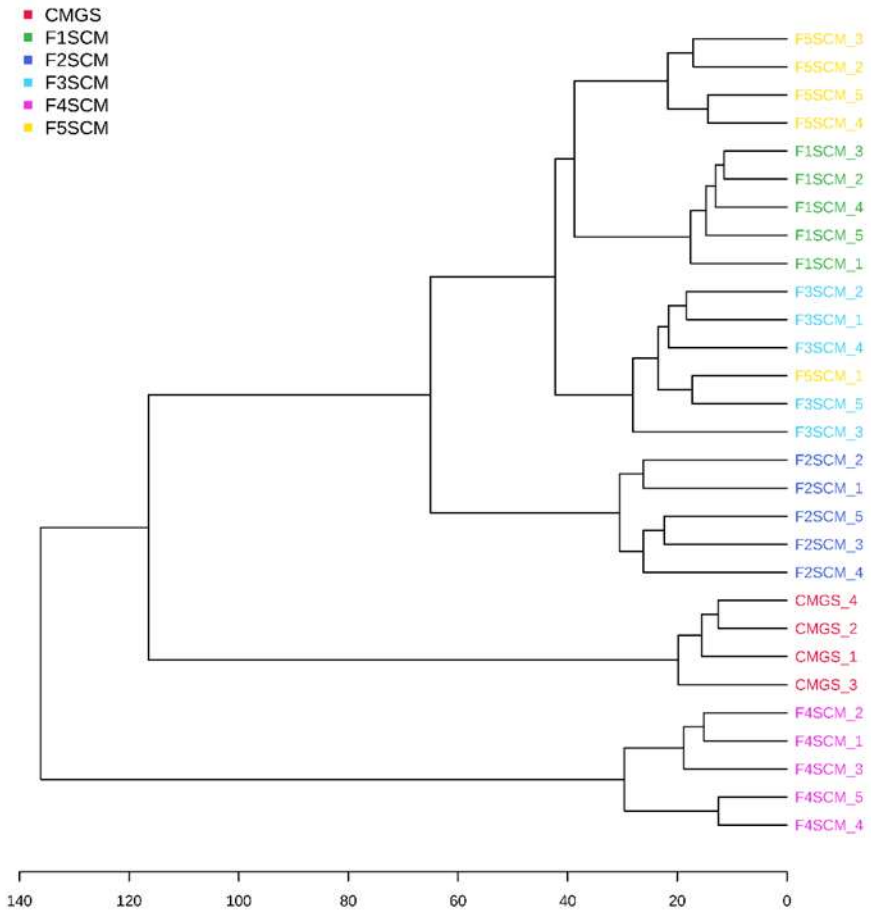
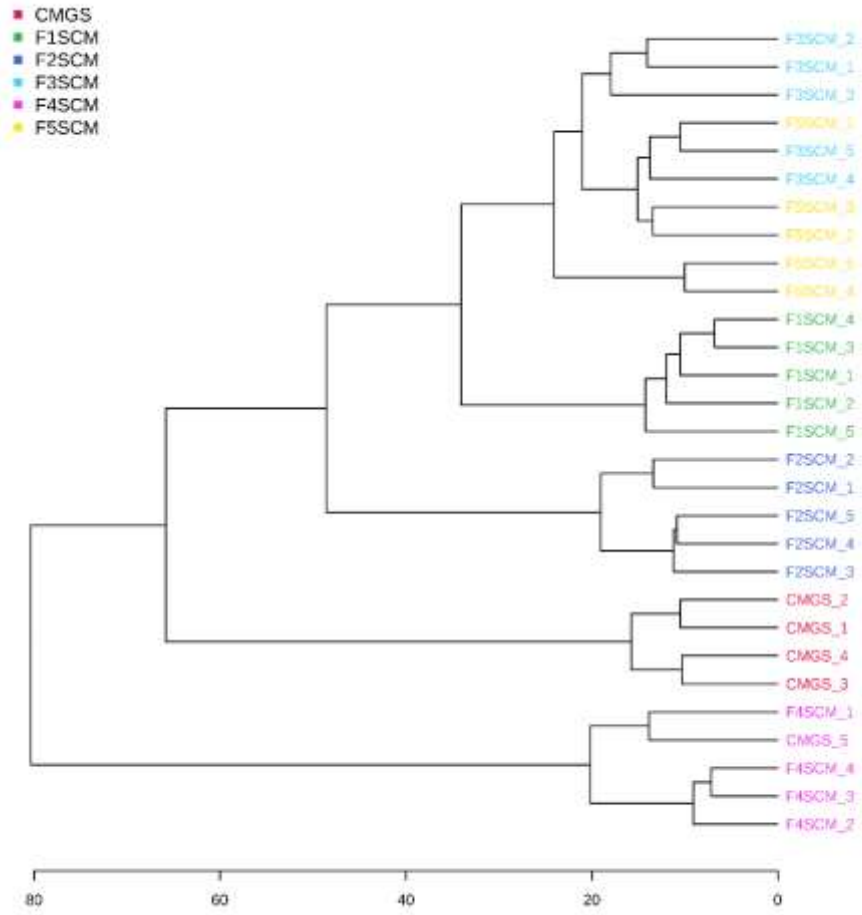
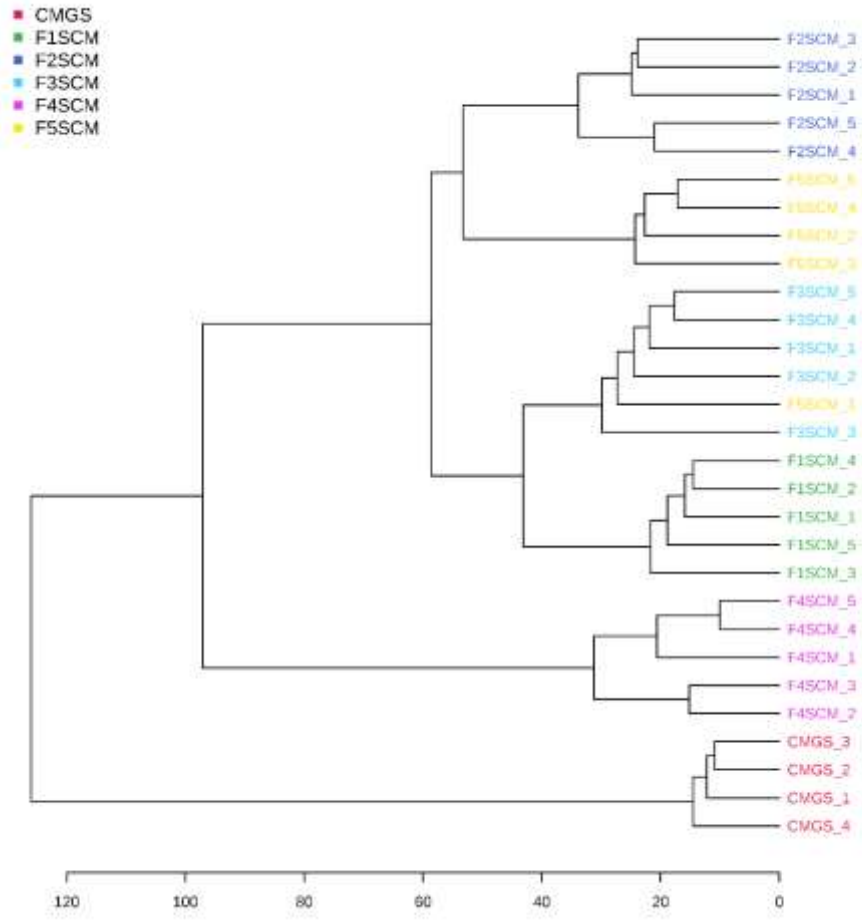


