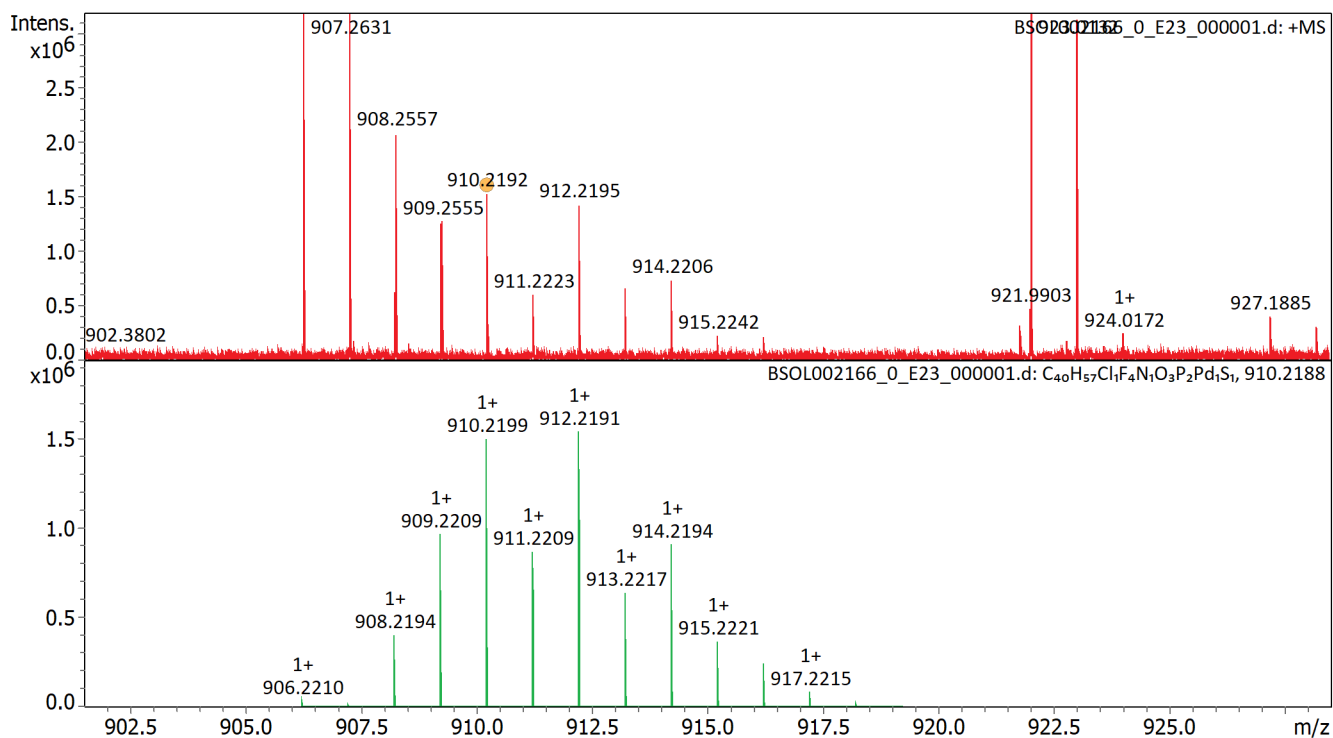
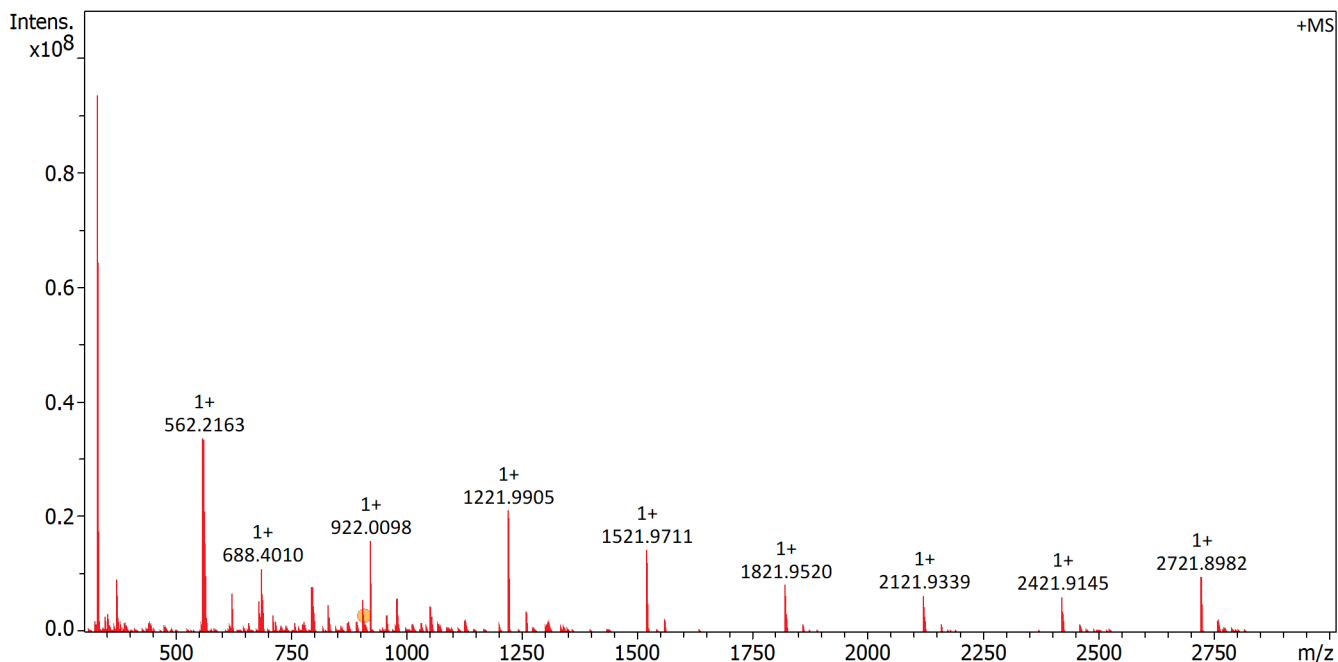


