LOT 230-08 **PHYTOMLS**

PLATE	NROW	NCOL
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4	H	12

Master List_NAME	SMILES	MOLECULAR FORMULA
Asiatic acid	OC[C@]1(C)[C@@H](O)[C@H](O)C[C@	C30H48O5
2-Undecanone	CCCCCCCCCC(C)=O	C11H22O
(-)-Bornyl acetate	CC(=O)O[C@@H]1CC2CC[C@@]1(C)C2	C12H20O2
Lipoamide	NC(=O)CCCCC1CCSS1	C8H15NOS2
Genistein	OC1=CC=C(C=C1)C1=COC2=CC(O)=CC(	C15H10O5
(±)-Naringenin	[H][C@]1(CC(=O)C2=C(O1)C=C(O)C=C2	C15H12O5
(−)-Catechin	O[C@@H]1CC2=C(O)C=C(O)C=C2O[C@	C15H14O6
(-)-Epigallocatechin	O[C@@H]1CC2=C(O[C@@H]1C1=CC((	C15H14O7
Carnosic acid	CC(C)C1=CC2=C(C(O)=C1O)[C@]1(CCC	C20H28O4
Rotenone	[H][C@@]12COC3=C(C=C(OC)C(OC)=C	C23H22O6
(−)-Epicatechin gallate	OC1=CC(O)=C2C[C@@H](OC(=O)C3=C	C22H18O10
Narirutin	CC1OC(OCC2OC(OC3=CC(O)=C4C(=O)C	C27H32O14
(R)-(+)-Limonene	CC(=C)[C@H]1CCC(C)=CC1	C10H16
Proline Beta	C[N+]1(C)CCC[C@H]1C([O-])=O (free b	C7H13NO2 (free base)
1,3,5-Trimethoxybenzene	COC1=CC(OC)=CC(OC)=C1	C9H12O3
10-Undecen-1-ol	OCCCCCCCCCC=C	C11H22O
(R)-lipoic acid	OC(=O)CCCC[C@@H]1CCSS1	C8H14O2S2
(±)-α-Bisabolol	[illegible])CCC=C(C)C	C15H26O
1'-Acetoxychavicol acetate	[illegible] C1	C13H14O4
(S)-Abscisic acid	OC(=O)\C=C(/C)\C=C\[C@@]1(O)C(C)=	C15H20O4
(R)-Glabridin	CC1(C)OC2=C(C=C1)C1=C(CC(CO1)C1=	C20H20O4
(-)-Matairesinol	[H][C@]1(CC2=CC=C(O)C(OC)=C2)COC	C20H22O6
(-)-Epigallocatechin-3-gallate	OC1=CC2=C(C[C@@H](OC(=O)C3=CC(	C22H18O11
(-)-Gossypol	CC(C)C1=C2C=C(C)C(=C(O)C2=C(C=O)C	C30H30O8
2-Pyrrolidinone	O=C1CCCN1	C4H7NO
2-Hexenal	CCCC=CC=O	C6H10O
1-Phenylethylamine	CC(N)C1=CC=CC=C1	C8H11N
2-Butylfuran	CCCCC1=CC=CO1	C8H12O
2-Octanone	CCCCCCC(C)=O	C8H16O
1-Methylnaphthalene	CC1=CC=CC2=CC=CC=C12	C11H10
1-Furfurylpyrrole	C(N1C=CC=C1)C1=CC=CO1	C9H9NO
1-Methoxy-4-(2-propenyl)benzene	COC1=CC=C(CC=C)C=C1	C10H12O

3-(Dimethylaminomethyl)indole	CN(C)CC1=CNC2=CC=CC=C12	C11H14N2
2-Tridecanone	CCCCCCCCCCCC(C)=O	C13H26O
3,3',4'5-Tetrahydroxystilbene	OC1=CC(\C=C\C2=CC(O)=C(O)C=C2)=C	C14H12O4
3,3',4',7-Tetrahydroxyflavone	COC1=CC=C(C=C1O)C1=C(O)C(=O)C2=	C16H12O6
alpha-Phellandrene	CC(C)C1CC=C(C)C=C1	C10H16
3-Indoleacetonitrile	N#CCC1=CNC2=C1C=CC=C2	C10H8N2
3-Methylsulfinylpropyl isothiocyanate	CS(=O)CCCN=C=S	C5H9NOS2
3,4-Dihydroxyhydrocinnamic acid	OC(=O)CCC1=CC=C(O)C(O)=C1	C9H10O4
7-Isopropyl-1,4-dimethylazulene	CC(C)C1=CC2=C(C)C=CC2=C(C)C=C1	C15H18
3-Indolebutyric acid	OC(=O)CCCC1=CNC2=C1C=CC=C2	C12H13NO2
3,3'-Dithiobis[2-methylfuran]	CC1=C(SSC2=C(C)OC=C2)C=CO1	C10H10O2S2
3-Methylcyclopentadecanone	CC1CCCCCCCCCCCCC(=O)C1	C16H30O
5,7-Dihydroxyflavone	OC1=CC(O)=C2C(=O)C=C(OC2=C1)C1=C	C15H10O4
Rhein	OC(=O)C1=CC2=C(C(O)=C1)C(=O)C1=C	C15H8O6
6beta-Hydroxyasiatic acid	[H][C@@]12[C@@H](C)[C@H](C)CC[C	C30H48O6
4,5-Di-O-caffeoylquinic acid	O[C@@H]1C[C@@](O)(C[C@@H](OC	C25H24O12
Acetophenone	CC(=O)C1=CC=CC=C1	C8H8O
alpha-Terpinene	CC(C)C1=CC=C(C)CC1	C10H16
D-Linalool	CC(C)=CCC[C@](C)(O)C=C	C10H18O
Aspirin	CC(=O)OC1=CC=CC=C1C(O)=O	C9H8O4
beta-Elemene	CC(=C)[C@@H]1CC[C@@](C)(C=C)[C@	C15H24
Bergapten	COC1=C2C=CC(=O)OC2=CC2=C1C=CO2	C12H8O4
Apigenin	OC1=CC=C(C=C1)C1=CC(=O)C2=C(O)C=	C15H10O5
Atropine	CN1[C@H]2CC[C@@H]1C[C@@H](C2	C17H23NO3
Boldine	COC1=C(O)C=C2CC3N(C)CCC4=CC(O)=	C19H21NO4
alpha-Mangostin	COC1=C(O)C=C2OC3=C(C(O)=C(CC=C(C	C24H26O6
Baicalin	O[C@@H]1[C@@H](O)[C@@H](OC2=	C21H18O11
Agnuside	OCC1OC(OC2OC=CC3C(O)C=C(COC(=O	C22H26O11
Cinnamyl alcohol	OCC=CC1=CC=CC=C1	C9H10O
Di-2-propenyl disulfide, 9CI	C=CCSSCC=C	C6H10S2
Carvone	CC(=C)C1CC=C(C)C(=O)C1	C10H14O
Camphor	[H][C@@]12CC[C@@](C)(C(=O)C1)C2(	C10H16O
Eucalyptol	CC12CCC(CC1)C(C)(C)O2	C10H18O
Cassiastearoptene	COC1=CC=CC=C1\C=C\C=O	C10H10O2

Biochanin A	COC1=CC=C(C=C1)C1=COC2=CC(O)=C(	C16H12O5
Capsaicin	COC1=C(O)C=CC(CNC(=O)CCCC\C=C\C	C18H27NO3
Bilobalide	[H][C@]12C[C@@](O)(C(C)(C)C)[C@]3	C15H18O8
Chlorogenic acid	O[C@@H]1C[C@](O)(C[C@@H](OC(=(	C16H18O9
Arctigenin	COC1=CC=C(C[C@H]2COC(=O)[C@@H	C21H24O6
Corilagin	O[C@@H]1[C@H]2COC(=O)C3=C(C(O)	C27H22O18
Camphene	CC1(C)C2CCC(C2)C1=C	C10H16
Cyclohexaneacetic acid	OC(=O)CC1CCCCC1	C8H14O2
Coumarin	O=C1OC2=CC=CC=C2C=C1	C9H6O2
D-Citronellol	C[C@@H](CCO)CCC=C(C)C	C10H20O
delta-Decalactone	CCCCCC1CCCC(=O)O1	C10H18O2
Curcumol	CC(C)C1CC23OC1(O)CC(=C)C2CCC3C	C15H24O2
Daidzein	OC1=CC=C(C=C1)C1=COC2=C(C=CC(O)	C15H10O4
Delphinidin	C1=C(C=C(C(=C1O)O)O)C2=C(C=C3C(=(	C15H11O7 (free base)
Dihydrocapsaicin	COC1=C(O)C=CC(CNC(=O)CCCCCCC(C)	C18H29NO3
Cryptochlorogenic acid	O[C@@H]1C[C@@](O)(C[C@@H](O)[	C16H18O9
Curcumin	COC1=CC(\C=C\C(=O)CC(=O)\C=C\C2=	C21H20O6
Daidzin	OC[C@H]1O[C@@H](OC2=CC3=C(C=C	C21H20O9
gamma-Terpinene	CC(C)C1=CCC(C)=CC1	C10H16
Benzyl isothiocyanate	S=C=NCC1=CC=CC=C1	C8H7NS
Geraniol	CC(C)=CCC\C(C)=C/CO	C10H18O
Eugenol	COC1=C(O)C=CC(CC=C)=C1	C10H12O2
Flavone	O=C1C=C(OC2=CC=CC=C12)C1=CC=CC	C15H10O2
Costunolide	C\C1=C\CC\C(C)=C/C2OC(=O)C(=C)C2(	C15H20O2
Farnesyl Acetate	CC(C)=CCC\C(C)=C\CC\C(C)=C\COC(C)=	C17H28O2
Emodin	CC1=CC2=C(C(O)=C1)C(=O)C1=C(C=C((	C15H10O5
gamma-Glutamylphenylalanine	N[C@@H](CCC(=O)N[C@@H](CC1=CC	C14H18N2O5
Diosmetin	COC1=C(O)C=C(C=C1)C1=CC(=O)C2=C(	C16H12O6
Diosgenin	CC1CCC2(C(C3C(O2)CC4C3(CCC5C4CC=	C27H42O3
Ganoderic acid A	CC(CC(=O)CC(C)C(O)=O)C1CC(O)C2(C)(	C30H44O7
Indole-3-carbinol	OCC1=CNC2=CC=CC=C12	C9H9NO
Hydrocinnamic acid	OC(=O)CCC1=CC=CC=C1	C9H10O2
Hydroxytyrosol	OCCC1=CC=C(O)C(O)=C1	C8H10O3

m-Coumaric acid	OC(=O)\C=C\C1=CC(O)=CC=C1	C9H8O3
Harmaline	COC1=CC2=C(C=C1)C1=C(N2)C(C)=NC(	C13H14N2O
Imperatorin	CC(C)=CCOC1=C2OC(=O)C=CC2=CC2=(	C16H14O4
Gingerol	CCCCCC(O)CC(=O)CCC1=CC=C(O)C(OC	C17H26O4
Glycerol Tributyrate	CCCC(=O)OCC(COC(=O)CCC)OC(=O)CC	C15H26O6
Ginkgolic acid	CCCCCC\C=C\CCCCCCCC1=C(C(O)=O)C	C22H34O3
Glycyrrhetinic acid	CC1(C)[C@@H](O)CC[C@@]2(C)C1CC	C30H46O4
Hesperetin 7-neohesperidoside	COC1=C(O)C=C(C=C1)C1CC(=O)C2=C(C	C28H34O15
Hypoletin 8-gentiobioside	OCC1OC(OCC2OC(OC3=C(O)C=C(O)C4=	C27H30O17
Menthol	CC(C)[C@@H]1CC[C@@H](C)C[C@H]1	C10H20O
Methyl cinnamate	COC(=O)\C=C/C1=CC=CC=C1	C10H10O2
Isoeugenol	COC1=CC(\C=C\C)=CC=C1O	C10H12O2
Menadione	CC1=CC(=O)C2=CC=CC=C2C1=O	C11H8O2
Isoliquiritigenin	OC1=CC=C(\C=C\C(=O)C2=C(O)C=C(O)	C15H12O4
Octadecanol	CCCCCCCCCCCCCCCCCCO	C18H38O
L-N-(1H-Indol-3-ylacetyl)aspartic acid	OC(=O)CC(NC(=O)CC1=CNC2=C1C=CC=	C14H14N2O5
Hesperetin	COC1=C(O)C=C(C=C1)[C@@H]1CC(=O	C16H14O6
Isoxanthohumol B	COC1=CC2=C(C(O)CC(C)(C)O2)C(O)=C1	C21H22O6
Luteolin-7-glucoside	OC[C@H]1O[C@@H](OC2=CC3=C(C(O	C21H20O11
Limonin	CC1(C)OC2CC(=O)OCC22C1CC(=O)C1((	C26H30O8
Madecassoside	CC1CCC2(CCC3(C)C(=CCC4C5(C)CC(O)(	C48H78O20
p-Cymene	CC(C)C1=CC=C(C)C=C1	C10H14
Nornicotine	C1CNC(C1)C1=CC=CN=C1	C9H12N2
Methylparaben	COC(=O)C1=CC=C(O)C=C1	C8H8O3
Methyleugenol	COC1=C(OC)C=C(CC=C)C=C1	C11H14O2
Methyl Jasmonate	CC\C=C/C[C@@H]1[C@@H](CC(=O)O	C13H20O3
Norizalpinin	OC1=CC(O)=C2C(OC(=C(O)C2=O)C2=C(	C15H10O5
Kaempferol	OC1=CC=C(C=C1)C1=C(O)C(=O)C2=C(C	C15H10O6
Myricetin	OC1=CC(O)=C2C(OC(=C(O)C2=O)C2=C(	C15H10O8
Neochlorogenic acid	OC1CC(O)(CC(OC(=O)\C=C\C2=CC=C(C	C16H18O9
Nobiletin	COC1=CC=C(C=C1OC)C1=CC(=O)C2=C(	C21H22O8
Oleanolic acid	CC1(C)CC[C@@]2(CC[C@]3(C)C(=CC[C	C30H48O3
Oleuropein	[H][C@]1(CC(=O)OCCC2=CC(O)=C(O)C=	C25H32O13
Pyrogallol	[H]OC1=CC=CC(O[H])=C1O[H]	C6H6O3

Pulegone	C[C@@H]1CCC(=C(C)C)C(=O)C1	C10H16O
Protocatechuic acid	OC(=O)C1=CC(O)=C(O)C=C1	C7H6O4
Sphingosine	CCCCCCCCCCCCC\C=C\[C@@H](O)[C@	C18H37NO2
Phthalic acid	OC(=O)C1=CC=CC=C1C(O)=O	C8H6O4
Resveratrol	OC1=CC=C(\C=C\C2=CC(O)=CC(O)=C2)	C14H12O3
Piperine	O=C(\C=C\C=C\C1=CC2=C(OCO2)C=C1	C17H19NO3
Quinine	[H][C@]1(C[C@@H]2CC[N@]1C[C@@	C20H24N2O2
Puerarin	OC[C@H]1O[C@H]([C@H](O)[C@@H]	C21H20O9
Quercitrin	C[C@@H]1O[C@@H](OC2=C(OC3=C(C	C21H20O11
Quercetin 3-O-glucuronide	OC1C(O)C(OC2=C(OC3=CC(O)=CC(O)=	C21H18O13
Rutin	=C(OC4=CC(=CC(=C4C3=O)O)O)C5=C	C27H30O16 (anhydrous)
Terpinolene	CC(C)=C1CCC(C)=CC1	C10H16
Thymol	CC(C)C1=C(O)C=C(C)C=C1	C10H14O
p-Octopamine	NC[C@H](O)C1=CC=C(O)C=C1 (free ba	C8H11NO2 (free base)
Sulforaphane	CS(=O)CCCCN=C=S	C6H11NOS2
Scopoletin	COC1=C(O)C=C2OC(=O)C=CC2=C1	C10H8O4
Scoparone	COC1=C(OC)C=C2C=CC(=O)OC2=C1	C11H10O4
trans-Nerolidol	CC(C)=CCCC(C)=CCCC(C)(O)C=C	C15H26O
Sclareol	CC(O)(CCC1C(C)(O)CCC2C(C)(C)CCCC1	C20H36O2
Stigmastanol	CC[C@H](CC[C@@H](C)[C@H]1CC[C@	C29H52O
Silibinin	COC1=C(O)C=CC(=C1)C1OC2=C(OC1C(	C25H22O10
Theaflavin	O[C@@H]1CC2=C(O)C=C(O)C=C2O[C@	C29H24O12
Secoisolariciresinol diglucoside	COC1=CC(CC(COC2OC(CO)C(O)C(O)C2	C32H46O16
(−)-β-Pinene	CC1(C)C2CC1C(=C)CC2	C10H16
Umbelliferone	OC1=CC2=C(C=C1)C=CC(=O)O2	C9H6O3
β-Caryophyllene	[H][C@]12CC(C)(C)[C@]1([H])CC\C(C)=	C15H24
Dihydrogenistein	OC1=CC=C(C=C1)C1COC2=CC(O)=CC(C	C15H12O5
Retinal	C\C(\C=C\C=C(/C)\C=C\C1=C(C)CCCC1	C20H28O
Luteolin	OC1=CC2=C(C(O)=C1)C(=O)C=C(O2)C1	C15H10O6
Vitamin D3	[H][C@@]1(CC[C@@]2([H])\C(CCC[C@	C27H44O
Ginkgolide A	CC1C(=O)OC2CC34C5CC(C(C)(C)C)C33	C20H24O9
Ginkgolide B	CC1C(=O)OC2C(O)C34C5CC(C(C)(C)C)C	C20H24O10
Ginkgolide C	CC1C(=O)OC2C(O)C34C5OC(=O)C3(OC	C20H24O11
Vitamin K1	CC(C)CCC[C@@H](C)CCC[C@@H](C)C	C31H46O2

