Supplementary Material

Anticancer Potential of Some Imidazole and Fused Imidazole Derivatives: Exploring mechanism via Epidermal Growth Factor Receptor (EGFR) Inhibition

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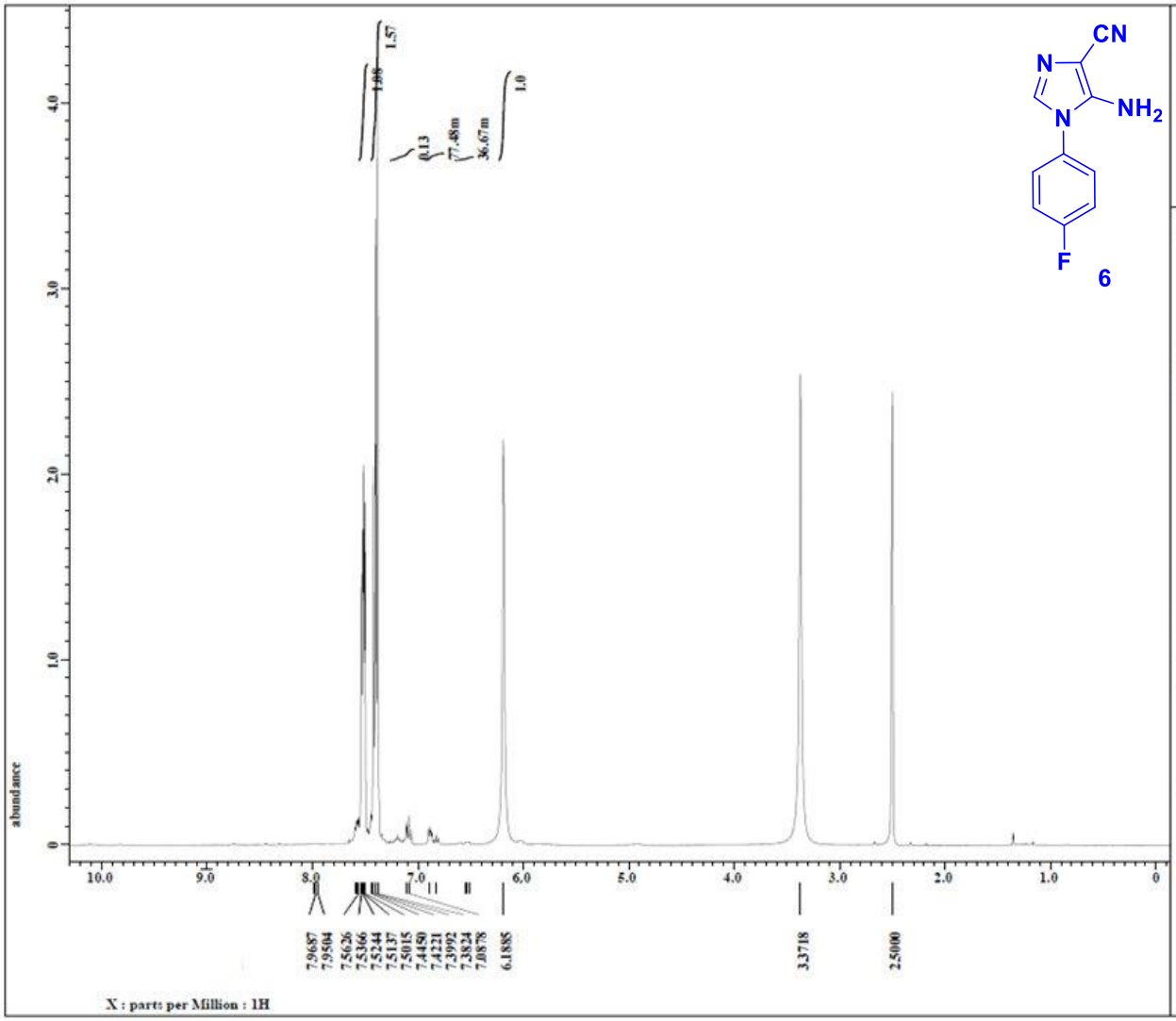
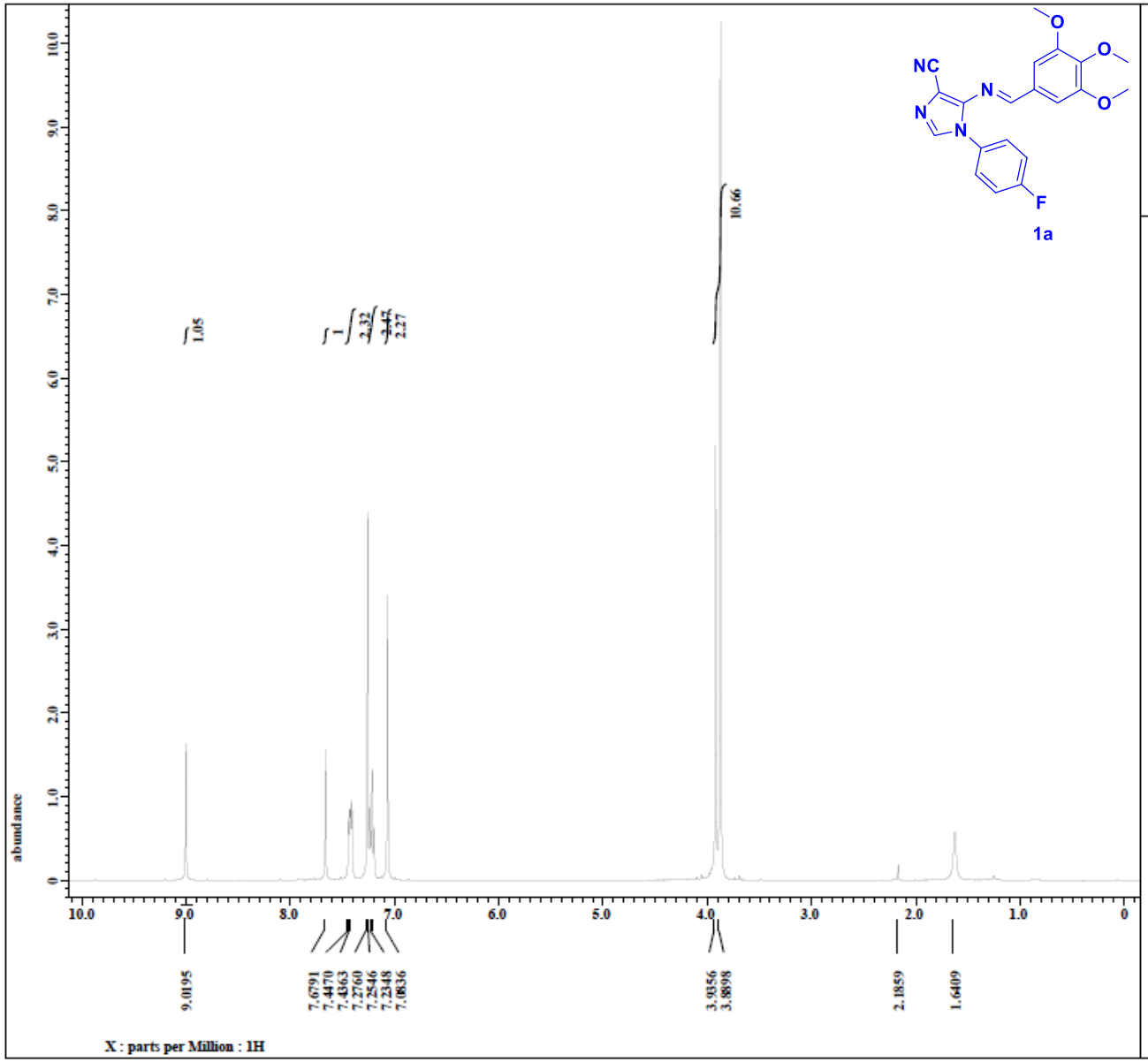
Spectra for representative compounds

Data ^{1}H , ^{13}C NMR, and HRMS

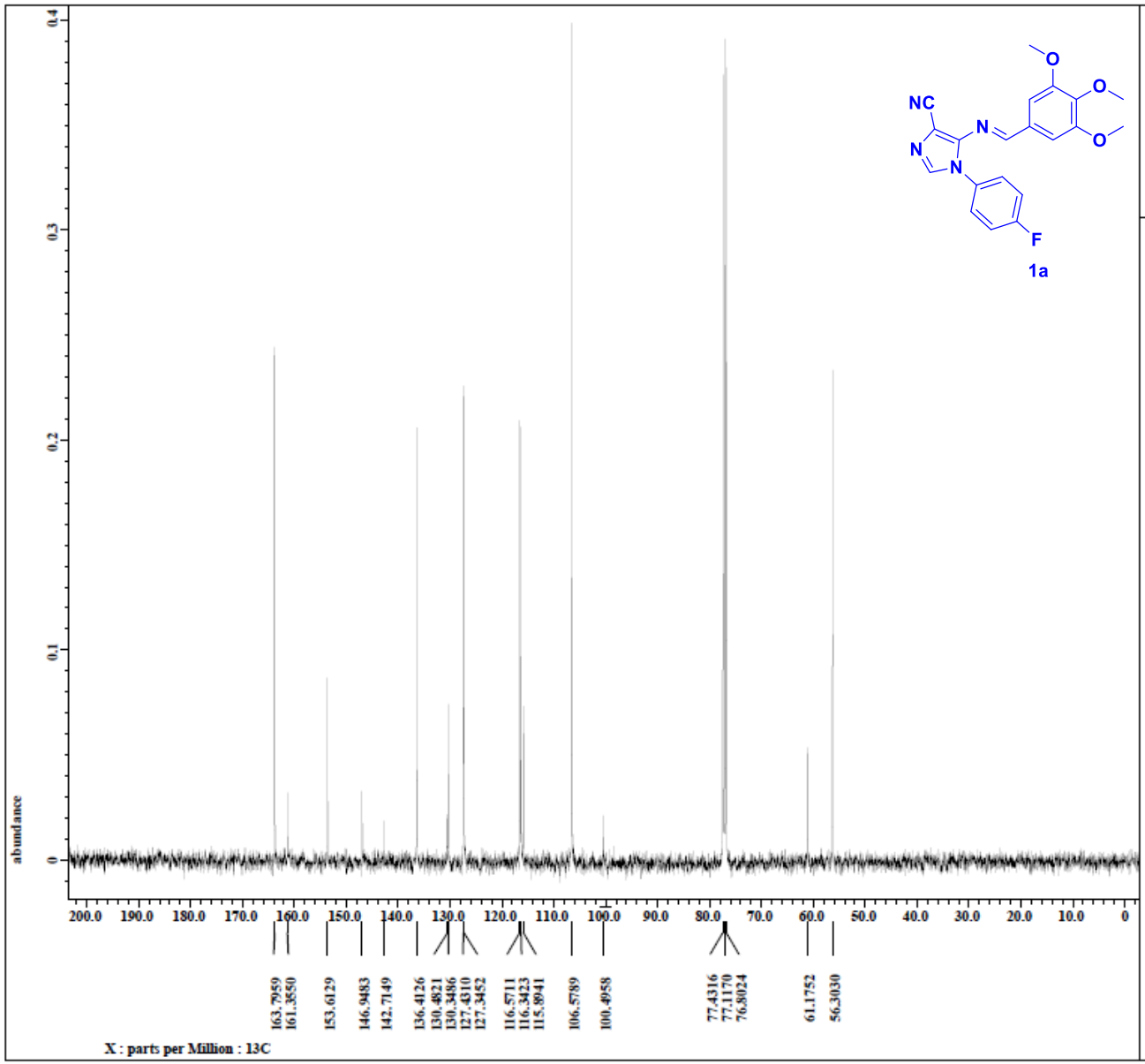



```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: SRK-1CU_PB_PROTON-1.jdf

Filename          = SRK-1CU_PB_PROTON-4.j
Author            = delta
Experiment        = single_pulse.ex2
Sample_id         = Z:\\SRK-1CU_PB
Solvent           = DMSO-D6
Creation_time     = 16-OCT-2016 17:12:11
Revision_time     = 16-OCT-2016 13:48:03
Current_time      = 16-OCT-2016 13:48:15

Comment           = Z:\\SRK-1CU_PB
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_strength    = 9.389766[T]  (400[MHz]
X_acq_duration    = 1.6384[s]
X_domain          = 1H
X_freq            = 399.78219838[MHz]
X_offset          = 9.0[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.61035156[Hz]
X_sweep           = 10[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 399.78219838[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 32
Total_scans       = 32

X_90_width        = 10.4214[us]
X_acq_time        = 1.6384[s]
X_angle           = 45[deg]
X_atn             = 0.4[dB]
X_pulse           = 5.2107[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 34
Relaxation_delay  = 2[s]
Repetition_time   = 3.6384[s]
Temp_get          = 19.4[dc]
```




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: A1_CU_PB_PROTON-1.jdf
```

Pilename	A1_CU_PB_PROTON-3.jdf
Author	delta
Experiment	single_pulse.ex2
Sample_id	Z:\\A1_CU_PB
Solvent	CHLOROFORM-D
Creation_time	17-OCT-2016 17:19:00
Revision_time	17-OCT-2016 14:39:58
Current_time	17-OCT-2016 14:40:09
Comment	Z:\\A1_CU_PB
Data_format	1D COMPLEX
Dim_size	13107
Dim_title	1H
Dim_units	[ppm]
Dimensions	X
Site	BCS 400
Spectrometer	JNM-BCS400
Field_strength	9.389766[T] (400[MHz]
X_acq_duration	1.6384[s]
X_domain	1H
X_freq	399.78219838[MHz]
X_offset	9.0[ppm]
X_points	16384
X_prescans	1
X_resolution	0.61035156[Hz]
X_sweep	10[kHz]
Irr_domain	1H
Irr_freq	399.78219838[MHz]
Irr_offset	5[ppm]
Tri_domain	1H
Tri_freq	399.78219838[MHz]
Tri_offset	5[ppm]
Clipped	FALSE
Mod_return	1
Scans	32
Total_scans	32
X_90_width	10.4214[us]
X_acq_time	1.6384[s]
X_angle	45[deg]
X_atn	0.4[dB]
X_pulse	5.2107[us]
Irr_mode	Off
Tri_mode	Off
Dante_presat	FALSE
Initial_wait	1[s]
Recvr_gain	42
Relaxation_delay	2[s]
Repetition_time	3.6384[s]
Temp_get	20.4[dC]




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: A1 CU PB  13C-1.jdf
```

Pilename	- A1 CU PB 13C-3.jdf
Author	- delta
Experiment	- single_pulse_dec
Sample_id	- Z:\\A1 CU PB 13C
Solvent	- CHLOROFORM-D
Creation_time	- 15-JUL-2017 06:56:21
Revision_time	- 15-JUL-2017 17:17:38
Current_time	- 15-JUL-2017 17:17:58
Comment	- single pulse decouple
Data_format	- 1D COMPLEX
Dim_size	- 26214
Dim_title	- 13C
Dim_units	- [ppm]
Dimensions	- X
Site	- ECS 400
Spectrometer	- JNM-ECS400
Field_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.04333312[s]
X_domain	- 13C
X_freq	- 100.52530333[MHz]
X_offset	- 100[ppm]
X_points	- 32768
X_prescans	- 4
X_resolution	- 0.95846665[Hz]
X_sweep	- 31.40703518[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 1000
Total_scans	- 1000
X_90_width	- 7.82792[us]
X_acq_time	- 1.04333312[s]
X_angle	- 90[deg]
X_atn	- 4.2[dB]
X_pulse	- 7.82792[us]
Irr_atn_dec	- 21.399[dB]
Irr_atn_noe	- 21.399[dB]
Irr_noise	- WALTZ
Decoupling	- TRUE
Initial_wait	- 1[s]
Noe	- TRUE
Noe_time	- 2[s]
Recvr_gain	- 60
Relaxation_delay	- 2[s]
Repetition_time	- 3.04333312[s]
Temp_get	- 19.9[dC]

Elemental Composition Report

Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

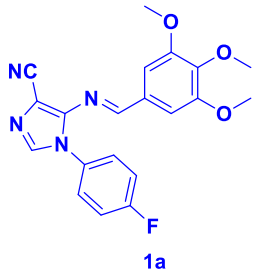
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-25 H: 11-30 N: 0-4 O: 0-3 F: 0-1

Sample Name : A-1
Test Name : HRMS-1
160120-A-1 17 (0.174)

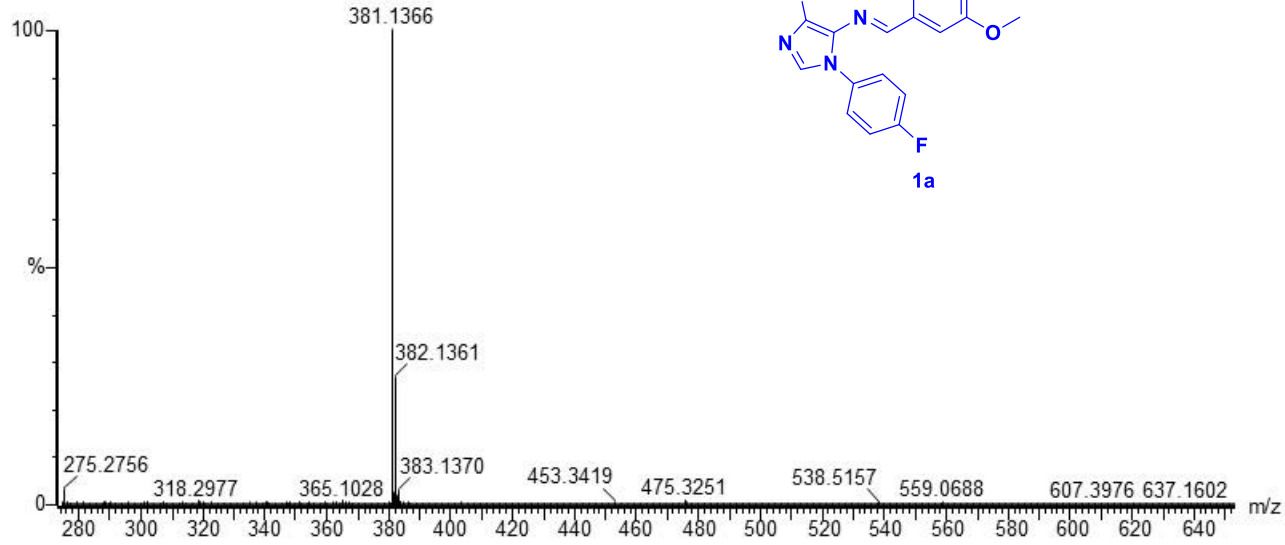
IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
2.77e+007

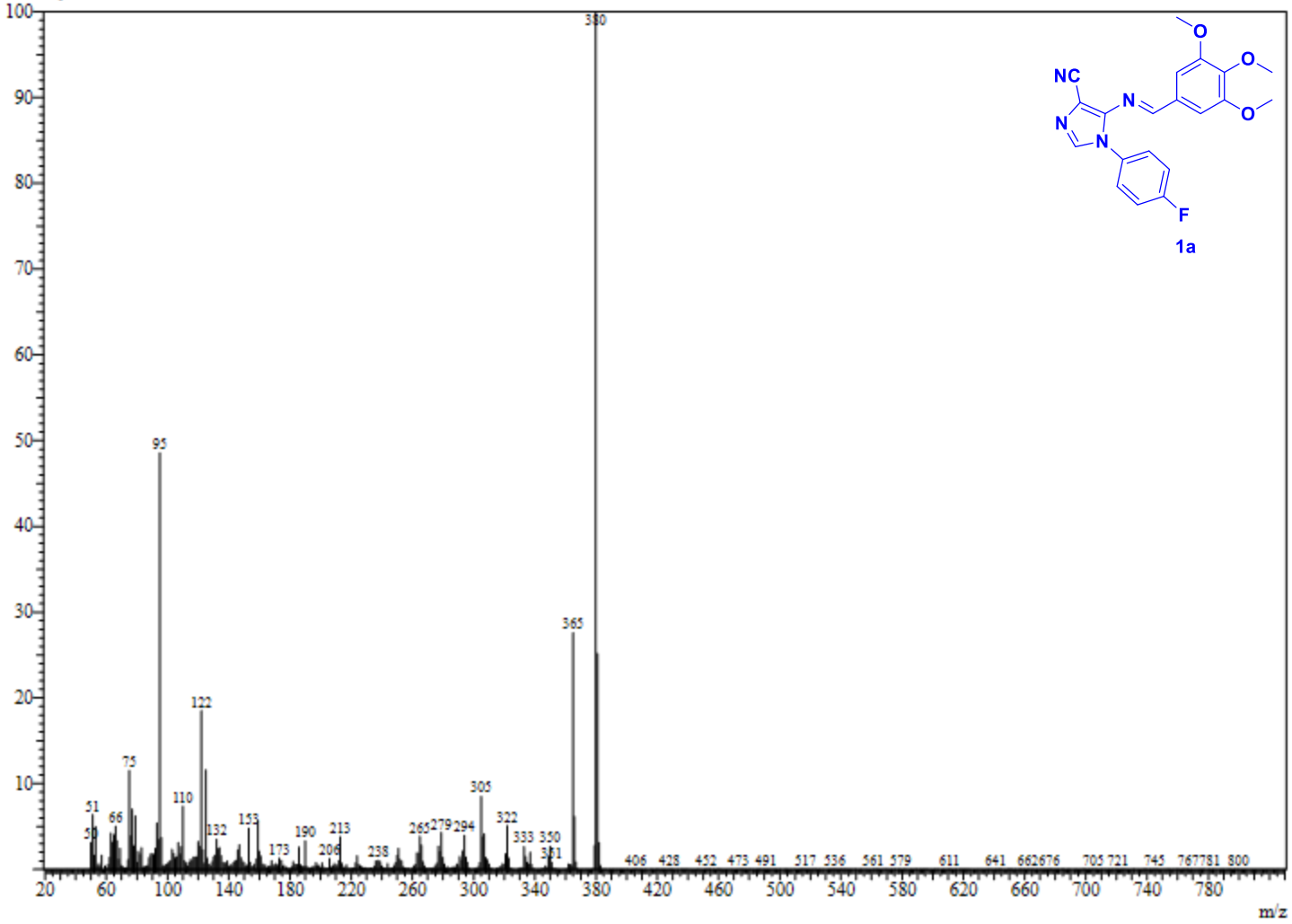


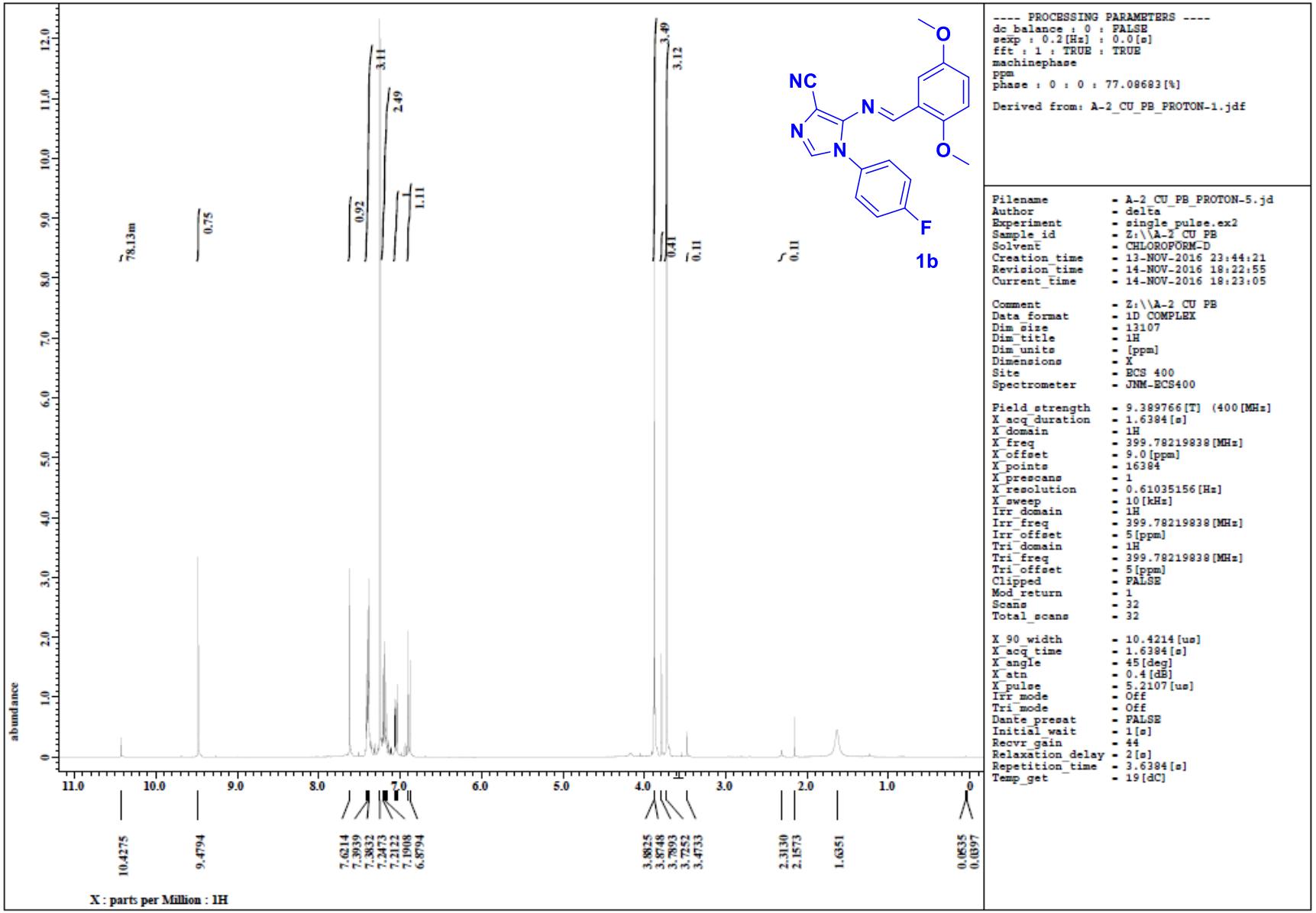
1a



Minimum:				-1.5				
Maximum:		5.0	3.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
381.1366	381.1363	0.3	0.8	13.5	1449.5	n/a	n/a	C20 H18 N4 O3 F

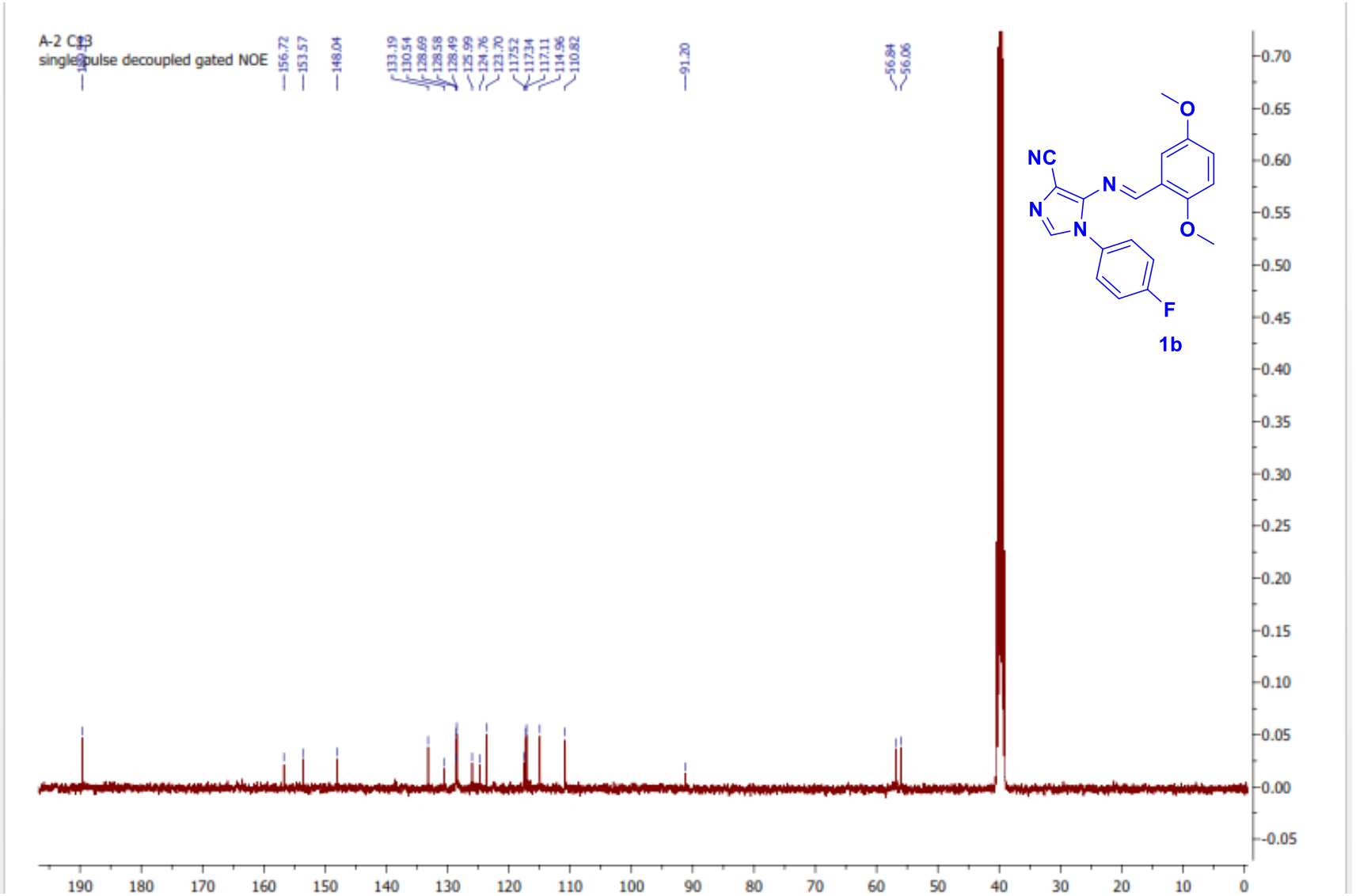
Line#:1 R.Time:4.860(Scan#:673)
MassPeaks:541
RawMode:Averaged 4.855-4.865(672-674) BasePeak:380(492565)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 77.08683[%]