Acquisition Parameter

| | | | |
|---------------------|---|----------------------------|-----------------------|
| Method: | MALDI_MS_POS_300-3000_2M_16AvScans | Acquisition Date: | 12/5/2023 11:19:56 AM |
| File Name: | D:\Data\ETH Data\BSOL0021xx\BSOL002166_0_E23_000001.d | Operator: | Daniel Wirz |
| Source | Dual (MALDI/ESI) | Polarity | Positive |
| Broadband Low Mass | 303.1 m/z | Nebulizer Gas | 1.0 bar |
| Broadband High Mass | 3000.0 m/z | Drying Gas Flow Rate | 4.0 L/min |
| No. of Cell Fills | 1 | Capillary | 4500.0 V |
| Apodization | Full-Sine | Drying Gas | 200.0 °C |
| | | Time of Flight to Detector | 0.002 sec |
| | | Temperature | |



Evaluation Spectra / Validation Formula:

| # | Ion Formula | Adduct | m/z | z | Meas. m/z | mSigma | N-Rule | err [mDa] | err [ppm] |
|---|--------------------|--------|----------|----|-----------|--------|--------|-----------|-----------|
| 1 | C40H57ClF4NO3P2PdS | M+H | 910.2188 | 1+ | 910.2192 | 98.8 | ok | -0.7 | -0.8 |

Calibration Info:

Internal calibration

Date: 12/5/2023 11:22:28 AM
Polarity: Positive
Calibration spectrum: +MS: Scan
Reference mass list: MALDI: DCTB Matrix + HP-Mix (pos)
Calibration mode: Quadratic
Standard deviation: 0.187 ppm

| Reference m/z | Resulting m/z | Intensity | Error [ppm] |
|---------------|---------------|-----------|-------------|
| 118.0863 | | | |
| 250.1464 | | | |
| 251.1543 | | | |
| 273.1362 | | | |
| 322.0481 | 322.0481 | 169836 | 0.010 |
| 332.2009 | 332.2009 | 94388528 | -0.018 |
| 500.2934 | 500.2935 | 307541 | 0.011 |
| 501.3013 | | | |
| 523.2832 | | | |
| 622.0290 | 622.0290 | 6926950 | 0.054 |
| 750.4404 | | | |
| 751.4483 | | | |
| 773.4302 | | | |
| 922.0098 | 922.0098 | 15979532 | -0.006 |
| 1000.5874 | | | |
| 1001.5953 | | | |
| 1023.5772 | | | |
| 1221.9906 | 1221.9905 | 21237474 | -0.109 |
| 1521.9715 | 1521.9711 | 14482298 | -0.217 |
| 1821.9523 | 1821.9520 | 8352601 | -0.149 |
| 2121.9332 | 2121.9339 | 6483236 | 0.329 |
| 2421.9140 | 2421.9145 | 6250278 | 0.194 |
| 2721.8948 | | | |