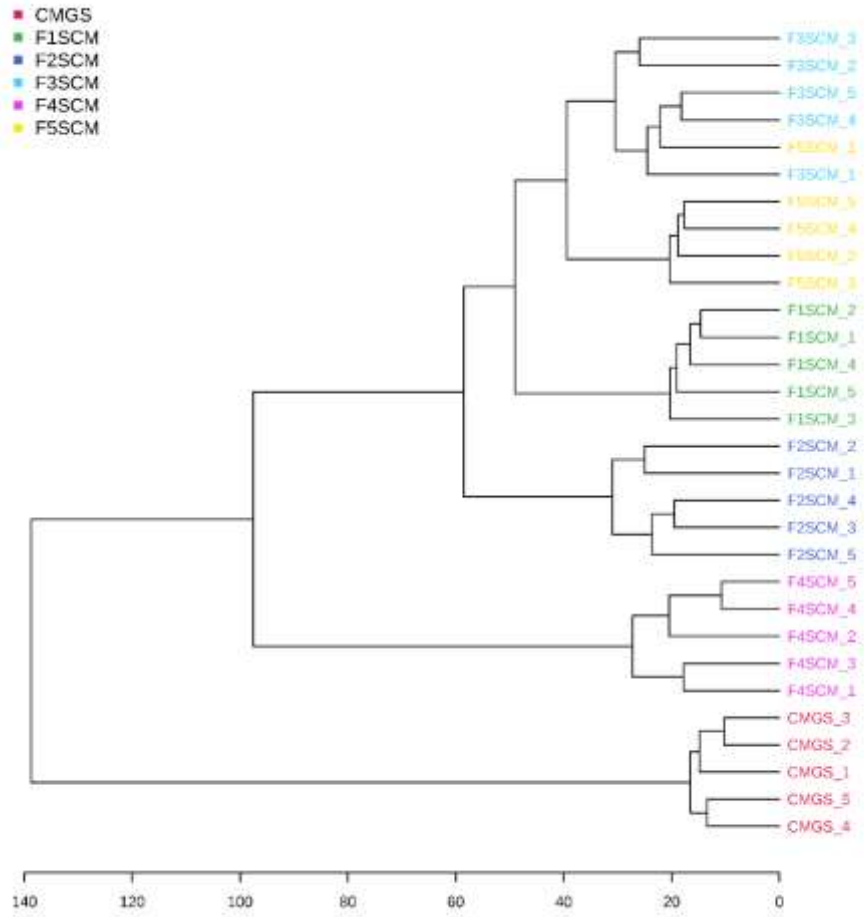

**Supplementary Figure 1.** Dendrogram showing the relationship between five soil CMs and CMGS medium based on their C18 negative ionization metabolite profiles. Dendrogram was constructed by ward clustering on the closest Euclidean distances between samples. Numbers represent sample ID.




**Supplementary Figure 2.** Dendrogram showing the relationship between five soil CMs and CMGS medium based on their C18 positive ionization metabolite profiles. Dendrogram was constructed by ward clustering on the closest Euclidean distances between samples. Numbers represent sample ID.

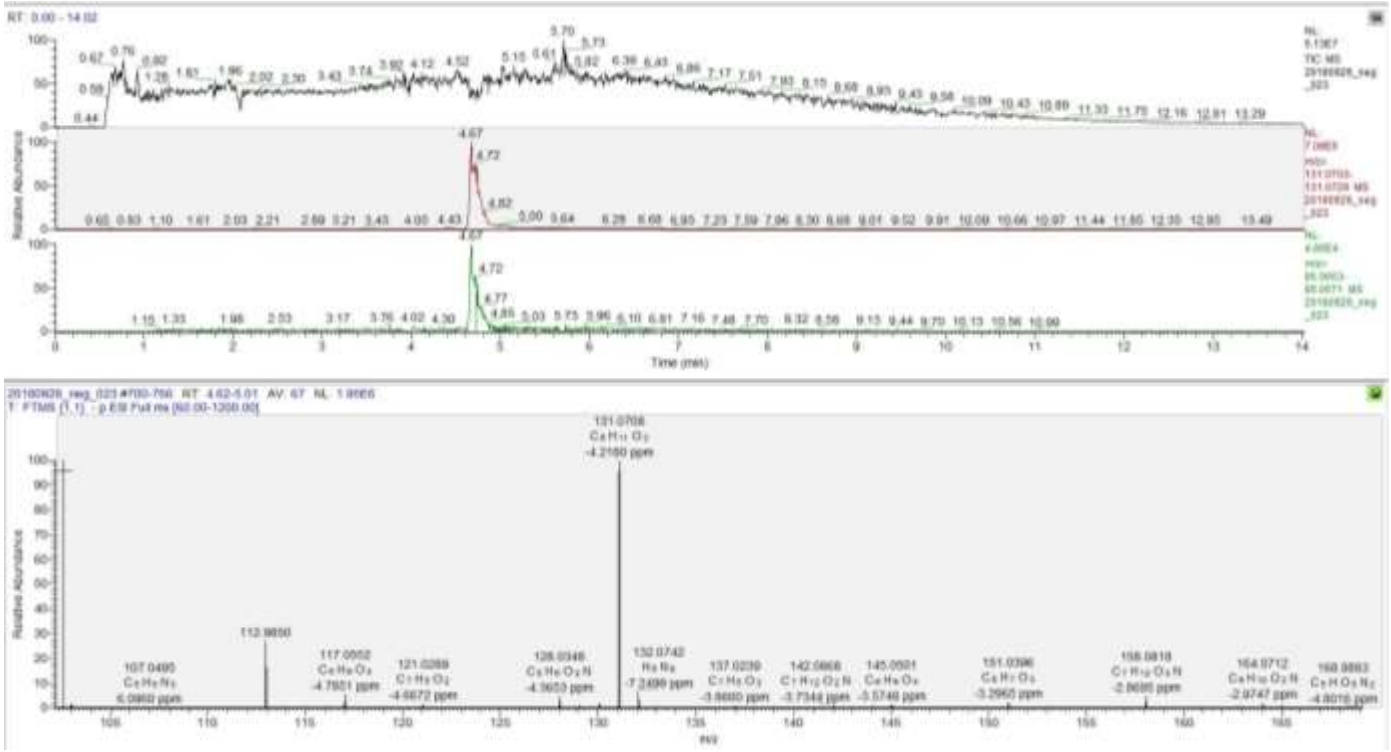



**Supplementary Figure 3.** Dendrogram showing the relationship between five soil CMs and CMGS medium based on their HILIC negative ionization metabolite profiles. Dendrogram was constructed by ward clustering on the closest Euclidean distances between samples. Numbers represent sample ID.