Eriocitrin	[H][C@]1(CC(=O)C2=C(C1)C=C(O[C@@	C27H32O15
Tetramethylpyrazine	CC1=NC(C)=C(C)N=C1C	C8H12N2
trans-Anethole	COC1=CC=C(\C=C/C)C=C1	C10H12O
Phenylacetylglutamine	NC(=O)CC[C@H](NC(=O)CC1=CC=CC=C	C13H16N2O4
5,7-dihydroxy-2-(4-hydroxyphenyl)-6-met	COC1=C(O)C2=C(OC(=CC2=O)C2=CC=C	C16H12O6
Quercetin	OC1=CC2=C(C(O)=C1)C(=O)C(O)=C(O2	C15H10O7 (anhydrous)
(+)-Gallocatechin	O[C@H]1CC2=C(O)C=C(O)C=C2O[C@@	C15H14O7
Casticin	COC1=C(O)C=C(C=C1)C1=C(OC)C(=O)C	C19H18O8
Celastrol	[H][C@@]12C[C@@](C)(CC[C@]1(C)C	C29H38O4
Astaxanthin	C\C(\C=C\C=C(/C)\C=C\C1=C(C)C(=O)[	C40H52O4
Hesperidine	COC1=CC=C(C=C1O)[C@@H]1CC(=O)C	C28H34O15
Acteoside	CC1OC(OC2C(O)C(OCCC3=CC(O)=C(O)C	C29H36O15
Melatonin	COC1=CC2=C(NC=C2CCNC(C)=O)C=C1	C13H16N2O2
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2-Furancarboxaldehyde	O=CC1=CC=CO1	C5H4O2
(E)-3-Hexen-1-ol	CC\C=C/CCO	C6H12O
2-Furoic acid	OC(=O)C1=CC=CO1	C5H4O3
2-Ethylbutyric Acid	CCC(CC)C(O)=O	C6H12O2
2,4-Dihydroxybutanoic acid	OCCC(O)C(O)=O (free acid)	C4H8O4 (free acid)
2-Acetylpyrazine	CC(=O)C1=CN=CC=N1	C6H6N2O
2-Hydroxyphenethylamine	NCC(O)C1=CC=CC=C1	C8H11NO
1,5-Anhydrosorbitol	@@H]1O	C6H12O5

(R)C(S)S-Alliin	NC(CS(=O)CC=C)C(O)=O	C6H11NO3S
2-Keto-D-gluconate	OCC(O)C(O)C(O)C(=O)C(O)=O	C6H10O7
Suberylglycine	OC(=O)CCCCCCC(=O)NCC(O)=O	C10H17NO5
Sinigrin	OC[C@H]1O[C@@H](S\C(=N\OS(O)(=(	C10H17NO9S2 (free acid
2-Methyl-1-butanol	CCC(C)CO	C5H12O
2-Methyltetrahydrofuran-3-one	CC1OCCC1=O	C5H8O2
3-Hydroxyisobutyric acid	C[C@H](CO)C(O)=O (free acid)	C4H8O3 (free acid)
3-Furoic acid	OC(=O)C1=COC=C1	C5H4O3
2-Methyl-2-pentenoic acid	CC\C=C(\C)C(O)=O	C6H10O2
2-Methylmalonic acid	CC(C(O)=O)C(O)=O	C4H6O4
2-Picolinic acid	OC(=O)C1=CC=CC=N1	C6H5NO2
Dihydrothymine	CC1CNC(=O)NC1=O	C5H8N2O2
3,4-Dihydroxybenzaldehyde	OC1=CC=C(C=O)C=C1O	C7H6O3
3,5-Dihydroxybenzoic acid	OC(=O)C1=CC(O)=CC(O)=C1	C7H6O4
3-(3,4-Dihydroxyphenyl)lactic acid	OC(CC1=CC(O)=C(O)C=C1)C(O)=O (free	C9H10O5 (free base)
3,4,5-Trimethoxycinnamic acid	COC1=CC(\C=C\C(O)=O)=CC(OC)=C1O(	C12H14O5
Acrylamide	NC(=O)C=C	C3H5NO
3-Aminoisobutanoic acid	CC(CN)C(O)=O	C4H9NO2
3-Hydroxyvaleric acid	CCC(O)CC(O)=O	C5H10O3
3-Methylthiopropionic acid	CSCCC(O)=O	C4H8O2S
4-hydroxy-3-methylbenzoic acid	CC1=CC(=CC=C1O)C(O)=O	C8H8O3
Arecoline	COC(=O)C1=CCCN(C)C1	C8H13NO2
4,5-Dihydroorotic acid	OC(=O)C1CC(=O)NC(=O)N1	C5H6N2O4
3-Methylxanthine	CN1C2=C(NC=N2)C(=O)NC1=O	C6H6N4O2
5-Methoxysalicylic acid	COC1=CC(C(O)=O)=C(O)C=C1	C8H8O4
D-Glucurono-6,3-lactone	O[C@@H]1O[C@@H]2[C@@H](O)C(=	C6H8O6
Arbutin	OCC1OC(OC2=CC=C(O)C=C2)C(O)C(O)(	C12H16O7
Amygdalin	OCC1OC(OCC2OC(OC(C#N)C3=CC=CC=	C20H27NO11
Cyclohexanone	O=C1CCCCC1	C6H10O
Ethyl isopropyl ketone	CCC(=O)C(C)C	C6H12O
3-Hydroxyisovaleric acid	CC(C)(O)CC(O)=O	C5H10O3
Cyclohexanecarboxylic Acid	OC(=O)C1CCCCC1	C7H12O2
Ethyl acetoacetate	CCOC(=O)CC(C)=O	C6H10O3
Citramalic acid	CC(O)(CC(O)=O)C(O)=O (free acid)	C5H8O5 (free acid)

alpha-Terpineol	CC1=CC[C@@H](CC1)C(C)(C)O	C10H18O
Betonicine	C[N+]1(C)C[C@H](O)C[C@H]1C([O-])=(	C7H13NO3
beta-Glycerophosphoric acid	OCC(CO)OP(O)(O)=O (anhydrous free a	C3H9O6P (anhydrous fre
Canavanine	N[C@@H](CCONC(N)=N)C(O)=O	C5H12N4O3
Ergothioneine	C[N+](C)(C)[C@@H](CC1=CNC(=S)N1)(	C9H15N3O2S
Deoxyinosine	OC[C@H]1O[C@H](C[C@@H]1O)N1C=	C10H12N4O4
3-Hydroxycoumarin	OC1=CC2=CC=CC=C2OC1=O	C9H6O3
Hydroquinone	OC1=CC=C(O)C=C1	C6H6O2
Ethyl pyruvate	CCOC(=O)C(C)=O	C5H8O3
L-Allothreonine	C[C@H](O)[C@H](N)C(O)=O	C4H9NO3
Isonicotinic acid	OC(=O)C1=CC=NC=C1	C6H5NO2
Kojic acid	OCC1=CC(=O)C(O)=CO1	C6H6O4
Gentisic acid	OC(=O)C1=C(O)C=CC(O)=C1	C7H6O4
Galactonic acid	OC[C@@H](O)[C@H](O)[C@H](O)[C@	C6H12O7 (free acid)
Glucaric acid	O[C@@H]([C@H](O)[C@@H](O)C(O)=	C6H10O8 (free acid)
Glycerophosphocholine	C[N+](C)(C)CCOP([O-])(=O)OC[C@H](C	C8H20NO6P
Geniposidic acid	OCC1OC(OC2OC=C(C3CC=C(CO)C23)C(	C16H22O10
Flavin mononucleotide	CC1=CC2=C(C=C1C)N(C[C@H](O)[C@H	C17H21N4O9P (anhydro
Levulinic acid	CC(=O)CCC(O)=O	C5H8O3
Niacinamide	NC(=O)C1=CC=CN=C1	C6H6N2O
Maltol	CC1=C(O)C(=O)C=CO1	C6H6O3
Methylcysteine	CSC[C@@H](N)C(O)=O	C4H9NO2S
Methyl nicotinate	COC(=O)C1=CN=CC=C1	C7H7NO2
Mesifurane	COC1=C(C)OC(C)C1=O	C7H10O3
Levoglucosan	[H][C@@]12OC[C@@H](O1)[C@@H](	C6H10O5
N2-Acetylornithine	CC(=O)N[C@@H](CCCN)C(O)=O	C7H14N2O3
scyllo-Inositol	O[C@H]1[C@H](O)[C@@H](O)[C@H](	C6H12O6
Lenticin	C[N+](C)(C)[C@@H](CC1=CNC2=CC=C	C14H18N2O2
Maltotriose	OC[C@H]1O[C@H](O[C@H]2[C@H](O	C18H32O16
Malonyl-CoA	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]	C24H38N7O19P3S (free
Senecioic acid	CC(C)=CC(O)=O	C5H8O2
o-Cresol	CC1=CC=CC=C1O	C7H8O
S-(2-Aminoethyl)-L-cysteine	NCCSCC(N)C(O)=O (free base)	C5H12N2O2S (free base)
Tropate	OCC(C(O)=O)C1=CC=CC=C1	C9H10O3

p-Hydroxymandelic acid	OC(C(O)=O)C1=CC=C(O)C=C1	C8H8O4
S-Carboxymethyl-L-cysteine	NC(CSCC(O)=O)C(O)=O	C5H9NO4S
L-Iditol	OC[C@H](O)[C@@H](O)[C@H](O)[C@	C6H14O6
Selenomethionine	C[Se]CCC(N)C(O)=O	C5H11NO2Se
Pilocarpine	CC[C@H]1[C@@H](CC2=CN=CN2C)CC	C11H16N2O2 (free base
Prephenate	OC1C=CC(CC(=O)C(O)=O)(C=C1)C(O)=(	C10H10O6 (free acid)
Ribothymidine	CC1=CN([C@@H]2O[C@H](CO)[C@@	C10H14N2O6
Salicin	OC[C@H]1O[C@@H](OC2=C(CO)C=CC	C13H18O7
2-Methylbenzoic acid	CC1=C(C=CC=C1)C(O)=O	C8H8O2
Tyrosol	OCCC1=CC=C(O)C=C1	C8H10O2
1-Phenyl-1,2-propanedione	CC(=O)C(=O)C1=CC=CC=C1	C9H8O2
(S)-Citronellal	C[C@H](CCC=C(C)C)CC=O	C10H18O
Vanillic acid	COC1=C(O)C=CC(=C1)C(O)=O	C8H8O4
L-Theanine	CCNC(=O)CC[C@H](N)C(O)=O	C7H14N2O3
(−)-Cotinine	CN1C(CCC1=O)C1=CN=CC=C1	C10H12N2O
1-Methyluric acid	CN1C(=O)NC2=C(NC(=O)N2)C1=O	C6H6N4O3
Adenosine phosphosulfate	NC1=NC=NC2=C1N=CN2[C@@H]1O[C	C10H14N5O10PS (free a
Genistin	OCC1OC(OC2=CC(O)=C3C(=O)C(=COC3	C21H20O10
Orientin	OCC1OC(C(O)C(O)C1O)C1=C(O)C=C(O)	C21H20O11
Myricitrin	CC1OC(OC2=C(OC3=CC(O)=CC(O)=C3C	C21H20O12
2-Phenylethanol	OCCC1=CC=CC=C1	C8H10O
Threonic acid	C(C(C(C(=O)O)O)O)O (FREE ACID)	C4H8O5 (free acid)
(+)-(S)-Carvone	CC(=C)[C@H]1CC=C(C)C(=O)C1	C10H14O
2',4'-Dihydroxyacetophenone	OCC(=O)C1=CC=C(O)C=C1	C8H8O3
Terpinen-4-ol	CC(C)C1(O)CCC(C)=CC1	C10H18O
2-Hydroxyoctanoic acid	CCCCCCC(O)C(O)=O	C8H16O3
Isoxanthopterin	NC1=NC(=O)C2=C(N1)NC(=O)C=N2	C6H5N5O2
(+)-Nootkatone	CC1CC(=O)C=C2CCC(CC12C)C(C)=C	C15H22O
Gibberellin A3	[H][C@@]12CC[C@]3(O)C[C@]1(CC3=	C19H22O6
Naringin	C[C@@H]1O[C@@H](O[C@@H]2[C@	C27H32O14
Diosmin	COC1=C(O)C=C(C=C1)C1=CC(=O)C2=C(	C28H32O15
Succinyl-CoA	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]:	C25H40N7O19P3S (free
2-Methylpentanal	CCCC(C)C=O	C6H12O

2-Ketohexanoic acid	CCCCC(=O)C(O)=O (free acid basis)	C6H10O3 (free acid basi
2,6-Dihydroxybenzoic acid	OC(=O)C1=C(O)C=CC=C1O	C7H6O
DL-2-Aminooctanoic acid	CCCCCCC(N)C(O)=O	C8H17NO2
7-Methylxanthine	CN1C=NC2=C1C(=O)NC(=O)N2	C6H6N4O2
Gallic acid	OC(=O)C1=CC(O)=C(O)C(O)=C1	C7H6O5
(-)-Epicatechin	O[C@@H]1CC2=C(O)C=C(O)C=C2O[C@	C15H14O6
7-Methylguanosine	CN1C=[N+]([C@@H]2O[C@H](CO)[C@	C11H16N5O5
Mangiferin	OCC1OC(C(O)C(O)C1O)C1=C(O)C2=C(C	C19H18O11
Dephospho-CoA	CC(C)(COP(O)(=O)OP(O)(=O)OC[C@H]:	C21H35N7O13P2S
Trigonelline	C[N+]1=CC=CC(=C1)C([O-])=O (non chl	C7H7NO2 (non chloride)
Methylmalonyl-CoA	C[C@@H](C(O)=O)C(=O)SCCNC(=O)CC	C25H40N7O19P3S (anhy
2-Oxohexane	CCCCC(C)=O	C6H12O
Ethyl propionate	CCOC(=O)CC	C5H10O2
Methylsuccinic acid	CC(CC(O)=O)C(O)=O	C5H8O4
3-Phenyl-1-propanol	OCCCC1=CC=CC=C1	C9H12O
2,4-Dihydroxybenzoic Acid	OC(=O)C1=C(O)C=C(O)C=C1	C7H6O4
7-Hydroxyoctanoic acid	CC(O)CCCCCC(O)=O	C8H16O3
3-Hydroxy-4,5-dimethyl-2(5H)-furanone	CC1OC(=O)C(O)=C1C	C6H8O3
2,4,6-Trihydroxybenzoic acid	OC(=O)C1=C(O)C=C(O)C=C1O (anhydr	C7H6O5 (anhydrous)
1,3,7-Trimethyluric acid	CN1C(=O)NC2=C1C(=O)N(C)C(=O)N2C	C8H10N4O3
Pseudouridine	OC[C@H]1O[C@H]([C@H](O)[C@@H]	C9H12N2O6
Monotropein	OCC1OC(OC2OC=C(C3C=CC(O)(CO)C2:	C16H22O11
Maltotetraose	OC[C@H]1O[C@H](O[C@H]2[C@H](O	C24H42O21
n-Butyl acetate	CCCCOC(C)=O	C6H12O2
D-Cysteine	N[C@H](CS)C(O)=O	C3H7NO2S
p-Anisidine	COC1=CC=C(N)C=C1	C7H9NO
Sesamol	OC1=CC2=C(OCO2)C=C1	C7H6O3
D-synephrine	CNC[C@H](O)C1=CC=C(O)C=C1 (free b	C9H13NO2 (free base)
N1-Acetylspermidine	CC(=O)NCCCNCCCCN (free base)	C9H21N3O (free base)
Pectic acid	O[C@H]1O[C@@H]([C@H](O)[C@H]((	C6H10O7 (free acid)
Homoveratric acid	COC1=CC=C(CC(O)=O)C=C1OC	C10H12O4
Cysteine-S-sulfate	N[C@@H](CSS(O)(=O)=O)C(O)=O	C3H7NO5S2
Neopterin	NC1=NC2=C(N=C(C=N2)C(O)C(O)CO)C(	C9H11N5O4
AICA-riboside	NC(=O)C1=C(N)N(C=N1)[C@@H]1O[C(	C9H14N4O5

