

Electronic Supporting Information

Ciprofloxacin tethered 1, 2, 3-triazole conjugates: new quinolone family compounds to upgrade our antiquated approach against bacterial infections

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***Corresponding Author**

Prof. Alka Agarwal

Department of Medicinal Chemistry

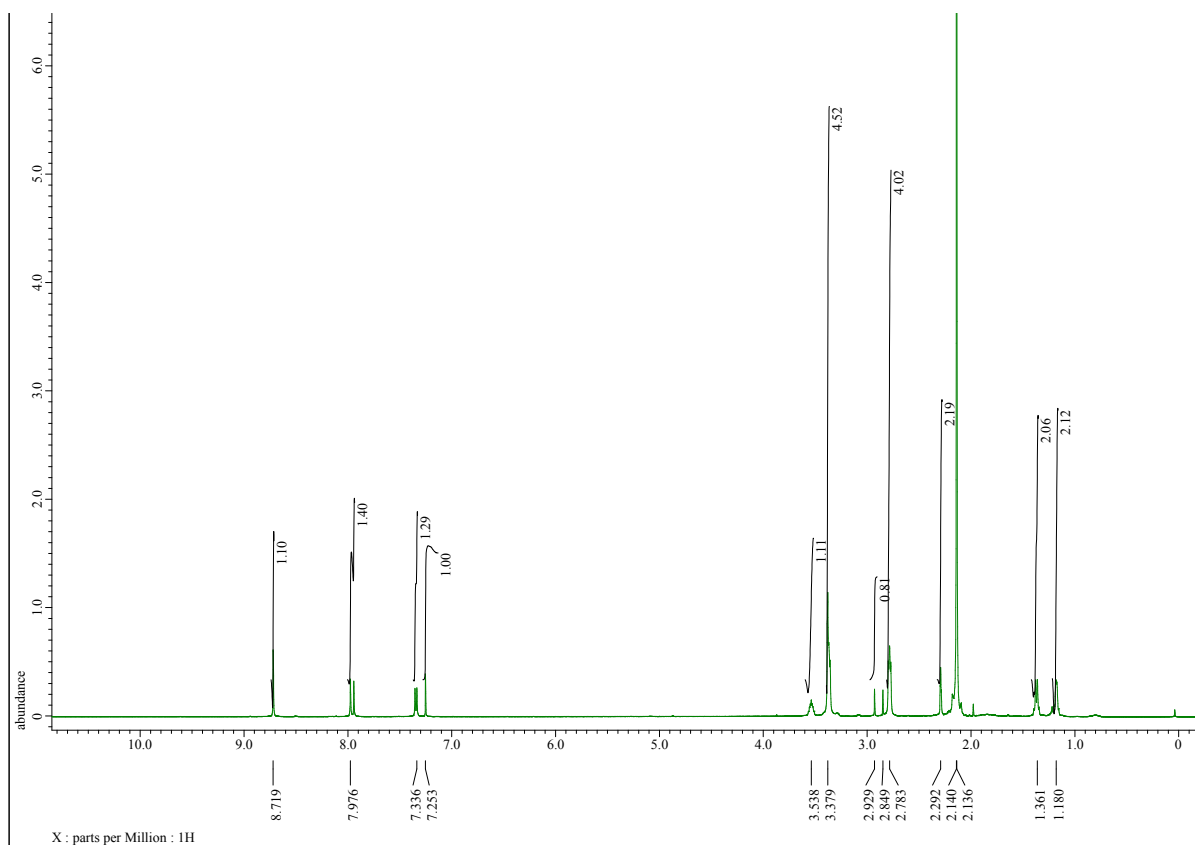
Institute of Medical Sciences

Banaras Hindu University

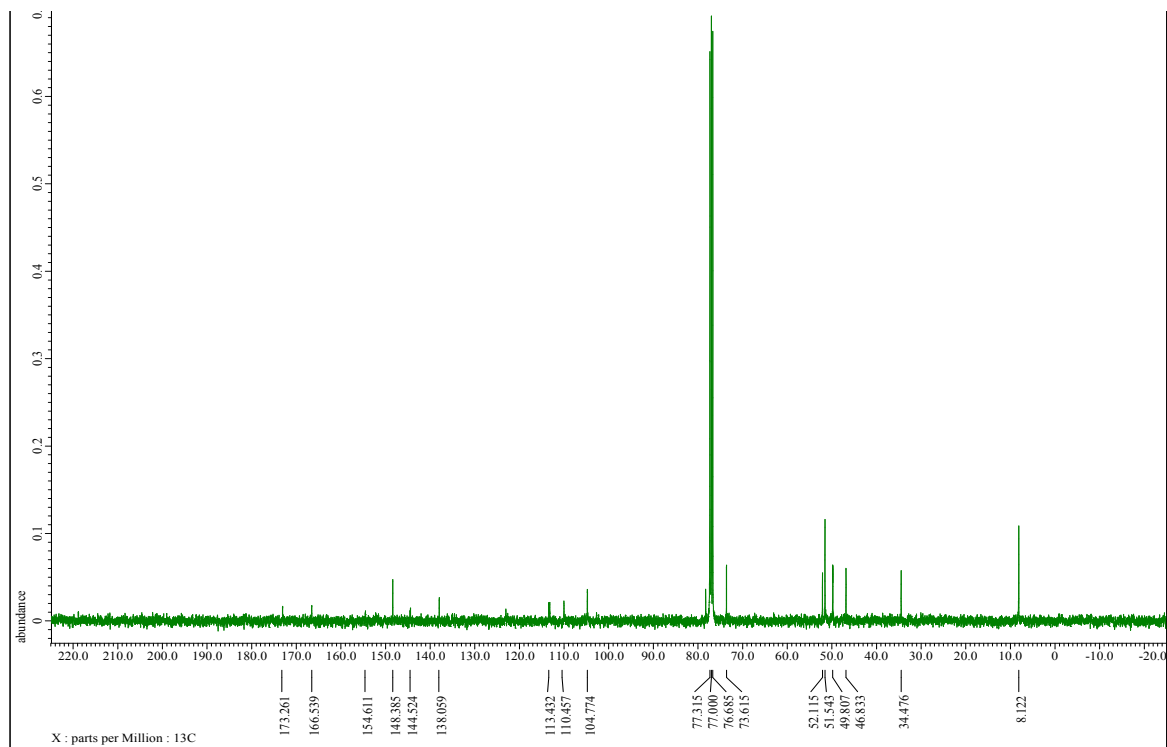
Varanasi, 221005, U.P. India

Email: agarwal.dralka@gmail.com

¹H NMR (400MHz, CDCl₃) (2):



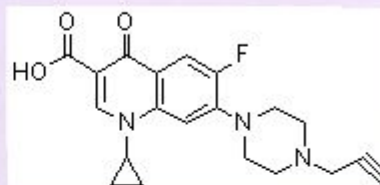
¹³C NMR (100MHz, CDCl₃) (2):



Qualitative Compound Report

Data File: RK-200.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo JK.m
 IRM Calibration Status: Success
 Comment:

Sample Name: RK-200
 Position: P1-C1
 User Name:
 Acquired Time: 25-06-2018 15:05:30
 DA Method: Default.m



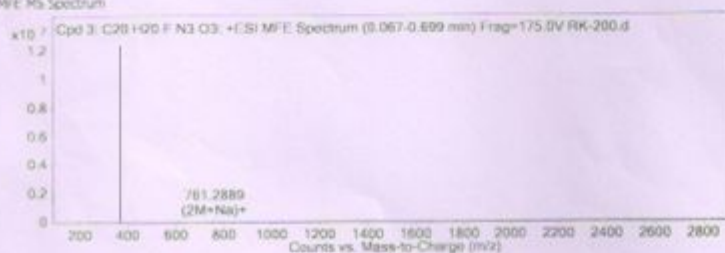
Sample Group: Info.
 Acquisition SW: 6200 series TOF/ESI series
 Version: Q-ToF B.05.01 (85125.1)

Compound Table

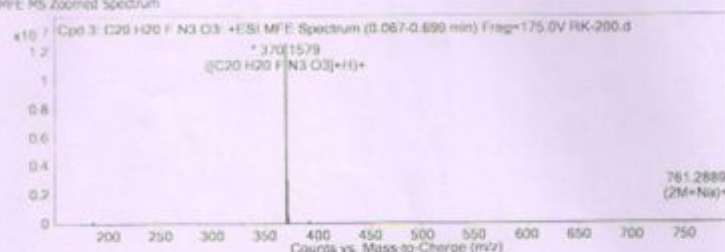
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|------------------------|-------|--------|-----------------|-----------------|----------------|-----------------|
| Cpd 3: C20 H20 F N3 O3 | 0.091 | 369.15 | C20 H20 F N3 O3 | C20 H20 F N3 O3 | -3.01 | C20 H20 F N3 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|-------|---------------------------|--------|
| Cpd 3: C20 H20 F N3 O3 | 370.1579 | 0.091 | Find by Molecular Feature | 369.15 |

M/E MS Spectrum



M/E MS Zoomed Spectrum

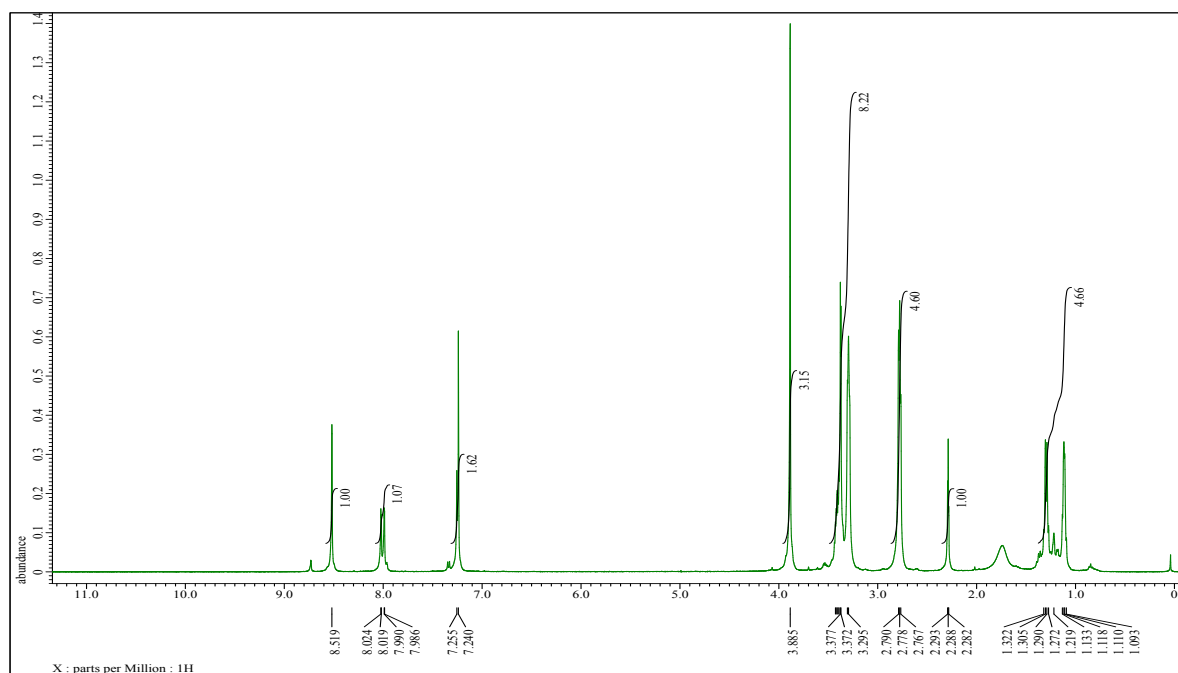


MS Spectrum Peak List

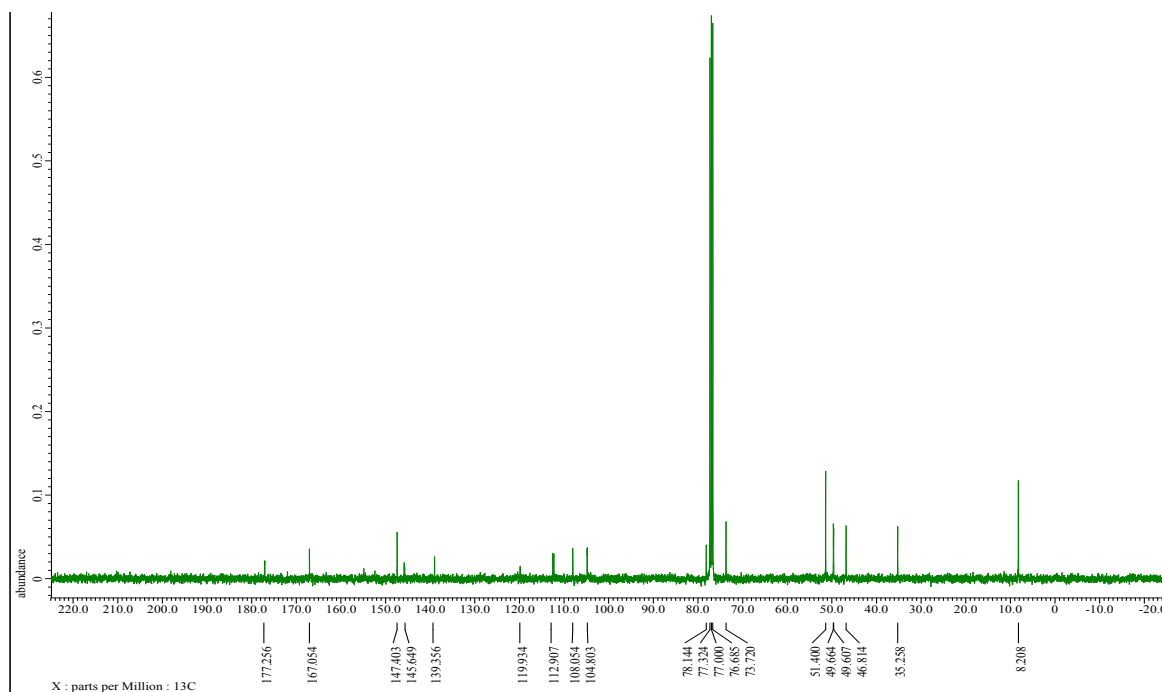
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|-----------------|----------|
| 185.5836 | 2 | 45616.8 | C20 H20 F N3 O3 | (M+2H)+2 |
| 370.1579 | 1 | 125851.35 | C20 H20 F N3 O3 | (M+H)+ |
| 371.1612 | 1 | 2888603.59 | C20 H20 F N3 O3 | (M+H)+ |
| 372.1639 | 1 | 292711.98 | C20 H20 F N3 O3 | (M+H)+ |
| 373.1662 | 1 | 45749 | C20 H20 F N3 O3 | (M+H)+ |
| 392.1397 | 1 | 63646.3 | C20 H20 F N3 O3 | (M+Na)+ |
| 729.3061 | 1 | 42064.08 | C20 H20 F N3 O3 | (2M+H)+ |
| 761.2889 | 1 | 179355.22 | | (2M+Na)+ |
| 762.2922 | 1 | 81797.65 | | (2M+Na)+ |
| 763.2953 | 1 | 21199.33 | | (2M+Na)+ |

— End Of Report. —

^1H NMR (400MHz, CDCl_3) (3a):



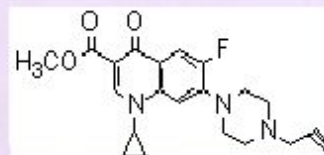
^{13}C NMR (100MHz, CDCl_3) (3a):



Qualitative Compound Report

Data File: RK-201.d
 Sample: Sample
 Instrument Name: Instrument 1
 Acq Method: Data_KL.M
 IRM Calibration Status: Success
 Comment:

Sample Name: RK-201
 Position: P1-C2
 User Name:
 Acquired Time: 25-06-2018 15:07:12
 DA Method: Default.m

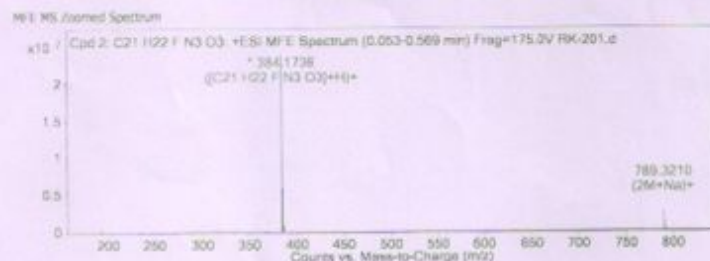
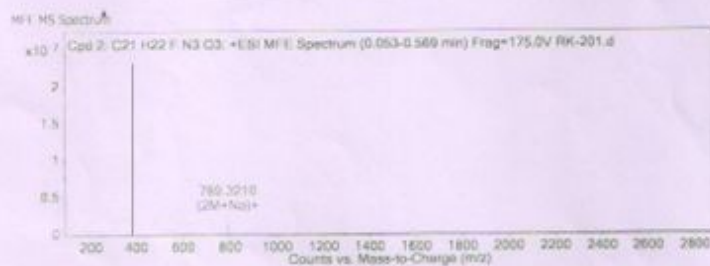


Sample Group: Info.
 Acquisition SW: 6700 series TOF/6500 series
 Version: Q-TOF 8.05.01 (RS175.1)

Compound Table

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|------------------------|-------|----------|-----------------|-----------------|----------------|-----------------|
| Cpd 2: C21 H22 F N3 O3 | 0.097 | 383.1666 | C21 H22 F N3 O3 | C21 H22 F N3 O3 | -5.5 | C21 H22 F N3 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|-------|---------------------------|----------|
| Cpd 2: C21 H22 F N3 O3 | 384.1736 | 0.097 | Find by Molecular Feature | 383.1666 |

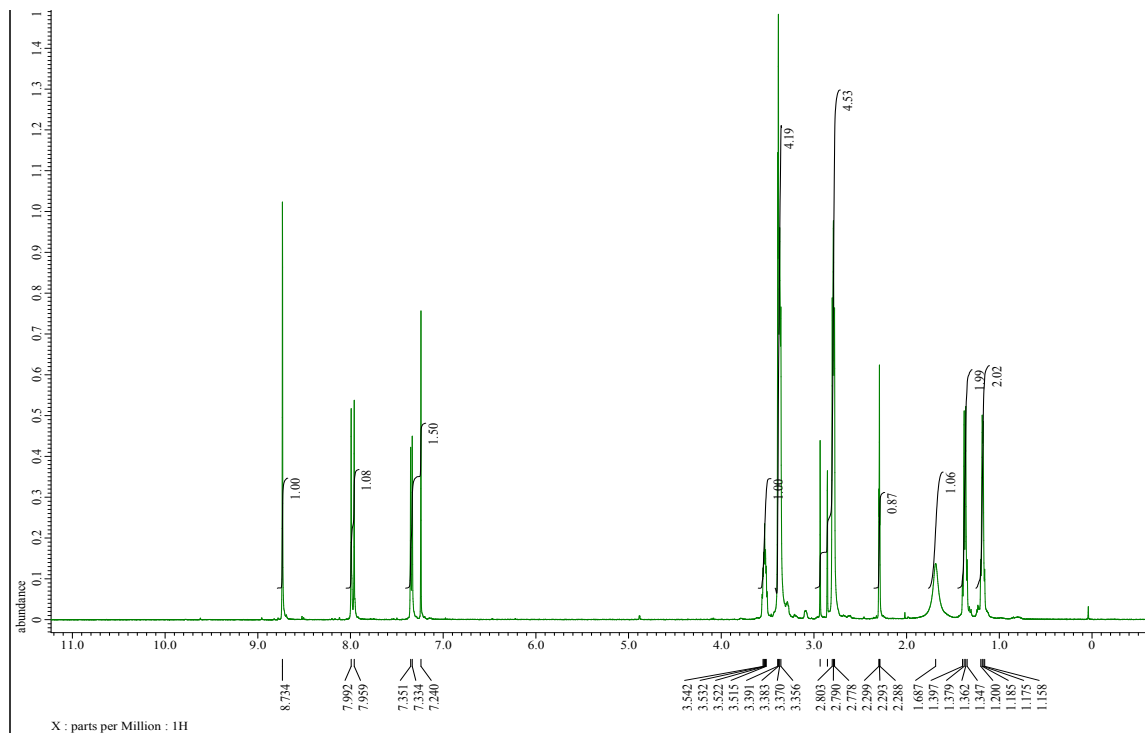


MS Spectrum Peak List

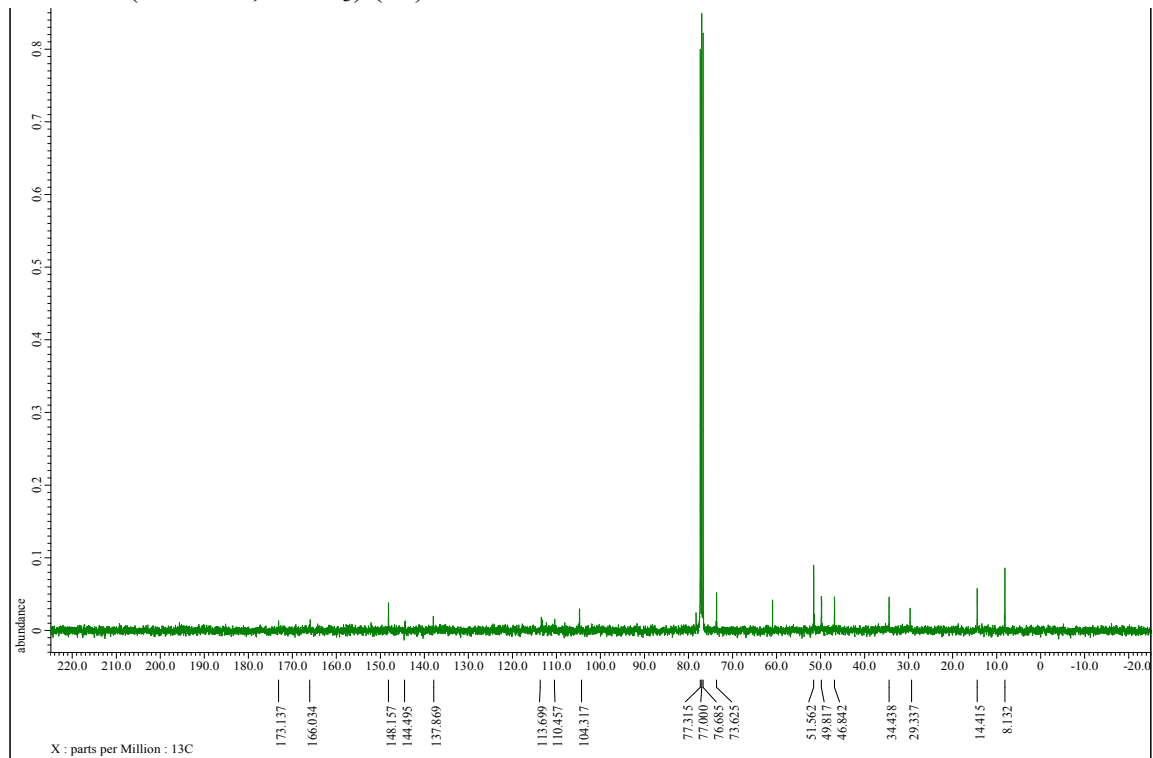
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|-----------------|----------|
| 150.1006 | 2 | 384309.69 | C21 H22 F N3 O3 | (M+2H)+2 |
| 193.0921 | 2 | 90383.72 | C21 H22 F N3 O3 | (M+2H)+2 |
| 384.1736 | 1 | 23774990 | C21 H22 F N3 O3 | (M+H)+ |
| 385.177 | 1 | 5704907.21 | C21 H22 F N3 O3 | (M+H)+ |
| 386.1799 | 1 | 756516.05 | C21 H22 F N3 O3 | (M+H)+ |
| 387.1821 | 1 | 75991.80 | C21 H22 F N3 O3 | (M+H)+ |
| 769.321 | 1 | 2659324.25 | | (2M+Na)+ |
| 790.3243 | 1 | 1282811.96 | | (2M+Na)+ |
| 791.3268 | 1 | 330750.84 | | (2M+Na)+ |
| 792.3292 | 1 | 60788.15 | | (2M+Na)+ |

-- End Of Report --

^1H NMR (400MHz, CDCl_3) (3b):



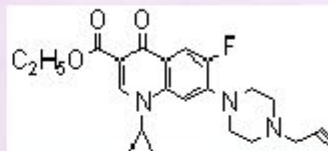
^{13}C NMR (100MHz, CDCl_3) (3b):



Qualitative Compound Report

Data File: RK-202.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo_K.M
 IRM Calibration Status: Success
 Comment:

Sample Name: RK-202
 Position: P1-06
 User Name:
 Acquired Time: 28-06-2018 14:41:44
 DA Method: Default.m



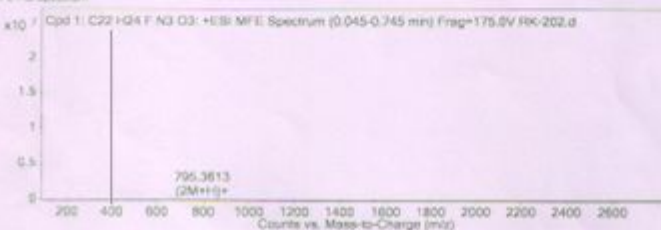
Sample Group: Info.
 Acquisition SW: 6500 series TOF/6500 series
 Version: Q-TOF 8.05.01 (85125.1)

Compound Table

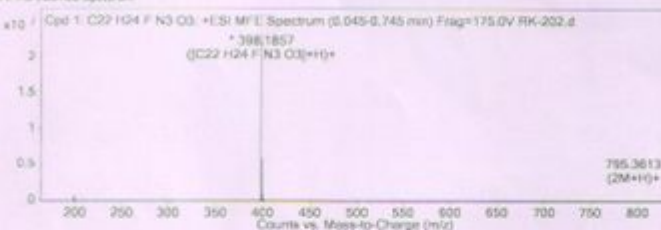
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | *DB Formula |
|------------------------|-------|----------|-----------------|-----------------|----------------|-----------------|
| Cpd 1: C22 H24 F N3 O3 | 0.092 | 397.1785 | C22 H24 F N3 O3 | C22 H24 F N3 O3 | 4.25 | C22 H24 F N3 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|-------|---------------------------|----------|
| Cpd 1: C22 H24 F N3 O3 | 398.1857 | 0.092 | Find by Molecular Feature | 397.1785 |

