavanine 2
86-48-6	6844	1-hydroxy-2-naphthoic acid
137-08-6	6613	pantothenic acid 2
86-74-8	6854	carbazole 2
3646-68-2	73563	D-glucosaminic acid 1
90-33-5	5280567	4-methylumbelliferone
0	439232	N-acetyl-ornithine 2
56-57-5	5955	4-nitroquinoline N-oxide
3646-68-2	73563	D-glucosaminic acid 1
503-66-2	68152	3-hydroxypropanoic acid 3
112-95-8	8222	eicosane
19246-18-5	65270	cysteinylglycine 2
90-33-5	5280567	4-methylumbelliferone
13382-27-9	128869	galactonic acid 2
104-98-3	1178	urocanic acid 2
69-89-6	1188	xanthine
2316-26-9	717531	3,4-Dimethoxycinnamic Acid 2
14769-73-4	26879	levamisole
68-94-0	790	hypoxanthine 2
87-73-0	5460673	D-saccharic acid
6133-30-8	97856	guanidinosuccinic acid 2
771-50-6	69867	indole-3-carboxylic acid
771-50-6	69867	indole-3-carboxylic acid

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CAS #	PubChem	Compound
63-37-6	6131	cytidine-5'-monophosphate 1
102916-66-5	25245723	2-deoxyribose 5-phosphate
1731-92-6	15609	methyl heptadecanoate
373-49-9	445638	palmitoleic acid
830-96-6	3744	indole 3-propionic acid 1
35608-63-0	110992	3-chloro-L-tyrosine 1
3646-68-2	73563	D-glucosaminic acid 2
64519-82-0	985	palmitic acid
1188-38-1	3679006	N-carbamyl-L-glutamic acid 5
1492-23-5	954	O-succinylhomoserine 2
3646-68-2	73563	D-glucosaminic acid 2
526-99-8	3037582	mucic acid
92-61-5	5280460	scopoletin
19246-18-5	65270	cysteinylglycine 3
530-59-6	637775	3,5-dimethoxy-4-hydroxycinnamic acid 1
298-81-7	4114	xanthotoxin 1
10094-62-9	101713	glucoheptonic acid 1
82-86-0	6724	acenaphthenequinone 1
2018-66-8	74840	N- carbobenzoxy-L-leucine 1
59-92-2	836	3,4 dihydroxyphenylalanine (DOPA) 1
2497-02-1	273260	N-acetyl-L-histidine 1
487-54-7	10253	salicylurate 2
57-92-7	6047	L-DOPA 1
367-93-1	656894	isopropyl beta-D-1-thiogalactopyranoside
492-27-3	3845	4-hydroxyquinoline-2-carboxylic acid(kynurenic acid)
35608-63-0	110992	3-chloro-L-tyrosine 2
97-59-6	204	allantoin 3
2018-66-8	74840	N- carbobenzoxy-L-leucine 2
7772-94-3	899	N-acetyl-D-mannosamine 1
484-20-8	2355	5-methoxypsoralen
7512-17-6	16218892	N-acetyl-D-glucosamine 1
830-96-6	3744	indolepropionic acid
3206-73-3	863	lipoamide 2
51-61-6	681	dopamine (hydroxytyramine)
830-96-6	3744	indole 3-propionic acid 2
537-33-7	5280507	sinapyl alcohol 2
6133-30-8	97856	guanidinosuccinic acid 3
7512-17-6	16218892	N-acetyl-D-glucosamine 2
1135-24-6	445858	ferulic acid
59-92-2	836	3,4 dihydroxyphenylalanine (DOPA) 2
66-22-8	1175	uric acid 1
7772-94-3	899	N-acetyl-D-mannosamine 2
65005-57-4	123831	N,N-dimethylarginine
87-89-8	892	myo-inositol
487-26-3	10251	flavanone 1

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CAS #	PubChem	Compound
113573-73-2	440053	S(-)willardiine 1
57-92-7	6047	L-DOPA 2
487-26-3	10251	flavonone 1
301-00-8	9316	methyl linolenate
4206-58-0	5280802	trans-3,5-dimethoxy-4-hydroxycinnamaldehyde
112-62-9	5364509	methyl oleate
879-37-8	397	indole-3-acetamide 2
487-26-3	10251	flavanone 2
2497-02-1	273260	N-acetyl-L-histidine 2
34522-32-2	108172	octopine 1
4376-20-9	20393	mono(2-ethylhexyl)phthalate
82-86-0	6724	acenaphthenequinone 2
487-26-3	10251	flavonone 2
21339-55-9	676159	1-methyl-L-tryptophan 1
15673-79-7	439167	D-ribose-5-phosphate 1
23279-22-3	160450	3-amino-L-tyrosine 1
15673-79-7	439167	D-ribose-5-phosphate 2
2107-77-9	5355836	4-Methyldaphnetin
484-17-3	10229	9-phenanthrenol
34522-32-2	108172	octopine 2
7365-44-8	446188	TES
108321-99-9	439184	ribulose-5-phosphate 3
10094-62-9	101713	glucoheptonic acid 2
21339-55-9	676159	1-methyl-L-tryptophan 2
112-61-8		Methyl Stearate
7541-49-3	5366244	phytol 1
7541-49-3	6430833	phytol 1
1214-20-6	71034	2-Methoxyxanthone
529-69-1	10729	isoxanthopterin
3471-31-6	18986	5-methoxy-3-indoleacetic acid 1
331-39-5	1549111	caffeic acid
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 1
879-37-8	397	indole-3-acetamide 3
506-12-7	10465	heptadecanoic acid
1821-52-9	92904	3-indolelactic acid 1
551-16-6	11082	(+)-6-aminopenicillanic acid 2
66-22-8	1175	uric acid 2
1214-47-7	5367146	2-hydroxychalcone 1
23279-22-3	160450	3-amino-L-tyrosine 2
51-41-2	5814	norepinephrine (noradrenalin)
22862-76-6	31549	Anisomycin
82-86-0	6724	acenaphthenequinone 3
3206-73-3	863	lipoamide 3
2922-83-0	161166	L-kynurenine 1
3471-31-6	18986	5-methoxy-3-indoleacetic acid 2

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CAS #	PubChem	Compound
70-18-8	124886	L-glutathione reduced
7541-49-3	5366244	phytol 2
7541-49-3	6430833	phytol 2
1821-52-9	92904	3-indolelactic acid 2
23279-22-3	160450	3-amino-L-tyrosine 3
31519-22-9	671	1,4-dihydroxy-2-naphthoic acid
113573-73-2	440053	S(-)willardiine 2
0	4130574	asp-glu 1
76-99-3	4095	Methaqualone
2922-83-0	161166	L-kynurenine 2
551-16-6	11082	(+)-6-aminopenicillanic acid 3
392-12-1	803	indole-3-pyruvic acid
73-22-3	6305	L-tryptophan 1
14721-66-5	26840	phytanic acid
138-81-8	61	2,3-diphosphoglycerate
3555-86-0	77093	phlorobenzophenone 1
1214-47-7	5367146	2-hydroxychalcone 2
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 2
124-20-9	1102	spermidine 1
469-62-5	10100	d-Propoxyphene
21339-55-9	676159	1-methyl-L-tryptophan 3
60-23-1	6058	2-aminoethanethiol 1
60-33-3	5280450	linoleic acid
621-44-3	65124	3-nitro-L-tyrosine 1
551-16-6	11082	(+)-6-aminopenicillanic acid 4
54-16-0	1826	5-hydroxyindole-3-acetic acid
73-22-3	6305	L-tryptophan 2
112-80-1	445639	oleic acid
481-39-0	3806	juglone
112-79-8	637517	elaidic acid
56-89-3	67678	L-cystine 1
0	4130574	asp-glu 2
481-06-1	221071	alpha-santonin 1
50-36-2	446220	Cocaine
693-71-0	6161490	trans-13-octadecenoic acid
53-96-3	5897	N-2-fluorenylacetamide 1
13956-29-1	644019	Cannabidiol
530-59-6	637775	3,5-dimethoxy-4-hydroxycinnamic acid 2
621-44-3	65124	3-nitro-L-tyrosine 2
525-82-6	10680	flavone
57-11-4	5281	stearic acid
41468-25-1	1051	pyridoxal 5'-phosphate 1
959-23-9	641818	4'-Methoxychalcone
60-11-7	6053	methyl yellow
298-81-7	4114	xanthotoxin 2

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CAS #	PubChem	Compound
462-20-4	421	dihydrolipoic acid
	4303260	Anhydrobrazilic Acid
124-20-9	1102	spermidine 2
481-06-1	221071	alpha-santonin 2
59-00-7	5699	4,8-dihydroxyquinoline-2-carboxylic acid (xanthurenic ac
	4303260	Anhydrobrazilic Acid 1
59-00-7	5699	xanthurenic acid
56-89-3	67678	L-cystine 2
3555-86-0	77093	phlorobenzophenone 2
10094-62-9	101713	glucoheptonic acid 3
	6708561	13-Methyl-4, 4-Bisnor-8, 11, 13-Podocarpatrien-3-One 1
129-43-1	8512	1-hydroxyanthraquinone
101-31-5	154417	L-hyoscyamine
359-83-1	441278	Pentazocine
101-31-5	3661	hyoscyamine (atropine)
	6708561	13-Methyl-4, 4-Bisnor-8, 11, 13-Podocarpatrien-3-One 2
52450-38-1	171161	N-gamma-acetyl-N-2-formyl-5-methoxykynurenamine 1
529-38-4	644006	Cocaethylene
56-89-3	67678	L-cystine 3
41468-25-1	1051	pyridoxal 5'-phosphate 2
	65161	2',3'-dideoxyuridine
577-85-5	11349	3-hydroxyflavone
519-09-5	448223	Benzoylecgonine
959-23-9	641818	4'-Methoxychalcone 1
959-23-9	641818	4'-Methoxychalcone 2
1464-44-4	65080	phenyl-beta-glucopyranoside
	1597617	(4-Hydroxy-2-oxo-1,2-dihydro-quinolin-3-yl)-acetic acid t
5626-99-3	3605363	5,6-dihydro-2'-deoxyuridine 1
7057-27-4	4085802	3'-deoxyuridine 1
5626-99-3	3605363	5,6-dihydro-2'-deoxyuridine 2
479-18-5	3182	dyphylline
56-73-5	439958	D-glucose-6-phosphate 1
5626-99-3	3605363	5,6-dihydro-2'-deoxyuridine 3
7057-27-4	4085802	3'-deoxyuridine 2
1120-28-1		Methyl Eicosanoate
7084-29-9	13845047	5-methyl-3'-deoxyuridine 1
56-73-5	439958	D-glucose-6-phosphate 2
41468-25-1	1051	pyridoxal 5'-phosphate 3
60-23-1	6058	2-aminoethanethiol 2
52450-38-1	171161	N-gamma-acetyl-N-2-formyl-5-methoxykynurenamine 2
951-78-0	13712	2-deoxyuridine 1
7084-29-9	13845047	5-methyl-3'-deoxyuridine 2
615-13-4	11983	2-indanone
2280-01-5	439917	N-acetyl-D-tryptophan 1
306-08-1	896	melatonin 1

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CAS #	PubChem	Compound
550-33-4	68368	purine riboside
52450-38-1	171161	N-gamma-acetyl-N-2-formyl-5-methoxykynurenamine 3
24607-05-4	3015189	Avocadyne
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
2280-01-5	439917	N-acetyl-D-tryptophan 2
0	4130574	asp-glu 3
306-08-1	896	melatonin2
481-05-0	65030	Artemisin
604-75-1	4616	Oxazepam
50-89-5	5789	thymidine
54965-21-8	2082	albendazole
0	4130574	asp-glu 4
646-31-1	12592	tetracosane
50-89-5	5789	thymidine
13114-27-7	449093	zeatin 1
6698-26-6	65166	2', 5'-Dideoxyadenosine
53-96-3	5897	N-2-fluorenylacetamide 2
0	4130574	asp-glu 5
63-37-6	6131	cytidine-5'-monophosphate 2
2091-39-6	5282805	eicosa-11,14-dienoic acid
1210-83-9	903	N-acetyl-5-hydroxytryptamine 1
487-90-1	1021	porphobilinogen
9/8/4350	439280	5-hydroxy-L-tryptophan 1
481-05-0	65030	Artemisin 1
608-07-1	1833	methoxytryptamine
53411-70-4	91493	6-phosphogluconic acid
306-08-1	896	melatonin 3
123-78-4	5280335	D-sphingosine 1
1/5/2280	439917	N-acetyl-D-tryptophan 3
9/8/4350	439280	5-hydroxy-L-tryptophan 2
514-10-3	10569	abietic acid
951-78-0	13712	2-deoxyuridine 2
123-78-4	5280335	D-sphingosine 2
506-30-9	10467	arachidic acid
626-72-2	439579	L-homocystine 1
58-96-8	6029	uridine
306-08-1	896	melatonin4
56-75-7	5959	chloramphenicol 1
521-35-7	2543	Cannabinol
363-24-6	62453	4-vinylphenol 2
123-78-4	5280335	D-sphingosine 3
50-67-9	5202	serotonin 1
13552-09-5	3126	DL-dihydrosphingosine 1
1812-30-2	2441	Bromazepam
22879-79-4	171548	biotin

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CAS #	PubChem	Compound
56-75-7	5959	chloramphenicol 2
303-49-1	2801	clomipramine
13552-09-5	3126	DL-dihydrosphingosine 2
65-46-3	596	cytidine 1
1210-83-9	903	N-acetyl-5-hydroxytryptamine 2
76-57-3	5284371	Codeine
16652-64-5	725701	O-benzyl-L-tyrosine 1
439-14-5	3016	Diazepam
604-75-1	4616	Oxazepam 1
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 1
1210-83-9	903	N-acetyl-5-hydroxytryptamine 3
626-72-2	439579	L-homocystine 2
50-67-9	5202	serotonin 2
404-86-4	1548943	capsaicin
13114-27-7	449093	zeatin 2
846-49-1	3958	Lorazepam
13552-09-5	3126	DL-dihydrosphingosine 3
13241-33-3	442439	neohesperidin
16652-64-5	725701	O-benzyl-L-tyrosine 2
629-98-1	5354168	cis-13-Docosanol
57-27-2	5288826	Morphine
626-72-2	439579	L-homocystine 3
466-99-9	5284570	Hydromorphone 1
	364106	4,4'-Dimethoxydalbergione 1
929-77-1		Methyl Docosanoate
658-79-7	92829	glycyl-L-tyrosine 1
	364106	4,4'-Dimethoxydalbergione 2
117-81-7	8343	dioctyl phthalate
	6728940	2,3-Dihydroxy-4-Methoxy-4'-Ethoxybenzophenone
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 2
305-84-0	9369	carnosine 1
466-99-9	5284570	Hydromorphone 2
146-22-5	4506	Nitrazepam
	688664	3,7-Dimethoxyflavone
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 3
	4000243	3,4-Didesmethyl-5-Deshydroxy-3'-Ethoxyscleroin
	6708739	2,3,4-Trihydroxy-4'-Ethoxybenzophenone
115-37-7	5324289	Thebaine
497-76-7	440936	arbutin
58-63-9	6021	inosine
76-41-5	5284604	Oxymorphone
72-48-0	6293	alizarin
62471-63-0	124925	8-oxo-2'-deoxyadenosine
554-62-1	122121	phytosphingosine 1
53-41-8	5879	androsterone

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CAS #	PubChem	Compound
	808242	3-methoxy-N-3-quinolinybenzamide 1
22316-47-8	2789	Clobazam
53-43-0	5881	trans-dehydroandrosterone 1
76-41-5	5284604	Oxymorphone 1
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
2018-66-8	74840	N- carbobenzoxy-L-leucine 3
958-09-8	13730	2'-deoxyadenosine
492-00-2	5393152	3,7-Dihydroxyflavone
554-62-1	122121	phytosphingosine 2
58-61-7	60961	adenosine
846-50-4	5391	Temazepam
131-48-6	445063	n-acetylneuraminic acid 1
4618-18-2	11333	lactulose 1
302-79-4	444795	retinoic acid
2140-79-6	317398	2-O-Methyladenosine
658-79-7	92829	glycyl-L-tyrosine 2
112-85-6	8215	behenic acid
521-18-6	10635	dihydrotestosterone 1
1086-80-2	5326566	7,8-dimethylalloxazine
53-43-0	5881	trans-dehydroandrosterone 2
42366-37-0	242332	5-alpha-androstane-3 beta,17 beta-diol
111-11-5	5988	Sucrose
0	242332	5alpha-androstane-3beta,17beta-diol
521-18-6	10635	dihydrotestosterone 2
10417-94-4	446284	eicosapentaenoic acid
19408-84-5	107982	dihydrocapsaicin
1622-62-4	3380	Flunitrazepam
1229-12-5	440114	5beta-androstane-3,17-dione
131-48-6	445063	n-acetylneuraminic acid 2
146-80-5	1189	xanthosine
846-46-8	439289	5alpha-Androstan-3, 17-Dione 1
	6708683	3-Deshydroxysappanol Trimethyl Ether
1622-61-3	2802	Clonazepam
2955-38-6	4890	Prazepam
50-28-2	5757	estradiol
846-46-8	439289	5alpha-Androstan-3, 17-Dione 2
593-49-7	11636	heptacosane
63-42-3	84571	lactose 1
53-16-7	5870	1,3,5(10)-estratrien-3-ol-17-one 1
53-16-7	5870	estrone 1
4618-18-2	11333	lactulose 3
4618-18-2	11333	lactulose 2
528-50-7	10712	cellobiose 1
501-36-0	445154	trans- resveratrol
53-16-7	5870	1,3,5(10)-estratrien-3-ol-17-one 2

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CAS #	PubChem	Compound
53-16-7	5870	estrone 2
501-36-0	445154	resveratrol
488-69-7	10267	fructose-1,6-diphosphate 1
60-82-2	4788	phloretin
63-42-3	84571	lactose 2
71-44-3	1103	spermine 2
897-06-3	6710699	Androsta-1, 4-Dien-3, 17-Dione 1
488-69-7	10267	fructose-1,6-diphosphate 2
897-06-3	6710699	Androsta-1, 4-Dien-3, 17-Dione 2
96-82-2	16219560	lactobionic acid 1
6889-80-1	97143	3-Hydroxy-3',4'-Dimethoxyflavone
6342-92-3	5355888	2',5'-Dihydroxy-4-Methoxychalcone
2442-49-1		Methyl Linocerate
53-43-0	6013	testosterone 2
53-43-0	6013	testosterone 1
		trans coutaric acid
2457-80-9	439176	5'-deoxy-5'-(methylthio)adenosine 1
305-84-0	9369	carnosine 2
63-05-8	6128	4-androsten-3,17-dione 1
62-84-0	65542	4-androsten-7-alpha-ol-3,17-dione 1
79786-40-6	676293	6,3'-Dimethoxyflavone
528-50-7	10712	cellobiose 2
69-79-4	6255	maltose 1
15763-06-1	16219662	1-methyladenosine 1
480-40-0	5281607	chrysin
578-86-9	1889	liquiritigenin 1
63-05-8	6128	4-androsten-3,17-dione 2
111-03-5	5283468	1 monoolein
118-00-3	6802	guanosine 1
6138-23-4	7427	D-(+) trehalose
64280-14-4	107885	(+/-)-11-nor-9-carboxy-delta-9-THC Standard
71-44-3	1103	spermine 1
35323-91-2	72276	(-)-epicatechin
3443-84-3	5319879	2-oleoylglycerol
35323-91-2	72276	epicatechin 1
547-25-1	5460935	turanose 1
5894-59-7	3294434	digalacturonic acid 1
62-84-0	65542	4-androsten-7-alpha-ol-3,17-dione 2
38183-03-8	1880	7,8-Dihydroxyflavone
118-00-3	6802	guanosine 2
96-82-2	91476	lactitol
15763-06-1	16219662	1-methyladenosine 2
96-82-2	16219560	lactobionic acid 2
0-00-0	440168	1,3,5(10)-estratrien-3,6- beta-17-beta-triol
123-94-4	24699	1 monostearin