Derived from: A-2_CU_PB_PROTON-1.jdf
```

Pilename	- A-2_CU_PB_PROTON-5.jd
Author	- delta
Experiment	- single_pulse.ex2
Sample_id	- Z:\\A-2_CU_PB
Solvent	- CHLOROPORM-D
Creation_time	- 13-NOV-2016 23:44:21
Revision_time	- 14-NOV-2016 18:22:55
Current_time	- 14-NOV-2016 18:23:05
Comment	- Z:\\A-2_CU_PB
Data_format	- 1D COMPLEX
Dim_size	- 13107
Dim_title	- 1H
Dim_units	- [ppm]
Dimensions	- X
Site	- BCS 400
Spectrometer	- JNM-ECS400
Pield_strength	- 9.389766[T] (400[MHz]
X_acq_duration	- 1.6384[s]
X_domain	- 1H
X_freq	- 399.78219838[MHz]
X_offset	- 9.0[ppm]
X_points	- 16384
X_prescans	- 1
X_resolution	- 0.61035156[Hz]
X_sweep	- 10[kHz]
Irr_domain	- 1H
Irr_freq	- 399.78219838[MHz]
Irr_offset	- 5[ppm]
Tri_domain	- 1H
Tri_freq	- 399.78219838[MHz]
Tri_offset	- 5[ppm]
Clipped	- FALSE
Mod_return	- 1
Scans	- 32
Total_scans	- 32
X_90_width	- 10.4214[us]
X_acq_time	- 1.6384[s]
X_angle	- 45[deg]
X_atn	- 0.4[dB]
X_pulse	- 5.2107[us]
Irr_mode	- Off
Tri_mode	- Off
Dante_presat	- FALSE
Initial_wait	- 1[s]
Recvr_gain	- 44
Relaxation_delay	- 2[s]
Repetition_time	- 3.6384[s]
Temp_get	- 19[dC]


A-2 C13
single pulse decoupled gated NOE
156.72
153.57
148.04
133.19
130.54
128.69
128.58
128.49
125.99
124.76
123.70
117.52
117.34
117.11
114.96
110.82
91.20
56.84
56.06
NC
N
N
N
O
O
F
1b

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

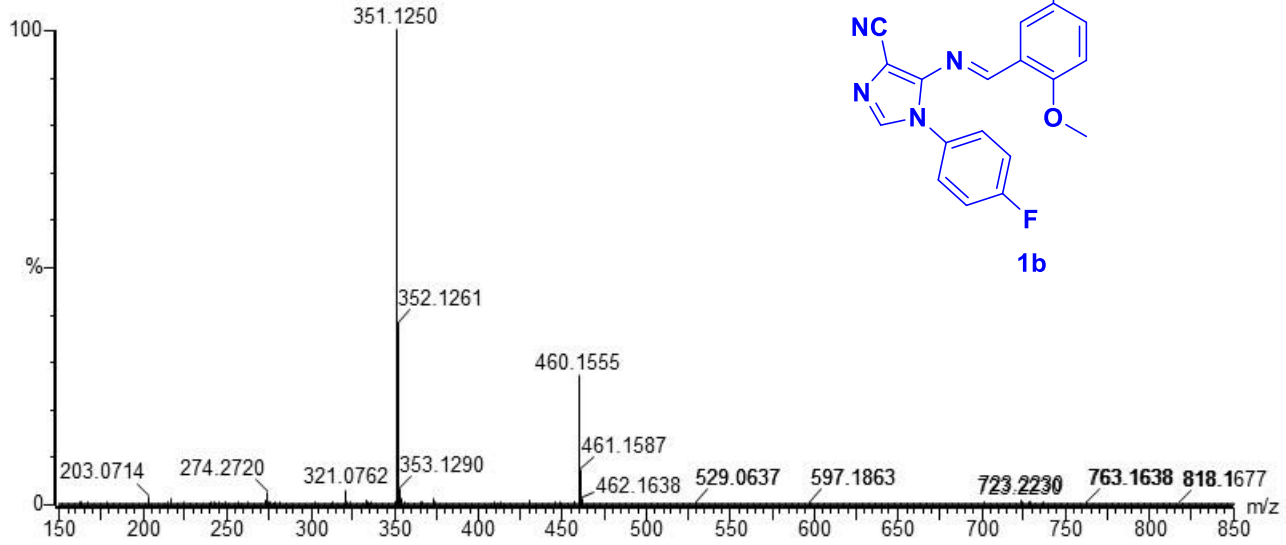
Monoisotopic Mass, Even Electron Ions
39 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-21 H: 8-25 N: 0-5 O: 0-3 F: 0-1

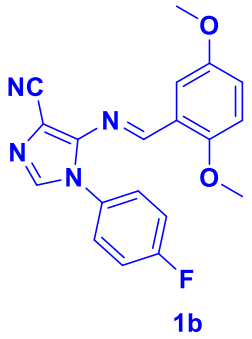
Sample Name : A-2
Test Name : HRMS-1
160120-A-2- 16 (0.165)

IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
4.44e+007

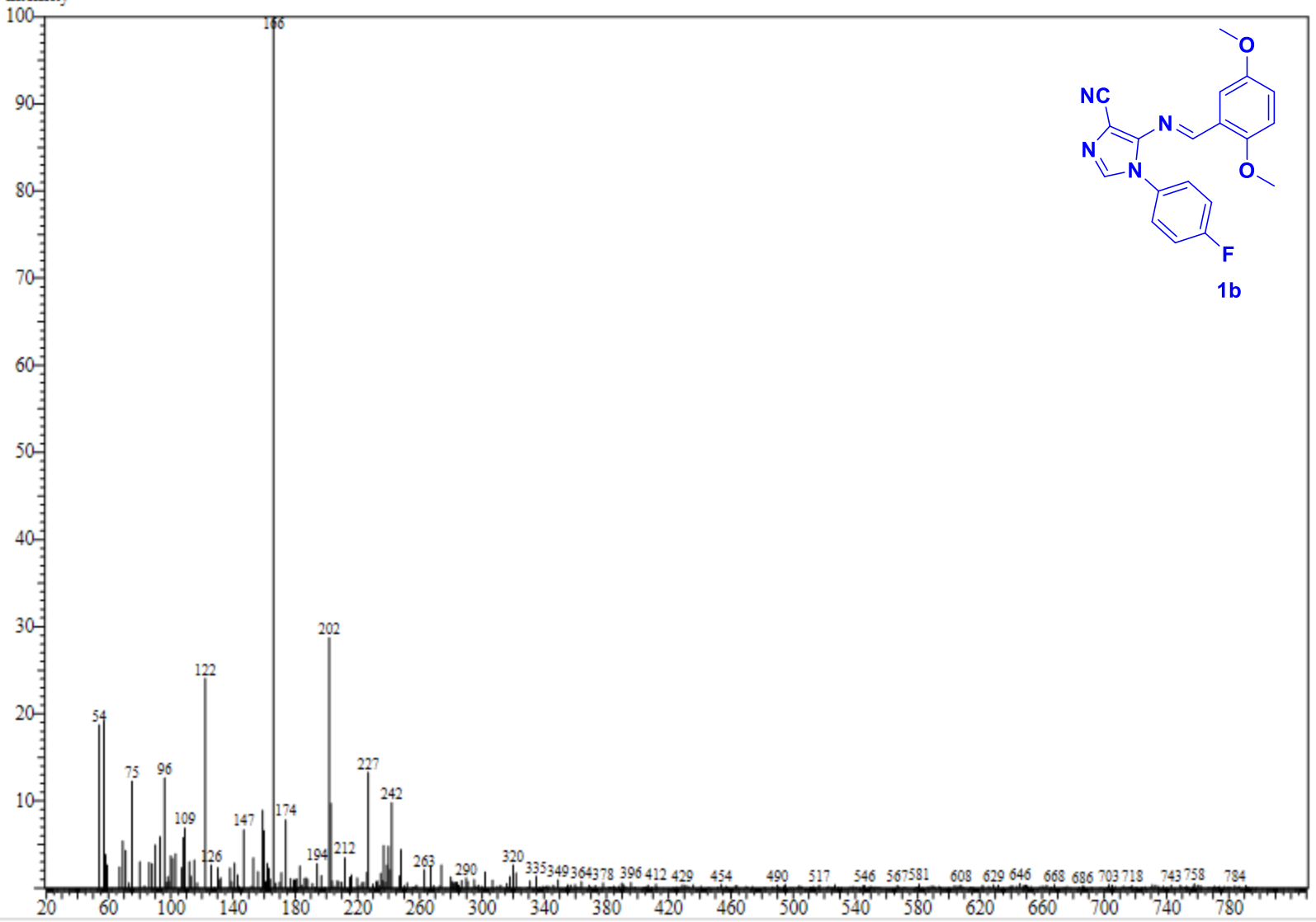


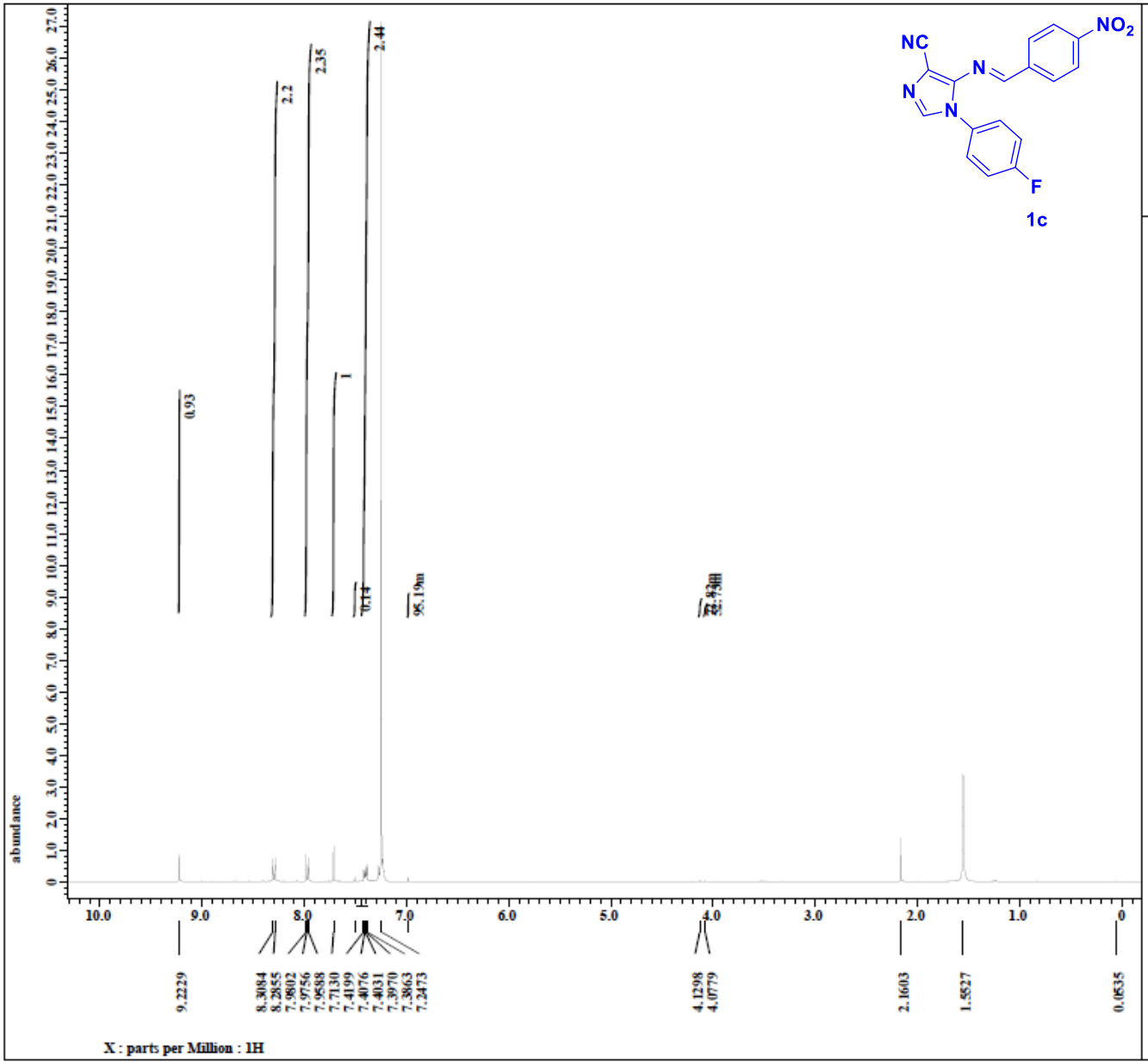


1b

Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
351.1250	351.1257	-0.7	-2.0	13.5	1726.8	n/a	n/a	C19 H16 N4 O2 F

Line#:1 R.Time:4.000(Scan#:501)
MassPeaks:336
RawMode:Averaged 4.000-4.005(501-502) BasePeak:166(3373)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.3[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 57.82848[%]
phase : 0.75 : -7 : 57.82848[%]
phase : 1 : 0 : 57.82848[%]

Derived from: A-3_CU_PB_PROTON-1.jdf
```

```
Pilename          - A-3_CU_PB_PROTON-7.jd
Author            - delta
Experiment        - single_pulse.ex2
Sample_id         - Z:\\A-3_CU_PB
Solvent           - CHLOROFORM-D
Creation_time     - 13-NOV-2016 23:33:43
Revision_time     - 14-NOV-2016 18:38:51
Current_time      - 14-NOV-2016 18:38:57

Comment           - Z:\\A-3_CU_PB
Data_format       - 1D COMPLEX
Dim_size          - 13107
Dim_title         - 1H
Dim_units         - [ppm]
Dimensions        - X
Site              - ECS 400
Spectrometer      - JNM-ECS400

Field_strength    - 9.389766[T] (400[MHz]
X_acq_duration    - 1.6384[s]
X_domain          - 1H
X_freq            - 399.78219838[MHz]
X_offset          - 9.0[ppm]
X_points          - 16384
X_prescans        - 1
X_resolution      - 0.61035156[Hz]
X_sweep           - 10[kHz]
Irr_domain        - 1H
Irr_freq          - 399.78219838[MHz]
Irr_offset        - 5[ppm]
Tri_domain        - 1H
Tri_freq          - 399.78219838[MHz]
Tri_offset        - 5[ppm]
Clipped           - FALSE
Mod_return        - 1
Scans             - 32
Total_scans       - 32

X_90_width        - 10.4214[us]
X_acq_time        - 1.6384[s]
X_angle           - 45[deg]
X_atn             - 0.4[dB]
X_pulse           - 5.2107[us]
Irr_mode          - Off
Tri_mode          - Off
Dante_presat      - FALSE
Initial_wait      - 1[s]
Recvr_gain        - 50
Relaxation_delay  - 2[s]
Repetition_time   - 3.6384[s]
Temp_get          - 19.2[dC]
```

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

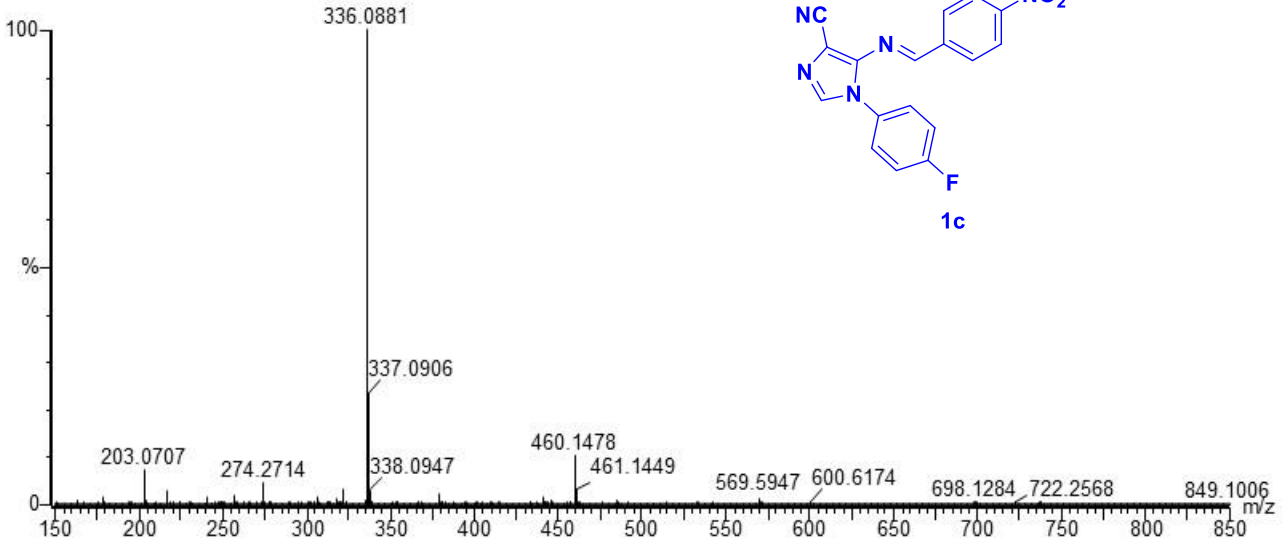
Monoisotopic Mass, Even Electron Ions
52 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-21 H: 11-30 N: 0-5 O: 0-3 F: 0-1

Sample Name : A-3
Test Name : HRMS-1
160120-A-3 14 (0.148)

IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
4.81e+007

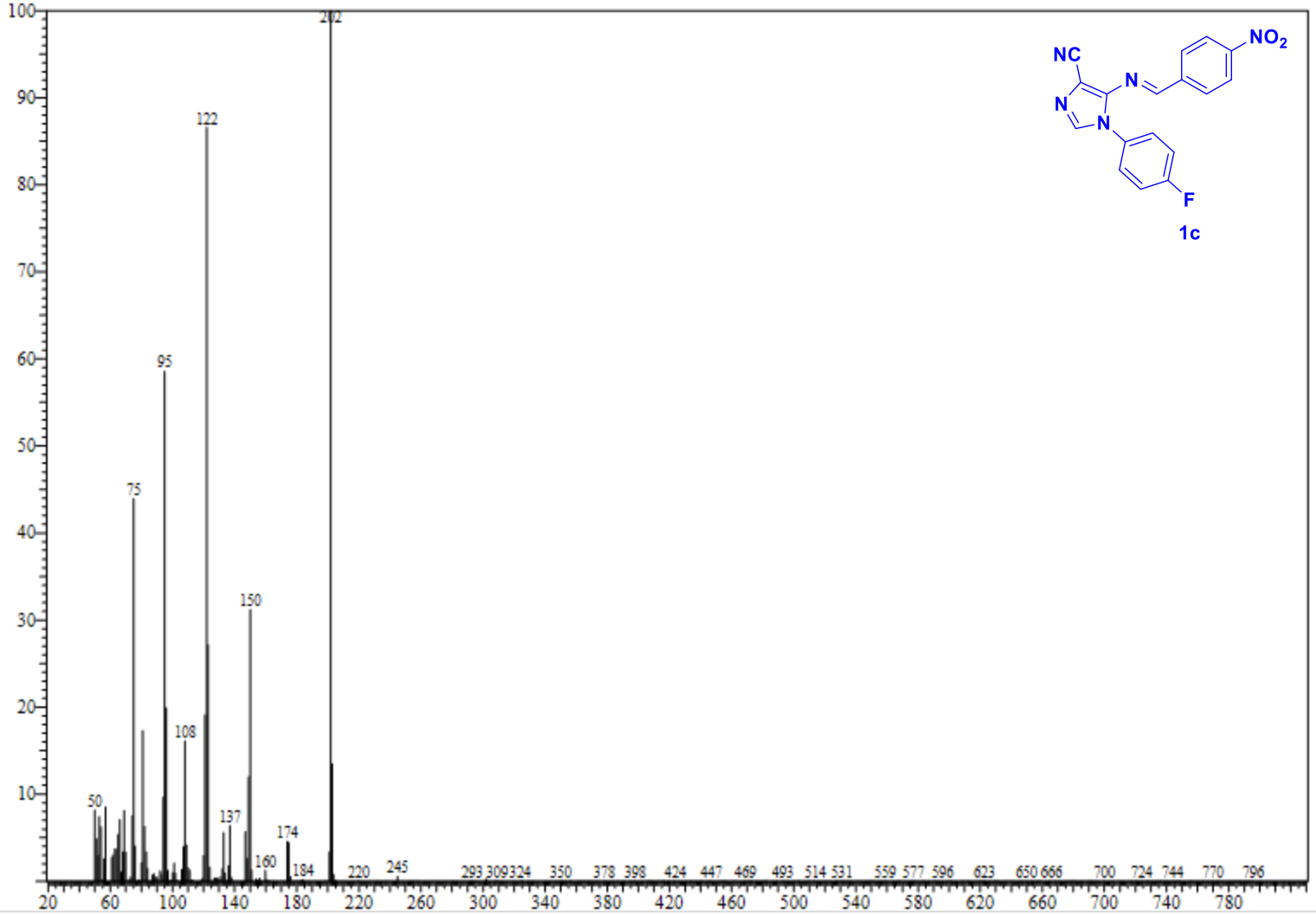


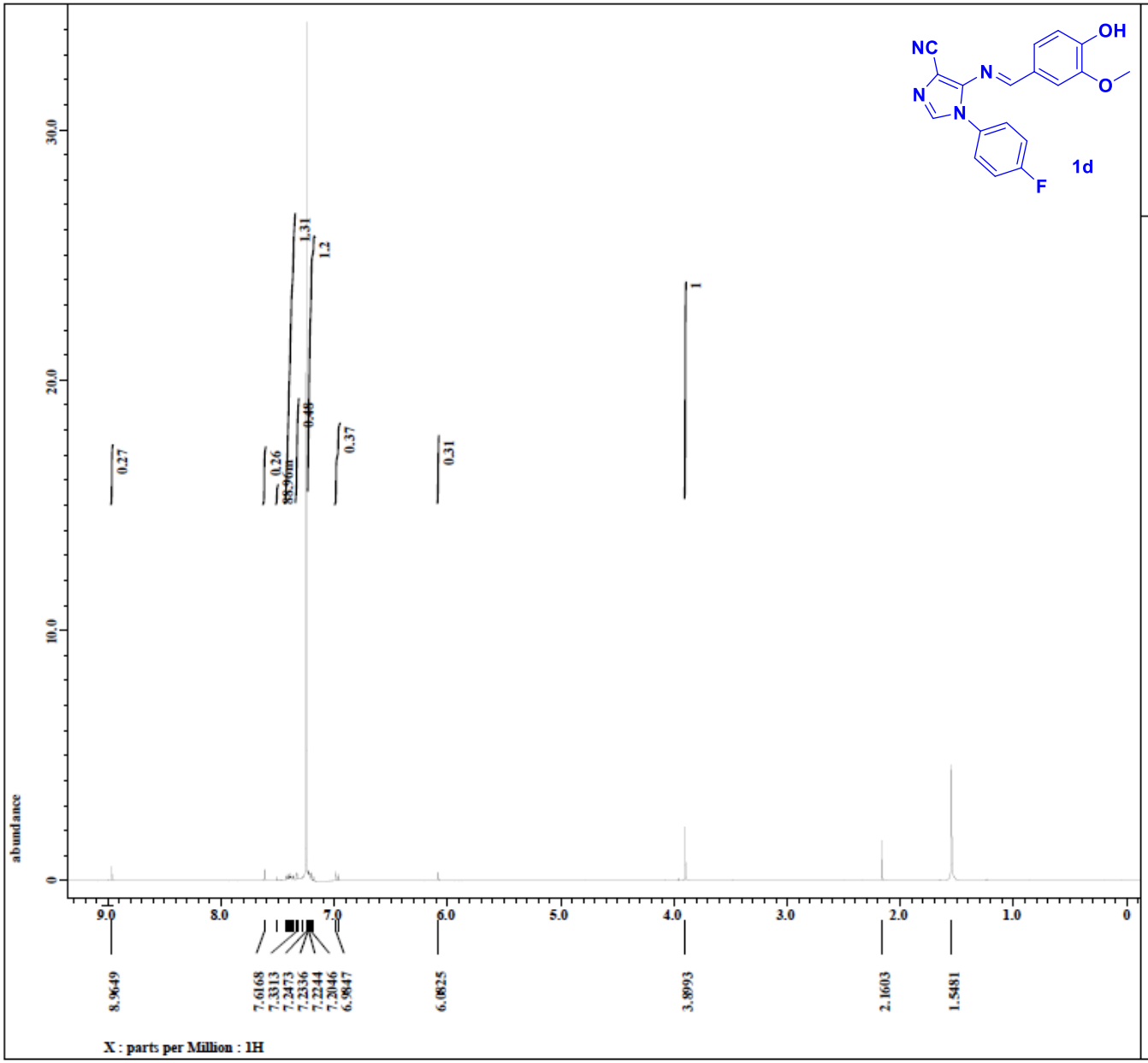
1c

Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
336.0881	336.0897	-1.6	-4.8	14.5	1585.4	n/a	n/a	C17 H11 N5 O2 F

x

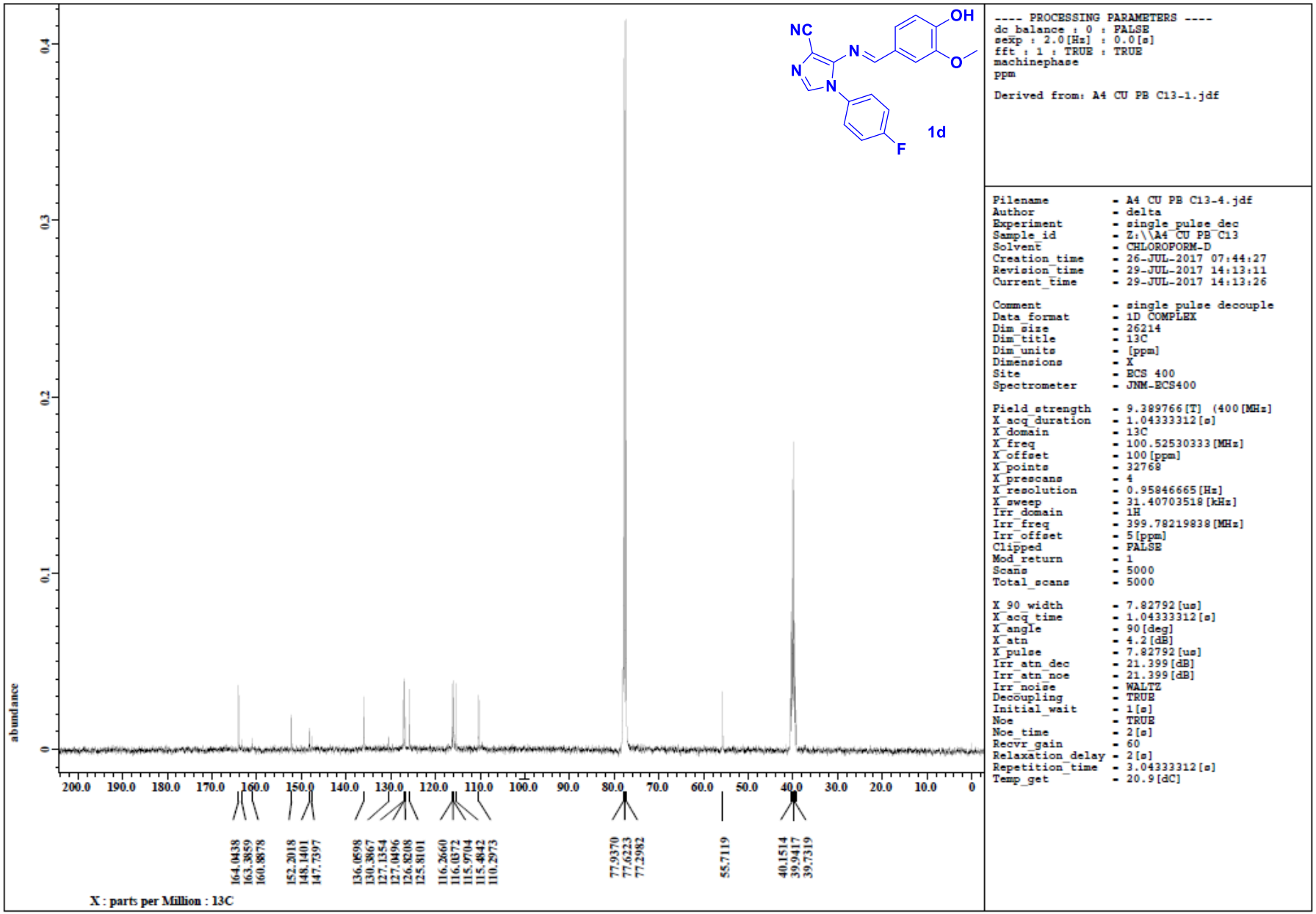
Line#:1 R.Time:3.420(Scan#:385)
MassPeaks:365
RawMode:Averaged 3.415-3.425(384-386) BasePeak:202(290256)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: A-4_CU_PB_PROTON-1.jdf
```

```
Pilename          - A-4_CU_PB_PROTON-4.jd
Author            - delta
Experiment        - single_pulse.ex2
Sample_id         - Z:\\A-4_CU_PB
Solvent           - CHLOROFORM-D
Creation_time     - 13-NOV-2016 23:23:38
Revision_time     - 14-NOV-2016 18:50:02
Current_time      - 14-NOV-2016 18:50:16

Comment           - Z:\\A-4_CU_PB
Data_format       - 1D COMPLEX
Dim_size          - 13107
Dim_title         - 1H
Dim_units         - [ppm]
Dimensions        - X
Site              - BCS 400
Spectrometer      - JNM-ECS400

