Effects of water deficit and heat stress on *Nicotiana Langsdorffii* metabolomic pattern modified by insertion of *rolD* gene from *Agrobacterium rhizogenes*.

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Table S1: Metabolites identified by untargeted metabolomic analysis at levels 2 and 3. Diagnostic fragments are in bold.

| Retention time (min) | Mass            | Formula         | Name                                                      | Fragments                                                                 | Error (ppm) | ID Level |
|----------------------|-----------------|-----------------|-----------------------------------------------------------|---------------------------------------------------------------------------|-------------|----------|
| 16,43                | 468.21310 (M - H) | C\(_{25}\)H\(_{31}\)N\(_3\)O\(_6\) | Dicaffeoyl spermidine                                      | 332.16077, 306.18170, 289.15533, 135.04524, 264.17065                     | -1.9        | 2        |
| 22,09                | 783.32617 (M - H) | C\(_{34}\)H\(_{56}\)O\(_20\) | Menthenetriol glucoside + ketoglutaric acid + octanoic acid | 739.33136, 652.68506, 491.28287, 287.14825, 215.12827, 143.10721            | -3.1        | 2        |
| 14,95                | 250.07155 (M - H) | C\(_{12}\)H\(_{13}\)NO\(_5\) | Phenylacetylaspartic acid                                  | 132.03020, 232.06131                                                     | -2.18       | 2        |
| 9,88                 | 315.07129 (M - H) | C\(_{13}\)H\(_{16}\)O\(_9\) | Glucopyranosyloxyhydroxybenzoic acid                       | 153.01921, 109.02940, 165.01924, 225.03976                                | -2.36       | 2        |
| 14,39                | 373.11310 (M - H) | C\(_{18}\)H\(_{22}\)O\(_{10}\) | Secologanate                                              | 358.08963, 211.06085, 196.03746, 179.07130, 153.0557, 304.91241, 265.07080, 195.02966, 180.04237, 139.04002 | -3.1        | 2        |
| 9,65                 | 367.12387 (M - H) | C\(_{14}\)H\(_{25}\)O\(_{11}\) | Acetyl methyl glucuronic acid + gamma hydroxyvaleric acid  | 349.11319, 323.09775, 249.06126, 231.05061                                 | -3.5        | 2        |
| Time | Fragment Masses | Formula | Description | Ions | RT | S* |
|------|----------------|---------|-------------|------|----|----|
| 15.06 | 472.2439 (M-H) | C_{23}H_{40}NO_3P | LysoPE (18:4; 0:0) | 381.17514, 350.20694, 308.19662, 186.16068, 121.02934, 137.06053, 266.08671 | -5.32 | 2 |
| 13.23 | 372.12909 (M + FA-H) | C_{15}H_{21}NO_7 | Phenylalanine glucopyranosyl | 304.91229, 236.09235, 179.05600, 161.04530 | -2.4 | 2 |
| 13.03 | 381.13959 | C_{15}H_{20}O_11 | Acetyl methyl glucuronic acid-hydroxy methyl pentanoic acid | 249.06136, 231.05087, 206.06825 | -2.4 | 2 |
| 16.09 | 385.11325 | C_{17}H_{22}O_10 | Acetyl methyl glucuronic acid hydroxy acetoephone | 267.07184, 249.06114 | -2.3 | 2 |
