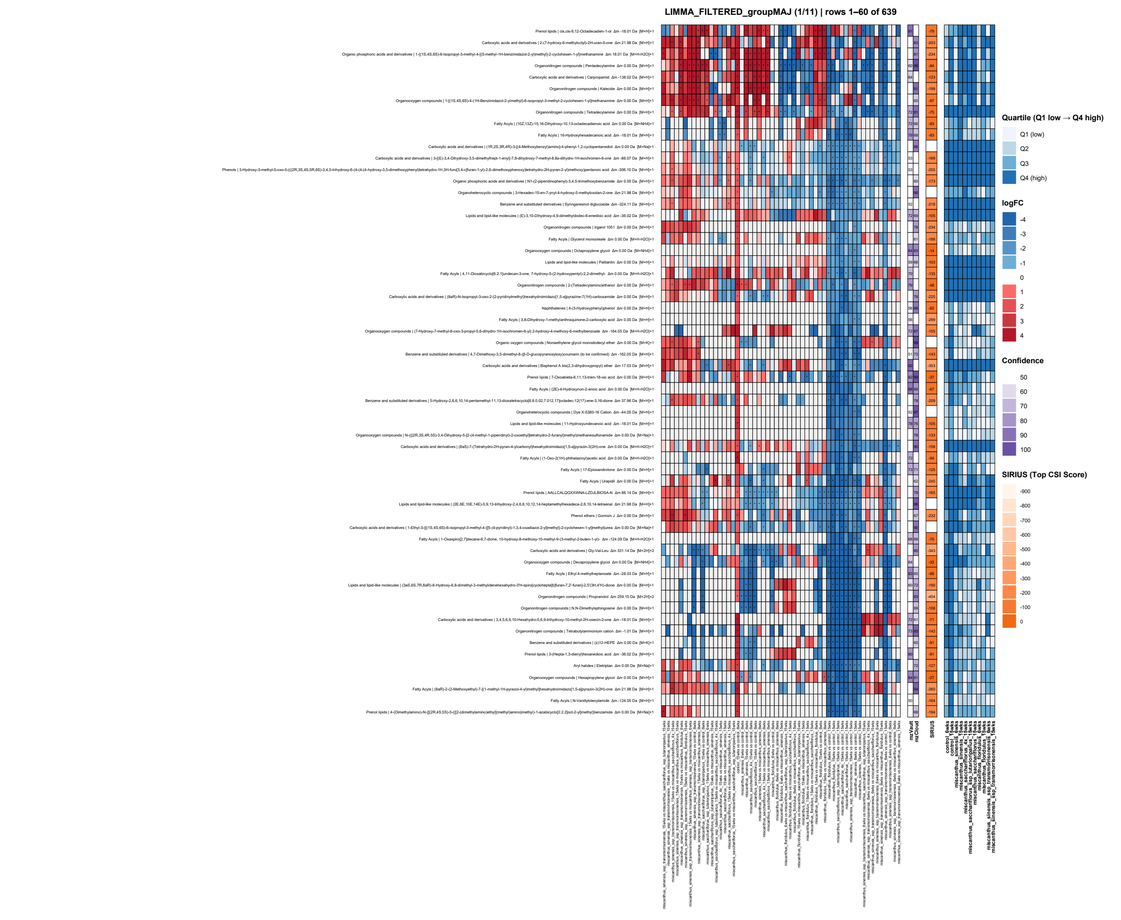
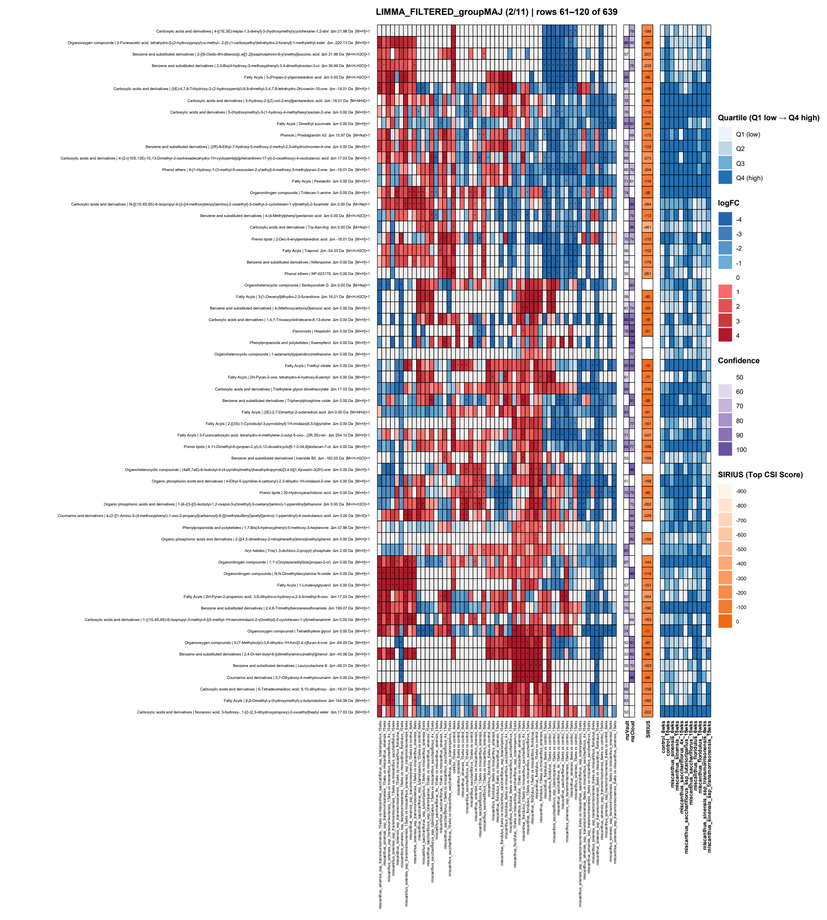
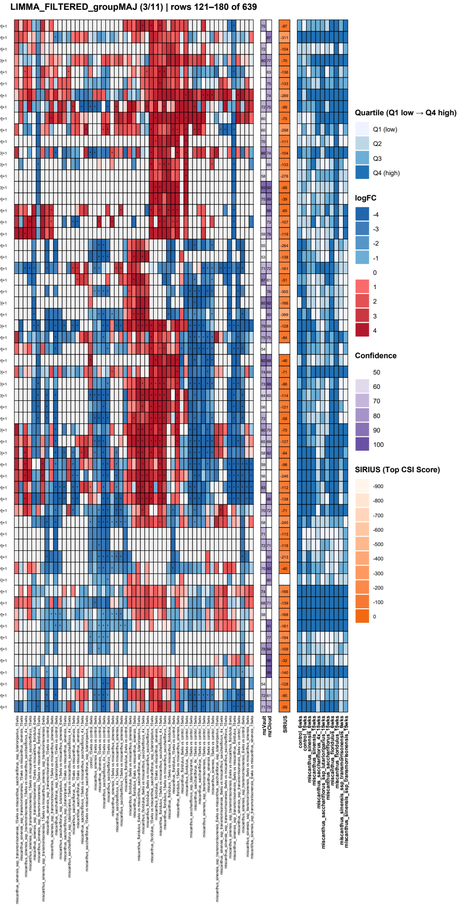
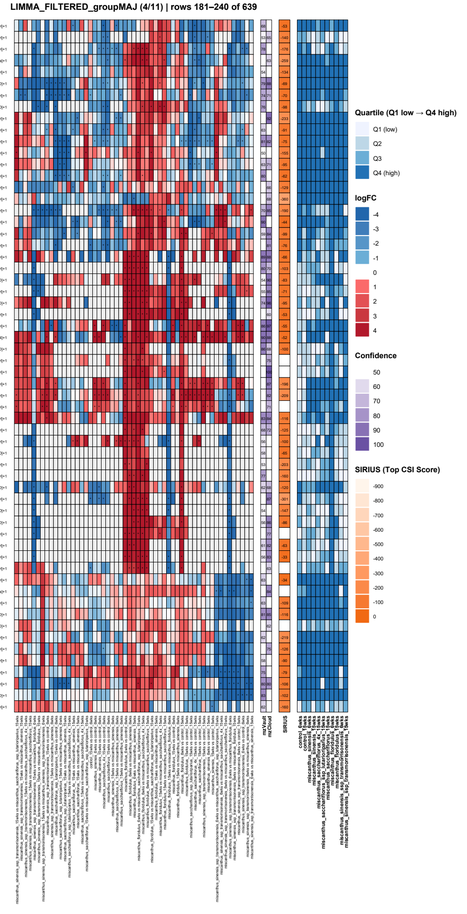
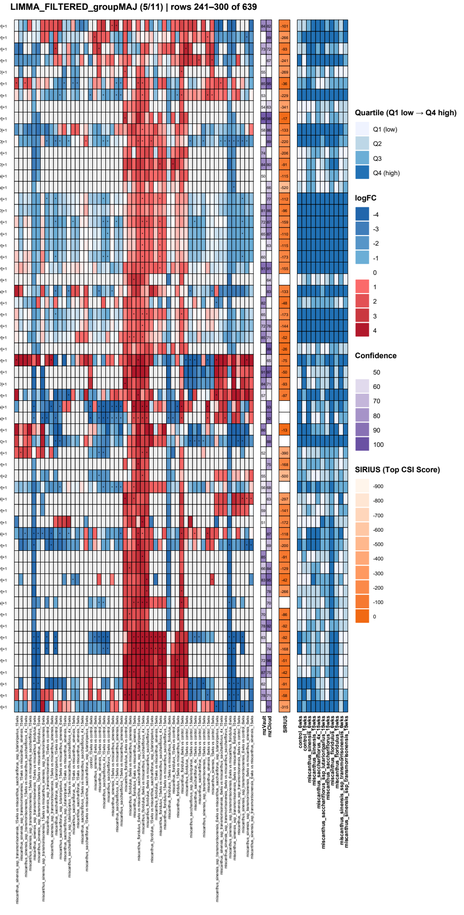
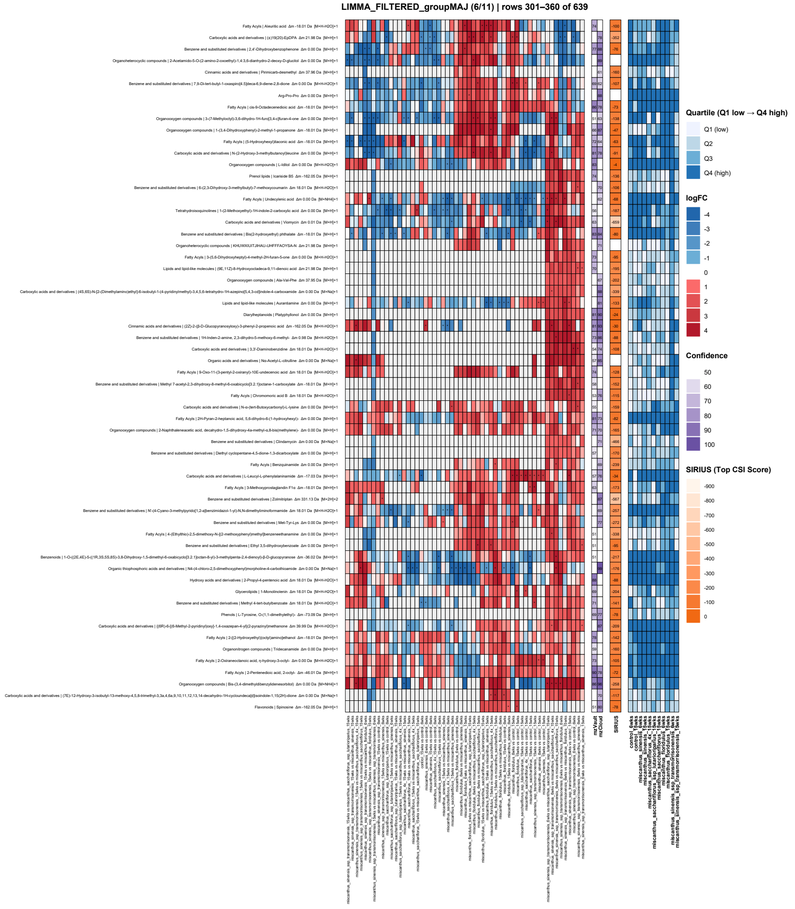

LIMMA_FILTERED_groupMAJ (1/11) | rows 1–60 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
pvalue
FDR
SIRIUS

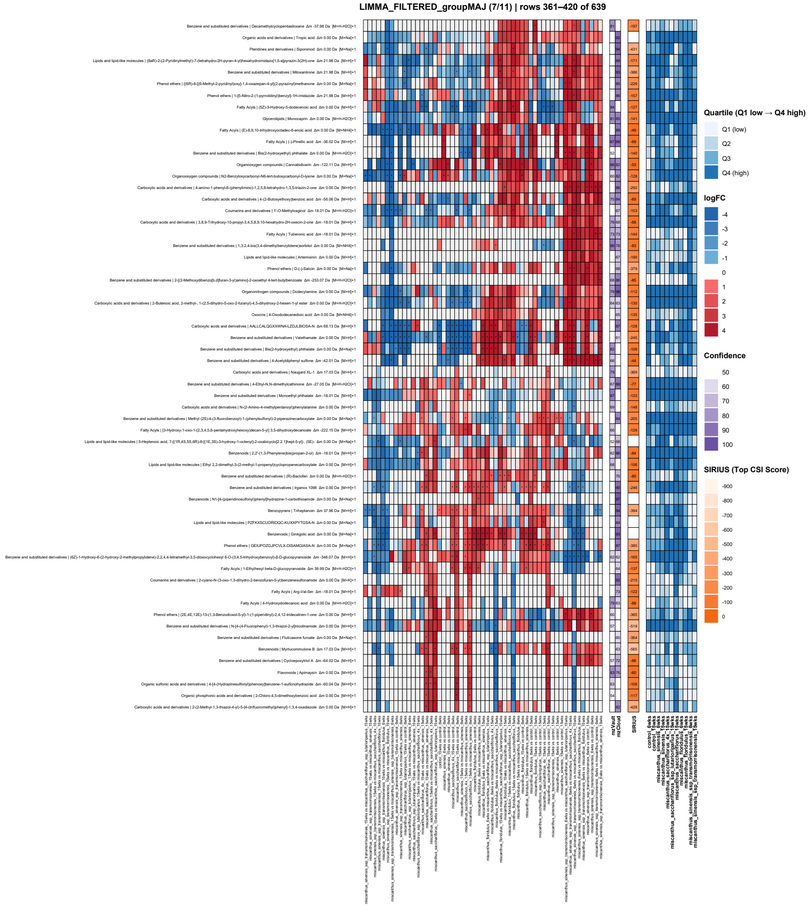

LIMMA_FILTERED_groupMAJ (2/11) | rows 61–120 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
pHSCDM
SIRIUS

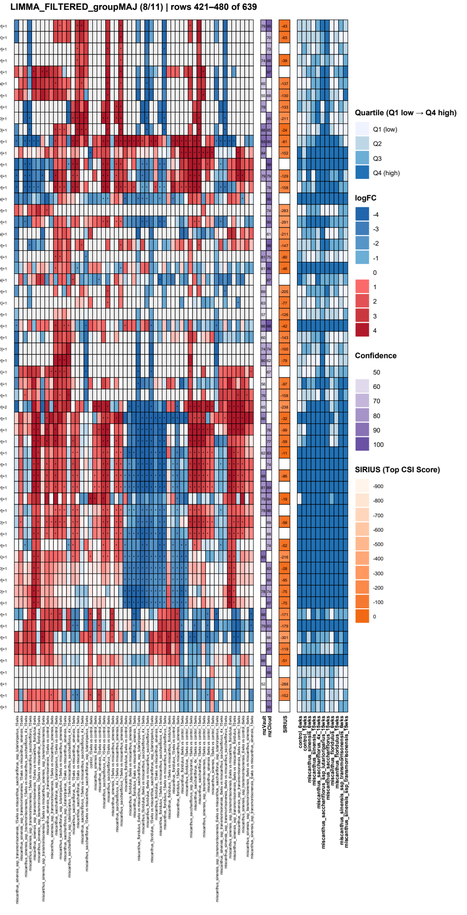

LIMMA_FILTERED_groupMAJ (3/11) | rows 121–180 of 639
Benzene and substituted derivatives | Benzyldimethyldodecylammonium cation Δm -1.01 Da [M+H]+
Fatty Acyls | Tegaserod Δm 0.00 Da [M+H]+
Fatty Acyls | NF-κB DSMB Δm -192.00 Da [M+H]+
Cinnamic acids and derivatives | 10-Hydroxy-6-methyl-3,7,12-trioxatricyclo[8.1.0.02,4]dodecan-8-one Δm -36.02 Da [M+H-H2O]+
Carboxylic acids and derivatives | Hirdatosaagatriazinone Δm 0.00 Da [M+H]+
Fatty Acyls | Monosaprin Δm -18.01 Da [M+H]+
Organooxygen compounds | [(3R,4S,6R)-6-[[8-(Hydroxymethyl)-1H-1,2,3-triazol-1-yl]methyl]-1-azabicyclo[2.2.2]oct-3-yl]β-morpholinylmethanone Δm 0.00 Da [M+H]+
Phenol ethers | Propanoic acid, 2-hydroxy-3-[(1-(4-methoxy-6-methyl-2-oxo-2H-pyran-3-yl)ethyl)thio] Δm -122.00 Da [M+H]+
Pyrans | Mirabotate A Δm -18.01 Da [M+H]+
Fatty Acyls | Benzenethiamine, 3,5-dimethoxy-α-methyl-4-propoxy- Δm 0.00 Da [M+H]+
Prenol lipids | (5Z)-3-Hydroxy-5-dodecenoic acid Δm -18.01 Da [M+H]+
Fatty Acyls | 3-(1-Hydroxyhexyl)-5-(hydroxymethyl)oxolan-2-one Δm 0.00 Da [M+H-H2O]+
Fatty Acyls | 1,16-Hexadecanediolic acid Δm 0.00 Da [M+H-H2O]+
Carboxylic acids and derivatives | Octyl α-ketoglutarate Δm 17.03 Da [M+H]+
Prenol lipids | [(3R,8aS)-Decahydro-2-naphthalenyl Δm 0.00 Da [M+H-H2O]+
Benzene and substituted derivatives | 3,4-Dihydroquinolin-1(2H)-yl]-β-propoxyphenylmethanone Δm -133.09 Da [M+H]+
Prenol lipids | Perfleximine Δm 0.00 Da [M+H]+
Prenol lipids | 1-[-(15,45,85)-6-Isopropyl-3-methyl-4-[(4-methyl-1H-benzimidazol-2-yl)methyl]-2-cyclohexen-1-yl]-N,N-dimethylmethanamine Δm 0.00 Da [M+H]+
Prenol lipids | Bicyclo[3.1.0]oxiba-6-ene,2,8-dol, 3-(hydroxymethyl)-5,6,10-trimethyl- Δm -36.02 Da [M+H]+
Fatty Acyls | 3a,2-Aminoethylthio,2-methylpropione acid Δm 163.07 Da [M+H]+
Fatty Acyls | 8-Nonenoic acid, 3-hydroxy-9-(4-methoxy-3-methyl-2-oxo-2H-pyran-6-yl)- Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | N-(4-tert-Butoxyphenyl)acetamide Δm 0.00 Da [M+H]+
Prenol lipids | 3,7,11-Dimethyl-6-ene-1,2,3-trol Δm -18.01 Da [M+H]+
Organooxygen compounds | Gln-Asp-Arg Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Methyl 2,4,6-tri-tert-butylbenzoate Δm -36.05 Da [M+H-H2O]+
Carboxylic acids and derivatives | 5-Acetoxy-2-(hydroxymethyl)-6-isopropyl-2-oxo-3-cyclohexen-1,yl 3-methylpentanoate Δm 21.98 Da [M+H]+
Organooxygen compounds | 10-Hydroxy-6-methyl-3,7,12-trioxatricyclo[8.1.0.02,4]dodecan-8-one Δm -18.01 Da [M+H-H2O]+
Fatty Acyls | 2-Decylmalonic acid Δm 0.00 Da [M+H]+
Organooxygen compounds | Glycopeptin C Δm 0.00 Da [M+H]+
Prenol lipids | γ-Nonalactone Δm -18.01 Da [M+H]+
Fatty Acyls | 10-Oxoundecanoic acid Δm 16.01 Da [M+H-H2O]+
Benzene and substituted derivatives | N,N-Diethylpentylone Δm -85.09 Da [M+H-H2O]+
Benzenoids | 3-[(1E,3E)-Hepta-1,3-dienyl]pentanedioic acid Δm -18.01 Da [M+H-H2O]+
Lipids and lipid-like molecules | 2,4-Dideoxy-2-(7-octen-1-yl)pentanoic acid Δm -18.01 Da [M+H]+
Fatty Acyls | 2-Ethyl-4-methylpentanoic acid Δm 0.00 Da [M+H]+
Hydroxy acids and derivatives | 2H-Pyran-2-one, tetrahydro-4-hydroxy-6-pentyl- Δm 18.01 Da [M+H-H2O]+
Benzene and substituted derivatives | Citrinin Δm 0.00 Da [M+H]+
Hydroxy acids and derivatives | 2-Oct-7-enylpentanedioic acid Δm 18.01 Da [M+H-H2O]+
Phenol ethers | 6H-2-Benzoxypyran-3-carboxylic acid, 7-ethyl-7,8-dihydro-8-hydroxy-6,7-dimethyl-6-oxo- Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 2-Aminoethyl-(1,8-dimethylimidazol)-2-ylpiperazate-4-yl]amine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Cocamidopropyl betaine Δm 0.00 Da [M+H]+
Fatty Acyls | Monoolatriam Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | Dodecanoic acid, 12-[(cyclohexylamino)carbonyl]amino] Δm -120.08 Da [M+H]+
Benzene and substituted derivatives | 1,4-Dibutoxy-2-nitrobenzene Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Tuberbilide Δm -36.02 Da [M+H]+
Carboxylic acids and derivatives | Propanoic acid, 2-hydroxy-3-[(1-(4-methoxy-6-methyl-2-oxo-2H-pyran-5-yl)ethyl)thio] Δm -122.00 Da [M+H]+
