

Figure S1: Plots of the root mean square deviation (RMSD) and ligand-protein contacts for 88 in the HAP pocket during the 10 ns simulation time.

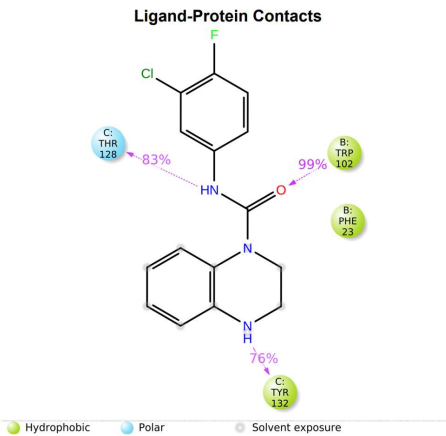
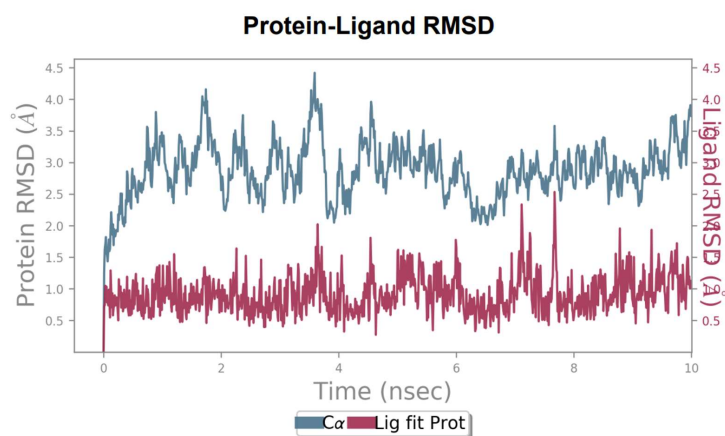


Figure S2: Plots of the root mean square deviation (RMSD) and ligand-protein contacts of 17 in the HAP pocket during the 10 ns simulation time.

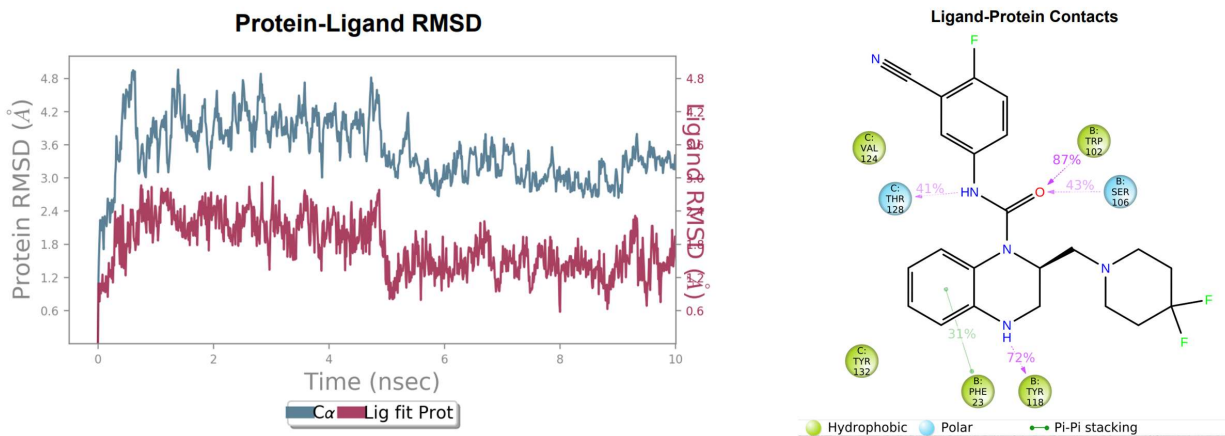


Figure S3: Plots of the root mean square deviation (RMSD) and ligand-protein contacts of 86 in the HAP pocket during the 10 ns simulation time.

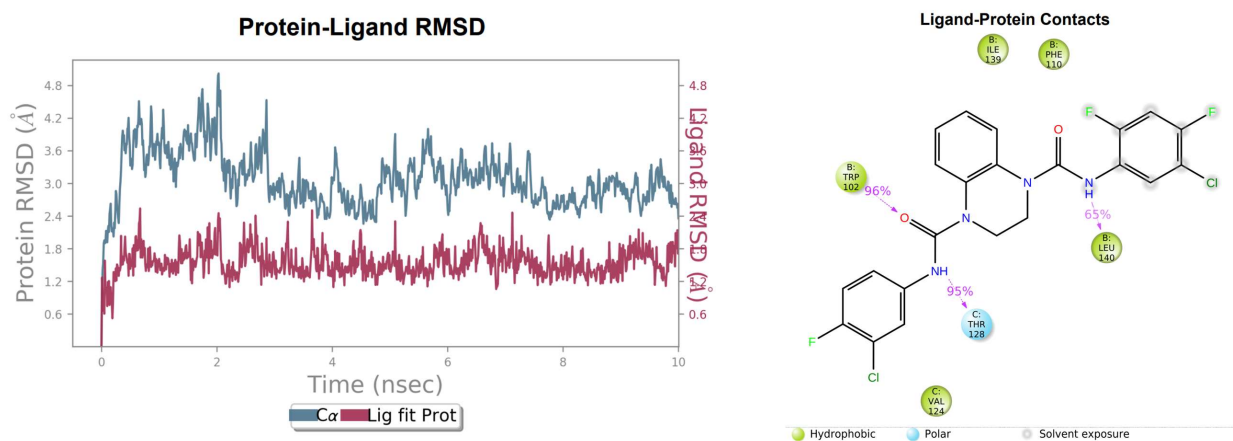


Figure S4: Plots of the root mean square deviation (RMSD) and ligand-protein contacts of 96 in the HAP pocket during the 10 ns simulation time.

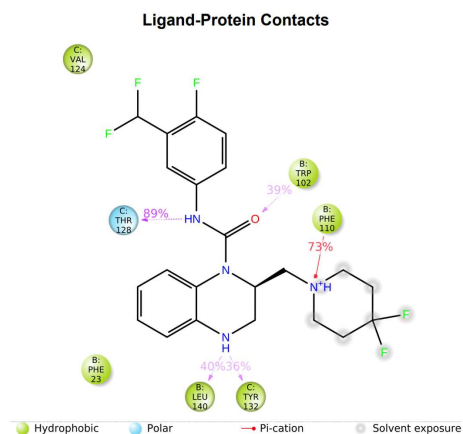
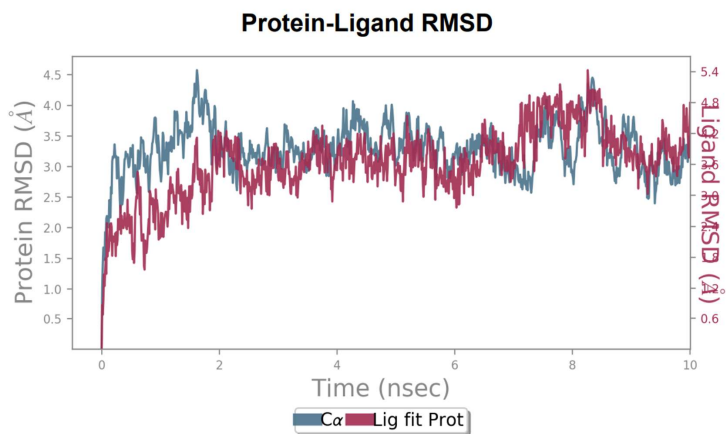
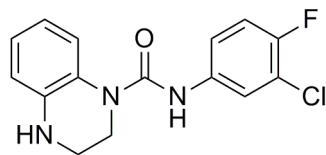
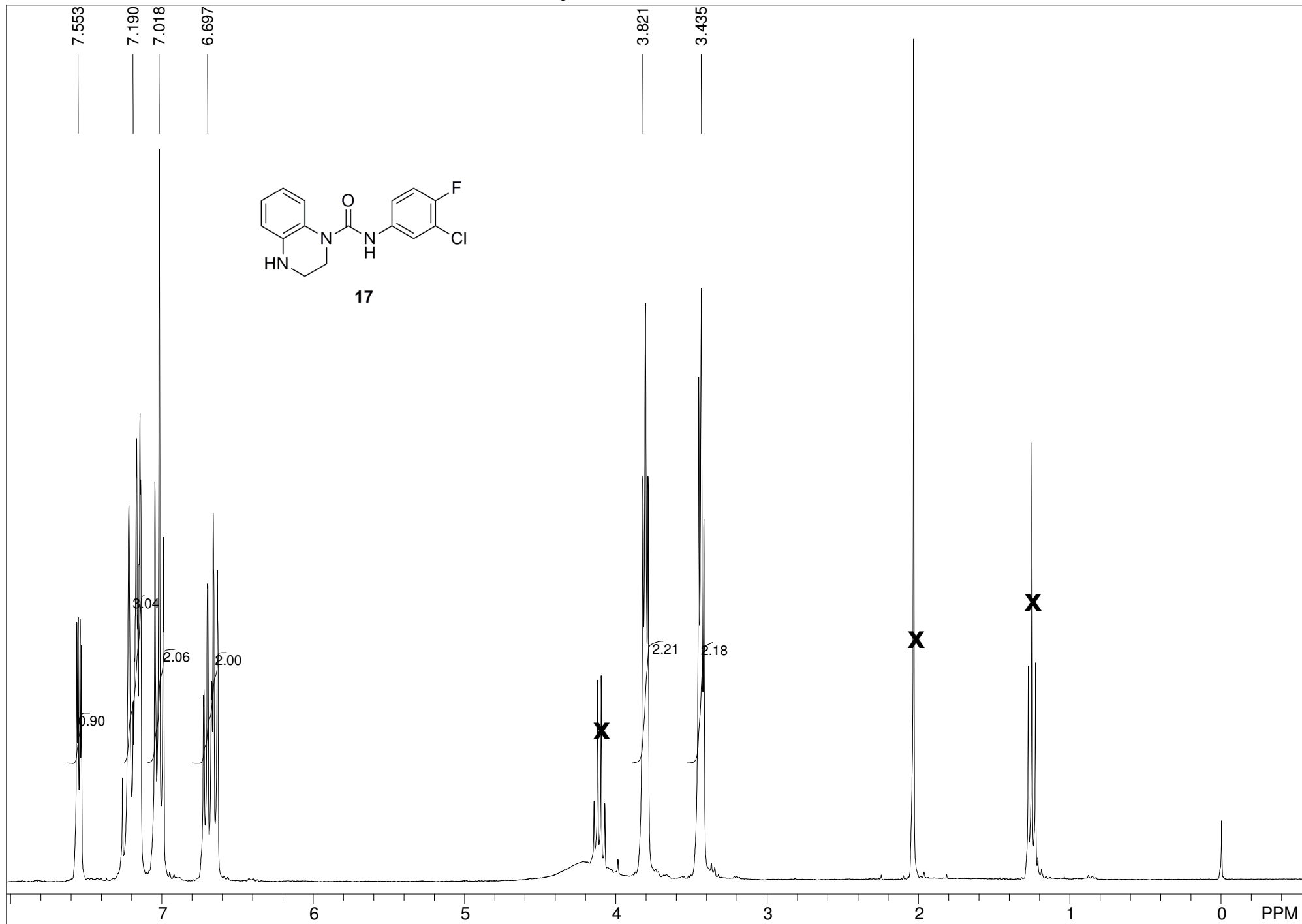


Figure S5: Plots of the root mean square deviation (RMSD) and ligand-protein contacts of 88 in the HAP pocket during the 10 ns simulation time.

<sup>1</sup>H NMR Spectrum (300 MHz, CDCl<sub>3</sub>) of 17



17



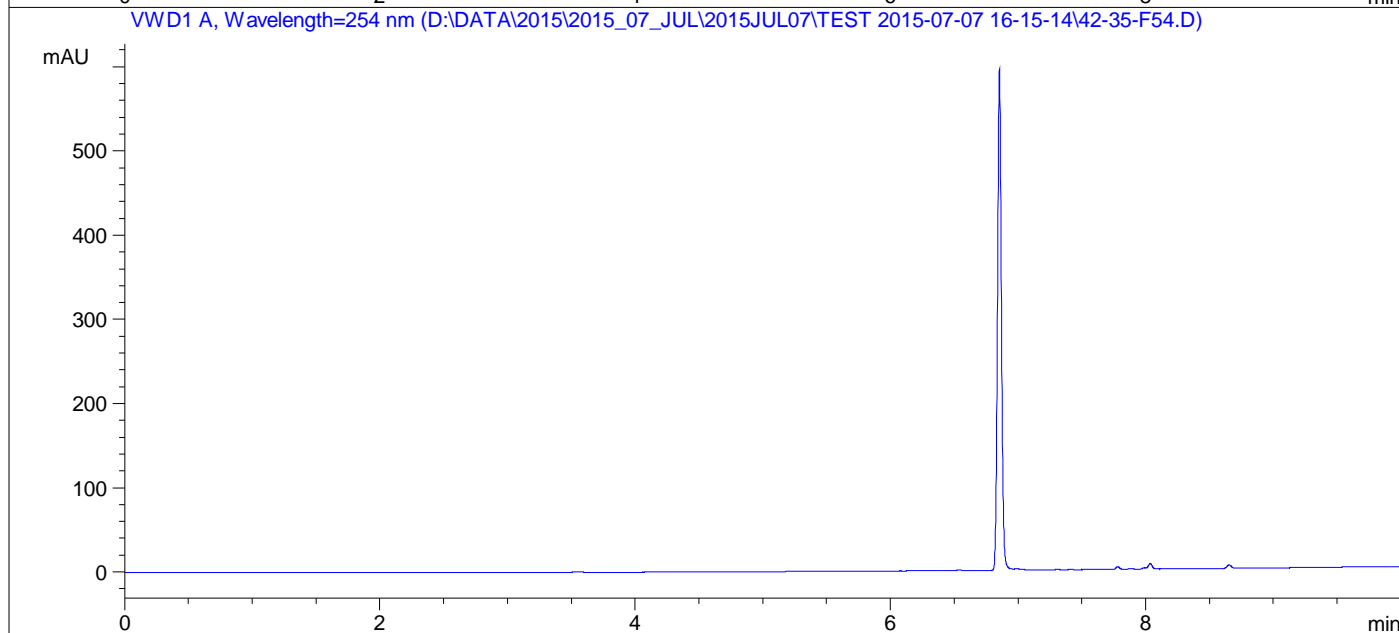
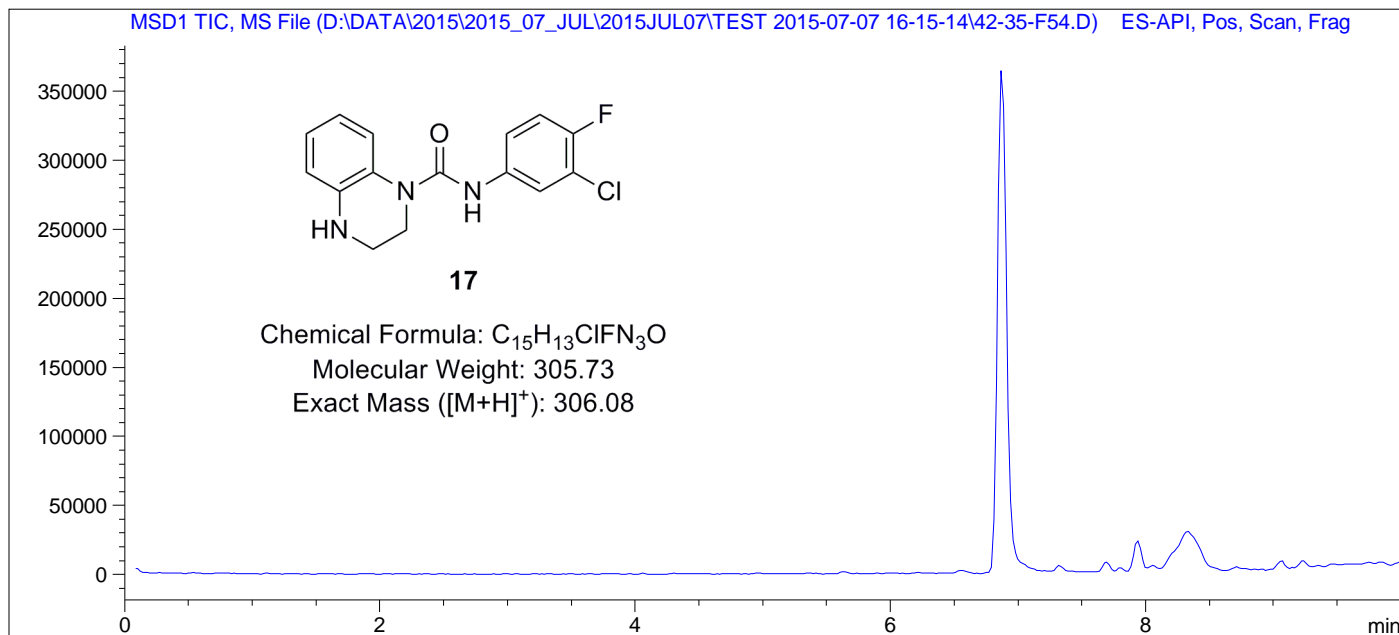
nh-43-98 20Nov2015

USER: -- DATE: Nov 20 2015 73:4

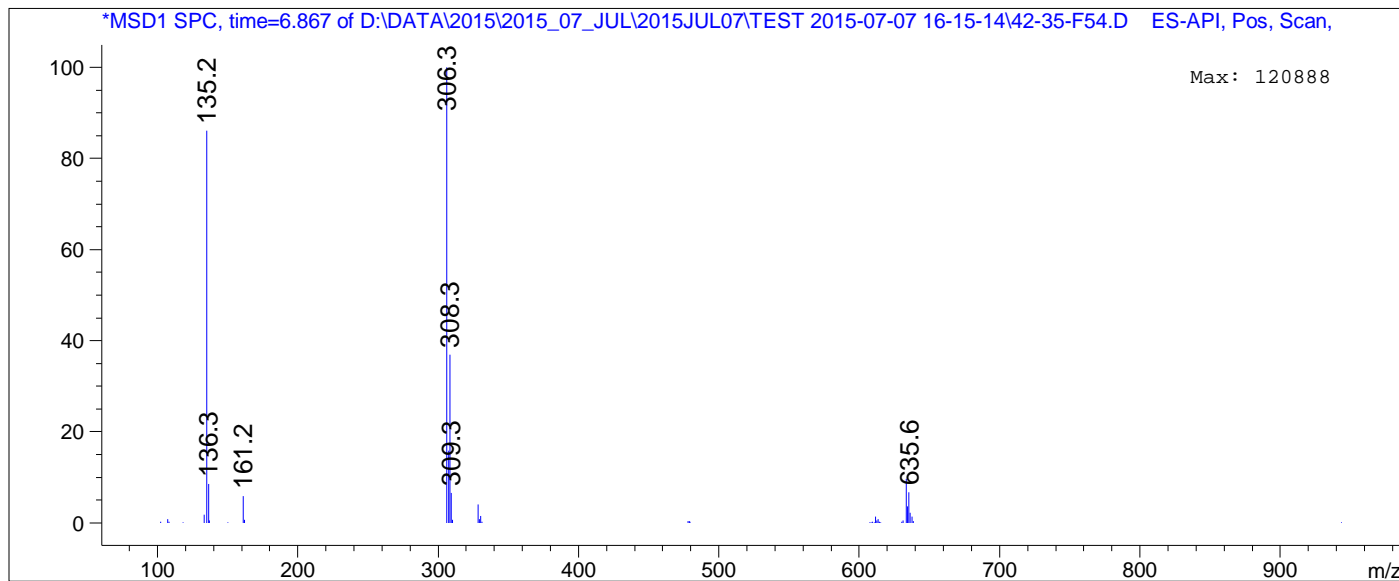
F1: 299.974	F2: 75.436	SW1: 4803	OF1: 1799.8	PTS1d: 9574	16384
EX: s2pul	PW: 6.6 us, 45deg	PD: 1.0 sec	NA: 16	LB: 0.3	Nuts - \$nh-43-98 PROTON.fid

## LCMS analysis of 17

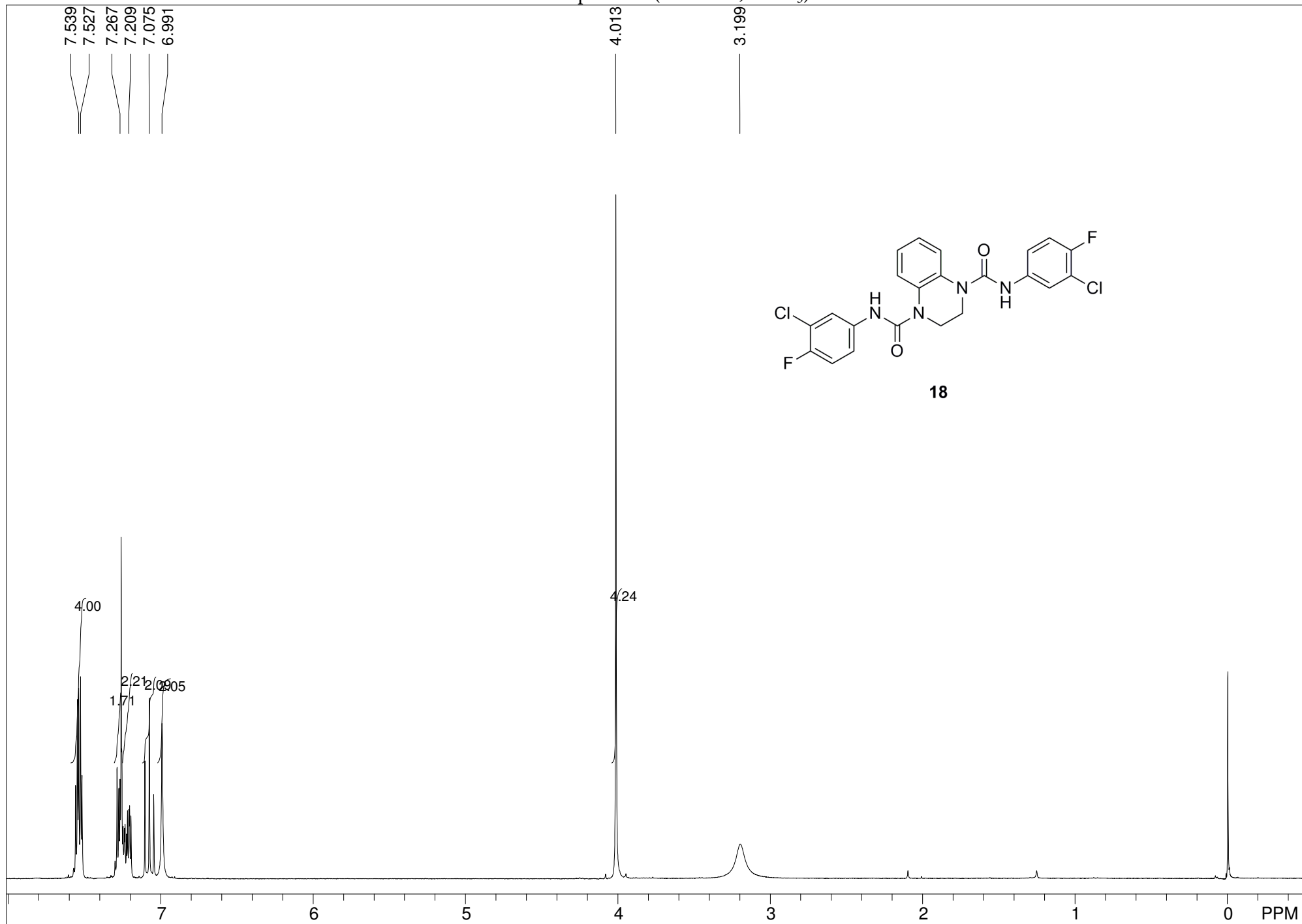
Current Chromatogram(s)



