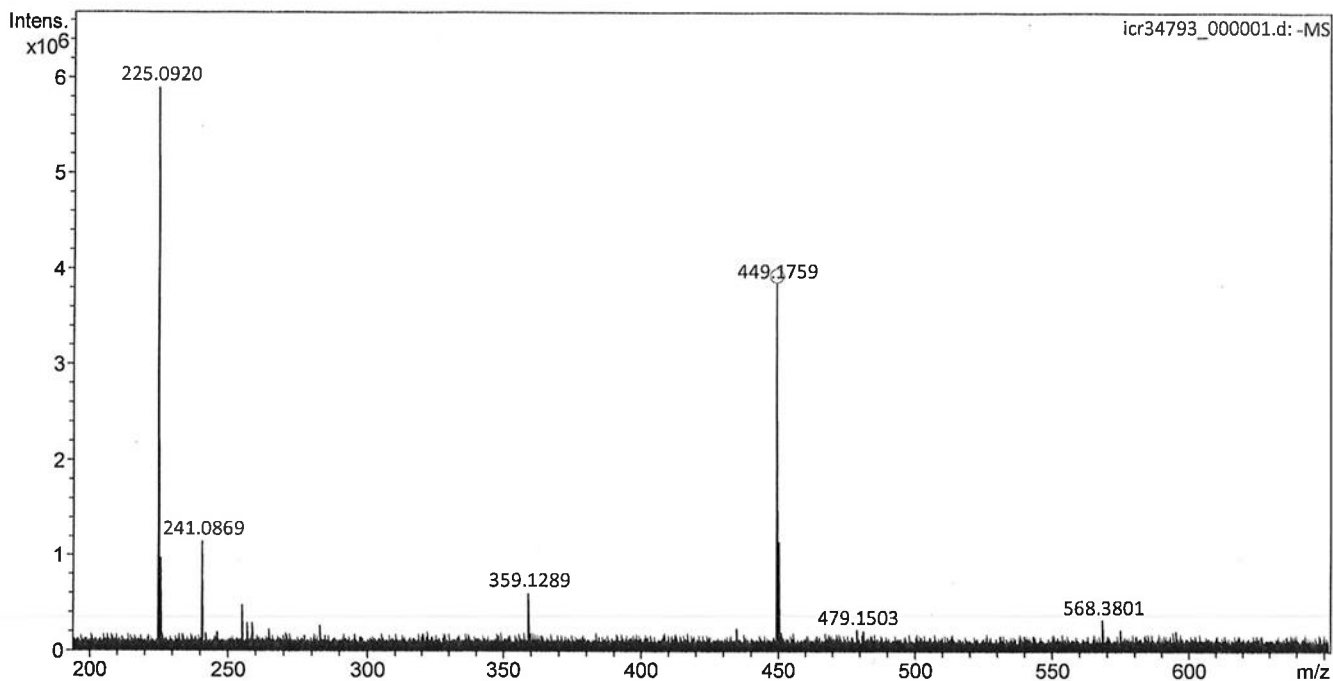


Mass Spectrum Formula Report

Analysis Info

Analysis Name D:\Data\Kopka DKFZ\icr34793_000001.d
Comment Krutzek, Kopka/DKFZ: FK_021.ml in CDCl3/MeOH

Acquisition Date 5/31/2019 7:59:44 AM



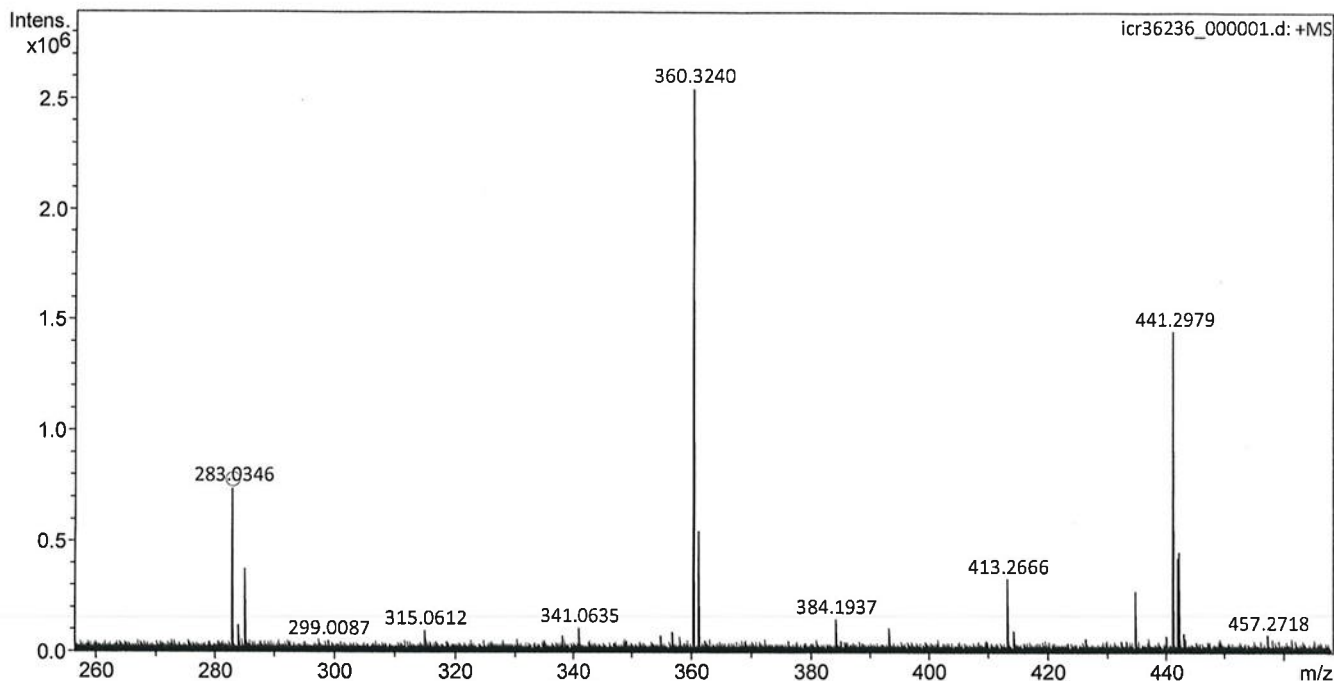
| Meas. m/z | Ion Formula | m/z | err [ppm] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|-------------|----------|-----------|--------|------|---------------------|--------|
| 225.0920 | C15H13O2 | 225.0921 | 0.6 | 7.4 | 9.5 | even | ok |
| 449.1759 | C30H25O4 | 449.1758 | -0.1 | 14.6 | 18.5 | even | ok |

