**Table 1. LC-MS/MS profile of methanolic extract of *P.betle* in the positive ion mode.**

| **Compound Identification** | | **General** | | | | | | **Database Search** | | **Library Search** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Cpd** | **Name** | **Formula** | **m/z** | **Mass** | **Start** | **RT** | **End** | **Score (DB)** | **Diff**  **(DB, ppm)** | **Score (Lib)** |
| 1 | 3,8-Dihydroxy-6-methoxy-7(11)-eremophilen-12,8-olide | C16 H24 O5 | 319.1505 | 296.161 | 1.703 | 1.712 | 1.72 | 93.26 | 3.86 | 0 |
| 2 | Mometasone Furoate | C27 H30 Cl2 O6 | 543.1322 | 520.143 | 1.904 | 1.912 | 1.92 | 65.99 | -2.29 | 0 |
| 3 | Dihydrocaffeic acid 3-O-glucuronide | C15 H18 O10 | 381.0796 | 358.09 | 1.928 | 1.937 | 1.945 | 81.23 | -0.04 | 0 |
| 4 | Choline | C5H14NO | 104.1076 | 104.108 | 1.879 | 1.987 | 2.096 |  | -5.74 | 95.28 |
| 5 | D-1-[(3-Carboxypropyl)amino]-1-deoxyfructose | C10 H19 N O7 | 266.1234 | 265.116 | 2.029 | 2.037 | 2.045 | 99.86 | -0.16 | 0 |
| 6 | L-Pinitol | C7 H14 O6 | 217.0685 | 194.079 | 2.004 | 2.125 | 2.246 | 99.41 | -1.36 | 0 |
| 7 | Sedoheptulose | C7 H14 O7 | 233.0636 | 210.074 | 2.129 | 2.237 | 2.346 | 99.14 | -1.91 | 91.37 |
| 8 | Deoxyfructosazine | C12 H20 N2 O7 | 327.1162 | 304.127 | 2.63 | 2.638 | 2.647 | 99.73 | 0.02 |  |
| 9 | (x)-1,2-Propanediol 1-O-b-D-glucopyranoside | C9 H18 O7 | 261.0949 | 238.106 | 2.705 | 2.714 | 2.722 | 99.01 | -1.65 | 0 |
| 10 | Pyroglutamic acid | C5 H7 N O3 | 130.0501 | 129.043 | 2.806 | 2.814 | 2.822 | 86.98 | -2.23 | 90.3 |
| 11 | Valinopine | C10 H17 N O6 | 270.0951 | 247.106 | 2.906 | 2.964 | 3.023 | 99.44 | -1.33 | 0 |
| 12 | N-Methyl-N,4-dinitrosoaniline | C7 H7 N3 O2 | 166.0613 | 165.054 | 3.106 | 3.115 | 3.123 | 96.66 | -1.5 | 0 |
| 13 | Adenosine | C10H13N5O4 | 268.1045 | 267.097 | 3.131 | 3.227 | 3.323 |  | -1.71 | 99.33 |
| 14 | Adenine | C5 H5 N5 | 136.0622 | 135.055 | 3.231 | 3.24 | 3.248 | 85.16 | -3.47 | 0 |
| 15 | Cellulose, microcrystalline | C14 H26 O11 | 393.1369 | 370.148 | 3.407 | 3.415 | 3.424 | 99.64 | -0.41 | 0 |
| 16 | Pro Leu | C11 H20 N2 O3 | 229.1548 | 228.148 | 3.432 | 3.49 | 3.549 | 98.96 | -0.74 | 96.61 |
| 17 | 2,3-Butanediol glucoside | C10 H20 O7 | 275.1103 | 252.121 | 3.632 | 3.641 | 3.649 | 99.78 | -0.49 | 0 |
| 18 | (Z)-2-Methyl-2-butene-1,4-diol 4-O-beta-D-Glucopyranoside | C11 H20 O7 | 287.1107 | 264.122 | 3.583 | 3.653 | 3.724 | 97.94 | -2.14 | 0 |
| 19 | (2S,4R,5S)-Muscarine | C9 H20 N O2 | 174.149 | 174.15 | 3.732 | 3.741 | 3.749 | 86.75 | -1.32 | 0 |
| 20 | Nonanoic acid, 3-amino-, (R)- | C9 H19 N O2 | 196.1311 | 173.142 | 3.833 | 3.841 | 3.849 | 86.81 | -2.02 | 0 |
| 21 | 3-(3,4-Dihydroxyphenyl)-1-propanol 3'-glucoside | C15 H22 O8 | 353.1208 | 330.132 | 3.808 | 3.879 | 3.949 | 98.88 | -0.49 | 0 |
| 22 | 3,4,5-Trimethoxyphenyl glucoside | C15 H22 O9 | 369.1159 | 346.127 | 3.908 | 3.916 | 3.925 | 99.57 | -0.53 | 0 |
| 23 | (R)-2-Hydroxybutane-1,2,4-tricarboxylate | C7 H10 O7 | 229.0322 | 206.043 | 4.008 | 4.017 | 4.025 | 99.22 | -1.51 | 0 |
| 24 | Glucosylisomaltol | C12 H16 O8 | 311.0736 | 288.085 | 4.109 | 4.117 | 4.125 | 85.36 | 0.11 | 0 |
| 25 | Isopropyl apiosylglucoside | C14 H26 O10 | 377.1419 | 354.153 | 4.133 | 4.142 | 4.15 | 97.15 | -0.62 | 0 |
| 26 | 1-(3-Methylbutanoyl)-6-apiosylglucose | C16 H28 O11 | 419.1522 | 396.163 | 4.209 | 4.217 | 4.225 | 90.31 | -0.5 | 0 |
| 27 | Dikegulac | C12 H18 O7 | 297.0945 | 274.105 | 4.234 | 4.242 | 4.25 | 98.84 | -0.24 | 0 |
| 28 | Pantoyllactone glucoside | C12 H20 O8 | 315.1052 | 292.116 | 4.434 | 4.442 | 4.451 | 83.99 | -1.79 | 0 |
| 29 | (1S,2R,4R,8S)-p-Menthane-2,8,9-triol 9-glucoside | C16 H30 O8 | 373.1833 | 350.194 | 4.409 | 4.468 | 4.526 | 99.47 | 0.23 | 0 |
| 30 | 7-(3-Methylbut-2-enyl)-L-tryptophan | C16 H20 N2 O2 | 273.1598 | 272.153 | 4.534 | 4.543 | 4.551 | 99.57 | -0.47 | 0 |
| 31 | 2'-Methoxy-3-(2,4-dihydroxyphenyl)-1,2-propanediol 4'-glucoside | C16 H24 O9 | 383.1313 | 360.142 | 4.61 | 4.618 | 4.626 | 99.48 | 0.08 | 0 |
| 32 | Butyl 3-O-beta-D-glucopyranosyl-butanoate | C14 H26 O8 | 345.1517 | 322.163 | 4.634 | 4.643 | 4.651 | 83.26 | 0.55 | 0 |
| 33 | 2-Hexenoylcholine | C11 H22 N O2 | 200.1648 | 200.165 | 5.136 | 5.144 | 5.152 | 87.01 | -1.5 | 0 |
| 34 | Glucosyl (E)-2,6-Dimethyl-2,5-heptadienoate | C15 H24 O7 | 339.1418 | 316.153 | 5.086 | 5.169 | 5.252 | 98.29 | -1.36 | 0 |
| 35 | Glucocaffeic acid | C15 H18 O9 | 365.0843 | 342.095 | 5.211 | 5.219 | 5.227 | 99.12 | -0.14 | 0 |
| 36 | Diethyl phenyl phosphate | C10 H15 O4 P | 231.0769 | 230.07 | 5.336 | 5.344 | 5.353 | 93.88 | 4.99 |  |
| 37 | D-Linalool 3-(6''-malonylglucoside) | C19 H30 O9 | 425.1783 | 402.189 | 5.411 | 5.42 | 5.428 | 83.27 | -0.24 | 0 |