MS Spectrum



<sup>1</sup>H NMR Spectrum (300 MHz, CDCl<sub>3</sub>) of **18**



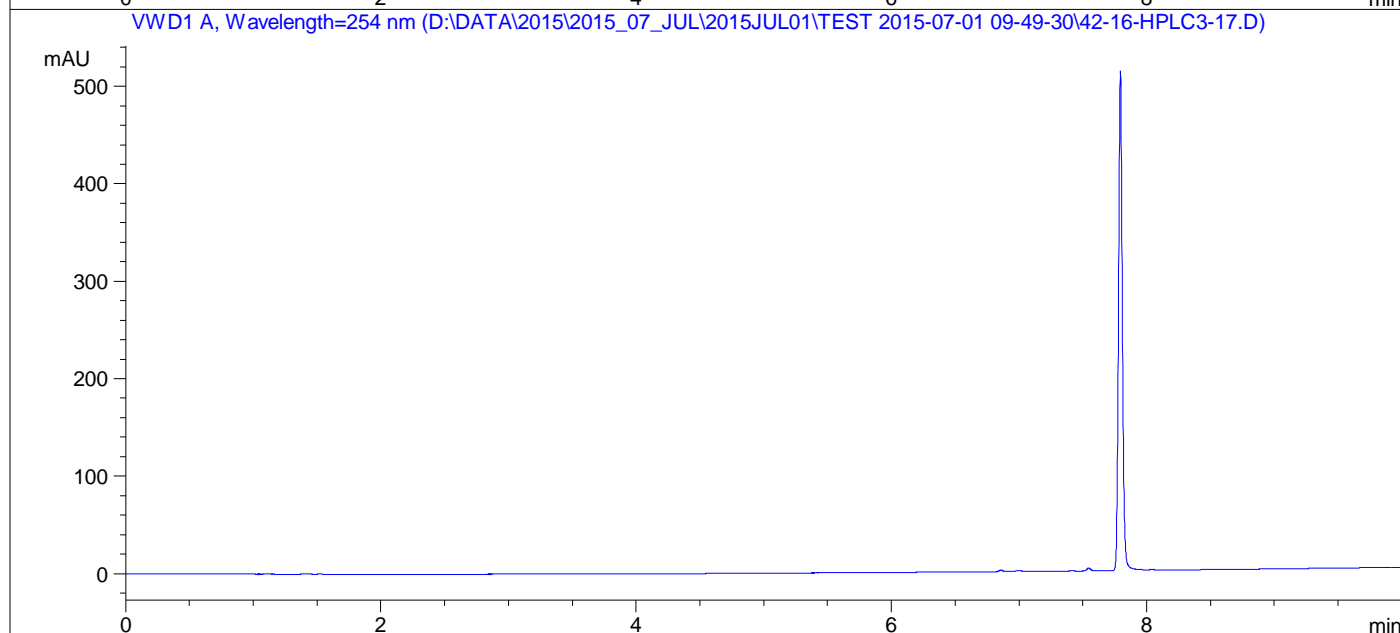
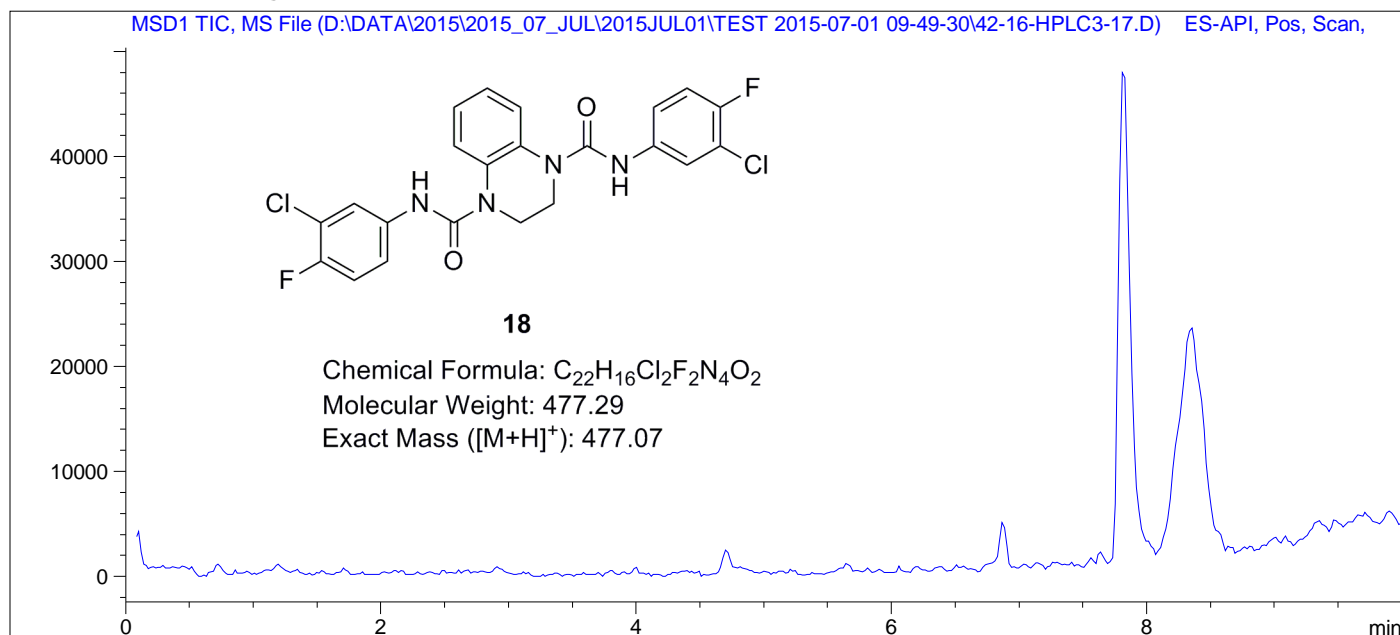
JL-42-16-DI 08Jul2015

USER: -- DATE: Jul 8 2015 "

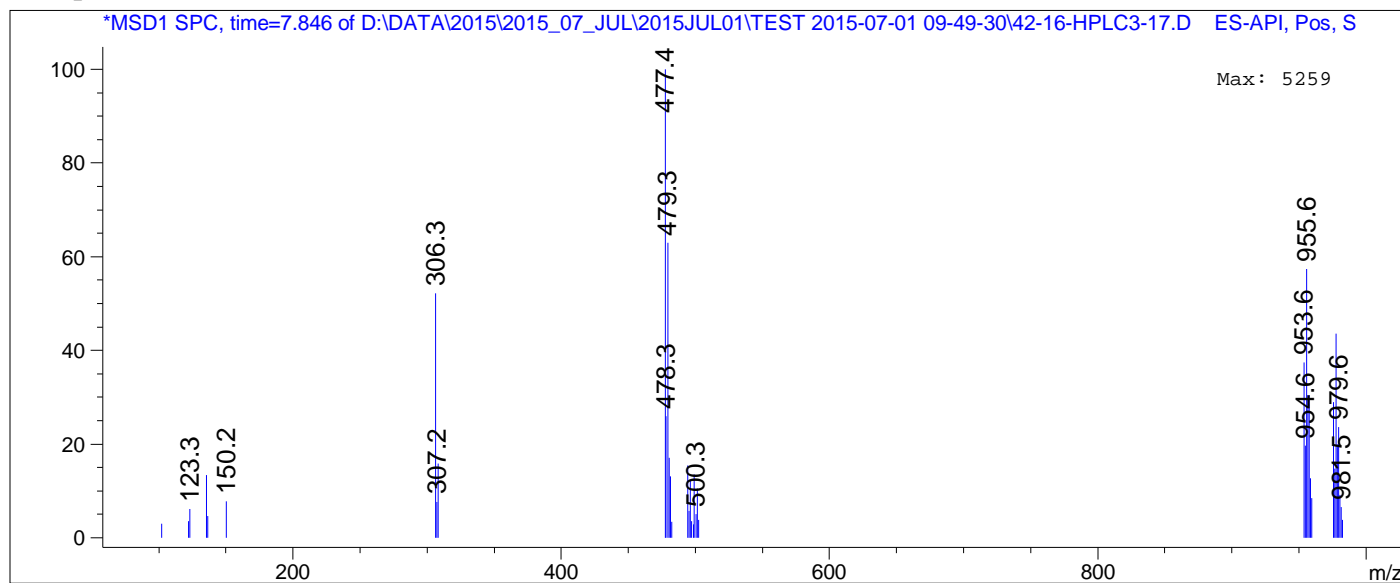
F1: 299.974	F2: 75.436	SW1: 4803		OF1: 1802.4		PTS1d: 9574 , 16384
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### LCMS analysis of 18

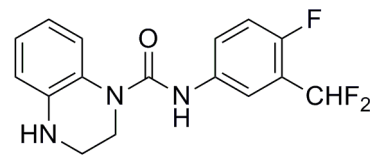
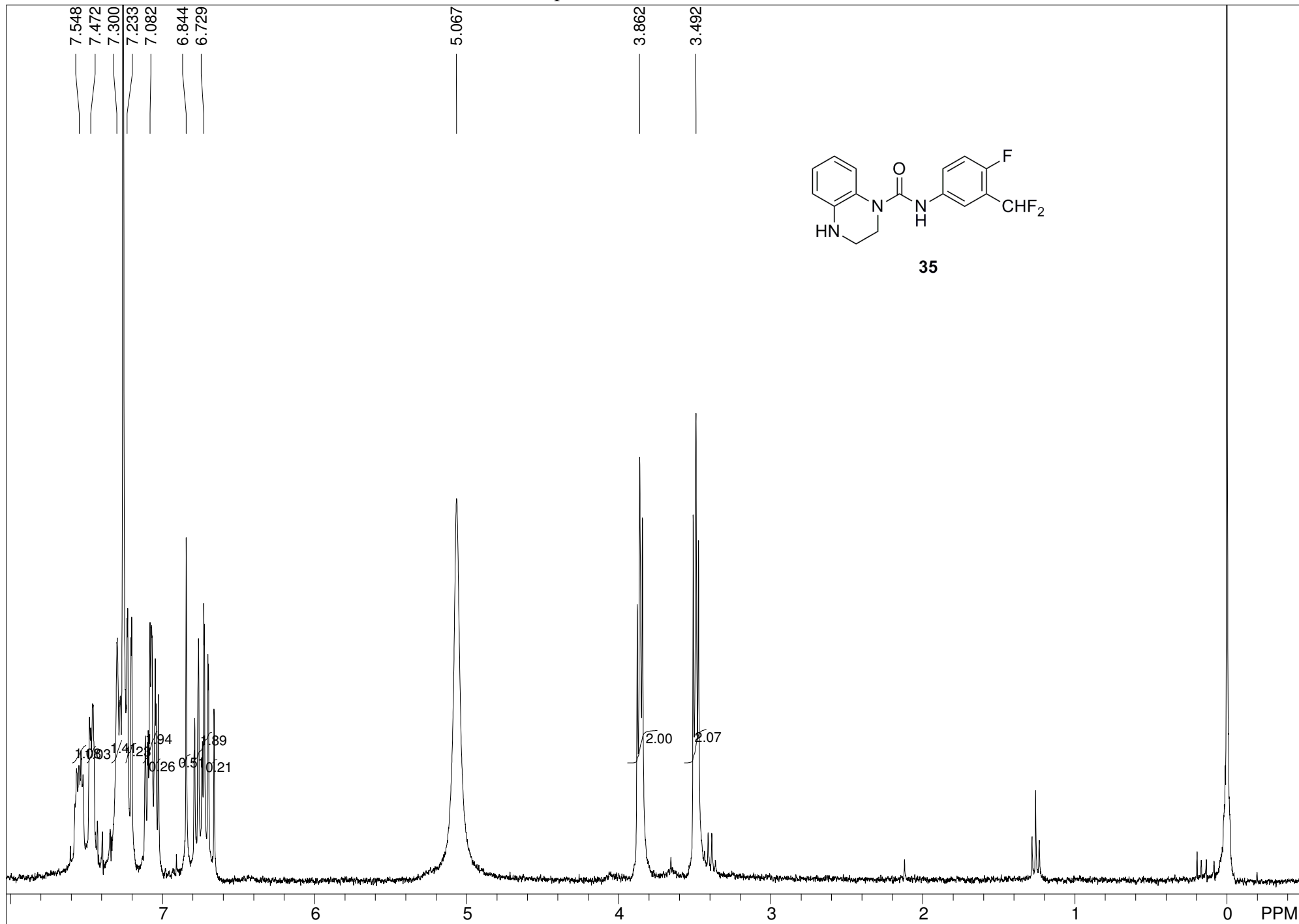
Current Chromatogram(s)



MS Spectrum



<sup>1</sup>H NMR Spectrum (300 MHz, CDCl<sub>3</sub>) of 35

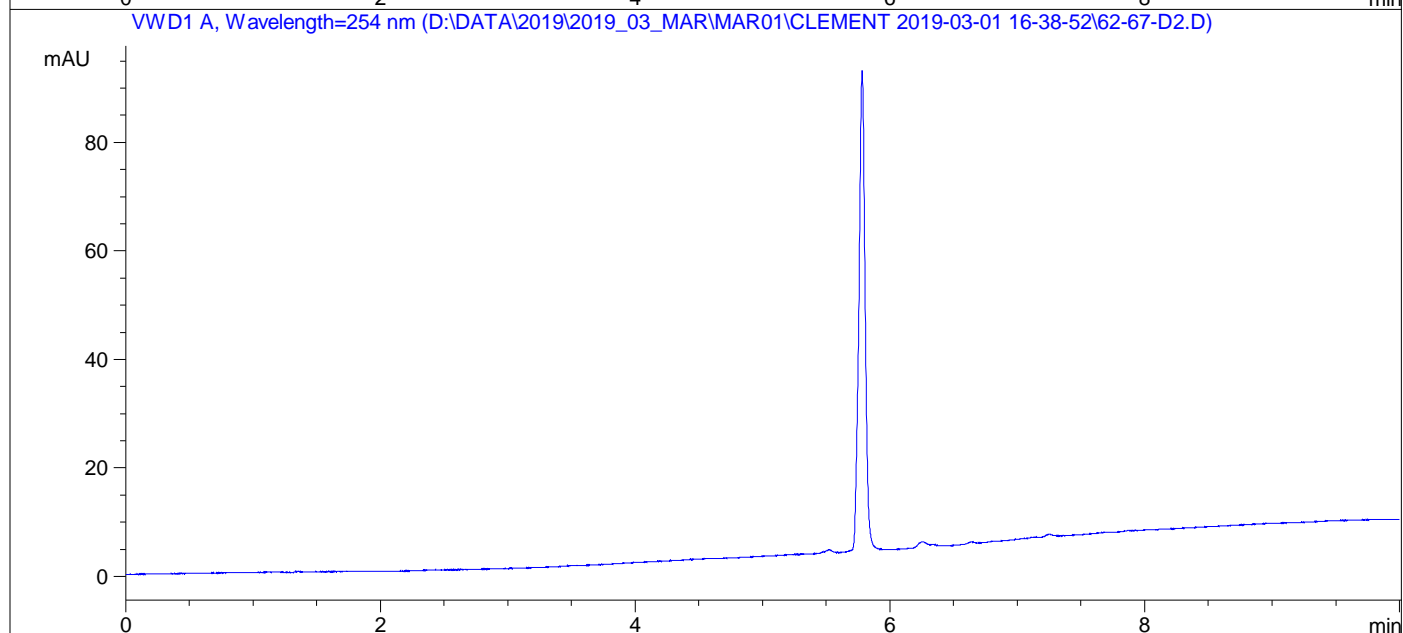
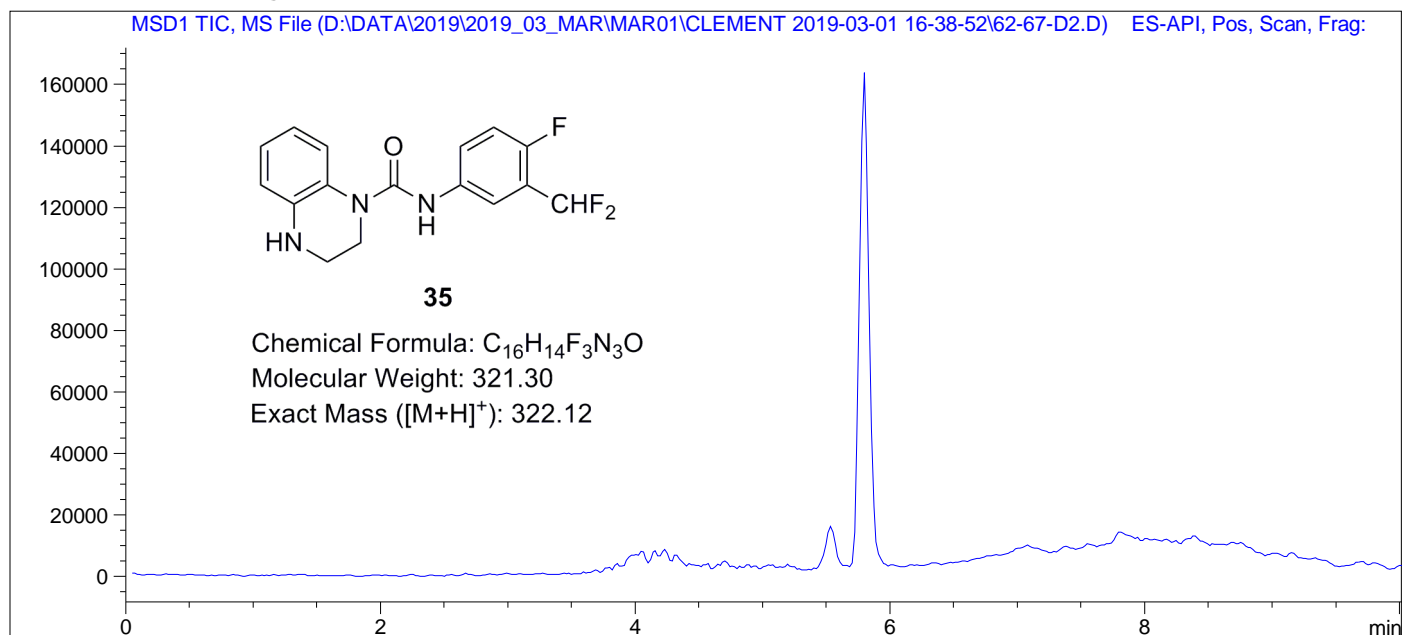


35

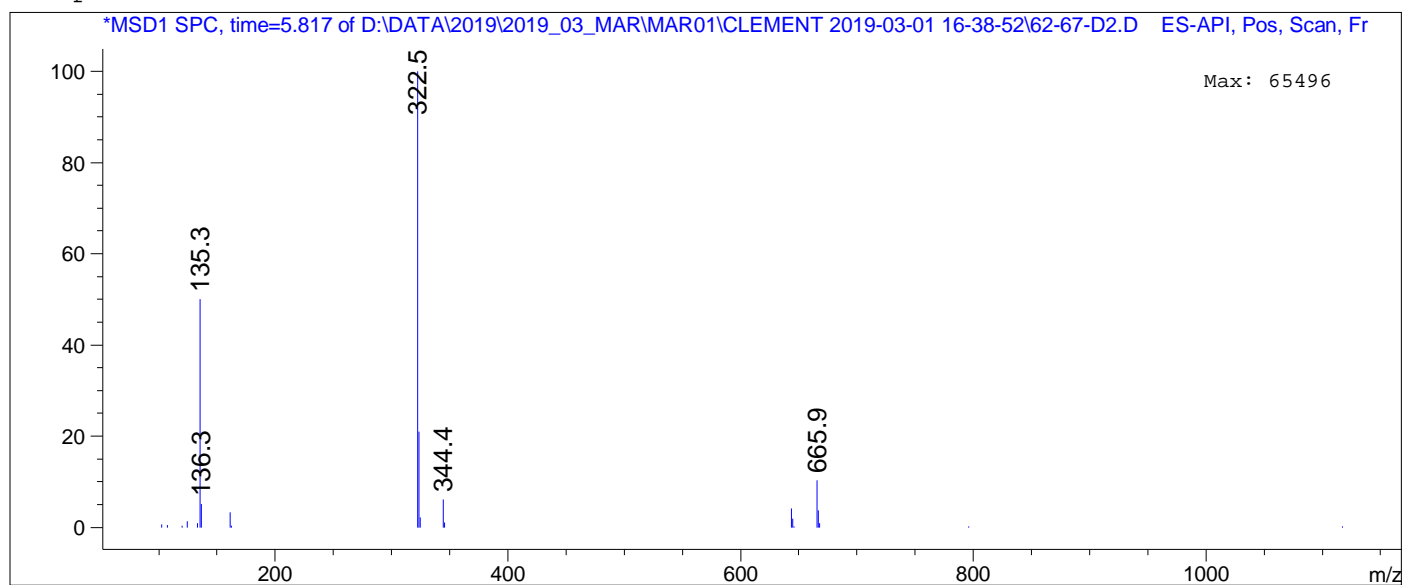


## LCMS analysis of 35

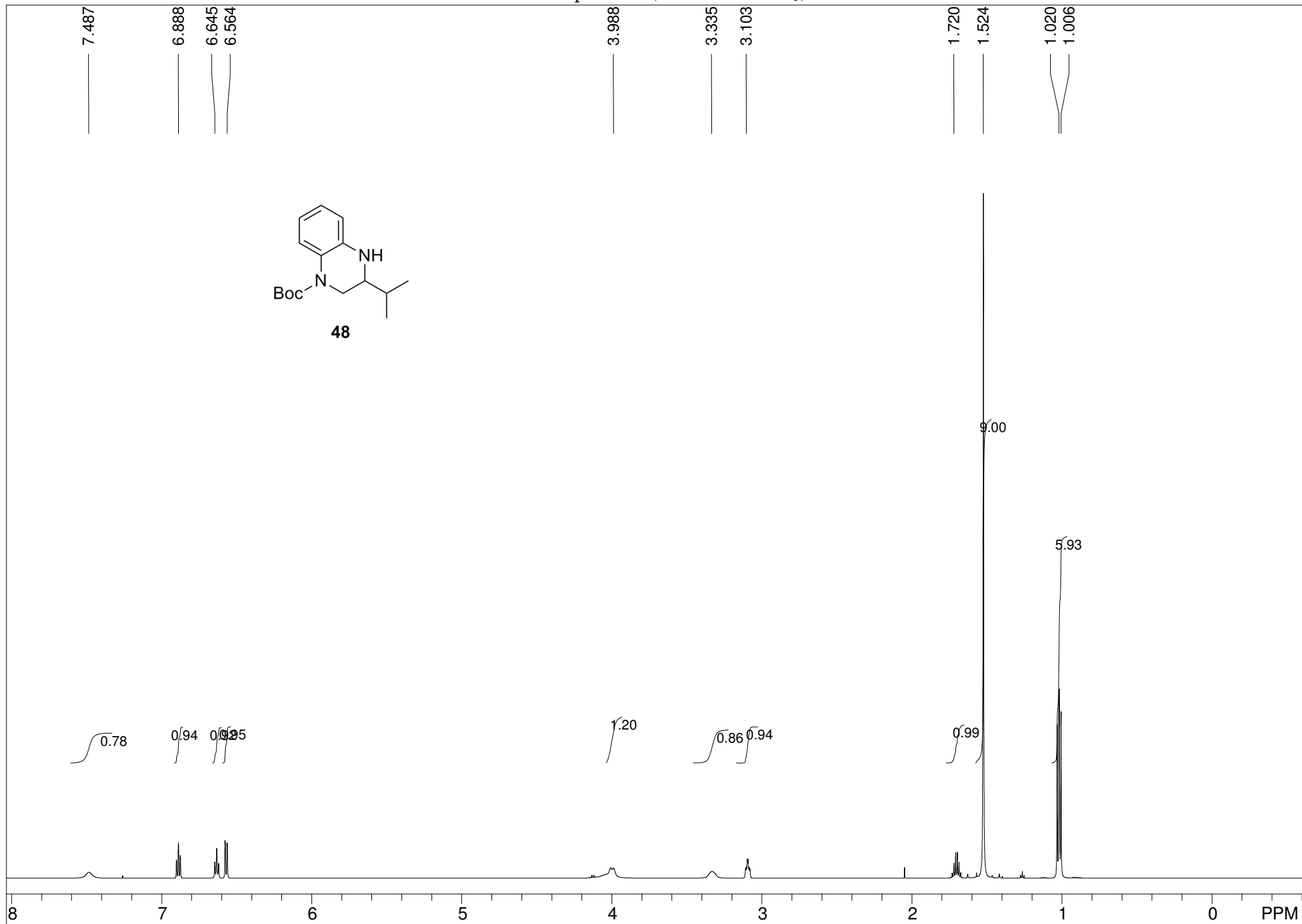
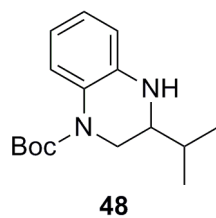
Current Chromatogram(s)