| 11.20 | 399.13171 | C_{15}H_{26}O_10S | Propyl-glucopyranosyl-2-tio-glucopyranoside | 136.99147 | -3.3 | 2 |
| 33.37 | 433.23569 | C_{17}H_{20}O_3P | PA (18:2/0:0) | 152.99603, 171.00659 | -0.5 | 2 |
| 10.70 | 395.02789 | C_{15}H_{16}O_5S | Periodic leaf movement factor, PLMF 3 (Glucopyranosyloxyhydroxybenzoic acid sulfate) | 351.03842, 377.01718, 241.00220, 153.01930, 241.00194, 253.02708, 109.02946 | -3.3 | 2 |
| 14.05 | 504.17111 (M + FA-H) | C_{20}H_{28}NO_11 | Cinnamido diglucoside | 357.10263, 311.09732, 293.08664, 251.07672, 221.06549, 191.05542, 161.04521 | -3.6 | 2 |
| 18.42 | 461.23703 (M + FA-H) | C_{13}H_{36}O_8 | Sesquiterpenoid | 467.12592, 441.14661, 423.13562, 349.08429, 305.09497, 232.09683, 190.03238 | -4.7 | 3 |
| 22.44 | 485.13596 | C_{24}H_{24}N_2O_5S | Caffeoyl indole-3-acetyl methionine | 467.12592, 441.14661, 423.13562, 349.08429, 305.09497, 232.09683, 190.03238 | -5.8 | 2 |
| Purity | M.S. | Formula | Name | M.W. | 1σ | Intensity |
|-------|------|---------|------|------|----|-----------|
| 19,59 | 483.20779 (M + FA - H) 437.20227 (M - H) | C₁₉H₅₆O₁₁ | Caprylic acid + xylopyranosyl glucopyranoside | 293,08746 | -4,04 | 2 |
| 26,24 | 552.24249 (M + FA - H) 506.23688 (M - H) | C₂₆H₉₅NO₃ | Octahydro-quinolizine-glucopyranosyl-hydroxy-methoxy-cinnamoyl | 362.12244, 200.07079, 305.15894, 260.09140, 117.03468 | -2,28 | 2 |
| 13,61 | 491.13986 (M + FA - H) 445.13428 (M - H) | C₁₉H₅₂O₁₁ | Benzoic acid difructofuranose dianhydride | 323.09787, 305.08676, 263.07663, 221.06628, 179.05598 | -3 | 2 |
| 19,94 | 555,22815 | C₂₉H₆₅O₁₅ | Menthenetriol diglucoside | 509.22238, 491.21146, 431.19080, 389.18036, 365.10730, 305.15909, 263.07663, 221.06628, 179.05598 | -2,3 | 2 |
| 22,06 | 649.30432 (M + 2FA - 2H) 1207.60474 (M - H) | C₃₈H₆₆O₂₆ | Diosgenin + 3glucoses + 1 dehydroxyglucose + 1 methyldehydroxyglucose (Methyldichotomin) | 626.30121 (-46), 603.29865 (-46), 1061.54749 (-146) | -5.8 | 2 |
| 18,04 | 645.25842 (M + FA - H) 599.25323 (M - H) | C₂₅H₄₄O₁₆ | Menthenetriol diglucoside + glycerol + galactose | 581.24353, 305.15909, 497.22095, 455.13800, 437.16897, 275.07568, 233.13835, 215.12788, 161.04489, 179.05542 | -4.7 | 2 |
| 26,62 | 653.26202 (M + FA - H) 607.25720 (M - H) | C₇H₁₄O₁₅ | Acylsucrose (S₄:15) | 627.54944, 565.24677, 56077814, 495.20340, 481.18893, 477.19397, 463.17798 | -5.8 | 2 |
| Retention Time | Mass/Charge | Formula | Name | Exact Mass | Charge | Intensity |
|---------------|-------------|---------|------|------------|--------|-----------|
| 18.26         | 645.25812 (M + FA - H) 599.25323 (M - H) | C_{28}H_{44}O_{16} | Menthenetriol diglucoside + carboxyethylglucose | 581.24353, 275.07599, 539.23181, 497.22095, 455.13800, 389.17941, 347.16898, 305.15884, 215.12823, 143.10721, 233.13835 | -3,1 | 2 |
| 27.16         | 721.36536 (M + FA - H) 675.35974 (M - H) | C_{33}H_{56}O_{14} | Diglucopyranosyl linolenylglycerol (C18:3) | 415.14557, 397.13477, 235.08237 | 0,2 | 2 |
| 33.01         | 723.38110 (M + FA - H) 677.37512 (M - H) | C_{33}H_{56}O_{14} | Acylsucrose (S3:21) | 593.31763, 551.27081, 533.26013 | -0,38 | 2 |