| 38 | Pisumionoside | C19 H32 O9 | 427.1936 | 404.205 | 5.436 | 5.444 | 5.453 | 92.95 | 0.05 | 0 |
| 39 | Prenyl arabinosyl-(1->6)-glucoside | C16 H28 O10 | 403.1577 | 380.169 | 5.536 | 5.545 | 5.553 | 99.02 | -0.61 | 0 |
| 40 | Phenethylamine glucuronide | C14 H19 N O6 | 320.1106 | 297.121 | 5.587 | 5.595 | 5.604 | 98.91 | -0.37 | 0 |
| 41 | (6RS)-22-oxo-23,24,25,26,27-pentanorvitamin D3 6,19-sulfur dioxide adduct / (6RS)-22-oxo-23,24,25,26,27-pentanorcholecalciferol 6,19-sulfurdioxide adduct | C22 H32 O4 S | 393.2096 | 392.203 | 5.637 | 5.645 | 5.653 | 87.3 | -1.05 | 0 |
| 42 | Ginkgolide J | C20 H24 O10 | 425.1422 | 424.135 | 5.712 | 5.758 | 5.804 | 88.49 | 4.54 | 82.67 |
| 43 | Octanoylglucuronide | C14 H24 O8 | 343.1365 | 320.147 | 5.812 | 5.821 | 5.829 | 98.47 | -0.67 | 0 |
| 44 | Dihydroroseoside | C19 H32 O8 | 411.199 | 388.21 | 5.737 | 5.833 | 5.929 | 98.59 | -0.19 | 0 |
| 45 | Coumarin | C9 H6 O2 | 147.0443 | 146.037 | 6.038 | 6.046 | 6.054 | 87.15 | -2.09 | 80.23 |
| 46 | Sonchuionoside C | C19 H30 O8 | 409.1834 | 386.194 | 6.138 | 6.146 | 6.154 | 83.62 | -0.25 | 0 |
| 47 | N-Carboxyacetyl-D-phenylalanine | C12 H13 N O5 | 274.0688 | 251.08 | 6.238 | 6.246 | 6.254 | 99.71 | -0.96 | 0 |
| 48 | 6-Feruloylglucose 2,3,4-trihydroxy-3-methylbutylglycoside | C21 H30 O12 | 497.1629 | 474.174 | 6.188 | 6.272 | 6.355 | 98.9 | 0.05 | 0 |
| 49 | N-Acetylanonaine | C19 H17 N O3 | 308.1284 | 307.121 | 6.313 | 6.322 | 6.33 | 99.75 | -0.7 | 0 |
| 50 | 2,6-Dimethyl-6-O-beta-D-quinovopyranosyl-7-octadecenoic acid | C16 H28 O7 | 355.1729 | 332.184 | 6.414 | 6.422 | 6.43 | 99.22 | -0.43 | 0 |
| 51 | 2-O-Acetylarbutin | C14 H18 O8 | 337.0897 | 314.101 | 6.438 | 6.497 | 6.555 | 98.29 | -1.38 | 0 |
| 52 | 1-O-2'-Hydroxy-4'-methoxycinnamoyl-b-D-glucose | C16 H20 O9 | 379.1002 | 356.111 | 6.589 | 6.597 | 6.606 | 99.18 | -0.62 | 0 |
| 53 | Diphenylcarbazide | C13 H14 N4 O | 265.105 | 242.116 | 6.689 | 6.698 | 6.706 | 93.47 | 3.64 | 0 |
| 54 | Bifenazate | C17 H20 N2 O3 | 301.1551 | 300.148 | 6.915 | 6.923 | 6.931 | 99.23 | -1.48 | 0 |
| 55 | 2-(Biaryl)carbapenems | C21 H19 N O4 | 350.1388 | 349.132 | 6.939 | 6.948 | 6.956 | 98.76 | -0.5 | 0 |
| 56 | CAY10485 | C27 H27 N O7 | 478.1862 | 477.179 | 6.99 | 6.998 | 7.007 | 96.84 | 0.11 |  |
| 57 | Linalool 3,7-oxide beta-primeveroside | C21 H36 O11 | 487.2151 | 464.226 | 7.24 | 7.248 | 7.257 | 99.4 | -0.2 | 0 |
| 58 | 1-(8-[5]-ladderane-octanoyl)-2-(8-[3]-ladderane-octanyl)-sn-glycerophosphocholine | C48 H81 N O7 P | 814.5776 | 814.578 | 7.215 | 7.286 | 7.357 | 86.86 | -3.48 | 0 |
| 59 | Dicyclohexylamine | C12 H23 N | 182.1908 | 181.184 | 7.291 | 7.299 | 7.307 | 86.58 | -2.3 | 0 |
| 60 | Gly Arg Tyr | C17 H26 N6 O5 | 395.2043 | 394.197 | 7.391 | 7.399 | 7.407 | 97.4 | -1.65 | 89.53 |
| 61 | 3''-HydroxyPravastatin | C23 H36 O8 | 441.2462 | 440.239 | 7.516 | 7.524 | 7.532 | 87.79 | 4.91 | 0 |
| 62 | 2-Hydroxymaprotiline glucuronide | C26 H31 N O7 | 492.2015 | 469.212 | 7.741 | 7.749 | 7.758 | 37.47 | -4.83 | 0 |
| 63 | Arg Tyr Thr | C19 H30 N6 O6 | 439.2303 | 438.224 | 7.817 | 7.825 | 7.833 | 72.32 | -2.75 | 86.85 |
| 64 | Deoxysappanone B 7,3'-Dimethyl Ether Acetate | C20 H20 O6 | 357.1336 | 356.126 | 7.917 | 7.925 | 7.933 | 99.02 | -0.78 | 0 |
| 65 | Citrusin C | C16 H22 O7 | 349.1262 | 326.137 | 7.892 | 7.95 | 8.009 | 98.53 | -1.34 | 0 |
| 66 | Isobutyl 2-furanpropionate | C11 H16 O3 | 197.1176 | 196.11 | 8.092 | 8.176 | 8.259 | 98.84 | -2.21 | 0 |
| 67 | Asperlicin | C31 H29 N5 O4 | 536.2282 | 535.221 | 8.117 | 8.238 | 8.359 | 96.39 | 1.92 | 0 |
| 68 | Kenposide B | C21 H36 O10 | 471.2204 | 448.231 | 8.393 | 8.401 | 8.41 | 97.98 | -0.58 | 0 |
| 69 | ZM 447439 | C29 H31 N5 O4 | 536.2281 | 513.239 | 8.443 | 8.451 | 8.459 | 96.07 | -2.48 | 0 |
| 70 | CAY10641 | C28 H27 N O6 | 474.1909 | 473.184 | 8.543 | 8.551 | 8.56 | 98.55 | 0.21 | 0 |
| 71 | NVP-BEZ235 | C30 H23 N5 O | 470.1966 | 469.189 | 8.719 | 8.727 | 8.735 | 97.78 | 1.97 | 0 |
| 72 | omega-Carboxy-N-acetyl-LTE4 | C25 H37 N O8 S | 534.2124 | 511.225 | 8.844 | 8.852 | 8.86 | 74.42 | -1.15 | 0 |
| 73 | 5-Hepten-3-yn-1-ol, 2,2-dimethyl-7-[methyl(1-naphthalenylmethyl)amino]-, (E)- glucuronide | C27 H33 N O7 | 506.2173 | 483.228 | 9.044 | 9.153 | 9.261 | 87.21 | -4.78 | 0 |
| 74 | N2-Maltulosylarginine | C18 H34 N4 O12 | 499.2229 | 498.216 | 9.22 | 9.228 | 9.236 | 81.4 | 3.24 | 0 |
| 75 | Nicardipine | C26 H29 N3 O6 | 480.2127 | 479.205 | 9.32 | 9.328 | 9.336 | 97.79 | 0.58 | 0 |
| 76 | SN-38 | C22 H20 N2 O5 | 393.1449 | 392.138 | 9.52 | 9.529 | 9.537 | 47.12 | -1.1 | 0 |
| 77 | (9R,10S,12Z)-9,10-Dihydroxy-8-oxo-12-octadecenoic acid | C18 H32 O5 | 351.2142 | 328.225 | 9.645 | 9.654 | 9.662 | 99.27 | 0.17 | 0 |
| 78 | Cyproterone acetate | C24 H29 Cl O4 | 439.1655 | 416.177 | 9.921 | 9.992 | 10.06 | 63.39 | -2.48 | 0 |
