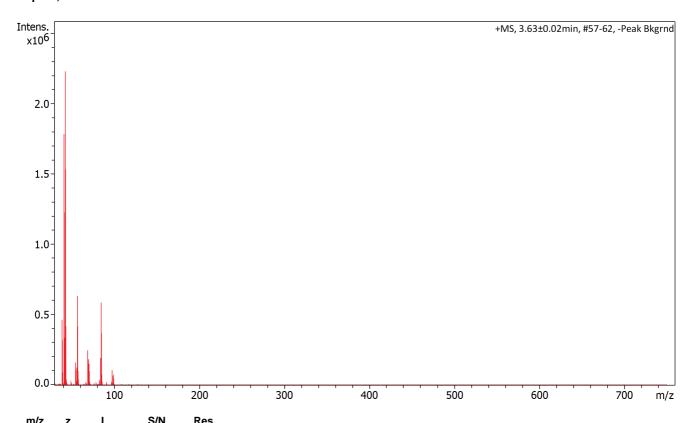


| # | RT [min] | Area     |
|---|----------|----------|
| 1 | 3.63     | 7996676  |
| 2 | 9.41     | 13042133 |
| 3 | 12.46    | 74677608 |

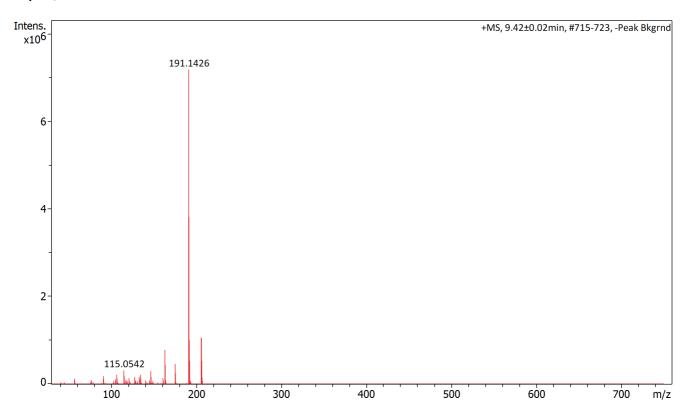
### Cmpd 1, 3.63 min



| m/z     | Z | ı       | S/N      | Res.  |
|---------|---|---------|----------|-------|
| 39.0228 |   | 465341  | 27026.9  | 57223 |
| 41.0383 |   | 1782971 | 103554.4 | 58939 |
| 42.0417 |   | 79118   | 4595.1   | 61852 |
| 42.0464 |   | 138769  | 8059.6   | 62727 |
| 43.0541 |   | 2230347 | 129537.9 | 34325 |
| 43.9892 |   | 61281   | 3559.2   | 65110 |
| 55.0542 |   | 163286  | 9483.6   | 79160 |
| 56.0620 |   | 127198  | 7387.6   | 59603 |
| 57.0697 |   | 634437  | 36847.9  | 77086 |
| 58.0731 |   | 59534   | 3457.7   | 79428 |
| 69.0698 |   | 248478  | 14431.5  | 77418 |
| 70.0733 |   | 20243   | 1175.7   | 97376 |
| 70.0776 |   | 185084  | 10749.6  | 54326 |
| 71.0855 |   | 153242  | 8900.3   | 96676 |
| 83.0854 |   | 36668   | 2129.7   | 62462 |
| 84.0933 |   | 192724  | 11193.4  | 95804 |
| 85.1009 |   | 587470  | 34120.1  | 63290 |
| 86.1043 |   | 40101   | 2329.0   | 64658 |
| 98.1089 |   | 108671  | 6311.6   | 89314 |
| 99.1167 |   | 74497   | 4326.8   | 72840 |