Organooxygen compounds | Oxyneroid Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 3-Benzylheptylmyoinositol-[1,2-dipyrophosphate]-1,4-diene Δm 0.00 Da [M+H]+
Organic oxygen compounds | Poly THF x7 Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 7,8-Dihydroxy-3,5,7-trimethyl-8,8a-dihydro-1H-isochromen-6-one Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | 2-(5-Decenyl)glutaconic acid Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 2-[(3aR,4S,7R,7aS)-1,3-Dioxoheksahydro-1H-4,7-methaneisoindol-2(3H)-yl]propanoic acid Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Cyclobexylpiprox Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | (-)-Arachidonoyl ethanolamine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Leu-Leu Δm 0.00 Da [M+H]+
Organonitrogen compounds | N-(4-Fluorophenyl)adamantane-1-carboxamide Δm 0.00 Da [M+H]+
Oxazinanes | N-Octyl-2-pyrrolidone Δm 0.00 Da [M+H]+
Fatty Acyls | trans-Vaccenic acid Δm 0.00 Da [M+H]+
Organooxygen compounds | (3aR,4R,7S,7aS)-3a,4,7,7a-Tetrahydro-4,7-methanoisobenzofuran-1,3-dione Δm -27.99 Da [M+H]+
Organooxygen compounds | Pentaoxyethyl glycol Δm 0.00 Da [M+H]+
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0


LIMMA_FILTERED_groupMAJ (4/11) | rows 181–240 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
pmDZNet
CSI:Net
SIRIUS


LIMMA_FILTERED_groupMAJ (5/11) | rows 241–300 of 639
Phenol ethers | O-Benzyl-L-tyrosine methyl ester Δm -60.02 Da [M+H]+
Piperidines | Bufadine A Δm 0.00 Da [M+H]+
Fatty Acyls | 8-(3-Octyl-2-oxiranyl)octanoic acid Δm -18.01 Da [M+H]+
Fatty Acyls | Anandamide (AEA) Δm 0.01 Da [M+H]+
Fatty Acyls | Leukotriene B4 ethanolamide Δm 0.00 Da [M+H-H2O]+
Benzene and substituted derivatives | Proscillorari Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | Naphtho[1,2-c]furan-1(3H)-one, 3a,5a,6,7,8,9,9a,9b-octahydro-6-hydroxy-3,7,9b-trimethyl-3-(1-vinylbutyl)- Δm 0.00 Da [M+H]+
Prenol lipids | N-(8-APDB) Fertistyl Δm 21.98 Da [M+H]+
Flavonoids | (1S)-1,5-Anhydro-2-O-(6-deoxy-α-L-mannopyranosyl)-1-(5,7-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-8-yl)-D-glucitol Δm -146.06 Da [M+H]+
Phenol ethers | Nardosinon Δm -58.04 Da [M+H-H2O]+
Phenols | Ginkgolic acid Δm 58.99 Da [M+H-H2O]+
Glycerophospholipids | Ophiobolin A Δm 21.98 Da [M+H]+
Fatty Acyls | 9,12-Dihydroxy-10-dodecenoic acid Δm 0.00 Da [M+H-H2O]+
Phenols | 5-Hexenoic acid, 4-hydroxy-4-methyl-6-(octahydro-1,7,8-trimethyl-3-oxo-1H-cyclopenta[c]pyran-5-yl)- Δm -60.02 Da [M+Na]+
Organooxygen compounds | Hemycloside Δm 0.00 Da [M+Na]+
Organooxygen compounds | Decoyinosinalone Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | 1,2-Dehydro-α-cupaenone Δm -38.05 Da [M+H-H2O]+
Benzene and substituted derivatives | NP-024019 Δm -162.05 Da [M+H]+
Phenols | 3-Allyl-4-ethoxy-5-methoxybenzaldehyde Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | ABRILZQRRNNMRY-UHFFFAOYSA-N Δm -18.01 Da [M+H]+
Lipids and lipid-like molecules | 1-Hepladecene-4,6-dyne-3,8,9,10-tetrol Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 3,5-Di-tert-butyl-4-hydroxyacetophenone Δm 18.01 Da [2M+K-CH]+
Lipids and lipid-like molecules | (6E,10E)-3-(methoxymethyl)-5,10-dimethyl-3a,4,5,8,9,11a-hexahydro-3H-cyclodeca[β]furan-2-one Δm 21.98 Da [M+H]+
Thiosthers | [(4E)-7-acetyloxy-8-hydroxy-2-methyl-10-oxo-2,3,6,7,8,9-hexahydrooxecin-3-yl] (E)-but-2-enoate Δm -40.03 Da [M+Na]+
Glycerolipids | Triproxydione glycol methyl ether Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Prosulfire Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | D-Tyrosine tert-butyl ester Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Ethanone, 1(2-(1-hydroxy-1-methylethyl)phenyl) Δm 0.00 Da [M+H]+
Flavonoids | Isoscoparin Δm 0.00 Da [M+H]+
Organooxygen compounds | PPG-n6 Δm 0.00 Da [M+H]+
Prenol lipids | Farnizhne Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | 2-Furanacetic acid, tetrahydro-5-(2-hydroxypropyl)-α-methyl-, 2-(5-(1-carboxyethyl)tetrahydro-2-furanyl)-1-methylethyl ester Δm -202.12 Da [M+H-H2O]+
Organooxygen compounds | μ-Methoxylotaderol Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | UFEZCKBFRMLAV-DBDKQAFGSA-N Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | DKEHGZXVPCCHN-OYKNDICUSA-N Δm 0.00 Da [M+Na]+
Organic metal salts | Tetradecamethylcyclohexylsiloxane Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | Spiroscale B Δm 0.00 Da [M+H]+