| 79 | Maculosin | C14 H16 N2 O3 | 261.1239 | 260.117 | 10.15 | 10.23 | 10.26 | 98.94 | -1.73 | 0 |
| 80 | Resolvin D2 | C22H32O5 | 399.2068 | 376.218 | 10.45 | 10.455 | 10.46 |  | 19.56 | 85.65 |
| 81 | Difenoxuron | C16 H18 N2 O3 | 309.1214 | 286.132 | 10.52 | 10.631 | 10.74 | 89.92 | -1.62 | 0 |
| 82 | 10-Hydroxycarbazepine | C15 H14 N2 O2 | 255.1133 | 254.106 | 10.55 | 10.656 | 10.76 | 97.22 | -1.93 | 0 |
| 83 | Palmitoyl glucuronide | C22 H42 O7 | 441.2823 | 418.293 | 10.82 | 10.831 | 10.84 | 98.96 | -0.05 | 0 |
| 84 | Metominostrobin | C16 H16 N2 O3 | 285.1236 | 284.116 | 11.02 | 11.032 | 11.04 | 98.87 | -1.06 | 0 |
| 85 | Tryptophyl-Tryptophan | C22 H22 N4 O3 | 413.157 | 390.169 | 11.25 | 11.257 | 11.27 | 88.54 | 1.52 | 0 |
| 86 | C16 Sphinganine | C16 H35 N O2 | 274.2744 | 273.267 | 11.2 | 11.27 | 11.34 | 98.84 | -1.17 | 0 |
| 87 | (7'x,8'x)-4,7'-Epoxy-3,8'-bilign-7-ene-3,5'-dimethoxy-4',9,9'-triol | C20 H22 O6 | 359.1492 | 358.142 | 11.3 | 11.37 | 11.44 | 98.94 | -0.89 | 0 |
| 88 | 13-Hydroxy-9-methoxy-10-oxo-11-octadecenoic acid | C19 H34 O5 | 365.2301 | 342.241 | 11.65 | 11.708 | 11.77 | 84.6 | -0.55 | 0 |
| 89 | Junosine | C19 H19 N O4 | 326.1391 | 325.132 | 11.63 | 11.733 | 11.84 | 98.34 | -1.05 | 0 |
| 90 | AK-toxin I | C23 H27 N O6 | 414.1913 | 413.184 | 11.9 | 11.959 | 12.02 | 98.72 | -0.65 | 0 |
| 91 | 7C-Aglycone | C18 H18 O4 | 299.1283 | 298.121 | 12.05 | 12.097 | 12.14 | 93.11 | -2.09 | 0 |
| 92 | 12,13-dihydroxy-11-methoxy-9-octadecenoic acid | C19 H36 O5 | 367.2462 | 344.257 | 12.25 | 12.259 | 12.27 | 97.42 | -2.28 | 0 |
| 93 | Gingerenone B | C22 H26 O6 | 387.1807 | 386.173 | 12.35 | 12.46 | 12.57 | 99.18 | -0.81 | 0 |
| 94 | Myristicanol B | C22 H28 O7 | 427.173 | 404.184 | 12.6 | 12.611 | 12.62 | 99.73 | -0.63 | 0 |
| 95 | Sonchifolin | C21 H26 O6 | 397.1625 | 374.173 | 12.63 | 12.686 | 12.74 | 99.65 | -0.79 | 0 |
| 96 | FIPI | C23 H24 F N5 O2 | 444.1809 | 421.192 | 12.7 | 12.711 | 12.72 | 99.19 | -0.88 |  |
| 97 | Gingerglycolipid A | C33 H56 O14 | 699.3561 | 676.367 | 12.8 | 12.861 | 12.92 | 99.65 | 0.16 | 0 |
| 98 | Phe Arg Thr | C19 H30 N6 O5 | 423.2357 | 422.229 | 13 | 13.086 | 13.17 | 98 | -1.68 | 89.99 |
| 99 | Morphine | C17 H19 N O3 | 286.1444 | 285.137 | 13.13 | 13.187 | 13.25 | 97.65 | -2.26 | 72.48 |
| 100 | 1-(4-Hydroxy-3-methoxyphenyl)-5-(4-hydroxyphenyl)-1,4-pentadien-3-one | C18 H16 O4 | 297.1124 | 296.105 | 13.33 | 13.337 | 13.35 | 92.4 | 0.05 | 0 |
| 101 | Acutilobin | C19 H20 O5 | 351.1204 | 328.131 | 13.35 | 13.362 | 13.37 | 93.93 | -0.18 | 0 |
| 102 | PC(18:3(6Z,9Z,12Z)/0:0) | C26 H49 N O7 P | 518.3242 | 518.325 | 13.45 | 13.462 | 13.47 | 99.08 | -0.24 | 0 |
| 103 | Clausarinol | C24 H30 O6 | 437.1937 | 414.204 | 13.5 | 13.513 | 13.57 | 99.7 | -0.51 | 0 |
| 104 | Met Tyr Glu | C19 H27 N3 O7 S | 442.1653 | 441.158 | 13.63 | 13.638 | 13.65 | 82.8 | -2.98 | 0 |
| 105 | Cys Trp Ala | C17 H22 N4 O4 S | 401.126 | 378.137 | 13.6 | 13.688 | 13.77 | 87.44 | -2.56 | 0 |
| 106 | Erysopine | C17 H19 N O3 | 286.1442 | 285.137 | 13.71 | 13.813 | 13.92 | 98.75 | -1.72 | 0 |
| 107 | Cetrimide | C17 H38 N | 256.3005 | 256.301 | 14.26 | 14.264 | 14.27 | 98.23 | -2.22 | 0 |
| 108 | Carpelastofuran | C30 H34 O8 | 545.2148 | 522.226 | 14.21 | 14.314 | 14.42 | 97.83 | -0.32 | 0 |
| 109 | 1-Naphthylacetylspermine | C22 H34 N4 O | 393.2616 | 370.272 | 14.43 | 14.439 | 14.45 | 94.26 | 2.36 | 0 |
| 110 | all-trans-heptaprenyl diphosphate | C35 H60 O7 P2 | 677.3721 | 654.383 | 14.53 | 14.54 | 14.55 | 92.81 | -2.17 | 0 |
| 111 | Corchorosol A | C29 H44 O9 | 537.3035 | 536.296 | 14.61 | 14.677 | 14.75 | 88.26 | 4.31 | 0 |
| 112 | N-trans-Feruloyl-4-O-methyldopamine | C19 H21 N O5 | 344.1495 | 343.142 | 14.71 | 14.765 | 14.82 | 98.44 | -0.84 | 0 |
| 113 | 2,3-dinor-8-iso-PGF2a | C18 H30 O5 | 349.1987 | 326.21 | 14.86 | 14.865 | 14.87 | 99.6 | -0.44 | 87.62 |
| 114 | (±)10-Gingerol | C21 H34 O4 | 351.2537 | 350.247 | 14.93 | 14.94 | 14.95 | 93.79 | -2.21 | 0 |
| 115 | Misoprostol (free acid) | C21 H36 O5 | 391.246 | 368.257 | 14.91 | 14.978 | 15.05 | 99.04 | -1.24 | 97.82 |
| 116 | (Z)-2-amino-1-hydroxyoctadec-4-en-3-one | C18 H35 N O2 | 320.2564 | 297.267 | 15.16 | 15.166 | 15.17 | 99.08 | -1.49 | 0 |
| 117 | Linoleamide | C18 H33 N O | 280.2638 | 279.257 | 15.13 | 15.191 | 15.25 | 99.2 | -0.97 | 0 |
| 118 | (4E,8E,10E-d18:3)sphingosine | C18 H33 N O2 | 318.2407 | 295.251 | 15.36 | 15.366 | 15.37 | 83.13 | -0.99 | 0 |
| 119 | Idoxanthin | C40 H54 O4 | 599.4093 | 598.402 | 15.46 | 15.466 | 15.48 | 99.17 | 0.31 | 0 |
| 120 | Lipoxin E4 | C23 H37 N O6 S | 478.2226 | 455.234 | 15.43 | 15.492 | 15.55 | 89.95 | 1.2 | 0 |