Mass Spectrum Formula Report

Analysis Info

Analysis Name D:\Data\Kopka DKFZ\icr36236_000001.d
Comment Krutzek, DKFZ/Kopka: FK_080.m1 in DCM/MeOH

Acquisition Date 10/15/2019 11:59:04 AM



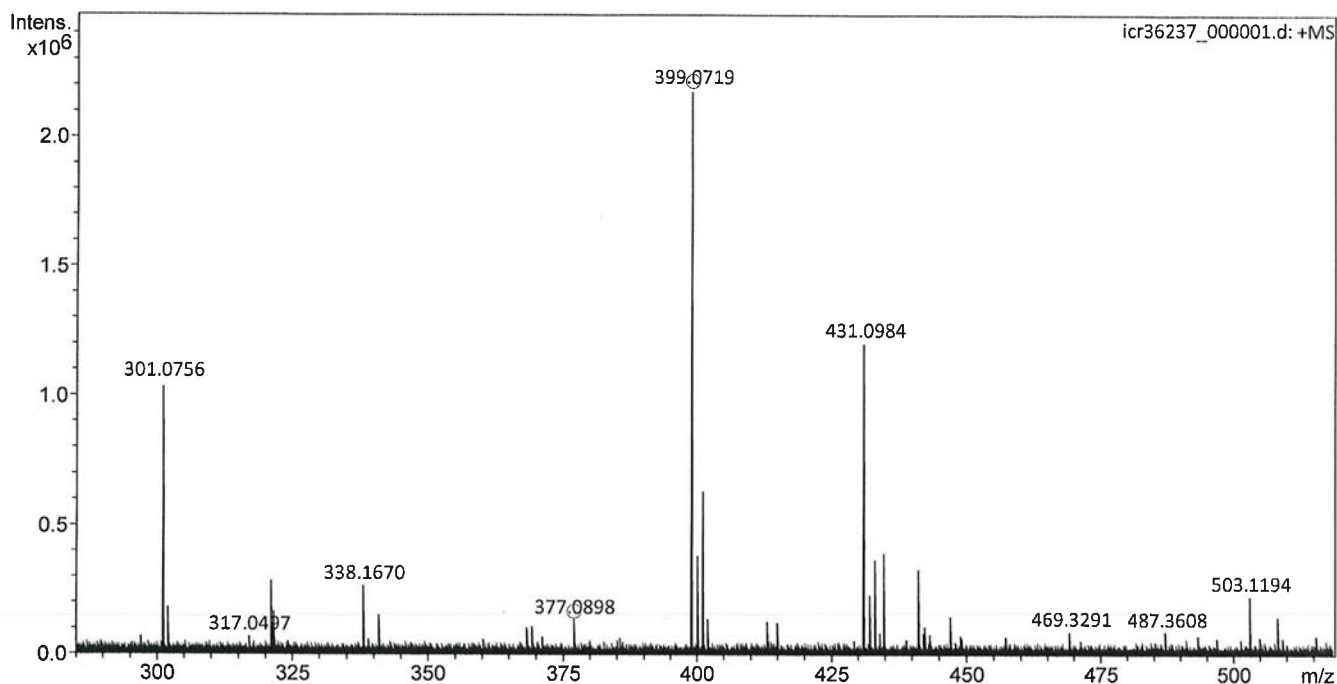
| Meas. m/z | Ion Formula | m/z | err [ppm] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|-----------------------------|----------|-----------|--------|------|---------------------|--------|
| 283.0346 | C14H7N2O5 | 283.0349 | 1.3 | 10.8 | 12.5 | even | ok |
| | C13HN9 | 283.0349 | 1.3 | 22.2 | 18.0 | odd | ok |
| | C11H13NaO5 ³⁵ Cl | 283.0344 | -0.8 | 28.3 | 4.5 | even | ok |
| | C10H7N7Na ³⁵ Cl | 283.0344 | -0.8 | 38.0 | 10.0 | odd | ok |

Mass Spectrum Formula Report

Analysis Info

Analysis Name D:\Data\Kopka DKFZ\icr36237_000001.d
Comment Krutzek, DKFZ/Kopka: FK_090.m1 in DCM/MeOH

