

Supplementary Table 4. The differential metabolites between

neg_1015; 5-Ethyl-2-(1-pyrro	neg_1002; Muricin E	neg_1037; (R)-3-Hydroxy-he	neg_11; 2,3-Butanedione
neg_1026; 4-Hydroxy-4-meth	neg_1010; 5-(2-Furanyl)-1,2,	neg_1040; Piperitine	neg_1148; 7,8-Dihydroxyango
neg_1044; Fumonisin AK1	neg_1013; Triterpenoid	neg_1046; 7-Methyl-3-methy	neg_1151; cis- and trans-Ethy
neg_105; Phe-Gly-OH	neg_1014; TG(10:0/10:0/10:(	neg_1049; Curzerenone	neg_1169; 10,11-dihydro-20-
neg_1054; 2,4-Dihydroxy-2H	neg_1017; xi-Dihydro-5-octy	neg_1093; Glyceric acid	neg_1237; Kanokoside D
neg_1064; Decanal	neg_1020; Rubraflavone C	neg_1104; 6,8-Tricosanedion	neg_1261; Myrcenol
neg_1075; 4-Ethyl-2-methoxy	neg_1022; Digoxigenin monc	neg_1217; Propyl 1-(propylth	neg_1285; trans-p-Menth-2-ei
neg_1078; Kamahine C	neg_1023; 1alpha-1-Hydroxy	neg_1249; Apo-12'-violaxant	neg_1458; Arecaidine
neg_1081; Desogestrel	neg_1024; 4-Acetoxy-2-hexy	neg_1347; (Z)-15-Oxo-11-eic	neg_1504; beta-Citraurin
neg_1085; AF Toxin II	neg_1031; Sativan	neg_1391; 28-Hydroxywithar	neg_1513; 5-Methoxytryptopl
neg_1104; 6,8-Tricosanedion	neg_1035; Glycerol 1-(5-hyd	neg_14; Serotonin hydrochlori	neg_154; 4-Gingerol
neg_1115; 3a,7b,21-Trihydro	neg_1046; 7-Methyl-3-methy	neg_1477; 2,5-Dimethyl-3-m	neg_1598; N-Desmethyltrama
neg_1140; Alectrol	neg_1047; (3S,7E,9S)-9-Hyd	neg_1505; L-Palmitoylcarniti	neg_1619; Phytolaccinic acid
neg_1148; 7,8-Dihydroxyango	neg_1050; D-Glycero-D-gala	neg_1529; LysoPE(0:0/20:4(i	neg_1728; Megastigmatrienoi
neg_1169; 10,11-dihydro-20-	neg_1051; Troxerutin	neg_1532; Perindoprilat gluci	neg_1833; Asimilobin
neg_117; 8,11-eicosadiynoic	neg_1053; trans-Jasmone	neg_1546; Esculentic acid (P	neg_1905; 19'-Hexanoyloxym
neg_1172; Lysyl-Tryptophan	neg_1058; 4-Methyl-2-(1-phen	neg_1553; 2,6 Dimethylhepta	neg_207; Artabsinolid D
neg_1179; 4-[(2-Methyl-3-fu	neg_1062; 3a,7a-Dihydroxy-5-	neg_157; 6-Gingerol	neg_2095; Nigelllic acid
neg_1191; Vulgarolide	neg_1066; Hovenine A	neg_1641; 5-Decanoyl-2-non	neg_2184; Ginsenoside Rh8
neg_1208; 1-Pentadecanecarl	neg_1073; Hordatine A	neg_1680; (S)-[10]-Gingerol	neg_2267; Ciliatine
neg_1212; Lentinic acid	neg_1079; Linoleic acid	neg_1690; LysoPE(0:0/18:0)	neg_2286; all-trans-Decapren
neg_1217; Propyl 1-(propylth	neg_108; p-Acetaminobenzal	neg_1691; Metabolite M6	neg_2371; cis-3-Hexenyl hex
neg_1220; 5-Hexyltetrahydro	neg_1088; D-Glucose	neg_1703; Lisuride	neg_2406; Naringenin
neg_1257; 13-Hydroxy-9-me	neg_1095; Mukonal	neg_1727; 4-Methyl-4-(meth	neg_2567; 3,5-Dimethyl-2-vi
neg_1259; Anatabine	neg_1113; (3R,7R)-1,3,7-Oct	neg_1771; PS(14:0/16:0)	neg_2645; 3-(1,1-Dimethylall
neg_1272; Vanilloloside	neg_1117; Cavipetin D	neg_1786; D8'-Merulinic acic	neg_2703; Methysergide
neg_1276; Momorcharaside I	neg_113; Nanaomycin	neg_1924; 7-HDoHE	neg_2705; Cocaethylene
neg_1278; Panaquinquecol 1	neg_1133; Methyl 3,4,5-trim	neg_1952; PG(18:1(11Z)/20:	neg_2744; Hexylresorcinol
neg_1285; trans-p-Menth-2-e	neg_1136; Oxytetracycline	neg_1967; 10-Hydroxy-3-me	neg_2750; Bambuterol
neg_1301; (E)-Arachidin II	neg_1153; (8R,8'R,9S)-9-Hy	neg_1999; Glabrolide	neg_2831; trans-p-Menthane-
neg_1307; Neopellitorine A	neg_1157; Neomycin	neg_2028; 24,25-Diacetyl vul;	neg_2900; Gossypurpurin
neg_1321; Asperxanthone	neg_1162; Neuromedin N (1-	neg_2033; PC(15:0/16:0)	neg_2913; LysoPE(0:0/20:1(1
neg_1323; Ivacaftor	neg_1164; Peralol	neg_2060; PC(22:6(4Z,7Z,10	neg_294; 5-Dodecenoic acid
neg_134; Lovastatin acid (Me	neg_1180; Zileuton	neg_2061; Docosapentaenoic	neg_295; (E,Z)-2,4-Heptadier
neg_1347; (Z)-15-Oxo-11-eic	neg_1192; 6-Methylnicotinan	neg_222; 13-Hydroxymarasn	neg_2988; Pyronaridine
neg_1359; Decarbamoylneos	neg_1194; D-1-[(3-Carboxyp	neg_2233; Scopolamine	neg_3017; Annopentocin A
neg_1363; Phenylalanyl-Isole	neg_1198; PE(20:5(5Z,8Z,11	neg_2251; (3beta,22E,24R)-E	neg_3056; Glutaminy-Methic
neg_1390; Fluvoxamine	neg_1200; Anandamide	neg_2310; 14-oxo-DoHE(1-	neg_310; 2-Carboxy-4-dodec
neg_14; Serotonin hydrochlori	neg_1207; Androstenedione	neg_2319; Solasodine	neg_3233; PGP(16:0/18:0)
neg_140; (𠄎)伪-CMBHC	neg_1213; Aloesol 7-glucosic	neg_2323; Falcaringidione	neg_3247; PC(DiMe(11,5)/M
neg_1418; 6-Hydroxymelator	neg_123; maltotetraose	neg_235; N-(14-Methylhexad	neg_3297; 2',6'-Dihydroxy-4'
neg_1420; All-trans-retinoic ;	neg_1230; N-Glycolylneuram	neg_2413; PS(MonoMe(11,3	neg_3361; PE(18:0/20:3(5Z,8
neg_1432; Tomatidine	neg_1234; Dihomo-gamma-li	neg_2450; PE(15:0/P-18:0)	neg_3370; PC(DiMe(11,3)/M
neg_1434; O-Desmethyltram;	neg_1238; xi-7-Hydroxyhexa	neg_246; Docosapentaenoic ;	neg_3468; L-Oxalylalbizziine
neg_1446; PGF2a ethanolami	neg_1239; Dihydrozeatin-7-T	neg_2466; Torvoside F	neg_3522; 15-keto-Prostaglar
neg_1449; Petasalbin	neg_1249; Apo-12'-violaxant	neg_2486; PG(16:0/22:5(7Z,	neg_3546; Valyl-Histidine
neg_1458; Arecaidine	neg_1253; 1-Undecanol	neg_2497; Musabalbisiiane B	neg_358;

neg_157; 6-Gingerol neg_1302; Inositol 1,3,4,5-tet neg_2946; Melilotoside D neg_59; Quadrone
 neg_1579; E-10-Hydroxyami neg_1312; Ethanolaminium(1 neg_2951; 3-Methyl-5-pentyl neg_596; alpha-Micropteroxa
 neg_1586; L-Leucine neg_1335; 2-Acetylpyrrole neg_2969; PE(14:0/20:4(5Z,8Z,11Z,14Z) neg_676; [8]-Paradol
 neg_1589; PE(20:2(11Z,14Z) neg_1336; 5-Acetylamino-6-I neg_3029; Isoleucyl-Asparag neg_743; Oxyphencyclimine
 neg_16; L-Tryptophan neg_1342; Plastoquinone 3 neg_306; Theaspirone A neg_749; Moracin O
 neg_1624; Procyclidine neg_1345; Furohyperforin neg_3069; Terniflorin neg_80; 19(R)-hydroxy-PGA:
 neg_1628; Dehydrocyanaropi neg_1362; Calenduloside B neg_3072; Heptylmalonic aci neg_823; Lysyl-Proline
 neg_1635; Indecainide neg_1367; Balenine neg_3077; 2-Methoxy-5-met neg_912; (1S,2S,4S,5R)-1,8-I
 neg_1640; (10Z,14E,16E)-10 neg_1370; DG(16:0/14:1(9Z) neg_308; 2-Hydroxy-6-tridec neg_934; Bisacurool
 neg_1668; Tacrolimus neg_1376; 4-Methoxy-3-gera neg_3129; Pipericine neg_942; Reticulataxanthin
 neg_1676; beta-Citraurinene neg_138; 15-Keto-protagland neg_3213; 3b,17b-Dihydroxy neg_957; alpha-Butyl-omega-
 neg_1680; (S)-[10]-Gingerol neg_1383; 2-O-(4-O-Methyl- neg_3217; Medicoside I pos_1007; Carisoprodol
 neg_1688; 2-Isopropyl-5-met neg_1384; 3'-Ketolactose neg_3287; Dimethylallylpyro pos_1020; 1-(3-Aminopropyl
 neg_1693; 3-carboxy-4-meth neg_139; Cellotetraose neg_3298; 20a,22b-Dihydrox pos_1043; 2-Heptanone
 neg_1703; Lisuride neg_1394; Hexylbenzene neg_3325; (5S)-hydroperoxy- pos_106; PG(20:5(5Z,8Z,11Z
 neg_1706; (5alpha,10alpha)- neg_1400; L-Galacto-2-heptu neg_3352; Crotamiton pos_1074; 10,20-Dihydroxyei
 neg_1754; 2-oleoyl-sn-glycer neg_1403; 3alpha,4,5,7alpha- neg_3400; 6beta-Hydroxytest pos_1081; Humulinic acid A
 neg_176; Val Asp Ile Arg neg_1404; Isophysalin G neg_3418; Nonadecanoic aci pos_1095; 3alpha-O-trans-Fei
 neg_177; Sequiterpene Lacto neg_1407; Italipyrone neg_3428; Helinorbisabone pos_111; 9Z,12E-Tetradecadi
 neg_1771; PS(14:0/16:0) neg_1408; L-Pyridosine neg_3429; Fludiazepam pos_1110; N(2)-phenylacetyl-
 neg_1774; Anhydrocinnzeyla neg_1426; Gamma-CEHC neg_3443; Yucalexin P21 pos_1138; Cellobiose
 neg_1778; 8,12-Epoxy-4(15) neg_1435; Uzarigenin 3-[xyl neg_3466; CDP-DG(16:0/16: pos_1157; 3-Methyl-3-buten-
 neg_1785; 6-Hydroxyfluvast neg_1437; (1E,4Z,6a,8b,10a) neg_3490; Asitrilobin D pos_1178; 2-Methylcyclodod
 neg_1786; D8'-Merulinic aci neg_1438; Phomopsin A neg_3535; Methyl linolenate pos_1179; (E)-2-Octen-1-ol
 neg_1788; Dirithromycin neg_1440; (E)-threo-1-(p-H neg_371; 2-Methylbutyrylgly pos_1353; 2,3-Dihydro-4-met
 neg_1789; PE(20:5(5Z,8Z,11 neg_1441; DG(15:0/20:5(5Z, neg_377; N-Jasmonoylisoleu pos_1402; Morphinone
 neg_179; 15(S)-HpEPE neg_1444; Quinquenoside III neg_380; Ustiloxin D pos_1565; (S)-Nerolidol 3-O-
 neg_1796; 6-Amino-9H-purir neg_1451; 3'-Sialyl-3-fucosyl neg_431; Dihydrodigoxin pos_1569; Alpha-ketoisovaler
 neg_1798; Gibberellin A94 neg_1452; Methyl 7-epi-12-h neg_478; (2'E,4'Z,7'Z,8E)-Co pos_1603; 3-(Acetyloxy)-2-hy
 neg_1801; 1-(beta-D-Ribofur neg_1453; Prednisolone neg_568; 15(R)-hydroperoxy pos_1680; 1-(2-Furanyl)-2-pr
 neg_1815; N6-Methylagmati neg_1461; Peltatol C neg_571; Ganodermic acid T pos_1714; xi-5-Hydroxydode
 neg_1825; 3a,4b,7a-Trihydro neg_1465; Prostaglandin C1(neg_574; 5-(10,13-Nonadeca pos_1748; 1-Hydroxy-3-meth
 neg_1833; Assimilobin neg_1475; 1,1'-(Tetrahydro-6 neg_575; (ent-2alpha,3beta,1 pos_1798; E-10-Hydroxynort
 neg_1873; Didesmethyl doxe neg_1480; 3-Acetyl-2,5-dime neg_585; 2-Palmitoylglycerol pos_1807; (3beta,5alpha,6bet
 neg_1903; Sphingosine 1-pho neg_1482; DG(20:3(5Z,8Z,11 neg_604; MG(0:0/20:1(11Z)/ pos_182; 9E,11-Dodecadiena
 neg_1905; 19'-Hexanoyloxyn neg_1488; 6-Hydroxyshogaol neg_631; Homocitrulline pos_1953; 2-Hexyl-4,5-dimet
 neg_1914; Cyperine neg_1495; Egonol gentiobios neg_640; 2,3-Dinor-6-keto-pi pos_1964; 7-Hydroxyglyclazic
 neg_1917; Methyl dihydrojas neg_1498; 3-Butylidene-1(3F neg_662; 1-Nonen-3-ol pos_1979; beta-D-Glucosylox
 neg_1924; 7-HDoHE neg_1501; Mocimycin neg_663; PE(14:1(9Z)/22:5(4 pos_2000; Polypodosaponin
 neg_1936; N2-Galacturonyl-I neg_1512; Fumonisin A2 neg_714; Kanzonol M pos_2016; 13-HOTE
 neg_194; 2-(N-morpholino)ei neg_1517; Prazepam neg_783; ent-8(17),13(16),14 pos_2030; DG(20:0/14:0/0:0)
 neg_1944; Prostaglandin H1 neg_1522; (3S,5R,6S,7E,9x)- neg_820; (R)-2-Hydroxyhexa pos_2073; 6-Deoxyfagomine
 neg_1951; 3-Nonen-5-one neg_153; Phe Asp Arg Asp neg_839; 15-dehydro-prostag pos_2086; 1-Arachidonoylgly
 neg_1953; Auberganol neg_1532; Perindoprilat gluc neg_840; Pregnanediol pos_2120; 14alpha-Hydroxyi
 neg_1990; 4-Hydroxystachyd neg_1535; Arbekacin neg_860; Desglucocheirotaxi pos_219; Glycerylphosphoryl
 neg_202; Leu Asn Arg Glu neg_1545; Litcubinine neg_889; 3-Oxo-octadecanoic pos_221; 12-OPDA
 neg_2021; 19-Oxoandrost-4- neg_1546; Esculentic acid (P neg_943; 3-Ethenyl-4-hydrox pos_2299; 2-Hexaprenyl-3-m
 neg_203; METAXALONE neg_1548; Gingerenone C neg_964; Sagittariol pos_2398; 25-Acetyl-6,7-dide
 neg_2033; PC(15:0/16:0) neg_155; Nabumetone pos_1014; 4-Hydroxy-all-trar pos_2476; Nicotinic acid mor
 neg_2037; Caffeoylcycloarte neg_1551; 3-Hydroxy-N6,N6 pos_1036; Acetaminophen cy pos_254; Oleoyl-EA(d2)
 neg_204; Glycerol 1-propano neg_1558; L-isoleucyl-L-prol pos_1058; 3-Methyl-alpha-io pos_2550; Dihydro-2-methox
 neg_2042; Crispanone neg_1563; 2-Hydroxy-6-pent pos_1108; L-Cysteine pos_2574; Squamoxinone
 neg_2046; PE(20:0/16:0) neg_1577; 12b-Hydroxy-5b-c pos_1206; (6S)-5-formyltetra pos_2576; Paricalcitol
 neg_2047; Cardoltriene neg_159; Nitrotyrosine pos_1212; Fasciculol C pos_2586; Alpha-Heptasacch
 neg_2053; Oryzaalexin E neg_1594; Gentian Violet pos_1268; Ginsenoside F5 pos_259; 2,4-Undecadienal
 neg_2059; Oxacyclotetradeca neg_1601; 2-Methoxyestrone pos_1330; PI(16:0/18:1(11Z) pos_2649; Malonoben
 neg_2060; PC(22:6(4Z,7Z,10 neg_1609; Calenduloside E pos_1340; Cyclocalopin D pos_2713; Lucidenic acid B
 neg_2061; Docosapentaenoic neg_1612; (E)-3-Heptenyl 2- pos_1350; AS 1-5 pos_2867; Cholest-5-ene