Organooxygen compounds | N-1,4-Dihydroxy-4-methylpentan-2-yl)-3-hydroxy-5-oxo-8-phenylhexanamide Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | Meplazine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | [2-[2-(2,2,2-Trifluoroethoxy)phenoxy]ethyl-1-amine Δm 235.08 Da [M+2H]+2
Organic phosphoric acids and derivatives | Tris(2-chloroethyl) phosphate Δm 0.00 Da [M+H]+
Fatty Acyls | Glycocholic acid Δm -111.02 Da [M+NH4]+
Benzopyrans | 8-(Glucopyr-3,4',5,7-tetrahydroxyflavonone Δm -120.06 Da [M+H]+
Benzene and substituted derivatives | 1H,3H-Furo[3,4-c]furan-1-one, 6-heptyl-4,6-dihydro- Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | (+)- (5S)-EET Ethanolamide Δm -35.04 Da [M+NH4]+
Organooxygen compounds | Imazamethabenz-methyl Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | N-Benzyl-N,N-dimethyl-1-tetradecanaminium cation Δm -1.01 Da [M+H]+
Benzenoids | Sembyosides C Δm 0.00 Da [M+H]+
Cinnamic acids and derivatives | L-Tyrosine, O,L-1-dimethylethyl- Δm -73.09 Da [M+H]+
Carboxylic acids and derivatives | Ile-Tip-Lys Δm 0.00 Da [M+H]+
Organic acids and derivatives | N-(2-Furylmethyl)-3-[(25,5a5,8a5)-1-methyl-9-(4-methylbenzyl)-5-oxodecahydropyrimido[3,4-E][1,4]diazepin-2-yl]propanamide Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | Benzyldimethylstearylammonium cation Δm -29.04 Da [M+H]+
Fatty Acyls | (11E,15Z)-9,10,13-Trihydroxyoctadeca-11,15-dienoic acid Δm -36.02 Da [M+H]+
Benzene and substituted derivatives | (4'-Furoyl)-7-hydroxy[3-a-carboxylic acid Δm 0.00 Da [M+H]+
Phenol ethers | 1-[5-Nitro-2-(1-pyrrolidinyl)benzyl]-5-1H-imidazole Δm 21.98 Da [M+H]+
Azoles | Triuvon PED Δm 0.00 Da [M+H]+
Prenol lipids | (2S)-5(1-1-Hydroxy-1-methylethyl)-2-methyl-2-(cyclohexen-1-one Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | 7-Oxabicyclo[2.2.1]hept-5-ene-2-butanoic acid, 3,3-dihydroxy-β,5-dimethyl- Δm -18.01 Da [M+H]+
Organooxygen compounds | 46-S-Tocopherol Δm -286.30 Da [M+H]+
Imidazopyrimidines | Pro-Ser-Arg Δm -18.01 Da [M+H]+
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0


LIMMA_FILTERED_groupMAJ (6/11) | rows 301–360 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
Fatty Acyls | Ricinoleic acid Δm -18.01 Da [M+H-H2O]+
Carboxylic acids and derivatives | [c(19)(20)(E)]DFA Δm 21.98 Da [M+H]+
Benzene and substituted derivatives | 2,4'-Dihydroxybenzophenone Δm 0.00 Da [M+H]+
Organoheterocyclic compounds | 2-Acetamido-D-O-(2-amino-2-oxoethyl)-1,4,3,6-dianhydro-2-deoxy-D-glucitol Δm 0.00 Da [M+H]+
Cinnamic acids and derivatives | Pimincarb-desmethyl Δm 37.96 Da [M+H]+
Benzene and substituted derivatives | 7-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione Δm 0.00 Da [M+H-H2O]+
Arg-Pro-Pro Δm 0.00 Da [M+H]+
Fatty Acyls | cis-9-Octadecenedioic acid Δm -18.01 Da [M+H]+
Organooxygen compounds | 3-(7-Methylhydq[3,5,6-dihydro-1H-furo[3,4-c]hexa]-4-one Δm 0.00 Da [M+H]+
Organooxygen compounds | 1-(3,4-Dihydroxyphenyl)-2-methyl-1-propanone Δm -18.01 Da [M+H]+
Fatty Acyls | (5-Hydroxyhexyl)tiacorsi acid Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | N-(2-Hydroxy-3-methylbutanoyl)leucine Δm 0.00 Da [M+H]+
Organooxygen compounds | L-Iditol Δm 0.00 Da [M+H-H2O]+
Prenol lipids | nardosin B3 Δm -162.05 Da [M+H]+
Benzene and substituted derivatives | 6(-)2-Dihydroxy-3-methylbutyl-7-methoxycoumarin Δm -18.01 Da [M+H-H2O]+
Fatty Acyls | Undecylenic acid Δm 0.00 Da [M+NH4]+
Tetrahydroisoquinolines | 1-(2-Methoxyethyl)-1H-indole-2-carboxylic acid Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Vismycin Δm 0.01 Da [M+H]+
Benzene and substituted derivatives | Bis(2-hydroxyethyl) phthalate Δm -18.01 Da [M+H]+
Organoheterocyclic compounds | HIVUWNXJFJNNLLJ-MFFFXOYSA-N Δm 21.98 Da [M+H]+
Fatty Acyls | 3-(5,6-Dihydroxyhexyl)-5-methyl-2H-furan-5-one Δm 0.00 Da [M+H-H2O]+
Lipids and lipid-like molecules | DE,11Z,6-Hydroxyoctadeca-9,11-dienoic acid Δm 21.98 Da [M+H]+
Organooxygen compounds | Ala-Val-Phe Δm 37.96 Da [M+H]+
Carboxylic acids and derivatives | (4S,8S)-N-[2-(Dimethylamino)ethyl]-6-iodo-pyl-1-(4-pyridinylmethyl)-5,6,7,8,9-tetrahydro-1H-azepino[4,5,4,3-cd]indole-4-carboxamide Δm 0.00 Da [M+Na]+
Lipids and lipid-like molecules | Aurantiamine Δm 0.00 Da [M+H]+
Diarylheptanoids | Platyphylloyl Δm 0.00 Da [M+H]+
Cinnamic acids and derivatives | (2Z)-2-[6-O-Glucopyranosyloxy]-5-phenyl-2-propenoic acid Δm -162.05 Da [M+H-H2O]+
Benzene and substituted derivatives | 1H-Inden-2-amine, 2,3-dihydro-5-methoxy-6-methyl- Δm 0.98 Da [M+H]+
Carboxylic acids and derivatives | 3,2'-Oxaminobenzoline Δm 18.01 Da [M+H-H2O]+
Organic acids and derivatives | Nor-Acetyl-L-citrulline Δm 0.00 Da [M+Na]+
