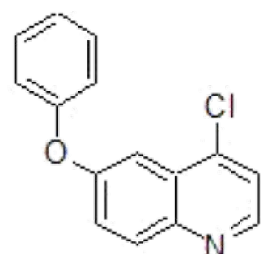
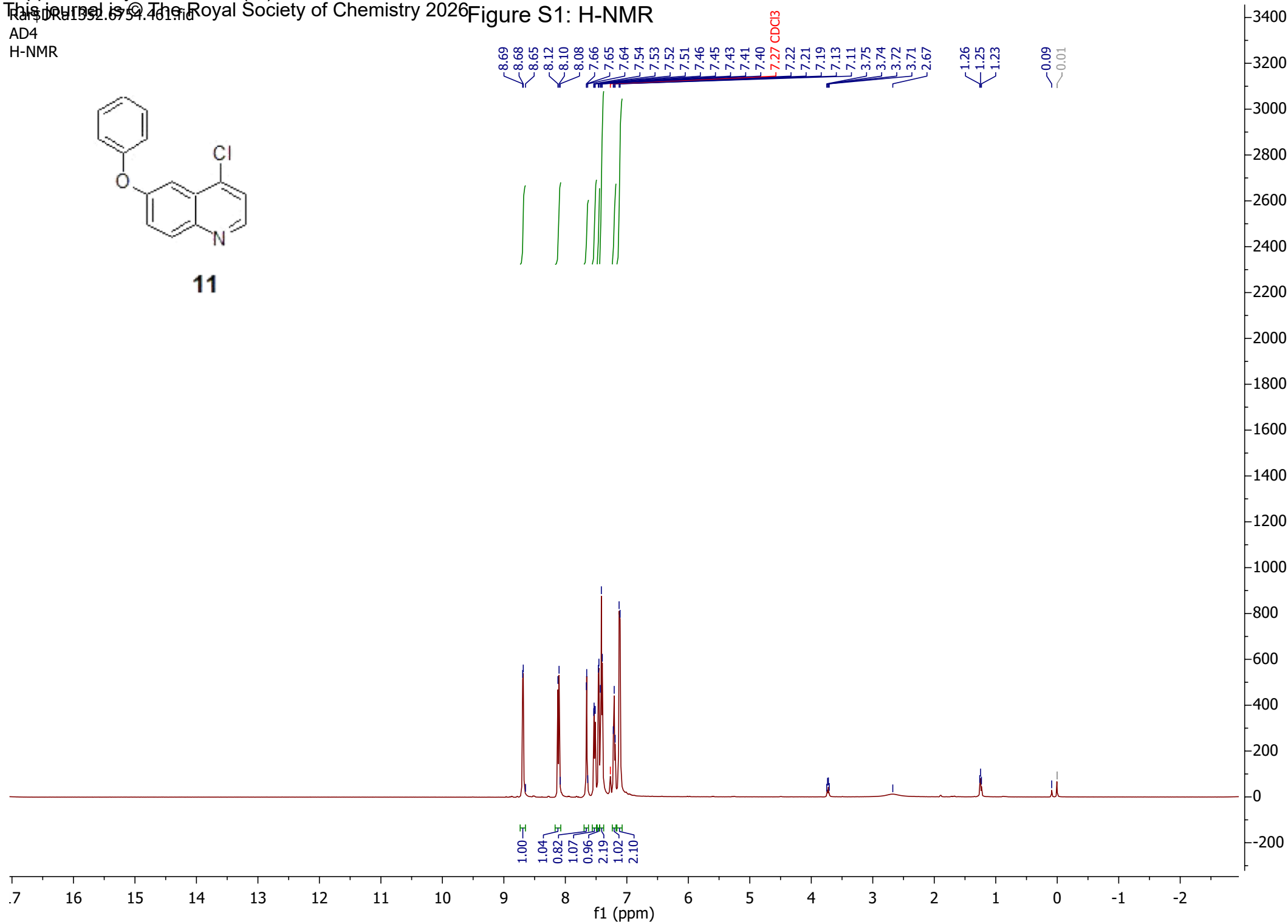


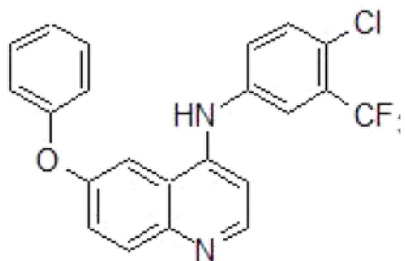
Figure S1: H-NMR

**11**

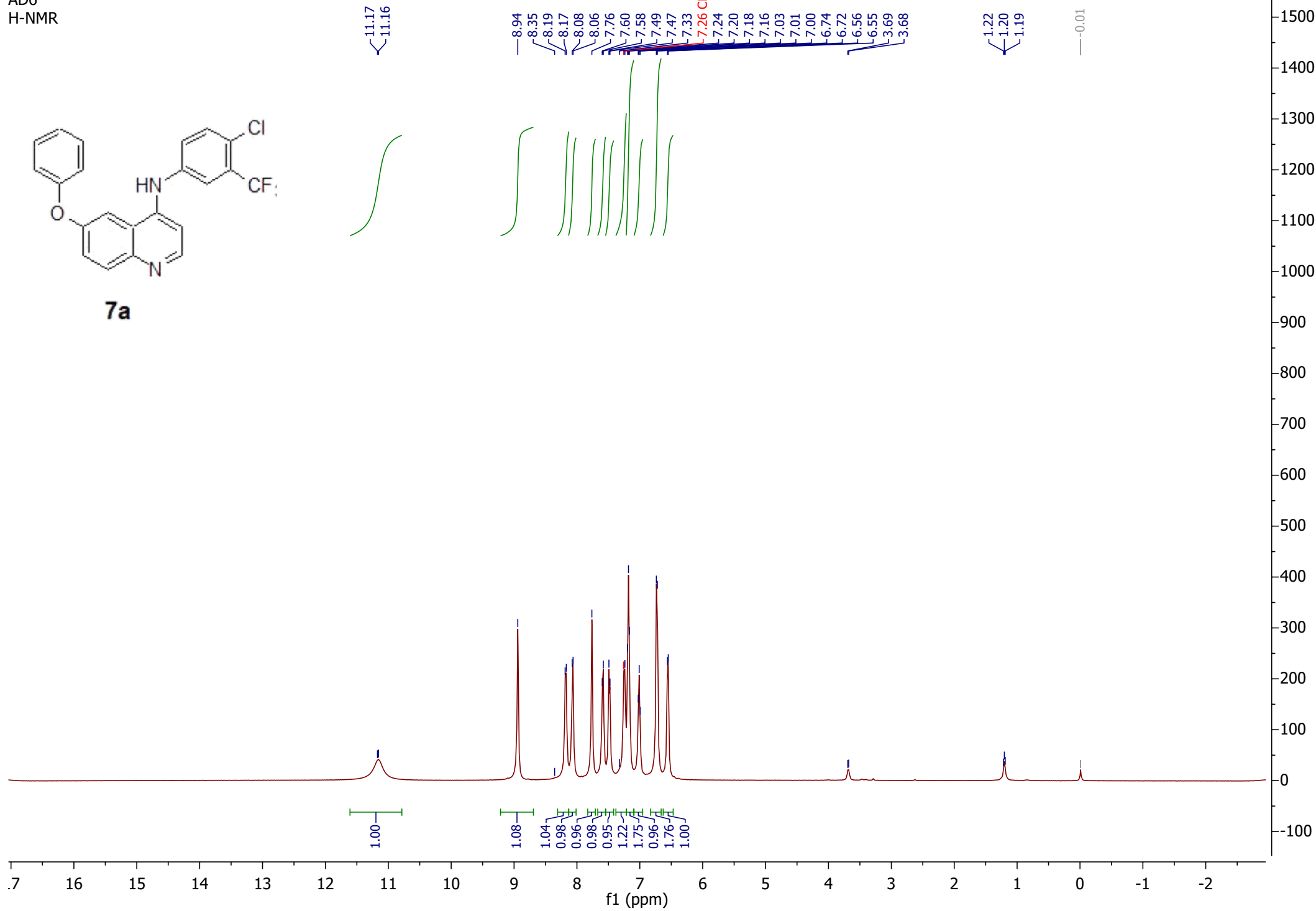
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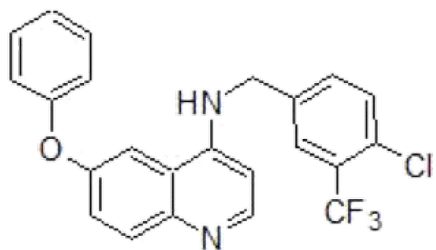
AD6

