Dyphylline
Eflornithine
p -Fluoroaniline
o -Fluorobenzoic acid
m -Fluorobenzoic acid
p -Fluorobenzoic acid
Ganciclovir
Gramine
Harman
Hexazinone
Hydroxyatrazine
2-Hydroxypyridine
Ibotenic acid
Ibuprofen
3-Indoleacetonitrile
3-Iodotyrosine
Ismelin
Isoniazid
Isoproterenol
Isoquinoline
Kanamycin A
Ketoprofen
Leupeptin
Lidocaine
Loperamide
Melamine
Mesalamine
Metamitron
Metaraminol
Metformin
Methotrimeprazine
Methoxamine
1-Methyl-4-phenyl-1,2,3,6-tetrahydropyridine
1-Methyl-2-pyrrolidone
4,4'-Methylene bis(o-chloroaniline)
Methysergide
Metronidazole
Muscimol
Nalidixic acid
Neomycin B
Neostigmine
Oleandomycin
Oxypurinol
Pargyline
Paromomycin
Penciclovir
Phenazopyridine
Phentolamine
Phenylephrine
Phosphoramidon
Phthalic acid
Piperazine
Pirimicarb
Pralidoxime
Prazosin
Propiconazole
Propranolol
Pseudopelletierine
Quisqualic acid
Ranitidine
Rhein
Ribavirin
Ribostamycin
Scopolamine
Sebacic acid
Simazine
Sisomicin
Spectinomycin
Stachydrine
Sulfanilamide
Sulfathiazole
p- Sulfobenzoic acid
Synephrine
Tacrine
Terbutaline
Terephthalic acid
1,2,3,4-Tetrahydroisoquinoline
Tetrahydrouridine
Timolol
Tobramycin
Tolazoline
Tolmetin
Triadimefon
2,4,5-Trichlorophenoxyacetic acid
Trientine
Triethanolamine
Trifluoperazine
3,3',5-Triiodothyronine
Trimethoprim
Tyrosine methyl ester
Verapamil
Xanthopterin

Compounds marked with numbers on their right shoulders cannot be distinguished as separated peaks, and their measured values are reported as the sum of the set.

C-SCOPE / CARCINOSCOPE

Central Carbon Metabolism

Acetyl CoA
cis-Aconitic acid
Argininosuccinic acid
Citric acid
CoA
Dihydroxyacetone phosphate
2,3-Diphosphoglyceric acid
Erythrose 4-phosphate
Fructose 1,6-diphosphate
Fructose 1-phosphate
Fructose 6-phosphate
Fumaric acid
Galactose 1-phosphate
Glucose 1-phosphate
Glucose 6-phosphate
Glyceraldehyde 3-phosphate
Glycerol 3-phosphate
Glycolic acid
Glyoxylic acid
2-Hydroxyglutaric acid
Isocitric acid
Lactic acid
Malic acid
2-Oxoglutaric acid
2-Oxoisovaleric acid
Phosphoenolpyruvic acid
2-Phosphoglyceric acid
3-Phosphoglyceric acid
6-Phosphogluconic acid
PRPP
Pyruvic acid
Ribose 1-phosphate
Ribose 5-phosphate
Ribulose 5-phosphate
Sedoheptulose 7-phosphate
Succinic acid
UDP-glucose
Xylulose 5-phosphate

Amino Acids

Ala
Arg
Asn
Asp
Cys
Gln
Glu
Gly
His
Ile
Leu
Lys
Met
Phe
Pro
Ser
Thr
Trp
Tyr
Val

Purine Metabolism

Adenine
Adenosine
Adenylosuccinic acid
ADP
ADP-ribose
AMP
ATP
cAMP
cGMP
GDP
GMP
GTP
Guanine
Guanosine
Hypoxanthine
IMP
Inosine
Uric acid
Xanthine
XMP

Others

Acetoacetyl CoA
N -Acetylglutamic acid
S-Adenosylhomocysteine
S-Adenosylmethionine
β-Ala
γ-Aminobutyric acid
Betaine
Betaine aldehyde
N -Carbamoylaspartic acid
Carbamoylphosphate
Carnitine
Carnosine
Choline
Citrulline
Creatine
Creatinine
Cystathionine
N ,*N* -Dimethylglycine
Folic acid
Glutathione (GSH)
Glutathione (GSSG)
HMG CoA
Homocysteine
Homoserine
Hydroxyproline
Malonyl CoA
Mevalonic acid
NAD^+
NADH
$NADP^+$
NADPH
Ornithine
Phosphocreatine
Putrescine
Sarcosine
Spermidine
Spermine
Urea

F-SCOPE

Anion

2-Oxoglutaric acid
2-Phosphoglyceric acid
3-Hydroxybutyric acid
3-Phosphoglyceric acid
6-Phosphogluconic acid
Acetyl CoA
ADP
AMP
ATP
cis-Aconitic acid
Citric acid
CoA
Dihydroxyacetone phosphate
Erythrose 4-phosphate
Fructose 1,6-diphosphate
Fructose 6-phosphate
Fumaric acid
Glucose 1-phosphate
Glucose 6-phosphate
Glyceraldehyde 3-phosphate
Isocitric acid
Lactic acid
Malic acid
Phosphoenolpyruvic acid
PRPP
Pyruvic acid
Ribose 5-phosphate
Ribulose 5-phosphate
Sedoheptulose 7-phosphate
Succinic acid

Cation

Ala
Arg
Asn
Asp
Citrulline
Cys
Gln
Glu
Glutathione (GSH)
Glutathione (GSSG)
Gly
His
Ile
Leu
Lys
Met
Ornithine
Phe
Pro
Ser
Thr
Trp
Tyr
Val

CE-MS Annotation List

HMT
ver.2.4a
CE: ver.7.4.6 (7.5.3)

Q110: Target compounds covered by "Q-OPTION 110"

