Supplementary Table 1. All the dysregulated metabolites detected by LC-MS in HR-HPV infection groups.

| No. | ID     | Ion mode | Metabolites                                           | Compound ID |
|-----|--------|----------|------------------------------------------------------|-------------|
| 1   | 0.80_103.03 | pos      | 2,4-Dihydroxybutanoic acid                          | HMDB0000360 |
| 2   | 90m/z 5.05_187.00 | neg      | p-Toluenesulfonic acid                               | HMDB0059933 |
| 3   | 73m/z 3.01_164.07 | neg      | L-Phenylalanine                                      | HMDB0000159 |
| 4   | 11.84_325.2 | pos      | 13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid    | HMDB0040901 |
| 5   | 376m/z 4.18_172.99 | pos      | 13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid    | HMDB0040901 |
| 6   | 15m/z 1.23_168.02 | neg      | Phenol sulphate                                      | HMDB0060015 |
| 7   | 99n 0.87_187.07 | neg      | Uric acid                                            | HMDB0000289 |
| 8   | 16m/z 6.08_137.02 | neg      | Serylthreonine                                       | HMDB0029049 |
| 9   | 36m/z 2.30_183.05 | neg      | Salicylic acid                                       | HMDB0000840 |
| 10  | 29m/z 7.96_239.09 | pos      | 3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid   | HMDB0061112 |
| 11  | 26m/z 4.75_263.10 | neg      | Phenylacetylglutamine                                | HMDB006344  |
| 12  | 30m/z 6.02_174.05 | neg      | Indoleacetic acid                                    | HMDB0000197 |
| 13  | 56m/z 4.18_204.09 | neg      | L-Tryptophan                                         | HMDB0000929 |
| 14  | 02n 9.34_392.29 | neg      | Ursodeoxycholic acid                                 | HMDB0000946 |
| 15  | 17n 0.73_156.07 | neg      | L-Histidine                                          | HMDB0000177 |
| 16  | 74m/z 9.72_448.30 | pos      | Deoxycholic acid conjugate                           | HMDB0000631 |
| 17  | 61m/z 7.32_368.16 | neg      | Dehydroepiandrosterone sulfate                       | HMDB0001032 |
| 18  | 59n 7.66_397.20 | neg      | Pregnanolone sulfate                                 | 3557        |
| 19  | 48m/z 7.82_528.26 | neg      | Glycochenodeoxycholate-3-sulfate                     | HMDB0002497 |
| 20  | 28m/z 0.92_426.01 | neg      | ADP                                                  | HMDB001341  |
| 21  | 98m/z 2.00_180.06 | neg      | L-Tyrosine                                           | 34          |
| 22  | 68m/z 9.05_279.23 | neg      | Alpha-Linolenic acid                                 | HMDB001388  |
| 23  | 17m/z 11.48_325.2 | neg      | 13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid    | HMDB0040901 |

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|   |   |   |   |   |
|---|---|---|---|---|
| 11.24_478.2 | 23 | 936m/z | neg | LysoPE(18:1(11Z)/0:0) | HMDB0011505 |
| 4.52_212.00 |   | 4.52_212.00 |   |   |   |
| 24m/z | neg | 24m/z | neg | Indoxyl sulfate | HMDB0000682 |
| 8.38_291.23 |   | 8.38_291.23 |   |   |   |
| 19m/z | pos | 19m/z | pos | Androsterone | HMDB0000031 |
| 5.50_204.06 |   | 5.50_204.06 |   |   |   |
| 63m/z | neg | 63m/z | neg | Indolelactic acid | HMDB0000671 |
| 6.05_191.08 |   | 6.05_191.08 |   |   |   |
| 30m/z | pos | 30m/z | pos | Carveol | HMDB0036083 |
| 10.86_454.2 |   | 10.86_454.2 |   |   |   |
| 963m/z | pos | 963m/z | pos | LysoPE(16:0/0:0) | HMDB0011503 |
| 7.56_369.17 |   | 7.56_369.17 |   | 5β-Androstan-3α-ol-17-one | 3564 |
| 35m/z | neg | 35m/z | neg | sulfate |   |
| 9.51_449.31 |   | 9.51_449.31 |   |   |   |
| 40n | neg | 40n | neg | Glycoursodeoxycholic acid | HMDB0000708 |
| 5.15_197.08 |   | 5.15_197.08 |   | a-Methyl-3,4- | 1515 |
| 02m/z | pos | 02m/z | pos | dihydroxyphenylpropionic acid |   |
| 6.02_340.13 |   | 6.02_340.13 |   |   |   |
| 29m/z | pos | 29m/z | pos | 4-methylbenzenesulfonamide | 3117 |
| 7.07_514.28 |   | 7.07_514.28 |   |   |   |
| 35m/z | neg | 35m/z | neg | Taurocholic acid | HMDB0000036 |
| 2.20_267.07 |   | 2.20_267.07 |   |   |   |
| 28m/z | neg | 28m/z | neg | Inosine | HMDB0000195 |
| 1.98_113.03 |   | 1.98_113.03 |   |   |   |
| 43m/z | pos | 43m/z | pos | Uracil | HMDB0000300 |
| 0.87_201.08 |   | 0.87_201.08 |   |   |   |
| 74m/z | neg | 74m/z | neg | Alanyl-Hydroxyproline | HMDB0028688 |
| 8.12_465.31 |   | 8.12_465.31 |   |   |   |
| 02n | pos | 02n | pos | Glycocholic acid | HMDB0000138 |
| 1.44_130.05 |   | 1.44_130.05 |   |   |   |
| 07m/z | pos | 07m/z | pos | Pyrrolidonecarboxylic acid | HMDB0000267 |
| 4.73_121.02 |   | 4.73_121.02 |   |   |   |
| 85m/z | neg | 85m/z | neg | 3-Hydroxybenzaldehyde | 65898 |
| 8.14_498.28 |   | 8.14_498.28 |   |   |   |
| 85m/z | neg | 85m/z | neg | Taurochenodesoxycholic acid | HMDB0000951 |
| 1.21_130.08 |   | 1.21_130.08 |   |   |   |
| 65m/z | pos | 65m/z | pos | L-Pipeolic acid | HMDB0000070 |
| 7.97_557.10 |   | 7.97_557.10 |   | Medicarpin 3-O-(6’- | LMPK12070006 |
| 31m/z | pos | 31m/z | pos | malonylglucisde) |   |
| 1.26_192.02 |   | 1.26_192.02 |   |   |   |
| 62n | neg | 62n | neg | Citric acid | HMDB0000094 |
| m/z   | Charge | Type    | Name                        | HMDB ID     |
|-------|--------|---------|-----------------------------|-------------|
| 3.83  | +      | dexpanthenol | 3978                       |             |
| 6.11  | +      |           |                             |             |
| 9.40  | -      | Vanillin  | HMDB0012308                 |             |
| 11.93 | +      | Metoprolol | 1250                       |             |
| 638   | -      | PE(21:0/0:0) | LMGP02050026               |             |
| 05    | +      | Cholic acid | HMDB0000619                |             |
| 57    | +      | 7-Methylxanthine | 58075                   |             |
| 6.32  | +      | 17α,20β-Hydroxyprogesterone | 3562        |             |
| 28    | -      | sulfate   |                             |             |
| 321   | -      | PE(19:0/0:0) | LMGP02050028               |             |
| 04    | -      | Hypoxanthine | HMDB0000157               |             |
| 281   | +      | 9-OxOODE  | HMDB0004669                 |             |
| 8.88  | -      | 3-alpha,20-alpha-dihydroxy-5-beta-pregnane 3-glucuronide | 57956       |             |
| 45    | -      | D-Maltose  | HMDB0000163                 |             |
| 21    | +      | LysoPE(18:0/0:0) | HMDB0011130               |             |
| 83    | -      | D-Mannitol | 142                        |             |
| 7.88  | +      | 3,4,5-trihydroxy-6-([5-methoxy-2,2-dimethyl-6-(3-oxo-3-phenylpropyl)-2H-chromen-7-yl]oxy)oxane-2-carboxylic acid | HMDB0125913 |             |
| 84    | +      | Taurodeoxycholic acid | HMDB0000896            |             |
| 44    | +      | NIPECOTIC ACID | 44223                   |             |
| 0.67  | -      | R-4-benzyl-3-((R)-3-hydroxy-2,2-dimethyloctanoyl)-5,5-dimethyl-oxazolidin-2-one | 65464      |             |
| 10.99 | +      |           |                             |             |
| m/z     | Charge | Intensity | Description                                                                 | HMDB ID     |
|---------|--------|-----------|------------------------------------------------------------------------------|-------------|
| 11.56   | 747.5  | 62        | SM(d18:1/16:0)                                                               | LMSP03010003|
| 3.86    | 384.11 | 62        | Succinyladenosine                                                            | HMDB0000912 |
| 4.80    | 153.01 | 64        | 2,6-Dihydroxybenzoic acid                                                   | HMDB0013676 |
| 11.33   | 530.3  | 65        | LysoPE(22:4(7Z,10Z,13Z,16Z)/0:0)                                             | HMDB0011523 |
| 9.51    | 449.31 | 66        | Chenodeoxycholic acid glycine conjugate                                      | HMDB0000637 |
| 10.26   | 512.2  | 69        | Heptadecanoylglycerophospho ethanolamine                                      | HMDB0061691 |
| 4.03    | 185.12 | 70        | N-Acetylisoputreanine                                                        | HMDB0094713 |
| 7.56    | 209.08 | 71        | 3,4-dimethyl-5-carboxymethyl-2-furanproanoic acid                            | LMFA01150048|
| 10.13   | 385.0  | 72        | 2-(1,3-Benzodioxol-5-y)-7-hydroxy-3,5,6,8-tetramethoxy-4H-1-benzopyran-4-one| LMK12113355 |
| 9.34    | 238.1  | 73        | Germacrenone                                                                | HMDB0035887 |
| 155     | 533.3  | 74        | PE(19:1(9Z)/0:0)                                                            | LMGP02050019|
| 0.87    | 292.09 | 75        | Edetic Acid                                                                 | HMDB0015109 |
| 5.86    | 151.03 | 77        | p-Hydroxyphenylacetic acid                                                  | HMDB0000020 |
| m/z | Charge | Peptide/Metabolite                                      | HMDB ID   |
|-----|--------|-------------------------------------------------------|-----------|
| 7.34 | pos    | 3,4,5-trihydroxy-6-{{5-methoxy-2,2-dimethyl-6-(3-oxo-3-phenylprop-1-en-1-yl)-2H-chromen-7-yl]oxy}oxane-2-carboxylic acid | HMDB0125912 |
| 2.28 | neg    | (R)-3-Hydroxybutyric acid                              | HMDB0000011 |
| 11.26 | neg    | PC(18:1(9Z)/0:0)                                       | LMGP01050032 |
| 10.80 | neg    | LysoPC(20:4(5Z,8Z,11Z,14Z))                            | HMDB0010395 |
| 11.46 | pol    | 2,3-Dihydrobenzofuran                                  | HMDB0013815 |
| 4.20 | neg    | Ascorbic acid-2-sulfate                                | HMDB0060649 |
| 0.89 | neg    | Theophylline                                           | 1458      |
| 0.86 | neg    | 1-O-(2-methoxy-4Z-hexadecenyl)-sn-glycero-3-phosphocholine | LMGP02010560 |
| 11.46 | pol    | LysoPC(17:0)                                           | HMDB0012108 |
| 11.74 | pol    | LysoPC(17:0)                                           | HMDB0010735 |
| 12.90 | pol    | LysoPC(17:0)                                           | HMDB0000874 |
| 11.74 | pol    | Trans-Hexa-dec-2-enoic acid                            | HMDB00141592 |
| 6.99 | neg    | 1,11-Undecanedicarboxylic acid                         | 6622      |
| 9.04 | neg    | Alloxanthin                                            | HMDB0036874 |
| 9.13 | pos    | gamma-Glutamylleucine                                  | HMDB0011171 |
| 3.31 | pol    | Ustiloxin B                                            | HMDB0041373 |
| 5.66 | pol    | 2-Hydroxycinnamic acid                                 | HMDB002641 |
| 9.66 | pol    | 1,11-Undecanedicarboxylic acid                         | 6622      |
| 4.31 | pol    | Alloxanthin                                            | HMDB0036874 |
| 5.31 | pol    | gamma-Glutamylleucine                                  | HMDB0011171 |
| 5.29 | pol    | Ustiloxin B                                            | HMDB0041373 |
| 5.66 | pol    | 2-Hydroxycinnamic acid                                 | HMDB002641 |
| m/z     | Charge | Isotope | Name                                                                 | HMDB_ID        |
|---------|--------|---------|----------------------------------------------------------------------|----------------|
| 11.68   | pos    |         | 4-Hydroxybenzoic acid                                               | HMDB0000500   |
| 6.90    | neg    |         | (2-{9-hydroxy-2-oxo-2H,8H,9H-furo[2,3-h]chromen-8-yl}-2-[(3-methylbut-2-enoyl)oxy]propoxy)sulfonic acid | HMDB0128935   |
| 12.13   | neg    |         | PE-Cer(d14:1(4E)/21:0)                                              | LMSP03020007  |
| 0.75    | neg    |         | L-Cysteinylglycine disulfide                                         | HMDB0000709   |
| 0.75    | pos    |         | Enoxacin                                                            | HMDB0014610   |
| 0.75    | neg    |         | PC(18:2(2E,4E)/0:0)                                                 | LMGP01050034  |
| 0.81    | pos    |         | 4-formyl Indole                                                     | 96392         |
| 10.89   | neg    |         | D-Galactose                                                         | HMDB0000143   |
| 3.85    | neg    |         | LysoPE(0:0/20:1(11Z))                                               | HMDB0011482   |
| 3.94    | pos    |         | Sylvopinol                                                          | HMDB0030570   |
| 4.51    | pos    |         | 2-hydroxy-3-[4-hydroxy-3-(3-methylbut-2-en-1-yl)phenyl]propanoic acid | HMDB0133182   |
| 97      | pos    |         | Melatonin glucuronide                                               | HMDB0060830   |
| 10.04   | neg    |         | Cucujolid IV                                                        | LMFA07040036  |
| 47      | pos    |         | Suberic acid                                                        | 4243          |
| 53      | pos    |         | Methylhydroxygliclazide                                             | HMDB0014029   |
| 59      | pos    |         | 4-Ipomeanol                                                         | HMDB0030472   |
| 72      | pos    |         | 5-Hydroxylysine                                                     | HMDB0000450   |
| m/z      | Charge | Valence | Compound Description                                      | HMDB ID   |
|----------|--------|---------|-----------------------------------------------------------|-----------|
| 1.21_362.04 |        | neg     | Guanosine monophosphate                                   | HMDB0001397 |
| 1.22_156.07 |        | pos     | L-2-Amino-3-(1-pyrazolyl)propanoic acid                   | HMDB0034267 |
| 12.55_277.2 |        |         |                                                           |           |
| 172m/z    |        | neg     | Gamma-Linolenic acid                                      | HMDB0003073 |
| 3.00_148.05 |      |         |                                                           |           |
| 17n       |        | pos     | Cinnamic acid                                             | HMDB0000567 |
| 4.76_178.05 |      |         |                                                           |           |
| 08m/z     |        | neg     | Hippuric acid                                             | HMDB0000714 |
| 10.27_467.3 |      |         |                                                           |           |
| 058n      |        | pos     | LysoPC(14:0/0:0)                                          | HMDB0010379 |
| 2.85_191.05 |      |         | xi-2,3-Dihydro-2-oxo-1H-indole-3-acetic acid              | HMDB0035514 |
| 12.55_277.2 |        |         |                                                           |           |
| 4.67_246.17 |      |         |                                                           |           |
| 13m/z     |        | pos     | 2-Methylbutyrylcarnitine                                  | HMDB0000378 |
| 2.00_244.06 |      |         |                                                           |           |
| 91n       |        | neg     | Uridine                                                  | HMDB0000296 |
| 5.22_139.03 |      |         |                                                           |           |
| 99m/z     |        | neg     | Furfuryl acetate                                          | HMDB0034246 |
| 5.22_183.02 |      |         |                                                           |           |
| 96m/z     |        | neg     | alpha-Furyl methyl diketone                               | HMDB0032920 |
| 10.61_285.2 |      |         |                                                           |           |
| 063m/z    |        | neg     | Hexadecanedioic acid                                      | 5642      |
| 11.48_592.3 |      |         |                                                           |           |
| 621m/z    |        | neg     | LysoPC(20:2(11Z,14Z))                                     | HMDB0010392 |
| 4.01_232.15 |      |         |                                                           |           |
| 62m/z     |        | pos     | Butyrylcarnitine                                          | HMDB0002013 |
| 3.76_220.11 |      |         |                                                           |           |
| 81m/z     |        | pos     | Pantothenic acid                                          | HMDB0000210 |
| 4.82_160.13 |      |         |                                                           |           |
| 36m/z     |        | pos     | 8-aminocaprylic acid                                      | LMFA01100059 |
| 5.04_319.16 |      |         | 5,8,11,14-Eicosatetraynoic acid                           | 35289     |
| 74m/z     |        | pos     |                                                           |           |
| 0.83_191.10 |      |         |                                                           |           |
| 34m/z     |        | pos     | Alanyl-Threonine                                          | HMDB0028697 |
| 11.28_526.3 |      |         |                                                           |           |
| 508m/z    |        | neg     | PC(O-16:0/0:0)                                            | LMGP01060010 |
| 11.46_189.1 |      |         |                                                           |           |
| 645m/z    |        | pos     | alpha-Irone                                               | HMDB0035631 |
| 8.24_273.22 |      |         | 16-fluoro-7Z-hexadecenoic acid                            | 96780     |
| 28m/z     |        | pos     |                                                           |           |
| 10.32_314.2 |      |         |                                                           |           |
| 447n      |        | pos     | (±)12,13-DiHOME                                           | 45199     |
| 0.83_191.10 |      |         |                                                           |           |
| Mass (m/z) | Charge | Chemical Name                                                                 | HMDB ID         |
|-----------|--------|-------------------------------------------------------------------------------|-----------------|
| 10.55_339.2 | pos    | 3-(2,4-Cyclopentadien-1-ylidene)-5alpha-androstan-17beta-ol                 | 70417           |
| 10.95_329.2 | pos    | 9Z,11Z,14Z-Eicosatrienoic acid                                                | LMFA01031060    |
| 4.86_303.14 |        | arabinofuranosylguanine                                                       | HMDB0061067     |
| 7.83_230.17 | pos    | Dihydro-3-coumaric acid                                                       | 4152            |
| 5.36_165.05 |        | 12-hydroxy-3Z,6Z-dodecadienoic acid                                           | LMFA01050171    |
| 8.12_601.26 |        | APC                                                                           | HMDB0060661     |
| 0.88_235.09 |        | L-beta-aspartyl-L-threonine                                                   | 62018           |
| 7.83_473.32 | pos    | 7-Hydroxygliclazide                                                           | HMDB0014027     |
| 6.26_340.13 |        | (23S,24S)-17,23-Epoxy-24,29-dihydroxy-27-norlanost-8-ene-3,15-dione          | HMDB0035843     |
| 6.01_178.08 |        | Lumichrome                                                                    | 64742           |
| 5.76_243.08 |        | Matricaric acid                                                               | HMDB0059663     |
| 10.47_452.2 |        | LysoPC(18:3(9Z,12Z,15Z))                                                      | HMDB0010388     |
| 10.87_490.3 |        | LysoPE(16:1(9Z)/0:0)                                                          | HMDB0011504     |
| 8.08_643.0 |        | Camelliagenin C                                                               | 90001           |
| 6.98_161.05 |        | Matricaric acid                                                               | LMFA01030751    |
| 10.11_512.2 |        | Coniferaldehyde                                                               | HMDB0141782     |
| 11.06_590.3 |        | PE(17:0/0:0)                                                                  | LMG02050030     |
| 464_983m/z  | neg    | LysoPC(20:3(5Z,8Z,11Z))                                                       | HMDB0010393     |
| m/z | Value | Charge | Name                                                                 | HMDB/NCI/HMDB ID     |
|-----|-------|--------|----------------------------------------------------------------------|----------------------|
| 12.31 | 269.2 | pos    | 17-hydroxy-heptadecanoic acid                                         | LMFA01050053         |
| 2.21  | 294.15| pos    | N-(1-Deoxy-1-fructosyl)isoleucine                                     | HMDB0039780          |
| 5.20  | 510.19| pos    | 4,2'-Dihydroxy-3,4',6'-trimethoxychalcone 4-glucoside                 | LMPK12120326         |
| 649   | pos   |        | Elaidic acid                                                          | HMDB0000573          |
| 796   | pos   |        | MG(0:0/16:0/0:0)                                                      | HMDB0011533          |
| 61    | pos   |        | 2-Piperidinone                                                        | HMDB0011749          |
| 9     | neg   |        | 2-Phenylacetamide                                                    | HMDB0010715          |
| 21    | neg   |        | N-lactoyl-Phenylalanine                                              | HMDB0062175          |
| 8.58  | 179.10| pos    | 1-(4-hydroxyphenyl)pentan-3-one                                       | HMDB0132981          |
| 9.14  | 387.25| pos    | 7α-Hydroxy-3-oxochola-1,4-dien-24-oic Acid                            | 42825                |
| 20    | neg   |        | (±)13-HpODE                                                          | 64784                |
| 146   | neg   |        | PE(0:0/18:0)                                                         | LMGP02050038         |
| 3,4,5-trihydroxy-6-((12,13,17-trihydroxy-3,4-dimethoxy-11-oxotricyclo[12.3.1.1
| 2,6]nonadeca-1(17),2,4,6(19),14(18),15-hexaen-5-y]oxy)oxane-2-carboxylic acid | HMDB0133715          |
| 15.37 | 860.6 | pos    | PC(20:3(8Z,11Z,14Z)/22:4(7Z,10Z,13Z,16Z))                             | 59862                |
| 6.06  | 300.12| pos    | 2-(3-Hydroxyphenyl)ethanol 1'-glucoside                               | HMDB0038332          |
| 1.21  | 243.06| neg    | Pseudouridine                                                         | HMDB0000767          |
| m/z     | Retention Time | Charge | Mol formula                     | Description                                      | HMDB ID      |
|---------|----------------|--------|---------------------------------|--------------------------------------------------|--------------|
| 44      | 1.34           | 123.05 | Niacinamide                     |                                                  |              |
| 10.38   | 6.38           | 562.3  | LysoPC(18:3(6Z,9Z,12Z))         | HMDB0010387                                      |              |
| 149     | 10.76          | 612.3  | LysoPC(22:6(4Z,7Z,10Z,13Z,19Z))| HMDB0010404                                      |              |
| 314     | 11.28          | 524.3  | LysoPC(P-16:0)                  | HMDB0010407                                      |              |
| 353     | 11.64          | 190    | 5-Hydroxyindoleacetic acid      |                                                  | 2975         |
| 06      | 5.60           | 479.16 | Capparilose B                   | HMDB0034938                                      |              |
| 67      | 6.73           | 188.07 | Indole-3-propionic acid         | HMDB0002302                                      |              |
| 15      | 8.14           | 339.27 | tetracosahexaenoic acid         | LMFA01030804                                     |              |
| 00      | 11.02          | 666.4  | Tragopogonsaponin A             | HMDB0037910                                      |              |
| 208     | 11.51          | 552.3  | LysoPC(24:1(15Z))               | HMDB0010406                                      |              |
| 67      | 11.96          | 614.3  | PC(22:5(4Z,7Z,10Z,13Z,16Z)/0:0)| LMGP01050142                                     |              |
| 60      |                |        | TUBERSTEMONINE                  |                                                  | 84994        |
| 36      | 0.80           | 492.19 | a-L-Arabinofuranosyl-(1->2)-    |                                                  |              |
|         |                |        | [a-D-mannopyranosyl-(1->6)]-D-mannose | HMDB0039818                                      |              |
| 357     | 10.96          | 614.3  | LysoPC(24:1(15Z))               | HMDB0010406                                      |              |
| 466     | 12.04          | 376.2  | PC(22:5(4Z,7Z,10Z,13Z,16Z)/0:0)| LMGP01050142                                     |              |
| 474     | 5.03           | 151.03 | TUBERSTEMONINE                  |                                                  |              |
| 95      | 7.63           | 352.07 | Methyl 2-hydroxybenzoate        | HMDB0034172                                      |              |
| 92      | 7.90           | 347.22 | Tyramine glucuronide            | HMDB0010328                                      |              |
| 30      | 9.33           | 374.28 | 15-hydroxy-tetracosa-6,9,12,16,18-pentaenoic acid | LMFA01050438                                     |              |
| 25      | 11.79          | 195.1  | 8-Hydroxy-4,8-dimethyl-4E,9-decadienoic acid | LMFA01050373                                     |              |
| 374     |                |        |                                |                                                  |              |
| m/z | Precursor | Type | Name                        | HMDB ID |
|-----|-----------|------|-----------------------------|---------|
| 12.43 | 403.3     | pos  | δ-Tocopherol                |         |
| 15.07 | 263.2     | pos  | Farnesyl acetone            |         |
| 576  | pos       | CD 1790 | Osmundalactone             | HMDB0031303 |
| 36m/z | pos       | Aspartyl-Hydroxyproline     | HMDB0028754 |
| 42m/z | pos       | PS(O-18:0/0:0)              | LMGP03060002 |
| 232  |           |      |                             |         |
| 13.03 | 449.3     | neg  | 6-Deoxodolichosterone       |         |
| 2.00 | 611.14    | neg  | Oxidized glutathione        | HMDB0003337 |
| 50m/z | neg       |      | Glycyl-Glutamine            | HMDB0028839 |
| 0.89 | 189.08    | neg  | 2,6-Nonadien-1-ol           | HMDB0031262 |
| 75m/z | pos       |      | L-3-Phenyllactic acid       | HMDB0000563 |
| 216m/z | neg      |      | 9(S)-HpODE                   | 36019   |
| 779  | neg       |      | LysoPC(20:1(11Z))           | HMDB0010391 |
| 7.70 | 263.12    | pos  | Undecanoic acid             | HMDB0000947 |
| 81m/z | neg       |      | γ-CEHC                      | 44822   |
| 695  | pos       |      | 6-Hydroxygliclazide         | HMDB0014028 |
| 6.39 | 340.13    | pos  | 7Z,9E-dodecadienoic acid    | LMFA01030237 |
| 39m/z | neg       |      | Dodecanedioic acid          | LMFA01170009 |
| 39m/z | neg       |      | (6S)-dehydrovomifoliol      | LMPR0103050009 |
| 0.80 | 365.10    | pos  | Trehalulose                 | HMDB0039727 |
| 73m/z | pos       |      | 3,4-Dihydroxyphenylvaleric  | HMDB0029233 |
| 5.43 | 255.08    | neg  | Isoquinoline                | HMDB0034244 |
| 74m/z | neg       |      | acid                        |         |
| m/z   | PPM   | Charge | Compound                                      | HMDB ID |
|-------|-------|--------|-----------------------------------------------|---------|
| 216   | 6.23_393.12 | pos    | cyclic N-Acetylserotonin glucuronide          | HMDB0060812 |
| 217   | 6.44_364.22 | pos    | Tetrahydrocortisone                           | 1915    |
| 218   | 6.57_293.06 | neg    | Aspartyl-Aspartate                            | HMDB0028749 |
|       | 9.77_236.17 |        |                                               |         |
| 219   | 75n_1.21_262.12 | pos    | 2-Hydroxyacorenone                            | HMDB0030916 |
| 220   | 99m/z_10.32_313.2 | pos    | O-methylmalonyl-L-carnitine                   | HMDB0062785 |
| 221   | 379m/z_4.00_247.12 | neg    | 12,13-DHOME                                   | HMDB0004705 |
| 222   | 92m/z_6.39_542.27 | pos    | Aspartyl-Leucine                              | HMDB0028757 |
| 223   | 39n_7.34_318.13 | pos    | Cortolone-3-glucuronide                       | HMDB0010320 |
| 224   | 9m/z_9.03_315.13 | pos    | Aspartyglycosamine                            | HMDB0000489 |
| 225   | 58m/z_10.40_586.3 | pos    | Panaquinquecol 2                              | HMDB0038938 |
| 226   | 157m/z_6.15_397.3 | neg    | LysoPC(20:5(5Z,8Z,11Z,14Z,17Z))                |         |
|       | 8.56_397.20 | pos    | 6'',6''-Dimethyl-5''-hydroxy-4''5''-dihydroprano[2''3''-2',3']-4'''-hydroxy-6''-methoxychalcone | LMPK12120239 |
| 227   | 64m/z_5.71_377.13 | pos    | 1-Hexanol arabinosylglucoside                 | 87865   |
| 228   | 62m/z_4.11_349.14 | pos    | 1-(1,2,3,4,5-Pentahydroxypent-1-yl)-1,2,3,4-tetrahydro-beta-carboline-3-carboxylate | HMDB0012492 |
| 229   | 05m/z_4.25_118.06 | pos    | Indole                                        | 286     |
| 230   | 55m/z_5.03_230.99 | neg    | (4-ethenyl-2,6-dihydroxyphenoxy) oxidanesulfonic acid | HMDB0128010 |
| 231   | 64m/z_6.57_414.30 | pos    | N-oleoyl methionine                          | LMFA08020110 |
| 232   | 41m/z_8.39_359.25 | pos    | 11beta-Hydroxy-6alpha,11-dimethylpregn-4-ene-3,20-dione | 70607 |
| 233   | 80m/z_8.39_359.25 | pos    |                                               |         |
| m/z | Charge | Name                                              | HMDB ID     |
|-----|--------|---------------------------------------------------|-------------|
| 8.94_615.24 | neg     | 8-Acetylegelolide                                 | HMDB0037772 |
| 9.20_467.11  | pos     | 5,4’-Dihydroxy-3,6,3’-trimethoxy-7-prenyloxyflavone | LMPK12112976 |
| 11.78_365.2   | neg     | Pregnanediol                                       | LMST02030202 |
| 4.11_367.15   | pos     | Tetrahydropentoxyline                              | HMDB0029992 |
| 5.83_245.04   | neg     | [3-(4-methoxyphenyl)propoxy]sulfonic acid          | HMDB0135750 |
| 10.53_374.2   | pos     | 12alpha-Hydroxy-5beta-chol-3-en-24-oic Acid       | LMST04010213 |
| 10.70_432.3   | neg     | Lithocholic acid glycine                          | HMDB0000698 |
| 11.87_889.5   | pos     | PGP(18:0/22:4(7Z,10Z,13Z,16Z))                    | HMDB0013513 |
| 2.17_173.04   | neg     | L-erythro-5-(1-Hydroxyethyl)-2(5H)-furanone        | HMDB0033285 |
| 5.14_121.02   | neg     | Benzoic acid                                      | HMDB0001870 |
| 5.38_317.11   | neg     | (2S,4R)-4-(9H-Pyrido[3,4-b]indol-1-yl)-1,2,4-butanetriol | HMDB0035191 |
| 7.32_435.14   | neg     | 3,4,5-trihydroxy-6-(((6E)-3-oxo-1,7-diphenylhepta-4,6-dien-1-yl)oxy)oxane-2-carboxylic acid | HMDB0133920 |
| 7.34_506.17   | neg     | Diosbulbinoside D                                 | HMDB0030084 |
| 7.83_359.16   | neg     | Oryzalide B                                       | HMDB0037592 |
| 9.52_105.07   | pos     | Styrene                                           | HMDB0034240 |
| 9.91_234.08   | pos     | Aspartyl-Threonine                                | HMDB0028763 |
| 11.40_708.4   | neg     | Aspartyl-Threonine                                | HMDB0008904 |
| m/z   | Charge | Ion Type | Molecule                                                                 | HMDB ID       |
|-------|--------|----------|--------------------------------------------------------------------------|---------------|
| 7.54  | 49     | pos      | Endomorphin-1                                                            | HMDB0005773   |
| 9.88  | 00     | neg      | 12-Oxo-2,3-dinor-10,15-phytodienoic acid                                 | HMDB0032090   |
| 1.16  | 24     | pos      | 3,4,5-trihydroxy-6-[(3-methylbut-2-enoyl)oxy]oxane-                        | HMDB0128920   |
| 1.25  | 18     | pos      | 5-(acetyloxy)-12,14-dihydroxy-9-oxo-8,17-dioxatetracyclo[8.7.0.0²,⁷.0¹¹,¹⁰]heptadeca-1(10),2(7),3,5,11(16),12,14-heptaen-13-yl acetate | HMDB0128415   |
| 10.79 | 747    | neg      | (+)-Scalarin                                                             | LMPR0105060001|
| 10.58 | 423.01 | pos      | LysoPC(20:4(8Z,11Z,14Z,17Z))                                             | HMDB0010396   |
| 11.13 | 622.2  | pos      | 11-[(2R)-3-[2-amino-3-methyl-4-(2-methyl-1,3-thiazol-4-yl)but-3-yl]-2-methyloxiran-2-yl]-3-hydroxy-4,4,6,8-tetramethyl-5-oxo-7-(sulfooxy)undecanoic acid | HMDB0127547   |
| 11.42 | 254.1  | pos      | 8-Hydroxy-4(6)-lactarente-5,14-diol                                       | HMDB0035780   |
| 11.83 | 421.3  | pos      | 3Alpha,7Alpha,12Alpha-trihydroxy-27-nor-5Beta-cholestan-24-one           | 84749         |
| 5.74  | 201.02 | pos      | 4-ethylphenylsulfate                                                   | HMDB0062551   |
| m/z  | Charge | Name                                                                                           | HMDB Number |
|------|--------|------------------------------------------------------------------------------------------------|-------------|
| 0.84 | pos    | 6-Methoxymusizin 8-O-[b-D-glucopyranosyl-(1->6)-b-D-glucopyranosyl-(1->3)-b-D-glucopyranosyl-(1->6)-b-D-glucopyranoside] | HMDB0034614 |
| 11.15| pos    | 16-hydroxy-9E-hexadecenoic acid                                                                | LMFA01050192|
| 4.06 | neg    | 1,3-Dimethyluric acid                                                                          | 2822        |
| 4.91 | pos    | Gravelliferone                                                                                  | HMDB0030729 |
| 5.43 | pos    | 3,4,5-Trimethoxycinnamic acid Eicosapentaenoic Acid ethyl                                        | 6705        |
| 7.80 | pos    | 5-Methoxyindoleacetate                                                                          | 45153       |
| 8.67 | neg    | 2,3-Dihydro-6-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one                                        | HMDB0041410 |
| 10.94| neg    | LysoPC(20:3(8Z,11Z,14Z))                                                                        | HMDB0010394 |
| 11.89| pos    | PE(18:0/0:0)                                                                                   | LMG002050001|
| 12.28| neg    | PC(O-18:0/0:0)                                                                                 | LMG001060014|
| 4.24 | neg    | p-CHLOROPHENYLALANINE                                                                          | 44308       |
| 5.62 | pos    | Neocnidilide                                                                                   | HMDB0034450 |
| 6.28 | pos    | N-[(3a,5b,7b)-7-hydroxy-24-oxo-3-(sulfoxy)cholan-24-yl]-Glycine                                | HMDB0002409 |
3-[(3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl)oxy]-5,7-dihydroxy-2-(3-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one

N-palmitoyl glutamine

Secologanin

{(6-[(2-(3,4-dihydroxyphenyl)-5,6,7-trihydroxy-4-oxo-4H-chromen-8-yl]-3,4,5-trihydroxyoxan-2-yl)methoxy)sulfonic acid

5,9,11-trihydroxyprosta-6E,14Z-dien-1-oate

MG(18:1(11Z)/0:0/0:0)

Leucylproline

(R)-2,4,5-Trimethoxydalbergiquinol

6-[1-(3,4-dimethoxyphenyl)-2-{2-(3,4-dimethoxyphenyl)ethyl]-C-hydroxycarbonimidoyl]ethoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid

3b,12a-Dihydroxy-5a-cholanoic acid

N-Acetylproline
| Retention Time | m/z     | Charge | Description                                      | HMDB ID       |
|---------------|---------|--------|-------------------------------------------------|---------------|
| 2.26_153.06   | 60 m/z  | pos    | N1-Methyl-2-pyridone-5-carboxamide               | HMDB0004193   |
| 3.92_232.15   |         |        |                                                 |               |
| 4.19_247.06   | 86 m/z  | pos    | 5-Phosphoribosylamine                            | HMDB0001128   |
| 4.73_212.00   | 12 m/z  | neg    | Paracetamol sulfate                              | HMDB0059911   |
| 5.75_305.11   |         |        |                                                 |               |
| 6.66_460.17   | 39 m/z  | pos    | Deoxyartemisinin                                 | HMDB00060569   |
| 6.36_597.28   |         |        |                                                 |               |
| 6.19_279.12   | 28 m/z  | pos    | Cyclocalopin C1                                  | HMDB0039812   |
| 7.32_347.16   | 14 m/z  | pos    | (6E,8E,10R,12Z)-10-Hydroxy-3-oxooctadecatrienoic acid | HMDB0062357   |
| 9.51_257.17   |         |        |                                                 |               |
| 5.26_173.14   | 10 m/z  | pos    | 3R-aminononanoic acid                            | LMFA01100019   |
| 5.39_393.3    |         |        |                                                 |               |
| 6.00_277.2    | 164 m/z | pos    | (9R,13R)-15,16-dihydro-12-oxo-10-phytenoic acid | LMFA02010004   |
| 6.33_393.3    |         |        |                                                 |               |
| 12.39_393.3   | 014 m/z | pos    | 11beta,12beta-Dihydroxy-5beta-cholan-24-oic Acid | LMST04010386   |
| 2.14_345.13   |         |        |                                                 |               |
| 3.04_107.04   | 34 m/z  | neg    | Gibberellin A3                                   | 6954          |
| 3.34_107.04   |         |        |                                                 |               |
| 4.50_146.06   | 99 m/z  | pos    | Benzaldehyde                                     | HMDB0006115   |
| 5.26_173.14   |         |        |                                                 |               |
| 10 m/z        | pos    |        |                                                 |               |
| 3.26_153.06   |         |        |                                                 |               |
| 2.26_153.06   |         |        |                                                 |               |
| 2.26_153.06   |         |        |                                                 |               |
5.76_188.07 11m/z  pos  Cinnamoylglycine  HMDB0011621
6.01_507.25 99m/z  pos  11-Hydroxyprogesterone 11-glucuronide  HMDB0010364
0.93_305.09
8.1m/z  neg  Glutamyl-Hydroxyproline  HMDB0028820
1.48_173.00
8.3m/z  neg  D-Glucaro-1,4-lactone  HMDB0041862
10.22_513.3 089n  pos  1-(2-methoxy-13-methylpentadecanyl)-sn-glycero-3-phosphoserine  LMGP03060009
10.41_560.2
8.60m/z  pos  Physagulin C  HMDB0038535
10.67_277.1
8.06m/z  neg  10-Deoxymethanolide  LMPK04000034
10.94_367.1 2,3-Butanediol
5.85m/z  pos  apiosylglucoside  HMDB0033063
5.04_512.21
3.6m/z  pos  Harpagoside  LMPR0102070010
6.24_255.11
3.7m/z  neg  Imazamethabenz  HMDB0034885
9.30_682.40
6.68m/z  pos  PS(12:0/18:4(6Z,9Z,12Z,15Z))  LMGP03010056
9.66_294.18
3.1m/z  neg  Tanacetol A  HMDB0035722
0.91_291.08
8.2n  neg  7-hydroxy-6-(3-hydroxy-3-methylbut-1-en-1-yl)-2H-chromen-2-one  HMDB0130516
0.91_425.07
9.2m/z  neg  Cysteine glutathione disulfide  HMDB0000656
10.53_299.2
12.85_328.2
8.2n  pos  3-ketosphinganine  3428
13.04_303.2
4.32n  pos  Docosahexaenoic acid  HMDB0002183
322
3.29m/z  neg  Arachidonic acid  HMDB0001043
2.01_249.05
3.8m/z  pos  2,3,4,5,6,7-Hexahydroxyheptanoic acid  HMDB0240292
4.41_261.00
7.41m/z  neg  3-(3,5-dihydroxyphenyl)-1-propanoic acid sulphate  HMDB0061117
| m/z     | Retention Time | Name                                      | HMDB ID    |
|---------|----------------|-------------------------------------------|------------|
| 325     | 4.92_203.00    | O-methoxycatechol-O-sulphate              | HMDB0060013|
| 326     | 6.14_336.06    | (S)-Annocherine A                         | HMDB0038723|
| 327     | 7.09_515.29    | Tauroursocholic acid                      | 57999      |
| 328     | 10.19_475.2    | 5,10-Methylene-THF                        | HMDB0001533|
| 329     | 10.80_279.2    | 10E,12Z-Octadecadienoic acid              | 34801      |
| 330     | 11.02_453.2    | Sambutoxin                                | 95518      |
| 331     | 20.19_715.2    | PE(15:0/22:2(13Z,16Z))                    | LMGP02010471|
| 332     | 20.60_168.04   | Theobromine                               | HMDB0002825|
| 333     | 3.85_181.07    | 1-Anilino-9,10-dioxo-2-anthoic acid       | 96354      |
| 334     | 4.83_177.09    | 3-Hydroxyphenyl-valeric acid              | HMDB0041666|
| 335     | 5.18_379.15    | Myricanone                                | HMDB0030798|
| 336     | 6.24_299.10    | fluvoxamino acid                          | HMDB0060950|
| 337     | 6.60_168.04    | Vanillic acid                             | HMDB0000484|
| 338     | 9.84_277.21    | (9S,13S)-15,16-dihydro-12-oxo-10-phytoenoic acid | LMFA02010005|
| 339     | 0.77_120.06    | 4-Amino-3-hydroxybutyrate                 | HMDB0061877|
| 340     | 10.46_660.4    | PS(P-16:0/13:0)                           | LMGP03030002|
| 341     | 12.32_531.3    | Acinospesigenin A                         | LMPR0106160001|
| 342     | 5.01_303.14    | Valproic acid glucuronide                 | HMDB0000901|
| 343     | 7.32_155.10    | 9-hydroxy-5Z-nonenoic acid                | LMFA01050232|
| 344     | 7.40_375.15    | Gravacridonetriol                         | HMDB0029330|
| 345     | 7.88_193.08    | Butylparaben                              | HMDB0032575|
| 346     | 9.30_644.40    | Ponasteroside A                           | HMDB0034091|
| 347     | 10.80_279.2    | 10E,12Z-Octadecadienoic acid              | 34801      |
1.26_147.02 2,3,4,5-Tetrahydroxypentanoic acid  HMDB0059750
10.58_309.2

347 91m/z  neg 13(S)-HpOTrE  36052
11.05_480.3

348 065m/z  neg  LysoPC(15:0)  HMDB0010381
14.34_673.5

349 099m/z  neg  PE-Cer(d15:1(4E)/20:0(2OH))  LMSP03020074

4.31_227.99 2-Hydroxyacetaminophen sulfate  HMDB0062547
4.81_321.14

351 65m/z  neg  Nicotine glucuronide  HMDB0001272
5.32_277.08

352 57m/z  pos  3',4'-dihydroxyflurbiprofen  2925
6.60_127.03

354 81m/z  pos  2-amino-4-({1-
[(carboxymethyl)-C-
hydroxycarbonimidoyl]-2-{{2-
hydroxy-3-(4-hydroxy-2-
methoxyphenyl)-1-
phenylpropyl}[sulfanyl]ethyl}-C-
hydroxycarbonimidoyl}butanoic acid  HMDB0130358
10.87_181.1

355 595m/z  pos  5Z-Dodecenoic acid  HMDB0000529

4.81_321.14

11.18_311.1  N-Undecylbenzenesulfonic acid  HMDB0032549
11.72_489.3

356 682m/z  neg  Alisol A  71704
11.72_489.3

357 575m/z  neg  4-HYDROXY-6-
METHYL PYRAN-2-ONE  44653
9.29_546.18

358 95m/z  pos  m-Carboxyphenyl
phenylacetamidomethylphosphonate  66239

7.63_350.08

359 05m/z  pos  2,10-dihydroxy-4,6,8-
decatriynoic acid  LMFA01050235
7.78_193.05

360 03m/z  pos  (+)-Myrtenyl formate  91711
8.62_181.12

361 18m/z  pos  (+)-Myrtenyl formate  91711
| m/z   | Charge | Name                                              | HMDB_ID   |
|-------|--------|---------------------------------------------------|-----------|
| 37m/z | neg    | 10-hydroxy capric acid                            | LMFA01050033 |
| 00m/z | pos    | 23-phenyl tricosanoic acid                         | LMFA01140072 |
| 752m/z| pos    | 2,6,10,10-Tetramethyl-1-oxaspiro[4.5]decan-6-ol    | HMDB0037907 |
| 379m/z| pos    | 2-Nor-1,3-seco-1α,25-dihydroxyvitamin D3           | 42605     |
| 15m/z | pos    | 6-amino-hexanoic acid                              | LMFA01100035 |
| 99m/z | pos    | 5-(3',4'-Dihydroxyphenyl)-gamma-valerolactone      | HMDB0029185 |
| 17m/z | pos    | Tephroleocarpin B                                  | LMPK12140183 |
| 35m/z | pos    | 9-J1-PhytoP                                       | LMFA02030069 |
| 34m/z | pos    | 2,5-Furandicarboxylic acid                         | HMDB0004812 |
| 382m/z| pos    | 2-Hydroxy-4,5,6-trimethoxydihydrochalcone          | 52412     |
| 241m/z| pos    | Benzoquinoneacetic acid                            | HMDB0002334 |
| 932m/z| neg    | PE(18:2(9Z,12Z)/21:0)                              | LMGP02010674 |
| 285m/z| neg    | Pentadecanal                                       | HMDB0031078 |
| 58m/z | neg    | but-2-enoic acid                                   | LMFA01030925 |
| 45m/z | pos    | 6-Ketoestriol                                      | HMDB0000530 |
| 37m/z | pos    | 10-Hydroxycarbazepine                              | HMDB0060676 |
| 65n   | pos    | Aleprylic acid                                     | LMFA01030189 |
| 84m/z | pos    | 11-deoxy-11-methylene-15-keto-PGD2                 | LMFA03010104 |
| 09m/z | pos    | Lansoprazole                                       | HMDB0005008 |
| 08m/z | pos    | L-Cystine                                          | HMDB0000192 |
| m/z     | Charge | Ion Mode | Compound Description                                                                 | HMDB ID     |
|---------|--------|----------|--------------------------------------------------------------------------------------|-------------|
| 0.77    | 265.09 | pos      | Xylobiose                                                                             | HMDB0029894|
| 0.91    | 897.24 | neg      | Rhamnetin 3-(3''''-p-coumaryl-rhamnosyl)(1->3)-rhamnosyl-(1->6)-galactoside            | LMPK12112606|
| 11.50   | 550.3  | neg      | LysoPC(P-18:1(9Z))                                                                   | HMDB0010408 |
| 12.15   | 448.3  | pos      | Typhasterol                                                                           | 64145       |
| 12.53   | 223.2  | pos      | Selina-6-en-4-ol                                                                      | 265102      |
| 2.05    | 247.05 | pos      | 2',2'-Difluorodeoxyuridine                                                            | HMDB0060727 |
| 2.14    | 277.03 | pos      | 4-Hydroxy-8-methoxy-2H-furo[2,3-h]-1-benzopyran-2-one                                  | HMDB0032659 |
| 2.35    | 203.05 | neg      | D-Glucose                                                                             | HMDB0000122 |
| 4.80    | 287.02 | pos      | 4-Hydroxy-5-(dihydroxyphenyl)-valeric acid-O-sulphate                                 | HMDB0059978 |
| 8.08    | 631.27 | pos      | Brassica napus non-fluorescent chlorophyll catabolite 3                               | HMDB0040917 |
| 8.17    | 229.14 | pos      | catabolite 3                                                                          | HMDB0040917 |
| 0.91    | 146.11 | neg      | Undecylenic acid                                                                      | LMFA01030036|
| 10.77   | 500.2  | pos      | Ethyl 4-pentenoate                                                                    | HMDB0031603 |
| 10.99   | 259.1  | neg      | PE(0:0/20:4(5Z,8Z,11Z,14Z))                                                           | LMGP02050051|
| 681     | 500    | pos      | CICUTOXIN                                                                             | LMFA05000647|
| 3.84    | 318.11 | pos      | (2R,4R)-tert-butyl 4-(hydroxymethyl)-2-phenylothiazolidine-3-carboxylate              | 65471       |
| 39      | 318.11 | pos      | (2R,4R)-tert-butyl 4-(hydroxymethyl)-2-phenylothiazolidine-3-carboxylate              | 65471       |
| 4.35    | 422.14 | pos      | cis-Resveratrol 3-O-glucuronide                                                       | HMDB0041711 |
| 53      | 318.11 | pos      | (E)-5,8-Megastigmadien-4-one                                                          | HMDB0034671 |
| 9.29    | 231.11 | pos      | (E)-5,8-Megastigmadien-4-one                                                          | HMDB0034671 |
10.78_504.3
399 094m/z  neg  PC(17:2(9Z,12Z)/0:0)  LMGP01050127

12.65_237.2
400 215m/z  pos  (Z)-13-Hexadecenoic acid  HMDB0035877
2.24_276.14
401 48m/z  pos  N-(1-Deoxy-1-
3.00_188.06
402 86m/z  pos  Triethanolamine  HMDB0032538

6.40_339.09
403 78m/z  pos  1,3-Diacetoxy-4,6,12-
tetradecatriene-8,10-diyn  HMDB0030922

8.59_407.28
404 03m/z  pos  3a,7a,12a,19-Tetrahydroxy-
8.81_285.12
405 51m/z  pos  11Z-Hexadecen-7,9-diynoic  acid  LMFA01031108
8.87_583.26

406 04m/z  pos  Biliverdin  HMDB0001008
9.19_347.16

407 19m/z  neg  Enalaprilat  2533
10.25_307.1

408 908m/z  neg  Methylgingerol  86546
10.43_302.3

409 075m/z  pos  Sphinganine  HMDB0000269
10.60_178.1

410 363n  pos  Quinceoxepine  HMDB0038107

11.73_494.3
411 626m/z  pos  1-(2-methoxy-nonadecanyl)-
3.89_208.13
412 38m/z  pos  phosphaethanolamine  LMGP02060022
4.22_245.09

413 55m/z  pos  Syneprine acetonide  HMDB0039939

5.50_205.07
414 46n  pos  3-Indolehydracrylic acid  HMDB0059765
5.79_187.09
415 72m/z  neg  4-ene-Valproic acid  LMFA01030982
6.25_254.10

416 64n  pos  (R)-MHD  HMDB0060701
6.34_333.14

417 52m/z  pos  Myrsinone  HMDB0040646

6.65_347.16
418 13m/z  pos  (6E,8E,10S,12Z)-10-Hydroxy-

3-oxooctadecatrienoic acid  HMDB0062359
| m/z   | Charge State | Retention Time (min) | Compound Name                                                                 | HMDB ID   |
|-------|--------------|----------------------|-------------------------------------------------------------------------------|-----------|
| 7.12  | pos          | 347.16               | Corchorifatty acid D                                                          | HMDB0033243 |
| 8.73  | pos          | 109.10               | 2,4,4-Trimethylcyclopentanone                                                 | HMDB0031197 |
|       |              | 151.14               | 4-undecenal                                                                  | LMFA06000066 |
| 9.66  | pos          | 221.15               | (1S,2S)-3-oxo-2-pentyl-cyclopentanebutanoic acid                             | LMFA02010016 |
| 9.76  | neg          | 584.35               | PS(O-20:0/0:0)                                                               | LMGP03060001 |
| 9.86  | pos          | 570.27               | Pipercyclobutanamide A                                                       | HMDB0036360 |
| 2.01  | neg          | 183.04               | 5-Oxo-2(5H)-isoaxolepropanenitrile                                           | HMDB0031338 |
| 4.24  | neg          | 162.05               | Beta-Tyrosine                                                                | HMDB0003831 |
| 4.92  | pos          | 510.19               | Okanin 3,4,3'-trimethyl ether glucoside                                        | LMPK12120174 |
| 5.95  | pos          | 342.09               | 5-hydroxy-2-[(1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)prop-2-en-1-ylidene]amino)-4-methoxybenzoic acid | HMDB0137670 |
| 6.05  | pos          | 333.14               | (4E)-7-(4-hydroxy-3-methoxyphenyl)-1-phenylhept-4-en-3-one                   | HMDB0138247 |
| 7.06  | pos          | 231.13               | Marasmen-3-one                                                               | HMDB0036040 |
| 9.83  | neg          | 239.12               | Cucujolide IX                                                                | LMFA07040037 |
| 0.79  | pos          | 118.08               | 5-Aminopentanoic acid                                                        | HMDB0003355 |
| 0.81  | neg          | 381.09               | 3,4,5-trihydroxy-6-[(2E)-3-phenylprop-2-enoyl]phenoxy]oxane-2-carboxylic acid | HMDB0135447 |
- 434: M/z = 17, Charge = neg, Compound: {3,5,6-trihydroxy-2-[3-(sulfooxy)phenyl]-7H-chromen-7-ylidene}oxidanium, HMDB0130444
- 435: M/z = 437, Charge = pos, Compound: (Z)-3-Methyl-3-decenoic acid, HMDB0031062
- 436: M/z = 915, Charge = pos, Compound: Tetraphyllin B sulfate, HMDB0038486
- 437: M/z = 644, Charge = pos, Compound: 8-Hydroxyhesperetin 7-[6-acetylglucosyl-(1->2)-glucoside], HMDB0041232
- 438: M/z = 22, Charge = pos, Compound: Isoachifolidiene, HMDB0038690
- 439: M/z = 63, Charge = neg, Compound: 4-Vinylphenol sulfate, HMDB0062775
- 440: M/z = 46, Charge = pos, Compound: N-docosahexaenoyl histidine, LMFA08020134
- 441: M/z = 56, Charge = pos, Compound: Sugeonyl acetate, LMPR0103450004
- 442: M/z = 35, Charge = pos, Compound: (S)-MHD, HMDB0060702
- 443: M/z = 8, Charge = pos, Compound: Neotenone, LMPK12050454
- 444: M/z = 17, Charge = pos, Compound: Δ-6 Testosterone Enanthate, 64682
- 445: M/z = 28, Charge = pos, Compound: 3,7,7,10-Tetramethyl-12-thiabicyclo[9.1.0]dodeca-3,7-diene, HMDB0036469
- 446: M/z = 59, Charge = neg, Compound: Benzyl gentiobioside, HMDB0041515
- 447: M/z = 70, Charge = neg, Compound: Quercetin 3-(6"-ferulylglucoside), LMPK12112145
- 448: M/z = 896, Charge = pos, Compound: 4-Oxoisotretinoin, 871
- 449: M/z = 856, Charge = neg, Compound: LysoPE(18:2(9Z,12Z)/0:0), HMDB0011507
2-amino-4-({1-\[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(2-hydroxy-5-oxo-1,7-diphenylheptyl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl)butanoic acid

HMDB0133948

PE-Cer(d14:2(4E,6E)/23:0)

LMSP03020041

N'-nitrosonornicotine

HMDB0041940

PS(P-20:0/19:1(9Z))

LMGP03030074

Methyl (3b,11x)-3-Hydroxy-8-oxo-6-eremophilen-12-oate

HMDB0041229

Phenoxyacetic acid

HMDB0031609

3-hydroxy-1-methyl-4,5-diphenylpiperidine-2,6-dione

HMDB0134789

N-[(3a,5b,7a)-3-hydroxy-24-oxo-7-(sulfooxy)cholan-24-yl]-Glycine

HMDB0002496

3'-Amino-3'-deoxythimidine glucuronide

HMDB0060751

Betaine

HMDB0000043

3,4,5-trihydroxy-6-((5-hydroxy-13,14-dimethoxy-9-oxo-8,17-dioxatetracyclo[8.7.0.0²,⁷.0¹¹,¹⁶]heptadeca-1(10),2,4,6,11,13,15-heptaen-4-yl)oxy)oxane-2-carboxylic acid

HMDB0128466
| m/z     | p/n   | Compound                                      | HMDB ID |
|---------|-------|-----------------------------------------------|---------|
| 10.51_493.3 | pos  | Tiamulin                                      | 43351   |
| 10.64_353.2 | pos  | LysoPC(22:4(7Z,10Z,13Z,16Z)                  |         |
| 11.36_616.3 | neg  | 15R-PGD2                                      | 36166   |
| 11.53_339.2 | neg  | 15(S)-HpEDE                                    | 35361   |
| 11.94_668.2 | pos  | Leukotriene C5                                | HMDB0012993 |
| 2.00_118.04 | pos  | Benzofuran                                     | HMDB0032929 |
| 2.44_316.09 | pos  | S-Nitrosoglutathione                           | HMDB0004645 |
| 3.01_147.04 | pos  | 4-Hydroxyproline galactoside                  | HMDB0029354 |
| 3.87_187.06 | neg  | trans-Cinnamic acid                            | HMDB0000930 |
| 5.58_315.21 | pos  | N-butyl-L-Homocysteine                        |         |
| 6.00_451.13 | pos  | 2,2-difluoro-hexadecanoic acid                | LMFA01090042 |
| 7.14_195.13 | neg  | Dihydrojasmonic acid                          | HMDB00129028 |
| 7.53_167.99 | pos  | 3,4,5-trihydroxy-6-{3-hydroxy-5-[(E)-2-(4hydroxyphenyl)ethenyl]-2-[(1E)-3-methylbuta-1,3-dien-1-yl]phenoxy}oxane-2-carboxylic acid | HMDB0033601 |
| 9.56_179.10 | pos  | 5S,6S-epoxy-7-undecynoic acid                 | LMFA01070039 |
| 11.18_337.2 | pos  | 2(3H)-Benzothiazolethione                     | HMDB0030524 |
| 11.93_678.4 | pos  | Leukotriene B4                                | HMDB0001085 |
| 11.95_339.2 | pos  | PE(18:4(6Z,9Z,12Z,15Z)/P-16:0)                | HMDB0009213 |
| 2.37_202.05 | pos  | Penmacric acid                                | HMDB0029436 |
| 3.79_188.98 | neg  | Pyrocatechol sulfate                          | HMDB0059724 |
| 3.91_211.10 | neg  | Pyroglutamylvaline                            | HMDB0094651 |
| m/z   | pos/neg | NAME                                                   | HMDB ID     |
|-------|---------|--------------------------------------------------------|-------------|
| 4.72  | neg     | Phthalic acid                                         | HMDB0002107|
| 4.75  |         | 6-hydroxy-2-hexynoic acid                             | LMFA01050273|
| 5.24  |         | Ascladiol                                              | HMDB0029610|
| 6.22  |         | (1xi,3S)-1,2,3,4-Tetrahydro-1-methyl-beta-carboline-1,3-dicarboxylic acid | HMDB0035115|
| 8.12  |         | 3-(2-Furanyl)-2-propenal                               | HMDB0037845|
| 8.38  |         | 10-Hydroxy-3-methoxy-1,3,5,7-cadinatetraen-9-one       | HMDB0036456|
| 4.97  |         | (2E)-3-(2,4-dihydroxy-5-methoxyphenyl)prop-2-enoic acid | HMDB0125514|
| 6.93  |         | Cyclopentac[c]pyrrole, benzoic acid deriv              | 3116        |
| 8.38  |         | Ethyl (4Z)-4,7-octadienoate                            | LMFA07010846|
(6-carboxy-3,4,5-trihydroxyoxan-2-yl)\{4-[6,11-dihydroxy-7-(4-hydroxy-3,5-dimethoxyphenyl)-2,8-dioxatricyclo[7.3.1.0^5,^1]^3|trideca-1(13),4,6,9,11-pentaen-3-yldiene]cyclohexa-2,5-dien-1-ylidene\}oxidanium

HMDB0134842

Veranisatin C

PE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))

LMGP02050060

(2R,3R,4R)-2-Amino-4-hydroxy-3-methylpentanoic acid

HMDB0029449

PA(P-18:0/17:2(9Z,12Z))

