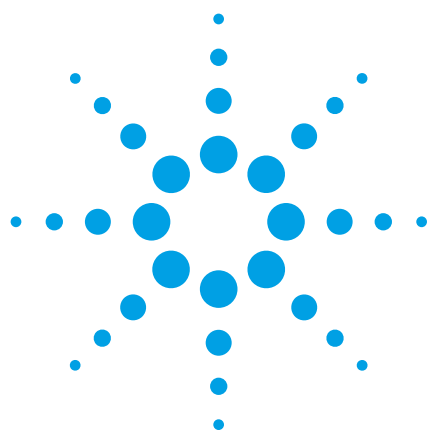




G1676AA Agilent Fiehn GC/MS Metabolomics RTL Library: List of Compounds

Data Sheet

More library compounds for more positive identifications

The Agilent Fiehn GC/MS Metabolomics RTL Library is the most comprehensive library of metabolite GC/MS spectra that is commercially available. This expanding library currently contains 1050 entries for approximately 700 common metabolites, including entries corresponding to partially derivatized metabolites for metabolites that do not always derivatize completely.

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



Agilent Technologies

CAS #	PubChem	Compound
1118-68-9	673	N,N-dimethylglycine
51-79-6	5641	carbamic acid ethyl ester (urethane)
105-60-2	7768	epsilon-caprolactam
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
127-17-3	1060	pyruvic acid
79-33-4	107689	L-(+) lactic acid
108-91-8	7965	cyclohexanamine
79-14-1	757	glycolic acid
72-18-4	6287	L-valine 1
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
3715-29-5	49	3-methyl-2-oxobutanoic acid 1
6600-40-4	65098	norvaline 1
141-97-9	96	acetoacetate 1
111-11-5	8091	octanoic acid methyl ester
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
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
61-90-5	6106	L-leucine 1
2043-43-8	94220	lactamide 2
100-61-8	5288725	N-methylalanine
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 1
4502-00-5	70	2-ketoisocaproic acid 1
147-85-3	145742	L-proline 1

CAS #	PubChem	Compound
443-79-8	791	DL-isoleucine 1
147-85-3	614	L-proline 1
122-78-1	998	phenylacetaldehyde 1
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
91-20-3	931	naphthalene
141-82-2	867	malonic acid 1
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
10569-71-9	64956	DL-3-aminoisobutyric acid 1
516-05-2	487	methylmalonic acid
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
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
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
124-07-2	379	caprylic acid
766-93-8	13017	N-cyclohexylformamide
535-75-1	439227	pipecolic acid 1
151-18-8	1647	3-aminopropionitrile 2
56-81-5	753	glycerol
61-90-5	6106	L-leucine 2

CAS #	PubChem	Compound
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
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
28954-12-3	99289	L-allothreonine 1
637-88-7	12511	1,4-cyclohexanedione 1
72-19-5	6288	L-threonine 1
443-79-8	791	DL-isoleucine 2
504-02-9	10434	1,3 cyclohexanedione 1
59-67-6	938	nicotinic acid
147-85-3	145742	L-proline 2
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
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
473-81-4	439194	glyceric acid
681295-24-9	66868	porphine 1
66-22-8	1174	uracil
13022-85-0	18407	4-acetylbutyric acid 2
765-87-7	13006	1,2-cyclohexanedione 1

CAS #	PubChem	Compound
97-65-4	811	itaconic acid
5391-40-5	638011	citral 2
17013-01-3	444972	fumaric acid
3012-37-1	18170	benzyl thiocyanate
634-97-9	12473	pyrrole -2-carboxylic acid
498-23-7	643798	citraconic acid 1
532-28-5	10758	mandelonitrile
6351-10-6	22819	1-indanol
532-28-5	10758	mandelonitrile
123-30-8	403	4-aminophenol 1
26016-99-9	3417	phosphonomycin
5391-40-5	638011	citral 3
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
56-41-7	5950	L-alanine 2
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
45159-34-0	439742	beta-cyano-L-alanine
103-84-4	904	acetanilide 2
108-46-3	5054	resorcinol
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 1
498-23-7	643798	citraconic acid 2
72-19-5	6288	L-threonine 2
92-52-4	7095	biphenyl
452-86-8	9958	4-methylcatechol
80-69-3	45	tartronic acid
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 2
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

CAS #	PubChem	Compound
5965-53-7	97750	diethyl oxalpropionate 2
108-13-4	7911	malonamide 1
488-17-5	340	3-methylcatechol
98-92-0	936	nicotinamide 1
123-31-9	785	hydroquinone
536-60-7	325	4-isopropylbenzyl alcohol
18457-55-1	369312	(-)-perillyl alcohol
103-81-1	7680	2-phenylacetamide 2
765-87-7	13006	1,2-cyclohexanedione 2
63-68-3	6137	L-methionine 1
501-52-0	107	hydrocinnamic acid
141-82-2	867	malonic acid 2
8/2/4298	440575	trans-3-hydroxy-L-proline 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
500-44-7	440473	L-mimosine 2
557-24-4	5280451	maleamic acid 1
498-23-7	643798	citraconic acid 3
95-43-2	439665	threose 1
498-23-7	643798	citraconic acid 4
504-15-4	10436	orcinol
100-83-4	101	3-hydroxybenzaldehyde
672-15-1	12647	L-homoserine 2
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

CAS #	PubChem	Compound
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
8/2/4298	440575	trans-3-hydroxy-L-proline 2
52-90-4	594	L-cysteine 1
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
611-73-4	11915	benzoylformic acid 1
3106-60-3	457	1-methyl nicotinamide 1
98-92-0	936	nicotinamide 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
123-08-0	126	4-hydroxybenzaldehyde 1
3025-96-5	18189	4-acetamidobutyric acid 1
59-31-4	6038	2-hydroxyquinoline 1
1504-06-9	150923	3-methyloxyindole 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
50-78-2	2244	O-acetylsalicylic acid
3025-96-5	18189	4-acetamidobutyric acid 2
1188-37-0	70914	N-acetyl-L-glutamic acid 1
119-84-6	660	dihydrocoumarin 1
69-72-7	338	salicylic acid
100-02-7	980	4-nitrophenol
4436-74-2	5351896	trans-3-hexenedioic acid
463-00-3	500	4-guanidinobutyric acid 1
14191-95-8	26548	4-hydroxybenzyl cyanide
63-68-3	6137	L-methionine 2

CAS #	PubChem	Compound
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
56-86-0	33032	L-glutamic acid 3 (dehydrated)
536-66-3	10820	4-isopropylbenzoic acid
100-09-4	7478	p-anisic acid
4385-35-7	78092	3-isochromanone
111-82-0		Methyl Laurate
5746-86-1	412	normicotine
71-30-7	597	cytosine 2
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
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
1504-06-9	150923	3-methyloxyindole 2
463-00-3	500	4-guanidinobutyric acid 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
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
119-68-6	67069	N-methylantranilic acid 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

CAS #	PubChem	Compound
56-57-5	77341	4-nitroquinoline
119-84-6	660	dihydrocoumarin 2
557-24-4	5280451	maleamic acid 3
6753-62-4	268779	N-methyl-DL-glutamic acid 2
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
119-67-5	8406	2-carboxybenzaldehyde 1
5006-66-6	72924	6-hydroxynicotinic acid
3237-44-3	36	2-isopropylmalic acid
501-94-0	10393	2-(4-hydroxyphenyl)ethanol
503-66-2	68152	3-hydroxypropanoic acid 2
328-50-7	51	alpha ketoglutaric acid
501-94-0	10393	4-(2-hydroxyethyl)phenol (tyrosol)
156-06-9	997	phenylpyruvate
828-01-3	3848	3-phenyllactic acid
0	444718	L-beta-phenyllactic acid
19253-88-4	159660	trimethyllysine
123-30-8	403	4-aminophenol 3
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
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
70-47-3	16217724	L-asparagine-15N2,d8 1
503-49-1	1662	3-hydroxy-3-methylglutaric acid (dicrotalic acid)
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

CAS #	PubChem	Compound
70-26-8	6262	L-ornithine 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
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
133-37-9	444305	tartaric acid
498-00-0	62348	4-hydroxy-3-methoxybenzyl alcohol
156-38-7	127	4-hydroxyphenylacetic acid
360-97-4	9679	5-aminoimidazole-4-carboxamide 1
108-73-6	359	phloroglucinol
99-98-9	7472	N,N-dimethyl-1,4-phenylenediamine 2
121-33-5	1183	vanillin
109-76-2	428	1,3-diaminopropane 1
39840-37-4	156807	D-lyxosylamine 1
1114-34-7	65550	D-lyxose 1
1114-34-7	439240	D-lyxose 1
689-31-6	71	2-ketoadipic acid 1
143-07-7	3893	lauric acid
7298-99-9	443239	threo-3-hydroxy-L-aspartate
997-55-7	65065	N-acetyl-L-aspartic acid 1
39840-37-4	156807	D-lyxosylamine 2
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
462-88-4	111	3-ureidopropionate 2
51268-88-3	440294	(1R,2S)-cis-1,2-dihydro-1,2-naphthalenediol
997-55-7	65065	N-acetyl-L-aspartic acid 2
660-88-8	138	5-aminovaleric acid 2
70-47-3	16217724	L-asparagine-15N2,d8 3
70-47-3	236	L-asparagine 2