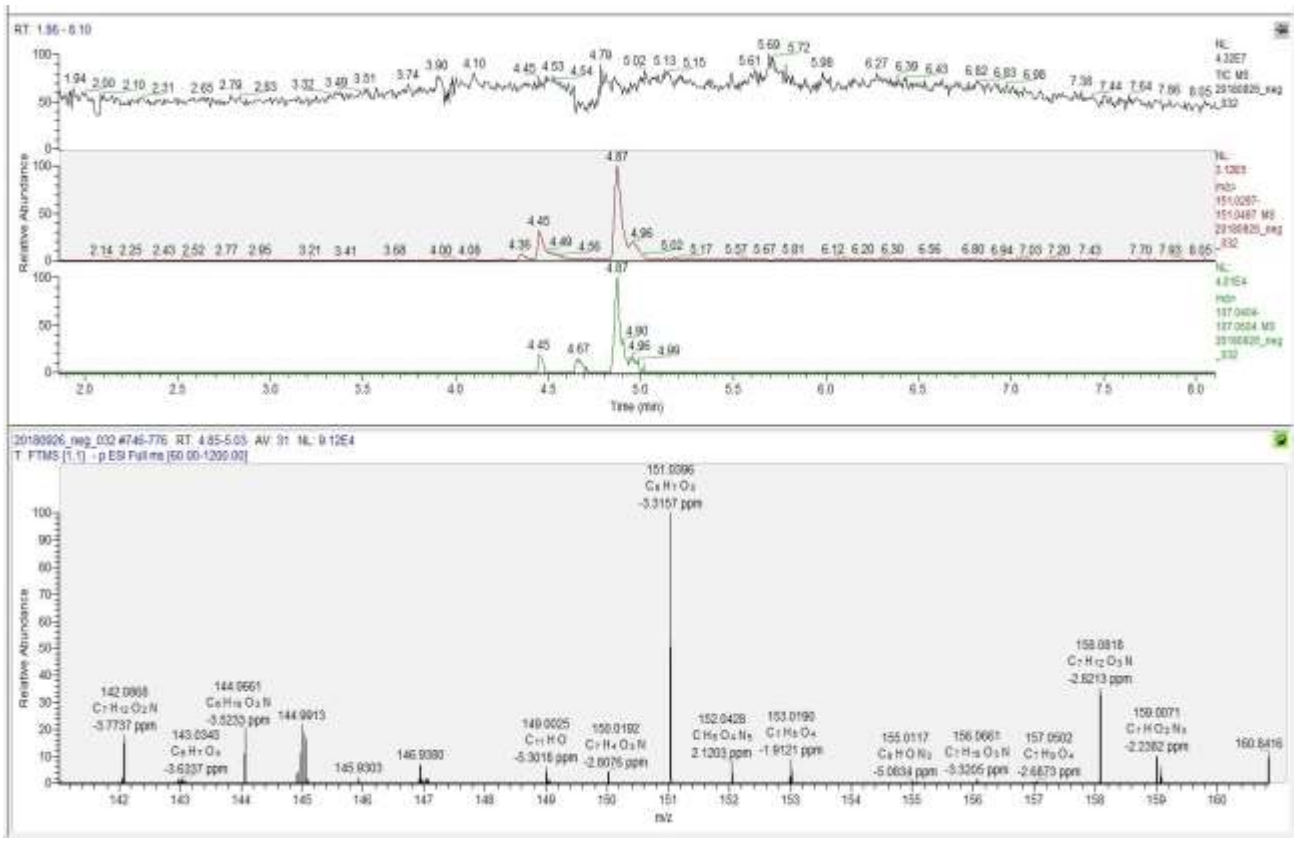

**Supplementary Figure 4.** Dendrogram showing the relationship between five soil CMs and CMGS medium based on their HILIC positive ionization metabolite profiles. Dendrogram was constructed by ward clustering on the closest Euclidean distances between samples. Numbers represent sample ID.

| Compound name | m/z | RT (sec) | Molecular formula | Adduct | Fragments (*m/z*) | Level of identification |
|---|---|---|---|---|---|---|
| 2-hydroxyisocaproic acid | 131.0708 | 284.2 | C6H12O3 | [M-H]- | 85.0662 | 2 |



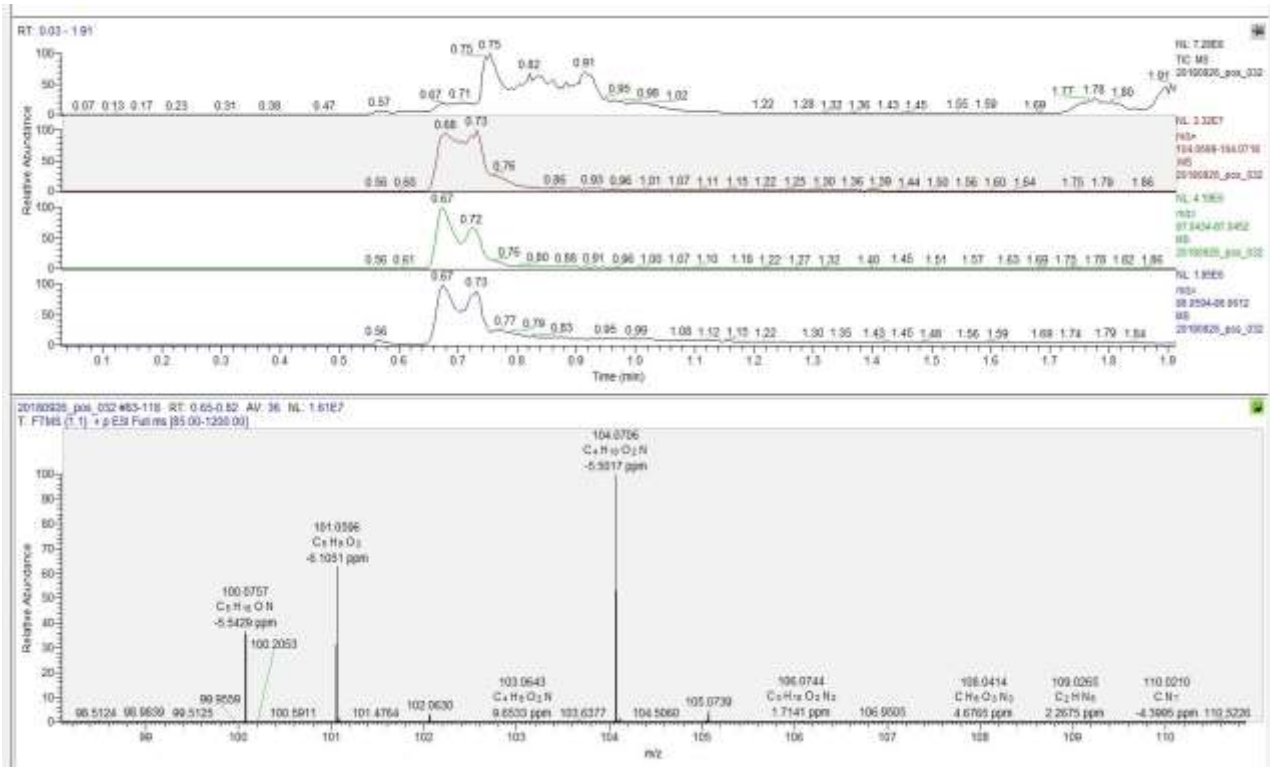
**Supplementary Figure 5.** Extracted ion chromatograms (C18 negative ionization) for parent masses and co-eluting diagnostic fragments of 2-hydroxyisocaproic acid in the public MS database.