| 35.08         | 751.44861 (M + FA - H) 705.44324 (M - H) | C_{36}H_{64}O_{13} | Dirhamnolipid C24:0 (C8:0, C16:0) | 561.32794, 543.31775 | 0,2 | 2 |
| 35.58         | 765.42755 (M + FA - H) 719.42200 (M - H) | C_{36}H_{64}O_{13} | Acylsucrose (S3:24) | 593.31781, 575.30658, 467.21338, 449.20279 | -0,4 | 2 |
| 33.54         | 773.43237 (M + FA - H) 727.42731 (M - H) | C_{38}H_{66}O_{13} | Dirhamnolipid C25:3 (C18:3, C7:0) | 583.31195, 565.30157, 277.21729 | -0,144 | 2 |
| 34.42         | 775.44818 (M + FA - H) 729.44269 (M - H) | C_{38}H_{66}O_{13} | Dirhamnolipid C25:2 (C18:2, C7:0) | 585.32806, 567.31610, 279.23318 | -0,5 | 2 |
| 37.25         | 807.43829 (M + FA - H) 761.43182 (M - H) | C_{38}H_{66}O_{15} | Acylsucrose S4:26 | 719.42218, 635.32861, 593.31799, 467.21503, 575.30829, 449.20309, 621.34656 | -1,4 | 2 |
| 15.79         | 470.22781 (M - H) | C_{23}H_{38}O_{7}NP | LysoPE (18:4; 0:0) | 334.17599, 291.17035, 121.02929, 137.02646, 169.13408, 180.06590, 237.12361, 249.12352 | -7,3 | 3 |
| 19,01         | 579.20538 (M - H) | C_{28}H_{56}O_{13} | Syringaresinol O-beta-D-glucoside | 417.15314 | -5,06 | 2 |
| 21,50         | 569.26837 (M + 2FA - 2H) 1047.53406 (M-H) | C_{31}H_{64}O_{22} | Diosgenin + 3glucoses + 1 hydroxyglucose (methylprotodioscin) | 546.26544 (-46) 523.26245 (-92) | -4,48 | 2 |
| M/z  | Molecular Formula | Molecular Weight | Name Description | M/z Values | Charge (+/-) | Retention Time (min) |
|------|-------------------|------------------|-----------------|------------|-------------|---------------------|
| 22,59| **C₇H₅O₈**       | 220.31822        | Allylgucose + caprylic acid | 143.10709  | -4.8        | 2                   |
| 21,02| **C₅H₄O₂₆**      | 619.29651 (-46), 596.29382 (-46), 523.26288 (-146), 1031.53821, 450.23441, 1047.53345, 901.47559, 1029.52332, 883.46600, 755.41864, 737.40845 | -3.05    | 2                   |
| 22,92| **C₇H₆O₂₅**      | 1029.52246 (-146), 883.46417 (-146), 737.40668 (-146), 557.34369 (-180), 865.45385, 806.02380, 766.13739, 719.39764, 671.37610, 653.36548, 575.35547, 599.04858, 509.32275 | -4.4     | 2                   |
| 26,06| **C₂₈H₄₂O₆₄N₄** | 511.28836, 407.19012, 293.21066, 253.09164, 275.20032 | -6.7     | 2                   |
| 20,23| **C₂₃H₃₈O₁₅**   | 509.22156, 389.17978, 347.16946, 305.15915, 263.07602, 233.13853, 161.04503, 179.05545 | -3.7     | 3                   |
| 21,34| **C₂₀H₂₀O₁₁**   | 297.06003, 315.07043, 152.01093, 179.03415 | -6.5     | 2                   |
| 12,27| **C₁₀H₁₃N₄O₄**  | 242.94350, 134.04739 | -0.44   | 2                   |
| 35,55| **C₁₆H₆O₂**     | 259.20651, 233.22757 | -0.7     | 2                   |
| 22,43| **C₁₆H₁₀NO₄**   | 297.09930, 270.11288, 242.94244, 178.05029, 148.05272, 135.04482 | -5.9     | 2                   |
| Mass (amu) | m/z (eV) | Formula | Molecular ion | Molecular mass (Da) | Identity | 2D/1D | Confi. % |
|-----------|----------|---------|---------------|---------------------|----------|-------|---------|
