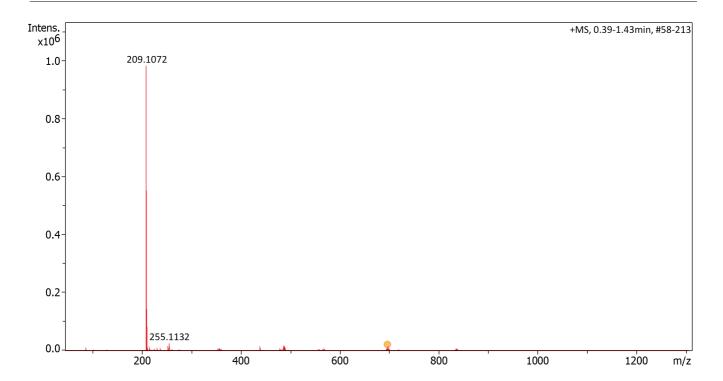
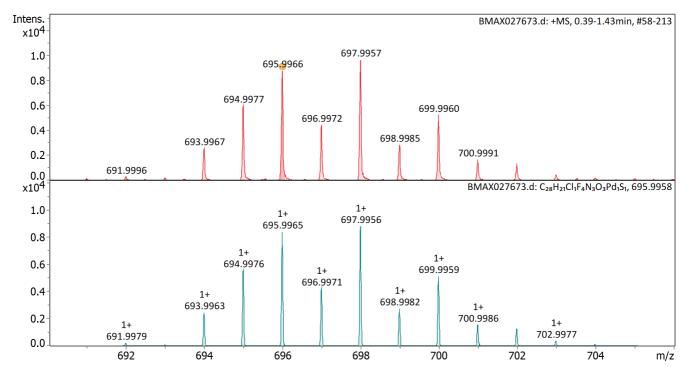
Acquisition Parameter

Method:ETH_HyStar_HPLC_QTOF_POS_LowMass_Loop-AS.mAcquisition Date:25.03.2024 09:04:29File Name:D:\Data\bmax0276xx\BMAX027673.dOperator:Michael Meier

Source Type ESI Ion Polarity Positive Set Nebulizer 1.6 Bar 4500 V Set Dry Heater 230 °C 10.0 l/min Active Set Capillary Focus -500 V Scan Begin 50 m/z Set End Plate Offset Set Dry Gas Scan End 1300 m/z Set Collision Cell RF 200.0 Vpp Set Divert Valve Source







Evaluation Spectra / Validation Formula:

| # | Ion Formula | Adduct | m/z | Z | Meas. m/z | mSigma | N-Rule | err [mDa] | err [ppm] |
|---|-------------------|--------|----------|----|-----------|--------|--------|-----------|-----------|
| 1 | C28H21CIF4N3O3PdS | M+H | 695.9958 | 1+ | 695.9966 | 22.2 | ok | -0.1 | -0.2 |