| Compound name | m/z | RT (sec) | Molecular formula | Adduct | Fragments (*m/z*) | Level of identification |
|---|---|---|---|---|---|---|
| 3-Hydroxyphenylacetic acid | 151.0395 | 295.3 | C8H8O3 | [M-H]- | 107.0504 | 2 |



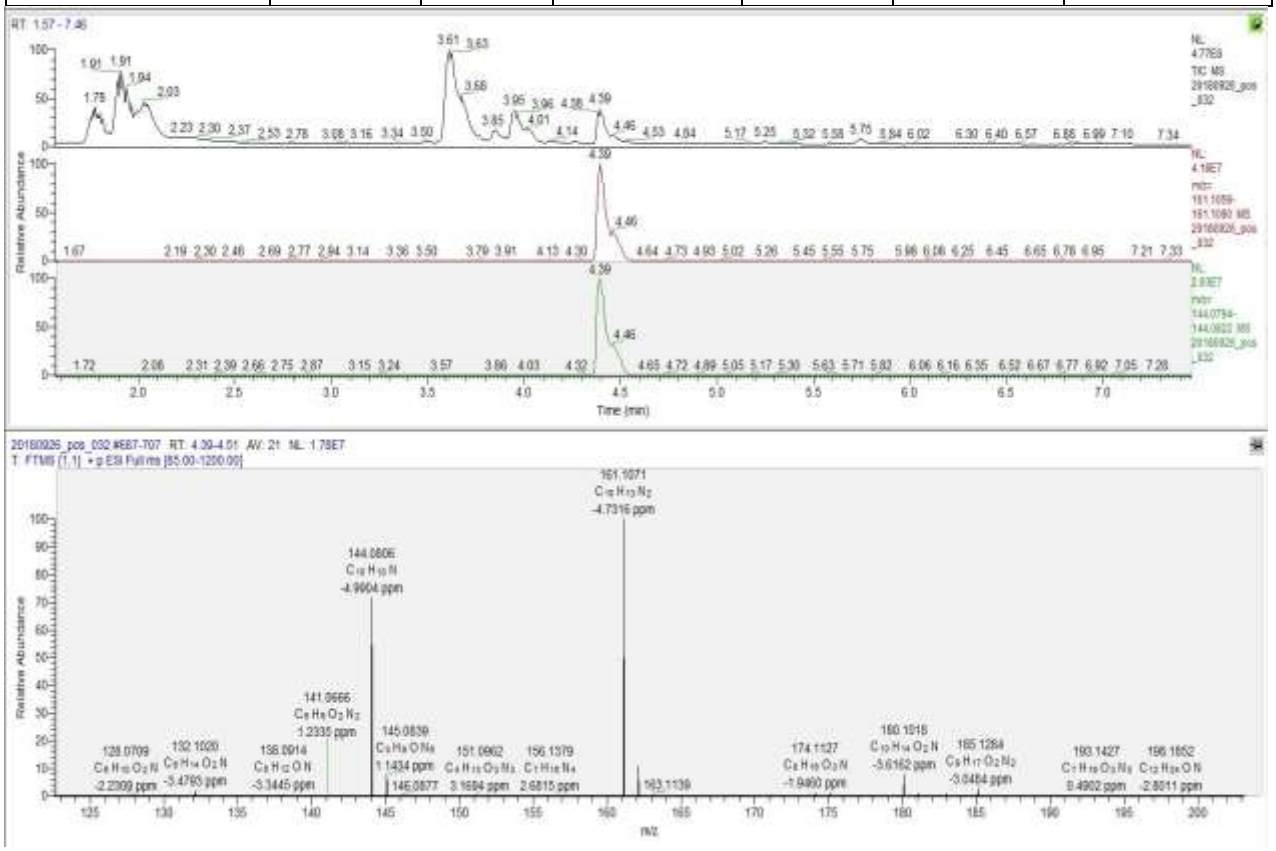

**Supplementary Figure 6.** Extracted ion chromatograms (C18 negative ionization) for parent masses and co-eluting diagnostic fragments of 3-hydroxyphenylacetic acid in the public MS database.

| Compound name | m/z | RT (sec) | Molecular formula | Adduct | Fragments (*m/z*) | Level of identification |
|---|---|---|---|---|---|---|
| γ-Aminobutyric acid | 104.0706 | 42.41 | C4H9NO2 | [M+H]+ | 87.0443, 86.0603 | 2 |



