

Supplementary information

**A NON-TARGETED LC-MS METABOLIC PROFILING OF PREGNANCY:
LONGITUDINAL EVIDENCE FROM HEALTHY AND PRE-ECLAMPTIC PREGNANCIES**

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Supplementary table 1: Results of the metabolomics study (ordered according to molecular mass)

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|--------------------------|----------|---|--|---------------|----------|---------------|----------|---------------|-----------|---------------|----------|-------|----------|------------------|-------------|----------|------------------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR _p | Value | raw p | FDR _p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_60_0323a0_9495243 | Hilic | + | 60.0323 | 0.95 | Urea | 2 | 10 eV: 44.0133 (100), 61.0401 (70) | (121.0721, 15746.633 122.0775, 606.077 123.0784, 204.266 83.0217, 642.821 78.0672, 156.2614 0.983, 419.813 362.9421, 691.726 63.0436, 205.5) | 171763.2 | 41675.37 | 153324.3 | 37866.51 | 172303.3 | 34207.08 | 221770.5 | 53922.98 | 0.01 | 0.981483 | 0.990277 | 1.30 | 1.34E-05 | 0.005768 |
| COMPOUND_68_0622a4_7624702 | Rp | + | 68.0622 | 4.76 | | | | (69.0698, 5334.49 70.0728, 412.9) | 19392.46 | 5336.748 | 19921.72 | 4031.242 | 20473.7 | 4378.354 | 19455.22 | 5162.023 | -0.34 | 0.2527 | 0.348701 | 0.26 | 0.468749 | 0.734042 |
| COMPOUND_85_0529a0_8500329 | Hilic | + | 85.0529 | 0.85 | | | | (171.1134, 282.94 86.06, 8444.94 87.0622, 268.39) | 10158.79 | 3372.965 | 10951.3 | 3501.109 | 13657.43 | 3464.032 | 14734.3 | 5109.426 | 0.79 | 0.002708 | 0.006529 | 0.09 | 0.763762 | 0.895777 |
| COMPOUND_89_0477a5_551579 | Hilic | + | 89.0477 | 5.55 | | | | (112.0371, 1981.51 113.0412, 134.81 201.0921, 287.74 90.055, 8697.23 91.0569, 246.96 92.0594, 96.86) | 19087.38 | 2746.593 | 20243.37 | 3137.107 | 24277.5 | 4356.908 | 26045.23 | 5255.566 | 1.21 | 3.52E-07 | 1.99E-06 | -0.05 | 0.852991 | 0.937499 |
| COMPOUND_103_0634a5_112903 | Hilic | + | 103.0634 | 5.11 | | | | (126.0562, 273.43 104.0707, 16203.7 105.0738, 595.69 106.0753, 186.77) | 50989.17 | 8448.219 | 52663.89 | 9057.901 | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.41 | 1.54E-13 | 1.25E-11 | -0.14 | 0.418222 | 0.699556 |
| COMPOUND_103_0998a1_4269782 | Hilic | + | 103.0998 | 4.14 | Choline | 2 | 10 eV: 104.1075 (100), 60.0812 (25), 46.0388 (5) | (207.2069, 3801.188 208.2103, 4932.08 209.2105, 513.94 104.107, 54639.89 105.1102, 2944.98 106.1127, 375.49) | 62789.26 | 63520.99 | 53932.93 | 40914.87 | 12483.43 | 4889.389 | 15913.51 | 8131.051 | -1.64 | 3.47E-10 | 4.44E-09 | 0.34 | 0.19379 | 0.505089 |
| COMPOUND_103_0999a10_346933 | Rp | + | 103.0999 | 10.35 | | | | (207.2079, 235.55 126.0914, 568.44 104.1073, 5429.49 105.1104, 432.79) | 45150.07 | 16833.65 | 46777.05 | 15855.33 | 24937 | 10521.29 | 24046.35 | 7438.76 | -0.65 | 0.019912 | 0.039301 | -0.08 | 0.816152 | 0.92157 |
| COMPOUND_108_0935a5_238501 | Rp | + | 108.0935 | 5.24 | | | | (109.1014, 5072.61 110.1043, 663.23 111.1165, 68.43) | 17256.13 | 4139.061 | 17369.93 | 3360.317 | 18423.73 | 4656.411 | 18206.21 | 4359.348 | 0.26 | 0.351159 | 0.453281 | -0.27 | 0.416625 | 0.699135 |
| COMPOUND_109_064a6_711251 | Hilic | + | 109.0640 | 6.71 | | | | (110.0713, 10463.09 111.0745, 1050.79 112.087, 310.83) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.62 | 0.019566 | 0.038754 | 0.01 | 0.968674 | 0.982722 |
| COMPOUND_110_1094a4_7634273 | Rp | + | 110.1094 | 4.76 | | | | (111.1169, 9512.58 112.1205, 1017.01 113.1226, 104.3) | 37439 | 10331.78 | 38187.13 | 7947.74 | 39293.77 | 8743.396 | 38010.06 | 11063.48 | 0.07 | 0.821818 | 0.873812 | -0.07 | 0.845973 | 0.93343 |
| COMPOUND_113_059a1_2121515 | Hilic | + | 113.0590 | 1.21 | Creatinine | 2 | 10 eV: 114.0671 (100), 44.0499 (85), 86.0718 (10) | (127.1257, 286196.84 228.1286, 30190.36 229.1304, 3118.65 230.1317, 233.56 136.0485, 21687.05 137.0517, 585.62 138.0558, 278.39 249.1075, 4435.64 250.1062, 461.47 251.1038, 122.89 114.0658, 1177171.5 115.0694, 57221.78 116.071, 4209.83) | 13622615 | 1645758 | 12932336 | 1889497 | 16721429 | 2062925 | 17701754 | 2885152 | 1.00 | 2.57E-06 | 1.16E-05 | 0.56 | 0.014344 | 0.179521 |
| COMPOUND_113_0842a2_9012837 | Rp | + | 113.0842 | 2.90 | | | | (227.1753, 581.27 228.1775, 61.06 136.0759, 250.35 137.0805, 23.79 249.1508, 565.74 250.1447, 307.29 114.0914, 30002.53 115.0944, 2195.38 116.0936, 32.87) | 44958.97 | 22081.96 | 49336.73 | 32384.05 | 47082.11 | 34701.17 | 83024.5 | 69201.06 | 0.13 | 0.559671 | 0.656827 | 0.31 | 0.24631 | 0.555348 |
| COMPOUND_113_0843a3_084201 | Rp | + | 113.0843 | 3.08 | | | | (227.1763, 47621.71 228.1791, 6980.99 229.1821, 612.46 136.0734, 10454.63 137.0757, 778.08 138.0776, 114.49 249.1582, 2492.78 250.1598, 335.97 251.1703, 36.52 152.0431, 1220.94 114.0912, 574859.8 115.0946, 37249.12 116.097, 2278.86) | 4247166 | 448273 | 4159536 | 463146.2 | 4483274 | 548903.7 | 4209974 | 352462.8 | 0.46 | 0.129038 | 0.202363 | -0.24 | 0.503519 | 0.754442 |
| COMPOUND_115_0633a4_706444 | Hilic | + | 115.0633 | 4.71 | Proline | 2 | 10 eV: 70.0655 (100), 116.0707 (40) | (231.1344, 7171.9 232.1387, 196.85 233.1284, 203.59 138.0529, 39656.23 139.0553, 2096.5 253.1165, 1233.65 254.1252, 238.3 255.1202, 44.71 116.0706, 952384.4 117.0742, 524.54) | 4092242 | 896065.5 | 4242154 | 951260.7 | 5146669 | 1009436 | 4509167 | 1122848 | 1.10 | 2.03E-05 | 7.55E-05 | -0.90 | 0.001827 | 0.061415 |
| COMPOUND_115_0636a7_1022463 | Hilic | + | 115.0636 | 7.10 | Ornithine (m/z 133.0974) | 1 | 10 eV: 70.0651 (100), 116.0700 (55), 133.0961 (3) | (138.0527, 268.88 133.0973, 58821.84 134.1005, 3725.79 135.1011, 478.01 116.0705, 24649.64 117.0735, 1389.89) | 143719.2 | 64241.31 | 161749.9 | 68720.46 | 152658.4 | 62940.56 | 133701.9 | 55456.93 | 0.23 | 0.440248 | 0.545645 | -0.60 | 0.095685 | 0.364606 |
| COMPOUND_117_0535a5_6224656 | Hilic | + | 117.0535 | 5.62 | Unknown betaine | 4 | 20 eV: 59.0724 (100), 118.0863 (45), 58.0650 (40) | (140.0431, 2405.27 141.0473, 76.76 118.0609, 11678.5 119.0652, 341.66 120.0642, 139.41) | 20275.04 | 3955.277 | 21921.3 | 4868.291 | 19188.92 | 4160.325 | 24255.68 | 8323.502 | -0.38 | 0.146498 | 0.223821 | 0.68 | 0.030544 | 0.234758 |
| COMPOUND_117_0787a3_4925504 | Hilic | + | 117.0787 | 3.49 | Glycine betaine | 1 | 10 eV: 118.0866 (100), 59.0733 (20), 58.0653 (15) | (235.1655, 5408.17 236.1678, 606.03 237.17, 626.53 140.0684, 11153.54 141.072, 117.05 142.0701, 119.74 257.1477, 1285.88 258.1521, 239.96 259.152, 154.83 118.0863, 961306.3 119.0896, 46030.71 120.0813, 41744.47) | 13708736 | 2459475 | 13975706 | 3722627 | 11518323 | 1685340 | 10912432 | 2615521 | -0.72 | 0.006574 | 0.014514 | -0.23 | 0.451336 | 0.723875 |
| COMPOUND_117_0795a4_6878123 | Hilic | + | 117.0795 | 4.69 | Valine | 2 | 20 eV: 55.0544 (100), 72.0810 (90), 118.0861 (5) | (140.0683, 4547.95 141.0719, 355.39 142.0829, 101.07 257.1474, 420.83 258.1561, 50.46 118.0865, 395519.9 119.0898, 21048.69 120.0915, 1776.9) | 963937.2 | 213159.6 | 97284.6 | 225804.5 | 805409.1 | 141052.8 | 861817.9 | 238901 | -0.70 | 0.009622 | 0.020461 | 0.11 | 0.724823 | 0.880421 |
| COMPOUND_119_0577a1_0233206 | Hilic | + | 119.0577 | 1.02 | | | | (239.1219, 272.34 142.048, 2603.53 143.0528, 93.71 137.0949, 155.19 120.0656, 35123.4 121.0683, 2529.38 122.0789, 418.6 256.1539, 149.66) | 47066.73 | 19694.44 | 39026.3 | 10585.3 | 51754.75 | 21862.45 | 63061.98 | 33551.39 | 0.47 | 0.05235 | 0.091176 | 0.36 | 0.205364 | 0.516497 |
| COMPOUND_119_058a5_7017784 | Hilic | + | 119.0580 | 5.70 | Threonine | 2 | 10 eV: 74.0603 (100), 56.0493 (45), 102.0548 (15), 120.0663 (5) | (142.0474, 16760.56 143.0509, 821.27 144.0542, 187.1 120.0659, 197510.62 121.0686, 11543.4 122.0799, 3614.87 123.0743, 146.51) | 165463.9 | 65594.6 | 166053.7 | 64612.18 | 322903.9 | 1337879.8 | 474757.5 | 192154.1 | 0.87 | 0.00026 | 0.000757 | 0.61 | 0.026496 | 0.225166 |
| COMPOUND_121_071a5_1081805 | Hilic | + | 121.0714 | 5.11 | | | | (144.0634, 3940.4 145.0653, 166.96 146.0658, 250.57 122.0813, 370562.62 123.0846, 17165.64 124.0859, 286.67) | 1143407 | 212425.7 | 1130958 | 258568.7 | 28918.18 | 18325.79 | 30239.62 | 64621.11 | -1.52 | 1.93E-12 | 6.99E-11 | -0.06 | 0.755951 | 0.895058 |
| COMPOUND_121_9174a2_9088342 | Hilic | + | 121.9174 | 2.91 | | | | (144.0034, 86.61 122.0245, 80129.39 123.0283, 983.32 124.0228, 10992.98) | 129719.6 | 10141.67 | 131939.8 | 9374.259 | 154199.1 | 85382.39 | 150230 | 20081.93 | -0.57 | 0.002125 | 0.005938 | -0.07 | 0.979761 | 0.913784 |
| COMPOUND_125_0147a5_236711 | Hilic | + | 125.0147 | 5.24 | Taurine | 1 | 10 eV: 126.0217 (100), 44.0499 (35) | (251.037, 1931.03 252.0399, 150.04 253.053, 247.28 148.0035, 2204.68 149.002, 105.18 149.9993, 143.15 273.0203, 452.84 143.049, 930.55 144.043, 37.72 126.0219, 18291.66 127.0259, 657.53 128.0179, 1113.89) | 47351.55 | 19360.23 | 51600.29 | 18004.49 | 45882.64 | 17275.37 | 47596.33 | 14539.52 | -0.09 | 0.752429 | 0.820964 | -0.08 | 0.818742 | 0.921903 |
| COMPOUND_125_059a1_8322271 | Hilic | + | 125.0590 | 1.83 | | | | (126.0665, 5635.72 127.0699, 285.49 128.0708, 63.48) | 15602.63 | 2253.826 | 16428.6 | 2838.101 | 14522.93 | 6013.422 | 14613.51 | 4998.777 | -0.28 | 0.324841 | 0.425562 | -0.22 | 0.520438 | 0.764408 |
| COMPOUND_126_1157a1_6098809 | Hilic | + | 126.1157 | 1.61 | | | | (149.1024, 166.6 127.123, 6422.11 128.1265, 765.84 129.1205, 65.51) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.93 | 0.000491 | 0.001369 | 0.01 | 0.970943 | 0.984052 |
| COMPOUND_128_0586a5_6120524 | Hilic | + | 128.0586 | 5.61 | Unknown | 4 | 20 eV: 83.0595 (100), 56.0495 (25), 129.0673 (5) | (151.0483, 3549.03 152.05, 115.42 279.1072, 639.62 129.0659, 48212.21 130.0688, 3422.31 131.0701, 458.61) | 70551.17 | 37482.76 | 75750.57 | 39786.96 | 60105.29 | 21826.27 | 104803.5 | 61818 | -0.35 | 0.082337 | 0.136743 | 1.03 | 3.72E-05 | 0.007614 |
| COMPOUND_129_0429a6_042503 | Hilic | + | 129.0429 | 6.04 | Glutamine | 1 | 10 eV: 130.0503 (100), 84.0443 (80), 147.0761 (20) | (152.032, 12190.3 153.0357, 929.59 154.0363, 162.36 147.0765, 782716.06 148.0799, 43904.18 149.0813, 6153.97 130.05, 175970.55 131.0533, 10557.22 132.0544, 1190.18) | 1472919 | 384827.9 | 1318936 | 486148 | 2176402 | 676675.1 | 2643025 | 798302.3 | 0.78 | 0.000826 | 0.002186 | 0.74 | 0.006545 | 0.125256 |
| COMPOUND_129_0433a4_067703 | Hilic | + | 129.0433 | 4.07 | | | | (259.0934, 486.05 260.0955, 98.37 152.0317, 3496.85 153.0351, 184.1 281.0756, 1300.58 282.0784, 222.53 283.0842, 23.12 130.0503, 6502.85 131.0537, 443.3 132.0601, 139.59 276.1226, 189.74) | 37003.87 | 9565.398 | 36562.85 | 13972.86 | 22403.36 | 10173.96 | 26333.41 | 11226.59 | -1.30 | 6.73E-06 | 2.78E-05 | 0.45 | 0.155998 | 0.466545 |
| COMPOUND_129_0576a3_7972538 | Hilic | + | 129.0576 | 3.80 | | | | (130.065, 3119.85 131.0697, 496.7 132.0645, 72.76) | 38505.15 | 7798.927 | 39437.98 | 7329.016 | 33601.07 | 8452.955 | 35000.23 | 8296.928 | -0.55 | 0.047493 | 0.083952 | -0.04 | 0.903147 | 0.956673 |
| COMPOUND_129_0786a4_8300214 | Hilic | + | 129.0786 | 4.83 | Pipecolic acid | 1 | 20 eV: 84.0807 (100), | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | | |
|-----------------------------|--------|----------|----------------|---|----------|---|--|---------------|-----------|---------------|----------|---------------|----------|---------------|-----------|----------|----------|----------|-------------|----------|----------|----------|----------|
| | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p | | |
| | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | | |
| COMPOUND_132_0244a_4539337 | Hilic | + | 132.0244 | 4.45 Methionine (m/z 150.0586) | 1 | 20 eV: 56.0492 (100), 61.0108 (55), 74.0603 (15), 104.0515 (10), 45.9869 (10), 87.0254 (9) | (265.0652, 89.171)(150.0586, 49836.59)(151.0616, 3532.7)(152.0553, 2510.78)(133.0321, 5471.86)(134.0341, 337.57)(135.0287, 317.66) | 34130.06 | 15607.68 | 37690.39 | 22493.29 | 102990.6 | 28559.31 | 121552.7 | 43618.18 | 1.38 | 2.11E-09 | 2.11E-08 | 0.15 | 0.515006 | 0.761025 | | |
| COMPOUND_132_0536a6_15403 | Hilic | + | 132.0536 | 6.15 Asparagine | 1 | 10 eV: 74.0241 (100), 87.0548 (95), 133.0610 (35), 116.0345 (25) | (155.043, 9908.62)(156.0457, 838.72)(133.0608, 31914.45)(134.0648, 1504.61)(135.0646, 538.52) | 47191.83 | 11727.11 | 46687.17 | 13641.2 | 76886.07 | 27037.79 | 83233.25 | 24888.71 | 1.25 | 8.54E-08 | 5.46E-07 | 0.19 | 0.418065 | 0.69956 | | |
| COMPOUND_135_0322a0_7497464 | Hilic | + | 135.0322 | 0.75 fragment of 2PY | 1 | 10 eV: 137.0460 (100), 119.0356 (5), 110.0350 (4), 94.0399 (3) | (271.079, 1591.95)(153.066, 153165.66)(154.0691, 12821.9)(155.0721, 1656.51)(136.0395, 14648.16)(137.0429, 1051.18)(138.0531, 185.66) | 336509.2 | 178787.1 | 296524.7 | 175827.6 | 311316.5 | 159380.3 | 513463.8 | 243751.8 | -0.11 | 0.665042 | 0.752222 | 1.08 | 0.000834 | 0.045795 | | |
| COMPOUND_136_0388a1_3568484 | Hilic | + | 136.0388 | 1.36 Hypoxanthine | 2 | 20 eV: 137.0460 (100), 119.0356 (5), 110.0350 (4), 94.0399 (3) | (1273.0848, 18746.45)(274.0869, 2460.75)(275.0922, 547.93)(159.0278, 121015.23)(160.0305, 8038.76)(161.0328, 611.76)(295.0668, 45767.58)(296.0694, 6148.97)(297.0724, 870.89)(298.0844, 95.27)(154.0715, 281.15)(137.0458, 403657.34)(138.0489, 23362.65)(139.0511, 1747.92) | 1945179 | 450572.9 | 2063340 | 429922.7 | 1572090 | 477914.1 | 1715478 | 1414438.3 | -0.83 | 0.004046 | 0.009316 | 0.04 | 0.911712 | 0.958977 | | |
| COMPOUND_136_0637a2_0840712 | Hilic | + | 136.0637 | 2.08 1-Methylnicotinamide | 1 | 20 eV: 137.0699 (100), 94.0645 (60), 92.0490 (55) | (175.1028, 884.55)(276.1058, 170.14)(160.0368, 12125.84)(161.04, 1050.28)(162.0442, 163.15)(297.0847, 1034.85)(298.087, 185.12)(299.0939, 79.32)(138.0547, 765883.5)(139.0584, 62203.91)(140.061, 4981.41)(292.1277, 267.54)(293.1173, 96.15) | 193383.8 | 88257.82 | 190411.7 | 93447.38 | 222314.9 | 90033.67 | 304174.7 | 169436 | 0.33 | 0.221768 | 0.315092 | 0.42 | 0.189123 | 0.504029 | | |
| COMPOUND_137_0481a4_037293 | Hilic | + | 137.0481 | 4.04 Trigonefine | 1 | 20 eV: 138.0555 (100), 94.0649 (70), 92.0500 (45), 78.0349 (10), 79.0409 (9) | (279.2786, 263.66)(162.128, 339.24)(301.2533, 530.54)(157.17, 157.55)(140.1431, 6981.32)(141.146, 691.09) | 609770.2 | 829792.5 | 551571.2 | 952817 | 1378993 | 1350694 | 597695.9 | 876805.2 | 0.83 | 0.002301 | 0.005632 | -0.56 | 0.069913 | 0.323961 | | |
| COMPOUND_138_0419a1_0292504 | Hilic | + | 138.0419 | 1.03 Urocanic acid | 1 | 10 eV: 139.0522 (100), 121.0378 (45), 95.0624 (5) | (139.0503, 26239.46)(140.0536, 2033.2)(141.0554, 301.66) | 22182.6 | 14917.04 | 21356.02 | 12764.02 | 38387.36 | 19021.83 | 26717.4 | 11943.7 | 1.13 | 0.000119 | 0.000364 | -0.61 | 0.064647 | 0.307286 | | |
| COMPOUND_139_1365a0_727119 | Hilic | + | 139.1365 | 0.73 | 1 | (279.2786, 263.66)(162.128, 339.24)(301.2533, 530.54)(157.17, 157.55)(140.1431, 6981.32)(141.146, 691.09) | 17623.06 | 3270.431 | 18841.71 | 2686.747 | 22073.21 | 5172.411 | 20686.3 | 3052.885 | 1.12 | 7.12E-05 | 0.000227 | -0.48 | 0.128746 | 0.425125 | | | |
| COMPOUND_140_0592a5_148521 | Hilic | + | 140.0592 | 5.15 | 1 | (141.0662, 21732.08)(142.0698, 1634.69)(143.0828, 288.11) | 20873.29 | 15773.61 | 17223.05 | 1551.56 | 22610.92 | 16281.26 | 27896.57 | 27127.15 | 0.17 | 0.514712 | 0.61525 | 0.46 | 0.128315 | 0.424949 | | | |
| COMPOUND_141_0794a1_2786746 | Hilic | + | 141.0794 | 1.28 | 1 | (164.0684, 2417.25)(165.0722, 263.9)(166.078, 33.62)(305.1475, 118.36)(142.0866, 97285.31)(143.0898, 8370.35)(144.0926, 606.3) | 5861 | 1854.936 | 8605.2 | 1683.105 | 105905 | 70117.49 | 189128.4 | 194126.2 | 0.93 | 2.28E-08 | 1.72E-07 | 0.46 | 0.009898 | 0.153413 | | | |
| COMPOUND_142_1105a1_4718053 | Hilic | + | 142.1105 | 1.47 | 1 | (143.1181, 8665.2)(144.1209, 788.6)(145.1316, 115.68) | 16575.87 | 6856.614 | 15862.15 | 4980.721 | 21772.5 | 4681.09 | 22980.18 | 6560.771 | 0.80 | 0.000953 | 0.002496 | 0.27 | 0.326359 | 0.633587 | | | |
| COMPOUND_143_0944a3_2846339 | Hilic | + | 143.0944 | 3.28 Proline betaine | 1 | 20 eV: 144.1022 (100), 58.0656 (25), 84.0816 (24) | (287.1971, 2658.26)(288.1996, 283.24)(289.1945, 210.44)(166.0846, 5687.51)(167.0904, 1144.52)(168.0918, 299.66)(309.175, 324.63)(310.1771, 94.87)(144.1014, 1450867.0)(145.1051, 98817.09)(146.1077, 7669.81) | 1812185.8 | 2032557.4 | 1666507.1 | 18431029 | 18796888 | 16581404 | 20866122 | 18635081 | 0.26 | 0.346151 | 0.447707 | 0.01 | 0.985314 | 0.992364 | | |
| COMPOUND_143_0946a3_9029844 | Hilic | + | 143.0946 | 3.90 | 1 | (144.102, 95526.16)(145.1053, 8282.14)(146.1086, 729.7) | 84920.62 | 58767.59 | 89475.11 | 60524.12 | 101882.6 | 58280.58 | 224224.3 | 171331.9 | 0.31 | 0.133053 | 0.207504 | 0.80 | 0.001338 | 0.058548 | | | |
| COMPOUND_143_0948a4_9968605 | Hilic | + | 143.0948 | 5.00 | 1 | (166.0856, 766.75)(144.1019, 5658.62)(145.1047, 646.35)(146.092, 539.5) | 13241.63 | 3577.532 | 14448.92 | 4260.488 | 16062.25 | 3533.222 | 20616.81 | 5215.788 | 0.32 | 0.167358 | 0.250925 | 0.82 | 0.003321 | 0.082317 | | | |
| COMPOUND_145_053a4_673086 | Rp | + | 145.0530 | 4.67 | 1 | (146.0603, 13883.18)(147.0634, 1509.62)(148.0552, 1409.93) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.11 | 4.56E-06 | 1.96E-05 | -0.01 | 0.966437 | 0.982565 |
| COMPOUND_145_0739a0_7994704 | Hilic | + | 145.0739 | 0.80 | 1 | (291.1528, 624.7)(168.0636, 2169.81)(169.0683, 152.92)(170.0634, 82.51)(313.1338, 232.06)(146.0817, 155426.14)(147.0847, 10036.62)(148.0875, 999.92)(308.1867, 1425.62) | 74456.79 | 76412.77 | 68000.98 | 74849.02 | 84655.36 | 60792.09 | 111955.9 | 114652.6 | 0.43 | 0.12291 | 0.194457 | 0.30 | 0.357049 | 0.665625 | | | |
| COMPOUND_145_074a0_78353864 | Hilic | + | 145.0740 | 0.78 | 1 | (291.1528, 624.7)(168.0635, 2231.98)(169.0669, 127.44)(170.0595, 241.15)(313.1312, 239.43)(146.0816, 127334.28)(147.085, 8990.95)(148.0875, 1286.03)(308.1855, 1313.39) | 67290.11 | 77161.07 | 65362.24 | 76290.01 | 71763.57 | 58440.02 | 92180.25 | 116548.3 | 0.51 | 0.07467 | 0.125584 | 0.15 | 0.659826 | 0.842895 | | | |
| COMPOUND_145_084a3_482057 | Hilic | + | 145.0848 | 3.48 | 1 | (146.0925, 10775.37)(147.095, 872.44)(148.096, 301.91) | 54875.23 | 23239.65 | 53230.28 | 18976.35 | 19228.3 | 18683.94 | 20922.03 | 20082.07 | -0.64 | 0.010617 | 0.022366 | -0.37 | 0.203399 | 0.5149 | | | |
| COMPOUND_145_1106a2_9687293 | Hilic | + | 145.1106 | 2.97 duplicate of 4-aminobutyric acid betaine | 1 | (146.1178, 62740.04)(147.1211, 5312.56)(148.1232, 604.17) | 174288.1 | 36939.47 | 189895.7 | 37498.38 | 150710.1 | 37679.53 | 164024.3 | 50375.38 | -0.57 | 0.044081 | 0.078288 | -0.06 | 0.861058 | 0.942428 | | | |
| COMPOUND_145_1109a3_0587182 | Hilic | + | 145.1109 | 3.06 4-Aminobutyric acid betaine | 1 | (146.1177, 24228.69)(147.1207, 1926.83)(148.1223, 289.17) | 79084.85 | 15501.9 | 80805.07 | 28247.23 | 7338.21 | 23142.21 | 83396 | 39660.34 | -0.46 | 0.123051 | 0.194464 | 0.36 | 0.313852 | 0.62054 | | | |
| COMPOUND_146_0942a5_80901 | Rp | - | 146.0942 | 5.81 | 1 | (145.0868, 11390.1)(146.0903, 935.53)(147.0918, 159.81) | 17924.58 | 8307.674 | 22270.27 | 9839.882 | 11764 | 1677.605 | 12633.13 | 2920.281 | -1.09 | 7.25E-07 | 3.78E-06 | -0.18 | 0.453647 | 0.725577 | | | |
| COMPOUND_147_0532a6_3011127 | Hilic | + | 147.0532 | 6.30 Glutamate | 1 | 10 eV: 84.0438 (100), 148.0589 (25), 130.0499 (20), 102.0549 (5) | (170.0425, 4258.46)(171.0457, 401.01)(317.0898, 214.69)(148.0608, 165728.64)(149.0639, 10732.5)(150.0653, 1867.89) | 143993.1 | 49687.64 | 177025 | 90122.76 | 96565.14 | 73286.66 | 88610.39 | 67704.38 | -0.78 | 0.002768 | 0.006652 | -0.43 | 0.154999 | 0.466404 | | |
| COMPOUND_147_0895a3_9679167 | Hilic | + | 147.0895 | 3.97 | 1 | (148.0969, 11739.22)(149.1009, 901.27)(150.11, 233.12) | 16831.74 | 6799.892 | 17980.67 | 7843.962 | 25699.36 | 10443.44 | 28422.98 | 14522.97 | 0.97 | 7.95E-05 | 0.00025 | -0.24 | 0.363561 | 0.668521 | | | |
| COMPOUND_148_0147a9_429351 | Rp | + | 148.0147 | 9.43 | 1 | (297.0457, 152.78)(335.0046, 131.18)(171.0047, 162.42)(149.0234, 26552.31)(150.0265, 2354.88) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.33 | 0.252432 | 0.348623 | 0.00 | 0.998689 | 0.999577 | |
| COMPOUND_148_0158a9_357669 | Rp | + | 148.0158 | 9.36 | 1 | (335.0002, 155.89)(171.003, 165.61)(319.0306, 125.5)(149.0234, 31700.56)(150.0262, 2924.31) | 108980.7 | 10317.62 | 109362.2 | 12775.93 | 109725.5 | 120991.4 | 108069.5 | 11782.21 | 0.05 | 0.869795 | 0.912333 | -0.17 | 0.617807 | 0.816971 | | | |
| COMPOUND_148_0163a11_066134 | Rp | + | 148.0163 | 11.07 | 1 | (186.9817, 12537.67)(187.9833, 1243.24)(149.0245, 19723.22)(150.0277, 1514.11)(151.0361, 381.97) | 43074.17 | 12509.38 | 36821.28 | 13006.56 | 57888.43 | 14161.43 | 61056.93 | 16628.28 | 0.87 | 0.000701 | 0.00189 | 0.55 | 0.062799 | 0.307286 | | | |
| COMPOUND_149_0514a0_8602325 | Hilic | + | 149.0514 | 0.86 | 1 | (172.0391, 386.81)(167.0917, 1189.51)(168.1002, 32.5)(150.0583, 40768.66)(151.0614, 3611.35)(152.0564, 1611.57)(1316.1389, 617.56) | 38407.23 | 10857.11 | 37577.63 | 9833.099 | 48986.07 | 12170.2 | 53896.67 | 16147.32 | 0.70 | 0.004252 | 0.00973 | 0.47 | 0.094988 | 0.36381 | | | |
| COMPOUND_150_1371a1_4405302 | Hilic | + | 150.1371 | 1.44 Trimethylamino N-oxide | 2 | 10 eV: 76.0760 (100), 151.1442 (5) | (301.2922, 107.04)(151.1438, 988447.0)(152.1475, 64746.88)(153.149, 5133.22)(76.0755, 4782.93)(76.57, 48.71) | 329913.2 | 1351085 | 275428.3 | 640911.3 | 257107.1 | 238474.1 | 318795.8 | 381445.9 | 0.53 | 0.067671 | 0.115803 | -0.11 | 0.748228 | 0.891783 | | |
| COMPOUND_152_0587a0_7483809 | Hilic | + | 152.0587 | 0.75 2PY (N-methyl-2-pyridone-5-carboxa | 2 | 20 eV: 136.0383 (100), 92.0506 (80), 109.0772 (45), 80.0500 (10) | (305.1109, 476.23)(175.048, 4180.01)(176.0514, 301.04)(153.0662, 96785.63)(154.0694, 7426.83)(155.0723, 1060.04)(156.0705, 49.96) | 31975.6 | 169556.9 | 280775.6 | 166017.6 | 296913.9 | 152901.9 | 492608.9 | 230300.9 | -0.11 | 0.689375 | 0.768618 | 1.03 | 0.001507 | 0.06002 | | |
| COMPOUND_152_0588a1_4972587 | Rp | + | 152.0588 | 1.50 Unknown | 4 | 20 eV: 153.0671 (100), 110.0584 (88), 108.0452 (60), 78.0329 (33), 135.0518 (25), 70.0276 (22), 122.0228 (20) | (175.0475, 739.31)(176.0478, 38.53)(191.0166, 171.83)(153.066, 18654.11)(154.0691, 1508.13)(155.0695, 246.12) | 75747.51 | 37421.05 | 61758.15 | 29974.59 | 50126.29 | 22210.45 | 84157.04 | 41750.7 | -0.71 | 0.010762 | 0.022608 | 1.26 | 0.002021 | 0.018868 | | |
| COMPOUND_152_1204a8_79496 | Rp | | | | | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|-----------------------------|----------|--|---|---------------|-----------|---------------|----------|---------------|----------|---------------|-----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_159_09a0_80897224 | Hilic | + | 159.0900 | 0.81 | | | | (319.2008, 176.35 182.08, 1151.74 183.0818, 218.36 341.1727, 226.21 160.0969, 30785.68 161.1008, 2368.6 162.1013, 271.59 336.2175, 2922.77 337.2204, 808.16) | 31352.45 | 18330.25 | 32321.96 | 14313.38 | 39499.36 | 17907.66 | 57163.67 | 36350.72 | 0.54 | 0.027893 | 0.052875 | 0.32 | 0.253985 | 0.566051 |
| COMPOUND_159_1264a_0211587 | Rp | + | 159.1260 | 4.02 | | | (160.1336, 10226.85 161.1363, 957.39 162.1295, 135.22) | 28743.08 | 16741.2 | 26197.58 | 10009.5 | 51337.21 | 85725.76 | 26752.34 | 14872.29 | 0.29 | 0.233347 | 0.328026 | -0.36 | 0.208107 | 0.518913 | |
| COMPOUND_159_1264a_19194915 | Hilic | + | 159.1264 | 1.92 | 5-Aminovaleric acid betaine | 1 | 10 eV: 160.1334 (100), 60.0809 (30), 101.0609 (25) | (341.2543, 438.82 342.2452, 119.31 177.1633, 56.41 160.1333, 181574.97 161.1364, 17522.03 162.1381, 1744.43 163.1407, 96.94) | 79419.9 | 211637.9 | 76504.92 | 25318.95 | 669165.7 | 163231.8 | 806496.6 | 266227.4 | -0.50 | 0.048847 | 0.075047 | 0.63 | 0.202807 | 0.219937 |
| COMPOUND_160_1096a6_332935 | Rp | - | 160.1096 | 6.33 | | | (159.1024, 9165.55 160.106, 725.64 161.1084, 134.08) | 17084.84 | 9378.35 | 16574.57 | 5177.725 | 13749.4 | 1336.556 | 13995.66 | 3716.272 | -0.70 | 0.005746 | 0.012838 | 0.16 | 0.574884 | 0.79068 | |
| COMPOUND_160_1098a6_856494 | Rp | - | 160.1098 | 6.86 | | | (159.1024, 9108.61 160.1061, 1882.38 161.1072, 239.18) | 20932.62 | 10954.83 | 18802.02 | 4009.22 | 22218.14 | 12731.54 | 19129.67 | 5176.444 | 0.11 | 0.709556 | 0.787658 | -0.15 | 0.671887 | 0.851748 | |
| COMPOUND_160_1213a6_7415733 | Hilic | + | 160.1213 | 6.74 | | | (183.1059, 595.51 161.1288, 75614.12 162.132, 6045.43 163.1338, 787.01) | 47896.77 | 28829.72 | 55562.34 | 35238.38 | 54003.79 | 40480.67 | 79282.91 | 58850.65 | 0.04 | 0.818224 | 0.872049 | 0.45 | 0.032582 | 0.244873 | |
| COMPOUND_161_1052a4_6681848 | Hilic | + | 161.1052 | 4.67 | L-Carnitine | 1 | 10 eV: 162.1130 (100), 103.0391 (15), 60.0811 (15) | (323.2164, 694.27 324.2295, 254.54 325.206, 273.48 184.0946, 28661.07 185.0988, 2437.93 186.0981, 430.18 345.201, 678.05 346.1981, 271.11 347.1853, 225.2 162.1128, 1180400.0 163.1165, 84337.64 164.1182, 11723.16 165.1204, 627.14) | 15620755 | 2296013 | 15868948 | 2771683 | 9735898 | 1715885 | 12387019 | 4095732 | -1.53 | 2.58E-08 | 1.89E-07 | 0.69 | 0.015419 | 0.185682 |
| COMPOUND_161_1055a5_3846574 | Hilic | + | 161.1055 | 5.38 | | | (184.0946, 596.14 162.1126, 8253.83 163.116, 712.81 164.1243, 86.26) | 11269.83 | 5101.885 | 1362.29 | 4482.939 | 9010.5 | 3328.291 | 8929.061 | 4287.766 | -0.62 | 0.028978 | 0.054747 | -0.14 | 0.681296 | 0.853001 | |
| COMPOUND_162_0674a7_166878 | Rp | + | 162.0674 | 7.17 | | | (162.0674, 22142.65 164.079, 2339.11 165.0853, 322.73) | 60017.23 | 24612.94 | 54521.98 | 21255.12 | 74084.14 | 13695.71 | 59465.66 | 21709.75 | 0.47 | 0.117742 | 0.187521 | -0.26 | 0.462826 | 0.731428 | |
| COMPOUND_162_0677a5_95999 | Rp | + | 162.0677 | 5.96 | | | (185.0578, 607.24 186.0624, 38.16 180.102, 944.06 181.1057, 146.39 163.0753, 14377.15 164.0788, 1666.86 165.0923, 289.49) | 37579.1 | 11163.32 | 38401.39 | 11998.57 | 36641.33 | 13697.4 | 37532.1 | 12940.22 | -0.12 | 0.696862 | 0.77844 | -0.08 | 0.820648 | 0.922833 | |
| COMPOUND_162_0682a7_1922607 | Rp | + | 162.0682 | 7.19 | | | (163.0758, 25239.6 164.0792, 2974.47 165.0891, 585.97) | 62121.33 | 25516.99 | 63412.45 | 22240.73 | 79000 | 31692.96 | 62447.17 | 22599.83 | 0.55 | 0.056334 | 0.096598 | -0.23 | 0.492686 | 0.748671 | |
| COMPOUND_162_0684a8_3995502 | Rp | + | 162.0684 | 8.40 | | | (363.0926, 144.05 163.0758, 22784.43 164.0791, 2964.67 165.0894, 320.91) | 46408.44 | 17770.79 | 36990.73 | 20098.19 | 51437.57 | 21782.33 | 43506.26 | 19047.61 | 0.39 | 0.232658 | 0.242754 | 0.02 | 0.951884 | 0.980885 | |
| COMPOUND_162_0688a8_3108421 | Rp | + | 162.0688 | 8.31 | | | (363.0925, 141.81 163.0756, 36728.90 164.0792, 4091.49 165.0839 165.0839, 371.92) | 67031.43 | 29380.55 | 54381.61 | 32425.66 | 77139.93 | 35848.18 | 66790.84 | 31094.85 | 0.17 | 0.629951 | 0.827657 | | | | |
| COMPOUND_162_1051a6_3720818 | Rp | + | 162.1051 | 6.37 | | | (163.1121, 26504.05 164.1157, 3107.88 165.1227, 332.44) | 37231.89 | 17771.51 | 35429.87 | 14838.65 | 32069 | 3701.655 | 32497.44 | 13884.15 | -1.24 | 3.86E-08 | 2.72E-07 | -0.02 | 0.914331 | 0.961085 | |
| COMPOUND_162_1262a5_6244516 | Rp | + | 162.1262 | 5.62 | | | (185.1168, 1229.52 186.1173, 148.13 187.1083, 84.44 180.1601, 1887.49 181.1615, 197.99 182.1629, 24.7 163.1333, 11266.86 164.1372, 1075.71 165.1305, 190.24) | 66818.94 | 8352.836 | 62576.74 | 6310.16 | 61503.36 | 7713.786 | 64478.75 | 8104.658 | -0.70 | 0.021584 | 0.042131 | 0.90 | 0.013152 | 0.173893 | |
| COMPOUND_163_0225a5_6991754 | Hilic | + | 163.0225 | 5.70 | | | (181.059, 1007.55 164.0296, 10013.45 165.0338, 613.42 166.0357, 143.67 344.0802, 157.63) | 34791.3 | 7220.134 | 38165.76 | 8950.592 | 42577.5 | 10286.61 | 49504.35 | 10446.24 | 0.76 | 0.002601 | 0.006305 | 0.27 | 0.346002 | 0.651869 | |
| COMPOUND_164_0476a4_975613 | Hilic | + | 164.0476 | 4.98 | Tyrosine (m/z 182.0811) | 1 | 10 eV: 136.0759 (100), 165.0551 (70), 123.0442 (25), 147.0444 (15), 182.0821 (10) | (329.1157, 343.96 182.0816, 67949.21 183.0849, 7110.25 184.0898, 1279.85 185.0851, 80.13 165.0546, 13304.5 166.0584, 1347.35 167.0660, 163.57) | 293362.4 | 56807.66 | 330078.2 | 80870.94 | 322662.1 | 52006.98 | 316936.7 | 82490.42 | 0.49 | 0.103933 | 0.168387 | -0.68 | 0.061113 | 0.302474 |
| COMPOUND_164_0834a5_493956 | Rp | + | 164.0834 | 5.49 | | | (329.1779, 2813.53 187.0758, 581.16 165.0914, 13299.32 166.0938, 1588.53) | 19711.59 | 6711.891 | 21950.55 | 10424.1 | 29925.25 | 13406.95 | 27887.27 | 13279.19 | -0.53 | 0.028711 | 0.054288 | -0.39 | 0.177227 | 0.491826 | |
| COMPOUND_164_1203a8_410994 | Rp | + | 164.1203 | 8.41 | | | (165.1279, 27714.15 166.1331, 3592.68) | 35214.58 | 15199.91 | 34954.54 | 12772.32 | 34411.33 | 4260.767 | 39523.29 | 10381.88 | -1.14 | 5.09E-07 | 2.74E-06 | -0.10 | 0.673133 | 0.848765 | |
| COMPOUND_165_0462a6_005415 | Hilic | + | 165.0462 | 6.01 | | | (188.0354, 18877.94 189.0387, 1348.49 190.0325, 903.43 353.0813, 1087.1 166.0535, 15283.03 167.0559, 907.31 168.0499, 835.69 169.0509, 34.21) | 11816.6 | 29835.73 | 18186.4 | 40105.43 | 34860.79 | 33283.22 | 31573.8 | 32192.45 | -1.17 | 1.43E-06 | 6.96E-06 | -0.34 | 0.192796 | 0.505089 | |
| COMPOUND_165_0654a1_4190111 | Hilic | + | 165.0654 | 1.42 | | | (331.1397, 413.73 332.1487, 73.14 188.0552, 708.89 166.0723, 24192.33 167.0755, 2107.92 168.0779, 253.98) | 60919.34 | 12610.77 | 62054.35 | 14436.27 | 129166.1 | 25643.78 | 121897.4 | 24490.95 | 1.66 | 1.58E-12 | 6.22E-11 | -0.12 | 0.599429 | 0.805439 | |
| COMPOUND_165_0789a1_9692475 | Rp | + | 165.0789 | 1.97 | Normetanephrine | 1 | 10 eV: 170.081(100), 103.0549(5), 166.0934(4) | (331.1524, 60.73 204.0338, 252.77 166.0863, 66450.02 167.0899, 62677.99 168.0921, 5057.16) | 5064084 | 925003.3 | 5061087 | 1008721 | 4985224 | 1080000 | 5081637 | 1151667 | -0.03 | 0.924058 | 0.950653 | 0.01 | 0.97179 | 0.984467 |
| COMPOUND_165_0792a3_5999737 | Hilic | + | 165.0792 | 3.60 | Phenylalanine | 2 | 10 eV: 120.0814 (100), 166.0876 (5) | (331.1578, 151.94 188.0682, 8406.81 189.0706, 970.98 190.0715, 114.71 353.1625, 272.18 166.0861, 79509.6 167.0897, 75220.42 168.0921, 6556.49 348.1968, 220.12) | 3202594 | 665554.3 | 3317060 | 666370 | 3149198 | 823712.1 | 3219243 | 838379.3 | 0.04 | 0.897854 | 0.933072 | -0.23 | 0.486477 | 0.747178 |
| COMPOUND_166_0629a4_513383 | Rp | - | 166.0629 | 4.51 | | | (201.025, 110.89 165.0555, 10954.59 166.0582, 1218.29 167.0706, 154.95 211.0615, 685.14 331.1223, 747.58) | 20162.82 | 10549 | 20692.4 | 11681.36 | 22361.38 | 7649.277 | 18871.29 | 9605.785 | 0.30 | 0.287381 | 0.386378 | -0.59 | 0.082054 | 0.343638 | |
| COMPOUND_166_1364a8_912118 | Rp | + | 166.1364 | 8.91 | | | (371.2352, 3531.2 372.2383, 966.78 373.2376, 207.53 167.1436, 44370.44 168.147, 5615.04 169.1533, 796.94) | 106125.5 | 35473.87 | 108805.2 | 40774.07 | 65125.5 | 35708.67 | 67663.27 | 35743.13 | -1.29 | 2.76E-09 | 2.64E-08 | -0.10 | 0.654348 | 0.841269 | |
| COMPOUND_168_9786a5_236611 | Hilic | + | 168.9786 | 5.24 | | | (159.986, 5457.63 170.9883, 262.78 171.982, 337.98) | 25426.04 | 4296.223 | 27767.33 | 4234.026 | 25487.38 | 2870.982 | 29442.09 | 3112.925 | -0.14 | 0.621305 | 0.713139 | -0.41 | 0.238046 | 0.543692 | |
| COMPOUND_169_0852a6_19915 | Hilic | + | 169.0852 | 6.20 | 1-Methylhistidine | 2 | 20 eV: 124.0871 (100), 83.0600 (45), 96.0673 (15), 170.0909 (5) | (339.1825, 181.29 192.0754, 4364.2 193.078, 400.18 194.0772, 75.56 170.0925, 124629.09 171.0955, 10290.07 172.0974, 1233.98) | 118778.4 | 35522.58 | 128595.6 | 40947.36 | 192434.4 | 123944.9 | 246632.4 | 186773.73 | 0.71 | 0.001309 | 0.003335 | 0.50 | 0.046305 | 0.273966 |
| COMPOUND_169_0852a6_288577 | Hilic | + | 169.0852 | 6.29 | | | (339.1848, 58.04 192.0745, 1128.6 193.0759, 39.77 194.0778, 37.63 170.0926, 105897.48 171.0956, 8616.52 172.098, 1152.79) | 72131.91 | 20648.94 | 80276.02 | 27092.84 | 111485.6 | 134476.3 | 142686.2 | 204807.6 | 0.62 | 0.820856 | 0.873202 | 0.44 | 0.165508 | 0.47786 | |
| COMPOUND_169_0852a6_804594 | Hilic | + | 169.0852 | 6.80 | 3-Methylhistidine | 2 | 20 eV: 96.0684 (100), 109.0756 (25), 68.0489 (15), 126.1045 (12), 125.0698 (9), 82.0641 (8), 170.0949 (5) | (192.0744, 342.53 161.1589, 202.93 170.0925, 280469.06 171.0957, 21349.58 172.0984, 2053.88) | 206835.9 | 273606.1 | 193946.9 | 288145.6 | 247750.1 | 273858.6 | 223370.4 | 230947.8 | 0.02 | 0.935699 | 0.957815 | 0.22 | 0.498762 | 0.753329 |
| COMPOUND_171_1136a1_2169836 | Hilic | + | 171.1136 | 1.22 | | | (172.1197, 4131.97 173.1219, 492.03 174.1246, 81.87) | 10785.59 | 2533.737 | 12527.24 | 4071.462 | 13016.86 | 3552.247 | 13092.75 | 3402.5 | 0.66 | 0.019837 | 0.039186 | -0.39 | 0.228651 | 0.535521 | |
| COMPOUND_173_1163a1_8126739 | Hilic | + | 173.1163 | 1.81 | | | (174.1234, 10491.71 175.1277, 1113.12 176.1338, 137.12) | 17933.83 | 9247.958 | 19511.627 | 10172.22 | 13361.1 | 9403.219 | 14880.53 | 13247.99 | -0.78 | 0.001992 | 0.004957 | -0.07 | 0.796948 | 0.91372 | |
| COMPOUND_173_1165a1_712097 | Hilic | + | 173.1165 | 1.71 | | | (174.1237, 14110.3 175.1264, 1197.38 176.1342, 312.36) | 22227.04 | 9475.665 | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|-----------------------------|--------|----------|----------|-----------|--------------------------|----------|---|--|--|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_180_0649a2_8124936 | Rp | + | 180.0649 | 2.81 | Paraxanthine | 1 | 10eV: 181.0709(100), 124.0497(15), 77.9675(4), 42.0308(1.5) | (203.054, 195.8789)(204.0553, 141.25)(181.0726, 68232.86)(182.0756, 6317.74)(183.0763, 538.56) | 175012.5 | 181781.8 | 170105.1 | 144207.9 | 237832.9 | 210050.5 | 145755.3 | 142679.6 | 0.69 | 0.0138 | 0.028459 | -0.76 | 0.020252 | 0.199159 | |
| COMPOUND_180_0652a2_3989115 | Rp | + | 180.0652 | 2.40 | | | (399.0835, 890.77)(203.0539, 4027.42)(204.0571, 359.5)(181.0723, 275140.12)(182.0752, 23901.78)(183.0772, 2138.58) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 139607.8 | 117585.6 | 156233 | 122502.8 | 269870.4 | 164228.6 | 183419.7 | 303147.6 | 1.06 | 0.00017 | 0.000559 | -0.96 | 0.003096 | 0.079218 | |
| COMPOUND_180_1157a6_7009764 | Rp | + | 180.1157 | 6.70 | | | (203.0550, 1030.19)(204.1044, 199.55)(181.1232, 16216.1)(182.1263, 1944.2)(183.1357, 482.16) | (183.0854, 25054.65) 39885.42 | 15054.65 | 35523.72 | 16717.44 | 25155.8 | 15609.17 | 26444 | 13759.8 | -1.24 | 3.17E-08 | 2.62E-07 | -0.10 | 0.067565 | 0.846185 | | |
| COMPOUND_181_0854a6_0349765 | Hilic | + | 181.0854 | 6.03 | | | (363.1674, 153.21)(204.0703, 71.17)(182.0925, 26466.98)(183.0957, 2407.42)(184.0983, 373.77) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 23672.94 | 26202.79 | 26664.71 | 23211 | 18175 | 13612.53 | 31905.27 | 21895.04 | -1.11 | 3.13E-06 | 1.39E-05 | -0.06 | 0.822181 | 0.922833 | |
| COMPOUND_182_0736a7_964954 | Rp | + | 182.0736 | 7.96 | | | (205.0851, 2071.04)(206.0851, 245.2)(200.1295, 2048.45)(183.1021, 9117.99)(184.1043, 1013.7)(185.0898, 392.87) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 71385.23 | 29963.26 | 56383.52 | 29387.98 | 82802.14 | 40825.25 | 70528.19 | 29706.34 | 0.39 | 0.192379 | 0.281323 | 0.03 | 0.9233 | 0.965307 | |
| COMPOUND_182_0948a5_4959054 | Rp | + | 182.0948 | 5.50 | | | (184.074, 10788.05)(185.0768, 767.26)(186.0786, 249.14) | (205.0851, 2071.04)(206.0851, 245.2)(200.1295, 2048.45)(183.1021, 9117.99)(184.1043, 1013.7)(185.0898, 392.87) | 19014.48 | 7326.411 | 22982.15 | 12335.54 | 36693.67 | 8835.101 | 30383.64 | 13761.5 | -0.71 | 0.004231 | 0.009712 | -0.23 | 0.424466 | 0.704939 | |
| COMPOUND_182_1054a0_7720168 | Hilic | + | 182.1054 | 0.77 | no msms | | (365.229, 585.7)(387.188, 522.05)(183.1132, 9611.53)(184.1136, 1433.97)(185.103, 499.13)(282.2559, 473.75) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 10701.5 | 3708.421 | 11099.53 | 4922.505 | 12996.8 | 5306.559 | 22699 | 11123.12 | -0.23 | 0.260733 | 0.357595 | 1.50 | 5.58E-08 | 0.000126 | |
| COMPOUND_183_0659a10_258124 | Rp | + | 183.0659 | 10.26 | | | (222.0197, 127.15)(184.0741, 18951.51)(185.0776, 1220.49)(186.0831, 241.15)(384.1897, 305.28) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 89557.02 | 8099.762 | 90011.67 | 8785.237 | 69119.07 | 8495.189 | 71241.86 | 10676.73 | -1.52 | 4.7E-10 | 5.74E-09 | 0.09 | 0.7188 | 0.876415 | |
| COMPOUND_183_0662a10_140341 | Rp | + | 183.0662 | 10.14 | | | (367.143, 204.38)(184.0739, 35737.41)(185.0771, 2288.61)(186.0781, 530.2) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 154455.3 | 18862.58 | 149769.2 | 30214.37 | 99520.36 | 19738.19 | 103132.4 | 23331.83 | -1.55 | 1.69E-09 | 1.75E-08 | 0.22 | 0.400334 | 0.690408 | |
| COMPOUND_183_0663a10_559524 | Rp | + | 183.0663 | 10.56 | | | (184.074, 10788.05)(185.0767, 908.39)(186.0797, 175.05) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 32578.89 | 6903.901 | 33013.33 | 7630.033 | 13323.88 | 2364.051 | 14646.74 | 2986.511 | -1.55 | 5.3E-13 | 2.86E-11 | -0.03 | 0.896441 | 0.954308 | |
| COMPOUND_183_0663a10_060661 | Hilic | + | 183.0663 | 1.06 | Phosphocholine | 2 | 10 eV: 184.0733 (100), 86.0966 (15) | (184.074, 10788.05)(185.0767, 908.39)(186.0797, 175.05) | 89152.09 | 21334.42 | 101458.3 | 18719.13 | 45740.57 | 11775.54 | 46801.2 | 12877.07 | -1.34 | 7.52E-10 | 8.73E-09 | -0.43 | 0.051292 | 0.283822 | |
| COMPOUND_183_0666a10_631687 | Rp | + | 183.0666 | 10.63 | | | (184.074, 10788.05)(185.0768, 767.26)(186.0786, 249.14) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 29950.69 | 5942.219 | 30377.71 | 5798.389 | 14882.43 | 2852.957 | 15953.35 | 3254.281 | -1.42 | 2.96E-11 | 6.17E-10 | -0.12 | 0.556281 | 0.781554 | |
| COMPOUND_183_1623a0_7821191 | Hilic | + | 183.1623 | 0.78 | | 4 | 10 eV: 102.0916 (100), 184.1686 (60), 128.1077 (12), 84.081 (10) | (367.3288, 270.57)(184.1697, 25207.48)(185.1732, 3375.01)(186.1853, 381.75) | 74998.64 | 7757.117 | 79599.09 | 10052.65 | 78103.86 | 8856.204 | 7706.93 | 8401.267 | 0.38 | 0.192173 | 0.281205 | 0.60 | 0.087933 | 0.350486 | |
| COMPOUND_184_1212a2_6085315 | Rp | + | 184.1212 | 2.61 | no msms | | (185.1289, 11922.88)(186.1321, 1202.92)(187.134, 279.18) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 28702.53 | 12291.72 | 24245.24 | 8456.348 | 20498.21 | 7503.059 | 37059.5 | 15507.18 | -0.64 | 0.01662 | 0.033477 | 1.59 | 2.87E-06 | 0.003234 | |
| COMPOUND_184_1468a8_186916 | Rp | + | 184.1468 | 8.19 | | | (207.1385, 5686.95)(208.1382, 1278.36)(202.1809, 205.152)(203.1819, 492.89)(204.1739, 228.37)(185.154, 8878.81)(186.1573, 1070.65)(187.1489, 903.53) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 41938.34 | 6148.01 | 38990.43 | 7299.021 | 30880.79 | 4099.841 | 6958.641 | -0.47 | 0.09962 | 0.162099 | 1.51 | 0.221505 | 0.532591 | | |
| COMPOUND_185_1054a3_7405825 | Hilic | + | 185.1054 | 3.74 | | | (208.0957, 1410.36)(203.1479, 152.79)(186.1128, 4164.26)(187.1161, 4803.88) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 86605.83 | 49263.37 | 84119.35 | 21538.66 | 80433.64 | 29277.96 | 86149.86 | 30528.06 | -0.27 | 0.262339 | 0.359141 | 0.21 | 0.460656 | 0.729797 | |
| COMPOUND_186_051a2_254241 | Rp | - | 186.0510 | 2.25 | | | (373.1106, 211.45)(187.0581, 14172.18)(188.0614, 981.26)(189.0595, 197.9) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 46713.3 | 17963.78 | 43215.89 | 17790.28 | 29594.14 | 10243.98 | 33474.91 | 11213.18 | -0.95 | 1.89E-06 | 8.84E-06 | 0.51 | 0.016467 | 0.189627 | |
| COMPOUND_186_1251a7_807181 | Rp | - | 186.1251 | 7.81 | | | (185.1182, 24697.62)(186.1213, 3026.49)(187.1254, 535.53)(231.1317, 57.95)(371.2418, 927.72)(372.2434, 203.41) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 27946.72 | 19136.21 | 30396.17 | 16556.16 | 24120.5 | 10452.43 | 21013.63 | 11335.31 | 0.00 | 0.999441 | 0.999465 | -0.73 | 0.026284 | 0.224785 | |
| COMPOUND_187_0278a6_014426 | Hilic | + | 187.0278 | 6.01 | | | (373.0652, 1656.56)(376.0667, 188.57)(377.0624, 127.47)(210.0172, 3206.02)(211.0203, 214.52)(212.0138, 372.38)(397.0456, 1181.82)(398.0476, 217.04)(399.041, 165.99)(188.0354, 16087.78)(189.0387, 1161.15)(190.0325, 739.17) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 65316.09 | 17010.83 | 70001 | 23596.26 | 24494.43 | 17270.8 | 22751.89 | 19528.13 | -1.17 | 1.46E-06 | 7.08E-06 | -0.37 | 0.164398 | 0.47785 | |
| COMPOUND_187_0636a3_785936 | Hilic | + | 187.0636 | 3.79 | Tryptophan (mz 205.0976) | 2 | 10 eV: 146.0598 (100), 188.0721 (50), 118.0650 (30), 144.0804 (30), 170.0587 (10) | (375.1458, 153.85)(210.0532, 604.23)(205.0974, 440130.62)(206.1008, 50505.11)(207.1033, 4483.31)(188.071, 143724.73)(189.0742, 18563.51) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 2796544 | 343687.4 | 2856336 | 506354.3 | 2304024 | 344382.6 | 2397651 | 566363.4 | -1.01 | 0.000303 | 0.000873 | 0.12 | 0.709479 | 0.869758 |
| COMPOUND_187_0639a2_564372 | Rp | + | 187.0639 | 2.56 | Tryptophan (205.0976) | | (205.0976, 64445.2)(206.1013, 739.79)(207.1039, 6671.9)(208.1058, 514.37)(188.0714, 229185.61)(189.0744, 27156.44)(190.0769, 2432.75) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 5645896 | 781598 | 5616848 | 970268.5 | 4738035 | 482281 | 4753862 | 1123508 | -0.92 | 0.000768 | 0.002052 | 0.05 | 0.87163 | 0.945212 | |
| COMPOUND_187_0642a2_0999832 | Rp | + | 187.0642 | 2.10 | | | (205.0979, 272103.06)(206.1011, 32757.86)(207.1034, 3051.91)(208.1057, 201.16)(188.071, 86773.01)(189.0744, 10498.27)(190.0766, 1152.76)(191.0757, 50.31) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 4048746 | 598970.6 | 4027903 | 76620.23 | 3415298 | 402566.7 | 3415608 | 822209.1 | -0.88 | 0.002184 | 0.005381 | 0.08 | 0.80458 | 0.917422 | |
| COMPOUND_187_1684a6_1041994 | Hilic | + | 187.1684 | 6.10 | | | (397.3411, 113.69)(188.1761, 7794.79)(189.179, 834.88)(190.1801, 87.63) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 22008.17 | 7993.375 | 25931.63 | 8320.817 | 18393 | 4450.978 | 22011.86 | 9155.733 | -0.42 | 0.142551 | 0.218998 | -0.08 | 0.807437 | 0.917894 | |
| COMPOUND_188_0661a1_5741142 | Hilic | + | 188.0661 | 1.57 | | | (399.1185, 346.57)(189.0737, 22285.49)(190.0772, 1622.76)(191.0777, 369.77) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 19875.6 | 16482.35 | 16207.86 | 13173.93 | 13803 | 8140.424 | 18056.88 | 11309.48 | -0.17 | 0.548497 | 0.646371 | 0.54 | 0.112637 | 0.398247 | |
| COMPOUND_188_1048a5_7491193 | Rp | - | 188.1048 | 5.75 | | | (223.0679, 66.07)(187.0974, 9655.9)(188.0993, 893.74)(189.1033, 226.63) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 15972.28 | 5530.807 | 17060 | 4220.602 | 14023.31 | 2446.397 | 13002.18 | 2398.997 | -0.52 | 0.04712 | 0.083422 | -0.70 | 0.024607 | 0.219303 | |
| COMPOUND_188_1163a5_572104 | Hilic | + | 188.1163 | 5.57 | | | (211.1057, 7095.35)(212.1078, 841.69)(213.1115, 384.93)(399.2307, 268.83)(189.1238, 7122.42)(190.1253, 665.93)(191.1258, 450.9) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 23157.81 | 4357.623 | 23312.13 | 4207.297 | 28977.29 | 6818.023 | 28041.68 | 5771.653 | 0.96 | 0.000443 | 0.001243 | -0.12 | 0.699099 | 0.862515 | |
| COMPOUND_188_1277a6_7667017 | Hilic | + | 188.1277 | 6.77 | | | (377.2644, 214.88)(211.1173, 1501.54)(212.1215, 282.18)(213.1257, 141.95)(399.2462, 270.41)(189.135, 6563.16)(190.1379, 5876.29)(191.1374, 601.48) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 98236.75 | 40298.06 | 109128.7 | 52353.61 | 139994.6 | 48366.49 | 132408.1 | 53187.17 | 0.76 | 0.002569 | 0.00624 | -0.27 | 0.329775 | 0.635357 | |
| COMPOUND_188_1409a8_30797 | Rp | - | 188.1409 | 8.31 | | | (301.1164, 815.94)(187.134, 94640.9)(188.1373, 10561.01)(189.1388, 1271.74) | (183.0809, 35081.98)(184.084, 5103.46)(185.0884, 894.72) | 45764.64 | 58193.98 | 40460.11 | 23449.42 | 39513.86 | 15578.5 | 29371.04 | 15736.63 | 0.11 | 0.682415 | 0.767632 | -0.76 | 0.015249 | 0.184632 | |
| COMPOUND_188_1414a7_952267 | Rp | - | 1 | | | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--------------|---|---------------|-------------------------------------|---------------|----------|---------------|----------|---------------|----------|----------|----------|-------|-------------|----------|-------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | | |
| COMPOUND_196_1218a3_4818578 | Rp | + | 196.1218 | 3.48 | | | | (197.1285, 5524.47)(198.1225, 350.72)(199.1293, 1962.199)(200.1308, 221.28)(201.1175, 59.15) (417.3393, 546.16)(418.3407, 235.3)(198.1858, 10339.55)(199.1886, 1738.27)(200.1981, 291.19) (199.1554, 3950.11)(200.1586, 4107.96)(201.1602, 387.32) (221.1537, 2978.61)(222.1555, 846.98)(199.1696, 11368.71)(200.1721, 1573.4)(201.1644, 1738.21) (200.0408, 6186.79)(201.0435, 474.91)(202.0457, 70.02) (224.0965, 1043.36)(202.1119, 10009.02)(203.1216, 1118.41)(204.1227, 601.22) (219.2116, 91.82)(202.1806, 270025.62)(203.1838, 33622.65)(204.1862, 332.73)(205.1872, 248.96) (225.1246, 1078.81)(226.1256, 188.12)(203.1395, 24550.99)(204.1418, 2799.69)(205.1418, 404.01) (203.1441, 9232.91)(204.1466, 1400.58)(205.1501, 254.86) (405.2031, 142.28)(203.1508, 123688.27)(204.1535, 10960.09)(205.1551, 1076.42) (225.132, 1563.5)(226.1349, 289.57)(203.1507, 76011.93)(204.1536, 7332.54)(205.1554, 850.7) (203.1799, 33231.36)(204.1835, 5486.97)(205.1893, 753.03) (226.0243, 1501.22)(227.0261, 153.89)(228.0236, 202.36)(429.0699, 120.72)(204.0426, 5548.88)(205.0456, 593.13)(206.0415, 342.04) (407.2396, 195.05)(408.2317, 93.84)(227.1061, 1454.53)(227.1084, 305.43)(228.1006, 188.13)(204.1229, 875433.2)(205.1266, 85177.6)(206.1286, 10555.83) | 4 | 20 eV: 100.0754 (100), 86.0966 (15) | 4164.96 | 19348.61 | 52275.45 | 27531.74 | 55071.92 | 18064.55 | 60161.95 | 32005.54 | 0.40 | 0.140349 | 0.216188 | -0.38 | 0.2375 | 0.531523 |
| COMPOUND_197_1785a7_8260665 | Rp | + | 197.1785 | 7.83 | | | | (197.1285, 5524.47)(198.1225, 350.72)(199.1293, 1962.199)(200.1308, 221.28)(201.1175, 59.15) (417.3393, 546.16)(418.3407, 235.3)(198.1858, 10339.55)(199.1886, 1738.27)(200.1981, 291.19) (199.1554, 3950.11)(200.1586, 4107.96)(201.1602, 387.32) (221.1537, 2978.61)(222.1555, 846.98)(199.1696, 11368.71)(200.1721, 1573.4)(201.1644, 1738.21) (200.0408, 6186.79)(201.0435, 474.91)(202.0457, 70.02) (224.0965, 1043.36)(202.1119, 10009.02)(203.1216, 1118.41)(204.1227, 601.22) (219.2116, 91.82)(202.1806, 270025.62)(203.1838, 33622.65)(204.1862, 332.73)(205.1872, 248.96) (225.1246, 1078.81)(226.1256, 188.12)(203.1395, 24550.99)(204.1418, 2799.69)(205.1418, 404.01) (203.1441, 9232.91)(204.1466, 1400.58)(205.1501, 254.86) (405.2031, 142.28)(203.1508, 123688.27)(204.1535, 10960.09)(205.1551, 1076.42) (225.132, 1563.5)(226.1349, 289.57)(203.1507, 76011.93)(204.1536, 7332.54)(205.1554, 850.7) (203.1799, 33231.36)(204.1835, 5486.97)(205.1893, 753.03) (226.0243, 1501.22)(227.0261, 153.89)(228.0236, 202.36)(429.0699, 120.72)(204.0426, 5548.88)(205.0456, 593.13)(206.0415, 342.04) (407.2396, 195.05)(408.2317, 93.84)(227.1061, 1454.53)(227.1084, 305.43)(228.1006, 188.13)(204.1229, 875433.2)(205.1266, 85177.6)(206.1286, 10555.83) | | | 95589.66 | 10274.99 | 96040.11 | 16402.26 | 99446.14 | 9602.834 | 102138.1 | 15835.03 | 0.34 | 0.252206 | 0.348623 | 0.18 | 0.605599 | 0.810674 |
| COMPOUND_198_1488a1_2070646 | Hilic | + | 198.1488 | 1.21 | | | | (197.1285, 5524.47)(198.1225, 350.72)(199.1293, 1962.199)(200.1308, 221.28)(201.1175, 59.15) (417.3393, 546.16)(418.3407, 235.3)(198.1858, 10339.55)(199.1886, 1738.27)(200.1981, 291.19) (199.1554, 3950.11)(200.1586, 4107.96)(201.1602, 387.32) (221.1537, 2978.61)(222.1555, 846.98)(199.1696, 11368.71)(200.1721, 1573.4)(201.1644, 1738.21) (200.0408, 6186.79)(201.0435, 474.91)(202.0457, 70.02) (224.0965, 1043.36)(202.1119, 10009.02)(203.1216, 1118.41)(204.1227, 601.22) (219.2116, 91.82)(202.1806, 270025.62)(203.1838, 33622.65)(204.1862, 332.73)(205.1872, 248.96) (225.1246, 1078.81)(226.1256, 188.12)(203.1395, 24550.99)(204.1418, 2799.69)(205.1418, 404.01) (203.1441, 9232.91)(204.1466, 1400.58)(205.1501, 254.86) (405.2031, 142.28)(203.1508, 123688.27)(204.1535, 10960.09)(205.1551, 1076.42) (225.132, 1563.5)(226.1349, 289.57)(203.1507, 76011.93)(204.1536, 7332.54)(205.1554, 850.7) (203.1799, 33231.36)(204.1835, 5486.97)(205.1893, 753.03) (226.0243, 1501.22)(227.0261, 153.89)(228.0236, 202.36)(429.0699, 120.72)(204.0426, 5548.88)(205.0456, 593.13)(206.0415, 342.04) (407.2396, 195.05)(408.2317, 93.84)(227.1061, 1454.53)(227.1084, 305.43)(228.1006, 188.13)(204.1229, 875433.2)(205.1266, 85177.6)(206.1286, 10555.83) | | | 31817.68 | 29847.44 | 166084.15 | 7103.036 | 29744.21 | 9869.836 | 29297.49 | 8705.993 | 0.05 | 0.056679 | 0.098302 | 0.47 | 0.154004 | 0.466404 |
| COMPOUND_198_1626a8_514762 | Rp | + | 198.1626 | 8.51 | | | | (197.1285, 5524.47)(198.1225, 350.72)(199.1293, 1962.199)(200.1308, 221.28)(201.1175, 59.15) (417.3393, 546.16)(418.3407, 235.3)(198.1858, 10339.55)(199.1886, 1738.27)(200.1981, 291.19) (199.1554, 3950.11)(200.1586, 4107.96)(201.1602, 387.32) (221.1537, 2978.61)(222.1555, 846.98)(199.1696, 11368.71)(200.1721, 1573.4)(201.1644, 1738.21) (200.0408, 6186.79)(201.0435, 474.91)(202.0457, 70.02) (224.0965, 1043.36)(202.1119, 10009.02)(203.1216, 1118.41)(204.1227, 601.22) (219.2116, 91.82)(202.1806, 270025.62)(203.1838, 33622.65)(204.1862, 332.73)(205.1872, 248.96) (225.1246, 1078.81)(226.1256, 188.12)(203.1395, 24550.99)(204.1418, 2799.69)(205.1418, 404.01) (203.1441, 9232.91)(204.1466, 1400.58)(205.1501, 254.86) (405.2031, 142.28)(203.1508, 123688.27)(204.1535, 10960.09)(205.1551, 1076.42) (225.132, 1563.5)(226.1349, 289.57)(203.1507, 76011.93)(204.1536, 7332.54)(205.1554, 850.7) (203.1799, 33231.36)(204.1835, 5486.97)(205.1893, 753.03) (226.0243, 1501.22)(227.0261, 153.89)(228.0236, 202.36)(429.0699, 120.72)(204.0426, 5548.88)(205.0456, 593.13)(206.0415, 342.04) (407.2396, 195.05)(408.2317, 93.84)(227.1061, 1454.53)(227.1084, 305.43)(228.1006, 188.13)(204.1229, 875433.2)(205.1266, 85177.6)(206.1286, 10555.83) | | | 133086.8 | 66366.87 | 151740 | 64650.66 | 383847.5 | 301078.8 | 370124.2 | 431863.4 | 1.22 | 2.47E-06 | 1.12E-05 | -0.29 | 0.295865 | 0.606268 |
| COMPOUND_199_0336a6_71391 | Hilic | + | 199.0336 | 6.71 | | | | (197.1285, 5524.47)(198.1225, 350.72)(199.1293, 1962.199)(200.1308, 221.28)(201.1175, 59.15) (417.3393, 546.16)(418.3407, 235.3)(198.1858, 10339.55)(199.1886, 1738.27)(200.1981, 291.19) (199.1554, 3950.11)(200.1586, 4107.96)(201.1602, 387.32) (221.1537, 2978.61)(222.1555, 846.98)(199.1696, 11368.71)(200.1721, 1573.4)(201.1644, 1738.21) (200.0408, 6186.79)(201.0435, 474.91)(202.0457, 70.02) (224.0965, 1043.36)(202.1119, 10009.02)(203.1216, 1118.41)(204.1227, 601.22) (219.2116, 91.82)(202.1806, 270025.62)(203.1838, 33622.65)(204.1862, 332.73)(205.1872, 248.96) (225.1246, 1078.81)(226.1256, 188.12)(203.1395, 24550.99)(204.1418, 2799.69)(205.1418, 404.01) (203.1441, 9232.91)(204.1466, 1400.58)(205.1501, 254.86) (405.2031, 142.28)(203.1508, 123688.27)(204.1535, 10960.09)(205.1551, 1076.42) (225.132, 1563.5)(226.1349, 289.57)(203.1507, 76011.93)(204.1536, 7332.54)(205.1554, 850.7) (203.1799, 33231.36)(204.1835, 5486.97)(205.1893, 753.03) (226.0243, 1501.22)(227.0261, 153.89)(228.0236, 202.36)(429.0699, 120.72)(204.0426, 5548.88)(205.0456, 593.13)(206.0415, 342.04) (407.2396, 195.05)(408.2317, 93.84)(227.1061, 1454.53)(227.1084, 305.43)(228.1006, 188.13)(204.1229, 875433.2)(205.1266, 85177.6)(206.1286, 10555.83) | | | 35662.23 | 9317.126 | 35808.58 | 8855.407 | 61502.57 | 12276.24 | 75492.86 | 23734.45 | 1.17 | 5.08E-08 | 3.49E-07 | 0.46 | 0.041687 | 0.265944 |
| COMPOUND_200_1325a4_476957 | Hilic | + | 202.1325 | 4.48 | Unknown | | | (197.1285, 5524.47)(198.1225, 350.72)(199.1293, 1962.199)(200.1308, 221.28)(201.1175, 59.15) (417.3393, 546.16)(418.3407, 235.3)(198.1858, 10339.55)(199.1886, 1738.27)(200.1981, 291.19) (199.1554, 3950.11)(200.1586, 4107.96)(201.1602, 387.32) (221.1537, 2978.61)(222.1555, 846.98)(199.1696, 11368.71)(200.1721, 1573.4)(201.1644, 1738.21) (200.0408, 6186.79)(201.0435, 474.91)(202.0457, 70.02) (224.0965, 1043.36)(202.1119, 10009.02)(203.1216, 1118.41)(204.1227, 601.22) (219.2116, 91.82)(202.1806, 270025.62)(203.1838, 33622.65)(204.1862, 332.73)(205.1872, 248.96) (225.1246, 1078.81)(226.1256, 188.12)(203.1395, 24550.99)(204.1418, 2799.69)(205.1418, 404.01) (203.1441, 9232.91)(204.1466, 1400.58)(205.1501, 254.86) (405.2031, 142.28)(203.1508, 123688.27)(204.1535, 10960.09)(205.1551, 1076.42) (225.132, 1563.5)(226.1349, 289.57)(203.1507, 76011.93)(204.1536, 7332.54)(205.1554, 850.7) (203.1799, 33231.36)(204.1835, 5486.97)(205.1893, 753.03) (226.0243, 1501.22)(227.0261, 153.89)(228.0236, 202.36)(429.0699, 120.72)(204.0426, 5548.88)(205.0456, 593.13)(206.0415, 342.04) (407.2396, 195.05)(408.2317, 93.84)(227.1061, 1454.53)(227.1084, 305.43)(228.1006, 188.13)(204.1229, 875433.2)(205.1266, 85177.6)(206.1286, 10555.83) | | | 23281.29 | 11055.98 | 23427 | 8172.656 | 25462 | 3270.533 | 25215.67 | 10743.85 | -1.05 | 6.56E-06 | 2.72E-05 | -0.08 | 0.756797 | 0.895589 |
| COMPOUND_200_1366a7_922454 | Rp | + | 202.1366 | 7.92 | | | | (197.1285, 5524.47)(198.1225, 350.72)(199.1293, 1962.199)(200.1308, 221.28)(201.1175, 59.15) (417.3393, 546.16)(418.3407, 235.3)(198.1858, 10339.55)(199.1886, 1738.27)(200.1981, 291.19) (199.1554, 3950.11)(200.1586, 4107.96)(201.1602, 387.32) (221.1537, 2978.61)(222.1555, 846.98)(199.1696, 11368.71)(200.1721, 1573.4)(201.1644, 1738.21) (200.0408, 6186.79)(201.0435, 474.91)(202.0457, 70.02) (224.0965, 1043.36)(202.1119, 10009.02)(203.1216, 1118.41)(204.1227, 601.22) (219.2116, 91.82)(202.1806, 270025.62)(203.1838, 33622.65)(204.1862, 332.73)(205.1872, 248.96) (225.1246, 1078.81)(226.1256, 188.12)(203.1395, 24550.99)(204.1418, 2799.69)(205.1418, 404.01) (203.1441, 9232.91)(204.1466, 1400.58)(205.1501, 254.86) (405.2031, 142.28)(203.1508, 123688.27)(204.1535, 10960.09)(205.1551, 1076.42) (225.132, 1563.5)(226.1349, 289.57)(203.1507, 76011.93)(204.1536, 7332.54)(205.1554, 850.7) (203.1799, 33231.36)(204.1835, 5486.97)(205.1893, 753.03) (226.0243, 1501.22)(227.0261, 153.89)(228.0236, 202.36)(429.0699, 120.72)(204.0426, 5548.88)(205.0456, 593.13)(206.0415, 342.04) (407.2396, 195.05)(408.2317, 93.84)(227.1061, 1454.53)(227.1084, 305.43)(228.1006, 188.13)(204.1229, 875433.2)(205.1266, 85177.6)(206.1286, 10555.83) | | | 169664 | 31966.13 | 172448.8 | 33906.5 | 222707 | 39267.03 | 273778.6 | 80293.16 | 0.96 | 7.17E-05 | 0.000228 | 0.44 | 0.101722 | 0.376156 |
| COMPOUND_200_1431a6_3173676 | Hilic | + | 202.1431 | 6.32 | | | | (197.1285, 5524.47)(198.1225, 350.72)(199.1293, 1962.199)(200.1308, 221.28)(201.1175, 59.15) (417.3393, 546.16)(418.3407, 235.3)(198.1858, 10339.55)(199.1886, 1738.27)(200.1981, 291.19) (199.1554, 3950.11)(200.1586, 4107.96)(201.1602, 387.32) (221.1537, 2978.61)(222.1555, 846.98)(199.1696, 11368.71)(200.1721, 1573.4)(201.1644, 1738.21) (200.0408, 6186.79)(201.0435, 474.91)(202.0457, 70.02) (224.0965, 1043.36)(202.1119, 10009.02)(203.1216, 1118.41)(204.1227, 601.22) (219.2116, 91.82)(202.1806, 270025.62)(203.1838, 33622.65)(204.1862, 332.73)(205.1872, 248.96) (225.1246, 1078.81)(226.1256, 188.12)(203.1395, 24550.99)(204.1418, 2799.69)(205.1418, 404.01) (203.1441, 9232.91)(204.1466, 1400.58)(205.1501, 254.86) (405.2031, 142.28)(203.1508, 123688.27)(204.1535, 10960.09)(205.1551, 1076.42) (225.132, 1563.5)(226.1349, 289.57)(203.1507, 76011.93)(204.1536, 7332.54)(205.1554, 850.7) (203.1799, 33231.36)(204.1835, 5486.97)(205.1893, 753.03) (226.0243, 1501.22)(227.0261, 153.89)(228.0236, 202.36)(429.0699, 120.72)(204.0426, 5548.88)(205.0456, 593.13)(206.0415, 342.04) (407.2396, 195.05)(408.2317, 93.84)(227.1061, 1454.53)(227.1084, 305.43)(228.1006, 188.13)(204.1229, 875433.2)(205.1266, 85177.6)(206.1286, 10555.83) | | | 115756.5 | 46942.36 | 115951.8 | 45002.59 | 138366.6 | 42205.39 | 167589.9 | 89370.95 | 0.68 | 0.014958 | 0.030457 | 0.21 | 0.519042 | 0.764125 |
| COMPOUND_200_1431a6_3645186 | Hilic | + | 202.1431 | 6.36 | | | | (197.1285, 5524.47)(198.1225, 350.72)(199.1293, 1962.199)(200.1308, 221.28)(201.1175, 59.15) (417.3393, 5 | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--|--|---|----------|---------------|-----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|-----------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_222_0899a7_359233 | Rp | + | 222.0899 | 7.36 | | | | (483.1288, 265.78)(245.0794, 6331.47)(246.0827, 1159.75)(247.0879, 267.05)(467.1531, 388.6)(468.1493, 61.28)(261.0534, 425.05)(223.0972, 3425.86)(224.1006, 5241.65)(225.1031, 786.73)(226.1017, 65.99) (479.2274, 3004.66)(480.2313, 786.62)(257.092, 100.54)(335.1001, 330.41)(221.1179, 8826.59)(222.1211, 1274.56)(223.1307, 260.53)(267.1233, 211.44)(268.1198, 60.67) | 171402.7 | 46982.07 | 161423.4 | 42163.67 | 166109.8 | 44359.36 | 175510.5 | 52546.31 | -0.05 | 0.864789 | 0.908351 | 0.37 | 0.308275 | 0.614305 | |
| COMPOUND_222_1255a7_407982 | Rp | - | 222.1255 | 7.41 | no msms | | | | 44747.7 | 5763.16 | 47022.74 | 5109.124 | 55508.07 | 8886.364 | 49382.35 | 6447.042 | 1.44 | 1.42E-06 | 6.9E-06 | -1.11 | 0.000863 | 0.046284 | |
| COMPOUND_222_1618a9_278769 | Rp | - | 222.1618 | 9.28 | | | | (257.1305, 563.07)(258.1318, 33.61)(259.1245, 58.28)(221.1545, 4316.78)(222.1584, 931.3)(223.1643, 94.44) (246.1109, 545.71)(247.1141, 102.24)(248.1086, 98.45)(224.1282, 25508.55)(225.1313, 3910.16)(226.1342, 260.25) (242.0513, 120.02)(225.0345, 3888.39)(226.0367, 622.47)(227.0315, 1657.29)(228.0345, 242.78)(229.0284, 61.63) (225.0352, 4365.48)(226.0377, 670.5)(227.0322, 1479.25)(228.0343, 162.89)(229.0334, 112.77) (483.2587, 658.53)(484.2601, 249.65)(259.1092, 335.76)(260.1109, 22.9)(261.1065, 219.98)(223.1337, 3376.55)(224.1367, 513.89)(225.1444, 111.55) (247.1284, 715.11)(248.1295, 49.63)(249.1132, 524.11)(225.1493, 12541.87)(226.1531, 1822.57)(227.1594, 559.82)(466.3167, 5600.15)(467.3214, 1773.92)(468.3213, 378.67) | 14841.21 | 2007.405 | 16279.54 | 2462.534 | 14128.5 | 1844.519 | 14954.65 | 1888.398 | -0.33 | 0.256184 | 0.352716 | -0.24 | 0.485576 | 0.747178 | |
| COMPOUND_223_1215a5_385399 | Hilic | + | 223.1215 | 5.39 | | | | | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.27 | 0.323939 | 0.424795 | -0.02 | 0.96165 | 0.981922 | |
| COMPOUND_224_0274a3_056523 | Hilic | + | 224.0274 | 3.06 | | | | | 63163.66 | 14362.03 | 64172.98 | 10595.91 | 60981.07 | 14960.23 | 61865.07 | 11970.63 | -0.19 | 0.526947 | 0.625888 | -0.02 | 0.947411 | 0.976462 | |
| COMPOUND_224_0278a3_0012653 | Hilic | + | 224.0278 | 3.00 | | | | | 41238.19 | 28840.59 | 35293.93 | 26610.72 | 31557.14 | 25184.92 | 40000.91 | 26685.17 | -0.69 | 0.024811 | 0.047634 | 0.65 | 0.073642 | 0.326462 | |
| COMPOUND_224_1408a7_7266345 | Rp | - | 224.1408 | 7.73 | | | | | 16742.49 | 2951.656 | 16433.02 | 2633.073 | 18174.93 | 3932.025 | 17063.6 | 2744.504 | 0.48 | 0.113146 | 0.181482 | -0.29 | 0.42549 | 0.705315 | |
| COMPOUND_224_1416a7_737181 | Rp | + | 224.1416 | 7.74 | | | | | 64269.09 | 6806.237 | 63514.52 | 6561.001 | 66566.71 | 6218.738 | 63473.33 | 7454.876 | 0.30 | 0.315065 | 0.417123 | -0.34 | 0.338127 | 0.642187 | |
| COMPOUND_225_0755a1_6014915 | Hilic | + | 225.0755 | 1.60 | | | | | 15988.37 | 5891.935 | 17521.51 | 6517.536 | 22702.5 | 6889.267 | 27230.49 | 9170.856 | 0.86 | 0.005512 | 0.001422 | 0.23 | 0.410974 | 0.694731 | |
| COMPOUND_225_1735a10_758327 | Rp | + | 225.1735 | 10.76 | | | | | (248.1632, 1114.71)(226.1811, 123859.27)(227.1841, 19428.05) (226.9517, 6660.35)(227.9555, 358.97)(228.956, 106.4)(469.9257, 811.68)(470.9291, 125.22) (226.9519, 145803.81)(227.9551, 5159.22)(228.956, 1990.64)(229.9587, 73.14) (249.0966, 3139.18)(250.0986, 432.4)(227.1142, 71632.97)(228.1172, 8533.14)(229.1195, 917.38) (250.1787, 7834.54)(251.1819, 1271.48)(252.1825, 267.93)(266.1508, 662.81)(267.1565, 218.87)(228.1969, 122100.52)(229.2, 16783.48)(230.2039, 1837.83)(231.197, 146.05) | 74394.1 | 43147.25 | 82613 | 39429.19 | 94825.23 | 83920.07 | 90098.29 | 67451.82 | 0.06 | 0.839285 | 0.887774 | -0.07 | 0.843605 | 0.93246 |
| COMPOUND_225_9443a5_387598 | Hilic | + | 225.9443 | 5.39 | | | | | 30162.45 | 6586.453 | 32041.85 | 4593.612 | 29360.86 | 4514.274 | 30643.75 | 5274.754 | -0.04 | 0.882494 | 0.922216 | -0.18 | 0.54664 | 0.77815 | |
| COMPOUND_225_9447a4_214626 | Hilic | + | 225.9447 | 4.21 | | | | | 1388692 | 89471.64 | 1348519 | 96128.94 | 1371412 | 112780.3 | 1400539 | 111171.8 | -0.16 | 0.595204 | 0.690571 | -0.17 | 0.0310186 | 0.234557 | |
| COMPOUND_226_1069a6_7047267 | Hilic | + | 226.1069 | 6.70 | | | | | 79950.34 | 52233.45 | 95496.11 | 67407.35 | 41059.82 | 47373.27 | 30638.16 | 43494.76 | -1.02 | 3.96E-05 | 0.000135 | -0.26 | 0.344143 | 0.650723 | |
| COMPOUND_227_1892a7_6200376 | Rp | + | 227.1892 | 7.62 | | | | | 356780.1 | 61471.7 | 392346.3 | 81801.15 | 383115.4 | 119746.5 | 386315 | 110476 | 0.17 | 0.568433 | 0.665338 | -0.31 | 0.389299 | 0.689231 | |
| COMPOUND_227_1896a8_620347 | Rp | + | 227.1896 | 8.62 | | | | | (493.3424, 1255.72)(494.3465, 792.03)(228.1966, 9905.08)(229.1979, 1543.51)(230.2047, 179.48) (250.1786, 61277.63)(251.1821, 8946.83)(252.1751, 645.06)(228.1966, 322520.44)(229.1998, 46013.67)(230.2026, 4519.31)(231.2027, 390.74)(472.4291, 809.2) (245.2274, 22876.42)(228.1966, 11734.01)(229.1997, 1560.72)(230.2055, 315.92) (228.233, 27619.0)(229.2361, 4260.13)(230.24, 324.58) (229.155, 56956.08)(230.1582, 7218.09)(231.1604, 886.59) (246.1732, 103.69)(229.155, 82398.07)(230.1581, 10938.51)(231.1608, 1199.66) (263.1721, 149.02)(227.2014, 75895.78)(228.2048, 12894.7)(229.2077, 1206.64)(230.2081, 104.05)(455.4067, 307.09)(273.2065, 3535.68)(274.2082, 661.38)(275.2028, 157.07) (459.3477, 469.85)(460.3518, 133.49)(252.1588, 694.82)(230.1753, 6655.6)(231.1779, 1049.15)(232.1721, 351.47) (231.1708, 28351.87)(232.1741, 3529.18)(233.1743, 495.72) (463.2527, 375.71)(254.1159, 54514.46)(255.1511, 6524.67)(256.1713, 785.93)(485.2338, 3643.82)(486.2361, 851.37)(232.1299, 13924.15)(233.1335, 1677.26)(234.1374, 336.42) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.22 | 0.434067 | 0.539172 | 0.01 | 0.987781 | 0.994046 |
| COMPOUND_227_1899a10_823332 | Rp | + | 227.1899 | 10.82 | Myristic acid | 1 | 10eV: 175.1501(100), 95.085(80), 228.1965(40), 151.469(25) | | 570268 | 287944 | 624098.5 | 302245.3 | 960393.6 | 780495.1 | 1011783 | 616985.6 | 0.66 | 0.021347 | 0.041766 | 0.10 | 0.771624 | 0.903639 | |
| COMPOUND_227_1904a10_4461565 | Rp | + | 227.1904 | 10.45 | | | | | 33678.04 | 14908.51 | 33999.57 | 19908.98 | 39968.31 | 12879.19 | 50570.15 | 26367.26 | 0.29 | 0.292926 | 0.392194 | 0.33 | 0.29801 | 0.60748 | |
| COMPOUND_227_2255a6_6411934 | Rp | + | 227.2255 | 6.64 | | | | | 75925 | 65304.77 | 52430.08 | 58068.72 | 64390.43 | 42181.94 | 77979.93 | 64244.22 | -0.02 | 0.939737 | 0.906639 | 0.81 | 0.015808 | 0.188356 | |
| COMPOUND_228_1477a4_747693 | Hilic | + | 228.1477 | 4.75 | | | | | 116959.4 | 67984.89 | 110218.3 | 70894.66 | 95927.43 | 64885.25 | 202111.7 | 267520.6 | -0.35 | 0.219751 | 0.31355 | 1.06 | 0.002155 | 0.067469 | |
| COMPOUND_228_1478a3_9028063 | Hilic | + | 228.1478 | 3.90 | | | | | 173543.8 | 57433.42 | 180197.4 | 47317.02 | 141666.9 | 48038.54 | 284149.3 | 290264.2 | -0.57 | 0.034999 | 0.064288 | 1.06 | 0.001131 | 0.055356 | |
| COMPOUND_228_2086a10_465194 | Rp | - | 228.2086 | 10.47 | Myristic acid | 1 | 10eV: 227.2014(100), 96.4889(4), 33.9118(4) | | 133361.8 | 43393.27 | 158022.9 | 50240.61 | 160939.1 | 47911.96 | 184268.1 | 49940.91 | 0.74 | 0.009882 | 0.020995 | -0.25 | 0.458371 | 0.727963 | |
| COMPOUND_229_1678a0_78063387 | Hilic | + | 229.1678 | 0.78 | | | | | 61645.9 | 4723.804 | 58889.21 | 4328.206 | 63363.67 | 3588.65 | 10182.86 | 6410.829 | -1.31 | 5E-09 | 4.38E-08 | 0.21 | 0.354928 | 0.664974 | |
| COMPOUND_230_1641a2_39293274 | Rp | + | 230.1641 | 2.39 | | | | | 39662.09 | 35016.9 | 42025.29 | 35228.47 | 59384.63 | 44463.76 | 36835.69 | 26015.71 | 0.04 | 0.859290 | 0.90493 | -0.59 | 0.027581 | 0.226687 | |
| COMPOUND_231_1247a5_709998 | Hilic | + | 231.1247 | 5.71 | | | | | 8835.706 | 5493.491 | 9998.615 | 4653.913 | 78955.31 | 49379.08 | 67358.22 | 41579.93 | 1.46 | 7.19E-13 | 3.45E-11 | -0.08 | 0.689659 | 0.856181 | |
| COMPOUND_231_1474a1_4667246 | Hilic | + | 231.1474 | 1.47 | | | | | (463.2917, 636.51)(254.1375, 414.67)(232.1545, 29015.84)(233.1578, 3550.21)(234.1596, 648.67)(235.1531, 51.88) (232.1549, 11476.8)(233.1574, 1570.67)(234.1557, 221.37) (41597.28, 19858.71, 37997.17, 16529.98, 35354.86, 13203.47, 41363.16, 17851.73) | 283293.7 | 126583 | 272225.8 | 130276.6 | 266461.6 | 96731.53 | 319448.8 | 139063.2 | -0.17 | 0.509196 | 0.609952 | 0.55 | 0.063734 | 0.307286 |
| COMPOUND_231_1477a1_9933995 | Rp | + | 231.1477 | 1.99 | Butyrcarnitine | 1 | 10eV: 85.0271(100), 232.1545(55), 190.9435(15), 33.8396(1) | | 41597.28 | 19858.71 | 37997.17 | 16529.98 | 35354.86 | 13203.47 | 41363.16 | 17851.73 | -0.30 | 0.273716 | 0.372453 | 0.60 | 0.0609 | 0.302474 | |
| COMPOUND_232_053a3_463621 | Rp | + | 232.0530 | 3.46 | | | | | (233.0607, 15935.77)(234.064, 1527.49)(235.0636, 291.24) (503.3413, 826.96)(504.3472, 375.81)(255.1787, 683.84)(256.1771, 181.62)(250.2168, 411.97)(233.191, 7604.74)(234.1941, 1273.62) (233.191, 23468.72)(234.1942, 4209.95)(235.1963, 488.55) (257.1039, 1337.05)(258.1062, 414.47)(235.1197, 17727.24)(236.1229, 2568.19)(237.125, 280.05) (233.1543, 18522.82)(234.1578, 3197.47)(235.1612, 452.36) (257.154, 941.24)(258.1577, 312.5)(259.1488, 2236.97)(235.1703, 99879.56)(236.1735, 16473.6)(237.1802, 2775.31)(238.1872, 233.49) (236.1137, 68388.15)(237.1169, 6933.62)(238.1189, 1441.67)(239.1205, 125.8) (349.0893, 143.39)(235.0973, 3751.64)(236.1007, 581.42)(237.108, 144.45) (271.1118, 349.58)(272.1139, 79.22)(273.1043, 182.28)(235.1339, 2915.71)(236.1371, 442.74)(237.138, 79.96) (259.207, 5427.44)(260.2107, 1138.89)(261.2099, 131.19)(237.2219, 4727.77)(238.225, 8694.57)(239.232, 1239.26) (239.0919, 13874.54)(240.0954, 1745.54)(241.0969, 461.98)(242.1059, 38.01) (251.1107, 8044.04)(262.1136, 1156.99)(263.1153, 94.87)(277.0839, 499.45)(239.1287, 39316.63)(240.1322, 5600.42)(241.1381, 872.92) (261.1106, 5288.05)(262.1159, 784.06)(263.1205, 183.6)(277.0835, 251.56)(278.0843, 50.67)(239.1286, 17091.99)(240.1318, 2766.61)(241.1391, 643.56) | 28555.76 | 11479.8 | 262626.61 | 9691.315 | 38534.36 | 13234.01 | 53308.89 | 24514.45 | 0.71 | 0.003068 | 0.007297 | 0.66 | 0.02096 | 0.204049 |
| COMPOUND_232_1836a8_81827 | Rp | + | 232.1836 | 8.82 | | | | | 67783.36 | 8995.027 | 69881.7 | 7555.289 | 67320.29 | 9551.525 | 67785.26 | 9739.637 | 0.03 | 0.906763 | 0.938328 | -0.19 | 0.594167 | 0.804125 | |
| COMPOUND_234_1136a1_7280852 | Hilic | + | 234.1136 | 1.73 | | | | | 28974.6 | 11796.77 | 32656.96 | 17894.02 | 22421.54 | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|--------------------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_242_177a1_4351301 | Hilic | + | 242.1770 | 1.44 | | | | (485.3592, 6696.91 486.3615, 2377.64 487.366, 602.24 243.184, 9873.84 244.1877, 1242.55 245.1816, 1288.61 246.1846, 117.61 247.1741, 105.19) (519.4035, 1180.89 241.217, 10650.08 242.2198, 1700.01 243.2234, 193.15 287.2214, 438.86 288.2158, 53.21) | 62230.72 | 20823.96 | 64129.8 | 24688.84 | 55997.14 | 37794.89 | 51955.89 | 27372.35 | -0.51 | 0.085593 | 0.141726 | -0.08 | 0.825709 | 0.923744 |
| COMPOUND_242_2238a10_637414 | Rp | - | 242.2238 | 10.64 | | | | (519.408, 263.11 241.171, 8995.49 242.2204, 1509.47 243.1212, 130.85 287.2223, 377.79 288.2296, 73.66) | 16368.69 | 4650.828 | 17925.86 | 4920.446 | 21119.71 | 8688.515 | 18290.82 | 6179.047 | 0.81 | 0.005723 | 0.0128 | -0.73 | 0.033931 | 0.248347 |
| COMPOUND_242_2244a10_659308 | Rp | - | 242.2444 | 10.66 | | | | (266.1394, 33308.27 509.284, 441.47 244.1546, 4608.02 245.1581, 787.69 246.1536, 94.93) | 16740.88 | 4877.989 | 34800.25 | 10260.69 | 29085.5 | 11541.89 | 41957.63 | 32961.91 | -0.62 | 0.023572 | 0.045487 | 0.54 | 0.091532 | 0.359093 |
| COMPOUND_243_1826a10_816747 | Rp | - | 243.1826 | 10.82 | | | | (521.3172, 305.79 278.1524, 2669.09 279.1574, 486.25 280.1501, 963.75 281.1411, 127.68 531.3635, 334.43 242.176, 16197.13 243.1795, 2995.44 244.1812, 239.45 485.9457, 473.24 486.3545, 166.15) | 19569.71 | 8143.41 | 21713.09 | 993.096 | 23525.36 | 12071.95 | 25841.8 | 12784.98 | 0.37 | 0.21352 | 0.306078 | -0.09 | 0.802917 | 0.916921 |
| COMPOUND_243_1833a7_493578 | Rp | - | 243.1833 | 7.49 | | | | (356.1555, 138.93 278.1525, 373.78 279.1567, 99.66 280.148, 173.38 242.176, 18290.99 243.1797, 2605.52 244.18, 297.58 599.3318, 167.22) | 26533.57 | 7657.591 | 28821.87 | 9401.18 | 28545.14 | 11275.37 | 28158.75 | 11803.91 | 0.13 | 0.657101 | 0.745111 | -0.27 | 0.456918 | 0.727709 |
| COMPOUND_243_184a10_81224 | Rp | + | 243.1840 | 10.81 | | | | (487.373, 2189.69 488.3759, 827.46 489.3674, 936.32 490.3673, 311.33 525.315, 295.64 266.173, 26197.24 267.1768, 4069.96 268.1775, 411.72 282.1393, 1100.4 244.1916, 2687.1747 245.1947, 36081.71 246.1967, 4622.3 504.3784, 719.11 505.3679, 1130.86) | 148776.5 | 86794.64 | 153981.1 | 100993.1 | 273891.5 | 248302.7 | 266464.9 | 141941.4 | 0.72 | 0.01068 | 0.022457 | 0.10 | 0.749224 | 0.891783 |
| COMPOUND_243_1841a7_5022793 | Rp | + | 243.1841 | 7.50 | | | | (266.1394, 33308.27 509.284, 441.47 244.1546, 4608.02 245.1581, 787.69 246.1536, 94.93) | 44051.7 | 13583.2 | 46111.91 | 15930.63 | 47457.43 | 20356.88 | 46669.65 | 20073.93 | 0.14 | 0.638801 | 0.728395 | -0.19 | 0.611766 | 0.814985 |
| COMPOUND_243_1843a10_825046 | Rp | + | 243.1843 | 10.83 | | | | (487.3751, 2729.14 488.3835, 1113.25 489.3872, 939.29 525.3134, 164.43 266.1735, 32028.64 267.1771, 5505.4 268.1776, 520.1 282.1373, 1400.01 244.192, 326917.2 245.1952, 45091.02 246.1977, 5778.93 504.3965, 450.56 505.4133, 261.29) | 165023.3 | 84958.01 | 185720.1 | 84705.65 | 309346.5 | 241401.8 | 317046.8 | 20852.2 | 0.83 | 0.003403 | 0.007991 | -0.06 | 0.851615 | 0.936901 |
| COMPOUND_244_0889a0_90353024 | Hilic | + | 244.0889 | 0.90 | | | | (489.1976, 155.02 267.0795, 435.89 511.1814, 160.77 245.096, 8626.18 246.0981, 870.23 247.094, 334.23 506.2238, 444.11) | 13939.04 | 3106.176 | 13051.91 | 2911.712 | 12119.36 | 2868.04 | 12617.65 | 3801.831 | -0.55 | 0.068207 | 0.116454 | 0.36 | 0.310295 | 0.616211 |
| COMPOUND_244_1789a1_7912574 | Hilic | + | 244.1789 | 1.79 | Leucine-Leucine | 2 | 10 eV: 86.0976 (100), 245.1856 (25), 132.1023 (20) | (489.3649, 324.21 490.3677, 90.97 267.1685, 7228.13 268.1717, 1035.25 269.1777, 147.81 511.3446, 592.47 245.1865, 44845.3 246.19, 6275.68 247.192, 574.9 506.4027, 95.67) | 30088.48 | 45157.59 | 36054.28 | 34802.36 | 70143 | 78696.13 | 38660.92 | 62747.22 | 0.38 | 0.180836 | 0.2681 | -1.08 | 0.001858 | 0.061536 |
| COMPOUND_244_1789a3_7724419 | Rp | + | 244.1789 | 3.77 | | | | (489.3658, 55.51 245.1869, 34080.21 246.1904, 4928.89 247.1921, 695.66 248.1853, 63.93) | 145576.1 | 225175.5 | 174184.7 | 188830.9 | 351590.8 | 410817.2 | 156263.3 | 254395.4 | 0.36 | 0.193183 | 0.282004 | -1.08 | 0.001717 | 0.06041 |
| COMPOUND_244_2201a10_460588 | Rp | + | 244.2201 | 10.46 | | | | (511.42, 504.43 245.2268, 5997.58 246.2317, 1075.22 247.2267, 88.46) | 22704.15 | 11388.55 | 25140.63 | 18762.9 | 27893.9 | 7745.313 | 42587.54 | 22538.24 | -0.02 | 0.934308 | 0.95693 | 0.95 | 0.002348 | 0.067469 |
| COMPOUND_245_1632a2_8370006 | Rp | + | 245.1632 | 2.84 | Isovalerylcarnitine | 1 | 10 eV: 246.1697(100), 85.0267(90), 179.9112(15), 60.0795(10) | (268.1553, 52329.32 246.1709, 261319.62 247.1742, 33896.7 248.176, 4330.24) | 67315.36 | 25639.23 | 140665.6 | 484357.6 | 53532.14 | 20128.7 | 71293.7 | 88994.74 | 0.43 | 0.144209 | 0.221225 | 0.05 | 0.881806 | 0.950612 |
| COMPOUND_246_1333a5_5420938 | Hilic | + | 246.1333 | 5.54 | | | | (493.2812, 208.49 269.1233, 597.01 270.1292, 135.03 247.1407, 52542.5 248.1439, 5190.8 249.1464, 784.95) | 38741.92 | 15012.74 | 46761.7 | 18291.17 | 19555.18 | 23832.47 | 18473.54 | 26963.03 | -0.98 | 0.000116 | 0.000355 | -0.37 | 0.201102 | 0.513471 |
| COMPOUND_246_1372a2_7683043 | Rp | + | 246.1372 | 2.77 | | | | (493.2878, 59.19 269.1292, 179.66 247.1451, 120905.54 248.148, 18546.61 249.1505, 1924.61) | 137921.9 | 246547.7 | 95156.17 | 85476.75 | 157320.4 | 232764.9 | 95340.36 | 94455.65 | -0.27 | 0.18999 | 0.279097 | 0.23 | 0.331907 | 0.636996 |
| COMPOUND_246_1375a1_3290383 | Hilic | + | 246.1375 | 1.33 | Tryptophan betaine | 1 | 20 eV: 146.061 (100), 188.072 (54), 60.082 (48) | (493.2818, 4203.65 494.2843, 1235.48 495.282, 196.74 269.1264, 13027.61 270.1292, 2130.36 271.1314, 250.29 515.264, 577.41 516.2686, 138.2 247.1442, 266633.2 248.1476, 41785.43 249.1506, 4658.8 250.1483, 421.84 510.297, 1775.38) | 434327.2 | 846558.7 | 307627.8 | 295149.6 | 471698.4 | 827318.2 | 284060 | 334351.1 | -0.31 | 0.12447 | 0.196155 | 0.18 | 0.433947 | 0.712127 |
| COMPOUND_246_2348a10_693114 | Rp | + | 246.2348 | 10.69 | no msm | | | (247.2426, 16749.08 248.2463, 3264.52 249.25, 308.2) | 18251.9 | 7366.659 | 16849.1 | 8589.885 | 16448 | 3937.029 | 29617.36 | 13166.24 | 0.04 | 0.863638 | 0.907566 | 1.14 | 6.28E-05 | 0.010097 |
| COMPOUND_247_142a3_9591537 | Hilic | + | 247.1420 | 3.96 | | | | (248.1495, 21818.15 249.1532, 2821.55 250.1532, 559.79) | 26616.48 | 15860.18 | 27099.66 | 11164.12 | 26789.5 | 15261.06 | 41813.77 | 29833.32 | 0.00 | 0.998069 | 0.999401 | 0.69 | 0.017798 | 0.195199 |
| COMPOUND_248_1267a4_403865 | Rp | + | 248.1267 | 4.40 | | | | (271.116, 1409.77 272.1178, 168.81 273.1057, 89.28 366.1606, 6450.47 267.1731, 1156.19 268.1673, 343.85 287.0944, 152.06 249.1342, 7763.65 250.1391, 1371.07 251.1401, 221.63) | 53461.3 | 10795.5 | 50974.98 | 9437.95 | 51859.38 | 8166.845 | 53876.65 | 9728.551 | -0.12 | 0.691203 | 0.774808 | 0.40 | 0.263417 | 0.574821 |
| COMPOUND_248_1782a9_118431 | Rp | + | 248.1782 | 9.12 | | | | (497.3697, 3031.81 498.3583, 1133.68 499.3584, 547.36 271.17, 4519.69 272.1742, 1096.24 273.1708, 486.1 519.3432, 507.24 520.3498, 888.37 249.1857, 48631.65 250.1892, 8771.26 251.1965, 1912.65 252.2006, 123.04) | 242039.9 | 27546.13 | 251239.5 | 28649.25 | 269103.4 | 47518.92 | 24797.3 | 29180.71 | 0.75 | 0.011555 | 0.02405 | -0.89 | 0.012435 | 0.169858 |
| COMPOUND_248_1989a8_150036 | Rp | + | 248.1989 | 8.15 | | | | (271.1915, 3786.38 272.1885, 541.32 273.1863, 576.24 519.3833, 2724.02 520.3852, 917.74 521.3825, 254.12 266.2331, 5137.54 267.2368, 782.04 268.2299, 233.67 249.2066, 34341.03 250.2101, 5085.53 251.2097, 740.2) | 138164.8 | 48968.61 | 128899.6 | 43658.61 | 139609.3 | 22706.27 | 138803 | 61659.15 | 0.29 | 0.323091 | 0.424408 | -0.24 | 0.490013 | 0.748114 |
| COMPOUND_249_0978a1_3501186 | Hilic | + | 249.0978 | 1.35 | | | | (272.0891, 779.21 250.1052, 16080.58 251.1084, 1797.74 252.108, 195.53) | 59730.91 | 12552.48 | 59180.26 | 9719.796 | 53796.93 | 12649.34 | 61783.46 | 13117.93 | -0.45 | 0.12197 | 0.193297 | 0.62 | 0.07453 | 0.328457 |
| COMPOUND_250_1211a8_072027 | Rp | + | 250.1211 | 8.07 | | | | (273.1108, 571.96 274.1224, 132.33 275.1207, 371.49 251.1284, 10775.26 252.134, 1447.77 253.1393, 455.92) | 46344.68 | 8576.673 | 42190.54 | 8741.787 | 46780.86 | 6231.903 | 47569.88 | 8196.722 | 0.09 | 0.754316 | 0.821829 | 0.57 | 0.094989 | 0.36381 |
| COMPOUND_250_1215a8_709986 | Rp | + | 250.1215 | 8.71 | Furan fatty acid 268.131 | 3 | 20 eV: 209.1195(100), 153.0548(30), 57.0699(20) | (251.1286, 63420.49 252.1316, 10166.53 253.1359, 1714.61) | 77844.51 | 42200.03 | 76906.8 | 33618.85 | 94997.79 | 21759.37 | 76799.65 | 34930.69 | 0.67 | 0.010227 | 0.021626 | -0.73 | 0.017232 | 0.194029 |
| COMPOUND_251_152a9_54126 | Rp | - | 251.1520 | 9.54 | | | | (250.1446, 13312.14 251.1477, 1958.07 252.1488, 201.38 501.2917, 17223.5) | 59233.68 | 8139.395 | 64172.54 | 7507.028 | 68091.93 | 36740.31 | 62042.49 | 13945.79 | 0.10 | 0.734624 | 0.807011 | -0.49 | 0.158543 | 0.468876 |
| COMPOUND_251_1658a8_569771 | Rp | - | 251.1658 | 8.57 | | | | (274.1556, 86.23 275.164, 330.32 252.1728, 16653.78 253.1774, 3535.15 254.1769, 1187.84) | 99214.46 | 26305.94 | 114239.8 | 31468.13 | 78894.89 | 30970.15 | 88641.42 | 33192.69 | -0.42 | 0.103786 | 0.16827 | -0.25 | 0.40295 | 0.691103 |
| COMPOUND_252_0994a7_5606976 | Rp | - | 252.0994 | 7.56 | | | | (251.0923, 4562.52 252.0965, 903.83 253.1019, 299.18) | 37760.89 | 4361.199 | 39311.11 | 3612.031 | 39601.79 | 4394.04 | 37507.25 | 3899.352 | 0.48 | 0.110578 | 0.177746 | -0.92 | 0.011672 | 0.167839 |
| COMPOUND_252_0996a7_1789227 | Rp | - | 252.0996 | 7.18 | | | | (365.0866, 585.93 366.0921, 87.62 251.092, 3688.06 252.0965, 937.46 253.1014, 295.97) | 25502.45 | 2339.001 | 25649.78 | 2751.427 | 24925.29 | 2124.006 | 25323.49 | 2176.978 | 0.19 | 0.206484 | 0.620038 | 0.08 | 0.832401 | 0.926681 |
| COMPOUND_252_2085a9_942671 | Rp | + | 252.2085 | 9.94 | | | | (543.3886, 2345.58 275.204, 1045.3 276.2122, 174.71 253.2173, 9889.61 254.2198, 1906.85) | 23305.79 | 5179.465 | 23577.83 | 6125.322 | 20786.46 | 5042.886 | 18282.76 | 4275.008 | -0.06 | 0.836989 | 0.886862 | -0.43 | 0.209467 | 0.518944 |
| COMPOUND_252_2093a9_446959 | Rp | + | 252.2093 | 9.45 | | | | (275.2012, 2517.97 276.2133, 860.34 253.2169, 11511.54 254.22, 228 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|-----------------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_255_2212a11_035777 | Rp | + | 255.2212 | 11.04 | | | | (549.4059, 5116.41) (550.4025, 3567.41) (551.4217, 8515.47) (552.4157, 4380.33) (278.2111, 545.87) (279.206, 47.96) (533.4238, 134.06) (534.4347, 860.51) (256.228, 17897.06) (257.2305, 3213.31) (258.237, 406.2) (258.497, 606.07) (511.5197, 2870.62) (512.524, 1216.42) (513.5244, 339.27) (278.2467, 2138.05) (279.261, 241.71) (533.506, 457.01) (256.2644, 213531.2) (257.2674, 37654.84) (258.2706, 3834.53) (259.2733, 301.63) | 44372.8 | 34197.27 | 40165.38 | 22782.62 | 84947 | 30658.91 | 67099.08 | 30110.78 | 1.02 | 0.000171 | 0.000514 | -0.30 | 0.31798 | 0.624317 |
| COMPOUND_255_2569a10_489768 | Rp | + | 255.2569 | 10.49 | Unknown | 4 | 10 ev: 256.2643(100), 88.0762(6) | (278.2488, 88.65) (256.2647, 174374.66) (257.2679, 29581.27) (258.2704, 2781.63) (259.2712, 243.74) | 499622.4 | 458577.5 | 310813.3 | 389057 | 422698.3 | 282442 | 518434.1 | 443547.2 | 0.01 | 0.958774 | 0.97523 | 0.82 | 0.016125 | 0.189073 |
| COMPOUND_255_2941a7_561388 | Rp | + | 255.2941 | 7.56 | | | | (549.5707, 58.6) (256.3006, 321390.84) (257.3041, 58558.19) (258.3072, 5181.29) (259.31, 291.86) | 3133687 | 294996.3 | 2960513 | 301013.6 | 3129539 | 211662.3 | 3163727 | 298409.7 | 0.00 | 0.99453 | 0.998768 | 0.82 | 0.014429 | 0.179521 |
| COMPOUND_256_0944a5_3326526 | Rp | - | 256.0944 | 5.33 | | | | (255.0874, 109273.94) (256.0906, 13964.63) (257.0929, 2349.25) (258.0946, 198.04) (301.1004, 357.97) | 92870.65 | 83370.2 | 67347.41 | 41595.17 | 51162.15 | 33703.32 | 39014.51 | 21711.87 | -0.89 | 1.32E-09 | 1.41E-08 | 0.17 | 0.23743 | 0.542834 |
| COMPOUND_256_1062a1_2656062 | Hilic | + | 256.1062 | 1.27 | | | | (279.0919, 289.38) (257.1139, 3778.88) (258.1162, 659.2) (259.1176, 205.45) (530.2454, 378.69) | 10274.96 | 1702.144 | 10513.7 | 1807.567 | 12318.43 | 2448.64 | 13523.91 | 2388.223 | 0.84 | 0.00965 | 0.002523 | 0.38 | 0.197478 | 0.508252 |
| COMPOUND_256_2201a9_888487 | Rp | + | 256.2201 | 9.89 | | | | (513.4352, 115.17) (257.2272, 45261.22) (258.2313, 9131.62) (259.2346, 790.33) | 24901.05 | 13069.03 | 25037.03 | 10819.87 | 45210.93 | 15630.64 | 37441.86 | 25550.01 | 1.41 | 5.66E-07 | 3E-06 | -0.93 | 0.002652 | 0.07283 |
| COMPOUND_256_2206a8_639969 | Rp | + | 256.2206 | 8.64 | | | | (257.2272, 36086.58) (258.2303, 7905.09) (259.2329, 940.01) | 16432.51 | 4908.077 | 16689.06 | 6783.403 | 40414.36 | 12329.76 | 37395.06 | 24712.49 | 1.51 | 2.25E-09 | 2.24E-08 | -0.33 | 0.198737 | 0.510852 |
| COMPOUND_256_2397a10_264209 | Rp | - | 256.2397 | 10.26 | | | | (547.4378, 59.82) (255.2328, 6331.71) (256.2361, 1163.75) (257.2379, 128.8) | 28477.36 | 3742.09 | 30976.89 | 4333.508 | 21496.36 | 4681.613 | 22788 | 5000.771 | -1.17 | 5.4E-06 | 2.28E-05 | -0.26 | 0.362918 | 0.668267 |
| COMPOUND_256_2398a10_160457 | Rp | - | 256.2398 | 10.16 | | | | (255.2327, 5437.9) (256.2361, 1107.43) (257.2358, 116.79) | 15834.75 | 2572.764 | 16936.67 | 2662.926 | 15479.92 | 4286.132 | 14027.6 | 3214.798 | -0.25 | 0.359286 | 0.461559 | -0.74 | 0.029407 | 0.231966 |
| COMPOUND_256_2398a10_853131 | Rp | - | 256.2398 | 10.85 | FA 16:0 | 1 | 10 ev: 255.2333(100) | (291.2091, 2730.24) (292.2125, 367.13) (293.2054, 929.37) (294.2052, 74.64) (295.1913, 42.71) (557.464, 206.91) (255.2323, 847006.1) (256.2361, 242204.56) (257.2389, 14248.2) (258.2412, 1059.03) (511.4733, 1365.01) (512.4768, 584.89) (513.474, 35.86) (301.238, 15199.55) (302.2414, 2519.85) (303.2371, 918.41) (304.2405, 82.68) (625.4577, 3502.73) (626.4543, 1796.57) (627.4384, 692.39) | 168917 | 628838.2 | 2057245 | 684419.7 | 1680787 | 484636.3 | 1746359 | 622056.4 | 0.11 | 0.71199 | 0.788624 | -0.50 | 0.155272 | 0.466404 |
| COMPOUND_257_1012a1_4381056 | Hilic | + | 257.1012 | 1.44 | | | | (515.2297, 1065.77) (516.2355, 367.78) (280.0924, 1132.84) (281.0959, 357.32) (282.1034, 205.66) (258.1089, 7081.81) (259.1113, 819.18) (260.1094, 175.57) | 13829.58 | 6033.565 | 12739.25 | 7229.818 | 21468.85 | 5033.676 | 22530.6 | 5939.553 | 0.96 | 2.2E-05 | 8.12E-05 | 0.26 | 0.298361 | 0.60748 |
| COMPOUND_257_1035a6_1399736 | Hilic | + | 257.1035 | 6.14 | Glycerophosphocholine | 1 | 10 ev: 104.1075 (100), 258.1101 (60), 184.0692 (5) | (515.2132, 15051.87) (516.2167, 2881.31) (517.2181, 709.66) (518.2208, 115.63) (280.0928, 216027.34) (281.0957, 18748.97) (282.0974, 3125.41) (537.1953, 142999.12) (538.1983, 25458.69) (539.2004, 5243.96) (540.2017, 730.75) (275.1275, 163.35) (258.1107, 244179.05) (259.1138, 21217.03) (260.1152, 3687.9) (261.1188, 335.85) | 802530.8 | 713954.1 | 497622.1 | 329782.2 | 461676.3 | 211280.6 | 1000174 | 754852.5 | -0.43 | 0.128833 | 0.202182 | 1.95 | 0.000173 | 0.018576 |
| COMPOUND_258_1986a10_330836 | Rp | + | 258.1986 | 10.33 | | | | (276.2304, 304.81) (259.2064, 5250.45) (260.2101, 1102.81) (261.2169, 488.86) | 31873.4 | 11233.49 | 28645 | 9092.699 | 23610.75 | 15589.8 | 27730.75 | 14405.64 | -1.19 | 6.3E-07 | 3.3E-06 | 0.17 | 0.500472 | 0.753664 |
| COMPOUND_258_1986a10_986215 | Hilic | + | 258.1986 | 1.00 | | | | (282.1674, 279.71) (541.3483, 914.65) (260.1861, 17556.66) (261.1894, 10986.93) (262.1198, 1668.97) | 49776.7 | 26219.1 | 51667.59 | 29477.26 | 47822.14 | 22552.18 | 77853.54 | 43588.39 | -0.04 | 0.879614 | 0.920296 | 0.79 | 0.014572 | 0.179825 |
| COMPOUND_259_1794a3_9611745 | Rp | + | 259.1794 | 3.96 | Hexanoylcarnitine | 1 | 10 ev: 260.1852(100), 85.0277(75), 201.1116(40), 60.0814(18) | (260.1868, 15609.43) (261.1903, 2352.62) (262.1901, 414.4) | 21282.21 | 9827.492 | 19464.03 | 9358.527 | 17579.92 | 9641.404 | 28981.83 | 15013.49 | -0.28 | 0.291732 | 0.390827 | 1.00 | 0.002803 | 0.074044 |
| COMPOUND_260_1379a3_1481564 | Rp | + | 260.1379 | 3.15 | | | | (261.1454, 18073.75) (262.1486, 2307.65) (263.1504, 368.61) | 76063.49 | 24796.31 | 73380.22 | 26785.41 | 59017.17 | 56724.15 | 39637.76 | 39961.56 | -1.17 | 4.33E-06 | 1.86E-05 | 0.05 | 0.844236 | 0.93246 |
| COMPOUND_261_1579a3_1249304 | Hilic | + | 261.1579 | 3.12 | | | | (262.1653, 6772.12) (263.1685, 1208.35) (264.1685, 287.97) | 32001.87 | 11010.6 | 32091.48 | 8480.484 | 20096.29 | 4539.232 | 31177.19 | 9254.666 | -1.04 | 3.7E-05 | 0.000128 | 0.93 | 0.009927 | 0.051018 |
| COMPOUND_262_194a9_176586 | Rp | + | 262.1940 | 9.18 | | | | (285.1852, 598.58) (286.1915, 162.35) (263.2012, 29168.34) (264.2042, 5755.56) (265.2034, 1495.53) (266.214, 150.35) | 49497.88 | 28368.05 | 63261.23 | 57936.74 | 59580.69 | 58508.15 | 84611.54 | 58373.6 | 0.52 | 0.019506 | 0.038669 | -0.07 | 0.796985 | 0.91372 |
| COMPOUND_262_2302a10_459587 | Rp | + | 262.2302 | 10.46 | | | | (285.2185, 1797.91) (280.2646, 11440.07) (263.2381, 156543.6) (264.2413, 31193.8) | 116749 | 59452.16 | 134133.5 | 85572.8 | 126471.1 | 60819.97 | 223484 | 114122.6 | 0.24 | 0.367628 | 0.469863 | 0.68 | 0.033571 | 0.247063 |
| COMPOUND_262_2303a10_443133 | Rp | + | 262.2303 | 10.44 | | | | (525.4533, 217.91) (285.2124, 836.66) (280.2646, 2411.17) (263.2384, 91457.25) (264.2418, 18173.09) | 98994.72 | 55238.48 | 12004.8 | 60093.76 | 100580.6 | 60292.73 | 134179.5 | 94991.11 | 0.03 | 0.920775 | 0.94911 | -0.08 | 0.82958 | 0.94046 |
| COMPOUND_264_1112a1_7612511 | Hilic | + | 264.1112 | 1.76 | | | | (287.1007, 44198.33) (288.1035, 6859.44) (289.1033, 1044.91) (290.0988, 118.59) (551.2114, 7184.15) (552.2151, 2237.54) (553.2168, 627.92) (554.218, 120.39) (265.1183, 12423.71) (266.1214, 1975.37) (267.1242, 455.84) (268.1315, 45.56) (546.2571, 252.56) | 251726.7 | 131978.3 | 233564.1 | 164354.2 | 364337.3 | 223228.9 | 296789.4 | 212138.8 | 0.50 | 0.064597 | 0.111133 | -0.16 | 0.616247 | 0.816971 |
| COMPOUND_264_112a3_427942 | Rp | + | 264.1120 | 3.43 | | | | (287.0941, 1775.38) (288.0975, 208.56) (303.0675, 824.22) (265.1189, 20162.09) (266.122, 2800.05) (267.1209, 274.03) | 92358.4 | 50601.29 | 83204.49 | 57841.36 | 132338.5 | 73676.05 | 110052.8 | 75387.07 | 0.52 | 0.059929 | 0.103656 | -0.11 | 0.737621 | 0.888668 |
| COMPOUND_264_1371a7_0381002 | Rp | + | 264.1371 | 7.04 | | | | (287.1257, 1431.96) (288.1276, 330.97) (289.135, 233.44) (303.0996, 3189.27) (265.1444, 11729.56) (266.1484, 1946.25) (267.153, 404.84) | 37186 | 10143.3 | 36726.13 | 11755.86 | 38799.29 | 14371.85 | 34309.43 | 8337.977 | 0.07 | 0.815834 | 0.870326 | -0.42 | 0.234775 | 0.54116 |
| COMPOUND_264_2447a10_448037 | Rp | + | 264.2447 | 10.45 | | | | (567.4494, 113.66) (287.2734, 6469.49) (288.2413, 1563.61) (282.2786, 602.31) (265.2518, 6542.12) (266.2587, 1165.61) | 30436.25 | 6844.763 | 31057.16 | 10193.93 | 34260 | 6351.317 | 40024.77 | 9602.071 | 0.50 | 0.056703 | 0.098302 | 0.63 | 0.04438 | 0.272788 |
| COMPOUND_264_2459a10_622422 | Rp | + | 264.2459 | 10.62 | | | | (529.5023, 309.48) (567.4587, 197.83) (287.2356, 23784.35) (288.2411, 4271.11) (289.2484, 702.66) (265.2533, 105627.15) (266.2563, 20294.19) (267.264, 3419.45) | 66596.92 | 50349.61 | 65340 | 65157.41 | 131421.1 | 52859.17 | 140618 | 62300.45 | 1.05 | 7.8E-05 | 0.000246 | 0.19 | 0.52806 | 0.7696 |
| COMPOUND_264_2463a10_692466 | Rp | + | 264.2463 | 10.69 | no msms | | | (529.5249, 466.56) (567.4615, 551.93) (287.2371, 3199.52) (288.241, 941.72) (289.2466, 236.41) (265.2536, 33804.48) (266.257, 6165.94) (267.2642, 1381.93) (268.266, 136.79) | 103348 | 54628.75 | 102701 | 58946.85 | 100482 | 42521.38 | 212343.8 | 95217.85 | -0.03 | 0.89068 | 0.926471 | 1.27 | 5.53E-05 | 0.009576 |
| COMPOUND_265_1662a10_830807 | Rp | + | 265.1662 | 10.83 | | | | (266.1733, 25593.86) (267.1772, 4422.21) (268.1796, 537.33) | 14714.83 | 5482.054 | 16241.68 | 4680.879 | 41780.11 | 23229.75 | 36014.23 | 20089.33 | 0.99 | 1.88E-06 | 8.8E-06 | 0.17 | 0.446283 | 0.72091 |
| COMPOUND_266_0517a3_329751 | Hilic | + | 266.0517 | 3.33 | | | | (289.0427, 238.28) (290.044, 61.8) (555.0963, 113.28) (267.0594, 4299.35) (268.0622, 398.62) (269.061, 82.52) | 21430.57 | 2973.34 | 24555.67 | 4085.338 | 25816.38 | 3359.709 | 28513.46 | 5921.824 | 0.63 | 0.009172 | 0.019596 | 0.52 | 0.064677 | 0.307286 |
| COMPOUND_266_1367a0_7758269 | Hilic | + | 266.1367 | 0.78 | | | | (533.2753, 226.49) (289.1264, 1791.15) (290.1164, 515.55) (291.1095, 35.03) (284.1707, 46862.45) (285.1753, 6699.67) (286.1791, 1312.68) (267.1441, 30950.32) (268.1472, 4152.77) (269.1486, 679.73) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.02 | 0.470078 | 0.573399 | -0.01 | 0.987866 | 0.994046 |
| COMPOUND_266_1566a10_47078 | Rp | + | 266.1566 | 10.47 | | | | (555.3131, 1165.99) (267.1642, 11201.08) (268.166, 2196.57) (269.1705, 410.1) | 22265.38 | 6659.349 | 24568.95 | 5946.83 | 28633.09 | 7258.67 | 27775.96 | 8108.915 | 0.65 | 0.021669 | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | 1st trimester | | | | | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|--------------------------------------|----------|---|---|----------|---------------|----------|----------|----------|---------------|----|---------------|-------|-------|-------|-------|-------|--|-------------|--|--|
| | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | | | | |
| | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | | | | |
| COMPOUND_269_2738a10_468469 | Rp | + | 269.2738 | 10.47 | | | | (539.5505, 8488.55)[540.5562, 4108.45][541.5635, 1093.02][542.5582, 129.05][292.2623, 1236474 147074.4 1217178 130153.6 1471131 68317.29 1493665 78865.69 | 1.33 | 3.35E-09 | 3.12E-08 | 0.31 | 0.180301 | 0.493854 | | | | | | | | | | | |
| COMPOUND_270_0855a1_6402763 | Hilic | + | 270.0855 | 1.64 | | | (541.187, 259.76)[293.075, 5495.54][294.0794, 889.51][295.0777, 97.07][288.1229, 440.21][271.0928, 4251.63][272.0971, 738.79][273.0974, 120.5] | -0.34 | 0.203623 | 0.294704 | 1.03 | 0.001501 | 0.06002 | | | | | | | | | | | | |
| COMPOUND_270_1994a7_383529 | Rp | + | 270.1994 | 7.38 | | | (293.191, 550.08)[294.2053, 163.03][288.233, 4369.72][289.2355, 934.41][290.2381, 161.93][271.2064, 30096.73][272.21, 6370.14][273.2139, 917.15][274.2261, 96.51] | -1.05 | 1.08E-06 | 5.32E-06 | -0.31 | 0.171894 | 0.487538 | | | | | | | | | | | | |
| COMPOUND_270_2189a9_938386 | Rp | - | 270.2189 | 9.94 | | | (305.1873, 187.44)[383.1971, 1019.37][384.1965, 136.3][269.2119, 5951.67][270.2157, 1277.0] | -0.94 | 0.0008 | 0.002124 | 0.18 | 0.571729 | 0.789098 | | | | | | | | | | | | |
| COMPOUND_270_2195a10_099287 | Rp | - | 270.2195 | 10.10 | | | (305.1865, 103.80)[269.2118, 6290.51][270.2155, 1255.34] | -0.68 | 0.003261 | 0.00769 | -0.30 | 0.253353 | 0.556462 | | | | | | | | | | | | |
| COMPOUND_270_2195a9_591034 | Rp | + | 270.2195 | 9.59 | | | (579.4014, 1257.27)[293.2071, 1720.05][294.2109, 580.6][295.192, 685.87][288.2542, 2438.58][289.2551, 210.15][290.2639, 463.09][271.227, 5817.47][272.2294, 1185.58][273.2351, 224.72] | 0.21 | 0.455949 | 0.561091 | -0.13 | 0.700573 | 0.863364 | | | | | | | | | | | | |
| COMPOUND_270_2217a9_94457 | Rp | + | 270.2217 | 9.94 | | | (541.4432, 127.41)[579.4145, 3745.43][293.2097, 2151.68][294.2095, 766.71][295.2203, 1757.58][288.2481, 1205.96][289.241, 336.3][290.236, 381.22][271.227, 9646.67][272.2298, 1602.74][273.2337, 858.51] | -0.32 | 0.212508 | 0.304821 | 0.50 | 0.099107 | 0.368908 | | | | | | | | | | | | |
| COMPOUND_270_2555a10_969355 | Rp | - | 270.2555 | 10.97 | | | (305.2121, 163.75)[269.2485, 41780.93][270.2515, 8595.62][271.2542, 876.15][315.2532, 1104.94][316.2544, 235.95][653.4723, 4150.38] | 0.82 | 0.006314 | 0.013967 | -0.86 | 0.016057 | 0.189073 | | | | | | | | | | | | |
| COMPOUND_270_2555a11_014253 | Rp | - | 270.2555 | 11.01 | FA 17.0 | 1 | (305.2191, 174.21)[269.2482, 6545.16][270.2514, 13027.23][271.2545, 1594.61][315.2539, 1405.51][316.2578, 355.08][317.2546, 41.80][653.4716, 4713.61] | 0.67 | 0.024428 | 0.046938 | -0.78 | 0.029459 | 0.213966 | | | | | | | | | | | | |
| COMPOUND_272_215a6_9161153 | Rp | + | 272.2150 | 6.92 | | | (273.2223, 10168.73)[274.2252, 2180.95][275.2296, 244.62] | -1.28 | 2.67E-10 | 3.62E-09 | -0.12 | 0.58836 | 0.719811 | | | | | | | | | | | | |
| COMPOUND_272_2343a9_512525 | Rp | - | 272.2343 | 9.51 | | | (271.2276, 5872.44)[272.2304, 1097.04][273.2216, 139.72] | -0.09 | 0.763308 | 0.828819 | -0.20 | 0.543746 | 0.776977 | | | | | | | | | | | | |
| COMPOUND_272_2347a9_940352 | Rp | - | 272.2347 | 9.94 | | | (307.1949, 813.03)[271.2274, 11261.97][272.2312, 271.09][273.2312, 188.55][317.2316, 78.12] | -0.73 | 0.009216 | 0.019673 | -0.05 | 0.867701 | 0.9447 | | | | | | | | | | | | |
| COMPOUND_272_2348a10_4309225 | Rp | - | 272.2348 | 10.43 | | | (307.2035, 448.54)[308.2066, 125.7][309.2024, 348.51][271.2275, 38872.18][272.2312, 6466.56][273.2324, 740.86][274.234, 66.86][543.4886, 147.66] | -1.45 | 3.35E-08 | 2.51E-07 | 0.34 | 0.212665 | 0.520001 | | | | | | | | | | | | |
| COMPOUND_273_1803a6_5916677 | Hilic | + | 273.1803 | 6.59 | | | (296.1692, 1247.85)[297.171, 201.59][274.1881, 23034.67][275.1909, 2974.71][276.1944, 486.76] | -0.38 | 0.12007 | 0.140243 | -0.38 | 0.12007 | 0.140243 | | | | | | | | | | | | |
| COMPOUND_273_1932a7_613201 | Rp | - | 273.1932 | 7.61 | | | (308.1466, 66.94)[386.1813, 469.89][272.1865, 3886.84][273.1897, 806.8][274.186, 274.78] | -0.23 | 0.395936 | 0.500048 | -0.61 | 0.058069 | 0.298567 | | | | | | | | | | | | |
| COMPOUND_276_0826a5_3917756 | Hilic | + | 276.0826 | 5.39 | | | (277.0898, 14265.17)[278.0931, 1474.74][279.0944, 321.01] | 0.61 | 0.027116 | 0.051575 | -0.37 | 0.246355 | 0.555348 | | | | | | | | | | | | |
| COMPOUND_276_172a8_981627 | Rp | - | 276.1720 | 8.98 | | | (275.165, 6989.59)[276.169, 1450.35][277.1732, 178.93] | -0.12 | 0.670847 | 0.758407 | -0.66 | 0.052846 | 0.286771 | | | | | | | | | | | | |
| COMPOUND_276_1736a8_209234 | Rp | + | 276.1736 | 8.21 | | | (299.1528, 509.73)[300.1607, 116.06][277.1807, 8912.24][278.1843, 2114.25][279.1879, 486.67] | 0.12 | 0.661057 | 0.748467 | 0.33 | 0.306224 | 0.613089 | | | | | | | | | | | | |
| COMPOUND_276_1738a9_035188 | Rp | + | 276.1738 | 9.04 | | | (299.1625, 1821.02)[300.1649, 397.68][301.1547, 22.63][294.2072, 4355.49][295.2203, 1520.62][315.1426, 384.34][316.1349, 58.09][317.1473, 917.26][277.1806, 16748.33][278.1852, 3463.44][279.1925, 1055.04][280.1886, 90.07] | 0.22 | 0.462527 | 0.567635 | 0.10 | 0.776863 | 0.905535 | | | | | | | | | | | | |
| COMPOUND_276_174a9_034545 | Rp | + | 276.1740 | 9.03 | | | (299.1624, 1583.63)[300.1651, 488.56][301.1559, 52.85][315.1481, 394.78][316.1394, 59.14][317.1496, 852.86][294.2078, 4071.77][295.2208, 1588.92][277.1811, 13403.19][278.186, 3074.46][279.1922, 996.68][280.1857, 82.28] | 0.09 | 0.768629 | 0.83299 | -0.35 | 0.332081 | 0.636996 | | | | | | | | | | | | |
| COMPOUND_276_209a9_656247 | Rp | + | 276.2090 | 9.66 | | | (277.2177, 41620.87)[278.2208, 8530.68] | -0.84 | 0.000691 | 0.001869 | -0.21 | 0.452895 | 0.72489 | | | | | | | | | | | | |
| COMPOUND_276_2096a9_609907 | Rp | + | 276.2096 | 9.61 | | | (591.4012, 925.15)[592.4058, 393.74][294.2423, 945.0][277.2176, 57559.31][278.2208, 12572.54] | -0.74 | 0.001728 | 0.004348 | -0.49 | 0.077782 | 0.333235 | | | | | | | | | | | | |
| COMPOUND_277_169a6_334597 | Rp | + | 277.1690 | 6.33 | | | (278.1759, 14308.44)[279.1783, 2821.84][280.1832, 395.59] | -1.24 | 2.5E-09 | 2.46E-08 | -0.18 | 0.399626 | 0.690408 | | | | | | | | | | | | |
| COMPOUND_278_0874a7_708572 | Rp | + | 278.0874 | 7.71 | | | (301.0752, 411.59)[302.0821, 144.11][303.0802, 178.86][317.063, 97.43][279.0941, 13901.83][280.0974, 2803.41][281.1002, 299.69] | -0.31 | 0.301177 | 0.401807 | -0.18 | 0.301177 | 0.401807 | | | | | | | | | | | | |
| COMPOUND_278_1529a9_435037 | Rp | + | 278.1529 | 9.44 | | | (301.1423, 5902.41)[302.1439, 1255.97][303.1493, 226.84][317.1179, 314.31][318.1116, 109.36][319.1176, 179.13][279.1599, 45370.24][280.1637, 8312.96][281.1688, 1636.57][574.3443, 314.24][575.3396, 115.53][576.3328, 126.12] | 0.11 | 0.700775 | 0.782034 | 0.31 | 0.373319 | 0.675816 | | | | | | | | | | | | |
| COMPOUND_278_1531a9_357016 | Rp | + | 278.1531 | 9.36 | Phthalic acid Mono-2-ethylhexyl Este | 2 | (301.1421, 14436.1)[302.1444, 2794.49][303.1485, 413.91][579.2999, 608.73][580.3093, 277.27][581.2925, 76.26][317.1151, 802.26][318.1191, 253.49][319.1125, 172.09][279.1605, 96397.19][280.1637, 16241.28][281.1688, 2456.58] | 0.10 | 0.736774 | 0.808584 | -0.09 | 0.806795 | 0.917894 | | | | | | | | | | | | |
| COMPOUND_278_1637a4_23307 | Rp | + | 278.1637 | 4.23 | | | (279.1712, 84385.31)[280.1743, 14206.51][281.1771, 1749.35][282.1797, 184.44][574.3615, 247.91] | 0.90 | 0.000799 | 0.002124 | -0.14 | 0.631835 | 0.828008 | | | | | | | | | | | | |
| COMPOUND_278_1637a1_5383792 | Hilic | + | 278.1637 | 1.54 | | | (557.3272, 64.49)[558.3184, 2646.74][301.1529, 2624.56][302.1558, 564.54][303.1603, 27.41][579.3411, 373.32][279.1709, 46646.07][280.174, 8146.26][281.1782, 1024.97][574.3316, 142.79] | 0.81 | 0.003453 | 0.008091 | -0.22 | 0.490219 | 0.748114 | | | | | | | | | | | | |
| COMPOUND_278_1637a4_3144116 | Rp | + | 278.1637 | 4.31 | | | (579.3094, 72.99)[279.1714, 61657.52][280.1745, 10260.07][281.1753, 1362.33][282.1662, 139.67][574.3576, 68.36] | 0.21 | 0.468045 | 0.572535 | -0.53 | 0.127595 | 0.424221 | | | | | | | | | | | | |
| COMPOUND_278_188a9_038569 | Rp | - | 278.1880 | 9.04 | | | (277.1808, 13204.08)[278.1843, 2705.09][279.1859, 409.01][280.1864, 39.51][323.1861, 663.59][324.1876, 55.49] | -0.50 | 0.067211 | 0.115136 | -0.40 | 0.205727 | 0.516497 | | | | | | | | | | | | |
| COMPOUND_278_2244a10_500361 | Rp | - | 278.2244 | 10.50 | FA 18.3 | 2 | (313.1339, 893.79)[314.1977, 81.43][315.1907, 469.74][277.2171, 67969.73][278.2204, 13554.81][279.2239, 1934.21][280.2219, 168.1][555.4215, 239.51][323.2168, 541.67] | 0.42 | 0.121906 | 0.193297 | -0.06 | 0.841703 | 0.93246 | | | | | | | | | | | | |
| COMPOUND_278_2254a9_403822 | Rp | + | 278.2254 | 9.40 | | | (296.2569, 813.09)[279.2326, 24512.28][280.2358, 4864.62][281.2434, 1682.18][282.2343, 106.84] | -0.90 | 0.000238 | 0.000701 | -0.19 | 0.494012 | 0.750179 | | | | | | | | | | | | |
| COMPOUND_278_2255a10_500704 | Rp | + | 278.2255 | 10.50 | | | (557.4462, 300.66)[595.4161, 2612.56][596.4126, 1705.44][597.4296, 6439.21][301.2077, 9565.57][302.2085, 3240.42][303.2, 757.85][296.259, 32994.05][297.2634, 7305.86][298.2723, 1601.44][279.2331, 39816.4][280.2366, 7864.84] | 0.71 | 0.00886 | 0.019026 | 0.18 | 0.565203 | 0.785799 | | | | | | | | | | | | |
| COMPOUND_278_2263a9_637026 | Rp | + | 278.2263 | 9.64 | | | (557.4574, 359.86)[301.2178, 286633.75][302.2211, 56658.69][279.2331, 495819.8][280.2369, 90665.09][281.2406, 10835.35][282.245, 953.62] | -0.65 | 0.011236 | 0.023452 | -0.66 | 0.030413 | 0.234557 | | | | | | | | | | | | |
| COMPOUND_279_1481a1_2006848 | Hilic | + | 279.1481 | 1.20 | | | (559.2983, 927.87)[280.155, 8786.51][281.158, 1658.22][282.1618, 272.37][576.3282, 2097.79] | -0.74 | 0.003234 | 0.007643 | 0.24 | 0.399987 | 0.690408 | | | | | | | | | | | | |
| COMPOUND_280_1059a2_741435 | Rp | + | 280.1059 | 2.74 | | | (281.1145, 7840.72)[282.1166, 1260.82][283.1207, 243.81] | 0.56 | 0.025944 | 0.049514 | -0.05 | 0.874238 | 0.946531 | | | | | | | | | | | | |
| COMPOUND_280_2405a10_7077675 | Rp | - | 280.2405 | 10.71 | FA 18.2 | 1 | (559.4466, 233.49)[315.2093, 4364.02][316.2127, 935.55][317.207, 1409.89][318.2093, 1030057 507266.5 1295928 680996.6 924758.5 438717 1240135 633049.7 | -0.09 | 0.740229 | 0.811585 | 0.06 | 0.854121 | 0.937825 | | | | | | | | | | | | |
| COMPOUND_280_2413a10_715105 | Rp | + | 280.2413 | 10.72 | | | (354.01)[279.2324, 597695.0][280.2361, 103159.23][281.2394, 11879.25][282.2423, 1246.29][595.4758, 217.2][527.2328, 304587.3] | 0.44 | 0.097989 | 0.160007 | 0.44 | 0.162723 | 0.476531 | | | | | | | | | | | | |
| COMPOUND_280_2416a9_988901 | Rp | + | 280.2416 | 9.99 | | | (551.4837, 826.65)[562.4736, 86.21][298.2747, 40154.15][299.2768, 8376.51][300.2835, 1634.54][281.2488, 23116.74][282.2528, 4766.0] | -0.44 | 0.136851 | 0.21225 | -0.04 | 0.909966 | 0.958935 | | | | | | | | | | | | |
| | | | | | | | (303.2328, 799857.44)[298.2781, 364.21][299.2888, 42.09][281.2482, 51955.91][282.2517, 9838.2] | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|-------------------|----------|---|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_280_2416a10_028688 | Rp | + | 280.2416 | 10.03 | | | | (303.2327, 810438.75)(298.2754, 361.29)(299.2772, 77.87)(281.2481, 50366.52)(282.2514, 9954.42) | 556628.3 | 887871.7 | 405069.1 | 676846.9 | 223828.1 | 143090.1 | 298760.6 | 470194.2 | -0.03 | 0.912153 | 0.942711 | 0.05 | 0.883915 | 0.951974 |
| COMPOUND_280_2417a10_084801 | Rp | + | 280.2417 | 10.08 | | | | (599.4343, 44729.37)(600.4358, 1640.41)(601.4286, 2120.54)(303.2323, 7284.5)(298.2739, 1714.24)(281.2483, 3327.75)(282.2518, 6706.07) | 84006.18 | 74959.96 | 76957.14 | 33828.53 | 80594.38 | 48901.03 | 94145.62 | 59730.26 | 0.11 | 0.70151 | 0.782467 | 0.04 | 0.90827 | 0.958319 |
| COMPOUND_280_243a10_235375 | Rp | + | 280.2430 | 10.24 | | | | (599.4398, 62135.09)(600.4438, 20635.38)(601.4437, 7315.62)(298.2753, 949.87)(281.2481, 2088.52)(282.2517, 3941.23) | 147067.4 | 84063.69 | 109318.9 | 54005.74 | 219756.4 | 34969.19 | 215317.9 | 55139.57 | 0.54 | 0.037037 | 0.0677 | 0.59 | 0.055005 | 0.294133 |
