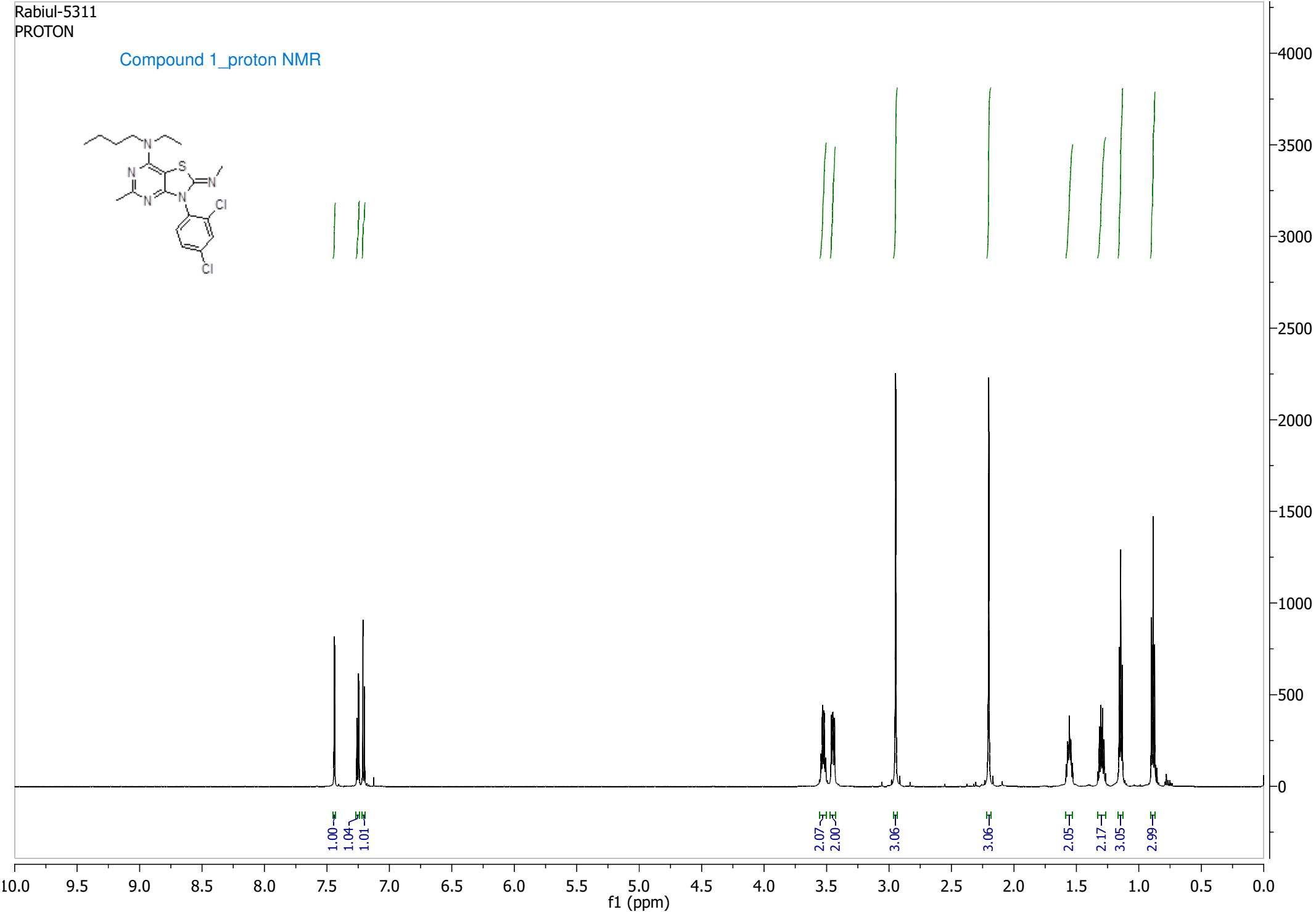
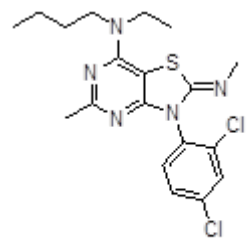


Rabiul-5311
PROTON

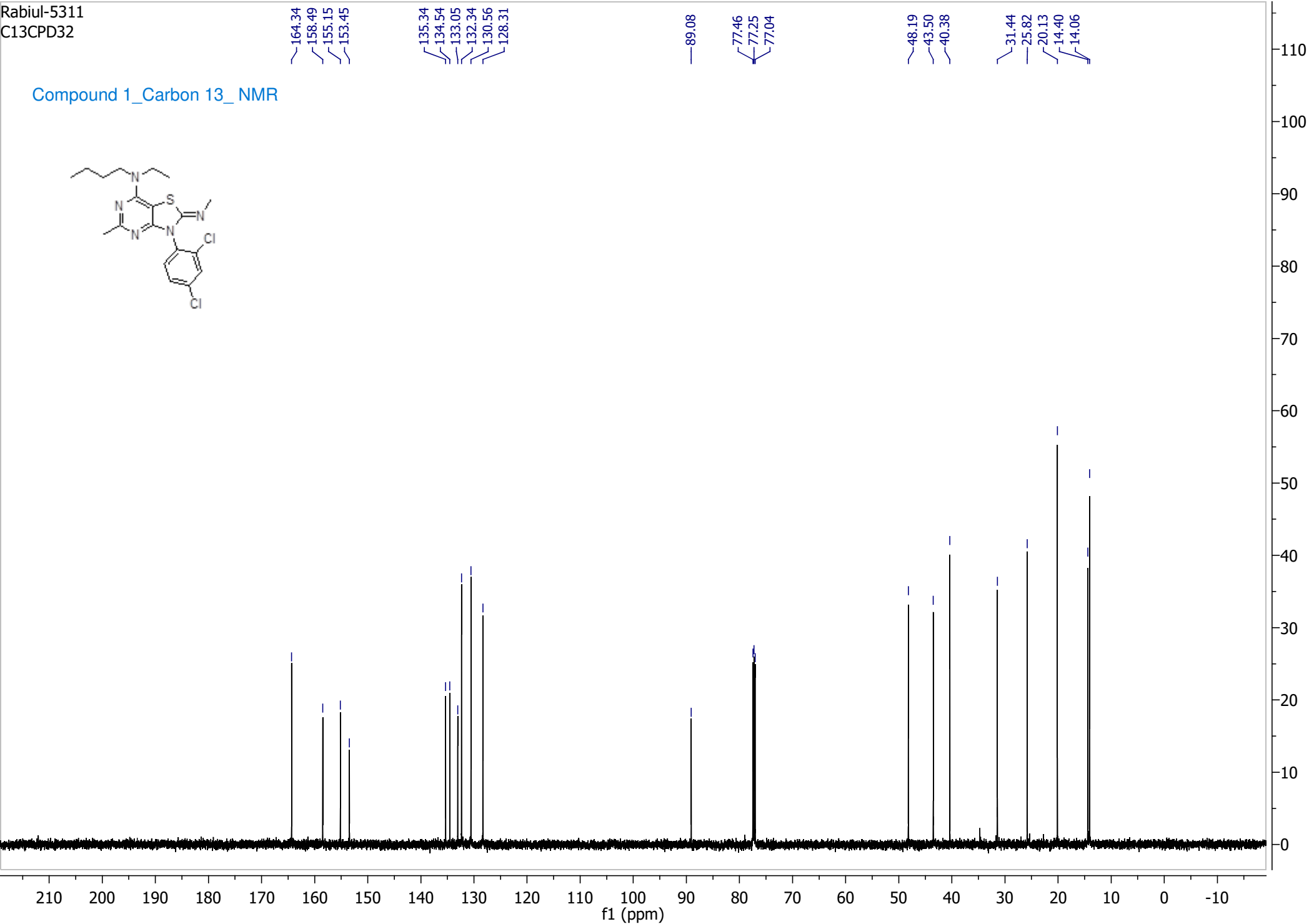
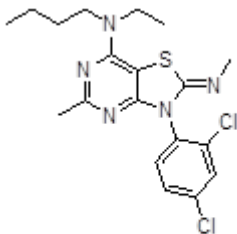
Compound 1_proton NMR



Rabiul-5311
C13CPD32

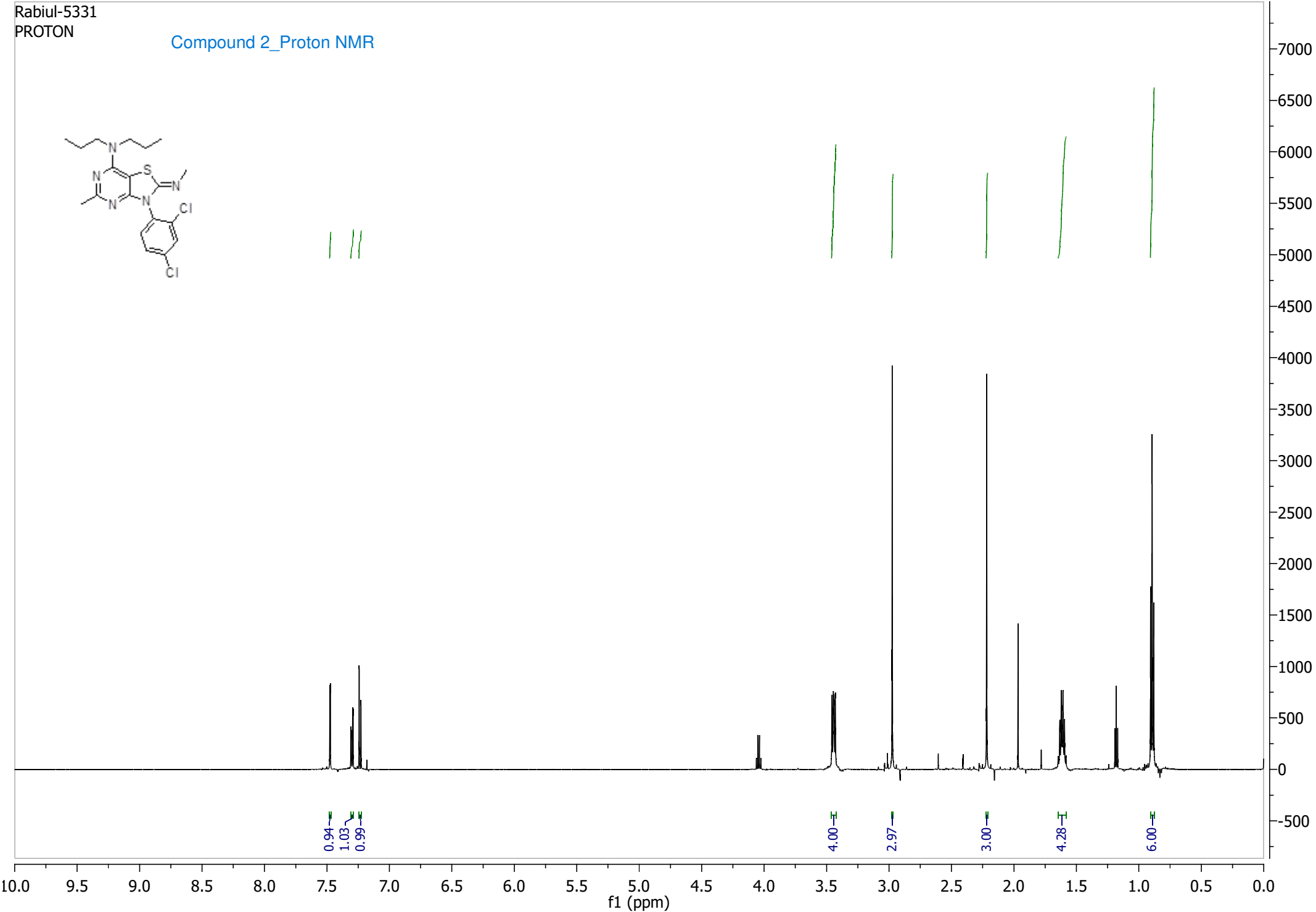
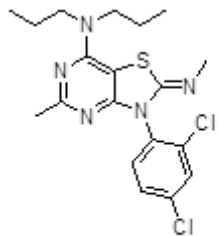
164.34 158.49 155.15 153.45 135.34 134.54 133.05 132.34 130.56 128.31 89.08 77.46 77.25 77.04 48.19 43.50 40.38 31.44 25.82 20.13 14.40 14.06

Compound 1_Carbon 13_NMR



Rabiul-5331
PROTON

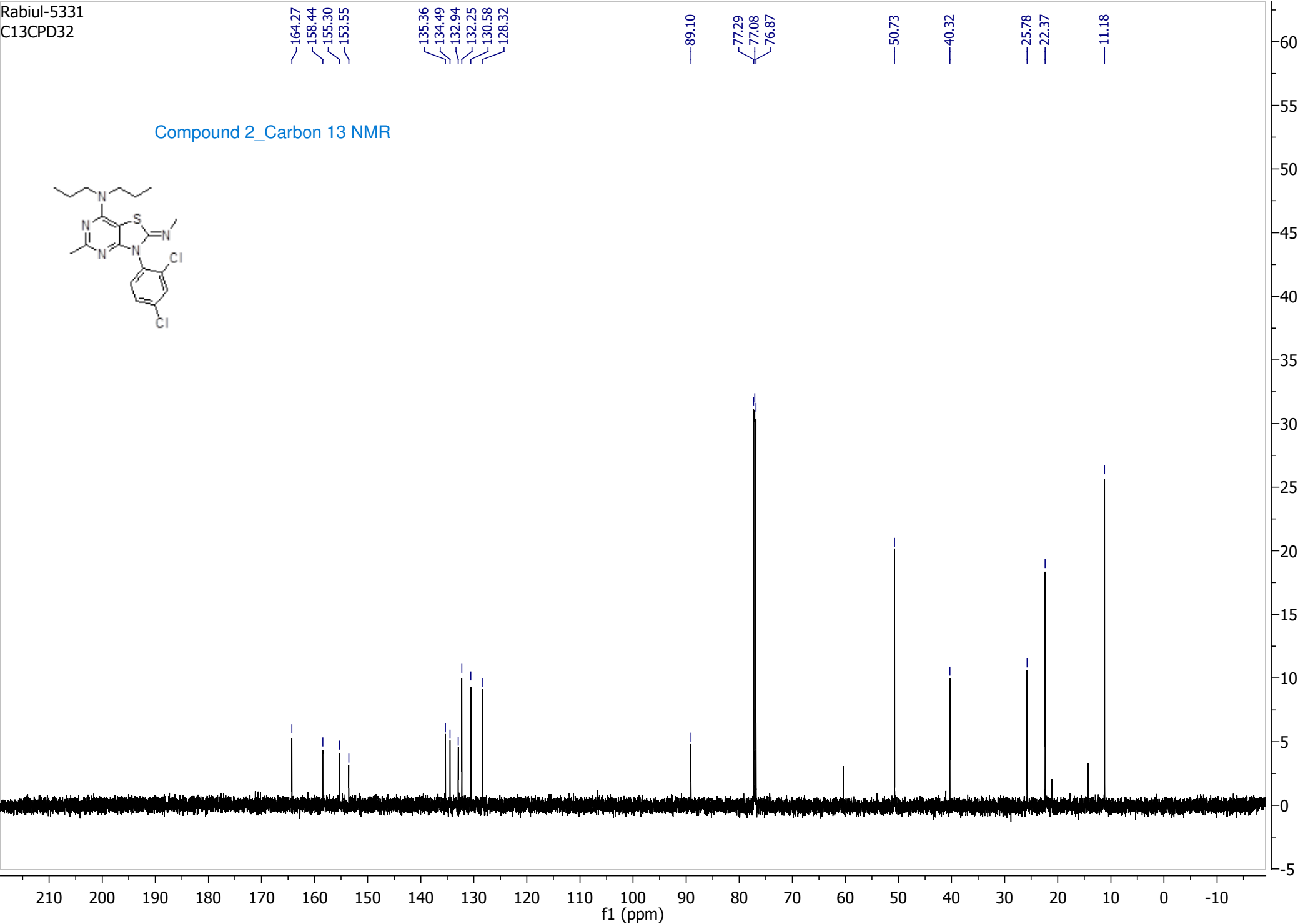
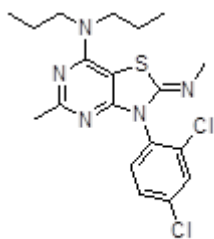
Compound 2_Proton NMR



Rabiul-5331
C13CPD32

164.27 158.44 155.30 153.55 135.36 134.49 132.94 132.25 130.58 128.32 89.10 77.29 77.08 76.87 50.73 40.32 25.78 22.37 11.18

Compound 2_Carbon 13 NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5331_000001.d
Method Bruker_11052015
Sample Name 5331
Comment

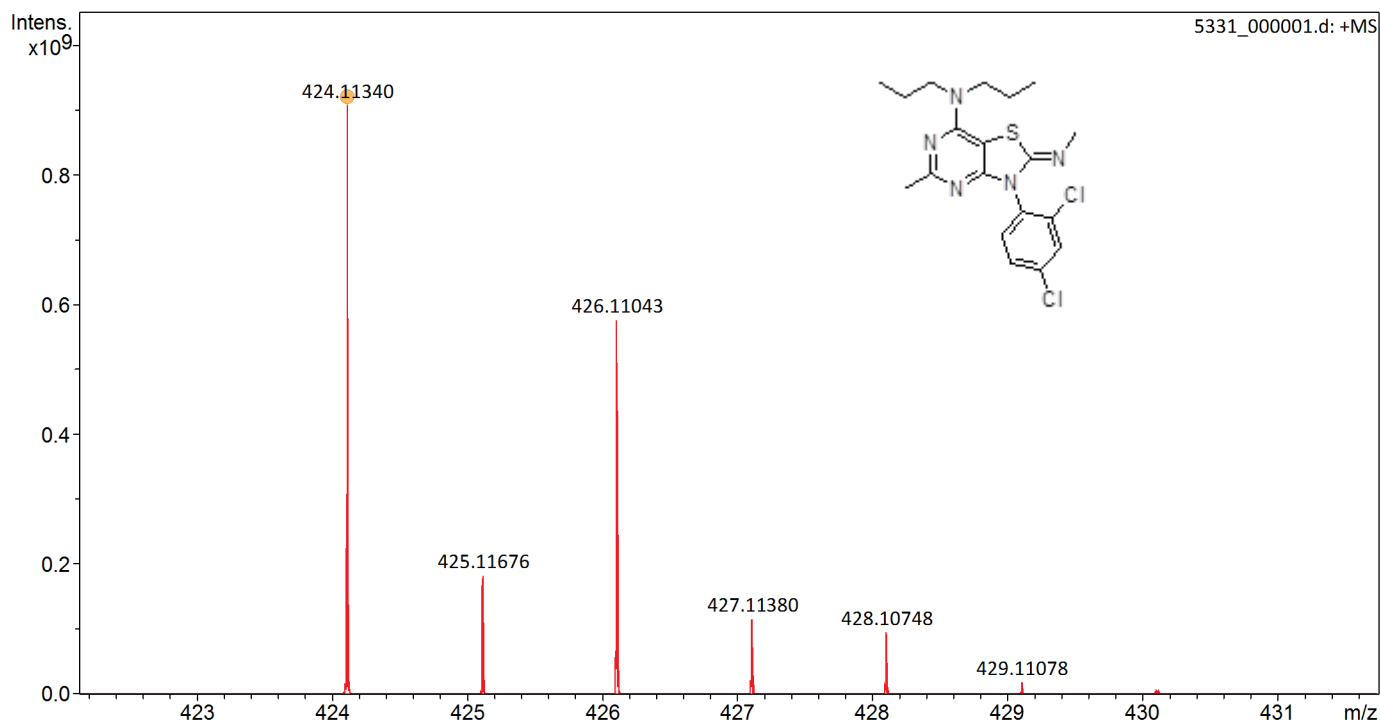
Acquisition Date 3/21/2019 5:32:27 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

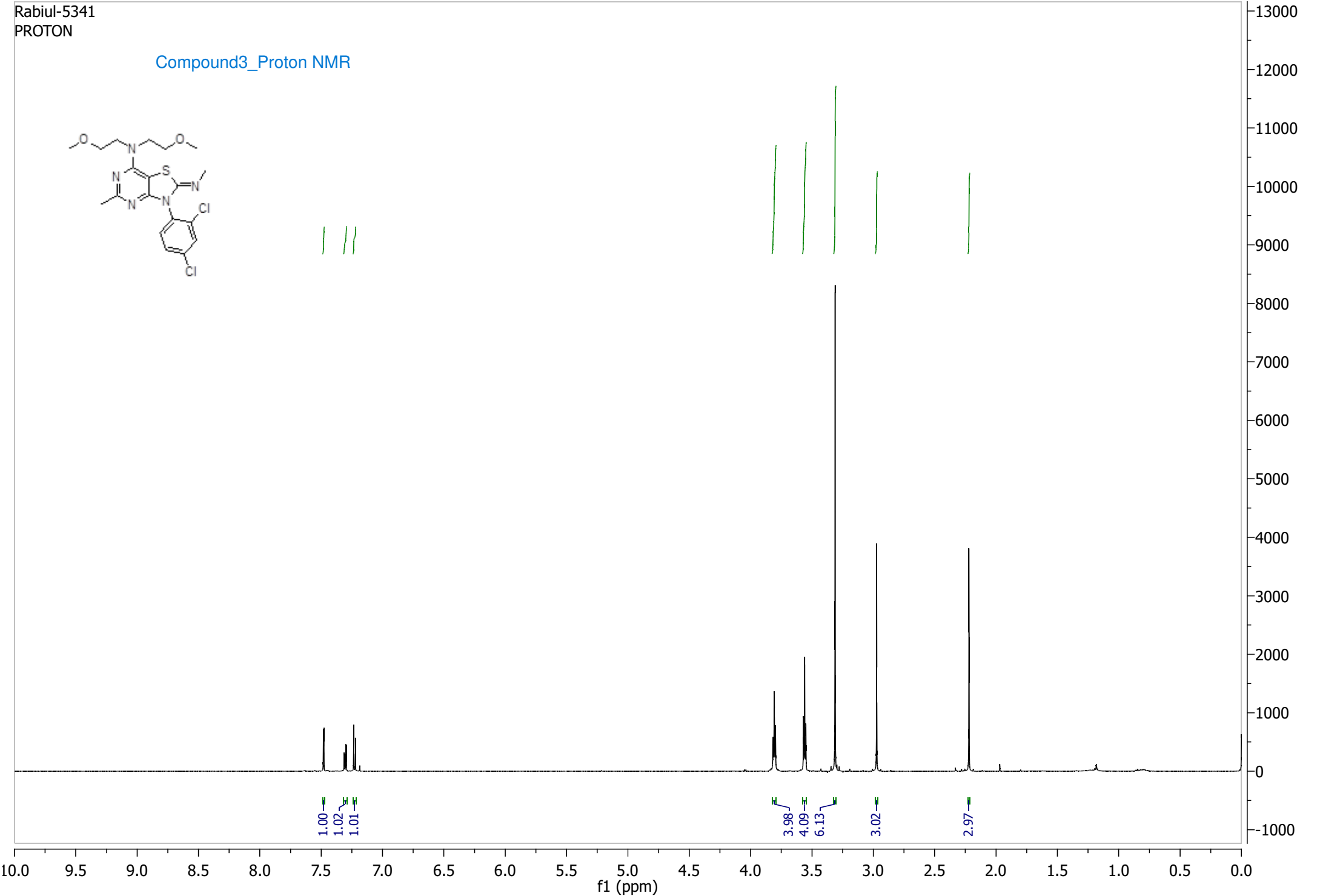
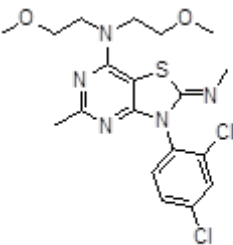
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	424.113399	1	C ₁₉ H ₂₄ Cl ₂ N ₅ S	100.00	424.112399	-2.4	-2.5	26.0	9.5	even		ok
M+Na	446.095180	1	C ₁₉ H ₂₃ Cl ₂ N ₅ NaS	100.00	446.094343	-1.9	-1.9	15.7	9.5	even		ok

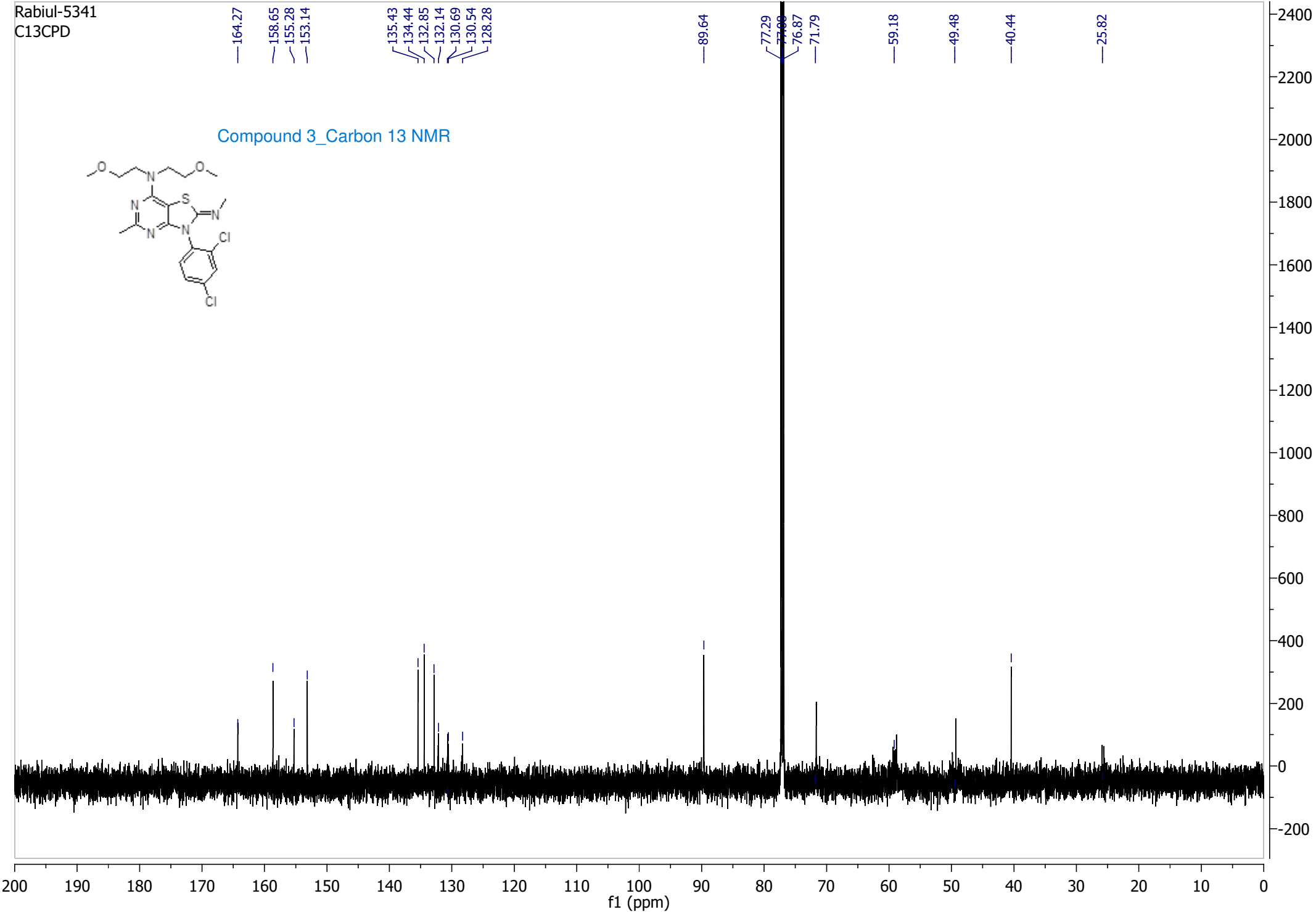
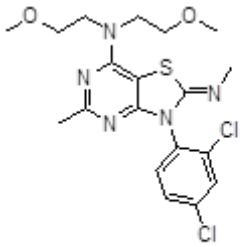
Rabiul-5341
PROTON

Compound3_Proton NMR



Rabiul-5341
C13CPD

Compound 3_Carbon 13 NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5341_000001.d
Method Bruker_11052015
Sample Name 5341
Comment

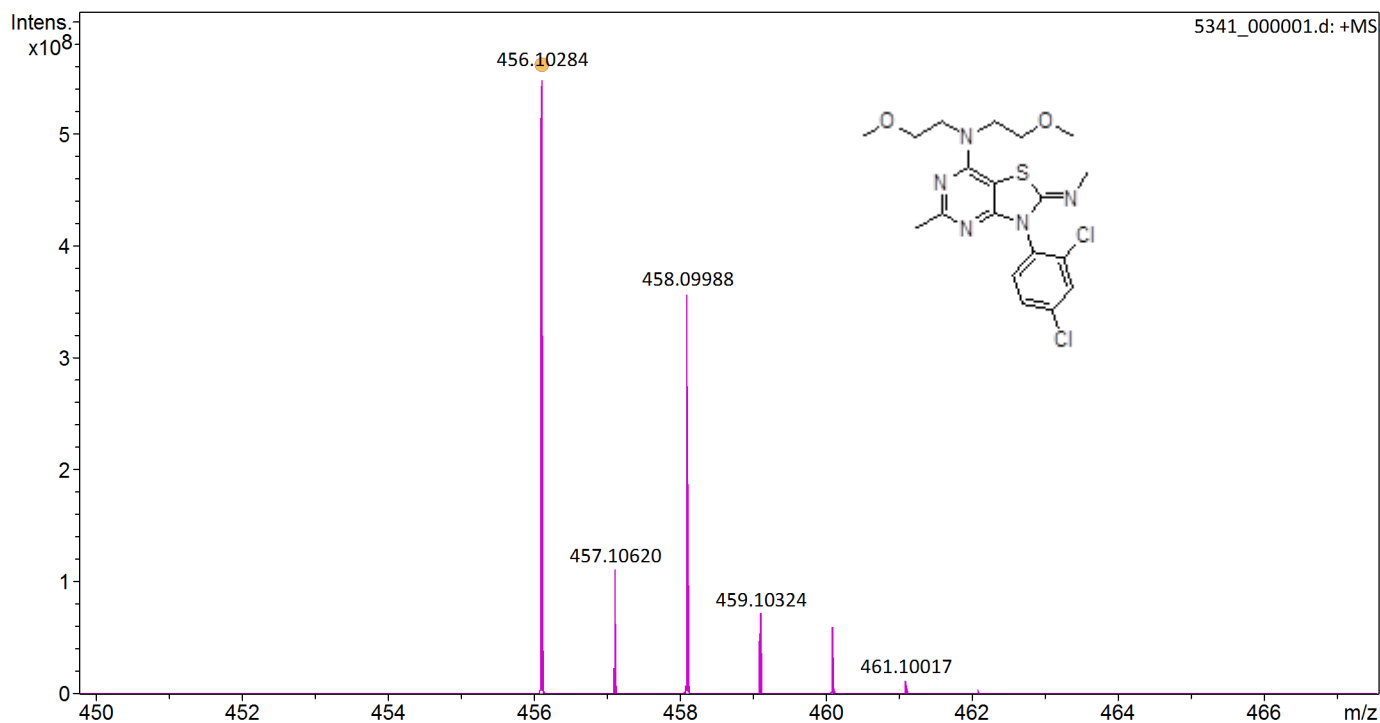
Acquisition Date 3/21/2019 5:47:59 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