| 12,72     | 372.0924 | C₉H₁₁NO₃| Acetyl methyl glucuronic acid | 249.06108, 231.05063 |          |       |         |
| 36,65     | 279.2328 | C₁₈H₃₂O₂| Linoleic acid  | 261.22223           | -0.4     | 2     |         |
| 16,57     | 403.1596 (M + FA - H) | 357.15430 (M - H) | C₁₇H₂₆O₈| Sesquiterpenoid | 161.04518 | -3.3 | 3 |
| 14,64     | 447.1495 (M + FA - H) | 401.14401 (M - H) | C₁₅H₂₆O₁₀| Benzyalcohol hexose-pentose | 269.10226, 293.08694, 356.13223, 233.06602, 161.04523, 277.09036, 251.09190, 262.06754 | -3.2 | 2 |
| 14,11     | 451.2178 (M + FA - H) | 405.21252 (M - H) | C₁₉H₃₄O₉| Megastigmenetetrol-glucopyranoside (Sesquiterpenoid) | 340.12256, 243.16002, 225.14966, 179.05597, 167.10770, 149.09705, 143.03485 | -1.1 | 2 |
| 28,01     | 474.2624 | C₂₃H₂₃NO₆P| LysoPE (18:3/0:0) | 277.21722, 233.22748, 259.20682 | -0.4 | 2 |
| 26,30     | 623,2367 | C₃₆H₅₈O₈| Grossamide | 486.15283, 460.17346, 445.14996, 297.11136, 283.09583, 268.07312, 471.12894, 427.13953, 352.08035 | -5.8 | 2 |
| 32,28     | 651.4111 (M + FA - H) | 605.40533 (M - H) | C₃₆H₆₂O₈| Saponin | -0.92 | 3 |
| 28,14     | 638,3311 | C₃₆H₅₈NO₁₂P| LysoPE (18:2/0:0) + hexose | 476.27805, 518.28864, 279.23279 | -0.05 | 2 |
| 34,03     | 637,4318 | C₃₆H₆₂O₈| Saponin | -0.35 | 3 |
| 42,19     | 673.46729 (M + FA) | C₃₆H₆₂O₈| Feruloyloxyfatty acid (C28:0) | -0.5 | 3 |
| M+FA | Mass/Charge (M+FA-H) | M-H | Mass/Charge (M-H) | Molecule | Masses (Da) | Molar Entropy (Kcal/Kmol) | Molar Volume (Å³) |
|------|----------------------|-----|-------------------|----------|-------------|--------------------------|-----------------|
| 31,03 | 695.35022 (M + FA - H) | 649.34393 (M - H) | C₃₁H₄₅O₁₄ | Acylsucrose (S3:19) | 565.28619, 551.27069, 523.23926 | -0.23 | 2 |
| 31,29 | 823.46887 (M - H) | C₄₄H₇₂O₁₄S | SQDG 35:6 | 805.46167, 585.24005, 567.22925, 415.14474, 397.13489, 661.41632 (-162), 643.40631 (-180), 187.09793 | 1.69 | 2 |
| 32,12 | 735.34393 (M + FA - H) | 691.35449 (M - H) | C₃₃H₅₄O₁₅ | Acylsucrose (S4:21) | -0.223 | 2 |
| 32,75 | 737.36023 (M + FA - H) | 705.37012 (M - H) | C₃₃H₅₆O₁₅ | Acylsucrose (S4:22) | 649.34418, 607.29761, 565.25488, 523.932, 481.19174 | -0.223 | 2 |
| 33,47 | 751.37561 (M + FA - H) | 709.39105 (M - H) | C₃₄H₅₈O₁₅ | Acylsucrose (S4:23) | 663.35950, 607.29712, 555.28638, 537.25513, 481.19266, 450.04047, 579.26575 | -0.2 | 2 |
| 34,12 | 583.31543 (M - H) | C₇₃H₉₅O₁₃S | Deoxysulfoquinovosylmonoaclglycerol | 522.35614, 299.04395, 225.00765, 297.27969 | -0.55 | 2 |
| 34,74 | 765.39105 (M + FA - H) | 719.38678 | C₃₅H₆₅O₁₅ | Acylsucrose (S4:24) | 677.37555, 635.32880, 593.28906, 551.27112, 566.47937, 548.46857 | -0.48 | 2 |
| 35,53 | 779.40680 (M + FA - H) | 733.40088 (M - H) | C₃₆H₆₅O₁₅ | Tetraacysucrose (S4:25) | 691.39069, 607.29718, 565.28638, 481.19226, 439.18195 | -0.9 | 2 |
| 41,51 | 837.48236 | C₃₈H₇₂O₁₅S | SQDG 36:6 (C:18/C:18) | 778.50342, 579.28290, 559.25781, 537.27264, 481.71002, 413.66330 | 0.1 | 2 |