CAS #	PubChem	Compound
9/3/2466	1023	pyrophosphate
1504-06-9	150923	3-methyloxyindole 3
5336-08-3	111064	ribonic acid-gamma-lactone 1
462-88-4	111	3-ureidopropionate 3
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
6753-62-4	268779	N-methylglutamic acid 4
3106-60-3	457	1-methyl nicotinamide 2
88-99-3	1017	phthalic acid
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
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
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
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

CAS #	PubChem	Compound
89-00-9	1066	quinolinic acid
582-60-5	675	5,6 - dimethylbenzimidazole 1
1211-29-6	62388	methyljasmonate 3
1211-29-6	62388	methyljasmonate 2
819-83-0	2526	beta-glycerolphosphate
488-81-3	827	ribitol
119-84-6	660	dihydrocoumarin 4
7568-93-6	1000	2-amino-1-phenylethanol
99-50-3	19	2,3-dihydroxybenzoic acid
110-60-1	1045	putrescine
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
2438-80-4	17106	L-(-)-fucose 1
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
585-84-2	444212	trans-aconitic acid
2041-14-7	339	ciliatine
3226-65-1	158980	L-methionine sulfoxide 1
1211-29-6	62388	methyljasmonate 4
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
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
34363-28-5	754	glycerol 1-phosphate
23945-44-0	90301	2,4-dihydroxypyrimidine-5-carboxylic acid
486-74-8	10243	4-quinolinecarboxylic acid
56-85-9	738	L-glutamine 3
82385-42-0	5143	saccharin 2
108-19-0	7913	biuret 2
490-79-9	3469	gentisic acid

CAS #	PubChem	Compound
7198-10-9	328	DL-4-hydroxymandelic acid
119-84-6	660	dihydrocoumarin 5
19317-11-4	5280598	farnesal 1
1114-81-4	3246323	O-phospho-L-threonine 1
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
407-41-0	68841	O-phospho-L-serine 1
3226-65-1	158980	L-methionine sulfoxide 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
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
28954-12-3	99289	L-allothreonine 2
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
68-94-0	790	hypoxanthine 1
673-49-4	69602	N-omega-acetylhistamine 2
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

CAS #	PubChem	Compound
2163-68-0	16553	atrazin-2-hydroxy 1
1679-53-4	74300	10-hydroxydecanoic acid
700-06-1	3712	indole-3-carbinol 1
628-94-4	12364	adipamide 3
119-53-9	8400	benzoin 1
85-01-8	995	phenanthrene
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
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
102-32-9	547	2-(3,4-dihydroxyphenyl)acetic acid
82385-42-0	5143	saccharin 1
186537-58-6	193653	S-carboxymethylcysteine 2
451-13-8	780	homogentisic acid
102-32-9	547	3,4-dihydroxyphenylacetic acid
150-13-0	978	4-aminobenzoic acid
60658-41-5		Myristic Acid d27
82-82-6	6723	4-pyridoxic acid 1
407-41-0	68841	O-phospho-L-serine 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
407-41-0	68841	O-phospho-L-serine 2
51-43-4	5816	adrenaline 1
490-83-5	835	dehydroascorbic acid 1
495-69-2	464	hippuric acid 2

CAS #	PubChem	Compound
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
1824-94-8	94214	methyl-beta-D-galactopyranoside
87-81-0	439312	D-tagatose 1
156-39-8	979	4-hydroxyphenylpyruvic acid 1
2163-68-0	16553	atrazin-2-hydroxy 3
923-16-0	601	D-Ala-D-Ala 4
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-methyloxyindole 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
73-24-5	190	adenine 1
548-93-6	86	3-hydroxyanthranilic acid 2
628-94-4	12364	adipamide 4
77-95-2	6508	quinic acid
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
87-81-0	439312	D-tagatose 2
490-83-5	835	dehydroascorbic acid 2
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 1
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
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
500-98-1	68144	phenaceturic acid 1

CAS #	PubChem	Compound
5934-29-2	6274	L-histidine 2
3615-56-3	1101	L- sorbose 2
87-89-8	892	allo-inositol
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
1188-38-1	3679006	N-carbamyl-L-glutamic acid 2
583-08-4	68499	nicotinoylglycin
0	16213445	L-tyrosine-3,3-d2 1
60-18-4	6057	tyrosine 1
97-59-6	204	allantoin 2
574-17-4	11321	acetylisatin 6
24940-57-6	440274	N,N-dimethyl-L-histidine
65-23-6	1054	pyridoxine
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
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
90-80-2	736	gluconic acid lactone 2
87-78-5	18950	D-mannose 2
6556-12-3	16213610	glucuronic acid 1
1990-29-0	441032	D (+)altrose 2
1120-25-8	643801	methyl palmitoleate
104-98-3	1178	urocanic acid 1
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

CAS #	PubChem	Compound
0	5459862	D-erythrose-4-phosphate 1
579-36-2	448388	D-allose 2
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
14883-87-5	85782	3,4-dihydroxymandelic acid
56-87-1	5962	L-lysine 2
1128-23-0	439373	L-gulonic acid gamma-lactone
50-66-8	5778	6-methylmercaptopurine 1
5934-29-2	6274	L-histidine 3
59-23-4	206	D (+) galactose 2
1002-57-9	66085	8-aminocaprylic acid
311-45-5	9395	paraoxon
90-80-2	736	gluconic acid lactone 3
112-39-0		Methyl Palmitate
6556-12-3	16213610	glucuronic acid 2
490-83-5	835	dehydroascorbic acid 4
1128-23-0	608	L-galactono-gamma-lactone 2
469-90-9	16219957	sedoheptulose anhydride monohydrate
2163-68-0	16553	atrazin-2-hydroxy 5
0	16213445	L-tyrosine-3,3-d2 2
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
490-83-5	835	dehydroascorbic acid 5
1138-80-3	14349	N-benzyloxycarbonylglycine
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 1
50-66-8	5778	6-methylmercaptopurine 2

CAS #	PubChem	Compound
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
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
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic acid
342385-52-8	159793	2-keto-L-gulonic acid 2
490-83-5	835	dehydroascorbic acid 6
149-91-7	370	gallic 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
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
4264-83-9	378	4-nitrophenyl phosphate
526-95-4	604	gluconic acid
583-93-7	865	2,6-diaminopimelic acid 2
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

CAS #	PubChem	Compound
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
19246-18-5	65270	cysteinylglycine 2
90-33-5	5280567	4-methylumbelliferone
104-98-3	1178	urocanic acid 2
69-89-6	1188	xanthine
68-94-0	790	hypoxanthine 2
87-73-0	5460673	D-saccharic acid
6133-30-8	97856	guanidinosuccinic acid 2
63-37-6	6131	cytidine-5'-monophosphate 1
1731-92-6	15609	methyl heptadecanoate
373-49-9	445638	palmitoleic acid
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- carbobenzoxo-L-leucine 1
2497-02-1	273260	N-acetyl-L-histidine 1
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- carbobenzoxo-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
3206-73-3	863	lipoamide 2

CAS #	PubChem	Compound
51-61-6	681	dopamine (hydroxytyramine)
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
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
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
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
529-69-1	10729	isoxanthopterin
3471-31-6	18986	5-methoxy-3-indoleacetic acid 1
331-39-5	1549111	caffeic acid

CAS #	PubChem	Compound
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)
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
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
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
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
21339-55-9	676159	1-methyl-L-tryptophan 3
60-23-1	6058	2-aminoethanethiol 1
60-33-3	5280450	linoleic acid
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
56-89-3	67678	L-cystine 1

CAS #	PubChem	Compound
0	4130574	asp-glu 2
481-06-1	221071	alpha-santonin 1
53-96-3	5897	N-2-fluorenylacetamide 1
530-59-6	637775	3,5-dimethoxy-4-hydroxycinnamic acid 2
525-82-6	10680	flavone
57-11-4	5281	stearic acid
41468-25-1	1051	pyridoxal 5'-phosphate 1
60-11-7	6053	methyl yellow
298-81-7	4114	xanthotoxin 2
462-20-4	421	dihydrolipoic 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
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
129-43-1	8512	1-hydroxyanthraquinone
101-31-5	154417	L-hyoscyamine
101-31-5	3661	hyoscyamine (atropine)
52450-38-1	171161	N-gamma-acetyl-N-2-formyl-5-methoxykynurenamine 1
56-89-3	67678	L-cystine 3
41468-25-1	1051	pyridoxal 5'-phosphate 2
577-85-5	11349	3-hydroxyflavone
1464-44-4	65080	phenyl-beta-glucopyranoside
56-73-5	439958	D-glucose-6-phosphate 1
1120-28-1		Methyl Eicosanoate
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
615-13-4	11983	2-indanone
2280-01-5	439917	N-acetyl-D-tryptophan 1
306-08-1	896	melatonin 1
550-33-4	68368	purine riboside
52450-38-1	171161	N-gamma-acetyl-N-2-formyl-5-methoxykynurenamine 3
2280-01-5	439917	N-acetyl-D-tryptophan 2
0	4130574	asp-glu 3

