CE-MS アノテーションリスト 1/4

本リストは、「ω Scan Advanced[*1]」「ω Scan」「Basic Scan」「Dual Scan[*2]」における測定対象物質の一覧です。

＊1 「ω Scan Advanced」では、本リストに含まれない物質も含め、CE-FTMSで検出されたすべてのピークについての結果をご報告いたします。

＊2 「Dual Scan」では、本リストの他に、「LC-MS アノテーションリスト」に記載のある物質についても測定対象となります。

☆は「ターゲット濃度計算（110物質定量）オプション」の対象となる物質を表します。

A

Abscisic acid
4-Acetamido-2-aminobutyric acid
★ 4-Acetamidobutanoic acid
Acetoacetamide
Acetoacetic acid
Acetoacetyl CoA
Acetohydrazide
☆ ★ Acetyl CoA
★ *N* -Acetyl-β-alanine
3-Acetylacrylic acid
★ *N* -Acetylalanine
N ^{2}-Acetylaminoadipic acid
★ 4-(β-Acetylaminoethyl)imidazole
6-(Acetylamino)hexanoic acid
N -α-Acetylarginine
★ *N* -Acetylasparagine
★ *N* -Acetylaspartic acid
N -Acetylaspartylglutamic acid
★ *O* -Acetylcarnitine
N -Acetylcarnosine
Acetylcholine
N -Acetylcysteine
N ^{4}-Acetylcytidine
N -Acetylgalactosamine
N -Acetylgalactosamine 4-sulfate
★ *N* -Acetylglucosamine
N -Acetylglucosamine 1-phosphate
N -Acetylglucosamine 6-phosphate
N -Acetylglucosylamine
★ *N* -Acetylglutamic acid
★ *N* -Acetylglutamine
★ *N* -Acetylglycine
★ *N* -Acetylhistidine
O -Acetylhomoserine
N -Acetylisoleucine
★ *N* -Acetylleucine
N -Acetyllysine
★ *N* ^{6}-Acetyllysine
N -Acetylmannosamine
★ *N* -Acetylmethionine
N -Acetylmuramic acid
★ *N* -Acetylneuraminic acid
★ *N* -Acetylornithine
N -Acetylphenylalanine
Acetylphosphate
★ *N* -Acetylproline
★ *N* -Acetylputrescine
Acetylpyrazine
N -Acetylserine
★ *O* -Acetylserine
N ^{1}-Acetylspermidine
N ^{8}-Acetylspermidine
★ *N* ^{1}-Acetylspermine
N -Acetyltaurine
N -Acetylthreonine
★ *N* -Acetyltryptophan
N -Acetyltyrosine
N -Acetylvaline
☆ ★ *cis* -Aconitic acid
☆ ★ Adenine
☆ ★ Adenosine
Adenosine 5'-phosphosulfate
Adenosine 5'-[γ-thio]triphosphate
S -Adenosylhomocysteine
☆ ★ *S* -Adenosylmethionine
Adenylosuccinic acid
Adipic acid
Adipic acid semialdehyde
ADMA
☆ ★ ADP
3',5'-ADP
ADP-glucose[1]
ADP-ribose
★ Adrenaline
★ Agmatine
☆ ★ Ala
☆ ★ β-Ala
★ Ala-Ala
Ala-Hyp
★ β-Ala-Lys
Albendazole
★ Allantoic acid
★ Allantoin
(+)-Alliin
(-)-Alliin
Allocryptopine
Alloisoleucine
S -Allylcysteine
Allysine
N -Amidinoglutamic acid
Amiloride
5-Amino-3,4-dihydro-2H-pyrrole-2-carboxylic acid
2-Amino-(3-hydroxy-5-methylisoxazole)-4-propionic acid
7-Amino-4-hydroxy-2-naphthalenesulfonic acid
3-Amino-1-hydroxy-2-pyrrolidone
★ 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-methyl-1-propanol
2-Amino-2-methylbutyric acid
★ 5-Amino-4-oxovaleric acid
2-Amino-4-phosphonobutyric 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
Aminomalonic acid
2-Aminooctanoic acid
Aminooxyacetic 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
☆ ★ AMP
★ 3'-AMP
Anabasine
Aniline
★ *p* -Anisic acid
★ Anserine
☆ ★ Anthranilic acid
Apigenin
Arabinonic acid
Arabinosylhypoxanthine
☆ ★ Arg
★ Arg-Glu
Argininic acid
Argininosuccinic acid
Argpyrimidine
Ascorbate 2-glucoside
★ Ascorbate 2-phosphate
★ Ascorbate 2-sulfate
Ascorbic acid
☆ ★ Asn
☆ ★ Asp
β-Asp-Leu
H-Asp(Gly-OH)-OH
H-Asp(Lys-OH)-OH
Aspartame
☆ ★ ATP
Atrolactic acid
★ Azelaic acid
Azetidine 2-carboxylic acid