Field_strength    - 9.389766[T] (400[MHz]
X_acq_duration    - 1.6384[s]
X_domain          - 1H
X_freq            - 399.78219838[MHz]
X_offset          - 9.0[ppm]
X_points          - 16384
X_prescans        - 1
X_resolution      - 0.61035156[Hz]
X_sweep           - 10[kHz]
Irr_domain        - 1H
Irr_freq          - 399.78219838[MHz]
Irr_offset        - 5[ppm]
Tri_domain        - 1H
Tri_freq          - 399.78219838[MHz]
Tri_offset        - 5[ppm]
Clipped           - FALSE
Mod_return        - 1
Scans             - 32
Total_scans       - 32

X_90_width        - 10.4214[us]
X_acq_time        - 1.6384[s]
X_angle           - 45[deg]
X_atn             - 0.4[dB]
X_pulse           - 5.2107[us]
Irr_mode          - Off
Tri_mode          - Off
Dante_presat      - FALSE
Initial_wait      - 1[s]
Recvr_gain        - 50
Relaxation_delay  - 2[s]
Repetition_time   - 3.6384[s]
Temp_get          - 19.1[dC]
```


NC
OH
N
N
N
O
F
1d
abundance
0.4
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
164.0438
163.3859
160.8878
152.2018
148.1401
147.7397
136.0898
130.3867
127.1354
127.0496
126.8208
125.8101
116.2660
116.0372
115.9704
115.4842
110.2973
77.9370
77.6223
77.2982
55.7119
40.1514
39.9417
39.7319
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: A4 CU PB C13-1.jdf
Pilename - A4 CU PB C13-4.jdf
Author - delta
Experiment - single_pulse_dec
Sample_id - Z:\\A4 CU PB C13
Solvent - CHLOROFORM-D
Creation_time - 26-JUL-2017 07:44:27
Revision_time - 29-JUL-2017 14:13:11
Current_time - 29-JUL-2017 14:13:26
Comment - single pulse decouple
Data_format - 1D COMPLEX
Dim_size - 26214
Dim_title - 13C
Dim_units - [ppm]
Dimensions - X
Site - ECS 400
Spectrometer - JNM-ECS400
Field_strength - 9.389766[T] (400[MHz]
X_acq_duration - 1.04333312[s]
X_domain - 13C
X_freq - 100.52530333[MHz]
X_offset - 100[ppm]
X_points - 32768
X_prescans - 4
X_resolution - 0.95846665[Hz]
X_sweep - 31.40703518[kHz]
Irr_domain - 1H
Irr_freq - 399.78219838[MHz]
Irr_offset - 5[ppm]
Clipped - FALSE
Mod_return - 1
Scans - 5000
Total_scans - 5000
X_90_width - 7.82792[us]
X_acq_time - 1.04333312[s]
X_angle - 90[deg]
X_atn - 4.2[dB]
X_pulse - 7.82792[us]
Irr_atn_dec - 21.399[dB]
Irr_atn_noe - 21.399[dB]
Irr_noise - WALTZ
Decoupling - TRUE
Initial_wait - 1[s]
Noe - TRUE
Noe_time - 2[s]
Recvr_gain - 60
Relaxation_delay - 2[s]
Repetition_time - 3.04333312[s]
Temp_get - 20.9[dC]

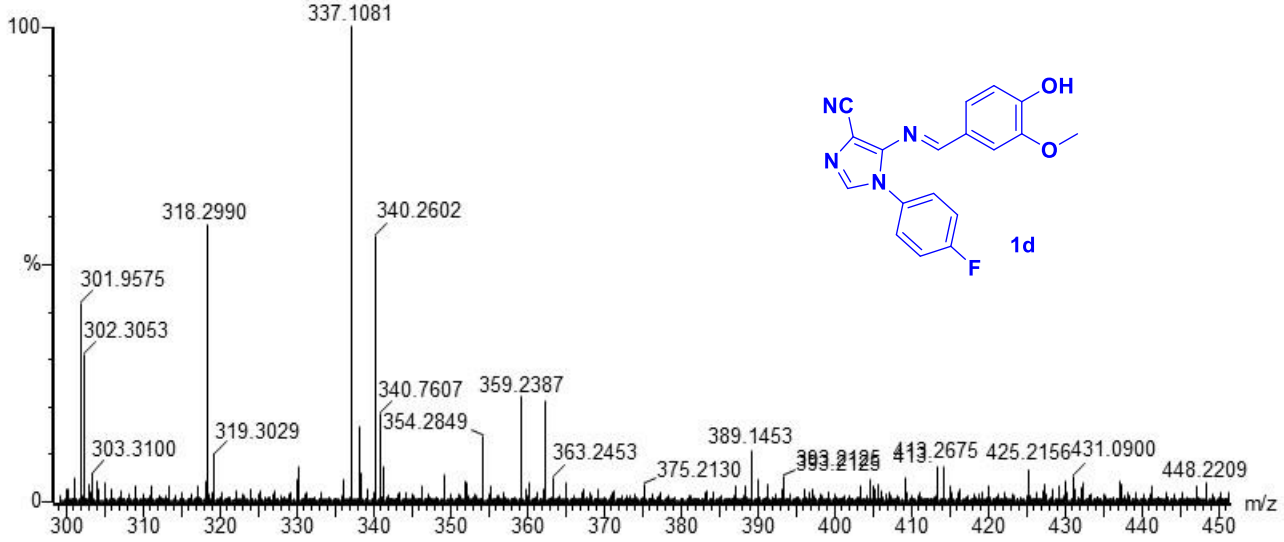
Elemental Composition Report

Single Mass Analysis

Tolerance = 6.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Odd and Even Electron Ions
46 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-20 H: 11-30 N: 0-5 O: 0-3 F: 0-1

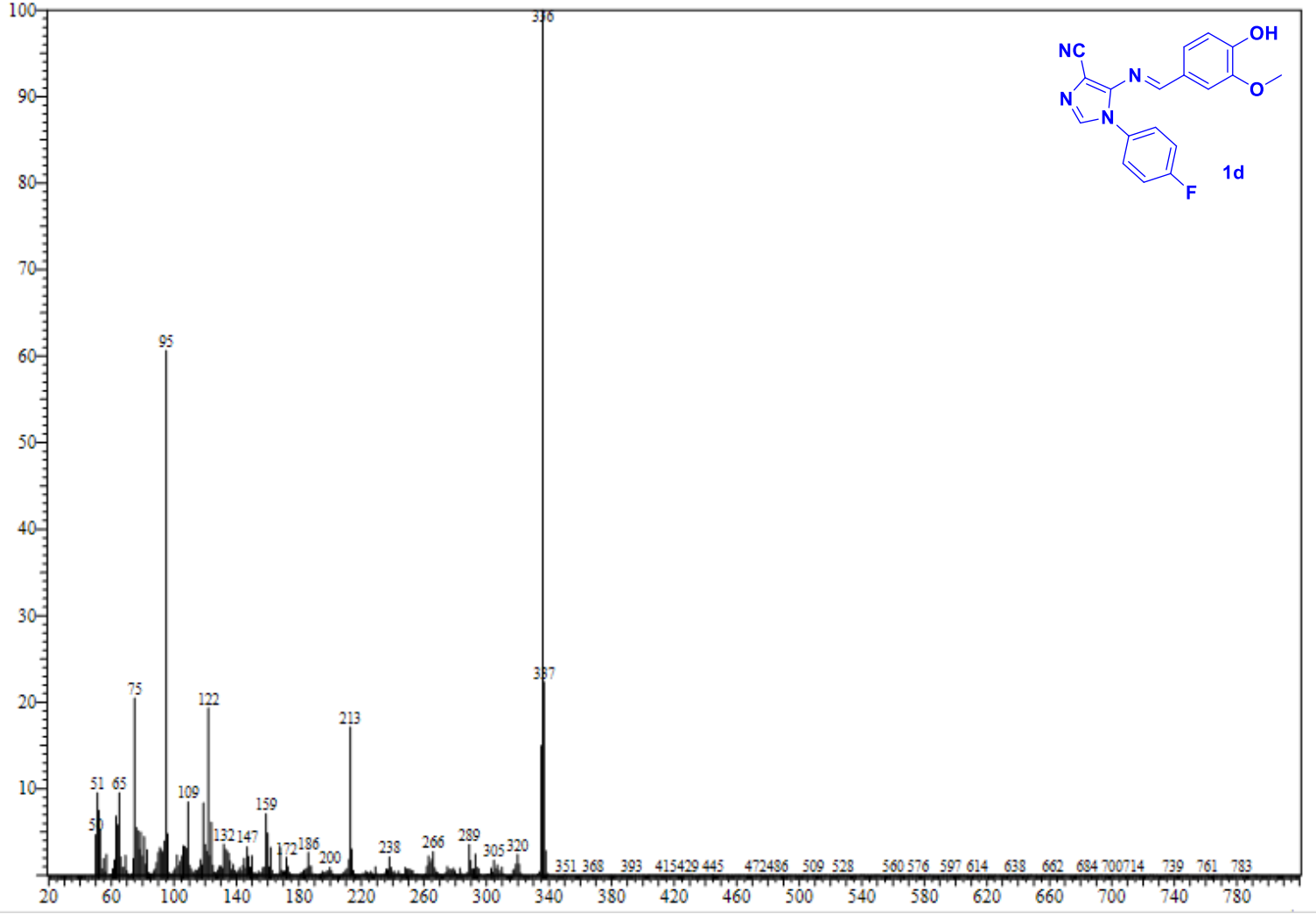
Sample Name : A-4 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
160120-A-4 16 (0.165) 1: TOF MS ES+
1.57e+005

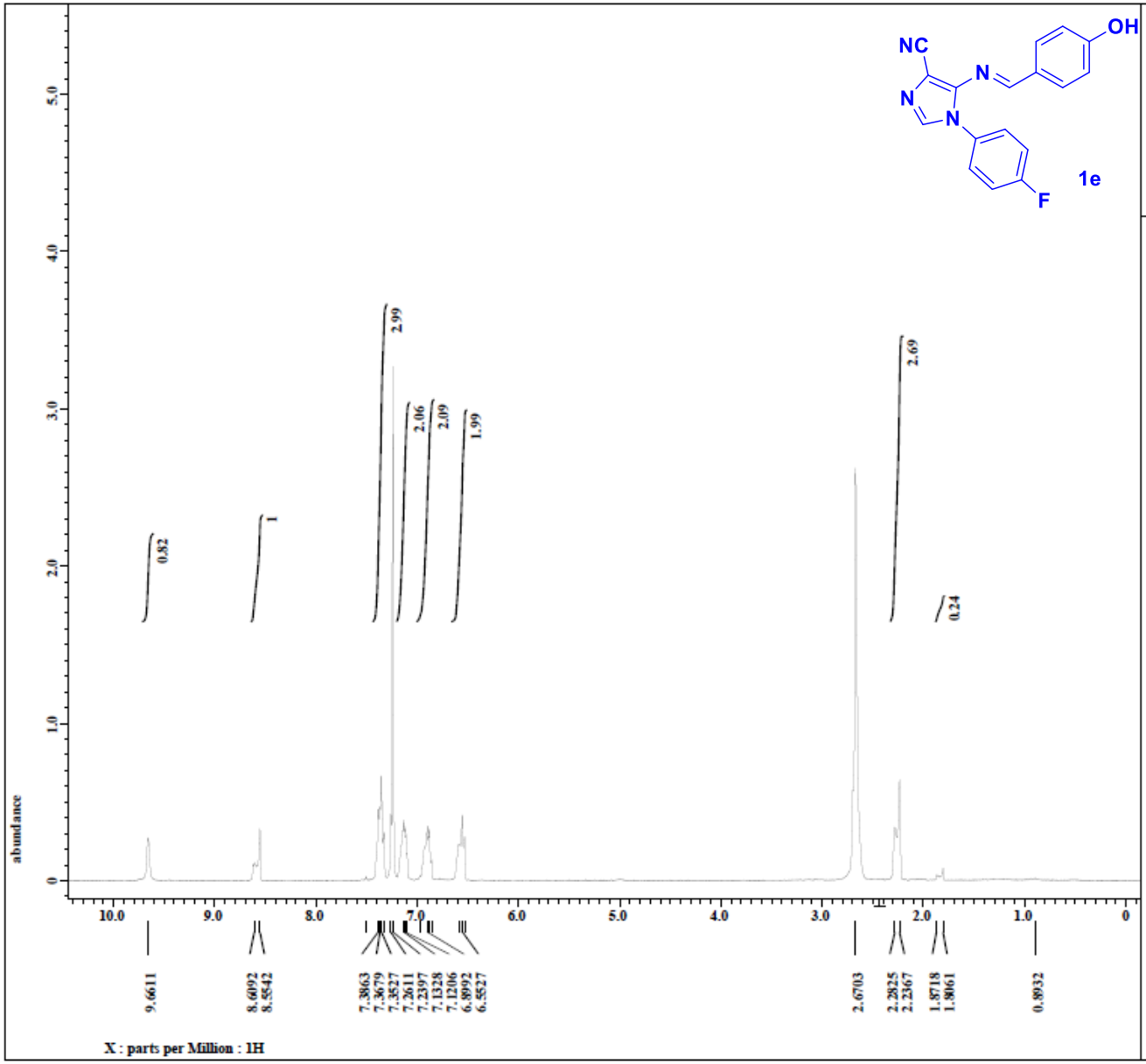


Minimum:				-1.5				
Maximum:		5.0	6.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
337.1081	337.1101	-2.0	-5.9	13.5	1087.3	n/a	n/a	C18 H14 N4 O2 F

Spectrum

Line#:1 R.Time:6.470(Scan#:995)
MassPeaks:582
RawMode:Averaged 6.465-6.475(994-996) BasePeak:336(1955400)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.5[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 50[%]
phase : 2 : -3 : 82.83992[%]

Derived from: A6_CU_PB_PROTON-1.jdf
```

```
Pilename            - A6_CU_PB_PROTON-6.jdf
Author              - delta
Experiment          - single_pulse.ex2
Sample_id           - Z:\\A6_CU_PB
Solvent             - CHLOROFORM-D
Creation_time       - 15-NOV-2016 14:43:45
Revision_time       - 15-NOV-2016 10:54:19
Current_time        - 15-NOV-2016 10:54:35

Comment             - Z:\\A6_CU_PB
Data_format         - 1D COMPLEX
Dim_size            - 13107
Dim_title           - 1H
Dim_units           - [ppm]
Dimensions          - X
Site                - BCS 400
Spectrometer        - JNM-ECS400

Field_strength      - 9.389766[T]  (400[MHz]
X_acq_duration      - 1.6384[s]
X_domain            - 1H
X_freq              - 399.78219838[MHz]
X_offset            - 9.0[ppm]
X_points            - 16384
X_prescans          - 1
X_resolution        - 0.61035156[Hz]
X_sweep             - 10[kHz]
Irr_domain          - 1H
Irr_freq            - 399.78219838[MHz]
Irr_offset          - 5[ppm]
Tri_domain          - 1H
Tri_freq            - 399.78219838[MHz]
Tri_offset          - 5[ppm]
Clipped             - FALSE
Mod_return          - 1
Scans               - 7
Total_scans         - 7

X_90_width          - 10.4214[us]
X_acq_time          - 1.6384[s]
X_angle             - 45[deg]
X_atn               - 0.4[dB]
X_pulse             - 5.2107[us]
Irr_mode            - Off
Tri_mode            - Off
Dante_presat        - FALSE
Initial_wait        - 1[s]
Recvr_gain          - 46
Relaxation_delay    - 2[s]
Repetition_time     - 3.6384[s]
Temp_get            - 18.9[dC]
```

Elemental Composition Report

Single Mass Analysis

Tolerance = 6.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

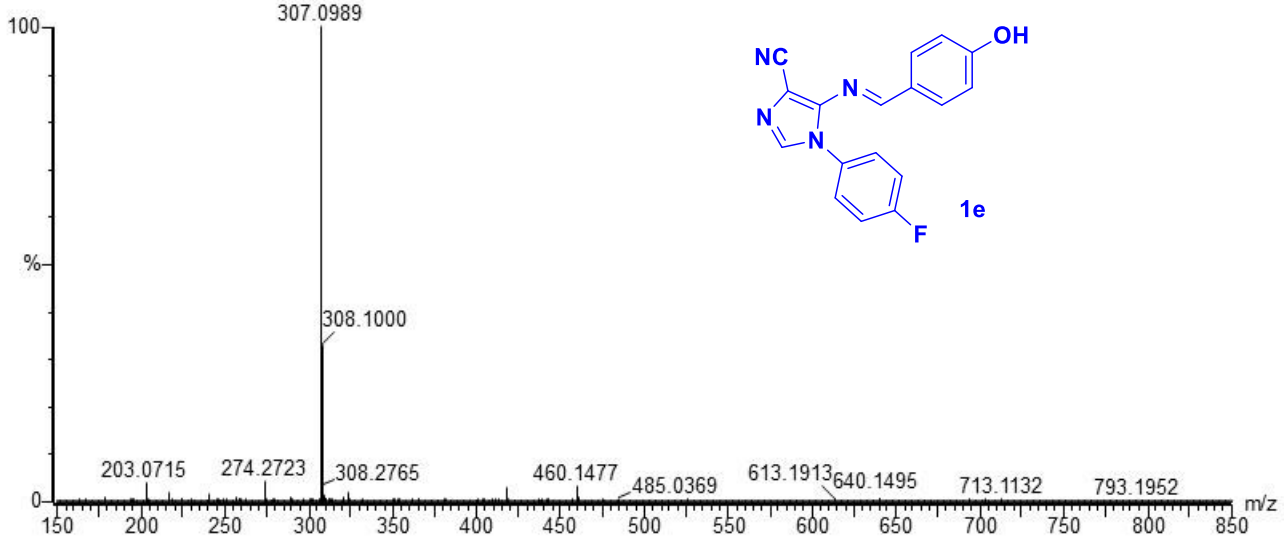
Monoisotopic Mass, Even Electron Ions
59 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-19 H: 11-30 N: 0-5 O: 0-3 F: 0-1

Sample Name : A-6
Test Name : HRMS-1
160120-A-6 15 (0.157)

IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
5.89e+007

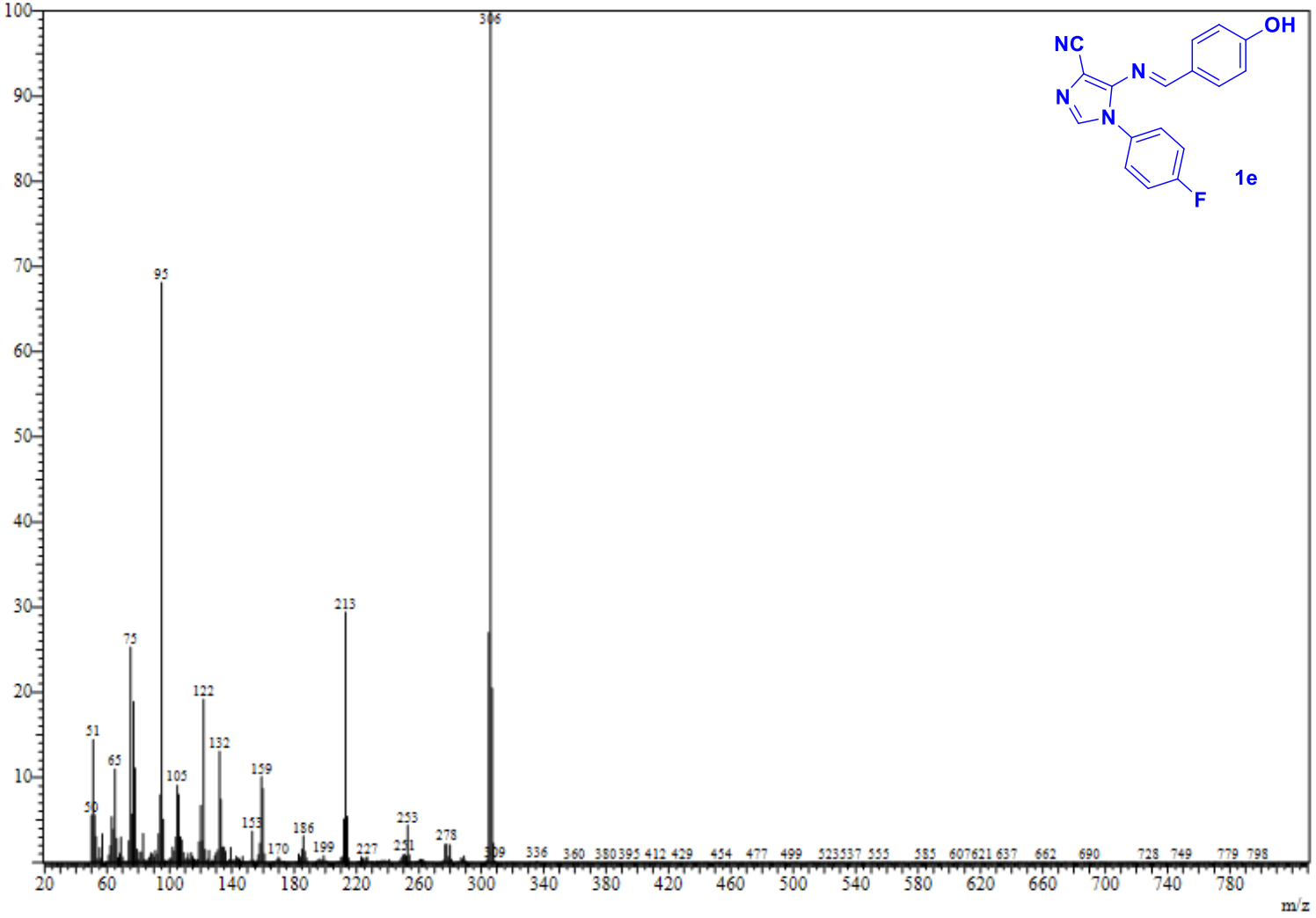


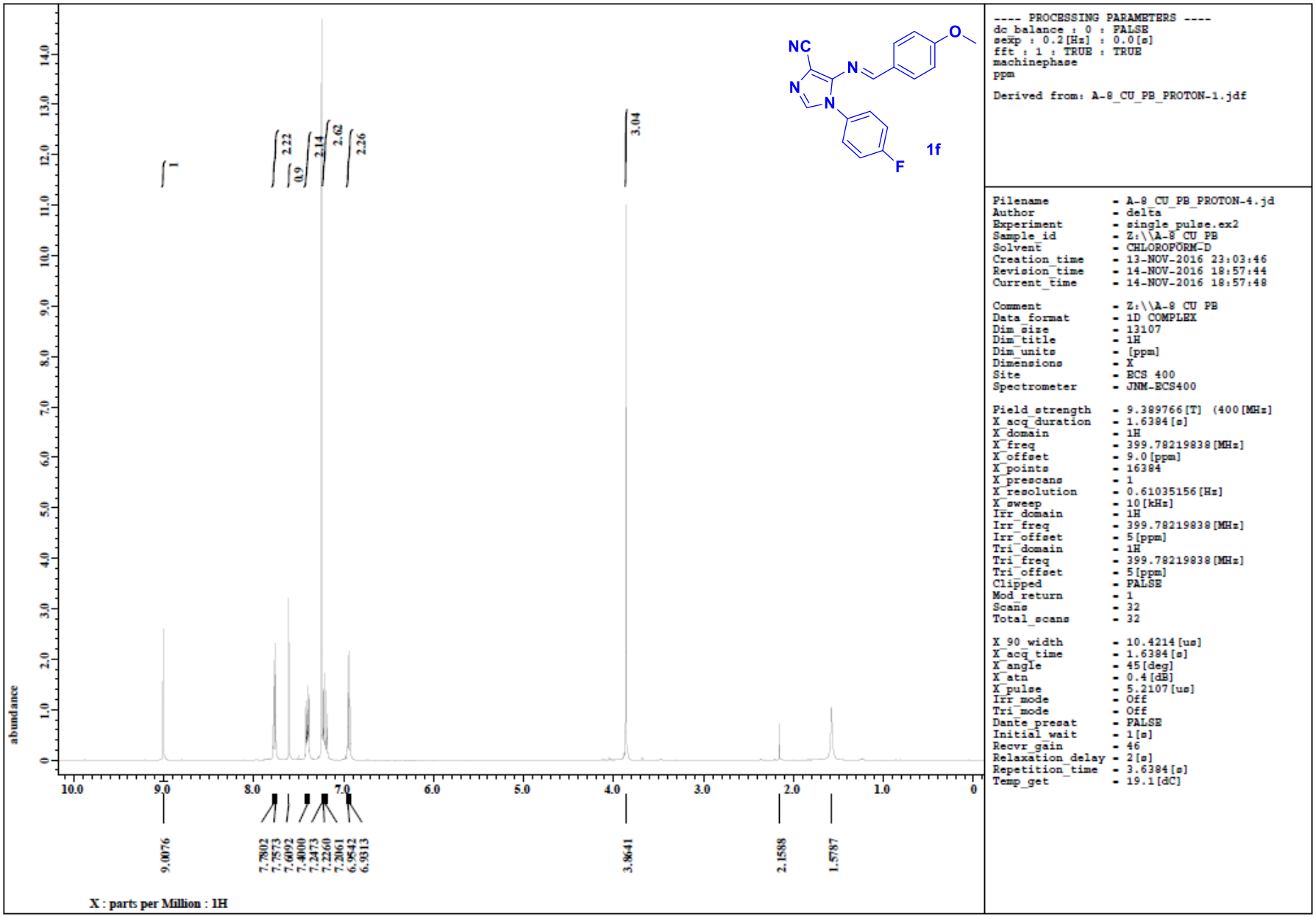
1e

Minimum:				-1.5				
Maximum:		5.0	6.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
307.0989	307.0995	-0.6	-2.0	13.5	1777.2	n/a	n/a	C17 H12 N4 O F

Spectrum

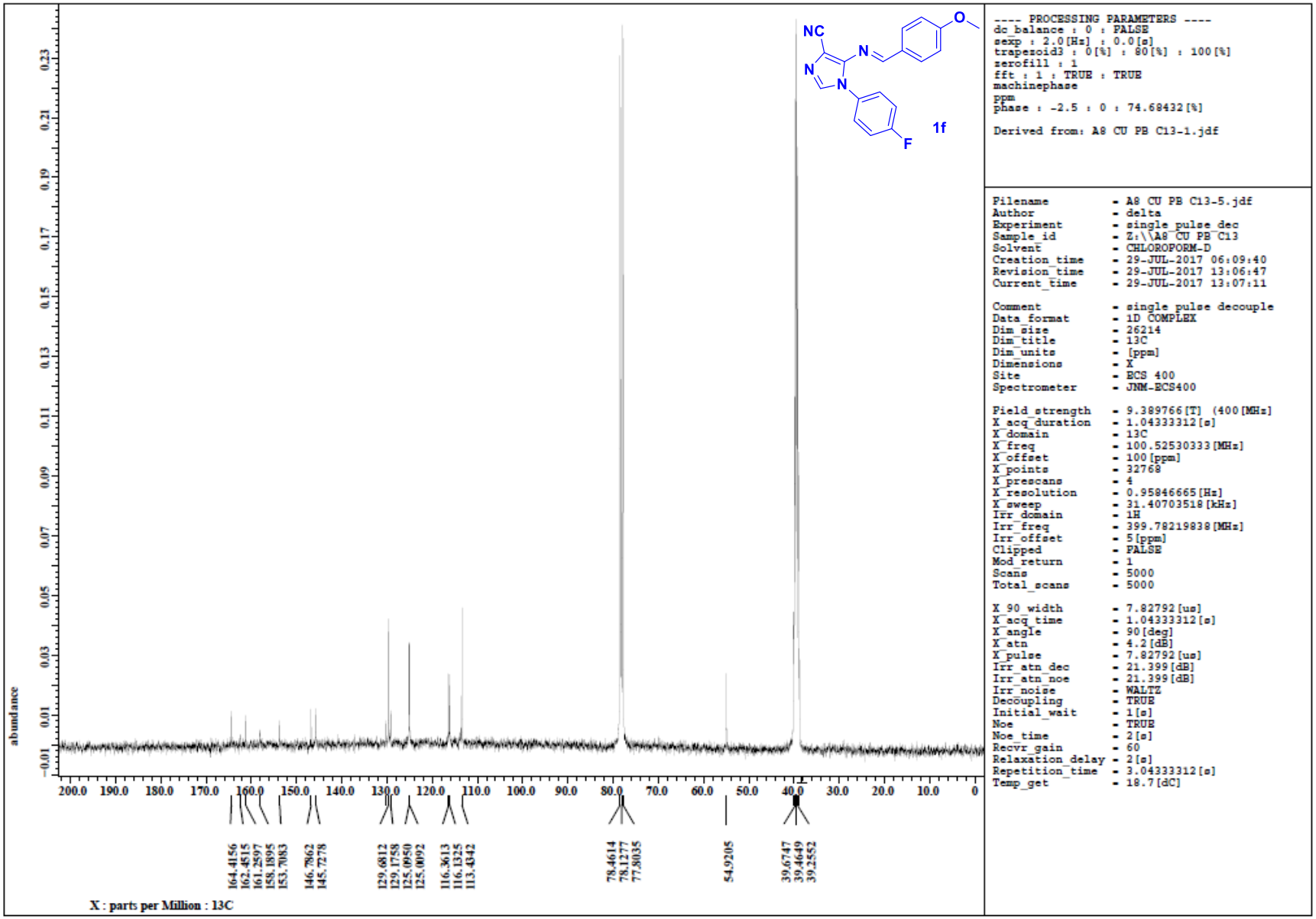
Line#:1 R.Time:6.270(Scan#:955)
MassPeaks:557
RawMode:Averaged 6.265-6.275(954-956) BasePeak:306(2138462)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: A-8_CU_PB_PROTON-1.jdf
```

```
Filename          - A-8_CU_PB_PROTON-4.jd
Author            - delta
Experiment        - single_pulse.ex2
Sample_id         - Z:\\A-8_CU_PB
Solvent           - CHLOROFORM-D
Creation_time     - 13-NOV-2016 23:03:46
Revision_time     - 14-NOV-2016 18:57:44
Current_time      - 14-NOV-2016 18:57:48