A

4-Acetamidobutanoic acid
Acetoacetamide
Acetoacetic acid
Acetoacetyl CoA
Acetohydrazide
Q110 Acetyl CoA
3-Acetylacrylic acid
N -Acetylalanine
N^2-Acetylaminoadipic acid
4-(β-Acetylaminoethyl)imidazole
N -Acetylasparagine
N -Acetylaspartic acid
O -Acetylcarnitine
Acetylcholine
N -Acetylcysteine
N -Acetylgalactosamine
N -Acetylglucosamine
N -Acetylglucosamine 1-phosphate
N -Acetylglucosamine 6-phosphate
N -Acetylglucosylamine
N -Acetylglutamic acid
N -Acetylglutamine
N -Acetylglycine
N -Acetylhistidine
O -Acetylhomoserine
N -Acetylleucine
N -Acetyllysine
N^6 -Acetyllysine
N -Acetylmannosamine
N -Acetylmethionine
N -Acetylmuramic acid
N -Acetylneuraminic acid
N -Acetylornithine
N -Acetylphenylalanine
N -Acetylputrescine
O -Acetylserine
N -Acetylserine
N^1 -Acetylspermidine
N^8 -Acetylspermidine
N^1 -Acetylspermine
N -Acetyltryptophan
N -Acetyltyrosine
N -Acetyl-β-alanine
Q110 *cis* -Aconitic acid
Q110 Adenine
Q110 Adenosine
Adenosine 5'-[γ-thio]triphosphate
Adenosine 5'-phosphosulfate
S -Adenosylhomocysteine
Q110 *S* -Adenosylmethionine
Adenylosuccinic acid
Adipic acid
ADMA
Q110 ADP
3',5'-ADP
ADP-glucose[5]
ADP-ribose
Adrenaline
Agmatine
Q110 Ala
Q110 β-Ala
Ala-Ala
β-Ala-Lys
Albendazole
Allantoic acid
Allantoin
Alliin
Allocryptopine
Alloisoleucine
N -Amidinoglutamic acid
Amiloride
4-Amino-3-hydroxybutyric acid
2-Amino-2-(hydroxymethyl)-1,3-propanediol
3-Amino-5-hydroxypyrazole
2-Amino-2-methyl-1,3-propanediol
2-Amino-2-methylbutyric acid
5-Amino-4-oxovaleric acid
2-Amino-3-phosphonopropionic acid
3-Amino-2-piperidone
Aminoacetone
2-Aminoadipic acid
2-Aminobenzenesulfonic acid
p -Aminobenzoic acid
2-Aminobutyric acid
3-Aminobutyric acid
1-Aminocyclopentanecarboxylic acid
1-Aminocyclopropane-1-carboxylic acid
1-Aminoethylphosphonic acid
2-Aminoethylphosphonic acid
6-Aminohexanoic acid
4-Aminohippuric acid
5-Aminoimidazole-4-carboxamide ribotide
2-Aminoisobutyric acid
3-Aminoisobutyric acid
6-Aminopenicillanic acid
o -Aminophenol
m -Aminophenol
p -Aminophenol
4-Aminophenylsulfone
Aminophylline
3-Aminopropane-1,2-diol
3-Aminopropionitrile
Aminopyrine
4-Aminosalicylic acid
11-Aminoundecanoic acid
5-Aminovaleric acid
Q110 AMP
3'-AMP
Anabasine
Aniline
p -Anisic acid
Anserine
Q110 Anthranilic acid
Apigenin
Q110 Arg
Arg-Glu
Argininosuccinic acid
Ascorbate 2-glucoside
Ascorbate 2-phosphate
Ascorbate 2-sulfate
Ascorbic acid
Q110 Asn
Q110 Asp
Aspartame
Q110 ATP
Atrolactic acid
Azelaic acid
Azetidine 2-carboxylic acid

B

Barbituric acid
Bentazone
Benzamide
Benzocaine
Benzoic acid
Benzoylformic acid
N^6 -Benzyladenine
Benzylamine
Benzylsuccinic acid
Q110 Betaine
Q110 Betaine aldehyde
Biopterin
Biotin
Bis(*p* -nitrophenyl)phosphate
4-Bromophenylalanine
Buformin
Butyric acid
γ-Butyrobetaine
Butyrylcarnitine

C

Cadaverine
Caffeic acid
Caffeine
Q110 cAMP
Canavanine
N -Carbamoylaspartic acid
Carbamoylphosphate
N -Carbamylglutamic acid
β-Carboline
2-Carboxybenzaldehyde
S -Carboxymethylcysteine
Carboxymethyllysine
Carnitine
Q110 Carnosine
cCMP[7]
2',3'-cCMP[7]
Q110 CDP
CDP-choline
Q110 cGMP
α-Chaconine
p -Chlorophenylacetic acid
Cholic acid
Q110 Choline
Cimetidine
cIMP
trans -Cinnamic acid
Citraconic acid
Citramalic acid
Q110 Citric acid
Q110 Citrulline
Q110 CMP
2'-CMP[9]
3'-CMP[9]
CMP-*N* -acetylneuraminate
Q110 CoA
Corosolic acid
o -Coumaric acid
p -Coumaric acid
Q110 Creatine
Q110 Creatinine
2-(Creatinine-3-yl)propionic acid
trans -Crocetin
Crotonic acid
cTMP
Q110 CTP
Cumic acid
β-Cyanoalanine
3',5'-Cyclic dAMP
Cyclohexanecarboxylic acid
Cyclohexylamine
Q110 Cys
Cys-Gly
Cystathionine
Cysteamine
Cysteic acid
Cysteine glutathione disulfide
Cysteinesulfinic acid
Cystine
Q110 Cytidine
Q110 Cytosine

D

dADP
DAMGO
Daminozide
dAMP
Q110 dATP
dCDP
dCMP
Q110 dCTP
Deamido-NAD^+
Decanoic acid
Decarboxylated *S* -Adenosylmethionine
3-Dehydroshikimic acid
N -(1-Deoxy-1-fructosyl)valine
5'-Deoxy-5'-methylthioadenosine
2'-Deoxyadenosine[2]
5'-Deoxyadenosine[2]
2'-Deoxycytidine
2-Deoxyglucose 6-phosphate
2'-Deoxyguanosine
2'-Deoxyinosine
2-Deoxyribose 1-phosphate
2'-Deoxyuridine
3'-Dephospho CoA
Desthiobiotin
dGDP
dGMP
dGTP
N^1,N^8-Diacetylspermidine
N^1,N^{12}-Diacetylspermine
P^1 , P^4 -Di(adenosine-5') tetraphosphate
2,4-Diaminobutyric acid
2,6-Diaminopimelic acid
1,3-Diaminopropane
2,3-Diaminopropionic acid
Diethanolamine
O ,*O* -Diethyl thiophosphate
Diethylaminomalonic acid
2,6-Diethylaniline
N^1,N^{11}-Diethylnorspermine
N^1,N^{12}-Diethylspermine
Digalacturonic acid
7,8-Dihydrobiopterin
7,8-Dihydrofolic acid
7,8-Dihydroneopterin
Dihydroorotic acid
Dihydrouracil
Q110 Dihydroxyacetone phosphate
2,3-Dihydroxybenzoic acid
2,4-Dihydroxybenzoic acid
2,5-Dihydroxybenzoic acid
3,4-Dihydroxybenzylamine
3,4-Dihydroxyhydrocinnamic acid
5,6-Dihydroxyindole
3,4-Dihydroxymandelic acid
3-(3,4-Dihydroxyphenyl)-2-methylalanine
3-(2,3-Dihydroxyphenyl) propionic acid
3,4-Dihydroxyphenylacetic acid
3,4-Dihydroxyphenylglycol
2,4-Dihydroxypyrimidine-5-carboxylic acid
4,6-Dihydroxyquinoline
Diisopropanolamine
Dimethylaminoethanol
N,*N* -Dimethylaniline[1]
5,6-Dimethylbenzimidazole
Q110 *N*,*N* -Dimethylglycine
N,*N* -Dimethylhistidine
2,5-Dimethylpyrazine
dIMP
Diphenylamine
2,3-Diphosphoglyceric acid
dITP
Dodecanedioic acid
DOPA
Dopamine
Q110 dTDP
dTDP-glucose
Q110 dTMP
Q110 dTTP
dUDP
dUMP
dUTP