CAS #	PubChem	Compound
306-08-1	896	melatonin2
50-89-5	5789	thymidine
54965-21-8	2082	albendazole
0	4130574	asp-glu 4
50-89-5	5789	thymidine
13114-27-7	449093	zeatin 1
53-96-3	5897	N-2-fluorenylacetamide 2
0	4130574	asp-glu 5
63-37-6	6131	cytidine-5'-monophosphate 2
1210-83-9	903	N-acetyl-5-hydroxytryptamine 1
487-90-1	1021	porphobilinogen
9/8/4350	439280	5-hydroxy-L-tryptophan 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
306-08-1	896	melatonin4
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
22879-79-4	171548	biotin
13552-09-5	3126	DL-dihydrosphingosine 2
65-46-3	596	cytidine 1
1210-83-9	903	N-acetyl-5-hydroxytryptamine 2
16652-64-5	725701	O-benzyl-L-tyrosine 1
1210-83-9	903	N-acetyl-5-hydroxytryptamine 3
626-72-2	439579	L-homocystine 2
50-67-9	5202	serotonin 2
13114-27-7	449093	zeatin 2
13552-09-5	3126	DL-dihydrosphingosine 3
13241-33-3	442439	neohesperidin

CAS #	PubChem	Compound
16652-64-5	725701	O-benzyl-L-tyrosine 2
626-72-2	439579	L-homocystine 3
929-77-1		Methyl Docosanoate
658-79-7	92829	glycyl-L-tyrosine 1
117-81-7	8343	dioctyl phthalate
497-76-7	440936	arbutin
58-63-9	6021	inosine
72-48-0	6293	alizarin
554-62-1	122121	phytosphingosine 1
53-41-8	5879	androsterone
2018-66-8	74840	N- carbobenzoxo-L-leucine 3
53-43-0	5881	trans-dehydroandrosterone 1
958-09-8	13730	2'-deoxyadenosine
554-62-1	122121	phytosphingosine 2
58-61-7	60961	adenosine
4618-18-2	11333	lactulose 1
302-79-4	444795	retinoic acid
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
0	242332	5alpha-androstane-3beta,17beta-diol
521-18-6	10635	dihydrotestosterone 2
19408-84-5	107982	dihydrocapsaicin
1229-12-5	440114	5beta-androstane-3,17-dione
146-80-5	1189	xanthosine
50-28-2	5757	estradiol
63-42-3	84571	lactose 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
53-16-7	5870	estrone 2
501-36-0	445154	resveratrol
60-82-2	4788	phloretin
63-42-3	84571	lactose 2
71-44-3	1103	spermine 2
53-43-0	6013	testosterone 1

CAS #	PubChem	Compound
96-82-2	16219560	lactobionic acid 1
2442-49-1		Methyl Linocerate
53-43-0	6013	testosterone 2
2457-80-9	439176	5'-deoxy-5'-(methylthio)adenosine 1
63-05-8	6128	4-androsten-3,17-dione 1
62-84-0	65542	4-androsten-7-alpha-ol-3,17-dione 1
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
118-00-3	6802	guanosine 1
6138-23-4	7427	D-(+) trehalose
71-44-3	1103	spermine 1
35323-91-2	72276	(-)-epicatechin
35323-91-2	72276	epicatechin 1
547-25-1	5460935	turanose 1
62-84-0	65542	4-androsten-7-alpha-ol-3,17-dione 2
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
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
534-46-3	4623424	sophorose 2
111-02-4	5280370	squalene

CAS #	PubChem	Compound
585-88-6	16217663	maltitol
382-45-6	223997	adrenosterone 1
96-82-2	16219560	lactobionic acid 3
362-06-1	440623	2-hydroxyestrone 1
3387-36-8	6030	uridine 5'-monophosphate 1
362-06-1	440623	2-hydroxyestrone 2
35323-91-2	72276	(-)-epicatechin
13718-94-2	439559	palatinose
35323-91-2	72276	epicatechin 2
0	194988	glycyl-tyrosyl-alanine 1
382-45-6	223997	adrenosterone 2
66009-10-7	440658	melibiose 1
10083-24-6	667639	piceatannol
499-40-1	439193	isomaltose 1
154-23-4	9064	catechin
3387-36-8	6030	uridine 5'-monophosphate 2
547-96-6	160520	5-beta-cholestan-3-alpha-7-alpha-12-alpha-triol 1
50-27-1	5756	estriol
66009-10-7	440658	melibiose 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
585-88-6	3034828	palatinitol 1
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
566-65-4	92810	5-alpha-pregnan-3,20-dione 3
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 1
5802-82-4		Methyl Hexacosanoate
94-62-2	638024	piperine 2
3687-64-7	439451	galactinol 1
382-44-5	94141	4-androsten-11-beta-ol-3,17-dione 2
41001-90-5	3593	hesperetin 1
446-72-0	5280961	4',5,7-trihydroxyisoflavone
41001-90-5	3593	hesperetin 2
480-18-2	439533	taxifolin

CAS #	PubChem	Compound
585-18-2	439762	sucrose-6-phosphate 1
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
699012-36-7	41211	adenosine-3'-monophosphate
327-97-9	6537496	chlorogenic acid 1
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
585-18-2	439762	sucrose-6-phosphate 2
41001-90-5	3593	hesperetin 3
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 1
146-14-5	643975	flavin adenine dinucleotide 1
84-21-9	224	adenosine-5-monophosphate 1
520-18-3	5280863	kaempferol 1
146-14-5	643975	flavin adenine dinucleotide 2
84-21-9	224	adenosine-5-monophosphate 2
68-42-8	65553	tetrahydrocorticosterone 2
520-18-3	5280863	kaempferol 2
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
327-97-9	6537496	chlorogenic acid 2
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
67-97-0	5280795	cholecalciferol 2
68-42-8	65553	tetrahydrocorticosterone 4
57-88-5	304	cholesterol
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
529-44-2	5281672	myricetin
566-88-1	92128	5alpha-cholestan-3-one 1
57-87-4	444679	ergosterol

CAS #	PubChem	Compound
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
110-15-6	5321515	stigmasterol
81-25-4	221493	cholic acid 1
79-36-0	440560	dihydrolanosterol
516-72-3	121935	20-hydroxycholesterol 1
516-72-3	121935	20-hydroxycholesterol 2
629-83-4		Methyl Triacontanoate
81-25-4	221493	cholic acid 2
79-36-0	246983	lanosterol
10236-47-2	25075	naringin
14167-59-0	26519	tetratriacontane
1109-28-0	192826	maltotriose 1
10030-67-8	92817	melezitose
10030-67-8	92817	D-(+)-melezitose
79-57-2	5280972	oxytetracycline
82950-64-9	1321	1,2-didecanoylglyceride
38819-01-1	439626	cellotetraose
1109-28-0	192826	maltotriose 2
32860-62-1	3625615	maltotriitol
21637-25-2	5280804	isoquercitrin 2
3681-93-4	5280441	vitexin 1
3681-93-4	5280441	vitexin 2
970-74-1	72277	epigallocatechin
681295-24-9	66868	porphine 2
0	122281	16-glucuronide-estriol
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
4502-00-5	70	2-ketoisocaproic acid 1
4502-00-5	70	2-ketoisocaproic acid 2
689-31-6	71	2-ketoadipic acid 1

CAS #	PubChem	Compound
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
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	adenine 2
124-04-9	196	adipic acid
97-59-6	204	allantoin 1
97-59-6	204	allantoin 2
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
65-85-0	243	benzoic acid

CAS #	PubChem	Compound
1133-63-7	254	2,3-dihydroxybiphenyl
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
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
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

CAS #	PubChem	Compound
102-32-9	547	3,4-dihydroxyphenylacetic 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
923-16-0	601	D-Ala-D-Ala 4
526-95-4	604	gluconic acid
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
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
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
93965-35-6	729	DL-glyceraldehyde 3-phosphate 1
93965-35-6	729	DL-glyceraldehyde 3-phosphate 2

CAS #	PubChem	Compound
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
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
451-13-8	780	homogentisic acid
123-31-9	785	hydroquinone
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
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

CAS #	PubChem	Compound
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
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
24259-59-4	993	ribose
85-01-8	995	phenanthrene
156-06-9	997	phenylpyruvate
122-78-1	998	phenylacetaldehyde 1
122-78-1	998	phenylacetaldehyde 2

CAS #	PubChem	Compound
7568-93-6	1000	2-amino-1-phenylethanol
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
65-71-4	1135	thymine
137-00-8	1136	4-methyl-5-thiazoleethanol
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
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
82950-64-9	1321	1,2-didecanoylglyceride

CAS #	PubChem	Compound
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 1
115-69-5	1531	2-amino-2-methyl-1,3-propanediol 2
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)
54-16-0	1826	5-hydroxyindole-3-acetic acid
608-07-1	1833	methoxytryptamine
578-86-9	1889	liquiritigenin 1
578-86-9	1889	liquiritigenin 2
578-86-9	1889	liquiritigenin 3
1188-21-2	1995	N-acetyl-L-leucine
54965-21-8	2082	albendazole
10191-41-0	2116	alpha tocophereol
50-78-2	2244	O-acetylsalicylic acid
55-21-0	2331	benzamide
484-20-8	2355	5-methoxypsoralen
819-83-0	2526	beta-glycerolphosphate
36653-82-4	2682	1-hexadecanol
36653-82-4	2682	1-hexadecanol, (cetyl alcohol)
95-48-7	2879	p-cresol
52-52-8	2901	cycloleucine 1
52-52-8	2901	cycloleucine 2
334-48-5	2969	capric acid
13552-09-5	3126	DL-dihydrosphingosine 1
13552-09-5	3126	DL-dihydrosphingosine 2
13552-09-5	3126	DL-dihydrosphingosine 3
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
127-07-1	3657	hydroxyurea
101-31-5	3661	hyoscyamine (atropine)
700-06-1	3712	indole-3-carbinol 1
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