LMGP10030038

3-Methyl-5-pentyl-2-furanpropanoic acid

HMDB0112084

CAY10587

45468

5-Acetylamino-6-formylamino-3-methyluracil

HMDB0011105

Austdiol

HMDB0030858

phenyl [1-(N-succinylamino)pentyl]phosphate

LMFA08020199

N-Undecanoylglycine

HMDB0013286

alpha-Tocopherol acetate

HMDB0034227

(Z)-3-Oxo-2-(2-pentenyl)-1-cyclopenteneacetic acid

HMDB0030197
| m/z | Charge | Description |
|-----|--------|-------------|
| 9.66_627.33 | pos | 25-Hydroxyvitamin D2-25-glucuronide | HMDB0010342 |
| 1.25_409.02 | pos | {5-hydroxy-11-methoxy-16,18-dioxo-6,8,19-trioxapentacyclo[10.7.0.0²,⁹.0³,⁷.0¹³,¹⁷]nonadeca-1(12),2(9),10,13(17)-tetraen-4-yl}oxidanesulfonic acid | HMDB0126048 |
| 777m/z | neg | PE(0:0/20:4(8Z,11Z,14Z,17Z)) | LMGP02050052 |
| 10.70_480.3 | pos | 1-(2-methoxy-octadecanyl)-sn-glycero-3-phosphoethanolamine | LMGP02060021 |
| 269m/z | neg | 9R,10S-EpOME | 43441 |
| 821m/z | neg | PE(P-16:0e/0:0) | HMDB0011152 |
| 314m/z | neg | Ambrettolic acid | LMFA01050106 |
| 10m/z | pos | Dyphylline | HMDB0014789 |
| 5.20_453.08 | pos | [(3E)-4-{4-[(E)-2-(3,4-dihydroxyphenyl)ethenyl]-2,6-dihydroxyphenyl]-2-methylbut-3-en-1-yl]oxy}sulfonic acid | HMDB0129084 |
| 47m/z | neg | 3-en-1-yloxy)sulfonic acid | HMDB0129084 |
| 6.78_408.27 | pos | Digoxigenin | LMST01120008 |
| 7.22_287.14 | pos | 2E,6Z,8Z,12E-hexadecatetraenoic acid | LMFA01030277 |
| 93m/z | pos | Piperyline | 68174 |
| m/z   | Parent Ion                      | Charge | Description                                                                 |
|-------|--------------------------------|--------|-----------------------------------------------------------------------------|
| 528   | 37m/z                          | pos    | 2-Oxomelatonin                                                              |
|       | 0.91_143.08                    |        | 4-Acetamido-2-aminobutanoic acid                                            |
| 529   | 15m/z                          | pos    | 3alpha,7alpha,12alpha-Trihydroxy-24-methyl-5beta-Cholestan-26-oic acid     |
|       | 12.27_463.3                    |        | Cholestan-26-oic acid                                                      |
| 530   | 417m/z                         | neg    | 3'-N'-Acetylfusarochromanone                                                |
|       | 15.45_550.4                    |        | N-(p-Hydroxyphenethyl)actinidine                                            |
| 531   | 218n                           | pos    | Cholestanyl glucoside                                                      |
|       | 4.18_247.12                    |        | 2',3,4',5-Tetrahydroxy-4-prenylstilbene                                     |
| 532   | 97m/z                          | pos    | 2E,4E-Undecadienoic acid                                                  |
|       | 5.93_286.20                    |        | Chenodeoxyglycocholate                                                      |
| 533   | 95m/z                          | pos    | 3,4,5-trihydroxy-6-([(1E)-5-oxo-1,7-diphenylhept-1-en-3-yl]oxy]oxane-2-carboxylic acid |
|       | 4.73_377.14                    |        | LysoSM(d18:0)                                                              |
| 534   | 82m/z                          | pos    | 1,17-dihydroxy-androstan-3-one                                             |
|       | 6.13_335.12                    |        | PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)                                             |
| 535   | 53m/z                          | pos    | Aspartyl-Isoleucine                                                        |
|       | 7.56_437.15                    |        | N-goshuyoyl lysine                                                         |
| 536   | 56m/z                          | pos    | Cholesteryl glucoside                                                       |
|       | 6.84_182.13                    |        | PC(O-18:1(11Z)/0:0)                                                        |
| 537   | 15n                            | pos    | N-(p-Hydroxyphenethyl)actinidine                                            |
|       | 8.17_448.30                    |        | 2E,4E-Undecadienoic acid                                                  |
| 538   | 93m/z                          | neg    | PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)                                             |
|       | 8.32_353.28                    |        | LysoSM(d18:0)                                                              |
| 539   | 58m/z                          | neg    | 1,17-dihydroxy-androstan-3-one                                             |
|       | 0.77_243.08                    |        | PC(O-18:1(11Z)/0:0)                                                        |
| 540   | 06m/z                          | pos    | LysoSM(d18:0)                                                              |
|       | 10.04_449.3                    |        | PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)                                             |
| 541   | 53n                            | neg    | LysoSM(d18:0)                                                              |
|       | 10.30_586.3                    |        | PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)                                             |
| 542   | 99m/z                          | pos    | LysoSM(d18:0)                                                              |
|       | 152m/z                         | neg    | LysoSM(d18:0)                                                              |
| 543   | 518m/z                         | pos    | LysoSM(d18:0)                                                              |
|       | 1.17-dihydroxy-androstan-3-one  |        | PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)                                             |
| 544   | 10.90_324.2                    |        | LysoSM(d18:0)                                                              |
|       | 4.73_377.14                    |        | PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)                                             |
| 545   | 547m/z                         | pos    | LysoSM(d18:0)                                                              |
|       | 12.24_552.3                    |        | PC(20:5(5Z,8Z,11Z,14Z,17Z)/0:0)                                             |
| 546   | 669m/z                         | neg    | LysoSM(d18:0)                                                              |
|       | 9.62_231.11                    |        | LysoSM(d18:0)                                                              |
| m/z      | Charge | Sign | Compound                                           | HMDB ID    |
|----------|--------|------|----------------------------------------------------|------------|
| 12.26_252.2 | 100n   | pos  | 8Z,10Z-hexadecadienoic acid                       | LMFA01030274 |
| 2.00_204.06 | 31m/z  | pos  | 4-Hydroxy-4-(3-pyridyl)-butanoic acid             | HMDB0001119 |
| 4.47_293.11 | 35m/z  | neg  | gamma-Glutamylphenylalanine                       | HMDB0000594 |
| 5.07_548.36 | 01m/z  | pos  | 3-keto Fusidic acid                               | HMDB0060745 |
| 5.36_629.11 | 82m/z  | neg  | {[5-((4,5-dihydroxy-2-[4-(7-hydroxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)phenoxy]-6-(hydroxymethyl)oxan-3-yl)oxy]-3,4-dihydroxyoxolan-3-yl]methoxy}sulfonic acid | HMDB0124936 |
| 5.97_255.11 | 34m/z  | neg  | 1-(9H-Pyrido[3,4-b]indol-1-yl)-1,4-butanediol     | HMDB0035193 |
| 8.22_241.14 | 39m/z  | neg  | 2E,4E-dodecadienoic acid                         | LMFA01030230 |
| 9.44_309.16 | 98m/z  | neg  | all-trans-7-hydroxyhexadecanoic acid             | LMFA01050502 |
| 9.60_242.21 | 23m/z  | pos  | Alepric acid                                     | LMFA01030191 |
| 0.87_248.10  | 00n    | neg  | gamma-Glutamylthreonine                          | HMDB0029159 |
| 0.92_144.10  | 24m/z  | pos  | xi-4-Hydroxy-4-methyl-2-cyclohexen-1-one         | HMDB0033629 |
| 10.55_403.1  | 357m/z | pos  | 8-Oxodiacetoxydicrinol                            | HMDB0037056 |
| 10.98_263.2  | 080m/z | pos  | Lysyl-Valine                                    | HMDB0028964 |
| No. | Retention Time (min) | m/z Value | Charge State | Molecular Formula | Database ID |
|-----|----------------------|-----------|--------------|-------------------|-------------|
| 560 | 405n                 | 11Z,15Z-octadecadienoic acid | pos | LMFA01030300 |
| 561 | 842m/z               | 2E,6Z-dodecadienoic acid        | neg | LMFA01030231 |
| 562 | 04nm/z               | Estradiol-17beta 3-sulfate      | pos | LMST05020005 |
| 563 | 26m/z                | N-oxide gliclazide              | pos | 3119         |
|     |                      | (3a,5b,7a,12a)-24-[(carboxymethyl)amino]-1,12-dihydroxy-24-oxocholan-3-yl-b-D-Glucopyranosiduronic acid | pos | LMST05010053 |
| 564 | 30m/z                | acid                                     | pos | LMST050010046 |
| 565 | 48m/z                | Ramiprilat                                | pos | HMDB0060579  |
|     |                      | 8Z,12E,14Z-eicosatrienoic acid        | pos | LMFA01030388 |
| 566 | 51n                  | Deoxycholic acid 3-glucuronide      | pos | LMFA02000135 |
|     |                      | 17-hydroxy stearic acid              | pos | HMDB0029061  |
| 567 | 940_318.30           | Threoninyl-Glycine                  | neg | HMDB0029061  |
|     |                      | 2-(2,6-dihydroxy-3,4-dimethoxycyclohexylidene)acetone |
|     |                      | 2-Hydroxyestrone-1-S-glutathione    | pos | HMDB0012623  |
| 568 | 188m/z               | OKHdiA-PE                               | neg | LMGP20020041 |
|     |                      | 2,6-dihydroxy-3,4-dimethoxycyclohexylideneacetone |
| 569 | 331m/z               | 2-Hydroxyestrone-1-S-glutathione    | pos | HMDB0012623  |
| 570 | 567m/z               | Glutaminyltryptophan                 | pos | HMDB0028808 |
|     |                      | gamma-Glutamylvaline                 | neg | HMDB0011172  |
| 571 | 37m/z                | Serotonin                               | pos | HMDB0000259  |
|     |                      | S-Lactoylglutathione                 | pos | HMDB0001066  |
| 572 | 4.19_159.09          | Rosmarinic acid                        | pos | HMDB0003572  |
| m/z | Charge | Intensity | Name | HMDB ID |
|-----|--------|-----------|------|---------|
| 4.69_243.13 | 44m/z | pos | gamma-Glutamylisoleucine | HMDB0011170 |
| 4.70_183.02 | | | 2-Methoxy-1,4-benzoquinone | HMDB0032576 |
| 5.54_376.12 | 65n | pos | 3,5-Pyridinedicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-2-hydroxyethyl | 1507 |
| 5.60_361.14 | 33m/z | pos | 6,11-Dihydroxy-3-methyl-3-(4-methyl-3-pentenyl)-3H,7H-pyran[2,3-c]xanthen-7-one | HMDB0040350 |
| 5.86_349.00 | 34m/z | neg | {4-[2,3-dioxo-3-(2,4,6-trihydroxyphenyl)propyl]phenyl}oxidanesulfonic acid | HMDB0125403 |
| 6.06_255.11 | 36m/z | neg | Naphazoline | HMDB0015656 |
| 6.84_405.18 | 89m/z | neg | Tryptophyl-Arginine | HMDB0029077 |
| 7.90_237.07 | 63m/z | pos | (S)-2,3-Dihydro-7-hydroxy-2-methyl-4-oxo-4H-1-benzopyran-5-acetic acid | 94916 |
| 8.14_499.29 | 94n | pos | 5β-CHOLANIC ACID-3α, 12α-DIOL N-(2-SULPHOETHYL)-AMIDE | 44688 |
| 9.31_663.35 | 92m/z | neg | Neomenthol-glucuronide | HMDB0060012 |
| 9.40_408.28 | 61n | neg | Allocholic acid | 5491 |
| 0.78_371.13 | 62m/z | neg | Loganin | LMPR0102070001 |
| 0.91_102.05 | 49m/z | pos | Hydroxyethyl glycine | HMDB0061148 |
| 1.25_111.00 | | | | |
| 10.97_550.3 | 77m/z | pos | 5-Hydroxy-2-furoic acid | HMDB0059784 |
| 11.97_550.3 | | | | |
| 516m/z | | neg | CerP(d18:1/8:0) | LMSP02050012 |
| m/z | Charge | Peak Type | Retention Time | Name | HMDB ID |
|-----|--------|-----------|----------------|------|---------|
| 593 | 188 m/z | neg       | 11.06 608.3 | OOB-PE | LMGP20020034 |
| 594 | 300 m/z  | pos       | 11.71 482.3 | 7-Dehydrocholesterol-3-sulfate-ester | LMST03010067 |
| 595 | 053 m/z  | pos       | 13.33 628.5 | CerP(d18:1/18:0) | LMSP02050004 |
| 596 | 736 m/z  | neg       | 13.64 467.3 | (5Z,9Z)-2-methoxy-hexacosadienoic acid | LMFA01080023 |
| 597 | 875 m/z  | pos       | 14.94 124.0 | L-Histidinol | HMDB0003431 |
| 598 | 93 m/z   | pos       | 4.63 195.08 | Caffeine | HMDB0001847 |
| 599 | 82 m/z   | pos       | 5.04 480.21 | Obtusaquinol | LMPK12100067 |
| 600 | 32 m/z   | pos       | 5.79 271.16 | Nicardipine | HMDB00014760 |
| 601 | 77 m/z   | pos       | 6.36 243.21 | 4-[3]-ladderane-butanoic acid | LMFA01140010 |
| 602 | 11 m/z   | pos       | 6.81 229.16 | 6-[1]-ladderene hexanol | LMFA01140088 |
| 603 | 71 n     | pos       | 7.04 345.14 | N-Decanoylglycine | HMDB0013267 |
| 604 | 64 m/z   | pos       | 7.92 177.03 | 5'-Carboxy-gamma-chromanol | HMDB0012799 |
| 605 | 89 m/z   | pos       | 8.73 175.14 | 4-(4-Methyl-3-pentenyl)-3-cyclohexene-1-carboxaldehyde | HMDB0031733 |
| 606 | 12 m/z   | neg       | 9.20 631.24 | Ichangin 4-glucoside | HMDB0039340 |
| 607 | 21 m/z   | pos       | 9.52 527.29 | 7',8'-Dihydro-8'-hydroxycitrani xanthin | HMDB0036884 |
| 608 | 99 m/z   | neg       | 1.48 177.03 | Gluconolactone | HMDB0000150 |
| 609 | 537 m/z  | neg       | 11.14 221.1 | (1R,2R)-3-oxo-2-pentyl-cyclopentane butanoic acid | LMFA02010017 |
| 610 | 547 n    | pos       | 13.55 688.5 | PE-Cer(d14:1(4E)/22:0) | 103047 |
| 611 | 189 m/z  | pos       | 13.98 380.2 | PE(12:0/0:0) | LMGP02050005 |
| 612 | 27 m/z   | pos       | 2.05 233.06 | D-altro-D-manno-Heptose | HMDB0029952 |
| m/z   | Type  | Retention Time | Name                                                                 | HMDB Code     |
|-------|-------|----------------|----------------------------------------------------------------------|---------------|
| 2.09  | pos   | 260.16         | 6E,8E,14E-Hexadecatriene-10,12-diynoic acid                          | LMFA01030704  |
| 4.03  | pos   | 125.08         | 6-Acetyl-1,2,3,4-tetrahydropyridine                                   | HMDB0030345   |
| 4.72  | neg   | 259.01         | 3-hydroxy-2-methyl-2-[(sulfooxy)methyl]propanoic acid                 | HMDB0127651   |
| 5.04  | pos   | 245.15         | 6E,8E,12E,14E-Hexadecatetraen-10-ynoic acid                          | LMFA01030703  |
| 6.15  | pos   | 377.13         | 7,14,16-trihydroxy-3-(hydroxymethyl)-3,4,5,6,7,8,9,10,11,12-decacyclo- | LMFA05000662  |
|       | pos   | 315.13         | benzoacyclotetradecin-1-one                                           |               |
| 6.80  | pos   | 315.13         | Ginsenoyne C                                                          |               |
|       | pos   | 336.10         | 3-(3-hydroxyphenyl)-1-(2,4,6-trihydroxy-3-methoxyphenyl)propane-1,2-dione | HMDB0128760   |
| 10.57 | pos   | 435.1          | Garcimangosone C                                                      | HMDB0036984   |
| 11.14 | pos   | 569.3          | LysoPC(22:5(7Z,10Z,13Z,16Z,19Z))                                      | HMDB0010403   |
|       | pos   | 201.10         | 8,8-Dimethoxy-2,6-dimethyl-2-octanol                                  | HMDB0040219   |
| 11.79 | pos   | 403.2          | 16,16-dimethyl-PGE2                                                  | 36136         |
| 11.99 | pos   | 209.1          | cis-tetradec-11-enoic acid                                           | LMFA01030770  |
| 12.85 | pos   | 256.2          | Palmitic amide                                                       | HMDB0012273   |
| 13.05 | pos   | 447.3          | KH 1049                                                             | 57904         |
| 15.26 | pos   | 429.3          | 13'-Hydroxy-alpha-tocopherol                                         | HMDB0012559   |
| 2.00  | neg   | 163.03         | Phenylpyruvic acid                                                  | HMDB0000205   |

**Additional Notes:**
- M/z values represent the mass-to-charge ratio of the detected ions.
- Retention times indicate the time it takes for the compound to pass through the chromatographic column.
- Type indicates whether the ion is positive (pos) or negative (neg).
- HMDB codes link to the Human Metabolome Database for more detailed information on each compound.
| m/z | Peaks | Name | HMDB Number |
|-----|-------|------|-------------|
| 2.00_322.07 | 84m/z | pos | Thymidine 3',5'-cyclic monophosphate | HMDB0001570 |
| 3.00_211.10 | 85m/z | pos | Hydroxyprolyl-Proline | HMDB0028871 |
| 4.54_333.14 | 44m/z | pos | (2E)-3-(3,4-dihydroxyphenyl)-N-[2-hydroxy-2-(4-hydroxyphenyl)ethyl]prop-2-enimide | HMDB0136320 |
| 4.68_400.22 | 18m/z | pos | Tofisopam | HMDB0015699 |
| 6.47_299.13 | 92m/z | pos | 3,6-dihydroxy-4,5-diphenyl-2,3,4,5-tetrahydropyridin-2-one | HMDB0134800 |
| 6.62_494.19 | 53m/z | pos | Erythroskyrin | HMDB0030464 |
| 9.94_337.23 | 00m/z | neg | (-)-Salvisyriacolide | LMPR0105040002 |
| 9.96_309.17 | 74m/z | neg | 12-epi Leukotriene B3 | 45638 |
| 1.19_203.01 | 93m/z | neg | methyl 8-[2-(2-formyl-vinyl)-3-hydroxy-5-oxo-cyclopentyl]-octanoate | LMFA01050151 |
| 1.96_307.11 | 46m/z | pos | 4-Carboxy-2-oxo-3-hexenedioate | 66310 |
| 10.69_392.2 | 919n | neg | 2-Phenylethyl beta-D-glucopyranoside | HMDB0029819 |
| 11.25_263.2 | 378m/z | pos | Stearic acid | LMFA01030455 |
| 13.04_445.3 | 313m/z | neg | Trihydroxycoprostanolic acid | LMST01010246 |
| 13.20_335.1 | 748m/z | pos | Quebrachidine | HMDB0030389 |
| 13.79_779.5 | 503n | pos | PE(19:0/20:5(5Z,8Z,11Z,14Z,17Z)) | LMG02010786 |
| 2.00_189.04 | 01m/z | neg | (E)-2-Methylglutaconic acid | HMDB0002266 |
| 4.51_137.06 | 03m/z | pos | Phenylacetic acid | HMDB0000209 |
4.83_241.11
647  85m/z  neg  Glutamylisoleucine  HMDB0028822

5.43_256.09
648  58n  pos  3-hydroxy-3-(3,4,5-
trimethoxyphenyl)propanoic acid  HMDB0141328

6.40_313.11
649  84m/z  neg  meta-O-Dealkylated flecainide  HMDB0060831
6.74_130.06
650  58m/z  pos  Indole-3-carbinol  HMDB0005785
7.32_452.13
651  46m/z  neg  Norfluoxetine glucuronide  HMDB0061170
9.60_209.15
652  46m/z  pos  Riesling acetal  HMDB0037562

9.69_290.11
653  22n  neg  N-Succinyl-L,L-2,6-
diaminopimelate  HMDB0012267

6.40_313.11
654  55n  pos  6-{3,5-dihydroxy-2-[3,4,5-
trihydroxy-6-(hydroxymethyl)oxan-2-
]phenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid  HMDB0132676

0.79_464.11
655  42m/z  neg  Myricetin 3-(2"-
galloylrhamnoside)  LMPK12112663
0.89_187.07
656  12m/z  pos  gamma-Glutamylglycine  HMDB0011667

1.96_200.97
657  10m/z  neg  2-(sulfooxy)acetic acid  HMDB0124940
10.68_335.2
658  215m/z  pos  8-iso PGF3α  36381
11.13_195.1
659  750m/z  pos  7-tridecenoic acid  LMFA01030595
11.23_258.2
660  423m/z  pos  Exaltolide  HMDB0034455

12.12_674.5
661  392n  pos  PE-Cer(d15:1(4E)/20:0)  LMSP03020016

12.22_391.2
662  843m/z  neg  2E,8E-dodecadienoic acid  LMFA01030232

12.68_391.2
663  844m/z  neg  (Z)-4-Hydroxy-6-dodecenoic acid lactone  LMFA07040067
| m/z  | Precursor | Charge | Name                                                                 | HMDB  |
|------|-----------|--------|----------------------------------------------------------------------|-------|
| 664  | 113       | pos    | 1α,25-Dihydroxy-21-(3-hydroxy-3-methylbutyl)vitamin D(3)             | 42539 |
| 665  | 333       | pos    | 4-Formylsalicylic acid                                                | 69795 |
| 666  | 12        | pos    | Citrusin D                                                            | HMDB0039334 |
|      |           |        | N-gamma-Glutamyl-S-(1-propenyl)cysteine                               | 93225 |
| 667  | 96        | pos    | 2α,25-Dihydroxy-5α-cholestan-3α-ol                                   |       |
|      |           |        | 5-(4-N-pentyl-2-pentylphenyl)-1H-indene                               |       |
| 668  | 57        | pos    | Ginsenosyne K                                                         | HMDB0040375 |
| 669  | 16        | neg    | D-Glucuronic acid 1-phosphate                                         | HMDB0003976 |
| 670  | 36        | neg    | Dityrosine                                                            | HMDB0006045 |
| 671  | 33        | pos    | ent-9-L1-PhytoP                                                       | LMFA02030003 |
|      |           |        | 2-([4-(2-Chlorophenyl)-3-ethoxycarbonyl-6-hydroxymethyl-2-|picolinyl]methoxyacetic acid | 976   |
| 672  | 94        | pos    | Lactacystin                                                           | 64856 |
|      |           |        | Lactacystin                                                           |       |
| 673  | 61        | pos    | Dodecanoic acid, trimethylsilyl ester                                 | HMDB0094677 |
| 674  | 68        | pos    | 3-Methyl sulfolene                                                    | HMDB0059667 |
| 675  | 38        | pos    | 5(S),6(R)-Lipoxin A4-d5                                              | 96397 |
|      |           |        | 5(S),6(R)-Lipoxin A4-d5                                              |       |
| 676  | 13        | pos    | S-Adenosylhomocysteine                                               | HMDB0000939 |
|      |           |        | S-Adenosylhomocysteine                                               |       |
| 677  | 37        | pos    | Trigonelline                                                          | HMDB0000875 |
|      |           |        | Trigonelline                                                          |       |
| 678  | 45        | pos    | 3-Methyl sulfolene                                                    | HMDB0059667 |
|      |           |        | 3-Methyl sulfolene                                                    |       |
| 679  | 435       | neg    | (S)-Bilobanone                                                        | HMDB0036110 |
|      |           |        | (S)-Bilobanone                                                        |       |
| 680  | 186       | neg    | PC(O-14:0/0:0)                                                       | LMGP01060007 |
|      |           |        | PC(O-14:0/0:0)                                                       |       |
| 681  | 793       | pos    | Tridihexethyl                                                         | HMDB0014648 |
|      |           |        | Tridihexethyl                                                         |       |
| 682  | 415       | neg    | 3a,7a-Dihydroxy-5b-cholestan-26-al                                    | HMDB0006894 |
|      |           |        | 3a,7a-Dihydroxy-5b-cholestan-26-al                                    |       |
| 683  | 2         | pos    | Gynocardin                                                            | HMDB0029913 |
| m/z       | Charge | Mass/Charge | Name                                                                                     | HMDB ID   |
|-----------|--------|-------------|------------------------------------------------------------------------------------------|-----------|
| 3.77_290.16 | pos    | 02          | 3-Methylglutaryl carnitine                                                               | HMDB0000552 |
| 4.82_289.12 | pos    | 32          | (1ααα,2ββα,3ααα,11ααα)-1α,2,3,11α-Tetrahydro-6,11-dimethylbenzo[6,7]phenanthro[               | HMDB062223 |
| 5.45_510.22 | pos    | 50          | 2-amino-4-{{1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(2,3-dihydroxy-2-pentyl-1-phenylpropyl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl}butanolic acid | HMDB0126538 |
| 5.53_766.45 | pos    | 65n         | PA(20:5(5Z,8Z,11Z,14Z,17Z)/2                                                             | HMDB0115221 |
| 6.28_414.30 | pos    | 11          | N-Docosahexaenoyl GABA                                                                    | HMDB0062332 |
| 6.57_321.05 | pos    | 80          | N-Formyl-L-aspartate                                                                     | HMDB0060495 |
| 7.04_647.27 | pos    | 07          | 2',7-Dihydroxy-4'-methoxy-8-prenylflavan 2',7-diglucoside                                 | HMDB0036400 |
| 7.96_195.10 | neg    | 27          | 11-oxo-undeca-5,8-dienoic acid                                                           | LMFA01060220 |
| 8.12_337.25 | pos    | 13          | delta2-THA                                                                               | LMFA01030852 |
| 10.03_547.2 | pos    | 14          | PS(12:0/0:0)                                                                             | LMGP03050008 |
| 10.45_616.4 | pos    | 236         | Aerobactin                                                                               | HMDB0004051 |
| 10.80_464.20 | pos    | 0.80        | delta2-THA                                                                               | LMFA01030852 |
| 11.37_359.2 | pos    | 317         | 1-(2-methoxy-18Z-pentacosenyl)-sn-glycero-3-phosphoethanolamine                           | LMGP02060030 |
| 11.37_359.2 | pos    | 317         | 1-(2-methoxy-18Z-pentacosenyl)-sn-glycero-3-phosphoethanolamine                           | LMGP02060030 |
| 11.37_359.2 | pos    | 317         | 1-(2-methoxy-18Z-pentacosenyl)-sn-glycero-3-phosphoethanolamine                           | LMGP02060030 |
| 11.37_359.2 | pos    | 317         | 1-(2-methoxy-18Z-pentacosenyl)-sn-glycero-3-phosphoethanolamine                           | LMGP02060030 |
| 11.37_359.2 | pos    | 317         | 1-(2-methoxy-18Z-pentacosenyl)-sn-glycero-3-phosphoethanolamine                           | LMGP02060030 |
| m/z  | Retention Time | Charge | Mass/Charge Ratio | Description                                                                                     | HMDB ID     |
|------|----------------|--------|-------------------|-------------------------------------------------------------------------------------------------|-------------|
| 687  | 000.20         | pos    | 12.30             | Behenic acid                                                                                   | HMDB0000944|
| 919  | 000.20         | pos    | 12.42             | Sphingosine                                                                                     | HMDB0000252|
| 317  | 000.20         | neg    | 13.51             | 24-keto-25 dehydrocholestanol                                                                     | LMST01010300|
| 95   | 000.30         | pos    | 12.42             | N6-Methyladenosine                                                                             | HMDB0004044|
| 52   | 000.30         | neg    | 5.14              | 4-Formyl-3-(formylmethyl)-4-hexenoic acid                                                        | HMDB0039650|
| 97   | 000.30         | pos    | 5.18              | Flutriafol                                                                                      | 72509       |
| 33   | 000.20         | pos    | 6.23              | 4-(dimethylamino)-1-(2-hydroxyphenyl)-3-methyl-2-phenylbutan-2-yl propanoate                   | HMDB0144291|
| 59   | 000.30         | pos    | 6.50              | (4E)-1-(4-hydroxy-3-methoxyphenyl)dec-4-en-3-one                                                | HMDB0137236|
| 96   | 000.30         | pos    | 6.53              | 5-Hydroxy-7,4-di-methoxy-6,8-di-C-prenylflavanone 5-O-galactoside                                | LMPK12140572|
| 99   | 000.20         | pos    | 6.86              | (S)-17-Hydroxy-9,11,13,15-octadecatetraynoic acid                                               | HMDB0038995|
| 25   | 000.30         | pos    | 7.02              | Linderic acid                                                                                  | LMFA01030038|
| 78   | 000.30         | pos    | 7.07              | Abscisic acid                                                                                  | HMDB0035140|
| 76   | 000.30         | pos    | 8.73              | (Z,Z)-3,6-Dodecadien-1-ol                                                                       | HMDB0031102|
| 86   | 000.30         | pos    | 8.87              | Postin                                                                                         | HMDB0005772|
| 951  | 000.30         | pos    | 9.51              | 1-(2-methoxy-5Z,19Z-hexacosadienyl)-sn-glycero-3-phosphoserine                                 | LMGP03060031|
| 49   | 000.30         | pos    | 9.73              | 6,9,12,15,18,21-                                                                              | HMDB0013025|
| 66   | 000.30         | pos    | 9.73              | Tetracosahexaenoic acid                                                                         |             |
| m/z | Charge | Compound Description                                    | HMDB ID       |
|-----|--------|--------------------------------------------------------|---------------|
| 713 | 14     | Pyranocyanin A                                         | HMDB0035420   |
| 0.79 | 389.13 | Semilepidinoside B                                     | HMDB0033108   |
| 0.89 | 217.08 | 5-(4-hydroxyphenyl)pentanoic acid                      | HMDB0132270   |
| 1.10 | 319.11 | Chavicol O-beta-glucopyranoside                        | HMDB0041617   |
| 11.64 | 417.3 | 24,25-hydroxyvitamin D3                                | 220           |
| 11.98 | 325.1 | 2-Dodecylenzenesulfonic acid                           |               |
| 13.97 | 539.4 | 16-hydroxy-9Z-hexadecenoic acid                         | LMFA01050193  |
| 319  | -0.02 | (S)-2-Hydroxyglutarate                                 | 4151          |
| 93   | -0.04 | 4-hydroxy ketorolac                                     | HMDB0060647   |
| 68   | 0.04  | 5-[2H-Pyrrol-4-(3H)-ylidenemethyl]-2-furanmethanol     | HMDB0040045   |
| 21   | 0.07  | Paraxanthine                                           | HMDB0001860   |
| 76   | 0.11  | Glycinexylidide                                        | HMDB0060679   |
| 91   | 0.08  | (+/-)-3-[(2-methyl-3-furyl)thio]-2-butanone            | HMDB0032401   |
| 75   | -0.03 | 3,4-Dihydroxymandelic acid                             | HMDB0001866   |
| 99   | -0.14 | S-aminomethyldihydrolipoamide                          | HMDB0006239   |
| 19   | 0.14  | Glutamyltryptophan                                     | HMDB0028830   |
| 5.07 | 360.10 | 5,15-dihydroxy-11-methoxy-6,8,20-trioxapentacyclo[10.8.0.0²,⁹.0³,⁷.0¹⁴,¹⁹]icosahexa-1(12),2(9),10,14,16,18-one | HMDB0140693   |
| m/z  | Retention Time | Charge | Description                                           | HMDB ID     |
|------|----------------|--------|-------------------------------------------------------|-------------|
| 5.26 | 257.15         | pos    | 4-Hydroxy-3-polyprenylbenzoate                         | HMDB0060388 |
| 5.53 | 299.13         | pos    | Carisoprodol                                          | HMDB0014539 |
| 6.01 | 466.22         | pos    | AM-toxin I                                            | 71340       |
| 6.75 | 309.09         | pos    | Salicin                                               | HMDB0003546 |
| 6.95 | 299.14         | pos    | Falcarindiol                                          | LMFA05000658|
| 7.10 | 159.10         | pos    | 5-Hydroxyvalproic acid                                 | HMDB0013898 |
| 7.30 | 215.12         | neg    | Isodecenoic acid                                      | LMFA01030032|
| 8.00 | 195.05         | neg    | (3S,5R,6R,7E)-3,5,6-Trihydroxy-7-megastigmen-9-one     | HMDB0038736 |
| 8.40 | 225.14         | pos    | (S)-a-Amino-2,5-dihydro-5-oxo-4-isoxazolepropanoic acid| HMDB0029404 |
| 10.04| 195.1          | neg    | N2-glicoside                                          | HMDB0029404 |
| 10.22| 283.1          | neg    | Cystophorene                                          | HMDB0030944 |
| 10.63| 312.1          | neg    | 2-Octenoic acid                                       | HMDB0000392 |
| 10.85| 241.1          | neg    | Piperettine                                            | HMDB00034371|
| 13.20| 858.5          | pos    | 4-(2,6,6-Trimethyl-1-cyclohexenyl)-2-butanol           | HMDB0036172 |
| 19(R) | 391.20         | pos    | PS(O-18:0/21:0)                                       | LMGP03020037|
| 19(R) | 391.20         | pos    | 19(R)-hydroxy-PGE2                                     | 3819        |
| 2.05 | 231.04         | neg    | Carisoprodol                                          | HMDB0003640 |
| 2.28 | 231.04         | neg    | Carbimazole                                            | HMDB0014533 |
| m/z     | Charge | Name                                                                                     | LMDB/LHMC ID     |
|---------|--------|-------------------------------------------------------------------------------------------|------------------|
| 4.67    | neg    | 2-iodo-hexadecanoic acid                                                                | LMFA01090037     |
| 6.28    | pos    | 1,8-Heptadecadiene-4,6-diyne-3,10-diol                                                    | LMFA05000584     |
| 6.37    | pos    | 7,8-diaminononanoic acid                                                                 | LMFA01100062     |
| 6.74    | pos    | Propanoic acid, 2-(methoxyimino)-, trimethylsilyl ester                                  | HMDB0094703      |
| 7.10    | neg    | Clitocine                                                                                 | HMDB00033718     |
| 7.18    | neg    | 12-oxo-5E,8E,10Z-dodecatrienoic acid                                                     | LMFA01060095     |
| 8.13    | pos    | Sodium glycocholate                                                                      | HMDB0032596      |
| 8.96    | neg    | Coriandrone B                                                                            | HMDB0037775      |
| 9.69    | neg    | 13-Oxo-9,11-tridecadienoic acid                                                          | LMFA01060202     |
| 0.81    | neg    | 4'-Hydroxy-5,7-dimethoxyflavanone 4'-[2-(5-Cinnamoyl)-beta-D-apiofuranosyl]glucoside     | LMPK12140594      |
| 0.87    | neg    | N6-Acetyl-5S-hydroxy-L-lysine                                                             | HMDB0033891      |
| 1.16    | pos    | Asymmetric dimethylarginine                                                               | HMDB0001539      |
| 1.42    | pos    | {[1-hydroxy-1-(1-oxo-1H-isochromen-3-yl)butan-2-yl]oxy}sulfonic acid                    | HMDB0130069      |
| 1.08    | neg    | Sphingosine 1-phosphate                                                                   | HMDB0000277      |
| 1.42    | neg    | Isohyodeoxycholic acid                                                                    | 5634             |
| m/z     | Ionization | Formula                                      | HMDB ID  |
|---------|------------|----------------------------------------------|----------|
| 10.61_337.2 | pos        | MG(0:0/18:2(9Z,12Z)/0:0)                      | HMDB0011538 |
| 10.66_361.2 | pos        | 9-deoxy-9-methylene-16,16-dimethyl-PGE2       | LMFA03010059   |
| 10.72_315.2 | neg        | (9S,10S)-9,10-dihydroxyoctadecanoate          | HMDB0059633   |
| 10.80_619.2 | neg        | 1-Arachidonoylglycerophosphoin                | HMDB0061690   |
| 11.69_251.2 | pos        | (1R,2R)-3-oxo-2-pentyl-cyclopentanohexanoic acid | LMFA02010014 |
| 12.40_324.3 | pos        | 9R,10S-Epoxy-3Z,6Z-heneicosadiene             | LMFA12000320 |
| 12.71_535.3 | neg        | (1S,2S)-3-oxo-2-pentyl-cyclopentanohexanoic acid | LMFA02010015 |
| 13.79_255.2 | neg        | Palmitic acid                                 | HMDB0000220   |
| 14_240.26   | pos        | N-methyl arachidonoyl amine                   | LMFA08020007   |
| 6.41_300.21  | pos        | 3-hydroxynonanoyl carnitine                   | HMDB0061635   |
| 7_345.14     | pos        | Tyrosyl-Tyrosine                             | 86009   |
| 9_490.27     | pos        | 12-Hydroxy-13-O-D-glucuronoside-octadec-9Z-enoate | HMDB0060118 |
| 9_435.22     | pos        | Valsartan                                    | HMDB0014323   |
| 9.60_208.14  | pos        | (5alpha,8beta,9beta)-5,9-Epoxy-3,6-megastigmadien-8-ol | HMDB0034672 |
| 9.66_361.16  | neg        | Thyrotropin releasing hormone                 | HMDB0060080   |
| 21m/z        | neg        |                                              |          |
| m/z     | Intensity | Charge | Name                          | HMDB ID       |
|---------|-----------|--------|-------------------------------|---------------|
| 62.01   | neg       | 0.94   | Thelephoric acid              | HMDB0030552   |
| 100.05  | pos       | 1.19   | 2-Methyltetrahydrofuran-3-one | HMDB0031178   |
| 103.05  | neg       | 1.24   | D-ribonucleotide              | 66231         |
| 326.05  | neg       | 16n    | (3S,6E)-Nerolidol             | HMDB0041629   |
| 339.1   | neg       | 10.35  | Octadecyl fumarate            | HMDB0038073   |
| 357.2   | pos       | 10.67  | 3beta-Hydroxy-chol-5-en-24-oic Acid | LMST04010201 |
| 362.1   | pos       | 11.05  | LysoPC(0:0/16:0)              | HMDB0240262   |
| 363.1   | pos       | 11.80  | 11,14,17-eicosatrienoic acid  | LMFA01030159  |
| 365.1   | pos       | 12.54  | 13-dimethylarsinoyl-tridecanoic acid | LMFA00000034 |
| 373.2   | pos       | 13.46  | 3-Methylpyrrolo[1,2-a]pyrazine | HMDB0033172   |
| 393.16  | pos       | 4.69   | 3-iodo-octadecanoic acid      | LMFA01090040  |
| 39.12   | pos       | 4.90   | Abyssinone II                 | LMPK12140037  |
| 283.10  | pos       | 5.37   | Furofoline                    | HMDB0034319   |
| 419.18  | pos       | 5.60   | Artocarpin                    | LMPK12110898  |
| 425.16  | pos       | 5.98   | Garcinone A                   | HMDB0029509   |
| 253.13  | neg       | 6.95   | (+)-Setoclavine               | HMDB0033428   |
| 471.24  | neg       | 7.31   | 3,16-DIDEOXYMEXICANOLIDE-3β-DIOL | 43636         |
| 326.23  | neg       | 8.20   | 16-J1-PhytoP                  | LMFA02030067  |
| 301.11  | pos       | 8.78   | Methyl 2-aminobenzoate        | HMDB0029703   |
| 255.15  | pos       | 8.89   | Heptanoylcholine              | HMDB0013239   |
| m/z | Charge | Extracted Ion | Compound Name | HMDB ID |
|-----|--------|---------------|---------------|---------|
| 9.61 | neg    | 663.35        | Unshuoside A  | HMDB0029784 |
| 9.66 | pos    | 123.04        | Salicylaldehyde | 66352     |
| 9.94 | pos    | 361.23        | Macrophorin A | 86989    |
| 0.78 | neg    | 241.09        | D-erythro-D-galacto-octitol | HMDB0029953 |
| 1.23 | neg    | 153.03        | Hydantoin-5-propionic acid | HMDB0001212 |
| 10.72 | neg  | 449.2          | 3alpha-androstanediol glururonide | LMST05010004 |
| 11.18 | neg  | 430.3          | 7alpha-Hydroxy-3-oxo-4-cholestenoate | HMDB0012458 |
| 11.44 | neg  | 363.2          | 3-undecynoic acid | LMFA01030611 |
| 11.75 | neg  | 228.2          | 9Z,11E-Tetradecadien-1-ol | LMFA05000187 |
| 11.93 | neg  | 508.3          | 1-heptadecanoyl-sn-glycero-3-phosphocholine | 24068 |
| 11.93 | pos  | 608.3          | OOB-PS | LMG20040019 |
| 13.99 | pos  | 281.2          | Oleic acid | HMDB0000207 |
| 15.33 | neg  | 390.2          | 5alpha-androstane-3alpha-ol-17-one sulfate | LMST05012001 |
| 17.04 | neg  | 396.19         | N1,N10- | 73018 |
| 21.68 | pos  | 229.14         | Dicoumaroylspermidine | HMDB0033469 |
| 7.04 | neg    | 476.19        | N1,N10- | 73018 |
| 6.56 | pos    | 418.14        | Ethyl 2-hydroxy-3-(3-indolyl)propanoate glucoside | HMDB0034873 |
| 6.68 | pos    | 229.14        | Trp-P-1 | 73018 |
| 5.88 | neg    | 370.18        | 5alpha-androstanediol-3alpha-ol-17-one sulfate | LMST05020001 |
| m/z | Intensity | Charge | Name                                                                 | HMDB ID     |
|-----|-----------|--------|----------------------------------------------------------------------|-------------|
| 7.96 | 262.08    | neg    | gamma-Glutamylaspartic acid                                          | HMDB0030419|
| 9.63 | 591.31    | pos    | I-Urobilin                                                           | HMDB004160  |
| 9.66 | 378.15    | neg    | 2-(Arabinosylamino)-3-(glucosylamino)propanenitrile                  | HMDB0039505|
| 9.66 | 591.31    | neg    | Ovalicin                                                             | HMDB0038120|
| 9.90 | 312.19    | pos    | N-desethyloxybutynin                                                 | HMDB0061042|
| 1.23 | 192.02    | pos    | 2,5-didehydro-D-gluconic acid                                        | LMFA01050471|
| 1.70 | 151.02    | neg    | 2,5-didehydro-D-gluconic acid                                        | LMFA01050471|
| 54   |           | pos    | N-desethyloxybutynin                                                 | HMDB0061042|
| 75   |           | neg    | 2,5-didehydro-D-gluconic acid                                        | LMFA01050471|
| 51   |           | neg    | Glycolic acid                                                        | HMDB0000115|
| 10.22| 828.4     | pos    | Digitoxigenin 3-[glucosyl-(1->6)-glucosyl-(1->4)-2,6-dideoxyribohexoside] | HMDB0034321|
| 10.41| 178.4     | pos    | 1-Amino-3-hydroxymethyl-5-methyl-adamantane                          | HMDB0060703|
| 343  |           | pos    | Imiquimod                                                            | 85419       |
| 914  |           | pos    | Leukotriene D4-d5                                                   | 96385       |
| 11.02| 331.2     | pos    | 12,15-Epoxy-13,14-dimethyleicosa-12,14,16-trienoic acid              | HMDB0112073|
| 644  |           | pos    | Formetanate                                                          | 72452       |
| 846  |           | neg    | 2E,8Z-dodecadienoic acid                                            | LMFA01030233|
| 646  |           | neg    | Stearic acid                                                         | 189         |
| 70   |           | pos    | (-)-3,5-Cadinadiene                                                 | HMDB0030673|
| 55   |           | pos    | Luteolin 7-methylgluronide                                          | LMPK12110646|
| m/z | Charge | Ion Type | Compound Name | HMDB ID |
|-----|--------|----------|---------------|---------|
| 5.03 | 186.11 | neg | (±)-Pelletierine | HMDB0030325 |
| 5.43 | 211.09 | neg | 3,4-Methyleneazelaic acid | HMDB0059744 |
| 6.26 | 161.07 | pos | 3-Allyl-1-cyclohexene | HMDB0061784 |
| 6.39 | 315.13 | pos | Cyclandelate | HMDB0015586 |
| 6.49 | 201.11 | neg | 2-Hydroxy-2,6,6-trimethylcyclohexanone | HMDB0037023 |
| 6.60 | 263.99 | pos | 3-Mercaptolactate-cysteine disulfide | HMDB0006512 |
| 6.82 | 527.21 | pos | Acetyl-N-formyl-5-methoxykynurenamine | HMDB0004259 |
| 8.38 | 540.25 | neg | Tetrahydroaldosterone-3-glucuronide | HMDB0010357 |
| 8.47 | 646.42 | pos | 1-(2-methoxy-19Z-hexacosenyl)-sn-glycero-3-phosphoethanolamine | LMGP02060033 |
| 9.30 | 440.27 | pos | N-docosahexaenoyl glutamic acid | LMFA08020089 |
| 9.74 | 409.16 | pos | 1,2-Dihydro-5-hydroxy-2-(1-hydroxy-1-methylethyl)-4-(isobutyl)-6-phenylfurano[2,3-| LMPK12100015 |
| 10.03 | 277.08 | pos | Galactosylglycerol | HMDB0006790 |
| 10.80 | 279.19 | pos | Ipomeatetrahydrofuran | HMDB0040904 |
| 12.88 | 116.07 | pos | L-Proline | HMDB0000162 |
| 11.46 | 494.3 | pos | Linoelaidyl carnitine | HMDB0006461 |
| 11.52 | 344.2 | pos | PC(16:0/0:0) | LMGP01050018 |
| 22.22 | 340.00 | pos | Piperolein B | HMDB0030340 |
| m/z    | Charge | Mass   | Name                                           | HMDB ID  |
|--------|--------|--------|------------------------------------------------|----------|
| 11.93  | neg    | 636.3  | Alodesmosine                                   | HMDB0040704 |
| 12.35  | pos    | 559.5  | 5-Hexatriacontanone                            | HMDB0030937 |
| 12.41  | neg    | 517.3  | Soyasapogenol D                                | HMDB0034507 |
| 13.39  | neg    | 445.3  | astrogorgiadiol B                              | LMST03020242 |
| 12.89  | pos    | 811.6  | PC(20:0/18:3(6Z,9Z,12Z))                       | LMGP01011794 |
| 14.00  | pos    | 123.04 | Hhypoxanthine                                  | HMDB0011140 |
| 14.47  | pos    | 251.2  | Ethyl maltol                                   | HMDB0031735 |
| 2.90   | pos    | 151.06 | 1-Methylhypoxanthine                           | HMDB0013141 |
| 4.60   | pos    | 326.19 | Heptaethylene glycol                           | HMDB0061835 |
| 5.64   | pos    | 516.16 | 2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-\[1-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-oxobutan-2-yl]sulfanyl\]ethyl}-C-hydroxycarbonimidoyl)butanoic acid | HMDB0135691 |
| 6.55   | pos    | 246.09 | Asparaginyl-Methionine                         | HMDB0028737 |
| 6.73   | pos    | 679.26 | Wanepeimicoside A                              | 50446    |
| 7.29   | pos    | 223.13 | Annuionone B                                   | 88204    |
| 7.79   | pos    | 427.21 | 7-Hydroxytacrine                               | 2617     |
| 8.17   | neg    | 427.21 | Harmaline                                      | 3350     |
| 8.37   | neg    | 301.12 | Acetaminophen                                  | HMDB0001859 |
| 9.34   | neg    | 145.12 | Caprylic acid                                  | LMFA01010008 |
| 9.66   | pos    | 593.33 | Mesobilirubinogen                              | HMDB0001898 |
| m/z     | Charge | Type   | Name                                | HMDB ID     |
|---------|--------|--------|-------------------------------------|-------------|
| 872     | 84m/z  | pos    | Pyridine-2-azo-p-dimethylaniline    | 96366       |
| 0.76    |        |        |                                     |             |
| 873     | 72m/z  | pos    | Choline                             | 56          |
| 0.81    |        |        |                                     |             |
| 874     | 31m/z  | neg    | N-Acetyl-D-fucosamine               | 70938       |
| 0.87    |        |        |                                     |             |
| 875     | 12m/z  | pos    | 1-Methylnicotinamide                | HMDB0000699 |
| 1.22    |        |        |                                     |             |
| 876     | 74n    | pos    | L-Acetylcarnitine                   | HMDB0000201 |
| 10.13   |        |        |                                     |             |
| 877     | 833m/z | pos    | Pefloxacin                          | HMDB0014630 |
| 10.39   |        |        |                                     |             |
| 878     | 033m/z | pos    | Butyl salicylate                    | HMDB0040730 |
| 10.71   |        |        |                                     |             |
| 879     | 436m/z | pos    | 2,7-dimethyl-6-nonenolic acid       | LMFA01020130|
| 11.11   |        |        |                                     |             |
| 880     | 512m/z | pos    | OKOHA-PA                            | LMGP20070025|
| 11.35   |        |        |                                     |             |
| 881     | 374m/z | neg    | 9,10-DiHOME                         | 35697       |
| 12.35   |        |        | 2-(5,8-Tetradecadienyl)cyclobutanone| HMDB0037519 |
| 882     | 312n   | pos    | Hydroxylated N-acetyl desmethyl frovatriptan | HMDB0061151|
| 3.76    |        |        |                                     |             |
| 883     | 28m/z  | neg    | Isovalerylalanine                   | HMDB0000747 |
| 3.91    |        |        |                                     |             |
| 884     | 22m/z  | pos    | Demethylated antipyrine             | HMDB0006240 |
| 4.05    |        |        |                                     |             |
| 885     | 84m/z  | pos    | Demethylated antipyrine             | HMDB006240  |
| 4.19    |        |        |                                     |             |
| 886     | 31m/z  | pos    | Dihydroaceanthrylene                | 73104       |
| 4.73    |        |        |                                     |             |
| 887     | 22m/z  | pos    | 5,6-Dihydro-5-hydroxy-6-methyl-2H-pyran-2-one | HMDB0034270|
| 4.74    |        |        |                                     |             |
| 888     | 32m/z  | pos    | 3,4-dimethyl-5-carboxyethyl-2-furanpentanoic acid | LMFA01150055|
| 5.24    |        |        |                                     |             |
| 889     | 78n    | pos    | 2-(3,4,5-trihydroxyphenyl)acetic acid | HMDB0130405 |
| 6.35    |        |        |                                     |             |
| 890     | 75m/z  | neg    | Estrone 3-glucuronide               | LMST05010011|
| 7.59    |        |        |                                     |             |
| 891     | 00m/z  | pos    | 2-Tetradecylcyclobutanone           | HMDB0037517 |
| 892 | 24m/z | neg | 9,10,13-TriHOME | HMDB0004710 |
| 893 | 61m/z | neg | Glucuronosylhyodeoxycholate | LMST05010016 |
| 894 | 5n | pos | 2-Amino-3-methylimidazo[4,5-f]quinoline | HMDB0029706 |
| 895 | 94m/z | pos | N6-goshuyoyl lysine | LMFA08020268 |
| 896 | 97m/z | neg | Valyl-Glutamine | HMDB0029125 |
| 897 | 63m/z | pos | (1R,2S,3S,4R)-p-Methane-2,3-diol | HMDB0035723 |
| 898 | 24m/z | pos | (+)-Limonene | HMDB0004321 |
| 899 | 69m/z | neg | Metoprolol acid | 1254 |
| 900 | 5m/z | pos | L-Histidinol phosphate | 3355 |
| 901 | 58m/z | pos | Isorhamnetin 3-rhamnosyl-(1->2)-galactoside-7-glucoside | LMPK12112331 |
| 902 | 53m/z | pos | 3-O-Methylcoumestrol | HMDB0029584 |
| 903 | 58m/z | pos | delta-Methylionone | HMDB0031737 |
| 904 | 914m/z | neg | Bismuth Subsalicylate | HMDB0015408 |
| 905 | 927m/z | neg | PC(15:1(9Z)/0:0) | LMGP01050125 |
| 906 | 929m/z | neg | PC(14:0/0:0) | LMGP01050012 |
| 907 | 592m/z | neg | Botrydial | LMPR0103640001 |
| 908 | 41m/z | pos | Droperidol | HMDB0014593 |
| 909 | 836m/z | neg | Acid | HMDB0059915 |
| 910 | 573m/z | neg | 5beta-Cholestane-3alpha,7alpha,26-triol | LMST04030020 |
| 911 | 677m/z | pos | Cyclohexylamine | HMDB0031404 |
| 912 | 45m/z | neg | gamma-Glutamylcysteine | HMDB0001049 |
| m/z   | Charge | Retention Time (min) | Name                                      | HMDB ID   |
|-------|--------|----------------------|-------------------------------------------|-----------|
| 3.42  | 309.10 | 83                   | gamma-Glutamyltyrosine                    | HMDB0011741 |
| 4.25  | 641.09 | 19                   | 6-Sinapoylglucoraphenin                    | HMDB0038405 |
| 4.60  | 372.26 | 05                   | Sannamycin A                              | 71872     |
| 5.04  | 347.16 | 22                   | 2,3-Epoxymenaquinone                      | HMDB0060359 |
| 5.51  | 516.16 | 45                   | 2-amino-4-({1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[[2-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-3-oxobuty][sulfanyl]ethyl]-C-hydroxycarbonimidoyl]butanoic acid | HMDB0135692 |
| 6.25  | 462.17 | 57                   | Dihydroisomorphine-3-glucuronide          | HMDB0060820 |
| 6.60  | 213.11 | 25                   | 6-Hydroxy-2,6-dimethyl-2,7-octadien-4-one  | HMDB0034670 |
| 7.20  | 601.26 | 97                   | Fosinopril                                | 2971      |
| 7.65  | 319.12 | 97                   | 1-(4-hydroxyphenyl)-7-phenylheptane-3,5-dione | HMDB0141090 |
| 8.13  | 527.29 | 55                   | 1,7-Diphenyl-4-hepten-3-one               | 87991     |
| 8.52  | 369.17 | 30                   | 5a-Dihydrotestosterone sulfate            | LMST05020042 |
| 8.85  | 279.09 | 56                   | 1-(beta-D-Ribofuranosyl)-1,4-dihydronicotinamide | HMDB0011648 |
| 8.99  | 255.15 | 96                   | 8-tridecynoic acid                        | LMFA01030601 |
| 9.03  | 181.15 | 97                   | Homodihydrojasmine                        | HMDB0031181 |
| m/z | Retention Time | Charge State | Compound Name                                                                 | HMDB ID       |
|-----|----------------|--------------|-------------------------------------------------------------------------------|---------------|
| 927 | 9.11_362.98    | neg          | 2-Oxo-4-phosphonobutanoate                                                     | 63606         |
|     | 9.25_362.98    |              |                                                                               |               |
| 928 | 9.58_172.17    | pos          | Capsidiol                                                                     | HMDB002352    |
|     | 10.04_172.17   |              |                                                                               |               |
| 929 | 9.82_239.09    | pos          | 3,4-dimethyl-5-carboxyethyl-2-furanacrylic acid                               |               |
|     | 10.12_424.9    |              |                                                                               |               |
| 930 | 10.54_333.1    | neg          | N-Trimethyl-2-aminoethylphosphonate                                           | 63594         |
|     | 10.66_172.1    |              |                                                                               |               |
| 931 | 10.81_528.3    | pos          | Eucalyptol                                                                    | HMDB0004472   |
|     | 11.48_465.2    |              |                                                                               |               |
| 932 | 10.97_99m/z    | neg          | PE(22:4(7Z,10Z,13Z,16Z)/0:0)                                                  | LMGP02050014  |
|     | 11.61_293.2    |              |                                                                               |               |
| 933 | 11.61_293.2    | pos          | Homodeoxycholic acid                                                          | LMST04070031  |
|     | 12.01_172.1    |              |                                                                               |               |
| 934 | 12.04_388.2    | pos          | Colnelenic acid                                                               | LMFA10000002  |
|     | 12.92_311.1    |              |                                                                               |               |
| 935 | 14.26_388.2    | pos          | 17-phenyl-trinor-PGF2alpha amide                                              | LMFA03010123  |
|     | 14.26_388.2    |              |                                                                               |               |
| 936 | 14.26_388.2    | pos          | 17-phenyl-trinor-PGF2alpha amide                                              |               |
|     | 14.46_388.2    |              |                                                                               |               |
| 937 | 15.46_388.2    | pos          | 17-phenyl-trinor-PGF2alpha amide                                              |               |
|     | 15.46_388.2    |              |                                                                               |               |
| 938 | 15.46_388.2    | pos          | 17-phenyl-trinor-PGF2alpha amide                                              |               |
|     | 15.46_388.2    |              |                                                                               |               |
| 939 | 15.46_388.2    | pos          | 17-phenyl-trinor-PGF2alpha amide                                              |               |
|     | 15.46_388.2    |              |                                                                               |               |
| 940 | 15.46_388.2    | pos          | 17-phenyl-trinor-PGF2alpha amide                                              |               |
|     | 15.46_388.2    |              |                                                                               |               |
| 941 | 18n            | neg          | Sinapinic acid-O-glucuronide isomer                                            | HMDB0060019   |
|     | 2.00_400.10    |              |                                                                               |               |
| 942 | 2.13_233.04    |              |                                                                               |               |
| 943 | 2.99_346.12    | pos          | 9-Aminoacridine                                                               | 43514         |
|     | 5.22_315.05    |              |                                                                               |               |
| 944 | 5.87_277.14    | pos          | 2-hydroxyflutamide                                                             | HMDB0060949   |
|     | 6.00_383.15    |              |                                                                               |               |
| 945 | 6.00_383.15    | pos          | Acetylpterosin C                                                               | HMDB0030764   |
|     | 6.06_355.12    |              |                                                                               |               |
| 946 | 26m/z          | neg          | S-(Hydroxymethyl)glutathione                                                   | HMDB0004662   |
|     | 6.06_355.12    |              |                                                                               |               |
| 947 | 65m/z          | pos          | Tetrobutylammonium                                                             | 85164         |
| m/z   | Name                                                                 |
|-------|----------------------------------------------------------------------|
| 97m/z | 2,9-heptadecadien-4,6-diyne-1,8-diol LMFA05000022                     |
| 89m/z | (3a,5b,7b)-24-[(carboxymethyl)amino]-7-hydroxy-24-oxocholan-3-yl-b-D-glucopyranosiduronic acid, 6724 |
| 84m/z | 9alpha-Fluoro-11beta,16alpha,17alpha,21-tetrahydroxypregn-4-ene-3,20-dione 70225 |
| 14m/z | Azatadine HMDB0014857                                                |
| 49m/z | (2E,6E)-1-Hydroxy-2,6,10-farnesatrien-9-one 87259                   |
| 13m/z | Undecylprodigiosin 69260                                             |
| 19m/z | 3-Pyridinebutanoic acid HMDB0001007                                  |
| 34m/z | L-Carnitine HMDB0000062                                             |
| 10m/z | Melibiitol HMDB0006791                                              |
| 55m/z | Creatinine HMDB0000562                                              |
| 84m/z | TEPP 72768                                                           |
| 61m/z | Ergothioneine HMDB0003045                                            |
| 787n  | (4OH,8Z,t18:1) sphingosine 53909                                     |
| Retention Time | M/z | Charge | Name                                                                 | HMDB ID   |
|----------------|-----|--------|----------------------------------------------------------------------|-----------|
| 10.16_226.1    | 214 | pos    | epi-4'-hydroxyjasmonic acid                                         | LMFA02020008 |
| 10.21_271.1    | 908 | neg    | 5-Tetradecenoic acid                                                | HMDB0000499 |
| 10.59_365.1    | 457 | pos    | Pyriminobac                                                          | 72651     |
| 10.74_595.2    | 892 | neg    | PI(18:2(9Z,12Z)/0:0)                                                | LMGP06050010 |
| 10.75_305.1    | 383 | pos    | 8-hydroxy-2-(hydroxymethyl)-2-(4-methylpent-3-en-1-yl)-2H-chromene-5-carboxylic acid | HMDB0134718 |
| 10.84_314.2    | 458 | pos    | 18-hydroxy-9R,10S-epoxy-stearic acid                                | LMFA02000003 |
| 10.91_608.3    | 187 | neg    | PHHdiA-PE                                                            | LMGP20020017 |
| 10.91_625.3    | 383 | neg    | HOMIDIUM                                                             | 44366     |
| 10.98_419.2    | 551 | pos    | 2-Hydroxy-4-oxo-5,12-heneicosadien-1-yl acetate                     | HMDB0039403 |
| 11.22_171.1    | 015 | pos    | 1,4-Ipomeadiol                                                       | 87001     |
| 11.25_325.2    | 374 | neg    | Bovinic acid                                                         | HMDB0003797 |
| 11.26_634.3    | 343 | neg    | Pentasine                                                            | HMDB0029803 |
| 11.26_714.3    | 451 | pos    | Fumonisin C4                                                         | LMSP01080030 |
| 11.61_334.2    | 518 | pos    | (±)5(6)-EET methyl ester                                             | 62931     |
| 11.75_464.3    | 517 | pos    | Hongguanggenin                                                       | LMST01080073 |
| 11.87_377.2    | 696 | neg    | 3-Hydroxy-1-phenyl-1-hexadecanone                                    | HMDB0035677 |
| 12.07_473.3    | 643 | pos    | Maslinic Acid                                                        | 44861     |
| 12.85_327.2    | 327 | neg    | DHA                                                                  | LMFA01030185 |
| 14.24_310.3    | 121 | pos    | Stearoylethanolamide                                                 | HMDB0013078 |
| 15.00_138.0    | 665 | pos    | Isoniazid                                                            | 848       |
| Retention Time | m/z   | Charge | Compound Name                                      | HMDB Number |
|----------------|-------|--------|---------------------------------------------------|-------------|
| 15.22          | 401.3 |        | Calcidiol                                         | HMDB0003550 |
| 15.56          | 187.1 |        | 7-Ethyl-5,6-dihydro-1,4-dimethylazulene           | 91006       |
| 4.35           | 291.1 |        | (E)-octadeca-15,17-dien-9,11,13-triynoic acid     | LMFA01031146|
| 4.75           | 179.0 |        | N-benzooylglycinate                                | HMDB0062583 |
| 5.47           | 381.1 |        | 3,4,5-trihydroxy-6-\{4-hydroxy-5-(3-methoxyphenyl)pentanoyl\}oxy-2-carboxylic acid | HMDB0127784 |
| 5.72           | 273.16|        | 1-Octen-3-yl glucoside                            | HMDB0032959 |
| 6.19           | 145.12|        | Hexyl acetate                                     | LMFA07010184|
| 7.93           | 567.31|        | (3a,5b,7a)-23-Carboxy-7-hydroxy-24-norcholan-3-yl-b-D-Glucopyranosiduronic acid | HMDB0002430 |
| 7.97           | 502.18|        | Limonexic acid                                    | HMDB0036075 |
| 9.72           | 257.17|        | 4-(3-Hydroxybutyl)-3,3,5-trimethylcyclohexanone   | HMDB0039805 |
| RT (min) | m/z     | Ionization | Compound Description                        | HMDB ID   |
|---------|---------|------------|---------------------------------------------|-----------|
| 9.93    | 942.18  | Pos        | 7-Methyl-3-oxo-6-octenoyl-CoA                | HMDB0060421 |
| 9.96    | 391.28  | Neg        | Hyodeoxycholic acid                         | 5701      |
| 0.67    | 285.02  | Pos        | 4-(1,2-dithiin-3-yl)-2-(prop-1-en-2-yloxy)but-3-yn-1-yl acetate | LMFA12000363 |
| 0.87    | 132.06  | Pos        | 6-Methyladenine                              | HMDB002099 |
| 0.92    | 455.15  | Pos        | Trioxsalen                                   | HMDB0015575 |
| 1.22    | 269.12  | Neg        | Hypephorine                                  | 67522     |
| 1.24    | 203.01  | Pos        | 4-(1,2-dithiin-3-yl)-2-(prop-1-en-2-yloxy)but-3-yn-1-yl acetate | LMFA07011020 |
| 1.43    | 335.2   | Pos        | Stearamide                                   | LMFA08010003 |
| 1.58    | 487.3   | Pos        | PGJ2                                         | LMFA03010019 |
| 1.64    | 335.1   | Neg        | Menthyl ethylene glycol carbonate           | HMDB0036141 |
| 1.06    | 452.2   | Pos        | 1,5-Dibutyl methyl hydroxyxycitrate         | HMDB0040461 |
| 1.97    | 171.1   | Pos        | LysoPE(0:0/16:0)                             | HMDB0011473 |
| 2.01    | 527.1   | Neg        | Azelaic acid                                 | LMFA01170054 |
| 1.12    | 464.3   | Neg        | 1'-Acetoxyeugenol acetate                   | HMDB0036544 |
| 1.33    | 267.1   | Pos        | 4,7,10-hexadecatrienoic acid                | LMFA08020133 |
| 1.14    | 399.2   | Pos        | 4-Hydroxy-3-methoxy-2,10-bisaboladien-9-one | 89616     |
| 1.16    | 305.0   | Pos        | Colupox b                                   | HMDB0039598 |
| 1.17    | 251.2   | Pos        | Mipafox                                      | 72759     |
| 0.87    | 267.1   | Pos        | 4-Hydroxy-3-methoxy-2,10-bisaboladien-9-one | 89616     |
| 1.01    | 103.1   | Pos        | 4,7,10-hexadecatrienoic acid                | LMFA01030134 |
| 1.12    | 15.2    | Pos        | 4,7,10-hexadecatrienoic acid                | LMFA01030134 |
| 1.17    | 15.2    | Neg        | 4,7,10-hexadecatrienoic acid                | LMFA01030134 |
| Retention Time (min) | m/z     | Ionization State | Compound Description                                           | Compound ID      |
|----------------------|---------|------------------|---------------------------------------------------------------|------------------|
| 12.19_483.3          | 14-hydroxy-5Z-tetradecenoic acid | neg              | LMFA01050181                                                  |                  |
| 12.30_223.2          | 9-Pentadecenoic acid | pos              | HMDB0029765                                                   |                  |
| 12.35_151.0          | 2-Aminobenzimidazole | pos              | 68671                                                        |                  |
| 12.35_563.5          | dirithromycin            | pos              | 3988                                                         |                  |
| 12.35_503.4          | Lyso-PAF C-16-d4              | pos              | 96524                                                        |                  |
| 14.98_129.1          | 2,5-Diethyltetrahydrofuran | pos              | 86355                                                        |                  |
| 15.71_129.1          | Caprylaldehyde            | pos              | LMFA06000028                                                  |                  |
| 15.71_200.05         | Ethosuximide M5           | neg              | 2600                                                         |                  |
| 14.98_479.22         | 11-Deacetylvaltrate 11-(3-hydroxy-3-methylbutanoate) | neg              | HMDB0033654                                                   |                  |
| 2.00_200.05          | N-Benzooxazol-2-yl-guanidine | neg              | 96363                                                        |                  |
| 2.00_479.22          | Tetraethylene glycol       | pos              | HMDB0094708                                                   |                  |
| 2.83_279.10          | [(2,3,4-trihydroxy-5-(hydroxymethyl)oxolan-2-yl)methoxy]sulfonic acid | neg              | HMDB0125613                                                   |                  |
| 3.01_351.13          | (E)-2-Octenal              | pos              | 75309                                                        |                  |
| 3.01_439.16          | 20-Hydroxy-leukotriene E4 | pos              | LMFA03020062                                                  |                  |
| 3.81_195.12          | p-Hydroxyl-ethotoin        | neg              | HMDB0061174                                                   |                  |
| 4.49_259.01          | S-4-benzyl-3-((S)-3-hydroxy-2,2-dimethyloctanoyl)oxazolidin-2-one | pos              | 65461                                                        |                  |
| 5.32_109.10          |                       | neg              |                                                              |                  |
| 5.46_494.19          |                       | pos              |                                                              |                  |
| 5.81_439.16          |                       | pos              |                                                              |                  |
| 6.89_365.24          |                       | pos              |                                                              |                  |
| 7.00_365.24          |                       | pos              |                                                              |                  |
| m/z   | Charge | Name                                                                 | HMDB ID   |
|-------|--------|----------------------------------------------------------------------|-----------|
| 6.93  | neg    | (3b,9R)-5-Megastigmene-3,9-diol 9-[apiosyl-(1->6)-glucoside]          | LMFA13010056 |
| 7.48  | pos    | 7-Hydroxyfluphenazine glucuronide                                     | 2779      |
| 7.96  | neg    | 4-O-Methyl-α-D-glucosyl-(1->2)-b-D-xylosyl-(1->4)-D-xylose             | HMDB0039742 |
| 7.97  | pos    | 2-(hydroxymethyl)-6-(2,4,6-trihydroxyphenyl)oxane-3,4,5-triol          | HMDB0132663 |
| 8.02  | neg    | (25S)-11α,20,26-trihydroxyecdysone                                   | LMST01010158 |
| 8.77  | pos    | INDOPROFEN                                                             | 44065     |
| 9.24  | pos    | Tridecanoylglycine                                                     | HMDB0013317 |
| 9.51  | neg    | 3,4,5-trihydroxy-6-(5-hydroxy-4-[2-hydroxy-3-[4-hydroxy-3-(3-methylbut-2-en-1-yl)phenyl]propanoyl]-2-(3-methylbut-2-en-1-yl)phenoxy)oxane-2-carboxylic acid | HMDB0133199 |
| 9.78  | neg    | 12-Hydroxydodecanoic acid                                             | HMDB0002059 |
| 9.86  | pos    | 2,2',3-Trihydroxydiphenylether                                         | 66734     |
| 0.59  | pos    | Ciliatine                                                              | HMDB0011747 |
| 0.61  | pos    | Rosoxacin                                                              | HMDB0014955 |
| 0.62  | pos    | Oxypurinol                                                             | HMDB0000786 |
| 0.64  | pos    | Lamivudine                                                             | HMDB0014847 |
| m/z     | Retention Time | Charge | Name                                                                                   | HMDB ID |
|---------|----------------|--------|----------------------------------------------------------------------------------------|---------|
| 0.73    | 169.98         | pos    | Iminoaspartic acid                                                                     | LMFA01170110 |
| 0.75    | 479.05         | pos    | 3,5-Dihydroxyphenyl 1-O-(6-O-galloyl-beta-D-glucopyranoside)                           | 93891   |
| 0.82    | 252.10         | pos    | Muramic acid                                                                           | 3381    |
| 0.82    | 203.05         | pos    | myo-Inositol                                                                           | 144     |
| 1.17    | 116.07         | neg    | Pyrrolidine                                                                             | HMDB0031641 |
| 1.22    | 219.01         | pos    | Methionine sulfoximine                                                                  | HMDB0029430 |
| 1.43    | 268.00         | pos    | Flonicamid                                                                              | 72269   |
| 10.37   | 295.1          | neg    | 2S-hydroxy-3-(10Z-tetradecenoyloxy)-propanoic acid                                      | LMFA07010692 |
| 10.41   | 437.1          | pos    | 2-(2,4-dihydroxy-5-methoxyphenyl)-3-(3,7-dimethylocta-2,6-dien-1-yl)-7-hydroxy-4H-chromen-4-one | HMDB0129645 |
| 10.61   | 619.2          | neg    | N-Desmethycitalopram                                                                    | HMDB0014021 |
| 10.93   | 526.2          | neg    | LysoPE(0:0/22:5(7Z,10Z,13Z,16Z,19Z))                                                   | HMDB0011495 |
| 11.02   | 452.2          | neg    | PE(0:0/16:0)                                                                            | LMGP02050036 |
| 11.89   | 183.1          | pos    | Cyclododecanone                                                                         | HMDB0031341 |
| 12.03   | 365.2          | neg    | 5alpha-Pregnane-3alpha,20alpha-diol                                                     | HMDB0060409 |
| 12.34   | 457.3          | neg    | N1,N8-Diacetylispermidine                                                               | HMDB0041947 |
| 12.70   | 333.3          | neg    | Panamine                                                                                | 68571   |
| 15.74   | 137.1          | pos    | (+)-Comphene                                                                            | LMPR0102120011 |
| 2.00    | 450.11         | pos    | Galβ1-4Glcβ-Sp                                                                          | 3607    |
| 23      | pos            |        |                                                                                         |         |
| m/z | Retention Time | Charge | Name | HMDB ID |
|-----|----------------|--------|------|---------|
| 2.12_448.21 | 1073 | 14m/z | pos | 2,2-Dimethyl-3,4-bis(4-methoxyphenyl)-2H-1-benzopyran-7-ol acetate | 70521 |
| 3.42_311.12 | 1074 | 58m/z | pos | 4'-Methoxymucidin | HMDB0030019 |
| 4.07_399.23 | 1075 | 99m/z | pos | Forasartan | HMDB0015434 |
| 4.11_301.09 | 1076 | 24m/z | neg | 2-Hydroxyadenine | HMDB0000403 |
| 4.93_289.12 | 1077 | 27m/z | pos | R-Soterenol | 69207 |
| 5.44_299.13 | 1078 | 96m/z | pos | Annolobine | 67612 |
| 6.19_229.14 | 1079 | 43m/z | pos | 3-Hydroxydodecanedioic acid | HMDB0000413 |
| 6.43_591.31 | 1080 | 87m/z | pos | Boc-Phe(NMe)-Pro-Phe(NMe)-Gly-OMe | 65475 |
| 7.32_487.10 | 1081 | 15m/z | neg | Citicoline | HMDB0001413 |
| 8.77_195.10 | 1082 | 36m/z | pos | 2-Amino-3,4-dimethylimidazo[4,5-f]quinoline | HMDB0029707 |
| 9.40_274.97 | 1083 | 67m/z | neg | Sodium citrate | 69553 |
| 9.40_372.26 | 1084 | 81n | pos | 3alpha-Hydroxy-5beta-chola-8,14-dien-24-oic Acid | LMST04010299 |
| 9.52_428.20 | 1085 | 83m/z | pos | 3-Isomangostin | HMDB0041521 |
| 0.66_275.05 | 1086 | 54m/z | neg | 3,4-Dihydroxybenzaldehyde | HMDB0059965 |
| 0.81_162.05 | 1087 | 22n | neg | 3-Hydroxymethylglutaric acid | HMDB0000355 |
| 0.85_391.00 | 1087 | 0 | neg | 3,3'-Biflaviolin | 72005 |
| 1.16_199.02 | 1089 | 35m/z | pos | 5-Carboxymethyl-2-hydroxymuconate | 63509 |
| m/z       | Compound Description                                                                 | HMDB ID  |
|-----------|--------------------------------------------------------------------------------------|----------|
| 66.02     | {5-[(E)-2-(3,5-dihydroxyphenyl)ethenyl]-2-hydroxyphenyl}oxidanesulfonic acid        | HMDB0128521 |
| 57.02     | RO 40-5966 (Methylmibefradil Metabolite)                                              | 1280     |
| 58.02     | PC(13:0/0:0)                                                                          | LMGP01050001 |
| 67.11     | Ergosine                                                                              | 67481    |
| 445.3     | 24,25-epoxy-cholesterol(d6)                                                          | 41655    |
| 1117.1    | Nonate                                                                                | HMDB0011717 |
| 141.1     | Metenamine                                                                            | HMDB0029598 |
| 417.2     | Androstan-3α,17β-diol                                                                 | 63341    |
| 785.5     | (+)-Dysideapalaunic acid                                                              | LMPR0105040001 |
| 185.1     | PC(18:1(14Z)/18:1(14Z))                                                               | LMGP01010853 |
| 265.02    | (3x,5Z)-1,5-Octadien-3-ol                                                             | HMDB0030966 |
| 429.15    | Anthralin                                                                             | 1030     |
| 294.09    | 6-O-(3R,4-dihydroxy-2-methylene-butanoyl)-beta-D-glucopyranose                      | LMSL05000003 |
| 245.18    | Leucyl-Leucine                                                                        | HMDB0028933 |
| 594.19    | Lipoxin E4                                                                            | LMFA03040006 |
| 255.11    | Nepafenac                                                                             | HMDB0015678 |
| 369.17    | 17β-Hydroxy-5α-androstan-3-one sulfate                                                | 3565     |
| 321.12    | Anthralin                                                                             | 1030     |
| m/z   | Charge |   |       |             |                  |                  |
|-------|--------|---|-------|-------------|------------------|------------------|
| 6.75  | 337.14 | neg | Fusarochromanone | HMDB0033514 | |
| 7.59  | 334.23 |   |       |              |                  |                  |
| 7.86  | 274.18 | pos | Cafestol | HMDB0035710 | |
| 7.86  | 591.25 | pos | Valyl-Arginine | HMDB0029121 | |
| 8.78  | 437.15 | neg | Bipindogulomethylene | HMDB0030623 | |
| 9.78  | 450.16 | pos | PE(6:0/6:0)[U] | 40503 | |
| 8.01  | 144.99 | neg | Tetrafluoroethylene | 73011 | |
| 8.05  | 285.12 |   |       |              |                  |                  |
| 8.59  | 181.15 | neg | Schradan | 72766 | |
| 8.73  | 147.11 | pos | 2-Methyl-3-(2-pentenyl)-2-cyclopenten-1-one | HMDB0037294 | |
| 9.44  | 237.15 | pos | Ferimzone | 72381 | |
| 9.45  | 253.14 | pos | C75 | 44901 | |
| 9.52  | 280.09 | neg | Gravolenic acid | 89591 | |
| 9.79  | 317.11 | pos | 5-Methoxy-2,2-dimethyl-8-phenyl-2H,6H-benzo[1,2-b:5,4-b']dipyran-6-one | 48615 | |
| 9.90  | 296.22 | pos | 9-Decenoylcarnitine | LMFA07070048 | |
| 0.67  | 301.14 | pos | 2-[5-(3,3-dimethyloxiran-2-yl)-3-methylpent-2-en-1-y]benzene-1,3,5-triol | HMDB0133086 | |
| 0.80  | 165.03 | neg | L-Lyxonate | 5524 | |
| 0.81  | 411.10 | neg | EUGENITOL | 44043 | |
| 0.81  | 423.04 | neg | Propane, 1,1,1,3,3-pentafluoro-2-(fluoromethoxy)-3-methoxy-(Compound B) | 2425 | |
| 0.81  | 423.04 | neg | Propane, 1,1,1,3,3-pentafluoro-2-(fluoromethoxy)-3-methoxy-(Compound B) | 2425 | |
0.87_293.10 (E)-1-O-Cinnamyl-beta-D-glucose HMDB0030293
0.88_256.01 Phosphophosphinate 69259
1.21_366.04 {3-[3-(3,4-dihydroxy-2-methoxyphenyl)prop-2-enoyl]phenyl}oxidanesulfonic acid HMDB0126072
1.30_180.91 Deoxypyridinoline HMDB0000569
1.30_430.23 3-Iodopropanoic acid HMDB0031252
10.66_543.3 Sphinganine 1-phosphate HMDB0001383
10.84_517.2 1,1,2-Triphenylpropane 69935
11.28_466.3 Lucidenic acid K HMDB0035890
11.35_592.3 PC(O-15:0/0:0) LMG01060009
11.50_594.3 PC(20:2(11Z,14Z)/0:0) LMG01050132
11.56_296.2 POV-PC 45370
11.56_433.2 9(R)-HODE 45660
11.66_580.3 N-Desmethylaminopyrine 85278
11.76_703.5 LysoPE(0:0/22:1(13Z)) HMDB0011491
11.87_330.2 GlcCer(d15:1/18:0) LMSP0501AA46
11.87_455.2 MG(16:0/0:0/0:0) LMGL01010009
12.67_227.2 Sulfolithocholic acid HMDB0000907
13.18_705.5 (Z)-4-Hepten-1-ol LMFA05000571
13.79_856.5 PC(20:5(5Z,8Z,11Z,14Z,17Z)/22:4(7Z,10Z,13Z,16Z)) 59961
11.29_28m/z pos
11.30_39m/z neg
| m/z  | Charge  | Compound Description                                                                 | HMDB ID  |
|------|---------|--------------------------------------------------------------------------------------|----------|
| 57   | pos     | 8-METHYLCAFFEINE                                                                     | 84980    |
| 76   | pos     | 5,8,11-heptadecatriynoic acid                                                       | LMFA01030479 |
| 46   | pos     | (2Z)-3-hydroxy-2-(phenylmethylidene)heptanoic acid                                    | HMDB0133171 |
| 2   | neg     | 4-hydroxy-7-methyl-5H-furo[2,3-g]isochromen-5-one                                     | HMDB0138947 |
| 80   | pos     | Hexazinone                                                                           | 68694    |
| 15   | neg     | {[1-(2-hydroxyphenyl)-3-oxopropan-2-y]oxy}sulfonic acid                              | HMDB0134069 |
| 65   | pos     | Sisomicin                                                                            | 43332    |
| 51   | pos     | 1,2,3-Tris(1-ethoxyethoxy)propane                                                    | HMDB0037162 |
| 84   | pos     | trans,trans-1,4-Diphenyl-1,3-butadiene                                               | 70315    |
| 14   | neg     | 7-Methylhypoxanthine                                                                 | HMDB0003162 |
| 64   | neg     | 2-Keto-3-deoxy-6-phosphogluconic acid                                                | HMDB0001376 |
| 49   | pos     | Carbofuran                                                                           | HMDB0031770 |
| 10   | pos     | Todatriol glucoside                                                                  | HMDB0037260 |
| 65   | pos     | (1E)-1-(4-hydroxy-3-methoxyphenyl)dec-1-en-3-one                                     | HMDB0137237 |
| 48   | pos     | Eflornithine                                                                         | 2531     |
| 73   | pos     | Glycerol 1-(5-hydroxydodecanoate)                                                    | 94704    |
| Mass (m/z) | Charge | Identity                                      | LMDB Code   |
|-----------|--------|-----------------------------------------------|-------------|
| 8.56      | 260.25 | Pentadecylic acid                             | LMFA01010015|
| 8.60      | 285.25 | 18-fluoro-octadecanoic acid                   | LMFA01090045|
| 8.98      | 236.98 | L-Ascorbate 6-phosphate                       | 63182       |
| 9.16      | 567.31 | (3alpha,5beta,7alpha)-23-Carboxy-7-hydroxy-24-nor-3-yl-beta-D-glucopyranosidouronic acid | LMST05010028|
| 9.26      | 255.15 | Glucopyranosidouronic acid                    |             |
| 9.52      | 267.12 | Cyclohexanecarboxylic acid                    | HMDB0031342 |
| 9.65      | 617.26 | Nevirapine                                    | HMDB0014383 |
| 9.88      | 404.21 | BEBEERINE                                     | 44247       |
| 0.78      | 219.04 | AKB48                                         | 85060       |
| 0.78      | 410.94 | 3-Hydroxyflavone                              | HMDB0031816 |
| 1.15      | 363.10 | Etidronic acid                                | 2629        |
| 1.43      | 360.03 | 2-[(hydroxy{(3,4,8,9,10-pentahydroxy-6-oxo-6H-benzo[c]chromen-1-yl)methyldiene}amino)acetic acid | HMDB0126665 |
| 10.05     | 583.2  | Geldanamycin                                  | 45547       |
| 10.39     | 151.1  | Cuminyl alcohol                               | HMDB0031817 |
| 10.68     | 268.1  | 2-[(5-Methyisufinyl)-4-penten-2-ynylidene]-1,6-dioxaspiro[4.4]non-3-ene | HMDB0032670 |
| 11.02     | 313.2  | Ricinoleic Acid methyl ester                  | 45190       |
| M/z | Retention Time | Charge | Description |
|-----|----------------|--------|-------------|
| 1181| 928 m/z        | neg    | LysoPE(0:0/20:3(11Z,14Z,17Z)) | HMDB0011484 |
| 1182| 366 m/z        | pos    | Nefopam PA(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | 1482 |
| 1183| 731 m/z        | pos    | Ricinoleic acid | 35485 |
| 1184| 429 m/z        | neg    | Verapamil metabolite D-617 | HMDB0013962 |
| 1185| 1227 m/z       | pos    | 1-(8-[5]-ladderane-octanyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphoethanolamine | LMGP02040014 |
| 1186| 387 m/z        | pos    | PG(18:0/22:4(7Z,10Z,13Z,16Z)) | LMGP04010883 |
| 1187| 346 m/z        | pos    | 5-Decanoyl-2-nonylpyridine | HMDB0035516 |
| 1188| 258 m/z        | pos    | 2,4-di-tert-butylphenol | 85271 |
| 1189| 483 m/z        | pos    | 3,4,5-trihydroxy-6-[(4-hydroxy-7-methoxy-2,2-dimethyl-6-(3-phenylpropanoyl)-3,4-dihydro-2H-1-benzopyran-5-yloxy)oxane-2-carboxylic acid | HMDB0125834 |
| 1190| 956 m/z        | pos    | 5-Ethyl-5-(1-methyl-3-carboxypropyl)barbituric acid | 1764 |
| 1191| 88 m/z         | pos    | dibucaine | 3979 |
| 1192| 93 m/z         | pos    | 12alpha-Fluoro-11beta,17beta-dihydroxyandrosta-1,4-dien-3-one | 70655 |
| 1193| 63 m/z         | pos    | Pipercide | HMDB0033449 |
| 1194| 30 m/z         | pos    | Trisphaeridine | 69349 |
| 1195| 62 m/z         | pos    | [8]-Shogaol | HMDB0031463 |
| 1196| 63 m/z         | pos    | Flecainide meta-O-dealkylated | 2702 |
| 1197| 86 m/z         | neg    | 11.02 502.2 LysoPE(0:0/20:3(11Z,14Z,17Z)) | HMDB0011484 |
| 1198| 11.05 276.1    |        | 11.05 771.4 Nefopam PA(P-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | 1482 |
| 1199| 11.36 297.2    |        | Ricinoleic acid | 35485 |
| 1200| 13.20 757.5    |        | 1-(8-[5]-ladderane-octanyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphoethanolamine | LMGP02040014 |
| 1201| 387 n          | pos    | PG(18:0/22:4(7Z,10Z,13Z,16Z)) | LMGP04010883 |
| 1202| 13.60 865.5    |        | 5-Decanoyl-2-nonylpyridine | HMDB0035516 |
| 1203| 346 m/z        | pos    | 2,4-di-tert-butylphenol | 85271 |
| 1204| 15.46 360.3    |        | 3,4,5-trihydroxy-6-[(4-hydroxy-7-methoxy-2,2-dimethyl-6-(3-phenylpropanoyl)-3,4-dihydro-2H-1-benzopyran-5-yloxy)oxane-2-carboxylic acid | HMDB0125834 |
| 1205| 15.92 279.0    |        | 5-Ethyl-5-(1-methyl-3-carboxypropyl)barbituric acid | 1764 |
| 1206| 956 m/z        | pos    | dibucaine | 3979 |
| 1207| 3.00 382.18    |        | 3,4,5-trihydroxy-6-[(4-hydroxy-7-methoxy-2,2-dimethyl-6-(3-phenylpropanoyl)-3,4-dihydro-2H-1-benzopyran-5-yloxy)oxane-2-carboxylic acid | HMDB0125834 |
| 1208| 5.28 571.15    |        | 12alpha-Fluoro-11beta,17beta-dihydroxyandrosta-1,4-dien-3-one | 70655 |
| 1209| 5.44 303.17    |        | Pipercide | HMDB0033449 |
| 1210| 6.06 241.09    |        | Trisphaeridine | 69349 |
| 1211| 6.09 315.13    |        | [8]-Shogaol | HMDB0031463 |
| 1212| 6.35 331.12    |        | Flecainide meta-O-dealkylated | 2702 |
| Time (min) | m/z  | Isotopic Position | Annotation                                                                 | HMDB ID       |
|-----------|------|-------------------|-----------------------------------------------------------------------------|---------------|
| 6.36_250.02 | 24n  | pos               | (S)-Spirobrassinin                                                          | HMDB0035974   |
| 6.84_361.20 | 32m/z | pos               | Aprindine                                                                  | HMDB0015498   |
| 6.99_195.13 | 72m/z | pos               | Traumatin                                                                  | LMFA01060093  |
| 7.02_294.18 | 36n  | pos               | Gingerol                                                                   | HMDB0005783   |
| 7.34_213.16 | 05m/z | pos               | 2-Methyl-2-phenyl-undecane                                                 | HMDB0013820   |
| 7.45_203.00 | 14m/z | pos               | 4-Sulfobenzoate                                                            | 65735         |
| 7.56_452.23 | 04n  | pos               | 2-(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl[oxy]propan-2-yl)-2-oxo-2H,8H,9H-furo[2,3-h]chromen-9-yl 3-methylbut-2-enoate | HMDB0128938   |
| 7.88_507.16 | 46m/z | pos               | 9-yI 3-methylbut-2-enoate                                                  |               |
| 8.28_471.24 | 03m/z | neg               | Oxatomide                                                                  | HMDB0240225   |
| 9.20_734.20 | 34m/z | pos               | Pelargonidin 3-(2G-xylosylrutinoside)                                       | LMPK12010023  |
| 9.60_245.08 | 01m/z | pos               | (2E,11Z)-Wyerone acid                                                      | HMDB0030946   |
| 9.66_236.10 | 51m/z | neg               | HC Blue No.1                                                               | 72968         |
| 0.61_219.05 | 06i/z | pos               | 11-Hydroxycanthin-6-one                                                    | 67521         |
| 0.76_259.07 | 78m/z | neg               | 4-Fluorocyclohexadiene-cis,cis-1,2-diol                                     | 71224         |
| 0.76_180.06 | 38n  | pos               | D-Mannose                                                                  | HMDB0000169   |
| 0.77_162.05 | 22n  | pos               | 2-Hydroxy-2-ethylsuccinic acid                                             | HMDB0059758   |
| 0.78_277.06 | 05m/z | neg               | 5-Hydroxypyrazinamide                                                       | HMDB0001978   |
| 0.78_269.07 | 85m/z | neg               |                                                                           |               |
| m/z  | Isotopes | Charge  | Compound                          | HMDB ID   |
|------|----------|---------|-----------------------------------|-----------|
| 82   | neg      | 1.00    | Isosyringinoside                  | 533.18    |
| 21   | pos      | 1.21    | Maltitol                          | 2928      |
| 47   | pos      | 1.22    | (-)-Nopol                          | 102.05    |
| 51   | pos      | 1.22    | L-Threonine                       | 100167    |
| 23   | pos      | 1.22    | 7-hydroxy-6-methoxy-3-phenyl-3,4-dihydro-2H-1-benzopyran-4-one | 132860    |
| 72   | neg      | 1.23    | Acenocoumarol                      | 15487     |
| 930  | pos      | 1.23    | Sodium Tetradecyl Sulfate          | 14607     |
| 683  | pos      | 1.23    | Usambarine                         | 7552      |
| 534  | neg      | 1.23    | Pelargonic acid                    | 10009     |
| 802  | pos      | 1.23    | 1-Hydroxyepiacorone                | 30918     |
| 961  | pos      | 1.23    | 4-Methylpentanal                   | 1318      |
| 416  | pos      | 1.24    | 8-methoxy-13-hydroxy-9,11-octadecadienoic acid | 108002    |
| 373  | neg      | 1.24    | 11-Cyclohexylundecanoic acid       | 114007    |
| 481  | pos      | 1.24    | 10-Hydroxy-3,7-dimethyl-2E,6E-decdienoic acid | 1030787   |
| 506  | pos      | 1.25    | Idanpramine                        | 71884     |
| 880  | pos      | 1.26    | 25-acetoxy-ergosta-3beta,5alpha,6beta-triol | 1031059   |
| 468  | pos      | 1.26    | MG(0:0/14:0/0:0)                   | 11530     |
| 575  | neg      | 1.26    | 5alpha-cholestan-3alpha,12alpha,16alpha-triol | 10335     |
| 548  | neg      | 1.26    | MG(0:0/14:0/0:0)                   | 11530     |
| m/z | Time | Charge | Description |
|-----|------|--------|-------------|
| 14.21 | 913.5 | pos | PG(22:2(13Z,16Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) LMGP04010786 |
| 14.97 | 107.0 | pos | 4-Methylocatechol 64945 |
| 2.00 | 383.11 | neg | Acetylmaltose 65717 |
| 2.13 | 261.05 | neg | 5-Fluorouridine 71273 |
| 2.28 | 191.0 | neg | 1-Propene, 1,3,3,3-tetrafluoro-2-(fluoromethoxy)-1-methoxy-, (Z)- (Compound C) 2426 |
| 2.83 | 277.08 | neg | gamma-Glutamylmethionine HMDB0034367 |
| 4.13 | 302.20 | pos | Latrepirdine HMDB0240240 |
| 4.18 | 333.03 | neg | 4,7-dihydroxy-3-[(4-hydroxy-2-oxo-2H-chromen-3-yl)methyl]-2H-chromen-2-one HMDB0143111 |
| 4.29 | 196.10 | pos | 4-(3-hydroxybutyl)-2-methoxyphenol HMDB0135672 |
| 4.52 | 379.20 | pos | Pentosidine HMDB0003933 |
| 4.64 | 188.09 | neg | Proline betaine HMDB0004827 |
| 5.12 | 339.00 | neg | Bis(4-nitrophenyl)phosphate 66043 |
| 5.62 | 275.23 | neg | 13-Heptadecyn-1-ol HMDB0013813 |
| 5.85 | 285.03 | pos | Mannitol 1-phosphate HMDB0001530 |
| 6.25 | 353.03 | pos | Repenone LMPK12060079 |
| 6.73 | 415.21 | neg | Isoelemicin HMDB0029867 |
| 6.74 | 223.17 | neg | 7-oxo-11Z-Tetradecenoic acid LMFA01060187 |
| 7.04 | 201.18 | pos | 16-phenyl-tetranor-PGE2 36137 |
| 7.70 | 186.22 | neg | 1-Dodecene HMDB0059874 |
| m/z  | Formula | Description |
|------|---------|-------------|
| 7.87_358.99 | 2-(Fluoromethoxy)-1,1,3,3,3-pentafluoro-1-propene (Compound A) | 2424 |
| 8.62_111.04 | 40m/z pos | Catechol HMDB0000957 |
| 9.62_309.16 | 99m/z neg | Valdiate HMDB0040980 |
| 9.75_195.10 | 39m/z pos | Chrysoidine free base 70207 |
| 9.77_181.15 | 93m/z pos | Methyl 10-undecenoate HMDB0029585 |
| 9.78_366.24 | 9-Fluoro-17beta-hydroxy-6alpha,17-dimethylandrost-4-ene-3,11-dione | 70584 |
| 9.84_288.29 | 37m/z pos | Oleic acid (d5) 45774 |
| 0.62_445.36 | 60m/z pos | 3-beta-Hydroxy-4-beta-methyl-5-alpha-cholest-7-ene-4-alpha-carboxylate HMDB0011662 |
| 0.66_261.04 | 01m/z neg | ISOBERGAPTENE 43733 |
| 0.69_145.09 | 76m/z neg | 3-Aminopropionaldehyde HMDB0001106 |
| 0.78_217.04 | 86m/z neg | Sodium (±)-2-(4-methoxyphenoxy)propionate 94786 |
| 0.78_399.00 | 61m/z neg | Sevoflurane 2422 |
| 0.80_279.00 | 37m/z pos | 2-C-Methyl-D-erythritol 2,4-cyclodiphosphate 64016 |
| 0.96_157.01 | 05m/z pos | L-Malic acid HMDB0000156 |
| 1.22_414.98 | 12m/z pos | 5-Iodotubercidin 45255 |
| 10.23_295.1 | 69m/z pos | 5-Iodotubercidin 45255 |
| 10.30_335.2 | 196m/z pos | Methionyl-Glutamate 85874 |
| 10.77_552.3 | 222m/z pos | 5-trans-PGE2 LMFA03010148 |
| 10.72_552.3 | 103m/z neg | LysoPE(0:0/24:6(6Z,9Z,12Z,15Z,18Z,21Z)) HMDB0011499 |
| m/z | Charge | Peak | Description                                                                 | HMDB/ID     |
|-----|--------|------|------------------------------------------------------------------------------|-------------|
| 10.94_333.2 | neg     | 2-Dimethylamino-5,6-dimethylpyrimidin-4-ol                                   | 68685       |
| 11.11_303.2 | pos     | 11,12-Epoxyeicosatrienoic acid                                              | HMDB0004673 |
| 11.17_375.2 | pos     | 17-phenyl trinor Prostaglandin F2α-d4                                         | 96575       |
| 11.56_459.2 | pos     | [6]-Gingerdiol 4'-O-beta-D-glucopyranoside                                   | HMDB0036122 |
| 11.64_337.1 | pos     | 1alpha,25-dihydroxyvitamin D3 LMST03020258                                  |             |
| 11.67_461.3 | neg     | 12,13-DiHOME(9) LMFA02000164                                                 |             |
| 11.89_304.2 | pos     | 1-O-(2R-hydroxy-tetradecyl)-sn-glycerol LMGL01020061                         |             |
| 11.91_646.2 | pos     | OXONITINE 43770                                                             |             |
| 12.16_336.3 | pos     | Anandamide (20:1, n-9) LMFA08040010                                          |             |
| 12.18_732.5 | pos     | Araliacerbroside HMDB0033621                                                 |             |
| 13.28_899.5 | pos     | PI(16:0/20:3(5Z,8Z,11Z)) 61172                                               |             |
| 15.99_153.0 | pos     | AMT 64865                                                                   |             |
| 2.35_249.05 | pos     | Glucoheptonic acid 3365                                                     |             |
| 4.19_409.18 | pos     | WIN 55212-2 43434                                                           |             |
| 4.63_138.06 | pos     | 2-Pyridylamide oxime 45425                                                  |             |
| 4.72_263.03 | pos     | Ammonium sulfate 92202                                                      |             |
| 5.19_307.11 | neg     | 3-carboxy-4-methyl-5-(4-hydroxypentyl)-2-furanpropanoic acid LMFA01150068   |             |
| 53m/z | pos     | fumaric acid                                                               |             |
| m/z | Charge | Name                                                                 | HMDB ID |
|-----|--------|----------------------------------------------------------------------|---------|
| 5.34_255.08 | 42 m/z | Glycerol 1-propanoate diacetate | HMDB0031640 |
| 5.55_317.11 |         | Fluvoxamine acid | 2951 |
| 5.64_177.11 | 94 m/z | 1-(4-Fluorobenzyl) piperazine | 96603 |
| 5.96_460.17 | 26 m/z | Pralatrexate | 85196 |
| 6.01_560.31 | 06 m/z | LysoPC(18:1(11Z)) | HMDB0010385 |
| 6.02_219.05 | 81 m/z | 3-((Isothiocyanatomethyl)-1-methoxy-1H-indole | HMDB0038463 |
| 6.03_213.01 |         | Deoxyribose 5-phosphate | HMDB001031 |
| 6.05_269.12 | 92 m/z | N-Methylformamide | 58023 |
| 6.06_331.12 |         | Pilosine | 68426 |
| 6.32_187.06 | 57 m/z | Eupolauridine | HMDB0030182 |
| 7.14_267.17 |         | Tributyl phosphate | 70062 |
| 7.27_647.26 | 96 m/z | CAY10626 | 64842 |
| 7.34_368.16 | 86 n | (2S)-2-Butanol O-[(b-D-Apiofuranosyl-(1->6)-b-D-glucopyranoside] | HMDB0041255 |
| 7.41_601.27 |         | PKODIA-PA | LMGP20070008 |
| 7.53_183.10 | 20 m/z | 9,10-dihydroxy-2-decenoic acid | LMFA01050428 |
| 7.59_299.13 |         | Balsoxine | 68395 |
| 7.91_313.11 | 85 m/z | N-Butyl-beta-carboline-3-carboxylate | 69712 |
| 7.97_336.05 |         | Phosphoribosylformylglycine | HMDB0000999 |
| 8.05_292.98 | 56 m/z | 2-Deoxy-D-ribose 1,5-bisphosphate | 66127 |
| 8.32_251.12 |         | Methyl sorbate | 86362 |
| 8.5_257.13 | 85 m/z | | |
| m/z  | Name                                                                 | P / N  |HMDB ID     |
|------|----------------------------------------------------------------------|--------|------------|
| 8.32 | N,N'-Diacetylbenzidine                                               | neg    | 72940      |
| 8.38 | Naphthyl dipeptide                                                  | neg    | 69283      |
| 8.65 | Scyphostatin A                                                      | pos    | LMSP01080060|
| 8.73 | Malyngamide H                                                       | pos    | 65446      |
| 9.12 | b-D-Glucopyranosiduronic acid, (3a,5b)-24-[(carboxymethyl)amino]-24-oxocholan-3-yl | neg    | 6694      |
| 9.15 | Eremopetasinorol                                                   | neg    | HMDB0029668|
| 9.24 | (R)-1-O-b-D-glucopyranosyl-1,3-octanediol                           | pos    | 86223      |
| 9.58 | 3a,7a-Dihydroxycholanoic acid                                      | neg    | HMDB0000384|
| 9.79 | 2,4,5,7alpha-Tetrahydro-1,4,4,7a-tetramethyl-1H-indene-2-ol         | neg    | HMDB0036684|
| 0.63 | Calcium formate                                                     | neg    | 72387      |
| 0.67 | Diplodiatoxin                                                       | pos    | 87705      |
| 0.68 | 5-L-Glutamyl-taurine                                                | pos    | HMDB0004195|
| 0.80 | 2-Cyanopyridine                                                    | neg    | 65730      |
| 0.83 | 6-[2-(2H-1,3-benzodioxol-5-yl)-1-hydroxyethyl]-4-methoxy-5,6-dihydro-2H-pyrans-2-one | pos    | HMDB0131687|
(5-{4-[2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-8-yl]-3,7-dihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl]-2-hydroxyphenyl}oxidanesulfonic acid)