MFE MS Spectrum



MFE MS Zoomed Spectrum

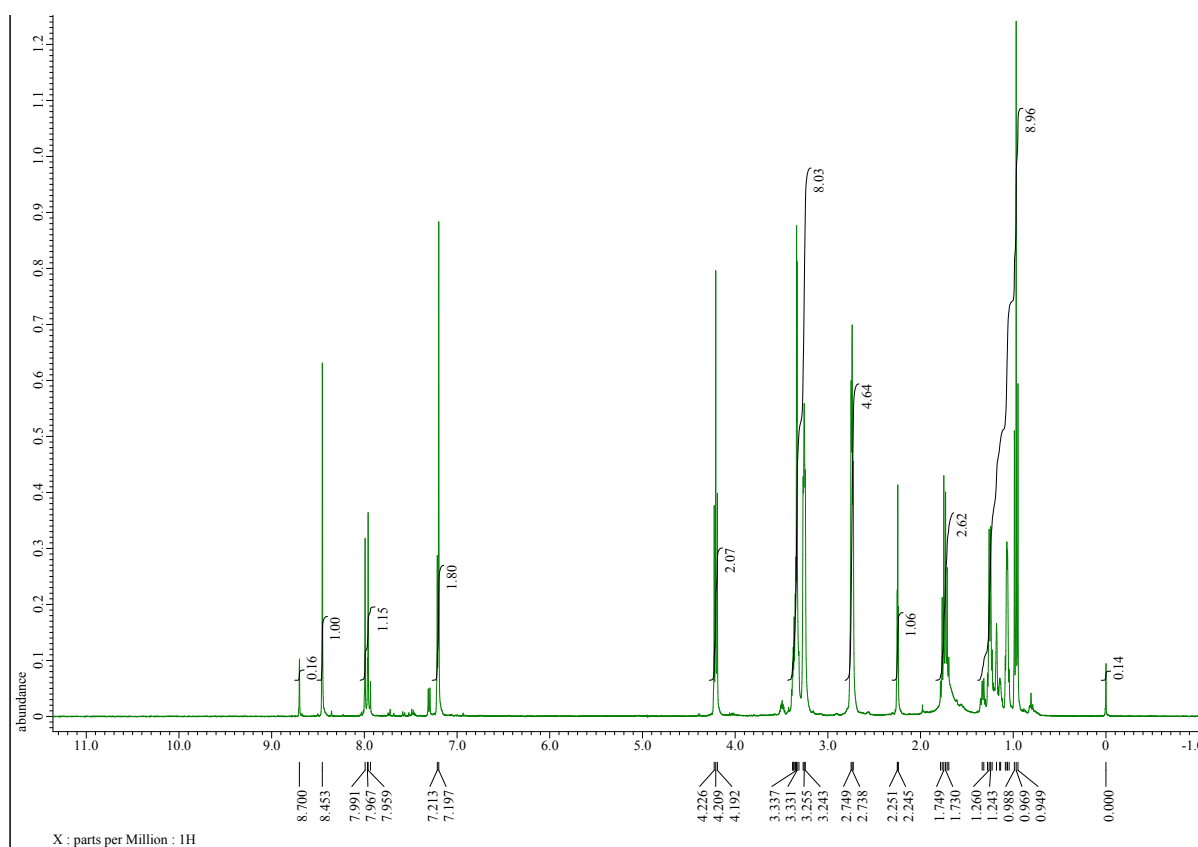


MS Spectrum Peak List

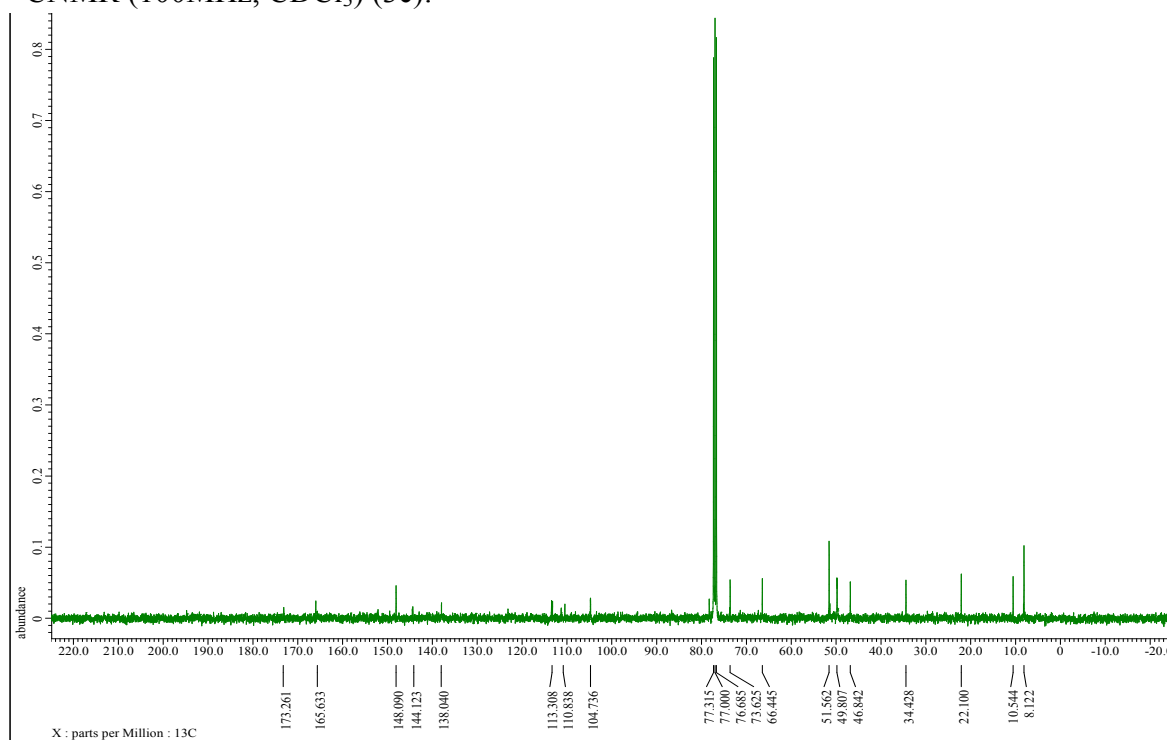
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|-----------------|----------|
| 199.5954 | 2 | 468728.25 | C22 H24 F N3 O3 | (M+2H)+2 |
| 200.9969 | 2 | 121913.5 | C22 H24 F N3 O3 | (M+2H)+2 |
| 200.9983 | 2 | 19372.27 | C22 H24 F N3 O3 | (M+2H)+2 |
| 398.1857 | 1 | 2334828 | C22 H24 F N3 O3 | (M+H)+ |
| 398.1889 | 1 | 5841546.73 | C22 H24 F N3 O3 | (M+H)+ |
| 400.1919 | 1 | 85147.43 | C22 H24 F N3 O3 | (M+H)+ |
| 401.1946 | 1 | 103297.76 | C22 H24 F N3 O3 | (M+H)+ |
| 417.1595 | 2 | 35592.49 | | (2M+H)+2 |
| 417.6604 | 2 | 17827.01 | | (2M+H)+2 |
| 418.171 | 2 | 14246.19 | | (2M+H)+2 |

--- End Of Report ---

^1H NMR (400MHz, CDCl_3) (3c):

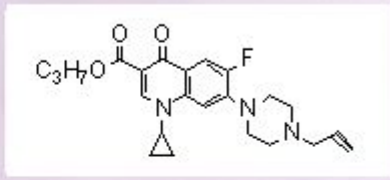


^{13}C NMR (100MHz, CDCl_3) (3c):



Qualitative Compound Report

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Sample Type Sample **Position** P1-B1
Instrument Name Instrument 1 **User Name**
Acq Method Data: 1K.m **Acquired Time** 04-07-2018 13:03:35
IRM Calibration Status Success **DA Method** Default.m
Comment

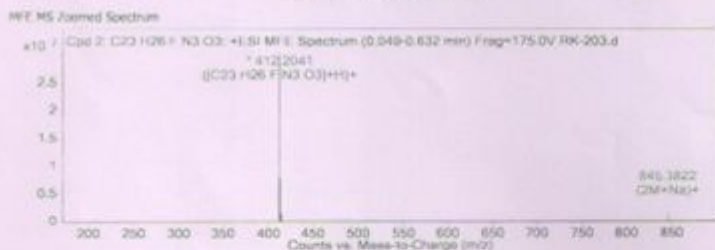


Sample Group Info.
Acquisition SW 6200 series TOF/MS00 series
Version Q-TOF 8.05.01 (06125.1)

Compound Table

| Compound Label | RT | Mass | Formula | MFG Formula | MFG DIF (ppm) | DB Formula |
|-------------------------|-------|----------|-----------------|-----------------|---------------|-----------------|
| Comp 2: C23 H26 F N3 O3 | 0.108 | 411.1965 | C23 H26 F N3 O3 | C23 H26 F N3 O3 | -1.7 | C23 H26 F N3 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|-------------------------|----------|-------|---------------------------|----------|
| Comp 2: C23 H26 F N3 O3 | 412.2041 | 0.108 | Find by Molecular Feature | 411.1965 |

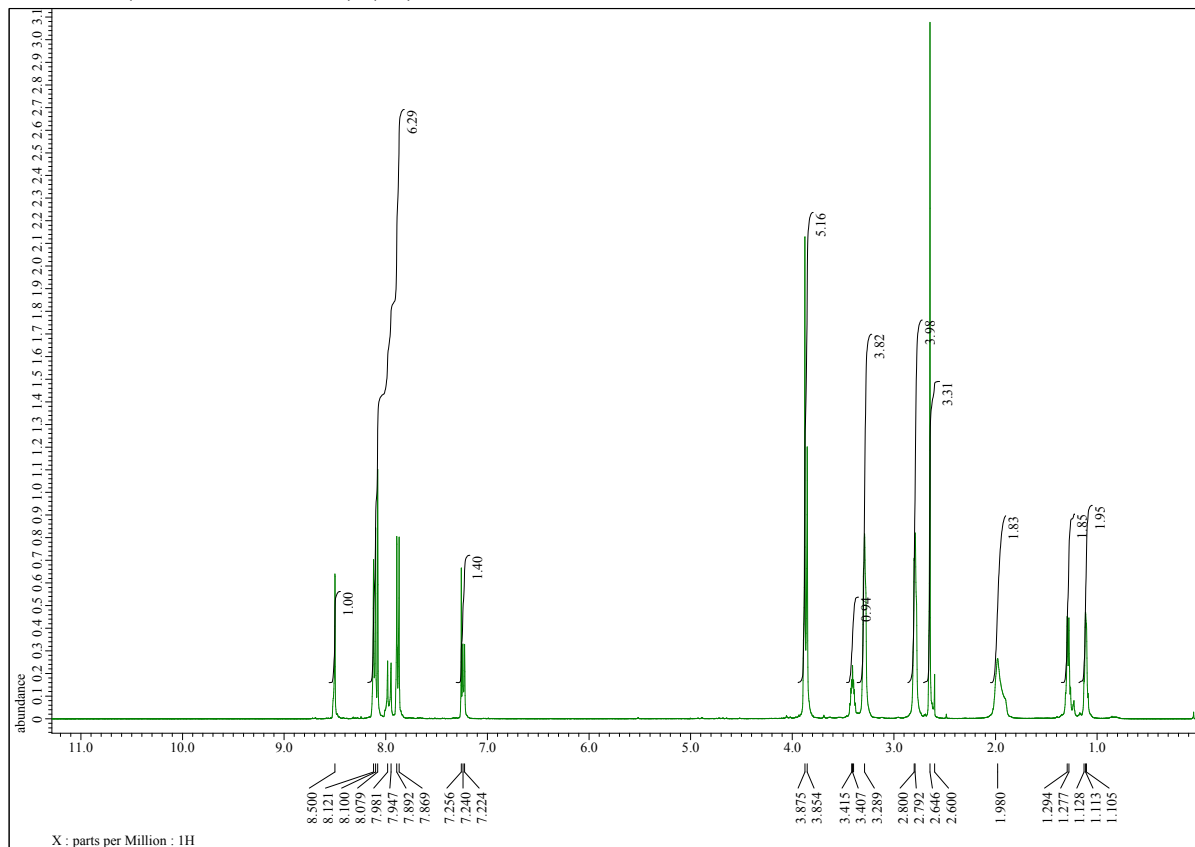


MS Spectrum Peak List

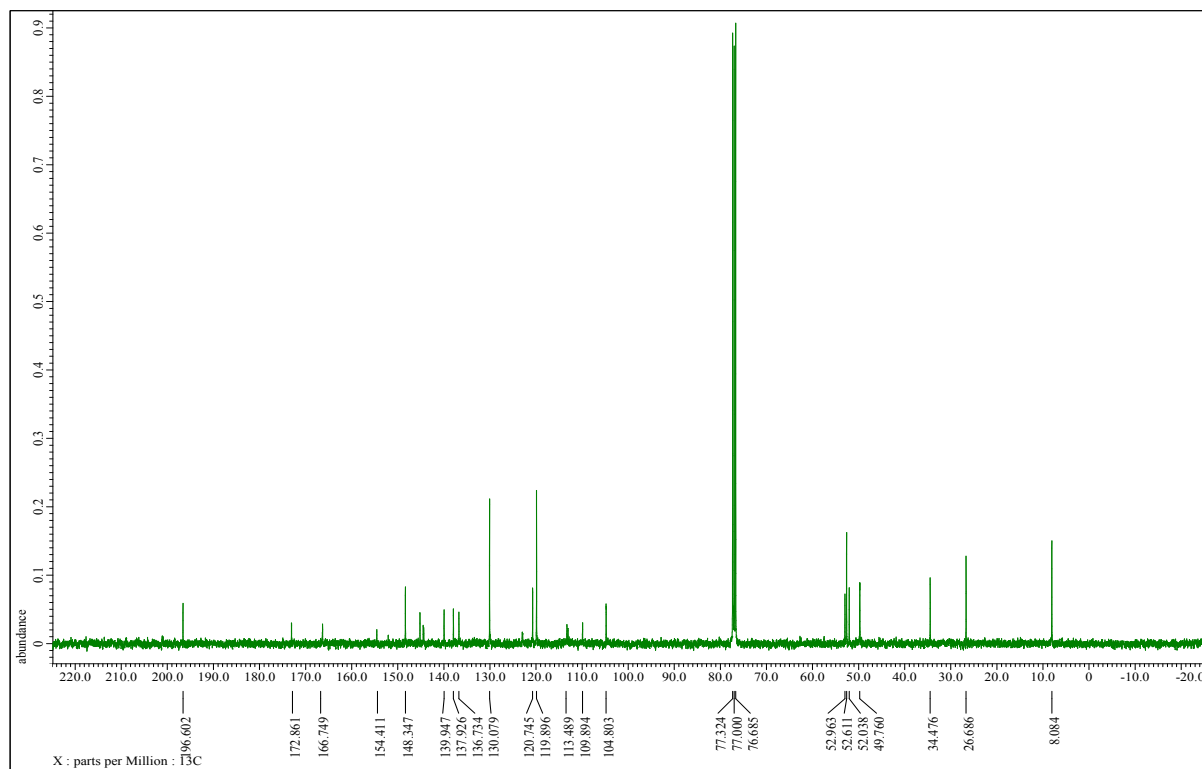
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|-----------------|----------|
| 206.6036 | 2 | 257996.24 | C23 H26 F N3 O3 | (M+2H)+2 |
| 207.1071 | 2 | 74624.24 | C23 H26 F N3 O3 | (M+2H)+2 |
| 412.2041 | 1 | 301997.76 | C23 H26 F N3 O3 | (M+H)+ |
| 413.2073 | 1 | 809385.26 | C23 H26 F N3 O3 | (M+H)+ |
| 414.2103 | 1 | 1192013.53 | C23 H26 F N3 O3 | (M+H)+ |
| 415.2132 | 1 | 140738.56 | C23 H26 F N3 O3 | (M+H)+ |
| 845.3822 | 1 | 1443680 | | (2M+Na)+ |
| 846.3853 | 1 | 771259.46 | | (2M+Na)+ |
| 847.3877 | 1 | 208680.85 | | (2M+Na)+ |
| 848.3901 | 1 | 40520.99 | | (2M+Na)+ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4a):



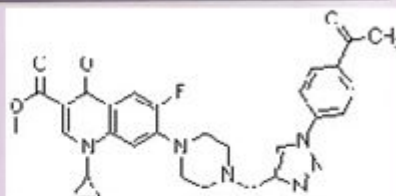
^{13}C NMR (100MHz, CDCl_3) (4a):



Qualitative Compound Report

Data File: RK-205.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo JK.m
 IRM Calibration Status: Success
 Comment:

Sample Name: RK-205
 Position: P1-04
 User Name:
 Acquired Time: 02-07-2018 15:46:00
 DA Method: Default.m



Sample Group: Info.
 Acquisition SW: 5200 series TOF/MSD series
 Version: Q-TOF 8.05.01 (86125.1)

Compound Table

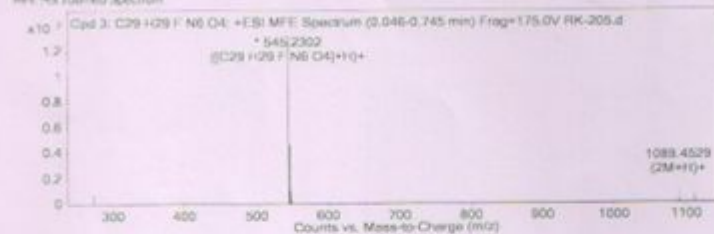
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|------------------------|-------|----------|-----------------|-----------------|----------------|-------------------|
| Cpd 3: C29 H29 F N6 O4 | 0.094 | 544.2226 | C29 H29 F N6 O4 | C29 H29 F N6 O4 | 1.48 | - C29 H29 F N6 O4 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|-------|---------------------------|----------|
| Cpd 3: C29 H29 F N6 O4 | 545.2302 | 0.094 | Find by Molecular Feature | 544.2226 |

MS Spectrum



MFE MS Zoomed Spectrum

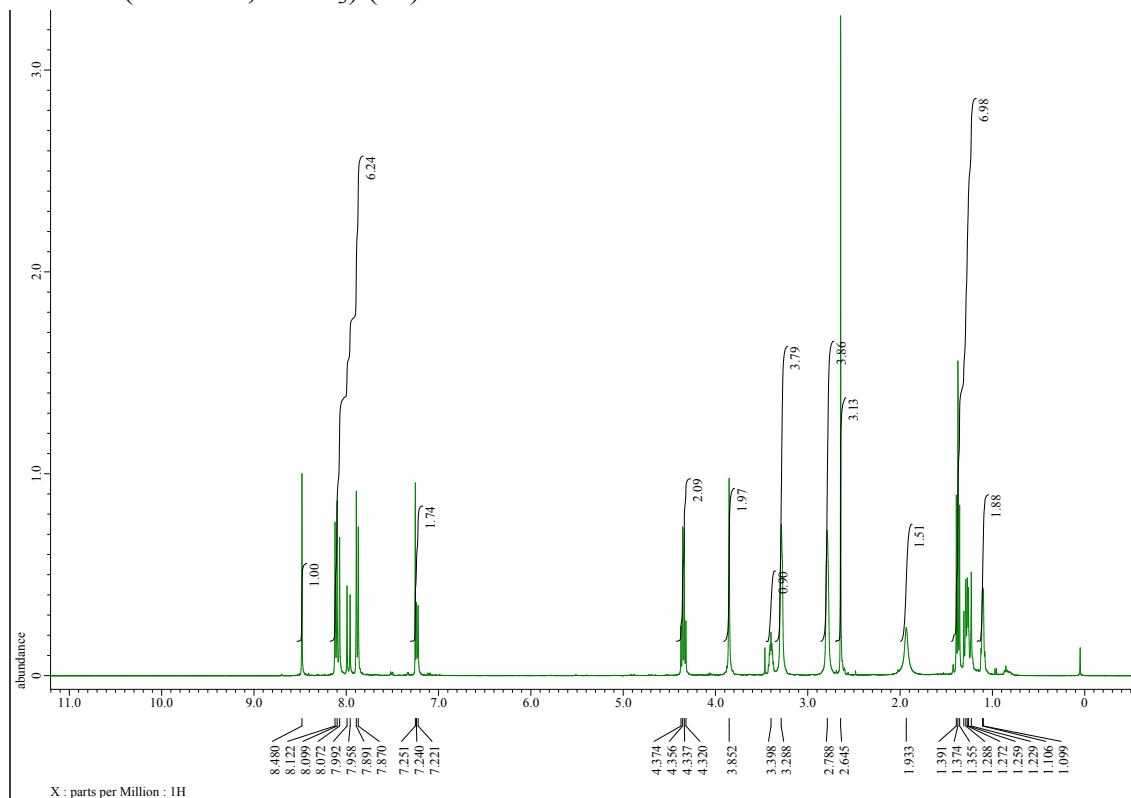


MS Spectrum Peak List

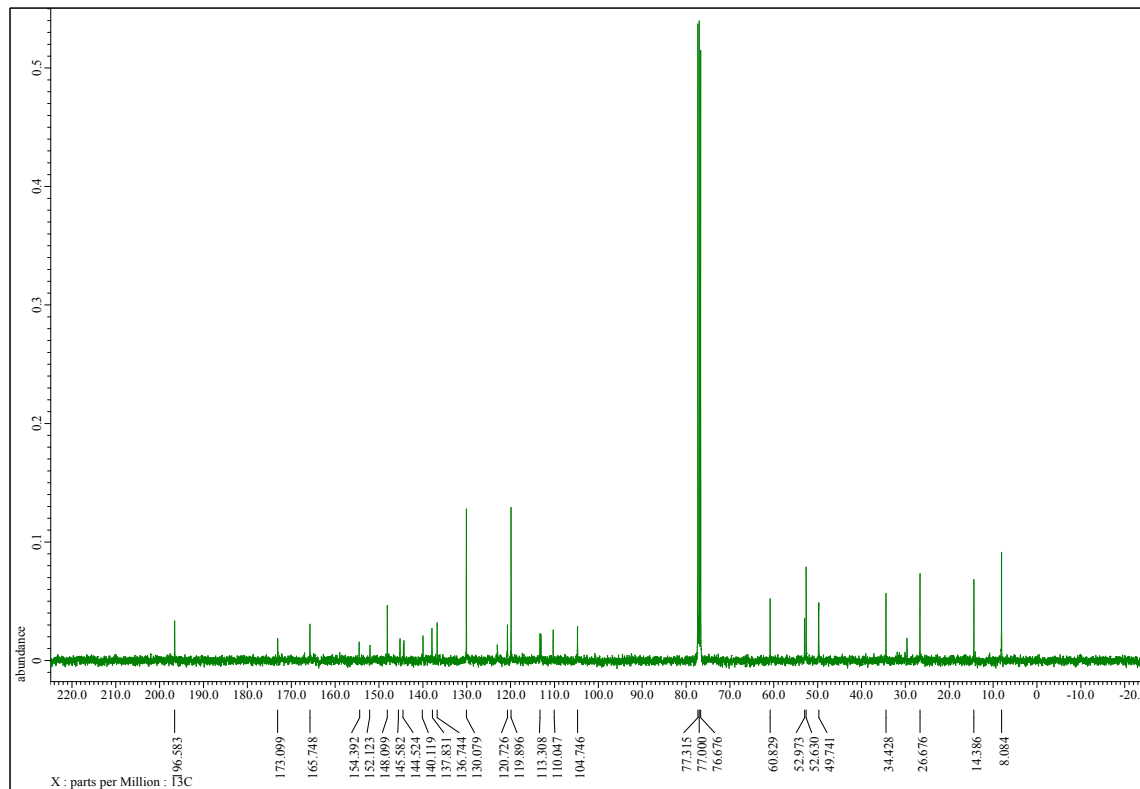
| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|-----------------|----------|
| 273.1186 | 2 | 751706.44 | C29 H29 F N6 O4 | (M+2H)+2 |
| 273.62 | 2 | 256403.25 | C29 H29 F N6 O4 | (M+2H)+2 |
| 545.2302 | 1 | 13157170 | C29 H29 F N6 O4 | (M+H)+ |
| 546.2333 | 1 | 4444756.69 | C29 H29 F N6 O4 | (M+H)+ |
| 547.2280 | 1 | 1096642.81 | C29 H29 F N6 O4 | (M+H)+ |
| 548.2235 | 1 | 210736.84 | C29 H29 F N6 O4 | (M+H)+ |
| 1089.4529 | 1 | 788981.44 | | (2M+H)+ |
| 1090.456 | 1 | 524201.06 | | (2M+H)+ |
| 1111.4396 | 1 | 616195.13 | | (2M+Na)+ |
| 1112.4376 | 1 | 407896.97 | | (2M+Na)+ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4b):



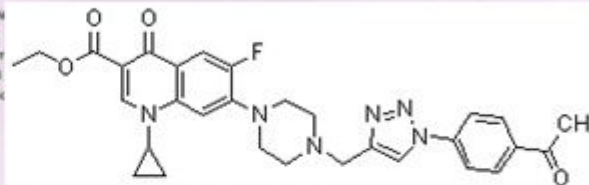
^{13}C NMR (100MHz, CDCl_3) (4b):



Qualitative Compound Report

Data File: RK-206.d
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 Instrument Name: Instrument 1
 Acq Method: Demo_K.M
 IRM Calibration Status: Success
 Comment:
 Sample Group:
 Acquisition SW Version: 6200 series TOF/6300 series Q-TOF B.05.01 (05.125.1)

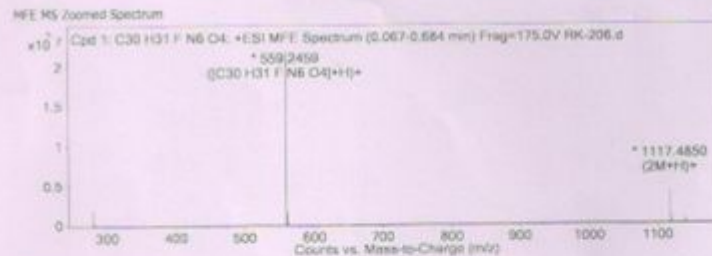
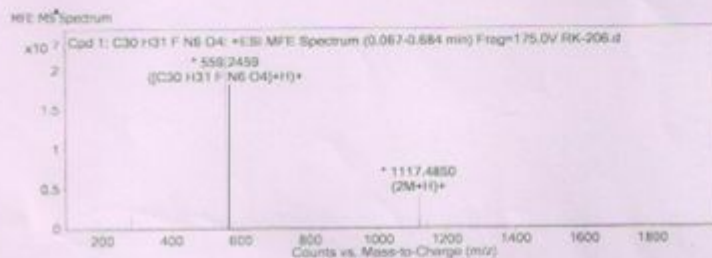
Sample Name:
 Position:
 User Name:
 Acquired:
 DA Meth:



Compound Table

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|------------------------|-------|----------|-----------------|-----------------|----------------|-----------------|
| Cpd 1: C30 H31 F N6 O4 | 0.109 | 558.2383 | C30 H31 F N6 O4 | C30 H31 F N6 O4 | 1.41 | C30 H31 F N6 O4 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|-------|---------------------------|----------|
| Cpd 1: C30 H31 F N6 O4 | 559.2459 | 0.109 | Find by Molecular Feature | 558.2383 |

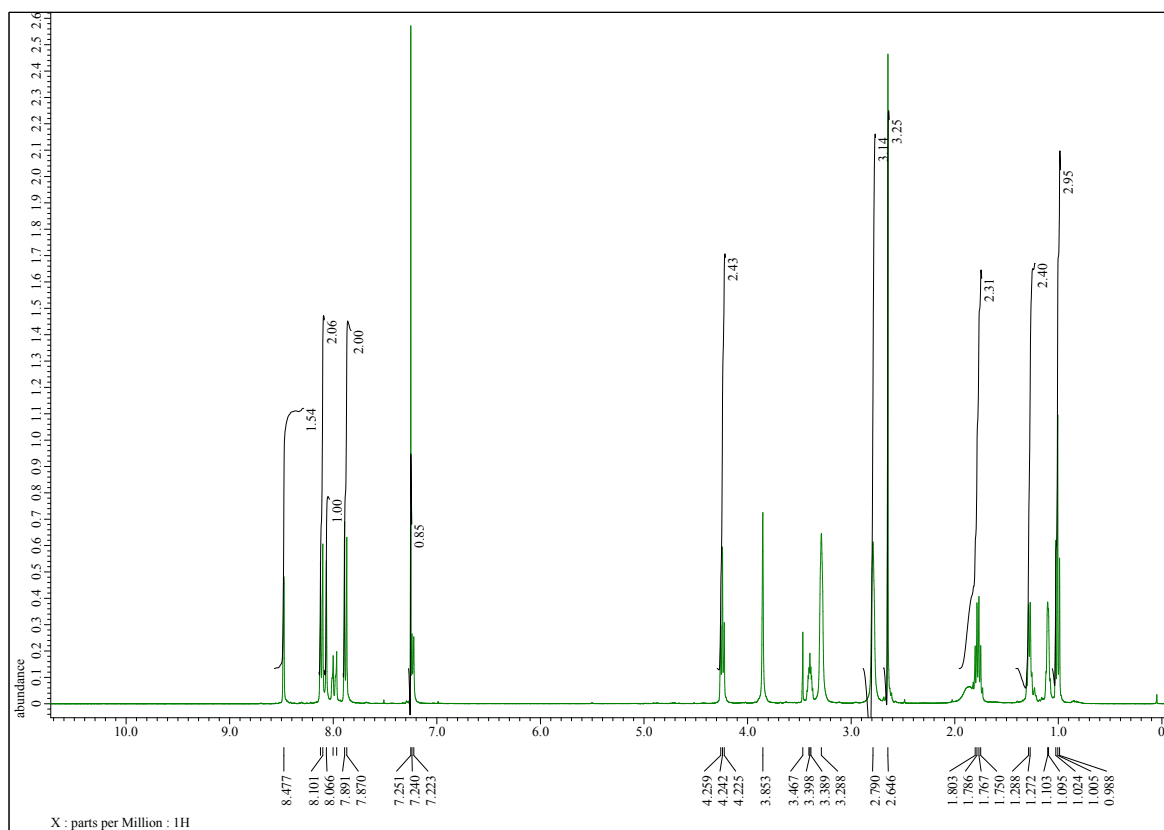


MS Spectrum Peak List

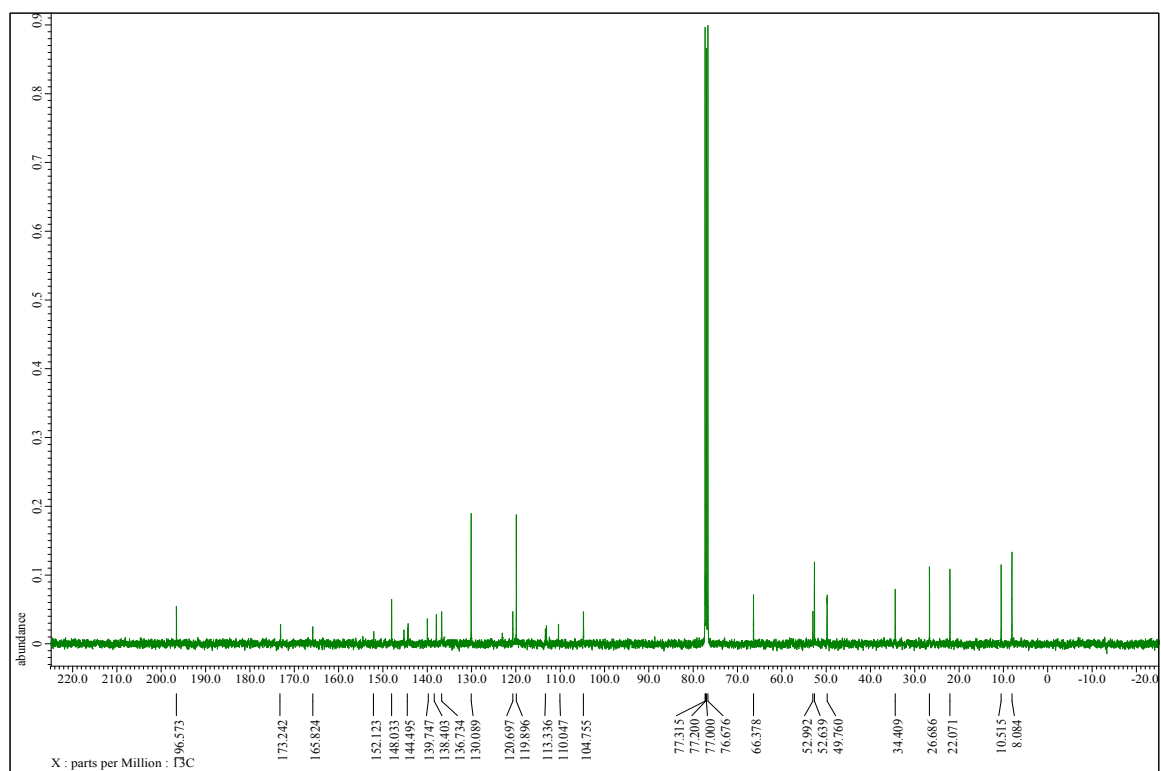
| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|-----------------|----------|
| 280.1264 | 2 | 1843615.38 | C30 H31 F N6 O4 | (M+2H)+2 |
| 280.678 | 2 | 671886.19 | C30 H31 F N6 O4 | (M+2H)+2 |
| 559.2459 | 1 | 21903958 | C30 H31 F N6 O4 | (M+1)+ |
| 560.3492 | 1 | 2634385.99 | C30 H31 F N6 O4 | (M+1)+ |
| 561.3492 | 1 | 5602234.76 | C30 H31 F N6 O4 | (M+1)+ |
| 1117.485 | 1 | 3967168.25 | | (2M+1)+ |
| 1118.4886 | 1 | 2801421.02 | | (2M+1)+ |
| 1119.4918 | 1 | 1050124.2 | | (2M+1)+ |
| 1139.4673 | 1 | 651719.88 | | (2M+Na)+ |
| 1140.4701 | 1 | 451261.72 | | (2M+Na)+ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4c):