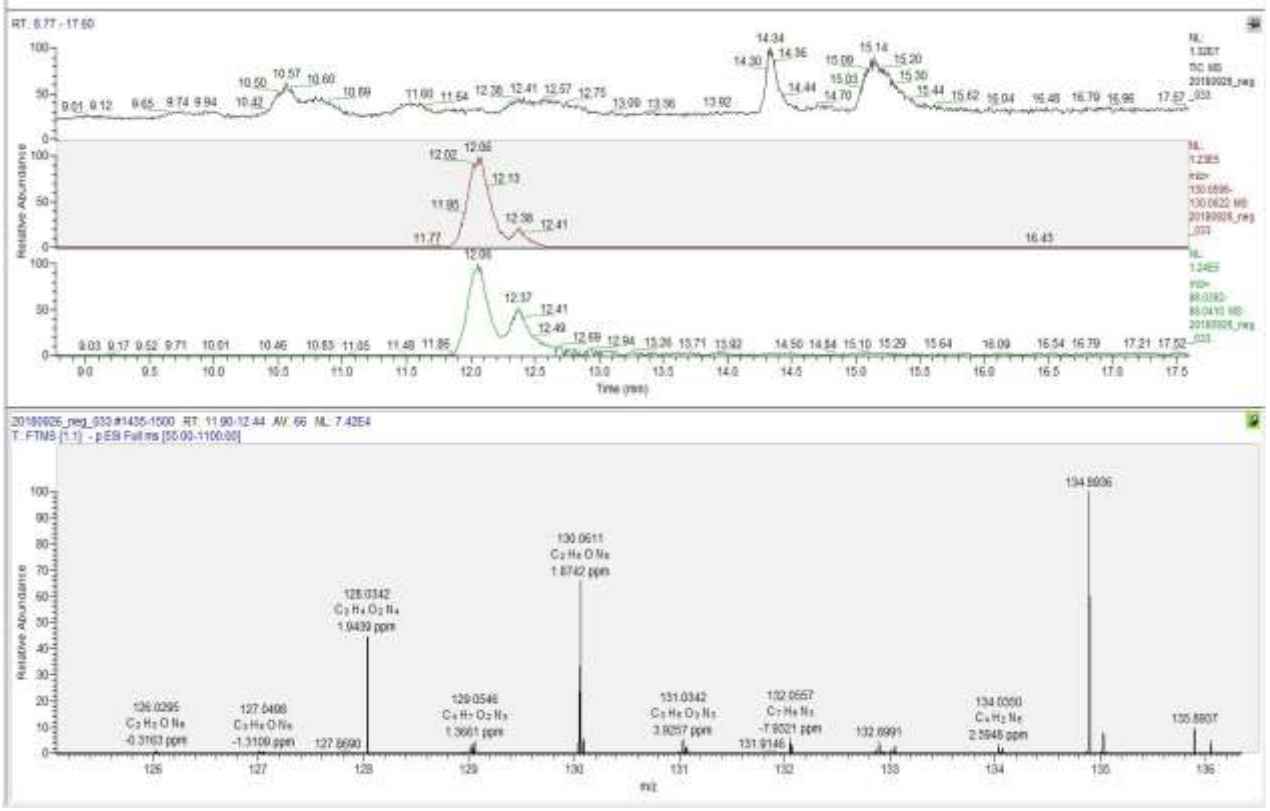

**Supplementary Figure 7.** Extracted ion chromatograms (C18 positive ionization) for parent masses and co-eluting diagnostic fragments of γ-aminobutyric acid in the public MS database.

| Compound name | m/z | RT (sec) | Molecular formula | Adduct | Fragments (*m/z*) | Level of identification |
|---|---|---|---|---|---|---|
| Tryptamine | 161.1071 | 262.45 | C10H12N2 | [M+H]+ | 144.0808 | 2 |



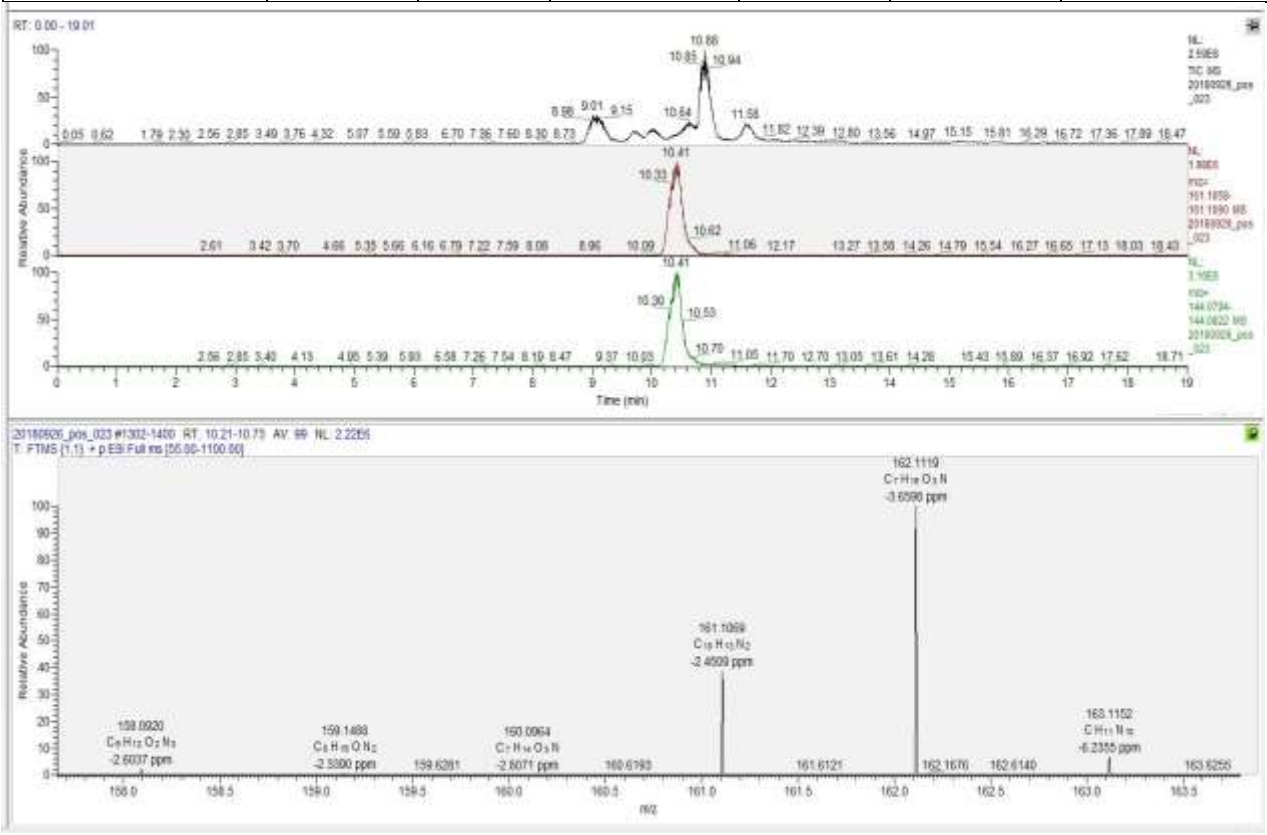

**Supplementary Figure 8.** Extracted ion chromatograms (C18 positive ionization) for parent masses and co-eluting diagnostic fragments of tryptamine in the public MS database.

| Compound name | m/z | RT (sec) | Molecular formula | Adduct | Fragments (*m/z*) | Level of identification |
|---|---|---|---|---|---|---|
| Creatine | 161.1071 | 723.24 | C4H9N3O2 | [M-H]- | 88.0401 | 2 |