Comment           - Z:\\A-8_CU_PB
Data_format       - 1D COMPLEX
Dim_size          - 13107
Dim_title         - 1H
Dim_units         - [ppm]
Dimensions        - X
Site              - ECS 400
Spectrometer      - JNM-ECS400

Field_strength    - 9.389766[T]  (400[MHz]
X_acq_duration    - 1.6384[s]
X_domain          - 1H
X_freq            - 399.78219838[MHz]
X_offset          - 9.0[ppm]
X_points          - 16384
X_prescans        - 1
X_resolution      - 0.61035156[Hz]
X_sweep           - 10[kHz]
Irr_domain        - 1H
Irr_freq          - 399.78219838[MHz]
Irr_offset        - 5[ppm]
Tri_domain        - 1H
Tri_freq          - 399.78219838[MHz]
Tri_offset        - 5[ppm]
Clipped           - FALSE
Mod_return        - 1
Scans             - 32
Total_scans       - 32

X_90_width        - 10.4214[us]
X_acq_time        - 1.6384[s]
X_angle           - 45[deg]
X_atn             - 0.4[dB]
X_pulse           - 5.2107[us]
Irr_mode          - Off
Tri_mode          - Off
Dante_presat      - FALSE
Initial_wait      - 1[s]
Recvr_gain        - 46
Relaxation_delay  - 2[s]
Repetition_time   - 3.6384[s]
Temp_get          - 19.1[dC]
```

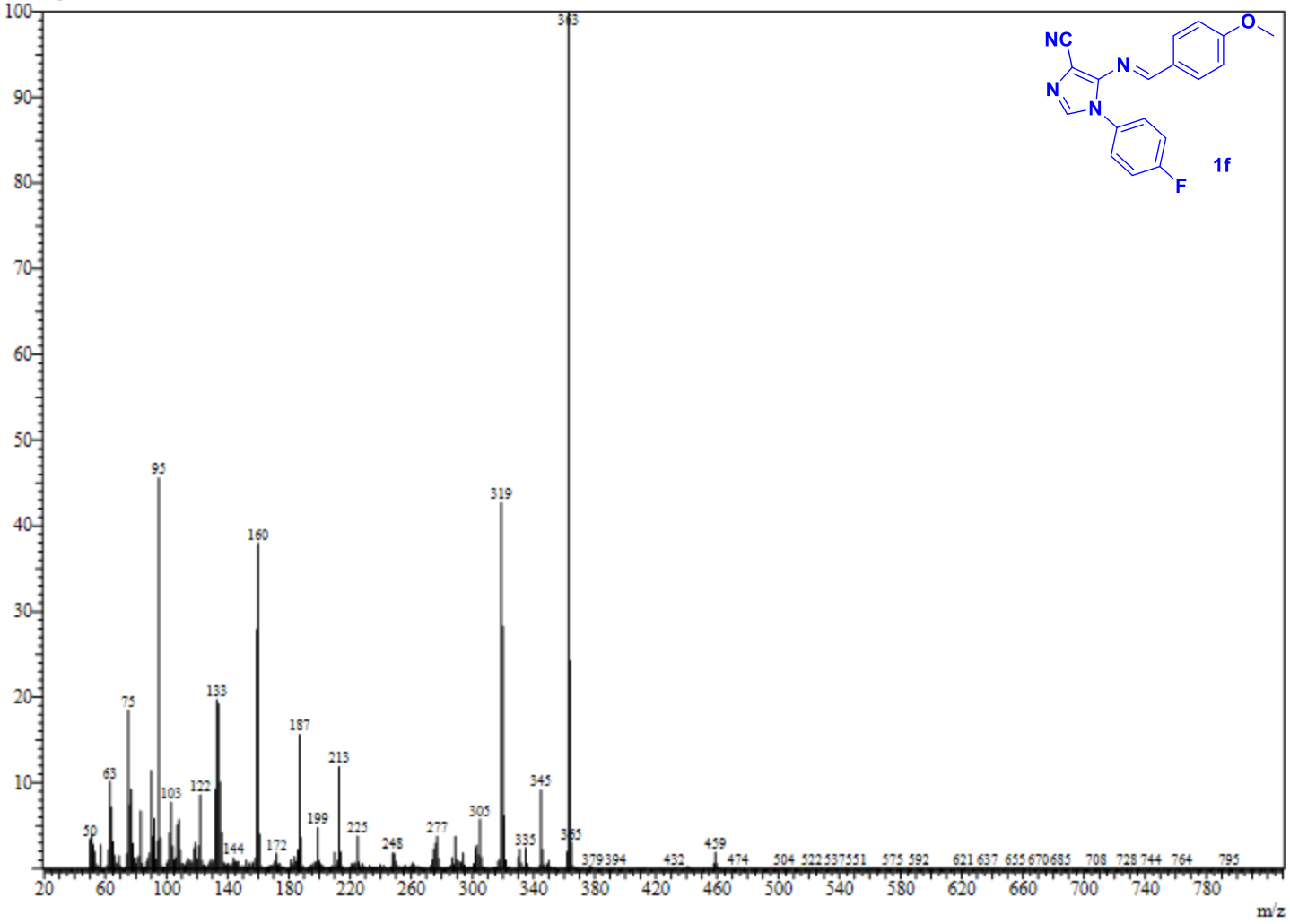


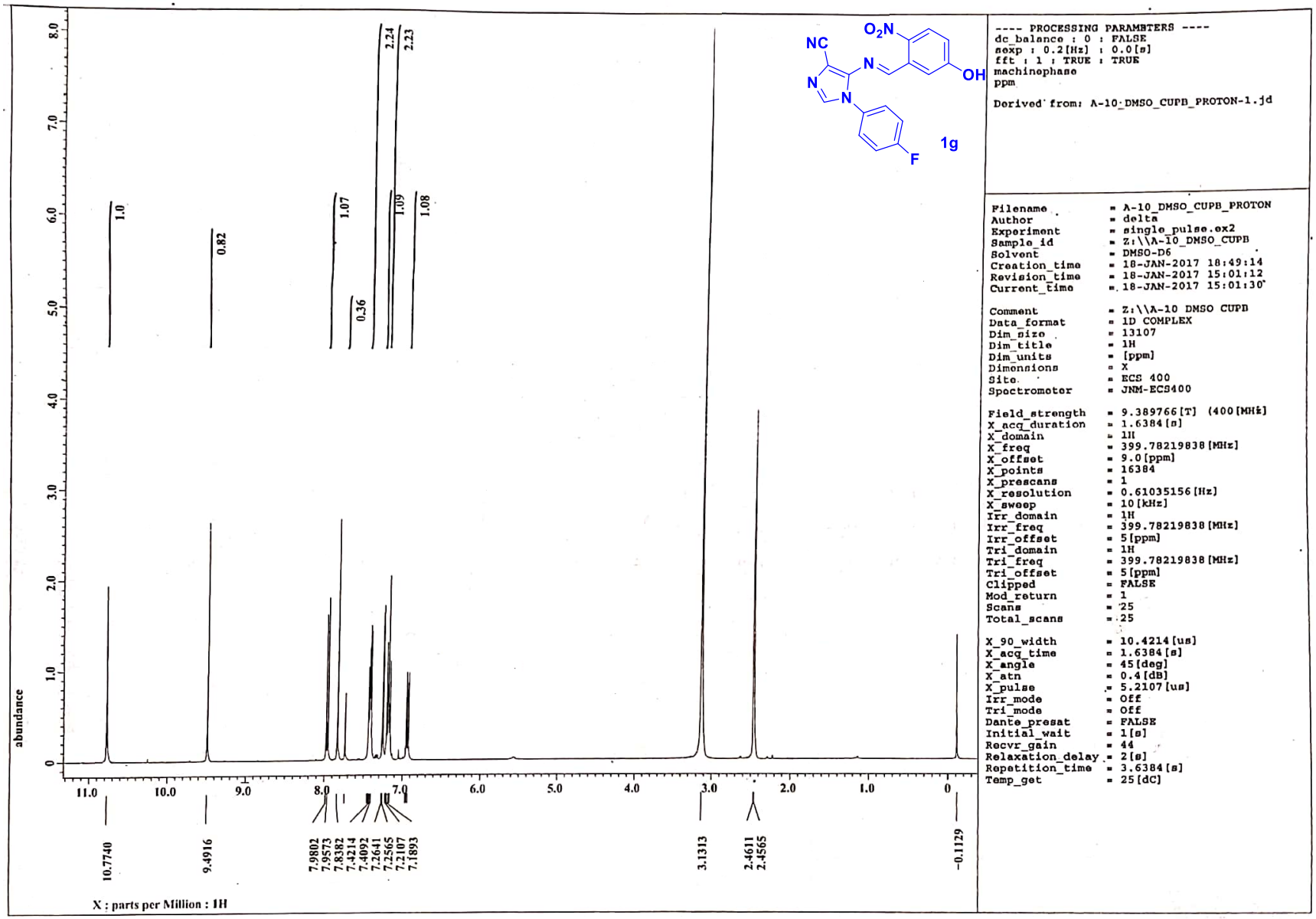

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : -2.5 : 0 : 74.68432[%]

Derived from: A8 CU PB C13-1.jdf
```

```
Pilename          - A8 CU PB C13-5.jdf
Author            - delta
Experiment        - single_pulse_dec
Sample_id         - Z:\\A8_CU_PB_C13
Solvent           - CHLOROFORM-D
Creation_time     - 29-JUL-2017 06:09:40
Revision_time     - 29-JUL-2017 13:06:47
Current_time      - 29-JUL-2017 13:07:11

Comment           - single pulse decouple
Data_format       - 1D COMPLEX
Dim_size          - 26214
Dim_title         - 13C
Dim_units         - [ppm]
Dimensions        - X
Site              - BCS 400
Spectrometer      - JNM-ECS400

Field_strength    - 9.389766[T] (400[MHz]
X_acq_duration    - 1.04333312[s]
X_domain          - 13C
X_freq            - 100.52530333[MHz]
X_offset          - 100[ppm]
X_points          - 32768
X_prescans        - 4
X_resolution      - 0.95846665[Hz]
X_sweep           - 31.40703518[kHz]
Irr_domain        - 1H
Irr_freq          - 399.78219838[MHz]
Irr_offset        - 5[ppm]
Clipped           - FALSE
Mod_return        - 1
Scans             - 5000
Total_scans       - 5000

X_90_width        - 7.82792[us]
X_acq_time        - 1.04333312[s]
X_angle           - 90[deg]
X_atn             - 4.2[dB]
X_pulse           - 7.82792[us]
Irr_atn_dec       - 21.399[dB]
Irr_atn_noe       - 21.399[dB]
Irr_noise         - WALTZ
Decoupling        - TRUE
Initial_wait      - 1[s]
Noe               - TRUE
Noe_time          - 2[s]
Recvr_gain        - 60
Relaxation_delay  - 2[s]
Repetition_time   - 3.04333312[s]
Temp_get          - 18.7[dC]
```

Spectrum

Line#:1 R.Time:7.815(Scan#:1264)
MassPeaks:479
RawMode:Averaged 7.810-7.820(1263-1265) BasePeak:363(347447)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity




abundance
X : parts per Million : 1H
1g
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: A-10-DMSO_CUPB_PROTON-1.jd
Filename = A-10_DMSO_CUPB_PROTON
Author = delta
Experiment = single_pulse.ex2
Sample_id = Z:\\A-10_DMSO_CUPB
Solvent = DMSO-D6
Creation_time = 18-JAN-2017 18:49:14
Revision_time = 18-JAN-2017 15:01:12
Current_time = 18-JAN-2017 15:01:30
Comment = Z:\\A-10 DMSO CUPB
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.6384[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 9.0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.61035156[Hz]
X_sweep = 10[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 25
Total_scans = 25
X_90_width = 10.4214[us]
X_acq_time = 1.6384[s]
X_angle = 45[deg]
X_atn = 0.4[dB]
X_pulse = 5.2107[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 2[s]
Repetition_time = 3.6384[s]
Temp_get = 25[dC]
10.7740
9.4916
7.9802
7.9573
7.8382
7.4214
7.4092
7.2641
7.2565
7.2107
7.1893
3.1313
2.4611
2.4565
-0.1129

Elemental Composition Report

Single Mass Analysis

Tolerance = 6.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

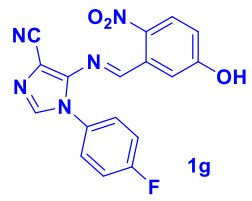
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-19 H: 11-30 N: 0-5 O: 0-3 F: 0-1

Sample Name : A-10
Test Name : HRMS-1
160120-A-10 17 (0.174)

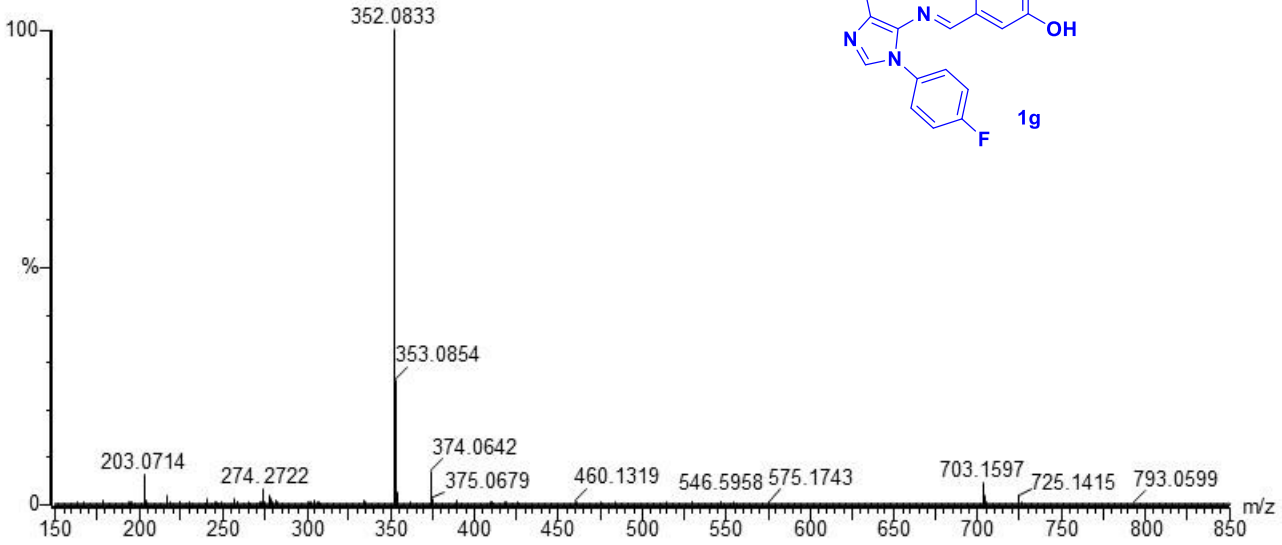
IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
3.04e+007



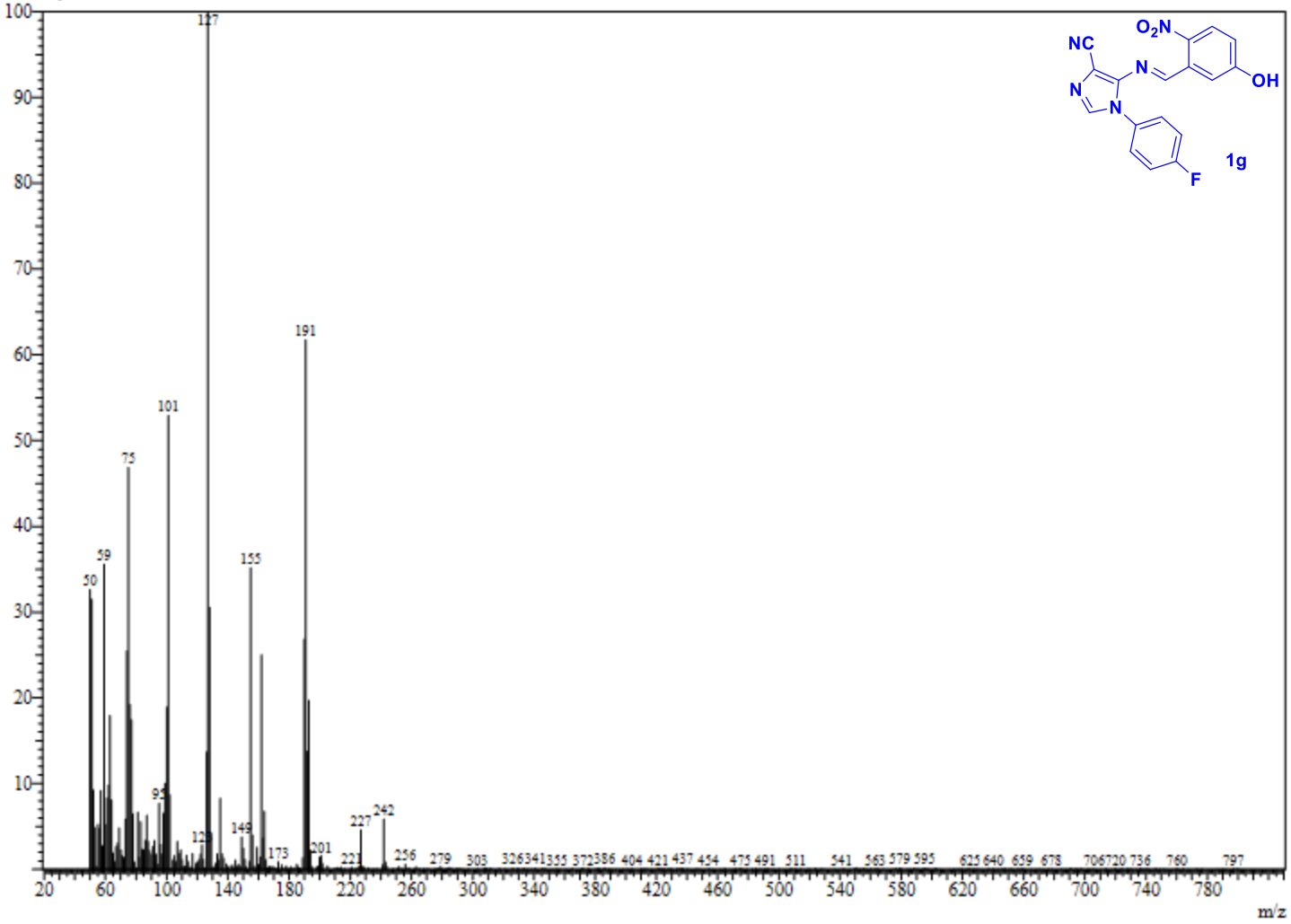
1g

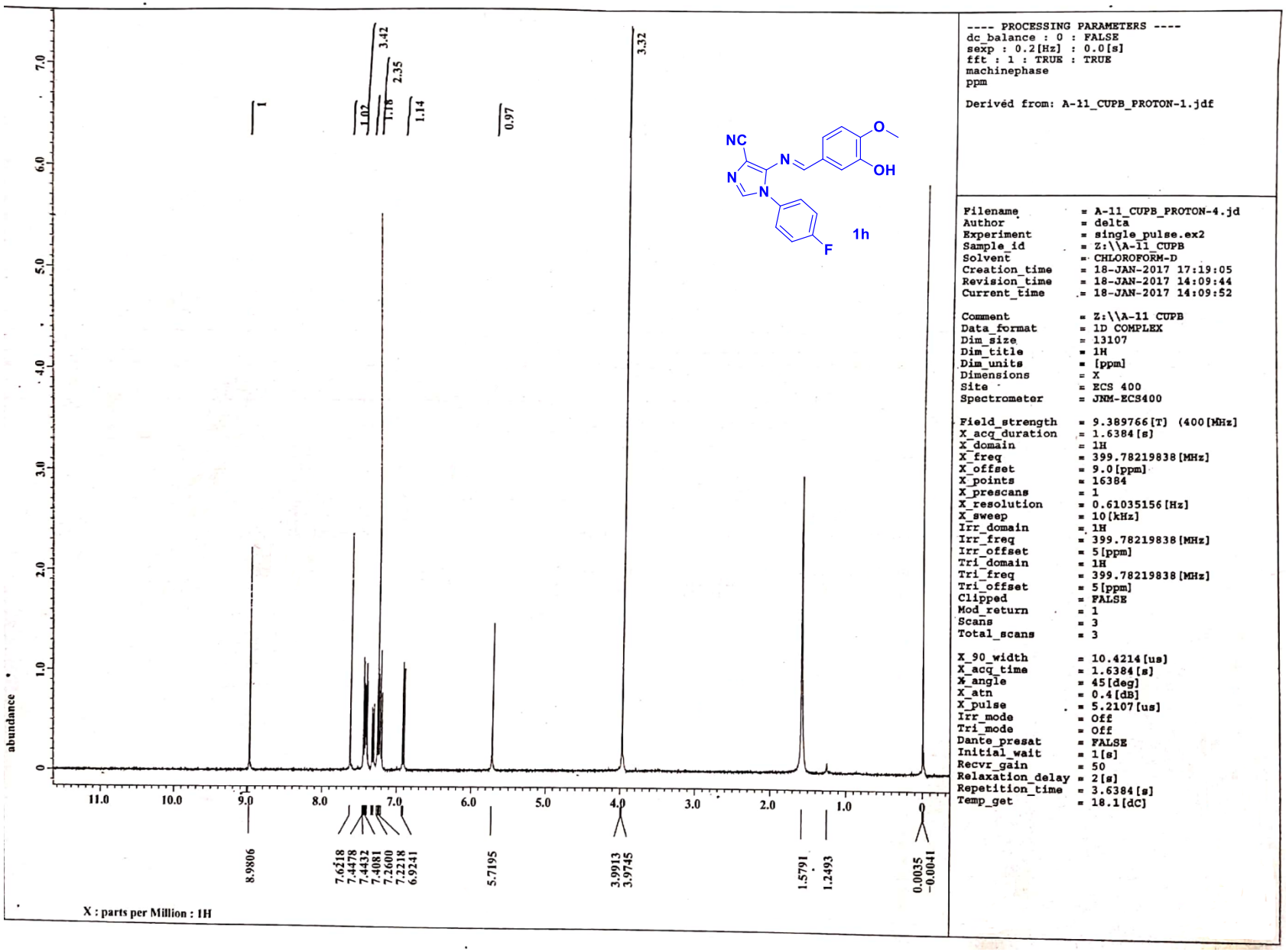


Minimum:				-1.5				
Maximum:		5.0	6.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
352.0833	352.0846	-1.3	-3.7	14.5	1530.9	n/a	n/a	C17 H11 N5 O3 F

Spectrum

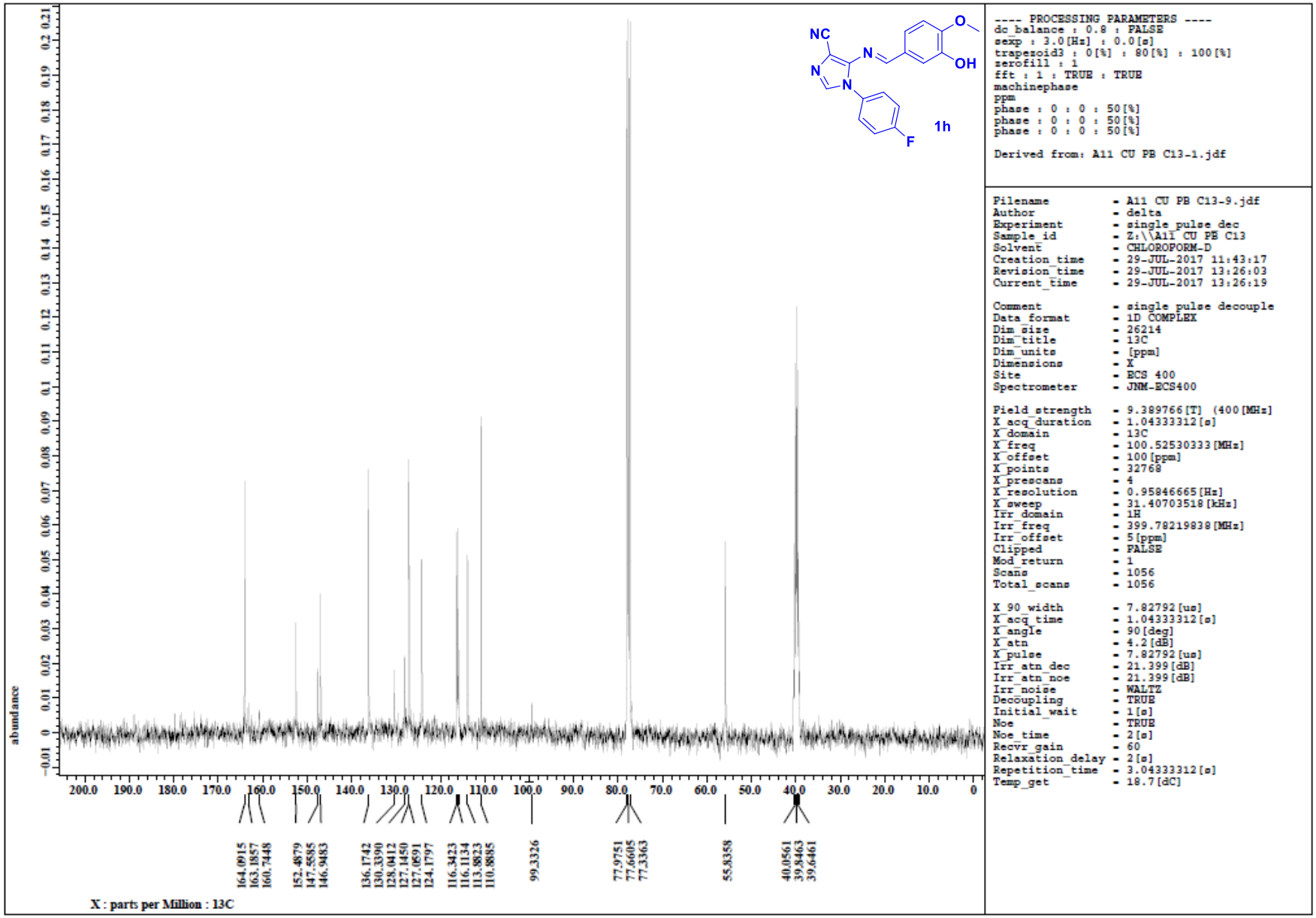
Line#:1 R.Time:2.155(Scan#:132)
MassPeaks:430
RawMode:Averaged 2.150-2.160(131-133) BasePeak:127(43367)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: A-11_CUPB_PROTON-1.jdf
```

Filename	= A-11_CUPB_PROTON-4.jd
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= z:\\A-11_CUPB
Solvent	= CHLOROFORM-D
Creation_time	= 18-JAN-2017 17:19:05
Revision_time	= 18-JAN-2017 14:09:44
Current_time	= 18-JAN-2017 14:09:52
Comment	= z:\\A-11 CUPB
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 1.6384[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 9.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.61035156[Hz]
X_sweep	= 10[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 3
Total_scans	= 3
X_90_width	= 10.4214[us]
X_acq_time	= 1.6384[s]
X_angle	= 45[deg]
X_atn	= 0.4[dB]
X_pulse	= 5.2107[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 50
Relaxation_delay	= 2[s]
Repetition_time	= 3.6384[s]
Temp_get	= 18.1[dC]




```
---- PROCESSING PARAMETERS ----
dc_balance : 0.8 : FALSE
sexp : 3.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
phase : 0 : 0 : 50[%]
phase : 0 : 0 : 50[%]
phase : 0 : 0 : 50[%]

Derived from: A11 CU PB C13-1.jdf
```

```
Filename            - A11 CU PB C13-9.jdf
Author              - delta
Experiment          - single_pulse_dec
Sample_id           - Z:\\A11 CU PB C13
Solvent             - CHLOROPORM-D
Creation_time       - 29-JUL-2017 11:43:17
Revision_time       - 29-JUL-2017 13:26:03
Current_time        - 29-JUL-2017 13:26:19

Comment             - single pulse decouple
Data_format         - 1D COMPLEX
Dim_size            - 26214
Dim_title           - 13C
Dim_units           - [ppm]
Dimensions          - X
Site                - ECS 400
Spectrometer        - JNM-ECS400

Field_strength      - 9.389766[T] (400[MHz]
X_acq_duration      - 1.04333312[s]
X_domain            - 13C
X_freq              - 100.52530333[MHz]
X_offset            - 100[ppm]
X_points            - 32768
X_prescans          - 4
X_resolution        - 0.95846665[Hz]
X_sweep             - 31.40703518[kHz]
Irr_domain          - 1H
Irr_freq            - 399.78219838[MHz]
Irr_offset          - 5[ppm]
Clipped             - FALSE
Mod_return          - 1
Scans               - 1056
Total_scans         - 1056