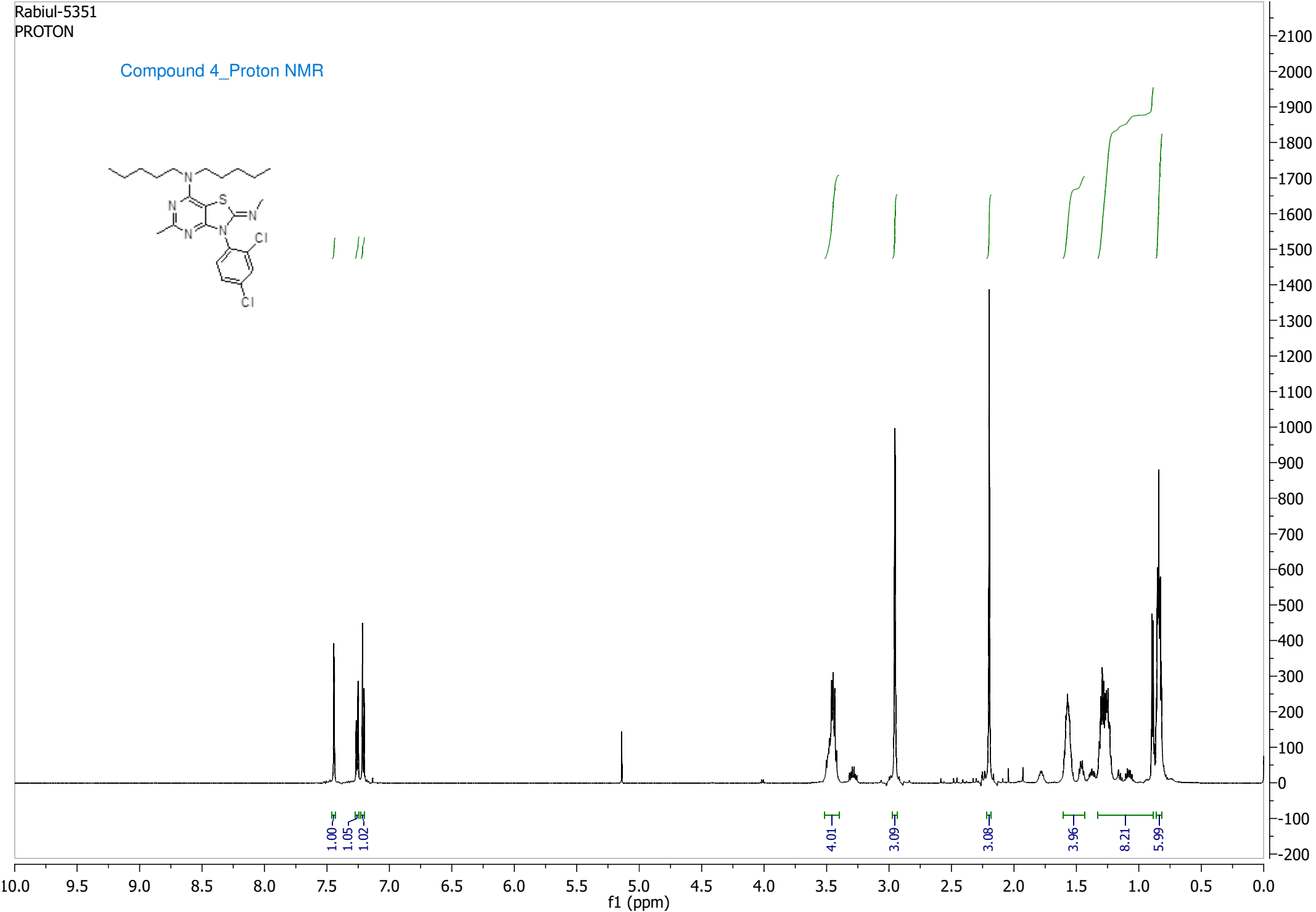
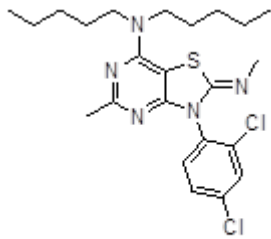
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	456.102845	1	C ₁₉ H ₂₄ Cl ₂ N ₅ O ₂ S	100.00	456.102228	-1.4	-1.4	22.0	9.5	even		ok

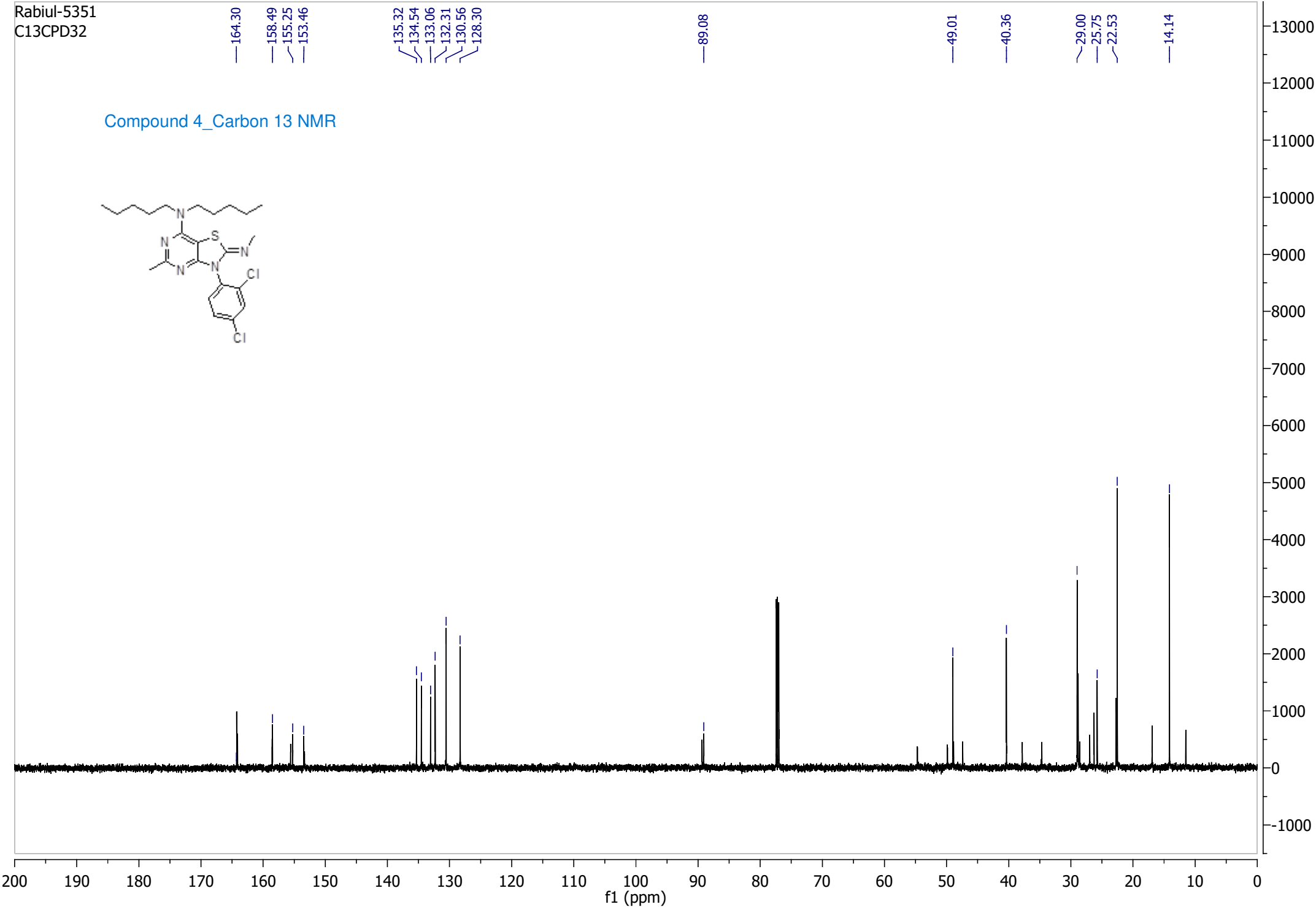
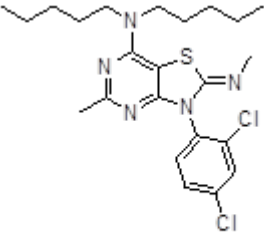
Rabiul-5351
PROTON

Compound 4_Proton NMR



Rabiul-5351
C13CPD32

Compound 4_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC_3-21-19\5351_000001.d
Method Bruker_11052015
Sample Name 5351
Comment

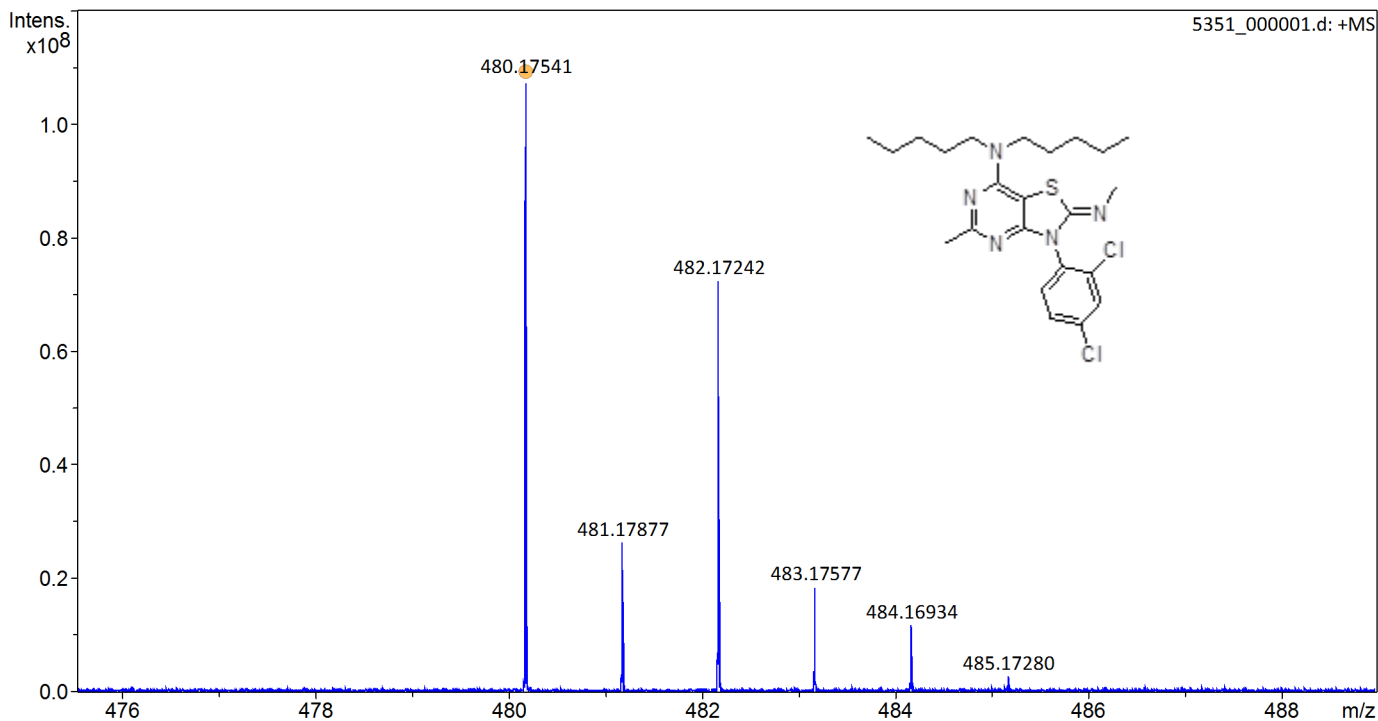
Acquisition Date 3/21/2019 5:51:19 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

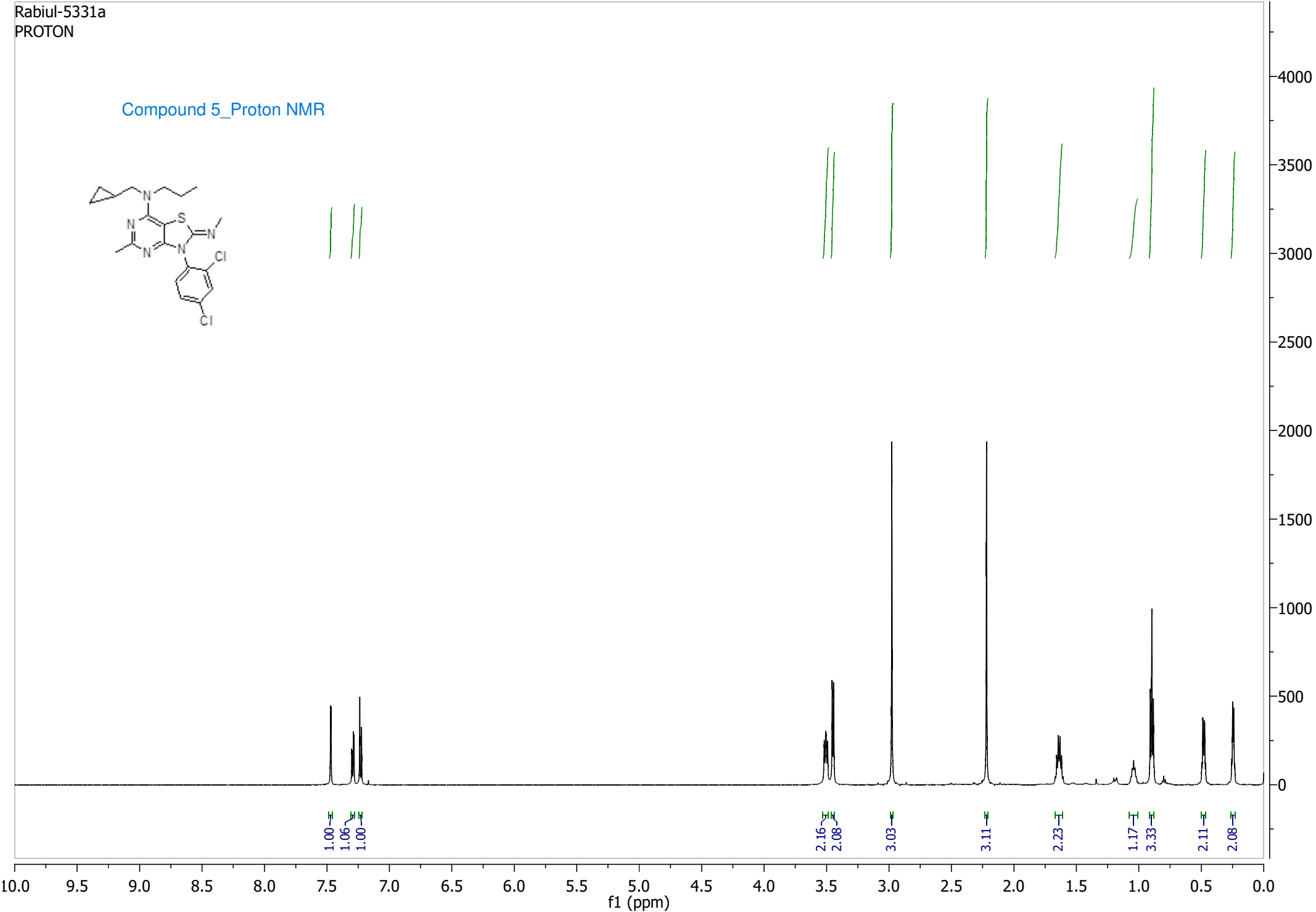
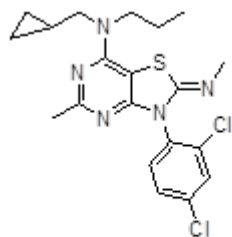
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	480.175406	1	C ₂₃ H ₃₂ Cl ₂ N ₅ S	100.00	480.174999	-0.8	-0.9	14.1	9.5	even		ok
M+Na	502.157142	1	C ₂₃ H ₃₁ Cl ₂ N ₅ NaS	100.00	502.156943	-0.4	-0.4	23.7	9.5	even		ok

Rabiul-5331a
PROTON

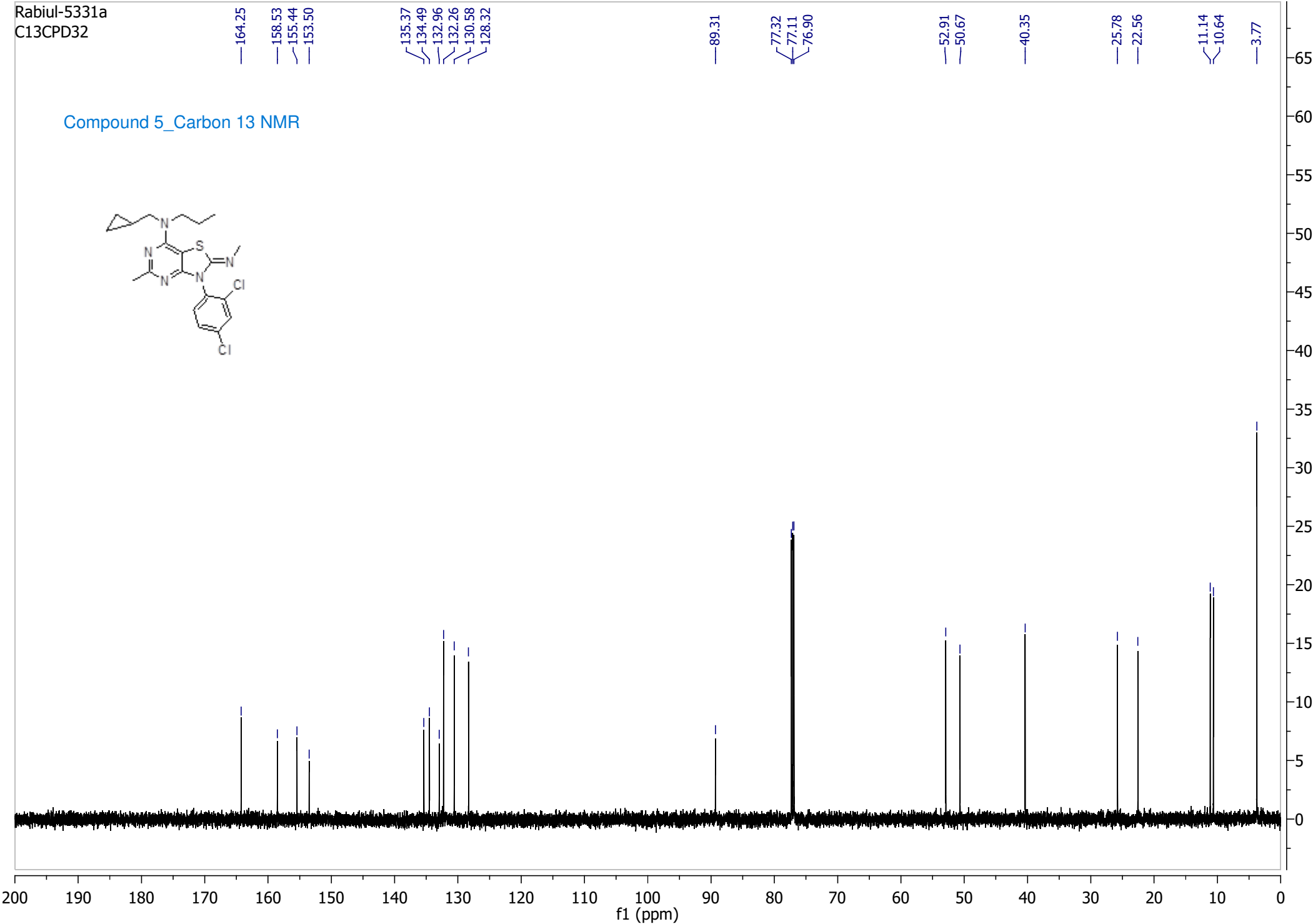
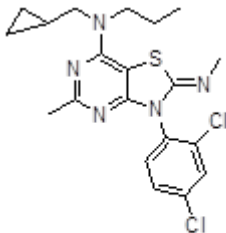
Compound 5_Proton NMR



Rabiul-5331a
C13CPD32

164.25 158.53 155.44 153.50 135.37 134.49 132.96 132.26 130.58 128.32 89.31 77.32 77.11 76.90 52.91 50.67 40.35 25.78 22.56 11.14 10.64 3.77

Compound 5_Carbon 13 NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5331a_000001.d
Method Bruker_11052015
Sample Name 5331a
Comment

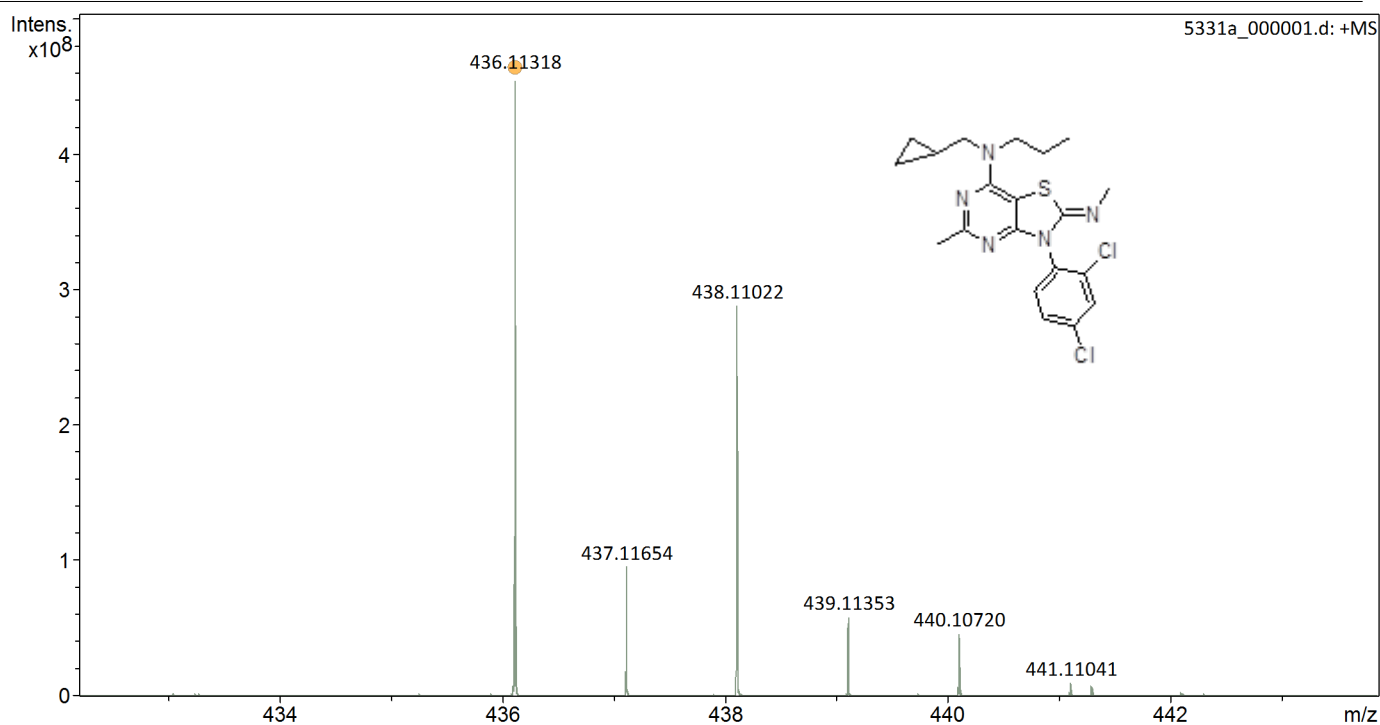
Acquisition Date 3/21/2019 7:13:29 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

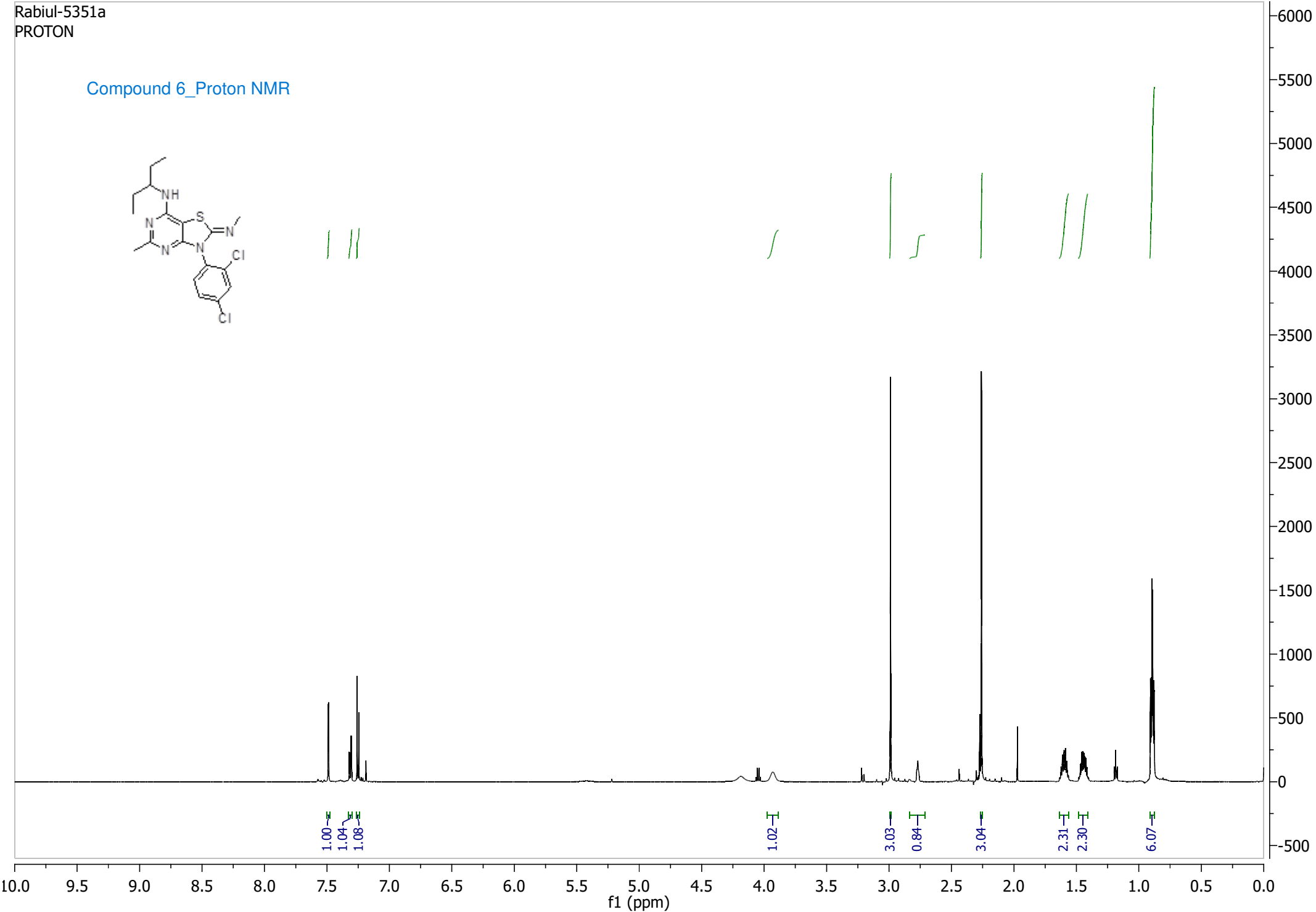
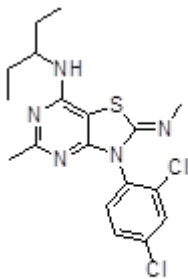
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	436.113182	1	C ₂₀ H ₂₄ Cl ₂ N ₅ S	100.00	436.112399	-1.8	-1.9	30.4	10.5	even		ok
M+Na	458.094930	1	C ₂₀ H ₂₃ Cl ₂ N ₅ NaS	100.00	458.094343	-1.3	-1.4	18.5	10.5	even		ok

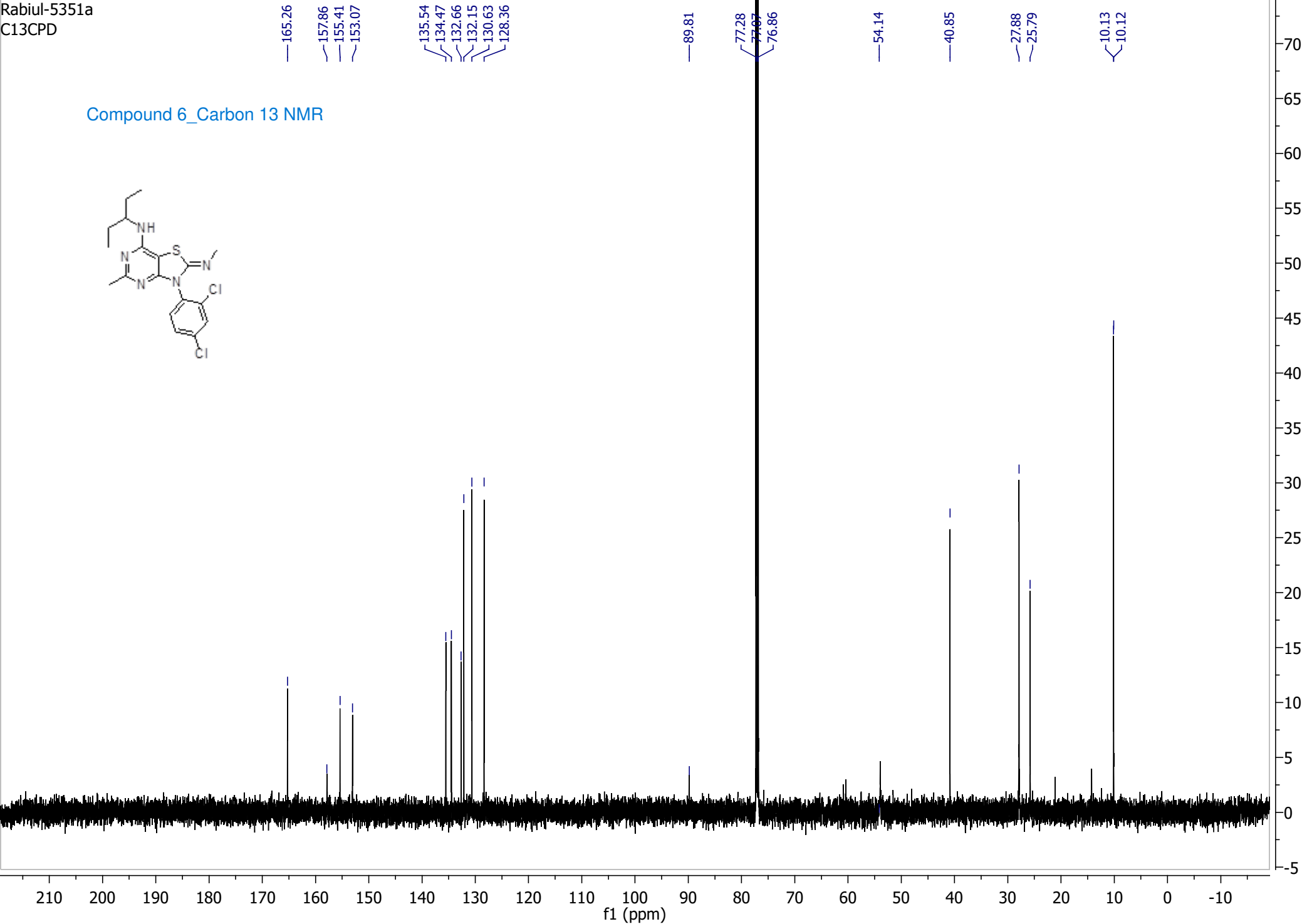
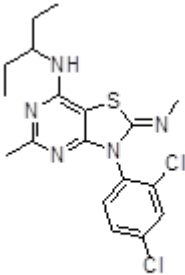
Rabiul-5351a
PROTON

Compound 6_Proton NMR



Rabiul-5351a
C13CPD

Compound 6_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC_3-21-19\5351a_000001.d
Method Bruker_11052015
Sample Name 5351a
Comment

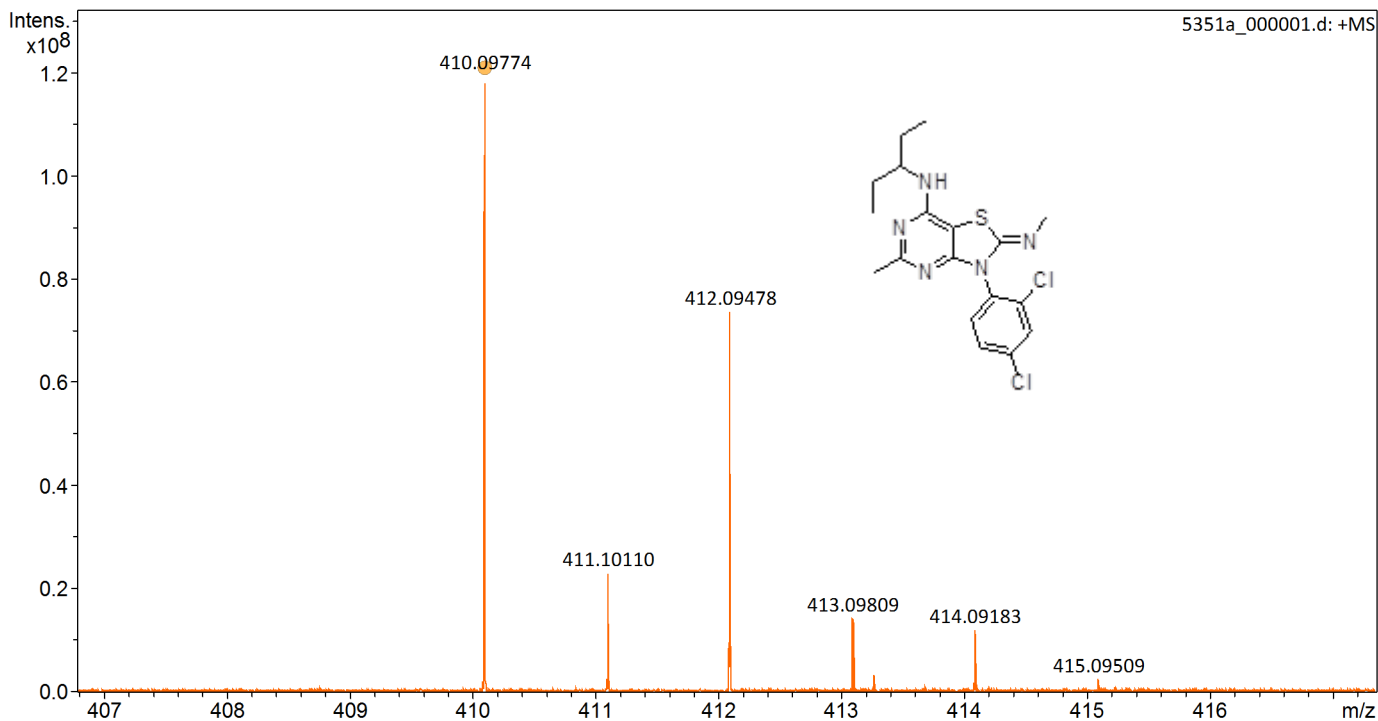
Acquisition Date 3/21/2019 7:10:30 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