CAS #	PubChem	Compound
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 3
884-33-3	3858	benzylsuccinic acid
143-07-7	3893	lauric acid
298-81-7	4114	xanthotoxin 1
298-81-7	4114	xanthotoxin 2
106-51-4	4650	p-benzoquinone
60-82-2	4788	phloretin
108-46-3	5054	resorcinol
82385-42-0	5143	saccharin 2
82385-42-0	5143	saccharin 1
90-01-7	5146	2-hydroxybenzyl alcohol
50-67-9	5202	serotonin 1
50-67-9	5202	serotonin 2
57-11-4	5281	stearic acid
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-methylmercaptopurine 1
50-66-8	5778	6-methylmercaptopurine 2
50-70-4	5780	D-sorbitol
50-81-7	5785	L-ascorbic acid
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)
51-43-4	5816	adrenaline 1
51028-73-0	5816	(-)-epinephrine 1
51-43-4	5816	adrenaline 2
51028-73-0	5816	(-)-epinephrine 2
53-16-7	5870	estrone 1
53-16-7	5870	estrone 2
53-41-8	5879	androsterone
53-43-0	5881	trans-dehydroandrosterone 1

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
56-84-8	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
53-43-0	6013	testosterone 1
53-43-0	6013	testosterone 2
58-63-9	6021	inosine
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
60-18-4	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
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
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

CAS #	PubChem	Compound
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
77-95-2	6508	quinic acid
137-08-6	6613	pantothenic acid 1
137-08-6	6613	pantothenic acid 2
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
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
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

CAS #	PubChem	Compound
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
98-79-3	7405	L-pyroglutamic acid
6138-23-4	7427	D-(+) trehalose
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
103-81-1	7680	2-phenylacetamide 1
103-81-1	7680	2-phenylacetamide 2
103-81-1	7680	2-phenylacetamide 3
105-60-2	7768	epsilon-caprolactam
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
111-11-5	8091	octanoic acid methyl ester
112-85-6	8215	behenic acid
116-09-6	8299	acetol 1
116-09-6	8299	acetol 2
116-09-6	8299	acetol 3
116-09-6	8299	acetol 4
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
121-34-6	8468	4-hydroxy-3-methoxybenzoic acid
129-43-1	8512	1-hydroxyanthraquinone
138-59-0	8742	shikimic acid
142-08-5	8871	2-hydroxypyridine

CAS #	PubChem	Compound
142-73-4	8897	iminodiacetic acid 1
142-73-4	8897	iminodiacetic acid 2
154-23-4	9064	catechin
301-00-8	9316	methyl linolenate
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
452-86-8	9958	4-methylcatechol
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	flavonone 1
487-26-3	10251	flavonone 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
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
532-28-5	10758	mandelonitrile
533-73-3	10787	benzene-1,2,4-triol

CAS #	PubChem	Compound
536-66-3	10820	4-isopropylbenzoic acid
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
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
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
615-58-7	11847	2,6-dibromophenol
13545-04-5	11848	2,3-dimethylsuccinic acid
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
628-94-4	12364	adipamide 1
628-94-4	12364	adipamide 2
628-94-4	12364	adipamide 3
628-94-4	12364	adipamide 4
634-97-9	12473	pyrrole -2-carboxylic acid
637-88-7	12511	1,4-cyclohexanedione 1
637-88-7	12511	1,4-cyclohexanedione 2
672-15-1	12647	L-homoserine 1
672-15-1	12647	L-homoserine 2

CAS #	PubChem	Compound
672-15-1	12647	L-homoserine 3
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
2438-80-4	17106	L-(-)-fucose 2
2438-80-4	17106	L-(-)-fucose 1
3012-37-1	18170	benzyl thiocyanate
3025-96-5	18189	4-acetamidobutyric acid 1
3025-96-5	18189	4-acetamidobutyric acid 2
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
4376-20-9	20393	mono(2-ethylhexyl)phthalate
327-57-1	21236	L-norleucine 1
327-57-1	21236	L-norleucine 2
6351-10-6	22819	1-indanol
59-23-4	24749	D-glucose 1
59-23-4	24749	D-glucose 2

CAS #	PubChem	Compound
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
16867-04-2	28115	2,3-dihydroxypyridine
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
699012-36-7	41211	adenosine-3'-monophosphate
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 2
1211-29-6	62388	methyljasmonate 3
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
368-16-1	64969	3-methyl-L-histidine
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
6600-40-4	65098	norvaline 1
6600-40-4	65098	norvaline 2
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
681295-24-9	66868	porphine 1

CAS #	PubChem	Compound
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
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
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	nicotinoylglycin
407-41-0	68841	O-phospho-L-serine 1
407-41-0	68841	O-phospho-L-serine 2
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
673-49-4	69602	N-omega-acetylhistamine 2
673-49-4	69602	N-omega-acetylhistamine 1
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
35323-91-2	72276	(-)-epicatechin
35323-91-2	72276	epicatechin 1
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
56-86-0	73064	beta-glutamic acid
3646-68-2	73563	D-glucosaminic acid 1
3646-68-2	73563	D-glucosaminic acid 2
1679-53-4	74300	10-hydroxydecanoic acid

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- carbobenzoxo-L-leucine 1
2018-66-8	74840	N- carbobenzoxo-L-leucine 2
2018-66-8	74840	N- carbobenzoxo-L-leucine 3
3555-86-0	77093	phlorobenzophenone 1
3555-86-0	77093	phlorobenzophenone 2
56-57-5	77341	4-nitroquinoline
4385-35-7	78092	3-isochromanone
704-15-4	79101	gly-pro
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
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 1
21598-06-1	88958	5-hydroxyindole-2-carboxylic acid 2
23945-44-0	90301	2,4-dihydroxypyrimidine-5-carboxylic acid
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
566-65-4	92810	5-alpha-pregnan-3,20-dione 3
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
1946-82-3	92907	N-alpha-acetyl-L-lysine 1
1946-82-3	92907	N-alpha-acetyl-L-lysine 2

CAS #	PubChem	Compound
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
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
10094-62-9	101713	glucoheptonic acid 1
10094-62-9	101713	glucoheptonic acid 2
10094-62-9	101713	glucoheptonic acid 3
79-33-4	107689	L-(+) lactic acid
566-26-7	107722	5-cholesten-3-beta-7-alpha-diol
300-84-5	107812	hypotaurine
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
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 3
20448-79-7	115288	2-amino-2-norbornanecarboxylic acid 4
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

CAS #	PubChem	Compound
65005-57-4	123831	N,N-dimethylarginine
70-18-8	124886	L-glutathione reduced
81-13-0	131204	D-panthenol 1
81-13-0	131204	D-panthenol 2
147-85-3	145742	L-proline 1
147-85-3	145742	L-proline 2
1504-06-9	150923	3-methyloxyindole 1
1504-06-9	150923	3-methyloxyindole 2
1504-06-9	150923	3-methyloxyindole 3
1504-06-9	150923	3-methyloxyindole 4
3685-22-1	151138	cis-4-hydroxycyclohexanecarboxylic acid
2734-48-7	151491	3-(1-pyrazolyl)-L-alanine
101-31-5	154417	L-hyoscyamine
39840-37-4	156807	D-lyxosylamine 1
39840-37-4	156807	D-lyxosylamine 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
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
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
961-07-9	187790	2'-deoxyguanosine
1109-28-0	192826	maltotriose 1

CAS #	PubChem	Compound
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
481-06-1	221071	alpha-santonin 1
481-06-1	221071	alpha-santonin 2
81-25-4	221493	cholic acid 1
81-25-4	221493	cholic acid 2
53-06-5	222786	cortisone
382-45-6	223997	adrenosterone 1
382-45-6	223997	adrenosterone 2
0	242332	5alpha-androstane-3beta,17beta-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
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
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
771-51-7	351795	3-indoleacetonitrile
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
820-11-1	439183	3-phosphoglycerate
80731-10-8	439183	3-phosphoglyceric acid
108321-99-9	439184	ribulose-5-phosphate 3
499-40-1	439193	isomaltose 1

CAS #	PubChem	Compound
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
14982-50-4	439215	galacturonic acid 1
14982-50-4	439215	galacturonic acid 2
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
9/8/4350	439280	5-hydroxy-L-tryptophan 1
9/8/4350	439280	5-hydroxy-L-tryptophan 2
87-81-0	439312	D-tagatose 1
87-81-0	439312	D-tagatose 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
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
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
56-73-5	439958	D-glucose-6-phosphate 1

CAS #	PubChem	Compound
56-73-5	439958	D-glucose-6-phosphate 2
113573-73-2	440053	S(-)-willardiine 1
113573-73-2	440053	S(-)-willardiine 2
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 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
497-76-7	440936	arbutin
1990-29-0	441032	D (+)altrose 1
1990-29-0	441032	D (+)altrose 2
2595-98-4	441035	talose 1
2595-98-4	441035	talose 2
13241-33-3	442439	neohesperidin
20549-47-7	443163	(-)-dihydrocarveol 1
20549-47-7	443163	(-)-dihydrocarveol 2
7298-99-9	443239	threo-3-hydroxy-L-aspartate
0	443239	DL-threo-beta-hydroxyaspartic acid
146255-66-5	443586	3,5-dihydroxyphenylglycine 1
146255-66-5	443586	3,5-dihydroxyphenylglycine 2
585-84-2	444212	trans-aconitic acid
110-16-7	444266	maleic acid
133-37-9	444305	tartaric acid
140-10-3	444539	cinnamic acid
57-87-4	444679	ergosterol
0	444718	L-beta-phenyllactic acid
302-79-4	444795	retinoic acid
17013-01-3	444972	fumaric acid
106-28-5	445070	trans-trans-farnesol