| COMPOUND_281_1132a4_2414556 | Hilic | + | 281.1132 | 4.24 | | | | (304.1024, 2565.79)(305.1045, 362.55)(282.1205, 4524.84)(283.1239, 689.92)(284.128, 119.91) | 25092.7 | 4256.56 | 25365.83 | 4704.075 | 40629.93 | 7683.702 | 43117.25 | 7053.76 | 1.44 | 2.49E-10 | 3.42E-09 | 0.13 | 0.556593 | 0.781554 |
| COMPOUND_281_2718a10_601354 | Rp | + | 281.2718 | 10.60 | Oleamide | 1 | 10 eV: 282.2817(100), 57.0699(82), 148.5324(78), 95.0881(50) | (563.5522, 16343.6)(564.5557, 6575.87)(565.557, 1517.28)(304.2622, 35179.18)(305.2637, 7783.41)(306.2707, 1176.51)(320.2363, 1760.85)(282.2806, 382545.72)(283.2835, 73064.03)(284.2894, 10231.9)(580.5751, 1057.19) | 234871.6 | 116440.3 | 317577.1 | 189581.7 | 561195.8 | 462092.8 | 554393.1 | 493933 | 1.02 | 0.000414 | 0.001165 | -0.98 | 0.003982 | 0.094399 |
| COMPOUND_282_0257a3_3187468 | Hilic | + | 282.0257 | 3.32 | | | | (305.016, 111.06)(283.0332, 5345.54)(384.0364, 547.66)(285.0332, 429.22) | 22630.91 | 4468.321 | 24758.24 | 5322.115 | 26547 | 5031.69 | 30793.49 | 6791.788 | 0.61 | 0.004549 | 0.010337 | 0.27 | 0.261476 | 0.572854 |
| COMPOUND_282_1299a10_470434 | Rp | + | 282.1299 | 10.47 | | | | (587.2442, 1495.4)(283.137, 6062.18)(284.1388, 1194.66)(285.137, 4274.02)(286.1398, 757.53)(287.132, 1786.83)(288.1252, 113.66) | 31913.51 | 6894.494 | 30381.22 | 5791.589 | 40060.93 | 6817.31 | 39568.77 | 6879.379 | 1.19 | 6.85E-06 | 2.82E-05 | -0.02 | 0.932826 | 0.970312 |
| COMPOUND_282_2359a8_031316 | Rp | + | 282.2359 | 8.03 | | | | (321.195, 721.39)(322.1983, 289.87)(283.2433, 38151.75)(284.2463, 8597.07)(285.2549, 1540.88) | 56633.33 | 24872.14 | 62171.51 | 38578.4 | 31266.71 | 9469.803 | 29683.94 | 12751.36 | -0.91 | 9.29E-05 | 0.000288 | -0.43 | 0.09223 | 0.359968 |
| COMPOUND_282_2557a10_931676 | Rp | - | 282.2557 | 10.93 | FA 18:1 | 1 | 10 eV: 281.2481(100) | (599.4821, 292.61)(317.2251, 7794.2)(318.2285, 1677.57)(319.2218, 2904.11)(320.2253, 595.48)(321.2181, 1086.27)(322.2187, 348.51)(281.248, 936368.7)(282.2519, 169994.42)(283.2553, 19343.86)(284.2597, 2150.62)(563.503, 496.53)(564.5011, 183.47)(565.5137, 109.49)(327.2533, 7541.66)(328.2562, 1413.36)(329.2539, 608.03)(330.2454, 79.47)(677.4872, 1741.84) | 1319349 | 936930.5 | 1676081 | 1385607 | 1548106 | 751639.3 | 2075641 | 1197834 | 0.34 | 0.215327 | 0.30808 | 0.20 | 0.527781 | 0.7696 |
| COMPOUND_282_2567a9_993883 | Rp | + | 282.2567 | 9.99 | | | | (305.2472, 67281.16)(306.2509, 13076.31)(283.2634, 17377.28)(284.2668, 3384.6)(285.2748, 620.8) | 71551.79 | 31914.91 | 114060.3 | 71940.13 | 62421.08 | 31237.76 | 56740.84 | 17777.17 | 0.78 | 0.001758 | 0.004409 | -0.22 | 0.446162 | 0.72091 |
| COMPOUND_282_2567a10_931917 | Rp | + | 282.2567 | 10.93 | | | | (565.5281, 885.97)(566.5413, 2128.71)(567.5302, 1249.7)(300.2898, 13859.76)(301.2932, 2934.85)(302.2962, 469.21)(283.2643, 28274.93)(284.2687, 5724.94)(582.5613, 3935.71) | 45561.92 | 19521.48 | 46580.74 | 24675.01 | 59060.29 | 22312.55 | 82953.75 | 29924.45 | 0.54 | 0.019645 | 0.038876 | 0.66 | 0.015558 | 0.186363 |
| COMPOUND_282_2569a10_455742 | Rp | + | 282.2569 | 10.46 | | | | (565.5372, 318.85)(305.348, 4903.83)(306.2516, 1081.42)(300.2902, 5840.85)(301.2932, 1120.36)(302.3008, 350.71)(283.2641, 23714.24)(284.2669, 4218.66)(285.2765, 372.13)(582.5467, 1905.24)(583.5558, 996.6)(584.5574, 270.7) | 193104.9 | 36839.71 | 180195.8 | 28102.86 | 225207.2 | 19960.02 | 231258.2 | 32788.77 | 0.60 | 0.014273 | 0.029303 | 0.53 | 0.065785 | 0.309933 |
| COMPOUND_283_2879a10_857864 | Rp | + | 283.2879 | 10.86 | | | | (567.5745, 3570.57)(568.5716, 1719.39)(605.5587, 1491.19)(306.2779, 80197.7)(307.2803, 17428.75)(308.2835, 2331.24)(589.5563, 2291.85)(590.5748, 1527.63)(322.2497, 2432.92)(323.2497, 287.17)(284.2962, 203213.31)(285.2991, 39619.43)(286.301, 4641.87)(584.614, 2782.73)(585.609, 275.84) | 85998.35 | 39804.15 | 107681.2 | 44622.33 | 212802.5 | 134678.3 | 178523.1 | 128597.6 | 1.42 | 8.06E-07 | 4.12E-06 | -0.78 | 0.01404 | 0.179521 |
| COMPOUND_283_2885a8_449652 | Rp | + | 283.2885 | 8.45 | | | | (284.2957, 21663.46)(285.299, 4141.85)(286.3024, 475.99) | 64256.02 | 54266.08 | 43199.83 | 48345.68 | 50488.36 | 32042.07 | 62586.54 | 53008.75 | -0.01 | 0.970706 | 0.983369 | 0.70 | 0.039287 | 0.261543 |
| COMPOUND_284_2156a9_926902 | Rp | + | 284.2156 | 9.93 | | | | (307.2054, 777.82)(308.1951, 142.55)(309.2111, 1932.13)(323.1641, 242.05)(285.2223, 27562.32)(286.2288, 6847.53)(287.2274, 3221.76)(288.2209, 312.73) | 144926.3 | 50050.12 | 152718.6 | 51732.33 | 169677.3 | 9763.875 | 152783.2 | 69066.04 | -0.96 | 4.8E-05 | 0.000216 | -0.18 | 0.487395 | 0.474693 |
| COMPOUND_284_2349a10_180572 | Rp | + | 284.2349 | 10.18 | | | | (569.4548, 185.31)(607.4257, 4840.64)(302.267, 755.46)(285.2433, 10436.88)(286.2459, 2195.29)(287.2322, 1675.22)(288.2266, 158.93) | 36171.1 | 13184.6 | 38600.82 | 16643.16 | 45595.78 | 15406.8 | 62790.02 | 32989.82 | 0.15 | 0.547952 | 0.646067 | 0.62 | 0.038469 | 0.259981 |
| COMPOUND_284_251a8_235709 | Rp | + | 284.2510 | 8.24 | | | | (591.514, 85.39)(302.2696, 300.19)(285.2589, 17787.68)(286.2619, 3178.9)(287.2656, 643.62) | 24289.96 | 9212.57 | 24212.92 | 9759.082 | 57567.07 | 19678.94 | 48495.84 | 22353.3 | 1.40 | 1.52E-08 | 1.19E-07 | -0.15 | 0.551989 | 0.780002 |
| COMPOUND_284_2515a8_853771 | Rp | + | 284.2515 | 8.85 | | | | (569.5082, 132.59)(285.259, 15904.64)(286.2622, 4074.5)(287.2657, 563.88)(288.2718, 46.63) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 1.55 | 3.21E-11 | 6.39E-10 | 0.01 | 0.962737 | 0.981922 |
| COMPOUND_284_2709a11_185121 | Rp | - | 284.2709 | 11.19 | Stearic acid | 1 | 10 eV: 283.2632(100) | (319.2401, 6441.77)(320.2438, 1500.33)(321.2253, 3119.46)(322.2248, 674.78)(323.2199, 419.66)(613.5219, 225.21)(283.2635, 1024397.5)(284.2675, 185898.08)(285.2703, 20044.0)(286.2735, 1841.71)(567.5338, 525.16)(568.5371, 282.08)(569.5459, 71.43)(329.2692, 13727.62)(330.2727, 2702.82)(331.2715, 216.08) | 3440636 | 1492739 | 4229792 | 1531885 | 3300295 | 1115388 | 3037785 | 1640165 | -0.06 | 0.819864 | 0.872719 | -0.78 | 0.024411 | 0.219303 |
| COMPOUND_284_2834a10_460715 | Rp | + | 284.2834 | 10.46 | | | | (569.5884, 212.06)(570.6038, 741.37)(307.2666, 1005.98)(591.5772, 341.1)(323.2609, 1086.97)(302.325, 755.6)(285.2919, 11029.5)(286.294, 2351.01)(287.3018, 563.34)(586.5878, 541.23) | 38489.85 | 9882.296 | 38605.28 | 7831.822 | 41628.77 | 10998.76 | 40080.13 | 9298.171 | 0.07 | 0.785767 | 0.844249 | 0.05 | 0.87172 | 0.945212 |
| COMPOUND_285_1378a8_28072 | Rp | + | 285.1378 | 8.28 | | | | (571.2818, 1712.07)(572.2862, 664.74)(573.2805, 236.46)(308.1276, 3842.56)(309.1292, 932.36)(310.1311, 83.22)(593.2654, 1126.98)(594.2674, 513.12)(595.266, 94.61)(324.0893, 790.12)(286.145, 407326.3)(287.1485, 70386.09)(288.1514, 8704.53)(289.1533, 953.59) | 471219 | 493905.6 | 508790.1 | 407741.6 | 432283.9 | 486602.2 | 238356.8 | 241053.8 | -0.02 | 0.948055 | 0.966948 | -0.79 | 0.022532 | 0.213113 |
| COMPOUND_285_1946a4_9806747 | Rp | + | 285.1946 | 4.98 | ACar 8:1 | 2 | 10 eV: 286.2037(100), 85.0288(40), 227.131(12), 125.0951(10), 55.0554(10) | (286.2022, 42941.66)(287.2058, 6716.69)(288.2071, 966.29)(289.2052, 99.52) | 110844.1 | 55860.03 | 115731.6 | 52731.15 | 114492.9 | 29859.63 | 133431.2 | 54660.65 | 0.15 | 0.57166 | 0.668263 | 0.21 | 0.491695 | 0.748114 |
| COMPOUND_285_195a0_9093032 | Hilic | + | 285.1950 | 0.91 | | | | (308.1862, 4675.11)(309.1897, 1031.25)(593.396, 356.33)(303.2251, 244.2)(286.2021, 66181.64)(287.2054, 11494.48)(288.2138, 2629.8)(289.2201, 289.66)(588.4375, 3253.6)(589.4406, 1046.1) | 315227.8 | 159611.9 | 334997.7 | 129521.3 | 310107.4 | 93165.84 | 349069.8 | 123547.8 | -0.01 | 0.96489 | 0.980123 | 0.15 | 0.613707 | 0.816343 |
| COMPOUND_285_195a5_092399 | Rp | + | 285.1953 | 5.09 | | | | (593.3834, 55.9)(286.2022, 11203.94)(287.2051, 1990.93)(288.2073, 229.47) | 28260.08 | 11756.49 | 29212.9 | 15386.37 | 30460.5 | 23160.98 | 26753.5 | 14803.63 | -0.12 | 0.674282 | 0.760763 | -0.07 | 0.822082 | 0.922833 |
| COMPOUND_285_2223a10_613533 | Rp | + | 285.2223 | 10.61 | | | | (593.441, 6672.1)(286.2304, 258041.5)(287.235, 71499.95)(288.2388, 10544.11) | 149906.8 | 35595.69 | 113983.8 | 26188.2 | 497062.6 | 184808.1 | 424602 | 149449.2 | 1.60 | 8.48E-16 | 3.82E-13 | -0.30 | 0.091687 | 0.359093 |
| COMPOUND_286_2156a9_812983 | Rp | + | 286.2156 | 9.81 | MAG 13:1 | 2 | 10 eV: 111.1163(100), 199.1695(35), 69.0693(10), 304.2394(1) | (611.4137, 668.63)(309.2054, 96129.01)(310.2101, 16229.86)(311.2152, 2648.57)(312.2194, 301.6)(595.4231, 10389.75)(596.4252, 3063.37)(325.1786, 3398.51)(326.1799, 677.99)(327.1776, 479.9)(328.1727, 36.25)(304.2493, 304911.03)(305.2525, 53063.19)(306.2549, 7277.05)(307.2557, 858.37)(287.2227, 198150.12)(288.2259, 33629.24)(289.2288, 4439.72) | 1436713 | 318036 | 1699943 | 307009 | 1536870 | 352737.3 | 1434123 | 348395.2 | 0.44 | 0.131945 | 0.206061 | -0.20 | 0.024906 | 0.219303 |
| COMPOUND_286_2373a5_8505173 | Hilic | + | 286.2373 | 5.85 | Unknown | 4 | 10 eV: 100.0759(100), 171.1502(50), 269.2285(20) | (287.2447, 3385.09)(288.248, 5802.66)(289.2509, 606.69)(144.1262, 2355.21)(144.6276, 409.21)(145.12, 235.43) | 11542.09 | 3110.856 | 10750.57 | 4722.91 | 46531.86 | 20969.72 | 64140.72 | 29987.5 | 1.11 | 1.28E-08 | 1.03E-07 | 0.71 | 0.000671 | 0.04444 |
| COMPOUND_287_2105a5_8078117 | Rp | + | 287.2105 | 5.81 | Octanoylcarnitine | 1 | 10eV: 288.2179(100), 85.0285(70), 60.0808(9), 127.1072(7) | (310.2027, 11664.4)(311.2055, 2280.0)(288.2181, 55420.46)(289.2215, 9434.36)(290.2236, 1317.2)(291.2223, 123.63) | 129823.4 | 6763.8 | 134504.3 | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|---|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|-----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_294_2189a9_363246 | Rp | - | 294.2189 | 9.36 | | | | (329.1829, 264.41)(330.1856, 81.17)(331.1924, 826.81)(293.2116, 7027.77)(294.2153, 1445.98)(295.2078, 202.87) (589.42, 117.07)(590.4107, 402.01)(617.4108, 208.44)(317.2107, 38613.58)(318.2144, 8471.55)(613.4417, 1160.63)(614.4563, 367.37)(615.4236, 298.01)(312.2497, 605.52)(313.239, 817.74)(333.1786, 2408.92)(334.1823, 558.27)(295.228, 41658.87)(296.2299, 10299.57)(297.2397, 3515.94)(298.2427, 328.09) | 29125.19 | 13891.22 | 39734.75 | 23142.32 | 37928.5 | 23916.97 | 45024.16 | 45622.66 | -0.58 | 0.024898 | 0.04772 | -0.38 | 0.217401 | 0.524815 |
| COMPOUND_294_2194a9_665863 | Rp | + | 294.2194 | 9.67 | | | | (589.4665, 132.79)(590.4634, 39.12)(627.3984, 720.64)(317.2102, 41690.54)(318.2142, 8954.08)(611.4297, 1808.53)(612.4319, 846.93)(613.4466, 2264.96)(614.4477, 823.84)(615.4483, 762.17)(333.1657, 4551.2)(334.1674, 1053.74)(312.2541, 22110.41)(313.2562, 4924.68)(314.2635, 986.78)(295.2286, 230221.64)(296.2316, 45408.76)(297.2353, 7160.15)(298.239, 840.09) (613.1192, 231.38)(296.0663, 73142.34)(297.0699, 7300.86)(298.0657, 6310.11)(299.0687, 549.46) (591.26, 1973.23)(592.2587, 759.35)(318.1065, 181.02)(334.0973, 261.74)(296.1319, 13993.38)(297.1342, 2701.93)(298.1318, 6074.33)(299.135, 1316.0)(300.1279, 2684.84) | 180416.3 | 121446.2 | 242658.8 | 170503.1 | 136073.5 | 97986.6 | 325372 | 264807.5 | -1.02 | 1.32E-05 | 5.15E-05 | -0.26 | 0.309896 | 0.615962 |
| COMPOUND_294_2201a9_608477 | Rp | + | 294.2201 | 9.61 | | | | (589.4665, 132.79)(590.4634, 39.12)(627.3984, 720.64)(317.2102, 41690.54)(318.2142, 8954.08)(611.4297, 1808.53)(612.4319, 846.93)(613.4466, 2264.96)(614.4477, 823.84)(615.4483, 762.17)(333.1657, 4551.2)(334.1674, 1053.74)(312.2541, 22110.41)(313.2562, 4924.68)(314.2635, 986.78)(295.2286, 230221.64)(296.2316, 45408.76)(297.2353, 7160.15)(298.239, 840.09) (613.1192, 231.38)(296.0663, 73142.34)(297.0699, 7300.86)(298.0657, 6310.11)(299.0687, 549.46) (591.26, 1973.23)(592.2587, 759.35)(318.1065, 181.02)(334.0973, 261.74)(296.1319, 13993.38)(297.1342, 2701.93)(298.1318, 6074.33)(299.135, 1316.0)(300.1279, 2684.84) | 317478.7 | 160793.1 | 437294 | 259861.9 | 492203.6 | 525447.5 | 461920 | 332631.7 | -0.68 | 0.003767 | 0.008747 | -0.58 | 0.035328 | 0.250187 |
| COMPOUND_295_0591a6_145353 | HiIic | + | 295.0591 | 6.15 | | | | (613.1192, 231.38)(296.0663, 73142.34)(297.0699, 7300.86)(298.0657, 6310.11)(299.0687, 549.46) (591.26, 1973.23)(592.2587, 759.35)(318.1065, 181.02)(334.0973, 261.74)(296.1319, 13993.38)(297.1342, 2701.93)(298.1318, 6074.33)(299.135, 1316.0)(300.1279, 2684.84) | 107745.8 | 63583.65 | 80204.83 | 40729.69 | 88536.21 | 34847.74 | 147609.6 | 62964.82 | -0.19 | 0.489146 | 0.589698 | 1.30 | 0.000171 | 0.018576 |
| COMPOUND_295_1249a9_949218 | Rp | + | 295.1249 | 9.95 | | | | (591.26, 1973.23)(592.2587, 759.35)(318.1065, 181.02)(334.0973, 261.74)(296.1319, 13993.38)(297.1342, 2701.93)(298.1318, 6074.33)(299.135, 1316.0)(300.1279, 2684.84) | 34435.88 | 9040.053 | 37935.44 | 10552.67 | 36391.07 | 8525.546 | 40401.26 | 11538.17 | 0.20 | 0.480134 | 0.582891 | 0.06 | 0.853745 | 0.937825 |
| COMPOUND_295_2162a9_045663 | Rp | + | 295.2162 | 9.05 | | | | (591.4234, 1530.37)(296.2232, 65593.04)(297.2275, 12653.97)(298.2308, 1849.63) (627.3484, 513.95)(637.367, 701.62)(295.189, 10510.62)(296.1923, 1653.15)(297.1941, 3315.7)(705.3638, 2124.82) | 304401 | 17437.3 | 292451.6 | 20559.16 | 320060 | 21152.69 | 323942.1 | 19600.04 | 0.68 | 0.00862 | 0.018594 | 0.69 | 0.024515 | 0.219303 |
| COMPOUND_296_1958a10_465157 | Rp | - | 296.1958 | 10.47 | | | | (591.4234, 1530.37)(296.2232, 65593.04)(297.2275, 12653.97)(298.2308, 1849.63) (627.3484, 513.95)(637.367, 701.62)(295.189, 10510.62)(296.1923, 1653.15)(297.1941, 3315.7)(705.3638, 2124.82) | 20059.4 | 5715.129 | 25147.07 | 7814.097 | 18400.93 | 5911.309 | 20974.06 | 6911.772 | -0.17 | 0.550283 | 0.647797 | -0.42 | 0.204697 | 0.516497 |
| COMPOUND_296_2347a9_623438 | Rp | - | 296.2347 | 9.62 | 9-HODE | 2 | 10 eV: 295.2276(100), 171.1023(15), 226.9689(3), 42.3797(2) | (311.2033, 8581.69)(332.2074, 1663.72)(333.2041, 3923.03)(334.2066, 674.36)(295.2276, 184656.31)(296.2308, 36121.01)(297.234, 4973.55)(298.2349, 561.62)(341.2294, 411.13) (320.0969, 3571.81)(321.1002, 545.77)(322.1125, 88.22)(315.1366, 292.93)(298.1149, 1412.08)(299.1159, 336.31)(300.1248, 44.5) (597.2823, 4418.58)(321.1207, 888.63)(322.1223, 253.72)(337.0881, 286.62)(299.1397, 28132.09)(300.1431, 6066.03)(301.143, 1050.85) (299.2051, 114866.73)(300.2051, 25114.96) (333.2122, 322.04)(297.243, 7799.13)(298.2467, 1776.81)(709.467, 624.5) (411.2202, 139.78)(333.2181, 544.57)(334.2208, 199.13)(335.2216, 290.5)(297.2431, 21109.53)(298.2465, 4395.11) (411.2223, 157.64)(333.2186, 508.11)(334.2209, 36.75)(335.2269, 456.28)(297.2434, 22417.84)(298.247, 4757.11) (411.2159, 173.94)(333.2189, 439.27)(334.2217, 58.95)(297.243, 15900.74)(298.2465, 3425.91) (333.2184, 439.96)(334.223, 94.46)(335.2238, 492.09)(297.2432, 21913.41)(298.2468, 4945.98) (333.2187, 420.57)(334.2225, 102.56)(335.2277, 393.77)(297.243, 17054.93)(298.2465, 3582.67) (321.2423, 26508.17)(322.2458, 5437.27)(323.2538, 2712.11)(619.478, 160.1)(337.2209, 1441.29)(338.2277, 428.23)(339.2228, 379.4)(316.286, 5539.53)(317.2882, 1111.67)(318.2695, 2532.39)(299.2588, 48532.73)(300.2621, 9784.09)(301.2641, 1735.07)(614.5651, 120.13) (321.2415, 1896.74)(322.2435, 487.82)(323.2374, 700.6)(324.2438, 154.79)(337.2228, 342.09)(316.2849, 1622.56)(317.2918, 65.69)(299.2587, 23506.19)(300.2626, 5144.49)(301.2653, 866.37) (321.2421, 18010.96)(322.2455, 3628.69)(323.2512, 2297.41)(619.4819, 129.23)(337.2113, 1726.07)(338.2198, 568.77)(339.215, 350.91)(316.2857, 6678.19)(317.2891, 1518.62)(318.2963, 1667.92)(299.2589, 55097.09)(300.2626, 11180.39)(301.2655, 1670.21)(614.5582, 103.81) (321.2423, 2705.51)(322.2418, 592.84)(323.2515, 878.85)(324.2562, 146.32)(337.2054, 159.04)(316.2856, 7097.62)(317.2879, 1577.4)(318.2975, 863.71)(299.2589, 18013.81)(300.2625, 3686.05)(301.2666, 642.11) (321.2412, 2215.86)(322.2439, 670.21)(323.2494, 1151.13)(324.252, 211.25)(337.2161, 350.65)(338.2073, 109.01)(316.2855, 6882.04)(317.2891, 1360.73)(318.2973, 856.84)(299.2585, 22961.75)(300.2623, 4379.28)(301.262, 753.01) (321.2423, 2687.59)(322.2476, 397.26)(323.2536, 944.54)(324.2559, 219.87)(337.2075, 150.12)(338.2135, 49.82)(316.2841, 3019.11)(317.2883, 674.19)(299.2584, 23506.22)(300.262, 3372.82)(301.2645, 829.33) (321.2415, 11385.57)(322.2452, 2173.46)(323.2517, 847.74)(619.4738, 126.15)(337.2197, 1235.35)(338.2289, 329.74)(339.2264, 395.67)(316.2857, 13176.39)(317.2883, 2708.11)(318.297, 2188.95)(299.2589, 42885.49)(300.2624, 8795.28)(301.2648, 1465.71)(614.5687, 106.32) (411.2601, 1170.01)(297.2796, 13446.61)(298.2832, 3114.99)(299.2848, 480.55)(343.2844, 233.69) (322.2719, 3440.48)(323.2763, 1259.44)(621.5594, 266.6)(300.2914, 21752.65)(301.2949, 4320.17)(302.2951, 627.45) (300.2905, 20197.81)(301.2933, 4544.01)(302.2963, 636.54)(303.3035, 72.33) (323.2018, 6437.12)(324.2074, 1884.33)(623.4093, 576.41)(624.4188, 192.58)(625.421, 525.39)(301.2171, 37552.09)(302.2205, 8310.45)(303.2227, 1784.23)(304.2272, 199.09) | 252869.2 | 123282.4 | 381172.8 | 233952.7 | 155666.5 | 237139.1 | 168937.2 | 295785.2 | -0.75 | 0.003359 | 0.007905 | -0.56 | 0.06042 | 0.302235 |
| COMPOUND_297_1077a1_8546703 | HiIic | + | 297.1077 | 1.85 | | | | (320.0969, 3571.81)(321.1002, 545.77)(322.1125, 88.22)(315.1366, 292.93)(298.1149, 1412.08)(299.1159, 336.31)(300.1248, 44.5) (597.2823, 4418.58)(321.1207, 888.63)(322.1223, 253.72)(337.0881, 286.62)(299.1397, 28132.09)(300.1431, 6066.03)(301.143, 1050.85) (299.2051, 114866.73)(300.2051, 25114.96) (333.2122, 322.04)(297.243, 7799.13)(298.2467, 1776.81)(709.467, 624.5) (411.2202, 139.78)(333.2181, 544.57)(334.2208, 199.13)(335.2216, 290.5)(297.2431, 21109.53)(298.2465, 4395.11) (411.2223, 157.64)(333.2186, 508.11)(334.2209, 36.75)(335.2269, 456.28)(297.2434, 22417.84)(298.247, 4757.11) (411.2159, 173.94)(333.2189, 439.27)(334.2217, 58.95)(297.243, 15900.74)(298.2465, 3425.91) (333.2184, 439.96)(334.223, 94.46)(335.2238, 492.09)(297.2432, 21913.41)(298.2468, 4945.98) (333.2187, 420.57)(334.2225, 102.56)(335.2277, 393.77)(297.243, 17054.93)(298.2465, 3582.67) (321.2423, 26508.17)(322.2458, 5437.27)(323.2538, 2712.11)(619.478, 160.1)(337.2209, 1441.29)(338.2277, 428.23)(339.2228, 379.4)(316.286, 5539.53)(317.2882, 1111.67)(318.2695, 2532.39)(299.2588, 48532.73)(300.2621, 9784.09)(301.2641, 1735.07)(614.5651, 120.13) (321.2415, 1896.74)(322.2435, 487.82)(323.2374, 700.6)(324.2438, 154.79)(337.2228, 342.09)(316.2849, 1622.56)(317.2918, 65.69)(299.2587, 23506.19)(300.2626, 5144.49)(301.2653, 866.37) (321.2421, 18010.96)(322.2455, 3628.69)(323.2512, 2297.41)(619.4819, 129.23)(337.2113, 1726.07)(338.2198, 568.77)(339.215, 350.91)(316.2857, 6678.19)(317.2891, 1518.62)(318.2963, 1667.92)(299.2589, 55097.09)(300.2626, 11180.39)(301.2655, 1670.21)(614.5582, 103.81) (321.2423, 2705.51)(322.2418, 592.84)(323.2515, 878.85)(324.2562, 146.32)(337.2054, 159.04)(316.2856, 7097.62)(317.2879, 1577.4)(318.2975, 863.71)(299.2589, 18013.81)(300.2625, 3686.05)(301.2666, 642.11) (321.2412, 2215.86)(322.2439, 670.21)(323.2494, 1151.13)(324.252, 211.25)(337.2161, 350.65)(338.2073, 109.01)(316.2855, 6882.04)(317.2891, 1360.73)(318.2973, 856.84)(299.2585, 22961.75)(300.2623, 4379.28)(301.262, 753.01) (321.2423, 2687.59)(322.2476, 397.26)(323.2536, 944.54)(324.2559, 219.87)(337.2075, 150.12)(338.2135, 49.82)(316.2841, 3019.11)(317.2883, 674.19)(299.2584, 23506.22)(300.262, 3372.82)(301.2645, 829.33) (321.2415, 11385.57)(322.2452, 2173.46)(323.2517, 847.74)(619.4738, 126.15)(337.2197, 1235.35)(338.2289, 329.74)(339.2264, 395.67)(316.2857, 13176.39)(317.2883, 2708.11)(318.297, 2188.95)(299.2589, 42885.49)(300.2624, 8795.28)(301.2648, 1465.71)(614.5687, 106.32) (411.2601, 1170.01)(297.2796, 13446.61)(298.2832, 3114.99)(299.2848, 480.55)(343.2844, 233.69) (322.2719, 3440.48)(323.2763, 1259.44)(621.5594, 266.6)(300.2914, 21752.65)(301.2949, 4320.17)(302.2951, 627.45) (300.2905, 20197.81)(301.2933, 4544.01)(302.2963, 636.54)(303.3035, 72.33) (323.2018, 6437.12)(324.2074, 1884.33)(623.4093, 576.41)(624.4188, 192.58)(625.421, 525.39)(301.2171, 37552.09)(302.2205, 8310.45)(303.2227, 1784.23)(304.2272, 199.09) | 18944.08 | 3460.183 | 20030.63 | 2758.775 | 23309.14 | 3344.942 | 24975.32 | 4059.803 | 1.00 | 0.434E-05 | 0.000146 | 0.09 | 0.751095 | 0.893065 |
| COMPOUND_298_1332a11_366976 | Rp | + | 298.1332 | 11.37 | | | | (597.2823, 4418.58)(321.1207, 888.63)(322.1223, 253.72)(337.0881, 286.62)(299.1397, 28132.09)(300.1431, 6066.03)(301.143, 1050.85) (299.2051, 114866.73)(300.2051, 25114.96) (333.2122, 322.04)(297.243, 7799.13)(298.2467, 1776.81)(709.467, 624.5) (411.2202, 139.78)(333.2181, 544.57)(334.2208, 199.13)(335.2216, 290.5)(297.2431, 21109.53)(298.2465, 4395.11) (411.2223, 157.64)(333.2186, 508.11)(334.2209, 36.75)(335.2269, 456.28)(297.2434, 22417.84)(298.247, 4757.11) (411.2159, 173.94)(333.2189, 439.27)(334.2217, 58.95)(297.243, 15900.74)(298.2465, 3425.91) (333.2184, 439.96)(334.223, 94.46)(335.2238, 492.09)(297.2432, 21913.41)(298.2468, 4945.98) (333.2187, 420.57)(334.2225, 102.56)(335.2277, 393.77)(297.243, 17054.93)(298.2465, 3582.67) (321.2423, 26508.17)(322.2458, 5437.27)(323.2538, 2712.11)(619.478, 160.1)(337.2209, 1441.29)(338.2277, 428.23)(339.2228, 379.4)(316.286, 5539.53)(317.2882, 1111.67)(318.2695, 2532.39)(299.2588, 48532.73)(300.2621, 9784.09)(301.2641, 1735.07)(614.5651, 120.13) (321.2415, 1896.74)(322.2435, 487.82)(323.2374, 700.6)(324.2438, 154.79)(337.2228, 342.09)(316.2849, 1622.56)(317.2918, 65.69)(299.2587, 23506.19)(300.2626, 5144.49)(301.2653, 866.37) (321.2421, 18010.96)(322.2455, 3628.69)(323.2512, 2297.41)(619.4819, 129.23)(337.2113, 1726.07)(338.2198, 568.77)(339.215, 350.9 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|---|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_300_2653a10_016575 | Rp | - | 300.2653 | 10.02 | | | | (335.2258, 463.49)[336.222, 70.0](299.2585, 9229.74)[300.2621, 1862.54][301.2663, 121.93] | 46720.53 | 7512.53 | 47459.93 | 6727.716 | 49599.5 | 10478.07 | 50936.11 | 11289.55 | 0.34 | 0.230509 | 0.325662 | -0.03 | 0.918208 | 0.962217 |
| COMPOUND_300_2658a10_777741 | Rp | - | 300.2658 | 10.78 | | | | (413.2471, 319.68)[335.22, 1424.97](299.2587, 12930.3)[300.2628, 2331.15][301.2662, 321.17] | 28472.88 | 9862.398 | 30997.22 | 9361.214 | 20622.07 | 5906.423 | 22622.02 | 5507.416 | -0.82 | 0.003966 | 0.00917 | -0.04 | 0.901603 | 0.955487 |
| COMPOUND_300_2661a10_737138 | Rp | - | 300.2660 | 10.74 | | | | (335.2245, 499.67)[413.2444, 282.69](299.2587, 12981.21)[300.2622, 2615.14][301.2663, 546.54] | 23106.94 | 9298.916 | 21551.78 | 9582.629 | 19328.86 | 6385.69 | 15689.81 | 4471.715 | -0.24 | 0.398019 | 0.501869 | -0.31 | 0.374287 | 0.677023 |
| COMPOUND_301_0754a9_211498 | Rp | - | 301.0754 | 9.21 | | | | (414.0649, 161.79)[300.0665, 4906.87](301.0678, 969.53)[302.0673, 234.12][60.1602, 871.25][602.156, 552.24][715.1528, 620.48][716.1366, 385.08] | 17171.35 | 4785.724 | 17375.12 | 4913.292 | 17333.79 | 3224.751 | 17161.4 | 4397.404 | 0.33 | 0.274953 | 0.37391 | -0.29 | 0.411174 | 0.694731 |
| COMPOUND_301_1895a1_4800488 | Hilic | - | 301.1895 | 1.48 | | | | (319.226, 358.91)[302.197, 32908.91](303.2006, 5333.69)[304.2087, 1386.27][305.2113, 134.29] | 10507.58 | 8066.564 | 11537.29 | 7184.235 | 90132.64 | 86269.97 | 74224.75 | 102865.4 | 1.53 | 2.51E-10 | 3.43E-09 | -0.16 | 0.497755 | 0.752946 |
| COMPOUND_301_1896a1_1891912 | Hilic | + | 301.1896 | 1.19 | | | | (603.394, 193.71)[302.1964, 32380.04](303.1996, 5512.14)[304.2019, 957.74][305.2052, 105.3] | 9666.022 | 6510.729 | 10607.38 | 8623.651 | 48679.21 | 35820.56 | 42752.39 | 48830.18 | 1.59 | 7.03E-10 | 8.21E-09 | -0.39 | 0.133839 | 0.434929 |
| COMPOUND_301_2095a8_116018 | Rp | + | 301.2095 | 8.12 | | | | (302.2161, 33821.04)[303.2193, 6370.21][304.2159, 2184.49] | 51398.34 | 23249.6 | 53920.2 | 2237.59 | 60613.29 | 36547.65 | 74267.96 | 30891.9 | 0.28 | 0.285599 | 0.384886 | 0.38 | 0.223404 | 0.531262 |
| COMPOUND_301_2243a0_7576121 | Hilic | + | 301.2243 | 0.76 | | | | (603.4524, 244.01)[324.218, 396.32][625.3986, 688.69][302.2314, 4953.26][303.2358, 1201.73][304.2313, 1689.24][305.2355, 230.99] | 78136.27 | 35618.59 | 83101.07 | 53745.09 | 64733.73 | 30618.74 | 93882.34 | 52640.29 | -0.44 | 0.039295 | 0.071135 | 0.06 | 0.804088 | 0.917422 |
| COMPOUND_301_2263a6_172385 | Rp | + | 301.2263 | 6.17 | ACar 9:0 | 2 | 10 eV: 302.2299(100), 60.0787(50), 243.1611(50) | (641.4048, 99.94)[302.2335, 8830.36][303.2367, 1424.59][304.2296, 570.49][305.2402, 48.6] | 35284 | 18898.93 | 34447.47 | 22800.87 | 27814.62 | 12320.84 | 33745.32 | 20504.91 | -0.22 | 0.331741 | 0.43284 | -0.09 | 0.721809 | 0.877707 |
| COMPOUND_302_2149a10_7173195 | Rp | + | 302.2149 | 10.72 | | | | (605.4288, 4122.97)[606.4326, 2397.37](607.433, 2564.14)[643.3741, 609.16][303.2213, 10436.01][304.2253, 3334.6][305.2176, 1552.05][306.2138, 165.77] | 47172 | 23105.7 | 45342.89 | 17627.2 | 49255.73 | 16822.28 | 56515.33 | 32255.78 | 0.63 | 0.016812 | 0.033834 | -0.21 | 0.502969 | 0.754119 |
| COMPOUND_302_2238a10_482109 | Rp | - | 302.2238 | 10.48 | | | | (337.1881, 4480.89)[338.1942, 994.07](301.2172, 308249.2)[302.2205, 64439.22][303.2235, 7671.46][304.2262, 722.07][347.2055, 586.88][717.4192, 1150.96][718.4268, 1726.53] | 234529.5 | 126446.8 | 288820.6 | 212010.5 | 143504.1 | 101115.3 | 159071.1 | 105620.8 | -0.95 | 7.24E-05 | 0.00023 | 0.03 | 0.896249 | 0.954308 |
| COMPOUND_302_2242a9_920079 | Rp | - | 302.2242 | 9.92 | | | | (301.2167, 23776.09)[302.22, 5315.76][303.2273, 977.96][304.2283, 115.98] | 51702.28 | 22511.67 | 56231.57 | 22815.6 | 45729.25 | 22831.01 | 61351 | 19387.57 | -1.00 | 1.49E-05 | 5.75E-05 | -0.27 | 0.285137 | 0.593016 |
| COMPOUND_302_2265a9_926412 | Rp | + | 302.2265 | 9.93 | | | | (605.4299, 2312.06)[606.4519, 651.87](607.4187, 1376.29)[608.4274, 968.26][325.2142, 16271.79][326.2178, 4277.21][627.4378, 3820.83][628.4264, 625.01][629.4319, 1235.03][320.2591, 333.71][341.1945, 2491.54][342.1853, 642.6][303.2328, 79995.74][304.2371, 160367.83][305.2456, 41993.32] | 152753.2 | 60484.54 | 160851.3 | 65769.7 | 155117.5 | 823001.4 | 153897.5 | 877524.9 | -1.00 | 1.87E-05 | 7.06E-05 | -0.23 | 0.369536 | 0.671661 |
| COMPOUND_302_2455a10_181607 | Rp | + | 302.2455 | 10.18 | | | | (643.4433, 3080.63)[644.4504, 1966.68][645.4515, 2046.95][325.2359, 14558.61][326.2403, 2736.97][327.2373, 1309.85][328.2277, 98.86][320.2803, 27284.57][321.2829, 5549.4][322.2845, 1108.03][341.208, 2421.62][342.2195, 472.88][343.2133, 1780.04][344.2223, 631.26][303.2542, 69987.6][304.2567, 13633.22][305.2493, 21330.05][306.2518, 4520.6] | 104262.5 | 54884.37 | 122670 | 70582.07 | 122026.2 | 66649.37 | 232681.3 | 154848.3 | 0.31 | 0.235478 | 0.329992 | 0.63 | 0.041652 | 0.265944 |
| COMPOUND_303_2047a4_3564334 | Rp | + | 303.2047 | 4.36 | | | | (304.2133, 16046.99)[305.2161, 3218.25][306.221, 364.86] | 25641.98 | 11254.91 | 26422.1 | 13972.91 | 22016.5 | 10960.49 | 22784.48 | 10379.37 | -0.68 | 0.012136 | 0.02519 | 0.53 | 0.092922 | 0.361416 |
| COMPOUND_303_2047a1_400974 | Hilic | + | 303.2047 | 1.40 | | | | (607.4056, 118.77)[326.2024, 288.79][327.1932, 95.52][328.2001, 1259.54][329.2064, 293.32][629.408, 122.64][304.2126, 64195.16][305.2161, 19098.52][306.2176, 2056.38][307.2205, 238.79][624.416, 130.08] | 74771.26 | 37446.02 | 79485.54 | 50824.84 | 58048.36 | 31849.75 | 72216.89 | 35347.75 | -0.65 | 0.022029 | 0.042878 | 0.57 | 0.083064 | 0.345768 |
| COMPOUND_304_2404a10_686863 | Rp | - | 304.2404 | 10.69 | | | | (643.442, 146.61)[644.4632, 73.41][645.4362, 301.34][339.2087, 5722.79][340.2126, 1313.31][341.2074, 2110.01][342.2099, 660.22][343.1981, 67.0][303.2323, 895668.94][304.2363, 176600.42][305.2392, 21101.61][306.2422, 1689.53][349.2398, 1313.2] | 1151397 | 320914.4 | 1387655 | 520570.1 | 929458.4 | 401620.1 | 991457.4 | 418179.3 | -0.66 | 0.00767 | 0.016689 | -0.21 | 0.451618 | 0.723875 |
| COMPOUND_304_2409a9_84599 | Rp | + | 304.2409 | 9.85 | | | | (327.2332, 94353.87)[328.2368, 22543.75](322.2747, 90.09)[305.249, 44715.91][306.2522, 9165.92][307.2585, 1884.37][308.2508, 199.66] | 186207.6 | 85042.96 | 213703.8 | 128493.6 | 217213.6 | 79399.85 | 189883.8 | 98112.94 | -0.69 | 0.01389 | 0.028618 | 0.05 | 0.876224 | 0.948226 |
| COMPOUND_304_2414a10_6913805 | Rp | + | 304.2414 | 10.69 | | | | (609.4705, 508.08)[610.4625, 274.02][611.4316, 4216.36][612.4345, 9276.05][327.2254, 834.75][328.2276, 2377.41][329.2163, 160.53][322.2746, 38234.28][323.2776, 10910.18][324.2818, 1638.64][305.2487, 55528.38][306.2523, 11958.46][307.255, 1783.95] | 175741 | 38990.68 | 192580.8 | 67377.02 | 154431.9 | 73752.42 | 147742.6 | 59613.55 | -0.27 | 0.299675 | 0.400041 | -0.28 | 0.348674 | 0.65489 |
| COMPOUND_304_2421a9_799166 | Rp | + | 304.2421 | 9.80 | | | | (609.515, 125.07)[327.2336, 128710.77](328.2366, 31097.42)[322.2888, 446.96][305.2572, 31098.41][306.2546, 4180.3][307.2543, 446.5] | 240005.5 | 78103.32 | 261694.5 | 144432.8 | 247791.8 | 28103.73 | 223710.1 | 156709 | -1.09 | 2.08E-05 | 7.7E-05 | 0.09 | 0.73781 | 0.888668 |
| COMPOUND_306_2552a10_840969 | Rp | - | 306.2552 | 10.84 | FA 20:3 | 2 | 10 eV: 305.2491(100), 88.5665(1) | (341.2244, 1166.55)[342.2268, 326.15][343.2238, 848.42][344.2274, 243.98][657.5035, 1020.12][658.5071, 328.14][305.2485, 115133.92][306.2517, 26220.29][307.2546, 3396.8][308.2566, 364.41][611.4864, 1972.96][725.4824, 2655.55][726.4705, 1652.19][727.4809, 1513.2] | 1738443 | 68879.97 | 213644.7 | 106812.9 | 125830.3 | 43849.76 | 169883.6 | 70977.18 | -0.85 | 0.00139 | 0.003524 | 0.37 | 0.21743 | 0.524815 |
| COMPOUND_308_2702a11_02445 | Rp | - | 308.2702 | 11.02 | | | | (651.5141, 153.44)[421.2449, 1073.37](422.2456, 344.73)[343.2367, 396.56][661.533, 763.45][662.5358, 381.06][307.2638, 27679.15][308.2673, 5773.44][309.2703, 752.59][310.2775, 85.59] | 27875.69 | 15124.26 | 37860.41 | 26251.42 | 34469.07 | 159264.1 | 50161.44 | 26433.51 | 0.53 | 0.041252 | 0.074142 | 0.07 | 0.80705 | 0.917894 |
| COMPOUND_309_1952a5_795485 | Rp | + | 309.1952 | 5.80 | | | | (310.2026, 25178.2)(311.2056, 4910.04)[312.2065, 714.13] | 31382.25 | 14776.53 | 33460.27 | 14119.08 | 49530.64 | 18609.53 | 53427.93 | 24237.3 | 0.94 | 0.000921 | 0.002423 | -0.08 | 0.80289 | 0.916921 |
| COMPOUND_309_1952a8_7701235 | Rp | + | 309.1952 | 8.77 | | | | (310.2022, 8801.47)[311.2039, 2011.08][312.2039, 664.42] | 33648.44 | 3014.259 | 32794.61 | 3046.738 | 33413.64 | 2837.681 | 33685.91 | 3076.03 | -0.05 | 0.874192 | 0.874192 | 0.29 | 0.421885 | 0.522902 |
| COMPOUND_309_1953a5_7616744 | Rp | + | 309.1953 | 5.76 | | | | (310.2026, 25178.2)(311.2056, 4910.04)[312.2065, 714.13] | 36509.04 | 15069.72 | 37215.33 | 14553.46 | 53733.31 | 18921.37 | 53888.09 | 23931.06 | 0.76 | 0.007196 | 0.01578 | 0.05 | 0.869108 | 0.945066 |
| COMPOUND_309_1956a5_458934 | Rp | + | 309.1956 | 5.46 | | | | (310.2022, 6419.38)[311.2063, 1229.53][312.2118, 619.54] | 17383.04 | 6799.966 | 15058.14 | 4597.563 | 18030.29 | 5830.875 | 21316.7 | 8588.062 | 0.83 | 0.000823 | 0.002181 | 0.14 | 0.62463 | 0.823156 |
| COMPOUND_309_2320a9_70118 | Rp | + | 309.2320 | 9.70 | | | | (332.2244, 325.27)[310.2386, 92590.45][311.2422, 10502.61][312.2476, 1756.43] | 172594.2 | 16422.75 | 17235.12 | 12210.02 | 164072.4 | 13837.94 | 171745.3 | 15289.71 | -0.52 | 0.082866 | 0.137519 | 0.40 | 0.258793 | 0.570391 |
| COMPOUND_309_3044a10_923578 | Rp | + | 309.3044 | 10.92 | | | | (619.6188, 15729.51)[620.633, 1130.92][621.6004, 19031.22][657.5949, 3001.48][332.2938, 13425.47][333.2941, 3354.42][334.3035, 784.93][335.3104, 94.73][348.265, 3727.91][349.2693, 1427.21][350.2701, 528.75][310.3113, 106478.91][311.3143, 25399.17][312.3194, 4297.01][313.3204, 528.97] | 236833.8 | 84850.9 | 256742.9 | 97034.51 | 418875.1 | 214655.9 | 376515.5 | 186107.8 | 1.16 | 2.96E-05 | 0.000105 | -0.40 | 0.193678 | 0.505089 |
| COMPOUND_310_1608a10_859484 | Rp | + | 310.1608 | 10.86 | | | | (621.3033, 1539.92)[622.3011, 562.46][623.3112, 1386.7](659.3096, 4065.11)[660.2861, 2819.45][643.2917, 1483.66][311.168, 21192.77][312.171, 4183.96][313.1683, 11957.45][314.1718, 2360.0][315.1642, 4549.44][316.167, 1184.59][317.1636, 970.27] | 92492.19 | 24648.96 | 93848.77 | 24504.42 | 143636.7 | 37709.68 | 1430 | | | | | | | |

| Compound | Column | Ion mode | Mass Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|------------------------------|--------|----------|----------------|----------------|-------------------|--------------|--|--|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|----------|
| | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | |
| | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_312_1376a_385394 | Rp | + | 312.1376 | 9.39 | | | (335.1257, 2514.72)(336.13, 589.73)(337.1326, 144.33)(351.0956, 643.44)(313.1441, 21264.02)(314.1475, 4388.67)(315.1494, 736.76) | 18311.57 | 8979.078 | 21230.24 | 15133.18 | 24888.58 | 10720.18 | 20803.82 | 16293.51 | 0.42 | 0.144655 | 0.221608 | -0.74 | 0.034807 | 0.249266 | |
| COMPOUND_312_1471a_4788327 | Rp | - | 312.1471 | 4.48 | | | (425.1283, 3350.27)(426.1322, 751.56)(347.1164, 7311.91)(348.1192, 1433.04)(349.1138, 2487.95)(350.1177, 548.67)(351.1202, 111.78)(311.14, 20610.81)(312.1432, 40379.48)(313.1462, 5059.0)(314.1484, 510.66)(623.2869, 25252.98)(624.2899, 10428.23)(625.2931, 2179.95)(626.2932, 448.67) | 439659.6 | 169693.1 | 477717.7 | 206422.2 | 479290.9 | 186283.8 | 487591.7 | 221295.6 | 0.08 | 0.765971 | 0.831309 | -0.12 | 0.708297 | 0.868783 | |
| COMPOUND_312_1482a_495519 | Rp | + | 312.1482 | 4.50 | | | (625.3042, 2364.66)(626.3043, 1085.69)(627.3064, 316.35)(628.3106, 65.38)(663.2586, 176.26)(664.2524, 82.62)(335.1346, 727.73)(336.1389, 247.76)(337.1223, 43.83)(647.2801, 61.57)(648.2765, 31.76)(649.2611, 67.24)(650.2743, 31.5)(330.181, 222.65)(351.1038, 1162.74)(313.1554, 951894.6)(314.159, 180588.81)(315.1617, 21652.04)(316.1643, 2471.78) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.10 | 0.736163 | 0.808307 | -0.01 | 0.967305 | 0.982576 | |
| COMPOUND_312_1483a_16320281 | Hilic | + | 312.1483 | 1.63 | | | (625.3026, 66313.67)(626.3056, 27334.73)(627.3081, 5858.52)(628.3109, 1065.64)(629.3176, 202.13)(335.137, 3193.41)(336.1409, 7429.08)(337.1435, 1761.03)(338.1584, 211.3)(647.2844, 4404.27)(648.2878, 1703.59)(649.2896, 843.34)(650.2894, 179.09)(651.288, 23.99)(313.1551, 680675.94)(314.1588, 128304.59)(315.1613, 16688.75)(316.1636, 1465.31)(642.3341, 268.7)(643.3398, 80.54) | 1249131 | 525330.3 | 1357152 | 660578.8 | 1317223 | 563553.1 | 1398477 | 741556 | -0.02 | 0.934409 | 0.95693 | -0.02 | 0.939927 | 0.972308 | |
| COMPOUND_312_2295a_604098 | Rp | - | 312.2295 | 9.60 | | | (347.1992, 5286.9)(348.2017, 1143.67)(349.1965, 1617.63)(350.2009, 398.47)(351.208, 202.29)(311.2223, 46507.95)(312.2256, 8637.88)(313.2296, 1651.18)(314.233, 191.09)(357.2176, 268.63) | 90553.15 | 44813.06 | 115815.4 | 64122.6 | 107925.3 | 89164.77 | 138279.1 | 75889.07 | -0.89 | 0.000148 | 0.000447 | -0.37 | 0.161943 | 0.475484 | |
| COMPOUND_312_2312a10_211772 | Rp | + | 312.2312 | 10.21 | | | (335.2208, 2104.9)(336.2239, 547.43)(337.2315, 645.03)(330.272, 5487.44)(313.2385, 16278.71)(314.2419, 3119.21)(315.2489, 1063.79) | 83715.98 | 8415.888 | 79787.24 | 9428.159 | 101704.1 | 14391.46 | 105687.8 | 14608.5 | 1.01 | 2.27E-05 | 8.33E-05 | 0.58 | 0.029257 | 0.231966 | |
| COMPOUND_312_2644a10_172118 | Rp | + | 312.2644 | 10.17 | | | (335.2563, 770.03)(330.3012, 1407.24)(331.2999, 274.34)(313.2728, 6213.93)(314.2758, 1508.06)(315.2679, 213.96) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.32 | 0.444081 | 0.339722 | 0.02 | 0.963262 | 0.981972 | |
| COMPOUND_312_2671a9_99728 | Rp | + | 312.2671 | 10.00 | | | (335.2468, 787.08)(647.5463, 106.24)(330.3008, 3135.38)(331.3034, 882.73)(332.307, 52.01)(313.2741, 7559.96)(314.276, 2494.37)(315.2752, 100.79) | 55907.3 | 16398.31 | 50864.79 | 14885.3 | 67171.5 | 21307.77 | 67195.84 | 21163.98 | 0.75 | 0.007306 | 0.01599 | -0.09 | 0.785234 | 0.909997 | |
| COMPOUND_312_2675a10_563439 | Rp | + | 312.2675 | 10.56 | | | (625.5199, 580.19)(535.2517, 1281.82)(336.2569, 454.04)(330.2976, 1387.81)(313.275, 217949.99)(314.278, 42423.14)(315.2812, 5822.7)(642.6, 671.47) | 290222.5 | 187814 | 239311.2 | 149641.2 | 168231.6 | 136961 | 208085.5 | 173479.5 | -0.63 | 0.020253 | 0.039938 | 0.41 | 0.192716 | 0.505089 | |
| COMPOUND_312_2681a10_60154 | Rp | + | 312.2681 | 10.60 | | | (625.52, 650.85)(335.2498, 900.6)(336.2475, 381.87)(330.3008, 1119.43)(313.2748, 242493.42)(314.2779, 51107.61)(315.2812, 6801.54)(642.5963, 719.83) | 380801.8 | 140574.2 | 364895.5 | 112626.8 | 269276.5 | 94403.05 | 381827 | 138227.9 | -0.85 | 0.004239 | 0.009721 | 0.92 | 0.008531 | 0.14883 | |
| COMPOUND_312_3024a11_580105 | Rp | - | 312.3024 | 11.58 | Arachidic acid | 1 | 10 eV: 311.2956(100), 51.5024(2), 135.1534(2) | (347.2713, 479.03)(348.2729, 94.41)(349.2678, 277.57)(311.2953, 45630.87)(312.2985, 9585.06)(313.3011, 1382.97)(314.3046, 171.96)(357.3004, 860.73)(358.3033, 96.62) | 98359.89 | 46493.09 | 119438 | 45350.61 | 125459.5 | 47007.97 | 114622 | 58925.25 | 0.63 | 0.034925 | 0.064204 | -0.74 | 0.038547 | 0.259981 |
| COMPOUND_312_3026a11_240537 | Rp | - | 312.3026 | 11.24 | | | (347.2673, 249.09)(311.2947, 11124.19)(312.2983, 2032.0)(313.2993, 208.64)(357.2913, 1376.6) | 15335.59 | 4808.62 | 16922.06 | 5169.478 | 19222.83 | 7445.196 | 19706.31 | 6838.353 | 0.61 | 0.022233 | 0.043237 | -0.08 | 0.790192 | 0.91097 | |
| COMPOUND_312_2258a0_7485032 | Hilic | + | 312.2258 | 0.75 | | | (336.2181, 2137.41)(337.2198, 579.46)(331.2508, 844.31)(314.2334, 158928.25)(315.2366, 30503.12) | 181607.6 | 98029.23 | 189389.6 | 108177.4 | 171554.5 | 110925.9 | 193681.3 | 89004.74 | -0.21 | 0.477545 | 0.580686 | 0.27 | 0.439915 | 0.715816 | |
| COMPOUND_313_2259a6_604511 | Rp | + | 313.2259 | 6.60 | Acar 10:1 | 2 | 10 eV: 314.2328(100), 85.0277(25), 281.9817(13) | (314.2335, 23465.77)(315.2369, 4546.92)(316.2402, 790.63)(317.2408, 74.01) | 65391.3 | 35461.1 | 67883.24 | 40328.84 | 53483.57 | 33840.01 | 62896.23 | 33906.75 | -0.46 | 0.122139 | 0.19343 | 0.51 | 0.143066 | 0.448726 |
| COMPOUND_313_2264a6_763148 | Rp | + | 313.2264 | 6.76 | | | (314.2339, 12049.53)(315.236, 2687.19)(316.2426, 499.67) | 28875.3 | 12707.83 | 25688.83 | 10519.21 | 23009.18 | 13258.1 | 21013.77 | 8696.694 | -0.58 | 0.038168 | 0.069543 | 0.11 | 0.742694 | 0.889653 | |
| COMPOUND_314_1263a7_063569 | Rp | - | 314.1263 | 7.06 | | | (427.1116, 1239.62)(428.1154, 321.05)(429.1252, 99.96)(349.0964, 1659.68)(350.101, 336.11)(351.092, 451.97)(313.1189, 6188.6)(314.1218, 999.77)(315.1265, 265.93)(316.1326, 33.44) | 28825.23 | 17051.22 | 24465.07 | 14248.55 | 20865.8 | 9513.077 | 20068.05 | 13517.39 | -0.64 | 0.005291 | 0.011914 | -0.37 | 0.155252 | 0.466404 | |
| COMPOUND_314_1274a7_0736856 | Rp | + | 314.1274 | 7.07 | | | (337.1198, 411.02)(315.1354, 22027.99)(316.1388, 4280.43)(317.1402, 735.75)(318.1316, 91.75) | 42477.62 | 27302.54 | 34537.96 | 19916.9 | 27555.92 | 15103.98 | 23006.18 | 21610.1 | -0.74 | 0.002233 | 0.005483 | -0.32 | 0.242461 | 0.549318 | |
| COMPOUND_314_1275a6_8774543 | Rp | + | 314.1275 | 6.88 | | | (313.1356, 14190.64)(316.138, 2663.9)(317.1426, 513.73) | 32214.86 | 19391.83 | 26802.98 | 14060.95 | 23888.45 | 12288.55 | 19671.2 | 11418.05 | -0.61 | 0.008787 | 0.0189 | -0.36 | 0.179345 | 0.493746 | |
| COMPOUND_314_2261a8_915458 | Rp | + | 314.2261 | 8.92 | | | (629.4547, 857.71)(630.4579, 602.3)(631.4508, 186.23)(337.2155, 17411.31)(338.2184, 3947.59)(339.2234, 791.46)(651.4393, 577.22)(652.44, 388.7)(332.2638, 4014.0)(333.2645, 1096.0)(334.259, 172.33)(353.1822, 380.1)(354.1884, 156.58)(355.1895, 1937.51)(315.2327, 562747.7)(316.2365, 117971.78)(317.2404, 15980.05)(318.2434, 1835.48) | 154259.4 | 41216.14 | 151100.6 | 50570 | 757768.7 | 198892.7 | 938244.2 | 398024.4 | 1.28 | 2.1E-09 | 2.11E-08 | 0.45 | 0.039475 | 0.261543 | |
| COMPOUND_314_2452a10_503139 | Rp | - | 314.2452 | 10.50 | | | (663.4815, 218.56)(427.2337, 5110.19)(428.236, 1868.46)(429.2337, 722.78)(673.4655, 124.44)(313.2382, 13394.39)(314.2414, 2484.68)(315.2464, 418.9) | 24598.67 | 11000.64 | 31038.26 | 15467.17 | 37007.86 | 17941.87 | 34035.68 | 18697.16 | 0.91 | 0.002633 | 0.006377 | -0.81 | 0.022617 | 0.213113 | |
| COMPOUND_314_284a10_898516 | Rp | + | 314.2840 | 10.90 | | | (629.5921, 7323.49)(337.2723, 21309.5)(338.2754, 4222.19)(339.2804, 1876.24)(651.5379, 848.61)(332.3293, 236.64)(315.2905, 32958.99)(316.2936, 7158.85)(317.3009, 1521.44)(646.6002, 9952.63)(647.5947, 2263.22) | 122214.2 | 33451.57 | 119489.4 | 31599.03 | 66387.5 | 28017.7 | 68778.88 | 23244.23 | -1.36 | 1.29E-09 | 1.39E-08 | 0.10 | 0.657718 | 0.842058 | |
| COMPOUND_314_3306a10_467288 | Rp | + | 314.3306 | 10.47 | | | (629.6558, 659.25)(353.2908, 260.78)(354.2711, 2554.04)(315.3378, 60538.92)(316.341, 12285.39)(317.3439, 1459.72)(318.3443, 108.93)(646.7039, 1589.6)(647.6951, 713.65)(648.7, 333.65) | 165802.6 | 99547 | 124976.8 | 90994.29 | 178291.8 | 64020.64 | 206704.5 | 111457.6 | 0.38 | 0.158537 | 0.239133 | 0.67 | 0.03471 | 0.249266 | |
| COMPOUND_315_2416a7_087783 | Rp | + | 315.2416 | 7.09 | Decanoylcarnitine | 1 | 10eV: 316.247(100), 85.0283(25), 257.1774(17), 155.143(9) | (316.2493, 93208.73)(317.2524, 17671.54)(318.255, 2543.31)(319.2608, 309.43) | 200916.7 | 145342.6 | 202770.2 | 151500.7 | 158562.1 | 122047.3 | 227608.8 | 153862.1 | -0.49 | 0.093722 | 0.15406 | 0.62 | 0.073562 | 0.326462 |
| COMPOUND_315_2419a0_71815705 | Hilic | + | 315.2419 | 0.72 | | | (631.4768, 328.13)(338.2331, 8867.36)(339.2358, 1983.02)(653.4468, 774.06)(316.2485, 383654.78)(317.252, 67376.16)(318.2547, 8559.69)(319.2566, 846.77)(648.5366, 349.17) | 318828.9 | 235801.4 | 348235.8 | 291974 | 290275.4 | 230174.4 | 404946 | 270638.7 | -0.25 | 0.384707 | 0.487541 | 0.45 | 0.185058 | 0.499463 | |
| COMPOUND_316_1725a10_502323 | Rp | + | 316.1725 | 10.50 | | | (633.3567, 1201.33)(634.3658, 652.92)(635.3568, 833.6)(339.1553, 1581.94)(317.1799, 18871.35)(318.1833, 3934.98)(319.1846, 730.55)(159.0944, 1067.99)(159.5951, 182.39)(160.0929, 415.43) | 20283.52 | 10114.6 | 22995.97 | 10768.43 | 30264.77 | 12372.28 | 33321.31 | 17143.91 | 0.88 | 0.00045 | 0.00126 | 0.03 | 0.926733 | 0.966461 | |
| COMPOUND_316_2051a9_232506 | Rp | + | 316.2051 | 9.23 | | | (339.1946, 5200.35)(340.1974, 1619.56)(334.2391, 14574.35)(317.2126, 47269.07)(318.2172, 11170.89) | 45637.63 | 27872.2 | 43885.84 | 27438.97 | 19025 | #DIV/0! | 14740 | 3729.281 | -1.25 | 5.76E-09 | 4.99E-08 | 0.09 | 0.676559 | 0.851655 | |
| COMPOUND_316_2051a9_221732 | Rp | + | 316.2051 | 9.22 | | | (339.1946, 5200.35)(340.1974, 1619.56)(334.2391, 14574.35)(317.2126, 47269.07)(318.2172, 11170.89) | 59644.52 | 39240.49 | 47425.08 | 2953.84 | 34666 | 25810.81 | 11165 | #DIV/0! | -1.16 | 4.76E-08 | 3.29E-07 | 0.07 | 0.738115 | 0.888668 | |
| COMPOUND_316_206a8_972682 | Rp | + | 316.2060 | 8.97 | | | (633.4437, 942.48)(634.4296, 273.87)(339.1942, 9836.98)(340.1981, 2295.87)(355.1847, 2409.61)(334.2377, 4128.26)(317.2125, 34606.7)(318.2167, 8944.28) | 72047.11 | 52080.14 | 73456.09 | 46341.44 | 31701 | 8865.055 | 27965.33 | 11091.05 | -1.43 | 2.37E-12 | 7.99E-11 | -0.04 | 0.816899 | 0.92157 | |
| COMPOUND_316_2405a8_828208 | Rp | + | 316.2405 | 8.83 | | | (671.4434, 155.7)(339.2 | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--------------|--|--|----------|---------------|----------|---------------|----------|---------------|----|-------|-------|-------|-------------|-------|-------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_318_2184a_643887 | Rp | + | 318.2184 | 9.64 | | | | (637.4417, 1638.82)(341.2101, 42343.65)(342.2143, 9982.0)(659.4298, 601.46)(357.1782, 113955.8) 68159.27 132743.3 86071.51 76515 67458.18 107209.3 113793.2 | -0.79 | 0.000589 | 0.002581 | -0.43 | 0.119188 | 0.408824 | | | | | | | | |
| COMPOUND_318_2189a_642285 | Rp | - | 318.2189 | 9.64 | | | | (431.1952, 2007.82)(432.1937, 580.46)(433.1821, 1576.77)(353.1882, 4577.98)(354.1916, 210967.5) 172638.5 244000 148299.9 231199.3 134957.3 243616.6 125562.5 | -0.93 | 4.97E-05 | 0.000165 | -0.35 | 0.171369 | 0.487277 | | | | | | | | |
| COMPOUND_318_2194a10_001665 | Rp | - | 318.2194 | 10.00 | | | | (671.4004, 123.14)(431.2007, 780.79)(432.2009, 195.64)(433.2091, 870.3)(434.202, 76250.54) 37687.39 83846.68 38813.64 104168 14969.78 95396.18 47945.14 | -0.88 | 0.000238 | 0.000701 | -0.24 | 0.366411 | 0.669574 | | | | | | | | |
| COMPOUND_318_2201a_668321 | Rp | + | 318.2201 | 9.67 | | | | (637.4406, 1369.25)(341.2101, 22405.57)(342.2143, 5570.8)(659.4385, 395.21)(357.1763, 140225.5) 111377.4 148844 92656.6 142215 130553.7 196171.4 140941.3 | -0.43 | 0.069643 | 0.118456 | -0.49 | 0.08388 | 0.346484 | | | | | | | | |
| COMPOUND_318_2203a_186296 | Rp | + | 318.2203 | 9.19 | | | | (341.2104, 27237.8)(342.2145, 6123.58)(659.4285, 471.4)(660.4217, 200.55)(336.2539, 204934.3) 63108.61 196290.1 69447.45 131009 166092.3 28022.33 13429.53 | -1.19 | 2.46E-08 | 1.83E-07 | 0.08 | 0.703777 | 0.86442 | | | | | | | | |
| COMPOUND_318_2209a_3014145 | Rp | + | 318.2209 | 9.30 | | | | (675.399, 1683.0)(341.2097, 55581.7)(342.2135, 11938.37)(659.4314, 214461.2) 77424.57 195802.3 80030.68 69061.5 72805.84 45899.5 26232.95 | -1.44 | 1.36E-12 | 5.69E-11 | 0.12 | 0.540422 | 0.776663 | | | | | | | | |
| COMPOUND_318_2209a_026607 | Rp | + | 318.2209 | 9.03 | | | | (341.2119, 28827.84)(342.2154, 6893.08)(659.4048, 614.2)(336.2461, 114.85)(337.2499, 189069.6) 83873.16 211243.6 96409.51 213719.3 132954.3 241408.5 98379.58 | -0.92 | 6.53E-05 | 0.000211 | -0.33 | 0.203202 | 0.5149 | | | | | | | | |
| COMPOUND_318_221a10_008217 | Rp | + | 318.2210 | 10.01 | | | | (637.4457, 9691.73)(638.4527, 2220.06)(639.434, 1260.72)(675.3839, 947.52)(341.2096, 100779.4) 43671.74 103557.1 47268.22 102222.6 82649.71 113172.5 72808.29 | -0.85 | 0.000315 | 0.000903 | -0.28 | 0.285185 | 0.593016 | | | | | | | | |
| COMPOUND_319_1642a_1318603 | Rp | + | 319.1642 | 6.13 | | | | (320.1711, 13290.75)(321.1746, 2195.29)(322.1772, 373.99) 34131.14 9582.073 31880.51 7100.308 30702.25 9899.278 34840.41 8405.245 | -0.15 | 0.600729 | 0.604311 | -0.47 | 0.179336 | 0.493746 | | | | | | | | |
| COMPOUND_320_2330a_90998 | Rp | + | 320.2330 | 9.91 | | | | (343.2257, 62111.8)(344.2302, 12634.09)(359.193, 9019.89)(338.2694, 251206.8) 123097 274162.9 140785.8 144158.6 122170.6 139870.9 112420.9 | -1.16 | 2.9E-07 | 1.66E-06 | -0.18 | 0.449073 | 0.72351 | | | | | | | | |
| COMPOUND_320_2345a_9747945 | Rp | - | 320.2345 | 9.75 | | | | (305.613)(321.2438, 29304.41)(322.2471, 6857.75)(323.2562, 1291.55) 355.2037 1459.71(356.2073, 276.17)(357.2018, 537.47)(358.2054, 73.14)(359.1872, 74856.55) 38271.28 110228.6 79097.48 74878.45 53983.24 107659.3 113581 | -0.52 | 0.072619 | 0.122501 | 0.20 | 0.560211 | 0.783425 | | | | | | | | |
| COMPOUND_320_2346a_793816 | Rp | - | 320.2346 | 9.79 | | | | (355.2037, 1459.71)(356.2073, 276.17)(357.2018, 537.47)(358.2054, 73.14)(359.1872, 123800.9) 82532.52 160388.6 109891.4 97164 104949.5 148115.2 185789.9 | -0.68 | 0.017588 | 0.035176 | 0.09 | 0.79397 | 0.913187 | | | | | | | | |
| COMPOUND_320_2347a_8436165 | Rp | - | 320.2347 | 9.84 | | | | (323.64)(365.2296, 709.75)(366.232, 205.36)(367.2386, 86.82) 465993.2 485766.5 528021.7 555941.1 110860.8 85706.56 168316.5 252784.1 | -0.97 | 0.00061 | 0.001672 | 0.04 | 0.908511 | 0.958319 | | | | | | | | |
| COMPOUND_320_2356a_889301 | Rp | - | 320.2356 | 9.89 | | | | (355.2042, 20506.49)(356.2079, 4309.65)(357.2028, 6996.43)(358.2043, 1160962) 528494.8 1290259 550275.2 472631 602448.4 358447.5 576553.1 | -1.19 | 3.64E-06 | 1.59E-05 | -0.15 | 0.584204 | 0.797833 | | | | | | | | |
| COMPOUND_320_3097a11_230653 | Rp | + | 320.3097 | 11.23 | | | | (17005.97)(322.2411, 2015.56)(639.4609, 595.66)(640.4664, 266.17) 17005.97 322.2411 2015.56 639.4609 595.66 640.4664 266.17 | 1.02 | 0.000308 | 0.000886 | -0.42 | 0.190574 | 0.505078 | | | | | | | | |
| COMPOUND_321_1805a_089787 | HiIic | + | 321.1805 | 6.09 | | | | (679.5785, 444.05)(680.6003, 310.97)(663.6252, 2315.57)(321.3159, 21855.95)(322.3196, 5189.78)(323.3245, 785.74)(658.6329, 215.54) 6433679 20325(344.1697, 1605.7)(345.1738, 324.16)(322.1882, 166771.77)(323.1912, 63772.62 17154.48 127905.3 129623.6 | -1.25 | 2.6E-07 | 1.49E-06 | -0.17 | 0.519271 | 0.764125 | | | | | | | | |
| COMPOUND_322_2118a10_580965 | Rp | - | 322.2118 | 10.58 | | | | (29754.04)(324.1936, 3615.59) 679.4191 653.31(689.4226, 964.09)(690.4306, 3395.01)(321.2047, 7380.83)(322.2079, 1261.34)(323.2158, 532.29)(324.2171, 68.72) | -0.56 | 0.038214 | 0.060957 | 0.48 | 0.130191 | 0.425921 | | | | | | | | |
| COMPOUND_322_2502a10_194824 | Rp | - | 322.2502 | 10.19 | | | | (357.2204, 1158.0)(358.2232, 283.33)(359.2181, 666.51)(321.2431, 34531.41)(322.2462, 29936.29) 17652.89 30305.64 15934.26 40390.75 19502.42 63896 34255.2 | -0.85 | 0.000745 | 0.001998 | -0.04 | 0.891784 | 0.953702 | | | | | | | | |
| COMPOUND_322_2502a_863129 | Rp | - | 322.2502 | 9.86 | | | | (7896.34)(323.2502, 847.25) 357.2152 2082.01(358.2167, 444.25)(359.2218, 3341.35)(360.2256, 822.9)(321.2431, 36695.09)(322.2464, 7863.83)(323.2517, 1144.07)(324.2564, 110.02) | -0.29 | 0.206946 | 0.297771 | -0.55 | 0.046292 | 0.273966 | | | | | | | | |
| COMPOUND_323_156a10_47007 | Rp | + | 323.1560 | 10.47 | | | | (685.284, 951.61)(686.2829, 706.84)(324.1633, 31519.52)(325.1663, 6642.0)(326.164, 19313.54)(327.1676, 4011.06)(328.1591, 8270.65)(329.1618, 1808.81)(330.1573, 1413.66) | 1.44 | 1.38E-08 | 1.1E-07 | -0.05 | 0.836432 | 0.929001 | | | | | | | | |
| COMPOUND_323_2289a10_958062 | Rp | + | 323.2289 | 10.96 | | | | (685.4168, 549.78)(346.2157, 894.4)(347.2173, 309.15)(324.2356, 11116.46)(325.2392, 3132.78)(326.2354, 1238.77) #DIV/0! #DIV/0! #DIV/0! #DIV/0! #DIV/0! #DIV/0! #DIV/0! #DIV/0! | 1.27 | 1.16E-08 | 9.44E-08 | -0.01 | 0.981333 | 0.990571 | | | | | | | | |
| COMPOUND_324_1804a11_034648 | Rp | + | 324.1804 | 11.03 | | | | (687.3088, 6598.04)(688.3214, 3699.79)(325.1837, 4704.62)(326.1856, 1098.23)(327.1843, 1932.72)(328.1917, 525.72)(329.1807, 764.34)(666.3685, 27699.63) | 0.41 | 0.116712 | 0.186408 | 0.24 | 0.447894 | 0.721588 | | | | | | | | |
| COMPOUND_324_2094a_208561 | Rp | + | 324.2094 | 9.21 | | | | (687.3782, 244.51)(347.1941, 347.98)(348.1962, 118.13)(349.1825, 408.64)(342.2382, 411.79)(325.217, 17147.14)(326.2207, 4846.8)(327.2297, 1132.46)(328.2231, 145.65) | -0.83 | 0.000719 | 0.00193 | -0.15 | 0.590563 | 0.820507 | | | | | | | | |
| COMPOUND_324_2104a_4589205 | Rp | + | 324.2104 | 9.46 | | | | (649.4136, 269.73)(650.4136, 180.95)(347.1946, 280.97)(348.2012, 83.21)(349.2008, 256.97)(342.2388, 800.32)(325.2175, 40774.29)(326.2209, 10439.91)(327.2273, 2013.98)(328.2219, 241.52) | -1.41 | 1.29E-11 | 3.06E-10 | 0.04 | 0.84468 | 0.93246 | | | | | | | | |
| COMPOUND_324_2104a_915277 | Rp | + | 324.2104 | 8.92 | | | | (325.2177, 3267.07)(326.2213, 8466.97)(327.2301, 3217.83) 148577.9 61870.55 161241.4 94798.96 147801 91196.07 134594.6 72942.05 | -1.06 | 3.74E-06 | 1.63E-05 | -0.21 | 0.407532 | 0.693371 | | | | | | | | |
| COMPOUND_324_28610_215273 | Rp | + | 324.2860 | 10.22 | | | | (325.2927, 15887.78)(326.2965, 4974.06)(327.2875, 1472.99) 31621.87 13824.27 26886.97 13458.37 27887.91 9209.25 37028.63 16609.63 | -0.26 | 0.358757 | 0.461252 | 0.65 | 0.063626 | 0.307286 | | | | | | | | |
| COMPOUND_326_0017a_006655 | Rp | + | 326.0017 | 8.01 | | | | (348.9904, 676.91)(349.9948, 129.94)(350.9871, 761.24)(351.9908, 71.78)(352.9846, 312.78)(344.0253, 81.05)(327.0087, 12211.81)(328.0118, 1355.07)(329.0058, 12040.13)(330.0092, 1341.88)(331.0027, 3717.74)(332.0066, 307.88)(333.0006, 644.97)(334.0031, 71.49)(335.0117, 145.92) | 0.20 | 0.490013 | 0.590427 | 0.48 | 0.173343 | 0.487961 | | | | | | | | |
| COMPOUND_326_0718a_964087 | Rp | + | 326.0718 | 8.96 | | | | (349.0607, 1646.08)(350.0629, 390.83)(351.0591, 32.03)(365.0269, 241.86)(344.1045, 968.93)(345.1132, 211.78)(346.099, 97.09)(327.0791, 18939.0)(328.0827, 3550.51)(329.087, 716.89)(330.083, 84.66) | 0.06 | 0.820015 | 0.872719 | -0.77 | 0.019027 | 0.196411 | | | | | | | | |
| COMPOUND_326_1433a_950292 | Rp | + | 326.1433 | 9.95 | | | | (349.1478, 405.05)(327.1502, 14178.48)(328.1554, 4293.73)(329.1595, 665.32) 20307.58 5591.677 21080.57 6559.315 23606.07 5025.68 28087.34 9079.107 | 0.57 | 0.03511 | 0.06444 | 0.23 | 0.465398 | 0.732912 | | | | | | | | |
| COMPOUND_326_2259a_978272 | Rp | + | 326.2258 | 9.98 | | | | (349.214, 1801.47)(350.2165, 2982.29)(351.214, 368.07)(365.1974, 1372.94)(366.1879, 26288.33)(346.2652, 4564.88)(347.264, 452.79)(327.2331, 127521.34)(328.2361, 30347.03)(329.2379, 1633.28) | -1.07 | 9.55E-06 | 3.84E-05 | 0.11 | 0.685169 | 0.853695 | | | | | | | | |
| COMPOUND_326_2259a10_325211 | Rp | + | 326.2259 | 10.33 | | | | (349.2086, 293.22)(350.2199, 136.67)(351.1986, 190.99)(344.2557, 3913.48)(345.2561, 477.97)(327.2336, 125374.38)(328.2367, 30189.58)(329.2425, 5303.17) | -1.03 | 1.73E-05 | 6.58E-05 | -0.08 | 0.773566 | 0.904971 | | | | | | | | |
| COMPOUND_326_226a_9745729 | Rp | + | 326.2260 | 9.75 | | | | | 237342 100680.5 311199.4 24527.9 182747.5 104209.9 253081 246501.6 | -1.03 | 1.73E-05 | 6.58E-05 | -0.08 | 0.773566 | 0.904971 | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_326_2263a9_990872 | Rp | + | 326.2263 | 9.99 | | | | (349.2143, 13569.49)(350.2179, 2969.74)(351.2174, 491.84)(365.1934, 1665.19)(366.202, 520.17)(344.2594, 59759.25)(345.2622, 16007.0)(346.272, 3700.87)(327.2332, 405537.06)(328.2367, 94508.63)(329.2412, 13549.51)(330.2456, 1603.01) | 415769.2 | 314535.2 | 509316.6 | 367142.1 | 896416 | 141227.7 | 817109.5 | 575176.2 | -0.74 | 0.002279 | 0.005586 | -0.29 | 0.287665 | 0.59707 |
| COMPOUND_327_2412a0_71427613 | Hilic | + | 327.2412 | 0.71 | | | | (655.4752, 97.27)(350.2319, 326.88)(328.2488, 2975.33)(329.2519, 5955.84)(330.2603, 4216.41)(331.2504, 460.74) | 97634.98 | 42210.89 | 96538.54 | 37959.49 | 114120.8 | 61157.01 | 135699.8 | 64422.54 | 0.24 | 0.354925 | 0.45726 | 0.45 | 0.148187 | 0.456493 |
| COMPOUND_327_2421a7_0652266 | Rp | + | 327.2421 | 7.07 | AcAr 11:1 | 2 | 10 eV: 328.2476(100), 85.0306(15), 210.8617(6), 279.8413(6) | (328.2492, 19541.63)(329.2526, 4116.41)(330.2537, 573.12)(331.255, 65.35) | 65621.58 | 29304.94 | 59899.26 | 23227.18 | 66271.57 | 32886.75 | 81154.02 | 37511.16 | -0.01 | 0.978324 | 0.987833 | 0.60 | 0.059765 | 0.300425 |
| COMPOUND_328_1348a10_465241 | Rp | - | 328.1348 | 10.47 | | | | (691.2495, 561.73)(441.1186, 2976.86)(442.1177, 957.33)(443.1171, 3645.39)(444.1231, 2033.7)(445.1164, 1598.4)(446.112, 355.06)(447.1076, 81.01)(363.1016, 2131.89)(364.1045, 572.37)(365.1015, 2739.95)(366.1051, 373.89)(367.1001, 1384.6)(368.1014, 344.95)(369.1064, 413.21)(701.2158, 965.01)(327.1265, 30333.52)(328.1303, 9246.19)(329.1296, 3597.93)(655.2805, 2480.9)(656.2918, 1576.48)(657.2926, 329.57)(373.1314, 8465.15)(374.1337, 2094.52)(375.1323, 16149.03)(376.1355, 2970.5)(377.1379, 15988.25)(378.1423, 5275.61)(379.1272, 716.88)(769.2434, 783.63)(770.2477, 553.27)(771.2498, 795.91) | 297959.7 | 46773.45 | 31179.33 | 54817.62 | 339764.9 | 42947.39 | 373146.8 | 46768.53 | 0.76 | 0.004106 | 0.009434 | 0.26 | 0.387593 | 0.68827 |
| COMPOUND_328_2404a10_66481 | Rp | - | 328.2404 | 10.66 | FA 22:6 | 1 | 10 eV: 327.2328(100), 283.2418(60), 59.0143(15), 229.1964(9) | (691.4745, 2548.66)(692.4788, 1315.84)(363.2087, 12558.54)(364.2121, 2748.17)(365.2064, 4022.82)(366.2095, 942.92)(367.2105, 131.21)(701.4681, 272.38)(702.433, 935.34)(327.2324, 832931.1)(328.2363, 172401.89)(329.2395, 24450.01)(330.2421, 2039.81)(655.4584, 1491.13)(769.478, 1056.21) | 1035360 | 330775.8 | 1262496 | 717304.1 | 969328.8 | 495142.9 | 1224065 | 591882.4 | -0.36 | 0.167904 | 0.25141 | 0.36 | 0.23679 | 0.542473 |
| COMPOUND_328_2422a10_646862 | Rp | + | 328.2422 | 10.65 | FA 22:5 | 2 | 10eV: 329.2456(100), 60.0821(75), 121.0977(25) | (695.4662, 2325.41)(696.4553, 3265.55)(351.2301, 58683.23)(352.2337, 14193.41)(353.2341, 1511.49)(679.4629, 3855.41)(680.452, 1525.21)(681.4566, 6137.9)(367.1982, 16337.65)(346.2756, 463141.9)(347.279, 106350.41)(348.2824, 13741.96)(349.2854, 1593.59)(329.2488, 36936.77)(330.2519, 9544.97)(331.255, 1284.46)(332.2476, 133.95) | 326242.6 | 230901.5 | 380123.1 | 235298.3 | 526153.6 | 249128.3 | 617653.9 | 345329.4 | 0.71 | 0.00814 | 0.017643 | 0.20 | 0.514369 | 0.761025 |
| COMPOUND_328_2614a10_473845 | Rp | - | 328.2614 | 10.47 | | | | (691.4716, 350.14)(441.2597, 1152.68)(442.2603, 507.39)(363.2261, 465.88)(364.2315, 100.96)(365.236, 934.3)(366.235, 148.33)(367.2441, 396.11)(327.2539, 9935.59)(328.2573, 2284.48)(329.2612, 337.53) | 89981.4 | 150465.9 | 95667.89 | 14823.5 | 100830.5 | 14394.23 | 101101.3 | 16329.98 | 0.69 | 0.018559 | 0.03702 | -0.38 | 0.267283 | 0.575669 |
| COMPOUND_328_2627a10_30045 | Rp | + | 328.2627 | 10.30 | no mms | | | (567.5435, 143.4)(695.4789, 1355.59)(696.4984, 2467.11)(697.4932, 1256.85)(351.2516, 25671.52)(352.2551, 11685.91)(353.2591, 1945.36)(354.2543, 258.13)(367.2246, 8512.11)(368.2282, 1731.04)(369.2286, 932.92)(346.296, 27332.45)(347.2995, 6172.97)(348.294, 2653.93)(349.2954, 219.49)(329.2692, 441415.53)(330.2728, 87962.29)(331.2756, 12719.81) | 142961.2 | 72888.16 | 147656.4 | 106326.2 | 159563.2 | 206134.9 | 548195.4 | 641414.1 | -0.05 | 0.035488 | 0.065081 | 1.35 | 0.000119 | 0.015703 |
| COMPOUND_328_2631a10_299084 | Rp | + | 328.2631 | 10.30 | | | | (657.5294, 199.77)(695.4847, 1716.68)(696.4694, 164.2)(697.5009, 2008.78)(351.2521, 40346.01)(352.2529, 8791.2)(353.2614, 1782.57)(354.2533, 234.36)(367.2258, 6151.53)(368.2278, 1360.17)(369.2313, 913.28)(364.2061, 33972.29)(347.2995, 7664.61)(348.2978, 1962.19)(349.2926, 259.37)(329.2699, 291557.66)(330.273, 59831.69)(331.2755, 7933.39) | 136551.4 | 73253.58 | 138557.3 | 90022.42 | 208458.8 | 160248.4 | 400855.3 | 372605 | 0.02 | 0.931907 | 0.956543 | 0.81 | 0.019158 | 0.196411 |
| COMPOUND_328_2635a10_486962 | Rp | + | 328.2635 | 10.49 | | | | (695.4855, 2411.25)(351.2516, 10714.91)(352.2559, 2448.03)(353.2552, 463.82)(346.2961, 21192.6)(347.2992, 4720.22)(348.2982, 1221.53)(329.2694, 4264.09)(330.2699, 1049.13)(331.2725, 282.79) | 187894.7 | 43783.86 | 178371.6 | 35586.04 | 285327.3 | 25201.86 | 277779.4 | 59270.83 | 1.35 | 1.13E-07 | 6.95E-07 | 0.09 | 0.744228 | 0.889952 |
| COMPOUND_328_3464a10_468469 | Rp | + | 328.3464 | 10.47 | | | | (657.7128, 1463.77)(658.7027, 338.23)(367.3014, 1479.14)(329.3539, 40406.95)(330.357, 9323.95)(331.3601, 1231.26)(332.361, 125.79) | 169396.2 | 19122.38 | 175495.9 | 19943.85 | 218133.2 | 17186.9 | 217855.6 | 15811.99 | 1.64 | 2.34E-11 | 5.11E-10 | -0.25 | 0.292525 | 0.602481 |
| COMPOUND_329_1057a9_944288 | Rp | - | 329.1057 | 9.94 | | | | (442.0994, 698.37)(328.098, 547.66)(329.1014, 1784.05)(330.1001, 551.01)(331.1015, 65.99)(771.2005, 363.45)(772.1998, 600.22)(773.1878, 363.08) | 29526.89 | 6407.85 | 32338.09 | 8173.33 | 32058.07 | 8189.155 | 36068.77 | 9004.274 | 0.29 | 0.30234 | 0.40312 | 0.16 | 0.631881 | 0.822008 |
| COMPOUND_329_2423a8_626431 | Rp | + | 329.2423 | 8.63 | | | | (330.2474, 7596.75)(331.2506, 1851.05)(332.2542, 615.87) | 27528.89 | 10657.92 | 30633.55 | 99627.93 | 28273.57 | 11237.95 | 35646.09 | 13577.58 | 0.23 | 0.406732 | 0.510438 | 0.26 | 0.436658 | 0.714128 |
| COMPOUND_330_16a7_132373 | Rp | + | 330.1600 | 7.13 | | | | (661.3323, 152.7)(662.3285, 112.77)(348.193, 30657.21)(349.1968, 7401.41)(350.1998, 1215.11)(331.1675, 8818.06)(332.1724, 1819.4)(333.1708, 381.89) | 60077.43 | 30901.59 | 62603.84 | 32275 | 39326.67 | 9886.799 | 19711.4 | 5497.313 | -1.31 | 6.77E-11 | 1.1E-09 | -0.14 | 0.46221 | 0.730967 |
| COMPOUND_330_2188a7_4728866 | Rp | + | 330.2188 | 7.47 | | | | (661.4374, 713.74)(353.2125, 597.2)(354.2147, 272.03)(355.2059, 65.23)(683.4011, 275.03)(331.2279, 11083.08)(332.231, 2920.31)(333.2398, 664.09) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 29888.64 | 6628.875 | 25699.65 | 10255.29 | 1.66 | 5.3E-19 | 1.19E-15 | -0.33 | 0.030023 | 0.234557 |
| COMPOUND_330_2202a8_229498 | Rp | + | 330.2202 | 8.23 | | | | (353.2103, 1258.05)(354.2173, 385.19)(331.2274, 33445.22)(332.231, 7684.6) | 11743.17 | 1278.26 | 12716.67 | 3395.199 | 28777.93 | 7862.018 | 25373.21 | 17370.57 | 1.70 | 9.19E-17 | 6.9E-14 | -0.42 | 0.019479 | 0.198488 |
| COMPOUND_330_2552a10_778889 | Rp | - | 330.2552 | 10.78 | FA 22:5 | 1 | 10 eV: 329.2473(100), 100.9339(7), 257.2244(4) | (695.491, 544.96)(696.5149, 81.0)(442.2297, 3022.66)(444.2272, 1278.61)(445.2319, 629.53)(325.2246, 2718.29)(366.2733, 509.02)(367.2228, 912.77)(329.2485, 191991.06)(330.2516, 46224.21)(331.2548, 6339.31)(332.258, 725.28)(375.2562, 577.77)(773.489, 873.67)(774.4812, 578.83)(775.4951, 1008.24) | 93605.75 | 40031.59 | 105687.1 | 63170.14 | 89229.21 | 49082.63 | 112930.6 | 52363.54 | -0.24 | 0.374469 | 0.476411 | 0.44 | 0.155166 | 0.466404 |
| COMPOUND_330_257a10_784361 | Rp | + | 330.2570 | 10.78 | | | | (661.5415, 250.21)(699.4825, 367.98)(353.2455, 13882.07)(354.2469, 4133.94)(355.2482, 1150.9)(360.2121, 7062.76)(348.2909, 15267.15)(349.2946, 3681.82)(350.3031, 1094.61)(351.2934, 131.96)(331.2644, 20381.43)(332.2689, 5601.08)(333.2748, 1252.46) | 71523.94 | 33394.25 | 79120.04 | 46756.59 | 87486 | 35837.28 | 116633.7 | 76381.9 | 0.01 | 0.978302 | 0.987833 | 0.66 | 0.04635 | 0.273966 |
| COMPOUND_330_2784a10_585497 | Rp | + | 330.2784 | 10.59 | | | | (661.5951, 127.49)(662.5915, 529.72)(353.2672, 63002.06)(354.271, 120611.75)(369.2408, 14092.14)(370.2431, 3075.29)(371.2489, 2236.48)(331.2847, 870523.25)(332.2887, 175353.5)(333.2912, 23645.0) | 1685094 | 1222032 | 1695435 | 1228679 | 1738036 | 665609.7 | 2298982 | 1178028 | 0.04 | 0.881504 | 0.921609 | 0.46 | 0.183448 | 0.497141 |
| COMPOUND_330_2787a10_601486 | Rp | + | 330.2787 | 10.60 | | | | (353.2672, 63002.06)(354.271, 120611.75)(355.2768, 17909.29)(356.2874, 2378.3)(683.5189, 911.13)(369.2403, 10165.97)(370.2434, 2382.29)(371.2463, 1371.61)(372.2476, 147.97)(348.3122, 101686.39)(349.3149, 21985.63)(350.3173, 3769.61)(351.3206, 512.68)(331.2851, 810365.75)(332.2891, 163279.95)(333.2917, 22492.22)(334.2942, 2342.13) | 2530304 | 983201.3 | 2468270 | 888107.2 | 1951994 | 742822.9 | 2847866 | 1075323 | -0.61 | 0.037845 | 0.06901 | 0.95 | 0.007607 | 0.138042 |
| COMPOUND_331_2365a6_1036196 | Rp | + | 331.2365 | 6.10 | | | | (332.2444, 13004.21)(333.2479, 2207.45)(334.2504, 402.67) | 21518.2 | 9365.92 | 22490.88 | 10632.78 | 17439.78 | 8475.423 | 17992.95 | 6986.355 | -0.52 | 0.049279 | 0.086362 | 0.22 | 0.47484 | 0.737985 |
| COMPOUND_331_2365a1_0914434 | Hilic | + | 331.2365 | 1.09 | | | | (332.2437, 9466.25)(333.2473, 2069.95)(334.2517, 530.23)(335.2504, 48.63) | 33717.02 | 20628.76 | 36886.04 | 24937.56 | 34800 | 25122.23 | 37553.25 | 20526.73 | -0.16 | 0.571673 | 0.668263 | 0.26 | 0.42952 | 0.707514 |
| COMPOUND_332_1376a6_4594316 | Rp | + | 332.1376 | 6.46 | | | | (333.1457, 11674.3)(334.1492, 2376.75)(335.1537, 428.44) | 15618.32 | 5073.064 | 14632.13 | 3374.047 | 24245.73 | 11521.35 | 18655.52 | 9951.862 | 0.90 | 5.76E-05 | 0.000189 | -0.31 | 0.209792 | 0.519177 |
| COMPOUND_332_138a6_158398 | Rp | + | 332.1380 | 6.16 | | | | (333.145, 15841.48)(334.1494, 3020.1)(335.1502, 429.94) | 21407.62 | 10657.55 | 18907.94 | 7468.096 | 29219 | 15616.04 | 22564.43 | 13873.25 | 0.74 | 0.005922 | 0.013179 | -0.26 | 0.394674 | 0.690408 |
| COMPOUND_332_138a45_941389 | Rp | + | 332.1384 | 5.94 | | | | (665.2964, 2364.32)(666.2925, 1455.15)(711.019, 7817.71)(372.1041, 3259.63)(373.1012, 1605.21)(333.1522, 30621.4)(334.1551, 6971.49)(335.1531, 22609.42)(336.1563, 5107.11)(337.149, 8233.98)(338.1601, 2838.45)(339.1506, 1355.62)(682.3447, 1568.71) | 18454.21 | 7440.537 | 16846.88 | 6139.437 | 29580.15 | 16824.95 | 22513.61 | 13611.73 | 0.93 | 4.84E-05 | 0.000161 | -0.11 | 0.655598 | 0.841269 |
| COMPOUND_332_1449a10_500881 | Rp | + | 332.1449 | 10.50 | | | | (329.2485, 191991.06)(330.2516, 46224.21)(331.2548, 6339.31)(332.258, 725.28)(375.2562, 577.77)(773. | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|---------------|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_334_1599a10_715213 | Rp | + | 334.1599 | 10.72 | | | | (669.3059, 536.85)(670.2815, 833.39)(707.3075, 2154.45)(691.295, 1550.05)(692.2785, 970.66)(373.1428, 619.79)(335.1683, 98335.97)(336.1709, 21641.61)(337.1688, 69396.33)(338.1711, 15596.69)(339.1649, 26384.77)(340.1673, 6700.04)(341.1638, 3828.16) (352.2495, 3526.84)(353.2563, 1274.01)(354.2609, 296.35)(373.3813, 1174.43)(335.2102, 22605.87)(336.2237, 4522.14)(337.2314, 1403.33)(686.4655, 746.07)(687.4652, 116.41)(688.4785, 601.7) (369.1824, 2926.96)(370.1853, 859.81)(371.188, 1690.91)(333.2069, 6851.78)(334.2101, 14278.03)(379.2111, 657.19)(380.215, 119.41) (369.1745, 5061.22)(370.1778, 1158.14)(333.2069, 16869.01)(334.21, 3390.53)(335.2189, 1056.97)(336.2222, 120.11)(379.2119, 2761.8)(380.2155, 698.49)(381.1943, 840.62) | 260892.3 | 102437.3 | 269029.2 | 99240.7 | 380858.9 | 129394.9 | 437567.7 | 155420.6 | 0.90 | 0.000716 | 0.001923 | 0.22 | 0.468524 | 0.734042 |
| COMPOUND_334_2125a9_609749 | Rp | + | 334.2125 | 9.61 | | | | (369.1745, 5061.22)(370.1778, 1158.14)(333.2069, 16869.01)(334.21, 3390.53)(335.2189, 1056.97)(336.2222, 120.11)(379.2119, 2761.8)(380.2155, 698.49)(381.1943, 840.62) | 41025.13 | 19104.43 | 43302.8 | 21770.31 | 55550.67 | 22724.75 | 53176.13 | 14062.76 | -0.63 | 0.005665 | 0.012681 | -0.51 | 0.056372 | 0.295234 |
| COMPOUND_334_2137a8_671635 | Rp | - | 334.2137 | 8.67 | | | | (369.1745, 5061.22)(370.1778, 1158.14)(333.2069, 16869.01)(334.21, 3390.53)(335.2189, 1056.97)(336.2222, 120.11)(379.2119, 2761.8)(380.2155, 698.49)(381.1943, 840.62) | 72759.72 | 59551.8 | 83076.27 | 48904.59 | 143484.3 | 6358.146 | 112613.9 | 46800.27 | -0.61 | 0.01136 | 0.023687 | -0.30 | 0.290319 | 0.600365 |
| COMPOUND_334_2139a8_443624 | Rp | - | 334.2139 | 8.44 | | | | (369.1745, 5061.22)(370.1778, 1158.14)(333.2069, 16869.01)(334.21, 3390.53)(335.2189, 1056.97)(336.2222, 120.11)(379.2119, 2761.8)(380.2155, 698.49)(381.1943, 840.62) | 72070.27 | 49660.84 | 83000.1 | 39455.76 | 63647 | 36480.39 | 101577 | 54722.82 | -0.95 | 5.2E-05 | 0.000172 | -0.20 | 0.440247 | 0.715839 |
| COMPOUND_334_2139a8_490905 | Rp | - | 334.2139 | 8.49 | | | | (369.1747, 2413.52)(370.1787, 538.62)(333.2069, 30792.12)(334.2102, 7016.31)(335.2169, 1727.85)(379.2116, 2431.32)(380.215, 389.84)(381.2214, 340.46)(667.4421, 66.85) (357.202, 18915.63)(358.2052, 3544.04)(691.3867, 286.18)(692.3939, 210.29)(373.1734, 1736.1)(374.1773, 438.52)(375.1699, 767.38)(385.2227, 23491.77)(336.227, 5252.62) | 41741.59 | 23131.61 | 52590.94 | 30746.35 | 44812.5 | 7265.522 | 54546.43 | 12635.53 | -0.79 | 0.000709 | 0.001908 | -0.10 | 0.717702 | 0.876415 |
| COMPOUND_334_2144a9_279192 | Rp | + | 334.2144 | 9.28 | | | | (357.202, 18915.63)(358.2052, 3544.04)(691.3867, 286.18)(692.3939, 210.29)(373.1734, 1736.1)(374.1773, 438.52)(375.1699, 767.38)(385.2227, 23491.77)(336.227, 5252.62) | 42305.08 | 20214.02 | 37107.43 | 19958.35 | 38909 | 4587.709 | 22874 | 6012.625 | -1.35 | 1.84E-10 | 2.6E-09 | 0.15 | 0.46706 | 0.733998 |
| COMPOUND_334_2157a8_971936 | Rp | + | 334.2157 | 8.97 | | | | (669.4412, 477.85)(357.2052, 10837.61)(358.2096, 2627.43)(352.2471, 7850.87)(353.2462, 2913.64)(373.1971, 3274.58)(335.2227, 18726.45)(336.228, 4358.08)(337.2257, 4596.27)(338.2209, 629.47) (671.4119, 2950.41)(672.4219, 2185.94)(353.2563, 6680.47)(354.2618, 3069.42)(336.2221, 15113.39)(337.2266, 4131.02)(338.2303, 766.63) (671.6248, 5452.98)(672.6448, 15925.84)(673.6294, 11347.73)(709.5785, 519.4)(358.3086, 14336.21)(359.3118, 4367.66)(360.3174, 1516.24)(361.3193, 142.69)(693.6559, 3543.42)(374.2852, 4810.98)(375.2828, 1710.17)(376.2817, 707.25)(336.3268, 490341.75)(337.3304, 111133.24)(338.3354, 15958.64)(688.6461, 6039.47) (336.3274, 17208.64)(337.3311, 4032.77)(338.3389, 1463.28)(339.3288, 141.73) (695.3668, 7060.56)(696.3648, 4769.61)(337.1833, 6108.06)(338.1861, 14960.71)(339.1884, 22536.58)(340.1863, 4725.32)(341.1797, 8536.91) (371.1976, 2251.26)(372.1999, 457.98)(373.2008, 2264.0)(374.2036, 490.41)(717.4341, 104.6)(335.2226, 57958.09)(336.2258, 12289.72)(337.2337, 2703.87)(338.2391, 353.79)(381.2277, 83.88) (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.2306, 158.3)(383.2385, 52.22) | 163023 | 47795 | 160469.8 | 63890.07 | 86432.33 | 22945.8 | 125610.9 | 84752.12 | -1.40 | 2.36E-10 | 3.2E-09 | 0.06 | 0.800923 | 0.916038 |
| COMPOUND_335_2143a10_856005 | Rp | + | 335.2143 | 10.86 | | | | (671.4119, 2950.41)(672.4219, 2185.94)(353.2563, 6680.47)(354.2618, 3069.42)(336.2221, 15113.39)(337.2266, 4131.02)(338.2303, 766.63) (671.6248, 5452.98)(672.6448, 15925.84)(673.6294, 11347.73)(709.5785, 519.4)(358.3086, 14336.21)(359.3118, 4367.66)(360.3174, 1516.24)(361.3193, 142.69)(693.6559, 3543.42)(374.2852, 4810.98)(375.2828, 1710.17)(376.2817, 707.25)(336.3268, 490341.75)(337.3304, 111133.24)(338.3354, 15958.64)(688.6461, 6039.47) (336.3274, 17208.64)(337.3311, 4032.77)(338.3389, 1463.28)(339.3288, 141.73) (695.3668, 7060.56)(696.3648, 4769.61)(337.1833, 6108.06)(338.1861, 14960.71)(339.1884, 22536.58)(340.1863, 4725.32)(341.1797, 8536.91) (371.1976, 2251.26)(372.1999, 457.98)(373.2008, 2264.0)(374.2036, 490.41)(717.4341, 104.6)(335.2226, 57958.09)(336.2258, 12289.72)(337.2337, 2703.87)(338.2391, 353.79)(381.2277, 83.88) (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.2306, 158.3)(383.2385, 52.22) | 41678.4 | 11214.76 | 42780.55 | 10259.89 | 71188.77 | 19493.12 | 77867.85 | 19881.21 | 1.10 | 1.4E-05 | 5.43E-05 | 0.08 | 0.78454 | 0.909997 |
| COMPOUND_335_3194a11_008178 | Rp | + | 335.3194 | 11.01 | | | | (671.6248, 5452.98)(672.6448, 15925.84)(673.6294, 11347.73)(709.5785, 519.4)(358.3086, 14336.21)(359.3118, 4367.66)(360.3174, 1516.24)(361.3193, 142.69)(693.6559, 3543.42)(374.2852, 4810.98)(375.2828, 1710.17)(376.2817, 707.25)(336.3268, 490341.75)(337.3304, 111133.24)(338.3354, 15958.64)(688.6461, 6039.47) (336.3274, 17208.64)(337.3311, 4032.77)(338.3389, 1463.28)(339.3288, 141.73) (695.3668, 7060.56)(696.3648, 4769.61)(337.1833, 6108.06)(338.1861, 14960.71)(339.1884, 22536.58)(340.1863, 4725.32)(341.1797, 8536.91) (371.1976, 2251.26)(372.1999, 457.98)(373.2008, 2264.0)(374.2036, 490.41)(717.4341, 104.6)(335.2226, 57958.09)(336.2258, 12289.72)(337.2337, 2703.87)(338.2391, 353.79)(381.2277, 83.88) (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.2306, 158.3)(383.2385, 52.22) | 343413 | 221952 | 548252.4 | 458553.8 | 635781.3 | 588465 | 510976.3 | 368020.4 | 0.74 | 0.010977 | 0.022973 | -0.76 | 0.026674 | 0.225828 |
| COMPOUND_335_3195a10_225195 | Rp | + | 335.3195 | 10.23 | | | | (336.3274, 17208.64)(337.3311, 4032.77)(338.3389, 1463.28)(339.3288, 141.73) (695.3668, 7060.56)(696.3648, 4769.61)(337.1833, 6108.06)(338.1861, 14960.71)(339.1884, 22536.58)(340.1863, 4725.32)(341.1797, 8536.91) (371.1976, 2251.26)(372.1999, 457.98)(373.2008, 2264.0)(374.2036, 490.41)(717.4341, 104.6)(335.2226, 57958.09)(336.2258, 12289.72)(337.2337, 2703.87)(338.2391, 353.79)(381.2277, 83.88) (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.2306, 158.3)(383.2385, 52.22) | 35166.18 | 20038.69 | 53557.87 | 39788.03 | 67036.29 | 62717.61 | 58181.72 | 37575.59 | 0.71 | 0.016359 | 0.033041 | -0.67 | 0.054984 | 0.292726 |
| COMPOUND_336_176a10_932189 | Rp | + | 336.1760 | 10.93 | | | | (695.3668, 7060.56)(696.3648, 4769.61)(337.1833, 6108.06)(338.1861, 14960.71)(339.1884, 22536.58)(340.1863, 4725.32)(341.1797, 8536.91) (371.1976, 2251.26)(372.1999, 457.98)(373.2008, 2264.0)(374.2036, 490.41)(717.4341, 104.6)(335.2226, 57958.09)(336.2258, 12289.72)(337.2337, 2703.87)(338.2391, 353.79)(381.2277, 83.88) (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.2306, 158.3)(383.2385, 52.22) | 124725.5 | 54128.38 | 124791.4 | 54792 | 222960 | 66472.41 | 171833.6 | 86319.62 | 1.05 | 4E-06 | 1.73E-05 | 0.47 | 0.061477 | 0.303349 |
| COMPOUND_336_2294a8_728184 | Rp | - | 336.2294 | 8.73 | | | | (371.1976, 2251.26)(372.1999, 457.98)(373.2008, 2264.0)(374.2036, 490.41)(717.4341, 104.6)(335.2226, 57958.09)(336.2258, 12289.72)(337.2337, 2703.87)(338.2391, 353.79)(381.2277, 83.88) (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.2306, 158.3)(383.2385, 52.22) | 96914.77 | 44889.42 | 118241.8 | 64343.28 | 143243.8 | 69267.33 | 185759.5 | 89458.2 | -0.80 | 0.00092 | 0.002423 | -0.33 | 0.232654 | 0.538289 |
| COMPOUND_336_2297a9_005535 | Rp | - | 336.2297 | 9.01 | | | | (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.2306, 158.3)(383.2385, 52.22) | 432433.2 | 220768.8 | 465870.6 | 282720.3 | 525572.3 | 323963.6 | 480645.8 | 294649.6 | -0.96 | 3.3E-05 | 0.000117 | -0.29 | 0.261321 | 0.572854 |
| COMPOUND_336_2297a8_870703 | Rp | - | 336.2297 | 8.87 | | | | (371.1976, 2251.26)(372.1999, 457.98)(373.2008, 2264.0)(374.2036, 490.41)(717.4341, 104.6)(335.2226, 57958.09)(336.2258, 12289.72)(337.2337, 2703.87)(338.2391, 353.79)(381.2277, 83.88) (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.2306, 158.3)(383.2385, 52.22) | 179076.3 | 83442.79 | 213900.4 | 103063.9 | 189643.5 | 93171.89 | 220316.4 | 114552.1 | -0.96 | 3.51E-05 | 0.000122 | -0.35 | 0.18055 | 0.493854 |
| COMPOUND_336_2297a8_816782 | Rp | - | 336.2297 | 8.82 | | | | (371.1976, 2251.26)(372.1999, 457.98)(373.2008, 2264.0)(374.2036, 490.41)(717.4341, 104.6)(335.2226, 57958.09)(336.2258, 12289.72)(337.2337, 2703.87)(338.2391, 353.79)(381.2277, 83.88) (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.2306, 158.3)(383.2385, 52.22) | 143594.5 | 71996 | 172334.9 | 85955.66 | 197020 | 99437.92 | 221289.5 | 114717.2 | -0.87 | 0.000245 | 0.000717 | -0.32 | 0.233159 | 0.538538 |
| COMPOUND_336_2298a9_017025 | Rp | - | 336.2298 | 9.02 | | | | (371.1976, 2251.26)(372.1999, 457.98)(373.2008, 2264.0)(374.2036, 490.41)(717.4341, 104.6)(335.2226, 57958.09)(336.2258, 12289.72)(337.2337, 2703.87)(338.2391, 353.79)(381.2277, 83.88) (449.2019, 517.03)(450.2021, 229.27)(371.1982, 9025.99)(372.2024, 1974.21)(373.1993, 5069.26)(374.2029, 1214.13)(335.2226, 210764.53)(336.2258, 44206.97)(337.2309, 7877.56)(338.2353, 878.82)(381.2274, 868.23)(382.23 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|---|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_340_3338a12_078226 | Rp | - | 340.3338 | 12.08 | | | | (339.262, 14134.37)(340.3295, 3278.42)(341.3333, 326.49)(385.3298, 136.48) | 19943.98 | 8747.392 | 22982.83 | 8224.438 | 19220 | 6771.418 | 18391.67 | 8229.71 | -0.06 | 0.841427 | 0.888787 | -0.61 | 0.071697 | 0.325554 | |
| COMPOUND_341_149a1_812361 | Rp | - | 341.1490 | 1.81 | | | (342.1571, 30752.99)(343.1601, 6500.67)(344.1621, 800.51)(171.5827, 757.26)(172.0835, 158.84) | 32585.12 | 40762.34 | 34160.29 | 29535.79 | 66098.91 | 73681.67 | 51902.73 | 65968.2 | | | 0.36 | 0.183634 | 0.271353 | -0.58 | 0.074229 | 0.327774 |
| COMPOUND_341_149a5_4751654 | Hilic | + | 341.1494 | 5.48 | His-Trp | 3 | 20 eV: 110.0712 (100), 324.1403 (10), 156.0774 (8), 342.1556 (5) | (364.1386, 3103.88)(365.1416, 742.7)(366.1413, 103.54)(342.1563, 40614.25)(343.1595, 790.64)(344.1622, 1142.25) | 29062.77 | 37588.9 | 34836.42 | 31567.78 | 58872.17 | 60872.08 | 34668.45 | 46245.77 | 0.28 | 0.334384 | 0.435531 | -0.77 | 0.027308 | 0.226687 | |
| COMPOUND_341_257a7_6879916 | Rp | + | 341.2574 | 7.69 | | | (364.2469, 50.93)(365.237, 30.73)(342.2649, 11355.71)(343.268, 2415.62)(344.2676, 436.73) | 23166.63 | 10536.65 | 21764.11 | 7419.721 | 20242.58 | 9302.552 | 23101.44 | 8504.696 | -0.47 | 0.1164 | 0.186174 | 0.44 | 0.216632 | 0.524744 | | |
| COMPOUND_341_258a7_5795503 | Rp | + | 341.2580 | 7.58 | ACar 12:1 | 2 | 20 eV: 85.0297(100), 342.2704(30), 283.1982(10) | (364.2491, 716.93)(365.2479, 286.26)(342.2649, 6259.26)(343.2699, 1259.93)(344.2694, 226.11)(345.2661, 30.16) | 49436.73 | 33717.39 | 44883.41 | 26675.92 | 38490.64 | 34858.66 | 50579 | 31721.04 | -0.48 | 0.096858 | 0.158406 | 0.67 | 0.051045 | 0.283822 | |
| COMPOUND_342_1496a10_620397 | Rp | - | 342.1496 | 10.62 | | | (455.1372, 6203.33)(377.1293, 693.67)(378.1278, 169.21)(379.1161, 569.86)(729.2758, 982.55)(841.1421, 3543.86)(342.145, 1252.77)(343.1476, 885.3)(344.1505, 46.19)(683.3217, 2275.32)(87.1485, 1256.14)(388.1551, 210.04)(389.1462, 3649.41)(390.148, 813.59)(391.1299, 2667.41)(392.1255, 709.58)(393.117, 931.23)(797.2481, 380.15)(798.2358, 585.34) | 37071.04 | 7819.579 | 38807.18 | 7705.813 | 43949.14 | 10426.4 | 49441.23 | 8227.825 | 0.77 | 0.003088 | 0.007337 | 0.32 | 0.28643 | 0.595057 | | |
| COMPOUND_342_1883a10_69024 | Rp | + | 342.1883 | 10.69 | | | (685.3863, 1473.14)(686.3979, 909.53)(687.3878, 1005.42)(707.3884, 1153.96)(708.3816, 662.9)(343.1958, 8954.92)(344.1998, 1856.52)(345.2041, 345.07) | 15457.98 | 3185.944 | 16700.34 | 5123.762 | 21557 | 7080.465 | 19865.76 | 7031.958 | 1.11 | 0.09E-05 | 0.000254 | -0.71 | 0.025042 | 0.219303 | | |
| COMPOUND_342_2187a9_899821 | Rp | + | 342.2187 | 9.90 | | | (685.4604, 343.05)(686.4627, 374.85)(365.2104, 4789.96)(366.2156, 1384.62)(381.1582, 1674.67)(382.159, 803.79)(383.1654, 615.88)(360.2544, 10280.12)(361.2571, 2662.79)(362.2659, 1853.28)(343.2254, 10182.21)(344.2289, 20968.43)(345.2385, 7098.06)(702.4769, 1427.96)(703.4782, 1163.29) | 205905.1 | 79197.9 | 215808.7 | 81159.25 | 92506.44 | 102630.4 | 78124.32 | 97255.67 | -1.19 | 2.79E-06 | 1.25E-05 | -0.11 | 0.700812 | 0.863364 | | |
| COMPOUND_342_2201a9_458428 | Rp | + | 342.2201 | 9.46 | | | (365.2097, 15821.84)(366.2135, 4183.66)(367.2152, 952.56)(368.2077, 102.38)(381.1932, 2654.83)(382.1955, 911.93)(383.1798, 263.46)(360.2542, 29026.35)(361.2587, 7504.62)(362.2638, 2193.44)(363.262, 244.93)(343.228, 10023.11)(344.2313, 2493.59)(345.2383, 763.16) | 162033.8 | 75768.64 | 151050.2 | 71381.06 | 78356.5 | 77199.8 | 81066.88 | 46953.03 | -1.47 | 5.46E-12 | 1.53E-10 | 0.33 | 0.538628 | 0.776408 | | |
| COMPOUND_342_2202a8_997395 | Rp | + | 342.2203 | 9.00 | | | (365.2093, 1304.36)(366.2162, 423.83)(343.2278, 34154.21)(344.2313, 8135.04)(345.2406, 2436.75) | 86697.53 | 35569.32 | 92583.64 | 51233.87 | 105857.8 | 70933.08 | 155555.1 | 86684.59 | -0.69 | 0.005508 | 0.012342 | -0.14 | 0.616421 | 0.816971 | | |
| COMPOUND_342_2692a10_860364 | Rp | + | 342.2692 | 10.86 | | | (685.5502, 623.55)(773.5022, 4119.33)(343.2728, 14544.52)(344.2745, 5347.65)(345.2709, 2866.83)(702.55, 323.53)(703.5644, 499.22) | 30269.63 | 10109.22 | 33270.57 | 10615.18 | 56515.8 | 18718.22 | 51479.16 | 19436.82 | 0.20 | 0.434694 | 0.539654 | -0.08 | 0.785698 | 0.909997 | | |
| COMPOUND_342_2896a8_817643 | Rp | + | 342.2896 | 8.82 | | | (365.2853, 672.53)(366.2954, 71.59)(367.271, 119.15)(707.5562, 166.33)(343.297, 35503.36)(344.2999, 7860.94)(345.3017, 1092.98) | 32952.38 | 21093.28 | 32838.35 | 13404.2 | 48645.79 | 39748.81 | 29724.86 | 15678.94 | 0.48 | 0.112636 | 0.180924 | -0.76 | 0.039191 | 0.261543 | | |
| COMPOUND_343_273a8_000297 | Rp | + | 343.2730 | 8.00 | ACar 12:0 | 2 | 10 eV: 344.2795(100), 60.0806(17), 144.0984(7) | (366.2624, 734.76)(367.2634, 333.61)(344.2807, 38715.42)(345.2844, 8059.8)(346.2859, 1185.47)(347.2907, 116.87) | 73683.94 | 43034.71 | 75345.33 | 40460.47 | 56941.29 | 42700.5 | 76654.89 | 40617.87 | -0.64 | 0.029771 | 0.055984 | 0.65 | 0.063073 | 0.307286 | |
| COMPOUND_344_2109a8_284668 | Rp | + | 344.2109 | 8.28 | | | (345.2184, 5841.06)(346.2209, 1382.44)(347.2222, 315.51)(348.2173, 35.48) | 44821.49 | 31781.63 | 44137.32 | 27629.44 | 36996.42 | 37541.33 | 24311.11 | 13766.75 | -0.02 | 0.927006 | 0.95325 | -0.81 | 0.012231 | 0.168989 | | |
| COMPOUND_344_2345a9_795691 | Rp | - | 344.2345 | 9.80 | | | (379.203, 1271.55)(380.2077, 288.08)(381.2033, 681.88)(382.203, 153.78)(343.2274, 10338.44)(344.2309, 2525.46)(345.2353, 489.43)(346.2432, 64.79)(687.4548, 225.04)(889.2296, 1518.25)(390.2316, 312.81)(391.2382, 40.37) | 162689.2 | 98979.54 | 236956.2 | 167470.2 | 145670.2 | 165381.1 | 123109.2 | 242907.2 | -0.97 | 0.000127 | 0.000385 | -0.15 | 0.589394 | 0.801519 | | |
| COMPOUND_344_2347a9_777399 | Rp | - | 344.2347 | 9.78 | | | (379.2036, 3954.09)(380.2058, 1125.53)(381.2039, 1492.83)(382.2059, 334.29)(343.2277, 116116.12)(344.231, 28715.71)(345.238, 4803.11)(389.228, 530.11)(390.2341, 97.32)(391.2399, 42.26) | 194868 | 81880.33 | 252006.4 | 155541.6 | 244786.6 | 214352.2 | 138822.9 | 244709.8 | -0.95 | 0.000258 | 0.000751 | -0.12 | 6.70713 | 0.847138 | | |
| COMPOUND_344_2351a9_914334 | Rp | + | 344.2351 | 9.91 | | | (367.2251, 20507.59)(368.2285, 5034.69)(383.1952, 2591.15)(384.1965, 835.15)(385.2032, 241.53)(386.2099, 2639.17)(363.2699, 977.03)(364.2814, 525.57)(345.2429, 16397.88)(346.2506, 3541.79)(347.2567, 1025.26) | 67403.73 | 30937.38 | 89514.74 | 60890.45 | 123980.3 | 34100.35 | 130536.3 | 68404.74 | -0.77 | 0.001201 | 0.003073 | -0.40 | 0.141226 | 0.447724 | | |
| COMPOUND_344_2352a10_011725 | Rp | - | 344.2352 | 10.01 | | | (457.2119, 2300.25)(344.2063, 1053.61)(379.204, 15299.33)(380.2077, 3618.16)(381.2021, 471.37)(382.2033, 1241.77)(383.2087, 384.85)(343.2273, 527995.44)(344.231, 120745.44)(345.2344, 16295.12)(346.2389, 1804.29)(687.464, 204.02) | 549147.3 | 264526.7 | 633578.7 | 329961.4 | 747185.5 | 325238 | 921542 | 433222.1 | -0.85 | 0.000493 | 0.001375 | -0.27 | 0.32981 | 0.635357 | | |
| COMPOUND_345_1746a10_4704075 | Rp | + | 345.1746 | 10.47 | | | (729.303, 492.63)(730.2649, 881.48)(368.1561, 260.58)(384.1246, 533.63)(346.1811, 31368.7)(347.1839, 6236.94)(348.1876, 1095.94) | 63276.46 | 10532.18 | 60273.7 | 10679 | 95226.07 | 14845.85 | 96485.61 | 13057.11 | 1.44 | 6.77E-10 | 7.94E-09 | 0.19 | 0.427114 | 0.706212 | | |
| COMPOUND_345_2679a9_974165 | Rp | + | 345.2679 | 9.97 | | | (729.5099, 667.57)(730.5157, 420.62)(346.275, 25480.29)(347.278, 6364.51)(348.2811, 1119.46) | 27790.67 | 15538.99 | 27192.3 | 18483.72 | 36485.67 | 8385.786 | 28278.17 | 14979.03 | -0.75 | 0.000766 | 0.002049 | 0.28 | 0.266821 | 0.575669 | | |
| COMPOUND_345_2889a10_488772 | Rp | + | 345.2889 | 10.49 | | | (713.5804, 236.22)(346.2958, 16734.89)(347.2986, 3964.32)(348.2946, 1095.66) | 100875.5 | 20854.37 | 95284.16 | 21348.99 | 137031.1 | 13342.03 | 138879.2 | 21362.83 | 1.18 | 1.77E-06 | 8.36E-06 | 0.32 | 0.226076 | 0.533671 | | |
| COMPOUND_346_2119a10_500157 | Rp | - | 346.2119 | 10.50 | | | (737.4525, 813.82)(345.2041, 10911.34)(346.207, 2362.57)(347.209, 365.14)(805.4421, 711.44) | 17988.13 | 6810.057 | 21637.5 | 9904.18 | 14984.7 | 5649.86 | 18072.94 | 7701.39 | 0.12 | 0.631808 | 0.721883 | -0.23 | 0.43427 | 0.712127 | | |
| COMPOUND_346_215a7_3962293 | Rp | + | 346.2150 | 7.40 | | | (693.4428, 223.53)(369.2038, 287.19)(370.2023, 135.03)(364.2499, 490.5)(365.2506, 219.01)(347.223, 13075.08)(348.2253, 3426.35)(349.2303, 529.71) | 15524.35 | 4347.437 | 14205.57 | 3117.73 | 26532.43 | 15184.64 | 26310.96 | 15883.78 | 1.27 | 1.22E-07 | 7.53E-07 | -0.28 | 0.469217 | 0.734042 | | |
| COMPOUND_346_2499a9_872088 | Rp | - | 346.2499 | 9.87 | | | (381.2298, 1888.74)(382.2336, 412.52)(383.226, 210.62)(345.2428, 22292.36)(346.2464, 5372.86)(347.2511, 793.11) | 31458.66 | 15036.11 | 43314.91 | 32445.94 | 50384 | 6017.296 | 66718.42 | 37515.82 | -0.88 | 0.000246 | 0.000718 | -0.25 | 0.351315 | 0.658752 | | |
| COMPOUND_346_2504a10_245456 | Rp | - | 346.2504 | 10.25 | | | (381.2307, 1508.06)(345.2431, 21978.94)(346.2463, 5000.31)(347.2496, 723.73) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.61 | 0.019304 | 0.03837 | -0.01 | 0.968555 | 0.982722 |
| COMPOUND_347_1073a10_465133 | Rp | - | 347.1073 | 10.47 | | | (729.2069, 458.79)(730.2046, 328.98)(731.2227, 254.12)(460.0977, 1882.32)(739.2512, 682.14)(346.1005, 36948.72)(347.1029, 9801.37)(348.098, 12517.7)(349.1014, 3346.6)(350.1008, 818.05)(693.1562, 416.75)(694.1758, 313.19)(807.203, 865.73)(808.228, 616.88)(809.2216, 351.89) | 58254.43 | 14224.76 | 61096.46 | 15818.71 | 88004.79 | 17190.81 | 98431.49 | 17754.5 | 1.24 | 1.03E-07 | 6.38E-07 | 0.26 | 0.298648 | 0.60748 | | |
| COMPOUND_347_1839a7_123690 | Rp | - | 347.1839 | 7.12 | | | (460.1687, 452.35)(461.172, 175.82)(462.164, 26.81)(382.1534, 6189.61)(383.1571, 1228.42)(384.1516, 2105.02)(385.156, 628.18)(386.1524, 87.96)(346.1768, 17995.71)(347.1803, 3794.73)(348.1835, 579.03)(392.183, 492.51)(393.188, 173.19) | 51955.94 | 27605.16 | 54656.02 | 29064.62 | 25898.75 | 8539.067 | 18554.57 | 6088.545 | -1.30 | 5.62E-11 | 8.98E-10 | -0.24 | 0.222124 | 0.531023 | | |
| COMPOUND_349_1708a10_581104 | Rp | + | 349.1708 | 10.58 | | | (737.2865, 1212.29)(738.2707, 1046.12)(739.3003, 560.87)(367.1964, 4340.84)(350.1789, 30947.1)(351.1815, 6798.02)(352.1795, 34969.13)(353.183, 7652.95)(354.1752, 14114.86)(355.1781, 405.185)(356.177, 2658.39) | 68574.33 | 48024.39 | 67864.11 | 49678.98 | 109524.2 | 65122.11 | 174515.8 | 84271.55 | 0.76 | 0.002115 | 0.005235 | 0.53 | 0.065033 | 0.308265 | | |
| COMPOUND_350_1185a6_711507 | Rp | + | 350.1185 | 6.71 | no msms | | (349.1112, 28613.2)(350. | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|---|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_352_2244a8_018731 | Rp | - | 352.2244 | 8.02 | | | | (465.1933, 1527.05)(466.194, 289.71)(467.1887, 327.77)(387.1902, 1413.54)(388.1932, 327.48)(389.1965, 5225.99)(390.2002, 1279.59)(351.2173, 24918.39)(352.2205, 5553.19)(397.2139, 1142.28)(398.2078, 114.16)(399.2207, 6597.28)(400.224, 1584.82) | 51515.07 | 52797.31 | 55531.93 | 49245.45 | 78812.67 | 78041.66 | 57886.44 | 29761.03 | -0.72 | 0.002344 | 0.005731 | -0.30 | 0.267796 | 0.575669 |
| COMPOUND_352_2246a8_980364 | Rp | - | 352.2246 | 8.98 | | | | (387.1938, 2033.28)(388.1966, 496.78)(389.1949, 834.39)(390.1955, 355.41)(351.2175, 10547.32)(352.2222, 2498.97)(353.2309, 1165.29)(354.2339, 143.13) | 59671.4 | 30869.54 | 62722.93 | 31179.95 | 54704.33 | 21010.04 | 52479.56 | 13676.02 | -1.16 | 1.67E-07 | 1.01E-06 | -0.18 | 0.438803 | 0.715597 |
| COMPOUND_352_2246a8_884727 | Rp | - | 352.2246 | 8.88 | | | | (387.1926, 1698.78)(388.1979, 324.06)(389.1941, 876.96)(390.1965, 262.22)(351.2174, 7625.38)(352.2205, 1713.2)(353.2304, 863.55)(354.2355, 103.51) | 43765.33 | 22858.72 | 53213.5 | 32346.22 | 29995 | 4887.84 | 34277.29 | 17058.5 | -0.92 | 3.1E-05 | 0.000109 | -0.27 | 0.263302 | 0.574821 |
| COMPOUND_352_2334a10_849869 | Rp | - | 352.2334 | 10.85 | | | | (739.4663, 3002.52)(465.2222, 1630.8)(466.2255, 501.87)(467.2075, 800.24)(387.2034, 323.5)(388.2105, 35.31)(389.2085, 916.54)(748.4806, 2065.21)(750.4746, 1354.58)(751.4845, 1145.47)(351.2289, 8405.42)(352.2322, 1410.73)(353.2392, 312.62)(703.4403, 1587.33)(397.2351, 7927.48)(398.2385, 2239.26)(399.2392, 468.21)(817.4799, 413.61) | 48732.02 | 12924.96 | 54949.84 | 18132.94 | 32393 | 12925.8 | 39754.7 | 11754.63 | -0.55 | 0.040667 | 0.073265 | 0.10 | 0.758569 | 0.896744 |
| COMPOUND_352_2625a10_223319 | Rp | + | 352.2625 | 10.22 | | | | (743.507, 835.97)(375.2523, 21943.56)(376.2555, 5380.07)(377.2672, 1578.56)(727.4951, 1299.93)(728.4879, 492.61)(729.5051, 1837.07)(730.5035, 463.9)(391.2261, 1241.94)(392.235, 566.23)(393.2176, 536.65)(370.297, 387.60)(371.2994, 10064.24)(372.3062, 1957.65)(373.3093, 254.16)(353.2699, 35681.61)(354.2736, 7504.13)(355.2796, 2428.41)(722.5338, 410.27) | 53595.8 | 35891.06 | 60830.04 | 45845.41 | 62079.42 | 32760.96 | 96460.53 | 55226.01 | 0.11 | 0.694125 | 0.777309 | 0.63 | 0.053571 | 0.288052 |
| COMPOUND_353_3313a10_579868 | Rp | + | 353.3313 | 10.58 | | | | (707.6758, 1040.11)(378.32, 13016.33)(377.3241, 3434.67)(378.3314, 919.95)(392.2931, 927.11)(371.364, 5782.72)(354.3373, 11227.82)(355.3399, 3130.68)(356.3454, 752.64)(357.3427, 67.2) | 31194.92 | 13265.66 | 38340.11 | 18508.8 | 49381.36 | 35074.49 | 47829.36 | 25510.29 | 0.80 | 0.006189 | 0.013717 | -0.47 | 0.166902 | 0.480028 |
| COMPOUND_354_1033a6_715043 | Hiic | + | 354.1033 | 6.72 | | | | (377.0918, 5976.57)(378.0951, 886.11)(379.0963, 129.88)(731.1942, 847.25)(732.2007, 350.63)(733.1929, 87.09)(355.1111, 1851.2)(356.1121, 183.4) | 19164.21 | 4606.613 | 21307.8 | 5518.484 | 25797.57 | 7116.442 | 29638.04 | 7896.351 | 0.91 | 0.000516 | 0.001432 | 0.11 | 0.712766 | 0.872838 |
| COMPOUND_354_1497a10_579311 | Rp | - | 354.1497 | 10.58 | | | | (743.2595, 270.39)(744.2707, 787.14)(467.1343, 5053.6)(468.1383, 666.06)(469.1306, 5409.23)(470.1259, 1653.7)(471.1311, 2192.56)(472.1321, 889.55)(473.1361, 742.44)(389.1155, 3490.72)(390.1179, 746.76)(391.1177, 3797.93)(392.1214, 796.96)(393.1159, 2175.43)(394.1252, 598.96)(395.1108, 547.94)(75.2307, 977.73)(754.3068, 602.46)(755.2983, 1110.79)(756.3058, 865.94)(757.2945, 732.41)(353.1422, 17526.06)(354.1461, 6464.64)(355.1502, 1967.09)(356.1638, 275.67)(707.2914, 972.23)(708.2786, 1580.04)(709.2856, 1127.81)(399.1465, 16942.69)(400.1502, 4288.83)(401.1474, 22152.98)(402.1514, 4481.55)(403.1437, 8626.87)(404.1483, 2625.21)(405.1464, 1708.06)(821.3058, 667.5)(822.2967, 499.51)(823.283, 726.02) | 201231.3 | 108120.4 | 209723.3 | 127643.9 | 238470.8 | 134219.9 | 361772.1 | 146516 | 0.32 | 0.215762 | 0.308505 | 0.75 | 0.017118 | 0.19372 |
| COMPOUND_354_1746a10_470297 | Rp | + | 354.1746 | 10.47 | | | | (747.3631, 1004.49)(748.3756, 155.43)(749.3469, 1273.51)(393.1238, 691.45)(372.1942, 1217.78)(355.1811, 35468.38)(356.1851, 8962.54)(357.1907, 1957.68)(726.3601, 955.59)(727.3787, 559.09)(728.3477, 931.0) | 65228.49 | 13390.02 | 61691.07 | 14134.94 | 100116.3 | 17830.99 | 100843.4 | 17812.68 | 1.36 | 2.73E-09 | 2.62E-08 | 0.19 | 0.413522 | 0.696003 |
| COMPOUND_354_2399a8_686489 | Rp | - | 354.2399 | 8.69 | | | | (389.2047, 695.07)(390.1975, 100.05)(391.2114, 1180.92)(392.2158, 266.17)(393.2232, 313.04)(353.2328, 14459.58)(354.2364, 3455.2)(355.2396, 590.08)(356.2428, 84.63) | 39033.92 | 21351.03 | 45866.15 | 22832.95 | 78488 | 33286.01 | 59721.2 | 21393.48 | -0.77 | 0.001028 | 0.002672 | -0.43 | 0.114755 | 0.401909 |
| COMPOUND_354_278a10_459615 | Rp | + | 354.2780 | 10.46 | no msms | | | (709.5937, 313.49)(377.2673, 587964.06)(378.271, 124014.46)(379.2805, 32846.94)(393.2408, 12969.22)(394.2449, 3718.19)(395.2433, 1642.85)(372.3119, 925775.5)(373.3158, 200988.2)(374.3189, 30050.97)(375.3215, 3470.26)(355.2853, 58358.9)(356.2889, 119046.83)(357.2911, 19798.4)(358.2953, 2820.99) | 978542.8 | 600135.2 | 1100807 | 944968.9 | 1100027 | 652355.7 | 2292947 | 1289399 | 0.00 | 0.996256 | 0.999963 | 1.10 | 0.000508 | 0.035763 |
| COMPOUND_354_2794a10_43812 | Rp | + | 354.2794 | 10.44 | | | | (12969.22)(394.2449, 3718.19)(372.3119, 925775.5)(373.3158, 200988.2)(374.3189, 30050.97)(355.2853, 58358.9)(356.2889, 119046.83)(357.2911, 19798.4)(358.2953, 2820.99) | 1003242 | 679554.3 | 671806.3 | 544888.9 | 795936.9 | 865848 | 1181000 | 1362139 | -0.39 | 0.197329 | 0.286885 | 0.85 | 0.01996 | 0.199116 |
| COMPOUND_355_2369a8_151008 | Rp | + | 355.2369 | 8.15 | | | | (356.2437, 9425.17)(357.2464, 2206.88)(358.2483, 593.65) | 26483.08 | 13246.41 | 21023.12 | 12181.61 | 27081.43 | 9457.592 | 29459.65 | 13805.08 | 0.17 | 0.55931 | 0.656827 | 0.42 | 0.220442 | 0.53038 |
| COMPOUND_355_273a7_978727 | Rp | + | 355.2730 | 7.98 | AcAr 13:1 | 2 | 10 eV: 356.2832(100), 163.1108(12), 278.4125(10), 44.1736(3) | (378.2645, 1994.92)(379.2665, 595.75)(380.2745, 247.06)(356.2804, 10711.06)(357.2843, 2509.35)(358.2863, 530.92)(359.2759, 71.16) | 36620.04 | 15851.6 | 33462.72 | 13243.7 | 32586.46 | 14302.57 | 33351.69 | 16220.04 | -0.40 | 0.153809 | 0.232938 | 0.29 | 0.38436 | 0.686423 |
| COMPOUND_356_144a9_927284 | Rp | + | 356.1440 | 9.93 | | | | (395.1274, 898.48)(374.166, 1369.41)(357.1521, 9657.59)(358.1567, 2643.34)(359.1538, 3289.6)(360.1585, 877.44)(361.1511, 1313.53) | 28660.65 | 10278.86 | 27837.96 | 9894.783 | 33343.67 | 1307.866 | 33935.11 | 10310.34 | -1.07 | 5.63E-06 | 2.37E-05 | -0.03 | 0.892679 | 0.953702 |
| COMPOUND_356_2713a10_901843 | Rp | - | 356.2713 | 10.90 | | | | (747.5002, 555.83)(355.2638, 34137.99)(356.2676, 9337.53)(357.2707, 1088.91)(358.2727, 139.79)(825.5267, 1709.25) | 21226.82 | 9170.031 | 31654 | 47118.16 | 23423.86 | 13320.34 | 36194.74 | 18501.76 | 0.50 | 0.034352 | 0.063307 | 0.31 | 0.250218 | 0.56013 |
| COMPOUND_356_2723a9_733602 | Rp | + | 356.2723 | 9.73 | | | | (713.5725, 145.14)(374.2927, 484.01)(357.2799, 108157.39)(358.2833, 27669.47)(359.2869, 3946.38)(360.2832, 560.57) | 79201.7 | 64569.95 | 87085 | 126026.7 | 64288.9 | 83119.62 | 91954.33 | 94833.81 | -0.54 | 0.029797 | 0.055984 | 0.60 | 0.038288 | 0.259981 |
| COMPOUND_356_2936a10_660318 | Rp | + | 356.2936 | 10.66 | | | | (379.283, 745789.94)(380.2869, 158695.0)(395.2567, 16036.79)(396.2583, 4549.44)(374.3275, 608008.44)(375.3313, 132881.06)(357.3009, 862338.8)(358.3049, 188872.89)(359.3076, 25796.81)(730.6216, 650.47) | 1043549 | 1023255 | 916011.9 | 847512.2 | 642301.4 | 815802.4 | 2290047 | 2422353 | -0.20 | 0.489057 | 0.589698 | 0.93 | 0.008713 | 0.14883 |
| COMPOUND_356_2946a10_693461 | Rp | + | 356.2946 | 10.69 | MAG 18:1 | 1 | 10eV: 265.2548(100), 339.2913(90), 247.2426(35), 109.1034(22), 357.3053(15) | (379.2834, 772951.25)(380.2875, 163999.9)(381.2905, 23961.18)(382.2947, 3337.33)(395.2567, 11830.38)(396.2595, 2815.79)(397.2607, 1649.75)(398.2596, 205.52)(374.3281, 347925.16)(375.3312, 78793.88)(376.3332, 11797.05)(377.3358, 1740.35)(378.3355, 185.76)(357.3016, 543354.8)(358.3053, 115006.61)(359.3077, 16585.91)(360.3115, 2372.08) | 1841413 | 1194453 | 1859414 | 1480080 | 1868554 | 1102725 | 4798112 | 2492278 | -0.11 | 0.642878 | 0.732302 | 1.39 | 7.61E-06 | 0.005716 |
| COMPOUND_357_1368a10_464027 | Rp | - | 357.1368 | 10.46 | | | | (749.2597, 619.73)(750.2573, 483.13)(751.2592, 608.1)(759.2915, 1070.04)(760.3028, 375.75)(761.2903, 881.29)(356.1293, 49132.06)(357.1325, 12701.01)(358.1335, 3287.28)(359.1352, 401.11)(713.2769, 1002.11)(714.278, 5218.61)(715.2816, 1880.44)(716.2794, 2937.59)(827.2409, 608.36)(828.2522, 471.03) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.74 | 0.0082 | 0.017755 | 0.01 | 0.975386 | 0.986465 |
| COMPOUND_357_1827a10_86012 | Rp | + | 357.1827 | 10.86 | | | | (715.3863, 6189.11)(716.391, 3248.64)(753.3467, 892.54)(754.3418, 3921.81)(737.3269, 1980.83)(738.3416, 1259.02)(396.1456, 519.85)(397.1434, 1149.01)(375.2154, 4228.63)(376.2184, 662.68)(377.2078, 75.11)(358.1892, 1565.61)(359.1939, 340.92)(360.1882, 2900.07)(361.1857, 1353.03)(362.1868, 1662.62)(732.3941, 3149.68) | 80490.89 | 19484.04 | 82801.56 | 19331.21 | 148404.8 | 43782.51 | 149869.9 | 30836.54 | 1.44 | 8.64E-08 | 5.51E-07 | -0.43 | 0.129455 | 0.425745 |
| COMPOUND_357_2894a8_258104 | Rp | + | 357.2894 | 8.26 | AcAr 13:0 | 2 | 10 eV: 358.3049(100), 165.099(55), 294.3479(27), 85.1828(5.5) | (380.2803, 5525.88)(358.2961, 10211.54)(359.3004, 2156.46)(360.3048, 411.29)(361.2934, 58.97) | 48013.74 | 42062.01 | 38529.48 | 26836.23 | 50598.15 | 47862.49 | 43430.7 | 32577.1 | -0.17 | 0.537618 | 0.636056 | 0.22 | 0.479188 | 0.742181 |
| COMPOUND_358_1615a10_691497 | Rp | + | 358.1615 | 10.69 | | | | (717.3439, 4632.95)(718.3458, 1130.17)(719.3449, 780.82)(755.2959, 1658.2)(739.3341, 1319.6)(376.1836, 1970.85)(359.1672, 24423.85)(360.1759, 6328.9)(361.1685, 15351.34)(362.1739, 3822.03)(363.1644, 5679.11)(364.1675, 1103.73)(365.1669, 722.45)(734.3701, 2556.17)(735.3772, 1375.71) | 87279.6 | 22716.81 | 91532.67 | 25997.22 | 110454.6 | 33372.41 | 116032.2 | 31712.79 | 0.70 | 0.015305 | 0.031136 | -0.12 | 0.720405 | 0.876947 |
| COMPOUND_358_1623a10_467041 | Rp | - | 358.1623 | 10.47 | | | | (715.2632, 853.37)(471.1609, 1400.68)(393.1486, 3183.81)(357.1552, 14321.77)(358.1594, 2976.09)(359.1696, 537.6)(715.3244, 621.72)(403.1494, 1825.64)(829.3143, 289.9)(830.3163, 532.44) | 23903 | 10108.27 | 29191.36 | 8227.041 | 37746.7 | 7781.894 | 36850.02 | 11911 | 0.95 | 3.91E-05 | 0.000133 | -0.16 | 0.528331 | 0.7696 |
| COMPOUND_358_1848a9_927043 | Rp | + | 358.1848 | 9.93 | | | | (717.3757, 499.28)(718.3608, 385.77)(719.3813, 308.57)(381.1586, | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_358_214a9_015355 | Rp | - | 358.2140 | 9.02 | | | | (751.378, 220.277)(752.3767, 55.67)(753.3983, 72.45)(471.1953, 1100.45)(472.1962, 244.56)(473.1883, 395.37)(474.1766, 27.51)(393.1803, 1878.89)(394.184, 439.46)(395.1933, 1273.32)(761.4113, 177.04)(762.3977, 40.7)(357.2068, 13829.13)(358.2097, 3212.07)(403.21, 4581.49)(404.2123, 1180.44)(405.217, 624.21)(406.228, 78.02) | 109223.5 | 52603.95 | 109024.4 | 56272.94 | 122863.7 | 22636 | 115057 | 53843.82 | -1.11 | 1.93E-06 | 8.98E-06 | -0.10 | 0.70283 | 0.86442 |
| COMPOUND_358_214a9_025965 | Rp | + | 358.2140 | 9.03 | | | | (381.2044, 7756.14)(382.208, 2303.53)(376.2496, 2285.35)(377.2404, 1009.76)(359.2204, 15331.95)(360.2249, 3440.15)(361.2312, 1110.41) | 78080.96 | 41770.17 | 81779.38 | 33972.59 | 119631 | 71990.3 | 88278.63 | 27892.38 | -0.94 | 3.39E-05 | 0.000119 | -0.31 | 0.213356 | 0.520562 |
| COMPOUND_358_2141a9_018258 | Rp | - | 358.2141 | 9.06 | | | | (751.3814, 147.34)(752.3782, 81.36)(753.3816, 146.14)(471.1965, 722.84)(472.1987, 199.26)(473.1936, 560.06)(474.2031, 99.66)(393.1806, 1806.82)(394.1835, 384.46)(395.1923, 947.47)(396.1977, 224.23)(761.4127, 172.75)(762.4118, 60.14)(357.2068, 12038.38)(358.2099, 2837.5)(403.2092, 6285.25)(404.2124, 1498.88)(405.2106, 608.23)(406.2246, 78.41) | 113952.6 | 70161.7 | 118153 | 66378.49 | 133000.7 | 26304.15 | 106309.5 | 58804.05 | -1.09 | 2.65E-06 | 1.2E-05 | -0.16 | 0.531456 | 0.771657 |
| COMPOUND_358_217a9_217477 | Rp | + | 358.2170 | 9.22 | | | | (381.2046, 7053.69)(382.2073, 1726.77)(397.1941, 1739.65)(398.2006, 534.86)(399.1939, 3305.37)(376.2498, 6117.01)(377.2553, 1327.02)(359.2223, 13347.84)(360.2263, 3323.02)(361.2359, 1184.0) | 100701.7 | 37802.12 | 90850.48 | 44344.01 | 20332.5 | 856.3063 | 29331.71 | 14938.33 | -1.47 | 2.41E-12 | 7.99E-11 | 0.13 | 0.500992 | 0.753664 |
| COMPOUND_358_309a10_909369 | Rp | + | 358.3094 | 10.91 | | | | (717.6525, 1593.16)(718.644, 554.23)(381.2981, 527484.06)(382.3019, 112025.93)(383.3046, 17468.8)(384.3086, 2559.93)(739.6043, 2565.71)(740.5953, 1153.63)(376.343, 64121.32)(377.3463, 15937.28)(378.3476, 2713.44)(397.2726, 12545.59)(398.2706, 3542.43)(399.2687, 1839.87)(359.3166, 208336.77)(360.3201, 49735.46)(361.323, 7298.81)(362.3221, 1045.23)(734.6606, 2029.67)(735.6565, 947.44) | 1315781 | 907638.4 | 1005062 | 79348.7 | 720776.3 | 455066.1 | 705666.6 | 569134.9 | -0.59 | 0.04875 | 0.085503 | 0.35 | 0.319119 | 0.625463 |
| COMPOUND_358_3101a10_927794 | Rp | + | 358.3101 | 10.93 | | | | (717.6395, 1969.11)(718.6271, 898.77)(381.2993, 290370.47)(382.3021, 65212.25)(383.3047, 10515.27)(384.3064, 1488.53)(385.2994, 154.61)(739.6034, 2288.99)(740.6256, 1303.55)(397.2718, 18155.11)(398.2749, 5383.89)(399.2713, 2554.13)(400.2832, 395.91)(376.3433, 169977.31)(377.3464, 40414.08)(378.3492, 7071.73)(379.3531, 1083.22)(359.3159, 948849.94)(360.3199, 203503.94)(361.3223, 28491.7)(362.3254, 3292.28)(734.6464, 4045.43)(735.6486, 2751.25) | 2159549 | 1057308 | 1947626 | 89662.4 | 984292.6 | 579064 | 1218670 | 777447.6 | -1.27 | 5.55E-06 | 2.33E-05 | 0.41 | 0.174909 | 0.48931 |
| COMPOUND_359_2471a9_455959 | Rp | + | 359.2471 | 9.46 | | | | (360.2539, 16419.92)(361.256, 5176.36)(362.2644, 2030.85)(363.2691, 303.13) | 126425.5 | 50172.55 | 116968.2 | 43226.26 | 65490.5 | 38969.36 | 74005.86 | 29550.63 | -1.41 | 2.65E-11 | 5.63E-10 | 0.10 | 0.615926 | 0.816971 |
| COMPOUND_359_2709a0_918676 | HiLic | + | 359.2709 | 0.92 | | | | (382.2591, 1437.25)(741.5306, 6538.96)(360.2751, 7538.63)(361.2787, 1653.63)(362.2795, 245.05)(736.5734, 1083.01) | 40121.39 | 20191.7 | 41666.85 | 16105.48 | 53904.44 | 27127.6 | 34271.95 | 18834.62 | 0.00 | 0.997735 | 0.999401 | -0.57 | 0.087615 | 0.350433 |
| COMPOUND_360_1944a6_5683947 | Rp | + | 360.1944 | 6.57 | Cortisone | 1 | 10eV: 361.2009(100), 322.2927(11), 121.0607(6) | (383.1844, 2612.5)(384.1878, 608.54)(385.1801, 35.81)(399.1564, 401.44)(400.1621, 78.36)(361.2023, 53727.71)(362.2051, 12594.35)(363.2088, 2200.11)(364.2099, 311.35) | 58121.53 | 16089.87 | 56191.28 | 14533.52 | 120306.6 | 24446.04 | 127249.2 | 48217.68 | 1.24 | 7.44E-06 | 3.04E-05 | -0.17 | 0.569133 | 0.788601 |