Fatty Acyls | 9-Oxo-11-(2-penta-2-ioxetane)-10E-undecenoic acid Δm 18.01 Da [M+H-H2O]+
Benzene and substituted derivatives | Methyl 7-euryl-2,3-dihydroxy-8-methyl-6-oxabicyclo[3.2.1]octane-1-carboxylate Δm -18.01 Da [M+H]+
Fatty Acyls | Dinomomoric acid B Δm 18.01 Da [M+H-H2O]+
Carboxylic acids and derivatives | N-α-(tert-Butoxycarbonyl)-L-lysine Δm 0.00 Da [M+H]+
Fatty Acyls | 2H-Pyran-2-heptanoic acid, 5,6-dihydro-6-(1-hydroxyhexyl)- Δm 0.00 Da [M+H]+
Organooxygen compounds | 2-Naphthaleneacetic acid, decahydro-1,5-dihydroxy-4a-methyl-α,8-bis(methylene)- Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Chlorbenzyn Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | Diethyl cyclopentane-4,5-dione-1,5-dicarboxylate Δm 0.00 Da [M+H]+
Fatty Acyls | Benzylsuramide Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | L-Leucyl-L-phenylalaninamide Δm -17.03 Da [M+H]+
Fatty Acyls | 3-Methoxyprostaglandin F1α Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | Zolmitriptan Δm 331.13 Da [M+2H]+2
Benzene and substituted derivatives | N'-(4-Cyano-3-methylpyridyl)-2-(p)tetrahydro-1-yl)-N,N-dimethylimidoformamide Δm 18.01 Da [M+H-H2O]+
Benzene and substituted derivatives | Met-Tyr-Lys Δm 0.00 Da [M+H]+
Fatty Acyls | 4-[E]Hydroxy-2,5-dimethoxy-N-[2-methoxyphenyl]methyl]benzoxeethanamine Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Ethyl 3,5-dihydroxybenzoate Δm 0.00 Da [M+H]+
Benzenoids | 1-O-α-[(3E,4E)-5-O-[R,3S,6S,8S]-3,8-Dihydroxy-1,5-dimethyl-6-oxabicyclo[3.2.1]octen-8-yl]-3-methylpentie-2,4-dienoyl]-β-D-glucopyranose Δm -36.02 Da [M+H]+
Organic thiophosphonic acids and derivatives | N4-(6-chloro-2,5-dimethoxyphenyl)methylidene-4-sulfolthiamide Δm 0.00 Da [M+Na]+
Hydroxy acids and derivatives | 2-Propyl-4-pentenoic acid Δm 18.01 Da [M+H-H2O]+
Glycerolipids | 1-Monolinolenin Δm 18.01 Da [M+H-H2O]+
Benzene and substituted derivatives | Methyl 4-tert-butylbenzoate Δm 18.01 Da [M+H-H2O]+
Phenols | L-Tyrosine, O,O,1-dimethylsilyl- Δm -73.08 Da [M+H]+
Carboxylic acids and derivatives | [DR]-6-[(8-Methyl-2-pyridinyl)oxy]-1,4-oxazepan-4-yl]2-pyrazolyl]methanone Δm 36.98 Da [M+H-H2O]+
Fatty Acyls | 2-[(2-Hydroxyethyl)oxy]propyl]methanol Δm -18.01 Da [M+H]+
Organonitrogen compounds | Tridecanamide Δm 0.00 Da [M+H]+
Fatty Acyls | 2-Octanecedarsoic acid, α-hydroxy-3-octyl- Δm 0.00 Da [M+H-H2O]+
Fatty Acyls | 2-Pentenedioic acid, 2-octyl- Δm -46.01 Da [M+H]+
Organooxygen compounds | Bis-(3,4-dimethylbiliverdyldeuteroporfirin) Δm 0.00 Da [M+NH4]+
Carboxylic acids and derivatives | (7E)-12-Hydroxy-3-iodoyl-13-methoxy-4,5,8-trimethyl-3,3a,4,8a,9,10,11,12,13,14-decahydro-1H-cyclooctadeca[d]pyrazolidin-1,10(2H)-dione Δm 0.00 Da [M+Na]+
Flavonoids | Spinosine Δm -162.05 Da [M+H]+
pmol/mg
dry tissue
stage
Tissue_Homogenate_Liver_Homogenate_Liver_Homogenate_Liver


LIMMA_FILTERED_groupMAJ (7/11) | rows 361–420 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0
pmzCHar
SIRIUS
Benzene and substituted derivatives | Decamethylcyclopentasiloxane Δm -37.96 Da [M+H+NQ]+
Organic acids and derivatives | Tropic acid Δm 0.00 Da [M+Na]+
Pteridines and derivatives | Sepiapterin Δm 0.00 Da [M+Na]+
Lipids and lipid-like molecules | (8aR)-2-(2-Pyridinylmethyl)-7,-Dehydrohis-2H-pyran-4-yl)hexahydrohimbiskol(1,5-dg)oxazin-3(2H)-one Δm -21.98 Da [M+H]+
Benzene and substituted derivatives | Mibisantrone Δm -21.98 Da [M+H]+
Phenol ethers | (6R)-6-[(8-Methyl-2-pyridinyl)oxy]-1,4-oxazepan-6-yl]-(2-pyrazinyl)methanone Δm 0.00 Da [M+Na]+
Phenol ethers | 1-[5-Nitro-2-(1-pyrrolidinyl)benzyl]-1H-imidazole Δm -21.98 Da [M+H]+
Fatty Acyls | (5Z)-3-Hydroxy-5-dodecenoic acid Δm 0.00 Da [M+H]+
Glycerolipids | Monoacyldiglycerol Δm 0.00 Da [M+H+NQ]+
Fatty Acyls | (E)-8,9,10-trihydroxyoctadec-6-enoic acid Δm 0.00 Da [M+NH4]+
Fatty Acyls | (-)-Prefic acid Δm -36.02 Da [M+H]+
Benzene and substituted derivatives | Bis(2-hydroxyethyl) phthalate Δm 0.00 Da [M+H+NQ]+
Organooxygen compounds | Cannabidiol Δm -122.11 Da [M+H]+
Organooxygen compounds | N,3-Benzylsuccinylcyl-N6-tert-butoxycarbonyl-D-lysine Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | 4-amino-1-phenyl-6-(phenylmino)-1,2,5,6-tetrahydro-1,3,5-triazin-2-one Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 4-(2-Butoxyethoxy)benzoic acid Δm -56.06 Da [M+H]+
Coumarins and derivatives | 7-O-Methylvaginol Δm 16.01 Da [M+H+NQ]+
Carboxylic acids and derivatives | 3,8,9-Trihydroxy-10-propyl-3,4,5,8,10-tetrahydro-2H-oxecin-2-one Δm -18.01 Da [M+H]+