H-NMR

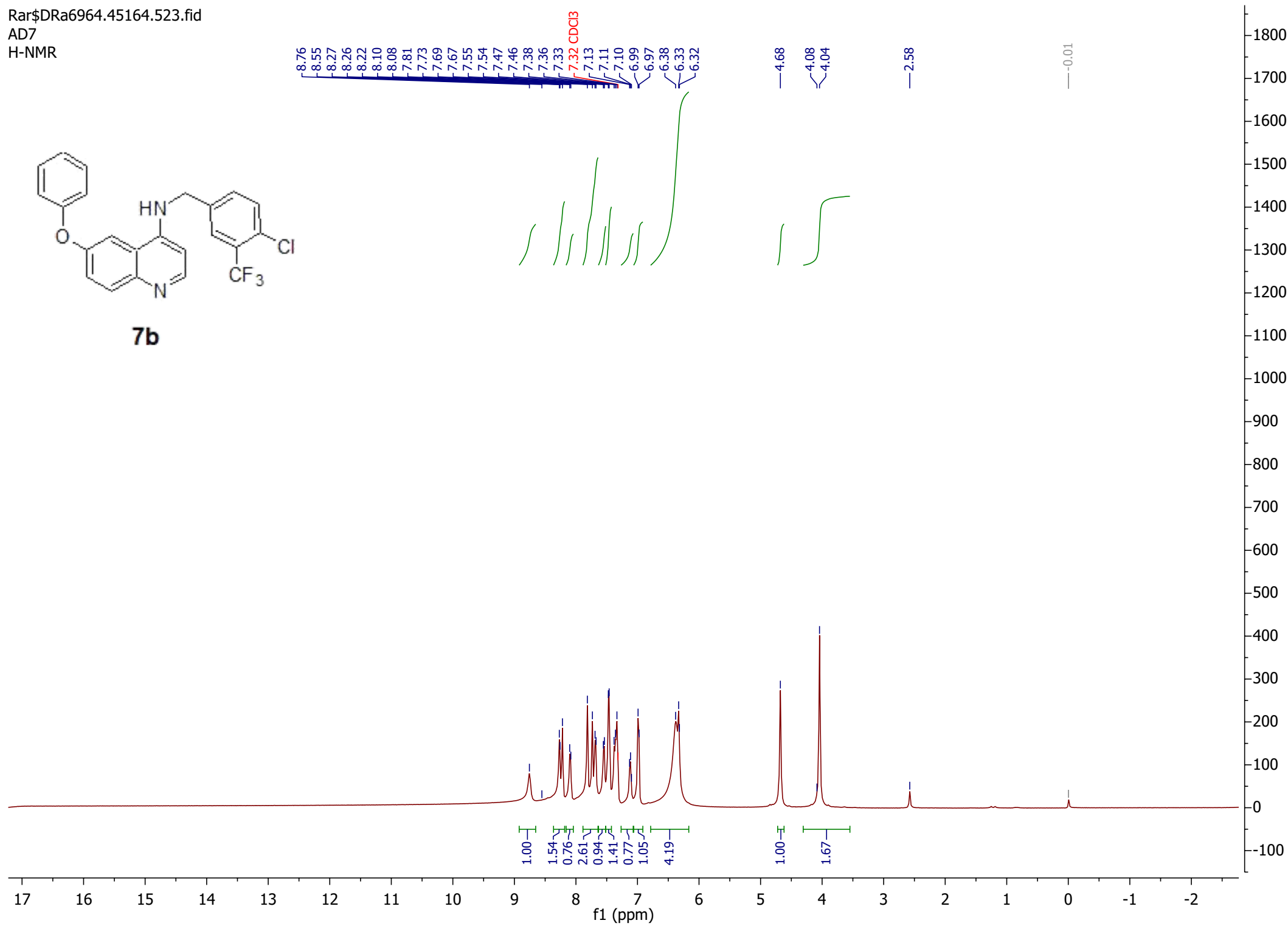


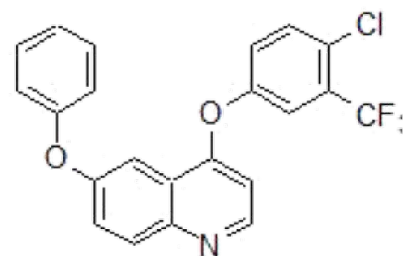
7a



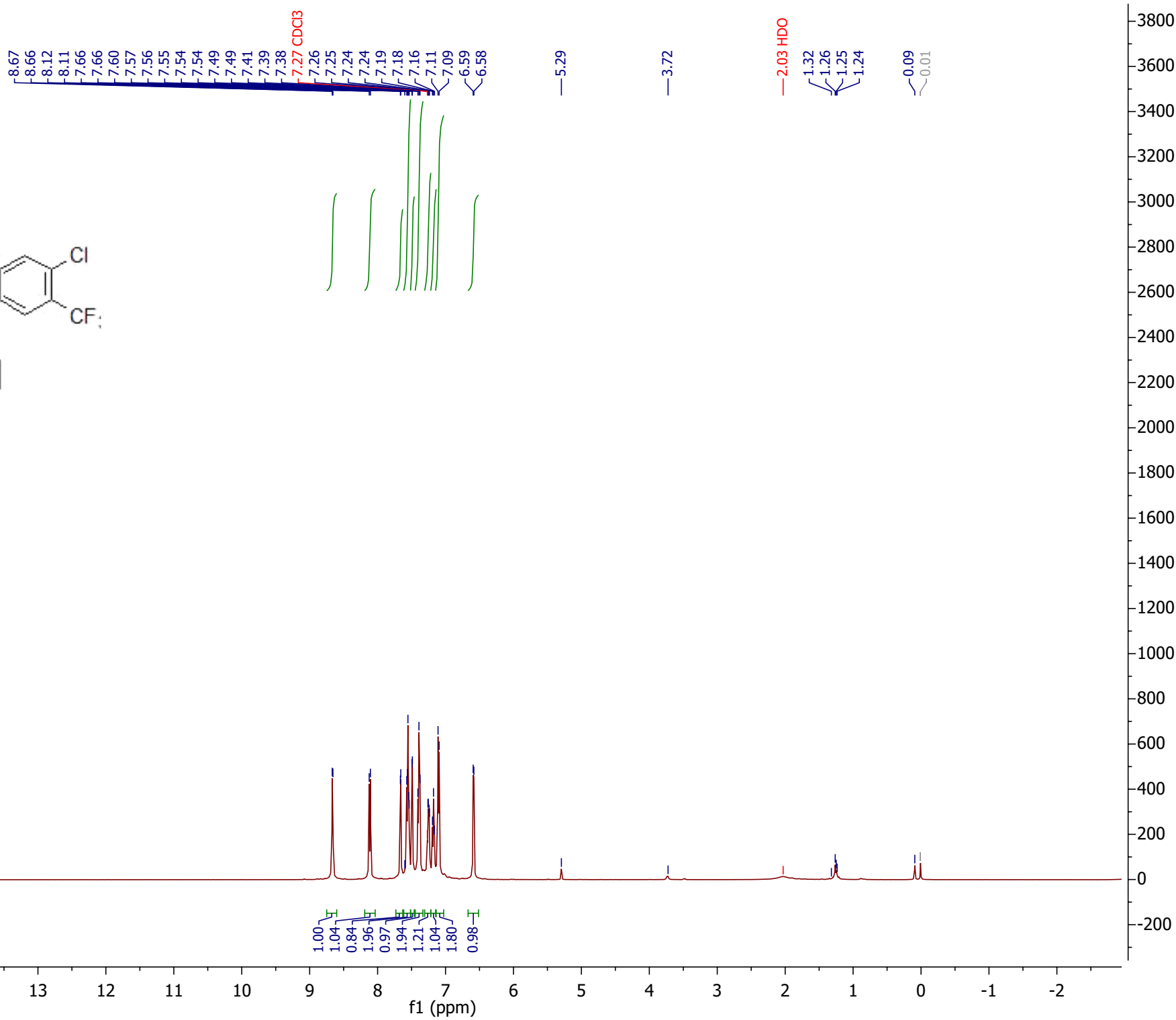


7b





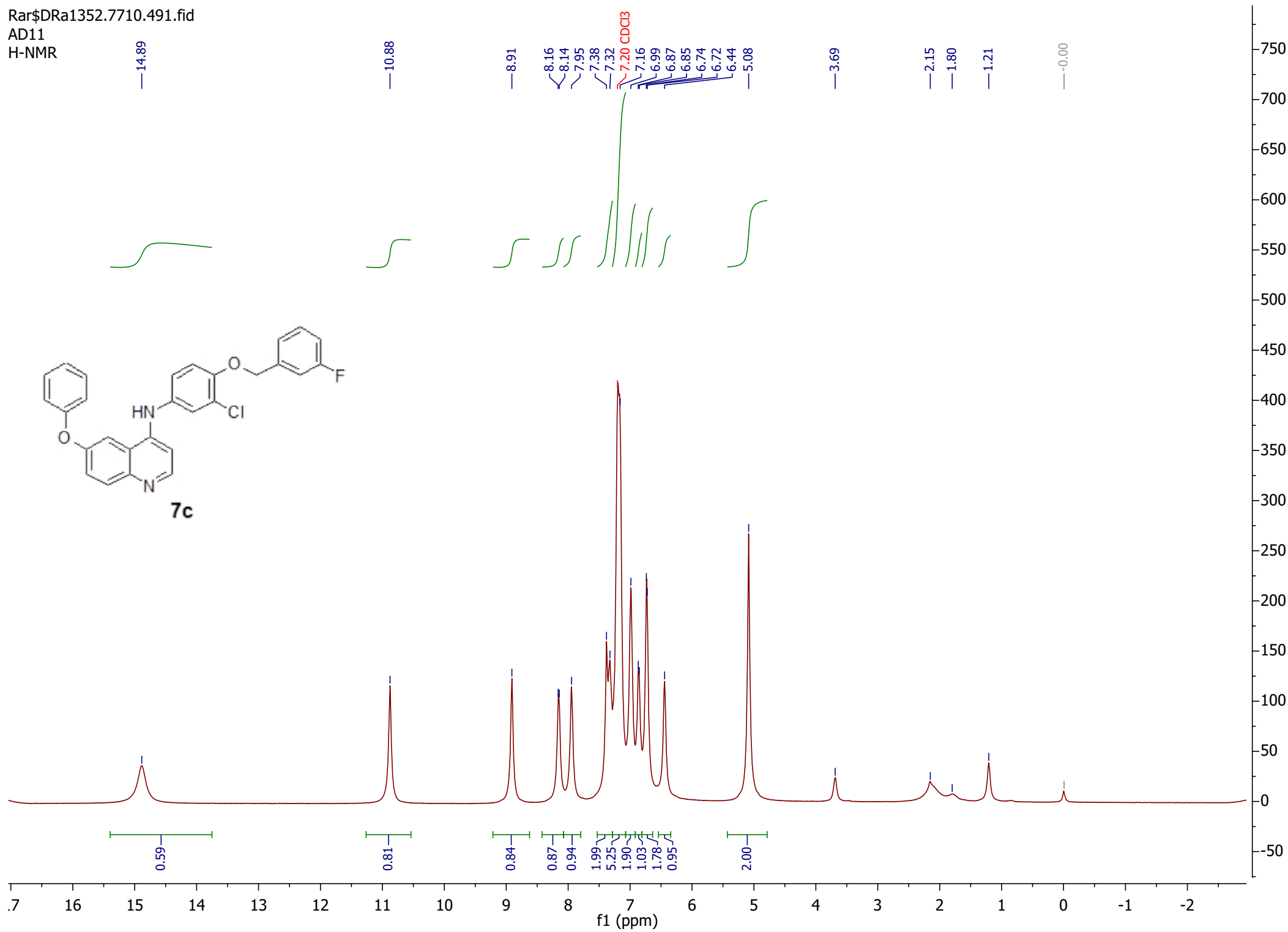
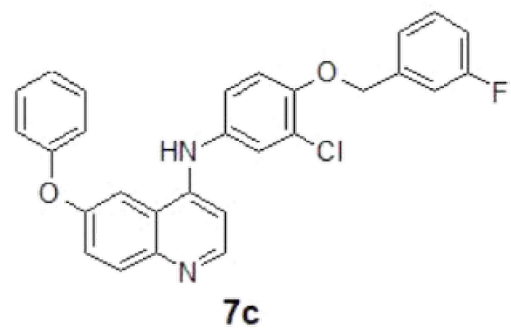