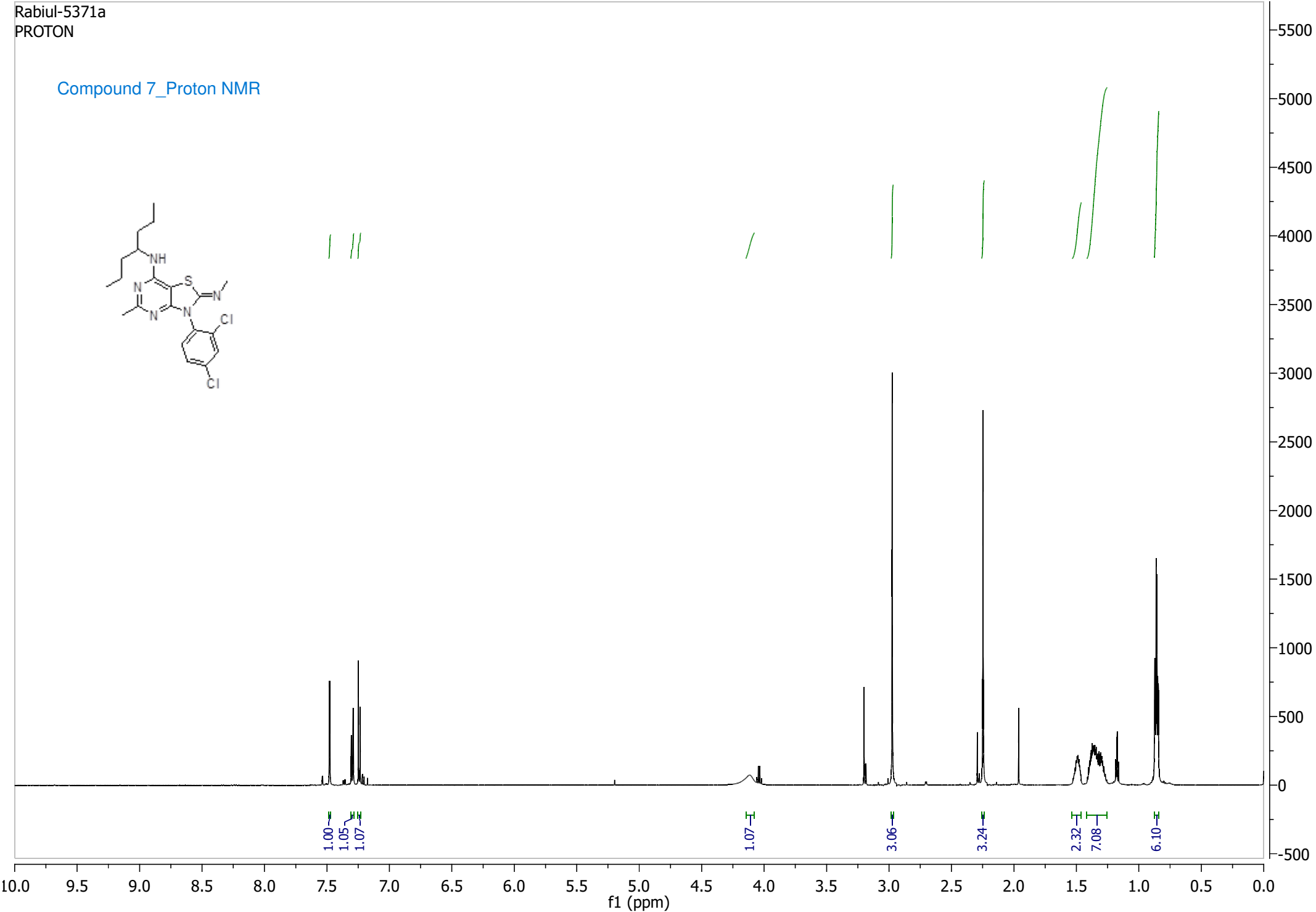
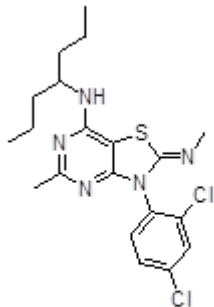
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdB	e ⁻	Conf	N-Rule
M+H	410.097742	1	C ₁₈ H ₂₂ Cl ₂ N ₅ S	100.00	410.096749	-2.4	-2.5	36.2	9.5	even		ok
M+Na	432.079523	1	C ₁₈ H ₂₁ Cl ₂ N ₅ NaS	100.00	432.078693	-1.9	-1.6	30.2	9.5	even		ok

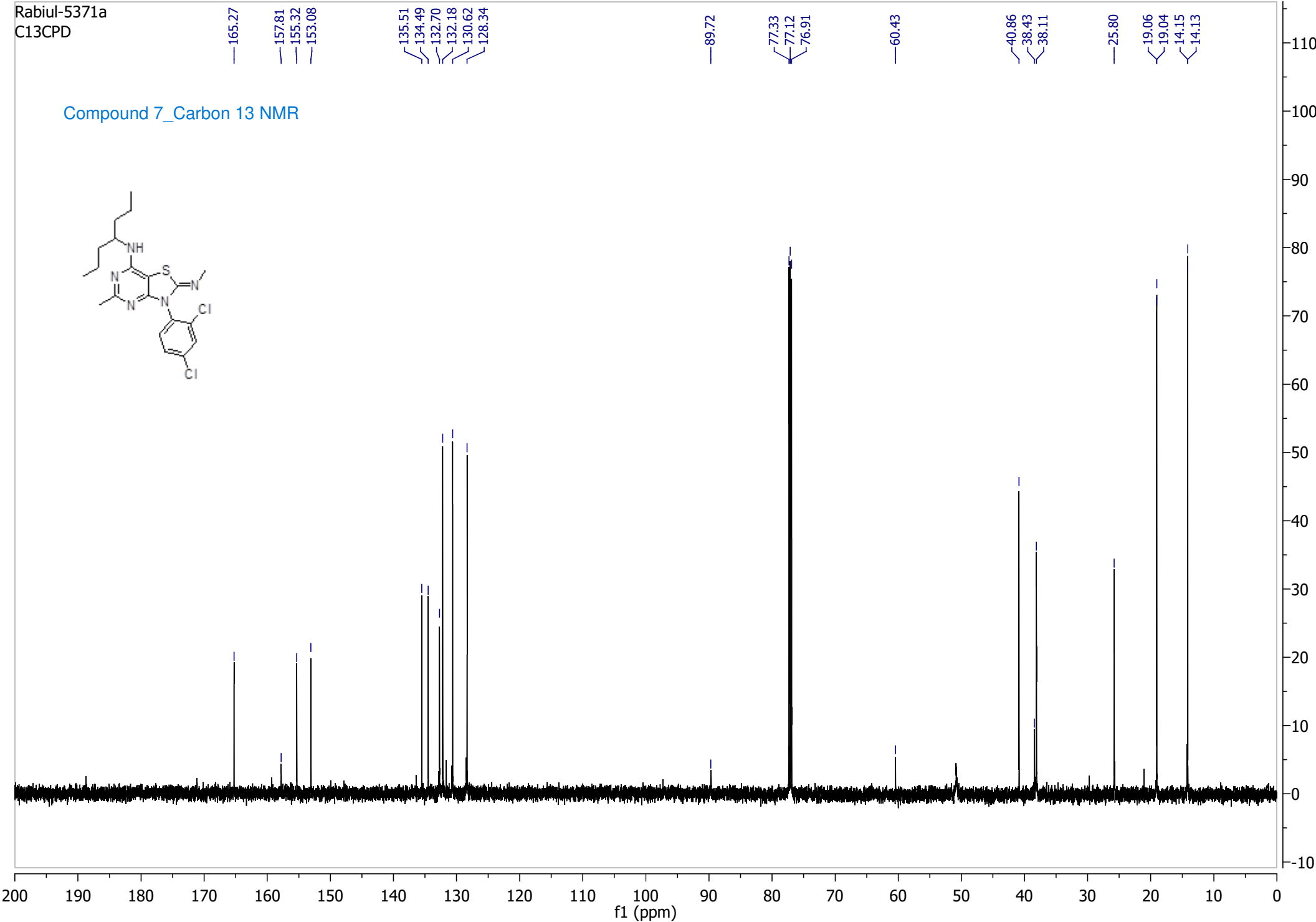
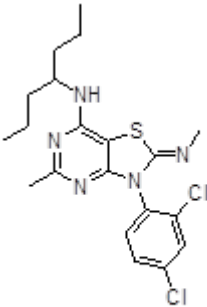
Rabiul-5371a
PROTON

Compound 7_Proton NMR



Rabiul-5371a
C13CPD

Compound 7_Carbon 13 NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5371a_000001.d
Method Bruker_11052015
Sample Name 5371a
Comment

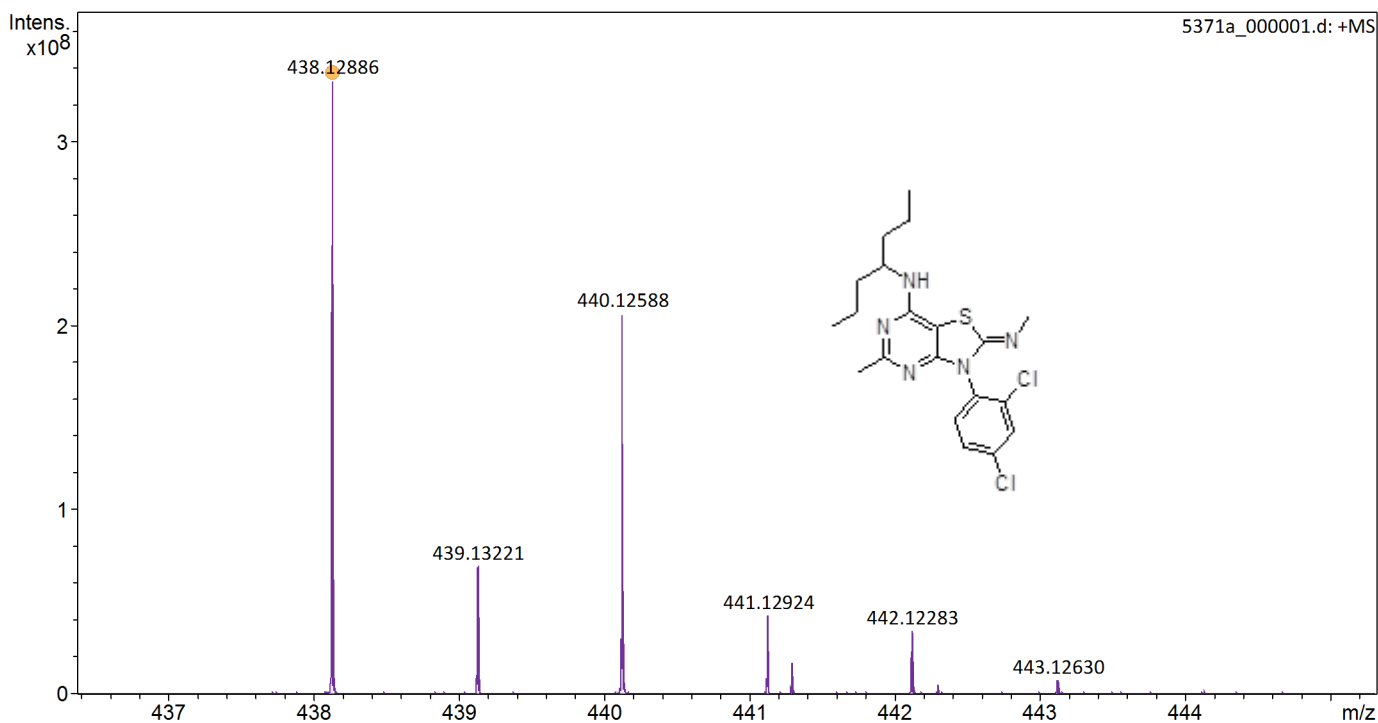
Acquisition Date 3/21/2019 6:54:32 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

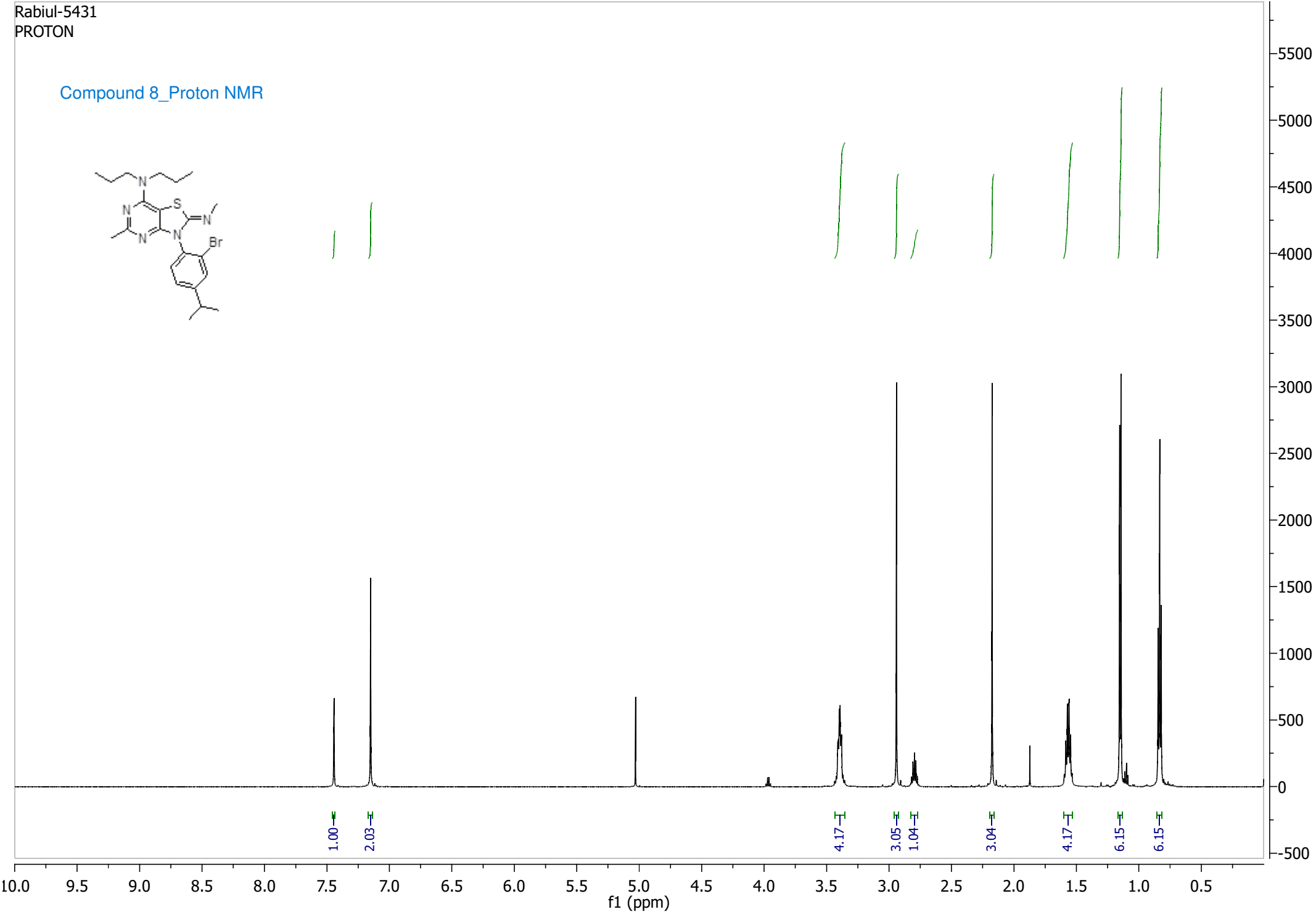
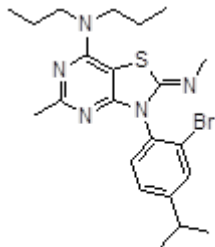
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	438.128862	1	C ₂₀ H ₂₆ Cl ₂ N ₅ S	100.00	438.128049	-1.9	-1.9	33.2	9.5	even		ok
M+Na	460.110633	1	C ₂₀ H ₂₅ Cl ₂ N ₅ NaS	100.00	460.109993	-1.4	-1.4	17.1	9.5	even		ok

Rabiul-5431
PROTON

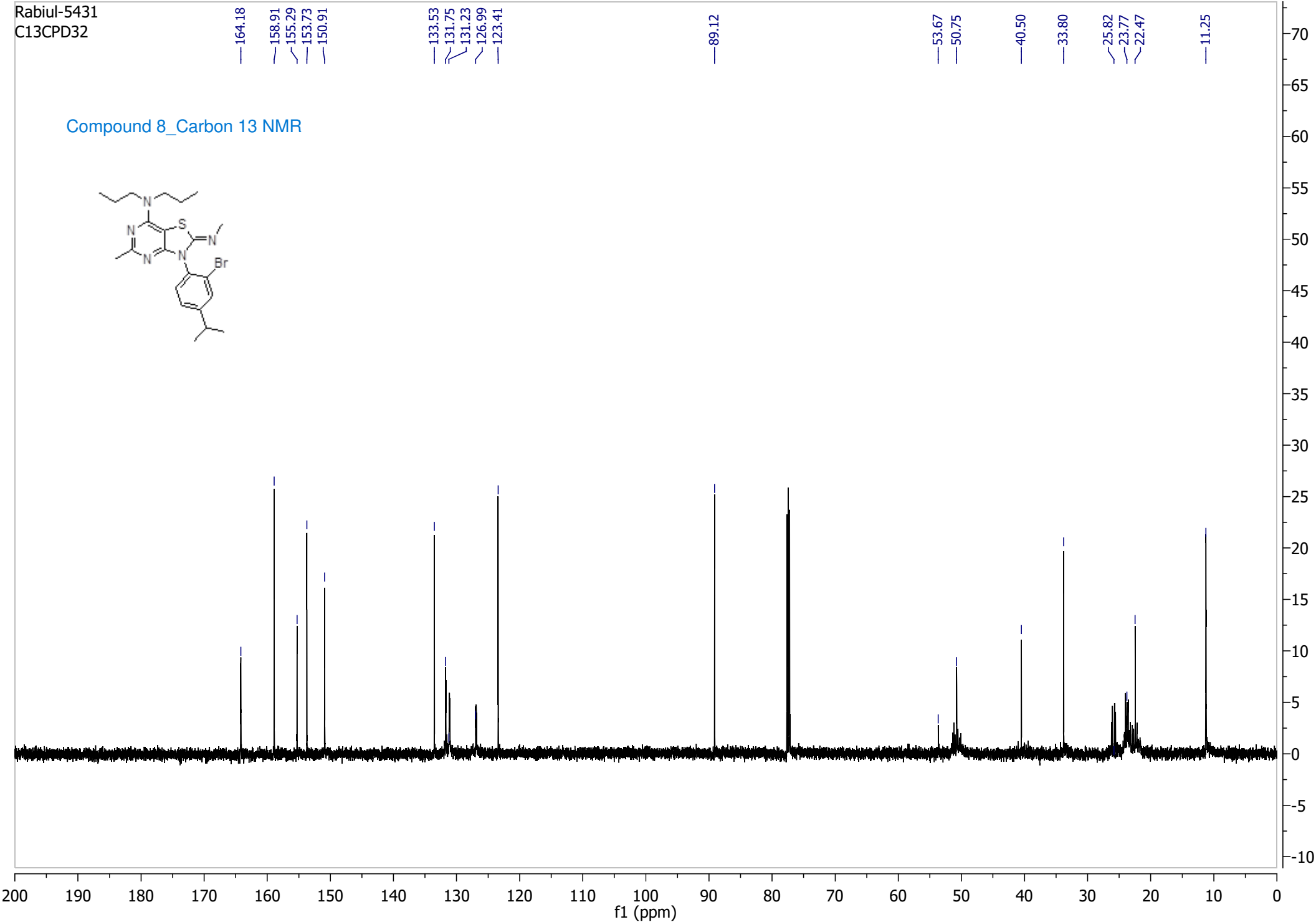
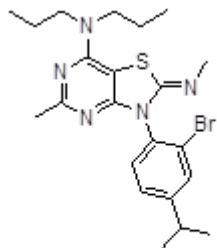
Compound 8_Proton NMR



Rabiul-5431
C13CPD32

164.18 158.91 155.29 153.73 150.91 133.53 131.75 131.23 126.99 123.41 89.12 53.67 50.75 40.50 33.80 25.82 23.77 22.47 11.25

Compound 8_Carbon 13 NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5431_000001.d
Method Bruker_11052015
Sample Name 5431
Comment

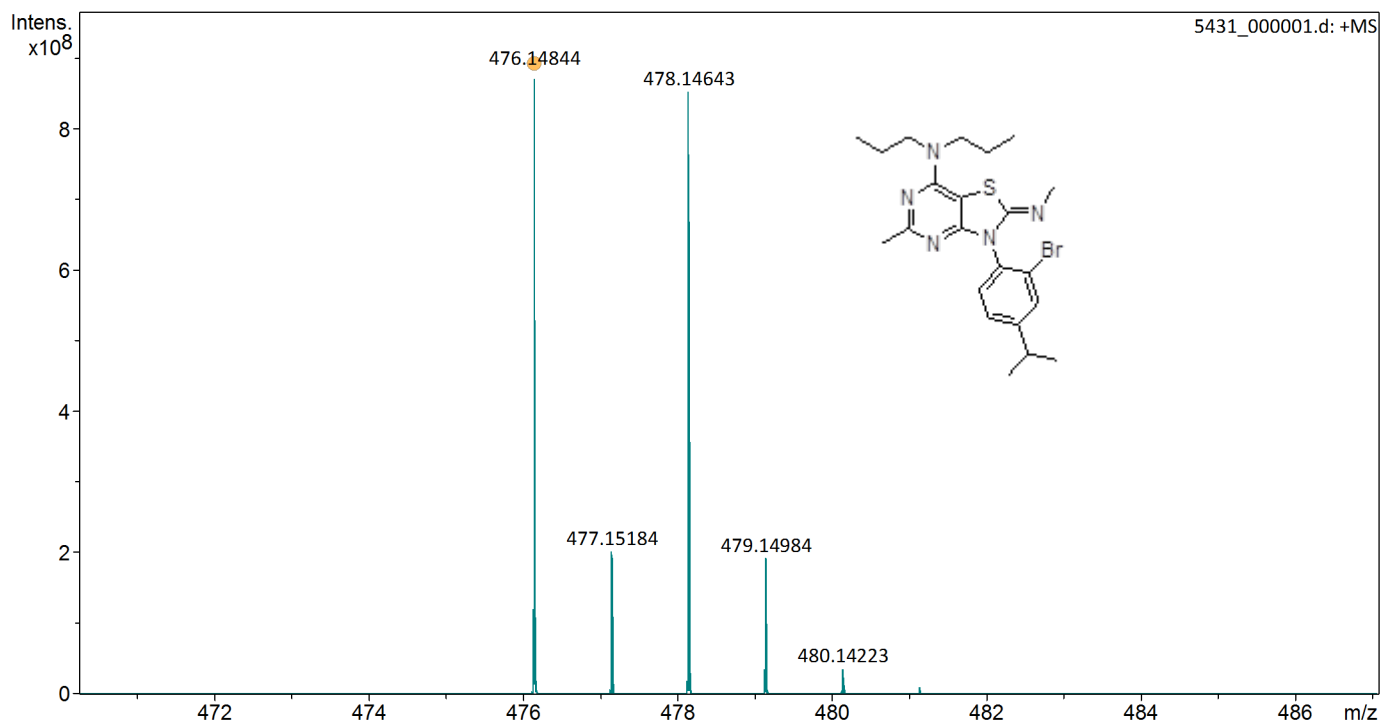
Acquisition Date 3/21/2019 5:58:22 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

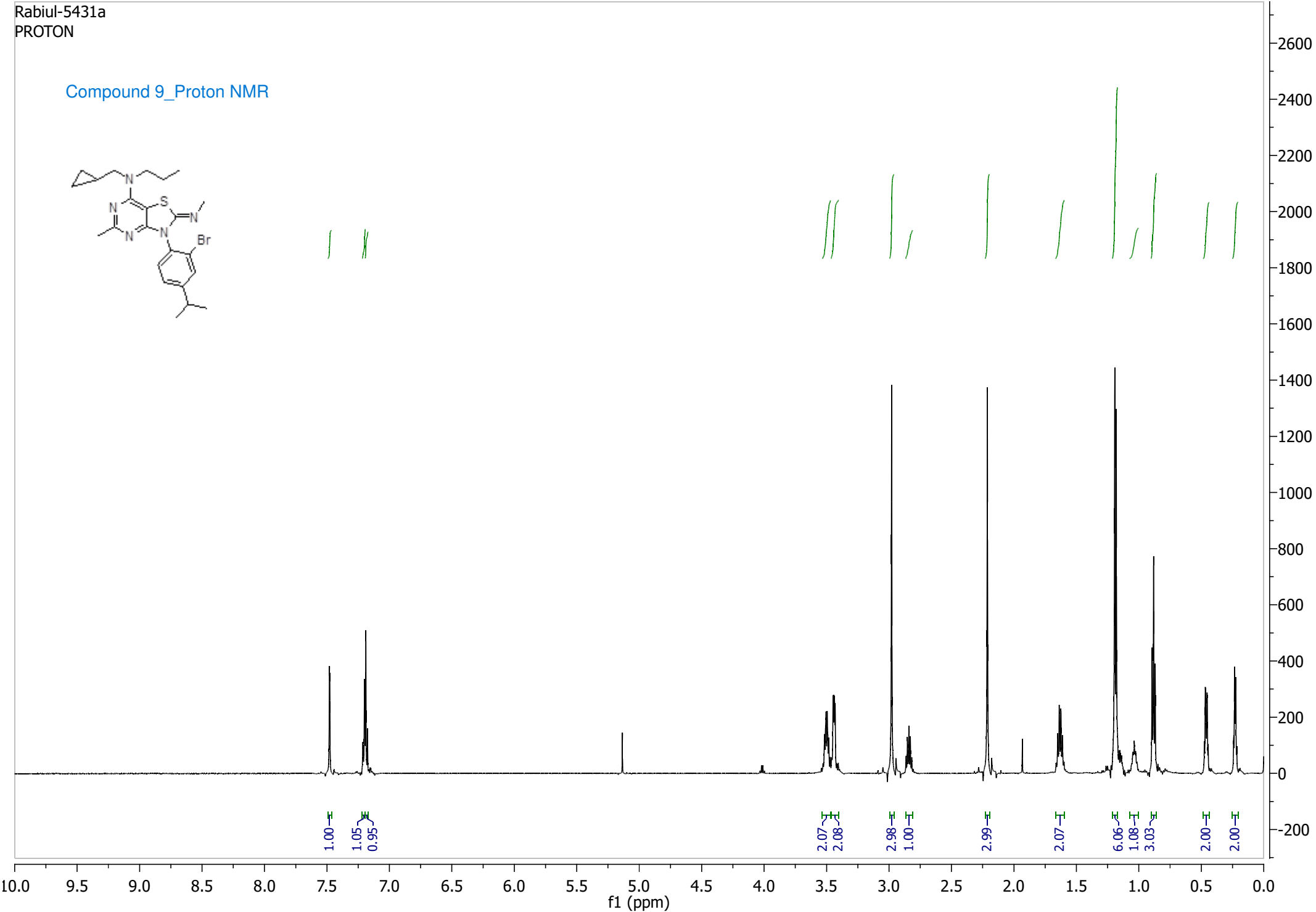
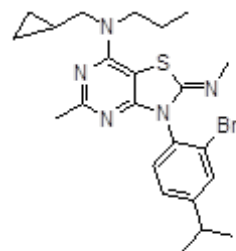
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



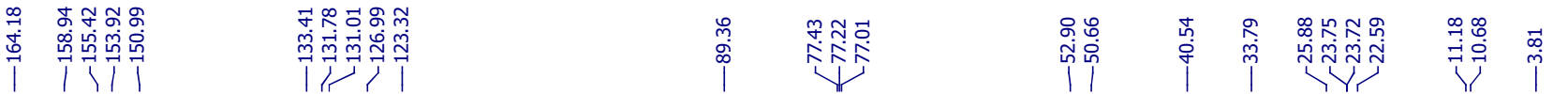
Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	476.148442	1	C22H31BrN5S	100.00	476.147806	-1.3	-1.4	21.3	9.5	even		ok
M+Na	498.130223	1	C22H30BrN5NaS	100.00	498.129750	-0.9	-0.9	17.4	9.5	even		ok

Rabiul-5431a
PROTON

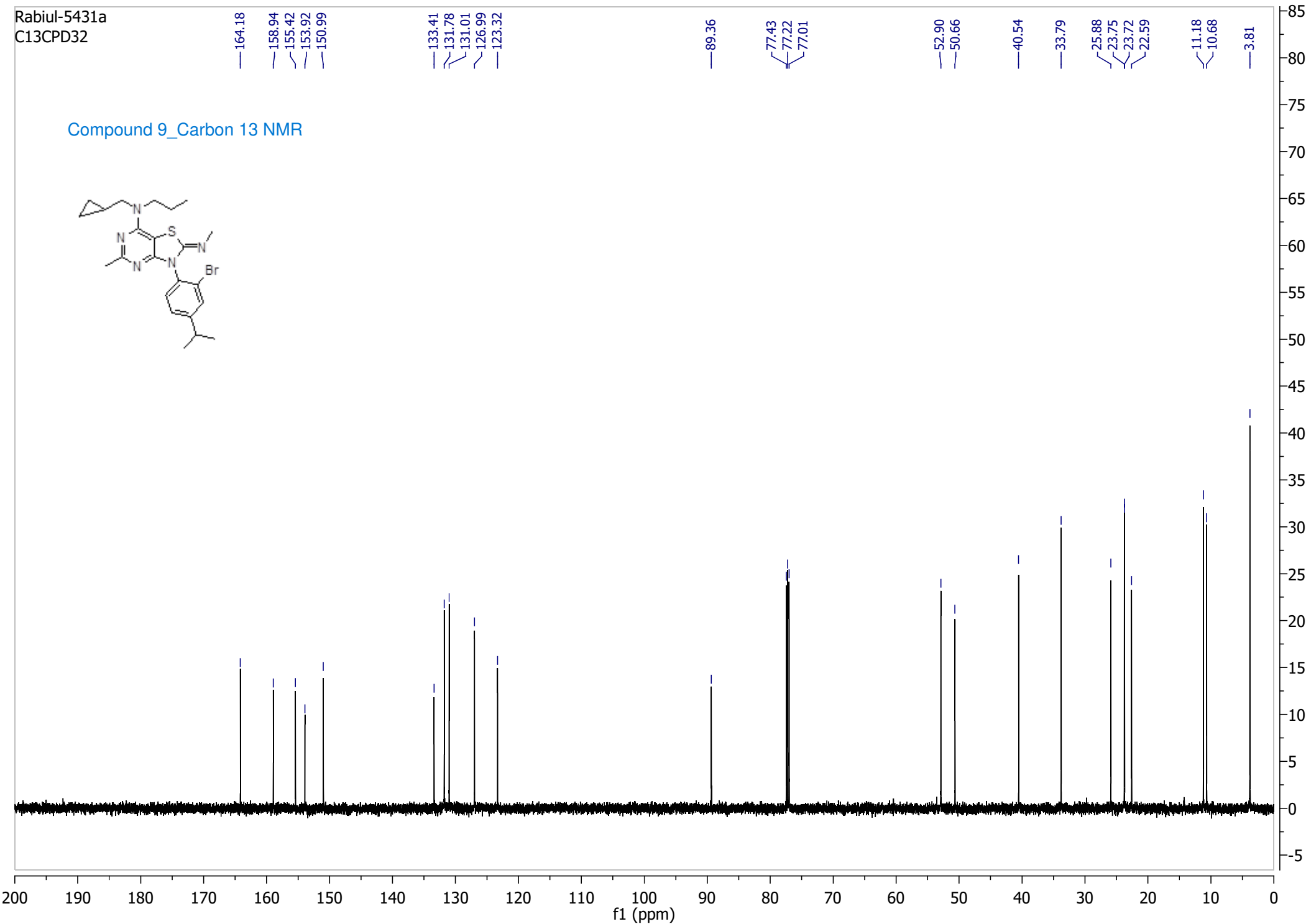
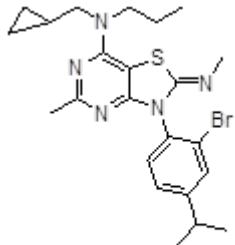
Compound 9_Proton NMR