Acetoacetyl-CoA	CC(=O)CC(=O)SCCNC(=O)CCNC(=O)C(C	C25H40N7O18P3S (anhy
2-Pentanone	CCCC(C)=O	C5H10O
3-(Methylthio)-1-propene	CSCC=C	C4H8S
Glycyrrhizin	CC1(C)C(CCC2(C)C1CCC1(C)C2C(=O)C=	C42H62O16
2-Phenylbutyric acid	CCC(C(O)=O)C1=CC=CC=C1	C10H12O2
2,6-Dimethoxybenzoic acid	COC1=CC=CC(OC)=C1C(O)=O	C9H10O4
5-Methoxytryptamine	COC1=CC2=C(NC=C2CCN)C=C1	C11H14N2O
alpha-Humulene	C\C1=C\CC(C)(C)\C=C/C\C(C)=C/CC1	C15H24
Phytanic acid	CC(C)CCCC(C)CCCC(C)CCCC(C)CC(O)=C	C20H40O2
Adipostatin A	CCCCCCCCCCCCCCCC1=CC(O)=CC(O)=	C21H36O2
Aesculin	OCC1OC(OC2=C(O)C=C3OC(=O)C=CC3=	C15H16O9 (anhydrous)
Aloin	OCC1OC(C(O)C(O)C1O)C1C2=C(C(O)=C	C21H22O9
Quercetin 3-galactoside	OC[C@H]1O[C@@H](OC2=C(OC3=C(C	C21H20O12
Angelicin	[H]C1=C([H])C2=C(O1)C([H])=C([H])C1=	C11H6O3
(S)-3-Butyl-1(3H)-isobenzofuranone	CCCCC1OC(=O)C2=C1C=CC=C2	C12H14O2
Farrerol	CC(C)=CCC\C(C)=C\CC\C(C)=C\CO	C15H26O
Coumesterol	OC1=CC2=C(C=C1)C1=C(O2)C2=C(OC1	C15H8O5
Enterodiol	OC[C@H](CC1=CC(O)=CC=C1)[C@H](C	C18H22O4
Isorhamnetin	COC1=C(O)C=CC(=C1)C1=C(O)C(=O)C2	C16H12O7
Berberine	COC1=CC=C2C=C3C4=CC5=C(OCO5)C=	C20H18NO4 (berberine)
Cosmosiin	OC[C@H]1O[C@@H](OC2=CC(O)=C3C	C21H20O10
Chicoric acid	OC(=O)[C@H](OC(=O)\C=C\C1=CC(O)=	C22H18O12
Amentoflavone	OC1=CC=C(C=C1)C1=CC(=O)C2=C(O)C=	C30H18O10
Canthaxanthin	C\C(\C=C\C=C(/C)\C=C\C1=C(C)C(=O)C	C40H52O2
Asiaticoside	CC1CCC2(CCC3(C)C(=CCC4C5(C)CC(O)C	C48H78O19
Phenylglyoxylic acid	OC(=O)C(=O)C1=CC=CC=C1	C8H6O3
Methyl 3-indolyacetate	COC(=O)CC1=CNC2=C1C=CC=C2	C11H11NO2
Phenylacetylglycine	OC(=O)CNC(=O)CC1=CC=CC=C1	C10H11NO3
Syringic acid	COC1=CC(=CC(OC)=C1O)C(O)=O	C9H10O5
Phenylpropionylglycine	OC(=O)CNC(=O)CCC1=CC=CC=C1	C11H13NO3
Sinapic acid	COC1=CC(\C=C\C(O)=O)=CC(OC)=C1O	C11H12O5
Phloretin	OC1=CC=C(CCC(=O)C2=C(O)C=C(O)C=C	C15H14O5
Morin	OC1=CC(O)=C(C=C1)C1=C(O)C(=O)C2=	C15H10O7 (anhydrous)
Sanguinarine	C[N+]1=C2C3=CC4=C(OCO4)C=C3C=CC	C20H14NO4 (Sanguinari

Tangeretin	COC1=CC=C(C=C1)C1=CC(=O)C2=C(OC	C20H20O7
Phloridzin	OC[C@H]1O[C@@H](OC2=CC(O)=CC((	C21H24O10 (anhydrous)
Calycosin 7-galactoside	COC1=CC=C(C=C1O)C1=COC2=CC(OC3	C22H22O10
Formononetin	COC1=CC=C(C=C1)C1=COC2=C(C=CC((	C16H12O4
(+)-Catechin	O[C@H]1CC2=C(O)C=C(O)C=C2O[C@(	C15H14O6 (anhydrous)
Solasodine	CC1C2C(CC3C4CC=C5CC(O)CCC5(C)C4(	C27H43NO2
Trifolirhizin	OCC1OC(OC2=CC=C3C4OC5=C(C=C6O(	C22H22O10
Nomilin	CC(=O)OC1CC(=O)OC(C)(C)C2CC(=O)C3	C28H34O9
Cucurbitacin B	CC(=O)OC(C)(C)\C=C\C(=O)C(C)(O)C1C	C32H46O8
INTENTIONALLY BLANK		
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KEGG ID_CSID	CAS ID	HMDB ID	NEUTRAL MONOISOTOI
C08617	464-92-6	NA	488.3501746
C01875	112-12-9	HMDB0033713	170.1670653
C09837	5655-61-8	HMDB0040397	196.1463299
C00248	940-69-2	HMDB0000962	205.0595055
C06563	446-72-0	HMDB0003217	270.0528234
C00509	67604-48-2	HMDB0002670	272.0684735
C14079	18829-70-4	HMDB0037953	290.0790382
C12136	970-74-1	HMDB0038361	306.0739528
CSID400886	3650-09-7	HMDB0002358	332.1987594
C07593	83-79-4	HMDB0034436	394.1416384
CSID97034	1257-08-5	HMDB0037944	442.0899968
C09793	14259-46-2	HMDB0033740	580.1792057
C00521	5989-54-8	HMDB0004321	136.1252005
C10172 (free base)	471-87-4 (free base)	HMDB0004827 (free bas	143.094628665 (free bas
CSID21111723	621-23-8	HMDB0059963	168.0786443
CSID7893	112-43-6	HMDB0031016	170.1670653
C16241	1200-22-2	HMDB0001451	206.0435211
C09621	23089-26-1	HMDB0036197	222.1983655
CSID354584	52946-22-2	HMDB0041005	234.0892089
C06082	21293-29-8	HMDB0035140	264.1361591
C10421	59870-68-7	HMDB0034188	324.1361591
C10682	580-72-3	HMDB0035698	358.1416384
C09731	989-51-5	HMDB0003153	458.0849114
C07667	90141-22-3	HMDB0040723	518.1940679
C11118	616-45-5	HMDB0002039	85.05276385
C08497	6728-26-3	HMDB0031496	98.07316494
C02455	98-84-0	HMDB0002017	121.0891494
CSID19338	4466-24-4	HMDB0040272	124.088815
CSID7802	111-13-7	HMDB0031294	128.1201151
C14082	90-12-0	HMDB0032860	142.0782503
CSID14312	1438-94-4	HMDB0030204	147.0684139
C10452	140-67-0	HMDB0034121	148.088815

C08304	87-52-5	HMDB0035762	174.1156985
CSID11132	593-08-8	HMDB0034148	198.1983655
C05901	10083-24-6	HMDB0004215	244.0735589
C10041	528-48-3	HMDB0029492	300.0633881
C09875	99-83-2	HMDB0035850	136.1252005
C02938	771-51-7	HMDB0006524	156.0687483
CSID10023	505-44-2	HMDB0006095	163.0125553
C10447	1078-61-1	HMDB0000423	182.0579088
C09675	489-84-9	HMDB0036648	198.1408506
C11284	133-32-4	HMDB0002096	203.0946287
CSID526624	28588-75-2	HMDB0040201	226.0122209
CSID10483	541-91-3	HMDB0034181	238.2296656
C10028	480-40-0	HMDB0036619	254.0579088
C10401	478-43-3	HMDB0032876	284.032088
CSID227128	18449-41-7	HMDB0036670	504.3450893
CSID4976335	57378-72-0	HMDB0030707	516.1267762
C07113	98-86-2	HMDB0033910	120.0575149
C09898	99-86-5	HMDB0036995	136.1252005
C11389	126-90-9	HMDB0036102	154.1357652
C01405	50-78-2	HMDB0001879	180.0422587
C17094	515-13-9	HMDB0061848	204.1878008
C01557	484-20-8	HMDB0030637	216.0422587
C01477	520-36-5	HMDB0002124	270.0528234
C01479	51-55-8	HMDB0014712	289.1677936
C09365	476-70-0	HMDB0039085	327.1470582
C10080	6147-11-1	HMDB0035796	410.1729386
C10025	21967-41-9	HMDB0041832	446.0849114
C09765	11027-63-7	HMDB0036561	466.1475117
C02394	104-54-1	HMDB0029697	134.0731649
C08369	2179-57-9	HMDB0033966	146.0223917
c01767	22327-39-5	HMDB0035824	150.1044651
C00808	464-49-3	HMDB0059838	152.1201151
C09844	470-82-6	HMDB0004472	154.1357652
CSID556589	1504-74-1	HMDB0033830	162.0680796

C00814	491-80-5	HMDB0002338	284.0684735
C06866	404-86-4	HMDB0002227	305.1990937
C07605	33570-04-6	HMDB0036735	326.1001676
C00852	327-97-9	HMDB0003164	354.0950822
C10545	7770-78-7	HMDB0030087	372.1572885
C10219	23094-69-1	HMDB0031457	634.0806139
C06076	79-92-5	HMDB0059839	136.1252005
CSID20080	5292-21-7	HMDB0031403	142.0993797
C05851	91-64-5	HMDB0001218	146.0367794
C09849	1117-61-9	HMDB0035093	156.1514153
CSID12282	705-86-2	HMDB0037116	170.1306798
CSID2797480	4871-97-0	HMDB0038122	236.17763
C10208	486-66-8	HMDB0003312	254.0579088
C05908 (free base)	528-53-0 (free base)	NA	303.049927 (free base)
C16952	19408-84-5	HMDB0038457	307.2147438
CSID22912773	905-99-7	HMDB0030653	354.0950822
C10443	458-37-7	HMDB0002269	368.1259884
C10216	552-66-9	HMDB0033991	416.1107322
C09900	99-85-4	HMDB0005806	136.1252005
C03098	622-78-6	HMDB0033969	149.0299199
C09871	106-25-2	HMDB0005812	154.1357652
C10453	97-53-0	HMDB0005809	164.0837296
C15608	525-82-6	HMDB0003075	222.0680796
C09382	553-21-9	HMDB0036688	232.1463299
CSID554014	4128-17-0	HMDB0240268	264.2089301
C10343	518-82-1	HMDB0035214	270.0528234
CSID99868	7432-24-8	HMDB0000594	294.1215717
C10038	520-34-3	HMDB0029676	300.0633881
C08898	512-04-9	NA	414.313385
CSID413668	81907-62-2	HMDB0034931	516.3087038
CSID3581	700-06-1	HMDB0005785	147.0684139
C05629	501-52-0	HMDB0000764	150.0680796
CSID74680	10597-60-1	HMDB0005784	154.0629942

C12621	14755-02-3	HMDB0001713	164.0473441
C06536	304-21-2	HMDB0030310	214.1106131
C09269	482-44-0	HMDB0034376	270.0892089
C10462	23513-14-6	HMDB0005783	294.1831093
C13870	60-01-5	HMDB0031094	302.1729386
C10794	22910-60-7	HMDB0033897	346.250795
C02283	471-53-4	HMDB0011628	470.33961
C09806	13241-33-3	HMDB0030748	610.1897704
C08902	467-55-0	HMDB0038824	626.1482995
C00400	2216-51-5	HMDB0003352	156.1514153
C06358	103-26-4	HMDB0033833	162.0680796
C10469	97-54-1	HMDB0005802	164.0837296
C05377	58-27-5	HMDB0001892	172.0524295
C08650	961-29-5	HMDB0037316	256.0735589
D01924	112-92-5	HMDB0002350	270.2922658
CSID3845644	2456-73-7	HMDB0038666	290.0902716
C01709	520-33-2	HMDB0005782	302.0790382
CSID35013938	521-48-2	HMDB0035499	370.1416384
C03951	5373-11-5	HMDB0035588	448.1005615
C03514	1180-71-8	HMDB0035921	470.1940679
CSID142124	34540-22-2	HMDB0040122	974.5086449
C06575	99-87-6	HMDB0005805	134.1095505
C06524	494-97-3	HMDB0001126	148.1000484
CSID7176	99-76-3	HMDB0032572	152.0473441
C10454	93-15-2	HMDB0031864	178.0993797
C11512	39924-52-2	HMDB0036583	224.1412445
C10044	548-83-4	HMDB0029521	270.0528234
C05903	520-18-3	HMDB0005801	286.0477381
C10107	529-44-2	HMDB0002755	318.0375673
CSID4475041	906-33-2	HMDB0040690	354.0950822
C10112	478-01-3	HMDB0029540	402.1314677
C17148	508-02-1	HMDB0002364	456.3603454
C09794	32619-42-4	HMDB0035872	540.1842911
C01108	87-66-1	HMDB0013674	126.0316941

C09893	89-82-7	HMDB0035604	152.1201151
C00230	99-50-3	HMDB0001856	154.0266087
C00319	123-78-4	HMDB0000252	299.2824294
C01606	88-99-3	HMDB0002107	166.0266087
C03582	501-36-0	HMDB0003747	228.0786442
C03882	94-62-2	HMDB0029377	285.1364935
C06526	130-95-0	HMDB0014611	324.183778
C10524	3681-99-0	HMDB0240265	416.1107322
C01750	522-12-3	HMDB0033751	448.1005615
CSID10176995	22688-79-5	HMDB0029212	478.0747407
C05625 (anhydrous)	153-18-4 (anhydrous)	HMDB0003249 (anhydrc	610.153384912 (anhydrc
C06075	586-62-9	HMDB0036994	136.1252005
C09908	89-83-8	HMDB0001878	150.1044651
C04227 (free base)	104-14-3 (free base)	HMDB0004825 (free bas	153.078978601 (free bas
CSID5157	4478-93-7	HMDB0005792	177.0282054
C01752	92-61-5	HMDB0034344	192.0422587
C09311	120-08-1	HMDB0030818	206.0579088
CSID8549	7212-44-4	HMDB0035662	222.1983655
C09183	515-03-7	HMDB0036827	308.2715304
CSID13078158	83-45-4	HMDB0000494	416.4018163
C07610	22888-70-6	HMDB0030583	482.1212969
CSID102754	4670-05-7	HMDB0005788	564.1267762
CSID8093627	158932-33-3	HMDB0036323	686.2785854
C09882	18172-67-3	HMDB0036560	136.1252005
C09315	93-35-6	HMDB0029865	162.0316941
C09629	87-44-5	HMDB0036792	204.1878008
C14458	21554-71-2	HMDB0005897	272.0684735
C00376	116-31-4	HMDB0001358	284.2140155
C01514	491-70-3	HMDB0005800	286.0477381
C05443	67-97-0	HMDB0000876	384.339216
C07601	15291-75-5	HMDB0036862	408.1420324
C07602	15291-77-7	HMDB0036861	424.136947
C07603	15291-76-6	HMDB0036860	440.1318616
C05850	84-80-0	HMDB0003555	450.3497807

C09732	13463-28-0	HMDB0005811	596.1741204
CSID13658	1124-11-4	HMDB0036584	136.1000484
C10428	4180-23-8	HMDB0030837	148.088815
C04148	28047-15-6	HMDB0006344	264.111007
C10058	1447-88-7	HMDB0128581	300.0633881
C00389 (anhydrous)	117-39-5 (anhydrous)	HMDB0005794 (anhydrc	302.042652674 (anhydrc
C12127	970-73-0	HMDB0038365	306.0739528
CSID4474632	479-91-4	HMDB0030660	374.1001676
CSID63959	34157-83-0	HMDB0002385	450.2770097
C08580	472-61-7	HMDB0002204	596.3865602
C09755	520-26-3	HMDB0003265	610.1897704
C10501	61276-17-3	HMDB0034843	624.2054205
C01598	73-31-4	HMDB0001389	232.1211778

C14279	98-01-1	HMDB0032914	96.02112937
C08492	928-96-1	HMDB0030003	100.088815
C01546	88-14-2	HMDB0000617	112.016044
CSID6649	88-09-5	HMDB0031221	116.0837296
CSID167259 (free acid)	1518-62-3 (free acid)	HMDB0000360 (free aci	120.042258744 (free aci
CSID28682	22047-25-2	HMDB0031861	122.0480128
C02735	7568-93-6	HMDB0001065	137.084064
C07326	154-58-5	HMDB0002712	164.0684735

C08265	556-27-4	HMDB0033592	177.0459639
C03342	669-90-9	HMDB0011732	194.0426527
CSID4956295	60317-54-6	HMDB0000953	231.1106727
C08427 (free acid)	534-69-0 (free acid)	HMDB0034070 (free aci	359.034472527 (free aci
CSID8398	1565-80-6	HMDB0031527	88.08881501
CSID17494	3188-00-9	HMDB0031178	100.0524295
CSID9392288 (free acid)	1910-47-0 (free acid)	HMDB0000336 (free aci	104.047344122 (free aci
CSID9849	488-93-7	HMDB0000444	112.016044
CSID4940988	3142-72-1	HMDB0031560	114.0680796
C02170	516-05-2	HMDB0000202	118.0266087
C10164	98-98-6	HMDB0002243	123.0320284
C00906	696-04-8	HMDB0000079	128.0585775
C16700	139-85-5	HMDB0059965	138.0316941
CSID7146	99-10-5	HMDB0013677	154.0266087
C01207 (free base)	67920-52-9 (free base)	HMDB0003503 (free bas	198.05282343 (free base
CSID642910	90-50-6	HMDB0002511	238.0841236
C01659	79-06-1	HMDB0004296	71.03711379
C05145	144-90-1	HMDB0003911	103.0633285
CSID96952	10237-77-1	HMDB0000531	118.0629942
C08276	646-01-5	HMDB0001527	120.0245002
CSID61446	499-76-3	HMDB0004815	152.0473441
C10129	300-08-3	HMDB0030353	155.0946287
C00337	155-54-4	HMDB0000528	158.0327567
C16357	1076-22-8	HMDB0001886	166.0490755
CSID68296	2612-02-4	HMDB0001868	168.0422587
C02670	32449-92-6	HMDB0006355	176.032088
C06186	497-76-7	HMDB0029943	272.0896029
C08325	29883-15-6	HMDB0035030	457.1584107
C00414	108-94-1	HMDB0003315	98.07316494
CSID10791	565-69-5	HMDB0005846	100.088815
CSID62571	625-08-1	HMDB0000754	118.0629942
C089822	98-89-5	HMDB0031342	128.0837296
C03500	141-97-9	HMDB0031216	130.0629942
C00815 (free acid)	597-44-4 (free acid)	HMDB0000426 (free aci	148.037173366 (free aci