B

Balenine
Barbituric acid
Benzamide
Benzocaine
★ Benzoic acid
★ Benzoylformic acid
N ^{6}-Benzyladenine
Benzylamine
Benzylsuccinic acid
☆ ★ Betaine
☆ ★ Betaine aldehyde
Biocytin
★ Biopterin
★ Biotin
Bis(*p* -nitrophenyl)phosphate
4-Bromophenylalanine
Buformin
Butyramide
Butyric acid
★ γ-Butyrobetaine
Butyrylcarnitine
★ *N* -Butyrylglycine

C

★ Cadaverine
Caffeic acid
★ Caffeine
☆ ★ cAMP
Canavanine
Capryloylglycine
★ *N* -Carbamoylaspartic acid
Carbamoylphosphate
N -Carbamylglutamic acid
β-Carboline
2-Carboxybenzaldehyde
N ^{7}-(1-carboxyethyl)arginine
S -(2-Carboxyethyl)cysteine
N $^{\varepsilon}$-(1-carboxyethyl)lysine
γ-Carboxyglutamic acid
N $^{\omega}$-(Carboxymethyl)arginine
S -Carboxymethylcysteine
Carboxymethyllysine
★ Carnitine
☆ ★ Carnosine
cCMP[2]
2',3'-cCMP[2]
☆ ★ CDP
★ CDP-choline
CDP-ethanolamine
☆ ★ cGMP
α-Chaconine
p -Chlorophenylacetic acid
3-Chlorotyrosine
Cholic acid
☆ ★ Choline
cIMP
Cinnabarinic acid
trans -Cinnamic acid
Cinnamoylglycine
★ Citraconic acid
★ Citramalic acid
☆ ★ Citric acid
☆ ★ Citrulline
☆ ★ CMP
2'-CMP[3]
3'-CMP[3]
CMP-*N* -acetylneuraminate
☆ ★ CoA
Corosolic acid
★ *o* -Coumaric acid
★ *p* -Coumaric acid
p -Coumaric acid sulfate
☆ ★ Creatine
☆ ★ Creatinine
p -Cresol glucuronide
p -Cresol sulfate
3-Cresotinic acid
trans -Crocetin
Crotonic acid
Crotonic acid betaine
Crotonoyl CoA
cTMP
☆ ★ CTP
Cumic acid
β-Cyanoalanine
Cyanuric acid
3',5'-Cyclic dAMP
Cyclohexanecarboxylic acid
Cyclohexylamine
☆ ★ Cys
★ Cys-Gly
★ Cystathionine
Cysteamine
★ Cysteic acid
Cysteine glutathione disulfide
Cysteinesulfinic acid
★ Cystine
☆ ★ Cytidine
☆ ★ Cytosine