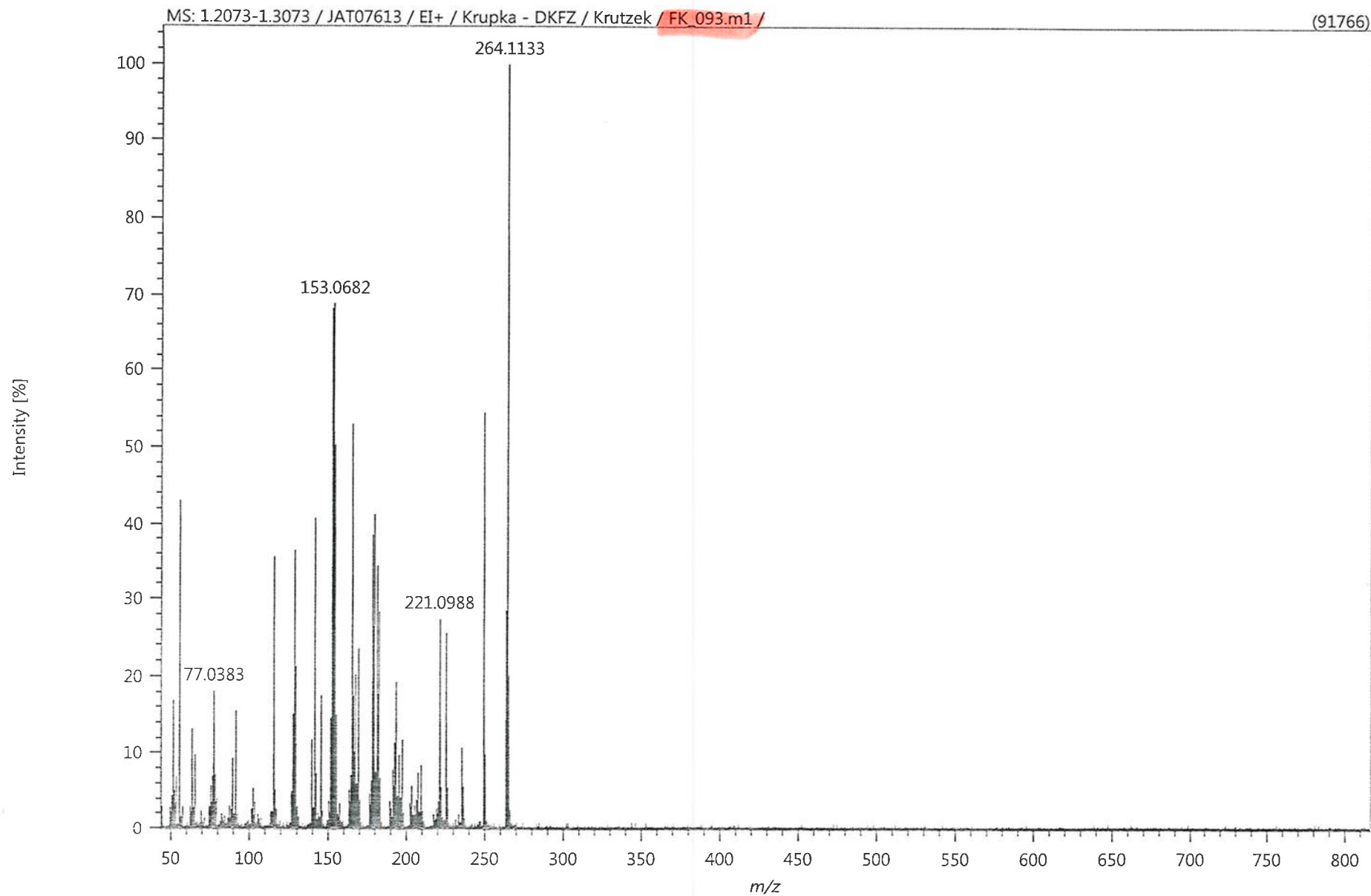
Acquisition Date 10/15/2019 1:06:14 PM



| Meas. m/z | Ion Formula | m/z | err [ppm] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|---|----------|-----------|--------|------|---------------------|--------|
| 377.0898 | C20H9N8O | 377.0894 | -1.2 | 88.1 | 20.5 | even | ok |
| | C17H12N9 ³⁵ Cl | 377.0899 | 0.1 | 89.8 | 16.0 | odd | ok |
| | C27H16 ³⁷ Cl | 377.0906 | 1.9 | 108.0 | 19.5 | even | ok |
| | C18H18N2O5 ³⁵ Cl | 377.0899 | 0.1 | 154.4 | 10.5 | even | ok |
| | C11H16N8O5 ³⁷ Cl | 377.0897 | -0.3 | 159.8 | 7.5 | even | ok |
| | C21H15NO6 | 377.0894 | -1.2 | 171.5 | 15.0 | odd | ok |
| | C12H22NO10 ³⁷ Cl | 377.0897 | -0.3 | 172.4 | 2.0 | odd | ok |
| 399.0719 | C20H8N8NaO | 399.0713 | -1.4 | 26.4 | 20.5 | even | ok |
| | C21H17N3O ³⁵ Cl ³⁷ Cl | 399.0714 | -1.3 | 27.8 | 14.0 | odd | ok |
| | C20H5N11 | 399.0724 | 1.3 | 29.6 | 24.0 | odd | ok |
| | C22H10N5NaO2 | 399.0727 | 2.0 | 34.1 | 20.0 | odd | ok |
| | C23H19O2 ³⁵ Cl ³⁷ Cl | 399.0727 | 2.1 | 44.2 | 13.5 | even | ok |
| | C27H15Na ³⁷ Cl | 399.0725 | 1.5 | 69.5 | 19.5 | even | ok |
| | C18H17N2NaO5 ³⁵ Cl | 399.0718 | -0.2 | 126.8 | 10.5 | even | ok |
| | C19H9N7O4 | 399.0711 | -2.1 | 128.6 | 19.0 | odd | ok |
| | C21H11N4O5 | 399.0724 | 1.3 | 128.9 | 18.5 | even | ok |
| | C20H15O9 | 399.0711 | -2.1 | 139.0 | 13.5 | even | ok |
| | C21H14NNaO6 | 399.0713 | -1.4 | 142.9 | 15.0 | odd | ok |



264.1173 [M]