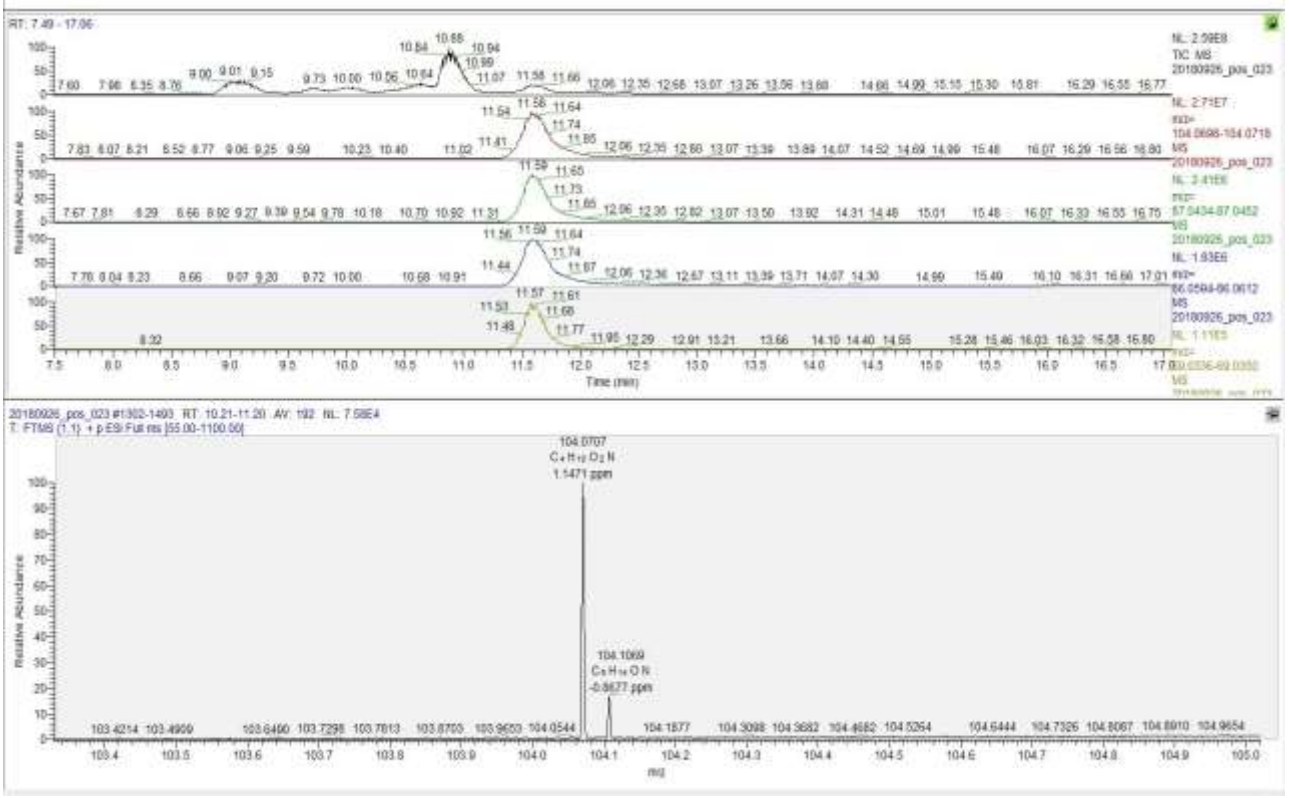
**Supplementary Figure 9.** Extracted ion chromatograms (HILIC negative ionization) for parent masses and co-eluting diagnostic fragments of creatine in the public MS database.

| Compound name | m/z | RT (sec) | Molecular formula | Adduct | Fragments (*m/z*) | Level of identification |
|---|---|---|---|---|---|---|
| Tryptamine | 161.107 | 622.03 | C10H12N2 | [M+H]+ | 427.0 | 2 |




**Supplementary Figure 10.** Extracted ion chromatograms (HILIC positive ionization) for parent masses and co-eluting diagnostic fragments of tryptamine in the public MS database.

| Compound name | m/z | RT (sec) | Molecular formula | Adduct | Fragments (*m/z*) | Level of identification |
|---|---|---|---|---|---|---|
| γ-Aminobutyric acid | 104.0706 | 692.68 | C4H9NO2 | [M+H]+ | 87.0443, 86.0603, 69.0343 | 2 |




**Supplementary Figure 11.** Extracted ion chromatograms (HILIC positive ionization) for parent masses and co-eluting diagnostic fragments of γ-aminobutyric acid in the public MS database.

**Supplementary Table 1.** Significantly high metabolite features in F4SCM group (top 50 features ranked based on the *p*-value).