D

dADP
Dalargin
DAMGO
dAMP
☆ ★ dATP
dCDP
dCMP
☆ ★ dCTP
Deamido-NAD^{+}
★ Decanoic acid
Decarboxylated *S* -Adenosylmethionine
3,4-Dehydroproline
3-Dehydroshikimic acid
Delphinidin 3,5-diglucoside
N -(1-Deoxy-1-fructosyl)glycine
N -(1-Deoxy-1-fructosyl)leucine
N -(1-Deoxy-1-fructosyl)threonine
N -(1-Deoxy-1-fructosyl)valine
3-Deoxy-D-manno-2-octulosonic acid
★ 5'-Deoxy-5'-methylthioadenosine
2'-Deoxyadenosine[4]
5'-Deoxyadenosine[4]
★ 2'-Deoxycytidine
2'-Deoxyguanosine
2'-Deoxyinosine
1-Deoxynojirimycin
4-Deoxypyridoxine
2-Deoxyribonic acid
2-Deoxyribose 1-phosphate
2'-Deoxyuridine
Deoxyxylulose 5-phosphate
3'-Dephospho CoA
Dethiobiotin
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
☆ ★ Dihydroxyacetone phosphate
2,3-Dihydroxybenzoic acid
2,4-Dihydroxybenzoic acid
2,5-Dihydroxybenzoic acid
2,6-Dihydroxybenzoic acid
3,5-Dihydroxybenzoic acid
3,4-Dihydroxybenzylamine
3,4-Dihydroxyhydrocinnamic acid
5,6-Dihydroxyindole
3,4-Dihydroxymandelic acid
(3,5-Dihydroxyphenyl)glycine
3-(3,4-Dihydroxyphenyl)-2-methylalanine
3-(2,3-Dihydroxyphenyl) propionic acid

※ 本資料記載の内容については予告なく変更する場合があります。

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ALA00WJ-03(25)

CE-MS アノテーションリスト 2/4

☆は「ターゲット濃度計算（110物質定量）オプション」の対象となる物質を表します。

ver.3.0a

3,4-Dihydroxyphenylacetic acid
3,4-Dihydroxyphenylglycol
2,4-Dihydroxypyrimidine-5-carboxylic acid
4,6-Dihydroxyquinoline
Diisopropanolamine
Dimethylallylpyrophosphate
Dimethylaminoethanol
N ,*N* -Dimethylaniline[5]
5,6-Dimethylbenzimidazole
☆ ★ *N* ,*N* -Dimethylglycine
N [2],*N* [2]-Dimethylguanosine
★ *N* ,*N* -Dimethylhistidine
N [6],*N* [6]-Dimethyllysine
2,5-Dimethylpyrazine
dIMP
Diphenylamine
★ 2,3-Diphosphoglyceric acid
5-Diphosphomevalonic acid
Diprotin A
dITP
Dodecanedioic acid
★ DOPA
★ Dopamine
Dopamine 3-*O* -sulfate
Dopamine 4-sulfate
☆ ★ dTDP
dTDP-glucose
☆ ★ dTMP
☆ ★ dTTP
dUDP
dUMP
dUTP

E

★ Ectoine
Emeriamine
Emideltide
Ephedrine
Ergothioneine
☆ ★ Erythrose 4-phosphate
★ Ethanolamine
★ Ethanolamine phosphate
Ethanolamine sulfate
Ethionine
m -Ethoxybenzoic acid
Ethyl glucuronide
Ethylacetimidate
Ethylenediaminetriacetic acid
★ *N* [5]-Ethylglutamine
★ *N* -Ethylglycine
2-Ethylhexanoic acid
2-Ethylhydracrylic acid
N -Ethylmaleimide
Ethylmalonic acid
Etidronic acid

F

FAD
Fagomine
Farnesyl pyrophosphate
★ Ferulic acid
3-Fluoro-4-hydroxybenzoic acid
FMN
Folic acid
Formiminoglutamic acid
N -Formylanthranilic acid
N -Formylaspartic acid
N -Formylglycine
N ′-Formylkynurenine
N [6]-Formyllysine
★ *N* -Formylmethionine
N -Formylphenylalanine
5-Formylsalicylic acid
☆ ★ Fructose 1,6-diphosphate
☆ ★ Fructose 6-phosphate
e -Fructoselysine
Fructosyllysine
☆ ★ Fumaric acid
Fumaric acid monomethyl ester
2-Furoic acid
3-Furoic acid
Furosemide

