| Compound name                                                                 | m/z Found [M+H]^+ | Mass error (ppm) |
|------------------------------------------------------------------------------|-------------------|------------------|
| 9.10-Octalin                                                                 | 137.1324          | 4.52             |
| Ectoin                                                                       | 143.0815          | 3.85             |
| 6-Methylsalicylic acid                                                       | 153.0547          | 2.63             |
| Allantoin                                                                    | 159.0502          | 10.36            |
| Hydroxyectoine                                                               | 159.0764          | 3.53             |
| Germicidin B                                                                 | 183.1015          | 3.41             |
| Germicidin                                                                   | 197.1171          | 3.04             |
| Kynurenone                                                                   | 209.0919          | 3.65             |
| (R)-3.5-Diethyl-4-hydroxy-5-[(E)-2-methylbuta-1.3-dienyl]thiophen-2(5H)-one | 239.1112          | 2.32             |
| CHEMBL3087384                                                                | 253.1407          | 13.08            |
| CHEMBL1242196                                                                | 285.0755          | 2.90             |
| (S)-DNPA                                                                     | 287.0911          | 2.96             |
| Kalafungin A                                                                 | 301.0703          | 3.16             |
| Dihydrokalafungin                                                            | 303.0859          | 2.92             |
| T3HN                                                                         | 305.1017          | 2.68             |
| Kinobscurinone                                                                | 307.0575          | 10.32            |
| Fluostatin K                                                                  | 309.0731          | 10.53            |
| DHK-OH                                                                       | 321.0942          | 10.20            |
| 3 Methyltetraphene 1.6.7.8.12 pentol                                         | 323.0958          | 11.96            |
| Fluostatin C                                                                 | 325.0679          | 10.14            |
| Cyclic AMP                                                                   | 330.0580          | 6.92             |
| Disaccharide (e.g., Trehalose)                                               | 343.1260          | 5.82             |
| Wallupemycin G                                                                | 347.0945          | 7.30             |
| Coelimycin P1                                                                 | 349.1211          | 3.25             |
| Roseoflavin                                                                  | 406.1773          | 11.49            |
| Fluostatin J                                                                  | 409.1325          | 9.19             |
| Fluostatin L                                                                  | 437.1637          | 8.41             |
| 3'-N-Demethyl-4'-hydroxystaurosporine                                       | 439.1793          | 5.27             |
| Granaticin                                                                   | 445.1091          | 9.75             |
| Oxytetracycline                                                              | 461.1612          | 11.24            |
| Brasiliquinone A                                                             | 466.1902          | 7.62             |
| Staurosporine M1                                                             | 481.1899          | 4.70             |
| 3'-N-Acetylholyrine A                                                        | 483.2055          | 4.61             |
| Mycothiol                                                                    | 487.1557          | 8.36             |
| 9-Hydroxyl-3'-N-acetyl-4'-Hydroxystaurosporine                              | 497.1848          | 4.58             |
| CHEMBL372196                                                                 | 561.1362          | 6.23             |
| Deferoxamine                                                                 | 561.3600          | 2.26             |
| 2-[[2-Amino-5-[(formyl(hydroxy)amino)pentanoyl]amino]-5-[[2-amino-5-[(formyl(hydroxy)amino)pentanoyl]amino]-3-hydroxybutanoyl]-hydroxyamino]pentanoic acid | 566.2774          | 2.21             |
| Difluostatin A                                                               | 599.1368          | 4.37             |
| Nocardamin                                                                   | 601.3549          | 2.06             |
| Tautomycetin                                                                 | 607.3418          | 10.51            |
| gamma-Actinorhodin                                                           | 631.1180          | 14.59            |
| epsilon-Actinorhodin                                                         | 640.1286          | 14.31            |