E

Ectoine
Ergothioneine
Q110 Erythrose 4-phosphate
Ethanolamine
Ethanolamine phosphate
Ethionine
m -Ethoxybenzoic acid
Ethyl glucuronide
Ethylacetimidate
N^5 -Ethylglutamine
N -Ethylglycine
N -Ethylmaleimide
Etidronic acid

F

FAD
Ferulic acid
FMN
Folic acid
Formiminoglutamic acid
Formylanthranilic acid
N -Formylaspartic acid
N -Formylglycine
N ′-Formylkynurenine
N -Formylmethionine
Q110 Fructose 1,6-diphosphate
Q110 Fructose 6-phosphate
Q110 Fumaric acid

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HMT

ver.2.4a
CE: ver.7.4.6 (7.5.3)

Fumaric acid monomethyl ester
2-Furoic acid
Furosemide

G

Q110 GABA
Galactosamine
Galacturonate 1-phosphate
Galacturonic acid
Gallic acid
Q110 GDP
3',5'-GDP
GDP-fucose[5]
GDP-galactose[8]
GDP-glucose
GDP-mannose[8]
Gibberellic acid
Q110 Gln
Q110 Glu
γ-Glu-Ala
γ-Glu-Arg
γ-Glu-Asn
γ-Glu-Asp
γ-Glu-Citrulline
γ-Glu-Cys
γ-Glu-Gln
Glu-Glu
γ-Glu-Glu
γ-Glu-Gly
γ-Glu-His
γ-Glu-Ile
γ-Glu-Leu
γ-Glu-Lys
γ-Glu-Met
γ-Glu-Ornitine
γ-Glu-Phe
γ-Glu-Ser
γ-Glu-Taurine
γ-Glu-Thr
γ-Glu-Trp
γ-Glu-Tyr
γ-Glu-Val
γ-Glu-Val-Gly
Glucaric acid
Q110 Gluconic acid
Gluconolactone
Glucosamine
Glucosamine 6-phosphate
Glucosamine 6-sulfuric acid
Glucosaminic acid
Q110 Glucose 1-phosphate
Q110 Glucose 6-phosphate
Glucurone
Glucuronic acid
trans -Glutaconic acid
γ-Glutamyl-*S* -Allylcysteine
Glutaric acid
Glutaryl CoA
Q110 Glutathione (GSH)
Q110 Glutathione (GSSG)
N^1-Glutathionylspermidine disulfide
Q110 Gly
Gly-Asp
Gly-Gly
Gly-Leu
Q110 Glyceraldehyde 3-phosphate
Glyceric acid
Glycerol
Glycerol 2-phosphate
Q110 Glycerol 3-phosphate
Glycerophosphocholine
Glycine anhydride
Glycocholic acid
Q110 Glycolic acid
N -Glycolylneuraminic acid
Glycyrrhetinic acid
Q110 Glyoxylic acid
Q110 GMP
Q110 GTP
2-Guanidinobenzimidazole
4-Guanidinobutyric acid
3-Guanidinopropionic acid
Guanidinosuccinic acid
Guanidoacetic acid
Q110 Guanine
Q110 Guanosine
Guanosine 5'-[γ-thio]triphosphate
Gulonolactone

H

Harmaline
Heptanoic acid
Hercynine
Hexamine
Hexanoic acid
Hexylamine
S -Hexylglutathione
Hippuric acid
Q110 His
His-Glu
Histamine
Histidinol
HMG CoA
Homoarginine
Homocarnosine
Homocitrulline
Homocysteic acid
Homocysteine
Homocysteinesulfinic acid
Homocysteinethiolactone
Homocystine
Homogentisic acid
Q110 Homoserine
Homoserinelactone
Homovanillic acid
Hordenine
8-Hydroxy-2'-deoxyguanosine
3-Hydroxy-2-methyl-4-pyrone
3-Hydroxy-3-methylglutaric acid
2-Hydroxy-4-methylvaleric acid
4-Hydroxy-3-methoxyphenylglycol sulfate
3-Hydroxyanthranilic acid
threo -3-Hydroxyaspartic acid
o -Hydroxybenzoic acid
m -Hydroxybenzoic acid
p -Hydroxybenzoic acid
Q110 2-Hydroxybutyric acid
Q110 3-Hydroxybutyric acid
10-Hydroxydecanoic acid
6-Hydroxydopamine
2-Hydroxyglutaric acid
6-Hydroxyhexanoic acid
o -Hydroxyhippuric acid
Hydroxyindole
5-Hydroxyindoleacetic acid
2-Hydroxyisobutyric acid
β-Hydroxyisovaleric acid
3-Hydroxykynurenine
5-Hydroxylysine
p -Hydroxymandelic acid
2-(Hydroxymethyl)benzoic acid
5-Hydroxymethyluracil
6-Hydroxynicotinic acid
2-Hydroxyoctanoic acid
8-Hydroxyoctanoic acid
5-Hydroxypentanoic acid
4-Hydroxyphenethyl alcohol
4-Hydroxyphenylacetaldehyde
3-Hydroxyphenylacetic acid
o -Hydroxyphenylacetic acid
p -Hydroxyphenylacetic acid
4-Hydroxyphenylglycine
4-Hydroxyphenylglyoxylic acid
Hydroxyphenyllactic acid
2-(4-Hydroxyphenyl)propionic acid
3-(2-Hydroxyphenyl)propionic acid
3-(3-Hydroxyphenyl)propionic acid
3-(4-Hydroxyphenyl)propionic acid
p -Hydroxyphenylpyruvic acid
Q110 Hydroxyproline
cis -4-Hydroxyproline
3-Hydroxypropionic acid
β-Hydroxypyruvic acid
4-Hydroxyquinoline
5-Hydroxytryptophan
Hydroxyurea
2-Hydroxyvaleric acid
Hypotaurine
Q110 Hypoxanthine