G

☆ ★ GABA
2-*O* -α-D-Galactopyranosyl-1-deoxynojirimycin
Galactosamine
Galacturonate 1-phosphate
Galacturonic acid
Gallic acid
☆ ★ GDP
GDP-fucose[1]
GDP-glucose
GDP-mannose
Geranyl diphosphate
Gibberellic acid
☆ ★ Gln
☆ ★ 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-Ornithine
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
Glucomoringin
☆ ★ Gluconic acid
Gluconolactone
Glucoraphanin
Glucosamine
★ Glucosamine 6-phosphate
Glucosamine 6-sulfuric acid
★ Glucosaminic acid
☆ ★ Glucose 1-phosphate
☆ ★ Glucose 6-phosphate
Glucurone
Glucuronic acid
trans -Glutaconic acid
Glutamic acid γ-methyl ester
γ-Glutamyl-*S* -Allylcysteine
★ Glutaric acid
Glutaryl CoA
Glutarylcarnitine
☆ ★ Glutathione (GSH)
☆ ★ Glutathione (GSSG)
Glutathione (GSH) monoisopropyl ester
N [1]-Glutathionylspermidine disulfide
☆ ★ Gly
★ Gly-Asp
★ Gly-Gly
Gly-Gly-Gly
Gly-Hyp
★ Gly-Leu
☆ ★ Glyceraldehyde 3-phosphate
★ Glyceric acid
Glycerol
Glycerol 2-phosphate
☆ ★ Glycerol 3-phosphate
★ Glycerophosphocholine
Glycerophosphorylethanolamine
Glycine anhydride
Glycocholic acid
☆ ★ Glycolic acid
★ *N* -Glycolylneuraminic acid
Glycylsarcosine
Glycyrrhetinic acid
☆ ★ Glyoxylic acid
Gly-Pro-Hyp
Gly-Thr-Trp-Tyr
☆ ★ GMP
GODIC
GOLA
GOLD
☆ ★ GTP
2-Guanidinobenzimidazole
★ 4-Guanidinobutyric acid
3-Guanidinopropionic acid
★ Guanidinosuccinic acid
★ Guanidoacetic acid
☆ ★ Guanine
☆ ★ Guanosine
Guanosine 5'-[γ-thio]triphosphate
Gulonolactone

H

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

I

★ IDP
☆ ★ Ile
Ile-Gly
Ile-Pro-Pro
Ile-Tyr
★ Imidazole-4-acetic acid
Imidazole-4-methanol
1*H* -Imidazole-4-propionic acid
★ Imidazolelactic acid
Iminodiacetic acid
☆ ★ IMP
Indole-3-acetaldehyde
Indole-3-acetaldoxime
★ Indole-3-acetamide
★ Indole-3-acetic acid
Indole-3-carboxylic acid
★ Indole-3-ethanol
★ Indole-3-glyoxylic acid
Indole-3-lactic acid
Indole-3-propionic acid
Indole-3-pyruvic acid
Indoleacrylic acid
3-Indolebutyric acid
★ 3-Indoxylsulfuric acid
☆ ★ Inosine
myo -Inositol 1-phosphate[6]
★ *myo* -Inositol 2-phosphate
myo -Inositol 3-phosphate[6]
3-Iodothyronamine
Isatin
★ Isethionic acid
★ Isoamylamine
Isoascorbic acid
★ Isobutylamine
Isobutyric acid
Isobutyryl CoA
Isobutyrylcarnitine
Isobutyrylglycine
☆ ★ Isocitric acid
Isoferulic acid
★ Isoglutamic acid
★ Isonicotinamide
★ Isonicotinic acid
N [6]-(*Δ* [2]-Isopentenyl)adenine
Isopentenyl diphosphate
Isopropanolamine
★ 2-Isopropylmalic acid
3-Isopropylmalic acid
Isovaleric acid
Isovalerylalanine
Isovalerylcarnitine
Isovalerylglycine
Isoxanthopterin
Itaconic acid
ITP

J

Jasmonic acid

K

Kinetin
Kojic acid
★ Kynurenic acid
★ Kynurenine

L

☆ ★ Lactic acid
N -Lactoylethanolamine

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ALA00WJ-03(25)