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CAS #	PubChem	Compound
5894-59-7	3294434	digalacturonic acid 2
123-94-4	24699	1-stearoyl-rac-glycerol
69-79-4	6255	maltose 2
94-62-2	638024	piperine 1
35850-13-6	5280887	15-keto-prostaglandin F2alpha
534-46-3	4623424	sophorose 1
961-07-9	187790	2'-deoxyguanosine
578-86-9	1889	liquiritigenin 2
35850-13-6	5280887	15-keto-prostaglandin F-2-alpha
7158-70-5	165577	leucrose
2457-80-9	439176	5'-deoxy-5'-(methylthio)adenosine 2
53-06-5	222786	cortisone
547-25-1	5460935	turanose 2
578-86-9	1889	liquiritigenin 3
65-46-3	596	cytidine 2
42155-08-8	18601100	2'-Deoxyuridine 5'-monophosphate 1
534-46-3	4623424	sophorose 2
17617-23-1	3393	Flurazepam
5996-00-9	441422	beta-gentiobiose 1
111-02-4	5280370	squalene
	4620898	12a-Hydroxy-6-Deoxydehydromunduserone
585-88-6	16217663	maltitol
382-45-6	223997	adrenosterone 1
96-82-2	16219560	lactobionic acid 3
67879-58-7	642609	trans caftaric acid 1
362-06-1	440623	2-hydroxyestrone 1
5996-00-9	441422	beta-gentiobiose 2
3387-36-8	6030	uridine 5'-monophosphate 1
362-06-1	440623	2-hydroxyestrone 2
	641605	trans fertaric acid
35323-91-2	72276	(-)-epicatechin
13718-94-2	439559	palatinose
365-07-1	1139	thymidine 5'-phosphate 1
35323-91-2	72276	epicatechin 2
0	194988	glycyl-tyrosyl-alanine 1
382-45-6	223997	adrenosterone 2
67879-58-7	642609	trans caftaric acid 2
66009-10-7	440658	melibiose 1
5894-59-7	3294434	digalacturonic acid 3
18829-70-4	73160	catechin
10083-24-6	667639	piceatannol
42155-08-8	18601100	2'-Deoxyuridine 5'-monophosphate 2
499-40-1	439193	isomaltose 1
154-23-4	9064	catechin
3387-36-8	6030	uridine 5'-monophosphate 2

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CAS #	PubChem	Compound
547-96-6	160520	5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol 1
50-27-1	5756	estriol
5894-59-7	3294434	digalacturonic acid 4
66009-10-7	440658	melibiose 2
630-03-5	12409	nonacosane
365-07-1	1139	thymidine 5'-phosphate 2
499-40-1	439193	isomaltose 2
566-65-4	92810	5-alpha-pregnan-3,20-dione 1
552-59-0	5281804	prunetin
0	194988	glycyl-tyrosyl-alanine 2
3371-27-5	9882981	gallocatechin
585-88-6	3034828	palatinitol 1
	5781145	2'-Methoxyformonetin
0	194988	glycyl-tyrosyl-alanine 3
566-65-4	92810	5-alpha-pregnan-3,20-dione 2
18524-94-2	16212335	loganin
486-66-8	5281708	daidzein
64519-82-0	3034828	palatinitol 2
	808242	3-methoxy-N-3-quinolinybenzamide 2
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 1
5802-82-4		Methyl Hexacosanoate
94-62-2	638024	piperine 2
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 2
41001-90-5	3593	hesperetin 1
3687-64-7	439451	galactinol 1
446-72-0	5280961	4',5,7-trihydroxyisoflavone
41001-90-5	3593	hesperetin 2
480-18-2	439533	taxifolin
585-18-2	439762	sucrose-6-phosphate 1
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 3
130-49-4	94136	adenosine 2'-monophosphate
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 4
699012-36-7	41211	adenosine-3'-monophosphate
38186-71-9	5379071	2',3-Dihydroxy-4,4',6'-Trimethoxychalcone
327-97-9	6537496	chlorogenic acid 1
63046-09-3	182362	6,4'-Dihydroxyflavone
131-99-7	797	inosine 5'-monophosphate
3687-64-7	439451	galactinol 2
68-42-8	65553	tetrahydrocorticosterone 1
67-97-0	5280795	cholecalciferol 1
69616-74-6	5955473	2',4-Dihydroxy-3,4',6'-Trimethoxychalcone
585-18-2	439762	sucrose-6-phosphate 2
41001-90-5	3593	hesperetin 3
2196-14-7	5282073	7,4'-Dihydroxyflavone
480-44-4	5280442	Acacetin 1

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CAS #	PubChem	Compound
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 1
	4646739	12a-Hydroxy-9-Demethylmunduserone-8-Carboxylic Aci
84-21-9	224	adenosine-5-monophosphate 1
520-18-3	5280863	kaempferol 1
56-65-5	5957	adenosine 5'-triphosphate
20398-34-9	6022	adenosine 5'-diphosphate
84-21-9	224	adenosine-5-monophosphate 2
4423-37-4	5281953	syringetin
53472-37-0	5282154	laricitrin
68-42-8	65553	tetrahydrocorticosterone 2
520-18-3	5280863	kaempferol 2
72003-83-9	188966	2' Deoxyadenosine 5'-diphosphate
2268-98-6	519975	11a-Acetoxyprogesterone 1
68-42-8	65553	tetrahydrocorticosterone 3
0	194988	glycyl-tyrosyl-alanine 4
653-63-4	621	2'-deoxyadenosine 5'-monophosphate
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 2
60-92-4	6076	adenosine 3',5'-cyclic monophosphate
2268-98-6	519975	11a-Acetoxyprogesterone 2
60-92-4	6076	cyclic AMP
6025-53-2	6440982	trans-Zeatin-riboside
327-97-9	6537496	chlorogenic acid 2
566-78-9	11276	21-Acetoxypregnenolone
28911-01-5	5556	Triazolam
520-36-5	5280443	Apigenin
566-26-7	107722	5-cholesten-3-beta-7-alpha-diol
5550-12-9	6804	guanosine-5'-monophosphate
55682-92-3		Methyl Octacosanoate
10191-41-0	2116	alpha tocophereol
547-96-6	160520	5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol 2
80-97-7	6665	5alpha-Cholestanol
4472-73-5	521171	3,4',5,6,7-Pentamethoxyflavone
133-05-1	101612	Asarinin (-)
67-97-0	5280795	cholecalciferol 2
68-42-8	65553	tetrahydrocorticosterone 4
1731-84-6	16213400	Cholestrol D6
57-88-5	304	cholesterol
93839-95-3	188955	2'-Deoxyadenosine 3' :5'-cyclic monophosphate
80-97-7	3240	5alpha-Cholestan-3-beta-ol
21637-25-2	5280804	isoquercitrin 1
7665-99-8	295	cyclic GMP
601-53-6	85881	coprostan-3-one
4484-88-2	122336	trehalose-6-phosphate
561-63-7	6453303	19-hydroxycholesterol
529-44-2	5281672	myricetin

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CAS #	PubChem	Compound
566-88-1	92128	5alpha-cholestan-3-one 1
57-87-4	444679	ergosterol
566-88-1	92128	5alpha-cholestan-3-one 2
601-57-0	91477	(+) -4-cholesten-3-one 1
601-57-0	91477	(+) -4-cholesten-3-one 2
17954-98-2	167685	22-hydroxycholesterol
110-15-6	5321515	stigmaterol
476-66-4	5281855	ellagic acid
123316-61-0		5-Hydroxy-2',4',7,8-Tetramethoxyflavone
79-36-0	440560	dihydrolanosterol
516-72-3	121935	20-hydroxycholesterol 1
1175-06-0	16219541	5alpha-Cholestan-3beta-OI-6-One 1
	6728949	3beta-Hydroxy-23, 24-Bisnorchol-5-Enic Acid
516-72-3	121935	20-hydroxycholesterol 2
629-83-4		Methyl Triacontanoate
83-46-5	5321342	beta-sitosterol
79-36-0	246983	lanosterol
566-28-9	91474	7-Oxocholesterol
10410-83-0	99980	Anthothecol
10236-47-2	25075	naringin
14167-59-0	26519	tetratriacontane
1175-06-0	16219541	5alpha-Cholestan-3beta-OI-6-One 2
470-69-9	440080	kestose
1109-28-0	192826	maltotriose 1
17629-30-0	439242	Raffinose
6906-39-4	443654	peonidin-3-glucoside
2140-46-7	65094	25-hydroxycholesterol
7228-78-6	443652	malvidin-3-glucoside
10030-67-8	92817	melezitose
6988-81-4	443651	petunidin-3-glucoside
10030-67-8	92817	D-(+)-melezitose
79-57-2	5280972	oxytetracycline
82950-64-9	1321	1,2-didecanoylglyceride
6906-38-3	443650	delphinidin 3-glucoside
38819-01-1	439626	cellotetraose
1109-28-0	192826	maltotriose 2
6906-38-3	443650	delphinidin 3-glucoside 2
32860-62-1	3625615	maltotriitol
27208-80-6	12314237	trans piceid
21637-25-2	5280804	isoquercitrin 2
3681-93-4	5280441	vitexin 1
5041-82-7	5318644	isorhamnetin-3--glucoside
3681-93-4	5280441	vitexin 2
6906-38-3	443650	delphinidin 3-glucoside 3
6906-39-4	443654	peonidin-3-glucoside 2

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CAS #	PubChem	Compound
989-51-5	1287	epigallocatechin gallate
970-74-1	72277	epigallocatechin
6988-81-4	443651	petunidin-3-glucoside 2
130405-40-2	6419835	catechin gallate
681295-24-9	66868	porphine 2
0	122281	16-glucuronide-estriol
1180-71-8	16219587	limonin

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CAS #	PubChem	Compound
0		L-glutamic acid-2,3,3,4,4-d5 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	443239	DL-threo-beta-hydroxyaspartic acid
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 1
0	16213445	L-tyrosine-3,3-d2 1
0	16217112	D-glucose-C-d7 1
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 2
0	5459862	D-erythrose-4-phosphate 1
0	5459862	D-erythrose-4-phosphate 2
0	16217112	D-glucose-C-d7 2
0	16213445	L-tyrosine-3,3-d2 2
0	439232	N-acetyl-ornithine 1
0	439232	N-acetyl-ornithine 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
0	242332	5alpha-androstane-3beta,17beta-diol
0	194988	glycyl-tyrosyl-alanine 1
0	194988	glycyl-tyrosyl-alanine 2
0	194988	glycyl-tyrosyl-alanine 3
0	194988	glycyl-tyrosyl-alanine 4
0	122281	16-glucuronide-estriol
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
	5176389	3,7-Epoxycaryophyllan-6-Ol
	5024745	2-Hydroxy-5 (6)Epoxy-Tetrahydrocaryophyllene
		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
	9925625	propofol hemisuccinate
	4303260	Anhydrobrazilic Acid
	4303260	Anhydrobrazilic Acid 1
	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
	65161	2',3'-dideoxyuridine
	1597617	(4-Hydroxy-2-oxo-1,2-dihydro-quinolin-3-yl)-acetic acid t
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 1
	364106	4,4'-Dimethoxydalbergione 1
	364106	4,4'-Dimethoxydalbergione 2
	6728940	2,3-Dihydroxy-4-Methoxy-4'-Ethoxybenzophenone

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CAS #	PubChem	Compound
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 2
	688664	3,7-Dimethoxyflavone
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 3
	4000243	3,4-Didesmethyl-5-Deshydroxy-3'-Ethoxyscleroin
	6708739	2,3,4-Trihydroxy-4'-Ethoxybenzophenone
	808242	3-methoxy-N-3-quinolinylbenzamide 1
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
	6708683	3-Deshydroxysappanol Trimethyl Ether
		trans coutaric acid
	4620898	12a-Hydroxy-6-Deoxydehydromunduserone
	641605	trans fertaric acid
	5781145	2'-Methoxyformonetin
	808242	3-methoxy-N-3-quinolinylbenzamide 2
	4646739	12a-Hydroxy-9-Demethylmunduserone-8-Carboxylic Aci
	6728949	3beta-Hydroxy-23, 24-Bisnorchol-5-Enic Acid
0-00-0	440168	1,3,5(10)-estratrien-3,6- beta-17-beta-triol
1/5/2280	439917	N-acetyl-D-tryptophan 3
100-02-7	980	4-nitrophenol
100-09-4	7478	p-anisic acid
1002-57-9	66085	8-aminocaprylic acid
10030-67-8	92817	melezitose
10030-67-8	92817	D-(+)-melezitose
100-46-9	7504	benzylamine
100-51-6	244	benzyl alcohol
100-52-7	240	benzaldehyde
100-61-8	5288725	N-methylalanine
10083-24-6	667639	piceatannol
100-83-4	101	3-hydroxybenzaldehyde
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
10094-62-9	101713	glucoheptonic acid 1
10094-62-9	101713	glucoheptonic acid 2
10094-62-9	101713	glucoheptonic acid 3
101-31-5	154417	L-hyoscyamine
101-31-5	3661	hyoscyamine (atropine)
10191-41-0	2116	alpha tocophereol
102-32-9	547	2-(3,4-dihydroxyphenyl)acetic acid
102-32-9	547	3,4-dihydroxyphenylacetic acid
10236-47-2	25075	naringin
102-71-6	7618	triethanolamine
102916-66-5	25245723	2-deoxyribose 5-phosphate
10323-20-3	66308	arabinose
103-26-4	637520	methyl cinnamate
1032-65-1	13945	2'-deoxycytidine 5'-monophosphoric acid
103-81-1	7680	2-phenylacetamide 1

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CAS #	PubChem	Compound
103-81-1	7680	2-phenylacetamide 2
103-81-1	7680	2-phenylacetamide 3
103-84-4	904	acetanilide 1
103-84-4	904	acetanilide 2
10410-83-0	99980	Anthothecol
10417-94-4	446284	eicosapentaenoic acid
104-51-8	7705	butylbenzene
104-55-2	637511	cinnamaldehyde 1
104-55-2	637511	cinnamaldehyde 2
104-76-7	7720	2-ethyl-1-hexanol
10482-56-1	17100	terpineol
104-98-3	1178	urocanic acid 1
104-98-3	1178	urocanic acid 2
105-60-2	7768	epsilon-caprolactam
10569-71-9	64956	DL-3-aminoisobutyric acid 1
10569-71-9	64956	DL-3-aminoisobutyric acid 2
106-24-1	637566	geraniol
106-24-1	637566	geraniol
106-28-5	445070	trans-trans-farnesol
106-32-1	7799	ethyl octanoate
106-33-2	7800	ethyl dodecanoate
106-51-4	4650	p-benzoquinone
106-57-0	7817	glycine anhydride 1
106-57-0	7817	glycine anhydride 2
1071-23-4	1015	O-phosphocolamine
107-35-7	1123	taurine
107-95-9	239	Beta- alanine 1
107-95-9	239	Beta- alanine 2
107-97-1	1088	sarcosine
1080-06-4	70652	tyrosine methyl ester 1
1080-06-4	70652	tyrosine methyl ester 2
108-13-4	7911	malonamide 1
108-13-4	7911	malonamide 2
108-13-4	7911	malonamide 3
108-19-0	7913	biuret 1
108-19-0	7913	biuret 2
108321-99-9	439184	ribulose-5-phosphate 3
108-39-4	342	m-cresol
108-46-3	5054	resorcinol
1086-80-2	5326566	7,8-dimethylalloxazine
108-73-6	359	phloroglucinol
108-91-8	7965	cyclohexanamine
109-00-2	7971	3-hydroxypyridine
109-76-2	428	1,3-diaminopropane 1
109-76-2	428	1,3-diaminopropane 2

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CAS #	PubChem	Compound
110-15-6	5321515	stigmasterol
110-16-7	444266	maleic acid
110-42-9		Methyl Caprate
110-60-1	1045	putrescine
110-65-6	8066	2-butyne-1,4-diol
1109-28-0	192826	maltotriose 1
1109-28-0	192826	maltotriose 2
110-93-0	9862	6-methyl-5-hepten-2-one
110-94-1	743	glutaric acid
111-02-4	5280370	squalene
111-03-5	5283468	1 monoolein
111-11-5		Methyl Caprylate
111-11-5	5988	Sucrose
111-14-8	8094	heptanoic acid
111-16-0	385	pimelic acid
1114-34-7	65550	D-lyxose 1
1114-34-7	439240	D-lyxose 1
1114-34-7	65550	D-lyxose 2
1114-34-7	439240	D-lyxose 2
1114-81-4	3246323	O-phospho-L-threonine 1
1114-81-4	3246323	O-phospho-L-threonine 2
111-82-0		Methyl Laurate
1118-68-9	673	N,N-dimethylglycine
111-87-5	957	1-octanol
1120-25-8	643801	methyl palmitoleate
1120-28-1		Methyl Eicosanoate
112-05-0	8158	pelargonic acid (nonanoic acid)
112-12-9	8163	2-undecanone 1
112-12-9	8163	2-undecanone 2
112-30-1	8174	1-decanol (decyl alcohol)
112-39-0		Methyl Palmitate
112-61-8		Methyl Stearate
112-62-9	5364509	methyl oleate
112-79-8	637517	elaidic acid
112-80-1	445639	oleic acid
1128-23-0	608	L-galactono-gamma-lactone 1
1128-23-0	439373	L-gulonic acid gamma-lactone
1128-23-0	608	L-galactono-gamma-lactone 2
112-85-6	8215	behenic acid
112-88-9	8217	1-octadecene
112-95-8	8222	eicosane
1133-63-7	254	2,3-dihydroxybiphenyl
1135-24-6	445858	ferulic acid
113573-73-2	440053	S(-)willardiine 1
113573-73-2	440053	S(-)willardiine 2

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CAS #	PubChem	Compound
1138-80-3	14349	N-benzyloxycarbonylglycine
114-63-6	135	4-hydroxybenzoic acid
115-37-7	5324289	Thebaine
115-38-8	8271	Mephobarbital
115-44-6	8275	Talbutal
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 1
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 2
116-09-6	8299	acetol 1
116-09-6	8299	acetol 2
116-09-6	8299	acetol 3
116-09-6	8299	acetol 4
1175-06-0	16219541	5alpha-Cholestan-3beta-OI-6-One 1
1175-06-0	16219541	5alpha-Cholestan-3beta-OI-6-One 2
117-81-7	8343	dioctyl phthalate
118-00-3	6802	guanosine 1
118-00-3	6802	guanosine 2
1180-71-8	16219587	limonin
118-74-1	8370	hexachlorobenzene
1188-21-2	1995	N-acetyl-L-leucine
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
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
1191-25-9	14490	6-hydroxyhexanoic acid
1191-25-9	14490	6-hydroxy caproic acid
1194-98-5	70949	2,5-dihydroxybenzaldehyde
119-53-9	8400	benzoin 1
119-53-9	8400	benzoin 2
119-67-5	8406	2-carboxybenzaldehyde 1
119-67-5	8406	2-carboxybenzaldehyde 2
119-68-6	67069	N-methylantranilic acid 1
119-68-6	67069	N-methylantranilic acid 2
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
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic acid
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic acid
120-14-9	8419	3,4-dimethoxybenzaldehyde
120-80-9	289	catechol

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CAS #	PubChem	Compound
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
1211-29-6	62388	methyljasmonate 1
1211-29-6	62388	methyljasmonate 1
1211-29-6	62388	methyljasmonate 2
1211-29-6	62388	methyljasmonate 3
1211-29-6	62388	methyljasmonate 2
1211-29-6	62388	methyljasmonate 4
121-33-5	1183	vanillin
121-34-6	8468	4-hydroxy-3-methoxybenzoic acid
1214-20-6	71034	2-Methoxyxanthone
1214-47-7	5367146	2-hydroxychalcone 1
1214-47-7	5367146	2-hydroxychalcone 2
122-03-2	326	4-isopropylbenzaldehyde
122-09-8	4771	Phentermine 1
122-09-8	4771	Phentermine 2
122-78-1	998	phenylacetaldehyde 1
122-78-1	998	phenylacetaldehyde 2
1229-12-5	440114	5beta-androstane-3,17-dione
123-08-0	126	4-hydroxybenzaldehyde 1
123-08-0	126	4-hydroxybenzaldehyde 2
123-30-8	403	4-aminophenol 1
123-30-8	403	4-aminophenol 2
123-30-8	403	4-aminophenol 3
123316-61-0		5-Hydroxy-2',4',7,8-Tetramethoxyflavone
123-31-9	785	hydroquinone
123-31-9	785	benzoquinone
123-35-3	31253	beta-myrcene
123-78-4	5280335	D-sphingosine 1
123-78-4	5280335	D-sphingosine 2
123-78-4	5280335	D-sphingosine 3
123-94-4	24699	1 monostearin
123-94-4	24699	1-stearoyl-rac-glycerol
123-99-9	2266	azelaic acid
124-04-9	196	adipic acid
124-07-2	379	caprylic acid
124-10-7		Methyl Myristate
124-20-9	1102	spermidine 1
124-20-9	1102	spermidine 2
125-64-4	4162	Methyprylon
127-07-1	3657	hydroxyurea
127-17-3	1060	pyruvic acid
128-37-0	31404	2,6-ditert-butyl-4-methylphenol 1
128-37-0	31404	2,6-ditert-butyl-4-methylphenol 2