CAS #	PubChem	Compound
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
579-36-2	448388	D-allose 1
579-36-2	448388	D-allose 2
13114-27-7	449093	zeatin 1
13114-27-7	449093	zeatin 2
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
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
94-62-2	638024	piperine 1
94-62-2	638024	piperine 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
146-14-5	643975	flavin adenine dinucleotide 1
146-14-5	643975	flavin adenine dinucleotide 2
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
16652-64-5	725701	O-benzyl-L-tyrosine 1
16652-64-5	725701	O-benzyl-L-tyrosine 2

CAS #	PubChem	Compound
458-35-5	1549095	coniferyl alcohol
331-39-5	1549111	caffeic acid
4896-77-9	2723970	glycine-d5 deuterated
87-81-0	2724552	tagatose 1
87-81-0	2724552	tagatose 2
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
14528-64-4	3505109	4-nitrocatechol
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
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
534-46-3	4623424	sophorose 1
534-46-3	4623424	sophorose 2
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
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
537-33-7	5280507	sinapyl alcohol 1
537-33-7	5280507	sinapyl alcohol 2
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 1

CAS #	PubChem	Compound
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
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
100-61-8	5288725	N-methylalanine
110-15-6	5321515	stigmasterol
1086-80-2	5326566	7,8-dimethylalloxazine
4436-74-2	5351896	trans-3-hexenedioic acid
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
1214-47-7	5367146	2-hydroxychalcone 1
1214-47-7	5367146	2-hydroxychalcone 2
0	5459862	D-erythrose-4-phosphate 1
0	5459862	D-erythrose-4-phosphate 2
87-73-0	5460673	D-saccharic acid
547-25-1	5460935	turanose 1
547-25-1	5460935	turanose 2
7541-49-3	6430833	phytol 1
7541-49-3	6430833	phytol 2

CAS #	PubChem	Compound
327-97-9	6537496	chlorogenic acid 1
327-97-9	6537496	chlorogenic acid 2
225101-69-9	12205373	L-alanine-2,3,3,3-d4
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
18524-94-2	16212335	loganin
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 2
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
96-82-2	16219560	lactobionic acid 1
96-82-2	16219560	lactobionic acid 2
96-82-2	16219560	lactobionic acid 3
15763-06-1	16219662	1-methyladenosine 1
15763-06-1	16219662	1-methyladenosine 2
469-90-9	16219957	sedoheptulose anhydride monohydrate
111-11-5		Methyl Caprylate
1731-84-6		Methyl Pelargonate
110-42-9		Methyl caprate
0		L-glutamic acid-2,3,3,4,4-d5 3 (dehydrated)
111-82-0		Methyl Laurate
0		L-glutamic acid-2,3,3,4,4-d5 1
0		L-glutamic acid-2,3,3,4,4-d5 2
124-10-7		Methyl Myristate
60658-41-5		Myristic Acid d27
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 1
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 2
112-39-0		Methyl Palmitate
112-61-8		Methyl Stearate
1120-28-1		Methyl Eicosanoate
929-77-1		Methyl Docosanoate

CAS #	PubChem	Compound
2442-49-1		Methyl Linocerate
5802-82-4		Methyl Hexacosanoate
55682-92-3		Methyl Octacosanoate
629-83-4		Methyl Triacontanoate
0		L-glutamic acid-2,3,3,4,4-d5 3 (dehydrated)
0		L-glutamic acid-2,3,3,4,4-d5 1
0	444718	L-beta-phenyllactic acid
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
0-00-0	440168	1,3,5(10)-estratrien-3,6- beta-17-beta-triol
2280-01-5	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
100-61-8	5288725	N-methylalanine

CAS #	PubChem	Compound
10083-24-6	667639	piceatannol
100-83-4	101	3-hydroxybenzaldehyde
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
103-26-4	637520	methyl cinnamate
1032-65-1	13945	2'-deoxycytidine 5'-monophosphoric acid
103-81-1	7680	2-phenylacetamide 1
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
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
106-28-5	445070	trans-trans-farnesol
106-51-4	4650	p-benzoquinone
1071-23-4	1015	O-phosphocolamine
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

CAS #	PubChem	Compound
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
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
111-02-4	5280370	squalene
111-11-5	8091	octanoic acid methyl ester
111-11-5		Methyl Caprylate
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
1120-25-8	643801	methyl palmitoleate
1120-28-1		Methyl Eicosanoate
112-39-0		Methyl Palmitate
112-61-8		Methyl Stearate
112-62-9	5364509	methyl oleate
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
1133-63-7	254	2,3-dihydroxybiphenyl
1135-24-6	445858	ferulic acid
113573-73-2	440053	S(-)-willardiine 1

CAS #	PubChem	Compound
113573-73-2	440053	S(-)-willardiine 2
1138-80-3	14349	N-benzyloxycarbonylglycine
114-63-6	135	4-hydroxybenzoic acid
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
117-81-7	8343	dioctyl phthalate
118-00-3	6802	guanosine 1
118-00-3	6802	guanosine 2
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
120-80-9	289	catechol
1210-83-9	903	N-acetyl-5-hydroxytryptamine 1

CAS #	PubChem	Compound
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 2
1211-29-6	62388	methyljasmonate 3
1211-29-6	62388	methyljasmonate 4
121-33-5	1183	vanillin
121-34-6	8468	4-hydroxy-3-methoxybenzoic acid
1214-47-7	5367146	2-hydroxychalcone 1
1214-47-7	5367146	2-hydroxychalcone 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
123-31-9	785	hydroquinone
123-78-4	5280335	D-sphingosine 1
123-78-4	5280335	D-sphingosine 2
123-78-4	5280335	D-sphingosine 3
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
127-07-1	3657	hydroxyurea
127-17-3	1060	pyruvic acid
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
13114-27-7	449093	zeatin 1
13114-27-7	449093	zeatin 2
131-99-7	797	inosine 5'-monophosphate
13241-33-3	442439	neohesperidin

CAS #	PubChem	Compound
132-64-9	568	dibenzofuran
133-37-9	444305	tartaric acid
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
140-10-3	444539	cinnamic acid
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
142-08-5	8871	2-hydroxypyridine
142-73-4	8897	iminodiacetic acid 1
142-73-4	8897	iminodiacetic acid 2
143-07-7	3893	lauric acid
144-62-7	971	oxalic acid
14528-64-4	3505109	4-nitrocatechol
1460-57-7	92886	trans-cyclohexane-1,2-diol
146-14-5	643975	flavin adenine dinucleotide 1
146-14-5	643975	flavin adenine dinucleotide 2
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
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
14883-87-5	85782	3,4-dihydroxymandelic acid
1492-23-5	954	O-succinylhomoserine 1

CAS #	PubChem	Compound
1492-23-5	954	O-succinylhomoserine 2
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-methyloxyindole 1
1504-06-9	150923	3-methyloxyindole 2
1504-06-9	150923	3-methyloxyindole 3
1504-06-9	150923	3-methyloxyindole 4
151-18-8	1647	3-aminopropionitrile 1
151-18-8	1647	3-aminopropionitrile 2
154-23-4	9064	catechin
156-06-9	997	phenylpyruvate
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
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
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
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
1731-92-6	15609	methyl heptadecanoate
1792-81-0	92903	cis-1,2-cyclohexanediol
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

CAS #	PubChem	Compound
18524-94-2	16212335	loganin
186537-58-6	193653	S-carboxymethylcysteine 1
186537-58-6	193653	S-carboxymethylcysteine 2
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- carbobenzoxyl-L-leucine 1
2018-66-8	74840	N- carbobenzoxyl-L-leucine 2
2018-66-8	74840	N- carbobenzoxyl-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
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
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
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

CAS #	PubChem	Compound
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
22059-21-8	535	1-aminocyclopropane-1-carboxylic acid
225101-69-9	12205373	L-alanine-2,3,3,3-d4
2280-01-5	439917	N-acetyl-D-tryptophan 1
2280-01-5	439917	N-acetyl-D-tryptophan 2
22879-79-4	171548	biotin
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 2
2438-80-4	17106	L-(-)-fucose 1
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
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
2734-48-7	151491	3-(1-pyrazolyl)-L-alanine
28822-73-3	91528	DL-3,4-dihydroxyphenyl glycol
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
298-81-7	4114	xanthotoxin 1

CAS #	PubChem	Compound
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
306-08-1	896	melatonin 1
306-08-1	896	melatonin2
306-08-1	896	melatonin 3
306-08-1	896	melatonin4
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
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
3237-44-3	36	2-isopropylmalic acid
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
3387-36-8	6030	uridine 5'-monophosphate 1
3387-36-8	6030	uridine 5'-monophosphate 2
342385-52-8	159793	2-keto-L-gulonic acid 1
342385-52-8	159793	2-keto-L-gulonic acid 2

CAS #	PubChem	Compound
34363-28-5	754	glycerol 1-phosphate
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
35323-91-2	72276	(-)-epicatechin
35323-91-2	72276	epicatechin 1
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
3588-17-8	5356793	trans,trans-muconic acid
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
3615-56-3	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
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