| COMPOUND_360_2294a8_915713 | Rp | - | 360.2294 | 8.92 | | | | (395.1975, 747.65)(396.2048, 120.92)(397.2051, 4023.11)(359.2222, 12385.22)(360.2254, 2720.37)(361.2352, 853.27)(362.2394, 105.66)(405.2176, 691.37)(406.2086, 65.84) | 128962.3 | 82121.36 | 162227.7 | 110607.1 | 183766 | 133515.6 | 226349 | 202293.2 | -0.86 | 0.000268 | 0.000778 | -0.34 | 0.20259 | 0.5149 |
| COMPOUND_360_2294a9_128733 | Rp | - | 360.2294 | 9.13 | | | | (395.1985, 1880.95)(396.2002, 389.02)(397.2053, 11452.22)(398.2086, 2985.29)(359.2222, 20340.73)(360.2255, 4662.58)(361.2309, 1170.11)(362.2359, 160.11)(405.2276, 11813.23)(406.2308, 2946.76)(407.2328, 553.21) | 424630.1 | 257530 | 518678 | 356820.5 | 3256000 | 4970357 | 1859066 | 1887534 | -0.87 | 0.000536 | 0.00148 | -0.10 | 0.721237 | 0.877485 |
| COMPOUND_360_2296a9_092889 | Rp | - | 360.2296 | 9.09 | | | | (395.1991, 1851.65)(396.203, 382.58)(397.207, 4751.86)(398.2109, 1185.44)(359.2225, 25264.85)(360.2258, 6007.6)(361.2316, 1399.45)(362.2416, 187.37)(405.2276, 15773.11)(406.2312, 4095.32)(407.2339, 789.66) | 235988.4 | 215181.7 | 208658.4 | 199614.8 | 2548341 | 4322325 | 762832.5 | 1434714 | -0.55 | 0.021563 | 0.042131 | -0.29 | 0.306297 | 0.613089 |
| COMPOUND_360_2311a9_514435 | Rp | + | 360.2311 | 9.51 | | | | (383.205, 9600.42)(384.2237, 2744.68)(385.2331, 1305.29)(399.1962, 1712.09)(400.2044, 467.53)(401.2013, 426.74)(378.2656, 74119.06)(379.2686, 18790.51)(380.2792, 11170.71)(361.2386, 8960.84)(362.2421, 2734.25)(363.2465, 797.67)(181.1274, 591.37)(181.6179, 22.96) | 124988.2 | 72005.61 | 128229.2 | 67799.07 | 112618.3 | 64513.66 | 153040.8 | 94950.71 | -1.05 | 9.9E-06 | 3.97E-05 | -0.14 | 0.598574 | 0.805251 |
| COMPOUND_361_2273a8_595282 | Rp | + | 361.2273 | 8.60 | | | | (362.2341, 5005.1)(363.2376, 1154.3)(364.2364, 235.18) | 29444.33 | 7041.994 | 27537.8 | 6672.233 | 28871.64 | 5214.131 | 27041.7 | 5055.614 | 0.05 | 0.866998 | 0.910247 | -0.11 | 0.759726 | 0.896853 |
| COMPOUND_361_2616a8_963542 | Rp | + | 361.2616 | 8.96 | | | | (379.3, 472.99)(362.2699, 21321.05)(363.2729, 5299.95)(364.2806, 2355.2) | 52505.35 | 32464.63 | 44803.28 | 30061.28 | 46898.67 | 10859.17 | 35966 | 22688.28 | -0.94 | 2.67E-05 | 9.62E-05 | 0.29 | 0.237365 | 0.542834 |
| COMPOUND_361_3202a10_602238 | Rp | + | 361.3202 | 10.60 | | | | (723.6681, 447.61)(384.3108, 99.91)(385.3102, 1564.35)(379.3452, 486.16)(362.327, 19203.13)(363.3301, 4405.7)(364.3317, 1078.06) | 20629.47 | 8560.757 | 16610.91 | 7494.388 | 15189.2 | 3799.416 | 21445.24 | 9747.781 | -0.24 | 0.357123 | 0.459566 | 0.85 | 0.007117 | 0.131884 |
| COMPOUND_362_2103a6_80662 | Rp | + | 362.2103 | 6.81 | Cortisol | 1 | 20 eV: 363.2204(100), 43.0158(75), 147.0816(75), 267.1743(65), 97.0611(55), 201.1308(55) | (725.4251, 136.36)(385.1994, 7870.78)(386.203, 2012.11)(387.2028, 316.51)(747.4063, 324.09)(748.4084, 159.39)(749.4092, 71.46)(401.2723, 876.57)(402.1782, 148.77)(403.1685, 86.55)(363.2178, 300556.06)(364.221, 67719.42)(365.2242, 10478.79)(366.2278, 1258.98) | 290636.7 | 97627.4 | 287770.5 | 92798.21 | 584199.9 | 164292.5 | 485252.7 | 269459.4 | 1.41 | 1.55E-06 | 7.5E-06 | -0.62 | 0.052324 | 0.286125 |
| COMPOUND_363_1912a6_3340254 | Rp | + | 363.1912 | 6.33 | | | | (727.4054, 118.0)(364.1978, 10924.07)(365.2019, 2040.9)(366.2045, 530.48) | 28398.27 | 7131.223 | 27166.5 | 5911.209 | 25804.64 | 7406.407 | 27580.94 | 7227.745 | -0.23 | 0.430728 | 0.535615 | 0.31 | 0.375003 | 0.67723 |
| COMPOUND_363_2784a9_301902 | Rp | + | 363.2784 | 9.30 | | | | (364.2855, 118077.09)(365.2887, 2192.21)(366.291, 4205.25)(367.2937, 493.0) | 237533 | 151323.8 | 166915.1 | 139195 | 160388.3 | 98588.55 | 115359.3 | 86957.02 | -1.33 | 9.07E-10 | 1.01E-08 | 0.18 | 0.420066 | 0.700732 |
| COMPOUND_363_2784a9_190326 | Rp | + | 363.2784 | 9.19 | | | | (364.2855, 53081.75)(365.289, 13053.08)(366.2854, 2417.37)(367.2921, 330.56) | 158121.8 | 98483.2 | 117556 | 89570.39 | 109611.5 | 60844.04 | 89896.2 | 64809.52 | -1.31 | 2.24E-09 | 2.24E-08 | 0.15 | 0.510716 | 0.757607 |
| COMPOUND_364_0983a6_384417 | HiLic | + | 364.0983 | 6.38 | | | | (729.2054, 120.73)(365.1061, 107234.94)(366.1097, 14646.54)(367.1111, 3460.11)(368.113, 412.79) | 11430 | 6212.934 | 12007.22 | 11979.33 | 30266.14 | 13553.71 | 41818.96 | 62155.56 | 1.40 | 1.61E-11 | 3.7E-10 | 0.02 | 0.921682 | 0.966461 |
| COMPOUND_364_0985a6_3290606 | HiLic | + | 364.0985 | 6.33 | Melibiose | 1 | 10 eV: 365.1044 (100), 203.0512 (5) | (387.0943, 66.69)(365.1061, 81302.7)(366.1095, 10603.95)(367.1111, 2667.58)(368.1144, 313.12) | 9745.382 | 6587.447 | 11021.72 | 14120.5 | 31323.64 | 12434.57 | 40147.67 | 46957.48 | 1.35 | 7.91E-10 | 9.09E-09 | 0.15 | 0.489757 | 0.748114 |
| COMPOUND_364_1822a10_469843 | Rp | + | 364.1822 | 10.47 | | | | (729.4031, 788.2)(730.3915, 882.86)(767.3036, 1475.06)(768.3271, 948.18)(769.3263, 810.45)(751.3701, 2064.68)(752.3848, 1178.21)(753.3693, 966.95)(403.1363, 805.82)(365.1884, 20820.28)(366.1927, 4975.55)(367.1906, 25866.97)(368.1942, 5481.98)(369.187, 10240.26)(370.1918, 2665.88)(371.1849, 1903.56)(746.398, 1946.1)(747.4001, 1307.15) | 122016.2 | 20817.01 | 126057 | 25213.26 | 166196.4 | 27686.23 | 170861.1 | 28964.57 | 1.30 | 5.6E-07 | 2.98E-06 | -0.03 | 0.91076 | 0.959323 |
| COMPOUND_364_2216a9_625648 | Rp | - | 364.2216 | 9.63 | | | | (363.2146, 11519.83)(364.218, 2555.95)(365.2169, 473.62) | 16303.55 | 5167.889 | 20828.97 | 10485.65 | 25145 | 6469.416 | 33710.67 | 9830.983 | -0.28 | 0.230332 | 0.325617 | -0.56 | 0.048511 | 0.279822 |
| COMPOUND_365_1795a10_715941 | Rp | + | 365.1795 | 10.72 | | | | (731.3713, 1278.28)(732.3707, 4534.16)(733.3752, 1951.09)(404.1571, 931.2)(366.1862, 73347.06)(367.1899, 17991.74)(368.1924, 3259.01)(748.4006, 3331.92) | 110127.5 | 38251.28 | 109080 | 39102.61 | 176181.2 | 46842.49 | 203705.4 | 67411.07 | 1.03 | 6.95E-05 | 0.000222 | 0.24 | 0.399441 | 0.690408 |
| COMPOUND_365_2025a11_020949 | Rp | + | 365.2025 | 11.02 | | | | (731.3864, 2546.55)(769.3513, 3095.47)(753.3866, 1711.63)(366.2097, 14554.79)(367.212, 4010.52)(368.2092, 6715.3)(369.2119, 1874.68)(370.2078, 2335.83)(371.2106, 1119.23)(372.2069, 515.51)(748.4538, 2322.35) | 40681.68 | 11460.39 | 41141.83 | 10304.93 | 66820.69 | 16364.64 | 68617.36 | 18469.3 | 1.11 | 5.88E-05 | 0.000192 | -0.39 | 0.211821 | 0.519471 |
| COMPOUND_365_3672a11_613963 | Rp | + | 365.3672 | 11.61 | | | | (731.7407, 5964.0)(732.7417, 3898.71)(733.7575, 1157.91)(769.6651, 1318.56)(388.3558, 19009.14)(389.3598, 5431.6)(390.3606, 970.93)(753.6 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|-----------------|----------|---|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_366_2527a10_596336 | Rp | - | 366.2527 | 10.60 | | | | (767.4744, 1097.78)(768.476, 1937.8)(365.2458, 15282.5)(366.2491, 3234.2)(367.2444, 5366.06)(368.2469, 1348.08)(369.2447, 213.75)(845.5135, 1675.86) | 36842.9 | 14170.5 | 41372.76 | 14480.27 | 21817.23 | 8503.286 | 28787.77 | 11942.53 | -1.16 | 7.39E-05 | 0.000234 | 0.37 | 0.266975 | 0.575669 |
| COMPOUND_366_3294a11_815989 | Rp | + | 366.3294 | 11.82 | | | | (771.5941, 800.98)(772.6088, 74.12)(755.6515, 1024.22)(367.337, 11070.7)(368.3402, 3163.9) | 38816 | 18776.25 | 34520.57 | 14943.25 | 29322.67 | 15231.19 | 16360.86 | 5198.457 | -1.26 | 2.72E-09 | 2.62E-08 | 0.02 | 0.929228 | 0.967463 |
| COMPOUND_366_3322a10_066952 | Rp | + | 366.3322 | 11.07 | | | | (733.6999, 3352.61)(734.6811, 1987.11)(735.6757, 1332.67)(367.3376, 16327.86)(368.3408, 5422.02)(369.3492, 2065.76)(370.349, 210.44)(750.7122, 4888.27)(751.6955, 1786.86)(752.6895, 1378.67) | 206300 | 46818.42 | 199944.7 | 44509.76 | 237686 | 141575.5 | 199417.9 | 106355.2 | -0.91 | 0.00016 | 0.000482 | 0.22 | 0.413326 | 0.696003 |
| COMPOUND_367_1953a10_932911 | Rp | + | 367.1953 | 10.93 | | | | (735.3932, 3121.81)(773.3658, 2925.3)(774.3454, 10489.79)(757.4067, 2711.84)(368.2035, 17385.8)(369.2064, 5223.75)(370.2117, 2036.29)(371.2067, 214.06)(752.4371, 1322.08)(753.4367, 1024.8)(754.4205, 1506.64) | 145677.8 | 56694.1 | 149706.9 | 60223.07 | 281086.7 | 77896.02 | 359892.9 | 116188.6 | 1.01 | 1.22E-05 | 4.82E-05 | 0.53 | 0.040193 | 0.246661 |
| COMPOUND_367_2726a7_9651318 | Rp | + | 367.2726 | 7.97 | ACar 14:2 | 2 | 10 eV: 368.282(100), 55.0523(6) | (390.369, 364.9)(391.3648, 85.84)(392.3553, 120.83)(406.3468, 381.96)(407.3502, 187.27)(368.3992, 12168.6)(369.3915, 3377.33)(370.3955, 482.5)(752.8073, 706.45)(753.8089, 209.33)(754.8289, 147.45) | 39913.33 | 19550.89 | 34554.79 | 16977.71 | 26485.85 | 19509 | 34766.76 | 16019.87 | -0.54 | 0.063448 | 0.109323 | 0.38 | 0.26442 | 0.575338 |
| COMPOUND_367_3816a12_037113 | Rp | + | 367.3816 | 12.04 | | | | (390.369, 364.9)(391.3648, 85.84)(392.3553, 120.83)(406.3468, 381.96)(407.3502, 187.27)(368.3992, 12168.6)(369.3915, 3377.33)(370.3955, 482.5)(752.8073, 706.45)(753.8089, 209.33)(754.8289, 147.45) | 15760.76 | 5135.549 | 18485.36 | 7080.267 | 22791.63 | 15345.63 | 17222.91 | 7219.606 | 0.23 | 0.402158 | 0.506238 | -0.48 | 0.139042 | 0.444794 |
| COMPOUND_368_1654a8_309799 | Rp | - | 368.1654 | 8.31 | | | | (367.1579, 28028.77)(368.1611, 6217.03) | 43747.35 | 29664.97 | 45829.14 | 16779.89 | 21133.62 | 4244.779 | 25049.64 | 10467.81 | -0.73 | 0.000219 | 0.000646 | -0.55 | 0.012228 | 0.168989 |
| COMPOUND_368_1658a7_434831 | Rp | - | 368.1658 | 7.43 | steroid sulfate | 3 | 10 eV: 367.158(100), 96.9599(6) | (367.1579, 794406.7)(368.1617, 164919.44)(369.1591, 45765.38)(735.3236, 3361.99)(736.326, 1470.59)(737.3237, 623.94)(738.322, 192.1)(739.3292, 38.76) | 2698883 | 1264167 | 2957206 | 1183172 | 983266.3 | 540257.5 | 1136107 | 747830.9 | -1.10 | 1.68E-07 | 1.01E-06 | -0.35 | 0.111675 | 0.397302 |
| COMPOUND_368_2195a7_7771025 | Rp | - | 368.2195 | 7.78 | | | | (403.1873, 941.47)(404.189, 295.33)(405.1923, 2109.41)(781.42, 107.15)(367.2122, 14592.46)(368.2155, 2874.96) | 43320.1 | 25127.78 | 47511.78 | 25989.84 | 30652.33 | 826.84 | 35168.89 | 14887.82 | -1.22 | 2.2E-08 | 1.67E-07 | -0.19 | 0.396591 | 0.690408 |
| COMPOUND_368_2195a8_789687 | Rp | - | 368.2195 | 8.79 | | | | (367.2122, 11017.15)(368.2149, 2836.24)(369.223, 1038.01)(370.2284, 116.71) | 24667.6 | 11475.76 | 27210.69 | 14564.25 | 22280.33 | 7511.632 | 21899.56 | 11373.14 | -1.18 | 9.12E-08 | 5.79E-07 | -0.16 | 0.483346 | 0.746055 |
| COMPOUND_368_2196a8_819054 | Rp | - | 368.2196 | 8.82 | | | | (367.2121, 16287.92)(368.2146, 3459.92)(369.2232, 870.44)(370.2241, 124.17) | 30600.02 | 14200.86 | 34018.16 | 15900.48 | 29994.33 | 8590.299 | 25953.7 | 8841.671 | -1.15 | 1.87E-07 | 1.11E-06 | -0.21 | 0.360172 | 0.666906 |
| COMPOUND_368_2236a11_193171 | Rp | + | 368.2236 | 11.19 | | | | (775.3974, 4066.44)(776.4029, 2246.48)(391.218, 819.69)(392.2166, 1103.61)(393.2162, 463.63)(407.1861, 8658.43)(408.1889, 1680.06)(409.1869, 3360.76)(410.2026, 1135.43)(411.1849, 1342.67)(369.2326, 9309.32)(754.4863, 1742.64)(755.489, 1232.28)(756.489, 597.52) | 33567.14 | 11055.77 | 27933.41 | 9601.435 | 127115.1 | 34982.28 | 126216.7 | 32445.49 | 1.04 | 1.4E-05 | 5.43E-05 | 0.22 | 0.400154 | 0.690408 |
| COMPOUND_368_3451a12_545252 | Rp | + | 368.3451 | 12.55 | | | | (386.3809, 12841.38)(387.383, 3874.06)(388.3791, 1170.35)(369.3528, 154639.45)(370.356, 44504.38)(371.3588, 6637.71) | 965742.9 | 109890.1 | 983616.9 | 118447.9 | 1025173 | 112841.3 | 983773.6 | 105902.5 | 0.53 | 0.078219 | 0.130869 | -0.55 | 0.13026 | 0.425921 |
| COMPOUND_368_3771a11_22971 | Rp | + | 368.3771 | 11.23 | | | | (737.3783, 1092.51)(775.7181, 2068.85)(759.7361, 1949.07)(760.7473, 280.41)(761.7262, 1308.71)(369.3843, 107556.59)(370.3868, 29125.66)(371.3875, 3860.65)(754.8012, 1401.72) | 76631.26 | 45143.27 | 80975.36 | 42998.21 | 177902.4 | 102696.6 | 186781 | 115896.5 | 0.77 | 0.001202 | 0.003074 | 0.41 | 0.129501 | 0.425745 |
| COMPOUND_369_2103a11_190524 | Rp | + | 369.2103 | 11.19 | | | | (777.3737, 4751.84)(761.4096, 1485.86)(762.4034, 2000.44)(370.2182, 31300.52)(371.2227, 13159.18)(372.2258, 2694.53) | 85975.14 | 18227.38 | 73506.46 | 16774.74 | 168229.6 | 56990.51 | 183992.6 | 46510.05 | 1.12 | 1.45E-06 | 7.03E-06 | 0.23 | 0.359636 | 0.666906 |
| COMPOUND_369_2882a8_350857 | Rp | + | 369.2882 | 8.35 | ACar 14:1 | 2 | 10 eV: 370.2965(100), 115.0756(11), 329.1844(7) | (370.2966, 55892.55)(371.2996, 12926.31)(372.2998, 2197.24)(373.300, 272.64) | 83991.21 | 58146.69 | 72548.09 | 42444.75 | 55106 | 45857.51 | 70551.33 | 42600.98 | -0.65 | 0.027428 | 0.052082 | 0.51 | 0.145118 | 0.452012 |
| COMPOUND_370_1808a6_951668 | Rp | - | 370.1808 | 6.95 | | | | (369.1737, 14897.16)(370.1764, 3297.32)(371.1744, 1145.48)(372.1729, 156.08) | 84836.45 | 38960.74 | 103393.3 | 45698.6 | 16526.15 | 9852.475 | 26555.73 | 11378.29 | -1.41 | 7.54E-12 | 2E-10 | -0.25 | 0.193744 | 0.505089 |
| COMPOUND_370_1808a7_689697 | Rp | - | 370.1808 | 7.69 | | | | (369.1736, 81939.73)(370.1768, 18554.74)(371.1749, 5743.57)(372.1761, 828.57)(739.3438, 219.94)(740.3426, 81.67)(741.3311, 85.49) | 290450.1 | 158121 | 261097.9 | 139489 | 122167.8 | 52710.75 | 113066.1 | 102557.6 | -0.95 | 7.18E-05 | 0.000228 | -0.18 | 0.495275 | 0.751527 |
| COMPOUND_370_1808a10_995727 | Rp | - | 370.1808 | 11.00 | | | | (775.3317, 378.41)(776.3485, 325.99)(777.3457, 250.66)(483.1661, 2614.65)(484.1628, 1556.13)(485.1632, 2493.17)(486.1601, 267.9)(487.1554, 1213.3)(405.1544, 3677.12)(406.1551, 1143.5)(407.1502, 1627.4)(408.1611, 601.29)(409.1537, 1195.77)(785.3667, 840.31)(786.3603, 563.78)(787.3821, 821.78)(369.1732, 7477.53)(370.1781, 3174.11)(371.1763, 1323.46)(372.1786, 195.76)(739.3594, 326.21)(740.3762, 148.48)(741.3566, 246.16)(415.1777, 9742.01)(416.1807, 2079.01)(417.1784, 18548.08)(418.1833, 4074.03)(419.1734, 6733.81)(420.1769, 1778.36)(421.1691, 1370.53)(853.3595, 666.44)(854.3756, 432.13)(855.3484, 317.82) | 146166.81 | 59668.79 | 146632 | 55388 | 160096.6 | 35066.3 | 151602.7 | 59222.01 | 0.53 | 0.082325 | 0.136743 | -0.35 | 0.338594 | 0.642388 |
| COMPOUND_370_1809a11_009078 | Rp | - | 370.1809 | 11.01 | | | | (775.3339, 373.68)(776.3391, 229.2)(777.3207, 90.3)(483.1673, 3050.98)(484.1624, 1684.23)(485.149, 1856.42)(486.1546, 503.91)(487.1492, 1717.34)(405.1535, 4226.26)(406.1557, 1184.91)(407.1489, 2771.95)(408.1521, 668.61)(409.1516, 1629.97)(785.3445, 1086.33)(786.3431, 547.34)(787.3411, 559.55)(369.1735, 7491.59)(370.1777, 3406.01)(371.1753, 1817.25)(372.1776, 249.59)(739.3278, 503.94)(740.3372, 410.11)(741.3472, 854.45)(415.1777, 11122.68)(416.1818, 2177.43)(417.1785, 21615.24)(418.1835, 5033.43)(419.1744, 8099.67)(420.177, 2130.62)(421.1732, 1555.68)(853.367, 618.83)(854.3825, 462.19)(855.3755, 839.33) | 911180.1 | 603976.8 | 913132.7 | 579794 | 538050.6 | 369605.3 | 517494.5 | 461508.4 | -0.62 | 0.003752 | 0.008719 | -0.22 | 0.360698 | 0.666906 |
| COMPOUND_370_1809a8_846407 | Rp | - | 370.1809 | 8.85 | | | | (4148.24)(740.3581, 1700.82)(741.3561, 827.82)(742.358, 176.87) | 93647.21 | 54770.41 | 105170.8 | 56444.53 | 123419.1 | 59392.55 | 84023.51 | 49773.25 | 0.56 | 0.022781 | 0.044113 | -0.94 | 0.001212 | 0.056309 |
| COMPOUND_370_181a8_184061 | Rp | - | 370.1810 | 8.18 | | | | (405.1576, 205.69)(483.1542, 936.24)(484.1572, 394.88)(485.1534, 201.41)(369.1738, 30616.29)(370.1768, 6588.29)(371.1747, 1792.25)(372.1748, 259.59)(739.3549, 3252.59)(740.3575, 1441.43)(741.3571, 644.08)(742.3623, 139.07) | 482512.5 | 500263.9 | 323358.2 | 490818.8 | 143700.6 | 208198.7 | 280464.5 | 410490.3 | -1.05 | 0.000611 | 0.001672 | 1.00 | 0.0056 | 0.118614 |
| COMPOUND_370_2113a10_48221 | Rp | - | 370.2113 | 10.48 | | | | (369.2038, 10587.05)(370.2074, 2095.68)(371.2137, 452.36)(372.2084, 59.85)(739.4372, 697.89)(740.4237, 1408.31) | 20747.23 | 9104.689 | 24803.28 | 14676.04 | 19137.75 | 7428.21 | 19523.5 | 8082.126 | -0.54 | 0.033843 | 0.062626 | -0.04 | 0.901497 | 0.955487 |
| COMPOUND_370_2346a7_587578 | Rp | - | 370.2346 | 7.59 | | | | (405.1972, 1459.94)(406.201, 334.72)(407.2069, 5148.65)(408.2102, 1163.22)(369.2277, 16681.71)(370.2313, 3760.93)(371.2377, 914.15)(372.2414, 134.22) | 97422.73 | 48039.02 | 108388.9 | 64554.81 | 85582.5 | 59088.1 | 57642.94 | 26544.34 | -1.02 | 4E-05 | 0.000136 | -0.17 | 0.532184 | 0.722216 |
| COMPOUND_370_3081a11_103045 | Rp | + | 370.3081 | 11.10 | | | | (741.6005, 81.64)(779.5524, 2761.57)(393.2927, 5467.37)(394.2933, 1194.59)(395.2944, 187.74)(409.2794, 114.39)(410.2652, 907.23)(371.3069, 8001.81)(372.3096, 2601.89)(373.3028, 1339.3)(374.3059, 170.56) | 47389.69 | 14820.81 | 43510.78 | 12494.55 | 69146.8 | 22347.71 | 70059.66 | 21825.53 | -0.42 | 0.012496 | 0.192954 | 0.41 | 0.193636 | 0.505089 |
| COMPOUND_371_2101a10_859324 | Rp | + | 371.2101 | 10.86 | | | | (743.4027, 2264.21)(744.3952, 1820.98)(745.3963, 1444.04)(765.4172, 2179.02)(766.4098, 1585.76)(410.1734, 9852.89)(411.1792, 2488.37)(412.1586, 926.41)(374.2127, 53617.54) | 131998.4 | 24265.87 | 127313 | 27932.68 | 255848 | 57951.44 | 266920.9 | 52084.24 | 1.12 | 4.08E-06 | 1.77E-05 | 0.07 | 0.793501 | 0.913114 |
| COMPOUND_371_2839a10_325151 | Rp | + | 371.2839 | 10.33 | | | | (781.5294, 1246.78)(394.2812, 844.32)(389.311, 694.75)(372.2906, 141129.3)(373.2938, 36517.66)(374.2969, 5652.38)(375.2997, 718.32) | 118826.7 | 71978.83 | 78890.3 | 69359.52 | 64975.25 | 43018.77 | 53305.46 | 39448.19 | -1.32 | 6.52E-09 | 5 | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | | | | | | | | Time | | | Interaction | | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--------------|---|---------------|----------|----------|---------------|---------------|----------|----------|----------|----------|----------|-------------|----------|----------|----------|
| | | | | | | | | 1st trimester | | | | 3rd trimester | | | | Value | raw p | FDR p | Value | raw p | FDR p | |
| | | | | | | | | Control | Pre-eclampsia | Mean | SD | Control | Pre-eclampsia | Mean | SD | | | | | | | |
| COMPOUND_374_155a9_926652 | Rp | + | 374.1550 | 9.93 | | | | (749.3241, 490.651)(750.3135, 324.43)(751.3256, 98.33)(375.1623, 7830.94)(376.1659, 2141.68)(377.163, 8916.04)(378.1651, 2211.74)(379.159, 3703.49)(380.1614, 1140.49)(381.1623, 371.1) | 14897.98 | 16072.15 | 44833.13 | 16985.5 | 39794.25 | 19809.52 | 46688 | 19782.68 | -1.02 | 1.52E-05 | 5.83E-05 | -0.16 | 0.530411 | 0.771657 |
| COMPOUND_374_2088a_513025 | Rp | - | 374.2088 | 8.51 | | | | (409.1779, 1673.12)(410.1647, 22.58)(373.2015, 10517.18)(374.2045, 2273.66)(419.2061, 25143.91) 8895.997 24428.16 10488.63 19788 9397.833 20491.67 7208.453 | 17372.53 | 11732.97 | 38471.02 | 14086.61 | 20347.69 | 7877.843 | 26202.89 | 10749.57 | -1.06 | 0.000207 | 0.000613 | 0.20 | 0.539935 | 0.76458 |
| COMPOUND_376_2821a10_598473 | Rp | - | 376.2820 | 10.60 | | | | (375.2746, 9198.58)(376.2785, 1974.94)(377.2789, 8121.09)(378.2689, 102.6)(421.2973, 176.74) | 17501 | 6271.961 | 20619.2 | 7027.135 | 15675.83 | 4761.182 | 16407.16 | 3827.597 | -0.53 | 0.069492 | 0.118289 | -0.06 | 0.86619 | 0.944172 |
| COMPOUND_377_2031a10_93219 | Rp | + | 377.2031 | 10.93 | | | | (755.4004, 6096.55)(756.3913, 3568.4)(793.3695, 1595.29)(794.3718, 1444.56)(795.3547, 265397.5) 111993 264966.9 112979.8 478941.9 141888.7 582769 183244.2 | 111993 | 264966.9 | 112979.8 | 478941.9 | 141888.7 | 582769 | 183244.2 | 1.06 | 8.29E-06 | 3.36E-05 | 0.43 | 0.103948 | 0.381877 | |
| COMPOUND_377_2572a9_505563 | Rp | + | 377.2572 | 9.51 | | | | (777.5297, 388.09)(378.2651, 18732.24)(379.2681, 5561.11)(380.2723, 1059.63)(381.262, 160.22) | 74348.4 | 36527.41 | 75194.89 | 34359.53 | 73136.5 | 40326.05 | 93538 | 48334.25 | -1.01 | 1.72E-05 | 6.56E-05 | -0.17 | 0.518147 | 0.763656 |
| COMPOUND_377_258a9_251448 | Rp | + | 377.2580 | 9.25 | | | | (378.2001, 200588.36)(379.2688, 48509.59)(380.2757, 11460.14) | 206398.3 | 105216.3 | 207524.4 | 100286.4 | 207391.8 | 118772.9 | 243370.5 | 143958.2 | -0.99 | 2.77E-05 | 9.96E-05 | -0.18 | 0.491728 | 0.748114 |
| COMPOUND_377_2929a9_299879 | Rp | + | 377.2929 | 9.30 | | | | (791.2838, 773.33)(491.1371, 2591.51)(492.1398, 1423.51)(493.1297, 3242.85)(494.1243, 948.63)(495.1282, 1178.35)(496.1354, 606.46)(497.1297, 492.02)(413.0988, 2814.46)(801.2774, 414.39)(802.292, 260.91)(803.2803, 795.94)(377.1336, 4498.06)(378.1388, 1202.18)(379.1288, 539.54)(380.117, 76.75)(755.2841, 810.05)(756.2796, 654.99)(757.2634, 673.29)(423.1469, 6936.83)(424.1476, 1755.85)(425.1467, 12138.69)(426.1505, 2670.52)(427.1431, 4090.01)(428.1455, 1415.65)(429.1416, 970.24)(869.2781, 348.45)(870.2788, 270.44)(871.2641, 369.79) | 116829.9 | 40854.53 | 101968.1 | 38568.97 | 48183 | 23280.46 | 51004 | 21454.55 | -1.49 | 1.1E-12 | 4.87E-11 | 0.14 | 0.486021 | 0.747178 |
| COMPOUND_378_1465a10_50011 | Rp | - | 378.1465 | 10.50 | | | | (791.2838, 773.33)(491.1371, 2591.51)(492.1398, 1423.51)(493.1297, 3242.85)(494.1243, 948.63)(495.1282, 1178.35)(496.1354, 606.46)(497.1297, 492.02)(413.0988, 2814.46)(801.2774, 414.39)(802.292, 260.91)(803.2803, 795.94)(377.1336, 4498.06)(378.1388, 1202.18)(379.1288, 539.54)(380.117, 76.75)(755.2841, 810.05)(756.2796, 654.99)(757.2634, 673.29)(423.1469, 6936.83)(424.1476, 1755.85)(425.1467, 12138.69)(426.1505, 2670.52)(427.1431, 4090.01)(428.1455, 1415.65)(429.1416, 970.24)(869.2781, 348.45)(870.2788, 270.44)(871.2641, 369.79) | 131118.1 | 52531.1 | 143905.9 | 59050.81 | 163781 | 53077.11 | 189990.9 | 59910.9 | 0.30 | 0.264734 | 0.361761 | 0.21 | 0.500683 | 0.753664 |
| COMPOUND_378_1938a9_921415 | Rp | - | 378.1938 | 9.92 | | | | (377.1865, 6909.99)(378.1894, 1415.49)(379.1868, 2342.62)(380.1876, 606.24)(381.1993, 79.33)(755.3501, 247.99)(756.3562, 195.19) | 16082.2 | 6301.635 | 17731.08 | 5331.25 | 17833.5 | 236.8808 | 19234 | 4800.668 | -0.94 | 4.65E-05 | 0.000155 | -0.16 | 0.52231 | 0.765284 |
| COMPOUND_378_2397a_97858 | Rp | - | 378.2397 | 8.98 | | | | (413.2076, 1258.25)(414.2119, 466.49)(415.1953, 973.36)(416.1885, 82.25)(417.1811, 1121.09)(377.2327, 21186.54)(378.2359, 5453.32)(379.2201, 3018.27)(380.216, 462.74)(755.4569, 54.17)(423.2381, 2474.94)(424.2409, 676.11) | 34366.3 | 21421.75 | 38747.56 | 21833.19 | 56824 | 13040.94 | 70271.9 | 26900.73 | -0.90 | 0.000275 | 0.000794 | -0.14 | 0.619017 | 0.817823 |
| COMPOUND_378_2774a10_447278 | Rp | + | 378.2774 | 10.45 | | | | (795.5212, 2803.14)(401.2766, 12881.11)(402.2796, 3978.07)(403.2861, 2414.99)(417.24, 1323.51)(418.2473, 607.26)(419.2358, 248.81)(396.3128, 85309.33)(397.3155, 21644.83)(398.3195, 3752.3)(379.284, 12176.12)(380.2853, 3806.79)(381.2884, 1333.58)(382.2869, 189.45)(774.5746, 496.05)(775.5868, 173.31)(776.5517, 1534.34) | 106328.8 | 58453.75 | 120333.6 | 122483.6 | 98136.92 | 55316.22 | 170162.7 | 93384.76 | 0.07 | 0.773955 | 0.833547 | 0.72 | 0.021012 | 0.199116 |
| COMPOUND_378_2925a10_860721 | Rp | + | 378.2925 | 10.86 | | | | (795.5388, 21262.57)(379.2956, 8735.38)(380.3016, 2420.43)(381.2989, 42268.68)(382.3018, 9692.21) | 86278.7 | 39238.88 | 74955.83 | 36999.67 | 94752.9 | 46046.77 | 93385.45 | 47789.32 | 0.28 | 0.279518 | 0.379202 | -0.10 | 0.741084 | 0.888965 |
| COMPOUND_379_2187a11_189893 | Rp | + | 379.2187 | 11.19 | | | | (759.4155, 1667.31)(797.3736, 4870.98)(798.363, 1208.37)(799.3926, 5055.43)(418.1813, 399.31)(380.2257, 82343.21)(381.2285, 19925.35)(382.2262, 35955.13)(383.2291, 9027.3)(384.2216, 15115.97)(385.224, 4168.74)(386.2212, 2194.37)(776.4692, 696.24)(777.4716, 615.37)(778.4787, 152.52) | 247264.8 | 50334.47 | 225822.5 | 51837.61 | 516646.2 | 173232.3 | 512284.3 | 149477.2 | 1.26 | 4.25E-07 | 2.37E-06 | 0.22 | 0.401307 | 0.690408 |
| COMPOUND_379_2729a9_27655 | Rp | + | 379.2723 | 9.28 | | | | (380.2805, 27882.69)(381.2835, 6664.5)(382.2911, 1996.5) | 53461.77 | 23179.89 | 45561.49 | 18184.66 | 66092.33 | 21889.73 | 47643.83 | 9648.144 | -1.17 | 9.32E-08 | 5.88E-07 | 0.06 | 0.786035 | 0.909997 |
| COMPOUND_380_378a11_01279 | Rp | + | 380.3780 | 11.01 | | | | (761.7973, 1670.69)(799.7292, 2605.38)(800.7174, 1925.64)(403.3787, 6057.42)(783.7488, 2734.44)(784.7294, 534.28)(785.7499, 2610.2)(381.3846, 100125.17)(382.3875, 27101.95)(383.3928, 4308.76)(384.3965, 565.79)(778.7644, 950.73) | 86710.07 | 36686 | 91328.74 | 40991.57 | 173480.8 | 115852.3 | 184249 | 160997.4 | 1.06 | 0.000155 | 0.000466 | -0.28 | 0.382371 | 0.685589 |
| COMPOUND_382_1098a6_195838 | Hiic | + | 382.1098 | 6.20 | | | | (383.1167, 10591.75)(384.1208, 1397.02)(385.1187, 176.59) | 7840.531 | 3125.66 | 6833.784 | 3378.778 | 9310.769 | 2106.677 | 10123.8 | 4702.338 | 0.39 | 0.142692 | 0.219047 | 0.55 | 0.085236 | 0.346484 |
| COMPOUND_382_1615a10_667491 | Rp | + | 382.1615 | 10.67 | | | | (765.353, 838.85)(383.1677, 31722.55)(384.1705, 7959.84)(385.1688, 17956.05)(386.1721, 4130.82)(387.1648, 6792.01)(388.1672, 1650.99)(389.1632, 883.23)(782.3612, 859.41) | 47576.15 | 16479.23 | 47937.35 | 19105.54 | 68336.29 | 27626.3 | 82394.84 | 38842.85 | 0.76 | 0.002877 | 0.006877 | 0.34 | 0.238609 | 0.543832 |
| COMPOUND_382_182a10_312435 | Rp | + | 382.1820 | 10.31 | no msms | | | (405.1598, 726.95)(421.1638, 1389.22)(383.1884, 14999.54)(384.1917, 3844.52)(385.1893, 6336.07)(386.1928, 1619.36)(387.1851, 3015.4)(388.1866, 695.02) | 12076.63 | 2125.312 | 16702.4 | 6333.529 | 19387 | 5676.229 | 31238.69 | 19188.14 | 0.32 | 0.074901 | 0.125878 | 0.85 | 0.000189 | 0.018868 |
| COMPOUND_382_2054a10_859109 | Rp | + | 382.2054 | 10.86 | | | | (765.4067, 3012.73)(803.345, 1888.33)(787.4163, 3693.73)(788.4213, 3996.25)(421.1788, 792.72)(400.2242, 1690.11)(383.2126, 61485.65)(384.2163, 16752.33)(385.2214, 3147.93)(782.418, 2786.44) | 150378.2 | 37426.69 | 137980.8 | 34614.5 | 250271.3 | 48672.64 | 277472.8 | 61868.7 | 1.15 | 5.26E-07 | 2.81E-06 | 0.52 | 0.035269 | 0.250187 |
| COMPOUND_382_2122a9_251608 | Rp | + | 382.2122 | 9.25 | | | | (383.2208, 9424.69)(384.2242, 2521.73)(385.2347, 787.28)(386.2223, 114.19) | 51004.57 | 22619.75 | 56499.35 | 25401.13 | 54704.25 | 29942.41 | 75066.7 | 31885.56 | -0.91 | 0.000139 | 0.000422 | -0.26 | 0.330998 | 0.636557 |
| COMPOUND_382_324a10_396373 | Rp | + | 382.3240 | 10.40 | | | | (383.3318, 9150.22)(384.3351, 2761.41)(385.3375, 621.95) | 14658.76 | 2585.681 | 13087.87 | 2571.217 | 19555.64 | 7435.435 | 18298.6 | 5452.75 | 1.09 | 1.35E-05 | 5.25E-05 | -0.20 | 0.461105 | 0.729797 |
| COMPOUND_382_3934a11_232425 | Rp | + | 382.3934 | 11.23 | | | | (765.754, 1247.91)(766.7343, 656.96)(787.7518, 1345.26)(383.4005, 41244.66)(384.4034, 11019.19)(385.4068, 1925.2)(386.4019, 220.26) | 351609.3 | 335382.7 | 283506.2 | 237286.3 | 869156.1 | 590360.9 | 147434 | 1061041 | 1.03 | 9.13E-05 | 0.000284 | 0.22 | 0.45469 | 0.725699 |
| COMPOUND_383_1524a10_576748 | Rp | - | 383.1524 | 10.58 | | | | (801.2459, 353.27)(802.258, 566.55)(803.2735, 491.22)(811.3231, 732.65)(812.3284, 426.18)(382.1448, 38867.64)(383.1474, 12789.82)(384.1497, 2980.16)(385.1474, 124.27)(765.2843, 454.76)(766.3046, 1534.02)(767.297, 1299.8)(879.3069, 453.84) | 183532.7 | 76179 | 199255.8 | 88403.68 | 214685 | 75312.17 | 254104.5 | 70800.73 | -0.05 | 0.848256 | 0.894514 | 0.65 | 0.054162 | 0.289719 |
| COMPOUND_383_3399a10_777776 | Rp | + | 383.3399 | 10.78 | | | | (767.7037, 1058.59)(406.3286, 6237.85)(407.3314, 1702.96)(422.2987, 976.3)(423.3047, 533.65)(384.3477, 11602.22)(385.3507, 3252.5)(386.3401, 189.87)(784.726, 1324.59)(785.7288, 1219.56) | 83765.26 | 19352.27 | 77950.8 | 21722.75 | 105442.6 | 33350.31 | 118967.8 | 19314.81 | 0.70 | 0.00899 | 0.019226 | 0.40 | 0.196835 | 0.507758 |
| COMPOUND_384_1601a5_617394 | Rp | - | 384.1601 | 5.62 | | | | (383.1529, 14388.69)(384.1565, 3483.78) | 18035.67 | 11693.39 | 18655.2 | 9784.407 | 40936.31 | 12567.61 | 30713.35 | 14319.51 | 1.52 | 3.1E-11 | 6.3E-10 | -0.72 | 0.001632 | 0.06002 |
| COMPOUND_384_1604a6_282825 | Rp | - | 384.1604 | 6.28 | | | | (383.1527, 4497.66)(384.1559, 10121.08)(385.1529, 2928.43)(386.1546, 437.55)(387.153, 32.0)(767.3124, 1501.41)(768.317, 721.72)(769.316, 327.62) | 181923.5 | 257969.2 | 172255.9 | 171457 | 541721.7 | 214533.2 | 370133.9 | 239933.1 | 1.55 | 9.76E-09 | 8.14E-08 | -0.73 | 0.009235 | 0.153413 |
| COMPOUND_384_1759a10_784266 | Rp | + | 384.1759 | 10.78 | | | | (769.3392, 1583.23)(770.3633, 1083.64)(807.3449, 1596.07)(791.3563, 1034.14)(423.1527, 176.79)(402.2216, 1071.06)(385.1822, 14920.04)(386.1869, 3505.01)(387.183, 6945.3)(388.186, 1702.57)(389.18, 2406.77)(390.1824, 1084.35)(391.1635, 784.9) | 28251.8 | 17763.11 | 28049.53 | 15558.99 | 24331.5 | 10224.39 | 38132.21 | 27354.59 | 0.02 | 0.944912 | 0.964615 | 0.83 | 0.002216 | 0.067469 |
| COMPOUND_384_3401a11_527961 | | | | | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--------------|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_385_1673a10_868931 | Rp | - | 385.1673 | 10.87 | | | | (805.335, 1344.03)(384.1606, 100249.88)(385.1655, 31212.05)(386.1646, 7995.63)(387.1673, 1174.14)(769.3231, 1809.42)(770.3383, 1199.81)(771.3452, 1154.3)(883.3443, 747.97) (403.3541, 17754.96)(404.3567, 6803.23)(386.3272, 11257.54)(387.3248, 4131.02)(388.3302, 189.53) (409.1628, 3140.61)(410.1684, 814.88)(411.1717, 218.01)(404.2077, 50154.91)(405.2108, 12894.66)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24) | 642139.5 | 69252.43 | 614268.4 | 72882.92 | 494991.3 | 162513.4 | 505132.6 | 105494.4 | -1.44 | 4.94E-08 | 3.4E-07 | 0.37 | 0.183835 | 0.497593 |
| COMPOUND_385_1919a10_459403 | Rp | + | 385.3199 | 10.46 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 56222.95 | 28204.55 | 42550.16 | 20641.11 | 64252.67 | 20376.43 | 101929.5 | 55430.48 | 0.32 | 0.214051 | 0.306643 | 0.63 | 0.037529 | 0.259604 |
| COMPOUND_386_1706a7_9313602 | Rp | + | 386.1706 | 7.93 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 124098.1 | 125022.5 | 72445.42 | 88761.32 | 60986 | 26048.11 | 48761.57 | 43092.16 | -1.23 | 1.08E-06 | 5.33E-06 | 0.42 | 0.127718 | 0.424221 |
| COMPOUND_386_1743a8_2173395 | Rp | + | 386.1743 | 8.22 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 25620.02 | 11284.57 | 23013.56 | 10018.04 | 10337 | #DIV/0! | 13825.15 | 3610.265 | -1.37 | 7.73E-10 | 8.93E-09 | 0.16 | 0.471118 | 0.734155 |
| COMPOUND_386_1749a7_864254 | Rp | + | 386.1749 | 7.86 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 231740.6 | 121617.8 | 199405.2 | 58936.45 | 43424.79 | 20240.69 | 51031.58 | 28797.09 | -1.77 | 1.32E-12 | 5.62E-11 | 0.40 | 0.096451 | 0.366905 |
| COMPOUND_386_1755a6_473585 | Rp | - | 386.1755 | 6.47 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 17159.05 | 6476.573 | 17023.43 | 5268.542 | 26232.31 | 10544.05 | 25202.11 | 18344.26 | 1.16 | 9.05E-07 | 4.54E-06 | -0.23 | 0.37013 | 0.671661 |
| COMPOUND_386_1755a5_6170444 | Rp | - | 386.1755 | 5.62 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 51040.15 | 21429.29 | 48735.87 | 15888.48 | 79661.07 | 54382.13 | 59109 | 44415.25 | 0.46 | 0.129254 | 0.20256 | -0.50 | 0.170552 | 0.485567 |
| COMPOUND_386_1756a7_296122 | Rp | - | 386.1756 | 7.30 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 24541.52 | 11408.51 | 24006.68 | 11677.58 | 57356.57 | 23443.14 | 47265.76 | 26738.99 | 1.51 | 3.44E-10 | 4.42E-09 | -0.54 | 0.024998 | 0.219303 |
| COMPOUND_386_1756a5_6674857 | Rp | - | 386.1756 | 5.67 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 58891.49 | 36097.24 | 55044.2 | 26589.45 | 138773.4 | 61236 | 104818.4 | 64203.22 | 1.32 | 3.61E-06 | 1.58E-05 | -0.50 | 0.109048 | 0.391669 |
| COMPOUND_386_1878a8_722836 | Rp | + | 386.1878 | 8.72 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 22611.27 | 4521.374 | 21098.2 | 6236.652 | 21481.71 | 6389.985 | 20522.98 | 4377.833 | -0.03 | 0.923778 | 0.950653 | 0.06 | 0.864182 | 0.943353 |
| COMPOUND_387_1618a9_927632 | Rp | + | 387.1618 | 9.93 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 17945.94 | 5710.612 | 18979.23 | 5899.716 | 20149 | 1013.468 | 23399.38 | 5960.526 | -1.00 | 2.6E-05 | 9.41E-05 | -0.02 | 0.94411 | 0.974642 |
| COMPOUND_387_2201a11_016309 | Rp | + | 387.2201 | 11.02 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 22942.92 | 6167.906 | 21631.08 | 5708.548 | 33947.83 | 8421.467 | 31020.63 | 9169.111 | 0.74 | 0.00748 | 0.016338 | 0.10 | 0.753439 | 0.890558 |
| COMPOUND_387_298a10_86685723 | Hilic | - | 387.2980 | 0.87 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 24670.76 | 9564.171 | 28688.81 | 8141.631 | 17269.92 | 7099.418 | 21673.8 | 9370.668 | -0.43 | 0.122961 | 0.194457 | 0.03 | 0.939042 | 0.97184 |
| COMPOUND_387_3392a10_695449 | Rp | + | 387.3392 | 10.70 | no mms | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 28836.85 | 18540.75 | 23233.91 | 9595.818 | 26997.56 | 7839.107 | 52698.11 | 33069.44 | 0.18 | 0.367564 | 0.469863 | 1.12 | 1.93E-05 | 0.005768 |
| COMPOUND_388_1912a6_901253 | Rp | - | 388.1912 | 6.90 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 28688.11 | 16267.13 | 29555.22 | 20055.4 | 69457.5 | 31273.67 | 57350.28 | 34559.55 | 1.23 | 1.07E-08 | 8.73E-08 | -0.33 | 0.125664 | 0.423013 |
| COMPOUND_388_222a9_917744 | Rp | - | 388.2220 | 9.92 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 66366.66 | 24892.88 | 74988.5 | 25421.89 | 60463.5 | 28805.16 | 61274.93 | 35157.31 | -0.99 | 1.93E-05 | 7.24E-05 | -0.32 | 0.214103 | 0.521709 |
| COMPOUND_389_0504a10_468301 | Rp | - | 389.0504 | 10.47 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 12579.65 | 2468.974 | 12756 | 1670.589 | 34310.93 | 9061.815 | 35200.67 | 10354.62 | 1.42 | 2.98E-14 | 4.19E-12 | 0.14 | 0.403246 | 0.691103 |
| COMPOUND_389_1546a11_008361 | Rp | - | 389.1546 | 11.01 | | | | (409.1651, 1401.51)(410.1627, 412.14)(411.1735, 130.57)(404.2086, 435.9)(405.2192, 232.75)(387.1817, 8364.55)(388.1853, 1797.99)(389.1926, 1213.37) (409.162, 3794.59)(410.1653, 995.6)(411.1694, 214.41)(425.1363, 972.18)(426.1396, 196.99)(427.1318, 174.51)(404.2075, 16760.91)(405.2107, 4535.62)(406.2152, 885.28)(407.2123, 130.28)(387.1812, 71342.19)(388.1843, 17480.46)(389.1886, 3839.24)(390.191, 516.63) | 17159.78 | 4952.057 | 17489.76 | 5362.747 | 25178.57 | 9688.534 | 24935.79 | 10015.73 | 1.09 | 8.72E-05 | 0.000272 | -0.22 | 0.476608 | 0.739711 |
| COMPOUND_389_1785a10_689982 | | | | | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|--------------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_395_1556a1_2353802 | Hilic | + | 395.1556 | 1.24 | | | | (418.1462, 336.68)(813.3099, 83.127)(396.1632, 4844.23)(397.1664, 866.81)(398.168, 105.93) | 12572.66 | 1914.18 | 12427.43 | 2254.02 | 18221.93 | 2741.019 | 16941.23 | 3912.285 | 1.41 | 5.07E-07 | 2.73E-06 | -0.31 | 0.298424 | 0.60748 |
| COMPOUND_395_187a10_686862 | Rp | - | 395.1870 | 10.69 | | | | (825.3765, 734.93)(432.1606, 27067.83)(835.3424, 635.98)(836.3493, 575.67)(837.344, 625.99)(394.1814, 5265.3)(395.1829, 1587.66)(396.1833, 506.25)(903.3247, 469.12)(904.3465, 423.58) | 137612.9 | 16439.48 | 138501 | 24609.81 | 118175.4 | 41568.61 | 115186.5 | 31931.4 | -0.74 | 0.003183 | 0.00753 | -0.28 | 0.325093 | 0.632765 |
| COMPOUND_395_2218a10_000543 | Rp | + | 395.2218 | 10.00 | | | | (396.2308, 13398.48)(397.2339, 3638.85)(398.2289, 5168.3)(399.2332, 1275.65)(400.2391, 354.27)(808.4717, 1417.35)(809.4604, 769.94) | 41958.12 | 15534.23 | 38076.62 | 12925.54 | 31773 | 4760.846 | 33468.25 | 11828.97 | -1.26 | 2.55E-08 | 1.88E-07 | 0.10 | 0.666092 | 0.845092 |
| COMPOUND_396_1699a6_5587883 | Rp | - | 396.1699 | 6.56 | | | | (395.1628, 12616.18)(396.1662, 2926.81)(397.1606, 4173.73)(398.1626, 982.1)(399.165, 192.73) | 16829.27 | 4331.436 | 18032.44 | 4529.683 | 32404 | 6834.184 | 35274.36 | 11439.02 | 1.27 | 3.77E-06 | 1.64E-05 | -0.27 | 0.365652 | 0.669574 |
| COMPOUND_396_1967a8_501419 | Rp | - | 396.1967 | 8.50 | steroid sulfate | 3 | 10 eV: 395.1874 (100), 96.9594 (25) | (509.168, 465.53)(395.1894, 34890.1)(396.1928, 8550.42)(397.1938, 3006.78)(398.1961, 458.97) | 165602.4 | 94476.1 | 193519.9 | 150129.3 | 304681 | 118993.6 | 188203.1 | 101332.5 | 1.30 | 7.88E-06 | 3.21E-05 | -1.34 | 6.74E-05 | 0.010116 |
| COMPOUND_396_2179a11_016559 | Rp | + | 396.2179 | 11.02 | | | | (793.4441, 336.89)(831.4018, 3865.22)(832.3984, 1048.51)(815.424, 1074.29)(397.2279, 8604.16)(398.232, 2707.32)(399.2372, 650.71) | 42031.05 | 12397.44 | 37312.21 | 9950.868 | 55784.08 | 34860.52 | 57551.6 | 20788.7 | 0.57 | 0.031669 | 0.059136 | 0.34 | 0.270725 | 0.579536 |
| COMPOUND_396_2201a11_018905 | Rp | + | 396.2201 | 11.02 | | | | (793.4243, 351.33)(831.3905, 1975.22)(832.4076, 799.49)(815.4231, 981.5)(397.2288, 7288.21)(398.2333, 2757.4)(399.2389, 719.31) | 38686.84 | 9992.376 | 35815.95 | 8254.826 | 44830.46 | 14768.18 | 49212.08 | 14166.06 | 0.69 | 0.006252 | 0.013844 | 0.34 | 0.249199 | 0.558959 |
| COMPOUND_396_2269a10_665085 | Rp | - | 396.2269 | 10.67 | | | | (827.4016, 997.84)(395.2197, 30907.36)(396.223, 7504.79)(397.2266, 1332.83)(398.2271, 123.94)(791.4443, 1416.21)(792.4428, 1262.19)(793.4432, 611.56) | 66087.11 | 17829.53 | 76138.61 | 30669.24 | 65232.21 | 26489.25 | 81254.39 | 31850.23 | -0.19 | 0.478577 | 0.581628 | 0.39 | 0.208994 | 0.518913 |
| COMPOUND_397_1213a10_497002 | Rp | - | 397.1213 | 10.50 | | | | (510.105, 943.69)(839.2209, 525.25)(840.2096, 493.61)(841.22, 433.2)(396.1164, 11989.19)(397.1203, 3465.99)(398.1146, 4070.99)(399.1178, 988.15)(400.1148, 291.42)(793.1998, 593.58)(794.2106, 528.37)(907.2064, 351.63)(908.2108, 291.09) | 44947 | 12716.25 | 50838 | 13063.43 | 52951.2 | 11846.56 | 62937.45 | 20142.59 | 0.49 | 0.400544 | 0.073162 | 0.30 | 0.284409 | 0.593016 |
| COMPOUND_397_2053a10_917028 | Rp | - | 397.2053 | 10.92 | | | | (829.4048, 794.18)(432.181, 33369.58)(433.1837, 8655.95)(434.1815, 4062.16)(839.3774, 525.06)(396.1986, 6814.79)(397.2, 2833.87)(398.2016, 434.13)(793.3661, 1357.64)(794.3793, 903.82)(907.4035, 290.07)(908.3953, 245.35)(909.3908, 369.64) | 115897 | 79768.53 | 91216.26 | 50077.41 | 122615.3 | 82257.99 | 94015.4 | 53599.67 | -0.72 | 0.0025 | 0.006086 | -0.09 | 0.755385 | 0.895058 |
| COMPOUND_397_3199a8_86249 | Rp | + | 397.3199 | 8.86 | ACar 16:1 | 2 | 10eV: 398.3277(100), 85.0287(6), 237.2237(4) | (420.3024, 1819.21)(421.3057, 376.56)(422.2914, 3252.86)(423.3053, 1547.02)(398.3276, 9511.78)(399.3313, 2604.08)(400.331, 468.5)(401.3415, 73.95) | 54508.08 | 24006.26 | 49437.89 | 19748.34 | 55194.57 | 29596.69 | 64438.79 | 26578.52 | -0.01 | 0.966729 | 0.980664 | 0.53 | 0.138817 | 0.444794 |
| COMPOUND_398_2119a9_107574 | Rp | - | 398.2119 | 9.11 | Unknown | 4 | 10 eV: 397.2047 (100), 243.9077 (5) | (511.1857, 1467.05)(512.1866, 67.88)(513.1862, 434.17)(397.2046, 763105.3)(398.2085, 164885.31)(399.2154, 88588.81)(795.416, 1786.83)(796.4203, 960.17)(797.429, 1221.94)(798.4328, 584.69)(799.4456, 630.36)(800.4473, 305.59)(801.4483, 107.76) | 342839.5 | 223399.3 | 320956.5 | 341254.5 | 6039262 | 4537443 | 3030805 | 2690834 | 1.86 | 5.2E-12 | 1.48E-10 | -0.92 | 0.000573 | 0.039109 |
| COMPOUND_398_2129a9_051908 | Rp | - | 398.2120 | 9.05 | | | | (511.1938, 670.13)(512.1869, 252.6)(513.2007, 4581.98)(397.2047, 728685.75)(398.2084, 154584.11)(399.2145, 74286.28)(795.4176, 1933.17)(796.4214, 965.96)(797.4327, 11868.54)(798.4355, 5506.51)(799.4477, 25246.61)(800.4511, 11568.13)(801.4499, 4935.67) | 157852.9 | 160128.7 | 139934 | 158689.9 | 603789.8 | 426374.8 | 1044924 | 1424371 | 1.22 | 1.56E-06 | 7.5E-06 | 0.14 | 0.611962 | 0.814985 |
| COMPOUND_398_2129a8_772959 | Rp | - | 398.2129 | 8.77 | | | | (397.2052, 25211.3)(398.208, 6148.52)(399.2126, 2121.6)(400.2059, 291.75)(795.4168, 3262.22)(796.4201, 1547.14)(797.421, 774.77)(798.4219, 238.11)(799.4172, 59.87) | 185079 | 98777.25 | 185162 | 104111.5 | 1878052 | 928775.9 | 1021511 | 882956.3 | 1.92 | 3.28E-13 | 1.99E-11 | -0.55 | 0.027374 | 0.226687 |
| COMPOUND_398_2129a8_106329 | Rp | - | 398.2129 | 8.11 | | | | (397.205, 64228.56)(398.2082, 15404.26)(399.2063, 5017.69)(400.2076, 703.41)(795.4174, 2931.44)(796.4203, 1575.54)(797.4214, 639.39) | 602163.8 | 292010.5 | 721258.4 | 650914.6 | 320121.3 | 116290.2 | 267184.5 | 123842.5 | -1.18 | 3.34E-07 | 1.9E-06 | -0.30 | 0.216702 | 0.527444 |
| COMPOUND_398_2293a7_8818645 | Rp | - | 398.2293 | 7.88 | | | | (397.222, 4177.43)(398.225, 1024.38)(399.2204, 3816.23)(400.2234, 832.16)(401.2208, 321.99) | 42119.04 | 18120.61 | 40271.15 | 14391.25 | 76817 | 25392.11 | 48144.27 | 23714.67 | -0.48 | 0.07197 | 0.121679 | 0.54 | 0.09458 | 0.36381 |
| COMPOUND_398_2445a9_604185 | Rp | + | 398.2445 | 9.60 | | | | (421.2332, 18751.93)(422.2357, 3855.46)(423.2444, 671.24)(437.2071, 798.18)(438.2112, 160.32)(439.2005, 185.53)(439.2515, 341585.3)(400.255, 66295.18)(401.2578, 10733.9)(402.2604, 1536.77)(814.5513, 470.21) | 101827.5 | 141082.3 | 110207.4 | 213710.7 | 96475.92 | 71303.23 | 83996.52 | 97720.25 | 0.20 | 0.499943 | 0.600465 | 0.05 | 0.895811 | 0.954308 |
| COMPOUND_398_2513a10_60243 | Rp | + | 398.2513 | 10.60 | | | | (797.5411, 3171.72)(835.4581, 1035.94)(437.208, 1331.48)(438.2197, 567.99)(439.2062, 2935.27)(440.2128, 719.58)(441.2032, 1466.47)(399.26, 5639.71)(400.264, 1675.22)(401.2589, 1837.39)(402.2641, 633.1) | 32203.8 | 7492.452 | 33491.54 | 8284.305 | 27645.44 | 6971.124 | 30448.63 | 8853.65 | -0.08 | 0.753312 | 0.821132 | 0.44 | 0.168116 | 0.480454 |
| COMPOUND_399_1832a11_005366 | Rp | - | 399.1832 | 11.01 | | | | (833.3732, 594.62)(834.3915, 331.01)(512.1608, 1789.02)(843.3808, 737.9)(844.3899, 665.35)(845.3832, 842.07)(398.1758, 23437.02)(399.1812, 7001.04)(401.1791, 2261.14)(401.1916, 265.36)(797.339, 781.47)(798.3584, 561.01)(799.3554, 481.48)(911.2945, 540.20)(912.3169, 437.25)(913.2876, 168.93) | 100051 | 18607.89 | 109990.1 | 34770.1 | 97920.07 | 9402.353 | 109210.6 | 41845.16 | -0.09 | 0.772054 | 0.833547 | -0.14 | 0.691778 | 0.857326 |
| COMPOUND_399_3364a10_449236 | Rp | + | 399.3364 | 10.45 | | | | (422.323, 3964.0)(423.3268, 2085.96)(438.2996, 12535.13)(439.3028, 28192.77)(417.3648, 1731.81)(400.3423, 14244.47)(401.3447, 4361.25)(402.344, 567.15) | 290038.8 | 84106.48 | 280762 | 85248.86 | 128922.8 | 117522 | 133388.9 | 83207.69 | -1.55 | 1.27E-08 | 1.02E-07 | 0.38 | 0.181997 | 0.495594 |
| COMPOUND_399_3364a9_184375 | Rp | + | 399.3364 | 9.18 | Palmitoylcarnitine | 1 | 10eV: 400.3445(100), 85.0271(7), 341.2713(4) | (400.343, 53203.54)(401.3464, 13585.63)(402.3489, 3114.25)(403.3462, 463.59) | 199278.4 | 60070.98 | 186998.8 | 49497.77 | 167695.6 | 53663.97 | 212192.1 | 62264.36 | -0.59 | 0.048549 | 0.085349 | 1.00 | 0.005671 | 0.118614 |
| COMPOUND_400_2277a7_921427 | Rp | - | 400.2277 | 7.92 | | | | (399.2203, 15890.24)(400.2239, 3807.35)(401.2211, 1224.01)(402.2213, 188.02) | 24308.06 | 9320.807 | 24818 | 8641.05 | 81344.07 | 22426.16 | 65369.14 | 36103.42 | 1.65 | 9.73E-11 | 1.47E-09 | -0.34 | 0.174503 | 0.488924 |
| COMPOUND_400_2281a8_326689 | Rp | - | 400.2281 | 8.33 | | | | (127425.15)(401.2217, 35794.13)(799.4449, 2826.81)(800.4512, 1450.08)(801.4506, 596.85)(802.452, 190.32) | 1067164 | 403522.5 | 1015878 | 461732.2 | 2486519 | 792380.4 | 1941831 | 949854.7 | 1.46 | 4.62E-08 | 3.2E-07 | -0.38 | 0.172426 | 0.487735 |
| COMPOUND_400_2283a9_027945 | Rp | - | 400.2283 | 9.03 | | | | (399.2198, 1095795.6)(400.2238, 241989.56)(401.222, 65890.29)(799.4481, 7313.84)(800.4514, 3242.13)(801.4501, 1406.52)(802.4502, 430.33)(803.4486, 101.72) | 902656.1 | 352283.7 | 993375.8 | 516136.8 | 4970717 | 5008438 | 3428228 | 2318867 | 1.69 | 2.22E-12 | 7.71E-11 | -0.35 | 0.117957 | 0.408047 |
| COMPOUND_400_2819a10_460036 | Rp | - | 400.2819 | 10.46 | | | | (835.5346, 1745.45)(836.5341, 1009.21)(837.5341, 520.48)(399.2746, 43311.87)(400.2777, 11243.61)(401.2794, 2237.73)(402.2824, 336.33) | 20834.62 | 8826.05 | 30206.16 | 25440.63 | 25041.78 | 9367.897 | 35491.84 | 20320.08 | 0.18 | 0.469136 | 0.572936 | 0.66 | 0.026351 | 0.224785 |
| COMPOUND_400_335a11_224104 | Rp | + | 400.3350 | 11.22 | | | | (423.3188, 1117.57)(424.3365, 510.04)(401.3425, 22143.68)(402.347, 7065.06)(403.3505, 35180.04) | 16978.41 | 32364.08 | 14298.67 | 16713.67 | 3838.865 | 15092.33 | 4105.087 | 1.19 | 9.51E-08 | 5.98E-07 | 0.04 | 0.870191 | 0.945212 | |
| COMPOUND_400_335a11_06124 | Rp | + | 400.3354 | 11.06 | | | | (801.6795, 1615.75)(423.3247, 9291.2)(424.3281, 2746.7)(425.3326, 645.94)(823.6516, 449.7)(418.3729, 1281.12)(401.3428, 11524.58)(402.3498, 4211.73)(403.3536, 996.16)(404.3535, 162.5)(818.6695, 2080.03) | 62722.3 | 37801.64 | 53681.18 | 27624.11 | 65365.43 | 38906.06 | 75599.6 | 52487.03 | 0.07 | 0.871615 | 0.84059 | -0.10 | 0.730694 | 0.885165 |
| COMPOUND_401_2364a11_1903715 | Rp | + | 401.2364 | 11.19 | | | | (841.4229, 637.66)(825.4316, 1075.33)(826.424, 732.68)(827.4375, 909.26)(402.2434, 58581.97)(403.2467, 14052.43)(404.2483, 2406.05) | 79677.57 | 16100.7 | 70006.75 | 13654.31 | 168385.1 | 58127.55 | 174501.4 | 49302.31 | 1.13 | 3.19E-06 | 1.41E-05 | 0.47 | 0.077779 | 0.333235 |
| COMPOUND_4 | | | | | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | | |
|-----------------------------|--------|----------|----------|-----------|----------------|--|--------------|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|---------|----------|----------|-------------|----------|----------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | | |
| COMPOUND_403_1595a9_920933 | Rp | - | 403.1595 | 9.92 | | | | (81.2975, 602.82) (842.3086, 359.61) (843.3161, 415.02) (438.1268, 555.81) (439.1303, 1347.55) (440.136, 345.08) (441.1397, 1381.45) (442.139, 1028.08) (851.3032, 317.61) (852.3264, 306.09) (853.3096, 454.23) (402.1559, 2661.09) (403.1525, 705.21) (404.1454, 6774.71) (448.1565, 4589.8) (449.1479, 81.41) (421.3091, 1810.86) (404.3018, 1996.03) (405.3051, 4973.4) (406.3029, 307.41) (439.188, 1312.73) (403.2091, 6227.34) (404.2133, 1280.64) (405.2122, 320.51) (439.1877, 153.55) (403.2116, 5046.15) (404.2148, 1155.31) (405.2125, 621.68) (406.2308, 74.54) (517.3056, 2874.93) (518.3082, 697.39) (439.2832, 423.93) (440.2824, 101.57) (403.3059, 36764.26) (404.3093, 8942.75) (405.3118, 1578.71) (406.3144, 235.88) (451.2909, 12333.44) | 34297.47 | 16709.95 | 36539.26 | 16255.11 | 29869 | #DIV/0! | 44198.43 | 10219.56 | -1.10 | 1.77E-06 | 8.36E-06 | -0.06 | 0.820023 | 0.922833 | | |
| COMPOUND_403_2946a10_85513 | Rp | + | 403.2946 | 10.86 | | | | (421.3091, 1810.86) (404.3018, 1996.03) (405.3051, 4973.4) (406.3029, 307.41) (439.188, 1312.73) (403.2091, 6227.34) (404.2133, 1280.64) (405.2122, 320.51) (439.1877, 153.55) (403.2116, 5046.15) (404.2148, 1155.31) (405.2125, 621.68) (406.2308, 74.54) (517.3056, 2874.93) (518.3082, 697.39) (439.2832, 423.93) (440.2824, 101.57) (403.3059, 36764.26) (404.3093, 8942.75) (405.3118, 1578.71) (406.3144, 235.88) (451.2909, 12333.44) | 63991.72 | 17946.65 | 58426.22 | 15494.28 | 113352.6 | 24027.32 | 122140.1 | 28795.13 | 1.17 | 4.42E-07 | 2.44E-06 | 0.45 | 0.071293 | 0.325554 | | |
| COMPOUND_404_2153a8_81256 | Rp | - | 404.2153 | 8.81 | | | | (439.188, 1312.73) (403.2091, 6227.34) (404.2133, 1280.64) (405.2122, 320.51) (439.1877, 153.55) (403.2116, 5046.15) (404.2148, 1155.31) (405.2125, 621.68) (406.2308, 74.54) (517.3056, 2874.93) (518.3082, 697.39) (439.2832, 423.93) (440.2824, 101.57) (403.3059, 36764.26) (404.3093, 8942.75) (405.3118, 1578.71) (406.3144, 235.88) (451.2909, 12333.44) | 25804.94 | 11728.33 | 27067.43 | 9992.113 | 26605.5 | 4608.215 | 26156.33 | 10854.09 | -1.09 | 1.96E-06 | 9.14E-06 | -0.15 | 0.554157 | 0.781442 | | |
| COMPOUND_404_2185a8_720452 | Rp | - | 404.2185 | 8.72 | | | | (439.188, 1312.73) (403.2091, 6227.34) (404.2133, 1280.64) (405.2122, 320.51) (439.1877, 153.55) (403.2116, 5046.15) (404.2148, 1155.31) (405.2125, 621.68) (406.2308, 74.54) (517.3056, 2874.93) (518.3082, 697.39) (439.2832, 423.93) (440.2824, 101.57) (403.3059, 36764.26) (404.3093, 8942.75) (405.3118, 1578.71) (406.3144, 235.88) (451.2909, 12333.44) | 25145.49 | 9301.792 | 26038.85 | 11038.82 | 16396.5 | 86.97413 | 21192 | 8522.468 | -1.31 | 5.87E-09 | 5.07E-08 | 0.12 | 0.99554 | 0.804532 | | |
| COMPOUND_404_3134a10_927403 | Rp | - | 404.3134 | 10.93 | | | | (517.3056, 2874.93) (518.3082, 697.39) (439.2832, 423.93) (440.2824, 101.57) (403.3059, 36764.26) (404.3093, 8942.75) (405.3118, 1578.71) (406.3144, 235.88) (451.2909, 12333.44) | 69639.87 | 33639.53 | 83423.82 | 37353.54 | 34854.67 | 25666.69 | 39821.44 | 34772.9 | -0.99 | 6.23E-05 | 0.000203 | -0.30 | 0.280094 | 0.587858 | | |
| COMPOUND_405_2892a9_249067 | Rp | + | 405.2892 | 9.25 | | | | (406.2957, 14165.16) (407.2989, 3961.12) (408.3036, 986.53) (409.3136, 145.99) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.93 | 8.22E-05 | 0.000257 | 0.01 | 0.966808 | 0.982565 | |
| COMPOUND_406_1982a6_558121 | Rp | - | 406.1982 | 6.56 | 4 | 10 eV: 329.1735(100), 301.1781(16), 405.1858(8), 129.873(8) | | (405.1915, 12883.21) (406.1944, 3017.74) (407.1986, 539.75) (408.1995, 63.84) (451.1964, 863.71) (452.2017, 225.27) | 20064.62 | 5250.175 | 21251.16 | 5105.504 | 37616.57 | 6814.944 | 41416.58 | 13086.58 | | | 1.25 | 7.21E-06 | 2.96E-05 | -0.28 | 0.360621 | 0.666906 |
| COMPOUND_406_2268a11_005156 | Rp | + | 406.2268 | 11.01 | | | | (813.4362, 2845.04) (851.4516, 5138.57) (429.2132, 335.71) (835.4424, 1933.21) (445.1843, 210.52) (407.2354, 8612.04) (408.2404, 2597.73) (409.2377, 6316.94) (410.2378, 1682.25) (411.2337, 2917.73) (412.2377, 885.55) (413.2242, 1065.05) | 48995.57 | 16542.03 | 45654.87 | 18072.65 | 59995.14 | 31526.98 | 54549.82 | 20583.48 | 0.53 | 0.066344 | 0.11379 | 0.08 | 0.813006 | 0.92097 | | |
| COMPOUND_406_2277a11_001731 | Rp | + | 406.2277 | 11.00 | | | | (813.4351, 391.78) (851.4515, 4977.15) (429.2084, 453.88) (835.4406, 1915.92) (445.1899, 212.97) (407.2368, 9846.65) (408.2403, 2528.95) (409.2378, 828.85) (410.2399, 2297.37) (411.2352, 3498.93) (412.2367, 1213.21) (413.2223, 213.14) | 45822.18 | 17845.26 | 48529 | 18175.51 | 55143.14 | 30784.56 | 52472.11 | 20943.63 | 0.44 | 0.13771 | 0.212996 | -0.04 | 0.907354 | 0.958319 | | |
| COMPOUND_406_2347a9_558533 | Rp | - | 406.2347 | 9.56 | | | | (405.2276, 20771.5) (406.2312, 5453.51) (407.2405, 2382.42) (408.2433, 289.11) | 58600.53 | 33730.41 | 61153.67 | 29633.09 | 53396.25 | 25668.55 | 71602.2 | 28696.27 | -1.02 | 1.3E-05 | 5.09E-05 | -0.19 | 0.465085 | 0.732912 | | |
| COMPOUND_406_2351a9_501248 | Rp | - | 406.2351 | 9.50 | | | | (405.2277, 15945.51) (406.2311, 4219.31) (407.236, 958.28) (408.2443, 138.84) | 42923.72 | 23753.85 | 45211.2 | 21258.5 | 38360.75 | 16455.02 | 53326.5 | 17786.22 | -1.03 | 1.1E-05 | 4.37E-05 | -0.18 | 0.486275 | 0.747178 | | |
| COMPOUND_406_2353a9_245045 | Rp | - | 406.2353 | 9.25 | | | | (405.2277, 3897.25) (406.2312, 9852.23) (407.234, 1833.7) (408.2353, 246.61) | 52391.81 | 29207.48 | 55324.02 | 26633.16 | 57345.67 | 6367.557 | 64747.8 | 24397.71 | -1.04 | 1E-05 | 4.01E-05 | -0.15 | 0.552234 | 0.780002 | | |
| COMPOUND_407_1523a10_501683 | Rp | - | 407.1523 | 10.50 | | | | (849.2845, 427.31) (850.2834, 380.81) (851.3005, 333.05) (520.1504, 460.85) (521.153, 236.49) (522.1511, 1263.99) (523.1447, 678.3) (859.3126, 468.94) (860.3299, 202.55) (861.3235, 272.44) (406.1449, 14157.24) (407.1503, 4640.42) (408.1505, 1347.83) (409.1465, 147.75) (813.3053, 581.9) (814.3061, 528.26) (815.2813, 482.25) (452.1701, 966.3) (453.1812, 455.76) (454.1645, 6394.53) (455.1661, 1723.13) (927.3322, 227.38) (928.3293, 176.42) (929.3132, 273.63) | 116957.9 | 50044.06 | 126983.7 | 56644.95 | 120265 | 43095.01 | 141817.2 | 51876.54 | -0.16 | 0.578874 | 0.675453 | 0.12 | 0.717289 | 0.876415 | | |
| COMPOUND_407_2472a11_585079 | Rp | + | 407.2472 | 11.59 | | | | (853.4761, 2656.4) (854.4609, 849.54) (837.4748, 905.0) (446.2181, 227.37) (408.2563, 9999.27) (409.2595, 3205.27) (410.2575, 4524.43) (411.2555, 1457.45) (412.2517, 1966.46) (413.2605, 661.04) (832.5003, 359.05) | 26970.14 | 8912.843 | 26129.83 | 7267.28 | 31603.43 | 8447.252 | 30241.02 | 9799.798 | 0.47 | 0.104978 | 0.169836 | -0.08 | 0.804999 | 0.917422 | | |
| COMPOUND_407_3021a10_822291 | Rp | + | 407.3021 | 10.82 | | | | (425.3235, 2599.57) (408.3097, 518468.53) (409.3133, 118893.58) (410.3157, 18611.31) (411.3171, 2467.95) | 166562.9 | 123284.2 | 280184.2 | 159471 | 584333.6 | 488235.5 | 618532.7 | 404298.6 | 1.26 | 1.73E-06 | 8.23E-06 | -0.37 | 0.196509 | 0.507758 | | |
| COMPOUND_407_3031a10_7575 | Rp | + | 407.3031 | 10.76 | | | | (408.31, 284984.28) (409.313, 65166.04) (410.3153, 10655.44) (411.3187, 1489.37) (412.3167, 167.92) | 300016 | 166329.1 | 385606.4 | 165800.3 | 583809.7 | 417515.9 | 602489.6 | 352927.8 | 0.99 | 0.000421 | 0.001182 | -0.25 | 0.439241 | 0.715597 | | |
| COMPOUND_408_1967a10_444244 | Rp | + | 408.1967 | 10.44 | | | | (817.3753, 500.44) (818.3445, 518.48) (855.391, 610.18) (856.3375, 449.77) (431.1869, 465.71) (432.2041, 56.34) (433.1905, 426.54) (839.3718, 287.47) (840.3918, 521.81) (426.2118, 1004.06) (409.2039, 30139.56) (410.2074, 7003.22) (411.2055, 11384.28) (412.2077, 3008.81) (413.2032, 4704.49) (414.2044, 1467.12) (415.2092, 1115.87) (205.1057, 299.91) (205.6049, 48.25) (206.1052, 287.37) (834.4653, 785.68) (835.4662, 690.41) | 26116.52 | 13628.76 | 31709.09 | 18836.71 | 29247.38 | 12493.11 | 51710.61 | 30291.26 | 0.22 | 0.352223 | 0.454039 | 0.60 | 0.0353 | 0.250187 | | |
| COMPOUND_408_2143a6_7962737 | Rp | - | 408.2143 | 6.80 | 4 | 20 eV: 331.1919(100), 44.9974(27), 282.1274(15), 125.0615(7) | | (407.2072, 86569.58) (408.2106, 21334.57) (409.2141, 3542.41) (410.2187, 499.93) (453.2114, 2474.95) (454.2141, 647.51) (455.2231, 844.83) | 808708.04 | 29996.61 | 96324.46 | 35808.68 | 191484.7 | 60492.18 | 155775.9 | 85486.29 | 1.45 | 8.51E-07 | 4.29E-06 | -0.82 | 0.010769 | 0.163867 | | |
| COMPOUND_408_2516a10_857087 | Rp | + | 408.2516 | 10.86 | | | | (855.4652, 879.08) (431.2541, 993.15) (447.207, 871.138) (409.2576, 22898.01) (410.26, 5714.49) (411.2629, 1621.05) (412.2633, 236.15) (834.5378, 25160.23) (835.5366, 12123.26) (836.5456, 352481.94) | 1157785 | 267362.9 | 1103329 | 381120.4 | 353864.1 | 504841.6 | 277933.8 | 416813.6 | -0.62 | 0.029724 | 0.055968 | 0.19 | 0.564402 | 0.785799 | | |
| COMPOUND_409_2484a8_333355 | Rp | + | 409.2484 | 8.33 | | | | (432.2391, 2317.33) (433.2424, 702.03) (434.249, 262.11) (410.2544, 15392.23) (411.2605, 3762.13) (412.2695, 101.141) | 38102.52 | 17972.18 | 32774.61 | 14092.26 | 24487 | #DIV/0! | 22681 | 15809.39 | -1.29 | 2.47E-09 | 2.44E-08 | 0.20 | 0.361079 | 0.667063 | | |
| COMPOUND_410_2115a10_692786 | Rp | + | 410.2115 | 10.69 | no mms | | | (821.4467, 869.73) (859.4208, 579.45) (860.4015, 385.13) (861.4114, 523.78) (843.4116, 1240.74) (844.3978, 864.86) (845.4017, 770.42) (428.2356, 423.84) (429.2393, 166.08) (411.2198, 36324.95) (412.2227, 8913.26) (413.2221, 14718.33) (414.2235, 2848.36) (415.2164, 5837.38) (416.2197, 1466.55) (417.2214, 882.43) | 35808.13 | 17250.28 | 35715.5 | 9126.48 | 43358.27 | 17403.81 | 79627.54 | 41759.72 | 0.09 | 0.704234 | 0.783952 | 1.20 | 4.79E-05 | 0.008997 | | |
| COMPOUND_410_2124a10_690761 | Rp | + | 410.2124 | 10.69 | no mms | | | (821.4476, 1328.53) (859.4135, 666.39) (860.4153, 336.67) (861.4142, 716.76) (843.4282, 844.72) (844.4369, 290.78) (845.4153, 376.8) (428.2271, 297.74) (429.227, 122.23) (411.2196, 40396.33) (412.2231, 9500.65) (413.2207, 15421.64) (414.223, 3613.58) (415.2151, 6025.9) (416.2193, 1705.22) (417.2205, 1216.51) | 36197.93 | 16500.29 | 34022.03 | 14252.87 | 38082.55 | 15848.79 | 71732.07 | 42615.66 | 0.09 | 0.712135 | 0.788624 | 1.11 | 0.000145 | 0.017228 | | |
| COMPOUND_410_2376a11_190169 | Rp | + | 410.2376 | 11.19 | | | | (843.4354, 5525.64) (449.2112, 763.91) (428.2541, 3538.06) (411.2437, 67155.2) (412.2476, 19429.28) (413.254, 3885.69) | 123467.8 | 24253.01 | 106951.2 | 21761.42 | 257305.1 | 85329.38 | 271160.9 | 78996.67 | 1.13 | 2.32E-06 | 1.07E-05 | 0.52 | 0.049732 | 0.282107 | | |
| COMPOUND_410_3175a11_228687 | Rp | + | 410.3175 | 11.23 | | | | (409.3103, 5853.23) (410.314, 1867.99) (411.317, 425.87) (933.6213, 480.36) (934.6334, 250.36) | 23360.13 | 2822.246 | 24523.67 | 2948.484 | 19191.43 | 3639.782 | 19058.75 | 3384.971 | -1.07 | 2.54E-05 | 9.24E-05 | -0.27 | 0.327449 | 0.634609 | | |
| COMPOUND_410_4245a11_614339 | Rp | + | 410.4245 | 11.61 | | | | (821.8348, 215.47) (822.8311, 414.4) (823.8474, 344.51) (859.7935, 264.97) (860.811, 129.33) (861.785, 769.37) (843.8053, 3267.02) (844.795, 435.09) (449.385, 681.05) (411.4314, 74452.07) (412.4347 | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--------------|--|---------------|-----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_413_1976a10_660368 | Rp | + | 413.1796 | 10.66 | | | | (827.3603, 430.721)(828.3765, 1290.75)(829.363, 359.35)(865.3265, 863.71)(866.3342, 482.66)(436.1741, 462.89)(431.2113, 13277.82)(432.2129, 3509.47)(433.2121, 9714.01)(414.1863, 14904.87)(415.1898, 3533.35)(416.1957, 756.75)(844.3875, 848.34) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.57 | 0.021589 | 0.042131 | 0.01 | 0.970608 | 0.984052 |
| COMPOUND_413_1973a10_598261 | Rp | - | 413.1973 | 10.60 | | | | (861.4038, 302.04)(862.4085, 290.97)(863.3807, 474.35)(448.1766, 690.83)(871.3648, 172.11)(872.3815, 381.3)(873.4073, 1474.4)(412.1919, 6763.06)(413.1935, 2331.47)(414.1768, 1369.85)(825.3892, 153.68)(826.3561, 429.93)(827.3829, 207.88)(939.4055, 366.46) | 16220.87 | 4189.969 | 15806.64 | 4663.607 | #DIV/0! | #DIV/0! | 12253.5 | 1981.561 | -0.87 | 0.00011 | 0.00034 | -0.03 | 0.890197 | 0.953702 |
| COMPOUND_413_2926a0_9439945 | Hilic | + | 413.2926 | 0.94 | | | | (827.5944, 761.43)(828.6049, 553.76)(849.5682, 8740.58)(431.311, 292.48)(414.301, 130725.42)(415.3044, 36811.69)(416.3074, 6024.66)(417.3116, 761.58) | 112826 | 54810.32 | 105091.1 | 50066.38 | 118269 | 107161 | 106246.6 | 154465.7 | -0.04 | 0.883173 | 0.922498 | -0.28 | 0.405451 | 0.6912 |
| COMPOUND_413_2937a0_0965185 | Rp | + | 413.2937 | 9.10 | | | | (849.5708, 328.45)(850.5794, 315.71)(414.3011, 389292.78)(415.3048, 10855.97)(416.3099, 21310.46)(417.3149, 3054.45) | 235782 | 171850.8 | 184936.5 | 123079.8 | 282136.9 | 252735.9 | 268071 | 370184.7 | 0.18 | 0.520481 | 0.620038 | -0.23 | 0.46937 | 0.734042 |
| COMPOUND_413_9736a8_737131 | Rp | - | 413.9736 | 8.74 | | | | (862.9127, 188.72)(863.935, 101.31)(526.9765, 140.13)(412.9659, 7745.85)(413.9679, 733.24)(414.9749, 135.5) | 15773.38 | 5963.183 | 18239.21 | 6048.873 | 12706.8 | 2386.555 | 14711.86 | 4751.888 | -0.51 | 0.000312 | 0.000895 | -0.09 | 0.543022 | 0.776977 |
| COMPOUND_414_2052a8_545986 | Rp | + | 414.2052 | 8.55 | | | | (437.1948, 2724.68)(438.1989, 546.02)(439.1904, 296.73)(453.1685, 532.41)(454.1759, 218.06)(455.1773, 157.89)(432.2388, 17564.25)(433.2417, 517.59)(434.2457, 855.08)(435.2475, 132.16)(415.213, 25194.39)(416.2161, 6330.29)(417.2202, 1287.26)(418.2227, 223.17) | 101241.2 | 59944.81 | 95157.04 | 55672.09 | 136730.5 | 35880.53 | 135164.8 | 39769.24 | 0.88 | 0.001793 | 0.004481 | 0.11 | 0.734748 | 0.888627 |
| COMPOUND_414_2066a7_793913 | Rp | - | 414.2066 | 7.79 | | | | (413.1996, 524736.0)(414.2032, 118528.36)(827.4075, 5751.37)(828.411, 2743.61)(829.4215, 7975.27)(830.4247, 3546.07)(831.4342, 3451.38)(832.4377, 1569.53)(833.4376, 657.42) | 15603.55 | 5411.732 | 19756.35 | 15328.06 | 371773.6 | 717894.8 | 175326.9 | 194885 | 1.73 | 8.42E-18 | 9.48E-15 | -0.28 | 0.091385 | 0.359093 |
| COMPOUND_414_2069a6_9546723 | Rp | - | 414.2069 | 6.95 | | | | (413.1997, 35411.78)(414.2026, 8695.66)(415.2023, 2993.49)(416.2052, 427.16) | 27039.67 | 14059.78 | 20596.63 | 8942.226 | 133181.5 | 65482.65 | 88284.28 | 78846.68 | 1.52 | 5.56E-13 | 2.91E-11 | -0.33 | 0.101424 | 0.37567 |
| COMPOUND_414_207a7_473809 | Rp | - | 414.2070 | 7.47 | | | | (413.1997, 36687.21)(414.2026, 8339.87)(415.2125, 11096.33)(416.216, 2570.99)(417.2135, 802.53)(827.4151, 176.47) | 199675.5 | 141824.2 | 215419.2 | 79139.81 | 91804 | 43502.4 | 89102.91 | 45316.78 | -0.91 | 2.03E-05 | 7.55E-05 | -0.59 | 0.012188 | 0.168989 |
| COMPOUND_414_2072a8_005874 | Rp | - | 414.2072 | 8.01 | | | | (413.1998, 21347.25)(414.2028, 5311.82)(415.2073, 2019.67)(416.2015, 321.38)(827.4107, 186.4)(828.4154, 73.49) | 21862.46 | 8162.23 | 26519.94 | 13157.74 | 207146.9 | 120607 | 153576.1 | 114379.5 | 1.84 | 1.04E-14 | 1.95E-12 | -0.51 | 0.018872 | 0.196411 |
| COMPOUND_414_3135a9_61439 | Rp | + | 414.3135 | 9.61 | | | | (437.3048, 1322.01)(438.2977, 760.41)(439.3103, 1808.66)(851.6132, 6254.42)(852.6166, 1848.37)(853.6156, 550.61)(415.3205, 7075.87)(416.3256, 2170.99)(417.3331, 1671.09) | 88289.29 | 35549.27 | 84847.3 | 35254.96 | 79466.43 | 38332.71 | 83454.3 | 41204.09 | 0.02 | 0.958396 | 0.97523 | 0.05 | 0.897823 | 0.954626 |
| COMPOUND_414_3155a10_468377 | Rp | + | 414.3155 | 10.47 | | | | (829.5919, 245.42)(867.5936, 536.07)(868.5806, 340.83)(869.5931, 423.91)(415.3204, 16079.34)(416.3249, 5376.27)(417.3324, 1359.03) | 302804 | #DIV/0! | 173338 | 41094.22 | 183091.6 | 112560.8 | 128974.6 | 81173.27 | 1.64 | 2.95E-15 | 7.92E-13 | -0.54 | 0.004309 | 0.100035 |
| COMPOUND_414_3824a10_219754 | Rp | + | 414.3824 | 10.22 | | | | (415.3904, 6068.53)(416.3899, 1889.64)(417.394, 469.64)(418.396, 64.77) | 23413.37 | 11177.95 | 23411.58 | 18820.14 | 24523.44 | 17118.31 | 26452.28 | 18317.62 | -0.09 | 0.752987 | 0.821132 | -0.10 | 0.755008 | 0.895058 |
| COMPOUND_415_2212a10_60256 | Rp | + | 415.2212 | 10.60 | | | | (831.491, 1169.11)(832.5149, 774.28)(869.3633, 697.91)(870.3504, 611.39)(871.3501, 293.64)(438.2174, 772.88)(853.4566, 809.03)(454.196, 877.74)(416.2274, 1252.66)(417.2293, 3710.91)(418.235, 516.8) | 23159.6 | 6673.859 | 23162.47 | 7810.851 | 21979.77 | 8501.781 | 9127.343 | -0.25 | 0.394424 | 0.498733 | 0.31 | 0.379495 | 0.67723 | |
| COMPOUND_415_3577a12_111721 | Rp | + | 415.3577 | 12.11 | | | | (869.6571, 1240.05)(438.3463, 1691.36)(439.3499, 588.63)(440.3544, 174.57)(853.7413, 1266.88)(854.7333, 660.38)(855.7384, 436.15)(454.324, 515.51)(455.3318, 296.04)(416.3657, 14026.61)(417.3704, 4457.32)(418.3713, 905.15)(419.3793, 104.18)(848.719, 8143.97)(849.7223, 5614.27) | 210257.5 | 122828.6 | 152880.5 | 111151.4 | 166345.9 | 80123.1 | 185612.5 | 118550 | -0.29 | 0.316493 | 0.418506 | 0.61 | 0.085211 | 0.346484 |
| COMPOUND_415_3678a11_101445 | Rp | + | 415.3678 | 11.10 | | | | (831.7513, 3753.03)(853.7281, 1123.77)(854.7292, 869.08)(416.374, 10677.23)(417.3762, 2839.15)(418.3758, 1398.95)(848.7646, 3491.44)(849.778, 317.73) | 250564.1 | 114099.94 | 23795.65 | 11675.69 | 36525.31 | 23718.5 | 46250.92 | 20882.44 | 0.72 | 0.00273 | 0.006569 | 0.50 | 0.075135 | 0.329961 |
| COMPOUND_416_2218a7_448072 | Rp | - | 416.2218 | 7.45 | | | | (415.2157, 81530.55)(416.2187, 19003.73)(417.2167, 6028.96)(418.2169, 1001.52)(831.4394, 117.98)(832.4375, 80.15)(461.2152, 414.88)(462.2232, 112.0) | 71413.85 | 34339.35 | 74809.2 | 31695.26 | 275317.6 | 130970.8 | 208154 | 128660 | 1.69 | 5.04E-11 | 9.14E-10 | -0.52 | 0.041026 | 0.265944 |
| COMPOUND_416_2222a6_1842346 | Rp | - | 416.2222 | 6.18 | | | | (867.433, 72.65)(415.2155, 15924.16)(416.2187, 3699.06)(417.2171, 1049.6)(418.2169, 178.21)(831.4458, 71.17) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 1.45 | 2.98E-15 | 7.92E-13 | 0.00 | 0.995923 | 0.998139 |
| COMPOUND_416_2222a7_77997 | Rp | - | 416.2222 | 7.78 | | | | (415.2157, 188867.06)(416.2188, 44725.54)(417.2171, 13219.07)(418.2183, 2261.99)(831.4323, 481.21)(832.4415, 164.87)(833.4375, 200.14)(834.4161, 25.87) | 107176.7 | 151020.7 | 110530 | 128286.3 | 96874.4 | 917832.7 | 598299.1 | 733715.7 | 1.58 | 8.48E-09 | 7.13E-08 | -0.66 | 0.020159 | 0.199116 |
| COMPOUND_416_2224a7_08239 | Rp | - | 416.2224 | 7.08 | | | | (415.2151, 19837.45)(416.2186, 5018.33)(417.216, 1401.49)(418.2168, 235.87) | 30570.04 | 17098.65 | 30082.93 | 23798.3 | 120298.6 | 48849.61 | 100392.1 | 81162.08 | 1.52 | 1.2E-09 | 1.29E-08 | -0.23 | 0.356442 | 0.665596 |
| COMPOUND_416_2224a8_630362 | Rp | - | 416.2224 | 8.63 | | | | (415.2154, 15773.05)(416.2192, 3929.71)(417.2165, 1154.13)(418.2166, 174.7) | 23164.29 | 10378.3 | 24891.44 | 10920.35 | 76027.14 | 48041.59 | 52397.59 | 37691.39 | 1.55 | 8.53E-08 | 5.46E-07 | -0.75 | 0.016778 | 0.1918 |
| COMPOUND_416_2225a8_2940235 | Rp | - | 416.2225 | 8.29 | | | | (415.2157, 47955.06)(416.2188, 10502.98)(417.2166, 3467.44)(418.2185, 582.7)(831.4383, 3710.75)(832.4417, 1547.27)(833.4407, 781.84) | 17044.08 | 6606.232 | 18554.61 | 10980 | 275101.8 | 667544.4 | 117750.6 | 134520.5 | 1.55 | 3.45E-14 | 4.32E-12 | -0.20 | 0.267018 | 0.575669 |
| COMPOUND_416_2227a7_795285 | Rp | - | 416.2227 | 7.80 | | | | (415.2157, 188867.06)(416.2188, 44725.54)(417.2171, 13219.07)(418.2183, 2261.99)(831.434, 3095.88)(832.4373, 1423.36)(833.4384, 616.73)(834.4537, 134.04) | 112845.5 | 133861 | 117890.1 | 115328.6 | 783140.7 | 757629.2 | 702961.4 | 877644.5 | 1.49 | 1.2E-11 | 2.9E-10 | -0.20 | 0.323725 | 0.630999 |
| COMPOUND_416_2227a8_400249 | Rp | - | 416.2227 | 8.40 | | | | (415.2154, 38361.23)(416.2185, 8659.52)(417.2153, 2899.92)(418.2184, 501.49)(831.4669, 71.36) | 20224.61 | 7935.229 | 15020.13 | 4047.682 | 48410.71 | 32498.62 | 48212.47 | 51886.71 | 1.39 | 9.38E-10 | 1.04E-08 | -0.24 | 0.291588 | 0.601884 |
| COMPOUND_416_3303a10_157481 | Rp | + | 416.3303 | 10.16 | | | | (439.3156, 1315.9)(440.3232, 724.88)(441.322, 1198.23)(455.2978, 15397.64)(417.3366, 13701.81)(418.3403, 4050.78)(419.3446, 1086.3) | 25022.33 | 4734.435 | #DIV/0! | #DIV/0! | 32510.31 | 12835.23 | 48485.62 | 20284.92 | 1.02 | 1.12E-10 | 1.67E-09 | 0.46 | 0.004464 | 0.102583 |
| COMPOUND_416_3623a10_757749 | Rp | + | 416.3623 | 10.76 | | | | (871.6541, 567.26)(839.3403, 1161.54)(855.6815, 1771.79)(856.7045, 1050.64)(434.386, 1599.39)(455.3334, 1583.57)(456.3307, 584.82)(417.3695, 38582.68)(418.3727, 10545.04)(419.3698, 2518.87)(420.3764, 405.4) | 70036.48 | 31969.53 | 66292.14 | 28044.34 | 80304.5 | 48254.96 | 90929.89 | 39517.78 | 0.29 | 0.324067 | 0.424795 | 0.35 | 0.305528 | 0.613089 |
| COMPOUND_416_3626a10_789158 | Rp | + | 416.3626 | 10.79 | | | | (871.6578, 811.28)(439.3587, 650.55)(855.7127, 257.7)(856.7136, 2205.67)(455.3355, 1009.9)(456.3328, 447.75)(434.3899, 4972.98)(417.3694, 19166.51)(418.3727, 4928.82)(419.3652, 1109.98)(420.3754, 148.93) | 800626.24 | 35178.93 | 66609.95 | 28842.59 | 108599.7 | 70584 | 120948.5 | 57807 | 0.32 | 0.246811 | 0.342042 | 0.55 | 0.094291 | 0.36381 |
| COMPOUND_418_3098a11_388098 | Rp | + | 418.3098 | 11.39 | | | | (441.2982, 4187.52)(442.3023, 1303.56)(443.3006, 420.44)(446.3442, 2427.24)(437.3552, 1132.7)(438.3533, 809.06)(419.3167, 39649.76)(420.3202, 11711.42)(421.3235, 2292.74)(422.3255, 391.19) | 128711.2 | 53697.51 | 113388 | 80964.42 | 257469.8 | 243194.1 | 211199 | 93727.88 | 0.94 | 0.000354 | 0.001009 | 0.38 | 0.202586 | 0.5149 |
| COMPOUND_418_3459a11_67529 | Rp | + | 418.3459 | 11.68 | | | | (837.7028, 990.3)(875.6495, 590.46)(413.334, 1692.99)(442.3332, 639.62)(443.3445, 173.31)(859.6639, 555.51)(457.3119, 453.64)(458.3069, 137.45)(459.3169, 279.82)(436.3786, 7560.39)(437.3835, 2309.3)(438.385, 668.15)(439.404, 103.21)(419.3529, 6597.22)(420.3556, 2188.57)(| | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|---|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_421_1419a10_575464 | Rp | - | 421.2419 | 10.58 | | | | (877.2499, 500.89)(878.2481, 325.94)(879.2264, 353.55)(534.1266, 1050.72)(887.2586, 23733.48 8405.882 23532.71 9872.408 | 31846.33 | 10214.87 | 43692.36 | 16792.85 | 0.61 | 0.010104 | 0.02144 | 0.52 | 0.064647 | 0.307286 | | | | |
| COMPOUND_422_2299a8_261905 | Rp | - | 422.2299 | 8.26 | | | | (328.48)(888.2737, 280.51)(889.2447, 532.26)(890.2673, 384.78)(891.2575, 388.09)(420.1364, 10259.94)(421.1387, 2701.57)(422.1341, 3944.1)(423.139, 1088.72)(434.1449, 257.52)(841.2713, 411.55)(842.2655, 341.54)(843.2995, 498.58)(466.1566, 3799.78)(955.2117, 409.37)(956.2411, 162.51) | 134624.9 | 74437.64 | 137868.8 | 62076.94 | 117583 | 6748.651 | 114254.1 | 46037.46 | -1.21 | 5.88E-08 | 3.94E-07 | -0.15 | 0.525258 | 0.768104 |
| COMPOUND_422_23a8_65038 | Rp | - | 422.2300 | 8.65 | | | | (421.2226, 56391.05)(422.226, 15376.61)(423.2277, 2969.35)(424.23, 435.2) | 82623.17 | 42679.51 | 82484.78 | 35341.95 | 90622.67 | 5087.67 | 88344 | 37954.1 | -1.09 | 2.79E-06 | 1.25E-05 | -0.15 | 0.548044 | 0.77853 |
| COMPOUND_422_2301a8_484494 | Rp | - | 422.2301 | 8.48 | | | | (421.2226, 12232.23)(422.2259, 3189.55)(423.2315, 794.63)(424.2378, 118.42) | 76150.08 | 41809.14 | 75759.49 | 37042.65 | 66231.67 | 4132.667 | 74187.78 | 22437.06 | -1.13 | 7.01E-07 | 3.66E-06 | -0.12 | 0.617675 | 0.816971 |
| COMPOUND_423_2755a10_812532 | Rp | + | 423.2755 | 10.81 | | | | (847.555, 34540.17)(885.5486, 6220.86)(462.2481, 833.39)(463.2418, 981.01)(464.2501, 569.05)(424.2836, 19138.72)(425.2864, 5469.79)(426.2842, 2398.35)(864.6022, 2051.78)(865.6045, 2692.48)(212.6382, 60.06)(213.1487, 1132.22) | 393176.8 | 198274.4 | 263080 | 224084.9 | 70836.91 | 37003.17 | 70821.98 | 26255.36 | 0.37 | 0.14871 | 0.226482 | -0.07 | 0.826177 | 0.923809 |
| COMPOUND_423_2778a10_781187 | Rp | + | 423.2778 | 10.78 | | | | (847.5553, 34283.11)(885.5375, 2839.68)(462.2496, 638.58)(463.2425, 335.04)(464.2518, 590.27)(424.2835, 22640.89)(425.286, 5746.37)(426.2865, 2559.8)(427.2893, 444.88)(212.6427, 50.3)(213.1484, 1269.42)(864.579, 12856.44)(865.5832, 6965.29) | 192400.7 | 106194.9 | 267976.3 | 246010.3 | 61356.09 | 29959.82 | 61044.77 | 22010.48 | 0.91 | 2.9E-05 | 0.000104 | -0.10 | 0.668864 | 0.846185 |
| COMPOUND_423_3348a9_032939 | Rp | + | 423.3348 | 9.03 | ACar 18:2 | 2 | 20 ev: 424.3428(100), 85.0278(75), 157.0459(10) | (446.3201, 562.18)(424.3437, 36929.04)(425.3467, 9967.41)(426.3478, 2423.03)(427.3436, 384.02) | 113263 | 42069.25 | 103441.4 | 30991.68 | 105162.7 | 32652.62 | 92861.37 | 29534.16 | -0.02 | 0.934149 | 0.95693 | -0.43 | 0.206677 | 0.518302 |
| COMPOUND_425_3519a9_302936 | Rp | + | 425.3519 | 9.30 | ACar 18:1 | 2 | 10 ev: 246.3608(100), 85.0283(18), 239.1203(7) | (426.3587, 100418.5)(427.3616, 28131.3)(428.3647, 4802.42)(429.3714, 708.69) | 371843 | 147464.8 | 328401.9 | 112081 | 326472.4 | 118922.9 | 358226.9 | 125795 | -0.33 | 0.276475 | 0.375752 | 0.57 | 0.116486 | 0.405455 |
| COMPOUND_425_3744a10_021565 | Rp | + | 425.3744 | 10.02 | | | | (464.9495, 156.83)(444.0168, 113.7)(426.9807, 5361.34)(427.983, 661.57)(428.9657, 636.16) | 22365.5 | 9567.346 | 18005.14 | 7074.333 | 22549.4 | 4505.37 | 25772.06 | 9146.837 | -0.16 | 0.564556 | 0.661488 | 1.06 | 0.001805 | 0.061415 |
| COMPOUND_426_3722a11_76912 | Rp | + | 426.3722 | 11.77 | | | | (853.7254, 1398.92)(854.7066, 479.91)(449.3601, 3644.62)(450.3629, 1646.17)(451.365, 507.02)(875.7425, 683.54)(876.7068, 943.79)(465.3392, 488.09)(466.3412, 229.75)(467.3434, 157.71)(444.4043, 4679.61)(445.407, 1139.86)(446.4262, 97.23)(427.3784, 22176.68)(428.3822, 6264.99)(429.3736, 33173.78)(430.3773, 11020.01)(431.3812, 4585.04)(432.3824, 1024.33)(433.3859, 351.45) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.33 | 9.56E-08 | 6E-07 | -1.01 | 0.964463 | 0.981972 |
| COMPOUND_426_4077a13_627346 | Rp | + | 426.4077 | 13.63 | | | | (891.7856, 700.12)(892.7925, 346.92)(449.4001, 813.23)(450.4027, 350.38)(451.4107, 79.22)(427.4163, 5391.55)(428.4193, 1687.79)(429.4102, 470.95)(430.4076, 69.92) | 38084.19 | 7593.869 | 36662.96 | 6480.603 | 37927.79 | 3456.077 | 38259.32 | 5666.328 | 0.05 | 0.87856 | 0.919812 | 0.22 | 0.542185 | 0.776977 |
| COMPOUND_427_178a10_57897 | Rp | - | 427.1780 | 10.58 | | | | (889.2607, 357.84)(890.2839, 305.65)(899.3749, 198.52)(900.3763, 330.34)(426.1704, 5179.33)(427.1747, 2273.12)(428.1663, 1838.37)(429.1541, 192.09)(853.3133, 326.83)(854.3305, 244.2)(855.323, 410.78) | 28508.42 | 9376.799 | 28415.7 | 11128.81 | 22708.25 | 7984.304 | 25329.26 | 8184.528 | -0.40 | 0.124812 | 0.196558 | 0.22 | 0.478036 | 0.740906 |
| COMPOUND_427_3671a9_576748 | Rp | + | 427.3671 | 9.58 | | | | (445.4066, 1915.77)(466.332, 2125.65)(467.3189, 346.71)(428.3745, 10758.37)(429.3779, 3112.93)(430.3818, 775.11)(431.3822, 109.3) | 69161.25 | 21520.49 | 65837.72 | 22700.42 | 49582.21 | 15888.3 | 54266.14 | 17734.1 | -1.02 | 0.000277 | 0.000799 | 0.39 | 0.207364 | 0.518872 |
| COMPOUND_427_3748a8_685235 | Rp | - | 427.3748 | 8.69 | | | | (540.9705, 124.11)(462.9336, 147.72)(900.9746, 193.0)(426.9676, 19413.36)(427.9707, 1956.34)(428.966, 947.03)(429.9655, 146.56)(472.9913, 117.01) | 81036.75 | 7385.623 | 82621.7 | 5278.883 | 80357 | 4573.439 | 80579.77 | 7078.906 | -0.07 | 0.812651 | 0.867341 | -0.26 | 0.480893 | 0.743153 |
| COMPOUND_428_166a10_663464 | Rp | - | 428.1660 | 10.66 | | | | (891.3191, 363.15)(541.1488, 3330.11)(542.1575, 1165.86)(543.1442, 3316.48)(544.1485, 1443.07)(545.1482, 1440.94)(546.1475, 813.86)(547.157, 599.35)(463.1292, 455.25)(464.1298, 1363.67)(465.1313, 3754.31)(466.1364, 618.97)(467.1346, 2110.46)(468.1484, 782.94)(901.3321, 458.1)(427.1576, 41350.06)(428.1603, 16327.95)(429.1618, 4537.06)(855.3403, 749.23)(473.1614, 10249.65)(474.165, 3231.36)(475.163, 18938.69)(476.1747, 7004.95)(477.1615, 574.33)(478.1671, 2722.61)(479.1634, 1386.79)(969.3356, 446.48)(970.3332, 133.76) | 151058.9 | 65738.22 | 175169.2 | 104423.9 | 137619.3 | 89649.95 | 180523.2 | 114192.6 | -0.41 | 0.146655 | 0.223909 | 0.34 | 0.308516 | 0.614305 |
| COMPOUND_428_3664a12_090394 | Rp | + | 428.3664 | 12.09 | | | | (429.3736, 13646.16)(430.3777, 4600.38)(431.357, 4040.59) | 51966.8 | 20184.64 | 47505.84 | 19339.8 | 40623.33 | 18687.7 | 34668.54 | 17918.06 | -0.78 | 0.001064 | 0.00276 | -0.16 | 0.548157 | 0.77853 |
| COMPOUND_428_3673a13_088575 | Rp | + | 428.3673 | 13.09 | | | | (895.674, 785.11)(896.651, 479.28)(429.3735, 24954.5)(430.3768, 77447.2)(431.3798, 13584.12)(432.3844, 1699.05)(433.3807, 145.02) | 974121.7 | 488898.3 | 790061.2 | 452268.8 | 436570.4 | 361050.3 | 353477.2 | 197560.5 | -1.41 | 2.34E-08 | 1.76E-07 | 0.22 | 0.397118 | 0.690408 |
| COMPOUND_428_3674a12_592195 | Rp | + | 428.3674 | 12.59 | Unknown | 4 | 20 ev: 429.3722(100), 163.1043(25), 71.0851(15), 234.1586(10) | (857.7341, 154.76)(858.7212, 153.74)(895.682, 438.94)(896.6834, 713.64)(897.6827, 514.36)(451.3557, 2656.94)(452.3503, 181.92)(429.3738, 15585.32)(430.3828, 6401.77)(431.3885, 2157.45)(432.3853, 317.58) | 78685.06 | 35261.99 | 62866.22 | 30180.65 | 26913.5 | 10901.47 | 41093.88 | 16239.6 | -1.82 | 2.82E-13 | 1.87E-11 | 0.85 | 0.000375 | 0.030145 |
| COMPOUND_428_3679a11_37579 | Rp | + | 428.3679 | 11.38 | | | | (877.7714, 1699.96)(879.7483, 1066.73)(880.7458, 784.81)(429.3737, 11574.41)(430.3796, 5887.58)(431.3866, 7506.85)(432.3894, 2473.79)(874.7911, 1638.8) | 44976.78 | 22933.52 | 39558.9 | 13622.12 | 70989.13 | 23214.89 | 49675.41 | 14748.48 | 0.62 | 0.0169 | 0.033982 | -0.14 | 0.650094 | 0.838541 |
| COMPOUND_428_3968a10_781774 | Rp | + | 428.3968 | 10.78 | | | | (857.799, 2887.51)(895.7457, 519.74)(896.7333, 164.75)(429.406, 17341.88)(430.4083, 5161.25)(874.8011, 1234.73) | 42732.05 | 19709.02 | 32397.55 | 14052.42 | 41074.23 | 12432.21 | 50155.81 | 22542.27 | 0.77 | 0.001072 | 0.002775 | 0.39 | 0.147692 | 0.456493 |
| COMPOUND_429_3736a12_432636 | Rp | + | 429.3736 | 12.43 | | | | (452.3622, 2822.22)(453.3667, 974.28)(454.3717, 190.84)(881.7369, 757.56)(882.7436, 416.23)(883.7427, 196.79)(468.3374, 614.71)(469.3448, 221.51)(470.3278, 106.07)(430.3797, 20607.15)(431.386, 101793.91)(432.39, 23002.4)(433.3944, 3221.02)(434.3922, 368.42) | 932115.8 | 300512.1 | 754370.7 | 239414.7 | 1016716 | 106848.1 | 1028706 | 264306.3 | -0.08 | 0.77912 | 0.883808 | 1.05 | 0.00154 | 0.06002 |
| COMPOUND_430_1733a11_847422 | Rp | + | 430.1733 | 11.85 | | | | (899.2976, 260.08)(900.2927, 191.74)(453.1686, 250.48)(883.3505, 954.98)(469.1331, 124.73)(431.1795, 65409.94)(432.1823, 17389.01)(433.1808, 4670.27)(878.3922, 693.34) | 159784.5 | 53186.58 | 135089 | 36423.19 | 144110.2 | 34687.08 | 157621.3 | 45823.84 | -0.29 | 0.333552 | 0.434951 | 0.74 | 0.040717 | 0.265782 |
| COMPOUND_430_2018a10_598564 | Rp | - | 430.2018 | 10.60 | | | | (543.1802, 1990.07)(465.166, 6254.74)(905.3905, 427.4)(429.1945, 6429.25)(430.1938, 2247.49)(431.1763, 2551.79)(432.1754, 515.31)(859.3716, 229.43)(860.3565, 485.1)(475.1939, 7263.75)(476.1969, 1834.46)(477.1944, 272.83)(973.391, 442.56)(974.3801, 97.71)(975.4008, 189.53) | 449256.5 | 14341.04 | 44758.11 | 13345.5 | 26031.75 | 7403.458 | 33560.32 | 12986.11 | -1.33 | 2.01E-06 | 9.34E-06 | 0.52 | 0.084567 | 0.346484 |
| COMPOUND_430_3072a9_780315 | Rp | - | 430.3072 | 9.78 | | | | (543.3006, 336.57)(544.2865, 208.72)(545.2872, 75.51)(465.2921, 1641.38)(466.2827, 268.71)(467.2906, 366.1)(468.3032, 28.88)(429.3004, 9474.79)(430.3034, 2988.92)(431.3126, 1193.49)(432.3139, 199.27)(475.3057, 4690.92)(476.3089, 1457.5)(477.3159, 484.29) | 54083.13 | 17420.02 | 51071.67 | 13304.56 | 59266.93 | 17900.41 | 70824.95 | 20188.54 | 0.32 | 0.235414 | 0.329992 | 0.64 | 0.045074 | 0.273371 |
| COMPOUND_430_3095a9_785857 | Rp | + | 430.3095 | 9.79 | | | | (899.5774, 255.22)(900.5933, 171.94)(453.2986, 2056.25)(454.2983, 876.61)(455.2988, 55.32)(469.2509, 268.08)(470.2588, 107.34)(431.3165, 30247.2)(432.3191, 10760.04)(433.3209, 7643.12)(434.3232, 1349.46) | 129359.8 | 33363.61 | 113191.2 | 29123.27 | 137420.5 | 30566.11 | 168155.9 | 47968.22 | 0.28 | 0.28356 | 0.383069 | 0.94 | 0.004019 | 0.094399 |
| COMPOUND_430_347a12_106378 | Rp | + | 430.3470 | 12.11 | | | | (861.7223, 341.64)(862.7389, 86.97)(469.3318, 1462.04)(470.3352, 613.31)(471.3446, 555.94)(431.3849, 76415.75)(432.3889, 20066.55)(433.3912, 30399.53)(434.3923, 3967.72)(435.3875, 399.99)(878.7761, 514.42)(879.7628, 450.27)(880.7564, 401.09) | 36878.22 | 10007.38 | 34688.77 | 12823.31 | 30310.86 | 9405.984 | 31392.11 | 11295.27 | -0.34 | 0.255139 | 0.351635 | 0.18 | 0.606527 | 0.810674 |
| COMPOUND_430_3797a10_820964 | Rp | + | 430.3797 | 12.43 | | | | (861.7829, 1311.81)(453.3588, 227.97)(883.7136, | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|------------------------------------|----------|---|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_430_3816a10_828956 | Rp | + | 430.3816 | 10.83 | | | | (861.781, 1296.85) (453.3669, 105.25) (454.3447, 876.37) (883.7733, 7907.61) (448.4049, 290.45) (469.3298, 5671.94) (470.3354, 1924.86) (431.3858, 51626.31) (432.3889, 13829.5) (433.3905, 2685.18) (434.3863, 479.44) (878.8174, 2642.58) | 431405.5 | 351993.2 | 383231.8 | 378216.6 | 1011105 | 948988.5 | 1219668 | 980836.8 | 0.66 | 0.018731 | 0.03733 | 0.34 | 0.295522 | 0.606116 |
| COMPOUND_431_3031a0_9478264 | Hilic | + | 431.3031 | 0.95 | | | | (863.6166, 2784.29) (864.6189, 526.36) (454.2934, 1693.78) (455.29, 702.83) (456.2864, 169.14) (449.3273, 537.53) (432.3117, 246696.78) (433.3149, 69447.63) (434.3178, 11673.19) (435.3206, 1298.55) (436.3211, 158.9) | 145681.2 | 86080.49 | 131570.2 | 60981.09 | 191655.4 | 150861.2 | 187732 | 267133.4 | 0.29 | 0.312052 | 0.413471 | -0.35 | 0.302609 | 0.610641 |
| COMPOUND_431_3043a9_096739 | Rp | + | 431.3043 | 9.10 | Chenodeoxycholic acid glycine conj | 1 | 10 ^{eV} : 414.3021(100), 432.3113(50), 339.266(17), 265.1939(7), 147.0952(6) | (449.338, 4173.45) (432.3117, 472287.0) (433.3152, 136238.45) (434.318, 21336.65) (435.3204, 2865.95) | 232074.4 | 163644.6 | 181764.3 | 115194 | 274572.8 | 237303.2 | 260209.8 | 351930.1 | 0.19 | 0.486064 | 0.587241 | -0.25 | 0.433929 | 0.712127 |
| COMPOUND_431_3271a11_147078 | Rp | + | 431.3271 | 11.15 | | | | (863.593, 658.82) (864.6122, 4320.11) (865.6012, 2035.08) (901.6314, 5407.38) (432.333, 22825.46) (433.3361, 6094.13) (434.3458, 1649.79) (880.7003, 2461.59) | 31618.04 | 12030.93 | 27073.5 | 9361.337 | 73329.67 | 48101.08 | 82725.55 | 44704.23 | -0.32 | 0.244383 | 0.339933 | 0.18 | 0.571563 | 0.789098 |
| COMPOUND_431_8104a9_787293 | Rp | + | 431.8104 | 9.79 | | | | (864.6256, 19122.69) (865.6286, 9287.06) (866.6302, 3055.3) (867.63, 722.17) (868.6328, 167.62) (432.8185, 10504.87) (433.8218, 1620.84) (434.8238, 538.4) | 237625.7 | 54047.93 | 208122.5 | 36743.57 | 256197.6 | 43372.05 | 252709.2 | 60635.47 | 0.24 | 0.396566 | 0.500317 | 0.61 | 0.076122 | 0.331641 |
| COMPOUND_432_3235a9_673759 | Rp | - | 432.3235 | 9.67 | | | | (467.2939, 864.39) (468.2991, 288.0) (469.2974, 265.66) (431.3161, 10061.07) (432.3194, 3019.56) (433.328, 1366.65) (434.3334, 241.28) (863.6331, 231.17) (864.6255, 72.19) (477.3234, 470.38) | 34413.05 | 11292.75 | 39169.52 | 16880.02 | 37582.08 | 10180.5 | 33597.61 | 14544.09 | 0.63 | 0.012767 | 0.034626 | -0.35 | 0.248207 | 0.557845 |
| COMPOUND_433_1201a6_149124 | Hilic | + | 433.1201 | 6.15 | | | | (434.128, 23234.52) (435.131, 3537.66) (436.1314, 643.65) | 18068.9 | 9878.533 | 13533.61 | 7298.18 | 17557.57 | 6863.499 | 29907.05 | 13422.2 | 0.10 | 0.683231 | 0.768166 | 1.26 | 8.73E-05 | 0.012291 |
| COMPOUND_433_1679a10_686771 | Rp | - | 433.1679 | 10.69 | | | | (901.3294, 366.63) (911.3649, 267.18) (912.36, 499.45) (913.367, 429.24) (432.1607, 29669.16) (433.1649, 13292.35) (434.1653, 3824.74) (865.353, 675.1) (866.3491, 560.69) (478.1737, 1974.69) (479.1636, 915.19) (480.1614, 16073.85) | 174934 | 22025.07 | 177679.9 | 33508.96 | 185107.2 | 50742.6 | 148476.7 | 35438.14 | -0.49 | 0.032599 | 0.060722 | -0.56 | 0.039487 | 0.261543 |
| COMPOUND_435_2115a6_702896 | Rp | + | 435.2115 | 6.70 | | | | (436.2178, 6068.63) (437.2224, 1318.9) (438.2299, 461.62) (439.244, 79.32) | 22320.23 | 5481.398 | 22732.49 | 4875.551 | 20496.08 | 6115.648 | 22409.5 | 4983.021 | -0.18 | 0.542353 | 0.640471 | 0.15 | 0.669116 | 0.846185 |
| COMPOUND_435_336a11_066518 | Rp | + | 435.3360 | 11.07 | | | | (909.6202, 2150.31) (901.6038, 2612.6) (911.6212, 2222.34) (453.3583, 1070.36) (436.3435, 140071.75) (437.3467, 39011.43) (438.3499, 6996.22) (439.3505, 1241.74) | 182179.9 | 103200.8 | 141102.4 | 81855.95 | 245317.9 | 67871.9 | 275010.1 | 112914.4 | 0.68 | 0.011075 | 0.023137 | 0.56 | 0.072481 | 0.326093 |
| COMPOUND_437_2898a10_448892 | Rp | - | 437.2898 | 10.45 | | | | (909.5503, 3381.13) (550.2873, 1172.37) (551.288, 598.29) (552.2949, 63.01) (436.2826, 13925.45) (437.2858, 34574.65) (438.2886, 5924.35) (439.2903, 964.85) (873.5331, 10937.14) | 247299.2 | 72730 | 253453.8 | 80418.28 | 83437.86 | 90669.81 | 68494.45 | 70496.87 | -1.28 | 1.74E-07 | 1.05E-06 | -0.20 | 0.43033 | 0.707891 |
| COMPOUND_437_2904a1_4497926 | Hilic | + | 437.2904 | 1.45 | | | | (875.5825, 353.52) (876.599, 299.16) (460.2795, 6907.03) (461.2824, 2058.39) (462.2926, 804.51) (463.2876, 126.95) (89.5484, 399.31) (898.569, 395.77) (899.5733, 147.55) (438.2983, 12030.29) (439.3019, 2940.4) (440.2908, 1033.96) (441.2879, 133.98) | 53940.13 | 16528.48 | 58279.89 | 18788.65 | 28394.5 | 26413.09 | 20897.82 | 20881.52 | -1.14 | 1.86E-06 | 8.73E-06 | -0.24 | 0.356955 | 0.665625 |
| COMPOUND_437_2908a10_447945 | Rp | + | 437.2908 | 10.45 | | | | (875.5737, 11355.81) (913.5591, 5185.14) (460.2804, 6600.42) (461.2818, 1740.19) (462.2919, 584.02) (897.566, 8127.91) (898.5746, 11739.46) (476.2593, 951.26) (477.2516, 575.9) (478.2445, 413.33) (438.2989, 87202.36) (439.3019, 20155.07) (440.3058, 3790.21) (441.3129, 671.19) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.37 | 5.17E-08 | 3.54E-07 | 0.00 | 0.995273 | 0.998139 |
| COMPOUND_438_1679a8_226983 | Rp | - | 438.1679 | 8.23 | | | | (473.1391, 736.94) (437.1612, 5545.66) (438.1629, 1147.58) (439.1625, 433.14) (440.1672, 66.12) | 23650.37 | 10171.31 | 25664.11 | 9312.98 | 16255.3 | 7186.263 | 19627.66 | 8328.65 | -0.58 | 0.010177 | 0.021539 | -0.18 | 0.469925 | 0.734155 |
| COMPOUND_438_2308a10_461539 | Rp | + | 438.2308 | 10.46 | | | | (877.4538, 136.02) (878.4435, 114.16) (879.4653, 300.47) (880.4879, 203.09) (881.4561, 329.29) (915.4216, 725.44) (916.4132, 367.52) (917.431, 560.47) (461.2197, 956.23) (899.4589, 783.31) (477.1822, 1109.74) (478.1783, 2334.71) (479.1802, 1156.39) (439.2374, 10668.49) (440.2414, 2558.73) (441.243, 1352.21) (442.2304, 111.11) | 40234.62 | 29571.09 | 32975.5 | 14116.68 | 19279 | 8599.527 | 13332.09 | 15158.47 | 0.18 | 0.432834 | 0.537937 | 0.17 | 0.01001 | 0.153413 |
| COMPOUND_439_3042a10_511937 | Rp | - | 439.3042 | 10.51 | | | | (913.5444, 1569.37) (552.2895, 524.01) (438.298, 6971.59) (439.2995, 2012.91) (440.3017, 424.98) (441.3068, 76.11) (484.2949, 715.77) (485.2901, 262.07) (991.5599, 1013.96) | 28838.65 | 10672.68 | 30153.36 | 14355.89 | 33359 | 7545.421 | 31228.11 | 7092.894 | -0.93 | 6E-05 | 0.000196 | -0.26 | 0.311507 | 0.617667 |
| COMPOUND_439_3074a10_509746 | Rp | + | 439.3074 | 10.51 | | | | (917.5848, 4687.16) (462.2946, 1656.84) (463.2975, 476.15) (901.5966, 1432.88) (478.258, 641.42) (479.2541, 349.78) (440.314, 25754.2) (441.3174, 6015.8) (442.3201, 1648.36) | 51169.38 | 27220.76 | 43659.59 | 24813.8 | 53774.33 | 25971.12 | 39980.38 | 8125.075 | -1.12 | 1E-06 | 4.98E-06 | 0.08 | 0.759716 | 0.896853 |
| COMPOUND_440_2145a10_688315 | Rp | - | 440.2145 | 10.69 | | | | (925.4103, 286.77) (926.4104, 269.51) (927.4138, 306.02) (439.2078, 7333.53) (440.2089, 2307.25) (441.2111, 1724.02) (879.3867, 361.18) (880.385, 348.24) | 19057.72 | 4792.49 | 20880.25 | 6610.861 | 18495.92 | 5689.36 | 21426.1 | 6160.303 | -0.06 | 0.833977 | 0.884235 | -0.04 | 0.892563 | 0.953702 |
| COMPOUND_441_1583a10_579119 | Rp | - | 441.1583 | 10.58 | | | | (927.2968, 187.98) (928.3009, 216.8) (929.3054, 165.07) (440.1496, 4494.43) (441.1498, 1703.67) (442.1536, 827.66) (443.1462, 58.33) (881.3337, 341.76) (882.3418, 181.97) (883.3135, 274.17) (884.3407, 232.72) (486.1438, 570.98) (487.1492, 170.77) (488.1499, 5488.77) (489.1506, 1800.02) (995.3034, 237.49) (996.3258, 146.09) | 24046 | 9172.581 | 24806.51 | 10890.67 | 55163.73 | 31708.69 | 47123.36 | 24917.42 | 0.61 | 0.029891 | 0.056095 | 0.18 | 0.580961 | 0.794368 |
| COMPOUND_442_2422a4_7021737 | Rp | + | 442.2422 | 4.70 | | | | (465.2317, 2359.26) (466.2345, 574.37) (467.2168, 273.53) (468.2108, 29.12) (907.4814, 84.04) (481.2047, 684.7) (482.1994, 198.89) (483.206, 69.49) (460.2765, 104341.76) (461.2797, 22452.09) (462.2816, 4440.82) (463.2854, 769.94) (464.2883, 92.75) (443.2494, 16494.92) (444.2528, 3776.75) (445.2531, 769.54) (446.258, 142.35) | 144487.2 | 214000.4 | 115581.7 | 171290.6 | 131898.7 | 183424.3 | 108890.1 | 159953.3 | 0.22 | 0.460381 | 0.56531 | 0.18 | 0.623601 | 0.823156 |
| COMPOUND_443_1729a10_855437 | Rp | - | 443.1729 | 10.86 | | | | (921.3042, 487.41) (922.3327, 325.0) (442.1657, 23276.35) (443.168, 7814.18) (444.1688, 2588.11) (445.1688, 475.54) (885.3307, 664.47) (886.3413, 542.55) (887.3337, 606.88) | 133563.3 | 19086.61 | 121977.9 | 22268.39 | 109798.8 | 24777.72 | 107948.3 | 15392.98 | -1.19 | 1.27E-05 | 4.98E-05 | 0.53 | 0.080258 | 0.339484 |
| COMPOUND_444_1141a11_330682 | Rp | + | 444.1141 | 11.33 | | | | (889.2099, 915.02) (467.1012, 405.49) (911.2383, 2037.41) (462.147, 5047.96) (463.1479, 2123.44) (464.1466, 1603.11) (465.1463, 220.49) (445.1192, 2250.26) (446.1205, 1091.13) (447.1224, 625.16) (908.2363, 2099.09) | 31805.79 | 5229.028 | 31826.78 | 11102.77 | 41977.5 | 7680.535 | 44074.42 | 7401.817 | 1.03 | 4.48E-05 | 0.00015 | 0.39 | 0.163556 | 0.47785 |
| COMPOUND_444_3616a11_450504 | Rp | + | 444.3616 | 11.45 | | | | (889.7006, 1300.37) (890.696, 741.34) (927.6604, 1085.31) (928.6523, 1283.08) (929.6587, 1094.31) (467.3606, 529.13) (468.377, 230.11) (911.6745, 1843.21) (445.3689, 126683.3) (446.3725, 39113.12) (447.3754, 6933.16) (448.378, 1203.09) (906.7938, 583.83) (907.7863, 281.43) (908.7861, 254.73) | 222128.3 | 149900 | 227093.8 | 142733.4 | 88401.3 | 90130 | 122868.7 | 104785.2 | -0.97 | 3.78E-05 | 0.00013 | -0.32 | 0.229404 | 0.535521 |
| COMPOUND_444_3617a12_4358635 | Rp | + | 444.3617 | 12.44 | | | | (462.3977, 514.82) (463.3918, 235.22) (445.3678, 24485.73) (446.371, 7764.98) (447.3752, 1702.27) (448.3817, 290.87) | 130653 | 22462.37 | 116443.7 | 17635.12 | 128634.7 | 11042.52 | 131674.4 | 19668.4 | 0.10 | 0.717058 | 0.792741 | 0.67 | 0.037723 | 0.259794 |
| COMPOUND_444_3621a11_444465 | Rp | + | 444.3621 | 11.44 | | | | (889.6995, 1407.93) (890.6989, 751.71) (927.688, 1178.98) (928.6692, 1029.11) (929.6829, 941.8) (467.3523, 536.02) (468.3608, 238.88) (911.7141, 581.4) (445.3687, 187987.97) (446.372, 58406.98) (447.375, 10426.29) (448.3793, 1561.79) (906.778, 516.21) (907.7883, 136.26) (908.7549, 606.37) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.96 | 0.000126 | 0.000383 | 0.00 | 0.999691 | 0.999832 |
| COMPOUND_444_3931a10_82522 | Rp | + | 444.3931 | 10.83 | | | | (467.3793, 760.87) (911.7762, 2106.0) (483.3673, 1439.28) (484.3775, 849.77) (485.3538, 379.28) (445.4017, 154659.14) (446.4047, 41910.83) (447.4063, 7415.87) (448.4042, 1073.12) (906.8492, 14338.2) (907.8527, 9041.42) | 119179.6 | 55538.81 | 137887.5 | 62043.24 | 202344.6 | 145068 | 214058.5 | 131621.6 | 0.81 | 0.003982 | 0.009198 | -0.07 | 0.822436 | 0.922833 |
| COMPOUND_444_3939a10_758215 | Rp | + | 444.3939 | 10.76 | | | | (889.8027, 827.87) (911.8194, 1173.54) (462.4117, | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_445_1025a9_919444 | Rp | - | 445.1025 | 9.92 | | | | (558.0926, 588.7815)(559.0852, 793.9661)(480.0687, 6260.76)(481.0739, 1726.62)(482.0666, 5659.47)(483.07, 1733.51)(484.0647, 1938.97)(485.0669, 626.17)(486.0616, 447.51)(935.2322, 1445.08)(444.0926, 131.49)(445.0972, 4691.19)(446.0918, 8768.16)(447.0969, 4001.13)(448.0954, 1878.03)(889.1787, 319.62)(890.1843, 270.57)(891.1747, 1469.28)(1003.2136, 697.96) (891.7126, 1363.03)(468.3656, 885.43)(469.3527, 275.07)(470.3477, 152.17)(463.3965, 665.93)(446.3753, 22432.34)(447.3797, 7292.81)(448.3836, 1976.69)(449.3914, 261.63) | 52357.79 | 24153.89 | 58206.91 | 27089 | 59683 | 10343.46 | 56611.17 | 26673.86 | -1.03 | 1.42E-05 | 5.5E-05 | -0.15 | 0.560247 | 0.783425 |
| COMPOUND_445_3677a10_910512 | Rp | + | 445.3677 | 10.91 | | | | (891.7126, 1363.03)(468.3656, 885.43)(469.3527, 275.07)(470.3477, 152.17)(463.3965, 665.93)(446.3753, 22432.34)(447.3797, 7292.81)(448.3836, 1976.69)(449.3914, 261.63) | 41620.91 | 20909.28 | 40296 | 19699.24 | 129596.5 | 47788.06 | 122279.7 | 40348.36 | 1.37 | 6.75E-11 | 1.1E-09 | 0.02 | 0.938276 | 0.97184 |
| COMPOUND_446_339a10_843731 | Rp | - | 446.3390 | 10.84 | | | | (559.3352, 1517.07)(481.3085, 418.36)(482.2939, 2612.31)(445.3315, 10011.88)(446.3351, 3152.71)(447.3441, 1305.19)(448.3509, 238.51)(491.3316, 784.45)(492.3417, 565.48)(493.3277, 77.55)(1005.6961, 298.54)(1006.671, 734.49) (929.3517, 614.90)(560.182, 1017.63)(561.1773, 421.49)(562.1751, 2988.64)(563.1681, 982.26)(564.1691, 1480.01)(565.1702, 550.39)(482.1654, 6156.71)(939.3529, 328.89)(940.3711, 236.97)(446.1972, 6937.68)(447.1996, 1579.71)(448.2046, 671.21)(449.2019, 99.61)(492.194, 16519.94)(893.4143, 394.66)(894.4113, 376.02)(895.4223, 439.55)(1007.3465, 197.65)(1008.365, 165.01)(1009.3668, 210.54) | 74531.92 | 30643.83 | 81768.46 | 30279.15 | 99142.07 | 30369.1 | 86077.3 | 33043.57 | 0.78 | 0.001274 | 0.00325 | -0.69 | 0.011997 | 0.168863 |
| COMPOUND_447_2029a10_993175 | Rp | - | 447.2029 | 10.99 | | | | (891.7126, 1363.03)(468.3656, 885.43)(469.3527, 275.07)(470.3477, 152.17)(463.3965, 665.93)(446.3753, 22432.34)(447.3797, 7292.81)(448.3836, 1976.69)(449.3914, 261.63) | 56947.64 | 31674.83 | 52370.93 | 26928.1 | 60183.33 | 25565.46 | 56294.2 | 26747.46 | -0.24 | 0.423908 | 0.528595 | 0.31 | 0.385724 | 0.687856 |
| COMPOUND_447_2037a11_014076 | Rp | - | 447.2037 | 11.01 | | | | (929.3501, 636.61)(560.1794, 786.95)(561.1802, 525.33)(562.178, 2331.33)(563.1738, 1010.07)(564.171, 1799.22)(565.1731, 334.4)(482.1655, 5482.66)(939.3692, 300.1)(940.3682, 283.03)(446.1972, 5757.59)(447.1992, 1858.97)(448.1991, 501.47)(449.2046, 79.94)(492.1931, 2725.0)(893.4133, 509.13)(894.4277, 353.43)(895.4393, 303.65)(1007.4456, 199.76)(1008.4242, 248.9)(1009.4058, 179.87) | 36475.21 | 14990.51 | 39282.5 | 19535.5 | 44734.85 | 22397.12 | 49170.22 | 21544.39 | 0.33 | 0.259268 | 0.356019 | 0.17 | 0.623966 | 0.823156 |
| COMPOUND_448_1408a8_923512 | Rp | - | 448.1408 | 8.92 | | | | (561.1026, 310.53)(562.1076, 205.56)(447.134, 9936.1)(448.1373, 1831.21)(449.1396, 722.05) | 36034.44 | 3302.194 | 36908.24 | 4028.59 | 31466.75 | 3515.997 | 30050.79 | 3060.67 | -0.46 | 0.091577 | 0.150974 | 0.15 | 0.632478 | 0.828105 |
| COMPOUND_449_3129a8_110696 | Rp | - | 449.3129 | 8.11 | | | | (484.2819, 2984.01)(485.286, 1120.73)(486.2794, 947.65)(562.2969, 10453.46)(563.2982, 3887.86)(448.3056, 1057400.9)(449.3097, 281169.97)(450.3124, 48557.41)(451.3152, 6504.77)(897.6204, 90356.41)(898.623, 52123.88)(899.627, 16158.52)(900.6278, 3308.23)(901.6285, 611.77) | 71804.43 | 85517.9 | 50464.24 | 54596.17 | 79972.09 | 181240.7 | 258178.5 | 1517567 | -0.39 | 0.116699 | 0.186408 | -0.15 | 0.608775 | 0.812181 |
| COMPOUND_449_3136a9_239955 | Rp | - | 449.3136 | 9.24 | | | | (562.2919, 3858.22)(563.2919, 1334.43)(564.2762, 3402.87)(565.2804, 992.25)(448.3062, 406948.28)(449.3097, 116274.84)(450.3124, 18429.24)(451.3114, 3416.19)(452.3092, 344.47)(897.62, 14728.94)(898.6236, 8476.66)(899.6257, 2891.02)(900.6281, 637.47) | 174282.8 | 135955.4 | 155921.9 | 96943.81 | 197152.9 | 123549.3 | 287929.6 | 419785.6 | 0.00 | 0.989436 | 0.995427 | 0.17 | 0.564808 | 0.785799 |
| COMPOUND_449_3138a9_090611 | Rp | - | 449.3138 | 9.09 | | | | (562.2956, 1764.88)(563.2945, 485.59)(564.2742, 1097.49)(565.272, 391.94)(566.2739, 104.33)(484.2804, 2923.45)(485.2839, 990.29)(486.2804, 997.79)(487.2809, 197.82)(448.3064, 143047.62)(449.3096, 41263.54)(450.3126, 7430.24)(451.3105, 1027.05)(452.3076, 136.52)(897.6208, 30603.72)(898.6238, 1727.49)(899.6272, 5159.73)(900.6292, 1476.19)(901.6253, 283.77) | 433764.2 | 329882.2 | 373668.9 | 234989.2 | 457001.1 | 343034.7 | 441020.1 | 563393.3 | 0.06 | 0.839991 | 0.888104 | -0.20 | 0.545903 | 0.77815 |
| COMPOUND_449_3143a0_9564283 | Hiic | + | 449.3143 | 0.96 | | | | (899.6363, 17919.18)(900.6394, 10658.91)(901.6425, 3291.92)(902.6455, 866.93)(903.6459, 202.13)(472.3035, 31094.47)(473.3072, 9400.9)(474.3093, 1619.66)(475.3111, 316.61)(921.6179, 46035.23)(922.6208, 27115.62)(923.6245, 8525.56)(924.6267, 1956.77)(925.6282, 536.23)(467.3488, 891.74)(468.3516, 337.67)(450.3223, 151678.39)(451.3256, 43684.09)(452.3286, 7386.77)(453.3315, 959.16)(916.6726, 1067.25) (899.6366, 29427.9)(900.6395, 17442.19)(901.641, 5738.53)(902.6448, 1176.51)(903.6457, 297.57)(937.5828, 2009.12)(938.5871, 1444.93)(939.5895, 540.29)(942.3034, 7745.2)(473.3055, 2407.59)(474.3007, 748.37)(475.3117, 119.56)(921.618, 21455.2)(922.6218, 12416.98)(923.6222, 4159.39)(924.6212, 1362.09)(925.6176, 318.99)(488.2712, 14410.39)(489.2752, 4482.73)(490.2799, 1358.74)(450.3227, 460478.25)(451.3262, 131858.67)(452.3286, 22545.83)(453.3332, 3170.13) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.45 | 0.100727 | 0.163781 | 0.00 | 0.988653 | 0.99433 |
| COMPOUND_449_3155a9_243959 | Rp | + | 449.3155 | 9.24 | | | | (929.3501, 636.61)(560.1794, 786.95)(561.1802, 525.33)(562.178, 2331.33)(563.1738, 1010.07)(564.171, 1799.22)(565.1731, 334.4)(482.1655, 5482.66)(939.3692, 300.1)(940.3682, 283.03)(446.1972, 5757.59)(447.1992, 1858.97)(448.1991, 501.47)(449.2046, 79.94)(492.1931, 2725.0)(893.4133, 509.13)(894.4277, 353.43)(895.4393, 303.65)(1007.4456, 199.76)(1008.4242, 248.9)(1009.4058, 179.87) | 130347.9 | 102876.3 | 110670.3 | 66646.11 | 154767.1 | 98757.64 | 255214.2 | 446159.5 | 0.05 | 0.841964 | 0.888937 | 0.19 | 0.52371 | 0.766338 |
| COMPOUND_449_3517a11_066475 | Rp | + | 449.3517 | 11.07 | ACar 20:3 | 2 | 10eV: 60.0812(100), 450.3234(4), 309.1472(2) | (921.7001, 1624.15)(450.3594, 60966.14)(451.3628, 17886.59)(452.3661, 3225.59)(453.3679, 557.82)(916.7305, 3709.03) | 136900.5 | 34593.8 | 133787.3 | 36095.61 | 208134.6 | 45688.96 | 208053.4 | 54463.65 | 1.35 | 2.89E-07 | 1.66E-06 | -0.04 | 0.896049 | 0.954308 |
| COMPOUND_450_261a9_890633 | Rp | - | 450.2610 | 9.89 | | | | (563.28, 1544.31)(564.2379, 473.19)(485.2285, 1543.69)(486.2289, 174.89)(487.2274, 342.05)(449.2537, 18698.85)(450.2592, 8779.08)(451.263, 1033.59)(452.2683, 180.65)(899.5161, 2488.42)(900.5179, 1519.24)(901.5227, 552.13)(902.5189, 211.79) | 130813.4 | 60785.94 | 145557.3 | 57549 | 276876.8 | 75637.42 | 215289.9 | 114458.7 | 1.20 | 3.59E-05 | 0.000125 | -1.01 | 0.002419 | 0.068106 |
| COMPOUND_451_2426a6_665682 | Rp | + | 451.2426 | 6.67 | | | | (490.21, 345.42)(491.2107, 80.35)(469.2731, 1542.11)(470.2743, 398.06)(452.2494, 5158.63)(453.2532, 1266.11)(454.2578, 289.18)(455.2678, 52.32) (474.2549, 2959.97)(475.2578, 771.1)(469.3015, 4186.63)(452.2786, 6402.13)(453.294, 2557.0)(454.2845, 1517.54)(455.2716, 213.38) | 21637.2 | 4684.758 | 19665.58 | 4125.23 | 21959.08 | 5820.558 | 23983.63 | 5842.819 | 0.32 | 0.262006 | 0.358903 | 0.23 | 0.491988 | 0.748114 |
| COMPOUND_451_2716a9_937766 | Rp | + | 451.2716 | 9.94 | | | | (939.572, 795.65)(940.5506, 1112.74)(941.5599, 792.45)(451.2908, 13658.45)(452.2932, 4576.05)(453.2908, 2055.69)(454.2919, 364.21)(497.3214, 143.83)(498.2967, 369.4) | 33739.38 | 11791.74 | 42460.88 | 21365.49 | 58133 | 22325.26 | 54625.69 | 25975.62 | 1.01 | 4.21E-05 | 0.000143 | -0.16 | 0.552574 | 0.780002 |
| COMPOUND_452_2981a11_1870985 | Rp | - | 452.2981 | 11.19 | | | | (939.572, 795.65)(940.5506, 1112.74)(941.5599, 792.45)(451.2908, 13658.45)(452.2932, 4576.05)(453.2908, 2055.69)(454.2919, 364.21)(497.3214, 143.83)(498.2967, 369.4) | 77986.29 | 56435.45 | 105293.1 | 81130.23 | 152099.2 | 122972.8 | 126553.2 | 111257.3 | 0.82 | 0.005942 | 0.01321 | -0.41 | 0.235744 | 0.541667 |
| COMPOUND_453_1911a10_7157135 | Rp | - | 453.1911 | 10.72 | | | | (941.327, 274.32)(942.3299, 192.06)(488.1523, 4725.34)(489.1533, 1448.62)(951.4337, 252.05)(952.4445, 163.14)(452.1858, 9113.65)(453.1922, 3331.13)(454.1844, 2243.28)(455.1721, 201.51)(905.3397, 355.18) | 46223.8 | 10771.43 | 50348.13 | 14240.85 | 32331.3 | 11792.14 | 31407.39 | 15064.15 | -0.68 | 0.007016 | 0.0154 | -0.33 | 0.268258 | 0.575898 |
| COMPOUND_453_2852a10_221464 | Rp | - | 453.2852 | 10.22 | LPE 16:0 | 2 | 10 eV: 452.2777(100), 255.2327(47), 196.038(4), 78.9588(2) | (566.2635, 357.54)(567.2576, 229.29)(452.2779, 250282.3)(453.2809, 56564.32)(454.2838, 996.96)(456.2898, 185.08)(905.5425, 1141.37)(906.5345, 2840.27)(907.5375, 1238.75) (907.5813, 119.95)(908.6063, 35.22)(909.5627, 127.37)(476.2845, 1985.8)(477.2765, 62.34)(478.2953, 2443.18)(929.5563, 333.29)(930.5692, 407.68)(471.3177, 124.76)(454.2931, 7903.8)(455.2965, 1896.44)(456.2985, 291.51) (907.5783, 1449.51)(908.585, 803.64)(909.583, 300.23)(910.5835, 20.58)(476.2751, 21255.27)(477.2783, 5198.93)(929.5606, 1849.02)(930.5645, 875.93)(931.5775, 937.98)(932.5794, 600.54)(933.5898, 323.65)(454.2933, 12973.41)(455.2965, 3085.44)(456.3004, 738.71)(457.2912, 137.34) (907.5735, 1542.61)(908.527, 5226.52)(909.5337, 2836.85)(910.5409, 3367.13)(945.5485, 393011.6) 84627.98 402405.6 141149.7 423145.5 225436.6 424688.3 163120.3 -0.14 0.633911 0.723918 0.31 0.388451 0.68827 | 520477.6 | 303979.3 | 534886.4 | 395678.4 | 248873.4 | 372721.6 | 324465.8 | 332258.4 | -1.02 | 0.000548 | 0.001512 | 0.30 | 0.367317 | 0.669574 |
| COMPOUND_453_2859a1_5489997 | Hiic | + | 453.2859 | 1.55 | | | | (907.5813, 119.95)(908.6063, 35.22)(909.5627, 127.37)(476.2845, 1985.8)(477.2765, 62.34)(478.2953, 2443.18)(929.5563, 333.29)(930.5692, 407.68)(471.3177, 124.76)(454.2931, 7903.8)(455.2965, 1896.44)(456.2985, 291.51) (907.5783, 1449.51)(908.585, 803.64)(909.583, 300.23)(910.5835, 20.58)(476.2751, 21255.27)(477.2783, 5198.93)(929.5606, 1849.02)(930.5645, 875.93)(931.5775, 937.98)(932.5794, 600.54)(933.5898, 323.65)(454.2933, 12973.41)(455.2965, 3085.44)(456.3004, 738.71)(457.2912, 137.34) | 27363.25 | 6214.642 | 30801.93 | 10937.52 | 23796.07 | 11943.39 | 23953.33 | 11566.33 | -0.58 | 0.048105 | 0.084701 | -0.21 | 0.543026 | 0.776977 |