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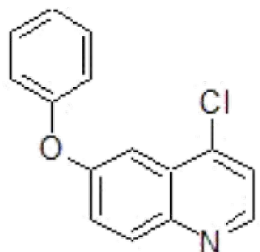


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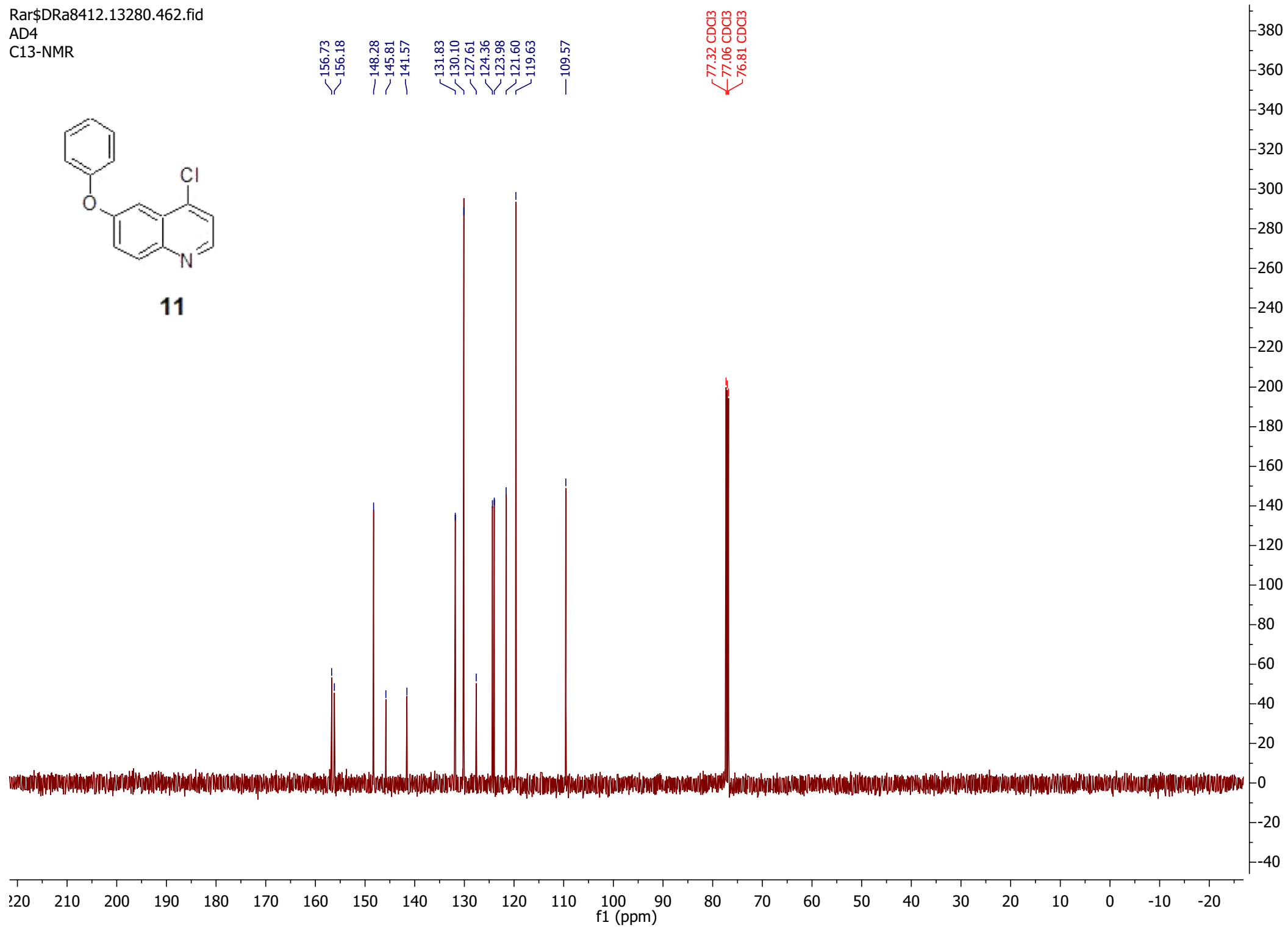
AD11