CAS #	PubChem	Compound
372-75-8	9750	citrulline 1
372-75-8	9750	citrulline 2
372-75-8	9750	citrulline 3
373-49-9	445638	palmitoleic acid
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
39840-37-4	156807	D-lyxosylamine 1
39840-37-4	156807	D-lyxosylamine 2
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
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
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
4436-74-2	5351896	trans-3-hexenedioic acid
443-79-8	791	DL-isoleucine 1
443-79-8	791	DL-isoleucine 2
446-72-0	5280961	4',5,7-trihydroxyisoflavone
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

CAS #	PubChem	Compound
452-86-8	9958	4-methylcatechol
458-35-5	1549095	coniferyl alcohol
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 1
458-36-6	5280536	4-hydroxy-3-methoxycinnamaldehyde 2
4618-18-2	11333	lactulose 1
4618-18-2	11333	lactulose 3
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
469-90-9	16219957	sedoheptulose anhydride monohydrate
473-81-4	439194	glyceric acid
480-18-2	439533	taxifolin
480-40-0	5281607	chrysin
481-06-1	221071	alpha-santonin 1
481-06-1	221071	alpha-santonin 2
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
487-90-1	1021	porphobilinogen
488-17-5	340	3-methylcatechol
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

CAS #	PubChem	Compound
490-83-5	835	dehydroascorbic acid 4
490-83-5	835	dehydroascorbic acid 5
490-83-5	835	dehydroascorbic acid 6
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
498-23-7	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 2
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	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)
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
504-15-4	10436	orcinol
506-12-7	10465	heptadecanoic acid
506-30-9	10467	arachidic acid

CAS #	PubChem	Compound
50-66-8	5778	6-methylmercaptopurine 1
50-66-8	5778	6-methylmercaptopurine 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
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	methylnalonic acid
51-61-6	681	dopamine (hydroxytyramine)
51-67-2	5610	tyramine
516-72-3	121935	20-hydroxycholesterol 1
516-72-3	121935	20-hydroxycholesterol 2
51-79-6	5641	carbamic acid ethyl ester (urethane)
520-18-3	5280863	kaempferol 1
520-18-3	5280863	kaempferol 2
521-18-6	10635	dihydrotestosterone 1
521-18-6	10635	dihydrotestosterone 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
52-52-8	2901	cycloleucine 1
52-52-8	2901	cycloleucine 2
525-82-6	10680	flavone

CAS #	PubChem	Compound
526-95-4	604	gluconic acid
526-99-8	3037582	mucic acid
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
529-44-2	5281672	myricetin
529-64-6	10726	tropic acid
529-69-1	10729	isoxanthopterin
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	estrone 1
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
533-73-3	10787	benzene-1,2,4-triol
53411-70-4	91493	6-phosphogluconic acid
53-41-8	5879	androsterone
53-43-0	5881	trans-dehydroandrosterone 1
53-43-0	5881	trans-dehydroandrosterone 2
53-43-0	6013	testosterone 1
53-43-0	6013	testosterone 2
534-46-3	4623424	sophorose 1
534-46-3	4623424	sophorose 2
535-75-1	439227	pipecolic acid 1
535-75-1	439227	pipecolic acid 2
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
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

CAS #	PubChem	Compound
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
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
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
56-40-6	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
566-65-4	92810	5-alpha-pregnan-3,20-dione 1
566-65-4	92810	5-alpha-pregnan-3,20-dione 2

CAS #	PubChem	Compound
566-65-4	92810	5-alpha-pregnan-3,20-dione 3
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
56-81-5	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)
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
57-11-4	5281	stearic acid
57-13-6	1176	urea
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
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

CAS #	PubChem	Compound
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
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	nicotinoylglycin
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
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
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
5949-29-1	311	citric 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
600-18-0	58	2-ketobutyric acid

CAS #	PubChem	Compound
600-18-0	58	2-ketobutyric acid
60-11-7	6053	methyl yellow
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
60-27-5	588	Creatinine
60-33-3	5280450	linoleic acid
60658-41-5		Myristic Acid d27
608-07-1	637542	4-hydroxycinnamic acid
608-07-1	1833	methoxytryptamine
60-82-2	4788	phloretin
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
61-90-5	6106	L-leucine 2
6192-52-5	6101	p-toluenesulfonic acid
620-24-6	102	3-hydroxybenzyl alcohol

CAS #	PubChem	Compound
621-37-4	12122	3-hydroxyphenylacetic acid
62147-49-3	668	dihydroxyacetone phosphate 1
62147-49-3	668	dihydroxyacetone phosphate 2
621-54-5	91	3-(3-hydroxyphenyl)propionic acid
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
627-01-0	316542	N-ethylglycine 1
627-01-0	316542	N-ethylglycine 2
62-84-0	65542	4-androsten-7- α -ol-3,17-dione 1
62-84-0	65542	4-androsten-7- α -ol-3,17-dione 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
629-83-4		Methyl Triacontanoate
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
63-42-3	84571	lactose 1
63-42-3	84571	lactose 2
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
64-04-0	1001	phenylethylamine
64519-82-0	985	palmitic acid
64519-82-0	3034828	palatinitol 2
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

CAS #	PubChem	Compound
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 2
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
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
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
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
67-97-0	5280795	cholecalciferol 1

CAS #	PubChem	Compound
67-97-0	5280795	cholecalciferol 2
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
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
68-94-0	790	hypoxanthine
68-94-0	790	hypoxanthine 2
6968-16-7	169019	D-threitol
69-72-7	338	salicylic acid
69-79-4	6255	maltose 1
69-79-4	6255	maltose 2
69-89-6	1188	xanthine
699012-36-7	41211	adenosine-3'-monophosphate
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
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
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

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
72-48-0	6293	alizarin
7298-99-9	443239	threo-3-hydroxy-L-aspartate
73-22-3	6305	L-tryptophan 1
73-22-3	6305	L-tryptophan 2
73-24-5	190	adenine 1
73-24-5	190	adenine 2
7365-44-8	446188	TES
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
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
771-51-7	351795	3-indoleacetonitrile
7772-94-3	899	N-acetyl-D-mannosamine 1
7772-94-3	899	N-acetyl-D-mannosamine 2
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
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

CAS #	PubChem	Compound
80-69-3	45	tartronic acid
80731-10-8	439183	3-phosphoglyceric acid
81-13-0	131204	D-panthenol 1
81-13-0	131204	D-panthenol 2
81-25-4	221493	cholic acid 1
81-25-4	221493	cholic acid 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
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
84-21-9	224	adenosine-5-monophosphate 1
84-21-9	224	adenosine-5-monophosphate 2
85-01-8	995	phenanthrene
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
87-51-4	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	439312	D-tagatose 1
87-81-0	2724552	tagatose 1
87-81-0	439312	D-tagatose 2
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

CAS #	PubChem	Compound
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
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
923-16-0	601	D-Ala-D-Ala 4
92-52-4	7095	biphenyl
92-61-5	5280460	scopoletin
929-77-1		Methyl Docosanoate
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
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
951-78-0	13712	2-deoxyuridine 1
951-78-0	13712	2-deoxyuridine 2
95-43-2	439665	threose 1

CAS #	PubChem	Compound
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
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
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
98-92-0	936	nicotinamide 1
98-92-0	936	nicotinamide 2
98-98-6	1018	picolonic acid
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
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

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
51268-88-3	440294	(1R,2S)-cis-1,2-dihydro-1,2-naphthalenediol
1200-22-2	6112	(R)-(+)-1,2-dithiolane-3-pentanoic 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
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	440168	1,3,5(10)-estratrien-3,6- beta-17-beta-triol
109-76-2	428	1,3-diaminopropane 1
109-76-2	428	1,3-diaminopropane 2
96-26-4	4180364	1,3-dihydroxyacetone
637-88-7	12511	1,4-cyclohexanedione 1
637-88-7	12511	1,4-cyclohexanedione 2
31519-22-9	671	1,4-dihydroxy-2-naphthoic acid
6892-68-8	439352	1,4-dithioerythritol
1679-53-4	74300	10-hydroxydecanoic acid
35850-13-6	5280887	15-keto-prostaglandin F2alpha
35850-13-6	5280887	15-keto-prostaglandin F-2-alpha
0	122281	16-glucuronide-estriol
22059-21-8	535	1-aminocyclopropane-1-carboxylic acid
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

CAS #	PubChem	Compound
102-32-9	547	2-(3,4-dihydroxyphenyl)acetic acid
501-94-0	10393	2-(4-hydroxyphenyl)ethanol
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
615-58-7	12005	2,4-dibromophenol
23945-44-0	90301	2,4-dihydroxypyrimidine-5-carboxylic acid
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
516-72-3	121935	20-hydroxycholesterol 1
516-72-3	121935	20-hydroxycholesterol 2
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
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
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 1
653-63-4	621	2'-deoxyadenosine 5'-monophosphate 2
653-63-4	621	2'-deoxyadenosine 5'-monophosphate
652157-52-3	637	2'-deoxycytidine
1032-65-1	13945	2'-deoxycytidine 5'-monophosphoric acid
961-07-9	187790	2'-deoxyguanosine
951-78-0	13712	2-deoxyuridine 1