Rabiul-5431a
C13CPD32



Compound 9_Carbon 13 NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5431a_000001.d
Method Bruker_11052015
Sample Name 5431a
Comment

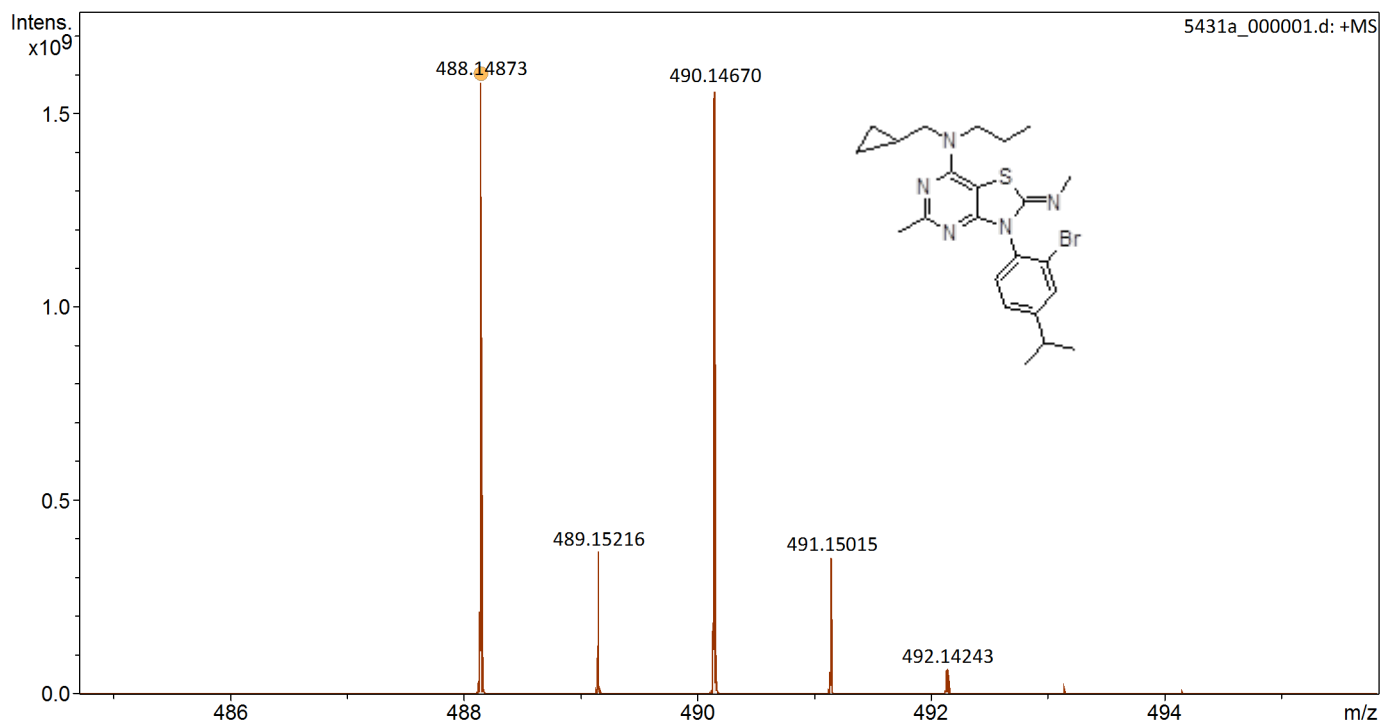
Acquisition Date 3/21/2019 6:49:00 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

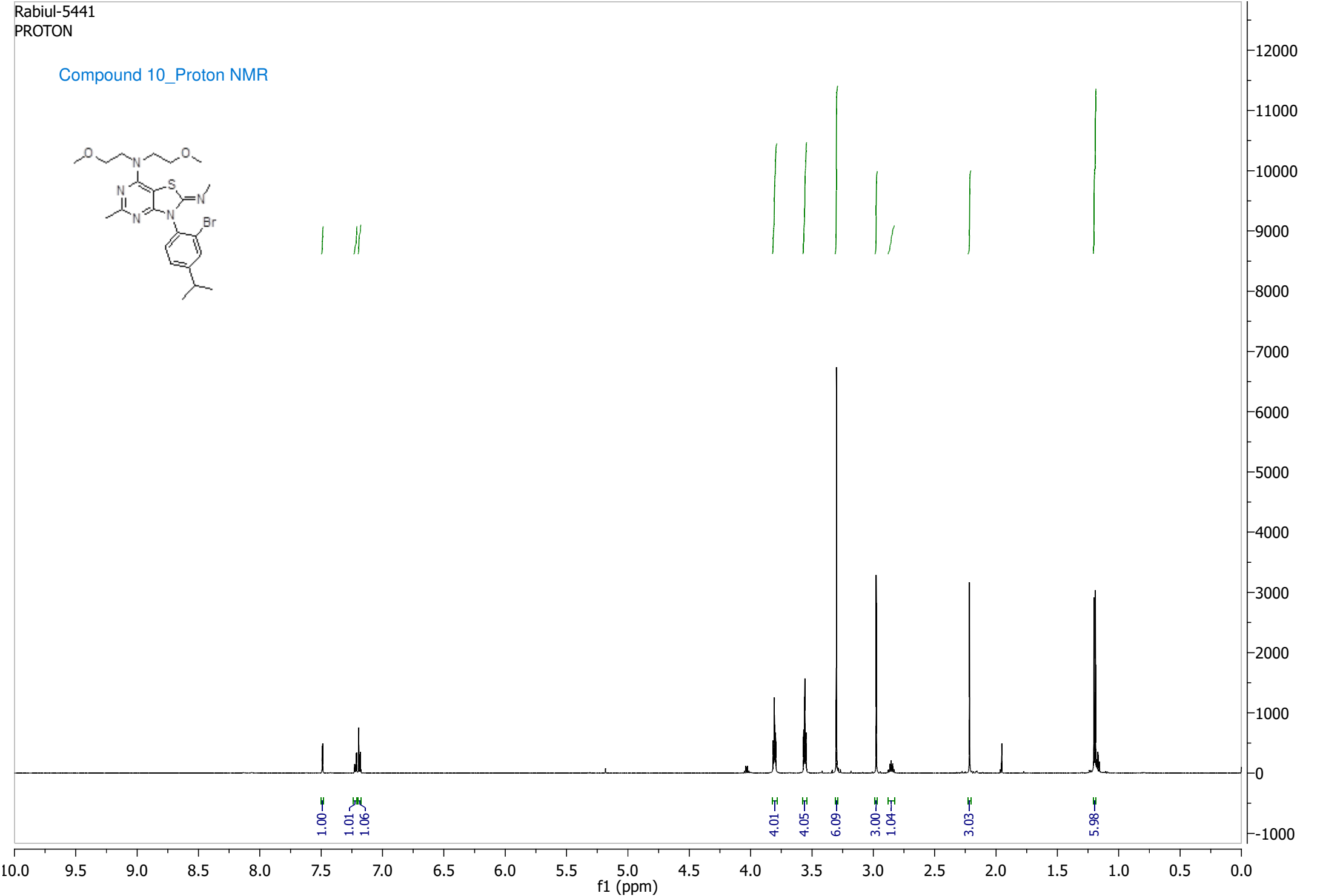
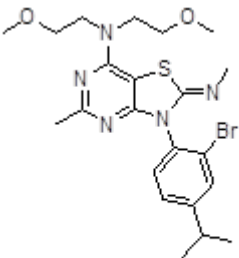
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	488.148727	1	C ₂₃ H ₃₁ BrN ₅ S	100.00	488.147806	-1.9	-1.9	18.7	10.5	even		ok
M+Na	510.130636	1	C ₂₃ H ₃₀ BrN ₅ NaS	100.00	510.129750	-1.7	-1.7	23.1	10.5	even		ok

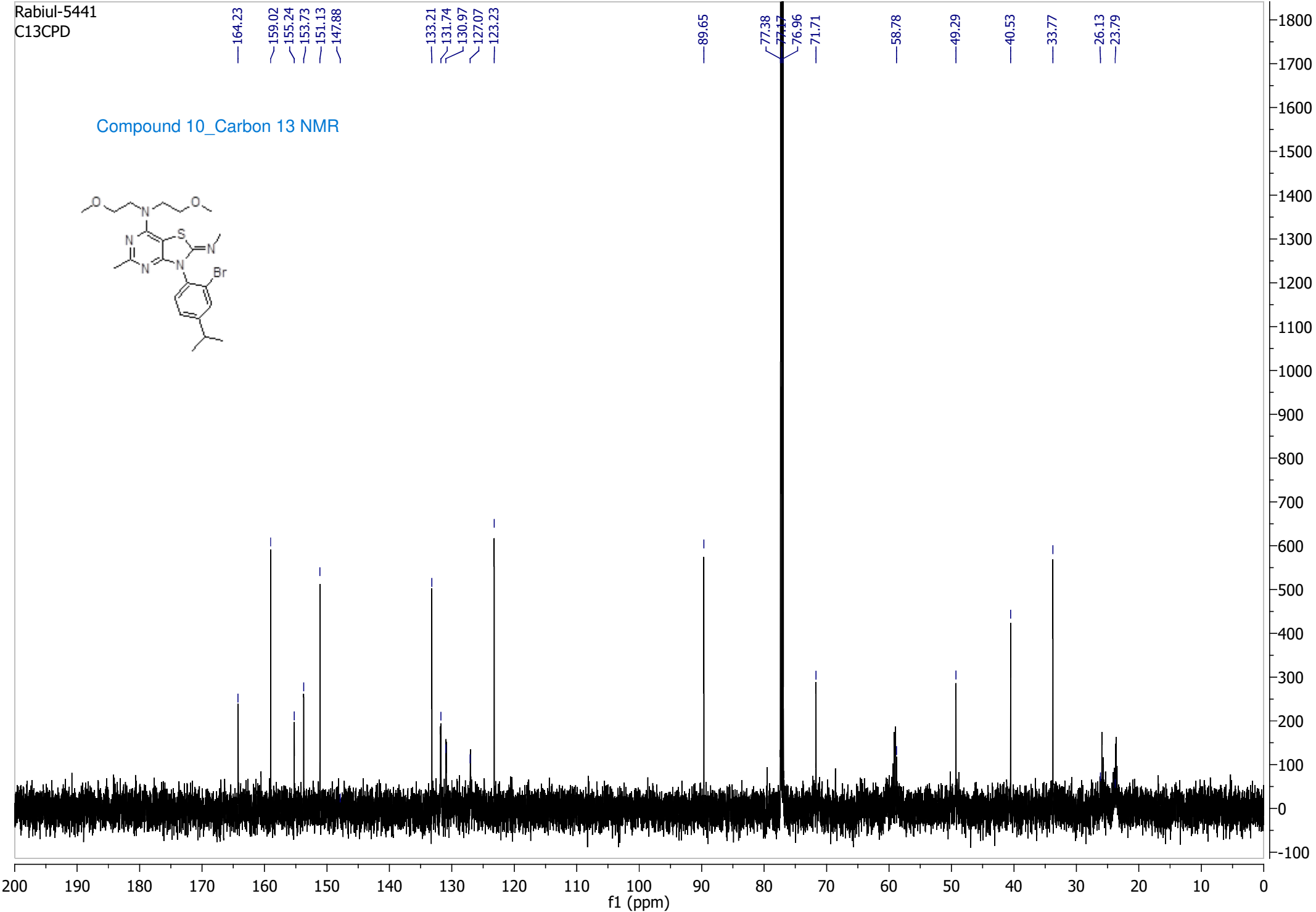
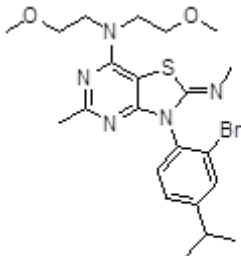
Rabiul-5441
PROTON

Compound 10_Proton NMR



Rabiul-5441
C13CPD

Compound 10_Carbon 13 NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5441_000001.d
Method Bruker_11052015
Sample Name 5441
Comment

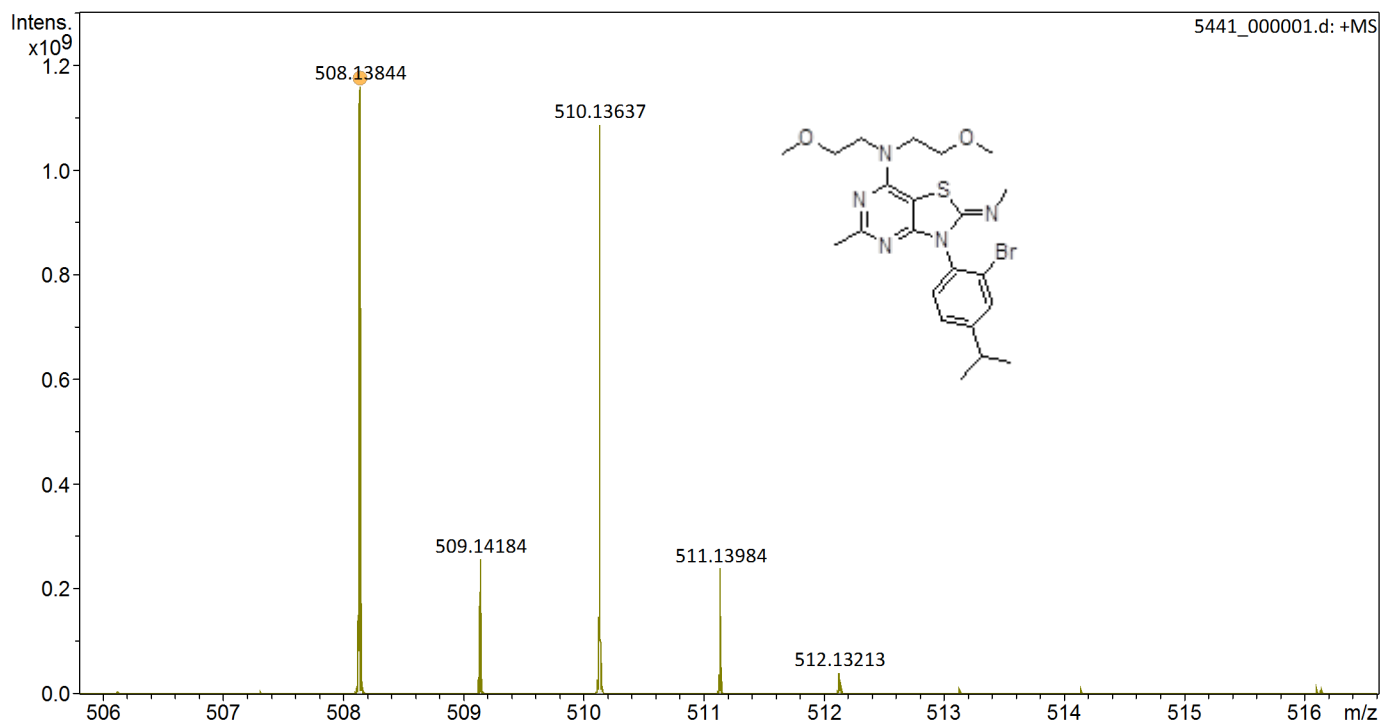
Acquisition Date 3/21/2019 6:51:37 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

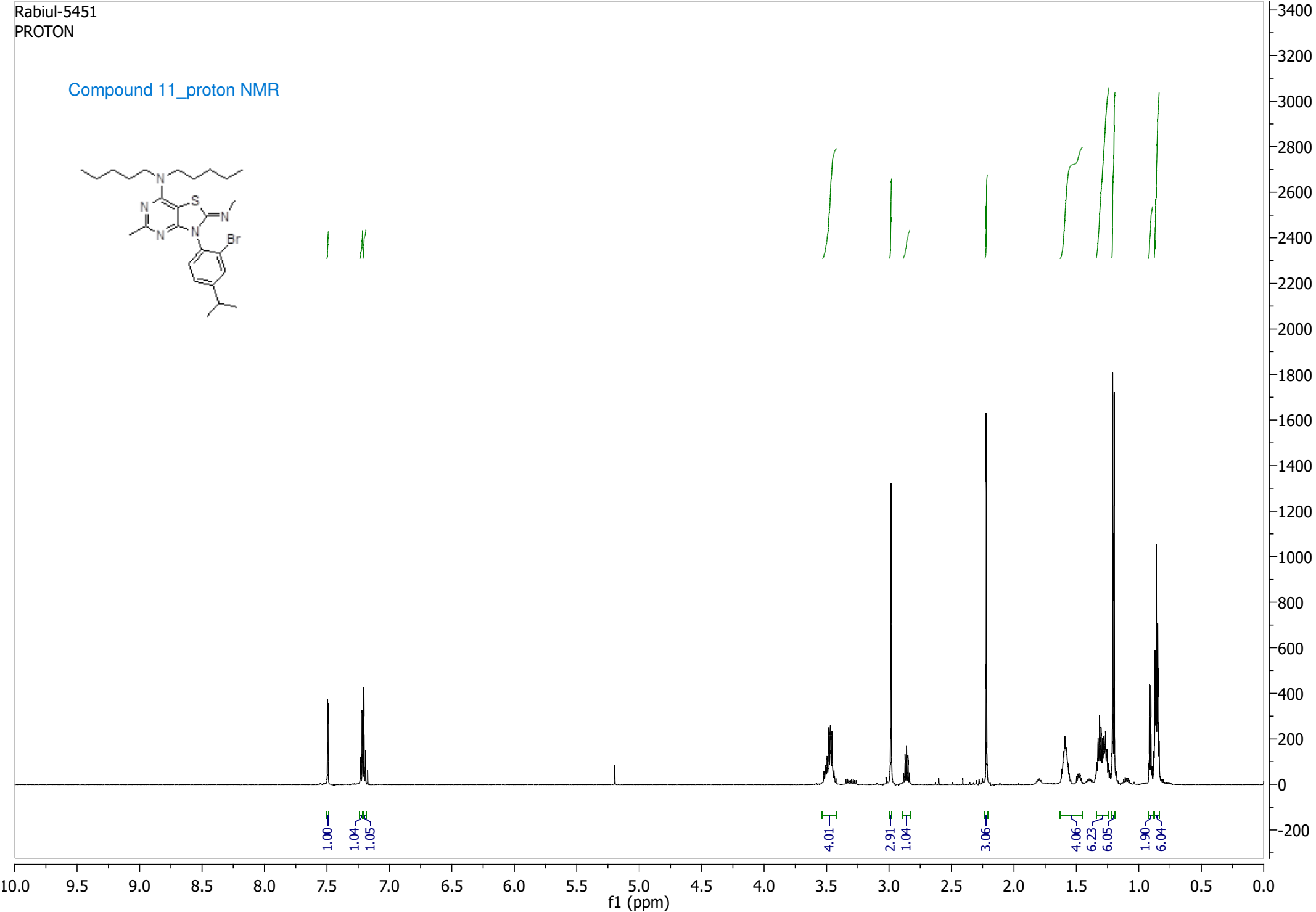
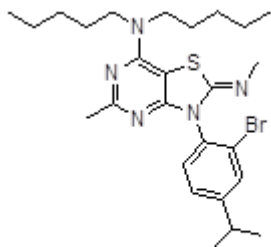
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	508.138436	1	C ₂₂ H ₃₁ BrN ₅ O ₂ S	100.00	508.137635	-1.6	-1.8	32.7	9.5	even		ok
M+Na	530.120311	1	C ₂₂ H ₃₀ BrN ₅ NaO ₂ S	100.00	530.119579	-1.4	-1.8	41.8	9.5	even		ok

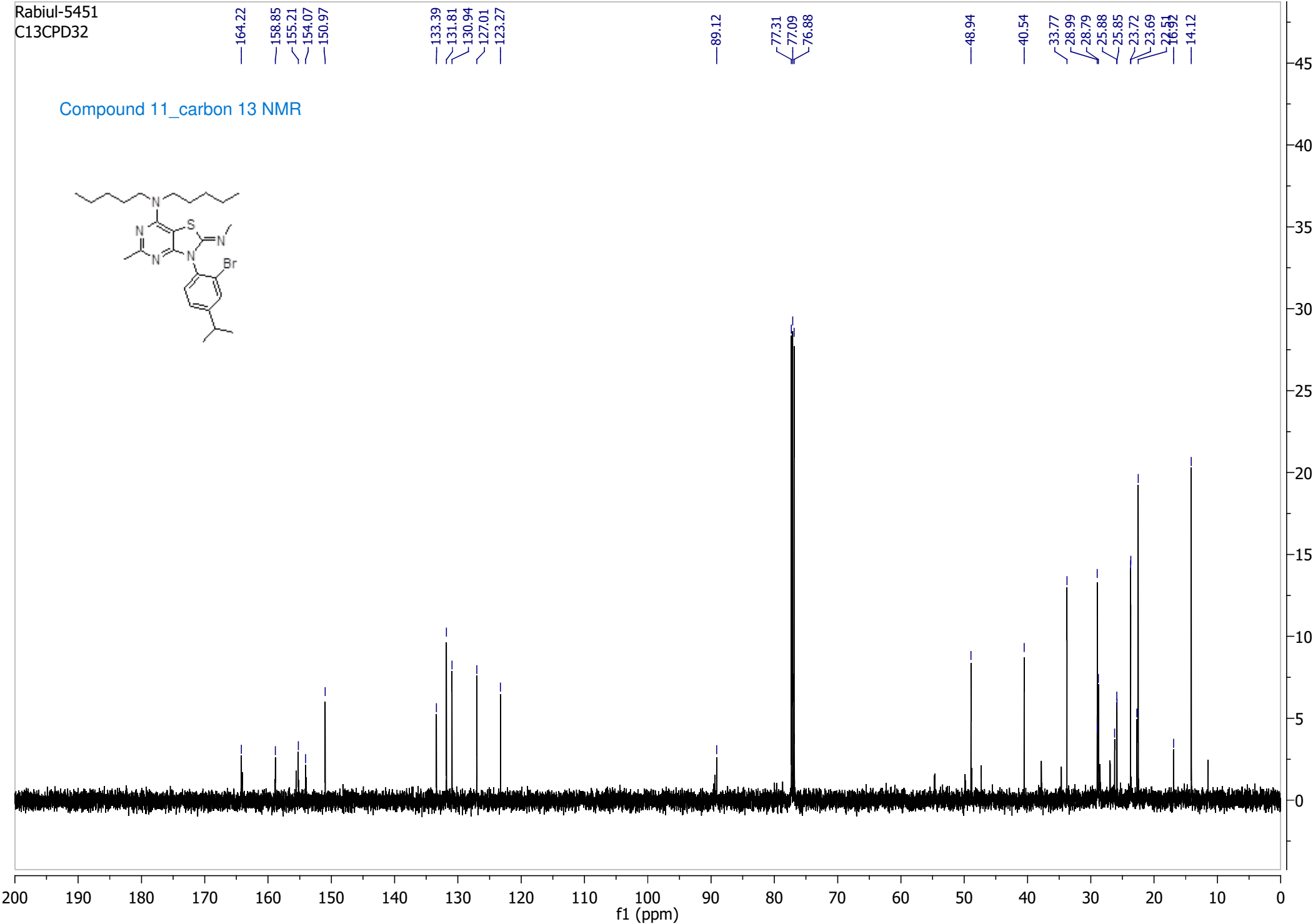
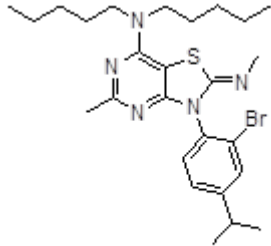
Rabiul-5451
PROTON

Compound 11_proton NMR



Rabiul-5451
C13CPD32

Compound 11_carbon 13 NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5451_000001.d
Method Bruker_11052015
Sample Name 5451
Comment

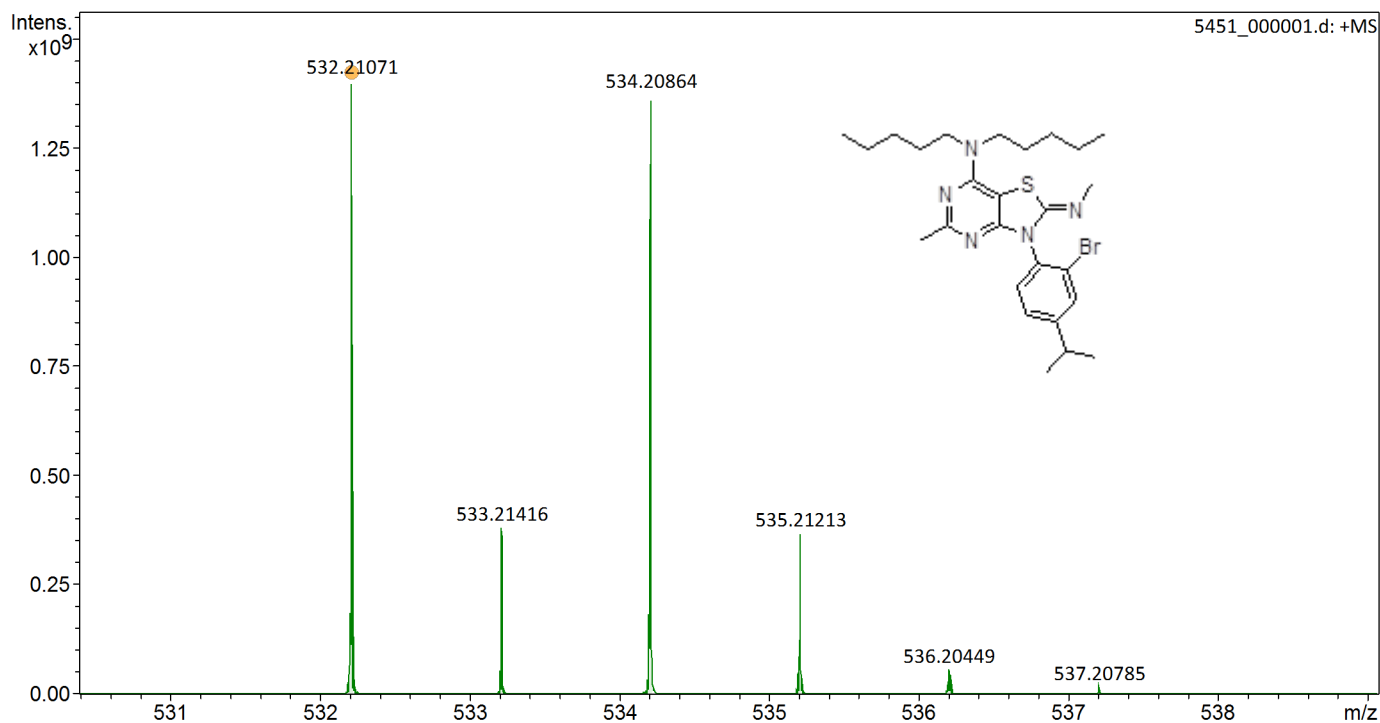
Acquisition Date 3/21/2019 6:41:40 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

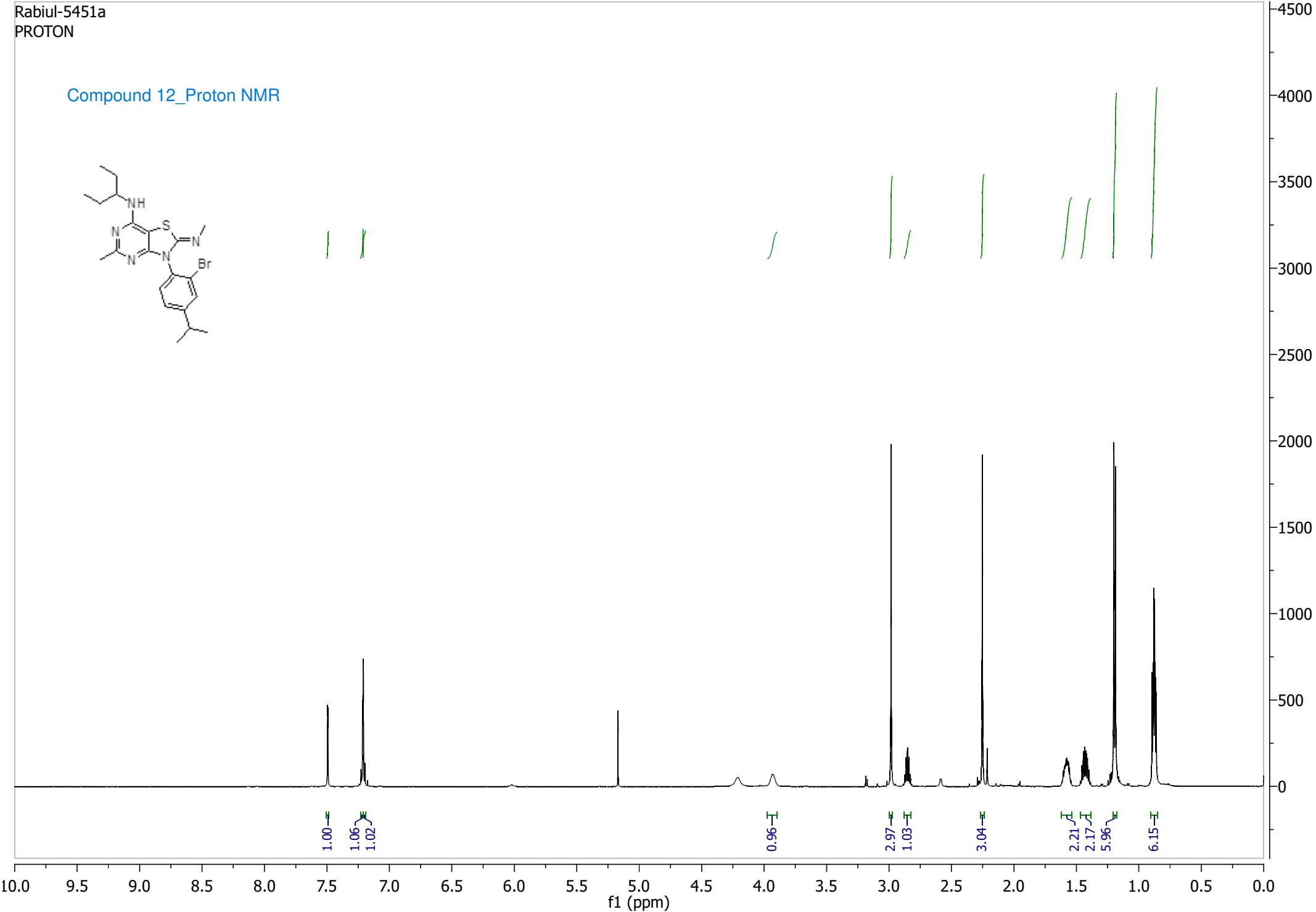
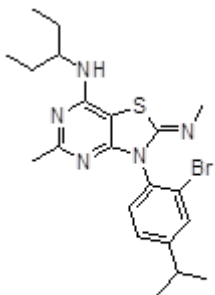
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	532.210706	1	C ₂₆ H ₃₉ BrN ₅ S	100.00	532.210406	-0.6	-0.8	29.7	9.5	even		ok
M+Na	554.192640	1	C ₂₆ H ₃₈ BrN ₅ NaS	100.00	554.192350	-0.5	-0.7	33.6	9.5	even		ok