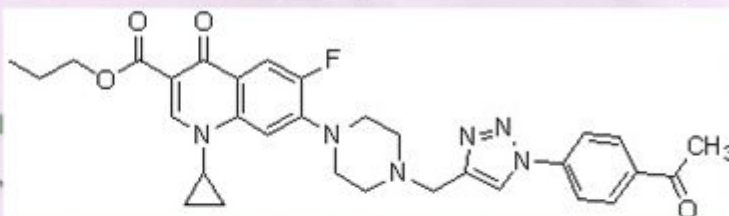


^{13}C NMR (100MHz, CDCl_3) (4c):



Qualitative Compound Report

Data File: RK-207.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo JK.m
 IRM Calibration Status: Success
 Comment:
 Sample Group:
 Acquisition SW: 6200 series TOF/6500 series
 Version: Q-TOF R.05.01 (09125.1)



Compound Table

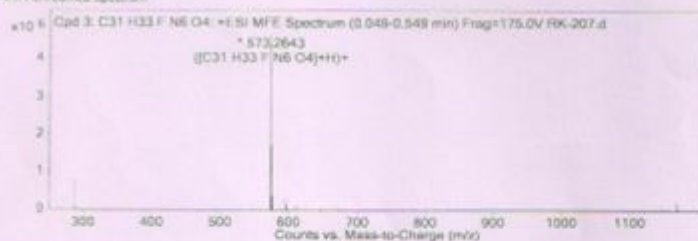
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|------------------------|------|----------|-----------------|-----------------|----------------|-----------------|
| Cpd 3: C31 H33 F N6 O4 | 0.14 | 572.2564 | C31 H33 F N6 O4 | C31 H33 F N6 O4 | -2.87 | C31 H33 F N6 O4 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|------|---------------------------|----------|
| Cpd 3: C31 H33 F N6 O4 | 573.2643 | 0.14 | Find by Molecular Feature | 572.2564 |

MFE MS Spectrum



MFE MS Zoomed Spectrum

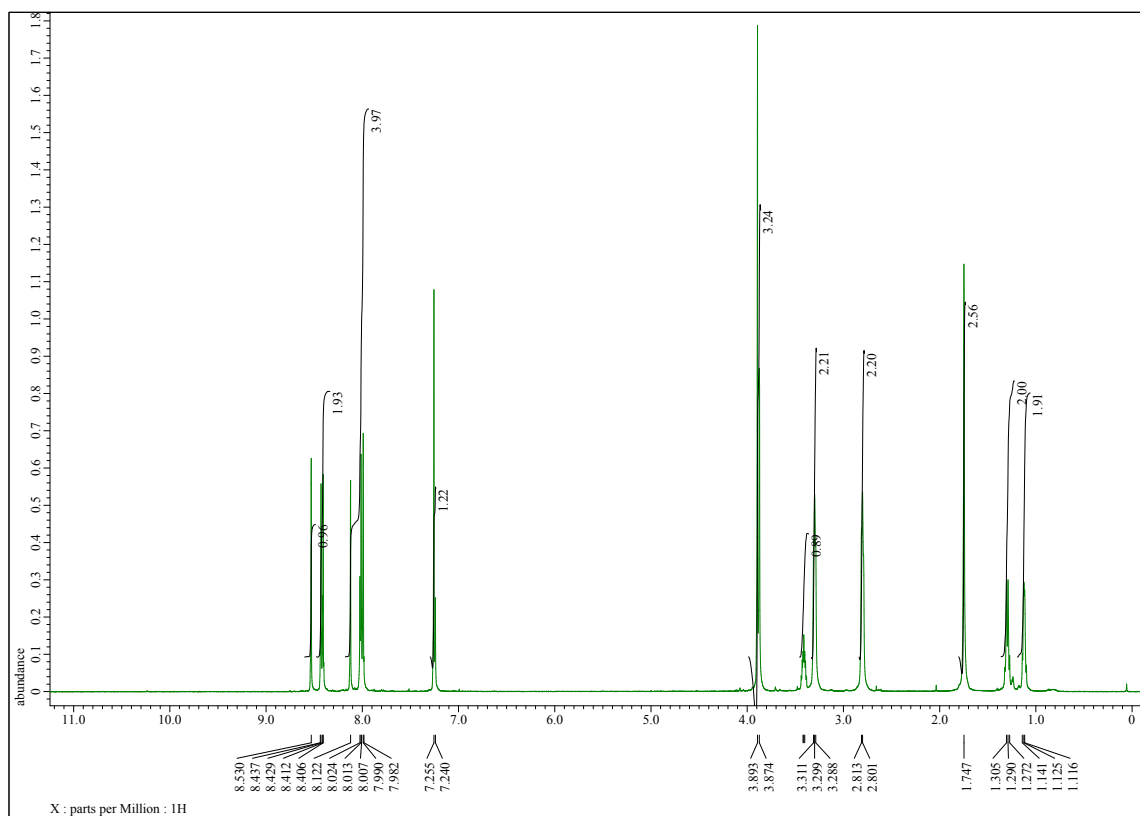


MS Spectrum Peak List

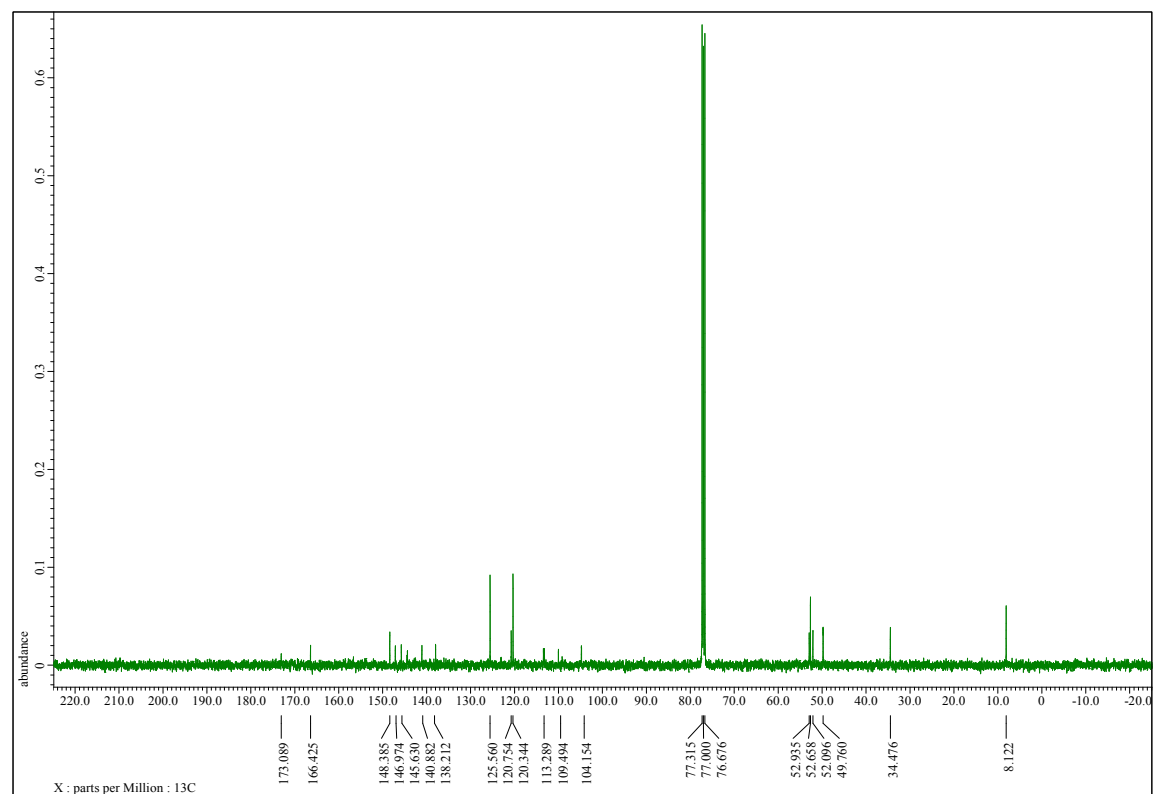
| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|-----------------|----------------------|
| 287.1367 | 2 | 778921.25 | C31 H33 F N6 O4 | (M+2H) ²⁺ |
| 287.6376 | 2 | 289348.32 | C31 H33 F N6 O4 | (M+2H) ²⁺ |
| 573.2643 | 1 | 4604809 | C31 H33 F N6 O4 | (M+H) ⁺ |
| 574.7876 | 1 | 1656201.71 | C31 H33 F N6 O4 | (M+H) ⁺ |
| 575.2682 | 1 | 353125.45 | C31 H33 F N6 O4 | (M+H) ⁺ |
| 585.246 | 1 | 279873.81 | C31 H33 F N6 O4 | (M+Na) ⁺ |
| 595.2487 | 1 | 96704 | C31 H33 F N6 O4 | (M+Na) ⁺ |
| 1143.5194 | 1 | 105373.3 | | (2M+H) ⁺ |
| 1167.5015 | 1 | 244892.14 | | (2M+Na) ⁺ |
| 1168.5049 | 1 | 175334.98 | | (2M+Na) ⁺ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4d):



^{13}C NMR (100MHz, CDCl_3) (4d):



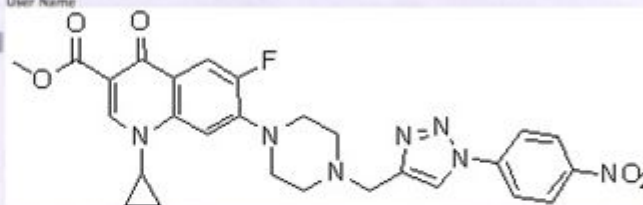
Qualitative Compound Report

Data File: RK-209.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Data XL.m
 IRM Calibration Status: Success
 Comment:

Sample Name: RK-209
 Position: P1-B1
 User Name:

Sample Group:
 Acquisition SW: 6200 series TOF/5500 series
 Version: Q-TOF B.05.01 (05125.1)

Info.

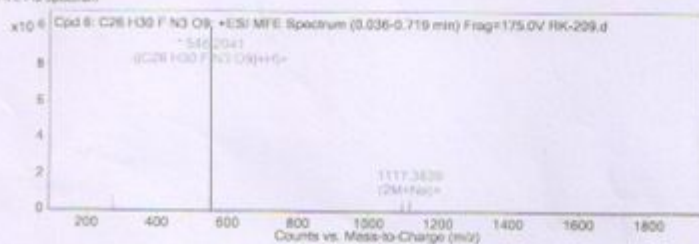


Compound Table

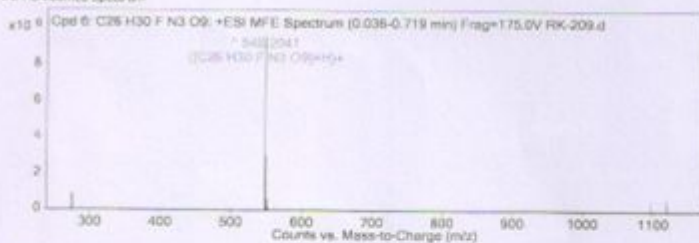
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|------------------------|-------|----------|-----------------|-----------------|----------------|-----------------|
| Cpd 6: C26 H30 F N3 O9 | 0.096 | 547.1964 | C26 H30 F N3 O9 | C26 H30 F N3 O9 | 0.35 | C26 H30 F N3 O9 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|-------|---------------------------|----------|
| Cpd 6: C26 H30 F N3 O9 | 548.2041 | 0.096 | Find by Molecular Feature | 547.1964 |

MFE MS Spectrum



MFE MS Zoomed Spectrum

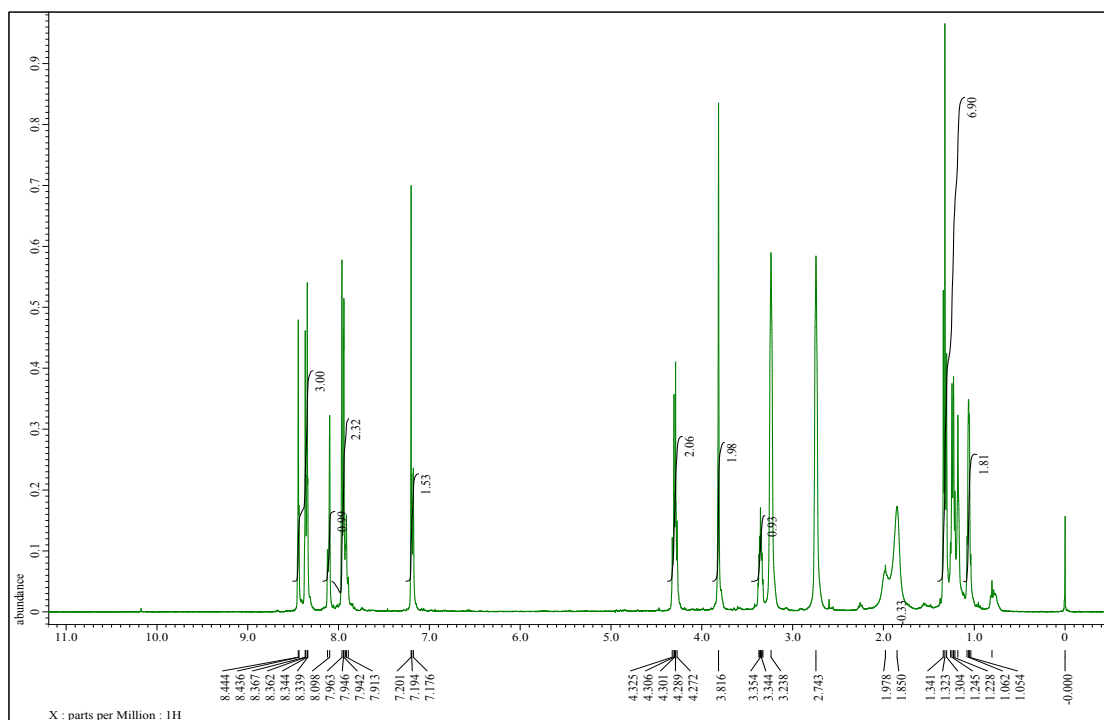


MS Spectrum Peak List

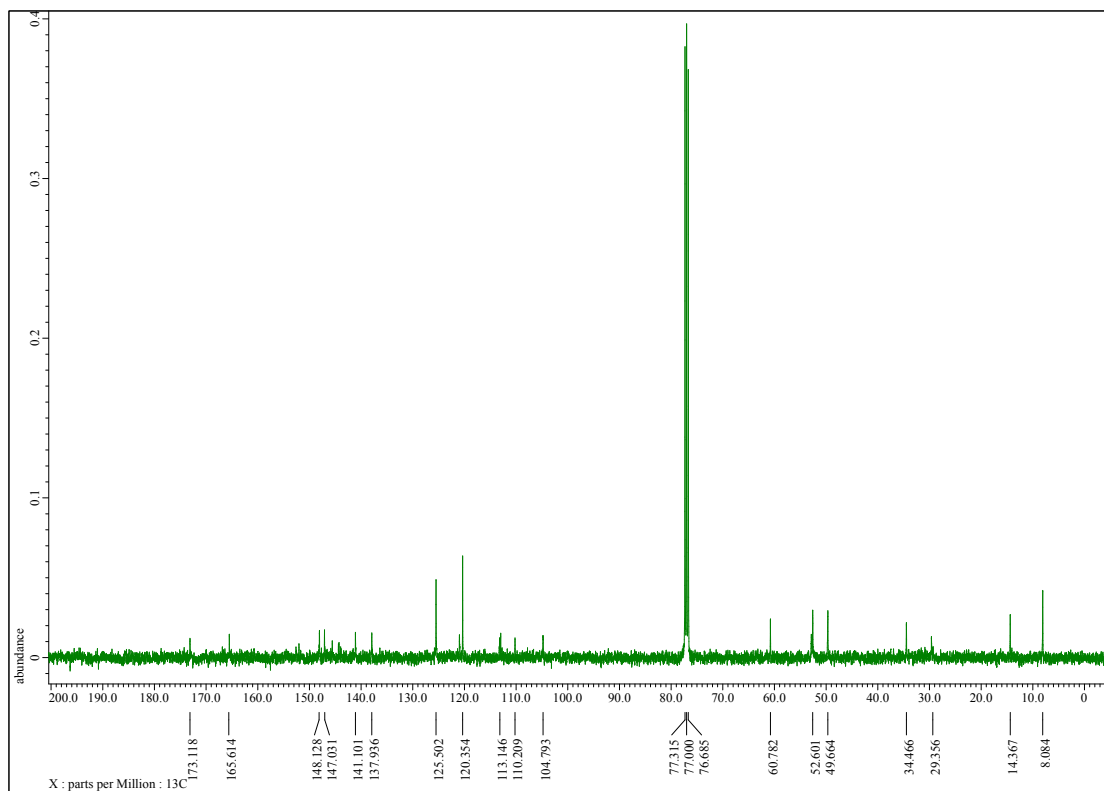
| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|-----------------|----------------------|
| 274.6056 | 2 | 796012.94 | C26 H30 F N3 O9 | (M+2H) ²⁺ |
| 275.1068 | 2 | 256414.09 | C26 H30 F N3 O9 | (M+2H) ²⁺ |
| 548.2041 | 1 | 9996801 | C26 H30 F N3 O9 | (M+H) ⁺ |
| 549.2673 | 1 | 3105845.64 | C26 H30 F N3 O9 | (M+H) ⁺ |
| 550.2087 | 1 | 581843.5 | C26 H30 F N3 O9 | (M+H) ⁺ |
| 1095.4015 | 1 | 474999.78 | | (2M+H) ⁺ |
| 1096.4044 | 1 | 301131.12 | | (2M+H) ⁺ |
| 1117.3839 | 1 | 695914.25 | | (2M+Na) ⁺ |
| 1118.3866 | 1 | 438854.79 | | (2M+Na) ⁺ |
| 1119.3889 | 1 | 148503.42 | | (2M+Na) ⁺ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4e):



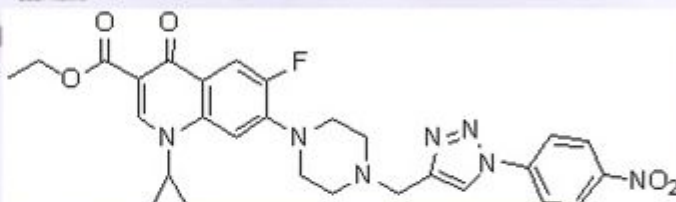
^{13}C NMR (100MHz, CDCl_3) (4e):



Qualitative Compound Report

Data File: RK-210.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo_3K.m
 IRM Calibration Status: Success
 Comment:
 Sample Group:
 Acquisition SW: 6200 series TOF/MS500 series
 Version: Q-TOF 8.05.01 (05125-1)

Sample Name: RK-210
 Position: P1-C3
 User Name:

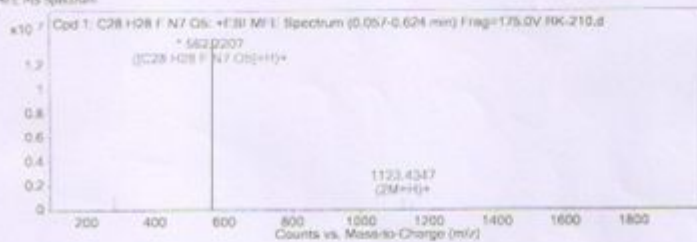


Compound Table

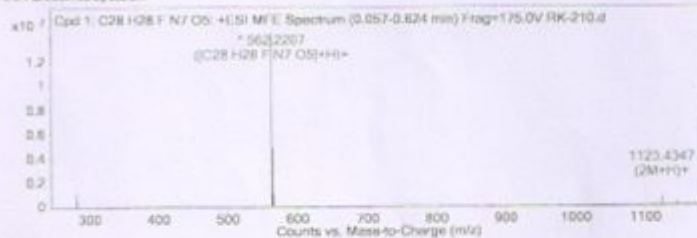
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|------------------------|-------|----------|-----------------|-----------------|----------------|-----------------|
| Cpd 1: C28 H28 F N7 O5 | 0.094 | 561.2133 | C28 H28 F N7 O5 | C28 H28 F N7 O5 | 0.55 | C28 H28 F N7 O5 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|-------|---------------------------|----------|
| Cpd 1: C28 H28 F N7 O5 | 562.2207 | 0.094 | Find by Molecular Feature | 561.2133 |

M/E MS Spectrum



M/E MS Zoomed Spectrum

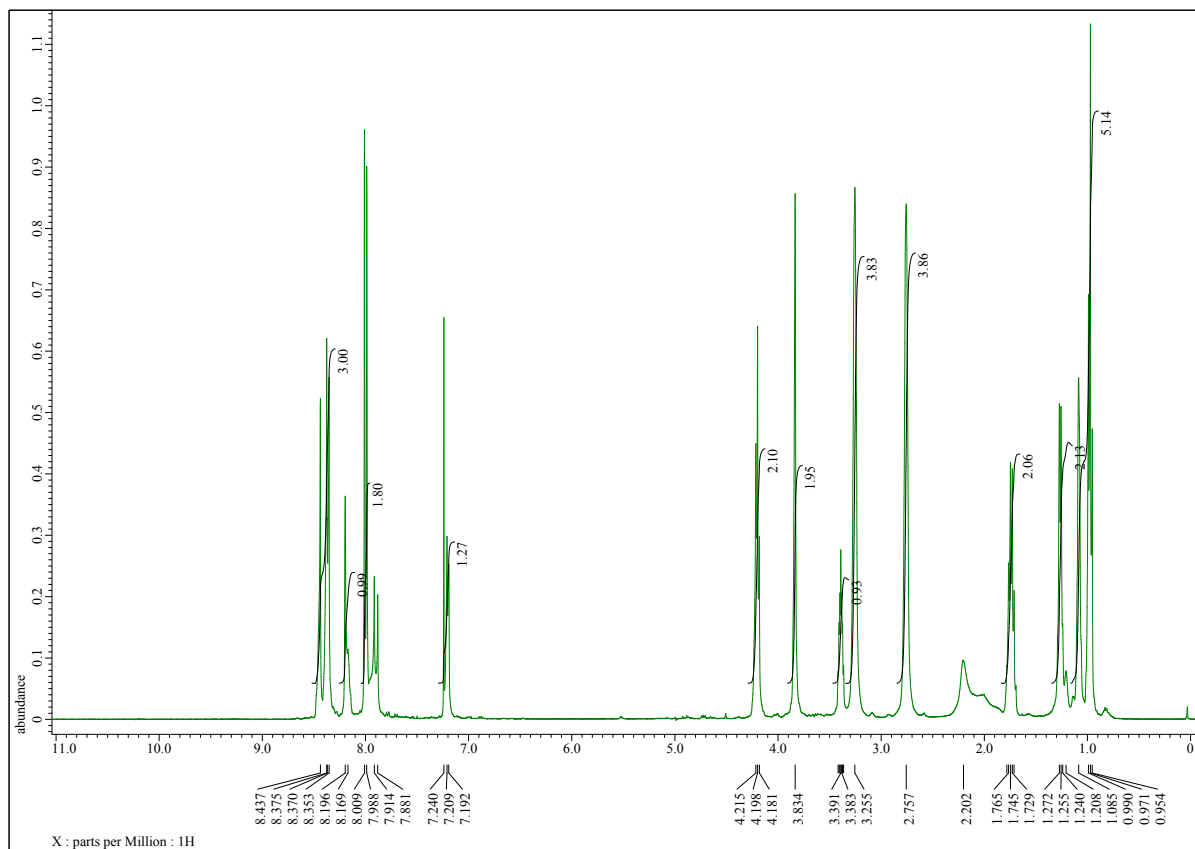


MS Spectrum Peak List

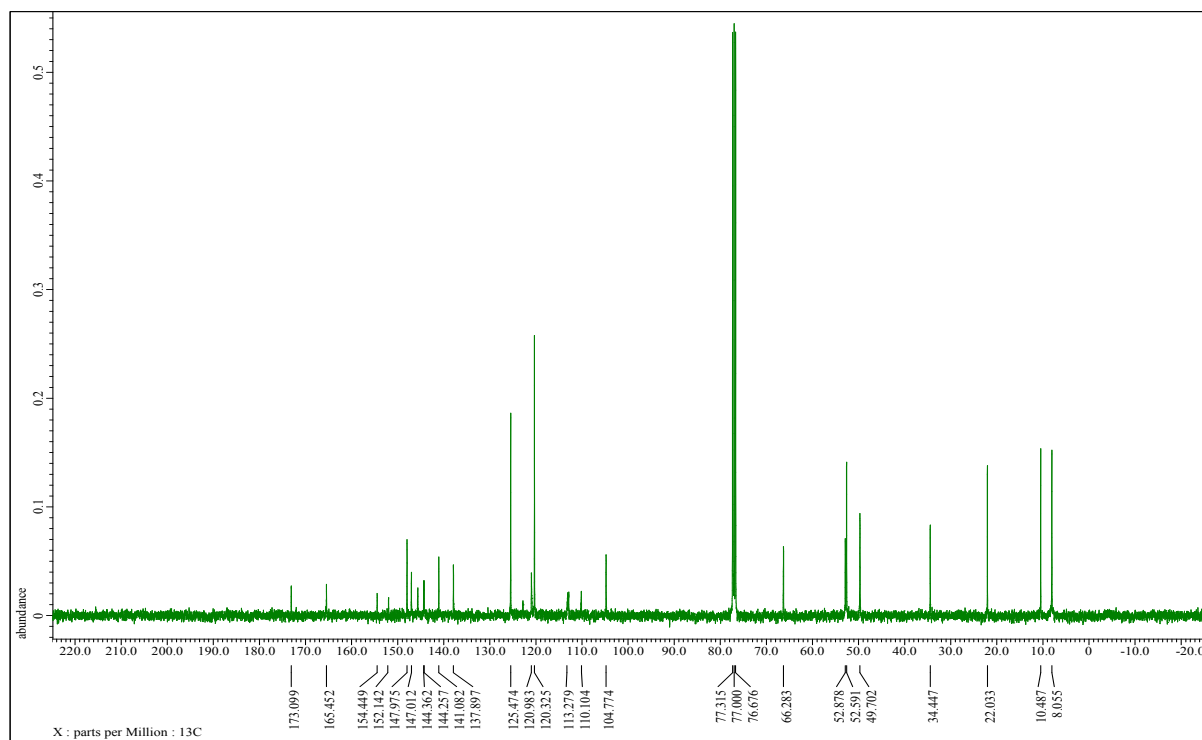
| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|-----------------|-----------|
| 281.6137 | 2 | 1080613.63 | C28 H28 F N7 O5 | [M+20]+2 |
| 282.115 | 2 | 379471.98 | C28 H28 F N7 O5 | [M+20]+2 |
| 562.2207 | 1 | 14387279 | C28 H28 F N7 O5 | [M+10]+ |
| 561.7227 | 1 | 4762086.58 | C28 H28 F N7 O5 | [M+10]+ |
| 564.2243 | 1 | 1042950.81 | C28 H28 F N7 O5 | [M+10]+ |
| 1123.4347 | 1 | 845899.54 | | [2M+10]+ |
| 1124.4372 | 1 | 372197.21 | | [2M+10]+ |
| 1125.439 | 1 | 708367.61 | | [2M+10]+ |
| 1145.4363 | 1 | 375576.34 | | [2M+16a]+ |
| 1146.4388 | 1 | 247862.56 | | [2M+16a]+ |