CAS #	PubChem	Compound
951-78-0	13712	2-deoxyuridine 2
88-14-2	6919	2-furoic acid
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
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
342385-52-8	159793	2-keto-L-gulonic acid 1
342385-52-8	159793	2-keto-L-gulonic acid 2
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
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
501-97-3	10394	3-(4-hydroxyphenyl)propionic acid
99-50-3	72	3,4-dihydroxybenzoic acid
14883-87-5	85782	3,4-dihydroxymandelic acid
102-32-9	547	3,4-dihydroxyphenylacetic acid

CAS #	PubChem	Compound
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
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 1
0		3-amino-3-(4-hydroxy-phenyl)-propionic acid 2
23279-22-3	160450	3-amino-L-tyrosine 1
23279-22-3	160450	3-amino-L-tyrosine 2
23279-22-3	160450	3-amino-L-tyrosine 3
151-18-8	1647	3-aminopropionitrile 1
151-18-8	1647	3-aminopropionitrile 2
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
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
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
1504-06-9	150923	3-methyloxyindole 1
1504-06-9	150923	3-methyloxyindole 2
1504-06-9	150923	3-methyloxyindole 3

CAS #	PubChem	Compound
1504-06-9	150923	3-methyloxyindole 4
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)
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
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
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

CAS #	PubChem	Compound
6851-36-1	166768	4-hydroxymandelonitrile 2
156-38-7	127	4-hydroxyphenylacetic acid
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)
536-66-3	10820	4-isopropylbenzoic acid
536-60-7	325	4-isopropylbenzyl alcohol
137-00-8	1136	4-methyl-5-thiazoleethanol
452-86-8	9958	4-methylcatechol
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
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
582-60-5	675	5,6 - dimethylbenzimidazole 1
582-60-5	675	5,6 - dimethylbenzimidazole 2
0	242332	5alpha-androstane-3beta,17beta-diol
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
566-65-4	92810	5-alpha-pregnan-3,20-dione 3
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

CAS #	PubChem	Compound
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
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
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
50-66-8	5778	6-methylmercaptopurine 1
50-66-8	5778	6-methylmercaptopurine 2
53411-70-4	91493	6-phosphogluconic acid
1086-80-2	5326566	7,8-dimethylalloxazine
1002-57-9	66085	8-aminocaprylic acid
486-25-9	10241	9-fluorenone
1689-64-1	74318	9-hydroxyfluorene
484-17-3	10229	9-phenanthrenol
514-10-3	10569	abietic acid
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
116-09-6	8299	acetol 2
116-09-6	8299	acetol 1
116-09-6	8299	acetol 3
116-09-6	8299	acetol 4
574-17-4	11321	acetylisatin 1

CAS #	PubChem	Compound
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
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
53-41-8	5879	androsterone
88-21-1	6926	aniline-o-sulfonic acid
488-82-4	94154	arabitol
506-30-9	10467	arachidic acid

CAS #	PubChem	Compound
497-76-7	440936	arbutin
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
112-85-6	8215	behenic acid
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
611-73-4	11915	benzoylformic acid 1
611-73-4	11915	benzoylformic acid 2
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
56-86-0	73064	beta-glutamic acid
819-83-0	2526	beta-glycerolphosphate
22879-79-4	171548	biotin
92-52-4	7095	biphenyl
108-19-0	7913	biuret 1
108-19-0	7913	biuret 2
331-39-5	1549111	caffeic acid
334-48-5	2969	capric acid
124-07-2	379	caprylic acid
51-79-6	5641	carbamic acid ethyl ester (urethane)
86-74-8	6854	carbazole 1
86-74-8	6854	carbazole 2

CAS #	PubChem	Compound
154-23-4	9064	catechin
120-80-9	289	catechol
528-50-7	10712	cellobiose 1
528-50-7	10712	cellobiose 2
38819-01-1	439626	cellotetraose
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
81-25-4	221493	cholic acid 1
81-25-4	221493	cholic acid 2
480-40-0	5281607	chrysin
2041-14-7	339	ciliatine
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
3685-22-1	151138	cis-4-hydroxycyclohexanecarboxylic 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	citruiline 2
372-75-8	9750	citruiline 3
458-35-5	1549095	coniferyl alcohol
601-53-6	85881	coprostan-3-one
53-06-5	222786	cortisone
60-27-5	588	Creatinine
7665-99-8	295	cyclic GMP
108-91-8	7965	cyclohexanamine
52-52-8	2901	cycloleucine 1

CAS #	PubChem	Compound
52-52-8	2901	cycloleucine 2
19246-18-5	65270	cysteinylglycine 1
19246-18-5	65270	cysteinylglycine 2
19246-18-5	65270	cysteinylglycine 3
65-46-3	596	cytidine 1
65-46-3	596	cytidine 2
63-37-6	6131	cytidine-5'-monophosphate 1
63-37-6	6131	cytidine-5'-monophosphate 2
71-30-7	597	cytosine 1
71-30-7	597	cytosine 2
71-30-7	597	cytosine 3
59-23-4	206	D (+) galactose 1
59-23-4	206	D (+) galactose 2
1990-29-0	441032	D (+)altrose 1
1990-29-0	441032	D (+)altrose 2
6138-23-4	7427	D-(+) trehalose
10030-67-8	92817	D-(+)-melezitose
486-66-8	5281708	daidzein
923-16-0	601	D-Ala-D-Ala 1
923-16-0	601	D-Ala-D-Ala 4
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
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
0	5459862	D-erythrose-4-phosphate 1
0	5459862	D-erythrose-4-phosphate 2
3646-68-2	73563	D-glucosaminic acid 1
3646-68-2	73563	D-glucosaminic acid 2
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

CAS #	PubChem	Compound
0	16217112	D-glucose-C-d7 2
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
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
521-18-6	10635	dihydrotestosterone 1
521-18-6	10635	dihydrotestosterone 2
62147-49-3	668	dihydroxyacetone phosphate 1
62147-49-3	668	dihydroxyacetone phosphate 2
117-81-7	8343	dioctyl phthalate
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 1
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 2
20263-06-3	3857	DL-2-amino-3-phosphonopropionic acid 3
28822-73-3	91528	DL-3,4-dihydroxyphenyl glycol
10569-71-9	64956	DL-3-aminoisobutyric acid 1
10569-71-9	64956	DL-3-aminoisobutyric acid 2
55-10-7	1245	DL-4-hydroxy-3-methoxymandelic acid
7198-10-9	328	DL-4-hydroxymandelic acid
13552-09-5	3126	DL-dihydrosphingosine 1
13552-09-5	3126	DL-dihydrosphingosine 2
13552-09-5	3126	DL-dihydrosphingosine 3
56-82-6	751	DL-glyceraldehyde 1
56-82-6	751	DL-glyceraldehyde 2
93965-35-6	729	DL-glyceraldehyde 3-phosphate 1
93965-35-6	729	DL-glyceraldehyde 3-phosphate 2
443-79-8	791	DL-isoleucine 1
443-79-8	791	DL-isoleucine 2
6482-98-0	9378	DL-p-hydroxyphenyllactic acid
0	443239	DL-threo-beta-hydroxyaspartic acid

CAS #	PubChem	Compound
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
39840-37-4	156807	D-lyxosylamine 1
39840-37-4	156807	D-lyxosylamine 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
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
87-81-0	439312	D-tagatose 1
87-81-0	439312	D-tagatose 2
6968-16-7	169019	D-threitol
35323-91-2	72276	epicatechin 1
35323-91-2	72276	epicatechin 2
970-74-1	72277	epigallocatechin
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
19317-11-4	5280598	farnesal 1
19317-11-4	5280598	farnesal 2
19317-11-4	5280598	farnesal 3
19317-11-4	5280598	farnesal 4
1135-24-6	445858	ferulic acid

CAS #	PubChem	Compound
487-26-3	10251	flavanone 1
487-26-3	10251	flavanone 2
146-14-5	643975	flavin adenine dinucleotide 1
146-14-5	643975	flavin adenine dinucleotide 2
525-82-6	10680	flavone
487-26-3	10251	flavonone 1
487-26-3	10251	flavonone 2
86-73-7	6853	fluorene
57-48-7	5984	fructose 1
57-48-7	5984	fructose 2
17013-01-3	444972	fumaric acid
3687-64-7	439451	galactinol 1
3687-64-7	439451	galactinol 2
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
490-79-9	3469	gentisic acid
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
90-80-2	736	gluconic acid lactone 1
90-80-2	736	gluconic acid lactone 2
90-80-2	736	gluconic acid lactone 3
6556-12-3	16213610	glucuronic acid 2
6556-12-3	16213610	glucuronic acid 1
473-81-4	439194	glyceric acid
56-81-5	753	glycerol
34363-28-5	754	glycerol 1-phosphate
56-40-6	750	glycine
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
0	194988	glycyl-tyrosyl-alanine 1
0	194988	glycyl-tyrosyl-alanine 2

CAS #	PubChem	Compound
0	194988	glycyl-tyrosyl-alanine 3
0	194988	glycyl-tyrosyl-alanine 4
704-15-4	79101	gly-pro
90-05-1	460	guaiacol
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
506-12-7	10465	heptadecanoic acid
41001-90-5	3593	hesperetin 1
41001-90-5	3593	hesperetin 2
41001-90-5	3593	hesperetin 3
118-74-1	8370	hexachlorobenzene
495-69-2	464	hippuric acid 1
495-69-2	464	hippuric acid 2
451-13-8	780	homogentisic acid
501-52-0	107	hydrocinnamic acid
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
879-37-8	397	indole-3-acetamide 1
879-37-8	397	indole-3-acetamide 2
879-37-8	397	indole-3-acetamide 3
700-06-1	3712	indole-3-carbinol 1
392-12-1	803	indole-3-pyruvic 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