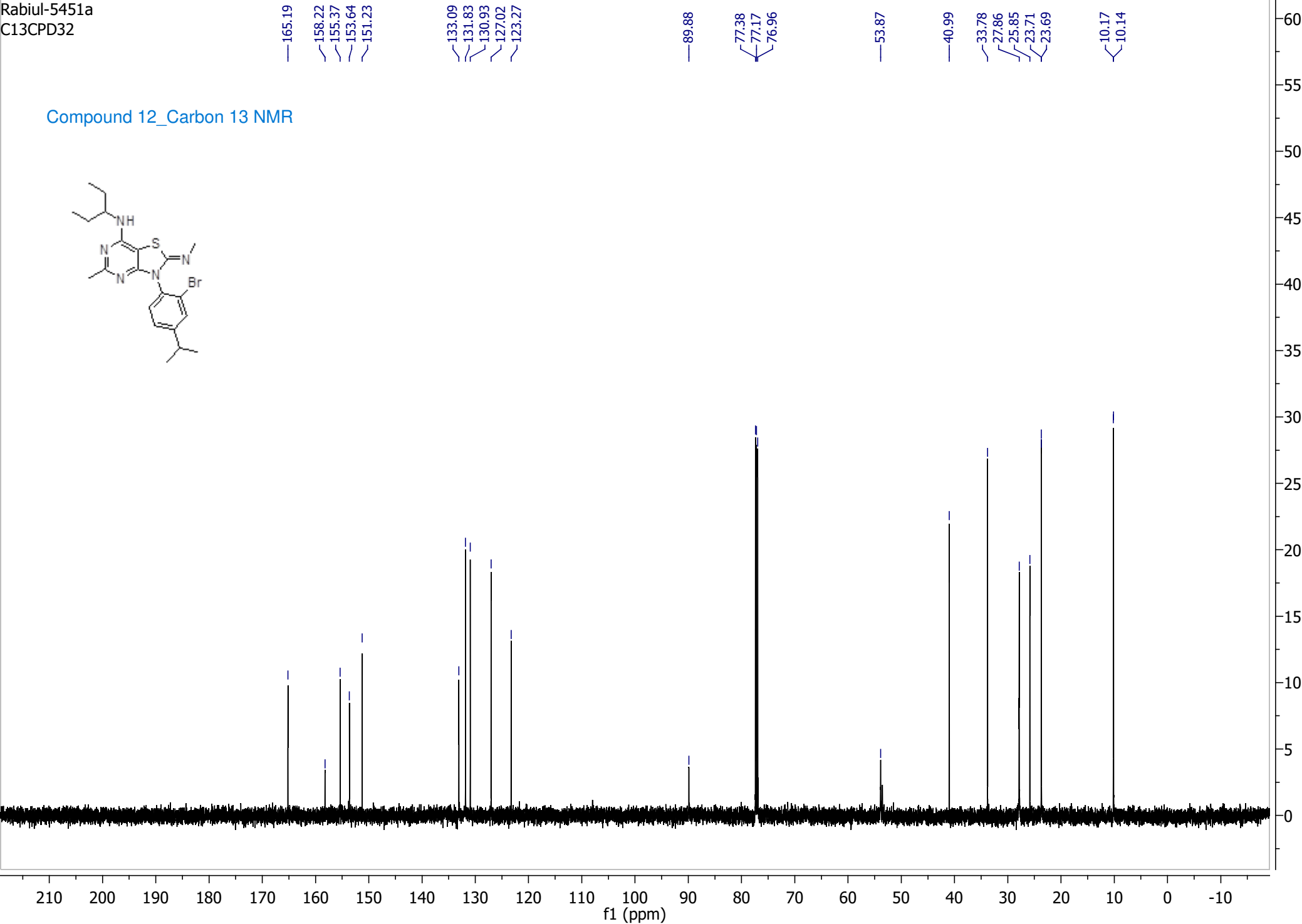
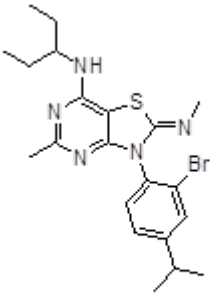
Rabiul-5451a
PROTON

Compound 12_Proton NMR



Rabiul-5451a
C13CPD32

Compound 12_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC_3-21-19\5451a_000001.d
Method Bruker_11052015
Sample Name 5451a
Comment

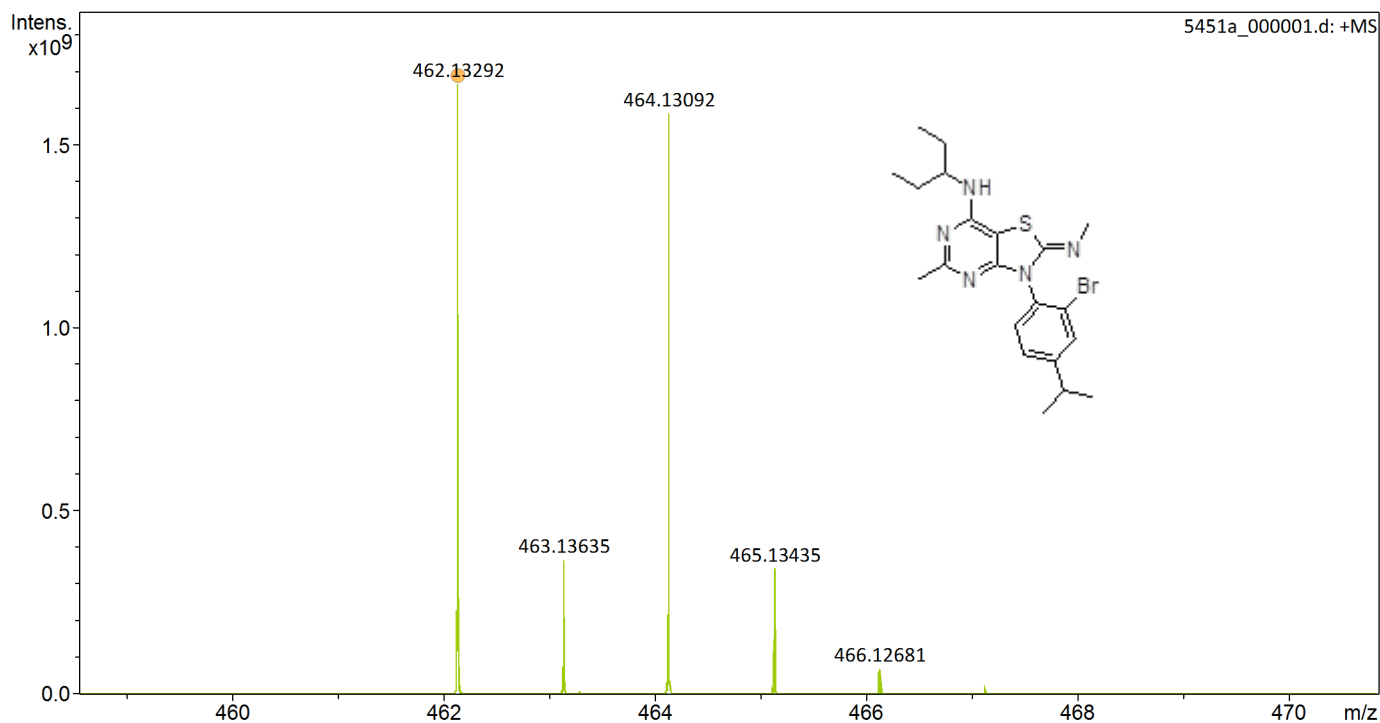
Acquisition Date 3/21/2019 6:27:21 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

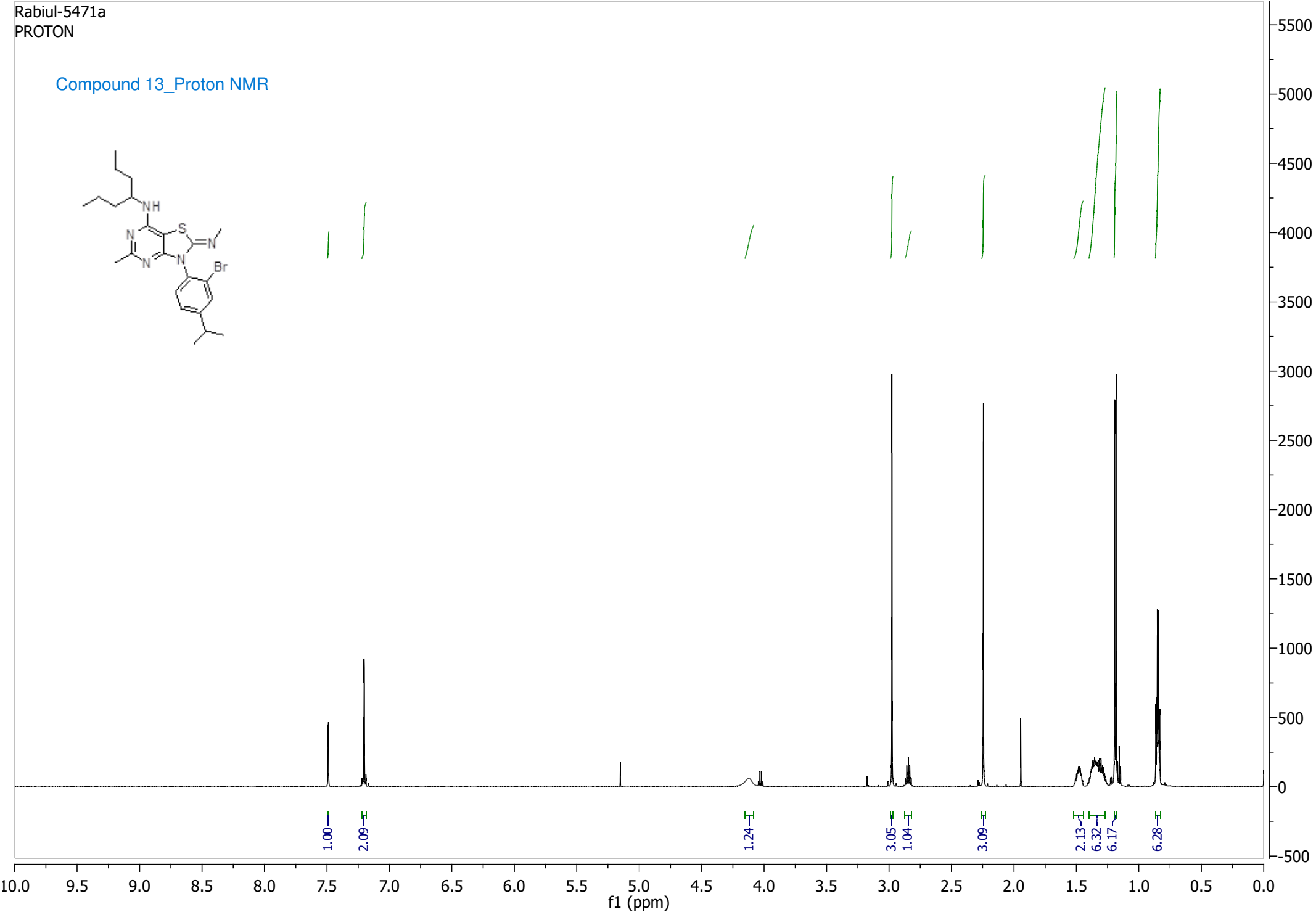
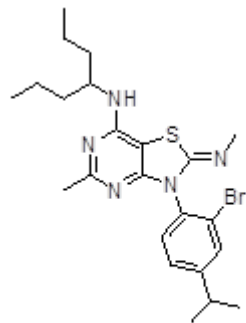
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	462.132924	1	C21H29BrN5S	100.00	462.132155	-1.7	-1.7	26.1	9.5	even		ok
M+Na	484.114796	1	C21H28BrN5NaS	100.00	484.114100	-1.4	-1.4	17.3	9.5	even		ok

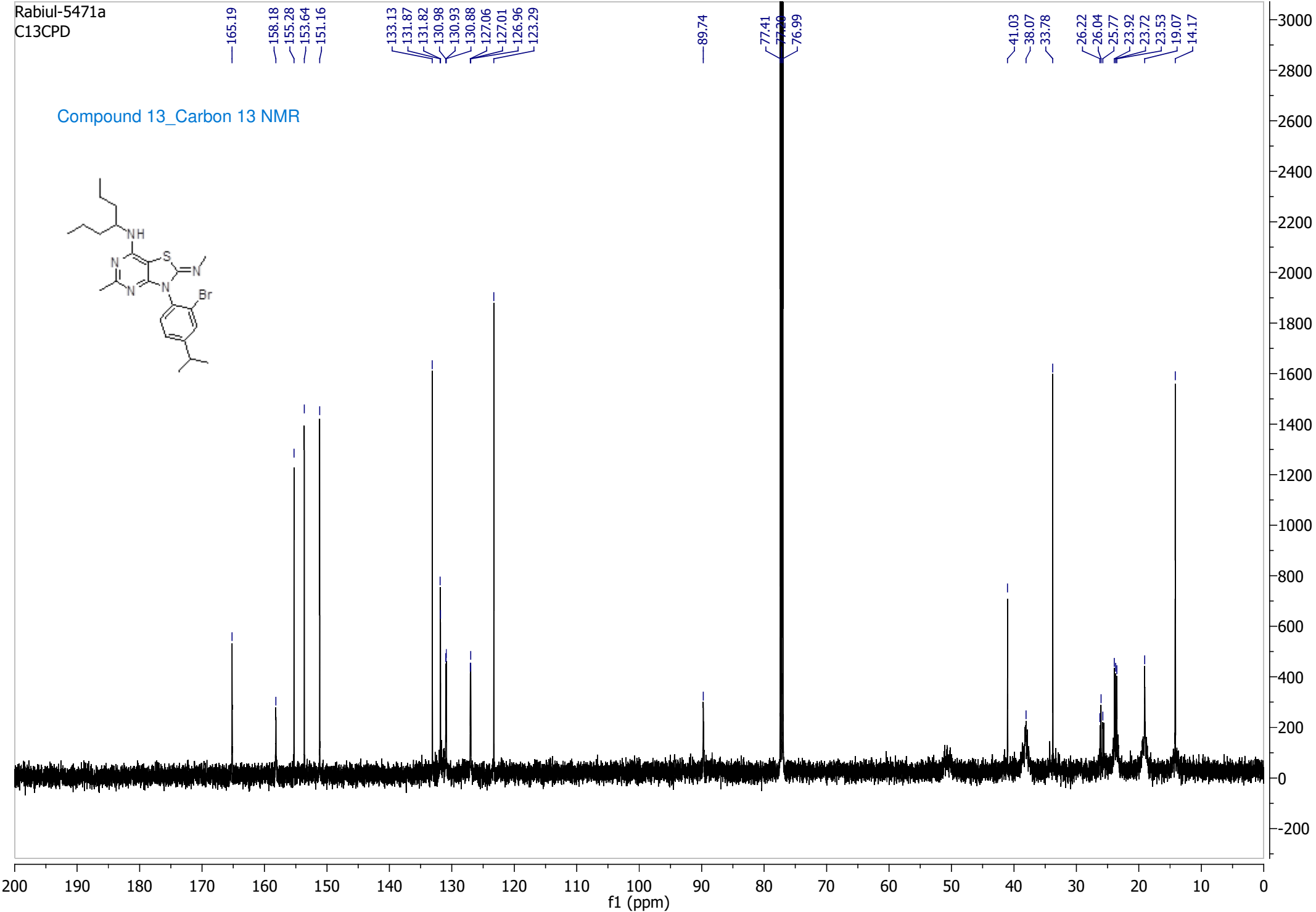
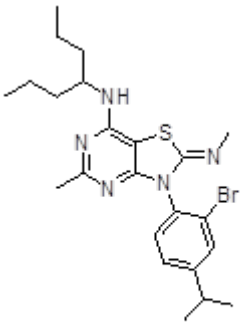
Rabiul-5471a
PROTON

Compound 13_Proton NMR



Rabiul-5471a
C13CPD

Compound 13_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC_3-21-19\5471a_000001.d
Method Bruker_11052015
Sample Name 5471a
Comment

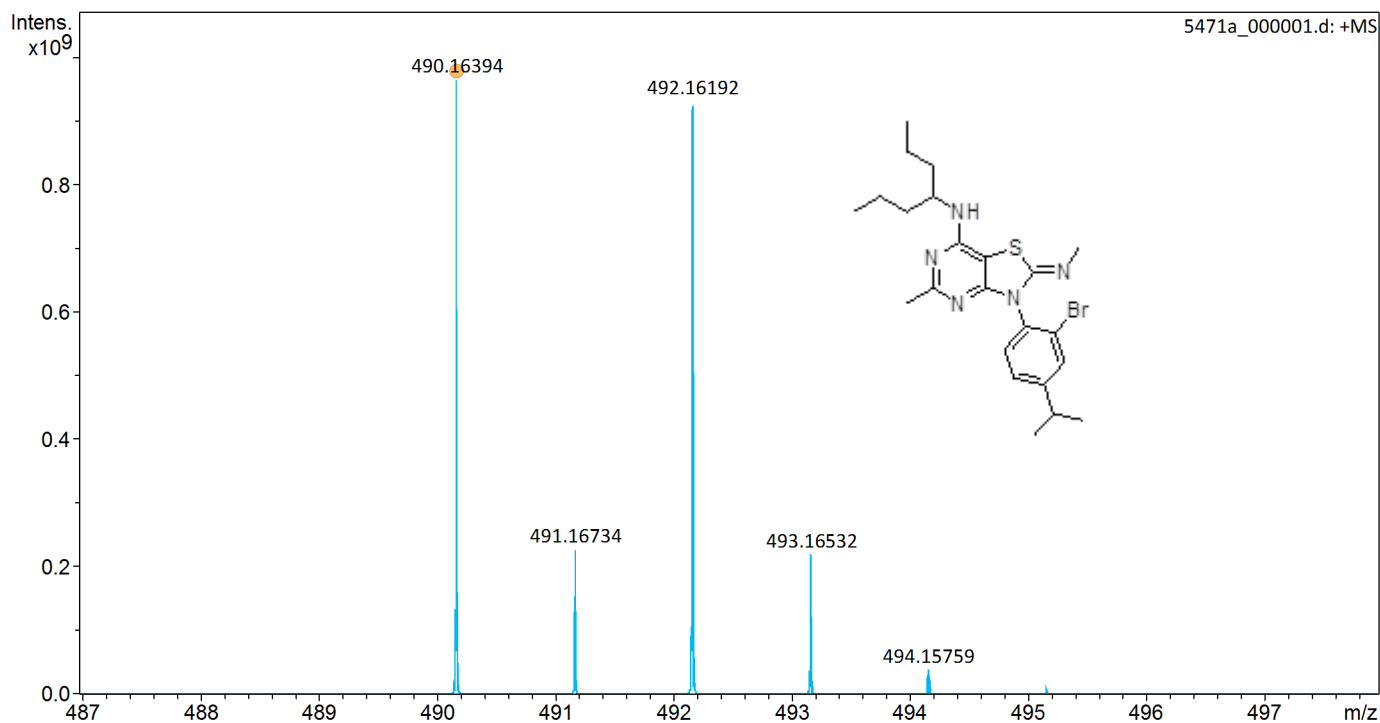
Acquisition Date 3/21/2019 6:44:55 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

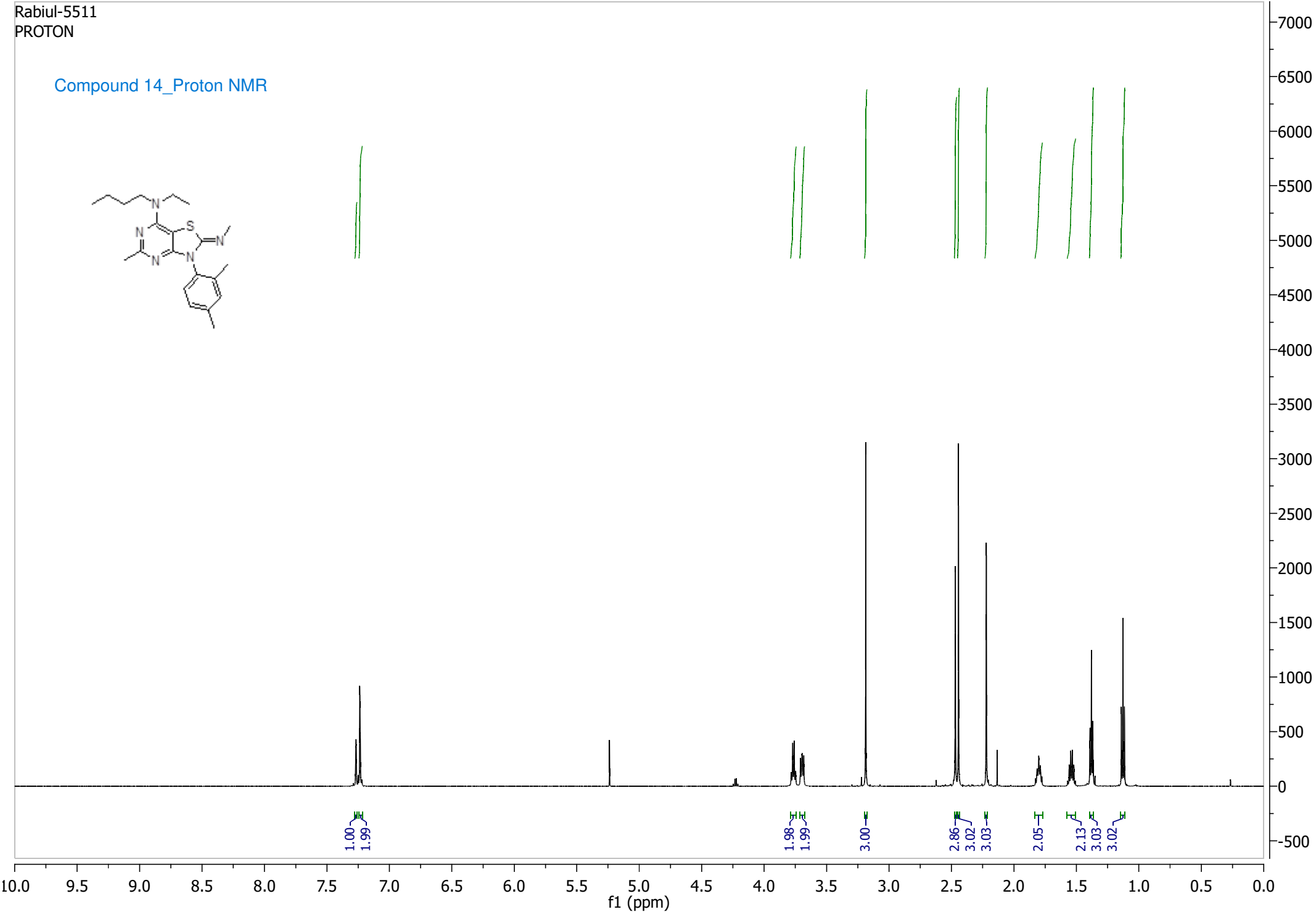
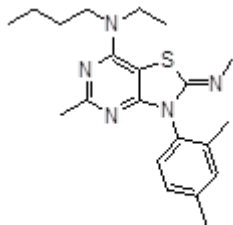
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	490.163944	1	C ₂₃ H ₃₃ BrN ₅ S	100.00	490.163456	-1.0	-1.0	22.6	9.5	even		ok
M+Na	512.145744	1	C ₂₃ H ₃₂ BrN ₅ NaS	100.00	512.145400	-0.7	-1.1	32.7	9.5	even		ok

Rabiul-5511
PROTON

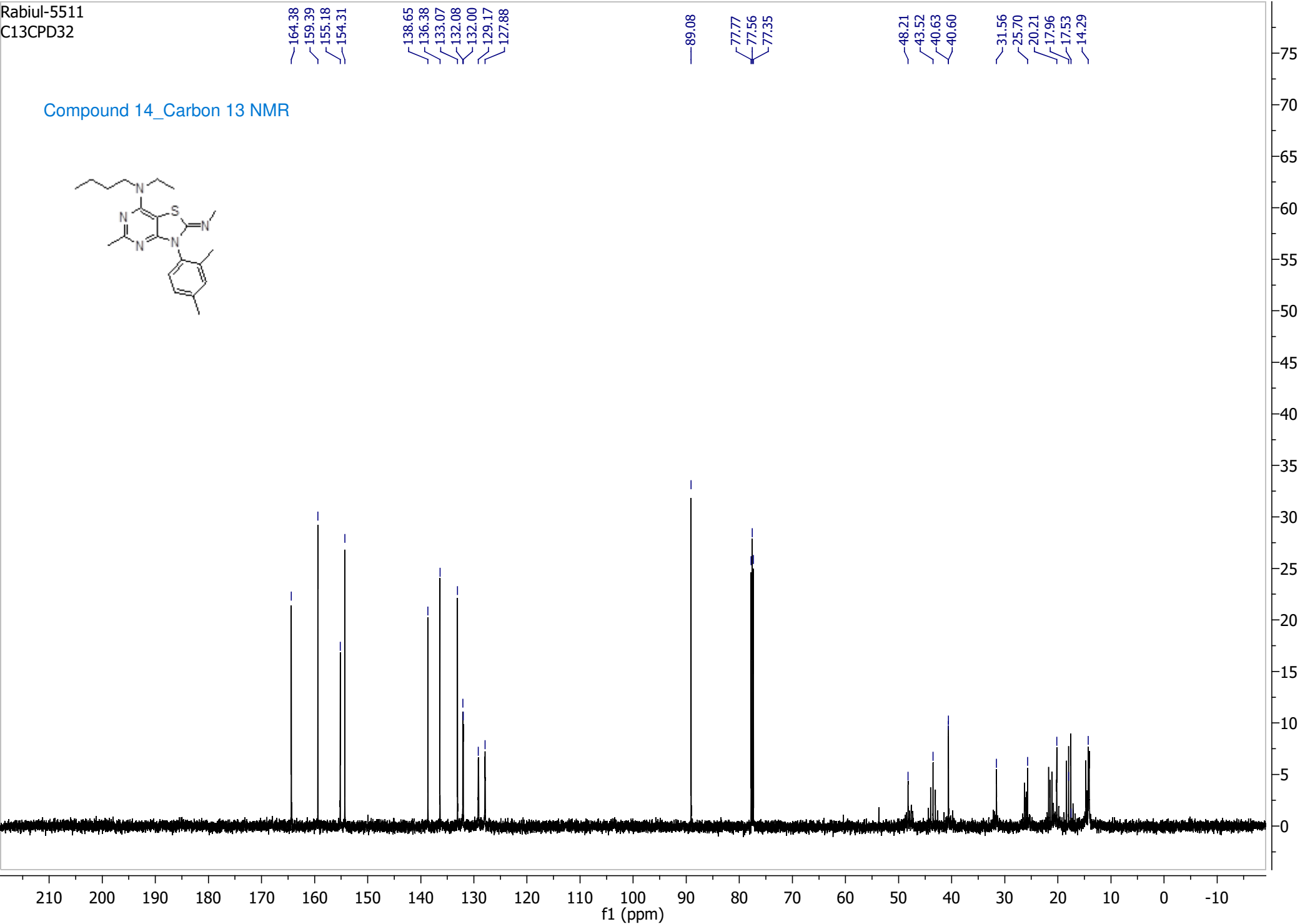
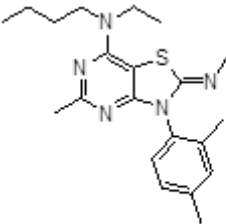
Compound 14_Proton NMR



Rabiul-5511
C13CPD32

164.38
159.39
155.18
154.31
138.65
136.38
133.07
132.08
132.00
129.17
127.88
89.08
77.77
77.56
77.35
48.21
43.52
40.63
40.60
31.56
25.70
20.21
17.96
17.53
14.29

Compound 14_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC_3-21-19\5511_000003.d
Method Bruker_11052015
Sample Name 5511
Comment

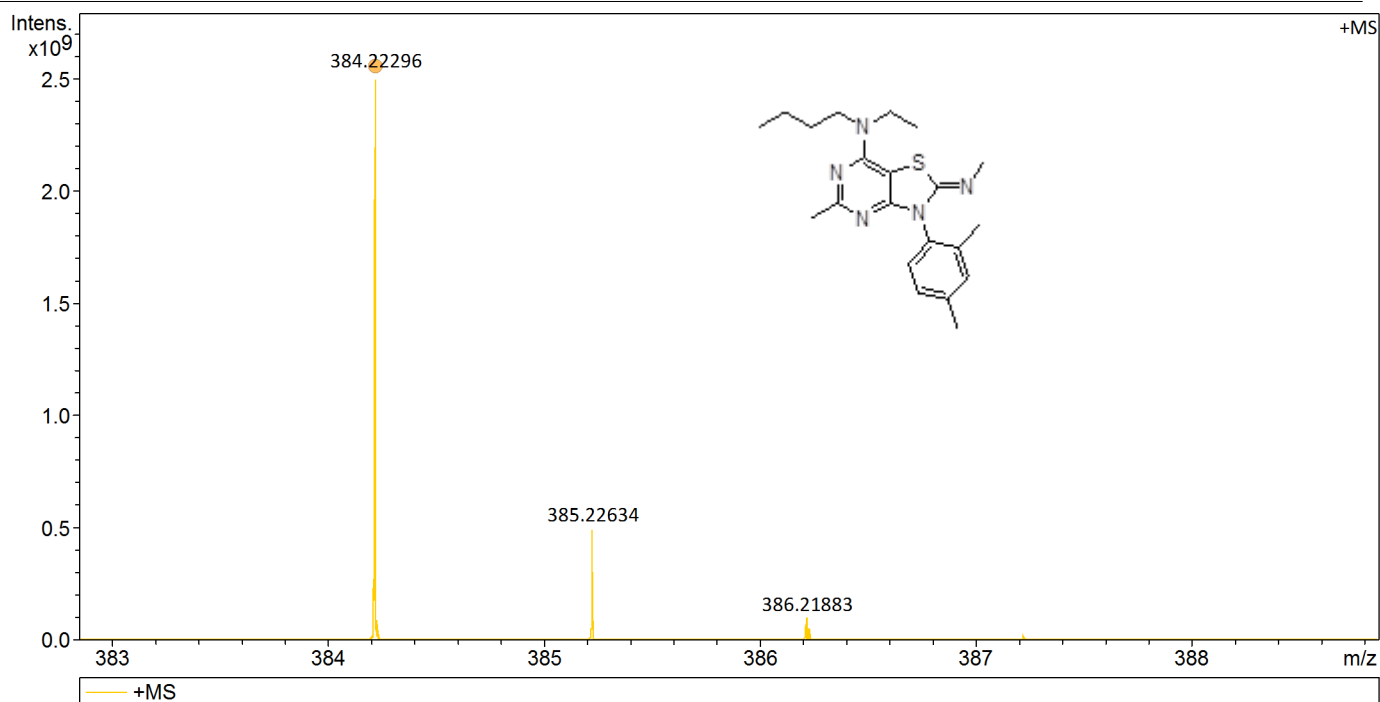
Acquisition Date 3/21/2019 6:11:07 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