| COMPOUND_453_2869a10_280065 | Rp | + | 453.2869 | 10.28 | LPE 16:0 | 2 | 10 eV: 454.2935(100), 313.2762(100), 44.049(95) | (907.5813, 119.95)(908.6063, 35.22)(909.5627, 127.37)(476.2845, 1985.8)(477.2765, 62.34)(478.2953, 2443.18)(929.5563, 333.29)(930.5692, 407.68)(471.3177, 124.76)(454.2931, 7903.8)(455.2965, 1896.44)(456.2985, 291.51) (907.5783, 1449.51)(908.585, 803.64)(909.583, 300.23)(910.5835, 20.58)(476.2 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--------------|---|---|----------|---------------|----------|---------------|----------|---------------|----------|----------|-------|----------|-------------|-------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_454_3013a11_232764 | Rp | + | 454.3013 | 11.23 | | | | (909.6243, 1557.47)(910.6107, 1208.011)(911.6394, 876.46)(477.2571, 286.29)(478.2509, 21163.86 10295.24 25013.43 10579.23 44358.17 22823.73 39124.45 16731.1 | 111.06(479.2698, 1170.69)(480.2665, 597.96)(931.6299, 1166.61)(455.3063, 12142.07)(456.3084, 3605.22)(457.3085, 869.211) | 21663.86 | 10295.24 | 25013.43 | 10579.23 | 44358.17 | 22823.73 | 39124.45 | 16731.1 | 1.08 | 4.35E-05 | 0.000146 | -0.26 | 0.383948 | 0.686377 |
| COMPOUND_455_1286a9_921174 | Rp | - | 455.1286 | 9.92 | | | | (915.67)(570.1048, 822.32)(571.1042, 527.57)(572.104, 452.62)(454.1207, 7846.78)(455.1164, 2434.94)(456.1177, 2710.2) | (568.1216, 1183.89)(569.1274, 481.02)(570.1194, 995.7)(490.1102, 13728.1)(491.113, 3297.87)(492.1075, 12371.17)(493.1112, 3112.75)(494.1058, 3946.55)(495.1103, 971.56)(496.1063, 698.46)(955.2775, 347.98)(956.2836, 299.5)(454.1339, 34633.83)(455.1371, 9083.12)(456.1313, 22448.43)(457.1316, 5750.03)(458.1279, 4127.81)(459.1116, 1836.06)(909.2471, 428.85)(910.2724, 149.08)(911.2403, 265.02)(1023.2259, 595.95) | 27648.96 | 8226.84 | 28602.33 | 9929.868 | 36308 | 2920.933 | 29210.56 | 10550.16 | -0.90 | 0.0001 | 0.00031 | -0.25 | 0.344614 | 0.651065 |
| COMPOUND_455_1408a10_597347 | Rp | - | 455.1408 | 10.60 | | | | (568.1216, 1183.89)(569.1274, 481.02)(570.1194, 995.7)(490.1102, 13728.1)(491.113, 3297.87)(492.1075, 12371.17)(493.1112, 3112.75)(494.1058, 3946.55)(495.1103, 971.56)(496.1063, 698.46)(955.2775, 347.98)(956.2836, 299.5)(454.1339, 34633.83)(455.1371, 9083.12)(456.1313, 22448.43)(457.1316, 5750.03)(458.1279, 4127.81)(459.1116, 1836.06)(909.2471, 428.85)(910.2724, 149.08)(911.2403, 265.02)(1023.2259, 595.95) | (568.15, 814.52)(569.1515, 287.42)(570.1415, 488.73)(490.1468, 5962.15)(491.1423, 2429.89)(955.2977, 233.9)(956.3164, 435.11)(957.326, 239.51)(454.1646, 7515.92)(455.1669, 2301.33)(456.175, 1021.69)(457.1609, 117.62)(909.3474, 292.07)(910.3496, 202.71)(500.1758, 13242.94)(501.1782, 4066.07) | 94734.98 | 40792.3 | 89847.85 | 37510.55 | 112562.4 | 41090.63 | 158908 | 54680.53 | 0.39 | 0.121666 | 0.193088 | 0.84 | 0.005846 | 0.118614 |
| COMPOUND_455_1723a10_50408 | Rp | - | 455.1723 | 10.50 | | | | (568.15, 814.52)(569.1515, 287.42)(570.1415, 488.73)(490.1468, 5962.15)(491.1423, 2429.89)(955.2977, 233.9)(956.3164, 435.11)(957.326, 239.51)(454.1646, 7515.92)(455.1669, 2301.33)(456.175, 1021.69)(457.1609, 117.62)(909.3474, 292.07)(910.3496, 202.71)(500.1758, 13242.94)(501.1782, 4066.07) | (949.6566, 2593.06)(950.6517, 2556.01)(478.3303, 5629.57)(479.3363, 1645.93)(480.3431, 1005.12)(456.3492, 6190.17)(457.351, 2170.67)(458.3505, 925.33)(928.6868, 1409.32) | 46377.94 | 18675.09 | 46867.07 | 19731.65 | 100134.2 | 22082.65 | 112303.9 | 32347.95 | 0.31 | 0.237059 | 0.331794 | 0.74 | 0.01915 | 0.196411 |
| COMPOUND_455_3402a10_948466 | Rp | + | 455.3402 | 10.95 | | | | (949.6566, 2593.06)(950.6517, 2556.01)(478.3303, 5629.57)(479.3363, 1645.93)(480.3431, 1005.12)(456.3492, 6190.17)(457.351, 2170.67)(458.3505, 925.33)(928.6868, 1409.32) | (456.1604, 13574.57)(457.1672, 6518.55)(458.1662, 2011.93)(459.172, 335.95)(913.3545, 507.62) | 45278.94 | 33255.79 | 40158.6 | 42896.23 | 41128.77 | 11099.65 | 44740.7 | 12257.37 | 0.00 | 0.99522 | 0.998768 | 0.27 | 0.440796 | 0.716214 |
| COMPOUND_457_1675a10_659327 | Rp | - | 457.1675 | 10.66 | | | | (456.1604, 13574.57)(457.1672, 6518.55)(458.1662, 2011.93)(459.172, 335.95)(913.3545, 507.62) | (949.3273, 408.21)(950.3328, 268.8)(951.3531, 280.37)(959.3299, 412.72)(960.3369, 384.12)(961.3518, 319.79)(456.1829, 1979.13)(457.1861, 980.56)(458.1963, 14580.56)(459.1996, 4482.5)(913.373, 529.63)(914.3838, 477.95)(915.3855, 325.04)(1027.3038, 283.12)(1028.3337, 284.11) | 44750.94 | 8013.6 | 43425.35 | 8040.38 | 32502.9 | 16084.75 | 34482 | 10592.72 | -0.85 | 0.00115 | 0.002954 | 0.05 | 0.87176 | 0.945212 |
| COMPOUND_457_1902a11_017043 | Rp | - | 457.1902 | 11.02 | | | | (949.3273, 408.21)(950.3328, 268.8)(951.3531, 280.37)(959.3299, 412.72)(960.3369, 384.12)(961.3518, 319.79)(456.1829, 1979.13)(457.1861, 980.56)(458.1963, 14580.56)(459.1996, 4482.5)(913.373, 529.63)(914.3838, 477.95)(915.3855, 325.04)(1027.3038, 283.12)(1028.3337, 284.11) | (959.4797, 3334.21)(456.2363, 14534.56)(457.2379, 6115.97)(458.2377, 2275.65)(459.2386, 357.05)(1027.487, 171.81) | 44750.94 | 8013.6 | 43425.35 | 8040.38 | 32502.9 | 16084.75 | 34482 | 10592.72 | -0.85 | 0.00115 | 0.002954 | 0.05 | 0.87176 | 0.945212 |
| COMPOUND_457_2445a10_789214 | Rp | - | 457.2445 | 10.79 | | | | (959.4797, 3334.21)(456.2363, 14534.56)(457.2379, 6115.97)(458.2377, 2275.65)(459.2386, 357.05)(1027.487, 171.81) | (915.5203, 408.98)(952.4734, 559.47)(953.4772, 383.65)(457.2283, 11337.64)(458.2307, 3194.44)(459.2253, 20425.6)(460.2272, 5786.91)(461.2219, 8185.82)(462.2253, 2201.45)(463.2209, 1618.84)(915.4657, 416.1)(916.4555, 414.99)(917.4655, 698.44)(1029.497, 667.07)(1030.5043, 1267.43) | 31580.52 | 14072.86 | 32971.29 | 15456.78 | 57723.29 | 21337.7 | 67673.89 | 20304.74 | 1.13 | 1.15E-06 | 5.64E-06 | 0.31 | 0.218258 | 0.526249 |
| COMPOUND_458_2359a11_579628 | Rp | - | 458.2359 | 11.58 | | | | (915.5203, 408.98)(952.4734, 559.47)(953.4772, 383.65)(457.2283, 11337.64)(458.2307, 3194.44)(459.2253, 20425.6)(460.2272, 5786.91)(461.2219, 8185.82)(462.2253, 2201.45)(463.2209, 1618.84)(915.4657, 416.1)(916.4555, 414.99)(917.4655, 698.44)(1029.497, 667.07)(1030.5043, 1267.43) | (915.5203, 408.98)(952.4734, 559.47)(953.4772, 383.65)(457.2283, 11337.64)(458.2307, 3194.44)(459.2253, 20425.6)(460.2272, 5786.91)(461.2219, 8185.82)(462.2253, 2201.45)(463.2209, 1618.84)(915.4657, 416.1)(916.4555, 414.99)(917.4655, 698.44)(1029.497, 667.07)(1030.5043, 1267.43) | 66015.54 | 15227.08 | 70379.85 | 15232.66 | 71942.36 | 21087.6 | 66501.73 | 22600.21 | 0.43 | 0.124933 | 0.196511 | -0.80 | 0.018156 | 0.195632 |
| COMPOUND_458_2437a1_3971556 | Hilic | + | 458.2437 | 1.40 | | | | (915.5203, 408.98)(952.4734, 559.47)(953.4772, 383.65)(457.2283, 11337.64)(458.2307, 3194.44)(459.2253, 20425.6)(460.2272, 5786.91)(461.2219, 8185.82)(462.2253, 2201.45)(463.2209, 1618.84)(915.4657, 416.1)(916.4555, 414.99)(917.4655, 698.44)(1029.497, 667.07)(1030.5043, 1267.43) | (915.5203, 408.98)(952.4734, 559.47)(953.4772, 383.65)(457.2283, 11337.64)(458.2307, 3194.44)(459.2253, 20425.6)(460.2272, 5786.91)(461.2219, 8185.82)(462.2253, 2201.45)(463.2209, 1618.84)(915.4657, 416.1)(916.4555, 414.99)(917.4655, 698.44)(1029.497, 667.07)(1030.5043, 1267.43) | 61025.43 | 41172.33 | 69269.66 | 37849.84 | 81611.45 | 49237.25 | 80209.56 | 25332.11 | 0.50 | 0.071339 | 0.120709 | -0.17 | 0.604434 | 0.810123 |
| COMPOUND_458_4091a11_081561 | Rp | + | 458.4091 | 11.08 | | | | (915.5203, 408.98)(952.4734, 559.47)(953.4772, 383.65)(457.2283, 11337.64)(458.2307, 3194.44)(459.2253, 20425.6)(460.2272, 5786.91)(461.2219, 8185.82)(462.2253, 2201.45)(463.2209, 1618.84)(915.4657, 416.1)(916.4555, 414.99)(917.4655, 698.44)(1029.497, 667.07)(1030.5043, 1267.43) | (917.8398, 1232.28)(918.8344, 809.83)(919.8211, 274.75)(955.7604, 115.75)(481.4111, 347.45)(939.7895, 940.35)(459.4161, 23194.81)(460.4188, 6754.1)(461.4188, 1241.02)(462.4104, 225.15)(934.8894, 967.75)(935.8738, 815.06)(936.8909, 252.71) | 44082 | 25837.03 | 32195.69 | 13120.35 | 73895.25 | 59952.42 | 75315.16 | 37617.03 | 0.54 | 0.038954 | 0.070689 | 0.46 | 0.14256 | 0.448182 |
| COMPOUND_458_4091a11_032743 | Rp | + | 458.4091 | 11.03 | | | | (917.8398, 1232.28)(918.8344, 809.83)(919.8211, 274.75)(955.7604, 115.75)(481.4111, 347.45)(939.7895, 940.35)(459.4161, 23194.81)(460.4188, 6754.1)(461.4188, 1241.02)(462.4104, 225.15)(934.8894, 967.75)(935.8738, 815.06)(936.8909, 252.71) | (917.8398, 1232.28)(918.8344, 809.83)(919.8211, 274.75)(955.7604, 115.75)(481.4111, 347.45)(939.7895, 940.35)(459.4161, 23194.81)(460.4188, 6754.1)(461.4188, 1241.02)(462.4104, 225.15)(934.8894, 967.75)(935.8738, 815.06)(936.8909, 252.71) | 38199.26 | 20773.94 | 28733.71 | 12539.22 | 46860.62 | 29724.82 | 51148.41 | 28356.74 | 0.46 | 0.029995 | 0.153089 | 0.41 | 0.203491 | 0.5149 |
| COMPOUND_459_9957a10_144271 | Rp | + | 459.9957 | 10.14 | | | | (917.8398, 1232.28)(918.8344, 809.83)(919.8211, 274.75)(955.7604, 115.75)(481.4111, 347.45)(939.7895, 940.35)(459.4161, 23194.81)(460.4188, 6754.1)(461.4188, 1241.02)(462.4104, 225.15)(934.8894, 967.75)(935.8738, 815.06)(936.8909, 252.71) | (917.8398, 1232.28)(918.8344, 809.83)(919.8211, 274.75)(955.7604, 115.75)(481.4111, 347.45)(939.7895, 940.35)(459.4161, 23194.81)(460.4188, 6754.1)(461.4188, 1241.02)(462.4104, 225.15)(934.8894, 967.75)(935.8738, 815.06)(936.8909, 252.71) | 43910.52 | 19002.43 | 34782.5 | 13550.54 | 49800 | 11730.96 | 53224.09 | 16914.46 | 0.23 | 0.393487 | 0.497827 | 0.78 | 0.020103 | 0.199116 |
| COMPOUND_463_2766a9_4074135 | Rp | + | 463.2766 | 9.41 | | | | (917.8398, 1232.28)(918.8344, 809.83)(919.8211, 274.75)(955.7604, 115.75)(481.4111, 347.45)(939.7895, 940.35)(459.4161, 23194.81)(460.4188, 6754.1)(461.4188, 1241.02)(462.4104, 225.15)(934.8894, 967.75)(935.8738, 815.06)(936.8909, 252.71) | (462.8902, 155.33)(463.8916, 305.09)(464.8929, 49.92)(465.8942, 228.53)(466.8956, 461.0042, 6601.39)(462.0056, 762.2)(462.9907, 1014.57)(464.0032, 119.68) | 50506.83 | 37765.59 | 53623.94 | 36754.1 | 274236.9 | 61777.6 | 148436.8 | 199837.7 | 0.57 | 0.002544 | 0.0483 | -0.04 | 0.896677 | 0.954308 |
| COMPOUND_463_3036a10_536387 | Rp | - | 463.3036 | 10.54 | | | | (462.8902, 155.33)(463.8916, 305.09)(464.8929, 49.92)(465.8942, 228.53)(466.8956, 461.0042, 6601.39)(462.0056, 762.2)(462.9907, 1014.57)(464.0032, 119.68) | (464.2838, 22592.01)(465.2875, 6400.58)(466.2887, 1962.45)(467.2886, 362.06) | 239965.7 | 72517.91 | 247174.3 | 82713.7 | 99067.56 | 92118.98 | 107383 | 89977.73 | -1.19 | 1.27E-07 | 7.8E-07 | -0.23 | 0.335126 | 0.63958 |
| COMPOUND_463_3066a1_3849862 | Hilic | + | 463.3066 | 1.38 | | | | (464.2838, 22592.01)(465.2875, 6400.58)(466.2887, 1962.45)(467.2886, 362.06) | (927.6145, 236.87)(928.6462, 521.98)(486.296, 4285.12)(487.2995, 1123.58)(488.3111, 2825.3)(949.5894, 276.13)(481.3323, 364.52)(464.3141, 12368.54)(465.3179, 3226.68) | 47263.45 | 15111.23 | 49605.74 | 18073.72 | 21616.63 | 19001.16 | 17717.86 | 18327.24 | -1.21 | 1.66E-07 | 1.01E-06 | -0.19 | 0.426584 | 0.705867 |
| COMPOUND_463_3083a10_537336 | Rp | + | 463.3083 | 10.54 | | | | (927.6145, 236.87)(928.6462, 521.98)(486.296, 4285.12)(487.2995, 1123.58)(488.3111, 2825.3)(949.5894, 276.13)(481.3323, 364.52)(464.3141, 12368.54)(465.3179, 3226.68) | (927.6204, 560.9)(928.6171, 865.94)(929.6275, 700.29)(965.5896, 1036.7)(966.5809, 1179.65)(967.5915, 897.18)(486.2963, 4236.74)(487.2951, 1453.91)(488.3009, 568.0)(949.5746, 1507.81)(950.5701, 1785.3)(951.587, 903.34)(502.294, 591.58)(503.2973, 323.32)(464.3146, 68359.01)(465.3177, 17323.0)(466.3235, 4779.5)(467.3166, 692.57)(944.6288, 542.55)(945.6153, 860.91) | 208666.9 | 67837.42 | 204597.1 | 64239.7 | 81871.75 | 90674.87 | 65212.43 | 76234.07 | -1.22 | 7.38E-07 | 3.83E-06 | -0.12 | 0.642189 | 0.834513 |
| COMPOUND_465_1576a9_919288 | Rp | - | 465.1576 | 9.92 | | | | (927.6204, 560.9)(928.6171, 865.94)(929.6275, 700.29)(965.5896, 1036.7)(966.5809, 1179.65)(967.5915, 897.18)(486.2963, 4236.74)(487.2951, 1453.91)(488.3009, 568.0)(949.5746, 1 | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|-----------------|----------|---|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_466_1709a10_715968 | Rp | - | 467.2709 | 10.72 | | | | (969.2925, 305.07)(970.274, 236.62)(580.174, 459.266)(581.1736, 2046.07)(979.3146, 295.5)(466.166, 812.147)(467.1693, 2704.32)(468.1671, 1044.91)(469.1743, 190.24)(933.3435, 395.52)(934.3408, 234.73)(935.361, 303.46)(936.3526, 270.72)(512.1785, 840.82)(513.1772, 85.69)(514.1658, 2577.94)(935.6091, 2432.96)(490.2911, 47804.33)(491.2943, 12196.35)(492.305, 4272.44)(957.5901, 1983.39)(468.3092, 52551.93)(469.3124, 13455.88)(470.3147, 2272.53)(471.3197, 431.47)(490.2931, 2986.0)(491.2955, 959.48)(492.3023, 265.17)(485.3461, 1038.09)(486.3463, 626.19)(468.3094, 15033.94)(469.3132, 3740.26)(470.3134, 827.35)(471.3131, 158.5) | 60983.09 | 10925.54 | 61832.07 | 18066.8 | 50566.78 | 19220.54 | 56263.03 | 16644.83 | -0.94 | 0.000778 | 0.002076 | 0.27 | 0.404114 | 0.6912 |
| COMPOUND_467_3017a1_1443499 | Hilic | + | 467.3017 | 1.14 | LPC 14:0 isomer | 2 | 10 eV: 468.3079 (100), 184.0733 (80) | (935.6091, 2432.96)(490.2911, 47804.33)(491.2943, 12196.35)(492.305, 4272.44)(957.5901, 1983.39)(468.3092, 52551.93)(469.3124, 13455.88)(470.3147, 2272.53)(471.3197, 431.47) | 164880.9 | 46343.7 | 129110.4 | 111653.3 | 112388.9 | 35189.9 | 87577.63 | 43050.65 | 0.58 | 0.042152 | 0.075398 | -1.16 | 0.000803 | 0.045795 |
| COMPOUND_467_3017a9_617346 | Rp | + | 467.3017 | 9.62 | LPC 14:0 isomer | 2 | 10 eV: 468.3131(100), 184.0753(15), 104.1084(11) | (490.2931, 2986.0)(491.2955, 959.48)(492.3023, 265.17)(485.3461, 1038.09)(486.3463, 626.19)(468.3094, 15033.94)(469.3132, 3740.26)(470.3134, 827.35)(471.3131, 158.5) | 97803.55 | 46461.07 | 128636.6 | 74630.19 | 101046.6 | 41699.43 | 83402.71 | 43616.55 | 0.01 | 0.962678 | 0.978317 | -0.61 | 0.056055 | 0.29488 |
| COMPOUND_467_3025a10_470193 | Rp | + | 467.3025 | 10.47 | | | | (935.6177, 403.98)(936.6313, 314.46)(937.6366, 539.62)(973.5746, 838.92)(974.5782, 752.21)(490.2948, 757.87)(491.2948, 300.34)(492.295, 394.55)(957.5686, 865.57)(506.273, 519.53)(507.2801, 243.88)(468.3098, 6954.84)(469.3132, 2152.2)(470.3048, 317.65)(952.6614, 1644.74)(953.661, 1339.82) | 50088.33 | 12834.41 | 51667.9 | 16061.07 | 29439.6 | 11589.57 | 27133.03 | 11234.1 | -1.02 | 3.44E-05 | 0.00012 | -0.04 | 0.877922 | 0.949606 |
| COMPOUND_467_3026a1_2767569 | Hilic | + | 467.3026 | 1.28 | LPC 14:0 | 2 | 10 eV: 468.3088 (100), 184.0734 (25), 104.1073 (15) | (935.6102, 4465.51)(936.6133, 2455.77)(937.6177, 760.34)(938.5983, 294.97)(490.291, 73432.02)(491.2943, 18967.02)(492.3048, 684.132)(957.592, 3968.97)(958.5948, 2274.64)(959.5991, 857.8)(960.6159, 211.71)(485.3317, 641.79)(468.3086, 70127.15)(469.3127, 163248.05)(470.3152, 28435.16)(471.3176, 3782.26)(472.3192, 498.8) | 1147623 | 666444.1 | 1742892 | 1101313 | 1159377 | 510672.8 | 932919.6 | 521910.5 | 0.07 | 0.783743 | 0.842477 | -1.02 | 0.002282 | 0.067469 |
| COMPOUND_467_303a9_7604685 | Rp | + | 467.3030 | 9.76 | LPC 14:0 | 2 | 10eV: 468.3104(100), 104.1076(25), 184.077(17) | (935.6113, 6131.02)(936.6152, 3084.25)(937.6173, 1071.12)(938.5954, 151.75)(490.2909, 9423.74)(491.2941, 2656.38)(492.307, 1023.06)(493.3086, 169.41)(957.6054, 1138.52)(958.587, 557.04)(959.5726, 904.68)(960.573, 451.68)(506.2644, 3146.84)(507.2661, 1183.67)(508.2723, 1194.33)(468.3103, 737854.94)(469.3141, 171333.94)(470.3163, 28110.07)(471.3199, 4429.43)(472.3109, 418.2) | 907722.4 | 499039.5 | 1293387 | 799978.1 | 945585.1 | 399904.3 | 769146 | 447486.1 | 0.08 | 0.770044 | 0.833358 | -0.95 | 0.002714 | 0.073638 |
| COMPOUND_468_1649a9_920559 | Rp | - | 468.1649 | 9.92 | | | | (467.1576, 8112.35)(468.1607, 1714.87)(469.1558, 3446.72)(470.1535, 1030.70)(471.1617, 792.67)(513.175, 715.8)(514.1628, 164.34) | 26846.57 | 7750.655 | 27775.7 | 7640.995 | 26865 | 3433.895 | 31984.7 | 9942.689 | -1.13 | 2.34E-06 | 1.07E-05 | -0.04 | 0.880417 | 0.950612 |
| COMPOUND_468_2145a9_028728 | Rp | - | 468.2145 | 9.03 | | | | (467.2075, 20390.52)(468.2108, 4933.65)(469.2114, 1751.87)(470.2102, 281.77) | 29299 | 9888.931 | 33679.2 | 15119.39 | 100275.9 | 47380.88 | 83096.4 | 36756.9 | 1.71 | 4.43E-13 | 2.56E-11 | -0.44 | 0.04669 | 0.275249 |
| COMPOUND_468_2155a8_328927 | Rp | - | 468.2155 | 8.33 | | | | (467.2078, 6304.44)(468.2115, 1721.58)(469.2099, 559.57)(470.2137, 96.57) | 19330.8 | 6337.55 | 19725.05 | 7534.179 | 38634.5 | 10801.23 | 32294.38 | 12464.14 | 1.43 | 1.76E-07 | 1.06E-06 | -0.51 | 0.076861 | 0.332868 |
| COMPOUND_468_3584a11_773093 | Rp | + | 468.3584 | 11.77 | | | | (975.7167, 794.14)(959.7309, 1211.85)(960.7148, 1248.73)(469.3668, 12206.89)(470.3692, 4328.61)(471.3709, 848.69)(472.3797, 149.11)(973.1678, 513.81)(504.0688, 2101.59)(505.0731, 764.43)(506.0662, 2156.68)(507.0678, 692.3)(508.0632, 693.82)(509.0779, 219.28)(983.1933, 417.34)(984.2173, 306.02)(468.092, 9589.48)(469.0973, 3958.86)(470.0896, 6458.42)(471.0952, 2687.32)(472.0911, 1384.63)(514.0844, 355.0)(937.1867, 659.91)(938.1991, 509.69)(939.2092, 488.95)(1051.2279, 425.78)(1052.2241, 418.75) | 52954.3 | 15137.96 | 53054.63 | 13862.92 | 23692.3 | 14325.75 | 21045.97 | 12929.04 | -1.31 | 4.77E-09 | 4.23E-08 | -0.19 | 0.409663 | 0.694731 |
| COMPOUND_469_1018a10_011417 | Rp | - | 469.1018 | 10.01 | | | | (973.1678, 513.81)(504.0688, 2101.59)(505.0731, 764.43)(506.0662, 2156.68)(507.0678, 692.3)(508.0632, 693.82)(509.0779, 219.28)(983.1933, 417.34)(984.2173, 306.02)(468.092, 9589.48)(469.0973, 3958.86)(470.0896, 6458.42)(471.0952, 2687.32)(472.0911, 1384.63)(514.0844, 355.0)(937.1867, 659.91)(938.1991, 509.69)(939.2092, 488.95)(1051.2279, 425.78)(1052.2241, 418.75) | 34970.02 | 16205.52 | 39666.33 | 16131.12 | 41931.25 | 19801.39 | 56005.6 | 23137.29 | -0.85 | 0.000521 | 0.00144 | -0.20 | 0.465718 | 0.732912 |
| COMPOUND_470_0011a9_978315 | Rp | + | 470.0011 | 9.98 | | | | (492.9948, 183.97)(494.0136, 415.75)(488.0574, 167.03)(508.9833, 160.5)(471.0082, 1155.62)(472.0109, 1168.21)(472.9929, 1725.81)(474.0027, 211.42)(475.004, 550.74) | 61593.83 | 23642.75 | 51015.26 | 18486.03 | 62760.62 | 11090.56 | 66216.27 | 19468.09 | 0.09 | 0.74521 | 0.814666 | 0.78 | 0.025023 | 0.219303 |
| COMPOUND_470_2331a7_9199367 | Rp | - | 470.2331 | 7.92 | | | | (469.2255, 6065.79)(470.2293, 1969.3)(471.2329, 869.09) | 13915.16 | 3129.989 | 12709.57 | 1945.359 | 18639.31 | 9726.876 | 17280.95 | 7060.772 | 1.12 | 2.11E-07 | 1.23E-06 | -0.50 | 0.02711 | 0.226687 |
| COMPOUND_470_4299a11_762702 | Rp | + | 471.4299 | 11.76 | | | | (943.9028, 455.19)(944.909, 405.2)(981.8043, 470.37)(494.412, 770.88)(489.4477, 329.02)(510.4159, 444.02)(472.4367, 2848.21)(473.44, 8866.34)(474.4419, 1793.52) | 91678.85 | 32687.25 | 74013.93 | 33032.31 | 91311.14 | 23867.08 | 99401.72 | 30612.89 | 0.04 | 0.88663 | 0.923966 | 0.83 | 0.014278 | 0.179521 |
| COMPOUND_472_3141a11_110396 | Rp | + | 472.3141 | 11.11 | | | | (495.3101, 685.52)(473.3197, 7591.19)(474.323, 2239.05)(475.3293, 685.42)(962.6642, 6099.84)(963.6672, 5891.05) | 30996.14 | 9905.527 | 26589.38 | 8071.212 | 45293.4 | 9624.523 | 46632.8 | 14167.93 | 0.44 | 0.105433 | 0.170449 | 0.36 | 0.266002 | 0.575669 |
| COMPOUND_473_2418a9_516804 | Rp | + | 473.2418 | 9.52 | | | | (474.2494, 5406.14)(475.2527, 1645.91)(476.2546, 362.67)(477.2516, 70.36) | 39484.42 | 8245.141 | 36050.65 | 6654.149 | 36166.71 | 4265.773 | 38288.28 | 7053.684 | -0.35 | 0.242391 | 0.337578 | 0.68 | 0.059651 | 0.300425 |
| COMPOUND_474_1659a9_920882 | Rp | - | 474.1659 | 9.92 | | | | (587.1383, 541.07)(588.124, 298.12)(509.1374, 648.34)(510.1356, 238.88)(511.1281, 303.86)(473.1624, 5298.44)(474.1647, 1927.95)(475.1589, 914.76)(476.1716, 107.98)(519.1577, 990.66)(520.1685, 261.55) | 18048.22 | 5786.546 | 20598.08 | 6584.556 | 21937.33 | 6339.429 | 24796.33 | 1932.44 | -0.76 | 0.0004 | 0.00113 | -0.51 | 0.039467 | 0.261543 |
| COMPOUND_474_4063a12_528065 | Rp | - | 474.4063 | 12.53 | | | | (509.3753, 2335.0)(510.3772, 819.51)(511.3742, 957.88)(512.3761, 480.14)(513.3736, 80.32)(993.7929, 103.32)(994.7905, 84.9)(973.3991, 24236.61)(474.4025, 8436.94)(475.4053, 1594.51)(476.4085, 268.73)(477.3953, 37.06)(519.4044, 1131.18)(520.4069, 1389.64)(521.4095, 466.18)(522.4132, 90.14) | 126604 | 40314.33 | 157849.6 | 45078.52 | 151205.3 | 56808.63 | 143314.3 | 46612.28 | 0.45 | 0.112897 | 0.181214 | -0.66 | 0.048748 | 0.279822 |
| COMPOUND_474_4064a12_427342 | Rp | - | 474.4064 | 12.43 | | | | (509.3756, 3599.3)(510.3787, 1141.81)(511.3743, 1263.96)(512.3754, 508.77)(513.3755, 71.48)(993.7995, 91.87)(994.8178, 93.38)(473.3989, 60688.42)(474.4027, 20750.52)(475.4057, 3694.89)(476.4087, 589.53)(477.4094, 84.41)(519.4044, 8978.74)(520.4076, 2833.01)(521.4106, 611.87)(522.4105, 115.13) | 400979.1 | 93797.4 | 457723.8 | 104540.4 | 387574.9 | 80133.57 | 380158 | 87355.66 | -0.09 | 0.744111 | 0.814256 | -0.78 | 0.020479 | 0.200518 |
| COMPOUND_474_4089a12_433876 | Rp | + | 474.4089 | 12.43 | | | | (497.3961, 6718.44)(498.4006, 2188.38)(499.4005, 476.49)(500.4102, 80.65)(513.3704, 958.84)(514.3736, 438.03)(515.3701, 654.99)(516.3687, 236.41)(492.442, 93049.78)(493.4452, 31171.89)(494.4484, 5951.79)(495.4504, 1020.79)(496.4576, 142.68)(475.4147, 32715.69)(476.4179, 11244.28)(477.4208, 1947.79)(478.4246, 365.27) | 684295.5 | 142997.1 | 612463.1 | 151841.8 | 598334.4 | 147154.3 | 625260.2 | 146674.3 | -0.50 | 0.0823 | 0.136743 | 0.59 | 0.080008 | 0.339484 |
| COMPOUND_474_6732a10_116064 | Rp | + | 474.6732 | 10.12 | | | | (950.3576, 227.09)(951.334, 151.77)(952.3405, 235.31)(953.3321, 103.69)(988.3231, 214.7)(989.3218, 155.64)(497.6427, 241.57)(972.3331, 125.27)(973.3555, 98.59)(974.3331, 277.63)(513.6525, 153.78)(475.6787, 13432.51)(476.681, 1659.95)(477.6644, 1166.25)(478.6735, 150.67)(967.4238, 214.51) | 56085.1 | 24173.01 | 43880.05 | 17889.02 | 61720.92 | 14939.19 | 67152.35 | 20200.42 | 0.21 | 0.442045 | 0.547572 | 0.90 | 0.006563 | 0.125256 |
| COMPOUND_475_0068a10_125416 | Rp | + | 475.0068 | 10.13 | | | | (497.9895, 495.88)(498.9857, 116.72)(476.0133, 7568.28)(477.0116, 616.06)(477.9969, 634.77) | 46403.91 | 21061.28 | 35777.08 | 14371.23 | 50470 | 8968.202 | 53275.74 | 15651.03 | 0.38 | 0.173092 | 0.257751 | 0.33 | 0.327174 | 0.634609 |
| COMPOUND_475_1985a10_596521 | Rp | - | 475.1985 | 10.60 | | | | (474.1912, 22951.97)(475.1942, 6312.7)(476.196, 1431.08)(477.2068, 283.34)(949.3523, 283.59)(1063.382, 289.93)(1064.3864, 319.91) | 64987.92 | 21760.8 | 61744.84 | 23991.82 | 35761.93 | 12416.04 | 47614.51 | 17354.91 | -1.23 | 2.89E-05 | 0.000103 | 0.69 | 0.03579 | 0.252664 |
| COMPOUND_475_1986a10_588313 | Rp | - | 475.1986 | 10.59 | | | | (474.1914, 19308.13)(475.1946, 5114.73)(476.1969, 1418.0)(477.2, 269.98)(949.3523, 283.59)(1063.3455, 277.44)(1064.3207, 190.71) | 48638.17 | 24333.56 | 53458.04 | 22280.14 | 32123.36 | 13627.54 | 42559.63 | 17397.32 | -0.75 | 0.010477 | 0.022133 | 0.33 | 0.332387 | 0.636996 |
| COMPOUND_475_269a9_859699 | Rp | - | | | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_477_2871a10_094607 | Rp | + | 477.2871 | 10.09 | LPE 18:2 | 2 | 10eV: 44.0493(100), 337.2768(80), 478.3379(12), 263.2394(12) | (955.5785, 4362.88)(956.5818, 2271.32)(957.5855, 906.41)(958.5834, 278.88)(993.5406, 385.59)(994.534, 343.66)(500.276, 7701.32)(501.2789, 2049.77)(977.5618, 320.15)(978.5597, 268.09)(979.5762, 3175.18)(980.5814, 1813.42)(975.2943, 736.37)(517.2494, 239.03)(518.2755, 96.23)(495.2337, 1931.41)(478.2942, 2089.19)(2)(479.2972, 53403.52)(480.3001, 9458.22)(481.3033, 1415.05)(972.6449, 299.75) | 288743.8 | 231607.6 | 344715.3 | 246447.4 | 494400.1 | 138325.5 | 468423.8 | 195979.6 | 0.79 | 0.004584 | 0.010385 | -0.13 | 0.686694 | 0.854077 |
| COMPOUND_477_2876a10_098582 | Rp | + | 477.2876 | 10.10 | LPE 18:2 duplicate | | | (955.577, 1973.99)(956.5834, 1264.86)(957.5877, 439.37)(958.582, 105.39)(993.5625, 371.81)(994.5686, 53.89)(500.275, 7855.6)(501.2797, 2327.42)(977.5631, 315.62)(978.5523, 191.8)(979.5768, 3525.26)(980.5817, 1774.49)(495.3306, 1865.56)(516.2442, 1373.65)(517.2637, 857.48)(518.2371, 107.93)(478.2941, 209498.39)(479.2974, 51041.89)(480.3005, 9994.51)(481.3017, 1275.59)(972.5928, 374.17) | 378153.8 | 257897.8 | 371149 | 234553.4 | 450575.4 | 321042.4 | 519064 | 281588.5 | 0.15 | 0.599542 | 0.693461 | 0.29 | 0.404677 | 0.6912 |
| COMPOUND_477_2212a11_0574329 | Hilic | + | 477.3221 | 1.06 | | | | (955.6719, 887.51)(500.2985, 255.88)(501.2889, 20.38)(478.3295, 13545.25)(479.3326, 3555.39)(972.678, 648.33) | 41510.64 | 8026.303 | 45338.76 | 7925.469 | 21249.5 | 6139.086 | 21852.88 | 6610.256 | -1.41 | 2.95E-10 | 3.97E-09 | -0.31 | 0.160245 | 0.472345 |
| COMPOUND_479_1411a10_46062 | Rp | - | 479.1411 | 10.46 | no msms | | | (993.2132, 295.33)(994.1896, 259.73)(592.1299, 751.84)(593.1232, 151.34)(514.1101, 11156.82)(515.1135, 2995.0)(516.1075, 11309.63)(517.1096, 3373.45)(518.1058, 3587.05)(519.107, 1163.76)(520.1093, 1085.15)(478.1344, 19155.57)(479.1387, 4962.55)(480.1313, 12017.74)(481.1333, 3203.56)(482.129, 3482.05)(483.127, 1036.91)(484.1345, 196.38)(524.1307, 582.84)(525.1211, 294.81) | 42366.29 | 21174.75 | 46542.38 | 30212.14 | 74615.56 | 26540.76 | 110294.7 | 54656.77 | 0.25 | 0.264942 | 0.361825 | 1.04 | 0.000223 | 0.020129 |
| COMPOUND_479_2212a11_580742 | Rp | - | 479.2212 | 11.58 | | | | (478.2143, 5213.71)(479.2171, 1335.79)(480.2133, 2859.34)(481.2146, 1103.06)(482.2066, 1360.25)(957.4533, 538.06)(958.4701, 283.29)(524.2127, 1051.35) | 26914.75 | 9435.771 | 25028.52 | 6060.143 | 37955.36 | 16961.63 | 29912.72 | 15247.04 | 0.76 | 0.012541 | 0.025958 | -0.65 | 0.071771 | 0.325554 |
| COMPOUND_479_2997a9_937698 | Rp | - | 479.2997 | 9.94 | | | | (478.2926, 8500.52)(479.2963, 2471.72)(480.301, 557.86)(481.3056, 85.64) | 32570.83 | 11855.33 | 38530.55 | 13827.33 | 29980.85 | 7016.233 | 28729 | 11980.4 | -0.13 | 0.628887 | 0.720006 | -0.73 | 0.019673 | 0.198675 |
| COMPOUND_479_3004a10_379412 | Rp | - | 479.3004 | 10.38 | LPE 18:1 | 2 | 10 eV: 478.2937(100), 281.2476(28), 196.0387(3) | (993.5703, 811.82)(994.5725, 580.15)(995.5734, 299.55)(996.5985, 96.15)(592.2784, 511.15)(593.2733, 297.37)(478.2935, 177998.72)(479.2966, 45400.98)(480.3024, 10076.92)(481.3057, 1912.91)(482.312, 271.25)(957.5654, 1138.13)(958.5403, 2677.11)(959.5407, 1407.54)(960.5455, 1884.27) | 523891.2 | 174914.6 | 530067.8 | 157261.7 | 442316.5 | 114229.8 | 496023.6 | 146930.5 | -0.50 | 0.098051 | 0.160007 | 0.28 | 0.422519 | 0.702743 |
| COMPOUND_479_3004a10_283007 | Rp | - | 479.3004 | 10.28 | | | | (993.5754, 587.31)(994.5774, 389.43)(995.5855, 265.08)(996.5976, 63.38)(592.2751, 543.03)(593.2723, 334.64)(478.2932, 143278.5)(479.2965, 36593.35)(480.3037, 9041.72)(481.3088, 1640.14)(957.6084, 2090.41)(958.6278, 385.54)(959.6424, 178.44)(960.6376, 68.61) | 89859.91 | 102180.5 | 110438.1 | 148895 | 73834.64 | 68402.1 | 68229.35 | 63307.23 | -0.36 | 0.234003 | 0.328538 | -0.04 | 0.912739 | 0.960508 |
| COMPOUND_479_3021a11_6692221 | Hilic | + | 479.3021 | 1.67 | | | | (959.6095, 481.19)(960.6113, 230.59)(961.6237, 513.75)(962.6278, 279.16)(502.2927, 25582.78)(503.2965, 6740.24)(981.5901, 806.05)(982.5954, 434.33)(983.6069, 857.06)(984.6096, 445.52)(985.6197, 413.97)(480.3087, 15113.82)(481.3123, 3767.88)(482.3236, 6456.17) | 229371.4 | 72906.44 | 232174.4 | 65762.26 | 169722.4 | 42753.28 | 198314.6 | 58561.44 | -0.91 | 0.002489 | 0.006067 | 0.42 | 0.229475 | 0.535521 |
| COMPOUND_479_3036a10_383264 | Rp | + | 479.3036 | 10.38 | LPE 18:1 | 2 | 10eV: 480.3121(100), 339.2917(65), 62.0591(25) | (959.6104, 4605.99)(960.6107, 2666.92)(961.6099, 1155.15)(962.5856, 375.31)(997.5841, 6452.09)(998.5828, 631.99)(999.5919, 868.34)(502.2913, 9804.21)(503.2957, 2731.68)(504.3042, 1018.16)(981.5848, 1081.06)(982.5861, 1019.03)(983.5879, 936.85)(480.31, 89422.38)(481.3128, 23490.74)(482.3174, 4469.56)(483.3197, 822.29)(484.3148, 118.03)(976.6096, 1224.93)(977.6038, 1031.78)(978.593, 827.77) | 454948.2 | 149436.1 | 431106.7 | 136479.7 | 467509.8 | 134784.9 | 525150 | 154331 | 0.09 | 0.748635 | 0.81722 | 0.52 | 0.123661 | 0.417518 |
| COMPOUND_479_3051a10_349595 | Rp | + | 479.3051 | 10.35 | | | | (959.6103, 4308.15)(981.6449, 1180.32)(480.3103, 101622.45)(481.3132, 26427.35)(482.3171, 5381.14)(483.324, 1036.93)(976.6096, 1224.93)(977.6038, 1031.78)(978.593, 827.77) | 372966.3 | 234442.8 | 272321 | 193008.9 | 303306.1 | 231461.5 | 391290.2 | 261493.1 | -0.28 | 0.33533 | 0.436459 | 0.88 | 0.014341 | 0.179521 |
| COMPOUND_479_3386a11_0067562 | Hilic | + | 479.3386 | 1.01 | | | | (959.6832, 4673.47)(960.6851, 2560.38)(961.6855, 984.02)(962.6777, 330.59)(502.327, 8182.47)(503.3312, 2114.01)(504.343, 2531.51)(505.3478, 678.73)(981.6645, 752.08)(982.6689, 441.0)(983.6677, 224.96)(497.3072, 190.65)(480.3461, 241358.69)(481.349, 63617.67)(482.3521, 10866.65)(483.3552, 1534.82)(484.3516, 211.97) | 971891.6 | 232271.1 | 1011474 | 273130.2 | 296402.8 | 188265.6 | 274901.8 | 173156.8 | -1.58 | 3.53E-12 | 1.09E-10 | -0.04 | 0.855222 | 0.938351 |
| COMPOUND_479_3394a10_438019 | Rp | + | 479.3394 | 10.44 | duplicate of LPE18:1 | | | (959.6779, 3830.33)(960.677, 2474.78)(961.6869, 777.59)(962.679, 310.37)(997.6679, 440.63)(998.6524, 618.82)(999.6308, 455.47)(502.3283, 26972.79)(503.3327, 7834.85)(981.6632, 1041.41)(982.6606, 571.28)(983.6541, 600.95)(480.3453, 59004.98)(481.3486, 15855.63)(482.3601, 20728.22)(483.3638, 5761.19)(484.3641, 1623.63) | 1297217 | 331607.6 | 1272403 | 381582.2 | 309047.6 | 251653.8 | 295313.5 | 215454.5 | -1.69 | 1.69E-12 | 6.46E-11 | 0.17 | 0.459969 | 0.729472 |
| COMPOUND_479_3404a10_222365 | Rp | + | 479.3404 | 10.22 | | | | (480.3482, 8976.34)(481.3489, 1467.6)(482.3326, 2834.86)(483.3331, 1209.17)(484.341, 1099.83) | 50435.05 | 13151.67 | 45447.53 | 9959.168 | 51280.33 | 13223.06 | 58513.06 | 20882.85 | -0.15 | 0.58411 | 0.679802 | 0.32 | 0.333879 | 0.638282 |
| COMPOUND_481_1587a10_686686 | Rp | - | 481.1587 | 10.69 | | | | (997.301, 221.57)(998.2834, 221.4)(999.2807, 360.26)(594.1527, 3394.28)(595.154, 1647.22)(516.1254, 10222.84)(517.134, 3235.77)(518.1224, 9768.49)(519.1332, 3315.88)(520.1229, 3502.74)(521.1319, 942.7)(522.1253, 479.85)(480.1499, 1584.12)(481.1502, 485.6)(482.1483, 944.9)(483.1576, 439.93)(484.1352, 878.11485.1392, 337.34)(485.1393, 661.35)(961.2934, 424.84)(962.2943, 256.84)(963.2897, 292.16)(526.149, 985.56)(527.1513, 819.56)(1075.3397, 74.34)(1076.3479, 28.63)(1077.3472, 64.85) | 40019.07 | 31963.76 | 38487.11 | 18286.49 | 76521.5 | 31118.88 | 163785 | 83591.45 | 0.63 | 0.000574 | 0.001576 | 0.71 | 0.001167 | 0.055917 |
| COMPOUND_481_3157a10_56611 | Rp | - | 481.3157 | 10.57 | | | | (997.5951, 477.15)(998.6191, 205.74)(480.3089, 85109.38)(481.312, 22155.23)(482.3147, 4124.21)(483.3135, 617.04)(484.3255, 52.78)(961.6231, 746.39)(962.627, 542.99)(963.6056, 839.76)(964.5808, 415.23) | 123792.6 | 149229.2 | 150974.3 | 176511.4 | 83116.5 | 77979.4 | 121184.6 | 158304.1 | -0.87 | 0.00253 | 0.006154 | -0.03 | 0.928641 | 0.967445 |
| COMPOUND_481_3159a10_257178 | Rp | - | 481.3159 | 10.26 | | | | (480.3087, 48573.28)(481.3119, 12398.32)(482.3146, 2239.86)(483.3164, 397.91)(484.3169, 54.22)(526.2941, 4181.18)(527.2973, 1405.5)(961.661, 789.03)(962.6354, 442.81) | 375190.5 | 37004.21 | 396915.6 | 36124.26 | 311730.6 | 36336.33 | 305552.5 | 39563.42 | -1.16 | 5.23E-07 | 2.8E-06 | -0.50 | 0.046246 | 0.273966 |
| COMPOUND_481_3161a10_146292 | Rp | - | 481.3160 | 10.15 | | | | (480.3088, 52579.06)(481.3121, 13021.43)(482.3145, 2354.45)(483.3178, 211.08)(961.6204, 359.23)(962.6047, 146.06)(526.2883, 7492.55)(527.2914, 1102.65) | 118233.4 | 37584.58 | 120394 | 16407.09 | 76741.36 | 13987.69 | 77926.7 | 16007.31 | -1.45 | 9.94E-11 | 1.49E-09 | -0.21 | 0.329304 | 0.635357 |
| COMPOUND_481_3162a10_6453085 | Rp | - | 481.3162 | 10.65 | LPE 18:0 | 2 | 10 eV: 480.3079(100), 283.2637(30), 78.9587(1) | (997.6243, 587.84)(998.6519, 299.65)(480.3092, 160373.53)(481.3123, 43772.92)(482.3148, 7177.47)(483.3141, 1462.64)(484.3236, 216.48)(961.5826, 2377.71)(962.5406, 2706.24)(963.5712, 718.92)(964.5239, 1242.18) | 478892.6 | 137549.8 | 524483.7 | 144391.8 | 291586.9 | 111366.3 | 302211.7 | 99430.7 | -1.29 | 3.95E-07 | 2.22E-06 | -0.15 | 0.571851 | 0.789098 |
| COMPOUND_481_317a11_6459244 | Hilic | + | 481.3170 | 1.65 | | | | (963.6428, 423.39)(964.6448, 344.26)(965.6592, 50.6)(504.3066, 10343.25)(505.31, 2639.79)(506.315, 857.06)(507.3233, 122.93)(965.6221, 674.87)(986.6241, 327.34)(987.6175, 54.24)(99.353, 362.89)(482.3245, 18985.23)(483.328, 5252.08)(484.33, 1114.38)(485.3327, 125.03)(980.6668, 224.15) | 145835.2 | 34382.72 | 157775.2 | 37956.54 | 87309.57 | 31978.38 | 93924.67 | 32543.2 | -1.29 | 5.07E-07 | 2.73E-06 | -0.13 | 0.645749 | 0.836838 |
| COMPOUND_481_3174a11_2258265 | Hilic | + | 481.3174 | 1.23 | | | | (963.6423, 10542.88)(504.324, 18686.58)(505.3283, 5216.87)(506.317, 495.7)(482.325, 210759.84)(483.328, 54887.24)(484.3307, 10086.01)(485.3334, 1468.11)(486.3348, 216.27)(980.6902, 1300.52) | 671625.7 | 208343.9 | 772496.2 | 252244.8 | 354509 | 120466 | 293807.7 | 123930.9 | -1.13 | 7.35E-08 | 4.8E-07 | -0.57 | 0.009473 | 0.153413 |
| COMPOUND_481_3176a11_0978168 | Hilic | + | 481.3176 | 1.10 | | | | (504.3065, 995.88)(505.3096, 275.0)(506.3225, 203.17)(482.3248, 31799.39)(483.3282, 9038.21)(484.3308, 1676.26)(485.3315, 175.02) | 112919.4 | 27592.44 | 123872.3 | 32298.34 | 74768.29 | 20793.54 | 64411.07 | 25273.63 | -1.04 | 7.15E-06 | 2.94E-05 | -0.54 | 0.033005 | 0.244873 |
| COMPOUND_481_3181a10_028497 | Rp | + | 481.3181 | 10.03 | LPC 15:0 | 2 | 10eV: 482.3257(100), 184.0733(24), 104.1062(20), 258.1098(4) | (969.6451, 117.14)(964.6449, 731.39)(965.6484, 177.9)(504.306, 28913.41)(505.3104, 7482.71)(506.3197, 1920.95)(520.2781, 700.2)(482.3255, 403392.38)(483.3289, 97274.88)(484.3325, 18369.54)(485.337, 2951.58) | 877932.8 | 255472.7 | 936323.3 | 320972.4 | 449817.5 | 149318 | 387912.5 | 157326.1 | -1.28 | 1.12E-09 | 1.12E-08 | -0.36 | 0.088516 | 0.352184 |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|---|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_481_3182a10_647905 | Rp | + | 481.3182 | 10.65 | LPE 18:0 | 2 | 20 eV: 341.3091(100), 44.0483(85), 216.0687(15), 421.2673(10) | (963.6374, 2573.37)(964.6361, 1452.37)(965.6124, 1262.27)(1001.6049, 840.45)(1002.6029, 667.95)(504.3068, 832.137)(505.3109, 2416.95)(506.3109, 406.35)(985.6021, 1407.76)(520.2798, 636.44)(521.2786, 376.76)(482.3256, 150379.14)(483.3287, 38870.39)(484.3314, 7393.67)(485.3401, 1179.78)(980.6254, 905.38)(981.607, 896.16) | 344673.5 | 70155.34 | 347075.2 | 91240.45 | 306478.4 | 125990 | 322058 | 91557.32 | -0.67 | 0.025025 | 0.047922 | 0.34 | 0.329477 | 0.635357 |
| COMPOUND_481_319a9_913841 | Rp | + | 481.3190 | 9.91 | | | (504.3065, 10937.63)(505.3103, 2912.06)(506.3133, 1205.83)(499.371, 10173.13)(482.3252, 111964.23)(483.328, 29664.07)(484.3405, 6598.98)(485.3403, 1186.74) | 151077 | 70882.81 | 159468.8 | 66858.19 | 128768.4 | 137476.9 | 183750.1 | 182845.2 | -0.68 | 0.01634 | 0.033032 | -0.08 | 0.812556 | 0.920924 | |
| COMPOUND_481_352a1_2328423 | Hilic | + | 481.3520 | 1.23 | | | (963.6636, 2709.18)(964.6456, 994.3)(504.3424, 15009.95)(505.3453, 4199.13)(506.3581, 3542.67)(985.6514, 670.91)(986.6418, 543.18)(482.3608, 198765.64)(483.3641, 51656.55)(484.3667, 9010.0)(485.3625, 1668.73)(486.37, 222.56) | 1093456 | 329327.3 | 1183969 | 386513.6 | 318020.1 | 255319.7 | 271731.5 | 199963.2 | -1.39 | 4.03E-10 | 5.01E-09 | -0.29 | 0.192785 | 0.505089 | |
| COMPOUND_481_3563a10_50593 | Rp | + | 481.3563 | 10.51 | LPC O-16:0 | 2 | 20 eV: 104.1068(100), 482.3619(37), 184.0714(14) | (963.7152, 1884.69)(964.7158, 1353.46)(965.7191, 552.68)(966.7224, 209.03)(1001.7434, 1102.85)(1002.7495, 539.55)(1003.7187, 407.76)(504.3465, 25814.78)(505.3474, 7216.89)(506.3586, 41249.01)(985.6879, 406.13)(986.7012, 226.32)(987.6897, 1520.01)(499.3774, 100.18)(500.3765, 273.28)(482.3624, 266383.88)(483.3653, 65722.41)(484.3671, 11903.25)(485.3664, 2062.82)(486.3639, 306.32)(980.7479, 1005.1) | 1614599 | 54097.6 | 1565750 | 519847.4 | 427676.9 | 435703.1 | 333292.8 | 293355 | -1.42 | 4.23E-10 | 5.23E-09 | -0.12 | 0.593797 | 0.804108 |
| COMPOUND_483_1723a10_929026 | Rp | - | 483.1723 | 10.93 | | | (1001.3236, 202.35)(1002.3026, 417.15)(518.1401, 2704.64)(519.1404, 837.69)(520.1384, 1937.33)(521.141, 745.35)(522.1369, 435.09)(1011.3098, 326.54)(1012.3183, 188.55)(482.1656, 17829.33)(483.1682, 5523.36)(484.1631, 11731.25)(485.162, 3928.84)(486.1601, 2492.29) | 86200.64 | 29682.98 | 73101.49 | 30747.93 | 95402 | 27457.19 | 95951.77 | 32820.99 | 0.13 | 0.620566 | 0.712655 | -0.42 | 0.168 | 0.480454 | |
| COMPOUND_484_3529a1_4378754 | Hilic | + | 484.3529 | 1.44 | | | (485.3592, 6696.9)(486.3615, 2377.64)(487.366, 602.24)(243.1837, 1715.38)(243.6853, 6031.15)(244.1872, 1487.24)(244.6876, 247.64) | 54401.43 | 17598.97 | 57037.72 | 23028.2 | 53681.71 | 37969.71 | 48485.35 | 26882.13 | -0.32 | 0.279917 | 0.379286 | -0.14 | 0.687233 | 0.854111 | |
| COMPOUND_484_6756a9_969427 | Rp | + | 484.6756 | 9.97 | | | (970.3852, 179.72)(971.3898, 136.71)(507.6791, 368.71)(523.6415, 176.52)(485.6837, 10728.71)(486.686, 1562.82)(487.669, 1609.61)(488.6587, 248.55)(489.6793, 713.75) | 75539.94 | 28291.62 | 62492.12 | 24240.59 | 72878.62 | 12045.36 | 77526.36 | 22626.79 | 0.00 | 0.988716 | 0.995346 | 0.77 | 0.028273 | 0.229862 | |
| COMPOUND_487_2856a12_53011 | Rp | - | 487.2856 | 12.53 | | | (522.2525, 324.43)(523.248, 129.18)(524.245, 43.16)(486.2781, 12400.5)(487.2807, 4614.47)(488.2817, 1284.47)(489.2802, 217.1)(532.257, 2166.61)(533.2435, 2042.23) | 54189.09 | 10797.68 | 58587.73 | 10052.06 | 54628.29 | 13600.94 | 9404.18 | 9542.958 | 0.03 | 0.904959 | 0.938291 | -0.71 | 0.028907 | 0.231966 | |
| COMPOUND_488_2207a9_978855 | Rp | + | 488.2207 | 9.98 | | | (511.2068, 636.67)(512.2117, 306.54)(513.2134, 148.02)(527.1664, 409.27)(506.2536, 1379.6)(507.2571, 450.15)(508.2666, 297.78)(489.228, 5650.92)(490.2316, 2131.67)(491.236, 550.54) | 21895.61 | 9179.286 | 21727.12 | 7084.98 | 12700 | #DIV/0! | 13488.67 | 2438.501 | -1.20 | 1.84E-08 | 1.43E-07 | -0.11 | 0.616569 | 0.816971 | |
| COMPOUND_489_2507a11_579841 | Rp | - | 489.2507 | 11.58 | | | (1013.4207, 510.69)(1014.4236, 300.08)(1015.4148, 423.57)(602.2208, 734.1)(603.2269, 477.25)(604.2227, 829.27)(605.2211, 367.53)(606.2236, 358.71)(488.2436, 7955.97)(489.2474, 2094.66)(490.2418, 1713.31)(491.244, 343.21) | 36019.85 | 9781.677 | 33761.48 | 8007.475 | 34235 | 11195.24 | 32968.65 | 7508.961 | -0.46 | 0.126768 | 0.19922 | 0.46 | 0.200493 | 0.512498 | |
| COMPOUND_489_4186a12_100817 | Rp | + | 489.4186 | 12.10 | | | (490.4268, 8818.71)(491.4305, 3148.52)(492.4401, 2391.88) | 23923.45 | 8478.968 | 26201.95 | 10755.45 | 24033.07 | 6561.224 | 22615.15 | 7294.035 | 0.22 | 0.403072 | 0.507105 | -0.53 | 0.094451 | 0.363881 | |
| COMPOUND_491_1816a10_687108 | Rp | - | 491.1816 | 10.69 | no mms | | (604.1659, 1004.02)(1027.3918, 218.27)(1028.4075, 216.48)(490.1776, 23162.13)(491.179, 6634.74)(492.1742, 7924.66)(493.1756, 1876.77)(494.1545, 3569.18)(981.3221, 339.32)(982.341, 167.78) | 57573.35 | 17046.67 | 47960.63 | 17003.45 | 47278.5 | 11688.09 | 72723.44 | 32611.35 | -0.21 | 0.371407 | 0.473886 | 1.25 | 3.22E-05 | 0.007252 | |
| COMPOUND_491_4321a11_773435 | Rp | + | 491.4321 | 11.77 | | | (983.9017, 250.71)(984.9164, 432.01)(1021.85, 471.12)(1005.8423, 282.75)(509.4442, 432.42)(492.4415, 80084.85)(493.4446, 25613.92)(494.4477, 5065.91)(495.4498, 801.06) | 178439.2 | 91147.68 | 139518.8 | 91547.61 | 96477.5 | 71491.47 | 82557.66 | 48293.78 | -1.16 | 8.54E-06 | 3.45E-05 | 0.19 | 0.506247 | 0.755512 | |
| COMPOUND_493_2006a10_866357 | Rp | - | 493.2006 | 10.87 | | | (492.1933, 6461.68)(493.1967, 1688.56)(494.1913, 2142.8)(495.1927, 807.63)(496.1779, 2887.23)(497.1791, 1086.43)(498.1782, 3501.74)(985.3685, 258.35)(986.3685, 155.55)(987.3919, 178.31) | 36335.41 | 13797.09 | 40416.38 | 16251.12 | 24148 | 10093.33 | 27043.2 | 13399.52 | -1.13 | 8.22E-07 | 4.19E-06 | 0.01 | 0.955938 | 0.980661 | |
| COMPOUND_493_2262a11_366556 | Rp | + | 493.2262 | 11.37 | | | (987.4649, 1675.61)(988.4622, 1549.11)(516.1869, 441.17)(494.2282, 7225.71)(495.232, 2338.21)(496.2362, 542.09) | 38422.62 | 21427.6 | 27248.73 | 9893.487 | 27544.6 | 14686.29 | 21209.93 | 12106.81 | 0.31 | 0.190755 | 0.279675 | 0.09 | 0.741566 | 0.888965 | |
| COMPOUND_493_3177a1_0837613 | Hilic | + | 493.3177 | 1.08 | | | (987.6443, 989.34)(516.3071, 2452.68)(517.3101, 656.1)(1009.6216, 262.04)(494.3247, 85389.75)(495.3278, 23202.18)(1004.6885, 1555.2) | 179276.6 | 62596.18 | 214341 | 7914.20 | 178250.4 | 41123.39 | 162389.1 | 76502.16 | -0.09 | 0.729018 | 0.803204 | -0.71 | 0.022851 | 0.214418 | |
| COMPOUND_493_3188a9_7975 | Rp | + | 493.3188 | 9.80 | | | (516.3059, 5845.44)(517.3096, 1552.59)(532.2904, 1149.59)(533.2891, 554.21)(511.3627, 1944.0)(494.3252, 129277.25)(495.3284, 35360.16)(496.3332, 8270.9)(497.3387, 1447.25) | 208954.4 | 89367.13 | 229561.2 | 99721.74 | 169685.8 | 45986.49 | 166747.3 | 79015.3 | -0.51 | 0.03936 | 0.071195 | -0.35 | 0.21117 | 0.519294 | |
| COMPOUND_493_3191a1_2026542 | Hilic | + | 493.3191 | 1.20 | | | (987.6403, 4501.15)(988.6442, 2493.7)(516.3066, 13189.24)(517.3102, 3915.49)(1009.6245, 1032.99)(1010.6302, 744.82)(1011.6391, 6285.4)(494.3241, 531382.4)(495.3281, 132933.17)(1004.7115, 14470.64) | 1147603 | 419477.1 | 1401814 | 591515.5 | 1018645 | 243328.1 | 946115.4 | 460477.2 | -0.35 | 0.163059 | 0.245296 | -0.66 | 0.025392 | 0.219937 | |
| COMPOUND_493_3198a9_925706 | Rp | + | 493.3198 | 9.93 | LPC 16:1 | 2 | 10eV: 499.3266(100), 104.1047(30), 184.0732(20), 258.1161(3) | (987.6423, 3422.64)(988.6458, 1682.65)(989.6516, 568.19)(1025.6024, 196.66)(516.308, 53597.34)(517.3119, 14621.11)(1009.6221, 679.99)(1010.6223, 334.76)(1011.6122, 631.5)(1012.6101, 475.34)(532.281, 2303.41)(533.2854, 1157.19)(534.2915, 2158.31)(511.3404, 400.1)(512.3363, 7622.08)(513.3423, 2505.93)(494.3261, 618151.7)(495.3302, 157898.69)(496.3329, 30218.62)(497.3409, 5675.5) | 1472723 | 655365.6 | 1764497 | 961093.3 | 1268945 | 365159.3 | 1243440 | 656917.4 | -0.38 | 0.129394 | 0.20264 | -0.39 | 0.80669 | 0.493854 |
| COMPOUND_493_354a10_570445 | Rp | + | 493.3540 | 10.57 | | | (987.7371, 1279.74)(988.7297, 570.83)(516.3429, 1388.67)(517.3479, 604.14)(518.3233, 5929.88)(494.3616, 29607.63)(495.3646, 8149.66) | 123999.7 | 50477.26 | 119864.6 | 63626.99 | 38279.43 | 22702.25 | 49606.47 | 31171.53 | -1.19 | 2.06E-06 | 9.52E-06 | 0.10 | 0.723129 | 0.878838 | |
| COMPOUND_494_0199a10_220755 | Rp | + | 494.0199 | 10.22 | | | (1026.9968, 142.33)(1028.0077, 120.43)(517.0235, 222.82)(518.0278, 451.22)(532.9828, 551.2)(495.027, 10310.16)(496.0301, 1477.55)(497.0117, 1823.56)(498.0143, 241.92)(498.9933, 178.1)(1006.1233, 292.38) | 48140.6 | 15406.18 | 41313.4 | 15249.26 | 65364.38 | 17514.53 | 65827.2 | 21029.1 | 0.59 | 0.029807 | 0.055984 | 0.52 | 0.106608 | 0.38909 | |
| COMPOUND_494_2867a8_815159 | Rp | - | 494.2867 | 8.82 | | | (607.8659, 138.28)(608.2667, 74.84)(609.2662, 68.7)(493.2794, 1606.97)(494.2809, 541.58)(495.2947, 543.57)(496.2978, 319.67)(987.5641, 587.88)(988.5528, 402.98)(989.5835, 3240.95) | 18634.33 | 11491.74 | 19419.86 | 10499.41 | 126976.9 | 70375.88 | 82839.77 | 55243.59 | 1.87 | 9.83E-14 | 9.22E-12 | -0.53 | 0.02425 | 0.219303 | |
| COMPOUND_494_2871a8_755209 | Rp | - | 494.2871 | 8.76 | | | (607.2617, 1004.28)(608.265, 410.26)(609.2567, 748.79)(493.2801, 35029.75)(494.2832, 11238.14)(495.2948, 13979.26)(496.2973, 4172.33)(497.3007, 699.43)(987.5661, 1109.76)(988.5727, 714.52)(989.5804, 217.24) | 23377.7 | 12190.9 | 30000.57 | 18326.26 | 305090.6 | 154376.4 | 209633.5 | 125852.9 | 1.95 | 1.49E-16 | 8.4E-14 | -0.56 | 0.007145 | 0.131884 | |
| COMPOUND_494_2873a9_267705 | Rp | - | 494.2873 | 9.27 | | | (493.28, 92364.91)(494.2832, 27799.48)(495.2862, 5791.66)(496.2888, 1062.07) | 18924.96 | 7185.801 | 20667 | 16769.82 | 209183 | 155191 | 185511.7 | 125362.5 | 1.48 | 9.3E-11 | 1.42E-09 | -0.49 | 0.02903 | 0.231966 | |
| COMPOUND_494_4354a12_537136 | Rp | + | 494.4354 | 12.54 | | | (495.4419, 13706.83)(496.4451, 4996.42)(497.446, 1285.14)(498.4485, 168.81) | 25880.94 | 21520.02 | 23457.39 | 15332.59 | 16135.09 | 4594.902 | 27824.36 | 18739.15 | -0.12 | 0.672235 | 0.759214 | 0.36 | 0.265357 | 0.575669 | |
| COMPOUND_494_482a11_230958 | Rp | + | 494.4820 | 11.23 | | | (517.4862, 1042.31)(511.9438, 1651.08)(512.5209, 182.15)(495.489, 12011.82)(496.4922, 4378.04)(497.4956, 771.75) | 29548.37 | 10520.9 | 34055.98 | 11513.75 | 43767 | 20025.34 | 42008.63 | 17159.55 | 0.91 | 0.001934 | 0.004818 | -0.46 | 0.175858 | 0.490747 | |
| COMPOUND_495_3328a1_1757683 | Hilic | + | 495.3328 | 1.18 | | | (991.6724, 30386.41)(992.6769, 17098.4)(993.6783, 4869.37)(994.6778, 976.57)(995.6787, 265.02)(518.3225, 84636.95)(519.3254, 222 | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|---------------------------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_495_3328a10_0589571 | Hilic | + | 495.3328 | 1.06 | | | | (991.672, 29057.14)(992.6751, 16058.74)(993.6786, 4766.42)(994.6813, 1477.52)(995.6883, 185.61)(18.3222, 63840.67)(519.326, 16340.98)(1013.6534, 3707.72)(1014.654, 1799.31)(1015.6722, 16688.67)(1016.6749, 9354.33)(1017.6875, 41425.62)(1018.6912, 21759.93)(1019.7042, 9896.28)(1019.7042, 834.02)(1019.7042, 1219908.1)(497.3437, 298859.9)(498.3462, 55659.13)(499.3479, 7692.34)(500.3546, 949.42)(1008.687, 484.12)(1009.6964, 843.41) | 14404974 | 2296360 | 15290129 | 2600131 | 7844737 | 2230531 | 8038482 | 2242212 | -1.46 | 3.19E-11 | 6.39E-10 | -0.22 | 0.294592 | 0.604759 |
| COMPOUND_495_3338a10_146823 | Rp | + | 495.3338 | 10.15 | | | | (991.6732, 36653.44)(992.6765, 18924.78)(993.6795, 5594.03)(994.6797, 1601.03)(995.6792, 428.61)(1029.6393, 1833.15)(518.323, 28452.49)(519.3267, 7517.75)(520.3384, 10211.66)(521.3423, 3219.92)(1013.6577, 3416.51)(1014.655, 2342.23)(1015.6676, 6465.8)(1016.6753, 2936.52)(1017.6731, 1042.37)(1018.6546, 683.15)(524.2974, 616.16)(513.3746, 7074.21)(496.4009, 381713.9)(497.3446, 96118.66)(498.3471, 17530.64)(499.3555, 3325.97)(1008.7201, 508.24)(1009.7108, 222.72) | 17896226 | 12723343 | 16075937 | 9149152 | 8148847 | 2474081 | 10091920 | 7493636 | -1.59 | 3.38E-10 | 4.37E-09 | 0.33 | 0.191881 | 0.505089 |
| COMPOUND_495_3344a10_254457 | Rp | + | 495.3344 | 10.25 | LPC 16:0 | 2 | 10eV: 184.074(100), 496.3416(90), 86.0972(2), 258.1104(1) | (991.6738, 2459.24)(992.6758, 1509.5)(993.6778, 523.5)(994.6754, 42.68)(1029.6075, 109.48)(1030.6252, 95.53)(1031.5989, 253.28)(1032.5836, 191.89)(1033.5847, 157.08)(1034.586, 88.66)(1035.59, 83.13)(518.3239, 29849.04)(519.3269, 8185.76)(520.3396, 14745.57)(521.3449, 4344.97)(1013.6548, 3614.31)(1014.6574, 1704.45)(1015.6329, 3878.15)(1016.643, 1116.06)(534.2968, 1339.11)(513.385, 6356.34)(496.3413, 1402052.9)(497.3461, 375985.0)(498.3486, 65725.84)(499.3507, 8944.04)(1008.7401, 1060.76)(1009.7502, 651.94) | 61771698 | 7075727 | 60867391 | 8063637 | 42671429 | 8275304 | 44522807 | 8432061 | -1.58 | 7.53E-11 | 1.2E-09 | 0.21 | 0.367493 | 0.669574 |
| COMPOUND_496_2532a5_9693127 | Rp | + | 496.2532 | 5.97 | | | | (991.6738, 2459.24)(992.6758, 1509.5)(993.6778, 523.5)(994.6754, 42.68)(1029.6075, 109.48)(1030.6252, 95.53)(1031.5989, 253.28)(1032.5836, 191.89)(1033.5847, 157.08)(1034.586, 88.66)(1035.59, 83.13)(518.3239, 29849.04)(519.3269, 8185.76)(520.3396, 14745.57)(521.3449, 4344.97)(1013.6548, 3614.31)(1014.6574, 1704.45)(1015.6329, 3878.15)(1016.643, 1116.06)(534.2968, 1339.11)(513.385, 6356.34)(496.3413, 1402052.9)(497.3461, 375985.0)(498.3486, 65725.84)(499.3507, 8944.04)(1008.7401, 1060.76)(1009.7502, 651.94) | 2843053 | 1406645 | 2650927 | 1500603 | 339459.8 | 169477.6 | 285588.6 | 131160.2 | 0.36 | 0.231363 | 0.326665 | -0.07 | 0.850752 | 0.936867 |
| COMPOUND_496_3027a8_848101 | Rp | - | 496.3027 | 8.85 | | | | (609.2806, 2868.97)(610.2816, 1205.85)(511.2709, 1703.71)(532.2608, 369.24)(495.2959, 341107.12)(496.2991, 94615.74)(497.3017, 19011.66)(498.3044, 2959.37)(499.3107, 398.12)(991.5994, 9084.15)(992.6027, 5220.3)(993.6065, 1988.97)(994.6086, 517.94)(995.6015, 120.48) | 282984.8 | 98287.45 | 314625.3 | 142708.2 | 1271915 | 576139.1 | 1184983 | 543002.2 | 1.52 | 7.37E-12 | 1.98E-10 | -0.04 | 0.832555 | 0.926681 |
| COMPOUND_496_3299a12_532405 | Rp | - | 496.3299 | 12.53 | | | | (531.3, 196.39)(1037.629, 406.11)(1038.6976, 224.7)(1039.6699, 323.73)(495.3277, 131393.75)(496.3261, 41028.5)(497.3289, 6149.37)(498.3326, 821.74)(499.3271, 117.35)(991.6799, 543.48)(992.6775, 484.88)(541.319, 693.22)(542.3123, 246.15)(543.3242, 37.8) | 546963.2 | 92444.58 | 581286.2 | 117767.8 | 641202.1 | 119020.3 | 650651.4 | 111792.1 | 0.73 | 0.00895 | 0.019159 | -0.14 | 0.657246 | 0.842058 |
| COMPOUND_497_2501a1_7669948 | Hilic | + | 497.2501 | 1.77 | | | | (995.5211, 280.67)(520.2431, 508.2)(521.2478, 254.95)(515.2824, 510.34)(498.2568, 7515.74)(499.2604, 1486.27)(500.273, 1172.35) | 43939.91 | 8613.9 | 50747.96 | 13787.32 | 33577.57 | 13704.3 | 35977.23 | 14534.74 | -0.82 | 0.003736 | 0.008697 | -0.19 | 0.550428 | 0.7796 |
| COMPOUND_498_6922a10_344574 | Rp | + | 498.6922 | 10.34 | | | | (998.4319, 813.37)(999.4298, 978.15)(521.6986, 399.03)(1020.4002, 448.02)(1021.4085, 518.13)(516.7411, 194.34)(499.6989, 10528.04)(500.7016, 1496.27)(501.6847, 1356.92)(502.6844, 261.55) | 59850.29 | 24919.13 | 44857.15 | 19794.15 | 53214.31 | 10283.61 | 58143.7 | 17291.68 | 0.18 | 0.482411 | 0.584006 | 0.76 | 0.018977 | 0.196411 |
| COMPOUND_499_0257a10_346504 | Rp | + | 499.0257 | 10.35 | | | | (999.0896, 390.48)(1000.0769, 530.05)(522.0084, 488.71)(1021.0486, 444.69)(537.9787, 424.22)(500.0332, 8615.83)(501.0276, 508.61)(502.0182, 576.54)(1016.0691, 400.17) | 44024.12 | 16154.15 | 36906.61 | 12368.61 | 44052.85 | 10281.36 | 47397.38 | 14878.45 | -0.04 | 0.890431 | 0.926471 | 0.91 | 0.008503 | 0.14883 |
| COMPOUND_499_2338a11_58046 | Rp | - | 499.2338 | 11.58 | | | | (612.2125, 261.18)(498.2265, 5609.38)(499.2288, 1764.08)(500.2321, 667.82)(501.2274, 133.68)(997.4743, 246.98)(998.4908, 333.65)(999.4995, 58.36)(1111.4974, 613.13)(1112.4825, 901.16)(1113.4849, 624.68)(1114.4836, 705.02) | 24442.58 | 3639.254 | 25381.56 | 4984.753 | 23042.2 | 2788.806 | 21483.82 | 5362.455 | -0.79 | 0.000788 | 0.002098 | -0.12 | 0.662619 | 0.844492 |
| COMPOUND_499_2692a9_864109 | Rp | - | 499.2692 | 9.86 | LPE 20:5 | 2 | 20 eV: 301.217(100), 498.2841(42), 196.0385(18), 140.0103(4) | (498.2618, 60075.57)(499.265, 17496.03)(500.2683, 3117.58)(501.2709, 621.68)(997.5291, 694.82)(998.5345, 412.44)(999.5411, 283.0) | 74139.06 | 54931.8 | 67983.27 | 49940.08 | 42754.9 | 17066.23 | 43161.44 | 24756.38 | -0.79 | 0.002279 | 0.005586 | 0.49 | 0.095271 | 0.36381 |
| COMPOUND_499_2706a9_868546 | Rp | + | 499.2706 | 9.87 | | | | (999.5341, 513.96)(1000.5509, 265.32)(1001.5308, 165.58)(522.2597, 2976.54)(523.2646, 1037.41)(524.2736, 528.06)(528.2284, 1164.74)(539.2304, 568.96)(540.2213, 194.28)(517.3111, 6716.06)(500.2785, 17632.49)(501.2809, 5174.59)(502.2864, 1480.74)(503.2719, 1466.01) | 76453.06 | 57244.65 | 71514.09 | 48397.25 | 50440.1 | 22233.09 | 46041.71 | 27139.6 | -0.72 | 0.008646 | 0.018615 | 0.90 | 0.783784 | 0.909997 |
| COMPOUND_499_2958a9_522447 | Rp | - | 499.2958 | 9.52 | Taurocholic acid | 1 | 40 eV: 498.2895(100), 106.981(3), 384.5558(2) | (1033.5697, 111.29)(1034.5839, 50.69)(1035.5591, 170.26)(612.2688, 2186.46)(613.2725, 248089.9) 291225.4 246726.7 194094 1145505 2687874 1116685 1640462 1012.72(498.2894, 248445.56)(499.2924, 73630.37)(500.2914, 21566.52)(501.2922, 4273.41)(502.2946, 649.06)(997.5858, 22488.22)(998.588, 14260.76)(999.5887, 6354.07)(1000.59, 2466.07)(1001.5907, 609.58) | 74139.06 | 54931.8 | 67983.27 | 49940.08 | 42754.9 | 17066.23 | 43161.44 | 24756.38 | -0.79 | 0.002279 | 0.005586 | 0.49 | 0.095271 | 0.36381 |
| COMPOUND_499_2959a9_756559 | Rp | - | 499.2959 | 9.76 | duplication of taurocholic acid | | | (1033.5665, 347.14)(1034.58, 261.52)(1035.5494, 314.77)(612.2681, 966.33)(613.2734, 448.41)(498.2889, 42177.32)(499.2923, 13001.38)(500.2918, 3938.82)(501.293, 822.83)(502.2876, 36.0)(997.5854, 9582.22)(998.5888, 5536.31)(999.5876, 2535.57)(1000.5898, 965.17) | 154303.8 | 190654 | 182384.7 | 120650.8 | 296305.3 | 267454.9 | 652998.4 | 751917 | 0.60 | 0.017312 | 0.034685 | 0.29 | 0.322157 | 0.628989 |
| COMPOUND_499_6875a9_962222 | Rp | + | 499.6875 | 9.96 | | | | (1038.289, 167.98)(522.6738, 344.59)(523.6993, 418.83)(538.6349, 146.56)(500.6927, 13289.25)(501.6952, 679.13)(502.6786, 936.06) | 52833.37 | 19725.82 | 45824.14 | 18344.97 | 54259.08 | 9672.222 | 56493.7 | 15774.07 | 0.11 | 0.704173 | 0.783952 | 0.62 | 0.07725 | 0.333235 |
| COMPOUND_499_9378a9_278484 | Rp | - | 499.9378 | 9.28 | | | | (612.9463, 179.79)(498.9301, 15360.33)(499.933, 1425.14)(500.9293, 840.5)(501.9281, 57.82)(544.9557, 145.45) | 37258.15 | 19845.14 | 43597.67 | 25397.85 | 27271 | 11419.23 | 32824.19 | 17169.54 | -0.40 | 0.003257 | 0.007689 | -0.19 | 0.210875 | 0.519294 |
| COMPOUND_500_0951a8_790591 | Rp | - | 500.0951 | 8.79 | | | | (535.0686, 569.11)(536.0647, 171.93)(537.0628, 283.21)(499.0874, 8065.55)(500.0912, 1650.07)(501.085, 2826.85)(502.09, 683.94)(503.0974, 100.05)(545.0958, 358.65)(546.1072, 219.09) | 29240.3 | 2983.167 | 30154.59 | 3323.837 | 24785 | 2265.338 | 27187.33 | 3779.74 | -1.24 | 1.84E-05 | 6.95E-05 | -0.42 | 0.189037 | 0.504029 |
| COMPOUND_500_149a9_034518 | Rp | - | 500.1490 | 9.03 | | | | (613.1325, 1882.57)(614.1307, 739.78)(615.1356, 2062.09)(616.1341, 994.71)(617.1341, 1382.18)(618.135, 1175.01)(619.136, 1254.52)(620.137, 1157.1809)(621.138, 1234.437.7)(539.1316, 1575.3)(499.1456, 7273.55)(500.1495, 2709.61)(501.1508, 1269.81)(502.1418, 128.89)(545.1447, 7973.79)(546.1496, 2603.98)(547.1475, 5340.26)(548.1569, 1505.54)(549.1462, 2231.16)(550.1474, 859.44)(551.1378, 2903.38) | 63378.67 | 15919.79 | 82379.13 | 26339.14 | 212676.1 | 138134.1 | 172076.7 | 87390.94 | 1.32 | 3.22E-08 | 2.31E-07 | -0.33 | 0.181994 | 0.495594 |
| COMPOUND_500_3898a12_96994 | Rp | + | 500.3898 | 12.97 | | | | (523.3808, 1723.08)(524.38, 1037.08)(525.3809, 286.55)(539.3547, 337.02)(540.3512, 140.03)(518.4245, 4840.45)(519.4279, 1705.88)(520.43, 588.81)(521.4352, 89.22)(501.3987, 6214.47)(502.4018, 1978.75)(503.3998, 842.79)(504.4067, 166.24) | 57102.51 | 18996.77 | 49184.89 | 17587.77 | 54432.14 | 12777.54 | 60514.47 | 18767.01 | -0.10 | 0.738212 | 0.809768 | 0.73 | 0.041676 | 0.265944 |
| COMPOUND_501_2844a10_033219 | Rp | - | 501.2844 | 10.03 | | | | (1003.5741, 824.59)(1004.5779, 404.54)(1005.5888, 824.5)(1006.5953, 368.29)(1007.6019, 510.26)(524.277, 1149.91)(525.2776, 3303.45)(1025.5555, 726.89)(1026.559, 455.06)(1027.5735, 907.58)(1028.5782, 586.25)(1029.5897, 524.53)(1030.5938, 283.58)(502.2926, 9177.85)(503.2961, 5619.49)(504.3067, 9152.55)(505.311, 2511.58)(506.3138, 672.01)(507.3268, 84.63)(1020.5796, 66.86)(1021.5412, 261.52) | 174945.8 | 171084.3 | 95927.57 | 95489.64 | 110139.9 | 105309.5 | 102819 | 97827.73 | -0.87 | 0.003312 | 0.007802 | 0.63 | 0.068426 | 0.319037 |
| COMPOUND_501_2849a10_113906 | Rp | - | 501.2849 | 10.11 | LPE 20:4 | 2 | 20 eV: 303.2318(100), 500.2763(35), 196.0371(8), 59.0131(5), 418.2086(2) | (500.2777, 114650.91)(501.2806, 31438.31)(502.2835, 5643.52)(503.2839, 1096.98)(1001.5623, 5324.79)(1002.5656, 2961.08)(1003.568, 1046.11)(1004.5776, 333.37) | 340047 | 103750.2 | 326194.5 | 104381 | 211330.4 | 64378.39 | 263017.4 | 94604.12 | -1.37 | 5.01E-06 | 2.13E-05 | 0.73 | 0.028786 | 0.231966 |
| COMPOUND_501_2849a1_619784 | Hilic | + | 501.2849 | 1.62 | | | | (1003.5741, 824.59)(1004.5779, 404.54)(1005.5888, 824.5)(1006.5953, 368.29)(1007.6019, 510.26)(524.277, 1149.91)(525.2776, 3303.45)(1025.5555, 726.89)(1026.559, 455.06)(1027.5735, 907.58)(1028.5782, 586.25)(1029.5897, 524.53)(1030.5938, 283.58)(502.2926, 9177.85)(503.2961, 5619.49)(504.3067, 9152.55)(505.311, 2511.58)(506.3138, 672.01)(507.3268, 84.63)(1020.5796, 66.86)(1021.5412, 261.52) | 328899.7 | 84616.16 | 344 | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-------------------------------|--------|----------|----------|-----------|----------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_501_2875a10_02062 | Rp | + | 501.2875 | 10.02 | | | | (1003.5721, 262.94)(1004.5721, 194.41)(1005.5563, 212.47)(524.2878, 1586.24)(525.2813, 1799.44)(540.2887, 1182.81)(541.2924, 616.85)(542.2699, 189.23)(502.2949, 26319.2)(503.2976, 7553.41)(504.3072, 15447.37)(505.3116, 3957.92)(506.3174, 788.68) | 111159.6 | 28390.13 | 112560.6 | 32062.16 | 59996.86 | 15660.22 | 68552 | 21812.78 | -1.06 | 5.51E-05 | 0.000181 | -0.04 | 0.898253 | 0.954633 |
| COMPOUND_501_2896a10_118062 | Rp | + | 501.2896 | 10.12 | | | | (1003.5798, 5106.05)(1004.5827, 2432.79)(1005.5949, 1235.58)(1006.6172, 475.15)(524.3006, 14008.0)(525.2996, 4980.8)(1025.5571, 592.09)(540.245, 788.49)(541.2571, 411.69)(502.2957, 131275.44)(503.2992, 34906.9)(504.3021, 6928.46)(505.3013, 1187.77)(1020.6341, 4889.14) | 307328.9 | 66672.27 | 273361.9 | 70013.67 | 228535.2 | 59571.31 | 285074.1 | 95376.03 | -1.07 | 0.000509 | 0.001416 | 1.14 | 0.001656 | 0.06002 |
| COMPOUND_503_3a10_28832 | Rp | - | 503.3000 | 10.29 | | | | (538.3175, 632.68)(539.3032, 206.98)(502.293, 24411.81)(503.2968, 6579.35)(504.2975, 1339.55)(505.2966, 227.34)(548.2891, 305.26)(549.2886, 6183.97)(550.2908, 2258.69) | 65500.58 | 26223.47 | 67788.15 | 32113.84 | 53549.21 | 17482.92 | 74470.81 | 31463.98 | -0.42 | 0.165725 | 0.248975 | 0.65 | 0.071992 | 0.325554 |
| COMPOUND_503_3005a1_2347902 | Hilic | + | 503.3005 | 1.23 | | | | (504.3069, 11265.45)(505.3097, 2808.13)(506.3088, 233.1) | 26323.18 | 10308.62 | 28647.43 | 10681.79 | 19006 | 5547.544 | 14786.25 | 5505.901 | -0.61 | 0.024268 | 0.046711 | -0.15 | 0.641503 | 0.834103 |
| COMPOUND_503_3036a10_293396 | Rp | + | 503.3036 | 10.29 | | | | (542.2772, 1125.11)(543.2722, 445.11)(544.283, 430.44)(521.343, 6521.31)(504.3095, 29545.69)(505.3131, 7946.14)(506.3156, 1753.56) | 69067.08 | 17108.93 | 64426.78 | 18748.09 | 60248.21 | 16006.8 | 74288.7 | 22327.69 | -0.33 | 0.25758 | 0.354133 | 0.98 | 0.00625 | 0.124555 |
| COMPOUND_504_0226a10_077409 | Rp | + | 504.0226 | 10.08 | | | | (1009.0809, 315.79)(527.0177, 536.85)(1031.0457, 249.85)(522.0412, 252.85)(543.0114, 175.75)(505.0309, 8213.95)(506.0342, 1157.61)(507.0161, 1302.53)(508.0156, 181.9)(509.0284, 699.63) | 77976.96 | 30889.64 | 63657.3 | 25668.6 | 83101.85 | 13326.89 | 87999.98 | 25065.94 | 0.21 | 0.457062 | 0.562154 | 0.80 | 0.018307 | 0.196324 |
| COMPOUND_505_1886a10_66283 | Rp | - | 505.1886 | 10.66 | | | | (504.1804, 10661.45)(505.1834, 3177.96)(506.189, 1026.57) | 21411.27 | 6025.36 | 19461.61 | 5884.237 | 23602.5 | 9303.247 | 28391.3 | 8378.38 | 0.30 | 0.244851 | 0.339954 | 0.79 | 0.01174 | 0.167839 |
| COMPOUND_505_3154a10_109535 | Rp | - | 505.3154 | 10.11 | | | | (504.3085, 19441.63)(505.3121, 5914.43)(506.3149, 1169.89)(507.3179, 241.59)(508.3176, 178.44)(551.3161, 49.29)(1123.6201, 2372.57)(1124.6262, 1069.74)(1125.6324, 425.29) | 137360.2 | 34443.93 | 149031.1 | 28569.74 | 101014.4 | 21540.51 | 91574.82 | 24346.29 | -1.00 | 2.64E-05 | 9.55E-05 | -0.50 | 0.057793 | 0.298567 |
| COMPOUND_505_3163a10_003307 | Rp | - | 505.3163 | 10.00 | | | | (504.309, 5444.23)(505.3125, 1707.39)(506.3207, 302.56)(507.3267, 62.01)(550.3113, 682.44)(551.3197, 177.11)(552.322, 1644.48)(553.3215, 471.68)(1123.6403, 227.77)(1124.6447, 159.7)(1125.6342, 725.08)(1126.6365, 395.96) | 31994.4 | 18318.29 | 32084.49 | 9326.166 | 33132.5 | 31742.48 | 25869.57 | 23445.32 | -0.38 | 0.170694 | 0.25474 | -0.52 | 0.120473 | 0.410445 |
| COMPOUND_505_3515a10_9708553 | Hilic | + | 505.3515 | 0.97 | | | | (1011.7013, 907.03)(1012.7141, 952.18)(1013.721, 753.24)(528.3433, 2245.4)(529.3471, 817.4)(530.3589, 2396.09)(531.3652, 804.78)(1033.7181, 1118.61)(506.3613, 57620.86)(507.3647, 16958.99)(508.3763, 36477.94)(509.38, 10470.07)(510.36, 15474.87) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.11 | 7.96E-06 | 3.24E-05 | 0.00 | 0.998259 | 0.999577 |
| COMPOUND_505_3527a10_534728 | Rp | + | 505.3527 | 10.53 | | | | (528.3502, 2754.64)(529.365, 1646.48)(530.3593, 13128.18)(531.364, 4319.93)(1033.7366, 1861.37)(1034.7391, 529.05)(506.3604, 6547.72)(507.3625, 2437.43)(508.3724, 2146.52)(509.3647, 80.83) | 283022.3 | 83130.61 | 284796 | 87821.88 | 97603.7 | 93906.3 | 88344.72 | 77184.87 | -1.38 | 1.47E-08 | 1.17E-07 | 0.04 | 0.881565 | 0.950612 |
| COMPOUND_506_129a8_312418 | Rp | - | 506.1290 | 8.31 | | | | (619.1146, 1593.71)(620.12, 395.13)(621.11, 1414.12)(622.1091, 400.28)(623.1271, 285.84)(541.0986, 1576.48)(542.1094, 551.36)(543.101, 653.93)(544.1091, 321.28)(545.1083, 133.58)(505.1198, 1036.19)(506.1223, 392.81)(507.1074, 155.13)(551.1265, 3883.45)(552.1316, 779.53)(553.1456, 301.94) | 27491.29 | 4826.948 | 27780.67 | 5171.314 | 27592.58 | 6287.922 | 7754.81 | 5289.959 | -0.32 | 0.487015 | 0.387015 | 0.17 | 0.643009 | 0.835096 |
| COMPOUND_507_3319a10_376232 | Rp | - | 507.3319 | 10.38 | | | | (1059.662, 922.33)(1060.6674, 572.93)(506.3344, 20397.93)(507.3276, 5787.86)(508.3295, 1104.59)(509.3338, 214.38)(552.3295, 3939.24)(553.3339, 1301.79) | 176262.6 | 27398.13 | 184445.7 | 32250.72 | 108145.3 | 18574.69 | 112622.8 | 25386.28 | -1.57 | 1.86E-12 | 6.88E-11 | -0.02 | 0.908957 | 0.958319 |
| COMPOUND_507_3319a10_366358 | Rp | + | 507.3319 | 10.37 | | | | (530.3198, 3455.17)(531.3201, 1280.04)(546.2868, 617.97)(525.3657, 19072.23)(508.3394, 9082.84)(509.3497, 3058.08) | 176978.1 | 40741.5 | 168248.6 | 43066.06 | 90562.5 | 30287.11 | 103042.2 | 27934.72 | -1.25 | 2.25E-07 | 1.3E-06 | 0.33 | 0.189045 | 0.504029 |
| COMPOUND_507_3329a1_0469726 | Hilic | + | 507.3329 | 1.05 | | | | (1015.6742, 57667.95)(1016.6775, 29849.48)(1017.6861, 23661.02)(1018.6906, 9779.13)(530.3571, 949.14)(531.35, 420.93)(532.3383, 3039.83)(533.3411, 1035.92)(1037.6542, 7739.43)(1038.6577, 4797.17)(1039.6693, 12482.79)(1040.6733, 6816.96)(1041.6864, 14641.06)(508.3414, 4988.19)(509.3453, 1336.84)(510.3561, 59062.14)(1032.7078, 1382.89) | 474864.2 | 126423 | 529554.9 | 115059.8 | 161434.6 | 59060.19 | 177255.6 | 106518.2 | -1.44 | 4.85E-09 | 5.88E-09 | -0.24 | 0.298884 | 0.60748 |
| COMPOUND_507_3333a1_1561561 | Hilic | + | 507.3333 | 1.16 | | | | (1015.6723, 6831.91)(1016.6759, 35864.08)(1017.6864, 42490.6)(1018.6897, 20749.91)(530.3579, 1632.26)(531.3617, 698.75)(532.3389, 6958.24)(533.3411, 1871.13)(1037.6559, 24833.93)(1038.6597, 14267.77)(1039.6724, 93591.88)(1040.6761, 51922.94)(1041.6877, 122455.48)(508.3763, 36111.95)(509.3798, 10200.6)(510.3567, 65323.19)(1032.7087, 15489.18) | 3132720 | 1060411 | 3422158 | 955536.3 | 1808703 | 488481 | 1755027 | 600216.3 | -1.22 | 5.89E-07 | 3.11E-06 | -0.28 | 0.281153 | 0.588984 |
| COMPOUND_507_3342a10_136346 | Rp | + | 507.3342 | 10.14 | | | | (1015.6755, 181896.17)(530.3126, 2213.02)(531.3232, 1419.03)(532.3273, 5668.18)(546.2964, 1164.91)(535.3762, 2461.71)(508.3399, 27478.92)(509.3434, 7702.64)(510.3471, 1724.21)(511.3445, 306.18) | 690763.4 | 210602.2 | 718481.5 | 234591.1 | 246942.9 | 104180.9 | 259028.7 | 126763.6 | -1.55 | 2.43E-11 | 5.21E-10 | -0.02 | 0.923184 | 0.965307 |
| COMPOUND_507_3683a10_95514464 | Hilic | + | 507.3683 | 0.96 | | | | (1015.7845, 877.24)(530.3601, 1490.14)(531.3661, 628.39)(532.3748, 2058.0)(533.3802, 716.54)(508.3765, 40444.21)(509.3803, 11595.99)(510.3735, 3849.34)(511.3701, 801.96) | 135592.5 | 41944.33 | 142484.5 | 49712.82 | 49245.92 | 34262.14 | 41850.18 | 25905.11 | -0.79 | 0.002205 | 0.005427 | -0.17 | 0.573388 | 0.790246 |
| COMPOUND_507_3688a1_1631838 | Hilic | + | 507.3688 | 1.16 | | | | (530.3608, 688.49)(531.3616, 171.16)(532.3741, 632.72)(533.38, 221.84)(508.3767, 154340.42)(509.3799, 42090.49) | 795767.1 | 176934.7 | 811685.8 | 191410.8 | 236793.3 | 54023.76 | 201317 | 32276.94 | -0.94 | 0.000207 | 0.000613 | 0.13 | 0.645438 | 0.836838 |
| COMPOUND_507_3695a10_783912 | Rp | + | 507.3695 | 10.78 | | | | (530.3649, 3729.5)(531.3719, 1964.88)(532.3779, 2110.45)(508.3768, 44672.52)(509.3796, 13194.99)(510.3804, 16924.49)(511.3927, 5313.84) | 175787.7 | 55083.81 | 170576.5 | 57795.8 | 97907.67 | 63616.02 | 80446.73 | 41686.3 | -1.34 | 3.18E-10 | 4.19E-09 | -0.03 | 0.888851 | 0.953702 |
| COMPOUND_507_3714a10_592616 | Rp | + | 507.3714 | 10.59 | LPC O-18:1 | 2 | 20eV: 104.1058(100), 508.3774(50), 184.0751(6) | (1015.7421, 3041.73)(1016.7484, 1831.57)(1017.7301, 1494.35)(530.3598, 27657.2)(531.3623, 8100.28)(532.3672, 2407.41)(533.3578, 512.01)(1037.704, 490.88)(1038.7261, 390.51)(508.3772, 536099.0)(509.381, 147956.77)(510.3816, 27576.99)(511.3802, 4392.93) | 1590641 | 492224.1 | 1556485 | 502789.9 | 511513.4 | 506177.7 | 407599 | 344758.1 | -1.42 | 4.99E-09 | 4.38E-08 | -0.06 | 0.824297 | 0.923541 |
| COMPOUND_508_6964a10_214169 | Rp | + | 508.6964 | 10.21 | | | | (1056.3112, 262.48)(531.6823, 275.01)(532.6888, 552.09)(547.6775, 420.54)(509.7021, 9152.34)(510.7061, 1465.79)(511.69, 1482.5)(512.6841, 251.38)(513.6896, 395.29)(514.6813, 43.69)(515.6821, 254.15) | 62052.13 | 22718.25 | 52151.84 | 20138.55 | 71888.92 | 13653.23 | 75799.18 | 24100.33 | 0.36 | 0.194778 | 0.283887 | 0.66 | 0.049862 | 0.282135 |
| COMPOUND_509_0289a10_21308 | Rp | + | 509.0289 | 10.21 | | | | (1019.0286, 302.79)(532.0112, 747.95)(533.0135, 357.44)(1041.036, 253.95)(527.0433, 351.6)(547.9696, 227.7)(510.0367, 16859.15)(511.0365, 946.9)(512.0209, 978.06) | 46422.47 | 19766.99 | 36064.81 | 15403.39 | 51488.83 | 12844.81 | 56787.26 | 20150.63 | 0.04 | 0.88534 | 0.923801 | 0.89 | 0.009747 | 0.153413 |
| COMPOUND_509_3476a10_651134 | Rp | - | 509.3476 | 10.65 | | | | (1053.663, 286.95)(1054.6544, 199.16)(1055.6805, 248.33)(1056.7012, 115.8)(1057.6534, 227.91)(622.3603, 810.69)(623.3713, 447.39)(544.3351, 1332.59)(1063.6935, 1921.74)(1064.694, 1438.19)(1065.6971, 1126.11)(1066.691, 493.52)(508.34, 20491.71)(509.3432, 5946.73)(510.3454, 1268.51)(511.3498, 219.42)(1017.6548, 2365.06)(1018.6313, 741.22)(554.3661, 3107.03)(555.3673, 680.42)(1131.6567, 366.6)(1132.6478, 332.0)(1133.6417, 435.15)(1134.6267, 282.09) | 230388 | 27171.14 | 241531.3 | 38423.9 | 137095.3 | 27580.07 | 13757.52 | 31900.57 | -0.30 | 0.268652 | 0.366447 | -0.33 | 0.309299 | 0.61532 |
| COMPOUND_509_3483a10_652478 | Rp | - | 509.3483 | 10.65 | | | | (1053.6694, 398.93)(1054.6906, 165.33)(1055.6669, 249.65)(1056.6722, 269.42)(1057.6392, 236.3)(622.3592, 364.34)(623.3712, 235.02)(544.3351, 1438.42)(1063.6917, 626.03)(1064.6938, 546.47)(1065.6831, 428.25)(1066.6984, 188.06)(1067.7017, 24.15)(508.3399, 22372.19)(509.3436, 5890.98)(510.3444, 1068.79)(511.3522, 214.71)(1017.666, 2157.4)(1018.6602, 863.74)(554.3696, 4509.39)(555.3658, 1057.47)(1131.6732, 465.88)(1132.6833, 293.3)(1133.6517, 479.11)(1134.6337, 187.68) | 238774.1 | 31336.72 | 251847.4 | 37994.47 | 144790.7 | 26715.49 | 139189.9 | 30494.02 | -1.40 | 1.58E-11 | 3.68E-10 | -0.36 | 0.073269 | 0.326093 |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|-----------------|----------|---|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_509_3488a1_0669302 | Hilic | + | 509.3488 | 1.07 | Unknown | 4 | 10 eV: 508.3764 (100), 104.1077 (20) | (1019.7023, 56398.47)(1020.7065, 27008.62)(1021.7092, 8191.34)(1022.713, 1952.99)(1023.7131, 451.79)(532.339, 3575.2)(533.3414, 941.83)(534.3542, 1540.7)(535.358, 382.95)(1041.6875, 5638.27)(1042.6914, 20650.83)(1043.704, 94675.53)(1044.7074, 52331.37)(1045.7195, 12427.24)(510.3564, 78683.48)(511.3597, 23029.53)(512.3622, 4078.07)(513.3647, 653.29)(514.3665, 88.4)(1036.7258, 437.69) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.01 | 0.965487 | 0.980203 | 0.78 | 0.017462 | 0.194676 |
| COMPOUND_509_3498a1_1393627 | Hilic | + | 509.3498 | 1.14 | | | (1019.7027, 105944.28)(1020.7065, 54416.98)(1021.7099, 17542.64)(1022.712, 4148.66)(1023.7102, 920.77)(532.3384, 2413.63)(533.3417, 699.53)(534.3546, 765.51)(535.3567, 210.18)(1041.6871, 36900.3)(1042.6907, 19196.09)(1043.7035, 63281.91)(1044.7072, 34448.86)(1045.7197, 12422.78)(510.3568, 299458.94)(511.3607, 83287.84)(512.3637, 15668.71)(513.3663, 2376.67)(514.3706, 370.17)(1036.7281, 982.37) | 2913774 | 485561.6 | 2941526 | 521974.1 | 1319528 | 368272.3 | 1183454 | 332028 | -1.49 | 3.41E-12 | 1.07E-10 | -0.18 | 0.359405 | 0.666906 | |
| COMPOUND_509_3503a10_413503 | Rp | + | 509.3503 | 10.41 | LPC 17:0 isomer | 2 | 10 eV: 510.3573(100), 104.1062(30), 184.073(26) | (1019.6951, 6829.97)(1057.658, 4682.74)(532.3388, 20343.31)(533.3427, 10405.63)(534.3474, 4242.41)(1041.6821, 4376.81)(527.3838, 1947.57)(528.3795, 3774.97)(548.3075, 4588.87)(510.3565, 224461.0)(511.3595, 58941.03)(512.363, 10972.67)(513.3662, 1993.14) | 1171403 | 262889.2 | 1226992 | 393840.7 | 387772.8 | 173770.7 | 383220.8 | 153944.1 | -1.59 | 6.31E-13 | 3.09E-11 | -0.06 | 0.76986 | 0.902789 |
| COMPOUND_509_3504a10_411854 | Rp | + | 509.3504 | 10.41 | | | (1019.6951, 6829.97)(1057.659, 5208.52)(532.3382, 20568.69)(533.3421, 9889.12)(534.3436, 3789.06)(1041.6802, 4599.28)(548.3075, 4588.87)(527.3745, 1107.65)(528.3847, 4247.14)(510.3565, 224461.0)(511.3595, 58941.03)(512.363, 10972.67)(513.3662, 1993.14) | 1053869 | 273351 | 1103243 | 382856.9 | 401870.1 | 134863.3 | 381332.8 | 145494.3 | -1.29 | 1.89E-08 | 1.46E-07 | -0.30 | 0.199304 | 0.510852 | |
| COMPOUND_509_3511a10_466734 | Rp | + | 509.3510 | 10.47 | LPC 17:0 | 2 | 11 eV: 510.3573(100), 104.1062(30), 184.073(26) | (1019.7024, 2502.18)(1020.7055, 1454.33)(1021.7068, 396.68)(532.3393, 34902.28)(533.3431, 10264.2)(534.3571, 3613.63)(535.3502, 437.74)(1041.6772, 2012.39)(1042.6794, 1480.31)(1043.6549, 76.07)(548.3144, 2425.93)(549.3177, 1404.61)(550.3136, 776.05)(527.3768, 1952.13)(510.3566, 384510.47)(511.3601, 101736.05)(512.3638, 21075.21)(513.3679, 3617.81) | 1574266 | 469388.9 | 1556930 | 720922.1 | 419941 | 160500.3 | 377145.4 | 129800.2 | -1.57 | 1.86E-12 | 6.88E-11 | -0.03 | 0.883794 | 0.951974 |
| COMPOUND_509_3861a10_855367 | Rp | + | 509.3861 | 10.86 | | | (1019.7932, 1229.89)(1020.7712, 1221.6)(532.3752, 14461.31)(533.379, 3925.58)(534.3917, 4998.39)(535.3947, 1631.31)(527.4464, 377.58)(510.3929, 134935.77)(511.3957, 38378.95)(512.3982, 7192.22)(513.4031, 1273.66)(514.4051, 194.41) | 489851.4 | 161113.3 | 498710 | 190630.5 | 160222 | 165906.7 | 120712.2 | 93879.12 | -1.22 | 1.18E-08 | 9.6E-08 | -0.37 | 0.095314 | 0.36381 | |
| COMPOUND_510_1233a_790389 | Rp | - | 510.1233 | 8.79 | | | (509.1161, 41548.05)(510.1196, 7896.63)(511.1215, 968.04)(512.133, 197.3) | 104222.0 | 9497.517 | 105948.8 | 8898.314 | 98584 | 8491.806 | 102639.9 | 7641.947 | -0.64 | 0.033043 | 0.061346 | 0.28 | 0.437514 | 0.714538 | |
| COMPOUND_510_2907a11_2283945 | Rp | + | 510.2907 | 11.23 | | | (549.2592, 726.65)(550.2638, 407.49)(551.2653, 720.84)(511.2959, 6148.11)(512.2989, 2337.22)(513.2927, 1005.75)(514.299, 140.65) | 18996.56 | 12039.27 | 13968.16 | 3579.012 | 28987.25 | 11082.56 | 28440.53 | 10561 | 1.11 | 9.24E-07 | 4.62E-06 | 0.08 | 0.744525 | 0.889952 | |
| COMPOUND_510_377a9_43281 | Rp | + | 510.3770 | 9.43 | | | (1021.7289, 91.32)(533.3658, 861.86)(534.3519, 113.01)(535.3733, 1290.58)(549.3304, 284.51)(528.4113, 16754.31)(529.412, 5187.15)(530.4144, 1142.94)(531.4093, 234.37)(511.3843, 2856.15)(512.3865, 919.01)(513.3689, 300.42)(256.1826, 433.9)(256.6951, 134.13) | 142365.4 | 34739.07 | 129294.3 | 24431.02 | 154050.3 | 25477.56 | 153207.6 | 37556.81 | 0.26 | 0.370363 | 0.472821 | 0.50 | 0.152875 | 0.465253 | |
| COMPOUND_511_3158a9_286957 | Rp | + | 511.3158 | 9.29 | | | (512.323, 29314.56)(513.3264, 8829.42)(514.3348, 2078.21)(515.3336, 349.13) | 14749.5 | 2870.798 | 26845.5 | 19403.72 | 83105 | 41409.07 | 82792.98 | 67472.21 | 1.41 | 8.88E-12 | 2.27E-10 | -0.36 | 0.076628 | 0.332499 | |
| COMPOUND_511_3274a8_750298 | Rp | + | 511.3274 | 8.75 | | | (534.319, 1252.25)(535.3228, 398.36)(536.3014, 636.68)(537.2891, 151.34)(512.3277, 32142.38)(513.3302, 9692.27)(514.3335, 2476.16)(515.336, 468.92) | 130139.2 | 38899.03 | 127585.2 | 44986.44 | 187372.8 | 112419.5 | 147908.7 | 81170.79 | 0.29 | 0.304002 | 0.404245 | -0.67 | 0.050772 | 0.283798 | |
| COMPOUND_511_3277a8_590921 | Rp | + | 511.3277 | 8.59 | | | (534.3292, 6125.13)(535.328, 2002.47)(512.3354, 5213.97)(513.3394, 1616.42)(514.342, 482.59) | 19625.76 | 7484.578 | 19386.24 | 6011.914 | 14065 | 2317.866 | 14251.9 | 3675.458 | -1.19 | 5.97E-08 | 3.99E-07 | -0.08 | 0.740788 | 0.888965 | |
| COMPOUND_511_3299a9_88206 | Rp | + | 511.3299 | 9.88 | | | (534.3185, 2331.58)(535.3241, 676.71)(536.3147, 301.17)(512.3357, 28177.65)(513.3389, 7725.79)(514.3442, 1840.51) | 114583.1 | 29567.04 | 108621.8 | 40487.16 | 52163.25 | 6688.069 | 60189.16 | 28542.07 | -1.58 | 7.65E-13 | 3.59E-11 | 0.35 | 0.09396 | 0.36381 | |
| COMPOUND_512_2974a8_635713 | Rp | - | 512.2974 | 8.64 | | | (511.2904, 30274.98)(512.2936, 8649.85)(513.2958, 2062.62)(514.2979, 405.7) | 62784.2 | 25817.84 | 62804.84 | 30600.85 | 213237.1 | 61633.1 | 175473 | 100936.9 | 1.66 | 1.3E-10 | 1.88E-09 | -0.36 | 0.155807 | 0.466545 | |
| COMPOUND_513_2754a9_351753 | Rp | - | 513.2754 | 9.35 | | | (1071.5552, 119.73)(1072.5687, 124.23)(512.2682, 11744.09)(513.2717, 3527.03)(514.2713, 1182.03)(515.2678, 192.78)(255.6308, 2720.49)(256.132, 814.23)(256.6317, 296.7) | 192051.7 | 243871.9 | 181209.9 | 130189.4 | 119436.6 | 108037.8 | 93882.85 | 66992.58 | -0.51 | 0.032515 | 0.060615 | -0.44 | 0.110802 | 0.396703 | |
| COMPOUND_513_2796a5_9541445 | Rp | + | 513.2796 | 5.95 | | | (1027.5135, 107.58)(514.2871, 106462.85)(515.2901, 25982.53)(516.2924, 5417.08)(517.2955, 1087.9) | 157109.8 | 122643.8 | 190166.8 | 142196 | 218486.9 | 156140.8 | 191681.4 | 129382.5 | 0.45 | 0.141805 | 0.218132 | -0.31 | 0.396553 | 0.690408 | |
| COMPOUND_513_3054a9_622855 | Rp | - | 513.3054 | 9.62 | LPC 14:0 | 1 | 10 eV: 452.2769(100), 152.2986(42), 227.2012(10), 44.9981(7) | (1071.6064, 140.59)(1072.6204, 105.5)(512.2981, 49025.72)(513.3011, 12178.05)(514.3033, 2407.46)(515.3072, 433.41)(516.3118, 43.61) | 93830.12 | 50198.35 | 127436.6 | 66685.46 | 118443.9 | 80706.87 | 86328.15 | 56360.56 | 0.42 | 0.141293 | 0.217493 | -1.14 | 0.001389 | 0.059009 |
| COMPOUND_513_3059a9_766879 | Rp | - | 513.3059 | 9.77 | LPC 14:0 isomer | 3 | 10 eV: 452.2769(100), 152.2986(42), 227.2012(10), 44.9981(7) | (1071.6272, 60.13)(512.2985, 375752.28)(513.302, 92454.06)(514.3042, 16811.23)(515.3069, 2741.51)(516.3078, 303.26) | 571460.8 | 284988.2 | 801812.9 | 432757.7 | 608628.3 | 215277.1 | 476258.1 | 252116.7 | 0.15 | 0.56304 | 0.660055 | -1.11 | 0.000739 | 0.045795 |
| COMPOUND_513_3317a8_852228 | Rp | + | 513.3317 | 8.85 | | | (552.3224, 807.58)(531.3756, 1341.23)(532.3685, 233.98)(514.3386, 14527.38)(515.3416, 4955.11)(516.3459, 1227.01)(517.3452, 252.58)(518.363, 36.73) | 82241.49 | 29502.19 | 88099.21 | 38976.69 | 333685.1 | 142236 | 325993.3 | 161506.1 | 1.44 | 1.07E-10 | 1.59E-09 | 0.11 | 0.593036 | 0.803855 | |
| COMPOUND_513_7017a10_334726 | Rp | + | 513.7017 | 10.33 | | | (1066.3882, 359.85)(1067.3962, 314.4)(1068.3846, 340.22)(536.6968, 412.97)(537.7156, 317.48)(514.7081, 11679.82)(515.7088, 771.22)(516.6949, 705.05) | 48342.88 | 18641.26 | 39251.63 | 14152.79 | 52078.08 | 10946.8 | 53300.85 | 16477.89 | 0.25 | 0.371765 | 0.474075 | 0.62 | 0.067317 | 0.315172 | |
| COMPOUND_514_0258a9_951875 | Rp | + | 514.0258 | 9.95 | | | (537.0279, 420.93)(538.031, 759.44)(1051.042, 141.27)(532.0343, 522.31)(515.0346, 8828.17)(516.0368, 1415.48)(517.02, 1760.4)(518.0096, 245.35)(519.0307, 658.53) | 73573 | 26320.92 | 61333.81 | 26695.29 | 72456.85 | 11386.02 | 74595.78 | 18252.63 | -0.03 | 0.904073 | 0.937804 | 0.75 | 0.032307 | 0.244873 | |
| COMPOUND_514_4067a13_4083 | Rp | + | 514.4067 | 13.41 | | | (537.3966, 3835.27)(538.3997, 121307.84)(539.3987, 36805.98)(540.3993, 752.95)(1051.7996, 2930.24)(1052.8044, 2248.6)(1053.8044, 992.47)(1054.8127, 427.3)(1055.809, 127.38)(553.3721, 19544.53)(554.3756, 7042.0)(555.3731, 3983.74)(556.3711, 861.92)(532.4398, 1133238.0)(533.4441, 372903.5)(534.4432, 103336.23)(535.4436, 22214.72)(536.4439, 3485.12)(515.4133, 1189855.5)(516.4179, 379318.5)(517.4168, 105856.15)(518.4167, 22623.58)(519.4182, 3130.08) | 55050943 | 10226918 | 50721739 | 8809059 | 55807143 | 5942217 | 56843860 | 7845404 | 0.12 | 0.687005 | 0.771253 | 0.54 | 0.132458 | 0.431688 | |
| COMPOUND_515_1731a10_66196 | Rp | - | 515.1731 | 10.66 | | | (550.1548, 815.74)(551.1458, 531.92)(552.1521, 357.93)(514.1656, 6661.06)(515.1677, 2469.29)(516.1673, 1181.05)(517.1799, 242.41) | 19489.08 | 4662.294 | 18619.57 | 5500.5 | 19577.09 | 6656.883 | 20041.45 | 6152.985 | -0.49 | 0.0952 | 0.156261 | 0.65 | 0.058999 | 0.30009 | |
| COMPOUND_515_2909a7_4732437 | Rp | - | 515.2909 | 7.47 | | | (514.2835, 51324.06)(515.2871, 16013.7)(516.2858, 5002.46)(517.2861, 960.33) | 29564.93 | 24795.27 | 27702.93 | 18983.05 | 95369.6 | 106335.4 | 73494.98 | 62938.62 | 0.66 | 0.001767 | 0.004425 | 0.21 | 0.378258 | 0.681469 | |
| COMPOUND_515_2911a8_730288 | Rp | - | 515.2911 | 8.73 | | | (1075.5514, 524.23)(1076.5552, 378.0)(514.2841, 306272.16)(515.2874, 87106.54)(516.2864, 26711.29)(517.2868, 5555.29)(518.2876, 864.57)(1029.5757, 28789.9)(1030.5785, 17006.33)(1031.5784, 7876.75)(1032.5786, 2912.65)(1033.5759, 890.36) | 145999.9 | 458780.4 | 95037.84 | 12735.58 | 2345539 | 7220578 | 1498032 | 2507149 | 1.10 | 1.69E-06 | 8.07E-06 | 0.26 | 0.295333 | 0.603136 | |
| COMPOUND_515_3049a1_2238518 | Hilic | + | 515.3049 | 1.22 | | | (1031.6315, 933.27)(1032.6498, 514.28)(1053.6196, 655.57)(533.3417, 851.12)(516.3066, 10083.76)(517.31, 3047.47)(1048.6256, 51.92)(1049.6616, 292.54)(1050.6708, 291.0) | 59115.74 | 12808.2 | 64271.61 | 17347.88 | 66259.93 | 11748.89 | 63756.38 | 14205.5 | 0.77 | 0.007265 | 0.015916 | -1.06 | 0.002306 | 0.067469 | |
| COMPOUND_515_4188a11_848802 | Rp | + | 515.4188 | 11.85 | | | (| | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|-----------------------------|--------|----------|----------------|----------------|----------|--------------|--|--|----------|---------------|----------|---------------|----------|---------------|----------|---------|----------|----------|-------------|----------|----------|----------|
| | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | |
| | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_517_3162a1_1540976 | Hilic | + | 517.3162 | 1.15 | | | (1035.638, 629.76) (1036.6412, 481.8) (1037.6552, 11728.55) (540.3075, 1204.05) (541.3119, 452.71) (542.3229, 8465.61) (543.3259, 2835.84) (1057.6355, 480.30) (1058.6322, 504.76) (1059.6366, 418.43) (1060.651, 238.33) (518.3233, 12458.33) (519.3266, 34056.87) | 1630681 | 544386.9 | 1702967 | 649682.4 | 1541913 | 229976.5 | 1540287 | 259118.5 | -0.09 | 0.756506 | 0.82302 | -0.14 | 0.702676 | 0.86442 | |
| COMPOUND_517_318a9_845915 | Rp | + | 517.3180 | 9.85 | LPC 18:3 | 2 | 10 eV: 518.3241(100), 104.107(18) | (1035.6384, 219.21) (1036.6392, 204.79) (1037.6555, 140.86) (540.3039, 7344.48) (541.3042, 3413.71) (556.2869, 777.25) (518.3256, 124474.67) (519.3289, 35002.93) (520.3333, 7486.69) (521.3389, 854.66) | 352557.3 | 172549.6 | 403034.1 | 208796.8 | 251813.3 | 93958.06 | 220031.3 | 100639 | -0.73 | 0.004247 | 0.00973 | -0.34 | 0.238832 | 0.543832 |
| COMPOUND_517_329a10_529172 | Rp | - | 517.3290 | 10.53 | | | (1079.6473, 369.66) (1080.665, 351.76) (516.3213, 6802.36) (517.3249, 2087.68) (518.3196, 2534.35) (519.3121, 748.36) (520.3045, 1235.97) | 42393.19 | 8462.973 | 43648.36 | 10993.91 | 24132.75 | 15487.86 | 20193.9 | 9135.36 | -1.25 | 2.46E-08 | 1.83E-07 | -0.22 | 0.338203 | 0.642187 | |
| COMPOUND_518_2862a8_854052 | Rp | + | 518.2862 | 8.85 | | | (541.3004, 420.51) (542.2871, 211.83) (557.2534, 320.26) (558.2555, 74.63) (519.2938, 13178.34) (520.297, 3910.27) (521.2975, 1081.57) (522.3092, 199.78) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 1.50 | 1.04E-12 | 4.7E-11 | 0.00 | 0.993167 | 0.997491 | |
| COMPOUND_519_3324a1_1471411 | Hilic | + | 519.3324 | 1.15 | | | (1039.6727, 21502.4) (1040.676, 12284.19) (1041.6888, 81182.96) (1042.6912, 46807.38) (542.3248, 441055.03) (543.329, 124839.65) (1061.6576, 8610.87) (1062.6602, 5096.96) (537.3769, 1794.46) (520.3397, 869338.75) (521.3441, 236528.58) (522.3552, 3288982.8) | 13824656 | 4909357 | 14473183 | 4207194 | 9239677 | 2466730 | 8553470 | 2707035 | -0.98 | 0.001116 | 0.000354 | -0.33 | 0.246264 | 0.555348 | |
| COMPOUND_519_333a10_411083 | Hilic | + | 519.3330 | 1.04 | | | (542.3245, 70841.04) (543.3276, 20542.25) (1061.6556, 5886.15) (1062.6586, 3560.5) (520.3396, 754564.06) (521.3437, 203585.92) (1056.7023, 640.31) (1057.6832, 1001.01) | 1691489 | 674244 | 1830499 | 572272.1 | 897008.8 | 236868.1 | 828787.7 | 306399.1 | -1.18 | 5.03E-07 | 2.72E-06 | -0.36 | 0.156518 | 0.46686 | |
| COMPOUND_519_334a10_012239 | Rp | + | 519.3341 | 10.01 | | | (1039.6724, 36113.35) (1040.6759, 19284.49) (1041.675, 7506.11) (1042.6912, 437.04) (1077.606, 975.01) (1078.6117, 2527.18) (1079.6162, 1674.84) (542.3231, 54205.82) (543.3257, 16910.29) (1061.6501, 8221.14) (1062.6512, 4836.95) (1063.6674, 17986.58) (1064.6726, 9727.92) (1065.6749, 5191.04) (1066.6741, 2825.08) (558.296, 4080.68) (559.3007, 2253.22) (560.3008, 1687.92) (537.3803, 1962.97) (520.3408, 1235781.1) (521.3459, 328856.3) (522.3476, 59266.63) (523.3436, 10527.79) | 2943646 | 3326904 | 3255308 | 4524378 | 1190243 | 1395285 | 2870652 | 4114157 | -0.09 | 0.000345 | 0.000984 | 0.13 | 0.682911 | 0.853695 | |
| COMPOUND_519_335a10_106271 | Rp | + | 519.3356 | 10.11 | LPC 18:2 | 2 | 10 eV: 520.3395(100), 184.0736(90), 104.1083(4), 258.1018(2) | (1039.6685, 5065.64) (1040.6703, 2961.41) (1041.6864, 8704.23) (1042.6907, 4310.57) (1043.6918, 1853.47) (1077.5944, 2826.03) (542.3238, 63893.44) (543.3271, 18710.74) (1061.6501, 8221.14) (1062.6512, 4836.95) (1063.6674, 17986.58) (1064.6726, 9727.92) (1065.6749, 5191.04) (537.3721, 2096.39) (538.3743, 1373.35) (558.2945, 5591.27) (520.3401, 133381.0) (521.3454, 361394.38) (522.3476, 65406.29) (523.3494, 4707.87) (1056.635, 3074.81) (1057.6375, 950.36) | 16365627 | 5118735 | 16600003 | 4672088 | 10449789 | 2540909 | 9942399 | 3408144 | -1.15 | 3.25E-06 | 1.44E-05 | -0.15 | 0.556783 | 0.781554 |
| COMPOUND_519_4676a12_437243 | Rp | + | 519.4676 | 12.44 | | | (520.4723, 23735.97) (521.4753, 8806.24) (522.4794, 1636.7) (523.4838, 242.82) | 38763.05 | 29811.58 | 24846.32 | 15085.51 | 27252.44 | 9346.254 | 32020.86 | 20019.77 | -0.32 | 0.219919 | 0.31355 | 0.62 | 0.041462 | 0.265944 | |
| COMPOUND_520_4106a10_754911 | Rp | + | 520.4106 | 10.75 | | | (543.3921, 2816.09) (544.3809, 1917.6) (545.3776, 730.03) (538.4246, 864.43) (521.4211, 11852.47) (522.4234, 4295.23) (523.4266, 1506.66) | 46607.6 | 27818.46 | 45655.56 | 18094.92 | 64839.85 | 40686.09 | 53909.06 | 34390.74 | 0.60 | 0.030587 | 0.057307 | -0.66 | 0.041202 | 0.265944 | |
| COMPOUND_520_4489a12_670413 | Rp | + | 520.4489 | 12.67 | | | (1041.932, 367.95) (1042.9244, 317.33) (1043.9117, 540.56) (1079.8967, 198.84) (521.4579, 41933.42) (522.4608, 14594.03) (523.4641, 3046.73) (524.4704, 550.41) (1058.9426, 620.4) (1059.9446, 470.61) (1060.9396, 388.63) | 59943.57 | 35211.42 | 62839.91 | 37213.28 | 54778.64 | 18341.3 | 90951.68 | 51647.01 | 0.11 | 0.671604 | 0.758882 | 0.65 | 0.045136 | 0.273371 | |
| COMPOUND_521_3482a1_1173073 | Hilic | + | 521.3482 | 1.12 | | | (1043.702, 21934.41) (1044.7068, 11460.52) (1045.7202, 82030.55) (1046.724, 46576.91) (1047.7362, 342104.4) (1048.7397, 194042.16) (1049.7423, 61991.49) (1050.7448, 14818.45) (1051.7463, 3565.73) (1052.72, 820.31) (544.3401, 135353.0) (545.3445, 377928.0) (1065.6865, 25891.92) (1066.6901, 13115.49) (1067.7037, 81354.4) (1068.7074, 46303.08) (1069.717, 57934.57) (1070.7213, 29600.16) (1071.7305, 17605.84) (1072.7349, 6160.95) (1073.7465, 6033.33) (539.3995, 9737.8) (540.3938, 1649.92) (522.3548, 1149114.9) (523.3597, 279622.5) (1060.7646, 2529.13) | 23575472 | 3356790 | 23597826 | 3381090 | 12698823 | 2414974 | 13573768 | 3342102 | -1.97 | 1.22E-14 | 2.11E-12 | 0.13 | 0.51501 | 0.761025 | |
| COMPOUND_521_349a10_368553 | Rp | + | 521.3490 | 10.37 | LPC 18:1 | 2 | 10 eV: 522.3558(100), 184.0736(50), 104.1087(15), 366.6751(6), 240.0936(4) | (1043.7034, 36613.24) (1044.7063, 10031.07) (1045.7087, 3796.67) (1046.7017, 1270.59) (1047.7046, 410.38) (1081.6136, 730.71) (1082.6215, 503.83) (1083.6224, 634.4) (544.339, 51415.71) (545.3421, 15101.63) (546.3551, 20301.62) (547.3583, 5621.64) (548.3708, 5829.9) (1065.6835, 4365.24) (1066.6876, 2849.35) (1067.6873, 3010.23) (1068.6807, 1507.61) (1069.7002, 515.88) (560.3122, 4181.32) (561.3124, 1595.95) (562.3186, 8262.27) (563.3173, 5589.42) (539.3807, 1579.66) (522.3572, 1229078.4) (523.3617, 328683.1) (524.3636, 58481.22) (525.3664, 8880.36) (526.366, 1432.56) | 20258491 | 3308057 | 19528261 | 3940314 | 10947889 | 2395487 | 11900727 | 3134930 | -1.74 | 1.66E-13 | 1.25E-11 | 0.32 | 0.134363 | 0.43508 |
| COMPOUND_521_3493a1_0073508 | Hilic | + | 521.3493 | 1.01 | | | (1043.7024, 8615.11) (1044.7067, 4637.08) (1045.7188, 16526.84) (1046.7217, 9051.48) (1047.7336, 16827.03) (1048.7382, 8806.6) (1049.74, 2784.53) (1050.7368, 839.43) (1051.7181, 312.97) (544.3404, 157027.1) (545.3437, 48177.14) (546.3556, 138752.39) (547.3592, 43072.89) (548.3678, 15795.34) (1065.6873, 13948.94) (1066.6912, 7208.66) (1067.7034, 17147.85) (1068.7074, 9930.56) (1069.7174, 11133.43) (1070.7214, 5194.06) (1071.7275, 2691.22) (1072.728, 1106.07) (1073.7393, 889.53) (522.3554, 609957.56) (523.3594, 161500.36) (1060.7684, 1014.83) | 2738550 | 592942 | 8232210 | 6020568 | 1297271 | 367085.7 | 1342191 | 389984 | -1.58 | 4.61E-13 | 2.6E-11 | -0.06 | 0.780935 | 0.909341 | |
| COMPOUND_521_3501a10_274176 | Rp | + | 521.3501 | 10.27 | | | (544.3392, 65996.72) (545.3432, 18387.91) (1065.6855, 10840.7) (1066.6884, 6210.83) (1067.6982, 5367.55) (560.3118, 4078.06) (561.3179, 1352.02) (539.3878, 9978.71) (540.3803, 1461.94) (522.3572, 919051.9) (523.3615, 246616.97) (524.3632, 44236.02) (525.3669, 7855.4) | 1473495 | 2724791 | 1040784 | 2197119 | 698238.6 | 82332.39 | 930347.2 | 1210631 | -1.81 | 5.49E-12 | 1.53E-10 | 0.71 | 0.005699 | 0.118614 | |
| COMPOUND_521_792a10_213077 | Rp | + | 521.7920 | 10.21 | | | (1044.5842, 24884.63) (1045.589, 20023.68) (1046.5958, 7738.09) (1047.6019, 3330.07) (544.7929, 692.72) (1066.6277, 4072.65) (1067.6108, 2434.82) (560.7507, 1038.65) (522.7984, 44536.32) (523.8031, 29192.87) (524.8035, 14621.86) (1061.6508, 6360.56) (1062.6553, 4301.86) | 511531.1 | 212380.8 | 480643 | 230132.2 | 537183.7 | 261445.7 | 516045.2 | 259793.7 | 0.12 | 0.68039 | 0.765736 | 0.29 | 0.414013 | 0.696309 | |
| COMPOUND_522_3295a12_530789 | Rp | - | 522.3295 | 12.53 | | | (557.313, 177.62) (558.3154, 282.56) (521.3218, 13860.63) (522.3222, 8890.68) (523.3246, 2231.1) (524.3256, 418.52) (567.3468, 246.17) (1043.6166, 460.5) (1044.6187, 342.07) | 91937.91 | 9901396 | 88079.24 | 12556.71 | 94828.21 | 8871.161 | 94008.32 | 12056.1 | 0.28 | 0.32212 | 0.423801 | 0.29 | 0.399547 | 0.690408 | |
| COMPOUND_522_4667a13_280933 | Rp | + | 522.4667 | 13.28 | | | (1045.9412, 7322.95) (1046.941, 4343.5) (1047.9431, 1852.9) (1048.9398, 506.48) (523.4732, 19825.12) (524.4762, 7199.14) (525.48, 1606.95) (526.4807, 262.33) | 123196.6 | 60084.04 | 158168.5 | 68708.54 | 156105.4 | 77745.94 | 141639.7 | 66815.93 | 0.62 | 0.037176 | 0.0679 | -0.79 | 0.026777 | 0.225849 | |
| COMPOUND_523_2641a6_903725 | Rp | + | 523.2641 | 6.90 | | | (524.2712, 6298.91) (525.2748, 1639.96) (526.2524, 3522.67) (527.2556, 965.91) (528.2577, 296.07) | 30659.59 | 8130.808 | 30133.81 | 6399.25 | 28664.36 | 9121.776 | 32525.62 | 8089.008 | -0.04 | 0.890506 | 0.926471 | 0.23 | 0.500899 | 0.753664 | |
| COMPOUND_523_363a10_0992484 | Hilic | + | 523.3634 | 1.10 | | | (1047.7318, 28528.98) (1048.7362, 13221.49) (1049.7393, 4154.69) (1050.7379, 1246.15) (1051.7214, 270.12) (546.3544, 159531.27) (547.3577, 42156.74) (548.3708, 6782.28) (549.374, 19664.15) (1069.7142, 8625.35) (1070.7194, 3966.51) (1071.7227, 1683.39) (1072.7223, 555.26) (541.4061, 721.69) (524.3704, 1464778.1) (525.3752, 374053.94) (526.3778, 67731.24) (527.3792, 8100.69) (528.3858, 1095.13) (1064.798, 656.19) | 25735849 | 4111573 | 25869565 | 3977261 | 10949717 | 2651341 | 10724784 | 2692486 | -1.56 | 6.74E-14 | 6.9E-12 | -0.07 | 0.720192 | 0.876947 | |
| COMPOUND_523_3639a0_9970972 | Hilic | + | 523.3639 | 1.00 | | | (1047.7333, 10931.65) (1048.7369, 5532.55) (1049.7378, 1860.72) (1050.7245, 784.74) (1051.7522, 81.54) (546.3547, 44676.52) (547.3582, 13109.07) (548.368, 5885.24) (549.3728, 1311.09) (1069.7145, 6600.01) (1070.7189, 3063.48) (1071.7268, 1894.26) (1072.7288, 794.76) (524.3706, 750840.6) (525.375, 204271.27) (526.3772, 36813.25) (527.38, 5937.3) (528.3841, 768.46) | 3371288 | 812641 | 3477854 | 696153.6 | 1243266 | 364751.5 | 1163599 | 333595.9 | -1.47 | 5.94E-13 | 2.98E-11 | -0.20 | 0.278347 | 0.585315 | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|-----------------|----------|--|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_523_3652a10_640335 | Rp | + | 523.3652 | 10.64 | LPC 18:0 | 2 | 10 eV: 524.3745(100), 184.073(70), 104.1067(3) | (1047.74, 18668.87)(1048.744, 10191.32)(1049.7434, 3755.41)(1050.7451, 1269.58)(1051.7399, 389.88)(1085.6548, 647.91)(1086.6654, 423.12)(1087.6859, 464.11)(1088.7172, 515.41)(1546.356, 184.63)(2054.47, 3587.48)(4644.29)(548.3629, 9627.82)(549.3706, 2105.26)(1069.7191, 3030.89)(1070.7155, 1819.39)(1071.7051, 1481.02)(1072.7054, 512.89)(541.3874, 1505.51)(542.4009, 655.55)(543.3706, 6008.54)(562.3281, 6255.94)(563.3327, 2177.15)(564.3326, 1424.41)(565.3209, 242.61)(524.3723, 1472801.6)(525.3767, 402439.5)(526.3791, 65702.59)(527.3812, 11436.44)(1064.724, 668.49) | 24650943 | 4250413 | 23647826 | 4484429 | 10706563 | 3239046 | 10564884 | 3129403 | -1.64 | 9.71E-14 | 9.22E-12 | 0.10 | 0.596494 | 0.805251 |
| COMPOUND_523_3662a10_548693 | Rp | + | 523.3662 | 10.55 | LPC 18:0 isomer | 2 | 10 eV: 524.3745(100), 184.073(70), 104.1067(3) | (1047.7385, 11020.18)(1048.741, 6199.97)(1049.7426, 2502.8)(1050.742, 818.39)(1051.7325, 111.43)(1085.6538, 505.47)(1086.6392, 424.35)(1546.3567, 1311.62)(1547.3587, 3709.9)(548.3625, 8067.74)(1069.7107, 1941.05)(1070.7191, 1325.57)(1071.7121, 901.7)(1072.7257, 400.7)(1073.7327, 66.68)(562.3288, 5306.5)(563.3301, 2081.29)(564.3297, 1404.77)(524.3732, 783535.4)(525.3772, 211042.19)(526.3794, 39284.11)(527.3809, 5907.48)(528.3845, 726.78) | 3848738 | 891366.9 | 4090050 | 2574789 | 2280830 | 3069934 | 1684168 | 2859787 | -1.06 | 6.44E-06 | 2.68E-05 | -0.36 | 0.157546 | 0.468065 |
| COMPOUND_523_7058a10_204601 | Rp | + | 523.7058 | 10.20 | | | | (546.691, 473.79)(547.7085, 478.77)(524.7117, 15649.51)(525.7137, 1130.09)(526.6979, 814.47) | 55060.31 | 24182.92 | 44815.58 | 21354.51 | 58988.54 | 11211.26 | 62242.22 | 19304.21 | 0.23 | 0.419877 | 0.524149 | 0.67 | 0.048994 | 0.280039 |
| COMPOUND_525_2845a10_05921 | Rp | - | 525.2845 | 10.06 | | | | (524.2778, 251396.61)(525.2811, 72879.71)(1049.5616, 4144.25)(1050.563, 2464.92) | 273142.4 | 205735.1 | 287159.1 | 250016.9 | 235648.6 | 214626.5 | 219202.6 | 237372.1 | -0.39 | 0.194888 | 0.283887 | 0.10 | 0.790949 | 0.911108 |
| COMPOUND_525_2851a1_3956394 | Hilic | + | 525.2851 | 1.40 | | | | (548.2751, 2352.06)(549.278, 723.55)(550.2895, 372.31)(551.2964, 35.61)(526.2921, 2180.79)(527.2953, 682.01)(528.3019, 4289.5)(529.3062, 1330.71) | 26965.9 | 6878.425 | 29446.96 | 9341.161 | 21991.23 | 8211.094 | 27677.22 | 12252.18 | -0.64 | 0.03303 | 0.061346 | 0.36 | 0.304921 | 0.613089 |
| COMPOUND_525_2852a10_103805 | Rp | - | 525.2852 | 10.10 | LPE 22:6 | 2 | 10 eV: 524.2775(100), 327.2131(18) | (1085.5209, 415.97)(1086.5138, 372.32)(524.2777, 243590.89)(525.2809, 70133.47)(526.2917, 16357.06)(527.2895, 2377.26)(1049.5616, 4144.25)(1050.563, 2464.92)(1051.5704, 836.81)(1052.576, 203.74)(1163.5862, 1122.63)(1164.5807, 600.31)(1165.6119, 1506.42) | 545500.2 | 137636.2 | 568914.3 | 196032.8 | 434123.3 | 185830.6 | 559061.5 | 242237.5 | -0.74 | 0.014462 | 0.029634 | 0.60 | 0.090948 | 0.385068 |
| COMPOUND_525_2853a1_586687 | Hilic | + | 525.2853 | 1.59 | | | | (1051.5754, 942.98)(1052.5809, 592.02)(1053.5894, 268.78)(1054.5936, 115.52)(548.275, 1010.02)(549.2788, 3036.97)(550.2898, 3107.6)(551.2937, 972.56)(1073.5565, 1106.09)(1074.5638, 707.89)(1075.5696, 333.67)(543.3251, 381.54)(526.2931, 14655.71)(527.2963, 4079.57)(528.3061, 1874.34)(529.31, 407.29) | 190245.9 | 48173.66 | 205790.1 | 71427.75 | 141554.6 | 56353.13 | 181744.7 | 78673.7 | -0.89 | 0.002935 | 0.007008 | 0.46 | 0.178081 | 0.492203 |
| COMPOUND_525_2865a10_022741 | Rp | + | 525.2865 | 10.02 | | | | (1051.5656, 4598.59)(1052.5752, 2601.52)(1053.5928, 1808.98)(548.2959, 3215.48)(549.2932, 1405.28)(550.2965, 1403.08)(1073.6085, 1558.32)(564.2497, 1708.76)(565.2574, 520.97)(526.2944, 171313.03)(527.2982, 50787.09)(528.301, 11821.77)(529.3002, 1991.91)(1068.5927, 9058.52)(1069.6084, 9193.84) | 119410.9 | 102119.2 | 119803.7 | 95606.47 | 76620.5 | 29084.05 | 173013.9 | 262651.4 | -0.80 | 0.000809 | 0.017393 | 0.68 | 0.053256 | 0.287606 |
| COMPOUND_525_2878a10_106169 | Rp | + | 525.2878 | 10.11 | LPE 22:6 | 2 | 10 eV: 526.2943(100), 35.2722(40), 62.0587(32), 44.0482(22), 198.0479(8) | (1051.5732, 4110.93)(1052.5806, 2803.67)(1053.5944, 2428.11)(548.2849, 990.35)(549.2984, 646.65)(550.3013, 831.58)(1073.6125, 1814.39)(564.2483, 1902.47)(565.2572, 1059.04)(526.2949, 195116.63)(527.2985, 61771.38)(528.3011, 12970.79)(529.3002, 2569.37)(1068.591, 10096.16)(1069.6013, 9016.42) | 513694.6 | 126090.3 | 474893.7 | 182535.3 | 482294 | 165494.4 | 619673.5 | 233355.4 | -0.26 | 0.379329 | 0.480996 | 0.90 | 0.012445 | 0.169858 |
| COMPOUND_525_3427a10_452606 | Rp | - | 525.3427 | 10.45 | LPC P-16:0 | 2 | 10 eV: 464.3136(100), 524.3348(30), 141.4541(3) | (1085.6787, 506.21)(1086.6794, 382.32)(1095.7026, 574.81)(1096.7212, 503.97)(1097.7172, 450.22)(524.3354, 149773.07)(525.3383, 39419.31)(526.3437, 11083.53)(527.348, 1681.05)(1049.6766, 866.37)(1050.6781, 534.64)(1051.6659, 563.61)(1052.6617, 334.69)(1053.6571, 376.27)(1163.6283, 661.78)(1164.6166, 370.88) | 685595.6 | 131185 | 707287.3 | 151431.1 | 252223.5 | 143935.4 | 232295.4 | 126220.2 | -1.69 | 7.2E-12 | 1.95E-10 | 0.28 | 0.228504 | 0.535521 |
| COMPOUND_527_3009a10_237866 | Rp | - | 527.3009 | 10.24 | LPE 22:5 | 2 | 20 eV: 329.248(100), 526.2932(37), 196.0365(7), 53.0058(4), 440.0885(4) | (1089.5819, 3181.16)(1090.5854, 1771.54)(1091.5836, 2938.65)(526.2936, 19072.98)(527.2964, 5609.15)(528.3003, 1151.08)(529.3007, 239.46)(1167.6259, 981.61)(1168.6296, 433.72) | 86221.6 | 33458.79 | 91104.02 | 38665.74 | 78929.36 | 32494.58 | 88863.11 | 23469.44 | -0.27 | 0.326201 | 0.464757 | 0.20 | 0.582594 | 0.796117 |
| COMPOUND_527_301a10_300283 | Rp | - | 527.3010 | 10.30 | | | | (1089.5807, 2205.98)(1090.5831, 1283.83)(1091.5826, 2106.18)(526.2936, 19072.98)(527.2964, 5609.15)(528.3003, 1151.08)(529.3007, 239.46)(1167.6075, 752.35)(1168.6068, 389.09) | 48130.28 | 28653.4 | 53682.31 | 40200.71 | 45885.15 | 30324.02 | 42427.81 | 20071.66 | -0.35 | 0.244546 | 0.339945 | 0.22 | 0.546392 | 0.77815 |
| COMPOUND_527_3103a8_223662 | Rp | + | 527.3103 | 8.22 | | | | (528.3185, 23057.2)(529.3213, 6738.28)(530.3259, 1664.11) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 44807 | 37355 | 27623.95 | 18921.86 | 1.33 | 2.4E-11 | 5.2E-10 | -0.33 | 0.09665 | 0.36704 |
| COMPOUND_527_3208a9_9053335 | Rp | - | 527.3208 | 9.91 | | | | (526.3143, 90461.38)(527.3176, 22764.48)(528.3175, 5519.24) | 90660.19 | 26164.2 | 118681.5 | 65630.41 | 89642.57 | 118648.9 | 55920.91 | 23295.65 | -0.84 | 0.000358 | 0.001017 | -0.75 | 0.005826 | 0.118614 |
| COMPOUND_527_3211a10_038401 | Rp | - | 527.3211 | 10.04 | LPC 15:0 | 1 | 241.217(13) | (526.3144, 124962.4)(527.3174, 22764.48)(528.3158, 8680.55)(529.3123, 1757.21)(530.3092, 233.54) | 469972.5 | 120944.7 | 516201.5 | 147295.3 | 26526.5 | 77413.79 | 220212.5 | 79892.71 | -1.22 | 4.27E-09 | 3.86E-08 | -0.50 | 0.019664 | 0.198675 |
| COMPOUND_527_3574a10_531313 | Rp | - | 527.3574 | 10.53 | LPC O-16:0 | 2 | 10 eV: 466.2927(100), 526.3123(45), 241.217(13) | (552.3356, 449.41)(526.3509, 162402.23)(527.3542, 45608.22)(528.3566, 8664.5)(529.3617, 1527.37) | 693196.1 | 151674.2 | 714493.1 | 194632 | 267222.5 | 184021.8 | 234234.9 | 139707.1 | -1.36 | 1.71E-09 | 1.76E-08 | -0.22 | 0.330727 | 0.636557 |
| COMPOUND_528_0424a10_324152 | Rp | + | 528.0424 | 10.32 | | | | (551.0315, 355.23)(552.0468, 876.32)(529.0501, 13578.04)(530.053, 2312.98)(531.0368, 2404.91)(532.0264, 218.84)(533.0413, 919.9) | 66390.96 | 26908.96 | 53049.16 | 20666.42 | 75482.92 | 14527.58 | 74788.33 | 28386.46 | 0.31 | 0.264282 | 0.361362 | 0.62 | 0.068056 | 0.317972 |
| COMPOUND_528_4232a13_922085 | Rp | + | 528.4232 | 13.92 | | | | (551.4111, 2578.58)(552.4166, 1047.87)(553.397, 412.62)(554.4027, 43.46)(567.407, 1012.35)(568.4103, 173.41)(546.4564, 7621.28)(547.4582, 2663.56)(548.459, 645.59)(529.4302, 7804.79)(530.4341, 2544.14)(531.4334, 890.95)(1074.8502, 141.49) | 98885.77 | 18450.5 | 97001.48 | 22977.95 | 102739.4 | 11937.19 | 103803.4 | 14841.2 | 0.22 | 0.466098 | 0.570463 | 0.25 | 0.486282 | 0.747178 |
| COMPOUND_528_702a9_944124 | Rp | + | 528.7020 | 9.94 | | | | (551.7078, 619.66)(529.7102, 12506.46)(530.7125, 1929.83)(531.6966, 1968.23)(532.6923, 287.04)(533.7051, 964.11) | 63202.48 | 24245.85 | 54234.53 | 24174.94 | 64603.23 | 13150.15 | 62985.8 | 17580.1 | 0.08 | 0.770819 | 0.833358 | 0.54 | 0.121374 | 0.411649 |
| COMPOUND_529_0355a9_946081 | Rp | + | 529.0355 | 9.95 | | | | (1059.0917, 138.81)(552.019, 764.43)(553.0158, 100.78)(547.0471, 323.17)(567.9837, 184.55)(568.9863, 119.24)(530.0449, 12442.26)(531.0443, 735.83)(532.031, 1294.21)(1076.1566, 584.44)(1077.1298, 375.38) | 48554.63 | 20008.24 | 43678.05 | 20751.63 | 45399.85 | 12519.55 | 46360.4 | 13741.81 | -0.11 | 0.705332 | 0.784399 | 0.44 | 0.211453 | 0.519294 |
| COMPOUND_529_2701a8_816477 | Rp | - | 529.2701 | 8.82 | | | | (528.2629, 12002.27)(529.2659, 3725.47)(530.2648, 1127.07)(531.2654, 229.82)(263.628, 791.96)(264.1294, 243.04)(264.6274, 77.23) | 102590.6 | 102800.1 | 104433.3 | 83833.42 | 211879.7 | 158585.1 | 126147 | 93477.14 | 0.68 | 0.006815 | 0.015002 | -0.58 | 0.044551 | 0.272788 |
| COMPOUND_529_2702a8_639005 | Rp | - | 529.2702 | 8.64 | | | | (528.265, 14272.67)(529.2653, 4378.11)(530.2647, 1281.82)(531.2564, 194.36)(263.6283, 3389.62)(264.1301, 381.24)(264.6294, 420.52) | 35882.77 | 38164.84 | 37492.39 | 33490.23 | 197426.3 | 492278.3 | 54985.5 | 107674.5 | 0.83 | 0.003555 | 0.008314 | -0.66 | 0.046226 | 0.273966 |
| COMPOUND_530_1842a9_033124 | Rp | - | 530.1842 | 9.03 | | | | (1105.3414, 317.47)(1106.3588, 120.92)(1107.3555, 129.41)(529.178, 5879.92)(530.1811, 1548.63)(531.18, 818.92)(532.1806, 158.28)(1059.3572, 261.14) | 14740.06 | 3387.914 | 16560.7 | 5758.249 | 49030.86 | 33497.44 | 39126.2 | 19270.93 | 1.59 | 2.39E-12 | 7.99E-11 | -0.27 | 0.203461 | 0.5149 |
| COMPOUND_530_1965a11_19501 | Rp | + | 530.1965 | 11.20 | | | | (553.1864, 559.91)(569.1538, 2548.53)(531.203, 2941.64)(532.2057, 2152.58)(533.1863, 10838.52)(534.188, 3426.94)(1078.4271, 848.27) | 32610.29 | 12358.28 | 23843.88 | 8095.714 | 51327 | 15321.7 | 55737.61 | 17416.71 | 0.77 | 0.001581 | 0.003982 | 0.74 | 0.009653 | 0.153413 |
| COMPOUND_530_4028a11_883773 | Rp | + | 530.4028 | 11.88 | | | | (1061.7737, 465.2)(1062.7631, 349.84)(1063.7789, 265.33)(1099.8055, 365.3)(1100.7847, 2000.69)(1101.788, 1936.92)(533.3919, 136343.48)(534.3949, 43676.13)(555.3936, 13752.78)(556.3948, 2822.44)(557.3868, 313.02)(1083.792, 36763.55)(1084.7957, 24690.98)(1085.7953, 11928.62)(1086.7951, 4504.12)(1087.7955, 1534.47)(1088.7979, 384.81)(569.3661, 13047.09)(570.3692, 4190.55)(571.3648, 2390.51)(572.3622, 570.92)(548.4115, 382.65)(531.4089, 832401.94)(532.4131, 260824.56)(533 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|---|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_531_276a12_5302 | Rp | - | 531.2760 | 12.53 | | | | (644.2597, 1590.61)(645.2632, 607.73)(646.2581, 778.39)(647.2572, 327.7)(648.2531, 346.58)(566.246, 79089.75)(567.2493, 27271.29)(568.2443, 27455.04)(569.2463, 8822.82)(570.2499, 1944.69)(571.2576, 473.6)(530.2679, 3863.73)(531.2685, 1752.99)(532.2751, 878.06)(533.2837, 62.45)(576.2746, 68865.68)(577.2776, 24515.66)(578.2708, 5642.26)(579.2833, 977.96) (1101.726, 550.61)(1102.7317, 742.34)(1103.7375, 838.16)(1085.7325, 1092.04)(1086.723, 611.17)(532.3754, 8951.49)(533.38, 2670.45)(534.391, 3114.92)(535.3926, 1291.42) | 724224.2 | 92660.43 | 695180.9 | 108358.3 | 778002.5 | 69506.33 | 764839.2 | 108356.8 | 0.64 | 0.029071 | 0.054877 | 0.12 | 0.730509 | 0.885165 |