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CAS #	PubChem	Compound
128-37-0	31404	3,5-Di-tert-butyl-4-hydroxytoluene
129-43-1	8512	1-hydroxyanthraquinone
13022-85-0	159664	2-ketocaproic acid
13022-85-0	18407	4-acetylbutyric acid 1
13022-85-0	18407	4-acetylbutyric acid 2
13031-04-4	39	dihydro-4,4-dimethyl-2,3-furandione 1
13031-04-4	39	dihydro-4,4-dimethyl-2,3-furandione 2
130405-40-2	6419835	catechin gallate
130-49-4	94136	adenosine 2'-monophosphate
13114-27-7	449093	zeatin 1
13114-27-7	449093	zeatin 2
131-48-6	445063	n-acetylneuraminic acid 1
131-48-6	445063	n-acetylneuraminic acid 2
131-99-7	797	inosine 5'-monophosphate
13241-33-3	442439	neohesperidin
132-64-9	568	dibenzofuran
133-05-1	101612	Asarinin (-)
133-37-9	444305	tartaric acid
13382-27-9	128869	galactonic acid 1
13382-27-9	128869	galactonic acid 2
13419-69-7	5282707	2-hexenoic acid
134-49-6	4762	Phenmetrazine
13545-04-5	11848	2,3-dimethylsuccinic acid
13552-09-5	3126	DL-dihydrosphingosine 1
13552-09-5	3126	DL-dihydrosphingosine 2
13552-09-5	3126	DL-dihydrosphingosine 3
137-00-8	1136	4-methyl-5-thiazoleethanol
137-08-6	6613	pantothenic acid 1
137-08-6	6613	pantothenic acid 2
13718-94-2	439559	palatinose
138-08-9	1005	phosphoenolpyruvic acid
138-59-0	8742	shikimic acid
138-81-8	61	2,3-diphosphoglycerate
13956-29-1	644019	Cannabidiol
140-10-3	444539	cinnamic acid
1401-55-4	16133892	tannic acid
141-12-8	1549026	neryl acetate 1
141-12-8	1549026	neryl acetate 2
141-43-5	700	ethanolamine
14167-59-0	26519	tetratriacontane
141-82-2	867	malonic acid 1
141-82-2	867	malonic acid 2
14191-95-8	26548	4-hydroxybenzyl cyanide
141-97-9	96	acetoacetate 1
141-97-9	96	acetoacetate 2

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CAS #	PubChem	Compound
142-08-5	8871	2-hydroxypyridine
142-62-1	8892	hexanoic acid
142-73-4	8897	iminodiacetic acid 1
142-73-4	8897	iminodiacetic acid 2
143-07-7	3893	lauric acid
143-08-8	8914	1-nonanol
144-62-7	971	oxalic acid
14528-64-4	3505109	4-nitrocatechol
1460-57-7	92886	trans-cyclohexane-1,2-diol
146-22-5	4506	Nitrazepam
146255-66-5	443586	3,5-dihydroxyphenylglycine 1
146255-66-5	443586	3,5-dihydroxyphenylglycine 2
1464-44-4	65080	phenyl-beta-glucopyranoside
146-80-5	1189	xanthosine
14721-66-5	26840	phytanic acid
14769-73-4	26879	levamisole
147-85-3	145742	L-proline 1
147-85-3	614	L-proline 1
147-85-3	145742	L-proline 2
147-85-3	614	L-proline 2
14838-15-4	26934	1R, 2S-Phenylpropylamine
14883-87-5	85782	3,4-dihydroxymandelic acid
14901-07-6	638014	beta-ionone 1
14901-07-6	638014	beta-ionone 2
1492-23-5	954	O-succinylhomoserine 1
1492-23-5	954	O-succinylhomoserine 2
149-57-5	8697	2-ethylhexanoic acid
149-57-5	8697	2-ethylhexanoic acid
149-57-5	8697	2-ethylcaproic acid
14982-50-4	445929	galacturonic acid 1
14982-50-4	439215	galacturonic acid 1
14982-50-4	445929	galacturonic acid 2
14982-50-4	439215	galacturonic acid 2
149-91-7	370	gallic acid
150-13-0	978	4-aminobenzoic acid
1504-06-9	150923	3-methoxyindole 1
1504-06-9	150923	3-methoxyindole 2
1504-06-9	150923	3-methoxyindole 3
1504-06-9	150923	3-methoxyindole 4
151-18-8	1647	3-aminopropionitrile 1
151-18-8	1647	3-aminopropionitrile 2
154-17-6	439268	deoxyglucose 1
154-17-6	439268	deoxyglucose 2
154-23-4	9064	catechin
154-41-6	441457	Phenylpropanolamine

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CAS #	PubChem	Compound
15450-76-7	97250	2,8-quinolinediol
154-58-5	64960	1,5-anhydroglucitol
154-58-5	219984	1,5-anhydro-D-sorbitol
156-06-9	997	phenylpyruvate
156-08-1	2341	Benzphetamine
156-38-7	127	4-hydroxyphenylacetic acid
156-39-8	979	4-hydroxyphenylpyruvic acid 1
156-39-8	979	4-hydroxyphenylpyruvic acid 2
15673-79-7	439167	D-ribose-5-phosphate 1
15673-79-7	439167	D-ribose-5-phosphate 2
1569-60-4	20745	6-methyl-5-hepten-2-ol
15763-06-1	16219662	1-methyladenosine 1
15763-06-1	16219662	1-methyladenosine 2
16096-97-2	439196	L-dithiothreitol 1
16096-97-2	439196	L-dithiothreitol 2
161886-59-5	11058264	(S)-Carnitine Mesylate Isobutylester
1622-61-3	2802	Clonazepam
1622-62-4	3380	Flunitrazepam
1637-73-6	1198	isocitric acid
16652-64-5	725701	O-benzyl-L-tyrosine 1
16652-64-5	725701	O-benzyl-L-tyrosine 2
1679-53-4	74300	10-hydroxydecanoic acid
16834-13-2	86073	5,10,15,20-tetra(4-pyridyl)-21H,23H-porphine
16867-04-2	28115	2,3-dihydroxypyridine
1689-64-1	74318	9-hydroxyfluorene
17013-01-3	444972	fumaric acid
17199-29-0	439616	mandelic acid
1731-84-6		Methyl Pelargonate
1731-84-6	16213400	Cholesterol D6
1731-92-6	15609	methyl heptadecanoate
17617-23-1	3393	Flurazepam
17629-30-0	439242	Raffinose
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
1792-81-0	92903	cis-1,2-cyclohexanediol
17954-98-2	167685	22-hydroxycholesterol
1812-30-2	2441	Bromazepam
1821-52-9	92904	3-indolelactic acid 1
1821-52-9	92904	3-indolelactic acid 2
1824-94-8	94214	methyl-beta-D-galactopyranoside
18457-55-1	369312	(-)-perillyl alcohol
18524-94-2	16212335	loganin

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CAS #	PubChem	Compound
18652-93-2	9034	Methohexital
186537-58-6	193653	S-carboxymethylcysteine 1
186537-58-6	193653	S-carboxymethylcysteine 2
18829-70-4	73160	catechin
19246-18-5	65270	cysteinylglycine 1
19246-18-5	65270	cysteinylglycine 2
19246-18-5	65270	cysteinylglycine 3
19253-88-4	159660	trimethyllysine
19317-11-4	5280598	farnesal 1
19317-11-4	5280598	farnesal 2
19317-11-4	5280598	farnesal 3
19317-11-4	5280598	farnesal 4
19408-84-5	107982	dihydrocapsaicin
1946-82-3	92907	N-alpha-acetyl-L-lysine 1
1946-82-3	92907	N-alpha-acetyl-L-lysine 2
1990-29-0	441032	D (+)altrose 1
1990-29-0	441032	D (+)altrose 2
2018-61-3	74839	N-acetyl-L-phenylalanine 1
2018-61-3	74839	N-acetyl-L-phenylalanine 2
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
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
20398-34-9	6022	adenosine 5'-diphosphate
2041-14-7	339	ciliatine
2043-43-8	94220	lactamide 1
2043-43-8	94220	lactamide 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
20549-47-7	443163	(-)-dihydrocarveol 1
20549-47-7	443163	(-)-dihydrocarveol 2
2078-54-8	4943	propofol
2091-39-6	5282805	eicosa-11,14-dienoic acid
2107-77-9	5355836	4-Methyldaphnetin
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
2140-46-7	65094	25-hydroxycholesterol
2140-79-6	317398	2-O-Methyladenosine
2152-75-2	740	alpha-D-glucosamine 1-phosphate
2152-75-2	740	alpha-D-glucosamine phosphate

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CAS #	PubChem	Compound
2152-75-2	740	alpha-glucosamine 1-phosphate
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 1
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 2
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
21637-25-2	5280804	isoquercitrin 1
21637-25-2	5280804	isoquercitrin 2
21784-30-5	12460	Phendimetrazine
21784-30-5	12460	Phendimetrazine 1
2196-14-7	5282073	7,4'-Dihydroxyflavone
22059-21-8	535	1-aminocyclopropane-1-carboxylic acid
22316-47-8	2789	Clobazam
225101-69-9	12205373	L-alanine-2,3,3,3-d4
2268-98-6	519975	11a-Acetoxyprogesterone 1
2268-98-6	519975	11a-Acetoxyprogesterone 2
2280-01-5	439917	N-acetyl-D-tryptophan 1
2280-01-5	439917	N-acetyl-D-tryptophan 2
22818-40-2	36143	4-hydroxyphenylglycine 1
22818-40-2	36143	4-hydroxyphenylglycine 2
22862-76-6	31549	Anisomycin
22879-79-4	171548	biotin
2316-26-9	717531	3,4-Dimethoxycinnamic Acid 1
2316-26-9	717531	3,4-Dimethoxycinnamic 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
23945-44-0	90301	2,4-dihydroxypyrimidine-5-carboxylic acid
24259-59-4	993	ribose
2438-80-4	17106	L-(-)-fucose 1
2438-80-4	17106	L-(-)-fucose 2
2442-49-1		Methyl Linocerate
2457-80-9	439176	5'-deoxy-5'-(methylthio)adenosine 1
2457-80-9	439176	5'-deoxy-5'-(methylthio)adenosine 2
24607-05-4	3015189	Avocadyne
2478-38-8	17198	Acetosyringone 1
2478-38-8	17198	Acetosyringone 2
24940-57-6	440274	N,N-dimethyl-L-histidine
2497-02-1	273260	N-acetyl-L-histidine 1
2497-02-1	273260	N-acetyl-L-histidine 2
2595-98-4	441035	talose 1
2595-98-4	441035	talose 2
26016-99-9	3417	phosphonomycin

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CAS #	PubChem	Compound
27208-80-6	12314237	trans piceid
2734-48-7	151491	3-(1-pyrazolyl)-L-alanine
2875-41-4	10034670	N-(3-Aminopropyl)glycine 1
2875-41-4	10034670	N-(3-Aminopropyl)glycine 2
28822-73-3	91528	DL-3,4-dihydroxyphenyl glycol
28911-01-5	5556	Triazolam
28954-12-3	99289	L-allothreonine 1
28954-12-3	99289	L-allothreonine 2
2922-42-1	80	3-dehydroshikimic acid 1
2922-42-1	80	3-dehydroshikimic acid 2
2922-83-0	161166	L-kynurenine 1
2922-83-0	161166	L-kynurenine 2
29267-67-2	121805	2-Methoxyresorcinol
2955-38-6	4890	Prazepam
298-12-4	760	glyoxylic acid
298-81-7	4114	xanthotoxin 1
298-81-7	4114	xanthotoxin 2
29915-38-6	1110	succinic acid
300-84-5	107812	hypotaurine
301-00-8	9316	methyl linolenate
3012-37-1	18170	benzyl thiocyanate
3025-96-5	18189	4-acetamidobutyric acid 1
3025-96-5	18189	4-acetamidobutyric acid 2
302-79-4	444795	retinoic acid
303-49-1	2801	clomipramine
305-84-0	9369	carnosine 1
305-84-0	9369	carnosine 2
306-08-1	1738	homovanillic acid (HVA)
306-08-1	896	melatonin 1
306-08-1	896	melatonin2
306-08-1	896	melatonin 3
306-08-1	896	melatonin4
306-23-0	9378	3-(4-hydroxyphenyl)lactic acid
3068-00-6	18302	butantriol
3081-61-6	228398	L-theanine 1
3081-61-6	228398	L-theanine 2
3106-60-3	457	1-methyl nicotinamide 1
3106-60-3	457	1-methyl nicotinamide 2
311-45-5	9395	paraoxon
3128-06-1	26447	L-menthone
31519-22-9	671	1,4-dihydroxy-2-naphthoic acid
3177-80-8	255720	2-amino-3-methoxybenzoic acid 1
3177-80-8	255720	2-amino-3-methoxybenzoic acid 2
3206-73-3	863	lipoamide 1
3206-73-3	863	lipoamide 2

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CAS #	PubChem	Compound
3206-73-3	863	lipoamide 3
3226-65-1	158980	L-methionine sulfoxide 1
3226-65-1	158980	L-methionine sulfoxide 2
3226-65-1	158980	L-methionine sulfoxide 3
3233-32-7	96009	4-Acetoxyphenol
3233-32-7	96009	4-Acetoxyphenol 1
3237-44-3	36	2-isopropylmalic acid
32449-92-6	439782	glucuronolactone 1
32449-92-6	439782	glucuronolactone 2
32449-92-6	439782	glucuronolactone 3
327-57-1	21236	L-norleucine 1
327-57-1	21236	L-norleucine 2
327-97-9	6537496	chlorogenic acid 1
327-97-9	6537496	chlorogenic acid 2
328-42-7	970	oxalacetic acid
328-50-7	51	alpha ketoglutaric acid
32860-62-1	3625615	maltotriitol
331-39-5	1549111	caffeic acid
334-48-5	2969	capric acid
3371-27-5	9882981	galocatechin
3387-36-8	6030	uridine 5'-monophosphate 1
3387-36-8	6030	uridine 5'-monophosphate 2
3391-86-4	2724898	1-octen-3-ol
342385-52-8	159793	2-keto-L-gulonic acid 1
342385-52-8	159793	2-keto-L-gulonic acid 2
34363-28-5	754	glycerol 1-phosphate
3443-84-3	5319879	2-oleoylglycerol
34522-32-2	108172	octopine 1
34522-32-2	108172	octopine 2
3471-31-6	18986	5-methoxy-3-indoleacetic acid 1
3471-31-6	18986	5-methoxy-3-indoleacetic acid 2
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
35323-91-2	72276	(-)-epicatechin
35323-91-2	72276	epicatechin 1
35323-91-2	72276	(-)-epicatechin
35323-91-2	72276	epicatechin 2
3555-86-0	77093	phlorobenzophenone 1
3555-86-0	77093	phlorobenzophenone 2
35608-63-0	110992	3-chloro-L-tyrosine 1
35608-63-0	110992	3-chloro-L-tyrosine 2
35850-13-6	5280887	15-keto-prostaglandin F2alpha
35850-13-6	5280887	15-keto-prostaglandin F-2-alpha

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CAS #	PubChem	Compound
3588-17-8	5356793	trans,trans-muconic acid
359-83-1	441278	Pentazocine
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
3615-41-6	220001	rhamnose 1
3615-41-6	220001	rhamnose 2
3615-56-3	1101	L- sorbose 1
3615-56-3	1101	L- sorbose 2
362-06-1	440623	2-hydroxyestrone 1
362-06-1	440623	2-hydroxyestrone 2
363-24-6	62453	4-vinylphenol 1
363-24-6	62453	4-vinylphenol 2
3646-68-2	73563	D-glucosaminic acid 1
3646-68-2	73563	D-glucosaminic acid 1
3646-68-2	73563	D-glucosaminic acid 2
3646-68-2	73563	D-glucosaminic acid 2
365-07-1	1139	thymidine 5'-phosphate 1
365-07-1	1139	thymidine 5'-phosphate 2
36653-82-4	2682	1-hexadecanol
36653-82-4	2682	1-hexadecanol, (cetyl alcohol)
367-93-1	656894	isopropyl beta-D-1-thiogalactopyranoside
368-16-1	64969	3-methyl-L-histidine
3681-93-4	5280441	vitexin 1
3681-93-4	5280441	vitexin 2
3685-22-1	151138	cis-4-hydroxycyclohexanecarboxylic acid
3687-64-7	439451	galactinol 1
3687-64-7	439451	galactinol 2
3715-29-5	49	3-methyl-2-oxobutanoic acid 1
3715-29-5	49	3-methyl-2-oxobutanoic acid 2
372-75-8	9750	citrulline 1
372-75-8	9750	citrulline 2
372-75-8	9750	citrulline 3
373-49-9	445638	palmitoleic acid
38183-03-8	1880	7,8-Dihydroxyflavone
38186-71-9	5379071	2',3-Dihydroxy-4,4',6'-Trimethoxychalcone
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 1
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 2
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 3
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 4
382-45-6	223997	adrenosterone 1
382-45-6	223997	adrenosterone 2
38819-01-1	439626	cellotetraose
392-12-1	803	indole-3-pyruvic acid
3943-74-6	19844	methyl 4-hydroxy-3-methoxybenzoate

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CAS #	PubChem	Compound
404-86-4	1548943	capsaicin
407-41-0	68841	O-phospho-L-serine 1
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 2
41001-90-5	3593	hesperetin 1
41001-90-5	3593	hesperetin 2
41001-90-5	3593	hesperetin 3
4104-45-4	77743	3-(methylthio)-propylamine
41468-25-1	1051	pyridoxal 5'-phosphate 1
41468-25-1	1051	pyridoxal 5'-phosphate 2
41468-25-1	1051	pyridoxal 5'-phosphate 3
4206-58-0	5280802	trans-3,5-dimethoxy-4-hydroxycinnamaldehyde
42155-08-8	18601100	2'-Deoxyuridine 5'-monophosphate 1
42155-08-8	18601100	2'-Deoxyuridine 5'-monophosphate 2
42366-37-0	242332	5-alpha-androstane-3 beta,17 beta-diol
42542-10-9	1615	3,4-MDMA
4264-83-9	378	4-nitrophenyl phosphate
4289-98-9	911	N-formyl-L-methionine 1
4289-98-9	911	N-formyl-L-methionine 2
4376-20-9	20393	mono(2-ethylhexyl)phthalate
4385-35-7	78092	3-isochromanone
439-14-5	3016	Diazepam
4423-37-4	5281953	syringetin
4436-74-2	5351896	trans-3-hexenedioic acid
443-79-8	791	DL-isoleucine 1
443-79-8	791	DL-isoleucine 2
4460-86-0	20525	Asarylaldehyde 1
4460-86-0	20525	Asarylaldehyde 2
446-72-0	5280961	4',5,7-trihydroxyisoflavone
4472-73-5	521171	3,4',5,6,7-Pentamethoxyflavone
4484-88-2	122336	trehalose-6-phosphate
4502-00-5	70	2-ketoisocaproic acid 1
4502-00-5	70	2-ketoisocaproic acid 2
451-13-8	780	homogentisic acid
45159-34-0	439742	beta-cyano-L-alanine
452-86-8	9958	4-methylcatechol
458-24-2	3337	Fenfluramine
458-24-2	3337	Fenfluramine 1
458-35-5	1549095	coniferyl alcohol
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 1
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 2
459-80-3	5275520	geranic acid
4618-18-2	11333	lactulose 1
4618-18-2	11333	lactulose 3