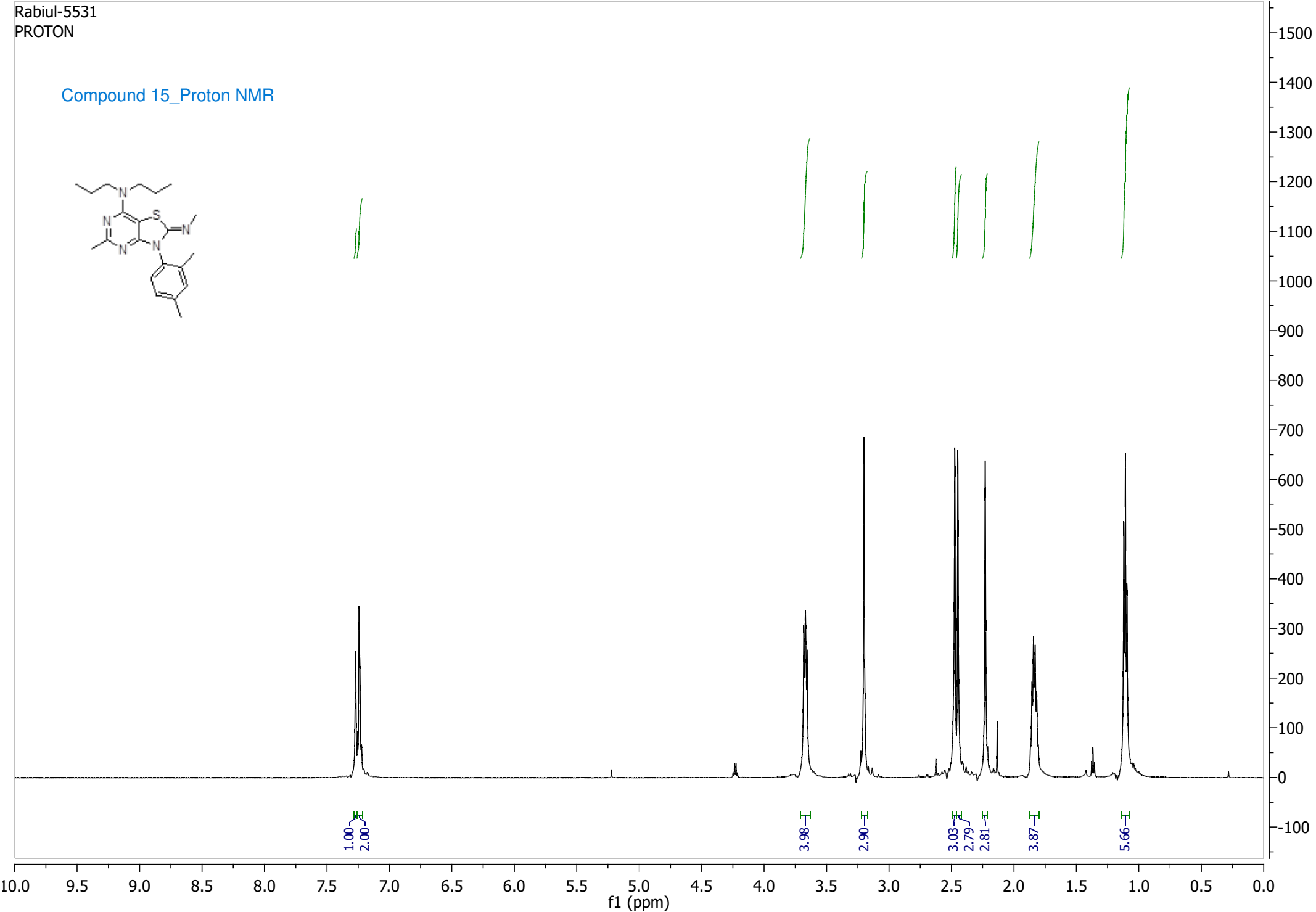
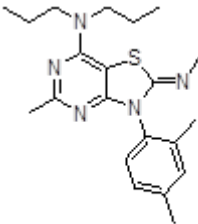
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	384.222957	1	C ₂₁ H ₃₀ N ₅ S	100.00	384.221643	-3.4	438.7	21.0	9.5	even		ok
M+Na	406.204814	1	C ₂₁ H ₂₉ N ₅ NaS	100.00	406.203588	-3.0	415.1	15.7	9.5	even		ok

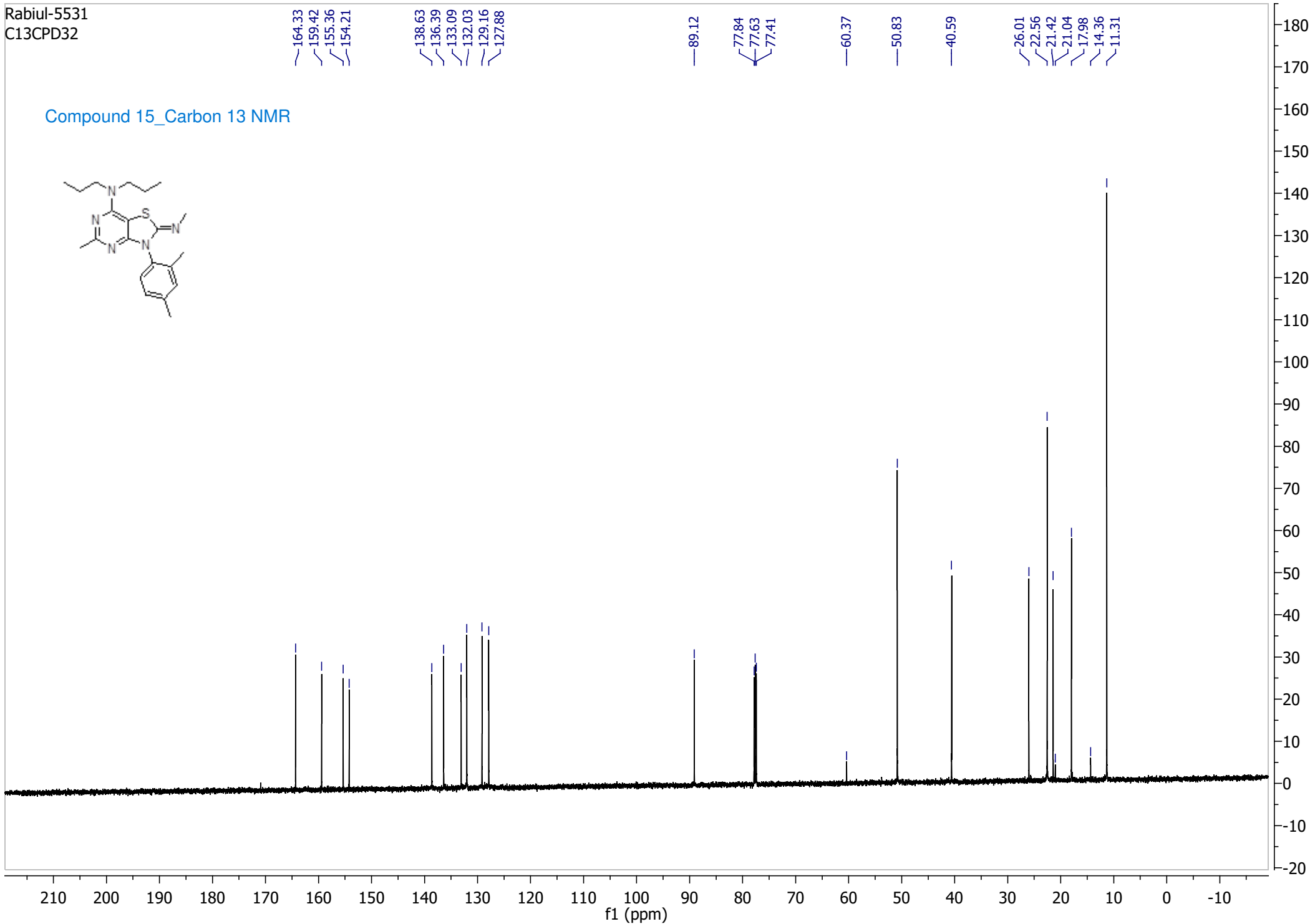
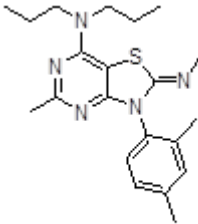
Rabiul-5531
PROTON

Compound 15_Proton NMR



Rabiul-5531
C13CPD32

Compound 15_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC\20191112\South Dakota\5531_000001.d
Method Bruker_11052015
Sample Name 5531
Comment

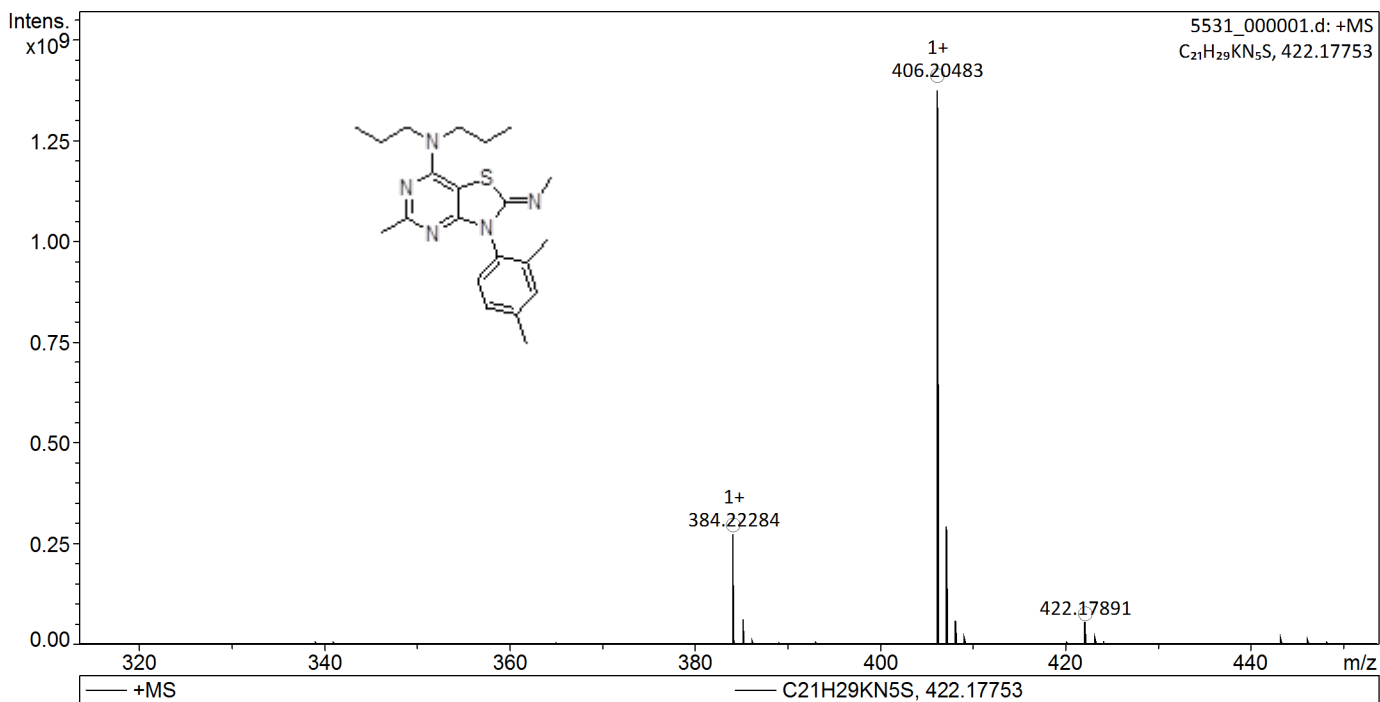
Acquisition Date 11/12/2019 2:39:57 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
n/a n/a
Broadband Low Mass 147.4 m/z
Broadband High Mass 3000.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 4000.0 V

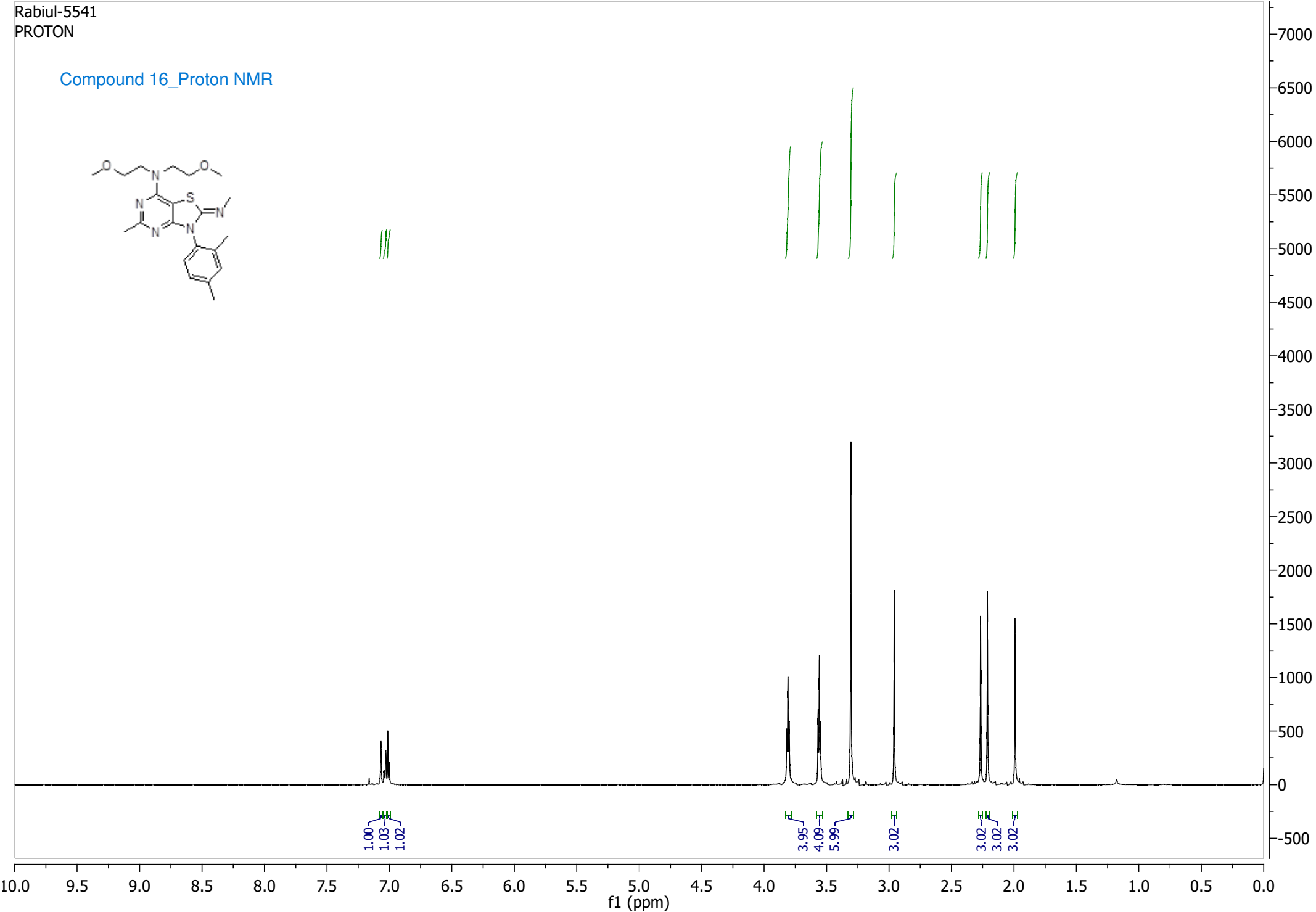
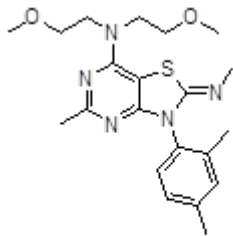
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Wed Jan 27 11:18:58 2016
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
384.222841	1	C ₂₁ H ₃₀ N ₅ S	100.00	384.221644	-3.1	-2.7	11.6	12.0	even	ok
406.204828	1	C ₂₁ H ₂₉ N ₅ NaS	100.00	406.203588	-3.1	-2.7	13.4	12.0	even	ok
422.178908	1	C ₂₁ H ₂₉ KN ₅ S	100.00	422.177525	-3.3	-2.7	31.0	12.0	even	ok

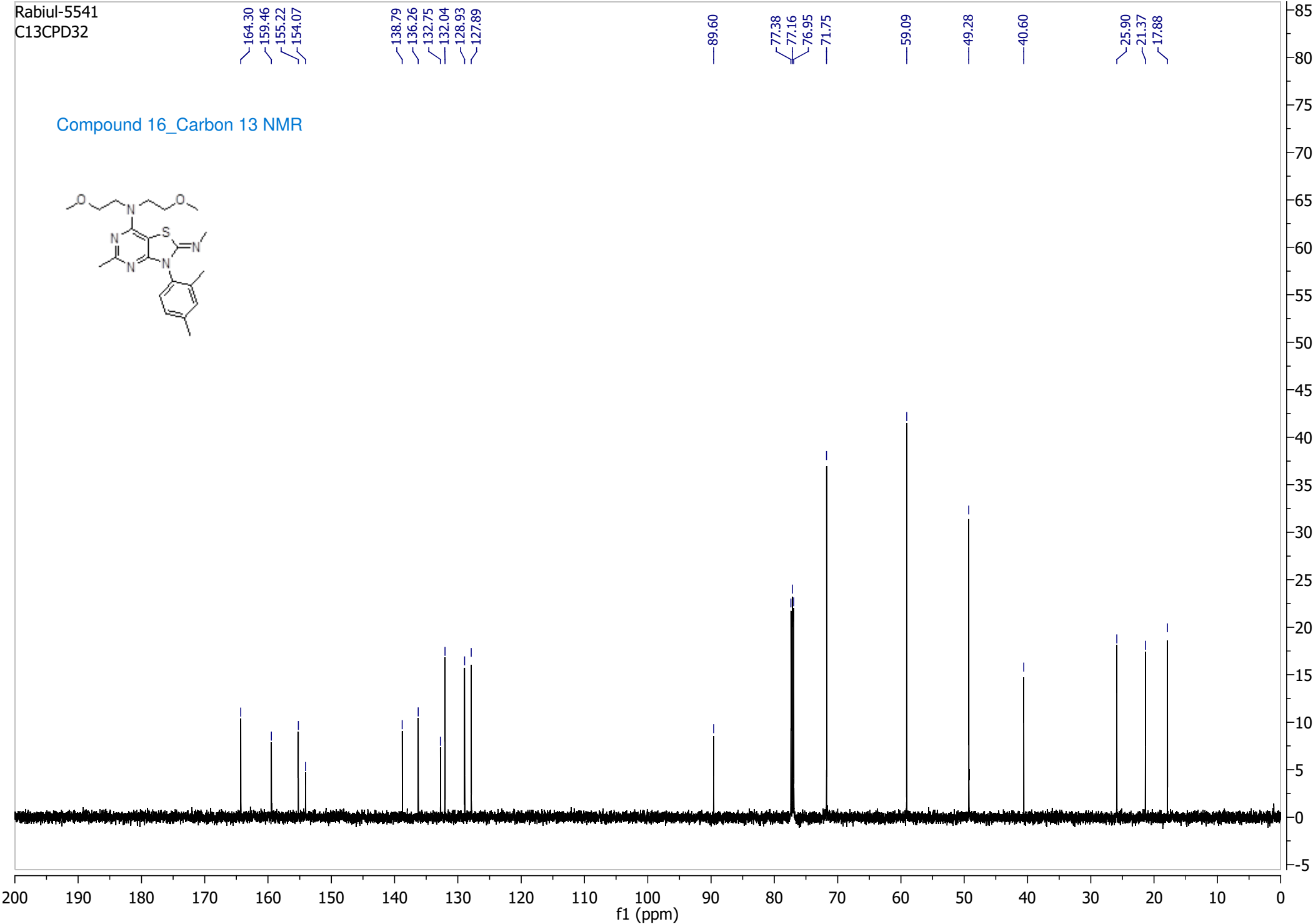
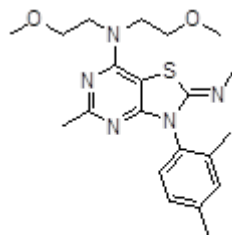
Rabiul-5541
PROTON

Compound 16_Proton NMR



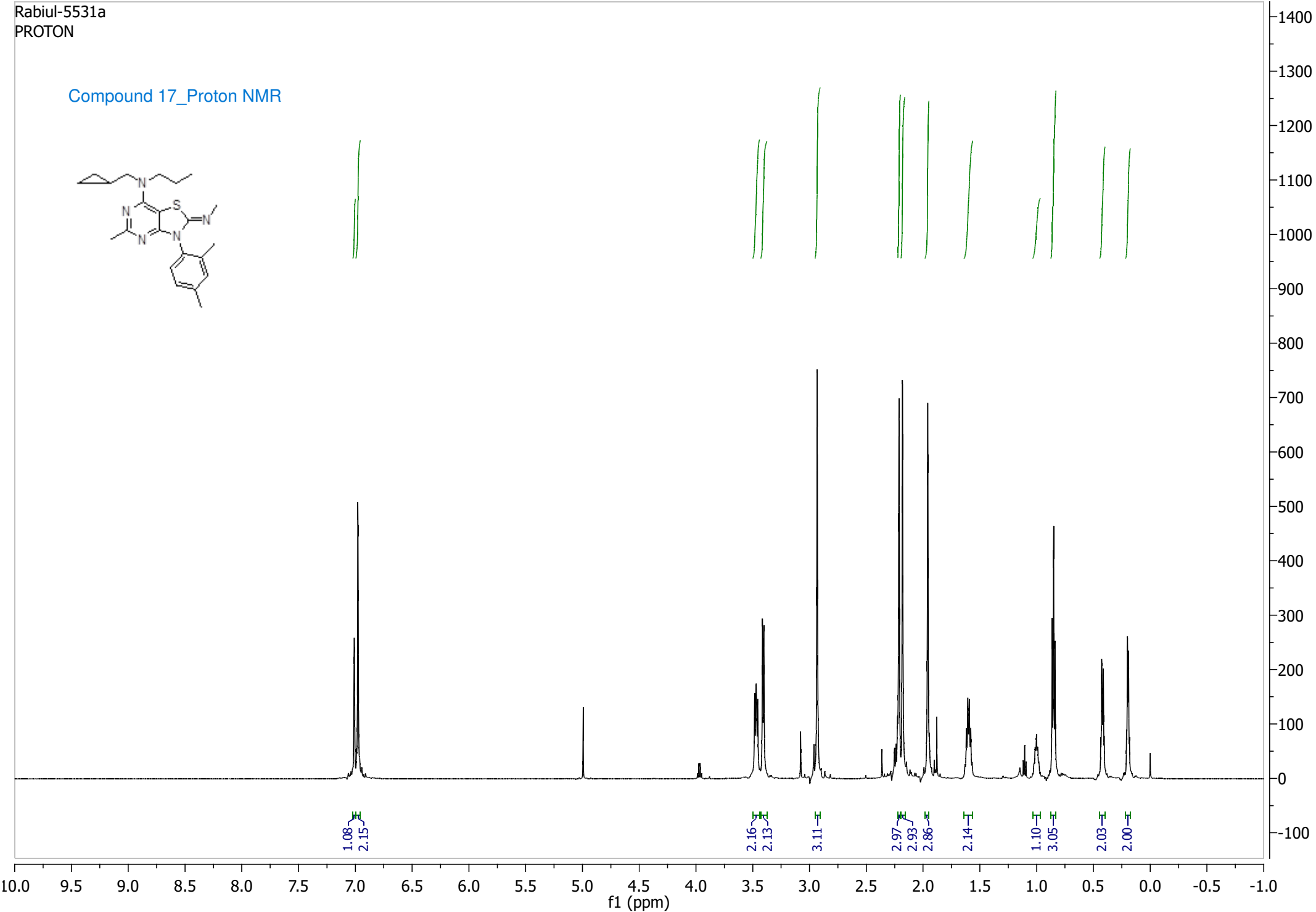
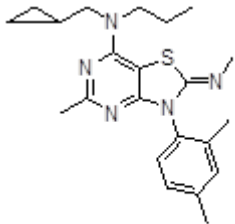
Rabiul-5541
C13CPD32

Compound 16_Carbon 13 NMR



Rabiul-5531a
PROTON

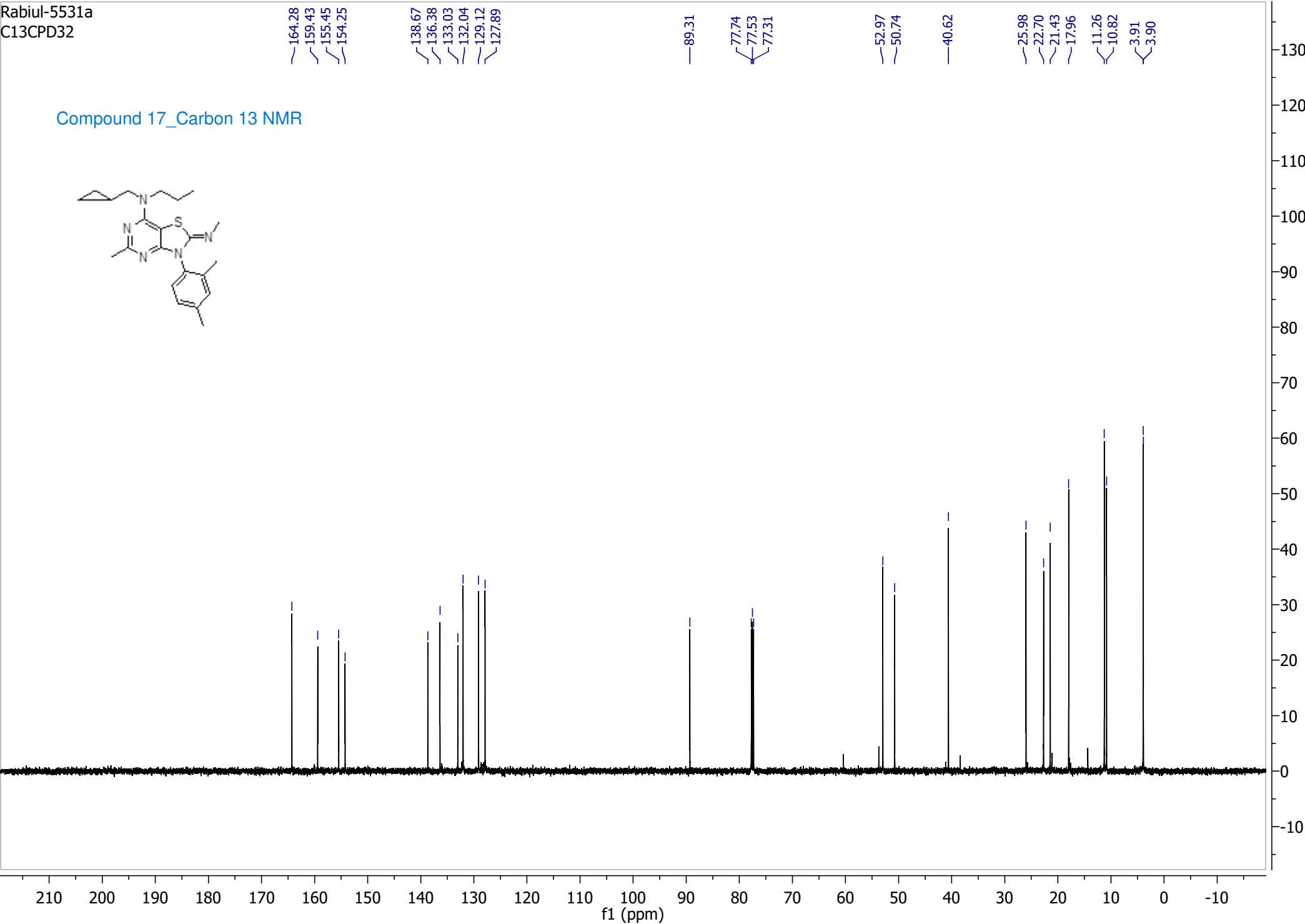
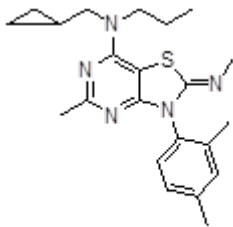
Compound 17_Proton NMR



Rabiul-5531a
C13CPD32

164.28 159.43 155.45 154.25 138.67 136.38 133.03 132.04 129.12 127.89 89.31 77.74 77.53 77.31 52.97 50.74 40.62 25.98 22.70 21.43 17.96 11.26 10.82 3.91 3.90

Compound 17_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC_3-21-19\5531a_000001.d
Method Bruker_11052015
Sample Name 5531a
Comment

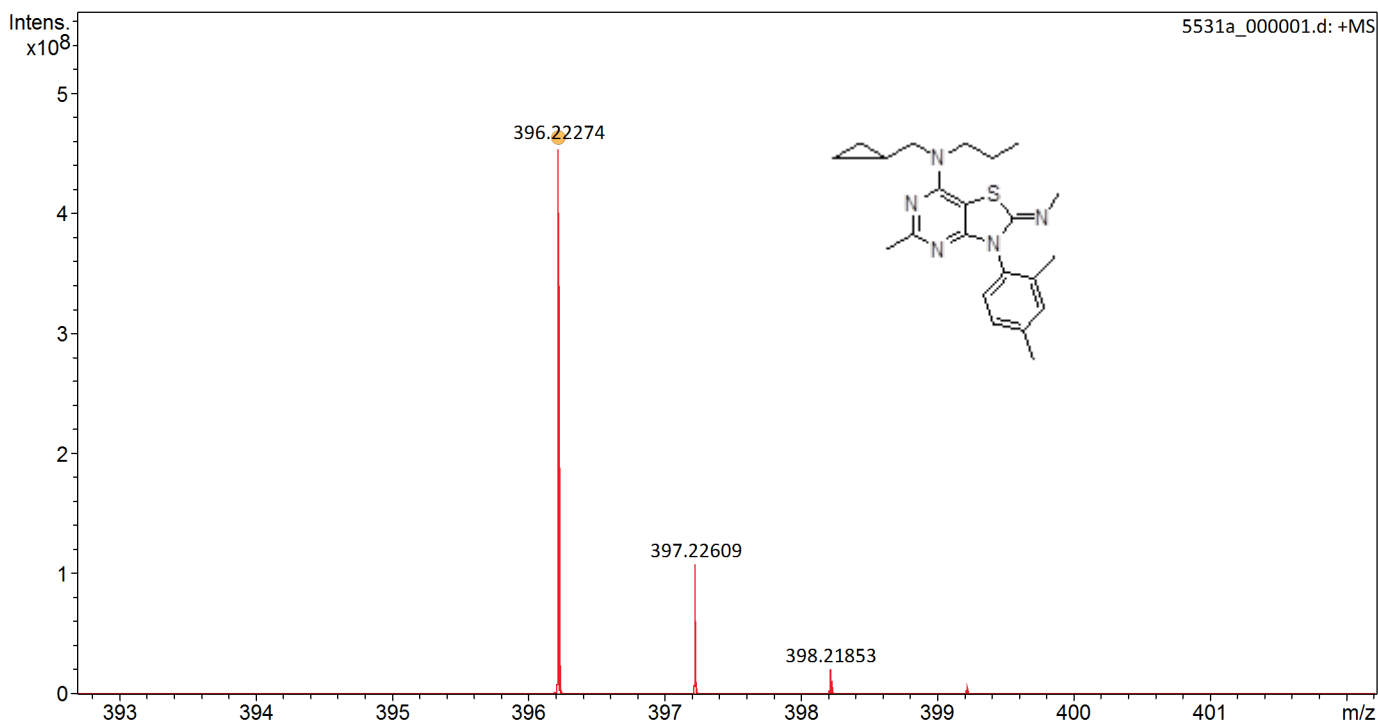
Acquisition Date 3/21/2019 7:43:27 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

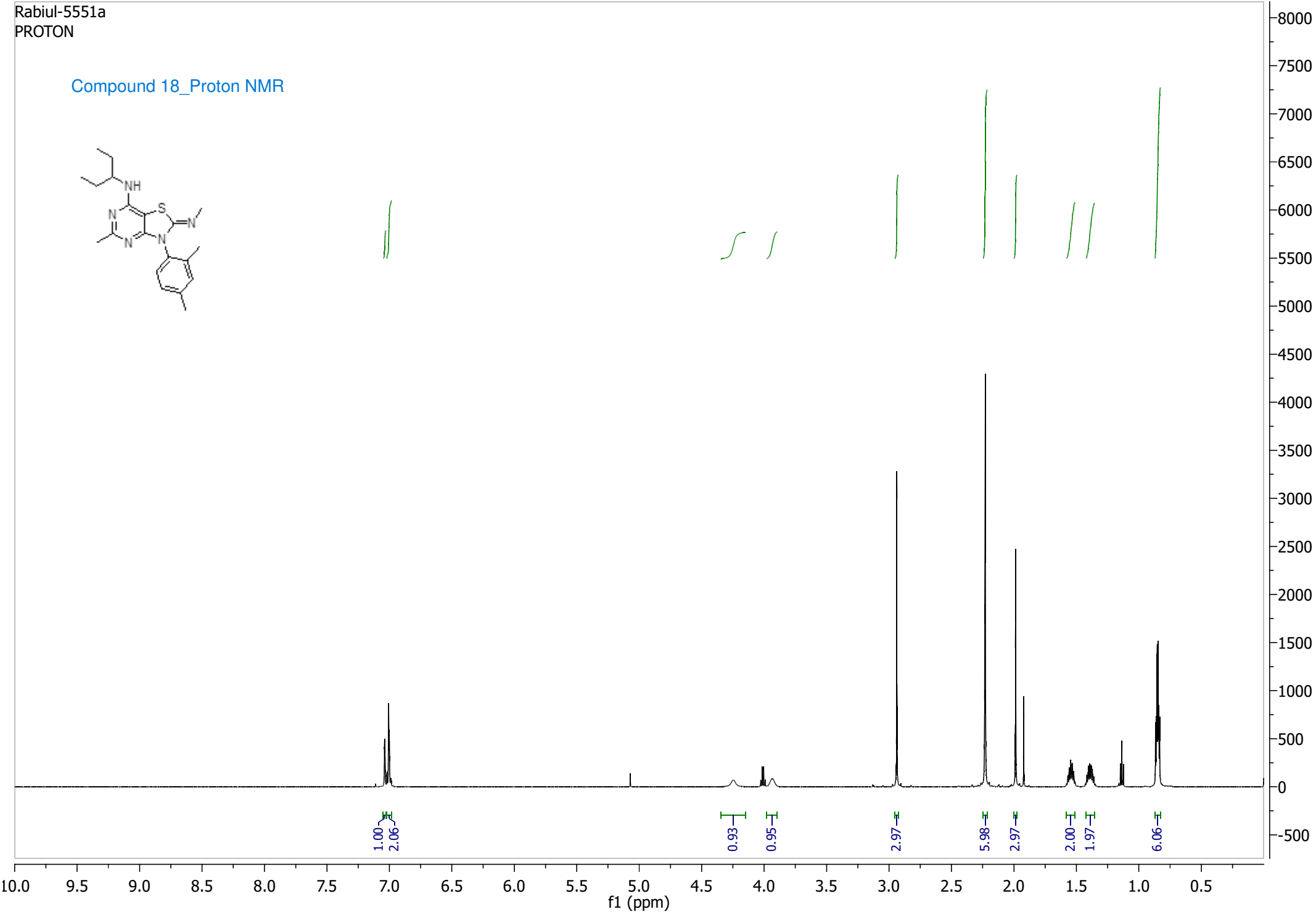
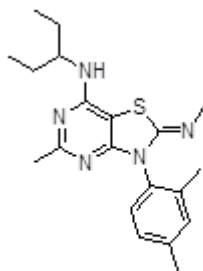
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	396.222739	1	C22H30N5S	100.00	396.221643	-2.8	-2.7	2.1	10.5	even		ok
M+Na	418.204475	1	C22H29N5NaS	100.00	418.203588	-2.1	-2.1	3.7	10.5	even		ok