Fatty Acyls | Tuberonic acid Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | 1,3-2,4-bis(3,4-dimethylbenzylidene)sorbitol Δm 0.00 Da [M+Na]+
Lipids and lipid-like molecules | Artemisinin Δm 0.00 Da [M+H]+
Phenol ethers | Cu (-)-Salvin Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | 2-[(2-Methoxycyclohexyl)-(5,6)furan-3-yl]amino]-2-oxoethyl 4-tert-butylbenzoate Δm -253.07 Da [M+H+NQ]+
Organonitrogen compounds | Clodesiamine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 2-Butenoic acid, 2-methyl-, 1-(2,5-dihydro-5-oxo-2-furanyl)-4,5-dihydroxy-2-hexen-1-yl ester Δm 0.00 Da [M+H+NQ]+
Oxocins | 4-Chlorobrassenolico acid Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | AALLCALQGVXWNLLZDLBOSA-N Δm 68.13 Da [M+H]+
Benzene and substituted derivatives | Valerbamate Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Bis(2-hydroxyethyl) phthalate Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | 4-Acetylbiphenyl sulfone Δm -42.01 Da [M+H]+
Carboxylic acids and derivatives | Naugard BL-1 Δm 17.03 Da [M+H]+
Benzene and substituted derivatives | 4-Ethyl-N,N-dimethylsulfamone Δm -27.05 Da [M+H+NQ]+
Benzene and substituted derivatives | Monoethyl phthalate Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | N-(2-Amino-4-methylpentanoyl)phenylalanine Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Methyl (2E)-4-(3-fluorobenzoyl)-1-(phenylsulfonyl)-2-(piperazinecarboxylate Δm 0.00 Da [M+H]+
Fatty Acyls | [(3-Hydroxy-1-oxo-1-(2,3,4,5,6-pentahydroxyhexoxy)decan-5-yl] 3,5-dihydroxybenzoate Δm -222.15 Da [M+H]+
Lipids and lipid-like molecules | 5-Heptenoic acid, 7-[(1R,4S,5S,6R)-6-[(1E,3S)-3-hydroxy-1-octenyl]-2-oxabicyclo[2.2.1]hept-5-yl]-, (9E)-, Δm 0.00 Da [M+Na]+
Benzenoids | 2,2'-(1,3-Phenylene)bis(propan-2-ol) Δm -18.01 Da [M+H]+
Lipids and lipid-like molecules | Ethyl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylate Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | (R)-Baclofen Δm 0.00 Da [M+H+NQ]+
Benzene and substituted derivatives | Ingenol 10B6 Δm 0.00 Da [M+H]+
Benzenoids | N1-[4-(pyrrolidinsulfonyl)phenyl]piperazine-1-carboxthioamide Δm 0.00 Da [M+Na]+
Benzopyranes | Trimethylanain Δm 37.98 Da [M+H]+
Lipids and lipid-like molecules | PZPXXSCUORDGC-KUXKPYTGSA-N Δm 0.00 Da [M+Na]+
Benzenoids | Ginkgolic acid Δm 0.00 Da [M+Na]+
Phenol ethers | GEXJPCOZLPCVLX-DISMIGASA-N Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | (6Z)-1-Hydroxy-6-(2-hydroxy-2-methylpropylidene)-2,2,4,4-tetramethyl-3,5-dioxocyclohexyl 6-O-(3,4,5-trihydroxybenzoyl)-β-D-glucopyranoside Δm -348.07 Da [M+H]+
Fatty Acyls | 1-Ethylhexyl beta-D-glucopyranoside Δm 38.99 Da [M+H+NQ]+
Coumarins and derivatives | 2-cyano-N-(2-oxo-1,2-dihydro-2-benzofuran-3-yl)benzenesulfonamide Δm 0.00 Da [M+H]+
Fatty Acyls | Arg-Val-Val-Val Δm -18.01 Da [M+H]+
Fatty Acyls | 4-Hydroxybiotecanoic acid Δm 0.00 Da [M+H+NQ]+
Phenol ethers | [(2E,4E,12E)-13-(1,3-Benzodioxol-5-yl)-1-(1-piperidinyl)-2,4,12-tridecatrien-1-one Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | N-[4-(4-Fluorophenyl)-1,3-thiazol-2-yl]ethoximate Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Fluticasone furoate Δm 0.00 Da [M+Na]+
Benzenoids | Myrtucommulone B Δm 17.03 Da [M+H]+
Benzene and substituted derivatives | Cyclopropylchlol A Δm -64.02 Da [M+H]+
Flavonoids | Apiharpin Δm 0.00 Da [M+H]+
Organic sulfonic acids and derivatives | 4-[4-(Hydroxiesulfonyl)phenoxy]benzene-1-sulfonylhydrazide Δm -60.04 Da [M+H]+
Organic phosphonic acids and derivatives | 2-Chloro-4,5-dimethoxybenzoic acid Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | (2-(2-Methyl-1,3-thiazol-4-yl)-(5-(8-(trifluoromethyl)phenyl)-1,3,4-oxadiazole Δm 0.00 Da [M+H]+


LIMMA_FILTERED_groupMAJ (8/11) | rows 421–480 of 639
Linear 1,3-diarylpropanoids | Liquiritigenin Δm 0.00 Da [M+H]+
Benzopyrans | Hymecromone Δm 0.00 Da [M+H]+
Organoheterocyclic compounds | N-(3,4-dichlorophenyl)-N'-(5-methyl-4-oxo-1-phenyl-1,4-dihydro-5H-pyrazolo[3,4-d]pyrimidin-6-yl)urea Δm 0.00 Da [M+H]+
Prenol lipids | Nevadensic acid Δm 0.00 Da [M+H]+
Benzenoids | 2-Chloro-1,3,8-trihydroxy-6-(hydroxymethyl)anthraquinone Δm 0.00 Da [M+H]+
Organonitrogen compounds | 10-Heptadecyn-4-one, 1,2-dihydroxy- Δm -21.98 Da [M+Na]+
Phenol ethers | (2E,5E)-3,5,7,7-trimethylocta-2,5-dienedioic acid Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | 2,5-Di-tert-butyl-1,4-benzoquinone Δm 0.00 Da [M+H]+
Organic sulfuric acids and derivatives | 5-nitro-N-[(1-{[1,3,4-oxadiazol-2-yl]methyl}azan-2-ca