MS Spectrum



<sup>1</sup>H NMR Spectrum (600 MHz, CDCl<sub>3</sub>) of **48**



Sample ID 65-074

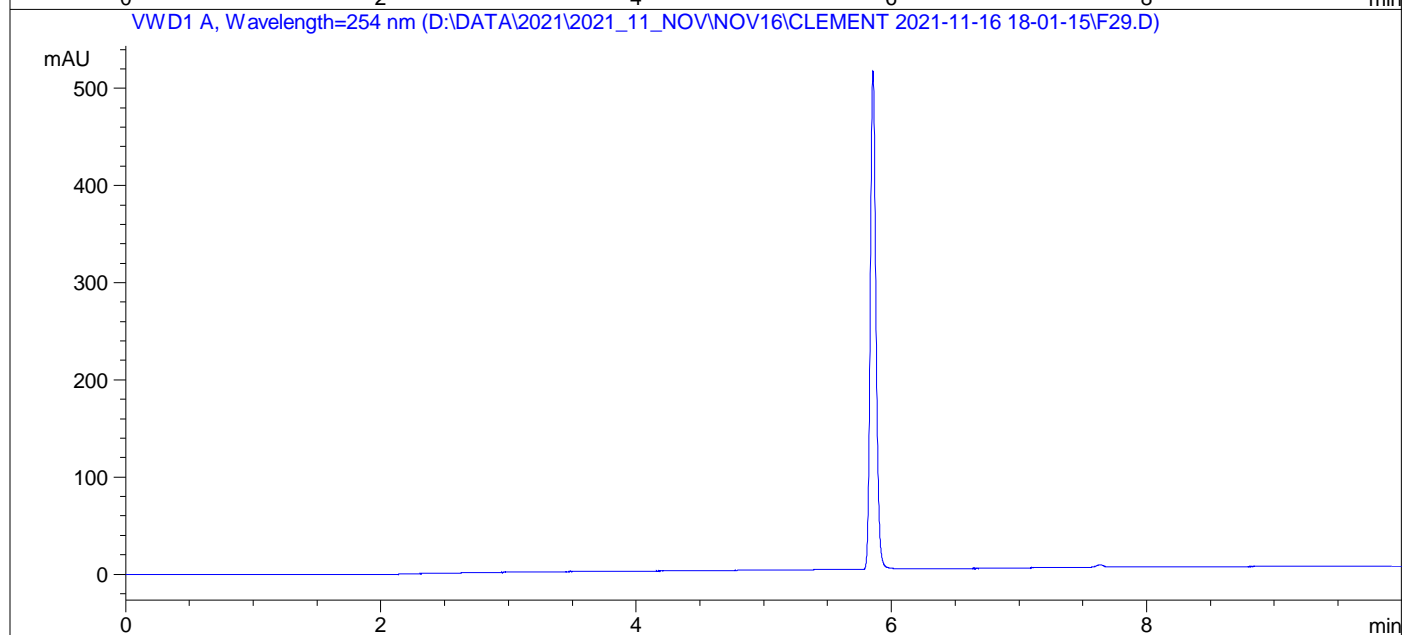
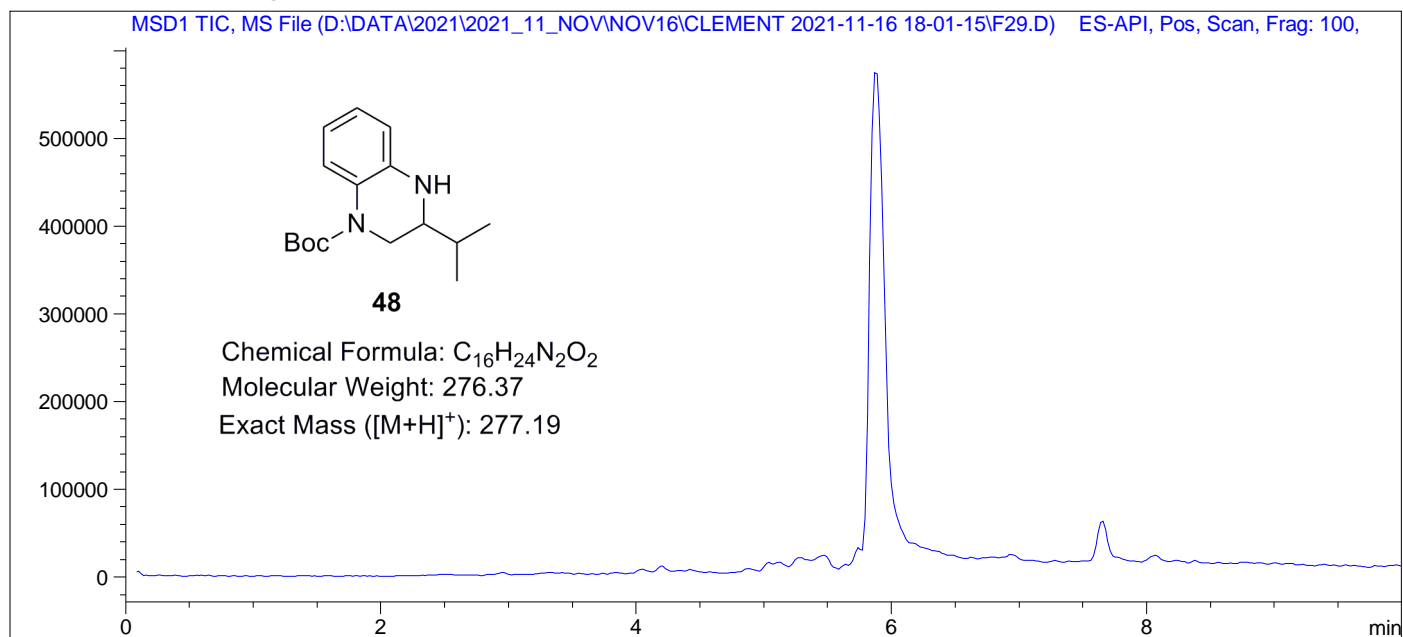
USER: undefined -- DATE: Thu Jan 20 16:05:47 2022

F1: 600.134	F2: 1.000	SW1: 12019	OF1: 3691.7	PTS1d: 32768 , 65536
EX:	PW: ? usec	PD: ? sec	NA: -1	LB: 0.0

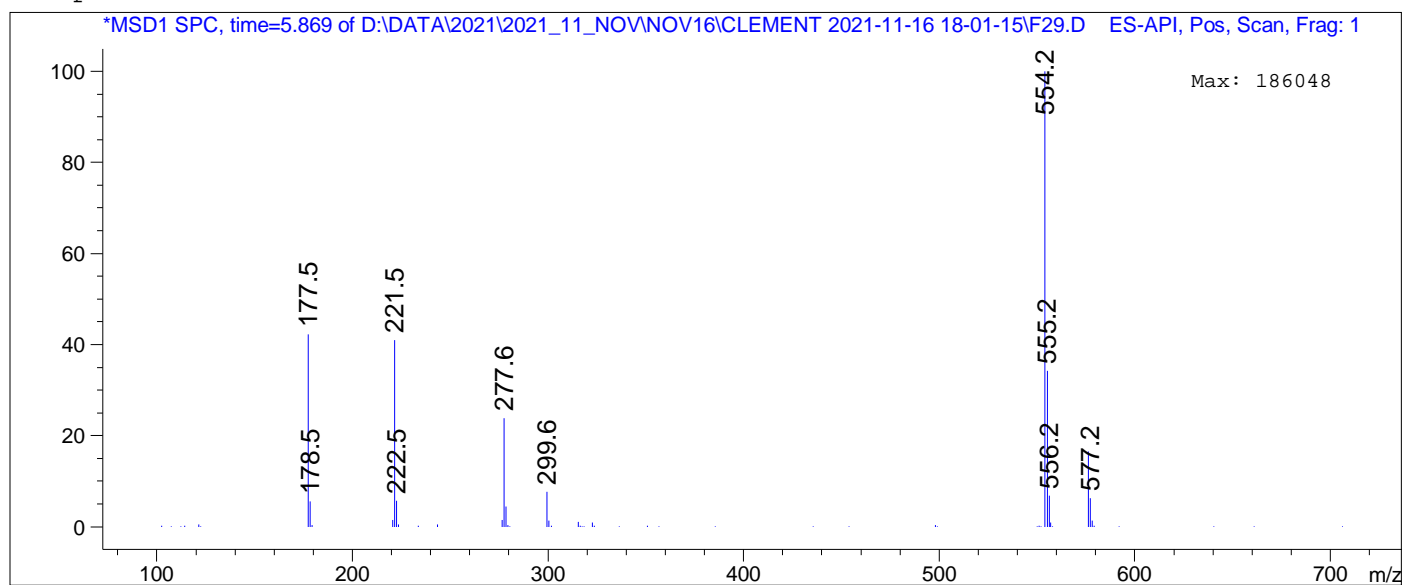
Nuts - \$65-074inCDCl3 1H.dx

## LCMS analysis of 48

Current Chromatogram(s)



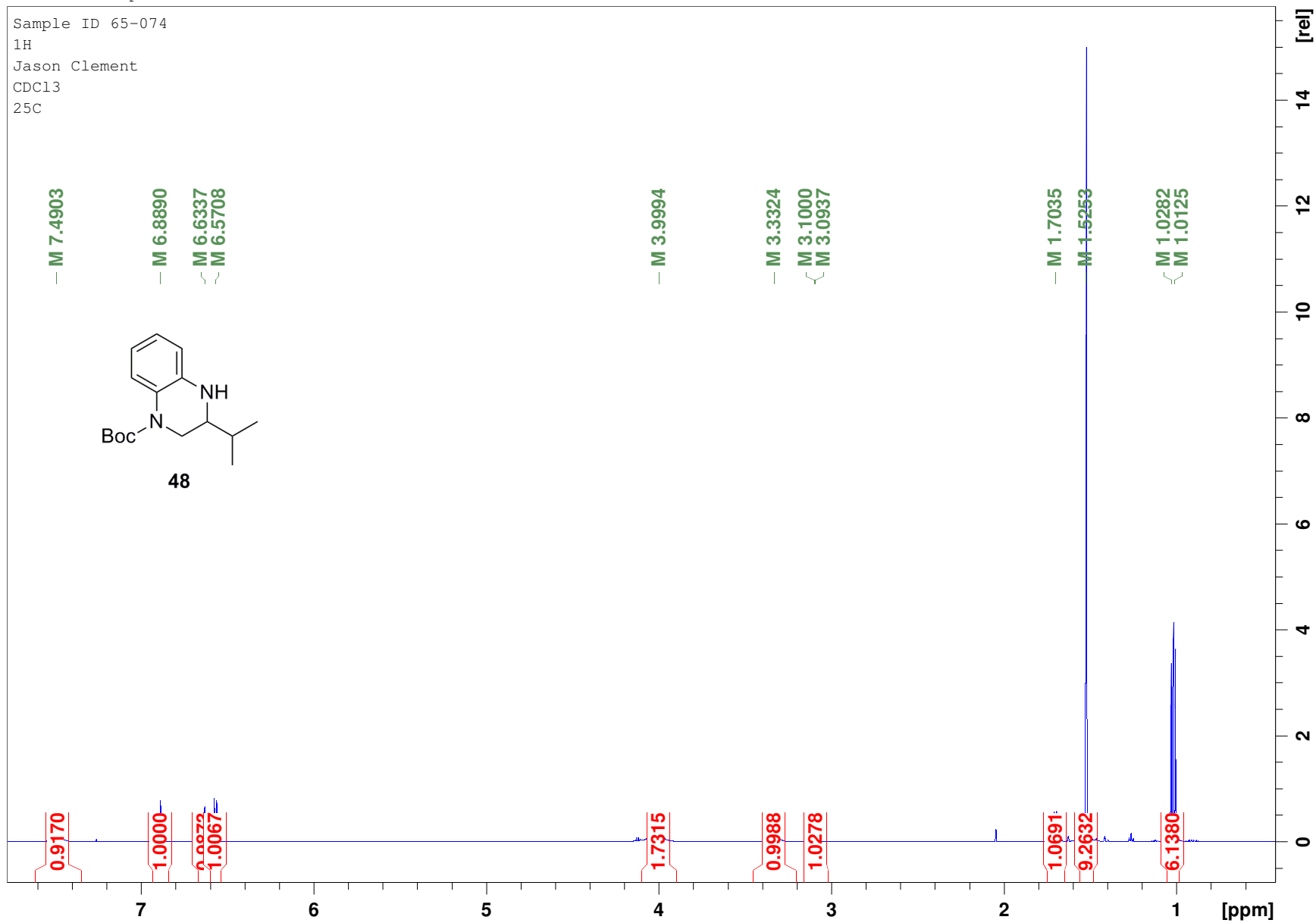
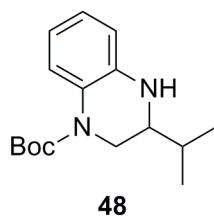
MS Spectrum



<sup>1</sup>H NMR Spectrum (600 MHz, CDCl<sub>3</sub>) of 48

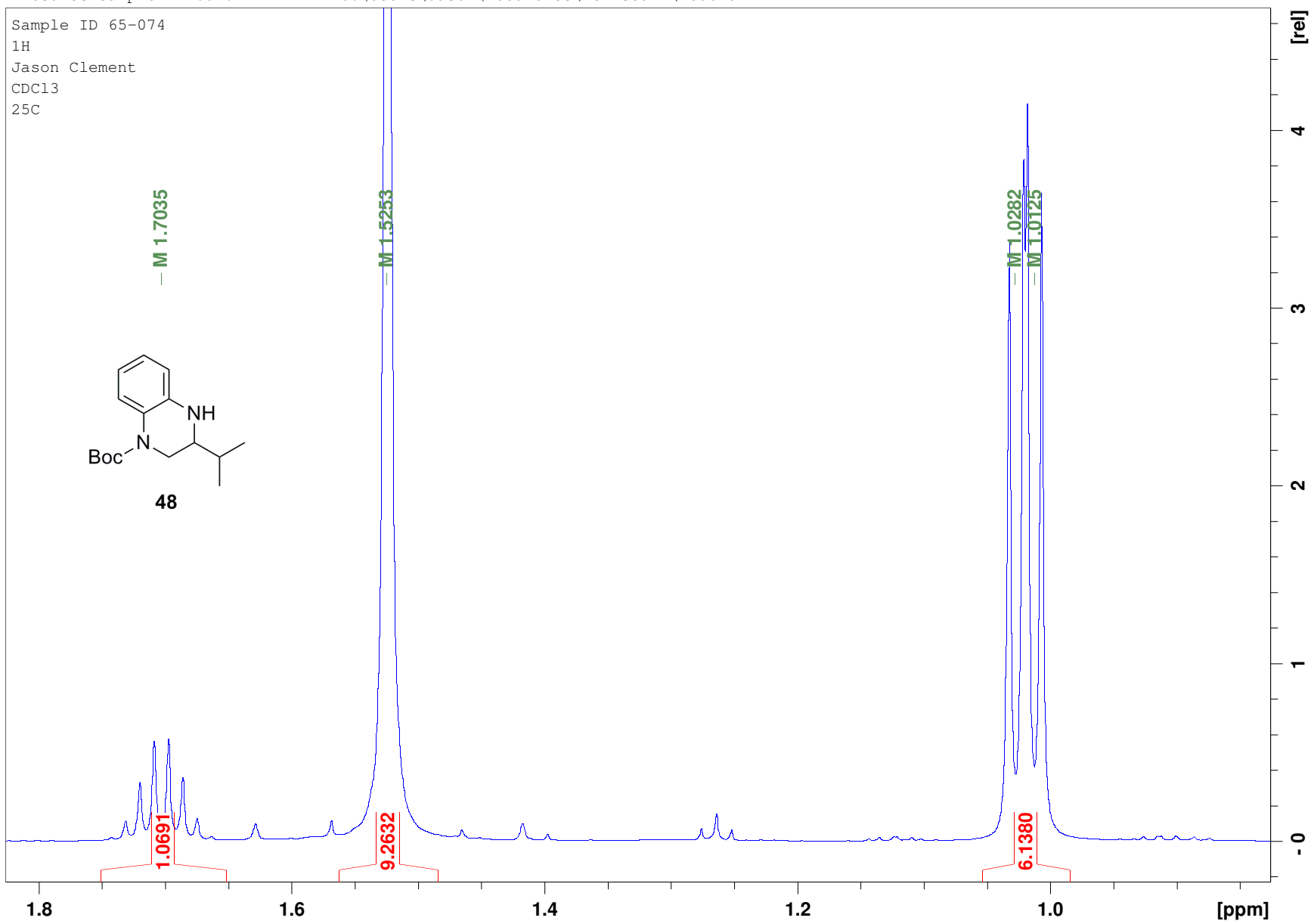
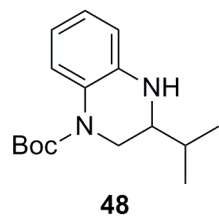
"Results sample ID 65-074" 1 1 C:\Users\Jason\Documents\BSBIstuff\MedChem

Sample ID 65-074  
1H  
Jason Clement  
CDCl<sub>3</sub>  
25C



"Results sample ID 65-074" 1 1 C:\Users\Jason\Documents\BSBIstuff\MedChem

Sample ID 65-074  
1H  
Jason Clement  
CDCl3  
25C



"Results sample ID 65-074" 1 1 C:\Users\Jason\Documents\BSBIstuff\MedChem

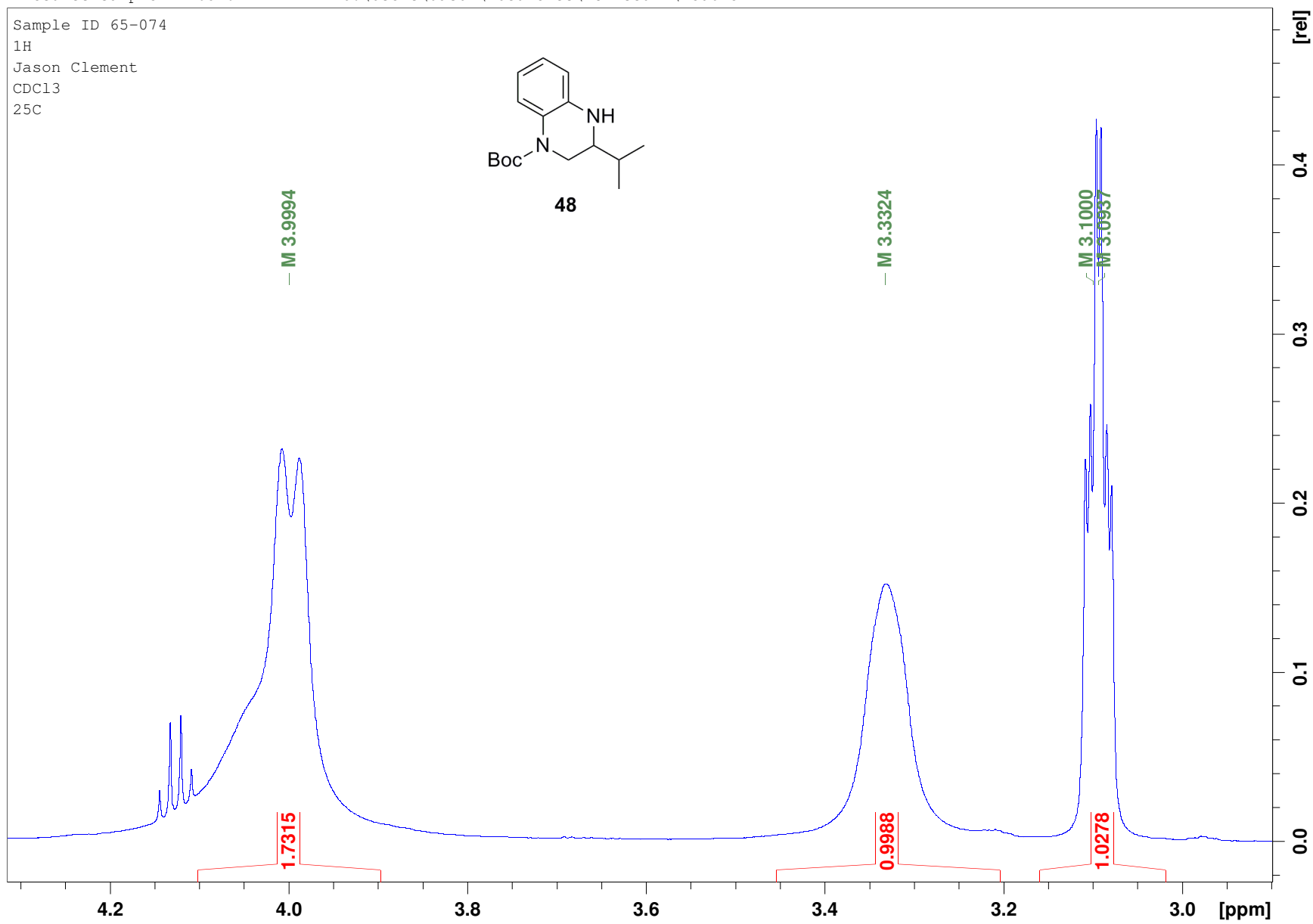
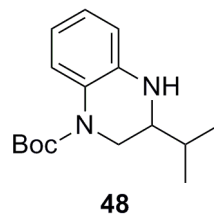
Sample ID 65-074

<sup>1</sup>H

Jason Clement

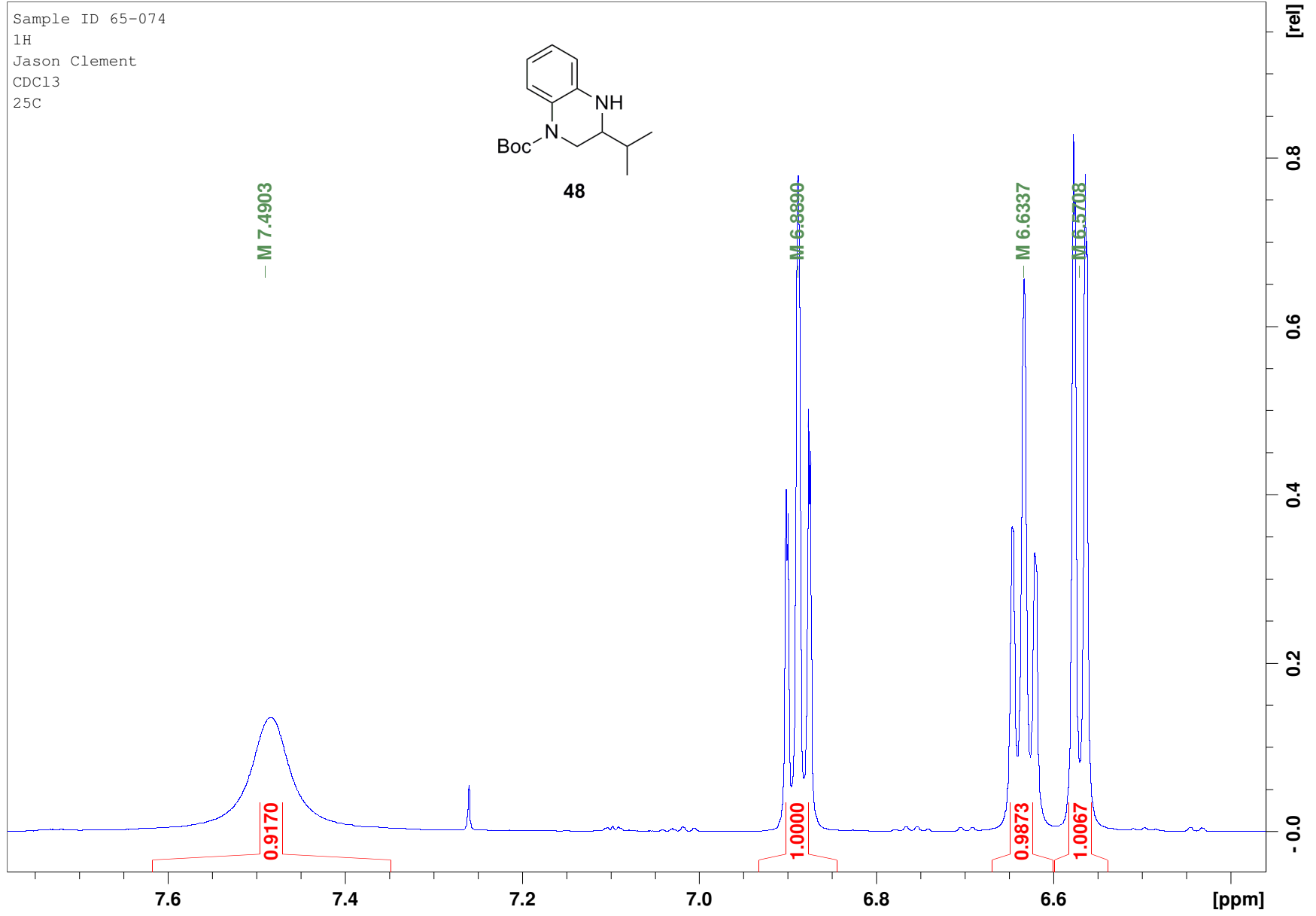
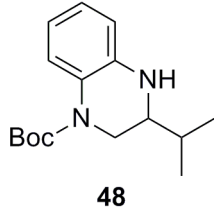
CDCl<sub>3</sub>