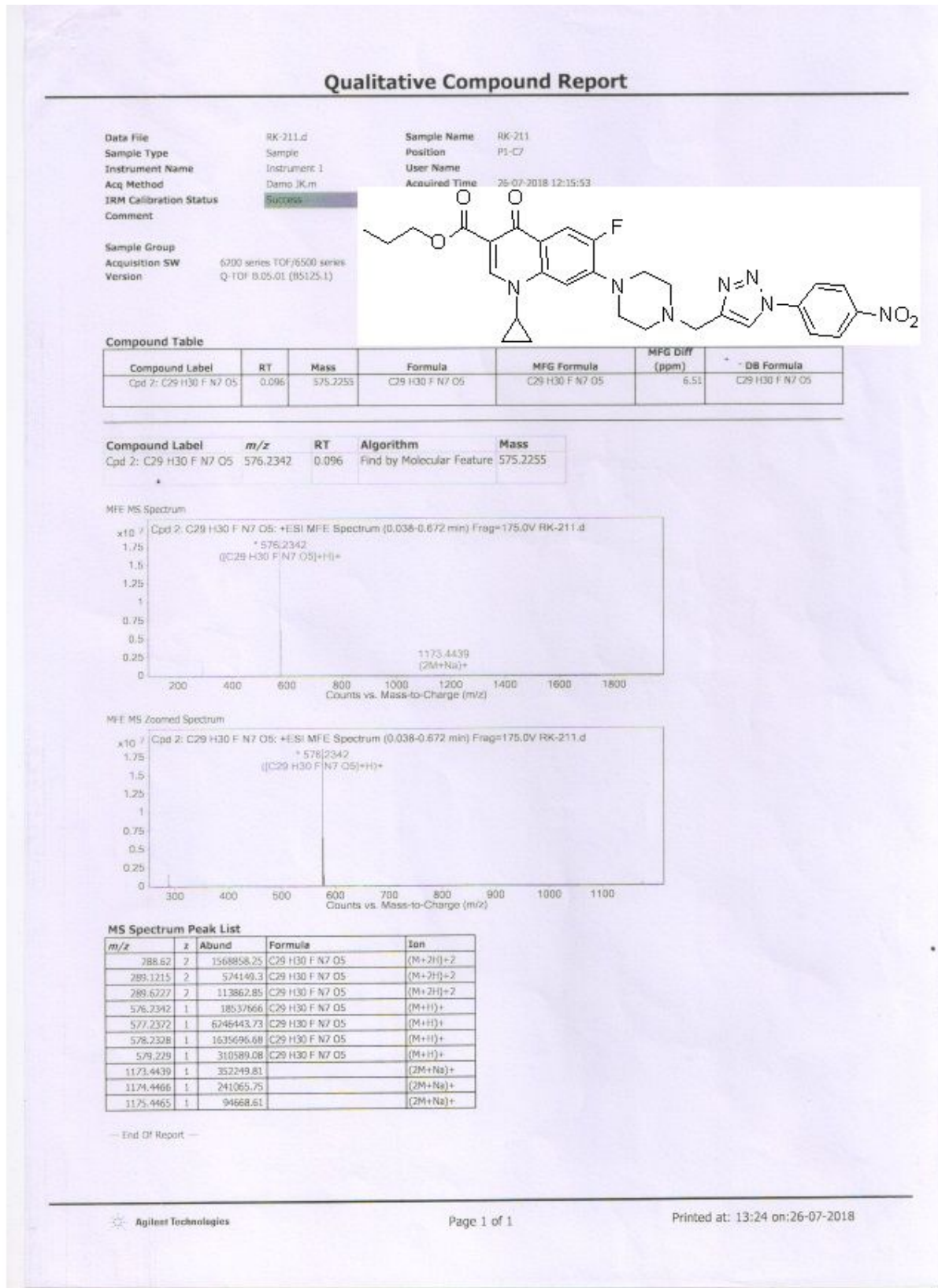
-- End Of Report --

^1H NMR (400MHz, CDCl_3) (4f):

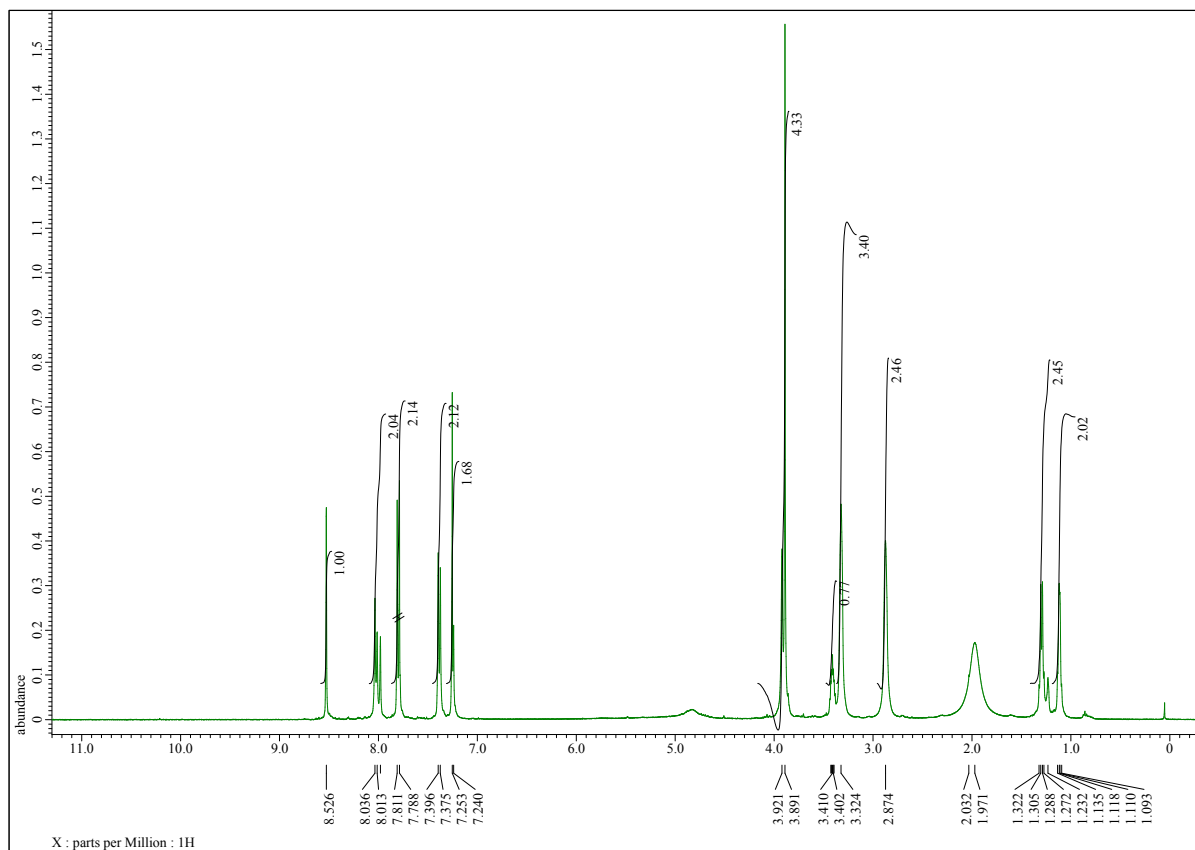


^{13}C NMR (100MHz, CDCl_3) (4f):

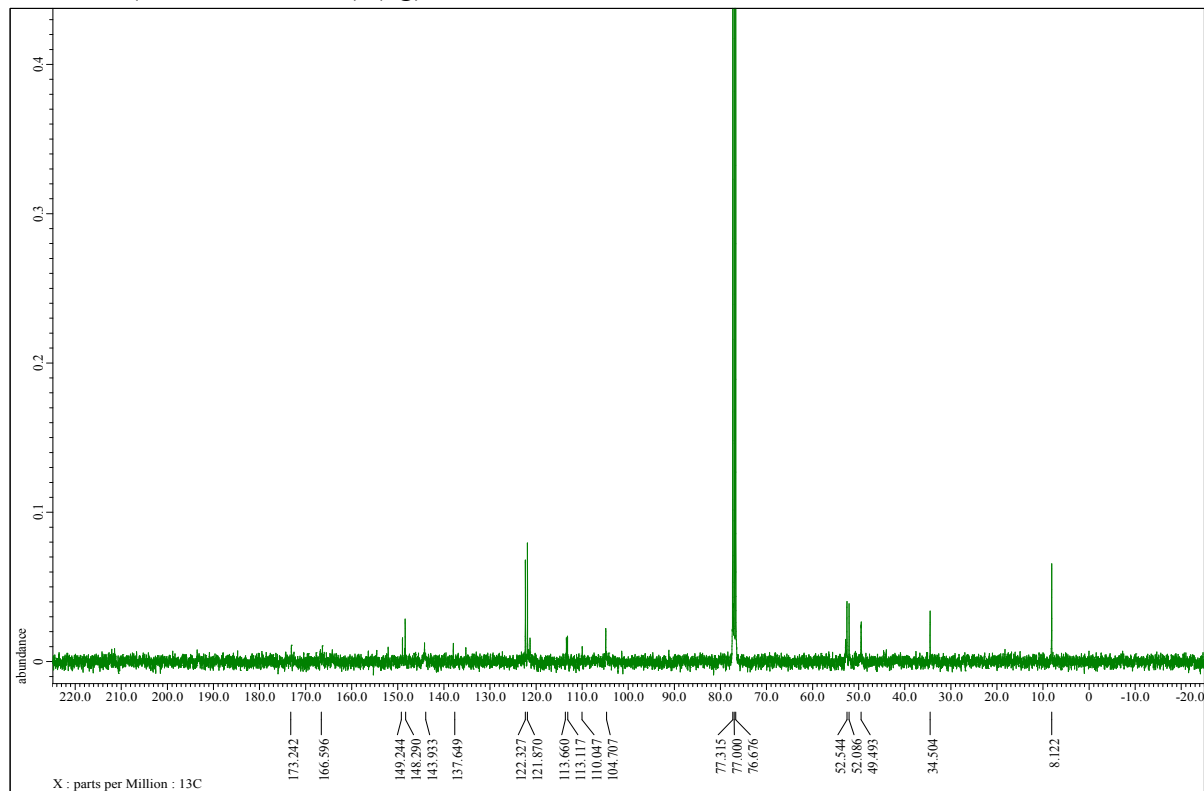




^1H NMR (400MHz, CDCl_3) (4g):



^{13}C NMR (100MHz, CDCl_3) (4g):



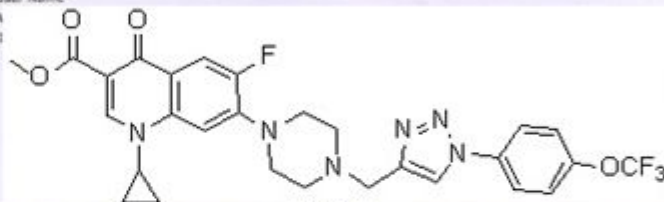
Qualitative Compound Report

Data File: RK-213.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo JK.m
 IRM Calibration Status: Success
 Comment:

Sample Name: RK-213
 Position: P1-E3
 User Name:

Sample Group:
 Acquisition SW: 6200 series TOF/MS00 Series
 Version: Q-ToF B.05.01 (05125.1)

Info.

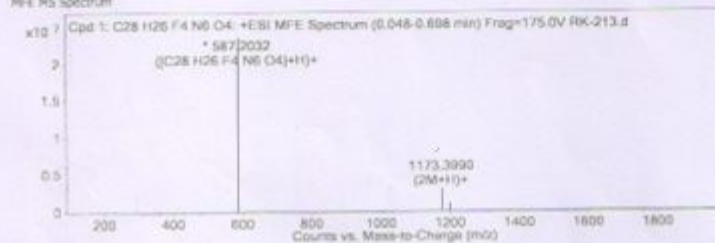


Compound Table

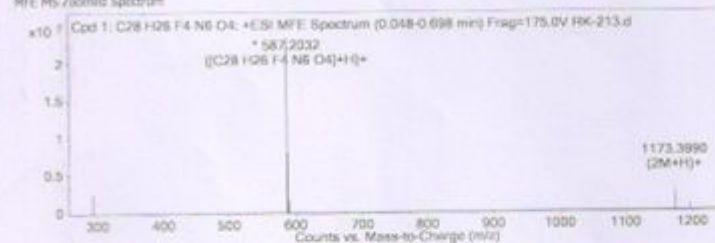
| Compound Label | RT | Mass | Formula | MFG Formula | MFu Unit (ppm) | DB Formula |
|-------------------------|-----|---------|------------------|------------------|----------------|------------------|
| Cpd 1: C28 H26 F4 N6 O4 | 0.1 | 586.196 | C28 H26 F4 N6 O4 | C28 H26 F4 N6 O4 | -1.43 | C28 H26 F4 N6 O4 |

| Compound Label | m/z | RT | Algorithm | Mass |
|-------------------------|----------|-----|---------------------------|---------|
| Cpd 1: C28 H26 F4 N6 O4 | 587.2032 | 0.1 | Find by Molecular Feature | 586.196 |

MFI MS Spectrum



MFE MS Zoomed Spectrum

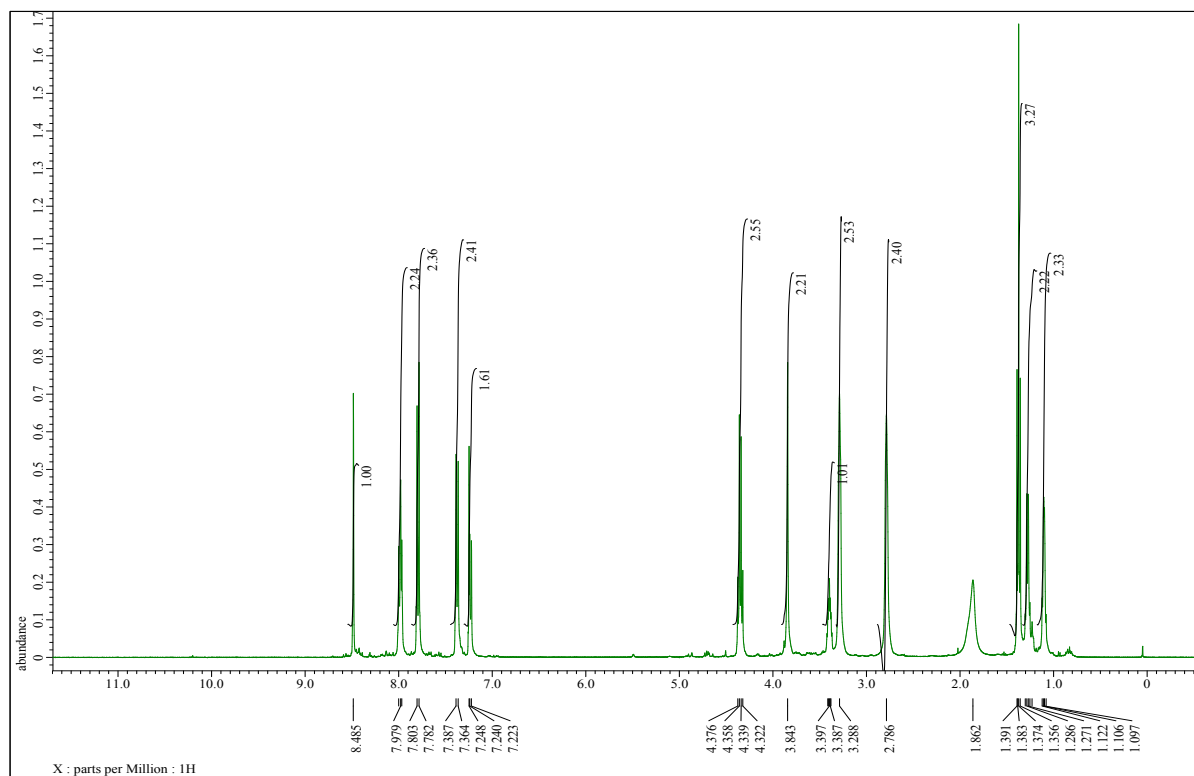


MS Spectrum Peak List

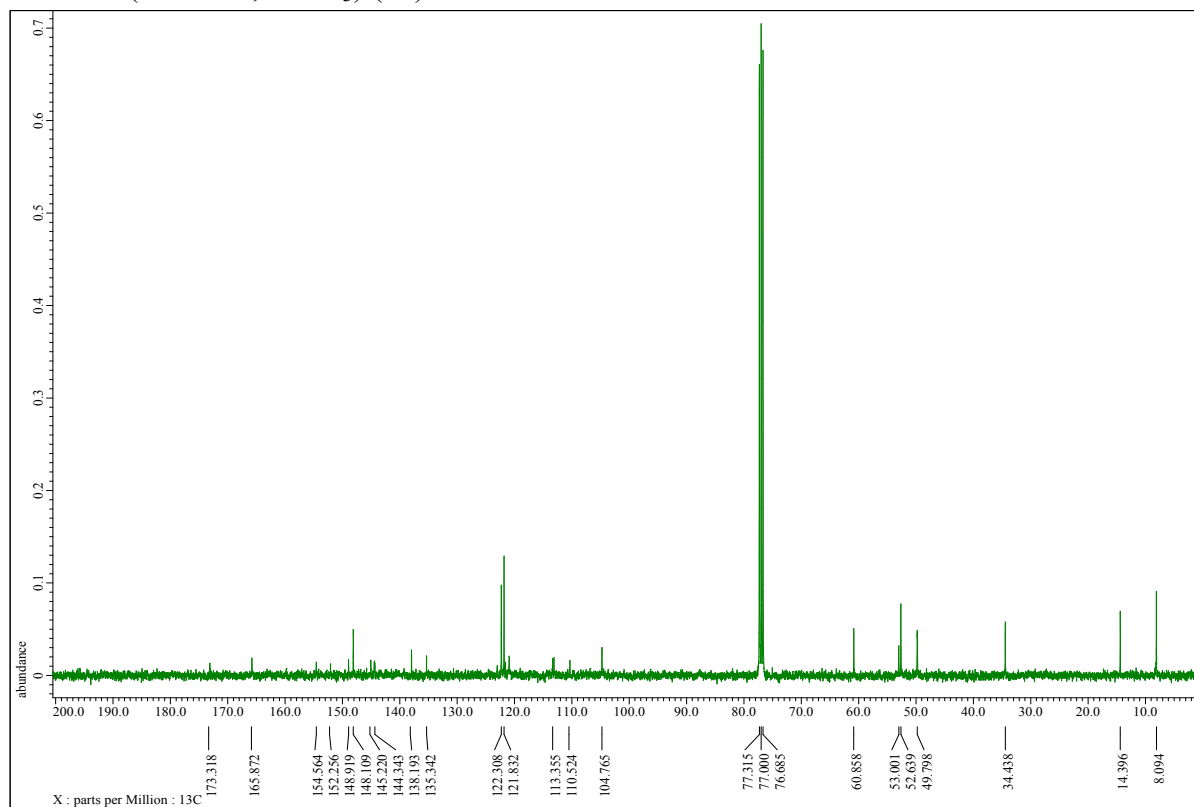
| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|------------------|----------------------|
| 294.1052 | 2 | 2413613 | C28 H26 F4 N6 O4 | (M+2H) ²⁺ |
| 294.607 | 2 | 832014.05 | C28 H26 F4 N6 O4 | (M+2H) ²⁺ |
| 587.2032 | 1 | 2333068 | C28 H26 F4 N6 O4 | (M+H) ⁺ |
| 588.2063 | 1 | 2548727.66 | C28 H26 F4 N6 O4 | (M+H) ⁺ |
| 589.2029 | 1 | 1728404.27 | C28 H26 F4 N6 O4 | (M+H) ⁺ |
| 1173.399 | 1 | 2863556.5 | | (2M+H) ⁺ |
| 1174.4024 | 1 | 1894933.18 | | (2M+H) ⁺ |
| 1175.4048 | 1 | 695657.05 | | (2M+H) ⁺ |
| 1195.3812 | 1 | 534554.75 | | (2M+Na) ⁺ |
| 1196.3841 | 1 | 619710.23 | | (2M+Na) ⁺ |

-- End Of Report --

^1H NMR (400MHz, CDCl_3) (4h):



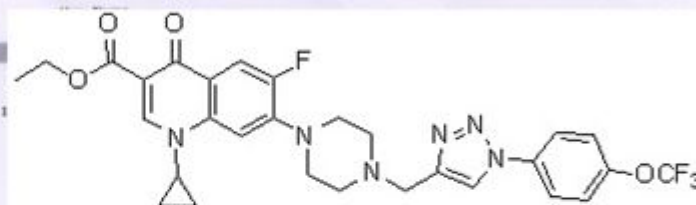
^{13}C NMR (100MHz, CDCl_3) (4h):



Qualitative Compound Report

Data File: RK-214.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo 3K.m
 IRM Calibration Status: Success
 Comment:
 Sample Group:
 Acquisition SW: 6200 series TOF/MS/MS series
 Version: Q-TOF 8.05.01 (05125.1)

Sample Name: RK-214
 Position: P1-77

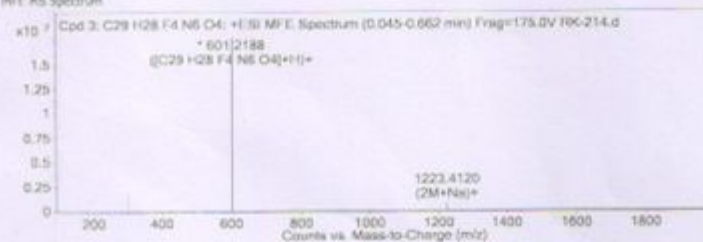


Compound Table

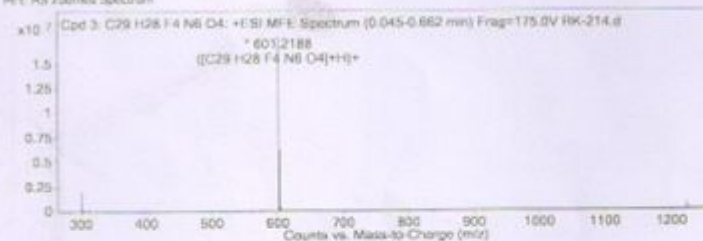
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|-------------------------|-------|----------|------------------|------------------|----------------|------------------|
| Cpd 3: C29 H28 F4 N6 O4 | 0.096 | 600.2118 | C29 H28 F4 N6 O4 | C29 H28 F4 N6 O4 | -1.28 | C29 H28 F4 N6 O4 |

| Compound Label | m/z | RT | Algorithm | Mass |
|-------------------------|----------|-------|---------------------------|----------|
| Cpd 3: C29 H28 F4 N6 O4 | 601.2188 | 0.096 | Find by Molecular Feature | 600.2116 |

MFE MS Spectrum



MFE MS Zoomed Spectrum

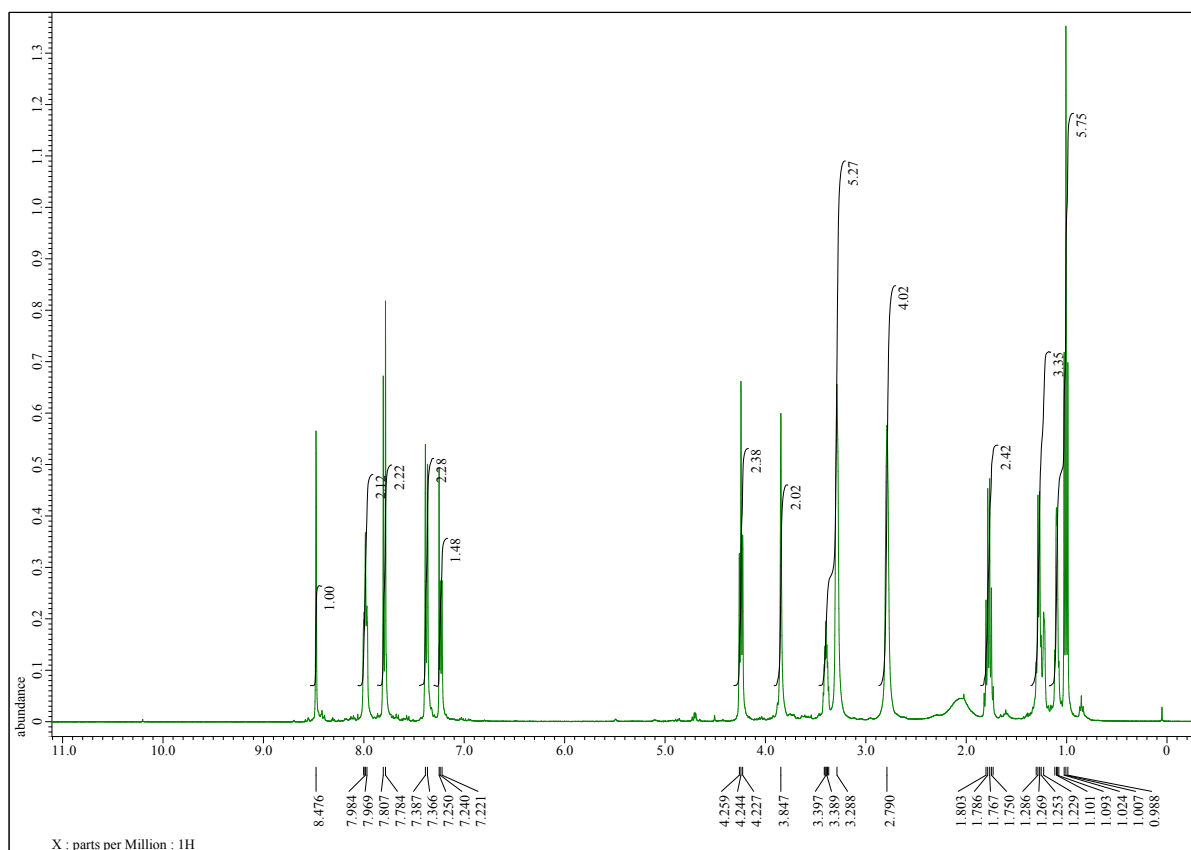


MS Spectrum Peak List

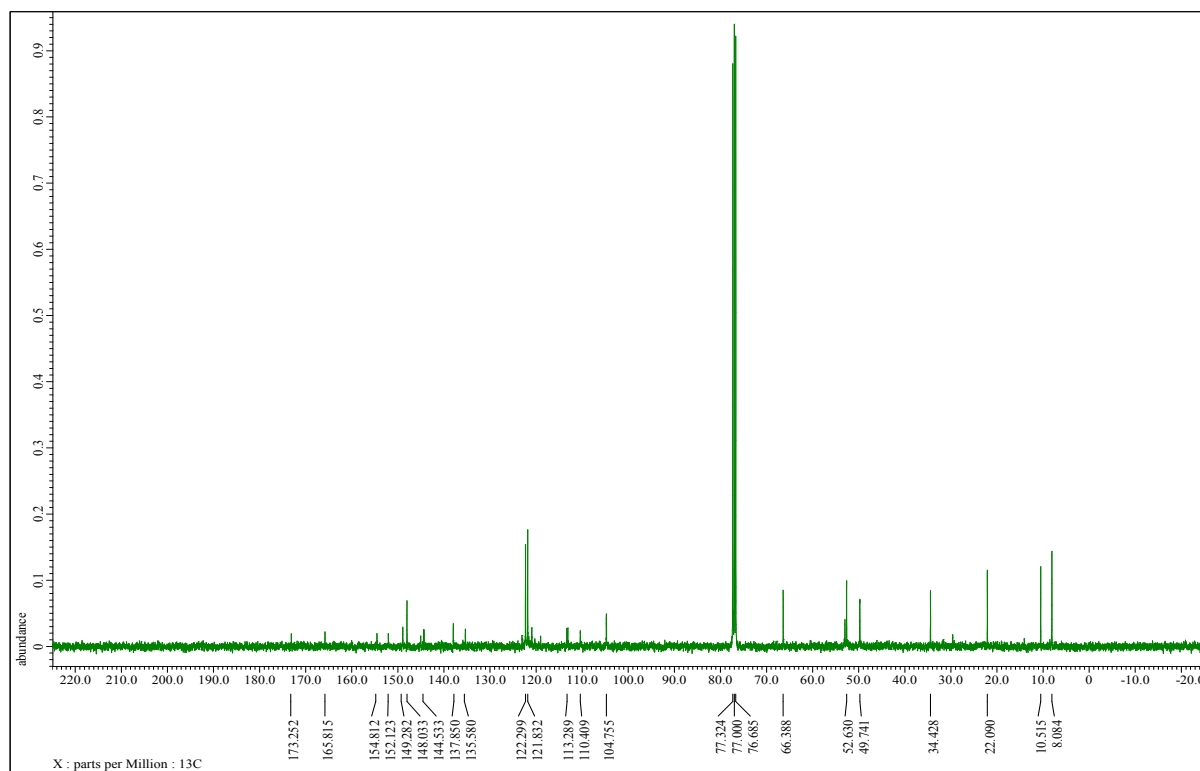
| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|------------------|----------|
| 301.1131 | 2 | 1980274.13 | C29 H28 F4 N6 O4 | (M+2H)+2 |
| 301.6146 | 2 | 713387 | C29 H28 F4 N6 O4 | (M+2H)+2 |
| 302.1158 | 2 | 134007.63 | C29 H28 F4 N6 O4 | (M+2H)+2 |
| 601.2188 | 1 | 17751898 | C29 H28 F4 N6 O4 | (M+H)+ |
| 602.2219 | 1 | 6074903.97 | C29 H28 F4 N6 O4 | (M+H)+ |
| 603.2159 | 1 | 1600136.88 | C29 H28 F4 N6 O4 | (M+H)+ |
| 604.2116 | 1 | 336915.82 | C29 H28 F4 N6 O4 | (M+H)+ |
| 1223.412 | 1 | 808314 | | (2M+N2)+ |
| 1224.4148 | 1 | 594606.62 | | (2M+N2)+ |
| 1225.4146 | 1 | 211569.69 | | (2M+N2)+ |

--- End Of Report ---

^1H NMR (400MHz, CDCl_3) (4i):



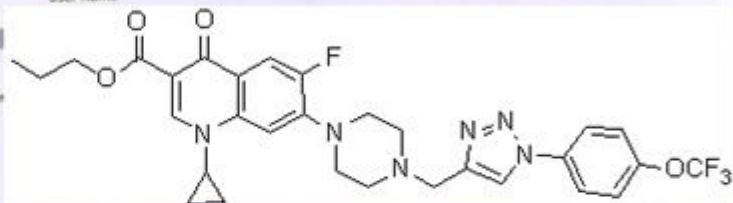
^{13}C NMR (100MHz, CDCl_3) (4i):



Qualitative Compound Report

Data File: RK-215.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Data JK.m
 IRM Calibration Status: Success
 Comment:
 Sample Group:
 Acquisition SW: 6200 series TOF/6500 series
 Version: Q-TOF R.05.01 (R0125-1)

Sample Name: RK-215
 Position: P1-01
 User Name:

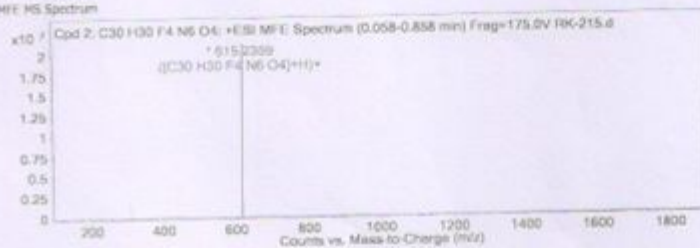


Compound Table

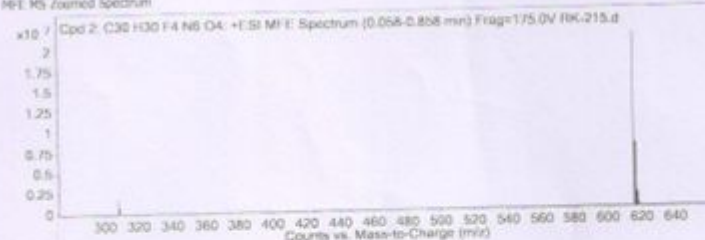
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|-------------------------|-------|----------|------------------|------------------|----------------|------------------|
| Cpd 2: C30 H30 F4 N6 O4 | 0.126 | 614.2292 | C30 H30 F4 N6 O4 | C30 H30 F4 N6 O4 | -4.45 | C30 H30 F4 N6 O4 |

| Compound Label | m/z | RT | Algorithm | Mass |
|-------------------------|----------|-------|---------------------------|----------|
| Cpd 2: C30 H30 F4 N6 O4 | 615.2359 | 0.126 | Find by Molecular Feature | 614.2292 |

MFE MS Spectrum



MFE MS Zoomed Spectrum

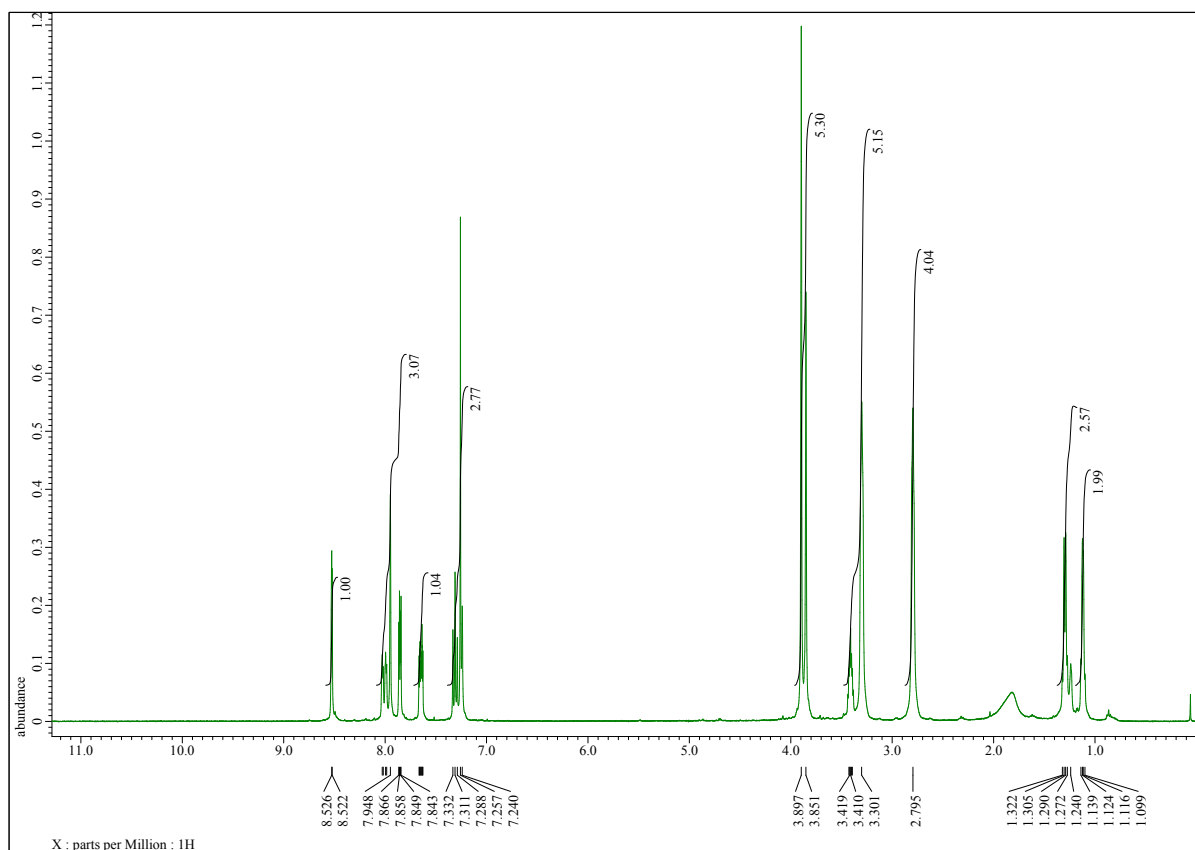


MS Spectrum Peak List

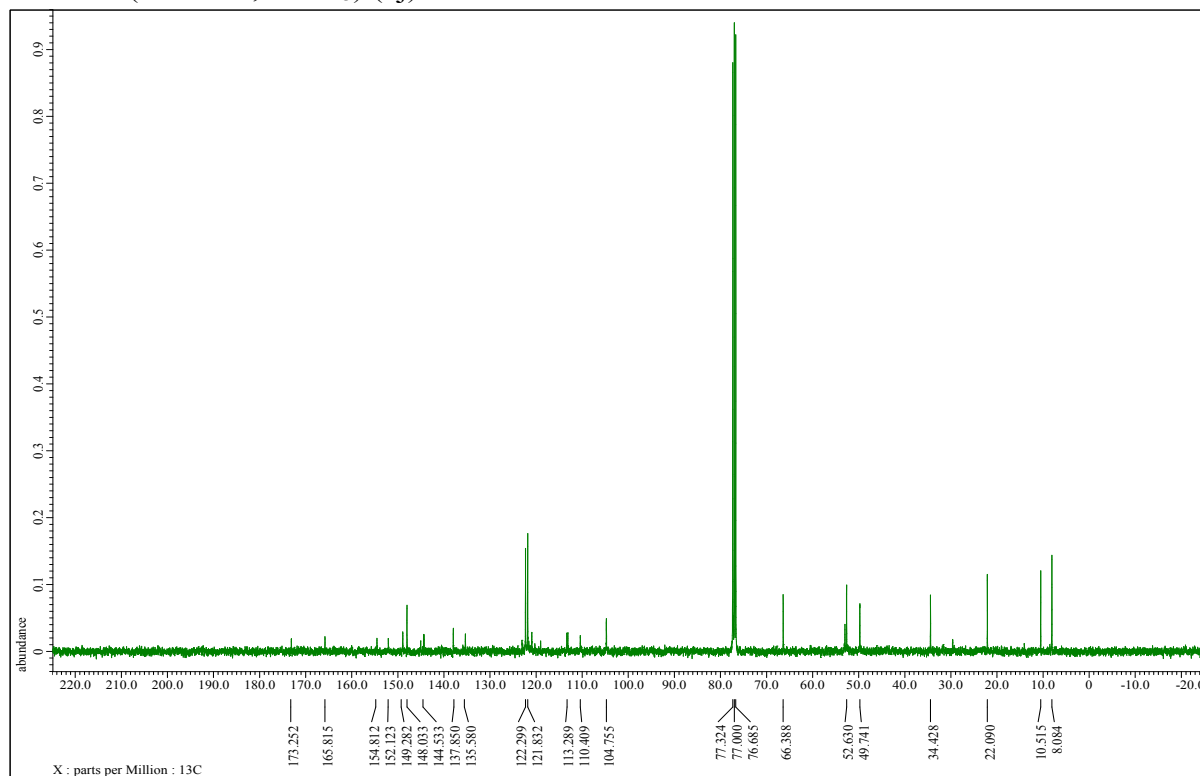
| m/z | z | Abund | Formula | Ion |
|----------|---|-------------|------------------|----------|
| 308.1219 | 2 | 1.780991.13 | C30 H30 F4 N6 O4 | (M+2H)+2 |
| 308.6234 | 2 | 6.30276.88 | C30 H30 F4 N6 O4 | (M+2H)+2 |
| 309.1245 | 2 | 12.0565.31 | C30 H30 F4 N6 O4 | (M+2H)+2 |
| 309.6259 | 2 | 18.700.14 | C30 H30 F4 N6 O4 | (M+2H)+2 |
| 615.2359 | 1 | 71.28575.7 | C30 H30 F4 N6 O4 | (M+H)+ |
| 616.239 | 1 | 241.3776.39 | C30 H30 F4 N6 O4 | (M+H)+ |
| 617.2318 | 1 | 205.7178.09 | C30 H30 F4 N6 O4 | (M+H)+ |
| 618.2276 | 1 | 421046.95 | C30 H30 F4 N6 O4 | (M+H)+ |
| 619.2263 | 1 | 66993.83 | C30 H30 F4 N6 O4 | (M+H)+ |
| 620.2283 | 1 | 18694.97 | C30 H30 F4 N6 O4 | (M+H)+ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4j):



^{13}C NMR (100MHz, CDCl_3) (4j):

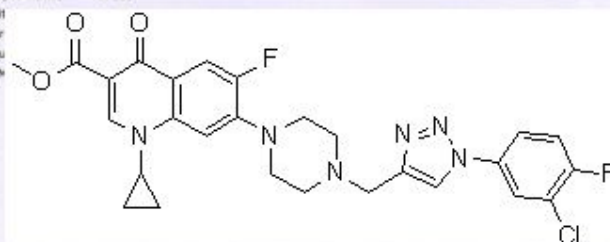


Qualitative Compound Report

Data File: RK-216.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo JK.m
 IRM Calibration Status: Success
 Comment:

Sample Name: RK-216
 Posit:
 User:
 Acq:
 DA M:

Sample Group:
 Acquisition SW: 6200 series TOF/6500 series
 Version: Q-TOF B.05.01 (B5125.1)

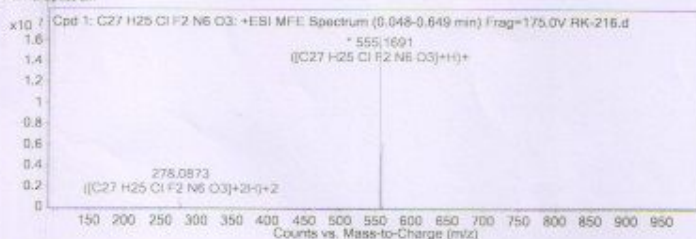


Compound Table

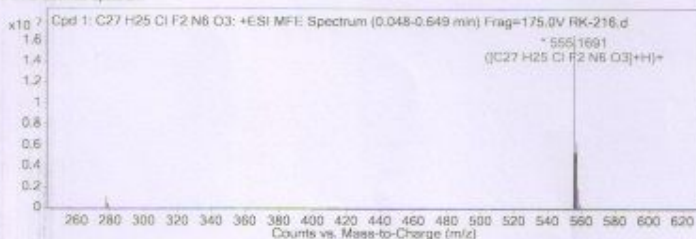
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|----------------------------|-------|----------|---------------------|---------------------|----------------|---------------------|
| Cpd 1: C27 H25 Cl F2 N6 O3 | 0.098 | 554.1615 | C27 H25 Cl F2 N6 O3 | C27 H25 Cl F2 N6 O3 | 5.31 | C27 H25 Cl F2 N6 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|----------------------------|----------|-------|---------------------------|----------|
| Cpd 1: C27 H25 Cl F2 N6 O3 | 555.1691 | 0.098 | Find by Molecular Feature | 554.1615 |

MFE MS Spectrum



MFE MS Zoomed Spectrum

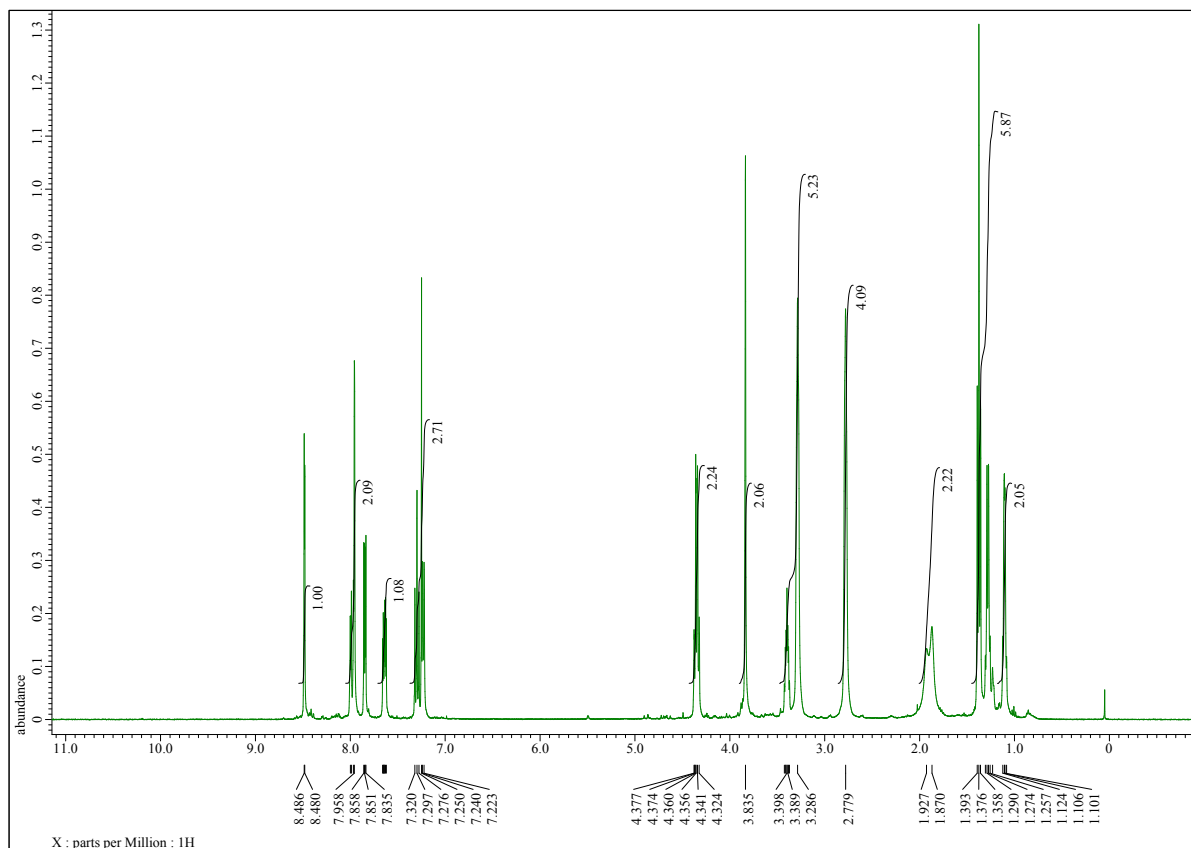


MS Spectrum Peak List

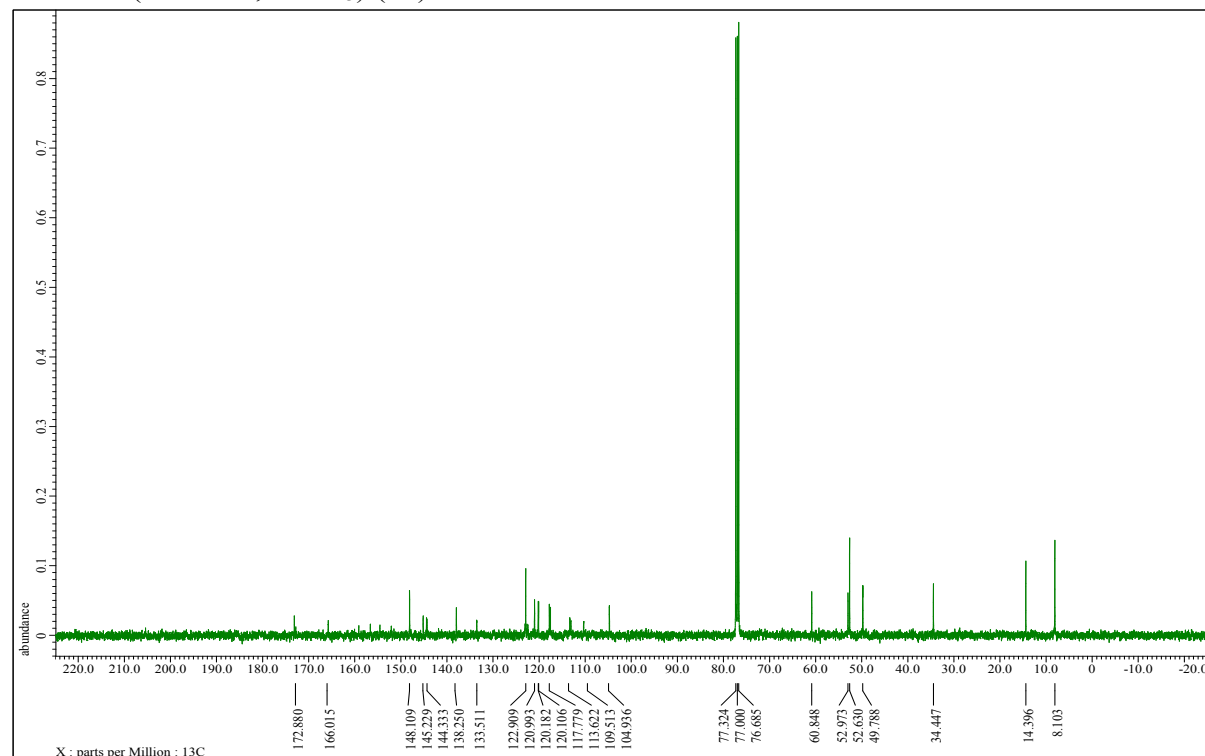
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|---------------------|----------|
| 278.0873 | 2 | 100778.81 | C27 H25 Cl F2 N6 O3 | (M+2H)+2 |
| 278.5885 | 2 | 378919.06 | C27 H25 Cl F2 N6 O3 | (M+2H)+2 |
| 279.0864 | 2 | 384401.68 | C27 H25 Cl F2 N6 O3 | (M+2H)+2 |
| 279.5872 | 2 | 110633.91 | C27 H25 Cl F2 N6 O3 | (M+2H)+2 |
| 555.1691 | 1 | 16964043 | C27 H25 Cl F2 N6 O3 | (M+H)+ |
| 555.172 | 1 | 5736108.86 | C27 H25 Cl F2 N6 O3 | (M+H)+ |
| 557.1666 | 1 | 6292320.78 | C27 H25 Cl F2 N6 O3 | (M+H)+ |
| 558.169 | 1 | 1851844.14 | C27 H25 Cl F2 N6 O3 | (M+H)+ |
| 559.1664 | 1 | 365034.67 | C27 H25 Cl F2 N6 O3 | (M+H)+ |
| 560.1621 | 1 | 58394.26 | C27 H25 Cl F2 N6 O3 | (M+H)+ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4k):



^{13}C NMR (100MHz, CDCl_3) (4k)

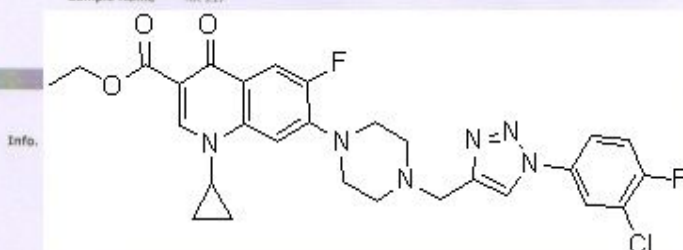


Qualitative Compound Report

Data File: RK-217.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo JK.m
 IRM Calibration Status: Success
 Comment:

Sample Name: RK-217

Sample Group:
 Acquisition SW: 6200 series TOF/6500 series
 Version: Q-TOF B.05.01 (HS125.1)

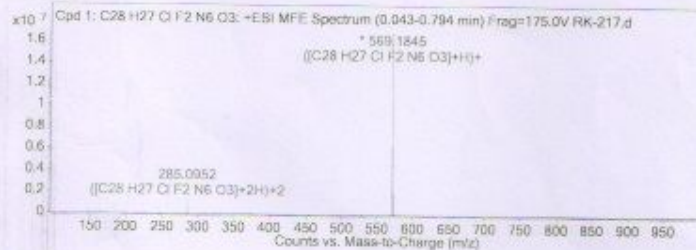


Compound Table

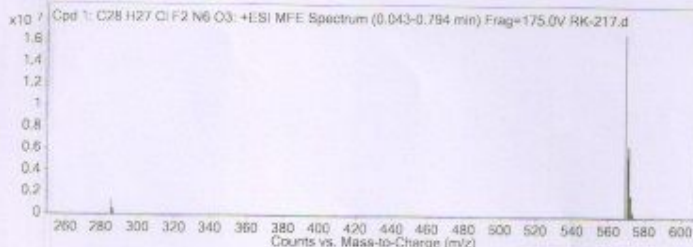
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|----------------------------|-------|----------|---------------------|---------------------|----------------|---------------------|
| Cpd 1: C28 H27 Cl F2 N6 O3 | 0.101 | 568.1773 | C28 H27 Cl F2 N6 O3 | C28 H27 Cl F2 N6 O3 | 4.99 | C28 H27 Cl F2 N6 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|----------------------------|----------|-------|---------------------------|----------|
| Cpd 1: C28 H27 Cl F2 N6 O3 | 569.1845 | 0.101 | Find by Molecular Feature | 568.1773 |

MFE MS Spectrum



MFE MS Zoomed Spectrum

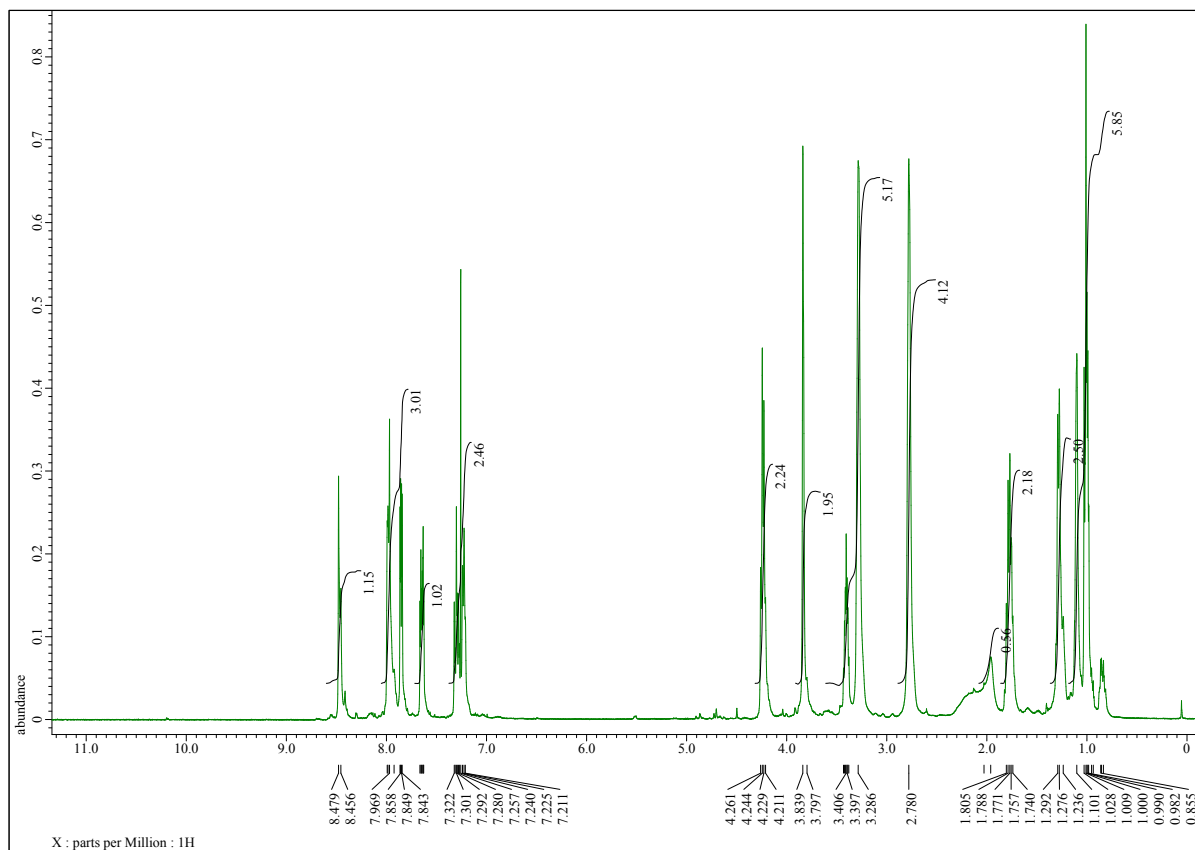


MS Spectrum Peak List

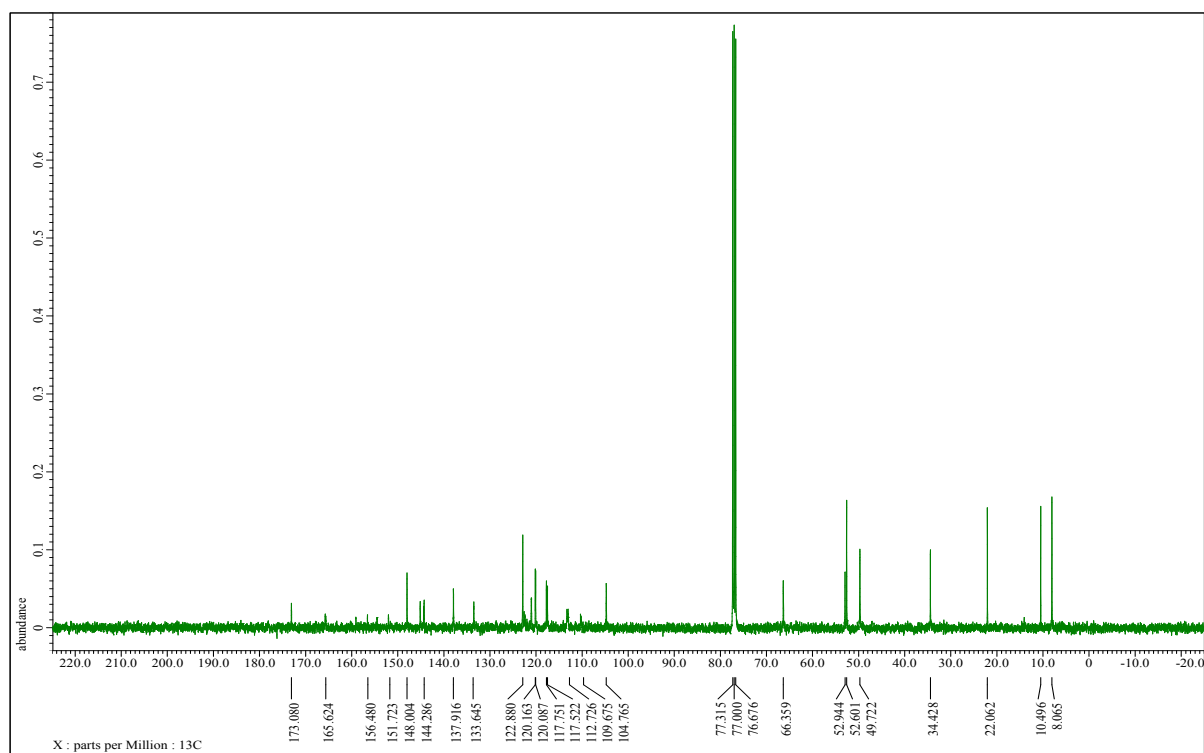
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|---------------------|----------|
| 285.0952 | 2 | 1318661.75 | C28 H27 Cl F2 N6 O3 | (M+2H)+2 |
| 285.5965 | 2 | 428011.33 | C28 H27 Cl F2 N6 O3 | (M+2H)+2 |
| 286.0943 | 2 | 500830.47 | C28 H27 Cl F2 N6 O3 | (M+2H)+2 |
| 286.5952 | 2 | 152558.64 | C28 H27 Cl F2 N6 O3 | (M+2H)+2 |
| 569.1845 | 1 | 16861050 | C28 H27 Cl F2 N6 O3 | (M+H)+ |
| 570.1878 | 1 | 5598747.26 | C28 H27 Cl F2 N6 O3 | (M+H)+ |
| 571.1829 | 1 | 6339970.97 | C28 H27 Cl F2 N6 O3 | (M+H)+ |
| 572.1854 | 1 | 1979875.38 | C28 H27 Cl F2 N6 O3 | (M+H)+ |
| 573.186 | 1 | 368464.47 | C28 H27 Cl F2 N6 O3 | (M+H)+ |
| 574.185 | 1 | 49790.05 | C28 H27 Cl F2 N6 O3 | (M+H)+ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4l):



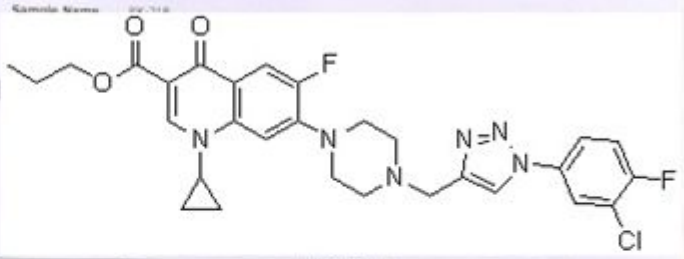
^{13}C NMR (100MHz, CDCl_3) (4l):



Qualitative Compound Report

Data File: RK-218.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Data 3K.m
 IRM Calibration Status: Success
 Comment:

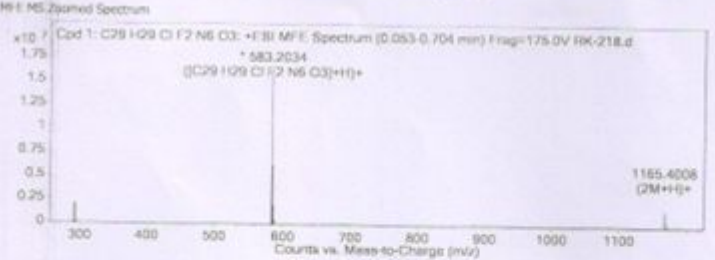
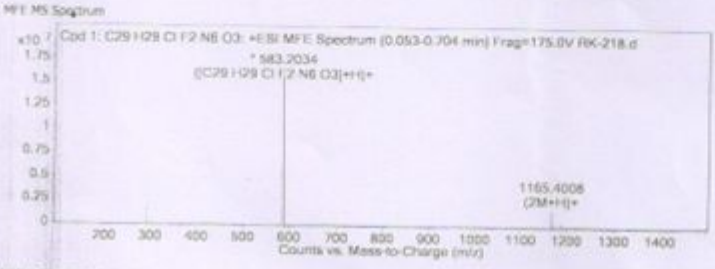
Sample Group: Info.
 Acquisition SW: 6.00 series 100/6500 series
 Version: Q-TOF 8.05.01 (R5125.1)



Compound Table

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|--|-------|---------|---|---|----------------|---|
| Cpd 1: C ₂₉ H ₂₉ O ₃ F ₂ N ₆ O ₃ | 0.095 | 583.196 | C ₂₉ H ₂₉ O ₃ F ₂ N ₆ O ₃ | C ₂₉ H ₂₉ O ₃ F ₂ N ₆ O ₃ | -6.33 | C ₂₉ H ₂₉ O ₃ F ₂ N ₆ O ₃ |

| Compound Label | m/z | RT | Algorithm | Mass |
|--|----------|-------|---------------------------|---------|
| Cpd 1: C ₂₉ H ₂₉ O ₃ F ₂ N ₆ O ₃ | 583.2034 | 0.095 | Find by Molecular Feature | 583.196 |

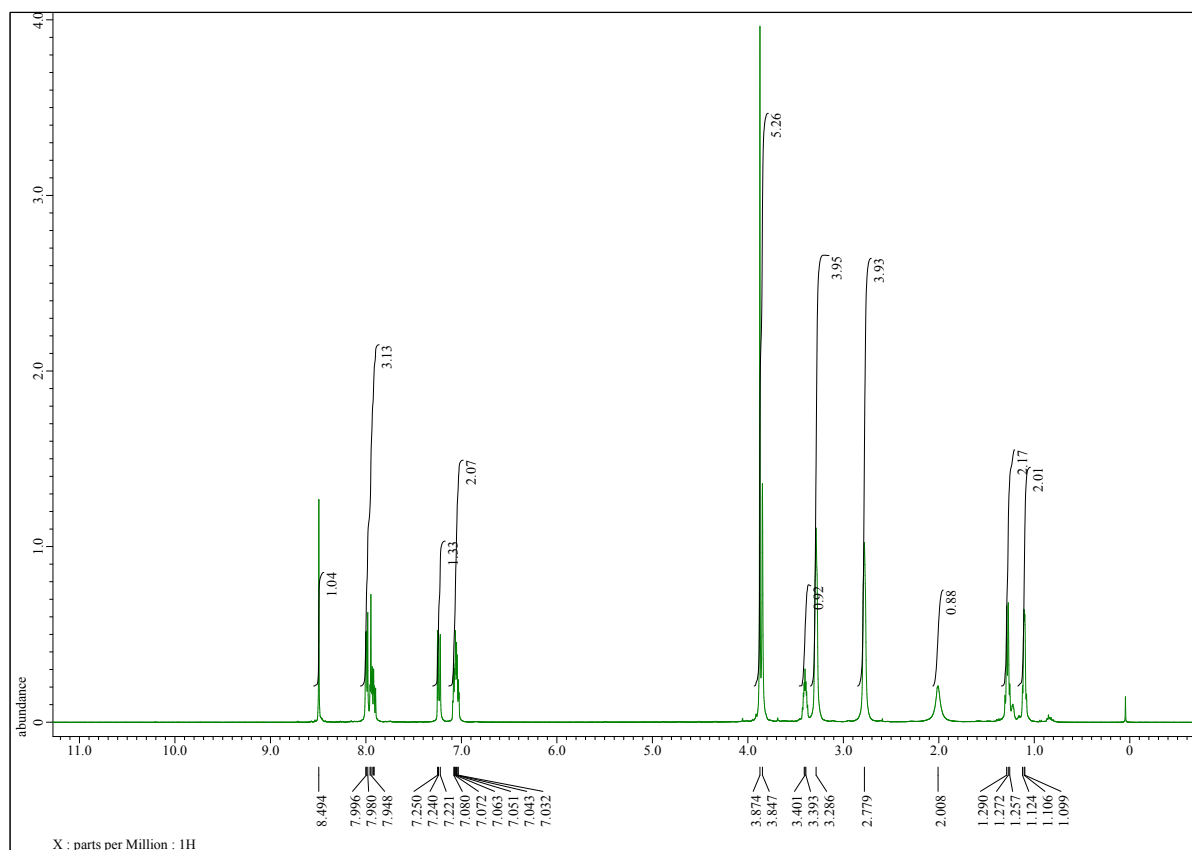


MS Spectrum Peak List

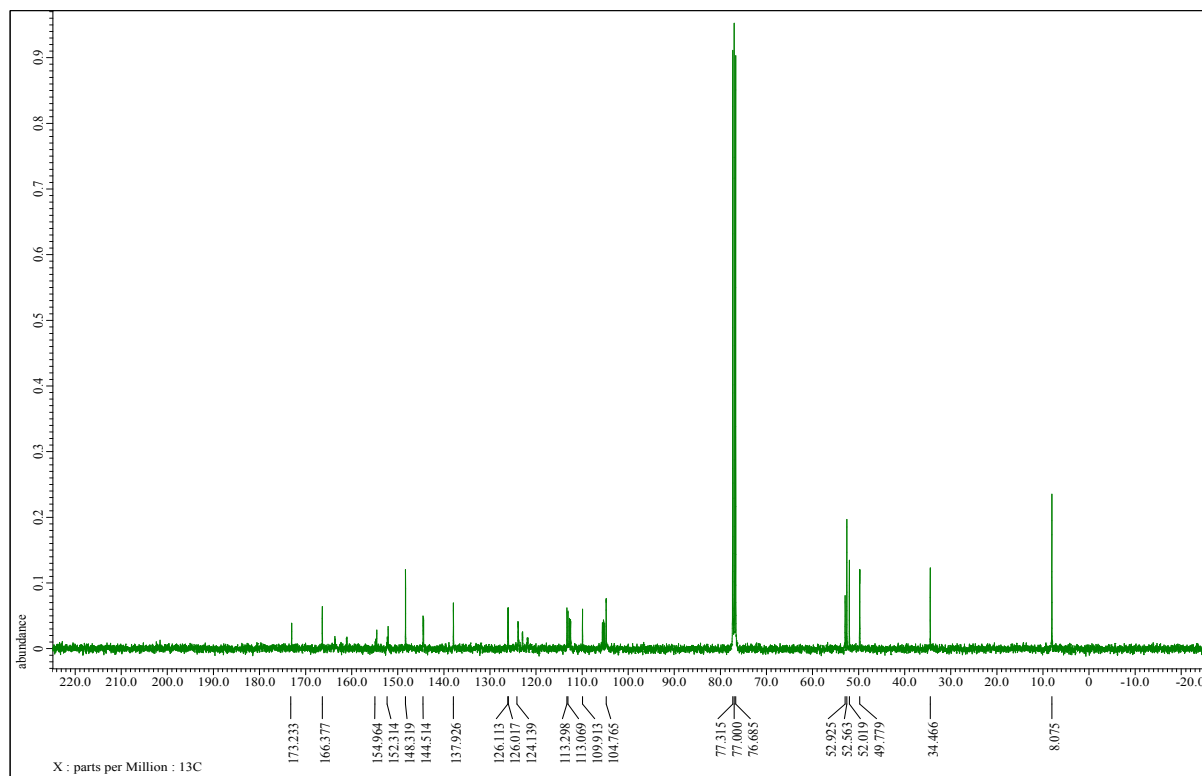
| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|---|----------------------|
| 202.1055 | 2 | 193015.38 | C ₉ H ₉ O ₃ F ₂ N ₆ O ₃ | (M+2H) ²⁺ |
| 293.1048 | 2 | 75482.32 | C ₉ H ₉ O ₃ F ₂ N ₆ O ₃ | (M+2H) ²⁺ |
| 583.2034 | 1 | 1588707 | C ₂₉ H ₂₉ O ₃ F ₂ N ₆ O ₃ | (M+H) ⁺ |
| 585.2067 | 1 | 5388134.93 | C ₂₉ H ₂₉ O ₃ F ₂ N ₆ O ₃ | (M+H) ⁺ |
| 585.2014 | 1 | 604468.87 | C ₂₉ H ₂₉ O ₃ F ₂ N ₆ O ₃ | (M+H) ⁺ |
| 586.2038 | 1 | 1939405.09 | C ₂₉ H ₂₉ O ₃ F ₂ N ₆ O ₃ | (M+H) ⁺ |
| 1165.4008 | 1 | 178899 | | (2M+H) ⁺ |
| 1166.4042 | 1 | 1230669.27 | | (2M+H) ⁺ |
| 1167.4003 | 1 | 158146.18 | | (2M+H) ⁺ |
| 1168.402 | 1 | 901856.32 | | (2M+H) ⁺ |

End Of Report

^1H NMR (400MHz, CDCl_3) (4m):



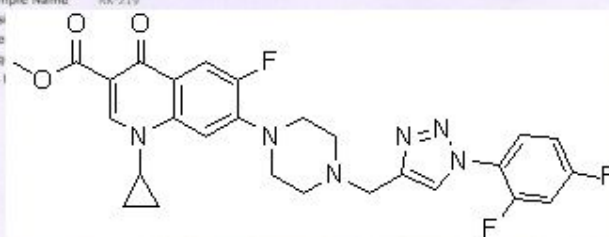
^{13}C NMR (100MHz, CDCl_3) (4m):



Qualitative Compound Report

Data File: RK-219.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Demo_KJ.m
 IRM Calibration Status: Success
 Comment:
 Sample Group:
 Acquisition SW: 6700 series TOF/6500 series
 Version: Q-TOF B.05.01 (85125.1)

Sample Name: RK-219
 Posi:
 Use:
 Acq: DA1

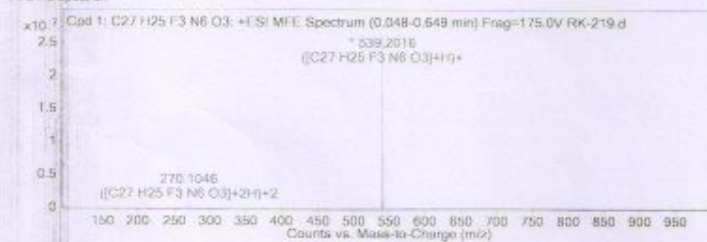


Compound Table

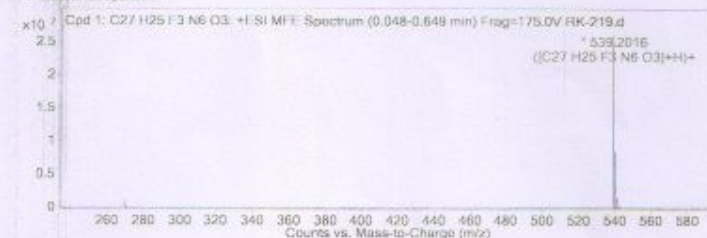
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|-------------------------|-------|----------|------------------|------------------|----------------|------------------|
| Cpd 1: C27 H25 F3 N6 O3 | 0.099 | 538.1946 | C27 H25 F3 N6 O3 | C27 H25 F3 N6 O3 | -1 | C27 H25 F3 N6 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|-------------------------|----------|-------|---------------------------|----------|
| Cpd 1: C27 H25 F3 N6 O3 | 539.2016 | 0.099 | Find by Molecular Feature | 538.1946 |

MFE MS Spectrum



MFE MS Zoomed Spectrum

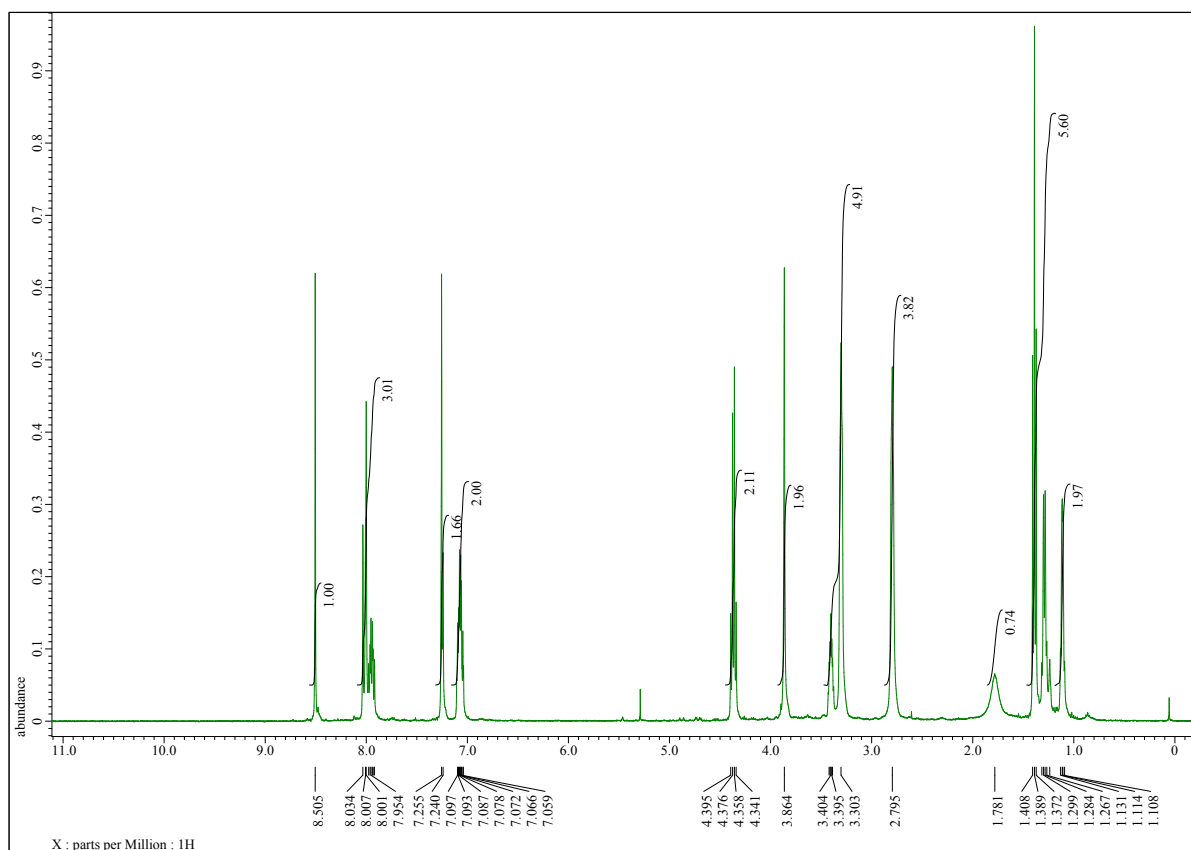


MS Spectrum Peak List

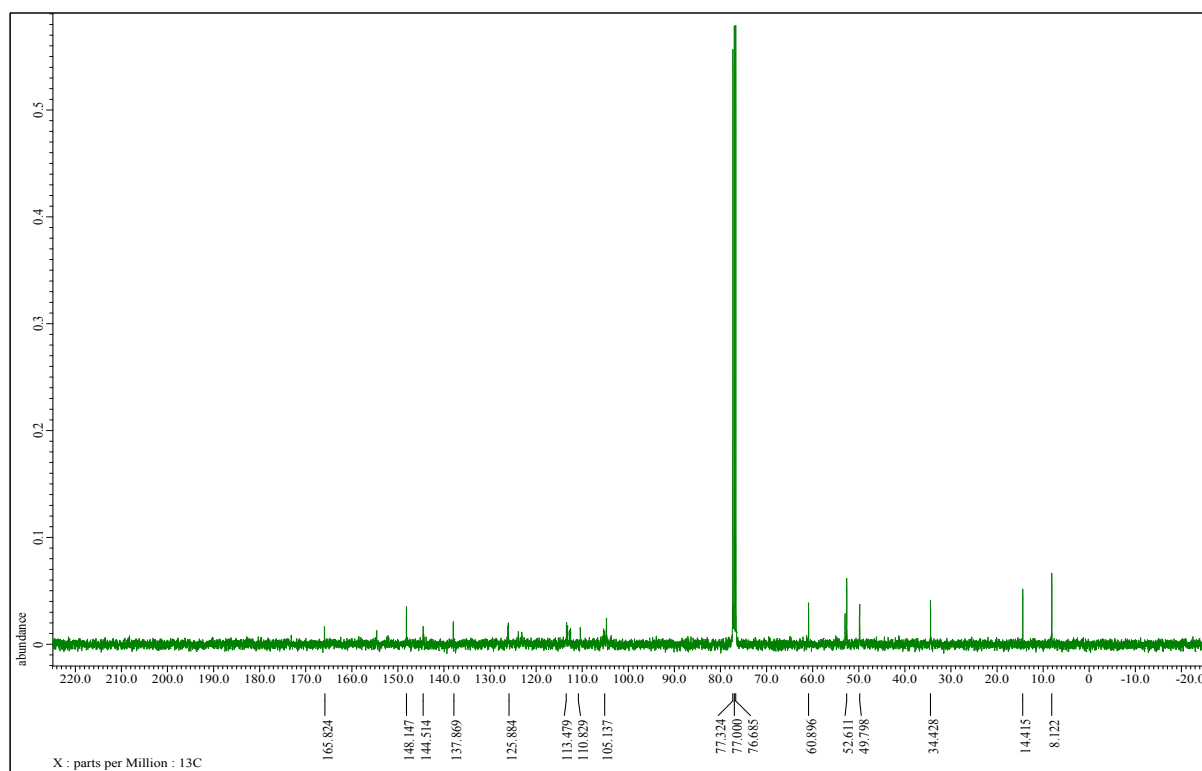
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|------------------|----------|
| 270.1046 | 2 | 892223.19 | C27 H25 F3 N6 O3 | (M+2H)+2 |
| 270.606 | 2 | 286426.11 | C27 H25 F3 N6 O3 | (M+2H)+2 |
| 271.107 | 2 | 51835.87 | C27 H25 F3 N6 O3 | (M+2H)+2 |
| 539.2016 | 1 | 2623386.7 | C27 H25 F3 N6 O3 | (M+H)+ |
| 540.2046 | 1 | 8222952.92 | C27 H25 F3 N6 O3 | (M+H)+ |
| 541.206 | 1 | 1558801.49 | C27 H25 F3 N6 O3 | (M+H)+ |
| 542.2059 | 1 | 207852.91 | C27 H25 F3 N6 O3 | (M+H)+ |
| 543.2024 | 1 | 27768.11 | C27 H25 F3 N6 O3 | (M+H)+ |
| 558.1781 | 2 | 20974.9 | | (2M+H)+2 |
| 558.6769 | 2 | 8405.48 | | (2M+H)+2 |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4n):



^{13}C NMR (100MHz, CDCl_3) (4n):



Qualitative Compound Report

Data File RK-220.d
Sample Type Sample
Instrument Name Instrument 1
Acq Method Demo 1K.m
IRM Calibration Status Success
Comment

Sample Group
Acquisition SW Version 6200 series TOF/6500 series
 Q-ToF B.05.01 (B0125.1)

Sample Name RK-220
Position P1-B4
User Name A

Info.

Compound Table

| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|-------------------------|-------|----------|------------------|------------------|----------------|------------------|
| Cpd 1: C28 H27 F3 N6 O3 | 0.125 | 552.2078 | C28 H27 F3 N6 O3 | C28 H27 F3 N6 O3 | 3.47 | C28 H27 F3 N6 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|-------------------------|----------|-------|---------------------------|----------|
| Cpd 1: C28 H27 F3 N6 O3 | 553.2148 | 0.125 | Find by Molecular Feature | 552.2078 |

M/E MS Spectrum

M/E MS Zoomed Spectrum

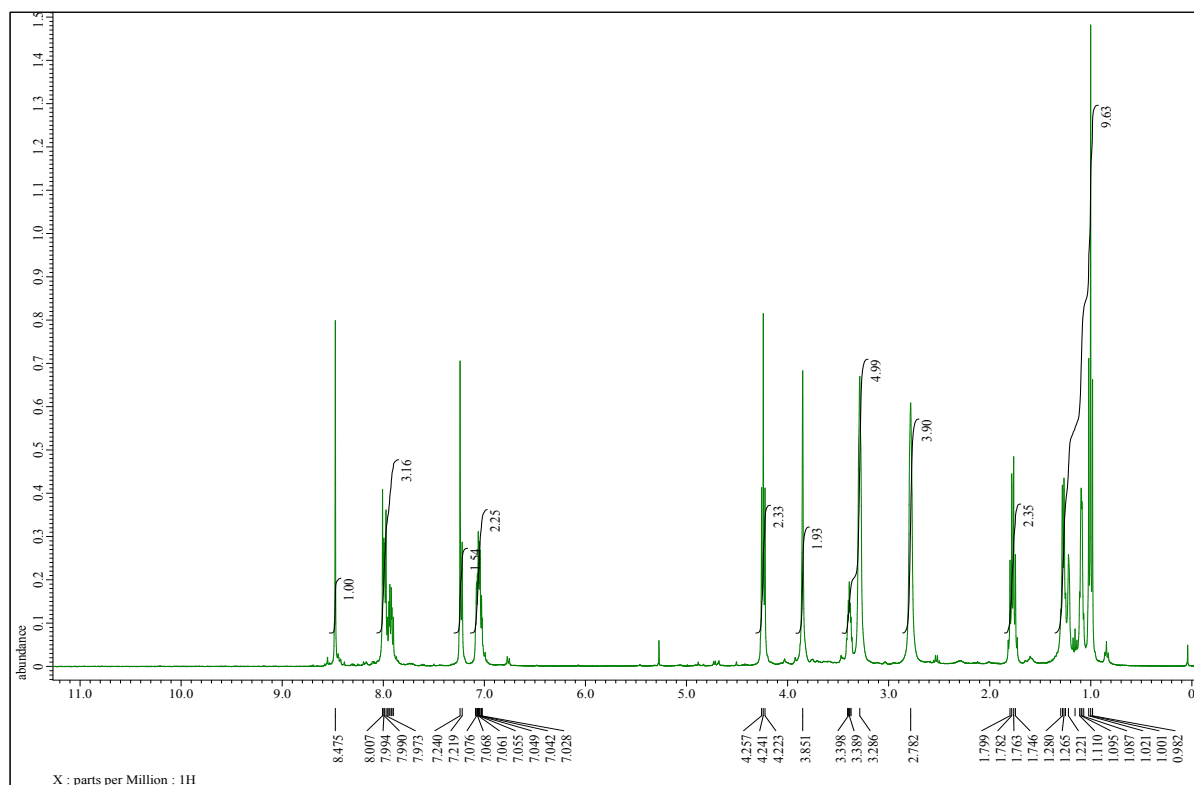
MS Spectrum Peak List

| m/z | z | Abund | Formula | Ion |
|----------|---|------------|------------------|-----------|
| 277.1112 | 2 | 171323.13 | C28 H27 F3 N6 O3 | (M-2H)+2 |
| 277.6126 | 2 | 560932.19 | C28 H27 F3 N6 O3 | (M+2H)+2 |
| 278.0136 | 2 | 102557.43 | C28 H27 F3 N6 O3 | (M+2H)+2 |
| 278.0152 | 2 | 13367.27 | C28 H27 F3 N6 O3 | (M+2H)+2 |
| 553.2148 | 1 | 23112674 | C28 H27 F3 N6 O3 | (M+H)+ |
| 554.2181 | 1 | 7494198.64 | C28 H27 F3 N6 O3 | (M+H)+ |
| 555.2181 | 1 | 1550787.26 | C28 H27 F3 N6 O3 | (M+H)+ |
| 556.2156 | 1 | 237181.26 | C28 H27 F3 N6 O3 | (M+H)+ |
| 557.212 | 1 | 29177.97 | C28 H27 F3 N6 O3 | (M+H)+ |
| 578.1933 | 2 | 25143.11 | C28 H27 F3 N6 O3 | (2M+1H)+2 |

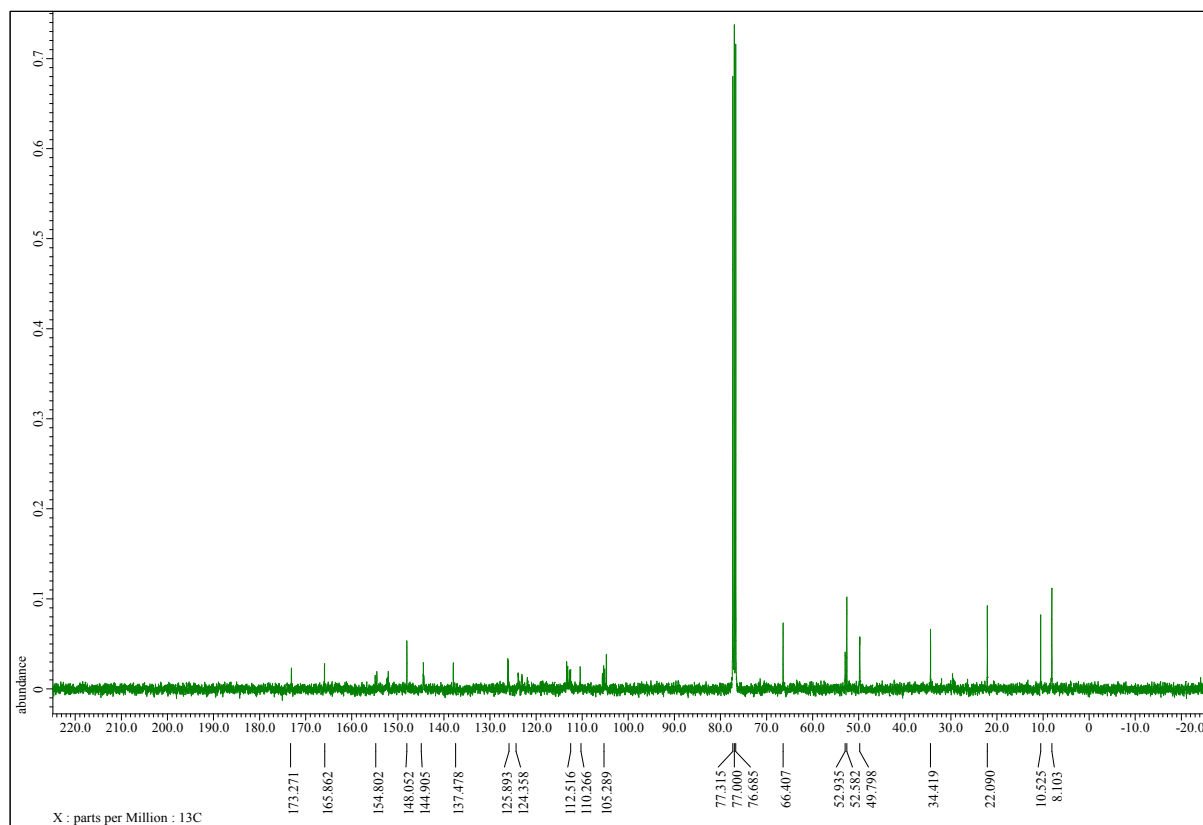
— End Of Report —

Agilent Technologies
Page 1 of 1
Printed at: 17:08 on:05-09-2018

^1H NMR (400MHz, CDCl_3) (4o):

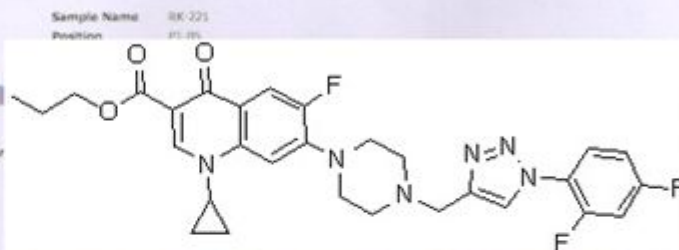


^{13}C NMR (100MHz, CDCl_3) (4o):



Qualitative Compound Report

Data File: RK-221.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Comp. ILCM
 IRM Calibration Status: Success
 Comment:
 Sample Group:
 Acquisition SW: 6200 series TOF/6300 series
 Version: Q-TOF B.05.01 (08125.1)



Compound Table

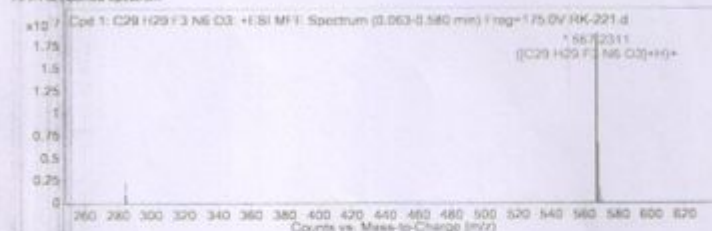
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|-------------------------|-------|----------|------------------|------------------|----------------|------------------|
| Cap 1: C29 H29 F3 N6 O3 | 0.123 | 566.2239 | C29 H29 F3 N6 O3 | C29 H29 F3 N6 O3 | 2.43 | C29 H29 F3 N6 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|-------------------------|----------|-------|-------------------------------------|------|
| Cap 1: C29 H29 F3 N6 O3 | 567.2311 | 0.123 | Find by Molecular Feature: 566.2239 | |