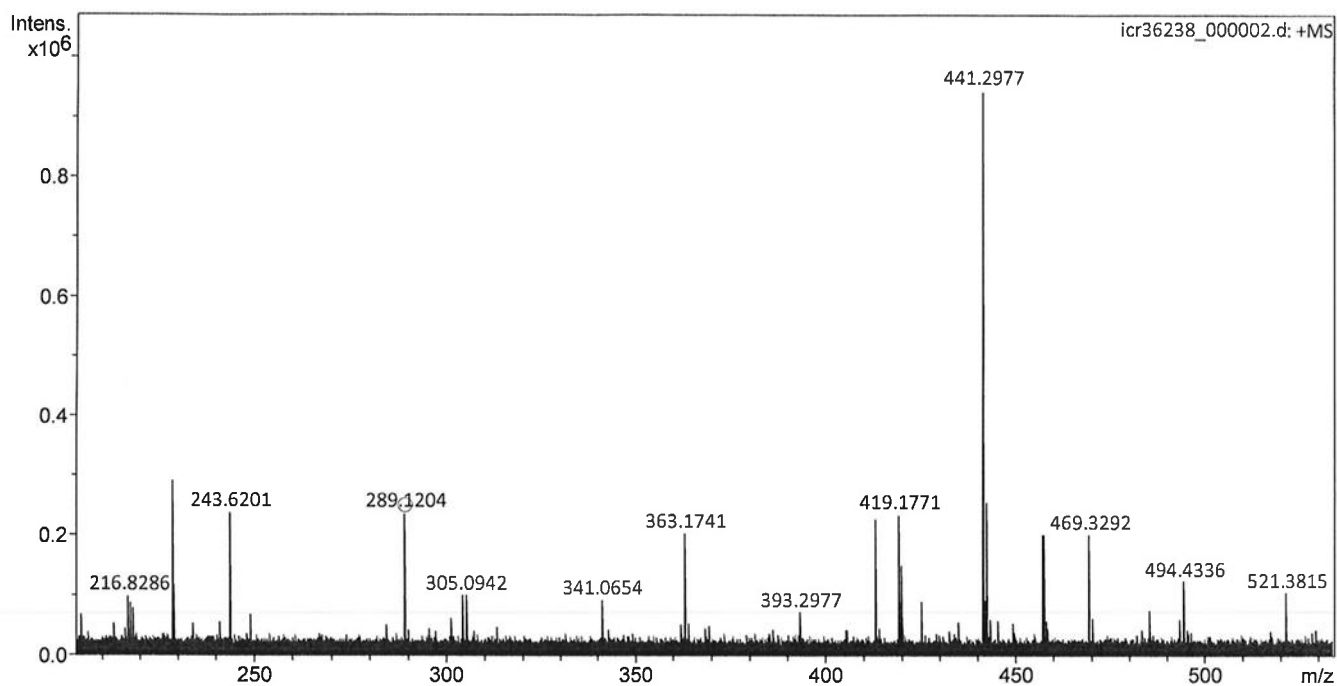
Mass Spectrum Formula Report

Analysis Info

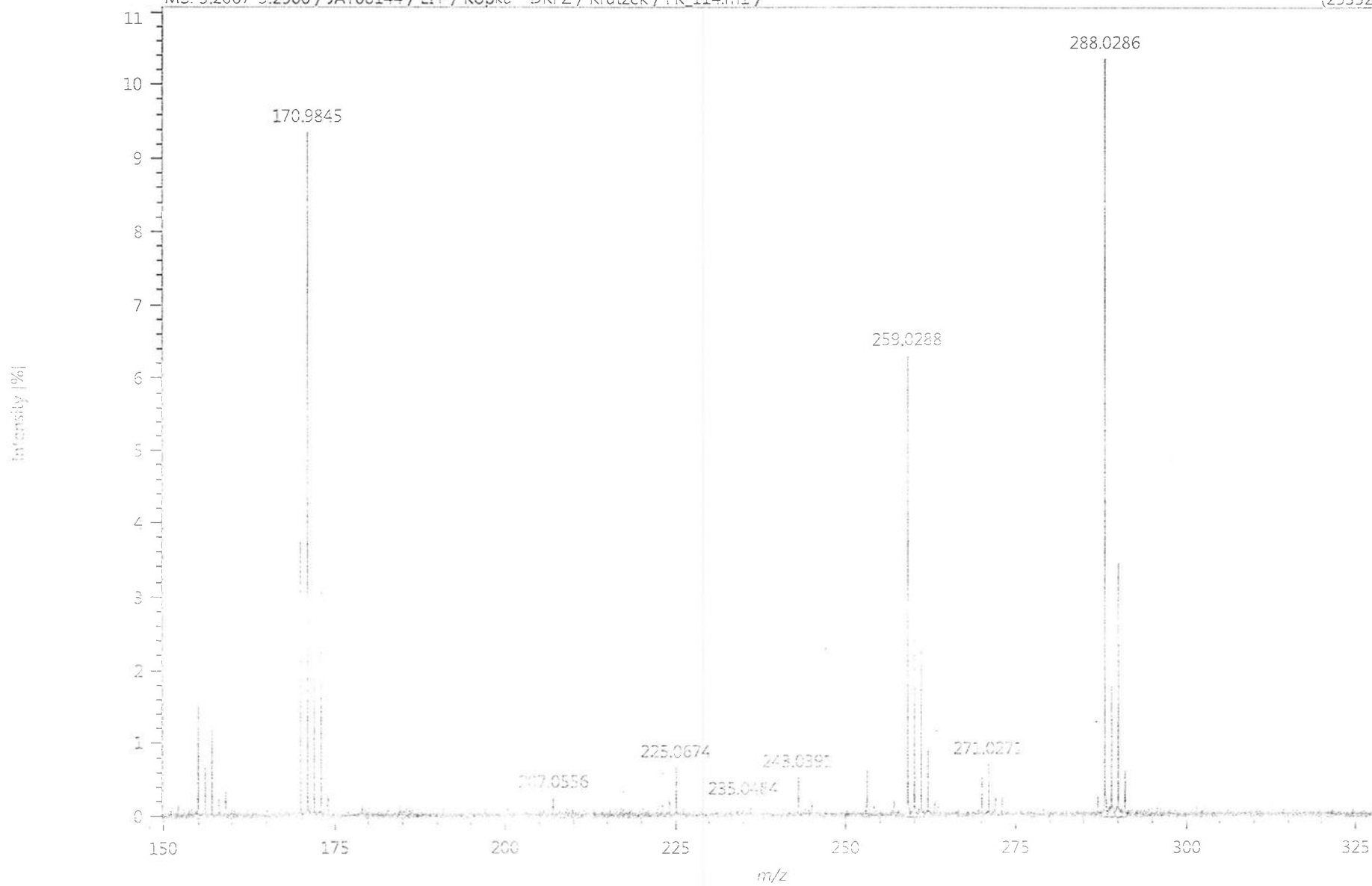
Analysis Name D:\Data\Kopka DKFZ\icr36238_000002.d