CAS #	PubChem	Compound
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
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
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
50-81-7	5785	L-ascorbic acid
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
0	444718	L-beta-phenyllactic acid

CAS #	PubChem	Compound
543-38-4	275	L-canavanine 1
543-38-4	275	L-canavanine 2
541-15-1	10918	L-carnitine 1
541-15-1	10918	L-carnitine 2
498-40-8	72886	L-cysteic acid
52-90-4	594	L-cysteine 1
52-90-4	594	L-cysteine 2
56-89-3	67678	L-cystine 1
56-89-3	67678	L-cystine 2
56-89-3	67678	L-cystine 3
16096-97-2	439196	L-dithiothreitol 1
16096-97-2	439196	L-dithiothreitol 2
57-92-7	6047	L-DOPA 1
57-92-7	6047	L-DOPA 2
7158-70-5	165577	leucrose
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
60-33-3	5280450	linoleic acid

CAS #	PubChem	Compound
3206-73-3	863	lipoamide 1
3206-73-3	863	lipoamide 2
3206-73-3	863	lipoamide 3
578-86-9	1889	liquiritigenin 1
578-86-9	1889	liquiritigenin 2
578-86-9	1889	liquiritigenin 3
2922-83-0	161166	L-kynurenine 1
2922-83-0	161166	L-kynurenine 2
61-90-5	6106	L-leucine 1
61-90-5	6106	L-leucine 2
56-87-1	5962	L-lysine 1
56-87-1	5962	L-lysine 2
3128-06-1	26447	L-menthone
63-68-3	6137	L-methionine 1
63-68-3	6137	L-methionine 2
3226-65-1	158980	L-methionine sulfoxide 1
3226-65-1	158980	L-methionine sulfoxide 2
3226-65-1	158980	L-methionine sulfoxide 3
500-44-7	440473	L-mimosine 2
327-57-1	21236	L-norleucine 1
327-57-1	21236	L-norleucine 2
18524-94-2	16212335	loganin
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	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
98-79-3	7405	L-pyroglutamic acid
56-45-1	5951	L-serine 1
56-45-1	5951	L-serine 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

CAS #	PubChem	Compound
0	16213445	L-tyrosine-3,3-d2 1
0	16213445	L-tyrosine-3,3-d2 2
487-21-8	10250	lumazine
72-18-4	6287	L-valine 1
72-18-4	6287	L-valine 2
557-24-4	5280451	maleamic acid 1
557-24-4	5280451	maleamic acid 2
557-24-4	5280451	maleamic acid 3
110-16-7	444266	maleic acid
108-13-4	7911	malonamide 1
108-13-4	7911	malonamide 2
108-13-4	7911	malonamide 3
141-82-2	867	malonic acid 1
141-82-2	867	malonic acid 2
585-88-6	16217663	maltitol
69-79-4	6255	maltose 2
69-79-4	6255	maltose 1
32860-62-1	3625615	maltotriitol
1109-28-0	192826	maltotriose 1
1109-28-0	192826	maltotriose 2
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
608-07-1	1833	methoxytryptamine
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
1731-92-6	15609	methyl heptadecanoate
5802-82-4		Methyl Hexacosanoate

CAS #	PubChem	Compound
111-82-0		Methyl Laurate
2442-49-1		Methyl Linocerate
301-00-8	9316	methyl linolenate
124-10-7		Methyl Myristate
55682-92-3		Methyl Octacosanoate
112-62-9	5364509	methyl oleate
112-39-0		Methyl Palmitate
1120-25-8	643801	methyl palmitoleate
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	methylnmalonic acid
4376-20-9	20393	mono(2-ethylhexyl)phthalate
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- carbobenzoxo-L-leucine 1
2018-66-8	74840	N- carbobenzoxo-L-leucine 2
2018-66-8	74840	N- carbobenzoxo-L-leucine 3
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 1
93-62-9	7152	N-(2-hydroxyethyl)iminodiacetic acid 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

CAS #	PubChem	Compound
1210-83-9	903	N-acetyl-5-hydroxytryptamine 2
1210-83-9	903	N-acetyl-5-hydroxytryptamine 3
7512-17-6	16218892	N-acetyl-D-glucosamine 1
7512-17-6	16218892	N-acetyl-D-glucosamine 2
7772-94-3	899	N-acetyl-D-mannosamine 1
7772-94-3	899	N-acetyl-D-mannosamine 2
2280-01-5	439917	N-acetyl-D-tryptophan 1
2280-01-5	439917	N-acetyl-D-tryptophan 2
1/5/2280	439917	N-acetyl-D-tryptophan 3
997-55-7	65065	N-acetyl-L-aspartic acid 1
997-55-7	65065	N-acetyl-L-aspartic acid 2
616-91-1	12035	N-acetyl-L-cysteine 1
616-91-1	12035	N-acetyl-L-cysteine 2
1188-37-0	70914	N-acetyl-L-glutamic acid 1
1188-37-0	70914	N-acetyl-L-glutamic acid 2
1188-37-0	70914	N-acetyl-L-glutamic acid 3
2497-02-1	273260	N-acetyl-L-histidine 1
2497-02-1	273260	N-acetyl-L-histidine 2
1188-21-2	1995	N-acetyl-L-leucine
2018-61-3	74839	N-acetyl-L-phenylalanine 1
2018-61-3	74839	N-acetyl-L-phenylalanine 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
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

CAS #	PubChem	Compound
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	nicotinoylglycin
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
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
111-11-5	8091	octanoic acid methyl ester
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

CAS #	PubChem	Compound
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
79-57-2	5280972	oxytetracycline
585-88-6	3034828	palatinitol 1
64519-82-0	3034828	palatinitol 2
13718-94-2	439559	palatinose
64519-82-0	985	palmitic acid
373-49-9	445638	palmitoleic acid
100-09-4	7478	p-anisic acid
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
500-98-1	68144	phenaceturic acid 1
500-98-1	68144	phenaceturic acid 2
85-01-8	995	phenanthrene
122-78-1	998	phenylacetaldehyde 1
122-78-1	998	phenylacetaldehyde 2
1464-44-4	65080	phenyl-beta-glucopyranoside
64-04-0	1001	phenylethylamine
701-64-4	12793	phenylphosphoric acid
156-06-9	997	phenylpyruvate
60-82-2	4788	phloretin
3555-86-0	77093	phlorobenzophenone 1
3555-86-0	77093	phlorobenzophenone 2
108-73-6	359	phloroglucinol
138-08-9	1005	phosphoenolpyruvic acid
95648-83-2	529	phosphoglycolic acid
26016-99-9	3417	phosphonomycin
7664-38-2	1004	phosphoric acid
88-99-3	1017	phthalic acid
14721-66-5	26840	phytanic acid
7541-49-3	5366244	phytol 1
7541-49-3	6430833	phytol 1

CAS #	PubChem	Compound
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
552-59-0	5281804	prunetin
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
108-46-3	5054	resorcinol
501-36-0	445154	resveratrol
302-79-4	444795	retinoic acid
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

CAS #	PubChem	Compound
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
107-97-1	1088	sarcosine
186537-58-6	193653	S-carboxymethylcysteine 2
186537-58-6	193653	S-carboxymethylcysteine 1
92-61-5	5280460	scopoletin
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
29915-38-6	1110	succinic acid
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
87-81-0	2724552	tagatose 1
87-81-0	2724552	tagatose 2
2595-98-4	441035	talose 1
2595-98-4	441035	talose 2
133-37-9	444305	tartaric acid
80-69-3	45	tartronic acid
480-18-2	439533	taxifolin
7365-44-8	446188	TES
53-43-0	6013	testosterone 1
53-43-0	6013	testosterone 2

CAS #	PubChem	Compound
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
7298-99-9	443239	threo-3-hydroxy-L-aspartate
95-43-2	439665	threose 1
95-43-2	439665	threose 2
50-89-5	5789	thymidine
50-89-5	5789	thymidine
65-71-4	1135	thymine
89-83-8	6989	thymol
3588-17-8	5356793	trans,trans-muconic 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
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
4484-88-2	122336	trehalose-6-phosphate
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
3387-36-8	6030	uridine 5'-monophosphate 1

CAS #	PubChem	Compound
3387-36-8	6030	uridine 5'-monophosphate 2
104-98-3	1178	urocanic acid 1
104-98-3	1178	urocanic acid 2
121-33-5	1183	vanillin
3681-93-4	5280441	vitexin 1
3681-93-4	5280441	vitexin 2
69-89-6	1188	xanthine
146-80-5	1189	xanthosine
298-81-7	4114	xanthotoxin 1
298-81-7	4114	xanthotoxin 2
59-00-7	5699	xanthurenic acid
87-99-0	6912	xylitol
13114-27-7	449093	zeatin 1
13114-27-7	449093	zeatin 2

www.agilent.com/chem

This item is intended for Research Use Only. Not for use in diagnostic procedures. Information, descriptions, and specifications in this publication are subject to change without notice.

Agilent Technologies shall not be liable for errors contained herein or for incidental or consequential damages in connection with the furnishing, performance, or use of this material.

© Agilent Technologies, Inc. 2009
Published in the U.S.A. January 13, 2009
5990-3311EN



Agilent Technologies