| 23,30 | 327.21603 | C₁₆H₃₂O₃ | Trihydroxyoctadecadienoic | 171.10214, 211.13322, 229.14371, 239.12776, 273.18454, 291.19528, 309.20554, 153.09113, 127.11237, 193.15909, 247.20549, 273.18460 | -4.6 | 2 |
| 23,13 | 1113.52881 (M + FA - H) 1067.52161 (M - H) | C₃₀H₄₄O₁₄ | Nicotianoside III | 921.46710 (-146), 903.45825, 757.39960, 613.35699, **775.40753** (-146), 629.35046 (-146), 467.29852 (-146), **575.31903**, 595.34308 | -4.4 | 2 |
|-------|-----------------------------------------------|------------|----------------|----------------------------------|--------|------|
| 28,87 | 476.27701                                     | C₂₀H₁₄NO₅P | LysoPE (18:2/0:0) | 279.23212, 261.2208 | -2.6 | 2 |
| 25,71 | 609.26501 (M - H)                             | C₂₀H₁₂O₅P  | PA (18:4/0:0) + glucose | 563.26831, 467.21176, 447.21265 (-162), 429.20215 (-180), 293.21054, 315.04654, 275.20016, 241.01062, 235.16841, 265.21635, 244.75534 | -5.15 | 2 |
| 14,05 | 172.09782                                     | C₁₃H₁₅NO₃ | Acetyl-leucine   | 130.08746 | -0.56 | 2 |
| 7,14  | 203.08176                                     | C₁₃H₁₃N₂O₂ | Tryptophan      | 159.09236, 186.05562, 142.06607, 116.05032 | -4.09 | 2 |
| 12.54 | 249.12405                                     | C₁₃H₁₈N₃O₃ | Caffeoylputrescine | 207.11348, 135.04503 | -1.6 | 2 |
| 11,56 | 192.0667                                      | C₁₀H₁₃NO₃ | Benzoylalanine  | 146.93811, 131.47552, 102.73841, 74.02512, 66.10155 | 0.43 | 2 |
| 11,92 | 215.13998                                     | C₁₀H₂₀N₂O₃ | Valyl valine    | 197.12953, 128.03546, 169.13451, 141.10333, 127.05141, 84.04576, 66.10163 | -0.63 | 2 |
| 13,23 | 321.14499                                     | C₁₃H₁₈N₂O₅ | Acetyl-tyrosil valine | 277.15555 | -1.88 | 2 |
| 14,39 | 373.11261                                     | C₁₃H₂₀O₁₀ | Propyl gallate glucoside | 358.08932, 304.91312, 328.13907, 211.06067, 195.02950, 153.05544, 180.04230, 179.07085, 196.03738 | -3.77 | 2 |
| 13,77 | 343.09238                                     | C₁₃H₂₀O₇ | Dihydroxyacetophenone glucoside | 328.08023, 299.10422, 275.07788, 181.05101, 166.02739, 234.04906 | -3   | 2 |
| MW      | M + FA (M - H)       | Formula       | Name                                               | Molecular Mass   | Delta MW | Delta Log E |
|---------|----------------------|---------------|---------------------------------------------------|------------------|----------|-------------|
| 20,53   | 381.164492 (M + FA - H) 305.15997 (M - H) | C₁₄H₂₆O₇       | Glucopyranosyloxyoctanone                          | 207.05090, 143.10780 (-162) | -1,62    | 2           |
| 13,91   | 386.14432 (M - H + FA) 340.13922 (M - H) | C₁₆H₂₂NO₇      | Acetyltyramine glucoside                           | 178.08691        | -2.8     | 2           |
| 13,23   | 329.08661             | C₁₄H₁₆O₅       | Trihydroxyacetophenone glucopyranoside             |                  |          |             |
| 15,67   | 321,15408             | C₁₄H₂₆O₈       | Octanoic acid glucoside                            | 311.83716, 303.14395, 159.10197, 141.09163 | -2.6     | 2           |