| COMPOUND_531_3678a10_857612 | Rp | + | 531.3678 | 10.86 | | | | (1101.765, 1010.56)(1102.7765, 1092.41)(1103.7605, 663.52)(570.3458, 322.9)(532.3928, 11985.21)(533.3955, 5496.94)(534.3908, 1173.64)(1080.7734, 1179.2)(1081.7982, 564.96)(1082.7654, 875.45) (1101.765, 1010.56)(1102.7765, 1092.41)(1103.7605, 663.52)(570.3458, 322.9)(532.3928, 11985.21)(533.3955, 5496.94)(534.3908, 1173.64)(1080.7734, 1179.2)(1081.7982, 564.96)(1082.7654, 875.45) | 100761.2 | 33005.84 | 113391.5 | 44983.04 | 39021.83 | 30850.47 | 33471.79 | 25714.59 | -1.07 | 4.02E-07 | 2.25E-06 | -0.51 | 0.028159 | 0.229762 |
| COMPOUND_531_3866a11_108429 | Rp | + | 531.3866 | 11.11 | | | | (1101.765, 1010.56)(1102.7765, 1092.41)(1103.7605, 663.52)(570.3458, 322.9)(532.3928, 11985.21)(533.3955, 5496.94)(534.3908, 1173.64)(1080.7734, 1179.2)(1081.7982, 564.96)(1082.7654, 875.45) (1101.765, 1010.56)(1102.7765, 1092.41)(1103.7605, 663.52)(570.3458, 322.9)(532.3928, 11985.21)(533.3955, 5496.94)(534.3908, 1173.64)(1080.7734, 1179.2)(1081.7982, 564.96)(1082.7654, 875.45) | 84251 | 16488.73 | 40166.21 | 14683.58 | 52171.38 | 9245.288 | 52306.69 | 14145.92 | 0.21 | 0.450206 | 0.555846 | 0.71 | 0.036714 | 0.255977 |
| COMPOUND_532_7128a10_43298 | Rp | + | 532.7128 | 10.43 | | | | (231.52)(537.7105, 432.89) (1067.1024, 312.13)(1105.0792, 222.98)(556.0474, 322.62)(557.0585, 527.92)(571.9969, 355.14)(551.0602, 353.56)(534.0558, 8786.99)(535.0603, 747.95)(536.0417, 946.25) | 37122.54 | 14049.95 | 28597.03 | 11988.99 | 40646.55 | 7772.888 | 40263.04 | 13607.21 | 0.07 | 0.793885 | 0.850538 | 0.80 | 0.018961 | 0.196411 |
| COMPOUND_532_283a10_251471 | Rp | + | 533.2830 | 10.25 | | | | (556.2771, 980.04)(556.7809, 697.89)(557.2848, 1244.82)(557.7897, 775.77)(558.2787, 816.86)(1067.5914, 853.35)(1105.5509, 1473.38)(556.2933, 1056.49)(557.3131, 230.98)(558.3, 474.05)(545.2847, 376.36)(545.7923, 568.71)(546.2788, 389.74)(1089.5652, 1668.9)(1090.5754, 1083.31)(1091.59, 4059.31)(1092.5939, 3088.9)(1093.582, 1854.58)(564.26, 2519.46)(564.7697, 2681.71)(565.2727, 1979.34)(565.774, 915.97)(566.2605, 330.0)(534.2953, 10181.1)(535.2989, 3315.31)(536.3059, 4632.85)(537.3075, 1971.11)(538.3051, 1823.41)(267.6488, 33273.44)(268.1505, 8966.75)(268.6516, 2135.61)(269.1552, 348.01) (556.2771, 980.04)(556.7809, 697.89)(557.2848, 1244.82)(557.7897, 775.77)(558.2787, 816.86)(1067.5914, 853.35)(1105.5509, 1473.38)(556.2933, 1056.49)(557.3131, 230.98)(558.3, 474.05)(545.2847, 376.36)(545.7923, 568.71)(546.2788, 389.74)(1089.5652, 1668.9)(1090.5754, 1083.31)(1091.59, 4059.31)(1092.5939, 3088.9)(1093.582, 1854.58)(564.26, 2519.46)(564.7697, 2681.71)(565.2727, 1979.34)(565.774, 915.97)(566.2605, 330.0)(534.2953, 10181.1)(535.2989, 3315.31)(536.3059, 4632.85)(537.3075, 1971.11)(538.3051, 1823.41)(267.6488, 33273.44)(268.1505, 8966.75)(268.6516, 2135.61)(269.1552, 348.01) | 448914.4 | 110080 | 408538.9 | 144166.9 | 470660.4 | 45479.31 | 464670.7 | 56994.4 | -0.09 | 0.772512 | 0.833547 | 0.24 | 0.50909 | 0.757224 |
| COMPOUND_533_2861a10_151148 | Rp | + | 533.2861 | 10.15 | | | | (556.2819, 808.22)(556.7777, 470.47)(557.2842, 866.68)(557.7805, 468.61)(558.2819, 524.08)(1067.631, 6078.28)(1105.5562, 705.0)(545.2845, 239.57)(545.7837, 257.13)(546.2768, 203.58)(556.2947, 3432.1)(564.2609, 1132.78)(564.7708, 1197.14)(565.2655, 1465.11)(565.7792, 710.74)(566.2556, 278.21)(1089.5662, 867.51)(1090.5763, 791.83)(1091.5918, 2554.17)(1092.6056, 2365.02)(1093.5991, 1480.62)(534.2954, 5880.01)(535.2988, 2358.72)(536.3073, 4472.39)(537.3092, 2280.84)(538.3094, 1284.64)(267.6493, 30446.66)(268.1509, 8256.29)(268.652, 1782.24)(269.1534, 366.8) (556.2819, 808.22)(556.7777, 470.47)(557.2842, 866.68)(557.7805, 468.61)(558.2819, 524.08)(1067.631, 6078.28)(1105.5562, 705.0)(545.2845, 239.57)(545.7837, 257.13)(546.2768, 203.58)(556.2947, 3432.1)(564.2609, 1132.78)(564.7708, 1197.14)(565.2655, 1465.11)(565.7792, 710.74)(566.2556, 278.21)(1089.5662, 867.51)(1090.5763, 791.83)(1091.5918, 2554.17)(1092.6056, 2365.02)(1093.5991, 1480.62)(534.2954, 5880.01)(535.2988, 2358.72)(536.3073, 4472.39)(537.3092, 2280.84)(538.3094, 1284.64)(267.6493, 30446.66)(268.1509, 8256.29)(268.652, 1782.24)(269.1534, 366.8) | 328545.6 | 51646.95 | 321092.1 | 43493.23 | 327030.1 | 116180.6 | 273343.9 | 76884.13 | -0.39 | 0.124059 | 0.195708 | -0.66 | 0.030294 | 0.234557 |
| COMPOUND_533_2885a1_0548054 | Hilic | + | 533.2885 | 1.05 | | | | (1068.6038, 401.31)(1069.5807, 94.81)(556.2855, 259.38)(1089.58, 619.97)(1090.5778, 1101.91)(1091.5734, 664.55)(551.3318, 557.56)(534.2963, 10553.75)(535.299, 2822.82)(536.2979, 1280.55)(537.3005, 258.45)(1084.6652, 769.91) (1068.6038, 401.31)(1069.5807, 94.81)(556.2855, 259.38)(1089.58, 619.97)(1090.5778, 1101.91)(1091.5734, 664.55)(551.3318, 557.56)(534.2963, 10553.75)(535.299, 2822.82)(536.2979, 1280.55)(537.3005, 258.45)(1084.6652, 769.91) | 68117.11 | 7441.158 | 73009.46 | 7263.458 | 63811.36 | 13063.97 | 66229.25 | 9185.799 | -0.34 | 0.23858 | 0.333581 | -0.43 | 0.219599 | 0.528917 |
| COMPOUND_533_2896a1_1620592 | Hilic | + | 533.2896 | 1.16 | | | | (1067.5598, 361.24)(1068.578, 812.73)(1069.6038, 818.3)(556.3005, 667.62)(557.3017, 314.43)(1089.5681, 270.31)(1090.5751, 517.35)(1091.5905, 566.98)(551.328, 398.97)(534.2962, 10210.61)(535.2997, 3015.3)(536.2991, 1267.81)(537.2996, 259.32)(1084.6467, 701.68) (1067.5598, 361.24)(1068.578, 812.73)(1069.6038, 818.3)(556.3005, 667.62)(557.3017, 314.43)(1089.5681, 270.31)(1090.5751, 517.35)(1091.5905, 566.98)(551.328, 398.97)(534.2962, 10210.61)(535.2997, 3015.3)(536.2991, 1267.81)(537.2996, 259.32)(1084.6467, 701.68) | 109809.2 | 20002.55 | 115580.4 | 27703.46 | 109156.4 | 7665.042 | 110242.1 | 8653.991 | -0.10 | 0.733531 | 0.806204 | -0.39 | 0.264411 | 0.575338 |
| COMPOUND_533_3075a10_783806 | Rp | - | 533.3075 | 10.78 | | | | (532.3006, 7855.75)(533.304, 2044.12)(534.3057, 568.49) (1067.5927, 262.98)(556.3021, 5993.7)(557.3051, 1844.89)(558.3181, 5137.98)(534.3183, 35084.64)(535.3216, 10380.87)(536.3338, 1311.782)(537.338, 3905.48)(538.3495, 2664.5)(539.3531, 724.11)(540.3645, 1294.49)(267.665, 925.84)(268.1676, 438.82)(268.6722, 23.65) (532.3006, 7855.75)(533.304, 2044.12)(534.3057, 568.49) | 19922.32 | 5427.853 | 21319 | 6831.156 | 13177 | 1241.68 | 12618.25 | 2472.042 | -1.33 | 2.42E-10 | 3.34E-09 | -0.02 | 0.934202 | 0.971294 |
| COMPOUND_533_3098a1_3927718 | Hilic | + | 533.3098 | 1.39 | | | | (1067.5927, 262.98)(556.3021, 5993.7)(557.3051, 1844.89)(558.3181, 5137.98)(534.3183, 35084.64)(535.3216, 10380.87)(536.3338, 1311.782)(537.338, 3905.48)(538.3495, 2664.5)(539.3531, 724.11)(540.3645, 1294.49)(267.665, 925.84)(268.1676, 438.82)(268.6722, 23.65) (1067.5927, 262.98)(556.3021, 5993.7)(557.3051, 1844.89)(558.3181, 5137.98)(534.3183, 35084.64)(535.3216, 10380.87)(536.3338, 1311.782)(537.338, 3905.48)(538.3495, 2664.5)(539.3531, 724.11)(540.3645, 1294.49)(267.665, 925.84)(268.1676, 438.82)(268.6722, 23.65) | 169809 | 157109.7 | 207830.8 | 110886.9 | 86359 | #DIV/0! | 74209.6 | 51413.28 | -0.92 | 1.92E-05 | 7.21E-05 | -0.22 | 0.359218 | 0.666906 |
| COMPOUND_533_3868a10_702347 | Rp | + | 533.3868 | 10.70 | | | | (1105.7347, 220.36)(1106.7107, 404.46)(1107.7002, 350.07)(556.3879, 2692.91)(557.3938, 1852.38)(558.3996, 1370.82)(1089.7137, 457.98)(1090.745, 231.97)(534.3888, 7970.38)(535.3889, 3142.97)(536.3874, 5948.64)(537.3904, 2578.79)(1084.7565, 225.12)(1085.7496, 141.69)(1086.7336, 137.34) (1105.7347, 220.36)(1106.7107, 404.46)(1107.7002, 350.07)(556.3879, 2692.91)(557.3938, 1852.38)(558.3996, 1370.82)(1089.7137, 457.98)(1090.745, 231.97)(534.3888, 7970.38)(535.3889, 3142.97)(536.3874, 5948.64)(537.3904, 2578.79)(1084.7565, 225.12)(1085.7496, 141.69)(1086.7336, 137.34) | 46590.69 | 16020.33 | 53406.14 | 26128.5 | 36442 | 19555.71 | 37439.43 | 17847.1 | -0.97 | 1.65E-05 | 6.31E-05 | -0.15 | 0.546474 | 0.77815 |
| COMPOUND_533_7078a10_0650425 | Rp | + | 533.7078 | 10.07 | | | | (556.6939, 595.85)(557.7019, 332.73)(534.7151, 16660.88)(535.7179, 1210.28)(536.7003, 1120.38) (1071.3276, 707.7)(1072.3239, 830.4)(1073.333, 857.57)(1074.335, 747.82)(1109.2837, 715.67)(1093.104, 380.17)(1094.3213, 594.73)(536.1659, 38785.71)(537.1663, 19286.2)(538.165, 13224.04)(1088.3312, 958.59) (556.6939, 595.85)(557.7019, 332.73)(534.7151, 16660.88)(535.7179, 1210.28)(536.7003, 1120.38) | 57692.73 | 24846.98 | 47374.4 | 20902.76 | 60973.08 | 11314.49 | 63254.84 | 18874.32 | 0.19 | 0.499444 | 0.600186 | 0.74 | 0.030401 | 0.234557 |
| COMPOUND_535_1591a11_6996555 | Rp | + | 535.1591 | 11.70 | | | | (1071.3276, 707.7)(1072.3239, 830.4)(1073.333, 857.57)(1074.335, 747.82)(1109.2837, 715.67)(1093.104, 380.17)(1094.3213, 594.73)(536.1659, 38785.71)(537.1663, 19286.2)(538.165, 13224.04)(1088.3312, 958.59) (1071.3276, 707.7)(1072.3239, 830.4)(1073.333, 857.57)(1074.335, 747.82)(1109.2837, 715.67)(1093.104, 380.17)(1094.3213, 594.73)(536.1659, 38785.71)(537.1663, 19286.2)(538.165, 13224.04)(1088.3312, 958.59) | 184821.8 | 17461.59 | 180130.6 | 16549.95 | 190287.2 | 21340.35 | 199013.4 | 18743.03 | 0.30 | 0.280115 | 0.379326 | 0.67 | 0.048832 | 0.279822 |
| COMPOUND_535_3277a1_4799759 | Hilic | + | 535.3277 | 1.48 | | | | (558.3179, 1620.36)(559.3215, 498.48)(560.3337, 1058.06)(561.3368, 317.34)(536.3345, 4131.89)(537.3382, 1181.47)(538.3496, 1336.83)(539.354, 376.89)(540.3661, 2267.01) (558.3179, 1620.36)(559.3215, 498.48)(560.3337, 1058.06)(561.3368, 317.34)(536.3345, 4131.89)(537.3382, 1181.47)(538.3496, 1336.83)(539.354, 376.89)(540.3661, 2267.01) | 107331.5 | 90594.99 | 136777.9 | 71630.77 | 86559.75 | 30415.68 | 139560.9 | 113399.2 | -0.96 | 2.79E-05 | 0.0001 | -0.38 | 0.139807 | 0.444883 |
| COMPOUND_535_3278a1_5378143 | Hilic | + | 535.3278 | 1.54 | | | | (558.3179, 1620.36)(559.3215, 498.48)(560.3337, 1058.06)(561.3368, 317.34)(536.3345, 4131.89)(537.3382, 1181.47)(538.3496, 1336.83)(539.354, 376.89)(540.3661, 2267.01) (558.3179, 1620.36)(559.3215, 498.48)(560.3337, 1058.06)(561.3368, 317.34)(536.3345, 4131.89)(537.3382, 1181.47)(538.3496, 1336.83)(539.354, 376.89)(540.3661, 2267.01) | 134400.2 | 91688.88 | 162963 | 94592.11 | 126829 | 60579.1 | 149219.6 | 72496.95 | -0.96 | 2.39E-05 | 8.71E-05 | -0.41 | 0.105918 | 0.387484 |
| COMPOUND_535_3285a_948308 | Rp | + | 535.3285 | 8.95 | LPC HODE | 2 | 20 eV : 518.3264(100), 104.1083(80), 184.0737(50), 454.9768(25) | (558.3206, 2564.3)(559.3223, 835.24)(560.3347, 2707.03)(561.3395, 912.58)(562.333, 232.01)(536.3363, 94582.22)(537.3397, 26135.66)(538.3434, 5067.09)(539.3468, 919.97) (558.3206, 2564.3)(559.3223, 835.24)(560.3347, 2707.03)(561.3395, 912.58)(562.333, 232.01)(536.3363, 94582.22)(537.3397, 26135.66)(538.3434, 5067.09)(539.3468, 919.97) | 129437.3 | 107060.1 | 179966.3 | 115023.7 | 119 | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|----------------------------|--------|----------|----------|-----------|----------------|----------|---|--|---------------|--------|---------------|---------|---------------|--------|---------------|----------|----------|-------|----------|-------------|-------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_539_3219a_802215 | Rp | - | 539.3219 | 9.80 | | | | (538.314, 38160.7)(539.3175, 10844.56)(540.324, 3184.95)(541.3287, 603.44)(542.3296, 91.19) (538.3145, 33004.1)(539.3179, 8813.05)(540.3217, 18930.29)(541.3251, 3317.2)(542.329, 522.27) (562.3503, 6874.04)(563.3534, 2141.53)(564.3643, 1932.0)(540.3659, 5378.41)(541.369, 1677.98)(542.3728, 312.7) (539.2493, 10108.05)(540.2525, 2969.57)(541.2554, 882.81)(542.2555, 186.6) (541.275, 6258.53)(542.2787, 1924.48)(543.2811, 522.34)(544.2778, 98.43) (1083.6344, 1810.76)(1084.6335, 952.29)(1085.653, 7927.2)(1086.6566, 5935.23)(1087.6711, 401.42.84)(1121.5801, 1215.24)(1122.5913, 4463.17)(561.3006, 2480.0)(561.794, 1761.26)(562.3138, 5473.55)(565.2925, 384.51)(565.3118, 4056.18)(565.7967, 2465.21)(564.3076, 4494.62)(564.7994, 1228.04)(565.2976, 5617.42)(1105.5735, 2898.7)(1106.5789, 6296.32)(301.6359, 1855.91)(302.1422, 907.87)(580.2907, 6103.56)(580.783, 551.2)(581.2793, 17502.36)(293.6323, 627.56)(294.1325, 289.08)(580.27, 572.67)(581.2791, 17069.09)(582.2821, 6483.93)(1100.5967, 1224.6)(271.6609, 4400.96)(272.1621, 1741.13)(272.662, 1015.86)(273.1625, 115.33) (1083.6595, 928.46)(1084.6608, 705.97)(1085.6573, 3777.5)(564.3134, 2383.54)(565.3176, 823.86)(569.3576, 685.18)(542.3245, 68152.59)(543.3275, 19867.57)(1100.6364, 900.77) (564.3078, 5200.53)(565.3111, 2139.39)(542.3245, 49405.5)(543.3281, 142677.77) (1083.6155, 80.88)(564.3072, 16774.8)(565.3114, 5570.23)(566.3185, 1881.97)(580.2604, 1035.79)(581.2639, 308.13)(542.3265, 142151.4)(543.3297, 43445.36)(544.3321, 8017.93)(545.3367, 1526.44)(1100.6532, 153.11) (1083.6375, 3405.19)(1084.6405, 2352.62)(1085.6447, 796.28)(564.3077, 21828.45)(565.3102, 6706.04)(566.3181, 2219.01)(567.3058, 309.83)(1105.6172, 814.57)(1106.6276, 452.19)(1107.6013, 951.79)(1108.6063, 636.64)(1109.612, 265.13)(580.2785, 3157.04)(581.2768, 981.81)(542.3258, 521416.88)(543.3295, 153956.36)(544.3322, 28875.86)(545.3334, 4585.91)(546.3338, 744.97)(1100.6376, 68.63)(271.6583, 499.65)(272.1619, 251.58)(272.6621, 61.87) (540.3295, 914958.6)(541.3335, 237716.08)(542.3357, 48358.0)(543.3383, 7105.4)(544.3362, 858.57) (1127.6696, 646.81)(1128.6735, 323.22)(1129.688, 1827.46)(540.3294, 1034370.9)(541.3325, 269025.56)(542.3356, 50257.91)(543.3384, 7916.24)(544.3345, 1248.39) (1084.4597, 460.77)(1085.4883, 494.07)(1086.4655, 374.04)(1106.4604, 430.78)(542.731, 8225.28)(543.7344, 618.87)(544.7296, 4499.21)(545.7334, 415.13)(546.7282, 1116.61)(547.7338, 88.51)(548.7253, 206.47) (560.7331, 854.52)(543.7253, 14219.59)(544.7301, 1637.55)(545.7137, 1741.76)(546.7081, 381.8)(547.7216, 698.76) (1087.0785, 546.38)(1125.0988, 316.28)(566.0373, 806.48)(567.0355, 213.27)(582.0081, 639.2)(583.0057, 275.81)(544.059, 16073.09)(545.0622, 1116.91)(546.0452, 965.52) | 91.19 | 668583 | 319518.9 | 1035996 | 397725.8 | 803952 | 172416.7 | 767833.7 | 345989.5 | -0.34 | 0.190162 | 0.279169 | -0.47 | 0.116794 | 0.405455 |
| COMPOUND_539_322a9_936208 | Rp | - | 539.3220 | 9.94 | LPC 16:1 | 2 | 10 eV: 478.2928(100), 538.3157(52), 253.218(10), 44.9987(6) | (538.3145, 33004.1)(539.3179, 8813.05)(540.3217, 18930.29)(541.3251, 3317.2)(542.329, 522.27) (562.3503, 6874.04)(563.3534, 2141.53)(564.3643, 1932.0)(540.3659, 5378.41)(541.369, 1677.98)(542.3728, 312.7) (539.2493, 10108.05)(540.2525, 2969.57)(541.2554, 882.81)(542.2555, 186.6) (541.275, 6258.53)(542.2787, 1924.48)(543.2811, 522.34)(544.2778, 98.43) (1083.6344, 1810.76)(1084.6335, 952.29)(1085.653, 7927.2)(1086.6566, 5935.23)(1087.6711, 401.42.84)(1121.5801, 1215.24)(1122.5913, 4463.17)(561.3006, 2480.0)(561.794, 1761.26)(562.3138, 5473.55)(565.2925, 384.51)(565.3118, 4056.18)(565.7967, 2465.21)(564.3076, 4494.62)(564.7994, 1228.04)(565.2976, 5617.42)(1105.5735, 2898.7)(1106.5789, 6296.32)(301.6359, 1855.91)(302.1422, 907.87)(580.2907, 6103.56)(580.783, 551.2)(581.2793, 17502.36)(293.6323, 627.56)(294.1325, 289.08)(580.27, 572.67)(581.2791, 17069.09)(582.2821, 6483.93)(1100.5967, 1224.6)(271.6609, 4400.96)(272.1621, 1741.13)(272.662, 1015.86)(273.1625, 115.33) (1083.6595, 928.46)(1084.6608, 705.97)(1085.6573, 3777.5)(564.3134, 2383.54)(565.3176, 823.86)(569.3576, 685.18)(542.3245, 68152.59)(543.3275, 19867.57)(1100.6364, 900.77) (564.3078, 5200.53)(565.3111, 2139.39)(542.3245, 49405.5)(543.3281, 142677.77) (1083.6155, 80.88)(564.3072, 16774.8)(565.3114, 5570.23)(566.3185, 1881.97)(580.2604, 1035.79)(581.2639, 308.13)(542.3265, 142151.4)(543.3297, 43445.36)(544.3321, 8017.93)(545.3367, 1526.44)(1100.6532, 153.11) (1083.6375, 3405.19)(1084.6405, 2352.62)(1085.6447, 796.28)(564.3077, 21828.45)(565.3102, 6706.04)(566.3181, 2219.01)(567.3058, 309.83)(1105.6172, 814.57)(1106.6276, 452.19)(1107.6013, 951.79)(1108.6063, 636.64)(1109.612, 265.13)(580.2785, 3157.04)(581.2768, 981.81)(542.3258, 521416.88)(543.3295, 153956.36)(544.3322, 28875.86)(545.3334, 4585.91)(546.3338, 744.97)(1100.6376, 68.63)(271.6583, 499.65)(272.1619, 251.58)(272.6621, 61.87) (540.3295, 914958.6)(541.3335, 237716.08)(542.3357, 48358.0)(543.3383, 7105.4)(544.3362, 858.57) (1127.6696, 646.81)(1128.6735, 323.22)(1129.688, 1827.46)(540.3294, 1034370.9)(541.3325, 269025.56)(542.3356, 50257.91)(543.3384, 7916.24)(544.3345, 1248.39) (1084.4597, 460.77)(1085.4883, 494.07)(1086.4655, 374.04)(1106.4604, 430.78)(542.731, 8225.28)(543.7344, 618.87)(544.7296, 4499.21)(545.7334, 415.13)(546.7282, 1116.61)(547.7338, 88.51)(548.7253, 206.47) (560.7331, 854.52)(543.7253, 14219.59)(544.7301, 1637.55)(545.7137, 1741.76)(546.7081, 381.8)(547.7216, 698.76) (1087.0785, 546.38)(1125.0988, 316.28)(566.0373, 806.48)(567.0355, 213.27)(582.0081, 639.2)(583.0057, 275.81)(544.059, 16073.09)(545.0622, 1116.91)(546.0452, 965.52) | 91.19 | 668583 | 319518.9 | 1035996 | 397725.8 | 803952 | 172416.7 | 767833.7 | 345989.5 | -0.26 | 0.325103 | 0.425658 | -0.60 | 0.051887 | 0.285695 |
| COMPOUND_539_3593a1_494732 | Hilic | + | 539.3593 | 1.49 | | | | (538.314, 38160.7)(539.3175, 10844.56)(540.324, 3184.95)(541.3287, 603.44)(542.3296, 91.19) (538.3145, 33004.1)(539.3179, 8813.05)(540.3217, 18930.29)(541.3251, 3317.2)(542.329, 522.27) (562.3503, 6874.04)(563.3534, 2141.53)(564.3643, 1932.0)(540.3659, 5378.41)(541.369, 1677.98)(542.3728, 312.7) (539.2493, 10108.05)(540.2525, 2969.57)(541.2554, 882.81)(542.2555, 186.6) (541.275, 6258.53)(542.2787, 1924.48)(543.2811, 522.34)(544.2778, 98.43) (1083.6344, 1810.76)(1084.6335, 952.29)(1085.653, 7927.2)(1086.6566, 5935.23)(1087.6711, 401.42.84)(1121.5801, 1215.24)(1122.5913, 4463.17)(561.3006, 2480.0)(561.794, 1761.26)(562.3138, 5473.55)(565.2925, 384.51)(565.3118, 4056.18)(565.7967, 2465.21)(564.3076, 4494.62)(564.7994, 1228.04)(565.2976, 5617.42)(1105.5735, 2898.7)(1106.5789, 6296.32)(301.6359, 1855.91)(302.1422, 907.87)(580.2907, 6103.56)(580.783, 551.2)(581.2793, 17502.36)(293.6323, 627.56)(294.1325, 289.08)(580.27, 572.67)(581.2791, 17069.09)(582.2821, 6483.93)(1100.5967, 1224.6)(271.6609, 4400.96)(272.1621, 1741.13)(272.662, 1015.86)(273.1625, 115.33) (1083.6595, 928.46)(1084.6608, 705.97)(1085.6573, 3777.5)(564.3134, 2383.54)(565.3176, 823.86)(569.3576, 685.18)(542.3245, 68152.59)(543.3275, 19867.57)(1100.6364, 900.77) (564.3078, 5200.53)(565.3111, 2139.39)(542.3245, 49405.5)(543.3281, 142677.77) (1083.6155, 80.88)(564.3072, 16774.8)(565.3114, 5570.23)(566.3185, 1881.97)(580.2604, 1035.79)(581.2639, 308.13)(542.3265, 142151.4)(543.3297, 43445.36)(544.3321, 8017.93)(545.3367, 1526.44)(1100.6532, 153.11) (1083.6375, 3405.19)(1084.6405, 2352.62)(1085.6447, 796.28)(564.3077, 21828.45)(565.3102, 6706.04)(566.3181, 2219.01)(567.3058, 309.83)(1105.6172, 814.57)(1106.6276, 452.19)(1107.6013, 951.79)(1108.6063, 636.64)(1109.612, 265.13)(580.2785, 3157.04)(581.2768, 981.81)(542.3258, 521416.88)(543.3295, 153956.36)(544.3322, 28875.86)(545.3334, 4585.91)(546.3338, 744.97)(1100.6376, 68.63)(271.6583, 499.65)(272.1619, 251.58)(272.6621, 61.87) (540.3295, 914958.6)(541.3335, 237716.08)(542.3357, 48358.0)(543.3383, 7105.4)(544.3362, 858.57) (1127.6696, 646.81)(1128.6735, 323.22)(1129.688, 1827.46)(540.3294, 1034370.9)(541.3325, 269025.56)(542.3356, 50257.91)(543.3384, 7916.24)(544.3345, 1248.39) (1084.4597, 460.77)(1085.4883, 494.07)(1086.4655, 374.04)(1106.4604, 430.78)(542.731, 8225.28)(543.7344, 618.87)(544.7296, 4499.21)(545.7334, 415.13)(546.7282, 1116.61)(547.7338, 88.51)(548.7253, 206.47) (560.7331, 854.52)(543.7253, 14219.59)(544.7301, 1637.55)(545.7137, 1741.76)(546.7081, 381.8)(547.7216, 698.76) (1087.0785, 546.38)(1125.0988, 316.28)(566.0373, 806.48)(567.0355, 213.27)(582.0081, 639.2)(583.0057, 275.81)(544.059, 16073.09)(545.0622, 1116.91)(546.0452, 965.52) | 91.19 | 668583 | 319518.9 | 1035996 | 397725.8 | 803952 | 172416.7 | 767833.7 | 345989.5 | -1.31 | 3.09E-07 | 1.76E-06 | -0.60 | 0.815253 | 0.92157 |
| COMPOUND_540_256a6_879685 | Rp | - | 540.2560 | 6.88 | | | | (538.314, 38160.7)(539.3175, 10844.56)(540.324, 3184.95)(541.3287, 603.44)(542.3296, 91.19) (538.3145, 33004.1)(539.3179, 8813.05)(540.3217, 18930.29)(541.3251, 3317.2)(542.329, 522.27) (562.3503, 6874.04)(563.3534, 2141.53)(564.3643, 1932.0)(540.3659, 5378.41)(541.369, 1677.98)(542.3728, 312.7) (539.2493, 10108.05)(540.2525, 2969.57)(541.2554, 882.81)(542.2555, 186.6) (541.275, 6258.53)(542.2787, 1924.48)(543.2811, 522.34)(544.2778, 98.43) (1083.6344, 1810.76)(1084.6335, 952.29)(1085.653, 7927.2)(1086.6566, 5935.23)(1087.6711, 401.42.84)(1121.5801, 1215.24)(1122.5913, 4463.17)(561.3006, 2480.0)(561.794, 1761.26)(562.3138, 5473.55)(565.2925, 384.51)(565.3118, 4056.18)(565.7967, 2465.21)(564.3076, 4494.62)(564.7994, 1228.04)(565.2976, 5617.42)(1105.5735, 2898.7)(1106.5789, 6296.32)(301.6359, 1855.91)(302.1422, 907.87)(580.2907, 6103.56)(580.783, 551.2)(581.2793, 17502.36)(293.6323, 627.56)(294.1325, 289.08)(580.27, 572.67)(581.2791, 17069.09)(582.2821, 6483.93)(1100.5967, 1224.6)(271.6609, 4400.96)(272.1621, 1741.13)(272.662, 1015.86)(273.1625, 115.33) (1083.6595, 928.46)(1084.6608, 705.97)(1085.6573, 3777.5)(564.3134, 2383.54)(565.3176, 823.86)(569.3576, 685.18)(542.3245, 68152.59)(543.3275, 19867.57)(1100.6364, 900.77) (564.3078, 5200.53)(565.3111, 2139.39)(542.3245, 49405.5)(543.3281, 142677.77) (1083.6155, 80.88)(564.3072, 16774.8)(565.3114, 5570.23)(566.3185, 1881.97)(580.2604, 1035.79)(581.2639, 308.13)(542.3265, 142151.4)(543.3297, 43445.36)(544.3321, 8017.93)(545.3367, 1526.44)(1100.6532, 153.11) (1083.6375, 3405.19)(1084.6405, 2352.62)(1085.6447, 796.28)(564.3077, 21828.45)(565.3102, 6706.04)(566.3181, 2219.01)(567.3058, 309.83)(1105.6172, 814.57)(1106.6276, 452.19)(1107.6013, 951.79)(1108.6063, 636.64)(1109.612, 265.13)(580.2785, 3157.04)(581.2768, 981.81)(542.3258, 521416.88)(543.3295, 153956.36)(544.3322, 28875.86)(545.3334, 4585.91)(546.3338, 744.97)(1100.6376, 68.63)(271.6583, 499.65)(272.1619, 251.58)(272.6621, 61.87) (540.3295, 914958.6)(541.3335, 237716.08)(542.3357, 48358.0)(543.3383, 7105.4)(544.3362, 858.57) (1127.6696, 646.81)(1128.6735, 323.22)(1129.688, 1827.46)(540.3294, 1034370.9)(541.3325, 269025.56)(542.3356, 50257.91)(543.3384, 7916.24)(544.3345, 1248.39) (1084.4597, 460.77)(1085.4883, 494.07)(1086.4655, 374.04)(1106.4604, 430.78)(542.731, 8225.28)(543.7344, 618.87)(544.7296, 4499.21)(545.7334, 415.13)(546.7282, 1116.61)(547.7338, 88.51)(548.7253, 206.47) (560.7331, 854.52)(543.7253, 14219.59)(544.7301, 1637.55)(545.7137, 1741.76)(546.7081, 381.8)(547.7216, 698.76) (1087.0785, 546.38)(1125.0988, 316.28)(566.0373, 806.48)(567.0355, 213.27)(582.0081, 639.2)(583.0057, 275.81)(544.059, 16073.09)(545.0622, 1116.91)(546.0452, 965.52) | 91.19 | 668583 | 319518.9 | 1035996 | 397725.8 | 803952 | 172416.7 | 767833.7 | 345989.5 | -0.38 | 0.172544 | 0.257161 | -0.02 | 0.960956 | 0.981885 |
| COMPOUND_540_2677a_2955306 | Hilic | + | 540.2677 | 2.30 | | | | (538.314, 38160.7)(539.3175, 10844.56)(540.324, 3184.95)(541.3287, 603.44)(542.3296, 91.19) (538.3145, 33004.1)(539.3179, 8813.05)(540.3217, 18930.29)(541.3251, 3317.2)(542.329, 522.27) (562.3503, 6874.04)(563.3534, 2141.53)(564.3643, 1932.0)(540.3659, 5378.41)(541.369, 1677.98)(542.3728, 312.7) (539.2493, 10108.05)(540.2525, 2969.57)(541.2554, 882.81)(542.2555, 186.6) (541.275, 6258.53)(542.2787, 1924.48)(543.2811, 522.34)(544.2778, 98.43) (1083.6344, 1810.76)(1084.6335, | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_550_417a11_0225315 | Rp | + | 550.4170 | 11.02 | | | | (1139.7617, 1209.08)(573.4069, 10675.19)(574.3987, 2255.55)(575.4102, 13377.23)(576.406, 5374.66)(577.4094, 9690.87)(551.4467, 102.62)(552.4496, 69.59)(553.457, 987.06)(551.5047, 20581.54)(552.508, 8122.08)(553.5084, 1568.05)(554.5122, 205.64) | 152980.5 | 107083 | 126811.3 | 85479.7 | 160336.6 | 58927.91 | 153027.9 | 65610.92 | 0.51 | 0.67355 | 0.128131 | 0.19 | 0.56486 | 0.785799 |
| COMPOUND_550_4976a14_295705 | Rp | + | 550.4976 | 14.30 | DG 16:0/16:0 | 1 | 10eV: 551.5036(100), 81.0666(7), 406.9026(2) | | 37809.31 | 19121.75 | 39795.5 | 25270.93 | 38435.5 | 13255.13 | 74553.07 | 47084.84 | 0.40 | 0.106354 | 0.171691 | 0.51 | 0.085065 | 0.346484 |
| COMPOUND_551_2798a12_528823 | Rp | - | 551.2798 | 12.53 | | | | (586.2409, 406.56)(587.224, 29.5)(588.2559, 538.47)(550.2731, 2476.53)(551.2751, 854.64)(552.2664, 30676.07) | 136355.7 | 15262.07 | 141275.3 | 13688.56 | 139355.6 | 16727.02 | 131179.1 | 14935.95 | 0.23 | 0.417873 | 0.522806 | -0.87 | 0.011953 | 0.168863 |
| COMPOUND_551_3224a8_9443245 | Rp | + | 551.3224 | 8.94 | | | | (1103.7042, 89.17)(574.3126, 3473.62)(575.316, 1169.26)(576.3283, 1735.52)(552.3307, 26860.33)(553.3336, 8072.81)(554.3364, 1736.9)(555.3387, 279.76) | 54570.7 | 46490.46 | 66469.11 | 55127.66 | 48406.67 | 22458.93 | 44884.22 | 15688.25 | -1.11 | 2.17E-07 | 1.26E-06 | -0.35 | 0.129181 | 0.425745 |
| COMPOUND_551_3229a11_386341 | Hilic | + | 551.3229 | 1.39 | | | | (574.3136, 10288.03)(575.3172, 3312.77)(576.3298, 10322.82)(577.3324, 3136.49)(552.33, 7232.06)(553.3329, 2309.22)(554.3453, 3936.33)(555.349, 1301.27)(556.3589, 1289.57) | 93638.57 | 99331.2 | 110998 | 77691.33 | 66633.75 | 47727.43 | 65858.18 | 37411.47 | -1.07 | 7.6E-07 | 3.91E-06 | -0.40 | 0.085157 | 0.346484 |
| COMPOUND_552_134a8_21079 | Rp | - | 552.1340 | 8.21 | | | | (551.1275, 4649.25)(552.1287, 1083.09)(553.1274, 260.78)(554.1357, 57.09) | 14119.49 | 1720.003 | 14611.69 | 1682.277 | 14630.07 | 1382.337 | 14694.74 | 1338.976 | 0.34 | 0.245265 | 0.340319 | -0.23 | 0.505359 | 0.754687 |
| COMPOUND_552_3546a13_408602 | Rp | + | 552.3546 | 13.41 | | | | (564.3585, 272.88)(564.8505, 146.11)(565.355, 227.12)(1127.6923, 155.73)(1128.6888, 190.34)(1129.717, 130.28)(553.372, 30846.66)(554.3754, 10281.57)(555.3717, 5088.5)(556.3716, 720.18)(1122.7103, 371.54)(1123.6936, 571.06)(1124.7002, 440.62)(277.1854, 6360.54)(277.6872, 2091.87)(278.1847, 975.65)(278.686, 222.66) | 387531.4 | 35312.32 | 397485.8 | 38232.79 | 411212.9 | 21732.68 | 401032.4 | 34117.63 | 0.70 | 0.021072 | 0.041336 | -0.47 | 0.191383 | 0.505089 |
| COMPOUND_552_7225a10_183379 | Rp | + | 552.7225 | 10.18 | | | | (553.7304, 14554.48)(554.7355, 2637.27)(555.717, 2870.93)(556.712, 429.91)(557.7295, 1252.9) | 70616.06 | 30393.94 | 58892.95 | 28526.39 | 72544.54 | 16029.45 | 76515.42 | 19893.54 | 0.08 | 0.772242 | 0.833547 | 0.77 | 0.025671 | 0.221494 |
| COMPOUND_553_0545a10_183234 | Rp | + | 553.0545 | 10.18 | | | | (576.0422, 715.15)(577.0335, 293.0)(554.0644, 6094.07)(555.0663, 462.06)(556.0474, 796.41)(557.0333, 82.27)(558.0583, 495.16)(1124.1644, 224.29) | 55758.1 | 22979.86 | 45808.4 | 22395.11 | 58586.08 | 12728.96 | 58942.96 | 16647.27 | 0.14 | 0.623081 | 0.714806 | 0.64 | 0.061096 | 0.302474 |
| COMPOUND_553_3272a10_105649 | Rp | - | 553.3272 | 10.11 | | | | (1141.6102, 1710.16)(1142.6088, 1035.21)(1143.6086, 1317.11)(1144.6123, 775.2)(666.3182, 507.49)(667.3211, 168.73)(1151.6497, 10139.19)(1152.6517, 6053.73)(1153.654, 2746.6)(1154.6517, 703.5)(552.3131, 3838.8)(553.317, 1138.64)(554.301, 41585.28)(1107.6625, 73042.99)(1108.6658, 44663.05) | 469128.1 | 99875.78 | 482884.7 | 83311.55 | 280693.5 | 52910.05 | 273030 | 17136.03 | -1.39 | 1.39E-09 | 1.46E-08 | -0.20 | 0.383476 | 0.686377 |
| COMPOUND_553_3369a10_175268 | Rp | - | 553.3369 | 10.18 | | | | (552.3299, 21650.23)(553.3329, 6443.04)(554.3376, 817.82) | 120763.4 | 27323.32 | 126958.9 | 29957.57 | 75283.57 | 15846.13 | 78796.59 | 24262.18 | -1.21 | 4.69E-07 | 2.56E-06 | 0.11 | 0.671643 | 0.847836 |
| COMPOUND_553_3376a10_353978 | Rp | - | 553.3376 | 10.35 | | | | (1151.6593, 53.36)(1152.7067, 58.61)(1153.6641, 1964.7)(552.3297, 3749.07)(553.3335, 1092.59)(554.3452, 21620.26)(555.3486, 6030.78)(598.3517, 363.83)(599.3423, 216.05) | 107592.1 | 19318.16 | 135623.7 | 87110.67 | 55475.5 | 13982.77 | 52945.19 | 13112.86 | -0.75 | 0.001041 | 0.002704 | -0.16 | 0.542035 | 0.767977 |
| COMPOUND_553_3725a10_618265 | Rp | - | 553.3725 | 10.62 | LPC O-18:1 | 1 | 20 eV: 492.3455(100), 44.9972(12), 168.0433(6) | (1141.7274, 490.06)(1142.7346, 237.09)(1143.7186, 1560.17)(666.3254, 1354.05)(588.3452, 910.3)(552.3664, 123964.84)(553.3696, 37666.96)(554.3691, 8022.92)(555.3659, 1721.81)(556.3557, 233.53)(1105.7545, 235.17)(1106.7579, 597.43)(598.37, 511.27)(599.3566, 778.64)(600.3687, 383.57)(577.3322, 1069.26)(578.3397, 742.44)(579.4016, 870.44)(593.356, 180.19)(594.3502, 129.83)(572.4376, 22120.68)(573.4387, 7155.16)(574.4391, 1760.57)(575.4441, 295.92)(555.4014, 2799.49)(556.4122, 1048.87)(557.4069, 331.89) | 521369.6 | 119190.3 | 533800.1 | 136735.5 | 222476 | 163736.6 | 186192.8 | 120839 | -1.25 | 1.44E-07 | 8.77E-07 | -0.25 | 0.311576 | 0.617667 |
| COMPOUND_554_4033a9_407668 | Rp | + | 554.4033 | 9.41 | | | | (577.3322, 1069.26)(578.3397, 742.44)(579.4016, 870.44)(593.356, 180.19)(594.3502, 129.83)(572.4376, 22120.68)(573.4387, 7155.16)(574.4391, 1760.57)(575.4441, 295.92)(555.4014, 2799.49)(556.4122, 1048.87)(557.4069, 331.89) | 204149.1 | 48106.26 | 181034.2 | 30474.77 | 221965.4 | 39450.25 | 219320.6 | 56041.62 | 0.27 | 0.330879 | 0.438821 | 0.54 | 0.114104 | 0.400254 |
| COMPOUND_555_2723a12_528823 | Rp | - | 555.2723 | 12.53 | | | | (554.2647, 10370.52)(555.267, 3352.24)(556.2682, 160.22) | 62754.15 | 6482.957 | 64105.09 | 5927.455 | 62783.43 | 8515.524 | 59506.07 | 7001.292 | -0.02 | 0.938928 | 0.960248 | -0.59 | 0.077834 | 0.333235 |
| COMPOUND_555_308a10_004767 | Rp | - | 555.3080 | 10.00 | | | | (1145.6086, 2133.07)(1146.6129, 1431.2)(1155.5892, 721.48)(1156.5912, 550.73)(1157.581, 746.09)(1158.5782, 753.38)(1159.574, 920.32)(554.3011, 17699.47)(555.305, 5563.43)(556.2997, 6887.97)(557.3099, 2792.12)(558.3113, 694.09)(559.3215, 165.53)(560.3201, 38.68)(1145.6459, 3651.59)(1146.6496, 1159.56)(668.3072, 1252.87)(1155.6796, 7035.19)(554.3458, 150733.58)(555.3489, 42390.2)(556.3491, 9816.44)(1109.6846, 748.66)(1110.6777, 319.38)(668.3245, 1241.56)(554.3456, 149046.23)(555.3488, 42237.11)(1109.6812, 1900.78)(1110.6794, 1122.36) | 819694.64 | 27751.94 | 89595.28 | 23285.03 | 87171.67 | 62498.78 | 77567.08 | 67471.31 | -0.70 | 0.014923 | 0.03044 | -0.17 | 0.062667 | 0.809307 |
| COMPOUND_555_3523a10_480261 | Rp | - | 555.3523 | 10.48 | LPC 17:0 | 2 | 20 eV: 269.2476(100), 44.9978(8), 78.9592(6) | (554.3458, 150733.58)(555.3489, 42390.2)(556.3491, 9816.44)(1109.6846, 748.66)(1110.6777, 319.38)(668.3245, 1241.56)(554.3456, 149046.23)(555.3488, 42237.11)(1109.6812, 1900.78)(1110.6794, 1122.36) | 759503.3 | 158041.6 | 738170.8 | 156488.7 | 371506.3 | 163080.8 | 339797.1 | 118383.5 | -1.58 | 8.15E-11 | 1.28E-09 | 0.08 | 0.728385 | 0.883795 |
| COMPOUND_555_3525a10_392928 | Rp | - | 555.3525 | 10.39 | | | | (668.3245, 1241.56)(554.3456, 149046.23)(555.3488, 42237.11)(1109.6812, 1900.78)(1110.6794, 1122.36) | 209292.8 | 147598.9 | 186407.2 | 154889.6 | 135524.1 | 50195.82 | 138591.4 | 54332.39 | -0.32 | 0.247958 | 0.343209 | -0.02 | 0.944853 | 0.974642 |
| COMPOUND_555_3886a10_904344 | Rp | - | 555.3886 | 10.90 | | | | (668.3533, 311.47)(554.3817, 23214.23)(555.3851, 7320.38)(556.3881, 1521.41)(557.3887, 287.61)(1109.7821, 881.97)(1110.794, 3868.43)(1111.7977, 2727.95) | 191635.2 | 44807.01 | 201368.4 | 60211.55 | 64963.83 | 54157.07 | 47117 | 35688.21 | -1.48 | 2.07E-11 | 4.66E-10 | -0.16 | 0.448269 | 0.721588 |
| COMPOUND_555_4868a12_667192 | Rp | + | 555.4868 | 12.67 | | | | (1149.935, 196.34)(1150.9408, 360.92)(1151.9482, 307.21)(556.495, 19671.57)(557.4985, 29605.43) | 19691.59 | 29661.7 | 18982.7 | 25039 | 9888.632 | 44588 | 28355.58 | 0.05 | 0.838029 | 0.886862 | 0.66 | 0.042626 | 0.268638 | |
| COMPOUND_557_2245a12_524318 | Rp | - | 557.2245 | 12.52 | | | | (556.2168, 18490.56)(557.2204, 6027.15)(558.2148, 11503.26)(559.2172, 3889.61)(560.2139, 2398.29)(561.2155, 944.8)(562.2164, 212.97) | 166695.9 | 43503.42 | 148548.5 | 35199.11 | 148133.8 | 34080.87 | 131598 | 38857.5 | -0.42 | 0.117725 | 0.187521 | -0.04 | 0.885909 | 0.952737 |
| COMPOUND_557_2831a10_034626 | Rp | - | 557.2831 | 10.03 | | | | (1115.5925, 1675.2)(580.267, 2375.93)(581.2428, 2463.77)(577.2672, 2461.09)(577.7512, 159000.2) | 124149.3 | 142937.2 | 106520 | 234929.7 | 166586.6 | 208498.8 | 192116.7 | 0.08 | 0.789623 | 0.84749 | -0.09 | 0.787397 | 0.909997 | |
| COMPOUND_557_2881a10_104622 | Rp | + | 557.2881 | 10.11 | | | | (1115.6082, 3210.68)(580.2683, 560.91)(581.2785, 13935.37)(577.2686, 2379.33)(577.7519, 2056.26)(578.2625, 2854.49)(1137.572, 1776.01)(1138.5819, 1735.89)(1139.5864, 3370.87)(1132.5732, 2541.88)(580.2912, 6099.23)(580.7874, 612.97)(581.2798, 15087.82)(569.2583, 678.98)(569.7747, 639.66)(588.2417, 3606.99)(588.7628, 1614.47)(589.2722, 1415.8)(589.7709, 678.79)(589.2957, 9959.88)(588.7971, 9271.57)(589.2997, 17485.37)(589.8006, 7563.53)(560.3015, 6985.16)(560.8037, 3393.27)(561.3012, 2958.17)(301.6354, 1923.7)(302.1423, 924.21)(302.6335, 337.09)(596.2637, 14528.67)(596.758, 1337.08)(597.2638, 5019.4)(596.2644, 12651.13)(575.3112, 2013.42)(558.295, 9001.48)(575.3093, 1409.74)(575.7997, 1046.87)(576.3205, 1548.28)(279.6485, 2194.39)(280.1518, 5226.93)(280.6518, 1077.63)(281.148, 220.41) | 355977.6 | 239795.1 | 274304.6 | 123459.2 | 326199.3 | 225485.4 | 311383.6 | 206974.2 | -0.69 | 0.015753 | 0.032018 | 0.27 | 0.418434 | 0.69956 |
| COMPOUND_557_3319a9_889187 | Rp | - | 557.3319 | 9.89 | | | | (556.3251, 30508.36)(557.3279, 8619.79)(558.3316, 1827.03)(559.333, 394.68) | 77353.17 | 17518.59 | 73427.26 | 23472.5 | 35472.93 | 8203.208 | 38499.05 | 16583.12 | -1.57 | 5.84E-11 | 1E-09 | 0.22 | 0.33492 | 0.63958 |
| COMPOUND_557_3319a8_742867 | Rp | - | 557.3319 | 8.74 | | | | (556.3249, 34999.91)(557.3282, 9608.62)(558.3304, 2085.69)(559.3341, 321.58) | 93189.09 | 29562.54 | 95353.13 | 35604.3 | 40125 | 12768.22 | 39941.87 | 14449.62 | -1.42 | 6.69E-11 | 1.1E-09 | -0.16 | 0.441887 | 0.717469 |
| COMPOUND_557_3954a10_311741 | Rp | + | 557.3954 | 10.31 | | | | (1153.7433, 326.62)(596.3838, 2692.46)(598.4001, 8723.4)(599.4014, 1831.56)(560.3901, 1857.34)(561.3951, 329.23)(562.3947, 1562.99) | 49505.86 | 16233.78 | 45321.84 | 20480.29 | 67797 | 22630.84 | 65199.77 | 28219.41 | -0.03</ | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--------------|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_558_4636a11_643689 | Rp | - | 558.4636 | 11.64 | no mms | | | (593.412, 82.93)(557.4563, 20682.40)(558.4597, 8405.4)(559.4637, 1784.9)(560.4666, 314.81) (1119.6008, 967.01)(579.2767, 2743.01)(579.7901, 653.19)(580.2869, 5517.12)(580.7897, 46725.01) 104810.9 479986.6 105431.7 322883 48197.92 327483.8 61904.4 359.53)(581.2799, 11112.36)(581.7978, 164.32)(582.2813, 4284.13)(582.2819, 1957.23)(583.2908, 934.93)(584.2793, 1443.89)(571.2995, 645.29)(571.7927, 889.01)(572.293, 897.54)(572.7873, 502.2)(573.2764, 359.05)(1141.5992, 1226.18)(1142.5973, 1081.39)(1143.6165, 2673.41)(1144.6215, 1768.41)(1145.6025, 1256.97)(1146.6077, 769.57)(1147.5983, 789.43)(590.2676, 1365.01)(590.7845, 1327.26)(591.2604, 2904.33)(591.7523, 1405.11)(592.2659, 2950.83)(560.3115, 5612.58)(561.3123, 2169.99)(562.3158, 6546.32)(563.3159, 4169.46)(280.6571, 18887.84)(281.1584, 5650.97)(281.6592, 1195.84)(282.1545, 274.93) | 154479.2 | 62708.28 | 176010.8 | 75184.89 | 213958.6 | 102257.5 | 134807.9 | 66641.39 | 0.66 | 0.016577 | 0.033451 | -1.27 | 0.000145 | 0.017228 |
| COMPOUND_559_2975a10_365007 | Rp | + | 559.2975 | 10.37 | | | | (1119.623, 890.58)(1120.6129, 947.59)(1121.622, 962.57)(1122.6295, 902.67)(1123.6394, 1142.02)(1141.6161, 439.44)(1142.6118, 458.29)(1143.5936, 850.28)(1144.5898, 1026.87)(1145.6182, 794.76)(560.3114, 6698.54)(561.314, 2115.56)(562.3272, 8998.58)(563.3312, 2727.22)(564.3149, 2703.81) (582.3175, 6507.34)(583.3212, 2033.48)(577.3359, 320.33)(560.335, 27512.37)(561.3384, 161360.7) 93561.59 192053.3 110459.1 103738.7 100935.7 138980 107604.5 8593.63)(562.3496, 12118.33)(563.3538, 3646.01)(564.3634, 2601.68)(565.3691, 772.65)(566.3801, 1300.97) (1153.6407, 353.04)(1154.6367, 370.36)(1155.6493, 315.35)(1163.6559, 1015.67)(1164.6569, 780.78)(1165.6504, 455.38)(558.3323, 21197.61)(559.3349, 6640.03)(560.3308, 8082.93)(561.3338, 2132.23)(562.3327, 439.82)(563.3341, 137.09)(604.357, 483.32)(1231.6364, 374.36)(1232.66, 365.8)(1233.6436, 273.21) (1153.6475, 763.05)(1154.6384, 353.36)(1155.6367, 381.32)(1156.6414, 274.38)(1157.6509, 621.02)(1158.6672, 318.56)(568.3324, 36189.23)(559.3355, 10675.7)(560.3306, 12775.75)(561.3333, 3547.09)(562.3361, 831.64)(563.3389, 145.29)(564.3315, 831.08) (560.3007, 4817.84)(561.3044, 1626.55)(562.2953, 7531.38)(606.3173, 684.31)(607.3208, 426.98)(608.323, 226.15) (1123.6394, 1146.22)(1124.6439, 739.49)(1125.6543, 1254.54)(1126.6619, 919.04)(1127.6613, 972.0)(584.3077, 1325.7)(585.3065, 307.19)(586.286, 1731.33)(1145.6332, 578.37)(1146.6484, 501.76)(1147.6405, 714.72)(1148.6196, 634.22)(1149.642, 636.08)(562.3275, 9122.47)(563.3316, 2735.17)(564.3318, 4426.82)(565.3126, 1472.6) (1123.6538, 1315.14)(1124.6443, 761.79)(1125.6603, 1125.76)(1126.6562, 681.26)(1127.6661, 1245.87)(584.3088, 1229.48)(585.3126, 257.88)(586.3112, 612.19)(1145.6305, 434.99)(1146.6625, 193.01)(1147.6403, 549.19)(1148.6425, 572.77)(1149.642, 560.63)(579.3368, 130.96)(562.3276, 4753.54)(563.3305, 1295.27)(564.3097, 2635.37)(565.3128, 1033.42) (1123.6427, 100.08)(584.3359, 4596.34)(585.3398, 1735.62)(586.3523, 1886.42)(587.3581, 666.69)(588.3478, 160.64)(579.3557, 1138.05)(562.3512, 13427.76)(563.3558, 4018.63)(564.3641, 1048.01) (584.4084, 315.22)(585.4045, 146.79)(586.4192, 298.58)(1145.8073, 569.77)(562.4232, 2169.88)(563.4264, 666.83)(564.4363, 889.69)(565.4352, 382.55)(566.4273, 1263.13) (584.4199, 499.97)(562.4232, 11223.75)(563.4272, 4091.06)(564.4391, 41950.18)(565.4426, 13856.24) (562.5197, 21967.05)(563.5229, 8675.02)(564.527, 2009.88)(565.528, 377.77) (1163.0828, 285.28)(585.0661, 440.13)(563.073, 6249.6)(564.0767, 1334.67)(565.0557, 1383.8)(566.0648, 301.76)(567.0703, 681.02) (675.3918, 908.31)(597.3328, 121.73)(598.344, 38.53)(599.3159, 820.12)(561.3787, 16870.88)(562.3621, 6455.56)(563.3848, 1452.44)(564.3875, 194.27)(607.3999, 1204.22) | 161360.7 | 93561.59 | 192053.3 | 110459.1 | 103738.7 | 100935.7 | 138980 | 107604.5 | -0.96 | 2.97E-05 | 0.000105 | -0.37 | 0.147901 | 0.456493 |
| COMPOUND_559_3051a1_1042868 | Hilic | + | 559.3051 | 1.10 | | | | (1119.623, 890.58)(1120.6129, 947.59)(1121.622, 962.57)(1122.6295, 902.67)(1123.6394, 1142.02)(1141.6161, 439.44)(1142.6118, 458.29)(1143.5936, 850.28)(1144.5898, 1026.87)(1145.6182, 794.76)(560.3114, 6698.54)(561.314, 2115.56)(562.3272, 8998.58)(563.3312, 2727.22)(564.3149, 2703.81) (582.3175, 6507.34)(583.3212, 2033.48)(577.3359, 320.33)(560.335, 27512.37)(561.3384, 161360.7) 93561.59 192053.3 110459.1 103738.7 100935.7 138980 107604.5 8593.63)(562.3496, 12118.33)(563.3538, 3646.01)(564.3634, 2601.68)(565.3691, 772.65)(566.3801, 1300.97) (1153.6407, 353.04)(1154.6367, 370.36)(1155.6493, 315.35)(1163.6559, 1015.67)(1164.6569, 780.78)(1165.6504, 455.38)(558.3323, 21197.61)(559.3349, 6640.03)(560.3308, 8082.93)(561.3338, 2132.23)(562.3327, 439.82)(563.3341, 137.09)(604.357, 483.32)(1231.6364, 374.36)(1232.66, 365.8)(1233.6436, 273.21) (1153.6475, 763.05)(1154.6384, 353.36)(1155.6367, 381.32)(1156.6414, 274.38)(1157.6509, 621.02)(1158.6672, 318.56)(568.3324, 36189.23)(559.3355, 10675.7)(560.3306, 12775.75)(561.3333, 3547.09)(562.3361, 831.64)(563.3389, 145.29)(564.3315, 831.08) (560.3007, 4817.84)(561.3044, 1626.55)(562.2953, 7531.38)(606.3173, 684.31)(607.3208, 426.98)(608.323, 226.15) (1123.6394, 1146.22)(1124.6439, 739.49)(1125.6543, 1254.54)(1126.6619, 919.04)(1127.6613, 972.0)(584.3077, 1325.7)(585.3065, 307.19)(586.286, 1731.33)(1145.6332, 578.37)(1146.6484, 501.76)(1147.6405, 714.72)(1148.6196, 634.22)(1149.642, 636.08)(562.3275, 9122.47)(563.3316, 2735.17)(564.3318, 4426.82)(565.3126, 1472.6) (1123.6538, 1315.14)(1124.6443, 761.79)(1125.6603, 1125.76)(1126.6562, 681.26)(1127.6661, 1245.87)(584.3088, 1229.48)(585.3126, 257.88)(586.3112, 612.19)(1145.6305, 434.99)(1146.6625, 193.01)(1147.6403, 549.19)(1148.6425, 572.77)(1149.642, 560.63)(579.3368, 130.96)(562.3276, 4753.54)(563.3305, 1295.27)(564.3097, 2635.37)(565.3128, 1033.42) (1123.6427, 100.08)(584.3359, 4596.34)(585.3398, 1735.62)(586.3523, 1886.42)(587.3581, 666.69)(588.3478, 160.64)(579.3557, 1138.05)(562.3512, 13427.76)(563.3558, 4018.63)(564.3641, 1048.01) (584.4084, 315.22)(585.4045, 146.79)(586.4192, 298.58)(1145.8073, 569.77)(562.4232, 2169.88)(563.4264, 666.83)(564.4363, 889.69)(565.4352, 382.55)(566.4273, 1263.13) (584.4199, 499.97)(562.4232, 11223.75)(563.4272, 4091.06)(564.4391, 41950.18)(565.4426, 13856.24) (562.5197, 21967.05)(563.5229, 8675.02)(564.527, 2009.88)(565.528, 377.77) (1163.0828, 285.28)(585.0661, 440.13)(563.073, 6249.6)(564.0767, 1334.67)(565.0557, 1383.8)(566.0648, 301.76)(567.0703, 681.02) (675.3918, 908.31)(597.3328, 121.73)(598.344, 38.53)(599.3159, 820.12)(561.3787, 16870.88)(562.3621, 6455.56)(563.3848, 1452.44)(564.3875, 194.27)(607.3999, 1204.22) | 107315.7 | 17090.3 | 110407.7 | 17113.6 | 125685.3 | 143344.5 | 125481.4 | 12058.21 | 1.18 | 6.01E-06 | 2.51E-05 | -0.20 | 0.480271 | 0.743153 |
| COMPOUND_559_3272a1_385052 | Hilic | + | 559.3272 | 1.39 | | | | (1119.623, 890.58)(1120.6129, 947.59)(1121.622, 962.57)(1122.6295, 902.67)(1123.6394, 1142.02)(1141.6161, 439.44)(1142.6118, 458.29)(1143.5936, 850.28)(1144.5898, 1026.87)(1145.6182, 794.76)(560.3114, 6698.54)(561.314, 2115.56)(562.3272, 8998.58)(563.3312, 2727.22)(564.3149, 2703.81) (582.3175, 6507.34)(583.3212, 2033.48)(577.3359, 320.33)(560.335, 27512.37)(561.3384, 161360.7) 93561.59 192053.3 110459.1 103738.7 100935.7 138980 107604.5 8593.63)(562.3496, 12118.33)(563.3538, 3646.01)(564.3634, 2601.68)(565.3691, 772.65)(566.3801, 1300.97) (1153.6407, 353.04)(1154.6367, 370.36)(1155.6493, 315.35)(1163.6559, 1015.67)(1164.6569, 780.78)(1165.6504, 455.38)(558.3323, 21197.61)(559.3349, 6640.03)(560.3308, 8082.93)(561.3338, 2132.23)(562.3327, 439.82)(563.3341, 137.09)(604.357, 483.32)(1231.6364, 374.36)(1232.66, 365.8)(1233.6436, 273.21) (1153.6475, 763.05)(1154.6384, 353.36)(1155.6367, 381.32)(1156.6414, 274.38)(1157.6509, 621.02)(1158.6672, 318.56)(568.3324, 36189.23)(559.3355, 10675.7)(560.3306, 12775.75)(561.3333, 3547.09)(562.3361, 831.64)(563.3389, 145.29)(564.3315, 831.08) (560.3007, 4817.84)(561.3044, 1626.55)(562.2953, 7531.38)(606.3173, 684.31)(607.3208, 426.98)(608.323, 226.15) (1123.6394, 1146.22)(1124.6439, 739.49)(1125.6543, 1254.54)(1126.6619, 919.04)(1127.6613, 972.0)(584.3077, 1325.7)(585.3065, 307.19)(586.286, 1731.33)(1145.6332, 578.37)(1146.6484, 501.76)(1147.6405, 714.72)(1148.6196, 634.22)(1149.642, 636.08)(562.3275, 9122.47)(563.3316, 2735.17)(564.3318, 4426.82)(565.3126, 1472.6) (1123.6538, 1315.14)(1124.6443, 761.79)(1125.6603, 1125.76)(1126.6562, 681.26)(1127.6661, 1245.87)(584.3088, 1229.48)(585.3126, 257.88)(586.3112, 612.19)(1145.6305, 434.99)(1146.6625, 193.01)(1147.6403, 549.19)(1148.6425, 572.77)(1149.642, 560.63)(579.3368, 130.96)(562.3276, 4753.54)(563.3305, 1295.27)(564.3097, 2635.37)(565.3128, 1033.42) (1123.6427, 100.08)(584.3359, 4596.34)(585.3398, 1735.62)(586.3523, 1886.42)(587.3581, 666.69)(588.3478, 160.64)(579.3557, 1138.05)(562.3512, 13427.76)(563.3558, 4018.63)(564.3641, 1048.01) (584.4084, 315.22)(585.4045, 146.79)(586.4192, 298.58)(1145.8073, 569.77)(562.4232, 2169.88)(563.4264, 666.83)(564.4363, 889.69)(565.4352, 382.55)(566.4273, 1263.13) (584.4199, 499.97)(562.4232, 11223.75)(563.4272, 4091.06)(564.4391, 41950.18)(565.4426, 13856.24) (562.5197, 21967.05)(563.5229, 8675.02)(564.527, 2009.88)(565.528, 377.77) (1163.0828, 285.28)(585.0661, 440.13)(563.073, 6249.6)(564.0767, 1334.67)(565.0557, 1383.8)(566.0648, 301.76)(567.0703, 681.02) (675.3918, 908.31)(597.3328, 121.73)(598.344, 38.53)(599.3159, 820.12)(561.3787, 16870.88)(562.3621, 6455.56)(563.3848, 1452.44)(564.3875, 194.27)(607.3999, 1204.22) | 161360.7 | 93561.59 | 192053.3 | 110459.1 | 103738.7 | 100935.7 | 138980 | 107604.5 | -0.96 | 2.97E-05 | 0.000105 | -0.37 | 0.147901 | 0.456493 |
| COMPOUND_559_3381a10_560094 | Rp | + | 559.3381 | 10.56 | | | | (1119.623, 890.58)(1120.6129, 947.59)(1121.622, 962.57)(1122.6295, 902.67)(1123.6394, 1142.02)(1141.6161, 439.44)(1142.6118, 458.29)(1143.5936, 850.28)(1144.5898, 1026.87)(1145.6182, 794.76)(560.3114, 6698.54)(561.314, 2115.56)(562.3272, 8998.58)(563.3312, 2727.22)(564.3149, 2703.81) (582.3175, 6507.34)(583.3212, 2033.48)(577.3359, 320.33)(560.335, 27512.37)(561.3384, 161360.7) 93561.59 192053.3 110459.1 103738.7 100935.7 138980 107604.5 8593.63)(562.3496, 12118.33)(563.3538, 3646.01)(564.3634, 2601.68)(565.3691, 772.65)(566.3801, 1300.97) (1153.6407, 353.04)(1154.6367, 370.36)(1155.6493, 315.35)(1163.6559, 1015.67)(1164.6569, 780.78)(1165.6504, 455.38)(558.3323, 21197.61)(559.3349, 6640.03)(560.3308, 8082.93)(561.3338, 2132.23)(562.3327, 439.82)(563.3341, 137.09)(604.357, 483.32)(1231.6364, 374.36)(1232.66, 365.8)(1233.6436, 273.21) (1153.6475, 763.05)(1154.6384, 353.36)(1155.6367, 381.32)(1156.6414, 274.38)(1157.6509, 621.02)(1158.6672, 318.56)(568.3324, 36189.23)(559.3355, 10675.7)(560.3306, 12775.75)(561.3333, 3547.09)(562.3361, 831.64)(563.3389, 145.29)(564.3315, 831.08) (560.3007, 4817.84)(561.3044, 1626.55)(562.2953, 7531.38)(606.3173, 684.31)(607.3208, 426.98)(608.323, 226.15) (1123.6394, 1146.22)(1124.6439, 739.49)(1125.6543, 1254.54)(1126.6619, 919.04)(1127.6613, 972.0)(584.3077, 1325.7)(585.3065, 307.19)(586.286, 1731.33)(1145.6332, 578.37)(1146.6484, 501.76)(1147.6405, 714.72)(1148.6196, 634.22)(1149.642, 636.08)(562.3275, 9122.47)(563.3316, 2735.17)(564.3318, 4426.82)(565.3126, 1472.6) (1123.6538, 1315.14)(1124.6443, 761.79)(1125.6603, 1125.76)(1126.6562, 681.26)(1127.6661, 1245.87)(584.3088, 1229.48)(585.3126, 257.88)(586.3112, 612.19)(1145.6305, 434.99)(1146.6625, 193.01)(1147.6403, 549.19)(1148.6425, 572.77)(1149.642, 560.63)(579.3368, 130.96)(562.3276, 4753.54)(563.3305, 1295.27)(564.3097, 2635.37)(565.3128, 1033.42) (1123.6427, 100.08)(584.3359, 4596.34)(585.3398, 1735.62)(586.3523, 1886.42)(587.3581, 666.69)(588.3478, 160.64)(579.3557, 1138.05)(562.3512, 13427.76)(563.3558, 4018.63)(564.3641, 1048.01) (584.4084, 315.22)(585.4045, 146.79)(586.4192, 298.58)(1145.8073, 569.77)(562.4232, 2169.88)(563.4264, 666.83)(564.4363, 889.69)(565.4352, 382.55)(566.4273, 1263.13) (584.4199, 499.97)(562.4232, 11223.75)(563.4272, 4091.06)(564.4391, 41950.18)(565.4426, 13856.24) (562.5197, 21967.05)(563.5229, 8675.02)(564.52 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | | | |
|------------------------------|--------|----------|----------------|----------------|----------|--------------|--|--|----------|---------------|-----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|----------|----------|----------|
| | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p | | | |
| | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | | | |
| COMPOUND_567_3324a10_0725617 | Hilic | + | 567.3324 | 1.07 | | | (1135.669, 3492.85) (1136.666, 2116.93) (1137.667, 2283.52) (1138.685, 1040.2) (1139.691, 969.5) (1140.705, 524.24) (1141.710, 316.67) (590.322, 915.96) (591.325, 2738.72) (592.326, 3473.34) (593.329, 1075.84) (157.612, 830.16) (158.605, 932.64) (159.602, 502.31) (160.622, 463.91) (585.3749, 2062.6.1) (586.378, 7234.58) (588.34, 420406.4) (589.348, 133996.77) (570.355, 142940.64) (571.3587, 43331.82) (572.3701, 41699.74) (1135.633, 1207.27) (590.3111, 1194.21) (591.3174, 1724.8) (592.3242, 674.56) (593.3321, 23430.1) 61874.45 235731.7 63585.83 140135.3 52363.72 149806.6 55732.03 -1.31 4.18E-07 2.33E-06 0.11 0.698489 0.862515 | 2344067 | 573313.6 | 2266273 | 591252.2 | 1306386 | 467429.1 | 1512970 | 607553.1 | -1.45 | 2.58E-08 | 1.89E-07 | 0.39 | 0.144435 | 0.451201 | | | |
| COMPOUND_567_3331a10_9777065 | Hilic | + | 567.3331 | 0.98 | | | (1135.669, 2564.16) (1136.6741, 1704.3) (1137.6636, 765.45) (1138.679, 378.09) (1173.5846, 577.48) (1174.5767, 832.93) (1175.553, 911.72) (590.3237, 13389.17) (591.3256, 4607.9) (592.3275, 961.96) (593.3455, 179.49) (1157.5702, 641.84) (1158.5865, 731.05) (1159.5782, 774.97) (1160.5789, 886.21) (568.3421, 349818.9) (569.3456, 109262.1) (570.3491, 25282.9) (571.3516, 3995.25) (1152.6687, 116.29) 1701706 446812.5 1523642 380324.1 908003.4 331576.4 1104965 471984.9 -1.50 1.89E-08 1.46E-07 0.65 0.019106 0.196411 | 428227.2 | 460496.7 | 687554.4 | 674013.3 | 367484.1 | 494280.1 | 291431.1 | 351334.2 | -0.91 | 0.001168 | 0.002997 | -0.12 | 0.699358 | 0.862515 | | | |
| COMPOUND_567_334a10_019982 | Rp | + | 567.3340 | 10.02 | | | (1135.669, 8036.09) (1136.6732, 5074.87) (1137.6752, 2215.89) (1138.6825, 618.82) (1173.5849, 493.23) (1174.5843, 1367.34) (1175.5479, 900.27) (590.3235, 24510.55) (591.3259, 8407.89) (592.3276, 1917.66) (593.334, 269.93) (1157.6025, 816.58) (1158.5958, 503.33) (1159.5897, 848.47) (1160.5764, 943.38) (568.3415, 308729.25) (569.3446, 97691.52) (570.3483, 21611.92) (571.3496, 3855.51) (572.3433, 673.41) (1152.6909, 207.82) 1701706 446812.5 1523642 380324.1 908003.4 331576.4 1104965 471984.9 -1.50 1.89E-08 1.46E-07 0.65 0.019106 0.196411 | 1701706 | 446812.5 | 1523642 | 380324.1 | 908003.4 | 331576.4 | 1104965 | 471984.9 | -1.50 | 1.89E-08 | 1.46E-07 | 0.65 | 0.019106 | 0.196411 | | | |
| COMPOUND_567_3353a10_088961 | Rp | + | 567.3353 | 10.09 | LPC 22:6 | 2 | 10eV: 568.3422(100), 104.1069(14), 184.0732(8), 311.2021(2) | (566.3452, 812793.1) (567.3492, 231045.34) (568.3517, 48095.76) (569.3544, 7251.78) (570.3586, 925.6) (612.3477, 2963.12) (613.3544, 1547.8) (1133.6906, 303.53) (1134.6779, 149.56) (1135.6831, 263.14) (1247.6469, 145.82) (1248.6647, 182.68) 1701706 446812.5 1523642 380324.1 908003.4 331576.4 1104965 471984.9 -1.50 1.89E-08 1.46E-07 0.65 0.019106 0.196411 | 8708403 | 1155285 | 8983571 | 1248465 | 5615457 | 832310.2 | 5891769 | 1114914 | -1.65 | 1.82E-13 | 1.28E-11 | 0.05 | 0.798141 | 0.913784 | | |
| COMPOUND_567_3523a10_376442 | Rp | - | 567.3523 | 10.38 | LPC 18:1 | 2 | 20 eV: 506.3236(100), 281.2477(75), 44.998(5), 168.041(3) | (566.3452, 685216.7) (567.3492, 195864.38) (568.3521, 38956.48) (569.3549, 6204.62) (570.3571, 991.6) (1133.6906, 370.45) (1134.6908, 163.0) (1135.6938, 835.1) (1136.6968, 626.5) (1137.7042, 350.28) (612.3298, 1735.83) (613.3341, 570.98) (1248.6956, 153.66) 432419.9 59709.5 831411.2 1881389 304078.4 36971.98 307969.3 48743.76 -1.55 4.44E-11 8.19E-10 0.04 0.857648 0.940019 | 432419.9 | 59709.5 | 831411.2 | 1881389 | 304078.4 | 36971.98 | 307969.3 | 48743.76 | -1.55 | 4.44E-11 | 8.19E-10 | 0.04 | 0.857648 | 0.940019 | | |
| COMPOUND_567_3524a10_27714 | Rp | - | 567.3524 | 10.28 | | | (566.3452, 685216.7) (567.3492, 195864.38) (568.3521, 38956.48) (569.3549, 6204.62) (570.3571, 991.6) (1133.6906, 370.45) (1134.6908, 163.0) (1135.6938, 835.1) (1136.6968, 626.5) (1137.7042, 350.28) (612.3298, 1735.83) (613.3341, 570.98) (1248.6956, 153.66) 432419.9 59709.5 831411.2 1881389 304078.4 36971.98 307969.3 48743.76 -1.55 4.44E-11 8.19E-10 0.04 0.857648 0.940019 | 432419.9 | 59709.5 | 831411.2 | 1881389 | 304078.4 | 36971.98 | 307969.3 | 48743.76 | -1.55 | 4.44E-11 | 8.19E-10 | 0.04 | 0.857648 | 0.940019 | | | |
| COMPOUND_567_4207a11_505867 | Rp | + | 567.4207 | 11.51 | | | (1173.794, 454.33) (1174.7769, 1454.12) (1175.7762, 1401.7) (1157.8789, 29.45) (1158.8417, 275.24) (585.4542, 1062.78) (568.429, 23271.97) (569.4319, 11263.9) (570.4347, 2814.59) (571.4294, 575.71) 570259.2 28398.73 53375.76 31210.84 123902.1 34276.39 103786.2 46986.94 1.30 1.88E-07 1.11E-06 -0.12 0.650196 0.838541 | 570259.2 | 28398.73 | 53375.76 | 31210.84 | 123902.1 | 34276.39 | 103786.2 | 46986.94 | 1.30 | 1.88E-07 | 1.11E-06 | -0.12 | 0.650196 | 0.838541 | | | |
| COMPOUND_567_4213a11_512313 | Rp | + | 567.4213 | 11.51 | | | (1173.7972, 489.53) (1174.7759, 1431.59) (1175.7762, 1404.25) (1157.8748, 304.55) (1158.856, 339.77) (585.4495, 472.36) (568.4288, 16106.9) (569.4325, 7321.55) (570.4364, 2215.58) (571.4502, 432.55) 53737.43 25163.06 49363.9 27766.14 114554.1 56425.76 94714.46 50075.26 1.18 3.41E-06 1.5E-05 -0.12 0.670227 0.846999 | 53737.43 | 25163.06 | 49363.9 | 27766.14 | 114554.1 | 56425.76 | 94714.46 | 50075.26 | 1.18 | 3.41E-06 | 1.5E-05 | -0.12 | 0.670227 | 0.846999 | | | |
| COMPOUND_567_4214a11_04483 | Rp | + | 567.4214 | 11.04 | | | (1173.7971, 306.97) (1174.774, 1265.09) (1175.7882, 1341.29) (590.4196, 5732.92) (606.3748, 664.04) (568.4288, 255825.66) (569.4319, 114242.6) (570.433, 26189.49) (571.419, 6268.25) 237442.7 85517.38 206235.9 105796.2 264768.9 319182.4 415283.2 332609.6 0.26 0.309356 0.41053 0.34 0.25905 0.570391 | 237442.7 | 85517.38 | 206235.9 | 105796.2 | 264768.9 | 319182.4 | 415283.2 | 332609.6 | 0.26 | 0.309356 | 0.41053 | 0.34 | 0.25905 | 0.570391 | | | |
| COMPOUND_567_4215a11_021897 | Rp | + | 567.4215 | 11.02 | | | (1173.853, 336.4) (1174.8417, 276.64) (1175.838, 182.86) (590.4227, 6127.24) (606.3802, 858.16) (568.4295, 306772.3) (569.4328, 129000.48) (570.4346, 28659.93) (571.4306, 5628.04) 286936.4 125470.3 273274 102504.1 769091.9 376971.8 682111.7 311220.1 1.53 2.19E-12 7.7E-11 -0.23 0.266655 0.575669 | 286936.4 | 125470.3 | 273274 | 102504.1 | 769091.9 | 376971.8 | 682111.7 | 311220.1 | 1.53 | 2.19E-12 | 7.7E-11 | -0.23 | 0.266655 | 0.575669 | | | |
| COMPOUND_569_2493a1_5842978 | Hilic | + | 569.2493 | 1.58 | | | (570.2569, 4862.8) (571.2605, 1464.6) (572.2677, 741.1) (573.2728, 177.79) 22942.02 5243.09 24599.24 8168.333 19431.93 8300.592 23243.26 9712.053 -0.74 0.012396 0.025705 0.53 0.126526 0.423869 | 22942.02 | 5243.09 | 24599.24 | 8168.333 | 19431.93 | 8300.592 | 23243.26 | 9712.053 | -0.74 | 0.012396 | 0.025705 | 0.53 | 0.126526 | 0.423869 | | | |
| COMPOUND_569_2518a12_529054 | Rp | - | 569.2518 | 12.53 | | | (568.2445, 25969.56) (569.2465, 8520.41) (570.2488, 1634.16) (571.2472, 365.09) 126477.6 20197.43 116436.1 19526.67 128724.4 11996.39 123025.1 19874.64 0.21 0.478946 0.581761 0.17 0.631748 0.828008 | 126477.6 | 20197.43 | 116436.1 | 19526.67 | 128724.4 | 11996.39 | 123025.1 | 19874.64 | 0.21 | 0.478946 | 0.581761 | 0.17 | 0.631748 | 0.828008 | | | |
| COMPOUND_569_3493a10_225313 | Rp | + | 569.3493 | 10.23 | LPC 22:5 | 2 | 10 eV: 570.3549(100), 104.1069(17), 303.1917(6) | (1139.7098, 501.45) (1177.6667, 167.48) (592.3391, 6552.65) (593.3419, 2245.11) (594.3475, 718.1) (595.3322, 158.01) (1161.7379, 308.55) (1162.7358, 205.97) (608.2984, 5591.14) (570.3573, 86172.02) (571.3603, 28682.88) (572.3638, 5851.93) (573.3639, 874.6) 259269.1 99749.44 225597.7 95552.17 90823.93 32081.21 125959 55784.05 -1.77 5.96E-13 2.98E-11 0.74 0.001626 0.06002 | 259269.1 | 99749.44 | 225597.7 | 95552.17 | 90823.93 | 32081.21 | 125959 | 55784.05 | -1.77 | 5.96E-13 | 2.98E-11 | 0.74 | 0.001626 | 0.06002 | | |
| COMPOUND_569_3494a10_285902 | Rp | + | 569.3494 | 10.29 | | | (1139.7098, 501.45) (1177.6669, 586.87) (592.3384, 10070.02) (593.3412, 3457.29) (594.3444, 1182.24) (595.3393, 138.22) (1161.7345, 665.15) (1162.7281, 412.19) (608.3413, 1800.21) (570.3573, 46439.5) (571.3604, 15448.08) (572.3596, 1560.02) (573.3549, 277.75) 166835.8 107110.6 162087.4 96645.14 75558.79 33691.45 104660.1 48043.67 -1.15 0.00014 0.000423 0.57 0.098144 0.36878 | 166835.8 | 107110.6 | 162087.4 | 96645.14 | 75558.79 | 33691.45 | 104660.1 | 48043.67 | -1.15 | 0.00014 | 0.000423 | 0.57 | 0.098144 | 0.36878 | | | |
| COMPOUND_569_3681a10_651824 | Rp | - | 569.3681 | 10.65 | LPC 18:0 | 2 | 10 eV: 508.3402(100), 568.3602(90), 283.2646(6), 44.9982(3) | (1183.7605, 759.21) (1184.762, 1387.05) (1185.7592, 1118.74) (568.3609, 817851.56) (569.365, 235295.88) (570.3673, 45687.98) (571.3697, 6984.99) (572.3715, 935.81) (614.3782, 565.77) 9505479 1154325 9723602 1292382 5141346 800222.8 5069928 971432.7 -1.50 1.67E-13 1.25E-11 -0.19 0.29948 0.607594 | 9505479 | 1154325 | 9723602 | 1292382 | 5141346 | 800222.8 | 5069928 | 971432.7 | -1.50 | 1.67E-13 | 1.25E-11 | -0.19 | 0.29948 | 0.607594 | | |
| COMPOUND_569_3686a10_558576 | Rp | - | 569.3686 | 10.56 | | | (1183.7562, 365.96) (1184.7513, 343.63) (1185.7622, 570.55) (1186.7675, 319.47) (1187.7695, 445.96) (568.3611, 422628.9) (569.3648, 120293.59) (570.3673, 25023.74) (571.3705, 3846.7) (572.369, 600.55) (1137.689, 317.15) (614.3631, 876.64) (615.3622, 1230.77) (1251.697, 261.8) (1252.7153, 331.39) (1253.7042, 392.75) 1759625 315060.7 1793996 3422235.6 727350.1 152789.4 728200.2 157510.2 -1.55 5.31E-14 5.69E-12 -0.11 0.558125 0.781981 | 1759625 | 315060.7 | 1793996 | 3422235.6 | 727350.1 | 152789.4 | 728200.2 | 157510.2 | -1.55 | 5.31E-14 | 5.69E-12 | -0.11 | 0.558125 | 0.781981 | | | |
| COMPOUND_570_2051a10_029141 | Rp | + | 570.2051 | 10.03 | | | (588.2224, 441.74) (589.2493, 1020.24) (590.2472, 741.78) (571.2131, 11748.16) (572.2183, 38883.98 12263.18 40601.04 14966.07 20181.86 7521.111 20048.07 7207.608 -1.20 2.93E-08 2.14E-07 -0.23 0.300424 0.60896 | 588.2224 | 441.74 | 589.2493 | 1020.24 | 590.2472 | 741.78 | 571.2131 | 11748.16 | 572.2183 | 38883.98 | 12263.18 | 40601.04 | 14966.07 | 20181.86 | 7521.111 | 20048.07 | 7207.608 |
| COMPOUND_570_2408a10_505557 | Rp | + | 570.2408 | 10.51 | | | (1141.4728, 206.77) (1142.474, 369.1) (1163.4769, 475.81) (571.2505, 9480.98) (572.2557, 1510.67) (573.2505, 4052.41) (1158.5597, 350.94) 37120.8 13354.18 35279.68 11997.72 25665.14 18029.5 21308.52 10281.59 -1.02 1.37E-05 5.33E-05 0.21 0.41737 0.699344 | 37120.8 | 13354.18 | 35279.68 | 11997.72 | 25665.14 | 18029.5 | 21308.52 | 10281.59 | -1.02 | 1.37E-05 | 5.33E-05 | 0.21 | 0.41737 | 0.699344 | | | |
| COMPOUND_571_366a10_434301 | Rp | + | 571.3660 | 10.43 | LPC 22:4 | 2 | 10 eV: 572.3744(100), 104.1071(14), 184.0766(7), 425.3099(5) | (1181.6447, 565.31) (594.3522, 6493.05) (595.3563, 2085.03) (610.3133, 1668.91) (572.3736, 12391.75) (573.3785, 3966.25) (574.3852, 1477.18) (575.3743, 222.88) 139250.2 45881.29 123274.8 46345.77 47881.2 29716.42 80664.48 27236.23 -1.14 1.08E-06 5.33E-06 0.31 0.21104 0.519294 | 139250.2 | 45881.29 | 123274.8 | 46345.77 | 47881.2 | 29716.42 | 80664.48 | 27236.23 | -1.14 | 1.08E-06 | 5.33E-06 | 0.31 | 0.21104 | 0.519294 | | |
| COMPOUND_572_0696a10_300524 | Rp | + | 572.0696 | 10.30 | | | (1183.0765, 236.5) (1167.1234, 396.17) (573.0763, 5164.93) (574.0804, 1077.98) (575.0646, 1201.9) (576.0701, 206.95) (577.0739, 548.08) (1162.1704, 361.22) 42116.98 19039.67 35565.09 | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|---|---|--|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_573_3109a1_0502512 | Hilic | + | 573.3109 | 1.05 | | | | (1147.6154, 652.75)(1148.6316, 493.49)(1149.6426, 519.96)(1150.64, 457.54)(596.3151, 49102.58 10414.87 48757.6 11072.39 77807.15 12764.19 86181.21 12839.69 | 49102.58 | 10414.87 | 48757.6 | 11072.39 | 77807.15 | 12764.19 | 86181.21 | 12839.69 | 1.00 | 3.59E-06 | 1.58E-05 | 0.66 | 0.00644 | 0.125019 | |
| COMPOUND_573_4807a13_921373 | Rp | + | 573.8007 | 13.92 | | | 98.64(1169.5741, 703.85)(574.3176, 9150.05)(575.3205, 2845.86)(576.3165, 1037.49)(577.3234, 157.04)(1164.618, 431.3) | 119038.3 | 38534.4 | 101506.6 | 39215.73 | 120071.8 | 25960.91 | 123825.2 | 32885.77 | -0.08 | 0.76918 | 0.833186 | 0.39 | 0.229155 | 0.535521 | | |
| COMPOUND_574_1353a9_321006 | Rp | - | 574.1353 | 9.32 | | | (1183.2289, 250.88)(1184.213, 80.14)(573.1284, 9138.84)(574.132, 2047.88)(575.1342, 50958.47 15536.13 47981.37 49715.95 | 50958.47 | 15536.13 | 47981.37 | 49715.95 | 49147.93 | 5764.338 | 49619.39 | 2460.262 | 0.06 | 0.837469 | 0.886862 | 0.14 | 0.693199 | 0.85806 | | |
| COMPOUND_574_1356a9_204304 | Rp | - | 574.1356 | 9.20 | | | 341.66(1177.2343, 191.38) | 83712.34 | 8944.078 | 83601 | 7998.938 | 78710 | 9558.823 | 81591.7 | 8859.027 | -0.55 | 0.070555 | 0.119735 | 0.31 | 0.396398 | 0.690408 | | |
| COMPOUND_574_1361a8_940168 | Rp | - | 574.1361 | 8.94 | | | (573.1289, 1632.91)(574.133, 3572.04)(575.1336, 320.35)(576.1204, 48.63) | 262570.7 | 25169.28 | 264084.3 | 17522.47 | 255557.5 | 17158.46 | 253024.4 | 16779.31 | -0.31 | 0.282092 | 0.381545 | -0.30 | 0.389863 | 0.689687 | | |
| COMPOUND_575_271a10_366332 | Rp | + | 575.2710 | 10.37 | | | (687.1254, 374.97)(688.1075, 257.81)(573.1288, 70382.42)(574.132, 13241.31)(575.1351, 1711.39)(576.134, 381.08) | 406294.8 | 52445.93 | 398389 | 55591.1 | 307596.5 | 37472.69 | 315048.7 | 45013.59 | -1.57 | 2.24E-10 | 3.14E-09 | 0.33 | 0.177599 | 0.491946 | | |
| COMPOUND_575_287a12_53095 | Rp | - | 575.2870 | 12.53 | | | (1151.5974, 572.74)(1152.6003, 699.63)(1189.5437, 811.43)(587.2635, 1206.95)(587.7565, 3021.66)(588.2587, 1586.94)(588.7521, 1188.97)(589.2705, 1037.61)(1173.5608, 894.26)(1174.5662, 655.23)(1175.5405, 779.59)(576.2761, 12295.04)(577.2784, 5223.47)(578.2591, 13699.62)(579.2608, 7214.17)(580.2687, 5362.65)(1168.573, 1717.18)(1169.5756, 1325.38)(1170.5686, 1382.36)(1171.5684, 870.07)(1172.5671, 495.98)(288.6428, 24614.0)(289.1443, 7880.57)(289.6438, 10419.45)(290.1455, 3204.0)(290.6415, 4480.43)(291.143, 1764.95)(291.6403, 854.82) | 171129.9 | 30428.66 | 165647.6 | 38054.55 | 204772 | 34896.56 | 209435.9 | 40640.71 | 0.29 | 0.29787 | 0.397867 | 0.03 | 0.931121 | 0.968985 | | |
| COMPOUND_575_4614a11_883623 | Rp | + | 575.4614 | 11.88 | | | (574.2799, 4542.82)(575.2835, 1538.52)(576.2746, 6865.68)(620.2934, 763.52)(621.3002, 194.54) | 2768946 | 1342957 | 2171220 | 1148124 | 746660.4 | 1048920 | 494488.5 | 671845.2 | -1.50 | 1.81E-09 | 1.85E-08 | 0.22 | 0.380999 | 0.683863 | | |
| COMPOUND_575_5302a14_105693 | Rp | + | 575.5302 | 14.11 | | | (1151.5931, 404.09)(576.4671, 524789.44)(577.4707, 182698.47)(578.4703, 52783.81)(579.4705, 12101.36)(580.4743, 2168.33) | 2324091 | 1055720 | 1868278 | 884061.1 | 2098360 | 511174.6 | 2361468 | 1001926 | 0.01 | 0.983145 | 0.99151 | 0.76 | 0.02457 | 0.219303 | | |
| COMPOUND_577_285a10_638372 | Rp | + | 577.2850 | 10.64 | | | (576.5357, 470167.5)(577.5394, 183963.9)(578.5421, 37939.93)(579.5446, 5489.85)(580.5481, 863.88) | 164389 | 48343.95 | 164287.3 | 48996.84 | 137889.6 | 29441.25 | 130252.7 | 26872.47 | -0.72 | 0.008913 | 0.019098 | 0.07 | 0.824864 | 0.923716 | | |
| COMPOUND_577_737a10_04196 | Rp | + | 577.7370 | 10.04 | | | (1155.6176, 599.92)(597.2768, 1828.79)(597.775, 1714.97)(598.29, 2605.77)(598.7918, 1288.78)(599.2805, 1911.76)(589.3074, 1026.31)(589.815, 1284.09)(590.3117, 902.05)(586.8074, 849.99)(587.2943, 625.68)(587.8073, 2133.09)(588.2952, 849.46)(588.7976, 1006.83)(578.2932, 2509.89)(579.2954, 1738.54)(580.3059, 3163.96)(581.3082, 1822.89)(582.3031, 1631.85)(1172.6097, 1670.61)(1173.6096, 856.87)(1174.6072, 1089.07)(1175.6044, 815.35)(1176.5996, 964.58)(289.6513, 11968.61)(290.1525, 3581.39)(290.6519, 5545.44)(291.1547, 1761.92)(291.6497, 1927.77)(292.151, 842.29)(292.6517, 264.54) | 46841.1 | 17356.94 | 43790.85 | 21931.88 | 48045.69 | 9062.49 | 48182.76 | 13676.47 | 0.04 | 0.886062 | 0.923801 | 0.30 | 0.397194 | 0.690408 | | |
| COMPOUND_578_2591a9_931467 | Rp | + | 578.2591 | 9.93 | | | (600.7304, 255.79)(601.7492, 707.84)(578.7434, 12129.77)(579.7475, 1394.01)(580.7307, 1395.19) | 68449.2 | 15742.98 | 74049.33 | 21612.77 | 52783.69 | 11814.45 | 51640.47 | 23124.37 | -0.07 | 0.80127 | 0.857257 | -0.34 | 0.280491 | 0.588143 | | |
| COMPOUND_578_2849a12_531047 | Rp | - | 578.2849 | 12.53 | | | 3399.83(581.2741, 129.42)(1174.5258, 155.31) | 60858.83 | 10062.72 | 61309.78 | 14682.66 | 74373.07 | 12188.7 | 75005.4 | 14369.37 | 0.89 | 0.00143 | 0.003617 | 0.08 | 0.796203 | 0.91372 | | |
| COMPOUND_579_3095a10_093017 | Rp | - | 579.3095 | 10.09 | | | (577.2775, 27458.93)(578.2807, 6224.90)(579.2834, 1085.61) | 87023.87 | 18834.36 | 91009.93 | 18616.77 | 58244.64 | 10092.12 | 68045.25 | 16207.41 | -1.28 | 2.48E-07 | 1.43E-06 | 0.18 | 0.481135 | 0.743153 | | |
| COMPOUND_579_3096a10_016066 | Rp | - | 579.3096 | 10.02 | no msm | | (576.5357, 470167.5)(577.5394, 183963.9)(578.5421, 37939.93)(579.5446, 5489.85)(580.5481, 863.88) | 29707.08 | 12819.57 | 26022.07 | 7218.974 | 18857 | 17665.73 | 36365.51 | 25652.45 | -1.51 | 7.6E-07 | 3.91E-06 | 1.50 | 2.47E-05 | 0.006177 | | |
| COMPOUND_579_3158a8_945963 | Rp | - | 579.3158 | 8.95 | | | (1193.6031, 1832.79)(1194.6058, 1304.02)(578.3006, 11979.54)(579.3035, 3307.39)(580.2998, 4079.04)(581.3093, 1735.41)(582.3127, 356.56)(583.325, 119.76)(624.2878, 2798.07) | 101098.8 | 79337.74 | 133956.9 | 92890.16 | 98990.67 | 11005.2 | 121144.7 | 33215 | -0.84 | 4.89E-05 | 0.000162 | -0.58 | 0.013204 | 0.173893 | | |
| COMPOUND_580_2727a10_193052 | Rp | + | 580.2727 | 10.19 | | | (1161.6006, 28.19)(1162.5645, 231.94)(1163.5286, 246.06)(1164.5469, 286.51)(1165.5283, 129.84)(1199.5153, 1425.89)(1200.519, 875.81)(1201.532, 820.47)(600.2622, 2717.27)(600.765, 222.58)(601.2501, 1047.14)(603.2721, 1887.33)(1183.5137, 633.24)(1184.5388, 698.29)(1185.544, 735.24)(581.2792, 32230.66)(582.2827, 10414.17)(583.2772, 2215.04)(584.2925, 454.34)(291.1451, 2439.09)(291.645, 915.21)(292.1453, 211.1)(1178.566, 286.17)(1179.5714, 105.25)(1180.5522, 262.92) | 121898.3 | 76035.76 | 144108.9 | 83159.53 | 158373.4 | 65233.04 | 154372 | 76343.78 | 0.50 | 0.095992 | 0.157217 | -0.16 | 0.655792 | 0.841269 | | |
| COMPOUND_580_2732a10_27787 | Rp | + | 580.2732 | 10.28 | | | (578.309, 12804.16)(579.3121, 4102.2)(580.3249, 95014.9) | 215157.4 | 161810.3 | 213216.7 | 160953.9 | 211724.6 | 66046.95 | 215597.5 | 75933.19 | 0.15 | 0.619309 | 0.711936 | 0.06 | 0.864083 | 0.943353 | | |
| COMPOUND_581_2457a8_853452 | Rp | + | 581.2457 | 8.85 | | | (1161.5712, 452.79)(1162.5829, 506.47)(1163.5892, 505.24)(1164.5903, 1080.93)(1165.6025, 1305.47)(1199.5483, 1148.1)(1200.5498, 768.14)(1201.5472, 1319.1)(600.2675, 4892.64)(600.7696, 854.27)(601.2581, 2618.77)(603.2454, 1570.27)(1183.5588, 551.63)(1184.561, 350.09)(1185.5536, 452.38)(581.2794, 25335.68)(582.2819, 7420.59)(583.2779, 1898.9)(584.2712, 350.53)(1178.5653, 492.48)(1179.5648, 615.78)(1180.5507, 322.47)(291.1422, 2423.18)(291.6454, 506.14)(292.1461, 217.52) | 14002.77 | 3336.531 | 15257.2 | 4214.689 | 38850.64 | 15348.05 | 37852.66 | 14020.02 | 1.55 | 1.47E-12 | 5.93E-11 | -0.13 | 0.531424 | 0.771657 | | |
| COMPOUND_581_2811a10_091351 | Rp | + | 581.2811 | 10.09 | | | (604.2358, 154.04)(605.2315, 401.23)(606.2431, 205.91)(582.253, 9356.74)(583.2553, 3563.3)(584.258, 1125.43) | 219383.7 | 45723.26 | 213499.8 | 42349.14 | 168278.8 | 25679.88 | 178249.3 | 40648 | -1.10 | 9.62E-05 | 0.000298 | 0.44 | 0.164315 | 0.47785 | | |
| COMPOUND_581_293a9_766728 | Rp | - | 581.2930 | 9.77 | | | (1163.5583, 1572.81)(1201.5413, 1181.23)(1202.5386, 981.64)(1203.5591, 481.99)(601.2631, 2107.67)(601.7606, 803.6)(602.2633, 3613.85)(602.7616, 2103.44)(603.2721, 1614.91)(593.2696, 2788.82)(593.7541, 2261.76)(612.2398, 2152.59)(612.7613, 269.06)(613.2589, 1071.77)(613.7658, 620.14)(1185.5658, 934.69)(1186.5521, 826.91)(1187.5411, 1033.41)(582.2854, 4375.11)(582.797, 1257.41)(583.2962, 2758.09)(583.7993, 829.11)(584.3013, 1537.61)(584.8019, 514.31)(585.298, 440.88)(313.6344, 690.41)(314.1385, 366.76)(314.6346, 123.14)(582.284, 6831.16)(583.2942, 3884.95)(1180.5612, 923.57)(291.649, 6469.1)(292.15, 1787.62)(292.6394, 845.61)(293.1344, 195.24) | 46658.17 | 20793.8 | 63008.3 | 30395.29 | 48698.29 | 15782.72 | 39901.53 | 18327.48 | 0.12 | 0.649587 | 0.737859 | -1.08 | 0.000956 | 0.050056 | | |
| COMPOUND_581_3317a8_946457 | Rp | - | 581.3317 | 8.95 | | | (580.3249, 30412.73)(581.3282, 9299.72)(582.3313, 1997.48)(583.3316, 344.67)(584.3373, 51.94)(1161.6785, 157.39)(1162.6741, 39.27) | 123570.8 | 98627.4 | 166195.3 | 118234.4 | 106465.8 | 52001.16 | 131680.4 | 69694.43 | -0.97 | 1.16E-05 | 4.62E-05 | -0.45 | 0.070864 | 0.325554 | | |
| COMPOUND_581_3675a10_571905 | Rp | - | 581.3675 | 10.57 | | | (1197.6528, 290.96)(1198.6599, 373.94)(1199.6671, 393.13)(580.3612, 6079.66)(581.3638, 2082.31)(582.3672, 500.41)(583.3747, 97.01)(626.3561, 454.51) | 50267.51 | 10808.66 | 53219.05 | 13092.65 | 27847.13 | 5874.314 | 29462.93 | 7647.221 | -1.27 | 4.3E-07 | 2.39E-06 | 0.20 | 0.446014 | 0.72091 | | |
| COMPOUND_581_5029a12_850153 | Rp | + | 581.5029 | 12.85 | | | (1201.9419, 223.67)(582.5099, 16554.86)(583.5132, 6304.59)(584.5177, 1578.73)(585.5216, 261.61)(1181.0645, 171.48) | 44657.74 | 21730.48 | 44317.54 | 21757.67 | 46485.14 | 19998.11 | 78821.68 | 38065.96 | 0.13 | 0.594921 | 0.690571 | 0.97 | 0.001028 | 0.051457 | | |
| COMPOUND_581_7475a10_490611 | Rp | + | 581.7475 | 10.49 | | | (1164.5211, 257.41)(1186.501, 173.15)(582.7524, 9651.86)(583.751, 1103.17)(584.7363, 32266.58) | 10176.33 | 28433.72 | 9392.561 | 30905.55 | 6819.133 | 31670.66 | 9233.548 | -0.12 | 0.679122 | 0.765074 | 0.62 | 0.071484 | 0.325554 | | | |
| COMPOUND_582_0725a10_165926 | Rp | + | 582.0725 | 10.17 | | | 838.61(1181.5577, 355.18) | 1165.1016 | 154.77(1203.076, 115.83)(1187.0844, 146.16)(583.0816, 10363.14)(584.085, 52283.85 23880.22 45263.95 23981.26 55014.31 8037.183 55861.33 15705.97 | 52283.85 | 23880.22 | 45263.95 | 23981.26 | 55014.31 | 8037.183 | 55861.33 | 15705.97 | 0.23 | 0.42644 | 0.531163 | 0.56 | 0.108749 | 0.391238 |
| COMPOUND_582_2076a9_9266615 | Rp | + | 582.2076 | 9.93 | | | (1967.06)(585.0681, 1972.32)(586.0582, 361.68)(587.079, 946.39)(1182.2294, 180.58) | 83253.96 | 24988.73 | 94210.51 | 35734.12 | 60238.57 | 17116.31 | 65285 | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_582_249a11_367533 | Rp | + | 582.2490 | 11.37 | Unknown | 4 | 20 eV: 583.2532(100), 297.1195(25), 478.3266(3) | (1165.5021, 1992.81)(1166.5079, 1458.82)(1167.5187, 8971.12)(605.238, 9088.46)(606.2463, 3992.91)(607.2522, 5784.6)(608.2546, 2469.9)(609.2464, 751.09)(610.187.5138, 220.34)(621.2037, 2587.25)(622.2089, 1060.63)(623.219, 2340.62)(600.3008, 2181.20)(583.257, 1501.64)(584.2621, 977.79)(23)(585.2711, 116165.55)(586.2747, 37597.11)(587.2769, 8747.16)(588.2791, 1621.16)(589.279, 1899.96)(590.2679, 761.27) | 495015.1 | 469934.1 | 325079.2 | 237956 | 690362.1 | 533419.9 | 517121 | 440433.8 | 0.52 | 0.05177 | 0.090237 | 0.02 | 0.95717 | 0.980661 |
| COMPOUND_582_3182a4_5278673 | Hilic | + | 582.3182 | 4.53 | | | (605.3063, 1134.48)(606.3136, 382.07)(1187.6501, 269.98)(600.3229, 199.79)(583.3246, 17837.55)(584.3275, 5341.26)(585.3298, 1185.81) | 17732.55 | 8914.625 | 19006.96 | 8780.493 | 11101 | 4755.373 | 8470.235 | 3924.751 | -1.32 | 8.85E-10 | 9.91E-09 | -0.16 | 0.452067 | 0.724079 | |
| COMPOUND_583_3274a1_3199148 | Hilic | + | 583.3274 | 1.32 | | | (606.3168, 2487.39)(607.3203, 878.7)(608.3315, 947.78)(609.334, 399.03)(584.3347, 15728.73)(585.3379, 5498.16)(586.3492, 6462.26)(587.3529, 2161.23)(588.3648, 1819.93) | 105010.8 | 73030.71 | 130389.1 | 79521.74 | 83071 | 66058.18 | 78284.59 | 88980.21 | -0.99 | 4.24E-05 | 0.000144 | -0.29 | 0.274252 | 0.583098 | |
| COMPOUND_583_5159a12_38974 | Rp | - | 583.5159 | 12.39 | | | (582.5093, 7657.53)(583.5131, 2972.73)(584.5143, 586.09)(585.5164, 144.06) | 16811.87 | 5865.533 | 17734.95 | 7981.128 | 21135.17 | 7861.154 | 21343.93 | 8639.133 | 0.40 | 0.150963 | 0.229398 | 0.08 | 0.807282 | 0.917894 | |
| COMPOUND_583_5169a13_459112 | Rp | + | 583.5169 | 13.46 | | | (584.5257, 32187.71)(585.5289, 12594.86)(586.5327, 3037.40)(587.526, 675.8) | 71911.66 | 33880.32 | 74643 | 41700.04 | 73904.36 | 28408.36 | 142854.1 | 78516.6 | 0.17 | 0.480527 | 0.583053 | 0.94 | 0.001125 | 0.056309 | |
| COMPOUND_583_5181a12_667186 | Rp | + | 583.5181 | 12.67 | | | (606.5105, 4684.04)(607.5147, 2007.96)(608.5122, 608.12)(1190.0555, 1116.58)(584.5253, 9179.22)(585.5286, 3732.82)(586.5305, 1000.83)(587.5393, 168.34) | 47015.77 | 29509.31 | 43045.91 | 23491.45 | 44635.71 | 22030.47 | 56930.57 | 28146.48 | -0.38 | 0.167533 | 0.251022 | 0.84 | 0.011668 | 0.167839 | |
| COMPOUND_584_2216a1_0488341 | Hilic | + | 584.2216 | 1.05 | | | (585.229, 3273.15)(586.2336, 1374.25)(587.2276, 1385.33)(588.2321, 732.5)(589.2427, 202.11)(1186.535, 312.41) | 15123.6 | 3523.452 | 15851.17 | 2884.691 | 23427.79 | 3281.435 | 24416.48 | 5042.285 | 1.43 | 1.01E-08 | 8.38E-08 | -0.14 | 0.577734 | 0.792726 | |
| COMPOUND_584_2246a10_30371 | Rp | + | 584.2246 | 10.30 | | | (1169.4655, 262.01)(1207.4556, 418.93)(602.2661, 2286.27)(603.2573, 1188.67)(604.2616, 2831.33)(585.2286, 25794.3)(586.2344, 13586.51)(587.2294, 10456.87)(1186.5098, 331.05)(1187.5148, 506.74)(1188.5232, 324.15)(1189.5438, 430.06) | 124560.2 | 39954.67 | 109412.6 | 30414.38 | 139953.2 | 23089.03 | 134931.7 | 32017.74 | 0.49 | 0.081401 | 0.135688 | 0.34 | 0.315222 | 0.621785 | |
| COMPOUND_584_2248a10_1615305 | Rp | + | 584.2248 | 10.16 | | | (1169.4971, 550.49)(1207.4517, 304.92)(1191.426, 348.29)(602.2616, 1357.98)(585.2286, 33188.7)(586.2346, 17752.76)(587.2299, 13124.5) | 145249.5 | 38488.36 | 129877.3 | 38550.41 | 144928.4 | 34696.4 | 149082 | 37251.67 | 0.11 | 0.712283 | 0.788624 | 0.44 | 0.211987 | 0.519471 | |
| COMPOUND_584_2623a6_9321017 | Rp | + | 584.2623 | 6.93 | | 4 | 10 eV: 583.2549(100), 227.1172(6), 74.5504(3) | (583.2556, 2081.44)(584.2585, 7484.91)(585.2608, 1421.13)(586.2566, 255.61)(1167.523, 249.33)(1168.5474, 185.94)(629.2584, 387.04) | 48504.57 | 31258.88 | 44736.98 | 26413.63 | 57035.07 | 33528.29 | 41573.35 | 21537.18 | 0.25 | 0.333921 | 0.43518 | -0.31 | 0.305237 | 0.613089 |
| COMPOUND_584_2623a5_6700606 | Rp | - | 584.2623 | 5.67 | | | (583.2553, 10003.74)(584.2581, 3880.14)(585.2613, 747.49)(586.2537, 115.78) | 27648.39 | 15365.06 | 25559.84 | 13409.14 | 28665.83 | 17321.25 | 20088.86 | 9368.648 | -0.09 | 0.699487 | 0.780984 | -0.11 | 0.665353 | 0.844963 | |
| COMPOUND_584_2634a5_6885524 | Rp | + | 584.2634 | 5.69 | | | (585.2718, 10673.63)(586.2749, 4007.42)(587.276, 975.91)(588.2792, 199.72)(589.2751, 35.86)(293.1407, 1623.54)(293.6415, 610.12)(294.1429, 187.91) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.16 | 0.533678 | 0.632881 | -0.01 | 0.96228 | 0.981922 | |
| COMPOUND_584_2644a1_1423072 | Hilic | + | 584.2644 | 1.14 | | | (607.2468, 127.66)(608.2399, 85.22)(609.2344, 801.7)(602.2935, 751.65)(603.2973, 404.54)(604.2825, 9482.93)(605.2849, 2670.41)(585.2708, 15896.39)(586.2744, 5928.95)(587.2783, 1357.67)(588.2773, 229.01)(1186.5634, 196.96)(1187.5511, 229.01)(1188.5521, 483.87) | 47629.9 | 38505.78 | 36198.59 | 28544.37 | 67379.36 | 41035.46 | 52190.75 | 30674.26 | 1.10 | 2.65E-05 | 9.59E-05 | -0.37 | 0.196003 | 0.507591 | |
| COMPOUND_584_2658a6_9457154 | Rp | + | 584.2658 | 6.95 | | | (1191.5342, 97.81)(602.2967, 233.54)(603.3083, 93.91)(585.2723, 87373.56)(586.2754, 31634.04)(587.2786, 6850.54)(588.2816, 1256.41)(589.2802, 184.44)(293.1379, 755.01)(293.6395, 74.3) | 233474.8 | 145036.8 | 200775.2 | 111711 | 265154.6 | 142697.7 | 198622.7 | 109022 | 0.26 | 0.310017 | 0.411165 | -0.24 | 0.4296 | 0.707514 | |
| COMPOUND_584_3676a1_055654 | Hilic | + | 584.3676 | 1.06 | | | (602.3943, 1168.27)(585.3752, 27010.02)(586.3786, 9464.27)(587.3822, 2097.93)(588.3789, 402.78)(293.1319, 6430.72)(293.6941, 2101.61)(294.197, 414.98) | 12341.12 | 7537 | 14327.77 | 10100.74 | 48816.36 | 39211.74 | 40538.02 | 40970.36 | 1.42 | 8.29E-10 | 9.47E-09 | -0.19 | 0.41327 | 0.696003 | |
| COMPOUND_585_2641a0_780989 | Hilic | + | 585.2641 | 0.78 | | | (603.2772, 640.88)(586.2712, 215743.84)(587.2741, 56288.03)(588.2769, 14715.48)(589.2802, 2589.76)(590.2823, 424.5) | 313674.2 | 420318 | 292372.8 | 402987.2 | 489121 | 525946.2 | 311151.6 | 438555.3 | 0.44 | 0.139498 | 0.215319 | -0.57 | 0.112648 | 0.398247 | |
| COMPOUND_585_363a9_362009 | Rp | - | 585.3630 | 9.36 | | | (584.3558, 5572.9)(585.3592, 1555.23)(586.362, 275.09) | 18655.14 | 5955.441 | 18404.68 | 6320.297 | #DIV/0! | #DIV/0! | 10754 | #DIV/0! | -1.37 | 4.13E-11 | 7.76E-10 | 0.10 | 0.624678 | 0.823156 | |
| COMPOUND_585_4464a9_695286 | Rp | + | 585.4464 | 9.70 | | | (586.4532, 16799.29)(587.4536, 6331.22)(588.4545, 1332.28)(589.4569, 227.11)(1188.89, 69.23) | 116988.7 | 31956.1 | 100598.4 | 19882.39 | 125676.5 | 22051.98 | 123583.5 | 31367.77 | 0.32 | 0.252488 | 0.348623 | 0.46 | 0.174554 | 0.488924 | |
| COMPOUND_585_5347a13_27537 | Rp | + | 585.5347 | 13.28 | | | (608.5253, 4194.5)(609.5284, 1683.38)(624.5084, 852.01)(625.5108, 330.87)(586.541, 12947.62)(587.5443, 5153.32)(588.5465, 1186.87)(589.5502, 238.43) | 42321 | 29667.22 | 35522.35 | 24253.1 | 30121.6 | 8894.083 | 55355.55 | 32664.21 | 0.15 | 0.520569 | 0.620038 | 0.71 | 0.014859 | 0.181233 | |
| COMPOUND_587_1693a8_431415 | Rp | + | 587.1693 | 8.43 | | | (588.175, 5095.27)(589.18, 1000.01)(590.1945, 181.06) | 16795.89 | 2251.171 | 16276.63 | 1953.49 | 16855.93 | 1638.52 | 17509.72 | 2091.254 | 0.03 | 0.910964 | 0.941916 | 0.38 | 0.28511 | 0.593016 | |
| COMPOUND_587_231a10_154449 | Rp | + | 587.2341 | 10.15 | | | (1213.4622, 205.67)(610.2255, 1364.94)(611.2333, 984.54)(612.2301, 805.33)(1197.4967, 337.63)(588.2353, 7432.48)(589.2441, 2633.37)(590.2343, 2518.11)(1192.519, 601.31)(1193.5226, 623.92)(1194.5244, 504.89) | 101785.7 | 36037.71 | 96809.3 | 39002.11 | 76318.73 | 60648.8 | 100359.3 | 60814.1 | 0.00 | 0.995081 | 0.998768 | 0.38 | 0.226834 | 0.53434 | |
| COMPOUND_587_3214a9_755528 | Rp | - | 587.3214 | 9.76 | | | (586.4532, 16799.29)(587.4536, 6331.22)(588.4545, 1332.28)(589.4569, 227.11)(1188.89, 69.23) | 98956.02 | 11276.9 | 60215.15 | 49735.99 | 55268.69 | 61962.01 | 33927.21 | 22365.42 | -1.00 | 0.000405 | 0.001142 | 0.20 | 0.537779 | 0.776408 | |
| COMPOUND_587_3217a9_850620 | Rp | - | 587.3217 | 9.86 | | | (608.5253, 4194.5)(609.5284, 1683.38)(624.5084, 852.01)(625.5108, 330.87)(586.541, 12947.62)(587.5443, 5153.32)(588.5465, 1186.87)(589.5502, 238.43) | 478975.1 | 348745 | 435900.8 | 253168.7 | 152963.4 | 90814.81 | 177554.1 | 111135 | -1.48 | 1.86E-09 | 1.88E-08 | 0.27 | 0.276368 | 0.585315 | |
| COMPOUND_587_3601a10_474119 | Rp | - | 587.3601 | 10.47 | | | (1209.7517, 258.26)(1210.7406, 364.71)(700.3145, 990.38)(701.3131, 380.28)(622.3328, 10869.27)(623.3344, 3495.51)(624.3314, 1920.22)(1219.6475, 189.57)(1220.6833, 307.15)(1221.6691, 377.45)(586.3528, 3608.13)(587.3562, 1497.35)(588.3474, 3202.01)(589.3371, 144.69)(590.3475, 1271.26)(1173.7606, 1464.67)(1174.7667, 905.52)(1175.7698, 463.95)(632.3644, 1292.49)(1287.6884, 280.47)(1288.6862, 281.47)(1289.6711, 311.6) | 120974.5 | 28329.14 | 130027.2 | 33314.1 | 71438.15 | 17823.72 | 76455.37 | 18514.38 | -1.23 | 2.61E-06 | 1.18E-05 | -0.06 | 0.822223 | 0.922833 | |
| COMPOUND_589_337a10_003053 | Rp | - | 589.3370 | 10.00 | | | (588.3299, 74826.82)(589.3332, 24207.17)(590.336, 5210.2)(591.3382, 854.52)(592.3467, 290693.2) | 74275.43 | 268550.7 | 75609.03 | 161018.7 | 1263650 | 171216.5 | 140589.3 | -1.43 | 5.43E-08 | 3.67E-07 | 0.28 | 0.306199 | 0.613089 | | |
| COMPOUND_589_3379a10_09891 | Rp | - | 589.3379 | 10.10 | LPC 20:4 | 1 | 20 eV: 303.2322(100), 528.3089(85),44.998(22) | (588.3298, 467615.78)(589.3334, 149190.55)(590.3361, 3101.83)(591.3384, 5275.85)(592.3394, 965.08)(1291.6294, 302.92)(1292.6422, 299.92) | 1565910 | 340017.2 | 1487614 | 356670.4 | 782209.2 | 172091 | 922980.7 | 282602.4 | -1.62 | 3.16E-13 | 1.98E-11 | 0.39 | 0.057927 | 0.298567 |
| COMPOUND_589_4475a1_0222793 | Hilic | + | 589.4475 | 1.02 | | | (612.4376, 634.94)(613.4311, 467.56)(590.4546, 13461.83)(591.4574, 5314.09)(592.4699, 39351.42) | 116276.2 | 43221.23 | 118707.9 | 52814.39 | 52842.86 | 20509.15 | 39810.54 | 18976.12 | -1.45 | 1.19E-11 | 2.9E-10 | -0.07 | 0.716552 | 0.876415 | |
| COMPOUND_590_2821a10_148812 | Rp | + | 590.2821 | 10.15 | | | (1181.5994, 955.32)(1219.5106, 652.35)(1220.5048, 787.28)(1221.5056, 903.94)(610.2747, 988.09)(610.7599, 567.37)(1203.5392, 980.23)(1198.631, 475.03)(296.1478, 14816.87)(296.6494, 4552.06)(297.1484, 8732.74)(297.6497, 2531.31)(298.1467, 3477.26)(298.6473, 987.58)(299.1445, 753.31)(299.6474, 228.96) | 123215.4 | 348321.15 | 116407.8 | 26400.68 | 90246.36 | 13613.91 | 95083.53 | 28405.44 | -1.38 | 7.64E-08 | 4.94E-07 | 0.35 | 0.186206 | 0.500401 | |
| COMPOUND_590_2823a10_250496 | Rp | + | 590.2823 | 10.25 | | | (1181.6033, 770.78)(1219.5126, 296.49)(1220.5114, 115.61)(1221.5386, | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------------|----------------|--------------------------------|--------------|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_591_3518a10_183858 | Rp | - | 591.3518 | 10.18 | | | (704.3142, 488.29)[705.3228, 228.73][590.3451, 57453.12][591.3485, 18743.37][592.3502, 4366.61][593.3542, 726.71][1181.7188, 173.37] (590.3453, 24095.48)[591.3487, 7927.77][592.3494, 2034.03][593.3532, 422.74][594.3446, 75.54] | 116848.7 | 37703.9 | 121409.9 | 44103.88 | 71700.57 | 15255.05 | 91093.51 | 37301.3 | -1.35 | 8.26E-07 | 4.2E-06 | 0.47 | 0.107032 | 0.38909 |
| COMPOUND_591_3528a10_293874 | Rp | - | 591.3528 | 10.29 | LPC 20:3 | 2 | 20 eV: 530.3234(100), 305.2479(45) | 497141.3 | 161938 | 507621.1 | 176593.9 | 361447.4 | 76703.73 | 438419.2 | 132937 | -0.94 | 0.000949 | 0.002488 | 0.49 | 0.127351 | 0.424221 |
| COMPOUND_591_4373a11_97843 | Rp | + | 591.4373 | 13.98 | | | (592.4444, 34689.73)[593.4473, 12627.48][594.4444, 5460.29][595.4464, 1358.87] | 391886.6 | 180808.6 | 305939.5 | 142099.2 | 355347.1 | 99966.45 | 375796.3 | 134169.9 | -0.01 | 0.965839 | 0.980203 | 0.54 | 0.129734 | 0.42589 |
| COMPOUND_591_4631a10_0163624 | Hiic | + | 591.4631 | 1.02 | | | (1183.9143, 153.47)[614.4788, 4104.72][615.4828, 1493.26][609.4744, 208.77][592.4702, 1192.53][593.4735, 1877.79][594.4855, 2142.07][595.4891, 795.05][596.4924, 128.83] | 113574.9 | 45051.7 | 116067.5 | 55189.7 | 42084.64 | 19112.34 | 32974.09 | 16658.79 | -1.29 | 1.42E-09 | 1.49E-08 | -0.33 | 0.122635 | 0.416475 |
| COMPOUND_591_4658a11_547967 | Rp | + | 591.4658 | 11.55 | | | (614.4467, 2975.33)[615.4414, 1460.08][1205.9482, 116.94][609.5182, 970.8][592.4742, 15962.67][593.4756, 5823.0][594.4757, 1412.79][595.4661, 229.12] | 102683.6 | 43060.83 | 114697.2 | 55105.27 | 47680.8 | 27437.41 | 36325.91 | 17069.61 | -0.87 | 6.78E-05 | 0.000218 | 0.14 | 0.574336 | 0.790589 |
| COMPOUND_591_7525a10_379943 | Rp | + | 591.7525 | 10.38 | | | (1184.5605, 581.82)[1222.4991, 519.02][609.7656, 948.59][592.7589, 11971.08][593.7615, 1670.73][594.7516, 1816.46][1201.5507, 2884.1][1202.5472, 1807.64][1203.545, 2170.13] | 76504.33 | 18609.01 | 72246.6 | 20940.64 | 72019.43 | 15357.32 | 76645.09 | 17910.81 | -0.04 | 0.899676 | 0.934535 | 0.50 | 0.155537 | 0.466404 |
| COMPOUND_592_396a11_245408 | Rp | - | 592.3960 | 11.25 | no msms | | (705.3738, 608.01)[706.367, 482.71][591.3892, 42053.09][592.3927, 15133.53][593.3953, 3748.35] | 10924.51 | 44902.02 | 13672.82 | 87814.43 | 51585.78 | 62345.95 | 26633.28 | 1.67 | 2.83E-09 | 2.69E-08 | -1.00 | 0.000445 | 0.034251 | |
| COMPOUND_593_279a10_09851 | Rp | - | 593.2729 | 10.10 | | | (592.2648, 7907.44)[593.2673, 3065.43][594.2783, 994.97][595.2771, 213.49][1299.5609, 685.45][1300.547, 655.61] | 24413.8 | 4765.198 | 25604.22 | 5805.366 | 27539.23 | 8314.436 | 31886.23 | 9209.84 | 0.22 | 0.418597 | 0.52284 | 0.55 | 0.086956 | 0.350026 |
| COMPOUND_593_3316a10_455811 | Rp | - | 593.3316 | 10.46 | | | (1221.6112, 296.01)[1222.6356, 376.89][706.3452, 417.33][1231.6184, 342.47][1232.6198, 319.73][1233.6128, 211.26][592.3222, 10987.7][593.3265, 3523.91][594.3308, 877.21][595.3287, 136.99][1185.6139, 517.23][1186.6112, 651.4][1187.6136, 760.86][1188.6187, 515.16][1189.6108, 550.51][1299.6531, 409.14][1300.6753, 148.78] | 53680.62 | 11394.13 | 56801.88 | 13714.13 | 23942 | 11452.18 | 24566.39 | 10182.69 | -1.26 | 3.37E-07 | 1.91E-06 | 0.08 | 0.766467 | 0.902291 |
| COMPOUND_593_367a10_514657 | Rp | - | 593.3670 | 10.51 | | | (1221.6809, 1336.94)[1222.6848, 934.78][706.3459, 562.32][707.3364, 225.81][708.3196, 68.6][628.3501, 2198.76][592.3608, 22984.89][593.3644, 7230.09][594.3421, 7734.78][595.3443, 2298.54][1185.7623, 877.71][1186.7653, 745.61][638.3626, 6476.47][639.3721, 3193.43][640.3766, 1248.55][1299.7045, 312.71][1300.7109, 329.6] | 208937.6 | 57507.03 | 242074.2 | 72039.28 | 124126.3 | 37494.78 | 150440.4 | 54636.89 | -1.13 | 1.21E-05 | 4.79E-05 | -0.17 | 0.55279 | 0.780002 |
| COMPOUND_593_3702a0_8402881 | Hiic | + | 593.3702 | 0.84 | | | (1187.7671, 170.92)[1188.7401, 176.07][616.3716, 930.21][617.3689, 689.08][618.3712, 1023.83][619.3863, 639.66][611.3883, 670.23][594.3766, 11616.16][595.38, 3859.86][596.3813, 963.58][597.3853, 214.69] | 94618.02 | 35866.16 | 91408.3 | 40117.73 | 35938.13 | 28290.28 | 29624.65 | 23994.83 | -1.33 | 9.61E-09 | 8.04E-08 | -0.76 | 0.762264 | 0.899225 |
| COMPOUND_593_3746a10_29375 | Rp | + | 593.3746 | 10.29 | | | (1187.7415, 474.64)[1188.7417, 320.38][1189.7605, 407.49][1225.7642, 499.25][1226.7352, 426.84][616.3591, 759.54][617.3579, 410.49][618.3406, 107.95][1209.7646, 484.05][1210.7452, 446.35][1211.7378, 298.84][611.4277, 2267.79][612.4334, 1510.72][594.3772, 12510.53][595.3866, 4787.51][596.3867, 1652.67][597.3738, 130.56] | 39120.16 | 33505.14 | 34147.44 | 18804.84 | 21502.33 | 8038.721 | 19811.43 | 9126.448 | -1.09 | 9.77E-07 | 4.88E-06 | -0.04 | 0.857789 | 0.940019 |
| COMPOUND_594_410a11_293655 | Rp | - | 594.4104 | 11.40 | | | (629.3661, 2604.86)[630.3685, 1060.31][593.4049, 5266.56][594.4072, 1749.39][595.4107, 664.02][596.4154, 117.56] | 16042.23 | 3715.1 | 18060.22 | 4280.69 | 21852.93 | 7522.033 | 20745.71 | 5967.281 | 1.02 | 0.000552 | 0.00152 | -0.64 | 0.059298 | 0.30009 |
| COMPOUND_594_4851a10_978287 | Rp | - | 594.4851 | 10.98 | | | (707.4704, 2762.83)[708.4706, 1590.74][709.4862, 3700.16][593.4773, 28451.71][594.4806, 10523.68][595.4929, 32767.63][596.4965, 12445.67][597.4998, 2839.08][598.4936, 788.04] | 184323.5 | 116065.7 | 210606.2 | 111887.3 | 216304 | 129016.9 | 145946.7 | 136772.6 | 0.03 | 0.920873 | 0.94911 | -0.84 | 0.014613 | 0.179825 |
| COMPOUND_595_2387a9_850974 | Rp | + | 595.2387 | 9.85 | | | (618.245, 1344.85)[618.7496, 1010.24][623.7334, 234.95][624.2475, 640.84][624.7445, 401.05][596.2437, 5463.56][597.2483, 1956.27][598.252, 2976.55][599.2494, 1179.37][600.2538, 1428.46][336.5837, 168.38][337.0783, 76.25][337.5864, 291.05][1208.5085, 413.75][1209.5092, 193.45][1298.6276, 9593.21][299.1281, 3605.49][299.6277, 4909.18][300.1286, 1508.28][300.6258, 1959.1] | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.05 | 2.67E-05 | 9.62E-05 | 0.01 | 0.984414 | 0.992345 |
| COMPOUND_595_2574a10_244268 | Rp | + | 595.2574 | 10.24 | | | (1191.5066, 285.42)[1192.5026, 315.2][1193.5079, 143.51][1229.4989, 134.65][1230.4934, 150.15][618.2481, 3866.2][619.2496, 1763.07][620.2497, 989.81][1213.4467, 70.92][1214.4615, 70.92][1215.4738, 102.3][1216.4784, 64.42][1217.4879, 117.79][634.238, 1030.72][596.2649, 21636.81][597.2679, 6184.94][598.2665, 10398.85][599.2692, 2780.34][600.2626, 4068.75][601.2579, 2003.0][602.2606, 1334.53][1208.5345, 258.08] | 132978.2 | 87880.28 | 131906.9 | 94052.18 | 184766.2 | 68512.07 | 154381.1 | 97445.18 | 0.51 | 0.060053 | 0.103715 | -0.03 | 0.915254 | 0.961085 |
| COMPOUND_595_259a10_259193 | Rp | + | 595.2590 | 10.26 | | | (1191.5555, 865.31)[1192.5529, 810.52][1193.5532, 1067.59][1229.5138, 397.52][1230.4875, 215.27][618.2613, 5047.28][619.2504, 1048.55][620.2561, 1926.37][1213.5092, 297.36][1214.5197, 177.32][1215.5306, 435.83][634.2431, 966.37][596.2655, 13561.38][597.2669, 4379.96][598.2666, 6906.84][599.2681, 2920.35][600.2659, 3641.69][601.2569, 2282.92][602.2698, 1722.11][1208.5813, 360.02] | 161599.2 | 96417.33 | 134938.9 | 78008.31 | 188431.9 | 93526.73 | 210355.2 | 95828.61 | 0.40 | 0.162613 | 0.244789 | 0.41 | 0.231067 | 0.537849 |
| COMPOUND_595_2595a10_152486 | Rp | + | 595.2595 | 10.15 | | | (1191.5322, 922.82)[1192.5258, 761.83][1229.51, 469.99][1230.4987, 501.54][1231.491, 365.7][1213.5109, 677.28][1214.5242, 514.93][1215.5331, 602.81][1216.5165, 533.24][1217.5203, 533.67][634.235, 3729.54][613.2645, 828.62][596.2643, 7318.43][597.2651, 2966.01][598.2636, 4704.42][599.2647, 1550.35][600.2662, 2421.49][601.2649, 1313.23][602.2638, 964.67] | 229381.3 | 50502.39 | 197837.1 | 48047.85 | 205644.6 | 29575.34 | 214324.1 | 41886.63 | -0.41 | 0.144926 | 0.221721 | 0.82 | 0.016302 | 0.18924 |
| COMPOUND_595_3054a12_4282465 | Rp | - | 595.3054 | 12.43 | | | (594.2975, 771.66)[595.299, 271.06][596.292, 6876.15] | 23718.12 | 4526.616 | 21341.27 | 3968.488 | 25339.21 | 2510.227 | 25034.69 | 3606.349 | 0.36 | 0.191423 | 0.280289 | 0.26 | 0.425632 | 0.705315 |
| COMPOUND_595_3082a10_039574 | Rp | - | 595.3082 | 10.04 | | | (594.3011, 10212.91)[595.3051, 2782.65][596.3017, 692.39][597.3036, 168.91] | 40978.89 | 10052.55 | 44764.37 | 11372.84 | 25036.79 | 6181.951 | 21921.53 | 6182.952 | -1.16 | 2.15E-08 | 1.65E-07 | -0.55 | 0.0111 | 0.165539 |
| COMPOUND_595_3473a10_218753 | Hiic | - | 595.3473 | 10.22 | | | (1225.5915, 308.26)[708.3186, 206.56][620.3146, 1040.35][631.3162, 396.61][594.3395, 10726.36][595.3431, 3347.07][596.3462, 879.62][597.3488, 164.59][640.3448, 429.03][641.3472, 210.44] | 28879.89 | 14674.46 | 25465.84 | 13072.42 | #DIV/0! | #DIV/0! | 106.17 | #DIV/0! | -1.34 | 5.82E-10 | 6.93E-09 | 0.38 | 0.082127 | 0.343638 |
| COMPOUND_595_3483a11_3578442 | Hiic | + | 595.3483 | 1.36 | | | (1191.7489, 111.75)[618.3392, 3869.23][619.3416, 1360.69][620.3476, 430.32][596.3565, 31718.48][597.3601, 9820.91][598.3624, 2287.68][599.3673, 508.04] | 74659.54 | 47750.68 | 66107.15 | 45631.5 | 8297 | 1858.894 | 8211.538 | 2618.689 | -1.63 | 2.12E-12 | 7.57E-11 | 0.19 | 0.38307 | 0.686295 |
| COMPOUND_595_3486a10_529693 | Rp | - | 595.3486 | 10.53 | | | (1225.6584, 318.2)[1226.6931, 380.42][594.3405, 8971.38][595.3432, 2829.8][596.3485, 701.04][597.3657, 94.97] | 58026.79 | 10989.36 | 63169.5 | 14544.61 | 26242.4 | 16203.07 | 28343.54 | 15287.36 | -0.97 | 2.44E-05 | 8.9E-05 | -0.23 | 0.370567 | 0.671914 |
| COMPOUND_595_3488a10_2031355 | Rp | + | 595.3488 | 10.20 | BMP 22:2 or PG 22:2 or PS 20:0 | 2 | 20 eV: 184.0742(100), 596.359(70), 89.0579(12), 514.3753(5) | 66014.1 | 40544.26 | 58222.3 | 35548.99 | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.45 | 3.88E-12 | 1.16E-10 | 0.23 | 0.247694 | 0.557807 |
| COMPOUND_595_3836a10_741276 | Rp | - | 595.3836 | 10.74 | | | (1225.7418, 287.3)[1226.766, 547.9][1227.7949, 312.31][708.3849, 287.62][709.4031, 457.83][1235.769, 453.7][1236.756, 495.44][594.3767, 43040.92][595.3799, 14065.34][596.3876, 5345.42][597.3894, 1168.45][1189.774, 103.26][1190.7418, 259.35][640.3985, 1039.29][641.4028, 656.25][1303.7832, 298.99][1304.7856, 323.97][1305.7903, 307.33] | 217402.2 | 58591.33 | 219351.3 | 52632.27 | 102723.2 | 33506.42 | 111121.8 | 28954.31 | -1.78 | 1.04E-12 | 4.7E-11 | 0.32 | 0.176496 | 0.491826 |
| COMPOUND_595_3849a10_650845 | Rp | - | 595.3849 | 10.65 | | | (1225.7347, 118.86)[1226.7407, 359.45][708.3468, 275.58][709.3392, 224.33][1235.8184, 90.19][1236.7942, 81.89][594.3769, 32386.25][595.3799, 10734.85][596.3869, 3849.45][597.3919, 942.65][640.3999, 3287.62][641.4028, 1361.96][1189.7694, 337.64][1190.7719, 264.65][1303.7927, 131.28][1304.782, 179.61][1305.7904, 139.4] | 65020.34 | 76209.58 | 82533.48 | 99145.3 | 31374.71 | 42122.88 | 24892.08 | 29598.26 | -0.89 | 6.37E-05 | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--------------|---|---------------|----------|---------------|-------|---------------|----------|---------------|----|-------|-------|-------|-------------|-------|-------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_596_4997a11_114499 | Rp | - | 596.4997 | 11.11 | | | | (631.4763, 1052.07)(709.4699, 4907.02)(710.4722, 2164.26)(711.4554, 134.73)(595.4932, 129729.7) 87613.1 102865.8 30701.71 130202.7 102879.8 108767.3 114957.1 | 0.10 | 0.70814 | 0.787133 | -0.28 | 0.390918 | 0.690408 | | | | | | | | |
| COMPOUND_596_5a11_068715 | Rp | - | 596.5000 | 11.07 | | | | (30074.08)(596.4966, 11988.68)(597.4995, 3420.29)(598.5044, 719.99)(641.468, 249.13)(131.9965, 331.02)(193.0126, 42.62) (631.4775, 4188.83)(709.4854, 3554.52)(710.4876, 1608.03)(711.4938, 1655.06)(595.4931, 49065.53)(596.4967, 18760.97)(597.4998, 4339.88)(598.5028, 819.85)(1191.9905, 397.98)(1193.0143, 69.16)(641.5162, 162.69) (1195.217, 124.29)(1233.1022, 156.51)(620.0817, 285.38)(621.0973, 617.84)(1217.1967, 139.58)(598.0904, 13318.37)(599.0935, 1123.98)(600.0727, 1617.09)(1212.2216, 79.95)(1213.2352, 229.49) (1195.5789, 990.18)(620.2931, 537.45)(598.3168, 2233.92)(599.3194, 775.48)(600.3322, 5553.55)(601.3357, 1769.18) 30395.74 8056.283 29351.96 8769.487 34250.29 9974.302 32872.51 7507.52 | -0.15 | 0.543599 | 0.641606 | -0.78 | 0.00887 | 0.149233 | | | | | | | | |
| COMPOUND_597_0816a10_156655 | Rp | + | 597.0816 | 10.16 | | | | (596.3199, 59294.01)(597.3232, 18102.47)(598.3253, 3975.96)(599.3274, 876.84) (1235.4622, 251.79)(1219.52, 255.62)(616.2644, 3163.28)(599.2453, 7135.56)(600.2507, 3964.09)(601.25, 4219.6)(1214.5215, 277.45) (621.4364, 2327.44)(622.4416, 1374.94)(637.3931, 3316.39)(599.4396, 26488.04)(600.4436, 9340.71)(601.4428, 17408.6)(602.4365, 8191.26)(603.4295, 1467.72) (621.49, 1162.35)(622.4918, 820.16)(1219.9811, 238.71)(1220.9763, 264.31)(1221.9823, 177.87)(637.449, 972.23)(638.4581, 633.55)(616.5157, 1111.98)(599.5044, 8205.58)(600.5088, 3427.17)(601.5082, 1092.36)(602.5061, 211.12) 37043.58 15243.51 31928.43 20084.64 40717.85 11551.75 37779.87 11976.98 | 0.26 | 0.362362 | 0.464714 | 0.46 | 0.18111 | 0.494376 | | | | | | | | |
| COMPOUND_597_3092a1_0271055 | Hilic | - | 597.3092 | 1.03 | | | | (1195.5789, 990.18)(620.2931, 537.45)(598.3168, 2233.92)(599.3194, 775.48)(600.3322, 5553.55)(601.3357, 1769.18) 30395.74 8056.283 29351.96 8769.487 34250.29 9974.302 32872.51 7507.52 | 0.53 | 0.076933 | 0.129004 | -0.05 | 0.893787 | 0.954308 | | | | | | | | |
| COMPOUND_597_3265a8_9442314 | Rp | - | 597.3265 | 8.94 | | | | (596.3199, 59294.01)(597.3232, 18102.47)(598.3253, 3975.96)(599.3274, 876.84) (1235.4622, 251.79)(1219.52, 255.62)(616.2644, 3163.28)(599.2453, 7135.56)(600.2507, 3964.09)(601.25, 4219.6)(1214.5215, 277.45) (621.4364, 2327.44)(622.4416, 1374.94)(637.3931, 3316.39)(599.4396, 26488.04)(600.4436, 9340.71)(601.4428, 17408.6)(602.4365, 8191.26)(603.4295, 1467.72) (621.49, 1162.35)(622.4918, 820.16)(1219.9811, 238.71)(1220.9763, 264.31)(1221.9823, 177.87)(637.449, 972.23)(638.4581, 633.55)(616.5157, 1111.98)(599.5044, 8205.58)(600.5088, 3427.17)(601.5082, 1092.36)(602.5061, 211.12) 55528.45 46639.18 65480.67 52749.17 51195 #DIV/0! 43533.57 14030.02 | -0.98 | 4.58E-06 | 1.96E-05 | -0.38 | 0.107121 | 0.38909 | | | | | | | | |
| COMPOUND_598_2383a10_454326 | Rp | + | 598.2383 | 10.45 | | | | (1235.4622, 251.79)(1219.52, 255.62)(616.2644, 3163.28)(599.2453, 7135.56)(600.2507, 3964.09)(601.25, 4219.6)(1214.5215, 277.45) (621.4364, 2327.44)(622.4416, 1374.94)(637.3931, 3316.39)(599.4396, 26488.04)(600.4436, 9340.71)(601.4428, 17408.6)(602.4365, 8191.26)(603.4295, 1467.72) (621.49, 1162.35)(622.4918, 820.16)(1219.9811, 238.71)(1220.9763, 264.31)(1221.9823, 177.87)(637.449, 972.23)(638.4581, 633.55)(616.5157, 1111.98)(599.5044, 8205.58)(600.5088, 3427.17)(601.5082, 1092.36)(602.5061, 211.12) 171776.47 25382.01 72039.76 33749.05 52335 19246.65 36097.53 9599.59 | -0.96 | 5.1E-05 | 0.000169 | 0.19 | 0.463264 | 0.731607 | | | | | | | | |
| COMPOUND_598_4347a10_256556 | Rp | + | 598.4347 | 10.26 | | | | (621.4364, 2327.44)(622.4416, 1374.94)(637.3931, 3316.39)(599.4396, 26488.04)(600.4436, 9340.71)(601.4428, 17408.6)(602.4365, 8191.26)(603.4295, 1467.72) (621.49, 1162.35)(622.4918, 820.16)(1219.9811, 238.71)(1220.9763, 264.31)(1221.9823, 177.87)(637.449, 972.23)(638.4581, 633.55)(616.5157, 1111.98)(599.5044, 8205.58)(600.5088, 3427.17)(601.5082, 1092.36)(602.5061, 211.12) 178994.2 61922.47 146416.9 60847.07 225823.5 39872.81 227258.3 40887.83 | 0.73 | 0.005892 | 0.013125 | 0.54 | 0.084252 | 0.346484 | | | | | | | | |
| COMPOUND_598_4978a11_762764 | Rp | + | 598.4978 | 11.76 | | | | (621.49, 1162.35)(622.4918, 820.16)(1219.9811, 238.71)(1220.9763, 264.31)(1221.9823, 177.87)(637.449, 972.23)(638.4581, 633.55)(616.5157, 1111.98)(599.5044, 8205.58)(600.5088, 3427.17)(601.5082, 1092.36)(602.5061, 211.12) 56745.9 30859.36 56233.43 22985.37 43255.25 25144.51 58148.73 30164.66 | -1.12 | 1.87E-06 | 8.79E-06 | -0.08 | 0.738715 | 0.888668 | | | | | | | | |
| COMPOUND_599_3261a1_0046843 | Hilic | + | 599.3261 | 1.00 | | | | (1199.649, 254.16)(622.3154, 1542.09)(623.3154, 582.44)(624.3303, 1269.53)(625.3316, 550.54)(617.3742, 260.02)(600.3325, 5924.14)(601.3349, 1877.18)(602.3478, 6075.38)(603.3514, 2001.34)(604.3513, 813.8)(605.3578, 183.69) (1237.8706, 119.23)(600.4688, 5464.06)(601.4666, 1874.78) (601.2663, 5745.87)(602.2697, 2251.81)(603.2717, 632.28)(604.2739, 135.25)(301.1316, 3414.22)(301.6338, 881.18)(302.1316, 328.87)(302.6313, 92.1) (601.5206, 69481.23)(602.5238, 29389.15)(603.526, 7410.71)(604.5261, 1403.47) (600.284, 61191.88)(601.2872, 19759.89)(602.2871, 6443.02)(603.2882, 1537.53)(604.2844, 251.81) (624.3263, 403.76)(625.3222, 154.6)(626.3031, 4050.55)(619.3584, 270.77)(602.3481, 7170.3)(603.3516, 2310.67)(604.3457, 920.83)(605.3606, 123.79) (637.1414, 27378.18)(638.1448, 5804.33)(639.1473, 862.19)(601.16, 1656.58)(602.1619, 518.23)(603.1521, 154.27)(1203.3563, 148.79) (602.3, 163911.81)(603.3029, 52615.02)(604.302, 16425.26)(605.3037, 4094.59)(606.3066, 773.78) (602.2999, 110280.84)(603.3027, 34572.08)(604.3022, 11315.06)(605.3045, 2672.43)(606.3071, 466.19) (1241.601, 933.23)(1242.6049, 823.56)(1243.6277, 1105.32)(1244.634, 631.01)(1245.6521, 233.15)(602.3007, 11318.58)(603.3035, 3651.22)(604.299, 4496.57)(605.3081, 1832.27)(606.3089, 796.47)(1319.5433, 569.5) (1209.5626, 682.28)(1210.5529, 712.43)(1211.5394, 680.43)(1247.4988, 625.87)(1248.4938, 410.87)(1249.4974, 496.86)(1250.4806, 531.49)(627.2509, 2748.13)(1251.5227, 322.31)(1252.497, 409.7)(1253.5172, 456.53)(1244.517, 536.48)(643.2524, 1007.55)(644.2535, 642.25)(605.2778, 13770.36)(606.2804, 5437.69)(607.2733, 831.77)(608.2891, 186.27)(1226.5468, 603.02)(1227.5319, 658.7) (1209.5647, 361.81)(1210.5529, 225.64)(1211.5468, 240.48)(1247.5123, 355.44)(1248.5, 433.47)(1249.5049, 468.03)(627.2717, 450.35)(1231.565, 206.51)(1232.5374, 138.13)(1233.5775, 176.87)(1234.5754, 105.09)(643.2549, 2709.96)(644.254, 1394.14)(645.2397, 700.67)(605.2795, 10792.86)(606.2829, 4192.95)(607.2714, 1253.14)(608.2873, 143.3)(1226.5608, 196.06)(1227.5488, 120.72) 58874.88 12934.36 60075.88 12958.59 46973.43 8757.667 51268.53 10434 | -0.49 | 0.095372 | 0.15643 | 0.06 | 0.86585 | 0.944172 | | | | | | | | |
| COMPOUND_599_4607a9_955438 | Rp | + | 599.4607 | 9.96 | | | | (1237.8706, 119.23)(600.4688, 5464.06)(601.4666, 1874.78) (601.2663, 5745.87)(602.2697, 2251.81)(603.2717, 632.28)(604.2739, 135.25)(301.1316, 3414.22)(301.6338, 881.18)(302.1316, 328.87)(302.6313, 92.1) (601.5206, 69481.23)(602.5238, 29389.15)(603.526, 7410.71)(604.5261, 1403.47) (600.284, 61191.88)(601.2872, 19759.89)(602.2871, 6443.02)(603.2882, 1537.53)(604.2844, 251.81) (624.3263, 403.76)(625.3222, 154.6)(626.3031, 4050.55)(619.3584, 270.77)(602.3481, 7170.3)(603.3516, 2310.67)(604.3457, 920.83)(605.3606, 123.79) (637.1414, 27378.18)(638.1448, 5804.33)(639.1473, 862.19)(601.16, 1656.58)(602.1619, 518.23)(603.1521, 154.27)(1203.3563, 148.79) (602.3, 163911.81)(603.3029, 52615.02)(604.302, 16425.26)(605.3037, 4094.59)(606.3066, 773.78) (602.2999, 110280.84)(603.3027, 34572.08)(604.3022, 11315.06)(605.3045, 2672.43)(606.3071, 466.19) (1241.601, 933.23)(1242.6049, 823.56)(1243.6277, 1105.32)(1244.634, 631.01)(1245.6521, 233.15)(602.3007, 11318.58)(603.3035, 3651.22)(604.299, 4496.57)(605.3081, 1832.27)(606.3089, 796.47)(1319.5433, 569.5) (1209.5626, 682.28)(1210.5529, 712.43)(1211.5394, 680.43)(1247.4988, 625.87)(1248.4938, 410.87)(1249.4974, 496.86)(1250.4806, 531.49)(627.2509, 2748.13)(1251.5227, 322.31)(1252.497, 409.7)(1253.5172, 456.53)(1244.517, 536.48)(643.2524, 1007.55)(644.2535, 642.25)(605.2778, 13770.36)(606.2804, 5437.69)(607.2733, 831.77)(608.2891, 186.27)(1226.5468, 603.02)(1227.5319, 658.7) (1209.5647, 361.81)(1210.5529, 225.64)(1211.5468, 240.48)(1247.5123, 355.44)(1248.5, 433.47)(1249.5049, 468.03)(627.2717, 450.35)(1231.565, 206.51)(1232.5374, 138.13)(1233.5775, 176.87)(1234.5754, 105.09)(643.2549, 2709.96)(644.254, 1394.14)(645.2397, 700.67)(605.2795, 10792.86)(606.2829, 4192.95)(607.2714, 1253.14)(608.2873, 143.3)(1226.5608, 196.06)(1227.5488, 120.72) 34179.46 9539.243 29402.9 6256.067 36208.85 6893.986 35909.07 9372.902 | 0.31 | 0.277487 | 0.376901 | 0.48 | 0.162292 | 0.475886 | | | | | | | | |