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CAS #	PubChem	Compound
4618-18-2	11333	lactulose 2
462-20-4	421	dihydrolipoic acid
462-88-4	111	3-ureidopropionate 1
462-88-4	111	3-ureidopropionate 2
462-88-4	111	3-ureidopropionate 3
463-00-3	500	4-guanidinobutyric acid 1
463-00-3	500	4-guanidinobutyric acid 2
4637-56-3	5460367	4-Hydroxyaminoquinoline-N-oxide
466-99-9	5284570	Hydromorphone 1
466-99-9	5284570	Hydromorphone 2
469-62-5	10100	d-Propoxyphene
469-90-9	16219957	sedoheptulose anhydride monohydrate
470-69-9	440080	kestose
4707-46-4	736228	3-Methylorsellinic Acid 1
4707-46-4	736228	3-Methylorsellinic Acid 2
473-81-4	439194	glyceric acid
476-66-4	5281855	ellagic acid
479-18-5	3182	dyphylline
480-18-2	439533	taxifolin
480-40-0	5281607	chrysin
480-44-4	5280442	Acacetin
480-44-4	5280442	Acacetin 1
481-05-0	65030	Artemisin
481-05-0	65030	Artemisin 1
481-06-1	221071	alpha-santonin 1
481-06-1	221071	alpha-santonin 2
481-37-8	91460	Ecgonine
481-39-0	3806	juglone
484-17-3	10229	9-phenanthrenol
484-20-8	2355	5-methoxypsoralen
486-25-9	10241	9-fluorenone
486-66-8	5281708	daidzein
486-74-8	10243	4-quinolinecarboxylic acid
487-21-8	10250	lumazine
487-26-3	10251	flavanone 1
487-26-3	10251	flavonone 1
487-26-3	10251	flavanone 2
487-26-3	10251	flavonone 2
487-54-7	10253	salicylurate 1
487-54-7	10253	salicylurate 2
487-89-8	10256	indole-3-carbaldehyde 1
487-89-8	10256	indole-3-carbaldehyde 2
487-90-1	1021	porphobilinogen
488-17-5	340	3-methylcatechol
488-69-7	10267	fructose-1,6-diphosphate 1

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CAS #	PubChem	Compound
488-69-7	10267	fructose-1,6-diphosphate 2
488-81-3	827	ribitol
488-82-4	94154	arabitol
4896-77-9	2723970	glycine-d5 deuterated
490-79-9	3469	gentisic acid
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
492-00-2	5393152	3,7-Dihydroxyflavone
492-27-3	3845	4-hydroxyquinoline-2-carboxylic acid(kynurenic acid)
495-69-2	464	hippuric acid 1
495-69-2	464	hippuric acid 2
495-78-3	873	3-(2-hydroxyphenyl)propanoic acid
497-76-7	440936	arbutin
498-00-0	62348	4-hydroxy-3-methoxybenzyl alcohol
498-07-7	2724705	1,6-anhydro-glucose
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
498-40-8	72886	L-cysteic acid
499-40-1	439193	isomaltose 1
499-40-1	439193	isomaltose 2
499-83-2	10367	pyridine-2,6-dicarboxylic acid
500-44-7	440473	L-mimosine 1
500-44-7	440473	L-mimosine 2
50-06-6	4763	Phenobarbital
5006-66-6	72924	6-hydroxynicotinic acid
5006-66-6	72924	6-hydroxynicotinic acid
500-98-1	68144	phenaceturic acid 1
500-98-1	68144	phenaceturic acid 2
501-36-0	445154	trans- resveratrol
501-36-0	445154	resveratrol
501-52-0	107	hydrocinnamic acid
501-94-0	10393	2-(4-hydroxyphenyl)ethanol
501-94-0	10393	4-(2-hydroxyethyl)phenol (tyrosol)
501-97-3	10394	3-(4-hydroxyphenyl)propionic acid
50-27-1	5756	estriol
50-28-2	5757	estradiol
503-49-1	1662	3-hydroxy-3-methylglutaric acid (dicrotalic acid)

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CAS #	PubChem	Compound
50-36-2	446220	Cocaine
503-66-2	68152	3-hydroxypropanoic acid 1
503-66-2	68152	3-hydroxypropanoic acid 2
503-66-2	68152	3-hydroxypropanoic acid 3
504-02-9	10434	1,3 cyclohexanedione 1
504-02-9	10434	1,3 cyclohexanedione 2
504-02-9	10434	1,3 cyclohexanedione 3
504-07-4	649	5,6-dihydrouracil 1
504-07-4	649	5,6-dihydrouracil 2
504-15-4	10436	orcinol
5041-82-7	5318644	isorhamnetin-3--glucoside
504-63-2	10442	1,3-propanediol
505-48-6	10457	suberic acid
506-12-7	10465	heptadecanoic acid
506-30-9	10467	arachidic acid
50-66-8	5778	6-methylmercaptapurine 1
50-66-8	5778	6-methylmercaptapurine 2
50-67-9	5202	serotonin 1
50-67-9	5202	serotonin 2
50-70-4	5780	D-sorbitol
50-78-2	2244	O-acetylsalicylic acid
50-81-7	5785	L-ascorbic acid
50887-69-9	967	orotic acid
50887-69-9	967	orotic acid
50-89-5	5789	thymidine
50-89-5	5789	thymidine
51028-73-0	5816	(-)-epinephrine 1
51028-73-0	5816	(-)-epinephrine 2
51268-88-3	440294	cis-1,2-dihydro-1,2-naphthalenediol
51268-88-3	440294	(1R,2S)-cis-1,2-dihydro-1,2-naphthalenediol
51-35-4	5810	trans-4-hydroxy-L-proline 1
51-35-4	5810	trans-4-hydroxy-L-proline 2
513-85-9	262	2,3-butanediol 1
513-85-9	262	2,3-butanediol 2
514-10-3	10569	abietic acid
51-41-2	5814	norepinephrine (noradrenalin)
51-43-4	5816	adrenaline 1
51-43-4	5816	adrenaline 2
5147-00-2	189	acetyl-L-serine 1
5147-00-2	189	acetyl-L-serine 2
516-05-2	487	methylmalonic acid
51-61-6	681	dopamine (hydroxytyramine)
51-64-9	5826	d-Amphetamine
51-67-2	5610	tyramine
516-72-3	121935	20-hydroxycholesterol 1

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CAS #	PubChem	Compound
516-72-3	121935	20-hydroxycholesterol 2
51-79-6	5641	carbamic acid ethyl ester (urethane)
519-09-5	448223	Benzoyllecgonine
520-18-3	5280863	kaempferol 1
520-18-3	5280863	kaempferol 2
520-36-5	5280443	Apigenin
521-18-6	10635	dihydrotestosterone 1
521-18-6	10635	dihydrotestosterone 2
521-35-7	2543	Cannabinol
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
52-52-8	2901	cycloleucine 1
52-52-8	2901	cycloleucine 2
525-82-6	10680	flavone
526-95-4	604	gluconic acid 1
526-95-4	604	gluconic acid 2
526-99-8	3037582	mucic acid
527-52-6	258531	digitoxose 1
527-52-6	258531	digitoxose 2
528-50-7	10712	cellobiose 1
528-50-7	10712	cellobiose 2
52-90-4	594	L-cysteine 1
52-90-4	594	L-cysteine 2
529-38-4	644006	Cocaethylene
529-44-2	5281672	myricetin
529-64-6	10726	tropic acid
529-69-1	10729	isoxanthopterin
530-57-4	10742	syringic acid
530-59-6	637775	3,5-dimethoxy-4-hydroxycinnamic acid 1
530-59-6	637775	3,5-dimethoxy-4-hydroxycinnamic acid 2
53-06-5	222786	cortisone
53-16-7	5870	1,3,5(10)-estratrien-3-ol-17-one 1
53-16-7	5870	estrone 1
53-16-7	5870	1,3,5(10)-estratrien-3-ol-17-one 2
53-16-7	5870	estrone 2
532-28-5	10758	mandelonitrile
532-28-5	10758	mandelonitrile
5336-08-3	111064	ribonic acid-gamma-lactone 1
5336-08-3	111064	ribonic acid-gamma-lactone 2
533-67-5	5460005	2-deoxy-D-ribose 1
533-67-5	5460005	2-deoxy-D-ribose 2
533-73-3	10787	benzene-1,2,4-triol
53411-70-4	91493	6-phosphogluconic acid
53-41-8	5879	androsterone

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CAS #	PubChem	Compound
53-43-0	5881	trans-dehydroandrosterone 1
53-43-0	5881	trans-dehydroandrosterone 2
53-43-0	6013	testosterone 2
53-43-0	6013	testosterone 1
534-46-3	4623424	sophorose 1
534-46-3	4623424	sophorose 2
53472-37-0	5282154	laricitrin
535-75-1	439227	pipecolic acid 1
535-75-1	439227	pipecolic acid 2
535-83-1	5570	trigonelline
536-60-7	325	4-isopropylbenzyl alcohol
536-66-3	10820	4-isopropylbenzoic acid
537-33-7	5280507	sinapyl alcohol 1
537-33-7	5280507	sinapyl alcohol 2
537-46-2	10836	Methamphetamine 1
537-46-2	10836	Methamphetamine 2
5391-40-5	638011	citral 1
5391-40-5	638011	citral 2
5391-40-5	638011	citral 3
5391-40-5	638011	citral 4
53-96-3	5897	N-2-fluorenylacetamide 1
53-96-3	5897	N-2-fluorenylacetamide 2
541-15-1	10918	L-carnitine 1
541-15-1	10918	L-carnitine 2
54-16-0	1826	5-hydroxyindole-3-acetic acid
543-38-4	275	L-canavanine 1
543-38-4	275	L-canavanine 2
544-63-8	11005	myristic acid
546-88-3	1990	acetohydroxamic acid
547-25-1	5460935	turanose 1
547-25-1	5460935	turanose 2
547-96-6	160520	5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol 1
547-96-6	160520	5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol 2
548-93-6	86	3-hydroxyanthranilic acid 1
548-93-6	86	3-hydroxyanthranilic acid 2
54965-21-8	2082	albendazole
550-33-4	68368	purine riboside
55-10-7	1245	DL-4-hydroxy-3-methoxymandelic acid
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
551-68-8	90008	psicose 1
551-68-8	90008	psicose 2
551-84-8	439204	xylulose

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CAS #	PubChem	Compound
55-21-0	2331	benzamide
552-59-0	5281804	prunetin
554-62-1	122121	phytosphingosine 1
554-62-1	122121	phytosphingosine 2
5550-12-9	6804	guanosine-5'-monophosphate
55682-92-3		Methyl Octacosanoate
557-24-4	5280451	maleamic acid 1
557-24-4	5280451	maleamic acid 2
557-24-4	5280451	maleamic acid 3
56-12-2	119	gamma-aminobutyric acid (GABA)
561-63-7	6453303	19-hydroxycholesterol
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
56-29-1	3608	Hexobarbital
56-40-6	750	glycine
56-41-7	5950	L-alanine 1
56-41-7	5950	L-alanine 2
56-45-1	5951	L-serine 1
56-45-1	5951	L-serine 2
565-70-8	11266	2-hydroxybutyric acid
56-57-5	77341	4-nitroquinoline
56-57-5	5955	4-nitroquinoline N-oxide
566-26-7	107722	5-cholesten-3-beta-7-alpha-diol
566-28-9	91474	7-Oxocholesterol
56-65-5	5957	adenosine 5'-triphosphate
566-65-4	92810	5-alpha-pregnan-3,20-dione 1
566-65-4	92810	5-alpha-pregnan-3,20-dione 2
566-78-9	11276	21-Acetoxypregnenolone
566-88-1	92128	5alpha-cholestan-3-one 1
566-88-1	92128	5alpha-cholestan-3-one 2
56-73-5	439958	D-glucose-6-phosphate 1
56-73-5	439958	D-glucose-6-phosphate 2
56-75-7	5959	chloramphenicol 1
56-75-7	5959	chloramphenicol 2
5680-79-5	69221	glycine methyl ester
56-81-5	753	glycerol
56-82-6	751	DL-glyceraldehyde 1
56-82-6	751	DL-glyceraldehyde 2
56-84-8	5960	aspartic acid 1
56-84-8	5960	aspartic acid 2
56-85-9	738	L-glutamine 1
56-85-9	738	L-glutamine 2
56-85-9	738	L-glutamine 3
56-86-0	33032	L-glutamic acid 3 (dehydrated)

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CAS #	PubChem	Compound
56-86-0	73064	beta-glutamic acid
56-86-0	33032	L-glutamic acid 1
56-86-0	33032	L-glutamic acid 2
56-87-1	5962	L-lysine 1
56-87-1	5962	L-lysine 2
56-89-3	67678	L-cystine 1
56-89-3	67678	L-cystine 2
56-89-3	67678	L-cystine 3
5704-04-1	79784	tricine 1
5704-04-1	79784	tricine 2
57-11-4	5281	stearic acid
57-13-6	1176	urea
57-27-2	5288826	Morphine
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
57-43-2	2164	Amobarbital
57-43-2	2164	Amobarbital 1
57-44-3	2294	Barbital
5746-86-1	412	nornicotine
57-48-7	5984	fructose 1
57-48-7	5984	fructose 2
577-85-5	11349	3-hydroxyflavone
57-87-4	444679	ergosterol
57-88-5	304	cholesterol
578-86-9	1889	liquiritigenin 1
578-86-9	1889	liquiritigenin 2
578-86-9	1889	liquiritigenin 3
57-92-7	6047	L-DOPA 1
57-92-7	6047	L-DOPA 2
579-36-2	448388	D-allose 1
579-36-2	448388	D-allose 2
5802-82-4		Methyl Hexacosanoate
58-08-2	2519	caffeine
582-24-1	68490	2-hydroxyacetophenone 1
582-24-1	68490	2-hydroxyacetophenone 2
582-60-5	675	5,6 - dimethylbenzimidazole 1
582-60-5	675	5,6 - dimethylbenzimidazole 2
583-08-4	68499	nicotinoylglycine
583-93-7	865	2,6-diaminopimelic acid 1
583-93-7	865	2,6-diaminopimelic acid 2
585-18-2	697	erythrose 4-phosphate 1

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CAS #	PubChem	Compound
585-18-2	697	erythrose 4-phosphate 2
585-18-2	439762	sucrose-6-phosphate 1
585-18-2	439762	sucrose-6-phosphate 2
585-84-2	444212	trans-aconitic acid
585-88-6	16217663	maltitol
585-88-6	3034828	palatinitol 1
58-61-7	60961	adenosine
58-63-9	6021	inosine
588-30-7	637541	3-hydroxycinnamic acid
58-86-6	6027	xylose 1
58-86-6	6027	xylose 2
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
58-96-8	6029	uridine
589-98-0	11527	3-octanol
59-00-7	5699	4,8-dihydroxyquinoline-2-carboxylic acid (xanthurenic ac
59-00-7	5699	xanthurenic acid
59-23-4	206	D (+) galactose 1
59-23-4	24749	D-glucose 1
59-23-4	24749	D-glucose 2
59-23-4	206	D (+) galactose 2
59-31-4	6038	2-hydroxyquinoline 1
59-31-4	6038	2-hydroxyquinoline 2
5934-29-2	6274	L-histidine 1
5934-29-2	6274	L-histidine 2
5934-29-2	6274	L-histidine 3
593-49-7	11636	heptacosane
5949-29-1	311	citric acid
595-98-2	136386	methyltartronic acid
5965-53-7	97750	diethyl oxalpropionate 1
5965-53-7	97750	diethyl oxalpropionate 2
5965-53-7	97750	diethyl oxalpropionate 3
59-67-6	938	nicotinic acid
5989-27-5	440917	limonene
599-04-2	989	pantolactone
59-92-2	836	3,4 dihydroxyphenylalanine (DOPA) 1
59-92-2	836	3,4 dihydroxyphenylalanine (DOPA) 2
5996-00-9	441422	beta-gentiobiose 1
5996-00-9	441422	beta-gentiobiose 2
600-18-0	58	2-ketobutyric acid
600-18-0	58	2-ketobutyric acid
60-11-7	6053	methyl yellow
60-12-8	6054	phenylethyl alcohol

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CAS #	PubChem	Compound
601-53-6	85881	coprostan-3-one
601-57-0	91477	(+) -4-cholesten-3-one 1
601-57-0	91477	(+) -4-cholesten-3-one 2
60-18-4	6057	L-tyrosine 1
60-18-4	6057	tyrosine 1
60-18-4	6057	L-tyrosine 2
60-18-4	6057	tyrosine 2
60-23-1	6058	2-aminoethanethiol 1
60-23-1	6058	2-aminoethanethiol 2
6025-53-2	6440982	trans-Zeatin-riboside
60-27-5	588	Creatinine
60-32-2	564	6-aminocaproic acid
60-33-3	5280450	linoleic acid
604-75-1	4616	Oxazepam
604-75-1	4616	Oxazepam 1
60658-41-5		Myristic Acid d27
608-07-1	637542	4-hydroxycinnamic acid
608-07-1	1833	methoxytryptamine
60-82-2	4788	phloretin
608-66-2	11850	galactitol
6090-95-5	119054	conduritol epoxide 1
6090-95-5	119054	conduritol epoxide 2
60-92-4	6076	adenosine 3',5'-cyclic monophosphate
60-92-4	6076	cyclic AMP
609-71-2	69114	2-hydroxynicotinic acid
611-14-3	11903	2-ethyltoluene
611-36-9	69141	4-hydroxyquinoline 1
611-36-9	69141	4-hydroxyquinoline 2
611-73-4	11915	benzoylformic acid 1
611-73-4	11915	benzoylformic acid 2
6133-30-8	97856	guanidinosuccinic acid 1
6133-30-8	97856	guanidinosuccinic acid 2
6133-30-8	97856	guanidinosuccinic acid 3
6138-23-4	7427	D-(+) trehalose
614-60-8	637540	2-hydroxycinnamic acid
614-75-5	11970	2-hydroxyphenylacetic acid
615-13-4	11983	2-indanone
615-58-7	11847	2,6-dibromophenol
615-58-7	12005	2,4-dibromophenol
616-04-6	69217	1-methylhydantoin 1
616-04-6	69217	1-methylhydantoin 2
616-91-1	12035	N-acetyl-L-cysteine 1
616-91-1	12035	N-acetyl-L-cysteine 2
617-48-1	92824	D-malic acid
61-90-5	6106	L-leucine 1

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CAS #	PubChem	Compound
61-90-5	6106	L-leucine 2
6192-52-5	6101	p-toluenesulfonic acid
6202-10-4	439216	dihydroorotic acid 1
6202-10-4	439216	dihydroorotic acid 2
6202-10-4	439216	dihydroorotic acid 3
620-24-6	102	3-hydroxybenzyl alcohol
621-37-4	12122	3-hydroxyphenylacetic acid
621-44-3	65124	3-nitro-L-tyrosine 1
621-44-3	65124	3-nitro-L-tyrosine 2
62147-49-3	668	dihydroxyacetone phosphate 1
62147-49-3	668	dihydroxyacetone phosphate 2
621-54-5	91	3-(3-hydroxyphenyl)propionic acid
622-78-6	2346	benzyl isothiocyanate
62471-63-0	124925	8-oxo-2'-deoxyadenosine
625-08-1	69362	beta-hydroxyisovalerate
6263-10-8	439766	citramalic acid
626-64-2	12290	4-hydroxypyridine
626-72-2	439579	L-homocystine 1
626-72-2	439579	L-homocystine 2
626-72-2	439579	L-homocystine 3
626-97-1	12298	valeramide 1
626-97-1	12298	valeramide 2
626-97-1	12298	valeramide 4
626-97-1	12298	valeramide 3
627-01-0	316542	N-ethylglycine 1
627-01-0	316542	N-ethylglycine 2
627-82-7	42953	diglycerol 1
627-82-7	42953	diglycerol 2
627-82-7	42953	diglycerol 3
62-84-0	65542	4-androsten-7-alpha-ol-3,17-dione 1
62-84-0	65542	4-androsten-7-alpha-ol-3,17-dione 2
628-48-8	5280498	glutaconic acid 1
628-48-8	5280498	glutaconic acid 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
629-73-2	12395	hexadecene
629-83-4		Methyl Triacontanoate
629-98-1	5354168	cis-13-Docosanol
630-03-5	12409	nonacosane
63046-09-3	182362	6,4'-Dihydroxyflavone
63-05-8	6128	4-androsten-3,17-dione 1
63-05-8	6128	4-androsten-3,17-dione 2
6307-89-7	238769	2,6-Dihydroxy-4-Methoxytoluene

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CAS #	PubChem	Compound
63-37-6	6131	cytidine-5'-monophosphate 1
63-37-6	6131	cytidine-5'-monophosphate 2
63-42-3	84571	lactose 1
63-42-3	84571	lactose 2
6342-92-3	5355888	2',5'-Dihydroxy-4-Methoxychalcone
634-97-9	12473	pyrrole -2-carboxylic acid
6351-10-6	22819	1-indanol
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
63-68-3	6137	L-methionine 1
63-68-3	6137	L-methionine 2
637-88-7	12511	1,4-cyclohexanedione 1
637-88-7	12511	1,4-cyclohexanedione 2
63-91-2	994	Phenylalanine 1
63-91-2	994	Phenylalanine 1
64-04-0	1001	phenethylamine
64-04-0	1001	phenylethylamine
642-71-7	69505	Antiarol
64280-14-4	107885	(+/-)-11-nor-9-carboxy-delta-9-THC Standard
644-90-6	69522	2-aminooctanoic acid 1
644-90-6	69522	2-aminooctanoic acid 2
64519-82-0	985	palmitic acid
64519-82-0	3034828	palatinitol 2
646-31-1	12592	tetracosane
6482-98-0	9378	DL-p-hydroxyphenyllactic acid
65005-57-4	123831	N,N-dimethylarginine
652157-52-3	637	2'-deoxycytidine
65-23-6	1054	pyridoxine
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 1
653-63-4	621	2'-deoxyadenosine 5'-monophosphate
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 2
65-46-3	596	cytidine 1
65-46-3	596	cytidine 2
6556-12-3	16213610	glucuronic acid 1
6556-12-3	16213610	glucuronic acid 3
6556-12-3	16213610	glucuronic acid 2
6556-12-3	16213610	glucuronic acid 4
65-71-4	1135	thymine
65-85-0	243	benzoic acid
658-79-7	92829	glycyl-L-tyrosine 1
658-79-7	92829	glycyl-L-tyrosine 2
6589-55-5	913	halostachine 1
6589-55-5	913	halostachine 2
6600-40-4	65098	norvaline 1
6600-40-4	65098	norvaline 2