| | C18 negative ionization | | | | C18 positive ionization | | | | HILIC negative ionization | | | | HILIC positive ionization | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | *m/z* | RT | *p*-value | FC | *m/z* | RT | *p*-value | FC | *m/z* | RT | *p*-value | FC | *m/z* | RT | *p*-value | FC |
| **01** | 172.0974 | 282.38 | $2.39X10^{-10}$ | 5.4 | 180.9041 | 37.57 | $4.52X10^{-9}$ | 2.3 | 374.1563 | 691.87 | $1.75X10^{-7}$ | 6.0 | 161.107 | 622.03 | $8.20X10^{-10}$ | 7972.2 |
| **02** | 362.9675 | 344.83 | $3.34X10^{-10}$ | 11.9 | 142.9482 | 37.5 | $1.33X10^{-8}$ | 2.2 | 336.1193 | 697.84 | $2.00X10^{-7}$ | 13.0 | 72.0811 | 629.24 | $1.41X10^{-9}$ | 60.7 |
| **03** | 131.0344 | 238.75 | $2.15X10^{-9}$ | 18.9 | 126.0524 | 40.93 | $1.06X10^{-7}$ | 15.3 | 261.0724 | 694.38 | $8.29X10^{-7}$ | 4.5 | 274.1657 | 622.65 | $1.77X10^{-9}$ | 13.8 |
| **04** | 61.9878 | 380.41 | $5.35X10^{-8}$ | 2.2 | 164.9301 | 37.27 | $1.29X10^{-7}$ | 2.8 | 245.125 | 869.8 | $8.67X10^{-7}$ | 5.0 | 141.0653 | 632.7 | $3.80X10^{-9}$ | 850.6 |
| **05** | 227.1399 | 267.28 | $5.91X10^{-8}$ | 3.1 | 89.1075 | 36.04 | $1.63X10^{-7}$ | 77.5 | 302.1352 | 690.07 | $9.53X10^{-7}$ | 3.7 | 143.0686 | 632.55 | $5.99X10^{-9}$ | 3.0 |
| **06** | 374.1566 | 247.69 | $6.22X10^{-8}$ | 3.4 | 141.0656 | 55.86 | $2.10X10^{-7}$ | 763.2 | 261.0877 | 681.74 | $1.36X10^{-6}$ | 2.7 | 92.0708 | 861.87 | $6.53X10^{-9}$ | 6.2 |
| **07** | 298.1517 | 209.11 | $6.42X10^{-8}$ | 2.2 | 104.0706 | 42.41 | $3.64X10^{-7}$ | 11.8 | 188.1033 | 781.06 | $2.66X10^{-6}$ | 8.4 | 123.0553 | 632.58 | $7.29X10^{-9}$ | 5452.1 |
| **08** | 390.1158 | 60.69 | $9.61X10^{-8}$ | 3.8 | 177.0741 | 343.31 | $3.93X10^{-7}$ | 343.31 | 242.1138 | 886.45 | $3.08X10^{-6}$ | 6.5 | 167.0812 | 657.18 | $8.25X10^{-9}$ | 3.3 |
| **09** | 250.0574 | 362.26 | $1.10X10^{-7}$ | 103.2 | 176.0707 | 343.59 | $4.13X10^{-7}$ | 111.2 | 258.0724 | 742.65 | $3.28X10^{-6}$ | 11.3 | 81.0449 | 632.74 | $1.02X10^{-8}$ | 9.3 |
| **10** | 256.0646 | 278.02 | $1.15X10^{-7}$ | 1493.9 | 188.1758 | 39.64 | $4.41X10^{-7}$ | 50.2 | 189.0509 | 695.32 | $3.49X10^{-6}$ | 3.4 | 100.0758 | 651.25 | $1.18X10^{-8}$ | 112.2 |
| **11** | 380.1825 | 290.49 | $1.29X10^{-7}$ | 3.1 | 148.0343 | 41.03 | $6.92X10^{-7}$ | 3.5 | 166.0172 | 591.4 | $4.13X10^{-6}$ | 3.7 | 144.0805 | 622.42 | $1.20X10^{-8}$ | 37.1 |
| **12** | 243.1348 | 240.69 | $1.35X10^{-7}$ | 11.3 | 202.144 | 343.19 | $1.68X10^{-6}$ | 42.7 | 61.9873 | 633.62 | $4.55X10^{-6}$ | 3.5 | 131.1178 | 655.11 | $1.27X10^{-8}$ | 2.8 |
| **13** | 107.0496 | 295.05 | $1.36X10^{-7}$ | 4.9 | 137.0267 | 61.99 | $2.09X10^{-6}$ | 3.0 | 204.0619 | 750.87 | $4.58X10^{-6}$ | 12.4 | 59.0493 | 650.66 | $2.01X10^{-8}$ | 20.0 |
| **14** | 131.0708 | 284.2 | $1.65X10^{-7}$ | 19.3 | 208.1335 | 314.05 | $2.85X10^{-6}$ | 314.8 | 232.0819 | 692.87 | $4.60X10^{-6}$ | 40.1 | 181.1043 | 550.47 | $4.02X10^{-8}$ | 4.0 |
| **15** | 102.0553 | 214.63 | $1.66X10^{-7}$ | 3106.1 | 184.1334 | 343.01 | $3.26X10^{-6}$ | 46.0 | 141.0537 | 634.1 | $4.71X10^{-6}$ | 88.8 | 87.0443 | 692.59 | $7.12X10^{-8}$ | 11.4 |
| **16** | 181.0362 | 207.4 | $2.39X10^{-7}$ | 13.7 | 199.144 | 214.91 | $3.31X10^{-6}$ | 48.4 | 139.0501 | 634.1 | $5.47X10^{-6}$ | 313.8 | 275.123 | 384.19 | $7.63X10^{-8}$ | 8.3 |
| **17** | 408.1411 | 259.96 | $2.64X10^{-7}$ | 9.5 | 131.1177 | 45.81 | $3.83X10^{-6}$ | 4.7 | 102.0186 | 324.23 | $8.06X10^{-6}$ | 2.0 | 86.0603 | 692.66 | $8.38X10^{-8}$ | 10.7 |
| **18** | 131.0344 | 225.55 | $2.72X10^{-7}$ | 29.2 | 264.1595 | 416.39 | $4.38X10^{-6}$ | 115.7 | 227.1143 | 875.22 | $8.55X10^{-6}$ | 3.9 | 180.1014 | 550.23 | $1.12X10^{-7}$ | 5289.9 |
| **19** | 101.0601 | 313.44 | $2.93X10^{-7}$ | 6818.2 | 115.0504 | 93.81 | $4.62X10^{-6}$ | 21.3 | 175.024 | 502.39 | $9.42X10^{-6}$ | 4.2 | 68.0497 | 692.68 | $1.26X10^{-7}$ | 57.8 |
| **20** | 213.0878 | 256.96 | $3.93X10^{-7}$ | 2.5 | 144.0806 | 262.44 | $4.65X10^{-6}$ | 798.8 | 167.9963 | 854.34 | $1.16X10^{-5}$ | 3.6 | 245.1492 | 591.97 | $1.48X10^{-7}$ | 13.1 |
| **21** | 85.0655 | 283.37 | $4.14X10^{-7}$ | 9.3 | 177.1027 | 231.18 | $5.81X10^{-6}$ | 59.2 | 152.0567 | 647.54 | $1.20X10^{-5}$ | 17.9 | 82.0652 | 650.63 | $1.64X10^{-7}$ | 1228.0 |
| **22** | 132.0742 | 282.84 | $4.32X10^{-7}$ | 19.8 | 133.0972 | 35.41 | $7.56X10^{-6}$ | 2.6 | 187.108 | 745.98 | $1.24X10^{-5}$ | 3.6 | 118.086 | 649.96 | $1.72X10^{-7}$ | 4.4 |
| **23** | 193.9946 | 268.55 | $4.57X10^{-7}$ | 28.7 | 105.0739 | 42.5 | $8.56X10^{-6}$ | 4.6 | 155.0817 | 650.65 | $1.30X10^{-5}$ | 20.8 | 61.0844 | 597.12 | $1.85X10^{-7}$ | 2892.2 |
| **24** | 346.198 | 273.22 | $5.30X10^{-7}$ | 90.1 | 100.0756 | 214.9 | $1.07X10^{-5}$ | 30.7 | 96.9686 | 747.63 | $1.31X10^{-5}$ | 2.2 | 119.0895 | 650.13 | $1.93X10^{-7}$ | 4.6 |
| **25** | 345.1499 | 242.3 | $5.62X10^{-7}$ | 5.3 | 229.1551 | 203.66 | $1.09X10^{-5}$ | 6.8 | 95.0604 | 634.1 | $1.43X10^{-5}$ | 41043.0 | 148.0964 | 690.6 | $2.40X10^{-7}$ | 4.8 |
| **26** | 279.0984 | 251.61 | $5.78X10^{-7}$ | 2.4 | 101.079 | 214.83 | $1.11X10^{-5}$ | 73.6 | 299.1145 | 651.04 | $1.46X10^{-5}$ | 11.9 | 245.1491 | 558.09 | $2.65X10^{-7}$ | 12.5 |
| **27** | 175.0243 | 116.1 | $6.38X10^{-7}$ | 37.8 | 161.1071 | 262.45 | $1.14X10^{-5}$ | 427.0 | 132.0293 | 692.36 | $1.50X10^{-5}$ | 2.8 | 101.0597 | 650.39 | $2.74X10^{-7}$ | 191.5 |
| **28** | 180.9993 | 312.17 | $6.43X10^{-7}$ | 2.3 | 121.0648 | 122.53 | $1.23X10^{-5}$ | 46.2 | 233.0232 | 739.66 | $1.57X10^{-5}$ | 3.5 | 74.0715 | 654.79 | $2.75X10^{-7}$ | 3.4 |
| **29** | 327.167 | 231.58 | $6.65X10^{-7}$ | 4.4 | 170.0926 | 38.67 | $1.63X10^{-5}$ | 8.6 | 257.1251 | 893.41 | $1.72X10^{-5}$ | 5.0 | 105.074 | 692.58 | $2.94X10^{-7}$ | 12.0 |
| **30** | 310.1406 | 272.94 | $6.71X10^{-7}$ | 30.9 | 138.0913 | 122.62 | $1.66X10^{-5}$ | 180.6 | 171.0403 | 693.86 | $1.77X10^{-5}$ | 3.8 | 134.0957 | 550.08 | $3.00X10^{-7}$ | 40.3 |
| **31** | 144.066 | 214.23 | $8.88X10^{-7}$ | 23.1 | 376.1723 | 246.56 | $1.68X10^{-5}$ | 3.4 | 431.1775 | 696.4 | $2.00X10^{-5}$ | 29.4 | 56.0497 | 650.38 | $3.23X10^{-7}$ | 32.7 |
| **32** | 231.0982 | 204.07 | $8.94X10^{-7}$ | 10.8 | 102.0801 | 214.58 | $2.07X10^{-5}$ | 7.8 | 121.0397 | 634.1 | $2.05X10^{-5}$ | 26.3 | 93.0701 | 636.27 | $3.48X10^{-7}$ | 1274.4 |
| **33** | 130.0867 | 344.67 | $8.97X10^{-7}$ | 4.2 | 100.0488 | 214.72 | $2.21X10^{-5}$ | 145.1 | 144.0657 | 650.53 | $2.27X10^{-5}$ | 2.2 | 103.0504 | 741.82 | $3.61X10^{-7}$ | 36.9 |
| **34** | 238.021 | 112.49 | $9.10X10^{-7}$ | 32.0 | 247.1292 | 235.16 | $2.36X10^{-5}$ | 2.4 | 129.0184 | 455.53 | $2.39X10^{-5}$ | 2.9 | 104.0706 | 692.68 | $3.64X10^{-7}$ | 10.1 |
| **35** | 151.0395 | 295.3 | $9.61X10^{-7}$ | 3.8 | 132.102 | 343.31 | $2.80X10^{-5}$ | 2.4 | 271.0568 | 785.47 | $2.60X10^{-5}$ | 79.9 | 170.0808 | 581.53 | $3.67X10^{-7}$ | 4.0 |
| **36** | 186.113 | 310.03 | $1.03X10^{-6}$ | 145.6 | 174.1129 | 270.86 | $2.89X10^{-5}$ | 120.4 | 206.9961 | 597.53 | $2.62X10^{-5}$ | 12.0 | 188.1279 | 583.53 | $3.70X10^{-7}$ | 5.4 |
| **37** | 179.0709 | 345.72 | $1.16X10^{-6}$ | 289.0 | 154.0972 | 55.62 | $3.43X10^{-5}$ | 455.6 | 214.035 | 695.33 | $2.64X10^{-5}$ | 4.8 | 376.1706 | 691.48 | $3.89X10^{-7}$ | 7.2 |
| **38** | 133.075 | 284.16 | $1.22X10^{-6}$ | 3.4 | 230.1752 | 411.4 | $3.55X10^{-5}$ | 52.7 | 146.0449 | 694.73 | $2.68X10^{-5}$ | 3.0 | 289.0834 | 648.77 | $3.91X10^{-7}$ | 478.0 |