neg_207; Artabsinolid D neg_1617; Piperochromenoic pos_1423; (S)-4',7-Dihydroxy pos_2868; Hoduloside IX
 neg_2078; Leukotriene B4 et neg_1623; Cortexolone pos_1429; Kiwiionoside pos_2899; D-Sedoheptulose 7
 neg_2089; PG(18:0/20:3(5Z,1 neg_1630; Nitroxoline pos_1437; PE(18:3(6Z,9Z,12 pos_2908; Notoginsenoside R
 neg_2091; 3alpha,7alpha,12a neg_1631; PI(16:0/20:2(11Z, pos_1442; Sildenafil pos_291; 9Z,12Z-Octadecadi
 neg_2102; Imidapril neg_1661; Serinyl-Tryptoph pos_1463; Hexaethylene glycol pos_2946; (S)-[8]-Gingerol
 neg_2103; Ineketone neg_1675; Soyasapogenol B pos_152; Val Ile Ile Asp pos_2950; Ganoderic acid J
 neg_213; Rishitin neg_1681; Melilotoside B pos_1527; Gingerglycolipid I pos_2984; N5-(3,4-Dioxo-1,5
 neg_2133; Gestrinone neg_1689; MG(18:0/0:0/0:0) pos_1567; PE(22:1(13Z)/22:(pos_2989; L-Proline
 neg_2141; PE(20:2(11Z,14Z) neg_1696; 45,46,47-Trinorye pos_1587; Protodioscin pos_3039; 4-Methyl-2-pentyl-
 neg_2154; Arginyl-Lysine neg_17; 16-Hydroxypalmitic pos_1624; 3-Hydroxyvaleric pos_3054; Macrophorin A
 neg_2159; N-Docosahexaeno neg_1700; 6beta-hydroxybud pos_1628; PC(24:1(15Z)/P-1 pos_3091; 5-Hydroxy-2-(5-m
 neg_2188; Falcarinone neg_1708; Murayenol pos_1629; Monoglucuronylgl pos_3115; Nandrolone
 neg_2197; Vulgarone A neg_1711; 1-Ethyl-1H-pyrrol pos_1685; DG(18:4(6Z,9Z,1 pos_3123; 3,4-Dimethyl-5-pe
 neg_2200; trans-O-Methylgra neg_173; (+)-Isomyristic acid pos_1686; 3b-Allotetrahydro pos_3134; Glyyunnansapoger
 neg_2226; 2-(14,15-Epoxyeic neg_1733; Nebularine pos_1688; Oleoylcarnitine pos_3193; (S)-4',5,7-Trihydr
 neg_2227; Cinn cassiol D2 neg_1734; Didymin pos_1706; Valorphin pos_3229; 5-Fluorouridine m
 neg_2233; Scopolamine neg_175; 1-Palmitoyl Lysoph pos_1717; Hebevinoside V pos_3337; Nonoxynol-9
 neg_2234; 1-(5Z,8Z,11Z,14Z neg_1750; Physapubenolide pos_1720; TR-Saponin C pos_3347; DG(20:5(5Z,8Z,11
 neg_2240; 3,5,5-Trimethyl-2- neg_1759; 20-Trihydroxy-leu pos_1721; Galabiosylceramic pos_3377; PE(15:0/24:0)
 neg_2247; N-(Heptan-4-yl)be neg_1777; L-N-(1H-Indol-3-yl pos_1724; 19-hydroxyprosta pos_3460; Ginsenoside Rc
 neg_225; Beta-Alanine neg_1779; delta3,5-Deoxytig pos_1730; Ganoderic acid M pos_3513; Ornithokin
 neg_2251; (3beta,22E,24R)-F neg_1782; 8(S)-HPETE pos_1738; Mulberranol pos_353; (6Z,9Z)-6,9-Pentade
 neg_2256; Cyperotundone neg_1793; Dulcoside A pos_1742; Squamosten A pos_3560; Dodecyl butyrate
 neg_2295; Cholestane-3,7,12 neg_1794; Nb-Methyltetrahy pos_1745; 2-Heptanethiol pos_3612; Eicosadienoic acid
 neg_2308; 8-Acetylgelelolide neg_1800; Chlorogenoquinor pos_1761; PS(18:2(9Z,12Z)/ pos_3632; N-[(4E,8E)-1,3-di
 neg_2312; Cyprodinil neg_1803; Ganoderic acid A pos_1846; Tsugaric acid A 2 pos_3636; 15-Acetoxyscirpen
 neg_2323; Falcarindione neg_181; IRIFLOPHENONE pos_1863; PE(24:0/18:3(6Z,9 pos_3638; Phenformin
 neg_2334; Cilastatin neg_1810; Dihydrojasnone pos_1864; PE(20:0/20:5(5Z,8 pos_3661; 4-(Glutamylamino
 neg_235; N-(14-Methylhexad neg_1817; Docosahexaenoyl pos_1865; Soyasaponin aa pos_3760; L-4-Chlorotryptop
 neg_2363; TG(22:6(4Z,7Z,10 neg_1822; Isolimononic acid 16 pos_1904; beta-Doradecin pos_3767; Valyl-Glutamate
 neg_2364; Bimatoprost neg_1823; Phenytoin methylc pos_1906; Blasticidin S pos_383; Glycyrrhiza flavono
 neg_2367; PGP(18:1(11Z)/22 neg_1834; 9alpha-(3-Methyl pos_1980; Corchorusoside A pos_3842; L-2,3-Dihydrodipi
 neg_2386; 1,6-Hexanedithiol neg_1838; 2-(3-Methylbutyl) pos_2022; Coutaric acid pos_3928; Celastrol
 neg_2390; N-[(4-Hydroxy-3- neg_1842; 2-Hydroxy-6-(8,11 pos_2054; LysoPE(0:0/24:0) pos_3982; 2-(Ethylsulfonylm
 neg_2412; 3beta,6beta-Dihyd neg_1844; 5-hydroxy-2-oxo- pos_2069; Polymyxin B Sulfate pos_4035; 1-O-Sinapoylglucc
 neg_2424; 3-Methylhistamin neg_1845; Oleoside dimethyl pos_2097; Crassostrea Secoc pos_4040; 5-Androstene-3b,1
 neg_2426; (2xi,3xi)-2,3-Dihy neg_186; Glutaric acid pos_2133; (R)-Laudanidine pos_4047; Gluten exorphin C
 neg_2431; Arachidyl carnitin neg_1866; Koryoginsenoside pos_2139; 11-beta-Hydroxya pos_4067; Benazepril
 neg_2436; 16b-Hydroxystanc neg_1867; Maltoheptaose pos_2172; CDP-DG(16:0/20: pos_4073; Trihexosylceramid
 neg_2465; cis-4-Decenoic aci neg_1868; Tracheloside pos_218; His Ile Leu Trp pos_4173; 3-Methylcyclopent
 neg_249; 3-Hydroxy-2-methyl neg_187; Lys-Lys-OH pos_2193; Roxatidine acetate pos_4189; 7-Hydroxy-2-meth
 neg_2501; Janthitrem C neg_1882; Vicine pos_2213; PE(22:5(7Z,10Z,1 pos_4306; DG(14:0/24:1(15Z
 neg_2502; PS(18:3(9Z,12Z,1 neg_1884; Halobetasol Propi pos_2214; PS(16:0/20:4(5Z,8 pos_4324; N-Methyltryptami
 neg_2508; PIP(18:2(9Z,12Z) neg_1888; Histidinyl-Serine pos_2234; Ginsenoside F2 pos_4331; Gonyautoxin VI
 neg_2521; Pondaplin neg_1892; (+)-Galeon pos_2237; AzII pos_4343; 3-(10-Heptadeceny
 neg_2540; DG(15:0/18:3(9Z, neg_1897; 4-HDoHE pos_2263; PC(18:2(9Z,12Z)/ pos_435; 2-Methylpropanoyl
 neg_2563; PS(DiMe(13,5)/M neg_19; Methyl vanillate pos_2264; PC(22:4(7Z,10Z,1 pos_4359; Betaine aldehyde
 neg_2567; 3,5-Dimethyl-2-vi neg_1907; 2-(trans-2-Penten pos_2325; Saringosterol 3-gl pos_4361; 7-Keto-8-aminope
 neg_2571; N-Acetyl-b-glucos neg_1909; 2-Oxo-3-hydroxy- pos_2338; 2-Dodecylbenzene pos_4414; Helenalin
 neg_2572; Eriojaposide B neg_1921; (-)-(E)-1-(4-Hydr pos_2343; Lucidenic acid G pos_492; 2-Methylpropanal C
 neg_2578; PE(20:3(5Z,8Z,11 neg_1945; Robustocin pos_2366; Fumonisin B2 pos_513; Spisulosine
 neg_2594; Ethyl (囟)-2-meth neg_1947; DG(14:1(9Z)/15:0 pos_2369; Galabiosylceramic pos_537; 5-Aminosalicyclic A
 neg_2599; Hebevinoside VII neg_1948; Sorbitan oleate pos_2382; Cabergoline pos_580; HEUDELOTTIN C
 neg_2606; 1-(2,3-Dihydro-6- neg_1958; 14alpha-Hydroxy pos_2403; Leucyl-Serine pos_595; Polyoxyethylene (6
 neg_2616; Muricatin C neg_1964; Phenylpropanolan pos_2405; omega-hydroxyfin pos_606; Nitramine
 neg_2635; Dihydrocumambri neg_1968; Mabioside C pos_2427; CDP-DG(16:0/22: pos_649; 11-Hydroxycanthin-
 neg_264; alpha-Amylcinnam neg_197; 3-hydroxy-hexadec pos_2471; dIDP pos_673; PI(22:5(4Z,7Z,10Z,
 neg_2645; 3-(1,1-Dimethylal neg_1970; PE(22:4(7Z,10Z,1 pos_2489; Azythromycin pos_686; 4,2'-Dihydroxychal