I

IDP
Q110 Ile
Ile-Pro-Pro
Imidazole-4-acetic acid
Imidazole-4-methanol
1*H* -Imidazole-4-propionic acid
Imidazolelactic acid
Q110 IMP
Indole-3-acetaldehyde
Indole-3-acetaldoxime[3]
Indole-3-acetamide[3]
Indole-3-acetic acid
Indole-3-carboxylic acid
Indole-3-ethanol
Indole-3-lactic acid
Indole-3-propionic acid
3-Indolebutyric acid
3-Indoxylsulfuric acid
Q110 Inosine
myo -Inositol 1-phosphate[11]
myo -Inositol 2-phosphate
myo -Inositol 3-phosphate[11]
Isatin
Isethionic acid
Isoamylamine
Isobutylamine
Isobutyric acid
Isobutyryl CoA
Isobutyrylcarnitine
Q110 Isocitric acid
Isoferulic acid
Isoglutamic acid
Isonicotinamide
Isonicotinic acid
Isopropanolamine
2-Isopropylmalic acid
Isovaleric acid
Isovalerylalanine
Isovalerylcarnitine
Itaconic acid
ITP

K

Kinetin
Kojic acid
Kynurenic acid
Kynurenine

L

Q110 Lactic acid
S -Lactoylglutathione
Lauric acid
Lauroyl CoA
Lauroylcarnitine
Q110 Leu
β-Leucine
Leu-Leu-Tyr
Lipoamide
Lumazine
Lupulone
Q110 Lys
Lysinamide

M

Maleamic acid
Maleic acid
Q110 Malic acid
Q110 Malonyl CoA
Malonylcarnitine
Mandelic acid
Mannosamine
Melatonin
3-Mercapto-2-oxopropanoate
3-Mercaptolactic acid
6-Mercaptopurine
Mesaconic acid
Q110 Met
Metanephrine
Metanilic acid
Methanesulfonic acid
Methionine sulfoxide
Methionine sulfoximine
5-Methoxy-*N*,*N* -dimethyltryptamine
3-Methoxy-4-hydroxyphenylethyleneglycol
3-Methoxyanthranilic acid
5-Methoxyindoleacetic acid
p -Methoxyphenylacetic acid
5-Methoxytryptamine
3-Methoxytyramine
3-Methoxytyrosine
15-Methyl prostaglandin $F_{2\alpha}$
Methyl sulfate
N^6-Methyl-2'-deoxyadenosine
5-Methyl-2'-deoxycytidine
1-Methyl-4-imidazoleacetic acid
3-Methyl-2-oxovaleric acid[10]
4-Methyl-2-oxovaleric acid[10]
N^1-Methyl-4-pyridone-5-carboxamide
4-Methyl-5-thiazoleethanol
4-Methyl-1,2,5-oxadiazol-3-amine
3-Methyladenine
N^6-Methyladenine
1-Methyladenosine
N -Methylalanine
N -Methylaniline
N -Methylanthranilic acid
N_ω -Methylarginine
N -Methylaspartic acid
threo -β-Methylaspartic acid
DL-2-Methylbutyric acid
2-Methylcholine
3-Methylcrotonyl CoA
S -Methylcysteine
S -Methylcysteine-*S* -oxide
5-Methylcytosine
N -Methylglutamic acid
S -Methylglutathione
Methylguanidine
3-Methylguanine
7-Methylguanine
N^1-Methylguanosine
1-Methylhistamine
3-Methylhistamine
1-Methylhistidine
3-Methylhistidine
1-Methylhydantoin
N^6-Methyllysine
Methylmalonic acid
Methylmalonyl CoA[6]
S -Methylmethionine
1-Methylnicotinamide
N -Methylnicotinamide
N -Methylnorsalsolinol
N -Methylphenylethanolamine
N -Methylproline
N -Methylputrescine
4-Methylpyrazole
2-Methylserine
N -Methylserotonin
Methylsuccinic acid
5-Methyltetrahydrofolic acid
2-Methylthiazolidine-4-carboxylic acid
(Methylthio)acetic acid
3-(Methylthio)propionic acid
4-Methylthio-2-oxobutyric acid
N -Methyltryptamine
N -Methyltryptophan
N -Methyltyramine
1-Methyluric acid
3-Methylxanthine
7-Methylxanthine
Mevalolactone
Mevalonic acid
Mimosine
Minocycline
Morpholine
Mucic acid
cis,cis -Muconic acid
Muramic acid
Myosmine
Myristic acid
Myristoleic acid

N

NAADP
Q110 NAD^+
NADH
Q110 $NADP^+$
NADPH
Neamine
Neopterin
Nicotinamide
Nicotinamide hypoxanthine dinucleotide
Nicotinamide riboside
Nicotine
Nicotinic acid
p -Nitrophenyl phosphate
3-Nitropropionic acid
N -Nitrosodiethanolamine
S -Nitrosoglutathione
3-Nitrotyrosine
NMN
Noradrenaline
Normetanephrine
Nornicotine
Norspermidine
Norvaline

O

Octanoic acid
Octanoyl CoA
Octanoylcarnitine
Octopamine
Octopine
Octylamine
Ophthalmic acid
Q110 Ornithine
Orotic acid
Orotidine
Orotidine 5'-monophosphate
Oxamic acid
5-Oxo-2-tetrahydrofurancarboxylic acid
2-Oxoadipic acid
2-Oxobutyric acid
Q110 2-Oxoglutaric acid
2-Oxohexanoic acid
4-Oxohexanoic acid
5-Oxohexanoic acid
Q110 2-Oxoisovaleric acid
2-Oxooctanoic acid
5-Oxoproline
4-Oxopyrrolidine-2-carboxylic acid
2-Oxovaleric acid
4-Oxovaleric acid