C09902	7785-53-7	HMDB0004043	154.1357652
C08269	515-25-3	HMDB0029412	159.0895433
C02979 (anhydrous free	17181-54-3 (anhydrous f	HMDB0002520 (anhydrc	172.013674532 (anhydrc
C00308	543-38-4	HMDB0002706	176.0909403
C05570	497-30-3	HMDB0003045	229.0884974
C05512	890-38-0	HMDB0000071	252.0858549
CSID13061	939-19-5	HMDB0002149	162.0316941
C00530	123-31-9	HMDB0002434	110.0367794
CSID11544	617-35-6	HMDB0031643	116.0473441
C05519	24830-94-2	HMDB0004041	119.0582432
C07446	55-22-1	HMDB0060665	123.0320284
C14516	501-30-4	HMDB0032923	142.0266087
C00628	490-79-9	HMDB0000152	154.0266087
C00880 (free acid)	13382-27-9 (free acid)	HMDB0000565 (free aci	196.058302738 (free aci
C00818 (free acid)	87-73-0 (free acid)	HMDB0029881 (free aci	210.037567296 (free aci
C00670	28319-77-9	HMDB0000086	257.1028244
C11673	27741-01-1	HMDB0034942	374.1212969
C00061 (anhydrous free	146-17-8 (anhydrous fre	HMDB0001520 (anhydrc	456.104614802 (anhydrc
CSID11091	123-76-2	HMDB0000720	116.0473441
C00153	98-92-0	HMDB0001406	122.0480128
C11918	118-71-8	HMDB0030776	126.0316941
CSID22826	1187-84-4	HMDB0002108	135.0353997
CSID21111785	93-60-7	HMDB0029806	137.0476785
CSID55261	4077-47-8	HMDB0034230	142.0629942
CSID9587432	498-07-7	HMDB0000640	162.0528234
C00437	6205-08-9	HMDB0003357	174.1004423
C06153	488-59-5	HMDB0006088	180.0633881
C09213	487-58-1	HMDB0061115	246.1368278
C01835	1109-28-0	HMDB0001262	504.169035
C00083 (free acid basis)	524-14-1 (free acid basis	HMDB0001175 (free aci	853.115602295 (free aci
CSID10468	541-47-9	HMDB0000509	100.0524295
C01542	95-48-7	HMDB0002055	108.0575149
CSID18889 (free base)	2936-69-8 (free base)	HMDB0033518 (free bas	164.061948328 (free bas
C01456	552-63-6	HMDB0062590	166.0629942

C11527	1198-84-1	HMDB0000822	168.0422587
C03727	638-23-3	-	179.0252285
C01507	488-45-9	HMDB0011632	182.0790382
C05335	3211-76-5	HMDB0003966	196.9955004
C07474 (free base)	54-71-7 (free base)	HMDB0015217 (free bas	208.121177766 (free bas
C00254 (free acid)	126-49-8 (free acid)	HMDB0012283 (free aci	226.047738052 (free aci
CSID393058	1463-10-1	HMDB0000884	258.0851862
C01451	138-52-3	HMDB0003546	286.1052529
C07215	118-90-1	HMDB0002340	136.0524295
C06044	501-94-0	HMDB0004284	138.0680796
C17268	579-07-7	HMDB0035243	148.0524295
C09848	5949-05-3	HMDB0035842	154.1357652
C06672	121-34-6	HMDB0000484	168.0422587
C01047	3081-61-6	HMDB0034365	174.1004423
CSID395	486-56-6	HMDB0001046	176.094963
C16359	708-79-2	HMDB0003099	182.0439901
C00224 (free acid)	102029-95-8 (free acid)	HMDB0001003 (free aci	427.019898895 (free aci
C09126	529-59-9	HMDB0033988	432.1056469
C10114	28608-75-5	HMDB0030614	448.1005615
C10108	17912-87-7	HMDB0034360	464.0954761
C05853	60-12-8	HMDB0033944	122.0731649
C21649 (FREE ACID)	3909-12-4 (free acid)	-	136.037173366 (free aci
C11383	2244-16-8	HMDB0004487	150.1044651
C13635	5706-85-4	HMDB0029657	152.0473441
C17073	562-74-3	HMDB0035833	154.1357652
CSID84994	617-73-2	HMDB0000711	160.1099444
C03975	529-69-1	HMDB0000704	179.0443244
C17914	4674-50-4	HMDB0013687	218.1670653
C01699	77-06-5	HMDB0003559	346.1416384
C09789	10236-47-2	HMDB0002927	580.1792057
C10039	520-27-4	HMDB0029548	608.1741204
C00091 (free acid basis)	604-98-8 (free acid basis	HMDB0001022 (free aci	867.131252359 (free aci
CSID28985	123-15-9	HMDB0031578	100.088815

C00902 (free acid basis)	2492-75-3 (free acid bas	HMDB0001864 (free aci	130.062994186 (free aci
CSID8974	303-07-1	HMDB0013676	154.0266087
CSID62727	1002-57-9	HMDB0000991	159.1259288
C16353	552-62-5	HMDB0001991	166.0490755
C01424	149-91-7	HMDB0005807	170.0215233
C09727	490-46-0	HMDB0001871	290.0790382
CSID393054	20244-86-4	HMDB0001107	298.1151436
C10077	4773-96-0	HMDB0034410	422.0849114
C00882	3633-59-8	HMDB0001373	687.148878
C01004 (non chloride)	535-83-1 (non chloride)	HMDB0000875 (non chl	137.047678473 (non chl
C00683 (anhydrous free	104809-02-1 (anhydrous	HMDB0001269 (anhydro	867.607 (anhydrous free
CSID11095	591-78-6	HMDB0005842	100.088815
CSID7463	105-37-3	HMDB0030058	102.0680796
CSID9922	498-21-5	HMDB0001844	132.0422587
CSID13871718	122-97-4	HMDB0033962	136.088815
CSID1446	89-86-1	HMDB0029666	154.0266087
CSID146647	17173-14-7	HMDB0000486	160.1099444
CSID56569	28664-35-9	HMDB0031306	166.0490755
CSID59891 (anhydrous)	83-30-7 (anhydrous)	HMDB0029649 (anhydro	170.021523302 (anhydro
C16361	5415-44-1	HMDB0002123	210.0752902
C02067	1445-07-4	HMDB0000767	244.0695361
C09788	5945-50-6	HMDB0035608	390.1162115
C02052	34612-38-9	HMDB0001296	666.2218584
C12304	123-86-4	HMDB0031325	116.0837296
C00793	921-01-7	HMDB0003417	121.0197496
C19326	104-94-9	HMDB0029300	123.0684139
C10832	533-31-3	HMDB0033812	138.0316941
C01869 (free base)	614-35-7 (free base)	HMDB0062811 (free bas	167.094628663 (free bas
C00612 (free base)	14278-49-0 (free base)	HMDB0001276 (free bas	187.168462309 (free bas
C00470 (free acid)	9046-40-6 (free acid)	HMDB0003363 (free aci	194.042652674 (free aci
CSID6872	93-40-3	HMDB0000434	196.0735589
C05824	1637-71-4	HMDB0000731	200.9765637
C05926	2009-64-5	HMDB0000845	253.0811039
CSID16560	2627-69-2	HMDB0062179	258.0964196

C00332 (anhydrous fee a	1420-36-6 (anhydrous fe	HMDB0001484 (anhydrc	851.136337737 (anhydrc
C01949	107-87-9	HMDB0034235	86.07316494
CSID21159856	10152-76-8	HMDB0031653	88.03467095
C02284	1405-86-3	HMDB0029843	822.4037859
CSID6745	90-27-7	HMDB0000329	164.0837296
CSID14381	1466-76-8	HMDB0029273	182.0579088
C05659	608-07-1	HMDB0004095	190.1106131
C09684	6753-98-6	HMDB0036467	204.1878008
C01607	14721-66-5	HMDB0000801	312.3028305
C10809	3158-56-3	HMDB0031009	320.2715304
C09264 (anhydrous)	531-75-9 (anhydrous)	HMDB0030820 (anhydrc	340.07943211 (anhydrou
CSID277139	8015-61-0	HMDB0035219	418.1263823
C10073	482-36-0	HMDB0030775	464.0954761
C09060	523-50-2	HMDB0033930	186.0316941
C17854	3413-15-8	HMDB0032064	190.0993797
C06081	24211-30-1	HMDB0004305	222.1983655
C10205	479-13-0	HMDB0002326	268.0371734
C18166	80226-00-2	HMDB0005056	302.1518092
C10084	480-19-3	HMDB0002655	316.0583027
C00757 (berberine)	2086-83-1 (berberine)	HMDB0003409 (berberi	336.123583069 (berberi
C04608	578-74-5	HMDB0037340	432.1056468
C10437	70831-56-0	HMDB0002375	474.079826
C10018	1617-53-4	HMDB0030832	538.0899968
C08583	514-78-3	HMDB0003154	564.3967309
C15428	16830-15-2	HMDB0036656	958.5137303
C02137	611-73-4	HMDB0001587	150.0316941
CSID67279	1912-33-0	HMDB0029738	189.0789786
C05598	500-98-1	HMDB0000821	193.0738932
C10833	530-57-4	HMDB0002085	198.0528234
CSID134261	56613-60-6	HMDB0000860	207.0895433
C00482	530-59-6	HMDB0032616	224.0684735
C00774	60-82-2	HMDB0003306	274.0841236
C10105 (anhydrous)	480-16-0 (anhydrous)	HMDB0030796 (anhydrc	302.042652674 (anhydrc
C06162 (Sanguinarine)	2447-54-3 (Sanguinarine	HMDB0029367 (Sanguin	332.092282941 (Sanguir

C10190	481-53-8	HMDB0030539	372.120903
C01604 (anhydrous)	7061-54-3 (anhydrous)	HMDB0036634 (anhydrc	436.136946988 (anhydrc
NA	20633-67-4	HMDB0038821	446.1212969
C00858	485-72-3	HMDB0005808	268.0735589
C06562 (anhydrous)	154-23-4 (anhydrous)	HMDB0002780 (anhydrc	290.07903818 (anhydrou
C10822	126-17-0	HMDB0035282	413.3293796
C10538	6807-83-6	HMDB0036630	446.1212969
C08773	1063-77-0	HMDB0035772	514.2202827
C08794	6199-67-3	HMDB0034927	558.3192684

METLIN ID	PC_CID	PC_SID	ChEBI
67079	119034	10810	2873
270650	8163	4989	17700
94906	6448	329773262	157
3372	863	374179440	17460
3398	5280961	24278036	28088
3401	932	57654457	17846
92745	73160	854316	33992
NA	72277	14283	42255
58123	455260	348275772	65585
48020	6758	9795	28201
43599	107905	160713153	70255
52724	85704	11981	28705
6911	439250	329759707	15383
7089 (free base)	115244 (free base)	12358 (free base)	35280 (free base)
43830	69301	24848368	31038
87349	8185	24900630	131344
126	6112	329748332	30314
41197	442343	329747043	125
NA	400072	348295957	469
91259	5702609	8348	18743
48257	4484219	12607	5369
44855	119205	12865	6698
3550	65064	11919	4806
41189	3505	9869	NA
6452	12025	24854414	36592
36524	5281168	24901149	19591
3246	7408	24896793	670
94798	20534	329778426	89750
87564	8093	24901181	87434
69781	7002	329756956	50717
318833	15037	24901608	NA
68335	8815	24890706	4867

66897	6890	10502	28948
89740	11622	329761808	77928
301154	667639	8189	28814
44206	5378244	348284896	42567
41106	7460	329830537	50035
3278	351795	24847904	17566
58356	10455	249934591	89494
5412	348154	24846583	48400
53446	3515	24895038	5550
6485	8617	329756816	33070
94735	526624	329830587	NA
89760	10947	348289394	NA
44046	5281607	12214	75095
2411	10168	12587	8825
43874	258809	NA	NA
87146	6474309	85340808	390480
44734	7410	329756199	27632
302598	7462	12084	10334
91265	67179	24901213	98
346	2244	4594	15365
71555	6918391	96023569	62855
43899	2355	4715	18293
3397	5280443	4649	18388
1163	174174	24890401	16684
43941	248507	348294082	95169
44383	5281650	12266	67547
49507	13654833	12211	2981
67924	3512643	11953	2515
65764	5280511	24846655	17177
66928	16590	329824979	4488
41072	7439	24847635	38265
41065	159055	329830466	15396
7060	2758	24893017	584235
89558	641298	24857378	NA

43566	5280373	24893597	17574
43476	1548943	329749614	3374
73567	545839	9807	3103
3498	1794427	57654010	16112
68372	64981	348285466	391051
58317	73568	12405	3884
64046	6616	24867879	3830
87656	21363	24892314	37277
3525	323	24892679	28794
41101	101977	12036	10360
92087	12810	348292157	87327
92870	3559861	312232900	NA
43572	5281708	12394	28197
3432 (free base)	68245 (free base)	162012105 (free base)	28436 (free base)
44747	107982	96023439	46932
87120	9798666	170474204	75491
44447	969516	24892408	3962
64304	107971	12402	42202
302517	7461	24853370	10577
65907	2346	24855213	17484
41105	643820	24849742	29452
4022	3314	24894609	4917
3359	10680	57654180	42491
67649	5367559	11573	3900
46229	638500	24860818	NA
41045	3220	12529	42223
86048	111299	348274644	89582
44398	5281612	12224	4630
43646	99474	24893501	4629
90313	14109402	348290750	NA
44445	3712	348276740	24814
4153	107	24848071	28631
58314	82755	348276739	68889

305	637541	24895159	32357
3350	3564	8766	28172
67564	10212	11460	5885
58313	3473	12645	10136
69736	6050	24900938	35020
43889	5281858	12977	5354
53782	18526330	5340	30853
3679	232990	11994	59016
43920	13988633	11095	5633
41062	16666	24901227	15409
66385	6428458	57653759	6857
58323	853433	329754773	50545
269705	4055	24897023	28869
44115	638278	10843	310312
6640	8221	24855658	32154
494239	4656408	24861361	21484
44508	72281	329815205	28230
90781	25244459	312231920	NA
NA	5280637	6673	27994
44458	235284	6323	16226
94663	161823	NA	66651
41091	7463	24892383	28768
1534	412	8755	28313
273890	7456	329823043	31835
68336	24901119	12637	4918
3361	5367719	13682	15929
45739	5281616	12230	5262
3410	5280863	8191	28499
3448	5281672	24278566	18152
86150	5315832	348295646	16384
44436	72344	12298	7602
43767	10494	96023600	37659
67938	5281544	11982	7747
65561	1057	24898098	16164

41112	442495	12079	35596
6350	72	3529	36062
392	5280335	3613	16393
6489	1017	329768344	29069
6979	445154	6374	45713
43568	638024	329766089	28821
2229	3034034	8757	15854
47528	5281807	329820231	8633
43747	5280459	4883	17558
86092	12004528	348284623	1030566
3677 (anhydrous)	5280805 (anhydrous)	329768121	28527 (anhydrous)
53322	11463	24901446	9457
4245	6989	57654643	27607
61 (free base)	440266 (free base)	24277791	44715 (free base)
58318	5350	26759585	47807
6956	5280460	4885	17488
67595	8417	11502	9055
301693	8888	329751635	7524
53595	521332	24861955	9053
425	15559396	363669299	89400
44434	5213	24899437	925392
44483	114777	85336343	136609
589297	74328989	348291423	NA
41109	14896	24865115	50025
44642	5281426	24895162	27510
64101	5281515	11819	10357
58334	9838356	17395458	34707
2276	638015	24899355	17898
3409	5280445	4680	15865
165	5280795	24871395	28940
41244	115221	9803	5355
41245	65243	9804	5356
41246	161120	9805	5357
7027	5284607	24871410	18067

52850	22833655	11920	28709
91653	14296	348291633	133246
43903	1549040	24847351	35616
58397	92258	329782653	17884
49584	5281628	12244	75902
409 (anhydrous)	5280343 (anhydrous)	3679 (anhydrous)	16243 (anhydrous)
NA	65084	14274	31018
51422	5315263	160712435	69355
43591	122724	135610657	63959
3671	5281224	10773	40968
3678	53477767	11943	28775
68367	5459010	12684	132853
73	896	24278103	16796

69936	7362	57647750	34768
271735	5281167	24901153	28857
2266	6919	24894811	30845
303246	6915	24901070	410868
5349 (free acid)	192742 (free acid)	329769561	86348 (free acid)
87980	30914	24855159	145236
59	1000	24891194	16343
3775	64960	24891181	16070