Organooxygen compounds | D-(+)-Cellobiose Δm 0.00 Da [M+H-H2O]+
Glycerolipids | 1-Palmitoylglycerol Δm 0.00 Da [M+H]+
Organooxygen compounds | [(6R,7R)-7-Hydroxy-7-methyl-8-oxo-3-[(E)-prop-1-enyl]-5,6-dihydro-1H-isochromen-6-yl] 3,6-dihydroxy-4-methoxy-2-methylbenzoate Δm -180.04 Da [M+H]+
Organoheterocyclic compounds | Sulfaphenazole Δm 37.96 Da [M+Na]+
Organooxygen compounds | 1,3-Benzenediol, 5-methyl-4-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]- Δm -94.06 Da [M+H]+
Pyridines and derivatives | Fenofibric acid Δm 21.98 Da [M+H]+
Benzenoids | N-2-(4-[[2,6-Dimethoxy-4-pyrimidinylamino]sulfonyl]phenyl)-2-furamide Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | Carfentrl Δm 0.00 Da [M+H]+
Phenol ethers | (4aS,9aR)-2-Benzyl-7-[(2-(2-oxo-1-imidazolidinyl)ethyl)thio]tetrahydro-6H-pyrido[3,4-d]pyrimidin-6-one Δm 21.98 Da [M+H]+
Carboxylic acids and derivatives | Terbumeton Δm 0.00 Da [M+Na]+
Organooxygen compounds | Hexadecenamide Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | N-Benzoyl-L-phenylalanine Δm 0.00 Da [M+H]+
Organonitrogen compounds | 1-Hexadecylamine Δm 0.00 Da [M+H]+
Organic acids and derivatives | 3,4-Dihydroisoyonoxinic acid Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | D-Pipecolinic acid Δm 126.08 Da [M+H]+
Prenol lipids | 2,6-Di-tert-butylbenzoquinone Δm 0.00 Da [M+H]+
Fatty Acyls | Tapanol Δm -54.03 Da [M+H]+
Organonitrogen compounds | n-Octadecylamine Δm 0.00 Da [M+H]+
Fatty Acyls | (8E)-Heptadeca-8,16-diene-1,2,4-triol Δm 0.00 Da [M+H]+
Prenol lipids | 2,6-Di-tert-butylbenzoquinone Δm 18.01 Da [M+H-H2O]+
Prenol lipids | 2H-Pyran-2-one, tetrahydro-6-hydroxy-6-pentyl- Δm -18.01 Da [M+H]+
Organic acids and derivatives | 1-(s-tert-pyridoxamine)-D-prolin-2-yl)amino]propan-1-one Δm -10.98 Da [M+H]+
Fatty Acyls | 4,4'-Oxydibenzoic-1-2-diamine Δm 0.00 Da [M+H]+
Organooxygen compounds | 8-Hydroxy-6-methoxy-3-methyl-3,4-dihydroisocoumarin-1-one Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 9-(2-Chlorophenyl)-7,8-dihydro[1,3]dioxolo[4,5-g]quinolin-6(5H)-one Δm 217.03 Da [M+2H]+2
Organometallic compounds | Octamethylcyclotetrasiloxane Δm 0.00 Da [M+H]+
Fatty Acyls | N-(1-Acetoxyoctyl)-2,2-[bis(3-(p)-3-chlorobenzoyloxy)-
Organometallic compounds | Butanol- Δm 0.00 Da [M+H]+
Organic metal salts | Dodecamethylcyclohexasiloxane Δm 0.00 Da [M+H]+
Organoheterocyclic compounds | Pyridalid Δm 0.00 Da [M+H]+
Organometallic compounds | 4-(4-Chlorophenyl)-2,6-pyperidinedione Δm 17.03 Da [M+H]+
Organometallic compounds | Hexamethylcyclotrisiloxane Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Benzophenone Δm 0.00 Da [M+H]+
Organometallic compounds | Hexamethylcyclotrisiloxane Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 3-(2,5-bis(trifluoromethyl)phenyl)6'-hydroxyspiro-2-eminiamide Δm 0.00 Da [M+H-H2O]+
Phenylpropanoids and polyketides | (E)-3-(8-hydroxy-6-methoxy-1-oxoisochromen-3-yl)prop-2-enoic acid Δm 0.00 Da [M+H]+
Organometallic compounds | N3-(2-Mercapto-4-oxo-3,4-dihydroquinazolin-3-yl)oxidiminamide Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Decamethylcyclopentasiloxane Δm -37.96 Da [M+H]+
Organometallic compounds | 3-Methylquinoline Δm 0.00 Da [M+H-H2O]+
Organonitrogen compounds | 3-Methylquinoline Δm 17.03 Da [M+H]+
Fatty Acyls | 5-Amino-2(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)-5-oxopentanoic acid Δm 21.98 Da [M+H-H2O]+
Fatty Acyls | 3-methyl-5-(4-methyl-1,2,3-thiadiazol-5-yl)-4-isoxazolecarboxamide Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Ethno-Dihydroquinopin Δm 0.00 Da [M+H]+
Organosulfur compounds | N,N-Dimethyl-3,4-DMA Δm 0.00 Da [M+H]+
Benzenoids | 17a-Methyl-androstan-3-hydroxyimine-17β-ol Δm 0.00 Da [M+H]+
Peptidomimetics | Avocadene 1-acetate Δm 21.98 Da [M+H]+
Organonitrogen compounds | 2-(Octadecylamino)ethanol Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Cyclopropyl[(3S)-3-(5-methyl- 1H-benzimidazol-2-yl)-1-pyrrolidinyl]methanone Δm 0.00 Da [M+H]+
Phenol ethers | (2S,3aR,8aR,8R,9S,10S,10aR,11R)-2,8,10-Trihydroxy-3a-methyl-12-methylenedodecahydro-1H-7H-5,7,10b-(epimethanetriyl)cyclopentaf[e]cyclodec-1,6-dione Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | 5,5-dimethyl-3-(methylthio)cyclohex-2-en-1-one Δm 0.00 Da [M+H]+
Phenylpropanoids and polyketides | ZEIOCTVSMTHEVQ-LGNFFFACHSLA- Δm 0.00 Da [M+H]+
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0

LIMMA_FILTERED_groupMAJ (9/11) | rows 481–540 of 639
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
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-800