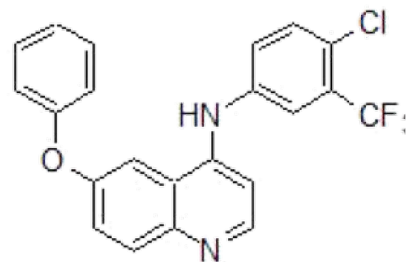
H-NMR



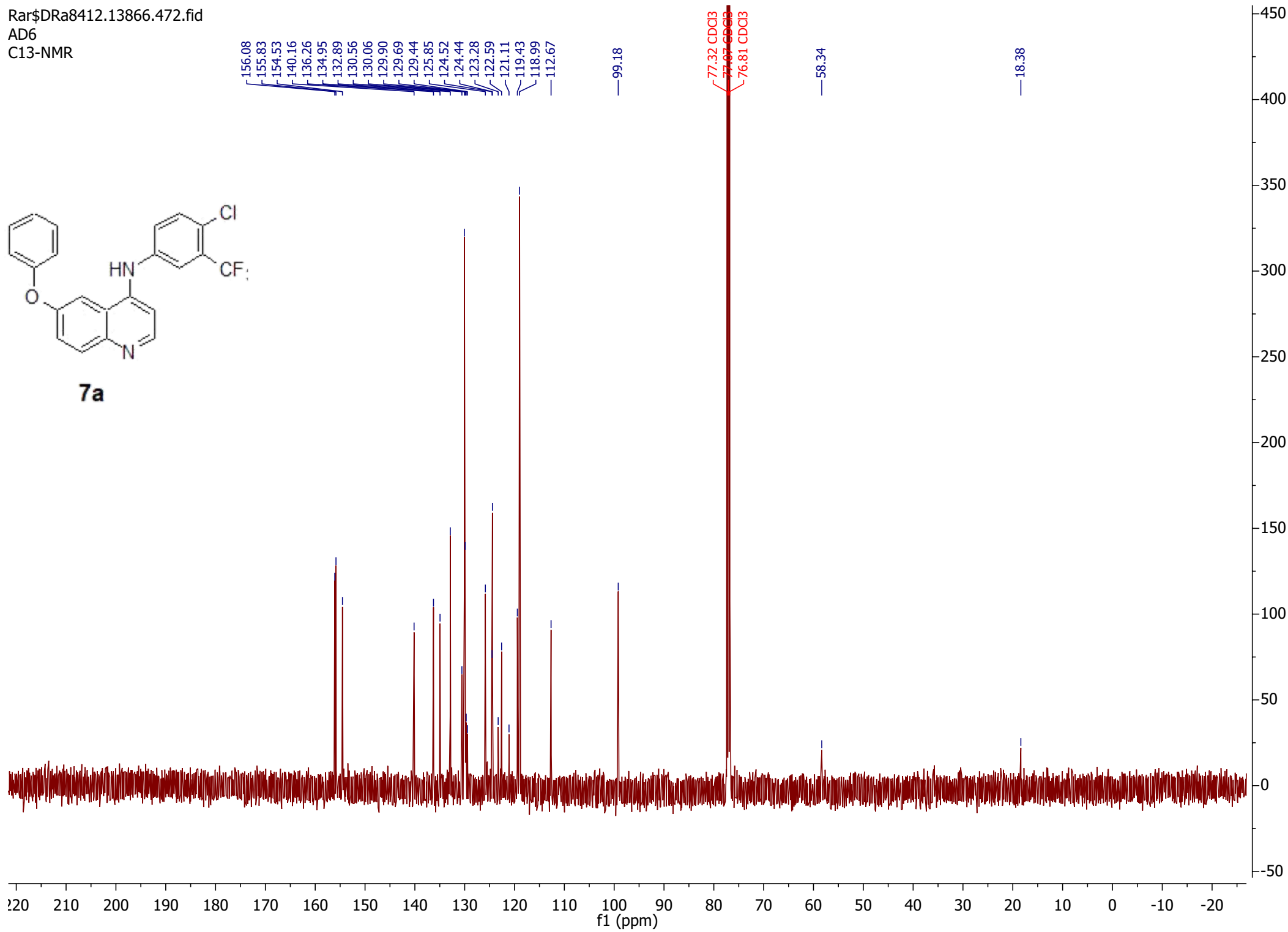


**11**

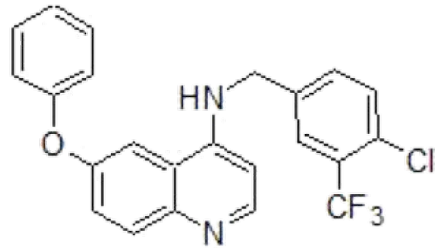




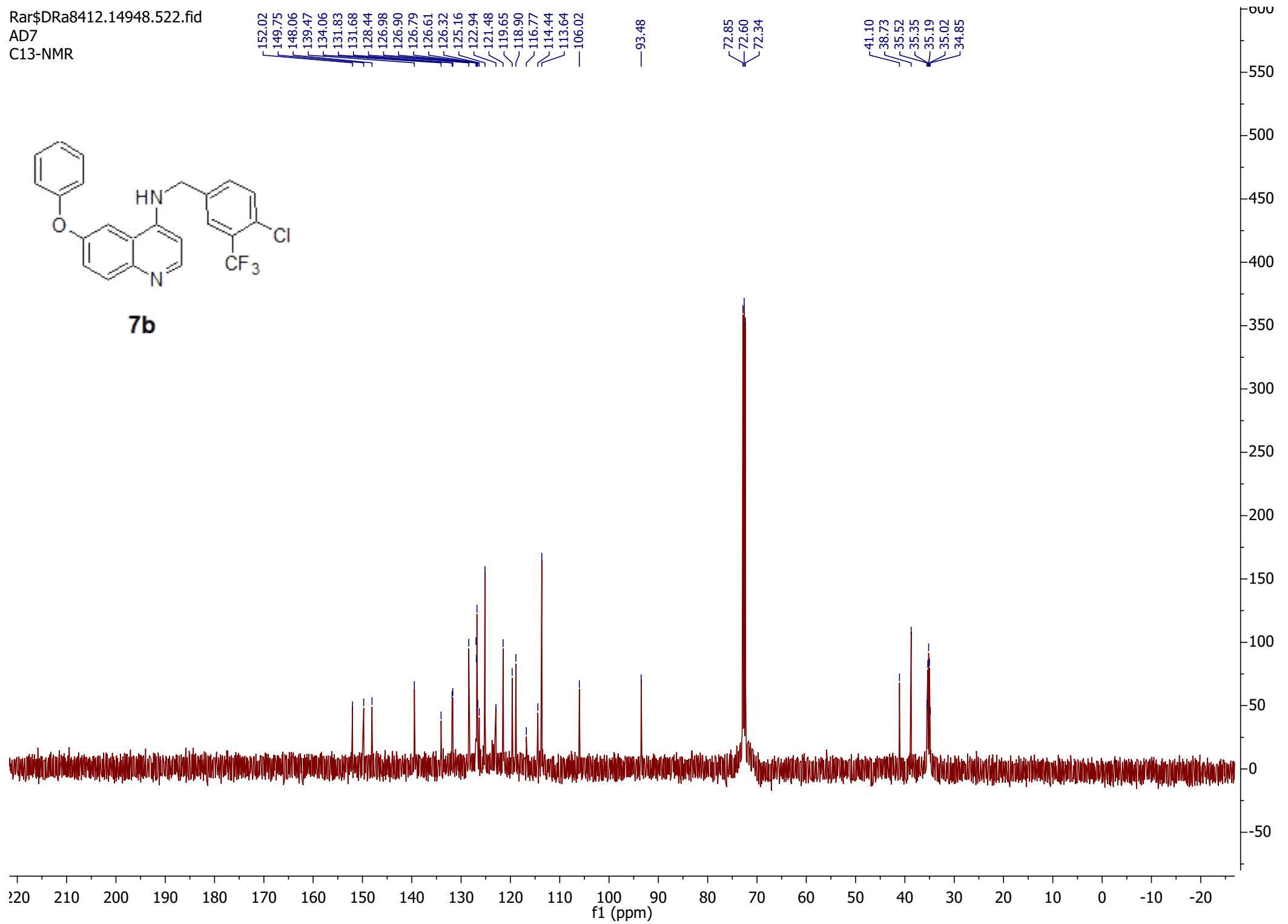
**7a**

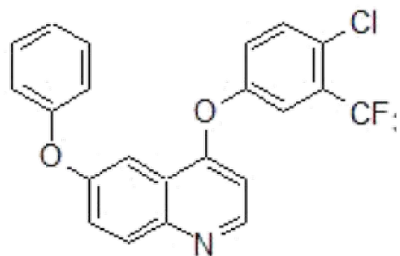