| 14,82   | 192,06606             | C₁₀H₁₃NO₃      | Phenylacetylglucose                                | 74,0251          | -2.8     | 2           |
| 11,99   | 340,13943             | C₁₆H₂₃NO₇      | Acetyl-hydroxy phenethylamine glucopyranose        |                  |          |             |
| 15,65   | 399,09238 (M + FA - H) 353.08685 (M - H) | C₁₆H₁₉O₇       | 3CQA                                              | 191,03455        | -2.7     | 1           |
| 15,87   | 461,16623 (M + FA - H) 415,16101 (M - H) | C₁₉H₂₆O₁₀      | Phenylethanol apiofuranosyl glucopyranoside        | 311.09796, 293.08740, 191.05603, 161.04555, 149.04562, 131.03503, 113.02453 | -4       | 2           |
| 32,28   | 481,25677             | C₂₂H₄₃O₂₃P     | PG (16:1/0:0)                                     | 253.21730, 245.04327, 152.99620 | -0.8     | 2           |
| 32,09   | 431,22028             | C₂₁H₃₅O₂₇P     | PA(18:3/0:0)                                      | 152.99603, 363.21521, 171.00633 | -0.309   | 2           |
| 19,32   | 483,20621 (M + FA - H) 437,20065 (M - H) | C₁₉H₃₅O₁₁      | Octanoic acid + dyhydroxymethylene butanoyl beta glucopyranoside | 403.69440, 293.08636, 191.05574, 149.04399, 131.03494, 125.02441, 101.02441, 89.02454 | -4.99    | 2           |
| 18,66   | 513,21667 (M - H + FA) 467,21097 (M - H) | C₂₀H₅₆O₁₂      | Sucrose octanoate                                  | 323.09671, 305.08640 | -5.2     | 2           |
| 18.04 | 675.25775 (M + FA - H) 599.25262 (M - H) | C₂₅H₄₆O₁₆ | Octenediol - diglucose - xylose | 305.15884, 581.24194, 539.23181, 497.22095, 455.13800, 389.17941, 347.16898, 275.07568, 233.13835, 161.04489 | -4.05 | 2 |
| 30.08 | 577.26654 | C₂₅H₄₆O₁₃S | SQMGC18:3 | 299.04263, 225.00653, 277.21597 | -3.925 | 2 |
| 17.65 | 245.09212 | C₃₅H₄₄N₂O₃ | Acetyl tryptophan | 203.08199, 186.05530, 159.09239, 142.06580, 116.05039 | -4.2 | 2 |
| 22.81 | 597.23712 (M + FA - H) 551.23236 | C₂₅H₆₆O₁₆ | Triacylsucrose (S₃:12) | 536.29572, 509.22107, 467.17386, 311.22119, 425.16483, 407.15314 | -4.8 | 2 |
| 22.97 | 597.23712 (M + FA - H) 551.23236 | C₂₅H₆₆O₁₆ | Triacylsucrose (S₃:12) | 536.29572, 509.22107, 467.17386, 311.22119, 425.16483, 407.15314 | -4.8 | 2 |
| 34.28 | 409.23572 | C₁₉H₃₉O₇ | LPA(0:0/16:0) | 152.99606, 369.90182, 340.20300, 171.00641 | -0.107 | 2 |
| 27.92 | 653.30243 (M + AF - H) 607.29736 (M-H) | C₂₈H₄₆O₁₄ | Triacylsucrose (S₃:16) | 523.23962, 509.22409, 491.21301, 425.16415, 407.15527, 319.07587, 439.18204, 396.82724, 323.09824 | -0.089 | 2 |
| 15.35 | 321.15442 | C₁₄H₂₆O₈ | Octanoic acid glucoside | 303.14401, 159.10231, 141.09180, 119.03476, 101.02428 | -3.35 | 2 |
| 28.30 | 681.29718 (M + FA - H) 635.29163 (M - H) | C₃₀H₆₈O₁₇ | Tetraacylsucrose (S₄:17) | 593.28168, 551.23468, 509.22233, 471.75043, 399.14078, 491.21207, 467.31448 | -0.32 | 2 |
| M.W (M + FA - H) | M.W (M - H) | Molecular Formula | Type of Substrate | Molecular Weight | Purity | Retention Time |
