



**B**

| fraction  | lipid name  | alkyl carbons | retention (minutes) | calculated $m/z$ | detected $m/z$ | volume (counts) |
|---|---|---------------|---------------------|------------------|----------------|-----------------|
| released  | carboxy-mycobactin,                                   | 6             | 10.95               | 759.2409         | 759.2416       | 2206923         |
|   | [M-2H+Fe] <sup>+</sup>                                | 7             | 11.37               | 773.2565         | 773.2568       | 4747524         |
|   |   | 8             | 11.93               | 787.2722         | 787.2706       | 3009866         |
|   |   | 9             | 12.81               | 801.2878         | 801.2871       | 513459          |
|   |   | 10            | 12.54               | 815.3035         | 815.3022       | 117289          |
|   |   | 11            | 13.06               | 829.3191         | 829.3180       | 90692           |
| acetone soluble   | mycobactin, [M-2H+Fe] <sup>+</sup>                    | 17            | 4.64                | 883.4388         | 883.4420       | 599635          |
|   |   | 18            | 4.68                | 897.4545         | 897.4556       | 1825330         |
|   |   | 19            | 5.38                | 911.4701         | 911.4635       | 13841471        |
|   |   | 20            | 5.44                | 925.4858         | 925.4825       | 28930836        |
|   | DDM, [M+H] <sup>+</sup>                               | 20            | 5.66                | 838.5688         | 838.5701       | 5812291         |
| acetone insoluble   | PDIM, [M+NH <sub>4</sub> ] <sup>+</sup>               | 47            | 3.16                | 1371.417         | 1371.409       | 13793           |
|   |   | 48            | 2.91                | 1385.433         | 1385.429       | 142067          |
|   |   | 50            | 2.89                | 1413.464         | 1413.461       | 293344          |
|   |   | 52            | 3.11                | 1441.495         | 1441.489       | 8606            |
|   |   | 53            | 2.87                | 1455.511         | 1455.508       | 221101          |
|   |   | 54            | 2.86                | 1469.526         | 1469.524       | 375121          |
|   |   | 55            | 2.86                | 1483.542         | 1483.536       | 94047           |
|   | alpha mycolic acid, [M+NH <sub>4</sub> ] <sup>+</sup> | 78            | 2.99                | 1155.207         | 1155.206       | 188841          |
|   |   | 80            | 2.98                | 1183.239         | 1183.238       | 211908          |
|   |   | 82            | 2.96                | 1211.270         | 1211.269       | 122709          |
|   |   | 84            | 2.94                | 1239.301         | 1239.292       | 133484          |
|   | 86  | 2.93          | 1267.333            | 1267.310         | 157711         |                 |
| diacyl sulfoglycolipid, [M+NH <sub>4</sub> ] <sup>+</sup> | 56  | 14.20         | 1268.937            | 1268.940         | 253252         |                 |
|   | 58  | 14.95         | 1296.968            | 1296.973         | 906964         |                 |
|   | 59  | 15.42         | 1310.984            | 1310.989         | 91129          |                 |