25C



"Results sample ID 65-074" 1 1 C:\Users\Jason\Documents\BSBIstuff\MedChem

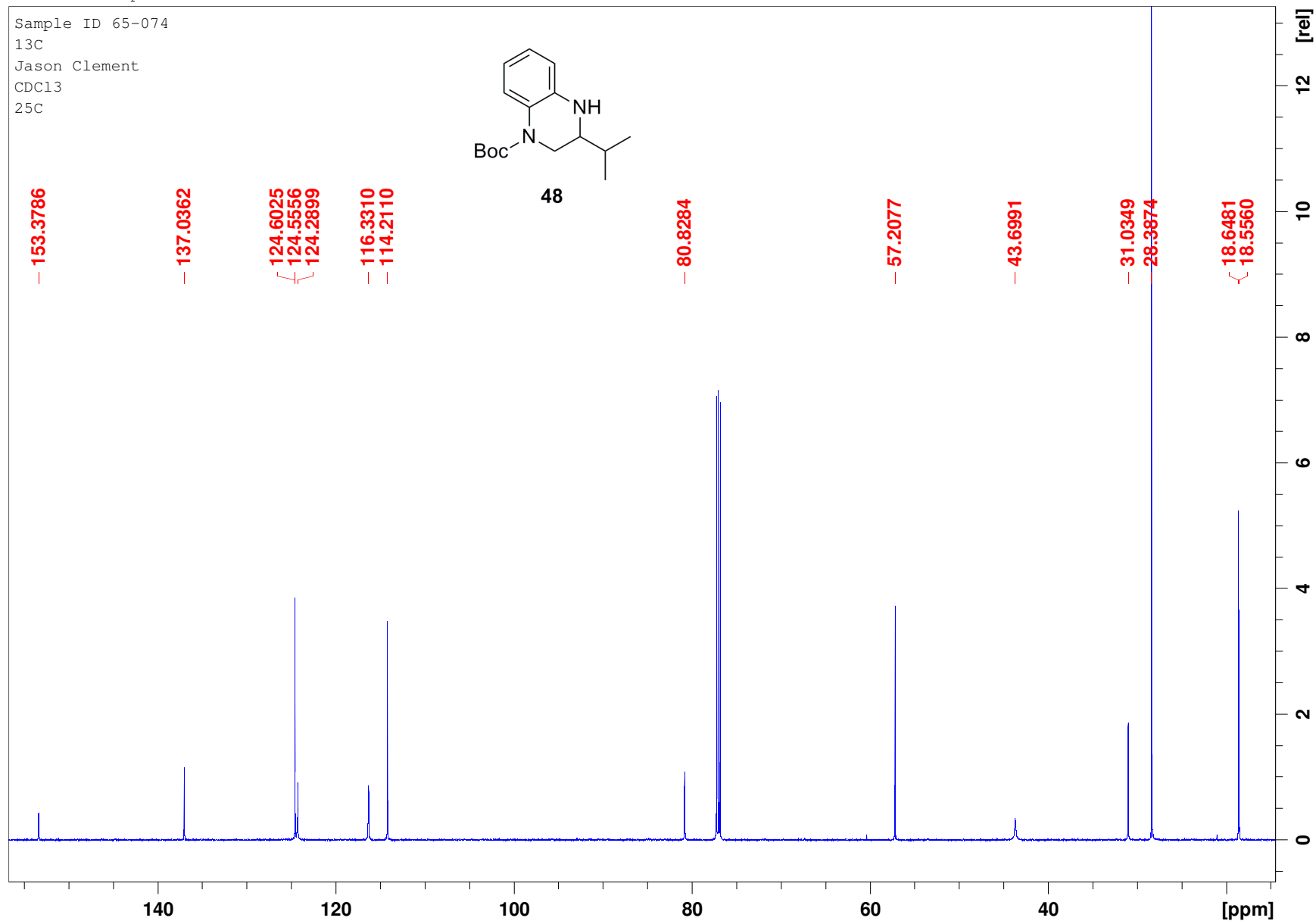
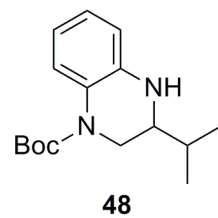
Sample ID 65-074  
1H  
Jason Clement  
CDCl3  
25C



<sup>13</sup>C NMR Spectrum (151 MHz, CDCl<sub>3</sub>) of 48

"Results sample ID 65-074" 4 1 C:\Users\Jason\Documents\BSBIstuff\MedChem

Sample ID 65-074  
13C  
Jason Clement  
CDCl<sub>3</sub>  
25C





"Results sample ID 65-074" 4 1 C:\Users\Jason\Documents\BSBIstuff\MedChem

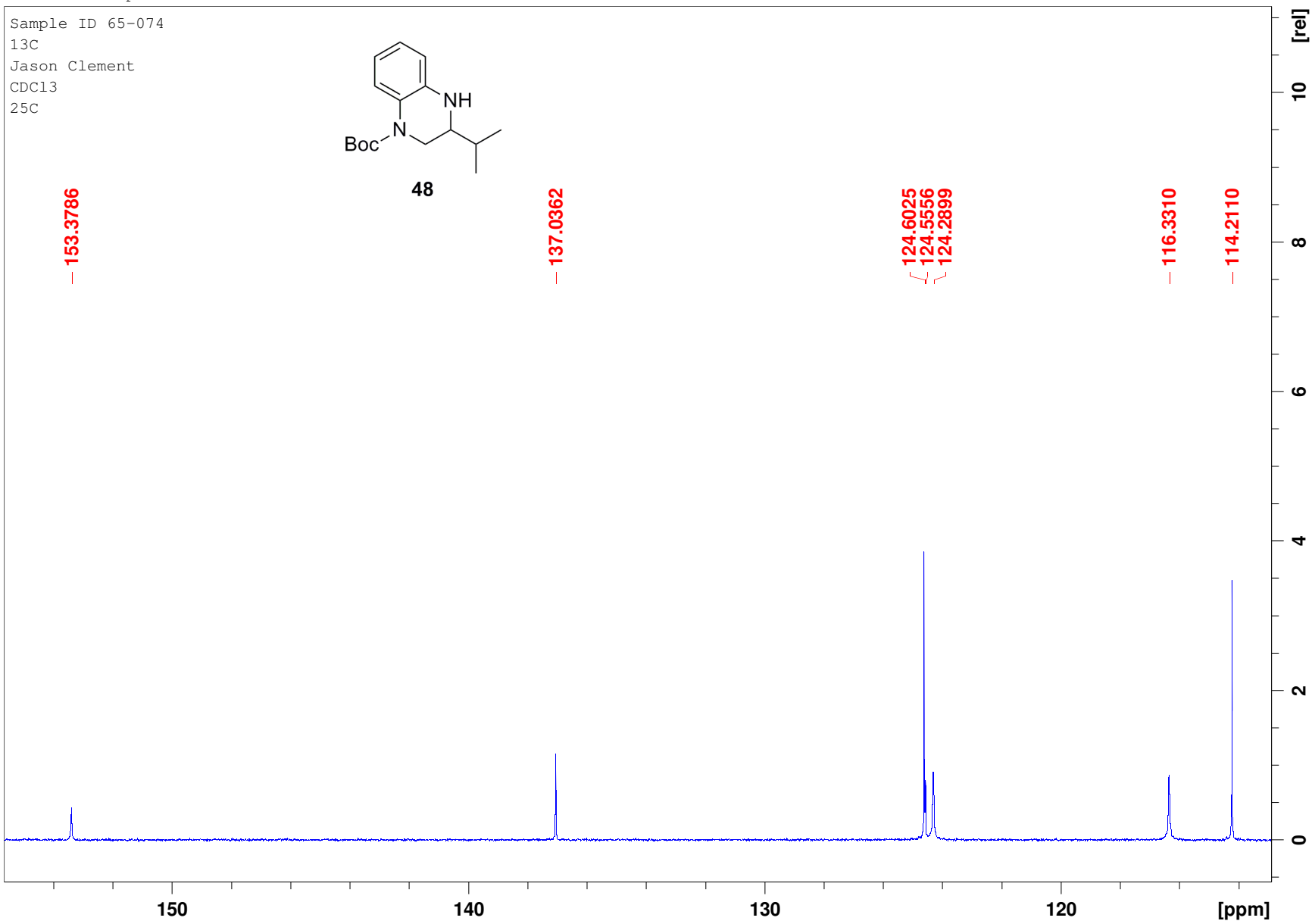
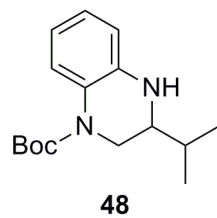
Sample ID 65-074

13C

Jason Clement

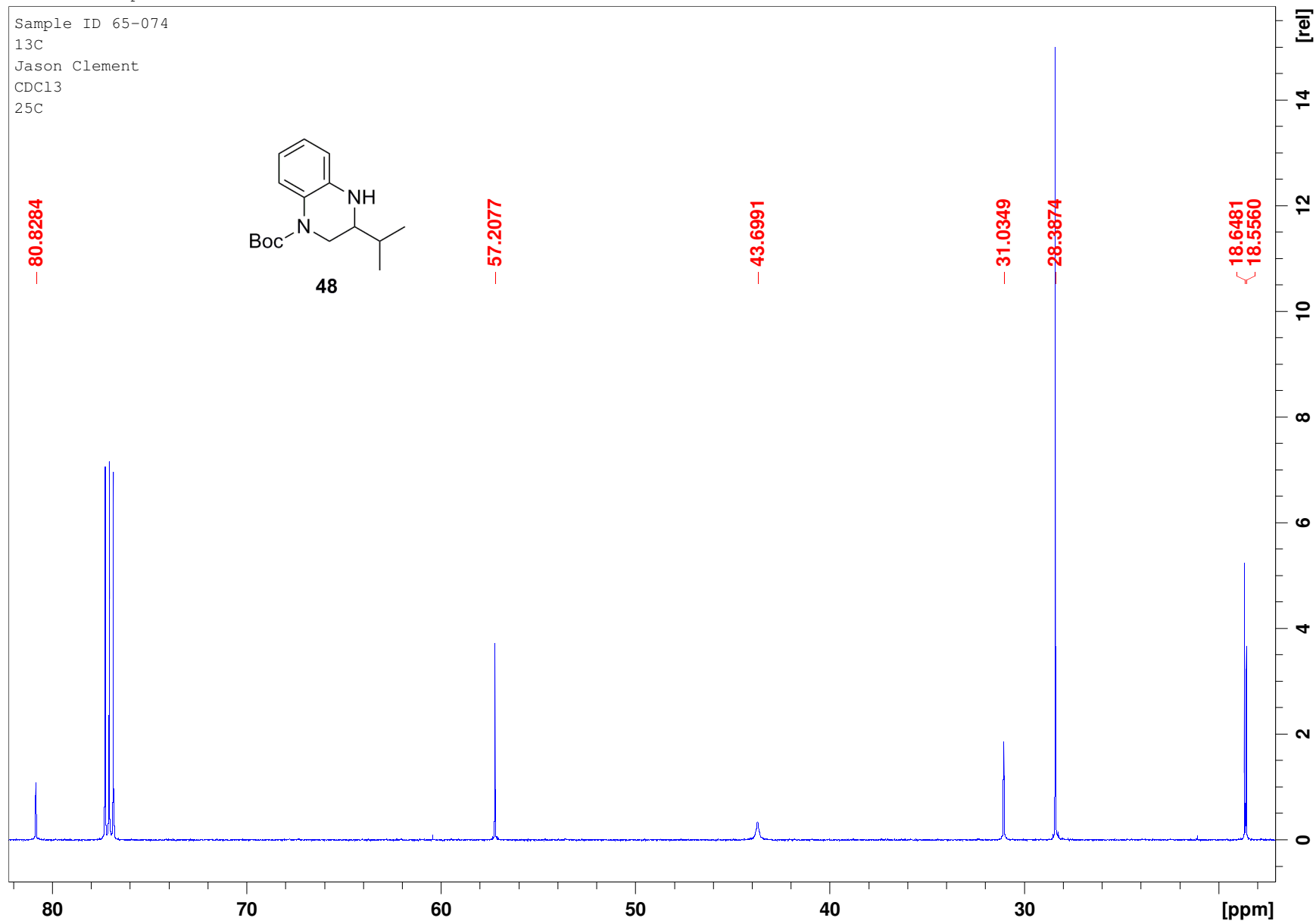
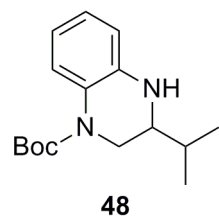
CDCl3

25C

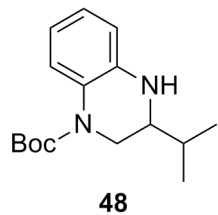


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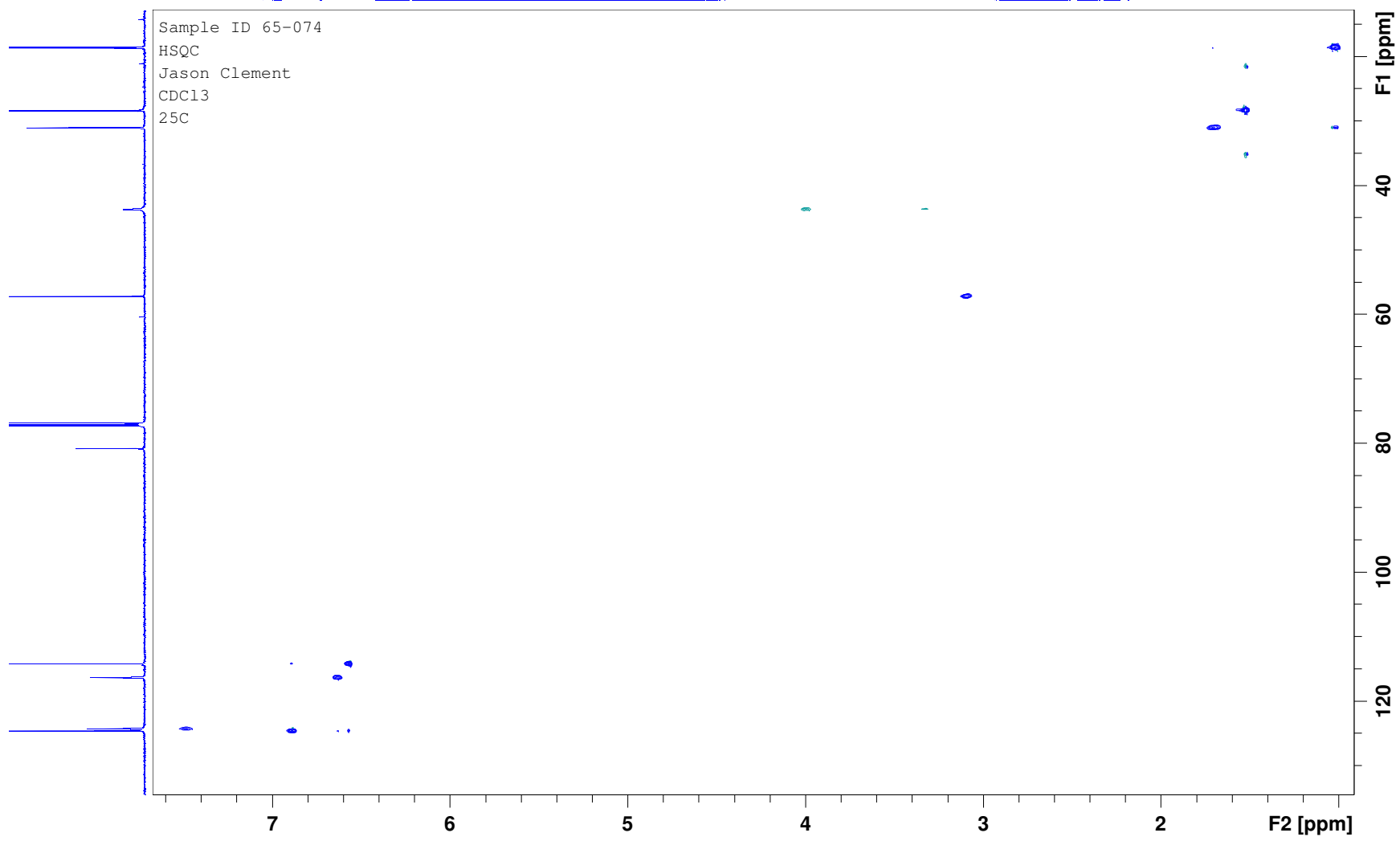
Sample ID 65-074  
13C  
Jason Clement  
CDCl3  
25C

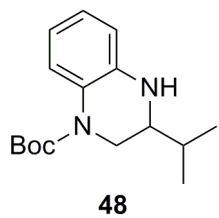


# HSQC Spectrum (CDCl<sub>3</sub>) of 48

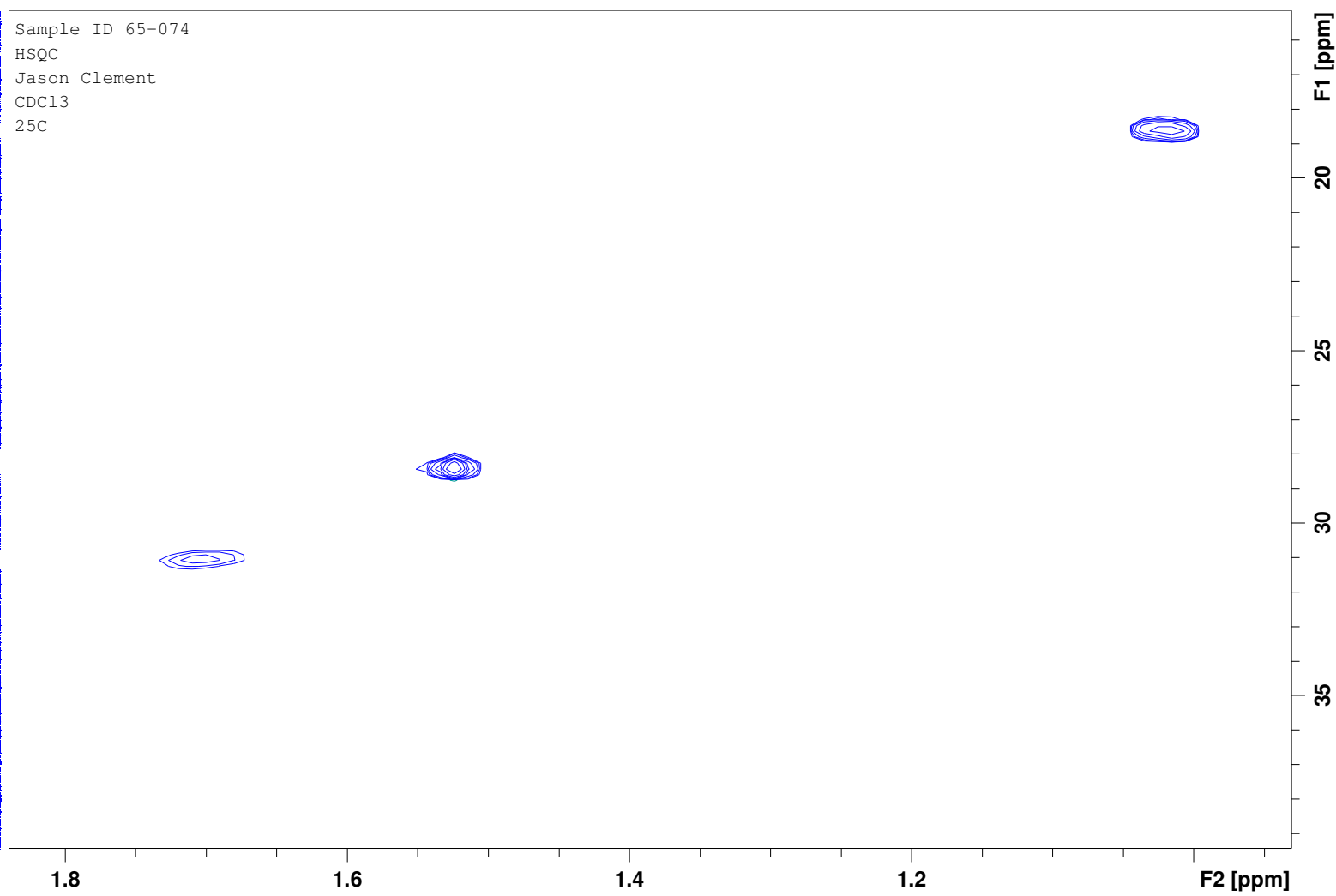


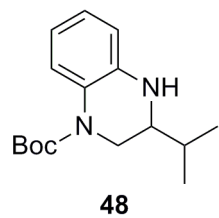
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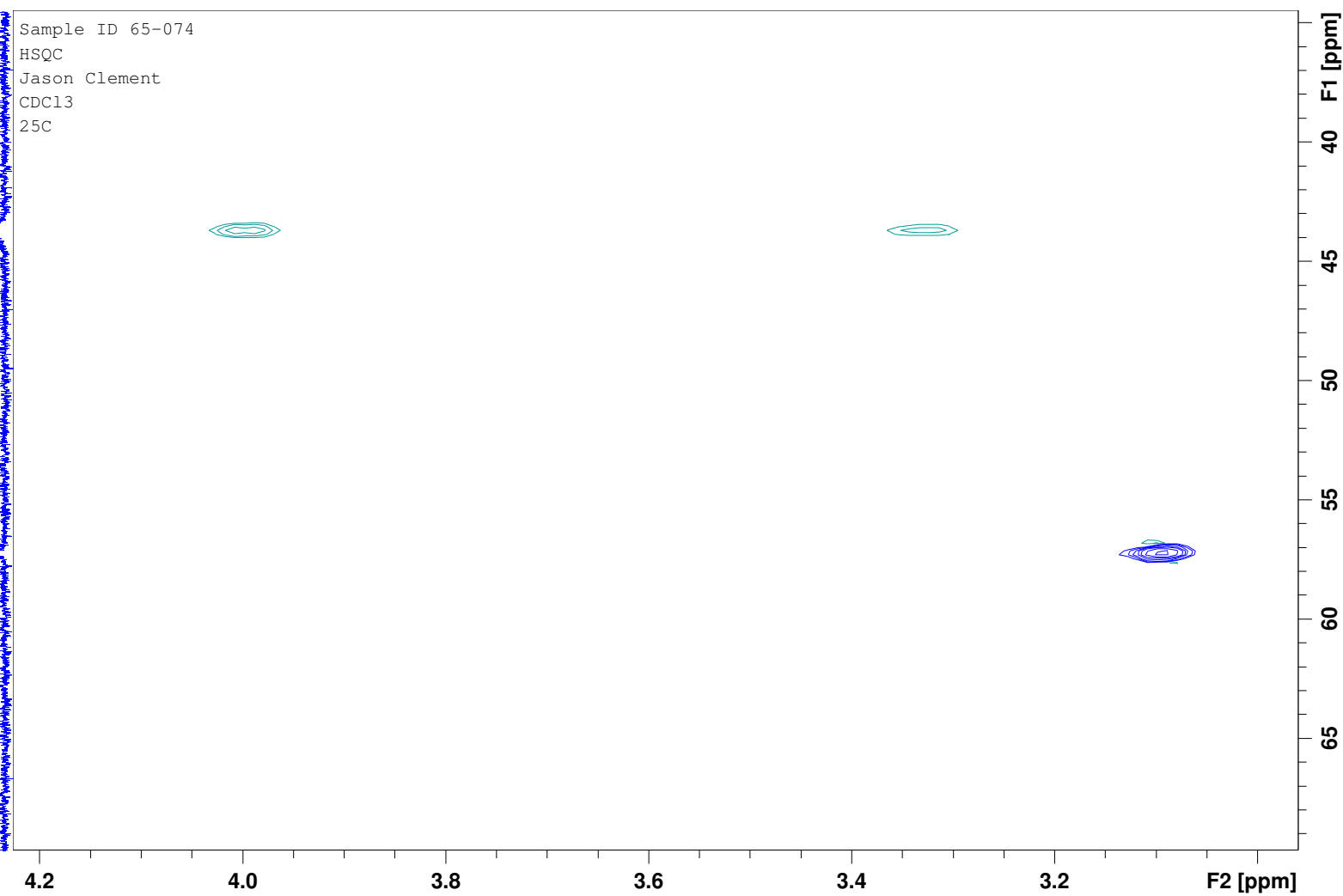