Mass List:

| # | m/z | Res. | S/N | I % | FWHM |
|----|-----------|--------|--------|-------|--------|
| 1 | 332.2009 | 583965 | 7936.0 | 100.0 | 0.0006 |
| 2 | 333.2042 | 581140 | 2004.7 | 25.3 | 0.0006 |
| 3 | 374.2115 | 518328 | 776.0 | 9.8 | 0.0007 |
| 4 | 558.2165 | 345124 | 983.9 | 14.5 | 0.0016 |
| 5 | 559.2175 | 343127 | 2050.2 | 30.2 | 0.0016 |
| 6 | 560.2159 | 343137 | 2409.3 | 35.7 | 0.0016 |
| 7 | 560.2208 | 316502 | 526.7 | 7.8 | 0.0018 |
| 8 | 561.2193 | 342998 | 701.1 | 10.4 | 0.0016 |
| 9 | 562.1965 | 343785 | 333.0 | 5.0 | 0.0016 |
| 10 | 562.2163 | 343132 | 2417.8 | 35.9 | 0.0016 |
| 11 | 563.1949 | 339766 | 403.5 | 6.0 | 0.0017 |
| 12 | 563.2197 | 341939 | 660.8 | 9.8 | 0.0016 |
| 13 | 564.2176 | 341664 | 1109.6 | 16.5 | 0.0017 |
| 14 | 565.1954 | 338398 | 388.7 | 5.8 | 0.0017 |
| 15 | 565.2209 | 342786 | 284.9 | 4.3 | 0.0016 |
| 16 | 622.0290 | 310242 | 469.8 | 7.3 | 0.0020 |
| 17 | 680.4803 | 281690 | 362.5 | 5.9 | 0.0024 |
| 18 | 688.4010 | 277982 | 725.3 | 11.9 | 0.0025 |
| 19 | 689.4044 | 275873 | 371.2 | 6.1 | 0.0025 |
| 20 | 795.2661 | 257102 | 384.3 | 6.7 | 0.0031 |
| 21 | 796.2646 | 235777 | 482.1 | 8.4 | 0.0034 |
| 22 | 798.2650 | 237605 | 485.5 | 8.5 | 0.0034 |
| 23 | 799.2684 | 238352 | 211.6 | 3.7 | 0.0034 |
| 24 | 832.2405 | 227389 | 288.3 | 5.1 | 0.0037 |
| 25 | 906.2593 | 207510 | 324.7 | 6.1 | 0.0044 |
| 26 | 907.2588 | 210187 | 203.8 | 3.8 | 0.0043 |
| 27 | 922.0098 | 205287 | 909.4 | 16.9 | 0.0045 |
| 28 | 980.2781 | 190336 | 328.7 | 6.3 | 0.0052 |
| 29 | 981.2773 | 214348 | 198.8 | 3.8 | 0.0046 |
| 30 | 1054.2968 | 177528 | 248.1 | 4.9 | 0.0059 |
| 31 | 1221.9905 | 151068 | 1089.1 | 22.5 | 0.0081 |
| 32 | 1222.9939 | 153047 | 271.9 | 5.6 | 0.0080 |
| 33 | 1259.9464 | 146229 | 183.5 | 3.9 | 0.0086 |
| 34 | 1521.9711 | 118907 | 705.0 | 15.3 | 0.0128 |
| 35 | 1522.9747 | 118233 | 208.9 | 4.6 | 0.0129 |
| 36 | 1821.9520 | 97407 | 382.0 | 8.8 | 0.0187 |
| 37 | 2121.9339 | 83791 | 280.3 | 6.9 | 0.0253 |
| 38 | 2421.9145 | 73467 | 248.8 | 6.6 | 0.0330 |
| 39 | 2721.8982 | 65276 | 392.5 | 10.3 | 0.0417 |
| 40 | 2722.9012 | 65798 | 223.6 | 5.9 | 0.0414 |

| # | m/z | Res. | S/N | I % | FWHM |
|----|----------|--------|-----|-------|--------|
| 1 | 906.2210 | 199106 | | 2.3 | 0.0046 |
| 2 | 907.2242 | 199326 | | 1.0 | 0.0046 |
| 3 | 908.2194 | 199545 | | 26.4 | 0.0046 |
| 4 | 909.2209 | 199765 | | 62.6 | 0.0046 |
| 5 | 910.2199 | 199985 | | 97.1 | 0.0046 |
| 6 | 911.2209 | 200205 | | 56.6 | 0.0046 |
| 7 | 912.2191 | 200424 | | 100.0 | 0.0046 |
| 8 | 913.2217 | 200644 | | 41.6 | 0.0046 |
| 9 | 914.2194 | 200863 | | 59.1 | 0.0046 |
| 10 | 915.2221 | 201084 | | 23.9 | 0.0046 |
| 11 | 916.2197 | 201303 | | 16.0 | 0.0046 |
| 12 | 917.2215 | 201523 | | 5.6 | 0.0046 |
| 13 | 918.2215 | 201743 | | 1.6 | 0.0046 |
| 14 | 919.2221 | 201963 | | 0.4 | 0.0046 |