66873	121922	10464	2596
NA	50	6185	88378
5899	6453952	348274942	88811
66966 (free acid)	6911854 (free acid)	10622 (free acid)	9162 (free acid)
288532	8723	24901965	48945
NA	18522	24856765	NA
NA	11217234 (free acid)	329755270	18064 (free acid)
5433	10268	24849746	30846
87765	6436344	24901545	NA
3712	487	24896996	30860
44803	1018	24898523	28747
291	93556	336225414	27468
63101	8768	96023224	50205
85250	7424	24893352	39912
6942 (free base)	23711819 (free base)	4430 (free base)	17807 (free base)
6705	735755	329748264	566519
65628	6579	329752440	28619
5472	64956	24853033	27389
5516	107802	NA	139272
6300	563	87572810	1438
58250	68138	24884411	85239
43570	2230	329753838	2814
5513	648	24894067	30865
2820	70639	24853339	62207
4164	75787	24848767	545920
44759	2724333	329748094	18268
43989	346	8437	18305
63626	2180	10523	27613
58147	7967	24864732	17854
58330	11265	24846819	89215
3792	69362	17425306	37084
67955	7413	24846554	36096
87501	8868	6312	4893
5415 (free acid)	1081 (free acid)	4073 (free acid)	15584 (free acid)

287641	442501	329753548	300
66877	164642	10468	85533
6708 (anhydrous free ac	2526 (anhydrous free ac	329799988	17270 (anhydrous free a
3238	439202	24892427	405237
53	5351619	7896	4828
3383	65058	24893935	28997
6512	13650	348275627	349245
505	785	57654278	17594
NA	12041	348286983	NA
3245	99289	7864	28718
849	5922	9649	6032
44532	3840	329770427	43572
618	3469	3901	17189
3336 (free acid)	128869 (free acid)	4136 (free acid)	16534 (free acid)
5633 (free acid)	33037 (free acid)	4076 (free acid)	16002 (free acid)
370	657272	3939	16870
64052	323273	13838	5301
6295 (anhydrous free ac	643976 (anhydrous free	3361 (anhydrous free ac	17621 (anhydrous free a
2195	11579	329756110	45630
1497	936	24897740	17154
285093	8369	24901222	142577
6490	24417	24897098	45658
86513	7151	329764069	451700
89789	61325	329830642	NA
5613	2724705	24859027	30997
3303	439232	3726	16543
NA	892	24896132	10642
67522	442106	11404	5832
3585	439586	4954	140999
6056 (free acid basis)	10663 (free acid basis)	348275093 (free acid ba	15531 (free acid basis)
4623	10931	24893422	37127
58085	335	329755539	28054
89330 (free base)	20049 (free base)	24890680	497734 (free base)
NA	10726	24900574	30765

5785	328	13695	16388
1525	193653	24892985	16163
62390	5460044	4675	18202
6993	15103	7713	27585
1936 (free base)	5910 (free base)	9677 (free base)	8207 (free base)
369 (free acid)	1028 (free acid)	3553 (free acid)	16666 (free acid)
85160	445408	24878114	45996
6948	439503	24899442	17814
6632	8373	24900155	36632
7044	10393	8315	1879
63534	11363	24853362	63552
41100	75427	12035	299
5471	8468	329770384	30816
44433	439378	4289	17394
1531	408	24278324	127762
2821	69726	47205667	68441
5933 (free acid)	10238 (free acid)	24890980	17709 (free acid)
45735	5264639	11318	27514
48900	5382105	12300	7781
50852	5352000	12294	544021
64740	6054	24901348	49000
35473 (FREE ACID)	151152 (free acid)	312225966 (FREE ACID)	49059 (free acid)
34489	16724	329752243	15399
69611	440082	24893343	35164
71541	11230	57646932	78884
5679	94180	24895793	86543
5672	10729	6694	16713
71939	20797	348282727	81377
6954	6466	4839	28833
3604	442428	57652274	28819
3676	5353588	12225	1188022
5951 (free acid basis)	439161 (free acid basis)	24899460	15380 (free acid basis)
87782	31245	24855648	89986

4144 (free acid basis)	159664 (free acid basis)	57654321	17308 (free acid basis)
85249	9338	24893351	68465
5923	69522	24853027	75145
58075	68374	47205661	48991
3295	370	4609	30778
3420	72276	11915	90
6008	445404	24896562	20794
68115	5358385	12263	6682
3689	439335	24893748	15468
273 (non chloride)	5570 (non chloride)	4250 (non chloride)	18123 (non chloride)
462 (anhydrous free acic	439291 (anhydrous free	24896685	15466 (anhydrous free a
NA	11583	329749014	421633
86695	7749	24901101	167460
6344	10349	24897223	91315
89643	31234	24901373	88817
86410	1491	24893350	248101
5473	167627	348274551	78949
87572	62835	24901819	67890
86397 (anhydrous)	66520 (anhydrous)	24862743 (anhydrous)	NA
58099	79437	47205669	691622
5734	15047	5155	17802
41157	3488508	11976	6988
4199	439639	5141	143180
69424	31272	329756481	31328
6925	92851	4051	16375
NA	7732	24891372	163384
68615	68289	24899539	9126
NA	854067 (free base)	4983 (free base)	119 (free base)
3323 (free base)	916 (free base)	329747292	17927 (free base)
6904 (free acid)	445929 (free acid)	329765362	33885 (free base)
5423	7139	24893270	86655
58010	115015	8119	27891
248	135398721	57654449	28670
313863	17513	24724407	28498

449 (anhydrous fee acid	92153 (anhydrous fee ac	3626 (anhydrous fee aci	15345 (anhydrous fee ac
NA	7895	24901343	16472
87837	66282	24890770	89856
53781	3495	5341	15939
5318	7012	24898271	86545
86145	15109	24893413	545935
7015	1833	24857245	2089
43510	6508206	11874	5768
5765	26840	4760	16285
68597	76617	12992	2120
43929 (anhydrous)	5351506 (anhydrous)	329748219	338261 (anhydrous)
90534	313325	348290351	73222
87190	5281643	12259	67486
67393	10658	11252	28928
88154	61361	163311856	NA
7048	445070	329825837	16619
48332	5281707	12391	3908
58292	115089	57650262	544560
3445	5281654	12270	6052
3471 (berberine)	2353 (berberine)	24891691	16118 (berberine)
NA	5280704	7199	16778
58128	5281764	12622	3594
47521	5281600	12204	2631
3597	5281227	10776	3362
70897	108062	329756318	79928
58059	11915	329768165	18280
86457	74706	24896162	72782
4237	68144	329770505	27480
2256	10742	329759879	68329
5823	152323	329770329	266653
45738	637775	57654131	15714
3405	4788	24278652	17276
3431 (anhydrous)	5281670 (anhydrous)	24278552	75092 (anhydrous)
311889 (Sanguinarine)	5154 (Sanguinarine)	8418 (Sanguinarine)	17183 (Sanguinarine)

NA	68077	12376	9400
3535 (anhydrous)	6072 (anhydrous)	329768518	8113 (anhydrous)
93458	91973796	329773327	86512
43917	5280378	329770326	18088
3419 (anhydrous)	9064 (anhydrous)	57653989	15600 (anhydrous)
41805	5250	13005	565242
64288	4485132	12721	9714
67191	326240	10966	7609
41667	5353545	10987	3941

SUPPLIER Name	SUPPLIER URL
Asiatic acid	https://www.sigmaaldrich.com/catalog/product
2-Undecanone	https://www.sigmaaldrich.com/catalog/product
(-)-Bornyl acetate	https://www.sigmaaldrich.com/catalog/product
DL-6,8-Thioctamide	https://www.aablocks.com/prod/940-69-2
Genistein	https://www.sigmaaldrich.com/catalog/product
(±)-Naringenin	https://www.sigmaaldrich.com/catalog/product
(−)-Catechin	https://www.sigmaaldrich.com/catalog/product
(-)-Epigallocatechin	https://www.caymanchem.com/product/11809
Carnosic acid	https://www.caymanchem.com/product/89820
Rotenone	https://www.caymanchem.com/product/13995
(−)-Epicatechin Gallate	https://www.caymanchem.com/product/11808
Narirutin	https://www.caymanchem.com/product/25124,
(+)-Limonene	https://www.sigmaaldrich.com/catalog/product
Stachydrine (hydrochloride)	https://www.caymanchem.com/product/20506
1,3,5-Trimethoxybenzene	https://www.sigmaaldrich.com/catalog/product
10-Undecen-1-ol	https://www.sigmaaldrich.com/catalog/product
(R)-(+)-α-Lipoic acid	https://www.sigmaaldrich.com/catalog/product
(−)-α-Bisabolol	https://www.sigmaaldrich.com/catalog/product
1’-Acetoxychavicol acetate	https://www.caymanchem.com/product/19649
(+)-Abscisic Acid	https://www.caymanchem.com/product/10073
Glabridin	https://www.caymanchem.com/product/11843,
Matairesinol	https://www.caymanchem.com/product/10005
(-)-Epigallocatechin-3-gallate	https://www.caymanchem.com/product/70935
Gossypol	https://www.caymanchem.com/product/14482,
2-Pyrrolidinone	https://www.sigmaaldrich.com/catalog/product
trans-2-Hexen-1-al	https://www.sigmaaldrich.com/catalog/product
α-Methylbenzylamine	https://www.sigmaaldrich.com/catalog/product
2-Butylfuran	https://www.sigmaaldrich.com/catalog/product
2-Octanone	https://www.sigmaaldrich.com/catalog/product
1-Methylnaphthalene	https://www.sigmaaldrich.com/catalog/product
1-Furfurylpyrrole	https://www.sigmaaldrich.com/catalog/product
4-Allylanisole	https://www.sigmaaldrich.com/catalog/product

Gramine	https://www.caymanchem.com/product/23401
2-Tridecanone	https://www.sigmaaldrich.com/catalog/product
Piceatannol	https://www.caymanchem.com/product/10009
Fisetin	https://www.caymanchem.com/product/15246
α-Phellandrene	https://www.sigmaaldrich.com/catalog/product
3-Indoleacetonitrile	https://www.sigmaaldrich.com/catalog/product
Iberin	https://www.caymanchem.com/product/14016
3,4-Dihydroxyhydrocinnamic acid	https://www.sigmaaldrich.com/catalog/product
Guaiazulene	https://www.sigmaaldrich.com/catalog/product
Indole-3-butyric acid	https://www.sigmaaldrich.com/catalog/product
Bis(2-methyl-3-furyl) Disulfide	https://www.sigmaaldrich.com/catalog/product
Muscone	https://www.caymanchem.com/product/16067
Chrysin	https://www.caymanchem.com/product/17402
Rhein	https://www.caymanchem.com/product/17345
Madecassic acid	https://www.caymanchem.com/product/11854
4,5-Dicaffeoylquinic Acid	https://www.caymanchem.com/product/27892
Acetophenone	https://www.sigmaaldrich.com/catalog/product
α-Terpinene	https://www.caymanchem.com/product/23178
L-Linalool	https://www.sigmaaldrich.com/catalog/product
Aspirin	https://www.caymanchem.com/product/70260
β-Elemene	https://www.caymanchem.com/product/19641
Bergapten	https://www.caymanchem.com/product/26254
Apigenin	https://www.sigmaaldrich.com/catalog/product
Atropine	https://www.caymanchem.com/product/12008
Boldine	https://www.caymanchem.com/product/18447
Mangostin	https://www.trc-canada.com/product-detail/?M
Baicalin	https://www.caymanchem.com/product/19843
Agnuside	https://www.aablocks.com/prod/11027-63-7
Cinnamyl alcohol	https://www.sigmaaldrich.com/catalog/product
Diallyl disulfide	https://www.sigmaaldrich.com/catalog/product
(R)-(−)-Carvone	https://www.sigmaaldrich.com/catalog/product
D-Camphor	https://www.sigmaaldrich.com/catalog/product
Eucalyptol	https://www.sigmaaldrich.com/catalog/product
2-Methoxycinnamaldehyde	https://www.scbt.com/p/2-methoxycinnamalde

Biochanin A	https://www.sigmaaldrich.com/catalog/product
Capsaicin	https://www.sigmaaldrich.com/catalog/product
Bilobalide	https://www.caymanchem.com/product/14272,
Chlorogenic acid	https://www.sigmaaldrich.com/catalog/product
Arctigenin	https://www.caymanchem.com/product/14913,
Corilagin	https://www.caymanchem.com/product/11832
Camphene	https://www.sigmaaldrich.com/catalog/product
Cyclohexaneacetic acid	https://www.sigmaaldrich.com/catalog/product
Coumarin	https://www.sigmaaldrich.com/catalog/product
(+)-β-Citronellol	https://www.caymanchem.com/product/23464,
delta-Decalactone	https://www.sigmaaldrich.com/catalog/product
Curcumol	https://www.caymanchem.com/product/26849
Daidzein	https://www.caymanchem.com/product/10005
Delphinidin (chloride)	https://www.caymanchem.com/product/11012,
Dihydrocapsaicin	https://www.caymanchem.com/product/92355,
Cryptochlorogenic acid	https://www.caymanchem.com/product/25098,
Curcumin	https://www.sigmaaldrich.com/catalog/product
Daidzin	https://www.caymanchem.com/product/13202,
γ-Terpinene	https://www.sigmaaldrich.com/catalog/product
Benzyl isothiocyanate	https://www.sigmaaldrich.com/catalog/product
Geraniol	https://www.sigmaaldrich.com/catalog/product
Eugenol	https://www.sigmaaldrich.com/catalog/product
Flavone	https://www.sigmaaldrich.com/catalog/product
Costunolide	https://www.caymanchem.com/product/14743,
Farnesyl Acetate	https://www.sigmaaldrich.com/catalog/product
Emodin	https://www.caymanchem.com/product/13109,
γ-Glutamylphenylalanine	https://www.carbosynth.com/carbosynth/webs
Diosmetin	https://www.caymanchem.com/product/18649,
Diosgenin	https://www.sigmaaldrich.com/catalog/product
Ganoderic acid A	https://www.caymanchem.com/product/26674,
Indole-3-carbinol	https://www.sigmaaldrich.com/catalog/product
Hydrocinnamic acid	https://www.sigmaaldrich.com/catalog/product
3,4-Dihydroxyphenyl ethanol	https://www.caymanchem.com/product/70604

trans-4-Hydroxycinnamic acid	https://www.sigmaaldrich.com/catalog/product
Harmaline	https://www.sigmaaldrich.com/catalog/product
Imperatorin	https://www.caymanchem.com/product/26070
6-Gingerol	https://www.caymanchem.com/product/11707,
Tributyrin	https://www.sigmaaldrich.com/catalog/product
Ginkgolic Acid C15:1	https://www.caymanchem.com/product/18422,
18β-Glycyrrhetinic Acid	https://www.caymanchem.com/product/11845,
Neohesperidin	https://www.caymanchem.com/product/23028,
Hecogenin	https://www.caymanchem.com/product/21372
L-Menthol	https://www.sigmaaldrich.com/catalog/product
Methyl cinnamate	https://www.sigmaaldrich.com/catalog/product
Isoeugenol	https://www.sigmaaldrich.com/catalog/product
Menadione	https://www.sigmaaldrich.com/catalog/product
Isoliquiritigenin	https://www.caymanchem.com/product/10739,
1-Octadecanol	https://www.sigmaaldrich.com/catalog/product
Indole-3-acetyl-l-aspartic acid	https://www.sigmaaldrich.com/catalog/building
Hesperetin	https://www.sigmaaldrich.com/catalog/product
Isoxanthohumol	https://www.trc-canada.com/product-detail/?I9
Luteoloside	https://www.caymanchem.com/product/25141,
Limonin	https://www.caymanchem.com/product/16932
Madecassoside	https://www.caymanchem.com/product/11855,
p-Cymene	https://www.sigmaaldrich.com/catalog/product
(±)-Nornicotine	https://www.caymanchem.com/product/20505
Methylparaben	https://www.sigmaaldrich.com/catalog/product
Methyl eugenol	https://www.sigmaaldrich.com/catalog/product
(±)-Jasmonic Acid methyl ester	https://www.caymanchem.com/product/90000
Galangin	https://www.caymanchem.com/product/15948,
Kaempferol	https://www.caymanchem.com/product/11852
Myricetin	https://www.sigmaaldrich.com/catalog/product
5-Caffeoylquinic Acid	https://www.caymanchem.com/product/25054,
Nobiletin	https://www.caymanchem.com/product/15421,
Oleanolic acid	https://www.caymanchem.com/product/11726
Oleuropein	https://www.caymanchem.com/product/21220,
Pyrogallol	https://www.sigmaaldrich.com/catalog/product

(R)-(+)-Pulegone	https://www.caymanchem.com/product/23163
Protocatechuic acid	https://www.caymanchem.com/product/14916
Sphingosine (d18:1)	https://www.caymanchem.com/product/10007
Phthalic acid	https://www.sigmaaldrich.com/catalog/product
Resveratrol	https://www.caymanchem.com/product/70675/
Piperine	https://www.sigmaaldrich.com/catalog/product
Quinine	https://www.caymanchem.com/product/23958/
Puerarin	https://www.sigmaaldrich.com/catalog/product
Quercitrin	https://www.caymanchem.com/product/19866/
Quercetin 3-O-glucuronide	https://www.aablocks.com/prod/22688-79-5
Rutin trihydrate	https://www.sigmaaldrich.com/catalog/product
Terpinolene	https://www.sigmaaldrich.com/catalog/product
Thymol	https://www.sigmaaldrich.com/catalog/product
(±)-Octopamine hydrochloride	https://www.sigmaaldrich.com/catalog/product
Sulforaphane	https://www.caymanchem.com/product/10496/
Scopoletin	https://www.caymanchem.com/product/20042
Scoparone	https://www.caymanchem.com/product/20046/
trans-Nerolidol	https://www.sigmaaldrich.com/catalog/product
Sclareol	https://www.sigmaaldrich.com/catalog/product
Stigmastanol	https://www.sigmaaldrich.com/catalog/product
Silibinin	https://www.sigmaaldrich.com/catalog/product
Theaflavin	https://www.caymanchem.com/product/25129
Secoisolariciresinol diglucoside	https://www.caymanchem.com/product/24974/
(−)-β-Pinene	https://www.sigmaaldrich.com/catalog/product
Umbelliferone	https://www.sigmaaldrich.com/catalog/product
β-Caryophyllene	https://www.caymanchem.com/product/21572
Dihydrogenistein	https://www.trc-canada.com/product-detail/?C
all trans-Retinal	https://www.sigmaaldrich.com/catalog/product
Luteolin	https://www.caymanchem.com/product/10004
Cholecalciferol (D3)	https://www.caymanchem.com/product/11792
Ginkgolide A	https://www.caymanchem.com/product/24970/
Ginkgolide B	https://www.caymanchem.com/product/14636
Ginkgolide C	https://www.caymanchem.com/product/19872
Phylloquinone (K1)	https://www.sigmaaldrich.com/catalog/product