| 121 | Methyl Robustone | C22 H18 O6 | 379.1179 | 378.111 | 15.56 | 15.567 | 15.58 | 99.28 | -0.85 | 97.53 |
| 122 | 1-(m-Methoxycinnamoyl)pyrrolidine | C14 H17 N O2 | 232.1338 | 231.127 | 15.63 | 15.642 | 15.65 | 98.45 | -2.53 | 0 |
| 123 | 1-Palmitoyllysophosphatidylcholine | C24 H51 N O7 P | 496.3402 | 496.341 | 15.66 | 15.755 | 15.85 | 96.24 | -1.08 | 99.41 |
| 124 | methyl 15-hydroperoxy-9Z,12Z,16E-octadecatrienoate | C19 H32 O4 | 347.2194 | 324.23 | 15.76 | 15.767 | 15.78 | 95.62 | -1.03 |  |
| 125 | Asn Arg Asp | C14 H25 N7 O7 | 426.1705 | 403.182 | 15.86 | 15.867 | 15.88 | 81.56 | 0.07 | 0 |
| 126 | N-Methyl-N-(2-phenylethenyl)-3-phenyl-2-oxiranecarboxamide | C18 H17 N O2 | 280.1337 | 279.127 | 16.11 | 16.118 | 16.13 | 98.71 | -1.9 | 0 |
| 127 | 3'-Demethylstaurosporine | C27 H24 N4 O3 | 475.1753 | 452.186 | 16.16 | 16.268 | 16.38 | 95.12 | -2.91 | 0 |
| 128 | Piperaduncin B | C29 H30 O8 | 529.1835 | 506.194 | 16.26 | 16.268 | 16.28 | 98.58 | -0.14 | 0 |
| 129 | Benzoyltropein | C15 H19 N O2 | 246.1494 | 245.142 | 16.56 | 16.569 | 16.58 | 98.74 | -2.11 | 0 |
| 130 | AT-56 | C25 H27 N5 | 420.2173 | 397.228 | 16.64 | 16.644 | 16.65 | 93.91 | -3.79 | 0 |
| 131 | PC(18:1(9Z)/0:0)[rac] | C26 H53 N O7 P | 522.3555 | 522.356 | 16.54 | 16.656 | 16.78 | 99.31 | -0.15 | 0 |
| 132 | OA-6129 D | C20 H33 N3 O8 S | 476.2069 | 475.2 | 16.81 | 16.87 | 16.93 | 84.2 | -2.34 | 0 |
| 133 | Cyclandelate | C17 H24 O3 | 277.1801 | 276.173 | 16.94 | 16.945 | 16.95 | 98.46 | -1.09 | 0 |
| 134 | Stearidonic Acid methyl ester | C19 H30 O2 | 291.2323 | 290.225 | 17.34 | 17.346 | 17.35 | 97.78 | -1.44 | 85.1 |
| 135 | (25S)-5alpha-cholestan-3beta,4beta,6alpha,8beta,15alpha,16beta,26-heptol | C27 H48 O7 | 507.3296 | 484.34 | 17.51 | 17.521 | 17.53 | 98.67 | -0.83 | 0 |
| 136 | Montanol | C21 H36 O4 | 353.2688 | 352.262 | 17.61 | 17.622 | 17.63 | 98.7 | -0.46 | 0 |
| 137 | Lucidenic acid M | C27 H42 O6 | 463.3035 | 462.296 | 17.66 | 17.671 | 17.68 | 87.06 | 4.45 | 0 |
| 138 | [8]-Paradol | C19 H30 O3 | 307.2271 | 306.22 | 17.86 | 17.872 | 17.88 | 99.35 | -1.09 | 0 |
| 139 | Spongipregnoloside B | C33 H52 O11 | 647.3409 | 624.351 | 17.94 | 17.947 | 17.96 | 90.05 | -0.59 | 0 |
| 140 | 9(Z),11(E),13(E)-Octadecatrienoic Acid methyl ester | C19 H32 O2 | 293.248 | 292.241 | 18.14 | 18.198 | 18.26 | 99.22 | -1.52 | 96.5 |
| 141 | 13(S)-HODE methyl ester | C19 H34 O3 | 333.2403 | 310.251 | 18.26 | 18.273 | 18.28 | 84.3 | -0.93 | 74.21 |
| 142 | Cyclopassifloside X | C37 H62 O12 | 721.4132 | 698.425 | 18.57 | 18.573 | 18.58 | 86.77 | -0.56 | 0 |
| 143 | Obtusilactone A | C19 H32 O3 | 309.2429 | 308.236 | 18.74 | 18.874 | 18.98 | 98.57 | -1.47 | 0 |
| 144 | Methyl acetyl ricinoleate | C21 H38 O4 | 377.2665 | 354.277 | 19.04 | 19.1 | 19.16 | 99.78 | -0.68 | 0 |
| 145 | Colupulone | C25 H36 O4 | 423.2507 | 400.261 | 19.24 | 19.25 | 19.26 | 99.73 | -0.1 | 0 |
| 146 | Avocadene 4-acetate | C19 H36 O4 | 351.2508 | 328.262 | 19.54 | 19.601 | 19.66 | 99.67 | -0.75 | 0 |
| 147 | Pseudoginsenoside RT3 | C41 H70 O13 | 793.4708 | 770.482 | 19.77 | 19.776 | 19.78 | 99.18 | 0.25 | 0 |
| 148 | Palmitic amide | C16 H33 N O | 256.2639 | 255.257 | 20.14 | 20.252 | 20.36 | 99.45 | -1.33 | 0 |
| 149 | N-stearoyl glutamic acid | C23 H43 N O5 | 436.3034 | 413.314 | 20.37 | 20.415 | 20.46 | 99.42 | -0.25 | 0 |
| 150 | Oleamide | C18 H35 N O | 282.2796 | 281.272 | 20.62 | 20.728 | 20.84 | 98.25 | -1.4 | 96.01 |
| 151 | MG(16:0/0:0/0:0)[rac] | C19 H38 O4 | 353.2667 | 330.278 | 20.97 | 21.029 | 21.09 | 99.17 | -1.38 | 0 |
| 152 | PG(12:0/16:0) | C34 H67 O10 P | 667.4543 | 666.447 | 21.27 | 21.329 | 21.39 | 95.88 | 0.78 | 0 |
| 153 | MG(18:1(9Z)/0:0/0:0)[rac] | C21 H40 O4 | 379.2821 | 356.293 | 21.47 | 21.567 | 21.66 | 99.49 | -0.63 | 96.93 |
| 154 | Oligomycin B | C45 H72 O12 | 827.4911 | 804.502 | 21.87 | 21.88 | 21.89 | 47.39 | 0.56 | 0 |
| 155 | Dinoflagellate luciferin | C33 H40 N4 O6 | 611.2862 | 588.297 | 21.97 | 22.018 | 22.06 | 92.29 | -3.77 | 0 |
| 156 | Azaspiracid 2 | C48 H73 N O12 | 856.5237 | 855.516 | 22.37 | 22.382 | 22.39 | 89.17 | -3.07 | 0 |
| 157 | 4-[N-(p-Coumaroyl)serotonin-4''-yl]-N-feruloylserotonin | C39 H36 N4 O7 | 673.2631 | 672.256 | 23.08 | 23.083 | 23.09 | 89.76 | 3.73 | 0 |
| 158 | 2,4,12-Octadecatrienoic acid isobutylamide | C22 H39 N O | 334.3106 | 333.303 | 23.28 | 23.284 | 23.29 | 99.6 | -0.54 | 0 |
| 159 | DG(14:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0) | C39 H62 O5 | 611.4672 | 610.46 | 23.88 | 23.985 | 24.09 | 99.63 | -0.28 | 0 |
| 160 | Oligomycin A | C45 H74 O11 | 813.5121 | 790.523 | 23.93 | 24.036 | 24.14 | 98.85 | 0.14 | 0 |
| 161 | Stearamide | C18 H37 N O | 284.2951 | 283.288 | 24.75 | 24.85 | 24.95 | 99.31 | -1.11 | 95.88 |