neg_266; cis-[8]-Shogaol neg_1979; Macrophorin B pos_2543; Ganodermic acid I pos_80; 1-Pyrroline
 neg_2695; 3-O-Sulfogalactos neg_1987; a-L-Arabinofuran pos_2563; (3b,5a,25R)-3-Hy pos_824; (Z)-1,5-Tridecadien
 neg_2697; Cotinine methoni neg_1989; N-Acetyl-D-glucos pos_2614; PIP2(18:3(9Z,12Z pos_866; Citronellyl cinnama
 neg_2703; Methysergide neg_1993; 5,8-Epoxy-5,8-dih pos_2628; Pseudoginsenoside pos_906; 2,5-Dimethyl-3(2H)
 neg_271; 14,19-Dihydroaspic neg_1995; Ginsenoside B2 pos_2653; Trigoneoside Xb pos_926; Shyobunol
 neg_2718; Enalapril neg_2010; Rivastigmine pos_2657; Spirolide F pos_972; 3-Furanmethanol gl
 neg_272; Asperagenin neg_2050; Methionyl-Threon pos_2668; Maslinic acid 3-O-b-D-glucoside
 neg_2727; PS(18:3(9Z,12Z,1 neg_2067; PIP(16:0/22:5(7Z, pos_2678; 3-O-Sulfogalactosylceramide (d18:1/24:1(15Z))
 neg_273; [8]-Gingerdione neg_2088; (3beta,9beta)-7-Di pos_2694; Jurubine
 neg_2733; Tetrahydrocortiso neg_209; trans-2-Hexyl-1-cyc pos_2697; Cervonoyl ethanolamide
 neg_2744; Hexylresorcinol neg_2096; Isopetasoside pos_271; Erinacine B
 neg_2747; Clidinium neg_2100; Maltol pos_2718; S-Formylglutathione
 neg_2750; Bambuterol neg_211; Avocadyne pos_2762; Kentsin
 neg_2751; PE(DiMe(11,5)/D neg_2121; 12,13-DHOME pos_2766; 5'-((Z)-Feruloyl) 3-(2'-methylarabinosylxylose)
 neg_278; Octanal neg_2134; 12-hydroxyicosan pos_2776; (3b,16a,21b,22a)-12-Oleanene-3,16,21,23,28-pe
 neg_2781; 6-[2,3-Dihydroxy- neg_214; Tetracosatetraenoic pos_2777; 3-Oxotetradecanoic acid
 neg_281; [6]-Dehydroshogao neg_2148; Gemcitabine pos_2824; (E)-1-Cinnamoylpyrrolidine
 neg_2810; Cepagenin neg_2151; 5'-Methylthioaden pos_2840; Trihexosylceramide (d18:1/20:0)
 neg_2812; Buspirone N-oxid neg_2152; Vitamin A2 aldeh pos_2857; 1-Oleoylglycerophosphoinositol
 neg_282; Isoleucyl-Methioni neg_2165; Allioesterol 1-rham pos_2892; Centellasaponin C
 neg_2822; Aldosine neg_2171; Brassilexin pos_2894; Dehydroaporheine
 neg_2853; L-2-Amino-5-(me neg_218; d-Tocotrienol pos_2910; Ginsenoside Rg5
 neg_2861; Ropivacaine neg_2194; Prostaglandin E1 pos_2911; 4,4-Dimethyl-14a-formyl-5a-cholesta-8,24-dien-
 neg_29; Corticosterone neg_2203; 28-[Glucosyl-(1-> pos_2973; Goyaglycoside e
 neg_2929; Arabsin neg_2204; Hydroxypropyl-Cy pos_3007; 1alpha,3beta,22R-Trihydroxyergosta-5,24E-dien
 neg_293; 5b-Cholestane-3a,7 neg_2208; Liquiritigenin 4'-[pos_3055; TG(14:0/22:4(7Z,10Z,13Z,16Z)/18:4(6Z,9Z,12Z
 neg_2943; 22b-Hydroxychole neg_2209; 3-(4-Hydroxy-3-m pos_3064; Tertatolol
 neg_295; (E,Z)-2,4-Heptadie neg_2212; Isomammein pos_3070; PS(20:4(5Z,8Z,11Z,14Z)/22:6(4Z,7Z,10Z,13Z,1
 neg_2956; Methyl aminolevu neg_222; 13-Hydroxymarasn pos_3114; (2E,4E,6Z)-2,4,6-Decatrienoic acid dehydropipe
 neg_2983; PI(18:2(9Z,12Z)/1 neg_2228; Gibberellin A3 pos_3166; alpha-Solamarine
 neg_2991; Glutamyl-Leucine neg_223; 5b-Cholestane-3a,7 pos_3175; Retrocalamin
 neg_3014; PG(18:3(6Z,9Z,12 neg_2230; Chrysophanol 8-g pos_3182; PS(DiMe(9,3)/DiMe(9,3))
 neg_302; Illicifolinoside A neg_2235; Methyl (Z,Z)-10-h pos_3202; M-Secociguatoxin 4A
 neg_304; 7-Aminonitrazepar neg_2238; N-Arachidonoyl ty pos_3224; Isepamicin
 neg_3052; UDP-4-dehydro-6 neg_2252; 1-Acetyl-3,27-dih pos_3272; 4'-N-desmethylolanzapine
 neg_306; Theaspirone A neg_2255; 4alpha-Formyl-4b pos_3381; Achyranthoside C
 neg_3067; LysoPC(18:4(6Z,9 neg_2280; Enalaprilat pos_340; 15-Octadecene-9,11,13-triynoic acid
 neg_3079; PG(16:1(9Z)/18:2 neg_2281; 6-Hydroxy-4,6-dir pos_342; Soyasaponin I
 neg_3086; PC(20:5(5Z,8Z,11 neg_2286; all-trans-Decapren pos_3461; PE(20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
 neg_3109; Dehydroascorbide neg_2289; Torvoside D pos_3466; Alliospiroside C
 neg_3121; S-(3-Methylbutan neg_2296; Polyporusterone C pos_3515; Anidulafungin
 neg_3126; Decyl propionate neg_2307; Dityrosine pos_3519; Sativoside R2
 neg_315; 11-Hydroxy-12-me neg_2316; PC(P-16:0/22:2(1 pos_3540; 1,7-Dimethylguanosine
 neg_3153; DG(20:4(8Z,11Z, neg_233; 3-Hydroxyisovalery pos_3570; Notoginsenoside R6
 neg_316; 11beta-Hydroxytest neg_2332; 3-Hydroxy-9-hexa pos_3575; Isobutyl N-methylanthranilate
 neg_3170; Epsilon-(gamma-C neg_2337; 2-Polyprenyl-3-m pos_3618; Pisatoside
 neg_3186; Capsoside A neg_2338; Cotinine glucuron pos_3653; Octyl 2-furoate
 neg_3190; Acorusnol neg_2339; Lc3Cer pos_3674; Sucrose acetate isobutyrate
 neg_3207; TG(14:1(9Z)/18:4 neg_2348; 18-Oxocortisol pos_3683; PG(16:0/16:1(9Z))
 neg_3213; 3b,17b-Dihydroxy neg_2355; Diethylcarbamazir pos_3694; DG(15:0/22:0/0:0)
 neg_3221; Prostaglandin F3a neg_2356; Prostaglandin E3 pos_3696; Oleanolic acid 3-[rhamnosyl-(1->4)-glucosyl-(1-
 neg_3233; PGP(16:0/18:0) neg_2370; 20-COOH-leukotr pos_3716; Lansioside B
 neg_3246; Carboxy-ibuprofe neg_2378; Caraganoside A pos_3728; PC(15:0/20:2(11Z,14Z))
 neg_3253; 2-Methylbutyroyl neg_241; 5-Nonyltetrahydro- pos_3773; Dynorphin A 9-17
 neg_328; Tryptamine neg_2413; PS(MonoMe(11,3 pos_3775; (S)-4',5,7-Trihydroxy-6-prenylflavanone
 neg_3293; 2-Pyrrolidineaceti neg_242; 2-Dodecenal pos_384; CDP-DG(18:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z
 neg_3297; 2',6'-Dihydroxy-4' neg_2425; Coriandrone D pos_3868; PE(18:3(6Z,9Z,12Z)/22:6(4Z,7Z,10Z,13Z,16Z,1
 neg_3306; DG(15:0/16:1(9Z) neg_2434; Dehydrocarpaine l pos_3903; 2-Amino-5-benzoylbenzimidazole

neg_3309; Dimethylbenzimid neg_2445; 3'-(gamma,gamma pos_3918; Erinacine G
 neg_331; Calamendiol neg_2449; Mabioside A pos_3950; Physalolactone B
 neg_3312; Glutamyl-Serine neg_2452; Butorphanol pos_3984; alpha-[3-[(Hydroxymethyl)nitrosoamino]propyl]
 neg_332; Ascaridole neg_2453; 2-Ethoxy-5-methy pos_4043; PE(22:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
 neg_3322; PS(18:3(9Z,12Z,1 neg_246; Docosapentaenoic acid pos_4046; PIP2(18:2(9Z,12Z)/20:2(11Z,14Z))
 neg_3325; (5S)-hydroperoxy- neg_2462; 9-Oxo-octadecanoic acid pos_4048; Mulberrofuran T
 neg_3326; 17-Hydroxyproge neg_2463; Bisoprolol pos_4077; PE(18:3(6Z,9Z,12Z)/22:1(13Z))
 neg_3347; Ganoderic acid th neg_2467; Ergocalciferol pos_4101; Tocophersolan
 neg_3350; Violanone neg_2471; Gibberellin A54 pos_4112; Quinquenoside IV
 neg_3359; 5-Dehydroepisterc neg_2473; PIP2(16:0/18:2(9Z pos_4127; Poppy acid
 neg_3364; 3beta-Acetoxy-11; neg_2476; 8-HDoHE pos_4138; Stevioside
 neg_3408; 3',5'-Dihydroxy-4', neg_2479; Suspensolide F pos_4152; Piperochromanoic acid
 neg_341; 5-Hydroxy-p-menth neg_2480; Idarubicin pos_4249; CDP-DG(18:0/20:4(8Z,11Z,14Z,17Z))
 neg_3410; 11-Oxo-octadecanoic neg_2487; Palmitoylstigmast pos_4251; Soyasaponin II
 neg_3440; Methyl 10-undec neg_2493; N-Carbamoyl-2-ar pos_4284; PIP(18:2(9Z,12Z)/18:1(11Z))
 neg_3442; Myristic acid neg_25; Sebacic acid pos_4335; Pefloxacin N-oxide
 neg_3443; Yucalexin P21 neg_2500; Prostaglandin D1 pos_4350; PE(20:1(11Z)/24:0)
 neg_3448; PC(22:0/22:4(7Z, neg_251; 6-Hydroxypentadec pos_4365; (+)-Mevalonolactone
 neg_3449; (3beta,19alpha)-3, neg_2515; Dide-O-methylsin pos_4372; 11(Z),14(Z)-Eicosadienoic Acid
 neg_3452; TG(20:4(5Z,8Z,11 neg_252; 4-Hydroxy-3-(16-m pos_44; Wogonin
 neg_347; 4-Hydroxy-3-meth neg_2520; Quinic acid pos_442; PE(12:0/16:1(9Z))
 neg_3472; Ethyl (3R,5Z)-3-h neg_2522; omega-Hydroxym pos_466; Panaquinquecol 4
 neg_349; Coprocholic acid neg_2530; Kudzusaponin SA pos_588; 3-Dimethylallyl-4-hydroxymandelic acid
 neg_3499; Imidaprilat neg_2541; 1-(7Z,10Z,13Z,16 pos_594; PS(12:0/19:0)
 neg_350; Trimipramine neg_2544; 2,3-Dimethyl-2-cy pos_610; (17Z)-1,25-dihydroxy-26,27-dimethyl-17,20,22
 neg_3516; Pyridostigmine ca neg_255; Imazamethabenz pos_655; PE(16:0/22:5(4Z,7Z,10Z,13Z,16Z))
 neg_3522; 15-keto-Prostagla neg_2552; 2-(1-Pentenyl)fura pos_706; PE(15:0/15:1(9Z))
 neg_3531; MG(18_2(9Z,12Z neg_2553; Corchorosol A pos_74; cis-12-Octadecenoic Acid methyl ester
 neg_3532; Compactin neg_2557; Oleanolic acid pos_750; Quinaprilat
 neg_3541; Valyl-Leucine neg_2569; Heterophyllin pos_797; 4-(Methylthio)-1-butanol
 neg_3545; 11-Deoxycorticost neg_2590; Dehydrocarpain pos_819; Pro Val Ser Leu
 neg_3546; Valyl-Histidine neg_2609; (E)-3-(Tetrahydro pos_848; 12-Hydroxy-12-octadecanoylcarnitine
 neg_3553; 13,14-Dihydro-15 neg_2613; 15-Hydroxyleptoc pos_991; Austroinulin
 neg_3554; Tridecanoic acid (neg_2614; Lysyl-Valine
 neg_3555; Venlafaxine neg_2621; Araliasaponin V
 neg_3556; 5-Hydroxytryptop neg_2622; Linalyl anthranilate
 neg_3566; Piperidione neg_2626; 2,4-Dihydroxy-6,7-dimethoxy-2H-1,4-benzoxazin-3(4H)-one
 neg_3572; p-Tolualdehyde neg_2629; 2,3-Dihydroxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanone
 neg_3580; Misoprostol (free neg_2631; 5'-Phosphoribosyl-N-formylglycinamide
 neg_3582; 4-Oxoretinol neg_2642; 3-trans-p-Coumaroylrotundic acid
 neg_3583; Nervonic acid neg_265; Cucurbitic acid
 neg_3588; Jasmonic acid neg_2651; Methyl acrylate-divinylbenzene, completely hydrolyzed, copolymer
 neg_359; Gabapentin neg_2657; Kaempferol 7-sophoroside
 neg_3604; (-)-Usnic acid neg_2662; Theogallin
 neg_374; 12-oxo-20-dihydro neg_2663; L-Fucose
 neg_380; Ustiloxin D neg_2675; 20-Dihydrodydrogesterone
 neg_386; (3S,6E)-Nerolidol neg_2690; (8R)-3',4'-Methylenedioxy-5,7-dimethylepicatechin
 neg_394; Neohesperidose neg_2692; N-Desmethyl sildenafil (UK-103,320)
 neg_4; Pantothenate neg_2698; Alpha-linolenyl carnitine
 neg_400; (S)-3-Methylthiohe neg_2701; Amprenavir
 neg_402; Isopropyl beta-D-gl neg_2728; Calendulose H methyl ester
 neg_406; Antibiotic X 14889 neg_2738; (8R,8'R)-Secoisolariciresinol 9,9'-bis-[4-carboxy-3-hydroxy-3-methylbutanoyl-
 neg_422; Prostaglandin F2a neg_2757; Zanthobisquinolone
 neg_425; 19-Hydroxytestoste neg_277; 9-Decenoic acid
 neg_430; ACRL Toxin II neg_2771; Muricoreacin
 neg_437; 3-keto Fusidic acid neg_2775; Trigofenoside F
 neg_446; (-)-trans-Carveol gl neg_2777; 5-O-beta-D-Xylopyranosyl-L-arabinose
 neg_455; Notoginsenoside J neg_2793; TG(15:0/20:5(5Z,8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))

neg_458; Oleoyl glycine neg_2799; L-2-Amino-3-(oxalylamino)propanoic acid
 neg_463; Fagomine neg_2800; Salsolinol 1-carboxylate
 neg_464; 3-Methylcrotonylgl neg_2806; Eremopetasitenin B2
 neg_473; Ginkgoic acid neg_2824; Goshonoside F4
 neg_478; (2'E,4'Z,7'Z,8E)-Co neg_2829; 6-Caffeoylsucrose
 neg_483; 1,3-Diphenylpropar neg_283; 1-Octen-3-yl glucoside
 neg_484; 5-(14-Nonadecenyl neg_2846; Albanin H
 neg_496; 2-Methylacetophen neg_2851; Oxytocin 1-8
 neg_498; alpha-Zearalenol neg_2855; 4,6-Heptadiyne-1,3-diol
 neg_500; Tyrosyl-Isoleucine neg_2856; Propyl propane thiosulfonate
 neg_508; 5'-Carboxy-gamma- neg_2882; 11-Hydroxy-9-tridecenoic acid
 neg_514; Oleic acid neg_2884; Nigellimine N-oxide
 neg_521; Cobinamide neg_2885; DL-Ornithino-L-alanine
 neg_522; Prolyl-Tyrosine neg_291; MG(0:0/14:1(9Z)/0:0)
 neg_532; Pantothenic acid neg_2920; Tragopogonsaponin C
 neg_535; 5-(8,11-Pentadecad neg_2923; L-phenylalanyl-L-hydroxyproline
 neg_540; 1,5,5,8-Tetramethyl neg_2933; Negletein 6-[rhamnosyl-(1->2)-fucoside]
 neg_541; 5beta-Cholestane-3 neg_2937; L-2-Amino-3-(1-pyrazolyl)propanoic acid
 neg_542; Phytocassane B neg_294; 5-Dodecenoic acid
 neg_55; 未-CEHC neg_2946; Melilotoside D
 neg_562; 3-Decenoic acid neg_2955; 1'-Acetoxyeugenol acetate
 neg_566; 1-Acetoxy-4,6-tetra neg_2958; L-alpha-glutamyl-L-hydroxyproline
 neg_574; 5-(10,13-Nonadeca neg_2959; 2-Decarboxybetanin
 neg_583; (14S)-14,15-Dihyd neg_296; Aflatoxin B1 dialcohol
 neg_59; Quadrone neg_2961; Cajaisoflavone
 neg_591; (3alphaOH,20S,24S neg_2967; Threoninyl-Phenylalanine
 neg_602; Rhazidigenine Nb- neg_2969; PE(14:0/20:4(5Z,8Z,11Z,14Z))
 neg_604; MG(0:0/20:1(11Z)/ neg_2973; PC(22:4(7Z,10Z,13Z,16Z)/24:1(15Z))
 neg_613; Alfalcacidol neg_2978; 8-Hydroxyoctanoate
 neg_618; 3-Oxo-1,4,11(13)-e neg_2981; 4-hydroxy ketorolac
 neg_626; Polyporusterone A neg_2982; 5'-Hydroxy-3',4',7-trimethoxyflavan
 neg_628; 3-Nonanon-1-yl ace neg_3006; C.I. Natural Red 20
 neg_633; Didanosine neg_301; Menthyl ethylene glycol carbonate
 neg_642; NAPQI neg_3020; Adrenorphin
 neg_655; (Z,Z)-2,9,16-Hepta neg_3021; 2-Hexenoylcholine
 neg_684; Isoleucyl-Lysine neg_3025; 1,2,3,4-Tetrahydro-2-methyl-b-carboline
 neg_692; 3-hydroxytridecano neg_3026; Lactucin
 neg_695; Cinchonidine neg_305; Jasmolone
 neg_696; Arginyl-Arginine neg_3050; 14R,15S-EpETrE
 neg_705; Copalic acid neg_3051; Niaziminin A
 neg_719; 3,7-Dihydroxy-12- neg_3055; S-nirvanol
 neg_737; Allyl thiohexanoate neg_3064; Withaperuvine H
 neg_743; Oxyphencyclimine neg_3068; Prostaglandin E2
 neg_746; Sterebin A neg_307; Setariol
 neg_76; 伪-Phenylcyclohexyl neg_3070; 3b,8b-Dihydroxy-6b-(3-chloro-2-hydroxy-2-methylbutanoyloxy)-7(11)-eremol
 neg_762; 5-Phenyl-1,3-oxazi neg_3078; 3-Hydroxymethylantipyrine
 neg_764; PC(MonoMe(11,3) neg_3082; Acrimarine N
 neg_772; Resveratrol 4'-(6-ga neg_3101; 16-Hydroxy hexadecanoic acid
 neg_783; ent-8(17),13(16),14 neg_311; Falcariindiol
 neg_784; (22Alpha)-hydroxy neg_3111; 1,2-Diacylglycerol-LD-PI-pool
 neg_791; Histidinyl-Isoleucine neg_3118; 5(S)-Hydroperoxyeicosatetraenoic acid
 neg_792; Secobarbital neg_3131; 8-oxo-dGDP
 neg_794; (14alpha,17beta,20 neg_3133; Ethyl 3-hydroxyoctanoate O-[glucosyl-(1->6)-glucoside]
 neg_80; 19(R)-hydroxy-PGA neg_3145; N-(1-Deoxy-1-fructosyl)tyrosine
 neg_802; Absindiol neg_3146; gamma-L-Glutamyl-L-methionine sulfoxide
 neg_803; Citreovirenone neg_3154; 10,12-Pentacosanedione
 neg_806; 1b,3a,7b-Trihydrox neg_3162; Fistuloside B
 neg_813; Talinolol neg_317; Hexyl acetate