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CAS #	PubChem	Compound
66009-10-7	440658	melibiose 1
66009-10-7	440658	melibiose 2
660-88-8	138	5-aminovaleric acid 1
660-88-8	138	5-aminovaleric acid 2
660-88-8	138	5-aminovaleric acid 3
66-22-8	1174	uracil
66-22-8	1175	uric acid 1
66-22-8	1175	uric acid 2
6698-26-6	65166	2', 5'-Dideoxyadenosine
672-15-1	12647	L-homoserine 1
672-15-1	12647	L-homoserine 2
672-15-1	12647	L-homoserine 3
673-49-4	69602	N-omega-acetylhistamine 2
673-49-4	69602	N-omega-acetylhistamine 1
67-47-0	237332	5-(hydroxymethylfurfural) 1
67-47-0	237332	5-(hydroxymethylfurfural) 2
675-10-5	12663	4-Hydroxy-6-Methylpyran-2-One
675-10-5	12663	4-hydroxy-6-methyl-2-pyrone
675-20-7	12665	2-piperidone 1
675-20-7	12665	2-piperidone 2
6753-62-4	268779	N-methylglutamic acid 1
6753-62-4	268779	N-methyl-DL-glutamic acid 1
6753-62-4	268779	N-methylglutamic acid 2
6753-62-4	268779	N-methyl-DL-glutamic acid 2
6753-62-4	268779	N-methylglutamic acid 3
6753-62-4	268779	N-methyl-DL-glutamic acid 3
6753-62-4	268779	N-methylglutamic acid 4
67879-58-7	642609	trans caftaric acid 1
67879-58-7	642609	trans caftaric acid 2
67-97-0	5280795	cholecalciferol 1
67-97-0	5280795	cholecalciferol 2
68-11-1	1133	thioglycolic acid
681295-24-9	66868	porphine 1
681295-24-9	66868	porphine 2
68-42-8	65553	tetrahydrocorticosterone 1
68-42-8	65553	tetrahydrocorticosterone 2
68-42-8	65553	tetrahydrocorticosterone 3
68-42-8	65553	tetrahydrocorticosterone 4
6851-36-1	166768	4-hydroxymandelonitrile 1
6851-36-1	166768	4-hydroxymandelonitrile 2
6889-80-1	97143	3-Hydroxy-3',4'-Dimethoxyflavone
6892-68-8	439352	1,4-dithioerythritol
689-31-6	71	2-ketoadipic acid 1
689-31-6	71	2-ketoadipic acid 2
68-94-0	790	hypoxanthine 1

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CAS #	PubChem	Compound
68-94-0	790	hypoxanthine
68-94-0	790	hypoxanthine 2
6906-38-3	443650	delphinidin 3-glucoside
6906-38-3	443650	delphinidin 3-glucoside 2
6906-38-3	443650	delphinidin 3-glucoside 3
6906-39-4	443654	peonidin-3-glucoside
6906-39-4	443654	peonidin-3-glucoside 2
693-71-0	26161490	trans-13-octadecenoic acid
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
69616-74-6	5955473	2',4-Dihydroxy-3,4',6'-Trimethoxychalcone
6968-16-7	169019	D-threitol
69-72-7	338	salicylic acid
69-79-4	6255	maltose 1
69-79-4	6255	maltose 2
6988-81-4	443651	petunidin-3-glucoside
6988-81-4	443651	petunidin-3-glucoside 2
69-89-6	1188	xanthine
699012-36-7	41211	adenosine-3'-monophosphate
700-06-1	3712	indole-3-carbinol (3-indolemethanol)
700-06-1	3712	indole-3-carbinol 1
701-64-4	12793	phenylphosphoric acid
70-18-8	124886	L-glutathione reduced
70-26-8	6262	L-ornithine 1
70-26-8	6262	L-ornithine 2
704-15-4	79101	gly-pro
704-15-4	79101	glycylproline
70-47-3	16217724	L-asparagine-15N2,d8 1
70-47-3	236	L-asparagine 1
70-47-3	16217724	L-asparagine-15N2,d8 2
70-47-3	16217724	L-asparagine-15N2,d8 3
70-47-3	236	L-asparagine 2
7057-27-4	4085802	3'-deoxyuridine 1
7057-27-4	4085802	3'-deoxyuridine 2
7084-29-9	13845047	5-methyl-3'-deoxyuridine 1
7084-29-9	13845047	5-methyl-3'-deoxyuridine 2
71-30-7	597	cytosine 1
71-30-7	597	cytosine 2
71-30-7	597	cytosine 3
71-44-3	1103	spermine 2
71-44-3	1103	spermine 1
7158-70-5	165577	leucrose
7198-10-9	328	DL-4-hydroxymandelic acid
72003-83-9	188966	2' Deoxyadenosine 5'-diphosphate

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CAS #	PubChem	Compound
72-18-4	6287	L-valine 1
72-18-4	6287	L-valine 2
72-19-5	6288	L-threonine 1
72-19-5	6288	L-threonine 2
7228-78-6	443652	malvidin-3-glucoside
72-48-0	6293	alizarin
7298-99-9	443239	threo-3-hydroxy-L-aspartate
7306-96-9	5460407	threonic acid
73-22-3	6305	L-tryptophan 1
73-22-3	6305	L-tryptophan 2
73-24-5	190	adenine 1
73-24-5	190	9H-purine-6-amine
73-24-5	190	adenine 2
7365-44-8	446188	TES
7507-89-3	24135	4-O-Methylphloracetophenone 1
7507-89-3	24135	4-O-Methylphloracetophenone 2
7507-89-3	24135	4-O-Methylphloracetophenone 3
7512-17-6	16218892	N-acetyl-D-glucosamine 1
7512-17-6	16218892	N-acetyl-D-glucosamine 2
7541-49-3	5366244	phytol 1
7541-49-3	6430833	phytol 1
7541-49-3	5366244	phytol 2
7541-49-3	6430833	phytol 2
7568-08-4	439746	6-deoxy-D-glucose 1
7568-08-4	439746	6-deoxy-D-glucose 2
7568-93-6	1000	2-amino-1-phenylethanol
76-41-5	5284604	Oxymorphone
76-41-5	5284604	Oxymorphone 1
76-57-3	5284371	Codeine
765-87-7	13006	1,2-cyclohexanedione 1
765-87-7	13006	1,2-cyclohexanedione 2
765-87-7	13006	1,2-cyclohexanedione 3
7664-38-2	1004	phosphoric acid
7665-99-8	295	cyclic GMP
766-93-8	13017	N-cyclohexylformamide
76-73-3	5193	Secobarbital
76-74-4	4737	Pentobarbital
76-99-3	4095	Methaqualone
77-02-1	6464	Aprobarbital
77-10-1	6468	Phencyclidine
771-50-6	69867	indole-3-carboxylic acid
771-50-6	69867	indole-3-carboxylic acid
771-51-7	351795	3-indoleacetonitrile
77-26-9	2481	Butalbital
7772-94-3	899	N-acetyl-D-mannosamine 1

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CAS #	PubChem	Compound
7772-94-3	899	N-acetyl-D-mannosamine 2
77-93-0	6506	triethyl citrate
77-95-2	6508	quinic acid
79-14-1	757	glycolic acid
79-33-4	107689	L-(+) lactic acid
79-36-0	440560	dihydrolanosterol
79-36-0	246983	lanosterol
79-57-2	5280972	oxytetracycline
79786-40-6	676293	6,3'-Dimethoxyflavone
8/2/4298	440575	trans-3-hydroxy-L-proline 1
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 2
80-69-3	45	tartronic acid
80731-10-8	439183	3-phosphoglyceric acid
80-97-7	6665	5alpha-Cholestanol
80-97-7	3240	5alpha-Cholestan-3-beta-ol
81-13-0	131204	D-panthenol 1
81-13-0	131204	D-panthenol 2
819-83-0	2526	beta-glycerolphosphate
820-11-1	439183	3-phosphoglycerate
82385-42-0	5143	saccharin 2
82385-42-0	5143	saccharin 1
828-01-3	3848	3-phenyllactic acid
82801-81-8	105039	3,4-MDEA
82-82-6	6723	4-pyridoxic acid 1
82-82-6	6723	4-pyridoxic acid 2
82-86-0	6724	acenaphthenequinone 1
82-86-0	6724	acenaphthenequinone 2
82-86-0	6724	acenaphthenequinone 3
82950-64-9	1321	1,2-didecanoylglyceride
830-96-6	3744	indole 3-propionic acid 1
830-96-6	3744	indolepropionic acid
830-96-6	3744	indole 3-propionic acid 2
83-46-5	5321342	beta-sitosterol
84-21-9	224	adenosine-5-monophosphate 1
84-21-9	224	adenosine-5-monophosphate 2
846-46-8	439289	5alpha-Androstan-3, 17-Dione 1
846-46-8	439289	5alpha-Androstan-3, 17-Dione 2
846-49-1	3958	Lorazepam
846-50-4	5391	Temazepam
84-66-2	6781	diethyl phthalate
85-01-8	995	phenanthrene
86-48-6	6844	1-hydroxy-2-naphthoic acid
86-73-7	6853	fluorene

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CAS #	PubChem	Compound
86-74-8	6854	carbazole 1
86-74-8	6854	carbazole 2
87-51-4	802	3-indoleacetic acid
87-66-1	1057	pyrogallol
87-73-0	5460673	D-saccharic acid
87-78-5	18950	D-mannose 1
87-78-5	18950	D-mannose 2
87-78-5	6251	D-mannitol
87-81-0	2724552	tagatose 1
87-81-0	2724552	tagatose 2
87-89-8	892	allo-inositol
87-89-8	892	myo-inositol
879-37-8	397	indole-3-acetamide 1
879-37-8	397	indole-3-acetamide 2
879-37-8	397	indole-3-acetamide 3
87-99-0	6912	xylitol
88-14-2	6919	2-furoic acid
88-21-1	6926	aniline-o-sulfonic acid
884-33-3	3858	benzylsuccinic acid
88-99-3	1017	phthalic acid
89-00-9	1066	quinolinic acid
897-06-3	6710699	Androsta-1, 4-Dien-3, 17-Dione 1
897-06-3	6710699	Androsta-1, 4-Dien-3, 17-Dione 2
89-83-8	6989	thymol
9/3/2466	1023	pyrophosphate
9/8/4350	439280	5-hydroxy-L-tryptophan 1
9/8/4350	439280	5-hydroxy-L-tryptophan 2
90-01-7	5146	2-hydroxybenzyl alcohol
90-05-1	460	guaiacol
90-33-5	5280567	4-methylumbelliferone
90-33-5	5280567	4-methylumbelliferone
90-43-7	7017	2-hydroxybiphenyl
90-80-2	736	gluconic acid lactone 1
90-80-2	736	gluconic acid lactone 2
90-80-2	736	gluconic acid lactone 3
91-20-3	931	naphthalene
91-22-5	6998	salicylaldehyde
923-16-0	601	D-Ala-D-Ala 1
923-16-0	601	D-Ala-D-Ala2
923-16-0	601	D-Ala-D-Ala3
92-52-4	7095	biphenyl
92-61-5	5280460	scopoletin
928-94-9	5318042	2-hexen 1-ol
929-77-1		Methyl Docosanoate
93-10-7	7124	quinaldinic acid

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CAS #	PubChem	Compound
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 1
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 2
93839-95-3	188955	2'-Deoxyadenosine 3' :5'-cyclic monophosphate
93965-35-6	729	DL-glyceraldehyde 3-phosphate 1
93965-35-6	729	DL-glyceraldehyde 3-phosphate 2
94-07-5	7172	synephrine 1
94-07-5	7172	synephrine 2
94-62-2	638024	piperine 1
94-62-2	638024	piperine 2
95-16-9	7222	benzothiazole
951-78-0	13712	2-deoxyuridine 1
951-78-0	13712	2-deoxyuridine 2
95-43-2	439665	threose 1
95-43-2	439665	threose 2
95-48-7	2879	p-cresol
95-55-6	5801	2-aminophenol 1
95-55-6	5801	2-aminophenol 2
95-55-6	5801	2-aminophenol 3
95648-83-2	529	phosphoglycolic acid
958-09-8	13730	2'-deoxyadenosine
959-23-9	641818	4'-Methoxychalcone
959-23-9	641818	4'-Methoxychalcone 1
959-23-9	641818	4'-Methoxychalcone 2
95-93-2	7269	1,2,4,5-tetramethylbenzene
961-07-9	187790	2'-deoxyguanosine
96-26-4	4180364	1,3-dihydroxyacetone
96-82-2	16219560	lactobionic acid 1
96-82-2	91476	lactitol
96-82-2	16219560	lactobionic acid 2
96-82-2	16219560	lactobionic acid 3
970-74-1	72277	epigallocatechin
97164-73-3	2479	Butabarbital
97-59-6	204	allantoin 1
97-59-6	204	allantoin 2
97-59-6	204	allantoin 3
97-65-4	811	itaconic acid
98-79-3	7405	L-pyroglutamic acid
98-89-5	7413	cyclohexanecarboxylic acid
98-92-0	936	nicotinamide 1
98-92-0	936	nicotinamide 2
989-51-5	1287	epigallocatechin gallate
98-98-6	1018	picolonic acid
99-04-7	7418	m-toluic acid
99-24-1	7428	methyl gallate
99-24-1	7428	methyl gallate

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CAS #	PubChem	Compound
99-50-3	19	2,3-dihydroxybenzoic acid
99-50-3	72	3,4-dihydroxybenzoic acid
997-55-7	65065	N-acetyl-L-aspartic acid 1
997-55-7	65065	N-acetyl-L-aspartic acid 2
99-87-6	7463	p-cymene
99-98-9	7472	N,N-dimethyl-1,4-phenylenediamine 1
99-98-9	7472	N,N-dimethyl-1,4-phenylenediamine 2

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CAS #	PubChem	Compound
99-50-3	19	2,3-dihydroxybenzoic acid
3237-44-3	36	2-isopropylmalic acid
13031-04-4	39	dihydro-4,4-dimethyl-2,3-furandione 1
13031-04-4	39	dihydro-4,4-dimethyl-2,3-furandione 2
80-69-3	45	tartronic acid
3715-29-5	49	3-methyl-2-oxobutanoic acid 1
3715-29-5	49	3-methyl-2-oxobutanoic acid 2
328-50-7	51	alpha ketoglutaric acid
600-18-0	58	2-ketobutyric acid
600-18-0	58	2-ketobutyric acid
138-81-8	61	2,3-diphosphoglycerate
4502-00-5	70	2-ketoisocaproic acid 1
4502-00-5	70	2-ketoisocaproic acid 2
689-31-6	71	2-ketoadipic acid 1
689-31-6	71	2-ketoadipic acid 2
99-50-3	72	3,4-dihydroxybenzoic acid
2922-42-1	80	3-dehydroshikimic acid 1
2922-42-1	80	3-dehydroshikimic acid 2
548-93-6	86	3-hydroxyanthranilic acid 1
548-93-6	86	3-hydroxyanthranilic acid 2
621-54-5	91	3-(3-hydroxyphenyl)propionic acid
141-97-9	96	acetoacetate 1
141-97-9	96	acetoacetate 2
100-83-4	101	3-hydroxybenzaldehyde
620-24-6	102	3-hydroxybenzyl alcohol
501-52-0	107	hydrocinnamic acid
462-88-4	111	3-ureidopropionate 1
462-88-4	111	3-ureidopropionate 2
462-88-4	111	3-ureidopropionate 3
56-12-2	119	gamma-aminobutyric acid (GABA)
123-08-0	126	4-hydroxybenzaldehyde 1
123-08-0	126	4-hydroxybenzaldehyde 2
156-38-7	127	4-hydroxyphenylacetic acid
114-63-6	135	4-hydroxybenzoic acid
660-88-8	138	5-aminovaleric acid 1
660-88-8	138	5-aminovaleric acid 2
660-88-8	138	5-aminovaleric acid 3
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	9H-purine-6-amine
73-24-5	190	adenine 2
124-04-9	196	adipic acid
97-59-6	204	allantoin 1
97-59-6	204	allantoin 2

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CAS #	PubChem	Compound
97-59-6	204	allantoin 3
59-23-4	206	D (+) galactose 1
59-23-4	206	D (+) galactose 2
84-21-9	224	adenosine-5-monophosphate 1
84-21-9	224	adenosine-5-monophosphate 2
70-47-3	236	L-asparagine 1
70-47-3	236	L-asparagine 2
107-95-9	239	Beta- alanine 1
107-95-9	239	Beta- alanine 2
100-52-7	240	benzaldehyde
65-85-0	243	benzoic acid
100-51-6	244	benzyl alcohol
1133-63-7	254	2,3-dihydroxybiphenyl
513-85-9	262	2,3-butanediol 1
513-85-9	262	2,3-butanediol 2
543-38-4	275	L-canavanine 1
543-38-4	275	L-canavanine 2
120-80-9	289	catechol
7665-99-8	295	cyclic GMP
57-88-5	304	cholesterol
5949-29-1	311	citric acid
536-60-7	325	4-isopropylbenzyl alcohol
122-03-2	326	4-isopropylbenzaldehyde
7198-10-9	328	DL-4-hydroxymandelic acid
69-72-7	338	salicylic acid
2041-14-7	339	ciliatine
488-17-5	340	3-methylcatechol
108-39-4	342	m-cresol
108-73-6	359	phloroglucinol
149-91-7	370	gallic acid
4264-83-9	378	4-nitrophenyl phosphate
124-07-2	379	caprylic acid
111-16-0	385	pimelic acid
879-37-8	397	indole-3-acetamide 1
879-37-8	397	indole-3-acetamide 2
879-37-8	397	indole-3-acetamide 3
123-30-8	403	4-aminophenol 1
123-30-8	403	4-aminophenol 2
123-30-8	403	4-aminophenol 3
5746-86-1	412	nornicotine
462-20-4	421	dihydrolipoic acid
109-76-2	428	1,3-diaminopropane 1
109-76-2	428	1,3-diaminopropane 2
3106-60-3	457	1-methyl nicotinamide 1
3106-60-3	457	1-methyl nicotinamide 2

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CAS #	PubChem	Compound
90-05-1	460	guaiacol
495-69-2	464	hippuric acid 1
495-69-2	464	hippuric acid 2
516-05-2	487	methylmalonic acid
463-00-3	500	4-guanidinobutyric acid 1
463-00-3	500	4-guanidinobutyric acid 2
95648-83-2	529	phosphoglycolic acid
22059-21-8	535	1-aminocyclopropane-1-carboxylic acid
102-32-9	547	2-(3,4-dihydroxyphenyl)acetic acid
102-32-9	547	3,4-dihydroxyphenylacetic acid
60-32-2	564	6-aminocaproic acid
132-64-9	568	dibenzofuran
60-27-5	588	Creatinine
52-90-4	594	L-cysteine 1
52-90-4	594	L-cysteine 2
65-46-3	596	cytidine 1
65-46-3	596	cytidine 2
71-30-7	597	cytosine 1
71-30-7	597	cytosine 2
71-30-7	597	cytosine 3
923-16-0	601	D-Ala-D-Ala 1
923-16-0	601	D-Ala-D-Ala2
923-16-0	601	D-Ala-D-Ala3
526-95-4	604	gluconic acid 1
526-95-4	604	gluconic acid 2
1128-23-0	608	L-galactono-gamma-lactone 1
1128-23-0	608	L-galactono-gamma-lactone 2
147-85-3	614	L-proline 1
147-85-3	614	L-proline 2
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 1
653-63-4	621	2'-deoxyadenosine 5'-monophosphate
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 2
652157-52-3	637	2'-deoxycytidine
504-07-4	649	5,6-dihydrouracil 1
504-07-4	649	5,6-dihydrouracil 2
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
62147-49-3	668	dihydroxyacetone phosphate 1
62147-49-3	668	dihydroxyacetone phosphate 2
31519-22-9	671	1,4-dihydroxy-2-naphthoic acid
1118-68-9	673	N,N-dimethylglycine
582-60-5	675	5,6 - dimethylbenzimidazole 1