Eriocitrin	https://www.trc-canada.com/product-detail/?E
2,3,5,6-Tetramethylpyrazine	https://www.caymanchem.com/product/30281,
trans-Anethole	https://www.caymanchem.com/product/29862,
Phenyl-Ac-Gln-OH	https://www.sigmaaldrich.com/catalog/product
Hispidulin	https://www.caymanchem.com/product/26383
Quercetin (hydrate)	https://www.caymanchem.com/product/10005
(+)-Gallocatechin	https://www.caymanchem.com/product/25125,
Casticin	https://www.caymanchem.com/product/16976,
Celastrol	https://www.caymanchem.com/product/70950
Astaxanthin	https://www.caymanchem.com/product/70685,
Hesperidin	https://www.caymanchem.com/product/18646,
Verbascoside	https://www.caymanchem.com/product/24965,
Melatonin	https://www.sigmaaldrich.com/catalog/product

Furfural	https://www.sigmaaldrich.com/catalog/product
cis-3-Hexen-1-ol	https://www.sigmaaldrich.com/catalog/product
2-Furoic acid	https://www.sigmaaldrich.com/catalog/product
2-Ethylbutyric Acid	https://www.sigmaaldrich.com/catalog/product
2,4-Dihydroxybutanoic acid lithium salt	https://www.sigmaaldrich.com/catalog/product
2-Acetylpyrazine	https://www.sigmaaldrich.com/catalog/product
2-Amino-1-phenylethanol	https://www.sigmaaldrich.com/catalog/product
1,5-Anhydro-D-glucitol	https://www.caymanchem.com/product/29874,

(+)-Alliin	https://www.caymanchem.com/product/14002/
2-Keto-d-gluconic acid	https://www.sigmaaldrich.com/catalog/building
N-Suberoylglycine	https://www.sigmaaldrich.com/catalog/product
Sinigrin potassium salt	https://www.sigmaaldrich.com/catalog/product
2-Methyl-1-butanol	https://www.sigmaaldrich.com/catalog/product
2-Methyltetrahydro-3-furanone	https://www.sigmaaldrich.com/catalog/product
(±)-Sodium β-hydroxyisobutyrate	https://www.sigmaaldrich.com/catalog/product
3-Furoic acid	https://www.sigmaaldrich.com/catalog/product
trans-2-Methyl-2-pentenoic Acid	https://www.sigmaaldrich.com/catalog/product
Methylmalonic acid	https://www.sigmaaldrich.com/catalog/product
2-Picolinic acid	https://www.sigmaaldrich.com/catalog/product
5,6-DIHYDRO-5-METHYLURACIL	https://www.sigmaaldrich.com/catalog/product
3,4-Dihydroxybenzaldehyde	https://www.caymanchem.com/product/27547
3,5-Dihydroxybenzoic acid	https://www.sigmaaldrich.com/catalog/product
Danshensu (sodium salt)	https://www.caymanchem.com/product/27222/
3,4,5-Trimethoxycinnamic acid	https://www.sigmaaldrich.com/catalog/product
Acrylamide	https://www.sigmaaldrich.com/catalog/product
DL-3-Aminoisobutyric acid	https://www.tcichemicals.com/US/en/p/A0324
rac-3-Hydroxypentanoic Acid	https://www.trc-canada.com/product-detail/?H
3-(Methylthio)propionic Acid	https://www.tcichemicals.com/eshop/en/us/co
4-hydroxy-3-methylbenzoic acid	https://www.sigmaaldrich.com/catalog/product
Arecoline hydrobromide	https://www.sigmaaldrich.com/catalog/product
DL-Dihydroorotic acid	https://www.sigmaaldrich.com/catalog/product
3-Methylxanthine	https://www.sigmaaldrich.com/catalog/product
2-Hydroxy-5-methoxybenzoic acid	https://www.sigmaaldrich.com/catalog/product
D-(+)-Glucuronic acid γ-lactone	https://www.sigmaaldrich.com/catalog/product
Arbutin	https://www.caymanchem.com/product/26407/
Amygdalin	https://www.caymanchem.com/product/26668
Cyclohexanone	https://www.sigmaaldrich.com/catalog/product
2-Methyl-3-Pentanone	https://www.sigmaaldrich.com/catalog/product
β-Hydroxyisovaleric Acid	https://www.trc-canada.com/product-detail/?H
Cyclohexanecarboxylic acid	https://www.sigmaaldrich.com/catalog/product
Ethyl acetoacetate	https://www.sigmaaldrich.com/catalog/product
D-(−)-Citramalic acid lithium salt	https://www.sigmaaldrich.com/catalog/product

α-Terpineol	https://www.sigmaaldrich.com/catalog/product
Betonicine	https://www.carbosynth.com/carbosynth/webs
β-Glycerophosphate disodium salt hydrate	https://www.sigmaaldrich.com/catalog/product
L-Canavanine	https://www.sigmaaldrich.com/catalog/product
L-(+)-Ergothioneine	https://www.caymanchem.com/product/14905/
2’-Deoxyinosine	https://www.sigmaaldrich.com/catalog/product
3-Hydroxycoumarin	https://www.sigmaaldrich.com/catalog/product
Hydroquinone	https://www.sigmaaldrich.com/catalog/product
Pyruvic acid ethyl ester	https://www.sigmaaldrich.com/catalog/product
D-Allothreonine	https://www.tcichemicals.com/US/en/search/?t
Isonicotinic acid	https://www.sigmaaldrich.com/catalog/product
Kojic acid	https://www.sigmaaldrich.com/catalog/product
Gentisic acid	https://www.caymanchem.com/product/27615/
D-GALACTONIC ACID, CALCIUM SALT	https://www.sigmaaldrich.com/catalog/product
D-Saccharic Acid 1,4-lactone (hydrate)	https://www.caymanchem.com/product/18896/
sn-glycero-3-Phosphocholine	https://www.caymanchem.com/product/20736
Geniposidic acid	https://www.caymanchem.com/product/28409/
Riboflavin 5'-Monophosphate Sodium Salt hyd	https://www.caymanchem.com/product/18167
Levulinic acid	https://www.sigmaaldrich.com/catalog/product
Niacinamide	https://www.sigmaaldrich.com/catalog/product
3-Hydroxy-2-methyl-4-pyrone	https://www.sigmaaldrich.com/catalog/product
S-Methyl-L-cysteine	https://www.sigmaaldrich.com/catalog/product
Methyl nicotinate	https://www.sigmaaldrich.com/catalog/product
2,5-Dimethyl-4-methoxy-3(2H)-furanone	https://www.sigmaaldrich.com/catalog/product
1,6-Anhydro-β-D-glucose	https://www.sigmaaldrich.com/catalog/product
N-alpha-Acetyl-L-ornithine	https://www.trc-canada.com/product-detail/?C
scyllo-Inositol	https://www.sigmaaldrich.com/catalog/product
Hypaphorine	https://www.carbosynth.com/carbosynth/webs
Maltotriose	https://www.caymanchem.com/product/20306/
Malonyl coenzyme A lithium salt	https://www.caymanchem.com/product/16455
3,3-Dimethylacrylic acid	https://www.sigmaaldrich.com/catalog/product
o-Cresol	https://www.sigmaaldrich.com/catalog/product
S-(2-Aminoethyl)-L-cysteine hydrochloride	https://www.sigmaaldrich.com/catalog/product
Tropic acid	https://www.sigmaaldrich.com/catalog/product

Benzeneacetic acid, α,4-dihydroxy-	https://www.aablocks.com/prod/1198-84-1
S-Carboxymethyl-L-cysteine	https://www.sigmaaldrich.com/catalog/product
L-Iditol	https://www.trc-canada.com/product-detail/?I1
L-Seleno-L-methionine	https://www.carbosynth.com/carbosynth/webs
Pilocarpine HCL	https://www.caymanchem.com/product/14487
Prephenic Acid Barium Salt	https://www.trc-canada.com/product-detail/?C
5-Methyluridine	https://www.sigmaaldrich.com/catalog/product
D-(-)-Salicin	https://www.sigmaaldrich.com/catalog/product
o-Toluic acid	https://www.sigmaaldrich.com/catalog/product
Tyrosol	https://www.caymanchem.com/product/27600
1-Phenyl-1,2-propanedione	https://www.sigmaaldrich.com/catalog/product
(S)-(−)-Citronellal	https://www.sigmaaldrich.com/catalog/product
Vanillic acid	https://www.sigmaaldrich.com/catalog/product
L-Theanine	https://www.caymanchem.com/product/20832
(−)-Cotinine	https://www.sigmaaldrich.com/catalog/product
1-Methyluric acid	https://www.trc-canada.com/product-detail/?M
Adenosine 5′-phosphosulfate sodium salt	https://www.sigmaaldrich.com/catalog/product
Genistin	https://www.caymanchem.com/product/14174,
Orientin	https://www.caymanchem.com/product/25143
Myricitrin	https://www.caymanchem.com/product/26902,
Phenethyl alcohol	https://www.sigmaaldrich.com/catalog/product
D-Threonic acid lithium salt	https://www.sigmaaldrich.com/catalog/product
(+)-Carvone	https://www.sigmaaldrich.com/catalog/product
2′,4′-Dihydroxyacetophenone	https://www.sigmaaldrich.com/catalog/product
(−)-Terpinen-4-ol	https://www.sigmaaldrich.com/catalog/product
(±)-2-Hydroxyoctanoic acid	https://www.sigmaaldrich.com/catalog/product
Isoxanthopterin	https://www.caymanchem.com/product/17564
Nootkatone	https://www.aablocks.com/prod/4674-50-4
Gibberellic acid	https://www.tcichemicals.com/US/en/p/G0029
Naringin	https://www.sigmaaldrich.com/catalog/product
Diosmin	https://www.caymanchem.com/product/19848,
Succinyl coenzyme A sodium salt	https://www.sigmaaldrich.com/catalog/product
2-Methylvaleraldehyde	https://www.sigmaaldrich.com/catalog/product

2-Ketohexanoic acid sodium salt	https://www.sigmaaldrich.com/catalog/product
2,6-Dihydroxybenzoic acid	https://www.sigmaaldrich.com/catalog/product
DL-2-Aminocaprylic acid	https://www.sigmaaldrich.com/catalog/product
7-Methylxanthine	https://www.carbosynth.com/carbosynth/webs
Gallic acid	https://www.caymanchem.com/product/11846
(−)-Epicatechin	https://www.caymanchem.com/product/11807/
7-Methylguanosine	https://www.sigmaaldrich.com/catalog/product
Mangiferin	https://www.caymanchem.com/product/22360/
3’-Dephosphocoenzyme A	https://www.sigmaaldrich.com/catalog/product
Trigonelline (chloride)	https://www.caymanchem.com/product/11904
Methylmalonyl coenzyme A tetralithium salt h	https://www.sigmaaldrich.com/catalog/product
2-Hexanone	https://www.sigmaaldrich.com/catalog/product
Ethyl propionate	https://www.sigmaaldrich.com/catalog/product
Methylsuccinic acid	https://www.sigmaaldrich.com/catalog/product
3-Phenyl-1-propanol	https://www.sigmaaldrich.com/catalog/product
2,4-Dihydroxybenzoic acid	https://www.sigmaaldrich.com/catalog/product
7-Hydroxyoctanoic acid	https://www.sigmaaldrich.com/catalog/building
4,5-Dimethyl-3-hydroxy-2,5-dihydrofuran-2-o	https://www.sigmaaldrich.com/catalog/product
2,4,6-Trihydroxybenzoic Acid Monohydrate	https://www.tcichemicals.com/eshop/en/us/co
1,3,7-Trimethyluric acid	https://www.caymanchem.com/product/16949
β-Pseudouridine	https://www.caymanchem.com/product/23383/
Monotropein	https://www.caymanchem.com/product/27595
Maltotetraose	https://www.caymanchem.com/product/24975
n-Butyl acetate	https://www.tcichemicals.com/US/en/p/A0024
D-Cysteine	https://www.sigmaaldrich.com/catalog/product
p-Anisidine	https://www.sigmaaldrich.com/catalog/product
Sesamol	https://www.sigmaaldrich.com/catalog/product
(±)-Synephrine (hydrochloride)	https://www.caymanchem.com/product/28398/
N1-Acetylspermine trihydrochloride	https://www.sigmaaldrich.com/catalog/product
D-Galacturonic acid sodium salt	https://www.sigmaaldrich.com/catalog/product
3,4-Dimethoxyphenylacetic acid	https://www.sigmaaldrich.com/catalog/product
S-Sulfo-L-cysteine	https://www.carbosynth.com/carbosynth/webs
D-(+)-Neopterin	https://www.sigmaaldrich.com/catalog/product
AICAR	https://www.sigmaaldrich.com/catalog/product

Acetoacetyl coenzyme A sodium salt hydrate	https://www.caymanchem.com/product/21219/
2-Pentanone	https://www.sigmaaldrich.com/catalog/product
Allyl methyl sulfide	https://www.sigmaaldrich.com/catalog/product
Glycyrrhizin	https://www.sigmaaldrich.com/catalog/product
2-Phenylbutyric acid	https://www.sigmaaldrich.com/catalog/product
2,6-Dimethoxybenzoic acid	https://www.sigmaaldrich.com/catalog/product
5-Methoxytryptamine	https://www.sigmaaldrich.com/catalog/product
α-Humulene	https://www.caymanchem.com/product/21574/
Phytanic acid	https://www.caymanchem.com/product/90360
Adipostatin A	https://www.caymanchem.com/product/22163/
Esculin hydrate	https://www.sigmaaldrich.com/catalog/product
Aloin	https://www.caymanchem.com/product/22435/
Quercetin 3-D-galactoside	https://www.caymanchem.com/product/18648
Angelicin	https://www.caymanchem.com/product/11683/
Forskolin	https://www.caymanchem.com/product/11018/
Farrerol	https://www.sigmaaldrich.com/catalog/product
Coumestrol	https://www.caymanchem.com/product/11730/
Enterodiol	https://www.sigmaaldrich.com/catalog/product
Isorhamnetin	https://www.caymanchem.com/product/16496/
Berberine chloride form	https://www.sigmaaldrich.com/catalog/product
Apigenin 7-glucoside	https://www.caymanchem.com/product/26813/
Chicoric acid	https://www.caymanchem.com/product/24960
Amentoflavone, Chamaecyparis obtusa (hinok	https://www.indofinechemical.com/details.aspx
all-trans-Canthaxanthin	https://www.trc-canada.com/product-detail/?C
Asiaticoside	https://www.caymanchem.com/product/11819/
Phenylglyoxylic acid	https://www.sigmaaldrich.com/catalog/product
Methyl 3-indolyacetate	https://www.sigmaaldrich.com/catalog/product
Phenylac-Gly-OH	https://www.sigmaaldrich.com/catalog/product
Syringic acid	https://www.sigmaaldrich.com/catalog/product
N-(3-Phenylpropionyl)glycine	https://www.sigmaaldrich.com/catalog/product
Sinapic acid	https://www.sigmaaldrich.com/catalog/product
Phloretin	https://www.sigmaaldrich.com/catalog/product
Morin hydrate	https://www.sigmaaldrich.com/catalog/product
Sanguinarine (chloride)	https://www.caymanchem.com/product/16951/

Tangeretin	https://www.caymanchem.com/product/10009
Phloridzin dihydrate	https://www.sigmaaldrich.com/catalog/product
Calycosin 7-O-β-D-Glucoside	https://www.caymanchem.com/product/25095
Formononetin	https://www.sigmaaldrich.com/catalog/product
(±)-Catechin hydrate	https://www.sigmaaldrich.com/catalog/product
Solasodine	https://www.sigmaaldrich.com/catalog/product
Trifolirhizin	https://www.sigmaaldrich.com/catalog/product
Nomilin	https://www.caymanchem.com/product/20836
Cucurbitacin B	https://www.caymanchem.com/product/14820