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AD7  
C13-NMR

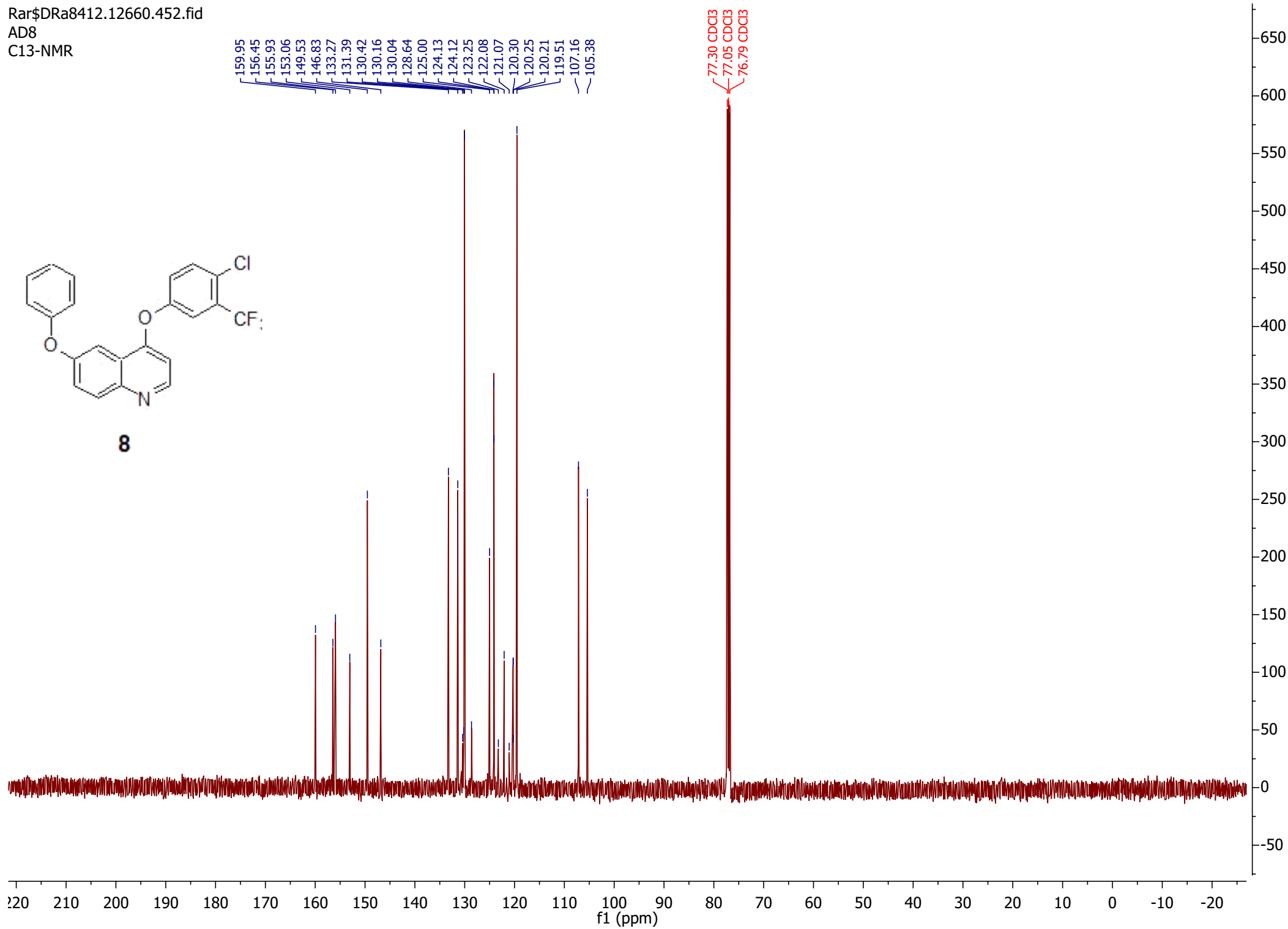


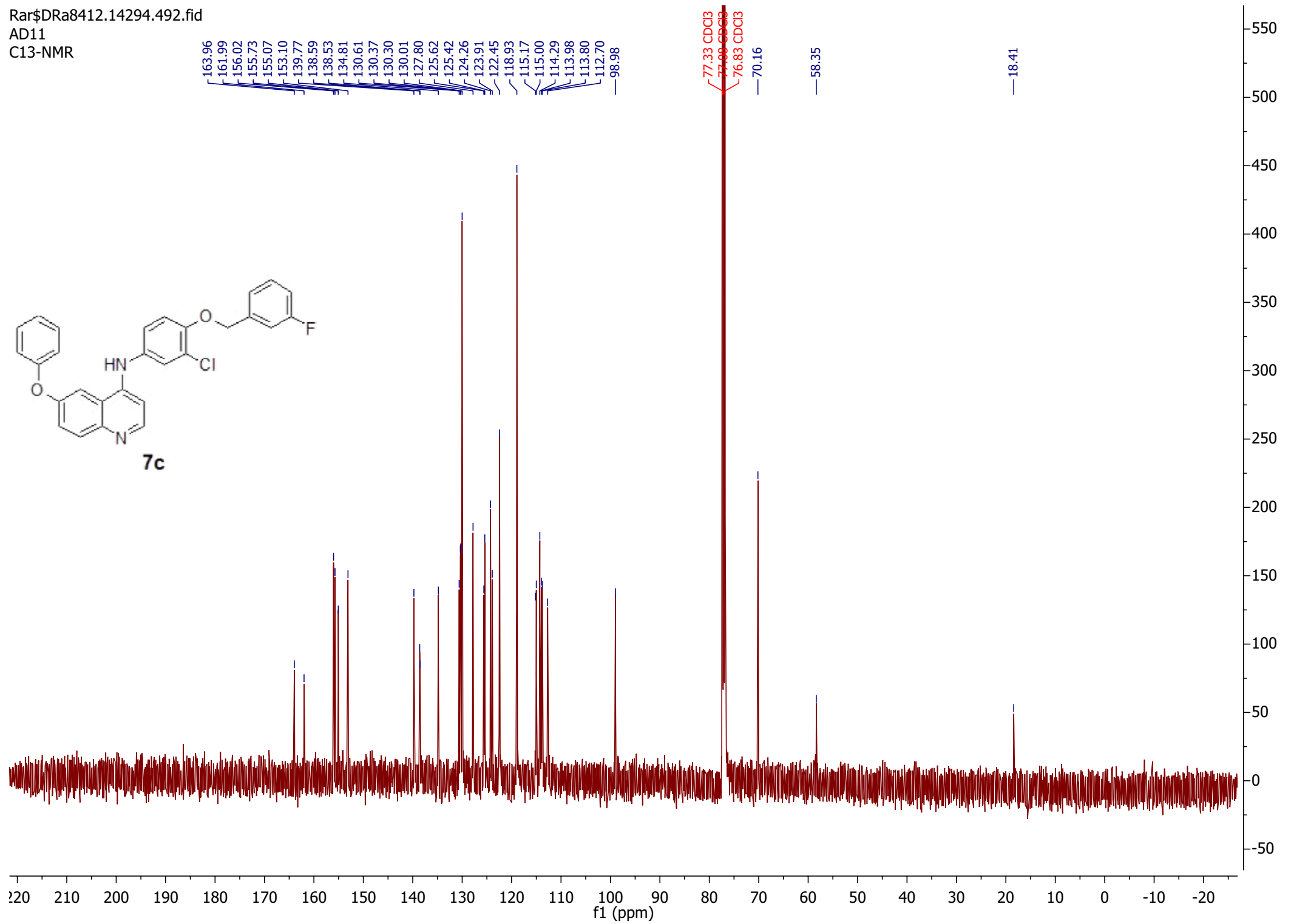
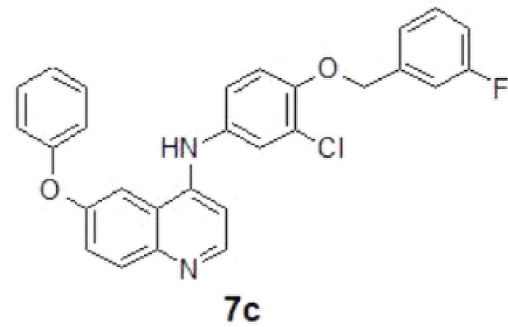
**7b**