| | C18 negative ionization | | | | C18 positive ionization | | | | HILIC negative ionization | | | | HILIC positive ionization | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | *m/z* | RT | *p*-value | FC | *m/z* | RT | *p*-value | FC | *m/z* | RT | *p*-value | FC | *m/z* | RT | *p*-value | FC |
| **39** | 165.0551 | 326.7 | $1.25X10^{-6}$ | 44.7 | 360.1925 | 288.38 | $3.60X10^{-5}$ | 2.2 | 164.0014 | 648.7 | $2.70X10^{-5}$ | 2.4 | 69.0338 | 692.48 | $4.14X10^{-7}$ | 32.6 |
| **40** | 180.0741 | 345.69 | $1.25X10^{-6}$ | 777.4 | 220.1006 | 304.23 | $3.74X10^{-5}$ | 6.9 | 228.0983 | 652.23 | $2.83X10^{-5}$ | 4.5 | 105.066 | 437.15 | $4.33X10^{-7}$ | 6.5 |
| **41** | 382.1729 | 224.02 | $1.28X10^{-6}$ | 11.7 | 194.1181 | 285.91 | $3.76X10^{-5}$ | 23.4 | 207.0879 | 655.51 | $3.11X10^{-5}$ | 10.5 | 139.0942 | 637.23 | $4.76X10^{-7}$ | 112.1 |
| **42** | 336.12 | 254.66 | $1.42X10^{-6}$ | 6.9 | 177.102 | 216.42 | $3.81X10^{-5}$ | 11.7 | 227.1031 | 674.94 | $3.16X10^{-5}$ | 3.9 | 121.0648 | 636.81 | $4.94X10^{-7}$ | 188.5 |
| **43** | 262.1446 | 417.53 | $1.58X10^{-6}$ | 106.0 | 188.1284 | 308.67 | $4.48X10^{-5}$ | 109.4 | 130.0501 | 748.19 | $3.42X10^{-5}$ | 4.9 | 76.076 | 664.05 | $5.41X10^{-7}$ | 190.1 |
| **44** | 263.1481 | 417.51 | $1.61X10^{-6}$ | 951.3 | 192.598 | 222.94 | $4.94X10^{-5}$ | 9.1 | 147.0288 | 455.34 | $3.69X10^{-5}$ | 3.0 | 55.0545 | 649.88 | $6.01X10^{-7}$ | 6.7 |
| **45** | 149.0603 | 380.88 | $1.73X10^{-6}$ | 107.6 | 190.0864 | 376.55 | $5.10X10^{-5}$ | 142.0 | 171.0403 | 844.2 | $3.71X10^{-5}$ | 3.3 | 138.0909 | 637.15 | $7.04X10^{-7}$ | 181.6 |
| **46** | 344.1461 | 242.32 | $1.77X10^{-6}$ | 101.4 | 360.2131 | 298.49 | $5.15X10^{-5}$ | 8.4 | 279.1094 | 641.69 | $3.72X10^{-5}$ | 2.4 | 405.0904 | 515.91 | $7.13X10^{-7}$ | 3234.7 |
| **47** | 245.114 | 236.91 | $1.88X10^{-6}$ | 2.4 | 141.0655 | 78.9 | $6.44X10^{-5}$ | 12.7 | 403.0761 | 516.58 | $3.84X10^{-5}$ | 338.7 | 229.1541 | 511.18 | $8.04X10^{-7}$ | 13.3 |
| **48** | 288.1198 | 200.13 | $2.05X10^{-6}$ | 6.3 | 155.0792 | 36.58 | $7.34X10^{-5}$ | 3.0 | 127.039 | 650.04 | $4.34X10^{-5}$ | 3.7 | 212.1025 | 529.08 | $8.14X10^{-7}$ | 5.6 |
| **49** | 383.158 | 223.78 | $2.06X10^{-6}$ | 7.7 | 318.1668 | 243.86 | $1.13X10^{-4}$ | 2.0 | 215.0667 | 833.28 | $4.69X10^{-5}$ | 2.6 | 145.133 | 639.18 | $8.28X10^{-7}$ | 10.5 |
| **50** | 188.0347 | 253.01 | $2.19X10^{-6}$ | 7.3 | 216.1596 | 382.5 | $1.17X10^{-4}$ | 93.7 | 214.0827 | 689.38 | $4.81X10^{-5}$ | 3.0 | 123.0998 | 601.36 | $9.35X10^{-7}$ | 1553.7 |

*m/z* – mass to charge ratio

RT – retention time (seconds)

*p*-value - *t*-test between F4SCM and CMGS groups

FC – fold change value (F4SCM/CMGS)