Acquisition Date 10/15/2019 1:20:00 PM

Comment Krutzek, DKFZ/Kopka: FK_094.m1 in DCM/MeOH

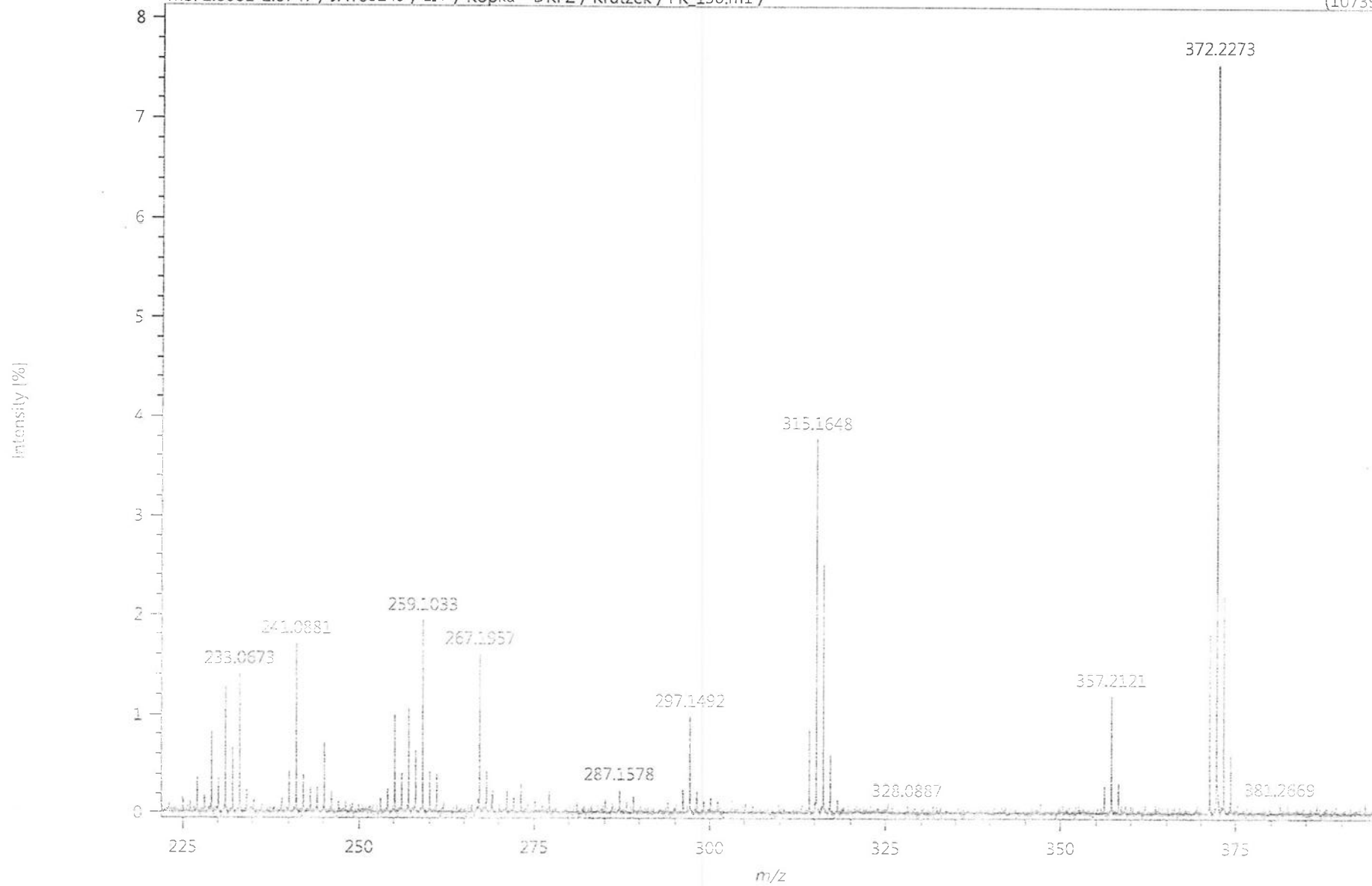


| Meas. m/z | Ion Formula | m/z | err [ppm] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|-------------|----------|-----------|--------|------|---------------------|--------|
| 289.1204 | C18H15N3O | 289.1210 | 2.0 | 11.7 | 13.0 | odd | ok |
| | C18H18NaO2 | 289.1199 | -1.7 | 12.1 | 9.5 | even | ok |



MS: 2.8081-2.8747 / JAT08149 / EI+ / Kopka - DKFZ / Krutzek / FK_130.ml /

(10739)