8





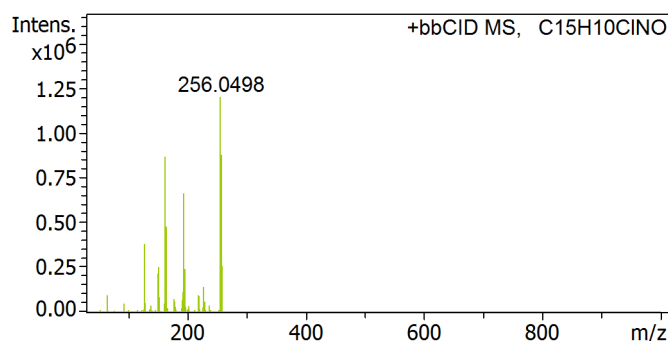
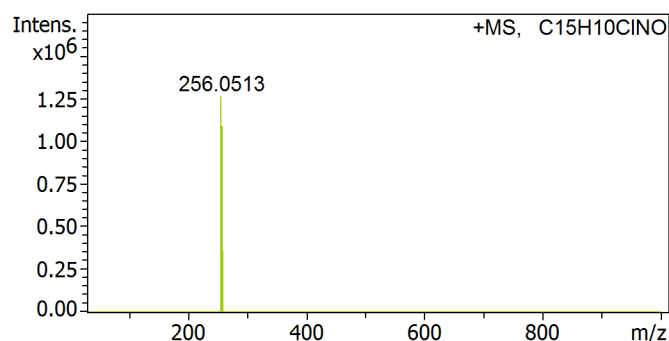
# Compound Spectrum List Report

Analysis Info QAD 4 Acquisition Date 9/09/2023  
Method Kailani\_MS/MS Operator Naba Hikma  
Instrument impact II 1825265.10265

## Acquisition Parameter

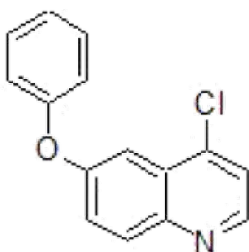
Source Type ESI Ion Polarity Positive Set Nebulizer 2.0 Bar  
Focus Active Set Capillary 2500 V Set Dry Heater 200 °C  
Scan Begin 30 m/z Set End Plate Offset -500 V Set Dry Gas 8.0 l/min  
Scan End 1000 m/z Set Charging Voltage 2000 V

## C15H10ClNO



| #  | m/z      | Res.  | S/N   | I       | I%    | FWHM   |
|----|----------|-------|-------|---------|-------|--------|
| 1  | 255.9523 | 13218 | 3.8   | 5269    | 0.4   | 0.0194 |
| 2  | 255.9924 | 8258  | 4.7   | 6453    | 0.5   | 0.0310 |
| 3  | 256.0513 | 11142 | 910.2 | 1262725 | 100.0 | 0.0230 |
| 4  | 256.1720 | 48651 | 22.1  | 30628   | 2.4   | 0.0053 |
| 5  | 256.2640 | 33506 | 12.2  | 16961   | 1.3   | 0.0076 |
| 6  | 256.5444 | 45370 | 61.1  | 84718   | 6.7   | 0.0057 |
| 7  | 257.0524 | 26109 | 637.6 | 884470  | 70.0  | 0.0098 |
| 8  | 258.0474 | 17565 | 784.1 | 1087719 | 86.1  | 0.0147 |
| 9  | 259.0493 | 37389 | 258.7 | 358946  | 28.4  | 0.0069 |
| 10 | 260.0524 | 34339 | 21.7  | 30166   | 2.4   | 0.0076 |

| #  | m/z      | Res.  | S/N   | I       | I%    | FWHM   |
|----|----------|-------|-------|---------|-------|--------|
| 1  | 128.0474 | 27357 | 311.7 | 381534  | 31.7  | 0.0047 |
| 2  | 151.0158 | 28006 | 208.0 | 254679  | 21.2  | 0.0054 |
| 3  | 163.0162 | 16987 | 709.4 | 868495  | 72.1  | 0.0096 |
| 4  | 165.0128 | 28454 | 392.5 | 480484  | 39.9  | 0.0058 |
| 5  | 195.0053 | 28421 | 541.8 | 663260  | 55.1  | 0.0069 |
| 6  | 197.0023 | 32122 | 198.4 | 242864  | 20.2  | 0.0061 |
| 7  | 256.0498 | 13465 | 983.4 | 1203855 | 100.0 | 0.0190 |
| 8  | 257.0523 | 27456 | 526.4 | 644439  | 53.5  | 0.0094 |
| 9  | 258.0460 | 20512 | 717.5 | 878421  | 73.0  | 0.0126 |
| 10 | 259.0493 | 38016 | 213.5 | 261402  | 21.7  | 0.0068 |



11

# Compound Spectrum List Report

Analysis Info

QAD 6

Acquisition Date

9/09/2023

Method

Kailani\_MS/MS

Operator

Naba Hikma

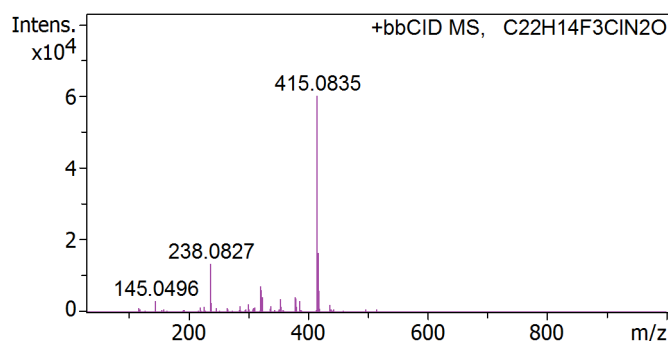
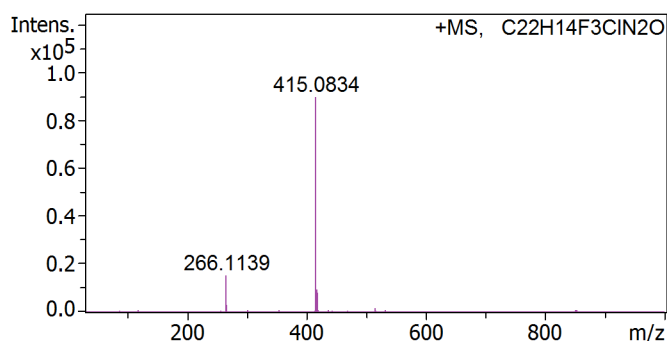
Instrument impact II

1825265.10265

## Acquisition Parameter

|             |          |                      |          |                |           |
|-------------|----------|----------------------|----------|----------------|-----------|
| Source Type | ESI      | Ion Polarity         | Positive | Set Nebulizer  | 2.0 Bar   |
| Focus       | Active   | Set Capillary        | 2500 V   | Set Dry Heater | 200 °C    |
| Scan Begin  | 30 m/z   | Set End Plate Offset | -500 V   | Set Dry Gas    | 8.0 l/min |
| Scan End    | 1000 m/z | Set Charging Voltage | 2000 V   |                |           |

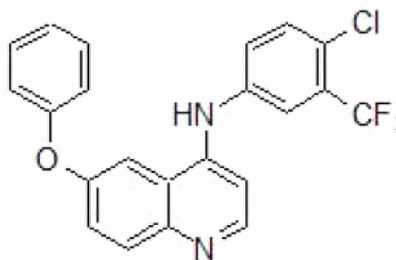
## C22H14F3ClN2O



| #  | m/z      | Res.  | S/N   | I     | I%    | FWHM   |
|----|----------|-------|-------|-------|-------|--------|
| 1  | 266.1139 | 34089 | 169.9 | 15521 | 17.3  | 0.0078 |
| 2  | 267.1173 | 30505 | 32.8  | 2995  | 3.3   | 0.0088 |
| 3  | 301.9958 | 34065 | 11.6  | 1063  | 1.2   | 0.0089 |
| 4  | 414.9764 | 14414 | 11.8  | 1081  | 1.2   | 0.0288 |
| 5  | 415.0834 | 11656 | 983.5 | 89837 | 100.0 | 0.0356 |
| 6  | 418.0767 | 45196 | 106.4 | 9720  | 10.8  | 0.0093 |
| 7  | 419.0799 | 42664 | 91.9  | 8391  | 9.3   | 0.0098 |
| 8  | 420.0832 | 36013 | 10.4  | 951   | 1.1   | 0.0117 |
| 9  | 515.1636 | 39021 | 17.5  | 1599  | 1.8   | 0.0132 |
| 10 | 851.1284 | 42273 | 11.5  | 1050  | 1.2   | 0.0201 |