| Calibration Info: | | | | Mass List: | | | | | |
|----------------------|---------------|---------------|-----------------|---------------|----------|-------|---------|-------|--------|
| Internal calibration | | | # | m/z | Res. | S/N | Ι% | FWHM | |
| Date: | 25.03.20 | 24 10:30:3 | 2 | # 1 | 87.0806 | 14369 | 360.6 | 0.7 | 0.0061 |
| Polarity: | Positive | | | 2 | 209.1072 | 36869 | 44349.0 | 100.0 | 0.0057 |
| Calibration spec | · | | #58-213: Scan | 3 | 210.1106 | 28083 | 6560.6 | 14.8 | 0.0037 |
| Reference mass | | | ESI-TOF Spezial | 4 | 211.1139 | 17221 | 410.3 | 0.9 | 0.0123 |
| Calibration mode | | ed Quadration | С | 5 | 215.0640 | 18452 | 438.8 | 1.0 | 0.0117 |
| Standard deviati | on: 0.894 pp | om | | 6 | 225.1024 | 17488 | 279.9 | 0.6 | 0.0129 |
| | | | | 7 | 231.0894 | 16766 | 380.3 | 0.9 | 0.0138 |
| Reference m/z | Resulting m/z | Intensity | Error [ppm] | 8 | 237.1027 | 17636 | 358.7 | 0.8 | 0.0134 |
| 118.0863 | 118.0863 | 716 | 0.025 | 9 | 237.1387 | 17128 | 299.6 | 0.7 | 0.0138 |
| 322.0481 | 322.0480 | 252 | -0.314 | 10 | 253.0976 | 19475 | 684.1 | 1.6 | 0.0130 |
| 622.0290 | 622.0291 | 560 | 0.276 | 11 | 255.1132 | 21013 | 1094.8 | 2.5 | 0.0121 |
| 922.0098 | 922.0094 | 315 | -0.433 | 12 | 277.0949 | 17475 | 180.1 | 0.4 | 0.0159 |
| 1221.9906 | 1221.9914 | 75 | 0.586 | 13 | 354.0441 | 17412 | 169.8 | 0.4 | 0.0203 |
| 1521.9715 | | | | 14 | 355.0428 | 16666 | 215.5 | 0.5 | 0.0213 |
| 1821.9523 | | | | 15 | 357.0424 | 16517 | 187.5 | 0.5 | 0.0216 |
| 2121.9332 | | | | 16 | 359.0018 | 17075 | 190.2 | 0.5 | 0.0210 |
| 2421.9140 | | | | 17 | 361.0013 | 17046 | 173.7 | 0.4 | 0.0212 |
| 2721.8948 | | | | 18 | 439.1895 | 18715 | 392.0 | 1.0 | 0.0235 |
| | | | | 19 | 479.1295 | 17060 | 217.4 | 0.6 | 0.0281 |
| | | | | 20 | 486.0020 | 19167 | 242.6 | 0.6 | 0.0254 |
| | | | | 21 | 486.5021 | 18453 | 268.1 | 0.7 | 0.0264 |
| | | | | 22 | 487.0020 | 19533 | 361.8 | 0.9 | 0.0249 |
| | | | | 23 | 487.5023 | 19759 | 371.5 | 1.0 | 0.0247 |
| | | | | 24 | 488.0019 | 19589 | 419.8 | 1.1 | 0.0249 |
| | | | | 25 | 488.5025 | 18693 | 329.6 | 0.9 | 0.0261 |
| | | | | 26 | 489.0024 | 19216 | 351.9 | 0.9 | 0.0254 |
| | | | | 27 | 489.5026 | 18903 | 221.9 | 0.6 | 0.0259 |
| | | | | 28 | 490.0022 | 19468 | 236.3 | 0.6 | 0.0252 |
| | | | | 29 | 567.1016 | 17648 | 221.1 | 0.6 | 0.0321 |
| | | | | 30 | 569.1013 | 17606 | 181.4 | 0.5 | 0.0323 |
| | | | | 31 | 694.9977 | 18606 | 266.1 | 0.6 | 0.0374 |
| | | | | 32 | 695.9966 | 18381 | 392.1 | 0.9 | 0.0379 |
| | | | | 33 | 696.9972 | 17997 | 197.6 | 0.5 | 0.0387 |
| | | | | 34 | 697.9957 | 18614 | 432.9 | 1.0 | 0.0375 |
| | | | | 35 | 699.9960 | 16970 | 236.4 | 0.5 | 0.0412 |
| | | | | 36 | 834.9967 | 17275 | 253.0 | 0.4 | 0.0483 |
| | | | | 37 | 835.4971 | 17658 | 286.6 | 0.5 | 0.0473 |
| | | | | 38 | 835.9973 | 17105 | 273.0 | 0.5 | 0.0489 |
| | | | | 39 | 836.4972 | 18085 | 294.8 | 0.5 | 0.0463 |
| | | | | 40 | 836.9973 | 18268 | 265.7 | 0.5 | 0.0458 |
| | | | | # | m/z | Res. | S/N | I % | FWHM |
| | | | | 1 | 691.9979 | 18275 | | 2.5 | 0.0379 |
| | | | | 2 | 693.0010 | 18302 | | 8.0 | 0.0379 |
| | | | | 3 | 693.9963 | 18328 | | 28.1 | 0.0379 |
| | | | | 4 | 694.9976 | 18354 | | 63.3 | 0.0379 |
| | | | | 5 | 695.9965 | 18381 | | 95.5 | 0.0379 |
| | | | | 6 | 696.9971 | 18407 | | 47.9 | 0.0379 |
| | | | | 7 | 697.9956 | 18434 | | 100.0 | 0.0379 |
| | | | | 8 | 698.9982 | 18460 | | 31.4 | 0.0379 |
| | | | | | | | | | |



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| # | m/z | Res. | S/N | I % | FWHM |
|----|----------|-------|-----|------|--------|
| 9 | 699.9959 | 18486 | | 58.4 | 0.0379 |
| 10 | 700.9986 | 18513 | | 17.9 | 0.0379 |
| 11 | 701.9955 | 18539 | | 14.4 | 0.0379 |
| 12 | 702.9977 | 18566 | | 4.0 | 0.0379 |
| 13 | 703.9965 | 18592 | | 1.1 | 0.0379 |
| 14 | 704.9971 | 18619 | | 0.2 | 0.0379 |