CE-MS アノテーションリスト 3/4

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ver.3.0a

S -Lactoylglutathione
N -Lactoylphenylalanine
Lauric acid
Lauroyl CoA
Lauroylcarnitine
Lenticin
☆ ★ Leu
Leu-Leu-Tyr
β-Leucine
Lipoamide
Lumazine
Lupulone
☆ ★ Lys
Lysinamide

M

Maleamic acid
★ Maleic acid
☆ ★ Malic acid
☆ ★ Malonyl CoA
Malonylcarnitine
Maltobionic acid
Maltosine
Mandelic acid
Mannosamine
★ Melatonin
3-Mercapto-2-oxopropanoate
3-Mercaptolactic acid
6-Mercaptopurine
Mesaconic acid
☆ ★ Met
Met-Val-Pro
Met-Val-Pro-Pro
Metanephrine
Metanilic acid
Methanesulfonic acid
★ Methionine sulfoxide
Methionine sulfoximine
5-Methoxy-*N* ,*N* -dimethyltryptamine
3-Methoxy-4-hydroxyphenylethyleneglycol
3-Methoxyanthranilic acid
5-Methoxyindoleacetic acid
o -Methoxyphenyl sulfate
p -Methoxyphenylacetic acid
5-Methoxytryptamine
★ 3-Methoxytyramine
3-Methoxytyrosine
Methyl aminolevulinate
15-Methyl prostaglandin $F_{2\alpha}$
Methyl sulfate
Methylcitric acid
N^6-Methyl-2'-deoxyadenosine
★ 5-Methyl-2'-deoxycytidine
1-Methyl-4-imidazoleacetic acid
4-Methyl-1,2,5-oxadiazol-3-amine
3-Methyl-2-oxovaleric acid[7]
4-Methyl-2-oxovaleric acid[7]
N^1-Methyl-4-pyridone-5-carboxamide
4-Methyl-5-thiazoleethanol
1-Methyladenine
★ 3-Methyladenine
N^6-Methyladenine
★ 1-Methyladenosine
N^6-Methyladenosine
3-Methyladipic acid
★ *N* -Methylalanine
3-(Methylamino)alanine
4-Methylaminobutyric acid
N -Methylaniline
★ *N* -Methylanthranilic acid
★ N^ω-Methylarginine
N -Methylaspartic acid
★ *threo* -β-Methylaspartic acid
DL-2-Methylbutyric acid
2-Methylbutyrylglycine
2-Methylcholine
3-Methylcrotonyl CoA
3-Methylcrotonylglycine
★ *S* -Methylcysteine
S -Methylcysteine-*S* -oxide
2'-*O* -Methylcytidine
3-Methylcytidine
5-Methylcytidine
★ 5-Methylcytosine
2-*C* -Methylerythritol 4-phosphate
5-Methylfuran-2-carboxylic acid
★ *N* -Methylglutamic acid
★ 2-Methylglutaric acid
S -Methylglutathione
★ Methylguanidine
3-Methylguanine
★ 7-Methylguanine
N^2-Methylguanine
N^1-Methylguanosine
1-Methylhistamine
3-Methylhistamine
1-Methylhistidine
3-Methylhistidine
1-Methylhydantoin
N^2-Methyllysine
★ N^6-Methyllysine
Methylmalonic acid
Methylmalonyl CoA[8]
S -Methylmethionine
★ 1-Methylnicotinamide
★ *N* -Methylnicotinamide
4-Methylpentanoic acid
N -Methylphenylethanolamine
N -Methylproline
★ *N* -Methylputrescine
4-Methylpyrazole
★ 2-Methylserine
★ *N* -Methylserotonin
Methylsuccinic acid
5-Methyltetrahydrofolic acid
2-Methylthiazolidine-4-carboxylic acid
4-Methylthio-2-oxobutyric acid
(Methylthio)acetic acid
3-(Methylthio)propionic acid
★ *N* -Methyltryptamine
★ *N* -Methyltryptophan
N -Methyltyramine
1-Methyluric acid
3-Methylxanthine
7-Methylxanthine
Metoprolol acid
★ Mevalolactone
Mevalonic acid
MG-H1
MG-H2
MG-H3
Mimosine
Minocycline
N -Monoacetylcystine
Monoethyl malonic acid
Monoethyl phosphate
Monomethyl glutaric acid
Morpholine
★ Mucic acid
cis,cis -Muconic acid
Muramic acid
Myosmine
Myristic acid
Myristoleic acid