HMDB0135073

Rizatriptan

HMDB0015088

Histidinyl-Isoleucine

HMDB0028888

F-Honaucin A

HMDB0036807

3,4-Dihydro-2H-1-benzopyran-2-one

HMDB0036626

dTDP

HMDB0001274

(2-Furanylmethyl) methyl disulfide

HMDB0062496

(2E)-4-hydroxy-3-methylbut-2-en-1-yl trihydrogen diphosphate

HMDB0036807

2-Polyprenyl-6-methoxyphenol

HMDB0060355

(1x,2x)-Guaiacylglycerol 3-glucoside

HMDB0040600

Lycodine

HMDB0062496

Ketanserin

HMDB0006510

2-Polypropenyl-6-methoxyphenol

HMDB0006510

N-Acetylaspartylglutamic acid

HMDB001067
| m/z      | RT      | Ions | Compound                           | HMDB ID   |
|----------|---------|------|------------------------------------|-----------|
| 11.18_453.3 | 1343    | neg  | 27-Norcholestanehexol              | HMDB0002157 |
| 11.21_237.1 | 1344    | pos  | Acorusnol                          | HMDB0030920 |
| 11.21_889.5 | 1345    | pos  | PG(20:2(11Z,14Z)/22:4(7Z,10Z,13Z,16Z)) | LMGP04010587 |
| 11.56_597.3 | 1346    | neg  | Neoacrimarine B                    | HMDB0040385 |
| 11.81_635.3 | 1347    | pos  | AGC                                | 43439     |
| 11.93_640.2 | 1348    | neg  | Madlongiside C                     | HMDB0037904 |
| 12.27_402.2 | 1349    | pos  | PS(15:0/24:0)                      | HMDB0112340 |
| 12.27_383.1 | 1350    | neg  | 20,24-Epoxy-25,26-dihydroxydammaran-3-one | HMDB0039692 |
| 12.27_383.1 | 1351    | pos  | N-desmethylimatinib                | HMDB0013862 |
| 12.27_383.1 | 1352    | neg  | Alanyl-Cysteine                    | HMDB0028684 |
| 14.02_492.4 | 1353    | pos  | Blighinone                          | HMDB0030643 |
| 15.47_497.2 | 1354    | pos  | 5-Acetamidopentanoate              | 63464     |
| 15.47_497.2 | 1355    | neg  | 3-[3-methoxy-4-(sulfoxy)phenyl]-2-oxopropanoic acid | HMDB0126595 |
| 5.80_171.10 | 1356    | pos  | cis- and trans-Ethyl 2,4-dimethyl-1,3-dioxolane-2-acetate | 88254     |
| 5.83_387.18 | 1357    | neg  | Argentine                           | 68550     |
| 6.05_347.00 | 1358    | neg  | Ellagic acid                        | HMDB0002899 |
| m/z  | wt | charge | Name                                      | HMDB/OtherID |
|------|----|--------|-------------------------------------------|--------------|
| 6.09 | 214.14 | neg | N-Nonanoylglycine                          | HMDB0013279  |
| 6.19 | 510.25 |    | N-Ac-Tyr-Val-Ala-Asp-CHO                   | 45363        |
| 6.25 | 241.09 |    | (E)-Monocrotophos                          | HMDB0031805  |
| 6.43 | 464.28 |    | N-arachidonoyl histidine                   | LMFA08020131 |
| 6.44 | 315.23 |    | Sannamycin B                               | 71873        |
| 6.80 | 362.21 |    | Isohumulone A                              | HMDB0030026  |
| 6.80 | 505.03 | neg| 5-(3'-Carboxy-3'-oxopropenyl)-4,6-dihydroxypicolinate | 63550        |
| 7.34 | 464.30 |    | Prostaglandin F2α isopropyl ester          |              |
| 7.44 | 505.03 |    | 17-phenoxy trinor                          |              |
| 7.63 | 111.04 |    | Hydroquinone                               | 505          |
| 7.83 | 295.22 |    | Dihydroxychaulmoogric acid                 | LMFA01140029 |
| 7.86 | 613.35 |    | Cuscutic resinoside A                      | LMSL05000008 |
| 7.88 | 499.12 |    | 6-[(6-{[3,4-di-hydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy}-3,4,5-trihydroxyoxan-2-yl)methoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid | HMDB0125617  |
| 7.91 | 480.21 |    | Leukotriene E3                             | LMFA03020074 |
| 7.96 | 297.04 |    | 6-(carboxymethoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid | HMDB0124938  |
| 8.02 | 497.27 |    | DIHYDROFLAVOPEREIRINE                      | 84953        |
| 8.04 | 287.14 |    | Fenothiocarb sulfoxide                     | 68827        |
| 8.30 | 151.11 |    | Perillyl aldehyde                          | LMPR0102090010|
| 8.44 | 221.08 |    | 2,2-dimethyl-2H-chromen-5-ol               | HMDB0126379  |
| m/z | Charge | Isotopic Label | Name                                                                 | HMDB00 ID      |
|-----|--------|---------------|----------------------------------------------------------------------|---------------|
| 8.48_167.10 | neg | Methyl propenyl ketone | 58028                                                                  |
| 8.71_424.15  | pos  | O-Methylandrocybmine     | 64398                                                                  |
| 9.53_431.16  | neg  | (2S,4S,6S)-2-[2-(4-Hydroxy-3-methoxyphenyl)ethyl]tetrahydr o-6-(4,5-dihydroxy-3-methoxyphenyl)-2H-pyran-4-yl | HMDB0030503  |
| 9.90_252.99  | pos  | 3-hydroxy-2-(hydroxymethyl)-2-[(sulfooxy)methyl]propanoic acid       | HMDB0127656  |
| 0.76_132.10  | pos  | L-Isoleucine              | HMDB0000172                                                           |
| 0.81_441.09  | pos  | 4-Hydroxylevamisole       | HMDB0000172                                                           |
| 0.83_979.16  | neg  | Glucuronide               | 728                                                                   |
| 0.87_132.02  | neg  | Calcium Gluceptate         | 85364                                                                 |
| 0.96_197.00  | neg  | L-Aspartic acid           | HMDB000191                                                            |
| 0.96_353.03  | pos  | [2-hydroxy-1-(7-hydroxy-1-oxo-1H-isochromen-3-yl)butoxy]sulfonic acid | HMDB0130071  |
| 1.09_227.1   | pos  | Adipic acid               | HMDB0000448                                                          |
| 1.21_503.07  | pos  | Hypericin                 | HMDB0034271                                                          |
| 1.24_165.00  | neg  | Hydroxymalonate           | 65746                                                                 |
| 1.28_427.00  | neg  | Olsalazine-O-sulfate      | HMDB0060600                                                          |
| 1.61_129.05  | neg  | 2-Dodecenal               | HMDB0031020                                                          |
10.13_428.1 7,14-dihydroxy-6-methoxy- 
4,12-dimethyl-5-(3-methylbut-
2-enoyl)-10-oxo-2,9-dioxatricyclo[9.4.0.0 
³,⁸]pentadeca-
1(11),3(8),4,6,12,14-hexaene-
15-carboxylic acid HMDB0139005

10.34_480.2 pos Retrocalamin HMDB0038159

10.35_310.0 pos Tetraphyllin B HMDB0029914

10.81_454.9 pos 3,5-Dinitrosalicylic acid 68986

10.84_405.1 pos HDMBOA-Glc HMDB0037265

10.87_179.1 pos Dihydro-5-(2-octenyl)-2(3H)-
furanone 87239

10.98_129.1 pos N-Acetyl-2,3-dihydro-1H-
pyrrole 87456

11.61_459.3 pos Pubesnolide 89500

12.62_245.2 pos 6,10,14-Trimethyl-5,9,13-
pentadecatrien-2-one 89972

12.62_337.2 pos PGF2alpha methyl ether LMFA03010073

12.72_313.2 pos 1-methylpropyl-tridecanolide LMFA07040053

13.30_672.5 pos PC(O-14:0/O-14:0) 40197

13.79_352.2 pos 4-Chloromethandienone HMDB0004634

15.89_568.4 pos 1-(2-methoxy-tricosanyl)-sn-
glycero-3-
phosphoethanolamine LMGP02060027

2.17_268.10 pos OR-1896 HMDB0060861

3.01_207.04 pos Benzthiazuron 72806
| Time  | M/z  | Charge | Name                                         | HMDB ID    |
|-------|------|--------|----------------------------------------------|------------|
| 4.15  | 304.06 | pos    | N5-Acetyl-N2-gamma-L-glutamyl-L-ornithine     | HMDB0039423|
| 4.19  | 275.06 | pos    | Hydroxyflutamide                             | 674        |
| 4.25  | 103.05 | pos    | Phenylacetaldehyde                           | HMDB0006236|
| 4.49  | 142.06 | neg    | (R)-Boschniakine                             | HMDB0030267|
| 5.03  | 188.12 | pos    | Phenformin                                   | HMDB0015050|
| 5.31  | 329.18 | pos    | 3-Hydroxyphenylacetic acid                   | HMDB0000440|
| 5.43  | 139.02 | pos    | 16alpha-Flouro-17alpha-hydroxyandrost-4-en-3-one | 70567     |
| 5.48  | 351.16 | neg    | Cinnamyl acetate                             | HMDB0029699|
| 5.50  | 426.15 | neg    | Chitobiose                                   | HMDB0003556|
| 5.61  | 195.13 | pos    | Capric acid                                  | HMDB0000511|
| 5.78  | 273.07 | pos    | Clidinium                                    | HMDB0014909|
| 5.94  | 586.36 | pos    | Oxaburimamide                                | 69231      |
| 7.96  | 151.11 | pos    | Fumonisin AK1                                | HMDB0033397|
| 7.79  | 513.26 | neg    | 8-Methylnonenoate                            | HMDB0012183|
| 8.43  | 165.02 | neg    | 3,17-Androstanediol glucuronide              | LMST05010037|
| 8.48  | 144.99 | neg    | Demethylphosphinothricin                     | 63600      |
| 9.03  | 424.15 | neg    | Flupropanate                                 | 72616      |
| 9.52  | 571.06 | pos    | Kreysigine                                   | 64402      |
| 9.68  | 312.41 | pos    | Polypassanone                                 |           |
| 9.98  | 274.06 | pos    | 16alpha-Flouro-17alpha-hydroxyandrost-4-en-3-one |           |
| 10.50 | 274.03 | pos    | 3-Hydroxyphenylacetic acid                   |           |
| 11.28 | 329.18 | pos    | 16alpha-Flouro-17alpha-hydroxyandrost-4-en-3-one |           |
| 11.78 | 426.15 | neg    | Chitobiose                                   |           |
| 12.30 | 273.07 | pos    | Clidinium                                    |           |
| 12.50 | 195.13 | pos    | Capric acid                                  |           |
| 13.00 | 513.26 | neg    | 8-Methylnonenoate                            |           |
| 13.50 | 274.03 | pos    | 3-Hydroxyphenylacetic acid                   |           |
9.24_479.28 STROPHANTHIDIN SEMICARBAZIDE 44254
9.34_197.15
9.38_265.10 3-carboxy-4-methyl-5-(4-oxopentyl)-2-furanproanoic acid LMFA01150067
9.44_306.26 (S)-10,16-Dihydroxyhexadecanoic acid HMDB0037798
9.55_455.24
9.65_238.99 6-Phosphonoglucono-D-lactone HMDB0001127
9.85_195.13
9.91_467.11 b-D-Xylopyranosyl-(1->4)-a-L-rhamnopyranosyl-(1->2)-L-arabinose HMDB0041221
0.62_265.01 3-(Phosphoacetylamido)-L-alanine 66116
0.68_239.16 5-Nonyltetrahydro-2-oxo-3-furancarboxylic acid HMDB0030993
0.75_203.01
0.79_243.11
0.80_102.09
0.87_159.11
0.97_255.05
1.18_463.09
1.18_463.09
1.25_414.0
1.36_251.1
1.36_251.1
1.45_309m/pos DMABA-d6 NHS ester 96492
6-{4-[(1E)-3-[(6-[(3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy)-3,4,5-trihydroxyoxan-2-yl)methoxy]-3-oxoprop-1-en-1-yl]-2-hydroxyphenoxy}-3,4,5-trihydroxyoxane-2-carboxylic acid

10.66_703.1

1452 688m/z  pos  HMDB0125601
1453 353m/z  pos  Palmitaldehyde  LMFA06000088
1454 539m/z  neg  Acorusdiol  HMDB0030919
1455 378m/z  pos  Arachidic acid  HMDB0002212
1456 440m/z  pos  Flavidulol C  HMDB0039150
1457 851m/z  pos  DL-PDMP (hydrochloride)  43407
1458 389m/z  neg  azaperone  3933
1459 488m/z  pos  13Z-Hexadecen-11-yn-1-ol  LMFA05000202
1460 784m/z  pos  Glucosyl 25-hydroxyhexacosanoate  LMFA13010053
1461 736m/z  pos  4-Trimethylammoniobutanoic acid  966
1462 073m/z  pos  Atherosperminine  HMDB0030304
1463 784m/z  pos  Cinn cassiol D2 glucoside  HMDB0034679

1H-1,2,4-Triazole-1-propanoic acid, 4,5-dihydro-3-(1-hydroxyethyl)-5-oxo-4-(2-phenoxyethyl)-

13.20_339.1

1464 656m/z  pos  1477

14.11_563.4

1465 346m/z  pos  Nb-Pentacosanoyltryptamine  HMDB0040820

2.13_305.16

1466 54m/z  pos  Akuammicine  67361
| m/z | intensity | charge | name                                                      | HMDB ID  |
|-----|-----------|--------|-----------------------------------------------------------|----------|
| 2.13_317.11 | 78m/z | pos | Karanjachromene                                           | LMPK12111544 |
| 2.13_410.25 | 66m/z | pos | Tropium                                                   | HMDB0014354 |
| 2.48_290.13 | 69m/z | pos | Codonopsine                                               | 68144    |
| 3.15_169.09 | 89m/z | pos | 2-Octanol                                                 | LMFA05000620 |
| 4.18_665.18 | 18m/z | neg | Ethalfuralin                                              | 72592    |
| 4.19_421.19 | 92m/z | pos | Sarcostin                                                 | 71890    |
| 4.19_650.22 | 51n | pos | 5-Hydroxy-7,3',4'-trimethoxy-8-methylisoflavone 5-O-neohesperidoside | LMPK12050358 |
| 4.44_511.05 | 62m/z | pos | {4-[3-(4-hydroxy-3,6-dioxo-2-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)cyclohexa-1,4-dien-1-yl}-3-oxoprop-1-en-1-yl]phenyl}oxidanesulfonic acid | HMDB0126625 |
| 4.91_474.29 | 47m/z | pos | PC(O-14:1(1E)/0:0)                                       | 40397    |
| 5.11_295.01 | 55m/z | pos | N1,N4-Diacetylsulfanilamide                               | 2528     |
| 5.33_253.07 | 59m/z | neg | L-Phosphoarginine                                         | HMDB0029438 |
| 5.55_485.16 | 07m/z | neg | Cytarabine                                                | HMDB0015122 |
| 5.83_146.06 | 14m/z | pos | 3-Fluorocatechol                                          | 71213    |
| 6.18_365.23 | 41m/z | pos | Indoramin                                                 | 830      |
| 6.25_464.19 | 41m/z | pos | Dihydroisomorphine-6-glucuronide                          | HMDB0061137 |
| 6.37_496.21 | 42m/z | pos | 10,11-Dihydro-12R-hydroxy-leukotriene E4                  | HMDB0012501 |
| 6.40_375.11 | 13m/z | pos | Miraxanthin-III                                          | 67062    |
1485 89m/z  pos  Allyl nonanoate  LMFA07010778
1486 29m/z  pos  D-Urobilin  HMDB0004161
1487 89m/z  neg  Methylisopelletierine  HMDB0030326

8-(1-hydroxy-2-[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy)propan-2-yl)-2-oxo-2H,8H,9H-furo[2,3-h]chromen-9-yl 3-methylbut-2-enoate  HMDB0128939

1488 62m/z  pos  Hexylbenzene  HMDB0061815
1490 29m/z  pos  Ustiloxin D  HMDB0041054
1491 39m/z  pos  Dihydrorhodamine 123  64881
1492 58m/z  pos  PHOOA-PE  LMGP20020023
1493 86m/z  neg  dihydro-α-ergocryptine  4042
1494 98m/z  neg  Dopamine quinone  64470
1495 17m/z  pos  2-thio-Acetyl MAGE  45189
1496 95m/z  pos  Temurin  HMDB0004328
1497 15m/z  neg  2Z,4E,6Z-Decatrienoic acid  LMFA01031053

7alpha-Hydroxy-3,12-dioxo-5beta-cholan-24-oic Acid  LMST04010194

(3E,7E)-4,8,12-Trimethyl-1,3,7,11-tridecatetraene  HMDB0034498

1500 16m/z  neg  Stearoylglycerophosphoglycerol  HMDB0061697

1501 58m/z  pos  4-Methylumbelliferone  HMDB0059622
1502 19m/z  neg  Erythrityl Tetranitrate  85532
2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]nona-3,8-diene
HMDB0030007

Bentazone-sodium
72395

α-Nitrobenzoate
71157

4-Fluorophenylacetic acid
1288

L-cis-3-Amino-2-pyrrolidinecarboxylic acid
86241

3,4,5-trihydroxy-6-((4-methoxy-6-(3-oxoprop-1-en-1-y1)-2H-1,3-benzodioxol-5-y1)oxy)oxane-2-carboxylic acid
HMDB0128691

Valdecoxib
HMDB0005033

1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione
HMDB0031670

Cyanosulfurous acid anion
HMDB0012916

Oxoglutaric acid
HMDB0000208

Chrycolide
HMDB0035145

N-Nitrosothiazolidine-4-carboxylic acid
HMDB0040192

1-hydroxy-2-(beta-D-glucosyloxy)-9,10-anthraquinone
LMFA13010061

Rhodanine
66618

Galactosylsphingosine
HMDB0000648

Merodesmosine
HMDB0030407

Epoxomicin
45091
10.53_253.1 3(4->5)-Abeo-4,11:4,12-diepoxy-3-eudesmanol HMDB0032122
1520 787m/z pos
10.53_447.2
1521 187m/z pos Dulciol A HMDB0029990
10.63_279.0
1522 946m/z pos Triphenylphosphine oxide alpha-N-(3-hydroxyhexadecanoyl) L-ornithine 64889
10.63_425.2
1523 791m/z pos
10.77_489.2
1524 770m/z neg Tropacocaine 68627
10.97_237.1
1525 851m/z pos Geranyl tiglate HMDB0032292
10.97_431.3
1526 157m/z neg 4-cholesten-7α,12α,24-triol-3-one HMDB0062399
11.18_293.2
1527 483m/z pos 3b,17b-Dihydroxyetiocholane HMDB0000369
11.19_179.1
1528 421m/z pos Nicotine imine HMDB0001010
11.52_492.3
1529 443m/z neg PC(P-17:0/0:0) LMGP01070007
11.76_243.2
1530 120m/z pos 6-[5]-ladderane-1-hexanol LMFA05000063
11.93_311.1
1531 656m/z pos 5-Hydroxy-7-(4-hydroxy-3-methoxyphenyl)-1-phenyl-3-heptanone 86319
12.00_429.3
1532 711m/z pos Nervonoylacetonone 91136
12.07_529.3
1533 539m/z pos 16-Glutaryloxy-1alpha,25-dihydroxyvitamin D3 LMST03020634
12.08_660.4
1534 237m/z pos PS(14:0/14:1(9Z)) LMGP03010094
12.24_507.3
1535 702m pos PC(O-18:1(9Z)/0:0) LMGP01060039
12.35_302.2
1536 468m/z pos Anandamide (18:4, n-3) LMFA08040006
13.20_221.2
1537 259m/z pos Hexadecenal HMDB060482
13.41_283.1
1538 756m/z pos Hexaethylene glycol HMDB0061822
14.40_519.4
1539 070m/z pos Ganoderiol C HMDB0037781
| m/z   | Precursor   | Charge | Name                                                                                   | HMDB ID |
|-------|-------------|--------|----------------------------------------------------------------------------------------|---------|
| 15.99 | 178 m/z     | pos    | N-butryl-L-Homoserine lactone-d5                                                       | 96403   |
| 1540  | 83 n        | pos    | m-Coumaric acid                                                                         | HMDB0001713 |
| 1541  | 81 m/z      | pos    | 3-METHYLCHOLANTHRENE                                                                     | 44182   |
| 1542  | 43 m/z      | neg    | 1-Propen, 1,3,3,3-tetrafluoro-2-(fluoromethoxy)-1-methoxy-, (E)-                        | 2427    |
| 1543  | 70 m/z      | pos    | Butyl (S)-3-hydroxybutyrate glucoside                                                   | HMDB0031694 |
| 1544  | 17 m/z      | neg    | 6-(2-Hydroxyethoxy)-6-oxohexanoic acid                                                  | HMDB0061681 |
| 1545  | 52 m/z      | pos    | Benzeneacetonitrile                                                                     | HMDB0034171 |
| 1546  | 82 m/z      | pos    | Dihydrosanguinarine                                                                     | 64356   |
| 1547  | 43 m/z      | neg    | Carboxyltolmetin Glucuronide                                                           | 2875    |
| 1548  | 51 m/z      | neg    | 2,4,6-Octatriynoic acid                                                                 | LMFA01030961 |
| 1549  | 51 m/z      | neg    | Kaempferol 7,4'-dimethyl ether                                                           | LMPK12112596 |
| 1550  | 94 m/z      | neg    | 3-O-sulfate                                                                             |         |
| 1551  | 51 m/z      | neg    | METHAMIDOPHOS                                                                           | 44566   |
| 1552  | 76 m/z      | pos    | 3,4,5-trihydroxy-6-((2E)-2-methyl-3-phenylprop-2-enoyl)oxyane-2-carboxylic acid         | HMDB0133621 |
| 1553  | 76 m/z      | pos    | Propionylcholine                                                                         | HMDB0013305 |
| 1554  | 92 m/z      | pos    | cis-4-Decenyl acetate                                                                   | HMDB0032214 |
| 1555  | 33 m/z      | pos    | SK&F 91581                                                                              | 69228   |
| 1556  | 01 m/z      | pos    | 5-NITRO-2-PHENYLPROPYLAMINO BENZOIC ACID [NPPB]                                         | 44306   |
| 1557  | 59 m/z      | pos    | L-Valine                                                                                | HMDB0000883 |
| m/z | Retention Time | Charge | Compound Name                        | HMDB ID   |
|-----|----------------|--------|--------------------------------------|-----------|
| 6.35_287.04 | 6.35_287.04 | neg    | Furamizole                           | 69954     |
| 6.74_285.03 | 6.74_285.03 | pos    | Sorbitol-6-phosphate                 | 58327     |
| 6.95_151.11 | 6.95_151.11 | pos    | trans-4,5-epoxy-2(E)-decenal          | HMDB0013105      |
| 7.04_289.13 | 6.95_151.11 | pos    | Furanizole                           | 69954     |
| 7.13_275.05 | 6.95_151.11 | pos    | Methionyl-Cysteine                   | HMDB0028970      |
| 7.28_442.16 | 6.95_151.11 | pos    | Hydroxydomperidone(M2b)              | 2377      |
| 7.66_519.22 | 6.95_151.11 | pos    | Glucarubin                           | HMDB0035626      |
| 7.78_315.13 | 6.95_151.11 | pos    | 1-Dehydro-9-fluoro-11-oxotestolactone | 70857     |
| 7.83_168.98 | 6.95_151.11 | pos    | 1,2,3,4-Tetrahydroisoquinoline       | HMDB0012489      |
| 8.01_274.18 | 6.95_151.11 | neg    | Thiazole                             | HMDB0029713      |
| 8.03_463.27 | 6.95_151.11 | pos    | Arginyl-Valine                       | HMDB0028722      |
| 8.28_442.16 | 6.95_151.11 | pos    | Retinyl beta-glucuronide             | HMDB0010340      |
| 8.30_334.23 | 6.95_151.11 | pos    | CARBETAPENTANE                       | 43477      |
| 8.93_334.23 | 6.95_151.11 | pos    | N,N'-Dicyclohexylurea                | 34503      |
| 9.16_621.37 | 6.95_151.11 | pos    | W123                                 | 64710      |
| 9.39_639.38 | 6.95_151.11 | neg    | PI(22:0/0:0)                         | LMGP06050024      |
| 9.66_356.17 | 6.95_151.11 | pos    | Histidinyl-Arginine                  | HMDB0028879      |
| 9.90_176.99 | 6.95_151.11 | pos    | 3-dimethylarsinoyl-propionic         | LMFA000000038      |
| 9.95_151.11 | 6.95_151.11 | pos    | 3-dimethylarsinoyl-propionic acid    | LMFA000000038      |
| 10m/z | 6.95_151.11 | neg    | L-cis-Cyclo(aspartylphenylalanyl)     | HMDB0031360      |
| 10.00_151.11 | 6.95_151.11 | neg    | 3-(Pyrazol-1-yl)-L-alanine           | 65565      |
| 10.84_315.04 | 6.95_151.11 | neg    | Calcium levulinate anhydrous         | 72192      |
| m/z  | Charge | Precursor | Name                                           | HMDB ID     |
|------|--------|-----------|------------------------------------------------|-------------|
| 0.89 389.05 | neg    | 3,4,5-trihydroxy-6-((8-methoxy-2-oxo-2H-furo[2,3-h]chromen-4-yl)oxy)oxane-2-carboxylic acid | HMDB0135849 |
| 0.89 797.26  | neg    | Oxmetidine |                                                | HMDB0041970 |
| 0.97 239.16 | pos    | 3-Hydroxydodecanoic acid |                                                | 5376        |
| 1.23 221.01 | neg    | Thiazafluron |                                                | 72835       |
| 1.42 144.02 | pos    | 3-Methylthiopropanamine |                                                | 65962       |
| 1.71 243.23 | pos    | Methyl tetradecanoate |                                                | 86999       |
| 10.08 397.2 | neg    | PGI2 |                                                | LMFA03010087 |
| 10.70 275.1 | neg    | Phytuberin |                                                | 67898       |
| 10.70 479.3 | neg    | 7-oxo-11E-Tetradecenoic acid |                                                | LMFA01060186 |
| 10.74 561.2 | neg    | Eriojaposide B |                                                | HMDB0038029 |
| 10.90 995.6 | neg    | PIM1(17:0/18:0) |                                                | LMGP15010012 |
| 10.90 512.3 | pos    | AGELASINE |                                                | 43731       |
| 10.74 512.3 | pos    | Makisterone A |                                                | 71399       |
| 11.03 580.2 | pos    | 19-Hydroxycinnzeylanol 19-glucoside |                                                | HMDB0036856 |
| 11.11 425.0 | pos    | Quercetin 7,3'-4'-trimethyl ether 3-sulfate |                                                | LMPK12112657 |
| 11.26 583.3 | pos    | POB-PC |                                                | LMGP20010021 |
| 11.37 293.2 | neg    | Thioperamide |                                                | 45306       |
| 11.40 580.3 | pos    | 12(13)Ep-9-KODE |                                                | HMDB0013623 |
| 11.83 636.3 | pos    | desferrioxamine G |                                                | LMFA08020171 |
| 11.89 341.3 | pos    | Glycidyl stearate |                                                | 73128       |
| m/z | Name                                                                 | HMDB ID       |
|-----|----------------------------------------------------------------------|---------------|
| 793 | (E)-6,10-Dimethyl-9-methylene-5-undecen-2-one                        | HMDB0035862   |
| 434 | 7-Epizucchini factor A                                              | HMDB0036405   |
| 133 | 2-N-Undecyltetrahydrothiophene                                       | 68825         |
| 594 | 2,6-Dimethyl-5-heptenal propyleneglycol acetal                      | HMDB0032235   |
| 37  | Palustrine                                                           | 68425         |
| 37  | Glucosamine                                                          | HMDB0001514   |
| 37  | (±)-erythro-Isoleucine                                              | HMDB0033923   |
| 76  | 2-Hydroxy-cis-hex-2,4-dienoate                                      | 69013         |
| 20  | Ethyl trans-p-methoxycinnamate                                      | HMDB0030762   |
| 37  | 14-O-(beta-D-glucopyranosyl)-7S,14R-dihydroxy-7,9,13,17-tetramethyl- | LMFA13010034  |
| 8.44| 2E,4E,8E,10E,12E,16E-octadecahexaenoic acid                          |               |
| 8.56| PARAROSANILINE                                                      | 43540         |
| 8.83| Leucyl-phenylalanine                                                | HMDB0013243   |
| 8.94| Burimamide                                                           | 66645         |
| 9.12| AG-490                                                              | 45246         |
| 9.22| Sphingosine 1-phosphate (d16:1-P)                                    | HMDB0060061   |
| 9.80| Apo-10'-violaxanthal                                                | 93624         |
| 9.91| Sedoheptulose 1,7-bisphosphate                                      | 156           |
1617 80 m/z  pos  Niazimicin A  HMDB0031944
1618 28 m/z  pos  Stearoylcarnitine  HMDB0000848
1619 73 m/z  pos  \{[(3E)-4-(5-hydroxy-1-oxo-1H-isochromen-3-yl)but-3-en-2-yloxy]sulfonic acid\}  HMDB0130051
1620 74 m/z  pos  Calopogoniumisoflavone A  47558
1621 16 m/z  pos  Desacetylcefotaxime  HMDB0041868
1622 84 m/z  neg  \{[(3E)-4-(5-hydroxy-1-oxo-1H-isochromen-3-yl)but-3-en-1-yloxy]sulfonic acid\}  HMDB0130058
1623 81 m/z  neg  FOSFOSAL  44294
1624 28 m/z  neg  6,11-dihydroxy-7-(4-hydroxy-3,5-dimethoxyphenyl)-3-[4-hydroxy-3-(sulfooxy)phenyl]-2λ⁴,8-dioxatricyclo[7.3.1.0⁵,¹³]trideca-1(13),2,4,6,9,11-hexaen-2-ylilum  HMDB0134859
1625 96 m/z  pos  De-O-methylsimmondsin  95628
1626 78 m/z  neg  Chrycorin  HMDB0035149
1627 100 m/z  pos  8'-Hydroxydihydroergotamine  2261
1628 964 m/z  pos  CRUSTECDYSONE  43863
1629 492 m/z  pos  15S-HETE-d8  36332
1630 884 m/z  pos  Geranylfarnesyl diphosphate  62877
1631 980 m/z  pos  Pederin  71091
1632 974 m/z  pos  Obacunone  HMDB0035858
| m/z (rt) | Intensity | Charge | Compound Description |
|---------|-----------|--------|----------------------|
| 10.93   | 351.2     |        | Propantheline        |
| 11.01   | 447.3     |        | 13'-Carboxy-gamma-tocopherol |
| 11.05   | 540.3     |        | (25R)-3alpha,7alpha-dihydroxy-5beta-cholestan-27-oyl taurine |
| 11.37   | 253.2     |        | 3-keto palmitic acid |
| 11.84   | 418.3     |        | PE(P-20:0/0:0)       |
| 12.04   | 780.1     |        | Malvidin 3-(6-malonylglucoside) 5-glucoside |
| 12.10   | 492.3     |        | Xeniasterol-a        |
| 12.97   | 899.4     |        | Hoduloside VIII      |
| 14.24   | 293.2     |        | Paullinic acid       |
| 15.47   | 549.4     |        | Monoanhydroescholtzanthin |
| 15.67   | 138.0     |        | 6-Aminonicotinamide  |
| 2.05    | 365.12    |        | 3,4,5-trihydroxy-6-{5-methoxy-2-[(1E)-3-oxopent-1-en-1-yl]phenoxy}oxane-2-carboxylic acid |
| 3.00    | 244.03    |        | {3-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenyl}oxidanesulfonic acid |
| 4.19    | 433.14    |        | cis-3-Hexenyl b-primeveroside |
| 4.19    | 531.10    |        | Americanin B         |
| 5.04    | 722.21    |        | Pteroyltriglutamic acid |