P

Palmatine
Palmitoylcarnitine
Pantothenic acid
Paraxanthine
Pelargonic acid
Penicillamine
Pentamidine
Perillic acid
Q110 Phe
Phenaceturic acid
o -Phenanthroline
Phenol
Phenoxyacetic acid
Phenoxybenzamine
Phenyl phosphate
N^2-Phenylacetylglutamine
trans -2-Phenylcyclopropylamine
1,3-Phenylenediamine
Phenylethanolamine
1-Phenylethylamine
2-Phenylethylamine
Phenylhydrazine
3-Phenyllactic acid
3-Phenylpropionic acid
Phenylpyruvic acid
Phloretin
Phosphocreatine
Q110 Phosphoenolpyruvic acid
Q110 6-Phosphogluconic acid
Q110 2-Phosphoglyceric acid
Q110 3-Phosphoglyceric acid
Phosphoglycolic acid
Phosphonoacetic acid
Phosphorylcholine
O -Phosphoserine
Phytic acid
Picolinamide
Picolinic acid
Pilocarpine
Pimelic acid
Pipecolic acid
Piperidine
Porphobilinogen
ppGpp
Pristanic acid
Q110 Pro
Procaine
Propionic acid
Propionyl CoA
Propionylcarnitine
Propylthiouracil
Prostaglandin E_2
Prostaglandin $F_{2\alpha}$
Protocatechuic acid
Q110 PRPP
Pseudouridine
Psychosine
Pterin
Purine
Purine riboside
Q110 Putrescine
Pyrazinamide
Pyrazole
Pyridine
Pyridine-2-carboxylic acid butyl ester
Pyridoxal
Pyridoxal 5-phosphate
Pyridoxamine
Pyridoxamine 5'-phosphate
4-Pyridoxic acid
Pyridoxine
Pyridoxol 5'-phosphate
Pyrimidine
Pyrophosphate
Pyrrole
Pyrrole-2-carboxylic acid
2,5-Pyrroledione
Q110 Pyruvic acid

Q

Quinic acid
Quinoline
2-Quinolinecarboxylic acid
Quinolinic acid

R

Retinoic acid
Riboflavin
Ribose 1-phosphate
Q110 Ribose 5-phosphate
Ribulose 1,5-diphosphate
Q110 Ribulose 5-phosphate

S

Saccharopine
Salsolinol
Q110 Sarcosine
SDMA
Q110 Sedoheptulose 7-phosphate
Semicarbazide
Sepiapterin
Q110 Ser
Ser-Glu
Serotonin
Shikimate 3-phosphate
Shikimic acid
Sinapic acid
α-Solanine
Sorbitol 6-phosphate
Q110 Spermidine
Q110 Spermine
Streptomycin sulfate
Suberic acid
Q110 Succinic acid
Succinic semialdehyde
Succinyl CoA[6]
N -Succinyl-5-aminoimidazole-4-carboxamide ribose 5'-phosphate
Succinylcholine
O -Succinylhomoserine
N^2-Succinylornithine
Sucrose 6'-phosphate
Sulfanilic acid
S -Sulfocysteine
O -Sulfoserine
Sulfotyrosine
Syringic acid

T

Tartaric acid
meso -Tartaric acid
Taurine
Taurocholic acid
Taurocyamine
5,6,7,8-Tetrahydrobiopterin
Tetrahydrofolic acid
Tetrahydropalmatine
Theobromine
Thiabendazole
Thiamine
Thiamine diphosphate
Thiamine phosphate
Thiamine triphosphate
Thiaproline
Thiazole
6,8-Thioctic acid
Thiodiglycolic acid
2-Thiopheneacetic acid
Thiourea
Q110 Thr
Thr-Asp
Threonic acid
allo -Threonine
Q110 Thymidine
Q110 Thymine
Tiglic acid
Tioconazole
o -Toluic acid
m -Toluic acid
p -Toluic acid
N -(*o* -Toluoyl)glycine
Topiramic acid
Trehalose 6-phosphate
TRH
2,4,4'-Trichloro-2'-hydroxydiphenyl ether
Tridecanoic acid
Trigonelline
Trimethylamine
Trimethylamine *N* -oxide
4-Trimethylammoniobutanal
N^6,N^6,N^6-Trimethyllysine
Trimethylsulfonium
Tropic acid
Tropine
Tropinone
Q110 Trp
Tryptamine
Tryptophanamide
Q110 Tyr
β-Tyr
Q110 Tyramine
Tyr-Arg
Tyr-Glu

U

Q110 UDP
UDP-*N* -acetylgalactosamine
UDP-*N* -acetylglucosamine
UDP-galactose[4]
UDP-glucose[4]
UDP-glucuronic acid
Q110 UMP
Undecanoic acid
Q110 Uracil
Urea
Ureidoglycolic acid
3-Ureidoisobutyric acid
3-Ureidopropionic acid
Uric acid
Q110 Uridine
Urocanic acid
Ursolic acid
Q110 UTP

V

Q110 Val
Val-Pro-Pro
Valeric acid
Vanillic acid
Vanillylmandelic acid

X

Xanthine
Xanthosine
Xanthurenic acid
XMP
XTP
Xylulose 5-phosphate

Z

trans- Zeatin

DRUGS

Acetanilide
Acetohydroxamic acid
Albizziine
Amantadine
Amikacin
3-Amino-1,2,4-triazole
2-Aminobenzimidazole
4-Aminoindole
5-Aminoindole
(Aminomethyl)phosphonic acid
Amrinone
8-Anilino-1-naphthalenesulfonic acid
Arginine ethyl ester
Atropine
Baclofen
Benzamidine
N α-Benzenol arginine ethylester
Benzimidazole
Benzyl viologen
Betonicine
Carbachol
Carbendazim
Castanospermine
Chelidonic acid
Chloramphenicol
Chloroacetic acid
3-Chloroalanine
o -Chlorobenzoic acid
p -Chlorobenzoic acid
p -Chlorophenoxyacetic acid
Ciprofloxacin
Clonidine
2-Cyanopyridine
Cycloserine
Cyprodinil
Daunorubicin
Deethylatrazine
Deisopropylatrazine
2-Deoxystreptamine
2,4-Dichlorobenzoic acid
2,4-Dichlorophenoxyacetic acid
Dichlorprop
Diclofenac
3,5-Diiodotyrosine
2,4-Dimethylaniline[1]
2,6-Dimethylaniline[1]
3,5-Dinitrosalicylic acid
Diphenylcarbazide
Disulfiram

Mediator Scan Annotation List

M: ver.6.1.1

Fatty acid

FA(10:0)	FA(19:0)
FA(11:0)	FA(19:1)
FA(11:1)	FA(19:2)
FA(12:0)	FA(20:0)
FA(12:1)	FA(20:1)
FA(13:0)	FA(20:2)
FA(13:1)	FA(20:3)
FA(14:0)	FA(20:4)
FA(14:1)	FA(20:5)
FA(15:0)	FA(21:0)
FA(15:1)	FA(21:1)
FA(16:0)	FA(22:0)
FA(16:1)	FA(22:1)
FA(16:2)	FA(22:2)
FA(17:0)	FA(22:3)
FA(17:1)	FA(22:4)
FA(18:0)	FA(22:5)
FA(18:1)	FA(22:6)
FA(18:2)	FA(23:0)
FA(18:3)	FA(23:1)
	FA(24:0)
	FA(24:1)