**Table 2. LC-MS/MS profile of methanolic extract of *P.betle* in the negative ion mode.**

| **Compound Identification** | | | | | | | | **Database Search** | | **Library Search** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Cpd** | **Name** | **Formula** | **m/z** | **Mass** | **Start** | **RT** | **End** | **Score (DB)** | **Diff**  **(DB, ppm)** | **Score (Lib)** |
| 1 | 2-(beta-D-Glucosyl)-sn-glycerol 3-phosphate | C9 H19 O11 P | 333.0593 | 334.067 | 1.7 | 1.708 | 1.716 | 99.84 | -0.21 | 0 |
| 2 | D-Lactose | C12H22O11 | 377.0856 | 342.116 | 1.825 | 1.833 | 1.842 |  | 0.03 | 85.47 |
| 3 | D-Mannonate | C6 H12 O7 | 195.0515 | 196.059 | 1.8 | 1.896 | 1.992 | 98.48 | -2.36 | 93.51 |
| 4 | L-Xylonate | C5 H10 O6 | 165.0408 | 166.048 | 1.9 | 1.971 | 2.042 | 99.16 | -2.16 | 0 |
| 5 | Glyceric acid | C3 H6 O4 | 105.0199 | 106.027 | 2.001 | 2.109 | 2.218 | 85.85 | -4.89 | 98.41 |
| 6 | Maleic acid | C4 H4 O4 | 115.0042 | 116.011 | 2.226 | 2.234 | 2.242 | 86.18 | -4.14 | 99.98 |
| 7 | Pyroglutamic acid | C5 H7 N O3 | 128.0356 | 129.043 | 2.276 | 2.335 | 2.393 | 87.13 | -2.48 | 100 |
| 8 | Malic acid | C4 H6 O5 | 133.0146 | 134.022 | 2.502 | 2.51 | 2.518 | 86.7 | -2.7 | 98.5 |
| 9 | 3-Deoxy-D-manno-octulosonate | C8 H14 O8 | 237.0617 | 238.069 | 2.702 | 2.71 | 2.719 | 98.02 | -0.7 | 0 |
| 10 | Sarmentosin epoxide | C11 H17 N O8 | 290.0883 | 291.096 | 2.727 | 2.735 | 2.743 | 86.95 | -2.04 | 0 |
| 11 | Sulfamethoxypyridazine | C11H12N4O3S | 279.0602 | 280.068 | 2.802 | 2.811 | 2.819 |  | -15.98 | 81.47 |
| 12 | 2,3-Dihydroxy-3-methylbutyric acid | C5 H10 O4 | 133.0509 | 134.058 | 2.827 | 2.886 | 2.944 | 91.34 | -0.24 | 0 |
| 13 | Pseudouridine | C9 H12 N2 O6 | 243.0628 | 244.07 | 2.903 | 2.961 | 3.019 | 98.53 | -2.11 | 0 |
| 14 | Calystegine B5 | C7 H13 N O4 | 174.0774 | 175.085 | 3.028 | 3.036 | 3.044 | 99.42 | -0.99 | 0 |
| 15 | Aminocaproic acid | C6 H13 N O2 | 130.0877 | 131.095 | 3.103 | 3.111 | 3.12 | 86.46 | -3.19 | 58.05 |
| 16 | Adenine | C5 H5 N5 | 134.0476 | 135.055 | 3.128 | 3.161 | 3.195 | 86.83 | -3.16 | 92.44 |
| 17 | Succinic acid | C4 H6 O4 | 117.0196 | 118.027 | 3.279 | 3.337 | 3.395 | 87.23 | -2.08 | 98.98 |
| 18 | Itaconic acid | C5 H6 O4 | 129.0196 | 130.027 | 3.504 | 3.512 | 3.52 | 87.07 | -2.26 | 84.64 |
| 19 | L-4-Hydroxy-3-methoxy-a-methylphenylalanine | C11 H15 N O4 | 224.0932 | 225.1 | 3.579 | 3.588 | 3.596 | 98.72 | -1.45 | 0 |
| 20 | D-Arabinono-1,4-lactone | C5 H8 O5 | 147.0302 | 148.038 | 3.629 | 3.637 | 3.645 | 86.66 | -2.21 | 0 |
| 21 | Trimethadione | C6 H9 N O3 | 142.0512 | 143.059 | 3.729 | 3.737 | 3.746 | 86.93 | -1.66 | 0 |
| 22 | (1x,2x)-Guaiacylglycerol 3-glucoside | C16 H24 O10 | 375.1298 | 376.137 | 3.78 | 3.788 | 3.796 | 99.61 | -0.12 | 0 |
| 23 | (±)-threo-1-(4-Hydroxyphenyl)-1,2,3-propanetriol | C9 H12 O4 | 183.0665 | 184.074 | 3.905 | 3.913 | 3.921 | 99.69 | -1.18 | 0 |
| 24 | 3,4,5-Trimethoxyphenyl glucoside | C15 H22 O9 | 345.1192 | 346.127 | 3.804 | 3.913 | 4.021 | 99.59 | -0.28 | 0 |
| 25 | 2,3-Dihydroxy-2,4-cyclopentadien-1-one | C5 H4 O3 | 111.0093 | 112.017 | 3.98 | 3.988 | 3.997 | 86.15 | -4.36 | 0 |
| 26 | (R)-2-Hydroxybutane-1,2,4-tricarboxylate | C7 H10 O7 | 205.0358 | 206.043 | 4.03 | 4.038 | 4.046 | 87.43 | -3.14 | 0 |
| 27 | 3,4-O-Dimethylgallic acid | C9 H10 O5 | 197.046 | 198.053 | 4.13 | 4.138 | 4.147 | 95.41 | -2.94 | 0 |
| 28 | 6'-Methoxypolygoacetophenoside | C15 H20 O10 | 359.0985 | 360.106 | 4.205 | 4.214 | 4.222 | 99.5 | -0.43 | 0 |
| 29 | 1-(2-Furanyl)-1-propanone | C7 H8 O2 | 123.0453 | 124.052 | 4.331 | 4.339 | 4.347 | 77.98 | 0.78 | 0 |
| 30 | Pantothenic Acid | C9 H17 N O5 | 218.104 | 219.111 | 4.381 | 4.389 | 4.398 | 98.24 | -2.46 | 0 |
| 31 | 1-(2-Furanyl)-1,3-butanedione | C8 H8 O3 | 151.0404 | 152.048 | 4.406 | 4.502 | 4.598 | 98.11 | -2.55 | 0 |
| 32 | (S)-beta-Methylindolepyruvate | C12 H11 N O3 | 216.0669 | 217.074 | 4.531 | 4.539 | 4.548 | 99.46 | -1.33 | 0 |
| 33 | (E)-2-Methyl-2-buten-1-ol O-beta-D-Glucopyranoside | C11 H20 O6 | 247.119 | 248.126 | 4.631 | 4.64 | 4.648 | 99.4 | -1.09 | 0 |
| 34 | p-Hydroxyphenylbutazone | C19H20N2O3 | 323.1348 | 324.142 | 4.782 | 4.79 | 4.799 |  | 16.32 | 87.22 |
| 35 | m-Coumaric acid | C9 H8 O3 | 163.0403 | 164.048 | 4.907 | 4.915 | 4.924 | 96.6 | -2.44 | 96.02 |
| 36 | Pyrocatechol | C6 H6 O2 | 109.0299 | 110.037 | 5.132 | 5.141 | 5.149 | 86.79 | -3.66 | 88.51 |
| 37 | 4-Acetoxyphenol | C8 H8 O3 | 151.0403 | 152.048 | 5.083 | 5.153 | 5.224 | 87.08 | -1.78 | 95.58 |
| 38 | 2',4'-Dihydroxy-6'-methoxyacetophenone | C9 H10 O4 | 181.051 | 182.058 | 5.108 | 5.178 | 5.249 | 99.09 | -2.04 | 0 |
| 39 | Glucocaffeic acid | C15 H18 O9 | 341.0883 | 342.096 | 5.183 | 5.254 | 5.324 | 99.13 | -1.18 | 0 |