HMDB IDs: Propantheline (HMDB0014920), 13'-Carboxy-gamma-tocopherol (HMDB0012557), (25R)-3alpha,7alpha-dihydroxy-5beta-cholestan-27-oyl taurine (LMST05040008), 3-keto palmitic acid (35745), PE(P-20:0/0:0) (LMGP02070004), Malvidin 3-(6-malonylglucoside) 5-glucoside (93459), Xeniasterol-a (LMST01031064), Hoduloside VIII (95138), Paullinic acid (HMDB0035159), Monoanhydroescholtzanthin (LMPR01070026), 6-Aminonicotinamide (44444), 3,4,5-trihydroxy-6-{5-methoxy-2-[(1E)-3-oxopent-1-en-1-yl]phenoxy}oxane-2-carboxylic acid (HMDB0132990), {3-[(1E)-3-hydroxy-2-methylprop-1-en-1-yl]phenyl}oxidanesulfonic acid (HMDB0133648), cis-3-Hexenyl b-primeveroside (HMDB0031690), Americanin B (92272), Pteroyltriglutamic acid (6381).
| m/z   | Charge | Name                                                                 | HMDB ID   |
|-------|--------|----------------------------------------------------------------------|-----------|
| 5.22_313.15 | 73m/z  | 5.24_268.03 Pos  | N-((3-oxo-hexanoyl)-Phenylalanylphenylalanine | HMDB0013302 |
| 95m/z  | Pos    | N-(3-oxo-hexanoyl)-homoserine thiolactone | LMFA08020240 |
| 95m/z  | Pos    | Oxoassoanine | 69383 |
| 6.00_213.05 | 51m/z  | 3-[[1(E)-but-1-en-1-yl]-5,6-dihydroxy-1H-isochromen-1-one | HMDB0130045 |
| 6.01_132.08 | 51m/z  | 3-Methylindole | HMDB0000466 |
| 6.18_558.29 | 90m/z  | LysoPC(18:2(9Z,12Z)) | HMDB0010386 |
| 6.29_369.17 | 90m/z  | Cyclomammein | HMDB0030711 |
| 6.78_535.04 | 30m/z  | PU-H71 | 96497 |
| 7.90_399.21 | 90m/z  | Nevskin | HMDB0030162 |
| 7.96_324.06 | 78m/z  | N-(7-Mercaptoheptanoyl)threonine 3-O-phosphate | 63904 |
| m/z   | Charge | Purity   | Name                          | HMDB ID       |
|-------|--------|----------|-------------------------------|---------------|
| 1670  | 77m/z  | pos      | 13-L-Hydroperoxylinoleic acid | HMDB0003871   |
| 1671  | 9.66_295.22 | neg | Halocins                      | HMDB0038173   |
| 1672  | 9.84_389.27 | pos      | Gentian Violet                | 4055          |
| 1673  | 0.61_279.04 | pos      | Caffeoylmalic acid            | HMDB0029318   |
| 1674  | 0.66_207.97 | neg      | 2-Thiothiazolidine-4-carboxylic acid | HMDB0041805   |
| 1675  | 0.77_302.04 | pos      | Quercetin                     | HMDB0005794   |
| 1676  | 0.80_148.03 | neg      | D-2-Hydroxyglutaric acid      | HMDB0000606   |
| 1677  | 21m/z  | neg      | N-Acetylhistidine              | HMDB0032055   |
| 1678  | 40m/z  | neg      | Phosphatidyl glycerol         | 186           |
| 1679  | 85m/z  | pos      | Canavaninosuccinate           | 62849         |
| 1680  | 58m/z  | neg      | Isradipine Metabolite (3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-d | 873           |
| 1681  | 0.83_657.19 | neg | Sulindac sulfide              | 2605          |
| 1682  | 72m/z  | neg      | Sulfamethoxazole sodium       | 71876         |
| 1683  | 16m/z  | pos      | 7-Methylpyrido[3,4-c]psoralen  | 73152         |
| 1684  | 0.83_679.17 | neg | 3,6,8-dodecatrien-1-ol        | LMFA05000058  |
| 1685  | 0.99_258.03 | pos      | Pyrroloquinoline quinone      | HMDB0013636   |
| 1686  | 10.04_421.3 | pos | Nb-Palmitoyltryptamine        | HMDB0040815   |
| 1687  | 208m/z | pos      | Furcelleran                   | 92382         |
| 1688  | 10.22_516.1 | pos | Undecanal                     | HMDB0030941   |
| Time (min) | m/z | Charge | Description | HMDB ID |
|-----------|-----|--------|-------------|---------|
| 10.27     | 587.2 | pos   | 2-{2,6-dihydroxy-4-[6-hydroxy-7-(3-methylbut-2-en-1-yl)-1-benzofuran-2-yl]-3-methoxyphenyl}-6-(2,4-dihydroxyphenyl)-4-methylcyclohex-3-ene-1-carboxylic acid | HMDB0126228 |
| 10.41     | 526.2 | neg   | LysoPE(22:5(4Z,7Z,10Z,13Z,16Z)/0:0) | HMDB0011524 |
| 10.65     | 632.3 | neg   | PHOOA-PS | LMGP20040005 |
| 10.79     | 551.3 | pos   | 24S-methylcholest-22E-en-3beta,4beta,5alpha,6alpha,8beta,a,14alpha,15alpha,25,28-nonol | 84029 |
| 10.87     | 277.1 | neg   | (2Z)-2-[(3-hydroxyphenyl)methylidene]octanal | HMDB0134125 |
| 10.98     | 427.3 | pos   | 1-O-(2R-hydroxy-eicosanyl)-sn-glycerol | LMGL01020066 |
| 11.18     | 901.5 | pos   | PGP(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | HMDB0013531 |
| 11.21     | 321.2 | pos   | 14,15-Epoxy-5,8,11-eicosatrienoic acid | HMDB0002283 |
| 11.70     | 480.3 | neg   | 1-(2-methoxy-6Z-heptadecenyl)-sn-glycero-3-phosphoethanolamine | LMGP02060019 |
| 11.87     | 841.5 | pos   | PI-Cer(t18:0/18:0(2OH)) | 103166 |
| 11.90     | 319.2 | pos   | 1-O-(2R-hydroxy-pentadecyl)-sn-glycerol | LMGL01020062 |
| m/z  | p/n   | Intensity | Name                                      | HMDB   |
|------|-------|-----------|-------------------------------------------|--------|
| 12.11 | 377.2 | neg       | Adrenic Acid                              | LMFA01030178 |
| 12.64 | 404.3 | pos       | Gamma-linolenyl carnitine                 | HMDB0006318 |
| 15.90 | 297.0 | neg       | 3,4,5-trihydroxy-6-[(2-hydroxyacetyl)oxy]oxane-2-carboxylic acid | HMDB0124939 |
| 2.00  | 279.03| neg       | 5-Hydroxypyrizinoic acid                  | 2198   |
| 2.00  | 306.05| neg       | Aminoparathion                            | HMDB0001504 |
| 2.01  | 169.06| neg       | Methylimidazole acetaldehyde              | HMDB0004181 |
| 4.19  | 220.08| pos       | 5-Hydroxy-L-tryptophan                    | HMDB0000472 |
| 4.82  | 385.31| pos       | Pinacidil-N-Oxide                        | 1942   |
| 5.04  | 289.00| pos       | Macamide                                  | LMFA08020159 |
| 5.64  | 389.09| pos       | 4-Methoxybenzenepropanol 1-(2-sulphoglucoside) | HMDB0034757 |
| 6.18  | 539.24| neg       | 7,11-Bisdeacetylvaltrate 7-(3-methylpentanoate) 11-(3-hydroxy-3-methylbutanoate) | HMDB0033655 |
| 6.49  | 159.10| neg       | 3-hydroxy caprylic acid                   | LMFA01050021 |
| 7.32  | 452.12| neg       | 5-[6-hydroxy-2-(4-hydroxyphenyl)-4-[(E)-2-(4-hydroxyphenyl)ethenyl]-1-benzofuran-3-yl]benzene-1,3-diol | HMDB0140527 |
| 7.34  | 505.13| neg       | Acridinium NHS ester                      | 64846  |
| 7.43  | 415.21| pos       | gamma-Asarone                             | HMDB0029872 |
| m/z | Charge | Isotope | Name                                           | HMDB ID   |
|-----|--------|---------|------------------------------------------------|-----------|
| 7.97 |     505.16 | pos     | Eriotriochin                                    | LMPK12050186 |
| 8.01 |     151.11 | pos     | Methyl octynecarboxylate                        | 87543     |
| 8.37 |     369.17 | neg     | 16-phenoxy tetranor                             | 45407     |
| 8.55 |     209.15 | pos     | Prostaglandin A2                                |           |
| 8.55 |     305.08 | pos     | 2,3-Dihydro-2,3-dihydroxy-4-(4-hydroxyphenyl)-1H-phenalen-1-one |           |
| 8.74 |     477.37 | pos     | 11-keto-Octacosanoic acid                       | LMFA01060204 |
| 8.95 |     446.28 | neg     | Trihydroxyoxocholanyl-Glycine                   | LMST05030007 |
| 9.29 |     450.32 | neg     | 2,3-Dihydroxyoxan-2-yl]methoxy]sulfonic acid    |           |
| 9.78 |     171.10 | pos     | 3-Sulfinoalanine                                | HMDB0000996 |
| 9.80 |     174.99 | pos     | 5-trans Latanoprost                             | 45709     |
| 9.78 |     234.05 | neg     | (+/-)-Ethyl 3-acetoxy-2-methylbutyrate          | HMDB0032258 |
| 0.68 |     237.14 | pos     | 4-Heptyloxybenzoic acid                         | 69931     |
| 0.77 |     127.03 | pos     | 5-Hydroxymethyl-2-furancarboxaldehyde           | HMDB0034355 |
| 0.77 |     565.06 | pos     | ((6-[5,6-dihydroxy-2-(4-hydroxyphenyl)-7-methoxy-4-oxo-4H-chromen-8-yl]-3,4,5-trihydroxyoxan-2-y| HMDB0127146 |
| 0.78 |     234.05 | pos     | Benzo[b]naphtho[2,1-d]thiophene                 | 73542     |
| 0.80 |     263.08 | pos     | FKGK 11                                         | 45480     |
| 0.85 |     607.13 | pos     | (±)-Conen                                       | 86377     |
| Retention Time | m/z     | Charge | Name                                      | HMDB ID    |
|----------------|---------|--------|-------------------------------------------|------------|
| 0.91_643.10    | 82m/z   | neg    | Fusaroskyrin                              | HMDB0034314|
| 1.01_241.06    | 49m/z   | neg    | Allura red AC                             | HMDB0032884|
| 1.21_154.06    | 94m/z   | pos    | Dinotefuran                               | 72315      |
| 1.21_265.08    | 17m/z   | neg    | 2-Oxoarginine                             | HMDB0004225|
| 1.21_319.12    | 77m/z   | pos    | 4-Methylburimamide                        | 69230      |
| 1.23_407.03    | 23m/z   | pos    | Didemethylcitalopram                      | HMDB0060472|
| 1.43_319.07    | 45m/z   | pos    | Thiamine pyrophosphate                    | 2832       |
| 1.24_381.02    | 77m/z   | neg    | [4-(5,7-dihydroxy-6-methoxy-4-oxo-3,4-dihydro-2H-1-benzopyran-2-yl)phenyl]oxidanesulfonic acid | HMDB0128600|
| 1.43_426.08    | 49m/z   | pos    | [4-(5-hydroxy-7-methoxy-8-methyl-4-oxo-4H-chromen-3-yl)-2-methoxyphenyl]oxidanesulfonic acid | HMDB0129590|
| 1.43_766.25    | 74m/z   | pos    | Aquifoliunine EIII                        | 89387      |
| 1.48_277.08    | 91m/z   | pos    | (2R)-1-O-beta-D-Galactopyranosylglycerol   | HMDB0038664|
| 1.65_243.23    | 23m/z   | pos    | Dodecyl propionate                        | 88298      |
| 1.98_298.99    | 83m/z   | pos    | [2-hydroxy-6-methoxy-4-(prop-2-en-1-yl)phenyl]oxidanesulfonic acid | HMDB0135261|
| 1.98_380.15    | 92n     | pos    | N-(1-Deoxy-1-fructosyl)tryptophan          | HMDB0037847|
| 10.17_379.0    | 930m/z  | pos    | Dolichin B                                | LMPK12070015|
| 10.46_361.2    | 1022m/z | pos    | JWH 210-d9                                | 96637      |
| m/z | Retention Time | rt | Name                                                                 | CID   |
|-----|---------------|----|----------------------------------------------------------------------|-------|
| 482 | 10.54_265.1   | neg| 6,7-Dihydro-4-(hydroxymethyl)-2-(p-hydroxyphenethyl)-7-methyl-5H-2-pyridinium | 89304 |
| 695 | 10.84_172.1   | pos| (R)-(+) alpha-Terpineol                                             | LMPR0102090028 |
| 763 | 10.90_100.0   | pos| 5-amino-pentanoic acid                                              | LMFA01100040 |
| 695 | 10.93_271.2   | pos| (R)-3-Hydroxy-hexadecanoic acid                                    | HMDB0010734 |
| 519 | 11.90_780.1   | pos| Malonylmalvin                                                       | LMPK12010388 |
| 491 | 12.11_447.3   | pos| 24-hydroxy-cholesterol(d6)                                         | 41656 |
| 682 | 12.27_483.3   | neg| 3-Oxotetradecanoic acid                                            | HMDB0010730 |
| 173 | 12.41_277.2   | pos| 13-Oxo-ODE                                                          | LMFA02000016 |
| 400 | 13.72_416.0   | pos| 6-Methylthioguanosine monophosphate                                | 71266 |
| 609 | 13.83_574.4   | pos| DG(15:0/18:4(6Z,9Z,12Z,15Z)/0:0)                                    | HMDB0007077 |
| 47  | 13.90_780.1   | neg| Moricizine sulfoxide                                               | 1346  |
| 99  | 2.04_262.03   | pos| (2-phenyl-7H-chromen-7-ylidene)oxidanium                            | HMDB0133410 |
| 34  | 2.04_275.11   | pos| Pantoyllactone glucoside                                           | 95683 |
| 87  | 2.12_516.21   | pos| Epothilone C                                                       | 71028 |
| 50  | 4.41_245.99   | pos| 4-Methyl-5-(2-phosphoethyl)-thiazole                                | 3360  |
| 50  | 4.50_453.05   | pos| Calcium gluconate                                                  | 66832 |
| 98  | 4.72_187.00   | neg| Dimethyl sulfone                                                   | 7236  |
| 4.74| 4.74_366.06   | pos| Dehydro-L-(+)-ascorbic acid dimer                                  | 45119 |
| 65  | 5.25_202.10   | pos| Lentiginosine                                                       | 68160 |
| m/z   | Intensity | Charge | Compound Name                                      | HMDB ID  |
|-------|-----------|--------|---------------------------------------------------|----------|
| 5.37_351.20 | 1768 | pos | trans-p-Menthane-1,7,8-triol 8-glucoside          | 90206    |
| 5.43_313.04 | 1769 | neg | 5’-Phosphoribosyl-N-formylglycinamide             | HMDB0001308 |
| 5.62_245.06 | 1770 | neg | (Z)-3-(1-Formyl-1-propenyl)pentanedioic acid     | HMDB0033091 |
| 5.83_532.33 | 1771 | pos | LysoPE(0:0/20:0)                                   | HMDB0011481 |
| 6.06_399.11 | 1772 | pos | Tegafur                                           | 69467    |
| 6.18_543.28 | 1773 | pos | Dipyridamole                                      | 2341     |
| 6.57_494.22 | 1774 | pos | Verruculogen                                      | 73523    |
| 6.69_172.16 | 1775 | pos | 2E-geraniol                                       | LMPR0102010016 |
| 6.81_275.23 | 1776 | pos | 3a,17a-Dihydroxy-5b-androstane                    | HMDB0000383 |
| 6.88_317.11 | 1777 | pos | 8-Hydroxyguanosine                                 | HMDB0002044 |
| 6.89_170.98 | 1778 | neg | 3-Hydroxy-4-aminopyridine                          | HMDB0061120 |
| 6.94_506.27 | 1779 | pos | 4-Megastigmene-6a,9R-diol 9-[apiosyl-(1->6)-glucoside] | HMDB0041580 |
| 7.50_451.06 | 1780 | neg | 3,5,7-Tris(acetoxy)-2-[4-(acetoxy)-3-hydroxyphenyl]-4H-1-benzopyran-4-one | 50719    |
| 7.54_139.11 | 1781 | pos | (3Z,6Z)-3,6-Nonadienal                             | HMDB0031152 |
| 8.28_641.35 | 1782 | pos | Arginy1-Phenylalanine                             | HMDB0028716 |
| 8.51_631.24 | 1783 | pos | Somniferine                                       | HMDB0038585 |
| m/z      | p/n | Compound Name                                                                 | HMDB ID |
|----------|-----|------------------------------------------------------------------------------|---------|
| 9.17     | 282.20 | N-(3-hydroxy-dodecanoyl)-homoserine lactone                                   | LMFA08030013 |
| 9.27     | 100.07 | N-Methyl-a-aminoisobutyric acid                                               | 6508    |
| 9.52     | 541.30 | Deoxyojirimycin Tetrabenzyl Ether                                              | 45345   |
| 0.02     | 184.93 | Thiomethylcarbamic acid                                                        |         |
| 0.61     | 182.06 | 8-Hydroxy-7-methylguanine                                                     |         |
| 0.62     | 148.95 | Trifluromethanesulfonic acid                                                   | 91649   |
| 0.66     | 389.03 | 4-iodo-SAHA                                                                  |         |
| 0.78     | 399.12 | Cyclomorusin                                                                 | HMDB0030687 |
| 0.80     | 232.04 | 1-(Malonylamino)cyclopropanecarboxylic acid                                   | 87876   |
| 0.92     | 959.31 | 3,4,5-trihydroxy-6-[(8-(2-hydroxypropan-2-yl)-2-oxo-4-propyl-2H,8H,9H-furo[2,3-h]chromen-5-yl]oxy]oxane-2-carboxylic acid | HMDB0130128 |
| 0.93     | 229.12 | Curcolone                                                                    | HMDB0038188 |
| 0.95     | 660.08 | UDP-N-acetyl-3-(1-carboxyvinyl)-D-glucosamine                                  | 63224   |
| 1.12     | 167.10 | (3R,5Z)-5-Octene-1,3-diol                                                     | HMDB0030368 |
| 1.21     | 136.06 | FAPy-adenine                                                                 | HMDB0004816 |
| 1.21     | 343.05 | Monomethylphenylphosphonate                                                   | 87986   |
| 1.21     | 507.19 | Maltotriitol                                                                 | 44774   |
| 1.21     | 511.13 | Dexamethasone phosphate                                                       | 3977    |
| Mass/Time   | M/z  | Intensity | Charge | Compound Name                                                       | HMDB ID       |
|------------|------|-----------|--------|-------------------------------------------------------------------|---------------|
| 10.20_253.1| 785m/z| pos       | 1,2-propanediol                                                   | HMDB0036133   |
| 10.27_251.1| 993m/z| pos       | Methoprene acid                                                   | 43446         |
| 10.76_629.3| 417m/z| pos       | Bis(glycerophospho)-glycerol                                     | 66064         |
| 10.79_287.1| 210m/z| neg       | Cytotrienin A                                                     | 44850         |
| 10.87_191.1| 363m/z| pos       | Subaphylline                                                      | HMDB0033463   |
| 10.98_463.3| 442m/z| pos       | 10-fluoro-capric acid                                            | 96778         |
| 11.22_610.3| 407m/z| pos       | Brassinolide                                                      | LMST01140001  |
| 11.35_483.3| 717m/z| pos       | PC(16:0/5:0(COOH))                                               | 82379         |
| 12.00_341.2| 676m/z| neg       | L-Menthol (R,S)-3-hydroxybutyrate                                 | HMDB0032370   |
| 12.83_283.1| 682m/z| neg       | 1-Ethylcarbamyl-4-methylpiperazine                                | 2006          |
| 13.79_397.2| 768m/z| pos       | Oxymetazoline                                                    | HMDB0015070   |
| 14.46_893.5| 219m/z| pos       | Isopetasoside                                                    | HMDB0029622   |
| 13.90_582.17| 660m/z| pos      | PG(20:2(11Z,14Z)/22:2(13Z,16Z))                                   | LMGP04010586  |
| 2.12_353.09| 90m/z | pos       | Apii                                                             | HMDB0030843   |
| 4.18_145.12| 45m/z | pos       | CAY10415                                                         | 63083         |
| 4.18_159.09| 19m/z | pos       | (3R,7R)-1,3,7-Octanetriol                                         | HMDB0033625   |
| 4.35_316.17| 32m/z | neg       | Tryptamine                                                       | HMDB0000303   |
| 4.25_455.00| 75m/z | pos       | 3-hydroxy-2-[3-methoxy-4-(sulfooxy)phenyl]-5-sulfino-3,4-dihydro-2H-1-benzopyran-7-olate | HMDB0127802   |
| 4.35_316.17| 65m/z | pos       | Toxin T2 tetrol                                                  | HMDB0036159   |
| Retention Time (min) | Mass/Charge (m/z) | Charge State | Name of Compound | HMDB ID |
|---------------------|------------------|-------------|-----------------|---------|
| 4.53_279.98         | 87 m/z           | neg         | 2-Methyl-4-amino-5-hydroxymethylpyrimidine diphosphate | 3426    |
| 4.66_475.22         | 28 m/z           | pos         | GW 9578         | 45313   |
| 5.12_480.18         | 12 m/z           | pos         | Vilazodone      | 85563   |
| 5.29_247.08         | 91 m/z           | pos         | 2,4-Diphenyl-1-butene | HMDB0032563 |
| 5.36_151.11         | 84 m/z           | pos         | PE(P-16:0/0:0)   | LMGP02070001 |
| 6.23_170.03         | 25 m/z           | pos         | (+/-)-Dihydromint lactone | 88269   |
| 6.47_171.10         | 64 m/z           | pos         | Tolylacetonitrile | 65797   |
| 7.39_515.28         | 23 m/z           | neg         | 2-Octen-4-one    | HMDB0031301   |
| 7.65_471.24         | 39 m/z           | neg         | L-Olivosyl-oleandolide | LMPK04000032   |
| 8.07_629.39         | 81 m/z           | pos         | Maprotiline glucuronide | 1067 |
| 8.41_240.19         | 65 m/z           | pos         | Ubiquinone 6     | HMDB0036062   |
| 8.48_516.32         | 65 m/z           | pos         | N-Lauroylglycine | HMDB0013272   |
| 8.59_100.07         | 23 m/z           | pos         | Oleyloxyethyl Phosphorylcholine | 63061   |
| 9.30_368.98         | 60 m/z           | pos         | Norvaline        | 85259   |
| 9.30_409.16         | 83 m/z           | neg         | dUDP             | HMDB0001000  |
| 9.30_599.25         | 77 m/z           | pos         | Bakkenolide D    | HMDB0034998  |
| 9.33_445.34         | 36 m/z           | pos         | Tiliacorine      | 67873   |
| 9.70_213.14         | 63 m/z           | pos         | 26:2(5Z,9Z)(25Me) | LMFA01020359 |
| 9.94_292.98         | 88 m/z           | neg         | 12-hydroxy-3Z-dodecenoic acid | LMFA01050170 |
| 4.53_210.13         | 45 m/z           | neg         | D-Ribose 1-diphosphate | 66359   |
| 5(S),6(R)-7-trihydroxymethyl | 5(S),6(R)-7-trihydroxymethyl | 44893 |
| 0.80_385.11         | 31 m/z           | pos         | Heptanoate       | 44893   |
| 0.77_210.13         | 17 m/z           | neg         | Toxoflavine      | 71343   |
| m/z | Charge | Intensity | Annotation | HMDB ID |
|-----|--------|-----------|------------|---------|
| 86 | +      | 0.82_283.08 | CAY10554 | 45242   |
| 81 | -      | 0.85_403.06 | AG-82 | 45247   |
| 69 | -      | 0.91_171.07 | meso-2,6-Diaminoheptanedioate | 63450   |
| 70 | +      | 0.95_363.10 | 5,8-dihydroxy-2-(1-hydroxy-3-methoxy-4-oxocyclohexyl)-3,7-dimethoxy-4H-chromen-4-one | HMDB0129296 |
| 35 | -      | 0.97_133.01 | Pyruvic acid | HMDB0000243 |
| 17 | -      | 1.17_317.10 | Guibourtinidol-7-methyl ether | LMPK12020008 |
| 60 | -      | 1.18_636.22 | Neoacmarine E | 95232   |
| 87 | +      | 1.19_396.23 | Eremopetasitenin C1 | HMDB0032770 |
| 10 | +      | 1.19_404.30 | Mangalkanyl glucoside | HMDB0036015 |
| 60 | -      | 1.20_355.07 | Cysteinyl-Glycine | 85689   |
| 39 | -      | 1.23_279.03 | 2'-Hydroxybiphenyl-2-sulfinate | 66515   |
| 30 | +      | 1.25_411.04 | Ceftibuten | HMDB0015485 |
| 73 | -      | 1.28_305.00 | 5-O-(1-Carboxyvinyl)-3-phosphoshikimate | 3454   |
| 51 | +      | 1.72_221.08 | Isopropyl β-D-ThiogalactoPyranoside | 44762   |
| 855 | - | 10.21_249.1 | (+)-1(10),4-Cadinadiene | HMDB0035084 |
| 10 | -      | 10.24_560.2 | Flocoumafen | 72474   |
| 879 | + | 10.27_500.2 | Mycalamide B | 71499   |
| 332 | + | 10.32_279.2 | 9(S)-HODE | 45662   |
| 639 | + | 10.35_236.1 | 5,7,9,11,13-tetradecapentaenoic acid | LMFA01030258 |
| m/z       | ion  | Time  | Name                                                                                     | HMDB_ID   |
|----------|------|-------|------------------------------------------------------------------------------------------|-----------|
| 945      | neg  | 10.39 | Pamidronate                                                                              | 1692      |
| 101      | neg  | 10.63 | 6-[(1-carboxy-8-hydroxy-3,5-dioxo-9-(sulfooxy)-1H,2H,3H,5H-cyclopenta[c]isochromen-7-yl)oxy]-3,4,5-trihydroxyoxane-2-carboxylic acid| HMDB0133722|
| 876      | pos  | 10.74 | Neocasomorphin (1-5)                                                                      | HMDB0060144|
| 654      | neg  | 10.75 | PS(20:4(5Z,8Z,11Z,14Z)/0:0)                                                               | LMGP03050007|
| 755      | pos  | 10.81 | MG(18:2(9Z,12Z)/0:0/0:0)                                                                   | HMDB0011568|
| 183      | neg  | 10.90 | OKOOA-PS                                                                                 | LMGP20040029|
| 404      | pos  | 11.05 | Koenimbine                                                                               | HMDB0030210|
| 216      | neg  | 11.53 | Tiocarbazil                                                                             | 72659     |
| 260      | pos  | 11.71 | 9-Thiastearic Acid                                                                       | 45061     |
| 64       | pos  | 11.75 | MG(18:0/0:0/0:0)                                                                          | HMDB0011131|
| 209      | pos  | 11.94 | OKHdiA-PA                                                                                | LMGP20070026|
| 636      | neg  | 12.35 | 2-Methyl-4-heptanone                                                                      | 85275     |
| 531      | pos  | 12.51 | 4alpha-Carboxy-5alpha-cholesta-8-en-3beta-ol                                            | HMDB0012166|
| 312      | pos  | 13.20 | Dynorphin A (6-8)                                                                         | HMDB0012932|
| 6       | pos  | 14.66 | GlcCer(t18:1(8Z)/20:0(2OH[S])                                                             | LMSP05010044|
| 460      | pos  | 14.66 | GlcCer(t18:1(8Z)/16:0(2OH[S])                                                             | LMSP05010042|
| 73       | neg  | 2.00  | 1-Nitro-5-hydroxy-6-glutathionyl-5,6-dihydronaphthalene                                   | HMDB0060327|
| 66       | pos  | 13.20 | 8-Isoquinoline methanamine (hydrochloride)                                               | 45036     |
| 50       | neg  | 13.20 | Indoleacrylic acid                                                                       | HMDB0000734|
Ohobanin  LMPK12120414
Phenylalanyl-Arginine  HMDB0028989
Thien-2-ylacetate  65796
(3-{{8,8-dimethyl-2-oxo-2H,8H-pyra}[2,3-f]chromen-3-yl}-2-hydroxy-6-methoxyphenyl)oxidanesulfonic acid  HMDB0135728
Gentamicin A2  71865
Benzothiazole  88833
Lamivudine-monophosphate  HMDB0060641
1-Isothiocyanato-7-(methylsulfinyl)heptane  HMDB0038441
Aspergillic acid  68394
Benzenepropanenitrile  HMDB0034236
6",6"-Dimethyl-3',4'-methylenedioxy[2",3":7,8]flavone  48477
(23R)-1α-hydroxy-25,27-didehydrovitamin D3 26,23-lactone  42528
Lubiminol  HMDB0029604
Glucosyl-limonin  66514
Ethacrynic acid M2  2586
2-N-Dodecyltetrahydrothiophene  68819
JSTX-3  69746
Hydroxydestruxin B  HMDB0040135
| m/z   | Intensity | Charge | Name                                         | HMDB/ID     |
|-------|-----------|--------|----------------------------------------------|-------------|
| 8.52  | 353.17    | 8      | Etiocholanolone sulfate                      | LMST05020044|
| 8.56  | 299.24    | 8      | 2-mercapto-octadecanoic acid                 | LMFA01130002|
| 9.39  | 401.34    | 44     | 22b-Hydroxycholesterol                       | HMDB0004035 |
| 9.71  | 364.08    | 54     | 4-Methylthiobutyl-desulfoglucosinolate       | 64514       |
| 0.88  | 189.08    | 74     | Threoninyl-Alanine                           | HMDB0029054 |
| 0.89  | 143.08    | 19     | N6-Hydroxy-L-lysine                          | 63466       |
| 0.94  | 361.08    | 74     | Meticillin                                   | HMDB0015541 |
| 1.08  | 457.17    | 13     | 6-Feruloylglucose 2,3,4-trihydroxy-3-         |             |
| 1.10  | 257.24    | 4      | methylbutylglycoside                         | HMDB0036214 |
| 1.22  | 295.06    | 83     | 4,8,12-trimethyl-tridecanoic acid            | LMFA01020249|
| 1.28  | 464.95    | 4      | (2-hydroxy-1,2-diphenylethoxy)sulfonic acid  | HMDB0135202 |
| 1.48  | 244.95    | 32     | Inositol 1,3,4-trisphosphate                 | HMDB0001143 |
| 10.13 | 452.3     | 17     | Thioxanthine monophosphate                   | HMDB0060876 |
| 10.35 | 597.2     | 117    | 17-phenyl trinor PGF2α cyclohexyl amide      | 64899       |
| 11.05 | 599.4     | 429    | Geranyl acetoacetate                         | 92981       |
| 10.52 | 677.1     | 489    | 3,4'-Dihydroxy-7,3',5'-trimethoxyflavone 3-   | LMPK12111575|
| 10.84 | 451.2     | 118    | galactosyl-(1->4)-xyloside                   |             |
| 11.05 | 313.2     | 488    | Sofalcone                                    | HMDB0042013 |
| 11.05 | 239.1     | 246    | MG(i-16:0/0:0/0:0)                            | HMDB0072844 |
| 11.05 | 599.4     | 645    | Geranyl acetoacetate                         |             |
| 11.05 | 599.4     | 429    | PA(P-16:0/15:1(9Z))                          | LMGP10030006|
| m/z   | Retention Time | Charge | Name                                      | HMDB ID       |
|-------|----------------|--------|-------------------------------------------|---------------|
| 11.49 | 355.2          | pos    | 3,6-Ditigloyloxytropan-7-ol               | HMDB0029325   |
| 11.65 | 191.1          | pos    | beta-Damascenone                          | 85264         |
| 11.71 | 630.4          | pos    | PE(14:0/P-16:0)                           | HMDB0008850   |
| 12.54 | 337.1          | pos    | 4-Oxoretinal                              | HMDB0012794   |
| 13.20 | 727.5          | pos    | SM(d18:2/18:1)                            | LMSP03010047  |
| 13.40 | 469.3          | pos    | (3beta,15alpha,22S,24E)-                  |               |
|       |                |        | 3,15,22-Trihydroxylanosta-24-acid        |               |
| 13.78 | 489.3          | pos    | Pitheduloside I                          | 89673         |
| 13.92 | 545.4          | pos    | PAF C-16-d4                               | 96561         |
| 2.14  | 362.12         | pos    | N-(1-Deoxy-1-fructosyl)histidine          | HMDB0037839   |
| 2.85  | 146.06         | neg    | 4-Oxo-1-(3-pyridyl)-1-butanone            |               |
| 5.01  | 381.07         | neg    | Brassicanal A                             | 68795         |
| 5.75  | 180.98         | neg    | 3,5-DINITROCATECHOL (OR-486)              | 44188         |
| 6.24  | 138.01         | neg    | 2-Aminomuconic acid                      | HMDB0001241   |
| 7.20  | 236.11         | pos    | Penciclovir                               | HMDB0014444   |
| 7.32  | 456.12         | pos    | Secogalioside                             | 69151         |
| 7.34  | 425.14         | pos    | Benzyl O-[arabinofuranosyl-(1->6)-glucoside] | 95898         |
| 7.34  | 432.16         | pos    | Glisoxepide                               | 85491         |
| 7.37  | 334.13         | neg    | O-Methylisoetharine sulfate              | 846           |
| 7.47  | 295.13         | pos    | Caffeoylputrescine                        | 3380          |
| 7.60  | 464.30         | pos    | N-palmitoyl tyrosine                     | LMFA08020098  |
| 7.91  | 491.11         | pos    | Glycitin                                  | HMDB0002219   |
| Time (min) | Mass/Charge | Charge State | Name                                      | HMDB ID     |
|-----------|-------------|--------------|-------------------------------------------|-------------|
| 7.95      | 409.27      | pos          | Azafrin                                   | 67076       |
| 7.97      | 304.10      | pos          | S-Glutaryl dihydro lipoamide              | HMDB0006832 |
| 8.38      | 303.14      | pos          | Arabinoside                               | 87702       |
| 8.38      | 539.24      | pos          | 10alpha-4,5-secosio-11-eudesmene-4,5-dione| HMDB0032681 |
| 9.29      | 663.22      | pos          | Desmosine                                 | HMDB0000572 |
| 9.70      | 179.14      | neg          | Nirurin                                   | LMPK12140614|
| 9.78      | 194.08      | neg          | 2-Aminopropiophenone                      | 2011        |
| 9.82      | 624.24      | pos          | Tigecycline                               | 69251       |
| 0.67      | 375.00      | pos          | beta-D-3-[5-Deoxy-5-(dimethylarsinyl)ribofuranosylxy]-2-hydroxy-1-propanesulfonic acid | HMDB0032686 |
| 0.71      | 824.73      | pos          | GlcCer(d18:0/26:0)                        | 41621       |
| 0.76      | 608.18      | pos          | AKLAVINE                                  | 43581       |
| 0.78      | 368.12      | neg          | Bialaphos                                 | 63603       |
| 0.80      | 403.11      | neg          | Gibberellin A55                           | HMDB0033420 |
| 0.82      | 390.19      | pos          | Clavamycin F                              | 71660       |
| 0.93      | 411.03      | neg          | 2-Hydroxy-4-trifluoromethyl benzoic acid  | HMDB0060715 |
| 0.96      | 201.00      | pos          | S-2-Propenyl 2-propene-1-sulfonothioate   | HMDB0039940 |
| 0.96      | 448.98      | neg          | C.I. Pigment Yellow 100                   | HMDB0037722 |
1957 04m/z  neg  Blue pigment  63889

1.19_580.16

1958 77m/z  pos  3,4,5-trihydroxy-6-[(7-
4H-chromen-5-yl)oxy]oxane-
2-carboxylic acid  HMDB0127263

10.08_237.1

1959 842m/z  pos  (4S)-Dihydrocurcumenone  HMDB0033083
11.33_528.3  pos  LysoPE(0:0/22:4(7Z,10Z,13Z,1
6Z))  HMDB0011493
160 092m/z  neg  OON-PA  LMGP20070023
11.35_608.3
161 926m/z  pos  (20R)-24-
11.53_340.2  pos  Hydroxygeminivitamin D3  42557
163 059m/z  pos  (+/-)N-(2-fluro-ethyl)-2,16,16-
tricosatetraenoyl amine  LMFA08020067
12.45_416.3  pos  (S)-2-methyl-5-(1-
Methylethenyl)-2-cyclohexen-
one  HMDB0061788
164 688m/z  pos  13.20_133.1  pos  27:3(5Z,9Z,20Z)  LMFA01030903
13.65_405.3
166 742m/z  pos  14.00_766.5
14.65_405.3
167 783m/z  pos  2-Amino-3-hydroxy-5-
nitrobenzophenone  1572
168 534m/z  pos  4.39_181.06  pos  Nicotinuric acid  HMDB0003269
169 11m/z  pos  4.50_152.01  pos  Thiobenzamide S,S-dioxide  71173
170 72m/z  pos  4.50_226.01  pos  N-acetyl-2-carboxy
171 76m/z  pos  Benzenesulfonamide  45011
| Year | m/z | Charge | Name                              | HMDB ID   |
|------|-----|--------|-----------------------------------|-----------|
| 1972 | 36  | neg    | 9-Fluoro-17-methyl-11-oxotestosterone | 70211     |
|      | 5.66 | 173.08 |                                   |           |
| 1973 | 26  | neg    | 2-Propylglutaric acid             | 2998      |
|      | 6.38 | 433.20 |                                   |           |
| 1974 | 66  | neg    | Alanyl-Glutamine                  | HMDB0028685 |
|      | 6.41 | 280.11 |                                   |           |
| 1975 | 64  | neg    | Saxitoxin                         | 69686     |
|      | 7.12 | 179.14 |                                   |           |
| 1976 | 29  | pos    | Propofol                          | 2155      |
|      | 7.23 | 249.11 |                                   |           |
| 1977 | 36  | pos    | SB 200646                         | 69188     |
|      | 7.59 | 137.13 |                                   |           |
| 1978 | 26  | pos    | 2-decenal                         | 75331     |
|      | 8.10 | 345.09 |                                   |           |
| 1979 | 07  | pos    | Piretanide                         | 1978      |
|      | 8.45 | 427.21 |                                   |           |
| 1980 | 44  | neg    | 4-Hydroxytacrine                  | 2618      |
|      | 8.55 | 307.09 |                                   |           |
| 1981 | 87  | pos    | Isomethiozin                       | 72849     |

| Year | m/z | Charge | Name                                                          | HMDB ID   |
|------|-----|--------|----------------------------------------------------------------|-----------|
| 1982 | 21  | pos    | Benzenesulfonamide                                            | 3115      |
|      | 9.32| 322.12 |                                                                |           |
| 1983 | 61  | pos    | 7-hydroxy coumarinyl-γ-Linolenate                              | 64760     |
|      | 9.59| 534.32 |                                                                |           |
| 1984 | 05  | pos    | PS(20:1(11Z)/0:0)                                              | LMGP03050020 |
|      | 9.62| 252.17 |                                                                |           |
| 1985 | 24  | pos    | Tridecanamide                                                  | LMFA08010012 |
|      | 0.02| 247.94 |                                                                |           |
| 1986 | 32  | pos    | Bismuth                                                        | HMDB0002196 |
|      | 0.62| 333.14 |                                                                |           |
| 1987 | 12  | pos    | Zanamivir                                                      | HMDB0014698 |
|      | 0.69| 403.03 |                                                                |           |
| 1988 | 04  | neg    | Distemonanthin                                                 | LMPK12113389 |
|      | 0.81| 453.03 |                                                                |           |
| 1989 | 16  | neg    | L-Glutamyl 5-phosphate                                         | 63480     |
|      | 0.84| 635.21 |                                                                |           |
| 1990 | 36  | neg    | Catechin 7,4’-dimethyl ether                                   | 47359     |
|      | 0.92| 209.06 |                                                                |           |
| 1991 | 58  | neg    | Sedoheptulose                                                  | 3344      |

N-
[[hexahydrocyclopenta[c]pyrr
ol-2(1H)-yl]amino]carbonyl]-4-
(hydroxymethyl)-
| Year | m/z     | Charge | Compound Description                                      | HMDB ID   |
|------|---------|--------|-----------------------------------------------------------|-----------|
| 1992 | 0.98    | pos    | DNDS                                                      | LMPK13090017 |
| 1993 | 1.22    | neg    | 3-AMINOPROPANESULPHONI C ACID                             | 43475     |
| 1994 | 1.29    | pos    | Methyl methanethiosulfonate                               | 87955     |
| 1995 | 0.71    | neg    | Diethyl disulfide                                         | HMDB0029572 |
| 1996 | 1.22    | pos    | Limonene aldehyde                                         | 86834     |
| 1997 | 3.45    | pos    | 2-{4-[(6-carboxy-3,4,5-trihydroxyoxan-2-yl)oxy]-3-hydroxyphenyl]-3,7-dihydroxy-5-[(3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yloxy)]-1λ⁴-chromen-1-ylium | HMDB0125133 |
| 1998 | 1.60    | neg    | N-lauroyl glycine                                         | LMFA08020261 |
| 1999 | 3.71    | neg    | Eremopetasidione                                          | HMDB0040778 |
| 2000 | 0.84    | pos    | Methional diethyl acetal                                  | HMDB0041608 |
| 2001 | 1.82    | pos    | 3α,7α,12α-trihydroxy-27-carboxymethyl-5β-cholestan-26-oic acid | 43164     |
| 2002 | 0.58    | pos    | Pivaloylcarnitine                                         | HMDB0041993 |
| 2003 | 1.82    | pos    | 11-Hydroxy-12-methoxydihydrokawain                      | HMDB0030766 |
| 2004 | 1.94    | pos    | Polyporusterone C                                         | HMDB0038497 |
| 2005 | 1.27    | pos    | NH125                                                    | 45320     |
| 2006 | 1.94    | pos    | 1-Lyso-2-arachidonoyl-phosphatidate                        | HMDB0012496 |
| 2007 | 1.64    | pos    | PC(22:2(13Z,16Z)/20:4(5Z,8Z,11Z,14Z))                    | LMGP01012058 |
2008 528m/z  pos  Byrsonic acid  LMFA01050424
12.48_487.4

2009 001m/z  pos  Arachidonyl carnitine  HMDB0006455
12.68_367.1

2010 916m/z  pos  Armillarivin  HMDB0038917

12.91_535.4

2011 026m/z  pos  Nb-Tricosanoyltrptamine  HMDB0040818

13.01_433.3  2-

2012 644m/z  pos  Hydroxyhexadecanoylcarnitine  LMFA07070113
13.80_842.6

2013 001m/z  pos  PE(16:0/24:0)  HMDB0008947
15.75_297.0

2014 844m/z  pos  flunixin  4044
2.02_195.04

2015 04m/z  neg  (S)-ACPA  69626
2.27_247.04

2016 94m/z  pos  L-Kynurenine  HMDB0000684
5.31_680.44

2017 25m/z  pos  Prostaglandin E2-biotin  44962

5.48_534.35  1-O-(2-methoxyhexadecyl)-sn-glycerol-3-phosphocholine  LMGP01060042

2018 24m/z  pos  Methiuron  72828
5.70_239.08

2019 56m/z  neg  Ribavirin  2298
5.82_144.04

2020 49m/z  neg  4-(3-Pyridyl)-3-butenoic acid  6236
7.59_403.00

2021 70m/z  neg  Porson  87208
8.16_367.15

2022 65m/z  neg  Dihydrodeoxystreptomycin  2507
8.16_566.27

2023 70m/z  neg  3-Oxo-14,15-dehydrorhazinilam  HMDB0035765
9.30_333.12

2024 72m/z  pos  Mannopine  71286
9.35_346.99

2025 16m/z  neg  Phenyl sulfate  1828
9.39_201.14

2026 91m/z  neg  p-Menth-3-ol  HMDB0039105
9.51_506.24

2027 44m/z  pos  Malyngamide L  65450
9.66_351.13

2028 37m/z  neg  NVP-AEW541  HMDB0039105
9.67_478.20

2029 01m/z  pos  3-Oxo-14,15-dehydrorhazinilam  HMDB0039105
| m/z  | Intensity | Charge | Name and Formula | HMDB ID |
|------|-----------|--------|------------------|---------|
| 64/254.99 | 9.90 | pos | [(7-hydroxy-1-oxo-1H-isochromen-3-yl)methoxy]sulfonic acid | HMDB0128634 |
| 68 | 0.04 | pos | Bay-K-8644 | 69687 |
| 34/311.02 | 0.14 | pos | [3-Deoxy-D-manno-octulonate 8-phosphate] | 63652 |
| 269/293.78 | 0.69 | pos | PC(24:0/22:0) | 60221 |
| 43/189.06 | 0.80 | neg | PE(18:3(9Z,12Z,15Z)/15:0) | HMDB0009153 |
| 13/202.06 | 0.81 | pos | (S)-F-Willardiine | 69624 |
| 20/135.02 | 0.83 | neg | 8-Hydroxyalanylclavam | 71633 |
| 91/445.03 | 0.92 | neg | L-Lactic acid | HMDB0000190 |
| 93/401.16 | 0.73 | pos | D-Gluconic acid Mn(II) salt | 92165 |
| 86/712.23 | 1.08 | neg | 6-Methoxy-2-naphthylacetic acid | HMDB0060787 |
| 50/401.16 | 1.21 | neg | BAY-41-8543 | 64714 |
| 53/671.10 | 1.23 | neg | (5-{8-[3,7-dihydroxy-2-(3-hydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-yl]-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl]-2-hydroxyphenyl)oxidanesulfonic acid | HMDB0135098 |
| 76/305.09 | 1.97 | neg | Fluconazole | HMDB0014342 |
| 181/463.2 | 10.18 | neg | 2-Oxo-10-methylthiodecanoic acid | 64510 |
| 263/619.3 | 10.43 | pos | PKOOA-PG | LMGP20060006 |
| 244/350.1 | 10.55 | neg | Rhizoctin A | 63578 |
| m/z   | Retention Time | Charge | Peak Area | Formula | HMDB ID |
|-------|----------------|--------|-----------|---------|----------|
| 10.63 | 442.9          | neg    | 2046      | 945     | Melarsoprol 66778 |
| 10.71 | 506.3          | pos    | 2047      | 597     | LysoPC(18:0) HMDB0010384 |
| 10.76 | 361.2          | pos    | 2048      | 767     | MG(0:0/20:4(8Z,11Z,14Z,17Z)/0:0) HMDB0011549 |
| 10.77 | 579.0          | neg    | 2049      | 067     | 5-(4-Acetoxy-3-oxo-1-butynyl)-2,2'-bithiophene 93147 |
| 11.29 | 309.1          | neg    | 2050      | 729     | 7-hydroxygranisetron HMDB0061062 |
| 11.80 | 363.2          | neg    | 2051      | 533     | 2,2,7,7-Tetramethyl-1,6-dioxaspiro[4.4]non-3-ene 86658 |
| 12.10 | 427.3          | pos    | 2052      | 300     | 1-diethyllarsinoyl-tricosane LMFA00000033 |
| 12.12 | 261.1          | pos    | 2053      | 875     | 2-ethyl-1,5-dimethyl-3,3-diphenylpyrrolinium (EDDP) HMDB0060931 |
| 12.27 | 361.2          | pos    | 2054      | 271     | N-Didesmethyl-tamoxifen HMDB0061086 |
| 12.68 | 369.1          | neg    | 2055      | 871     | 9-(beta-D-Ribofuranosyl)zeatin HMDB0030388 |
| 14.43 | 850.6          | pos    | 2056      | 660     | PC(22:0/P-18:1(11Z)) HMDB0008556 |
| 14.54 | 868.5          | pos    | 2057      | 122     | P(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) LMGP06010128 |
| 2.01  | 269.04         | neg    | 2058      | 74      | Sulfamethoxazole N4-hydroxylamine HMDB0013852 |
| 2.06  | 219.00         | neg    | 2059      | 85      | SQ 26180 71381 |
| 4.31  | 319.10         | neg    | 2060      | 26      | Glutaminyl-Glutamate 85710 |
| 4.51  | 348.99         | neg    | 2061      | 48      | Diflubenzuron 70053 |
| 4.70  | 525.03         | pos    | 2062      | 40      | Quercetin 3-(3''-sulfatoglucoside) LMPK12112165 |
| 5.24  | 406.06         | neg    | 2063      | 46      | Gluconasturtiin HMDB0038423 |
| 5.34  | 339.04         | pos    | 2064      | 21      | Sodium 3-ethyl-7-isopropyl-1-azulenesulfonate 69570 |
| m/z | Charge | Isotopic Label | Description | HMDB ID |
|-----|--------|----------------|-------------|---------|
| 5.39 | 315.13 | pos | Longifolone | 67811 |
| 5.79 | 561.20 | pos | Juzirine | HMDB0033954 |
| 5.93 | 240.04 | neg | p-Nitrophenyl-O-ethyl ethylphosphonate | 69527 |
| 6.02 | 267.00 | pos | Mevalonic acid-5P | HMDB001343 |
| 6.29 | 528.26 | neg | N-[(3a,5b,7b)-7-hydroxy-24-oxo-3-(sulfoxy)cholan-24-yl]-Glycine | LMST05030012 |
| 7.25 | 253.13 | neg | Ergoline-8-methanol, 10-methoxy-, (8b)- | 1516 |
| 7.88 | 427.13 | neg | Farnesyl pyrophosphate | 403 |
| 8.13 | 512.26 | neg | Sulfoglycolithocholic acid | LMST05030015 |
| 8.19 | 214.99 | pos | Isorenieratene/ (Leprotene) | LMPR01070124 |
| 8.14 | 511.37 | neg | Salithion | 72740 |
| 8.39 | 465.24 | neg | Etiocholan-3alpha-ol-17-one 3-glucuronide | LMST05010014 |
| 9.15 | 209.15 | neg | 7-methoxy-dodec-4-enoic acid | LMFA01080012 |
| 9.17 | 400.33 | neg | 7a-Hydroxy-cholestene-3-one | HMDB0001993 |
| 9.90 | 319.29 | pos | Thromboxane | HMDB0003208 |
| 9.94 | 320.23 | pos | 19(R)-HETE | 45085 |
| 0.03 | 205.08 | pos | Tafluprost ethyl amide | 96555 |
| 0.61 | 455.27 | pos | gamma-Glutamyl-beta-(isoxazolin-5-on-2-yl)alanine | 95006 |
| 0.69 | 199.06 | pos | Diphenylmethylphosphine | 518 |
| 0.69 | 393.08 | neg | Bensulfuron-methyl | 68703 |
| m/z | m/z 1 | Compound Name | HMDB ID |
|-----|-------|---------------|---------|
| 0.76_261.01 | tert-Butylbicyclophosphorothionate | 73434 |
| 2085 | 14m/z | pos | |
| 0.80_487.08 | | | |
| 0.81_463.06 | | | |
| 2087 | 79m/z | neg | 11-O-Demethylpradinone I |
| 0.81_818.30 | | | 66535 |
| 2088 | 19m/z | neg | Docetaxel M4 |
| 0.83_349.02 | | | 741 |
| 2089 | 22m/z | pos | Mefluidide |
| 0.96_188.07 | | | 72517 |
| 2090 | 38m/z | pos | acetate |
| 1.17_333.07 | | | HMDB0032234 |
| 2091 | 41m/z | neg | Phenylacetothiohydroximate |
| 10.70_433.3 | | | 64521 |
| 2092 | 225n | pos | N-heneicosanoyl taurine |
| 10.75_312.1 | | | LMFA08020250 |
| 2093 | 375m/z | pos | Tolazamide |
| 10.75_753.1 | | | HMDB0014977 |
| 2094 | 631m/z | pos | Isorientin 4’-O-glucoside 2”-O- p-hydroxybenzoate |
| | | | 48980 |
| 10.77_466.9 | | | |
| 2095 | 967m/z | neg | 5-Hydroxy-1-(4-sulfophenyl)-4-[(E)-(4- sulfophenyl)diazenyl]-1H-pyrazole-3-carboxylic acid |
| 10.80_585.3 | | | HMDB0059914 |
| 2096 | 425m/z | pos | PI(P-18:0/0:0) |
| 10.85_614.3 | | | LMGP06070002 |
| 2097 | 456m/z | pos | OHOOA-PE |
| 10.87_474.3 | | | LMGP20020046 |
| 2098 | 631m/z | pos | N-nervonoyl taurine |
| 10.90_515.3 | | | LMFA08020257 |
| 2099 | 186m/z | pos | IC202B |
| 11.27_281.1 | | | LMFA08020183 |
| 2100 | 608m/z | pos | Pentoxifylline alcohol |
| 11.54_433.3 | | | 1768 |
| 2101 | 044m/z | pos | N-oleoyl glutamine |
| 11.57_262.2 | | | 75510 |
| 2102 | 300n | pos | 6-[3]-ladderane-1-hexanol |
| 11.78_185.1 | | | LMFA05000065 |
| 2103 | 177m/z | neg | 3-Oxodecanoic acid |
| 12.32_517.3 | | | HMDB0010724 |
| 2104 | 889m/z | neg | Theonellasterol D |
| 12.43_495.3 | | | LMST01040182 |
| 2105 | 901m/z | pos | Leucettamol A |
| | | | LMSP01080040 |
| m/z       | Name                                                                 | Retention Time | PubChem CID |
|-----------|----------------------------------------------------------------------|----------------|-------------|
| 2106 14.43, 343.2 | Docosahexaenoic Acid methyl ester                                    | 644 m/z, pos   | 44958       |
| 2107 2.27, 205.99 | 2,3-Dimercaptopropane-1-sulfonic acid                                | 73 m/z, pos    | 68691       |
| 2108 4.09, 205.02 | Hydroxyanthraquinone                                                  | 95 m/z, neg    | 65876       |
| 2109 4.18, 649.21 | Citalopram (propionic acid derivative)                                | 23 m/z, neg    | 1785        |
| 2110 4.29, 337.15 | Ergoline-1-carboxaldehyde, 8-(hydroxymethyl)-10-methoxy-6-methyl-, (8b)- | 26 m/z, pos    | 1520        |
| 2111 4.69, 158.09 | Cystamine                                                             | 23 m/z, neg    | 55          |
| 2112 5.43, 339.03 | N-Acetyltrylcypromine                                                | 60 m/z, pos    | 2896        |
| 2113 5.67, 340.27 | Gallic acid                                                           | 78 m/z, neg    | HMDB0005807 |
| 2114 6.16, 375.11 | (-)-Ormosanine                                                       | 10 m/z, pos    | 68570       |
| 2115 6.29, 363.21 | N-Acetylsertotonin glucuronide                                        | 83 m/z, neg    | HMDB0060833 |
| 2116 7.16, 314.23 | 3-hydroxydecanoyl carnitine                                          | 94 m/z, pos    | 45298       |
| 2117 7.59, 225.14 | 7-Hydroxyterpineol 8-glucoside                                       | 41 m/z, pos    | HMDB0033019 |
| 2118 7.61, 331.17 | (23S)-1alpha-hydroxy-25,27-didehydrovitamin D3 26,23-lactone        | 92 m/z, neg    | LMST03020599|
| 2119 7.78, 409.27 | O-Desmethylcardedilol                                                 | 50 m/z, pos    | HMDB0013949 |
| 2120 7.88, 415.16 | Rhoifolin                                                             | 50 m/z, pos    | HMDB0038848 |
| 2121 7.97, 617.12 | (R)-Lisofylline                                                       | 32 m/z, pos    | 45571       |
| 2122 8.01, 303.14 | Tricycloekasantalol                                                  | 80 m/z, pos    |             |
| 2123 8.01, 303.14 | 7-Hydroxyterpineol 8-glucoside                                       | 20 m/z, pos    |             |
| m/z  | Charge | Sample   | Molecular Formula          | Hyperlink |
|------|--------|----------|----------------------------|-----------|
| 8.30 | 299.24 | Octadecanoic acid, 2-mercapto-; alpha-Mercaptostearic acid | 74887     |
| 8.77 | 157.08 | Ethyladipic acid                                     | 45928     |
| 9.07 | 625.35 | Ecdysone 25-O-D-glucopyranoside                       | LMST01010192 |
| 9.33 | 472.27 | Isomigrastatin                                       | 71110     |
| 9.48 | 479.30 | 3alpha,7alpha,12alpha-Trihydroxy-5beta-23E-cholestan-26-oic acid | LMST04030199 |
| 9.77 | 276.19 | (all-E)-1,8,10-Heptadecatriene-4,6-diyn-3,12-diol      | HMDB0039737 |
| 0.59 | 238.20 | 1,2-Bis(1-ethoxyethoxy)propane                       | HMDB0037163 |
| 0.64 | 402.37 | Type IV cyanolipid 22:0 ester                        | LMFA07030004 |
| 0.69 | 775.34 | Beta-D-Glucopyranosyl-11-hydroxyjasmonic acid         | HMDB0039964 |
| 0.72 | 912.55 | PI(17:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))              | LMGP06010245 |
| 0.81 | 783.18 | Tiotropium                                            | HMDB0015479 |
| 0.82 | 543.10 | 6-Caffeoylsucrose                                     | 90768     |
| 0.93 | 318.06 | Beta-nicotinamide D-ribonucleotide                    | HMDB0059645 |
| 1.23 | 545.04 | Orange B                                              | HMDB0037522 |
| 1.27 | 271.0  | 5,6-Dihydrouridine                                    | 5483      |
| 10.22| 459.2  | Armillaripin                                           | HMDB0030404 |
| 10.27| 558.2  | Zafirlukast                                            | HMDB0014689 |
| 10.38| 579.3  | Diisopentyl thiomalate                                 | LMFA07010835 |
| m/z   | Retention Time | Charge | Name                                      | External ID |
|-------|----------------|--------|-------------------------------------------|-------------|
| 2142  | 10.43          | 311.2  | Undecanoylcholine                         | LMFA07011030|
| 2143  | 10.49          | 591.3  | S-Farnesyl Thioacetic acid                | 43440       |
| 2144  | 10.54          | 478.9  | Ponceau SX                                | 73193       |
| 2145  | 10.76          | 568.2  | PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)        | LMGP03050013|
| 2146  | 10.78          | 623.4  | OH-Spheroidenone                          | LMPR01070151|
| 2147  | 10.90          | 523.3  | OH-Spheroidenone                          |             |
| 2148  | 11.11          | 191.1  | 2-(Octylthio)ethanol                      | 72625       |
| 2149  | 11.26          | 580.4  | Cholesterol glucuronide                   | LMST05010043|
| 2150  | 11.37          | 407.2  | Nandrolone phenpropionate                 |             |
| 2151  | 11.54          | 540.3  | Oleic Acid-biotin                         | 45287       |
| 2152  | 15.09          | 703.5  | Ropinirole                                | 2361        |
| 2153  | 15.10          | 610.4  | Campesterol elaidate                      | 91433       |
| 2154  | 15.46          | 431.3  | 5alpha,6beta-dihydroxy-24-methylenecholestan-3-one | LMST01031062|
| 2155  | 2.26           | 233.06 | Thiolactomycin                            | 68888       |
| 2156  | 3.80           | 145.12 | {4-[(1E)-3-oxoprop-1-en-1-yl]phenyl}oxidanesulfonic acid | HMDB0135289|
| 2157  | 4.55           | 273.00 | 2-Ethylhexanoic acid                      | HMDB0031230 |
| 2158  | 5.28           | 446.30 | 1,2-Benzisothiazol-3(2H)-one              | HMDB0034413 |
| 2159  | 5.31           | 232.06 | Alpha-linolenyl carnitine                 | 58390       |
| 2160  | 5.71           | 488.30 | 3-amino-2-naphthoic acid                  | 34509       |
| 2161  | 10.49          | 478.9  | LysoPE(20:2(11Z,14Z)/0:0)                 | HMDB0011513 |
5.81_256.15
2163 50m/z  neg  N-Butylscopolamine metabolite  2399

6.06_620.38
2164 76m/z  pos  1-(2-methoxy-docosanyl)-sn-
glycero-3-phosphoserine  LMG03060021

6.57_385.16
2165 71m/z  neg  5-Deoxymyricanone  87204
6.91_498.27
2166 37m/z  pos  Alangimarckine  64421
7.66_550.24
2167 46m/z  neg  Endoxifen O-glucuronide  HMDB0060622

8.35_651.26
2168 67m/z  pos  Myricanol 5-[arabinosyl-(1->6)-
glucoside]  HMDB0035627

8.41_550.22
2169 07m/z  pos  2-amino-4-{{1-
[(carboxymethyl)-C-
hydroxycarbonimidoyl]-2-[(1,3-
dihydroxy-2-pentyl-1-
phenylpropan-2-
yl)sulfonyl]ethyl}-C-
hydroxycarbonimidoyl}butanoic acid  HMDB0126539
9.46_212.14
2170 62m/z  pos  2-Heptyl-4,5-dimethylthiazole  94633
9.46_329.16
2171 99n  neg  Hydroxyethylpromethazine  HMDB0240229
9.60_440.33
2172 89m/z  pos  Cholic Acid Methyl Ester  73574
0.61_267.02
2173 97m/z  pos  4-phenylbutanolic acid-O-
sulphate  HMDB0059983
0.70_838.70
2174 64m/z  neg  PC(24:0/P-18:0)  HMDB0008785
0.93_313.06
2175 43m/z  neg  Vat Yellow 4  73222
0.96_231.06
2176 11m/z  neg  Kifunensine  45180
1.21_273.09
2177 93n  pos  L-Thyronine  HMDB0000667
1.21_566.20  6-[(10-butanoyl-3-hydroxy-6-(2-hydroxypropyl)-2,2-dimethyl-8-oxo-2H,3H,4H,8H-pyran[3,2-g]chromen-5-yloxy)-3,4,5-trihydroxyoxan-2-carboxylic acid  HMDB0130103
1.22_233.98  40m/z  pos  Carbocysteine sulfoxide  1527
10.11_212.1  10.12_382.0  460m/z  pos  4-Ethyl-2-heptylthiazole  94654
10.38_498.2  10.51_275.1  294m/z  pos  SB 206553  69189
10.57_503.2  8-Hydroxyondansetron  glucuronide  1654
10.68_292.1  2-(1-hydroxy-3-phenylpropyl)-5-methoxybenzene-1,3-diol  HMDB0140889
10.78_539.3  27-nor-24S-methylcholestan-3beta,4beta,5alpha,6alpha,7beta,8beta,14alpha,15alpha,24-nonol  84028
10.94_477.3  183m/z  pos  Rockogenin  LMST01080017
10.98_225.0  2-Amino-5-nitrobenzophenone  1570
11.05_267.1  957m/z  neg  (-)-alpha-Bisabolol  LMPR0103060001
11.05_268.1  11.84_535.3  514m/z  pos  Isovalerylcarnitine  HMDB0000688
11.89_276.1  11.92_275.0  996m/z  neg  Aragusteroketal  LMST01110016
12.62_431.3  2(E,4E,6Z)-2,4,6-Decatrienoic acid dehydropiperide  HMDB0033530
156m/z  neg  Shibic acid  LMFA01030831
|      |     |     |                                   |                        |
|------|-----|-----|-----------------------------------|------------------------|
| 2194 | 941 | m/z | PS(O-18:0/19:1(9Z))               | LMGP03020033           |
| 2195 | 077 | m/z | Eicosadienoic acid                | HMDB0005060            |
| 2196 | 330 | m/z | Sulfasalazine                     | HMDB0014933            |
| 2197 | 713 | m/z | Cyanidin 3-O-dimalonyl-laminaribioside | 86120                |
| 2198 | 27  | m/z | Dhurrin                           | 63619                  |
| 2199 | 18  | m/z | 1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-glycero-3-phosphate | HMDB0062307 |
| 2200 | 71  | n   | Methyl acrylate-divinylbenzene, completely hydrolyzed, copolymer | HMDB0032389 |
| 2201 | 70  | m/z | 4,13,14-trihydroxy-9-oxo-8,17-dioxatetracyclo[8.7.0.0²,⁷.0¹¹,¹⁶]heptadeca-1(10),2,4,6,11(16),12,14-heptaen-5-yl acetate | HMDB0128437 |
| 2202 | 68  | n   | N6,N6-Dimethyladenosine            | 65975                  |
| 2203 | 30  | n   | aminopentamide                    | 3998                   |
| 2204 | 31  | m/z | 2,15,16-trihydroxy palmitic acid   | 35476                  |
| 2205 | 77  | m/z | Bouillonamide B                   | 65413                  |
| 2206 | 25  | m/z | Methyl 2-undecynoate               | LMFA07010946           |
| 2207 | 74  | n   | (+)-Calycanthine                  | HMDB0029561            |
| 2208 | 88  | m/z | Glucosylgalactosyl                | HMDB0000585            |
| 2209 | 03  | n   | Stearidonyl carnitine             | LMFA07070106           |
DIHYDRO-7-DESACETYLDEOXYGEDUNI
43755

L-2-Aminoadipate adenylate
HMDB0006941

Hesperetin
HMDB0005782

Buddledin A
67850

Desethylene-N-acetylnorfloxacin
1603

Glu-P-1
72965

Suprofen S-oxide
HMDB0060924

CDP-DG(16:1(9Z)/18:2(9Z,12Z))
HMDB0115952

Echothiophate
HMDB0015190

Glucolimnanthin
66955

(-)-Epicatechin sulfate
HMDB0012467

Methyl 3-carbazolecarboxylate
HMDB0029744

Pelargonidin 3-O-3",6"-O-dimalonylglucoside
64249

2-(3,4-dimethoxyphenyl)-5,7-dihydroxy-3,6,8-trimethoxy-4H-chromen-4-one
HMDB0136121

3,4-Dehydrothiomorpholine-3-carboxylate
66183

1-(5-Methyl-2-thienyl)-1-propanone
HMDB0040231

Erosnin
HMDB0029465

Bisnorbadioquinone A
HMDB0033267

Tazobactam
HMDB0015544
10.03_198.1
2229 281m/z  pos  trans-Stilbene  96322

10.08_409.2
2230 737m/z  pos  (23R)-1alpha-hydroxy-25,27-
didehydrovitamin D3 26,23-
lactone  LMST03020600

10.12_428.0
2231 092n  neg  Ticarcillin disodium  69762

10.76_272.1
2233 620m/z  pos  N,O-Didesmethylvenlafaxine  HMDB0060852

11.34_449.3
2234 612m/z  pos  Hexacosanedioic acid  LMFA01170040

12.15_467.3
2235 736m/z  pos  6alpha-Hydroxycastasterone  LMST01030128

12.39_441.3
2236 575m/z  neg  DG(8:0/15:0/0:0)  HMDB0092917

13.05_359.1
2237 749m/z  pos  4-Chloro-17alpha-methyl-
17beta-hydroxy-4-androsten-
3-one  70830

13.79_450.3
2238 701m/z  pos  C-8 Ceramine  43406

14.06_647.5
2239 166m/z  pos  CE(15:1)  HMDB0060056

14.15_715.5
2240 783m/z  pos  PE-Cer(d14:1(4E)/24:0(2OH))  LMSP03020064

2.15_411.12
2241 93m/z  neg  2,3-dihydro-2-oxo-1H-
Benzimidazole-1-propanoic
acid  2386

3.18_241.09
2242 97m/z  pos  (±)-Anisoxide  87068

4.19_430.16
2243 17n  pos  3,7-Dihydroxy-2-[3-(4-
hydroxy-3-methylbutyl)-4-
methoxyphenyl]-5,6-
dimethoxy-4H-1-benzopyran-
4-one  LMPK12112858