| COMPOUND_600_259a5_2416496 | Rp | + | 600.2590 | 5.24 | | | | (1237.8706, 119.23)(600.4688, 5464.06)(601.4666, 1874.78) (601.2663, 5745.87)(602.2697, 2251.81)(603.2717, 632.28)(604.2739, 135.25)(301.1316, 3414.22)(301.6338, 881.18)(302.1316, 328.87)(302.6313, 92.1) (601.5206, 69481.23)(602.5238, 29389.15)(603.526, 7410.71)(604.5261, 1403.47) (600.284, 61191.88)(601.2872, 19759.89)(602.2871, 6443.02)(603.2882, 1537.53)(604.2844, 251.81) (624.3263, 403.76)(625.3222, 154.6)(626.3031, 4050.55)(619.3584, 270.77)(602.3481, 7170.3)(603.3516, 2310.67)(604.3457, 920.83)(605.3606, 123.79) (637.1414, 27378.18)(638.1448, 5804.33)(639.1473, 862.19)(601.16, 1656.58)(602.1619, 518.23)(603.1521, 154.27)(1203.3563, 148.79) (602.3, 163911.81)(603.3029, 52615.02)(604.302, 16425.26)(605.3037, 4094.59)(606.3066, 773.78) (602.2999, 110280.84)(603.3027, 34572.08)(604.3022, 11315.06)(605.3045, 2672.43)(606.3071, 466.19) (1241.601, 933.23)(1242.6049, 823.56)(1243.6277, 1105.32)(1244.634, 631.01)(1245.6521, 233.15)(602.3007, 11318.58)(603.3035, 3651.22)(604.299, 4496.57)(605.3081, 1832.27)(606.3089, 796.47)(1319.5433, 569.5) (1209.5626, 682.28)(1210.5529, 712.43)(1211.5394, 680.43)(1247.4988, 625.87)(1248.4938, 410.87)(1249.4974, 496.86)(1250.4806, 531.49)(627.2509, 2748.13)(1251.5227, 322.31)(1252.497, 409.7)(1253.5172, 456.53)(1244.517, 536.48)(643.2524, 1007.55)(644.2535, 642.25)(605.2778, 13770.36)(606.2804, 5437.69)(607.2733, 831.77)(608.2891, 186.27)(1226.5468, 603.02)(1227.5319, 658.7) (1209.5647, 361.81)(1210.5529, 225.64)(1211.5468, 240.48)(1247.5123, 355.44)(1248.5, 433.47)(1249.5049, 468.03)(627.2717, 450.35)(1231.565, 206.51)(1232.5374, 138.13)(1233.5775, 176.87)(1234.5754, 105.09)(643.2549, 2709.96)(644.254, 1394.14)(645.2397, 700.67)(605.2795, 10792.86)(606.2829, 4192.95)(607.2714, 1253.14)(608.2873, 143.3)(1226.5608, 196.06)(1227.5488, 120.72) 25302.64 11319.7 22256.4 9673.97 16563.4 5107.665 16408.87 6671.785 | -0.87 | 6.53E-05 | 0.000211 | -0.25 | 0.302436 | 0.610641 | | | | | | | | |
| COMPOUND_600_5127a13_950206 | Rp | + | 600.5127 | 13.95 | | | | (1237.8706, 119.23)(600.4688, 5464.06)(601.4666, 1874.78) (601.2663, 5745.87)(602.2697, 2251.81)(603.2717, 632.28)(604.2739, 135.25)(301.1316, 3414.22)(301.6338, 881.18)(302.1316, 328.87)(302.6313, 92.1) (601.5206, 69481.23)(602.5238, 29389.15)(603.526, 7410.71)(604.5261, 1403.47) (600.284, 61191.88)(601.2872, 19759.89)(602.2871, 6443.02)(603.2882, 1537.53)(604.2844, 251.81) (624.3263, 403.76)(625.3222, 154.6)(626.3031, 4050.55)(619.3584, 270.77)(602.3481, 7170.3)(603.3516, 2310.67)(604.3457, 920.83)(605.3606, 123.79) (637.1414, 27378.18)(638.1448, 5804.33)(639.1473, 862.19)(601.16, 1656.58)(602.1619, 518.23)(603.1521, 154.27)(1203.3563, 148.79) (602.3, 163911.81)(603.3029, 52615.02)(604.302, 16425.26)(605.3037, 4094.59)(606.3066, 773.78) (602.2999, 110280.84)(603.3027, 34572.08)(604.3022, 11315.06)(605.3045, 2672.43)(606.3071, 466.19) (1241.601, 933.23)(1242.6049, 823.56)(1243.6277, 1105.32)(1244.634, 631.01)(1245.6521, 233.15)(602.3007, 11318.58)(603.3035, 3651.22)(604.299, 4496.57)(605.3081, 1832.27)(606.3089, 796.47)(1319.5433, 569.5) (1209.5626, 682.28)(1210.5529, 712.43)(1211.53 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|---------------|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_608_3721a10_5784855 | Rp | - | 608.3721 | 10.58 | | | | (943.3316, 261.79)(644.3334, 576.28)(645.34, 201.84)(721.3492, 1635.38)(607.3658, 9427.71)(608.3683, 4004.24)(609.366, 18075.55)(610.3691, 7330.01)(611.3621, 7912.14)(612.3652, 3697.03)(613.3649, 1867.1)(614.3618, 1093.0)(615.3603, 2140.5)(616.3648, 1679.64)(1329.6528, 346.28)(1330.6254, 136.11)(1331.6326, 338.29) | 46484.31 | 31198.25 | 54551.36 | 51063.54 | 51908.83 | 31710.86 | 71667.67 | 42471.42 | -0.09 | 0.718123 | 0.79314 | 0.81 | 0.005799 | 0.118614 |
| COMPOUND_609_1781a10_093475 | Rp | - | 609.1781 | 12.09 | | | | (1219.3135, 1588.34)(1220.3116, 1342.51)(610.185, 43769.18)(611.1857, 24975.33)(612.1834, 17824.51)(1236.3606, 637.65)(1237.3866, 315.06)(608.3173, 46736.48)(609.3205, 13628.42)(610.3221, 2951.0)(611.3247, 528.68)(1217.5789, 609.96)(1218.5544, 271.89)(608.317, 56959.8)(609.3205, 15599.15)(610.3225, 3695.19)(611.3283, 681.33)(1217.6484, 2205.68)(1218.65, 1224.21)(1219.6458, 562.67)(608.3172, 53156.0)(609.3205, 16249.65)(610.3238, 3477.43)(611.3286, 795.73)(1217.6481, 1809.81)(1218.6534, 1088.73)(1219.6484, 447.36)(632.3542, 1817.39)(633.3606, 516.25)(634.3699, 482.48)(610.372, 90615.27)(611.3755, 31457.0)(612.3783, 6317.9)(613.3806, 1441.04)(1219.7352, 666.47)(632.3553, 7566.27)(633.3578, 2692.49)(634.3706, 1553.55)(635.3722, 383.6)(627.4, 395.49)(648.3221, 1941.48)(610.3741, 174823.47)(611.3766, 55633.27)(612.3809, 11685.33)(613.3908, 2550.36)(722.512, 337.71)(723.5155, 14914.84)(724.5175, 4208.95)(725.5192, 1177.34)(726.5177, 347.04)(608.5249, 9443.13)(609.5274, 3991.63)(610.5305, 1028.62)(611.5326, 157.72)(654.4984, 219.73)(1242.0602, 599.49)(1243.0623, 660.84)(610.5421, 50728.67)(611.5449, 20979.19)(612.5498, 5143.26)(613.552, 926.93)(614.5543, 121.97)(1242.063, 289.79)(1243.0474, 297.51)(1244.0656, 235.35)(610.5419, 72649.63)(611.5448, 29355.51)(612.5486, 6996.27)(613.5523, 1133.4)(614.5486, 189.54)(1237.0634, 86.99)(1221.5262, 417.24)(1259.4862, 482.5)(1260.4958, 230.44)(633.2512, 1165.6)(1243.5286, 393.33)(628.2697, 1646.03)(629.2684, 740.94)(630.2722, 1048.16)(611.2446, 33038.63)(612.249, 16520.45)(613.2451, 12977.61)(1238.54, 392.79)(1239.5498, 276.77)(1240.534, 338.61)(1222.5187, 285.73)(1244.5511, 316.13)(611.771, 5232.23)(612.7714, 1793.54)(613.7541, 940.56)(614.7732, 229.49)(1239.544, 288.02)(1240.5497, 145.74)(612.3227, 7142.37)(613.3262, 2165.52)(614.3285, 604.29)(615.3245, 106.4)(634.5411, 4162.13)(635.5457, 1821.21)(636.5526, 945.46)(637.5381, 58.45)(650.5127, 510.96)(651.5182, 289.08)(652.5275, 2322.82)(613.5607, 9874.28)(614.564, 2336.47)(615.5687, 358.21)(1241.1774, 1173.43)(1225.554, 416.18)(1226.5427, 221.83)(1263.5457, 421.6)(1264.5151, 324.75)(635.2715, 1650.85)(1247.542, 272.27)(651.2497, 1194.01)(630.2883, 1964.42)(631.2843, 691.96)(632.2908, 2284.21)(633.2948, 837.46)(634.2865, 1560.27)(613.2609, 27930.26)(614.2659, 16380.36)(615.2611, 11391.36)(1242.5588, 386.81)(1225.492, 55.8)(1226.4543, 333.31)(1263.5323, 159.22)(1264.5435, 119.33)(635.27, 722.28)(1247.5325, 271.53)(651.2444, 1031.85)(630.2837, 1680.72)(631.2913, 1152.45)(632.2846, 2124.33)(633.2964, 1087.25)(634.2857, 1593.45)(613.2603, 23278.77)(614.2657, 13846.76)(615.2615, 10309.82)(1242.556, 258.28) | 278611.7 | 44950.3 | 249146 | 44008.72 | 268749.3 | 43768.27 | 274301.4 | 46709.23 | -0.30 | 0.297546 | 0.39767 | 0.72 | 0.03758 | 0.259604 |
| COMPOUND_609_3241a10_150996 | Rp | - | 609.3241 | 10.15 | | | | (608.3173, 46736.48)(609.3205, 13628.42)(610.3221, 2951.0)(611.3247, 528.68)(1217.5789, 609.96)(1218.5544, 271.89)(608.317, 56959.8)(609.3205, 15599.15)(610.3225, 3695.19)(611.3283, 681.33)(1217.6484, 2205.68)(1218.65, 1224.21)(1219.6458, 562.67)(608.3172, 53156.0)(609.3205, 16249.65)(610.3238, 3477.43)(611.3286, 795.73)(1217.6481, 1809.81)(1218.6534, 1088.73)(1219.6484, 447.36)(632.3542, 1817.39)(633.3606, 516.25)(634.3699, 482.48)(610.372, 90615.27)(611.3755, 31457.0)(612.3783, 6317.9)(613.3806, 1441.04)(1219.7352, 666.47)(632.3553, 7566.27)(633.3578, 2692.49)(634.3706, 1553.55)(635.3722, 383.6)(627.4, 395.49)(648.3221, 1941.48)(610.3741, 174823.47)(611.3766, 55633.27)(612.3809, 11685.33)(613.3908, 2550.36)(722.512, 337.71)(723.5155, 14914.84)(724.5175, 4208.95)(725.5192, 1177.34)(726.5177, 347.04)(608.5249, 9443.13)(609.5274, 3991.63)(610.5305, 1028.62)(611.5326, 157.72)(654.4984, 219.73)(1242.0602, 599.49)(1243.0623, 660.84)(610.5421, 50728.67)(611.5449, 20979.19)(612.5498, 5143.26)(613.552, 926.93)(614.5543, 121.97)(1242.063, 289.79)(1243.0474, 297.51)(1244.0656, 235.35)(610.5419, 72649.63)(611.5448, 29355.51)(612.5486, 6996.27)(613.5523, 1133.4)(614.5486, 189.54)(1237.0634, 86.99)(1221.5262, 417.24)(1259.4862, 482.5)(1260.4958, 230.44)(633.2512, 1165.6)(1243.5286, 393.33)(628.2697, 1646.03)(629.2684, 740.94)(630.2722, 1048.16)(611.2446, 33038.63)(612.249, 16520.45)(613.2451, 12977.61)(1238.54, 392.79)(1239.5498, 276.77)(1240.534, 338.61)(1222.5187, 285.73)(1244.5511, 316.13)(611.771, 5232.23)(612.7714, 1793.54)(613.7541, 940.56)(614.7732, 229.49)(1239.544, 288.02)(1240.5497, 145.74)(612.3227, 7142.37)(613.3262, 2165.52)(614.3285, 604.29)(615.3245, 106.4)(634.5411, 4162.13)(635.5457, 1821.21)(636.5526, 945.46)(637.5381, 58.45)(650.5127, 510.96)(651.5182, 289.08)(652.5275, 2322.82)(613.5607, 9874.28)(614.564, 2336.47)(615.5687, 358.21)(1241.1774, 1173.43)(1225.554, 416.18)(1226.5427, 221.83)(1263.5457, 421.6)(1264.5151, 324.75)(635.2715, 1650.85)(1247.542, 272.27)(651.2497, 1194.01)(630.2883, 1964.42)(631.2843, 691.96)(632.2908, 2284.21)(633.2948, 837.46)(634.2865, 1560.27)(613.2609, 27930.26)(614.2659, 16380.36)(615.2611, 11391.36)(1242.5588, 386.81)(1225.492, 55.8)(1226.4543, 333.31)(1263.5323, 159.22)(1264.5435, 119.33)(635.27, 722.28)(1247.5325, 271.53)(651.2444, 1031.85)(630.2837, 1680.72)(631.2913, 1152.45)(632.2846, 2124.33)(633.2964, 1087.25)(634.2857, 1593.45)(613.2603, 23278.77)(614.2657, 13846.76)(615.2615, 10309.82)(1242.556, 258.28) | 260367.1 | 30197.06 | 277329.3 | 33104.51 | 212359.8 | 30189.63 | 219256.2 | 31683.22 | -1.20 | 2.44E-06 | 1.11E-05 | -0.23 | 0.400943 | 0.690408 |
| COMPOUND_609_3244a10_274486 | Rp | - | 609.3244 | 10.27 | | | | (608.317, 56959.8)(609.3205, 15599.15)(610.3225, 3695.19)(611.3283, 681.33)(1217.6484, 2205.68)(1218.65, 1224.21)(1219.6458, 562.67)(608.3172, 53156.0)(609.3205, 16249.65)(610.3238, 3477.43)(611.3286, 795.73)(1217.6481, 1809.81)(1218.6534, 1088.73)(1219.6484, 447.36)(632.3542, 1817.39)(633.3606, 516.25)(634.3699, 482.48)(610.372, 90615.27)(611.3755, 31457.0)(612.3783, 6317.9)(613.3806, 1441.04)(1219.7352, 666.47)(632.3553, 7566.27)(633.3578, 2692.49)(634.3706, 1553.55)(635.3722, 383.6)(627.4, 395.49)(648.3221, 1941.48)(610.3741, 174823.47)(611.3766, 55633.27)(612.3809, 11685.33)(613.3908, 2550.36)(722.512, 337.71)(723.5155, 14914.84)(724.5175, 4208.95)(725.5192, 1177.34)(726.5177, 347.04)(608.5249, 9443.13)(609.5274, 3991.63)(610.5305, 1028.62)(611.5326, 157.72)(654.4984, 219.73)(1242.0602, 599.49)(1243.0623, 660.84)(610.5421, 50728.67)(611.5449, 20979.19)(612.5498, 5143.26)(613.552, 926.93)(614.5543, 121.97)(1242.063, 289.79)(1243.0474, 297.51)(1244.0656, 235.35)(610.5419, 72649.63)(611.5448, 29355.51)(612.5486, 6996.27)(613.5523, 1133.4)(614.5486, 189.54)(1237.0634, 86.99)(1221.5262, 417.24)(1259.4862, 482.5)(1260.4958, 230.44)(633.2512, 1165.6)(1243.5286, 393.33)(628.2697, 1646.03)(629.2684, 740.94)(630.2722, 1048.16)(611.2446, 33038.63)(612.249, 16520.45)(613.2451, 12977.61)(1238.54, 392.79)(1239.5498, 276.77)(1240.534, 338.61)(1222.5187, 285.73)(1244.5511, 316.13)(611.771, 5232.23)(612.7714, 1793.54)(613.7541, 940.56)(614.7732, 229.49)(1239.544, 288.02)(1240.5497, 145.74)(612.3227, 7142.37)(613.3262, 2165.52)(614.3285, 604.29)(615.3245, 106.4)(634.5411, 4162.13)(635.5457, 1821.21)(636.5526, 945.46)(637.5381, 58.45)(650.5127, 510.96)(651.5182, 289.08)(652.5275, 2322.82)(613.5607, 9874.28)(614.564, 2336.47)(615.5687, 358.21)(1241.1774, 1173.43)(1225.554, 416.18)(1226.5427, 221.83)(1263.5457, 421.6)(1264.5151, 324.75)(635.2715, 1650.85)(1247.542, 272.27)(651.2497, 1194.01)(630.2883, 1964.42)(631.2843, 691.96)(632.2908, 2284.21)(633.2948, 837.46)(634.2865, 1560.27)(613.2609, 27930.26)(614.2659, 16380.36)(615.2611, 11391.36)(1242.5588, 386.81)(1225.492, 55.8)(1226.4543, 333.31)(1263.5323, 159.22)(1264.5435, 119.33)(635.27, 722.28)(1247.5325, 271.53)(651.2444, 1031.85)(630.2837, 1680.72)(631.2913, 1152.45)(632.2846, 2124.33)(633.2964, 1087.25)(634.2857, 1593.45)(613.2603, 23278.77)(614.2657, 13846.76)(615.2615, 10309.82)(1242.556, 258.28) | 468845.8 | 99826.8 | 493242.5 | 102290.9 | 530295.9 | 121597.8 | 419730.8 | 170894.1 | 0.67 | 0.01972 | 0.03899 | -1.09 | 0.001679 | 0.06002 |
| COMPOUND_609_3245a10_26004 | Rp | - | 609.3245 | 10.26 | | | | (608.317, 56959.8)(609.3205, 15599.15)(610.3225, 3695.19)(611.3283, 681.33)(1217.6484, 2205.68)(1218.65, 1224.21)(1219.6458, 562.67)(608.3172, 53156.0)(609.3205, 16249.65)(610.3238, 3477.43)(611.3286, 795.73)(1217.6481, 1809.81)(1218.6534, 1088.73)(1219.6484, 447.36)(632.3542, 1817.39)(633.3606, 516.25)(634.3699, 482.48)(610.372, 90615.27)(611.3755, 31457.0)(612.3783, 6317.9)(613.3806, 1441.04)(1219.7352, 666.47)(632.3553, 7566.27)(633.3578, 2692.49)(634.3706, 1553.55)(635.3722, 383.6)(627.4, 395.49)(648.3221, 1941.48)(610.3741, 174823.47)(611.3766, 55633.27)(612.3809, 11685.33)(613.3908, 2550.36)(722.512, 337.71)(723.5155, 14914.84)(724.5175, 4208.95)(725.5192, 1177.34)(726.5177, 347.04)(608.5249, 9443.13)(609.5274, 3991.63)(610.5305, 1028.62)(611.5326, 157.72)(654.4984, 219.73)(1242.0602, 599.49)(1243.0623, 660.84)(610.5421, 50728.67)(611.5449, 20979.19)(612.5498, 5143.26)(613.552, 926.93)(614.5543, 121.97)(1242.063, 289.79)(1243.0474, 297.51)(1244.0656, 235.35)(610.5419, 72649.63)(611.5448, 29355.51)(612.5486, 6996.27)(613.5523, 1133.4)(614.5486, 189.54)(1237.0634, 86.99)(1221.5262, 417.24)(1259.4862, 482.5)(1260.4958, 230.44)(633.2512, 1165.6)(1243.5286, 393.33)(628.2697, 1646.03)(629.2684, 740.94)(630.2722, 1048.16)(611.2446, 33038.63)(612.249, 16520.45)(613.2451, 12977.61)(1238.54, 392.79)(1239.5498, 276.77)(1240.534, 338.61)(1222.5187, 285.73)(1244.5511, 316.13)(611.771, 5232.23)(612.7714, 1793.54)(613.7541, 940.56)(614.7732, 229.49)(1239.544, 288.02)(1240.5497, 145.74)(612.3227, 7142.37)(613.3262, 2165.52)(614.3285, 604.29)(615.3245, 106.4)(634.5411, 4162.13)(635.5457, 1821.21)(636.5526, 945.46)(637.5381, 58.45)(650.5127, 510.96)(651.5182, 289.08)(652.5275, 2322.82)(613.5607, 9874.28)(614.564, 2336.47)(615.5687, 358.21)(1241.1774, 1173.43)(1225.554, 416.18)(1226.5427, 221.83)(1263.5457, 421.6)(1264.5151, 324.75)(635.2715, 1650.85)(1247.542, 272.27)(651.2497, 1194.01)(630.2883, 1964.42)(631.2843, 691.96)(632.2908, 2284.21)(633.2948, 837.46)(634.2865, 1560.27)(613.2609, 27930.26)(614.2659, 16380.36)(615.2611, 11391.36)(1242.5588, 386.81)(1225.492, 55.8)(1226.4543, 333.31)(1263.5323, 159.22)(1264.5435, 119.33)(635.27, 722.28)(1247.5325, 271.53)(651.2444, 1031.85)(630.2837, 1680.72)(631.2913, 1152.45)(632.2846, 2124.33)(633.2964, 1087.25)(634.2857, 1593.45)(613.2603, 23278.77)(614.2657, 13846.76)(615.2615, 10309.82)(1242.556, 258.28) | 376782.9 | 202576.7 | 313742.8 | 233595.5 | 543037.6 | 132567.1 | 486932.1 | 127651.3 | 0.91 | 0.002142 | 0.005295 | -0.37 | 0.278131 | 0.585315 |
| COMPOUND_609_3643a11_1230482 | Hilic | - | 609.3643 | 1.12 | | | | (632.3542, 1817.39)(633.3606, 516.25)(634.3699, 482.48)(610.372, 90615.27)(611.3755, 31457.0)(612.3783, 6317.9)(613.3806, 1441.04)(1219.7352, 666.47)(632.3553, 7566.27)(633.3578, 2692.49)(634.3706, 1553.55)(635.3722, 383.6)(627.4, 395.49)(648.3221, 1941.48)(610.3741, 174823.47)(611.3766, 55633.27)(612.3809, 11685.33)(613.3908, 2550.36)(722.512, 337.71)(723.5155, 14914.84)(724.5175, 4208.95)(725.5192, 1177.34)(726.5177, 347.04)(608.5249, 9443.13)(609.5274, 3991.63)(610.5305, 1028.62)(611.5326, 157.72)(654.4984, 219.73)(1242.0602, 599.49)(1243.0623, 660.84)(610.5421, 50728.67)(611.5449, 20979.19)(612.5498, 5143.26)(613.552, 926.93)(614.5543, 121.97)(1242.063, 289.79)(1243.0474, 297.51)(1244.0656, 235.35)(610.5419, 72649.63)(611.5448, 29355.51)(612.5486, 6996.27)(613.5523, 1133.4)(614.5486, 189.54)(1237.0634, 86.99)(1221.5262, 417.24)(1259.4862, 482.5)(1260.4958, 230.44)(633.2512, 1165.6)(1243.5286, 393.33)(628 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--------------|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_628_1193a9_061208 | Rp | - | 628.1193 | 9.06 | | | | (741.0756, 535.97)(742.0801, 434.84)(663.078, 666.47)(664.0733, 310.32)(665.0739, 645.24)(627.113, 175.1663)(628.1161, 3663.05)(629.1099, 5745.91)(630.1129, 1106.07)(631.1073, 245.37)(1255.2314, 123.23)(1256.2126, 129.96)(673.0951, 1240.59)(674.1011, 669.37)(675.101, 1595.78)(676.1114, 736.28)(677.1053, 1415.31) | 104839.5 | 10185.83 | 105468.4 | 9484.196 | 95097.14 | 9783.255 | 97357.61 | 10692.24 | -0.94 | 0.001026 | 0.002671 | 0.15 | 0.639954 | 0.83305 |
| COMPOUND_628_1201a9_296112 | Rp | - | 628.1201 | 9.30 | | | | (627.1122, 10215.31)(628.116, 2192.65)(629.1093, 3417.05)(630.112, 802.45)(631.116, 193.25) | 59796.75 | 5347.91 | 59049.76 | 3675.786 | 57257.79 | 4365.68 | 57542.7 | 4458.322 | -0.55 | 0.068847 | 0.117368 | 0.16 | 0.658919 | 0.842895 |
| COMPOUND_628_2742a10_085511 | Rp | + | 628.2742 | 10.09 | | | | (1257.5173, 411.11)(1258.5002, 392.29)(1295.4783, 433.21)(1296.4727, 350.93)(651.2666, 652.73)(1279.5376, 309.69)(667.2543, 2794.7)(629.2793, 7724.77)(630.2814, 3056.8)(631.2606, 1274.27)(1274.5479, 249.02) | 43885.03 | 15414.07 | 37484.61 | 13719.19 | 28966 | 5741.462 | 41093.76 | 12444.25 | -0.91 | 0.00122 | 0.003116 | 1.02 | 0.002337 | 0.067469 |
| COMPOUND_628_2844a10_154417 | Rp | - | 628.2844 | 10.15 | | | | (1291.5294, 505.37)(1292.534, 353.14)(1293.5198, 428.81)(1294.5373, 324.62)(1295.5477, 429.43)(741.2635, 677.87)(742.2748, 2169.05)(663.273, 999.86)(1301.5688, 483.01)(1302.5452, 477.33)(1303.5819, 244.09)(627.278, 13530.3)(628.2797, 4484.82)(629.2822, 845.65)(630.267, 43.36)(1255.5757, 392.42)(1256.5702, 185.13)(1257.5885, 748.0)(1258.5892, 598.36)(1259.583, 303.14)(673.2816, 973.07)(1369.5402, 171.17)(1370.4996, 289.44) | 140526.3 | 31198.66 | 139356.3 | 33789.48 | 119782.1 | 48744.34 | 125590.2 | 46444.78 | -0.94 | 0.00134 | 0.00341 | 0.26 | 0.449699 | 0.722351 |
| COMPOUND_628_3806a8_966238 | Rp | - | 628.3806 | 8.97 | | | | (741.3396, 129.12)(627.3743, 6490.65)(628.3777, 2211.7)(629.3797, 588.0)(630.3833, 103.24)(1255.7858, 101.46)(1256.7642, 71.38) | 32746.21 | 13045.64 | 35595.72 | 10594.07 | 46148.64 | 28750.53 | 35736.39 | 16169.85 | 0.68 | 0.01305 | 0.026937 | -0.77 | 0.016504 | 0.189627 |
| COMPOUND_629_4718a9_663932 | Rp | + | 629.4718 | 9.66 | | | | (1259.9899, 67.07)(1261.9622, 71.77)(630.4791, 23085.24)(631.4796, 8162.3)(632.4763, 1835.59)(633.4826, 243.04) | 183354.9 | 49543.39 | 159464.1 | 30644.51 | 200937.7 | 34534.76 | 199228.7 | 51756.2 | 0.09 | 0.744074 | 0.814256 | 0.75 | 0.029366 | 0.231966 |
| COMPOUND_631_3713a13_408046 | Rp | + | 631.3713 | 13.41 | | | | (1301.6873, 152.95)(1302.7052, 106.3)(654.3553, 303.28)(655.3431, 102.61)(656.341, 3513.37)(670.3662, 381.07)(671.3492, 268.96)(632.3781, 12193.22)(633.3813, 4621.72)(634.3797, 1619.1)(635.3686, 172.86) | 98558.68 | 12603.17 | 98408.2 | 11595.75 | 104272.6 | 58364.56 | 100953.1 | 11996.31 | 0.51 | 0.096091 | 0.157266 | -0.27 | 0.455779 | 0.726923 |
| COMPOUND_632_2471a8_341707 | Rp | - | 632.2471 | 8.34 | | | | (631.2401, 11598.25)(632.2427, 4165.22)(633.2457, 994.91)(634.2522, 206.92) | 20888.31 | 9860.171 | 17130.57 | 7113.454 | 35990 | 20679.33 | 24428.84 | 14602.39 | 1.13 | 2.75E-06 | 1.24E-05 | -0.21 | 0.410399 | 0.694731 |
| COMPOUND_632_2479a8_347881 | Rp | + | 632.2479 | 8.35 | | | | (655.2375, 316.66)(656.2305, 167.52)(633.2572, 3351.64)(634.2607, 12652.3)(635.2618, 3028.49)(636.2677, 656.4) | 38035.77 | 22524.48 | 27604.33 | 15290.99 | 73320.86 | 42969.64 | 54255.84 | 35098.78 | 1.20 | 5.2E-06 | 2.2E-05 | -0.17 | 0.542998 | 0.776977 |
| COMPOUND_633_3245a10_110965 | Rp | - | 633.3245 | 10.11 | | | | (632.3169, 28624.94)(633.3206, 8679.49)(634.3227, 2141.8)(635.3257, 484.92) | 199888.3 | 36178.61 | 219086.8 | 36925.69 | 191424 | 30346.28 | 172567.9 | 35375.25 | -0.27 | 0.303023 | 0.403553 | -0.90 | 0.005169 | 0.111932 |
| COMPOUND_635_3401a10_379357 | Rp | - | 635.3401 | 10.38 | | | | (634.3331, 42354.2)(635.3364, 12960.27)(636.3404, 3069.79)(637.3422, 673.1)(638.358, 119.29) | 468863.9 | 68930.54 | 503956.6 | 64113.87 | 391899.3 | 54369.81 | 401535.4 | 65331.28 | -1.03 | 4.89E-05 | 0.000162 | -0.25 | 0.362721 | 0.668267 |
| COMPOUND_635_4167a0_7054705 | Hiic | + | 635.4167 | 0.71 | | | | (658.4204, 1309.92)(659.422, 595.47)(660.4244, 4081.37)(661.429, 1739.99)(662.438, 3069.49)(635.4643, 6418.05)(636.4241, 26944.14)(637.4276, 9809.72)(638.428, 2506.67)(639.4269, 666.61) | 398546.7 | 176504.9 | 360210.8 | 166514.6 | 62280.08 | 63714.81 | 53780.33 | 55044.05 | -1.47 | 4.84E-11 | 8.86E-10 | -0.04 | 0.842739 | 0.93246 |
| COMPOUND_635_4198a10_456654 | Rp | + | 635.4198 | 10.46 | | | | (658.4129, 3482.45)(659.4116, 1192.29)(660.4259, 21101.91)(636.4268, 11596.88)(637.4313, 4689.78)(638.4278, 4744.22)(639.436, 2630.07) | 128238.3 | 56475.52 | 123203.1 | 52869.51 | 86714.25 | 48602.58 | 51772.62 | 33990.61 | -1.15 | 1.34E-06 | 6.57E-06 | 0.04 | 0.890715 | 0.953702 |
| COMPOUND_635_5493a13_090127 | Rp | + | 635.5493 | 13.09 | | | | (1310.075, 62.69)(1311.028, 205.86)(658.5401, 3345.45)(659.5434, 1637.98)(660.5566, 4315.58)(661.5602, 2022.09)(1294.0208, 128.26)(636.5566, 19465.95)(637.5601, 8610.1)(638.5632, 2053.83)(639.5696, 399.85) | 88492.49 | 37213.17 | 95888.36 | 48601.7 | 96456.7 | 48014.79 | 136459.3 | 82056.96 | 0.16 | 0.522267 | 0.621521 | 0.61 | 0.04427 | 0.272788 |
| COMPOUND_635_5499a13_93558 | Rp | + | 635.5499 | 13.94 | | | | (1294.0326, 158.86)(636.5579, 134530.4)(637.5607, 56367.32)(638.5638, 13572.48)(639.5674, 2541.39)(640.5714, 463.43) | 49530 | 153698.3 | 512197.6 | 185960.9 | 574350.4 | 179786.4 | 771810.1 | 381324.3 | 0.37 | 0.19322 | 0.282004 | 0.43 | 0.208348 | 0.518913 |
| COMPOUND_635_5502a13_155785 | Rp | + | 635.5502 | 13.16 | | | | (1310.0504, 58.05)(658.5411, 17086.98)(659.5446, 7835.27)(660.5501, 2694.92)(661.5565, 742.51)(1294.0977, 188.48)(636.5559, 8712.93)(637.5594, 3581.18)(638.5635, 1088.14)(639.5649, 244.3) | 118274.5 | 55419.45 | 112092.8 | 63210.2 | 145161.9 | 43649.45 | 191117.7 | 98042.2 | 0.45 | 0.089549 | 0.147848 | 0.59 | 0.064589 | 0.307286 |
| COMPOUND_635_7758a10_339983 | Rp | + | 635.7758 | 10.34 | | | | (1272.5817, 264.16)(1310.4886, 254.85)(658.7882, 391.86)(659.7938, 1161.96)(636.7845, 10096.16)(637.7848, 1262.94)(638.7898, 1431.77) | 28083.3 | 17454.17 | 27922.48 | 15211.26 | 26559.78 | 5042.852 | 25395.26 | 6912.853 | -0.11 | 0.69545 | 0.77802 | -0.02 | 0.945212 | 0.974642 |
| COMPOUND_636_2998a10_393211 | Rp | + | 636.2998 | 10.39 | | | | (1273.6082, 626.17)(1274.6196, 359.47)(1275.5933, 194.65)(1311.5023, 283.39)(1312.5107, 324.99)(659.2877, 11863.67)(660.2928, 5112.41)(661.2859, 1827.87)(662.2713, 411.81)(1295.581, 1953.01)(1296.5897, 1259.38)(1297.6029, 770.91)(1298.576, 330.79)(654.3339, 32672.72)(655.3374, 12720.37)(656.3404, 2818.6)(657.342, 724.46)(637.3073, 56460.81)(638.3098, 19450.78)(639.3132, 4445.51)(640.3166, 1051.01)(641.3095, 193.59)(1290.6824, 416.47)(1291.725, 607.42) | 234195.2 | 80708.72 | 188720.4 | 80559.55 | 280929.4 | 91292.97 | 291158.2 | 109048.4 | 0.54 | 0.054443 | 0.094676 | 0.50 | 0.130311 | 0.425921 |
| COMPOUND_637_2869a10_376145 | Rp | - | 637.2869 | 10.38 | | | | (1309.5222, 353.03)(1310.5295, 339.37)(1311.5425, 376.11)(1319.5529, 326.96)(1320.5411, 394.42)(1321.5558, 275.71)(636.2827, 1346.52)(637.2767, 593.79)(638.276, 19992.51)(1273.5651, 970.56)(1274.5679, 658.55)(1275.5712, 663.04)(1276.5886, 363.28)(1277.5833, 583.69)(1278.5905, 472.47)(1279.575, 460.71)(1387.5345, 285.51)(1388.5399, 203.71)(1389.5358, 294.57) | 190867.8 | 22154.82 | 196504.3 | 22812.54 | 150242.1 | 16370.88 | 152515.4 | 23611.63 | -1.31 | 7.49E-08 | 4.88E-07 | -0.08 | 0.738034 | 0.888668 |
| COMPOUND_637_3555a10_62855 | Rp | - | 637.3555 | 10.63 | | | | (1309.6761, 135.08)(1310.6665, 50.38)(1311.6763, 204.11)(1312.672, 239.73)(1313.6458, 523589.2) | 173499.2 | 545538.2 | 207256.1 | 299722.6 | 200614.5 | 333546.7 | 180303.7 | -1.14 | 1.47E-05 | 5.69E-05 | -0.13 | 0.655605 | 0.841269 | |
| COMPOUND_637_3559a10_605653 | Rp | - | 637.3559 | 10.61 | | | | (520.03)(750.3196, 562.77)(751.3157, 467.83)(1319.7122, 227.79)(1320.7106, 274.44)(1321.7196, 250.96)(636.3485, 54855.3)(637.3517, 17231.3)(638.3528, 3973.48)(639.357, 818.04)(1273.7301, 303.93)(1274.7046, 122.69)(1275.7378, 337.08)(1276.7511, 327.96)(1277.764, 311.61)(1387.7448, 183.51)(1388.7648, 152.72)(1389.756, 214.31) | 314202.2 | 235039.5 | 306105.7 | 24126.2 | 307613.9 | 214418.4 | 354739.3 | 185798.9 | -0.52 | 0.086909 | 0.1437 | 0.29 | 0.422303 | 0.702743 |
| COMPOUND_637_396a1_0536169 | Hiic | + | 637.3960 | 1.05 | | | | (288.96)(1321.7155, 268.63)(636.3485, 52306.32)(637.3516, 16579.47)(638.3533, 3723.69)(639.3527, 685.77)(1273.7311, 333.73)(1274.758, 233.56)(1275.7677, 421.38)(1276.7664, 314.44)(1277.7595, 427.24)(1387.7183, 175.27)(1388.7351, 215.06)(1389.7449, 186.96) | 86499.47 | 72092.99 | 83276.76 | 62821.67 | 6375 | 353534 | 6451.75 | 531.3325 | -1.46 | 1.73E-13 | 1.26E-11 | -0.03 | 0.867294 | 0.9447 |
| COMPOUND_637_5662a13_674904 | Rp | + | 637.5662 | 13.67 | | | | (650.3859, 3700.71)(661.3984, 1701.63)(662.4031, 13851.36)(655.4257, 165.85)(638.4033, 60589.44)(639.4063, 20437.56)(640.4093, 4889.68)(641.4138, 896.26) | 196039.5 | 87855.06 | 209771.2 | 108764.2 | 171400.4 | 73710.97 | 314168.4 | 173952.2 | -0.25 | 0.341027 | 0.441883 | 1.02 | 0.00202 | 0.065137 |
| COMPOUND_637_5663a13_736985 | Rp | + | 637.5663 | 13.74 | | | | (1276.1637, 72.24)(660.5573, 4831.94)(661.5595, 2276.06)(662.5716, 4316.06)(638.5721, 53357.39)(639.5754, 22665.21)(640.5791, 5183.55)(641.5816, 968.34)(642.5857, 181.92) | 250680.4 | 120949.6 | 249141 | 115546.5 | 191151.6 | 53002.55 | 310526.5 | 169895 | -0.49 | 0.092439 | 0.152285 | 0.84 | 0.015907 | 0.188539 |
| COMPOUND_638_1482a9_060878 | Rp | - | 638.1482 | 9.06 | | | | (1276.0898, 53.34)(660.5572, 6084.68)(661.5594, 3030.01)(662.5676, 1732.09)(638.5725, 30207.86)(639.5758, 13138.52)(640.5788, 3244.9)(641.5842, 659.19)(642.5875, 106.75) | 303850.2 | 28681.78 | 306722.4 | 20998.68 | 272919.1 | 24369.26 | 286254.2 | 25046.94 | -1.21 | 3.83E-05 | 0.000131 | 0.40 | 0.2278 | 0.535498 |
| COMPOUND_638_1483a9_407069 | Rp | - | 638.1483 | 9.41 | | | | (1986.77)(640.162, 426.76) | 159407.5 | 13912.72 | 160929.6 | 11670.22 | 157919 | 10169.64 | 159794.7 | 12276.94 | -0.09 | 0.773046 | 0.833547 | -0.02 | 0.960606 | 0.981885 |
| COMPOUND_638_1487a9_295998 | Rp | - | 638.1487 | 9.30 | | | | (1311.2484, 280.36)(1312.2366, 83.19)(637.1414, 27378.18)(638.1448, 5804.33)(639.1473, 862.19)(640.1438, 199.13)(683.1476, 374.74)(684.1413, 60.25)(685.1299, 474.26) | 193931 | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--------------|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|-----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_639_3168a10_649515 | Rp | - | 639.3168 | 10.65 | | | | (674.2783, 1165.32)(675.2682, 506.29)(752.3089, 195.5)(753.2745, 300.51)(754.2992, 218.59)(755.2917, 448.72)(1325.6141, 266.29)(1324.6093, 247.25)(1328.3088, 1961.8)(639.3087, 743.44)(640.2918, 1645.08)(1277.5972, 747.73)(1278.5991, 412.31)(1279.6025, 362.07)(684.34, 1537.61) | 128032.9 | 14837.43 | 128656.9 | 18242.15 | 113490.2 | 12058.12 | 105329.6 | 24339.23 | -0.88 | 0.00098 | 0.002559 | -0.21 | 0.491039 | 0.748114 |
| COMPOUND_639_3305a12_429419 | Rp | - | 639.3305 | 12.43 | | | | (674.3081, 221.38)(675.3059, 166.42)(676.3095, 183.0)(677.3075, 140.57)(678.3092, 202.94)(638.3244, 633.43)(639.3219, 266.4)(640.3185, 716.93)(684.3111, 836.55)(685.3094, 409.62)(686.2995, 448.88) | 32866.83 | 4924.137 | 29726.48 | 4344.908 | 33720.21 | 4898.628 | 33211.16 | 5290.533 | 0.21 | 0.465334 | 0.569838 | 0.47 | 0.183022 | 0.496585 |
| COMPOUND_640_2871a10_397091 | Rp | - | 640.2871 | 10.40 | | | | (1315.5411, 416.82)(1316.5573, 447.18)(1317.5668, 341.81)(1318.5723, 365.03)(1319.5656, 295.06)(753.2747, 884.34)(754.2745, 522.8)(755.2686, 594.42)(1325.5577, 272.32)(1326.5422, 309.85)(1327.5695, 402.58)(1328.5569, 296.59)(1329.5686, 140.29)(1330.5247, 291.83)(1331.515, 271.44)(639.2785, 6808.39)(640.2862, 8263.77)(641.2892, 3155.52)(642.286, 585.35)(685.3623, 3109.64)(686.2653, 2561.36)(687.2658, 1188.93)(1279.586, 328.24)(1280.5596, 414.05)(1281.536, 271.57)(1393.558, 142.68)(1394.5698, 124.39)(1395.5388, 210.01)(1396.5214, 189.15)(1397.4978, 313.6) | 179087.7 | 80244.28 | 180806.4 | 79441.95 | 151951.8 | 36402.22 | 142909.5 | 39256.87 | 0.14 | 0.579626 | 0.67598 | -0.18 | 0.548635 | 0.77853 |
| COMPOUND_640_4301a10_924666 | Rp | - | 640.4301 | 10.92 | | | | (675.3858, 446.58)(676.4041, 1053.33)(677.3959, 657.17)(753.4051, 1279.58)(1325.8892, 56413.19)19815.21 64929.95 23512.69 100060.7 41699.35 121862.7 35233.18 259.53(1326.897, 368.79)(1327.8778, 383.41)(1328.8894, 382.56)(1329.9099, 320.09)(639.4149, 3703.47)(640.4159, 1411.61)(641.4187, 2175.47)(642.4172, 1181.32)(643.4178, 844.47)(1279.8237, 720.83)(1280.815, 987.95)(1281.8224, 1040.12)(685.4213, 8478.50)(686.4178, 7933.86)(1393.896, 264.03)(1394.859, 346.7) | 56413.19 | 19815.21 | 64929.95 | 23512.69 | 100060.7 | 41699.35 | 121862.7 | 35233.18 | 0.39 | 0.079284 | 0.132426 | 0.61 | 0.023655 | 0.219225 |
| COMPOUND_641_2616a10_1700945 | Rp | - | 641.2616 | 10.17 | | | | (1317.4768, 79.29)(1318.4911, 226.01)(1319.4976, 104.37)(754.2359, 1220.67)(755.2359, 223508.9)75566.47 211286.2 92490.52 205610.4 50599.3 205271.7 56836.37 645.04(756.2381, 2465.33)(757.2377, 1512.47)(758.2421, 1378.77)(759.2452, 672.53)(760.2526, 1044.63)(676.2324, 1220.89)(677.2316, 613.04)(678.2274, 1594.58)(679.2198, 818.35)(680.2405, 1671.86)(1327.4847, 240.31)(1328.4899, 373.99)(640.2547, 10661.26)(641.2576, 3497.53)(642.2597, 1483.22)(643.2609, 388.93)(1281.5015, 459.53)(1282.5096, 368.99)(1283.5144, 406.09)(686.258, 7324.82)(687.2613, 2401.63)(688.2604, 8799.33)(689.2637, 2626.46)(690.2588, 3854.08)(691.2589, 1376.80)(692.2611, 1194.49) | 75566.47 | 211286.2 | 92490.52 | 205610.4 | 50599.3 | 205271.7 | 56836.37 | -0.40 | 0.186667 | 0.274755 | 0.30 | 0.405977 | 0.691573 | |
| COMPOUND_641_2624a10_211116 | Rp | - | 641.2624 | 10.21 | | | | (1317.5281, 336.94)(1318.5327, 236.73)(1319.5255, 393.26)(754.242, 1072.24)(755.2449, 170560.9)96379.98 165740.1 95713.9 301790 139478.9 264060.4 137604.2 590.38(756.2402, 2588.25)(757.2384, 1559.57)(758.2442, 1423.14)(759.2417, 604.81)(760.2554, 1244.43)(676.2493, 1591.71)(677.2348, 459.28)(678.232, 1083.37)(679.2423, 461.02)(680.2419, 1754.22)(1327.4965, 279.9)(1328.5145, 241.91)(640.2549, 13408.94)(641.2583, 4853.79)(642.2584, 1594.69)(643.2622, 399.22)(1281.5015, 348.33)(1282.5073, 348.44)(1283.5107, 304.63)(686.2589, 5714.86)(687.2605, 1940.42)(688.2608, 9601.57)(689.2619, 3328.98)(690.2585, 3551.54)(691.2615, 1235.43)(692.2653, 1131.23) | 96379.98 | 165740.1 | 95713.9 | 301790 | 139478.9 | 264060.4 | 137604.2 | 1.00 | 0.000573 | 0.001576 | -0.19 | 0.571159 | 0.789098 | |
| COMPOUND_641_2959a10_507441 | Rp | - | 641.2959 | 10.51 | | | | (1317.5942, 160.67)(1318.5979, 141.14)(1319.6156, 169.84)(1320.5879, 214.86)(1321.5869, 136.97)(754.2249, 1254.21)(755.2412, 710.4)(676.288, 913.05)(677.2886, 485.95)(678.3041, 1159.13)(1327.5646, 259.25)(1328.5602, 319.05)(1329.5847, 275.61)(1330.5415, 255.95)(640.2908, 10045.78)(641.2929, 3849.65)(642.2935, 1613.45)(643.2986, 388.42)(686.2637, 580.31)(687.2691, 275.84)(688.2805, 910.91)(1281.5895, 352.53)(1282.5938, 313.02)(1283.594, 222.94)(1395.6398, 110.02)(1396.6156, 131.53)(1397.601, 116.49)(1398.6307, 130.53)(1399.6588, 84.89) | 49993.92 | 101639.9 | 48662.11 | 48736.45 | 26596.08 | 38239.06 | 16511.71 | -1.20 | 7.45E-07 | 3.85E-06 | -0.18 | 0.501774 | 0.75374 | |
| COMPOUND_641_2971a10_514763 | Rp | - | 641.2971 | 10.51 | | | | (1317.5942, 160.67)(1318.5979, 141.14)(1319.6156, 169.84)(1320.5879, 214.86)(1321.5869, 136.97)(754.2249, 1254.21)(755.2412, 710.4)(676.288, 913.05)(677.2886, 485.95)(678.3041, 1159.13)(1327.5646, 259.25)(1328.5602, 319.05)(1329.5847, 275.61)(1330.5415, 255.95)(640.2908, 10045.78)(641.2929, 3849.65)(642.2935, 1613.45)(643.2986, 388.42)(686.2637, 580.31)(687.2691, 275.84)(688.2805, 910.91)(1281.5895, 352.53)(1282.5938, 313.02)(1283.594, 222.94)(1395.6398, 110.02)(1396.6156, 131.53)(1397.601, 116.49)(1398.6307, 130.53)(1399.6588, 84.89) | 49993.92 | 101639.9 | 48662.11 | 48736.45 | 26596.08 | 38239.06 | 16511.71 | -1.20 | 7.45E-07 | 3.85E-06 | -0.18 | 0.501774 | 0.75374 | |
| COMPOUND_641_2985a10_65236 | Rp | - | 641.2985 | 10.65 | | | | (1317.6144, 131.47)(1318.5908, 133.8)(1319.6039, 98.29)(1320.5817, 85.16)(1321.5807, 85.02)(754.2331, 1097.73)(755.2379, 777.21)(676.2909, 928.33)(677.2863, 376.45)(678.3034, 1126.32)(1327.5696, 316.78)(1328.5768, 347.66)(1329.5891, 201.56)(1330.5928, 167.92)(640.2912, 1071.12)(641.2938, 4304.36)(642.295, 1523.63)(643.2983, 374.4)(644.2966, 68.31)(1281.603, 277.83)(1282.5929, 210.66)(1283.591, 306.0)(686.2634, 499.07)(687.2735, 232.67)(688.2764, 961.87)(1395.6431, 161.71)(1396.6395, 175.91)(1397.6374, 144.81)(1398.6307, 134.38)(1399.6115, 81.42) | 16197.22 | 17415.4 | 21649.01 | 151231.3 | 15922.82 | 147209.1 | 21394.05 | -0.87 | 0.001096 | 0.002831 | -0.30 | 0.323905 | 0.630999 | |
| COMPOUND_641_3025a10_552493 | Rp | - | 641.3025 | 10.55 | | | | (1317.5886, 125.41)(1318.57, 143.55)(1319.5796, 159.71)(1320.5814, 215.21)(1321.58, 200.61)(754.2364, 1046.95)(755.2392, 692.82)(676.2886, 1126.28)(677.2878, 541.1)(678.3054, 1748.95)(1327.626, 169.21)(1328.6381, 234.33)(1329.6229, 235.76)(1330.6213, 55.45)(640.2919, 12652.96)(641.2939, 5378.59)(642.2949, 1786.56)(643.2974, 479.19)(1281.6295, 222.4)(1282.6132, 302.0)(1283.6321, 167.11)(686.281, 586.75)(687.2625, 352.82)(688.2838, 945.86)(1395.6886, 133.89)(1396.6598, 160.25)(1397.6377, 176.61)(1398.6548, 105.81)(1399.6912, 111.44) | 17898.92 | 18399.41 | 72467.58 | 15655.96 | 40588.36 | 7059.905 | 48524.8 | 37150.78 | -1.44 | 0.404E-08 | 2.83E-07 | 0.21 | 0.449705 | 0.722351 |
| COMPOUND_641_5245a11_608373 | Rp | + | 641.5245 | 11.61 | | | | (1321.9551, 127.01)(1322.9895, 37.6)(680.4832, 1402.69)(681.4916, 1949.68)(682.4882, 1484.1)(659.5804, 912.05)(642.5309, 10921.14)(643.5352, 4563.61)(644.5394, 1444.48)(645.5365, 320.1) | 56638.56 | 75521.24 | 41286.43 | 40785.33 | 15195.65 | 40406.13 | 15236.24 | -1.07 | 2.08E-06 | 9.6E-06 | -0.05 | 0.831972 | 0.926681 | |
| COMPOUND_642_1857a10_314848 | Rp | + | 642.1857 | 10.31 | | | | (1285.3422, 268.43)(681.1549, 5486.32)(682.146, 1540.01)(683.1473, 721.61)(643.1901, 11027.72)(644.1964, 3296.93)(645.1871, 6289.26)(646.1907, 2519.11)(647.1949, 2396.88)(648.1969, 913.29)(649.1864, 424.61) | 11826.17 | 18763.64 | 13164.28 | 60583.14 | 13383.2 | 55969.72 | 13537.55 | 1.10 | 3.72E-05 | 0.000128 | 0.15 | 0.604101 | 0.810123 | |
| COMPOUND_642_5223a13_782367 | Rp | + | 642.5223 | 13.78 | | | | (665.5123, 8118.39)(666.5155, 3687.54)(667.5199, 988.71)(668.5178, 243.53)(681.4879, 848.15)(682.4949, 453.99)(683.4863, 310.16)(660.557, 19341.23)(661.5599, 8632.42)(662.5641, 2470.33)(663.5668, 622.67)(643.5313, 3990.37)(644.5374, 1991.74)(645.5373, 465.71)(646.5478, 97.43) | 42610.12 | 110781.3 | 49833.5 | 133653.1 | 67954.86 | 183684.1 | 81932.55 | 0.58 | 0.021627 | 0.042167 | 0.47 | 0.10824 | 0.391238 | |
| COMPOUND_643_4869a9_914848 | Rp | + | 643.4869 | 9.91 | | | | (1309.9836, 69.35)(644.495, 12158.0)(645.4961, 4533.27) | 81806.54 | 22779.34 | 70779.43 | 13436.16 | 89901.08 | 16251.57 | 89148.49 | 23278.34 | 0.27 | 0.323206 | 0.424408 | 0.68 | 0.043589 | 0.271169 |
| COMPOUND_644_2833a11_357574 | Rp | - | 644.2833 | 11.36 | | | | (757.276, 323.97)(758.2833, 174.29)(679.2473, 709.0)(680.2498, 358.99)(681.2478, 452.56)(682.2503, 261.6)(643.2767, 9632.56)(644.2791, 4106.78)(645.287, 1957.07)(646.2943, 501.81)(689.2505, 269.29)(690.2406, 264.56) | 30692.23 | 28714.54 | 30835 | 22075.85 | 61620.08 | 46047.46 | 38144.1 | 29467.11 | 0.72 | 0.006089 | 0.01351 | -0.34 | 0.252974 | 0.565176 |
| COMPOUND_644_2858a11_367559 | Rp | + | 644.2858 | 11.37 | | | | (1289.6403, 552.6)(667.2802, 5109.19)(668.2848, 2946.52)(669.2919, 1374.09)(670.2828, 357.79)(662.3138, 2959.88)(663.3001, 1861.84)(664.3294, 1863.17)(683.2395, 910.62)(645.293, 22696.91)(646.2961, 10340.67)(647.2983, 3432.83)(648.2994, 843.86) | 83462.02 | 110071.8 | 67535.66 | 164780.2 | 89381.31 | 130048.1 | 69293.41 | 0.41 | 0.075463 | 0.126728 | -0.29 | 0.282602 | 0.591468 | |
| COMPOUND_644_4898a0_916681 | Hiic | + | 644.4898 | 0.92 | | | | (667.4774, 275.8)(668.4738, 169.66)(669.4934, 1303.89)(670.4961, 577.56)(645.4968, 13008.84)(646.4998, 5411.64)(647.5123, 38549.45)(648.5154, 15176.74) | 37841.29 | 155833.2 | 45907.22 | 141992.3 | 36027.58 | 132602 | 41616.64 | 0.05 | 0.848512 | 0.894514 | -0.69 | 0.024655 | 0.219303 | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_645_4017a0_71836036 | Hilic | + | 645.4017 | 0.72 | | | | (668.3963, 1161.42)[669.3981, 330.98][670.4032, 461.46][671.4109, 239.84][646.4085, 46263.61][647.412, 16908.5][648.4204, 8835.16][649.4239, 2379.76] | 200577.4 | 96596.24 | 185253.3 | 88853.72 | 63681 | 29637.6 | 62031.67 | 22442.01 | -1.45 | 1.08E-11 | 2.68E-10 | 0.15 | 0.472005 | 0.734155 |
| COMPOUND_645_4017a10_47807 | Rp | + | 645.4017 | 10.48 | | | | (668.3923, 11369.09)[669.3977, 4456.17][670.4053, 3648.86][671.4142, 990.85][684.3875, 3241.37][663.4175, 6865.61][646.4101, 133691.85][647.414, 12558.78][648.4233, 12743.35][649.4326, 4831.2] | 338839.2 | 159438.7 | 261931.5 | 134138.6 | 96537.67 | 17355.17 | 105105.8 | 46400.86 | -1.35 | 2.15E-10 | 3.02E-09 | 0.19 | 0.378565 | 0.681478 |
| COMPOUND_645_4052a10_856795 | Rp | + | 645.4052 | 10.86 | | | | (1291.7972, 1387.12)[1329.7812, 734.99][1330.7706, 914.83][1331.7892, 1056.78][1332.7675, 766.12][1333.7627, 776.58][668.4026, 384.72][669.4118, 4616.3][670.419, 2532.66][1313.7673, 668.63][1314.7957, 973.52][1315.7802, 1002.01][684.3759, 5320.9][685.3759, 2904.0][686.3776, 6869.89][687.3822, 3335.2][646.4106, 19650.35][647.4132, 7526.24][648.4304, 5921.49][1308.8217, 612.09][1309.711, 705.48] | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.03 | 0.900188 | 0.934635 | 0.01 | 0.964075 | 0.981972 |
| COMPOUND_646_4198a10_843989 | Rp | - | 646.4198 | 10.84 | | | | (1327.7659, 736.31)[1328.7782, 624.78][1329.7699, 927.27][759.3795, 1039.52][1337.8843, 266.2][1338.8657, 295.17][1339.8442, 263.51][645.4146, 18097.91][646.4157, 5810.35][1291.8107, 431.71][1292.7845, 447.2][691.4596, 1177.62] | 27029.44 | 7165.596 | 30191.68 | 9951.74 | 26618.14 | 4583.083 | 31398.36 | 6666.988 | -0.67 | 0.013021 | 0.026902 | 0.67 | 0.032451 | 0.244873 |
| COMPOUND_646_4537a11_671692 | Rp | + | 646.4537 | 11.67 | | | | (669.4754, 968.87)[670.4738, 666.56][685.4322, 1467.28][686.4351, 774.33][687.4207, 365.68][647.4595, 69544.77][648.4626, 32330.21][649.4659, 7770.28][650.468, 1798.96][651.4511, 177.03] | 905607 | 299841.2 | 663036 | 216569.2 | 1071931 | 404482.7 | 1112322 | 378620.7 | 0.39 | 0.137464 | 0.212908 | 0.88 | 0.006026 | 0.121164 |
| COMPOUND_646_5049a0_916627 | Hilic | + | 646.5049 | 0.92 | | | | (659.4948, 1962.23)[670.5002, 847.47][671.5103, 850.2][664.5323, 393.69][647.5123, 38549.45][648.5154, 15176.74][649.5194, 3698.87][650.5126, 747.32][651.5323, 133.78] | 135478.7 | 37454.99 | 153252.4 | 46023.56 | 137897.1 | 35659.5 | 128681.1 | 40851.56 | 0.00 | 0.996714 | 0.999377 | -0.68 | 0.027559 | 0.226687 |
| COMPOUND_646_5058a11_263703 | Rp | + | 646.5058 | 11.26 | SM d30:1 | 2 | 20 eV: 184.0743(100), 647.5073(10), 89.0603(9) | (669.4752, 5891.05)[670.4743, 4665.07][671.4798, 8959.94][647.5138, 29694.61][648.516, 11731.71][649.5176, 2797.01][650.5101, 569.4] | 198070.5 | 52117.68 | 189297.8 | 58450.14 | 181041.3 | 41094.43 | 188588.1 | 44991.26 | -0.40 | 0.13698 | 0.212305 | 0.26 | 0.402158 | 0.691103 |
| COMPOUND_649_4368a10_522202 | Rp | + | 649.4368 | 10.52 | | | | (672.4246, 12533.83)[673.4295, 5108.53][674.4375, 4175.28][650.4397, 13131.24][651.4436, 5014.43][652.4255, 2721.24][653.4266, 356.35] | 300812.4 | 133891.1 | 303184.9 | 126017.9 | 72985.5 | 62411.38 | 37668.67 | 18657.21 | -0.76 | 0.00039 | 0.001104 | -0.31 | 0.203442 | 0.5149 |
| COMPOUND_651_1819a8_603599 | Rp | + | 651.1819 | 8.60 | | | | (652.1872, 6161.9)[653.1902, 1432.59][654.1854, 256.79][1320.4149, 132.9] | 18185.08 | 3527.807 | 17746.24 | 3561.262 | 20095 | 3732.392 | 18778.16 | 3497.315 | 0.26 | 0.366875 | 0.469434 | -0.04 | 0.915146 | 0.961085 |
| COMPOUND_651_2815a10_040113 | Rp | - | 651.2815 | 10.04 | | | | (1337.5013, 292.67)[1338.4937, 357.63][1339.5161, 307.57][764.2627, 404.04][765.2571, 154.41][766.2608, 404.86][767.2621, 73.88][686.259, 5546.99][687.261, 1864.19][688.2589, 9183.69][1347.5311, 315.93][1348.5214, 248.71][1349.5084, 237.38][650.2757, 2078.87][651.2777, 8872.2][652.2785, 2637.3][653.2798, 721.57][1301.5693, 426.41][1302.5452, 409.14][1303.5834, 221.61][696.2733, 2616.36][697.2719, 840.15][1415.4854, 232.26][1416.4403, 207.0] | 169796.4 | 128308.9 | 216103 | 137439.8 | 193617.9 | 117677.1 | 162650.6 | 112602.1 | -0.11 | 0.710548 | 0.788253 | -0.68 | 0.053067 | 0.287276 |
| COMPOUND_651_3547a12_427157 | Rp | - | 651.3547 | 12.43 | | | | (650.3476, 10792.92)[651.351, 4511.67][652.3538, 1206.89][653.3561, 296.56] | 87915.15 | 6931.52 | 88385.98 | 5841.067 | 88983.36 | 7621.055 | 88722.21 | 6587.239 | 0.19 | 0.498777 | 0.599888 | 0.54 | 0.120231 | 0.410243 |
| COMPOUND_652_2754a10_083093 | Rp | + | 652.2754 | 10.08 | | | | (1343.4572, 219.49)[1344.4543, 187.23][1327.4915, 185.34][691.3336, 1074.97][692.2273, 781.48][693.2295, 181.69][653.2791, 6033.22][654.2843, 2154.09][655.2765, 889.79][656.2906, 223.98] | 22438.67 | 6555.603 | 19317.03 | 3833.98 | 18517.38 | 5381.784 | 22918.44 | 6006.372 | -0.73 | 0.00887 | 0.019026 | 0.73 | 0.027385 | 0.226687 |
| COMPOUND_653_3194a10_597453 | Rp | - | 653.3194 | 10.60 | | | | (1341.6101, 217.83)[1342.5958, 209.56][1343.5715, 229.71][688.2804, 1141.39][689.2767, 828.14][690.2747, 684.41][766.3045, 1786.16][767.2983, 1423.57][768.2949, 997.49][769.2958, 194.93][1351.73, 259.09][1352.7029, 217.26][652.3145, 3725.22][653.3211, 1123.44][654.3072, 39198.9][698.3172, 5284.36][699.309, 4365.81][700.3073, 1698.62][701.312, 504.38][1305.6095, 320.74][1306.6147, 268.74][1307.6104, 405.23][149.5688, 228.61] | 262828.9 | 148108.8 | 233004 | 144706.9 | 255308 | 170496.9 | 237250.8 | 139679 | -0.64 | 0.030382 | 0.056969 | 0.19 | 0.580069 | 0.794113 |
| COMPOUND_653_3208a10_647613 | Rp | - | 653.3208 | 10.65 | | | | (766.3045, 1786.16)[767.2983, 1423.57][768.2949, 997.49][769.2958, 194.93][1351.73, 259.09][1352.7029, 217.26][652.3145, 3725.22][653.3211, 1123.44][654.3072, 39198.9][698.3172, 5284.36][699.309, 4365.81][700.3073, 1698.62][701.312, 504.38][1305.6095, 320.74][1306.6147, 268.74][1307.6104, 405.23][149.5688, 228.61] | 474389.9 | 48467.69 | 465951.3 | 97305.23 | 369551.6 | 97956.62 | 383780.5 | 59610.67 | -1.21 | 5.12E-06 | 2.17E-05 | 0.08 | 0.76792 | 0.902789 |
| COMPOUND_653_5592a11_6700115 | Rp | + | 653.5592 | 11.67 | | | | (1043.999)[698.3184, 6563.41][699.3097, 5363.67][700.31, 2097.91][701.3119, 592.55][1305.6178, 246.77][1306.6222, 176.37][1307.6351, 436.43][1308.6284, 253.12] | 262828.9 | 148108.8 | 233004 | 144706.9 | 255308 | 170496.9 | 237250.8 | 139679 | -1.18 | 5.47E-07 | 2.92E-06 | 0.19 | 0.439253 | 0.715597 |
| COMPOUND_654_5058a11_672439 | Rp | - | 654.5058 | 11.67 | | | | (1330.156, 88.97)[671.5682, 2666.77][672.5686, 898.2][654.5673, 2081.75][655.5704, 9128.46][656.5674, 2980.81][657.5774, 514.58] | 143941.1 | 86927.02 | 121220.1 | 75829.63 | 140204.7 | 48053.8 | 93784.17 | 62516.07 | -1.18 | 7.69E-08 | 4.97E-07 | -0.25 | 0.284287 | 0.593016 |
| COMPOUND_655_139a9_063978 | Rp | - | 655.1390 | 9.06 | | | | (653.4985, 21537.19)[654.5016, 9328.94][655.5041, 2293.3][656.5057, 468.6] | 63756.15 | 34742.27 | 72520.91 | 30012.92 | 39430.25 | 19526.95 | 53688.36 | 25661.81 | -1.18 | 7.69E-08 | 4.97E-07 | -0.25 | 0.284287 | 0.593016 |
| COMPOUND_655_3087a9_856484 | Rp | - | 655.3087 | 9.86 | | | | (768.1448, 250.64)[769.1407, 3828.7][770.1437, 1033.83][690.1124, 224.87][691.1204, 998.13][692.1134, 517.34][654.132, 6775.35][655.1337, 1476.21][656.1364, 322.7] | 25223.11 | 27322.73 | 18234.12 | 4368.089 | 19807.5 | 7055.327 | 20579.64 | 4917.659 | -0.71 | 0.006703 | 0.014784 | 0.78 | 0.013001 | 0.173893 |
| COMPOUND_655_3176a10_095957 | Rp | - | 655.3176 | 10.10 | | | | (654.3012, 17953.63)[655.3051, 5644.1][656.3065, 1446.25][657.3076, 362.47] | 38062.28 | 21979.54 | 34390.29 | 17557.97 | 22592.33 | 7040.171 | 25963.07 | 8458.036 | -1.18 | 4.35E-07 | 2.41E-06 | 0.25 | 0.301058 | 0.609696 |
| COMPOUND_656_3167a10_65436 | Rp | - | 656.3167 | 10.65 | | | | (654.3087, 2698.71)[655.313, 1263.56][656.3162, 8959.67] | 69998.11 | 18731.41 | 73936.33 | 15508.37 | 45905.55 | 7592.888 | 53782.8 | 11836.44 | -0.27 | 0.321974 | 0.423801 | -0.07 | 0.822056 | 0.922833 |
| COMPOUND_656_471a9_638034 | Rp | + | 656.4710 | 9.64 | | | | (1347.5841, 262.23)[1348.5775, 150.16][1349.5895, 245.51][769.2862, 618.07][770.2789, 498.79][771.2799, 96.63][691.2838, 570.28][1357.68, 287.7][1358.6558, 242.67][655.3088, 13960.76][656.3105, 4891.58][657.3125, 1097.27][658.3183, 219.8][659.314, 28.84][1311.6564, 247.79][1312.6826, 159.58][1313.6428, 567.51][1314.6466, 529.39][1315.6292, 377.36][701.3099, 853.6][702.3047, 721.06] | 271641.6 | 67986.5 | 252091.6 | 51076.81 | 291942.3 | 51663.97 | 294476.2 | 72556.57 | 0.20 | 0.482366 | 0.58406 | 0.44 | 0.208449 | 0.518913 |
| COMPOUND_656_4989a11_759014 | Rp | + | 656.4989 | 11.76 | | | | (346.2788, 989.51)[346.773, 209.71][1313.9813, 60.28][679.4592, 1291.73][680.4596, 603.82][681.4575, 404.35][695.4593, 364.44][674.5054, 20904.73][675.5076, 7716.32][676.4923, 3143.82][677.5105, 446.33][678.5174, 78.86][657.4769, 3173.26][658.4804, 1287.48][659.4741, 518.66][329.246, 3058.73][329.7387, 50.99][330.2522, 517.25] | 134638.3 | 54635.09 | 151552.2 | 53232.36 | 114361.3 | 65631.25 | 169024.4 | 54619.7 | -0.97 | 3.02E-05 | 0.000107 | -0.31 | 0.230558 | 0.537492 |
| COMPOUND_657_3229a10_032313 | Rp | - | 657.3229 | 10.03 | | | | (1313.9818, 171.61)[674.5079, 5185.12][657.508, 21569.58][658.5117, 8990.35][659.5163, 2498.0][660.5195, 537.76] | 22603.81 | 16597.53 | 29321.63 | 24040.15 | 36363.91 | 16694.23 | 37625.2 | 18978.52 | -0.01 | 0.973736 | 0.985552 | -0.05 | 0.880023 | 0.950612 |
| COMPOUND_657_3237a10_083144 | Rp | - | 657.3237 | 10.08 | | | | (770.2938, 281.34)[1359.6316, 51.98][1360.6042, 111.47][656.3168, 7354.64][657.3174, 2609.87][658.3216, 856.28][659.3233, 93.02] | 67541.91 | 26484.34 | 66170.63 | 27771.17 | 44109.85 | 12774.42 | 54854.6 | 16654.15 | -1.10 | 0.00025 | 0.000729 | 0.50 | 0.142192 | 0.448182 |
| COMPOUND_659_3395a10_30282 | Rp | - | 659.3395 | 10.30 | | | | (1204.53)[659.3217, 260.49] | 67541.91 | 26484.34 | 66170.63 | 27771.17 | 44109.85 | 12774.42 | 54854.6 | 16654.15 | -1.10 | 0.00025 | 0.000729 | 0.50 | 0.142192 | 0.448182 |
| COMPOUND_659_4197a10_549629 | Rp | + | 659.4197 | 10.55 | | | | (658.3325, 7008.41)[659.3353, 2206.22][660.3397, 885.53][661.3402, 184.8] | 26039.62 | 8281.057 | 27551.09 | 8168.247 | 32893.93 | 31610.99 | 29081.73 | 8341.729 | 0.10 | 0.730068 | 0.803968 | 0.08 | 0.815103 | 0.92157 |
| COMPOUND_659_4814a9_375362 | Rp | + | 659.4814 | 9.38 | | | | (682.4062, 17897.64)[683.4108, 7033.72][684.4151, 4196.56][685.4337, 975.76][698.4088, 1969.03][699.3924, 201.33 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | | | | | | | | |
|------------------------------|--------|----------|----------------|----------------|----------|--------------|---|---------------|----------|---------------|----------|---------------|-----------|---------------|----------|--------------------|----------|----------|-------------|----------|----------|---------|---------|------|----------|----------|-------|----------|----------|
| | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | | | | | | | | |
| | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | | | | | | | | |
| COMPOUND_660_5218a0_9025708 | Hilic | + | 660.5218 | 0.90 | | | (683.5173, 713.06)(684.5128, 298.81)(685.5283, 341.1)(678.5578, 6018.52)(661.5281, 11326.26)(662.5316, 4601.78)(663.5336, 967.97)(664.5351, 243.22) | 66336.27 | 16374.19 | 72766.8 | 22973 | 66664.64 | 15633.62 | 61348.14 | 16240.21 | 0.00 | 0.987379 | 0.994444 | -0.62 | 0.047169 | 0.27735 | | | | | | | | |
| COMPOUND_661_3967a1_0089915 | Hilic | + | 661.3967 | 1.01 | | | (684.3899, 2825.81)(685.3901, 803.43)(686.4031, 1047.96)(687.4194, 589.64)(662.4032, 22510.94)(663.408, 8233.37)(664.4169, 4105.82)(665.4248, 1156.22) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.39 | 5.7E-12 | 1.57E-10 | -0.01 | 0.96453 | 0.981972 | | | | | | | | |
| COMPOUND_661_5655a13_280865 | Rp | + | 661.5655 | 13.28 | | | (684.5564, 1700.98)(685.5594, 825.65)(686.5722, 10365.06)(662.5724, 35360.2)(663.5755, 16253.5)(664.5783, 4125.1)(665.5823, 804.92)(666.5867, 136.71) | 125896.1 | 65684.05 | 115605.4 | 69650.57 | 141229.2 | 36095.49 | 188441.1 | 112294.5 | 0.42 | 0.134079 | 0.208527 | 0.53 | 0.113907 | 0.400254 | | | | | | | | |
| COMPOUND_662_4503a12_871078 | Rp | + | 662.4503 | 12.87 | | | (1325.8964, 4112.47)(1326.9025, 3740.35)(1327.904, 1823.14)(1328.9048, 702.42)(1329.9103, 210.08)(1330.9148, 353.89)(1331.9184, 262.37)(685.4369, 15036.00)(686.4396, 7387.51)(687.4435, 1766.21)(688.4466, 338.03)(689.4363, 70.63)(1347.8374, 881.59)(1348.8241, 639.09)(1349.8071, 682.06)(1350.81, 634.0)(701.4103, 1445.56)(702.4144, 731.64)(703.4131, 411.74)(680.482, 1260.92)(681.4829, 505.63)(682.4875, 70.43)(663.4561, 177122.25)(664.4589, 81878.22)(665.4619, 18639.52)(666.4643, 3289.35)(667.4661, 645.46)(668.4632, 96.32)(1342.926, 1351.52)(1343.9319, 1201.44)(1344.9347, 568.0)(1345.9473, 294.08)(1346.9417, 118.76)(686.5722, 4281.22)(687.5753, 2054.35)(688.583, 1201.93)(664.5881, 60944.59)(665.5912, 27802.11)(666.5945, 6693.88)(667.5943, 1386.02)(668.5978, 265.48) | 2831840 | 862529.2 | 2489481 | 515762 | 2300344 | 497108.2 | 2416858 | 749479.6 | -0.66 | 0.026341 | 0.050186 | 0.44 | 0.211017 | 0.519294 | | | | | | | | |
| COMPOUND_663_5814a13_940646 | Rp | + | 663.5814 | 13.94 | | | (1365.5002, 323.92)(1366.4836, 198.53)(1367.5173, 222.88)(778.2322, 1055.0)(779.2278, 210873.8) (2735.24, 210055.7) (37273.55, 210072.6) (21091.64, 192515.2) (28435.33, 865.42)(703.2354, 388.87)(704.2439, 1058.58)(1375.4968, 199.21)(1376.4762, 237.76)(1377.4882, 310.21)(664.2546, 5777.17)(665.2575, 2082.42)(666.2691, 1462.62)(667.259, 292.98)(1329.5039, 249.27)(1330.4996, 289.27)(1331.4679, 394.93)(1332.4946, 316.86)(1333.5079, 259.72)(710.2522, 2367.26)(711.254, 744.92)(712.2591, 5164.42)(713.2622, 1734.73)(714.2575, 2296.48)(715.2597, 869.97)(716.2596, 1010.0)(1443.4474, 240.75)(1444.476, 197.13) | 246000.9 | 136052.9 | 224636.8 | 142738.5 | 248943.1 | 93455.68 | 383503.7 | 257729.7 | 0.24 | 0.39613 | 0.500048 | 0.63 | 0.068653 | 0.319436 | | | | | | | | |
| COMPOUND_665_2605a10_106638 | Rp | - | 665.2605 | 10.11 | | | (1365.5002, 323.92)(1366.4836, 198.53)(1367.5173, 222.88)(778.2322, 1055.0)(779.2278, 210873.8) (2735.24, 210055.7) (37273.55, 210072.6) (21091.64, 192515.2) (28435.33, 865.42)(703.2354, 388.87)(704.2439, 1058.58)(1375.4968, 199.21)(1376.4762, 237.76)(1377.4882, 310.21)(664.2546, 5777.17)(665.2575, 2082.42)(666.2691, 1462.62)(667.259, 292.98)(1329.5039, 249.27)(1330.4996, 289.27)(1331.4679, 394.93)(1332.4946, 316.86)(1333.5079, 259.72)(710.2522, 2367.26)(711.254, 744.92)(712.2591, 5164.42)(713.2622, 1734.73)(714.2575, 2296.48)(715.2597, 869.97)(716.2596, 1010.0)(1443.4474, 240.75)(1444.476, 197.13) | 150873.8 | 2735.24 | 210055.7 | 37273.55 | 210072.6 | 21091.64 | 192515.2 | 28435.33 | -0.15 | 0.588852 | 0.683906 | -0.58 | 0.080919 | 0.340768 | | | | | | | | |
| COMPOUND_665_2821a10_3792715 | Rp | - | 665.2821 | 10.38 | | | (1365.539, 262.11)(1366.5197, 275.53)(1367.5381, 382.64)(1368.525, 236.43)(1369.5162, 273.7)(778.2324, 1118.07)(1375.6078, 137.26)(1376.5886, 156.62)(1377.6038, 150.76)(664.2683, 943.68)(665.273, 581.43)(666.2703, 12541.6)(1329.5496, 388.47)(1443.4968, 225.56)(1444.4974, 183.81)(1445.4807, 155.29) | 700.2938 | 390.37 | 701.2941 | 149.14 | 702.2963 | 86.55 | 664.3176 | 4752.85 | 665.3211, 17877.92 | 4029.204 | 17958.65 | 4994.608 | 20654.73 | 6709.355 | 18145.7 | 4845.24 | 0.38 | 0.180981 | 0.268138 | -0.33 | 0.332924 | 0.636996 |
| COMPOUND_665_3256a5_558744 | Rp | - | 665.3256 | 5.56 | | | (1681.06)(666.3237, 445.05)(667.3223, 52.63)(1443.5835, 108.15) | 1681.06 | 666.3237 | 445.05 | 667.3223 | 52.63 | 1443.5835 | 108.15 | | | | | | | | | | | | | | | |
| COMPOUND_665_326a0_84776014 | Hilic | + | 665.3260 | 0.85 | | | (668.3166, 1037.07)(689.3185, 399.69)(690.3177, 279.62)(666.3333, 48279.41)(667.3364, 15614.73)(668.344, 7047.74)(669.3491, 1972.76)(670.3526, 403.08)(333.6723, 374.29)(334.175, 193.91) | 157357.5 | 66770.38 | 185143 | 79911.73 | 207142.3 | 89945.11 | 183271.4 | 71894.06 | 0.37 | 0.203465 | 0.294704 | -0.42 | 0.231965 | 0.537875 | | | | | | | | |
| COMPOUND_665_33a5_5597057 | Rp | + | 665.3300 | 5.56 | | | (688.3151, 1445.12)(689.3175, 461.93)(690.3212, 129.22)(363.6369, 182.49)(364.1428, 72.82)(352.6458, 1651.65)(353.1475, 612.33)(353.6447, 256.42)(344.6649, 6151.27)(345.1671, 2172.39)(345.6667, 722.45)(346.176, 205.35)(704.2891, 134.69)(342.1858, 540117.04)(342.6874, 20641.86)(343.1891, 4677.26)(343.6906, 1089.22)(666.3338, 18414.08)(667.3371, 6271.91)(668.3398, 1732.81)(669.345, 385.05)(333.6727, 1813.15)(334.1752, 908.88)(334.6722, 140.89) | 237082.1 | 95833.92 | 228826.3 | 85760.94 | 276916.5 | 120284.4 | 257300.7 | 107648 | 0.39 | 0.185906 | 0.273992 | -0.11 | 0.759856 | 0.896853 | | | | | | | | |
| COMPOUND_665_3573a11_082845 | Rp | + | 665.3573 | 11.08 | | | (1369.7261, 414.07)(688.3359, 3719.17)(1353.7106, 152.39)(1354.7219, 217.81)(1355.7274, 288.06)(704.3263, 10302.49)(705.3245, 3481.17)(706.3235, 2314.57)(683.3886, 842.97)(666.3686, 50153.41)(667.3716, 19718.92)(668.3723, 4619.56)(669.3699, 924.52) | 111745.3 | 51255.45 | 110238.8 | 53053.51 | 178112.8 | 21501.7 | 185670.9 | 72978.24 | 0.95 | 1.24E-05 | 4.88E-05 | 0.22 | 0.360257 | 0.666906 | | | | | | | | |
| COMPOUND_665_4067a10_706241 | Rp | - | 665.4067 | 10.71 | | | (1365.7634, 335.15)(1366.7332, 468.86)(1367.7592, 310.7)(778.3765, 1288.35)(779.3936, 1819.39)(780.4021, 822.93)(1375.8785, 563.34)(1376.8574, 74.84)(1377.8679, 570.39)(664.3988, 2964.97)(665.3993, 1414.17)(666.394, 6149.21)(667.398, 4574.72)(668.3997, 1989.22)(1329.7875, 382.45)(1330.7861, 235.07)(1331.8132, 242.33)(1332.828, 334.91)(1333.8344, 605.1)(710.4112, 6295.46)(1443.8156, 463.91)(1444.8206, 299.75) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.69 | 0.008213 | 0.017767 | 0.01 | 0.968758 | 0.982722 | | | | | | | | |
| COMPOUND_665_4237a10_47626 | Rp | - | 665.4237 | 10.48 | | | (778.4352, 1095.77)(700.4107, 2021.63)(701.404, 749.66)(702.4043, 2055.64)(1375.9225, 97294.59) (50678.3, 117444.2) (74811.24, 12594.67) (2096.101, 24009.75) (9791.371, 414.86)(1376.9128, 534.46)(1377.883, 854.03)(1378.8798, 672.84)(1379.8861, 1090.39)(664.419, 38658.23)(665.4222, 14373.77)(666.4241, 3791.79)(667.4247, 985.46)(1329.8396, 521.69)(1330.8403, 378.79)(1331.8395, 762.31)(710.4195, 1603.16)(711.4187, 705.67) | 97294.59 | 50678.3 | 117444.2 | 74811.24 | 12594.67 | 2096.101 | 24009.75 | 9791.371 | -1.28 | 2.96E-09 | 2.79E-08 | -0.10 | 0.660869 | 0.843694 | | | | | | | | |
| COMPOUND_666_1793a9_475972 | Rp | - | 666.1793 | 9.48 | | | (1367.3328, 159.29)(1368.3423, 76.63)(779.1754, 594.84)(780.1865, 351.6)(781.1638, 582.89)(701.1539, 37055.0)(702.157, 9110.67)(703.1585, 1371.19)(704.1597, 328.18)(665.1775, 2210.88)(666.195, 1676.98)(667.201, 582.3) | 243531.9 | 24865.48 | 244877.5 | 21265.96 | 254153.2 | 28347.59 | 246508.3 | 24604.25 | 0.43 | 0.156885 | 0.236958 | -0.45 | 0.221802 | 0.531023 | | | | | | | | |
| COMPOUND_666_523a13_601004 | Rp | + | 666.5230 | 13.60 | | | (1334.0464, 73.83)(1335.0754, 52.83)(689.5121, 10581.56)(690.5154, 4507.15)(691.5186, 1187.71)(692.5213, 328.71)(705.4866, 1000.77)(706.4969, 478.97)(707.496, 276.03)(684.5571, 32073.3)(685.5605, 15165.89)(686.5636, 4005.03)(687.5676, 838.6)(688.5717, 2305.23)(689.5752, 1223.07)(689.5752, 452.47)(670.5507, 127.04) | 58634.1 | 31866.3 | 67459.23 | 50445.34 | 104743.6 | 46614.13 | 189001.9 | 118363.2 | 0.87 | 0.000113 | 0.000349 | 0.51 | 0.042358 | 0.268638 | | | | | | | | |
| COMPOUND_667_2983a10_647927 | Rp | - | 667.2983 | 10.65 | | | (1369.5591, 351.18)(1370.5465, 208.31)(1371.5219, 261.06)(780.2558, 833.63)(666.2892, 1001.58)(667.2904, 493.72)(668.286, 13890.82)(1333.5704, 308.52)(1334.5706, 264.71) | 82358.59 | 9002.124 | 80994.17 | 14637.15 | 70499.21 | 8286.453 | 69480.91 | 11817.38 | -0.54 | 0.044014 | 0.078231 | -0.12 | 0.685538 | 0.853695 | | | | | | | | |
| COMPOUND_667_4769a10_860655 | Rp | - | 667.4769 | 10.86 | | | (1369.9388, 635.91)(1370.9515, 364.3)(780.4847, 1390.4)(781.491, 819.38)(782.4596, 2638.73)(702.4608, 850.4)(703.4592, 520.79)(704.462, 11351.56)(1379.9253, 655.54)(1380.931, 517.89)(1381.9167, 843.08)(1382.9232, 624.16)(1383.9328, 954.39)(666.4697, 8175.77)(667.4723, 4447.23)(668.4705, 1896.47)(669.4718, 231.2)(1333.9087, 423.23)(1334.9443, 192.39)(1447.9388, 443.95)(1448.9524, 481.79)(1449.9454, 487.13)(1450.945, 585.0)(1451.9475, 691.99) | 90377.6 | 16603.63 | 91059.15 | 15345.41 | 114285.1 | 15926.51 | 114551.2 | 12624.85 | 1.25 | 2.41E-06 | 1.1E-05 | -0.03 | 0.915421 | 0.961085 | | | | | | | | |
| COMPOUND_668_1981a10_400407 | Rp | + | 668.1981 | 10.40 | | | (1337.3989, 208.28)(686.2458, 647.14)(687.2375, 988.63)(707.1875, 2772.11)(669.204, 9776.51)(670.2091, 3412.49)(671.2017, 6361.58)(672.208, 3204.02)(673.2048, 1693.59)(674.205, 697.55)(675.2079, 296.2)(1354.4165, 193.89) | 40769.64 | 23767.59 | 35853.41 | 14576.24 | 88967.57 | 27692.92 | 84699.42 | 34057.12 | 1.49 | 5.18E-11 | 9.34E-10 | -0.08 | 0.703785 | 0.86442 | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|---|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_669_2917a10_615242 | Rp | - | 669.2917 | 10.62 | | | | (1373.5986, 220.39)(1374.6218, 218.49)(782.2666, 1033.36)(783.2662, 511.16)(784.2721, 1507.51)(785.2588, 1104.23)(786.2656, 792.02)(787.2644, 420.17)(788.2747, 341.49)(404.2655, 1861.66)(705.2706, 452.88)(706.2824, 1574.94)(707.2867, 728.13)(708.2759, 1208.74)(1383.5466, 168.03)(1384.5385, 384.68)(668.2862, 9745.67)(669.2889, 3840.15)(670.2899, 1448.05)(671.2757, 122.99)(1337.5691, 311.71)(1338.5732, 363.22)(1339.5782, 233.94)(714.2892, 5064.96)(715.2891, 1696.2)(716.2913, 5176.29)(717.2949, 1676.34)(718.2857, 2210.51)(719.2886, 933.72)(720.2857, 1110.62)(721.2935, 652.0) | 188777.9 | 82233.21 | 204495.3 | 70851.55 | 150250.1 | 86103.57 | 170040.6 | 81994.06 | -0.63 | 0.033888 | 0.062656 | 0.06 | 0.861682 | 0.942452 |
| COMPOUND_669_5541a11_606946 | Rp | + | 669.5541 | 11.61 | | | | (1379.336, 366.22)(709.1943, 2190.42)(710.1776, 1039.69)(711.1903, 916.81)(688.2807, 1057.49)(671.22, 1009.25)(672.2254, 4277.22)(673.2169, 7388.2)(674.2198, 2391.01)(675.2216, 2036.78)(676.2241, 861.65)(677.2249, 389.34) | 13400.79 | 92144.07 | 102611.5 | 65574.59 | 99789.67 | 35771.85 | 96212.44 | 42999.59 | -1.23 | 9.62E-08 | 6.01E-07 | 0.14 | 0.568306 | 0.788601 |
| COMPOUND_670_2151a10_66635 | Rp | + | 670.2151 | 10.67 | | | | (1379.336, 366.22)(709.1943, 2190.42)(710.1776, 1039.69)(711.1903, 916.81)(688.2807, 1057.49)(671.22, 1009.25)(672.2254, 4277.22)(673.2169, 7388.2)(674.2198, 2391.01)(675.2216, 2036.78)(676.2241, 861.65)(677.2249, 389.34) | 31440.6 | 8046.064 | 22480.33 | 8422.645 | 95274.3 | 24947.4 | 85905.39 | 33088.74 | 1.08 | 3.57E-09 | 3.31E-08 | 0.26 | 0.164711 | 0.47785 |
| COMPOUND_670_5009a11_60244 | Rp | - | 670.5009 | 11.60 | | | | (783.4829, 583.04)(669.4934, 1283.58)(670.4965, 5267.92)(671.4999, 1410.28)(672.4934, 363.27)(673.5038, 68.2)(715.4882, 625.82)(716.4826, 303.08)(717.5061, 2664.27)(718.5097, 1279.23) | 100868.4 | 54490.18 | 113067.7 | 52544.53 | 57723.67 | 27162.77 | 69885.89 | 18655.99 | -1.26 | 2.57E-09 | 2.5E-08 | -0.21 | 0.332808 | 0.636996 |
| COMPOUND_672_2846a10_161604 | Rp | - | 672.2846 | 10.16 | | | | (707.2647, 1396.26)(671.2781, 10060.74)(672.2798, 3561.05)(673.2836, 807.89)(717.2908, 122.44)(1343.5175, 387.35)(1344.5215, 330.8) | 70467.1 | 29979.23 | 64022.79 | 25965.72 | 60696.21 | 26881.37 | 62522.54 | 28151.65 | -0.61 | 0.040873 | 0.073578 | 0.43 | 0.227378 | 0.535063 |
| COMPOUND_672_285a10_268594 | Rp | - | 672.2850 | 10.27 | | | | (707.2677, 1671.17)(671.2779, 1325.76)(672.2809, 4009.04)(673.2822, 1503.12)(1343.5262, 99.79)(1344.5149, 80.33)(717.2697, 1057.06) | 119234.7 | 50848.06 | 102574.3 | 54383.39 | 119943.4 | 40687.84 | 120759.4 | 46720.48 | 0.02 | 0.942512 | 0.963038 | 0.55 | 0.116813 | 0.405455 |
| COMPOUND_672_4958a11_685205 | Rp | + | 672.4958 | 11.69 | | | | (695.4936, 1801.26)(696.489, 1112.88)(673.5031, 17391.64)(674.5065, 7898.01)(1363.0574, 83.71) | 93279.02 | 50692.61 | 104832.5 | 53223.07 | 58304 | 47380.94 | 91112.38 | 31386.15 | -0.96 | 1.99E-05 | 7.45E-05 | -0.26 | 0.30464 | 0.613089 |
| COMPOUND_672_5204a11_339026 | Rp | + | 672.5204 | 11.34 | SM d32.2 | 2 | 10 eV: 673.528(100), 184.072(50), 561.4149(4), 414.042(4), 86.0952(4) | (1345.9983, 215.32)(695.5033, 8065.68)(696.4997, 5748.37)(697.4961, 3766.66)(711.5006, 4436.08)(690.526, 1481.54)(673.5301, 83999.55)(674.5326, 34397.33)(675.5354, 8276.67)(676.5309, 1731.01)(677.5528, 340.94) | 418777.3 | 97773.5 | 414742.2 | 134407.4 | 337609.4 | 107554.1 | 324201.1 | 92552.36 | -0.82 | 0.000114 | 0.000351 | -0.03 | 0.89272 | 0.953702 |
| COMPOUND_672_5207a0_8844271 | Hilic | + | 672.5207 | 0.88 | | | | (695.5104, 2779.22)(696.5133, 1320.85)(697.5257, 8654.32)(698.5292, 4144.41)(699.543, 6984.78)(673.5286, 88253.3)(674.5318, 37185.59)(675.5444, 356427.66) | 957721.9 | 234854 | 1050988 | 355962 | 1088848 | 238616.5 | 1035566 | 266731.1 | 0.55 | 0.041429 | 0.0744 | -0.59 | 0.058464 | 0.299231 |
| COMPOUND_673_4975a9_63872 | Rp | + | 673.4975 | 9.64 | | | | (1385.953, 58.14)(1369.9958, 54.59)(346.2702, 900.59)(346.7726, 288.28)(347.2599, 348.88)(674.5052, 19880.7)(675.5076, 7817.14)(676.4995, 2319.22)(677.5102, 394.59)(678.5183, 78.11)(337.7578, 422.97)(338.2658, 1821.53)(338.7642, 24.8) | 249748 | 64750.95 | 214576 | 42520.4 | 268561.8 | 44541.65 | 268163 | 67877.76 | 0.30 | 0.285478 | 0.384886 | 0.59 | 0.082221 | 0.343638 |
| COMPOUND_674_2725a10_392099 | Rp | + | 674.2725 | 10.39 | | | | (1371.5741, 145.97)(713.2408, 790.22)(714.24, 808.8)(675.2808, 6235.89)(676.2777, 2405.2)(677.2596, 1288.19)(678.2837, 292.15) | 34679.57 | 13175.86 | 29909.15 | 12970.14 | 41551.08 | 10852.66 | 37750.46 | 9586.416 | 0.87 | 0.000812 | 0.002154 | 0.02 | 0.952667 | 0.980085 |
| COMPOUND_674_54a11_606961 | Rp | + | 674.5400 | 11.61 | SM d32.1 | 2 | 10eV: 675.5446(100), 184.073(35), 388.867(3) | (1330.0846, 710.89)(1351.0935, 588.13)(1352.082, 264.24)(1308.0002, 156.58)(697.5274, 21819.92)(698.5306, 9572.64)(699.5363, 2927.31)(700.5573, 231.35)(1372.0112, 232.74)(713.5016, 1757.86)(714.4983, 1189.02)(715.5121, 1112.26)(692.5535, 2255.93)(693.5555, 1122.95)(675.5459, 310016.28)(676.5492, 125283.59)(677.5515, 26677.19)(678.557, 5112.04) | 1510548 | 404228.4 | 1607133 | 684530.7 | 1488993 | 354308 | 1412110 | 370291.4 | 0.00 | 0.991959 | 0.997273 | -0.31 | 0.322109 | 0.628989 |
| COMPOUND_675_5249a11_220736 | Rp | + | 675.5249 | 11.22 | | | | (693.5324, 951.78)(676.5333, 20974.51)(677.536, 9481.15)(678.5343, 14321.73)(679.5351, 6350.34)(680.531, 5763.94) | 23836.11 | 9057.114 | 31498.6 | 14588.07 | 99951.7 | 44505.02 | 71912.3 | 29796.93 | 1.09 | 2.35E-06 | 1.07E-05 | 0.01 | 0.957092 | 0.980661 |
| COMPOUND_675_5406a0_88432986 | Hilic | + | 675.5406 | 0.88 | | | | (698.5294, 6236.98)(699.5429, 7996.6)(700.5464, 3545.12)(693.5645, 392.61)(676.5479, 112781.45)(677.5513, 26413.68)(678.5555, 4956.43)(679.5589, 973.98)(680.5647, 157.46) | 392383.5 | 97023.87 | 434429.4 | 142034.3 | 448677.7 | 98007.66 | 421864.7 | 109994.3 | 0.55 | 0.044449 | 0.078879 | -0.67 | 0.036127 | 0.252742 |
| COMPOUND_676_5522a11_792699 | Rp | + | 676.5522 | 11.79 | | | | (699.5236, 1194.14)(700.5473, 970.22)(694.5993, 2237.45)(695.602, 1490.61)(677.5559, 3117.34)(678.5655, 3854.64)(679.5733, 2408.13)(680.5827, 9941.78) | 90449.92 | 38099.3 | 87788.09 | 48611.35 | 43104.6 | 15637.33 | 46773.58 | 19970.66 | -0.14 | 0.60716 | 0.700115 | 0.23 | 0.470222 | 0.734155 |
| COMPOUND_677_3063a10_304156 | Rp | - | 677.3063 | 10.30 | | | | (790.2787, 679.15)(791.287, 403.28)(712.2663, 2901.88)(676.2994, 9776.01)(677.3001, 3461.84)(678.3014, 1268.82)(679.292, 336.99) | 87129.94 | 24081.66 | 84246.96 | 19593.13 | 86644.57 | 16795.16 | 83258.7 | 19519.1 | 0.08 | 0.80168 | 0.857257 | -0.04 | 0.906962 | 0.958319 |
| COMPOUND_677_3082a10_222234 | Rp | - | 677.3082 | 10.22 | | | | (712.2655, 2567.3)(790.2755, 474.28)(791.2746, 263.14)(676.2999, 7425.59)(677.3029, 2488.91)(678.3035, 1005.06)(679.3025, 269.27) | 39675.35 | 15869.28 | 42490.25 | 13664.81 | 42906.33 | 30829.36 | 38361.13 | 28842.74 | 0.48 | 0.083807 | 0.138877 | -0.22 | 0.512878 | 0.75937 |
| COMPOUND_677_5013a11_656002 | Rp | + | 677.5013 | 11.66 | PC 28.0 | 2 | 20 eV: 184.074(100), 678.5107(90) | (700.4913, 4493.86)(701.5005, 1493.33)(1377.964, 188.93)(716.469, 471.05)(678.5073, 31683.83)(679.5102, 12618.59)(680.5128, 3237.09)(681.5031, 795.9) | 161324 | 90170.64 | 175333.9 | 99085.49 | 167482.1 | 84587.18 | 186676.3 | 106561.4 | 0.57 | 0.023322 | 0.045082 | -0.15 | 0.593254 | 0.803855 |
| COMPOUND_677_5598a11_508577 | Rp | + | 677.5598 | 11.51 | | | | (700.5481, 3956.77)(678.567, 22666.42)(679.5703, 10178.6)(680.576, 4531.2)(681.5659, 843.63) | 144243.4 | 80623.47 | 142826.3 | 93472.94 | 176122.8 | 119990.5 | 208413.1 | 133015.3 | -0.70 | 0.003919 | 0.009069 | -0.19 | 0.510586 | 0.757607 |
| COMPOUND_679_5756a11_755592 | Rp | + | 679.5756 | 11.76 | | | | (1360.1598, 210.11)(1398.155, 143.03)(697.5817, 14308.78)(680.583, 55868.91)(681.5863, 24642.31)(682.5848, 7113.09)(683.5821, 1994.05) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.02 | 2.22E-05 | 8.16E-05 | -0.01 | 0.974689 | 0.986465 |
| COMPOUND_680_1589a8_665838 | Rp | - | 680.1589 | 8.67 | | | | (679.1525, 3474.99)(680.156, 936.16)(681.1713, 218.96)(682.1542, 61.81)(725.1436, 345.44)(726.1331, 239.21)(727.1438, 372.81) | 14706.09 | 2831.089 | 15195.07 | 2766.856 | 14988.64 | 3047.039 | 15377.02 | 2599.436 | 0.06 | 0.855055 | 0.900226 | -0.03 | 0.937288 | 0.97184 |
| COMPOUND_680_1594a8_602407 | Rp | - | 680.1594 | 8.60 | | | | (679.151, 4470.21)(680.1528, 1201.34)(681.1536, 338.82)(682.1419, 45.68)(725.1604, 319.12)(726.1436, 211.05)(727.1444, 331.6) | 18298.98 | 2275.179 | 18039.59 | 1915.246 | 18903.14 | 3135.381 | 19144.39 | 2614.266 | 0.30 | 0.318976 | 0.421063 | 0.17 | 0.634244 | 0.828972 |
| COMPOUND_680_5212a11_757137 | Rp | - | 680.5212 | 11.76 | | | | (679.5143, 9103.44)(680.5176, 3976.64)(681.5197, 1027.82)(682.5216, 244.29)(683.539, 481.13)(1360.0446, 113.88)(725.5029, 816.41)(726.5039, 372.96)(727.5141, 2821.27)(728.5145, 1379.33) | 150371.7 | 64535.01 | 170958.5 | 61637.75 | 121590.5 | 75172.1 | 178936.5 | 95802.33 | -1.06 | 8.91E-06 | 3.59E-05 | -0.17 | 0.509654 | 0.757224 |
| COMPOUND_681_3219a1_1681348 | Hilic | + | 681.3219 | 1.17 | | | | (704.309, 356.29)(705.3157, 215.56)(682.3282, 9048.2)(683.3322, 3273.78)(684.336, 817.41)(685.3386, 152.22) | 19920.61 | 7299.881 | 20936.64 | 9352.378 | 29496.15 | 15075.75 | 28517.42 | 12774.39 | 0.73 | 0.010592 | 0.022335 | -0.15 | 0.649492 | 0.838541 |
| COMPOUND_681_3225a10_086524 | Rp | - | 681.3225 | 10.09 | | | | (680.3165, 13665.75)(681.3201, 4568.78)(682.3222, 1076.37)(683.3287, 296.26) | 40418.74 | 8114.936 | 34909.3 | 8160.291 | 29329.14 | 9610.092 | 33601.82 | 8970.777 | -1.13 | 1.06E-05 | 4.22E-05 | 0.56 | 0.044697 | 0.27288 |
| COMPOUND_681_3582a10_395896 | Rp | + | 681.3582 | 10.40 | | | | (1363.7657, 520.03)(1364.7784, 161.39)(1401.65, 317.09)(704.3399, 824.45)(720.326, 656.73)(721.3119, 366.68)(699.4085, 733.64)(682.3641, 78912.15)(683.3673, 30392.42)(684.3704, 6789.34)(685.3756, 1154.36)(686.3805, 246.55) | 78223.1 | 66045.82 | 53962.58 | 58479.57 | 102399.7 | 52920.66 | 116347.8 | 78147.73 | 0.59 | 0.02252 | 0.043718 | 0.55 | 0.072698 | 0.326093 |
| COMPOUND_681_4761a10_928599 | Rp | - | 681.4761 | 10.93 | | | | (1397.9069, 1592.98)(1398.909, 1273.19)(1399.9196, 1786.1)(794.4573, 750.28)(795.4833, 455.91)(716.446, 6492.6)(717.4442, 2247.01)(1407.8773, 764.48)(1408.8798, 743.69)(680.467, 9328.01)(681.4717, 4405.12)(682.4755, 1177.77)(683.4822, 223.43)(726.4688, 1351.15)(727.4661, 728.64)(7 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--|---|---------------|----------|-------------------|-------------------|-------------------|-------------------|---------------|----------|----------|----------|----------|-------------|----------|----------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | | |
| COMPOUND_684_5764a0_8690934 | Hilic | + | 684.5764 | 0.87 | | | | (685.5475, 521.09)(343.2954, 17475.92)(343.7887, 857.01)(344.2991, 3380.95)(344.7913, 90.25)(345.302, 350.28) | 41701.93 | 20231.79 | 46297.56 | 17740.09 | 60661.45 | 39539.81 | 45436.26 | 21603.02 | 0.41 | 0.147351 | 0.224821 | -0.08 | 0.816931 | 0.92157 | | |
| COMPOUND_685_4348a10_680474 | Rp | + | 685.4348 | 10.68 | | | | (1409.8856, 1899.4)(708.4253, 4770.46)(709.437, 2538.3)(710.4374, 6021.82)(711.4449, 2205.37)(712.4458, 4231.71)(703.4679, 7214.48)(686.4414, 16917.18)(687.4538, 8366.79)(688.4556, 19923.99)(689.4618, 8270.16)(690.4494, 10414.12) | 347312.5 | 136628.7 | 346924.5 | 121509 | #DIV/0! | #DIV/0! | 254472 | #DIV/0! | -1.07 | 7.35E-07 | 3.82E-06 | 0.32 | 0.173954 | 0.488459 | | |
| COMPOUND_686_5365a0_8701679 | Hilic | + | 686.5365 | 0.87 | | | | (709.5234, 861.61)(710.5327, 478.45)(711.5416, 4923.99)(712.5436, 2036.73)(687.5439, 10422.59)(688.5453, 4560.33)(689.5597, 111729.45) | 297793.4 | 75895.85 | 318505 | 120360.4 | 330989.6 | 78384.95 | 303671.1 | 77881.79 | 0.36 | 0.19691 | 0.28646 | -0.45 | 0.165421 | 0.47785 | | |
| COMPOUND_686_5381a11_517818 | Rp | + | 686.5381 | 11.52 | | | | (709.5104, 3811.89)(710.5086, 2626.34)(704.5772, 2139.73)(705.5795, 931.53)(687.5453, 7512.12)(688.548, 3470.33)(689.5466, 1157.34) | 44416.96 | 14355.97 | 52141.97 | 26079.16 | 43574.5 | 18003.31 | 37513.93 | 15589.02 | -0.45 | 0.067231 | 0.115136 | -0.21 | 0.457736 | 0.727948 | | |
| COMPOUND_687_3214a10_29665 | Rp | + | 687.3214 | 10.30 | | | | (1375.6824, 308.65)(726.3059, 872.17)(688.328, 8577.99)(689.3315, 3660.26)(690.3282, 3738.31)(691.3301, 1205.80)(692.319, 345.96)(1392.7479, 379.41) | 29435.98 | 9775.082 | 24565.95 | 9845.062 | 32686.64 | 12237.18 | 33374.15 | 13355.07 | 0.34 | 0.232371 | 0.327267 | 0.49 | 0.148192 | 0.456493 | | |
| COMPOUND_687_3876a10_863252 | Rp | + | 687.3876 | 10.86 | | | | (688.3946, 28117.34)(689.3975, 10989.49)(690.3969, 3499.3)(691.3945, 835.74) | 11227 | #DIV/0! | #DIV/0! | #DIV/0! | 77370.64 | 12190.16 | 79488.2 | 16618.45 | 1.04 | 1.3E-09 | 1.39E-08 | 0.30 | 0.092029 | 0.359807 | | |
| COMPOUND_687_4119a0_9568352 | Hilic | + | 687.4119 | 0.96 | | | | (710.4127, 1246.91)(711.4176, 455.35)(712.4268, 1900.88)(713.4288, 735.42)(705.4512, 808.34)(688.4196, 17133.05)(689.4233, 6425.55)(690.4347, 14650.79)(691.4384, 5712.42)(692.4429, 2260.56)(693.4503, 781.71)(694.4528, 1042.74) | 54401.64 | 40840.51 | 59238.57 | 34787.37 | #DIV/0! | #DIV/0! | 16711 | 14584.13 | -1.30 | 3.68E-09 | 3.39E-08 | 0.10 | 0.650503 | 0.838541 | | |
| COMPOUND_687_5141a9_882115 | Rp | + | 687.5141 | 9.88 | | | | (1375.982, 60.23)(1414.0369, 69.09)(353.2721, 1321.24)(353.7755, 67.03)(688.5212, 20793.59)(689.523, 7982.51)(344.7615, 384.37)(345.2685, 410.29)(345.7617, 46.51) | 155038.9 | 42117.97 | 134849.1 | 27071.95 | 167786.4 | 27226.22 | 166484.8 | 43125.96 | 0.25 | 0.375652 | 0.477409 | 0.57 | 0.098038 | 0.36878 | | |
| COMPOUND_687_5806a13_782784 | Rp | + | 687.5806 | 13.78 | | | | (688.5883, 11804.9)(689.5911, 5619.4)(690.5951, 1461.88)(691.5986, 272.13) | 33561.24 | 22973.15 | 31312.51 | 18889.98 | 40165.71 | 13432.82 | 63707.7 | 36506.63 | 0.56 | 0.025956 | 0.055774 | 0.62 | 0.040467 | 0.265689 | | |
| COMPOUND_688_5536a11_812392 | Rp | + | 688.5536 | 11.81 | SM d33:1 | 2 | 10 eV: 689.5641(100), 184.0735(15), 81.0719(3) | (1378.1638, 162.11)(1416.0829, 110.33)(711.5407, 3247.7)(712.5351, 1978.97)(713.5491, 610.58)(714.5534, 49.29)(1400.1448, 180.26)(706.5894, 2245.67)(707.5987, 559.69)(689.5614, 17125.76)(690.5641, 30426.04)(691.5672, 7146.9)(692.5558, 1107.35)(1395.1685, 248.96) | 456196.2 | 124668.7 | 459250.4 | 190965 | 467819.4 | 118680.4 | 420165.5 | 107008.5 | 0.10 | 0.712886 | 0.788904 | -0.27 | 0.409398 | 0.694731 | | |
| COMPOUND_689_2666a10_208906 | Rp | - | 689.2666 | 10.21 | | | | (597.0202, 691.2575, 5470.02)(691.2575, 1584.73)(692.2632, 1501.42)(693.2662, 502.69)(1377.5009, 162.38)(1378.5055, 176.76)(1379.5317, 131.82)(1380.5016, 148.95)(1381.5043, 184.97)(734.2508, 1592.92)(735.2498, 882.59)(736.2575, 2002.06)(737.2596, 937.12)(1491.458, 123.71) | 89302.22 | 58474.49 | 64651.82 | 46435.3 | 146232.5 | 51276.64 | 112215.6 | 54098.57 | 0.60 | 0.03441 | 0.063362 | 0.13 | 0.698105 | 0.862515 | | |
| COMPOUND_689_2678a10_278288 | Rp | - | 689.2678 | 10.28 | | | | (1413.451, 147.81)(1414.4779, 192.01)(802.2362, 689.13)(688.2601, 12205.91)(689.2643, 4671.72)(690.2571, 5075.03)(691.2592, 1887.07)(692.261, 1374.22)(693.2674, 512.57)(1377.4868, 151.15)(1378.495, 240.88)(1379.4929, 244.3)(1380.5096, 141.9)(1381.4899, 166.25)(734.2573, 1857.14)(735.2603, 1032.89)(736.2591, 1745.05)(737.2594, 587.27)(1401.526, 153.91) | 159948 | 86809.19 | 127257.8 | 86634.97 | 196234.4 | 55198.86 | 140443.3 | 68583.91 | 0.42 | 0.15291 | 0.231731 | -0.27 | 0.443553 | 0.71862 | | |
| COMPOUND_689_4929a9_112516 | Rp | + | 689.4929 | 9.11 | | | | (720.493, 679.38)(720.9908, 424.39)(354.2662, 2559.64)(354.7706, 416.05)(355.2645, 12697.86)(690.5004, 7740.61)(691.4986, 3665.2)(692.4974, 1087.94)(693.5057, 216.49)(345.7549, 500.72)(346.2549, 1182.7)(346.7559, 21.71) | 137695 | 33970.67 | 127178.4 | 37745.96 | 126752.2 | 21062.32 | 123378.6 | 38117.81 | -0.39 | 0.191408 | 0.280289 | 0.43 | 0.229451 | 0.535521 | | |
| COMPOUND_689_4987a12_1908 | Rp | - | 689.4987 | 12.19 | | | | (688.4915, 9709.51)(689.4946, 3902.25)(690.4979, 1232.48)(691.5021, 235.01) | 12210 | #DIV/0! | 14749.33 | 5452.56 | 24127.5 | 9546.464 | 38071.29 | 20842.76 | 1.01 | 2.89E-11 | 6.09E-10 | 0.45 | 0.003326 | 0.082317 | | |
| COMPOUND_689_5557a0_8700491 | Hilic | + | 689.5557 | 0.87 | | | | (712.5433, 1055.61)(713.5583, 1738.85)(714.5609, 1026.24)(707.5914, 3332.83)(708.5941, 464.96)(690.5628, 46213.26)(691.5659, 11325.58)(692.5691, 1920.69)(693.5691, 324.82) | 138786.6 | 35666.44 | 150618 | 54747.37 | 154555.5 | 39215.54 | 140088.7 | 36487.1 | 0.34 | 0.220554 | 0.314161 | -0.52 | 0.108689 | 0.391238 | | |
| COMPOUND_691_4231a10_704643 | Rp | - | 691.4231 | 10.70 | | | | (1417.7834, 312.26)(1418.753, 204.17)(804.3781, 964.32)(805.3968, 177.9)(726.4116, 1932.58)(690.4036, 28236.34)(691.4056, 15468.79)(692.4084, 5238.95)(693.4094, 1539.07)(1381.7625, 274.34)(1382.7426, 396.27)(736.4184, 3010.57)(737.4055, 1551.57)(1405.8741, 581.81)(1496.8597, 563.45) | 88017.37 | 30469.29 | 97170.12 | 45775.01 | 79088 | 35014.44 | 89161.45 | 40961.7 | -0.75 | 0.004583 | 0.010385 | 0.06 | 0.833841 | 0.927314 | | |
| COMPOUND_692_5062a11_310362 | Rp | - | 692.5062 | 11.31 | | | | (1429.9694, 196.89)(691.5017, 8041.77)(692.505, 3411.83)(693.5026, 1151.41)(694.5072, 83513.33) | 20237.91 | 101268.9 | 29082.37 | 105642.9 | 26767.02 | 111999.5 | 38371.16 | 1.86 | 0.001095 | 0.002831 | -0.07 | 0.811819 | 0.920552 | | | |
| COMPOUND_693_489a12_86907 | Rp | + | 693.4890 | 12.87 | | | | (199.04)(1383.9637, 115.01)(737.4969, 1400.09) | 138794.74 | 344.46 | 1425.9443, 263.58 | 1426.9309, 306.14 | 1427.9523, 268.92 | 694.496, 56140.17 | 22317.85 | 45998.18 | 17215.5 | 46598.21 | 14211.43 | 49369.6 | 18757.84 | -0.41 | 0.157492 | 0.237716 |
| COMPOUND_695_2695a10_272763 | Rp | - | 695.2695 | 10.27 | | | | (1425.4901, 182.61)(1426.4784, 205.26)(1427.457, 220.75)(808.2409, 646.06)(809.2524, 387.01)(730.2085, 805.01)(731.2213, 551.56)(732.2077, 208.48)(694.262, 7081.29)(695.2648, 3131.38)(696.2624, 1259.56)(697.2524, 249.04)(1389.5197, 222.74)(740.2927, 1840.25) | 58777.92 | 40784.27 | 79549.62 | 46085.21 | 44775.43 | 40921.07 | 62952.94 | 53563.08 | 0.38 | 0.179246 | 0.266093 | -0.50 | 0.139048 | 0.444794 | | |
| COMPOUND_695_3701a10_391698 | Rp | + | 695.3701 | 10.39 | | | | (1391.791, 613.28)(1429.7736, 389.38)(1413.7523, 454.63)(734.3386, 437.56)(713.4161, 1222.27)(696.3804, 17161.62)(697.3834, 6962.67)(698.3858, 1895.15)(699.3882, 521.35)(1408.7917, 576.02) | 41723.34 | 9407.973 | 39976.5 | 9366.083 | 42027.14 | 12641.44 | 41871.02 | 13007.91 | 0.27 | 0.336637 | 0.437453 | 0.31 | 0.356046 | 0.665596 | | |
| COMPOUND_695_5708a11_684356 | Rp | + | 695.5708 | 11.68 | | | | (718.5598, 3500.47)(719.5666, 1808.27)(734.5176, 620.16)(735.522, 1640.57)(736.5208, 1360.99)(713.5915, 892.74)(696.5781, 11635.73)(697.5791, 5635.21)(698.5804, 1650.09)(699.5832, 466.27)(700.5967, 93.77)(1409.1765, 185.62) | 162700.7 | 126893.5 | 128519.5 | 97981.99 | 157918.3 | 143492.5 | 109367.9 | 100551.1 | -1.29 | 1.19E-08 | 9.65E-08 | 0.13 | 0.578 | 0.792726 | | |
| COMPOUND_696_5162a11_681318 | Rp | - | 696.5162 | 11.68 | | | | (809.5339, 789.78)(810.5502, 1363.36)(695.5093, 49707.27)(696.5126, 22736.35)(697.5158, 5799.3)(698.5182, 1190.56)(699.5199, 210.86) | 158887.9 | 89381.86 | 160669.5 | 79294.48 | 107277.3 | 77385.34 | 119364.1 | 68076.25 | -1.27 | 1.01E-08 | 8.39E-08 | -0.08 | 0.716857 | 0.876415 | | |
| COMPOUND_698_2994a10_378443 | Rp | - | 698.2994 | 10.38 | | | | (733.2599, 737.52)(697.2936, 8166.38)(698.293, 2874.73)(699.2875, 1262.89)(700.27, 247.68)(1395.5325, 325.07)(743.3187, 526.76)(744.3188, 352.16) | 96861.79 | 11946.43 | 98562.32 | 11092.28 | 87479.29 | 11465.28 | 85835.58 | 11889.17 | -0.71 | 0.009322 | 0.019842 | -0.15 | 0.638268 | 0.831817 | | |
| COMPOUND_698_3517a5_478739 | Rp | + | 698.3517 | 5.48 | | | | (699.3311, 151.43)(350.1835, 8649.64)(350.6846, 3369.63)(351.1848, 875.02)(351.6862, 141.96) | 26856.44 | 10189.64 | 24016.53 | 9450.935 | 35005 | 12871.58 | 35985.82 | 15304.86 | 0.33 | 0.244694 | 0.339945 | 0.18 | 0.598336 | 0.805251 | | |
| COMPOUND_699_2819a10_087934 | Rp | - | 699.2819 | 10.09 | | | | (1433.5039, 157.29)(812.2636, 470.43)(813.264, 314.43)(814.2759, 210.94)(734.2467, 1766.7)(735.2461, 1010.91)(736.2536, 1706.04)(737.2564, 662.5)(738.2707, 2664.19)(739.267, 1664.47)(740.2578, 1149.84)(698.276, 7147.15)(699.2769, 3029.62)(700.2961, 2446.86)(1397.4895, 193.72)(1398.5009, 273.24) | 89531.58 | 16811.33 | 84711.31 | 22920.16 | 71019.64 | 16108.03 | 76018.75 | 15402.98 | -0.73 | 0.012454 | 0.025801 | 0.38 | 0.261123 | 0.572854 | | |
| COMPOUND_699_3817a7_8125954 | Rp | - | 699.3817 | 7.81 | | | | (812.3547, 379.33)(698.3752, 22620.21)(699.3781, 9017.83)(700.3802, 2405.22)(701.3827, 498.13)(702.3908, 105.65) | 16005.87 | 4960.95 | 15521.88 | 4838.97 | 58543.71 | 30792.37 | 73006.32 | 53726.24 | 1.35 | 3.18E-10 | 4.19E-09 | -0.13 | 0.538941 | 0.776408 | | |
| COMPOUND_699_4492a10_746508 | Rp | + | 699.4492 | 10.75 | | | | (722.439, 5812.83)(723.4416, 2731.17)(724.4498, 3908.94)(725.4681, 2080.26)(726.4383, 635.74)(700.4576, 7560.8)(701.4631, 8390.67)(702.4712, 24891.42)(703.4754, 11242.73)(704.4725, 6163.97)(705.4731, 2827.69) | 281458.4 | 120399.8 | 256973.1 | 101022.2 | 88604 | #DIV/0! | 68153.5 | 43678.69 | -1.07 | 1.02E-06 | 5.05E-06 | 0.34 | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|---|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_700_5534a0_85892963 | Hilic | + | 700.5534 | 0.86 | | | | (723.542, 31714.26)(724.5455, 15006.13)(725.5572, 51306.06)(726.5609, 21731.3)(727.5739, 25477.74)(728.5784, 10674.77)(729.5934, 8382.53)(730.5969, 2479.93)(731.5596, 554447.0)(732.5747, 234702.9)(733.5747, 795642.1)(704.579, 337836.8)(705.5827, 76802.6)(706.5862, 14693.21)(707.5889, 2399.16)(708.5962, 425.62)(351.2837, 487.63)(351.7851, 127.51)(352.2952, 435.22) | 7404810 | 1895624 | 7871857 | 2608108 | 8583046 | 2126883 | 8208371 | 2230865 | 0.50 | 0.089172 | 0.147334 | -0.31 | 0.367119 | 0.669574 |
| COMPOUND_700_556a11_700257 | Rp | + | 700.5560 | 11.70 | SM d34:2 | 2 | 20 eV: 184.0735(100), 701.5584(25) | (1402.1117, 2461.05)(1403.1143, 2132.1)(1404.1187, 1231.23)(1405.1064, 615.61)(1440.1324, 182.55)(723.5427, 47503.5)(724.5454, 19802.28)(725.5499, 5038.56)(726.5454, 1014.39)(1424.0918, 667.55)(1425.0978, 596.26)(1426.1166, 446.56)(739.5161, 3101.27)(740.5215, 2246.82)(741.5234, 2276.08)(718.5595, 2341.27)(719.5669, 1257.14)(701.5603, 676346.4)(702.5644, 281432.38)(703.5671, 66395.42)(704.5685, 10195.03)(705.5738, 1498.18) | 3388843 | 835956.5 | 3503888 | 1275485 | 3517332 | 923504.9 | 3358623 | 818712.1 | 0.07 | 0.790288 | 0.84749 | -0.07 | 0.832594 | 0.926681 |
| COMPOUND_701_4618a10_771543 | Rp | + | 701.4618 | 10.77 | | | | (724.4549, 7192.09)(725.4588, 3233.17)(726.4734, 3040.84)(740.4597, 1513.94)(719.4982, 6531.89)(720.4836, 3794.24)(721.4916, 2165.84)(702.4713, 17836.06)(703.4756, 8841.54)(704.4835, 9779.23)(705.4816, 4864.5) | 203382.6 | 101428.2 | 174464.4 | 92422.98 | 150589.7 | 66701.45 | 90778.83 | 43767.34 | -1.19 | 5.23E-08 | 3.57E-07 | 0.08 | 0.738527 | 0.888668 |
| COMPOUND_701_5296a10_098768 | Rp | + | 701.5296 | 10.10 | | | | (702.5367, 6858.37)(703.5361, 2909.02)(351.7638, 70.51)(352.2479, 796.53) | 46008.56 | 11968.22 | 40455.8 | 7695.957 | 53470.15 | 9706.096 | 52166.35 | 23764.84 | 0.44 | 0.106784 | 0.172261 | 0.55 | 0.098994 | 0.368908 |
| COMPOUND_702_1608a9_162468 | Rp | - | 702.1608 | 9.16 | | | | (815.1586, 374.82)(816.1583, 200.79)(701.1539, 48303.08)(702.1568, 11882.92)(703.1553, 1737.61)(704.152, 424.99) | 255684.8 | 29134.86 | 258780.4 | 22524.82 | 238630.9 | 16154.44 | 243050.3 | 22684.53 | -0.68 | 0.020949 | 0.041131 | 0.03 | 0.935755 | 0.97184 |
| COMPOUND_702_161a9_473247 | Rp | - | 702.1610 | 9.47 | | | | (737.1244, 677.85)(701.1533, 40844.41)(702.1571, 10564.34)(703.1584, 1182.52)(704.1613, 354.28)(747.1545, 408.82)(748.1654, 177.64)(749.1359, 561.41) | 244656.4 | 30103.07 | 242703.6 | 32992.02 | 241217.6 | 28086.19 | 238965.3 | 23462.21 | -0.11 | 0.721322 | 0.796283 | -0.13 | 0.711192 | 0.871385 |
| COMPOUND_702_161a9_376014 | Rp | - | 702.1610 | 9.38 | | | | (815.1345, 434.65)(816.1376, 365.57)(817.1287, 538.31)(701.1534, 45202.1)(702.1568, 10713.89)(703.1595, 1562.98)(704.1528, 269.31)(1403.317, 138.84)(747.1379, 592.61)(748.1457, 427.02)(749.1345, 862.59) | 223413.6 | 19668.02 | 223319.3 | 18052.03 | 224694.2 | 15063.02 | 219477.6 | 15479.95 | 0.09 | 0.760988 | 0.827496 | -0.30 | 0.417361 | 0.699344 |
| COMPOUND_702_5718a12_023964 | Rp | + | 702.5718 | 12.02 | SM d34:1 | 2 | 10 eV: 703.5757(100), 184.0735(27) | (1406.1422, 3154.3)(1407.1462, 2803.78)(1408.1521, 1428.89)(1409.1451, 695.87)(1410.16, 264.09)(1441.1129, 309.26)(1445.1304, 346.47)(1446.1108, 279.98)(725.5598, 38082.6)(726.5625, 16292.11)(727.5682, 4783.21)(728.5686, 1159.18)(1428.1646, 531.62)(1429.1449, 262.81)(1430.1495, 317.59)(1431.1731, 366.52)(1432.1722, 101.09)(741.5357, 5537.61)(742.5411, 2299.74)(743.5402, 1410.19)(703.5762, 747841.2)(704.5803, 30611.70)(705.583, 71694.56)(706.5834, 10203.77)(707.5844, 1484.76)(1423.193, 268.43)(1424.1917, 363.86)(1425.1874, 230.67) | 5418515 | 1675107 | 5311868 | 2129967 | 5401172 | 994209.6 | 5138594 | 1498241 | 0.09 | 0.745031 | 0.814666 | -0.09 | 0.802801 | 0.916921 |
| COMPOUND_703_3249a10_391383 | Rp | - | 703.3249 | 10.39 | | | | (816.2822, 298.03)(817.2755, 282.83)(702.3182, 6578.68)(703.3204, 2409.29)(704.3178, 872.81)(705.3238, 191.05) | 64867.07 | 13344.93 | 67781.98 | 13678.5 | 65526.71 | 10785.53 | 68938.5 | 13250.24 | 0.34 | 0.236422 | 0.331108 | -0.19 | 0.588651 | 0.800992 |
| COMPOUND_703_5082a9_365048 | Rp | + | 703.5082 | 9.37 | | | | (363.7527, 184.94)(364.2551, 625.77)(364.746, 29.12)(361.2681, 3633.09)(361.7783, 942.09)(362.2668, 1382.12)(704.5161, 17249.73)(705.5162, 7128.07)(706.5176, 2020.77)(707.5258, 350.98)(352.7639, 926.42)(353.2661, 3808.33)(353.7623, 105.78) | 237163.7 | 52068.35 | 209310 | 49444.1 | 257985.5 | 50525.88 | 261556.3 | 73276.71 | 0.22 | 0.455052 | 0.560294 | 0.54 | 0.124252 | 0.418884 |
| COMPOUND_703_5179a11_742987 | Rp | + | 703.5179 | 11.74 | PC 30:1 | 2 | 20 eV: 184.0737(100), 704.5271(60), 499.1125(3) | (1408.0359, 375.66)(1409.0463, 233.28)(1410.0162, 133.5)(726.5058, 12924.29)(727.5099, 5810.29)(728.5221, 5433.41)(1430.0778, 254.99)(742.4852, 1047.29)(743.4943, 420.17)(744.4835, 80.92)(721.5825, 2271.25)(704.5237, 163256.08)(705.5267, 67617.2)(706.5292, 16133.56)(707.5311, 3403.69) | 311906.1 | 148546.4 | 359848.9 | 181610.1 | 545782.9 | 163396.1 | 738889.2 | 402921.3 | 0.96 | 2.89E-05 | 0.000103 | 0.27 | 0.27446 | 0.583908 |
| COMPOUND_704_584a12_243275 | Rp | + | 704.5840 | 12.24 | | | | (1410.2134, 299.04)(727.5277, 61.17)(728.5569, 1346.74)(1432.2102, 226.64)(705.5906, 22775.95)(706.591, 10078.83)(707.5939, 2322.21)(708.5992, 457.53)(1427.2242, 223.8)(1428.2289, 204.53)(1429.2169, 174.5) | 58524.83 | 20715.07 | 59800.07 | 30126.85 | 53312.71 | 14010.69 | 51337.96 | 16454.18 | -0.20 | 0.470279 | 0.573399 | -0.40 | 0.908579 | 0.958319 |
| COMPOUND_705_344a10_567998 | Rp | - | 705.3442 | 10.57 | | | | (1445.6733, 182.09)(1446.6447, 154.17)(818.3112, 530.89)(819.2993, 391.06)(704.3345, 6573.55)(705.339, 2456.48)(706.3363, 604.43)(707.3389, 84.1)(1409.7028, 178.4)(1410.6826, 135.84) | 27132.46 | 16192.24 | 24893.82 | 6726.496 | 16948.93 | 3400.961 | 33584.28 | 27866.96 | -0.88 | 0.003174 | 0.007515 | 0.45 | 0.193953 | 0.505089 |
| COMPOUND_705_4199a10_552607 | Rp | - | 705.4199 | 10.55 | | | | (1445.8651, 539.06)(818.3668, 512.22)(819.3732, 312.33)(1455.8931, 936.62)(1456.9003, 603.52)(704.4135, 9736.42)(705.4165, 3749.84)(706.4246, 2425.26)(707.4299, 697.6)(1523.8417, 445.99)(1524.8602, 553.72)(1525.8243, 730.6)(1526.8239, 360.16) | 78016.71 | 27386.93 | 70320.39 | 29623.24 | 12359 | #DIV/0! | #DIV/0! | #DIV/0! | -1.26 | 3.71E-09 | 3.41E-08 | 0.26 | 0.234161 | 0.540298 |
| COMPOUND_705_5347a12_080148 | Rp | + | 705.5347 | 12.08 | PC 30:0 | 2 | 20 eV: 184.0742(100), 706.5421(45) | (1412.079, 625.53)(1413.0729, 504.34)(1414.0846, 218.59)(728.5122, 7547.84)(729.5244, 2496.02)(730.5387, 17209.34)(1434.1039, 369.53)(1435.1118, 299.17)(1436.122, 172.17)(706.5406, 162599.44)(707.5435, 65630.13)(708.5454, 15520.92)(709.5459, 3046.68)(710.5429, 648.38)(1429.1304, 851.2) | 711161.5 | 339273.4 | 707714.1 | 341988.1 | 821733.9 | 171783.3 | 952724 | 363663.3 | 0.52 | 0.0313 | 0.058495 | 0.17 | 0.537426 | 0.776400 |
| COMPOUND_707_5067a12_868767 | Rp | + | 707.5067 | 12.87 | | | | (1415.9202, 332.56)(1416.9304, 435.09)(1453.9211, 315.79)(708.513, 34131.38)(709.5164, 165648.77)(710.5193, 39356.31)(711.5215, 6693.27)(712.5273, 1225.54)(713.5171, 185.99)(1432.9744, 182.18) | 1173202 | 728799.9 | 881877.4 | 611240.2 | 931654.2 | 408944.5 | 1021035 | 595187.9 | -0.27 | 0.351232 | 0.453281 | 0.48 | 0.161092 | 0.473602 |
| COMPOUND_709_6457a2_89473 | Hilic | + | 709.6457 | 2.89 | | | | (710.6531, 3903.79)(711.6556, 509.66)(712.6519, 2934.01)(713.6572, 360.67)(714.6512, 910.58)(715.6515, 105.07)(716.6485, 189.06) | 20095.57 | 4654.196 | 23843.07 | 5656.808 | 20860.86 | 4531.677 | 20980.95 | 5686.464 | 0.30 | 0.302962 | 0.403553 | -0.70 | 0.043194 | 0.270201 |
| COMPOUND_710_5108a11_688845 | Rp | - | 710.5108 | 11.69 | | | | (1456.0209, 78.16)(1466.0364, 312.99)(709.5047, 9138.52)(710.5076, 3537.61)(711.5037, 3578.11)(712.5, 1401.56)(713.5049, 362.16)(755.539, 261.34)(756.5133, 1094.14)(757.5283, 781.95)(1534.0665, 322.54) | 97224 | 27745.75 | 103666.5 | 36397.55 | 127376.7 | 32848.94 | 127542.9 | 38518.46 | 0.25 | 0.37211 | 0.474245 | -0.37 | 0.256536 | 0.56678 |
| COMPOUND_711_5809a13_60106 | Rp | + | 711.5809 | 13.60 | | | | (712.5886, 17881.63)(713.5923, 8934.46)(714.5948, 2479.46)(715.5921, 734.55) | 28711.49 | 15181.31 | 27502.09 | 16620.46 | 36994.57 | 17730.42 | 71824.39 | 44630.97 | 0.61 | 0.008355 | 0.018057 | 0.72 | 0.010014 | 0.153413 |
| COMPOUND_713_3628a5_4239244 | Rp | + | 713.3628 | 5.42 | | | | (357.6894, 6069.55)(358.1913, 2114.95)(358.6898, 569.09)(359.1907, 117.91) | 17545.09 | 3712.884 | 14448.19 | 3381.014 | 20520.2 | 7507.248 | 27780.4 | 9121.826 | 0.29 | 0.224508 | 0.318383 | 0.84 | 0.004024 | 0.094399 |
| COMPOUND_713_498a12_015046 | Rp | - | 713.4980 | 12.02 | | | | (1471.986, 174.24)(1472.987, 147.53)(712.4912, 10304.19)(713.4944, 4422.59)(714.4991, 2345.87)(715.5029, 678.7)(1425.9266, 128.53) | 20981.97 | 6188.262 | 26390.54 | 16357.09 | 66571.38 | 37422.49 | 50996.28 | 27981.09 | 1.45 | 8.4E-11 | 1.3E-09 | -0.06 | 0.797274 | 0.91372 |
| COMPOUND_713_4988a12_034298 | Rp | - | 713.4988 | 12.03 | | | | (1471.9922, 198.44)(1473.0048, 172.07)(712.4909, 13276.89)(713.4942, 6179.83)(714.4973, 2197.39)(715.4984, 588.25)(716.4963, 73.97)(1425.9183, 110.14) | 23635.25 | 6594.967 | 33218.59 | 14823.9 | 75694.43 | 31818.03 | 84409.18 | 35558.39 | 1.38 | 1.24E-10 | 1.83E-09 | -0.04 | 0.832361 | 0.926681 |
| COMPOUND_713_5024a12_0111265 | Rp | + | 713.5024 | 12.01 | | | | (1465.9199, 81.72)(736.4961, 1045.22)(737.4976, 510.48)(738.508, 20044.43)(1449.9257, 102.99)(714.5085, 11307.34)(715.5129, 5198.87)(716.5166, 1507.71)(717.5206, 450.25) | 72115 | 34781.28 | 55065 | 18292.34 | 149010.2 | 73357.04 | 180737.6 | 90594.18 | 1.23 | 4.03E-13 | 2.39E-11 | 0.22 | 0.158819 | 0.468876 |
| COMPOUND_713_5039a11_964554 | Rp | + | 713.5039 | 11.96 | | | | (1465.935, 253.74)(736.514, 977.86)(737.5061, 489.77)(738.5093, 13640.78)(1449.9316, 126.15)(714.5078, 15125.9)(715.5114, 6719.42)(716.5145, 1791.75)(717.5124, 497.82) | #DIV/0! | #DIV/0! | 107515.8 | 69971.53 | 56601.18 | 41937.8 | 62263.25 | 62604.05 | 1.14 | 2.02E-09 | 2.03E-08 | 0.03 | 0.873639 | 0.946337 |
| COMPOUND_714_2937a10_646723 | Rp | - | 714.2937 | 10.65 | | | | (1463.5586, 135.22)(1464.5554, 169.49)(713.2841, 1555.47)(714.2868, 3339.75)(715.2872, 1040.96)(1427.5626, 128.3)(1428.5977, 152.24)(759.3231, 724.57) | 50045.27 | 8126.123 | 47518.48 | 9219.662 | 44922.31 | 6088.527 | 43682.13 | 8985.028 | -0.56 | 0.042799 | 0.076374 | 0.29 | 0.37003 | 0.671661 |
| COMPOUND_714_566a11_9216795 | Rp | + | 714.5660 | 11.92 | | | | (1430.1312, 410.67)(737.5313, 1 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_715_4937a10_8657 | Rp | - | 715.4973 | 10.87 | | | | (1465.893, 493.44)(1466.878, 224.16)(1467.9196, 377.78)(1468.9204, 267.23)(1469.9242, 296.37)(150.4716, 1263.47)(151.4699, 344.01)(152.4865, 429.3)(153.4885, 2087.83)(154.4972, 4825.28)(155.4951, 404.67)(1476.9688, 526.81)(1477.9834, 298.35)(1478.9763, 483.09)(1479.9794, 423.56)(149.4909, 5480.19)(151.4936, 2686.21)(152.4929, 908.03)(153.4914, 186.62)(1429.9536, 339.49)(1430.9744, 497.5)(1431.9642, 366.26)(1543.9741, 369.78)(1544.9672, 243.52)(1545.977, 321.84)(1546.9857, 263.31)(1547.9834, 330.56)(1476.0791, 302.87)(1477.0791, 1079.09)(151.5105, 4742.35)(156.5133, 1565.56)(157.5152, 2156.28)(158.5186, 345.35)(1429.9418, 34.07)(1430.9739, 75.87)(1544.0833, 630.62)(1545.0723, 689.63)(1546.0837, 2222.43)(1432.0249, 158.21)(1433.0347, 163.95)(1434.0396, 66.14)(1738.5188, 372.73)(1739.5117, 134.06)(1740.5241, 11598.35)(1741.5269, 5326.76)(1742.5299, 42660.29)(1743.5295, 18535.76)(1748.5322, 4860.35)(1749.5371, 919.37)(1449.104, 220.65) | 116898 | 37695.67 | 123101.5 | 37044.28 | 83854.77 | 25641.43 | 84604.56 | 19958.16 | -0.97 | 0.000681 | 0.001843 | 0.05 | 0.878547 | 0.949827 |
| COMPOUND_715_5139a12_343616 | Rp | - | 715.5139 | 12.34 | PE 34:2 | 2 | 20 eV: 714.5073(100), 279.2328(42), 434.2677(4) | (1476.0791, 302.87)(1477.0791, 1079.09)(151.5105, 4742.35)(156.5133, 1565.56)(157.5152, 2156.28)(158.5186, 345.35)(1429.9418, 34.07)(1430.9739, 75.87)(1544.0833, 630.62)(1545.0723, 689.63)(1546.0837, 2222.43)(1432.0249, 158.21)(1433.0347, 163.95)(1434.0396, 66.14)(1738.5188, 372.73)(1739.5117, 134.06)(1740.5241, 11598.35)(1741.5269, 5326.76)(1742.5299, 42660.29)(1743.5295, 18535.76)(1748.5322, 4860.35)(1749.5371, 919.37)(1449.104, 220.65) | 74799.62 | 24523.94 | 95000.26 | 43092.66 | 309433.7 | 96381.98 | 399183.3 | 159105 | 1.35 | 2.11E-11 | 4.71E-10 | 0.12 | 0.536762 | 0.776357 |
| COMPOUND_715_5197a12_3454075 | Rp | - | 715.5197 | 12.35 | PE 34:2 | 2 | 10 eV: 716.5234(100), 575.5043(60), 43.0539(7) | (1476.0791, 302.87)(1477.0791, 1079.09)(151.5105, 4742.35)(156.5133, 1565.56)(157.5152, 2156.28)(158.5186, 345.35)(1429.9418, 34.07)(1430.9739, 75.87)(1544.0833, 630.62)(1545.0723, 689.63)(1546.0837, 2222.43)(1432.0249, 158.21)(1433.0347, 163.95)(1434.0396, 66.14)(1738.5188, 372.73)(1739.5117, 134.06)(1740.5241, 11598.35)(1741.5269, 5326.76)(1742.5299, 42660.29)(1743.5295, 18535.76)(1748.5322, 4860.35)(1749.5371, 919.37)(1449.104, 220.65) | 62922.96 | 33620.06 | 70378.14 | 37048.25 | 180807 | 53626.73 | 232326.9 | 77344.59 | 1.33 | 1.6E-09 | 1.67E-08 | 0.18 | 0.405165 | 0.6912 |
| COMPOUND_716_5838a12_270833 | Rp | + | 716.5838 | 12.27 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 56076.94 | 18210 | 54732.96 | 23456.45 | 46601.85 | 7482.646 | 44939.36 | 11849.52 | -0.60 | 0.026262 | 0.050686 | 0.06 | 0.851514 | 0.936901 |
| COMPOUND_717_2988a10_644881 | Rp | - | 717.2988 | 10.64 | | | | (1476.0791, 302.87)(1477.0791, 1079.09)(151.5105, 4742.35)(156.5133, 1565.56)(157.5152, 2156.28)(158.5186, 345.35)(1429.9418, 34.07)(1430.9739, 75.87)(1544.0833, 630.62)(1545.0723, 689.63)(1546.0837, 2222.43)(1432.0249, 158.21)(1433.0347, 163.95)(1434.0396, 66.14)(1738.5188, 372.73)(1739.5117, 134.06)(1740.5241, 11598.35)(1741.5269, 5326.76)(1742.5299, 42660.29)(1743.5295, 18535.76)(1748.5322, 4860.35)(1749.5371, 919.37)(1449.104, 220.65) | 94457.06 | 11976.07 | 95612.83 | 15568.04 | 78878.07 | 20731.72 | 78629.37 | 19403.1 | -0.81 | 0.001112 | 0.002864 | -0.09 | 0.373927 | 0.888604 |
| COMPOUND_717_5246a9_619151 | Rp | + | 717.5246 | 9.62 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 307257 | 75627.83 | 266788.9 | 52464.22 | 335087.1 | 56285.27 | 334457.1 | 84663.06 | 0.27 | 0.337057 | 0.437747 | 0.63 | 0.064599 | 0.307286 |
| COMPOUND_717_5294a12_769517 | Rp | - | 717.5294 | 12.77 | PE 16_0:18:1 | 1 | 10 eV: 716.5214(100), 281.2485(6) | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 24619.58 | 8582.44 | 28905.24 | 11776.89 | 73656.86 | 28953.85 | 101407.4 | 38328.46 | 1.34 | 3.2E-10 | 4.19E-09 | 0.17 | 0.41194 | 0.694898 |
| COMPOUND_717_5337a11_952413 | Rp | + | 717.5337 | 11.95 | PC 31:1 | 2 | 20 eV: 184.0735(100), 718.5437(90), 494.0215(5) | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 85071.7 | 35271.86 | 92989.96 | 46583.39 | 110666.4 | 30534.76 | 146327.1 | 72917.07 | 0.78 | 0.000291 | 0.000837 | 0.43 | 0.073932 | 0.327102 |
| COMPOUND_717_5339a12_766433 | Rp | + | 717.5339 | 12.77 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 40357 | #DIV/0! | 47369.8 | 16307.81 | 78440.73 | 21186.28 | 107568.6 | 48626.83 | 0.96 | 4.96E-10 | 5.97E-09 | 0.48 | 0.0028 | 0.074044 |
| COMPOUND_717_5671a12_931534 | Rp | + | 717.5671 | 12.93 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 67749.88 | 32289.55 | 57134.33 | 29358.87 | 56827 | 15173.15 | 62625.6 | 23208.2 | -0.27 | 0.364002 | 0.462728 | 0.10 | 0.780485 | 0.909288 |
| COMPOUND_717_5674a12_571076 | Rp | + | 717.5674 | 12.57 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 149858.5 | 50866.98 | 140861 | 52685.75 | 134304.9 | 42081.22 | 126073.7 | 47385.58 | -0.44 | 0.078495 | 0.131233 | 0.14 | 0.633405 | 0.828355 |
| COMPOUND_717_9053a11_05774 | Rp | + | 717.9053 | 11.06 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 91296.92 | 57809.11 | 91837.97 | 69875.81 | 86737.54 | 23951.75 | 88324.09 | 23547.98 | 0.40 | 0.152624 | 0.231454 | -0.13 | 0.691616 | 0.857326 |
| COMPOUND_718_525a11_379731 | Rp | - | 718.5250 | 11.38 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 213835.9 | 56163.89 | 218910.1 | 60691.96 | 212635.4 | 46188.3 | 231164.7 | 56871.41 | -0.70 | 0.00579 | 0.012923 | 0.06 | 0.843717 | 0.93246 |
| COMPOUND_719_1516a9_161084 | Rp | - | 719.1516 | 9.16 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 17832.02 | 3423.469 | 17267 | 3166.995 | 16009.57 | 2704.825 | 17138.86 | 4282.706 | -0.51 | 0.094291 | 0.154883 | 0.35 | 0.335729 | 0.639647 |
| COMPOUND_719_5536a12_241971 | Rp | + | 719.5536 | 12.24 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 52008.82 | 27817.67 | 53754.99 | 29738.58 | 67949.55 | 14826.23 | 73798.36 | 25941.96 | 0.27 | 0.282295 | 0.38159 | 0.49 | 0.095145 | 0.36381 |
| COMPOUND_719_5831a13_133488 | Rp | + | 719.5831 | 13.13 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 45569.54 | 24653.3 | 49123.13 | 28336.01 | 41375.77 | 17590.64 | 45660.52 | 28386.52 | -0.11 | 0.689141 | 0.773266 | 0.14 | 0.667713 | 0.846185 |
| COMPOUND_720_5402a11_690141 | Rp | - | 720.5402 | 11.69 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 981455 | 256322.8 | 1078396 | 372634.2 | 1085899 | 241661.5 | 1083365 | 302289.2 | 0.40 | 0.145596 | 0.222595 | -0.36 | 0.274045 | 0.583098 |
| COMPOUND_721_5045a12_198856 | Rp | - | 721.5045 | 12.20 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 40495.65 | 24998.42 | 38597.04 | 24407.97 | 33661.64 | 15439.93 | 36898.63 | 18946.74 | -0.16 | 0.5334 | 0.632881 | 0.20 | 0.506653 | 0.755617 |
| COMPOUND_721_5228a12_871885 | Rp | + | 721.5228 | 12.87 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 495190 | 535556.7 | 4482359 | 436826.7 | 4105132 | 456796.6 | 4400573 | 541576.4 | -0.85 | 0.002423 | 0.005918 | 0.04 | 0.890663 | 0.953702 |
| COMPOUND_722_1006a9_06127 | Rp | - | 722.1006 | 9.06 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 116912.4 | 18869.79 | 127689.5 | 18202.61 | 103204.7 | 12619.83 | 106271 | 14075.47 | -0.69 | 0.011405 | 0.02376 | -0.39 | 0.223049 | 0.531262 |
| COMPOUND_723_2995a10_647959 | Rp | - | 723.2995 | 10.65 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 88217.3 | 16559.44 | 88565.83 | 18780.41 | 95963.21 | 14912.71 | 92328.88 | 15784.51 | 0.47 | 0.107899 | 0.179395 | -0.24 | 0.481093 | 0.743153 |
| COMPOUND_723_5057a11_708447 | Rp | - | 723.5057 | 11.71 | PC 28:0 | 2 | 20 eV: 662.4759(100), 227.2026(22), 722.5332(10) | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 77572.16 | 50888.17 | 99009.61 | 74142.89 | 144303.9 | 86693.1 | 156252.7 | 89449.2 | 0.57 | 0.026169 | 0.0499 | 0.06 | 0.841526 | 0.93246 |
| COMPOUND_723_5191a12_532415 | Rp | - | 723.5191 | 12.53 | PE 36:5e | 2 | 20 eV: 722.513(100), 303.2328(52), 436.285(7) | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 334914.6 | 269074.2 | 361978.8 | 267481.5 | 452061.1 | 296055.7 | 451936 | 237630.7 | 0.56 | 0.033106 | 0.061413 | -0.05 | 0.871739 | 0.945212 |
| COMPOUND_723_5206a12_5318985 | Rp | + | 723.5206 | 12.53 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 171922.9 | 42129.23 | 64446.2 | 50770.2 | 15866.08 | 29550.76 | 68431.9 | 51930.44 | -0.12 | 0.673401 | 0.760149 | 0.26 | 0.442418 | 0.717814 |
| COMPOUND_724_0943a9_296961 | Rp | - | 724.0943 | 9.30 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 69570.64 | 11152.63 | 75226.02 | 10619.14 | 66929.07 | 9489.962 | 67521.32 | 10563.37 | -0.25 | 0.376458 | 0.477624 | -0.42 | 0.221903 | 0.531023 |