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CAS #	PubChem	Compound
582-60-5	675	5,6 - dimethylbenzimidazole 2
51-61-6	681	dopamine (hydroxytyramine)
585-18-2	697	erythrose 4-phosphate 1
585-18-2	697	erythrose 4-phosphate 2
141-43-5	700	ethanolamine
93965-35-6	729	DL-glyceraldehyde 3-phosphate 1
93965-35-6	729	DL-glyceraldehyde 3-phosphate 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
56-85-9	738	L-glutamine 1
56-85-9	738	L-glutamine 2
56-85-9	738	L-glutamine 3
2152-75-2	740	alpha-D-glucosamine 1-phosphate
2152-75-2	740	alpha-D-glucosamine phosphate
2152-75-2	740	alpha-glucosamine 1-phosphate
110-94-1	743	glutaric acid
56-40-6	750	glycine
56-82-6	751	DL-glyceraldehyde 1
56-82-6	751	DL-glyceraldehyde 2
56-81-5	753	glycerol
34363-28-5	754	glycerol 1-phosphate
79-14-1	757	glycolic acid
298-12-4	760	glyoxylic acid
352-97-6	763	guanidinoacetic acid 1
352-97-6	763	guanidinoacetic acid 2
451-13-8	780	homogentisic acid
123-31-9	785	hydroquinone
123-31-9	785	benzoquinone
68-94-0	790	hypoxanthine 1
68-94-0	790	hypoxanthine
68-94-0	790	hypoxanthine 2
443-79-8	791	DL-isoleucine 1
443-79-8	791	DL-isoleucine 2
131-99-7	797	inosine 5'-monophosphate
87-51-4	802	3-indoleacetic acid
392-12-1	803	indole-3-pyruvic acid
97-65-4	811	itaconic acid
488-81-3	827	ribitol
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

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CAS #	PubChem	Compound
59-92-2	836	3,4 dihydroxyphenylalanine (DOPA) 1
59-92-2	836	3,4 dihydroxyphenylalanine (DOPA) 2
3206-73-3	863	lipoamide 1
3206-73-3	863	lipoamide 2
3206-73-3	863	lipoamide 3
583-93-7	865	2,6-diaminopimelic acid 1
583-93-7	865	2,6-diaminopimelic acid 2
141-82-2	867	malonic acid 1
141-82-2	867	malonic acid 2
495-78-3	873	3-(2-hydroxyphenyl)propanoic acid
87-89-8	892	allo-inositol
87-89-8	892	myo-inositol
306-08-1	896	melatonin 1
306-08-1	896	melatonin2
306-08-1	896	melatonin 3
306-08-1	896	melatonin4
7772-94-3	899	N-acetyl-D-mannosamine 1
7772-94-3	899	N-acetyl-D-mannosamine 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
103-84-4	904	acetanilide 1
103-84-4	904	acetanilide 2
4289-98-9	911	N-formyl-L-methionine 1
4289-98-9	911	N-formyl-L-methionine 2
6589-55-5	913	halostachine 1
6589-55-5	913	halostachine 2
91-20-3	931	naphthalene
98-92-0	936	nicotinamide 1
98-92-0	936	nicotinamide 2
59-67-6	938	nicotinic acid
1492-23-5	954	O-succinylhomoserine 1
1492-23-5	954	O-succinylhomoserine 2
111-87-5	957	1-octanol
50887-69-9	967	orotic acid
50887-69-9	967	orotic acid
328-42-7	970	oxalacetic acid
144-62-7	971	oxalic acid
150-13-0	978	4-aminobenzoic acid
156-39-8	979	4-hydroxyphenylpyruvic acid 1
156-39-8	979	4-hydroxyphenylpyruvic acid 2
100-02-7	980	4-nitrophenol
64519-82-0	985	palmitic acid
599-04-2	989	pantolactone
24259-59-4	993	ribose

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CAS #	PubChem	Compound
63-91-2	994	Phenylalanine 1
63-91-2	994	Phenylalanine 1
85-01-8	995	phenanthrene
156-06-9	997	phenylpyruvate
122-78-1	998	phenylacetaldehyde 1
122-78-1	998	phenylacetaldehyde 2
7568-93-6	1000	2-amino-1-phenylethanol
64-04-0	1001	phenethylamine
64-04-0	1001	phenylethylamine
7664-38-2	1004	phosphoric acid
138-08-9	1005	phosphoenolpyruvic acid
1071-23-4	1015	O-phosphocolamine
88-99-3	1017	phthalic acid
98-98-6	1018	picolonic acid
487-90-1	1021	porphobilinogen
9/3/2466	1023	pyrophosphate
110-60-1	1045	putrescine
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
127-17-3	1060	pyruvic acid
89-00-9	1066	quinolinic acid
107-97-1	1088	sarcosine
3615-56-3	1101	L- sorbose 1
3615-56-3	1101	L- sorbose 2
124-20-9	1102	spermidine 1
124-20-9	1102	spermidine 2
71-44-3	1103	spermine 2
71-44-3	1103	spermine 1
29915-38-6	1110	succinic acid
107-35-7	1123	taurine
68-11-1	1133	thioglycolic acid
65-71-4	1135	thymine
137-00-8	1136	4-methyl-5-thiazoleethanol
365-07-1	1139	thymidine 5'-phosphate 1
365-07-1	1139	thymidine 5'-phosphate 2
66-22-8	1174	uracil
66-22-8	1175	uric acid 1
66-22-8	1175	uric acid 2
57-13-6	1176	urea
104-98-3	1178	urocanic acid 1
104-98-3	1178	urocanic acid 2
121-33-5	1183	vanillin

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CAS #	PubChem	Compound
69-89-6	1188	xanthine
146-80-5	1189	xanthosine
1637-73-6	1198	isocitric acid
55-10-7	1245	DL-4-hydroxy-3-methoxymandelic acid
989-51-5	1287	epigallocatechin gallate
82950-64-9	1321	1,2-didecanoylglyceride
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 1
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 2
42542-10-9	1615	3,4-MDMA
151-18-8	1647	3-aminopropionitrile 1
151-18-8	1647	3-aminopropionitrile 2
503-49-1	1662	3-hydroxy-3-methylglutaric acid (dicrotalic acid)
306-08-1	1738	homovanillic acid (HVA)
54-16-0	1826	5-hydroxyindole-3-acetic acid
608-07-1	1833	methoxytryptamine
38183-03-8	1880	7,8-Dihydroxyflavone
578-86-9	1889	liquiritigenin 1
578-86-9	1889	liquiritigenin 2
578-86-9	1889	liquiritigenin 3
546-88-3	1990	acetohydroxamic acid
1188-21-2	1995	N-acetyl-L-leucine
54965-21-8	2082	albendazole
10191-41-0	2116	alpha tocophereol
57-43-2	2164	Amobarbital
57-43-2	2164	Amobarbital 1
50-78-2	2244	O-acetylsalicylic acid
123-99-9	2266	azelaic acid
57-44-3	2294	Barbital
55-21-0	2331	benzamide
156-08-1	2341	Benzphetamine
622-78-6	2346	benzyl isothiocyanate
484-20-8	2355	5-methoxypsoralen
1812-30-2	2441	Bromazepam
97164-73-3	2479	Butabarbital
77-26-9	2481	Butalbital
58-08-2	2519	caffeine
819-83-0	2526	beta-glycerolphosphate
521-35-7	2543	Cannabinol
36653-82-4	2682	1-hexadecanol
36653-82-4	2682	1-hexadecanol, (cetyl alcohol)
22316-47-8	2789	Clobazam
303-49-1	2801	clomipramine
1622-61-3	2802	Clonazepam
95-48-7	2879	p-cresol
52-52-8	2901	cycloleucine 1

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CAS #	PubChem	Compound
52-52-8	2901	cycloleucine 2
334-48-5	2969	capric acid
439-14-5	3016	Diazepam
13552-09-5	3126	DL-dihydrosphingosine 1
13552-09-5	3126	DL-dihydrosphingosine 2
13552-09-5	3126	DL-dihydrosphingosine 3
479-18-5	3182	dyphylline
80-97-7	3240	5alpha-Cholestan-3-beta-ol
458-24-2	3337	Fenfluramine
458-24-2	3337	Fenfluramine 1
1622-62-4	3380	Flunitrazepam
17617-23-1	3393	Flurazepam
26016-99-9	3417	phosphonomycin
490-79-9	3469	gentisic acid
41001-90-5	3593	hesperetin 1
41001-90-5	3593	hesperetin 2
41001-90-5	3593	hesperetin 3
56-29-1	3608	Hexobarbital
127-07-1	3657	hydroxyurea
101-31-5	3661	hyoscyamine (atropine)
700-06-1	3712	indole-3-carbinol (3-indolemethanol)
700-06-1	3712	indole-3-carbinol 1
830-96-6	3744	indole 3-propionic acid 1
830-96-6	3744	indolepropionic acid
830-96-6	3744	indole 3-propionic acid 2
481-39-0	3806	juglone
492-27-3	3845	4-hydroxyquinoline-2-carboxylic acid(kynurenic acid)
828-01-3	3848	3-phenyllactic acid
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
884-33-3	3858	benzylsuccinic acid
143-07-7	3893	lauric acid
846-49-1	3958	Lorazepam
76-99-3	4095	Methaqualone
298-81-7	4114	xanthotoxin 1
298-81-7	4114	xanthotoxin 2
125-64-4	4162	Methyprylon
146-22-5	4506	Nitrazepam
604-75-1	4616	Oxazepam
604-75-1	4616	Oxazepam 1
106-51-4	4650	p-benzoquinone
76-74-4	4737	Pentobarbital
134-49-6	4762	Phenmetrazine
50-06-6	4763	Phenobarbital

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CAS #	PubChem	Compound
122-09-8	4771	Phentermine 1
122-09-8	4771	Phentermine 2
60-82-2	4788	phloretin
2955-38-6	4890	Prazepam
2078-54-8	4943	propofol
108-46-3	5054	resorcinol
82385-42-0	5143	saccharin 2
82385-42-0	5143	saccharin 1
90-01-7	5146	2-hydroxybenzyl alcohol
76-73-3	5193	Secobarbital
50-67-9	5202	serotonin 1
50-67-9	5202	serotonin 2
57-11-4	5281	stearic acid
846-50-4	5391	Temazepam
28911-01-5	5556	Triazolam
535-83-1	5570	trigonelline
51-67-2	5610	tyramine
51-79-6	5641	carbamic acid ethyl ester (urethane)
59-00-7	5699	4,8-dihydroxyquinoline-2-carboxylic acid (xanthurenic ac
59-00-7	5699	xanthurenic acid
50-27-1	5756	estriol
50-28-2	5757	estradiol
50-66-8	5778	6-methylmercaptapurine 1
50-66-8	5778	6-methylmercaptapurine 2
50-70-4	5780	D-sorbitol
50-81-7	5785	L-ascorbic acid
50-89-5	5789	thymidine
50-89-5	5789	thymidine
95-55-6	5801	2-aminophenol 1
95-55-6	5801	2-aminophenol 2
95-55-6	5801	2-aminophenol 3
51-35-4	5810	trans-4-hydroxy-L-proline 1
51-35-4	5810	trans-4-hydroxy-L-proline 2
51-41-2	5814	norepinephrine (noradrenalin)
51028-73-0	5816	(-)-epinephrine 1
51028-73-0	5816	(-)-epinephrine 2
51-43-4	5816	adrenaline 1
51-43-4	5816	adrenaline 2
51-64-9	5826	d-Amphetamine
53-16-7	5870	1,3,5(10)-estratrien-3-ol-17-one 1
53-16-7	5870	estrone 1
53-16-7	5870	1,3,5(10)-estratrien-3-ol-17-one 2
53-16-7	5870	estrone 2
53-41-8	5879	androsterone
53-43-0	5881	trans-dehydroandrosterone 1

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CAS #	PubChem	Compound
53-43-0	5881	trans-dehydroandrosterone 2
53-96-3	5897	N-2-fluorenylacetamide 1
53-96-3	5897	N-2-fluorenylacetamide 2
56-41-7	5950	L-alanine 1
56-41-7	5950	L-alanine 2
56-45-1	5951	L-serine 1
56-45-1	5951	L-serine 2
56-57-5	5955	4-nitroquinoline N-oxide
56-65-5	5957	adenosine 5'-triphosphate
56-75-7	5959	chloramphenicol 1
56-75-7	5959	chloramphenicol 2
56-84-8	5960	aspartic acid 1
56-84-8	5960	aspartic acid 2
56-87-1	5962	L-lysine 1
56-87-1	5962	L-lysine 2
57-48-7	5984	fructose 1
57-48-7	5984	fructose 2
111-11-5	5988	Sucrose
53-43-0	6013	testosterone 2
53-43-0	6013	testosterone 1
58-63-9	6021	inosine
20398-34-9	6022	adenosine 5'-diphosphate
58-86-6	6027	xylose 1
58-86-6	6027	xylose 2
58-96-8	6029	uridine
3387-36-8	6030	uridine 5'-monophosphate 1
3387-36-8	6030	uridine 5'-monophosphate 2
59-31-4	6038	2-hydroxyquinoline 1
59-31-4	6038	2-hydroxyquinoline 2
57-92-7	6047	L-DOPA 1
57-92-7	6047	L-DOPA 2
60-11-7	6053	methyl yellow
60-12-8	6054	phenylethyl alcohol
60-18-4	6057	L-tyrosine 1
60-18-4	6057	tyrosine 1
60-18-4	6057	L-tyrosine 2
60-18-4	6057	tyrosine 2
60-23-1	6058	2-aminoethanethiol 1
60-23-1	6058	2-aminoethanethiol 2
60-92-4	6076	adenosine 3',5'-cyclic monophosphate
60-92-4	6076	cyclic AMP
6192-52-5	6101	p-toluenesulfonic acid
61-90-5	6106	L-leucine 1
61-90-5	6106	L-leucine 2
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic acid

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CAS #	PubChem	Compound
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic acid
63-05-8	6128	4-androsten-3,17-dione 1
63-05-8	6128	4-androsten-3,17-dione 2
63-37-6	6131	cytidine-5'-monophosphate 1
63-37-6	6131	cytidine-5'-monophosphate 2
63-68-3	6137	L-methionine 1
63-68-3	6137	L-methionine 2
87-78-5	6251	D-mannitol
69-79-4	6255	maltose 1
69-79-4	6255	maltose 2
70-26-8	6262	L-ornithine 1
70-26-8	6262	L-ornithine 2
5934-29-2	6274	L-histidine 1
5934-29-2	6274	L-histidine 2
5934-29-2	6274	L-histidine 3
72-18-4	6287	L-valine 1
72-18-4	6287	L-valine 2
72-19-5	6288	L-threonine 1
72-19-5	6288	L-threonine 2
72-48-0	6293	alizarin
73-22-3	6305	L-tryptophan 1
73-22-3	6305	L-tryptophan 2
77-02-1	6464	Aprobarbital
77-10-1	6468	Phencyclidine
77-93-0	6506	triethyl citrate
77-95-2	6508	quinic acid
137-08-6	6613	pantothenic acid 1
137-08-6	6613	pantothenic acid 2
80-97-7	6665	5alpha-Cholesterol
82-82-6	6723	4-pyridoxic acid 1
82-82-6	6723	4-pyridoxic acid 2
82-86-0	6724	acenaphthenequinone 1
82-86-0	6724	acenaphthenequinone 2
82-86-0	6724	acenaphthenequinone 3
84-66-2	6781	diethyl phthalate
118-00-3	6802	guanosine 1
118-00-3	6802	guanosine 2
5550-12-9	6804	guanosine-5'-monophosphate
86-48-6	6844	1-hydroxy-2-naphthoic acid
86-73-7	6853	fluorene
86-74-8	6854	carbazole 1
86-74-8	6854	carbazole 2
87-99-0	6912	xylitol
88-14-2	6919	2-furoic acid
88-21-1	6926	aniline-o-sulfonic acid

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CAS #	PubChem	Compound
89-83-8	6989	thymol
91-22-5	6998	salicylaldehyde
90-43-7	7017	2-hydroxybiphenyl
92-52-4	7095	biphenyl
93-10-7	7124	quinaldinic acid
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 1
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 2
94-07-5	7172	synephrine 1
94-07-5	7172	synephrine 2
95-16-9	7222	benzothiazole
95-93-2	7269	1,2,4,5-tetramethylbenzene
98-79-3	7405	L-pyroglutamic acid
98-89-5	7413	cyclohexanecarboxylic acid
99-04-7	7418	m-toluic acid
6138-23-4	7427	D-(+) trehalose
99-24-1	7428	methyl gallate
99-24-1	7428	methyl gallate
99-87-6	7463	p-cymene
99-98-9	7472	N,N-dimethyl-1,4-phenylenediamine 1
99-98-9	7472	N,N-dimethyl-1,4-phenylenediamine 2
100-09-4	7478	p-anisic acid
100-46-9	7504	benzylamine
102-71-6	7618	triethanolamine
103-81-1	7680	2-phenylacetamide 1
103-81-1	7680	2-phenylacetamide 2
103-81-1	7680	2-phenylacetamide 3
104-51-8	7705	butylbenzene
104-76-7	7720	2-ethyl-1-hexanol
105-60-2	7768	epsilon-caprolactam
106-32-1	7799	ethyl octanoate
106-33-2	7800	ethyl dodecanoate
106-57-0	7817	glycine anhydride 1
106-57-0	7817	glycine anhydride 2
108-13-4	7911	malonamide 1
108-13-4	7911	malonamide 2
108-13-4	7911	malonamide 3
108-19-0	7913	biuret 1
108-19-0	7913	biuret 2
108-91-8	7965	cyclohexanamine
109-00-2	7971	3-hydroxypyridine
110-65-6	8066	2-butyne-1,4-diol
111-14-8	8094	heptanoic acid
112-05-0	8158	pelargonic acid (nonanoic acid)
112-12-9	8163	2-undecanone 1
112-12-9	8163	2-undecanone 2

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CAS #	PubChem	Compound
112-30-1	8174	1-decanol (decyl alcohol)
112-85-6	8215	behenic acid
112-88-9	8217	1-octadecene
112-95-8	8222	eicosane
115-38-8	8271	Mephobarbital
115-44-6	8275	Talbutal
116-09-6	8299	acetol 1
116-09-6	8299	acetol 2
116-09-6	8299	acetol 3
116-09-6	8299	acetol 4
117-81-7	8343	dioctyl phthalate
118-74-1	8370	hexachlorobenzene
119-53-9	8400	benzoin 1
119-53-9	8400	benzoin 2
119-67-5	8406	2-carboxybenzaldehyde 1
119-67-5	8406	2-carboxybenzaldehyde 2
120-14-9	8419	3,4-dimethoxybenzaldehyde
121-34-6	8468	4-hydroxy-3-methoxybenzoic acid
129-43-1	8512	1-hydroxyanthraquinone
149-57-5	8697	2-ethylhexanoic acid
149-57-5	8697	2-ethylhexanoic acid
149-57-5	8697	2-ethylcaproic acid
138-59-0	8742	shikimic acid
142-08-5	8871	2-hydroxypyridine
142-62-1	8892	hexanoic acid
142-73-4	8897	iminodiacetic acid 1
142-73-4	8897	iminodiacetic acid 2
143-08-8	8914	1-nonanol
18652-93-2	9034	Methohexital
154-23-4	9064	catechin
301-00-8	9316	methyl linolenate
305-84-0	9369	carnosine 1
305-84-0	9369	carnosine 2
306-23-0	9378	3-(4-hydroxyphenyl)lactic acid
6482-98-0	9378	DL-p-hydroxyphenyllactic acid
311-45-5	9395	paraoxon
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
372-75-8	9750	citrulline 1
372-75-8	9750	citrulline 2
372-75-8	9750	citrulline 3
110-93-0	9862	6-methyl-5-hepten-2-one
452-86-8	9958	4-methylcatechol
469-62-5	10100	d-Propoxyphene