| 40 | Dihydrocaffeic acid 3-O-glucuronide | C15 H18 O10 | 357.083 | 358.09 | 5.408 | 5.416 | 5.425 | 99.38 | -0.75 | 0 |
| 41 | 3,4-Methylenedioxybenzoic acid | C8 H6 O4 | 165.0196 | 166.027 | 5.508 | 5.517 | 5.525 | 96.72 | -2.52 | 0 |
| 42 | Phenylethyl primeveroside | C19 H28 O10 | 415.1611 | 416.169 | 5.484 | 5.604 | 5.725 | 98.37 | -0.59 | 0 |
| 43 | CAY10487 | C13 H15 N O5 | 264.0881 | 265.095 | 5.633 | 5.642 | 5.65 | 99.36 | -1.16 | 0 |
| 44 | Verbasoside | C20 H30 O12 | 461.1665 | 462.174 | 5.684 | 5.767 | 5.85 | 99.35 | -0.1 | 0 |
| 45 | Benzyl O-[arabinofuranosyl-(1->6)-glucoside] | C18 H26 O10 | 401.1457 | 402.153 | 5.784 | 5.793 | 5.801 | 99.33 | -0.74 | 0 |
| 46 | Asp Trp Glu | C20 H24 N4 O8 | 447.1509 | 448.158 | 5.809 | 5.817 | 5.826 | 93.43 | 2.5 | 0 |
| 47 | Trp Asp Ile | C21 H28 N4 O6 | 431.1924 | 432.2 | 5.884 | 5.893 | 5.901 | 78.76 | 2.68 | 0 |
| 48 | 2,5-Dihydroxybenzaldehyde | C7 H6 O3 | 137.025 | 138.032 | 5.985 | 6.093 | 6.202 | 85.34 | -4.31 | 92.51 |
| 49 | Saponarin | C27 H30 O15 | 593.151 | 594.158 | 6.235 | 6.281 | 6.327 | 98.55 | 0.28 | 0 |
| 50 | Hydrojuglone glucoside | C16 H18 O8 | 337.0931 | 338.1 | 6.335 | 6.343 | 6.352 | 99.68 | -0.48 | 0 |
| 51 | 3,4-Dihydroxybenzaldehyde | C7 H6 O3 | 137.0247 | 138.032 | 6.285 | 6.356 | 6.427 | 87.16 | -1.95 | 92.98 |
| 52 | Niazirin | C14 H17 N O5 | 278.1039 | 279.111 | 6.386 | 6.394 | 6.402 | 98.8 | -1.69 | 0 |
| 53 | Propyl 2-furanacrylate | C10 H12 O3 | 179.0719 | 180.079 | 6.535 | 6.544 | 6.552 | 98.39 | -2.4 | 0 |
| 54 | Scutellarein 7,4'-dirhamnoside | C27 H30 O14 | 577.1562 | 578.164 | 6.486 | 6.569 | 6.652 | 99.21 | 0.09 | 0 |
| 55 | 1-O-2'-Hydroxy-4'-methoxycinnamoyl-b-D-glucose | C16 H20 O9 | 355.1038 | 356.111 | 6.586 | 6.594 | 6.603 | 81.61 | 0.54 | 0 |
| 56 | Diphenylcarbazide | C13 H14 N4 O | 241.1084 | 242.116 | 6.686 | 6.757 | 6.828 | 93 | 4.14 | 0 |
| 57 | Mahaleboside | C15 H16 O8 | 323.0776 | 324.085 | 6.736 | 6.769 | 6.803 | 84.84 | -0.95 | 0 |
| 58 | 1-(2,4,5-Trimethoxyphenyl)-1,2-propanedione | C12 H14 O5 | 237.0771 | 238.084 | 6.836 | 6.844 | 6.853 | 99.36 | -1.02 | 0 |
| 59 | Gibberellin A87 | C19 H22 O7 | 361.1298 | 362.137 | 6.912 | 6.92 | 6.928 | 98.7 | -1.25 | 0 |
| 60 | (7E)-2-acetyl-2,3,4,5-tetrahydrooxonine-6,9-dione | C10 H12 O4 | 195.0669 | 196.074 | 6.887 | 7.008 | 7.128 | 96.98 | -3.07 | 0 |
| 61 | cis-p-Coumaric acid | C9 H8 O3 | 163.0404 | 164.048 | 6.936 | 7.02 | 7.104 | 86.75 | -2.17 | 0 |
| 62 | 8-Hydroxypinoresinol | C20 H22 O7 | 373.1295 | 374.137 | 7.037 | 7.045 | 7.053 | 83.68 | -0.57 | 0 |
| 63 | 3-(3-Furanyl)-2-methyl-2-propenal | C8 H8 O2 | 135.0454 | 136.053 | 7.237 | 7.245 | 7.254 | 87.5 | -1.55 | 0 |
| 64 | 4-Hydroxybenzaldehyde | C7 H6 O2 | 121.0298 | 122.037 | 7.212 | 7.283 | 7.354 | 86.66 | -3.03 | 90.43 |
| 65 | Leu Thr Trp | C21 H30 N4 O5 | 417.2131 | 418.22 | 7.437 | 7.446 | 7.454 | 94.31 | 2.95 | 0 |
| 66 | p-Hydroxymandelic acid | C8 H8 O4 | 167.0356 | 168.043 | 7.538 | 7.546 | 7.554 | 97.88 | -3.57 | 84.98 |
| 67 | 3-Hydroxychavicol 1-glucoside | C15 H20 O7 | 311.1135 | 312.12 | 7.638 | 7.696 | 7.755 | 80.5 | 2.35 | 0 |
| 68 | 7-Ethoxy-4-methyl-2H-1-benzopyran-2-one | C12 H12 O3 | 203.0717 | 204.079 | 7.713 | 7.722 | 7.73 | 97.94 | -1.55 | 0 |
| 69 | 2-(2-Furanyl)-3-methyl-2-butenal | C9 H10 O2 | 149.0613 | 150.069 | 7.613 | 7.734 | 7.855 | 86.21 | -3.17 | 0 |
| 70 | Gibberellin A92 | C19 H22 O6 | 345.1348 | 346.142 | 7.889 | 7.897 | 7.905 | 99.19 | -1.09 | 0 |
| 71 | Ethyl 2-furanacrylate | C9 H10 O3 | 165.0561 | 166.063 | 7.914 | 7.922 | 7.93 | 99.04 | -2.38 | 0 |
| 72 | 1,5,8-Trihydroxy-3-methyl-2-prenylxanthone | C19 H18 O6 | 341.1035 | 342.111 | 8.139 | 8.147 | 8.156 | 84.04 | -1.28 | 0 |
| 73 | Edulisin III | C21 H24 O7 | 387.1453 | 388.153 | 8.29 | 8.298 | 8.306 | 82.83 | -0.81 | 0 |
| 74 | 1-phenyl-1H-pyrazolo[3,4-d]pyrimidine-4-thiol | C11 H8 N4 S | 227.0386 | 228.046 | 8.339 | 8.348 | 8.356 | 93.08 | 4.05 | 0 |
| 75 | p-Hydroxycinnamaldehyde | C9H8O2 | 147.0459 | 148.053 | 8.39 | 8.498 | 8.607 |  | -4.76 | 84.66 |
| 76 | Isoplumbagin | C11 H8 O3 | 187.0404 | 188.048 | 8.715 | 8.724 | 8.732 | 98.23 | -2.27 | 0 |
| 77 | Scytalone | C10 H10 O4 | 193.0513 | 194.059 | 8.84 | 8.849 | 8.857 | 97.49 | -3.4 | 93.26 |
| 78 | (R)-(-)-Mellein | C10 H10 O3 | 177.0563 | 178.064 | 8.791 | 8.912 | 9.033 | 84.87 | -3.2 | 0 |
| 79 | 2,3-dihydro-1,4-benzodioxin-2-ylmethyl dimethylcarbamate | C12 H15 N O4 | 236.093 | 237.1 | 9.317 | 9.325 | 9.333 | 97.11 | -0.23 | 0 |
| 80 | 6,11-Dihydroxy-2,2-dimethylpyrano[3,2-c]xanthen-7(2H)-one | C18 H14 O5 | 309.077 | 310.084 | 9.442 | 9.45 | 9.458 | 85.1 | -0.51 | 0 |
| 81 | Diosbulbin B | C19 H20 O6 | 343.1191 | 344.127 | 9.392 | 9.463 | 9.534 | 90.31 | -1.73 | 0 |