|-------------------|--------------|-------------------|------------------|-----------------|--------|----------------|
| 28,01             | 679.28137    | C₃₀H₄₇O₁₇       | Tetraacylsucrose (S4:17) | 591.26581, 551.23230, 509.22476, 415.14536, 397.13455 | -0.74  | 2              |
| 28,72             | 681.29718    | C₃₀H₅₀O₁₇ + CH₃O₂ | Tetraacylsucrose (S4:17) | 593.28168, 551.23468, 509.22263, 399.14078, 491.21207 | -3     | 2              |
| 15,98             | 353.11301    | C₃₁H₂₄NO₈S      | Homomethionine + quinic acid | 309.12335, 191.05563 | -5.5   | 2              |
| 30,42             | 709.32623    | C₃₁H₅₁O₁₅ + CH₃O₂ | Tetraacylsucrose (S4:19) | 621.30927, 579.26245, 523.23724, 537.25281, 505.22699 | -4.3   | 2              |
| 29,72             | 695.31165    | C₃₁H₅₈O₁₄      | Tetraacylsucrose (S4:18) | 607.29517, 565.24805, 523.23773, 467.17517, 509.22223, 491.21164, 407.15445, 551.23254 | -3.59  | 2              |
| 30,66             | 709.3277     | C₃₁H₅₁O₁₅ + CH₃O₂ | Tetraacylsucrose (S4:19) | 621.30927, 523.23724, 537.25281, 565.25739, 421.17258 | -1.6   | 2              |
| 27,33             | 721.36536    | C₃₃H₅₆O₁₄       | Digalactopyranosyl lineoylglycerol (C18:3) | 397.13483 | 0.016  | 2              |
| 33,01             | 723.38092    | C₃₃H₅₈O₁₄ + AF  | Triacylsucrose (S3:21) | 677.37500, 551.27081, 593.31763, 533.26019 | 0.33   | 2              |
| 22,47             | 453.13809    | C₂₁H₂₅O₁₁       | Dihydroferulic acid glucuronide + methylfurane | 435.12799, 371.09631, 353.08560, 331.10107, 249.06006 | -4.7   | 2              |
| 41,73             | 787.46674    | C₄₁H₇₂O₂₂S      | SQDG 16:3 18:0 | 537.27368, 559.25854 | -0.5   | 2              |
| 23,76             | 1007.46606   | C₄₇H₇₆O₂₃      | Nicotianoside IV | 963.47504, 903.45404, 921.46436, 775.40692, 757.39697 | -4.36  | 2              |
| 26,98             | 1059.53882   | C₅₁H₆₆O₂₀      | Diosgenin tetraglicoside | 868.47736, 722.41968, 576.35822 | -0.866 | 2              |
| 19,51 | 1074.54419 (M - H + FA) 1028.53674 (M - H) | C_{51}H_{63}NO_{20} | Solanidine tetrabioside | -6,6 | 3 |
| 20,40 | 1119.63293 (M + FA - H) | C_{51}H_{58}NO_{22} | Glykoalkaloid | -7,8 | 3 |
| 17,37 | 675.26807 (M + FA - H) 629.26263 (M - H) | C_{26}H_{16}O_{17} | Sucrose + hexose octanoate | 611.25220, 551.23083, 467.21072, 341.10675, 323.09659 | -5,7 | 2 |
| 1,67 | 116.0709 (M + H) | C_{5}H_{9}NO_{2} | Proline | -2.58 | 2 |
| 1,54 | 175.1192 (M + H) | C_{6}H_{14}N_{4}O_{2} | Arginine | 116.0706, 130.0961 | 1,71 | 2 |
| 1,7 | 132.1015 (M + H) | C_{6}H_{13}NO_{2} | Leucine + Isoleucine | 86.0967 | 3,02 | 2 |
| 1,7 | 166.0857 (M + H) | C_{6}H_{11}NO_{2} | Phenylalanine | 120.0804 | 3,34 | 2 |
| 1,65 | 182.0807 (M + H) | C_{6}H_{11}NO_{3} | Tyrosine | 165.0548, 136.0750 | 2,19 | 2 |
| 2,05 | 174.0827 (M - H) | C_{10}H_{6}NO_{2} | 3-Indole acetic acid | 130.0639, 128.0485 | 1,14 | 2 |
| 14,28 | 265.14344 (M + H) | C_{13}H_{20}O_{4} | Abscisic acid | 247.1290, 187.1115 | 3,449 | 2 |