X_90_width          - 7.82792[us]
X_acq_time          - 1.04333312[s]
X_angle             - 90[deg]
X_atn               - 4.2[dB]
X_pulse             - 7.82792[us]
Irr_atn_dec         - 21.399[dB]
Irr_atn_noe         - 21.399[dB]
Irr_noise           - WALTZ
Decoupling          - TRUE
Initial_wait        - 1[s]
Noe                 - TRUE
Noe_time            - 2[s]
Recvr_gain          - 60
Relaxation_delay    - 2[s]
Repetition_time     - 3.04333312[s]
Temp_get            - 18.7[dC]
```

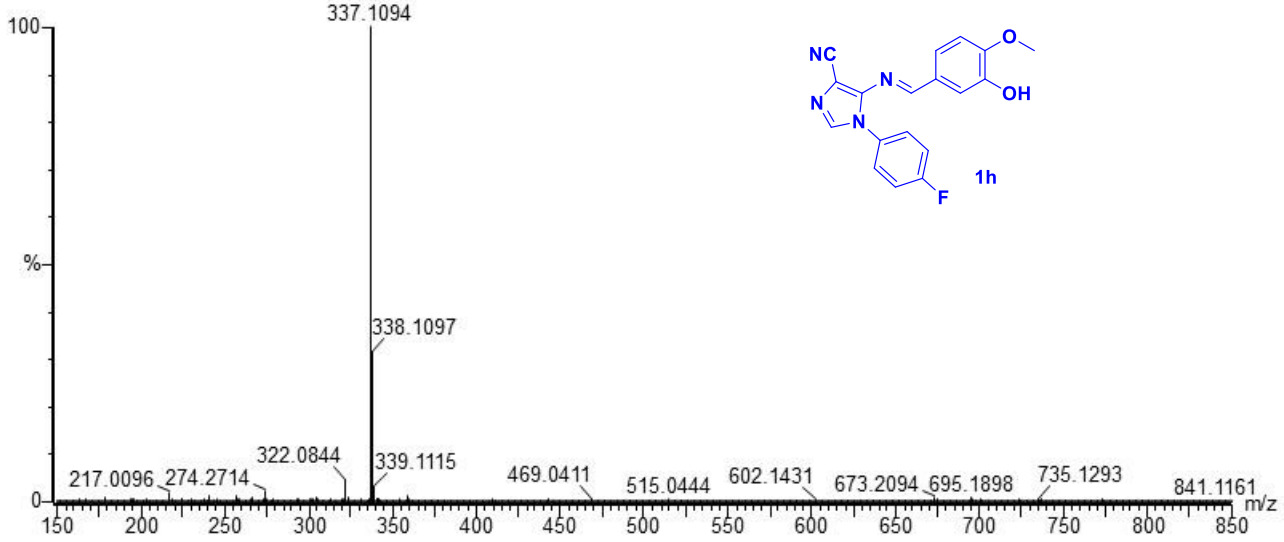
Elemental Composition Report

Single Mass Analysis

Tolerance = 6.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
43 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-19 H: 11-30 N: 0-5 O: 0-3 F: 0-1

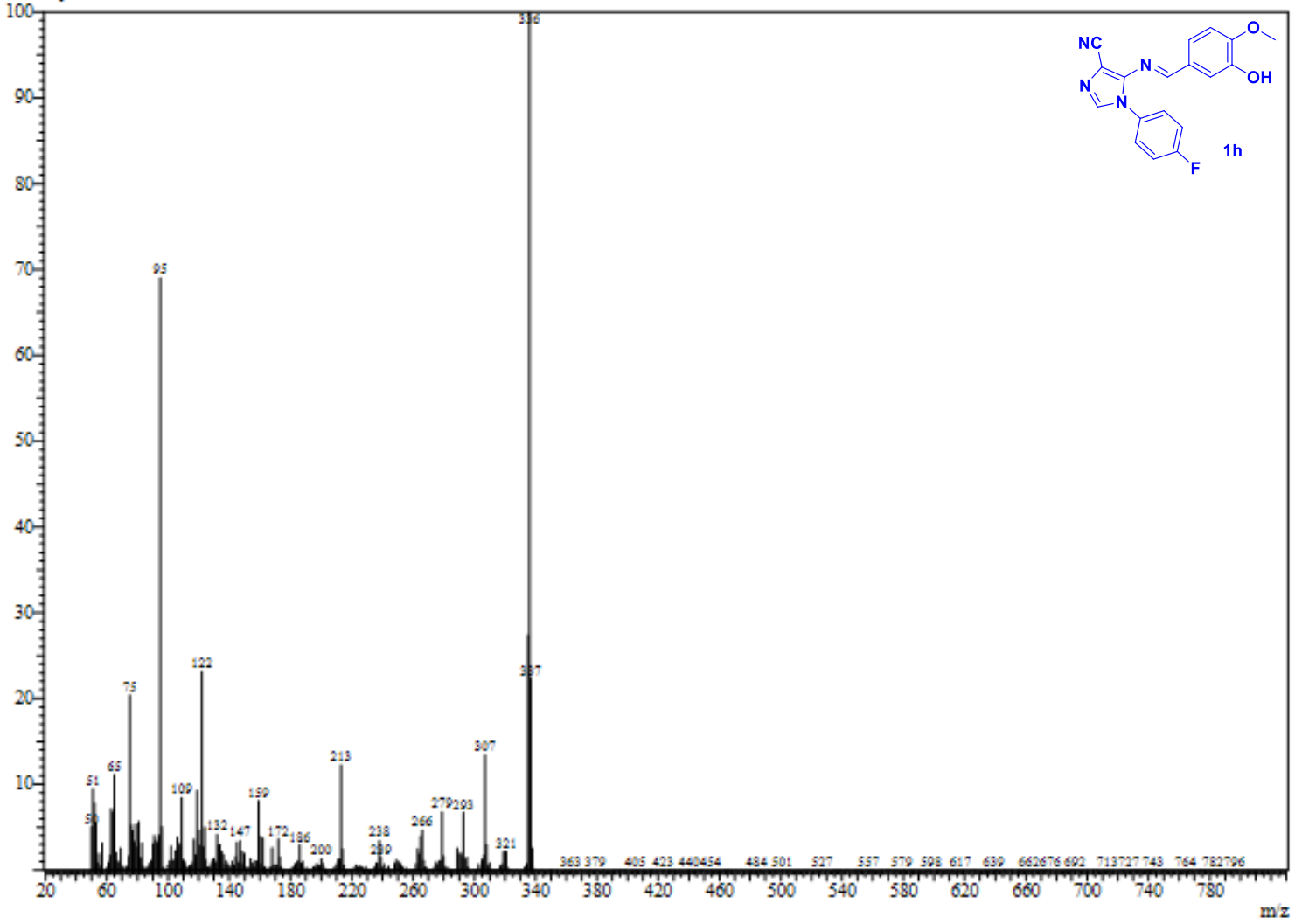
Sample Name : A-11 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
160120-A-11 17 (0.174) 1: TOF MS ES+
3.46e+007

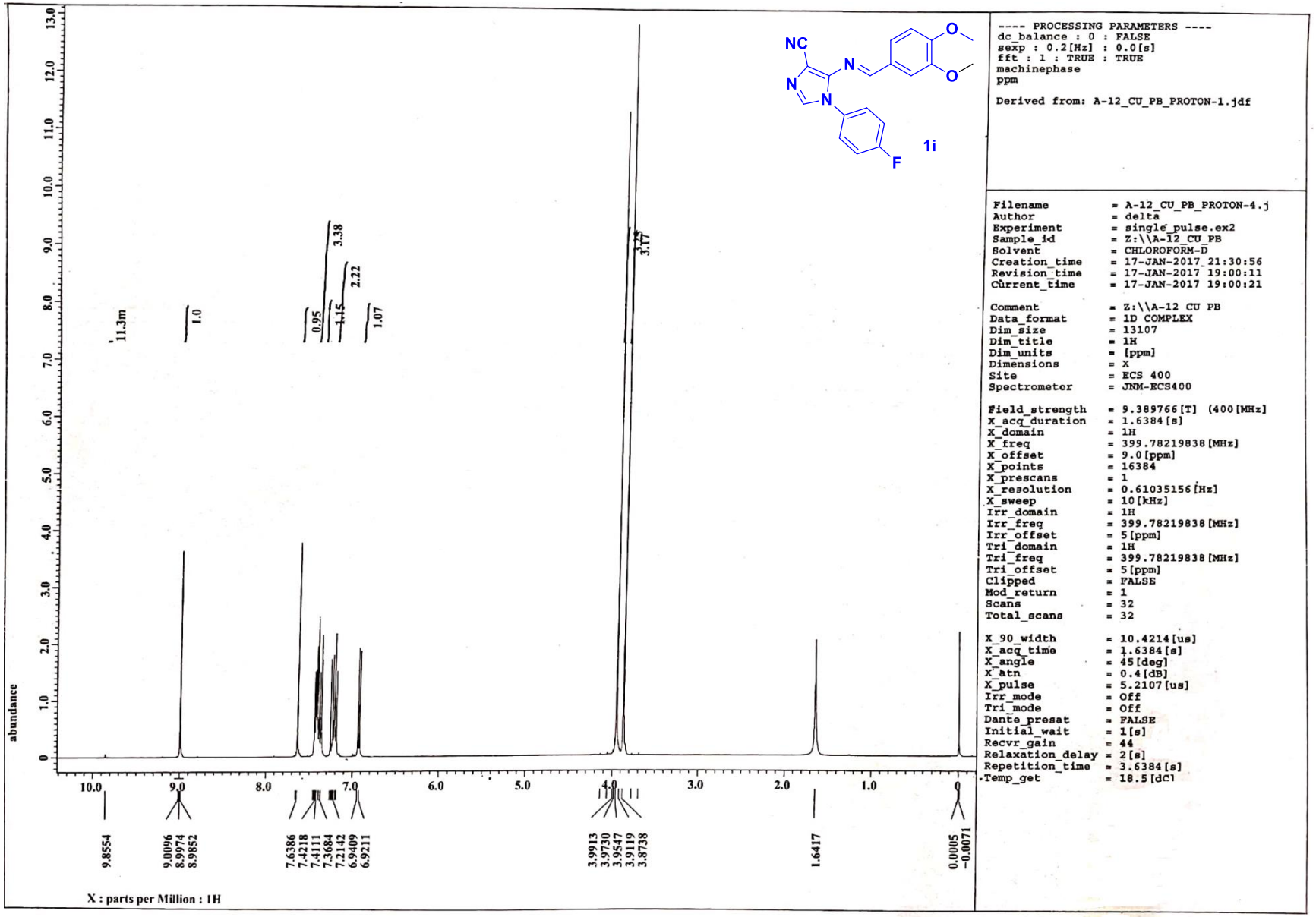


Minimum:				-1.5				
Maximum:		5.0	6.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
337.1094	337.1101	-0.7	-2.1	13.5	2165.1	n/a	n/a	C18 H14 N4 O2 F

Spectrum

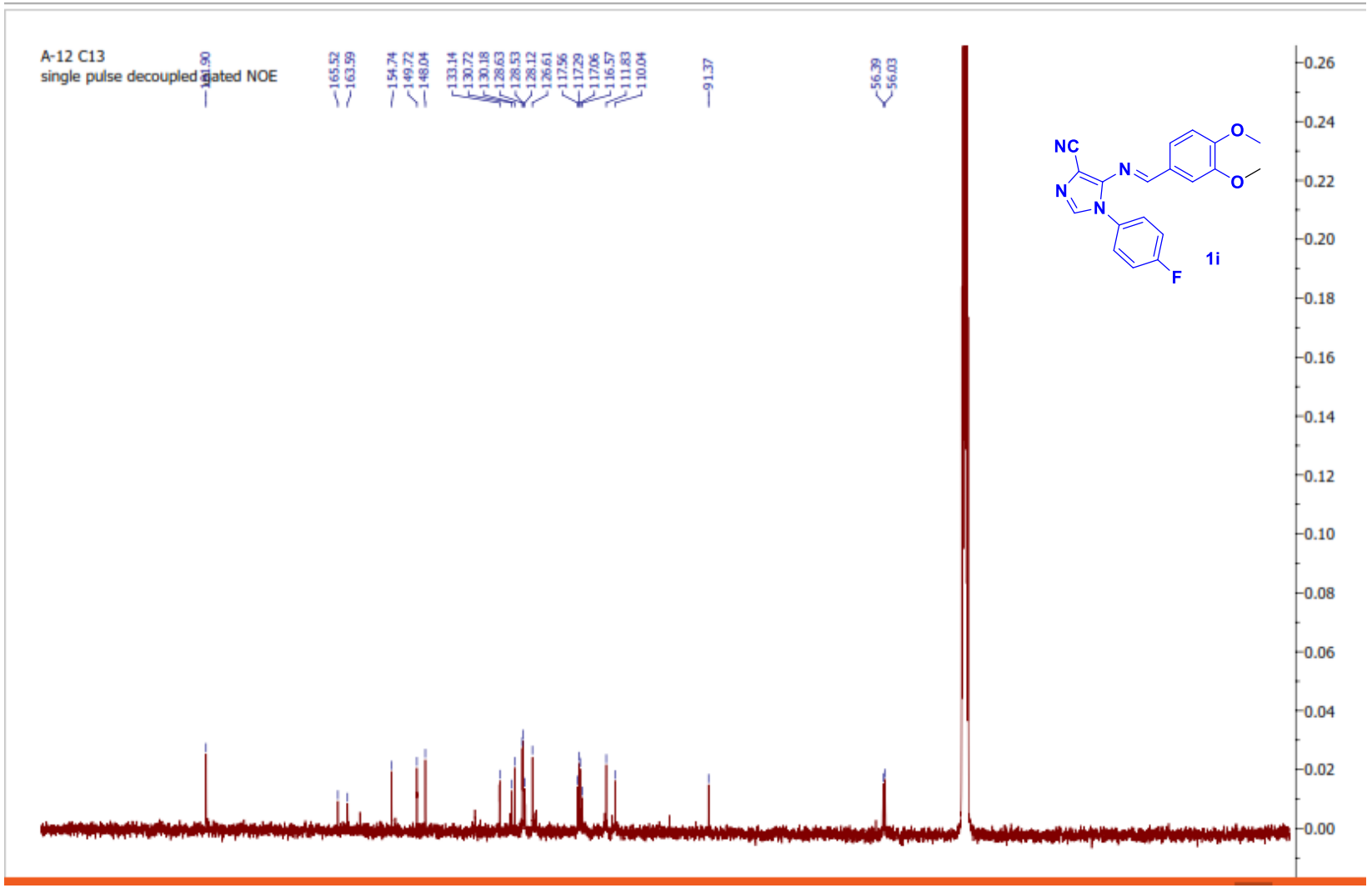
Line#:1 R.Time:6.180(Scan#:937)
MassPeaks:522
RawMode:Averaged 6.175-6.185(936-938) BasePeak:336(307885)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity






```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: A-12_CU_PB_PROTON-1.jdf
```

Filename	= A-12_CU_PB_PROTON-4.j
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= Z:\\A-12_CU_PB
Solvent	= CHLOROFORM-D
Creation_time	= 17-JAN-2017_21:30:56
Revision_time	= 17-JAN-2017 19:00:11
Current_time	= 17-JAN-2017 19:00:21
Comment	= Z:\\A-12 CU PB
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= ECS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 1.6384[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 9.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.61035156[Hz]
X_sweep	= 10[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 32
Total_scans	= 32
X_90_width	= 10.4214[us]
X_acq_time	= 1.6384[s]
X_angle	= 45[deg]
X_atn	= 0.4[dB]
X_pulse	= 5.2107[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 44
Relaxation_delay	= 2[s]
Repetition_time	= 3.6384[s]
Temp_get	= 18.5[dC]


A-12 C13
single pulse decoupled gated NOE
165.52
163.59
154.74
149.72
148.04
133.14
130.72
130.18
128.63
128.53
128.12
126.61
117.56
117.29
117.06
116.57
111.83
110.04
91.37
56.39
56.03
NC
N
N
N
O
O
F
1i
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00

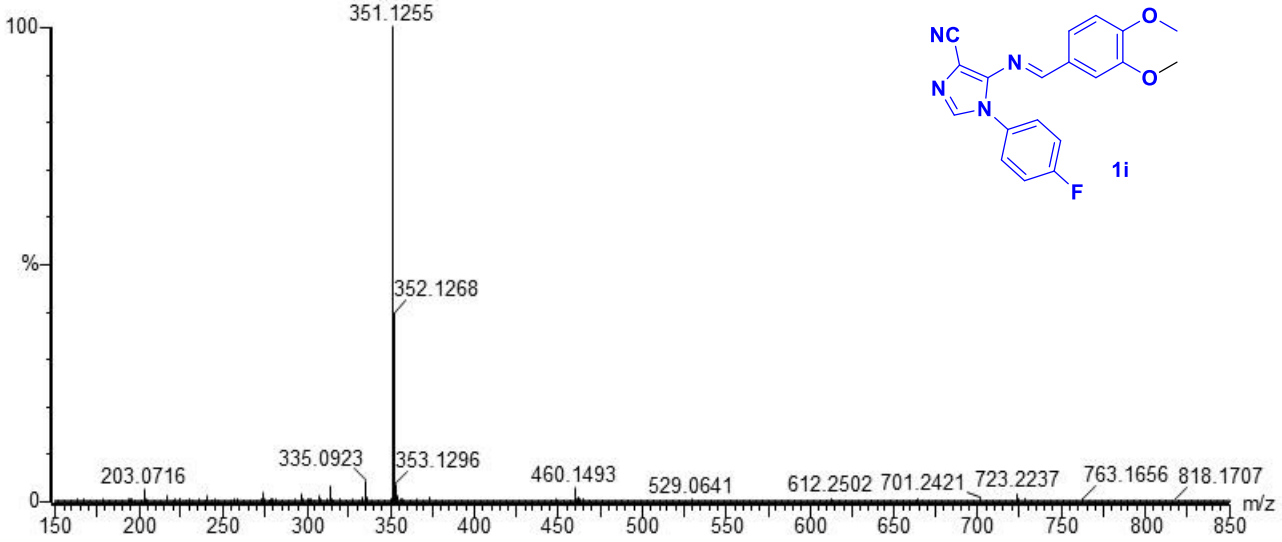
Elemental Composition Report

Single Mass Analysis

Tolerance = 6.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

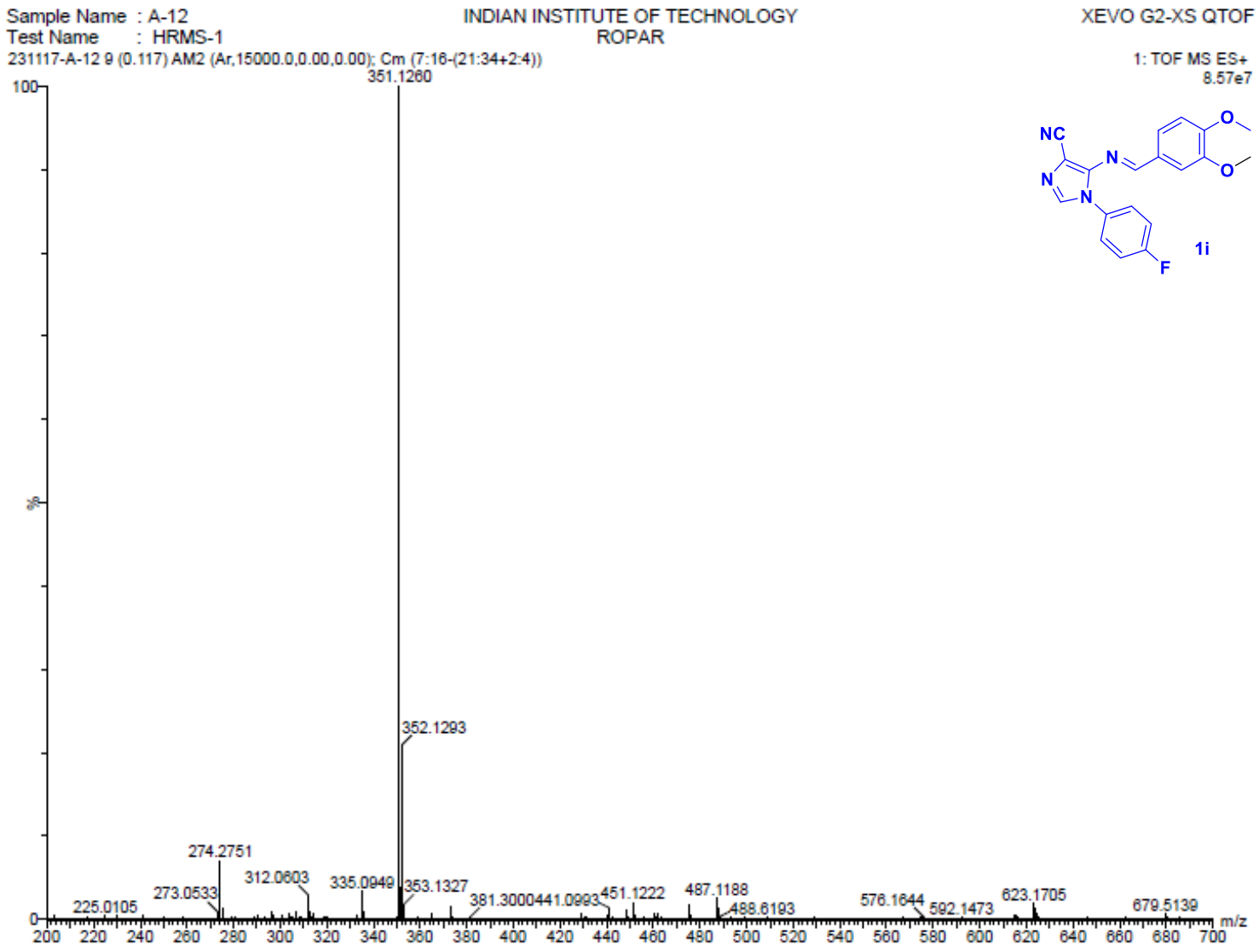
Monoisotopic Mass, Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-19 H: 11-30 N: 0-5 O: 0-3 F: 0-1

Sample Name : A-12 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
160120-A-12 17 (0.174) 1: TOF MS ES+
4.64e+007



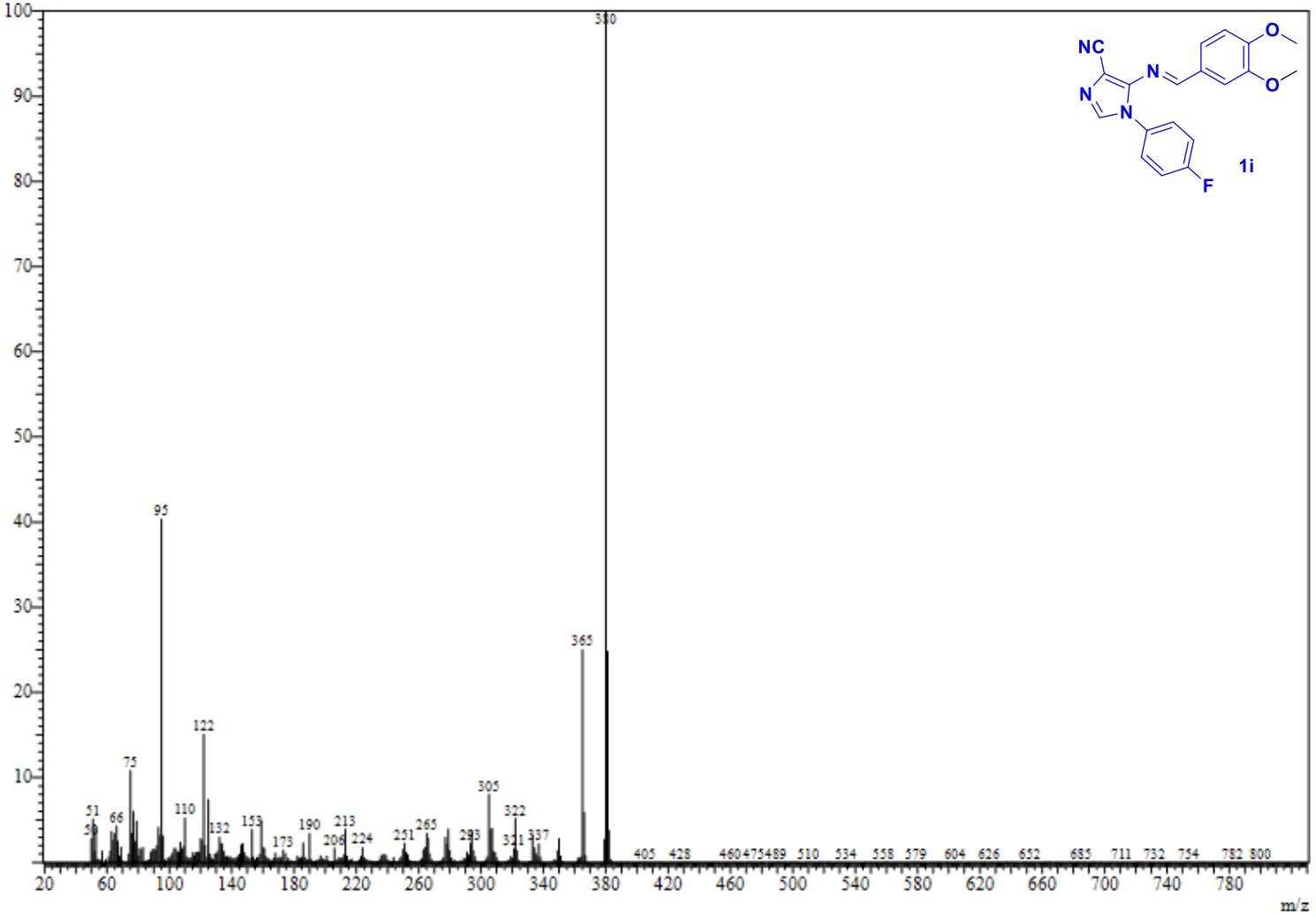
1i

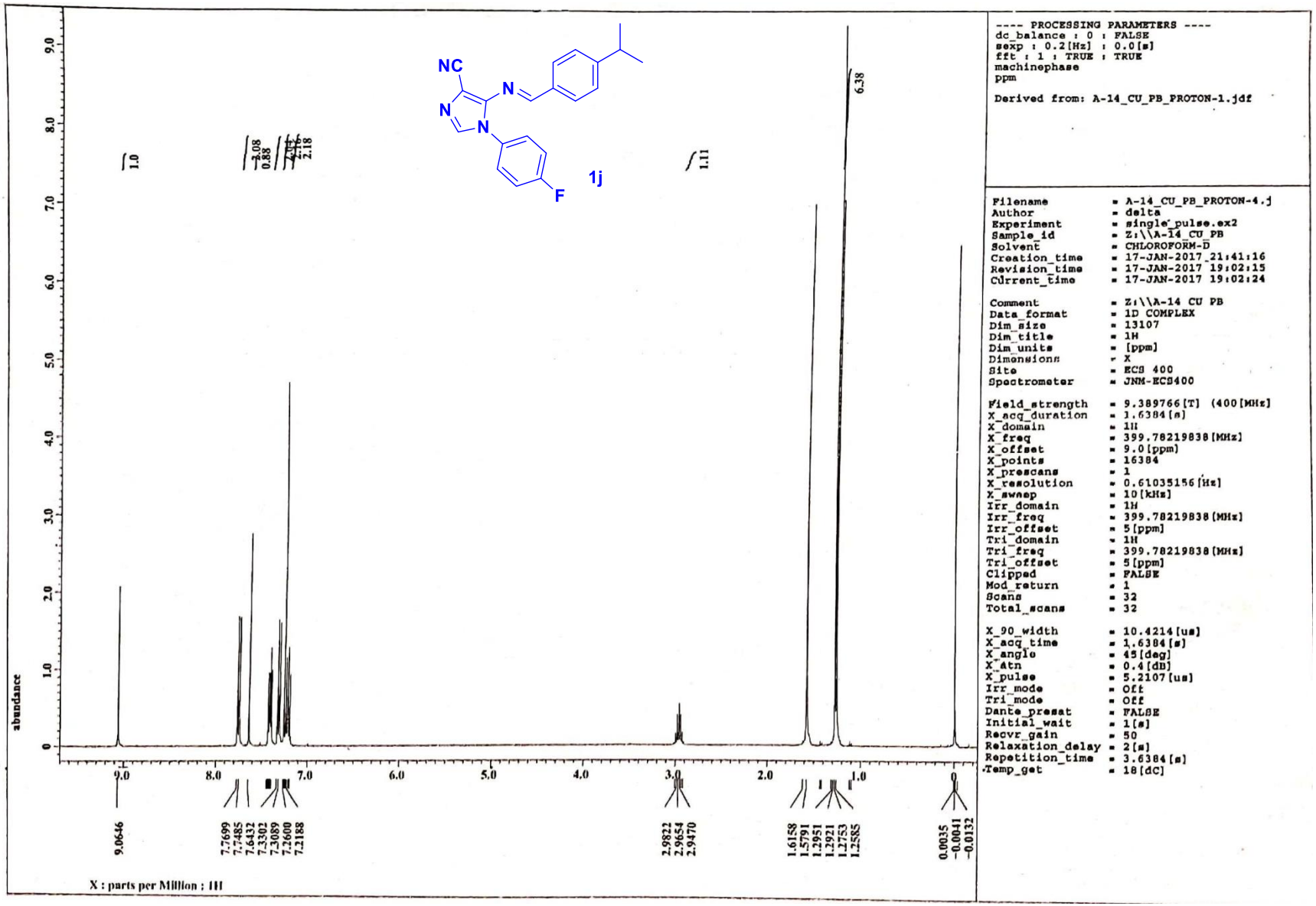
Minimum:				-1.5				
Maximum:		5.0	6.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
351.1255	351.1257	-0.2	-0.6	13.5	1738.3	n/a	n/a	C19 H16 N4 O2 F

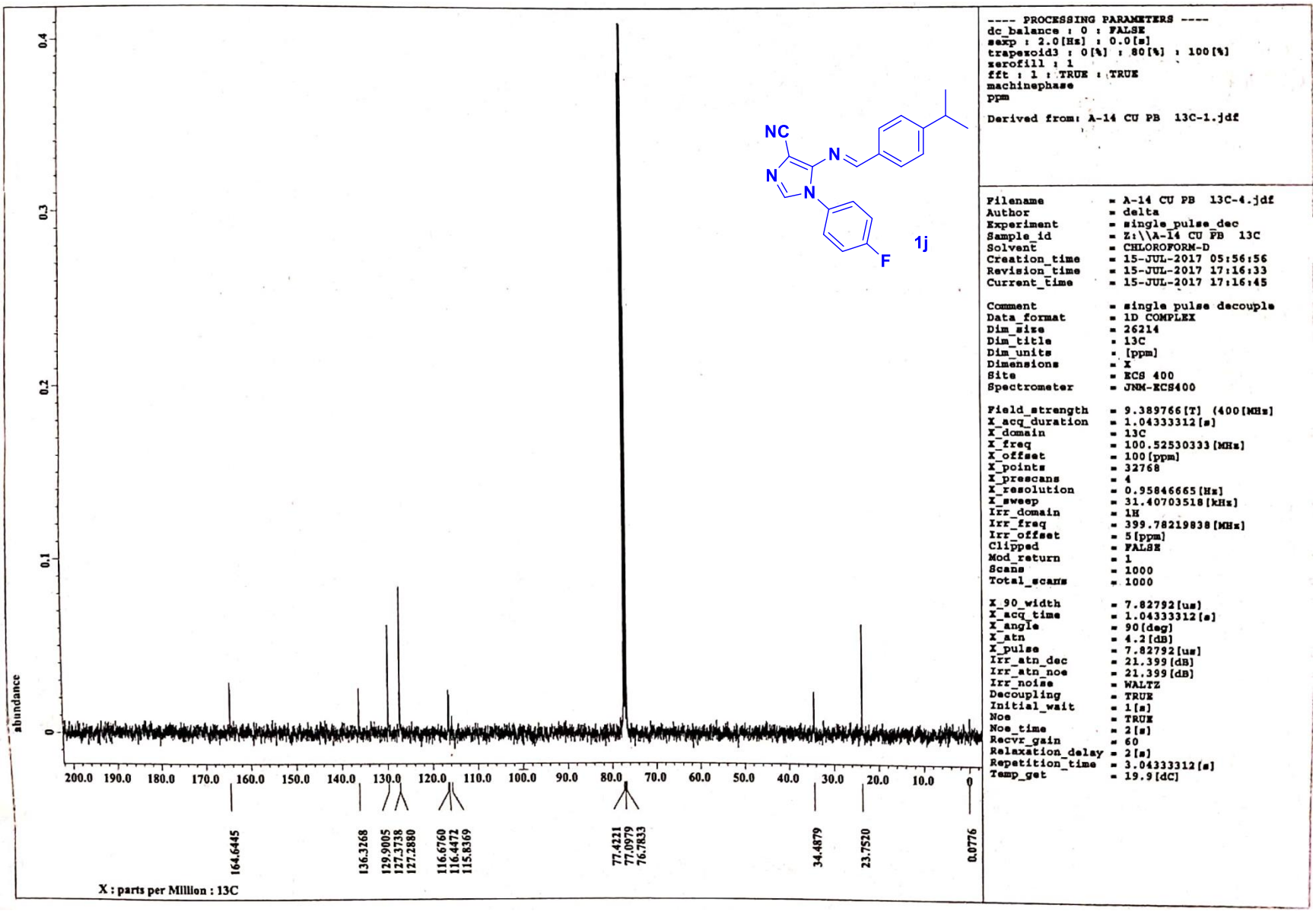

Sample Name : A-12
Test Name : HRMS-1
231117-A-12 9 (0.117) AM2 (Ar,15000.0,0.00,0.00); Cm (7:16-(21:34+2:4))
INDIAN INSTITUTE OF TECHNOLOGY
ROPAR
XEVO G2-XS QTOF
1: TOF MS ES+
8.57e7
NC
N
N
N
O
O
F
1i
100
%
0
351.1260
352.1293
274.2751
312.0603
335.0949
353.1327
273.0533
225.0105
381.3000
441.0993
451.1222
487.1188
488.6193
576.1644
592.1473
623.1705
679.5139
m/z
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700

Spectrum

Line#:1 R.Time:7.425(Scan#:1186)
MassPeaks:583
RawMode:Averaged 7.420-7.430(1185-1187) BasePeak:380(6661844)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity

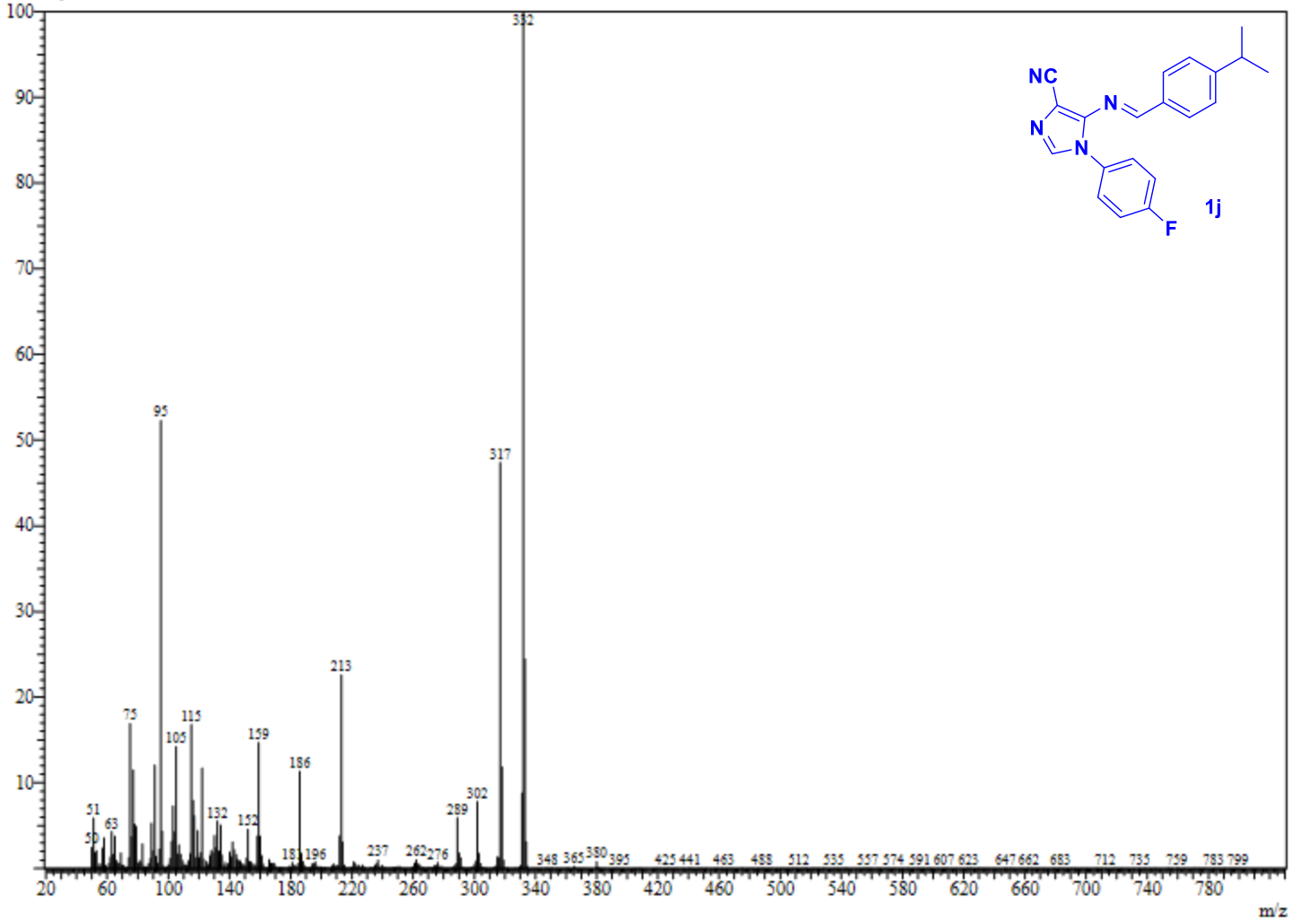



NC
N
N
N
F
1j
abundance
X : parts per Million : 1H
9.0646
7.7699
7.7485
7.6432
7.3302
7.3089
7.2600
7.2188
2.9822
2.9654
2.9470
1.6158
1.5791
1.2951
1.2921
1.2753
1.2585
0.0035
-0.0041
-0.0132
6.38
1.0
3.08
0.88
4.04
2.16
2.18
1.11
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: A-14_CU_PB_PROTON-1.jdf
Filename = A-14_CU_PB_PROTON-4.j
Author = delta
Experiment = single_pulse.ex2
Sample_id = Z:\\A-14_CU_PB
Solvent = CHLOROFORM-D
Creation_time = 17-JAN-2017 21:41:16
Revision_time = 17-JAN-2017 19:02:15
Current_time = 17-JAN-2017 19:02:24
Comment = Z:\\A-14 CU PB
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = 1H
Dim_units = [ppm]
Dimension = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.6384[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 9.0[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.61035156[Hz]
X_sweep = 10[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 32
Total_scans = 32
X_90_width = 10.4214[us]
X_acq_time = 1.6384[s]
X_angle = 45[deg]
X_Atn = 0.4[dB]
X_pulse = 5.2107[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.6384[s]
Temp_get = 18[dC]

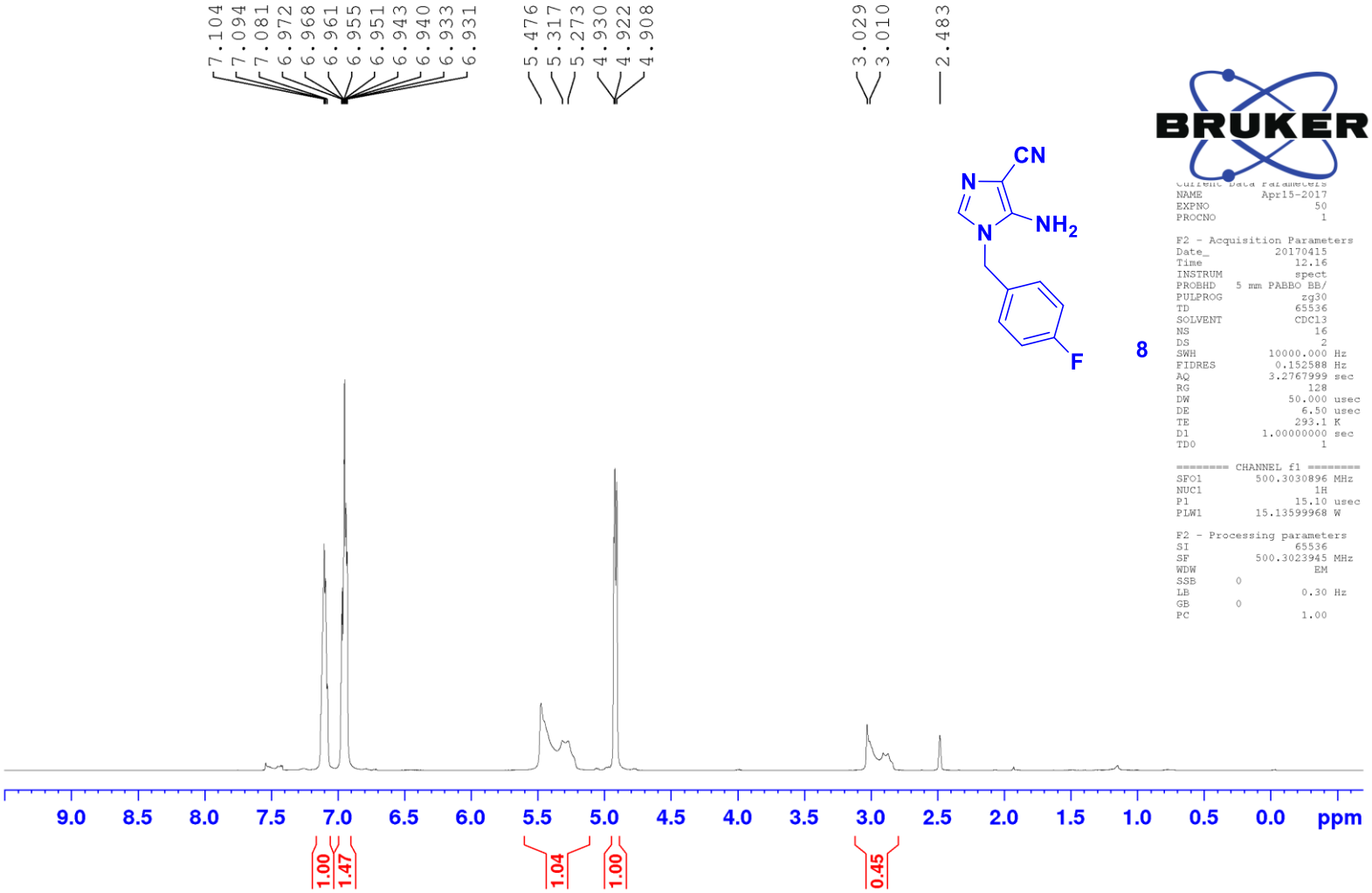

NC
N
N
N
F
1j
abundance
0.4
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
164.6445
136.3268
129.9005
127.3738
127.2880
116.6760
116.4472
115.8369
77.4221
77.0979
76.7833
34.4879
23.7520
0.0776
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: A-14 CU PB 13C-1.jdf
Filename = A-14 CU PB 13C-4.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = Z:\\A-14 CU PB 13C
Solvent = CHLOROFORM-D
Creation_time = 15-JUL-2017 05:56:56
Revision_time = 15-JUL-2017 17:16:33
Current_time = 15-JUL-2017 17:16:45
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = ECS 400
Spectrometer = JNM-ECS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 7.82792[us]
X_acq_time = 1.04333312[s]
X_angle = 90[deg]
X_atn = 4.2[dB]
X_pulse = 7.82792[us]
Irr_atn_dec = 21.399[dB]
Irr_atn_noe = 21.399[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 19.9[dC]

Spectrum

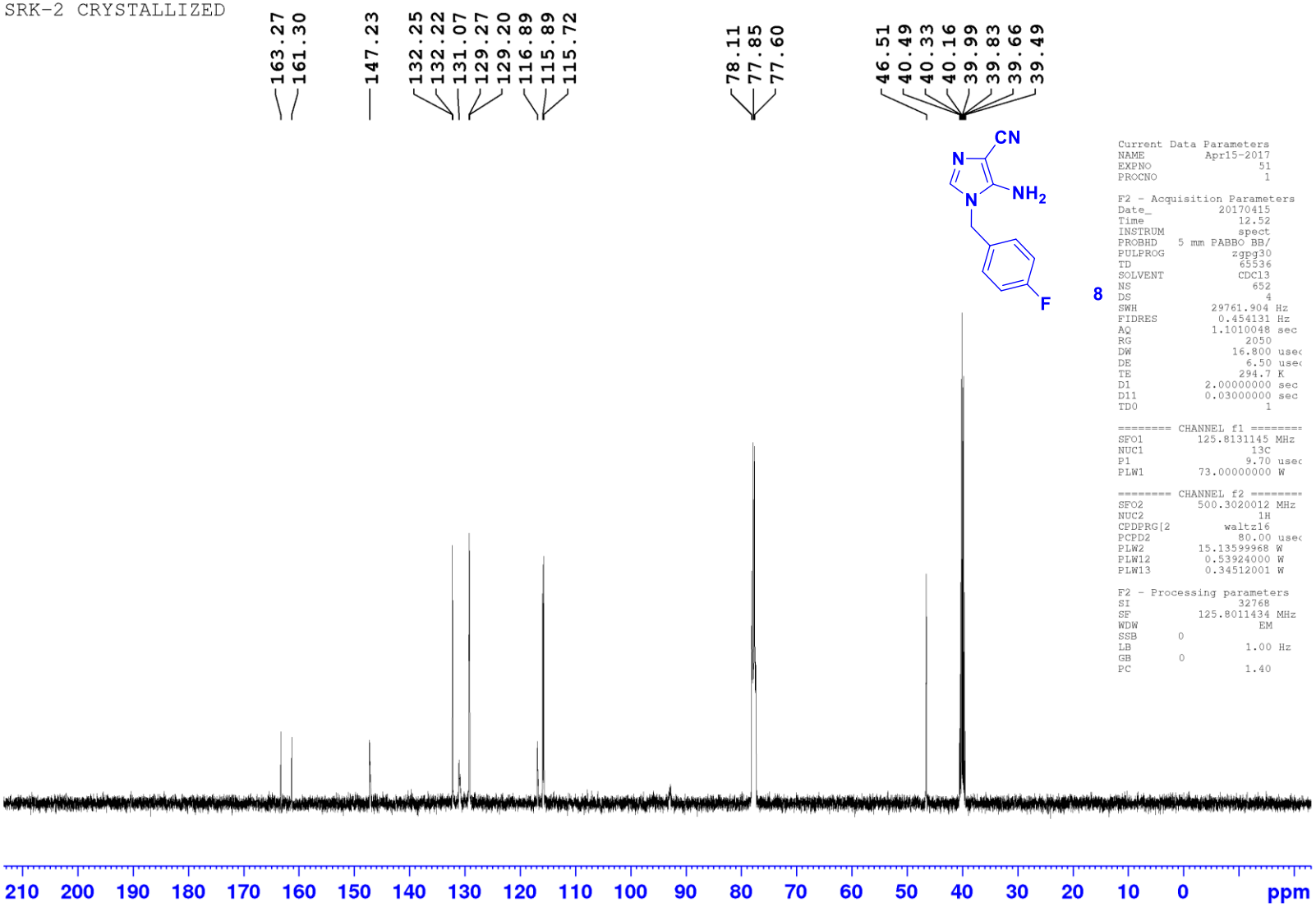
Line#:1 R.Time:4.880(Scan#:677)
MassPeaks:519
RawMode:Averaged 4.875-4.885(676-678) BasePeak:332(535382)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity



SRK-2 CRYSTALLIZED

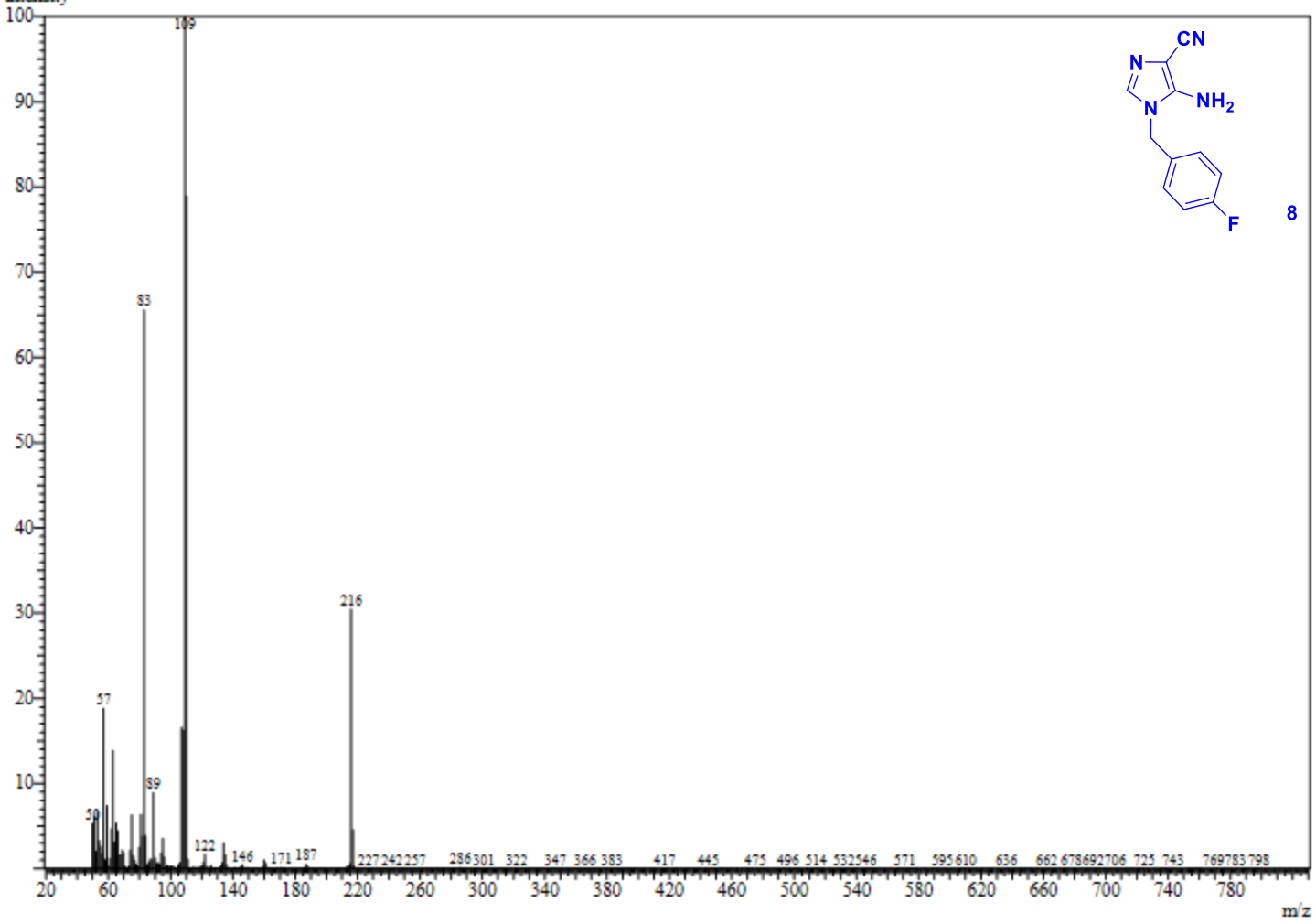


SRK-2 CRYSTALLIZED



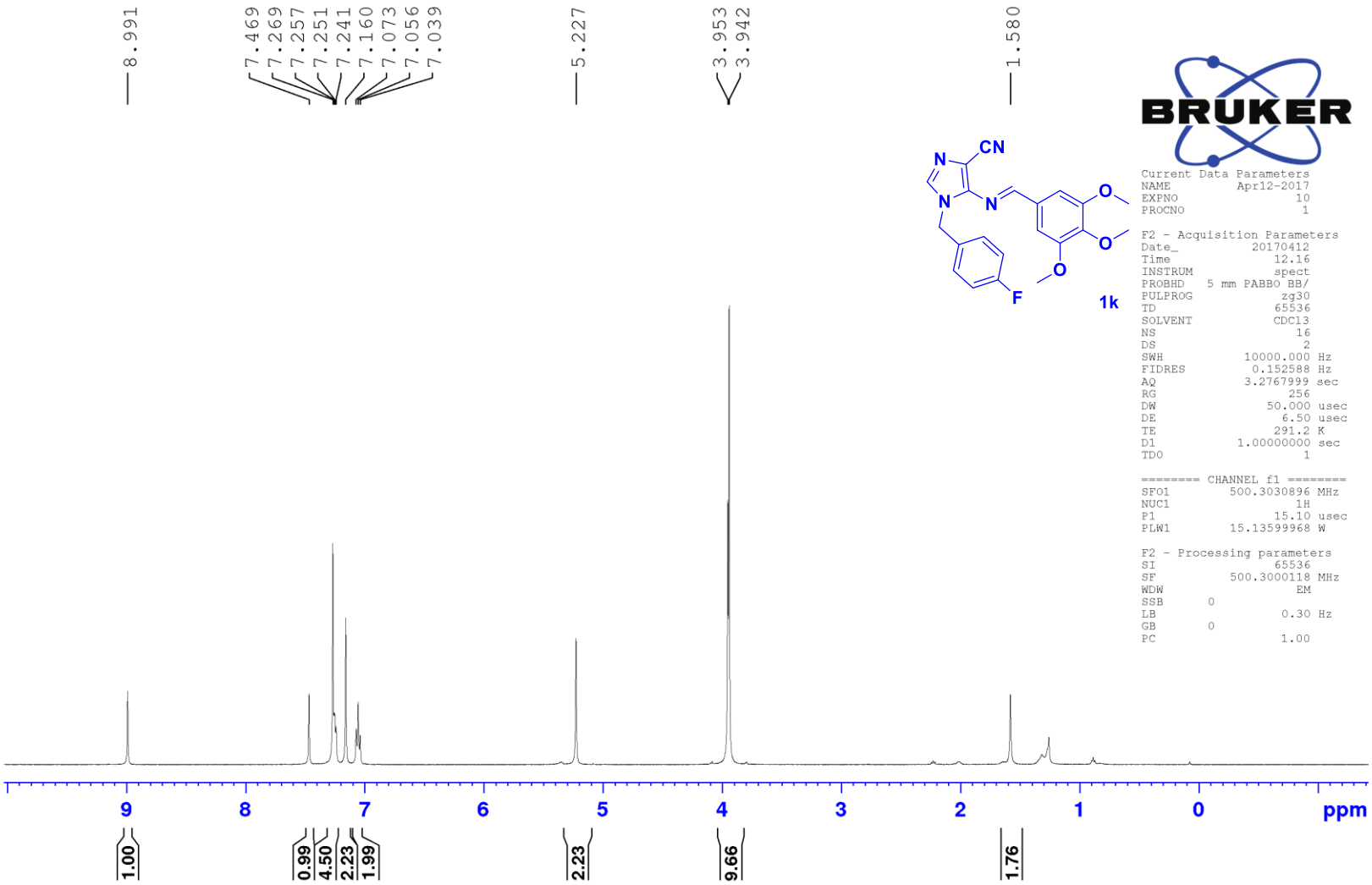
Spectrum

Line#:1 R.Time:6.290(Scan#:959)
MassPeaks:642
RawMode:Averaged 6.285-6.295(958-960) BasePeak:109(7591332)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity



8

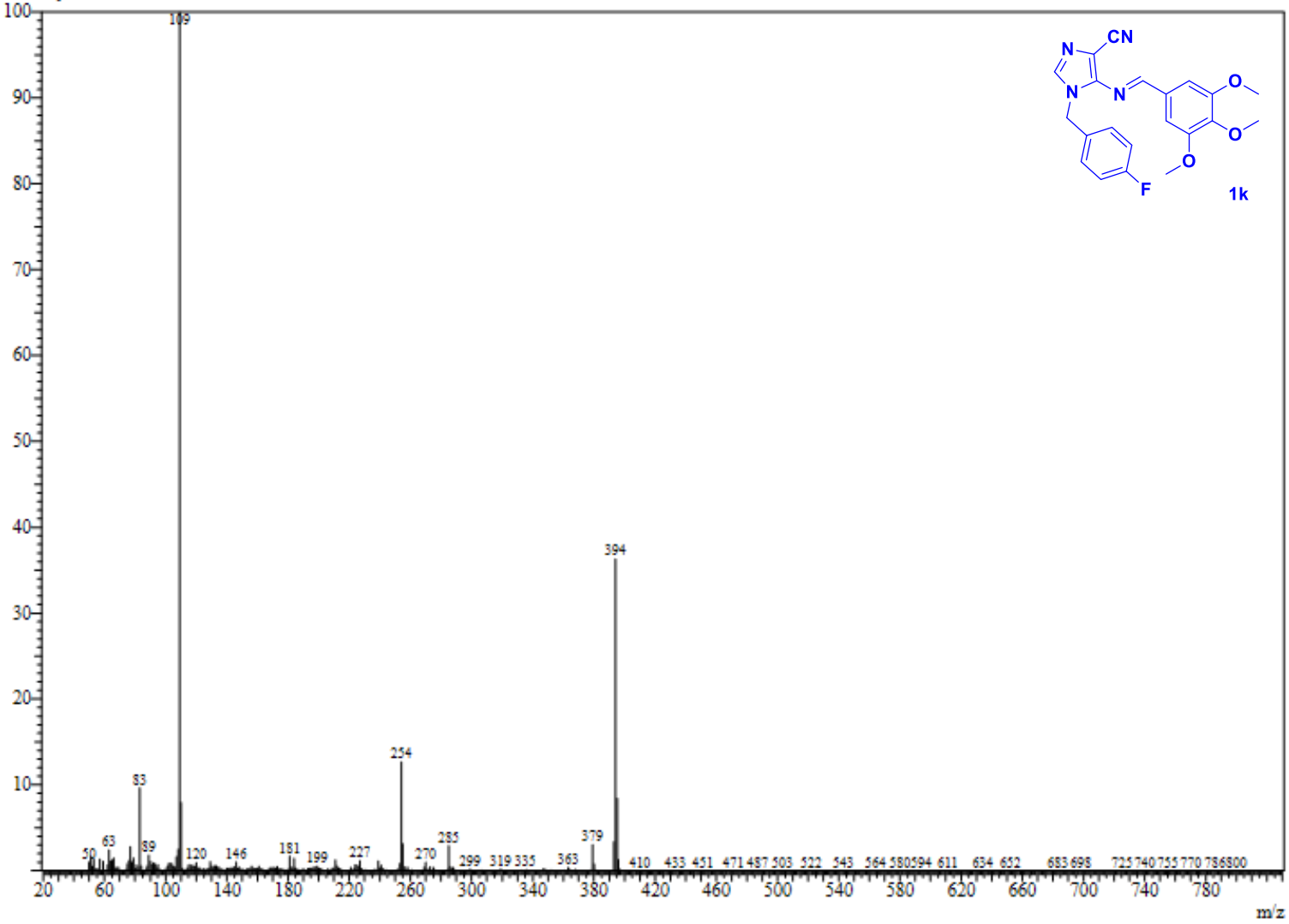
SA-1

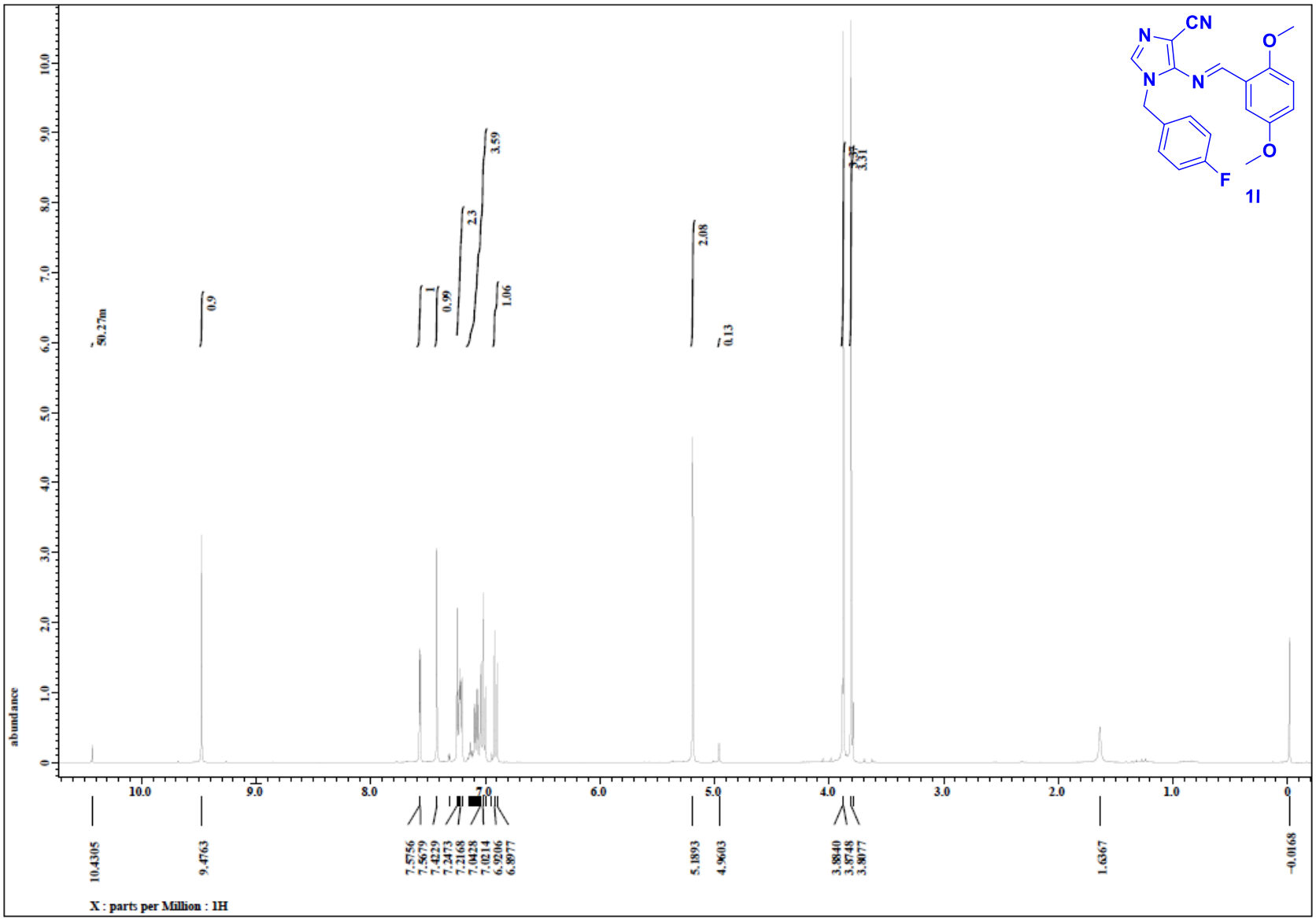


BRUKER