| 82 | 6'-O-Formylmarmin | C20 H24 O6 | 359.1501 | 360.157 | 9.492 | 9.563 | 9.634 | 99.28 | -0.4 | 0 |
| 83 | Cardamonin | C16 H14 O4 | 269.0822 | 270.09 | 9.593 | 9.601 | 9.609 | 99.16 | -1.1 | 84 |
| 84 | 5,6,7,8-tetrahydro-2-Quinolone | C9 H11 N O | 148.077 | 149.084 | 9.642 | 9.651 | 9.659 | 87.2 | -1.21 | 85.14 |
| 85 | Ferulic acid | C10 H10 O4 | 193.051 | 194.058 | 9.693 | 9.776 | 9.859 | 98.49 | -2.24 | 0 |
| 86 | 2-Fluoro-3-guanidinopropionic acid | C4 H8 F N3 O2 | 148.0533 | 149.061 | 9.943 | 10.04 | 10.14 | 45.76 | -3.8 | 0 |
| 87 | Hispolone | C12 H12 O4 | 219.0666 | 220.074 | 10.14 | 10.15 | 10.16 | 99.49 | -1.3 | 0 |
| 88 | omega-Hydroxymoracin N | C19 H18 O5 | 325.1083 | 326.116 | 10.22 | 10.33 | 10.44 | 92.77 | -1.21 | 0 |
| 89 | 7C-Aglycone | C18 H18 O4 | 297.1134 | 298.121 | 10.6 | 10.7 | 10.81 | 99.13 | -0.81 | 0 |
| 90 | 2,4-Dihydroxy-6,4'-dimethoxychalcone | C17 H16 O5 | 299.0928 | 300.1 | 11.1 | 11.15 | 11.21 | 98.44 | -1.18 | 0 |
| 91 | (7'x,8'x)-4,7'-Epoxy-3,8'-bilign-7-ene-3,5'-dimethoxy-4',9,9'-triol | C20 H22 O6 | 357.1344 | 358.142 | 11.3 | 11.36 | 11.41 | 97.98 | -0.46 | 0 |
| 92 | N-[2-(3,4-Dimethoxyphenyl)ethyl]-3,4-dimethoxycinnamic acid amide | C21 H25 N O5 | 370.1665 | 371.174 | 11.42 | 11.43 | 11.44 | 98.35 | -1.2 | 0 |
| 93 | 7-Hydroxyenterolactone | C18 H18 O5 | 313.1084 | 314.115 | 11.65 | 11.66 | 11.66 | 91.81 | 0.54 | 0 |
| 94 | Junosine | C19 H19 N O4 | 324.1244 | 325.131 | 11.72 | 11.73 | 11.74 | 84.85 | 2.43 | 0 |
| 95 | 6-Methoxyflavanone | C16 H14 O3 | 253.0875 | 254.095 | 11.7 | 11.76 | 11.81 | 98.88 | -1.82 | 0 |
| 96 | Gancaonin V | C19 H20 O4 | 311.129 | 312.136 | 11.82 | 11.89 | 11.96 | 99.09 | -0.52 | 0 |
| 97 | AK-toxin I | C23 H27 N O6 | 412.1767 | 413.184 | 11.9 | 11.91 | 11.91 | 98.25 | -0.55 | 0 |
| 98 | 1-(4-Hydroxy-3-methoxyphenyl)-5-(4-hydroxyphenyl)-1,4-pentadien-3-one | C18 H16 O4 | 295.098 | 296.105 | 11.92 | 11.93 | 11.94 | 97.25 | -1.93 | 0 |
| 99 | N-(2-phenylethyl)-Indomethacin amide | C27 H25 Cl N2 O3 | 459.1479 | 460.155 | 12.5 | 12.51 | 12.52 | 63.65 | 0.44 | 0 |
| 100 | 1,2,3,4-Tetrahydro-1-[1-hydroxy-3-(4-hydroxyphenyl)-2-propenyl]-7-methoxy-2,6-naphthalenediol | C20 H22 O5 | 341.1398 | 342.147 | 12.6 | 12.61 | 12.62 | 99 | -0.7 | 0 |
| 101 | Myristicanol B | C22 H28 O7 | 403.1764 | 404.184 | 12.65 | 12.66 | 12.67 | 99.72 | -0.36 | 0 |
| 102 | Sonchifolin | C21 H26 O6 | 373.166 | 374.173 | 12.62 | 12.7 | 12.77 | 99.06 | -0.85 | 0 |
| 103 | PD 98059 | C16 H13 N O3 | 266.0828 | 267.09 | 12.72 | 12.73 | 12.74 | 98.01 | -1.67 | 0 |
| 104 | Gingerglycolipid A | C33 H56 O14 | 675.3594 | 676.367 | 12.82 | 12.83 | 12.84 | 98.75 | 0.54 | 0 |
| 105 | 1-(2H-1,3-Benzodioxol-5-yl)-2-[2,6-dimethoxy-4-(prop-2-en-1-yl)phenoxy]propyl benzoate | C28 H28 O7 | 475.1781 | 476.185 | 13.03 | 13.03 | 13.04 | 92.25 | -3.17 | 0 |
| 106 | Acutilobin | C19 H20 O5 | 327.124 | 328.131 | 13.13 | 13.18 | 13.24 | 98.42 | -0.69 | 0 |
| 107 | Demethoxyegonol | C18 H16 O4 | 295.0982 | 296.105 | 13.1 | 13.22 | 13.34 | 97.51 | -1.85 | 0 |
| 108 | Met Tyr Glu | C19 H27 N3 O7 S | 440.1505 | 441.158 | 13.6 | 13.66 | 13.72 | 83.45 | -2.65 | 0 |
| 109 | Dehydroisochalciporone | C16 H19 N O | 240.1399 | 241.147 | 13.73 | 13.85 | 13.97 | 98.16 | -2.15 | 0 |
| 110 | Lauryl hydrogen sulfate | C12 H26 O4 S | 265.1483 | 266.156 | 13.9 | 14.02 | 14.14 | 97.54 | -1.44 | 0 |
| 111 | 8-Prenyllepidissipyrone | C29 H30 O7 | 489.1922 | 490.199 | 14.25 | 14.26 | 14.27 | 95.56 | 0.07 | 0 |
| 112 | Carpelastofuran | C30 H34 O8 | 521.2179 | 522.225 | 14.53 | 14.54 | 14.55 | 98.95 | 0.25 | 0 |
| 113 | N-Undecylbenzenesulfonic acid | C17 H28 O3 S | 311.169 | 312.176 | 14.63 | 14.72 | 14.82 | 96.82 | -1.17 |  |
| 114 | Pandamarilactone 32 | C18 H21 N O3 | 298.1453 | 299.153 | 14.75 | 14.76 | 14.77 | 99.17 | -1.32 | 0 |
| 115 | Euchrenone b4 | C27 H28 O7 | 463.1763 | 464.184 | 14.73 | 14.79 | 14.85 | 98.08 | -0.23 | 0 |
| 116 | 13(S)-HOTrE | C18 H30 O3 | 293.2127 | 294.22 | 14.85 | 14.86 | 14.87 | 99 | -1.42 | 98.13 |
| 117 | Triptophenolide | C20H24O3 | 311.1691 | 312.176 | 14.9 | 15.01 | 15.12 |  | -12.21 | 98.15 |
| 118 | Isopulegone caffeate | C19 H24 O4 | 315.1604 | 316.168 | 15.53 | 15.59 | 15.65 | 97.78 | -0.8 | 0 |
| 119 | 13(S)-HODE | C18 H32 O3 | 295.2283 | 296.236 | 15.66 | 15.66 | 15.67 | 99.2 | -1.37 | 99.79 |
| 120 | PG(16:0/0:0)[U] | C22 H45 O9 P | 483.273 | 484.28 | 15.76 | 15.76 | 15.77 | 99.62 | -0.22 | 0 |
| 121 | Triamcinolone | C21 H27 F O6 | 393.1719 | 394.179 | 15.73 | 15.8 | 15.87 | 93.98 | -0.04 | 0 |
| 122 | 2-Dodecylbenzenesulfonic acid | C18 H30 O3 S | 325.1847 | 326.192 | 15.81 | 15.92 | 16.02 | 96.9 | -1.13 | 0 |
| 123 | Sodium Tetradecyl Sulfate | C14 H30 O4 S | 293.1794 | 294.187 | 15.83 | 15.95 | 16.07 | 97.16 | -0.84 |  |