4.35_111.11
2244 68m/z  pos  (Z)-5-Octen-1-ol  HMDB0031298
| m/z   | Charge | Compound                                                                 | HMDB  |
|-------|--------|--------------------------------------------------------------------------|-------|
| 5.04  | +      | Bis(1-aziridinyl)morpholinophosphine sulfide                               | 73052 |
| 6.67  | +      | Serratanidine                                                             | 67995 |
| 5.25  | +      | 1,3-Benzenedisulfonamide                                                 | 69857 |
| 6.92  | +      | Normethadone                                                              | 1185  |
| 5.71  | -      | N-acetyl-LTE4                                                             | LMFA03020008|
| 6.67  | -      | coumarin-SAHA                                                            | 64949 |
| 9.86  | -      | Adefovir Dipivoxil                                                        | 85417 |
| 6.92  | +      | TOLPERISONE                                                               | 43502 |
| 6.71  | +      | Pyrantel                                                                  | 2191  |
| 0.72  | +      | CDP-DG(18:2(9Z,11Z)/i-14:0)                                              | HMDB0116054|
| 0.78  | +      | threeo-Syringoylglycerol                                                  | 87513 |
| 0.71  | -      | Inosine triphosphate                                                      | 3589  |
| 0.81  | -      | alpha-Viniferin                                                           | HMDB0030603|
| 0.83  | -      | 1-O-alpha-D-Glucopyranosyl-D-mannitol                                     | HMDB0029911|
| 1.18  | -      | 4',5-Dihydroxy-3,3'-dimethoxy-6,7-methylenedioxyflavone 4'-glucuronide    |       |
| 1.19  | +      | 1-O-alpha-D-Glucopyranosyl-D-mannitol                                     |       |
| 7.50  | -      | threo-Syringoylglycerol                                                   |       |
| 7.76  | -      | Inosine triphosphate                                                      |       |
| 0.71  | -      | alpha-Viniferin                                                           |       |
| 0.61  | +      | CDP-Ethanolamine                                                          | HMDB0001564|
| 0.81  | -      | Pelargonidin 3,5-di-(6-acetylglucoside)                                    | LMPK12010045|
| 0.78  | +      | Pelargonidin 3,5-di-(6-acetylglucoside)                                    |       |
| 1.21  | +      | CDP-Ethanolamine                                                          |       |
| 0.81  | +      | CDP-Ethanolamine                                                          |       |
| 1.21  | +      | CDP-Ethanolamine                                                          |       |
| 10.00 | +      | Pelargonidin 3,5-di-(6-acetylglucoside)                                    |       |
| 10.11 | +      | Formylmethionyl-leucyl-phenylalanine methyl ester                         | 68923 |
| 10.11 | +      | Formylmethionyl-leucyl-phenylalanine methyl ester                         |       |
| m/z    | Retention Time | Charge | Name                                                                 | HMDB ID   |
|--------|----------------|--------|----------------------------------------------------------------------|-----------|
| 869m/z | 10.26_580.2    | neg    | POB-PS                                                               | LMGP20040017 |
| 616m/z | 10.48_450.2    | neg    | LysoPE(0:0/16:1(9Z))                                                | HMDB0011474 |
| 945m/z | 10.60_876.4    | pos    | PE(22:5(4Z,7Z,10Z,13Z,16Z)/2                                        | 61028     |
| 086m/z | 10.80_699.0    | neg    | {3-hydroxy-5-oxo-2-[(3-(sulfooxy)phenyl)-5H-chromen-7-yl]oxidanium}  | HMDB0125156 |
| 429m/z | 10.89_508.3    | pos    | Gymnodimine                                                          | HMDB0041430 |
| 837m/z | 10.99_208.1    | pos    | 2-Cyclotetradecen-1-one                                              | HMDB0039884 |
| 946m/z | 11.22_409.2    | pos    | 3alpha,9alpha,11beta-Trihydroxy-5beta-cholan-24-oic Acid            | LMST04010104 |
| 12.35_149.1 | 11.37_362.1 | pos    | Thaumatin b, recombinant                                             | HMDB0032529 |
| 317m/z | 12.62_340.3    | pos    | 2,4-Undecadienal                                                    | HMDB0031359 |
| 242m/z | 12.66_798.5    | pos    | PE(22:5(4Z,7Z,10Z,13Z,16Z)/P-18:1(11Z))                              | 61033     |
| 170m/z | 13.20_147.1    | pos    | 1-(1-Methoxy-1-methyl-4-methylbenzene                                | HMDB0029653 |
| 999m/z | 13.20_763.5    | pos    | 3-Demethylubiquinone-9                                               | HMDB0060370 |
| 550m/z | 13.37_567.4    | pos    | 36:4(21Z,24Z,27Z,30Z)                                               | LMFA01030829 |
| 471m/z | 13.88_447.3    | neg    | Linalyl isobutyrate                                                 | 86967     |
| 637m/z | 14.15_591.4    | neg    | 13-HODE                                                              | HMDB0061708 |
| 93m/z  | 2.12_418.31    | pos    | Philanthotoxin 343                                                  | 69713     |
| 38m/z  | 5.53_393.25    | pos    | RCS-8                                                                | 64777     |
| 29m/z  | 5.83_480.28    | pos    | Perindopril erbumine                                                | 66719     |
| Mass/Charge (m/z) | Charge Status | Compound Name                          | HMDB ID |
|------------------|---------------|----------------------------------------|---------|
| 6.62_464.21      | pos           | Diprenorphine                          | 69224   |
| 6.75_333.25      | pos           | Bremazocine                            | 69221   |
| 6.81_228.15      | neg           | Tecostanine                            | 68068   |
| 7.32_757.30      | neg           | Kasugamycin                            | 71964   |
| 7.57_222.11      | neg           | Phenmetrazine                          | HMDB0014968 |
| 7.65_319.13      | neg           | Carboxyprimaquine                      | 2082    |
| 7.88_471.13      | neg           | 2-amino-4-[(2-carboxy-2-hydroxy-1-phenylethyl)sulfonyl]-1-[(carboxymethyl)-C-hydroxycarbonimidoyl][ethyl]-C-hydroxycarbonimidoyl]butanoic acid | HMDB0126549 |
| 8.41_256.19      | neg           | Ethyl menthane carboxamide             | 92642   |
| 8.62_651.26      | pos           | (3a,5b,7b,12a)-(1,3-dihydro-5-nitro-1,3-dioxo-2H-isooindol-2-yl)methyl ester-3,7,12-trihydroxy-Cholan | 6688    |
| 8.76_468.27      | pos           | Prostaglandin E2 p-acetamidophenyl ester | 45604   |
| 9.43_191.10      | pos           | Tris(1-aziridinyl)phosphine oxide      | 73220   |
| 9.51_506.26      | neg           | Isodesmosine                           | 5707    |
| 9.60_213.18      | pos           | 10-Undecenyl acetate                   | 87350   |
| 9.96_209.15      | neg           | 5-Ethyl-3-methyl-2E,4E,6E-nonenatriene  | LMFA11000051 |
| 0.63_134.95      | neg           | (E)-S-1-Propenyl thiosulfate           | HMDB0041079 |
| m/z     | Retention Time (min) | Charge    | Molecular Formula | HMDB ID   |
|---------|----------------------|-----------|-------------------|-----------|
| 2298_73 | 0.65 390.99          | neg       | (E)-4-(6-methyl-1,2-dithiin-3-yl)but-1-en-3-yn-1-ol | LMFA12000367 |
| 2299_06 | 0.72 844.58          | pos       | PE(22:2(13Z,16Z)/20:3(5Z,8Z,11Z)) | HMDB0009562 |
| 2300_03 | 0.73_975.29          | pos       | Asiaticoside B    | 86571     |
| 2301_69 | 0.73 306.15          | neg       | trans-tetradec-2-enoyl-CoA | LMFA07050396 |
| 2302_50 | 0.76 205.01          | pos       | Histidinyl-Lysine  | 85796     |
| 2303_68 | 0.81 387.11          | neg       | Thiacremonone      | HMDB0035901 |
| 2304_07 | 0.83 367.99          | neg       | CRESOPYRINE        | 43914     |
| 2305_53 | 0.87 292.20          | pos       | NAc-DNP-Cys        | 69126     |
| 2306_19 | 0.92 262.06          | pos       | Allyxycarb         | 72707     |
| 2307_68 | 1.21 484.11          | neg       | Propetamphos       | 72453     |
| 2308_97 | 1.42 315.31          | pos       | Lucuminamide       | HMDB0031697 |
| 2309_91 | 10.14 388.9          | neg       | 6-Hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid | HMDB0034022 |
| 2310_96 | 10.63 333.2          | neg       | Nitroglycerin      | HMDB0014865 |
| 2311_06 | 10.76 977.5          | neg       | Dehydroepiandrosterone | HMDB0000077 |
| 2312_64 | 10.86 465.3          | neg       | PIM1(18:0/16:2(9Z,12Z)) | LMGP15010017 |
| 2313_53 | 10.87 468.3          | pos       | DG(8:0/0:0/15:0)   | HMDB0092918 |
| 2314_49 | 10.87 468.3          | pos       | N-(7Z,10Z,13Z-16Z-docosatetraenoyl) dopamine | LMFA08020274 |
| 2315_31 | 11.03 314.0          | pos       | (2S)-2-amino-3-[4-hydroxy-3-(sulfoxy)phenyl]-2-methylpropanoic acid | HMDB0142153 |
| 2316_68 | 11.07 596.2          | pos       | Z-Gly-Pro-Leu-Gly-Pro | 65925     |
11.11_643.1  Malvidin 3-glucoside-4-vinylcatechol  LMPK12010436
2317  887 m/z  pos
11.78_249.1  (6R,7S)-6,7-Epoxy-1,3-tetradecadiyne  HMDB0031776
2318  491 m/z  neg
11.81_295.2
2319  268 m/z  neg  (±)9-HODE  35487
12.02_483.3
2320  675 m/z  neg  6-Ketomyristic acid  HMDB0030982
11.19_522.3  6-O-alpha-L-rhamnopyranosyl-3-hydroxydecanoyl-3-hydroxydecanoic acid  LMFA13030001
2321  621 m/z  pos
12.70_515.3
2322  756 m/z  pos  16-Acetylpriverogenin A  HMDB0034529
12.92_503.3
2323  386 m/z  pos  Medicagenic acid  HMDB0034551
2.08_258.09
2324  19 m/z  neg  Glutamylmethionine  HMDB0028803
4.18_317.06
2325  07 m/z  neg  Pyrifthalid  72291
4.18_507.09
2326  56 m/z  neg  Farnesyl triphosphate  LMPR0103010023
4.18_635.24
2327  85 m/z  pos  Dehydroisococoporphyrinogen  HMDB0002242
4.24_650.03
2328  15 m/z  neg  Adenophostin A  69662
4.64_333.14  (2E)-N-[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-3-(4-hydroxyphenyl)prop-2-enimidic acid  HMDB0136318
2329  45 m/z  pos
5.11_534.31
2330  67 m/z  pos  POV-PE  LMGP20020030
7.61_469.11
2331  20 m/z  pos  Luteolin 5-galactoside  LMPK12110638
7.65_469.22
2332  32 m/z  neg  Licoricidin  LMPK12080045
8.14_647.23
2333  94 m/z  pos  Bis(5-hydroxynoracronycine)  88197
8.54_399.21
2334  96 m/z  neg  Lucidone B  HMDB0035834
| m/z   | RT (min) | Adduct | m/z  | Name                                                      | HMDB ID   |
|-------|----------|--------|------|-----------------------------------------------------------|-----------|
| 8.99  | 9.52     | neg    | 397.20 | Pregnanalone sulfate (Allopregnanolone sulfate)           | 3560      |
| 42m/z |          |        |       | Butyl isopropyl disulfide                                 | HMDB0033050 |
| 68m/z |          | pos    |       | Elatoside G                                               | HMDB0041347 |
| 46m/z |          | pos    | 3560  | 4-phenyl-5-methyl-1,2,3-Thiadiazole                       | 45304     |
| 52m/z |          | neg    | 795.73| TG(15:0/17:1(9Z)/15:0)                                    | 46630     |
| 51n   |          | neg    | 926m/z| CDP-DG(16:0/18:0)                                         | 58604     |
| 70m/z |          | pos    | 780.41| Leucomycin A6                                             | 69773     |
| 87m/z |          | neg    | 320.04| Nitrazepam                                                | HMDB0015534 |
| 25m/z |          | pos    | 320.04| Isophylloflavanine                                        | LMPK12020080 |
| 45m/z |          | pos    | 337.13| 2,9-Dimethyl-2,9-diazatricyclo[10.2.2.25,8]octadeca-5,7,12,14,15,17-hexaene-3,10-diol, 9CI | HMDB0038832 |
| 58m/z |          | pos    | 689.21| 1-dimethylarsinoyl-decane                                 | LMFA11000719 |
| 51.022|          |        |       | Cellotetraose                                             | 63206     |
| 926m/z|          | neg    | 643.2 | LysoPE(0:0/20:3(5Z,8Z,11Z))                               | HMDB0011485 |
| 729m/z|          | pos    | 509.3 | Lanceotoxin A                                             | 67237     |
| 370m/z|          | pos    | 552.0 | Ambolic acid                                              | HMDB0035713 |
| 186n  |          | neg    |       | Myricatín                                                 | HMDB0029513 |
| 599m/z|          | pos    | 178.1 | 3-Amino-1-hydroxy-5,7-dimethyl-adamantane                 | HMDB0060738 |
| 326m/z|          | pos    |       | ARCAINE                                                   | 43946     |
| 625m/z|          | pos    | 727.5 | Cholesteryl 11-hydroperoxy-eicosatetraenoate              | 41724     |
| m/z | Retention Time | Charge | Name | HMDB ID |
|-----|----------------|--------|------|---------|
| 2354 727 | 11.46 | pos | Oleanderolide 3-acetate | HMDB0034647 |
| 2355 667 | 11.93 | pos | L-Hexanoylcarnitine | HMDB0000756 |
| 2356 727 | 11.94 | neg | CPX | 44518 |
| 2357 025 | 12.70 | pos | PA(O-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | 82236 |
| 2358 112 | 12.92 | pos | Polyporusterone B | HMDB0038496 |
| 2359 572 | 13.13 | neg | Schleicherastatin 5 | HMDB0035804 |
| 2360 114 | 13.76 | pos | Vecuronium | 3000 |
| 2361 388 | 13.97 | pos | PS(16:0/18:0) | LMGP03010906 |
| 2362 388 | 14.78 | pos | TG(8:0/8:0/a-13:0)[rac] | HMDB0071246 |
| 2363 793 | 13.79 | neg | Cohibin A | HMDB0031168 |
| 2364 55 | 4.25 | pos | {4-[3-(5-hydroxy-2,2-dimethyl-2H-chromen-6-yl)propanoyl]phenyl}oxidanesulfonic acid | HMDB0125896 |
| 2365 96 | 4.64 | pos | talinolol | 96207 |
| 2366 20 | 5.04 | pos | {3-[2-(3,5-dihydroxyphenyl)ethyl]phenyl}oxidanesulfonic acid | HMDB0129951 |
| 2367 65 | 5.20 | neg | (beta-1-O-[N-(2-methyl-3-chlorophenyl-4-hydroxy)anthraniloyl]-D-glucopyranuronic acid) | HMDB0060035 |
| 2368 77 | 5.81 | pos | Hericerin | HMDB0038587 |
| 2369 96 | 6.06 | neg | (±)-Rollipyrrole | HMDB0037554 |
| 2370 58 | 6.09 | pos | (23S)-1α-hydroxy-25,27-didehydrovitamin D3 26,23-lactone | 42527 |
| m/z   | Name                                                   | HMDB ID   |
|-------|--------------------------------------------------------|-----------|
| 6.11  | 3-[4-hydroxy-2-methoxy-3-(3-methylbut-2-en-1-yl)phenyl]-1-(3-hydroxyphenyl)propan-1-one | HMDB0124820 |
| 7.02  | Terbinafine metabolite glucuronide                      | 2748      |
| 7.77  | N,2,3-Trimethyl-2-(1-methylethyl)butanamide             | 91344     |
| 8.02  | 3'-Deoxystreptomycin 6-phosphate                       | 2500      |
| 8.12  | LysoPC(22:0)                                           | 61707     |
| 8.16  | Jasmonic acid                                          |           |
| 8.78  | BENZANTHRONE                                           | 44054     |
| 9.56  | Toonacil                                               | 67202     |
| 0.73  | Virginiamycin                                          |           |

| m/z   | Name                                                   | HMDB ID   |
|-------|--------------------------------------------------------|-----------|
| 0.73  | Malvidin 3-O-(6-O-(4-O-feruloyl-alpha-rhamnopyranosyl)-beta-glucopyranoside)-5-beta-glucopyranoside | LMPK12010409 |
| 0.82  | MONOCROTALINE                                          | 44128     |
| 0.87  | Wy 14643                                               | 43447     |
| 0.92  | CDP-3,6-dideoxy-D-glucose                              | 63230     |
| 1.21  | Methoxybrassinin                                        |           |
| 1.21  | Bufferin                                               | 69567     |
| 10.11 | 1-Phenyl-1,3-eicosanedione                             |           |
| m/z    | Intensity | Charge | Compound                                      | HMDB ID       |
|--------|-----------|--------|-----------------------------------------------|---------------|
| 2388   | 253       | pos    | 2-amino-4-({1-[carboxymethyl]-C-hydroxycarbonimidoyl]-2-{[3-hydroxy-4-(7-methoxy-2-oxo-2H-chromen-8-yl)-2-methylbutan-2-yl]sulfanyl}ethyl}-C-hydroxycarbonimidoyl)butanoic acid | HMDB0132694   |
| 2389   | 133       | pos    | Phaeophorbide b                               | HMDB0031149   |
| 2390   | 430       | pos    | Bitertanol                                    | 68944         |
| 2391   | 569       | pos    | CAY10594                                      | 45492         |
| 2392   | 366       | pos    | (±)14(15)-EET-SI                              | 45177         |
| 2393   | 390       | pos    | 13-sophorosyloxydocosanoic acid               | LMFA13020004  |
| 2394   | 839       | pos    | LysoPE(20:0/0:0)                              | HMDB0011511   |
| 2395   | 186       | neg    | Etidocaine                                    | 66669         |
| 2396   | 781       | neg    | Granisetron                                   | HMDB0015026   |
| 2397   | 521       | pos    | Schleicherastatin 6                          | 90794         |
| 2398   | 5         | pos    | Viniferal                                     | HMDB0029790   |
| 2399   | 46        | pos    | 6-({2-[(acetyloxy)methyl]-4,5,6-trihydroxyoxan-3-yl}oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid | HMDB0125228   |
| 2400   | 17        | neg    | N-Benzylphthalimide                           | 69922         |
| 2401   | 99        | neg    | Coumestrol                                    | 48332         |
| 2402   | 49        | neg    | 5-Hydroxylansoprazole sulfone                 | 923           |
4.93_232.06  2403 04m/z    neg  N-Phenylacetylaspartic acid  HMDB0029355
          5.22_285.04

2404 07m/z    pos  Bracteatin  LMPK12130044
          6.08_335.12

2405 47m/z    neg  Dinocton 6  72683
          6.27_236.09

2406 54m/z    neg  Trihomomethionine  64500

          6.80_424.19  O-Desmethyltramadol glucuronide  HMDB0060856

2407 63m/z    neg  7.51_313.11

2408 86m/z    neg  Lysergic acid  66676
          7.65_465.18  Hydrocortisone sodium succinate  66842

2409 97m/z    neg  7.97_260.08

2410 21m/z    pos  Indirubin-3'-monoxime  45531

          7.98_450.17

2411 06m/z    pos  6-Hydroxyfluvastatin  HMDB0014037
          8.27_517.24

2412 66m/z    pos  2-O-Methyl-L-fucose  89534
          8.52_491.19

2413 22m/z    pos  3,4,5-trihydroxy-6-((2-[(2-[(2-methylbut-3-en-2-yl)-7-oxo-2H,3H,7H-furo[3,2-g]chromen-2-yl]propan-2-yl)oxy]oxy)oxane-2-carboxylic acid  HMDB0130297

          0.62_452.34  5b-Cholestane-3a,7a,12a,23S,25-pentol  LMST01010241

2414 82n      pos  0.63_679.31

2415 40m/z    neg  Asteridoside L  84931
          0.63_687.30

2416 45m/z    neg  Physagulin E  94248
          0.73_708.45  PE(14:0/20:5(5Z,8Z,11Z,14Z,17Z))  HMDB0008840

2417 87m/z    neg  0.84_361.08

2418 76m/z    neg  Bumetanide M1  1395
          0.97_197.05

2419 39m/z    neg  1.21_433.15

2420 19m/z    pos  1.22_205.98  BRUCINE  43921

2421 95m/z    pos  Thioguanine  HMDB0014496
| m/z | Time  | Name                          | Database ID |
|-----|-------|-------------------------------|-------------|
| 11-dehydro-TXB3 | 10.06_411.2 | 2422 | LMFA03030009 |
| Phenobarbital | 10.20_213.0 | 2423 | HMDB0015305 |
| Nalbuphine-3-glucuronide | 10.75_556.2 | 2424 | 1402 |
| Benzosimuline | 10.98_285.2 | 2425 | 88044 |
| Avocadyne | 11.13_289.1 | 2426 | HMDB0035473 |
| Sodium lauryl sulfate | 11.33_203.1 | 2427 | 58284 |
| Tetradecan-7,9-diynoic acid | 11.72_455.3 | 2428 | LMFA01031094 |
| Solacapine | 11.76_640.2 | 2429 | 68604 |
| S-(PGA2)-glutathione | 11.92_289.1 | 2430 | HMDB0013062 |
| JWH 200 4-hydroxyindole metabolite | 12.85_383.1 | 2431 | 96658 |
| Pubescenol | 13.20_475.3 | 2432 | HMDB0030085 |
| 20a,22b-Dihydroxycholesterol | 13.45_463.3 | 2433 | HMDB0006763 |
| 3'-Deoxystreptomycin 3'α,6-bisphosphate | 13.98_780.1 | 2434 | 2518 |
| PC(22:0/18:4(6Z,9Z,12Z,15Z)) | 14.27_860.6 | 2435 | HMDB0008536 |
| DG(14:1(9Z)/22:2(13Z,16Z)/0) | 14.53_601.5 | 2436 | HMDB0007059 |
| 1-(1-Propanylthio)propyl propyl disulfide | 15.83_223.0 | 2437 | 88933 |
| Brassica oleracea Alkaloid | 2.01_270.03 | 2438 | 89404 |
| N4-Acetylsulfadoxine | 2.14_351.07 | 2439 | 2543 |
| 2440 | 29m/z | pos | 4.19_510.13 | 2-amino-4-{{1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-[(2,3-dihydroxy-2-methyl-1-phenylpropyl)sulfanyl]ethyl}-C-hydroxycarbonimidoyl}butanoic acid | HMDB0133654 |
| 2441 | 35m/z | neg | 4.72_214.03 | Brassicanal B | 93257 |
| 2442 | 58m/z | neg | 5.27_258.05 | PPM-18 | 64815 |
| 2443 | 61m/z | pos | 5.37_349.22 | JWH 018 2-hydroxyindole metabolite-d9 | 96646 |
| 2444 | 54m/z | pos | 6.37_418.14 | Meperidinic acid glucuronide | 1135 |
| 2445 | 58m/z | neg | 6.73_230.98 | 4-Hydroxyriluzole | 2323 |
| 2446 | 77m/z | neg | 9.02_239.05 | trans-Ferulic acid | HMDB0000954 |
| 2447 | 07m/z | neg | 9.05_248.08 | Adenosine | HMDB0000050 |
| 2448 | 20m/z | pos | 0.62_415.04 | 5,8-dihydroxy-2-(1-hydroxy-3-methoxy-4-oxocyclohexa-2,5-dien-1-yl)-3,7-dimethoxy-4H-chromen-4-one | HMDB0129273 |
| 2449 | 42m/z | neg | 0.63_663.33 | Minosaminomycin | 71965 |
| 2450 | 33m/z | neg | 0.63_797.27 | Difloxacín | 68932 |
| 2451 | 59m/z | neg | 0.69_417.04 | NORSTICTIC ACID | 43603 |
| 2452 | 60m/z | pos | 0.83_976.13 | 1,4-Dihydroxy-2-naphthoyl-CoA | 63987 |
| 2453 | 98m/z | pos | 1.23_129.01 | Di-2-propenyl disulfide, 9CI | HMDB0033966 |
| 2454 | 813m/z | pos | 10.12_258.0 | 2-Amino-6-(benzylthio)purine | 70755 |
3,6-dihydroxy-2-[3-methoxy-4-(sulfooxy)phenyl]-5-sulfino-3,4-dihydro-2H-1-benzopyran-7-olate

10.12_448.0
2455 117n  neg HMDB0127804

10.13_261.1
2456 832m/z  pos Guaidiol HMDB0033228

10.67_345.1
2457 678m/z  neg Spenolimycin 71966

10.79_300.1
2458 367m/z  pos Acrifoline 67964

10.91_481.3
2459 123m/z  neg Latanoprost-d4 96388

10.98_826.5
2460 626m/z  neg PC(16:0/20:4(5Z,8Z,11Z,14Z)) 39120

12.62_773.5
2461 827m/z  neg SM(d18:1/18:1(11Z)) HMDB0012100

14.76_663.4
2462 597m/z  pos PG(a-13:0/i-16:0) HMDB0116646

2.00_552.39
2463 32m/z  pos Dendrogenin A LMST05050025

2.13_650.23
2464 76m/z  pos Tri-N-acetylchitotriose HMDB0006698

3.02_299.97
2465 33m/z  neg 5-Trifluoromethyl-2,4-disulfamoylaniline 3181

4.19_841.32
2466 74m/z  pos Dermorphin 73515

4.25_104.05
2467 01m/z  pos Aminofluoropropionic acid 690

4.38_231.17
2468 29m/z  pos 2-Decylfuran 88266

6.62_230.98
2469 58m/z  neg 5-Hydroxyriluzole 2324

6.76_262.06
2470 49m/z  pos ZLJ-6 45512

7.75_565.29
2471 99m/z  neg 24,25-Diacetylvulgaroside HMDB0041366

9.50_284.18
2472 50n  pos Melanostatin 58299

9.52_213.07
2473 02m/z  pos Hexanethioic acid S-propyl ester HMDB0039466

9.60_247.08
2474 58m/z  pos Perlolyrine HMDB0030327

9.93_944.18
2475 57m/z  pos Salviadelphin LMPK12010302
| m/z | Intensity | Charge | Compound                             | HMDB ID     |
|-----|-----------|--------|--------------------------------------|-------------|
| 29n | 0.73_769.42| neg    | Niddamycin                           | 69327       |
| 85m/z | 0.77_430.15 | neg    | Minoxidil-O-glucuronide              | 1320        |
| 41m/z | 0.80_395.09 | neg    | 4-Methyl dibenzothiophene             | 94701       |
| 82m/z | 0.80_441.06 | pos    | Glucoiberin                          | HMDB0038406 |
| 06m/z | 0.81_198.07 | neg    | 1-aminopyrene                        | 96142       |
| 27n | 0.82_630.12 | pos    | 2'-C-Methyl myricetin 3-rhamnoside-5'-gallate | 50846       |
| 94m/z | 1.23_447.04 | neg    | 4,5-diphenyl-1,2,3-Thiadiazole       | 45303       |
| 89m/z | 1.26_303.03 | neg    | Cysteinyll-Cysteine                  | HMDB0028772 |
| 16m/z | 1.47_213.01 | neg    | IPSP                                 | 72751       |
| 21m/z | 10.43_263.1 | neg    | Cyclobrassinone                      | HMDB0034209 |
| 644m/z | 10.52_606.3 | neg    | Nookatone                            | HMDB0013687 |
| 029m/z | 10.86_876.4 | pos    | PE(22:5(7Z,10Z,13Z,16Z,19Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) | HMDB0009672 |
| 1130.99_144.1 | pos    | Aminocyclohexanecarboxylic acid      | 6589        |
| 013m/z | 11.05_523.3 | pos    | Ganoderic acid beta                 | HMDB0033234 |
| 030m/z | 11.53_405.2 | pos    | 1b-Hydroxycholic acid                | HMDB0000307 |
| 633m/z | 11.83_622.4 | neg    | Enniatin B                           | 71071       |
| 083m/z | 11.94_627.4 | pos    | OLEANANOIC ACID ACETATE              | 44453       |
| 755m/z | 13.00_501.3 | pos    | PA(O-16:0/17:2(9Z,12Z))              | LMGP10020010 |
| 961m/z | 13.14_682.3 | pos    | OKOHA-PC                             | LMGP20010031 |
| 719m/z | 14.43_883.5 | pos    | Pitheduloside B                      | HMDB0034865 |
| 14.47_515.3 | 783m/z | pos | Hexafluronium | 85446 |
| 2.14_394.14 | 03m/z | neg | Anisessine | 68452 |
| 4.67_347.12 | 67m/z | pos | 3,6-Dimethoxy-6",6"-dimethylpyran[2,3:7,8]flavone | LMPK12111585 |
| 4.90_345.10 | 58m/z | neg | meta-O-Dealkylated flecainide lactam | HMDB0060832 |
| 5.33_350.14 | 98m/z | neg | Arginyl-Methionine | 85630 |
| 5.80_327.22 | 83m/z | pos | Boc-DVal(NMe)-Val-OMe | 65479 |
| 5.86_285.27 | 92m/z | pos | ethyl hexadecanoate | LMFA07010471 |
| 6.51_198.13 | 6.80_282.16 | pos | Cycloate | 72550 |
| 6.91_479.22 | 6.97_268.98 | pos | Xanomeline | 69206 |
| 7.12_397.16 | 7.57_331.26 | pos | 4-thiodimethylarsenobutanoic acid | LMFA00000041 |
| 7.12_397.16 | 8.08_327.09 | pos | Sclareol | HMDB0036827 |
| 8.28_660.39 | 8.95_447.13 | pos | Nifedipine | HMDB0015247 |
| 8.95_447.13 | 8.95_447.13 | pos | PC(10:0/14:0)[U] | 39128 |
| 9.30_252.17 | 9.51_484.28 | pos | 3-methyl-4-(methylamino)-1,2-diphenylbutan-2-ol | HMDB0144299 |
| 9.84_433.32 | 9.84_433.32 | pos | 24-Noroleana-3,12-diene | 265081 |
| 10.0_103.95 | 10.0_103.95 | pos | 3,6-Dimethoxy-6",6"-dimethylpyran[2,3:7,8]flavone | LMPK12111585 |
| 10.0_104.92 | 10.0_104.92 | pos | meta-O-Dealkylated flecainide lactam | HMDB0060832 |
| 10.0_104.92 | 10.0_104.92 | pos | Arginyl-Methionine | 85630 |
| 10.0_104.92 | 10.0_104.92 | pos | Boc-DVal(NMe)-Val-OMe | 65479 |
| 10.0_104.92 | 10.0_104.92 | pos | ethyl hexadecanoate | LMFA07010471 |
| 10.0_104.92 | 10.0_104.92 | pos | Cycloate | 72550 |
| 10.0_104.92 | 10.0_104.92 | pos | Xanomeline | 69206 |

| 10.0_104.92 | 10.0_104.92 | pos | 4-thiodimethylarsenobutanoic acid | LMFA00000041 |
| 10.0_104.92 | 10.0_104.92 | pos | Sclareol | HMDB0036827 |
| 10.0_104.92 | 10.0_104.92 | pos | Nifedipine | HMDB0015247 |
| 10.0_104.92 | 10.0_104.92 | pos | PC(10:0/14:0)[U] | 39128 |
| 10.0_104.92 | 10.0_104.92 | pos | 3-methyl-4-(methylamino)-1,2-diphenylbutan-2-ol | HMDB0144299 |
| 10.0_104.92 | 10.0_104.92 | pos | 24-Noroleana-3,12-diene | 265081 |
0.01_108.93
2518 67n  pos
0.01_122.89
2519 32m/z  neg
0.01_124.89
2520 05m/z  neg
0.01_143.86
2521 47m/z  neg
0.01_150.98
2522 21m/z  neg
0.01_156.93
2523 88m/z  neg
0.01_167.88
2524 25m/z  neg
0.01_169.89
2525 42n  neg
0.01_171.91
2526 25n  neg
0.01_178.97
2527 76m/z  neg
0.01_180.91
2528 27m/z  neg
0.01_182.96
2529 48m/z  pos
0.01_189.85
2530 94m/z  neg
0.01_197.90
2531 10m/z  neg
0.01_206.97
2532 25m/z  neg
0.01_216.87
2533 98m/z  neg
0.01_241.89
2534 62m/z  neg
0.01_243.89
2535 88m/z  neg
0.01_245.89
2536 19m/z  neg
0.01_250.90
2537 68m/z  neg
0.01_252.99
2538 60m/z  neg
0.01_261.87
2539 26m/z  neg
0.01_307.85
2540 53m/z  neg
0.01_316.86
2541 51m/z  neg
0.01_320.88
2542 38m/z  neg
| Mass (m/z) | Charge (z) | Status |
|-----------|-----------|--------|
| 326.84    | neg       |        |
| 336.85    | neg       |        |
| 341.83    | neg       |        |
| 120.96    | pos       |        |
| 122.96    | pos       |        |
| 137.96    | pos       |        |
| 140.94    | neg       |        |
| 142.87    | neg       |        |
| 145.86    | neg       |        |
| 145.86    | neg       |        |
| 147.87    | neg       |        |
| 148.87    | neg       |        |
| 149.87    | neg       |        |
| 152.97    | neg       |        |
| 179.84    | pos       |        |
| 116.92    | neg       |        |
| 116.97    | pos       |        |
| 126.96    | pos       |        |
| 152.96    | pos       |        |
| 171.87    | neg       |        |
| 173.86    | neg       |        |
| 177.84    | neg       |        |
| 206.91    | neg       |        |
| 81.91     | pos       |        |
| m/z | Charge | Status |
|-----|--------|--------|
| 213.89 | pos | 0.03 |
| 213.92 | pos | 0.03 |
| 217.86 | pos | 0.03 |
| 213.95 | pos | 0.03 |
| 217.86 | pos | 0.03 |
| 224.89 | pos | 0.03 |
| 249.93 | pos | 0.03 |
| 256.95 | pos | 0.03 |
| 263.86 | pos | 0.03 |
| 270.89 | pos | 0.03 |
| 289.88 | pos | 0.03 |
| 301.86 | pos | 0.03 |
| 610.18 | pos | 0.04 |
| 684.20 | pos | 0.04 |
| 613.96 | pos | 0.04 |
| 630.00 | pos | 0.04 |
| 638.96 | pos | 0.04 |
| 171.97 | pos | 0.04 |
| 181.98 | pos | 0.04 |
| 201.92 | pos | 0.04 |
| 213.11 | pos | 0.04 |
| 230.89 | pos | 0.04 |
| 234.85 | pos | 0.04 |
| 241.88 | pos | 0.04 |
| 243.88 | pos | 0.04 |
0.04 244.91
2593 33n  pos
0.04 247.84
2594 24m/z  neg
0.04 258.88
2595 76m/z  pos
0.04 273.89
2596 68n  pos
0.04 287.89
2597 15m/z  pos
0.04 293.85
2598 76m/z  pos
0.04 295.87
2599 18n  pos
0.04 297.88
2600 63n  pos
0.04 519.14
2601 21m/z  pos
0.05 124.96
2602 67m/z  pos
0.05 181.83
2603 80n  neg
0.06 203.85
2604 50m/z  neg
0.06 232.86
2605 21m/z  neg
0.06 249.84
2606 83m/z  neg
0.06 322.87
2607 69m/z  pos
0.08 151.88
2608 83m/z  neg
0.08 163.84
2609 58m/z  neg
0.08 281.85
2610 72m/z  neg
0.08 324.84
2611 87m/z  neg
0.09 157.86
2612 23m/z  neg
0.09 159.85
2613 94m/z  neg
0.09 179.99
2614 68m/z  pos
0.09 207.83
2615 61m/z  neg
0.09 209.83
2616 32m/z  neg
0.09 262.86
2617 82m/z  pos
| m/z   | Charge | Status |
|-------|--------|--------|
| 16     | 0.10   | pos    |
| 48     | 0.11   | neg    |
| 94     | 0.12   | pos    |
| 55     | 0.12   | neg    |
| 88     | 0.12   | pos    |
| 21     | 0.13   | neg    |
| 11     | 0.13   | pos    |
| 93     | 0.14   | neg    |
| 37     | 0.14   | pos    |
| 22     | 0.14   | neg    |
| 04     | 0.14   | pos    |
| 61     | 0.15   | pos    |
| 56     | 0.15   | pos    |
| 36     | 0.15   | pos    |
| 17     | 0.16   | pos    |
| 73     | 0.16   | neg    |
| 09     | 0.16   | pos    |
| 73     | 0.17   | neg    |
| 42     | 0.17   | pos    |
| 70     | 0.18   | neg    |
| 51     | 0.18   | pos    |
| 38     | 0.18   | pos    |
| 98     | 0.18   | neg    |
| 44     | 0.18   | pos    |
0.18_234.86
2643 39m/z pos
0.18_303.88
2644 66m/z pos
0.18_320.87
2645 72m/z pos
0.20_278.85
2646 79m/z neg
0.22_171.98
2647 43m/z pos
0.22_186.99
2648 13m/z pos
0.22_195.91
2649 51m/z pos
0.22_786.26
2650 05m/z pos
0.23_145.93
2651 02m/z neg
0.28_179.99
2652 10m/z pos
0.35_178.92
2653 11m/z pos
0.38_179.99
2654 07m/z pos
0.53_179.99
2655 32m/z pos
0.57_126.96
2656 80m/z pos
0.57_150.91
2657 94n neg
0.57_217.86
2658 21m/z pos
0.58_105.93
2659 51m/z pos
0.58_113.96
2660 38m/z pos
0.58_170.88
2661 30m/z neg
0.58_194.90
2662 49m/z neg
0.58_194.94
2663 47m/z pos
0.58_225.92
2664 50m/z neg
0.58_258.88
2665 80m/z pos
0.58_294.86
2666 94m/z pos
0.58_308.86
2667 98m/z neg
0.58  324.84  
2668  86m/z  neg  
0.59  101.95  
2669  01m/z  pos  
0.59  105.03  
2670  33m/z  pos  
0.59  137.96  
2671  45m/z  pos  
0.59  142.97  
2672  80m/z  pos  
0.59  146.93  
2673  75n  pos  
0.59  156.89  
2674  06m/z  pos  
0.59  180.91  
2675  22m/z  neg  
0.59  183.91  
2676  43m/z  neg  
0.59  197.90  
2677  12m/z  neg  
0.59  205.91  
2678  01m/z  pos  
0.59  208.93  
2679  57m/z  neg  
0.59  210.93  
2680  22m/z  pos  
0.59  222.90  
2681  49m/z  pos  
0.59  228.89  
2682  77m/z  pos  
0.59  230.89  
2683  31m/z  pos  
0.59  239.88  
2684  04m/z  pos  
0.59  241.89  
2685  70n  pos  
0.59  243.23  
2686  36m/z  pos  
0.59  247.89  
2687  37m/z  neg  
0.59  251.90  
2688  25m/z  pos  
0.59  255.82  
2689  22m/z  neg  
0.59  265.87  
2690  90m/z  neg  
0.59  275.90  
2691  48m/z  neg  
0.59  281.85  
2692  50m/z  neg
0.59_292.88
2693 80n  neg
0.59_299.89
2694 15m/z  pos
0.59_327.85
2695 83m/z  neg
0.59_338.89
2696 06m/z  neg
0.59_342.87
2697 12m/z  pos
0.59_353.85
2698 36m/z  pos
0.59_367.85
2699 85m/z  pos
0.59_379.86
2700 32m/z  neg
0.59_492.83
2701 35m/z  neg
0.59_509.81
2702 99m/z  neg
0.59_786.25
2703 85m/z  pos
0.61_109.67
2704 70m/z  pos
0.61_131.01
2705 96m/z  pos
0.61_152.91
2706 75m/z  neg
0.61_157.89
2707 77m/z  pos
0.61_164.08
2708 58n  pos
0.61_165.93
2709 79m/z  neg
0.61_171.94
2710 62m/z  pos
0.61_179.90
2711 31m/z  pos
0.61_182.40
2712 60m/z  pos
0.61_188.91
2713 82m/z  pos
0.61_192.95
2714 71m/z  neg
0.61_201.88
2715 81m/z  pos
0.61_215.86
2716 89m/z  neg
0.61_220.87
2717 68m/z  pos
2718 68m/z   pos  0.61_235.90
2719 29m/z   pos  0.61_238.11
2720 19m/z   pos  0.61_246.88
2721 78n     pos  0.61_249.92
2722 02m/z   pos  0.61_253.96
2723 40n     pos  0.61_260.97
2724 62m/z   pos  0.61_261.04
2725 56m/z   pos  0.61_271.91
2726 74m/z   pos  0.61_279.54
2727 93m/z   pos  0.61_292.88
2728 11n     pos  0.61_297.14
2729 09m/z   pos  0.61_300.88
2730 26n     pos  0.61_307.88
2731 90m/z   pos  0.61_310.86
2732 96m/z   neg  0.61_327.86
2733 74n     pos  0.61_336.89
2734 70n     pos  0.61_348.91
2735 75m/z   neg  0.61_376.85
2736 93m/z   pos  0.61_397.36
2737 28m/z   pos  0.61_416.86
2738 57n     pos  0.61_421.84
2739 03m/z   neg  0.61_431.01
2740 94m/z   pos  0.61_440.86
2741 49n     pos  0.61_454.10
2742 50n     pos
| m/z | isotope | charge | status |
|-----|---------|--------|--------|
| 2743 | 39 | 0.61 | neg |
| 2744 | 40 | 0.61 | neg |
| 2745 | 17 | 0.61 | pos |
| 2746 | 94 | 0.61 | pos |
| 2747 | 26 | 0.61 | pos |
| 2748 | 39 | 0.61 | pos |
| 2749 | 59 | 0.62 | pos |
| 2750 | 76 | 0.62 | pos |
| 2751 | 93 | 0.62 | neg |
| 2752 | 40 | 0.62 | pos |
| 2753 | 60 | 0.62 | pos |
| 2754 | 72 | 0.62 | pos |
| 2755 | 46 | 0.62 | neg |
| 2756 | 57 | 0.62 | neg |
| 2757 | 65 | 0.62 | pos |
| 2758 | 48 | 0.62 | pos |
| 2759 | 86 | 0.62 | pos |
| 2760 | 29 | 0.62 | neg |
| 2761 | 93 | 0.62 | pos |
| 2762 | 27 | 0.62 | pos |
| 2763 | 02 | 0.62 | neg |
| 2764 | 34 | 0.62 | pos |
| 2765 | 81 | 0.62 | pos |
| 2766 | 80 | 0.62 | pos |
| 2767 | 57 | 0.62 | neg |
| m/z  | Charge | Status |
|------|--------|--------|
| 289.93 | pos    |        |
| 294.88 |        | neg    |
| 313.88 | neg    |        |
| 357.40 |        | pos    |
| 359.94 | pos    |        |
| 360.93 | pos    |        |
| 369.88 | neg    |        |
| 372.89 |        | pos    |
| 378.87 | pos    |        |
| 391.40 | pos    |        |
| 394.38 | pos    |        |
| 396.85 | pos    |        |
| 408.86 | neg    |        |
| 410.86 |        | neg    |
| 422.38 | neg    |        |
| 424.84 | pos    |        |
| 426.90 | neg    |        |
| 429.85 | pos    |        |
| 435.86 | pos    |        |
| 440.83 | pos    |        |
| 444.36 | neg    |        |
| 450.36 | pos    |        |
| 456.37 | pos    |        |
| 459.36 | pos    |        |
| 459.36 | pos    |        |
0.62_459.88
2793 35n  pos
0.62_471.84
2794 79n  pos
0.62_477.85
2795 18n  neg
0.62_478.87
2796 11m/z  neg
0.62_482.85
2797 31n  pos
0.62_487.35
2798 82m/z  pos
0.62_494.84
2799 75m/z  neg
0.62_501.35
2800 15n  pos
0.62_502.35
2801 28m/z  pos
0.62_509.33
2802 72n  pos
0.62_512.82
2803 44m/z  neg
0.62_516.35
2804 02m/z  pos
0.62_528.86
2805 33m/z  pos
0.62_538.82
2806 72m/z  neg
0.62_544.84
2807 48m/z  pos
0.62_551.82
2808 80n  pos
0.62_551.83
2809 28m/z  pos
0.62_552.33
2810 56m/z  pos
0.62_553.33
2811 56m/z  pos
0.62_555.83
2812 13m/z  pos
0.62_557.84
2813 95n  pos
0.62_560.33
2814 54m/z  pos
0.62_566.33
2815 18n  pos
0.62_573.33
2816 80m/z  pos
0.62_574.31
2817 73n  pos
2818 0.62_581.33
2819 0.62_612.81
2820 0.62_627.80
2821 0.62_631.31
2822 0.62_639.29
2823 0.62_646.30
2824 0.62_665.30
2825 0.62_668.79
2826 0.62_668.82
2827 0.62_695.78
2828 0.62_696.28
2829 0.62_701.76
2830 0.62_704.27
2831 0.62_708.77
2832 0.62_711.28
2833 0.62_742.77
2834 0.62_763.77
2835 0.62_770.77
2836 0.62_772.77
2837 0.62_778.76
2838 0.62_782.75
2839 0.62_804.76
2840 0.62_809.71
2841 0.62_811.75
2842 0.62_811.75
| m/z | Charge State | Isotope | Intensity |
|-----|--------------|---------|-----------|
| 2843 | 33m/z | pos | 0.62_840.74 |
| 2844 | 30m/z | pos | 0.62_854.74 |
| 2845 | 67n | pos | 0.62_866.74 |
| 2846 | 62n | pos | 0.62_87.019 |
| 2847 | 8n | pos | 0.62_875.27 |
| 2848 | 00n | neg | 0.62_974.23 |
| 2849 | 31n | neg | 0.63_114.98 |
| 2850 | 78m/z | neg | 0.63_118.96 |
| 2851 | 57m/z | neg | 0.63_130.96 |
| 2852 | 56m/z | neg | 0.63_131.97 |
| 2853 | 53m/z | neg | 0.63_136.92 |
| 2854 | 38m/z | neg | 0.63_139.95 |
| 2855 | 55n | neg | 0.63_146.96 |
| 2856 | 04m/z | neg | 0.63_175.96 |
| 2857 | 58m/z | neg | 0.63_178.94 |
| 2858 | 84m/z | neg | 0.63_195.93 |
| 2859 | 86m/z | neg | 0.63_244.95 |
| 2860 | 85m/z | neg | 0.63_260.92 |
| 2861 | 62n | neg | 0.63_261.95 |
| 2862 | 20m/z | neg | 0.63_272.95 |
| 2863 | 84m/z | neg | 0.63_277.92 |
| 2864 | 68n | neg | 0.63_288.04 |
| 2865 | 46m/z | neg | 0.63_288.93 |
| 2866 | 64m/z | neg | 0.63_289.94 |
| 2867 | 24m/z | neg | 0.63_289.94 |
0.63_292.93
2868 04m/z  neg
0.63_303.97
2869 19m/z  neg
0.63_304.91
2870 38m/z  neg
0.63_325.89
2871 63m/z  neg
0.63_377.86
2872 67m/z  neg
0.63_402.91
2873 55m/z  neg
0.63_417.59
2874 67m/z  neg
0.63_418.89
2875 39m/z  neg
0.63_433.52
2876 42m/z  neg
0.63_438.86
2877 28m/z  neg
0.63_451.86
2878 07m/z  neg
0.63_455.85
2879 24m/z  neg
0.63_461.87
2880 26n   neg
0.63_505.87
2881 86m/z  neg
0.63_532.87
2882 38m/z  neg
0.63_548.85
2883 22m/z  neg
0.63_564.82
2884 98m/z  neg
0.63_581.81
2885 90m/z  neg
0.63_585.81
2886 20m/z  neg
0.63_589.81
2887 12n   neg
0.63_609.85
2888 47n   neg
0.63_614.33
2889 37m/z  neg
0.63_622.32
2890 40m/z  neg
0.63_624.85
2891 55n   neg
0.63_630.31
2892 49m/z  neg
0.63_649.83
2893 58n  neg
0.63_650.81
2894 55m/z  neg
0.63_671.32
2895 41m/z  neg
0.63_675.31
2896 37n  neg
0.63_682.80
2897 38m/z  neg
0.63_686.79
2898 89m/z  neg
0.63_689.78
2899 82m/z  neg
0.63_695.29
2900 44m/z  neg
0.63_711.77
2901 82m/z  neg
0.63_720.81
2902 55m/z  neg
0.63_727.81
2903 22m/z  neg
0.63_728.31
2904 35m/z  neg
0.63_731.29
2905 61m/z  neg
0.63_736.30
2906 37m/z  neg
0.63_739.78
2907 67m/z  neg
0.63_740.28
2908 45m/z  neg
0.63_744.29
2909 37m/z  neg
0.63_744.79
2910 83n  neg
0.63_751.79
2911 03m/z  neg
0.63_752.28
2912 38m/z  neg
0.63_764.79
2913 96m/z  neg
0.63_777.81
2914 13m/z  neg
0.63_779.29
2915 17n  neg
0.63_782.77
2916 06m/z  neg
0.63_785.30
2917 24m/z  neg
2918 30m/z neg 0.63_785.79
2919 10m/z neg 0.63_792.79
2920 30m/z neg 0.63_801.28
2921 31m/z neg 0.63_804.77
2922 69n neg 0.63_806.26
2923 10m/z neg 0.63_808.76
2924 91m/z neg 0.63_809.27
2925 35m/z neg 0.63_814.73
2926 21m/z neg 0.63_820.79
2927 93n neg 0.63_824.74
2928 68m/z neg 0.63_836.28
2929 10n neg 0.63_844.27
2930 11n neg 0.63_850.28
2931 15m/z neg 0.63_852.76
2932 02m/z neg 0.63_858.27
2933 17m/z neg 0.63_861.77
2934 54n neg 0.63_866.26
2935 19m/z neg 0.63_869.74
2936 78m/z neg 0.63_883.26
2937 22n neg 0.63_897.74
2938 51m/z neg 0.63_901.27
2939 12m/z neg 0.63_903.25
2940 45m/z neg 0.63_909.25
2941 10n neg 0.63_914.74
2942 81m/z neg
| Time (min) | Mass/Charge Ratio (m/z) | Charge State |
|-----------|-------------------------|--------------|
| 0.63      | 915.25                  | neg          |
| 0.63      | 923.25                  | neg          |
| 0.63      | 931.24                  | neg          |
| 0.63      | 931.75                  | neg          |
| 0.63      | 938.72                  | neg          |
| 0.63      | 940.24                  | neg          |
| 0.63      | 958.24                  | neg          |
| 0.63      | 966.23                  | neg          |
| 0.63      | 980.23                  | neg          |
| 0.63      | 988.22                  | neg          |
| 0.63      | 996.21                  | neg          |
| 0.63      | 997.71                  | neg          |
| 0.64      | 146.99                  | pos          |
| 0.64      | 151.03                  | pos          |
| 0.64      | 157.92                  | pos          |
| 0.64      | 167.01                  | pos          |
| 0.64      | 182.90                  | pos          |
| 0.64      | 186.92                  | pos          |
| 0.64      | 202.93                  | pos          |
| 0.64      | 214.26                  | pos          |
| 0.64      | 219.89                  | pos          |
| 0.64      | 233.06                  | pos          |
| 0.64      | 243.96                  | pos          |
| 0.64      | 295.89                  | pos          |
| 0.64      | 316.88                  | pos          |
| 0.64      | 316.88                  | pos          |
| m/z   | Value  | Charge |
|-------|--------|--------|
| 2968  | 332.89 |        |
| 2969  | 361.88 | +      |
| 2970  | 365.87 | +      |
| 2971  | 386.89 | +      |
| 2972  | 409.85 | +      |
| 2973  | 430.86 | +      |
| 2974  | 463.84 | +      |
| 2975  | 491.82 | +      |
| 2976  | 494.83 | +      |
| 2977  | 498.84 | +      |
| 2978  | 500.84 | +      |
| 2979  | 515.84 | +      |
| 2980  | 559.81 | +      |
| 2981  | 565.82 | +      |
| 2982  | 602.81 | +      |
| 2983  | 621.78 | +      |
| 2984  | 652.79 | +      |
| 2985  | 674.82 | +      |
| 2986  | 702.79 | +      |
| 2987  | 709.79 | +      |
| 2988  | 714.92 | +      |
| 2989  | 135.90 | -      |
| 2990  | 174.42 | -      |
| 2991  | 200.97 | -      |
| 2992  | 214.93 | -      |
| Index | Value    | Description | Unit | Z Value | Intensity |
|-------|----------|-------------|------|---------|-----------|
| 2993  | 0.65_504.97 | neg | 69m/z | 0.65 | 588.83    |
| 2994  | 0.65_617.84 | neg | 69m/z | 0.65 | 633.82    |
| 2995  | 0.66_158.97 | neg | 81m/z | 0.66 | 179.97    |
| 2996  | 0.66_158.97 | neg | 81m/z | 0.66 | 242.94    |
| 2997  | 0.66_245.06 | neg | 22m/z | 0.66 | 259.93    |
| 2998  | 0.66_245.06 | neg | 22m/z | 0.66 | 329.02    |
| 2999  | 0.66_356.92 | neg | 27m/z | 0.66 | 372.89    |
| 3000  | 0.66_356.92 | neg | 27m/z | 0.66 | 375.01    |
| 3001  | 0.66_356.92 | neg | 27m/z | 0.66 | 390.89    |
| 3002  | 0.66_356.92 | neg | 27m/z | 0.66 | 408.93    |
| 3003  | 0.66_356.92 | neg | 27m/z | 0.66 | 424.90    |
| 3004  | 0.66_440.88 | neg | 97m/z | 0.66 | 457.87    |
| 3005  | 0.66_440.88 | neg | 97m/z | 0.66 | 479.01    |
| 3006  | 0.66_440.88 | neg | 97m/z | 0.66 | 487.88    |
| 3007  | 0.66_440.88 | neg | 97m/z | 0.66 | 492.89    |
| 3008  | 0.66_440.88 | neg | 97m/z | 0.66 | 502.85    |
| 3009  | 0.66_440.88 | neg | 97m/z | 0.66 | 508.87    |
| 3010  | 0.66_440.88 | neg | 97m/z | 0.66 | 508.87    |
| 3011  | 0.66_440.88 | neg | 97m/z | 0.66 | 508.87    |
| 3012  | 0.66_440.88 | neg | 97m/z | 0.66 | 508.87    |
3018 18m/z  neg  0.66_544.90
3019 40m/z  neg  0.66_560.88
3020 17m/z  neg  0.66_576.86
3021 26m/z  neg  0.66_593.85
3022 15m/z  neg  0.66_593.86
3023 19n    neg  0.66_594.95
3024 98m/z  neg  0.66_644.84
3025 93m/z  neg  0.66_647.88
3026 75n    neg  0.66_708.83
3027 83n    neg  0.66_712.82
3028 13m/z  neg  0.66_768.78
3029 60m/z  neg  0.66_780.80
3030 18m/z  neg  0.66_836.77
3031 89m/z  neg  0.67_181.96
3032 71n    neg  0.67_181.96
3033 92n    pos  0.67_186.93
3034 01m/z  neg  0.67_202.11
3035 88n    pos  0.67_243.93
3036 99n    pos  0.67_249.95
3037 39n    neg  0.67_265.93
3038 12n    neg  0.67_267.05
3039 66m/z  neg  0.67_276.05
3040 22n    pos  0.67_311.92
3041 74n    pos  0.67_333.91
3042 84n    neg
3043 13n  pos
3044 92n  neg
3045 74m/z  neg
3046 10m/z  pos
3047 57m/z  neg
3048 37m/z  neg
3049 71m/z  neg
3050 41n  pos
3051 66m/z  pos
3052 73m/z  pos
3053 23m/z  pos
3054 95m/z  pos
3055 95m/z  neg
3056 05m/z  neg
3057 02n  pos
3058 84m/z  neg
3059 61n  pos
3060 19m/z  neg
3061 57m/z  pos
3062 30m/z  pos
3063 72n  neg
3064 97m/z  pos
3065 23m/z  pos
3066 48n  neg
3067 76m/z  pos
| Mass/Time | Charge | Status |
|-----------|--------|--------|
| 0.67_686.81 | 79m/z  | pos    |
| 0.67_702.86 |        |        |
| 0.67_718.85 | 86m/z  | neg    |
| 0.67_734.82 | 12m/z  | neg    |
| 0.67_809.80 | 29m/z  | neg    |
| 0.67_814.31 | 74m/z  | neg    |
| 0.68_154.07 | 85n    | neg    |
| 0.68_168.08 | 69m/z  | neg    |
| 0.68_249.95 | 50n    | neg    |
| 0.68_281.90 | 77m/z  | neg    |
| 0.68_304.06 | 25n    | pos    |
| 0.68_340.93 | 84n    | pos    |
| 0.68_389.02 | 32n    | pos    |
| 0.68_401.90 |        |        |
| 0.68_404.06 | 37n    | pos    |
| 0.68_408.92 | 46m/z  | pos    |
| 0.68_437.91 |        |        |
| 0.68_456.84 | 07m/z  | pos    |
| 0.68_475.90 | 84n    | pos    |
| 0.68_510.98 | 30n    | pos    |
| 0.68_516.99 | 92m/z  | pos    |
| 0.68_521.90 |        |        |
3093 89n  pos  0.68_525.85
3094 33m/z pos  0.68_541.12
3095 79m/z pos  0.68_557.09
3096 07m/z pos  0.68_599.00
3097 22n  pos  0.68_605.87
3098 34m/z pos  0.68_612.88
3099 98n  pos  0.68_673.85
3100 67n  pos  0.68_690.81
3101 81m/z pos  0.68_708.34
3102 54m/z pos  0.68_741.84
3103 71n  pos  0.68_775.82
3104 33n  pos  0.68_776.33
3105 42m/z pos  0.68_784.32
3106 24m/z pos  0.68_818.32
3107 12m/z pos  0.68_826.80
3108 70m/z pos  0.68_851.80
3109 56m/z pos  0.68_865.80
3110 02n  pos  0.68_886.30
3111 38m/z pos  0.68_935.78
3112 66n  pos  0.68_999.80
3113 16n  pos  0.68_935.78
3114 27m/z pos  0.68_958.77
3115 98m/z pos  0.68_961.77
3116 49n  pos  0.68_962.29
3117 17m/z pos
| M/z | Charge State | Value |
|-----|--------------|-------|
| 3143| -            | 0.69_384.93 |
| 3144| -            | 0.69_390.88 |
| 3145| +            | 0.69_400.90 |
| 3146| -            | 0.69_416.88 |
| 3147| -            | 0.69_430.91 |
| 3148| +            | 0.69_444.11 |
| 3149| +            | 0.69_452.92 |
| 3150| -            | 0.69_462.86 |
| 3151| +            | 0.69_463.89 |
| 3152| +            | 0.69_468.89 |
| 3153| -            | 0.69_471.01 |
| 3154| -            | 0.69_475.91 |
| 3155| -            | 0.69_485.03 |
| 3156| -            | 0.69_485.87 |
| 3157| -            | 0.69_491.88 |
| 3158| +            | 0.69_493.86 |
| 3159| -            | 0.69_531.01 |
| 3160| +            | 0.69_536.88 |
| 3161| -            | 0.69_543.90 |
| 3162| +            | 0.69_552.85 |
| 3163| -            | 0.69_588.89 |
| 3164| -            | 0.69_598.83 |
| 3165| +            | 0.69_604.87 |
| 3166| -            | 0.69_611.89 |
| 3167| +            | 0.69_614.14 |
| m/z     | Charge | Status | MRM Value |
|---------|--------|--------|-----------|
| 41      | neg    | 0.69_620.84 |
| 61      | pos    | 0.69_656.88 |
| 35      | neg    | 0.69_662.36 |
| 14      | pos    | 0.69_669.84 |
| 70      | pos    | 0.69_672.85 |
| 76      | neg    | 0.69_675.83 |
| 14      | pos    | 0.69_676.35 |
| 1      | pos    | 0.69_679.87 |
| 82      | pos    | 0.69_683.82 |
| 86      | pos    | 0.69_688.82 |
| 65      | neg    | 0.69_693.34 |
| 2       | pos    | 0.69_704.80 |
| 60      | neg    | 0.69_724.86 |
| 99      | neg    | 0.69_727.83 |
| 9       | pos    | 0.69_729.80 |
| 54      | pos    | 0.69_732.83 |
| 20      | neg    | 0.69_733.36 |
| 11      | neg    | 0.69_734.81 |
| 52      | pos    | 0.69_740.84 |
| 52      | neg    | 0.69_744.33 |
| 76      | pos    | 0.69_744.84 |
| 58      | pos    | 0.69_746.79 |
| 58      | neg    | 0.69_749.78 |
| 79      | pos    | 0.69_749.83 |
| 59      | neg    | 0.69_749.83 |
0.69_752.32
3193  73n  pos
0.69_756.81
3194  88m/z  neg
0.69_760.82
3195  12m/z  pos
0.69_763.84
3196  01n  pos
0.69_766.82
3197  25m/z  neg
0.69_768.35
3198  52n  neg
0.69_770.85
3199  52m/z  pos
0.69_772.33
3200  13n  pos
0.69_778.33
3201  09n  pos
0.69_778.82
3202  57m/z  pos
0.69_783.33
3203  01m/z  neg
0.69_786.32
3204  08n  pos
0.69_791.81
3205  31n  neg
0.69_793.84
3206  20n  neg
0.69_806.32
3207  60m/z  neg
0.69_810.33
3208  68n  neg
0.69_811.81
3209  67n  pos
0.69_817.32
3210  40m/z  neg
0.69_821.32
3211  73m/z  pos
0.69_825.31
3212  15m/z  neg
0.69_828.80
3213  98m/z  pos
0.69_833.96
3214  3n  pos
0.69_830.76
3215  75m/z  neg
0.69_831.78
3216  34n  pos
0.69_831.82
3217  80n  pos
| M/z   | Intensity | Charge | Result   |
|-------|-----------|--------|----------|
| 0.69  | 833.80    | 48n    | neg      |
| 0.69  | 835.83    | 03n    | neg      |
| 0.69  | 836.78    | 25m/z  | pos      |
| 0.69  | 843.78    | 36n    | pos      |
| 0.69  | 843.82    | 26n    | pos      |
| 0.69  | 845.28    | 45n    | neg      |
| 0.69  | 846.31    | 53m/z  | pos      |
| 0.69  | 847.79    | 81n    | pos      |
| 0.69  | 850.79    | 64m/z  | neg      |
| 0.69  | 852.31    | 95m/z  | neg      |
| 0.69  | 854.30    | 99n    | neg      |
| 0.69  | 858.78    | 39n    | pos      |
| 0.69  | 859.76    | 31m/z  | neg      |
| 0.69  | 863.82    | 20n    | pos      |
| 0.69  | 871.29    | 70n    | pos      |
| 0.69  | 877.33    | 42m/z  | pos      |
| 0.69  | 880.31    | 05m/z  | neg      |
| 0.69  | 880.81    | 29n    | pos      |
| 0.69  | 890.81    | 11m/z  | pos      |
| 0.69  | 898.74    | 82m/z  | neg      |
| 0.69  | 901.78    | 40n    | neg      |
| 0.69  | 903.77    | 48n    | pos      |
| 0.69  | 905.82    | 48n    | pos      |
| 0.69  | 906.31    | 20n    | pos      |
| 0.69  | 908.76    | 68n    | pos      |
| 0.69  | 908.76    | 76m/z  | neg      |
| m/z   | Charge | State |
|-------|--------|-------|
| 3243  | 45     | neg   |
| 3244  | 18     | neg   |
| 3245  | 16     | pos   |
| 3246  | 61     | pos   |
| 3247  | 51     | neg   |
| 3248  | 56     | pos   |
| 3249  | 75     | neg   |
| 3250  | 50     | neg   |
| 3251  | 59     | pos   |
| 3252  | 03     | neg   |
| 3253  | 47     | pos   |
| 3254  | 17     | neg   |
| 3255  | 19     | pos   |
| 3256  | 69     | neg   |
| 3257  | 07     | pos   |
| 3258  | 61     | neg   |
| 3259  | 83     | pos   |
| 3260  | 02     | neg   |
| 3261  | 90     | neg   |
| 3262  | 71     | neg   |
| 3263  | 84     | pos   |
| 3264  | 33     | pos   |
| 3265  | 30     | neg   |
| 3266  | 07     | pos   |
| 3267  | 88     | neg   |
| Mass/Charge (m/z) | Value 1   | Value 2   | Modality |
|------------------|-----------|-----------|----------|
| 0.69_995.76      | 80n neg   |           |          |
| 0.69_997.76      | 73n pos   |           |          |
| 0.69_998.26      | 71n pos   |           |          |
| 0.70_238.93      | 09m/z neg |           |          |
| 0.70_240.92      | 81m/z neg |           |          |
| 0.70_245.90      | 24n neg   |           |          |
| 0.70_248.19      | 34m/z neg |           |          |
| 0.70_271.90      | 10n neg   |           |          |
| 0.70_279.88      | 76n neg   |           |          |
| 0.70_308.91      | 11m/z neg |           |          |
| 0.70_315.96      | 89m/z neg |           |          |
| 0.70_331.88      | 79n neg   |           |          |
| 0.70_366.87      | 30m/z neg |           |          |
| 0.70_374.90      | 62m/z neg |           |          |
| 0.70_380.85      | 43m/z neg |           |          |
| 0.70_405.83      | 80n neg   |           |          |
| 0.70_413.87      | 52n neg   |           |          |
| 0.70_432.86      | 28m/z neg |           |          |
| 0.70_434.86      | 07m/z neg |           |          |
| 0.70_448.83      | 93m/z neg |           |          |
| 0.70_461.87      | 52n neg   |           |          |
| 0.70_473.82      | 44n neg   |           |          |
| 0.70_483.84      | 19n neg   |           |          |
| 0.70_500.84      | 85m/z neg |           |          |
| 0.70_508.79      | 38m/z neg |           |          |
| m/z  | Retention Time | Charge | Peak |     |
|------|----------------|--------|------|-----|
| 54   | 0.70           | neg    | 516.82 |
| 73   | 0.70           | neg    | 534.79 |
| 62   | 0.70           | neg    | 545.87 |
| 17   | 0.70           | neg    | 548.78 |
| 29   | 0.70           | neg    | 560.80 |
| 58   | 0.70           | neg    | 568.82 |
| 75   | 0.70           | neg    | 574.78 |
| 48   | 0.70           | neg    | 576.78 |
| 11   | 0.70           | neg    | 586.81 |
| 12   | 0.70           | neg    | 590.75 |
| 99   | 0.70           | neg    | 592.75 |
| 62   | 0.70           | neg    | 602.78 |
| 34   | 0.70           | neg    | 608.73 |
| 43   | 0.70           | neg    | 610.82 |
| 26   | 0.70           | neg    | 613.86 |
| 49   | 0.70           | neg    | 616.76 |
| 93   | 0.70           | neg    | 619.80 |
| 85   | 0.70           | neg    | 626.79 |
| 95   | 0.70           | neg    | 629.80 |
| 04   | 0.70           | neg    | 634.74 |
| 00   | 0.70           | neg    | 644.76 |
| 74   | 0.70           | neg    | 651.76 |
| 07   | 0.70           | neg    | 661.79 |
| 37   | 0.70           | neg    | 668.78 |
| 40   | 0.70           | neg    | 683.78 |
| 3318 | 0.70_677.76 | 39n | neg |
| 3319 | 0.70_684.76 | 66m/z | neg |
| 3320 | 0.70_702.72 | 80m/z | neg |
| 3321 | 0.70_719.75 | 87n | neg |
| 3322 | 0.70_729.77 | 73n | neg |
| 3323 | 0.70_745.75 | 48n | neg |
| 3324 | 0.70_789.78 | 59n | neg |
| 3325 | 0.70_854.69 | 31m/z | neg |
| 3326 | 0.70_990.65 | 80m/z | neg |
| 3327 | 0.71_186.91 | 40m/z | pos |
| 3328 | 0.71_190.91 | 25m/z | pos |
| 3329 | 0.71_196.09 | 38n | pos |
| 3330 | 0.71_209.90 | 88n | pos |
| 3331 | 0.71_211.90 | 54n | pos |
| 3332 | 0.71_216.92 | 41m/z | pos |
| 3333 | 0.71_236.89 | 44m/z | pos |
| 3334 | 0.71_266.84 | 33m/z | pos |
| 3335 | 0.71_342.86 | 71m/z | pos |
| 3336 | 0.71_345.88 | 54n | pos |
| 3337 | 0.71_352.89 | 94m/z | pos |
| 3338 | 0.71_387.86 | 88n | pos |
| 3339 | 0.71_397.89 | 85n | pos |
| 3340 | 0.71_416.80 | 32m/z | pos |
| 3341 | 0.71_422.88 | 55m/z | pos |
| 3342 | 0.71_445.83 | 39n | pos |
0.71_667.76
3368 55n  pos
0.71_691.77
3369 20n  pos
0.71_693.77
3370 18n  pos
0.71_706.73
3371 07m/z  pos
0.71_717.77
3372 95n  pos
0.71_719.78
3373 67n  pos
0.71_724.79
3374 12m/z  pos
0.71_736.76
3375 54m/z  pos
0.71_768.79
3376 01m/z  pos
0.71_775.74
3377 69n  pos
0.71_782.74
3378 93m/z  pos
0.71_783.77
3379 52n  pos
0.71_791.77
3380 15n  pos
0.71_804.74
3381 15m/z  pos
0.71_807.75
3382 23n  pos
0.71_827.75
3383 29n  pos
0.71_829.74
3384 84n  pos
0.71_833.75
3385 32n  pos
0.71_837.74
3386 73m/z  pos
0.71_875.74
3387 27n  pos
0.71_878.77
3388 33m/z  pos
0.71_894.72
3389 06m/z  pos
0.71_901.73
3390 97n  pos
0.71_905.72
3391 75n  pos
0.71_908.70
3392 29m/z  pos
| m/z | Charge | Status |
|-----|--------|--------|
| 44n | pos    | 0.71_909.72 |
| 31m/z | pos  | 0.71_936.70 |
| 28n  | pos    | 0.71_937.74 |
| 40n  | pos    | 0.71_951.71 |
| 48n  | pos    | 0.71_955.69 |
| 28m/z | pos  | 0.71_962.70 |
| 50m/z | pos  | 0.71_969.68 |
| 76n  | pos    | 0.71_982.69 |
| 95m/z | pos  | 0.71_988.69 |
| 43m/z | pos  | 0.71_998.69 |
| 27m/z | pos  | 0.72_104.95 |
| 30m/z | neg   | 0.72_112.89 |
| 56m/z | pos  | 0.72_114.89 |
| 31m/z | pos    | 0.72_170.94 |
| 37m/z | neg   | 0.72_177.05 |
| 31n  | pos    | 0.72_199.87 |
| 86n  | pos    | 0.72_206.89 |
| 23m/z | pos  | 0.72_210.88 |
| 88m/z | pos  | 0.72_212.84 |
| 55m/z | pos  | 0.72_218.87 |
| 34m/z | neg    | 0.72_220.87 |
| 04m/z | neg   | 0.72_226.86 |
| 39m/z | pos    | 0.72_228.90 |
| 21m/z | neg    | 0.72_230.89 |
| 91m/z | neg    |
0.72_231.83
3418 38n  pos  
0.72_240.84
3419 46m/z  pos  
0.72_253.88
3420 75n  neg  
0.72_264.84
3421 51m/z  pos  
0.72_276.83
3422 16m/z  neg  
0.72_278.82
3423 87m/z  neg  
0.72_286.86
3424 05m/z  neg  
0.72_288.85
3425 76m/z  neg  
0.72_296.88
3426 80m/z  neg  
0.72_369.80
3427 65n  pos  
0.72_409.27
3428 38m/z  pos  
0.72_418.79
3429 89m/z  pos  
0.72_442.81
3430 40m/z  pos  
0.72_601.73
3431 04n  pos  
0.72_610.73
3432 91m/z  pos  
0.72_617.71
3433 29n  pos  
0.72_620.62
3434 84m/z  neg  
0.72_625.71
3435 91n  neg  
0.72_628.66
3436 18m/z  neg  
0.72_633.69
3437 67n  neg  
0.72_644.68
3438 90m/z  pos  
0.72_645.71
3439 26n  pos  
0.72_649.67
3440 28n  neg  
0.72_651.67
3441 90n  pos  
0.72_655.74
3442 01n  pos  
| m/z | Charge State | 0.72_737.59 |
|-----|-------------|-------------|
| 3468 | 20m/z      | neg         |
| 3469 | 84m/z      | neg         |
| 3470 | 79m/z      | pos         |
| 3471 | 15n        | neg         |
| 3472 | 93m/z      | neg         |
| 3473 | 22m/z      | pos         |
| 3474 | 76n        | pos         |
| 3475 | 08m/z      | pos         |
| 3476 | 39n        | neg         |
| 3477 | 76n        | pos         |
| 3478 | 91m/z      | neg         |
| 3479 | 97n        | neg         |
| 3480 | 65n        | pos         |
| 3481 | 04n        | neg         |
| 3482 | 89n        | pos         |
| 3483 | 67m/z      | neg         |
| 3484 | 26n        | neg         |
| 3485 | 11n        | pos         |
| 3486 | 36n        | neg         |
| 3487 | 40m/z      | neg         |
| 3488 | 56n        | pos         |
| 3489 | 76m/z      | neg         |
| 3490 | 65m/z      | neg         |
| 3491 | 07n        | neg         |
| 3492 | 42m/z      | neg         |
| M/Z | Charge State | Mass/Charge Ratio |
|-----|--------------|------------------|
| 19n | pos          | 0.72_855.59      |
| 34n | neg          | 0.72_859.57      |
| 25m/z| neg         | 0.72_866.54      |
| 78n | pos          | 0.72_871.59      |
| 15n | pos          | 0.72_881.51      |
| 85m/z| neg         | 0.72_882.52      |
| 35m/z| neg         | 0.72_885.59      |
| 25n | pos          | 0.72_904.56      |
| 85n | pos          | 0.72_907.51      |
| 91n | pos          | 0.72_908.50      |
| 71m/z| pos         | 0.72_913.57      |
| 63n | pos          | 0.72_915.58      |
| 27n | pos          | 0.72_920.56      |
| 31m/z| pos         | 0.72_933.49      |
| 71n | neg          | 0.72_935.50      |
| 01n | neg          | 0.72_940.48      |
| 87m/z| neg         | 0.72_940.56      |
| 16m/z| pos         | 0.72_943.52      |
| 02n | neg          | 0.72_943.57      |
| 03n | pos          | 0.72_945.55      |
| 67n | pos          | 0.72_947.56      |
| 09n | pos          | 0.72_951.50      |
| 77n | neg          | 0.72_951.50      |
0.72_965.50
3518 04n  neg
0.72_967.56
3519 22n  pos
0.72_972.53
3520 39m/z  pos
0.72_973.50
3521 39n  neg
0.72_973.54
3522 98n  pos
0.72_977.49
3523 40n  neg
0.72_982.46
3524 20m/z  neg
0.72_985.49
3525 09n  neg
0.72_993.47
3526 81n  neg
0.72_994.53
3527 33m/z  pos
0.72_997.53
3528 93n  pos
0.73_110.07
3529 24m/z  pos
0.73_110.89
3530 81m/z  neg
0.73_141.94
3531 15n  pos
0.73_150.88
3532 59m/z  neg
0.73_152.88
3533 32m/z  neg
0.73_157.08
3534 88n  pos
0.73_170.09
3535 34m/z  pos
0.73_177.02
3536 58m/z  pos
0.73_192.99
3537 74m/z  pos
0.73_196.87
3538 26m/z  pos
0.73_198.86
3539 34m/z  pos
0.73_208.84
3540 46m/z  neg
0.73_210.84
3541 15m/z  neg
0.73_212.83
3542 88m/z  neg
| M/Z   | Charge | Status |
|-------|--------|--------|
| 226.81| 55     | neg    |
| 266.80| 21     | pos    |
| 268.80| 31     | neg    |
| 271.80| 03     | neg    |
| 284.77| 37     | neg    |
| 286.77| 12     | neg    |
| 288.76| 85     | neg    |
| 300.74| 76     | neg    |
| 321.75| 45     | neg    |
| 325.76| 81     | neg    |
| 326.75| 92     | neg    |
| 342.73| 94     | neg    |
| 379.71| 20     | neg    |
| 384.72| 84     | neg    |
| 386.71| 24     | neg    |
| 401.69| 84     | neg    |
| 442.67| 87     | neg    |
| 444.67| 52     | neg    |
| 459.65| 71     | neg    |
| 460.64| 70     | neg    |
| 475.63| 05     | neg    |
| 476.62| 00     | neg    |
3568 64m/z  neg
0.73_481.65
3569 65n  neg
0.73_500.63
3570 67m/z  neg
0.73_502.63
3571 66m/z  neg
0.73_518.60
3572 67m/z  neg
0.73_532.58
3573 67m/z  neg
0.73_535.62
3574 66n  neg
0.73_558.59
3575 58m/z  neg
0.73_575.57
3576 51n  neg
0.73_579.56
3577 56n  neg
0.73_581.60
3578 69n  neg
0.73_590.54
3579 20m/z  neg
0.73_595.58
3580 29n  neg
0.73_606.52
3581 31m/z  neg
0.73_611.55
3582 62n  neg
0.73_619.59
3583 57n  neg
0.73_626.53
3584 24m/z  neg
0.73_631.53
3585 51n  neg
0.73_633.53
3586 51n  neg
0.73_635.53
3587 21n  neg
0.73_640.51
3588 73m/z  neg
0.73_649.51
3589 15n  neg
0.73_655.53
3590 97n  neg
0.73_664.49
3591 48m/z  neg
0.73_668.47
3592 48m/z  neg
0.73_668.50
3593 58m/z   pos
0.73_671.51
3594 29n   neg
0.73_691.50
3595 67n   neg
0.73_700.47
3596 42m/z   neg
0.73_711.46
3597 21n   neg
0.73_712.45
3598 39m/z   neg
0.73_715.46
3599 36n   neg
0.73_725.48
3600 30n   neg
0.73_745.44
3601 76n   neg
0.73_749.45
3602 46n   neg
0.73_759.43
3603 27m/z   neg
0.73_767.42
3604 77n   neg
0.73_771.45
3605 87n   neg
0.73_772.41
3606 92m/z   neg
0.73_782.40
3607 83m/z   neg
0.73_796.41
3608 37m/z   neg
0.73_805.37
3609 93n   pos
0.73_805.41
3610 18n   neg
0.73_807.40
3611 63n   neg
0.73_809.40
3612 69n   neg
0.73_810.39
3613 77m/z   neg
0.73_811.38
3614 79n   pos
0.73_813.38
3615 54n   pos
0.73_819.38
3616 82n   pos
0.73_826.38
3617 80m/z   pos
0.73_827.36
3618 13n  pos
0.73_830.36
3619 60m/z pos
0.73_832.36
3620 38m/z pos
0.73_832.36
3621 81m/z neg
0.73_835.40
3622 63n neg
0.73_841.36
3623 01n neg
0.73_843.39
3624 27n neg
0.73_845.39
3625 00n neg
0.73_847.38
3626 72n neg
0.73_849.38
3627 59n neg
0.73_857.37
3628 81n neg
0.73_860.32
3629 20m/z neg
0.73_870.35
3630 09m/z neg
0.73_874.33
3631 25m/z neg
0.73_881.34
3632 67n neg
0.73_883.35
3633 62n neg
0.73_885.33
3634 92n neg
0.73_891.35
3635 37n neg
0.73_898.31
3636 83m/z neg
0.73_901.32
3637 02n neg
0.73_902.30
3638 61m/z neg
0.73_904.31
3639 04m/z neg
0.73_907.32
3640 02m/z neg
0.73_921.30
3641 50m/z neg
0.73_933.30
3642 43n neg
0.73_934.30
3643 12m/z   neg
    0.73_941.31
3644 50n    neg
    0.73_943.32
3645 67n    neg
    0.73_945.29
3646 45n    neg
    0.73_948.28
3647 66m/z  neg
    0.73_960.26
3648 49m/z  neg
    0.73_970.27
3649 99m/z  neg
    0.73_972.27
3650 24m/z  neg
    0.73_982.26
3651 89m/z  neg
    0.73_984.27
3652 54m/z  neg
    0.73_999.28
3653 00n    neg
    0.75_108.90
3654 08m/z  neg
    0.75_154.88
3655 03m/z  neg
    0.75_184.02
3656 51n    pos
    0.75_191.04
3657 12m/z  pos
    0.75_234.86
3658 58m/z  neg
    0.75_260.99
3659 04m/z  neg
    0.75_294.82
3660 15m/z  neg
    0.75_308.79
3661 94m/z  neg
    0.75_309.99
3662 71n    pos
    0.75_325.95
3663 96n    pos
    0.75_350.78
3664 33m/z  neg
    0.75_352.78
3665 09m/z  neg
    0.75_368.75
3666 50m/z  neg
    0.75_368.96
3667 02m/z  pos
| m/z   | RT  | Charge | Status |
|-------|-----|--------|--------|
| 0.75  | 427.76 | 04n    | neg    |
| 0.75  | 429.75 | 68n    | neg    |
| 0.75  | 468.69 | 54m/z  | neg    |
| 0.75  | 484.67 | 10m/z  | neg    |
| 0.76  | 106.05 | 13m/z  | pos    |
| 0.76  | 124.00 | 63m/z  | neg    |
| 0.76  | 146.06 | 84m/z  | neg    |
| 0.76  | 152.03 | 28m/z  | pos    |
| 0.76  | 154.92 | 70m/z  | neg    |
| 0.76  | 158.84 | 58m/z  | neg    |
| 0.76  | 160.84 | 18m/z  | neg    |
| 0.76  | 162.83 | 87m/z  | neg    |
| 0.76  | 164.83 | 54m/z  | neg    |
| 0.76  | 166.83 | 34m/z  | neg    |
| 0.76  | 168.05 | 12n    | pos    |
| 0.76  | 183.96 | 23m/z  | neg    |
| 0.76  | 189.13 | 57m/z  | pos    |
| 0.76  | 193.81 | 44m/z  | neg    |
| 0.76  | 195.81 | 10m/z  | neg    |
| 0.76  | 197.80 | 78m/z  | neg    |
| 0.76  | 199.80 | 48m/z  | neg    |
| 0.76  | 201.80 | 12m/z  | neg    |
| 0.76  | 236.86 | 29m/z  | neg    |
| 0.76  | 265.01 | 84m/z  | neg    |
| 0.76  | 292.82 | 42m/z  | neg    |
0.76_310.79
3693 68m/z  neg
0.76_351.13
3694 79m/z  pos
0.76_400.05
3695 22m/z  pos
0.76_610.18
3696 87m/z  pos
0.77_147.05
3697 18n  neg
0.77_153.05
3698 81m/z  pos
0.77_156.92
3699 42m/z  neg
0.77_170.89
3700 96m/z  neg
0.77_177.84
3701 52m/z  neg
0.77_192.11
3702 64n  pos
0.77_203.79
3703 81m/z  neg
0.77_207.83
3704 59m/z  neg
0.77_212.88
3705 49m/z  neg
0.77_217.93
3706 48n  neg
0.77_224.85
3707 64n  neg
0.77_243.96
3708 41m/z  neg
0.77_250.83
3709 97m/z  neg
0.77_263.02
3710 89m/z  pos
0.77_265.02
3711 73m/z  pos
0.77_271.10
3712 24m/z  neg
0.77_271.97
3713 82m/z  pos
0.77_272.13
3714 52m/z  pos
0.77_272.84
3715 03m/z  neg
0.77_275.89
3716 33n  neg
0.77_282.00
3717 52m/z  pos
| m/z values | Charge | Status |
|------------|--------|--------|
| 286.05     | neg    |        |
| 298.00     |        |        |
| 301.92     | neg    |        |
| 306.21     | pos    |        |
| 308.10     |        |        |
| 313.97     |        |        |
| 322.14     | pos    |        |
| 333.97     |        |        |
| 347.78     | neg    |        |
| 350.02     | neg    |        |
| 353.01     | neg    |        |
| 372.14     | pos    |        |
| 382.98     |        |        |
| 396.91     |        |        |
| 397.10     | pos    |        |
| 409.97     | neg    |        |
| 454.07     |        |        |
| 484.10     |        |        |
| 484.10     |        |        |
| 51.02      |        |        |
| 138.91     | pos    |        |
| 141.86     | neg    |        |
| 144.86     | neg    |        |
| 146.86     | neg    |        |
| 148.86     | neg    |        |
| 159.85     | neg    |        |
| 168.02     | neg    |        |
| 77.00      | neg    |        |
0.78_168.85
3743 72m/z  neg
0.78_172.89
3744 77m/z  neg
0.78_174.08
3745 75m/z  neg
0.78_211.08
3746 99m/z  neg
0.78_228.85
3747 93m/z  neg
0.78_228.85
3748 40m/z  neg
0.78_230.85
3749 95m/z  neg
0.78_262.99
3750 16m/z  neg
0.78_266.00
3751 30m/z  neg
0.78_275.00
3752 77m/z  neg
0.78_287.98
3753 42m/z  neg
0.78_288.81
3754 42m/z  neg
0.78_288.81
3755 32m/z  neg
0.78_290.97
3756 93m/z  neg
0.78_327.13
3757 95m/z  neg
0.78_339.06
3758 99m/z  neg
0.78_367.10
3759 99m/z  neg
0.78_370.13
3760 99m/z  neg
0.78_394.96
3761 67m/z  neg
0.79_146.05
3762 92n   pos
0.79_158.06
3763 95n   pos
0.79_182.08
3764 22n   pos
0.79_194.57
3765 35m/z  pos
0.79_199.09
3766 20m/z  pos
0.79_204.44
3767 39m/z  pos
| m/z   | Charge | Status |
|-------|--------|--------|
| 3768  | 43     | pos    |
| 3769  | 03     | pos    |
| 3770  | 32     | pos    |
| 3771  | 51     | pos    |
| 3772  | 17     | pos    |
| 3773  | 17     | pos    |
| 3774  | 18     | pos    |
| 3775  | 15     | pos    |
| 3776  | 57     | pos    |
| 3777  | 26     | pos    |
| 3778  | 13     | pos    |
| 3779  | 30     | pos    |
| 3780  | 13     | pos    |
| 3781  | 23     | neg    |
| 3782  | 14     | neg    |
| 3783  | 38     | neg    |
| 3784  | 18     | neg    |
| 3785  | 06     | pos    |
| 3786  | 31     | pos    |
| 3787  | 70     | neg    |
| 3788  | 08     | neg    |
| 3789  | 65     | neg    |
| 3790  | 09     | neg    |
| 3791  | 28     | pos    |
| 3792  | 12     | neg    |
3793 22m/z  neg
    0.80_218.37
3794 88m/z  neg
    0.80_267.96
3795 02m/z  neg
    0.80_269.95
3796 93m/z  neg
    0.80_271.95
3797 64m/z  neg
    0.80_283.94
3798 30m/z  neg
    0.80_303.92
3799 17m/z  neg
    0.80_305.93
3800 47m/z  neg
    0.80_307.93
3801 25m/z  neg
    0.80_309.93
3802 08m/z  neg
    0.80_323.22
3803 08m/z  pos
    0.80_323.97
3804 68m/z  neg
    0.80_339.89
3805 67m/z  neg
    0.80_341.90
3806 46m/z  neg
    0.80_343.90
3807 49m/z  neg
    0.80_344.13
3808 43n  pos
    0.80_358.97
3809 84m/z  neg
    0.80_383.97
3810 05m/z  pos
    0.80_427.08
3811 13m/z  pos
    0.80_429.09
3812 24m/z  neg
    0.80_434.18
3813 77m/z  pos
    0.80_442.08
3814 56n  pos
    0.80_445.05
3815 86m/z  neg
    0.80_483.09
3816 76m/z  neg
    0.80_483.19
3817 55n  pos
| m/z | Charge | Value |
|-----|--------|-------|
| 0.80_485.03 | neg | 3818 |
| 0.80_487.02 | neg | 3819 |
| 0.80_491.02 | neg | 3820 |
| 0.80_512.98 | neg | 3821 |
| 0.80_514.03 | neg | 3822 |
| 0.80_516.03 | neg | 3823 |
| 0.80_535.17 | neg | 3824 |
| 0.80_541.05 | neg | 3825 |
| 0.80_549.06 | neg | 3826 |
| 0.80_549.20 | neg | 3827 |
| 0.80_551.18 | neg | 3828 |
| 0.80_580.13 | neg | 3829 |
| 0.80_602.19 | neg | 3830 |
| 0.80_665.11 | neg | 3831 |
| 0.80_709.23 | neg | 3832 |
| 0.80_844.17 | neg | 3833 |
| 0.80_846.17 | neg | 3834 |
| 0.81_116.92 | neg | 3835 |
| 0.81_146.08 | neg | 3836 |
| 0.81_149.04 | neg | 3837 |
| 0.81_240.08 | neg | 3838 |
| 0.81_258.07 | neg | 3839 |
| 0.81_372.99 | neg | 3840 |
| 0.81_377.92 | neg | 3841 |
| 0.81_401.95 | neg | 3842 |
| n  | m/z | charge | status |
|----|-----|--------|--------|
| 97 | 402.08 | neg |        |
| 61 | 425.04 | neg |        |
| 70 | 433.01 | neg |        |
| 84 | 439.05 | neg |        |
| 71 | 452.18 | neg |        |
| 67 | 456.07 | neg |        |
| 57 | 468.13 | neg |        |
| 65 | 469.98 | neg |        |
| 53 | 474.16 | neg |        |
| 65 | 511.99 | neg |        |
| 85 | 518.07 | neg |        |
| 19 | 521.02 | neg |        |
| 97 | 523.02 | neg |        |
| 68 | 540.20 | neg |        |
| 43 | 548.05 | neg |        |
| 45 | 568.94 | neg |        |
| 96 | 570.94 | neg |        |
| 71 | 573.99 | neg |        |
| 07 | 598.16 | neg |        |
| 28 | 600.16 | neg |        |
| 44 | 656.11 | neg |        |
| 99 | 681.15 | neg |        |
| 48 | 695.15 | neg |        |
| 10 | 710.10 | neg |        |
| 72 |       | neg |        |
| m/z   | Charge | Status |
|-------|--------|--------|
| 0.81_717.13 | 07m/z  | neg    |
| 0.81_739.11  |        |        |
| 0.81_746.08  |        |        |
| 0.81_768.06  |        | neg    |
| 0.81_781.19  | 64m/z  | neg    |
| 0.81_781.19  |        | neg    |
| 0.81_788.24  |        | neg    |
| 0.81_839.14  |        | neg    |
| 0.81_841.14  |        | neg    |
| 0.81_971.26  |        | neg    |
| 0.82_234.09  | 66m/z  | pos    |
| 0.82_283.59  |        | pos    |
| 0.82_314.07  | 04m/z  | pos    |
| 0.82_498.13  | 57n    | pos    |
| 0.82_527.08  | 20n    | pos    |
| 0.82_601.14  | 48n    | pos    |
| 0.82_606.16  | 47m/z  | pos    |
| 0.82_628.14  | 80n    | pos    |
| 0.82_658.20  | 61n    | pos    |
| 0.82_659.07  | 82n    | pos    |
| 0.82_680.19  | 75n    | pos    |
| 0.82_682.16  | 02n    | pos    |
| 0.82_688.26  | 81n    | pos    |
| 0.82_689.13  | 69n    | pos    |
| 0.82_734.11  | 88n    | pos    |
| 0.82_748.11  | 25m/z  | pos    |
| 0.82_748.11  |        |        |
| 0.82_49m/z   |        | pos    |
| m/z | Charge | Status |Retention Time |
|-----|--------|--------|---------------|
| 53  | 0.82   | pos    | 750.08        |
| 10n | 0.82   | pos    | 831.21        |
| 25n | 0.82   | pos    | 843.14        |
| 68n | 0.82   | pos    | 990.12        |
| 94  | 0.83   | pos    | 227.12        |
| 25n | 0.83   | pos    | 238.98        |
| 57n | 0.83   | neg    | 240.05        |
| 65n | 0.83   | pos    | 302.02        |
| 22n | 0.83   | pos    | 307.11        |
| 16n | 0.83   | neg    | 308.12        |
| 6n  | 0.83   | pos    | 315.08        |
| 21n | 0.83   | pos    | 316.05        |
| 33n | 0.83   | pos    | 338.09        |
| 48n | 0.83   | pos    | 338.59        |
| 62n | 0.83   | pos    | 341.10        |
| 67n | 0.83   | neg    | 348.01        |
| 82n | 0.83   | pos    | 406.11        |
| 86n | 0.83   | neg    | 412.03        |
| 53n | 0.83   | neg    | 433.11        |
| 57n | 0.83   | neg    | 463.94        |
| 66n | 0.83   | neg    | 513.12        |
| 88n | 0.83   | pos    | 631.13        |
| 12n | 0.83   | pos    | 653.07        |
| 45n | 0.83   | neg    | 673.16        |
| 78n | 0.83   | neg    |               |
0.83_675.17
3918 99m/z    pos
0.83_684.05
3919 07m/z    pos
0.83_688.12
3920 52m/z    neg
0.83_725.11
3921 00m/z    neg
0.83_744.27
3922 90m/z    neg
0.83_751.16
3923 46m/z    pos
0.83_756.04
3924 10m/z    neg
0.83_766.26
3925 05m/z    neg
0.83_797.18
3926 21m/z    neg
0.83_808.08
3927 34m/z    neg
0.83_923.22
3928 68m/z    pos
0.83_969.18
3929 01n      pos
0.83_974.16
3930 13m/z    pos
0.83_982.23
3931 03m/z    pos
0.84_159.57
3932 54m/z    pos
0.84_298.00
3933 75m/z    neg
0.84_365.08
3934 25m/z    neg
0.84_608.14
3935 66n      pos
0.84_624.13
3936 24m/z    neg
0.84_624.16
3937 71n      pos
0.84_637.23
3938 76m/z    pos
0.84_638.10
3939 60m/z    pos
0.84_651.09
3940 48m/z    neg
0.84_653.12
3941 44n      pos
0.84_658.06
3942 70m/z    neg
| M/z | Charge | Type |
|-----|--------|------|
| 59  | neg    |      |
| 66  | neg    |      |
| 98  | neg    |      |
| 80  | neg    |      |
| 70  | neg    |      |
| 68  | pos    |      |
| 80  | neg    |      |
| 70  | pos    |      |
| 76  | neg    |      |
| 43  | neg    |      |
| 97  | neg    |      |
| 86  | neg    |      |
| 94  | neg    |      |
| 50  | pos    |      |
| 86  | neg    |      |
| 34  | neg    |      |
| 37  | neg    |      |
| 60  | neg    |      |
| 77  | neg    |      |
| 80  | neg    |      |
| 76  | neg    |      |
| 50  | pos    |      |
| 915 | pos    |      |
| 85  | neg    |      |
0.85_636.08
3968 52m/z neg
0.85_674.03
3969 97m/z neg
0.85_710.97
3970 90m/z neg
0.85_726.95
3971 24m/z neg
0.85_959.16
3972 11m/z neg
0.86_901.25
3973 04m/z pos
0.86_983.11
3974 75m/z pos
0.87_145.09
3975 66m/z neg
0.87_157.09
3976 73m/z neg
0.87_226.97
3977 53m/z neg
0.87_227.98
3978 29m/z neg
0.87_246.33
3979 22m/z neg
0.87_272.23
3980 08m/z neg
0.87_291.19
3981 30n neg
0.87_291.93
3982 73m/z neg
0.87_292.49
3983 21m/z neg
0.87_300.00
3984 42m/z neg
0.87_345.00
3985 19n neg
0.87_352.99
3986 76m/z neg
0.87_354.99
3987 27m/z neg
0.87_356.99
3988 13m/z neg
0.87_414.96
3989 22m/z neg
0.87_415.96
3990 14m/z neg
0.87_420.96
3991 33m/z neg
0.87_584.20
3992 29n pos
0.87  603.27  
3993  42m/z   neg
     0.87  656.06
3994  97m/z   neg
     0.87  667.06
3995  95m/z   neg
     0.87  669.05
3996  75m/z   neg
     0.87  671.07
3997  12m/z   neg
     0.87  687.00
3998  48m/z   neg
     0.87  699.99
3999  84m/z   neg
     0.87  708.98
4000  77m/z   neg
     0.88  292.24
4001  38m/z   neg
     0.88  292.59
4002  73m/z   neg
     0.88  342.93
4003  17m/z   neg
     0.88  348.00
4004  22m/z   neg
     0.88  418.96
4005  11m/z   neg
     0.88  634.08
4006  95m/z   neg
     0.89  348.99
4007  75m/z   neg
     0.89  850.18
4008  02m/z   neg
     0.89  966.12
4009  89m/z   neg
     0.91  339.99
4010  90m/z   neg
     0.91  505.17
4011  65m/z   neg
     0.91  551.18
4012  83m/z   neg
     0.91  603.14
4013  52m/z   neg
     0.91  799.34
4014  76m/z   pos
     0.91  819.25
4015  03m/z   neg
     0.91  913.21
4016  92m/z   neg
     0.91  919.22
4017  78m/z   neg
| m/z   | Retention Time | Intensity | Charge |
|-------|----------------|-----------|--------|
| 87.07 | 0.91           | 935.19    | neg    |
| 369.00| 0.92           | neg       |
| 396.95| 0.92           | neg       |
| 457.18| 0.92           | pos       |
| 506.18| 0.92           | pos       |
| 146.02| 0.93           | pos       |
| 168.06| 0.93           | pos       |
| 192.03| 0.93           | pos       |
| 207.05| 0.93           | pos       |
| 319.02| 0.93           | pos       |
| 328.13| 0.93           | pos       |
| 329.03| 0.93           | neg       |
| 332.05| 0.93           | neg       |
| 345.00| 0.93           | pos       |
| 358.00| 0.93           | pos       |
| 482.10| 0.93           | neg       |
| 504.08| 0.93           | neg       |
| 526.06| 0.93           | neg       |
| 541.15| 0.93           | neg       |
| 543.14| 0.93           | neg       |
| 568.17| 0.93           | neg       |
| 668.23| 0.93           | neg       |
| 703.20| 0.93           | neg       |
| 192.02| 0.94           | neg       |
| 192.02| 0.94           | neg       |
| m/z   | Retention Time | Charge | Mass-to-Charge Ratio | Ionization Mode |
|-------|---------------|--------|----------------------|-----------------|
| 31    | 0.94          | neg    | 363.10               |                 |
| 84    | 0.94          | neg    | 431.13               |                 |
| 90    | 0.95          | neg    | 343.00               |                 |
| 87    | 0.96          | pos    | 141.06               |                 |
| 59    | 0.96          | neg    | 154.99               |                 |
| 61    | 0.96          | neg    | 185.84               |                 |
| 46    | 0.96          | neg    | 191.01               |                 |
| 79    | 0.96          | pos    | 242.02               |                 |
| 50    | 0.96          | neg    | 342.01               |                 |
| 49    | 0.96          | neg    | 366.98               |                 |
| 50    | 0.96          | neg    | 393.00               |                 |
| 49    | 0.96          | neg    | 556.99               |                 |
| 97    | 0.96          | neg    | 600.06               |                 |
| 03    | 0.96          | neg    | 659.07               |                 |
| 89    | 0.96          | pos    | 677.05               |                 |
| 64    | 0.96          | pos    | 690.00               |                 |
| 82    | 0.96          | pos    | 702.02               |                 |
| 85    | 0.97          | neg    | 129.05               |                 |
| 61    | 0.97          | pos    | 144.96               |                 |
| 51    | 0.97          | neg    | 158.00               |                 |
| 46    | 0.97          | pos    | 277.04               |                 |
| 07    | 0.97          | neg    | 285.98               |                 |
| 83    | 0.97          | neg    | 318.05               |                 |
| 31    | 0.97          | neg    | 324.00               |                 |
| 50    | 0.97          | pos    | 366.98               |                 |
0.97_367.00
4068 24n  pos  0.97_376.05
4069 93m/z  neg  0.97_385.97
4070 43m/z  pos  0.97_398.04
4071 01m/z  neg  0.97_401.95
4072 24m/z  neg  0.97_413.00
4073 08m/z  pos  0.97_414.01
4074 12m/z  neg  0.97_454.99
4075 76n  neg  0.97_463.94
4076 35m/z  neg  0.97_479.91
4077 33m/z  neg  0.98_183.84
4078 76m/z  neg  0.98_218.81
4079 65m/z  neg  0.98_220.81
4080 44m/z  neg  0.98_241.99
4081 83m/z  neg  0.98_245.03
4082 48m/z  neg  0.98_373.00
4083 35m/z  neg  0.98_451.96
4084 72m/z  neg  0.98_486.93
4085 11m/z  neg  0.99_448.00
4086 21n  pos  0.99_530.17
4087 92m/z  pos  1.00_101.05
4088 90m/z  pos  1.00_146.96
4089 41m/z  neg  1.00_157.08
4090 65m/z  pos  1.00_186.85
4091 89m/z  neg  1.00_267.03
4092 84m/z  pos
| 1.00  | 411.98 |
|-------|--------|
| 1.00  | 422.97 |
| 1.00  | 442.97 |
| 1.00  | 450.99 |
| 1.00  | 473.95 |
| 1.00  | 513.94 |
| 1.00  | 465.96 |
| 1.01  | 489.92 |
| 1.03  | 249.84 |
| 1.03  | 262.99 |
| 1.03  | 269.95 |
| 1.03  | 518.13 |
| 1.04  | 166.83 |
| 1.04  | 183.97 |
| 1.04  | 233.95 |
| 1.04  | 475.99 |
| 1.05  | 193.81 |
| 1.06  | 193.81 |
| 1.06  | 460.92 |
| 1.07  | 145.12 |
| 1.07  | 334.04 |
| 1.07  | 112.95 |
| 1.08  | 150.98 |
| 1.08  | 168.94 |
| 1.08  | 411.98 |
| 1.09  | 242.97 |
| 1.09  | 442.97 |
| 1.09  | 540.99 |
| 1.09  | 465.96 |
| 1.10  | 489.92 |
| 1.10  | 249.84 |
| 1.10  | 262.99 |
| 1.10  | 269.95 |
| 1.10  | 518.13 |
| 1.10  | 166.83 |
| 1.10  | 183.97 |
| 1.10  | 233.95 |
| 1.10  | 475.99 |
| 1.11  | 193.81 |
| 1.11  | 460.92 |
| 1.12  | 145.12 |
| 1.12  | 334.04 |
| 1.12  | 112.95 |
| 1.13  | 150.98 |
| 1.13  | 168.94 |
| 1.13  | 411.98 |
| 1.14  | 242.97 |
| 1.14  | 442.97 |
| 1.14  | 540.99 |
| 1.14  | 465.96 |
| 1.15  | 489.92 |
| 1.15  | 249.84 |
| 1.15  | 262.99 |
| 1.15  | 269.95 |
| 1.15  | 518.13 |
| 1.15  | 166.83 |
| 1.15  | 183.97 |
| 1.15  | 233.95 |
| 1.15  | 475.99 |
| 1.16  | 193.81 |
| 1.16  | 460.92 |
| 1.16  | 145.12 |
| 1.16  | 334.04 |
| 1.16  | 112.95 |
| 1.17  | 150.98 |
| 1.17  | 168.94 |
| 1.17  | 411.98 |