neg_823; Lysyl-Proline neg_3180; 4-Hydroxy-3-polyprenylbenzoate
 neg_828; 24-Ethyllophenol neg_3193; (S)-Oleuropeic acid
 neg_829; 16-Acetylpriveroge neg_3200; 2-Ethylidihydro-3(2H)-thiophenone
 neg_83; 1,11-Undecanedicarbal neg_3202; Ethyl 2,4-dioxohexanoate
 neg_869; 13'-Carboxy-gamm neg_3204; LysoPE(0:0/18:4(6Z,9Z,12Z,15Z))
 neg_877; (S)-Verimol F neg_3217; Medicoside I
 neg_884; 17a,21-Dihydroxy-! neg_3220; Thiamine monophosphate
 neg_892; Glyuranolide neg_3222; Edultin
 neg_894; 2-Acetyl-5-methylf neg_3224; Methylphenidate
 neg_897; Prolyl-Arginine neg_3225; 3-Hydroxyglabrol
 neg_898; thymidine 3'-mono neg_3226; Chlorophyll d
 neg_899; D-Glucuronic acid neg_3228; 3-Hydroxy-beta-ionol 3-[glucosyl-(1->6)-glucoside]
 neg_900; Furanofukinin neg_3230; Ganoderic acid H
 neg_908; 3-Acetoxyscirpene- neg_3243; Hydroxyclo mipramine glucuronide
 neg_910; Valdiate neg_3247; PC(DiMe(11,5)/MonoMe(11,3))
 neg_924; 2beta,9xi-Dihydrox neg_325; 4,6-Pentacosanedione
 neg_929; CD 1790 neg_3257; Hexadecanedioic acid mono-L-carnitine ester
 neg_957; alpha-Butyl-omega- neg_3258; TG(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))[iso6]
 neg_96; N-Alpha-acetyllysine neg_3271; 4'-hydroxytrazodone
 neg_961; Clarithromycin neg_3289; N-[2-(4-Prenyloxyphenyl)ethyl]tiglamide
 neg_962; 22-Acetylpriveroge neg_329; Phenylethanolaminium
 neg_973; (+)-(S)-Carvone neg_3300; Withaperuvine E
 neg_975; Methionyl-Proline neg_3301; xi-7-Octen-2-ol
 neg_979; Ganoderic acid G neg_3311; (E,E)-Boviquinone 3
 neg_999; PI(16:1(9Z)/16:1(9 neg_3313; Cysteinyl-Glutamate
 pos_100; Val Ile Ile neg_3315; Gentisin
 pos_1004; Porrigenin A neg_3318; PC(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
 pos_1005; (Z)-4-Heptenal neg_3329; PS(DiMe(11,3)/MonoMe(13,5))
 pos_1009; Wyrone neg_333; 5a-Cholestane-3a,7a,12a,25-tetrol
 pos_1010; D-Alanyl-D-alanin neg_3334; MG(0:0/20:0/0:0)
 pos_1014; 4-Hydroxy-all-trar neg_334; Lepidiumterpenyl ester
 pos_1015; 5,6-Dihydro-11-m neg_3345; beta-D-Galactopyranosyl-(1->4)-2-amino-2-deoxy-beta-D-glucopyranosyl-(1->
 pos_102; Pro Pro Ala Thr neg_335; 1-heptadecanoyl-glycero-3-phosphate
 pos_1021; 2-Acetyl-3-ethylid neg_3351; [6]-Gingerdiol 3-acetate
 pos_1024; Ethinamate neg_3358; DG(20:5(5Z,8Z,11Z,14Z,17Z)/22:2(13Z,16Z)/0:0)
 pos_1027; 3,4,5,6-Tetrahydro neg_336; delta-Methylinone
 pos_1072; xi-2,3-Dihydro-3,5 neg_3372; Amylopectin
 pos_1077; (R)-2-Hydroxy-4- neg_3394; L-Menthyl (R,S)-3-hydroxybutyrate
 pos_1081; Humulinic acid A neg_3404; P1,P4-Bis(5'-uridyl) tetraphosphate
 pos_1083; 3-keto-Digoxigenin neg_3414; 6,8-Heneicosanedione
 pos_1103; Valerianol neg_3421; Niazicin A
 pos_1120; meta-O-Dealkylate neg_3429; Fludiazepam
 pos_1139; p-Mentha-1,3,8-tri neg_3434; Allyl butyrate
 pos_1141; 1alpha,23(S),25-tr neg_3451; Amaranthussaponin I
 pos_116; Eremolactone neg_3460; Deoxyinosine
 pos_1169; Filifiline neg_3468; L-Oxalylalbizziine
 pos_1173; Australigenin neg_3480; Glycerol tripropanoate
 pos_1180; N-Acetylanonaine neg_3482; Schinifoline
 pos_1210; Pentacosanoylglyc neg_3488; 13E-Tetranor-16-carboxy-LTE4
 pos_1213; Glutaminyl-Hydro neg_3500; Momordicoside G
 pos_1216; Dipthamide neg_3502; Parasiloxanthin
 pos_123; 3-Deoxyestradiol neg_3504; Myricatomentoside II
 pos_1231; Austalide K neg_3505; (6b,7b,13R)-6,7-Diacetoxy-8,14-labdadiene-13-ol
 pos_1247; Pyridoxamine neg_3506; Cepanone
 pos_1253; 13-L-Hydroperoxy neg_3511; Harmalol
 pos_1255; Pyrazinemethanetl neg_3518; Deoxycoryformycin
 pos_1258; Idoxuridine neg_3525; 1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine
 pos_1260; 6-Methylthiopurin neg_3527; (+)-Absciscic acid

pos_1268; Ginsenoside F5 neg_3540; delta-Tocotrienol
 pos_1270; 2-beta-hydroxy me neg_3563; 1-Palmitoylglycerol
 pos_1272; Enol-3-Ethyl-1,2- α neg_3569; Androstendione
 pos_1276; 1-Methoxy-3-methyl neg_3571; 3-Methylcyclohexanethiol
 pos_1278; 24-Hydroxycholesterol neg_3573; Phenylalanyl-Glutamine
 pos_1281; 4-Methyl-1-phenyl neg_3578; Leucyl-Glutamine
 pos_1284; 7-hydroxygraniset neg_3579; 2'-O-methylinosine
 pos_1290; Sorbitan palmitate neg_3593; Serotonin
 pos_1292; Cymorcin monoglucoside neg_3602; 9Z,12Z-Linoleic acid
 pos_1294; 1-Acetoxy-2-hydroxy neg_3603; Geldanamycin
 pos_13; Duloxetine neg_361; Ribothymidine
 pos_1305; 1,4'-Bipiperidine-1,4'-diol neg_37; Tetradecanedioic acid
 pos_1308; 7 α ,12 α ,26-trihydroxy neg_377; N-Jasmonoylisoleucine
 pos_133; 5 β -Androst-16-en-3-one neg_388; Armillaripin
 pos_1330; PI(16:0/18:1(11Z)) neg_389; 3-Oxohexadecanoic acid
 pos_1332; Illudin C2 neg_393; Amyl salicylate
 pos_1335; Ethyl menthane carboxylate neg_405; (2S,2'S)-Pyrosaccharopine
 pos_1337; 15(S)-Hydroxyeicosanoic acid neg_407; Lyciumoside III
 pos_134; (22E)-3 β ,7 β ,12 β -Trihydroxy-13,14-dihydro-2H-pyran-2-one neg_415; 2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-diene
 pos_1349; cis-Hydroxy Perhexilene neg_418; 13-Nor-6-eremophilene-8,11-dione
 pos_135; m-Xylene neg_420; (S)-3-Octanol glucoside
 pos_1354; Tetrahydropersin neg_423; trans-p-Menthane-7,8-diol 7-glucoside
 pos_1358; Mupirocin neg_438; 5,9-Epidioxy-3-hydroxyergost-7-en-6-one
 pos_136; Val Glu Val Arg neg_440; 17,23-Epoxy-29-hydroxy-27-norlanost-8-ene-3,15,24-trione
 pos_1367; 41-O-demethylrapamycin neg_444; alpha-D-Xylopyranosyl-(1 $\rightarrow$ 6)-beta-D-glucopyranosyl-(1 $\rightarrow$ 4)-D-glucose
 pos_137; Lys Lys Met Gln neg_449; DG(16:1(9Z)/16:1(9Z)/0:0)
 pos_1388; LysoPC(18:0) neg_454; Polyethylene, oxidized
 pos_139; PG(16:0/0:0)[U] neg_460; LysoPE(0:0/14:0)
 pos_1410; Tolbutamide neg_465; 6-beta-hydrocortisol
 pos_1421; 4-Butyl-2-methylol neg_469; Muricin H
 pos_1423; (S)-4',7-Dihydroxy neg_482; (+)-threo-2-Amino-3,4-dihydroxybutanoic acid
 pos_1432; 6-Succinoaminopterin neg_486; Capecitabine
 pos_1437; PE(18:3(6Z,9Z,12Z)) neg_497; Arachidonic acid
 pos_1453; Spirolide B neg_50; 5-cis Carbaprostacyclin
 pos_1465; PE(18:4(6Z,9Z,12Z)) neg_513; (1R*,2R*,4R*,8S*)-p-Menthane-1,2,8,9-tetrol 9-glucoside
 pos_1466; 1-Phenyl-1-pentanol neg_518; 8-Hydroxynevirapine
 pos_147; 1 β -hydroxy-23,24-dihydroxy neg_52; 2-Isopropylmalic acid
 pos_1482; isobutyrylcarnitine neg_533; Ascorbalamic acid
 pos_1491; 4-(2,6,6-Trimethyl-2-oxocyclohexyl) neg_538; 3-hydroxyropivacaine
 pos_1497; (2E,11Z)-Wyeroneg_539; Ganodermatriol
 pos_1511; 3-Methyl-1-(2,4,6-trimethylphenyl) neg_54; 6-keto PGE1
 pos_152; Val Ile Ile Asp neg_551; 7(14)-Bisabolene-2,3,10,11-tetrol
 pos_1520; (3E,7E)-4,8,12-Trihydroxy neg_552; Neryl glucoside
 pos_1527; Gingerglycolipid I neg_553; Goshonoside F1
 pos_1538; 5-b-Cholestane-3 α neg_556; LysoPE(0:0/14:1(9Z))
 pos_1540; N-Succinyl-2-amino-6-aminocaproic acid neg_58; (R)-12,13-DiHOME
 pos_1560; Hovenidulcioside neg_580; Dihydro-3-(2-octenyl)-2,5-furandione
 pos_1577; LysoPE(0:0/24:6(11Z)) neg_581; Lamivudine-monophosphate
 pos_158; 13-METHYL-4,4-E neg_585; 2-Palmitoylglycerophosphocholine
 pos_1580; Octreotide neg_590; 12-Oxo-20-trihydroxy-leukotriene B4
 pos_1581; Cloversaponin I neg_593; MG(0:0/22:2(13Z,16Z)/0:0)
 pos_1585; Alpha-Cryptoxanthin neg_594; 3-hydroxyhexadecanoyl carnitine
 pos_1587; Protodioscin neg_595; 22-Angeloylbarringtonol C
 pos_1603; 3-(Acetyloxy)-2-hydroxy neg_598; Stercurensin
 pos_1604; Fucoxanthin neg_600; (R)-Oxypeucedanin
 pos_1606; 24,25,26,27-Tetrahydro-2H-pyran-2-one neg_601; Ganoderic acid L
 pos_1607; 3-Hydroxyhexadecanoic acid neg_606; Obtustylene
 pos_1609; Arginyl-Histidine neg_609; N-Formyl-L-methionine