| COMPOUND_724_388a10_8601265 | Rp | + | 724.3880 | 10.86 | | | | (1472.0872, 777.95)(1473.0739, 419.4)(1739.5653, 865.11)(1717.5902, 7845.07)(1718.5936, 3510.9)(1719.5874, 1082.77) | 23166.23 | 8574.473 | 19858.82 | 7897.725 | 76685.43 | 51942.72 | 87008.8 | 22121.05 | 1.2 | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------------------|----------|--|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_726_5682a11_813656 | Rp | + | 726.5682 | 11.81 | | | | (1454.188, 146.78)(1492.045, 463.71)(749.5317, 1871.16)(750.5429, 1266.26)(751.5463, 1035.8)(744.5719, 1283.04)(745.5787, 803.36)(746.5922, 854.31)(727.5755, 20420.08)(728.5791, 11248.04)(729.5814, 3553.34)(1471.2064, 456.48) | 164522.9 | 48469.36 | 175957 | 64406.46 | 176308.1 | 61523.76 | 165618.7 | 48064.33 | 0.18 | 0.483741 | 0.585062 | -0.48 | 0.11517 | 0.397302 |
| COMPOUND_727_5157a11_618334 | Rp | + | 727.5157 | 11.62 | | | | (1456.033, 531.89)(1494.0156, 319.51)(750.5402, 4468.43)(751.5505, 2488.06)(1478.0322, 50.12)(1479.0782, 306.96)(728.5221, 1371.23)(729.5252, 6237.5)(730.5386, 106435.63)(731.5422, 47029.83)(1473.0588, 213.62)(840.5301, 715.96)(841.534, 411.46)(842.5355, 799.73)(843.5376, 401.16)(726.5432, 5051.13)(727.5461, 2282.1)(728.5498, 803.71)(729.5522, 201.12)(751.5727, 11965.02)(752.5755, 5816.54)(753.5876, 8783.52)(754.5911, 3968.61)(755.6049, 8038.11)(746.5977, 2826.09)(747.5879, 1503.18)(748.5729, 432.25)(729.5912, 145731.42)(730.5944, 67866.17)(731.605, 68051.16)(732.6085, 27643.09)(733.612, 7373.01)(734.6147, 1410.92)(735.6246, 427.05)(365.2992, 275.14)(365.798, 20.25) | 104250.5 | 58375.21 | 122422.9 | 73122.87 | 207638.1 | 109854 | 187362.5 | 80108.24 | 1.13 | 2.28E-05 | 8.36E-05 | -0.26 | 0.369208 | 0.671613 |
| COMPOUND_727_5493a11_368302 | Rp | - | 727.5493 | 13.37 | | | | (751.5727, 11965.02)(752.5755, 5816.54)(753.5876, 8783.52)(754.5911, 3968.61)(755.6049, 8038.11)(746.5977, 2826.09)(747.5879, 1503.18)(748.5729, 432.25)(729.5912, 145731.42)(730.5944, 67866.17)(731.605, 68051.16)(732.6085, 27643.09)(733.612, 7373.01)(734.6147, 1410.92)(735.6246, 427.05)(365.2992, 275.14)(365.798, 20.25) | 43735.35 | 16526.7 | 50489 | 22212.8 | 49193.93 | 11628.39 | 44731.34 | 17937.3 | 0.47 | 0.099101 | 0.161604 | -0.63 | 0.060528 | 0.302235 |
| COMPOUND_728_5831a0_8363836 | Hilic | + | 728.5831 | 0.84 | | | | (751.5727, 11965.02)(752.5755, 5816.54)(753.5876, 8783.52)(754.5911, 3968.61)(755.6049, 8038.11)(746.5977, 2826.09)(747.5879, 1503.18)(748.5729, 432.25)(729.5912, 145731.42)(730.5944, 67866.17)(731.605, 68051.16)(732.6085, 27643.09)(733.612, 7373.01)(734.6147, 1410.92)(735.6246, 427.05)(365.2992, 275.14)(365.798, 20.25) | 1379251 | 381935.3 | 1467393 | 466881.3 | 1501340 | 462471.8 | 1472812 | 460912.4 | 0.25 | 0.399515 | 0.499958 | -0.25 | 0.458038 | 0.727948 |
| COMPOUND_728_5854a12_142221 | Rp | + | 728.5854 | 12.14 | SM d36.2 | 20 | 20 eV: 184.0729(100), 729.5946(28) | (1458.1833, 424.82)(1459.2611, 562.16)(1460.1631, 384.68)(1496.0734, 5401.72)(751.573, 10728.49)(752.5726, 5910.76)(753.5739, 2001.06)(1480.1365, 157.6)(1481.1244, 285.16)(1482.1196, 197.11)(767.5397, 5645.48)(729.5929, 202307.62)(730.5954, 91009.86)(731.5981, 22392.93)(1475.1733, 133.57)(1476.2089, 169.98)(1477.2091, 113.26) | 933099.2 | 285836.4 | 897211.6 | 366108.4 | 892635.7 | 274777.4 | 863040.5 | 280008.6 | -0.11 | 0.703677 | 0.783952 | 0.04 | 0.897205 | 0.954419 |
| COMPOUND_729_533a11_862355 | Rp | + | 729.5330 | 11.86 | PC 14.0_18.2 | 1 | 20 eV: 184.0737(100), 730.5359(75), 104.1071(3), 451.2971(1) | (1460.0708, 4809.18)(1461.0725, 4429.33)(1462.076, 2094.02)(1463.0789, 818.38)(1464.0867, 379.85)(1498.08, 517.01)(752.5277, 44956.04)(753.5259, 19559.12)(1482.052, 1193.93)(1483.057, 1172.29)(1484.0692, 1971.78)(1485.0775, 1430.76)(1486.0756, 1003.06)(1487.0812, 787.3)(1488.0872, 631.18)(768.5111, 1666.24)(769.5086, 1284.46)(770.5283, 1367.07)(730.5407, 387487.47)(731.5445, 164436.6)(732.547, 39038.51)(733.5488, 7561.62)(734.5517, 1493.77)(735.5558, 266.81)(1477.1459, 191.48) | 2062161 | 742333.5 | 2414727 | 857698 | 3674738 | 1322215 | 3678019 | 1276568 | 1.27 | 1.89E-07 | 1.11E-06 | -0.33 | 0.194471 | 0.505132 |
| COMPOUND_730_0318a12_024141 | Rp | + | 730.0318 | 12.02 | | | | (1499.08, 880.95)(748.0358, 548.39)(731.038, 10299.61)(732.0391, 2823.5)(733.0378, 995.34)(734.0269, 162.65)(1478.1075, 770.49)(1479.1123, 906.69)(1480.1135, 708.17) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.10 | 0.724184 | 0.798344 | 0.00 | 0.993505 | 0.997491 |
| COMPOUND_730_5978a12_575648 | Rp | + | 730.5978 | 12.58 | N-Stearoyl-D-sphingomyelin | 1 | 20 eV: 184.0738(100), 731.6159(21), 104.1027(4), 590.5249(3) | (1462.206, 179.16)(1463.2266, 267.1)(1464.2318, 186.05)(1465.213, 221.68)(1500.1243, 341419.9) 113208.6 347000.2 141050.3 326137.1 100432.5 322446.3 114598.9 780.48(1501.1353, 672.83)(1502.1489, 1103.61)(753.5848, 5414.95)(754.5852, 2678.38)(755.5948, 1019.1)(1484.123, 604.13)(1485.122, 560.49)(731.6068, 38584.87)(732.6087, 17978.63)(733.6107, 4507.28)(734.6129, 342.45)(1479.206, 257.59)(1480.2054, 208.15)(1481.1923, 200.01)(1482.1906, 96.04) | 326137.1 | 100432.5 | 322446.3 | 114598.9 | -0.07 | 0.817885 | 0.872049 | -0.11 | 0.748274 | 0.891783 | | | | |
| COMPOUND_731_5085a11_177976 | Rp | - | 731.5085 | 11.18 | | | | (1497.992, 232.75)(1499.0273, 262.77)(766.4652, 5903.33)(767.4678, 2954.71)(768.4698, 1030.39)(1507.9865, 534.62)(1508.998, 660.63)(1510.0013, 474.33)(730.502, 56249.29)(731.505, 24732.77)(732.5062, 7631.18)(733.4984, 2013.24)(1461.9976, 368.51)(1462.9973, 567.44)(1464.0038, 714.58)(1465.0035, 823.19)(1466.0052, 580.71) | 103187.9 | 28107.66 | 119460.5 | 41648.58 | 180205.3 | 64704.19 | 224558.1 | 100724.8 | -0.63 | 0.010662 | 0.022439 | -0.42 | 0.149132 | 0.45818 |
| COMPOUND_731_5415a9_853401 | Rp | + | 731.5415 | 9.85 | | | | (1464.1158, 63.68)(1486.1377, 74.92)(377.7692, 316.65)(378.2676, 1338.33)(378.7781, 66.31)(770.537, 1752.61)(375.2911, 2781.55)(375.793, 1180.14)(376.2861, 2410.21)(376.7963, 76.77)(386.29, 507.37)(386.7955, 127.85)(732.5469, 21005.56)(733.5494, 8500.72)(734.5482, 1106.35)(366.7785, 2081.91)(367.2819, 1130.66)(367.7829, 232.63) | 235920.4 | 64020.62 | 202242.8 | 41829.07 | 272375.8 | 42167.38 | 270329.8 | 70017.29 | 0.44 | 0.113225 | 0.181482 | 0.54 | 0.107417 | 0.38954 |
| COMPOUND_731_5497a12_171762 | Rp | + | 731.5497 | 12.17 | PC 32.1 | 2 | 40eV: 184.0733(100), 86.0963(4) | (1464.1012, 12294.17)(1465.1095, 10954.99)(1466.107, 5057.69)(1467.1075, 1982.37)(1468.1073, 537.48)(1469.122, 198.64)(1470.1488, 36.87)(754.538, 17590.37)(755.541, 7661.45)(756.5562, 247497.5)(1486.1024, 1769.04)(1487.116, 1562.33)(1488.1029, 2662.06)(1489.1052, 2024.98)(1490.1141, 1817.13)(1491.1125, 1338.9)(1492.1172, 771.78)(1493.1168, 386.79)(1494.0981, 245.42)(732.5555, 830709.75)(733.5597, 348721.34)(734.5625, 83366.52)(735.5646, 14678.25)(736.5666, 2523.83)(737.561, 433.04) | 3786019 | 1359359 | 3762709 | 1927352 | 6137051 | 1812338 | 8278111 | 3408405 | 0.89 | 6.5E-05 | 0.000211 | 0.60 | 0.01762 | 0.194764 |
| COMPOUND_733_5197a9_113487 | Rp | + | 733.5197 | 9.11 | | | | (1468.0625, 57.36)(1505.9615, 67.31)(764.5262, 554.73)(765.0149, 305.72)(376.281, 3205.74)(736.7851, 704.61)(377.279, 1294.63)(734.5264, 5876.51)(735.5266, 2689.98)(736.5265, 725.58)(737.5367, 185.34)(367.7686, 987.56)(368.2692, 552.89)(368.7709, 138.54)(1485.1165, 53.82) | 97625.87 | 27370.29 | 87901.46 | 22618.48 | 105096.8 | 19324.99 | 99833.16 | 27130.94 | 0.17 | 0.565207 | 0.661907 | 0.45 | 0.192143 | 0.505089 |
| COMPOUND_733_5645a12_636991 | Rp | + | 733.5645 | 12.64 | PC 16.0_16.0 | 1 | 10 eV: 734.5685(100), 184.074(16) | (1468.142, 518.88)(1469.1357, 418.58)(1470.1539, 349.62)(1471.1361, 176.73)(1506.1434, 1313.43)(756.5535, 16865.63)(757.5569, 7401.85)(1490.1252, 421.86)(734.571, 71559.41)(735.5741, 30629.69)(736.5761, 7517.03)(737.5767, 1676.46)(738.5713, 365.47)(739.5713, 50.42) | 800363 | 325728.3 | 814631.8 | 409732.3 | 795206.6 | 200400.1 | 929792.7 | 346716.8 | 0.08 | 0.771264 | 0.833439 | 0.41 | 0.225889 | 0.533671 |
| COMPOUND_735_5388a12_870843 | Rp | + | 735.5388 | 12.87 | | | | (1509.991, 156.04)(736.5394, 7865.36)(737.5434, 3830.06)(738.5411, 1793.33)(739.5372, 64137.47) 9353.328 60828.02 9030.602 55085.29 7475.654 55429.15 8596.102 | -0.80 | 0.004453 | 0.010139 | 0.45 | 0.168038 | 0.480454 | | | | | | | | |
| COMPOUND_736_5279a11_778821 | Rp | - | 736.5279 | 11.78 | | | | (1508.018, 199.92)(1509.0118, 130.35)(1509.9768, 219.41)(1518.0739, 301.13)(1519.1025, 484.17)(1520.1025, 469.09)(735.5245, 14054.51)(736.52, 7991.92)(737.5187, 6488.74)(781.5492, 1136.09)(1586.073, 324.78)(1587.1077, 495.14) | 217339.3 | 57781.27 | 241380.4 | 72946.09 | 257305.8 | 63385.02 | 262402.3 | 61501.83 | -0.49 | 0.063055 | 0.108729 | 0.12 | 0.692104 | 0.857326 |
| COMPOUND_737_3602a12_429183 | Rp | - | 737.3602 | 13.43 | | | | (736.3535, 6545.75)(737.3566, 2961.15)(738.3511, 4150.92)(739.354, 1708.92)(740.3504, 1041.92)(741.3499, 343.94)(742.3429, 158.9)(1473.7129, 122.91) | 27248.96 | 11914.37 | 27906.8 | 13635.46 | 27829.07 | 8545.028 | 51266.23 | 25061.34 | 0.27 | 0.23878 | 0.333581 | 0.87 | 0.001783 | 0.061415 |
| COMPOUND_737_5032a11_989126 | Rp | + | 737.5032 | 11.99 | | | | (1476.0896, 360.73)(1477.0658, 200.66)(760.5006, 598.41)(761.4981, 86.96)(762.518, 321.77)(776.4389, 496.15)(738.5086, 7428.95)(739.5126, 3328.47)(740.5229, 1578.97)(741.5289, 492.45)(1493.0782, 632.36) | 38950.1 | 17712.04 | 42628.95 | 22809.41 | 93206.31 | 28075.06 | 112898.1 | 49723.87 | 1.19 | 8.44E-10 | 9.56E-09 | 0.29 | 0.138454 | 0.44479 |
| COMPOUND_738_5093a0_85949695 | Hilic | + | 738.5093 | 0.86 | | | | (761.4953, 1366.03)(739.5159, 6201.25)(740.5202, 3349.42)(741.5305, 9835.75)(742.5385, 5159.82)(743.5393, 1892.21)(744.5539, 1297.56) | 78591.97 | 21494.39 | 90283.91 | 25783.52 | 91888.1 | 18125.93 | 95995.36 | 20250.61 | 0.32 | 0.219695 | 0.31355 | 0.24 | 0.446933 | 0.720983 |
| COMPOUND_738_5423a12_0963545 | Rp | - | 738.5423 | 12.10 | | | | (1512.0677, 279.85)(1513.0886, 376.75)(1514.0793, 394.12)(1522.0833, 950.05)(1523.0825, 589.17)(1524.0706, 363.48)(1525.0396, 121.28)(737.535, 16968.31)(738.5334, 3991.83)(739.5292, 5333.28)(740.5207, 4161.19)(741.5225, 1634.77)(742.5109, 927.12)(743.5166, 368.67)(1476.1368, 445.29)(783.5398, 304.76)(784.5505, 1368.78)(1500.0673, 605.64)(1591.0891, 659.05)(1592.0824, 958.79) | 209658.4 | 53987.73 | 209194.2 | 60332.25 | 240834.3 | 50782.21 | 243935.5 | 47933.55 | -0.12 | 0.660362 | 0.748056 | -0.40 | 0.221354 | 0.531023 |
| COMPOUND_739_5143a12_282022 | Rp | - | 739.5143 | 12.28 | | | | (852.4661, 271.86)(853.4769, 138.29)(854.4745, 168.19)(1524.081, 931.8)(738.5074, 16693.48)(739.5106, 7813.27)(740.5141, 2286.61)(741.515, 516.96)(742.5018, 42.11)(1478.0275, 432.31)(1479.0394, 369.84)(1480.0575, 261.61) | 135605.1 | 39257.84 | 151750.3 | 54322.36 | 435699.4 | 139734 | 551810.6 | 178694.7 | 1.33 | 6.68E-11 | 1.1E-09 | 0.26 | 0.185196 | 0.499463 |
| COMPOUND_739_5174a12_2786 | Rp | + | 739.5174 | 12.28 | PE 16.0_20.4 | 1 | 20 eV: 599.5108(100), 313.2788(7), 740.535(6), 95.0878(4) | (1480.0438, 590.98)(1481.0404, 440.64)(1482.0619, 301.52)(1483.0471, 111.71)(762.5074, 2872.34)(763.5104, 1237.84)(778.4539, 392.01)(779.4625, 355.66)(757.5566, 10231.63)(740.5258, 80403.89)(741.5291, 36202.14)(742.5325, 9172.67)(743.5359, 1964.46)(1497.0763, 3942.52) | 93238.83 | 26753.12 | 103164.7 | 41229.96 | 286070 | 74939.54 | 345734.1 | 93522.65 | 1.26 | 5.91E-10 | 7.01E-09 | 0.44 | 0.034661 | 0.249266 |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|---|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_741_4565a0_74391323 | Hilic | + | 741.4565 | 0.74 | | | | (764.459, 456.121)(765.4618, 246.67)(766.4763, 530.07)(759.4813, 417.16)(742.4668, 13964.59)(743.4705, 6411.64)(744.479, 7601.09)(745.4844, 3178.43)(746.5001, 1908.99) | 113944.3 | 45200.37 | 105648.3 | 44985.58 | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -1.25 | 4.8E-09 | 4.24E-08 | 0.12 | 0.563903 | 0.788601 |
| COMPOUND_741_5217a10_943338 | Rp | - | 741.5217 | 10.94 | | | | (1517.9631, 161.76)(1518.9701, 166.56)(1519.9526, 204.88)(1520.9694, 166.33)(1521.9978, 121.93)(854.5196, 7897.19)(855.5234, 3947.43)(776.4873, 1955.49)(777.491, 1101.9)(1527.9801, 163.67)(1528.9911, 177.41)(1529.9797, 208.77)(1530.9877, 232.73)(740.5055, 3526.14)(741.5095, 1824.22)(742.4917, 2064.57)(743.489, 1093.9)(1481.9828, 214.66)(1482.9655, 247.58)(1483.9377, 344.73)(1596.0605, 397.32) | 146171.6 | 52259.02 | 119530 | 33446.64 | 59184.18 | 4576.772 | 66953.52 | 25917.04 | 0.17 | 0.511655 | 0.612246 | 0.43 | 0.164565 | 0.47785 |
| COMPOUND_741_5299a12_466389 | Rp | - | 741.5299 | 12.47 | | | | (1518.0876, 235.56)(1518.1086, 431.19)(1529.0872, 127.27)(1530.0914, 1296.79)(1531.0975, 1178.14)(1532.1025, 1631.72)(1533.1082, 1118.31)(740.5224, 62852.03)(741.5258, 28007.84)(742.5319, 10680.2)(743.5369, 2914.9)(744.5401, 654.83)(1482.0841, 794.28)(1483.0914, 517.53)(1484.0916, 247.84)(1596.0323, 85.39)(1597.0518, 60.16) | 158458.6 | 64447.21 | 165200 | 67433.36 | 307227.1 | 78602.56 | 337022.6 | 122351.3 | 1.23 | 4.35E-08 | 3.03E-07 | 0.09 | 0.683985 | 0.853695 |
| COMPOUND_741_5331a11_827901 | Rp | + | 741.5331 | 11.83 | | | | (1484.0762, 1202.82)(1485.0748, 926.82)(1486.082, 1135.51)(1487.0859, 831.05)(1522.0565, 278.86)(764.5191, 3368.56)(765.5232, 1533.55)(1506.0946, 339.96)(1507.0807, 490.83)(742.5391, 10026.49)(743.5418, 4810.33)(744.5441, 1579.14)(745.5257, 416.53)(1501.1027, 195.99) | 56844.67 | 25286.92 | 69139.24 | 37812.4 | 89319.42 | 45828.82 | 80434.11 | 35081.84 | 0.88 | 0.000239 | 0.000702 | 0.10 | 0.718561 | 0.876415 |
| COMPOUND_741_5358a12_454743 | Rp | + | 741.5358 | 12.45 | PE 3e:3 | 2 | 10 ev: 742.542(100), 601.5214(42), 412.2839(5), 80.6082(2) | (1484.0807, 417.37)(1485.0726, 234.83)(1486.0717, 234.47)(764.5225, 4473.33)(765.5271, 2122.68)(742.54, 56559.71)(743.543, 25878.83)(744.5474, 8012.49)(745.5525, 2006.63)(1501.1123, 1781.42)(1502.121, 1250.02)(1503.1324, 706.15) | 135881.7 | 32171.24 | 160873.6 | 49197.08 | 316528 | 83320.56 | 371625.4 | 129611.1 | 1.29 | 3.1E-13 | 1.98E-11 | 0.19 | 0.239191 | 0.5441 |
| COMPOUND_741_5698a12_588807 | Rp | + | 741.5698 | 12.59 | PC 34:3e | 2 | 10 ev: 742.5762(100), 184.0758(12), 601.5229(4) | (1484.1216, 966.14)(1485.12, 1015.89)(1486.131, 641.47)(1487.1416, 352.53)(1522.1718, 19797.21)(1523.1733, 6617.17)(1524.165, 2409.95)(764.5569, 16908.52)(765.5596, 8454.84)(766.5752, 82104.55)(1506.1367, 1044.25)(1507.1218, 280.93)(1508.1172, 1510.57)(742.5758, 276611.78)(743.5791, 126787.34)(744.5822, 34590.27)(745.5855, 7174.06)(1501.1267, 749.2) | 2240311 | 685058.4 | 2059151 | 797766.6 | 1848022 | 546725.1 | 1826567 | 606346.8 | -0.49 | 0.074599 | 0.125558 | 0.17 | 0.597527 | 0.805251 |
| COMPOUND_743_5453a12_994272 | Rp | - | 743.5453 | 12.99 | | | | (742.5381, 6802.22)(743.5411, 3083.68)(744.5518, 3563.15)(745.5549, 1946.26)(746.5547, 580.74)(1486.091, 242.44)(1487.0936, 135.51)(1488.1095, 82.87) | 120728.8 | 44162.22 | 148282.1 | 59751.55 | 262888.8 | 94984.69 | 319737.6 | 121302.3 | 1.32 | 2.05E-08 | 1.58E-07 | -0.04 | 0.859495 | 0.941431 |
| COMPOUND_743_5453a12_921009 | Rp | - | 743.5453 | 12.92 | | | | (742.5381, 14835.32)(743.5411, 6702.18)(744.5513, 6731.67)(745.5552, 2846.64)(1486.1033, 219.85) | 113207.9 | 71889 | 130599.2 | 111708.4 | 169111.4 | 147236.7 | 172181.4 | 101547.7 | 0.82 | 0.001099 | 0.002836 | 0.09 | 0.743586 | 0.889774 |
| COMPOUND_743_5466a12_34561 | Rp | - | 743.5466 | 12.35 | | | | (1532.1022, 1326.73)(1533.1086, 1096.11)(742.5383, 15152.77)(743.5413, 7262.89)(744.5444, 1692.66) | 177276.7 | 19462.7 | 194507.8 | 21386.35 | 205209.4 | 30763.69 | 195844.5 | 40815.74 | 0.90 | 0.002584 | 0.006271 | -0.88 | 0.011776 | 0.167839 |
| COMPOUND_743_5501a12_082787 | Rp | + | 743.5501 | 12.08 | PC 15:0_18:2 | 1 | 10 ev: 744.554(100), 184.0742(15) | (1488.0997, 2398.51)(1489.1044, 1995.41)(1490.1106, 1104.68)(1491.1007, 622.74)(1492.1038, 253.66)(766.5397, 871.04)(767.5442, 4825.70)(768.5548, 60209.89)(1510.13, 5300.95)(1511.1271, 4202.56)(744.556, 139956.17)(745.5589, 60553.45)(746.5612, 15468.46)(747.5625, 3315.35)(748.563, 681.85)(1505.0992, 1797.38) | 1627148 | 382391.5 | 1626234 | 532839.8 | 1861054 | 494565.9 | 1627406 | 429487.5 | 0.98 | 0.17878 | 0.265575 | -0.36 | 0.279738 | 0.587659 |
| COMPOUND_743_5539a12_984675 | Rp | + | 743.5539 | 12.98 | PE 3e:2 | 2 | 20 ev: 603.5355(100), 184.076(32), 744.5828(32), 306.274(5) | (1488.0985, 368.95)(1489.1083, 214.41)(1490.1002, 163.84)(1526.1271, 368.36)(766.5427, 3800.33)(767.5475, 1854.46)(744.5577, 61212.6)(745.5613, 26872.08)(746.5652, 8968.9)(747.5693, 2349.61)(1505.1592, 786.62) | 91882.33 | 6049.352 | 162881.6 | 47566.75 | 255333.7 | 91662.09 | 311057.2 | 122223.5 | 0.93 | 4.49E-07 | 2.47E-06 | 0.26 | 0.185547 | 0.499463 |
| COMPOUND_743_584a12_730444 | Rp | + | 743.5840 | 12.73 | PC 34:2e | 2 | 20 ev: 184.074(100), 744.5898(65), 423.7637(3) | (1488.1492, 286.63)(1489.1503, 172.37)(1490.1603, 164.28)(766.5761, 8420.09)(767.5793, 4056.03)(1501.1224, 1044.49)(744.5904, 2767.08)(745.5941, 12899.96)(746.5905, 4428.05)(747.5878, 1213.3)(748.5672, 180.55) | 612557.2 | 308401.4 | 552718.2 | 194905 | 582021.7 | 206778.5 | 508325.6 | 221818.1 | -0.10 | 0.686187 | 0.77072 | -0.15 | 0.598212 | 0.805251 |
| COMPOUND_743_5866a12_077679 | Rp | + | 743.5866 | 13.08 | PC 34:2e | 2 | 20 ev: 184.0732(100), 744.5867(70) | (1488.2507, 166.91)(1489.2606, 183.61)(1490.258, 195.92)(1526.2097, 153.22)(1527.2037, 140.71)(766.5671, 4702.47)(767.5717, 2229.47)(768.5865, 5839.69)(769.589, 2663.5)(770.6047, 19008.3)(771.6136, 9886.41)(1510.1852, 132.73)(744.5871, 25231.51)(745.5905, 11634.96)(746.6051, 31169.39)(747.6089, 13658.45)(748.6082, 4102.05)(1505.162, 305.73) | 505042.9 | 317290.8 | 445444.7 | 276307.5 | 421956.5 | 207731 | 330340.4 | 184862.7 | -0.64 | 0.014793 | 0.030259 | -0.08 | 0.791641 | 0.911439 |
| COMPOUND_744_1193a11_028072 | Rp | + | 744.1193 | 11.03 | | | | (767.1271, 3381.78)(783.066, 340.17)(762.1285, 2177.58)(745.1244, 9530.09)(746.1183, 5064.03)(747.104, 2270.03) | 66140.32 | 38425.62 | 71695.32 | 53366.3 | 55201.85 | 17626.64 | 67453.46 | 22459.88 | 0.08 | 0.788942 | 0.847257 | 0.10 | 0.767928 | 0.902789 |
| COMPOUND_744_1705a8_785409 | Rp | - | 744.1705 | 8.79 | | | | (1533.4058, 69.79)(743.1644, 3973.59)(744.1691, 1231.44)(745.17, 358.48)(1488.3391, 78.69)(790.2031, 150.67)(791.1945, 57.76) | 13618.85 | 1905.094 | 13500.74 | 2285.515 | 14041.25 | 1934.6 | 14019.15 | 2284.153 | -0.59 | 0.041809 | 0.075022 | 0.24 | 0.475918 | 0.739151 |
| COMPOUND_744_1709a8_742204 | Rp | - | 744.1709 | 8.74 | | | | (1533.3369, 134.15)(743.1639, 3047.41)(744.1659, 1656.95)(745.1681, 813.61)(1487.1183, 126.91)(1488.4235, 51.51)(789.1479, 256.05)(790.1404, 220.04)(791.1466, 322.32) | 13183.92 | 1999.542 | 13255.36 | 2891.092 | 13411 | 2056.928 | 15126.26 | 5665.965 | -0.36 | 0.22908 | 0.324051 | 0.67 | 0.063462 | 0.307286 |
| COMPOUND_744_1724a9_074611 | Rp | - | 744.1724 | 9.07 | | | | (1523.252, 104.21)(1524.2648, 95.64)(857.1748, 210.24)(858.1582, 196.55)(859.1687, 205.31)(1533.2814, 72.59)(743.1641, 3034.56)(744.1672, 950.01)(745.1578, 378.84)(746.1406, 90.31)(789.1006, 487.06)(790.1162, 159.47) | 28888.64 | 8213.995 | 30909.67 | 6409.164 | 27634.21 | 7945.805 | 27502.81 | 8257.289 | -0.14 | 0.631504 | 0.721883 | -0.35 | 0.322315 | 0.628989 |
| COMPOUND_745_5551a10_064624 | Rp | + | 745.5551 | 10.06 | | | | (1492.185, 127.21)(76.5565, 614.01)(77.0263, 489.44)(77.5422, 2012.3)(778.0045, 1397.93)(382.2966, 1711.58)(382.8012, 716.84)(383.292, 804.79)(746.5632, 13012.64)(747.5641, 5474.17)(748.5644, 442.03)(373.7866, 947.78)(374.2881, 699.63)(374.7923, 160.67) | 101725.9 | 34054.11 | 84905.97 | 19694.24 | 110588.3 | 19997.14 | 111566.1 | 30413.83 | 0.27 | 0.326643 | 0.42693 | 0.65 | 0.052058 | 0.285939 |
| COMPOUND_745_56a12_786839 | Rp | - | 745.5600 | 12.79 | | | | (858.5233, 2117.51)(859.5297, 1042.63)(1536.1354, 885.41)(1537.1361, 739.03)(744.5532, 9549.91)(745.5565, 4555.73)(746.5586, 1169.81) | 125462 | 21525.07 | 130497.2 | 26229.76 | 150153.4 | 26420 | 170927.5 | 28868.73 | 0.67 | 0.004362 | 0.009963 | 0.52 | 0.053778 | 0.288355 |
| COMPOUND_745_5677a12_445017 | Rp | + | 745.5677 | 12.45 | PC 33:1 | 2 | 20 ev: 184.0732(100), 746.5687(65), 482.3166(6) | (1492.1234, 328.24)(1493.1448, 276.86)(1494.1198, 143.81)(1495.0905, 41.46)(768.5787, 13139.44)(768.5796, 4009.27)(770.5804, 1103.7)(1514.1185, 1445.69)(1515.1193, 1417.06)(746.5711, 174025.75)(747.574, 76380.46)(748.5661, 20668.23)(749.5744, 2194.63)(750.5736, 354.11)(1509.1072, 1898.65) | 913791.3 | 297202 | 822914.2 | 285355.8 | 980659 | 147039.7 | 1123755 | 329025.4 | 0.40 | 0.095948 | 0.157217 | 0.65 | 0.02149 | 0.206818 |
| COMPOUND_745_5993a13_282169 | Rp | + | 745.5993 | 13.28 | PC 34:1e | 2 | 10 ev: 746.6066(100), 184.0723(25) | (1492.2437, 136.59)(768.5886, 5883.64)(769.5916, 2933.61)(770.6047, 24607.68)(771.6093, 11803.67)(1514.2533, 161.75)(746.6063, 53747.46)(747.6097, 24530.16)(748.6125, 6455.42)(749.6136, 1252.56)(750.6277, 215.36)(1509.243, 168.05)(1510.2402, 124.13) | 529242 | 217320.3 | 474269.8 | 229661 | 454537.4 | 193163.7 | 419520.7 | 210703 | -0.49 | 0.069749 | 0.118546 | 0.22 | 0.470784 | 0.734155 |
| COMPOUND_746_5564a11_781273 | Rp | - | 746.5564 | 11.78 | SM d3:2 | 2 | 20 ev: 685.5281(100), 745.5506(8), 41.0579(2) | (1528.0573, 1496.66)(1529.0609, 1203.3)(1530.0624, 952.54)(859.5299, 3678.16)(1538.0928, 362.19)(1539.0793, 375.1)(1540.0712, 284.67)(745.5493, 115490.57)(746.5524, 50785.64)(747.5553, 12709.24)(748.5544, 1899.35)(749.5557, 337.71)(1492.0992, 437.69) | 2195169 | 478458.2 | 2303688 | 704939 | 2325469 | 484600 | 2278689 | 517604 | 0.21 | 0.43874 | 0.544076 | -0.18 | 0.57079 | 0.789098 |
| COMPOUND_746_9255a11_077844 | Rp | + | 746.9255 | 11.08 | | | | (769.9304, 3436.88)(764.9423, 3858.43)(747.9288, 14375.16)(748.9256, 6221.3)(749.9249, 2711.54) | 83202.67 | 54685.42 | 84814.53 | 64904.44 | 70109.62 | 30692.88 | 71776.8 | 24630.34 | 0.61 | 0.020639 | 0.040592 | -0.10 | 0.736708 | 0.888668 |
| COMPOUND_747_1229a11_073729 | Rp | + | 747.1229 | 11.07 | | | | (770.1196, 3004.61)(748.1295, 18586.34)(749.1199, 6617.17)(750.1117, 2253.02) | 61410.1 | 35797.78 | 64456.67 | 41257.52 | 46607.56 | 8083.817 | 57453.56 | 17894.61 | -0.37 | 0.152504 | 0.231428 | 0.61 | 0.049648 | 0.282107 |
| COMPOUND_747_5191a12_323417 | Rp | - | 747.5191 | 12.3 | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|-------------------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_747_5355a9_359567 | Rp | + | 747.5355 | 9.36 | | | | (778.538, 532.597)(779.0193, 157.43)(779.5303, 346.35)(385.7685, 665.77)(386.2697, 450.69)(386.777, 146.29)(383.2912, 3318.28)(383.7918, 1308.36)(384.3015, 603.87)(748.542, 1397.24)(749.544, 6046.18)(750.5453, 1801.9)(751.5507, 422.34)(1513.0688, 66.95)(374.7763, 2360.24)(375.2766, 1526.50)(375.7779, 456.05) | 216414.6 | 50097.46 | 187509.7 | 3925.14 | 225863.9 | 41292.19 | 223611.6 | 58308.93 | 0.04 | 0.890622 | 0.926471 | 0.68 | 0.050786 | 0.283798 |
| COMPOUND_748_3746a5_343451 | Hiic | + | 748.3746 | 5.34 | | | | (771.3658, 3079.24)(772.3672, 1198.82)(773.3691, 355.67)(749.3832, 10233.13)(750.387, 4404.29)(751.3899, 1119.15)(752.3963, 226.89)(375.1969, 497.43)(375.6994, 178.99) | 11679.18 | 8041.885 | 14497.16 | 9593.04 | 29803.67 | 9949.195 | 27378.19 | 15162.73 | 1.02 | 4.83E-06 | 2.06E-05 | 0.02 | 0.934965 | 0.971639 |
| COMPOUND_748_3749a4_594323 | Rp | - | 748.3749 | 4.59 | | | | (747.3672, 27452.4)(748.3701, 11338.0)(749.372, 2720.76)(750.3726, 522.7)(751.3639, 81.98) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 1.05 | 8.1E-06 | 3.29E-05 | 0.00 | 0.997595 | 0.99937 |
| COMPOUND_748_3761a4_607116 | Rp | + | 748.3761 | 4.61 | | | | (771.3713, 200.2)(394.1707, 9641.79)(394.6714, 3904.05)(395.1732, 906.34)(395.6719, 250.88)(386.1839, 1137.52)(386.6873, 493.9)(387.1761, 7108.76)(387.6777, 2630.19)(787.3251, 210.43)(749.3847, 54798.9)(750.3879, 22236.04)(751.3881, 5674.61)(752.3922, 1113.77)(753.3955, 263.89)(413.145, 659.46)(413.6434, 200.37)(414.1455, 73.23)(375.1978, 2578.32)(375.698, 999.94)(376.2017, 251.65)(376.6935, 67.37) | 73041.81 | 71753.98 | 77540.4 | 76337.25 | 259096.2 | 114158.9 | 245435.2 | 145509.1 | 0.93 | 0.000252 | 0.000733 | 0.19 | 0.505101 | 0.754687 |
| COMPOUND_748_5726a12_090697 | Rp | - | 748.5726 | 12.09 | SM d34:1 | 2 | 20 ev: 687.543(100), 747.566(14), 399.842(2), 152.1508(1) | (1532.0952, 3942.56)(1533.0941, 3217.87)(747.565, 405617.1)(748.5685, 173234.52)(749.5712, 42389.85)(750.5702, 5811.3)(751.5728, 873.63) | 2670060 | 711880.9 | 2702743 | 940262.8 | 2605528 | 491948.4 | 2477125 | 615124.5 | -0.01 | 0.969727 | 0.982819 | -0.19 | 0.585736 | 0.798957 |
| COMPOUND_749_5206a11_796187 | Rp | - | 749.5206 | 11.80 | | | | (1534.0793, 351.960)(1535.0698, 358.47)(862.4909, 1794.1)(863.4995, 1233.85)(784.4908, 850.34)(785.5052, 1159.78)(748.5126, 66627.53)(749.5158, 27455.67)(750.5188, 7272.59)(751.5212, 1591.05)(752.5272, 266.61)(794.5291, 1441.62)(795.539, 1236.24)(796.5186, 307.59) | 183342.6 | 78362.33 | 201367.6 | 102962 | 336342.3 | 113564.8 | 444975.2 | 239209.3 | 1.04 | 7.34E-06 | 3.01E-05 | 0.23 | 0.346413 | 0.651869 |
| COMPOUND_749_5347a12_651332 | Rp | - | 749.5347 | 12.65 | | | | (862.4908, 580.4)(863.4748, 221.81)(864.5114, 1127.38)(748.5279, 49183.29)(749.5311, 22916.92)(750.5346, 6159.56)(751.5379, 1314.72)(1498.0781, 387.75)(1499.081, 310.02)(1500.0914, 303.11)(794.5331, 4259.19)(795.5386, 5104.72)(796.5429, 2746.0) | 265913.2 | 104790.3 | 266148.8 | 119626.6 | 270837.7 | 100226.3 | 234104 | 84506.85 | 0.09 | 0.721827 | 0.79645 | -0.33 | 0.275106 | 0.58392 |
| COMPOUND_749_5389a12_641697 | Rp | + | 749.5389 | 12.64 | PE 38:6e | 2 | 20 ev: 390.2767(100), 609.5197(28), 137.1271(23), 484.2974(15) | (1500.1339, 1058.19)(1501.1393, 934.98)(1538.0012, 168.71)(1538.9836, 143.65)(788.4941, 479.5)(789.4933, 332.97)(750.5441, 62598.79)(751.5472, 29252.09)(752.5511, 8070.21)(753.5654, 2080.08) | 293269.9 | 122272.3 | 264641.1 | 99798.61 | 295396.3 | 99934.46 | 258617.5 | 76434.41 | 0.17 | 0.49893 | 0.599888 | -0.13 | 0.651883 | 0.83936 |
| COMPOUND_750_122a10_973539 | Rp | + | 750.1220 | 10.97 | | | | (773.1258, 2408.1)(774.1408, 6875.95)(780.0541, 731.9)(751.127, 11072.71)(752.1212, 4838.64)(753.1103, 2299.99) | 66787.16 | 37619.08 | 63636 | 43998.49 | 68523.11 | 41227.77 | 78475.73 | 46210.14 | -0.20 | 0.453016 | 0.558703 | 0.43 | 0.180672 | 0.438954 |
| COMPOUND_751_5153a11_583241 | Rp | + | 751.5153 | 11.58 | PC 34:5 | 2 | 20 ev: 184.0728(100), 752.5426(80), 86.0977(5), 287.2077(4), 441.5945(3) | (1503.997, 202.26)(1541.9987, 342.93)(774.4916, 5284.28)(1525.9878, 536.36)(769.5529, 2112.5)(770.5496, 2490.71)(771.5479, 1640.92)(752.5245, 49165.13)(753.5276, 23159.97)(754.5304, 6801.24)(755.5323, 1973.0) | 123664.7 | 78059.67 | 143203.8 | 91782.07 | 105315.8 | 99160.33 | 98917.11 | 70620.55 | 0.09 | 0.731639 | 0.805246 | 0.06 | 0.831128 | 0.926681 |
| COMPOUND_751_5358a12_125399 | Rp | - | 751.5358 | 12.13 | | | | (1538.0728, 211.86)(1539.086, 415.0)(864.5318, 1419.42)(865.5359, 724.08)(866.5483, 1803.93)(786.508, 428.21)(1548.0729, 1537.21)(1549.0797, 997.44)(750.5287, 55184.12)(751.5316, 24023.35)(752.5338, 6297.49)(753.5355, 1489.79)(754.5166, 341.51)(1502.1023, 477.88) | 243826.4 | 112198.5 | 263473.3 | 117438 | 298913.7 | 66590.88 | 345746.9 | 113750.2 | 0.60 | 0.014952 | 0.030457 | 0.08 | 0.788772 | 0.909997 |
| COMPOUND_751_5516a13_248221 | Rp | - | 751.5516 | 13.25 | | | | (1538.1427, 600.9)(1539.1523, 311.28)(786.5659, 1280.82)(787.5577, 976.41)(864.5346, 706.41)(865.5298, 390.92)(866.5401, 511.15)(750.543, 27710.7)(751.5463, 13391.32)(752.5498, 4106.92)(753.5509, 1018.16)(796.5677, 2786.65)(797.5653, 2391.7)(798.5605, 1201.52) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.50 | 0.050743 | 0.088721 | -0.01 | 0.965914 | 0.982565 |
| COMPOUND_751_5526a12_230772 | Rp | + | 751.5526 | 13.23 | PC 35:5e | 2 | 40 ev: 69.0696(100), 361.2729(52), 752.713(12), 572.8602(11) | (774.5428, 1352.23)(775.5487, 594.58)(776.5608, 1219.9)(1526.1188, 105.86)(790.5118, 764.2)(791.4993, 335.34)(792.5079, 37.21)(760.5931, 3487.93)(752.5592, 24766.83)(753.5624, 12265.78)(754.5648, 3654.81)(755.5691, 1037.03) | 134471.6 | 67292 | 124103.1 | 75490.61 | 121506.8 | 59952.68 | 113185 | 47322.93 | -0.15 | 0.537674 | 0.636056 | 0.13 | 0.650438 | 0.838541 |
| COMPOUND_753_1226a11_019529 | Rp | + | 753.1226 | 11.02 | | | | (776.1276, 2957.81)(771.1385, 2791.37)(754.1344, 15818.87)(755.124, 6746.13)(756.1151, 2026.51) | 65403.02 | 41790.67 | 69936.53 | 45152.08 | 62510.91 | 15412.82 | 59177.45 | 18310.98 | 0.03 | 0.907078 | 0.938328 | 0.08 | 0.810111 | 0.919078 |
| COMPOUND_753_5327a11_815522 | Rp | + | 753.5327 | 11.82 | PC 34:4 | 2 | 10 ev: 754.5403(100), 184.0738(15), 55.0517(2) | (1508.0669, 1276.07)(1509.0692, 1450.42)(1510.0801, 2167.87)(1511.0869, 1556.54)(1546.0602, 559.14)(776.5228, 17818.56)(777.5274, 8618.16)(778.5412, 75459.88)(779.5435, 35811.36)(780.5569, 179420.17)(781.5597, 82722.81)(1530.0591, 578.83)(1531.0743, 716.03)(1532.0627, 1026.09)(792.4579, 2965.9)(793.4589, 2600.44)(754.5409, 251810.92)(755.5437, 113333.91)(756.5468, 30073.1)(757.5443, 7231.39) | 1138011 | 466549.7 | 1182417 | 477681.8 | 1757745 | 768476 | 1657625 | 57826.6 | 1.03 | 0.000176 | 0.000526 | -0.25 | 0.418873 | 0.699556 |
| COMPOUND_753_592a13_915185 | Rp | + | 753.5920 | 13.92 | | | | (754.5997, 8794.68)(755.6031, 4818.47)(756.6001, 1940.1)(757.6233, 574.17) | 58613.33 | 27656.34 | 51885.52 | 20051.99 | 40536.67 | 1144.43 | 33237 | 11801.74 | -1.27 | 4.28E-09 | 3.86E-08 | 0.05 | 0.804179 | 0.917422 |
| COMPOUND_753_9893a10_244545 | Rp | + | 753.9893 | 10.24 | | | | (1508.9885, 40680.93)(1509.9111, 33622.91)(1510.9928, 16207.77)(1511.991, 6353.98)(1546.9331, 1228.44)(1547.9062, 1752.04)(1548.9067, 2035.94)(1549.9115, 1378.45)(1550.9156, 1312.93)(1551.9196, 1107.44)(1552.9283, 959.46)(776.948, 3417.53)(777.9391, 1636.8)(1530.9526, 1291.75)(754.9949, 7248.84)(756.0154, 6422.04)(757.0157, 1677.98)(758.0041, 309.16) | 285490.8 | 53767.5 | 274715.4 | 43895.18 | 289039.6 | 16050.13 | 298507.6 | 36728.74 | 0.11 | 0.695974 | 0.77822 | 0.51 | 0.144604 | 0.451201 |
| COMPOUND_755_5479a11_088077 | Rp | + | 755.5479 | 11.09 | | | | (778.5399, 12099.68)(779.5424, 59183.2)(780.553, 69754.84)(1534.0808, 736.36)(397.7605, 1027.79)(398.2621, 603.07)(398.7686, 699.16)(389.7691, 1251.98)(390.2734, 790.9)(390.7726, 647.03)(756.5571, 477299.34)(757.5611, 21274.83)(758.5618, 58134.77)(759.5594, 13941.22)(416.7359, 5101.96)(417.2388, 3213.81)(378.7822, 1213.19)(379.2977, 984.25)(379.7844, 83.0) | 1649371 | 809010.8 | 1694209 | 740801.4 | 1488923 | 886681.8 | 1388438 | 632521.6 | -1.06 | 2.32E-06 | 1.07E-05 | -0.26 | 0.292851 | 0.602481 |
| COMPOUND_755_5492a11_9932575 | Rp | + | 755.5492 | 11.99 | PC(16:1_18:2) duplicate | | | (1512.1018, 11629.54)(1513.1046, 10361.32)(1514.1063, 5251.61)(1515.107, 2212.84)(1516.1082, 985.62)(1550.1006, 5532.11)(1551.101, 3987.04)(1552.0929, 2536.76)(778.5371, 25451.26)(779.5407, 12675.13)(780.5555, 672716.56)(1534.0872, 4045.04)(1535.092, 4111.21)(1536.1003, 17769.83)(1537.1038, 16130.86)(1538.1102, 15801.29)(1539.1151, 10615.37)(1540.115, 5228.02)(794.5504, 8645.19)(773.6152, 594.35)(756.5564, 751765.2)(757.5604, 339736.84)(758.5634, 88802.87)(759.5662, 17307.7)(760.5757, 4126.16)(1529.1024, 686.79)(1530.0876, 702.5) | 15362032 | 5866578 | 15229628 | 5890574 | 22635714 | 5719146 | 23621053 | 6255590 | 0.97 | 0.000132 | 0.0004 | 0.17 | 0.550093 | 0.7796 |
| COMPOUND_755_5503a11_170548 | Rp | + | 755.5503 | 11.17 | PC 34:3 | 2 | 20 ev: 756.5538(100), 184.0737(85) | (778.5395, 7390.31)(779.5476, 5291.96)(780.5563, 74930.2)(1534.0996, 785.05)(1535.0989, 502.03)(1536.1237, 190.67)(397.7602, 1931.52)(398.2584, 1341.15)(398.7718, 1131.21)(389.768, 3293.15)(390.2695, 2142.99)(390.772, 1237.13)(756.5549, 719076.9)(757.559, 319297.44)(758.5618, 87530.7)(759.5627, 18177.21)(378.7845, 5670.65)(379.2858, 2633.37)(379.7884, 814.95) | 4239682 | 966992.4 | 4268790 | 1024213 | 3341303 | 2593144 | 3647098 | 1845634 | -0.99 | 1.5E-05 | 5.78E-05 | -0.26 | 0.304305 | 0.613089 |
| COMPOUND_755_5507a11_965143 | Rp | + | 755.5507 | 11.97 | PC 16:1_18:2 | 1 | 10 ev: 756.5551(100), 184.0743(10) | (1512.1007, 9956.59)(1513.103, 9262.87)(1514.1053, 4811.16)(1515.1096, 2042.05)(1516.1064, 951.94)(1550.0813, 1839.54)(1551.0797, 1489.68)(1552.0886, 825.27)(778.5369, 23317.08)(779.5398, 11981.6)(780.5552, 519573.22)(1534.0905, 2603.2)(1535.093, 2610.39)(1536.1008, 8751.83)(1537.1025, 8312.71)(1538.1123, 9669.33)(1539.1149, 7106.73)(1540.1167, 3608.0)(773.5504, 1570.53)(794.5499, 6824.95)(756.5559, 777350.8)(757.5605, 346212.47)(758.5631, 90033.48)(759.5669, 17168.6)(760.5753, 4056.2)(1529.1112, 1329.28)(1530.0981, 1078.51) | 6030459 | 5990580 | 5624574 | 5305051 | 6039651 | 5557031 | 5950080 | 5840752 | 0.47 | 0.093441 | 0.153711 | -0.13 | 0.698132 | 0.862515 |
| COMPOUND_756_1442a9_242933 | Rp | - | 756.1442 | 9.24 | | | | (869.0893, 126.25)(870.1058, 285.89)(871.0889, 278.08)(791.134, 412.34)(792.1455, 151.7)(793.1427, 453.72)(755.1371, 12010.11)(756.1407, 3242.73)(757.1361, 3894.75)(758.1373, 1163.0)(759.1387, 517.46)(760.1274, 249.05)(801.136, 808.24)(802.1526, 378.15) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.57 | 0.054734 | 0.095108 | 0.00 | 0.999832 | 0.999832 |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|---|---|---------------|----------|---------------|----------|---------------|---------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_757_5605a11_226129 | Rp | + | 757.5605 | 11.23 | | | | (1554.085, 1020.77)(1555.0707, 700.91)(1556.1051, 1499.25)(1557.1051, 1348.45)(1558.1272, 1928.55)(1559.1296, 1456.76)(1560.1248, 2311.57)(780.5563, 173445.95)(781.5593, 81532.25)(1538.0461, 702.54)(1539.0385, 581.03)(758.5698, 45608.08)(759.5726, 20405.94)(760.584, 22026.92)(761.5872, 8770.57)(1516.1355, 23609.54)(1517.1406, 21656.95)(1518.1401, 10809.06)(1519.145, 4115.02)(1520.1562, 1292.38)(1521.1552, 422.02)(780.5519, 29431.81)(781.5562, 13746.27)(782.5707, 78842.3)(1538.12, 21362.11)(1539.1232, 20521.71)(1540.1289, 15663.63)(796.5274, 1680.55)(797.5285, 1154.91)(798.5416, 7864.87)(799.5422, 4385.55)(758.5705, 1394080.1)(759.5749, 610906.7)(760.5778, 157150.3)(761.5814, 28391.69)(762.5827, 5027.26)(763.5895, 931.33)(1533.119, 5405.26)(1534.1272, 2762.23)(1554.0796, 79.59)(1555.0878, 204.78)(1556.0865, 224.11)(1557.0836, 377.11)(1558.0908, 168.46)(1564.0941, 299.18)(1565.0929, 360.17)(1566.0972, 323.64)(1567.1079, 348.45)(1568.1151, 278.83)(1569.1127, 194.6)(1570.1094, 132.82)(758.533, 10252.37)(759.5363, 5282.82)(760.5401, 1361.4)(761.5398, 424.78)(1518.07, 68.76)(1519.101, 363.43)(1520.1038, 285.92)(1520.1632, 14861.03)(1521.1665, 13148.03)(1522.1694, 6828.42)(1523.175, 2316.85)(1524.1807, 854.19)(1525.2186, 189.13)(782.5684, 74705.47)(783.5711, 35495.89)(784.5846, 475963.12)(1542.1448, 3839.31)(1543.1492, 3275.27)(1544.1564, 9582.53)(1545.1616, 7822.79)(1546.1711, 10916.35)(788.5423, 2756.61)(799.5453, 923.93)(800.5515, 2281.98)(801.5694, 1321.2)(760.5857, 1176076.0)(761.5899, 511765.62)(762.5928, 124819.09)(763.5945, 24120.88)(764.5944, 4004.87)(765.5799, 639.61)(795.5416, 1355.38)(796.5419, 1039.74)(797.5465, 6422.29)(760.5675, 3071.39)(761.5742, 1136.96)(762.5916, 311.18)(805.5636, 1067.01)(806.5371, 1207.76)(807.5271, 709.5)(400.6931, 144.79)(401.183, 66.82)(392.7006, 955.76)(393.2144, 534.97)(393.715, 112.31)(779.4091, 68.44)(390.2242, 8895.4)(390.7264, 3443.35)(391.2183, 2401.21)(391.7276, 320.38)(762.4122, 5349.72)(763.4154, 2079.69)(764.421, 661.0)(765.4122, 127.6)(381.7124, 1410.24)(382.2133, 632.03)(382.7173, 98.07)(383.2062, 26.23)(1558.0182, 262.32)(1559.0293, 244.94)(874.4771, 1682.31)(796.443, 389.35)(797.4571, 155.85)(1568.0522, 497.85)(1569.0548, 451.17)(760.4915, 13682.44)(761.4949, 6291.07)(762.5096, 3211.43)(763.5082, 563.37)(1522.096, 100.02)(1523.0746, 723.06)(806.4949, 1266.81)(807.5045, 1389.48)(808.5188, 1130.09)(784.5373, 390.55)(392.7743, 1026.27)(393.2777, 787.85)(393.7767, 209.29)(390.2969, 5906.64)(390.7998, 2107.28)(391.2978, 866.76)(391.8016, 255.8)(409.2787, 314.0)(409.7893, 118.91)(410.2718, 912.15)(762.5581, 18924.81)(763.5608, 8090.96)(764.5602, 2568.21)(765.5624, 565.99)(766.5735, 128.68)(811.7846, 4540.54)(382.2866, 2074.97)(382.7873, 675.68)(784.9422, 2252.58)(800.8853, 1180.26)(779.9452, 4009.54)(762.9367, 12221.21)(763.9313, 4924.81)(764.9314, 2629.07)(762.359, 6179.04)(763.3725, 2578.93)(764.3669, 4223.65)(765.3694, 1865.29)(766.3663, 1020.53)(767.3693, 366.02)(768.3655, 123.7)(876.4975, 365.31)(877.5228, 2079.46)(798.4618, 199.86)(799.4671, 86.63)(762.5077, 283883.9)(763.5109, 129447.1)(764.5142, 33674.28)(765.5182, 6497.2)(1526.0334, 2138.83)(1527.0408, 1976.23)(1528.0468, 1092.06)(1529.0472, 480.43)(1530.0452, 131.97)(798.5131, 728.56)(799.5292, 59.97)(876.5016, 1393.31)(762.5072, 7471.32)(763.5103, 3889.08)(764.5231, 23256.92)(1525.98, 166.74)(1527.0115, 137.2)(1528.0093, 157.59)(808.5107, 4007.74)(809.5145, 1394.35)(1538.0554, 3210.25)(1529.0589, 3107.53)(1530.06, 1670.16)(1531.0669, 773.41)(1532.0735, 366.39)(786.5268, 7034.45)(787.5273, 3432.91)(788.5361, 4811.89)(1550.0162, 413.41)(802.5196, 4142.5)(803.5117, 1956.42)(764.525, 245985.36)(765.528, 111609.7)(766.5314, 28878.7)(767.5344, 6403.61)(1545.102, 2689.04)(1546.0885, 4762.29)(1547.0912, 4444.65)(1548.0985, 4814.09)(763.1505, 4792.96)(764.153, 1299.33)(765.1662, 43731.81)(766.1696, 10815.7)(764.5231, 23256.92)(765.5261, 112155.85)(766.5291, 29087.6)(767.5317, 5516.38)(150600.8, 42699.38, 163183.5, 57951.3, 170544.6, 90585.62, 166366.1, 68437.44, 84420.17, 55776.98, 99917.16, 61106.33, 240761.7, 129508.2, 322034, 210913.8) | 1726247 | 780725.8 | 1504299 | 729598.7 | 1800574 | 1343115 | 1839616 | 986480.5 | -0.95 | 6.35E-05 | 0.000206 | -0.06 | 0.808527 | 0.918373 |
| COMPOUND_757_5641a12_321749 | Rp | + | 757.5641 | 12.32 | PC 16:0_18:2 | 1 | 10 eV: 758.57(100), 184.0731(9), 86.1007(1) | (1516.1355, 23609.54)(1517.1406, 21656.95)(1518.1401, 10809.06)(1519.145, 4115.02)(1520.1562, 1292.38)(1521.1552, 422.02)(780.5519, 29431.81)(781.5562, 13746.27)(782.5707, 78842.3)(1538.12, 21362.11)(1539.1232, 20521.71)(1540.1289, 15663.63)(796.5274, 1680.55)(797.5285, 1154.91)(798.5416, 7864.87)(799.5422, 4385.55)(758.5705, 1394080.1)(759.5749, 610906.7)(760.5778, 157150.3)(761.5814, 28391.69)(762.5827, 5027.26)(763.5895, 931.33)(1533.119, 5405.26)(1534.1272, 2762.23)(1554.0796, 79.59)(1555.0878, 204.78)(1556.0865, 224.11)(1557.0836, 377.11)(1558.0908, 168.46)(1564.0941, 299.18)(1565.0929, 360.17)(1566.0972, 323.64)(1567.1079, 348.45)(1568.1151, 278.83)(1569.1127, 194.6)(1570.1094, 132.82)(758.533, 10252.37)(759.5363, 5282.82)(760.5401, 1361.4)(761.5398, 424.78)(1518.07, 68.76)(1519.101, 363.43)(1520.1038, 285.92)(1520.1632, 14861.03)(1521.1665, 13148.03)(1522.1694, 6828.42)(1523.175, 2316.85)(1524.1807, 854.19)(1525.2186, 189.13)(782.5684, 74705.47)(783.5711, 35495.89)(784.5846, 475963.12)(1542.1448, 3839.31)(1543.1492, 3275.27)(1544.1564, 9582.53)(1545.1616, 7822.79)(1546.1711, 10916.35)(788.5423, 2756.61)(799.5453, 923.93)(800.5515, 2281.98)(801.5694, 1321.2)(760.5857, 1176076.0)(761.5899, 511765.62)(762.5928, 124819.09)(763.5945, 24120.88)(764.5944, 4004.87)(765.5799, 639.61)(795.5416, 1355.38)(796.5419, 1039.74)(797.5465, 6422.29)(760.5675, 3071.39)(761.5742, 1136.96)(762.5916, 311.18)(805.5636, 1067.01)(806.5371, 1207.76)(807.5271, 709.5)(400.6931, 144.79)(401.183, 66.82)(392.7006, 955.76)(393.2144, 534.97)(393.715, 112.31)(779.4091, 68.44)(390.2242, 8895.4)(390.7264, 3443.35)(391.2183, 2401.21)(391.7276, 320.38)(762.4122, 5349.72)(763.4154, 2079.69)(764.421, 661.0)(765.4122, 127.6)(381.7124, 1410.24)(382.2133, 632.03)(382.7173, 98.07)(383.2062, 26.23)(1558.0182, 262.32)(1559.0293, 244.94)(874.4771, 1682.31)(796.443, 389.35)(797.4571, 155.85)(1568.0522, 497.85)(1569.0548, 451.17)(760.4915, 13682.44)(761.4949, 6291.07)(762.5096, 3211.43)(763.5082, 563.37)(1522.096, 100.02)(1523.0746, 723.06)(806.4949, 1266.81)(807.5045, 1389.48)(808.5188, 1130.09)(784.5373, 390.55)(392.7743, 1026.27)(393.2777, 787.85)(393.7767, 209.29)(390.2969, 5906.64)(390.7998, 2107.28)(391.2978, 866.76)(391.8016, 255.8)(409.2787, 314.0)(409.7893, 118.91)(410.2718, 912.15)(762.5581, 18924.81)(763.5608, 8090.96)(764.5602, 2568.21)(765.5624, 565.99)(766.5735, 128.68)(811.7846, 4540.54)(382.2866, 2074.97)(382.7873, 675.68)(784.9422, 2252.58)(800.8853, 1180.26)(779.9452, 4009.54)(762.9367, 12221.21)(763.9313, 4924.81)(764.9314, 2629.07)(762.359, 6179.04)(763.3725, 2578.93)(764.3669, 4223.65)(765.3694, 1865.29)(766.3663, 1020.53)(767.3693, 366.02)(768.3655, 123.7)(876.4975, 365.31)(877.5228, 2079.46)(798.4618, 199.86)(799.4671, 86.63)(762.5077, 283883.9)(763.5109, 129447.1)(764.5142, 33674.28)(765.5182, 6497.2)(1526.0334, 2138.83)(1527.0408, 1976.23)(1528.0468, 1092.06)(1529.0472, 480.43)(1530.0452, 131.97)(798.5131, 728.56)(799.5292, 59.97)(876.5016, 1393.31)(762.5072, 7471.32)(763.5103, 3889.08)(764.5231, 23256.92)(1525.98, 166.74)(1527.0115, 137.2)(1528.0093, 157.59)(808.5107, 4007.74)(809.5145, 1394.35)(1538.0554, 3210.25)(1529.0589, 3107.53)(1530.06, 1670.16)(1531.0669, 773.41)(1532.0735, 366.39)(786.5268, 7034.45)(787.5273, 3432.91)(788.5361, 4811.89)(1550.0162, 413.41)(802.5196, 4142.5)(803.5117, 1956.42)(764.525, 245985.36)(765.528, 111609.7)(766.5314, 28878.7)(767.5344, 6403.61)(1545.102, 2689.04)(1546.0885, 4762.29)(1547.0912, 4444.65)(1548.0985, 4814.09)(763.1505, 4792.96)(764.153, 1299.33)(765.1662, 43731.81)(766.1696, 10815.7)(764.5231, 23256.92)(765.5261, 112155.85)(766.5291, 29087.6)(767.5317, 5516.38)(150600.8, 42699.38, 163183.5, 57951.3, 170544.6, 90585.62, 166366.1, 68437.44, 84420.17, 55776.98, 99917.16, 61106.33, 240761.7, 129508.2, 322034, 210913.8) | 87701887 | 11589460 | 85180435 | 1331217 | 97121429 | 8969451 | 98256140 | 13504008 | 0.76 | 0.004969 | 0.011213 | 0.28 | 0.360358 | 0.666906 |
| COMPOUND_759_5408a11_4646635 | Rp | - | 759.5408 | 11.46 | | | | (1554.085, 1020.77)(1555.0707, 700.91)(1556.1051, 1499.25)(1557.1051, 1348.45)(1558.1272, 1928.55)(1559.1296, 1456.76)(1560.1248, 2311.57)(780.5563, 173445.95)(781.5593, 81532.25)(1538.0461, 702.54)(1539.0385, 581.03)(758.5698, 45608.08)(759.5726, 20405.94)(760.584, 22026.92)(761.5872, 8770.57)(1516.1355, 23609.54)(1517.1406, 21656.95)(1518.1401, 10809.06)(1519.145, 4115.02)(1520.1562, 1292.38)(1521.1552, 422.02)(780.5519, 29431.81)(781.5562, 13746.27)(782.5707, 78842.3)(1538.12, 21362.11)(1539.1232, 20521.71)(1540.1289, 15663.63)(796.5274, 1680.55)(797.5285, 1154.91)(798.5416, 7864.87)(799.5422, 4385.55)(758.5705, 1394080.1)(759.5749, 610906.7)(760.5778, 157150.3)(761.5814, 28391.69)(762.5827, 5027.26)(763.5895, 931.33)(1533.119, 5405.26)(1534.1272, 2762.23)(1554.0796, 79.59)(1555.0878, 204.78)(1556.0865, 224.11)(1557.0836, 377.11)(1558.0908, 168.46)(1564.0941, 299.18)(1565.0929, 360.17)(1566.0972, 323.64)(1567.1079, 348.45)(1568.1151, 278.83)(1569.1127, 194.6)(1570.1094, 132.82)(758.533, 10252.37)(759.5363, 5282.82)(760.5401, 1361.4)(761.5398, 424.78)(1518.07, 68.76)(1519.101, 363.43)(1520.1038, 285.92)(1520.1632, 14861.03)(1521.1665, 13148.03)(1522.1694, 6828.42)(1523.175, 2316.85)(1524.1807, 854.19)(1525.2186, 189.13)(782.5684, 74705.47)(783.5711, 35495.89)(784.5846, 475963.12)(1542.1448, 3839.31)(1543.1492, 3275.27)(1544.1564, 9582.53)(1545.1616, 7822.79)(1546.1711, 10916.35)(788.5423, 2756.61)(799.5453, 923.93)(800.5515, 2281.98)(801.5694, 1321.2)(760.5857, 1176076.0)(761.5899, 511765.62)(762.5928, 124819.09)(763.5945, 24120.88)(764.5944, 4004.87)(765.5799, 639.61)(795.5416, 1355.38)(796.5419, 1039.74)(797.5465, 6422.29)(760.5675, 3071.39)(761.5742, 1136.96)(762.5916, 311.18)(805.5636, 1067.01)(806.5371, 1207.76)(807.5271, 709.5)(400.6931, 144.79)(401.183, 66.82)(392.7006, 955.76)(393.2144, 534.97)(393.715, 112.31)(779.4091, 68.44)(390.2242, 8895.4)(390.7264, 3443.35)(391.2183, 2401.21)(391.7276, 320.38)(762.4122, 5349.72)(763.4154, 2079.69)(764.421, 661.0)(765.4122, 127.6)(381.7124, 1410.24)(382.2133, 632.03)(382.7173, 98.07)(383.2062, 26.23)(1558.0182, 262.32)(1559.0293, 244.94)(874.4771, 1682.31)(796.443, 389.35)(797.4571, 155.85)(1568.0522, 497.85)(1569.0548, 451.17)(760.4915, 13682.44)(761.4949, 6291.07)(762.5096, 3211.43)(763.5082, 563.37)(1522.096, 100.02)(1523.0746, 723.06)(806.4949, 1266.81)(807.5045, 1389.48)(808.5188, 1130.09)(784.5373, 390.55)(392.7743, 1026.27)(393.2777, 787.85)(393.7767, 209.29)(390.2969, 5906.64)(390.7998, 2107.28)(391.2978, 866.76)(391.8016, 255.8)(409.2787, 314.0)(409.7893, 118.91)(410.2718, 912.15)(762.5581, 18924.81)(763.5608, 8090.96)(764.5602, 2568.21)(765.5624, 565.99)(766.5735, 128.68)(811.7846, 4540.54)(382.2866, 2074.97)(382.7873, 675.68)(784.9422, 2252.58)(800.8853, 1180.26)(779.9452, 4009.54)(762.9367, 12221.21)(763.9313, 4924.81)(764.9314, 2629.07)(762.359, 6179.04)(763.3725, 2578.93)(764.3669, 4223.65)(765.3694, 1865.29)(766.3663, 1020.53)(767.3693, 366.02)(768.3655, 123.7)(876.4975, 365.31)(877.5228, 2079.46)(798.4618, 199.86)(799.4671, 86.63)(762.5077, 283883.9)(763.5109, 129447.1)(764.5142, 33674.28)(765.5182, 6497.2)(1526.0334, 2138.83)(1527.0408, 1976.23)(1528.0468, 1092.06)(1529.0472, 480.43)(1530.0452, 131.97)(798.5131, 728.56)(799.5292, 59.97)(876.5016, 1393.31)(762.5072, 7471.32)(763.5103, 3889.08)(764.5231, 23256.92)(1525.98, 166.74)(1527.0115, 137.2)(1528.0093, 157.59)(808.5107, 4007.74)(809.5145, 1394.35)(1538.0554, 3210.25)(1529.0589, 3107.53)(1530.06, 1670.16)(1531.0669, 773.41)(1532.0735, 366.39)(786.5268, 7034.45)(787.5273, 3432.91)(788.5361, 4811.89)(1550.0162, 413.41)(802.5196, 4142.5)(803.5117, 1956.42)(764.525, 245985.36)(765.528, 111609.7)(766.5314, 28878.7)(767.5344, 6403.61)(1545.102, 2689.04)(1546.0885, 4762.29)(1547.0912, 4444.65)(1548.0985, 4814.09)(763.1505, 4792.96)(764.153, 1299.33)(765.1662, 43731.81)(766.1696, 10815.7)(764.5231, 23256.92)(765.5261, 112155.85)(766.5291, 29087.6)(767.5317, 5516.38)(150600.8, 42699.38, 163183.5, 57951.3, 170544.6, 905 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|-----------------------------|--------|----------|----------|-----------|---------------------------|----------|--------------|---|--|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_775_5508a11_108693 | Rp | - | 775.5508 | 13.11 | | | | (1596.1447, 414.477)(774.5428, 16215.62)(775.5467, 8189.79)(776.5493, 3506.05)(777.55, 1150.11) | 81038.98 | 35677.56 | 83835.65 | 44493.35 | 102681.5 | 45942.34 | 85529.19 | 33008.6 | 0.51 | 0.065653 | 0.11269 | -0.32 | 0.316832 | 0.622922 | |
| COMPOUND_775_5689a_826908 | Rp | + | 775.5680 | 9.83 | | | | (796.1017, 180.81)(796.601, 131.69)(999.7829, 1034.58)(400.2845, 772.38)(400.7904, 167.13)(397.3052, 644.129)(397.807, 2583.62)(398.3092, 1079.6)(398.8056, 147.02)(416.2958, 758.12)(416.7924, 140.56)(776.5732, 19880.76)(777.5762, 8685.56)(778.5638, 2947.04)(779.5447, 910.03)(780.5654, 219.8)(888.7922, 4628.99)(889.2932, 2080.88)(889.7942, 609.18) | 356720.3 | 90761.51 | 309647 | 64398.71 | 383174.6 | 60668.14 | 383195 | 99497.7 | 0.23 | 0.418276 | 0.52284 | 0.59 | 0.088828 | 0.352184 | |
| COMPOUND_775_5682a11_317031 | Rp | + | 775.5682 | 11.32 | | | | (1590.1255, 514.37)(1591.13, 563.4)(1592.1157, 598.08)(1574.1295, 1610.11)(1575.133, 979.79)(1576.1313, 528.66)(1577.1154, 226.76)(776.5796, 16659.11)(777.5841, 6684.22)(778.5709, 2069.38)(779.5817, 483.41) | 246784.2 | 100858.6 | 236272.6 | 93269.51 | 157445.7 | 21870.55 | 192122.8 | 43638.14 | -1.02 | 4.25E-06 | 1.83E-05 | -0.14 | 0.568542 | 0.788601 | |
| COMPOUND_776_1413a11_090051 | Rp | + | 776.1413 | 11.09 | | | | (799.1483, 1426.65)(777.1495, 13990.97)(778.1424, 5860.36)(779.1313, 2011.57) | 48886 | 30670.06 | 47710.09 | 31834.5 | 57448.55 | 10291.94 | 58077.52 | 19774.02 | 0.37 | 0.181743 | 0.26909 | 0.07 | 0.837049 | 0.929046 | |
| COMPOUND_776_6028a12_662439 | Rp | - | 776.6028 | 12.66 | N-Stearyl-D-sphingomyelin | 1 | 40 | 10 eV: 715.5744(100), 168.0425(37), 279.2326(22), 78.9582(12) | 203085.8 | 65694.47 | 206193.1 | 79039.39 | 204006.2 | 60123.09 | 192039.1 | 58173.5 | 0.08 | 0.799881 | 0.856553 | -0.22 | 0.527076 | 0.7696 | |
| COMPOUND_777_534a11_744952 | Rp | + | 777.5340 | 11.74 | PC 36:6 | 2 | 10 | 10 eV: 778.5372(100), 184.0763(13), 585.1288(4) | 528276.4 | 259159.9 | 580013 | 33967.3 | 740998.5 | 283798.6 | 818888 | 415139.1 | 0.31 | 0.190326 | 0.279227 | 0.27 | 0.329273 | 0.635357 | |
| COMPOUND_777_5515a12_213564 | Rp | - | 777.5515 | 12.21 | | | | (775.5439, 4848.1325)(777.5477, 215318.0)(778.5501, 55602.03)(779.5529, 11251.1)(780.5541, 1898.91)(781.5527, 298.75) | 1284858 | 446382.2 | 1384043 | 658074.9 | 1999348 | 612527.8 | 2648651 | 998300.2 | 0.87 | 0.000196 | 0.000585 | 0.42 | 0.108008 | 0.39105 | |
| COMPOUND_778_9422a11_136764 | Rp | + | 778.9422 | 11.14 | | | | (801.9089, 1330.29)(796.9613, 1354.52)(779.9503, 14007.39)(780.9449, 5283.59)(781.9488, 2130.03) | 29616.61 | 26615.07 | 35332.79 | 31476.66 | 46184.8 | 22729.25 | 49288.05 | 22500.02 | 0.38 | 0.161682 | 0.243714 | 0.06 | 0.844004 | 0.93246 | |
| COMPOUND_779_1459a11_136102 | Rp | + | 779.1459 | 11.14 | | | | (802.1548, 985.34)(818.0683, 1293.23)(780.1501, 16921.94)(781.1434, 3181.35)(782.1343, 936.83) | 38867.12 | 25196.52 | 33534.41 | 28561.61 | 40311.6 | 9359.385 | 44995.09 | 17622.27 | 0.04 | 0.870411 | 0.912554 | 0.61 | 0.047602 | 0.279163 | |
| COMPOUND_779_5084a10_922651 | Rp | - | 779.5084 | 10.92 | | | | (778.5019, 15678.32)(779.5055, 7546.3)(780.5157, 10811.33)(781.5189, 5067.64)(782.5216, 3420.9)(783.5304, 1075.51)(784.5194, 884.38)(1557.9875, 216.44)(1559.0018, 268.31)(1560.007, 283.12) | 139970.3 | 75405.06 | 139430.6 | 62675.36 | 140676.7 | 28274.73 | 142340.6 | 44338.55 | -1.01 | 1.39E-05 | 5.4E-05 | -0.09 | 0.735057 | 0.888627 | |
| COMPOUND_779_5098a11_194105 | Rp | - | 779.5098 | 11.19 | | | | (1593.9358, 174.6)(778.5021, 8832.79)(779.5052, 4305.64)(780.5147, 4307.64)(781.5191, 310177.9) | 116592.6 | 375131.9 | 234922.1 | 611269.5 | 173609.5 | 639118.2 | 282940.9 | -0.64 | 0.010799 | 0.022665 | -0.35 | 0.231189 | 0.537849 | | |
| COMPOUND_779_5345a12_288433 | Rp | + | 779.5345 | 12.29 | | | | (1598.1229, 3883.23)(791.5436, 10166.67)(792.0331, 1899.89)(792.5518, 3910.89)(793.0345, 729.92)(409.7412, 1087.58)(410.2378, 748.93)(800.0403, 2890.02)(800.5489, 1809.46)(801.0415, 13863.15)(818.5058, 823.69)(819.0125, 446.12)(818.5396, 1289.71)(780.5521, 72005.9)(781.5552, 33811.2)(782.5703, 1098514.1)(783.5743, 506261.75)(1577.132, 4204.65)(390.7767, 6980.09)(391.2773, 4444.33)(391.7772, 3136.3)(392.2724, 963.97)(392.7734, 158.74) | 19511214 | 4800319 | 15655826 | 6966814 | 8933607 | 9625509 | 12210064 | 9634828 | -0.71 | 0.016931 | 0.034014 | 0.61 | 0.073255 | 0.326093 | |
| COMPOUND_779_5478a11_878703 | Rp | + | 779.5478 | 11.88 | PC 16:1_20:4 | 1 | 10 | 10 eV: 780.5553(100), 184.0729(10), 494.0954(3) | 7188953 | 8996697 | 2920316 | 4510985 | 8071244 | 9008944 | 5237687 | 7961148 | 0.28 | 0.284481 | 0.388853 | 0.25 | 0.428701 | 0.707279 | |
| COMPOUND_779_5488a11_980451 | Rp | + | 779.5488 | 11.98 | PC(16:1_20:4) duplicate | | | | (1560.0961, 9639.33)(1561.1, 8245.0)(1562.1108, 9476.21)(1563.1149, 6439.66)(1564.1115, 3107.91)(1565.105, 1551.79)(1598.0374, 1397.99)(1599.0468, 1675.92)(802.5379, 6127.32)(803.5369, 3258.42)(804.5571, 146720.44)(1582.069, 2797.75)(1583.073, 2500.68)(1584.0868, 2632.0)(1585.0919, 2420.06)(818.5162, 4562.53)(819.5176, 2962.44)(820.5293, 3129.27)(797.5471, 4160.73)(780.555, 992129.9)(781.5593, 465964.88)(782.5662, 20382.08)(783.5704, 60975.91)(1577.0771, 2059.4) | 12643831 | 6643172 | 11387092 | 5683450 | 13631398 | 5996660 | 13779005 | 6554713 | -0.01 | 0.974675 | 0.98606 | 0.42 | 0.189996 | 0.505078 |
| COMPOUND_779_5516a11_206111 | Rp | + | 779.5516 | 11.21 | | | | (1560.097, 17668.04)(1561.1001, 16317.86)(1562.1108, 21588.36)(1563.1143, 15609.61)(1564.1138, 9003.92)(1565.1068, 4066.67)(1598.0554, 2409.82)(1599.0562, 2266.53)(802.5365, 40018.91)(803.5369, 19739.46)(804.5539, 47337.24)(805.5568, 22349.94)(1582.0717, 4059.56)(1583.0767, 3478.14)(1584.0918, 5384.03)(1585.0925, 5235.28)(797.5483, 4958.11)(818.5109, 4112.02)(819.511, 3544.16)(820.5248, 3927.44)(780.5566, 388594.97)(781.5602, 180066.66)(782.5699, 216934.73)(783.5744, 89331.72)(784.5785, 26334.7)(785.5813, 6673.65)(1577.076, 2483.09) | 2977510 | 1374666 | 2835822 | 1550505 | 3686688 | 1849743 | 2639746 | 1553208 | -0.95 | 3.33E-05 | 0.000117 | -0.08 | 0.747636 | 0.891783 | |
| COMPOUND_779_5658a12_689466 | Rp | - | 779.5658 | 12.69 | PC 16:0_16:0 | 1 | 10 | 10 eV: 778.5577(100), 255.2323(6), 23.7679(2) | 778.5592, 66019.84(779.5621, 30991.03)(780.5642, 8808.21)(781.5639, 2864.11)(1558.1257, 2066.04)(1559.145, 2128.29)(1560.1359, 2103.28)(824.5701, 6938.04)(825.5758, 3476.34) | 382831.8 | 133023.8 | 397585.1 | 156155.6 | 345168.6 | 100819.1 | 381927 | 162739.2 | -0.32 | 0.246333 | 0.341589 | 0.26 | 0.429787 | 0.707514 |
| COMPOUND_781_5515a12_730271 | Rp | + | 781.5515 | 12.73 | | | | (802.0546, 1768.46)(802.5579, 2012.48)(803.0557, 12008.11)(782.5684, 130418.77)(783.5713, 59567.62)(1581.1733, 2676.39)(391.7831, 5057.99)(392.2844, 2902.44)(392.7843, 1531.02)(393.2848, 452.56)(393.7792, 91.69) | 1336533 | 309123.2 | 1364066 | 280569.2 | 1509853 | 308422.4 | 1365399 | 306867.2 | 0.55 | 0.070523 | 0.119735 | -0.66 | 0.07062 | 0.325554 | |
| COMPOUND_781_5619a11_260242 | Rp | + | 781.5619 | 11.26 | PC 36:4 | 2 | 20 | 20 eV: 782.5784(100), 184.0736(65), 338.2386(4) | (1564.1177, 20372.01)(804.5576, 96837.49)(805.5601, 48000.33)(1586.0994, 6822.34)(1587.1011, 6775.34)(1588.1122, 10366.58)(1589.1158, 7826.63)(1590.124, 7954.45)(782.5703, 110902.2)(783.5735, 50056.48)(784.5859, 104388.0)(785.5894, 46141.52)(786.5928, 22223.45)(787.5934, 7438.69)(391.7908, 416.08)(392.2895, 3598.95)(392.7951, 72.51) | 2758260 | 1353608 | 2175217 | 1306743 | 3015929 | 2690905 | 1871654 | 1397726 | -1.04 | 5.09E-06 | 2.16E-05 | 0.10 | 0.674185 | 0.849616 |
| COMPOUND_781_5672a12_260051 | Rp | + | 781.5672 | 12.26 | PC 36:4 | 2 | 20 | 20 eV: 782.5729(100), 184.0737(85), 502.3351(1) | (1564.1317, 36288.83)(1565.138, 33906.4)(1566.1326, 41399.55)(1567.1318, 28859.98)(1568.1305, 14284.63)(1569.1208, 581.79)(1570.1208, 2697.27)(804.5511, 49176.46)(805.5546, 24956.89)(1586.1093, 3888.67)(1587.1106, 3371.77)(1588.1304, 19553.95)(1589.1345, 19285.18)(1590.1426, 29942.8)(1591.1486, 24591.18)(1592.149, 12509.81)(1593.1414, 5236.18)(1594.1206, 2624.61)(799.5609, 1123.63)(800.5259, 2729.16)(820.5574, 3470.99)(821.5816, 616.86)(822.5538, 4120.34)(782.5691, 1415447.8)(783.5731, 669907.44)(784.5768, 174998.72)(785.579, 30857.43)(786.5824, 5478.22) | 3206037 | 6803657 | 28950000 | 6844649 | 33214286 | 4671494 | 35242105 | 7546616 | 0.44 | 0.072678 | 0.122508 | 0.45 | 0.116847 | 0.405455 |
| COMPOUND_781_5642a12_085624 | Rp | + | 781.5642 | 12.09 | | | | (1564.1305, 11869.55)(1565.1344, 10807.01)(1566.1366, 5750.96)(1567.138, 2369.86)(1568.1184, 1073.47)(804.5537, 42300.05)(805.5556, 21088.63)(806.5731, 48967.82)(1586.1134, 8569.11)(1587.118, 8383.96)(1588.1128, 11623.68)(1589.1327, 8858.68)(1590.1329, 4759.93)(1591.1265, 2167.2)(1592.1042, 1313.25)(1593.0898, 1250.66)(1594.0878, 1672.31)(820.5351, 3775.67)(821.5346, 2923.48)(822.5538, 3578.48)(823.5434, 2335.69)(782.571, 1052432.4)(783.5752, 485193.84)(784.5781, 124764.13)(785.5802, 23593.98)(786.5822, 4766.05)(787.5904, 545.82)(1581.0857, 1066.62)(1582.0784, 2038.21) | 9736373 | 3096082 | 9349826 | 3467017 | 9657695 | 2753277 | 8941926 | 3673717 | -0.04 | 0.901289 | 0.935347 | -0.11 | 0.747568 | 0.891783 | |
| COMPOUND_782_1479a11_030399 | Rp | + | 782.1479 | 11.03 | | | | (805.1448, 2119.99)(806.1595, 3508.35)(800.2177, 2315.85)(783.1537, 9281.18)(784.1434, 4715.41)(785.1366, 2376.96) | 95947.84 | 53712.83 | 83111.34 | 57912.63 | 104330.8 | 40075.56 | 76939.2 | 36436.25 | 0.21 | 0.457534 | 0.562427 | -0.08 | 0.816812 | 0.92157 | |
| COMPOUND_782_5681a13_892386 | Rp | - | 782.5680 | 13.89 | | | | (781.5618, 14135.55)(782.5648, 7242.05)(783.5689, 2435.53)(784.5719, 687.12)(785.5813, 151.46)(827.5641, 2608.49) | 77598.83 | 49376.42 | 73020.71 | 37377 | 33175.33 | 4497.657 | 29613.11 | 14012.31 | -1.41 | 3.04E-11 | 6.26E-10 | 0.03 | 0.881525 | 0.950612 | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_782_5688a14_010123 | Rp | - | 782.5688 | 14.01 | | | | (781.5611, 13787.71) (782.5648, 7127.21) (783.5691, 2449.86) (784.5726, 642.42) (785.5737, 116.69) (827.5629, 1804.28) (782.1553, 5568.79) (783.1567, 1387.68) (784.1541, 544.88) (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 73715.28 | 47032.39 | 73153.3 | 36493.17 | 35816 | 914.0804 | 40766.14 | 13392.9 | -1.25 | 5.38E-09 | 4.68E-08 | -0.09 | 0.680483 | 0.853001 |
| COMPOUND_783_1643a9_241846 | Rp | - | 783.1643 | 9.24 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 17075.65 | 2987.297 | 15804.43 | 3067.72 | 15817.29 | 1442.8 | 16547.48 | 3501.936 | -0.29 | 0.322367 | 0.423801 | 0.48 | 0.175802 | 0.490747 |
| COMPOUND_783_5771a11_348161 | Rp | + | 783.5771 | 11.35 | PC 36:3 | 2 | 40 eV: 184.0725(100), 86.0952(8), 524.800(1) | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 1048162 | 434972.8 | 1020556 | 492590.9 | 986512.3 | 536335.8 | 114441.3 | 550933.7 | -1.07 | 6.54E-06 | 2.71E-05 | -0.08 | 0.768095 | 0.902789 |
| COMPOUND_783_5789a12_453448 | Rp | + | 783.5789 | 12.45 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 22971698 | 12625149 | 25328261 | 11072702 | 20007143 | 3361882 | 30567904 | 21654933 | -0.07 | 0.82357 | 0.874436 | 0.08 | 0.818036 | 0.92157 |
| COMPOUND_783_5797a11_452839 | Rp | + | 783.5797 | 11.45 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 1827091 | 679945.1 | 1873837 | 730887.4 | 1245792 | 742685 | 1042510 | 524416.1 | -1.25 | 4.14E-09 | 3.78E-08 | -0.20 | 0.363649 | 0.668521 |
| COMPOUND_783_5803a12_51953 | Rp | + | 783.5803 | 12.52 | PC 36:3 | 2 | 10 eV: 784.5882(100), 184.0719(10) | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 36052830 | 10404319 | 35776087 | 11185987 | 41542857 | 6782411 | 50052632 | 13005083 | 0.64 | 0.008645 | 0.018615 | 0.51 | 0.070148 | 0.324382 |
| COMPOUND_784_6445a0_8248375 | Hilic | + | 784.6445 | 0.82 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 495413.9 | 190207.9 | 541693.8 | 215655.8 | 367758.8 | 138194.6 | 410167.4 | 152035.1 | -0.74 | 0.011965 | 0.024858 | 0.08 | 0.817438 | 0.92157 |
| COMPOUND_784_6452a0_7917568 | Hilic | + | 784.6452 | 0.79 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 588455.4 | 299260 | 70953.3 | 359701.5 | 410053.1 | 161386 | 413748.4 | 176885.1 | -0.65 | 0.018315 | 0.036565 | -0.36 | 0.254614 | 0.566592 |
| COMPOUND_784_9497a11_077688 | Rp | + | 784.9497 | 11.08 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 80973.12 | 61397.66 | 77898.95 | 77158.59 | 87654.63 | 28667.72 | 73653.98 | 28137.4 | 0.28 | 0.286786 | 0.385808 | 0.20 | 0.520694 | 0.764408 |
| COMPOUND_785_1398a11_079318 | Rp | + | 785.1398 | 11.08 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 87854.47 | 60549.64 | 82691.22 | 64132.36 | 78663.11 | 24221.63 | 78975.07 | 23015.98 | -0.01 | 0.976596 | 0.987116 | 0.23 | 0.491564 | 0.748114 |
| COMPOUND_785_472a12_178252 | Rp | + | 785.4720 | 12.18 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 17947.03 | 5156.04 | 20262.2 | 7889.815 | 26860.69 | 7989.537 | 32744.57 | 9272.643 | 0.84 | 0.001149 | 0.002954 | 0.02 | 0.95771 | 0.980661 |
| COMPOUND_785_5946a12_972127 | Rp | + | 785.5946 | 12.97 | PC 36:2 | 2 | 10 eV: 786.6024(100), 184.0735(10) | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 32233962 | 8136195 | 3496791 | 10374693 | 32657143 | 5867999 | 32063158 | 10663131 | 0.09 | 0.743604 | 0.814256 | -0.47 | 0.158644 | 0.468876 |
| COMPOUND_787_5381a11_02854 | Rp | - | 787.5381 | 11.03 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 1844093 | 1063453 | 1942637 | 966363.4 | 1325593 | 1142049 | 1492476 | 808482.6 | -0.94 | 1.99E-05 | 7.44E-05 | -0.37 | 0.133467 | 0.434347 |
| COMPOUND_787_5721a12_641872 | Rp | - | 787.5721 | 12.64 | | | | (1568.1046, 3807.45) (806.5701, 47893.04) (807.5732, 22706.62) (808.5853, 53846.89) (809.5887, 25914.29) (810.5884, 13662.83) (795.5563, 2306.14) (796.0605, 612.88) (1590.1272, 88.74) (422.7497, 645.51) (423.2541, 8610.38) (411.774, 1195.43) (412.2739, 657.14) (412.7833, 677.66) (413.2904, 262.47) (413.7797, 175.22) (403.7842, 914.01) (404.2886, 829.41) (404.7865, 567.54) (784.5881, 163490.72) (785.5911, 75326.05) (786.5923, 31548.52) (787.5925, 9929.67) (430.7584, 1297.97) (431.2646, 1160.25) (431.7655, 2102.42) (432.2719, 1175.88) (1585.1199, 1651.42) (392.8006, 441.27) (393.2987, 499.95) (393.7978, 86.09) | 709765.3 | 170049.5 | 724033.1 | 201291.2 | 545571.6 | 141905.2 | 532897 | 130208.7 | -1.02 | 8.19E-05 | 0.000256 | 0.07 | 0.81452 | 0.92157 |
| COMPOUND_787_61a13_585232 | Rp | + | 787.6100 | 13.59 | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|---|--|---------------|----------|---------------|----------|---------------|----------|---------------|------------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_789_5655a12_40603 | Rp | + | 789.5655 | 12.41 | | | | (812.5593, 10053.52)(813.5527, 3990.45)(814.5524, 6246.6)(790.5748, 56600.09)(791.5779, 2737.52)(792.5909, 72185.19)(793.594, 34001.44)(794.5921, 10899.14)(795.5823, 4266.09)(796.5854, 2222.28) (812.5429, 619.01)(813.0577, 616.63)(813.5598, 1024.97)(1580.1956, 83.73)(406.7935, 720.18)(407.298, 664.23)(407.7912, 155.83)(828.5557, 1027.0)(829.5667, 846.14)(807.6484, 195.24)(423.2752, 389.79)(423.7871, 50.15)(424.2626, 551.39)(404.3113, 1786.26)(404.8151, 2562.17)(405.312, 1242.87)(405.8187, 173.08)(790.589, 16392.5)(791.5915, 7182.02)(792.5834, 1262.64)(793.5916, 194.04)(395.7994, 2985.94)(396.3011, 1677.05)(396.8036, 490.1) | 661771.2 | 229214.9 | 591519.9 | 177724.9 | 658516.1 | 154366.3 | 718389.2 | 156640.7 | 0.13 | 0.615634 | 0.708436 | 0.51 | 0.094008 | 0.36381 |
| COMPOUND_789_5832a10_038973 | Rp | + | 789.5832 | 10.04 | | | | (812.5593, 10053.52)(813.5527, 3990.45)(814.5524, 6246.6)(790.5748, 56600.09)(791.5779, 2737.52)(792.5909, 72185.19)(793.594, 34001.44)(794.5921, 10899.14)(795.5823, 4266.09)(796.5854, 2222.28) (812.5429, 619.01)(813.0577, 616.63)(813.5598, 1024.97)(1580.1956, 83.73)(406.7935, 720.18)(407.298, 664.23)(407.7912, 155.83)(828.5557, 1027.0)(829.5667, 846.14)(807.6484, 195.24)(423.2752, 389.79)(423.7871, 50.15)(424.2626, 551.39)(404.3113, 1786.26)(404.8151, 2562.17)(405.312, 1242.87)(405.8187, 173.08)(790.589, 16392.5)(791.5915, 7182.02)(792.5834, 1262.64)(793.5916, 194.04)(395.7994, 2985.94)(396.3011, 1677.05)(396.8036, 490.1) | 182562.9 | 56442.33 | 162125.2 | 44068.84 | 198321 | 35206.88 | 199646.2 | 55051.81 | 0.63 | 0.015782 | 0.032048 | 0.29 | 0.346486 | 0.651869 |
| COMPOUND_789_5869a13_163428 | Rp | - | 789.5869 | 13.16 | | | | (824.55, 3336.2)(825.5507, 1590.78)(788.5795, 18142.78)(789.5835, 8730.51)(790.5843, 4185.07)(791.5915, 1367.03)(1578.1458, 879.88)(1579.1478, 747.33)(1580.1458, 1033.98) | 202173.4 | 73219.02 | 206264.5 | 80499.96 | 134269.4 | 64040.22 | 125869.7 | 49403.2 | -1.04 | 0.00011 | 0.000338 | 0.33 | 0.266257 | 0.575669 |
| COMPOUND_790_9459a11_021012 | Rp | + | 790.9459 | 11.02 | | | | (813.9518, 2536.2)(829.905, 1127.66)(808.963, 2318.55)(791.9531, 9763.2)(792.9483, 48284.97) 28607.75 43564.78 35361.25 42520.92 14432.01 46878.57 15520.89 4797.73(793.9366, 1568.62) | 86277.58 | 56332.6 | 71713.14 | 58842.09 | 94177.23 | 41544.74 | 86221.91 | 45630.58 | 0.39 | 0.140338 | 0.216188 | -0.28 | 0.36587 | 0.669574 |
| COMPOUND_791_1564a11_02265 | Rp | + | 791.1564 | 11.02 | | | | (814.157, 650.71)(815.1727, 5898.55)(816.1707, 3418.99)(809.1683, 4806.29)(792.1573, 16567.94)(793.1465, 5175.89)(794.1449, 1814.4) | 132452.7 | 44402.75 | 154252.7 | 48971.42 | 80143.67 | 64537.93 | 81902.87 | 65923.35 | -0.56 | 0.034112 | 0.062967 | 0.20 | 0.515656 | 0.761481 |
| COMPOUND_791_5324a10_973565 | Rp | - | 791.5324 | 10.97 | | | | (790.5174, 14510.29)(791.5207, 9329.75)(792.5158, 9408.52)(793.5177, 4072.6)(794.5191, 1956.14)(1582.0681, 281.32)(1583.071, 226.21)(1584.0758, 256.31) | 312452.7 | 44402.75 | 154252.7 | 48971.42 | 80143.67 | 64537.93 | 81902.87 | 65923.35 | -0.56 | 0.034112 | 0.062967 | 0.20 | 0.515656 | 0.761481 |
| COMPOUND_791_5456a11_954262 | Rp | + | 791.5456 | 11.95 | PC 37:6 | 2 | 10 ev: 792.5549(100), 184.0727(11), 463.4809(4) | (1584.091, 8603.26)(814.5301, 4587.05)(815.5285, 2561.8)(816.5156, 1654.53)(817.4988, 447.65)(792.5549, 6774.52)(793.5577, 33511.42)(794.5559, 10365.23)(795.5539, 1069.88) (790.5382, 53994.85)(791.5413, 26547.45)(792.5451, 8268.0)(793.5484, 2112.56)(1582.1462, 867.19)(1583.1497, 732.84) (814.5424, 4251.93)(815.5456, 2871.43)(792.5571, 71108.27)(793.5599, 34746.49) | 99071.44 | 42931.04 | 126933.7 | 49018.02 | 228122.6 | 91397.97 | 280680.9 | 123064.9 | 1.24 | 6.55E-08 | 4.37E-07 | 0.10 | 0.683153 | 0.853695 |
| COMPOUND_791_5461a12_792073 | Rp | - | 791.5461 | 12.79 | | | | (1584.1375, 3568.22)(1585.1382, 4064.14)(1586.1375, 3825.15)(814.5728, 15589.18)(815.5691, 10219.43)(816.5843, 13469.11)(792.5921, 17709.97)(793.5951, 85871.67)(794.5933, 30697.11)(795.5874, 9503.90) (904.6086, 398.62)(905.6095, 246.31)(790.5954, 17057.15)(791.5988, 8049.72)(792.5997, 2321.55)(793.5988, 705.22) | 1670060 | 665426.6 | 1443174 | 620766.1 | 1826664 | 597496.6 | 1907686 | 626622.1 | 0.22 | 0.046855 | 0.510438 | 0.04 | 0.890389 | 0.953702 |
| COMPOUND_791_6024a13_421187 | Rp | - | 791.6024 | 13.42 | | | | (792.5912, 41583.51)(793.534, 19366.67)(794.5304, 16748.29) (1588.1338, 107374.44)(1589.1373, 101669.52)(1616.5391, 3274.47)(817.5529, 3045.77)(811.5887, 2321.23)(812.6009, 403.22)(813.6191, 69.34)(794.5705, 21892.5)(795.5711, 10793.69)(796.5581, 4492.05)(797.5758, 511.55) (1588.1493, 2568.0)(816.5811, 13595.86)(817.5824, 7935.82)(794.6076, 256538.0)(795.6105, 127614.98)(796.6121, 34654.71)(797.611, 7350.52) (816.9172, 1234.21)(832.8935, 823.76)(811.9962, 2522.81)(794.9571, 12795.73)(795.9506, 4876.3)(796.9347, 1037.14) (907.174, 605.26)(908.1531, 176.27)(909.1773, 563.16)(829.1787, 68254.48)(830.1818, 18894.55)(831.1797, 2983.14)(832.1747, 451.1)(793.1974, 2368.05)(794.2004, 894.08)(795.1862, 458.37)(796.179, 148.54)(1587.3474, 110.7) (907.1916, 589.35)(908.1858, 304.28)(909.1701, 458.06)(829.1784, 27087.46)(793.1965, 2579.27)(794.1976, 960.14)(795.2086, 346.79)(1587.4265, 71.74)(1588.428, 76.93)(839.1872, 375.55)(840.1797, 279.84)(841.1774, 247.81) (794.4978, 8944.86)(795.501, 4457.38)(796.5115, 4890.53)(797.5161, 2482.91)(798.5264, 5779.39)(799.5307, 2608.22)(1590.076, 635.84)(1591.0842, 487.9) | 287325.3 | 97755.54 | 304435.1 | 129285.7 | 260547.1 | 70677.5 | 233943.9 | 80782.65 | -0.30 | 0.261012 | 0.35776 | -0.34 | 0.273223 | 0.583098 |
| COMPOUND_793_5387a12_398204 | Rp | - | 793.5387 | 12.40 | | | | (792.5912, 41583.51)(793.534, 19366.67)(794.5304, 16748.29) (1588.1338, 107374.44)(1589.1373, 101669.52)(1616.5391, 3274.47)(817.5529, 3045.77)(811.5887, 2321.23)(812.6009, 403.22)(813.6191, 69.34)(794.5705, 21892.5)(795.5711, 10793.69)(796.5581, 4492.05)(797.5758, 511.55) (1588.1493, 2568.0)(816.5811, 13595.86)(817.5824, 7935.82)(794.6076, 256538.0)(795.6105, 127614.98)(796.6121, 34654.71)(797.611, 7350.52) (816.9172, 1234.21)(832.8935, 823.76)(811.9962, 2522.81)(794.9571, 12795.73)(795.9506, 4876.3)(796.9347, 1037.14) (907.174, 605.26)(908.1531, 176.27)(909.1773, 563.16)(829.1787, 68254.48)(830.1818, 18894.55)(831.1797, 2983.14)(832.1747, 451.1)(793.1974, 2368.05)(794.2004, 894.08)(795.1862, 458.37)(796.179, 148.54)(1587.3474, 110.7) (907.1916, 589.35)(908.1858, 304.28)(909.1701, 458.06)(829.1784, 27087.46)(793.1965, 2579.27)(794.1976, 960.14)(795.2086, 346.79)(1587.4265, 71.74)(1588.428, 76.93)(839.1872, 375.55)(840.1797, 279.84)(841.1774, 247.81) (794.4978, 8944.86)(795.501, 4457.38)(796.5115, 4890.53)(797.5161, 2482.91)(798.5264, 5779.39)(799.5307, 2608.22)(1590.076, 635.84)(1591.0842, 487.9) | 733119.8 | 104808 | 753265.2 | 133403.9 | 718598.7 | 87528.69 | 664651 | 88793.93 | -0.07 | 0.811707 | 0.866745 | -0.68 | 0.053594 | 0.288052 |
| COMPOUND_793_5633a12_2282915 | Rp | + | 793.5633 | 12.23 | | | | (792.5912, 41583.51)(793.534, 19366.67)(794.5304, 16748.29) (1588.1338, 107374.44)(1589.1373, 101669.52)(1616.5391, 3274.47)(817.5529, 3045.77)(811.5887, 2321.23)(812.6009, 403.22)(813.6191, 69.34)(794.5705, 21892.5)(795.5711, 10793.69)(796.5581, 4492.05)(797.5758, 511.55) (1588.1493, 2568.0)(816.5811, 13595.86)(817.5824, 7935.82)(794.6076, 256538.0)(795.6105, 127614.98)(796.6121, 34654.71)(797.611, 7350.52) (816.9172, 1234.21)(832.8935, 823.76)(811.9962, 2522.81)(794.9571, 12795.73)(795.9506, 4876.3)(796.9347, 1037.14) (907.174, 605.26)(908.1531, 176.27)(909.1773, 563.16)(829.1787, 68254.48)(830.1818, 18894.55)(831.1797, 2983.14)(832.1747, 451.1)(793.1974, 2368.05)(794.2004, 894.08)(795.1862, 458.37)(796.179, 148.54)(1587.3474, 110.7) (907.1916, 589.35)(908.1858, 304.28)(909.1701, 458.06)(829.1784, 27087.46)(793.1965, 2579.27)(794.1976, 960.14)(795.2086, 346.79)(1587.4265, 71.74)(1588.428, 76.93)(839.1872, 375.55)(840.1797, 279.84)(841.1774, 247.81) (794.4978, 8944.86)(795.501, 4457.38)(796.5115, 4890.53)(797.5161, 2482.91)(798.5264, 5779.39)(799.5307, 2608.22)(1590.076, 635.84)(1591.0842, 487.9) | 605653.4 | 300873.4 | 578824.1 | 319361.8 | 737706 | 446035.5 | 684964.1 | 298830.9 | 0.35 | 0.232743 | 0.327385 | 0.14 | 0.684839 | 0.853695 |
| COMPOUND_793_5991a12_7826185 | Rp | + | 793.5991 | 12.78 | PC 38:5e | 2 | 40 ev: 184.0734(100), 86.0966(5), 478.3244(1) | (1584.1375, 3568.22)(1585.1382, 4064.14)(1586.1375, 3825.15)(814.5728, 15589.18)(815.5691, 10219.43)(816.5843, 13469.11)(792.5921, 17709.97)(793.5951, 85871.67)(794.5933, 30697.11)(795.5874, 9503.90) (904.6086, 398.62)(905.6095, 246.31)(790.5954, 17057.15)(791.5988, 8049.72)(792.5997, 2321.55)(793.5988, 705.22) | 2380827 | 685267.9 | 2135413 | 697407.8 | 2225368 | 342187 | 2109981 | 487480.2 | -0.15 | 0.585378 | 0.680925 | 0.21 | 0.511387 | 0.757661 |
| COMPOUND_793_9485a11_066964 | Rp | + | 793.9485 | 11.07 | | | | (792.5912, 41583.51)(793.534, 19366.67)(794.5304, 16748.29) (1588.1338, 107374.44)(1589.1373, 101669.52)(1616.5391, 3274.47)(817.5529, 3045.77)(811.5887, 2321.23)(812.6009, 403.22)(813.6191, 69.34)(794.5705, 21892.5)(795.5711, 10793.69)(796.5581, 4492.05)(797.5758, 511.55) (1588.1493, 2568.0)(816.5811, 13595.86)(817.5824, 7935.82)(794.6076, 256538.0)(795.6105, 127614.98)(796.6121, 34654.71)(797.611, 7350.52) (816.9172, 1234.21)(832.8935, 823.76)(811.9962, 2522.81)(794.9571, 12795.73)(795.9506, 4876.3)(796.9347, 1037.14) (907.174, 605.26)(908.1531, 176.27)(909.1773, 563.16)(829.1787, 68254.48)(830.1818, 18894.55)(831.1797, 2983.14)(832.1747, 451.1)(793.1974, 2368.05)(794.2004, 894.08)(795.1862, 458.37)(796.179, 148.54)(1587.3474, 110.7) (907.1916, 589.35)(908.1858, 304.28)(909.1701, 458.06)(829.1784, 27087.46)(793.1965, 2579.27)(794.1976, 960.14)(795.2086, 346.79)(1587.4265, 71.74)(1588.428, 76.93)(839.1872, 375.55)(840.1797, 279.84)(841.1774, 247.81) (794.4978, 8944.86)(795.501, 4457.38)(796.5115, 4890.53)(797.5161, 2482.91)(798.5264, 5779.39)(799.5307, 2608.22)(1590.076, 635.84)(1591.0842, 487.9) | 63513.61 | 35197.6 | 45401.16 | 32968.7 | 42236.38 | 21179.32 | 44122.18 | 20798.22 | -0.15 | 0.554135 | 0.651651 | 0.55 | 0.082247 | 0.343638 |
| COMPOUND_794_2038a9_581989 | Rp | - | 794.2038 | 9.58 | | | | (792.5912, 41583.51)(793.534, 19366.67)(794.5304, 16748.29) (1588.1338, 107374.44)(1589.1373, 101669.52)(1616.5391, 3274.47)(817.5529, 3045.77)(811.5887, 2321.23)(812.6009, 403.22)(813.6191, 69.34)(794.5705, 21892.5)(795.5711, 10793.69)(796.5581, 4492.05)(797.5758, 511.55) (1588.1493, 2568.0)(816.5811, 13595.86)(817.5824, 7935.82)(794.6076, 256538.0)(795.6105, 127614.98)(796.6121, 34654.71)(797.611, 7350.52) (816.9172, 1234.21)(832.8935, 823.76)(811.9962, 2522.81)(794.9571, 12795.73)(795.9506, 4876.3)(796.9347, 1037.14) (907.174, 605.26)(908.1531, 176.27)(909.1773, 563.16)(829.1787, 68254.48)(830.1818, 18894.55)(831.1797, 2983.14)(832.1747, 451.1)(793.1974, 2368.05)(794.2004, 894.08)(795.1862, 458.37)(796.179, 148.54)(1587.3474, 110.7) (907.1916, 589.35)(908.1858, 304.28)(909.1701, 458.06)(829.1784, 27087.46)(793.1965, 2579.27)(794.1976, 960.14)(795.2086, 346.79)(1587.4265, 71.74)(1588.428, 76.93)(839.1872, 375.55)(840.1797, 279.84)(841.1774, 247.81) (794.4978, 8944.86)(795.501, 4457.38)(796.5115, 4890.53)(797.5161, 2482.91)(798.5264, 5779.39)(799.5307, 2608.22)(1590.076, 635.84)(1591.0842, 487.9) | 442228.8 | 51879.9 | 450866.5 | 52618.14 | 435458.9 | 45479.2 | 433723.7 | 55302.29</ | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-------------------------------|--------|----------|----------|-----------|----------------|----------|--|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_801_5916a11_457064 | Rp | + | 801.5916 | 11.46 | | | | (824.5819, 170840.44)(825.5848, 82887.73)(826.5969, 146394.58)(827.6007, 65906.66)(802.598, 753303.8)(803.6018, 350087.78)(804.6046, 90901.58)(805.6054, 18587.0) | 5278350 | 1979765 | 5606918 | 2056242 | 3574470 | 2141549 | 3206084 | 1573134 | -1.22 | 7.44E-09 | 6.33E-08 | -0.26 | 0.23951 | 0.544276 |
| COMPOUND_803_5349a12_255897 | Rp | + | 803.5349 | 12.26 | PC 38:7 | 2 | 40 eV: 146.9805(100), 621.4828(65), 745.4794(10), 502.3124(13) | (815.5353, 2982.2)(816.0318, 1909.51)(816.5406, 1614.28)(817.0421, 1022.57)(824.0408, 1356.29)(824.5388, 1450.44)(825.04, 7113.81)(825.5423, 10130.99)(804.5527, 96227.03)(805.556, 46849.9)(402.7753, 3377.54)(403.2762, 2321.25)(403.7767, 1167.86)(404.2791, 388.28)(404.7722, 95.33) | 821350 | 117834.1 | 766902.4 | 104254.6 | 755783 | 103578.6 | 741381.6 | 112072.9 | -0.45 | 0.099495 | 0.162099 | 0.23 | 0.471616 | 0.734155 |
| COMPOUND_803_5474a11_831466 | Rp | + | 803.5474 | 11.83 | PC 18:2_20:5 | 1 | 40 eV: 184.0756(100), 124.9984(6), 437.1869(2), 804.5533(1) | (826.536, 5635.78)(827.5344, 3131.94)(828.5446, 1451.38)(829.5394, 404.81)(842.4857, 175.27)(821.5569, 1658.28)(804.5547, 146578.02)(805.5758, 70205.84)(806.5616, 21833.16)(807.5636, 5120.09) | 795199.9 | 466866.5 | 817518.7 | 396650.5 | 1078540 | 543982.9 | 3110827 | 636632.3 | 0.62 | 0.011003 | 0.023007 | 0.40 | 0.154078 | 0.466404 |
| COMPOUND_803_5483a11_835721 | Rp | + | 803.5483 | 11.84 | | | | (826.5586, 15824.46)(827.5519, 8580.84)(828.5752, 4775.75)(829.5971, 1528.45)(821.5565, 1706.52)(842.4929, 2695.08)(804.5544, 39677.08)(805.5575, 28910.47)(806.569, 37453.32)(807.5717, 16671.41)(808.5769, 6801.45) | 902590 | 348499.8 | 884833.5 | 311409.7 | 1237540 | 595049.1 | 1340124 | 562643.7 | 0.78 | 0.001133 | 0.002916 | 0.27 | 0.329625 | 0.635357 |
| COMPOUND_803_5511a11_19134 | Rp | + | 803.5511 | 11.19 | | | | (804.5584, 96629.78)(805.5606, 48872.27)(806.5678, 50200.71)(402.7797, 1406.22)(403.2775, 683.9) | 966300.6 | 280005.8 | 897852.8 | 359074.7 | 678911.5 | 566634.8 | 829092.5 | 597761.8 | -0.75 | 0.001426 | 0.003613 | -0.15 | 0.587047 | 0.799293 |
| COMPOUND_803_5668a12_344101 | Rp | - | 803.5668 | 12.34 | PC 16:0_18:2 | 2 | 10 eV: 802.5593(100), 279.2329(3) | (802.5591, 780535.0)(803.563, 359118.0)(804.566, 94938.71)(805.5687, 19080.78)(806.57, 3340.83)(807.5736, 635.99) | 24769811 | 2528346 | 26919565 | 2457426 | 27450000 | 1935001 | 26001754 | 2889482 | 0.90 | 0.001017 | 0.002652 | -0.92 | 0.00381 | 0.093266 |
| COMPOUND_803_5991a10_217415 | Rp | + | 803.5991 | 10.22 | | | | (842.5788, 991.5)(843.0888, 470.54)(843.5889, 6115.16)(411.3178, 1922.39)(411.8226, 592.25)(412.3228, 525.76)(412.8252, 48.27)(804.6047, 3883.48)(805.6058, 1753.32)(806.5993, 819.81)(807.6027, 100.68)(422.3147, 981.82)(422.8076, 61.51)(423.3114, 496.47)(402.8037, 491.38)(403.2886, 1105.07)(403.7922, 103.5) | 6942786 | 24451.36 | 60721.52 | 22096.46 | 83807.92 | 19488.24 | 84528.89 | 22579.69 | 0.49 | 0.071878 | 0.130869 | 0.43 | 0.197401 | 0.508252 |
| COMPOUND_803_6023a10_707655 | Rp | - | 803.6023 | 10.71 | | | | (802.595, 17728.34)(803.5977, 9312.33)(804.5983, 2535.52)(805.5965, 613.83)(806.5962, 152.94) | 48935.32 | 27850.17 | 60386.44 | 34336.37 | 50822.56 | 23730.63 | 50145.73 | 25546.64 | -0.08 | 0.767305 | 0.832356 | -0.41 | 0.20429 | 0.516343 |
| COMPOUND_805_5482a11_072999 | Rp | - | 805.5482 | 11.07 | | | | (804.539, 13815.38)(805.5421, 6410.18)(806.5261, 6497.0)(807.5258, 3034.17)(850.5426, 7000.87)(851.5453, 3578.36)(852.5397, 7279.53)(853.5419, 3727.33) | 129805.3 | 42554.08 | 136832.8 | 46374.74 | 141980 | 46336.65 | 121089.3 | 26959.39 | -1.11 | 2.96E-07 | 1.69E-06 | -0.29 | 0.214916 | 0.521996 |
| COMPOUND_805_5626a12_181954 | Rp | + | 805.5626 | 12.18 | PC 16:0_22:6 | 1 | 10 eV: 806.5684(100), 184.074(12), 86.0942(1) | (828.5539, 56676.38)(829.5558, 29112.66)(830.5606, 11347.54)(831.5591, 3468.65)(823.6028, 3217.87)(824.6039, 1378.04)(844.5245, 5603.15)(845.525, 2978.73)(846.5365, 2503.22)(806.5709, 1273137.2)(807.5747, 633189.75)(808.5812, 222204.48)(809.5839, 60083.6) | 27277358 | 6224074 | 24628261 | 6234658 | 28221429 | 4755916 | 29092982 | 9545672 | 0.19 | 0.494946 | 0.596053 | 0.56 | 0.103883 | 0.381877 |
| COMPOUND_805_5658a12_035259 | Rp | + | 805.5658 | 12.04 | | | | (828.5505, 11121.51)(829.5481, 6356.61)(830.5699, 41800.48)(831.5736, 20772.05)(823.6224, 2083.41)(806.5712, 366537.38)(807.5745, 184610.11)(808.5768, 51209.79)(809.5759, 11049.31)(810.5735, 2542.01)(811.5935, 442.01) | 3284945 | 1095565 | 3015891 | 951562.4 | 2996978 | 792800.4 | 3090031 | 680516.6 | -0.23 | 0.413082 | 0.517387 | 0.39 | 0.243186 | 0.550407 |
| COMPOUND_805_5784a9_587811 | Rp | + | 805.5784 | 9.59 | | | | (414.7896, 1535.67)(415.2841, 1353.72)(415.7934, 338.06)(412.3103, 15044.86)(412.8122, 6648.35)(413.3103, 2416.62)(413.8134, 604.41)(806.5843, 11449.46)(807.5867, 5259.83)(808.5888, 1538.19)(809.591, 472.4)(810.5772, 117.34)(423.2918, 352.51)(423.8, 133.8)(424.3029, 905.66)(403.7971, 5073.21)(404.2961, 3111.87)(404.8025, 755.37) | 407003.1 | 108947.4 | 356083.2 | 68887.13 | 425602.6 | 69719.25 | 430639.9 | 110623.1 | 0.15 | 0.597071 | 0.691669 | 0.60 | 0.086036 | 0.348516 |
| COMPOUND_805_5821a12_793038 | Rp | - | 805.5821 | 12.79 | PC 34:1 | 2 | 20 eV: 744.5547(100), 804.5764(30), 281.2487(10), 44.9998(4), 480.309(1) | (804.5747, 840188.3)(805.5788, 393290.88)(806.5816, 99340.09)(807.5843, 19944.06)(808.5851, 3548.98)(809.5846, 613.74) | 16481132 | 2661120 | 17186957 | 3174664 | 19335714 | 2430767 | 21200000 | 2808533 | 0.86 | 0.000198 | 0.000591 | 0.26 | 0.305317 | 0.613089 |
| COMPOUND_806_6259a10_7969206 | HiLic | | 806.6259 | 0.80 | | | | (829.6211, 3373.51)(830.6236, 1784.76)(831.6365, 7460.25)(832.6376, 4449.45)(833.6501, 8206.34)(834.6295, 3779.95)(807.6357, 21252.9)(808.6363, 10831.37)(809.6352, 24555.1)(810.6522, 13467.68)(811.6689, 87503.69)(404.3232, 1372.97)(404.824, 687.28)(405.3318, 1301.27)(405.8309, 537.69)(406.3341, 255.31) | 412257.3 | 130593.9 | 446832.3 | 136913 | 465967 | 211999.2 | 422644.3 | 174983.7 | 0.30 | 0.291571 | 0.390827 | -0.23 | 0.496013 | 0.751527 |
| COMPOUND_807_5611a10_627024 | Rp | + | 807.5611 | 10.63 | | | | (830.556, 122831.57)(831.5588, 56107.81)(832.5699, 82065.22)(833.5735, 34886.83)(808.56, 3324.11)(809.5596, 1509.14)(810.5408, 2308.17)(811.5405, 1333.38) | 521163.6 | 337188.5 | 501894.7 | 258146.1 | 301976.6 | 261383.5 | 317317 | 216371.9 | -1.03 | 6.25E-06 | 2.6E-05 | -0.10 | 0.680276 | 0.853001 |
| COMPOUND_807_5798a12_375857 | Rp | + | 807.5798 | 12.38 | PC 38:5 | 2 | 10 eV: 808.5857(100), 184.0758(10) | (830.5668, 25291.13)(831.5705, 13168.28)(832.5835, 23087.27)(833.5878, 11313.86)(834.6001, 31714.34)(846.5265, 3583.93)(847.5254, 2225.38)(808.5871, 716565.3)(809.591, 352037.56)(810.5935, 94814.47)(811.5906, 20258.47)(812.5776, 4126.2)(813.599, 460.64) | 6769973 | 1965862 | 5730694 | 1658790 | 5557741 | 893049 | 6227971 | 1463985 | -0.52 | 0.048664 | 0.085485 | 0.92 | 0.00323 | 0.081732 |
| COMPOUND_807_5818a12_500268 | Rp | + | 807.5818 | 12.50 | | | | (830.5674, 17935.56)(831.5707, 9215.15)(832.584, 15292.02)(833.5885, 7831.64)(846.5336, 4507.27)(808.5864, 713420.8)(809.5903, 345694.22)(810.5944, 106151.98)(811.5918, 27011.77) | 4441667 | 1800302 | 3786734 | 1489590 | 3712439 | 1005470 | 4362628 | 1439769 | -0.38 | 0.149179 | 0.226993 | 0.80 | 0.011414 | 0.166978 |
| COMPOUND_808_6454a10_7934525 | HiLic | + | 808.6454 | 0.79 | | | | (831.6365, 6177.56)(832.6373, 3743.83)(833.6512, 9585.27)(834.6484, 4765.35)(835.6631, 5006.98)(826.6506, 6853.56)(809.6524, 22511.88)(810.6537, 10253.37)(811.6691, 65469.05)(812.6721, 34287.64)(813.6833, 37830.06)(405.3311, 1277.32)(405.8311, 656.67)(406.3371, 317.04) | 617268.5 | 225006 | 666514.5 | 266007.2 | 516080 | 178635.2 | 553829.4 | 243455.1 | -0.23 | 0.426942 | 0.531495 | -0.14 | 0.678524 | 0.851748 |
| COMPOUND_809_4733a11_166188 | Rp | + | 809.4733 | 11.17 | | | | (837.847, 282.03)(838.8205, 526.43)(405.743, 15297.81)(406.2452, 8188.39) | 108300.6 | 27441.99 | 1096664 | 29088.43 | 104847.5 | 40648.4 | 111796.9 | 36544.84 | -0.99 | 1.66E-05 | 6.35E-05 | -0.20 | 0.426592 | 0.705867 |
| COMPOUND_809_5331a11_179161 | Rp | - | 809.5331 | 11.18 | | | | (808.5259, 20224.93)(809.5297, 8990.91)(810.5245, 9096.98)(811.5265, 3528.03)(812.525, 1616.08)(854.5216, 7488.35) | 213578.2 | 77130.4 | 239064.8 | 90794.24 | 241186.7 | 11592.74 | 253655.1 | 74357.69 | -0.94 | 2.23E-05 | 8.18E-05 | -0.31 | 0.209232 | 0.518933 |
| COMPOUND_809_5559a12_19905 | Rp | - | 809.5559 | 12.20 | | | | (844.5322, 17790.44)(845.5352, 7915.89)(846.5477, 3231.56)(847.5721, 835.7)(808.5481, 6901.29)(809.5514, 3593.02)(810.5553, 1455.96)(811.5661, 450.11) | 138575.3 | 26295.49 | 139313.4 | 32146.77 | 134976.3 | 32574.42 | 156108.1 | 35423.94 | -0.13 | 0.649722 | 0.737859 | 0.62 | 0.083666 | 0.346484 |
| COMPOUND_809_5951a12_8862915 | Rp | + | 809.5951 | 12.89 | PC 18:0_20:4 | 1 | 10 eV: 810.6015(100), 184.0735(8) | (832.583, 44462.23)(833.5867, 22232.24)(834.6018, 92460.52)(835.605, 45325.59)(836.6135, 58411.31)(848.5538, 4700.25)(849.5531, 2845.73)(850.5569, 3288.2)(827.6411, 417.93)(810.6011, 781.902.7)(811.6051, 386191.7)(812.6081, 103516.8)(813.5953, 25177.91)(814.6077, 3148.33)(815.6131, 438.62) | 12568897 | 3512020 | 11415812 | 3793958 | 10396884 | 2662643 | 10606833 | 3324973 | -0.53 | 0.038551 | 0.07007 | 0.28 | 0.33564 | 0.639647 |
| COMPOUND_809_5959a12_640725 | Rp | + | 809.5959 | 12.64 | PC 18:1_20:3 | 1 | 10 eV: 810.6038(100), 184.0718(8), 522.3501(1) | (832.5841, 23141.67)(833.5866, 12320.6)(834.6012, 34660.84)(835.6052, 17610.52)(836.605, 5616.98)(827.6414, 357.3)(810.6016, 486332.6)(811.6056, 235236.88)(812.6079, 63556.43)(813.6094, 12829.68) | 2878208 | 1043306 | 2851766 | 1107611 | 3634284 | 1100444 | 4223037 | 1484344 | 0.48 | 0.047555 | 0.083973 | 0.53 | 0.063348 | 0.307286 |
| COMPOUND_810_6609a13_636442 | Rp | + | 810.6609 | 13.64 | SM d42:3 | 2 | 10 eV: 811.6664(100), 184.0711(15), 458.2399(1) | (833.6336, 10426.67)(834.6229, 3011.95)(835.6118, 1100.79)(811.6694, 58748.79)(812.6709, 31085.18)(813.6724, 8606.25)(814.6658, 1240.29)(815.6755, 111.81)(406.3459, 389.2)(406.8439, 79.7)(407.3502, 161.99) | 1084407 | 461677.4 | 1205156 | 494301.6 | 757650 | 276685.4 | 786873.8 | 352280.1 | -0.46 | 0.071006 | 0.12032 | 0.35 | 0.249795 | 0.559739 |
| COMPOUND_810_6614a10_78531355 | HiLic | + | 810.6614 | 0.79 | | | | (834.5391, 9140.24)(834.6519, 4764.41)(835.6644, 5050.08)(836.6671, 2410.59)(837.6753, 1146.13)(828.6692, 3957.46)(829.6727, 3163.31)(811.6695, 138088.38)(812.6724, 72649.15)(813.6834, 76592.25)(814.6875, 35158.29)(815.6926, 12063.62)(816.6967, 3150.09)(817.7009, 947.1)(406.3364, 273.64)(406.8383, 150.21)(407.337 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|---------------------|----------|--|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_811_6117a13_244986 | Rp | + | 811.6117 | 13.24 | PC 18_0_20_3 | 1 | 10eV: 812.6133(100), 184.0732(16), 310.348(1) | (834.5997, 38355.43)(853.6031, 19358.69)(836.6169, 56407.12)(837.6208, 27587.21)(838.6246, 9948.98)(839.6076, 3625.89)(840.6336, 480.42)(850.5748, 3131.69)(851.5749, 2371.38)(852.573, 1649.26)(859.6265, 338.65)(830.8366, 866.58)(831.6556, 179.65)(812.6186, 31782.75)(813.622, 15737.39)(814.6243, 41904.05)(815.6265, 8807.96)(816.6141, 1936.42)(817.633, 166.37)(926.5021, 1129.49)(927.4941, 919.07)(812.5438, 29748.08)(813.5469, 15489.9)(814.52, 17415.14)(858.5067, 4195.9) | 201296.4 | 50363.78 | 178954.5 | 69867.52 | 202147.9 | 47379.6 | 191381.4 | 52266.29 | 0.11 | 0.696358 | 0.778262 | 0.17 | 0.604357 | 0.810123 |
| COMPOUND_813_5493a12_0586405 | Rp | - | 813.5493 | 12.06 | | | (926.5213, 683.92)(927.5299, 391.33)(928.5045, 606.87)(929.5197, 217.51)(930.5317, 325.28)(812.5444, 79233.59)(813.5474, 39179.75)(814.5524, 12646.22)(815.5566, 2953.84)(816.5613, 746.99) | 65275.3 | 34110.95 | 85342.85 | 60840.48 | 76004.75 | 45014.55 | 74945.2 | 44159.58 | -0.99 | 4.59E-06 | 1.96E-05 | -0.38 | 0.106967 | 0.38909 | |
| COMPOUND_813_5508a9_927079 | Rp | - | 813.5508 | 9.93 | | | (836.5413, 42397.38)(837.5442, 21234.7)(838.5602, 141386.04)(839.563, 66532.3)(814.5623, 214146.45)(815.5649, 101460.88)(816.5767, 274427.0)(817.5801, 123498.23)(818.5893, 107215.16) | 4281641 | 1786020 | 4332267 | 2107547 | 4342261 | 4167380 | 3416063 | 1970627 | -0.71 | 0.002145 | 0.005297 | -0.25 | 0.346337 | 0.651869 | |
| COMPOUND_813_5874a12_718801 | Rp | - | 813.5874 | 12.72 | PC 36_4e | 2 | 20 eV: 752.5582(100), 812.5812(40), 303.2318(13), 44.9986(4) | (926.5322, 1887.85)(812.5807, 149352.84)(813.5837, 72358.63)(814.5865, 20523.76)(815.5883, 4021.67)(858.5863, 993.02)(859.5654, 501.38)(860.583, 171.9) | 1052377 | 264331 | 1048928 | 314290.1 | 909985.3 | 168979.8 | 877705.2 | 192954.6 | -0.52 | 0.037311 | 0.068092 | -0.08 | 0.786519 | 0.909997 |
| COMPOUND_814_542a11_783751 | Rp | - | 814.5420 | 11.78 | | | (813.537, 25170.07)(814.5382, 12081.66)(815.5392, 3609.64)(859.5299, 3678.16) | 250388.6 | 65313.07 | 259889.3 | 103245.6 | 280105.4 | 74532.05 | 275525.3 | 68199.84 | 0.75 | 0.002836 | 0.006801 | -0.18 | 0.523679 | 0.766338 | |
| COMPOUND_814_5568a10_857167 | Rp | + | 814.5568 | 10.86 | | | (837.5473, 94675.16)(815.5645, 130106.38)(816.5719, 66235.13)(817.576, 22662.44) | 1791534 | 477262 | 1706405 | 594200 | 1969205 | 389498.6 | 1355709 | 655616.4 | -1.03 | 5.75E-06 | 2.41E-05 | -0.17 | 0.490692 | 0.748114 | |
| COMPOUND_815_4156a7_49421 | Rp | + | 815.4156 | 7.49 | | | (838.4176, 112.87)(838.9306, 62.72)(839.421, 160.63)(835.4034, 230.27)(835.8987, 26.44)(427.6758, 358.75)(428.1633, 237.11)(419.7085, 583.51)(420.2099, 2484.57)(420.709, 791.82)(421.2026, 265.21)(417.2301, 40351.89)(417.7317, 17450.98)(418.2338, 5109.34)(418.7349, 1295.71)(419.2359, 274.08)(816.4225, 23440.42)(817.4271, 9230.44)(818.4283, 2962.88)(819.431, 795.04)(820.4374, 206.73)(408.7175, 1695.51)(409.2123, 1087.87)(409.72, 262.73) | 289591.5 | 125220.8 | 270890.5 | 97462.96 | 255968.8 | 118485.2 | 299302.3 | 115858.6 | -0.20 | 0.504384 | 0.604832 | 0.55 | 0.12102 | 0.411311 | |
| COMPOUND_815_5666a12_244778 | Rp | - | 815.5666 | 12.24 | | | (814.5588, 15490.13)(815.5599, 10589.22)(860.5915, 1508.76)(861.5954, 896.67)(862.5766, 1044.12) | 107093.8 | 38129.25 | 111719.9 | 42090.81 | 124663.5 | 42860.77 | 109010.4 | 31887.83 | 0.40 | 0.144327 | 0.221256 | -0.24 | 0.464171 | 0.732257 | |
| COMPOUND_815_5766a12_533583 | Rp | + | 815.5766 | 12.53 | | | (838.5596, 1963.58)(839.5572, 1872.79)(840.5481, 2119.79)(841.5447, 2003.56)(842.531, 3681.57)(815.5882, 28038.14)(817.592, 13697.78)(818.5916, 13868.81)(819.5907, 6473.85)(820.5858, 16382.99) | 201979.9 | 57854.22 | 183344 | 73771.47 | 199218.5 | 78966.62 | 216752 | 65373.75 | -0.02 | 0.933611 | 0.95693 | 0.19 | 0.536122 | 0.776357 | |
| COMPOUND_815_6011a12_916941 | Rp | - | 815.6011 | 12.92 | | | (814.5953, 19225.41)(815.5991, 9562.5)(816.5921, 3234.32)(817.5863, 1102.95) | 240846.9 | 100210.6 | 253804.9 | 101287.4 | 252160.4 | 63082.25 | 256493.6 | 98175.52 | 0.36 | 0.168105 | 0.251544 | -0.32 | 0.297896 | 0.60748 | |
| COMPOUND_817_5a11_98166 | Rp | + | 817.5000 | 11.98 | | | (827.0369, 1131.78)(827.5355, 3311.09)(828.0305, 601.92)(838.027, 2084.45)(838.5096, 1194.98)(839.0194, 1469.36)(835.522, 2093.5)(437.2387, 211.84)(437.7353, 177.19)(835.5069, 1566.04)(836.0247, 1626.14)(836.5172, 2078.51)(837.0143, 1920.15)(837.5073, 2051.38)(838.0088, 1692.72)(838.5049, 1864.7)(839.0057, 1451.77)(839.5024, 1169.25)(818.511, 9028.8)(819.5124, 5160.78)(820.5258, 4573.91)(409.756, 13012.07)(410.2579, 6285.33)(410.7589, 1890.51)(411.245, 218.83) | 274114 | 105007.1 | 238393 | 71194.81 | 322030.7 | 180285.3 | 362388.5 | 201183.8 | -0.01 | 0.960528 | 0.976573 | 0.45 | 0.188222 | 0.504013 | |
| COMPOUND_817_5442a11_094098 | Rp | - | 817.5442 | 11.09 | | | (930.5168, 2607.76)(931.5158, 1396.68)(816.5387, 1729.52)(817.5419, 32912.88)(818.5542, 119539.96)(819.5576, 54013.21)(820.5464, 28124.41)(821.5433, 10524.25) | 860761.3 | 271580.6 | 956846.2 | 338345.9 | 1104397 | 498964.8 | 1033231 | 718424.4 | -0.83 | 0.000618 | 0.00169 | -0.33 | 0.235144 | 0.541455 | |
| COMPOUND_817_5456a11_323749 | Rp | - | 817.5456 | 11.32 | | | (930.544, 18454.35)(931.5453, 8938.16)(932.5351, 4415.7)(816.5393, 199318.89)(817.5424, 91943.16)(818.5536, 154064.05)(819.5573, 66263.33)(820.563, 22473.28) | 609302.9 | 253434.1 | 706220.8 | 226577.9 | 437550.5 | 25808.69 | 425996 | 152393.9 | -1.16 | 4.37E-08 | 3.04E-07 | -0.18 | 0.430792 | 0.708135 | |
| COMPOUND_817_5811a11_319503 | Rp | + | 817.5811 | 11.32 | | | (840.5747, 122685.97)(841.5787, 53043.07)(818.593, 576618.56)(819.5968, 275583.1) | 1755671 | 1018789 | 1691806 | 1095638 | 1424605 | 1396018 | 1103060 | 439309.1 | -1.23 | 7.64E-09 | 6.47E-08 | -0.13 | 0.548464 | 0.77853 | |
| COMPOUND_817_5818a12_677716 | Rp | - | 817.5818 | 12.68 | | | (930.5763, 1662.33)(931.5666, 1040.81)(816.5751, 81552.77)(817.5785, 38582.41)(818.5607, 17672.8)(862.5948, 15315.4)(863.5985, 8251.9) | 967133.5 | 262128.9 | 1030982 | 358333.5 | 920517.4 | 126885 | 824789.2 | 163198.2 | 0.27 | 0.238705 | 0.333581 | -0.06 | 0.832861 | 0.926681 | |
| COMPOUND_817_5841a11_419728 | Rp | + | 817.5841 | 11.42 | | | (840.5753, 87328.65)(841.578, 43904.13)(842.5909, 89357.38)(843.5961, 41477.06)(844.59, 33865.07)(856.5588, 9741.06)(857.5605, 5257.42)(858.572, 6545.43)(818.5919, 755353.94)(819.5957, 358122.25)(820.5946, 103918.57)(821.5897, 22160.71) | 4362272 | 2389116 | 4704741 | 2337041 | 2100707 | 1575192 | 1403329 | 1123330 | -1.28 | 4.01E-10 | 5.01E-09 | -0.22 | 0.283092 | 0.591944 | |
| COMPOUND_817_5923a11_075347 | Rp | + | 817.5923 | 13.08 | | | (840.5816, 1568.96)(841.5754, 1459.82)(842.5683, 2072.84)(818.6043, 14823.06)(819.6081, 7957.08)(820.6199, 11992.83)(821.6232, 6012.43)(822.6184, 2472.6) | 127646.8 | 75733.08 | 155878.7 | 123501.3 | 117600.4 | 62409.39 | 116982.2 | 68722.24 | 0.36 | 0.208391 | 0.299487 | -0.30 | 0.376378 | 0.678626 | |
| COMPOUND_817_598a12_667346 | Rp | + | 817.5980 | 12.67 | PC 40_7e | 2 | 10 eV: 818.6086(100), 184.0724(10), 502.3357(1) | (840.5851, 7936.13)(841.5869, 4265.08)(842.5741, 2009.46)(843.5812, 676.51)(818.608, 122063.43)(819.6108, 64435.84)(820.6123, 19112.28)(821.6045, 4302.22) | 652747.7 | 226878 | 575437.3 | 209045.8 | 783495.5 | 235278.3 | 760750.8 | 242919.8 | 0.61 | 0.025702 | 0.049092 | 0.18 | 0.573735 | 0.790246 |
| COMPOUND_819_5134a12_24219 | Rp | + | 819.5134 | 12.24 | | | (427.7837, 357.27)(428.2786, 309.7)(839.5329, 1931.28)(840.0298, 1625.34)(840.5294, 1250.59)(841.0281, 704.03)(831.4783, 171.35)(831.9649, 53.2)(842.5225, 2863.64)(843.5278, 2600.92)(844.5256, 4563.04)(845.5268, 2124.48)(846.5354, 1851.63)(820.5281, 6279.9)(821.0386, 1596.34)(821.5325, 922.66)(822.0345, 6317.85)(822.5374, 6259.41)(848.0355, 929.94)(848.5354, 1117.34)(840.0343, 1094.44)(840.524, 1403.19)(841.0284, 793.53)(837.5374, 4914.91)(840.7641, 24008.21)(411.266, 11745.35)(411.7668, 3287.74)(412.2652, 1053.48) | 307153.6 | 59896.03 | 269892.2 | 68384.5 | 278439.6 | 342655.4 | 279469.7 | 62348.34 | -0.04 | 0.871118 | 0.91287 | 0.30 | 0.358907 | 0.666906 | |
| COMPOUND_819_5438a10_837796 | Rp | + | 819.5438 | 10.84 | | | (440.7478, 327.78)(441.2422, 2328.19)(441.7387, 1271.03)(442.7419, 554.38)(422.2438, 429.09)(422.7528, 1048.16)(820.5502, 131462.34)(821.5535, 65467.13)(822.5565, 77319.15)(823.569, 33049.17)(824.575, 27575.78)(410.78, 1395.63)(411.2857, 885.68)(411.7856, 653.44) | 1410195 | 518734.9 | 1246255 | 504508.3 | 1293648 | 784437 | 1244569 | 693224.8 | -1.11 | 1.7E-06 | 8.12E-06 | -0.02 | 0.938657 | 0.97184 | |
| COMPOUND_819_5542a12_535168 | Rp | - | 819.5542 | 12.54 | | | (818.5472, 44526.77)(819.5499, 22296.55)(820.5464, 18957.68) | 1150659 | 112495.5 | 1201137 | 96691.82 | 1239264 | 91913.75 | 1239531 | 104818.1 | 0.70 | 0.007909 | 0.017193 | -0.37 | 0.224636 | 0.532591 | |
| COMPOUND_819_56a11_121188 | Rp | - | 819.5600 | 11.12 | | | (818.5548, 342638.66)(819.5584, 155717.14)(820.5609, 42408.7)(821.5629, 8690.7)(864.5445, 1347.98)(865.5467, 792.57) | 497549.6 | 191774 | 575202 | 112793.9 | 202564.1 | 208299.5 | 211946.2 | 225662.1 | -1.20 | 6.28E-07 | 3.3E-06 | -0.22 | 0.396073 | 0.690408 | |
| COMPOUND_819_5614a11_190397 | Rp | - | 819.5614 | 11.19 | PC 16_0_HOHE | 1 | 10 eV: 818.553(100), 758.5311(30), 295.2285(2) | (818.5541, 486499.88)(819.5581, 223002.31)(820.5607, 60852.2)(821.5632, 12273.88)(822.5547, 2661.39)(823.5613, 415.56)(864.5429, 3760.12)(865.5448, 2054.21) | 5713077 | 1147957 | 6229103 | 1319915 | 1820508 | 2795350 | 1221215 | 2486766 | -1.07 | 1.71E-05 | 6.5E-05 | -0.38 | 0.172652 | 0.487735 |
| COMPOUND_819_576a12_380157 | Rp | + | 819.5760 | 12.38 | duplicate of PC39:6 | | | (837.5778, 2707.34)(838.5562, 1342.73)(820.585, 20964.87)(821.5884, 11389.41)(822.57, 1359.71)(823.5794, 559.05)(824.5749, 113.94) | 169275 | 91198.34 | 152177.7 | 50896.43 | 134631.3 | 59745.57 | 138665.7 | 72474.41 | -0.05 | 0.854374 | 0.89993 | 0.19 | 0.56113 | 0.783425 |
| COMPOUND_819_5786a12_398953 | Rp | + | 819.5786 | 12.40 | PC 39:6 | 2 | 20 eV: 820.5784(100), 184.0733(80), 504.2071(3) | (837.6058, 3373.15)(838.6215, 460.19)(820.5871, 27382.19)(821.59, 14504.56)(822.5843, 4407.46)(823.5811, 864.16) | 1713259 | 109568.7 | 141823.2 | 81779.93 | 115060.4 | 46807.93 | 133020.9 | 89624.22 | -0.55 | 0.039457 | 0.071314 | 0.46 | 0.139873 | 0.444883 |
| COMPOUND_819_5932a9_808102 | Rp | + | 819.5932 | 9.81 | | | (421.7983, 1292.42)(422.3047, 1260.47)(422.7952, 263.07)(419.3181, 18867.05)(419.8197, 8572.4)(420.3231, 2373.12)(420.8243, 681.05)(820.6003, 20186.13)(821.6027, 9210.48)(822.6003, 2975.88)(823.5992, 870.38)(824.611, 223.92)(410.8057, | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--------------|--|--|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p | |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | | |
| COMPOUND_820_1584a9_309281 | Rp | - | 820.1584 | 9.31 | | | | (819.15, 765.701)(820.1528, 2254.58)(821.1484, 2557.89)(822.1491, 823.56)(823.164, 325.07)(865.1605, 527.23)(866.1573, 235.62)(867.1379, 371.69) (844.5394, 4440.38)(845.5405, 2220.07)(846.5408, 2351.7)(847.5402, 1426.23)(848.5477, 2464.96)(842.0408, 1031.99)(842.5245, 5029.74)(843.0363, 933.38)(843.7552, 447.54)(41.2611, 323.94)(431.7592, 1495.58)(839.5497, 2191.71)(840.0458, 1317.38)(840.5364, 2110.2)(841.0372, 2085.1)(841.5354, 2028.21)(842.0376, 1279.02)(842.5279, 5315.06)(843.0344, 1246.6)(843.5298, 3265.34)(822.5725, 12264.78)(823.5969, 2568.53)(824.5559, 4402.94)(825.5563, 2270.38)(411.7714, 7715.57)(412.2717, 4039.48)(412.7791, 8196.72)(413.2809, 3790.25)(413.7701, 343.19) | 62871.87 | 11228.62 | 63520.26 | 9549.255 | 60350.57 | 12383.98 | 60667.67 | 12061.02 | -0.25 | 0.400789 | 0.504797 | -0.04 | 0.91513 | 0.961085 | |
| COMPOUND_821_5294a12_543394 | Rp | + | 821.5294 | 12.54 | | | | (820.5624, 33251.39)(821.5654, 17312.54)(822.5618, 14973.74) (857.5178, 4967.62)(821.5492, 10338.53)(822.5533, 3570.35)(823.5603, 1200.38) (849.4222, 419.489)(849.4166, 318.51)(850.4338, 675.19)(843.4623, 443.3)(826.4261, 3836.98)(827.4297, 1965.65)(828.4369, 8579.11)(829.44, 4086.98)(830.4378, 5262.95)(831.4406, 2051.55)(832.4374, 1400.55)(833.4368, 463.36) (824.5211, 16338.22)(825.524, 7392.56)(826.5218, 7675.22)(827.5253, 3176.62)(828.537, 2884.79) (824.5441, 228025.05)(825.5474, 106831.27)(826.5574, 107511.66)(827.5617, 44390.11)(828.5659, 13004.87)(829.569, 3202.28) (849.4222, 2139.84)(844.1776, 1193.58)(827.1835, 7132.12)(828.1696, 3377.31)(829.1597, 1584.6) (839.528, 3096.71)(840.0272, 2029.85)(840.5214, 2397.47)(858.4855, 3103.39)(859.0066, 792.81)(855.9923, 368.03)(856.4876, 5352.73)(857.0101, 883.0)(848.0447, 1358.4)(848.538, 1450.94)(849.0408, 7676.29)(828.553, 112791.29)(829.5557, 56788.36)(830.5596, 17082.13)(831.5609, 4747.28)(414.7762, 3397.04)(415.2772, 2404.72)(415.7748, 1253.51)(416.2737, 358.89)(416.7612, 86.22) (826.5591, 886736.75)(827.5662, 427021.16)(828.5662, 114750.37)(829.5687, 23190.27)(830.5722, 4432.67)(831.5744, 874.55) (826.5597, 391094.9)(827.5633, 183340.25)(828.5659, 50689.39)(829.5689, 10737.18)(830.5729, 2492.89)(831.584, 463.74) (826.5961, 78262.14)(827.599, 38688.81)(828.602, 11490.13)(829.6045, 2499.39) (850.5962, 57091.14)(851.5994, 29618.08)(852.6096, 27148.98)(828.612, 87676.74)(829.6155, 38502.21)(830.6187, 13892.97)(831.6204, 3662.94) (852.5488, 4795.12)(853.5515, 2601.85)(854.5703, 39661.95)(830.5711, 24834.12)(831.5748, 12920.52)(832.5783, 4242.53)(833.5774, 1301.65)(834.5717, 226.13) | 70566.56 | 159014.7 | 679612.6 | 119280.1 | 808118.7 | 282751.5 | 897225.9 | 333028.4 | 0.59 | 0.022539 | 0.043718 | -0.25 | 0.398797 | 0.690408 | |
| COMPOUND_821_5692a13_040231 | Rp | - | 821.5692 | 13.04 | PC 18_0_18_2 | 1 | 10 | ev: 820.5637(100), 417.1003(5) | (820.5624, 33251.39)(821.5654, 17312.54)(822.5618, 14973.74) (857.5178, 4967.62)(821.5492, 10338.53)(822.5533, 3570.35)(823.5603, 1200.38) (849.4222, 419.489)(849.4166, 318.51)(850.4338, 675.19)(843.4623, 443.3)(826.4261, 3836.98)(827.4297, 1965.65)(828.4369, 8579.11)(829.44, 4086.98)(830.4378, 5262.95)(831.4406, 2051.55)(832.4374, 1400.55)(833.4368, 463.36) (824.5211, 16338.22)(825.524, 7392.56)(826.5218, 7675.22)(827.5253, 3176.62)(828.537, 2884.79) (824.5441, 228025.05)(825.5474, 106831.27)(826.5574, 107511.66)(827.5617, 44390.11)(828.5659, 13004.87)(829.569, 3202.28) (849.4222, 2139.84)(844.1776, 1193.58)(827.1835, 7132.12)(828.1696, 3377.31)(829.1597, 1584.6) (839.528, 3096.71)(840.0272, 2029.85)(840.5214, 2397.47)(858.4855, 3103.39)(859.0066, 792.81)(855.9923, 368.03)(856.4876, 5352.73)(857.0101, 883.0)(848.0447, 1358.4)(848.538, 1450.94)(849.0408, 7676.29)(828.553, 112791.29)(829.5557, 56788.36)(830.5596, 17082.13)(831.5609, 4747.28)(414.7762, 3397.04)(415.2772, 2404.72)(415.7748, 1253.51)(416.2737, 358.89)(416.7612, 86.22) (826.5591, 886736.75)(827.5662, 427021.16)(828.5662, 114750.37)(829.5687, 23190.27)(830.5722, 4432.67)(831.5744, 874.55) (826.5597, 391094.9)(827.5633, 183340.25)(828.5659, 50689.39)(829.5689, 10737.18)(830.5729, 2492.89)(831.584, 463.74) (826.5961, 78262.14)(827.599, 38688.81)(828.602, 11490.13)(829.6045, 2499.39) (850.5962, 57091.14)(851.5994, 29618.08)(852.6096, 27148.98)(828.612, 87676.74)(829.6155, 38502.21)(830.6187, 13892.97)(831.6204, 3662.94) (852.5488, 4795.12)(853.5515, 2601.85)(854.5703, 39661.95)(830.5711, 24834.12)(831.5748, 12920.52)(832.5783, 4242.53)(833.5774, 1301.65)(834.5717, 226.13) | 1269711 | 192797.5 | 1386168 | 202340.3 | 1336690 | 136252.5 | 1282157 | 202150.6 | 0.18 | 0.512159 | 0.612524 | -0.72 | 0.028912 | 0.231966 |