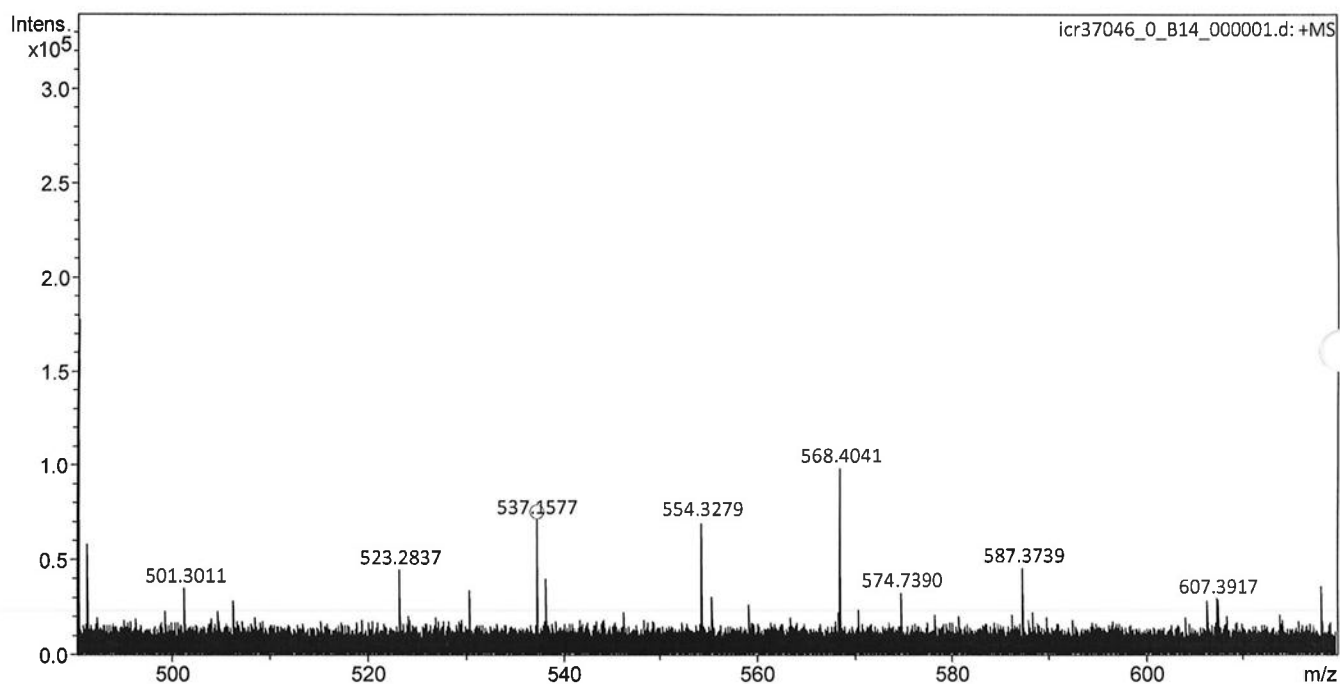
Mass Spectrum Formula Report

Analysis Info

Analysis Name D:\Data\Kopka DKFZ\icr37046_0_B14_000001.d

Acquisition Date 12/16/2019 1:50:36 PM

Comment Krutzek, AK Kopka (DKFZ): FK_158.m1 in DCM Matrix: DCTB



| Meas. m/z | Ion Formula | m/z | err [ppm] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|--|----------|-----------|--------|------|---------------------|--------|
| 537.1577 | C ₃₂ H ₂₆ N ₂ O ₄ ³⁵ Cl | 537.1576 | -0.3 | 140.2 | 20.5 | even | ok |

Analysis Info

Analysis Name D:\Data\Kopka DKFZ\icr37196_000001.d
Method ESI pos HPmix 200-1800
Sample Name FK_169.m1
Comment Krutzek, DKFZ/Kopka: FK_169.m1 in DCM/MeOH

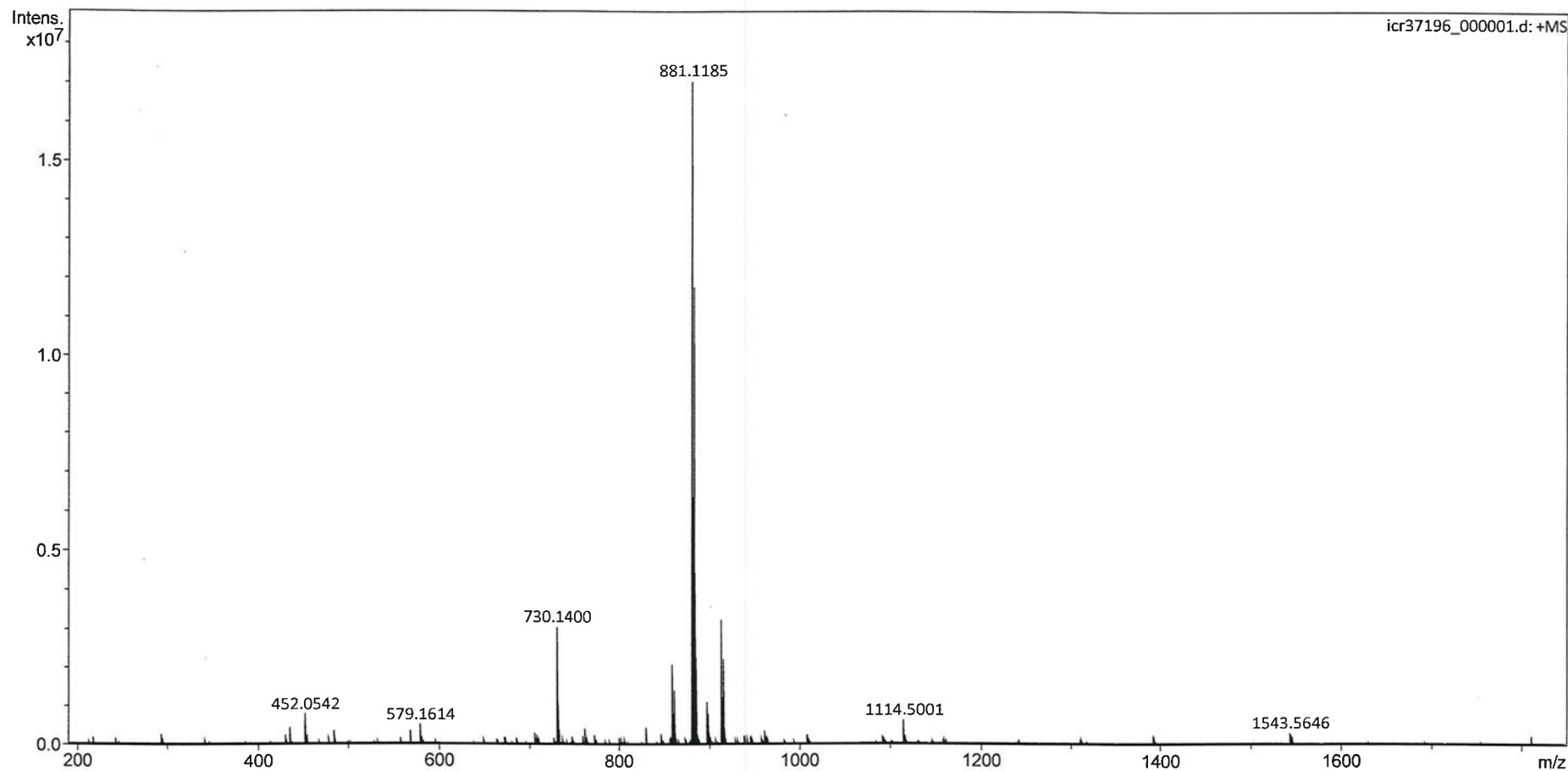
Acquisition Date 1/16/2020 8:49:06 AM
Instrument ICR Apex-Qe
Operator I.Mitsch