Acylcarnitine

AC(10:0)	AC(19:0)
AC(11:0)	AC(19:1)
AC(11:1)	AC(20:0)
AC(12:0)	AC(20:1)
AC(12:1)	AC(20:2)
AC(13:0)	AC(20:3)
AC(13:1)	AC(20:4)
AC(14:0)	AC(20:5)
AC(14:1)	AC(22:0)
AC(15:0)	AC(22:1)
AC(15:1)	AC(22:2)
AC(16:0)	AC(22:3)
AC(16:1)	AC(22:4)
AC(17:0)	AC(22:5)
AC(17:1)	AC(22:6)
AC(18:0)	AC(24:0)
AC(18:1)	AC(24:1)
AC(18:2)	
AC(18:3)	

Endocannabinoid

Acylethanolamine(16:0)
Acylethanolamine(18:0)
Acylethanolamine(18:1)
Acylethanolamine(18:2)
Acylethanolamine(18:3)
Acylethanolamine(20:3)
Acylethanolamine(20:4)
Acylethanolamine(20:5)
Acylethanolamine(22:4)
Acylethanolamine(22:6)
2-Arachidonoylglycerol

Platelet-activating factor (PAF)

PAF(14:0)	PAF(19:0)
PAF(15:0)	PAF(20:4)
PAF(16:0)	PAF(20:5)
PAF(16:1)	PAF(20:6)
PAF(16:2)	PAF(22:4)
PAF(17:0)	PAF(22:5)
PAF(18:0)	PAF(22:6)
PAF(18:1)	
PAF(18:2)	
PAF(18:3)	

LysoPAF

LysoPAF(16:0)	LysoPAF(18:0)

Arachidonic acid metabolites

15-deoxy Prostaglandin J2
5,6-diHETE
5,15-diHETE
8,15-diHETE
5-HETE
12-HETE
15-HETE
20-hydroxy Leukotriene B4
6-keto Prostaglandin F1α
Leukotriene B4
Lipoxin A4
Lipoxin B4
5-oxoETE
15-oxoETE
Prostaglandin D2
Prostaglandin F2α
Prostaglandin H2
Prostaglandin I2
Thromboxane B2

EPA metabolites

5-HEPE
12-HEPE
15-HEPE
18-HEPE
Lipoxin A5
Prostaglandin D3
Prostaglandin E3
Resolvin E1

DHA metabolites

7,17-diHDoHE
4-HDoHE
7-HDoHE
10-HDoHE
13-HDoHE
14-HDoHE
17-HDoHE
20-HDoHE
Protectin DX
Resolvin D1
Resolvin D2

Steroid

Aldosterone
Chenodeoxycholic acid
Cholic acid
Corticosterone
Cortisol
Cortisone
7-Dehydrocholesterol
Deoxycholic acid
Desmosterol
DHEA-S
Estradiol
Estriol
Estrone
20-Hydroxycholesterol
22-Hydroxycholesterol
17-Hydroxyprogesterone
Lanosterol
Lithocholic acid
Pregnenolone
Progesterone
Squalene
Testosterone
Thyroxine
Triiodothyronine
Ursodeoxycholic acid

Lysophosphatidic acid (LPA)

LPA(12:0)	LPA(20:0)
LPA(14:0)	LPA(20:1)
LPA(15:0)	LPA(20:2)
LPA(16:0)	LPA(20:3)
LPA(16:1)	LPA(20:4)
LPA(17:0)	LPA(20:5)
LPA(18:0)	LPA(22:0)
LPA(18:1)	LPA(22:1)
LPA(18:2)	LPA(22:2)
LPA(18:3)	LPA(22:3)
LPA(19:0)	LPA(22:4)
	LPA(22:5)
	LPA(22:6)
	LPA(24:0)
	LPA(24:1)

Lysophosphatidylcholine (LPC)

LPC(12:0)	LPC(20:0)
LPC(14:0)	LPC(20:1)
LPC(15:0)	LPC(20:2)
LPC(16:0)	LPC(20:3)
LPC(16:1)	LPC(20:4)
LPC(17:0)	LPC(20:5)
LPC(18:0)	LPC(22:0)
LPC(18:1)	LPC(22:1)
LPC(18:2)	LPC(22:2)
LPC(18:3)	LPC(22:3)
LPC(19:0)	LPC(22:4)
	LPC(22:5)
	LPC(22:6)
	LPC(24:0)
	LPC(24:1)

Lysophosphatidylethanolamine (LPE)

LPE(12:0)	LPE(20:0)
LPE(14:0)	LPE(20:1)
LPE(15:0)	LPE(20:2)
LPE(16:0)	LPE(20:3)
LPE(16:1)	LPE(20:4)
LPE(17:0)	LPE(20:5)
LPE(18:0)	LPE(22:0)
LPE(18:1)	LPE(22:1)
LPE(18:2)	LPE(22:2)
LPE(18:3)	LPE(22:3)
LPE(19:0)	LPE(22:4)
	LPE(22:5)
	LPE(22:6)
	LPE(24:0)
	LPE(24:1)

Sphinganine

Sphinganine(d16:0)
Sphinganine(d18:0)
Sphinganine(d20:0)
Sphinganine(d22:0)
Sphinganine(d24:0)

Sphingosine

Sphingosine(d16:1)
Sphingosine(d18:1)
Sphingosine(d20:1)
Sphingosine(d22:1)
Sphingosine(d24:1)

Lysophosphatidylglycerol (LPG)

LPG(12:0)	LPG(20:0)
LPG(14:0)	LPG(20:1)
LPG(15:0)	LPG(20:2)
LPG(16:0)	LPG(20:3)
LPG(16:1)	LPG(20:4)
LPG(17:0)	LPG(20:5)
LPG(18:0)	LPG(22:0)
LPG(18:1)	LPG(22:1)
LPG(18:2)	LPG(22:2)
LPG(18:3)	LPG(22:3)
LPG(19:0)	LPG(22:4)
	LPG(22:5)
	LPG(22:6)
	LPG(24:0)
	LPG(24:1)

Lysophosphatidylinositol (LPI)

LPI(12:0)	LPI(20:0)
LPI(14:0)	LPI(20:1)
LPI(15:0)	LPI(20:2)
LPI(16:0)	LPI(20:3)
LPI(16:1)	LPI(20:4)
LPI(17:0)	LPI(20:5)
LPI(18:0)	LPI(22:0)
LPI(18:1)	LPI(22:1)
LPI(18:2)	LPI(22:2)
LPI(18:3)	LPI(22:3)
LPI(19:0)	LPI(22:4)
	LPI(22:5)
	LPI(22:6)
	LPI(24:0)
	LPI(24:1)