SUPPLIER CAT_NO	SUB CLASS OR CLASS	FOOD SOURCE EXAMPLES	SOLVENT USED FOR PLA
546712	triterpenoid	Variety of plants, including	HIGH-QUALITY ETHANOl
74038	Carbonyl compounds	oils, cloves	HIGH-QUALITY ETHANOl
B55203	Monoterpenoids	nutmeg, rosemary	HIGH-QUALITY ETHANOl
AA003M07	Lipoamides	spinach, broccoli, yeast	HIGH-QUALITY ETHANOl
G6649	Isoflavonoids	soy products	HIGH-QUALITY ETHANOl
N5893	Flavonoids	citrus frutis	HIGH-QUALITY ETHANOl
PHL80992	Flavonoids	fruits, green tea, chocolate	HIGH-QUALITY ETHANOl
11809	Flavonoids	cauliflower, cabbage, pasta	HIGH-QUALITY ETHANOl
89820	Diterpenoids	rosemary, sage	HIGH-QUALITY ETHANOl
13995	Isoflavonoids	yam bean	HIGH-QUALITY ETHANOl
11808	Flavonoids	walnuts, carrots, pecans	HIGH-QUALITY ETHANOl
25124	Flavonoids	artichokes,, tea, frutis	HIGH-QUALITY ETHANOl
218367	Monoterpenoids	citrus fruits	HIGH-QUALITY ETHANOl
20506	Amino acids, peptides, and	citrus fruits, capers, oats	HIGH-QUALITY ETHANOl
138827	Flavonoids	brassicas, rocket salad, tarc	HIGH-QUALITY ETHANOl
U2008	Fatty alcohol	flavoring agent	HIGH-QUALITY ETHANOl
7039	Lipoic acids and derivatives	spinach, broccoli, potatoes	HIGH-QUALITY ETHANOl
14462	Sesquiterpenoids	chamomile, sage	HIGH-QUALITY ETHANOl
19649	Phenol esters	herbs, spices	HIGH-QUALITY ETHANOl
10073	Sesquiterpenoids	fruits, vegetables	HIGH-QUALITY ETHANOl
11843	Pyranoisoflavonoids	herbs, spices, tea	HIGH-QUALITY ETHANOl
10005174	Tetrahydrofuran lignans	sesame, flaxseeds, oats, as	HIGH-QUALITY ETHANOl
70935	Flavonoids	green tea	HIGH-QUALITY ETHANOl
14482	Sesquiterpenoids	cottonseed	HIGH-QUALITY ETHANOl
240338	Pyrrolidones	soybean	HIGH-QUALITY ETHANOl
W256005	Carbonyl compounds	apricots, kiwi, also used in	HIGH-QUALITY ETHANOl
M31104	Amine	chocolate	HIGH-QUALITY ETHANOl
CDS001204	Heteroaromatic compounc	chick peas, carob	HIGH-QUALITY ETHANOl
W280208	Carbonyl compounds	tortilla chips, cloves, tea, c	HIGH-QUALITY ETHANOl
45795	Naphthalenes	black walnuts, asian pears	HIGH-QUALITY ETHANOl
W328405	Pyrroles	alcoholic beverages, cereal	HIGH-QUALITY ETHANOl
A29208	Anisoles	citrus, chinese cinnamons,	HIGH-QUALITY ETHANOl

23401	Indoles	barley, brassicas, cereals a	HIGH-QUALITY ETHANOL
69620	Carbonyl compounds	fruits, citrus, milk and milk	HIGH-QUALITY ETHANOL
10009366	Stilbenes	red wine	HIGH-QUALITY ETHANOL
15246	Flavonoids	strawberry, apple, persimn	HIGH-QUALITY ETHANOL
814893	Monoterpenoids	ceylon cinnamon, dill, turm	HIGH-QUALITY ETHANOL
129453	Indoles and derivatives	cabbage, cauliflower, broc	HIGH-QUALITY ETHANOL
14016	Sulfoxides	brussel sprouts, broccoli, c	HIGH-QUALITY ETHANOL
102601	Phenylpropanoic acids	coffee	HIGH-QUALITY ETHANOL
G11004	Sesquiterpenoids	fats and oils	HIGH-QUALITY ETHANOL
45532	Indoles	leaves and seeds of maize	HIGH-QUALITY ETHANOL
W325900	Heteroaromatic compounc	tea	HIGH-QUALITY ETHANOL
16067	Organooxygen compounds	musk fragrance	HIGH-QUALITY ETHANOL
17402	Flavones	carrots, sour cherries, swe	HIGH-QUALITY ETHANOL
17345	Anthracenes	docks, garden rhubarbs, an	HIGH-QUALITY ETHANOL
11854	triterpenoids	green vegetables	HIGH-QUALITY ETHANOL
27892	Organooxygen compounds	coffee and coffee products	HIGH-QUALITY ETHANOL
42163	Carbonyl compounds	fruit flavors	HIGH-QUALITY ETHANOL
23178	Monoterpenoids	cardamom and marjoram c	HIGH-QUALITY ETHANOL
W263516	Monoterpenoids	apricot, cranberry essentia	HIGH-QUALITY ETHANOL
70260	Benzoic acids and derivativ	jasmine, beans, peas, clove	HIGH-QUALITY ETHANOL
19641	sesquiterpenoids	herbs, spices, and root veg	HIGH-QUALITY ETHANOL
26254	5-methoxypsoralens	anises, figs, carrots, fennel	HIGH-QUALITY ETHANOL
SMB00702	flavones	fruits and vegetables	HIGH-QUALITY ETHANOL
12008	Tropane alkaloids	solanaceae	HIGH-QUALITY ETHANOL
18447	Aporphines	sweet bay	HIGH-QUALITY ETHANOL
M164500	1-benzopyrans	fruits	HIGH-QUALITY ETHANOL
19843	Macrolides and analogues	skull cap	HIGH-QUALITY ETHANOL
AA008QXV	Terpene glycosides	chasteberry	HIGH-QUALITY ETHANOL
108197	Cinnamyl alcohols	ceylon cinnamons, star ani	HIGH-QUALITY ETHANOL
SMB00378	Allyl sulfur compounds	garlics	HIGH-QUALITY ETHANOL
124931	Monoterpenoids	spearmint oil (Mentha spic	HIGH-QUALITY ETHANOL
W223023	Monoterpenoids	camphor basil	HIGH-QUALITY ETHANOL
C80601	monoterpene	eucalyptus oil, the herbs ar	HIGH-QUALITY ETHANOL
sc-230476A	Cinnamaldehydes	chinese cinnamons	HIGH-QUALITY ETHANOL

D2016	Isoflavonoids	red clover in soy, in alfalfa	HIGH-QUALITY ETHANOl
12084	Methoxyphenols	Capsicum fruits	HIGH-QUALITY ETHANOl
14272	Terpene lactones	Ginkgo biloba	HIGH-QUALITY ETHANOl
C3878	Alcohols and polyols	coffee	HIGH-QUALITY ETHANOl
14913	Tetrahydrofuran lignans	Arctium lappa, Saussurea h	HIGH-QUALITY ETHANOl
11832	Hydrolyzable tannins	pomegranate	HIGH-QUALITY ETHANOl
442505	Monoterpenoids	dill, caraway, hyssop, and f	HIGH-QUALITY ETHANOl
C104507	carboxylic acids	Cyclohexaneacetic acid is a	HIGH-QUALITY ETHANOl
C4261	Coumarins and derivatives	tonka bean, cassia (bastarc	HIGH-QUALITY ETHANOl
23464	Monoterpenoids	herbs and spices, as well as	HIGH-QUALITY ETHANOl
74026	Delta valerolactones	coconuts, evergreen blackb	HIGH-QUALITY ETHANOl
26849	Sesquiterpenoids	tumeric	HIGH-QUALITY ETHANOl
10005166	Isoflavonoids	soybeans and soy products	HIGH-QUALITY ETHANOl
11012	anthocyanidin	red wine and berries	HIGH-QUALITY ETHANOl
92355	Methoxyphenols	yellow bell peppers, red be	HIGH-QUALITY ETHANOl
25098	Alcohols and polyols	coffee, robusta coffee, and	HIGH-QUALITY ETHANOl
C1386	Linear diarylheptanoids	tumeric	HIGH-QUALITY ETHANOl
13202	Isoflavonoids	soy beans, soy yogurts, and	HIGH-QUALITY ETHANOl
223190	Branched unsaturated hyd	cumins, caraway, sweet or	HIGH-QUALITY ETHANOl
252492	Benzene and substituted d	horseradish	HIGH-QUALITY ETHANOl
163333	monoterpenoid	oil-of-rose and palmarosa c	HIGH-QUALITY ETHANOl
E51791	Methoxyphenols	certain essential oils espec	HIGH-QUALITY ETHANOl
F2003	flavonoid	forms the "backbone" for r	HIGH-QUALITY ETHANOl
14743	Terpene lactones	lettuce	HIGH-QUALITY ETHANOl
340480	sesquiterpenoids	blueberries	HIGH-QUALITY ETHANOl
13109	Anthraquinones	docks, garden rhubarbs, an	HIGH-QUALITY ETHANOl
FG36323	Amino acids, peptides, and	adzuki bean, onion (Allium	HIGH-QUALITY ETHANOl
18649	O-methylated flavonoids	common sages, lemons, dil	HIGH-QUALITY ETHANOl
D1634	steroidal sapogenin	fenugreek seeds and yam t	HIGH-QUALITY ETHANOl
26674	triterpenoids	Ganoderma mushrooms	HIGH-QUALITY ETHANOl
I7256	Indoles	cabbage, radishes, cauliflo	HIGH-QUALITY ETHANOl
135232	Phenylpropanoic acids	macadamia nuts, watercre	HIGH-QUALITY ETHANOl
70604	Tyrosols and derivatives	cloves, fruits, and rapes	HIGH-QUALITY ETHANOl

H23007	Hydroxycinnamic acids and	pepper (c. frutescens), pine	HIGH-QUALITY ETHANOL
51330	Harmala alkaloids	fruits and herbs and spices	HIGH-QUALITY ETHANOL
26070	Furanocoumarins	root vegetables, lambsqua	HIGH-QUALITY ETHANOL
11707	Methoxyphenols	pepper (spice), cumins, sw	HIGH-QUALITY ETHANOL
W222305	Triradylcglycerols	butter, also a flavor ingredi	HIGH-QUALITY ETHANOL
18422	Benzoic acids and derivativ	cashew nuts, fats and oils,	HIGH-QUALITY ETHANOL
11845	Triterpenoids	licorice component, flavori	HIGH-QUALITY ETHANOL
23028	Flavonoid glycosides	grapefruits, grapefruit/pun	HIGH-QUALITY ETHANOL
21372	Flavonoid glycosides	herbs and spices, root vege	HIGH-QUALITY ETHANOL
W266523	Monoterpenoids	peppermint or other mint (	HIGH-QUALITY ETHANOL
96410	Cinnamic acid esters	ceylan cinnamon	HIGH-QUALITY ETHANOL
34038	Methoxyphenols	certain essential oils espec	HIGH-QUALITY ETHANOL
M5625	Naphthoquinones	collards, spinach, kale, and	HIGH-QUALITY ETHANOL
10739	Chalcones and dihydrochal	oval-leaf huckleberries, elli	HIGH-QUALITY ETHANOL
258768	Fatty alcohols	soft-necked garlic and pota	HIGH-QUALITY ETHANOL
COM964463226	Amino acids, peptides, and	garden tomato (var.), opiu	HIGH-QUALITY ETHANOL
H4125	O-methylated flavonoids	limes, persian limes, sweet	HIGH-QUALITY ETHANOL
I918213	Chalcones and dihydrochal	alcoholic beverages and ce	HIGH-QUALITY ETHANOL
25141	Flavonoid glycosides	mexican oregano, anises,w	HIGH-QUALITY ETHANOL
16932	Triterpenoids	citrus fruits	HIGH-QUALITY ETHANOL
11855	Terpene glycosides	pennywort herb	HIGH-QUALITY ETHANOL
C121452	Monoterpenoids	oil of cumin and thyme	HIGH-QUALITY ETHANOL
20505	Pyrrolidinylpyridines	tobacco plant	HIGH-QUALITY ETHANOL
PHR1012	Benzoic acids and derivativ	alcoholic beverages, saffro	HIGH-QUALITY ETHANOL
W247502	Methoxybenzenes	soy beans, evergreen black	HIGH-QUALITY ETHANOL
9000059	Lineolic acids and derivativ	apple, raspberry	HIGH-QUALITY ETHANOL
15948	Flavones	lingonberries, garden onio	HIGH-QUALITY ETHANOL
11852	Flavones	saffrons, capers, and cumir	HIGH-QUALITY ETHANOL
M6760	Flavones	common walnuts, carobs, a	HIGH-QUALITY ETHANOL
25054	Alcohols and polyols	coffee and coffee products	HIGH-QUALITY ETHANOL
15421	O-methylated flavonoids	citrus, grapefruits, lemons,	HIGH-QUALITY ETHANOL
11726	Triterpenoids	Olive pomace oil, olives, ra	HIGH-QUALITY ETHANOL
21220	Terpene glycosides	olives	HIGH-QUALITY ETHANOL
P0381	Benzenetriols and derivativ	coffee, arabica coffee, and	HIGH-QUALITY ETHANOL

23163	Monoterpenoids	cornmint, orange mint, pe	HIGH-QUALITY ETHANOl
14916	Benzoic acids and derivativ	garden onions, cocoa pow	HIGH-QUALITY ETHANOl
10007907	Amines	beans, figs, and pomegran	HIGH-QUALITY ETHANOl
79255	Benzoic acids and derivativ	food contact materials; pla	HIGH-QUALITY ETHANOl
70675	Stilbenes	red wines, less in white wi	HIGH-QUALITY ETHANOl
75047	Alkaloids and derivatives	pepper (spice)	HIGH-QUALITY ETHANOl
23958	Cinchona alkaloids	quinine-containing soft dri	HIGH-QUALITY ETHANOl
P5555	Isoflavonoid C-glycosides	found in a number of plant	HIGH-QUALITY ETHANOl
19866	Flavonoid glycosides	lingonberries, american cra	HIGH-QUALITY ETHANOl
AA0039RW	Flavonoid glycosides	wine	HIGH-QUALITY ETHANOl
78095	Flavonoid glycosides	buckwheat, apricots, cherr	HIGH-QUALITY ETHANOl
43909	Monoterpenoids	nutmeg, cumin, and apples	HIGH-QUALITY ETHANOl
T0501	Monoterpenoids	thyme oil or other volatile	HIGH-QUALITY ETHANOl
O0250	1-hydroxy-2-unsubstituted	mandarin orange (clement	HIGH-QUALITY ETHANOl
10496	Sulfoxides	brussel sprouts, broccoli, c	HIGH-QUALITY ETHANOl
20042	Hydroxycoumarins	green vegetables, carrots, t	HIGH-QUALITY ETHANOl
20046	Coumarins and derivatives	limes, citrus, wild celeries,	HIGH-QUALITY ETHANOl
18143	Sesquiterpenoids	neroli, ginger, jasmine, lave	HIGH-QUALITY ETHANOl
357995	Diterpenoids	sage	HIGH-QUALITY ETHANOl
S462330	Stigmastanes and derivativ	various vegetables, legume	HIGH-QUALITY ETHANOl
S0417	Flavonolignans	coffee and coffee products	HIGH-QUALITY ETHANOl
25129	Flavans	teas	HIGH-QUALITY ETHANOl
24974	Lignan glycosides	flaxseeds, ryes, oriental wh	HIGH-QUALITY ETHANOl
402753	Monoterpenoids	lime peel oil, ginger, nutm	HIGH-QUALITY ETHANOl
H24003	Hydroxycoumarins	buckwheats, sweet orange	HIGH-QUALITY ETHANOl
21572	Sesquiterpenoids	allspice, fig, pot marjoram,	HIGH-QUALITY ETHANOl
D449710	Isoflavanones	soy beans and other soy pr	HIGH-QUALITY ETHANOl
R2500	Retinoids	fruits and vegetables conta	HIGH-QUALITY ETHANOl
10004161	Flavones	celery, parsley, broccoli, or	HIGH-QUALITY ETHANOl
11792	Vitamin D and derivatives	mushrooms	HIGH-QUALITY ETHANOl
24970	Sesquiterpenoids	Ginkgo biloba	HIGH-QUALITY ETHANOl
14636	Terpene lactones	Ginkgo biloba	HIGH-QUALITY ETHANOl
19872	Terpene lactones	Ginkgo biloba	HIGH-QUALITY ETHANOl
47773	Quinone and hydroquinon	Brussels sprouts, cabbage,	HIGH-QUALITY ETHANOl

E600070	Phenylnaphthalenes	peppermints, lemons, and	HIGH-QUALITY ETHANOl
30281	Pyrazines	pepper (c. annuum), milk a	HIGH-QUALITY ETHANOl
29862	Anisoles	nutmegs, cumins, lemon b	HIGH-QUALITY ETHANOl
CDS006238	Amino acids, peptides, and	grape juice and chocolate	HIGH-QUALITY ETHANOl
26383	O-methylated flavonoids	sunflowers and tarragons	HIGH-QUALITY ETHANOl
10005169	Flavones	red grapes, citrus fruit, tom	HIGH-QUALITY ETHANOl
25125	Flavans	tea, broad beans, and cott	HIGH-QUALITY ETHANOl
16976	O-methylated flavonoids	fruits and herbs and spices	HIGH-QUALITY ETHANOl
70950	Triterpenoids	root extracts of Tripterygiu	HIGH-QUALITY ETHANOl
70685	Tetraterpenoids	red plant foods	HIGH-QUALITY ETHANOl
18646	Flavonoid glycosides	sweet orange and lemon	HIGH-QUALITY ETHANOl
24965	Hydroxycinnamic acids and	bitter gourds, fruits, and se	HIGH-QUALITY ETHANOl
M5250	Indoles	nuts, mushrooms, cereals a	HIGH-QUALITY ETHANOl

185914	Carbonyl compounds	apple, apricot, sweet cherr	HIGH-QUALITY WATER
H12900	Fatty alcohols	black elderberry	HIGH-QUALITY WATER
F20505	Furoic acid and derivatives	Fabaceae, beer; preservati	HIGH-QUALITY WATER
W242918	Fatty acids and conjugates	geranium oil, tobacco vap	HIGH-QUALITY WATER
89921	Short-chain hydroxy acids a	mushrooms	HIGH-QUALITY WATER
W312606	Carbonyl compounds	seeds, nuts	HIGH-QUALITY WATER
A72405	Amines	Catharanthus roseus and V	HIGH-QUALITY WATER
29874	Carbohydrates and carboh	soybeans, rice	HIGH-QUALITY WATER