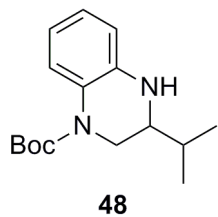
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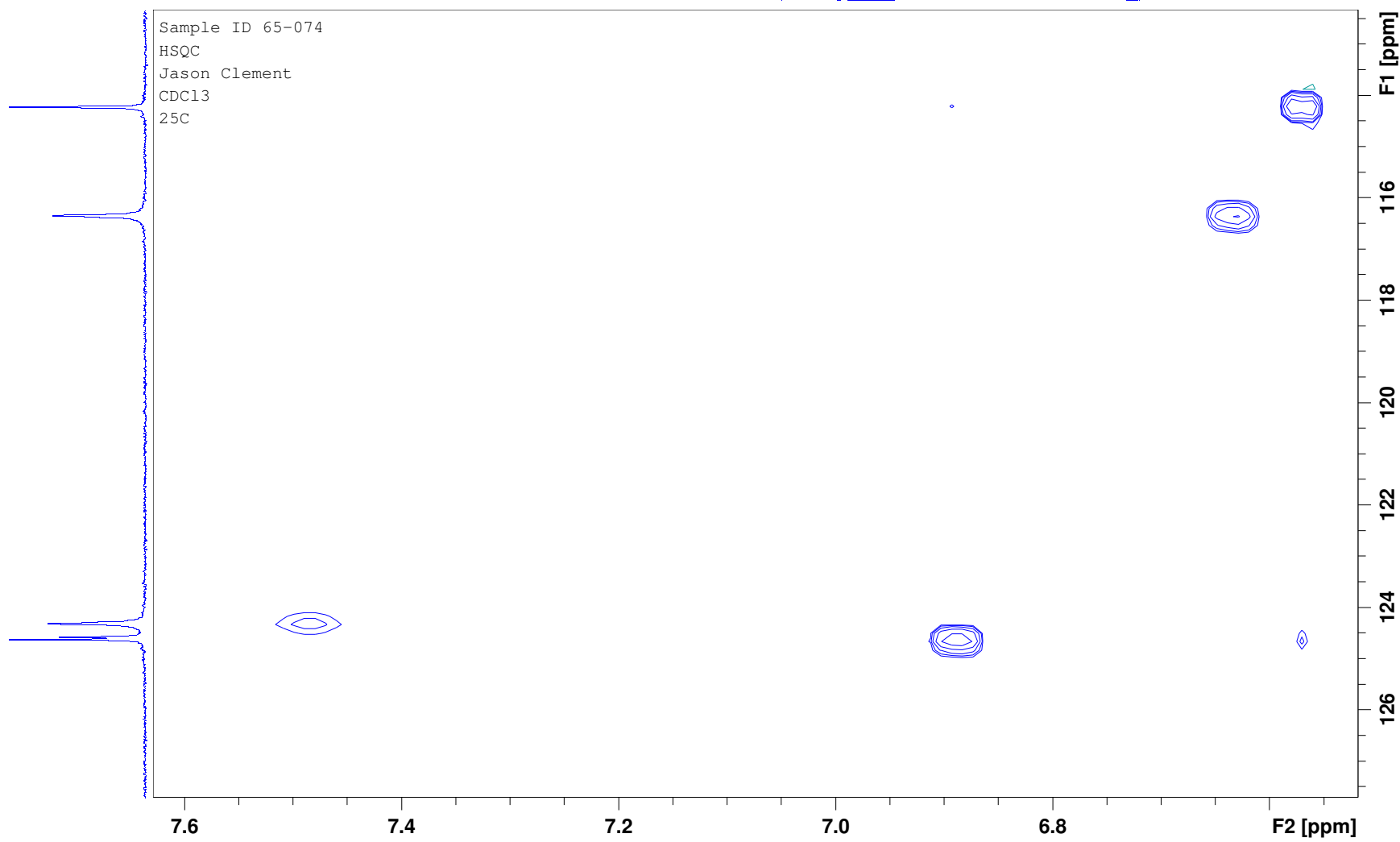


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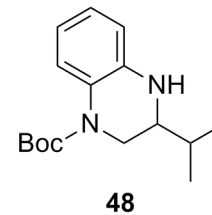




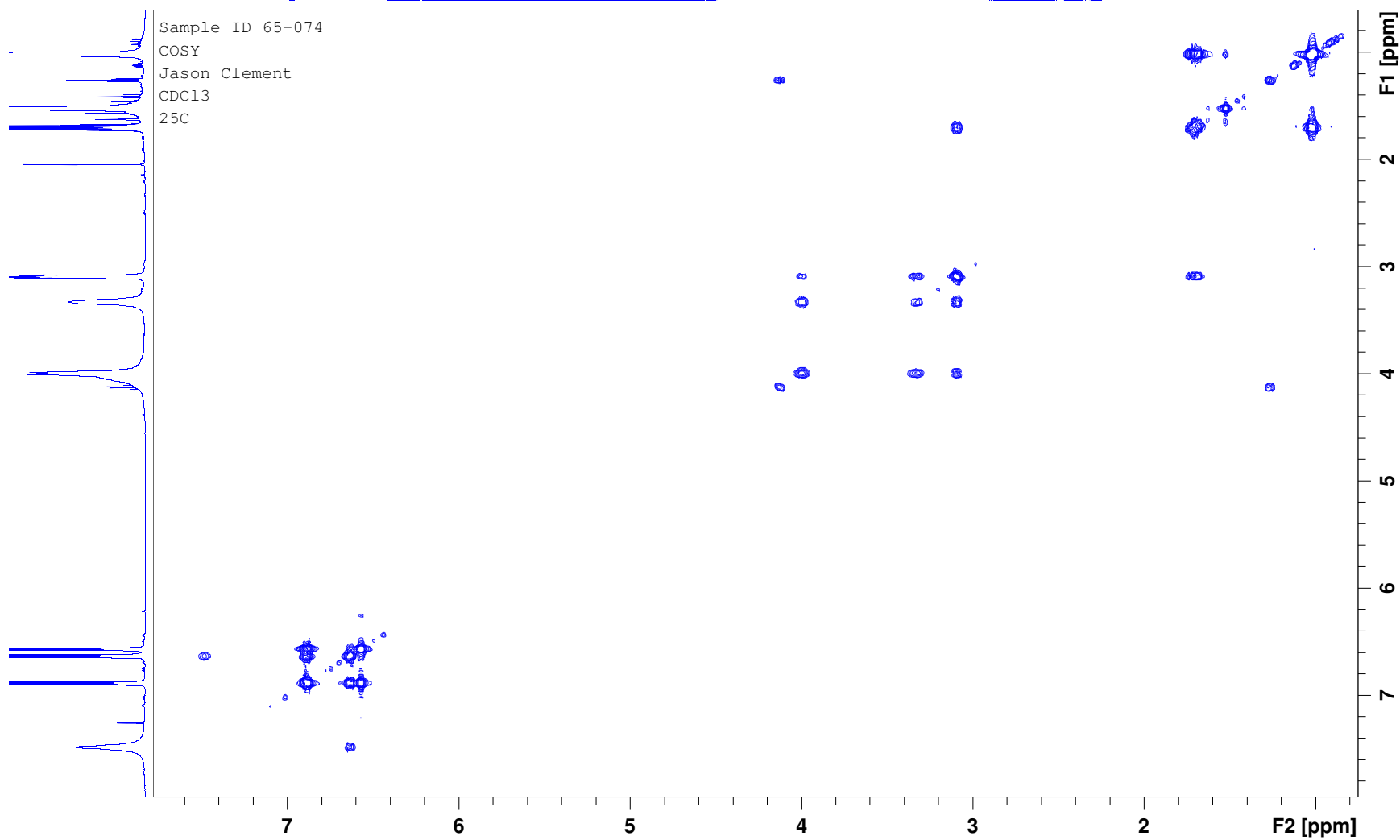
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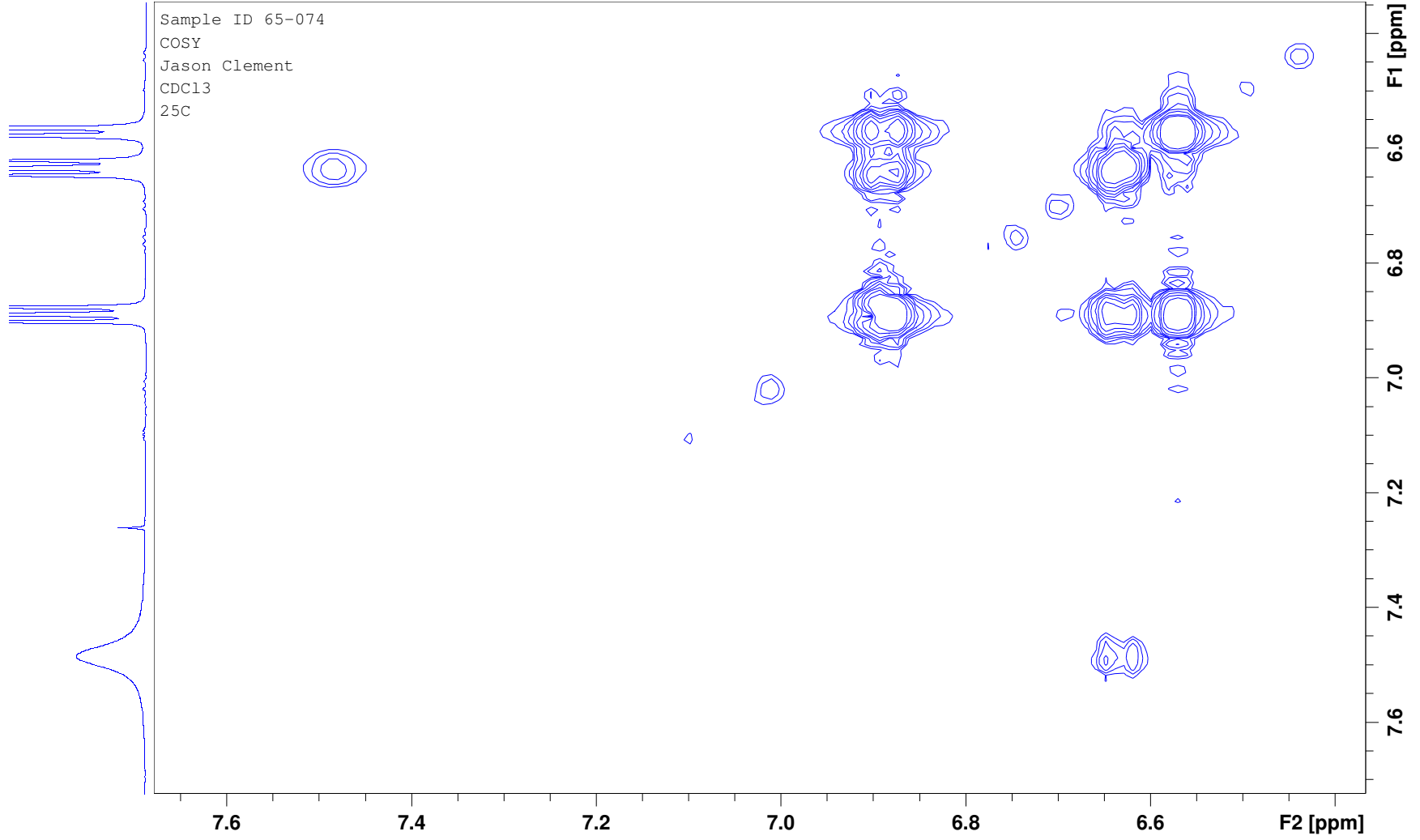
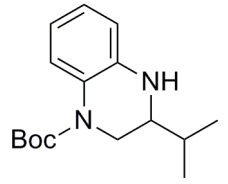
COSY Spectrum (CDCl<sub>3</sub>) of 48



"Results sample ID 65-074" 12 1 C:\Users\Jason\Documents\BSB\stuff\MedChem

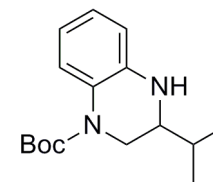


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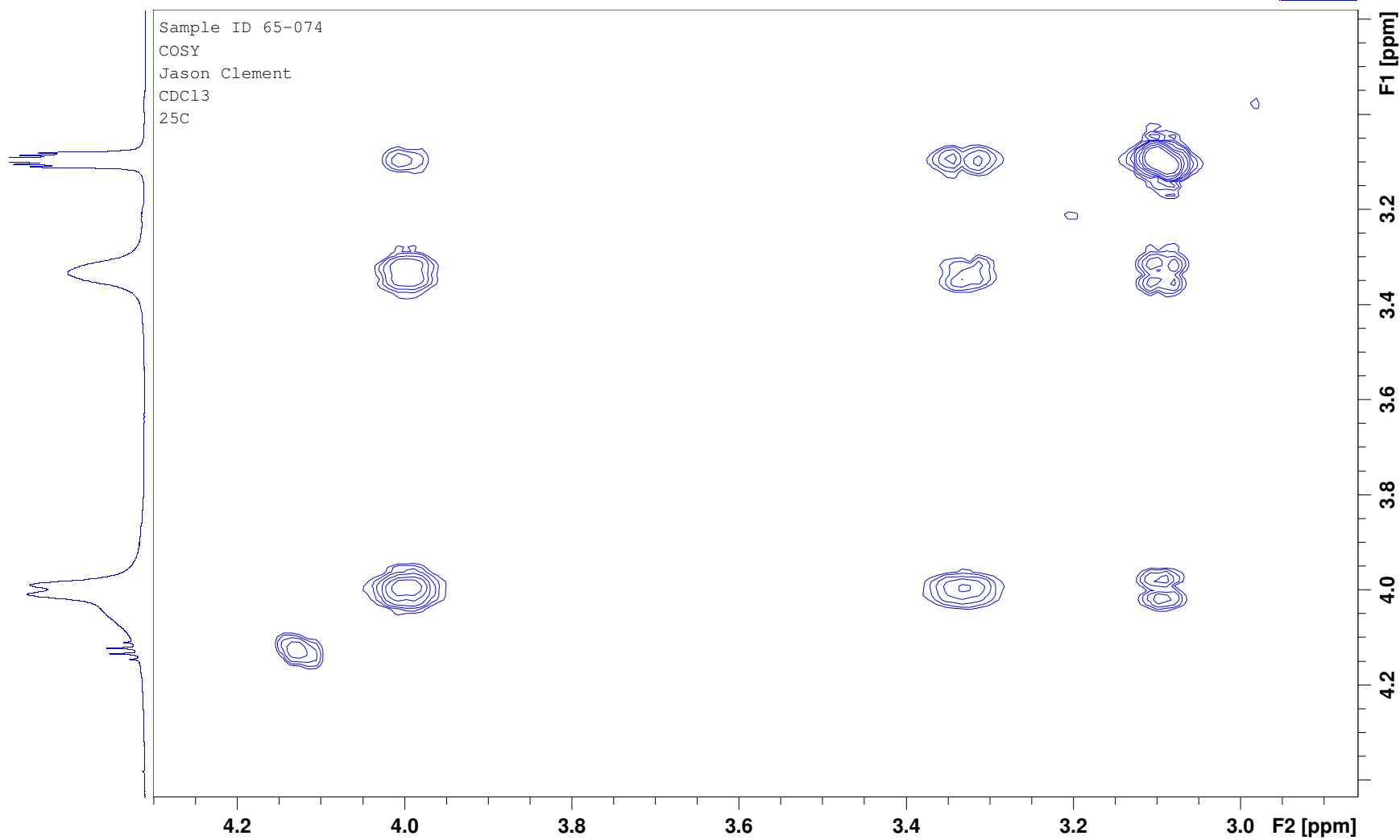




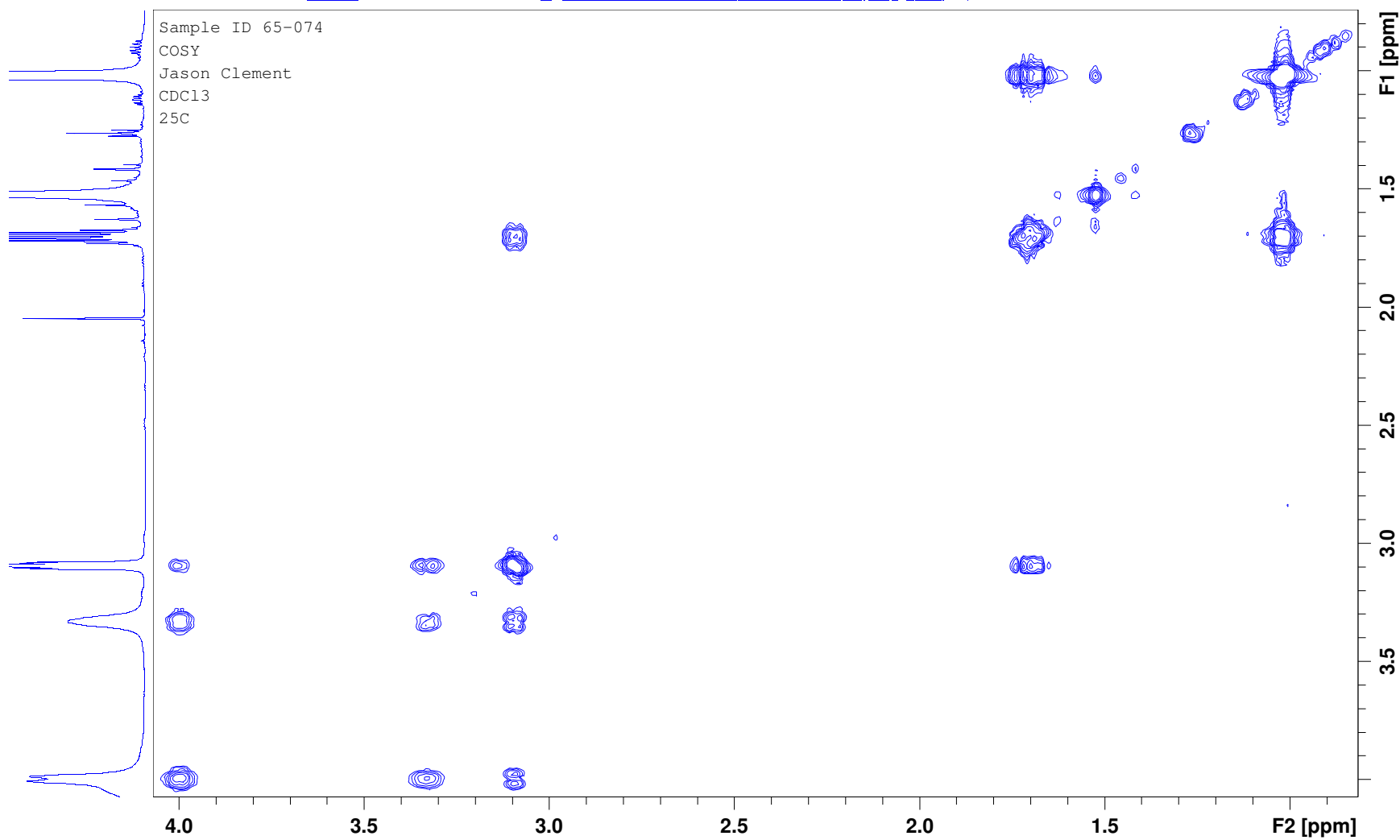
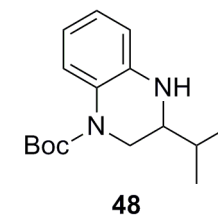
"Results sample ID 65-074" 12 1 C:\Users\Jason\Documents\BSBIstuff\MedChem



48

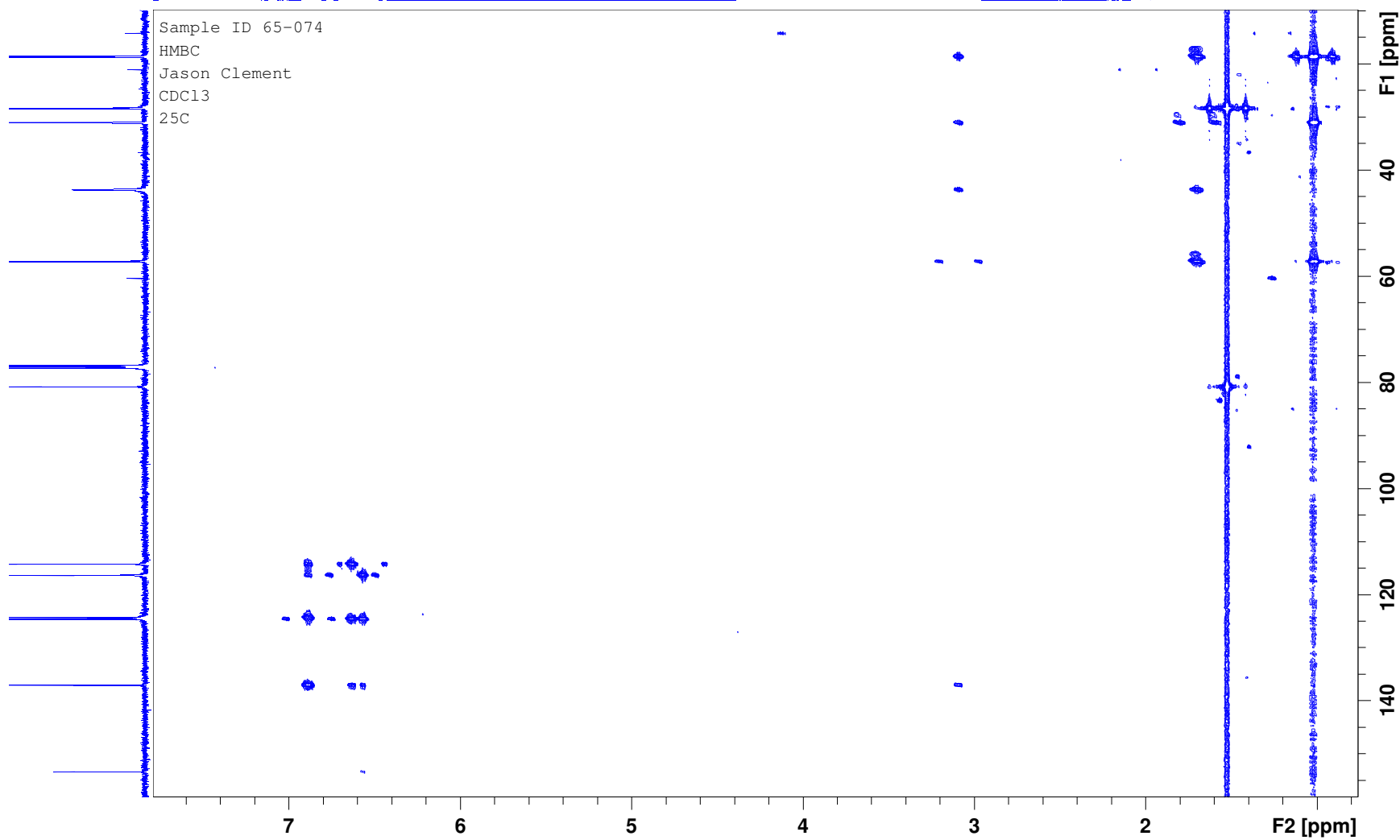
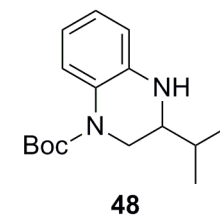