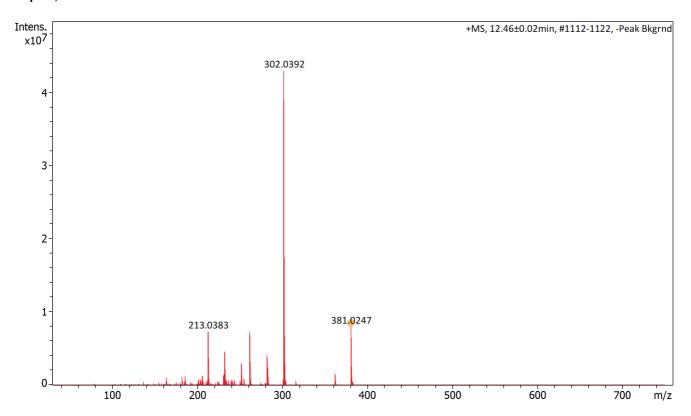


#### Cmpd 2, 9.41 min



| m/z      | Z | I       | S/N      | Res.   |
|----------|---|---------|----------|--------|
| 57.0699  |   | 126266  | 3186.5   | 50751  |
| 77.0385  |   | 93668   | 2363.9   | 106118 |
| 91.0541  |   | 175300  | 4424.0   | 73525  |
| 105.0698 |   | 115635  | 2918.2   | 84189  |
| 107.0491 |   | 216783  | 5470.9   | 77505  |
| 115.0542 |   | 308308  | 7780.7   | 83968  |
| 117.0699 |   | 97224   | 2453.6   | 81218  |
| 121.0648 |   | 137839  | 3478.6   | 78722  |
| 128.0621 |   | 168473  | 4251.7   | 75600  |
| 133.0648 |   | 173729  | 4384.3   | 74463  |
| 135.0805 |   | 215958  | 5450.1   | 75433  |
| 147.0804 |   | 302221  | 7627.0   | 74837  |
| 161.0960 |   | 135487  | 3419.2   | 68032  |
| 163.1117 |   | 786181  | 19840.5  | 71537  |
| 164.1150 |   | 91191   | 2301.4   | 70977  |
| 175.1116 |   | 454543  | 11471.1  | 71339  |
| 191.1426 |   | 7178627 | 181164.0 | 67953  |
| 192.1462 |   | 994954  | 25109.2  | 68571  |
| 206.1663 |   | 1065575 | 26891.5  | 65491  |
| 207.1697 |   | 150336  | 3794.0   | 64331  |

#### Cmpd 3, 12.46 min

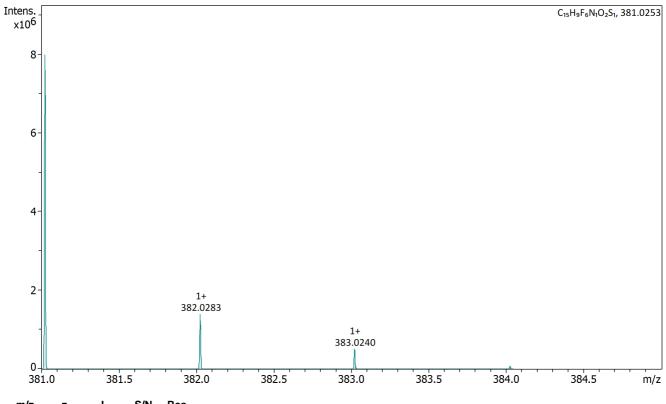


| m/z      | Z | ı        | S/N     | Res.  |
|----------|---|----------|---------|-------|
| 164.0494 |   | 996258   | 536.6   | 70027 |
| 182.0400 |   | 1147627  | 618.1   | 70399 |
| 186.0275 |   | 1287337  | 693.4   | 69232 |
| 206.0337 |   | 1257158  | 677.1   | 64544 |
| 213.0383 |   | 7300954  | 3932.3  | 65531 |
| 214.0419 |   | 794930   | 428.1   | 62416 |
| 231.0289 |   | 1305932  | 703.4   | 62120 |
| 232.0369 |   | 1517900  | 817.5   | 62903 |
| 233.0446 |   | 4562654  | 2457.4  | 62880 |
| 252.0430 |   | 2980524  | 1605.3  | 60143 |
| 255.0227 |   | 831561   | 447.9   | 59275 |
| 262.0273 |   | 7300955  | 3932.3  | 59113 |
| 263.0302 |   | 971596   | 523.3   | 57196 |
| 282.0334 |   | 4022165  | 2166.3  | 56766 |
| 283.0417 |   | 2470904  | 1330.8  | 54999 |
| 302.0392 |   | 42941400 | 23128.1 | 55568 |
| 303.0442 |   | 7354180  | 3960.9  | 48552 |
| 362.0266 |   | 1634914  | 880.6   | 50529 |
| 381.0247 |   | 7988194  | 4302.4  | 50203 |
| 382.0283 |   | 1262050  | 679.7   | 48291 |

# Ion Formula Adduct m/z z Meas. m/z mSigma N-Rule err [mDa] err [ppm] 1 C15H9F6NO2S M 381.0253 1+ 381.0247 16.0 ok 0.6 1.5

Cmpd 3, 12.46 min





| m/z      | z  | I       | S/N | Res.  |
|----------|----|---------|-----|-------|
| 381.0253 | 1+ | 7988194 |     | 50203 |
| 382.0283 | 1+ | 1402581 |     | 50335 |
| 383.0240 | 1+ | 506057  |     | 50466 |
| 384 0258 | 1+ | 71659   |     | 50598 |



Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich

**General Acquisition Paramet** 

File Name: D:\Data\TGC0021xx\TGC0002152\_GC.cdf Acquisition Date: 12/12/2023 20:41:51

Operator: Xcalibur\_System

**GC-Parameter Info:** 

please see infos logged in Thermo

Software

**Calibration Info:** 

please see infos logged in Thermo

Software

Initial calibration from acquisition

Date: <unknown>
Polarity: Positive
Calibration mode: Linear
Coverage: -nan(ind)%