| #  | m/z      | Res.  | S/N   | I     | I%    | FWHM   |
|----|----------|-------|-------|-------|-------|--------|
| 1  | 238.0827 | 32448 | 223.9 | 13495 | 22.4  | 0.0073 |
| 2  | 321.0352 | 33409 | 123.4 | 7442  | 12.4  | 0.0096 |
| 3  | 322.0427 | 34866 | 105.6 | 6364  | 10.6  | 0.0092 |
| 4  | 324.0399 | 31348 | 73.1  | 4407  | 7.3   | 0.0103 |
| 5  | 354.0328 | 33063 | 63.2  | 3809  | 6.3   | 0.0107 |
| 6  | 379.0995 | 35585 | 73.4  | 4423  | 7.4   | 0.0107 |
| 7  | 380.1058 | 31392 | 67.3  | 4057  | 6.7   | 0.0121 |
| 8  | 415.0835 | 11096 | 997.5 | 60135 | 100.0 | 0.0374 |
| 9  | 418.0765 | 45010 | 275.8 | 16627 | 27.6  | 0.0093 |
| 10 | 419.0796 | 42586 | 102.7 | 6192  | 10.3  | 0.0098 |

Type text here



7a

# Compound Spectrum List Report

Analysis Info

QAD 7

Acquisition Date

9/09/2023

Method

Kailani\_MS/MS

Operator

Naba Hikma

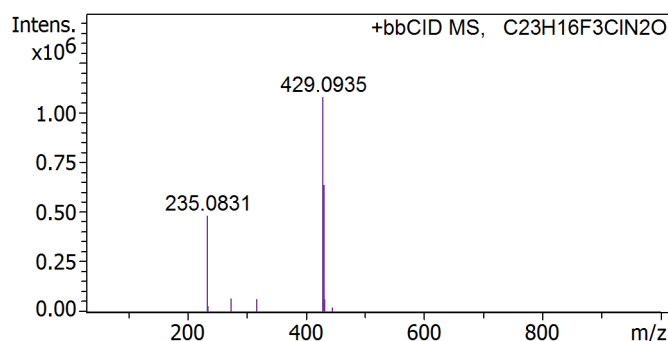
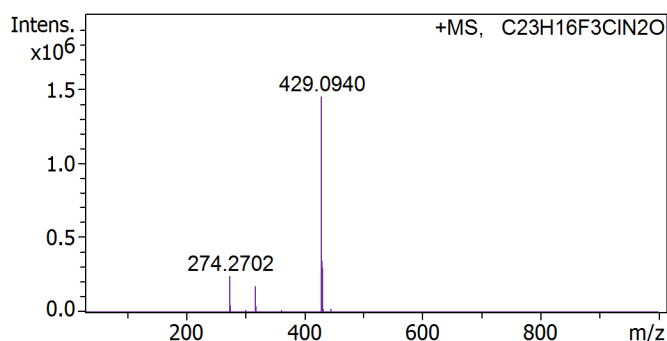
Instrument impact II

1825265.10265

## Acquisition Parameter

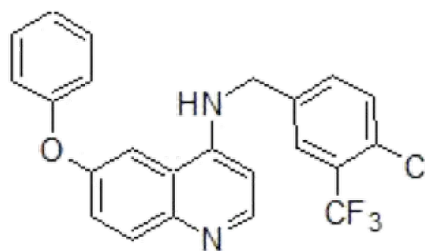
|             |          |                      |          |                |           |
|-------------|----------|----------------------|----------|----------------|-----------|
| Source Type | ESI      | Ion Polarity         | Positive | Set Nebulizer  | 2.0 Bar   |
| Focus       | Active   | Set Capillary        | 2500 V   | Set Dry Heater | 200 °C    |
| Scan Begin  | 30 m/z   | Set End Plate Offset | -500 V   | Set Dry Gas    | 8.0 l/min |
| Scan End    | 1000 m/z | Set Charging Voltage | 2000 V   |                |           |

## C23H16F3ClN2O



| #  | m/z      | Res.  | S/N   | I       | I %   | FWHM   |
|----|----------|-------|-------|---------|-------|--------|
| 1  | 274.2702 | 36172 | 161.2 | 247282  | 17.0  | 0.0076 |
| 2  | 275.2736 | 33459 | 28.8  | 44200   | 3.0   | 0.0082 |
| 3  | 318.2961 | 37424 | 115.0 | 176342  | 12.1  | 0.0085 |
| 4  | 319.2995 | 34928 | 25.3  | 38880   | 2.7   | 0.0091 |
| 5  | 429.0940 | 19165 | 946.2 | 1451508 | 100.0 | 0.0224 |
| 6  | 429.7299 | 56700 | 23.6  | 36128   | 2.5   | 0.0076 |
| 7  | 430.0951 | 36794 | 227.0 | 348206  | 24.0  | 0.0117 |
| 8  | 431.0894 | 31350 | 197.5 | 302897  | 20.9  | 0.0138 |
| 9  | 432.0920 | 46603 | 15.9  | 24459   | 1.7   | 0.0093 |
| 10 | 445.0866 | 38934 | 14.2  | 21714   | 1.5   | 0.0114 |

| #  | m/z      | Res.  | S/N   | I       | I %   | FWHM   |
|----|----------|-------|-------|---------|-------|--------|
| 1  | 235.0831 | 24910 | 445.9 | 485355  | 44.9  | 0.0094 |
| 2  | 236.0891 | 32676 | 28.0  | 30525   | 2.8   | 0.0072 |
| 3  | 274.2701 | 35749 | 66.5  | 72376   | 6.7   | 0.0077 |
| 4  | 318.2960 | 37770 | 62.4  | 67903   | 6.3   | 0.0084 |
| 5  | 429.0935 | 19148 | 992.1 | 1079857 | 100.0 | 0.0224 |
| 6  | 429.7300 | 57748 | 24.6  | 26727   | 2.5   | 0.0074 |
| 7  | 430.0950 | 36583 | 392.0 | 426701  | 39.5  | 0.0118 |
| 8  | 431.0892 | 31558 | 585.8 | 637565  | 59.0  | 0.0137 |
| 9  | 432.0920 | 46686 | 64.3  | 69967   | 6.5   | 0.0093 |
| 10 | 445.0865 | 39215 | 20.6  | 22464   | 2.1   | 0.0113 |



**7b**

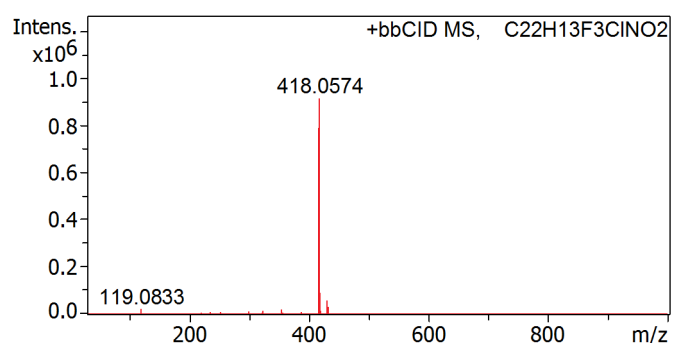
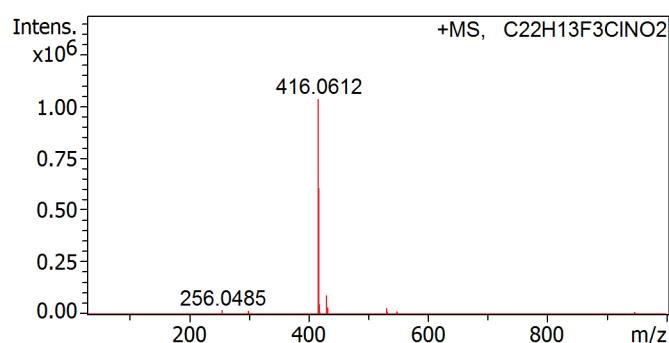
# Compound Spectrum List Report

Analysis Info QAD 8 Acquisition Date 9/09/2023  
Method Kailani\_MS/MS Operator Naba Hikma  
Instrument impact II 1825265.10265