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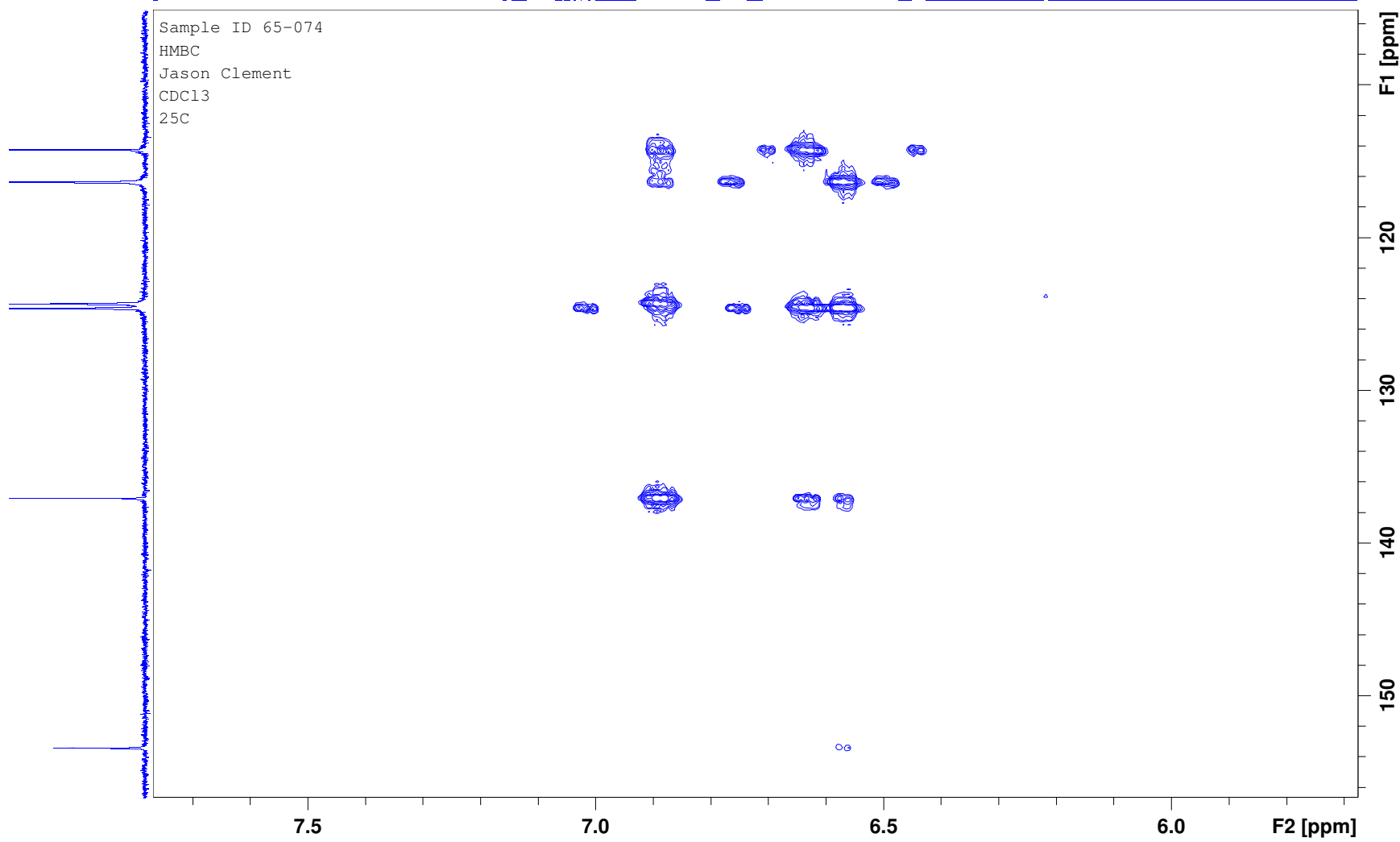
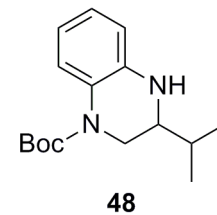


# HMBC Spectrum (CDCl<sub>3</sub>) of 48

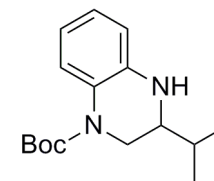
"Results sample ID 65-074" 7 1 C:\Users\Jason\Documents\BSBIstuff\MedChem



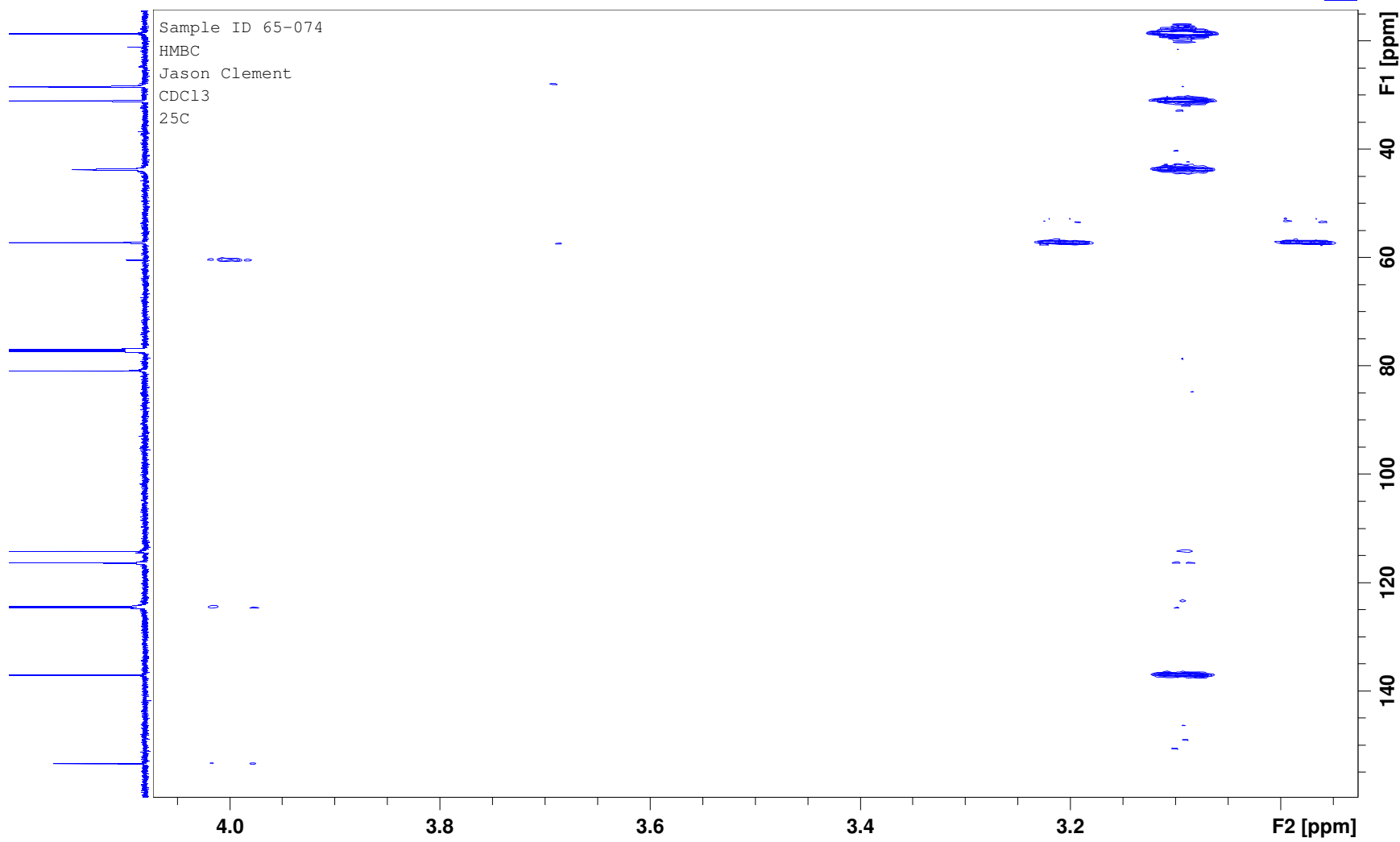
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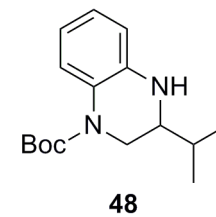


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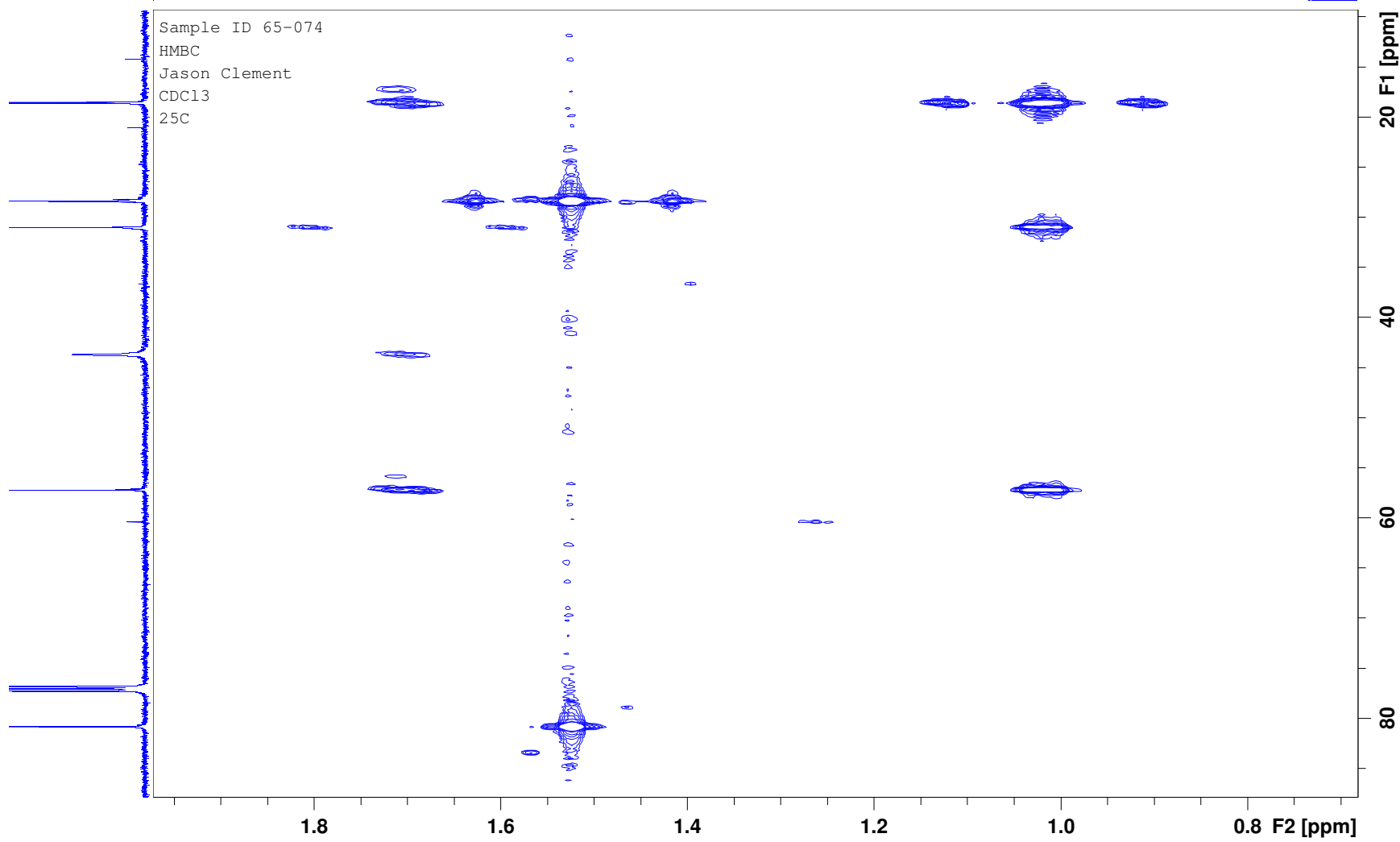


48

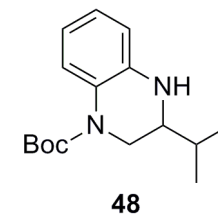




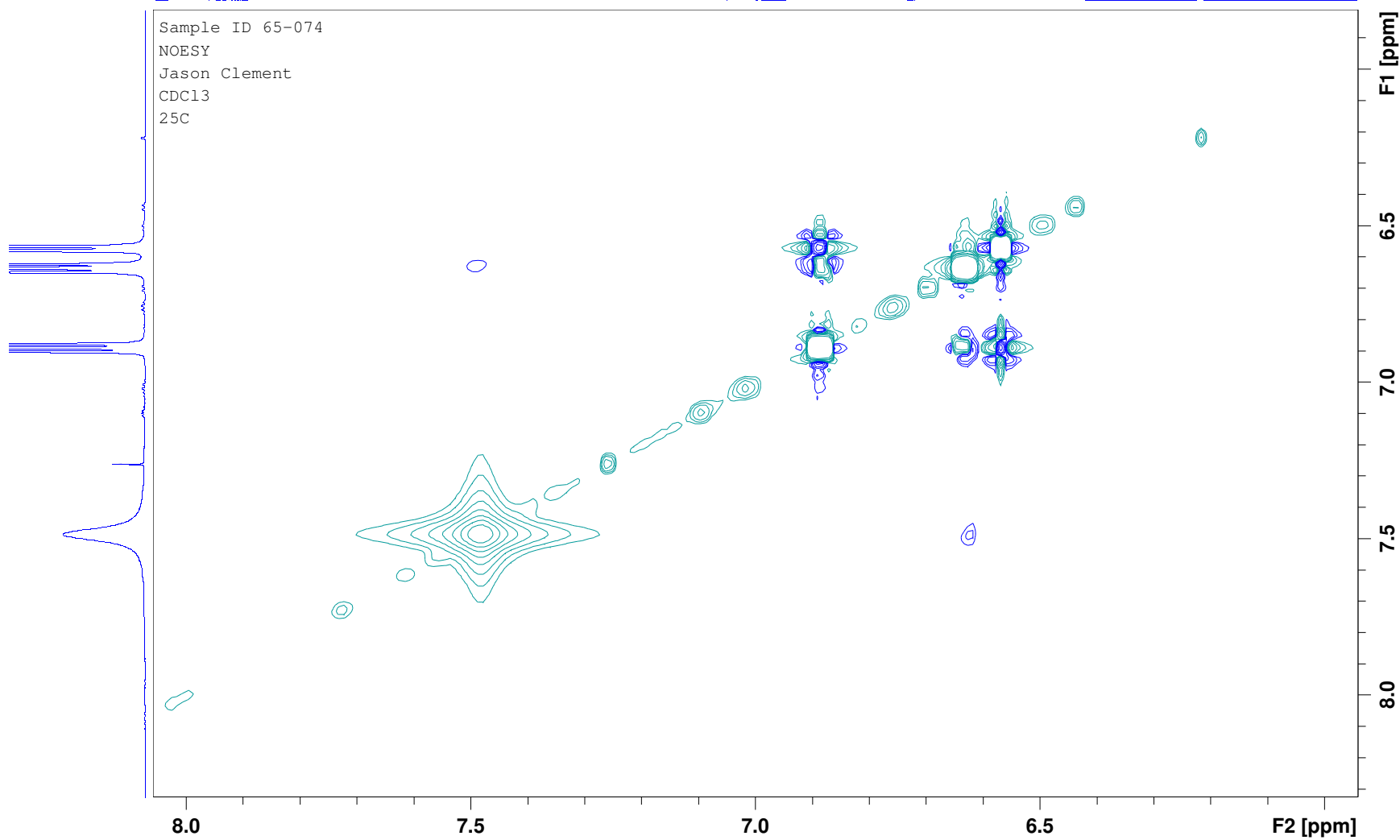
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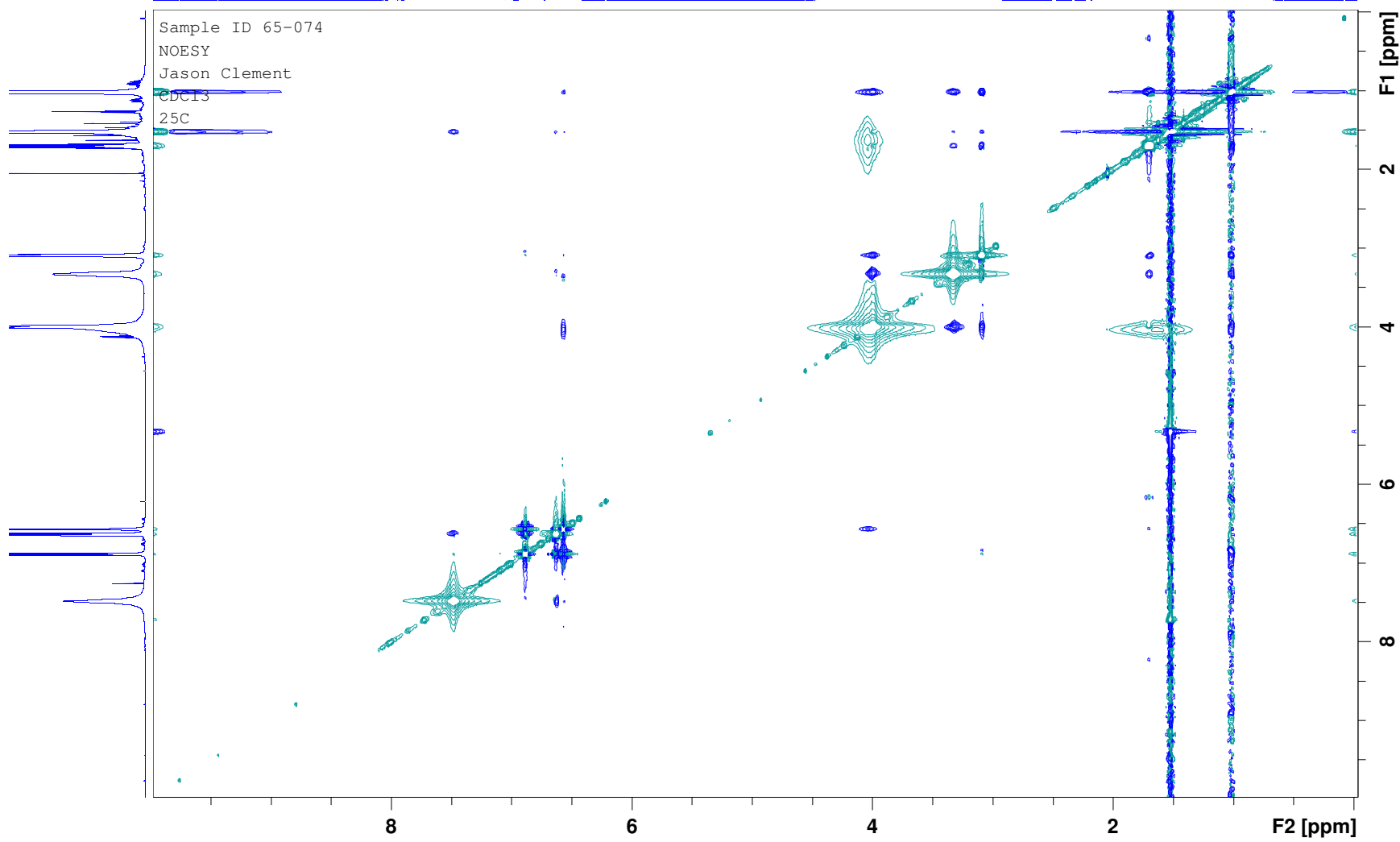
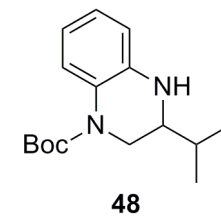
# NOESY Spectrum (CDCl<sub>3</sub>) of 48



"Results sample ID 65-074" 9 1 C:\Users\Jason\Documents\BSBISstuff\MedChem

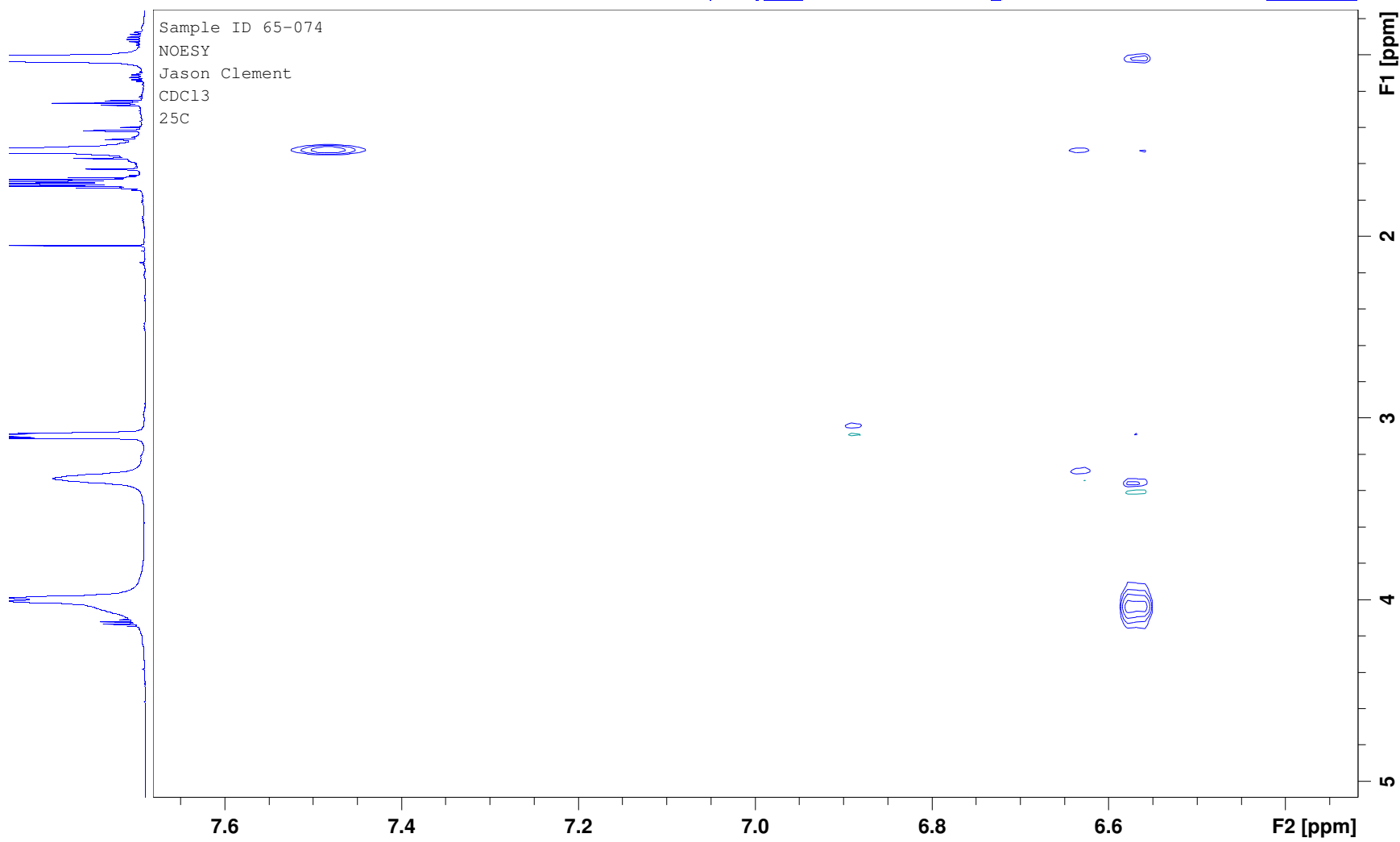
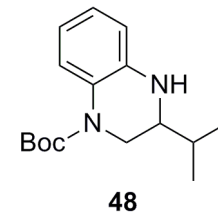


"Results sample ID 65-074" 9 1 C:\Users\Jason\Documents\BSBIstuff\MedChem

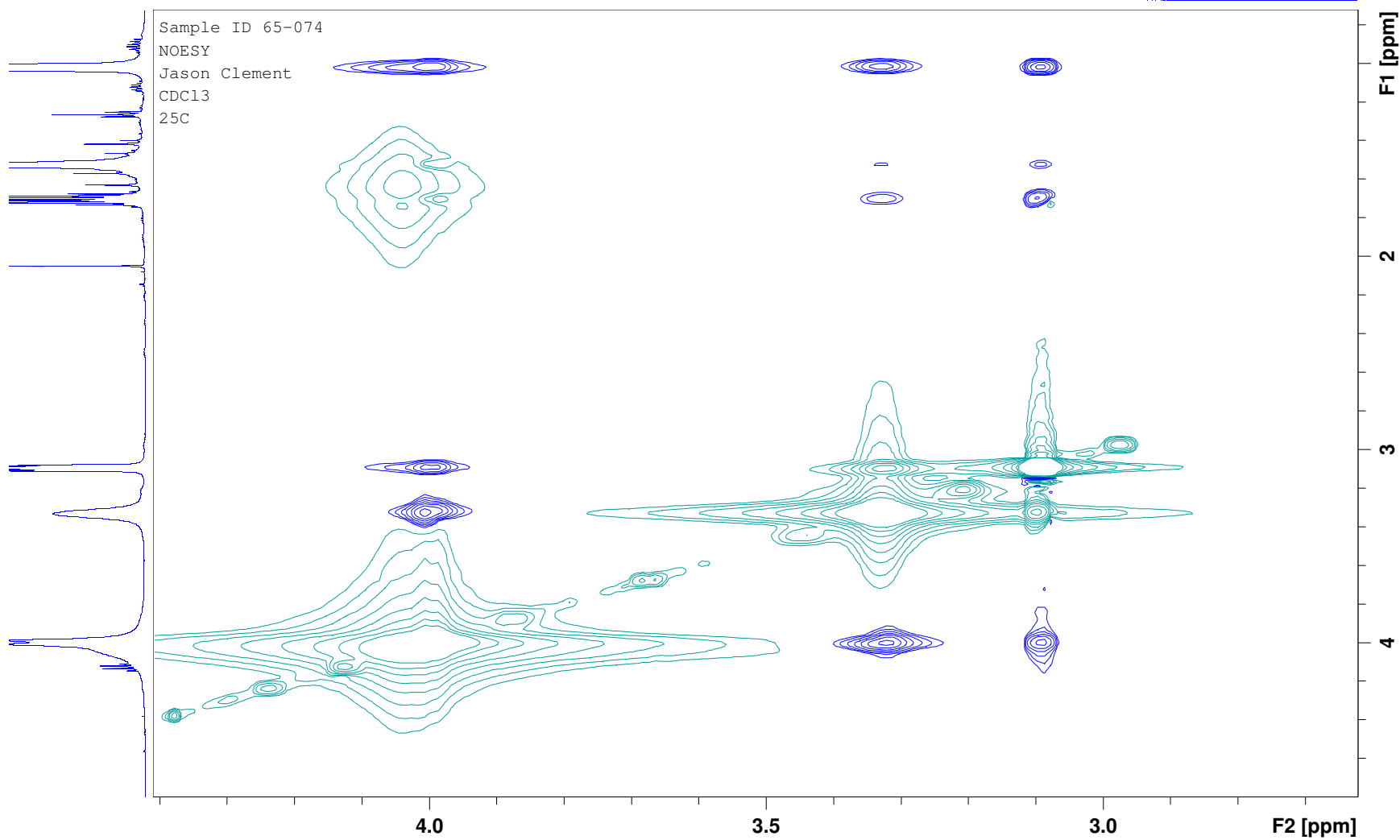
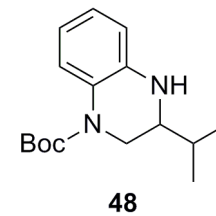