N

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

O

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

P

Palmatine
Palmitoylcarnitine
Pantoic acid
★ Pantothenic acid
Pantothenol
★ Paraxanthine
★ Pelargonic acid
Penicillamine
Pentamidine
Pentosidine
★ Perillic acid
☆ ★ Phe
★ Phenaceturic acid
o -Phenanthroline
Phenol
Phenol sulphate
p -Phenolsulfonic acid
★ 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
Phenylpropionylglycine
Phenylpyruvic acid
Phloretin
Phloroglucinol
★ Phosphocreatine
☆ ★ Phosphoenolpyruvic acid
☆ ★ 6-Phosphogluconic acid
☆ ★ 2-Phosphoglyceric acid
☆ ★ 3-Phosphoglyceric acid
Phosphoglycolic acid
Phosphomevalonic acid
Phosphonoacetic acid
★ Phosphorylcholine
★ *O* -Phosphoserine
Phytic acid
Picolinamide
★ Picolinic acid
Pilocarpine
★ Pimelic acid
★ Pipecolic acid
★ Piperidine
Porphobilinogen
ppGpp
☆ ★ Pro
Pro-Hyp
Procaine
1,2,3-Propanetricarboxylic acid
★ Propionic acid
Propionyl CoA
N -Propionylalanine
Propionylcarnitine
Propionylglycine
Propylthiouracil
Prostaglandin E_2
Prostaglandin $F_{2\alpha}$
Protocatechuic acid
☆ ★ PRPP
Pseudoephedrine
Pseudouridine
Psychosine
★ Pterin
Purine
Purine riboside
☆ ★ Putrescine
Pyrazinamide
Pyrazinoic acid
Pyrazole
Pyridine
Pyridine-2-carboxylic acid butyl ester
★ Pyridoxal
Pyridoxal 5-phosphate
★ Pyridoxamine
Pyridoxamine 5'-phosphate
★ 4-Pyridoxic acid
★ Pyridoxine
Pyridoxol 5'-phosphate
Pyrimidine
Pyrocatechol sulfate
Pyrogallol
Pyroglutamine
Pyroglutamylhistidylglycine
Pyrophosphate
Pyrraline
Pyrrole-2-carboxylic acid
2,5-Pyrroledione
Pyrroloquinoline quinone
☆ ★ Pyruvic acid

Q

★ Quinic acid
Quinine
Quinoline
2-Quinolinecarboxylic acid
★ Quinolinic acid

R

Retinoic acid
★ Riboflavin
Ribose 1-phosphate
☆ ★ Ribose 5-phosphate
Ribulose 1,5-diphosphate
☆ ★ Ribulose 5-phosphate

S

Saccharopine
Salsolinol
☆ ★ Sarcosine
SDMA
☆ ★ Sedoheptulose 7-phosphate
Selenocystine
Selenomethionine
Semicarbazide
Sepiapterin
☆ ★ Ser
★ Ser-Glu
★ Serotonin
Shikimate 3-phosphate
★ Shikimic acid
Sinapic acid
α-Solanine
★ Sorbitol 6-phosphate
☆ ★ Spermidine
☆ ★ Spermine
Streptomycin sulfate
Subaphylline
★ Suberic acid
☆ ★ Succinic acid
Succinic semialdehyde
Succinyl CoA[8]
N -Succinyl-5-aminoimidazole-4-carboxamide ribose 5'-phosphate
Succinylacetone
Succinyladenosine
N^α-Succinylarginine
Succinylcarnitine
Succinylcholine
O -Succinylhomoserine
N^2-Succinylornithine
Sucrose 6'-phosphate
Sulfanilic acid
S -Sulfocysteine
3-Sulfopropanediol
5-Sulfosalicylic acid
O -Sulfoserine
Sulfotyrosine
Syringic acid