## Acquisition Parameter

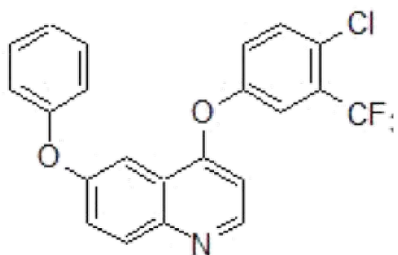
Source Type ESI Ion Polarity Positive Set Nebulizer 2.0 Bar  
Focus Active Set Capillary 2500 V Set Dry Heater 200 °C  
Scan Begin 30 m/z Set End Plate Offset -500 V Set Dry Gas 8.0 l/min  
Scan End 1000 m/z Set Charging Voltage 2000 V

## C22H13F3ClNO2



| #  | m/z      | Res.  | S/N   | I       | I%    | FWHM   |
|----|----------|-------|-------|---------|-------|--------|
| 1  | 256.0485 | 34866 | 18.7  | 19516   | 1.9   | 0.0073 |
| 2  | 299.9974 | 35562 | 14.8  | 15404   | 1.5   | 0.0084 |
| 3  | 416.0612 | 23142 | 994.2 | 1036211 | 100.0 | 0.0180 |
| 4  | 417.0633 | 47170 | 258.6 | 269504  | 26.0  | 0.0088 |
| 5  | 418.0572 | 43528 | 581.6 | 606146  | 58.5  | 0.0096 |
| 6  | 419.0605 | 45316 | 47.5  | 49512   | 4.8   | 0.0092 |
| 7  | 430.0755 | 41993 | 89.5  | 93273   | 9.0   | 0.0102 |
| 8  | 431.0790 | 38481 | 31.5  | 32797   | 3.2   | 0.0112 |
| 9  | 432.0730 | 37444 | 29.7  | 30948   | 3.0   | 0.0115 |
| 10 | 531.2667 | 41526 | 26.5  | 27650   | 2.7   | 0.0128 |

| #  | m/z      | Res.  | S/N   | I      | I%    | FWHM   |
|----|----------|-------|-------|--------|-------|--------|
| 1  | 119.0833 | 25123 | 23.5  | 21670  | 2.4   | 0.0047 |
| 2  | 323.0269 | 37869 | 17.5  | 16136  | 1.8   | 0.0085 |
| 3  | 355.0168 | 37179 | 21.0  | 19330  | 2.1   | 0.0095 |
| 4  | 416.0615 | 20361 | 856.2 | 789017 | 86.2  | 0.0204 |
| 5  | 417.0634 | 45359 | 466.4 | 429794 | 47.0  | 0.0092 |
| 6  | 418.0574 | 38135 | 993.1 | 915213 | 100.0 | 0.0110 |
| 7  | 419.0606 | 45862 | 101.1 | 93196  | 10.2  | 0.0091 |
| 8  | 430.0755 | 42544 | 65.3  | 60187  | 6.6   | 0.0101 |
| 9  | 431.0788 | 39564 | 29.7  | 27376  | 3.0   | 0.0109 |
| 10 | 432.0729 | 37809 | 34.8  | 32110  | 3.5   | 0.0114 |



8

# Compound Spectrum List Report

Analysis Info

QAD 11

Acquisition Date

9/09/2023

Method

Kailani\_MS/MS

Operator

Naba Hikma

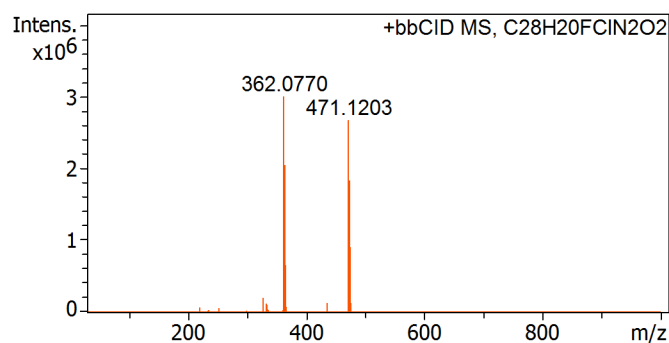
Instrument impact II

1825265.10265

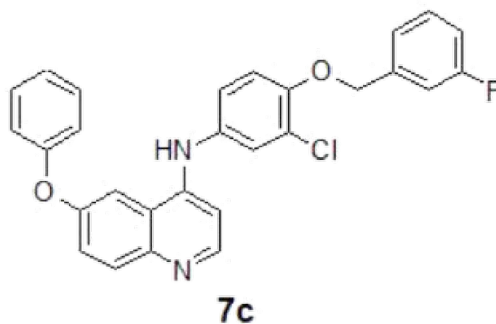
## Acquisition Parameter

|             |          |                      |          |                |           |
|-------------|----------|----------------------|----------|----------------|-----------|
| Source Type | ESI      | Ion Polarity         | Positive | Set Nebulizer  | 2.0 Bar   |
| Focus       | Active   | Set Capillary        | 2500 V   | Set Dry Heater | 200 °C    |
| Scan Begin  | 30 m/z   | Set End Plate Offset | -500 V   | Set Dry Gas    | 8.0 l/min |
| Scan End    | 1000 m/z | Set Charging Voltage | 2000 V   |                |           |

## C28H20FCIN2O2

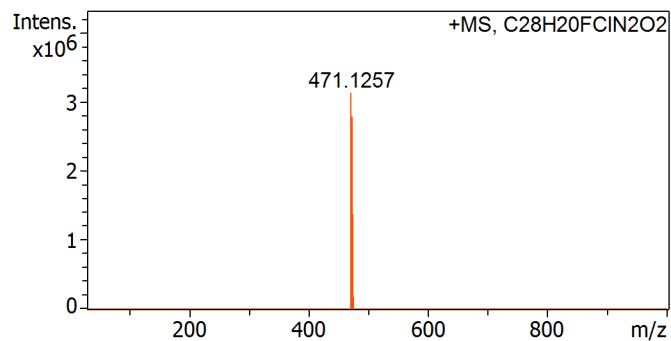


| #  | m/z      | Res.  | S/N        | I       | I %   | FWHM   |
|----|----------|-------|------------|---------|-------|--------|
| 1  | 327.1077 | 36821 | 1277755.3  | 210678  | 7.0   | 0.0089 |
| 2  | 362.0770 | 19829 | 18252024.0 | 3009413 | 100.0 | 0.0183 |
| 3  | 363.0798 | 31022 | 11087186.0 | 1828067 | 60.7  | 0.0117 |
| 4  | 364.0743 | 25125 | 12424277.0 | 2048528 | 68.1  | 0.0145 |
| 5  | 365.0766 | 39461 | 3988196.3  | 657578  | 21.9  | 0.0093 |
| 6  | 435.1443 | 40530 | 789934.5   | 130245  | 4.3   | 0.0107 |
| 7  | 471.1203 | 20052 | 16168759.0 | 2665922 | 88.6  | 0.0235 |
| 8  | 472.1244 | 27032 | 10902825.0 | 1797669 | 59.7  | 0.0175 |
| 9  | 473.1185 | 24229 | 11141909.0 | 1837090 | 61.0  | 0.0195 |
| 10 | 474.1216 | 48615 | 5508679.0  | 908277  | 30.2  | 0.0098 |



# Compound Spectrum List Report

C28H20FCIN2O2



| #  | m/z      | Res.  | S/N        | I       | I %   | FWHM   |
|----|----------|-------|------------|---------|-------|--------|
| 1  | 471.0115 | 13923 | 92330.3    | 12981   | 0.4   | 0.0338 |
| 2  | 471.1257 | 15153 | 22255818.0 | 3128971 | 100.0 | 0.0311 |
| 3  | 471.2871 | 68322 | 259092.5   | 36426   | 1.2   | 0.0069 |
| 4  | 471.4120 | 43227 | 216421.5   | 30427   | 1.0   | 0.0109 |
| 5  | 471.7900 | 57501 | 785442.4   | 110426  | 3.5   | 0.0082 |
| 6  | 472.1253 | 26686 | 18789296.0 | 2641609 | 84.4  | 0.0177 |
| 7  | 473.1204 | 23577 | 19804288.0 | 2784308 | 89.0  | 0.0201 |
| 8  | 474.1216 | 47332 | 9783370.0  | 1375455 | 44.0  | 0.0100 |
| 9  | 475.1246 | 44551 | 1367273.9  | 192227  | 6.1   | 0.0107 |
| 10 | 476.1277 | 38222 | 88705.5    | 12471   | 0.4   | 0.0125 |