| m/z   | 1.00 | neg |
|-------|------|-----|
| 12     | 1.00 | neg |
| 69     | 1.00 | neg |
| 88     | 1.00 | pos |
| 83     | 1.00 | pos |
| 16     | 1.00 | neg |
| 75     | 1.00 | neg |
| 89     | 1.01 | neg |
| 49     | 1.01 | pos |
| 83     | 1.01 | pos |
| 47     | 1.03 | neg |
| 66     | 1.03 | neg |
| 77     | 1.03 | neg |
| 87     | 1.03 | neg |
| 56     | 1.04 | pos |
| 29     | 1.04 | neg |
| 01     | 1.04 | pos |
| 61     | 1.04 | neg |
| 55     | 1.06 | pos |
| 45     | 1.06 | neg |
| 03     | 1.07 | neg |
| 16     | 1.07 | pos |
| 36     | 1.08 | pos |
| 63     | 1.08 | pos |
| 21     | 1.08 | neg |
| 79     | 1.08 | neg |
| Mass/Charge | Retention Time | Charge State |
|-------------|----------------|--------------|
| 32/1.08     | 176.97         | neg          |
| 31/1.08     | 191.94         | neg          |
| 57/1.08     | 205.83         | neg          |
| 87/1.08     | 207.83         | neg          |
| 59/1.08     | 308.11         | neg          |
| 70/1.08     | 358.00         | pos          |
| 95/1.08     | 89.989         | neg          |
| 3n          | 164.92         | neg          |
| 79/1.09     | 185.87         | neg          |
| 56/1.09     | 209.83         | neg          |
| 29/1.09     | 217.86         | neg          |
| 54/1.09     | 235.92         | neg          |
| 53/1.10     | 360.02         | pos          |
| 76/1.10     | 372.06         | pos          |
| 61/1.10     | 400.94         | pos          |
| 40/1.11     | 102.01         | pos          |
| 44/1.11     | 130.96         | pos          |
| 55/1.11     | 206.97         | neg          |
| 15/1.11     | 225.92         | neg          |
| 54/1.11     | 243.23         | neg          |
| 49/1.12     | 146.02         | pos          |
| 90/1.12     | 192.03         | pos          |
| 54/1.12     | 195.91         | pos          |
| 53/1.12     | 211.99         | pos          |
| 91/1.12     | 176.97         | neg          |
1.12_273.94
4143 76m/z  neg
1.12_308.28
4144 24m/z  pos
1.12_786.25
4145 86m/z  pos
1.13_259.81
4146 53m/z  neg
1.13_361.08
4147 64m/z  neg
1.15_124.99
4148 12m/z  pos
1.15_156.97
4149 67m/z  pos
1.15_166.99
4150 59m/z  neg
1.15_252.03
4151 82m/z  pos
1.16_183.97
4152 18m/z  pos
1.17_184.05
4153 86m/z  neg
1.17_187.86
4154 13m/z  neg
1.17_198.01
4155 35n   neg
1.17_217.00
4156 31n   neg
1.17_236.00
4157 31m/z  neg
1.17_240.93
4158 55m/z  neg
1.17_242.93
4159 41m/z  neg
1.17_246.02
4160 87m/z  neg
1.17_249.03
4161 04m/z  neg
1.17_255.13
4162 21m/z  neg
1.17_260.00
4163 14m/z  neg
1.17_265.90
4164 95m/z  neg
1.17_268.96
4165 24m/z  neg
1.17_275.96
4166 71m/z  neg
1.17_281.98
4167 44m/z  neg
1.17_294.97
4168 38m/z   neg
1.17_299.88
4169 98m/z   neg
1.17_316.95
4170 66m/z   neg
1.17_330.04
4171 85m/z   neg
1.17_335.07
4172 65n    neg
1.17_366.10
4173 93m/z   neg
1.17_373.03
4174 69m/z   neg
1.17_389.01
4175 30m/z   neg
1.18_158.00
4176 14m/z   pos
1.19_250.11
4177 84n    pos
1.19_258.03
4178 13m/z   pos
1.19_263.91
4179 23m/z   neg
1.19_275.01
4180 19m/z   pos
1.19_301.88
4181 69m/z   neg
1.19_310.97
4182 81m/z   pos
1.19_331.12
4183 09n    pos
1.19_332.06
4184 14m/z   neg
1.19_334.18
4185 81m/z   pos
1.19_444.08
4186 73m/z   pos
1.19_459.06
4187 59m/z   pos
1.19_488.39
4188 73m/z   pos
1.19_646.17
4189 78m/z   pos
1.19_710.24
4190 08m/z   pos
1.20_101.02
4191 34m/z   neg
1.20_350.05
4192 79m/z   neg
4218 43 m/z neg
   1.21_395.96
4219 10 n pos
   1.21_416.01
4220 41 m/z neg
   1.21_441.11
4221 42 m/z pos
   1.21_448.06
4222 37 n pos
   1.21_452.13
4223 68 n pos
   1.21_460.03
4224 44 m/z neg
   1.21_468.12
4225 40 m/z pos
   1.21_477.08
4226 53 n neg
   1.21_482.10
4227 01 m/z neg
   1.21_491.07
4228 71 n neg
   1.21_514.08
4229 29 m/z neg
   1.21_515.13
4230 34 n pos
   1.21_524.14
4231 29 m/z pos
   1.21_529.17
4232 56 m/z pos
   1.21_543.02
4233 38 n pos
   1.21_550.03
4234 66 m/z pos
   1.21_552.04
4235 05 m/z neg
   1.21_555.98
4236 94 m/z neg
   1.21_582.00
4237 72 m/z pos
   1.21_590.00
4238 27 m/z neg
   1.21_597.18
4239 46 m/z pos
   1.21_672.11
4240 71 n pos
   1.21_674.70
4241 46 m/z pos
   1.21_678.21
4242 33 m/z pos
| n  | 1.21_682.07 | pos |
|----|-------------|-----|
| n  | 1.21_682.11 |     |
| n  | 1.21_693.09 |     |
| n  | 1.21_704.09 |     |
| n  | 1.21_770.21 |     |
| n  | 1.21_830.29 |     |
| n  | 1.21_919.31 |     |
| n  | 1.21_991.33 |     |
| n  | 1.21_993.35 |     |
| n  | 1.21_997.31 |     |
| n  | 1.22_110.07 |     |
| n  | 1.22_110.97 |     |
| n  | 1.22_115.95 |     |
| n  | 1.22_178.03 |     |
| n  | 1.22_204.02 |     |
| n  | 1.22_282.14 |     |
| n  | 1.22_336.12 |     |
| n  | 1.22_347.06 |     |
| n  | 1.22_358.02 |     |
| n  | 1.22_360.05 |     |
| n  | 1.22_379.01 |     |
| n  | 1.22_457.01 |     |
| n  | 1.22_478.00 |     |
| n  | 1.22_531.04 |     |
| n  | 1.22_553.05 |     |
| m/z   | Retention Time | Charge | Sign |
|-------|----------------|--------|------|
| 0.559 | 1.22           | pos    |      |
| 0.841 | 1.22           |        |      |
| 1.14  | 1.23           |        |      |
| 1.14  | 1.23           |        |      |
| 0.841 | 1.23           |        |      |
| 1.155 | 1.23           |        |      |
| 1.166 | 1.23           |        |      |
| 0.57  | 1.23           |        |      |
| 0.52  | 1.23           |        |      |
| 0.8  | 1.23           |        |      |
| 0.77  | 1.23           |        |      |
| 1.85  | 1.23           |        |      |
| 1.85  | 1.23           |        |      |
| 1.8  | 1.23           |        |      |
| 0.98  | 1.23           |        |      |
| 1.67  | 1.23           |        |      |
| 1.85  | 1.23           |        |      |
| 1.85  | 1.23           |        |      |
| 1.8  | 1.23           |        |      |
| 1.8  | 1.23           |        |      |
| 1.8  | 1.23           |        |      |
| 1.8  | 1.23           |        |      |
| 1.8  | 1.23           |        |      |
| 1.8  | 1.23           |        |      |
| 1.8  | 1.23           |        |      |
| 1.8  | 1.23           |        |      |

...
1.23_393.01  
4293 96m/z    neg  
      1.23_393.98
4294 71m/z    pos  
      1.23_399.99
4295 53m/z    neg  
      1.23_404.04
4296 75n      neg  
      1.23_421.97
4297 67m/z    neg  
      1.23_434.00
4298 18m/z    neg  
      1.23_435.98
4299 04m/z    pos  
      1.23_454.01
4300 62m/z    neg  
      1.23_476.98
4301 77m/z    neg  
      1.23_477.99
4302 39m/z    neg  
      1.23_488.06
4303 05n      neg  
      1.23_499.97
4304 33m/z    neg  
      1.23_525.05
4305 43m/z    neg  
      1.23_534.00
4306 33m/z    neg  
      1.23_541.02
4307 41m/z    neg  
      1.23_556.99
4308 65m/z    neg  
      1.23_563.01
4309 29m/z    neg  
      1.23_566.05
4310 79n      neg  
      1.23_571.01
4311 45m/z    neg  
      1.23_668.00
4312 21m/z    neg  
      1.23_720.06
4313 17m/z    neg  
      1.23_724.01
4314 70m/z    neg  
      1.23_737.04
4315 75m/z    neg  
      1.24_171.94
4316 58m/z    neg  
      1.24_411.96
4317 04m/z    neg
1.24_430.05
4318 98m/z  neg
1.24_516.06
4319 33n  neg
1.25_133.00
4320 90m/z  pos
1.25_212.00
4321 98m/z  pos
1.25_216.99
4322 59m/z  pos
1.25_217.00
4323 45m/z  neg
1.25_234.99
4324 91m/z  pos
1.25_237.00
4325 03m/z  pos
1.25_305.03
4326 60m/z  pos
1.25_334.98
4327 10m/z  pos
1.25_396.99
4328 65m/z  neg
1.25_419.04
4329 29m/z  neg
1.25_437.97
4330 62m/z  pos
1.25_450.98
4331 82m/z  pos
1.25_456.00
4332 43m/z  neg
1.25_615.04
4333 13m/z  pos
1.26_252.97
4334 49m/z  neg
1.26_285.98
4335 69m/z  pos
1.26_292.20
4336 16m/z  pos
1.26_310.96
4337 81m/z  neg
1.26_319.00
4338 21m/z  pos
1.26_345.96
4339 46m/z  neg
1.26_348.99
4340 66m/z  pos
1.26_418.98
4341 54m/z  pos
1.26_444.96
4342 37m/z  neg
| m/z | Charge/State |
|-----|--------------|
| 49.98 | pos          |
| 61.03 | pos          |
| 162.99 | pos        |
| 198.98 | pos        |
| 243.96 | pos        |
| 287.98 | pos        |
| 130.02 | pos        |
| 190.43 | neg        |
| 199.93 | neg        |
| 263.01 | neg        |
| 130.00 | neg        |
| 275.00 | neg        |
| 279.90 | neg        |
| 315.89 | neg        |
| 318.89 | neg        |
| 325.01 | neg        |
| 326.98 | neg        |
| 333.96 | neg        |
| 355.94 | neg        |
| 360.01 | neg        |
| 403.97 | neg        |
| 407.00 | neg        |
| 420.99 | neg        |
| 428.97 | neg        |
| 435.95 | neg        |
| 435.98 | neg        |
1.28 442.97
4368 85m/z  neg  1.28 450.02
4369 46n  neg  1.28 450.96
4370 87m/z  neg  1.28 457.93
4371 88m/z  neg  1.28 480.92
4372 81m/z  neg  1.28 524.97
4373 86m/z  neg  1.28 613.01
4374 85m/z  neg  1.29 104.00
4375 88m/z  pos  1.29 270.95
4376 86m/z  neg  1.29 277.97
4377 29m/z  neg  1.29 291.95
4378 38m/z  pos  1.29 291.96
4379 16m/z  neg  1.29 297.97
4380 79m/z  neg  1.29 313.95
4381 07m/z  neg  1.29 460.96
4382 82m/z  pos  1.30 136.04
4383 02n  pos  1.30 144.95
4384 85m/z  neg  1.30 181.99
4385 21m/z  pos  1.30 205.93
4386 91m/z  neg  1.30 385.97
4387 31m/z  pos  1.30 389.99
4388 32m/z  pos  1.32 133.00
4389 84m/z  neg  1.32 169.89
4390 86m/z  neg  1.32 176.99
4391 72m/z  neg  1.32 193.98
4392 80m/z  neg
1.32_218.98
4393 24m/z  neg
1.33_213.88
4394 82m/z  neg
1.33_259.81
4395 54m/z  neg
1.35_187.86
4396 10m/z  neg
1.35_235.97
4397 10m/z  neg
1.37_102.01
4398 35m/z  pos
1.42_243.89
4399 92m/z  neg
1.42_256.95
4400 42m/z  neg
1.42_376.01
4401 51m/z  pos
1.43_246.98
4402 04n   pos
1.43_312.00
4403 69n   pos
1.43_475.05
4404 39m/z  pos
1.44_200.97
4405 44m/z  pos
1.44_214.00
4406 35m/z  pos
1.44_227.98
4407 48m/z  pos
1.44_348.99
4408 42m/z  pos
1.45_156.97
4409 55m/z  pos
1.45_230.99
4410 10m/z  pos
1.46_139.00
4411 27m/z  pos
1.46_242.02
4412 04m/z  neg
1.46_288.87
4413 60m/z  neg
1.46_290.87
4414 28m/z  neg
1.47_110.00
4415 88m/z  pos
1.47_128.03
4416 42m/z  neg
1.47_196.02
4417 17m/z  neg
| Mass 1.47 | Value | Charge | Status |
|----------|-------|--------|--------|
| 202.98   | 74n   | neg    |        |
| 212.99   |       |        |        |
| 166.00   | 43n   | neg    |        |
| 227.95   |       |        |        |
| 217.93   | 89m/z | neg    |        |
| 217.93   |       |        |        |
| 227.95   | 90m/z | neg    |        |
| 252.89   |       |        |        |
| 263.02   |       |        |        |
| 264.95   |       |        |        |
| 274.98   |       |        |        |
| 279.05   |       |        |        |
| 292.87   |       |        |        |
| 296.03   |       |        |        |
| 303.00   |       |        |        |
| 310.99   |       |        |        |
| 331.00   |       |        |        |
| 339.99   |       |        |        |
| 358.01   |       |        |        |
| 424.06   |       |        |        |
| 424.06   |       |        |        |
| 424.06   |       |        |        |
| 174.99   |       |        |        |
| 174.99   |       |        |        |
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| 174.99   |       |        |        |
| 174.99   |       |        |        |
| 174.99   |       |        |        |
1.77_105.93
4443 63m/z    pos
  1.78_163.98
4444 57m/z    pos
  1.79_257.25
4445 00m/z    pos
  1.86_195.91
4446 38m/z    pos
  1.91_144.95
4447 96m/z    pos
  1.92_404.01
4448 58m/z    neg
  1.95_204.99
4449 27m/z    neg
  1.95_243.89
4450 67m/z    neg
  1.96_172.95
4451 42m/z    neg
  1.96_201.99
4452 47m/z    neg
  1.96_217.96
4453 10m/z    neg
  1.96_232.98
4454 81m/z    neg
  1.96_233.93
4455 70m/z    neg
  1.96_241.88
4456 67m/z    neg
  1.96_277.86
4457 03m/z    neg
  1.96_281.85
4458 49m/z    neg
  1.96_360.02
4459 61m/z    pos
  1.98_135.90
4460 66m/z    pos
  1.98_234.99
4461 34m/z    pos
  1.98_244.07
4462 09n    pos
  1.98_271.97
4463 77m/z    pos
  1.98_273.97
4464 48m/z    pos
  1.98_567.18
4465 01n    pos
  10.01_182.9
4466 621m/z    pos
  10.01_280.2
4467 605m/z    pos
| Time (s) | m/z | Charge | Intensity |
|---------|-----|--------|-----------|
| 10.01   | 356.0 | neg    | 10.01     |
| 10.01   | 364.9 | neg    | 10.01     |
| 10.03   | 435.3 | pos    | 10.03     |
| 10.03   | 426.3 | neg    | 10.03     |
| 10.04   | 774.3 | pos    | 10.04     |
| 10.04   | 234.3 | pos    | 10.04     |
| 10.04   | 512.3 | neg    | 10.04     |
| 10.04   | 564.3 | pos    | 10.04     |
| 10.04   | 979.3 | pos    | 10.04     |
| 10.04   | 484.3 | pos    | 10.04     |
| 10.04   | 516.3 | pos    | 10.04     |
| 10.04   | 295.3 | neg    | 10.04     |
| 10.04   | 412.3 | neg    | 10.04     |
| 10.04   | 181.3 | pos    | 10.05     |
| 10.04   | 375.2 | neg    | 10.05     |
| 10.05   | 375.2 | neg    | 10.05     |
| 10.05   | 407.2 | neg    | 10.05     |
| 10.05   | 407.2 | neg    | 10.05     |
| 10.05   | 412.3 | neg    | 10.05     |
| 10.05   | 430.2 | pos    | 10.05     |
| 10.05   | 484.3 | pos    | 10.05     |
| 10.05   | 516.3 | pos    | 10.05     |
| 10.05   | 516.3 | pos    | 10.05     |
| 10.05   | 582.2 | pos    | 10.05     |
| 10.08   | 484.3 | pos    | 10.08     |
| 10.08   | 416.2 | pos    | 10.08     |
| 10.09   | 181.1 | pos    | 10.09     |
| 10.09   | 191.1 | pos    | 10.09     |
| 10.09   | 443.2 | pos    | 10.09     |
| 10.11   | 194.1 | pos    | 10.11     |
| 10.11   | 378.0 | pos    | 10.11     |
| 10.11   | 418.9 | pos    | 10.11     |
| 10.11   | 414.3 | neg    | 10.11     |
| 10.11   | 194.1 | pos    | 10.11     |
| 10.11   | 378.0 | pos    | 10.11     |
| 10.11   | 414.3 | neg    | 10.11     |
| m/z   | retention time |
|-------|----------------|
| 4493  | 10.11_445.2    |
| 138m/z| pos            |
| 4494  | 10.11_468.3    |
| 084n  | pos            |
| 4495  | 10.11_490.2    |
| 942m/z| pos            |
| 4496  | 10.11_529.2    |
| 10.12 | 151.1          |
| 130m/z| pos            |
| 4497  | 10.12_180.1    |
| 499m/z| pos            |
| 4498  | 10.12_211.1    |
| 350m/z| pos            |
| 4500  | 10.12_234.1    |
| 354m/z| pos            |
| 4501  | 10.12_238.1    |
| 141m/z| pos            |
| 4502  | 10.12_238.3    |
| 605m/z| pos            |
| 4503  | 10.12_325.9    |
| 977n  | neg            |
| 4504  | 10.12_440.9    |
| 955m/z| neg            |
| 4505  | 10.12_505.0    |
| 032m/z| neg            |
| 4506  | 10.12_542.0    |
| 168n  | neg            |
| 4507  | 10.13_159.1    |
| 395m/z| pos            |
| 4508  | 10.13_271.0    |
| 876n  | pos            |
| 4509  | 10.13_418.2    |
| 527m/z| pos            |
| 4510  | 10.13_430.8    |
| 883m/z| pos            |
| 4511  | 10.13_458.2    |
| 989m/z| pos            |
| 4512  | 10.14_304.9    |
| 863m/z| neg            |
| 4513  | 10.14_392.9    |
| 878m/z| neg            |
| 4514  | 10.14_416.0    |
| 020n  | neg            |
| 4515  | 10.14_556.0    |
| 211n  | neg            |
| 4516  | 10.15_313.1    |
| 814m/z| pos            |
|     |     |     |
|-----|-----|-----|
| 4518 | 10.15_391.2 | pos |
| 4519 | 10.15_529.2 | pos |
| 4520 | 10.16_155.1 | pos |
| 4521 | 10.16_244.2 | pos |
| 4522 | 10.16_455.3 | pos |
| 4523 | 10.17_203.1 | pos |
| 4524 | 10.17_343.1 | pos |
| 4525 | 10.18_441.2 | neg |
| 4526 | 10.18_446.2 | neg |
| 4527 | 10.19_246.2 | neg |
| 4528 | 10.19_330.2 | pos |
| 4529 | 10.19_379.2 | pos |
| 4530 | 10.19_477.2 | pos |
| 4531 | 10.20_313.2 | pos |
| 4532 | 10.20_458.9 | pos |
| 4533 | 10.21_294.1 | neg |
| 4534 | 10.22_197.1 | neg |
| 4535 | 10.22_209.1 | pos |
| 4536 | 10.22_227.5 | pos |
| 4537 | 10.22_410.1 | pos |
| 4538 | 10.22_414.2 | pos |
| 4539 | 10.22_440.3 | pos |
| 4540 | 10.22_507.1 | pos |
| 4541 | 10.22_623.3 | pos |
| 4542 | 10.22_644.3 | pos |
| Time  | Mass/Charge | Signal  |
|-------|-------------|---------|
| 10.23 | 316.9       | neg     |
| 10.23 | 413.9       |         |
| 10.23 | 426.2       |         |
| 10.23 | 428.2       |         |
| 10.23 | 455.2       |         |
| 10.23 | 476.1       |         |
| 10.24 | 483.2       |         |
| 10.24 | 488.3       |         |
| 10.24 | 502.2       |         |
| 10.24 | 519.2       |         |
| 10.25 | 476.0       |         |
| 10.25 | 502.2       |         |
| 10.25 | 529.2       |         |
| 10.27 | 214.1       |         |
| 10.27 | 245.1       |         |
| 10.27 | 253.6       |         |
| 10.27 | 267.2       |         |
| 10.27 | 466.8       |         |
| 10.27 | 551.2       |         |
| 10.28 | 288.2       |         |
| 10.30 | 165.1       |         |
| 10.30 | 251.1       |         |
| 10.30 | 284.1       |         |
10.31_115.9
4568 624m/z  pos
10.31_540.2
4569 632m/z  neg
10.31_561.2
4570 180n  pos
10.32_209.1
4571 551m/z  pos
10.32_307.2
4572 436m/z  pos
10.32_401.3
4573 073m/z  pos
10.32_462.3
4574 260m/z  pos
10.34_320.9
4575 808m/z  neg
10.34_348.9
4576 914m/z  pos
10.34_353.9
4577 958n  neg
10.34_404.0
4578 077n  neg
10.34_431.0
4579 846m/z  pos
10.34_440.0
4580 129n  neg
10.34_474.2
4581 681m/z  neg
10.35_182.9
4582 625m/z  pos
10.35_321.2
4583 247m/z  pos
10.35_360.0
4584 075n  neg
10.35_446.0
4585 020n  neg
10.35_480.3
4586 123m/z  pos
10.35_490.0
4587 032n  neg
10.36_223.1
4588 723m/z  pos
10.36_381.2
4589 690n  pos
10.36_479.2
4590 183m/z  pos
10.36_486.3
4591 857m/z  pos
10.37_282.9
4592 825m/z  neg
| m/z     | Time  | Charge | Status |
|---------|-------|--------|--------|
| 869     | 10.38 | +      |
| 959     | 10.38 | +      |
| 312     | 10.39 | +      |
| 180     | 10.39 | +      |
| 089     | 10.39 | -      |
| 645     | 10.39 | +      |
| 127     | 10.39 | -      |
| 566     | 10.39 | +      |
| 945     | 10.39 | +      |
| 147     | 10.40 | -      |
| 055     | 10.41 | -      |
| 265     | 10.41 | +      |
| 212     | 10.41 | +      |
| 031     | 10.41 | +      |
| 739     | 10.41 | +      |
| 177     | 10.41 | +      |
| 274     | 10.41 | -      |
| 164     | 10.41 | -      |
| 217     | 10.41 | +      |
| 259     | 10.42 | +      |
| 151     | 10.42 | +      |
| 175     | 10.42 | +      |
| 425     | 10.42 | +      |
| 755     | 10.42 | +      |
| 326     | 10.42 | +      |
| Time  | Charge | m/z  | Status |
|-------|--------|------|--------|
| 10.43 | 208.1  | pos  |        |
| 10.43 | 253.2  | pos  |        |
| 205m/z|        | pos  |        |
| 10.43 | 372.3  | pos  |        |
| 195m/z|        | pos  |        |
| 10.43 | 440.3  | pos  |        |
| 257m/z|        | pos  |        |
| 10.43 | 490.3  | pos  |        |
| 614m/z|        | pos  |        |
| 10.44 | 484.0  | neg  |        |
| 156n  |        | neg  |        |
| 10.44 | 504.0  |     |        |
| 131n  |        | neg  |        |
| 10.44 | 508.9  | neg  |        |
| 951m/z|        | neg  |        |
| 10.44 | 592.0  |     |        |
| 177n  |        | neg  |        |
| 10.45 | 260.2  |     |        |
| 154n  |        | pos  |        |
| 10.45 | 318.2  | pos  |        |
| 429m/z|        | pos  |        |
| 10.45 | 334.2  | pos  |        |
| 187m/z|        | pos  |        |
| 10.45 | 464.3  | pos  |        |
| 133m/z|        | pos  |        |
| 10.45 | 528.3  | pos  |        |
| 775m/z|        | pos  |        |
| 10.46 | 271.1  | pos  |        |
| 356m/z|        | pos  |        |
| 10.46 | 407.2  | pos  |        |
| 635m/z|        | pos  |        |
| 10.47 | 155.8  | pos  |        |
| 651m/z|        | neg  |        |
| 10.47 | 422.3  |     |        |
| 310m/z|        | pos  |        |
| 10.47 | 457.3  | pos  |        |
| 374m/z|        | pos  |        |
| 10.48 | 348.9  |     |        |
| 894m/z|        | neg  |        |
| 10.49 | 122.9  |     |        |
| 639m/z|        | pos  |        |
| 10.49 | 197.1  |     |        |
| 898m/z|        | pos  |        |
| 10.49 | 396.3  |     |        |
| 136m/z|        | pos  |        |
| 10.49 | 409.2  |     |        |
| 787m/z|        | pos  |        |
10.49_446.3
4643 322m/z   pos
10.49_603.5
4644 386m/z   pos
10.50_610.2
4645 453m/z   neg
10.51_266.6
4646 418m/z   pos
10.51_274.6
4647 263m/z   pos
10.51_306.2
4648 657m/z   pos
10.51_351.1
4649 620m/z   neg
10.51_492.8
4650 050m/z   pos
10.51_528.2
4651 860m/z   neg
10.51_548.2
4652 464m/z   pos
10.51_555.3
4653 052m/z   neg
10.51_577.2
4654 733n   pos
10.51_584.2
4655 235m/z   pos
10.51_594.2
4656 443m/z   pos
10.52_312.1
4657 611m/z   pos
10.52_414.2
4658 090n   pos
10.52_417.2
4659 217m/z   pos
10.52_473.2
4660 702m/z   pos
10.52_498.3
4661 644m/z   pos
10.52_504.3
4662 296m/z   pos
10.52_555.3
4663 224m/z   pos
10.52_640.1
4664 687n   pos
10.52_758.4
4665 655m/z   neg
10.53_195.1
4666 390m/z   pos
10.53_458.2
4667 514m/z   pos
| m/z   | Charge | Mass/Charge Ratio | Description |
|-------|--------|-------------------|-------------|
| 159   | pos    | 0.54_264.3        |             |
| 310   | neg    | 0.54_512.0        |             |
| 049   | neg    | 0.54_516.0        |             |
| 173   | neg    | 0.54_527.0        |             |
| 002   | neg    | 0.54_536.0        |             |
| 180   | neg    | 0.54_543.0        |             |
| 011   | neg    | 0.54_550.0        |             |
| 098   | neg    | 0.54_553.0        |             |
| 020   | neg    | 0.54_583.0        |             |
| 041   | neg    | 0.54_586.0        |             |
| 212   | neg    | 0.54_590.0        |             |
| 198   | neg    | 0.54_605.0        |             |
| 047   | neg    | 0.54_619.0        |             |
| 077   | neg    | 0.54_652.0        |             |
| 240   | neg    | 0.55_214.1        |             |
| 824   | pos    | 0.55_258.1        |             |
| 853   | pos    | 0.55_323.1        |             |
| 488   | pos    | 0.55_405.1        |             |
| 364   | pos    | 0.55_436.0        |             |
| 131   | neg    | 0.55_459.2        |             |
| 716   | neg    | 0.55_613.0        |             |
| 078   | neg    | 0.56_243.1        |             |
| 853   | pos    | 0.57_234.1        |             |
| 365   | pos    | 0.57_376.1        |             |
| 935   | pos    |                   |             |
10.57_413.2
4693  815m/z   pos
10.57_442.3
4694  565m/z   pos
10.57_448.2
4695  882n    pos
10.57_588.2
4696  531m/z   pos
10.58_520.0
4697  147n    neg
10.59_275.2
4698  030m/z   pos
10.59_297.1
4699  528m/z   neg
10.59_310.2
4700  168n    pos
10.59_345.2
4701  560n    pos
10.59_529.1
4702  919n    pos
10.61_141.1
4703  139m/z   pos
10.61_254.2
4704  131m/z   pos
10.61_286.2
4705  397m/z   pos
10.61_386.3
4706  290m/z   pos
10.61_398.3
4707  334m/z   pos
10.61_477.3
4708  078n    pos
10.61_526.0
4709  139n    neg
10.61_887.5
4710  656m/z   pos
10.63_231.1
4711  460n    pos
10.63_268.1
4712  243m/z   pos
10.63_293.2
4713  362n    pos
10.63_399.7
4714  690m/z   pos
10.63_406.7
4715  500m/z   pos
10.63_440.2
4716  870m/z   pos
10.63_618.0
4717  222n    neg
| Number | Time (min) | m/z | Charge | Status |
|--------|------------|-----|--------|--------|
| 4718   | 10.64      | 667 |        | pos    |
| 4719   | 10.64      | 031 |        | pos    |
| 4720   | 10.64      | 539 |        | pos    |
| 4721   | 10.64      | 226 |        | pos    |
| 4722   | 10.65      | 122 |        | neg    |
| 4723   | 10.65      | 404 |        | neg    |
| 4724   | 10.65      | 212 |        | neg    |
| 4725   | 10.65      | 612 |        | neg    |
| 4726   | 10.65      | 086 |        | neg    |
| 4727   | 10.66      | 411 |        | pos    |
| 4728   | 10.66      | 272 |        | pos    |
| 4729   | 10.66      | 498 |        | pos    |
| 4730   | 10.66      | 370 |        | pos    |
| 4731   | 10.66      | 929 |        | neg    |
| 4732   | 10.66      | 228 |        | pos    |
| 4733   | 10.66      | 896 |        | pos    |
| 4734   | 10.66      | 854 |        | neg    |
| 4735   | 10.66      | 392 |        | pos    |
| 4736   | 10.66      | 111 |        | pos    |
| 4737   | 10.66      | 577 |        | pos    |
| 4738   | 10.66      | 771 |        | pos    |
| 4739   | 10.66      | 026 |        | neg    |
| 4740   | 10.66      | 372 |        | neg    |
| 4741   | 10.66      | 602 |        | pos    |
| 4742   | 10.66      | 786 |        | pos    |
| m/z     | RT     | Charge |
|---------|--------|--------|
| 10.66   | 796.5  |        |
| 10.67   | 320.2  | neg    |
| 10.67   | 374.1  |        |
| 10.67   | 392.2  |        |
| 10.67   | 661.2  |        |
| 10.68   | 294.2  | pos    |
| 10.68   | 304.3  | pos    |
| 10.68   | 307.2  |        |
| 10.68   | 313.2  |        |
| 10.68   | 324.2  |        |
| 10.68   | 360.2  |        |
| 10.68   | 392.2  |        |
| 10.68   | 404.3  |        |
| 10.68   | 475.2  |        |
| 10.68   | 488.2  |        |
| 10.68   | 542.6  |        |
| 10.68   | 598.2  |        |
| 10.68   | 630.2  |        |
| 10.68   | 634.2  |        |
| 10.69   | 427.2  |        |
| 10.69   | 459.2  |        |
| 10.69   | 578.3  |        |
| 10.69   | 605.3  |        |
| 10.69   | 656.3  |        |
| 10.70   | 221.1  |        |
| 10.70   | 297.1  |        |
| 10.70   | 372.2  |        |
| 10.70   | 408.3  |        |
| 10.70   | 408.3  |        |
| 10.70   | 488.2  |        |
10.70_410.9
4768 893 m/z  neg
10.70_418.7
4769 504 m/z  pos
10.70_430.9
4770 918 m/z  neg
10.70_438.3
4771 780 m/z  pos
10.70_627.5
4772 397 m/z  pos
10.71_257.2
4773 307 m/z  pos
10.71_450.2
4774 684 n  pos
10.71_462.3
4775 401 n  pos
10.71_470.3
4776 357 m/z  pos
10.71_603.5
4777 397 m/z  pos
10.71_753.5
4778 664 m/z  pos
10.71_882.4
4779 984 m/z  pos
10.72_100.9
4780 554 m/z  pos
10.72_197.1
4781 549 m/z  pos
10.72_241.8
4782 846 m/z  pos
10.72_281.2
4783 500 m/z  pos
10.72_292.2
4784 059 n  pos
10.72_299.2
4785 615 m/z  pos
10.72_314.0
4786 892 n  pos
10.72_339.2
4787 608 m/z  pos
10.72_348.9
4788 931 m/z  pos
10.72_411.2
4789 690 m/z  pos
10.72_419.2
4790 544 m/z  pos
10.72_472.3
4791 465 m/z  pos
10.72_498.9
4792 334 m/z  neg
4793 394m/z    pos
10.72_871.5
4794 797m/z    neg
10.72_967.4
4795 044m/z    pos
10.72_969.4
4796 272m/z    pos
10.74_390.9
4797 858m/z    neg
10.74_397.3
4798 151m/z    pos
10.74_405.2
4799 526n     pos
10.74_477.2
4800 893n     pos
10.74_488.1
4801 649n     pos
10.74_509.3
4802 385m/z   pos
10.74_532.2
4803 151m/z   pos
10.74_580.2
4804 149m/z   pos
10.74_617.1
4805 926m/z   pos
10.74_742.5
4806 656m/z   pos
10.74_263.2
4807 324m/z   pos
10.74_266.6
4808 116m/z   pos
10.75_303.6
4809 504m/z   pos
10.75_476.8
4810 239m/z   pos
10.75_566.5
4811 922m/z   pos
10.75_596.3
4812 002n     pos
10.75_622.2
4813 602n     pos
10.75_657.2
4814 331m/z   pos
10.75_658.2
4815 349m/z   pos
10.75_703.1
4816 675m/z   pos
10.75_715.1
4817 898m/z   pos
10.75_824.5
4818 594m/z   pos
10.75_955.5
4819 893m/z   pos
10.75_979.5
4820 862m/z   pos
10.76_200.2
4821 022m/z   pos
10.76_249.1
4822 866m/z   pos
10.76_311.6
4823 361m/z   pos
10.76_366.9
4824 866m/z   neg
10.76_412.2
4825 197m/z   pos
10.76_448.3
4826 487m/z   pos
10.76_526.7
4827 822m/z   pos
10.76_530.7
4828 949m/z   pos
10.76_538.2
4829 792m/z   pos
10.76_538.7
4830 794m/z   pos
10.76_563.3
4831 152m/z   pos
10.76_563.8
4832 179m/z   pos
10.76_567.3
4833 375n     pos
10.76_585.2
4834 553m/z   neg
10.76_619.2
4835 624n     pos
10.76_627.3
4836 020m/z   pos
10.76_678.4
4837 172m/z   pos
10.76_680.3
4838 178m/z   neg
10.76_692.4
4839 569m/z   pos
10.76_712.3
4840 326m/z   pos
10.76_808.5
4841 016n     pos
10.76_997.6
4842 356m/z   pos
| Retention Time (m/z) | Spectrum Status |
|----------------------|-----------------|
| 10.77_512.9          | neg             |
| 976m/z               | neg             |
| 10.77_559.0          | neg             |
| 006m/z               | neg             |
| 10.77_563.0          | neg             |
| 003m/z               | neg             |
| 10.77_602.3          | neg             |
| 010m/z               | neg             |
| 10.77_607.0          | neg             |
| 060m/z               | neg             |
| 10.77_609.0          | neg             |
| 067m/z               | neg             |
| 10.77_622.0          | neg             |
| 214n                 | neg             |
| 10.77_623.0          | neg             |
| 031m/z               | neg             |
| 10.77_639.0          | neg             |
| 088m/z               | neg             |
| 10.77_646.0          | neg             |
| 259n                 | neg             |
| 10.77_648.0          | neg             |
| 151n                 | neg             |
| 10.77_672.0          | neg             |
| 245n                 | neg             |
| 10.77_674.0          | neg             |
| 220n                 | neg             |
| 10.77_675.0          | neg             |
| 112m/z               | neg             |
| 10.77_684.0          | neg             |
| 270n                 | neg             |
| 10.77_684.2          | neg             |
| 635m/z               | neg             |
| 10.77_688.0          | neg             |
| 257n                 | neg             |
| 10.77_707.0          | neg             |
| 126m/z               | neg             |
| 10.77_800.4          | neg             |
| 730m/z               | neg             |
| 10.77_899.0          | neg             |
| 186m/z               | neg             |
| 10.78_248.6          | pos             |
| 708n                 | pos             |
| 10.78_278.6          | pos             |
| 295m/z               | pos             |
| 10.78_279.6          | pos             |
| 499m/z               | pos             |
| 10.78_286.6          | pos             |
| 368m/z               | pos             |
| 10.78_335.1          | pos             |
| 681m/z               | pos             |
| Retention Time (min) | m/z     | Charge State | Ion Type |
|----------------------|---------|--------------|----------|
| 10.78                | 424.3   |              | pos      |
| 10.78                | 468.2   |              | pos      |
| 10.78                | 518.7   |              | pos      |
| 10.78                | 519.8   |              | pos      |
| 10.78                | 520.8   |              | pos      |
| 10.78                | 534.3   |              | pos      |
| 10.78                | 535.8   |              | pos      |
| 10.78                | 539.8   |              | pos      |
| 10.78                | 547.3   |              | pos      |
| 10.78                | 547.8   |              | pos      |
| 10.78                | 548.3   |              | pos      |
| 10.78                | 548.8   |              | pos      |
| 10.78                | 551.8   |              | pos      |
| 10.78                | 552.5   |              | pos      |
| 10.78                | 554.3   |              | pos      |
| 10.78                | 555.3   |              | pos      |
| 10.78                | 556.8   |              | pos      |
| 10.78                | 557.8   |              | pos      |
| 10.78                | 558.3   |              | pos      |
| 10.78                | 559.8   |              | pos      |
| 10.78                | 562.5   |              | pos      |
| 10.78                | 574.2   |              | pos      |
| 10.78                | 575.0   |              | neg      |
| 10.78                | 577.0   |              | neg      |
| 10.78                | 575.0   |              | neg      |
| 10.78                | 581.3   |              | neg      |
| 10.78                | 612.0   |              | neg      |
| 10.78                | 615.2   |              | neg      |
| 10.78                | 616.2   |              | pos      |
| 10.78                | 624.2   |              | neg      |
| 10.78                | 636.2   |              | neg      |
| 10.78                | 636.2   |              | neg      |
10.78_643.2
4893 897m/z  neg
10.78_644.0
4894 260n   neg
10.78_647.4
4895 394m/z  pos
10.78_649.3
4896 077m/z  neg
10.78_660.0
4897 262n   neg
10.78_665.2
4898 645n   neg
10.78_680.0
4899 173n   neg
10.78_685.0
4900 094m/z  neg
10.78_696.0
4901 279n   neg
10.78_701.0
4902 106m/z  neg
10.78_705.2
4903 555m/z  neg
10.78_712.2
4904 625m/z  neg
10.78_715.0
4905 115m/z  neg
10.78_717.0
4906 114m/z  neg
10.78_723.0
4907 132m/z  neg
10.78_728.0
4908 301n   neg
10.78_739.0
4909 141m/z  neg
10.78_765.0
4910 157m/z  neg
10.78_783.9
4911 585n   pos
10.78_787.0
4912 155m/z  neg
10.78_796.0
4913 347n   neg
10.78_798.9
4914 899m/z  pos
10.78_799.4
4915 880m/z  pos
10.78_807.4
4916 734m/z  pos
10.78_808.0
4917 337n   neg
| m/z | Value | Charge | Retention Time |
|-----|-------|--------|----------------|
| 810 | 10.78 | pos    | 810.9          |
| 359 | 10.78 | neg    | 818.9          |
| 726 | 10.78 | pos    | 819.4          |
| 716 | 10.78 | pos    | 943.6          |
| 819 | 10.78 | pos    | 104.1          |
| 066 | 10.78 | pos    | 291.6          |
| 505 | 10.79 | pos    | 299.6          |
| 360 | 10.79 | pos    | 542.6          |
| 652 | 10.79 | pos    | 598.2          |
| 628 | 10.79 | pos    | 620.3          |
| 002 | 10.80 | pos    | 190.9          |
| 928 | 10.80 | neg    | 391.2          |
| 251 | 10.80 | neg    | 428.8          |
| 954 | 10.80 | pos    | 430.8          |
| 907 | 10.80 | pos    | 432.8          |
| 877 | 10.80 | pos    | 434.8          |
| 876 | 10.80 | pos    | 570.0          |
| 193 | 10.80 | neg    | 586.5          |
| 033 | 10.80 | neg    | 622.2          |
| 902 | 10.80 | neg    | 643.2          |
| 802 | 10.80 | pos    | 667.3          |
| 094 | 10.80 | neg    | 668.0          |
| 240 | 10.80 | neg    | 681.0          |
| 096 | 10.80 | neg    | 694.2          |
| 885 | 10.80 | neg    |                |
10.80_700.3  
4943  053m/z neg  
10.80_704.2  
4944  517m/z neg  
10.80_768.0  
4945  220n neg  
10.80_810.0  
4946  350n neg  
10.80_815.0  
4947  162m/z neg  
10.80_825.0  
4948  171m/z neg  
10.80_838.0  
4949  353n neg  
10.80_840.0  
4950  356n neg  
10.80_886.0  
4951  372n neg  
10.81_486.9  
4952  952m/z neg  
10.81_578.3  
4953  017m/z neg  
10.81_594.3  
4954  406m/z neg  
10.81_605.3  
4955  210m/z neg  
10.81_640.2  
4956  905m/z neg  
10.81_660.2  
4957  613m/z neg  
10.81_673.3  
4958  077m/z neg  
10.81_691.0  
4959  104m/z neg  
10.81_799.0  
4960  151m/z neg  
10.81_801.0  
4961  154m/z neg  
10.81_823.0  
4962  179m/z neg  
10.82_284.2  
4963  625m/z pos  
10.82_316.3  
4964  261m/z pos  
10.83_242.2  
4965  095m/z pos  
10.83_379.2  
4966  537m/z pos  
10.83_416.2  
4967  187m/z pos
10.84_197.1
4968 551m/z   pos
10.84_266.1
4969 738m/z   pos
10.84_269.2
4970 159m/z   pos
10.84_317.2
4971 151m/z   pos
10.84_473.2
4972 821m/z   neg
10.86_100.9
4973 554m/z   pos
10.86_234.1
4974 365m/z   pos
10.86_293.1
4975 779m/z   pos
10.86_297.2
4976 682m   pos
10.86_406.7
4977 495m/z   pos
10.86_410.7
4978 643m/z   pos
10.86_490.2
4979 877m/z   pos
10.86_491.2
4980 947m/z   pos
10.86_575.5
4981 047m/z   pos
10.86_875.4
4982 897m/z   pos
10.86_901.4
4983 990m/z   pos
10.86_967.4
4984 102m/z   pos
10.87_306.2
4985 264m   pos
10.87_347.2
4986 251m/z   pos
10.87_384.3
4987 269m/z   pos
10.87_565.0
4988 004m/z   neg
10.88_435.3
4989 105m/z   neg
10.89_304.2
4990 531m/z   pos
10.89_363.2
4991 782m/z   pos
10.89_382.3
4992 252m/z   pos
4993  389m/z   pos  10.89_466.3
4994  272m/z   pos  10.89_637.2
4995  595m/z   pos  10.89_679.1
4996  731m/z   pos  10.89_828.5
4997  504m/z   pos  10.90_184.0
4998  743m/z   pos  10.90_222.1
4999  638n    pos  10.90_226.1
5000  815m/z   pos  10.90_236.6
5001  721n    pos  10.90_256.2
5002  303m/z   pos  10.90_267.6
5003  493m/z   pos  10.90_296.6
5004  496m/z   pos  10.90_484.8
5005  394n    pos  10.90_494.8
5006  146m/z   pos  10.90_495.3
5007  373n    pos  10.90_515.8
5008  205m/z   pos  10.90_562.2
5009  612n    pos  10.90_586.2
5010  397m/z   pos  10.90_590.2
5011  575n    pos  10.90_595.2
5012  594n    pos  10.90_615.2
5013  591m/z   pos  10.90_666.4
5014  169m/z   pos  10.90_770.9
5015  709m/z   pos  10.90_771.4
5016  734m/z   pos  10.90_991.6
5017  804m/z   pos
| Mass/Charge | Retention Time | Charge | Isotopic Pattern |
|------------|----------------|--------|-----------------|
| 5018       | 10.91          | 196.1  | pos             |
| 5019       | 10.91          | 402.2  | pos             |
| 5020       | 10.91          | 538.6  | neg             |
| 5021       | 10.91          | 557.3  | neg             |
| 5022       | 10.91          | 592.2  | neg             |
| 5023       | 10.91          | 598.2  | neg             |
| 5024       | 10.91          | 612.2  | neg             |
| 5025       | 10.91          | 640.2  | neg             |
| 5026       | 10.91          | 676.3  | neg             |
| 5027       | 10.91          | 688.2  | neg             |
| 5028       | 10.93          | 528.3  | pos             |
| 5029       | 10.93          | 530.2  | pos             |
| 5030       | 10.93          | 627.5  | pos             |
| 5031       | 10.94          | 253.1  | pos             |
| 5032       | 10.94          | 276.2  | pos             |
| 5033       | 10.94          | 291.1  | pos             |
| 5034       | 10.94          | 312.2  | pos             |
| 5035       | 10.94          | 369.1  | pos             |
| 5036       | 10.94          | 397.3  | pos             |
| 5037       | 10.94          | 415.3  | pos             |
| 5038       | 10.94          | 444.3  | pos             |
| 5039       | 10.94          | 481.3  | pos             |
| 5040       | 10.94          | 607.3  | pos             |
| 5041       | 10.95          | 462.3  | pos             |
| 5042       | 10.95          | 462.3  | pos             |
10.95_467.3
5043 656n  pos
10.97_118.1
5044 248n  pos
10.97_241.8
5045 847m/z  pos
10.97_242.2
5046 100m/z  pos
10.97_406.2
5047 755n  pos
10.97_431.3
5048 241m/z  pos
10.97_536.5
5049 300n  pos
10.97_756.5
5050 629m/z  pos
10.98_116.9
5051 272m/z  neg
10.98_182.9
5052 653m/z  pos
10.98_253.2
5053 178m/z  pos
10.98_324.2
5054 330n  pos
10.98_400.3
5055 473m/z  pos
10.98_523.3
5056 635m/z  pos
10.98_614.3
5057 423m/z  pos
10.98_764.5
5058 555m/z  neg
10.98_792.5
5059 354m/z  neg
10.98_794.5
5060 468m/z  neg
10.98_816.5
5061 395m/z  neg
10.98_837.5
5062 235n  pos
10.98_882.4
5063 990m/z  pos
10.98_887.5
5064 553m/z  neg
10.98_894.5
5065 485m/z  neg
10.98_899.4
5066 905m/z  pos
10.98_901.5
5067 010m/z  pos
| m/z  | Fragment | Charge | Retention Time |
|------|----------|--------|----------------|
| 471  | 5068     | 10.99  | pos            |
| 509  | 5069     | 10.99  | pos            |
| 446  | 5070     | 10.99  | pos            |
| 568  | 5071     | 10.99  | pos            |
| 499  | 5072     | 10.99  | pos            |
| 024  | 5073     | 10.99  | pos            |
| 005  | 5074     | 10.99  | pos            |
| 372  | 5075     | 10.99  | pos            |
| 645  | 5076     | 10.99  | pos            |
| 409  | 5077     | 10.99  | pos            |
| 369  | 5078     | 10.99  | pos            |
| 753  | 5079     | 10.99  | pos            |
| 787  | 5080     | 10.99  | neg            |
| 796  | 5081     | 10.99  | pos            |
| 880  | 5082     | 10.99  | pos            |
| 617  | 5083     | 11.01  | pos            |
| 713  | 5084     | 11.01  | pos            |
| 285  | 5085     | 11.01  | pos            |
| 479  | 5086     | 11.01  | pos            |
| 335  | 5087     | 11.01  | pos            |
| 648  | 5088     | 11.01  | neg            |
| 811  | 5089     | 11.01  | pos            |
| 677  | 5090     | 11.01  | pos            |
| 811  | 5091     | 11.01  | pos            |
| 660  | 5092     | 11.01  | pos            |
| M/Z   | Value | Status |
|-------|-------|--------|
| 380m/ | 1866.5| pos    |
| 291m/ | 436.3 | pos    |
| 679n  | 502.7 | pos    |
| 824m/ | 504.3 | pos    |
| 216m/ | 537.2 | pos    |
| 554m/ | 552.2 | pos    |
| 027m/ | 585.2 | neg    |
| 326m/ | 587.2 | pos    |
| 387m/ | 603.3 | pos    |
| 016m/ | 613.2 | pos    |
| 545m/ | 642.1 | pos    |
| 824n  | 688.3 | pos    |
| 304m/ | 947.6 | pos    |
| 122m/ | 296.6 | neg    |
| 499m/ | 496.9 | pos    |
| 873m/ | 534.7 | pos    |
| 941m/ | 550.2 | pos    |
| 620m/ | 554.3 | pos    |
| 971m/ | 576.2 | pos    |
| 803n  | 578.2 | pos    |
| 687m/ | 591.2 | pos    |
| 671m/ | 596.2 | pos    |
| 741n  | 754.9 | pos    |
| 962m/ | 766.4 | pos    |
| 965m/ |       | pos    |
11.03_948.6
5118 252n pos
11.04_152.0
5119 633m/z neg
11.04_239.0
5120 652m/z neg
11.04_706.0
5121 140n neg
11.04_711.0
5122 121m/z neg
11.04_738.0
5123 273n neg
11.04_750.0
5124 284n neg
11.04_766.0
5125 235n neg
11.04_778.0
5126 244n neg
11.04_792.0
5127 244n neg
11.04_805.0
5128 196m/z neg
11.05_134.8
5129 939m/z neg
11.05_139.3
5130 758m/z pos
11.05_139.6
5131 413m/z pos
11.05_139.9
5132 030m/z pos
11.05_151.7
5133 988m/z neg
11.05_267.6
5134 528m/z pos
11.05_273.1
5135 603n pos
11.05_275.6
5136 362m/z pos
11.05_409.2
5137 353m/z neg
11.05_478.8
5138 193m/z neg
11.05_494.8
5139 143m/z pos
11.05_507.8
5140 302m/z pos
11.05_511.3
5141 289m/z pos
11.05_515.3
5142 222m/z pos
| m/z  | Retention Time | Charge | Sign |
|------|---------------|--------|------|
| 199  | 11.05_522.8   | pos    |      |
| 019  | 11.05_523.8   | pos    |      |
| 048  | 11.05_527.3   | pos    |      |
| 246  | 11.05_530.3   | pos    |      |
| 023  | 11.05_538.6   | neg    |      |
| 542  | 11.05_555.5   | neg    |      |
| 907  | 11.05_570.3   | neg    |      |
| 405  | 11.05_579.3   | neg    |      |
| 411  | 11.05_582.3   | neg    |      |
| 371  | 11.05_592.2   | neg    |      |
| 947  | 11.05_612.2   | neg    |      |
| 615  | 11.05_640.2   | neg    |      |
| 562  | 11.05_688.2   | neg    |      |
| 621  | 11.05_761.0   | neg    |      |
| 140  | 11.05_762.9   | neg    |      |
| 894  | 11.05_763.4   | pos    |      |
| 869  | 11.05_768.0   | pos    |      |
| 211  | 11.05_769.0   | neg    |      |
| 125  | 11.05_770.9   | neg    |      |
| 744  | 11.05_787.0   | pos    |      |
| 153  | 11.05_794.0   | neg    |      |
| 345  | 11.05_798.0   | neg    |      |
| 343  | 11.05_808.0   | neg    |      |
| 340  | 11.05_816.0   | neg    |      |
| 250  | 11.05_816.0   | neg    |      |
| m/z     | Charge | Status |
|---------|--------|--------|
| 11.05_821.0 | 196 m/z | neg |
| 11.05_825.0 | 188 m/z | neg |
| 11.05_828.0 | 360 n | neg |
| 11.05_836.0 | 202 m/z | neg |
| 11.05_830.0 | 359 n | neg |
| 11.05_849.0 | 203 m/z | neg |
| 11.05_860.0 | 187 m/z | neg |
| 11.05_864.0 | 380 n | neg |
| 11.05_975.6 | 960 m/z | neg |
| 11.05_988.6 | 064 m/z | pos |
| 11.05_991.6 | 798 m/z | pos |
| 11.06_104.1 | 062 m/z | pos |
| 11.06_607.3 | 362 m/z | neg |
| 11.06_624.2 | 925 m/z | neg |
| 11.06_819.0 | 163 m/z | neg |
| 11.06_867.0 | 214 m/z | neg |
| 11.06_869.0 | 218 m/z | neg |
| 11.06_876.0 | 409 n | neg |
| 11.06_877.0 | 206 m/z | neg |
| 11.06_890.0 | 390 n | neg |
| 11.06_901.0 | 238 m/z | neg |
| 11.08_580.3 | 199 m/z | neg |
| 11.08_598.2 | 896 m/z | neg |
| 11.08_625.3 | 073 m/z | neg |
| M/z | Retention Time |
|-----|----------------|
| 5193 | 11.08_676.3   |
| 5194 | 11.09_529.2   |
| 5195 | 11.09_790.5   |
| 5196 | 11.10_279.2   |
| 5197 | 11.10_426.3   |
| 5198 | 11.11_295.2   |
| 5199 | 11.11_563.2   |
| 5200 | 11.11_569.3   |
| 5201 | 11.11_585.2   |
| 5202 | 11.11_595.2   |
| 5203 | 11.11_615.2   |
| 5204 | 11.12_583.3   |
| 5205 | 11.13_280.6   |
| 5206 | 11.13_288.6   |
| 5207 | 11.13_445.3   |
| 5208 | 11.13_476.3   |
| 5209 | 11.13_520.7   |
| 5210 | 11.14_128.1   |
| 5211 | 11.14_203.1   |
| 5212 | 11.14_204.1   |
| 5213 | 11.14_421.2   |
| 5214 | 11.14_774.5   |
| 5215 | 11.15_146.9   |
| 5216 | 11.15_175.1   |
| 5217 | 11.15_384.3   |
| 5218 | 11.15_384.3   |