pos_1617; 4,5-Dimethyl-2-he neg_612; Procainamide
 pos_1626; O-Desmethyloango neg_616; (17alpha,23S)-17,23-Epoxy-29-hydroxy-27-norlanosta-1,8-diene-3,15,24-trione
 pos_1627; Ganoderiol H neg_629; (2E,6E)-Piperamide-C7:2
 pos_1629; Monoglucuronylg neg_630; Cyclocalopin C1
 pos_1656; Kukoamine B neg_634; N-Acetylmuramoyl-Ala
 pos_1663; 3b-Hydroxy-6b-m neg_639; Ramiprilat
 pos_1669; 3beta-Acetoxy-19; neg_645; (S)-alpha-Amino-4-carboxy-3-furanpropanoic acid
 pos_1677; 2-Methyl-1-hydro; neg_650; LysoPE(0:0/15:0)
 pos_1681; Palmitoyl glucuro; neg_656; D-Glucaro-1,4-lactone
 pos_1686; 3b-Allotetrahydro; neg_66; HU-211
 pos_169; 5,8,11-Octadecatriy neg_661; eta-Tocopherol
 pos_1706; Valorphin neg_664; Achillicin
 pos_1707; 2-Deoxycastastero neg_669; hydroxyrepaglinide
 pos_1717; Hebevinoside V neg_672; (3beta,5alpha,6alpha,7alpha,22E,24R)-5,6-Epoxyergosta-8,14,22-triene-3,7-dio
 pos_1720; TR-Saponin C neg_675; MG(0:0/22:1(13Z)/0:0)
 pos_1724; 19-hydroxyprosta; neg_68; (𐄀)-Catechin
 pos_1726; 4-oxo-Retinoic aci neg_680; Oxybuprocaine
 pos_1729; PE(14:1(9Z)/18:4(neg_682; Tavulin
 pos_1732; 7-Ethyl-2,3,6,7-tet neg_683; Myricanene B 5-[arabinosyl-(1->6)-glucoside]
 pos_1757; Hydroxyhomodest neg_693; N-Ethyl trans-2-cis-6-nonadienamide
 pos_1761; PS(18:2(9Z,12Z)/. neg_698; Calendulose H
 pos_178; Glechomanolide neg_703; Caffeic acid
 pos_1785; 4-Hydroxyretinoic neg_706; Melleolide
 pos_1802; Araliasaponin III neg_709; Digitoxin
 pos_1807; (3beta,5alpha,6bet neg_712; (9R,10S,12Z)-9,10-Dihydroxy-8-oxo-12-octadecenoic acid
 pos_1808; PG(16:0/18:3(6Z,4 neg_718; 3-hydroxyundecanoyl carnitine
 pos_181; LysoPC(20:4(5Z,8Z neg_729; trans-3-Hydroxycotinine glucuronide
 pos_1820; 9alpha-(3-Methyl- neg_736; 2,2'-Dithenyl sulfide
 pos_1835; PS(20:4(5Z,8Z,11 neg_747; 5alpha-Cholestanone
 pos_1836; 1,2-Dihydrodehyd neg_75; 13,14-dihydro Prostaglandin E1-d4
 pos_1842; Collettiside I neg_753; 3-(2-Heptenyloxy)-2-hydroxypropyl undecanoate
 pos_1846; Tsugaric acid A 2; neg_756; Tetracosanoylglycine
 pos_1860; 11-Hydroxyandro; neg_757; Vitamin K2
 pos_1871; 3-[(3-Methylbutyl neg_759; 3-trans-Caffeoyltormentic acid
 pos_1904; beta-Doradecin neg_763; 2,4-Dihydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one 2-glucoside
 pos_1908; Hydroxyclo miprar neg_773; 3-Fucosyllactose
 pos_1918; PS(18:0/18:2(9Z,1 neg_778; Physapubescin
 pos_1920; Eicosapentaenoyl neg_781; Norbutorphanol
 pos_1922; Pteroside A neg_79; 11(R)-HEDE
 pos_1924; Hexyl benzoate neg_790; Notoginsenoside T2
 pos_1926; Hoduloside V neg_796; Desglucocorolose
 pos_1931; 4-(3-Hydroxybuty neg_8; trans-3-Coumaric acid
 pos_1935; 3-O-Sulfogalactos neg_800; 9,12-Hexadecadienoylcarnitine
 pos_1941; Testolactone neg_815; 2-Arachidonoylglycerophosphocholine
 pos_1952; (3beta,24xi)-Cyclc neg_821; Maltotriose
 pos_1960; 23S,25,26-Trihyd neg_824; (3b,6b,8b,12a)-8,12-Epoxy-7(11)-eremophilene-6-angeloyloxy-8,12-dimethoxy
 pos_1964; 7-Hydroxyglyclazi neg_827; 3-Hexaprenyl-4-hydroxy-5-methoxybenzoic acid
 pos_1969; Ganoderic acid C2 neg_830; Pentadecanoylglycine
 pos_1980; Corchorusoside A neg_834; 3-Hydroxynevirapine glucuronide
 pos_1988; (25S)-26-Hydroxy neg_838; Campesteryl caffeate
 pos_2012; 1-(4-Hydroxy-3-m neg_84; DIHYDROJASMONIC ACID
 pos_2014; 3a,7a-Dihydroxyc neg_862; 2-Amino-4-ethoxy-3-hydroxybutanoic acid
 pos_2015; Phytolaccoside D neg_87; 1-Dehydro-12-gingerdione
 pos_2016; 13-HOTE neg_90; D-Xylulose
 pos_2022; Coutaric acid neg_904; Prosapogenin
 pos_2023; Furaneol 4-glucosi neg_920; DG(15:0/18:4(6Z,9Z,12Z,15Z)/0:0)
 pos_203; (S)-11,12,13-Trino; neg_938; L-Menthyl acetoacetate
 pos_2031; PC(18:3(9Z,12Z,1 neg_939; N2-Succinoylarginine

pos_2032; 2,4-Diamino-6-nit neg_942; Reticulatexanthin
pos_2042; Pyrrolidine neg_944; Oleanolic acid 3-[glucosyl-(1->4)-xyloside]
pos_2048; RPR112698 neg_945; 3,7,11,15,23-Pentaoxolanost-8-en-26-oic acid
pos_2049; Grevilline B neg_947; N-Arachidonoyl GABA
pos_2054; LysoPE(0:0/24:0) neg_978; 13'-Hydroxy-alpha-tocotrienol
pos_2069; Polymyxin B Sulfate neg_982; 3-Hydroxy-1-phenyl-1-eicosanone
pos_207; Cicutoxin neg_985; (2S,24S)-17,23-Epoxy-24,29-dihydroxy-27-norlanost-8-ene-3,15-dione
pos_2072; 2-Hydroxymyristic acid neg_997; (3beta,4alpha,5alpha,24S)-4,14-Dimethylstigmasta-8,25-dien-3-ol
pos_2078; Pipazethate pos_10; Xanthurenic acid
pos_2083; 10,11-dihydro-20-pos_1008; 6,8-Dihydroxypurine
pos_2096; Difluprednate pos_1016; Dihydrozeatin-O-glucoside
pos_2098; Glucosylceramide pos_1018; 6-Cinnamoyl-1-galloylglucose
pos_2100; Trypanothione dis pos_1022; Kobusone
pos_2104; 24-Hydroxyglabro pos_1026; Butyl 3-methylbutanoate
pos_2114; Carbamazepine pos_1036; Acetaminophen cysteine
pos_2119; Persenone B pos_1044; 7a,12a-Dihydroxy-cholestene-3-one
pos_212; 3-Deoxyestrone pos_1058; 3-Methyl-alpha-ionyl acetate
pos_2126; Beta-D-Glucopyranose pos_1059; MG(0:0/15:0/0:0)
pos_2137; 4,4-Dimethyl-14-al pos_106; PG(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)
pos_2139; 11-beta-Hydroxyoctadecanoic acid pos_1061; 2(R)-hydroxyicosanoic acid
pos_215; delta2-THA pos_1062; Almotriptan
pos_2158; DG(22:1n9/0:0/22 pos_1063; (1beta,2beta,5beta)-p-Menth-3-ene-1,2,5-triol
pos_2169; (1R,2R,4S)-p-Mercuric chloride pos_1068; 2-Methylpropyl butanoate
pos_2170; (-)-Matairesinol 4' pos_1069; Butyl propionate
pos_2172; CDP-DG(16:0/20:0) pos_1071; 5-Octadecynoic acid
pos_2177; 2-Ethylsuccinic acid pos_1074; 10,20-Dihydroxyeicosanoic acid
pos_2193; Roxatidine acetate pos_1076; 4-Hydroxyphenylpyruvic acid
pos_220; Val Val Val pos_1079; Zerumbone oxide
pos_2208; Capsicum annuum pos_1080; Dopamine quinone
pos_2214; PS(16:0/20:4(5Z,8Z,11Z,14Z,17Z)) pos_1082; Phytosphingosine-1-P
pos_2218; Secoeremopetasitol pos_1086; (R)-3-Hydroxy-Octadecanoic acid
pos_2224; Cedryl acetate pos_1089; Alkaloid AQC2
pos_2248; 2-Hydroxy-2,6,6-trimethyl-2,6-heptanedioic acid pos_1095; 3alpha-O-trans-Feruloyl-2alpha-hydroxy-12-ursen-28-oic acid
pos_2254; Mamea B/BC cy pos_1096; CE(20:4(8Z,11Z,14Z,17Z))
pos_2255; 7Z,10Z-Hexadecaenoic acid pos_1100; 5'-Deoxy-5-fluorocytidine
pos_2260; 2,3-Decanedion pos_1107; 6,11-Dihydroxy-2,2-dimethylpyrano[3,2-c]xanthen-7(2H)-one
pos_2264; PC(22:4(7Z,10Z,13Z,16Z)) pos_1108; L-Cysteine
pos_2270; PE(18:2(9Z,12Z))/POSH pos_1111; Lepidiumterpenoid
pos_2286; 3-Hydroxy-3-(3,4-dihydroxyphenyl)-2-methylpropanoic acid pos_1112; 2-Acetyl-4,5-dihydrothiazole
pos_2294; Citreoviridin C pos_1115; Glyceryl 5-hydroxydecanoate
pos_2299; 2-Hexaprenyl-3-methyl-2,4,6-trimethylbenzoate pos_1116; Santene hydrate
pos_2310; S-Adenosylhomocysteinine pos_1117; Yuzu lactone
pos_234; 2-Methyl-4-phenyl-2-methylpent-3-enoic acid pos_1125; 4,6-Dihydroxy-2-quinolinecarboxylic acid
pos_2354; Tridemorph pos_1128; (S)-Bilobanone
pos_2369; Galabiosylceramide pos_1131; 1-pentadecanoyl-glycero-3-phosphate
pos_2382; Cabergoline pos_1143; N-Lauroylglycine
pos_2388; (all-E)-1,8,10-Hepatria pos_1147; Lotaustralin
pos_2403; Leucyl-Serine pos_1148; (-)-3-Cyanomethyl-3-hydroxy-1H-indol-2(3H)-one
pos_2407; Amaranthusaponin pos_1149; 4-Hydroxybenzylamine
pos_2410; (2E,5E,12Z,15Z)-Farnesol pos_1150; TG(15:0/20:3(5Z,8Z,11Z)/20:4(5Z,8Z,11Z,14Z))
pos_2423; Ethyl 7-epi-12-hydroxyheptadecanoate pos_1152; DHBOA-Glc
pos_2427; CDP-DG(16:0/22:0) pos_1153; 6'-Hydroxyenterolactone
pos_2429; 2-acetyl-1-alkyl-sn-glycerol pos_1157; 3-Methyl-3-buten-2-one
pos_2443; Gomphidic acid pos_1159; (Z)-6-Tetradecene-1,3-diyn-5,8-diol
pos_2467; 3'-Hydroxy-4'-methoxyacetophenone pos_1163; Tetranor 12-HETE
pos_2471; diIDP pos_1164; 3-Hydroxy-2-(4-methylbenzoyl)-4H-1-benzopyran-4-one
pos_2473; Capsicoside C3 pos_118; 6-Methylpretetramide
pos_2478; Ricinine pos_1183; 5-(3',4',5'-Trihydroxyphenyl)-gamma-valerolactone-3'-O-glucuronide

pos_2505; 3-Epinobilin pos_1185; Dulciol D
 pos_2508; Fluorometholone pos_1186; DG(22:4(7Z,10Z,13Z,16Z)/16:1(9Z)/0:0)
 pos_2519; Asparaginy-Hydro pos_119; 3-ketosphinganine
 pos_2522; (5Z,8Z)-1,5,8-Hept pos_1190; Cerebronic acid
 pos_2536; Terretinin pos_1191; Floribundine
 pos_2539; Trandolapril-d5 D pos_1193; Bovolide
 pos_2541; 2'-Oxoaloesol 7-gl pos_1196; Kanzonol N
 pos_2543; Ganodermic acid I pos_1198; Camelliagenin B
 pos_2560; 3-Oxo-alpha-ionol pos_1199; Oxsolavetivone
 pos_2562; Physagulin G pos_12; Bis(2-ethylhexyl) phthalate
 pos_2563; (3b,5a,25R)-3-Hydro pos_120; Zerumbone
 pos_2568; PC(14:0/22:5(7Z,1 pos_1204; (2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid
 pos_2572; Melilotussaponin (pos_121; p-CHLOROPHENYLALANINE
 pos_2573; Lucidumol A pos_1219; N-methyl-L-glutamic Acid
 pos_2578; Hydroxychloroqui pos_122; R1128B
 pos_2581; Enoxacin pos_1232; hydroxytorsemide
 pos_2598; L-Histidinol pos_1234; Portensterol
 pos_2599; 1,1'-Ethylidenebis pos_1237; Taraxinic acid glucosyl ester
 pos_2600; 3-cis-Hydroxy-b,e pos_1239; 5,8-Epoxy-5,8-dihydro-10'-apo-b,y-carotene-3,10'-diol
 pos_2602; 1,20-Eicosanediol pos_1251; 3beta-3-Hydroxy-18-lupen-21-one
 pos_2614; PIP2(18:3(9Z,12Z pos_1252; Anileridine
 pos_2617; 4-Methyl-1-phenyl pos_1257; Lenalidomide
 pos_2628; Pseudoginsenoside pos_126; 24-Dehydroprovitamin D3
 pos_2629; Gravelliferone pos_1263; Lysyl-Lysine
 pos_2630; Momordicoside E pos_1266; PC(18:4(6Z,9Z,12Z,15Z)/20:3(5Z,8Z,11Z))
 pos_264; Neocembrene pos_1277; Feruloyl-beta-sitosterol
 pos_2648; Coniferan pos_1279; (17alpha,23S)-Epoxy-28,29-dihydroxy-27-norlanost-8-ene-3,24-dione
 pos_2653; Trigoneoside Xb pos_1282; Ethylsuberenol
 pos_2662; (1S,2R,4R,8S)-p- pos_1283; D-Pantothenoyl-L-cysteine
 pos_2663; N-Nitrosoproline pos_1289; (S)-10,16-Dihydroxyhexadecanoic acid
 pos_2668; Maslinic acid 3-O pos_1298; 1-Stearoylglycerophosphoserine
 pos_2676; Digoxigenin bisdi pos_1300; alpha-Tocopherolquinone
 pos_2678; 3-O-Sulfogalactos pos_1313; 5,10-Methylene-THF
 pos_2703; 8-Hydroxypinores pos_1316; Pentazocine
 pos_271; Erinacine B pos_1317; 5,6-epoxy,18R-HEPE
 pos_2720; Balanitoside pos_1322; (R)-Pterosin B
 pos_2723; 6,7-Dihydro-7-hydro pos_1324; Phytosphingosine
 pos_2725; Trihydroxycoprosta pos_1326; Momorcharaside A
 pos_2728; Pregeijerene pos_1327; Oleuroside
 pos_2731; Bethanechol pos_1336; 6-Hydroxy-1H-indole-3-acetamide
 pos_2732; Ethanolamine pos_1338; Propyl cinnamate
 pos_2736; Cortol pos_1339; Thiamine(1+) Diphosphate(1-)
 pos_2761; Crustecdysone pos_1341; PI(16:0/16:0)
 pos_277; Demethoxycurcumi pos_1346; (E)-4-[5-(4-Hydroxyphenoxy)-3-penten-1-ynyl]phenol
 pos_2773; Gingerglycolipid A pos_1356; Ketotifen-N-glucuronide
 pos_2775; DG(14:0/0:0/18:2) pos_1361; Isofucosterol glucoside
 pos_2776; (3b,16a,21b,22a)- pos_1362; Dihydrojasmonic acid
 pos_2779; PE(DiMe(11,5)/D pos_1378; Vanillic acid-4-O-glucuronide
 pos_278; Maculine pos_1379; Methyl 3,4-dihydroxy-5-prenylbenzoate 3-glucoside
 pos_2799; Minaprine pos_1381; Lacto-N-hexaose
 pos_2819; Gibberellin A62 pos_1383; 4-Hydroxyproline
 pos_2840; Trihexosylceramic pos_1384; 7a-Hydroxytestosterone
 pos_2886; N-(2,14-Eicosadie pos_1391; PGP(18:0/22:4(7Z,10Z,13Z,16Z))
 pos_2888; Alanyl-Serine pos_1392; Tranexamic Acid
 pos_2894; Dehydroaporphine pos_1393; Glucosamine 6-phosphate
 pos_2916; 11beta,20-Dihydro pos_1395; Vanillin
 pos_2932; Cerebroside B pos_1398; Pteroside B
 pos_2938; 1-Methylhistidine pos_1399; Methyl 5-hydroxyoxindole-3-acetate