Lysophosphatidylserine (LPS)

LPS(12:0)	LPS(20:0)
LPS(14:0)	LPS(20:1)
LPS(15:0)	LPS(20:2)
LPS(16:0)	LPS(20:3)
LPS(16:1)	LPS(20:4)
LPS(17:0)	LPS(20:5)
LPS(18:0)	LPS(22:0)
LPS(18:1)	LPS(22:1)
LPS(18:2)	LPS(22:2)
LPS(18:3)	LPS(22:3)
LPS(19:0)	LPS(22:4)
	LPS(22:5)
	LPS(22:6)
	LPS(24:0)
	LPS(24:1)

Sphinganine-1P

Sphinganine-1P(d16:0)
Sphinganine-1P(d18:0)
Sphinganine-1P(d20:0)
Sphinganine-1P(d22:0)
Sphinganine-1P(d24:0)

Sphingosine-1P

Sphingosine-1P(d16:1)
Sphingosine-1P(d18:1)
Sphingosine-1P(d20:1)
Sphingosine-1P(d22:1)
Sphingosine-1P(d24:1)

Glucosylceramide

Glucosylceramide(d18:1/14:0)
Glucosylceramide(d18:1/16:0)
Glucosylceramide(d18:1/16:1)
Glucosylceramide(d18:1/18:0)
Glucosylceramide(d18:1/18:1)
Glucosylceramide(d18:1/20:0)
Glucosylceramide(d18:1/20:1)
Glucosylceramide(d18:1/22:0)
Glucosylceramide(d18:1/22:1)
Glucosylceramide(d18:1/22:2)
Glucosylceramide(d18:1/24:0)
Glucosylceramide(d18:1/24:1)
Glucosylceramide(d18:1/24:2)

Lactosylceramide

Lactosylceramide(d18:1/14:0)
Lactosylceramide(d18:1/16:0)
Lactosylceramide(d18:1/16:1)
Lactosylceramide(d18:1/18:0)
Lactosylceramide(d18:1/18:1)
Lactosylceramide(d18:1/20:0)
Lactosylceramide(d18:1/20:1)
Lactosylceramide(d18:1/22:0)
Lactosylceramide(d18:1/22:1)
Lactosylceramide(d18:1/22:2)
Lactosylceramide(d18:1/24:0)
Lactosylceramide(d18:1/24:1)
Lactosylceramide(d18:1/24:2)

Ceramide

Ceramide-1P(d18:1/14:0)
Ceramide-1P(d18:1/16:0)
Ceramide-1P(d18:1/16:1)
Ceramide-1P(d18:1/18:0)
Ceramide-1P(d18:1/18:1)
Ceramide-1P(d18:1/20:0)
Ceramide-1P(d18:1/20:1)
Ceramide-1P(d18:1/22:0)
Ceramide-1P(d18:1/22:1)
Ceramide-1P(d18:1/22:2)
Ceramide-1P(d18:1/24:0)
Ceramide-1P(d18:1/24:1)
Ceramide-1P(d18:1/24:2)

Ganglioside

GD1(d18:1/16:0)
GD1(d18:1/18:0)
GD3(d18:1/16:0)
GD3(d18:1/18:0)
GM3(d18:1/12:0)
GM3(d18:1/12:1)
GM3(d18:1/14:0)
GM3(d18:1/14:1)
GM3(d18:1/16:0)
GM3(d18:1/16:1)
GM3(d18:1/18:0)
GM3(d18:1/18:1)
GT1(d18:1/16:0)
GT1(d18:1/18:0)

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LC-MS Annotation List

ver. 2.4b
LC: ver.3.7.3

Steroids

Adrenosterone
Aldosterone
Androstanediol
Androstanolone
4-Androstene-3,17-dione
Androsterone
Asiatic acid
Betulinic acid
Brassinolide
Campesterol
Cepharanthine
5α-Cholestan-3-one
Cholesterol
Cholesterol sulfate
Cortexolone
Corticosterone
Cortisol
Cortisone
Cycloartenol
7-Dehydrocholesterol
Dehydroisoandrosterone
Dehydroisoandrosterone 3-sulfate
Deoxycorticosterone
21-Deoxycortisol
Desmosterol
3α,21-Dihydroxy-5α-pregnan-20-one
Diosgenin
16-Epiestriol
17α-Estradiol
Ergocalciferol
Ergosterol
β-Estradiol
β-Estradiol 17-glucuronide
Estriol
Estriol 16α-glucuronide
Estrone
Estrone 3-glucuronide
Estrone 3-sulfate
Ethynyl estradiol
Etiocholan-3α-ol-17-one
Etiocholan-3α-ol-17-one glucuronide
Hecogenin
11β-Hydroxyandrost-4-ene-3,17-dione
19-Hydroxyandrostenedione
20α-Hydroxycholesterol[13]
22-Hydroxycholesterol[13]
18-Hydroxycorticosterone
2-Hydroxyestradiol
16α-Hydroxyestrone
2-Hydroxyestrone
17α-Hydroxypregnenolone[12]
21-Hydroxypregnenolone[12]
17α-Hydroxyprogesterone
20α-Hydroxyprogesterone
Hydroxyprogesterone caproate
19-Hydroxytestosterone
Lanosterol
Lathosterol
Medroxyprogesterone
Methoxyestradiol
Ouabain
5α-Pregnan-20α-ol-3-one
5α-Pregnan-3α-ol-20-one
5α-Pregnane-3,20-dione
5β-pregnane-3α,21-diol-11,20-dione
Pregnenolone
Pregnenolone sulfate
Progesterone
Sitosterol
Solanidine
Stigmasterol
Testosterone
Testosterone acetate
Testosterone glucuronide

Bile acids

Chenodeoxycholic acid
Cholic acid
Deoxycholic acid
Hyodeoxycholic acid
Glycochenodeoxycholic acid
Glycocholic acid
Glycodeoxycholic acid
Glycolithocholic acid
Glycoursodeoxycholic acid
Lithocholic acid
Taurochenodeoxycholic acid
Taurocholic acid
Taurodeoxycholic acid
Taurolithocholic acid
Taurolithocholic acid 3-sulfate
Tauroursodeoxycholic acid
Ursodeoxycholic acid