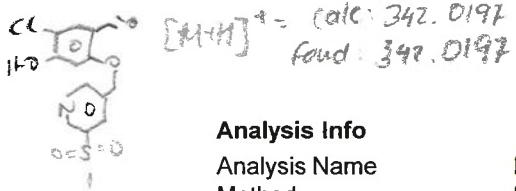
Acquisition Parameters

Accumulations 16
Broadband Low Mass 173.2 m/z
Broadband High Mass 2500.0 m/z
Data Acquisition Size 2097152

Collision Gas Flow Rate 0.5 L/sec
Collision Energy 0.5 eV
Collision Cell RF 1200.0 V
Q1 Resolution 5.0
Q1 Mass 200.000 m/z

Capillary Entrance 4200.0 V
Calibration Date Tue Jan 14 02:13:10 2020





Analysis Info

Analysis Name D:\Data\Kopka DKFZ\icr37197_000001.d
Method ESI pos HPmix 200-1800
Sample Name FK_174.m1
Comment Krutzek, DKFZ/Kopka: FK_174.m1 in DCM/MeOH

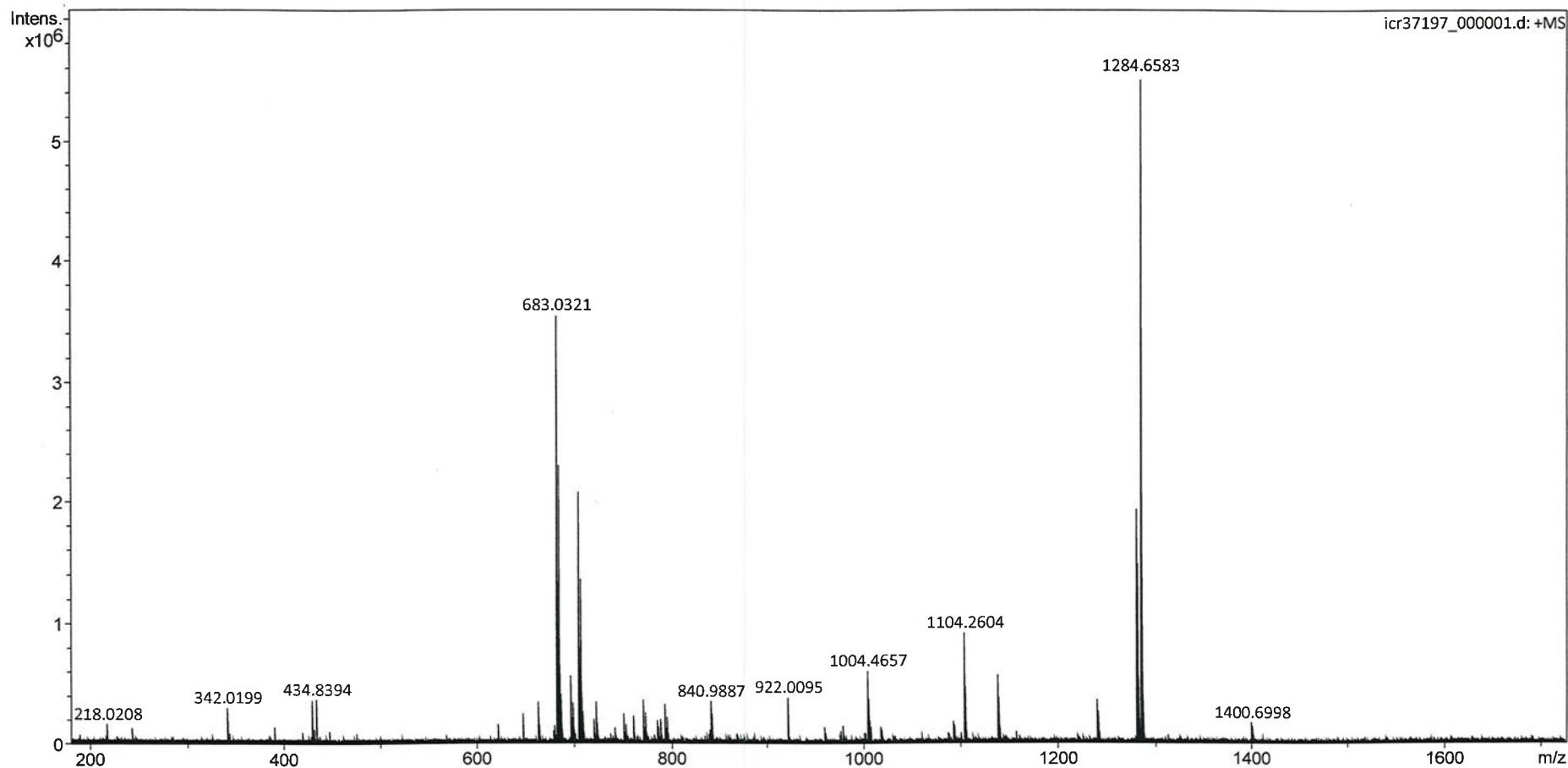
Acquisition Date 1/16/2020 9:02:16 AM
Instrument ICR Apex-Qe
Operator I.Mitsch