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CAS #	PubChem	Compound
484-17-3	10229	9-phenanthrenol
486-25-9	10241	9-fluorenone
486-74-8	10243	4-quinolinecarboxylic acid
487-21-8	10250	lumazine
487-26-3	10251	flavanone 1
487-26-3	10251	flavonone 1
487-26-3	10251	flavanone 2
487-26-3	10251	flavonone 2
487-54-7	10253	salicylurate 1
487-54-7	10253	salicylurate 2
487-89-8	10256	indole-3-carbaldehyde 1
487-89-8	10256	indole-3-carbaldehyde 2
488-69-7	10267	fructose-1,6-diphosphate 1
488-69-7	10267	fructose-1,6-diphosphate 2
499-83-2	10367	pyridine-2,6-dicarboxylic acid
501-94-0	10393	2-(4-hydroxyphenyl)ethanol
501-94-0	10393	4-(2-hydroxyethyl)phenol (tyrosol)
501-97-3	10394	3-(4-hydroxyphenyl)propionic acid
504-02-9	10434	1,3 cyclohexanedione 1
504-02-9	10434	1,3 cyclohexanedione 2
504-02-9	10434	1,3 cyclohexanedione 3
504-15-4	10436	orcinol
504-63-2	10442	1,3-propanediol
505-48-6	10457	suberic acid
506-12-7	10465	heptadecanoic acid
506-30-9	10467	arachidic acid
514-10-3	10569	abietic acid
521-18-6	10635	dihydrotestosterone 1
521-18-6	10635	dihydrotestosterone 2
525-82-6	10680	flavone
528-50-7	10712	cellobiose 1
528-50-7	10712	cellobiose 2
529-64-6	10726	tropic acid
529-69-1	10729	isoxanthopterin
530-57-4	10742	syringic acid
532-28-5	10758	mandelonitrile
532-28-5	10758	mandelonitrile
533-73-3	10787	benzene-1,2,4-triol
536-66-3	10820	4-isopropylbenzoic acid
537-46-2	10836	Methamphetamine 1
537-46-2	10836	Methamphetamine 2
541-15-1	10918	L-carnitine 1
541-15-1	10918	L-carnitine 2
544-63-8	11005	myristic acid
551-16-6	11082	(+)-6-aminopenicillanic acid 1

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CAS #	PubChem	Compound
551-16-6	11082	(+)-6-aminopenicillanic acid 2
551-16-6	11082	(+)-6-aminopenicillanic acid 3
551-16-6	11082	(+)-6-aminopenicillanic acid 4
565-70-8	11266	2-hydroxybutyric acid
566-78-9	11276	21-Acetoxypregnenolone
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
4618-18-2	11333	lactulose 1
4618-18-2	11333	lactulose 3
4618-18-2	11333	lactulose 2
577-85-5	11349	3-hydroxyflavone
589-98-0	11527	3-octanol
593-49-7	11636	heptacosane
615-58-7	11847	2,6-dibromophenol
13545-04-5	11848	2,3-dimethylsuccinic acid
608-66-2	11850	galactitol
611-14-3	11903	2-ethyltoluene
611-73-4	11915	benzoylformic acid 1
611-73-4	11915	benzoylformic acid 2
614-75-5	11970	2-hydroxyphenylacetic acid
615-13-4	11983	2-indanone
615-58-7	12005	2,4-dibromophenol
616-91-1	12035	N-acetyl-L-cysteine 1
616-91-1	12035	N-acetyl-L-cysteine 2
621-37-4	12122	3-hydroxyphenylacetic acid
626-64-2	12290	4-hydroxypyridine
626-97-1	12298	valeramide 1
626-97-1	12298	valeramide 2
626-97-1	12298	valeramide 4
626-97-1	12298	valeramide 3
628-94-4	12364	adipamide 1
628-94-4	12364	adipamide 2
628-94-4	12364	adipamide 3
628-94-4	12364	adipamide 4
629-73-2	12395	hexadecene
630-03-5	12409	nonacosane
21784-30-5	12460	Phendimetrazine
21784-30-5	12460	Phendimetrazine 1
634-97-9	12473	pyrrole -2-carboxylic acid
637-88-7	12511	1,4-cyclohexanedione 1
637-88-7	12511	1,4-cyclohexanedione 2

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CAS #	PubChem	Compound
646-31-1	12592	tetracosane
672-15-1	12647	L-homoserine 1
672-15-1	12647	L-homoserine 2
672-15-1	12647	L-homoserine 3
675-10-5	12663	4-Hydroxy-6-Methylpyran-2-One
675-10-5	12663	4-hydroxy-6-methyl-2-pyrone
675-20-7	12665	2-piperidone 1
675-20-7	12665	2-piperidone 2
701-64-4	12793	phenylphosphoric acid
765-87-7	13006	1,2-cyclohexanedione 1
765-87-7	13006	1,2-cyclohexanedione 2
765-87-7	13006	1,2-cyclohexanedione 3
766-93-8	13017	N-cyclohexylformamide
951-78-0	13712	2-deoxyuridine 1
951-78-0	13712	2-deoxyuridine 2
958-09-8	13730	2'-deoxyadenosine
1032-65-1	13945	2'-deoxycytidine 5'-monophosphoric acid
1138-80-3	14349	N-benzyloxycarbonylglycine
1191-25-9	14490	6-hydroxyhexanoic acid
1191-25-9	14490	6-hydroxy caproic acid
1731-92-6	15609	methyl heptadecanoate
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
10482-56-1	17100	terpineol
2438-80-4	17106	L-(-)-fucose 1
2438-80-4	17106	L-(-)-fucose 2
2478-38-8	17198	Acetosyringone 1
2478-38-8	17198	Acetosyringone 2
3012-37-1	18170	benzyl thiocyanate
3025-96-5	18189	4-acetamidobutyric acid 1
3025-96-5	18189	4-acetamidobutyric acid 2
3068-00-6	18302	butantriol
13022-85-0	18407	4-acetylbutyric acid 1
13022-85-0	18407	4-acetylbutyric acid 2
87-78-5	18950	D-mannose 1
87-78-5	18950	D-mannose 2
3471-31-6	18986	5-methoxy-3-indoleacetic acid 1
3471-31-6	18986	5-methoxy-3-indoleacetic acid 2
3943-74-6	19844	methyl 4-hydroxy-3-methoxybenzoate
4376-20-9	20393	mono(2-ethylhexyl)phthalate
4460-86-0	20525	Asarylaldehyde 1
4460-86-0	20525	Asarylaldehyde 2

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CAS #	PubChem	Compound
1569-60-4	20745	6-methyl-5-hepten-2-ol
327-57-1	21236	L-norleucine 1
327-57-1	21236	L-norleucine 2
6351-10-6	22819	1-indanol
7507-89-3	24135	4-O-Methylphloracetophenone 1
7507-89-3	24135	4-O-Methylphloracetophenone 2
7507-89-3	24135	4-O-Methylphloracetophenone 3
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
123-94-4	24699	1 monostearin
123-94-4	24699	1-stearoyl-rac-glycerol
59-23-4	24749	D-glucose 1
59-23-4	24749	D-glucose 2
10236-47-2	25075	naringin
3128-06-1	26447	L-menthone
14167-59-0	26519	tetratriacontane
14191-95-8	26548	4-hydroxybenzyl cyanide
14721-66-5	26840	phytanic acid
14769-73-4	26879	levamisole
14838-15-4	26934	1R, 2S-Phenylpropylamine
16867-04-2	28115	2,3-dihydroxypyridine
123-35-3	31253	beta-myrcene
128-37-0	31404	2,6-ditert-butyl-4-methylphenol 1
128-37-0	31404	2,6-ditert-butyl-4-methylphenol 2
128-37-0	31404	3,5-Di-tert-butyl-4-hydroxytoluene
22862-76-6	31549	Anisomycin
56-86-0	33032	L-glutamic acid 3 (dehydrated)
56-86-0	33032	L-glutamic acid 1
56-86-0	33032	L-glutamic acid 2
22818-40-2	36143	4-hydroxyphenylglycine 1
22818-40-2	36143	4-hydroxyphenylglycine 2
699012-36-7	41211	adenosine-3'-monophosphate
627-82-7	42953	diglycerol 1
627-82-7	42953	diglycerol 2
627-82-7	42953	diglycerol 3
58-61-7	60961	adenosine
498-00-0	62348	4-hydroxy-3-methoxybenzyl alcohol
1211-29-6	62388	methyljasmonate 1
1211-29-6	62388	methyljasmonate 1
1211-29-6	62388	methyljasmonate 2
1211-29-6	62388	methyljasmonate 3
1211-29-6	62388	methyljasmonate 2

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CAS #	PubChem	Compound
1211-29-6	62388	methyljasmonate 4
363-24-6	62453	4-vinylphenol 1
363-24-6	62453	4-vinylphenol 2
10569-71-9	64956	DL-3-aminoisobutyric acid 1
10569-71-9	64956	DL-3-aminoisobutyric acid 2
154-58-5	64960	1,5-anhydroglucitol
368-16-1	64969	3-methyl-L-histidine
481-05-0	65030	Artemisin
481-05-0	65030	Artemisin 1
997-55-7	65065	N-acetyl-L-aspartic acid 1
997-55-7	65065	N-acetyl-L-aspartic acid 2
1464-44-4	65080	phenyl-beta-glucopyranoside
2140-46-7	65094	25-hydroxycholesterol
6600-40-4	65098	norvaline 1
6600-40-4	65098	norvaline 2
621-44-3	65124	3-nitro-L-tyrosine 1
621-44-3	65124	3-nitro-L-tyrosine 2
	65161	2',3'-dideoxyuridine
6698-26-6	65166	2', 5'-Dideoxyadenosine
19246-18-5	65270	cysteinylglycine 1
19246-18-5	65270	cysteinylglycine 2
19246-18-5	65270	cysteinylglycine 3
62-84-0	65542	4-androsten-7-alpha-ol-3,17-dione 1
62-84-0	65542	4-androsten-7-alpha-ol-3,17-dione 2
1114-34-7	65550	D-lyxose 1
1114-34-7	65550	D-lyxose 2
68-42-8	65553	tetrahydrocorticosterone 1
68-42-8	65553	tetrahydrocorticosterone 2
68-42-8	65553	tetrahydrocorticosterone 3
68-42-8	65553	tetrahydrocorticosterone 4
1002-57-9	66085	8-aminocaprylic acid
10323-20-3	66308	arabinose
681295-24-9	66868	porphine 1
681295-24-9	66868	porphine 2
119-68-6	67069	N-methylantranilic acid 1
119-68-6	67069	N-methylantranilic acid 2
56-89-3	67678	L-cystine 1
56-89-3	67678	L-cystine 2
56-89-3	67678	L-cystine 3
353-09-3	67701	guanidinopropionic acid 1
353-09-3	67701	guanidinopropionic acid 2
500-98-1	68144	phenaceturic acid 1
500-98-1	68144	phenaceturic acid 2
503-66-2	68152	3-hydroxypropanoic acid 1
503-66-2	68152	3-hydroxypropanoic acid 2

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CAS #	PubChem	Compound
503-66-2	68152	3-hydroxypropanoic acid 3
550-33-4	68368	purine riboside
582-24-1	68490	2-hydroxyacetophenone 1
582-24-1	68490	2-hydroxyacetophenone 2
583-08-4	68499	nicotinoylglycine
407-41-0	68841	O-phospho-L-serine 1
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 2
609-71-2	69114	2-hydroxynicotinic acid
611-36-9	69141	4-hydroxyquinoline 1
611-36-9	69141	4-hydroxyquinoline 2
616-04-6	69217	1-methylhydantoin 1
616-04-6	69217	1-methylhydantoin 2
5680-79-5	69221	glycine methyl ester
625-08-1	69362	beta-hydroxyisovalerate
642-71-7	69505	Antiarol
644-90-6	69522	2-aminooctanoic acid 1
644-90-6	69522	2-aminooctanoic acid 2
673-49-4	69602	N-omega-acetylhistamine 2
673-49-4	69602	N-omega-acetylhistamine 1
771-50-6	69867	indole-3-carboxylic acid
771-50-6	69867	indole-3-carboxylic acid
1080-06-4	70652	tyrosine methyl ester 1
1080-06-4	70652	tyrosine methyl ester 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
1194-98-5	70949	2,5-dihydroxybenzaldehyde
1214-20-6	71034	2-Methoxyxanthone
35323-91-2	72276	(-)-epicatechin
35323-91-2	72276	epicatechin 1
35323-91-2	72276	(-)-epicatechin
35323-91-2	72276	epicatechin 2
970-74-1	72277	epigallocatechin
498-40-8	72886	L-cysteic acid
5006-66-6	72924	6-hydroxynicotinic acid
5006-66-6	72924	6-hydroxynicotinic acid
56-86-0	73064	beta-glutamic acid
18829-70-4	73160	catechin
3646-68-2	73563	D-glucosaminic acid 1
3646-68-2	73563	D-glucosaminic acid 1
3646-68-2	73563	D-glucosaminic acid 2
3646-68-2	73563	D-glucosaminic acid 2
1679-53-4	74300	10-hydroxydecanoic acid

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CAS #	PubChem	Compound
1689-64-1	74318	9-hydroxyfluorene
2018-61-3	74839	N-acetyl-L-phenylalanine 1
2018-61-3	74839	N-acetyl-L-phenylalanine 2
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
3555-86-0	77093	phlorobenzophenone 1
3555-86-0	77093	phlorobenzophenone 2
56-57-5	77341	4-nitroquinoline
4104-45-4	77743	3-(methylthio)-propylamine
4385-35-7	78092	3-isochromanone
704-15-4	79101	gly-pro
704-15-4	79101	glycylproline
5704-04-1	79784	tricine 1
5704-04-1	79784	tricine 2
63-42-3	84571	lactose 1
63-42-3	84571	lactose 2
14883-87-5	85782	3,4-dihydroxymandelic acid
601-53-6	85881	coprostan-3-one
16834-13-2	86073	5,10,15,20-tetra(4-pyridyl)-21H,23H-porphine
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 1
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 2
551-68-8	90008	psicose 1
551-68-8	90008	psicose 2
23945-44-0	90301	2,4-dihydroxypyrimidine-5-carboxylic acid
481-37-8	91460	Ecgonine
566-28-9	91474	7-Oxocholesterol
96-82-2	91476	lactitol
601-57-0	91477	(+) -4-cholesten-3-one 1
601-57-0	91477	(+) -4-cholesten-3-one 2
53411-70-4	91493	6-phosphogluconic acid
28822-73-3	91528	DL-3,4-dihydroxyphenyl glycol
566-88-1	92128	5alpha-cholestan-3-one 1
566-88-1	92128	5alpha-cholestan-3-one 2
566-65-4	92810	5-alpha-pregnan-3,20-dione 1
566-65-4	92810	5-alpha-pregnan-3,20-dione 2
10030-67-8	92817	melezitose
10030-67-8	92817	D-(+)-melezitose
617-48-1	92824	D-malic acid
658-79-7	92829	glycyl-L-tyrosine 1
658-79-7	92829	glycyl-L-tyrosine 2
1460-57-7	92886	trans-cyclohexane-1,2-diol
1792-81-0	92903	cis-1,2-cyclohexanediol
1821-52-9	92904	3-indolelactic acid 1
1821-52-9	92904	3-indolelactic acid 2

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CAS #	PubChem	Compound
1946-82-3	92907	N-alpha-acetyl-L-lysine 1
1946-82-3	92907	N-alpha-acetyl-L-lysine 2
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
130-49-4	94136	adenosine 2'-monophosphate
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 1
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 2
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 3
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 4
488-82-4	94154	arabitol
1824-94-8	94214	methyl-beta-D-galactopyranoside
2043-43-8	94220	lactamide 1
2043-43-8	94220	lactamide 2
3233-32-7	96009	4-Acetoxyphenol
3233-32-7	96009	4-Acetoxyphenol 1
6889-80-1	97143	3-Hydroxy-3',4'-Dimethoxyflavone
15450-76-7	97250	2,8-quinolinediol
5965-53-7	97750	diethyl oxalpropionate 1
5965-53-7	97750	diethyl oxalpropionate 2
5965-53-7	97750	diethyl oxalpropionate 3
6133-30-8	97856	guanidinosuccinic acid 1
6133-30-8	97856	guanidinosuccinic acid 2
6133-30-8	97856	guanidinosuccinic acid 3
28954-12-3	99289	L-allothreonine 1
28954-12-3	99289	L-allothreonine 2
10410-83-0	99980	Anthothecol
133-05-1	101612	Asarinin (-)
10094-62-9	101713	glucoheptonic acid 1
10094-62-9	101713	glucoheptonic acid 2
10094-62-9	101713	glucoheptonic acid 3
82801-81-8	105039	3,4-MDEA
79-33-4	107689	L-(+) lactic acid
566-26-7	107722	5-cholesten-3-beta-7-alpha-diol
300-84-5	107812	hypotaurine
64280-14-4	107885	(+/-)-11-nor-9-carboxy-delta-9-THC Standard
19408-84-5	107982	dihydrocapsaicin
34522-32-2	108172	octopine 1
34522-32-2	108172	octopine 2
35608-63-0	110992	3-chloro-L-tyrosine 1
35608-63-0	110992	3-chloro-L-tyrosine 2
5336-08-3	111064	ribonic acid-gamma-lactone 1
5336-08-3	111064	ribonic acid-gamma-lactone 2
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 1
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 2

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CAS #	PubChem	Compound
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 3
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 4
6090-95-5	119054	conduritol epoxide 1
6090-95-5	119054	conduritol epoxide 2
29267-67-2	121805	2-Methoxyresorcinol
516-72-3	121935	20-hydroxycholesterol 1
516-72-3	121935	20-hydroxycholesterol 2
554-62-1	122121	phytosphingosine 1
554-62-1	122121	phytosphingosine 2
0	122281	16-glucuronide-estriol
4484-88-2	122336	trehalose-6-phosphate
65005-57-4	123831	N,N-dimethylarginine
70-18-8	124886	L-glutathione reduced
62471-63-0	124925	8-oxo-2'-deoxyadenosine
13382-27-9	128869	galactonic acid 1
13382-27-9	128869	galactonic acid 2
81-13-0	131204	D-panthenol 1
81-13-0	131204	D-panthenol 2
595-98-2	136386	methyltartronic acid
147-85-3	145742	L-proline 1
147-85-3	145742	L-proline 2
1504-06-9	150923	3-methoxyindole 1
1504-06-9	150923	3-methoxyindole 2
1504-06-9	150923	3-methoxyindole 3
1504-06-9	150923	3-methoxyindole 4
3685-22-1	151138	cis-4-hydroxycyclohexanecarboxylic acid
2734-48-7	151491	3-(1-pyrazolyl)-L-alanine
101-31-5	154417	L-hyoscyamine
3226-65-1	158980	L-methionine sulfoxide 1
3226-65-1	158980	L-methionine sulfoxide 2
3226-65-1	158980	L-methionine sulfoxide 3
19253-88-4	159660	trimethyllysine
13022-85-0	159664	2-ketocaproic acid
342385-52-8	159793	2-keto-L-gulonic acid 1
342385-52-8	159793	2-keto-L-gulonic 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
547-96-6	160520	5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol 1
547-96-6	160520	5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol 2
2922-83-0	161166	L-kynurenine 1
2922-83-0	161166	L-kynurenine 2
7158-70-5	165577	leucrose
6851-36-1	166768	4-hydroxymandelonitrile 1
6851-36-1	166768	4-hydroxymandelonitrile 2

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CAS #	PubChem	Compound
17954-98-2	167685	22-hydroxycholesterol
6968-16-7	169019	D-threitol
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
22879-79-4	171548	biotin
63046-09-3	182362	6,4'-Dihydroxyflavone
961-07-9	187790	2'-deoxyguanosine
93839-95-3	188955	2'-Deoxyadenosine 3' :5'-cyclic monophosphate
72003-83-9	188966	2' Deoxyadenosine 5'-diphosphate
1109-28-0	192826	maltotriose 1
1109-28-0	192826	maltotriose 2
186537-58-6	193653	S-carboxymethylcysteine 1
186537-58-6	193653	S-carboxymethylcysteine 2
0	194988	glycyl-tyrosyl-alanine 1
0	194988	glycyl-tyrosyl-alanine 2
0	194988	glycyl-tyrosyl-alanine 3
0	194988	glycyl-tyrosyl-alanine 4
154-58-5	219984	1,5-anhydro-D-sorbitol
3615-41-6	220001	rhamnose 1
3615-41-6	220001	rhamnose 2
481-06-1	221071	alpha-santonin 1
481-06-1	221071	alpha-santonin 2
53-06-5	222786	cortisone
382-45-6	223997	adrenosterone 1
382-45-6	223997	adrenosterone 2
3081-61-6	228398	L-theanine 1
3081-61-6	228398	L-theanine 2
67-47-0	237332	5-(hydroxymethylfurfural) 1
67-47-0	237332	5-(hydroxymethylfurfural) 2
6307-89-7	238769	2,6-Dihydroxy-4-Methoxytoluene
0	242332	5alpha-androstane-3beta,17beta-diol
42366-37-0	242332	5-alpha-androstane-3 beta,17 beta-diol
79-36-0	246983	lanosterol
3177-80-8	255720	2-amino-3-methoxybenzoic acid 1
3177-80-8	255720	2-amino-3-methoxybenzoic acid 2
527-52-6	258531	digitoxose 1
527-52-6	258531	digitoxose 2
6753-62-4	268779	N-methylglutamic acid 1
6753-62-4	268779	N-methyl-DL-glutamic acid 1
6753-62-4	268779	N-methylglutamic acid 2
6753-62-4	268779	N-methyl-DL-glutamic acid 2
6753-62-4	268779	N-methylglutamic acid 3
6753-62-4	268779	N-methyl-DL-glutamic acid 3
6753-62-4	268779	N-methylglutamic acid 4