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CE-MS アノテーションリスト 4/4

☆は「ターゲット濃度計算（110物質定量）オプション」の対象となる物質を表します。

ver.3.0a

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
6,8-Thioctic acid
Thiodiglycolic acid
2-Thiopheneacetic acid
Thiourea
☆ ★ Thr
★ Thr-Asp
Thr-Hyp
★ Threonic acid
allo -Threonine
☆ ★ Thymidine
☆ ★ Thymine
Tiglic acid
Tiglylcarnitine
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
Trigalacturonic acid
★ Trigonelline
★ Trimethylamine
★ Trimethylamine *N* -oxide
4-Trimethylammoniobutanal
N^6,N^6,N^6-Trimethyllysine
Trimethylsulfonium
Tropic acid
Tropine
Tropinone
☆ ★ Trp
Tryptamine
Tryptophanamide
☆ ★ Tyr
★ β-Tyr
★ Tyr-Arg
★ Tyr-Glu
☆ ★ Tyramine

U

☆ ★ UDP
UDP-*N* -acetylgalactosamine
UDP-*N* -acetylglucosamine
UDP-galactose[9]
UDP-glucose[9]
★ UDP-glucuronic acid
☆ ★ UMP
3'-UMP
Undecanedioic acid
Undecanoic acid
☆ ★ Uracil
★ Urea
Ureidoglycolic acid
3-Ureidoisobutyric acid
★ 3-Ureidopropionic acid
Uric acid
☆ ★ Uridine
★ Urocanic acid
Ursolic acid
☆ ★ UTP

V

☆ ★ Val
Val-Pro-Pro
★ Valeric acid
N -Valerylglycine
★ Vanillic acid
Vanillylmandelic acid
Veratric acid

X

★ Xanthine
★ Xanthosine
★ Xanthurenic acid
★ XMP
XTP
Xylulose 5-phosphate

Z

★ *trans*- Zeatin
trans -Zeatin riboside

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
N^{α} -Benoylarginine ethylester
Benzamidine
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
2,4-Dichlorobenzoic acid
2,4-Dichlorophenoxyacetic acid
Dichlorprop
Diclofenac
3,5-Diiodotyrosine
2,4-Dimethylaniline[5]
2,6-Dimethylaniline[5]
3,5-Dinitrosalicylic acid
Diphenylcarbazide
Disulfiram
Eflornithine
p -Fluoroaniline
o -Fluorobenzoic acid
m -Fluorobenzoic acid
p -Fluorobenzoic acid
Gramine
Harman
Hexazinone
Homotaurine
Hydroxyatrazine
2-Hydroxypyridine
Ibotenic acid
Ibuprofen
3-Indoleacetonitrile
3-Iodotyrosine
Ismelin
Isoniazid
Isoproterenol
Isoquinoline
Kainic acid
Kanamycin A
Leupeptin
Lidocaine
Loperamide
Melamine
Mesalamine
Metamitron
Metaraminol
Methotrimeprazine
Methoxamine
1-Methyl-4-phenyl-1,2,3,6-tetrahydropyridine
★ 1-Methyl-2-pyrrolidone
4,4'-Methylene bis(*o* -chloroaniline)
Methysergide
Muscimol
Nalidixic acid
Neomycin B
Neostigmine
Oleandomycin
Oxypurinol
Pargyline
Paromomycin
Phenazopyridine
Phentolamine
Phenylephrine
Phosphoramidon
Phthalic acid
Piperazine
Pralidoxime
Prazosin
Propiconazole
Propranolol
Pseudopelletierine
Pyridine-3-methanol
Quisqualic acid
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
Tranexamic acid
Triadimefon
2,4,5-Trichlorophenoxyacetic acid
Trientine
Triethanolamine
Trifluoperazine
3,3',5-Triiodothyronine
Trimethoprim
★ Tyrosine methyl ester
Verapamil
Xanthopterin

右肩に数字が付記されている物質につきましては、同じ数字が付記された物質同士の判別がなされません。それらの物質の報告値は合算値となります。

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