Rabiul-5551a
PROTON

Compound 18_Proton NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5551a_000001.d
Method Bruker_11052015
Sample Name 5551a
Comment

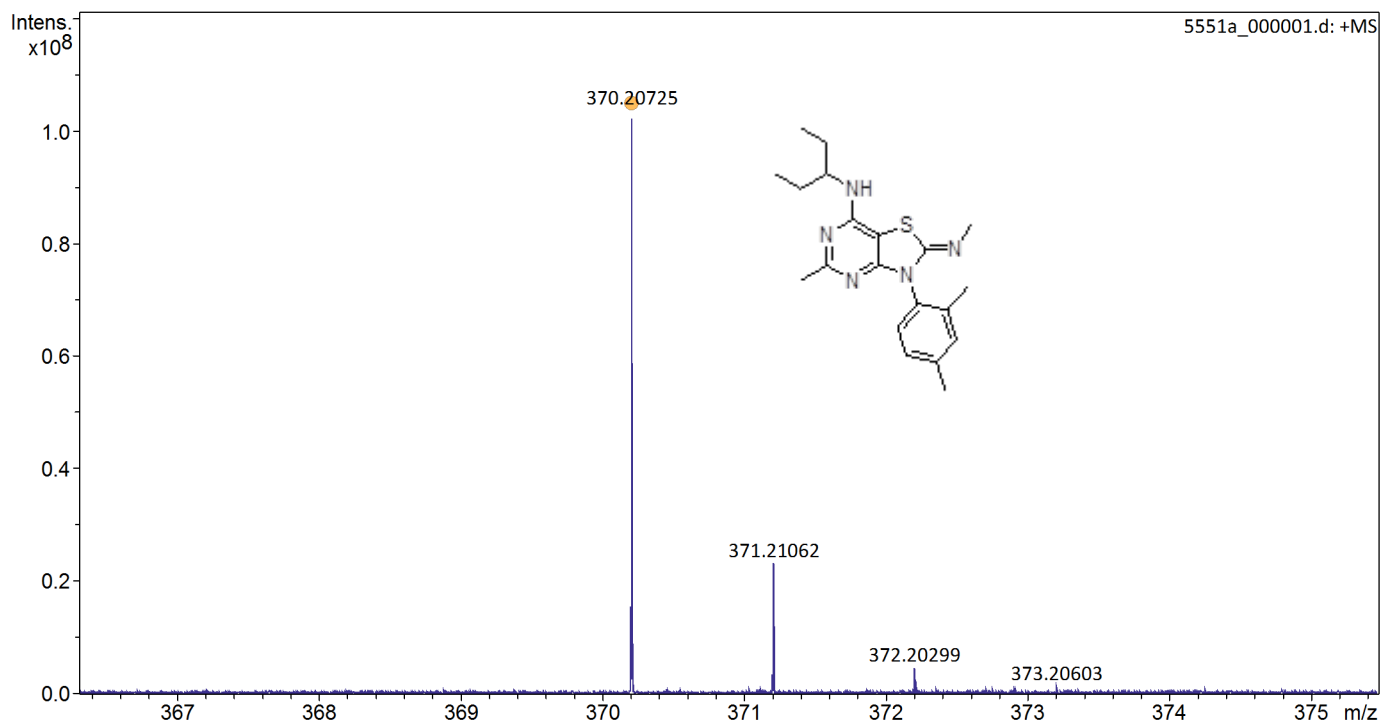
Acquisition Date 3/21/2019 7:40:43 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

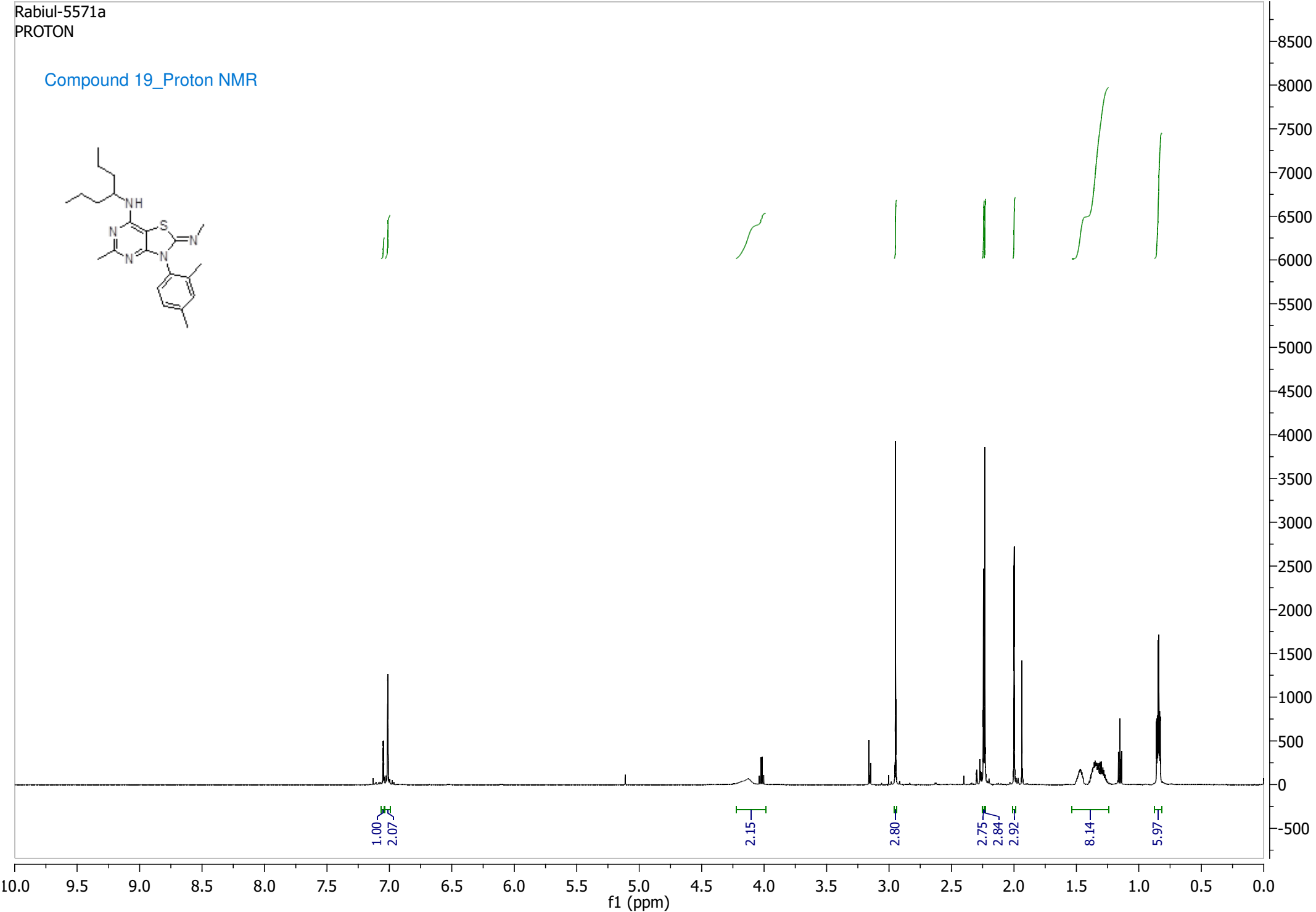
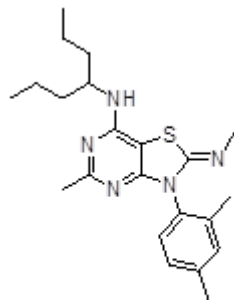
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	370.207246	1	C20H28N5S	100.00	370.205993	-3.4	-3.5	4.7	9.5	even		ok
M+Na	392.189038	1	C20H27N5NaS	100.00	392.187938	-2.8	431.3	13.1	9.5	even		ok

Rabiul-5571a
PROTON

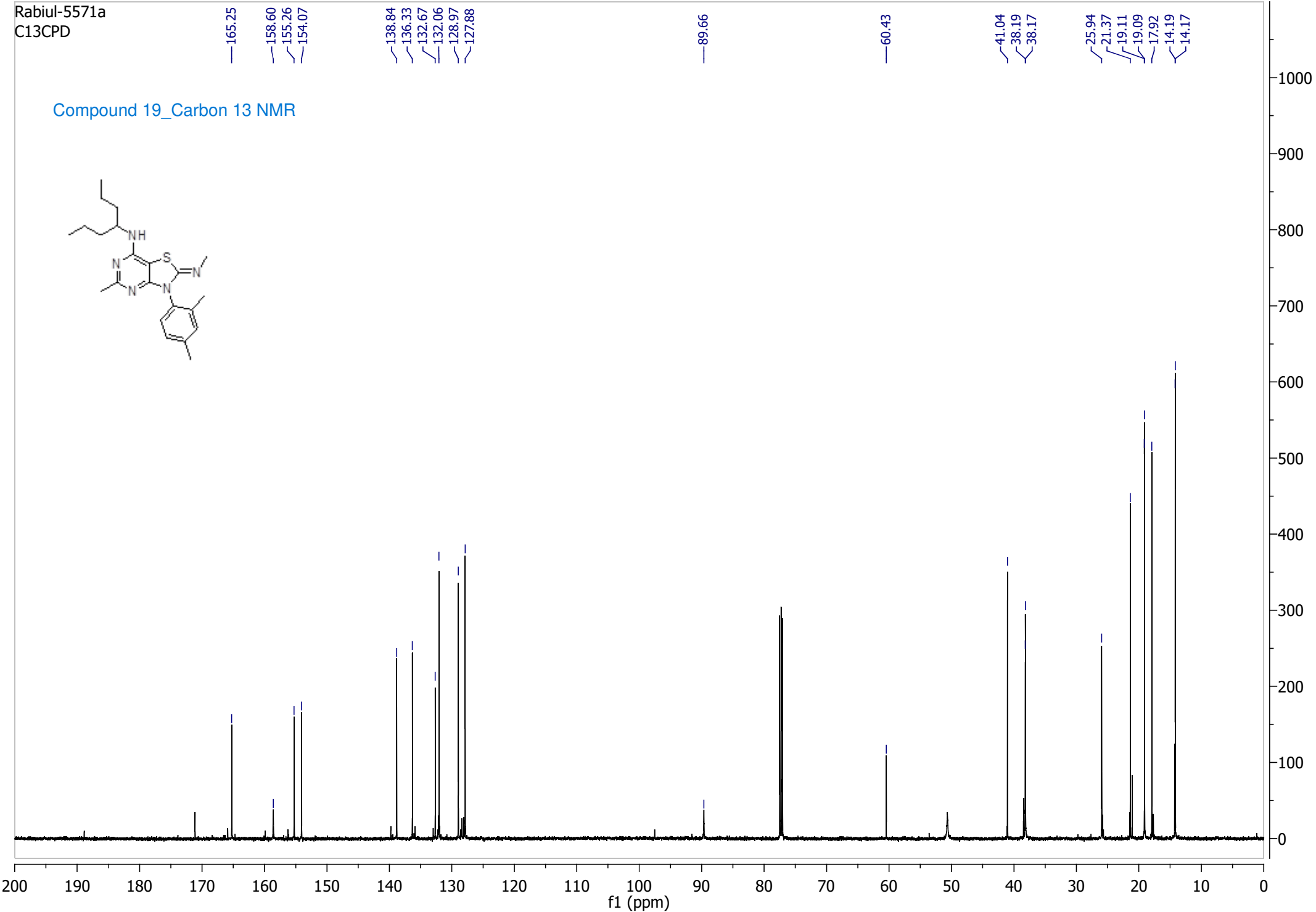
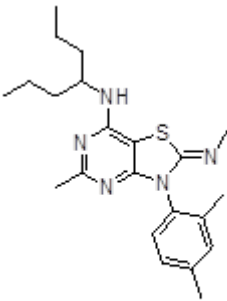
Compound 19_Proton NMR



Rabiul-5571a
C13CPD

165.25 158.60 155.26 154.07 138.84 136.33 132.67 132.06 128.97 127.88 89.66 60.43 41.04 38.19 38.17 25.94 21.37 19.11 19.09 17.92 14.19 14.17

Compound 19_Carbon 13 NMR



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5571a_000001.d
Method Bruker_11052015
Sample Name 5571a
Comment

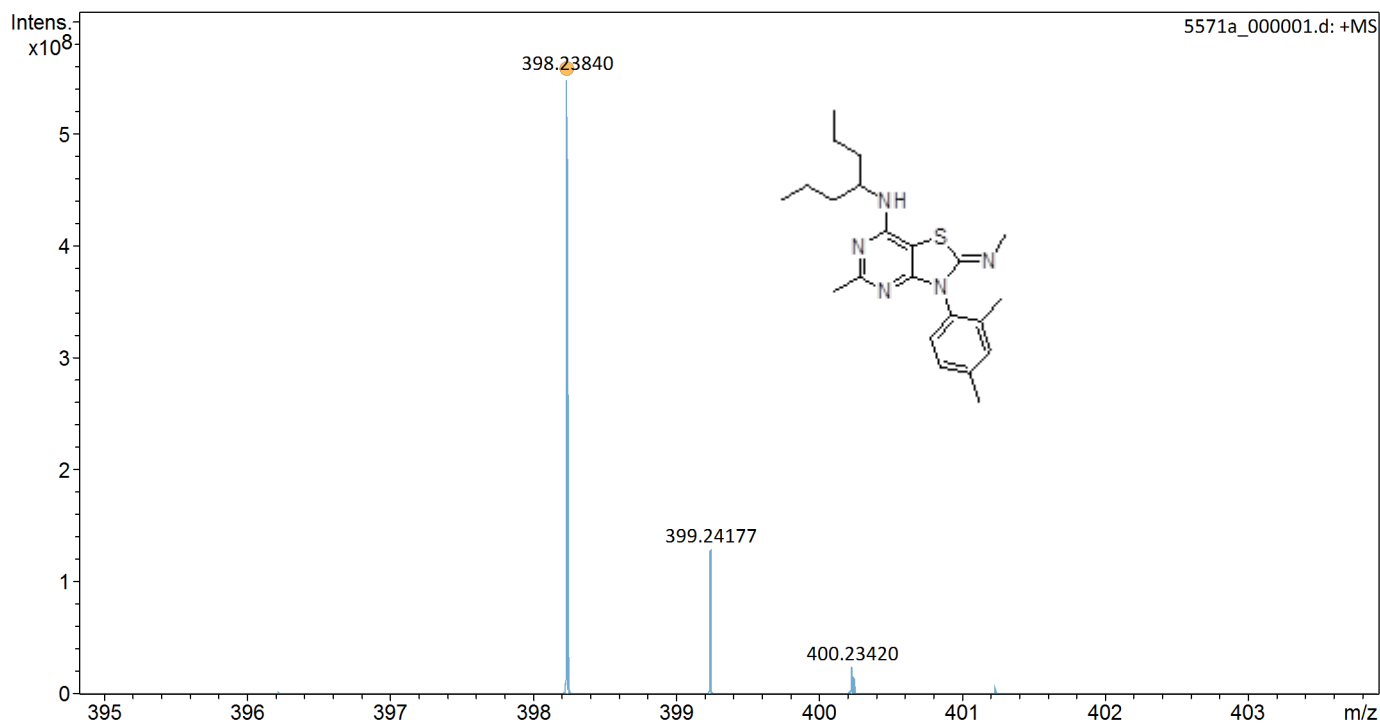
Acquisition Date 3/21/2019 7:34:51 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

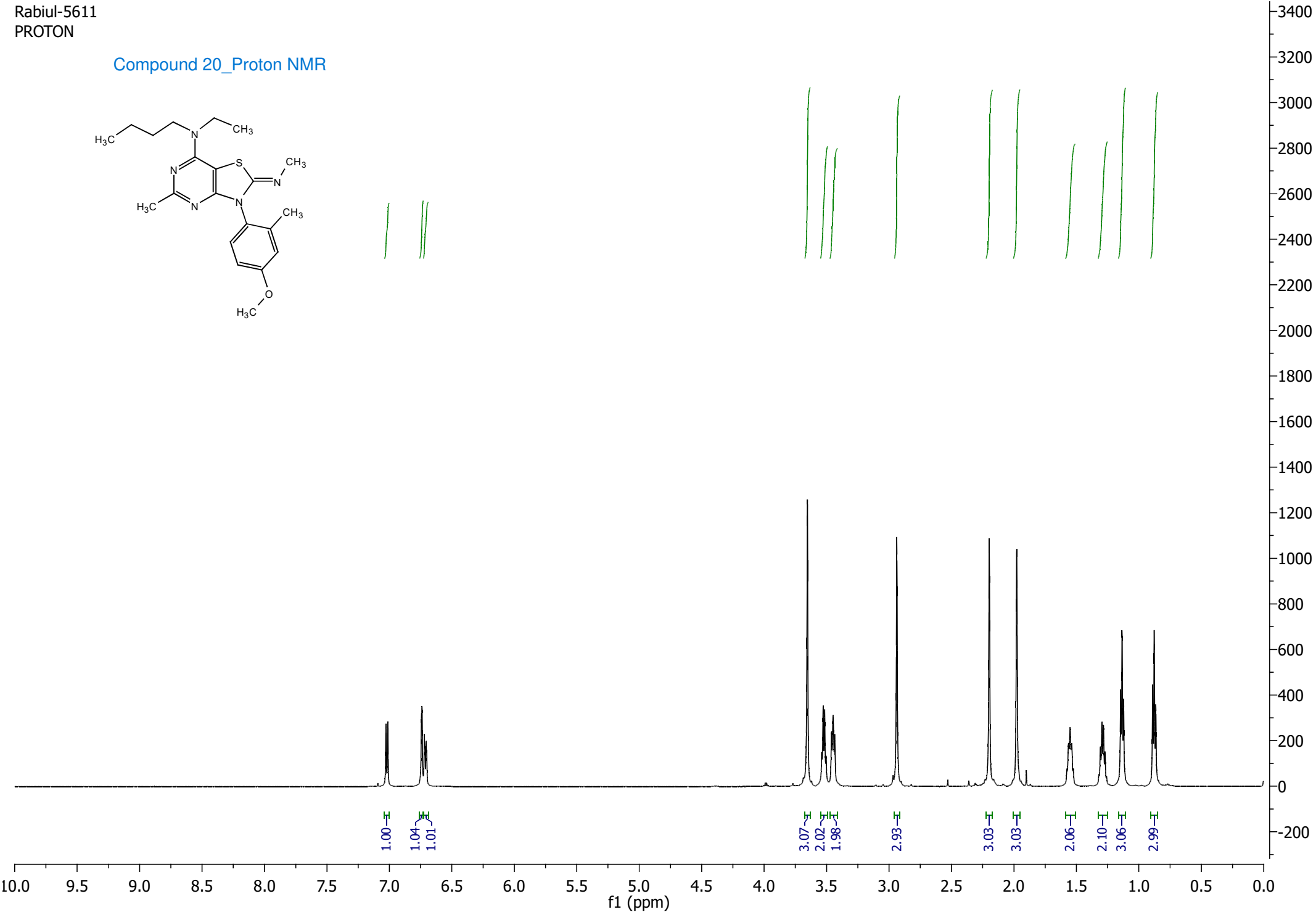
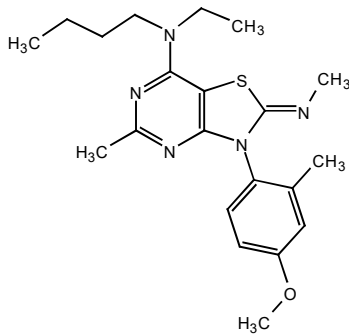
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	398.238398	1	C22H32N5S	100.00	398.237293	-2.8	1274.1	14.1	9.5	even		ok
M+Na	420.220155	1	C22H31N5NaS	100.00	420.219238	-2.2	1207.9	14.9	9.5	even		ok

Rabiul-5611
PROTON

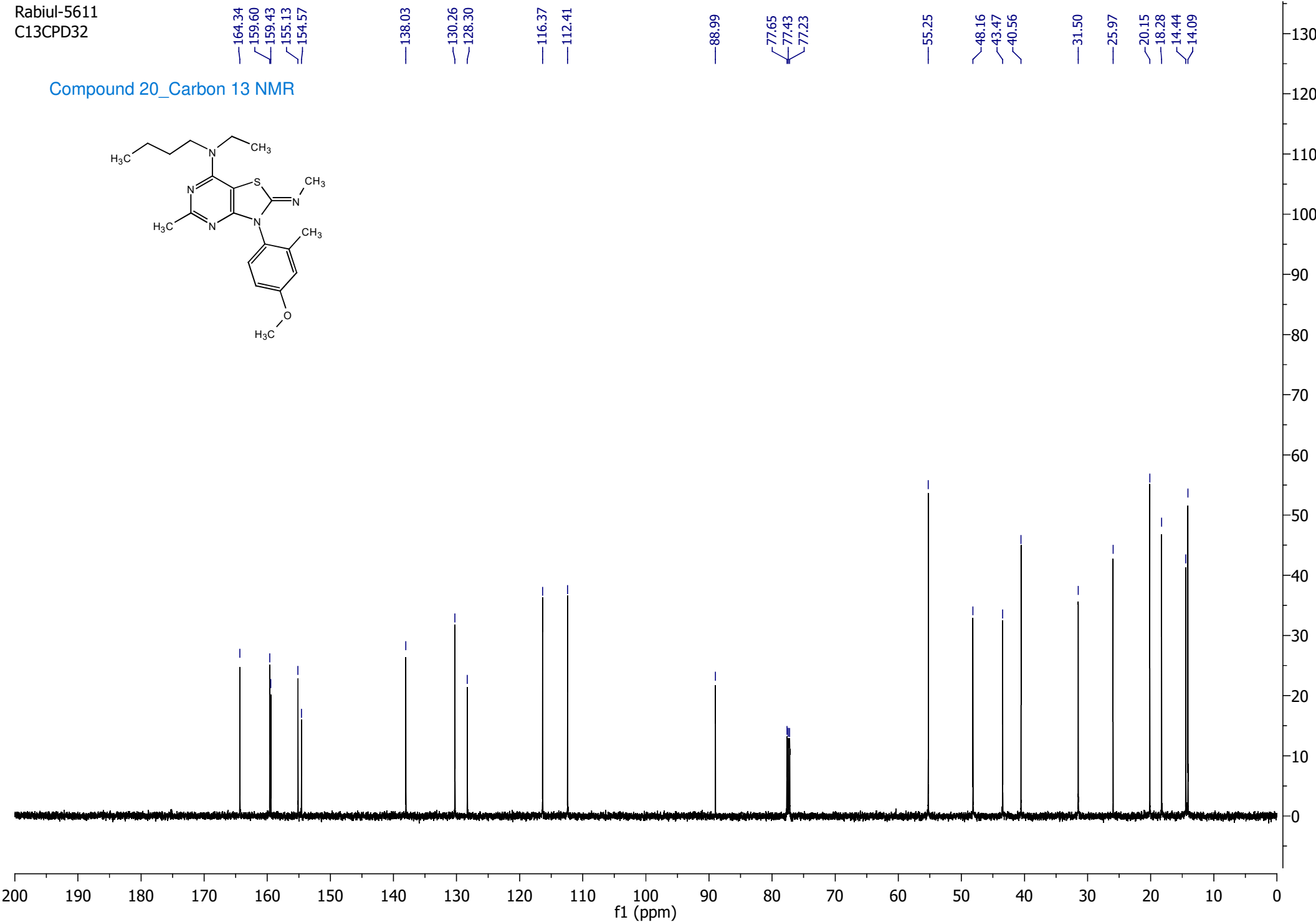
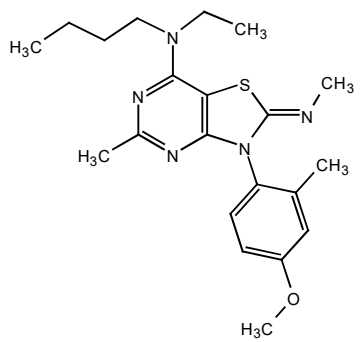
Compound 20_Proton NMR



Rabiul-5611
C13CPD32



Compound 20_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC_3-21-19\5611_000001.d
Method Bruker_11052015
Sample Name 5611
Comment

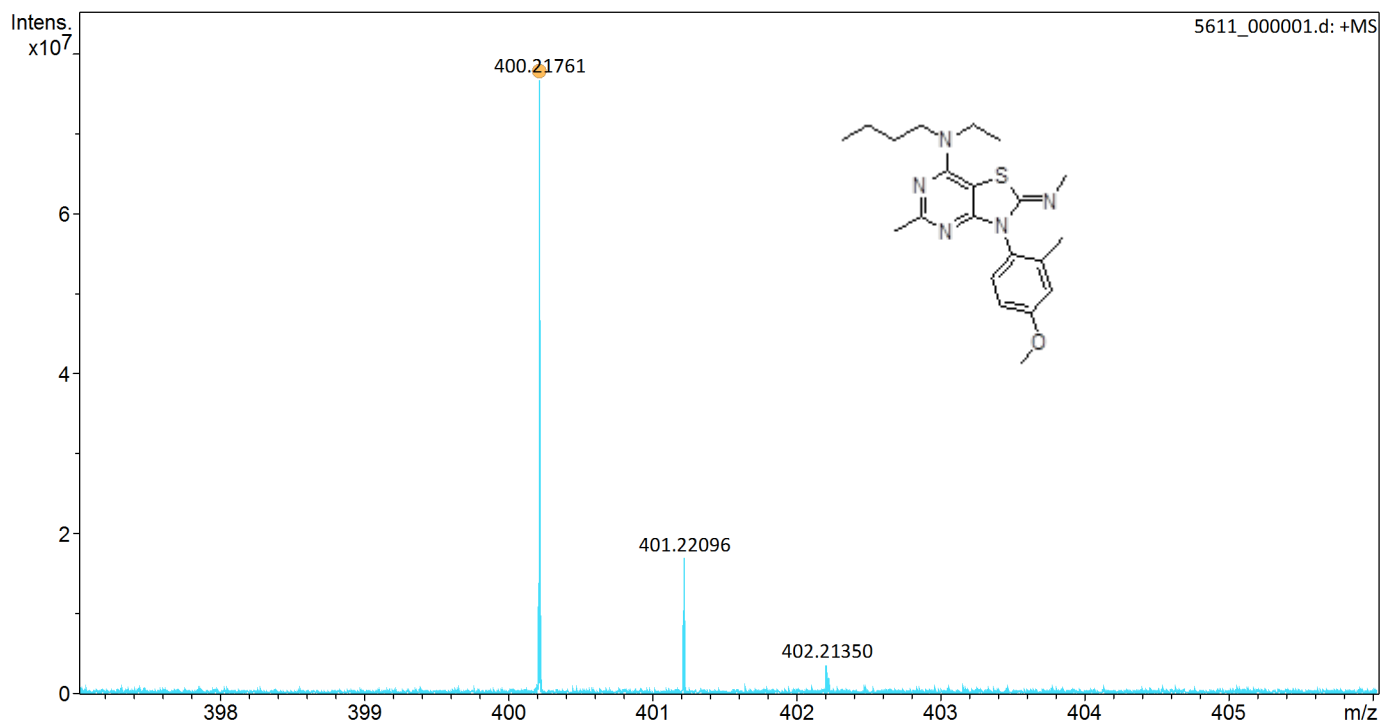
Acquisition Date 3/21/2019 7:29:44 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

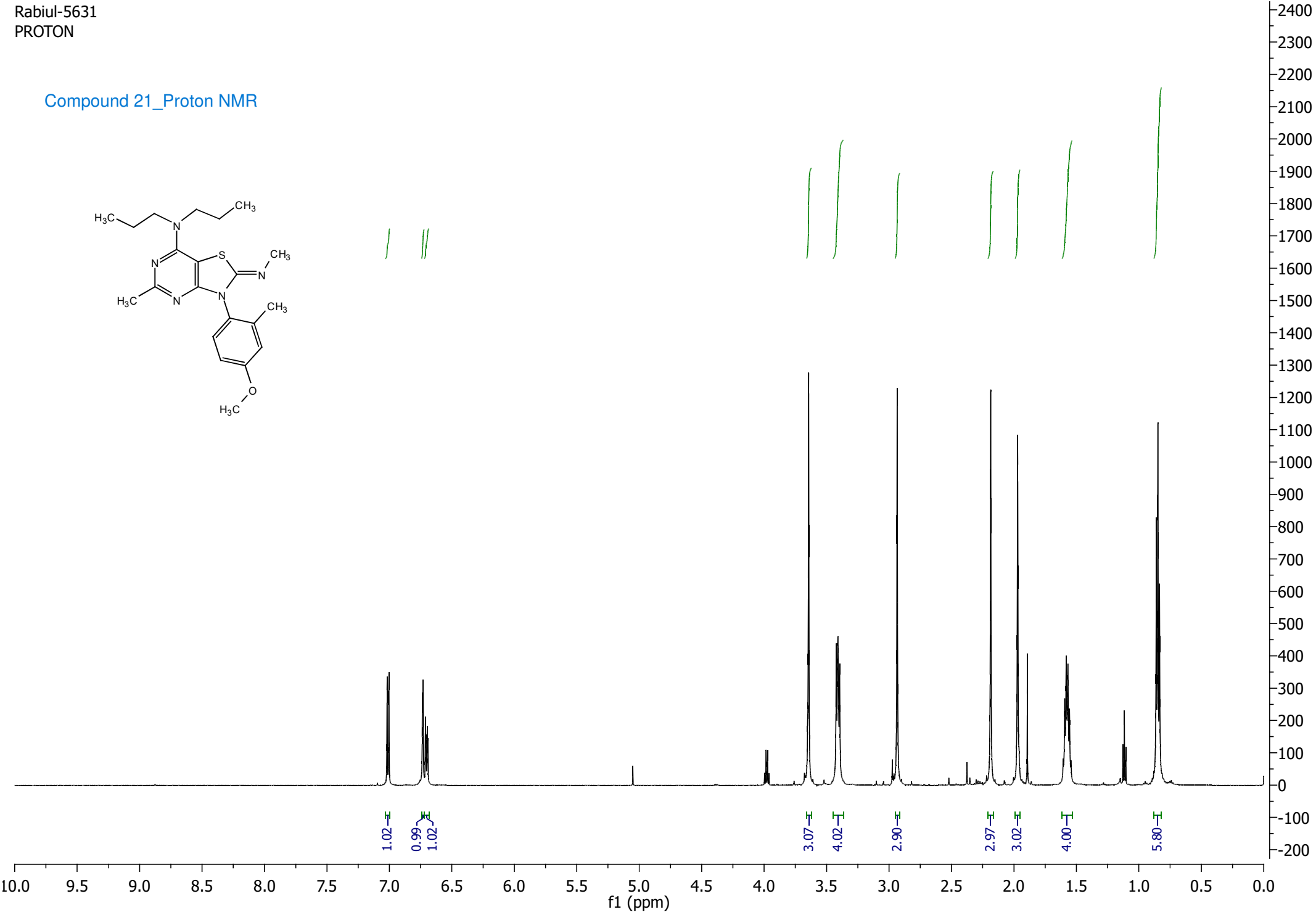
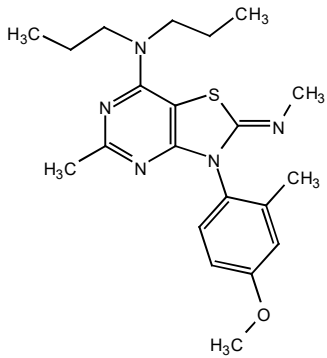
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	400.217609	1	C ₂₁ H ₃₀ N ₅ OS	100.00	400.216558	-2.6	-2.7	4.8	9.5	even		ok
M+Na	422.199350	1	C ₂₁ H ₂₉ N ₅ NaOS	100.00	422.198502	-2.0	-2.1	2.9	9.5	even		ok