-700
-600
-500
-400
-300
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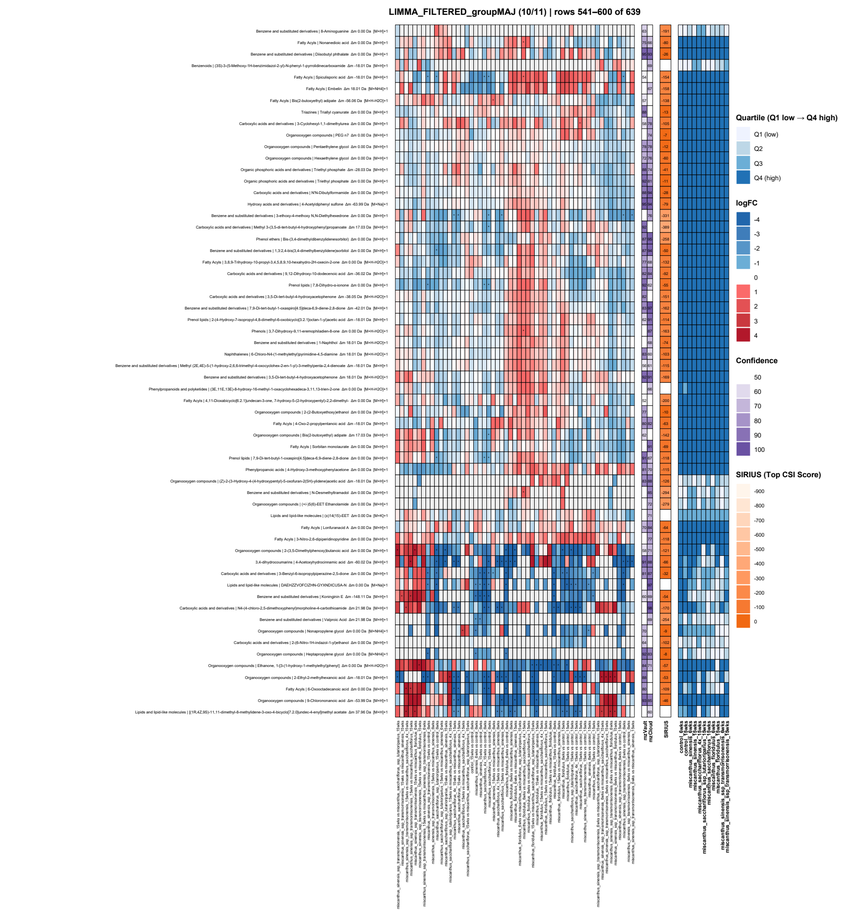
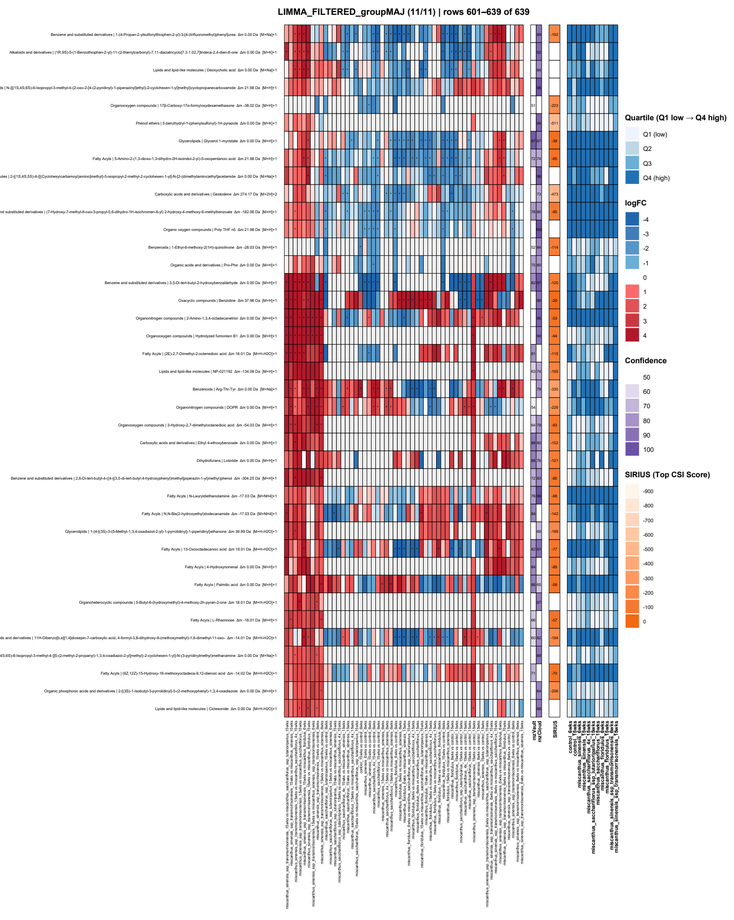

LIMMA_FILTERED_groupMAJ (10/11) | rows 541–600 of 639
Benzene and substituted derivatives | 8-Aminoguanine Δm 0.00 Da [M+H]+
Fatty Acyls | Nonanedioic acid Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | Dibutoxyethyl phthalate Δm 0.00 Da [M+H]+
Benzenoids | (3S)-3-(5-Methoxy-1H-benzimidazol-2-yl)-N-phenyl-1-pyrrolidinecarboxamide Δm -16.01 Da [M+H]+
Fatty Acyls | Spiculisporic acid Δm -18.01 Da [M+H]+
Fatty Acyls | Embelin Δm 18.01 Da [M+NH4]+
Fatty Acyls | Bis(2-butoxyethyl) adipate Δm -56.96 Da [M+H-H2O]+
Triazines | Triallyl cyanurate Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 2-Cyclohexyl-1,1-dimethylurea Δm 0.00 Da [M+H]+
Organooxygen compounds | PEG n7 Δm 0.00 Da [M+H]+
Organooxygen compounds | Pentaethylene glycol Δm 0.00 Da [M+H]+
Organooxygen compounds | Hexaethylene glycol Δm 0.00 Da [M+H]+
Organic phosphoric acids and derivatives | Triethyl phosphate Δm -28.03 Da [M+H]+
Organic phosphoric acids and derivatives | Triethyl phosphate Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | N,N-Dibutylformamide Δm 0.00 Da [M+H]+
Hydroxy acids and derivatives | 4-Acetylphenyl sulfone Δm -63.99 Da [M+Na]+
Benzene and substituted derivatives | 3-ethoxy-4-methoxy N,N-Diethylbenzidine Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | Methyl 3-(5,5-di-tert-butyl-4-hydroxyphenyl)propanoate Δm 17.03 Da [M+H]+
Phenol ethers | Bis-(3,4-dimethylbenzylidene)sorbitol Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 1,3,2,4-bis(2,4-dimethylbenzylidene)sorbitol Δm 0.00 Da [M+H]+
Fatty Acyls | 9,8,9-Trihydroxy-10-propyl-5,6,3',8,10-hexahydro-2H-oxecin-2-one Δm 0.00 Da [M+H-H2O]+
Carboxylic acids and derivatives | 9,12-Dihydroxy-10-dodecenoic acid Δm -36.02 Da [M+H]+
Prenol lipids | 7,8-Dihydro-α-ionone Δm 0.00 Da [M+H]+
Carboxylic acids and derivatives | 3,5-Di-tert-butyl-4-hydroxyacetophenone Δm -38.05 Da [M+H-H2O]+
Benzene and substituted derivatives | 7,9-Di-tert-butyl-1-oxaspiro[5.5]deca-6,9-diene-2,8-dione Δm -42.01 Da [M+H]+
Prenol lipids | 2-(4-Hydroxy-7-oxaspiro[5.6-dimethyl-8-oxobicyclo[2.2.1]octan-1-yl]pentyl) acid Δm -18.01 Da [M+H]+
Phenols | 3,7-Dihydroxy-3,11-eremophiladien-8-one Δm 0.00 Da [M+H-H2O]+
Benzene and substituted derivatives | 1-Naphthol Δm 18.01 Da [M+H-H2O]+
Naphthalenes | 6-Chloro-N4-(1-methylethyl)pyrimidine-4,5-diamine Δm 18.01 Da [M+H-H2O]+
Benzene and substituted derivatives | Methyl (2E,4E)-5-(1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl)-3-methylpenta-2,4-dienoate Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | 3,5-Di-tert-butyl-4-hydroxyacetophenone Δm 18.01 Da [M+H-H2O]+
Phenylpropanoids and polyketides | (3E,11E,13E)-8-Hydroxy-16-methyl-1-oxacyclohexadeca-3,11,13-trien-2-one Δm 0.00 Da [M+H-H2O]+
Fatty Acyls | 4,11-Dioxabicyclo[8.2.1]tridecan-3-one, 7-hydroxy-5-(2-hydroxypentyl)-2,2-dimethyl- Δm 0.00 Da [M+H]+
Organooxygen compounds | 2-(2-Butoxyethoxy)ethanol Δm 0.00 Da [M+H]+
Fatty Acyls | 4-Oxo-2-propylpentanoic acid Δm -18.01 Da [M+H]+
Organooxygen compounds | Bis(2-butoxyethyl) adipate Δm 17.03 Da [M+H]+
Fatty Acyls | Sorbitan monostearate Δm 0.00 Da [M+H]+
Prenol lipids | 7,9-Di-tert-butyl-1-oxaspiro[5.5]deca-6,9-diene-2,8-dione Δm 0.00 Da [M+H]+
Phenylpropanoic acids | 4-Hydroxy-3-methoxyphenylacetone Δm 0.00 Da [M+H]+
Organooxygen compounds | (2r)-2-(3-Hydroxy-4-oh-hydroxyperhydy)-5-oxofuran-2(5H)-ylidene]acetic acid Δm -18.01 Da [M+H]+
Benzene and substituted derivatives | N-Desmethyldiranazol Δm 0.00 Da [M+H]+
Organooxygen compounds | >= (EtO)-DET Ethanolamide Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | (±)18(19)-EET Δm 0.00 Da [M+H]+
Fatty Acyls | Lumbaroacid A Δm 0.00 Da [M+H]+
Fatty Acyls | 3-Nitro-2,6-dipiperidinopyridine Δm 0.00 Da [M+H]+
Organooxygen compounds | (-)-3,5-Dimethylphenoxy)butenoic acid Δm 0.00 Da [M+H]+
3,4-dihydrocoumarins | 4-Acetoxyphthalocrisantaric acid Δm -60.02 Da [M+H]+
Carboxylic acids and derivatives | 3-Benzyl-N-isopropylpiperazine-2,5-dione Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | CHEMZEOFCQUHN-OYNNDCUSA-N Δm 0.00 Da [M+Na]+
Benzene and substituted derivatives | Kisinoligin E Δm -146.11 Da [M+H]+
Carboxylic acids and derivatives | N4-(4-chloro-2,5-dimethoxyphenyl)nicotinic-4-carbothioamide Δm 21.98 Da [M+H]+
Benzene and substituted derivatives | Valproic Acid Δm 21.98 Da [M+H]+