MFE MS Spectrum



MFE MS Zoomed Spectrum

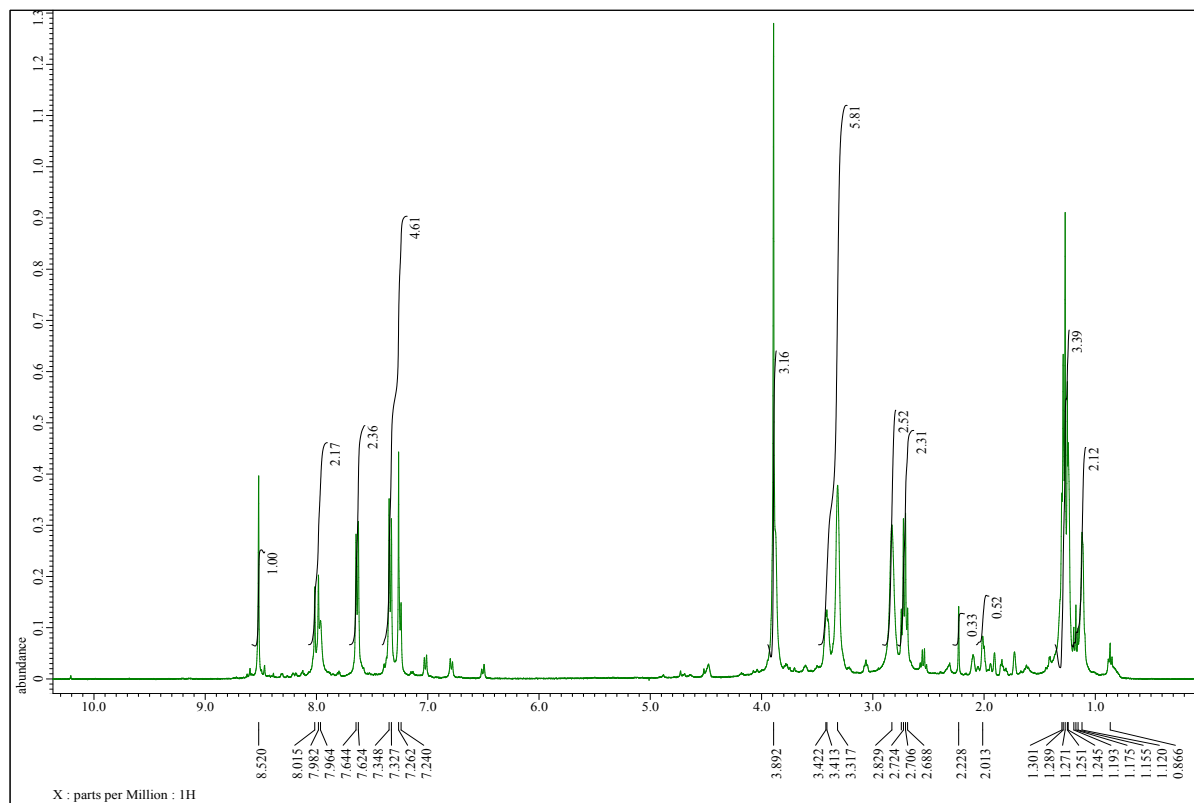


MS Spectrum Peak List

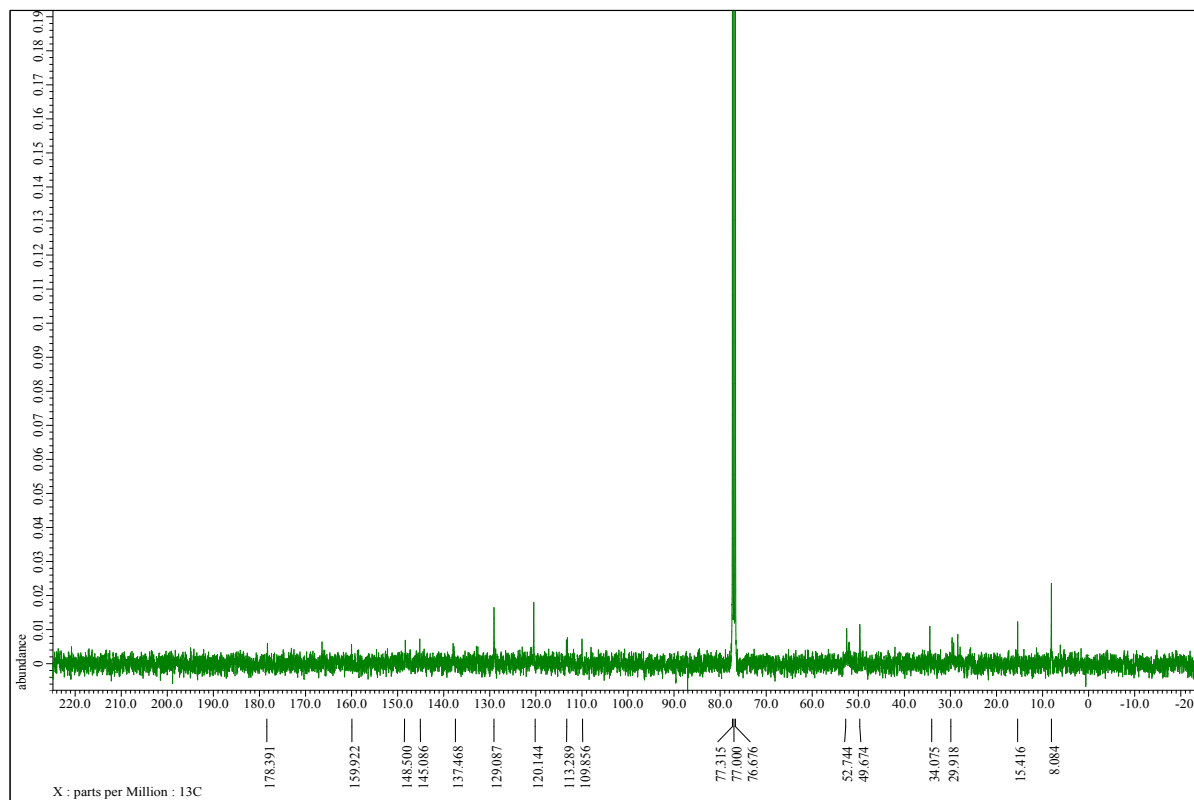
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|------------------|----------|
| 264.1191 | 2 | 21881.72.5 | C29 H29 F3 N6 O3 | (M+2H)+2 |
| 284.6208 | 2 | 797136.35 | C29 H29 F3 N6 O3 | (M+2H)+2 |
| 285.1216 | 2 | 148385.06 | C29 H29 F3 N6 O3 | (M+2H)+2 |
| 295.3302 | 2 | 58504.63 | C29 H29 F3 N6 O3 | (M+2H)+2 |
| 295.6117 | 2 | 20834.4 | C29 H29 F3 N6 O3 | (M+2H)+2 |
| 567.2311 | 1 | 18881684 | C29 H29 F3 N6 O3 | (M+H)+ |
| 568.2341 | 1 | 6286122.62 | C29 H29 F3 N6 O3 | (M+H)+ |
| 569.2290 | 1 | 1712819.02 | C29 H29 F3 N6 O3 | (M+H)+ |
| 570.2242 | 1 | 35260.97 | C29 H29 F3 N6 O3 | (M+H)+ |
| 571.2202 | 1 | 57262.22 | C29 H29 F3 N6 O3 | (M+H)+ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4p):



^{13}C NMR (100MHz, CDCl_3) (4p):



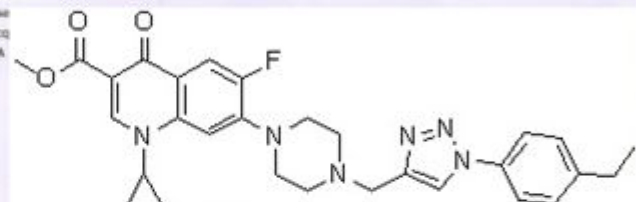
Qualitative Compound Report

Data File: RK-222.d
 Sample Type: Sample
 Instrument Name: Instrument 1
 Acq Method: Data_XC.m
 IRM Calibration Status: **Sustone**
 Comment:

Sample Name: RK-222
 Position: P1-06
 Use:
 Acq: DA

Sample Group:
 Acquisition SW: 6300 series TQF/6500 series
 Version: Q-TOF R.05.01 (06125.1)

Info.

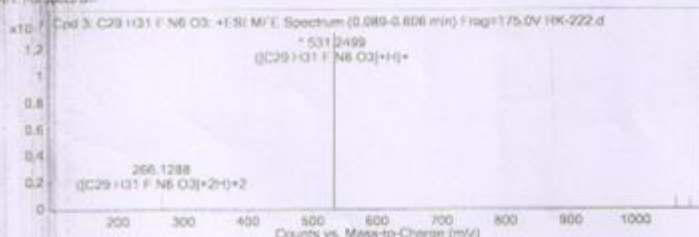


Compound Table

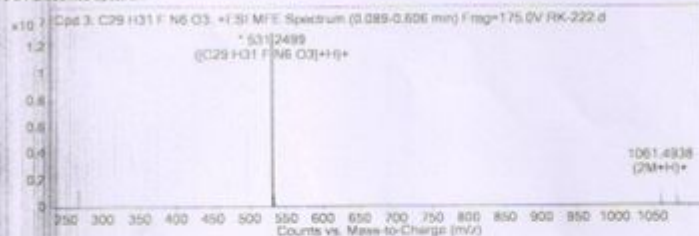
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|------------------------|-------|----------|-----------------|-----------------|----------------|-----------------|
| Cpd 3: C29 H31 F N6 O3 | 0.132 | 530.2429 | C29 H31 F N6 O3 | C29 H31 F N6 O3 | 2.43 | C29 H31 F N6 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|-------|---------------------------|----------|
| Cpd 3: C29 H31 F N6 O3 | 531.2499 | 0.132 | Find by Molecular Feature | 530.2429 |

MFI MS Spectrum



MFI MS Zoomed Spectrum

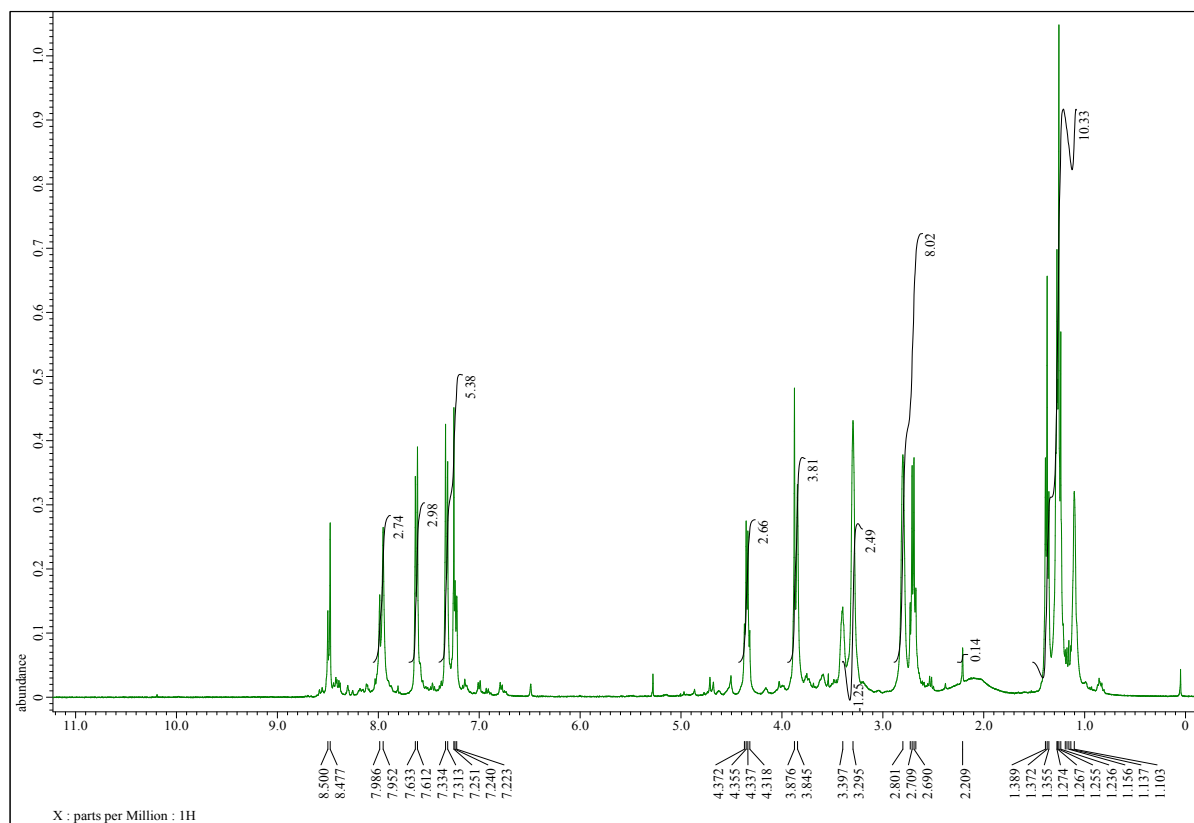


MS Spectrum Peak List

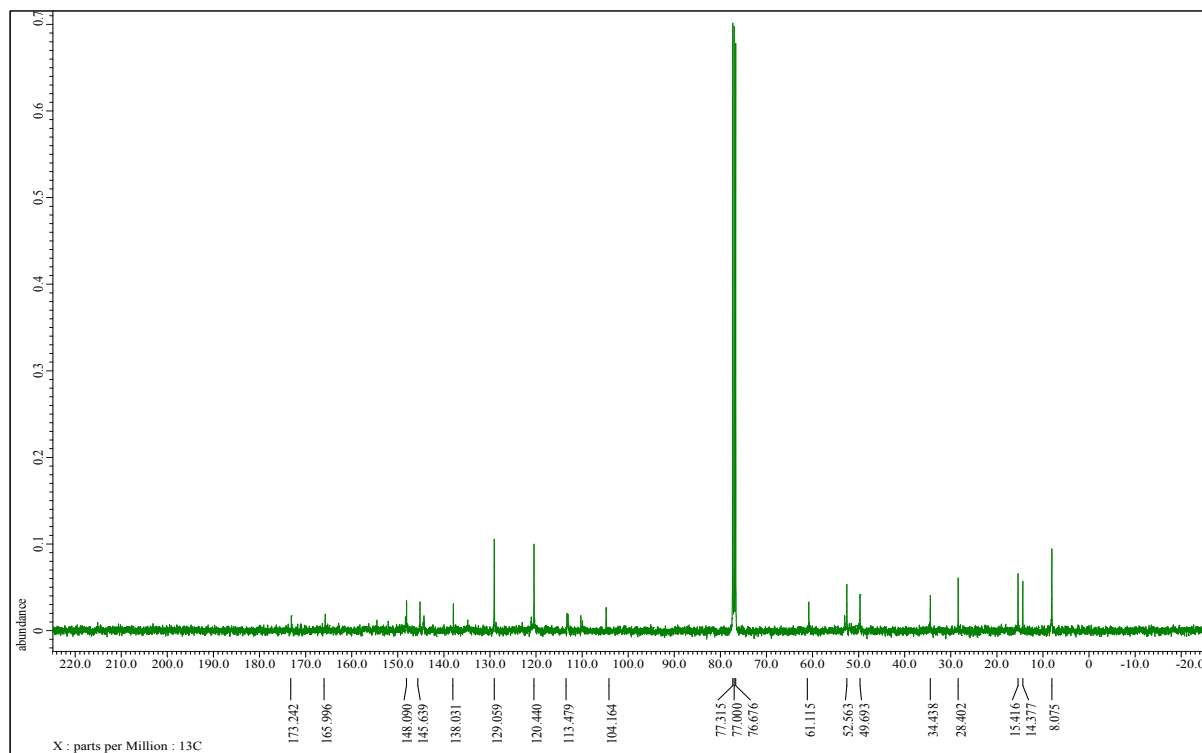
| m/z | z | Abund | Formula | Ion |
|-----------|---|------------|-----------------|----------|
| 266.1288 | 2 | 1230593.5 | C29 H31 F N6 O3 | (M+2H)+2 |
| 266.6301 | 2 | 400289.06 | C29 H31 F N6 O3 | (M+2H)+2 |
| 531.2499 | 1 | 1304136.7 | C29 H31 F N6 O3 | (M+H)+ |
| 532.2532 | 1 | 4662970.98 | C29 H31 F N6 O3 | (M+H)+ |
| 533.2497 | 1 | 1071134.57 | C29 H31 F N6 O3 | (M+H)+ |
| 1061.4938 | 1 | 911160.19 | | (2M+H)+ |
| 1062.4963 | 1 | 630822.46 | | (2M+H)+ |
| 1063.4984 | 1 | 218054.72 | | (2M+H)+ |
| 1063.4751 | 1 | 793893.75 | | (2M+Na)+ |
| 1064.4782 | 1 | 539913.34 | | (2M+Na)+ |

— End Of Report —

^1H NMR (400MHz, CDCl_3) (4q):



^{13}C NMR (100MHz, CDCl_3) (4q):

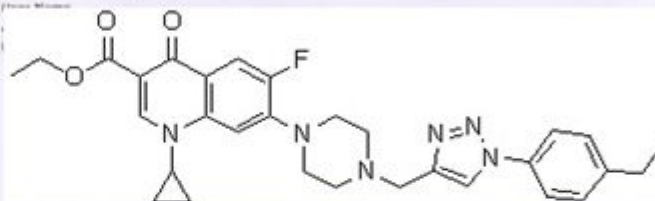


Qualitative Compound Report

Data File: RK-223.d
 Sample Type: Instrument 1
 Instrument Name: Demo 3K.m
 IRM Calibration Status: Success
 Comment:

Sample Name: RK-223
 Position: P1-04

Sample Group: Info.
 Acquisition SW: 6300 series TOF/MS00 series
 Version: Q-TOF B.05.01 (R6125.1)

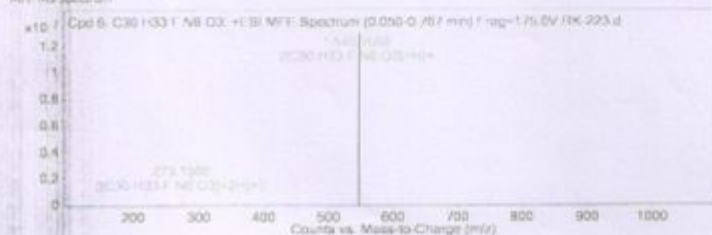


Compound Table

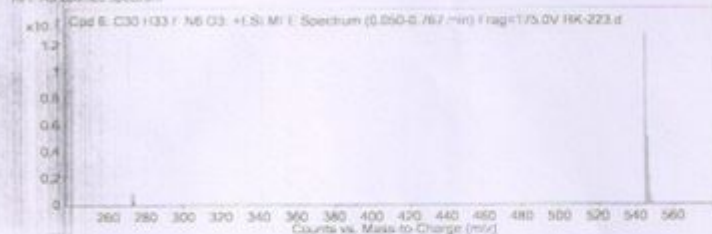
| Compound Label | RT | Mass | Formula | MFG Formula | MFG DIFF (ppm) | DB Formula |
|------------------------|-------|----------|-----------------|-----------------|----------------|-----------------|
| Cpd 6: C30 H33 F N6 O3 | 0.117 | 544.2585 | C30 H33 F N6 O3 | C30 H33 F N6 O3 | 2.47 | C30 H33 F N6 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|------------------------|----------|-------|---------------------------|----------|
| Cpd 6: C30 H33 F N6 O3 | 545.2658 | 0.117 | Find by Molecular Feature | 544.2585 |

MFT MS Spectrum



MFI MS Zoomed Spectrum

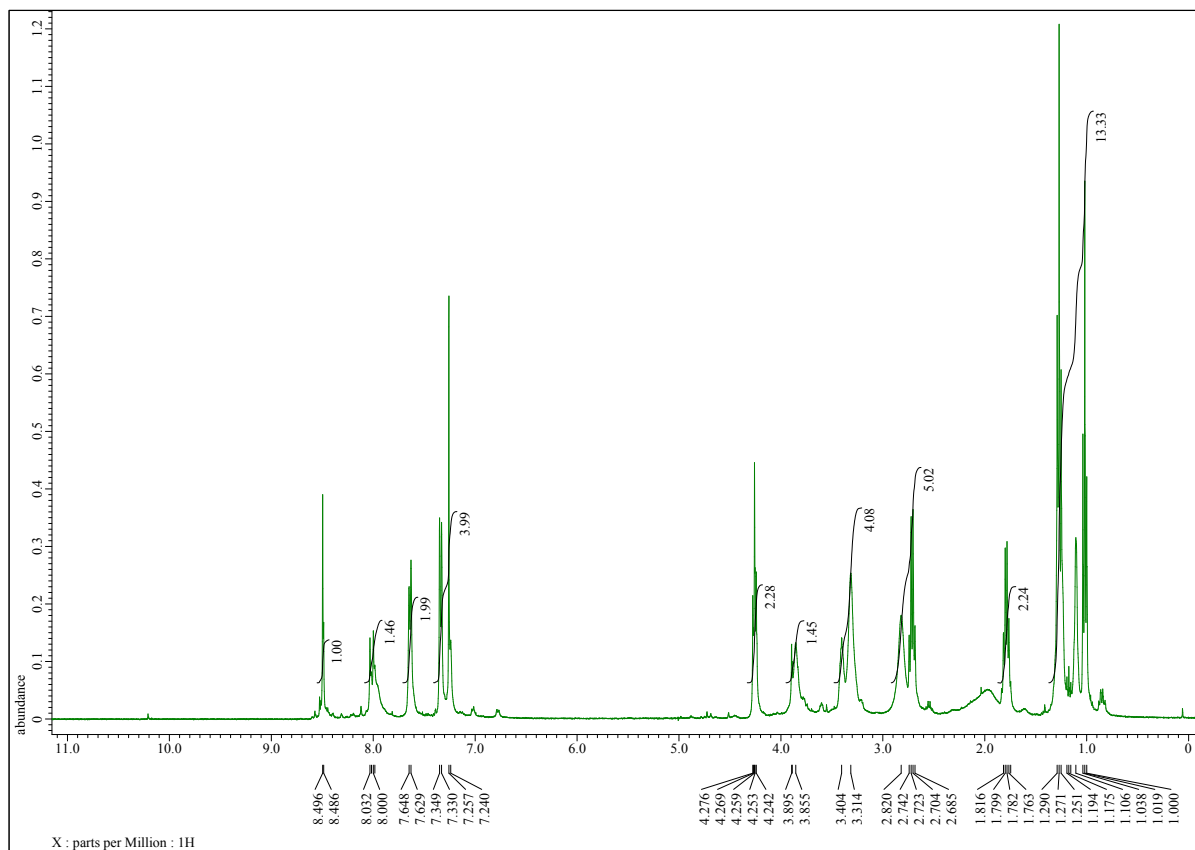


MS Spectrum Peak List

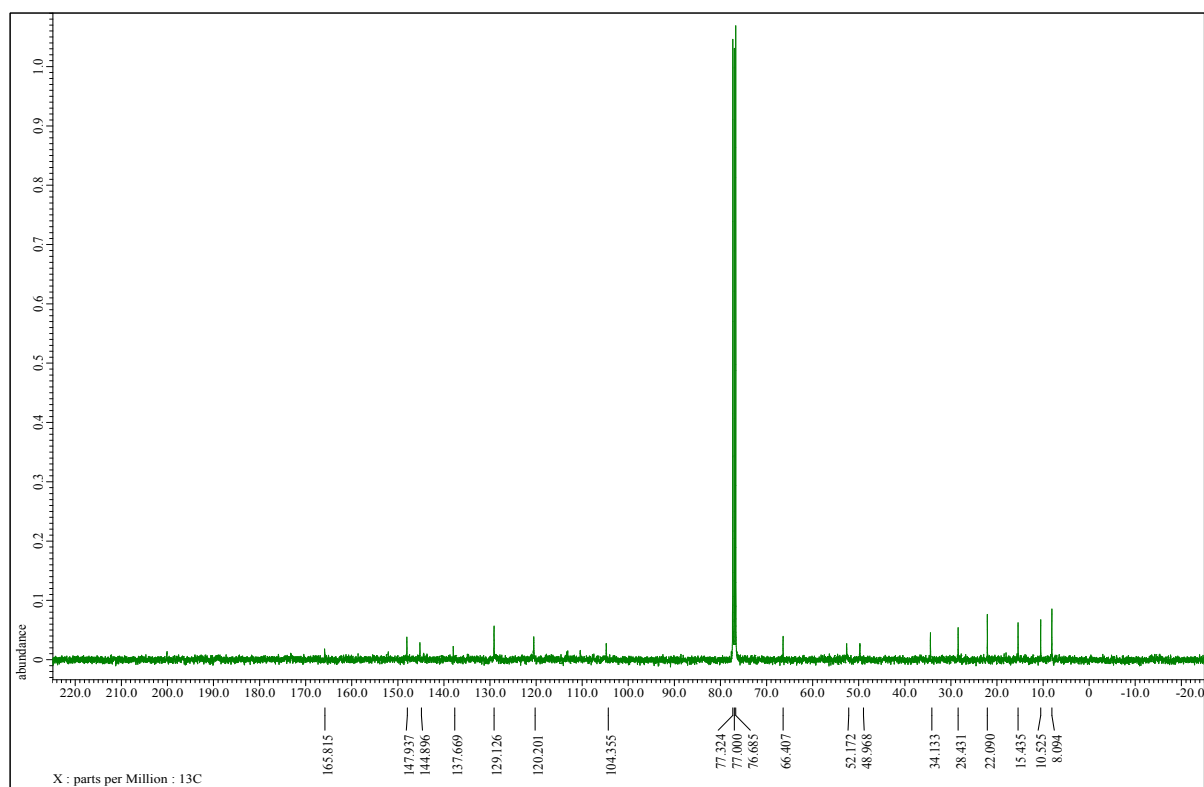
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|-----------------|----------|
| 273.1366 | 2 | 817735.56 | C30 H33 F N6 O3 | (M+2H)+2 |
| 273.0378 | 2 | 281213.79 | C30 H33 F N6 O3 | (M+2H)+2 |
| 276.139 | 2 | 56438.3 | C30 H33 F N6 O3 | (M+2H)+2 |
| 274.6407 | 2 | 8343.39 | C30 H33 F N6 O3 | (M+2H)+2 |
| 545.2658 | 1 | 12866832 | C30 H33 F N6 O3 | (M+H)+ |
| 546.2688 | 1 | 4557393.05 | C30 H33 F N6 O3 | (M+H)+ |
| 547.265 | 1 | 2206495.5 | C30 H33 F N6 O3 | (M+H)+ |
| 548.2625 | 1 | 658963.57 | C30 H33 F N6 O3 | (M+H)+ |
| 549.2532 | 1 | 129486.85 | C30 H33 F N6 O3 | (M+H)+ |
| 550.2548 | 1 | 19097.85 | C30 H33 F N6 O3 | (M+H)+ |

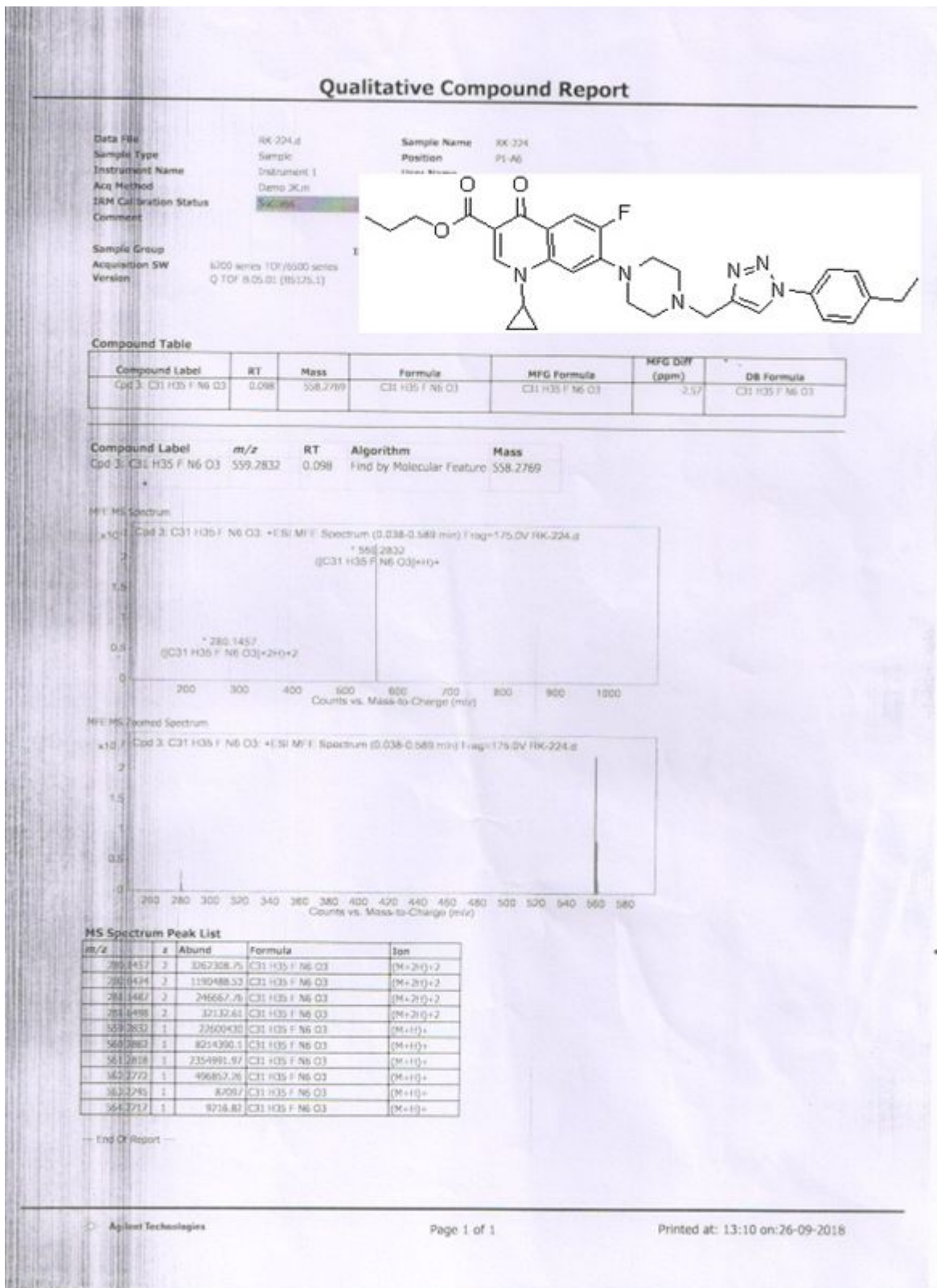
--- End Of Report ---

^1H NMR (400MHz, CDCl_3) (4r):