Acquisition Parameters

Accumulations 16
Broadband Low Mass 173.2 m/z
Broadband High Mass 2500.0 m/z
Data Acquisition Size 2097152

Collision Gas Flow Rate 0.5 L/sec
Collision Energy 0.5 eV
Collision Cell RF 1200.0 V
Q1 Resolution 5.0
Q1 Mass 200.000 m/z

Capillary Entrance 4200.0 V
Calibration Date Tue Jan 14 02:13:10 2020



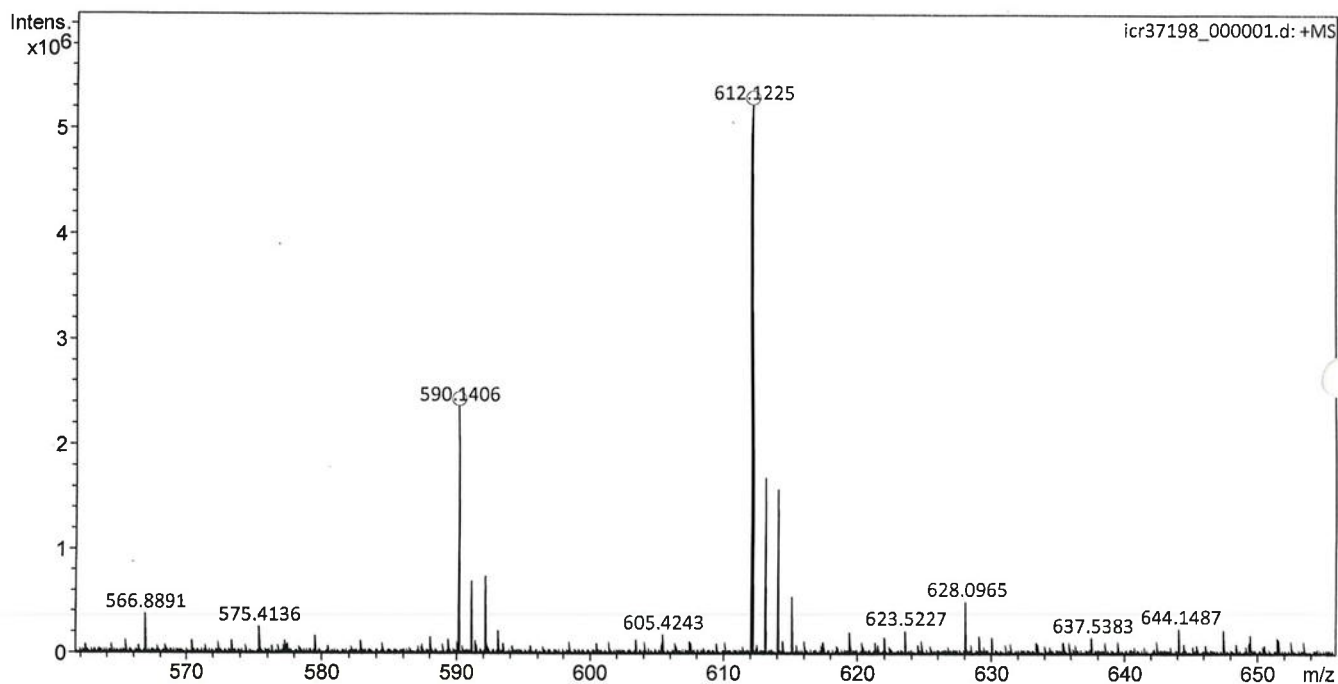
Mass Spectrum Formula Report

Analysis Info

Analysis Name D:\Data\Kopka DKFZ\icr37198_000001.d

Acquisition Date 1/16/2020 9:17:25 AM

Comment Krutzek, DKFZ/Kopka: FK_177.m1 in DCM/MeOH



| Meas. m/z | Ion Formula | m/z | err [ppm] | mSigma | rdb | e ⁻ Conf | N-Rule |
|-----------|-------------------|----------|-----------|--------|------|---------------------|--------|
| 590.1406 | C33H23N5O4^37Cl | 590.1404 | -0.3 | 49.1 | 24.5 | even | ok |
| | C35H25N2O5^37Cl | 590.1417 | 1.9 | 61.9 | 24.0 | odd | ok |
| | C34H20N7O2S | 590.1394 | -2.0 | 107.0 | 28.5 | even | ok |
| | C35H26O7S | 590.1394 | -2.0 | 107.6 | 23.0 | odd | ok |
| | C32H29NO6S^35Cl | 590.1399 | -1.2 | 111.4 | 18.5 | even | ok |
| | C33H25N5O2S^35Cl | 590.1412 | 1.1 | 113.1 | 23.5 | even | ok |
| | C36H22N4O3S | 590.1407 | 0.3 | 113.7 | 28.0 | odd | ok |
| | C38H30S^35Cl^37Cl | 590.1410 | 0.8 | 116.3 | 23.0 | odd | ok |
| | C34H19N9^37Cl | 590.1417 | 1.9 | 140.9 | 29.5 | even | ok |
| 612.1225 | C32H23N4O7^37Cl | 612.1220 | -0.7 | 46.0 | 23.0 | odd | ok |
| | C32H28NNaO6S^35Cl | 612.1218 | -1.1 | 100.6 | 18.5 | even | ok |
| | C32H25N4O5S^35Cl | 612.1229 | 0.7 | 105.2 | 22.0 | odd | ok |