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CAS #	PubChem	Compound
2497-02-1	273260	N-acetyl-L-histidine 1
2497-02-1	273260	N-acetyl-L-histidine 2
627-01-0	316542	N-ethylglycine 1
627-01-0	316542	N-ethylglycine 2
2140-79-6	317398	2-O-Methyladenosine
771-51-7	351795	3-indoleacetonitrile
	364106	4,4'-Dimethoxydalbergione 1
	364106	4,4'-Dimethoxydalbergione 2
18457-55-1	369312	(-)-perillyl alcohol
15673-79-7	439167	D-ribose-5-phosphate 1
15673-79-7	439167	D-ribose-5-phosphate 2
2457-80-9	439176	5'-deoxy-5'-(methylthio)adenosine 1
2457-80-9	439176	5'-deoxy-5'-(methylthio)adenosine 2
80731-10-8	439183	3-phosphoglyceric acid
820-11-1	439183	3-phosphoglycerate
108321-99-9	439184	ribulose-5-phosphate 3
499-40-1	439193	isomaltose 1
499-40-1	439193	isomaltose 2
473-81-4	439194	glyceric acid
16096-97-2	439196	L-dithiothreitol 1
16096-97-2	439196	L-dithiothreitol 2
551-84-8	439204	xylulose
14982-50-4	439215	galacturonic acid 1
14982-50-4	439215	galacturonic acid 2
6202-10-4	439216	dihydroorotic acid 1
6202-10-4	439216	dihydroorotic acid 2
6202-10-4	439216	dihydroorotic acid 3
535-75-1	439227	pipecolic acid 1
535-75-1	439227	pipecolic acid 2
0	439232	N-acetyl-ornithine 1
0	439232	N-acetyl-ornithine 2
1114-34-7	439240	D-lyxose 1
1114-34-7	439240	D-lyxose 2
17629-30-0	439242	Raffinose
154-17-6	439268	deoxyglucose 1
154-17-6	439268	deoxyglucose 2
9/8/4350	439280	5-hydroxy-L-tryptophan 1
9/8/4350	439280	5-hydroxy-L-tryptophan 2
846-46-8	439289	5alpha-Androstan-3, 17-Dione 1
846-46-8	439289	5alpha-Androstan-3, 17-Dione 2
6892-68-8	439352	1,4-dithioerythritol
1128-23-0	439373	L-gulonic acid gamma-lactone
3687-64-7	439451	galactinol 1
3687-64-7	439451	galactinol 2
480-18-2	439533	taxifolin

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CAS #	PubChem	Compound
13718-94-2	439559	palatinose
626-72-2	439579	L-homocystine 1
626-72-2	439579	L-homocystine 2
626-72-2	439579	L-homocystine 3
17199-29-0	439616	mandelic acid
38819-01-1	439626	cellotetraose
95-43-2	439665	threose 1
95-43-2	439665	threose 2
45159-34-0	439742	beta-cyano-L-alanine
7568-08-4	439746	6-deoxy-D-glucose 1
7568-08-4	439746	6-deoxy-D-glucose 2
585-18-2	439762	sucrose-6-phosphate 1
585-18-2	439762	sucrose-6-phosphate 2
6263-10-8	439766	citramalic acid
32449-92-6	439782	glucuronolactone 1
32449-92-6	439782	glucuronolactone 2
32449-92-6	439782	glucuronolactone 3
1/5/2280	439917	N-acetyl-D-tryptophan 3
2280-01-5	439917	N-acetyl-D-tryptophan 1
2280-01-5	439917	N-acetyl-D-tryptophan 2
56-73-5	439958	D-glucose-6-phosphate 1
56-73-5	439958	D-glucose-6-phosphate 2
113573-73-2	440053	S(-)willardiine 1
113573-73-2	440053	S(-)willardiine 2
470-69-9	440080	kestose
1229-12-5	440114	5beta-androstane-3,17-dione
0-00-0	440168	1,3,5(10)-estratrien-3,6- beta-17-beta-triol
24940-57-6	440274	N,N-dimethyl-L-histidine
51268-88-3	440294	cis-1,2-dihydro-1,2-naphthalenediol
51268-88-3	440294	(1R,2S)-cis-1,2-dihydro-1,2-naphthalenediol
500-44-7	440473	L-mimosine 1
500-44-7	440473	L-mimosine 2
79-36-0	440560	dihydrolanosterol
8/2/4298	440575	trans-3-hydroxy-L-proline 1
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 2
362-06-1	440623	2-hydroxyestrone 1
362-06-1	440623	2-hydroxyestrone 2
66009-10-7	440658	melibiose 1
66009-10-7	440658	melibiose 2
5989-27-5	440917	limonene
497-76-7	440936	arbutin
1990-29-0	441032	D (+)altrose 1
1990-29-0	441032	D (+)altrose 2

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CAS #	PubChem	Compound
2595-98-4	441035	talose 1
2595-98-4	441035	talose 2
359-83-1	441278	Pentazocine
5996-00-9	441422	beta-gentiobiose 1
5996-00-9	441422	beta-gentiobiose 2
154-41-6	441457	Phenylpropanolamine
13241-33-3	442439	neohesperidin
20549-47-7	443163	(-)-dihydrocarveol 1
20549-47-7	443163	(-)-dihydrocarveol 2
0	443239	DL-threo-beta-hydroxyaspartic acid
7298-99-9	443239	threo-3-hydroxy-L-aspartate
146255-66-5	443586	3,5-dihydroxyphenylglycine 1
146255-66-5	443586	3,5-dihydroxyphenylglycine 2
6906-38-3	443650	delphinidin 3-glucoside
6906-38-3	443650	delphinidin 3-glucoside 2
6906-38-3	443650	delphinidin 3-glucoside 3
6988-81-4	443651	petunidin-3-glucoside
6988-81-4	443651	petunidin-3-glucoside 2
7228-78-6	443652	malvidin-3-glucoside
6906-39-4	443654	peonidin-3-glucoside
6906-39-4	443654	peonidin-3-glucoside 2
585-84-2	444212	trans-aconic acid
110-16-7	444266	maleic acid
133-37-9	444305	tartaric acid
140-10-3	444539	cinnamic acid
57-87-4	444679	ergosterol
302-79-4	444795	retinoic acid
17013-01-3	444972	fumaric acid
131-48-6	445063	n-acetylneuraminic acid 1
131-48-6	445063	n-acetylneuraminic acid 2
106-28-5	445070	trans-trans-farnesol
501-36-0	445154	trans- resveratrol
501-36-0	445154	resveratrol
373-49-9	445638	palmitoleic acid
112-80-1	445639	oleic acid
1135-24-6	445858	ferulic acid
14982-50-4	445929	galacturonic acid 1
14982-50-4	445929	galacturonic acid 2
7365-44-8	446188	TES
50-36-2	446220	Cocaine
10417-94-4	446284	eicosapentaenoic acid
519-09-5	448223	Benzoyllecgonine
579-36-2	448388	D-allose 1
579-36-2	448388	D-allose 2
13114-27-7	449093	zeatin 1

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CAS #	PubChem	Compound
13114-27-7	449093	zeatin 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
2268-98-6	519975	11a-Acetoxyprogesterone 1
2268-98-6	519975	11a-Acetoxyprogesterone 2
4472-73-5	521171	3,4',5,6,7-Pentamethoxyflavone
104-55-2	637511	cinnamaldehyde 1
104-55-2	637511	cinnamaldehyde 2
112-79-8	637517	elaidic acid
103-26-4	637520	methyl cinnamate
614-60-8	637540	2-hydroxycinnamic acid
588-30-7	637541	3-hydroxycinnamic acid
608-07-1	637542	4-hydroxycinnamic acid
106-24-1	637566	geraniol
106-24-1	637566	geraniol
530-59-6	637775	3,5-dimethoxy-4-hydroxycinnamic acid 1
530-59-6	637775	3,5-dimethoxy-4-hydroxycinnamic acid 2
5391-40-5	638011	citral 1
5391-40-5	638011	citral 2
5391-40-5	638011	citral 3
5391-40-5	638011	citral 4
14901-07-6	638014	beta-ionone 1
14901-07-6	638014	beta-ionone 2
94-62-2	638024	piperine 1
94-62-2	638024	piperine 2
498-23-7	638129	citraconic acid
	641605	trans fertaric acid
959-23-9	641818	4'-Methoxychalcone
959-23-9	641818	4'-Methoxychalcone 1
959-23-9	641818	4'-Methoxychalcone 2
67879-58-7	642609	trans caftaric acid 1
67879-58-7	642609	trans caftaric acid 2
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
1120-25-8	643801	methyl palmitoleate
529-38-4	644006	Cocaethylene
13956-29-1	644019	Cannabidiol
367-93-1	656894	isopropyl beta-D-1-thiogalactopyranoside
10083-24-6	667639	piceatannol
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

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CAS #	PubChem	Compound
79786-40-6	676293	6,3'-Dimethoxyflavone
	688664	3,7-Dimethoxyflavone
2316-26-9	717531	3,4-Dimethoxycinnamic Acid 1
2316-26-9	717531	3,4-Dimethoxycinnamic Acid 2
16652-64-5	725701	O-benzyl-L-tyrosine 1
16652-64-5	725701	O-benzyl-L-tyrosine 2
4707-46-4	736228	3-Methylorsellinic Acid 1
4707-46-4	736228	3-Methylorsellinic Acid 2
	808242	3-methoxy-N-3-quinolinybenzamide 1
	808242	3-methoxy-N-3-quinolinybenzamide 2
404-86-4	1548943	capsaicin
141-12-8	1549026	neryl acetate 1
141-12-8	1549026	neryl acetate 2
458-35-5	1549095	coniferyl alcohol
331-39-5	1549111	caffeic acid
	1597617	(4-Hydroxy-2-oxo-1,2-dihydro-quinolin-3-yl)-acetic acid k
4896-77-9	2723970	glycine-d5 deuterated
87-81-0	2724552	tagatose 1
87-81-0	2724552	tagatose 2
498-07-7	2724705	1,6-anhydro-glucose
3391-86-4	2724898	1-octen-3-ol
24607-05-4	3015189	Avocadyne
585-88-6	3034828	palatinitol 1
64519-82-0	3034828	palatinitol 2
526-99-8	3037582	mucic acid
1114-81-4	3246323	O-phospho-L-threonine 1
1114-81-4	3246323	O-phospho-L-threonine 2
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
14528-64-4	3505109	4-nitrocatechol
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
	3554670	2-Methylene-5-(2,5-Dioxotetrahydrofuran-3-YL)-6-OXO-
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
32860-62-1	3625615	maltotriitol
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
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 1

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CAS #	PubChem	Compound
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 2
	3908719	2,3,4'-Trihydroxy-4-Methoxybenzophenone 3
	4000243	3,4-Didesmethyl-5-Deshydroxy-3'-Ethoxyscleroin
7057-27-4	4085802	3'-deoxyuridine 1
7057-27-4	4085802	3'-deoxyuridine 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
96-26-4	4180364	1,3-dihydroxyacetone
	4303260	Anhydrobrazilic Acid
	4303260	Anhydrobrazilic Acid 1
	4620898	12a-Hydroxy-6-Deoxydehydromunduserone
534-46-3	4623424	sophorose 1
534-46-3	4623424	sophorose 2
	4646739	12a-Hydroxy-9-Demethylmunduserone-8-Carboxylic Aci
	5024745	2-Hydroxy-5 (6)Epoxy-Tetrahydrocaryophyllene
	5176389	3,7-Epoxycaryophyllan-6-Ol
459-80-3	5275520	geranic acid
123-78-4	5280335	D-sphingosine 1
123-78-4	5280335	D-sphingosine 2
123-78-4	5280335	D-sphingosine 3
111-02-4	5280370	squalene
3681-93-4	5280441	vitexin 1
3681-93-4	5280441	vitexin 2
480-44-4	5280442	Acacetin
480-44-4	5280442	Acacetin 1
520-36-5	5280443	Apigenin
60-33-3	5280450	linoleic acid
557-24-4	5280451	maleamic acid 1
557-24-4	5280451	maleamic acid 2
557-24-4	5280451	maleamic acid 3
92-61-5	5280460	scopoletin
628-48-8	5280498	glutaconic acid 1
628-48-8	5280498	glutaconic acid 2
537-33-7	5280507	sinapyl alcohol 1
537-33-7	5280507	sinapyl alcohol 2
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 1
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 2
90-33-5	5280567	4-methylumbelliferone
90-33-5	5280567	4-methylumbelliferone
19317-11-4	5280598	farnesal 1
19317-11-4	5280598	farnesal 2
19317-11-4	5280598	farnesal 3

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CAS #	PubChem	Compound
19317-11-4	5280598	farnesal 4
67-97-0	5280795	cholecalciferol 1
67-97-0	5280795	cholecalciferol 2
4206-58-0	5280802	trans-3,5-dimethoxy-4-hydroxycinnamaldehyde
21637-25-2	5280804	isoquercitrin 1
21637-25-2	5280804	isoquercitrin 2
520-18-3	5280863	kaempferol 1
520-18-3	5280863	kaempferol 2
35850-13-6	5280887	15-keto-prostaglandin F2alpha
35850-13-6	5280887	15-keto-prostaglandin F-2-alpha
446-72-0	5280961	4',5,7-trihydroxyisoflavone
79-57-2	5280972	oxytetracycline
480-40-0	5281607	chrysin
529-44-2	5281672	myricetin
486-66-8	5281708	daidzein
552-59-0	5281804	prunetin
476-66-4	5281855	ellagic acid
4423-37-4	5281953	syringetin
2196-14-7	5282073	7,4'-Dihydroxyflavone
53472-37-0	5282154	laricitrin
13419-69-7	5282707	2-hexenoic acid
2091-39-6	5282805	eicosa-11,14-dienoic acid
111-03-5	5283468	1 monoolein
76-57-3	5284371	Codeine
466-99-9	5284570	Hydromorphone 1
466-99-9	5284570	Hydromorphone 2
76-41-5	5284604	Oxymorphone
76-41-5	5284604	Oxymorphone 1
100-61-8	5288725	N-methylalanine
57-27-2	5288826	Morphine
928-94-9	5318042	2-hexen 1-ol
5041-82-7	5318644	isorhamnetin-3--glucoside
3443-84-3	5319879	2-oleoylglycerol
83-46-5	5321342	beta-sitosterol
110-15-6	5321515	stigmasterol
115-37-7	5324289	Thebaine
1086-80-2	5326566	7,8-dimethylalloxazine
4436-74-2	5351896	trans-3-hexenedioic acid
629-98-1	5354168	cis-13-Docosanol
2107-77-9	5355836	4-Methylaphnetin
6342-92-3	5355888	2',5'-Dihydroxy-4-Methoxychalcone
3588-17-8	5356793	trans,trans-muconic acid
112-62-9	5364509	methyl oleate
7541-49-3	5366244	phytol 1
7541-49-3	5366244	phytol 2

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CAS #	PubChem	Compound
1214-47-7	5367146	2-hydroxychalcone 1
1214-47-7	5367146	2-hydroxychalcone 2
38186-71-9	5379071	2',3-Dihydroxy-4,4',6'-Trimethoxychalcone
492-00-2	5393152	3,7-Dihydroxyflavone
0	5459862	D-erythrose-4-phosphate 1
0	5459862	D-erythrose-4-phosphate 2
533-67-5	5460005	2-deoxy-D-ribose 1
533-67-5	5460005	2-deoxy-D-ribose 2
4637-56-3	5460367	4-Hydroxyaminoquinoline-N-oxide
7306-96-9	5460407	threonic acid
87-73-0	5460673	D-saccharic acid
547-25-1	5460935	turanose 1
547-25-1	5460935	turanose 2
	5781145	2'-Methoxyformonetin
69616-74-6	5955473	2',4-Dihydroxy-3,4',6'-Trimethoxychalcone
693-71-0	6161490	trans-13-octadecenoic acid
130405-40-2	6419835	catechin gallate
7541-49-3	6430833	phytol 1
7541-49-3	6430833	phytol 2
6025-53-2	6440982	trans-Zeatin-riboside
561-63-7	6453303	19-hydroxycholesterol
327-97-9	6537496	chlorogenic acid 1
327-97-9	6537496	chlorogenic acid 2
	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
	6708683	3-Deshydroxysappanol Trimethyl Ether
	6708739	2,3,4-Trihydroxy-4'-Ethoxybenzophenone
897-06-3	6710699	Androsta-1, 4-Dien-3, 17-Dione 1
897-06-3	6710699	Androsta-1, 4-Dien-3, 17-Dione 2
	6728940	2,3-Dihydroxy-4-Methoxy-4'-Ethoxybenzophenone
	6728949	3beta-Hydroxy-23, 24-Bisnorchol-5-Enic Acid
3371-27-5	9882981	galocatechin
	9925625	propofol hemisuccinate
2875-41-4	10034670	N-(3-Aminopropyl)glycine 1
2875-41-4	10034670	N-(3-Aminopropyl)glycine 2
161886-59-5	11058264	(S)-Carnitine Mesylate Isobutylester
225101-69-9	12205373	L-alanine-2,3,3,3-d4
27208-80-6	12314237	trans piceid
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
7084-29-9	13845047	5-methyl-3'-deoxyuridine 1
7084-29-9	13845047	5-methyl-3'-deoxyuridine 2
1401-55-4	16133892	tannic acid
18524-94-2	16212335	loganin
1731-84-6	16213400	Cholestrol D6

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CAS #	PubChem	Compound
0	16213445	L-tyrosine-3,3-d2 1
0	16213445	L-tyrosine-3,3-d2 2
6556-12-3	16213610	glucuronic acid 1
6556-12-3	16213610	glucuronic acid 3
6556-12-3	16213610	glucuronic acid 2
6556-12-3	16213610	glucuronic acid 4
0	16217112	D-glucose-C-d7 1
0	16217112	D-glucose-C-d7 2
585-88-6	16217663	maltitol
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
7512-17-6	16218892	N-acetyl-D-glucosamine 1
7512-17-6	16218892	N-acetyl-D-glucosamine 2
1175-06-0	16219541	5alpha-Cholestan-3beta-OI-6-One 1
1175-06-0	16219541	5alpha-Cholestan-3beta-OI-6-One 2
96-82-2	16219560	lactobionic acid 1
96-82-2	16219560	lactobionic acid 2
96-82-2	16219560	lactobionic acid 3
1180-71-8	16219587	limonin
15763-06-1	16219662	1-methyladenosine 1
15763-06-1	16219662	1-methyladenosine 2
469-90-9	16219957	sedoheptulose anhydride monohydrate
42155-08-8	18601100	2'-Deoxyuridine 5'-monophosphate 1
42155-08-8	18601100	2'-Deoxyuridine 5'-monophosphate 2
102916-66-5	25245723	2-deoxyribose 5-phosphate
0		L-glutamic acid-2,3,3,4,4-d5 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		3-amino-3-(4-hydroxy-phenyl)-propionic acid 1
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 2
		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
		trans coutaric acid
110-42-9		Methyl Caprate
111-11-5		Methyl Caprylate
111-82-0		Methyl Laurate
1120-28-1		Methyl Eicosanoate
112-39-0		Methyl Palmitate
112-61-8		Methyl Stearate
123316-61-0		5-Hydroxy-2',4',7,8-Tetramethoxyflavone
124-10-7		Methyl Myristate

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CAS #	PubChem	Compound
1731-84-6		Methyl Pelargonate
2442-49-1		Methyl Linocerate
55682-92-3		Methyl Octacosanoate
5802-82-4		Methyl Hexacosanoate
60658-41-5		Myristic Acid d27
629-83-4		Methyl Triacontanoate
929-77-1		Methyl Docosanoate