14002	Amino acids, peptides, and	garden onions, garlics, and	HIGH-QUALITY WATER
COM448647947	Carbohydrates and carboh	fruit, honey and wine	HIGH-QUALITY WATER
52888	Amino acids, peptides, and	walnuts	HIGH-QUALITY WATER
PHL89279	Carbohydrates and carboh	white cabbages, garden cre	HIGH-QUALITY WATER
W399817	Alcohols and polyols	red raspberries, nectarines	HIGH-QUALITY WATER
277487	Furanones	coffee and coffee products	HIGH-QUALITY WATER
36105	Beta hydroxy acids and der	plant metabolite	HIGH-QUALITY WATER
163392	Furoic acid and derivatives	honeydew	HIGH-QUALITY WATER
W319503	Fatty acids and conjugates	snake fruit, wild strawberr	HIGH-QUALITY WATER
M54058	Dicarboxylic acids and deri	mushrooms	HIGH-QUALITY WATER
P42800	Pyridinecarboxylic acids an	medicinal herbs	HIGH-QUALITY WATER
S412295	Pyrimidines and pyrimidine	plant metabolite	HIGH-QUALITY WATER
27547	Carbonyl compounds	orange bell peppers, comm	HIGH-QUALITY WATER
D110000	Benzoic acids and derivativ	whole grain wheat	HIGH-QUALITY WATER
27222	Phenylpropanoic acids	rosemaries	HIGH-QUALITY WATER
T70408	Hydroxycinnamic acids and	lon pepper, medicinal plan	HIGH-QUALITY WATER
23701	Carboximidic acids	potato products, grain proc	HIGH-QUALITY WATER
A0324	Amino acids, peptides, and	tomatoes and other major	HIGH-QUALITY WATER
H949470	Fatty acids and conjugates	valerian parent	HIGH-QUALITY WATER
M0811	Fatty acids and conjugates	cassava, pickling melon	HIGH-QUALITY WATER
659282	Benzoic acids and derivativ	vanilla and other plant extr	HIGH-QUALITY WATER
31593	Alkaloids and derivatives	betel, areca nut	HIGH-QUALITY WATER
D7003	Amino acids, peptides, and	many	HIGH-QUALITY WATER
222526	Purines and purine derivat	tea, coffee and cacao	HIGH-QUALITY WATER
146188	Benzoic acids and derivativ	herbs and spices and tea	HIGH-QUALITY WATER
5566	Isosorbides	pant gums	HIGH-QUALITY WATER
26407	Organooxygen compounds	bilberries, quinces, pears, a	HIGH-QUALITY WATER
26668	Carbohydrates and carboh	almonds, kernels of cherrie	HIGH-QUALITY WATER
398241	Carbonyl compounds	basil oil, bell pepper, greer	HIGH-QUALITY WATER
108707	Carbonyl compounds	clover, corn	HIGH-QUALITY WATER
H943605	Fatty acids and conjugates	aloe	HIGH-QUALITY WATER
W353108	Carboxylic acids	coffee	HIGH-QUALITY WATER
W241512	Beta-keto acids and deriva	coffee and coffee products	HIGH-QUALITY WATER
06711	Fatty acids and conjugates	apple peel	HIGH-QUALITY WATER

30627	Monoterpenoids	cardamom seed, marjoram	HIGH-QUALITY WATER
FB34887	Amino acids, peptides, and	fruit juices of yellow orang	HIGH-QUALITY WATER
G9422	Glycerophosphates	plant metabolite	HIGH-QUALITY WATER
C1625	Amino acids, peptides, and	leguminous plants	HIGH-QUALITY WATER
14905	Amino acids, peptides, and	oat seed	HIGH-QUALITY WATER
D5287	Purine 2'-deoxyribonucleos	green bean	HIGH-QUALITY WATER
642673	Hydroxycoumarins	fruits, green tea, chicory	HIGH-QUALITY WATER
H9003	Benzenediols	anise, bilberry, ligonberry,	HIGH-QUALITY WATER
E47808	Alpha-keto acids and deriv	wheat bread, cocoa, white	HIGH-QUALITY WATER
A1518	Amino acids, peptides, and	plant metabolite	HIGH-QUALITY WATER
I17508	Pyridinecarboxylic acids and	derivatives	HIGH-QUALITY WATER
95197	Pyranones and derivatives	Japanese sake, soy sauce, a	HIGH-QUALITY WATER
27615	Benzoic acids and derivativ	Tarragons, common thyme	HIGH-QUALITY WATER
S960098	Medium-chain hydroxy aci	guava, yellow wax bean, cc	HIGH-QUALITY WATER
18896	Medium-chain hydroxy aci	apples and grapefruit	HIGH-QUALITY WATER
20736	Glycerophosphocholines	plant metabolite	HIGH-QUALITY WATER
28409	Terpene glycosides	gardenia fructus, Eucommi	HIGH-QUALITY WATER
18167	Flavin nucleotides	plant metabolite	HIGH-QUALITY WATER
41474	Gamma-keto acids and der	cereals and cereal products	HIGH-QUALITY WATER
N5535	Pyridinecarboxylic acids an	cacao bean, fenugreek see	HIGH-QUALITY WATER
W265608	Pyranones and derivatives	milk and milk products, nu	HIGH-QUALITY WATER
M6626	Amino acids, peptides, and	dried and cooked beans, ga	HIGH-QUALITY WATER
72420	Pyridinecarboxylic acids an	alcoholic beverages, coffee	HIGH-QUALITY WATER
W366412	Furanones	arctic brambles, mangoes,	HIGH-QUALITY WATER
316555	Oxepanes	sugar beet, sugar cane, cor	HIGH-QUALITY WATER
A187240	Amino acids, peptides, and	legume seeds	HIGH-QUALITY WATER
I8132	Alcohols and polyols	rice bran, wheat kernels, b	HIGH-QUALITY WATER
FH74222	Amino acids, peptides, and	lentil extracts	HIGH-QUALITY WATER
20306	Carbohydrates and carboh	beer wort, blueberries	HIGH-QUALITY WATER
16455	Fatty acyl thioesters	rapes, mamey sapotes, jew	HIGH-QUALITY WATER
D138606	Fatty acids and conjugates	celery, carrot, parsley fami	HIGH-QUALITY WATER
36922	Cresols	oils from jasmine, cassia, E	HIGH-QUALITY WATER
A2636	Amino acids, peptides, and	mushrooms	HIGH-QUALITY WATER
T89206	Hydroxy acids and derivati	Solanaceae family	HIGH-QUALITY WATER

AA000PLU	Phenols	wheat, barley, rye and oat	HIGH-QUALITY WATER
C7757	Amino acids, peptides, and	root vegetables	HIGH-QUALITY WATER
I175000	Carbohydrates and carboh	saffrons, adzuki beans, cus	HIGH-QUALITY WATER
FS09881	Amino acids, peptides, and	breads, grains, Brazil nuts,	HIGH-QUALITY WATER
14487	Alkaloids and derivatives	Pilocarpus	HIGH-QUALITY WATER
P2384	Gamma-keto acids and der	American pokeweeds, brea	HIGH-QUALITY WATER
535893	Pyrimidine nucleosides	wheat seadlings	HIGH-QUALITY WATER
S0625	Carbohydrates and carboh	white willow, poplars	HIGH-QUALITY WATER
T36404	Benzoic acids and derivativ	abiyuchs, lemon grass, bea	HIGH-QUALITY WATER
27600	Tyrosols and derivatives	virgin olive oil, wines, verm	HIGH-QUALITY WATER
223034	Phenylpropanes	coffee and coffee products	HIGH-QUALITY WATER
373753	Monoterpenoids	cocoa and cocoa products,	HIGH-QUALITY WATER
94770	Benzoic acids and derivativ	vanilla, wine, whole wheat	HIGH-QUALITY WATER
20832	Amino acids, peptides, and	mushrooms, tea	HIGH-QUALITY WATER
C5923	Pyrrolidinylpyridines	medlars, arrowhead, lotus,	HIGH-QUALITY WATER
M338180	Purines and purine derivat	major metabolite of caffeir	HIGH-QUALITY WATER
A5508	Purine ribonucleotides	chia, yardlong beans, swiss	HIGH-QUALITY WATER
14174	Isoflavonoid O-glycosides	soy beans, soy yogurts, and	HIGH-QUALITY WATER
25143	Flavonoid glycosides	spelts, triticales, red rices,	HIGH-QUALITY WATER
26902	Flavonoid glycosides	rubus (blackberry, raspberi	HIGH-QUALITY WATER
W285803	Benzene and substituted d	red wines, black walnuts, g	HIGH-QUALITY WATER
79272	Carbohydrates and carboh	Capers, Muscadine grapes,	HIGH-QUALITY WATER
22070	Monoterpenoids	seeds of caraway, spearmi	HIGH-QUALITY WATER
D107409	Carbonyl compounds	Paeonia lactiflora	HIGH-QUALITY WATER
11584	Monoterpenoids	blackberry, cauliflower, cel	HIGH-QUALITY WATER
H7396	Fatty acids and conjugates	plant metabolite	HIGH-QUALITY WATER
17564	Pterins and derivatives	soybean	HIGH-QUALITY WATER
AA003T7K	Sesquiterpenoids	grapefruit	HIGH-QUALITY WATER
G0029	Diterpenoids	hormone found in plants	HIGH-QUALITY WATER
71162	Flavonoid glycosides	rosemaries, grapefruit/pur	HIGH-QUALITY WATER
19848	Flavonoid glycosides	hyssops, peppermints, lem	HIGH-QUALITY WATER
S1129	Fatty acyl thioesters	soybean, cacao, gourds, leg	HIGH-QUALITY WATER
258563	Organic oxides	leeks, beers, rice, coffee, b	HIGH-QUALITY WATER

K6625	Medium-chain keto acids a	Solanaceae family	HIGH-QUALITY WATER
D109606	Benzoic acids and derivativ	beers and olives	HIGH-QUALITY WATER
217700	Alpha amino acids	Grapes, hops, turf; found ir	HIGH-QUALITY WATER
FM25575	Purines and purine derivat	tea leaves, yerba mate, cof	HIGH-QUALITY WATER
11846	Benzoic acids and derivativ	gallnuts, sumac, witch haze	HIGH-QUALITY WATER
11807	Flavans	teas	HIGH-QUALITY WATER
M0627	Purine nucleosides	plant metabolite	HIGH-QUALITY WATER
22360	1-benzopyrans	mango	HIGH-QUALITY WATER
D3385	Purine ribonucleotides	wild leeks, summer savour	HIGH-QUALITY WATER
11904	Alkaloids and derivatives	arabica coffee, fenugreeks,	HIGH-QUALITY WATER
M1762	Fatty acyl thioesters	plant metabolite	HIGH-QUALITY WATER
103004	Carbonyl compounds	hyssops, milk (cow), corns,	HIGH-QUALITY WATER
W245607	Carboxylic acid derivatives	apple, beer, fig, white grap	HIGH-QUALITY WATER
M81209	Fatty acids and conjugates	plant metabolite aloes	HIGH-QUALITY WATER
W288500	Benzene and substituted d	mushrooms, alcoholic beve	HIGH-QUALITY WATER
D109401	Benzoic acids and derivativ	alcoholic beverages, coffee	HIGH-QUALITY WATER
EN300-267726	Medium-chain hydroxy aci	plant metabolite	HIGH-QUALITY WATER
W363405	Furanones	coffee	HIGH-QUALITY WATER
P0601	Benzoic acids and derivativ	onion-family vegetables	HIGH-QUALITY WATER
16949	Purines and purine derivat	soybean, cacao, gourds, leg	HIGH-QUALITY WATER
23383	Nucleoside and nucleotide	cereal products, red bell p	HIGH-QUALITY WATER
27595	Terpene glycosides	cranberry, ligonberry, bilbe	HIGH-QUALITY WATER
24975	Carbohydrates and carboh	welsh onions, kales, romai	HIGH-QUALITY WATER
A0024	Carboxylic acid derivatives	many types of fruit	HIGH-QUALITY WATER
30095	Amino acids, peptides, and	chervils, fruits, lichee, nuts	HIGH-QUALITY WATER
A88255	Aminophenyl ethers	found in foods of plant orig	HIGH-QUALITY WATER
S3003	Benzodioxoles	sesame seeds and sesame	HIGH-QUALITY WATER
28398	1-hydroxy-2-unsubstituted	citrus	HIGH-QUALITY WATER
1467	Carboximidic acids	jutes, yams, pineapples ,an	HIGH-QUALITY WATER
73960	Carbohydrates and carboh	Pectic acid exists in the cell	HIGH-QUALITY WATER
D135909	Methoxybenzenes	olives	HIGH-QUALITY WATER
FC172487	Amino acids, peptides, and	hazelnut, star anise, agar, a	HIGH-QUALITY WATER
N3386	Pterins and derivatives	soy foods	HIGH-QUALITY WATER
A9978	Imidazole ribonucleosides	plant metabolite	HIGH-QUALITY WATER

21219	Aminopiperidines	plant metabolic intermedia	HIGH-QUALITY WATER
W284203	Carbonyl compounds	fats and oils, corns, apples,	HIGH-QUALITY METHAN
A34201	Allyl sulfur compounds	garden onions, gingers, oni	HIGH-QUALITY METHAN
PHL89217	Terpene glycosides	licorice	HIGH-QUALITY METHAN
P20955	Phenylpropanes	grape seeds	HIGH-QUALITY METHAN
D131601	Benzoic acids and derivativ	rices, herbs of Curculigo or	HIGH-QUALITY METHAN
286583	Tryptamines and derivative	alternative synthetic pathv	HIGH-QUALITY METHAN
21574	Sesquiterpenoids	hops, cannabis, sage, and g	HIGH-QUALITY METHAN
90360	Diterpenoids	any food of purely vegetab	HIGH-QUALITY METHAN
22163	Benzenediols	ryes, hard wheats, commoi	HIGH-QUALITY METHAN
6212	Coumarin glycosides	Horse Chestnut, basil, chic	HIGH-QUALITY METHAN
22435	Anthracenes	aloe	HIGH-QUALITY METHAN
18648	Flavonoid glycosides	common walnuts, black ch	HIGH-QUALITY METHAN
11683	Furanocoumarins	parsnips, fats and oils, figs,	HIGH-QUALITY METHAN
11018	Benzofuranones	wild celeries, lovages, cele	HIGH-QUALITY METHAN
SML1389	Sesquiterpenoids	plant metabolite	HIGH-QUALITY METHAN
11730	Coumestans	soybeans, clover, alfalfa sp	HIGH-QUALITY METHAN
45198	Dibenzylbutanediol lignans	soy beans and other soy pr	HIGH-QUALITY METHAN
16496	Flavones	parsley, green bell peppers	HIGH-QUALITY METHAN
B3251	Protoberberine alkaloids a	barberry, goldenseal, gold	HIGH-QUALITY METHAN
26813	Flavonoid glycosides	thyme, white lupine, comn	HIGH-QUALITY METHAN
24960	Tetracarboxylic acids and d	chicory, globe and Jerusale	HIGH-QUALITY METHAN
021057S	Biflavonoids and polyflavoi	Ginkgo,Chamaecyparis obt	HIGH-QUALITY METHAN
C175735	Tetraterpenoids	all young leaves and in etic	HIGH-QUALITY METHAN
11819	Terpene glycosides	Gotu Kola, pennywort	HIGH-QUALITY METHAN
78610	Benzoyl derivatives	plant metabolite	HIGH-QUALITY METHAN
I9770	Indolyl carboxylic acids and	apple	HIGH-QUALITY METHAN
96408	Amino acids, peptides, and	consumption of fruits and	HIGH-QUALITY METHAN
63627	Benzoic acids and derivativ	common walnuts, swiss ch	HIGH-QUALITY METHAN
94348	Carboxylic acids and deriva	phenylacetonitrile metabo	HIGH-QUALITY METHAN
D7927	Hydroxycinnamic acids and	strawberry guava, purple	HIGH-QUALITY METHAN
P7912	Chalcones and dihydrochal	apples, pears and tomatoe	HIGH-QUALITY METHAN
M4008	Flavones	strawberries, redcurrants,	HIGH-QUALITY METHAN
16951	Quaternary benzophenanth	opium poppy, bloodroot,, I	HIGH-QUALITY METHAN

10009911	O-methylated flavonoids	sweet oranges, sweet bay,	HIGH-QUALITY METHAN
P3449	Flavonoid glycosides	epazotes, durians, chinese	HIGH-QUALITY METHAN
25095	Isoflavonoid O-glycosides	herbs and spices, pulses, a	HIGH-QUALITY METHAN
94334	O-methylated isoflavonoid	soy beans, sunflowers, soy	HIGH-QUALITY METHAN
C1788	Flavans	blackcurrants, cocoa powd	HIGH-QUALITY METHAN
SML1141	Steroidal alkaloids	family Solanaceae such as	HIGH-QUALITY METHAN
PHL80547	Furanoisoflavonoids	pulses	HIGH-QUALITY METHAN
20836	Triterpenoids	citrus fruits	HIGH-QUALITY METHAN
14820	Cucurbitacins	pumpkins, gourds, cucumb	HIGH-QUALITY METHAN

added 9/3/20