pos_294; Rhubafuran pos_1407; Melleolide H
 pos_2945; Nomilinic acid 17 pos_1415; o-Tyrosine
 pos_2946; (S)-[8]-Gingerol pos_1420; Colupulone
 pos_2954; 12-Hydroxy-13-O pos_1429; Kiwiionoside
 pos_2955; Tuberoside A (All pos_1430; Docosanamide
 pos_2967; Tragopogonsaponin pos_1438; Stigmasta-4,6-dien-3-one
 pos_297; 1 β ,25-dihydroxy-3 pos_144; 26,26,26-trifluoro-25-hydroxyvitamin D3 / 26,26,26-trifluoro-25-hydroxycholesterol
 pos_2987; PE(15:0/20:1(11Z pos_1440; MG(20:1(11Z)/0:0/0:0)
 pos_2990; Molybdopterin precursor pos_1449; Pivampicillin
 pos_30; rac-Glycerol 1-myristate pos_1450; 1,2,3,4,5,6-Hexahydro-5-(1-hydroxyethylidene)-7H-cyclopenta[b]pyridin-7-one
 pos_3035; Methyl Arachidonate pos_1461; Furazolidone
 pos_305; 1-H-Inden-1-one,2,3-dione pos_1467; N,N-Dimethylsphingosine
 pos_3050; N-Acetyl-L-phenylethylamine pos_1470; Cinitapride
 pos_3051; Diadenosine diphosphate pos_1472; Margaroylglycine
 pos_3055; TG(14:0/22:4(7Z,8Z) pos_1475; Galabiosylceramide (d18:1/25:0)
 pos_3064; Tertatolol pos_1478; Petroselinic acid
 pos_3070; PS(20:4(5Z,8Z,11Z) pos_1486; Propylene glycol alginate
 pos_3089; (3b,9R)-5-Megastrol pos_1494; 6-Hydroxydopamine
 pos_3108; PC(20:5(5Z,8Z,11Z) pos_1501; 2,4-Di-tert-butylphenol
 pos_3109; Capryloylcholine pos_1505; Valechlorin
 pos_315; ANETHOLE pos_1506; Alpha-Linolenoyl ethanolamide
 pos_3163; 6,11-Dihydroxy-3-oxo-2-octadecanoic acid pos_1510; Arjunolic acid
 pos_3164; Austdiol pos_1512; L-argininium(1+)
 pos_3165; Melilotin pos_1516; 3-(Acetyloxy)-2-hydroxypropyl icosanoate
 pos_3167; 8-Nonen-2-one pos_1519; 23-Hydroxy-3-oxocycloart-24-en-26-oic acid
 pos_3182; PS(DiMe(9,3)/DiMe(9,3)) pos_1533; Acarbose
 pos_3187; Hoduloside VIII pos_1535; 5-Hydroxytryptophol glucuronide
 pos_3193; (S)-4',5,7-Trihydroxyflavone pos_1543; (Z)-N-Feruloyl-5-hydroxyanthranilic acid
 pos_3202; M-Secociguatoxin pos_1545; Irisolidone 7-O-glucuronide
 pos_3203; (3x,5x,10x)-9,10-Isopropylidene-1,2,3,4,5,6-hexahydro-2H-pyran-2-one pos_1546; Streptomycin
 pos_3204; gamma-Chaconine pos_1547; 12-Oxo-2,3-dinor-10,15-phytodienoic acid
 pos_3207; N-Cyclopropyl-tryptamine pos_1549; N-Stearoyl GABA
 pos_3224; Isepamicin pos_1579; D-1-Amino-2-pyrrolidinecarboxylic acid
 pos_323; Farfugin A pos_1584; TG(15:0/18:1(11Z)/18:4(6Z,9Z,12Z,15Z))
 pos_3241; 18-Deoxysagittarone pos_1591; Aesculin
 pos_3245; DG(15:0/18:0/0:0) pos_1597; (1S,2S,4R,8S)-p-Menthane-1,2,8,9-tetrol 2-glucoside
 pos_3249; Xylometazoline pos_1611; Valganciclovir
 pos_3259; Tryptophyl-Tryptamine pos_1616; Stearoylglycine
 pos_3272; 4'-N-desmethylolamide pos_1618; 3-Methyluric acid
 pos_3281; Quassamarin pos_163; 11-Deoxocucurbitacin I
 pos_3295; 11-Hydroxyprogestin pos_1630; Demethylphylloquinone
 pos_3301; DHAP(10:0) pos_1634; Octyl 4-methoxycinnamic acid
 pos_3304; Phytolaccoside A pos_1641; erythro-7,9-Hexatriacontanediol
 pos_3312; Oleoside 11-methyl pos_1642; Fludrocortisone
 pos_3323; Tricosanoylglycine pos_1643; Homoferreirin
 pos_3331; 3-O-Sulfogalactosyl pos_1644; Pyridinoline
 pos_3338; Hebevinoside II pos_1646; 13'-Hydroxy-gamma-tocotrienol
 pos_334; 10,13,16-Docosatriene pos_1650; Cinnamic acid
 pos_335; 13-Oxo-9,11-tridecenoic acid pos_1651; Benzaldehyde
 pos_3365; Neosilyhermin A pos_1658; DG(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)
 pos_341; Ethyl (2E,4Z,7Z)-D-glucuronide pos_1660; Mabioside D
 pos_344; 7-Ethyl-3,11-dimethyl-2-octadecanoic acid pos_1664; Ginsenoyne J
 pos_3441; PC(22:2(13Z,16Z)) pos_167; Ganoderic acid beta
 pos_3451; PE(15:0/22:1(13Z) pos_1671; (3S,3'R,4xi)-beta,beta-Carotene-3,3',4-triol
 pos_3474; Emtricitabine pos_1680; 1-(2-Furanyl)-2-propanone
 pos_3485; Myricatomentoside pos_1684; Octahydro-2H-1-benzopyran-2-one
 pos_350; 7-Ethyl-3,11-dimethyl-2-octadecanoic acid pos_1687; 24,25-Dihydroxyvitamin D
 pos_3514; 54-Deoxyciguatoxin pos_1689; Fencamfamine

pos_3519; Sativoside R2 pos_1694; Oxytocin
pos_354; TrHA pos_1695; Milrinone
pos_3542; Aspartylglycosami pos_1699; 3-Hydroxy-4-butanolide
pos_3545; TG(22:5(4Z,7Z,1 pos_170; 7,8-Dehydro-3,4-dihydro-beta-ionol
pos_3546; Hoduloside X pos_1702; Estradiol
pos_355; Ala Thr Tyr His pos_1704; (3beta,17alpha,23S,24S)-17,23-Epoxy-3,24,29-trihydroxy-27-norlanost-8-en-1
pos_3566; PE(14:0/22:2(13Z pos_1710; Lycopersiconolide
pos_3568; DG(16:0/22:1(13Z pos_1715; 5-(3',4'-Dihydroxyphenyl)-gamma-valerolactone
pos_3574; Aegle marmelos A pos_1716; 5-Hydroxy-L-tryptophan
pos_3576; Tsugaric acid A pos_1738; Mulberranol
pos_3596; Docetaxel pos_174; 1,25-Dihydroxy-24-oxo-16-ene-vitamin D3
pos_3600; Glucosylceramide pos_1743; Ginsenoyne N
pos_3611; 1-(9Z-tetradeceno pos_1744; 1,2-Di-(9Z,12Z-octadecadienoyl)-sn-glycero-3-phosphate
pos_3613; PS(DiMe(13,5)/M pos_1748; 1-Hydroxy-3-methoxy-7-primeverosyloxanthone
pos_3625; DG(22:6(4Z,7Z,1 pos_1760; Oryzalide A
pos_364; (Z)-2-hexacos-17-e pos_1767; (-)-beta-Elementene
pos_3640; 3'-p-Hydroxypacli pos_1773; 3-Hydroxyanthranilic acid
pos_3645; Oleamide pos_1774; 4-Hydroxybenzaldehyde
pos_3653; Octyl 2-furoate pos_1776; Ginsenoside Rh5
pos_366; Peroxysimulenoline pos_1780; Ac-Ser-Asp-Lys-Pro-OH
pos_3660; Epsilon-caprolact pos_1781; Octadecadienoate
pos_3661; 4-(Glutamylamino pos_1787; Polyporusterone B
pos_3666; 7-a,25-Dihydroxy pos_1788; 1-Heptadecanoylglycerophosphoethanolamine
pos_3671; DG(16:0e/18:0/0:(pos_1791; Salsoline-1-carboxylate
pos_3674; Sucrose acetate is pos_1795; SM(d18:1/12:0)
pos_3695; DG(14:1(9Z)/22:1 pos_1806; 2-oxoglutarate(2-)
pos_3696; Oleanolic acid 3-[pos_1811; MG(0:0/14:0/0:0)
pos_3697; PG(16:1(9Z)/20:4 pos_1818; Linatine
pos_3705; Notoginsenoside F pos_1823; Bisbynin
pos_3707; Cyclotricuspidoge pos_1826; Ceanothenic acid
pos_3715; Resolvin D5 pos_1828; beta-Citraurol
pos_3717; Methyl 3,4,5-trim pos_1831; 27-Norcholestanehexol
pos_3720; Alpha-Tocotrienol pos_1833; Theaflagallin
pos_3723; (+)-15,16-Dihydro pos_1834; Butyric acid
pos_3741; 2-Hexaprenyl-6-m pos_184; Cynaroside A
pos_3767; Valyl-Glutamate pos_1840; 1b-Furanoedesm-4(15)-en-1-ol acetate
pos_3773; Dynorphin A 9-17 pos_1845; (R)-1-O-[b-D-Glucopyranosyl-(1->6)-b-D-glucopyranoside]-1,3-octanediol
pos_3778; 3,6,10-Trimethylt pos_1848; Azaspiracid 3
pos_379; 6-Valerene-11-ol pos_1855; 3-O-alpha-D-Glucopyranuronosyl-D-xylose
pos_3816; Dihydromelilotosi pos_1868; Neferine
pos_3828; Demethylcalabaxa pos_1884; Primidone
pos_3848; Rubraflavone B pos_1890; L-Homoserine
pos_3868; PE(18:3(6Z,9Z,12 pos_1892; N-Stearoyl phenylalanine
pos_3885; Serotinose pos_1893; Norketamine
pos_3905; Zingiberenol pos_1897; Galactosylceramide (d18:1/14:0)
pos_3906; DG(14:1(9Z)/20:0 pos_1906; Blasticidin S
pos_3914; Melilotoside C pos_1907; 2-Propionylpyrrole
pos_3932; PG(16:0/18:2(9Z, pos_1910; 2-phosphonato-D-glycerate(3-)
pos_3939; (9S,10S)-9,10-dih pos_1913; DG(18:1(11Z)/14:1(9Z)/0:0)
pos_3983; 10-Undecenal pos_1914; PC(22:1(13Z)/22:5(4Z,7Z,10Z,13Z,16Z))
pos_3993; Ginsenoside III pos_1927; Cyclohexanecarboxylic acid
pos_400; Constanolactone E pos_1928; gamma-Tocopheryl quinone
pos_4000; Diosbulbin H pos_1929; Asparaginy-Proline
pos_401; 5alpha-androst-16-e pos_193; 25-hydroxy-16,17,23,24-tetradehydrovitamin D3 / 25-hydroxy-16,17,23,24-tetr
pos_4035; 1-O-Sinapoylgluc pos_1932; xi-2,3-Dihydro-2-oxo-1H-indole-3-acetic acid
pos_4041; Phytol diphosphat pos_1936; Amasterol
pos_4046; PIP2(18:2(9Z,12Z pos_1949; Matesaponin 3
pos_4048; Mulberrofuran T pos_1953; 2-Hexyl-4,5-dimethyl-1,3-dioxolane

pos_4049; xi-2,2,6-Trimethyl pos_1956; 8,11-Heptadecadienal
 pos_4064; Dezocine pos_1957; Cinnzeylanine
 pos_407; diethyltoluamide pos_196; 20(17+mm12尾)-abeo-1伪,25-Dihydroxy-24-dihomo-21-norvitamin D3
 pos_4081; 2-(4-Methyl-5-thia pos_1962; 4a-Carboxy-4b-methyl-5a-cholesta-8,24-dien-3b-ol
 pos_4087; Glucoconringiin pos_197; 4-Hydroxy-2-quinolone
 pos_4092; Brassicanal C pos_1977; 2-(2-Thienylmethylene)-1,6-dioxaspiro[4.4]non-3-ene
 pos_4103; DG(18:3(6Z,9Z,12Z)) pos_1979; beta-D-Glucosyloxydestruxin B
 pos_4112; Quinquenoside IV pos_1984; PE(20:4(5Z,8Z,11Z,14Z)/P-16:0)
 pos_4113; PE(18:2(9Z,12Z))/ pos_1986; Methylthio 2-(propanoyloxy)propanoate
 pos_4114; 3-alpha-Androstan pos_1991; Artenolide
 pos_413; 3-(3,4-Dihydroxypl pos_1992; N-Acetylaminooctanoic acid
 pos_4136; Kuwanon F pos_1994; N-di-Demethyl roxithromycin
 pos_4137; Sambubiose pos_2001; PE(14:0/P-16:0)
 pos_4138; Stevioside pos_2017; Ubiquinone-4
 pos_414; 5alpha-Gonane pos_2019; Treprostinil
 pos_4144; N-Acetylneuramin pos_2026; (2alpha,3alpha,5alpha,22R,23R)-2,3,22,23-Tetrahydroxy-25-methylergost-24(28E)-ol
 pos_416; Docosahexaenoic A pos_2027; Armexifolin
 pos_4161; 4,14-Dimethylergost pos_2033; PE(14:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))
 pos_4164; 2-Methoxy-estradi pos_2036; 4-[2,2'-Bithiophen-5-yl]-3-butyne-1-ol
 pos_4169; Pomonic acid pos_2039; LysoSM(d18:0)
 pos_4172; Ganoderic acid C1 pos_2053; DG(14:0/14:0/0:0)
 pos_4176; 5-Ethynyl-5'-(1-pr pos_2056; Annomutacin
 pos_4190; cis-3-Hexenyl tig pos_2066; Alitame
 pos_4192; PC(16:0/24:0) pos_2074; MG(0:0/22:0/0:0)
 pos_4220; Jubanine A pos_2077; (S)-Homostachydrine
 pos_4239; Lucyoside R pos_208; Longicamphenylone
 pos_4255; Galactonic acid pos_2092; Deoxynivalenol
 pos_4284; PIP(18:2(9Z,12Z)) pos_2093; 4-Hydroxytamoxifen-O-glucuronide
 pos_4301; PE(DiMe(13,5)/D pos_2099; DG(18:2(9Z,12Z)/18:3(9Z,12Z,15Z)/0:0)
 pos_4305; erythro-6,8-Tricos pos_2108; alpha-Terpineol butanoate
 pos_4319; PC(DiMe(9,3)/Mc pos_2111; 1-(3,5-Dihydroxyphenyl)-2-pentadecanone
 pos_4331; Gonyautoxin VI pos_2113; 5-(2-Hydroxyethyl)-4-methylthiazole acetate
 pos_4335; Pefloxacin N-oxid pos_2121; 6-Deoxodolichosterone
 pos_434; alatolide pos_2140; SM(d17:1/24:1(15Z))
 pos_4358; alpha-Linolenic ac pos_2153; Dimethyl 2-galloylgalactarate
 pos_436; 3-Deoxy-25-hydrox pos_2157; LysoSM(d18:1)
 pos_4362; Stearidonic Acid pos_2163; Glycylproline
 pos_4373; Eicosapentaenoic pos_2164; Norepinephrine
 pos_4382; C-8 Ceramide pos_2168; Avocadyne 2-acetate
 pos_4386; Epitestosterone pos_2173; Linalyl propionate
 pos_4393; 25-hydroxyvitamin pos_2186; 2-Pyrrolyl glycine
 pos_4411; Cholecalciferol (V pos_219; Glycerylphosphorylethanolamine
 pos_4429; cis-9-Palmitoleic a pos_2194; N-arachidonoylglycinate
 pos_447; (+)-alpha-Longipin pos_2197; 13'-Hydroxy-gamma-tocopherol
 pos_45; cholesta-5,22E-dien- pos_2200; 13'-Carboxy-gamma-tocotrienol
 pos_450; 2-Phenylethanol pos_2204; Latanoprost
 pos_458; toxisterol3 E1 pos_2207; DG(14:1n5/0:0/18:3n6)
 pos_495; 5a-androstane pos_2216; 13'-Carboxy-alpha-tocopherol
 pos_498; 2-Butyl-3-phenyl-2- pos_222; DG(16:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z)/0:0)[iso2]
 pos_500; (20S,22E)-3尾-Hyd pos_2228; Lamivudine sulfoxide
 pos_502; toxisterol3 D1 pos_223; Ganoderic acid delta
 pos_503; Lathosterol pos_2233; [10]-Gingerdione
 pos_506; 2-hexadecenal pos_2239; (22Alpha)-hydroxy-5alpha-campestan-3-one
 pos_510; Cholesterol pos_2241; Heptadecanoyl carnitine
 pos_512; 17-Methyl-18-norai pos_2256; PC(o-22:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))
 pos_524; 2,4,6-Heptatrienoic pos_2267; 20-Hydroxy-leukotriene E4
 pos_528; 11H-Benz[bc]acear pos_2277; Pandamarilactam 3x
 pos_532; 1-Naphthol pos_2281; 5-[2H-Pyrrol-4-(3H)-ylidenemethyl]-2-furanmethanol