- **neg**: Negative ion mode
- **pos**: Positive ion mode
11.17_124.9
5218 646m/z  pos
11.17_174.1
5219 294m/z  pos
11.17_234.1
5220 355m/z  pos
11.17_323.2
5221 151m/z  pos
11.17_348.9
5222 926m/z  pos
11.17_368.2
5223 971n   pos
11.17_406.2
5224 776n   pos
11.17_412.3
5225 020n   pos
11.17_418.7
5226 503m/z  pos
11.17_430.3
5227 110n   pos
11.17_451.3
5228 395m/z  pos
11.17_461.3
5229 331m/z  pos
11.17_464.3
5230 526n   pos
11.18_189.1
5231 313m/z  pos
11.18_409.7
5232 560n   pos
11.18_420.7
5233 646m/z  pos
11.18_454.3
5234 327n   pos
11.18_481.3
5235 509m/z  neg
11.18_540.9
5236 953m/z  neg
11.18_603.5
5237 395m/z  pos
11.18_871.5
5238 790m/z  neg
11.18_876.4
5239 957m/z  pos
11.18_885.5
5240 156n   pos
11.18_887.5
5241 576m/z  pos
11.18_894.5
5242 485m/z  neg
11.22_536.5
5268 304n    pos
11.22_605.2
5269 951m/z   pos
11.22_718.5
5270 786m/z   pos
11.22_893.5
5271 616m/z   pos
11.23_332.3
5272 340m/z   pos
11.23_413.3
5273 596n    pos
11.23_479.3
5274 056n    pos
11.23_532.3
5275 748m/z   pos
11.23_596.3
5276 764m/z   pos
11.23_668.1
5277 961n    pos
11.23_705.1
5278 934m/z   pos
11.23_798.6
5279 541n    pos
11.24_546.2
5280 805m/z   neg
11.25_265.1
5281 837m/z   pos
11.25_298.2
5282 533n    pos
11.25_568.3
5283 444m/z   pos
11.25_959.6
5284 489m/z   pos
11.26_249.6
5285 781n    pos
11.26_250.1
5286 828n    pos
11.26_279.6
5287 388m/z   pos
11.26_438.3
5288 022m/z   pos
11.26_510.8
5289 577n    pos
11.26_558.3
5290 165m/z   neg
11.26_564.5
5291 881m/z   neg
11.26_606.3
5292 084m/z   pos
| Mass (m/z) | Time (s) | Charge Status |
|-----------|----------|---------------|
| 513       | 11.26    | +              |
| 508       | 11.26    | +              |
| 816       | 11.26    | +              |
| 086       | 11.26    | -              |
| 756       | 11.26    | +              |
| 045       | 11.26    | -              |
| 816       | 11.26    | +              |
| 086       | 11.26    | -              |
| 756       | 11.26    | +              |
| 045       | 11.26    | -              |
| 71        | 11.26    | -              |
| 759       | 11.26    | +              |
| 083       | 11.26    | -              |
| 234       | 11.26    | +              |
| 317       | 11.26    | +              |
| 208       | 11.26    | -              |
| 205       | 11.27    | -              |
| 061       | 11.27    | +              |
| 582       | 11.27    | +              |
| 502       | 11.27    | +              |
| 567       | 11.27    | +              |
| 464       | 11.27    | +              |
| 495       | 11.27    | +              |
| 085       | 11.27    | +              |
| 155       | 11.27    | +              |
| 165       | 11.27    | +              |
| m/z | RT (min) | Charge State | Ion Type |
|-----|---------|--------------|----------|
| 11.27_529.8 | 197 | pos |
| 11.27_533.3 | 572 | pos |
| 11.27_537.3 | 262 | pos |
| 11.27_541.3 | 572 | pos |
| 11.27_541.8 | 341 | pos |
| 11.27_554.3 | 357 | pos |
| 11.27_625.4 | 538 | pos |
| 11.27_802.0 | 648 | pos |
| 11.27_809.9 | 053 | pos |
| 11.27_809.9 | 053 | pos |
| 11.27_819.0 | 057 | neg |
| 11.27_821.0 | 186 | neg |
| 11.27_823.0 | 408 | neg |
| 11.27_833.0 | 389 | neg |
| 11.27_819.0 | 140 | neg |
| 11.28_821.0 | 140 | neg |
| 11.28_823.0 | 181 | neg |
| 11.28_833.0 | 177 | neg |
| 11.28_845.0 | 186 | neg |
| 11.28_845.0 | 186 | neg |
| 11.28_850.0 | 164 | neg |
| 11.29_268.6 | 164 | neg |
| 11.29_268.6 | 164 | neg |
| 11.29_479.3 | 457 | pos |
| 11.29_479.3 | 457 | pos |
| 11.29_482.3 | 401 | pos |
| 11.30_276.2 | 641 | pos |
| 11.30_276.2 | 641 | pos |
| 11.31_253.1 | 327 | pos |
| 11.31_253.1 | 327 | pos |
| 11.31_515.3 | 821 | pos |
| 11.31_515.3 | 821 | pos |
| 11.33_379.2 | 760 | pos |
| 11.33_379.2 | 760 | pos |
| 11.33_379.2 | 760 | pos |
| 11.33_379.2 | 760 | pos |
| 11.33_379.2 | 760 | pos |
| m/z | Time | Charge State |
|-----|------|--------------|
| 654 | 11.33 | pos          |
| 541 | 11.34 | pos          |
| 457 | 11.34 | pos          |
| 700 | 11.34 | pos          |
| 788 | 11.34 | pos          |
| 347 | 11.35 | pos          |
| 334 | 11.35 | pos          |
| 717 | 11.35 | pos          |
| 682 | 11.36 | pos          |
| 366 | 11.36 | neg          |
| 210 | 11.37 | pos          |
| 344 | 11.37 | pos          |
| 619 | 11.37 | pos          |
| 512 | 11.37 | neg          |
| 905 | 11.37 | pos          |
| 439 | 11.38 | pos          |
| 372 | 11.38 | pos          |
| 861 | 11.38 | pos          |
| 644 | 11.38 | pos          |
| 788 | 11.40 | pos          |
| 681 | 11.40 | neg          |
| 111 | 11.40 | pos          |
| 111 | 11.41 | pos          |
| 326 | 11.41 | neg          |
| 974 | 11.41 | pos          |
| 084 | 11.41 | pos          |
5368 470 m/z  pos  11.41_286.2
5369 405 m/z  pos  11.41_664.4
5370 688 m/z  pos  11.41_969.4
5371 296 m/z  pos  11.42_100.9
5372 556 m/z  pos  11.42_319.2
5373 412 m/z  pos  11.42_319.2
5374 635 m/z  neg  11.42_329.2
5375 495 m/z  pos  11.42_364.2
5376 640 n  pos  11.42_421.3
5377 329 m/z  pos  11.42_603.5
5378 409 m/z  pos  11.42_620.4
5379 423 m/z  pos  11.42_860.5
5380 167 m/z  pos  11.44_365.2
5381 720 m/z  pos  11.44_371.3
5382 371 n  pos  11.44_466.2
5383 928 m/z  neg  11.44_468.3
5384 176 m/z  pos  11.44_576.4
5385 159 m/z  pos  11.45_330.2
5386 443 n  pos  11.45_434.3
5387 096 n  pos  11.46_253.2
5388 179 m/z  pos  11.46_282.6
5389 453 m/z  pos  11.46_357.2
5390 850 m/z  pos  11.46_472.3
5391 463 m/z  pos  11.46_487.3
5392 512 n  pos
| Time (min) | m/z 11.46 | Charge | Status | m/z 11.47 | Charge | Status | m/z 11.48 | Charge | Status | m/z 11.49 | Charge | Status | m/z 11.50 | Charge | Status | m/z 11.51 | Charge | Status | m/z 11.52 | Charge | Status | m/z 11.53 | Charge | Status | m/z 11.54 | Charge | Status |
|-----------|------------|--------|--------|------------|--------|--------|------------|--------|--------|------------|--------|--------|------------|--------|--------|------------|--------|--------|------------|--------|--------|------------|--------|--------|------------|--------|--------|------------|--------|--------|------------|--------|--------|
| 5393      | 508.7      |        | +      | 51.3       |        | -      | 462.2      |        | +      | 409.2      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5394      | 571.3      |        | -      | 462.2      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 571.3      |        | -      |
| 5395      | 622.3      |        | -      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5396      | 365.0      |        | -      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5397      | 340.0      |        | -      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5398      | 346.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5399      | 313.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5400      | 341.3      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5401      | 341.3      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5402      | 510.3      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5403      | 521.0      |        | -      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5404      | 690.3      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5405      | 385.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5406      | 675.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5407      | 538.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5408      | 237.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5409      | 568.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5410      | 732.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5411      | 571.3      |        | -      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5412      | 373.0      |        | -      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5413      | 246.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5414      | 529.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5415      | 733.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5416      | 777.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
| 5417      | 645.0      |        | +      | 409.2      |        | +      | 444.3      |        | +      | 464.3      |        | +      | 508.7      |        | +      |
5443 030m/z  pos  11.63_816.5
5444 401m/z  neg  11.64_296.1
5445 322m/z  pos  11.64_339.1
5446 632m/z  pos  11.64_439.3
5447 417m/z  neg  11.64_454.3
5448 932m/z  pos  11.64_639.4
5449 062n  pos  11.65_360.2
5450 175n  pos  11.65_404.3
5451 294n  pos  11.66_463.3
5452 415m/z  neg  11.66_570.9
5453 980m/z  neg  11.66_764.5
5454 549m/z  neg  11.66_848.5
5455 847m/z  neg  11.67_388.1
5456 068n  pos  11.67_627.5
5457 391m/z  pos  11.68_148.5
5458 724m/z  pos  11.68_278.1
5459 542n  pos  11.68_379.0
5460 871m/z  pos  11.68_419.2
5461 593m/z  pos  11.68_462.3
5462 379n  pos  11.68_620.3
5463 924m/z  pos  11.69_278.0
5464 497m/z  pos  11.71_452.3
5465 271m/z  pos  11.72_267.1
5466 980m/z  pos  11.72_377.2
5467 729m/z  pos
11.72_511.3
5468 404m/z  neg
11.72_586.4
5469 556m/z  pos
11.73_285.1
5470 739m/z  pos
11.73_415.3
5471 556m/z  pos
11.73_542.4
5472 290m/z  pos
11.73_811.0
5473 117m/z  neg
11.74_808.0
5474 274n  neg
11.74_825.0
5475 126m/z  neg
11.75_281.6
5476 648m/z  pos
11.75_289.6
5477 513m/z  pos
11.75_522.7
5478 593m/z  pos
11.75_523.3
5479 678n  pos
11.75_623.2
5480 913n  pos
11.75_643.2
5481 904m/z  pos
11.76_260.2
5482 155n  pos
11.76_353.1
5483 986m/z  neg
11.76_444.2
5484 910n  pos
11.76_558.3
5485 329m/z  neg
11.76_570.3
5486 676m/z  neg
11.76_585.3
5487 521m/z  neg
11.76_636.3
5488 498m/z  neg
11.76_777.0
5489 110m/z  neg
11.77_331.2
5490 663m/z  pos
11.77_366.2
5491 844n  pos
11.77_410.3
5492 543m/z  pos
11.77_717.5
5493 591m/z  pos
11.78_387.2
5494 508m/z  neg
11.79_255.2
5495 329m/z  pos
11.79_364.2
5496 649n  pos
11.79_531.3
5497 694m/z  pos
11.79_574.3
5498 882m/z  pos
11.79_776.5
5499 681m/z  pos
11.80_252.1
5500 625m/z  pos
11.80_319.2
5501 632m/z  neg
11.80_319.2
5502 654m/z  pos
11.80_382.2
5503 999m/z  pos
11.80_471.3
5504 505m/z  pos
11.80_533.3
5505 833m/z  pos
11.80_838.6
5506 129n  pos
11.81_654.4
5507 263m/z  pos
11.81_893.5
5508 605m/z  pos
11.83_438.3
5509 398n  pos
11.83_462.3
5510 388n  pos
11.83_534.3
5511 325n  pos
11.83_630.4
5512 808m/z  pos
11.83_871.5
5513 787m/z  neg
11.84_405.3
5514 308m/z  pos
11.84_424.3
5515 589m/z  pos
11.84_436.3
5516 248n  pos
11.84_461.3
5517 261m/z  neg
| m/z value | Charge Status |
|-----------|---------------|
| 11.89_580.2 | neg |
| 11.89_748.5 | pos |
| 11.89_753.5 | neg |
| 11.89_763.5 | pos |
| 11.89_799.6 | pos |
| 11.89_846.5 | pos |
| 11.90_295.2 | pos |
| 11.90_366.3 | pos |
| 11.90_389.2 | pos |
| 11.90_391.2 | pos |
| 11.90_410.3 | pos |
| 11.90_480.8 | pos |
| 11.90_536.4 | pos |
| 11.90_548.2 | pos |
| 11.90_720.5 | pos |
| 11.90_963.6 | pos |
| 11.91_631.3 | pos |
| 11.91_643.2 | pos |
| 11.92_628.3 | pos |
| 11.93_290.1 | pos |
| 11.93_311.6 | pos |
| 11.93_535.3 | pos |
| 11.93_535.8 | pos |
| 11.93_538.3 | pos |
| 11.93_558.3 | pos |
| 333m/z | neg |
11.93_566.5
5568 974m/z  neg
   11.93_585.3
5569 529m/z  neg
   11.93_598.3
5570 716m/z  neg
   11.93_619.2
5571 959m/z  pos
   11.93_623.2
5572 943m/z  pos
   11.93_626.3
5573 011m/z  pos
   11.93_652.3
5574 236m/z  neg
   11.93_718.2
5575 899m/z  neg
   11.93_768.0
5576 159n   neg
   11.93_770.0
5577 266n   neg
   11.93_779.0
5578 097m/z  neg
   11.93_783.0
5579 097m/z  neg
   11.93_790.0
5580 277n   neg
   11.93_837.0
5581 117m/z  neg
   11.93_842.0
5582 303n   neg
   11.93_847.0
5583 137m/z  neg
   11.93_863.0
5584 144m/z  neg
   11.93_875.0
5585 160m/z  neg
   11.93_879.0
5586 135m/z  neg
   11.94_281.6
5587 661m/z  pos
   11.94_289.1
5588 581m/z  pos
   11.94_289.6
5589 524m/z  pos
   11.94_522.7
5590 588m/z  pos
   11.94_523.3
5591 704n   pos
   11.94_543.8
5592 503m/z  pos
11.94_551.8
5593 375m/z pos 11.94_552.3
5594 357m/z pos 11.94_555.3
5595 563m/z pos 11.94_612.3
5596 762m/z neg 11.94_620.3
5597 240m/z neg 11.94_626.3
5598 208m/z neg 11.94_708.2
5599 783m/z neg 11.94_716.2
5600 934m/z neg 11.94_813.0
5601 198m/z pos 11.94_813.5
5602 215m/z pos 11.94_843.0
5603 129m/z neg 11.94_878.0
5604 238n neg 11.94_897.0
5605 163m/z neg 11.94_914.0
5606 343n neg 11.94_930.0
5607 356n neg 11.95_104.1
5608 063m/z pos 11.96_481.3
5609 513m/z neg 11.96_505.3
5610 524m/z neg 11.96_704.3
5611 366m/z neg 11.96_794.0
5612 189n neg 11.96_848.5
5613 750m/z neg 11.96_905.0
5614 175m/z neg 11.96_907.0
5615 164m/z neg 11.98_634.4
5616 590m/z pos 11.99_324.2
5617 912m/z pos
| m/z | Retention Time | Charge | Intensity |
|-----|----------------|--------|-----------|
| 310 | 11.99          | 590.4  | pos       |
| 573 | 12.00          | 480.3  | pos       |
| 505 | 12.00          | 718.5  | pos       |
| 713 | 12.00          | 730.5  | pos       |
| 443 | 12.00          | 816.5  | neg       |
| 729 | 12.02          | 353.2  | pos       |
| 341 | 12.02          | 397.3  | pos       |
| 446 | 12.02          | 462.3  | pos       |
| 395 | 12.03          | 644.4  | pos       |
| 261 | 12.04          | 130.0  | pos       |
| 885 | 12.04          | 259.1  | pos       |
| 712 | 12.04          | 366.2  | pos       |
| 806 | 12.04          | 414.3  | pos       |
| 256 | 12.04          | 458.3  | pos       |
| 515 | 12.04          | 504.3  | pos       |
| 209 | 12.07          | 390.2  | pos       |
| 816 | 12.07          | 636.4  | pos       |
| 245 | 12.07          | 887.5  | pos       |
| 518 | 12.08          | 382.2  | pos       |
| 999 | 12.08          | 441.3  | pos       |
| 396 | 12.08          | 465.3  | pos       |
| 564 | 12.08          | 537.5  | neg       |
| 422 | 12.08          | 764.5  | pos       |
| 535 | 12.08          | 764.5  | neg       |
| Time  | m/z   | Charge | Status |
|-------|-------|--------|--------|
| 12.08 | 845.5 |        |        |
| 12.09 | 491.3 |        |        |
| 12.10 | 124.9 |        |        |
| 12.10 | 279.2 |        |        |
| 12.10 | 329.2 |        |        |
| 12.10 | 475.3 |        |        |
| 12.10 | 603.5 |        |        |
| 12.11 | 198.1 |        |        |
| 12.11 | 298.2 |        |        |
| 12.11 | 361.2 |        |        |
| 12.11 | 379.2 |        |        |
| 12.11 | 419.3 |        |        |
| 12.12 | 319.2 |        |        |
| 12.12 | 471.3 |        |        |
| 12.12 | 538.4 |        |        |
| 12.13 | 537.4 |        |        |
| 12.14 | 212.1 |        |        |
| 12.14 | 549.3 |        |        |
| 12.15 | 776.5 |        |        |
| 12.15 | 823.6 |        |        |
| 12.15 | 824.5 |        |        |
| 12.16 | 255.2 |        |        |
| 12.16 | 490.3 |        |        |
| 12.16 | 519.4 |        |        |
| 12.16 | 519.4 |        |        |
| 12.16 | 519.4 |        |        |
12.18_317.2
5668 738m/z  pos
12.19_281.2
5669 496m/z  pos
12.19_421.3
5670 362m/z  pos
12.19_422.3
5671 342n  pos
12.19_502.4
5672 089m/z  pos
12.20_289.2
5673 440m/z  pos
12.22_456.3
5674 972m/z  pos
12.22_893.5
5675 617m/z  pos
12.23_392.2
5676 959n  pos
12.23_626.4
5677 652n  pos
12.23_633.4
5678 776m/z  pos
12.24_340.2
5679 894m/z  pos
12.24_350.3
5680 121m/z  pos
12.24_410.3
5681 323m/z  pos
12.26_489.3
5682 571m/z  neg
12.26_582.4
5683 387n  pos
12.26_808.0
5684 920m/z  pos
12.27_273.1
5685 029m/z  pos
12.27_908.5
5686 133m/z  pos
12.28_489.2
5687 313m/z  pos
12.28_510.3
5688 954m/z  pos
12.28_538.3
5689 921m/z  pos
12.28_538.4
5690 120n  pos
12.30_494.3
5691 855n  pos
12.32_236.2
5692 124n  pos
12.32_278.2
5693 265m/z   pos
12.32_450.3
5694 582n     pos
12.32_451.3
5695 652m/z   pos
12.32_484.2
5696 922n     pos
12.32_608.3
5697 907m/z   pos
12.34_195.1
5698 239m/z   pos
12.34_318.2
5699 900n     pos
12.34_376.3
5700 195m/z   pos
12.34_406.3
5701 324n     pos
12.34_650.4
5702 439m/z   pos
12.35_175.1
5703 478m/z   pos
12.35_179.1
5704 326n     pos
12.35_299.2
5705 611m/z   pos
12.35_362.3
5706 060n     pos
12.35_421.3
5707 756m/z   pos
12.35_458.3
5708 626n     pos
12.36_391.2
5709 894m/z   pos
12.36_428.3
5710 403m/z   pos
12.36_456.3
5711 548n     pos
12.38_314.2
5712 725m/z   pos
12.38_552.4
5713 111n     pos
12.39_352.3
5714 260m/z   pos
12.39_375.2
5715 925m/z   pos
12.39_389.3
5716 438m/z   pos
12.39_532.3
5717 785n     pos
12.40_419.3
5718 183m/z    pos
12.41_518.4
5719 000n    pos
12.42_466.3
5720 617n    pos
12.43_799.6
5721 501m/z    pos
12.45_286.2
5722 171n    pos
12.45_303.2
5723 347m/z    pos
12.45_480.3
5724 709m/z    pos
12.45_622.4
5725 098m/z    pos
12.47_275.2
5726 603m/z    pos
12.47_299.2
5727 638m/z    pos
12.47_538.3
5728 918m/z    pos
12.48_410.3
5729 349m/z    pos
12.49_357.2
5730 790n    pos
12.49_650.4
5731 424m/z    pos
12.52_497.3
5732 418m/z    pos
12.52_579.4
5733 074m/z    pos
12.54_278.2
5734 270n    pos
12.54_412.3
5735 252n    pos
12.54_690.4
5736 384m/z    pos
12.55_489.3
5737 572m/z    neg
12.56_237.1
5738 864m/z    pos
12.56_268.2
5739 679m/z    pos
12.56_452.4
5740 003n    pos
12.58_295.2
5741 299m/z    pos
12.60_433.3
5742 370m/z    pos
| m/z   | retention time |
|-------|----------------|
| 007   | 12.60          |
| 293   | 12.61          |
| 826   | 12.61          |
| 242   | 12.61          |
| 282   | 12.62          |
| 716   | 12.62          |
| 813   | 12.62          |
| 966   | 12.62          |
| 418   | 12.64          |
| 355   | 12.65          |
| 630   | 12.65          |
| 840   | 12.65          |
| 561   | 12.65          |
| 210   | 12.66          |
| 550   | 12.66          |
| 656   | 12.66          |
| 873   | 12.66          |
| 608   | 12.68          |
| 804   | 12.68          |
| 904   | 12.69          |
| 327   | 12.69          |
| 923   | 12.70          |
| 894   | 12.70          |
| 729   | 12.70          |
| 116   | 12.70          |