| 124 | Piperaduncin B | C29 H30 O8 | 505.1867 | 506.194 | 16.16 | 16.27 | 16.37 | 98.46 | 0.26 | 0 |
| 125 | 4-(3-Hydroxy-7-phenyl-6-heptenyl)-1,2-benzenediol | C19 H22 O3 | 297.15 | 298.157 | 16.43 | 16.5 | 16.57 | 99.45 | -1.17 |  |
| 126 | Norethindrone Acetate | C22H28O3 | 339.2003 | 340.208 | 16.51 | 16.62 | 16.73 |  | -10.95 | 94.4 |
| 127 | S-Octyl GSH | C18 H33 N3 O6 S | 418.2025 | 419.21 | 16.63 | 16.64 | 16.65 | 84.34 | -2.37 | 0 |
| 128 | 6-Hydroxydexamethasone | C22 H29 F O6 | 407.1876 | 408.195 | 16.66 | 16.77 | 16.88 | 91.94 | 0.66 | 0 |
| 129 | 4-Androsten-3,17-dione 19-aldehyde | C19 H24 O3 | 299.1655 | 300.173 | 16.83 | 16.94 | 17.05 | 99.15 | -0.84 | 84.64 |
| 130 | 6-Azaequilenin | C17 H17 N O2 | 266.1188 | 267.126 | 17.36 | 17.41 | 17.45 | 99.76 | -0.78 | 0 |
| 131 | Isosteviol | C20 H30 O3 | 317.2123 | 318.22 | 17.96 | 17.97 | 17.98 | 97.5 | -0.81 | 77.52 |
| 132 | Fluvastatin | C24 H26 F N O4 | 410.1763 | 411.184 | 18.11 | 18.22 | 18.33 | 96.93 | 2.41 | 0 |
| 133 | 1α,25-dihydroxy-22-oxavitamin D3 3-hemiglutarate/ 1α,25-dihydroxy-22-oxacholecalciferol 3-hemiglutarate | C31 H48 O7 | 531.3322 | 532.339 | 18.46 | 18.47 | 18.48 | 95.46 | 1.49 | 0 |
| 134 | Perindopril | C19H32N2O5 | 367.2279 | 368.235 | 18.61 | 18.62 | 18.63 |  | -11.13 | 87.77 |
| 135 | α-Linolenic Acid | C18 H30 O2 | 277.2176 | 278.225 | 18.64 | 18.73 | 18.83 | 98.44 | -1.18 | 86.11 |
| 136 | Pinolenic Acid | C18 H30 O2 | 277.2174 | 278.225 | 18.94 | 19.01 | 19.08 | 95.38 | -0.98 | 86.95 |
| 137 | 16-hydroxy hexadecanoic acid | C16 H32 O3 | 271.2282 | 272.235 | 19.01 | 19.1 | 19.18 | 99.39 | -1.08 | 94.96 |
| 138 | Colupulone | C25 H36 O4 | 399.2549 | 400.262 | 19.11 | 19.17 | 19.23 | 97.31 | -1.84 | 0 |
| 139 | 5beta-Chola-3,11-dien-24-oic Acid | C24 H36 O2 | 355.2643 | 356.272 | 19.26 | 19.27 | 19.28 | 98.39 | 0.08 | 0 |
| 140 | 17beta-Hydroxy-7alpha-methylandrost-4-en-3-one propionate | C23 H34 O3 | 357.2438 | 358.251 | 19.31 | 19.39 | 19.46 | 98.85 | -0.5 | 0 |
| 141 | 1,1'-[1,11-Undecanediylbis(oxy)]bisbenzene | C23 H32 O2 | 339.2331 | 340.24 | 19.34 | 19.41 | 19.48 | 99.04 | -0.28 | 0 |
| 142 | 6,8a-Seco-6,8a-deoxy-5-oxoavermectin ''2b'' aglycone | C33 H48 O8 | 571.3276 | 572.335 | 19.36 | 19.45 | 19.53 | 97.39 | 0.25 | 0 |
| 143 | Hypercalin B | C33 H42 O5 | 517.2954 | 518.303 | 19.84 | 19.85 | 19.86 | 98.67 | 0.73 | 0 |
| 144 | Physapruin B | C34 H50 O9 | 601.3373 | 602.345 | 20.17 | 20.17 | 20.18 | 97.18 | 1.27 | 0 |
| 145 | PG(12:0/22:0) | C40 H79 O10 P | 749.5316 | 750.539 | 20.14 | 20.26 | 20.38 | 91.75 | 3.12 | 0 |
| 146 | Ginkgolic Acid | C22 H34 O3 | 345.2435 | 346.251 | 20.34 | 20.35 | 20.36 | 98.7 | 0.28 | 88.77 |
| 147 | 10E,12Z-Octadecadienoic acid | C18 H32 O2 | 279.2332 | 280.241 | 20.42 | 20.53 | 20.63 | 99.57 | -1 | 98.92 |
| 148 | DG(18:3(6Z,9Z,12Z)/22:3(10Z,13Z,16Z)/0:0)[iso2] | C43 H72 O5 | 667.5325 | 668.54 | 21.07 | 21.08 | 21.08 | 91.62 | -2.38 | 0 |
| 149 | cis-7-Hexadecenoic Acid | C16 H30 O2 | 253.2173 | 254.225 | 21.22 | 21.3 | 21.38 | 86.65 | -0.05 | 56.94 |
| 150 | Hebevinoside V | C46 H74 O14 | 849.499 | 850.506 | 21.52 | 21.53 | 21.54 | 45.16 | 1.83 | 0 |
| 151 | Sorbitan palmitate | C22 H42 O6 | 401.2908 | 402.298 | 21.57 | 21.58 | 21.59 | 99.53 | 0.41 | 0 |
| 152 | DG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:2(13Z,16Z)/0:0) | C47 H76 O5 | 719.5633 | 720.57 | 21.67 | 21.68 | 21.69 | 90.52 | -1.46 | 0 |
| 153 | Polyporusterone A | C28 H46 O6 | 477.322 | 478.329 | 21.74 | 21.84 | 21.94 | 98.6 | 0.48 | 0 |
| 154 | Persicachrome | C25 H36 O3 | 383.259 | 384.266 | 22.75 | 22.75 | 22.76 | 83.11 | 0.49 | 0 |
| 155 | Cyclopassifloic acid C | C31 H52 O7 | 535.3636 | 536.371 | 22.72 | 22.79 | 22.86 | 99.21 | 0.84 | 0 |
| 156 | Isopalmitic acid | C16 H32 O2 | 255.2333 | 256.241 | 22.92 | 23.03 | 23.14 | 98.27 | -1.45 | 100 |
| 157 | 13-methoxy-heneicosanoic acid | C22 H44 O3 | 355.3219 | 356.329 | 23.22 | 23.33 | 23.44 | 99.8 | -0.35 | 0 |
| 158 | Elaidic Acid | C18 H34 O2 | 281.2491 | 282.257 | 23.62 | 23.73 | 23.84 | 97.09 | -2.12 | 100 |
| 159 | 9-deoxy-9-methylene-PGE2 | C21H34O4 | 349.2363 | 350.244 | 23.77 | 23.78 | 23.79 |  | 6.22 | 87.78 |
| 160 | Oligomycin A | C45 H74 O11 | 789.5153 | 790.522 | 23.95 | 24.06 | 24.17 | 98.84 | 0.86 | 0 |
| 161 | Avermectin A2a | C49 H76 O15 | 903.5074 | 904.515 | 24.27 | 24.28 | 24.29 | 87.67 | 4.06 | 0 |
| 162 | Roxithromycin | C41 H76 N2 O15 | 835.5204 | 836.528 | 24.33 | 24.4 | 24.47 | 91.05 | -3.61 | 0 |
| 163 | SQDG(22:5(5Z,8Z,11Z,14Z,17Z)/16:1(13Z)) | C45 H76 O12 S | 839.4979 | 840.505 | 24.73 | 24.83 | 24.94 | 98.33 | 0.8 | 0 |
| 164 | PI(P-16:0/17:2(9Z,12Z)) | C42 H77 O12 P | 803.5095 | 804.517 | 25.63 | 25.74 | 25.84 | 95.35 | -1.64 | 0 |