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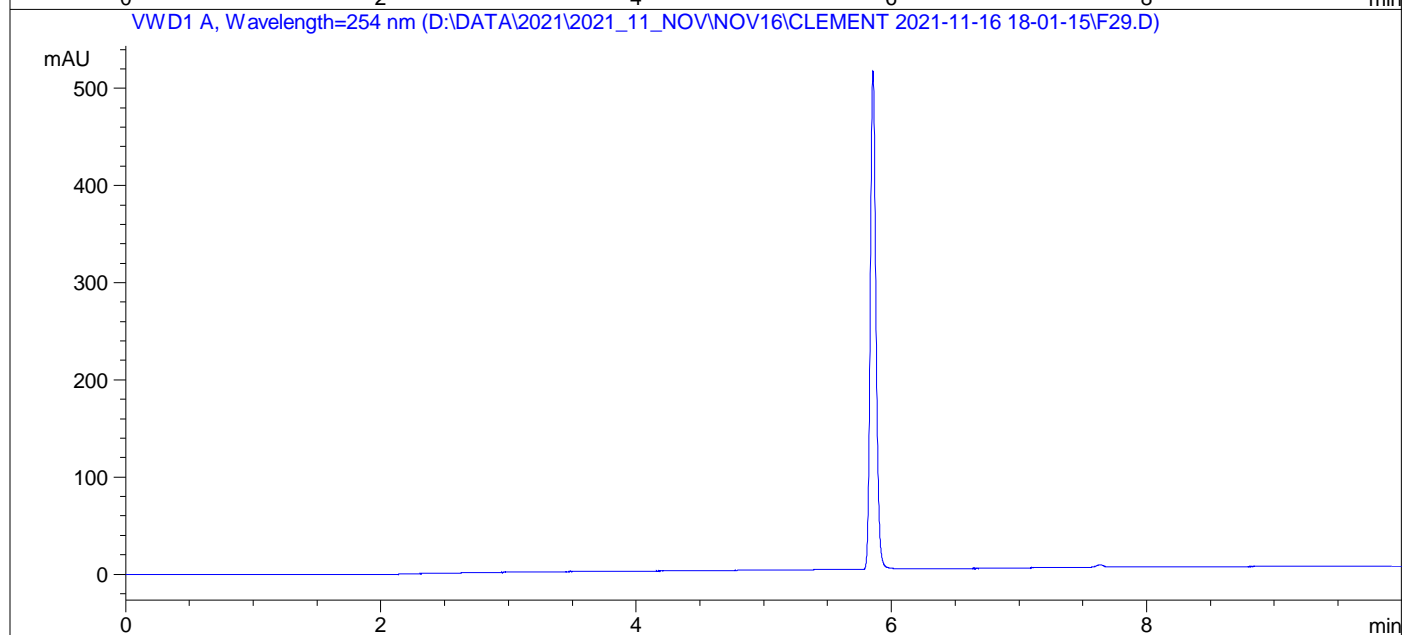
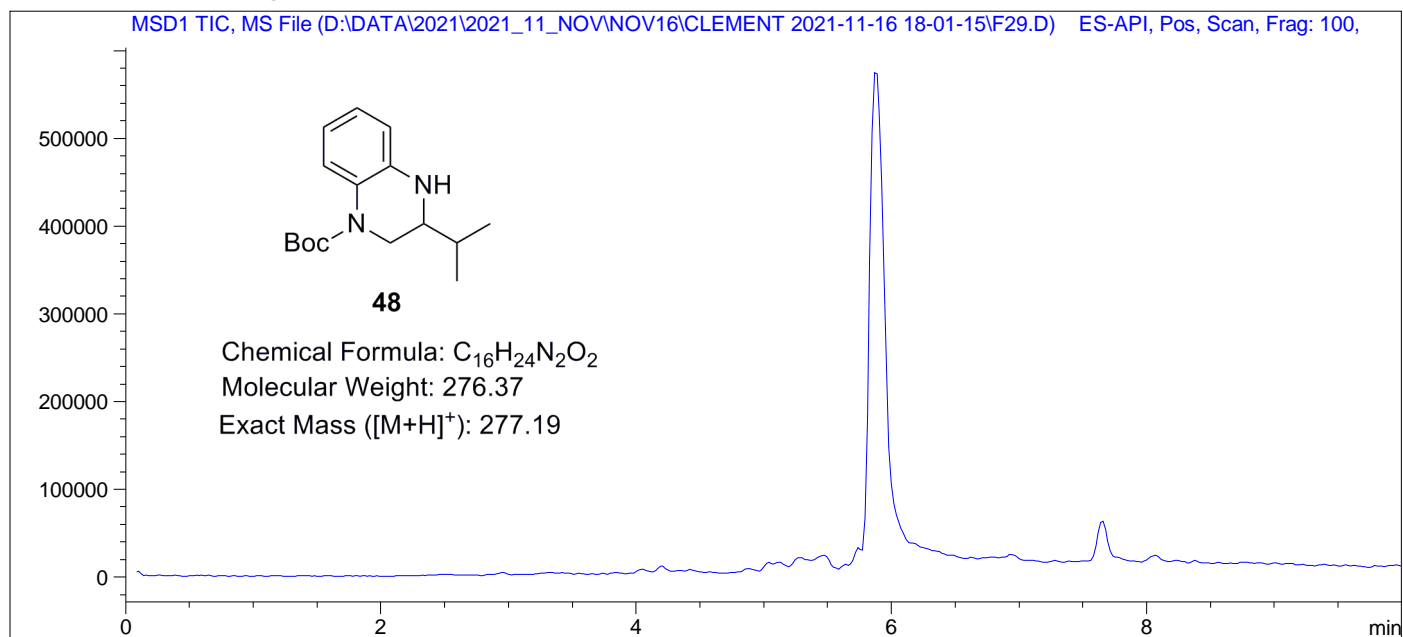


"Results sample ID 65-074 9 1 C:\Users\Jason\Documents\BSBIstuff\MedChem

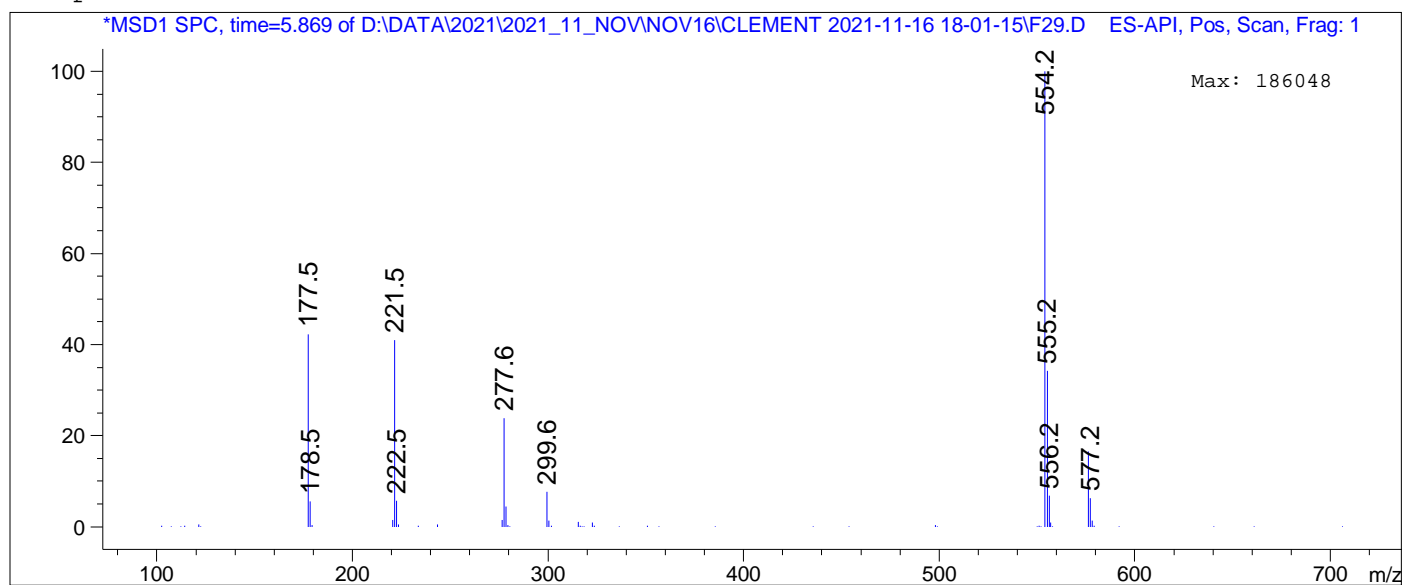


## LCMS analysis of 48

Current Chromatogram(s)



MS Spectrum



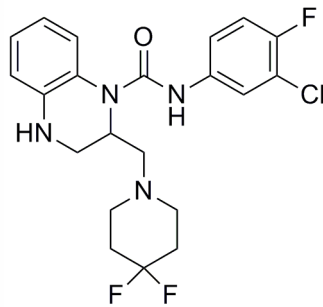
<sup>1</sup>H NMR Spectrum (300 MHz, CDCl<sub>3</sub>) of 61

STANDARD 1H OBSERVE

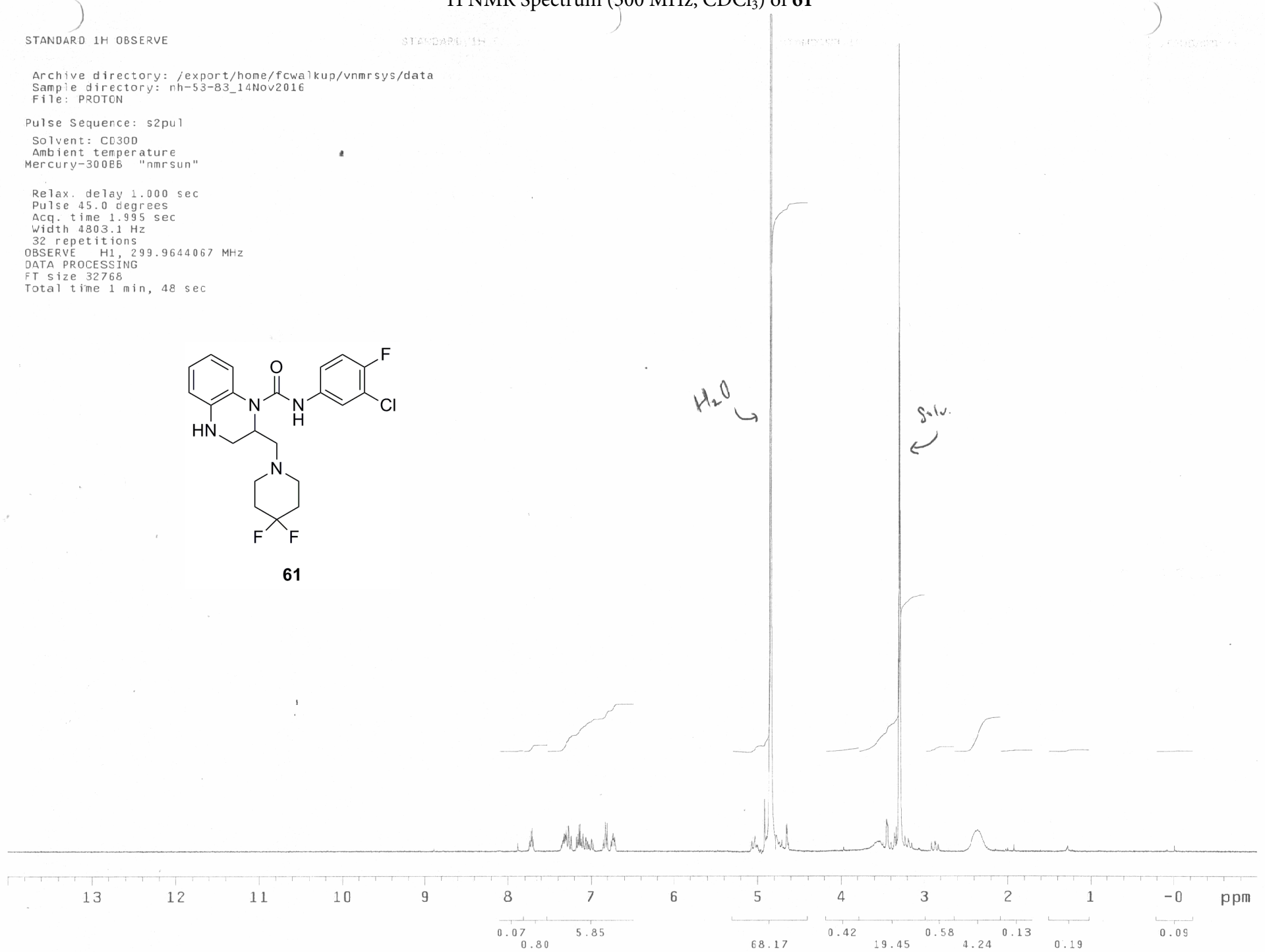
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Sample directory: nh-53-83\_14Nov2016  
File: PROTON

Pulse Sequence: s2pu1  
Solvent: CD300  
Ambient temperature  
Mercury-300B6 "nmrsun"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.995 sec  
Width 4803.1 Hz  
32 repetitions  
OBSERVE H1, 299.9644067 MHz  
DATA PROCESSING  
FT size 32768  
Total time 1 min, 48 sec



61



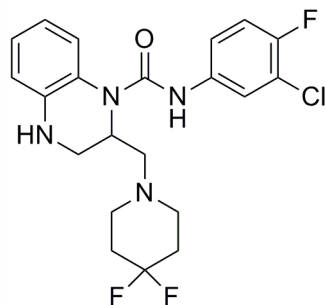
<sup>1</sup>H NMR Spectrum (300 MHz, CDCl<sub>3</sub>) of 61

STANDARD 1H OBSERVE

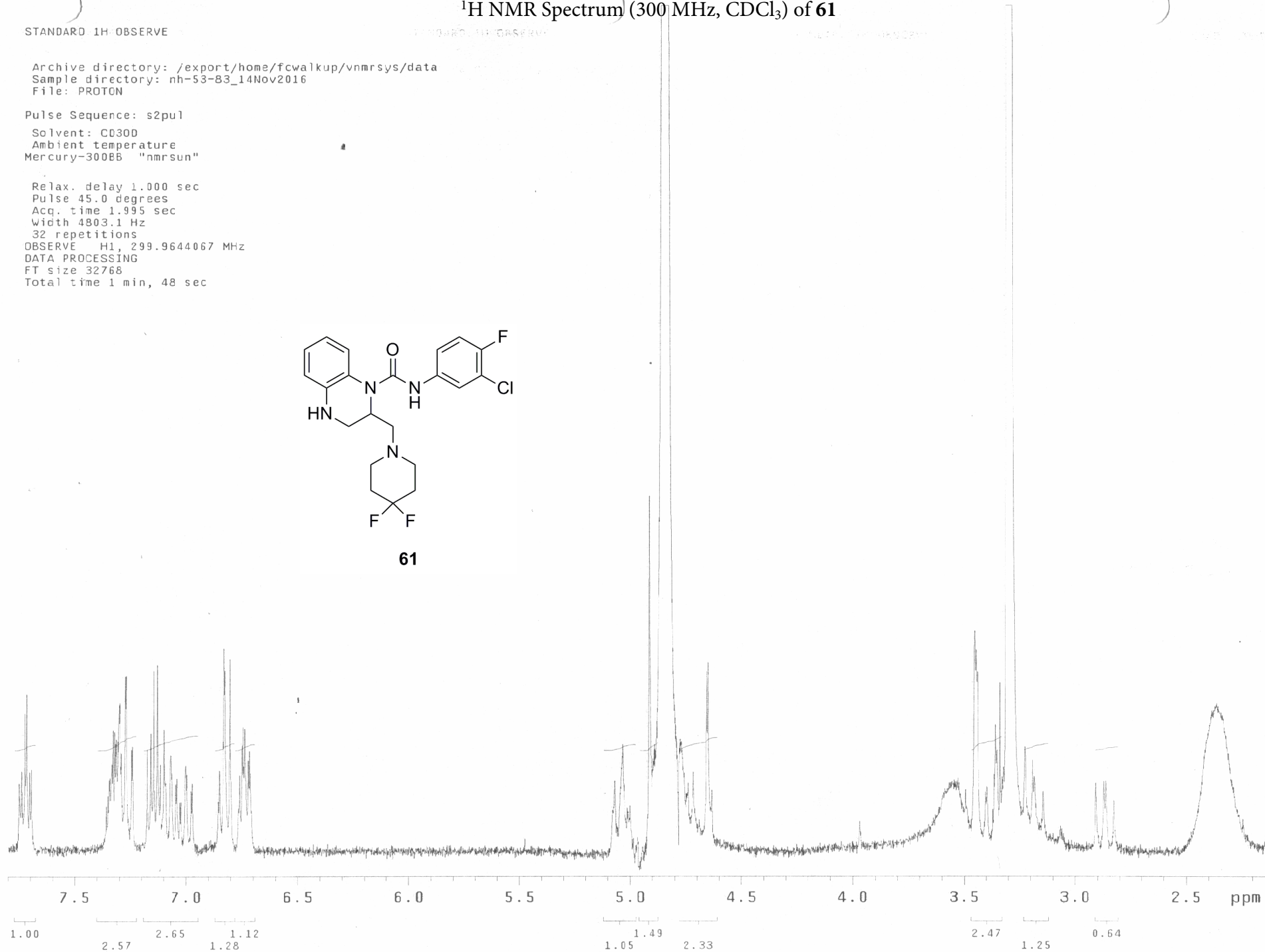
Archive directory: /export/home/fcwalkup/vnmrsys/data  
Sample directory: nh-53-83\_14Nov2016  
File: PROTON

Pulse Sequence: s2pul  
Solvent: CD3OD  
Ambient temperature  
Mercury-300B5 "nmrsun"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.995 sec  
Width 4803.1 Hz  
32 repetitions  
OBSERVE H1, 299.9644067 MHz  
DATA PROCESSING  
FT size 32768  
Total time 1 min, 48 sec

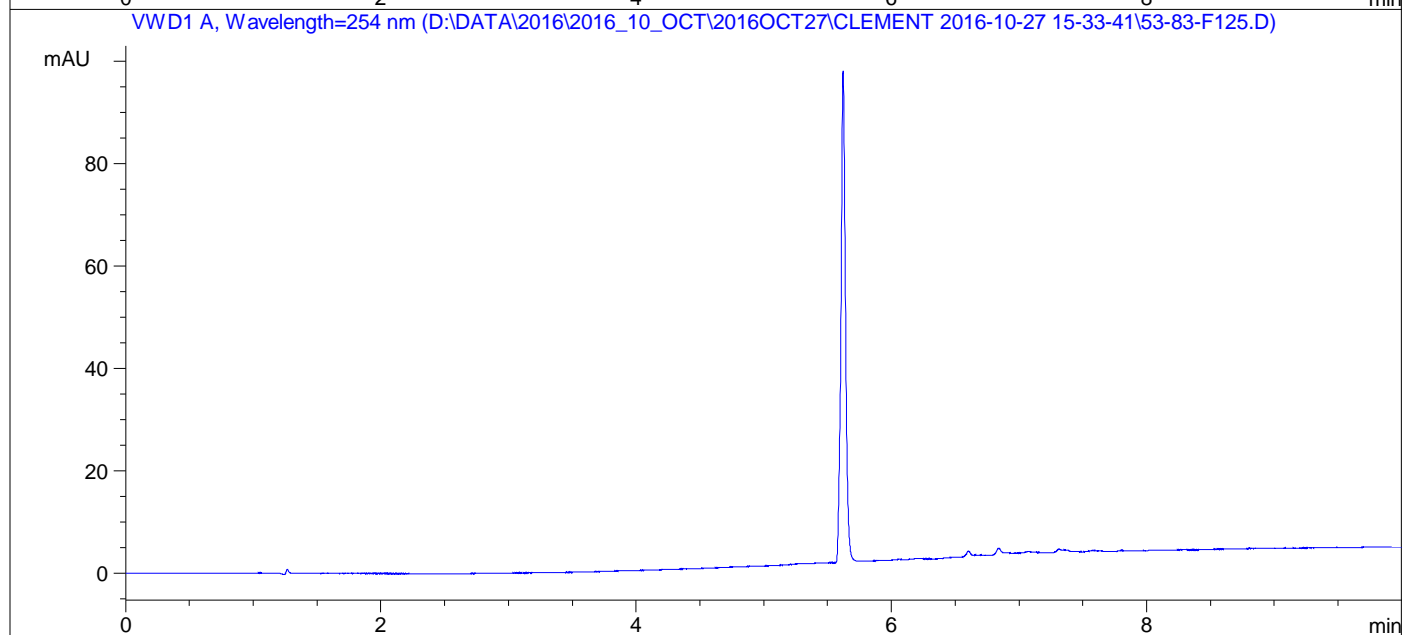
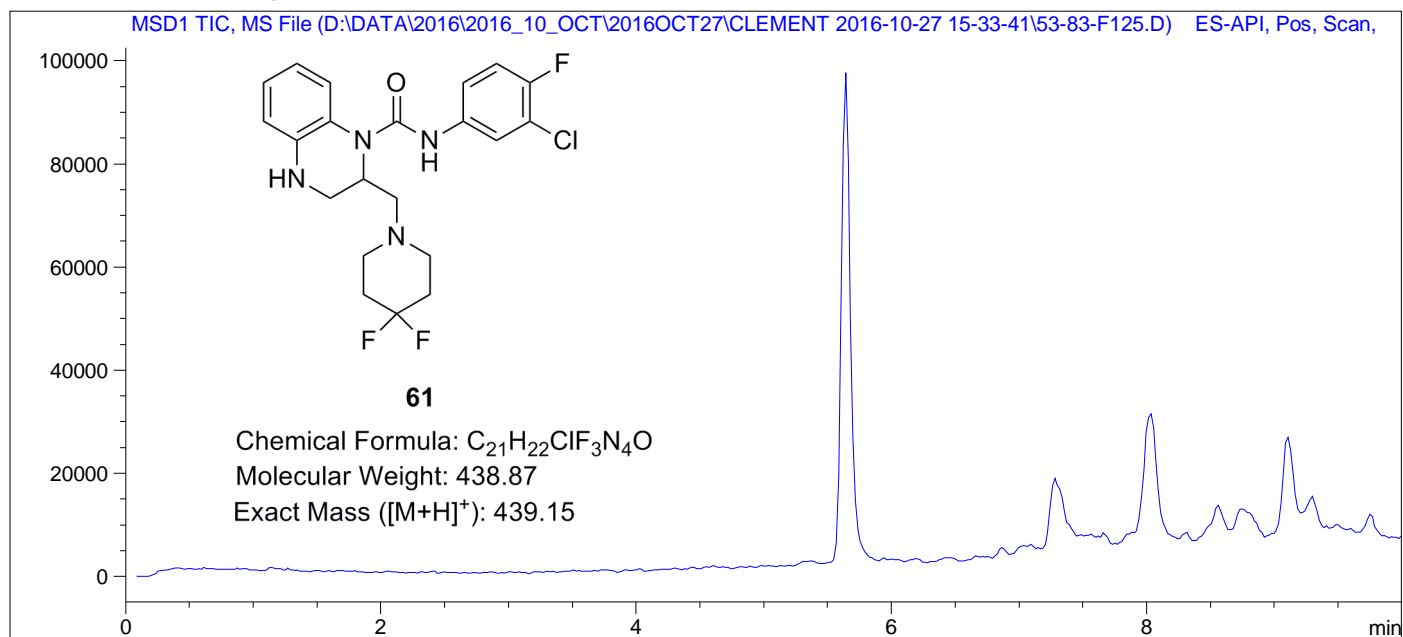