Rabiul-5631
PROTON

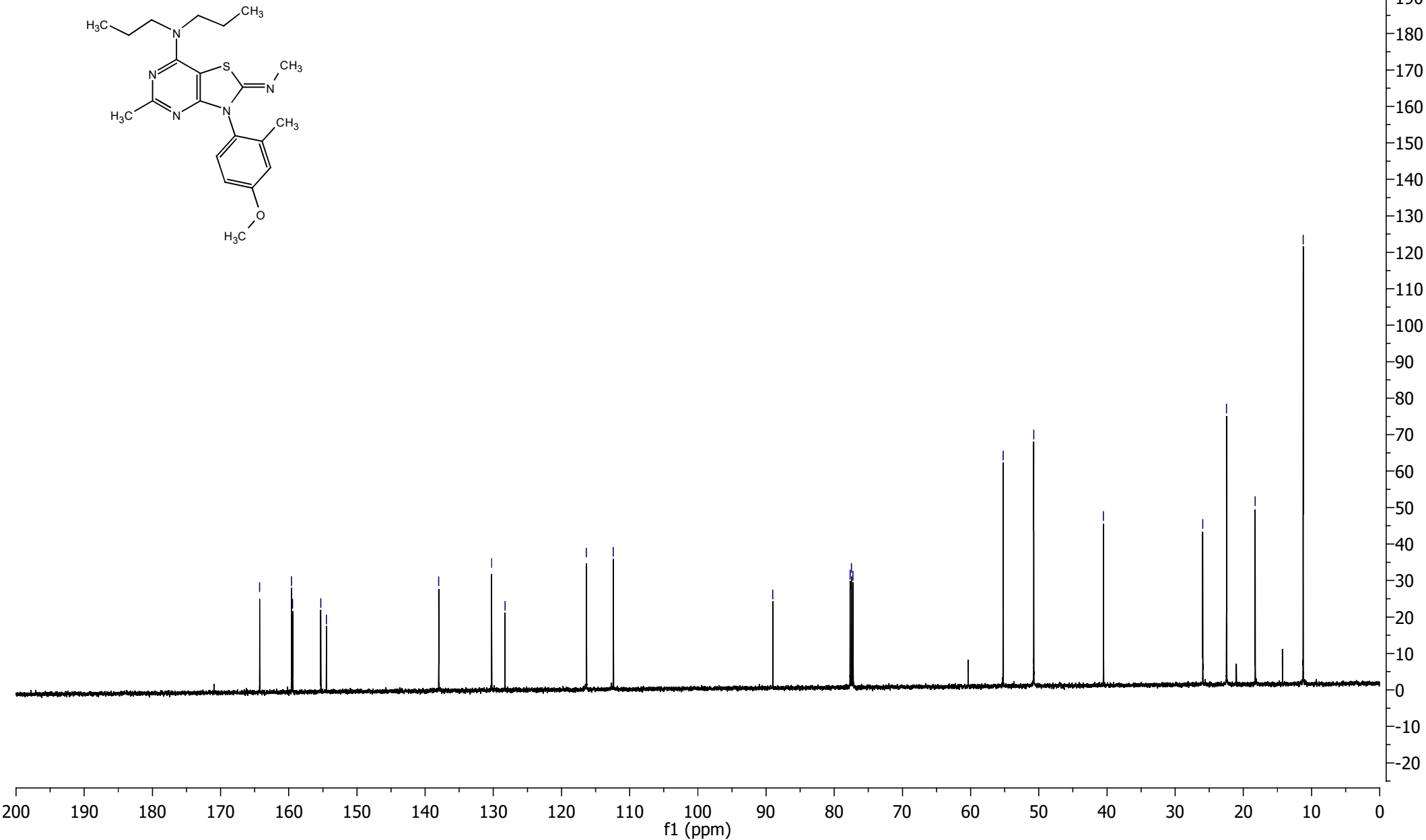
Compound 21_Proton NMR



Rabiul-5631
C13CPD32



Compound 21_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC_3-21-19\5631_000001.d
Method Bruker_11052015
Sample Name 5631
Comment

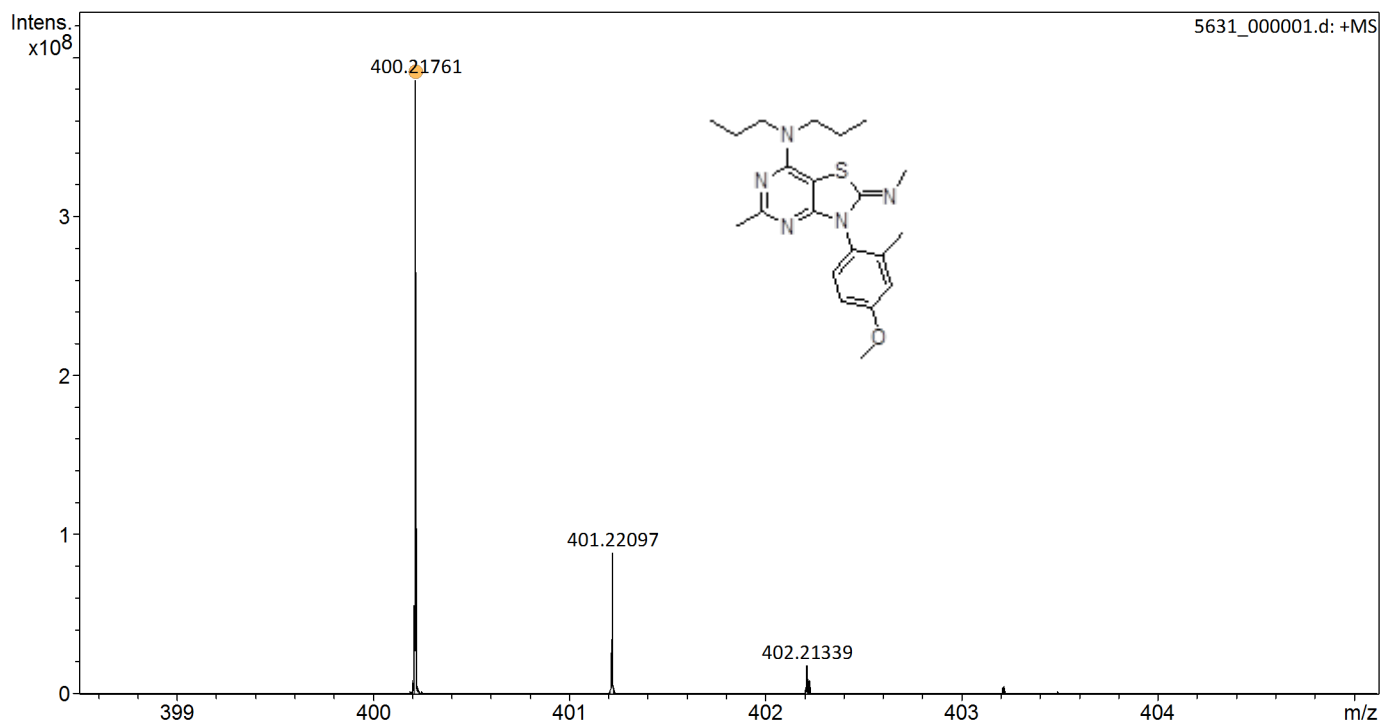
Acquisition Date 3/21/2019 7:24:09 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

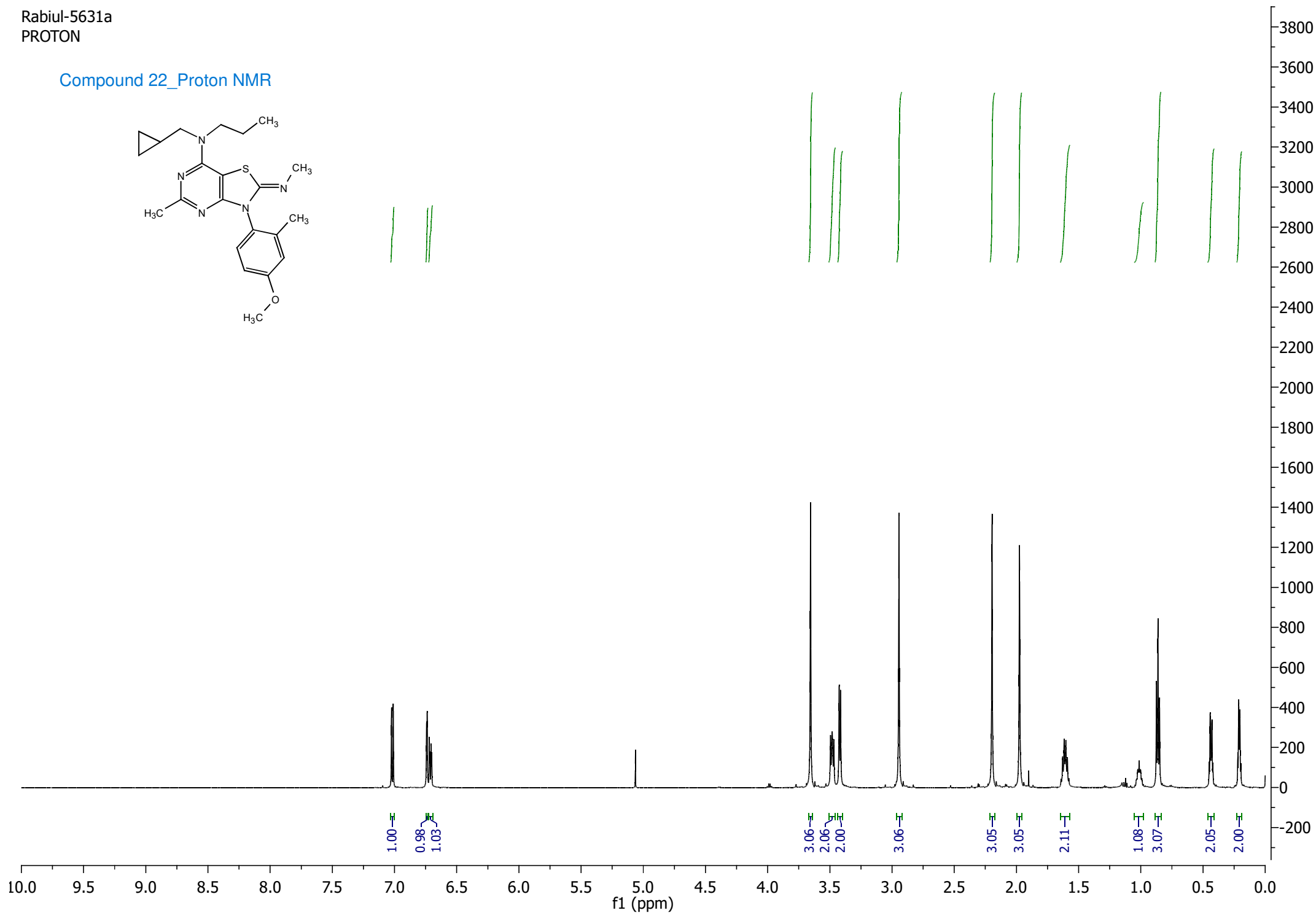
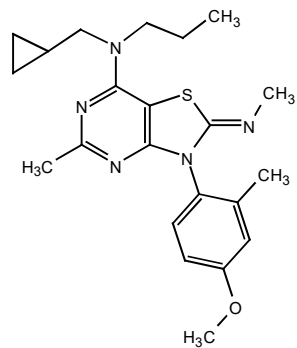
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	400.217611	1	C ₂₁ H ₃₀ N ₅ OS	100.00	400.216558	-2.6	-2.7	2.3	9.5	even		ok
M+Na	422.199362	1	C ₂₁ H ₂₉ N ₅ NaOS	100.00	422.198502	-2.0	-2.1	2.9	9.5	even		ok

Rabiul-5631a
PROTON

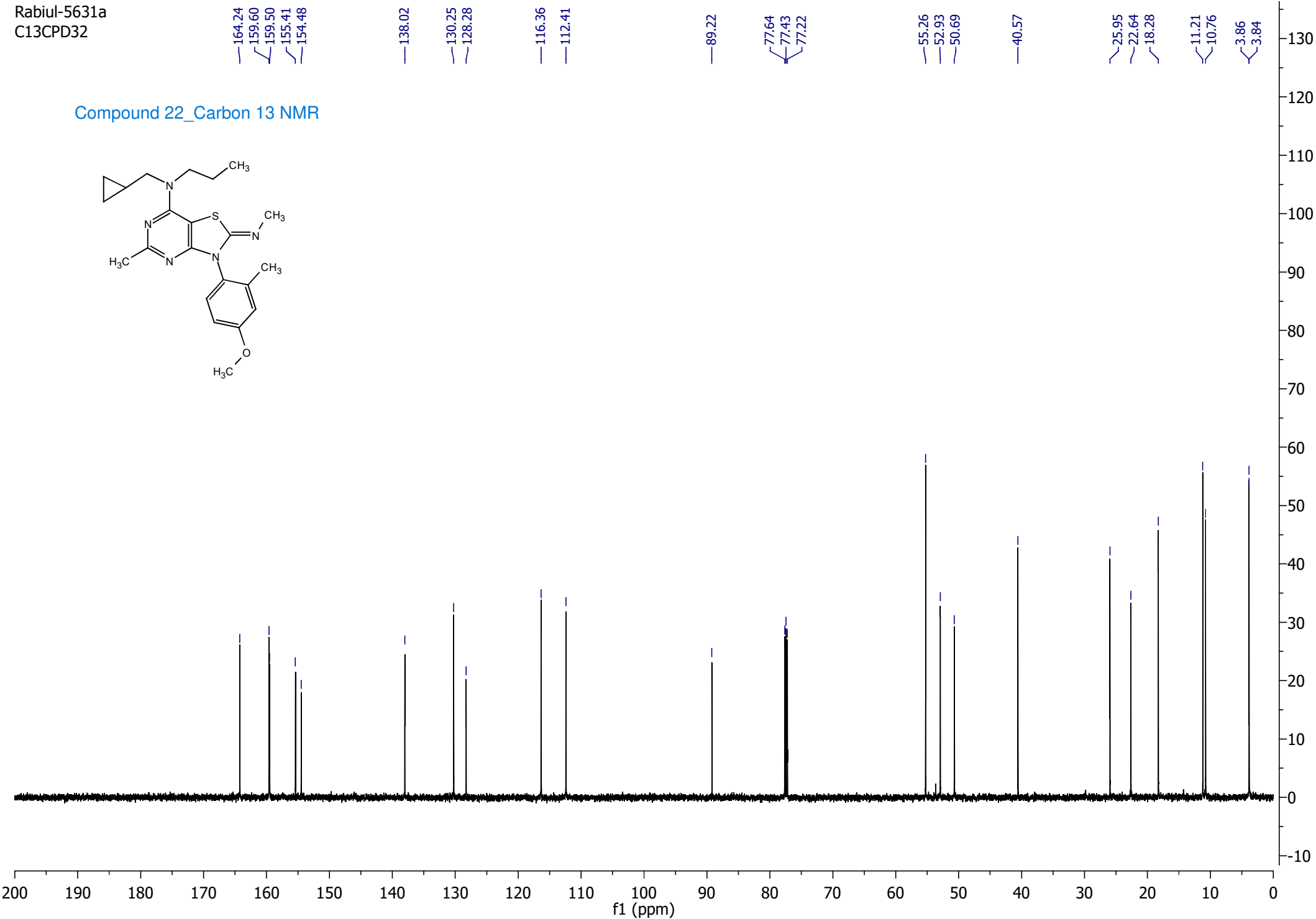
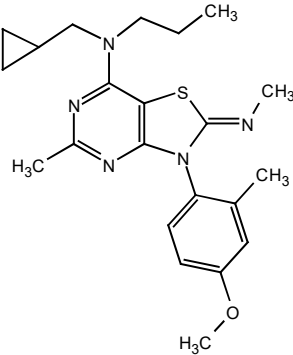
Compound 22_Proton NMR



Rabiul-5631a
C13CPD32



Compound 22_Carbon 13 NMR



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Analysis Info

Analysis Name D:\Data\IC_3-21-19\5631a_000001.d
Method Bruker_11052015
Sample Name 5631a
Comment

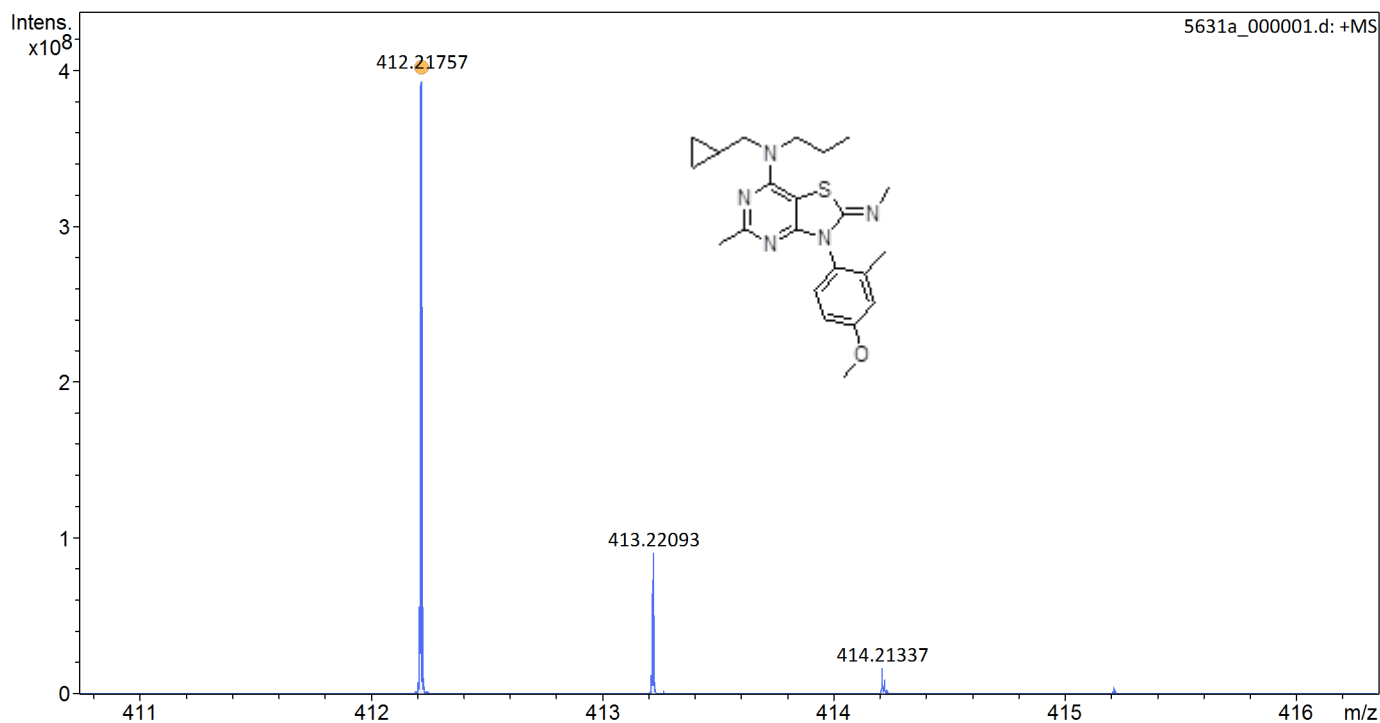
Acquisition Date 3/21/2019 7:20:02 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

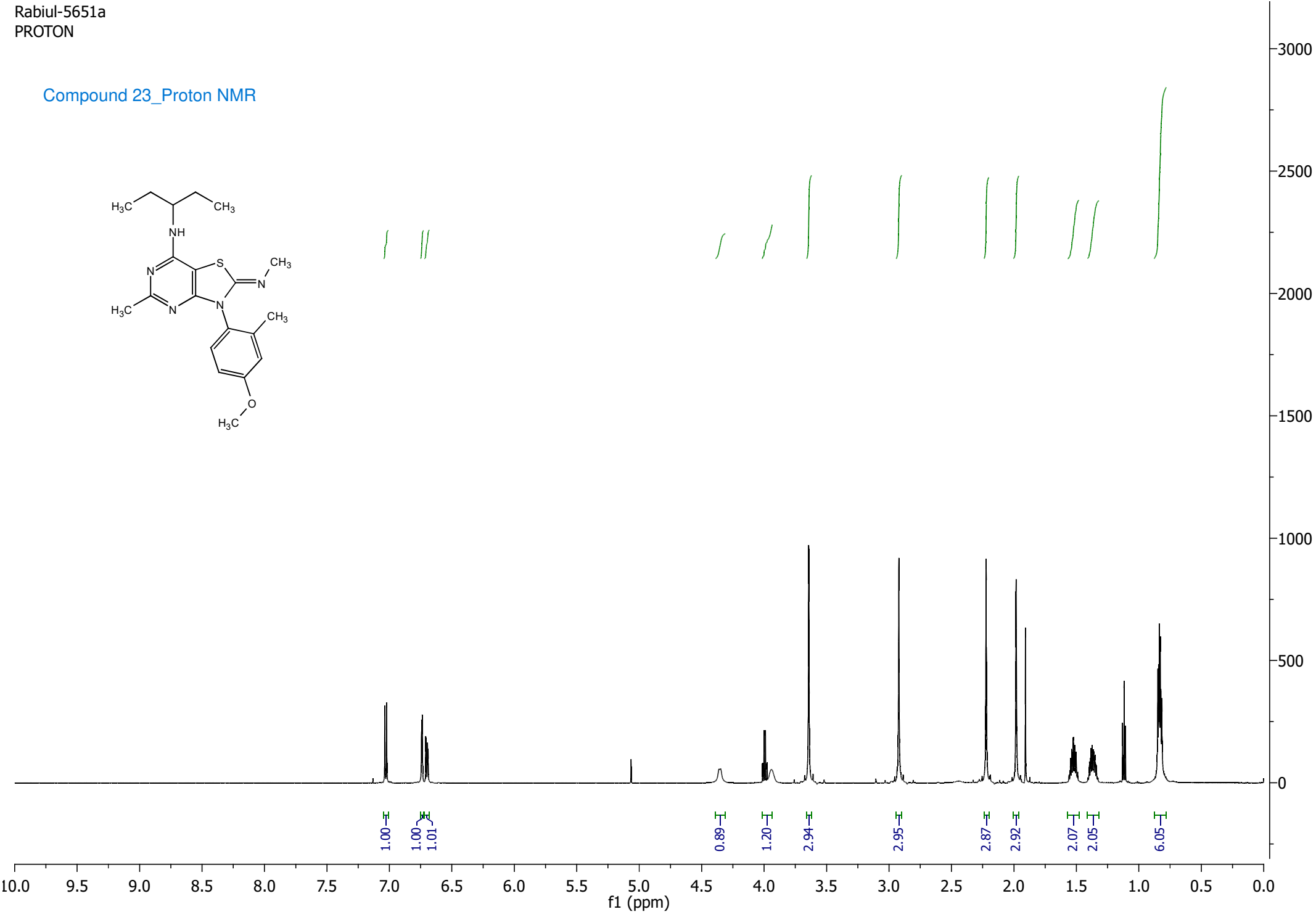
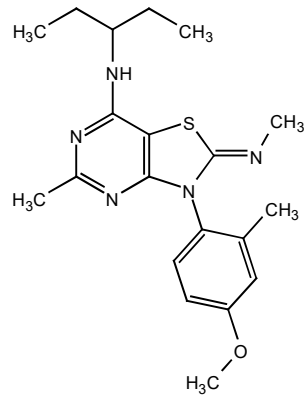
Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	412.217566	1	C22H30N5OS	100.00	412.216558	-2.4	-2.5	7.1	10.5	even		ok
M+Na	434.199303	1	C22H29N5NaOS	100.00	434.198502	-1.8	-1.9	6.0	10.5	even		ok

Rabiul-5651a
PROTON

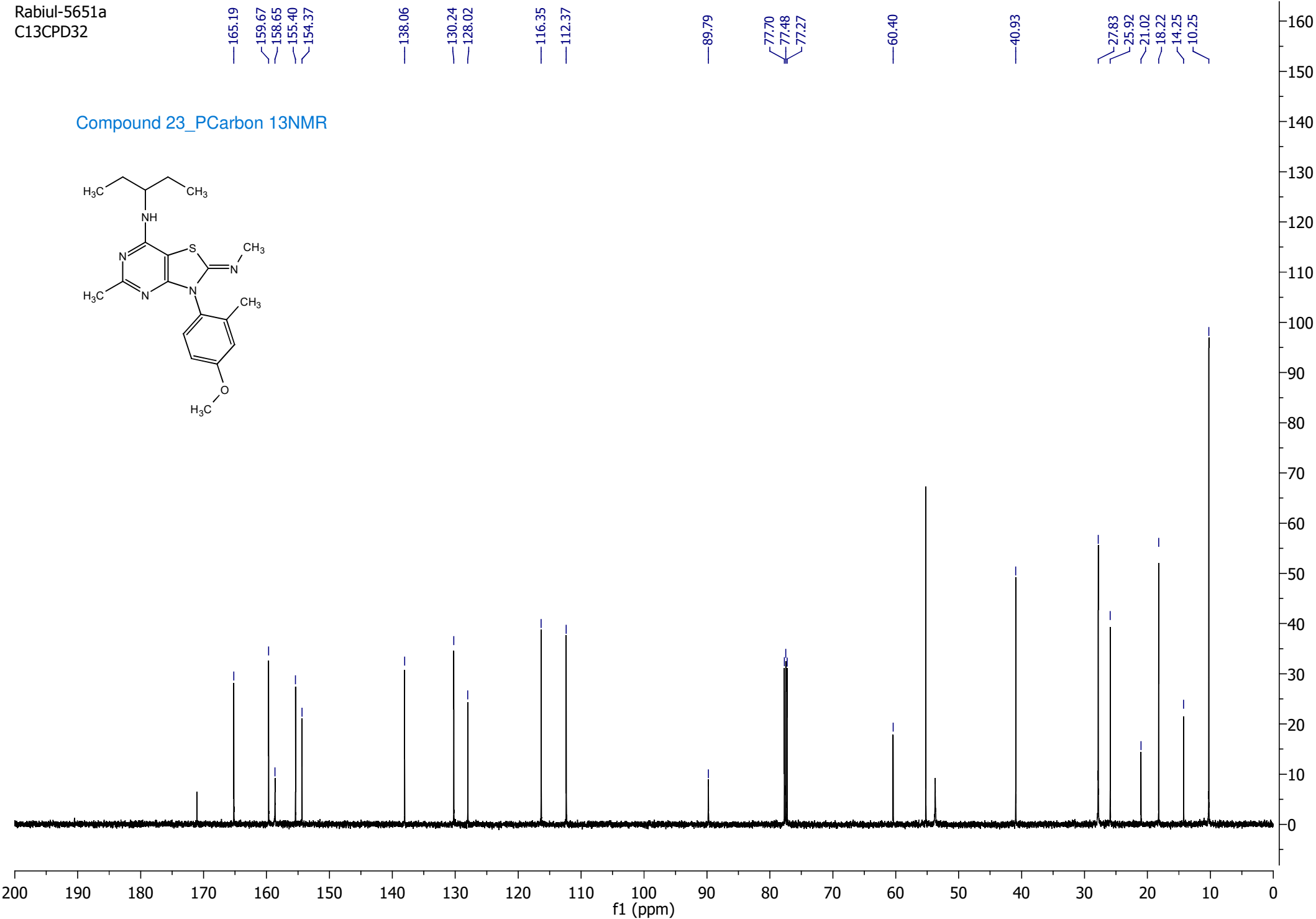
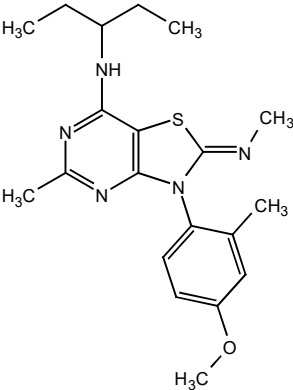
Compound 23_Proton NMR



Rabiul-5651a
C13CPD32



Compound 23_PC



UB Mass Spectrometry Facility - SmartFormula Report

Analysis Info

Analysis Name D:\Data\IC_3-21-19\5651a_000001.d
Method Bruker_11052015
Sample Name 5651a
Comment

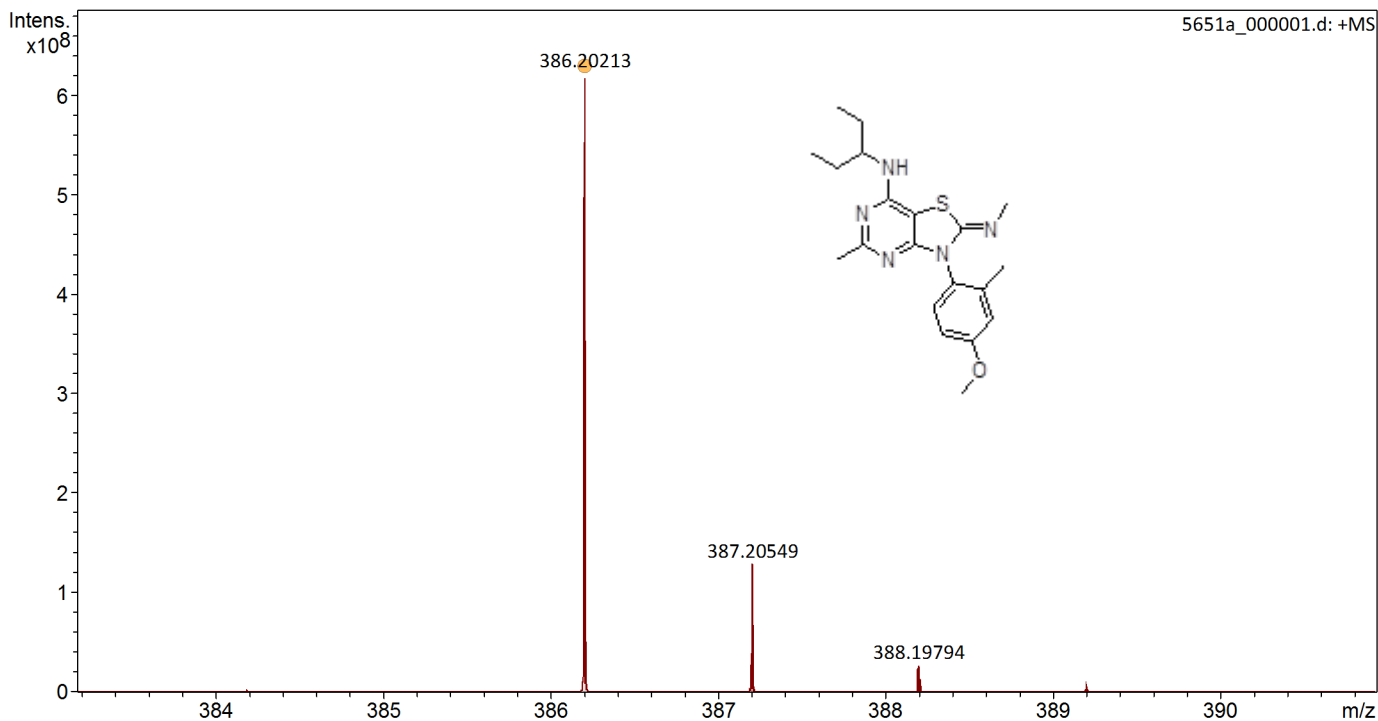
Acquisition Date 3/21/2019 7:16:36 PM

Operator
Instrument solariX

Acquisition Parameters

Acquisition Mode Single MS
Polarity Positive
Broadband Low Mass 147.4 m/z
Broadband High Mass 1500.0 m/z
Time of Flight to Detector 0.001 sec
Ion Accumulation Time 0.100 sec
Acquired Scans 20
Capillary 6000.0 V

Nebulizer gas flow rate 1.2 bar
Drying Gas Temperature 180.0 °C
Drying Gas Flow Rate 4.2 L/min
Calibration Date Thu Sep 27 10:56:48 2018
Data Acquisition Size 1048576
Data Processing Size (SI) 2097152
Apodization Full-Sine



Adduct	Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
M+H	386.202134	1	C ₂₀ H ₂₈ N ₅ OS	100.00	386.200908	-3.2	437.7	14.4	9.5	even		ok
M+Na	408.183871	1	C ₂₀ H ₂₇ N ₅ NaOS	100.00	408.182852	-2.5	414.5	14.4	9.5	even		ok