| COMPOUND_822_5555a12_53386 | Rp | - | 822.5555 | 12.53 | | | | (820.5624, 33251.39)(821.5654, 17312.54)(822.5618, 14973.74) (857.5178, 4967.62)(821.5492, 10338.53)(822.5533, 3570.35)(823.5603, 1200.38) (849.4222, 419.489)(849.4166, 318.51)(850.4338, 675.19)(843.4623, 443.3)(826.4261, 3836.98)(827.4297, 1965.65)(828.4369, 8579.11)(829.44, 4086.98)(830.4378, 5262.95)(831.4406, 2051.55)(832.4374, 1400.55)(833.4368, 463.36) (824.5211, 16338.22)(825.524, 7392.56)(826.5218, 7675.22)(827.5253, 3176.62)(828.537, 2884.79) (824.5441, 228025.05)(825.5474, 106831.27)(826.5574, 107511.66)(827.5617, 44390.11)(828.5659, 13004.87)(829.569, 3202.28) (849.4222, 2139.84)(844.1776, 1193.58)(827.1835, 7132.12)(828.1696, 3377.31)(829.1597, 1584.6) (839.528, 3096.71)(840.0272, 2029.85)(840.5214, 2397.47)(858.4855, 3103.39)(859.0066, 792.81)(855.9923, 368.03)(856.4876, 5352.73)(857.0101, 883.0)(848.0447, 1358.4)(848.538, 1450.94)(849.0408, 7676.29)(828.553, 112791.29)(829.5557, 56788.36)(830.5596, 17082.13)(831.5609, 4747.28)(414.7762, 3397.04)(415.2772, 2404.72)(415.7748, 1253.51)(416.2737, 358.89)(416.7612, 86.22) (826.5591, 886736.75)(827.5662, 427021.16)(828.5662, 114750.37)(829.5687, 23190.27)(830.5722, 4432.67)(831.5744, 874.55) (826.5597, 391094.9)(827.5633, 183340.25)(828.5659, 50689.39)(829.5689, 10737.18)(830.5729, 2492.89)(831.584, 463.74) (826.5961, 78262.14)(827.599, 38688.81)(828.602, 11490.13)(829.6045, 2499.39) (850.5962, 57091.14)(851.5994, 29618.08)(852.6096, 27148.98)(828.612, 87676.74)(829.6155, 38502.21)(830.6187, 13892.97)(831.6204, 3662.94) (852.5488, 4795.12)(853.5515, 2601.85)(854.5703, 39661.95)(830.5711, 24834.12)(831.5748, 12920.52)(832.5783, 4242.53)(833.5774, 1301.65)(834.5717, 226.13) | 114688.6 | 24000.92 | 108972.9 | 21582.47 | 106437.9 | 23138.39 | 110779.3 | 20829.33 | -0.41 | 0.138175 | 0.213422 | 0.47 | 0.147713 | 0.456493 | |
| COMPOUND_825_4188a0_89871585 | Hilic | + | 825.4188 | 0.90 | | | | (820.5624, 33251.39)(821.5654, 17312.54)(822.5618, 14973.74) (857.5178, 4967.62)(821.5492, 10338.53)(822.5533, 3570.35)(823.5603, 1200.38) (849.4222, 419.489)(849.4166, 318.51)(850.4338, 675.19)(843.4623, 443.3)(826.4261, 3836.98)(827.4297, 1965.65)(828.4369, 8579.11)(829.44, 4086.98)(830.4378, 5262.95)(831.4406, 2051.55)(832.4374, 1400.55)(833.4368, 463.36) (824.5211, 16338.22)(825.524, 7392.56)(826.5218, 7675.22)(827.5253, 3176.62)(828.537, 2884.79) (824.5441, 228025.05)(825.5474, 106831.27)(826.5574, 107511.66)(827.5617, 44390.11)(828.5659, 13004.87)(829.569, 3202.28) (849.4222, 2139.84)(844.1776, 1193.58)(827.1835, 7132.12)(828.1696, 3377.31)(829.1597, 1584.6) (839.528, 3096.71)(840.0272, 2029.85)(840.5214, 2397.47)(858.4855, 3103.39)(859.0066, 792.81)(855.9923, 368.03)(856.4876, 5352.73)(857.0101, 883.0)(848.0447, 1358.4)(848.538, 1450.94)(849.0408, 7676.29)(828.553, 112791.29)(829.5557, 56788.36)(830.5596, 17082.13)(831.5609, 4747.28)(414.7762, 3397.04)(415.2772, 2404.72)(415.7748, 1253.51)(416.2737, 358.89)(416.7612, 86.22) (826.5591, 886736.75)(827.5662, 427021.16)(828.5662, 114750.37)(829.5687, 23190.27)(830.5722, 4432.67)(831.5744, 874.55) (826.5597, 391094.9)(827.5633, 183340.25)(828.5659, 50689.39)(829.5689, 10737.18)(830.5729, 2492.89)(831.584, 463.74) (826.5961, 78262.14)(827.599, 38688.81)(828.602, 11490.13)(829.6045, 2499.39) (850.5962, 57091.14)(851.5994, 29618.08)(852.6096, 27148.98)(828.612, 87676.74)(829.6155, 38502.21)(830.6187, 13892.97)(831.6204, 3662.94) (852.5488, 4795.12)(853.5515, 2601.85)(854.5703, 39661.95)(830.5711, 24834.12)(831.5748, 12920.52)(832.5783, 4242.53)(833.5774, 1301.65)(834.5717, 226.13) | 63475.85 | 18972.29 | 64877.73 | 20669.54 | 100021.5 | 20665.55 | 108449.5 | 22771.76 | 0.94 | 9.73E-05 | 0.000301 | 0.50 | 0.065663 | 0.309933 | |
| COMPOUND_825_5297a11_150297 | Rp | - | 825.5297 | 11.15 | | | | (820.5624, 33251.39)(821.5654, 17312.54)(822.5618, 14973.74) (857.5178, 4967.62)(821.5492, 10338.53)(822.5533, 3570.35)(823.5603, 1200.38) (849.4222, 419.489)(849.4166, 318.51)(850.4338, 675.19)(843.4623, 443.3)(826.4261, 3836.98)(827.4297, 1965.65)(828.4369, 8579.11)(829.44, 4086.98)(830.4378, 5262.95)(831.4406, 2051.55)(832.4374, 1400.55)(833.4368, 463.36) (824.5211, 16338.22)(825.524, 7392.56)(826.5218, 7675.22)(827.5253, 3176.62)(828.537, 2884.79) (824.5441, 228025.05)(825.5474, 106831.27)(826.5574, 107511.66)(827.5617, 44390.11)(828.5659, 13004.87)(829.569, 3202.28) (849.4222, 2139.84)(844.1776, 1193.58)(827.1835, 7132.12)(828.1696, 3377.31)(829.1597, 1584.6) (839.528, 3096.71)(840.0272, 2029.85)(840.5214, 2397.47)(858.4855, 3103.39)(859.0066, 792.81)(855.9923, 368.03)(856.4876, 5352.73)(857.0101, 883.0)(848.0447, 1358.4)(848.538, 1450.94)(849.0408, 7676.29)(828.553, 112791.29)(829.5557, 56788.36)(830.5596, 17082.13)(831.5609, 4747.28)(414.7762, 3397.04)(415.2772, 2404.72)(415.7748, 1253.51)(416.2737, 358.89)(416.7612, 86.22) (826.5591, 886736.75)(827.5662, 427021.16)(828.5662, 114750.37)(829.5687, 23190.27)(830.5722, 4432.67)(831.5744, 874.55) (826.5597, 391094.9)(827.5633, 183340.25)(828.5659, 50689.39)(829.5689, 10737.18)(830.5729, 2492.89)(831.584, 463.74) (826.5961, 78262.14)(827.599, 38688.81)(828.602, 11490.13)(829.6045, 2499.39) (850.5962, 57091.14)(851.5994, 29618.08)(852.6096, 27148.98)(828.612, 87676.74)(829.6155, 38502.21)(830.6187, 13892.97)(831.6204, 3662.94) (852.5488, 4795.12)(853.5515, 2601.85)(854.5703, 39661.95)(830.5711, 24834.12)(831.5748, 12920.52)(832.5783, 4242.53)(833.5774, 1301.65)(834.5717, 226.13) | 209193.6 | 48752.43 | 211711.1 | 56470.52 | 180064.5 | 7149.557 | 156932.9 | 43793.38 | -1.22 | 1.61E-08 | 1.26E-07 | -0.14 | 0.543395 | 0.776977 | |
| COMPOUND_825_5297a12_011763 | Rp | - | 825.5297 | 12.01 | PC 16_1_20_4 | 1 | 20 | ev: 764.5209(100), 824.5395(37), 44.9981(11), 303.2318(5) | (820.5624, 33251.39)(821.5654, 17312.54)(822.5618, 14973.74) (857.5178, 4967.62)(821.5492, 10338.53)(822.5533, 3570.35)(823.5603, 1200.38) (849.4222, 419.489)(849.4166, 318.51)(850.4338, 675.19)(843.4623, 443.3)(826.4261, 3836.98)(827.4297, 1965.65)(828.4369, 8579.11)(829.44, 4086.98)(830.4378, 5262.95)(831.4406, 2051.55)(832.4374, 1400.55)(833.4368, 463.36) (824.5211, 16338.22)(825.524, 7392.56)(826.5218, 7675.22)(827.5253, 3176.62)(828.537, 2884.79) (824.5441, 228025.05)(825.5474, 106831.27)(826.5574, 107511.66)(827.5617, 44390.11)(828.5659, 13004.87)(829.569, 3202.28) (849.4222, 2139.84)(844.1776, 1193.58)(827.1835, 7132.12)(828.1696, 3377.31)(829.1597, 1584.6) (839.528, 3096.71)(840.0272, 2029.85)(840.5214, 2397.47)(858.4855, 3103.39)(859.0066, 792.81)(855.9923, 368.03)(856.4876, 5352.73)(857.0101, 883.0)(848.0447, 1358.4)(848.538, 1450.94)(849.0408, 7676.29)(828.553, 112791.29)(829.5557, 56788.36)(830.5596, 17082.13)(831.5609, 4747.28)(414.7762, 3397.04)(415.2772, 2404.72)(415.7748, 1253.51)(416.2737, 358.89)(416.7612, 86.22) (826.5591, 886736.75)(827.5662, 427021.16)(828.5662, 114750.37)(829.5687, 23190.27)(830.5722, 4432.67)(831.5744, 874.55) (826.5597, 391094.9)(827.5633, 183340.25)(828.5659, 50689.39)(829.5689, 10737.18)(830.5729, 2492.89)(831.584, 463.74) (826.5961, 78262.14)(827.599, 38688.81)(828.602, 11490.13)(829.6045, 2499.39) (850.5962, 57091.14)(851.5994, 29618.08)(852.6096, 27148.98)(828.612, 87676.74)(829.6155, 38502.21)(830.6187, 13892.97)(831.6204, 3662.94) (852.5488, 4795.12)(853.5515, 2601.85)(854.5703, 39661 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|----------------|----------|--|---|---------------|----------|---------------|-----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_837_5021a11_498895 | Rp | + | 837.5021 | 12.50 | | | | (430.757, 378.341)(431.2558, 315.41)(431.7586, 1534.73)(432.2617, 955.61)(419.7582, 6603.31)(420.2599, 3354.51)(420.7596, 1904.23)(421.2583, 569.11) | 183900 | 28540.84 | 176756 | 28562.75 | 212161 | 28944.67 | 210302.6 | 34922.67 | 0.80 | 0.002689 | 0.006491 | 0.19 | 0.520208 | 0.764408 |
| COMPOUND_837_5506a11_985389 | Rp | - | 837.5506 | 11.99 | | | | (950.5295, 476.07)(836.5437, 32130.73)(837.5472, 16858.51)(838.5454, 5644.38)(839.544, 1688.51) | 187957.2 | 57487.78 | 181838.8 | 66687.74 | 215062.4 | 95351.38 | 195125.8 | 65290.21 | 0.29 | 0.291381 | 0.390822 | -0.08 | 0.790424 | 0.91097 |
| COMPOUND_837_5549a10_855005 | Rp | + | 837.5549 | 10.86 | | | | (860.5452, 132054.03)(861.5478, 64274.79)(862.5573, 64692.66)(863.5613, 27184.33)(864.5748, 39702.54)(865.5789, 19612.3)(866.5769, 15403.27)(838.5626, 280632.5)(839.5661, 133280.89)(840.5756, 145597.3)(841.579, 61393.86)(842.5838, 45433.48)(843.5856, 18807.21)(419.777, 1082.0)(420.2814, 683.58) | 6645907 | 2064785 | 6251599 | 2260206 | 4679524 | 3999423 | 5598147 | 3503666 | -1.08 | 3.43E-06 | 1.51E-05 | -0.10 | 0.69873 | 0.862515 |
| COMPOUND_837_5621a11_493071 | Rp | - | 837.5621 | 11.49 | | | | (836.5553, 7866.89)(837.5599, 3619.13)(838.5559, 3658.61)(839.5577, 1414.14)(840.5475, 2648.39)(882.5559, 3599.92)(883.5505, 2255.0)(884.5615, 12080.28)(885.5649, 6469.42) | 212199.6 | 138130.9 | 242615.3 | 148099.2 | 319164.7 | 63394.92 | 306739.9 | 108163.1 | -0.63 | 0.007618 | 0.016607 | -0.22 | 0.434776 | 0.712127 |
| COMPOUND_837_5871a12_651116 | Rp | - | 837.5871 | 12.65 | | | | (872.5635, 3500.71)(873.5758, 1408.05)(874.5836, 478.82)(950.5019, 2205.05)(951.5125, 1257.66)(952.516, 1636.76)(836.5801, 53792.73)(837.5834, 28835.99)(838.5867, 9286.66)(839.5895, 2365.0)(882.5732, 1362.22)(883.5616, 375.86) | 438520.9 | 125731.6 | 424145.9 | 136751.4 | 426574.9 | 123716.7 | 427441.6 | 109523.4 | -0.02 | 0.938265 | 0.960006 | 0.27 | 0.421538 | 0.702667 |
| COMPOUND_839_5174a12_975627 | Rp | + | 839.5174 | 12.98 | | | | (840.5051, 237.58)(420.7655, 7106.43)(421.2671, 3835.82)(421.7676, 1799.18)(422.27, 644.58) | 154742 | 23972.77 | 158831.8 | 32957.39 | 167772.3 | 20600.12 | 156592.4 | 24895.52 | 0.47 | 0.104869 | 0.169781 | -0.53 | 0.128704 | 0.425125 |
| COMPOUND_839_6025a12_830119 | Rp | - | 839.6025 | 12.83 | | | | (874.5696, 6198.27)(875.5703, 1499.08)(876.579, 559.74)(838.5958, 63200.59)(839.5992, 31762.14)(840.6005, 9558.31)(841.6001, 2294.57) | 891316.5 | 186112.4 | 877433.1 | 204628.5 | 865890.8 | 146327.7 | 774753.7 | 166041.7 | -0.12 | 0.658034 | 0.745794 | -0.41 | 0.190426 | 0.505078 |
| COMPOUND_840_6351a0_8306668 | Hilic | + | 840.6351 | 0.83 | | | | (293.6162, 3292.77)(864.6185, 498.54)(865.635, 2115.41)(858.6744, 742.72)(841.643, 896.79)(842.6451, 15601.36)(843.6582, 37235.21)(844.6608, 20379.7)(845.6679, 9049.09)(846.6715, 4129.02)(847.676, 1466.55) | 219159.8 | 118464.4 | 239060.9 | 143443.8 | 92929.8 | 64385.88 | 73186.63 | 55353.65 | -1.31 | 3.53E-10 | 4.47E-09 | -0.21 | 0.326174 | 0.633587 |
| COMPOUND_841_5387a12_21047 | Rp | - | 841.5387 | 12.21 | | | | (840.5316, 12929.77)(841.5375, 6490.76)(842.5357, 7739.24)(843.5399, 3689.78)(844.5365, 6498.16) | 425455.4 | 63257.31 | 416863.8 | 66969.13 | 395830.9 | 53671.69 | 363245.4 | 77089.9 | -0.45 | 0.083714 | 0.138825 | -0.25 | 0.40105 | 0.690408 |
| COMPOUND_841_5463a11_111553 | Rp | - | 841.5463 | 11.11 | | | | (840.5399, 157625.58)(841.5422, 75717.93)(842.5533, 118932.28)(843.5573, 51879.09)(844.5641, 24727.83) | 1435265 | 461075.3 | 1525346 | 469578.2 | 1590718 | 248183 | 1615442 | 390554.8 | -1.05 | 2.68E-06 | 1.21E-05 | -0.16 | 0.499897 | 0.753664 |
| COMPOUND_841_5824a12_602464 | Rp | - | 841.5824 | 12.60 | | | | (876.5722, 2181.46)(877.5757, 1155.11)(840.5744, 14422.15)(841.5776, 7199.01)(842.555, 7566.97)(843.5606, 4208.61) | 211307.7 | 79084.89 | 215800.5 | 91977 | 138492.1 | 49490.64 | 160872.1 | 42889.67 | -0.67 | 0.012657 | 0.026173 | -0.21 | 0.507669 | 0.75635 |
| COMPOUND_843_5089a12_177403 | Rp | + | 843.5089 | 12.18 | | | | (863.4988, 5635.0)(864.0132, 1165.49)(864.5028, 3661.96)(865.016, 821.09)(865.5057, 1612.18)(866.0142, 963.7)(855.5065, 2049.25)(856.0202, 1539.72)(853.0107, 805.85)(853.5202, 1200.96)(871.9999, 755.59)(872.4751, 2236.88)(861.5061, 1588.66)(862.009, 1151.41)(844.5215, 4802.28)(845.523, 2743.51)(846.5205, 2144.41)(847.4984, 666.76)(422.7646, 22262.95)(423.2667, 11277.59)(423.7682, 3952.95)(424.2689, 1085.11) | 262062.5 | 71253.53 | 280847.1 | 92031.44 | 292927.4 | 94027.72 | 265440.9 | 84790.3 | 0.36 | 0.223561 | 0.31724 | -0.67 | 0.056798 | 0.296083 |
| COMPOUND_843_5233a11_918069 | Rp | - | 843.5233 | 11.92 | | | | (956.4877, 1858.02)(957.4897, 1111.55)(958.4861, 1222.69)(959.4784, 992.84)(878.4758, 119269.9) | 42689.53 | 141762 | 47272.44 | 197370.5 | 59157.61 | 187565.4 | 62760.25 | 1.38 | 5.71E-08 | 3.85E-07 | -0.52 | 0.048035 | 0.279822 | |
| COMPOUND_843_5448a11_193773 | Rp | + | 843.5448 | 11.19 | | | | (842.5161, 15421.51)(843.5192, 6976.63)(844.5374, 2930.06)(845.5176, 654.3)(846.5348, 109.97)(888.5141, 3554.3)(889.5136, 2223.36) | 896802.4 | 284914.7 | 818996.3 | 339878.6 | 865036 | 504626.8 | 1000700 | 591399.9 | -0.57 | 0.016603 | 0.033474 | -0.10 | 0.727753 | 0.883503 |
| COMPOUND_843_5544a12_41593 | Rp | - | 843.5544 | 12.42 | | | | (842.5464, 9807.26)(843.5487, 5000.24)(844.544, 5153.56)(845.5468, 2251.03) | 77755.66 | 27096.7 | 64867.83 | 172722.65 | 73814.79 | 2576.69 | 80605.2 | 23209.89 | 0.19 | 0.476484 | 0.580023 | 0.77 | 0.018669 | 0.196411 |
| COMPOUND_843_5617a12_3645315 | Rp | - | 843.5617 | 11.36 | | | | (30952.59)(846.586, 242580.2)(847.5893, 114349.02)(848.5918, 32012.82)(849.5938, 7254.95) | 2364827 | 1714728 | 2602692 | 1466770 | 1856893 | 2964121 | 1221505 | 2468429 | -0.52 | 0.031068 | 0.058111 | -0.20 | 0.467769 | 0.734042 |
| COMPOUND_843_5637a11_075828 | Rp | - | 843.5637 | 11.08 | PC 17_0_20.4 | 1 | 20 eV: 782.533(100), 842.555(37), 295.2257(6) | (878.5656, 9810.22)(879.5692, 4210.36)(880.5415, 5152.79)(881.5398, 2400.51)(842.5532, 87912.63)(843.5568, 40084.68)(844.5634, 17794.39)(845.5676, 5789.32)(846.5649, 930.11) | 887995.9 | 306850.2 | 999519 | 303545.7 | 410953 | 378851.7 | 351502.2 | 427210.8 | -1.24 | 2.49E-08 | 1.85E-07 | -0.23 | 0.31531 | 0.621785 |
| COMPOUND_843_5976a12_88655 | Rp | - | 843.5976 | 12.89 | | | | (956.6061, 212.42)(957.5932, 206.83)(842.5908, 12985.37)(843.5935, 6415.49)(888.61, 1626.03)(889.6127, 1031.0)(890.6145, 387.86) | 114461.6 | 24417.07 | 113635.3 | 34409.66 | 100680.4 | 21592.73 | 104962 | 22457.79 | -0.41 | 0.169042 | 0.252441 | 0.27 | 0.446567 | 0.72091 |
| COMPOUND_845_5402a12_228107 | Rp | - | 845.5402 | 12.23 | | | | (844.5321, 18620.79)(845.5348, 8395.05)(846.5389, 2444.2)(847.5447, 753.99)(890.5245, 1725.29)(891.5266, 1135.33) | 76498.16 | 25772 | 8635.26 | 38296.54 | 88700.57 | 31409.08 | 104533.6 | 38635.38 | 0.46 | 0.101508 | 0.164813 | 0.14 | 0.681416 | 0.853001 |
| COMPOUND_845_5697a12_936705 | Rp | - | 845.5697 | 12.94 | | | | (844.5631, 7445.44)(845.5668, 3775.37)(846.5662, 4609.89)(847.5712, 2688.53)(848.5768, 1410.37)(849.5802, 603.36) | 313308.2 | 30298.72 | 112098.3 | 25321.01 | 118864 | 19898.31 | 126667.8 | 24244.14 | 0.14 | 0.629375 | 0.7202 | 0.43 | 0.205213 | 0.516497 |
| COMPOUND_845_57a12_689569 | Rp | - | 845.5700 | 12.69 | | | | (844.564, 11263.72)(845.5654, 6217.92)(846.5549, 9120.13)(847.5569, 4275.37)(848.5712, 2135.95)(849.5786, 888.01) | 38608.53 | 9259.682 | 36617.13 | 10885.88 | 38887.54 | 5501.294 | 39507.42 | 12177.07 | -0.18 | 0.553542 | 0.651294 | 0.43 | 0.232813 | 0.538289 |
| COMPOUND_847_1737a9_568081 | Rp | - | 847.1737 | 9.57 | | | | (960.1473, 594.48)(846.1685, 3284.04)(847.1741, 1544.67)(848.1782, 413.6)(892.1787, 744.53) | 386805.8 | 141493.1 | 392426.2 | 120748.8 | 363507.8 | 91220.24 | 397294.4 | 116410.3 | 0.09 | 0.746612 | 0.815803 | -0.10 | 0.739796 | 0.888787 |
| COMPOUND_847_5844a13_380447 | Rp | - | 847.5844 | 13.38 | | | | (882.5545, 6499.76)(846.586, 403208.3)(847.5896, 193135.11)(848.5921, 5620.31)(849.5948, 12015.87)(850.5769, 2989.23) | 2565134 | 902716.9 | 2870553 | 987657.1 | 1011715 | 1117313 | 663626.2 | 1008531 | -1.28 | 1.04E-08 | 8.59E-08 | -0.26 | 0.259107 | 0.570391 |
| COMPOUND_847_5929a11_493024 | Rp | - | 847.5929 | 11.49 | PC 18_0_H0DE | 1 | 10 eV: 846.5862(100), 786.563(25), 131.4722(2) | (870.587, 475.49)(871.0964, 253.23)(871.6019, 574.58)(870.5927, 152.96)(871.5695, 764.35)(878.5903, 648.24)(879.1041, 620.9)(879.6055, 956.07)(876.1117, 351.67)(876.6233, 481.89)(868.0923, 429.12)(868.586, 372.96)(886.6066, 558.98)(887.1143, 582.67)(887.6152, 3988.65)(835.4108, 286.84)(436.2919, 979.27)(436.8019, 100.77)(437.2975, 375.52)(433.3343, 8486.05)(433.8353, 2929.59)(434.337, 1038.59)(434.8275, 223.24)(452.2833, 528.26)(452.7917, 60.96)(453.2985, 1259.7)(444.3312, 852.87)(444.8238, 50.13)(445.3252, 531.3)(848.6306, 6752.53)(849.6337, 3269.59)(850.6051, 3420.3)(851.5964, 1871.53)(424.821, 2170.1)(425.3216, 1138.25)(425.825, 555.55) | 158331 | 58580 | 131501.9 | 38648.28 | 154732.2 | 30778.03 | 150978.2 | 50752.83 | -0.03 | 0.906257 | 0.938328 | 0.53 | 0.134658 | 0.43508 |
| COMPOUND_847_6225a10_199461 | Rp | + | 847.6225 | 10.20 | | | | (870.587, 475.49)(871.0964, 253.23)(871.6019, 574.58)(870.5927, 152.96)(871.5695, 764.35)(878.5903, 648.24)(879.1041, 620.9)(879.6055, 956.07)(876.1117, 351.67)(876.6233, 481.89)(868.0923, 429.12)(868.586, 372.96)(886.6066, 558.98)(887.1143, 582.67)(887.6152, 3988.65)(835.4108, 286.84)(436.2919, 979.27)(436.8019, 100.77)(437.2975, 375.52)(433.3343, 8486.05)(433.8353, 2929.59)(434.337, 1038.59)(434.8275, 223.24)(452.2833, 528.26)(452.7917, 60.96)(453.2985, 1259.7)(444.3312, 852.87)(444.8238, 50.13)(445.3252, 531.3)(848.6306, 6752.53)(849.6337, 3269.59)(850.6051, 3420.3)(851.5964, 1871.53)(424.821, 2170.1)(425.3216, 1138.25)(425.825, 555.55) | 657891.2 | 285796.8 | 752723 | 276179.8 | 911857.2 | 362546.9 | 990408.4 | 295063.8 | 0.67 | 0.007661 | 0.016685 | -0.03 | 0.907398 | 0.958319 |
| COMPOUND_849_5531a11_884156 | Rp | - | 849.5531 | 11.88 | | | | (962.5049, 2142.81)(963.5114, 1418.6)(848.5441, 57258.01)(849.5472, 29906.15)(850.5572, 36012.08)(851.5617, 16036.13)(852.5655, 4917.92)(894.559, 7134.01) | 963155.8 | 514470.2 | 1023460 | 443831.7 | 806899.3 | 561867.9 | 939969 | 331245.8 | -1.09 | 1.15E-06 | 5.64E-06 | -0.20 | 0.397464 | 0.690408 |
| COMPOUND_849_5893a11_479956 | Rp | + | 849.5893 | 11.48 | | | | (872.5779, 12642.25)(873.5809, 6947.27)(874.5873, 7394.11)(875.5905, 3850.51)(888.567, 6910.1 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|---------------------|----------|--|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|-----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_853_1224a9_243353 | Rp | - | 853.1224 | 9.24 | | | | (888.0863, 257.88) (889.0962, 290.25) (890.0971, 98.64) (852.1149, 117.10.53) (853.1143, 3143.33) (854.1184, 671.04) (855.1392, 129.9) (876.5483, 5511.58) (877.5547, 3105.33) (878.5661, 3196.29) (879.5709, 1776.32) (854.5707, 50089.09) (855.5741, 27265.34) (856.5764, 8257.41) (857.5795, 1935.89) (858.5912, 519.67) (852.5613, 36155.73) (853.5644, 17475.78) (854.5664, 5787.77) (855.5674, 1374.1) (852.5756, 18297.38) (853.5787, 93563.52) (854.5813, 27139.1) (855.5841, 6024.84) (856.5859, 1389.09) (857.5958, 256.71) (852.5753, 385136.03) (853.5789, 194315.25) (854.5817, 55112.57) (855.5838, 11677.96) (856.5848, 2346.59) (857.5844, 412.47) (966.5678, 359.82) (967.5604, 2713.36) (968.5703, 1536.22) (888.5882, 2683.45) (852.65, 23592.36) (853.6534, 18394.81) (854.6559, 5698.44) (855.6583, 1990.65) (856.6652, 373.99) (898.6794, 637.37) (899.6781, 3525.79) (878.471, 7446.8) (879.4713, 6944.16) (878.5007, 5725.57) (874.4921, 4060.42) (875.493, 3434.38) (856.4843, 6461.08) (857.4902, 3517.68) (858.4861, 3529.13) (859.4933, 2125.74) (860.4888, 2277.36) (428.7468, 89.15) (429.2323, 71.21) (429.7465, 539.79) | 56583.87 | 11129.95 | 62383.15 | 11670.84 | 54252.57 | 9922.074 | 53810.68 | 9888.124 | -0.20 | 0.481825 | 0.583999 | -0.50 | 0.150267 | 0.460409 |
| COMPOUND_853_5644a11_888902 | Rp | + | 853.5644 | 11.89 | PC 42:10 | 2 | 10 eV: 854.5741(100), 184.0707(15), 308.9499(5) | (878.471, 7446.8) (879.4713, 6944.16) (878.5007, 5725.57) (874.4921, 4060.42) (875.493, 3434.38) (856.4843, 6461.08) (857.4902, 3517.68) (858.4861, 3529.13) (859.4933, 2125.74) (860.4888, 2277.36) (428.7468, 89.15) (429.2323, 71.21) (429.7465, 539.79) (878.551, 2808.02) (879.5238, 3138.55) (880.5135, 2122.49) (894.5348, 6062.56) (895.0384, 1684.35) (894.5311, 4920.75) (895.5354, 3061.72) (896.529, 3156.49) (897.5282, 2010.92) (898.5246, 2444.24) (899.5284, 15269.99) (851.5854, 7943.64) (858.5778, 3423.29) (859.586, 309.54) (428.7857, 600.43) (429.2877, 463.72) (429.7906, 498.34) (430.2922, 283.9) (878.5646, 1332.38) (879.5682, 812.49) (880.5853, 1366.04) (881.6067, 1181.81) (856.586, 16187.36) (857.5896, 9569.68) (858.5924, 2911.69) (859.5901, 924.66) | 112991.6 | 42104.23 | 101166.4 | 41463.25 | 250838 | 106989.9 | 284874.9 | 132818.7 | 1.34 | 2.91E-09 | 2.75E-08 | 0.17 | 0.459546 | 0.729315 |
| COMPOUND_853_5679a10_619556 | Rp | - | 853.5679 | 10.62 | | | | (852.5613, 36155.73) (853.5644, 17475.78) (854.5664, 5787.77) (855.5674, 1374.1) (852.5756, 18297.38) (853.5787, 93563.52) (854.5813, 27139.1) (855.5841, 6024.84) (856.5859, 1389.09) (857.5958, 256.71) (852.5753, 385136.03) (853.5789, 194315.25) (854.5817, 55112.57) (855.5838, 11677.96) (856.5848, 2346.59) (857.5844, 412.47) (966.5678, 359.82) (967.5604, 2713.36) (968.5703, 1536.22) (888.5882, 2683.45) (852.65, 23592.36) (853.6534, 18394.81) (854.6559, 5698.44) (855.6583, 1990.65) (856.6652, 373.99) (898.6794, 637.37) (899.6781, 3525.79) (878.471, 7446.8) (879.4713, 6944.16) (878.5007, 5725.57) (874.4921, 4060.42) (875.493, 3434.38) (856.4843, 6461.08) (857.4902, 3517.68) (858.4861, 3529.13) (859.4933, 2125.74) (860.4888, 2277.36) (428.7468, 89.15) (429.2323, 71.21) (429.7465, 539.79) | 104249.6 | 59975.47 | 124140.3 | 90262.18 | 61760.75 | 37317.29 | 45632 | 25008.38 | -0.81 | 0.00137 | 0.000414 | -0.56 | 0.021021 | 0.204049 |
| COMPOUND_853_5824a12_488253 | Rp | - | 853.5824 | 12.49 | | | | (852.5613, 36155.73) (853.5644, 17475.78) (854.5664, 5787.77) (855.5674, 1374.1) (852.5756, 18297.38) (853.5787, 93563.52) (854.5813, 27139.1) (855.5841, 6024.84) (856.5859, 1389.09) (857.5958, 256.71) (852.5753, 385136.03) (853.5789, 194315.25) (854.5817, 55112.57) (855.5838, 11677.96) (856.5848, 2346.59) (857.5844, 412.47) (966.5678, 359.82) (967.5604, 2713.36) (968.5703, 1536.22) (888.5882, 2683.45) (852.65, 23592.36) (853.6534, 18394.81) (854.6559, 5698.44) (855.6583, 1990.65) (856.6652, 373.99) (898.6794, 637.37) (899.6781, 3525.79) (878.471, 7446.8) (879.4713, 6944.16) (878.5007, 5725.57) (874.4921, 4060.42) (875.493, 3434.38) (856.4843, 6461.08) (857.4902, 3517.68) (858.4861, 3529.13) (859.4933, 2125.74) (860.4888, 2277.36) (428.7468, 89.15) (429.2323, 71.21) (429.7465, 539.79) | 2213187 | 706405.2 | 2191848 | 663083.7 | 1895173 | 347820 | 2096032 | 520902.9 | -0.46 | 0.191943 | 0.189485 | -0.26 | 0.045464 | 0.725699 |
| COMPOUND_853_5825a12_405809 | Rp | - | 853.5825 | 12.41 | | | | (852.5613, 36155.73) (853.5644, 17475.78) (854.5664, 5787.77) (855.5674, 1374.1) (852.5756, 18297.38) (853.5787, 93563.52) (854.5813, 27139.1) (855.5841, 6024.84) (856.5859, 1389.09) (857.5958, 256.71) (852.5753, 385136.03) (853.5789, 194315.25) (854.5817, 55112.57) (855.5838, 11677.96) (856.5848, 2346.59) (857.5844, 412.47) (966.5678, 359.82) (967.5604, 2713.36) (968.5703, 1536.22) (888.5882, 2683.45) (852.65, 23592.36) (853.6534, 18394.81) (854.6559, 5698.44) (855.6583, 1990.65) (856.6652, 373.99) (898.6794, 637.37) (899.6781, 3525.79) (878.471, 7446.8) (879.4713, 6944.16) (878.5007, 5725.57) (874.4921, 4060.42) (875.493, 3434.38) (856.4843, 6461.08) (857.4902, 3517.68) (858.4861, 3529.13) (859.4933, 2125.74) (860.4888, 2277.36) (428.7468, 89.15) (429.2323, 71.21) (429.7465, 539.79) | 2572910 | 638087.2 | 2350576 | 565459.7 | 2147142 | 408088.8 | 2354627 | 530459.8 | -0.60 | 0.022668 | 0.043932 | 0.66 | 0.029916 | 0.234557 |
| COMPOUND_853_6569a10_853576 | Rp | - | 853.6569 | 10.85 | | | | (852.5613, 36155.73) (853.5644, 17475.78) (854.5664, 5787.77) (855.5674, 1374.1) (852.5756, 18297.38) (853.5787, 93563.52) (854.5813, 27139.1) (855.5841, 6024.84) (856.5859, 1389.09) (857.5958, 256.71) (852.5753, 385136.03) (853.5789, 194315.25) (854.5817, 55112.57) (855.5838, 11677.96) (856.5848, 2346.59) (857.5844, 412.47) (966.5678, 359.82) (967.5604, 2713.36) (968.5703, 1536.22) (888.5882, 2683.45) (852.65, 23592.36) (853.6534, 18394.81) (854.6559, 5698.44) (855.6583, 1990.65) (856.6652, 373.99) (898.6794, 637.37) (899.6781, 3525.79) (878.471, 7446.8) (879.4713, 6944.16) (878.5007, 5725.57) (874.4921, 4060.42) (875.493, 3434.38) (856.4843, 6461.08) (857.4902, 3517.68) (858.4861, 3529.13) (859.4933, 2125.74) (860.4888, 2277.36) (428.7468, 89.15) (429.2323, 71.21) (429.7465, 539.79) | 97375.77 | 20839.58 | 104889.1 | 18277.08 | 114915.3 | 24150.44 | 119300.9 | 24190.98 | 0.78 | 0.00701 | 0.0154 | -0.21 | 0.539555 | 0.776408 |
| COMPOUND_855_4734a12_004098 | Rp | + | 855.4734 | 12.00 | | | | (878.471, 7446.8) (879.4713, 6944.16) (878.5007, 5725.57) (874.4921, 4060.42) (875.493, 3434.38) (856.4843, 6461.08) (857.4902, 3517.68) (858.4861, 3529.13) (859.4933, 2125.74) (860.4888, 2277.36) (428.7468, 89.15) (429.2323, 71.21) (429.7465, 539.79) (878.551, 2808.02) (879.5238, 3138.55) (880.5135, 2122.49) (894.5348, 6062.56) (895.0384, 1684.35) (894.5311, 4920.75) (895.5354, 3061.72) (896.529, 3156.49) (897.5282, 2010.92) (898.5246, 2444.24) (899.5284, 15269.99) (851.5854, 7943.64) (858.5778, 3423.29) (859.586, 309.54) (428.7857, 600.43) (429.2877, 463.72) (429.7906, 498.34) (430.2922, 283.9) (878.5646, 1332.38) (879.5682, 812.49) (880.5853, 1366.04) (881.6067, 1181.81) (856.586, 16187.36) (857.5896, 9569.68) (858.5924, 2911.69) (859.5901, 924.66) | 291678.4 | 66628.31 | 273586.8 | 70583.47 | 314920.2 | 140314.5 | 33860.1 | 132360.3 | 0.42 | 0.138149 | 0.213422 | 0.48 | 0.153475 | 0.465803 |
| COMPOUND_855_5737a12_795058 | Rp | + | 855.5737 | 12.80 | PC 42:9 | 2 | 40 eV: 673.5219(100), 86.0965(45), 504.3401(9), 797.5095(18), 856.5798(15) | (878.551, 2808.02) (879.5238, 3138.55) (880.5135, 2122.49) (894.5348, 6062.56) (895.0384, 1684.35) (894.5311, 4920.75) (895.5354, 3061.72) (896.529, 3156.49) (897.5282, 2010.92) (898.5246, 2444.24) (899.5284, 15269.99) (851.5854, 7943.64) (858.5778, 3423.29) (859.586, 309.54) (428.7857, 600.43) (429.2877, 463.72) (429.7906, 498.34) (430.2922, 283.9) (878.5646, 1332.38) (879.5682, 812.49) (880.5853, 1366.04) (881.6067, 1181.81) (856.586, 16187.36) (857.5896, 9569.68) (858.5924, 2911.69) (859.5901, 924.66) | 749492.3 | 276242.1 | 775141 | 251352 | 542181.5 | 197617 | 613668.3 | 218392.7 | -0.66 | 0.02044 | 0.040237 | 0.18 | 0.595448 | 0.804532 |
| COMPOUND_855_5781a12_068871 | Rp | + | 855.5781 | 12.07 | | | | (878.551, 2808.02) (879.5238, 3138.55) (880.5135, 2122.49) (894.5348, 6062.56) (895.0384, 1684.35) (894.5311, 4920.75) (895.5354, 3061.72) (896.529, 3156.49) (897.5282, 2010.92) (898.5246, 2444.24) (899.5284, 15269.99) (851.5854, 7943.64) (858.5778, 3423.29) (859.586, 309.54) (428.7857, 600.43) (429.2877, 463.72) (429.7906, 498.34) (430.2922, 283.9) (878.5646, 1332.38) (879.5682, 812.49) (880.5853, 1366.04) (881.6067, 1181.81) (856.586, 16187.36) (857.5896, 9569.68) (858.5924, 2911.69) (859.5901, 924.66) | 59531.6 | 27650.77 | 50818.41 | 19528.46 | 98108.29 | 23919.67 | 125558.5 | 49637.96 | 1.03 | 0.606E-06 | 2.53E-05 | 0.55 | 0.031021 | 0.237615 |
| COMPOUND_855_5972a12_688698 | Rp | - | 855.5972 | 12.69 | PC 18:1_20:3 | 1 | 10 eV: 854.5909(100), 293.1318(4), 112.9855(2) | (854.5906, 136689.77) (855.5939, 68488.06) (856.5966, 19761.73) (857.5985, 4490.92) (858.5961, 1054.44) (859.6026, 163.81) (854.5907, 505598.25) (855.5949, 254650.99) (856.5975, 72126.91) (857.5998, 15288.09) (858.6015, 2907.63) (859.5997, 620.06) (970.5227, 3586.53) (856.5334, 40229.61) (857.5365, 20344.39) (858.5486, 67221.84) (859.552, 31603.2) (860.5615, 25529.21) (861.5654, 10264.87) (862.5632, 3631.53) (863.5671, 847.59) (858.6018, 6323.54) (859.6084, 3734.54) (860.6046, 1128.06) (861.6064, 182.46) (972.4877, 1782.32) (973.5339, 1081.56) (974.523, 306.46) (975.5279, 265.33) (858.5493, 14496.89) (859.5526, 69863.63) (860.5634, 91865.18) (861.5671, 40783.84) (862.5701, 12104.31) (863.5738, 2020.85) (882.5651, 1342.87) (883.5839, 799.65) (884.6046, 177.66) (860.6156, 13095.83) (861.6209, 6749.96) (862.6244, 3054.75) (863.6259, 819.61) (864.632, 213.3) | 1574187 | 523990.4 | 1566756 | 424338.6 | 1629485 | 429566.6 | 1889253 | 398687.3 | 0.08 | 0.776736 | 0.836143 | 0.63 | 0.04967 | 0.282107 |
| COMPOUND_855_5988a12_93301 | Rp | - | 855.5988 | 12.93 | duplicate of PC38.3 | | | (854.5906, 136689.77) (855.5939, 68488.06) (856.5966, 19761.73) (857.5985, 4490.92) (858.5961, 1054.44) (859.6026, 163.81) (854.5907, 505598.25) (855.5949, 254650.99) (856.5975, 72126.91) (857.5998, 15288.09) (858.6015, 2907.63) (859.5997, 620.06) (970.5227, 3586.53) (856.5334, 40229.61) (857.5365, 20344.39) (858.5486, 67221.84) (859.552, 31603.2) (860.5615, 25529.21) (861.5654, 10264.87) (862.5632, 3631.53) (863.5671, 847.59) (858.6018, 6323.54) (859.6084, 3734.54) (860.6046, 1128.06) (861.6064, 182.46) (972.4877, 1782.32) (973.5339, 1081.56) (974.523, 306.46) (975.5279, 265.33) (858.5493, 14496.89) (859.5526, 69863.63) (860.5634, 91865.18) (861.5671, 40783.84) (862.5701, 12104.31) (863.5738, 2020.85) (882.5651, 1342.87) (883.5839, 799.65) (884.6046, 177.66) (860.6156, 13095.83) (861.6209, 6749.96) (862.6244, 3054.75) (863.6259, 819.61) (864.632, 213.3) | 5548839 | 1382421 | 5295836 | 1546768 | 4446272 | 1160565 | 4591829 | 1251005 | -0.71 | 0.003485 | 0.008158 | 0.23 | 0.395701 | 0.690408 |
| COMPOUND_857_5441a10_777037 | Rp | - | 857.5400 | 10.78 | | | | (854.5906, 136689.77) (855.5939, 68488.06) (856.5966, 19761.73) (857.5985, 4490.92) (858.5961, 1054.44) (859.6026, 163.81) (854.5907, 505598.25) (855.5949, 254650.99) (856.5975, 72126.91) (857.5998, 15288.09) (858.6015, 2907.63) (859.5997, 620.06) (970.5227, 3586.53) (856.5334, 40229.61) (857.5365, 20344.39) (858.5486, 67221.84) (859.552, 31603.2) (860.5615, 25529.21) (861.5654, 10264.87) (862.5632, 3631.53) (863.5671, 847.59) (858.6018, 6323.54) (859.6084, 3734.54) (860.6046, 1128.06) (861.6064, 182.46) (972.4877, 1782.32) (973.5339, 1081.56) (974.523, 306.46) (975.5279, 265.33) (858.5493, 14496.89) (859.5526, 69863.63) (860.5634, 91865.18) (861.5671, 40783.84) (862.5701, 12104.31) (863.5738, 2020.85) (882.5651, 1342.87) (883.5839, 799.65) (884.6046, 177.66) (860.6156, 13095.83) (861.6209, 6749.96) (862.6244, 3054.75) (863.6259, 819.61) (864.632, 213.3) | 704765.5 | 376638.8 | 674808.4 | 217443.2 | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|--|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_877_6384a9_982376 | Rp | + | 877.6384 | 9.98 | | | | (897.6023, 321.55)(898.1133, 108.3)(889.6105, 117.03)(890.1113, 159.47)(890.6018, 295.86)(906.1191, 178.75)(906.6399, 397.22)(907.1318, 162.04)(916.6289, 401.69)(917.1293, 277.55)(917.6197, 406.14)(950.817, 3083.42)(951.3211, 2159.51)(951.8158, 660.37)(916.6174, 532.08)(917.6237, 278.69)(448.3401, 20932.01)(448.8407, 10944.47)(449.3435, 3607.41)(449.8421, 1033.67)(450.3423, 288.91)(878.6417, 16077.99)(879.6449, 7689.43)(880.6339, 2953.61)(881.6383, 696.72)(882.6482, 117.91)(439.8263, 9235.6)(440.3276, 4658.19)(440.8293, 1553.74) | 463928 | 125658.7 | 396042.5 | 83952.69 | 514945.5 | 83915.47 | 514964.2 | 129762.6 | 0.29 | 0.296057 | 0.396151 | 0.68 | 0.045482 | 0.273371 |
| COMPOUND_878_5307a12_098638 | Rp | - | 878.5307 | 12.10 | | | (877.5222, 8412.8)(878.5182, 6831.33)(879.5174, 3065.41) | 88700.03 | 18471.64 | 90934.29 | 22261.73 | 84751 | 10277.35 | 78439.95 | 15814.81 | 0.03 | 0.923033 | 0.950466 | -0.47 | 0.156467 | 0.46686 | |
| COMPOUND_879_5981a12_817843 | Rp | - | 879.5981 | 12.82 | | | (878.5912, 16854.11)(879.5943, 89959.1)(880.5977, 29492.33)(881.6009, 7851.69)(882.5984, 2170.23)(919.5423, 4041.15) | 2023915 | 556989.4 | 1971626 | 508965.1 | 1907878 | 642211.1 | 1974150 | 619831.7 | -0.14 | 0.58824 | 0.683887 | 0.21 | 0.47205 | 0.734155 | |
| COMPOUND_881_489a12_250776 | Rp | + | 881.4890 | 12.25 | | | (889.523, 5651.88)(900.5009, 939.74)(901.5177, 1960.77)(902.5027, 1367.77)(882.4955, 22374.69)(883.4994, 11990.29)(884.497, 16945.2)(885.5002, 8274.24)(886.4954, 7542.45)(887.498, 3894.02)(888.4969, 2476.76) | 209625.1 | 57174.67 | 170458.5 | 42218.44 | 179080.9 | 40667.16 | 191052.8 | 50658.45 | -0.58 | 0.048728 | 0.085503 | 0.96 | 0.007258 | 0.132885 | |
| COMPOUND_881_5915a10_865179 | Rp | - | 881.5915 | 10.87 | | | (880.5873, 13788.63)(881.5918, 7163.23) | 35215 | 19581.95 | 41335.26 | 25072.6 | 16619 | 797.6164 | 17343.8 | 3956.93 | -1.11 | 6.74E-08 | 4.47E-07 | -0.34 | 0.115199 | 0.402603 | |
| COMPOUND_883_5567a10_840087 | Rp | - | 883.5567 | 10.84 | | | (996.5294, 2137.47)(997.5313, 1238.26)(998.5302, 874.19)(999.5435, 234.96)(882.5497, 109292.85)(883.5528, 54177.65)(884.5626, 58550.98)(885.5668, 25211.99)(886.5753, 19730.6)(887.5791, 8356.82) | 2725266 | 847508.2 | 2688474 | 760442.4 | 2285760 | 1243093 | 2180059 | 1585163 | -1.13 | 2.23E-06 | 1.03E-05 | -0.04 | 0.873494 | 0.946337 | |
| COMPOUND_889_5578a13_074443 | Rp | - | 889.5578 | 13.07 | | | (888.5495, 6976.01)(889.5523, 3654.57)(890.5413, 3749.53)(891.5415, 1814.07)(892.5388, 926.91)(893.5371, 348.83)(894.5497, 1041.26)(895.5643, 404.06)(896.5625, 1926.88)(897.5667, 1062.48) | 211839.5 | 71866.59 | 222843.3 | 73584.51 | 243939 | 71084.53 | 224649.5 | 64686.26 | 0.36 | 0.204774 | 0.29561 | -0.71 | 0.034706 | 0.249266 | |
| COMPOUND_889_6013a11_607544 | Rp | - | 889.6013 | 11.61 | | | (924.5597, 602.06)(925.555, 502.77)(926.5351, 1450.49)(888.5959, 50135.07)(889.5996, 24614.44)(890.6051, 10061.99)(891.6096, 3353.93)(892.6118, 577.11) | 528832.4 | 262733.3 | 503227 | 219526.5 | 257459.3 | 147759.5 | 305291 | 154986.6 | -1.33 | 3.31E-10 | 4.3E-09 | -0.04 | 0.865373 | 0.944172 | |
| COMPOUND_891_649a10_170948 | Rp | + | 891.6490 | 10.17 | | | (911.6021, 176.97)(912.1275, 218.77)(922.6463, 463.15)(923.1315, 593.05)(923.6352, 872.49)(930.5511, 934.05)(931.0673, 58.97)(457.8254, 1117.72)(458.337, 591.98)(458.8256, 339.08)(455.3465, 15239.83)(455.8487, 7845.38)(456.3475, 2745.44)(456.8493, 598.01)(930.5747, 327.87)(892.6567, 9875.08)(893.6602, 5047.94)(894.6522, 2072.91)(895.6415, 659.64)(446.8344, 4609.31)(447.3353, 3267.82)(447.8357, 788.13) | 247244.4 | 60807.96 | 211653.6 | 47135.13 | 277628.5 | 46371.09 | 277614.3 | 63707.1 | 0.42 | 0.128419 | 0.201673 | 0.62 | 0.061559 | 0.303349 | |
| COMPOUND_893_5765a11_273696 | Rp | - | 893.5765 | 11.27 | | | (928.5396, 10092.85)(929.5382, 5371.49)(930.5496, 17115.15)(931.5501, 9735.66)(932.5352, 6014.14)(933.532, 3166.45)(934.5389, 8715.35)(892.5696, 10318.91)(893.5731, 5803.1)(894.5845, 19181.92) | 343466.6 | 53871.24 | 374664.6 | 56108.02 | 421611.3 | 72098.6 | 459885.8 | 134475.4 | -0.66 | 0.007557 | 0.01649 | -0.37 | 0.196685 | 0.507758 | |
| COMPOUND_893_6332a9_570584 | Rp | + | 893.6332 | 9.57 | | | (466.7625, 146.72)(467.2653, 1467.1)(467.7825, 311.92)(458.8152, 1493.44)(459.3267, 5306.9)(459.8199, 276.97)(460.3319, 1030.8)(456.3374, 13402.72)(456.8395, 6551.44)(456.8493, 598.01)(930.5747, 327.87)(892.6567, 9875.08)(893.6602, 7786.54)(895.6397, 3958.09)(896.6417, 1387.64)(897.6436, 331.26)(485.7973, 274.55)(486.2935, 100.68)(447.824, 5301.19)(448.3268, 2672.19)(448.8258, 1083.97)(449.3135, 104.06) | 441258.8 | 112116.6 | 387192.7 | 83135.28 | 478367.5 | 75095.92 | 472050.8 | 119569 | 0.28 | 0.320082 | 0.422275 | 0.52 | 0.127345 | 0.424221 | |
| COMPOUND_894_198a9_36771 | Rp | - | 894.1980 | 9.37 | | | (1007.188, 68.72)(1008.1517, 259.23)(1009.1497, 231.27)(893.1906, 16254.78)(894.1943, 5038.86)(895.1872, 1053.42)(896.1681, 228.12) | 99390.45 | 18902.42 | 101281.1 | 16366.54 | 95794.79 | 18397.92 | 95743.7 | 14877.06 | -0.20 | 0.4958 | 0.596762 | -0.16 | 0.65175 | 0.83936 | |
| COMPOUND_894_1982a9_601177 | Rp | - | 894.1982 | 9.60 | | | (929.1535, 689.54)(930.1559, 233.75)(931.1781, 116.25)(893.1916, 49612.45)(894.1947, 15166.77)(895.189, 2594.41)(896.1909, 425.9)(939.1847, 442.81)(940.1873, 171.42)(941.171, 588.31)(942.1549, 245.24) | 435860 | 62463.41 | 456282.8 | 35884.43 | 445469.1 | 75562.39 | 444507.8 | 61298.3 | 0.14 | 0.644327 | 0.733582 | -0.34 | 0.347179 | 0.652628 | |
| COMPOUND_895_553a12_135263 | Rp | - | 895.5530 | 12.14 | | | (894.5462, 22440.07)(895.5488, 11389.73)(896.5526, 3764.92)(897.5523, 1014.25)(898.5531, 252.6) | 276875 | 65064.81 | 307974.8 | 72464.45 | 267027.2 | 53129.91 | 257246.5 | 66785.84 | -0.28 | 0.252334 | 0.348623 | -0.44 | 0.12635 | 0.423869 | |
| COMPOUND_895_5538a12_271391 | Rp | - | 895.5538 | 12.27 | | | (894.5467, 4381.01)(895.5497, 21827.82)(896.5534, 6413.34)(897.5567, 1646.05)(898.5634, 443.1) | 375929.7 | 50902.68 | 379699.7 | 49352.73 | 325185.9 | 36284.19 | 312153.4 | 38689.73 | -0.90 | 0.000404 | 0.00114 | -0.31 | 0.278159 | 0.585315 | |
| COMPOUND_898_1732a9_573771 | Rp | - | 898.1732 | 9.57 | | | (897.1666, 5020.61)(898.1702, 1538.96)(899.1703, 453.02)(900.1721, 107.06) | 33209.23 | 4581.528 | 34135.07 | 4924.677 | 33494.21 | 6557.933 | 32330.74 | 4535.858 | -0.03 | 0.914173 | 0.944366 | -0.32 | 0.376247 | 0.678626 | |
| COMPOUND_899_5665a11_92443 | Rp | - | 899.5665 | 11.92 | | | (1012.5221, 452.65)(1013.4799, 711.62)(1014.4615, 712.8)(898.5591, 31560.48)(899.5625, 17280.23)(900.5654, 6019.47)(901.5609, 1534.85)(902.5658, 3139.98) | 68053.83 | 27645.48 | 67449.36 | 30240.02 | 158888.5 | 59810.08 | 180752.3 | 76227.6 | 1.34 | 1.05E-08 | 8.64E-08 | 0.18 | 0.464327 | 0.732257 | |
| COMPOUND_899_5852a13_039803 | Rp | - | 899.5852 | 13.04 | | | (898.5782, 41874.7)(899.5812, 20610.94)(900.5842, 6536.51)(901.5816, 1668.43)(902.5885, 436.88)(903.5704, 90.56) | 1559499 | 254725.4 | 1729365 | 261760 | 1607628 | 121940.3 | 1553018 | 260302.8 | 0.09 | 0.713944 | 0.805246 | -0.75 | 0.01796 | 0.195392 | |
| COMPOUND_903_4644a4_8528066 | Rp | + | 903.4644 | 4.85 | | | (463.7295, 936.27)(464.2278, 527.74)(464.7201, 2938.53)(465.22, 1725.26)(921.4823, 71.67)(904.4676, 2539.88)(905.4719, 1283.39)(906.4742, 387.59)(907.4844, 120.77)(452.7395, 85923.87)(453.2409, 45526.49)(453.7419, 13922.13)(454.2424, 3041.78)(454.7438, 634.47)(455.24, 139.59) | 189838.4 | 316024.4 | 185812.9 | 237665.5 | 55037.9 | 83216.77 | 54250.82 | 46149.14 | -1.02 | 4.3E-05 | 0.000145 | 0.03 | 0.899521 | 0.955487 | |
| COMPOUND_904_4797a3_2558017 | Rp | + | 904.4797 | 3.26 | | | (472.2245, 404.35)(472.7171, 382.96)(905.4819, 372.21)(906.4873, 203.98)(453.2469, 15486.71)(453.7486, 7784.79)(454.2503, 2361.68)(454.7524, 551.96)(455.2505, 101.12) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 1.27 | 1.4E-09 | 1.48E-08 | 0.00 | 0.984112 | 0.992345 | |
| COMPOUND_904_48a3_5165477 | Rp | + | 904.4800 | 3.52 | | | (472.2245, 404.35)(472.7171, 382.96)(905.4819, 372.21)(906.4873, 203.98)(453.2469, 15486.71)(453.7486, 7784.79)(454.2503, 2361.68)(454.7524, 551.96)(455.2505, 101.12) | 20074 | 8417.811 | 15210.71 | 3855.661 | 58713.91 | 48802.32 | 48808.98 | 31754.25 | 1.18 | 2.24E-08 | 1.7E-07 | -0.11 | 0.631534 | 0.828008 | |
| COMPOUND_905_4823a12_187387 | Rp | + | 905.4823 | 12.19 | | | (923.5099, 6233.35)(924.5069, 4207.27)(925.5046, 2259.75)(926.5056, 699.04)(906.4948, 16727.14)(907.4978, 9855.23)(908.4962, 12735.04)(909.4978, 6093.85)(910.4943, 5760.36)(911.497, 3307.46)(912.498, 2046.64) | 347077.5 | 83684.11 | 286070.6 | 78830.11 | 305436.6 | 75833.92 | 328772.5 | 95065.54 | -0.55 | 0.060055 | 0.103715 | 0.92 | 0.009814 | 0.153413 | |
| COMPOUND_905_5132a11_185645 | Rp | - | 905.5132 | 11.19 | | | (940.4681, 3910.69)(941.4782, 2404.09)(904.5027, 15973.27)(905.5045, 8846.51)(906.5052, 3656.38)(907.5076, 1419.05) | 149502.6 | 26404.41 | 155434.8 | 38777.61 | 163479.5 | 55713.52 | 167096.5 | 36982.75 | -0.51 | 0.028379 | 0.053706 | -0.47 | 0.087351 | 0.350026 | |
| COMPOUND_905_5216a10_583235 | Rp | - | 905.5216 | 10.58 | | | (904.5161, 9087.81)(905.5196, 4604.88)(906.5237, 13418.11)(907.5365, 7065.51)(908.5481, 9691.09)(909.5515, 4670.76)(910.5513, 4080.46)(950.5337, 3060.92)(951.5389, 2165.07)(952.5387, 2543.29)(953.5384, 1275.72)(954.5193, 1731.32) | 166887 | 80360.92 | 159711.8 | 77739.91 | 60780 | 45283.8 | 76360.14 | 38617.5 | -1.38 | 6.24E-11 | 1.06E-09 | 0.01 | 0.95557 | 0.980661 | |
| COMPOUND_905_6039a12_530823 | Rp | - | 905.6039 | 12.53 | | | (904.5953, 370.46)(1018.6027, 504.26)(1019.6084, 295.25)(1020.6168, 412.65)(904.5977, 1900.55)(905.6019, 1052.34)(906.5946, 23870.64)(950.5916, 597.15)(951.5843, 403.79)(952.5644, 455.4) | 49634.33 | 13417.48 | 55494.27 | 14289.45 | 56108 | 21590.51 | 50343.32 | 14602.04 | 0.52 | 0.068525 | 0.116907 | -0.90 | 0.008689 | 0.148883 | |
| COMPOUND_905_6875a10_929913 | Rp | - | 905.6875 | 10.93 | | | (1018.6479, 1298.64)(940.6833, 2073.8)(904.6791, 7735.18)(905.678, 4248.78)(906.6767, 1518.37) | 30146.6 | 14786.8 | 32306.28 | 20031.42 | 22973.64 | 10684.67 | 30087.87 | 12489.23 | -0.13 | 0.635845 | 0.725759 | 0.32 | 0.307045 | 0.613089 | |
| COMPOUND_907_5935a12_848889 | Rp | - | 907.5935 | 12.85 | | | (1020.5579, 225.99)(1021.5567, 299.4)(906.5866, 6029.31)(907.5896, 3036.67)(908.5886, 58263.88) | 13718.23 | 56352.39 | 15457.5 | 46675.17 | 10261.64 | 40251.17 | 11817.44 | -0.88 | 0.000325 | 0.00093 | -0.04 | 0.895295 | 0.954308 | | |
| COMPOUND_907_6489a9_774024 | Rp | + | 907.6489 | 9.77 | | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|----------|-----------|---|----------|--------------|-------------------|---------------|----------|---------------|----------|---------------|----------|---------------|----------|----------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_912_5049a12_247652 | Rp | + | 912.5049 | 12.25 | (935.5116, 947.07)(936.5111, 567.26)(913.5127, 15671.73)(914.5132, 8686.17)(915.516, 3123.28) | | | | 95520.05 | 28662.73 | 82724.46 | 29297.58 | 81165.69 | 19949.23 | 79038.93 | 25881.16 | 0.00 | 0.993205 | 0.99808 | 0.57 | 0.07221 | 0.325884 |
| COMPOUND_913_5148a12_269906 | Rp | - | 913.5148 | 12.27 | (1026.503, 679.94)(1027.5068, 4367.13)(948.4898, 4985.22)(912.5063, 13215.81)(913.5086, 7397.49)(914.5113, 3162.36)(915.514, 1058.05) | | | | 93472.21 | 32916.76 | 93760.43 | 28319 | 90736.38 | 30665.89 | 79307.68 | 30318.5 | 0.17 | 0.559703 | 0.656827 | -0.47 | 0.168987 | 0.481172 |
| COMPOUND_914_1366a12_309307 | Rp | - | 914.1366 | 9.31 | (913.1279, 1334.18)(914.129, 428.72)(915.1242, 20248.82)(959.1566, 700.39)(960.1395, 261.16) | | | | 95853.96 | 20568.9 | 104574.85 | 21877.0 | 92917.79 | 20957.06 | 87190.75 | 18062.15 | -0.17 | 0.53668 | 0.635772 | -0.65 | 0.043384 | 0.270638 |
| COMPOUND_915_529a12_559266 | Rp | - | 915.5290 | 12.56 | (1028.5164, 889.45)(1029.5219, 2851.55)(1030.5216, 1781.24)(950.4932, 4530.12)(951.4983, 2190.62)(914.5222, 6855.21)(915.5245, 4271.03)(916.5344, 4480.81)(917.5385, 2575.4)(960.5202, 2756.69)(961.5094, 1063.26)(962.4946, 179.44) | | | | 287578.5 | 83001.84 | 244871.2 | 87031.05 | 317357 | 87277.14 | 293796.6 | 77012.99 | 0.41 | 0.149455 | 0.22726 | 0.18 | 0.584763 | 0.798113 |
| COMPOUND_915_5799a11_493208 | Rp | - | 915.5799 | 11.49 | (914.574, 11941.05)(915.577, 6151.0)(916.5765, 2340.69)(917.5757, 764.68)(918.6014, 161.52) | | | | 263555.9 | 91768.39 | 321957.4 | 102218 | 210488.8 | 108082.7 | 223934 | 112560.6 | -1.06 | 4.89E-07 | 2.66E-06 | -0.48 | 0.037481 | 0.259604 |
| COMPOUND_915_6362a12_531209 | Rp | - | 915.6362 | 12.53 | (1028.6108, 307.85)(1029.6234, 241.75)(950.5921, 739.46)(951.6013, 440.52)(914.6272, 2174.44)(915.6315, 1407.96)(916.6238, 3113.38)(960.6775, 896.6)(961.696, 3766.21)(962.6985, 2199.0) | | | | 45578.49 | 16656.19 | 54227.46 | 20027.25 | 66077.93 | 26675.58 | 63177.68 | 22338.57 | 0.86 | 0.002151 | 0.005305 | -0.50 | 0.121637 | 0.411918 |
| COMPOUND_916_5338a12_9877825 | Rp | + | 916.5338 | 12.99 | (939.5324, 2097.15)(940.5283, 1516.15)(917.543, 15312.62)(918.5433, 9280.5)(919.5415, 4046.52)(920.5265, 1455.17) | | | | 323387.4 | 102756.1 | 301198.4 | 10426.25 | 314065.9 | 88369.9 | 339743.4 | 100685.9 | 0.04 | 0.883924 | 0.922855 | 0.67 | 0.048737 | 0.279822 |
| COMPOUND_917_1344a9_309351 | Rp | - | 917.1344 | 9.31 | (952.1052, 221.19)(953.114, 207.93)(916.1275, 8028.36)(917.1285, 2397.19)(918.1361, 537.37)(919.1581, 155.26) | | | | 44334.53 | 9640.836 | 48489.04 | 11451.58 | 41895.86 | 8166.263 | 39814.95 | 9999.81 | -0.25 | 0.376402 | 0.477624 | -0.55 | 0.10308 | 0.379929 |
| COMPOUND_918_6339a12_530645 | Rp | - | 918.6339 | 12.53 | (917.6265, 17429.23)(918.6293, 5848.55)(919.6328, 1735.7)(920.6414, 294.58) | | | | 37210.55 | 13686.03 | 44357.2 | 16821.71 | 54464.36 | 21820.69 | 51431.07 | 18346.35 | 0.82 | 0.003991 | 0.009208 | -0.45 | 0.168791 | 0.481172 |
| COMPOUND_919_553a12_113661 | Rp | - | 919.5530 | 12.11 | (918.5464, 48548.1)(919.5497, 26086.08)(920.5519, 8323.51)(921.5536, 2086.78)(922.5638, 603.9) | | | | 306827.2 | 237822.7 | 248235.6 | 217198.4 | 146494.1 | 125350.3 | 152232.6 | 144208.2 | -0.66 | 0.017017 | 0.034155 | 0.44 | 0.173221 | 0.487961 |
| COMPOUND_919_5536a12_211285 | Rp | - | 919.5536 | 12.21 | (918.5464, 48548.1)(919.5497, 26086.08)(920.5519, 8323.51)(921.5536, 2086.78)(922.5638, 603.9) | | | | 537185.5 | 66336.24 | 548511.6 | 97302.73 | 374408.4 | 130733.8 | 338079.4 | 106291.9 | -1.25 | 1.77E-07 | 1.06E-06 | -0.28 | 0.274269 | 0.583098 |
| COMPOUND_921_469a11_911196 | Rp | - | 921.4690 | 11.91 | (1034.4365, 863.53)(1035.4424, 696.56)(1036.446, 1218.64)(920.4588, 5839.12)(921.4634, 2964.73)(922.4619, 3447.23)(923.4651, 1724.66)(924.4603, 1688.38)(925.4696, 1085.09)(926.4778, 1063.37) | | | | 92185 | 20583.55 | 84465.59 | 32355.13 | 111431.5 | 32223.41 | 116761.3 | 32860.89 | 0.89 | 8.86E-05 | 0.000276 | 0.03 | 0.916312 | 0.961472 |
| COMPOUND_921_5693a12_415492 | Rp | - | 921.5693 | 12.42 | (920.5518, 19515.81)(921.5553, 10859.47)(922.5643, 3443.05)(923.5721, 1051.99) | | | | 187459.8 | 88687.44 | 160468.1 | 88547.39 | 122647.5 | 82063.37 | 133953.7 | 79119.83 | -0.50 | 0.04976 | 0.087138 | 0.40 | 0.177337 | 0.491826 |
| COMPOUND_921_6659a9_963869 | Rp | + | 921.6658 | 9.96 | (472.8303, 4124.21)(473.3312, 2785.37)(473.8314, 1014.2)(470.3525, 38680.61)(470.8541, 19269.33)(471.3478, 19453.51)(471.8513, 1979.2)(472.3498, 2579.58)(489.3428, 1104.14)(489.8476, 925.77)(481.3439, 1987.1)(481.8278, 513.62)(922.6677, 13839.85)(923.6704, 6817.66)(924.6696, 2471.99)(925.6705, 735.17)(926.6814, 189.99)(461.8404, 4773.75)(462.3441, 2527.63)(462.8434, 967.04)(463.3285, 91.01) | | | | 634286.2 | 167638 | 539681.3 | 109985.3 | 689690.9 | 106143.9 | 693499.1 | 173598.1 | 0.26 | 0.356125 | 0.458544 | 0.68 | 0.044618 | 0.272788 |
| COMPOUND_923_5829a12_6915455 | Rp | - | 923.5829 | 12.69 | (922.5774, 15796.63)(923.5811, 8190.74)(924.5823, 2941.8)(925.5771, 728.34) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | 0.24 | 0.360613 | 0.462735 | 0.01 | 0.982715 | 0.99152 |
| COMPOUND_923_585a12_936366 | Rp | - | 923.5850 | 12.94 | (922.5781, 20685.83)(923.5816, 11346.83)(924.5837, 3792.66)(925.5841, 1171.09)(926.5822, 224.62) | 458105.2 | 101138.2 | 447293.8 | 123031.1 | 374819.1 | 86227.32 | 364483.8 | 82523.94 | -0.69 | 0.005316 | 0.011952 | -0.07 | 0.809897 | 0.919078 | | | |
| COMPOUND_925_7311a10_862317 | Rp | - | 925.7311 | 10.86 | (924.7239, 5252.72)(925.7261, 3420.68)(926.7277, 1683.01)(927.7277, 639.23)(970.7322, 260.61)(971.7333, 237.99)(972.7098, 886.76) | 31370.39 | 4824.686 | 33910.09 | 4786.042 | 24793.14 | 2568.129 | 24952.76 | 4647.074 | -0.34 | 0.227189 | 0.321983 | -0.14 | 0.677089 | 0.851683 | | | |
| COMPOUND_927_575a11_035155 | Rp | - | 927.5750 | 11.04 | (1040.5254, 1703.56)(1041.5111, 1110.74)(1042.5006, 778.47)(962.5143, 1871.0)(963.4952, 1074.93)(964.4981, 1339.66)(926.569, 21174.84)(927.5725, 10846.02)(928.5834, 12837.66)(929.588, 5823.7)(930.5824, 4035.45)(931.5807, 3180.13)(972.5424, 5037.89)(973.5209, 2361.78)(974.5112, 2575.63) | 372178.1 | 155871.3 | 329120.6 | 173366.4 | 283109 | 100245.9 | 307651.7 | 64130.92 | -1.17 | 2.2E-07 | 1.28E-06 | 0.27 | 0.256034 | 0.56678 | | | |
| COMPOUND_929_2315a9_578919 | Rp | + | 929.2315 | 9.58 | (947.2752, 80.09)(930.2999, 5911.61)(931.2431, 1834.93)(932.2489, 295.22)(933.2593, 65.51) | 41453.06 | 13671.97 | 43615.78 | 11985.92 | 48293.43 | 9163.936 | 44822.02 | 11388.78 | 0.60 | 0.048369 | 0.085098 | -0.48 | 0.1807 | 0.493854 | | | |
| COMPOUND_929_2324a9_597884 | Rp | + | 929.2324 | 9.60 | (947.2633, 78.78)(930.2389, 5197.16)(931.2429, 1796.66)(932.2451, 383.56)(933.2677, 52.2) | 40573.13 | 14896.16 | 40097.78 | 13882.95 | 50050 | 10423.63 | 42534.44 | 15287.8 | 0.72 | 0.018235 | 0.036439 | -0.53 | 0.140063 | 0.444883 | | | |
| COMPOUND_930_4808a0_8089563 | Hilic | + | 930.4808 | 0.81 | (953.5101, 2883.78)(953.9858, 1318.66)(953.4723, 456.26)(954.4648, 375.28)(955.4772, 309.92)(948.51, 3845.94)(949.5035, 2172.32)(950.5138, 2528.69)(931.4971, 3623.49)(466.2479, 5797.99)(466.7499, 2741.59)(467.2509, 1107.98)(467.7556, 329.89) | 60203.15 | 16340.16 | 62237.38 | 13009.82 | 49767.69 | 22781.42 | 42683.54 | 12010.56 | 0.14 | 0.617404 | 0.710109 | -0.39 | 0.248728 | 0.55846 | | | |
| COMPOUND_933_524a12_4057045 | Rp | - | 933.5240 | 12.41 | (932.5172, 14085.96)(933.5207, 6955.51)(934.5244, 2634.4)(935.5274, 813.58) | 215452.8 | 54276.35 | 239324.2 | 77017.58 | 201509.9 | 59015.88 | 173093.3 | 39680.45 | -0.29 | 0.27121 | 0.369365 | -0.62 | 0.050563 | 0.283798 | | | |
| COMPOUND_935_539a12_808606 | Rp | - | 935.5390 | 12.81 | (934.532, 15838.18)(935.5357, 7498.59)(936.5381, 3037.75)(937.5391, 923.38) | 301652.9 | 45378.31 | 326694.1 | 50651.34 | 321576.8 | 55843.14 | 315877.2 | 69692.23 | 0.35 | 0.24185 | 0.337243 | -0.34 | 0.349981 | 0.656798 | | | |
| COMPOUND_935_5503a12_240658 | Rp | - | 935.5503 | 11.24 | (1048.51, 891.09)(1049.5109, 528.12)(1050.5245, 650.45)(934.5143, 14351.48)(935.5447, 273096.1) | 93313.9 | 318455.4 | 164499.7 | 359771 | 118448.2 | 350351.3 | 147092.4 | -0.74 | 0.001816 | 0.004534 | -0.38 | 0.167383 | 0.480454 | | | | |
| COMPOUND_935_672a10_148822 | Rp | + | 935.6762 | 10.15 | (479.836, 1703.93)(480.3468, 6998.45)(480.8377, 494.48)(477.3599, 14708.01)(477.8613, 382448.6) | 105051.3 | 327295.3 | 69900.7 | 440015.6 | 70933.57 | 436123.1 | 114222 | 0.42 | 0.132057 | 0.206093 | 0.60 | 0.071898 | 0.325554 | | | | |
| COMPOUND_935_7423a13_247795 | Rp | + | 935.7423 | 13.25 | (7830.78)(478.3546, 1551.19)(478.8449, 520.57)(974.6298, 2461.23)(936.6833, 7362.33)(937.686, 3828.02)(938.6794, 1579.13)(939.6671, 617.15)(940.6708, 73.34)(488.3415, 513.4)(488.8439, 156.25)(489.3492, 2556.53)(468.8471, 5854.11)(469.3489, 3425.15)(469.8495, 1245.09) | 96519.1 | 62693.42 | 104134.9 | 91949.35 | 52164 | 17472.61 | 28528.38 | 14994.02 | -1.28 | 9.85E-10 | 1.09E-08 | -0.15 | 0.490322 | 0.748114 | | | |
| COMPOUND_936_5026a12_1799933 | Rp | + | 936.5026 | 12.18 | (959.4828, 1701.01)(960.4778, 1315.33)(975.4839, 2350.42)(937.5126, 17159.91)(938.5157, 9598.12)(939.5164, 3640.06)(940.5133, 1411.63) | 127808.9 | 52798.59 | 106894.7 | 56532.95 | 120220.2 | 25352.81 | 135961 | 51786.75 | -0.15 | 0.597012 | 0.691669 | 0.37 | 0.270446 | 0.57949 | | | |
| COMPOUND_937_6605a9_559114 | Rp | + | 937.6605 | 9.56 | (499.8081, 75.83)(500.3052, 4759.49)(500.7982, 128.25)(480.8275, 2472.23)(481.3344, 2254.48)(481.8317, 713.62)(482.3309, 283.44)(478.35, 2123.93)(478.8512, 10997.86)(479.3528, 3644.23)(479.8518, 1126.25)(480.3477, 199.0)(938.663, 4753.09)(939.6649, 2531.03)(940.6671, 890.45)(941.6731, 299.23)(507.792, 220.53)(508.3047, 102.86)(469.8366, 8728.23)(470.3387, 4890.52)(470.8408, 1785.28) | 413760.3 | 110504.3 | 355619.5 | 70839.87 | 438953.7 | 71157.87 | 455624.9 | 103904.5 | 0.18 | 0.519089 | 0.619167 | 0.79 | 0.020144 | 0.199116 | | | |
| COMPOUND_941_4652a4_883823 | Rp | + | 941.4652 | 4.88 | (964.4519, 85.85)(965.4321, 43.44)(966.4324, 215.12)(942.4731, 474.52)(942.9925, 40.87)(943.4767, 196.61)(943.9956, 208.69)(944.4874, 129.95)(501.6987, 416.86)(502.1896, 133.5)(502.6965, 409.39)(961.9465, 96.36)(962.4526, 61.34)(490.714, 4800.06)(491.2138, 2483.73)(491.7168, 780.75)(492.2101, 161.66)(493.7202, 234.84)(494.2254, 114.23)(494.7059, 397.63)(482.7366, 261.66)(483.2311, 36.51)(483.7176, 830.15)(484.2308, 630.23)(484.7323, 172.62)(959.5191, 104.24)(980.4167, 234.46)(942.4678, 7976.82)(943.4719, 4545.23)(944.4729, 1300.92)(9 | | | | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MS/MS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-----------------------------|--------|----------|----------|-----------|----------------|----------|---------------|--|---------------|----------|---------------|-----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_948_6168a10_193423 | Rp | - | 948.6168 | 10.19 | | | | (947.6099, 74510.8)(948.6129, 36445.68)(949.6159, 11252.29)(950.6185, 2696.49)(951.6257, 595.03) (947.6101, 60998.27)(948.6132, 29220.2)(949.6161, 9226.11)(950.619, 2023.71)(951.6245, 439.88) (971.6075, 6351.67)(972.6099, 3367.35)(973.6173, 1361.83)(974.6216, 412.43)(987.5647, 1098.46)(988.5488, 958.66)(989.5404, 1179.04)(949.6267, 42760.6)(950.63, 20649.35)(951.6346, 6248.35)(952.638, 1611.97)(953.6432, 447.77) | 72221.19 | 77375.15 | 94174.89 | 108399.91 | 80019.07 | 123368.6 | 104039.8 | 115789.7 | -0.59 | 0.051469 | 0.089781 | 0.26 | 0.461146 | 0.729797 |
| COMPOUND_948_617a10_273766 | Rp | - | 948.6170 | 10.27 | | | | (971.6075, 6351.67)(972.6099, 3367.35)(973.6173, 1361.83)(974.6216, 412.43)(987.5647, 1098.46)(988.5488, 958.66)(989.5404, 1179.04)(949.6267, 42760.6)(950.63, 20649.35)(951.6346, 6248.35)(952.638, 1611.97)(953.6432, 447.77) | 186228.8 | 36448.33 | 204273.1 | 61762.77 | 184256.9 | 86605.8 | 188251.7 | 78597.97 | -0.45 | 0.133459 | 0.207993 | 0.03 | 0.93651 | 0.97184 |
| COMPOUND_948_6197a10_273863 | Rp | + | 948.6197 | 10.27 | | | | (971.6075, 6351.67)(972.6099, 3367.35)(973.6173, 1361.83)(974.6216, 412.43)(987.5647, 1098.46)(988.5488, 958.66)(989.5404, 1179.04)(949.6267, 42760.6)(950.63, 20649.35)(951.6346, 6248.35)(952.638, 1611.97)(953.6432, 447.77) | 98104.06 | 22124.84 | 104185.7 | 34578.31 | 85337.93 | 49485.49 | 87204.81 | 39471.06 | -0.69 | 0.021135 | 0.041425 | 0.09 | 0.785857 | 0.909997 |
| COMPOUND_949_498a12_408281 | Rp | - | 949.4980 | 12.41 | | | | (1062.4736, 761.1)(1063.4758, 547.18)(1064.4745, 576.11)(948.4904, 11262.56)(949.4931, 6076.05)(950.4911, 6508.06)(951.4955, 3017.78)(952.4895, 2720.6)(953.4924, 1307.56)(954.4983, 1066.25)(994.5172, 548.92)(995.5005, 532.43) | 192432.3 | 37813.91 | 200304.9 | 49616.88 | 181653.2 | 35456.06 | 171007.3 | 38699.95 | -0.20 | 0.482654 | 0.58406 | -0.46 | 0.17283 | 0.487735 |
| COMPOUND_949_5325a11_446433 | Rp | - | 949.5325 | 11.45 | | | | (984.5247, 2840.94)(985.5014, 909.1)(948.5253, 14817.97)(949.5274, 9068.72)(950.5279, 4154.48)(951.5231, 1429.86) (980.6749, 358.15)(981.1743, 302.56)(988.5789, 517.03)(989.0996, 289.2)(486.842, 1012.13)(487.3353, 1836.34)(488.8362, 173.76)(967.6841, 281.46)(503.3411, 2521.28)(503.8581, 1348.53)(484.3675, 9150.38)(484.8698, 4691.55)(485.3587, 8632.67)(485.8464, 564.89)(486.3543, 1008.47)(950.6983, 3151.34)(951.7013, 1872.04)(952.6934, 692.17)(953.7071, 226.51)(495.3599, 5659.01)(495.8675, 1193.68)(475.8545, 2634.92)(476.3555, 1752.86)(476.8585, 4900.87) (487.8356, 2843.7)(488.3382, 1656.35)(488.838, 662.78)(489.3264, 252.56)(485.359, 21907.79)(485.8608, 11792.12)(486.361, 4136.36)(486.8607, 1250.77)(487.3589, 347.35)(504.3484, 788.27)(504.8565, 610.24)(952.6783, 7984.13)(953.6807, 4210.1)(954.6834, 1353.32)(955.6859, 416.91)(956.684, 45.31)(476.845, 12712.91)(477.3468, 7754.02)(477.8486, 2897.43) (994.4793, 420.07)(956.5153, 13866.8)(957.5179, 7210.72)(958.5118, 2932.66)(959.4934, 631.76) (992.4855, 905.03)(993.4795, 825.06)(994.4757, 1291.74)(956.5142, 12232.02)(957.5176, 6414.78)(958.51, 2582.38)(959.518, 582.54) (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 88664.94 | 30900.41 | 92481.3 | 45062.05 | 72192.5 | 5714.13 | 49006.14 | 9946.424 | -1.26 | 6.37E-10 | 7.52E-09 | -0.22 | 0.278362 | 0.585315 |
| COMPOUND_949_6942a10_31658 | Rp | + | 949.6942 | 10.32 | | | | (980.6749, 358.15)(981.1743, 302.56)(988.5789, 517.03)(989.0996, 289.2)(486.842, 1012.13)(487.3353, 1836.34)(488.8362, 173.76)(967.6841, 281.46)(503.3411, 2521.28)(503.8581, 1348.53)(484.3675, 9150.38)(484.8698, 4691.55)(485.3587, 8632.67)(485.8464, 564.89)(486.3543, 1008.47)(950.6983, 3151.34)(951.7013, 1872.04)(952.6934, 692.17)(953.7071, 226.51)(495.3599, 5659.01)(495.8675, 1193.68)(475.8545, 2634.92)(476.3555, 1752.86)(476.8585, 4900.87) (487.8356, 2843.7)(488.3382, 1656.35)(488.838, 662.78)(489.3264, 252.56)(485.359, 21907.79)(485.8608, 11792.12)(486.361, 4136.36)(486.8607, 1250.77)(487.3589, 347.35)(504.3484, 788.27)(504.8565, 610.24)(952.6783, 7984.13)(953.6807, 4210.1)(954.6834, 1353.32)(955.6859, 416.91)(956.684, 45.31)(476.845, 12712.91)(477.3468, 7754.02)(477.8486, 2897.43) (994.4793, 420.07)(956.5153, 13866.8)(957.5179, 7210.72)(958.5118, 2932.66)(959.4934, 631.76) (992.4855, 905.03)(993.4795, 825.06)(994.4757, 1291.74)(956.5142, 12232.02)(957.5176, 6414.78)(958.51, 2582.38)(959.518, 582.54) (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 171722 | 54951.78 | 144578.6 | 43142.57 | 234727.5 | 50588.97 | 253043.5 | 78766.69 | 0.65 | 0.011667 | 0.024261 | 0.65 | 0.03481 | 0.249266 |
| COMPOUND_951_6769a9_75777 | Rp | + | 951.6769 | 9.76 | | | | (971.6075, 6351.67)(972.6099, 3367.35)(973.6173, 1361.83)(974.6216, 412.43)(987.5647, 1098.46)(988.5488, 958.66)(989.5404, 1179.04)(949.6267, 42760.6)(950.63, 20649.35)(951.6346, 6248.35)(952.638, 1611.97)(953.6432, 447.77) | 681616.3 | 176561.8 | 588766.9 | 120576.1 | 744510.4 | 115321.5 | 737630.4 | 188774.3 | 0.30 | 0.279853 | 0.379286 | 0.58 | 0.088803 | 0.352184 |
| COMPOUND_957_5185a12_268805 | Rp | - | 957.5185 | 12.27 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 80764.15 | 16872.88 | 81237.41 | 11446.5 | 66630.23 | 11922.39 | 62790.54 | 11279.76 | -0.74 | 0.004029 | 0.009288 | -0.34 | 0.255985 | 0.56678 |
| COMPOUND_957_5199a12_141909 | Rp | - | 957.5199 | 12.14 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 60482.7 | 15647.6 | 66436.03 | 17706.07 | 63902 | 11660.07 | 65788.82 | 18777.58 | -0.27 | 0.296604 | 0.396646 | 0.13 | 0.668885 | 0.846185 |
| COMPOUND_958_2103a9_640239 | Rp | - | 958.2103 | 9.64 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 190114.4 | 45561.55 | 203671.2 | 52315.32 | 176522.1 | 43242.93 | 196151.3 | 75019.23 | -0.23 | 0.446609 | 0.551672 | -0.02 | 0.957643 | 0.980661 |
| COMPOUND_958_2109a9_585631 | Rp | - | 958.2109 | 9.59 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 149026 | 43705.1 | 158872.5 | 30471.39 | 130216.7 | 25633.01 | 145712.9 | 29560.98 | -0.60 | 0.04241 | 0.075799 | 0.20 | 0.554675 | 0.781554 |
| COMPOUND_961_515a12_025444 | Rp | - | 961.5150 | 12.03 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 90414.26 | 31597.79 | 100574.5 | 36846.67 | 78579.6 | 21511.13 | 120176.4 | 62281.03 | -0.82 | 0.001507 | 0.003801 | 0.22 | 0.448171 | 0.721588 |
| COMPOUND_961_5525a13_040233 | Rp | - | 961.5525 | 13.04 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 453071 | 76115.21 | 497721.5 | 78049.46 | 645500 | 55643.14 | 446483.9 | 71415.56 | 0.00 | 0.999965 | 0.999965 | -0.70 | 0.022517 | 0.213113 |
| COMPOUND_962_6334a1_1547581 | Hilic | + | 962.6334 | 1.15 | no msm | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 16741.63 | 8005.605 | 24460.07 | 13148.19 | 19631.79 | 7412.439 | 16006.16 | 7785.645 | 0.38 | 0.168697 | 0.252094 | -1.23 | 0.00029 | 0.024157 |
| COMPOUND_963_774a13_243681 | Rp | + | 963.7740 | 13.24 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 73018.91 | 53671.27 | 75473.38 | 62277.13 | 41779.67 | 15673.42 | 26698 | 9084.847 | -1.13 | 1.8E-07 | 1.07E-06 | -0.11 | 0.62724 | 0.825147 |
| COMPOUND_965_69a9_930252 | Rp | + | 965.6900 | 9.93 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 1227567 | 243750.1 | 1151574 | 289225.5 | 1160777 | 183496.1 | 1138928 | 283432.3 | -0.33 | 0.231905 | 0.326815 | 0.22 | 0.498686 | 0.753329 |
| COMPOUND_968_5249a12_560808 | Rp | + | 968.5249 | 12.56 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 133221.6 | 53793.31 | 100672.5 | 38046.45 | 146654.6 | 5788.17 | 124716.1 | 51625.68 | -0.02 | 0.943361 | 0.963469 | 0.54 | 0.119695 | 0.409655 |
| COMPOUND_972_6176a10_133184 | Rp | - | 972.6176 | 10.13 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | #DIV/0! | -0.51 | 0.082069 | 0.136701 | 0.00 | 0.994829 | 0.998139 |
| COMPOUND_972_6185a10_130318 | Rp | + | 972.6185 | 10.13 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 63169 | 26969 | 66021.75 | 29854.9 | 39708.54 | 15520.83 | 44492.33 | 18175.64 | -0.89 | 0.001746 | 0.004388 | 0.10 | 0.755277 | 0.895058 |
| COMPOUND_973_4935a12_144854 | Rp | - | 973.4935 | 12.14 | | | | (1071.1797, 1290.9)(957.2039, 35559.72)(958.2075, 12148.84)(959.1922, 2881.62)(960.2099, 458.51)(1003.2007, 379.63)(1004.1908, 141.05)(1005.182, 438.0)(1006.1899, 94.4)(1007.1644, 1071.08)(1008.1393, 352.26)(1009.1637, 663.33) | 87691.7 | 20533.89 | 94441.88 | 26795.85 | 89971.46 | 25272.57 | 85122.89 | 27489.2 | -0.01 | 0.984679 | 0.992613 | -0.15 | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|-------------------------------|--------|----------|-----------|-----------|----------------|----------|--------------|--|---------------|----------|---------------|-----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR_p | Value | raw p | FDR_p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_980_5134a12_426218 | Rp | - | 980.5134 | 12.43 | | | | (1093.465, 440.79)(1094.407, 837.1)(1095.479, 653.4)(1096.487, 377.11)(1097.502, 383.56)(979.5075, 723.02)(980.5095, 4626.61)(981.5096, 2289.07)(1025.5128, 1061.92)(1026.5155, 2147.66) | 24235.54 | 17030.72 | 34717.52 | 19483.95 | 65290 | 45711.7 | 53616.39 | 28337.04 | 0.02 | 0.931047 | 0.956096 | 0.67 | 0.032896 | 0.244873 |
| COMPOUND_980_6074a9_766103 | Rp | - | 980.6074 | 9.77 | | | | (979.6002, 19190.13)(980.6025, 9544.59)(981.6063, 3191.99)(982.6105, 744.56)(983.6146, 173.79) | 23351.58 | 12522.32 | 33295.58 | 24921.96 | 19456.75 | 11214.52 | 20346.55 | 8983.811 | 0.01 | 0.951878 | 0.96951 | -0.73 | 0.009286 | 0.153413 |
| COMPOUND_990_3552a9_064262 | Rp | - | 990.3552 | 9.06 | | | | (1103.3616, 731.52)(1025.3315, 762.57)(1026.3243, 464.83)(989.3482, 13401.98)(990.3516, 5793.31)(991.3623, 10019.32)(992.3654, 4121.26)(993.3669, 1519.8)(994.3635, 487.45) | 17389 | 6428.867 | 19196.31 | 4826.99 | 120085.6 | 79817.11 | 65442.2 | 53002.01 | 1.81 | 3.16E-15 | 7.92E-13 | -0.65 | 0.002025 | 0.065137 |
| COMPOUND_990_5354a12_2677145 | Rp | - | 990.5354 | 12.27 | | | | (1025.5077, 1826.55)(1026.498, 986.43)(989.5286, 6364.43)(990.5312, 3886.56)(991.5325, 1517.74)(992.538, 452.06)(993.5475, 105.5) | 37024.04 | 4938.511 | 34931.39 | 8798.07 | 32581.36 | 7195.816 | 32806.68 | 8039.762 | 0.07 | 0.024052 | 0.046353 | 0.44 | 0.214873 | 0.521996 |
| COMPOUND_995_7027a9_744923 | Rp | + | 995.7027 | 9.74 | | | | (509.8495, 3718.13)(510.3583, 3091.75)(510.8522, 889.55)(511.3458, 272.11)(526.3597, 667.86)(526.8662, 576.07)(1034.6754, 101.1)(996.7044, 4466.34)(997.7071, 2585.8)(998.7095, 888.78)(999.7108, 272.91)(998.8582, 12416.31)(999.3602, 7517.24)(999.862, 2735.28) | 723248.6 | 195329.9 | 626149.5 | 139798.78 | 779848 | 134845.1 | 779017.5 | 194616.8 | 0.23 | 0.408696 | 0.512463 | 0.61 | 0.075258 | 0.329961 |
| COMPOUND_996_6177a10_121729 | Rp | + | 996.6177 | 10.12 | | | | (1019.6216, 3868.1)(1020.617, 2505.17)(1021.6256, 1227.01)(1035.6207, 1479.9)(1036.619, 1025.69)(997.6271, 24282.12)(998.6297, 13915.19)(999.6346, 4270.97)(1000.634, 1146.46) | 116784.9 | 39260.91 | 124821.4 | 41009.2 | 58848 | 22639.24 | 67427.39 | 29168.44 | -1.28 | 1.13E-06 | 5.53E-06 | 0.09 | 0.739998 | 0.888787 |
| COMPOUND_996_7274a10_134578 | Rp | + | 996.7274 | 10.13 | | | | (1019.6891, 436.22)(1020.2083, 217.8)(1017.2995, 168.88)(1017.789, 157.67)(1014.8, 150.07)(997.6897, 183.2)(998.6761, 148.21)(499.3728, 32162.57)(499.876, 16325.82)(500.374, 6979.08)(500.8735, 2014.94)(501.3755, 414.13) | 341201.1 | 105446.6 | 272741.9 | 69657.62 | 364529.2 | 65424.96 | 374743.9 | 99540.63 | 0.52 | 0.051093 | 0.089195 | 0.43 | 0.178128 | 0.492203 |
| COMPOUND_997_4946a12_208357 | Rp | - | 997.4946 | 12.21 | | | | (1110.4624, 1132.24)(1111.4587, 785.1)(996.4891, 13036.41)(997.4928, 7150.63)(998.491, 7765.71)(999.4959, 4027.41)(1000.4914, 3253.93)(1001.4930, 1858.11)(1002.4951, 1281.28) | 147499.6 | 29836.89 | 141326.8 | 24456.51 | 139776.9 | 49869.14 | 122253.6 | 63849.39 | -0.41 | 0.155839 | 0.235695 | -0.12 | 0.720402 | 0.876947 |
| COMPOUND_998_6333a10_2881 | Rp | - | 998.6333 | 10.29 | | | | (997.6259, 9826.39)(998.6297, 5197.04)(999.6337, 1841.88)(1000.6354, 647.43)(1001.6572, 164.79) | 19955.64 | 6587.849 | 20658 | 8709.31 | 18611.08 | 5362.498 | 22597.6 | 8546.567 | -0.35 | 0.231771 | 0.326815 | 0.54 | 0.11901 | 0.408824 |
| COMPOUND_999_5143a12_421767 | Rp | - | 999.5143 | 12.42 | | | | (998.5038, 5490.17)(999.5084, 3441.4)(1000.506, 4855.77)(1001.5127, 2771.68)(1002.5084, 1904.36)(1003.5109, 1858.33)(1004.5087, 1362.98) | 46919.4 | 15904.9 | 39839.58 | 13346.92 | 40256.7 | 17190.28 | 57395.23 | 17461.78 | -0.25 | 0.364003 | 0.466024 | 0.73 | 0.027757 | 0.227301 |
| COMPOUND_1000_6486a10_379304 | Rp | - | 1000.6486 | 10.38 | | | | (999.6412, 51982.82)(1000.6445, 27133.7)(1001.6473, 9000.53)(1002.6509, 2044.62)(1003.6519, 525.74)(1004.6479, 123.74) | 166473.8 | 60489.2 | 166963.8 | 50853.35 | 128556.1 | 38391.22 | 148647.8 | 52460.12 | -0.72 | 0.015992 | 0.032444 | 0.36 | 0.307089 | 0.613089 |
| COMPOUND_1000_6509a10_3721895 | Rp | + | 1000.6509 | 10.37 | | | | (1023.638, 6253.57)(1024.638, 4109.66)(1025.6373, 1952.32)(1026.6534, 666.19)(1039.6033, 115.87)(1040.5927, 4372.56)(1001.6566, 9898.21)(1002.6596, 4896.66)(1003.6669, 1781.8)(1004.6806, 671.11)(1005.6681, 176.92) | 76298.04 | 26414.45 | 76395.48 | 27243.1 | 39634.15 | 15432.81 | 51399.94 | 22118.96 | -1.13 | 8.56E-05 | 0.000267 | 0.42 | 0.188073 | 0.504013 |
| COMPOUND_1004_6794a10_647412 | Rp | - | 1004.6794 | 10.65 | | | | (1003.6723, 41139.26)(1004.6757, 22964.71)(1005.6783, 7804.82)(1006.6793, 1817.54)(1007.6905, 517.35) | 139241.6 | 29490.76 | 147706.4 | 34557.15 | 76033.79 | 36802.44 | 79997.88 | 31468.18 | -1.35 | 5.8E-08 | 3.9E-07 | -0.12 | 0.637282 | 0.831083 |
| COMPOUND_1009_7204a9_927808 | Rp | + | 1009.7204 | 9.93 | | | | (1019.1796, 101.34)(1019.6879, 141.55)(504.8574, 265.63)(525.3698, 1911.16)(525.8648, 121.4)(526.3668, 1417.6)(1038.2471, 180.25)(1038.7307, 163.4)(1039.2444, 113.16)(516.8569, 5475.77)(517.3571, 3617.61)(517.86, 1192.81)(533.3692, 1361.74)(533.8734, 735.55)(514.3788, 43606.86)(514.8804, 23998.54)(515.3767, 12924.97)(515.8816, 2410.32)(516.3756, 782.85)(525.3712, 1903.09)(525.8571, 466.82)(526.3581, 1367.57)(1010.7196, 4550.29)(1011.7223, 2659.82)(1012.7228, 944.78)(1013.7235, 335.92)(1014.7082, 72.47)(505.8657, 15683.75)(506.368, 8917.06)(506.8691, 3174.5) | 787687.6 | 211204.2 | 679467.6 | 148957.2 | 855091.3 | 144107.5 | 872955.7 | 223716.7 | 0.23 | 0.404854 | 0.509063 | 0.69 | 0.044246 | 0.272788 |
| COMPOUND_1014_6712a10_116928 | Rp | + | 1014.6712 | 10.12 | | | | (1019.6547, 967.28)(1019.6573, 7175.09)(1039.6749, 563440.56)(530.3097, 3882.91)(530.7972, 1186.35)(531.3245, 3353.02)(1032.696, 93.27)(1033.7023, 252.27)(1053.6226, 2136.9)(1015.6738, 73053.36)(1016.6767, 37753.26)(1017.6779, 11807.49)(1018.6598, 4870.87)(1019.6701, 420.76)(508.3388, 12813.95)(508.8311, 1120.15)(509.3449, 3612.88)(509.8477, 738.9)(510.36, 3026.26) | 1886662 | 886419.8 | 2053240 | 840665.9 | 611636.1 | 274983.5 | 639546.1 | 377686.9 | -1.38 | 8.71E-10 | 9.81E-09 | -0.18 | 0.410757 | 0.694731 |
| COMPOUND_1016_6807a10_3650675 | Rp | + | 1016.6807 | 10.37 | | | | (1039.6683, 5456.83)(1040.6716, 3140.27)(1041.6761, 5915.1)(1042.6818, 4384.6)(1034.6987, 1179.54)(1035.688, 706.77)(1017.6903, 46877.29)(1018.6935, 25412.14)(1019.6993, 8583.36)(1020.6992, 2146.06)(1021.6894, 601.0)(509.3497, 3183.05)(509.8501, 1568.43) | 226461 | 61637.27 | 242495 | 62157.08 | 63317.25 | 32060.99 | 80562.21 | 37163.19 | -1.24 | 4.32E-08 | 3.02E-07 | -0.14 | 0.545976 | 0.77815 |
| COMPOUND_1020_6175a10_113955 | Rp | - | 1020.6175 | 10.11 | | | | (1019.6102, 40933.0)(1020.6133, 22641.46)(1021.6165, 7721.65)(1022.6225, 1889.1) | 114153.8 | 33642.56 | 113552.8 | 33014.26 | 73848.86 | 24843.94 | 86616.58 | 32801.14 | -1.21 | 3.56E-05 | 0.000124 | 0.41 | 0.215103 | 0.521996 |
| COMPOUND_1020_6177a10_137846 | Rp | + | 1020.6177 | 10.14 | | | | (1043.6053, 1525.32)(1044.586, 17486.55)(1032.6365, 1031.69)(1033.1246, 995.04)(1033.6216, 910.5)(1034.1287, 715.57)(533.3103, 392.91)(533.8219, 120.93)(534.296, 9060.22)(1059.5961, 1355.85)(1038.6573, 8735.42)(1021.6273, 16293.2)(1022.6327, 10728.72)(1023.6399, 4271.8)(1024.638, 1681.64)(511.3123, 2625.2)(511.8156, 1065.26)(512.313, 338.57) | 222510.1 | 33007.31 | 217314.2 | 36671.38 | 133872.9 | 34121.91 | 143045.1 | 48491.95 | -1.64 | 3.23E-11 | 6.39E-10 | 0.45 | 0.056586 | 0.295663 |
| COMPOUND_1022_2229a9_673863 | Rp | - | 1022.2229 | 9.67 | | | | (1021.2151, 32571.47)(1022.2195, 7992.21)(1023.2077, 1856.88)(1024.2231, 280.65)(1067.2083, 436.9)(1068.2094, 200.2)(1069.1823, 482.92) | 230566.5 | 33960.02 | 240353.7 | 38009.14 | 213537.1 | 43803.94 | 233723.2 | 34529.05 | -0.39 | 0.188062 | 0.276446 | 0.19 | 0.586233 | 0.79915 |
| COMPOUND_1023_7316a10_095456 | Rp | + | 1023.7316 | 10.10 | | | | (1043.6929, 223.38)(1044.2104, 140.46)(1044.7086, 59.54)(523.8644, 3476.63)(524.3733, 12819.21)(524.8648, 831.67)(540.3781, 1418.58)(540.882, 837.83)(541.3714, 1085.62)(541.8755, 235.45)(1024.7358, 6759.5)(1025.7382, 3800.85)(1026.7384, 1488.67)(1027.7363, 357.51)(512.8736, 11037.23)(513.3737, 6295.56)(513.8784, 2467.03) | 226596.6 | 74146.67 | 196918.4 | 51565 | 286446 | 35260.9 | 297558.6 | 70624.63 | 0.73 | 0.006568 | 0.014514 | 0.39 | 0.217347 | 0.524815 |
| COMPOUND_1024_7574a10_434175 | Rp | + | 1024.7574 | 10.43 | | | | (1025.726, 196.0)(513.3885, 7839.62)(513.8909, 4133.34)(514.3775, 4867.84)(514.8772, 911.57)(515.3691, 1107.36) | 109335.6 | 37043.36 | 97929.59 | 29466.19 | 130585.5 | 39092.4 | 124431.2 | 34074.59 | -0.97 | 0.000214 | 0.000631 | 0.57 | 0.056174 | 0.29488 |
| COMPOUND_1026_5424a10_198213 | Rp | + | 1026.5424 | 10.20 | | | | (1049.5684, 922.38)(1038.6113, 825.49)(1039.0958, 321.55)(1057.4962, 642.8)(1057.975, 42.34)(1027.5498, 1863.33)(1028.0491, 229.04)(1028.5566, 1032.36)(1029.0496, 95.85)(1029.5435, 775.5)(1030.0402, 91.72)(1030.5457, 297.19)(1036.1531, 1402.89)(1036.6462, 1820.74)(1037.1324, 478.84)(1055.0695, 453.07)(1055.5464, 389.98)(1065.4843, 265.25)(1066.4792, 144.93)(1044.5853, 12106.71)(1045.602, 11369.0)(1046.6094, 5616.31)(1047.611, 1779.69)(1048.6096, 558.62)(1027.5522, 2187.47)(1028.5583, 1140.38)(1029.5465, 846.36)(1030.5458, 341.93)(1031.5629, 43.92)(514.2775, 2163.95)(514.7788, 1036.77)(515.2798, 276.35)(515.7751, 99.56) | 52112.04 | 19277.08 | 56185.02 | 20190.44 | 23958 | 6007.281 | 17763.07 | 6641.928 | -1.45 | 1.08E-12 | 3.24E-12 | -0.12 | 0.522902 | 0.522902 |
| COMPOUND_1026_6403a10_160824 | Rp | - | 1026.6403 | 10.16 | | | | (1025.6335, 16209.99)(1026.6367, 8679.38)(1027.6333, 7517.2)(1028.6345, 3206.82)(1029.6372, 1009.49)(1030.6361, 198.24) | 87532.68 | 46265.52 | 80482.8 | 38490.45 | 60747.29 | 46984.79 | 60604.18 | 46950.38 | -1.15 | 1.88E-05 | 7.07E-05 | -0.02 | 0.954304 | 0.980661 |
| COMPOUND_1030_696a10_383612 | Rp | + | 1030.6960 | 10.38 | | | | (1053.6836, 2616.91)(1031.7035, 9476.59)(1032.7056, 5526.61)(1033.7065, 2213.97)(1034.6927, 867.64)(1035.7133, 103.43)(516.3585, 2618.07)(516.8548, 291.45)(517.3615, 890.35) | 80799.43 | 26145.52 | 83833.11 | 31992.67 | 26451.5 | 10075.06 | 25310.28 | 9470.864 | -1.42 | 2.85E-12 | 9.15E-11 | -0.16 | 0.393714 | 0.690408 |
| COMPOUND_1030_7301a10_632225 | Rp | + | 1030.7301 | 10.63 | | | | (530.8735, 2444.79)(531.3713, 2082.63)(531.8714, 712.05)(528.3941, 20638.12)(528.8957, 12373.01)(529.3878, 10171.7)(529.8912, 1469.88)(1076.6724, 864.37)(1077.6757, 460.44)(1038.7502, 3503.48)(1039.7533, 2209.78)(1040.7507, 945.92)(1041.7561, 77.9)(519.8814, 8412.21)(520.381, 1643.57)(520.8846, 1694.09) | 145106.2 | 51058.61 | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|-----------|-----------|----------------|----------|--------------|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_1042_6993a10_368553 | Rp | + | 1042.6993 | 10.37 | | | | (1065.6876, 4745.77) (1066.6909, 27842.24) (1067.6976, 29238.47) (1068.7, 13894.47) (1069.6885, 6023.95) (1043.7069, 451348.6) (1044.7112, 250218.55) (1045.7129, 81457.39) (1046.7144, 18016.57) (1047.7147, 3975.75) (1048.7047, 1014.55) | 2060465 | 694679.8 | 2086819 | 77796.3 | 486975.2 | 247440.9 | 623123 | 368265.9 | -1.72 | 2.5E-14 | 3.75E-12 | 0.18 | 0.367028 | 0.669574 |
| COMPOUND_1043_5793a10_248927 | Rp | + | 1043.5793 | 10.25 | | | | (1061.6074, 1342.32) (1062.5963, 1083.6) (1044.5854, 70259.56) (1045.5887, 40444.18) (1046.5914, 14053.05) | 493434.5 | 96858 | 436981.9 | 89360.55 | 542759.5 | 74748.01 | 549982.5 | 80941.06 | 0.51 | 0.047493 | 0.083952 | 0.66 | 0.032001 | 0.243467 |
| COMPOUND_1044_5898a10_241842 | Rp | + | 1044.5898 | 10.24 | | | | (1064.5604, 1804.85) (1065.0771, 553.61) (1065.5712, 1058.54) (1066.09, 541.78) (1066.5721, 1034.61) (1066.6189, 2804.61) (1067.1423, 728.55) (1067.6052, 2155.95) (1068.1108, 542.83) (1068.5994, 1272.56) (1069.0958, 459.26) (1069.5948, 1843.95) (1069.1318, 716.52) (1069.6047, 1005.05) (1069.1313, 1012.4) (1069.6322, 2558.74) (1069.1403, 1526.75) (1069.6807, 605.8) (1069.5905, 678.0) (1069.0865, 569.99) (1069.2787, 1508.98) (1069.7731, 688.88) (1069.543, 2765.1101.64) (1069.543, 7775, 348.71) (1069.5925, 433.13) (1069.5781, 437.12) (1069.583, 417.07) (1069.5876, 40071.02) (1069.5905, 14493.35) (1069.3026, 68383.26) (1069.3028, 33677.92) (1069.3034, 35749.46) (1069.3049, 18152.76) (1069.3053, 15786.26) (1069.3053, 7713.09) (1069.3017, 4791.31) (1069.3015, 1595.24) (1069.2999, 5615.76) | 914721.3 | 133846.8 | 829703.5 | 146873.4 | 898389.6 | 84320.05 | 909216.4 | 90442.38 | -0.25 | 0.372957 | 0.474788 | 0.87 | 0.009976 | 0.153413 |
| COMPOUND_1044_5939a10_125637 | Rp | + | 1044.5939 | 10.13 | | | | (1064.5928, 154.5) (1065.1143, 842.31) (1066.6208, 2300.63) (1067.1167, 1373.02) (1067.6102, 2196.99) (1068.1113, 1621.98) (1069.5836, 3297.66) (1070.0771, 300.35) (1070.1086, 812.03) (1073.6096, 1382.92) (1074.1337, 761.17) (1065.1134, 628.74) (1065.5919, 138.44) (1066.1302, 11646.09) (1068.5662, 2032.79) (1068.0813, 451.46) (1068.602, 2072.88) (1069.2959, 8601.04) (1069.534, 7981, 7009.51) (1069.535, 3001, 11056.33) (1069.8012, 4638.18) (1069.5306, 5002.43) (1069.8037, 2038.24) (1069.537, 2998, 2263.15) (1069.5669, 5700.34) (1069.6111, 19849.83) (1069.6196, 10176.84) (1069.622, 4294.8) (1069.6188, 1673.42) (1069.6129, 1558.35) (1069.6176, 1237.99) (1069.62816, 2036.97) (1069.622, 42805.41) (1069.623, 19916.34) (1069.624, 20308, 25051.48) (1069.624, 11850.21) (1069.623, 11366.72) (1069.623, 5332.93) (1069.623, 526.3016, 3961.29) (1069.6202, 2011.92) | 856840.4 | 107760.4 | 813041 | 132309.7 | 639385.2 | 158485.2 | 767009.7 | 217410.6 | -0.79 | 0.005414 | 0.012156 | 0.80 | 0.016204 | 0.189073 |
| COMPOUND_1044_6176a10_105027 | Rp | - | 1044.6176 | 10.11 | | | | (1157.5953, 1886.14) (1079.5605, 577.37) (1080.5643, 325.45) (1043.6101, 19019.02) (1044.6129, 11736.02) (1045.6168, 3870.94) (1046.6217, 1233.85) (1047.6309, 415.92) (1048.6438, 107.96) | 125370 | 29809.24 | 131767.9 | 39289.35 | 95103.79 | 38699.83 | 111509.6 | 48436.78 | -0.80 | 0.007372 | 0.016119 | 0.25 | 0.469079 | 0.734042 |
| COMPOUND_1046_727a10_64033 | Rp | + | 1046.7270 | 10.64 | | | | (1069.7178, 82444.88) (1070.7212, 48369.3) (1071.7166, 19190.94) (1072.71, 6680.41) (1047.7346, 993780.06) (1048.7384, 564931.06) (1049.7418, 178479.23) (1050.7433, 41029.23) (1051.7433, 8177.72) (1052.7393, 1909.09) | 3700068 | 1240544 | 3671931 | 1119289 | 469053.3 | 360520 | 427876.8 | 315734.5 | -1.55 | 1.44E-13 | 1.25E-11 | -0.08 | 0.685239 | 0.853695 |
| COMPOUND_1050_721a10_554148 | Rp | - | 1050.7210 | 10.55 | | | | (1085.7153, 77.75) (1086.7045, 260.08) (1087.701, 243.52) (1049.7137, 7253.72) (1050.7166, 4088.13) (1051.721, 1570.63) (1052.7158, 561.09) (1053.7217, 89.74) (1055.7354, 806.12) (1096.7372, 273.21) | 280607.8 | 11445.53 | 29162 | 11155.03 | 12356.5 | 3322.695 | 12757.8 | 1804.714 | -1.09 | 1.05E-07 | 6.48E-07 | -0.27 | 0.199707 | 0.511069 |
| COMPOUND_1051_763a10_412446 | Rp | + | 1051.7630 | 10.41 | | | | (1052.7661, 977.92) (1053.2467, 135.13) (1053.77, 552.68) (1054.2896, 84.65) (1072.3185, 301.3) (1072.8335, 94.57) (1073.878, 1312.17) (1073.8885, 3892.82) (1073.876, 434.32) (1073.4011, 1274.02) (1073.9043, 4111.08) (1073.386, 4216.11) (1073.8826, 443.82) (1073.3794, 1610.32) (1073.8131, 275.41) (1073.3917, 1876.36) (1073.8828, 2066.57) (1073.3933, 2530.08) (1073.7687, 1324.96) (1073.7711, 811.45) (1073.763, 313.92) (1073.749, 52.59) (1073.8873, 2469.13) (1073.8828, 2233.59) (1073.8878, 806.52) | 177453 | 49126.95 | 145832.9 | 33158.44 | 208517.3 | 41328.42 | 202185.4 | 63118.6 | 0.26 | 0.346317 | 0.447707 | 0.64 | 0.056127 | 0.29488 |
| COMPOUND_1052_5844a10_237459 | Rp | + | 1052.5844 | 10.24 | | | | (1064.559, 1800.46) (1065.0684, 518.83) (1065.5667, 1114.81) (1066.0856, 485.02) (1066.5671, 1072.19) (1066.5935, 1242.37) (1066.1108, 665.62) (1066.606, 878.95) (1066.1143, 665.23) (1066.1088, 417.49) (1066.623, 338.15) (1066.0952, 216.85) (1066.5769, 97.79) (1066.2837, 557.73) (1066.7993, 467.67) (1066.59, 1214.14) (1066.5994, 835.93) (1066.6097, 2490.27) (1066.3001, 4832.76) (1066.8008, 2314.72) (1066.3094, 11250.4) (1066.8055, 1845.57) (1066.3089, 4372.18) (1066.7969, 896.15) (1066.3121, 1485.88) (1066.807, 315.57) | 151308.5 | 41530.93 | 152105.2 | 20768.26 | 152973.7 | 36327.08 | 159431.2 | 28950.66 | -0.24 | 0.389666 | 0.493547 | 0.87 | 0.01271 | 0.172426 |
| COMPOUND_1053_7465a9_911521 | Rp | + | 1053.7465 | 9.91 | | | | (1054.7465, 1691.7) (1055.237, 69.3) (1056.8599, 272.66) (1057.3547, 743.28) (1057.8451, 644.91) (1058.3514, 514.56) (1058.8377, 277.6) (1059.225, 87.51) (1059.7491, 170.21) (1059.8701, 4154.19) (1059.3743, 3605.83) (1059.8723, 1094.42) (1059.3566, 184.25) (1059.3827, 1287.85) (1059.8858, 770.88) (1059.3798, 797.19) (1059.7454, 3631.63) (1059.7485, 2107.43) (1059.7512, 871.26) (1059.7493, 281.09) (1059.8795, 12147.13) (1059.7481, 7481.44) (1059.8836, 2970.22) | 846679.3 | 218980.5 | 737788 | 154824 | 913433.1 | 148725.4 | 922636.7 | 227497.5 | 0.24 | 0.393361 | 0.497827 | 0.64 | 0.063493 | 0.307286 |
| COMPOUND_1054_3676a9_157458 | Rp | - | 1054.3676 | 9.16 | | | | (1089.3416, 641.42) (1090.3436, 293.13) (1053.361, 44080.02) (1054.3647, 19966.87) (1055.369, 10003.46) (1056.3717, 3017.87) (1057.372, 748.26) (1058.3688, 185.66) | 19415.89 | 8016.267 | 24051.54 | 12663.03 | 94038.08 | 85176.27 | 58749.82 | 43654.87 | 1.54 | 3.14E-09 | 2.95E-08 | -0.88 | 0.001427 | 0.059516 |
| COMPOUND_1054_5461a5_432122 | Rp | + | 1054.5461 | 5.43 | | | | (1057.2589, 905.62) (1057.7567, 575.47) (1058.2626, 126.58) (1059.2732, 273.89) (1059.7646, 158.41) (1055.5527, 339.29) (1056.5533, 247.96) (1058.2818, 15551.89) (1058.7836, 9313.14) (1059.2849, 3320.43) (1059.7836, 1026.59) (1059.30285, 315.4) (1059.7824, 63.37) | 48990.91 | 44962.71 | 71509.97 | 70186.03 | 12816 | #DIV/0! | 13201 | 2789.776 | -0.83 | 6.7E-05 | 0.000215 | -0.41 | 0.079756 | 0.339484 |
| COMPOUND_1054_7773a10_289623 | Rp | + | 1054.7773 | 10.29 | | | | (1077.737, 163.85) (1078.2217, 140.66) (1078.7164, 176.12) (1077.729, 340.75) (1079.3868, 1498.95) (1079.8766, 520.76) (1079.369, 5360.99) (1079.8842, 879.85) (1079.8127, 105.5) (1079.8911, 579.32) (1079.3942, 1134.85) (1079.7295, 188.92) (1079.3945, 12408.25) (1079.8957, 7114.96) (1079.3849, 16280.99) (1079.8837, 2090.68) (1079.3686, 273.94) | 162065.4 | 65970.21 | 119934 | 40484.28 | 162868.1 | 44391.39 | 189558.7 | 66831.57 | -0.23 | 0.406366 | 0.510394 | 0.58 | 0.086046 | 0.348516 |
| COMPOUND_1060_6418a10_100553 | Rp | + | 1060.6418 | 10.10 | | | | (1083.6375, 4373.85) (1084.1332, 2044.28) (1084.6278, 2283.36) (1085.1204, 965.09) (1085.6523, 16583.19) (1086.1298, 1325.46) (1072.6309, 2541.53) (1073.1285, 1146.07) (1073.6357, 1838.21) (1074.1307, 1525.41) (1083.6343, 3564.61) (1084.6337, 1904.58) (1085.653, 14986.12) (1086.6562, 11254.09) (1087.6718, 79635.05) (1088.6747, 46553.86) (1089.6758, 16388.35) (1080.5879, 3717.17) (1081.1127, 1496.95) (1081.5898, 2894.64) (1082.117, 1244.76) (1082.6245, 1711.94) (1091.6349, 12364.53) (1092.132, 6236.81) (1091.3012, 4710.66) (1091.7961, 3245.35) (1092.2899, 3044.9) (1092.787, 1510.61) (1089.1152, 1041.53) (1089.617, 223.32) (1090.1257, 3493.54) (1091.3013, 1837.49) (1091.7961, 1157.46) (1091.6552, 24615.28) (1092.6584, 20607.58) (1093.6757, 439281.58) (1093.3256, 7993.39) (1093.8279, 4388.07) (1093.3271, 4541.58) (1093.8282, 2211.12) (1093.3289, 1069.5) (1093.8272, 384.6) | 1002624 | 367506 | 991184.5 | 316743.6 | 295526.1 | 127747.2 | 349238.4 | 207650.2 | -1.53 | 3.85E-11 | 7.54E-10 | 0.03 | 0.887399 | 0.953446 |
| COMPOUND_1060_669a10_133247 | Rp | - | 1060.6690 | 10.13 | | | | (1059.6625, 77633.11) (1060.6656, 43884.13) (1061.6683, 14900.43) (1062.6704, 3472.79) (1063.6727, 1007.99) (1064.6759, 194.64) | 311983.4 | 78428.12 | 349574.7 | 69720.59 | 170189 | 42703.95 | 166681.1 | 56800.62 | -1.31 | 4.16E-09 | 3.78E-08 | -0.40 | 0.080955 | 0.340768 |
| COMPOUND_1063_67a10_101033 | Rp | + | 1063.6700 | 10.10 | | | | (1086.6573, 13021.73) (1087.6285, 7586.99) (1088.6335, 6130.7) (1089.6351, 5516.27) (1089.1356, 3690.76) (1089.6375, 315.87) (1089.6392, 2659.61) (1089.6394, 7664.79) (1089.6256, 2347.22) (1089.6708, 3064.72) (1089.6761, 1117.38) (1089.6731, 173.32) (1089.6807, 53.34) (1089.6824, 1809.21) (1089.6835, 1081.19) (1089.6806, 195.73) | 416342.2 | 171568 | 408402.6 | 144432.2 | 128955.8 | 52348.97 | 150753.7 | 89217.51 | -1.57 | 3.71E-12 | 1.13E-10 | 0.13 | 0.556443 | 0.781554 |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|-----------|-----------|----------------|----------|--------------|---|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_1067_7596a10_07238 | Rp | + | 1067.7596 | 10.07 | | | | (553.8711, 408.72)(554.3957, 7050.24)(1106.7122, 319.75)(1107.2314, 88.8)(545.8784, 3817.31)(546.3893, 895.95)(546.8797, 1091.74)(547.3906, 466.55)(543.3998, 39804.82)(543.3923, 2153.88)(544.3972, 4364.65)(544.9001, 1569.49)(1085.7598, 119.59)(1086.7412, 113.6)(562.3917, 1583.3)(562.8952, 1203.42)(1085.7719, 165.49)(1086.2906, 257.74)(1068.7618, 3928.47)(1069.7653, 2303.33)(1070.7668, 1033.85)(1071.7676, 363.6)(554.3953, 5319.88)(554.8779, 677.12)(534.8865, 13066.96)(535.388, 9703.53)(535.8899, 2967.3)(1103.5648, 533.76)(1104.5417, 483.08)(1105.5557, 134.02)(1067.6099, 7699.94)(1068.6129, 4799.97)(1069.6117, 1845.86)(1070.6191, 565.17)(1071.6403, 177.47)(1096.5927, 1751.88)(1074.5951, 8465.68)(1075.5974, 6251.72)(1076.5986, 2644.55)(1077.5992, 1022.75)(537.8092, 894.93)(538.2066, 2114.92)(1072.815, 36494.11)(1073.8185, 23919.27)(1074.8214, 8665.76)(1075.8254, 2271.5)(1076.8254, 680.36)(1077.8145, 132.28)(1118.804, 354.06)(1119.8195, 208.13)(535.9018, 536.4)(536.3867, 188.84)(536.8988, 277.96)(1189.1545, 208.83)(1190.1405, 239.81)(1111.1934, 253.44)(1112.1841, 123.03)(1075.1998, 6477.11)(1076.2023, 2471.08)(1077.2008, 2547.79)(1078.2018, 916.75)(1079.2098, 343.84)(1080.208, 312.71)(1081.1904, 182.79)(1099.5715, 2902.96)(1100.0836, 618.09)(1096.5962, 2053.91)(1097.106, 870.64)(1097.5867, 1712.5)(1098.097, 670.52)(1107.5848, 3375.67)(1108.096, 958.12)(1077.623, 2898.34)(1078.128.854)(1078.6295, 13577.36)(1079.1316, 10996.87)(1079.6339, 6880.16)(1105.0936, 950.25)(1105.5709, 4684.42)(1106.0825, 717.02)(558.2953, 8024.97)(558.7973, 8731.9)(559.2994, 15751.36)(559.8018, 6369.38)(560.3017, 7108.34)(560.8028, 3341.48)(561.3008, 2711.92)(1115.5972, 2658.93)(1116.1263, 684.26)(1116.5786, 14182.69)(561.3011, 1719.29)(561.7918, 870.68)(562.31, 6778.45)(562.8086, 4206.62)(563.3114, 4849.26)(550.2921, 4113.49)(550.7913, 2295.34)(551.309, 16676.01)(551.8098, 4083.42)(552.3139, 8424.76)(1077.6176, 2613.56)(539.3132, 14304.0)(539.8176, 7625.98)(540.3099, 5245.74)(540.8068, 2018.03)(541.3012, 3568.06)(1075.7295, 11208.55)(1076.7336, 6977.42)(1077.734, 2470.33)(1078.7323, 632.68)(1079.7443, 156.82)(1121.7177, 117.6)(1122.6818, 839.15)(1098.5948, 4693.71)(1081.5653, 19196.84)(1082.5627, 15154.54)(560.8721, 270.86)(561.3791, 1128.92)(561.8911, 294.08)(552.8857, 3707.96)(553.3887, 371377.1)(95107.54, 315124.8, 73104.42, 463706.3, 752157.9, 465181.5, 110690.6, 372.49)(553.8883, 885.63)(569.3958, 1457.21)(569.9009, 415.35)(1099.7684, 177.85)(550.4089, 28097.02)(550.9106, 17241.8)(551.4097, 7099.86)(551.909, 2222.31)(552.4079, 736.4)(1120.705, 238.79)(1082.777, 491.83)(1083.7806, 2034.01)(1084.7784, 886.92)(1085.7695, 313.99)(541.8948, 9498.85)(542.3962, 6597.29)(542.8989, 2191.82)(1081.696, 12669.65)(1082.6993, 7036.84)(1083.696, 5977.67)(1084.6984, 2801.55)(1085.699, 798.44)(562.8549, 404.23)(561.8796, 569.84)(562.3659, 430.24)(553.876, 2534.34)(554.3842, 3004.87)(554.8763, 755.32)(555.3596, 196.72)(551.3989, 13280.33)(551.9, 7758.32)(552.3994, 3269.71)(552.8978, 1050.79)(570.386, 578.68)(570.8894, 451.41)(1101.7623, 94.64)(1102.2771, 333.74)(562.3753, 566.22)(562.8637, 364.41)(1084.7559, 1318.01)(1085.7588, 839.38)(1086.757, 313.45)(1087.7611, 109.74)(542.8848, 9060.38)(543.3878, 5867.67)(543.8877, 2253.51)(1083.6633, 202087.77)(1084.6666, 117553.05)(1085.669, 38922.19)(1086.6715, 9253.99)(1087.6731, 2197.4)(1088.6715, 363.67)(1102.1315, 3630.56)(1102.6305, 5194.77)(1103.1317, 4040.44)(1103.6302, 3113.48)(1113.0988, 431.05)(1113.6288, 826.26)(1114.102, 717.25)(1121.0801, 763.91)(1121.5743, 1423.39)(1122.0739, 685.62)(1131.5667, 4405.65)(1132.079, 772.67)(1132.5734, 2046.08)(1133.0854, 579.07)(1133.5712, 1393.12)(1134.0919, 347.49)(1134.564, 1045.2)(558.2953, 8024.97)(558.7973, 8731.9)(559.2994, 15751.36)(559.8018, 6369.38)(560.3017, 7108.34)(560.8028, 3341.48)(561.3008, 2711.92)(561.7967, 1687.43)(1131.5647, 8025.87)(1132.5634, 3374.53)(1133.5623, 1544.67)(555.7964, 4881.4)(556.2977, 3827.84)(556.7949, 1782.45)(1093.5883, 6796.05)(1094.5886, 2712.39)(1095.5857, 1172.53)(1096.5893, 161.35)(585.2347, 5479.09)(585.7362, 576.33)(547.302, 29909.7)(547.8034, 14633.33)(548.302, 14773.35)(548.8034, 6654.05)(549.3012, 6329.88)(549.7957, 3678.69)(550.2866, 3832.51)(1205.7405, 1016.5)(1206.7592, 481.81)(1207.7681, 508.3)(1091.7257, 190107.83)(1092.7288, 109704.0)(1093.7313, 36525.83)(1094.7344, 9033.92)(1095.7384, 2018.13)(1096.7408, 538.49)(1097.724, 115.08)(1117.7344, 383.33)(1118.7404, 212.94)(1119.7411, 171.64)(1115.2618, 189.43)(1115.78, 909216.2)(257404.1, 780178.7, 178248.6, 986437.2, 169061.9, 992926.3, 246040.3, 250.31)(559.3946, 3476.41)(559.888, 712.36)(560.3772, 626.26)(575.9122, 172.94)(576.3863, 631.02)(576.8773, 642.74)(1112.787, 2533.23)(1113.7906, 1674.34)(1114.79, 670.52)(1115.7974, 228.14)(567.8937, 2918.73)(568.4, 3463.46)(568.8939, 519.76)(569.3793, 61.06)(1095.7667, 293.32)(1096.7583, 203.49)(548.3859, 4401.79)(548.8874, 1552.54)(549.3912, 9760.56)(549.8918, 1021.49)(550.4031, 6344.51)(1128.7645, 139.16)(1129.246, 270.76)(568.8448, 136.52)(569.3448, 5448.52)(560.8847, 819029.8)(212133.8, 712792.8, 154891.6, 852830.3, 158252.7, 864609.3, 216123.7, 3556.76)(561.3843, 2822.82)(561.8843, 1156.22)(562.3769, 463.35)(577.3977, 1390.71)(577.899, 828.24)(569.3948, 1546.53)(569.8793, 365.44)(570.3933, 1213.89)(570.8996, 833.47)(571.3848, 1132.71)(1098.7704, 2174.99)(1099.773, 1405.55)(1100.7765, 543.18)(1101.7872, 157.43)(549.8928, 5640.34)(550.3947, 4038.03)(550.8965, 1664.81)(551.3813, 240.41)(1135.7767, 202.01)(1133.2784, 113.81)(1133.7513, 121.76)(576.4033, 2144.11)(576.907, 174609.8)(50426.29, 123864.2, 32112.4, 182619, 61394.49, 186823.8, 65935.3, 1785.36)(577.407, 2153.92)(568.4076, 3009.69)(568.8919, 646.91)(569.399, 2302.51)(569.9039, 1296.49)(570.3963, 1176.62)(576.9074, 1216.05)(577.4065, 1326.45)(1113.772, 202.56)(557.4142, 15260.35)(557.9164, 8724.96)(558.4049, 9150.74)(558.9073, 1895.11)(559.3983, 2228.09)(580.9132, 749.48)(581.4029, 869.82)(574.8989, 4749.52)(575.3991, 3372.29)(575.899, 1182.1)(576.3821, 234.01)(577.4217, 16814.04)(577.9243, 10806.01)(578.4209, 5439.7)(579.9210, 1640.04)(574.418, 370.69)(591.4175, 3966.29)(591.9118, 888.23)(583.4142, 6371.76)(583.9034, 525.44)(584.4101, 2429.62)(584.9101, 983.25)(1126.8038, 2314.96)(1127.8053, 1482.08)(1128.8074, 691.01)(1129.801, 201.19)(1130.8136, 41.68)(601.8511, 78.76)(602.326, 279.79)(563.9079, 12193.92)(564.4105, 8066.71)(564.9114, 2906.45) | 721025.4 | 221903.3 | 603945.5 | 136739.3 | 863539.3 | 129468.5 | 868073.9 | 205594.3 | 0.35 | 0.211831 | 0.304237 | 0.60 | 0.071857 | 0.325554 |
| COMPOUND_1068_6165a10_101867 | Rp | - | 1068.6165 | 10.10 | | | | (1103.5648, 533.76)(1104.5417, 483.08)(1105.5557, 134.02)(1067.6099, 7699.94)(1068.6129, 4799.97)(1069.6117, 1845.86)(1070.6191, 565.17)(1071.6403, 177.47)(1096.5927, 1751.88)(1074.5951, 8465.68)(1075.5974, 6251.72)(1076.5986, 2644.55)(1077.5992, 1022.75)(537.8092, 894.93)(538.2066, 2114.92)(1072.815, 36494.11)(1073.8185, 23919.27)(1074.8214, 8665.76)(1075.8254, 2271.5)(1076.8254, 680.36)(1077.8145, 132.28)(1118.804, 354.06)(1119.8195, 208.13)(535.9018, 536.4)(536.3867, 188.84)(536.8988, 277.96)(1189.1545, 208.83)(1190.1405, 239.81)(1111.1934, 253.44)(1112.1841, 123.03)(1075.1998, 6477.11)(1076.2023, 2471.08)(1077.2008, 2547.79)(1078.2018, 916.75)(1079.2098, 343.84)(1080.208, 312.71)(1081.1904, 182.79)(1099.5715, 2902.96)(1100.0836, 618.09)(1096.5962, 2053.91)(1097.106, 870.64)(1097.5867, 1712.5)(1098.097, 670.52)(1107.5848, 3375.67)(1108.096, 958.12)(1077.623, 2898.34)(1078.128.854)(1078.6295, 13577.36)(1079.1316, 10996.87)(1079.6339, 6880.16)(1105.0936, 950.25)(1105.5709, 4684.42)(1106.0825, 717.02)(558.2953, 8024.97)(558.7973, 8731.9)(559.2994, 15751.36)(559.8018, 6369.38)(560.3017, 7108.34)(560.8028, 3341.48)(561.3008, 2711.92)(1115.5972, 2658.93)(1116.1263, 684.26)(1116.5786, 14182.69)(561.3011, 1719.29)(561.7918, 870.68)(562.31, 6778.45)(562.8086, 4206.62)(563.3114, 4849.26)(550.2921, 4113.49)(550.7913, 2295.34)(551.309, 16676.01)(551.8098, 4083.42)(552.3139, 8424.76)(1077.6176, 2613.56)(539.3132, 14304.0)(539.8176, 7625.98)(540.3099, 5245.74)(540.8068, 2018.03)(541.3012, 3568.06)(1075.7295, 11208.55)(1076.7336, 6977.42)(1077.734, 2470.33)(1078.7323, 632.68)(1079.7443, 156.82)(1121.7177, 117.6)(1122.6818, 839.15)(1098.5948, 4693.71)(1081.5653, 19196.84)(1082.5627, 15154.54)(560.8721, 270.86)(561.3791, 1128.92)(561.8911, 294.08)(552.8857, 3707.96)(553.3887, 371377.1)(95107.54, 315124.8, 73104.42, 463706.3, 752157.9, 465181.5, 110690.6, 372.49)(553.8883, 885.63)(569.3958, 1457.21)(569.9009, 415.35)(1099.7684, 177.85)(550.4089, 28097.02)(550.9106, 17241.8)(551.4097, 7099.86)(551.909, 2222.31)(552.4079, 736.4)(1120.705, 238.79)(1082.777, 491.83)(1083.7806, 2034.01)(1084.7784, 886.92)(1085.7695, 313.99)(541.8948, 9498.85)(542.3962, 6597.29)(542.8989, 2191.82)(1081.696, 12669.65)(1082.6993, 7036.84)(1083.696, 5977.67)(1084.6984, 2801.55)(1085.699, 798.44)(562.8549, 404.23)(561.8796, 569.84)(562.3659, 430.24)(553.876, 2534.34)(554.3842, 3004.87)(554.8763, 755.32)(555.3596, 196.72)(551.3989, 13280.33)(551.9, 7758.32)(552.3994, 3269.71)(552.8978, 1050.79)(570.386, 578.68)(570.8894, 451.41)(1101.7623, 94.64)(1102.2771, 333.74)(562.3753, 566.22)(562.8637, 364.41)(1084.7559, 1318.01)(1085.7588, 839.38)(1086.757, 313.45)(1087.7611, 109.74)(542.8848, 9060.38)(543.3878, 5867.67)(543.8877, 2253.51)(1083.6633, 202087.77)(1084.6666, 117553.05)(1085.669, 38922.19)(1086.6715, 9253.99)(1087.6731, 2197.4)(1088.6715, 363.67)(1102.1315, 3630.56)(1102.6305, 5194.77)(1103.1317, 4040.44)(1103.6302, 3113.48)(1113.0988, 431.05)(1113.6288, 826.26)(1114.102, 717.25)(1121.0801, 763.91)(1121.5743, 1423.39)(1122.0739, 685.62)(1131.5667, 4405.65)(1132.079, 772.67)(1132.5734, 2046.08)(1133.0854, 579.07)(1133.5712, 1393.12)(1134.0919, 347.49)(1134.564, 1045.2)(558.2953, 8024.97)(558.7973, 8731.9)(559.2994, 15751.36)(559.8018, 6369.38)(560.3017, 7108.34)(560.8028, 3341.48)(561.3008, 2711.92)(561.7967, 1687.43)(1131.5647, 8025.87)(1132.5634, 3374.53)(1133.5623, 1544.67)(555.7964, 4881.4)(556.2977, 3827.84)(556.7949, 1782.45)(1093.5883, 6796.05)(1094.5886, 2712.39)(1095.5857, 1172.53)(1096.5893, 161.35)(585.2347, 5479.09)(585.7362, 576.33)(547.302, 29909.7)(547.8034, 14633.33)(548.302, 14773.35)(548.8034, 6654.05)(549.3012, 6329.88)(549.7957, 3678.69)(550.2866, 3832.51)(1205.7405, 1016.5)(1206.7592, 481.81)(1207.7681, 508.3)(1091.7257, 190107.83)(1092.7288, 109704.0)(1093.7313, 36525.83)(1094.7344, 9033.92)(1095.7384, 2018.13)(1096.7408, 538.49)(1097.724, 115.08)(1117.7344, 383.33)(1118.7404, 212.94)(1119.7411, 171.64)(1115.2618, 189.43)(1115.78, 909216.2)(257404.1, 780178.7, 178248.6, 986437.2, 169061.9, 992926.3, 246040.3, 250.31)(559.3946, 3476.41)(559.888, 712.36)(560.3772, 626.26)(575.9122, 172.94)(576.3863, 631.02)(576.8773, 642.74)(1112.787, 2533.23)(1113.7906, 1674.34)(1114.79, 670.52)(1115.7974, 228.14)(567.8937, 2918.73)(568.4, 3463.46)(568.8939, 519.76)(569.3793, 61.06)(1095.7667, 293.32)(1096.7583, 203.49)(548.3859, 4401.79)(548.8874, 1552.54)(549.3912, 9760.56)(549.8918, 1021.49)(550.4031, 6344.51)(1128.7645, 139.16)(1129.246, 270.76)(568.8448, 136.52)(569.3448, 5448.52)(560.8847, 819029.8)(212133.8, 712792.8, 154891.6, 852830.3, 158252.7, 864609.3, 216123.7, 3556.76)(561.3843, 2822.82)(561.8843, 1156.22)(562.3769, 463.35)(577.3977, 1390.71)(577.899, 828.24)(569.3948, 1546.53)(569.8793, 365.44)(570.3933, 1213.89)(570.8996, 833.47)(571.3848, 1132.71)(1098.7704, 2174.99)(1099.773, 1405.55)(1100.7765, 543.18)(1101.7872, 157.43)(549.8928, 5640.34)(550.3947, 4038.03)(550.8965, 1664.81)(551.3813, 240.41)(1135.7767, 202.01)(1133.2784, 113.81)(1133.7513, 121.76)(576.4033, 2144.11)(576.907, 174609.8)(50426.29, 123864.2, 32112.4, 182619, 61394.49, 186823.8, 65935.3, 1785.36)(577.407, 2153.92)(568.4076, 3009.69)(568.8919, 646.91)(569.399, 2302.51)(569.9039, 1296.49)(570.3963, 1176.62)(576.9074, 1216.05)(577.4065, 1326.45)(1113.772, 202.56)(557.4142, 15260.35)(557.9164, 8724.96)(558.4049, 9150.74)(558.9073, 1895.11)(559.3983, 2228.09)(580.9132, 749.48)(581.4029, 869.82)(574.8989, 4749.52)(575.3991, 3372.29)(575.899, 1182.1)(576.3821, 234.01)(577.4217, 16814.04)(577.9243, 10806.01)(578.4209, 5439.7)(579.9210, 1640.04)(574.418, 370.69)(591.4175, 3966.29)(591.9118, 888.23)(583.4142, 6371.76)(583.9034, 525.44)(584.4101, 2429.62)(584.9101, 983.25)(1126.8038, 2314.96)(1127.8053, 1482.08)(1128.8074, 691.01)(1129.801, 201.19)(1130.8136, 41.68)(601.8511, 78.76)(602.326, 279.79)(5 | | | | | | | | | | | | | | |

| Compound | Column | Ion mode | Mass | Retention | Identification | ID level | MSMS spectra | CompositeSpectrum | 1st trimester | | | | 3rd trimester | | | | Time | | | Interaction | | |
|------------------------------|--------|----------|-----------|-----------|----------------|----------|--------------|--|---------------|----------|---------------|----------|---------------|----------|---------------|----------|-------|----------|----------|-------------|----------|----------|
| | | | | | | | | | Control | | Pre-eclampsia | | Control | | Pre-eclampsia | | Value | raw p | FDR p | Value | raw p | FDR p |
| | | | | | | | | | Mean | SD | Mean | SD | Mean | SD | Mean | SD | | | | | | |
| COMPOUND_1135_618a10_640722 | Rp | + | 1135.6180 | 10.64 | | | | (1158.6073, 5359.03) (1159.6107, 4493.61) (1160.6086, 3544.94) (1174.6038, 1564.32) (1153.6445, 1265.47) (1154.641, 877.53) (1155.6536, 389.09) (1136.6241, 12167.77) (1137.6304, 8170.6) (1138.6254, 7202.92) (1139.627, 3439.31) (1140.623, 1162.42) | 120221.4 | 32875.35 | 107679.3 | 28744.9 | 114646.3 | 24804.53 | 114926.2 | 40237.71 | 0.06 | 0.826559 | 0.877196 | 0.31 | 0.355709 | 0.665596 |
| COMPOUND_1139_8173a10_349059 | Rp | + | 1139.8173 | 10.35 | | | | (589.9019, 471.03) (590.995, 1413.58) (590.9121, 1139.2) (581.907, 2267.04) (582.4121, 2759.03) (582.9068, 699.86) (583.3902, 658.65) (579.4255, 10886.18) (579.9286, 6591.55) (580.4186, 4284.01) (580.921, 1834.89) (581.4061, 1851.74) (598.4163, 1877.53) (598.9178, 1909.34) (1140.8195, 1305.2) (1141.8248, 983.31) (1142.821, 516.49) (570.9137, 3118.54) (571.4134, 2930.65) (571.9162, 1130.5) | 308681.7 | 86199.11 | 244989.3 | 64473.16 | 331206.7 | 54955.86 | 319804.2 | 85051.64 | 0.39 | 0.168598 | 0.252094 | 0.43 | 0.203328 | 0.5149 |
| COMPOUND_1154_5446a10_36111 | Rp | + | 1154.5446 | 10.36 | | | | (1177.545, 634.31) (1178.0344, 77.94) (1178.556, 510.87) (1177.5481, 588.38) (1178.5577, 500.63) (1179.5614, 553.87) (1185.5674, 507.87) (1186.0498, 62.64) (600.2574, 3648.8) (600.7514, 463.46) (601.2545, 3340.36) (589.2682, 1078.0) (589.7702, 706.71) (590.2758, 1525.67) (590.7855, 1899.1) (591.2713, 2003.17) (591.7709, 1288.26) (1172.5641, 577.26) (1173.0483, 342.53) (1173.5588, 591.42) (1174.0701, 236.43) (1174.5397, 275.52) (1175.0441, 219.24) (1155.5796, 2098.6) (578.282, 6155.0) (578.7826, 2043.11) (579.2846, 3103.0) (579.7949, 1319.72) (580.2853, 3786.11) (580.7884, 606.74) (581.2788, 6485.33) (581.771, 307.91) (582.2822, 2576.89) | 216308.6 | 42864.62 | 208567 | 52443.97 | 139050.6 | 14067.04 | 138835.6 | 21397.38 | -0.15 | 0.581683 | 0.678028 | -0.02 | 0.94447 | 0.974642 |
| COMPOUND_1155_8156a10_045544 | Rp | + | 1155.8156 | 10.05 | | | | (597.8999, 318.72) (598.4212, 2560.46) (589.9068, 4501.87) (590.4055, 3619.3) (590.9076, 1117.93) (591.4004, 448.51) (606.4133, 1756.01) (606.9207, 931.25) (607.4234, 1643.83) (1156.8132, 1718.11) (1157.817, 1284.87) (1158.8204, 613.14) (1159.8015, 149.59) (598.4237, 5518.46) (598.9139, 288.89) (578.9128, 12407.64) (579.4141, 11908.36) (579.9177, 3632.77) | 803967 | 221970.5 | 681474.7 | 164885.6 | 893279.8 | 155693.7 | 891624 | 218532.9 | 0.32 | 0.256236 | 0.352716 | 0.66 | 0.050463 | 0.283798 |
| COMPOUND_1169_8315a10_19566 | Rp | + | 1169.8315 | 10.20 | | | | (1198.3396, 71.81) (1198.8466, 79.58) (604.91, 238.48) (605.4003, 1366.28) (605.8941, 532.79) (596.9132, 5402.94) (597.4151, 4440.27) (597.9148, 1514.18) (594.4347, 29400.79) (594.9364, 18793.95) (595.4363, 7963.57) (595.9364, 2667.37) (596.4317, 947.21) (1208.7393, 270.52) (613.4303, 3221.18) (613.9255, 598.33) (614.4215, 2633.11) (614.9282, 384.01) (615.4315, 1444.74) (1170.8298, 1899.79) (1171.8336, 1230.54) (1172.8328, 583.6) (1173.8323, 217.69) (585.9219, 10477.1) (586.4236, 7273.27) (586.9259, 2806.01) | 566638.2 | 155890.6 | 479553.9 | 108583.6 | 646033.6 | 112773.8 | 638014.1 | 161511.6 | 0.36 | 0.187928 | 0.27643 | 0.65 | 0.052504 | 0.286293 |
| COMPOUND_1170_8593a10_492284 | Rp | + | 1170.8593 | 10.49 | | | | (597.4275, 7652.67) (597.9165, 1094.25) (598.4064, 4611.57) (598.9242, 2375.38) (613.9326, 1506.34) (614.4277, 1992.0) (614.9235, 797.14) (1171.7983, 155.84) (586.4361, 14807.61) (586.938, 9199.98) (587.4321, 5651.45) (587.9258, 2304.84) | 110801.4 | 31829.81 | 91129.23 | 25444.52 | 124195 | 26801.78 | 120069.1 | 33408.53 | 0.41 | 0.114775 | 0.183836 | 0.57 | 0.066707 | 0.313621 |
| COMPOUND_1185_279a9_739681 | Rp | + | 1185.2790 | 9.74 | | | | (1208.2289, 409.23) (1186.289, 6912.78) (1187.2909, 2907.3) (1188.297, 715.75) (1189.3033, 137.45) | 74950.3 | 13891.02 | 70200.65 | 13748.68 | 78099.93 | 10306.86 | 75789.96 | 18387.84 | 0.23 | 0.43537 | 0.540195 | 0.15 | 0.680752 | 0.853001 |
| COMPOUND_1197_8564a10_469222 | Rp | + | 1197.8564 | 10.47 | | | | (1209.8568, 98.58) (1210.3401, 75.16) (1198.8555, 480.05) (1199.362, 56.35) (1199.8634, 453.31) (618.9232, 505.29) (619.4175, 1296.3) (1236.7979, 117.54) (1237.2968, 104.15) (610.9269, 1905.82) (611.4286, 2407.73) (611.9191, 764.48) (608.4492, 11746.91) (608.9518, 7671.42) (609.4459, 4092.41) (609.9421, 1827.04) (610.4444, 307.61) (1198.861, 523.01) (1199.8667, 459.77) (1200.8691, 215.83) (599.9352, 3426.26) (600.4304, 3271.9) (600.9356, 1190.42) | 148884.4 | 38233.61 | 129892.2 | 27483.85 | 177960.5 | 38360.54 | 177035 | 46809.84 | 0.54 | 0.043004 | 0.076617 | 0.56 | 0.077534 | 0.333235 |

Legend: ACar, acetylcarnitine; FA, fatty acid; MAG, monoacylglyceride; PC, phosphatidylcholine; PE, phosphatidylethanolamine; p-values are from linear mixed model (both raw and FDR corrected are shown)