61

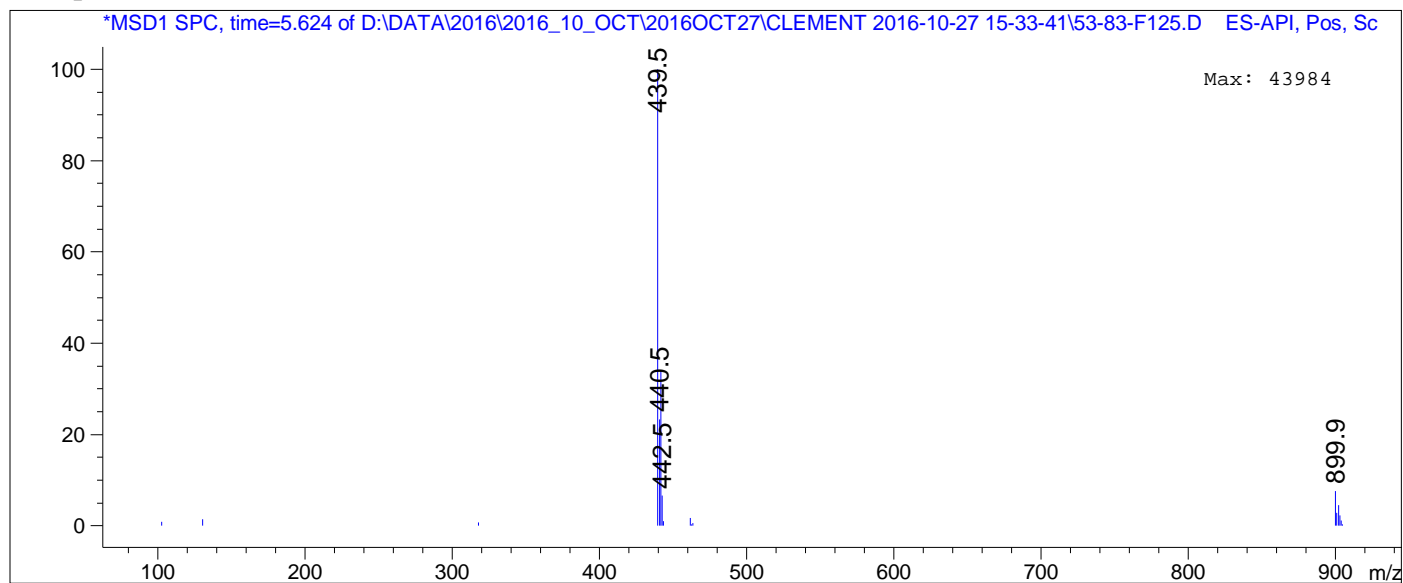


LCMS analysis of **61**

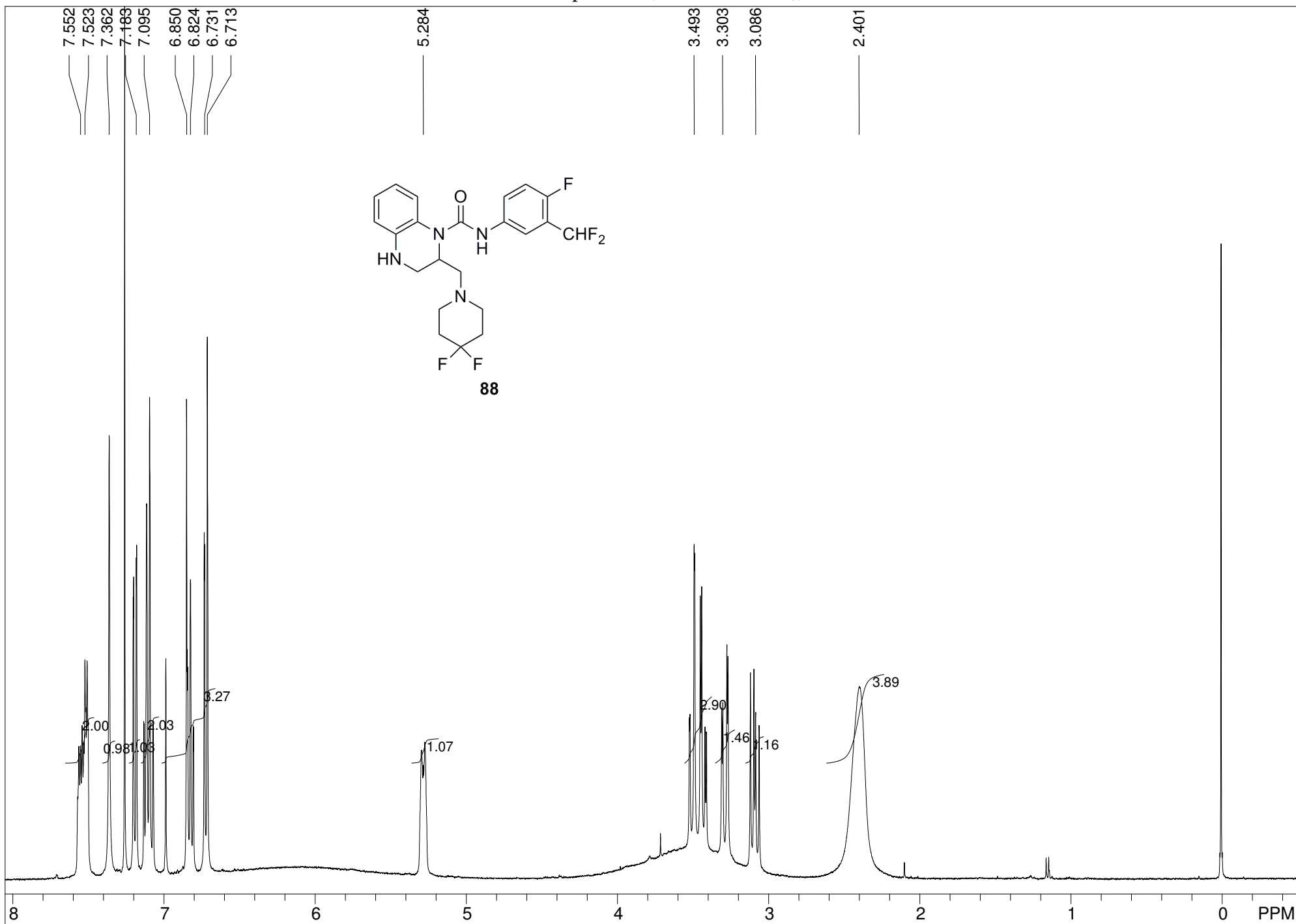
Current Chromatogram(s)



MS Spectrum



<sup>1</sup>H NMR Spectrum (400 MHz, CDCl<sub>3</sub>) of **88**



BSB1-65012-D 1

USER: qiuf -- DATE: Tue Oct 20 17:11:42 2020

F1: 400.133 F2: 400.133

SW1: 7211

OF1: 2794.5

PTS1d: 32734

EX: <zg30>

PW: 0.0 us

PD: ? sec

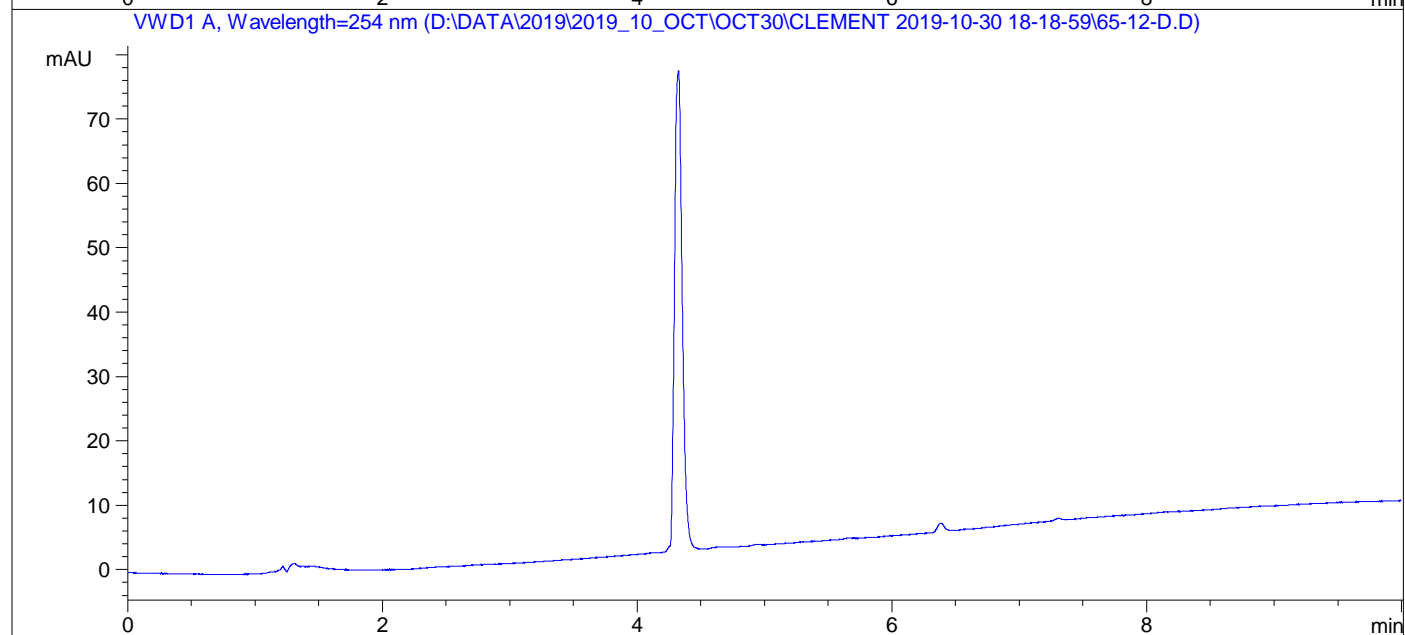
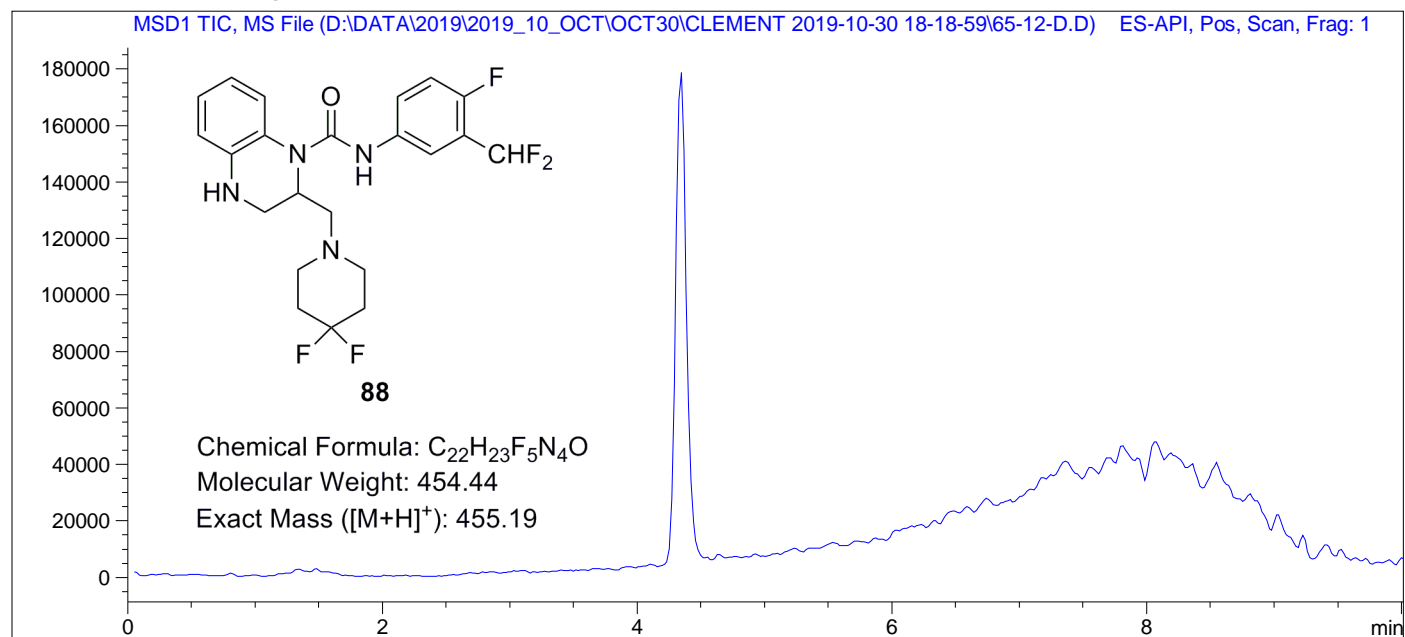
NA: 16

LB: 0.0

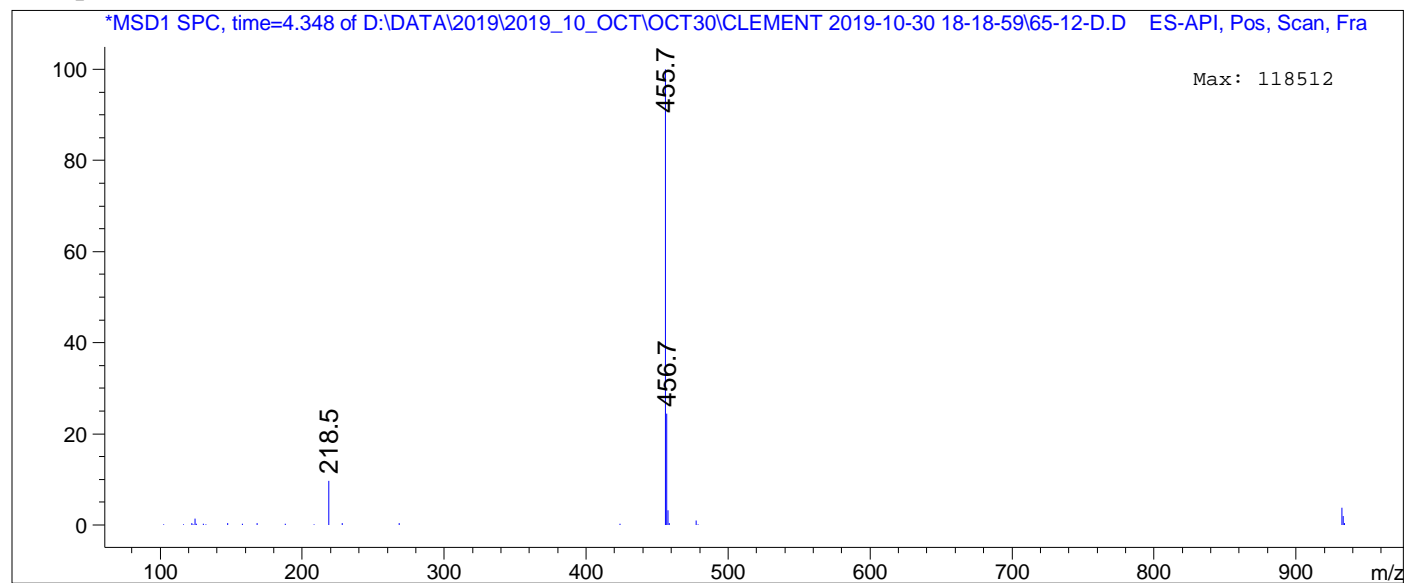
Nuts - \$BSB1-65012-D 1.dx

LCMS analysis of **88**

Current Chromatogram(s)



MS Spectrum





## Analysis Info

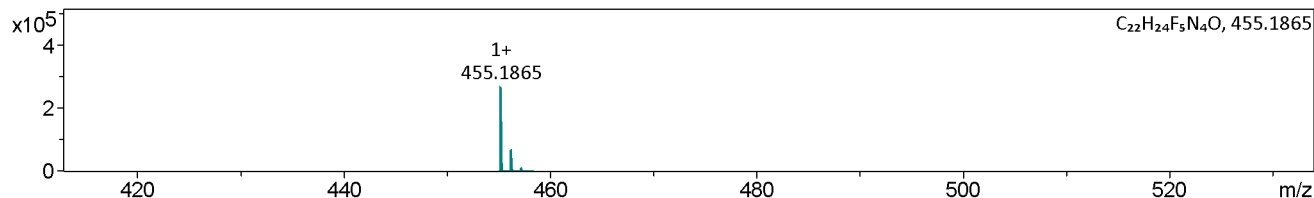
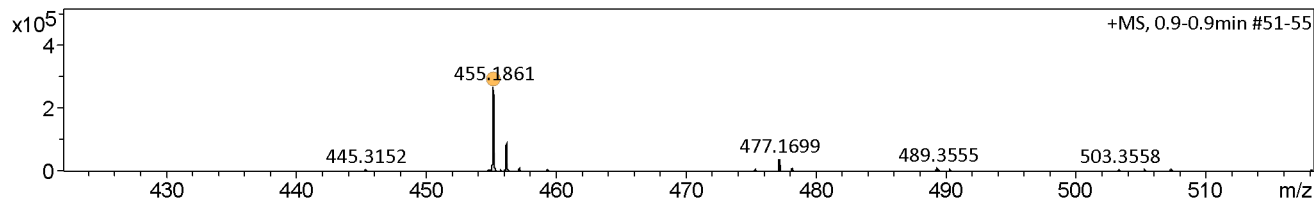
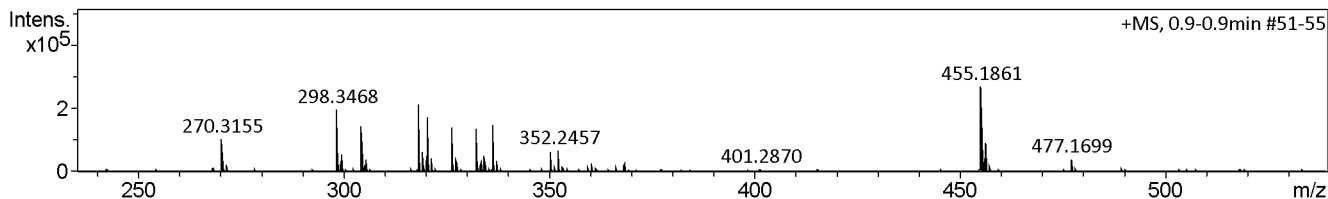
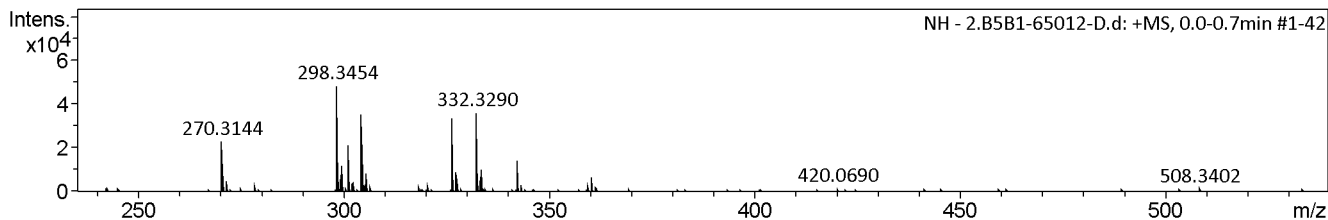
Analysis Name D:\Data\1022\NH - 2.B5B1-65012-D.d  
 Method 1019\_tune low.m  
 Sample Name 2.B5B1-65012-D  
 Comment direct infusion

Acquisition Date 10/22/2020 2:46:14 PM

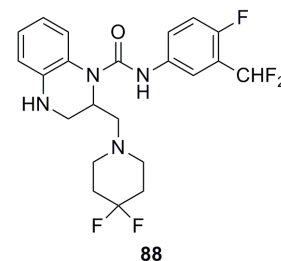
Operator BDAL@DE  
 Instrument / Ser# micrOTOF II 8213750.1  
 0314

## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1650 m/z	n/a	n/a	Set Divert Valve	Source

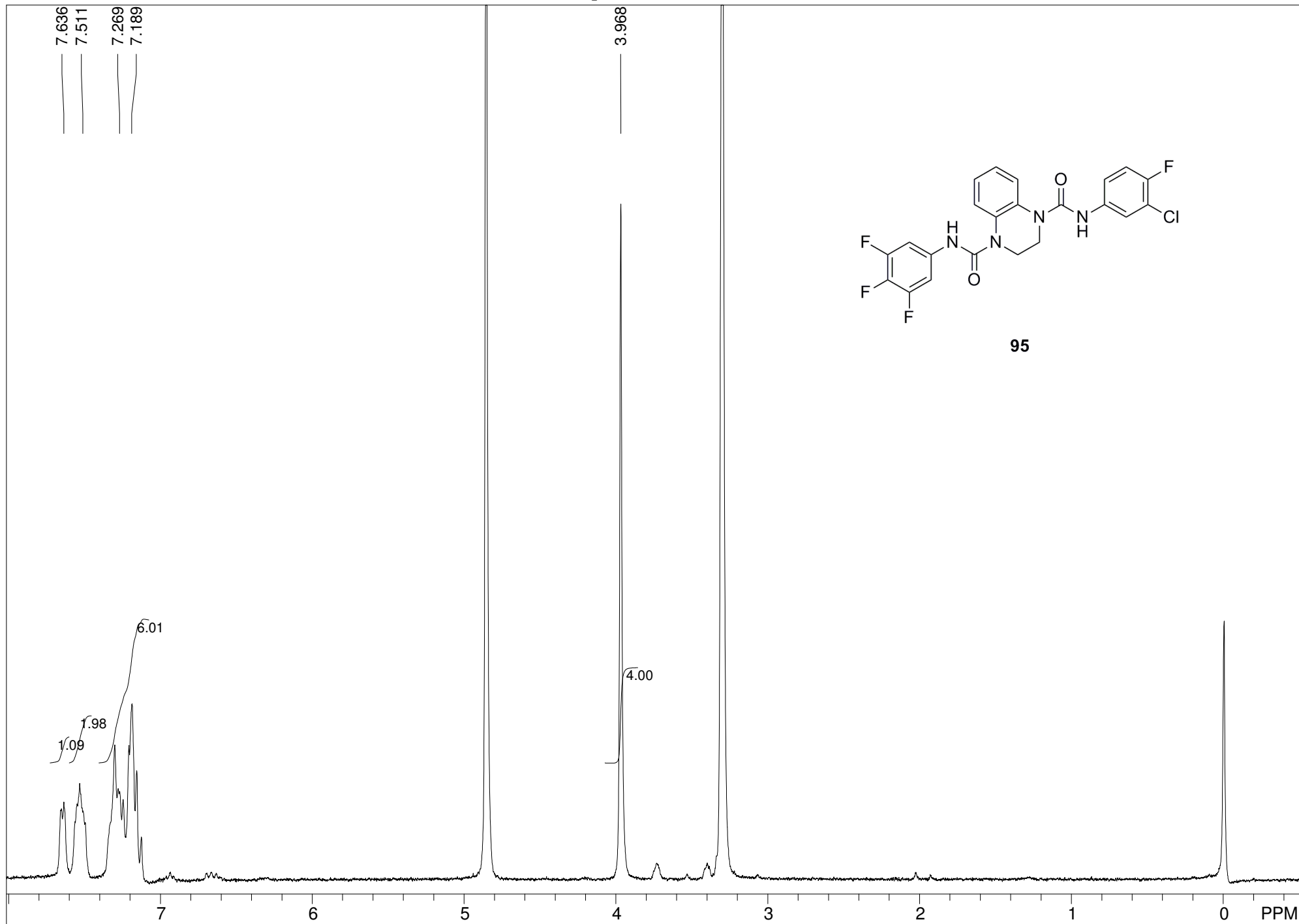


Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e <sup>-</sup>	Conf
455.186146	1	C22H24F5N4O	455.186479	0.7	-0.7	10.5	ok	even	



Chemical Formula: C<sub>22</sub>H<sub>23</sub>F<sub>5</sub>N<sub>4</sub>O  
 Molecular Weight: 454.44  
 Exact Mass ([M+H]<sup>+</sup>): 455.19

<sup>1</sup>H NMR Spectrum (300 MHz, CD<sub>3</sub>OD) of 95



nh-58-91-a

USER: -- DATE: Dec 20 2017 11:25

F1: 299.965

F2: 75.433

SW1: 4799

OF1: 1799.9

PTS1d: 8192 , 16384

EX: s2pul

PW: 6.8 us, 45deg

PD: 1.0 sec

NA: 64

LB: 0.3

Nuts - \$nh-58-91-a PROTON 01.fid

### LCMS analysis of 95

Current Chromatogram(s)