Fatty acids/Lipids

N -Acetylsphingosine
AEA(18:1)
AEA(18:3)
AEA(20:3)
AEA(20:5)
AEA(22:4)
AEA(22:6)
Anandamide
Arachidic acid
Arachidonic acid
2-Arachidonoylglycerol
Behenic acid
Decanoic acid
1,2-Dipalmitoyl-glycero-3-phosphoethanolamine
1,2-Dipalmitoyl-glycero-3-phosphoglycerol
1,2-Distearoyl-glycero-3-phosphocholine
cis -4,7,10,13,16,19-Docosahexaenoic acid
cis -11,14-Eicosadienoic acid
cis -5,8,11,14,17-Eicosapentaenoic acid
cis -8,11,14-Eicosatrienoic acid
cis -11-Eicosenoic acid
cis -13-Eicosenoic acid
Erucic acid
Ethyl arachidonate
Fatty Acid(12:0)
Fatty Acid(12:1)
Fatty Acid(13:0)
Fatty Acid(14:1)
Fatty Acid(14:2)
Fatty Acid(14:3)
Fatty Acid(15:0)
Fatty Acid(15:1)
Fatty Acid(16:2)
Fatty Acid(16:3)
Fatty Acid(17:0)
Fatty Acid(17:1)
Fatty Acid(17:2)
Fatty Acid(17:3)
Fatty Acid(19:0)
Fatty Acid(19:1)
Fatty Acid(19:2)
Fatty Acid(20:3)
Fatty Acid(22:2)
Fatty Acid(22:3)
Fatty Acid(22:4)
Fatty Acid(22:5)
Fatty Acid(24:0)
Fatty Acid(24:2)
Fatty Acid(24:4)
Fatty Acid(24:5)
Fatty Acid(25:0)
Fatty Acid(25:3)
Fatty Acid(26:0)
Fatty Acid(26:2)
Glucosylceramide(d18:1/24:1)
Heneicosanoic acid
Heptadecanoic acid
15(S)-HETE
1-Hexadecyl-2-acetyl-glycero-3-phosphocholine
N -Hexanoylsphingosine
2-Hydroxytetradecanoic acid
3-Hydroxytetradecanoic acid
Lactosylceramide(d18:1/24:1)
Leukotriene B4
Linoleic acid
Linolenic acid
Linoleyl ethanolamide
LPA(14:0)
LPC(12:0)
LPC(24:0)
LPE(16:0)
LPE(18:1)
LPG(16:0)
LPG(18:1)
LPS(18:0)
LysoPAF(16:0)
19-Methylarachidic acid
Myristic acid
1-Myristoyl-glycero-3-phosphocholine
1-Myristoyl-glycero-3-phosphoethanolamine
Nervonic acid
Oleic acid
Oleoyl ethanolamide
1-Oleoyl-glycero-3-phosphocholine
PAF(17:0)
Palmitic acid
Palmitoleic acid
Palmitoylethanolamide
1-Palmitoyl-glycero-3-phosphocholine
1-Palmitoyl-glycero-3-phosphoethanolamine
Pentadecanoic acid
Phytosphingosine
Ricinoleic acid
Sphinganine
Sphinganine 1-phosphate
Sphinganine(d20:0)
Sphingomyelin(d18:1/16:0)
Sphingomyelin(d18:1/18:0)
Sphingosine
Sphingosine 1-phosphate
Sphingosine(d20:1)
Stearic acid
Stearidonic acid
Stearoyl ethanolamide
1-Stearoyl-glycero-3-phosphocholine
Tricosanoic acid
Trilaurin

Acylcarnitines

Acylcarnitine(10:0)
Acylcarnitine(12:0)
Acylcarnitine(12:1)
Acylcarnitine(13:1)
Acylcarnitine(14:0)
Acylcarnitine(14:1)
Acylcarnitine(14:2)
Acylcarnitine(14:3)
Acylcarnitine(15:0)
Acylcarnitine(16:1)
Acylcarnitine(16:2)
Acylcarnitine(17:0)
Acylcarnitine(17:1)
Acylcarnitine(18:0)
Acylcarnitine(18:1)
Acylcarnitine(18:2)
Acylcarnitine(20:0)
Acylcarnitine(20:1)
Acylcarnitine(21:0)
Acylcarnitine(22:0)
Acylcarnitine(23:0)
Palmitoylcarnitine

Polyphenols

Apigenin 7-glucoside
Apigenin 8-glucoside
Arctigenin
Baicalein
Baicalin
Capillarisin
Catechin
Catechin gallate
Chlorogenic acid
Chrysin
Chrysoeriol
Curcumin
Cyanidin-3-*O* -Glucoside
Daidzein
Datiscetin
Delphinidin
7,8-Dihydroxycoumarin
Eleutheroside B
Eleutheroside E
Epicatechin
Epicatechin gallate
Epigallocatechin 3-*O* -(3-*O* -methyl)gallate
Epigallocatechin gallate
Eriocitrin
Eriodictyol
Eriodictyol 7-neohesperidoside
Flavanone
Formononetin
Formononetin 7-glucoside
Galangin
Gallocatechin
Gallocatechin gallate
Genistein
Glabridin
Glycitein
Hesperidin
7-Hydroxycoumarin
Hyperoside
Isofraxidin
Isoliquiritigenin
Isoorientin
Isoquercetin
Kaempferol
Liquiritigenin
Luteolin
Luteolin 7-glucoside
Malvidin
Myricetin 3-rhamnoside
Naringenin
Naringenin 7-neohesperidoside
Peonidin 3-glucoside
Poncirin
Procyanidin B_1
Procyanidin B_2
Quercetin
Quercetin 3-rutinoside
Resveratrol
Saponarin
Taxifolin
Tectorigenin
Theaflavin
Theaflavin-3-gallate

Others

N -Acetylserotonin
N -Acetyltyrosine ethyl ester
p -Anisic acid
5,7-Dimethoxyflavone
5-Methoxyindoleacetic acid
6-Hydroxymelatonin
6-Ketoprostaglandin E_1
Abietic acid
Astaxanthin
Biotin
Caffeic acid
Carvone
Coenzyme Q10
Corosolic acid
trans -Crocetin
β-Cryptoxanthin
Dethiobiotin
N -Formylanthranilic acid
Gymnemic acid
Humulone
Indole-3-carboxaldehyde
Kynurenic acid
Lupulone
Lutein
Monoglucosyl hesperidin
Oleanolic acid
Piperine
Prostaglandin B_2
Prostaglandin D_1
Prostaglandin D_2
Prostaglandin E_1
PGI2
Riboflavin
Retinol
Sesamin
Thyroxine
α-Tocopherol
α-Tocopherol acetate
γ-Tocopherol
Triptolide
Tropic acid
Zeaxanthin

Compounds marked with numbers on their right shoulders cannot be distinguished as separated peaks, and their measured values are reported as the sum of the set.