*pos* indicates a positive ion, *neg* indicates a negative ion.
5793 261 n  pos  12.91_254.2
5794 833 m/z  pos  12.91_427.3
5795 221 m/z  pos  12.92_309.2
5796 445 m/z  pos  12.92_495.4
5797 042 m/z  pos  12.92_499.3
5798 826 m/z  pos  12.93_420.3
5799 483 n  pos  12.95_151.0
5800 974 m/z  pos  12.95_332.2
5801 948 n  pos  12.95_376.3
5802 215 n  pos  12.95_403.3
5803 248 m/z  pos  12.97_313.2
5804 767 m/z  pos  12.97_383.3
5805 364 m/z  pos  12.99_677.5
5806 602 m/z  pos  12.99_860.5
5807 155 m/z  pos  13.00_499.3
5808 837 m/z  pos  13.00_517.3
5809 916 m/z  pos  13.00_536.4
5810 133 n  pos  13.00_808.0
5811 925 m/z  pos  13.00_896.4
5812 572 m/z  pos  13.03_495.4
5813 068 m/z  pos  13.03_859.5
5814 981 m/z  pos  13.03_909.5
5815 233 n  pos  13.05_304.2
5816 418 n  pos  13.05_533.3
5817 854 m/z  pos
13.06_551.4
5818 008n  pos
13.07_645.5
5819 025m/z  pos
13.08_656.4
5820 331n  pos
13.09_462.3
5821 623m/z  pos
13.09_485.3
5822 942m/z  pos
13.09_503.4
5823 111m/z  pos
13.12_170.1
5824 552m/z  pos
13.12_247.2
5825 435m/z  pos
13.12_265.2
5826 543m/z  pos
13.12_281.2
5827 742n  pos
13.12_281.4
5828 137m/z  pos
13.13_293.2
5829 509m/z  pos
13.13_918.5
5830 826m/z  pos
13.14_403.3
5831 596m/z  pos
13.14_490.3
5832 678n  pos
13.14_575.4
5833 707m/z  pos
13.14_636.3
5834 032n  pos
13.14_681.2
5835 968m/z  neg
13.14_695.3
5836 695m/z  pos
13.16_286.2
5837 345m/z  pos
13.16_512.4
5838 098n  pos
13.17_269.2
5839 286m/z  pos
13.17_279.2
5840 345m/z  pos
13.17_876.6
5841 948m/z  pos
13.18_100.9
5842 334m/z  neg
13.18_239.2
5843 408m/z       pos
13.20_134.8
5844 941m/z       neg
13.20_138.1
5845 428n         pos
13.20_175.1
5846 491m/z       pos
13.20_182.1
5847 329n         pos
13.20_184.1
5848 478n         pos
13.20_188.1
5849 438n         pos
13.20_196.1
5850 483n         pos
13.20_210.1
5851 632n         pos
13.20_225.1
5852 864m/z       pos
13.20_245.2
5853 285m/z       pos
13.20_280.2
5854 427n         pos
13.20_347.2
5855 195m/z       neg
13.20_560.4
5856 845n         pos
13.20_581.4
5857 543m/z       neg
13.20_720.5
5858 908m/z       pos
13.20_742.5
5859 783m/z       pos
13.20_756.2
5860 276m/z       pos
13.20_773.5
5861 621n         pos
13.20_778.1
5862 412m/z       pos
13.20_778.5
5863 509m/z       pos
13.20_780.1
5864 515m/z       pos
13.20_808.0
5865 929m/z       pos
13.20_819.5
5866 496n         pos
13.20_820.6
5867 140m/z       pos
13.20_825.5
5868 926n  pos
13.20_832.5
5869 888m/z  pos
13.20_844.6
5870 315m/z  pos
13.21_151.1
5871 108m/z  pos
13.21_329.2
5872 476m/z  neg
13.21_364.2
5873 098m/z  neg
13.21_536.4
5874 124n  pos
13.21_578.4
5875 283m/z  pos
13.21_718.5
5876 773m/z  pos
13.24_455.3
5877 758m/z  pos
13.24_896.4
5878 542m/z  pos
13.27_716.5
5879 516m/z  pos
13.27_795.0
5880 803m/z  pos
13.28_340.3
5881 603m/z  pos
13.28_770.0
5882 696m/z  pos
13.30_447.3
5883 493m/z  pos
13.32_494.3
5884 964m/z  pos
13.33_533.3
5885 888m/z  pos
13.33_608.4
5886 794m/z  pos
13.33_633.4
5887 660m/z  pos
13.36_566.4
5888 433n  pos
13.36_781.0
5889 582m/z  pos
13.37_353.3
5890 329n  pos
13.38_522.4
5891 156n  pos
13.38_575.4
5892 722m/z  pos
| 5893  | 712m/z     | pos |
|-------|------------|-----|
| 13.40 | 223.1      |     |
| 5894  | 896n       | pos |
| 13.41 | 478.3      |     |
| 5895  | 395m/z     | pos |
| 13.44 | 239.1      |     |
| 5896  | 505m/z     | pos |
| 13.44 | 434.3      |     |
| 5897  | 634n       | pos |
| 13.45 | 195.1      |     |
| 5898  | 240m/z     | pos |
| 13.45 | 390.3      |     |
| 5899  | 369n       | pos |
| 13.45 | 487.3      |     |
| 5900  | 481m/z     | pos |
| 13.46 | 364.3      |     |
| 5901  | 446m/z     | pos |
| 13.46 | 369.3      |     |
| 5902  | 023m/z     | pos |
| 13.46 | 874.4      |     |
| 5903  | 930m/z     | neg |
| 13.48 | 537.4      |     |
| 5904  | 156m/z     | neg |
| 13.49 | 415.0      |     |
| 5905  | 397m/z     | pos |
| 13.49 | 446.3      |     |
| 5906  | 421n       | pos |
| 13.49 | 484.4      |     |
| 5907  | 047m/z     | pos |
| 13.49 | 537.4      |     |
| 5908  | 222m/z     | pos |
| 13.51 | 223.1      |     |
| 5909  | 711m/z     | pos |
| 13.51 | 403.3      |     |
| 5910  | 600m/z     | pos |
| 13.52 | 519.4      |     |
| 5911  | 072m/z     | pos |
| 13.55 | 279.2      |     |
| 5912  | 344m/z     | pos |
| 13.57 | 346.3      |     |
| 5913  | 130n       | pos |
| 13.58 | 857.5      |     |
| 5914  | 139n       | pos |
| 13.61 | 377.2      |     |
| 5915  | 720m/z     | neg |
| 13.62 | 261.2      |     |
| 5916  | 236m/z     | neg |
| 13.64 | 537.4      |     |
| 5917  | 159m/z     | neg |
| m/z | Value | Position |
|-----|-------|----------|
| 13.65 | 379.2 | pos |
| 13.65 | 397.3 | pos |
| 13.65 | 432.3 | pos |
| 13.65 | 468.3 | pos |
| 13.66 | 720.5 | pos |
| 13.66 | 503.4 | pos |
| 13.66 | 535.4 | pos |
| 13.67 | 720.5 | pos |
| 13.68 | 535.4 | pos |
| 13.69 | 770.0 | pos |
| 13.69 | 848.4 | pos |
| 13.69 | 889.5 | pos |
| 13.69 | 948.4 | pos |
| 13.70 | 781.0 | pos |
| 13.71 | 590.4 | pos |
| 13.71 | 904.4 | pos |
| 13.72 | 515.4 | pos |
| 13.72 | 519.4 | pos |
| 13.72 | 781.0 | pos |
| 13.74 | 635.4 | pos |
| 13.76 | 281.2 | pos |
| 13.76 | 317.2 | pos |
| 13.76 | 565.4 | pos |
| 13.78 | 475.3 | pos |
| 13.78 | 872.5 | pos |
| 13.78 | 876.6 | pos |
| 13.79 | 256.2 | pos |
| 13.80 | 466.2 | pos |
13.79_395.2
5943 256 m/z    pos
13.79_778.1
5944 413 m/z    pos
13.79_778.5
5945 478 m/z    pos
13.79_790.5
5946 887 m/z    pos
13.79_799.5
5947 777 n      pos
13.79_804.5
5948 577 m/z    pos
13.79_823.6
5949 518 n      pos
13.80_825.5
5950 705 n      pos
13.82_878.5
5951 925 m/z    neg
13.83_279.2
5952 339 m/z    pos
13.83_795.0
5953 740 m/z    pos
13.84_554.1
5954 802 m/z    pos
13.85_433.3
5955 687 m/z    pos
13.85_468.3
5956 851 n      pos
13.85_566.4
5957 607 n      pos
13.87_535.4
5958 045 m/z    pos
13.88_523.4
5959 402 m/z    pos
13.88_577.4
5960 885 m/z    pos
13.89_383.3
5961 421 n      pos
13.89_483.3
5962 525 m/z    pos
13.90_338.3
5963 446 m/z    pos
13.95_317.2
5964 761 m/z    pos
13.95_567.4
5965 650 m/z    pos
13.97_281.2
5966 506 m/z    pos
13.97_519.4
5967 074 m/z    pos
13.97_589.4
5968 526m/z  pos
13.97_591.4
5969 705m/z  pos
13.97_592.4
5970 755n   pos
13.98_100.9
5971 334m/z  neg
13.98_227.2
5972 042m/z  pos
13.98_842.6
5973 075m/z  pos
13.99_283.2
5974 598m/z  neg
14.00_247.2
5975 466m/z  pos
14.00_282.2
5976 590n   pos
14.00_778.1
5977 464m/z  pos
14.00_780.5
5978 579m/z  pos
14.00_789.5
5979 791n   pos
14.00_833.6
5980 083n   pos
14.01_523.4
5981 425m/z  pos
14.01_717.5
5982 911m/z  pos
14.01_831.5
5983 833n   pos
14.01_840.6
5984 218m/z  pos
14.02_473.3
5985 609m/z  neg
14.06_284.2
5986 969m/z  pos
14.08_577.4
5987 879m/z  pos
14.09_475.3
5988 800m/z  pos
14.09_539.4
5989 372m/z  pos
14.10_740.5
5990 510m/z  pos
14.13_696.5
5991 400m/z  pos
14.13_805.5
5992 681n   pos
14.15_519.4
5993 072m/z  pos
14.15_610.5
5994 102m/z  pos
14.15_794.0
5995 667m/z  pos
14.16_523.4
5996 394m/z  pos
14.16_592.4
5997 747n  pos
14.17_652.5
5998 029m/z  pos
14.18_765.5
5999 526n  pos
14.19_608.4
6000 796m/z  pos
14.19_804.0
6001 768m/z  pos
14.21_492.4
6002 080m/z  pos
14.21_799.6
6003 604m/z  pos
14.22_590.4
6004 586m/z  pos
14.26_411.2
6005 803m/z  pos
14.26_519.4
6006 084m/z  pos
14.26_524.4
6007 524n  pos
14.28_867.5
6008 517m/z  neg
14.29_523.4
6009 399m/z  pos
14.29_578.4
6010 948m/z  pos
14.29_711.5
6011 206m/z  pos
14.33_391.3
6012 600m/z  pos
14.33_784.5
6013 909m/z  pos
14.34_695.5
6014 161m/z  pos
14.36_667.4
6015 865m/z  pos
14.37_358.3
6016 122n  pos
14.38_573.4
6017 601m/z  pos
| m/z | pos | m/z | pos | m/z | pos |
|-----|-----|-----|-----|-----|-----|
| 14.73 | 546.4 | 14.73 | 876.6 | 14.74 | 569.4 |
| 14.74 | 616.5 | 14.75 | 279.2 | 14.76 | 319.2 |
| 14.76 | 336.2 | 14.76 | 591.4 | 14.77 | 591.4 |
| 14.79 | 594.4 | 14.79 | 576.4 | 14.79 | 594.4 |
| 14.80 | 405.3 | 14.80 | 573.4 | 14.81 | 429.3 |
| 14.81 | 521.4 | 14.81 | 592.4 | 14.81 | 908.5 |
| 14.82 | 344.0 | 14.82 | 575.4 | 14.84 | 368.3 |
| 14.84 | 699.5 | 14.85 | 522.4 | 14.91 | 435.3 |
| 14.91 | 435.3 | 14.91 | 435.3 | 14.91 | 435.3 |
| Time   | m/z    | Charge | Status |
|--------|--------|--------|--------|
| 14.91  | 577.4  |        |        |
| 14.93  | 593.4  |        |        |
| 14.96  | 128.0  |        | pos    |
| 14.96  | 279.2  |        | pos    |
| 14.96  | 361.0  |        | pos    |
| 14.98  | 574.4  |        | pos    |
| 15.00  | 285.2  |        | pos    |
| 15.03  | 191.1  |        | pos    |
| 15.04  | 123.7  |        | pos    |
| 15.04  | 628.1  |        | pos    |
| 15.07  | 294.2  |        | pos    |
| 15.22  | 153.0  |        | pos    |
| 15.24  | 437.3  |        | pos    |
| 15.25  | 138.0  |        | pos    |
| 15.27  | 636.5  |        | pos    |
| 15.29  | 547.4  |        | pos    |
| 15.29  | 579.5  |        | pos    |
| 15.33  | 261.1  |        | pos    |
| 15.33  | 584.4  |        | pos    |
| 15.33  | 803.5  |        | pos    |
| 15.35  | 138.0  |        | pos    |
| 15.37  | 312.3  |        | pos    |
| 15.37  | 624.4  |        | pos    |
| 15.39  | 595.4  |        | pos    |
| 15.98  | 987.4  |        | pos    |
15.39_904.4
6093 817m/z pos
15.40_121.0
6094 658m/z pos
15.40_153.0
6095 461m/z pos
15.41_564.4
6096 018m/z pos
15.41_580.5
6097 049m/z pos
15.43_476.3
6098 680m/z pos
15.43_656.4
6099 369m/z pos
15.45_584.4
6100 272m/z pos
15.46_320.3
6101 115n pos
15.46_574.4
6102 655n pos
15.46_575.4
6103 712m/z pos
15.46_675.6
6104 811m/z pos
15.48_115.0
6105 509m/z pos
15.48_566.4
6106 162m/z pos
15.48_587.5
6107 543m/z pos
15.49_473.2
6108 825m/z neg
15.49_617.4
6109 810m/z pos
15.49_850.6
6110 353m/z pos
15.51_474.2
6111 936n pos
15.51_548.3
6112 869m/z pos
15.52_565.5
6113 726m/z pos
15.53_107.0
6114 508m/z pos
15.53_619.4
6115 966m/z pos
15.55_191.1
6116 806m/z pos
15.60_579.5
6117 037m/z pos
15.60 597.5
6118 101m/z  pos
15.64_191.1
6119 813m/z  pos
15.75_341.0
6120 200m/z  pos
15.75_776.2
6121 379m/z  pos
15.77_326.9
6122 687m/z  pos
15.85_429.3
6123 759m/z  pos
15.86_201.1
6124 649m/z  pos
15.87_107.0
6125 499m/z  pos
15.87_131.9
6126 029m/z  pos
15.88_283.0
6127 348m/z  pos
15.88_355.0
6128 727m/z  pos
15.89_267.0
6129 005m/z  pos
15.91_117.0
6130 709m/z  pos
15.91_119.0
6131 860m/z  pos
15.91_128.0
6132 626m/z  pos
15.91_203.1
6133 799m/z  pos
15.93_207.0
6134 336m/z  pos
15.93_371.1
6135 039m/z  pos
15.93_430.8
6136 881m/z  pos
15.97_191.1
6137 807m/z  pos
15.98_125.9
6138 688m/z  pos
2.00_135.66
6139 47m/z   pos
2.00_179.51
6140 51m/z   neg
2.00_238.02
6141 45m/z   neg
2.00_249.06
6142 04n    neg
| m/z | Time (s) | Charge | Status |
|-----|----------|--------|--------|
| 68  | 2.00_266.05 | 8n     | neg    |
| 66  | 2.00_282.02 | 2n     | neg    |
| 77  | 2.00_296.03 | 2n     | neg    |
| 56  | 2.00_300.00 | m/z    | neg    |
| 60  | 2.00_305.93 | m/z    | neg    |
| 80  | 2.00_307.58 | m/z    | neg    |
| 69  | 2.00_332.95 | m/z    | neg    |
| 72  | 2.00_334.95 | m/z    | neg    |
| 52  | 2.00_340.90 | m/z    | neg    |
| 74  | 2.00_348.99 | m/z    | neg    |
| 87  | 2.00_359.02 | m/z    | pos    |
| 87  | 2.00_359.97 | m/z    | neg    |
| 68  | 2.00_367.92 | m/z    | neg    |
| 67  | 2.00_369.92 | m/z    | neg    |
| 34  | 2.00_378.11 | m/z    | neg    |
| 45  | 2.00_441.11 | n      | pos    |
| 67  | 2.00_451.03 | n      | pos    |
| 64  | 2.00_453.05 | m/z    | neg    |
| 36  | 2.00_461.06 | m/z    | pos    |
| 35  | 2.00_468.09 | m/z    | neg    |
| 81  | 2.00_476.08 | m/z    | neg    |
| 41  | 2.00_478.05 | n      | pos    |
| 49  | 2.00_483.05 | m/z    | neg    |
| 76  | 2.00_483.09 | m/z    | neg    |
| 99  | 2.00_484.11 | m/z    | pos    |
| 50  | 2.00_484.11 | m/z    | pos    |
| m/z | RT/minute | Charge | Status |
|-----|-----------|--------|--------|
| 90   | 2.00      |        | neg    |
| 88   | 2.00      |        | pos    |
| 86   | 2.01      |        | pos    |
| 80   | 2.01      |        | neg    |
| 11   | 2.01      |        | pos    |
| 44   | 2.01      |        | neg    |
| 40   | 2.01      |        | neg    |
| 43   | 2.01      |        | pos    |
| 77   | 2.01      |        | neg    |
| 93   | 2.01      |        | neg    |
| 92   | 2.01      |        | neg    |
| 39   | 2.01      |        | neg    |
| 75   | 2.03      |        | neg    |
| 46   | 2.03      |        | pos    |
| 44   | 2.04      |        | pos    |
| 64   | 2.04      |        | pos    |
| 73   | 2.04      |        | pos    |
| 89   | 2.04      |        | neg    |
| 06   | 2.04      |        | pos    |
| 01   | 2.05      |        | pos    |
| 89   | 2.05      |        | pos    |
| 13   | 2.05      |        | pos    |
| 30   | 2.05      |        | pos    |
| 85   | 2.05      |        | pos    |
| 23   | 2.05      |        | pos    |
2.05_274.09
6193 84m/z  pos
2.05_351.10
6194 25m/z  pos
2.06_171.02
6195 66m/z  neg
2.06_202.96
6196 43m/z  neg
2.06_232.99
6197 75m/z  neg
2.06_256.11
6198 56m/z  neg
2.06_318.08
6199 56m/z  neg
2.07_200.00
6200 12m/z  pos
2.08_227.90
6201 42m/z  neg
2.08_229.06
6202 89m/z  neg
2.08_229.90
6203 13m/z  neg
2.09_177.10
6204 63m/z  pos
2.12_111.04
6205 38m/z  pos
2.12_220.08
6206 00m/z  pos
2.12_341.15
6207 22n   pos
2.12_399.34
6208 87m/z  pos
2.12_417.24
6209 45n   pos
2.12_431.23
6210 23n   pos
2.12_549.34
6211 62m/z  pos
2.12_724.25
6212 64m/z  pos
2.13_131.70
6213 25m/z  pos
2.13_294.22
6214 85m/z  pos
2.13_319.13
6215 50m/z  pos
2.13_458.10
6216 51m/z  pos
2.13_459.09
6217 55n   pos
2.13_502.41
6218 26m/z  pos
  2.14_188.04
6219 55m/z  neg
  2.14_198.07
6220 41m/z  neg
  2.14_215.06
6221 44m/z  neg
  2.14_230.01
6222 15m/z  neg
  2.14_250.01
6223 93m/z  neg
  2.14_252.01
6224 37m/z  neg
  2.14_254.95
6225 13m/z  neg
  2.14_265.98
6226 92m/z  neg
  2.14_267.00
6227 48m/z  neg
  2.14_281.97
6228 25m/z  neg
  2.14_283.16
6229 31m/z  neg
  2.14_293.00
6230 67m/z  neg
  2.14_295.03
6231 45n  neg
  2.14_361.10
6232 53m/z  neg
  2.14_430.22
6233 14m/z  neg
  2.14_462.23
6234 80m/z  neg
  2.15_145.03
6235 57m/z  pos
  2.15_226.82
6236 35m/z  neg
  2.15_256.11
6237 61m/z  neg
  2.15_332.15
6238 28n  neg
  2.15_379.11
6239 57n  neg
  2.15_446.19
6240 42m/z  neg
  2.21_151.06
6241 23m/z  pos
  2.22_136.03
6242 91m/z  pos
| MS/MS Number | Time [min] | RT [min] | m/z | Charge | Ionization Status |
|--------------|------------|----------|-----|--------|------------------|
| 6243         | 2.22       | 185.87   | 51  | neg    |                  |
| 6244         | 2.24       | 164.92   | 89  | neg    |                  |
| 6245         | 2.26       | 200.00   | 37  | neg    |                  |
| 6246         | 2.27       | 130.00   | 27  | pos    |                  |
| 6247         | 2.27       | 146.01   | 83  | pos    |                  |
| 6248         | 2.27       | 181.98   | 98  | pos    |                  |
| 6249         | 2.27       | 189.00   | 96  | pos    |                  |
| 6250         | 2.27       | 221.08   | 94  | pos    |                  |
| 6251         | 2.27       | 262.01   | 44  | pos    |                  |
| 6252         | 2.28       | 158.97   | 51  | neg    |                  |
| 6253         | 2.28       | 171.02   | 54  | neg    |                  |
| 6254         | 2.28       | 192.93   | 58  | neg    |                  |
| 6255         | 2.28       | 221.98   | 21  | neg    |                  |
| 6256         | 2.28       | 224.96   | 58  | neg    |                  |
| 6257         | 2.28       | 227.90   | 44  | neg    |                  |
| 6258         | 2.28       | 229.90   | 16  | neg    |                  |
| 6259         | 2.28       | 232.99   | 77  | neg    |                  |
| 6260         | 2.28       | 235.99   | 86  | neg    |                  |
| 6261         | 2.28       | 249.98   | 81  | neg    |                  |
| 6262         | 2.28       | 261.00   | 54  | neg    |                  |
| 6263         | 2.28       | 285.98   | 54  | neg    |                  |
| 6264         | 2.28       | 308.02   | 92  | neg    |                  |
| 6265         | 2.29       | 363.10   | 2.33 | neg    |                  |
| 6266         | 30         | 235.14   | 43  | neg    |                  |
| 6267         | 30         | 30n      | 30  | pos    |                  |
| m/z | Precursor Mass | Charge | Status |
|-----|---------------|--------|--------|
| 59n | 2.35_144.02   | pos    |        |
|     | 2.40_166.08   |        |        |
| 88m/z | 2.45_196.15  | pos    |        |
| 45m/z | 2.47_145.03  | pos    |        |
| 40m/z | 2.48_162.06  | pos    |        |
| 26m/z | 2.50_105.93  | pos    |        |
| 43m/z | 2.52_179.10  | pos    |        |
| 68m/z | 2.56_252.13  | pos    |        |
| 93n | 2.59_308.28   | pos    |        |
| 35m/z | 2.64_212.00  | pos    |        |
| 12m/z | 2.65_244.99  | pos    |        |
| 72m/z | 2.72_229.14  | neg    |        |
| 60m/z | 2.85_342.21  | pos    |        |
| 23m/z | 2.91_104.00  | pos    |        |
| 79m/z | 2.95_308.28  | pos    |        |
| 30m/z | 2.98_119.07  | pos    |        |
| 35m/z | 2.98_520.20  | pos    |        |
| 37m/z | 2.99_511.20  | pos    |        |
| 36n | 2.99_519.19   | pos    |        |
| 55n | 2.99_536.40   | pos    |        |
| 80m/z | 2.99_786.25  | pos    |        |
| 74m/z | 3.00_102.04  | pos    |        |
| 72n | 3.00_165.58   | pos    |        |
| 22m/z | 3.00_421.06  | pos    |        |
| 38m/z | 3.01_233.06  | pos    |        |
| 59n | 3.01_233.06   | neg    |        |
| m/z | Charge | Status |
|-----|--------|--------|
| 249.04 | 95 | neg |
| 265.00 | 32 | neg |
| 280.04 | 06 | neg |
| 285.99 | 68 | neg |
| 288.93 | 55 | neg |
| 289.94 | 28 | neg |
| 294.02 | 06 | neg |
| 297.03 | 89 | neg |
| 300.98 | 95 | neg |
| 315.95 | 71 | neg |
| 316.96 | 22 | neg |
| 328.01 | 23 | neg |
| 347.02 | 62 | neg |
| 429.07 | 39 | neg |
| 266.01 | 34 | pos |
| 269.03 | 46 | neg |
| 285.02 | 87 | neg |
| 419.04 | 65 | neg |
| 445.11 | 73 | neg |
| 462.10 | 95 | neg |
| 162.98 | 23 | neg |
| 308.28 | 41 | pos |
| 105.93 | 49 | pos |
| 142.03 | 56 | pos |
| 105.93 | 38 | pos |
| m/z | z | 6318 | pos 3.74 | 105.93 |
|-----|---|------|---------|---------|
| m/z | 6319 | pos 3.83 | 253.14 |
| m/z | 6320 | pos 4.00 | 142.08 |
| m/z | 6321 | pos 4.00 | 145.12 |
| m/z | 6322 | pos 4.07 | 125.09 |
| m/z | 6323 | pos 4.08 | 142.08 |
| m/z | 6324 | pos 4.08 | 176.07 |
| m/z | 6325 | pos 4.09 | 117.05 |
| m/z | 6326 | neg 4.09 | 202.03 |
| m/z | 6327 | neg 4.09 | 247.01 |
| m/z | 6328 | neg 4.09 | 264.00 |
| m/z | 6329 | neg 4.09 | 280.99 |
| m/z | 6330 | neg 4.10 | 172.99 |
| m/z | 6331 | neg 4.10 | 216.98 |
| m/z | 6332 | neg 4.10 | 171.01 |
| m/z | 6333 | neg 4.17 | 124.04 |
| m/z | 6334 | pos 4.18 | 116.05 |
| m/z | 6335 | neg 4.18 | 187.49 |
| m/z | 6336 | pos 4.18 | 202.45 |
| m/z | 6337 | neg 4.18 | 226.07 |
| m/z | 6338 | neg 4.18 | 257.96 |
| m/z | 6339 | neg 4.18 | 263.03 |
| m/z | 6340 | neg 4.18 | 278.01 |
| m/z | 6341 | neg 4.18 | 288.05 |
| m/z | 6342 | neg 4.18 | 288.05 |
4.19_294.99
6368 58m/z    pos
4.19_394.05
6369 83n    pos
4.19_462.10
6370 16n    pos
4.19_522.11
6371 76n    pos
4.19_532.09
6372 56n    pos
4.19_575.40
6373 98m/z    pos
4.19_598.14
6374 99n    pos
4.19_636.22
6375 95n    pos
4.19_885.29
6376 03m/z    pos
4.20_124.89
6377 08m/z    neg
4.20_162.98
6378 25m/z    neg
4.21_204.47
6379 22m/z    pos
4.22_204.13
6380 94m/z    pos
4.22_238.14
6381 41n    pos
4.22_284.20
6382 85m/z    pos
4.22_471.22
6383 47m/z    pos
4.24_136.05
6384 12n    neg
4.24_181.00
6385 63m/z    neg
4.24_183.00
6386 30m/z    neg
4.24_187.86
6387 06m/z    neg
4.24_200.03
6388 01m/z    neg
4.24_267.02
6389 69n    neg
4.24_268.01
6390 68m/z    neg
4.24_285.00
6391 64m/z    neg
4.24_316.96
6392 78m/z    pos
| m/z   | Value     | Charge | Status |
|-------|-----------|--------|--------|
| 58     | 4.25_138.00 | neg    |        |
| 64n    | 4.25_140.00 | pos    |        |
| 35n    | 4.25_143.00 | pos    |        |
| 73m/z  | 4.25_153.57 | pos    |        |
| 58m/z  | 4.25_182.01 | pos    |        |
| 44n    | 4.25_184.01 | pos    |        |
| 21n    | 4.25_197.42 | pos    |        |
| 48m/z  | 4.25_199.43 | neg    |        |
| 78m/z  | 4.25_222.03 | pos    |        |
| 04m/z  | 4.25_224.02 | pos    |        |
| 91m/z  | 4.25_236.99 | pos    |        |
| 53n    | 4.25_255.99 | neg    |        |
| 07m/z  | 4.25_257.98 | neg    |        |
| 81m/z  | 4.25_260.03 | neg    |        |
| 05m/z  | 4.25_284.00 | pos    |        |
| 24m/z  | 4.25_288.00 | pos    |        |
| 25m/z  | 4.25_289.94 | neg    |        |
| 78m/z  | 4.25_298.98 | pos    |        |
| 25m/z  | 4.25_300.98 | neg    |        |
| 31m/z  | 4.25_300.99 | neg    |        |
| 13m/z  | 4.25_302.98 | pos    |        |
| 84m/z  | 4.25_315.99 | pos    |        |
| 96m/z  | 4.25_316.97 | neg    |        |
| 45n    | 4.25_319.96 | neg    |        |
| 33m/z  | 4.25_319.96 | neg    |        |
| Peak Number | retention time | m/z | Charge | Ionisation |
|-------------|----------------|-----|--------|------------|
| 6443        | 4.25_333.02    |     | 14n    | neg        |
| 6444        | 4.25_334.94    |     | 09n    | neg        |
| 6445        | 4.25_334.95    | 08m/z | neg    |            |
| 6446        | 4.25_352.92    | 76m/z | neg    |            |
| 6447        | 4.25_354.91    | 05m/z | neg    |            |
| 6448        | 4.25_358.87    | 83m/z | neg    |            |
| 6449        | 4.25_360.87    | 14m/z | neg    |            |
| 6450        | 4.25_361.97    | 02m/z | neg    |            |
| 6451        | 4.25_362.86    | 44n   | neg    |            |
| 6452        | 4.25_377.94    | 71m/z | neg    |            |
| 6453        | 4.25_436.03    | 15m/z | neg    |            |
| 6454        | 4.25_438.03    | 45n   | neg    |            |
| 6455        | 4.25_452.00    | 21n   | neg    |            |
| 6456        | 4.25_465.04    | 30n   | pos    |            |
| 6457        | 4.25_468.04    | 64m/z | neg    |            |
| 6458        | 4.25_470.99    | 76n   | neg    |            |
| 6459        | 4.25_477.04    | 48m/z | neg    |            |
| 6460        | 4.25_480.19    | 36n   | pos    |            |
| 6461        | 4.25_488.96    | 96m/z | pos    |            |
| 6462        | 4.25_488.98    | 54m/z | neg    |            |
| 6463        | 4.25_490.96    | 62m/z | pos    |            |
| 6464        | 4.25_504.03    | 27m/z | neg    |            |
| 6465        | 4.25_506.02    | 07m/z | neg    |            |
| 6466        | 4.25_515.00    | 84m/z | neg    |            |
| 6467        | 4.25_515.00    | 78n   | neg    |            |
| Time (s)  | m/z   | Charge | P/1 | Time (s)  | m/z   | Charge | P/1 | Time (s)  | m/z   | Charge | P/1 | Time (s)  | m/z   | Charge | P/1 |
|----------|-------|--------|-----|----------|-------|--------|-----|----------|-------|--------|-----|----------|-------|--------|-----|
| 4.25     | 51    | neg    |     | 4.25     | 31    | pos    |     | 4.25     | 82    | pos    |     | 4.25     | 12    | neg    |     |
| 5.98     | 4.25  | 51m/z  |     | 4.25     | 31m/z | pos    |     | 4.25     | 82m/z | pos    |     | 4.25     | 12m/z | neg    |     |
| 5.98     | 4.25  | 526.05 |     | 4.25     | 528.04| pos    |     | 4.25     | 530.03| pos    |     | 4.25     | 532.02| neg    |     |
| 5.98     | 4.25  | 31m/z  |     | 4.25     | 82m/z | pos    |     | 4.25     | 12m/z | pos    |     | 4.25     | 622.09| pos    |     |
| 6.05     | 4.25  | 32     |     | 4.25     | 635.07| pos    |     | 4.25     | 636.05| pos    |     | 4.25     | 637.07| neg    |     |
| 6.05     | 4.25  | 636.07 |     | 4.25     | 638.07| pos    |     | 4.25     | 646.07| pos    |     | 4.25     | 652.05| pos    |     |
| 6.05     | 4.25  | 637.07 |     | 4.25     | 654.04| pos    |     | 4.25     | 661.07| pos    |     | 4.25     | 654.04| pos    |     |
| 6.05     | 4.25  | 860.06 |     | 4.25     | 685.06| pos    |     | 4.25     | 685.07| pos    |     | 4.25     | 661.07| pos    |     |
| 6.05     | 4.25  | 821.13 |     | 4.25     | 823.12| pos    |     | 4.25     | 865.09| pos    |     | 4.25     | 865.09| pos    |     |
| 6.05     | 4.25  | 823.12 |     | 4.25     | 823.12| pos    |     | 4.25     | 865.09| pos    |     | 4.25     | 865.09| pos    |     |
| 6.05     | 4.25  | 867.09 |     | 4.25     | 867.09| pos    |     | 4.25     | 867.09| pos    |     | 4.25     | 867.09| pos    |     |
| 6.05     | 4.26  | 155.56 |     | 4.25     | 208.13| neg    |     | 4.25     | 253.18| pos    |     | 4.25     | 208.13| neg    |     |
| 6.05     | 4.29  | 134.09 |     | 4.25     | 253.18| pos    |     | 4.25     | 253.18| pos    |     | 4.25     | 253.18| pos    |     |
| 6.05     | 4.29  | 512.79 |     | 4.31     | 208.13| pos    |     | 4.31     | 253.18| pos    |     | 4.31     | 208.13| pos    |     |
| 6.05     | 4.31  | 208.13|     | 4.31     | 253.18| pos    |     | 4.31     | 208.13| pos    |     | 4.31     | 253.18| pos    |     |
| 6.05     | 4.31  | 208.13|     | 4.31     | 253.18| pos    |     | 4.31     | 208.13| pos    |     | 4.31     | 253.18| pos    |     |
| 6.05     | 4.31  | 208.13|     | 4.31     | 253.18| pos    |     | 4.31     | 208.13| pos    |     | 4.31     | 253.18| pos    |     |
4.32_409.58
6493 13m/z pos
4.32_464.76
6494 57m/z pos
4.32_465.26
6495 84m/z pos
4.39_300.01
6496 73m/z neg
4.39_338.13
6497 90m/z pos
4.40_199.98
6498 91m/z pos
4.41_243.99
6499 75m/z pos
4.41_437.72
6500 59m/z pos
4.42_104.00
6501 87m/z pos
4.42_282.17
6502 01n pos
4.42_375.70
6503 25m/z pos
4.42_500.59
6504 75m/z pos
4.43_218.99
6505 57m/z neg
4.44_304.91
6506 30m/z neg
4.44_328.23
6507 41m/z pos
4.44_333.00
6508 61m/z neg
4.46_296.14
6509 73n pos
4.46_342.21
6510 34m/z pos
4.46_448.23
6511 84m/z pos
4.47_156.03
6512 91m/z pos
4.47_166.08
6513 83m/z pos
4.47_203.00
6514 13m/z neg
4.47_623.12
6515 77m/z pos
4.48_138.05
6516 52m/z neg
4.49_129.05
6517 49m/z neg
6518 94m/z  4.49_276.00  neg
6519 29m/z  4.49_289.89  neg
6520 63m/z  4.50_118.06  neg
6521 58m/z  4.50_246.13  pos
6522 92n   4.50_254.00  pos
6523 09m/z  4.50_455.04  pos
6524 45m/z  4.50_460.21  pos
6525 44m/z  4.50_635.34  pos
6526 42m/z  4.51_141.05  neg
6527 82n   4.51_248.99  neg
6528 15m/z  4.51_281.94  neg
6529 73m/z  4.51_291.89  neg
6530 30m/z  4.51_292.99  neg
6531 27m/z  4.51_308.96  neg
6532 58m/z  4.51_343.06  neg
6533 96m/z  4.52_137.02  neg
6534 36m/z  4.52_270.00  neg
6535 37n   4.52_296.97  pos
6536 92m/z  4.52_379.70  neg
6537 94m/z  4.52_475.01  pos
6538 48m/z  4.52_475.51  pos
6539 25m/z  4.53_341.95  pos
6540 99m/z  4.55_253.16  neg
6541 11m/z  4.55_298.22  pos
6542 46m/z  pos
| m/z | Retention Time | Charge |
|-----|----------------|--------|
| 4.57 | 448.56         | pos    |
| 4.57 | 448.90         |        |
| 4.58 | 125.98         |        |
| 4.63 | 318.19         |        |
| 4.64 | 340.17         |        |
| 4.66 | 410.54         |        |
| 4.67 | 213.11         |        |
| 4.69 | 222.14         |        |
| 4.69 | 222.14         |        |
| 4.70 | 268.21         |        |
| 4.70 | 272.92         |        |
| 4.70 | 308.90         |        |
| 4.70 | 310.89         |        |
| 4.70 | 335.92         |        |
| 4.70 | 337.91         |        |
| 4.70 | 346.96         |        |
| 4.70 | 350.00         |        |
| 4.70 | 362.94         |        |
| 4.70 | 364.94         |        |
| 4.70 | 363.01         |        |
| 4.71 | 263.01         |        |
| 4.72 | 527.05         |        |
| 4.72 | 129.05         |        |
| 4.72 | 197.04         |        |
| 4.72 | 276.00         |        |
| 4.72 | 343.07         |        |
| 4.72 | 360.05         |        |
| 4.73 | 360.05         |        |
4.73_226.01
6568 77m/z  pos
4.73_250.01
6569 24n   neg
4.73_265.97
6570 43m/z  neg
4.73_281.94
6571 73m/z  neg
4.73_289.89
6572 62m/z  neg
4.73_291.89
6573 32m/z  neg
4.73_294.00
6574 34n   neg
4.73_308.96
6575 59m/z  neg
4.73_325.85
6576 99m/z  neg
4.74_248.09
6577 53m/z  pos
4.74_253.99
6578 93m/z  pos
4.74_416.28
6579 63m/z  pos
4.74_460.21
6580 27m/z  pos
4.75_231.02
6581 28m/z  pos
4.75_327.85
6582 68m/z  neg
4.76_348.08
6583 05m/z  neg
4.78_384.20
6584 26n   pos
4.79_304.18
6585 26m/z  pos
4.79_338.89
6586 16m/z  neg
4.79_643.34
6587 17m/z  pos
4.81_733.33
6588 72m/z  pos
4.83_743.39
6589 32m/z  pos
4.84_703.95
6590 99m/z  pos
4.86_125.98
6591 60m/z  pos
4.86_414.24
6592 60n   pos
| m/z | Time (s) | Charge | Status |
|-----|----------|--------|--------|
| 4.86 | 460.31   |        | pos    |
| 4.86 | 880.20   |        | pos    |
| 4.87 | 703.76   |        | pos    |
| 4.89 | 266.17   |        | pos    |
| 4.90 | 377.13   |        |        |
| 4.90 | 312.23   |        | pos    |
| 4.91 | 704.16   |        | pos    |
| 4.91 | 879.94   |        |        |
| 4.95 | 171.13   |        | neg    |
| 4.95 | 213.11   |        | pos    |
| 4.95 | 323.90   |        | pos    |
| 4.95 | 569.30   |        | neg    |
| 4.95 | 569.80   |        | pos    |
| 4.96 | 236.00   |        | pos    |
| 4.96 | 458.27   |        | pos    |
| 4.96 | 504.33   |        | pos    |
| 4.96 | 531.63   |        | pos    |
| 4.98 | 234.00   |        | pos    |
| 5.00 | 130.98   |        | pos    |
| 5.01 | 518.31   |        | neg    |
| 5.03 | 123.11   |        | pos    |
| 5.03 | 311.98   |        | pos    |
| 5.03 | 315.97   |        | pos    |
| 5.04 | 36m/z    |        | neg    |
6618  5.03_379.19  pos
6619  74m/z  pos
6620  5.04_111.11
6621  5.04_151.11
6622  27m/z  pos
6623  5.04_232.98
6624  03m/z  pos
6625  5.04_226.97
6626  05m/z  pos
6627  5.04_245.00
6628  86n  pos
6629  5.04_310.20
6630  11n  pos
6631  5.04_324.99
6632  66m/z  pos
6633  5.04_350.99
6634  17m/z  pos
6635  5.04_432.01
6636  41m/z  pos
6637  5.04_745.28
6638  83m/z  pos
6639  5.05_107.04
6640  95m/z  neg
6641  5.05_271.98
6642  41m/z  neg
6643  5.05_274.98
6644  22m/z  neg
6645  5.05_316.96
6646  46m/z  neg
6647  5.05_333.95
6648  37m/z  neg
6649  5.05_350.94
6650  43m/z  neg
6651  5.05_397.00
6652  21m/z  neg
6653  5.06_124.89
6654  03m/z  neg
6655  5.06_186.43
6656  30m/z  neg
6657  5.06_244.96
6658  52m/z  neg
6659  5.06_306.94
6660  89m/z  neg
6661  5.06_413.98
6662  35n  neg
6663  5.06_420.07
6664  75m/z  neg
| m/z | Time | Charge | Nature |
|-----|------|--------|--------|
| 5.06_475.96 | 17 | neg |
| 5.07_167.10 | 84 | pos |
| 5.07_502.29 | 85 | pos |
| 5.08_141.09 | 25 | pos |
| 5.08_246.07 | 58 | neg |
| 5.08_282.22 | 86 | pos |
| 5.09_207.01 | 05 | neg |
| 5.10_452.33 | 91 | pos |
| 5.10_498.40 | 47 | pos |
| 5.11_220.03 | 58 | pos |
| 5.11_233.99 | 88 | neg |
| 5.11_239.51 | 04 | neg |
| 5.11_259.51 | 19 | neg |
| 5.11_260.01 | 76 | neg |
| 5.11_267.17 | 85 | pos |
| 5.11_312.23 | 54 | pos |
| 5.11_438.06 | 10 | neg |
| 5.12_188.00 | 36 | pos |
| 5.12_189.99 | 98 | pos |
| 5.12_203.00 | 44 | pos |
| 5.12_210.05 | 54 | pos |
| 5.12_231.99 | 28 | neg |
| 5.12_234.00 | 95 | pos |
| 5.12_236.00 | 68 | pos |
| 5.12_264.97 | 52 | pos |
| m/z | Charge | Time (s) |
|-----|--------|----------|
| 43  | pos    | 5.12_266.97 |
| 84  | pos    | 5.12_312.00 |
| 58  | pos    | 5.12_355.99 |
| 16  | neg    | 5.12_369.88 |
| 58  | neg    | 5.12_372.06 |
| 56  | pos    | 5.12_564.08 |
| 44  | neg    | 5.12_786.25 |
| 69  | pos    | 5.14_125.98 |
| 61  | pos    | 5.14_277.03 |
| 17  | neg    | 5.14_282.98 |
| 97  | neg    | 5.14_294.02 |
| 23  | neg    | 5.14_361.93 |
| 81  | neg    | 5.14_371.88 |
| 31  | neg    | 5.14_373.88 |
| 03  | neg    | 5.16_546.32 |
| 54  | pos    | 5.17_377.13 |
| 38  | neg    | 5.18_151.02 |
| 68  | pos    | 5.18_402.27 |
| 22  | pos    | 5.18_592.39 |
| 00  | pos    | 5.19_344.20 |
| 75  | pos    | 5.20_230.99 |
| 39  | neg    | 5.20_266.51 |
| 98  | neg    | 5.20_267.02 |
| 59  | neg    | 5.20_330.19 |
| 30  | pos    | 5.20_330.19 |
|   | Time (min) | m/z   | Charge | Status |
|---|------------|-------|--------|--------|
| 6693 | 5.20 | 437.05 | neg    |        |
| 6694 | 5.21 | 555.02 | neg    |        |
| 6695 | 5.22 | 218.52 | neg    |        |
| 6696 | 5.23 | 168.98 | neg    |        |
| 6697 | 5.24 | 217.01 | neg    |        |
| 6698 | 5.25 | 493.05 | pos    |        |
| 6699 | 5.26 | 240.98 | pos    |        |
| 6700 | 5.27 | 308.90 | neg    |        |
| 6701 | 5.28 | 310.89 | neg    |        |
| 6702 | 5.29 | 332.00 | neg    |        |
| 6703 | 5.30 | 335.92 | neg    |        |
| 6704 | 5.31 | 337.91 | neg    |        |
| 6705 | 5.32 | 346.96 | neg    |        |
| 6706 | 5.33 | 362.93 | neg    |        |
| 6707 | 5.34 | 364.94 | neg    |        |
| 6708 | 5.35 | 125.02 | pos    |        |
| 6709 | 5.36 | 132.51 | pos    |        |
| 6710 | 5.37 | 241.03 | pos    |        |
| 6711 | 5.38 | 247.03 | pos    |        |
| 6712 | 5.39 | 280.18 | pos    |        |
| 6713 | 5.40 | 393.03 | pos    |        |
| 6714 | 5.41 | 421.99 | pos    |        |
| 6715 | 5.42 | 196.98 | pos    |        |
| 6716 | 5.43 | 372.06 | neg    |        |
| 6717 | 5.44 | 55m/z  | pos    |        |
| m/z | Charge | Status |
|-----|--------|--------|
| 5.25_590.35 | 12n | pos |
| 5.25_636.41 | 63m/z | pos |
| 5.27_224.56 | 42m/z | neg |
| 5.27_225.07 | 00n | neg |
| 5.27_351.16 | 22m/z | neg |
| 5.27_471.11 | 19m/z | neg |
| 5.27_615.10 | 28m/z | neg |
| 5.28_203.00 | 18m/z | pos |
| 5.28_226.82 | 33m/z | neg |
| 5.28_255.21 | 47m/z | pos |
| 5.28_353.18 | 03m/z | pos |
| 5.28_554.18 | 96m/z | pos |
| 5.28_566.42 | 85m/z | pos |
| 5.28_616.11 | 44n | pos |
| 5.29_304.25 | 03m/z | pos |
| 5.30_226.99 | 47m/z | neg |
| 5.31_194.11 | 68m/z | pos |
| 5.31_260.18 | 91m/z | pos |
| 5.31_317.19 | 00n | pos |
| 5.31_326.71 | 09m/z | pos |
| 5.31_479.58 | 49m/z | pos |
| 5.31_479.92 | 01m/z | pos |
| 5.31_631.01 | 58m/z | pos |
| 5.31_631.35 | 16m/z | pos |
| 5.31_631.68 | 50m/z | pos |
| m/z   | Charge | Status |
|-------|--------|--------|
| 634.37| +      | pos    |
| 718.87| +      | 5.31   |
| 719.37| +      | 5.31   |
| 946.51| +      | 5.31   |
| 718.87| -      | 5.31   |
| 719.37| -      | 5.31   |
| 415.90| -      | 5.31   |
| 210.05| -      | 5.34   |
| 413.91| -      | 5.34   |
| 415.90| -      | 5.34   |
| 210.05| +      | 5.34   |
| 304.21| +      | 5.34   |
| 142.99| +      | 5.34   |
| 158.00| +      | 5.36   |
| 385.16| -      | 5.36   |
| 630.13| -      | 5.36   |
| 267.00| +      | 5.36   |
| 272.18| +      | 5.36   |
| 630.13| +      | 5.36   |
| 267.00| +      | 5.36   |
| 301.00| +      | 5.36   |
| 339.20| +      | 5.36   |
| 348.72| +      | 5.36   |
| 490.32| +      | 5.36   |
| 568.20| +      | 5.36   |
| 478.40| +      | 5.36   |
| 333.00| +      | 5.36   |
| 478.40| -      | 5.36   |
| 284.19| -      | 5.40   |
| 238.57| +      | 5.41   |
| 238.57| -      | 5.41   |
| 239.08| -      | 5.41   |
| 239.08| -      | 5.41   |
| 239.08| -      | 5.41   |
| m/z   | t   | Charge State | Isotope | Name |
|-------|-----|--------------|---------|------|
| 51    | 5.41| neg          | 362.04  |      |
| 73    | 5.41| neg          | 415.92  |      |
| 19    | 5.43| pos          | 179.07  |      |
| 51    | 5.43| pos          | 193.08  |      |
| 73    | 5.43| pos          | 230.08  |      |
| 28    | 5.43| pos          | 278.07  |      |
| 55    | 5.43| neg          | 283.24  |      |
| 56    | 5.43| pos          | 334.03  |      |
| 97    | 5.43| pos          | 340.06  |      |
| 29    | 5.43| neg          | 355.01  |      |
| 02    | 5.43| neg          | 356.02  |      |
| 94    | 5.43| neg          | 381.21  |      |
| 35    | 5.43| pos          | 334.03  |      |
| 25    | 5.43| pos          | 441.00  |      |
| 57    | 5.44| neg          | 238.36  |      |
| 25    | 5.44| pos          | 698.78  |      |
| 83    | 5.44| pos          | 699.29  |      |
| 11    | 5.46| pos          | 224.16  |      |
| 78    | 5.46| pos          | 361.21  |      |
| 63    | 5.46| pos          | 370.73  |      |
| 69    | 5.46| pos          | 722.42  |      |
| 94    | 5.48| pos          | 224.56  |      |
| 39    | 5.48| neg          | 225.06  |      |
| 97    | 5.50| neg          | 125.98  |      |
| 59    | 5.50| pos          | 289.04  |      |
| 13    | 5.51| neg          | 239.58  |      |
| 73    | 5.51| neg          |         |      |
5.51_240.08
6793 53m/z  neg  5.51_255.21
6794 34m/z  pos  5.51_282.99
6795 15m/z  neg  5.51_285.26
6796 49m/z  pos  5.53_242.17
6797 96m/z  pos  5.53_292.98
6798 83m/z  neg  5.53_375.11
6799 84m/z  neg  5.53_383.22
6800 91n   pos  5.54_504.20
6801 80m/z  pos  5.56_432.88
6802 69m/z  pos  5.57_383.15
6803 22m/z  neg  5.58_274.13
6804 10n   neg  5.60_405.24
6805 19n   pos  5.61_186.14
6806 71m/z  pos  5.61_344.20
6807 94m/z  pos  5.61_359.12
6808 33m/z  neg  5.62_245.56
6809 91m/z  neg  5.65_601.26
6810 85m/z  pos  5.66_294.20
6811 59n   pos  5.66_600.28
6812 30m/z  neg  5.67_234.98
6813 43m/z  neg  5.69_198.12
6814 88m/z  pos  5.69_274.20
6815 33m/z  pos  5.69_427.25
6816 50n   pos  5.69_436.77
6817 53m/z  pos
| M/Z  | Time  | Charge | Status |
|------|-------|--------|--------|
| 6818 | 5.70  | 543.28 | neg    |
| 6819 | 5.71  | 375.11 | neg    |
| 6820 | 5.72  | 125.98 | pos    |
| 6821 | 5.73  | 285.99 |        |
| 6822 | 5.74  | 358.04 | neg    |
| 6823 | 5.74  | 360.06 | neg    |
| 6824 | 5.76  | 312.19 |        |
| 6825 | 5.76  | 449.26 |        |
| 6826 | 5.78  | 267.00 |        |
| 6827 | 5.79  | 301.09 |        |
| 6828 | 5.80  | 338.23 |        |
| 6829 | 5.80  | 341.11 |        |
| 6830 | 5.83  | 242.98 |        |
| 6831 | 5.83  | 266.15 | neg    |
| 6832 | 5.83  | 328.21 |        |
| 6833 | 5.83  | 384.29 |        |
| 6834 | 5.84  | 348.23 |        |
| 6835 | 5.84  | 471.28 |        |
| 6836 | 5.85  | 541.26 |        |
| 6837 | 5.86  | 219.13 | neg    |
| 6838 | 5.89  | 343.08 |        |
| 6839 | 5.90  | 361.14 | neg    |
| 6840 | 5.90  | 511.33 |        |
| 6841 | 5.91  | 413.19 |        |
| 6842 | 5.70  | 543.28 | neg    |
5.95_576.36
6843  28m/z  pos
      5.96_539.24
6844  89m/z  neg
      5.97_228.16
6845  26m/z  pos
      5.99_300.11
6846  82n   pos
      5.99_367.16
6847  04m/z  pos
      6.00_218.21
6848  28m/z  pos
      6.01_176.07
6849  30m/z  pos
      6.01_227.09
6850  13m/z  neg
      6.01_312.21
6851  45n   pos
      6.01_348.23
6852  21n   pos
      6.01_348.99
6853  27m/z  pos
      6.01_541.26
6854  49m/z  neg
      6.02_130.06
6855  55m/z  neg
      6.04_137.13
6856  21m/z  pos
      6.04_165.11
6857  31n   pos
      6.04_217.04
6858  17m/z  neg
      6.04_271.18
6859  66m/z  pos
      6.05_394.12
6860  41m/z  neg
      6.06_186.04
6861  98m/z  pos
      6.06_213.11
6862  47m/z  pos
      6.06_256.11
6863  44m/z  pos
      6.06_416.10
6864  59m/z  neg
      6.07_315.12
6865  93m/z  neg
      6.08_194.98
6866  97m/z  neg
      6.08_237.15
6867  00m/z  pos
| 6.08_261.88 | 84m/z   | neg   |
| 6.08_376.62 | 84m/z   | pos   |
| 6.11_197.14 | 25n     | pos   |
| 6.11_234.13 | 52m/z   | pos   |
| 6.12_318.26 | 73m/z   | pos   |
| 6.13_262.23 | 97m/z   | pos   |
| 6.13_267.12 | 69m/z   | pos   |
| 6.14_208.16 | 70m/z   | neg   |
| 6.14_361.14 | 75m/z   | pos   |
| 6.15_111.04 | 32m/z   | pos   |
| 6.15_197.15 | 34m/z   | pos   |
| 6.16_310.98 | 27m/z   | neg   |
| 6.16_515.28 | 55m/z   | neg   |
| 6.17_234.20 | 83m/z   | pos   |
| 6.17_363.21 | 95m/z   | pos   |
| 6.17_681.21 | 70m/z   | pos   |
| 6.18_133.06 | 50m/z   | neg   |
| 6.18_213.02 | 15m/z   | neg   |
| 6.18_290.11 | 32m/z   | pos   |
| 6.18_331.21 | 02m/z   | pos   |
| 6.18_348.99 | 22m/z   | pos   |
| 6.19_252.22 | 10m/z   | pos   |
| 6.19_263.62 | 79n     | neg   |
| 6.19_412.28 | 86m/z   | pos   |
| ID  | m/z   | Charge | Status |
|-----|-------|--------|--------|
| 6918| 47    | pos    | 6.37   |
| 6919| 14    | pos    | 6.37   |
| 6920| 87    | pos    | 6.38   |
| 6921| 61    | neg    | 6.38   |
| 6922| 31    | neg    | 6.39   |
| 6923| 60    | pos    | 6.39   |
| 6924| 12    | pos    | 6.39   |
| 6925| 20    | pos    | 6.39   |
| 6926| 51    | neg    | 6.41   |
| 6927| 42    | neg    | 6.43   |
| 6928| 58    | pos    | 6.43   |
| 6929| 92    | neg    | 6.43   |
| 6930| 33    | neg    | 6.45   |
| 6931| 92    | neg    | 6.47   |
| 6932| 97    | neg    | 6.47   |
| 6933| 73    | neg    | 6.47   |
| 6934| 78    | neg    | 6.49   |
| 6935| 51    | pos    | 6.50   |
| 6936| 71    | pos    | 6.51   |
| 6937| 14    | pos    | 6.51   |
| 6938| 36    | pos    | 6.52   |
| 6939| 32    | pos    | 6.52   |
| 6940| 93    | pos    | 6.52   |
| 6941| 56    | pos    | 6.53   |
| 6942| 74    | pos    |        |
6.53_311.22
6943 73m/z   pos
6.55_143.08
6944 98m/z   pos
6.55_184.11
6945 63m/z   pos
6.55_261.04
6946 52m/z   pos
6.55_304.24
6947 91m/z   pos
6.56_272.09
6948 07m/z   pos
6.57_284.95
6949 61n    neg
6.57_319.92
6950 53m/z   neg
6.57_321.91
6951 98m/z   neg
6.57_323.91
6952 92m/z   neg
6.60_104.00
6953 58m/z   pos
6.60_132.00
6954 45m/z   pos
6.60_132.50
6955 20m/z   pos
6.60_209.05
6956 67n    pos
6.60_267.00
6957 16m/z   pos
6.60_292.90
6958 67m/z   neg
6.60_314.99
6959 62m/z   neg
6.60_346.94
6960 58m/z   neg
6.61_430.29
6961 79m/z   pos
6.62_213.11
6962 48m/z   pos
6.62_298.23
6963 40n    pos
6.62_413.19
6964 93m/z   neg
6.62_498.17
6965 61m/z   neg
6.62_622.32
6966 29m/z   neg
6.63_272.21
6967 72n    pos
| m/z   | Retention Time | Charge | Type |
|-------|----------------|--------|------|
| 70/379.19 | 6.63 | pos |
| 47/310.20 | 6.64 | pos |
| 265.18 | 6.65 | pos |
| 142.99 | 6.66 | pos |
| 310.20 | 6.66 | pos |
| 265.18 | 6.66 | pos |
| 125.98 | 6.69 | pos |
| 236.98 | 6.69 | neg |
| 332.25 | 6.69 | pos |
| 475.16 | 6.69 | pos |
| 313.22 | 6.69 | neg |
| 331.12 | 6.69 | neg |
| 288.22 | 6.69 | pos |
| 464.30 | 6.69 | pos |
| 481.24 | 6.69 | pos |
| 241.12 | 6.70 | pos |
| 681.27 | 6.70 | pos |
| 260.05 | 6.73 | pos |
| 300.21 | 6.73 | pos |
| 318.02 | 6.73 | pos |
| 348.91 | 6.73 | pos |
| 400.29 | 6.73 | neg |
| 496.20 | 6.73 | neg |
| 378.14 | 6.74 | pos |
| 626.35 | 6.74 | pos |
6.75_141.09 6993 06m/z pos 6.75_186.99
6.75_350.17 6994 76m/z neg
6.75_624.33 6995 56n neg
6.80_294.24 6996 91m/z neg
6.80_397.17 6997 45m/z pos
6.81_528.22 6998 04m/z neg
6.84_147.11 6999 49n pos
6.84_326.20 7000 68m/z pos
6.84_245.22 7001 23m/z pos
6.86_125.98 7002 28m/z pos
6.86_317.63 7003 58m/z pos
6.86_348.99 7004 44m/z pos
6.86_633.25 7005 19m/z pos
6.89_502.04 7006 67m/z pos
6.89_640.33 7007 74m/z pos
6.91_336.21 7008 46m/z neg
6.91_336.21 7009 89m/z pos
6.92_235.10 7010 12m/z pos
6.92_308.99 7011 67m/z neg
6.93_119.04 7012 98m/z pos
6.93_168.98 7013 98m/z neg
6.94_234.13 7014 53m/z pos
6.94_412.29 7015 02m/z pos
6.95_348.99 7016 14m/z pos
6.98_397.20 7017 37m/z neg
6.98_633.26
7018 06m/z   pos
6.99_223.17
7019 07m/z   pos
6.99_463.27
7020 57n     pos
7.00_294.98
7021 33m/z   neg
7.00_415.19
7022 44m/z   neg
7.00_442.16
7023 30m/z   pos
7.00_674.32
7024 17m/z   neg
7.01_213.11
7025 56m/z   pos
7.01_489.20
7026 30n     pos
7.02_430.29
7027 85m/z   pos
7.03_253.14
7028 74m/z   pos
7.03_412.28
7029 86m/z   pos
7.03_465.31
7030 35n     pos
7.04_302.23
7031 39m/z   pos
7.04_356.24
7032 99m/z   pos
7.05_178.10
7033 11m/z   pos
7.05_239.18
7034 94n     pos
7.06_216.44
7035 61m/z   pos
7.06_324.24
7036 22n     pos
7.06_412.21
7037 37m/z   neg
7.08_375.15
7038 36m/z   pos
7.09_312.22
7039 16m/z   pos
7.09_371.18
7040 85m/z   neg
7.09_479.27
7041 17n     pos
7.10_167.07
7042 44m/z   pos
7.10 234.13
7043 47m/z pos
  7.10 345.14
7044 45m/z neg
  7.12 186.99
7045 79m/z neg
  7.12 191.08
7046 49m/z pos
  7.12 281.12
7047 42m/z neg
  7.12 300.99
7048 02m/z neg
  7.12 317.63
7049 46m/z pos
  7.12 496.20
7050 78m/z neg
  7.12 497.22
7051 35n pos
  7.13 367.27
7052 00m/z pos
  7.14 281.62
7053 98n neg
  7.14 369.90
7054 70m/z neg
  7.14 371.90
7055 42m/z neg
  7.14 528.26
7056 25m/z neg
  7.14 584.23
7057 27m/z neg
  7.18 195.10
7058 54m/z pos
  7.18 254.11
7059 83n pos
  7.18 581.29
7060 78m/z pos
  7.19 176.99
7061 70m/z neg
  7.19 302.23
7062 52m/z pos
  7.19 355.26
7063 69m/z pos
  7.23 208.98
7064 30m/z neg
  7.23 312.21
7065 94m/z pos
  7.23 344.20
7066 99m/z pos
  7.24 352.99
7067 28m/z neg
7.34_624.23
7093  89m/z   pos
   7.34_683.25
7094  58m/z   pos
   7.35_179.10
7095  78m/z   pos
   7.38_213.11
7096  56m/z   pos
   7.41_137.13
7097  22m/z   pos
   7.43_409.27
7098  50m/z   pos
   7.43_649.25
7099  32m/z   pos
   7.44_402.28
7100  77m/z   pos
   7.44_437.05
7101  33m/z   neg
   7.44_522.03
7102  01m/z   neg
   7.44_583.31
7103  15m/z   neg
   7.45_301.04
7104  03m/z   pos
   7.47_326.98
7105  83m/z   neg
   7.49_346.15
7106  49n    pos
   7.50_253.14
7107  75m/z   pos
   7.50_303.66
7108  79n    neg
   7.50_431.30
7109  78n    pos
   7.51_111.04
7110  67m/z   pos
   7.51_302.23
7111  53m/z   pos
   7.53_342.17
7112  31m/z   pos
   7.54_211.01
7113  33n    pos
   7.54_346.26
7114  08m/z   pos
   7.56_272.21
7115  93n    pos
   7.56_370.18
7116  53n    pos
   7.56_454.15
7117  01m/z   neg
| m/z       | Charge | Retention Time | Mass  | Charge | Retention Time |
|-----------|--------|----------------|-------|--------|----------------|
| 7.59_181.16 | neg    | 94 m/z         | 7.59_190.13 | neg    | 71 n           |
| 7.59_243.18 | pos    | 7.57_222.99   |       |        |                |
| 7.59_300.13 | pos    | 7.59_326.12   |       |        |                |
| 7.59_327.15 | neg    | 7.59_327.15   |       |        |                |
| 7.59_384.30 | neg    | 7.59_384.30   |       |        |                |
| 7.60_447.30 | pos    | 7.60_447.30   |       |        |                |
| 7.61_244.90 | neg    | 7.61_466.31   |       |        |                |
| 7.61_248.90 | neg    | 7.61_248.90   |       |        |                |
| 7.61_292.98 | neg    | 7.61_292.98   |       |        |                |
| 7.62_313.11 | neg    | 7.62_313.11   |       |        |                |
| 7.63_288.05 | neg    | 7.63_288.05   |       |        |                |
| 7.65_223.17 | pos    | 7.65_223.17   |       |        |                |
| 7.65_246.24 | pos    | 7.65_246.24   |       |        |                |
| 7.65_257.23 | pos    | 7.65_257.23   |       |        |                |
| 7.65_264.63 | pos    | 7.65_264.63   |       |        |                |
| 7.66_300.24 | pos    | 7.66_300.24   |       |        |                |
| 7.66_330.28 | pos    | 7.66_330.28   |       |        |                |
7.66_381.21
7143 33m/z   pos
7.67_357.05
7144 95m/z   neg
7.68_338.23
7145 56m/z   pos
7.68_777.69
7146 81m/z   pos
7.69_775.68
7147 39m/z   neg
7.70_151.07
7148 65m/z   pos
7.70_442.16
7149 26m/z   pos
7.72_234.13
7150 57m/z   pos
7.72_286.98
7151 13m/z   neg
7.72_358.26
7152 29m/z   pos
7.72_371.18
7153 84m/z   neg
7.74_599.25
7154 51m/z   pos
7.75_190.99
7155 32m/z   neg
7.76_145.00
7156 70m/z   neg
7.76_372.26
7157 89n   pos
7.76_584.34
7158 57m/z   pos
7.76_649.25
7159 48m/z   pos
7.77_181.15
7160 71m/z   pos
7.78_161.13
7161 30m/z   pos
7.78_402.09
7162 75n   pos
7.78_469.07
7163 16m/z   neg
7.80_232.18
7164 17m/z   pos
7.80_338.23
7165 50m/z   pos
7.81_191.11
7166 21m/z   pos
7.81_222.99
7167 92m/z   neg
| m/z | Retention Time | Charge | Isotope Pattern |
|-----|----------------|--------|----------------|
| 7168 | 7.81_640.37    | pos    |                |
| 7169 | 7.82_155.10    | pos    |                |
| 7170 | 7.82_353.23    | pos    |                |
| 7171 | 7.82_358.26    | pos    |                |
| 7172 | 7.82_414.30    | pos    |                |
| 7173 | 7.82_431.30    | pos    |                |
| 7174 | 7.82_529.27    | pos    |                |
| 7175 | 7.83_262.23    | neg    |                |
| 7176 | 7.84_412.28    | pos    |                |
| 7177 | 7.86_255.63    | pos    |                |
| 7178 | 7.86_402.31    | neg    |                |
| 7179 | 7.86_436.29    | pos    |                |
| 7180 | 7.86_511.26    | pos    |                |
| 7181 | 7.86_532.23    | pos    |                |
| 7182 | 7.86_578.35    | neg    |                |
| 7183 | 7.86_614.37    | pos    |                |
| 7184 | 7.87_230.21    | pos    |                |
| 7185 | 7.87_308.99    | pos    |                |
| 7186 | 7.88_368.03    | neg    |                |
| 7187 | 7.88_370.18    | neg    |                |
| 7188 | 7.88_430.89    | pos    |                |
| 7189 | 7.88_475.21    | pos    |                |
| 7190 | 7.88_508.19    | pos    |                |
| 7191 | 7.88_530.19    | pos    |                |
| 7192 | 7.88_530.19    | pos    |                |
| m/z | Value  | Charge | Status |
|-----|--------|--------|--------|
| 7193 | 8.8_533.11 | neg    |        |
| 7194 | 9.9_443.15 | neg    |        |
| 7195 | 7.9_285.26 | neg    |        |
| 7196 | 7.9_314.23 | pos    |        |
| 7197 | 7.9_430.30 | pos    |        |
| 7198 | 0.9_441.10 | pos    |        |
| 7199 | 0.9_476.30 | pos    |        |
| 7200 | 7.9_246.15 | pos    |        |
| 7201 | 7.9_246.98 | pos    |        |
| 7202 | 7.9_327.98 | pos    |        |
| 7203 | 7.9_186.99 | neg    |        |
| 7204 | 7.9_357.28 | neg    |        |
| 7205 | 7.9_625.35 | pos    |        |
| 7206 | 7.9_640.37 | pos    |        |
| 7207 | 7.9_321.14 | pos    |        |
| 7208 | 7.9_340.03 | pos    |        |
| 7209 | 7.9_356.00 | pos    |        |
| 7210 | 7.9_359.99 | pos    |        |
| 7211 | 7.9_363.95 | pos    |        |
| 7212 | 7.9_365.95 | pos    |        |
| 7213 | 7.9_386.00 | pos    |        |
| 7214 | 7.9_397.99 | pos    |        |
| 7215 | 7.9_399.93 | pos    |        |
| 7216 | 7.9_401.93 | pos    |        |
| 7217 | 0.2_401.93 | pos    |        |
7.96_408.01
7218 84m/z    neg
7.96_425.00
7219 35m/z    neg
7.96_501.17
7220 11m/z    neg
7.97_139.04
7221 08m/z    pos
7.97_153.05
7222 56m/z    pos
7.97_195.10
7223 42m/z    pos
7.97_238.35
7224 69m/z    neg
7.97_240.10
7225 12n      pos
7.97_318.98
7226 54m/z    neg
7.97_329.06
7227 02m/z    neg
7.97_346.05
7228 06m/z    neg
7.98_187.12
7229 75m/z    pos
8.00_214.99
7230 33m/z    neg
8.00_280.98
7231 34m/z    neg
8.02_477.29
7232 01m/z    pos
8.03_269.22
7233 91m/z    pos
8.03_641.35
7234 34m/z    neg
8.04_417.21
7235 17m/z    neg
8.06_451.32
7236 85m/z    pos
8.06_642.37
7237 87n      pos
8.07_111.04
7238 55m/z    pos
8.07_125.98
7239 60m/z    pos
8.08_284.22
7240 35m/z    pos
8.08_625.35
7241 17n      pos
8.08_627.37
7242 33m/z    neg
8.12_252.63
7243 64m/z  pos
8.12_663.26
7244 66m/z  pos
8.13_264.99
7245 10m/z  neg
8.13_510.25
7246 08m/z  neg
8.14_253.14
7247 72m/z  pos
8.14_350.99
7248 08m/z  pos
8.14_464.28
7249 49m/z  pos
8.14_529.21
7250 14m/z  pos
8.14_532.28
7251 69m/z  neg
8.14_544.26
7252 98m/z  pos
8.14_549.27
7253 67m/z  neg
8.14_665.24
7254 94m/z  pos
8.15_226.62
7255 76m/z  pos
8.15_235.63
7256 48m/z  pos
8.15_414.30
7257 24m/z  pos
8.15_449.31
7258 59n  pos
8.15_568.35
7259 18m/z  pos
8.16_663.22
7260 99m/z  neg
8.17_234.13
7261 49m/z  pos
8.17_511.30
7262 07m/z  neg
8.17_516.29
7263 28m/z  neg
8.18_633.25
7264 83m/z  pos
8.19_130.99
7265 12m/z  neg
8.19_327.98
7266 80m/z  neg
8.19_337.20
7267 61m/z  pos
8.21_321.14
7268 61m/z neg
8.22_175.12
7269 54m/z pos
8.24_360.28
7270 12m/z pos
8.24_465.24
7271 69m/z neg
8.24_484.29
7272 36m/z pos
8.26_268.98
7273 66m/z neg
8.26_601.26
7274 87m/z pos
8.28_174.99
7275 26m/z pos
8.28_328.25
7276 09m/z pos
8.28_373.27
7277 63m/z pos
8.30_255.21
7278 52m/z pos
8.30_296.99
7279 62m/z neg
8.30_633.25
7280 94m/z pos
8.31_340.25
7281 21m/z pos
8.32_389.98
7282 64m/z neg
8.32_460.29
7283 00m/z neg
8.32_679.26
7284 17m/z neg
8.32_681.28
7285 02m/z pos
8.33_234.13
7286 52m/z pos
8.33_268.27
7287 08m/z pos
8.33_360.28
7288 01m/z pos
8.35_316.25
7289 28m/z pos
8.37_321.14
7290 62m/z neg
8.38_272.21
7291 91m pos
8.38_285.26
7292 45m/z pos
8.56_242.28
7318  69m/z    pos
  8.59_232.07
7319  83m/z    pos
  8.59_280.27
7320  05m/z    pos
  8.59_324.98
7321  96m/z    neg
  8.61_509.27
7322  35m/z    neg
  8.61_627.37
7323  24m/z    neg
  8.62_202.18
7324  02m/z    pos
  8.62_314.14
7325  54m/z    pos
  8.62_331.25
7326  02m/z    pos
  8.62_512.26
7327  72m/z    neg
  8.62_549.20
7328  37m/z    pos
  8.63_213.11
7329  60m/z    pos
  8.63_295.22
7330  91m/z    pos
  8.63_340.25
7331  27m/z    pos
  8.64_329.23
7332  22m/z    neg
  8.65_125.98
7333  72m/z    pos
  8.65_276.20
7334  07m/z    pos
  8.65_494.33
7335  30m/z    pos
  8.65_556.32
7336  53m/z    neg
  8.66_426.97
7337  56m/z    neg
  8.67_137.09
7338  77m/z    pos
  8.67_235.09
7339  91m/z    pos
  8.69_143.10
7340  51m/z    pos
  8.69_387.18
7341  28m/z    pos
  8.70_111.08
7342  19m/z    pos
8.71_135.90
7343 51m/z   pos
     8.71_141.09
7344 10m/z   pos
     8.71_243.23
7345 30m/z   pos
     8.73_133.90
7346 50m/z   pos
     8.73_210.16
7347 35n   pos
     8.73_210.52
7348 69m/z   pos
     8.73_234.20
7349 52m/z   pos
     8.73_273.25
7350 58m/z   pos
     8.73_312.15
7351 07m/z   pos
     8.73_344.29
7352 16m/z   pos
     8.74_133.57
7353 62m/z   pos
     8.74_214.18
7354 14m/z   pos
     8.74_266.15
7355 60m/z   pos
     8.74_326.98
7356 88m/z   neg
     8.75_290.19
7357 62m/z   neg
     8.75_294.61
7358 97m/z   neg
     8.76_181.12
7359 46m/z   pos
     8.77_384.27
7360 83m/z   pos
     8.77_466.25
7361 51m/z   neg
     8.77_601.27
7362 28m/z   pos
     8.78_317.95
7363 12m/z   neg
     8.78_460.29
7364 00m/z   neg
     8.78_556.32
7365 96m/z   neg
     8.79_125.98
7366 60m/z   pos
     8.79_462.31
7367 52m/z   pos
| m/z     | Retention Time | Charge | Ionization Status |
|---------|----------------|------|------------------|
| 341.28  | 8.80           | pos  |                  |
| 415.31  | 8.80           | pos  |                  |
| 633.25  | 8.80           | pos  |                  |
| 256.63  | 8.80           | pos  |                  |
| 282.16  | 8.81           | neg  |                  |
| 534.24  | 8.81           | neg  |                  |
| 552.23  | 8.81           | pos  |                  |
| 593.26  | 8.81           | pos  |                  |
| 330.26  | 8.83           | pos  |                  |
| 430.31  | 8.85           | pos  |                  |
| 285.26  | 8.87           | pos  |                  |
| 294.24  | 8.89           | pos  |                  |
| 329.24  | 8.89           | pos  |                  |
| 158.15  | 8.91           | pos  |                  |
| 345.98  | 8.91           | pos  |                  |
| 329.24  | 8.91           | pos  |                  |
| 353.24  | 8.91           | neg  |                  |
| 609.32  | 8.91           | neg  |                  |
| 282.98  | 8.92           | pos  |                  |
| 408.29  | 8.92           | neg  |                  |
| 408.29  | 8.92           | neg  |                  |
| 318.30  | 8.93           | neg  |                  |
| 454.32  | 8.93           | pos  |                  |
| 628.37  | 8.93           | pos  |                  |
| 616.26  | 8.94           | pos  |                  |
| 237.15  | 8.95           | pos  |                  |
| 362.32  | 8.95           | pos  |                  |
| 362.32  | 8.95           | pos  |                  |
| 362.32  | 8.95           | pos  |                  |
| m/z | RT  | Charge |
|-----|-----|--------|
| 7393| 8.95 | 47.30  |
|     | 24n  | pos    |
| 7394| 8.95 | 585.27 |
|     | 41m/z| pos    |
| 7395| 8.97 | 447.17 |
|     | 41m/z| pos    |
| 7396| 8.97 | 228.10 |
|     | 62n  | pos    |
| 7397| 8.98 | 208.98 |
|     | 14m/z| pos    |
| 7398| 8.98 | 386.17 |
|     | 29m/z| neg    |
| 7399| 8.98 | 256.98 |
|     | 74n  | pos    |
| 7400| 8.98 | 256.98 |
|     | 54m/z| neg    |
| 7401| 8.99 | 373.27 |
|     | 16m/z| neg    |
| 7402| 9.01 | 207.03 |
|     | 83m/z| pos    |
| 7403| 9.01 | 223.02 |
|     | 36m/z| pos    |
| 7404| 9.01 | 386.29 |
|     | 72m/z| neg    |
| 7405| 9.01 | 227.50 |
|     | 78m/z| pos    |
| 7406| 9.02 | 263.06 |
|     | 05m/z| pos    |
| 7407| 9.02 | 409.27 |
|     | 81m/z| pos    |
| 7408| 9.03 | 295.22 |
|     | 51m/z| pos    |
| 7409| 9.03 | 313.11 |
|     | 88m/z| pos    |
| 7410| 9.03 | 313.24 |
|     | 86m/z| neg    |
| 7411| 9.03 | 321.11 |
|     | 01m/z| pos    |
| 7412| 9.03 | 329.23 |
|     | 49n  | pos    |
| 7413| 9.03 | 480.07 |
|     | 26m/z| neg    |
| 7414| 9.05 | 265.14 |
|     | 00m/z| pos    |
| 7415| 9.05 | 600.26 |
|     | 31m/z| neg    |
| 7416| 9.06 | 230.98 |
|     | 18n  | pos    |
| 7417| 9.06 | 230.98 |
|     | 62m/z| neg    |
9.06_315.25
7418 64m/z  pos
9.07_414.31
7419 60n  pos
9.07_474.31
7420 34m/z  pos
9.07_626.37
7421 20n  pos
9.09_151.11
7422 38m/z  pos
9.09_330.98
7423 35m/z  neg
9.10_111.04
7424 32m/z  pos
9.10_366.26
7425 76m/z  pos
9.12_135.90
7426 54m/z  pos
9.12_246.08
7427 23m/z  pos
9.12_261.04
7428 58m/z  pos
9.12_287.22
7429 55m/z  pos
9.12_434.33
7430 21m/z  pos
9.12_610.36
7431 58m/z  pos
9.14_111.08
7432 38m/z  pos
9.14_234.13
7433 62m/z  pos
9.14_254.15
7434 35n  pos
9.14_300.21
7435 87m/z  pos
9.14_342.26
7436 81m/z  pos
9.16_161.13
7437 30m/z  pos
9.16_330.26
7438 75m/z  pos
9.16_350.98
7439 77m/z  pos
9.18_233.18
7440 43m/z  pos
9.20_111.04
7441 63m/z  pos
9.20_255.82
7442 14m/z  neg
7468 84m/z  pos  9.30_366.26
7469 35m/z  pos  9.30_479.19
7470 98m/z  pos  9.30_718.29
7471 10m/z  pos  9.30_718.78
7472 74m/z  pos  9.31_625.35
7473 83m/z  neg  9.32_624.23
7474 98m/z  pos  9.33_336.25
7475 17m/z  pos  9.33_338.25
7476 96n  pos  9.33_342.27
7477 02m/z  pos  9.34_142.08
7478 85m/z  pos  9.34_314.98
7479 81m/z  neg  9.35_315.13
7480 60m/z  neg  9.36_346.24
7481 41m/z  pos  9.37_527.29
7482 16m/z  pos  9.38_516.23
7483 75n  pos  9.39_273.26
7484 93n  pos  9.39_307.23
7485 16m/z  pos  9.40_288.24
7486 89m/z  pos  9.40_386.29
7487 20m/z  pos  9.40_620.34
7488 30m/z  neg  9.42_125.98
7489 59m/z  pos  9.42_246.18
7490 93m/z  pos  9.42_264.19
7491 87m/z  pos  9.42_362.32
7492 84m/z  pos
9.42_473.33
7493  85n   pos
   9.43_189.09
7494  22m/z   pos
   9.44_330.17
7495  02n   pos
   9.45_286.98
7496  44m/z   neg
   9.46_195.17
7497  60m/z   pos
   9.46_223.17
7498  11m/z   pos
   9.46_240.19
7499  84m/z   pos
   9.46_253.14
7500  73m/z   pos
   9.46_286.14
7501  50n   pos
   9.46_332.20
7502  71m/z   pos
   9.46_578.41
7503  56m/z   pos
   9.47_280.12
7504  48m/z   neg
   9.47_367.34
7505  20m/z   pos
   9.47_444.29
7506  09n   pos
   9.47_498.34
7507  50m/z   pos
   9.47_581.23
7508  96m/z   neg
   9.47_582.25
7509  02n   pos
   9.47_583.76
7510  02m/z   pos
   9.48_290.27
7511  09m/z   pos
   9.48_548.21
7512  65m/z   pos
   9.50_430.89
7513  41m/z   pos
   9.51_235.63
7514  49m/z   pos
   9.51_243.63
7515  22n   pos
   9.51_338.26
7516  08n   pos
   9.51_413.02
7517  89m/z   pos
| m/z   | Mass   | Charge | Retention Time |
|-------|--------|--------|----------------|
| 9.51_414.30 | pos   | 7518   |
| 9.51_440.34 | pos   | 7519   |
| 9.51_468.29 | pos   | 7520   |
| 9.51_471.29 | pos   | 7521   |
| 9.51_516.29 | pos   | 7522   |
| 9.51_533.28 | neg   | 7523   |
| 9.51_546.27 | neg   | 7524   |
| 9.51_550.26 | pos   | 7525   |
| 9.51_593.33 | pos   | 7526   |
| 9.51_635.26 | pos   | 7527   |
| 9.51_698.63 | pos   | 7528   |
| 9.51_119.05 | pos   | 7529   |
| 9.51_213.57 | pos   | 7530   |
| 9.52_385.99 | pos   | 7531   |
| 9.52_386.17 | pos   | 7532   |
| 9.52_437.73 | pos   | 7533   |
| 9.52_447.22 | pos   | 7534   |
| 9.52_460.27 | pos   | 7535   |
| 9.52_471.13 | pos   | 7536   |
| 9.52_474.25 | pos   | 7537   |
| 9.52_488.12 | pos   | 7538   |
| 9.52_503.28 | pos   | 7539   |
| 9.52_772.35 | pos   | 7540   |
| 9.52_858.47 | pos   | 7541   |
| 9.53_533.27 | neg   | 7542   |
9.54_165.12
7543  84m/z  pos
9.54_284.22
7544  33m/z  pos
9.54_432.24
7545  55m/z  pos
9.56_182.04
7546  66m/z  pos
9.56_323.13
7547  04n   pos
9.56_323.14
7548  24m/z  pos
9.56_380.30
7549  61n   pos
9.56_482.05
7550  08m/z  pos
9.56_484.04
7551  88m/z  pos
9.56_646.26
7552  09n   pos
9.58_171.14
7553  69m/z  pos
9.58_202.06
7554  00m/z  pos
9.58_374.28
7555  47n   pos
9.58_464.24
7556  62m/z  pos
9.59_378.99
7557  52m/z  neg
9.59_412.30
7558  99m/z  pos
9.60_181.16
7559  00m/z  pos
9.60_214.18
7560  16m/z  pos
9.60_241.18
7561  18m/z  pos
9.60_257.20
7562  10n   pos
9.60_303.26
7563  62m/z  pos
9.60_397.31
7564  25m/z  pos
9.61_607.34
7565  80m/z  neg
9.62_151.11
7566  28m/z  pos
9.62_302.27
7567  31m/z  pos
| Mass (m/z) | Retention Time (min) | Charge State |
|-----------|----------------------|--------------|
| 50        | 9.63                 | +            |
| 73        | 9.64                 | -            |
| 88        | 9.64                 | -            |
| 60        | 9.65                 | -            |
| 47        | 9.65                 | +            |
| 64n       | 9.65                 | -            |
| 03n       | 9.65                 | -            |
| 61n       | 9.65                 | +            |
| 01m/z     | 9.65                 | -            |
| 19m/z     | 9.65                 | -            |
| 24m/z     | 9.65                 | -            |
| 97m/z     | 9.66                 | +            |
| 10m/z     | 9.66                 | +            |
| 76m/z     | 9.66                 | +            |
| 17m/z     | 9.66                 | +            |
| 15n       | 9.66                 | +            |
| 71m/z     | 9.66                 | +            |
| 12m/z     | 9.66                 | -            |
| 58n       | 9.66                 | +            |
| 00m/z     | 9.66                 | +            |
| 94m/z     | 9.66                 | +            |
| 90m/z     | 9.66                 | -            |
| 27m/z     | 9.66                 | -            |
| 26m/z     | 9.67                 | -            |
| 86m/z     | 9.67                 | +            |
| Retention Time | m/z | Charge | Ion Mode |
|---------------|-----|--------|----------|
| 7593          | 39  | +      | 9.67_368.28 |
| 7594          | 86  | -      | 9.69_254.15 |
| 7595          | 38  | +      | 9.69_388.31 |
| 7596          | 25  | +      | 9.70_153.05 |
| 7597          | 80  | +      | 9.70_219.13 |
| 7598          | 93  | +      | 9.70_268.13 |
| 7599          | 29  | +      | 9.70_330.08 |
| 7600          | 10  | +      | 9.70_332.13 |
| 7601          | 91  | +      | 9.70_368.06 |
| 7602          | 64  | -      | 9.70_575.21 |
| 7603          | 79  | +      | 9.72_511.30 |
| 7604          | 05  | -      | 9.72_516.29 |
| 7605          | 34  | -      | 9.73_234.13 |
| 7606          | 51  | +      | 9.73_235.63 |
| 7607          | 52  | +      | 9.73_244.64 |
| 7608          | 08  | +      | 9.73_248.17 |
| 7609          | 94  | +      | 9.73_344.28 |
| 7610          | 36  | +      | 9.73_414.30 |
| 7611          | 28  | +      | 9.73_449.31 |
| 7612          | 69  | +      | 9.73_519.31 |
| 7613          | 66  | -      | 9.74_147.08 |
| 7614          | 70  | +      | 9.74_230.24 |
| 7615          | 91  | +      | 9.74_237.11 |
| 7616          | 51  | +      | 9.75_318.22 |
| 7617          | 30  | +      |            |
| m/z | Retention Time | Charge State |
|-----|----------------|--------------|
| 36 | 9.75 | pos |
| 359.22 | 9.75 | 464.34 |
| 17 | 9.75 | pos |
| 264.99 | 9.76 | 345.99 |
| 04 | 9.76 | neg |
| 9.76 | 364.22 | |
| 45 | 9.77 | neg |
| 328.23 | 9.77 | 380.30 |
| 34 | 9.78 | pos |
| 328.23 | 9.78 | 380.30 |
| 87 | 9.78 | pos |
| 318.35 | 9.78 | 485.05 |
| 87 | 9.78 | pos |
| 410.37 | 9.78 | 540.37 |
| 77 | 9.79 | pos |
| 215.12 | 9.79 | 304.01 |
| 20 | 9.80 | neg |
| 458.35 | 9.80 | 485.05 |
| 88 | 9.80 | pos |
| 334.98 | 9.81 | 434.98 |
| 53 | 9.82 | neg |
| 442.34 | 9.82 | 447.31 |
| 07 | 9.82 | pos |
| 447.31 | 9.82 | 603.53 |
| 39 | 9.82 | pos |
| 252.17 | 9.83 | 252.17 |
| 84 | 9.83 | pos |
| 430.29 | 9.83 | 482.29 |
| 16 | 9.83 | pos |
| 312.23 | 9.84 | 312.23 |
| 25 | 9.85 | pos |
| 280.98 | 9.85 | 377.19 |
| 26 | 9.85 | pos |
| 377.19 | 9.86 | 151.11 |
| 33 | 9.86 | pos |
| 359.22 | 9.86 | 151.11 |
| m/z  | mass/charge | ionization | mass (Da) |
|------|-------------|------------|-----------|
| 9.86 | 285.13      | pos        | 86n       |
| 9.86 | 426.25      | pos        |           |
| 9.86 | 524.23      | pos        |           |
| 9.86 | 583.25      | pos        |           |
| 9.87 | 406.99      | neg        | 20m/z     |
| 9.87 | 414.20      | pos        | 82n       |
| 9.87 | 418.22      | pos        |           |
| 9.87 | 460.27      | pos        | 62m/z     |
| 9.87 | 488.33      | pos        |           |
| 9.87 | 555.32      | pos        | 29m/z     |
| 9.88 | 383.33      | pos        | 25m/z     |
| 9.88 | 387.17      | pos        | 97n       |
| 9.88 | 431.17      | neg        |           |
| 9.88 | 432.24      | neg        |           |
| 9.89 | 611.38      | pos        | 14m/z     |
| 9.90 | 147.11      | pos        |           |
| 9.90 | 174.99      | pos        |           |
| 9.90 | 210.16      | pos        |           |
| 9.90 | 230.89      | pos        |           |
| 9.90 | 242.21      | pos        |           |
| 9.90 | 251.00      | pos        |           |
| 9.90 | 297.25      | pos        |           |
| 9.90 | 298.25      | pos        |           |
| 9.90 | 322.99      | pos        |           |
| 9.90 | 326.00      | neg        |           |
| 9.90 | 35n         | pos        |           |
| m/z      | Time  |
|----------|-------|
| 9.90_328.00 | pos  |
| 9.90_329.99 | pos  |
| 9.90_358.19 | pos  |
| 9.90_412.96 | pos  |
| 9.90_419.06 | pos  |
| 9.90_427.95 | pos  |
| 9.90_428.28 | pos  |
| 9.91_312.99 | neg  |
| 9.91_415.07 | neg  |
| 9.91_417.07 | pos  |
| 9.91_478.19 | pos  |
| 9.91_480.21 | neg  |
| 9.91_647.27 | pos  |
| 9.92_395.24 | pos  |
| 9.93_419.25 | neg  |
| 9.94_213.11 | pos  |
| 9.94_330.26 | pos  |
| 9.94_334.21 | pos  |
| 9.94_338.00 | pos  |
| 9.95_330.98 | neg  |
| 9.96_386.99 | neg  |
| 9.97_191.14 | neg  |
| 9.97_651.16 | pos  |
| 9.98_252.17 | pos  |
| 9.98_265.30 | pos  |
| 9.99_50n      | pos  |
| m/z | Charge | Status |
|-----|--------|--------|
| 9.98 | 339.27 | pos |
| 9.98 | 374.28 | pos |
| 9.99 | 455.24 | pos |
| 9.99 | 488.24 | pos |
| 61m/z | neg |
| 60m/z | pos |