pos_547; Methylripariochron pos_2287; Taurocholic acid 3-sulfate
 pos_551; Val Phe Arg Val pos_2289; 3-Acetyl-2,5-dimethylthiophene
 pos_552; Gly Ile Met Ala pos_2292; Licoricone
 pos_553; methyl 9-butylperoxy pos_2300; Tragopogonsaponin A
 pos_558; 3-Gymnomitrene pos_2303; N-Linoleoyl GABA
 pos_573; 3-Isopropyl-2-methyl pos_2312; Kaempferol 3-sophorotrioside
 pos_594; PS(12:0/19:0) pos_2328; PE(24:0/P-18:0)
 pos_597; ent-7alpha-hydroxy pos_233; JWH 302
 pos_605; 5beta-pregnane-3,20-dione pos_2335; Acidissiminol epoxide
 pos_619; Ala Leu pos_2336; Isovalerylcarnitine
 pos_641; Ser His Cys Arg pos_2339; (3beta,22E,24R)-3-Hydroxyergosta-5,8,22-trien-7-one
 pos_649; 11-Hydroxycanthin pos_2340; 4,4-Dimethylcholesta-8(9),14-dien-3beta-ol
 pos_655; PE(16:0/22:5(4Z,7Z)) pos_2344; Zeranol
 pos_656; Irehine pos_2353; Betavulgaroside I
 pos_673; PI(22:5(4Z,7Z,10Z)) pos_237; (3S,6E)-6-Caryophyllen-15-ol
 pos_682; NERYL ACETATE pos_2374; (6R,7S)-6,7-Epoxy-1,3-tetradecadiyne
 pos_692; Coriandrone E pos_2375; PC(20:3(5Z,8Z,11Z)/20:4(5Z,8Z,11Z,14Z))
 pos_697; MG(20:3(5Z,8Z,11Z)) pos_2378; Galbanic acid
 pos_7; Lumichrome pos_2385; 4-Nonylphenol
 pos_70; Sphingosine pos_2392; 1-O-all-trans-retinoyl-beta-glucuronic Acid
 pos_701; PS(17:0/18:4(6Z,9Z)) pos_2399; Herniarin
 pos_706; PE(15:0/15:1(9Z)) pos_240; 2,5-Diisopropyl-4-methylphenol
 pos_713; 2,4,6-undecatrienal pos_2400; keratan sulfate I
 pos_724; Triazamate pos_2405; omega-hydroxyfinasteride
 pos_727; Leu Phe Trp pos_2408; Dehydrophytosphingosine
 pos_73; 7-Ethyl-3,6-dihydro- pos_2411; 9'-Carboxy-gamma-chromanol
 pos_732; Ganolucidic acid B pos_2418; N2-Succinyl-L-glutamic acid 5-semialdehyde
 pos_739; Erogorgiaene pos_2424; (24E)-3alpha,15alpha-Diacetoxy-23-oxo-7,9(11),24-lanostatrien-26-oic acid
 pos_755; Selina-6-en-4-ol pos_2433; PE(16:0/20:3(5Z,8Z,11Z))
 pos_78; (S)-gamma-Calacore pos_2450; Carnosol
 pos_781; 5-(2-hydroxyethyl)pos_2451; Lithocholate 3-O-glucuronide
 pos_785; Ile Ile Leu pos_2453; 1-(3-Methylbutanoyl)-6-apiosylglucose
 pos_787; Senkirkine pos_2463; Oxypinnatanine
 pos_793; (6R)-6,19-epidioxy pos_248; 4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde
 pos_797; 4-(Methylthio)-1-butanol pos_2480; Juzirine
 pos_803; Ala His Gln Thr pos_2492; 28-Hydroxymangiferonic acid
 pos_806; 2-(2-Methylpropoxy)pos_2493; Epimetendiol
 pos_816; Lysyl-Isoleucine pos_2496; Congmunoside XV
 pos_819; Pro Val Ser Leu pos_2498; Dronabinol
 pos_834; 3-Oxo-delta4-steroid pos_2499; Mizoribine
 pos_838; 5a-Androst-3-en-17-one pos_2501; Melibiose
 pos_841; Ala Val pos_2504; Aucubin
 pos_846; Vitispirane pos_2507; Sarmentosin
 pos_85; 12-O-Hydroxy-3-oxo pos_251; Galactose-beta-1,4-xylose
 pos_853; Dodecanoic acid pos_2513; 4,5-Dihydroorotic acid
 pos_861; Tolterodine pos_2514; Avenalunic acid
 pos_864; 15-Hexadecanolide pos_2515; Norrubrofusarin 6-beta-gentiobioside
 pos_866; Citronellyl cinnamate pos_2526; 5beta-Coprostanol
 pos_873; N-Decanoylglycine pos_2564; Megestrol
 pos_886; 3a,7a-Dihydroxy-5beta pos_2585; Lacto-N-difucopeptase II
 pos_894; Tetrahydro-6-(2-hydroxy)pos_2594; DG(14:1(9Z)/20:4(5Z,8Z,11Z,14Z)/0:0)
 pos_898; 4,4alpha,5,6-Tetrahydro pos_2597; Pitheduloside B
 pos_90; L-Methionine pos_2605; para-hydroxyrosiglitazone
 pos_903; Pseudomonine pos_2612; 3-phosphonato-D-glyceroyl Phosphate(4-)
 pos_92; N-(3-Indolylacetyl)-I pos_2613; triazolopropionic acid
 pos_925; Propyl hexanoate pos_2638; 2-Keto-6-acetamidocaproate
 pos_933; N,N,O-Tridesmethylen pos_2649; Malonoben
 pos_934; (R)-lipoic acid pos_265; (6E,8E)-4,6,8-Megastigmatriene

pos_936; 4-Ethyl-2-methyl-5- pos_2652; Myricanol 5-laminaribioside
 pos_95; xi-3-(4-Isopropylphe pos_2664; Oleacein
 pos_956; Pipereicosalidine pos_2665; Glucosinalbin
 pos_958; Propiverine pos_2675; 7a-Hydroxycholesterol
 pos_962; (all-Z)-8,11,14-Hep pos_268; (E)-Suberenol
 pos_965; 5-Aminopentanal pos_2683; PC(DiMe(11,3)/MonoMe(11,3))
 pos_977; MG(0:0/24:6(6Z,9Z pos_2690; Bisacurone epoxide
 pos_978; Tetracosapentaenoi pos_2696; 3-(2-Furanylmethyl)-1H-pyrrole
 pos_982; Obtusilactone A pos_2713; Lucidenic acid B
 pos_991; Austroinulin pos_274; 1-(1-Pyrrolidinyl)-2-propanone
 pos_2765; Phenylbutyrylglutamine
 pos_2774; (-)-Quebrachamine
 pos_2780; Ceanothine B
 pos_2784; (R)-2-Hydroxysterculic acid
 pos_2791; DG(16:1(9Z)/22:2(13Z,16Z)/0:0)
 pos_2794; O-Desmethylnaproxen
 pos_2796; Zymosterol intermediate 2
 pos_2800; Shoyuflavone B
 pos_2803; trans-2-Dodecenoylcarnitine
 pos_2814; N-desmethylrosglitazone
 pos_2816; 11,12,13-Trinor-1(10)-spirovetivene-2,7-dione
 pos_282; 4E,6Z-Hexadecadienyl acetate
 pos_2823; 3beta-3-Hydroxy-11-oxolanosta-8,24-dien-26-al
 pos_2825; DG(18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)
 pos_2828; 3-Nonyl-1H-pyrazole
 pos_2829; (Z)-6-(2-Methoxyvinyl)-7-methyl-2H-1-benzopyran-2-one
 pos_2836; PE(15:0/P-16:0)
 pos_2847; lysoPC(26:1(5Z))
 pos_2849; Chinenoside II
 pos_285; Nitrosylsulfuric acid
 pos_2854; alpha-Crocetin glucosyl ester
 pos_2867; Cholest-5-ene
 pos_2870; Corchoroside A
 pos_2872; 4-Hydroxydiphenylamine
 pos_2887; Maslinic acid
 pos_289; N1,N10-Dicoumaroylspermidine
 pos_2898; Ganoderic acid W
 pos_290; Eremopetasinorol
 pos_2903; Citranaxanthin
 pos_2919; Glutamyl-Tryptophan
 pos_292; 3,4-Dihydroxybenzaldehyde
 pos_2921; (2S,3S,4S)-5,7,9,11-Tridecatetrayne-1,2,3,4-tetrol
 pos_2925; MG(20:2(11Z,14Z)/0:0/0:0)
 pos_2944; Glutamyl-Arginine
 pos_2947; Lacinilene C
 pos_2950; Ganoderic acid J
 pos_2951; Erucic acid
 pos_2952; 2'-Apo-beta-carotenal
 pos_2959; Oltipraz
 pos_2964; Oxalic acid
 pos_2966; arabinofuranosylguanine
 pos_2979; 1,9-Nonanedithiol
 pos_2984; N5-(3,4-Dioxo-1,5-cyclohexadien-1-yl)-L-glutamine
 pos_2989; L-Proline
 pos_3001; (3b,16a,20R)-25-Acetoxy-3,16,20,22-tetrahydroxy-5-cucurbiten-11-one 3-gluc
 pos_3003; Foeniculoside VIII
 pos_3004; trans-isoeugenol-O-glucuronide
 pos_3011; Ethyladipic acid

pos_3014; Pentadecanal
pos_3015; 2,4-Heptadecanedione
pos_3016; 3-Hydroxy-9Z-octadecenoylcarnitine
pos_3023; Hypoglycin B
pos_3026; 4-(2-Furanylmethylene)-3,4-dihydro-2H-pyrrole
pos_3029; (S)-3-Butyl-1(3H)-isobenzofuranone
pos_3030; 3a,7a,12a-Trihydroxy-5b-cholest-24-enoyl-CoA
pos_3032; Avocadene 1-acetate
pos_3034; Ganglioside GM3 (d18:1/18:1(11Z))
pos_3037; Glucosyl 6-hydroxy-2,6-dimethyl-2E,7-octadienoate
pos_3062; Tenuazonic acid
pos_3065; alpha-Carissanol
pos_3071; 1,21-Heneicosanediol
pos_3074; Okadaic acid
pos_3075; Isocolumbin
pos_3085; Smilagenin 3-[2"-glucosyl-6"-arabinosylglucoside]
pos_3087; 3-Hydroxy-5, 8-tetradecadienecarnitine
pos_3093; 2,4-Difurfurylfuran
pos_3096; (S)-2,2'-Iminobispropanoic acid
pos_3099; 1-nonadecanoyl-glycero-3-phosphate
pos_3106; Dihydroxyacetone Phosphate Acyl Ester
pos_3107; Nonate
pos_311; Cer(d18:0/16:0)
pos_3110; Muricin G
pos_3111; PE(24:1(15Z)/24:1(15Z))
pos_3114; (2E,4E,6Z)-2,4,6-Decatrienoic acid dehydropiperidide
pos_3115; Nandrolone
pos_3118; 5S,6S-epoxy-15R-hydroxy-ETE
pos_3119; Ganglioside GM3 (d18:1/16:0)
pos_3132; Triethanolamine
pos_3133; Methylegonovine
pos_3134; Glyyunnansapogenin B
pos_314; 1,4,5-Naphthalenetriol
pos_3153; 3 alpha,7 alpha,26-Trihydroxy-5beta-cholestane
pos_3154; Momordol
pos_3157; Pyranomammea C
pos_3159; Betavulgaroside VII
pos_3162; 8-Methoxykynurenate
pos_3166; alpha-Solamarine
pos_3181; (1xi,4xi,6xi)-Carvone oxide
pos_3184; N-Dodecane
pos_3201; Secoisolariciresinol
pos_3206; 5'-O-Methylmelledonal
pos_3211; PE(24:0/22:1(13Z))
pos_322; Benzyl trans-2-methyl-2-butenate
pos_3227; Momordicoside D
pos_3228; Linalyl isobutyrate
pos_3229; 5-Fluorouridine monophosphate
pos_324; Ile Val Leu Ile
pos_3243; lysoPC(28:0)
pos_3248; PE(14:0/14:1(9Z))
pos_3266; Dapiprazole
pos_3269; Tetracosanoic acid
pos_327; Oleanolic aldehyde
pos_3280; 2,2-dichloro-1,1-ethanediol
pos_3284; (S)-Aegeline
pos_3286; 3-Mercapto-2-butanol
pos_3294; 20-Oxo-leukotriene E4

pos_3297; CerP(d18:1/12:0)
pos_330; Val Leu
pos_3306; Debenzoylzucchini factor B
pos_3311; Cysteiny-Lysine
pos_3319; (3beta,11alpha,13beta)-3,11,13-Oleananetriol
pos_3322; Hericene C
pos_333; Adynerin
pos_3336; alpha-Terpinyl pentanoate
pos_3349; Astin I
pos_3355; PG(16:0/20:3(5Z,8Z,11Z))
pos_3356; Ganglioside GM3 (d18:0/14:0)
pos_3357; (Z)-8-Tetradecenal
pos_3362; Tryptophyl-Threonine
pos_3363; TG(8:0/8:0/15:0)
pos_3369; Nigroxanthin
pos_3372; Melongoside G
pos_3373; Methylgingerol
pos_3380; Erythrose
pos_3394; 3-Hydroxytamoxifen (Droloxifene)
pos_3395; TG(14:1(9Z)/14:1(9Z)/14:1(9Z))
pos_3399; NPC
pos_3413; N-Acetyl-6-O-L-fucosyl-D-glucosamine
pos_342; Soyasaponin I
pos_3423; Cibaric acid
pos_3436; 4-Hydroxy-3-prenylbenzoic acid glucoside
pos_3438; alpha-Chaconine
pos_345; LG 100268
pos_3450; Farnesiferol A
pos_347; Anofinic acid
pos_3478; Perflutren
pos_3498; 7a,17-dimethyl-5b-Androstane-3a,17b-diol
pos_35; LysoPE(15:0/0:0)
pos_3502; Nicotine imine
pos_3513; Ornithokinine
pos_3516; Methionine sulfoximine
pos_352; 2-(1-Pyrrolidinyl)-3-pentanone
pos_3537; Glutaminy-L-Tryptophan
pos_3540; 1,7-Dimethylguanosine
pos_3552; Periandrin V
pos_3559; lysoPC(6:0)
pos_3560; Dodecyl butyrate
pos_3564; HMBOA-Glc
pos_3567; 13'-Carboxy-alpha-tocotrienol
pos_357; Arachidonic Acid-biotin
pos_3573; Ginsenoyne M
pos_3578; 1-Ethenylhexyl butanoate
pos_3581; N1-trans-Feruloylagmatine
pos_3583; Tetrahydrodeoxycorticosterone
pos_3591; Sonchifolin
pos_3595; Testosterone glucuronide
pos_3597; APC
pos_3608; Campesterol 6'-(9Z-octadecenoyl)-glucoside
pos_3609; Hv-NCC-1
pos_361; R-4-benzyl-3-((R)-3-hydroxy-2,2-dimethyloctanoyl)-5,5-dimethyloxazolidin-2-c
pos_3623; Armillarin
pos_3632; N-[(4E,8E)-1,3-dihydroxyoctadeca-4,8-dien-2-yl]hexadecanamide
pos_3636; 15-Acetoxyscirpene-3,4-diol 4-O-a-D-glucopyranoside
pos_3638; Phenformin