Organooxygen compounds | Nonapropylene glycol Δm 0.00 Da [M+NH4]+
Carboxylic acids and derivatives | 2-(6-Nitro-1H-indazol-1-yl)ethanol Δm 0.00 Da [M+H]+
Organooxygen compounds | Heptapropylene glycol Δm 0.00 Da [M+NH4]+
Organooxygen compounds | Ethanone, 1-[2h-(1-hydroxy-1-methylethyl)phenyl] Δm 0.00 Da [M+H-H2O]+
Organooxygen compounds | 2,6'dhp-2-methylheneoxo acid Δm -18.01 Da [M+H]+
Fatty Acyls | 9-Oxooctadecanoic acid Δm 0.00 Da [M+H]+
Organooxygen compounds | 9-Chlorononanoic acid Δm -53.98 Da [M+H]+
Lipids and lipid-like molecules | [1R,4Z,6S)-11,11-dimethyl-8-methylidene-3-oxo-4-bicyclo[7.2.1]undec-4-enyl]methyl acetate Δm 37.99 Da [M+H]+
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0


LIMMA_FILTERED_groupMAJ (11/11) | rows 601–639 of 639
Benzene and substituted derivatives | 1-(4-Propan-2-ylsulfonylthiophen-2-yl)-3,2h-2h-furoromethyl)phenylurea Δm 0.00 Da [M+Na]+
Alkaloids and derivatives | (1R,9S)-5-(1-Benzylthiophen-2-yl)-11-(2-thienylcarbonyl)-7,11-diazatricyclo[7.3.1.02,7]trideca-2,4-dien-6-one Δm 0.00 Da [M+Na]+
Lipids and lipid-like molecules | Deoxycholic acid Δm 0.00 Da [M+Na]+
Organoheterocyclic compounds | N-[(1S,4S,6S)-6-Isopropyl-3-methyl-4,2-oxo-2-[4-(2-pyridinyl)-1-piperazinylethyl]-2-cyclohexen-1-yl]methylcyclopropanecarboxamide Δm 21.98 Da [M+H]+
Organooxygen compounds | 17β-Carboxy-17α-formylsulpiteanethesone Δm -38.02 Da [M+H]+
Phenol ethers | 5-Ketohydrohyl-1-(phenylsulfonyl)-1H-pyrazole Δm 0.00 Da [M+K]+
Glycerolipids | Glycerol 1-myristate Δm 0.00 Da [M+H]+
Fatty Acyls | 5-Amino-2-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)-5-oxopentanoic acid Δm 21.98 Da [M+H]+
Lipids and lipid-like molecules | 2-[(1S,4S,5S)-4-[[Cyclohexylcarbamoyl]amino]methyl]-5-isopropyl-2-methyl-2-cyclohexen-1-yl]-N-[(-)dimethylamino]ethylpentanide Δm 0.00 Da [M+Na]+
Carboxylic acids and derivatives | Gestodene Δm 374.17 Da [M+2H]+2
Benzene and substituted derivatives | (7-Hydroxy-7-methyl-8-oxo-3-propyl-5,6-dihydro-1H-isochromen-8-yl) 2-hydroxy-4-methoxy-6-methylbenzoate Δm -182.06 Da [M+H]+
Organic oxygen compounds | Poly THF-10 Δm 21.98 Da [M+H]+
Benzenoids | 1-Ethyl-6-methoxy-2(1H)-quinolinone Δm -28.03 Da [M+H]+
Organic acids and derivatives | Pro-Pro Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 3,5-Di-tert-butyl-2-(3-hydroxybenzaldehyde Δm 0.00 Da [M+H]+
Oxacyclic compounds | Benzidine Δm 37.96 Da [M+H]+
Organonitrogen compounds | 2-Amino-1,3,4-octadecanetriol Δm 0.00 Da [M+H]+
Organooxygen compounds | Hydrolyzed fumonisin B1 Δm 0.00 Da [M+H]+
Fatty Acyls | (3E)-2,7-Dimethyl-2-octenedioic acid Δm 18.01 Da [M+H-H2O]+
Lipids and lipid-like molecules | NP-021192 Δm -134.08 Da [M+H]+
Benzenoids | Arg-Tm-Tyr Δm 0.00 Da [M+Na]+
Organonitrogen compounds | DOPR Δm 0.00 Da [M+H]+
Organooxygen compounds | 3-Hydroxy-2,7-dimethylocta-2-enedioic acid Δm -54.03 Da [M+H]+
Carboxylic acids and derivatives | Ethyl 4-ethoxybenzoate Δm 0.00 Da [M+H]+
Dihydrofuranes | Loliolide Δm 0.00 Da [M+H]+
Benzene and substituted derivatives | 2,6-Di-tert-butyl-4-[4-[[3,5-di-tert-butyl-4-hydroxyphenyl]methyl]piperazin-1-yl]methyl]phenol Δm -304.25 Da [M+H]+
Fatty Acyls | N-Lauroylethanolamine Δm -17.03 Da [M+NH4]+
Fatty Acyls | N,N-Bis(2-hydroxyethyl)dodecanamide Δm -17.03 Da [M+NH4]+
Glycerolipids | 1-(9-[(3S)-3-(5-Methyl-1,3,4-oxadiazol-2-yl)-1-pyrrolidinyl]-1-piperidinyl)ethanone Δm 39.99 Da [M+H-H2O]+
Fatty Acyls | 13-Oxooctadecanoic acid Δm 18.01 Da [M+H-H2O]+
Fatty Acyls | 4-Hydroxynonenal Δm 0.00 Da [M+H]+
Fatty Acyls | Palmitic acid Δm 0.00 Da [M+H]+
Organoheterocyclic compounds | 5-Butyl-6-(hydroxymethyl)-4-methoxy-2h-pyran-2-one Δm 18.01 Da [M+H-H2O]+
Fatty Acyls | L-Rhamnose Δm -18.01 Da [M+H]+
Carboxylic acids and derivatives | 11H-Dibenz[b,e][1,4]dioxepin-7-carboxylic acid, 4-formyl-3,8-dihydroxy-9-(methoxymethyl)-1,6-dimethyl-11-oxo- Δm -14.01 Da [M+H-H2O]+
Lipids and lipid-like molecules | 1-[(1S,4S,6S)-6-Isopropyl-3-methyl-4-[[5-(2-methyl-2-propanyl)-1,3,4-oxadiazol-2-yl]methyl]-2-cyclohexen-1-yl]-N-(3-pyridinylmethyl)methanamine Δm 0.00 Da [M+Na]+
Fatty Acyls | (9Z,12Z)-15-Hydroxy-16-methoxycycladea-9,12-dienoic acid Δm -14.02 Da [M+H-H2O]+
Organic phosphonic acids and derivatives | [(3S)-1-Iodobutyl-3-pyrrolidinyl]-5-(2-methoxyphenyl)-1,3,4-oxadiazole Δm 0.00 Da [M+H]+
Lipids and lipid-like molecules | Colosevole Δm 0.00 Da [M+H-H2O]+
Quartile (Q1 low → Q4 high)
Q1 (low)
Q2
Q3
Q4 (high)
logFC
-4
-3
-2
-1
0
1
2
3
4
Confidence
50
60
70
80
90
100
SIRIUS (Top CSI Score)
-900
-800
-700
-600
-500
-400
-300
-200
-100
0