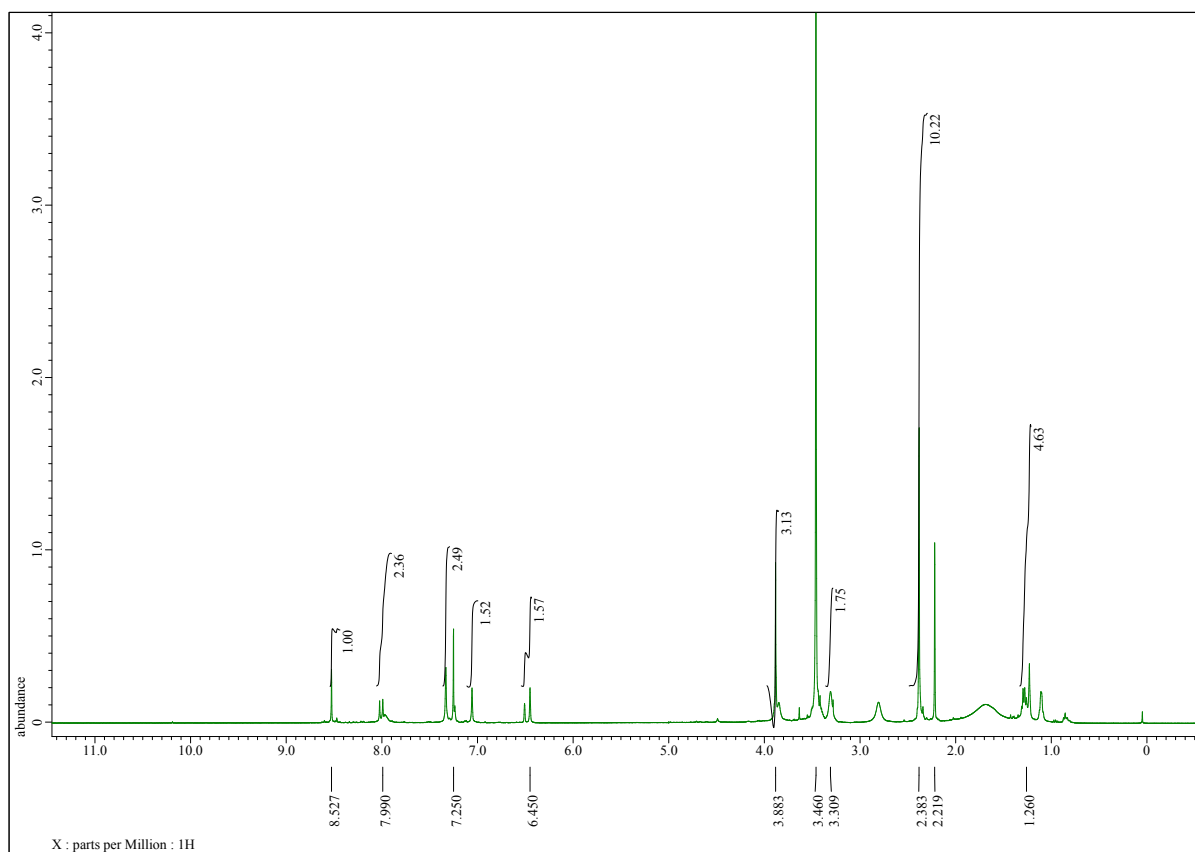


^{13}C NMR (100MHz, CDCl_3) (4r):

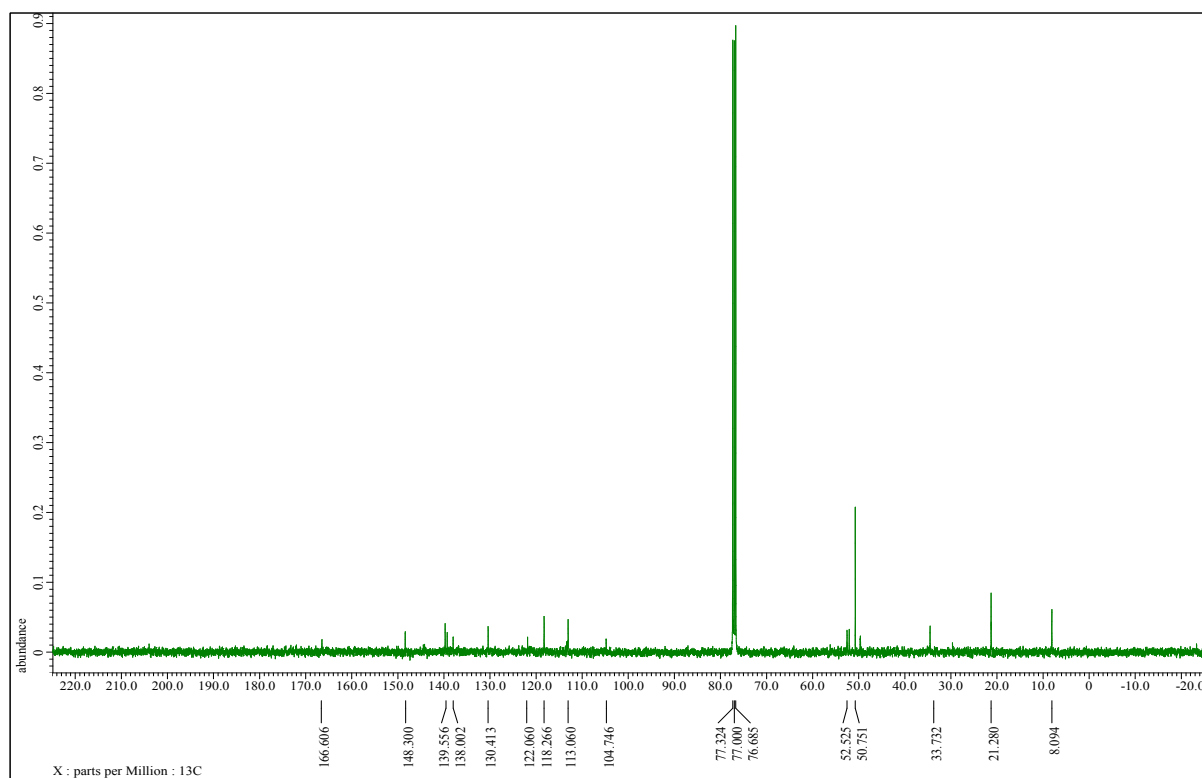


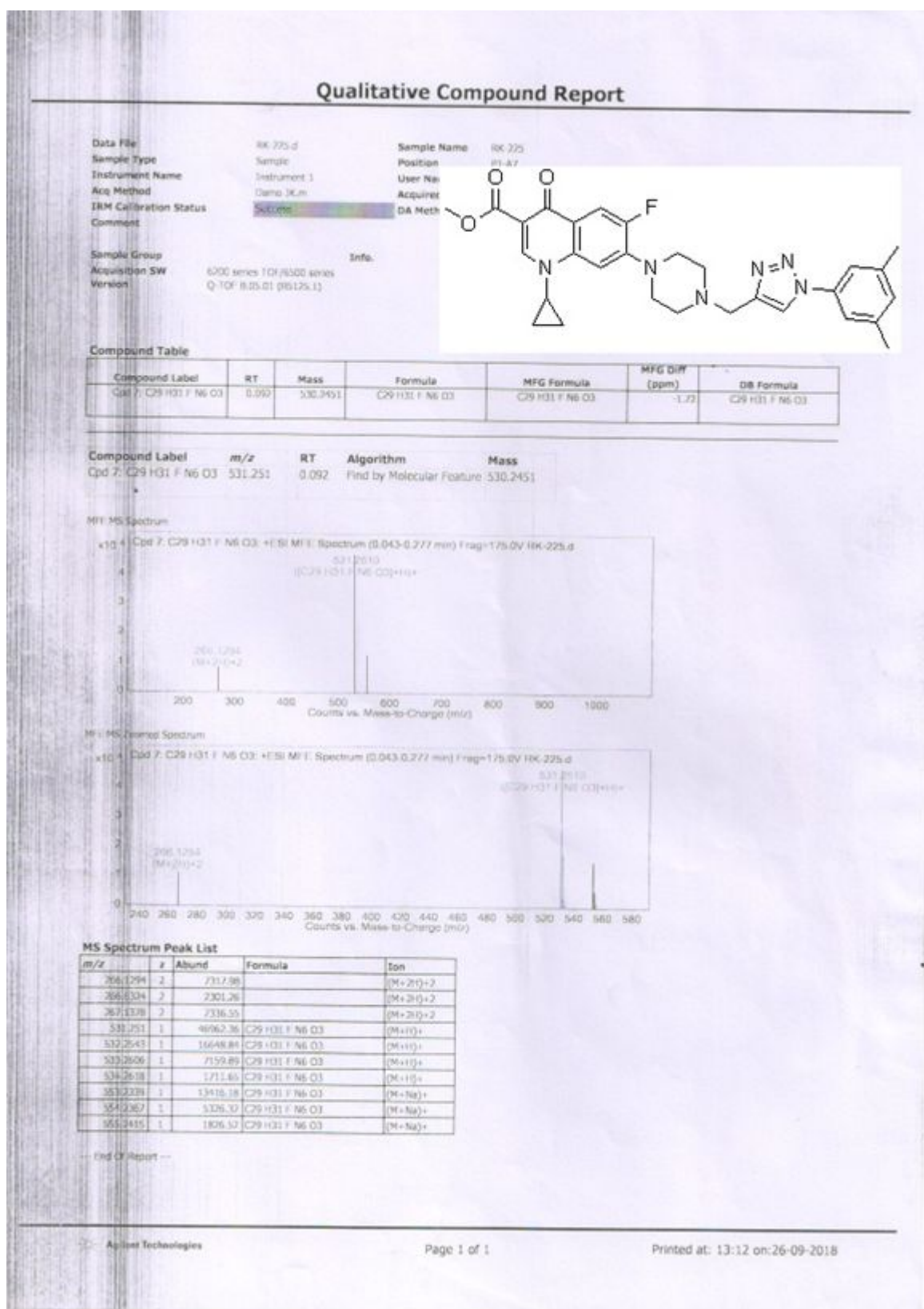


^1H NMR (400MHz, CDCl_3) (4s):

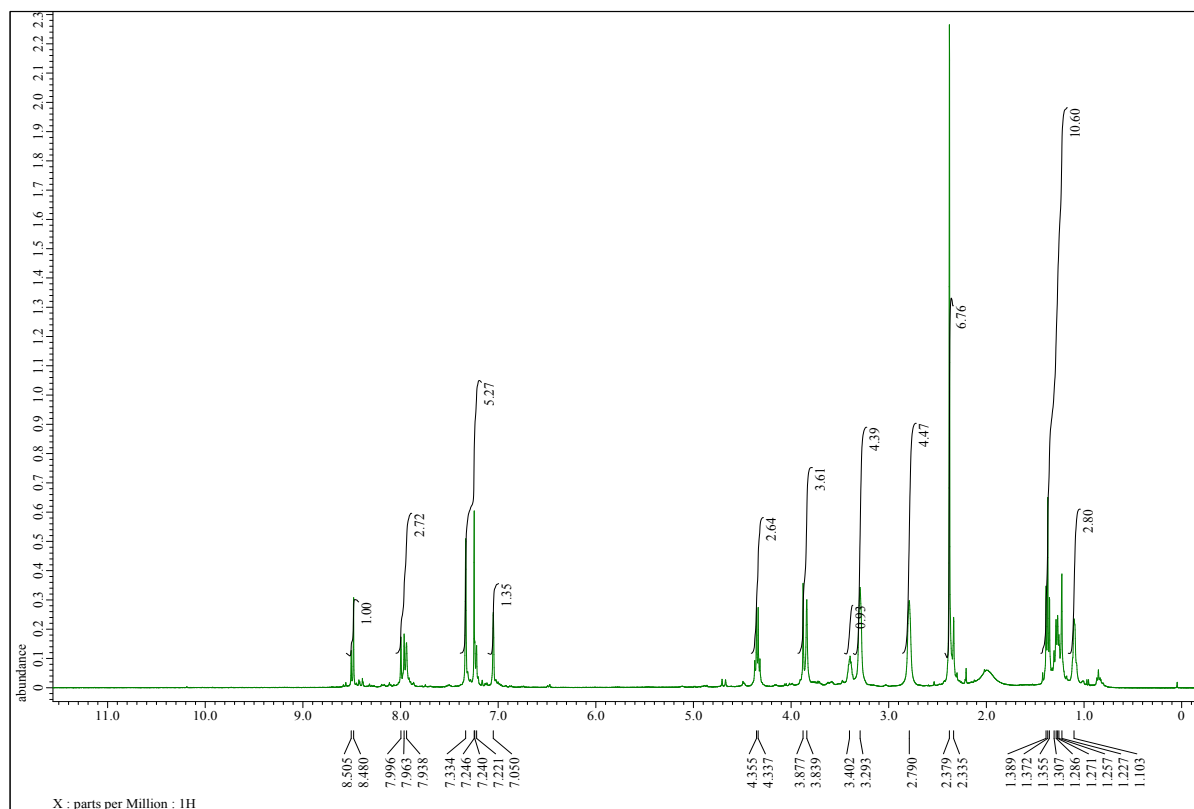


^{13}C NMR (100MHz, CDCl_3) (4s):

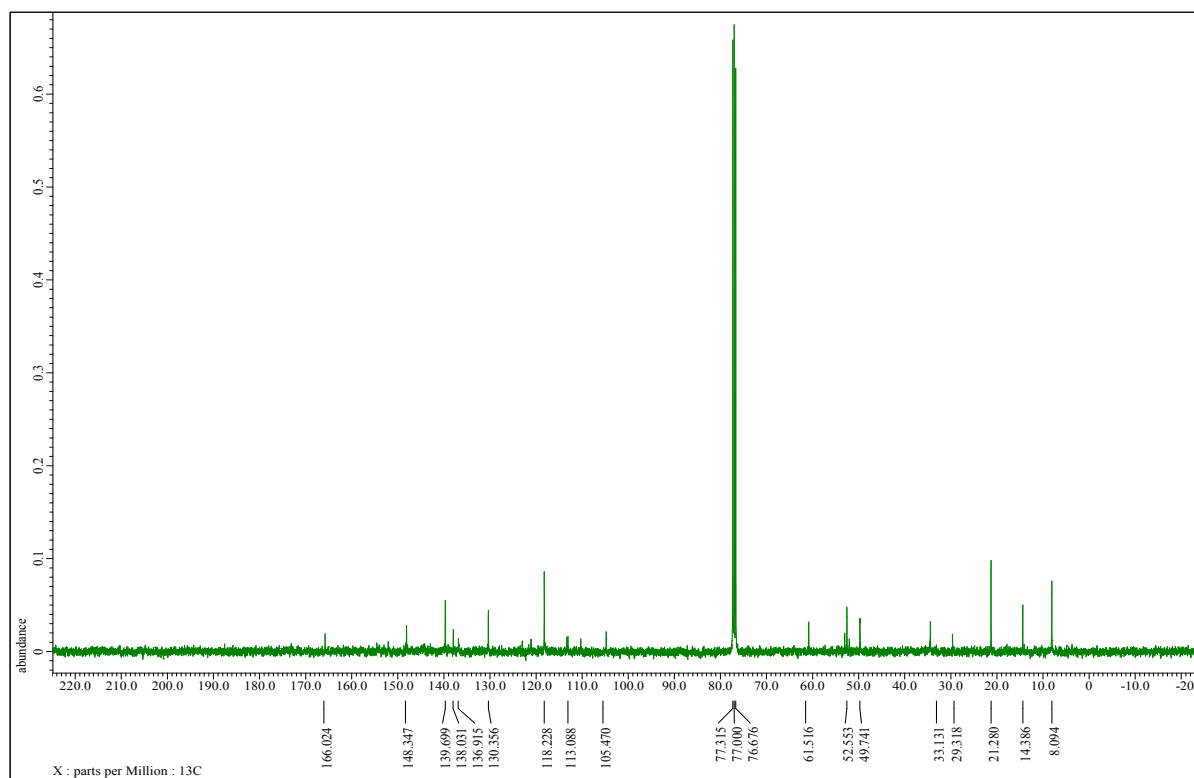




^1H NMR (400MHz, CDCl_3) (4t):



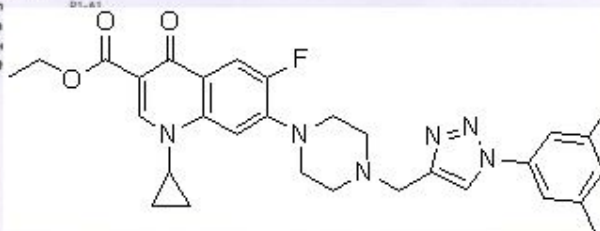
^{13}C NMR (100MHz, CDCl_3) (4t):



Qualitative Compound Report

| | | | |
|-------------------------------|--------------|--------------------|--------|
| Data File | RK-226.d | Sample Name | RK-226 |
| Sample Type | Sample | Position | D1_61 |
| Instrument Name | Instrument 1 | User Na | |
| Acq Method | Demo JK.m | Acquire | |
| IRM Calibration Status | Success | DA Mett | |
| Comment | | | |

| | | |
|-----------------------|-----------------------------|--------------|
| Sample Group | | Info. |
| Acquisition SW | 6200 series TOF/6500 series | |
| Version | Q-TOF B.05.01 (B5125.1) | |

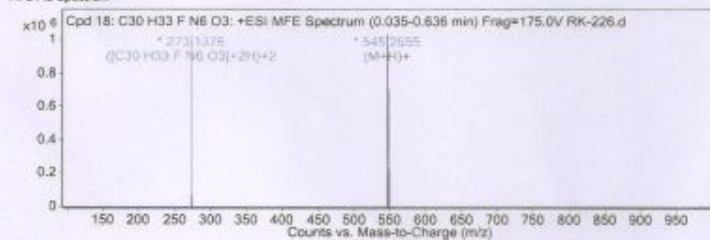


Compound Table

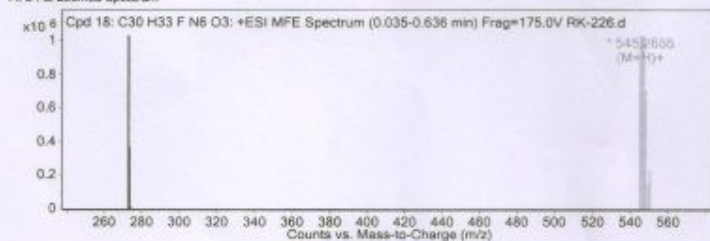
| Compound Label | RT | Mass | Formula | MFG Formula | MFG Diff (ppm) | DB Formula |
|-------------------------|-------|----------|-----------------|-----------------|----------------|-----------------|
| Cpd 18: C30 H33 F N6 O3 | 0.109 | 544.2606 | C30 H33 F N6 O3 | C30 H33 F N6 O3 | -1.49 | C30 H33 F N6 O3 |

| Compound Label | m/z | RT | Algorithm | Mass |
|-------------------------|----------|-------|---------------------------|----------|
| Cpd 18: C30 H33 F N6 O3 | 545.2655 | 0.109 | Find by Molecular Feature | 544.2606 |

MFE MS Spectrum



MFE MS Zoomed Spectrum

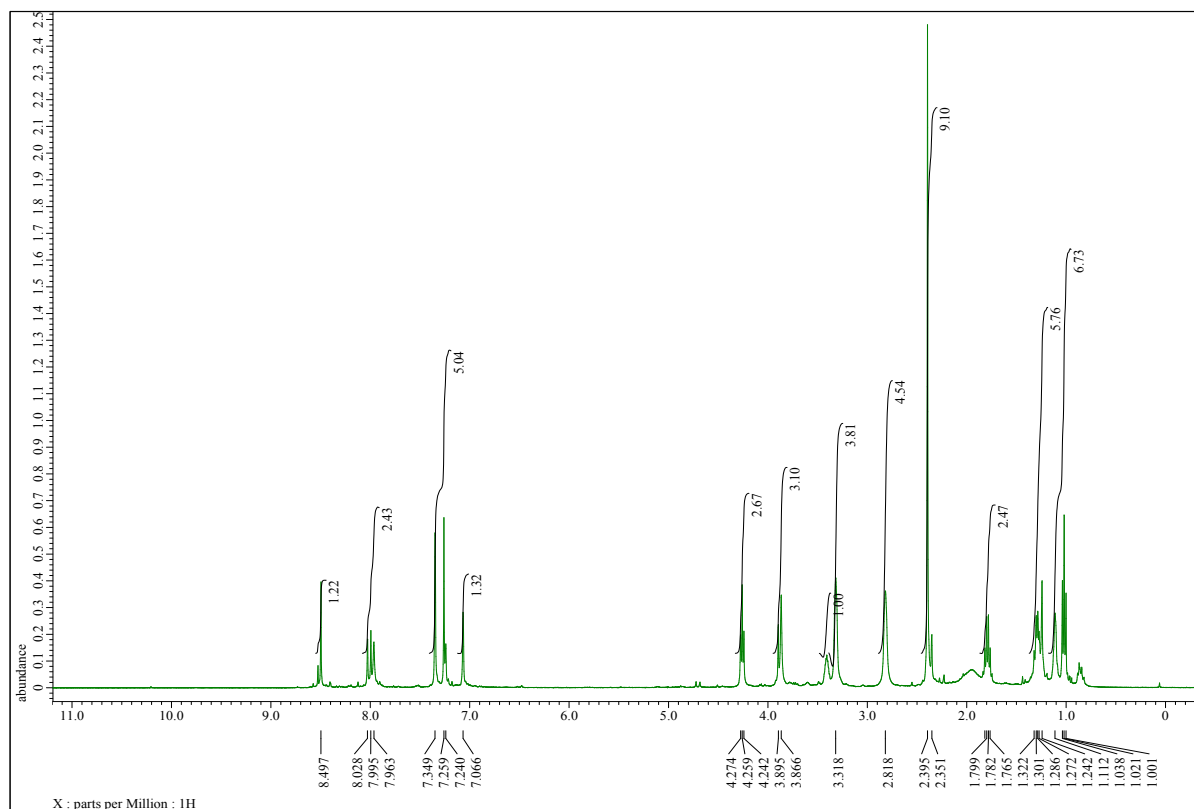


MS Spectrum Peak List

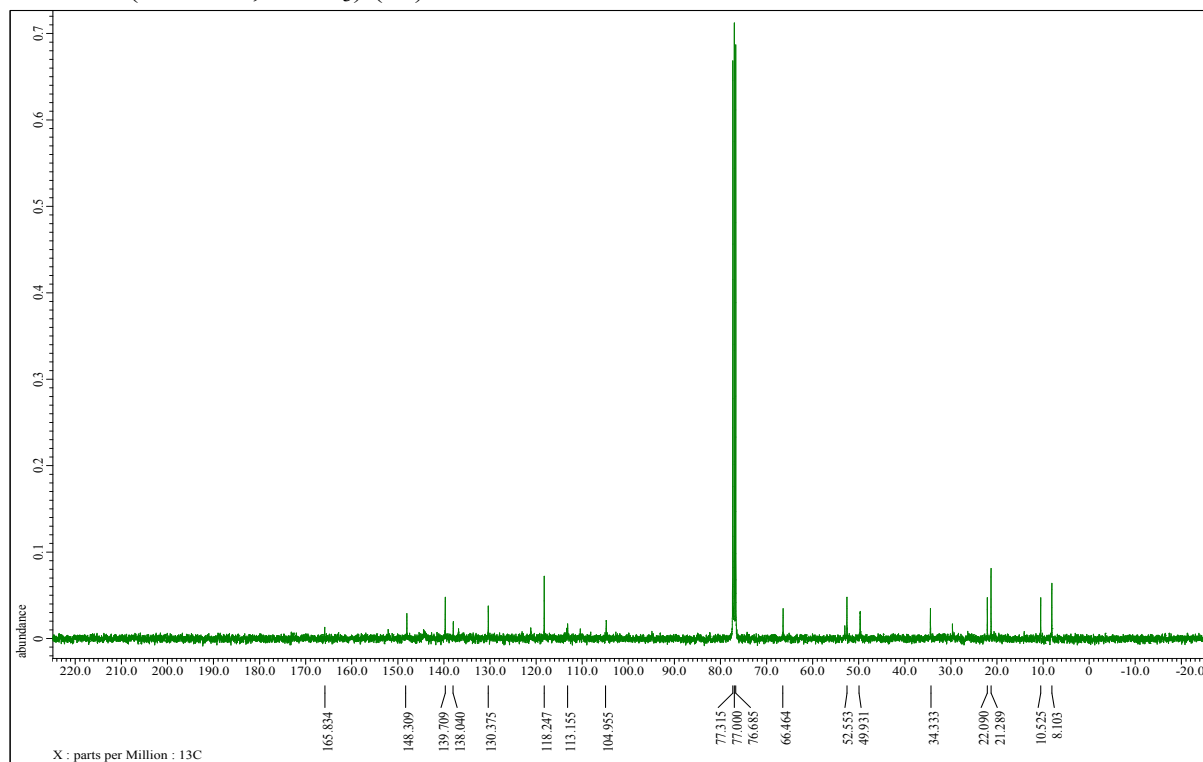
| m/z | z | Abund | Formula | Ion |
|----------|---|------------|-----------------|----------|
| 273.1376 | 2 | 1032085.63 | C30 H33 F N6 O3 | (M+2H)+2 |
| 273.6392 | 2 | 365649.5 | C30 H33 F N6 O3 | (M+2H)+2 |
| 274.1401 | 2 | 74582.3 | C30 H33 F N6 O3 | (M+2H)+2 |
| 274.6411 | 2 | 10967.38 | C30 H33 F N6 O3 | (M+2H)+2 |
| 545.2655 | 1 | 5966244.5 | | (M+H)+ |
| 546.2677 | 1 | 2037548.07 | | (M+H)+ |
| 547.2494 | 1 | 2157937.15 | | (M+H)+ |
| 548.2499 | 1 | 705076.48 | | (M+H)+ |
| 549.2532 | 1 | 153351.73 | | (M+H)+ |
| 550.2508 | 1 | 227633.96 | | (M+H)+ |

--- End Of Report ---

^1H NMR (400MHz, CDCl_3) (4u):



^{13}C NMR (100MHz, CDCl_3) (4u):

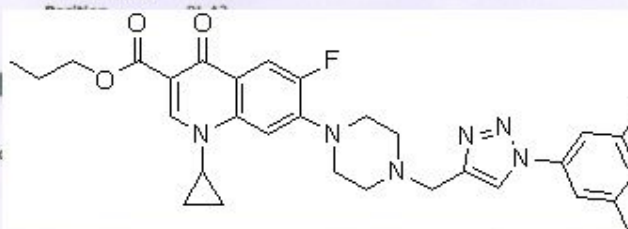


Qualitative Compound Report

Data File RK-227.d
Sample Type Sample
Instrument Name Instrument 1
Acq Method Demo JK.m
IRM Calibration Status Success
Comment

Sample Group
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Sample Name RK-227

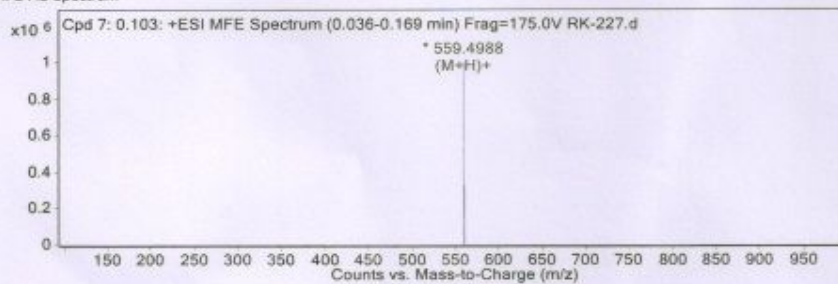


Compound Table

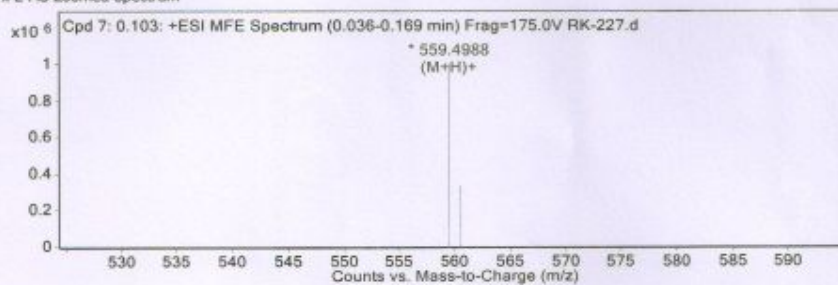
| Compound Label | RT | Mass | MFG Formula |
|----------------|-------|----------|-------------|
| Cpd 7: 0.103 | 0.103 | 558.4915 | <none> |

| Compound Label | m/z | RT | Algorithm | Mass |
|----------------|----------|-------|---------------------------|----------|
| Cpd 7: 0.103 | 559.4988 | 0.103 | Find by Molecular Feature | 558.4915 |

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

| m/z | z | Abund | Ion |
|----------|---|------------|--------|
| 559.4988 | 1 | 1001560.63 | (M+H)+ |
| 560.4992 | 1 | 327256 | (M+H)+ |

--- End Of Report ---