pos_3650; 3-Hydroxyadipic acid 3,6-lactone
pos_3651; Glyoxylic acid
pos_3659; 2,4-Dimethyloxazole
pos_3675; 2-(Arabinosylamino)-3-(glucosylamino)propanenitrile
pos_3676; CDP-DG(18:0/22:3(10Z,13Z,16Z))
pos_369; Benzarone
pos_3700; (Z)-13-Hexadecenoic acid
pos_3738; PG(16:1(9Z)/16:1(9Z))
pos_3742; 9-Hydroxy-10-O-D-glucuronoside-12Z-octadecenoate
pos_3743; (24E)-3beta,15alpha,22S-Triacetoxylanosta-7,9(11),24-trien-26-oic acid
pos_3748; Rigin
pos_375; Mayolene-18
pos_3752; Gamma-Glutamyltyrosine
pos_3759; Thioguanosine 5'-diphosphate
pos_3760; L-4-Chlorotryptophan
pos_3765; Genipic acid
pos_3779; 12-O-D-Glucuronoside-13-hydroxyoctadec-9Z-enoate
pos_3785; Diflunisal
pos_3795; 1-Butanethiol
pos_3797; Octahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-one
pos_380; 4-O-Methylpinosylvic acid
pos_3801; Ganglioside GA2 (d18:1/9Z-18:1)
pos_3805; TG(14:0/14:1(9Z)/22:2(13Z,16Z))
pos_3806; PE(14:1(9Z)/16:1(9Z))
pos_3807; Bepotastine
pos_3808; Jujuboside B
pos_3827; PC(22:1(13Z)/24:0)
pos_3834; PI(16:0/22:4(10Z,13Z,16Z,19Z))
pos_3854; 3-Phenylpropyl isovalerate
pos_3860; 2,3-Dihydrowithanolide E
pos_3864; Vilazodone
pos_3893; cis-3-Chloroallyl aldehyde
pos_3896; Stearidonyl carnitine
pos_3897; Menthone 1,2-glyceryl ketal
pos_3907; Cer(d18:0/22:1(13Z))
pos_3928; Celastrol
pos_393; Sphinganine
pos_3935; Calendulose G methyl ester
pos_3936; (1R,4R,5S)-5-Hydroxyfenchone glucoside
pos_3942; (Z)-Resveratrol 3,4'-diglucoside
pos_3952; 19alpha-19-Hydroxy-3,11-dioxo-12-ursen-28-oic acid
pos_3954; Chloroxine
pos_3957; 3-Pyridylacetic acid
pos_3960; 2-Tetradecanone
pos_3963; Irinotecan
pos_3964; Vindesine
pos_3975; Mabiogenin 3-[rhamnosyl-(1->6)-[glucosyl-(1->2)]-glucoside]
pos_3979; 2-Ethylacrylic acid
pos_3988; N-(1-Deoxy-1-fructosyl)threonine
pos_3991; PE(20:1(11Z)/P-18:1(11Z))
pos_3994; TG(14:1(9Z)/20:3(5Z,8Z,11Z)/22:5(7Z,10Z,13Z,16Z,19Z))
pos_3996; 1-Acetyl-2-methylcyclopentene
pos_40; PE(17:0/0:0)
pos_4002; Hydroxyisonobilin
pos_4011; Gibberellin A45
pos_4015; CPA(18:2(9Z,12Z)/0:0)
pos_4016; Azukisaponin I
pos_4018; Shikimic acid

pos_402; PUROMYCIN
pos_4023; MG(16:0/0:0/0:0)
pos_4024; PE(14:1(9Z)/15:0)
pos_4026; N-lactoyl-Methionine
pos_4028; 3-Methyluridine
pos_403; Rhodovibrin
pos_4034; Fevicordin B 2-gentiobioside
pos_4039; Ethambutol
pos_404; Aricine
pos_4045; Faradiol myristate
pos_405; 未-Tocotrienol
pos_4054; (1R*,3R*,3'S*)-1,2,3,4-Tetrahydro-1-(2-thio-3-pyrrolidinyl)-beta-carboline-3-ol
pos_406; 4-Hydroxyquinoline
pos_4062; 9-(2-Carboxyphenyl)-3,6-bis(diethylamino)xanthylium(1+)
pos_4071; Aegelinol
pos_4093; 24-Oxo-1alpha,25-dihydroxyvitamin D3
pos_4094; 2-(5-Methyl-2-furanyl)piperidine
pos_4096; Tirofiban
pos_4118; Sanguisorbic acid dilactone
pos_4121; Hydroxypropyl-Asparagine
pos_4126; Histidinyl-Cysteine
pos_4127; Poppy acid
pos_4132; 1'-O-Acetylpaxilline
pos_4142; Trimeprazine
pos_4147; psi-Pelletierine
pos_4168; Ethyl 3-methyl-9H-carbazole-9-carboxylate
pos_417; 3-Formyl-4,6-dihydroxy-2-methoxy-5-methylchalcone
pos_4173; 3-Methylcyclopentadecanone
pos_418; desethyletomidate
pos_4188; (N-acetylneuraminosyl(a2-6)lactosamine)
pos_4189; 7-Hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5-acetic acid
pos_4204; (E)-10-Hydroxy-2-decene-4,6-diynoic acid
pos_4205; Ascorbic acid
pos_4207; Erinapyrone C
pos_421; p-Mentha-2,4(8)-dien-9,3-olide
pos_4212; Suxibuzone
pos_4213; Telithromycin
pos_4228; Vanillin 1,2-butylene glycol acetal
pos_4245; TG(22:5(4Z,7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z))
pos_4247; Ganglioside GM3 (d18:1/14:0)
pos_4253; Hebevinoside XIII
pos_4254; 4-Methyl-2-methylene-1-(1methylethylidene)-cyclohexane
pos_4258; Histamine
pos_4261; Secaloside A
pos_4262; L-dopachromate
pos_4264; Gossypetin 8-glucoside 3-sulfate
pos_4265; Curcumin II
pos_4269; Erythrityl Tetranitrate
pos_4273; TG(14:0/22:4(7Z,10Z,13Z,16Z)/o-18:0)
pos_4280; 7-Hexadecenoic acid, methyl ester
pos_4281; Galabiosylceramide (d18:1/24:0)
pos_4283; Olanzapine
pos_4287; Dinitolmide
pos_4292; 2-Oxo-4-methylthiobutanoic acid
pos_4295; 2-methyl-1,3-thiazolidine-2-carboxamide
pos_4303; 4,4-Dimethyl-5a-cholesta-8-en-3b-ol
pos_4307; Thiophene
pos_4309; 2-Hydroxyundecanoate

pos_4313; Xanthochymol
pos_4322; TG(8:0/14:0/10:0)
pos_4323; (5E)-6-Oxo-5-(phenylhydrazono)-5,6-dihydro-2-naphthalenesulfonic acid
pos_4327; Lucyoside J
pos_4336; Hexacosanoic acid
pos_4343; 3-(10-Heptadecenyl)phenol
pos_4356; 16-hydroxy hexadecanoic acid
pos_4377; Glycerol 1-myristate
pos_4381; Phenylalanyl-Histidine
pos_440; Vinyl caffeate
pos_4400; Baccatin III
pos_4402; dodecanamide
pos_4403; Estradiol Cypionate
pos_4409; Caffeine
pos_4413; DL-Methionine sulfoxide
pos_4414; Helenalin
pos_4415; 5alpha-Androstane-3,17-dione
pos_4420; .beta.-Cryptoxanthin
pos_4425; Azacitidine
pos_4431; cis-4-Hydroxy-D-proline
pos_4432; 3-Methyl-2-oxopentanoate
pos_446; 11-Oxo-beta-amyrin
pos_463; 3',4',5'-Trimethoxycinnamyl alcohol acetate
pos_468; PC(6:0/6:0)
pos_471; Herculin
pos_473; Bombykol
pos_475; Gly Pro Gly Asp
pos_485; 2',3',5'-triacetyl-5-Azacytidine
pos_489; 3,7,11,15-Tetramethyl-6,10,14-hexadecatrien-1-ol
pos_490; 4,7,10,13-Docosatetraynoic acid
pos_492; 2-Methylpropanal O-methyloxime
pos_5; Uracil
pos_504; 3"-Hydroxy-geranylhydroquinone
pos_518; Propapyriogenin A2
pos_526; 2-hydroxyestradiol
pos_527; LEVULINIC ACID, 3-BENZYLIDENYL-
pos_531; 12-amino-octadecanoic acid
pos_535; Gly Gln Trp Pro
pos_536; Gestodene metabolite 4
pos_537; 5-Aminosalicylic Acid
pos_541; PC(24:0/20:2(11Z,14Z))
pos_544; azido-FTY720
pos_549; Pro Ile Phe Ile
pos_559; Asp Pro Ile
pos_564; 22-Deoxocucurbitacin D
pos_57; PE(16:0/0:0)
pos_571; 1-Nitronaphthalene-7,8-oxide
pos_572; Glutathione amide
pos_575; alpha-Santalyl acetate
pos_579; beta-Hydroxy-2',6'-dimethoxy-3',4'-methylenedioxydihydrochalcone
pos_588; 3-Dimethylallyl-4-hydroxymandelic acid
pos_592; Morpholine
pos_595; Polyoxyethylene (600) mono- ricinoleate
pos_596; Ricinoleic Acid methyl ester
pos_60; Guanine
pos_601; Norsanguinine
pos_603; Bisindolylmaleimide IV
pos_608; Glu Ile Leu Ile

pos_609; PI(21:0/16:0)
pos_610; (17Z)-1,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-hexadehydrovitamin
pos_615; 14-METHOXY-4,4-BISNOR-4,8,11,13-PODOCARPATETRAEN-3-ONE
pos_617; 8-Hydroxyalanylclavam
pos_618; Methyl(2-furoylamino)acetic acid
pos_628; 3-(2-chloro-10H-phenothiazin-10-yl)propan-1-amine
pos_631; U-46619
pos_635; Tylactone
pos_64; Mandelonitrile
pos_644; Ergoline-1,8-dimethanol, 10-methoxy-, (8b)-
pos_648; 2-docosanamidoethanesulfonic acid
pos_657; 16-oxo-octadecanoic acid
pos_664; Ser Asp Thr Leu
pos_675; Leu Leu Met Ile
pos_68; 4E,6E,11Z-Hexadecatrienal
pos_681; N-Carboxyethyl-L-aminobutyric acid
pos_685; Cys Tyr Glu Trp
pos_686; 4,2'-Dihydroxychalcone 4-glucoside
pos_691; 3,5-diethyloctahydroindolizine
pos_693; (22S)-1,22,25-trihydroxy-26,27-dimethyl-23,23,24,24-tetrahydrovitamin D
pos_694; Thuyl 19-trachylobanoate
pos_700; Gly Asp Lys
pos_707; 1,2,4,5-Tetrahydrotestolactone
pos_712; (S)-Dulcitol E
pos_718; 4-tert-Octylphenol
pos_720; Phenolic steroid
pos_735; Thr Ile His Ile
pos_736; Dihydroshikonofuran
pos_737; (23R)-23,25-dihydroxyvitamin D3 / (23R)-23,25-dihydroxycholecalciferol
pos_74; cis-12-Octadecenoic Acid methyl ester
pos_740; Edulan I
pos_747; 6-Deoxyjacareubin
pos_75; Pfaffic acid
pos_750; Quinaprilat
pos_756; Gly Gly Trp
pos_759; 3-Hydroxy-1-phenyl-1-heneicosanone
pos_769; 2-Oxo-7-methylthioheptanoic acid
pos_77; (6 α ,22E)-6-Hydroxy-4,7,22-ergostatrien-3-one
pos_775; YM-53601
pos_782; Gly Ala Lys Trp
pos_79; Ectocarpin
pos_801; Geranylhydroquinone
pos_802; Elaidamide
pos_812; Tyr Leu Gly
pos_815; N-methyl arachidonoyl amine
pos_828; Ergosterol
pos_83; 1,25-dihydroxy-11-[(1R)-oxiranyl]vitamin D3 / 1,25-dihydroxy-11-[(1S)-oxiranyl]vitamin D3
pos_831; His Pro Trp Trp
pos_835; HECOGENIN ACETATE
pos_839; Pro Leu Arg Arg
pos_842; 2-Amino-3-methoxy-benzoic acid
pos_845; Nookatone
pos_851; Azaspiracid 4
pos_852; 2(R)-hydroxydocosanoic acid
pos_855; Dodecanal dimethyl acetal
pos_856; 13-Heptadecyn-1-ol
pos_859; Dioscorine
pos_86; Alisol C

pos_860; p-Hydroxynonanophenone
pos_862; 2-Hydroxy-desipramine glucuronide
pos_869; (3beta,5alpha,9alpha,22E,24R)-5,9-Epidioxy-3-hydroxyergosta-7,22-dien-6-one
pos_870; 2-(1,2,3,4-Tetrahydroxybutyl)-6-(2,3,4-trihydroxybutyl)pyrazine
pos_874; 4-Hydroxybenzyl alcohol
pos_875; Cyclandelate
pos_876; (E)-6,10-Dimethyl-9-methylene-5-undecen-2-one
pos_878; cis-3-Hexenyl pentanoate
pos_882; Monoethylhexyl phthalic acid
pos_884; 2,2,4,4,-Tetramethyl-6-(1-oxopropyl)-1,3,5-cyclohexanetrione
pos_888; 1-(2,3-Dihydro-1H-pyrrolizin-5-yl)-2-propen-1-one
pos_891; N-Methyltyramine
pos_893; (E)-5,8-Megastigmadien-4-one
pos_9; D-(+)-Trehalose dihydrate
pos_900; 5,10-Pentadecadien-1-ol
pos_901; Behenoylglycine
pos_902; Bilirubin
pos_909; Curlone
pos_91; D-erythro-Sphingosine C-17
pos_922; 3-Hydroxy-5Z-octenyl acetate
pos_93; 1伪,25-dihydroxy-24-nor-22-oxavitamin D3 / 1伪,25-dihydroxy-24-nor-22-oxaci
pos_931; 10-Oxo-11-octadecen-13-olide
pos_932; Ovalicin
pos_941; Niazinin A
pos_943; Cryptoxanthin diepoxide
pos_945; 1,4-Ipomeadiol
pos_953; Dihydroceramide
pos_954; S-Carboxymethyl-L-cysteine
pos_960; Cappariloside A
pos_963; (S)-a-Amino-2,5-dihydro-5-oxo-4-isoxazolepropanoic acid N2-glucoside
pos_968; N-Desmethylterbinafine
pos_970; 3-hydroxypristanic acid
pos_973; 5-Acetylamino-6-amino-3-methyluracil
pos_983; Tricycloekasantalol
pos_988; Gynocardin
pos_999; L-alpha-Amino-1H-pyrrole-1-hexanoic acid

!,22,23,23-hexadehydrovitamin D3 / (17Z)-1伪,25-dihydroxy-26,27-dimethyl-17,20,22,22,23,23-hexadehydrochole

calciferol