```
Current Data Parameters
NAME          Apr12-2017
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170412
Time               12.16
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                  256
DW               50.000 usec
DE                6.50 usec
TE                291.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SF01        500.3030896 MHz
NUC1                1H
P1                15.10 usec
PLW1        15.13599968 W

F2 - Processing parameters
SI                65536
SF          500.3000118 MHz
WDW                 EM
SSB       0
LB              0.30 Hz
GB        0
PC                1.00
```

Line#:2 R.Time:6.590(Scan#:1019)
MassPeaks:567
RawMode:Averaged 6.585-6.595(1018-1020) BasePeak:109(2294380)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity




CN
N
N
N
O
O
F
1l
abundance
50.27m
0.9
1
0.99
2.3
3.59
1.06
2.08
0.13
3.37
3.31
10.4305
9.4763
7.5756
7.5679
7.4229
7.2473
7.2168
7.0428
7.0214
6.9206
6.8977
5.1893
4.9603
3.8840
3.8748
3.8077
1.6367
-0.0168
X : parts per Million : 1H

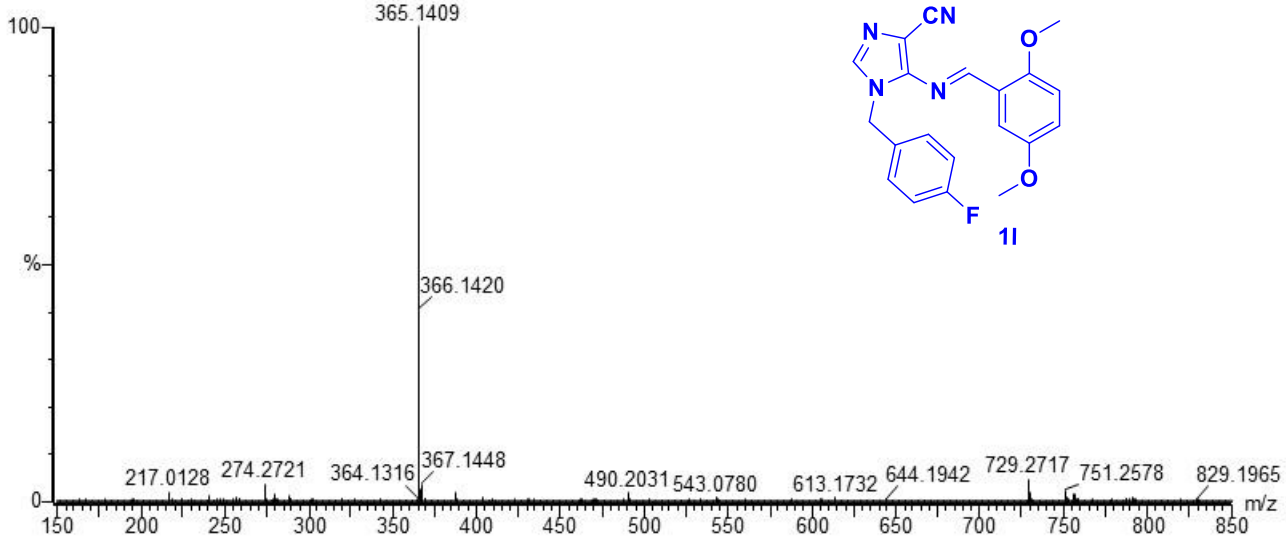
Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
43 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-22 H: 11-30 N: 0-5 O: 0-3 F: 0-1

Sample Name : SA-2 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
160120-SA-2 12 (0.131) 1: TOF MS ES+
1.44e+008

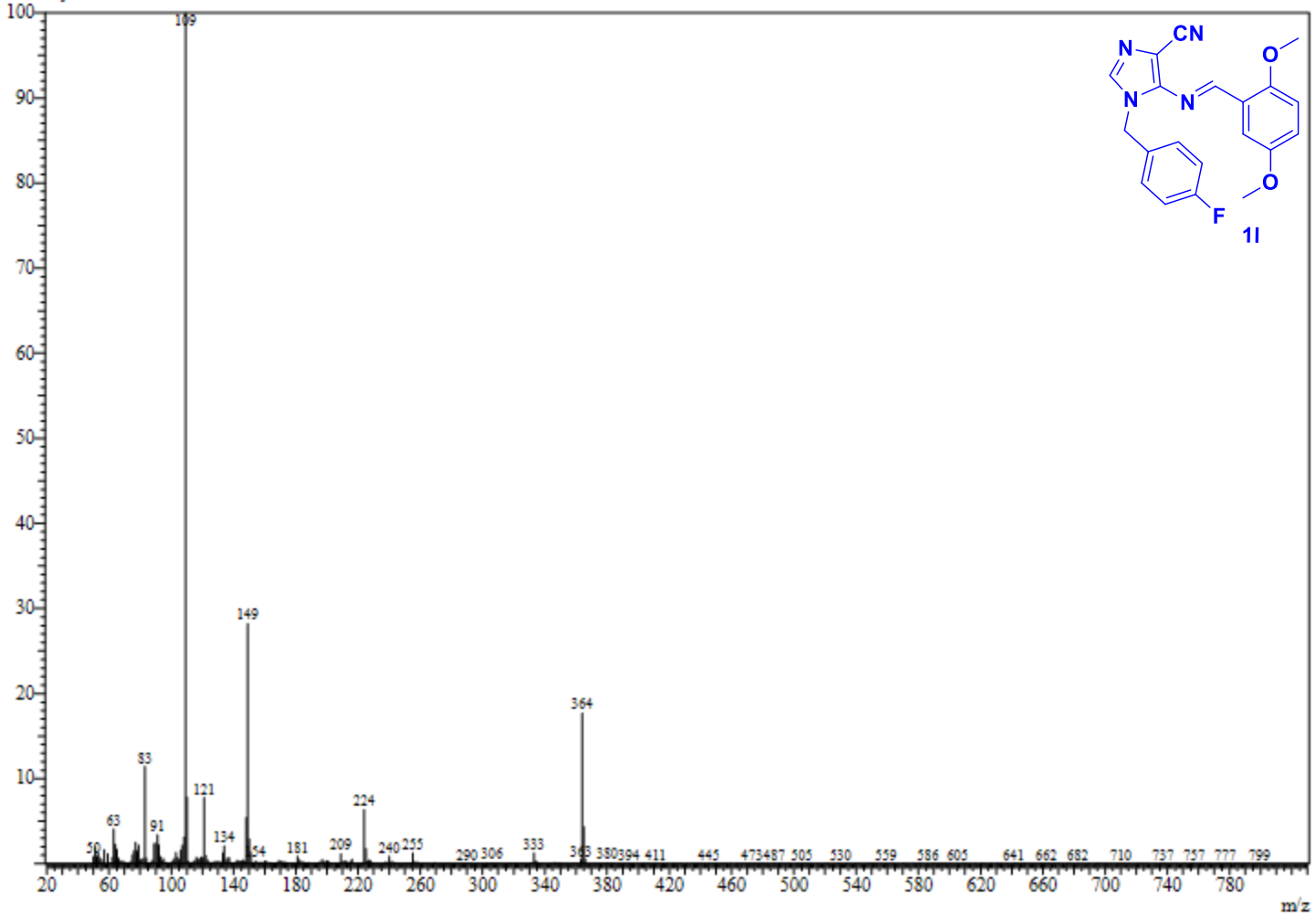


1l

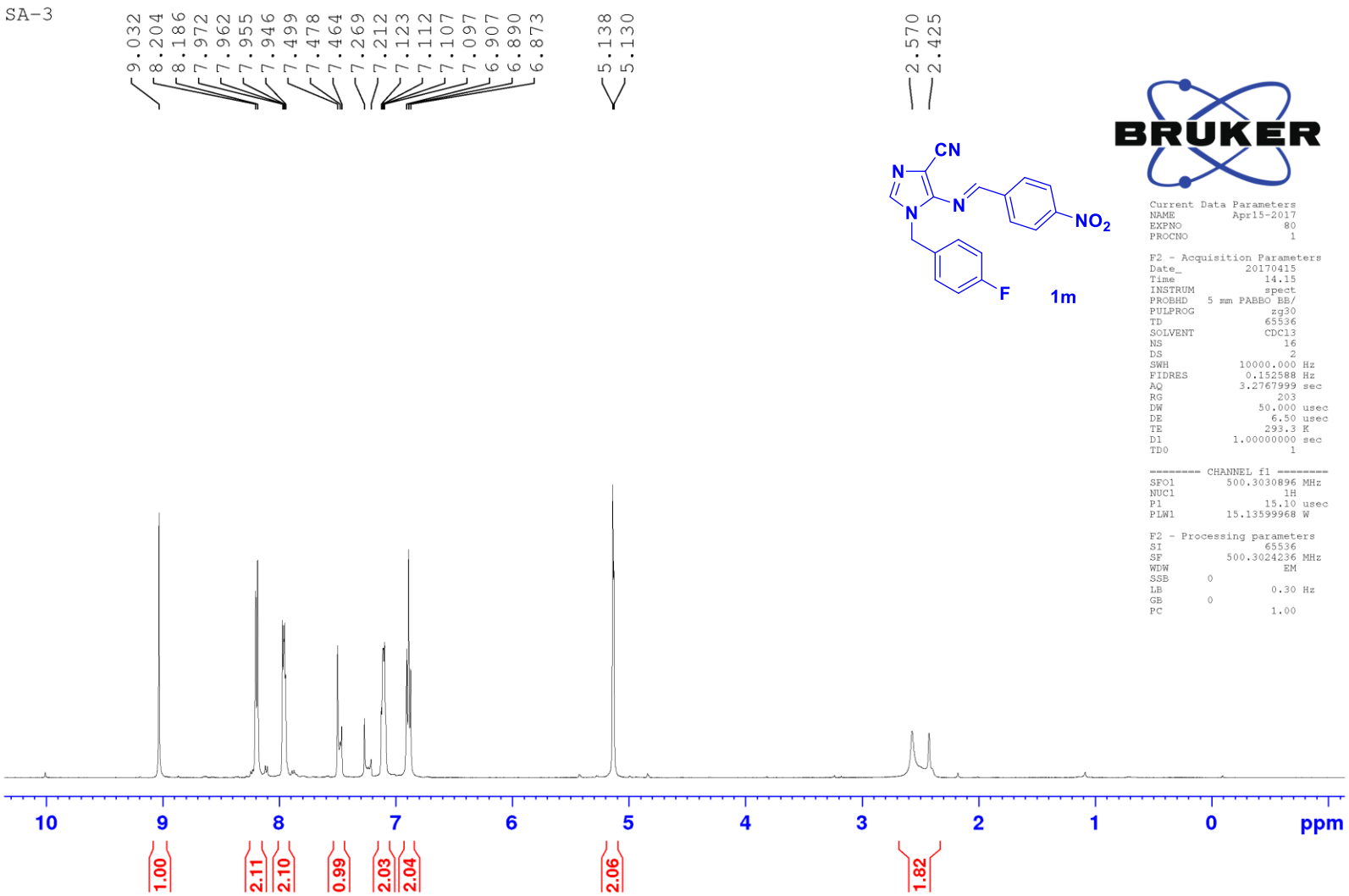
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
365.1409	365.1414	-0.5	-1.4	13.5	1846.9	n/a	n/a	C20 H18 N4 O2 F

Spectrum

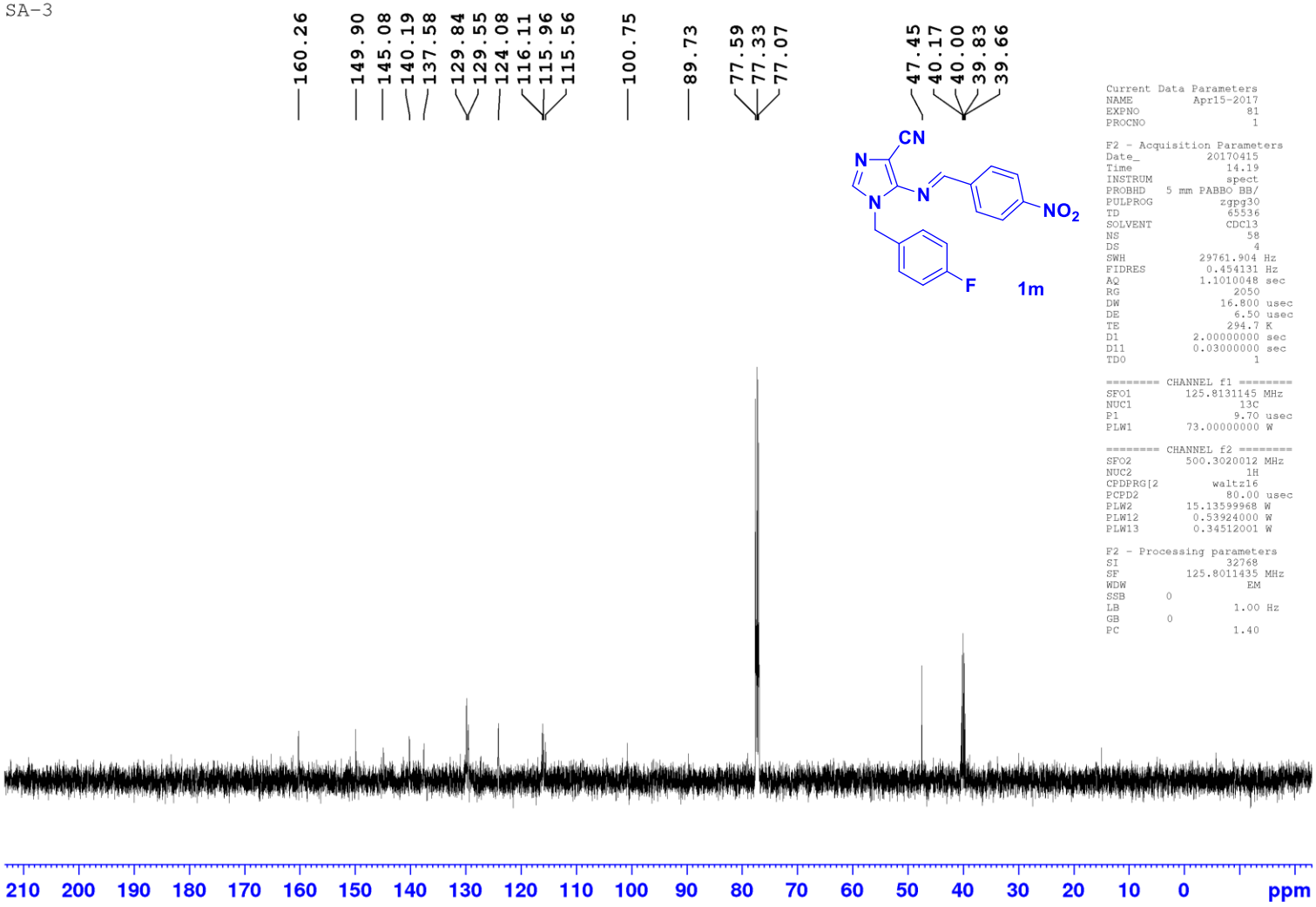
Line#:1 R.Time:5.230(Scan#:747)
MassPeaks:585
RawMode:Averaged 5.225-5.235(746-748) BasePeak:109(5182759)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity



1l


SA-3
9.032
8.204
8.186
7.972
7.962
7.955
7.946
7.499
7.478
7.464
7.269
7.212
7.123
7.112
7.107
7.097
6.907
6.890
6.873
5.138
5.130
2.570
2.425
CN
N
N
N
NO2
F
1m
BRUKER
Current Data Parameters
NAME Apr15-2017
EXPNO 80
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170415
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W
F2 - Processing parameters
SI 65536
SF 500.3024236 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.11
2.10
0.99
2.03
2.04
2.06
1.82

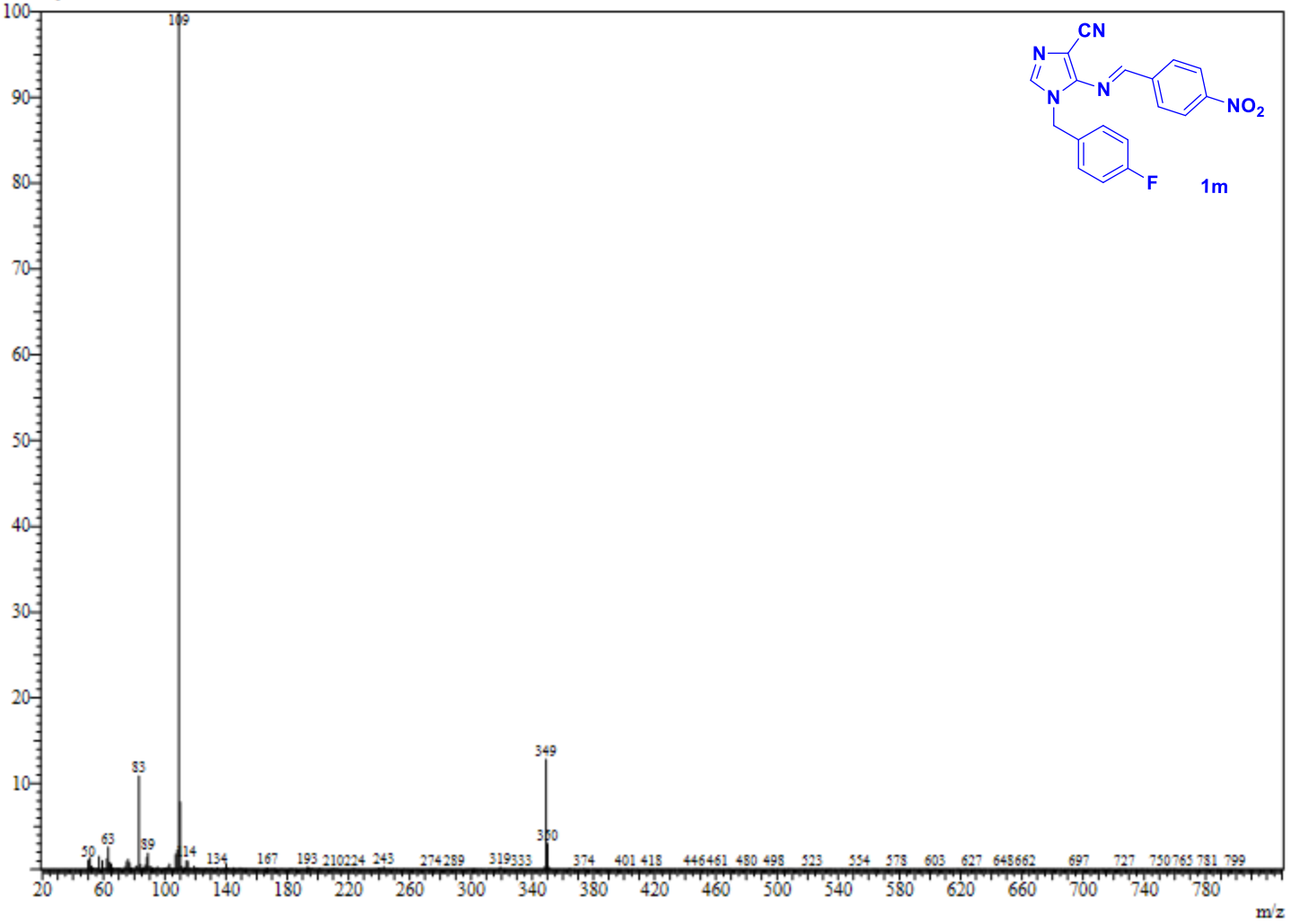
SA-3

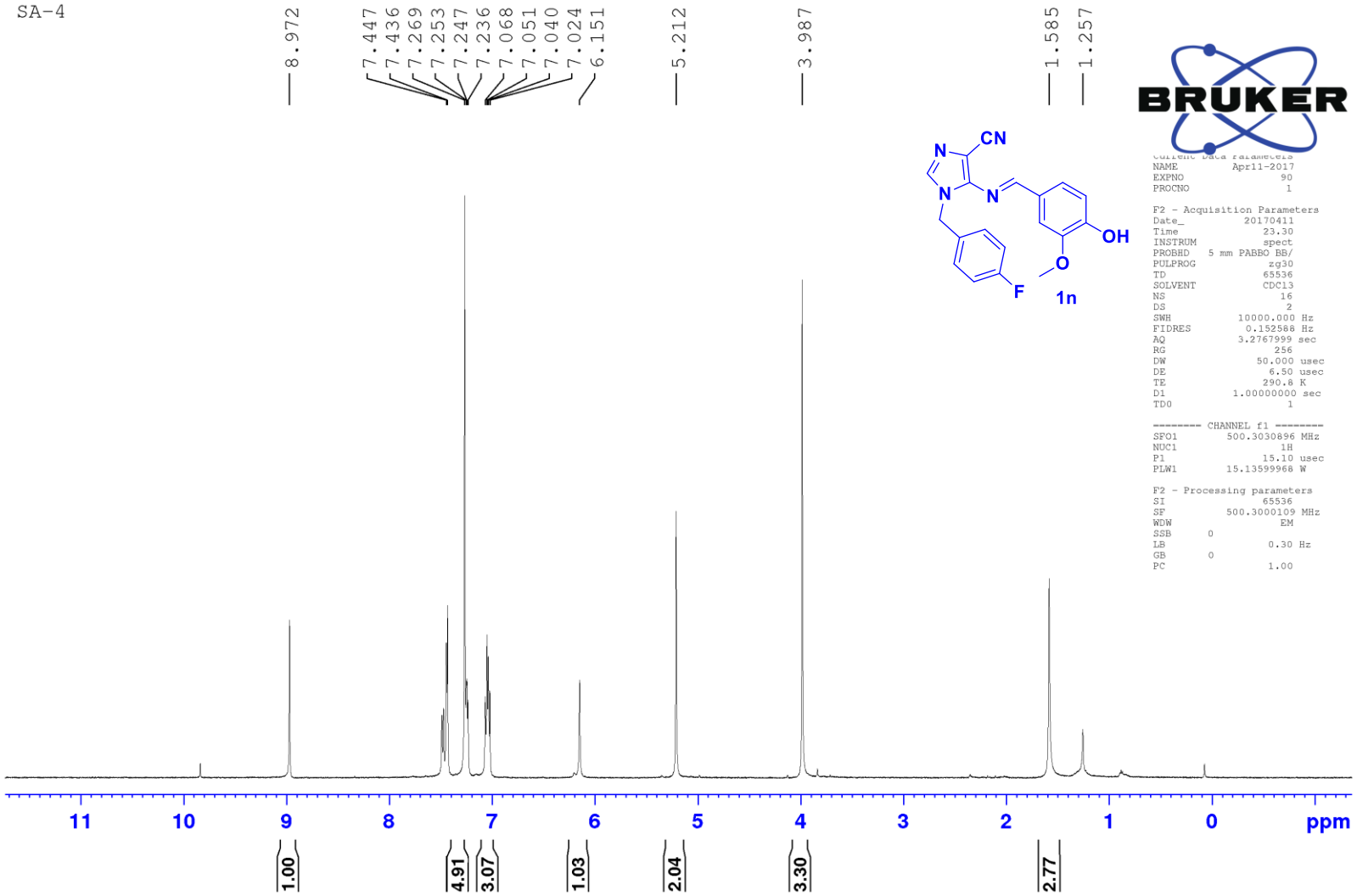



```
Current Data Parameters
NAME          Apr15-2017
EXPNO                 81
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170415
Time              14.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                  58
DS                   4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                2050
DW              16.800 usec
DE               6.50 usec
TE               294.7 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        125.8131145 MHz
NUC1               13C
P1                9.70 usec
PLW1       73.00000000 W

======== CHANNEL f2 ========
SFO2        500.3020012 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2       15.13599968 W
PLW12       0.53924000 W
PLW13       0.34512001 W

F2 - Processing parameters
SI               32768
SF          125.8011435 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

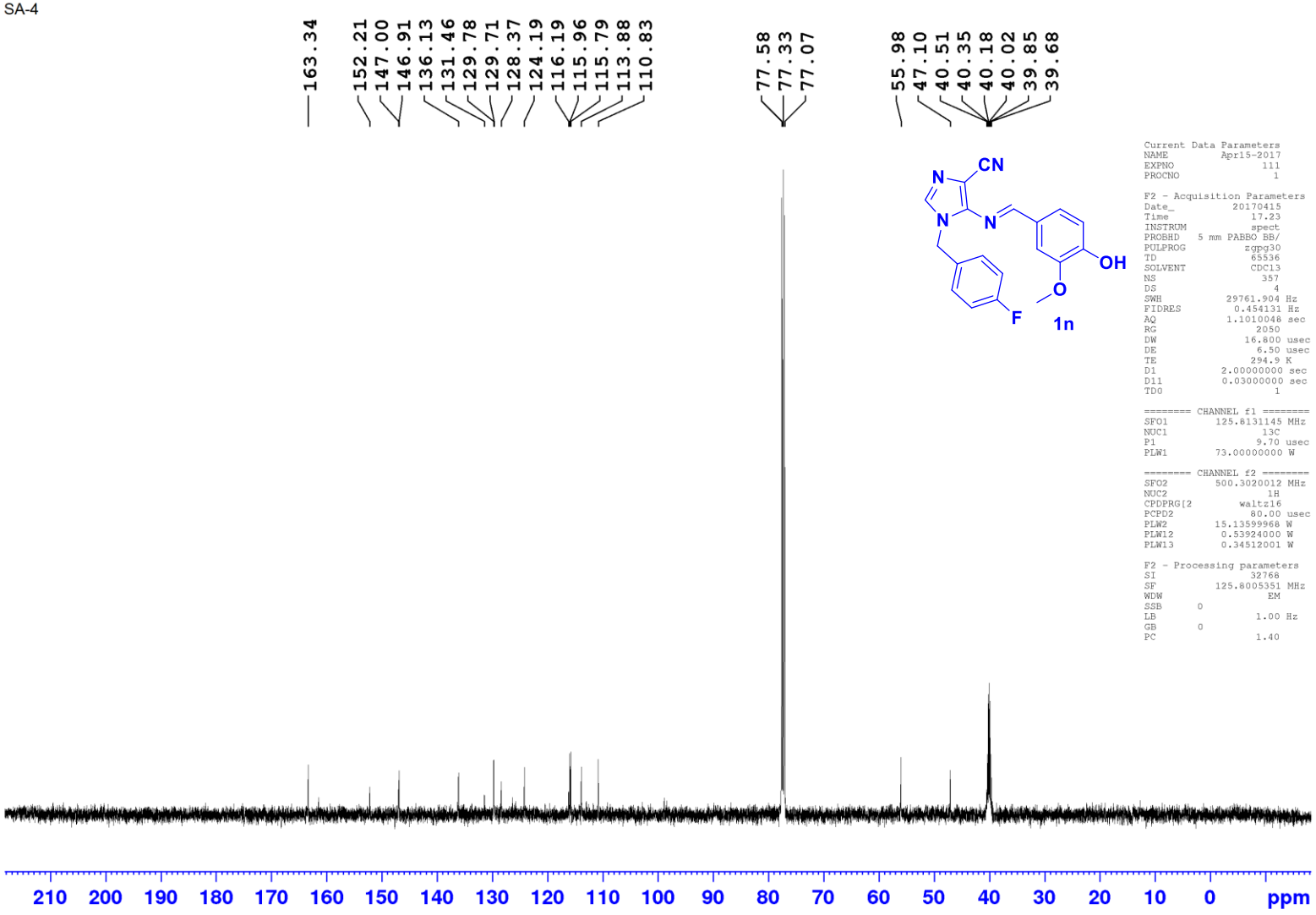
Spectrum

Line#:1 R.Time:5.910(Scan#:883)
MassPeaks:561
RawMode:Averaged 5.905-5.915(882-884) BasePeak:109(2769141)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity



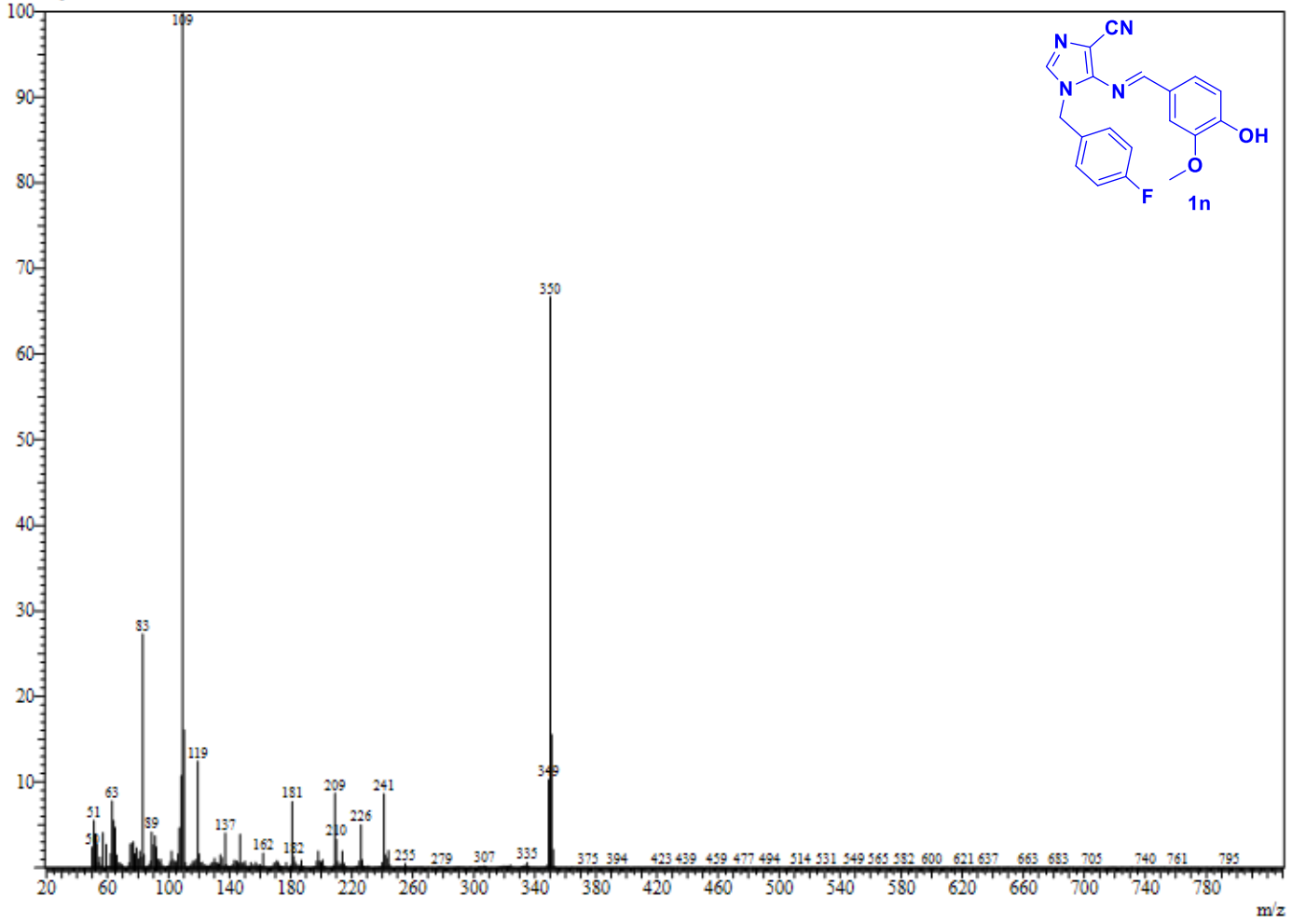

SA-4
8.972
7.447
7.436
7.269
7.253
7.247
7.236
7.068
7.051
7.040
7.024
6.151
5.212
3.987
1.585
1.257
CN
N
N
N
OH
O
F
1n
BRUKER
NAME Apr11-2017
EXPNO 90
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170411
Time 23.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 256
DW 50.000 usec
DE 6.50 usec
TE 290.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W
F2 - Processing parameters
SI 65536
SF 500.3000109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
4.91
3.07
1.03
2.04
3.30
2.77

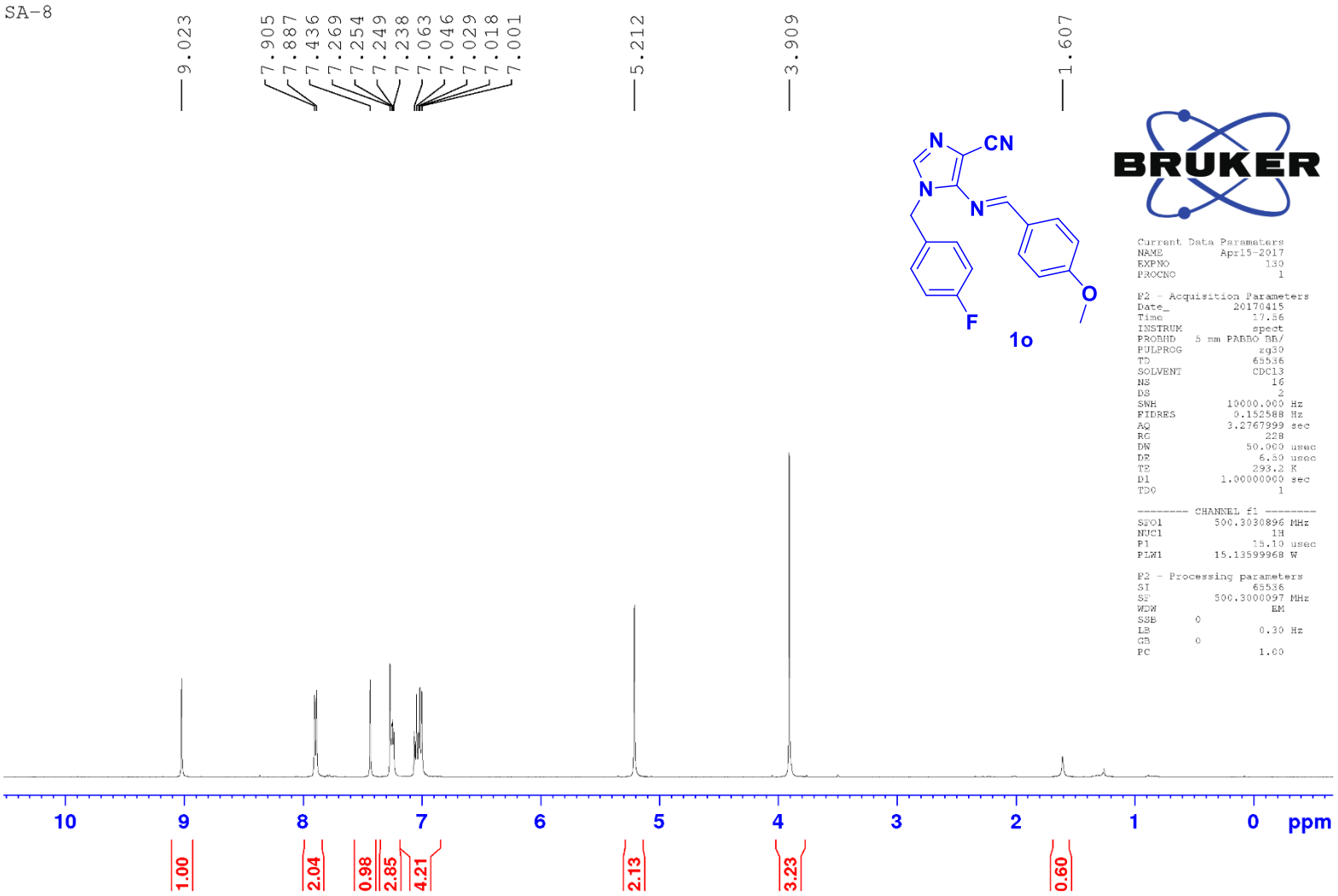
SA-4


163.34
152.21
147.00
146.91
136.13
131.46
129.78
129.71
128.37
124.19
116.19
115.96
115.79
113.88
110.83
77.58
77.33
77.07
55.98
47.10
40.51
40.35
40.18
40.02
39.85
39.68
CN
N
N
N
OH
O
F
1n
Current Data Parameters
NAME Apr15-2017
EXPNO 111
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170415
Time 17.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 357
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.8131145 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
======== CHANNEL f2 ========
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.34512001 W
F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

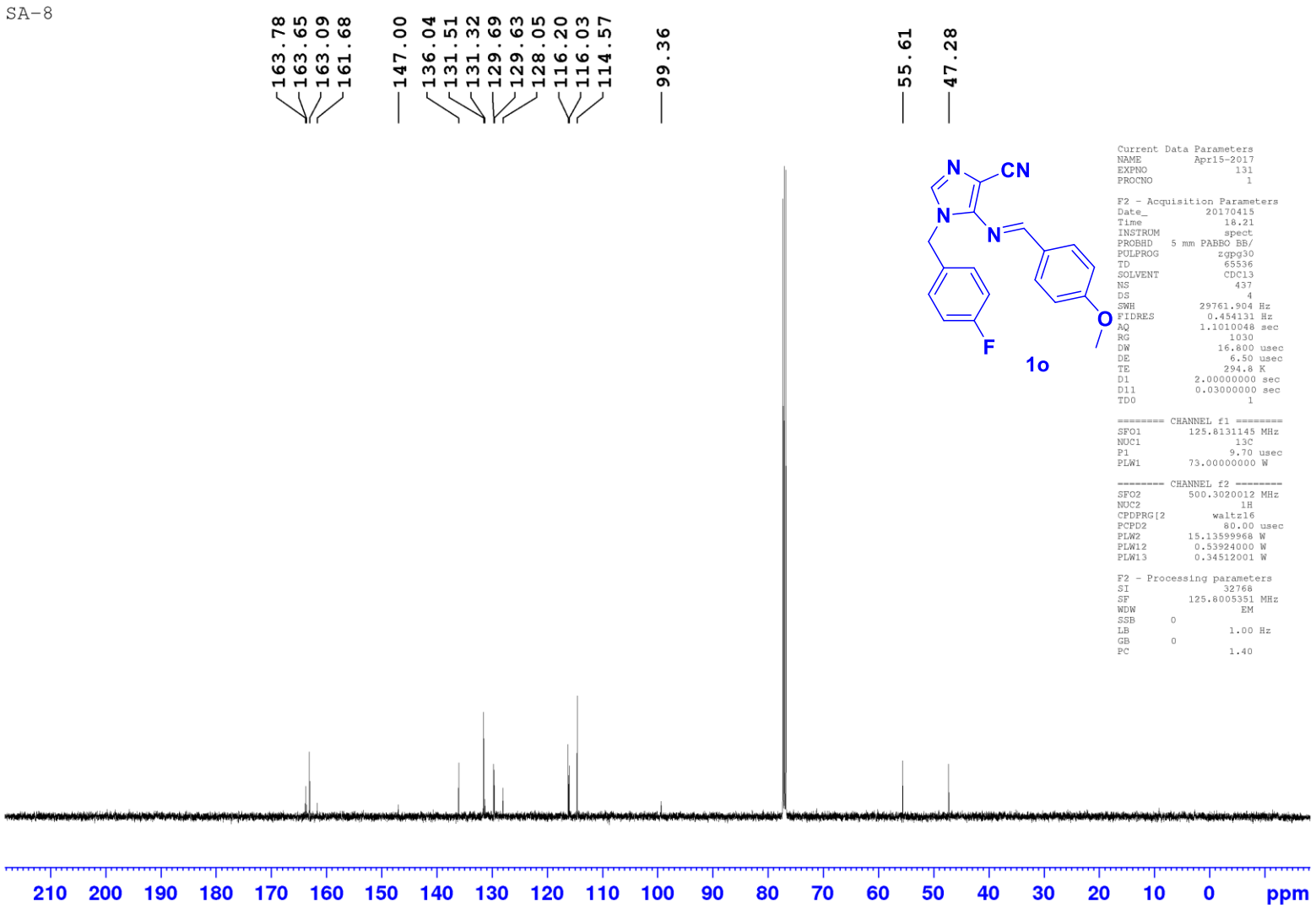
Spectrum

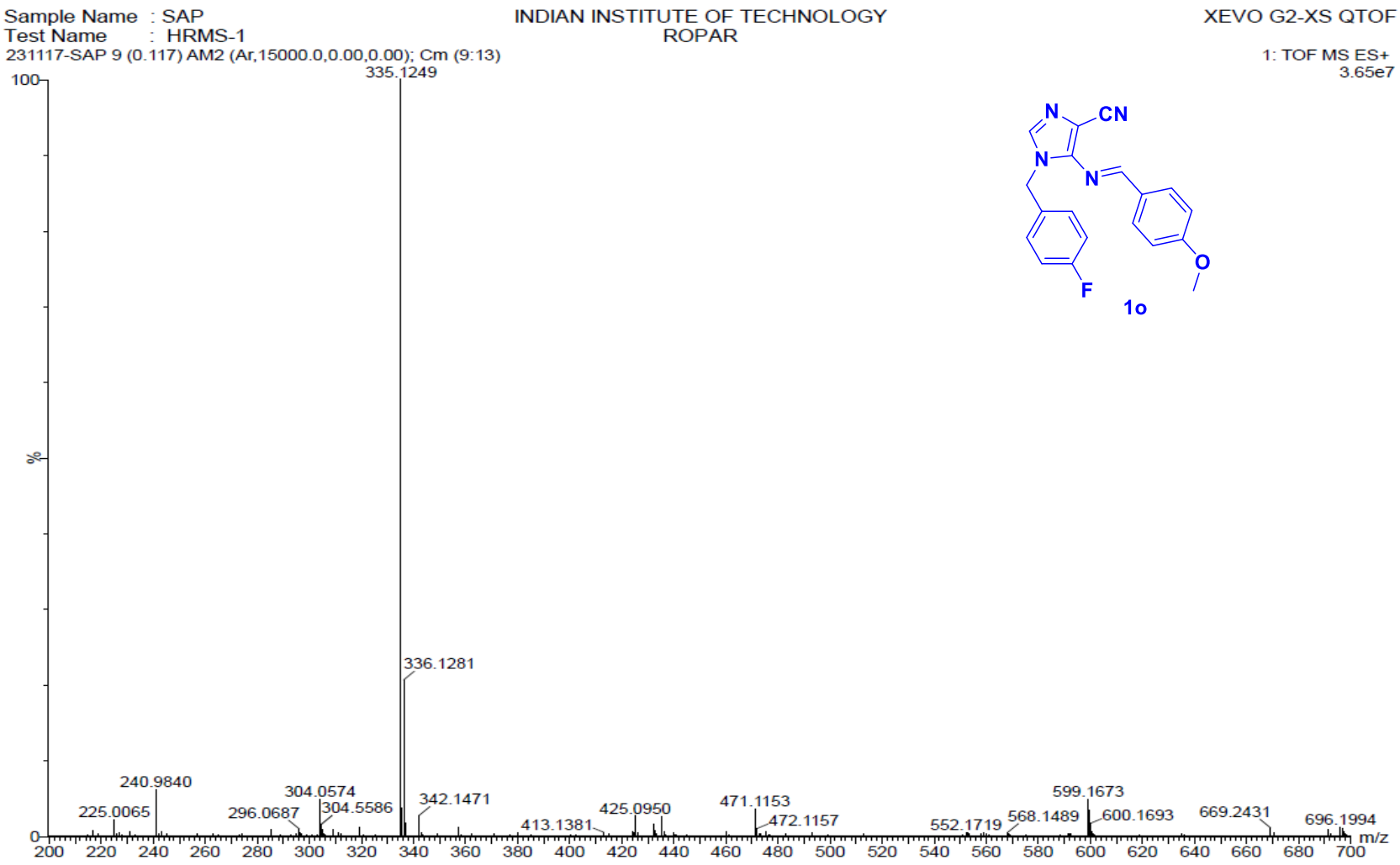
Line#:1 R.Time:6.445(Scan#:990)
MassPeaks:621
RawMode:Averaged 6.440-6.450(989-991) BasePeak:109(7420310)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity



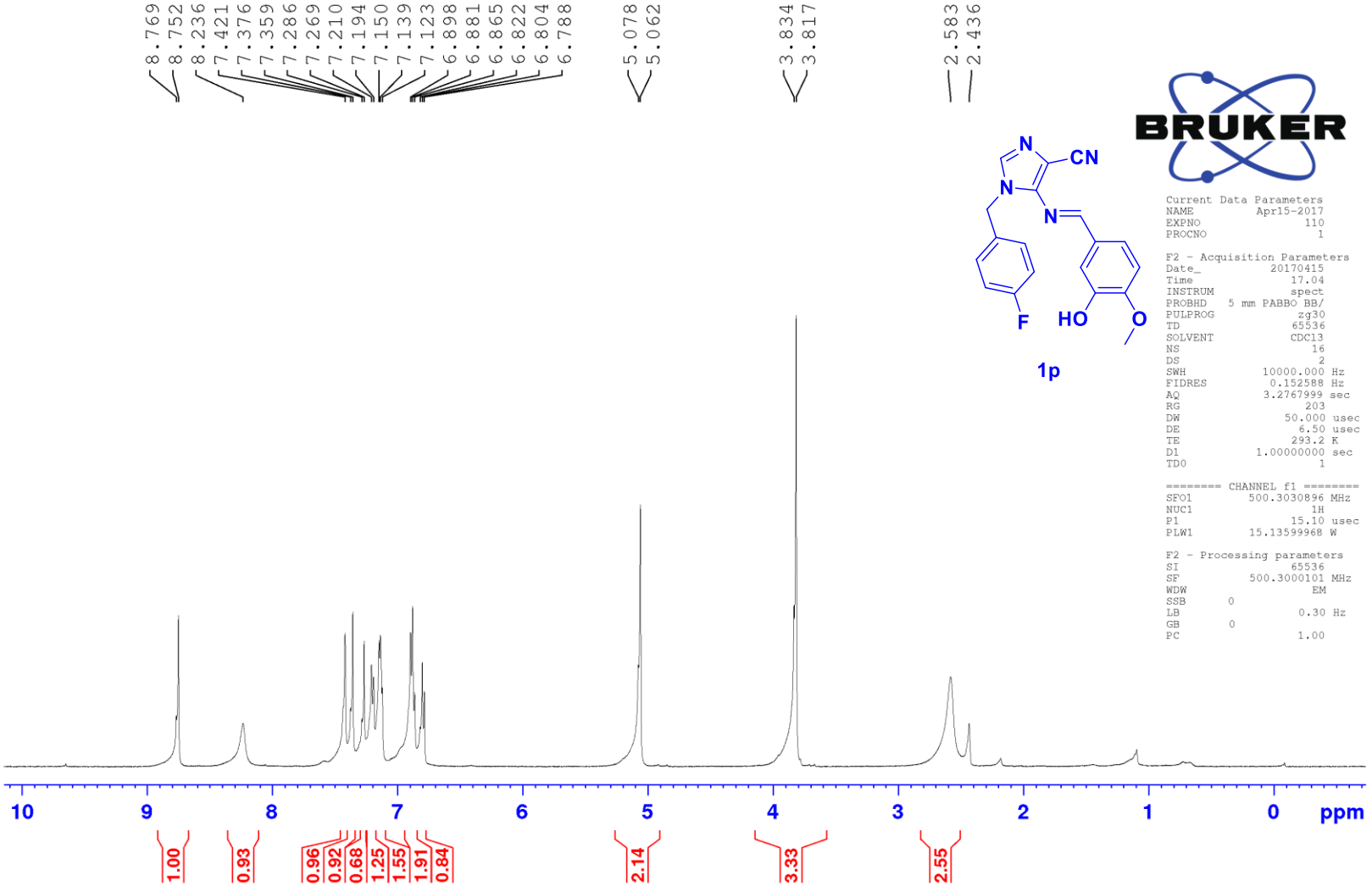

SA-8
9.023
7.905
7.887
7.436
7.269
7.254
7.249
7.238
7.063
7.046
7.029
7.018
7.001
5.212
3.909
1.607
N
CN
N
N
F
O
1o
BRUKER
Current Data Parameters
NAME Apr15-2017
EXPNO 130
PROCNO 1
P2 - Acquisition Parameters
Date_ 20170415
Time 17.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 228
DW 50.000 usec
DE 6.50 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1
-------- CHANNEL f1 --------
SFO1 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W
P2 - Processing parameters
SI 65536
SF 500.3000097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.04
0.98
2.85
4.21
2.13
3.23
0.60

SA-8

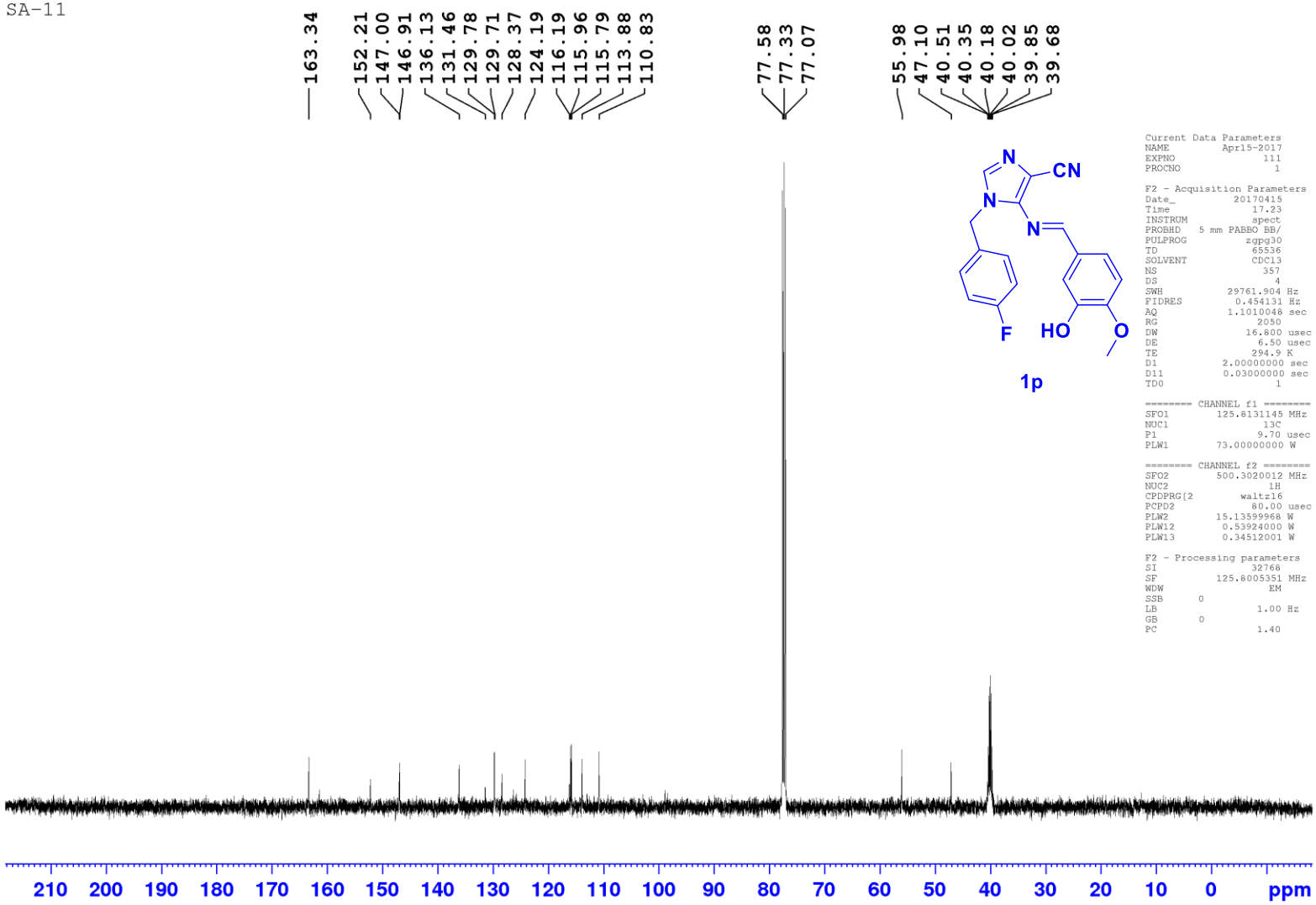

163.78
163.65
163.09
161.68
147.00
136.04
131.51
131.32
129.69
129.63
128.05
116.20
116.03
114.57
99.36
55.61
47.28
N
CN
N
N
O
F
1o
Current Data Parameters
NAME Apr15-2017
EXPNO 131
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170415
Time 18.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 437
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 1030
DW 16.800 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.8131145 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
======== CHANNEL f2 ========
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.34512001 W
F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Sample Name : SAP
Test Name : HRMS-1
231117-SAP 9 (0.117) AM2 (Ar,15000.0,0.00,0.00); Cm (9:13)
INDIAN INSTITUTE OF TECHNOLOGY
ROPAR
XEVO G2-XS QTOF
1: TOF MS ES+
3.65e7
100
%
0
335.1249
336.1281
240.9840
225.0065
304.0574
304.5586
296.0687
342.1471
413.1381
425.0950
471.1153
472.1157
552.1719
568.1489
599.1673
600.1693
669.2431
696.1994
200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 660 680 700
m/z
N
CN
N
N
O
F
1o

SA-11

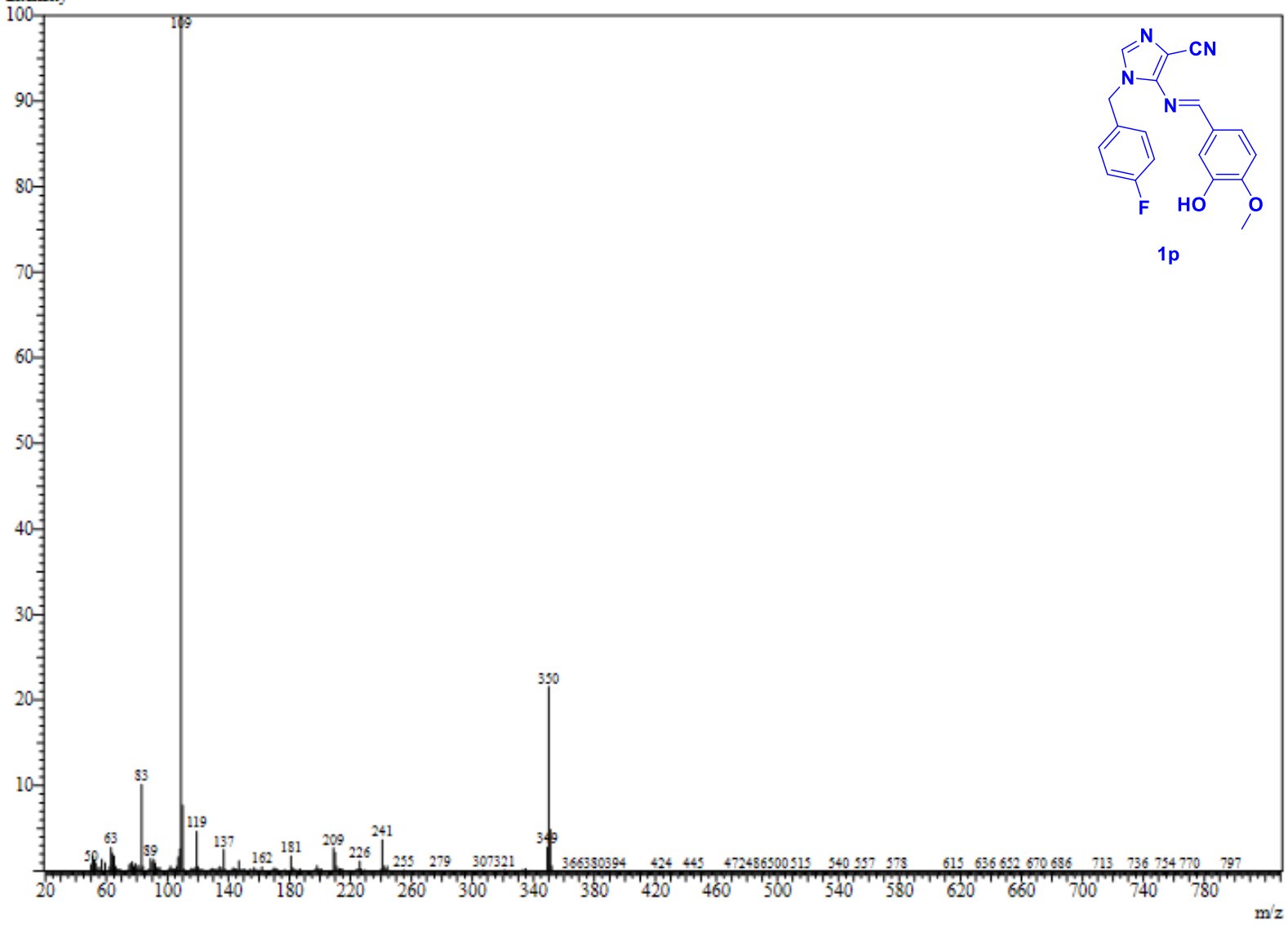

8.769
8.752
8.236
7.421
7.376
7.359
7.286
7.269
7.210
7.194
7.150
7.139
7.123
6.898
6.881
6.865
6.822
6.804
6.788
5.078
5.062
3.834
3.817
2.583
2.436
N
CN
N
N
F
HO
O
1p
BRUKER
Current Data Parameters
NAME Apr15-2017
EXPNO 110
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170415
Time 17.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W
F2 - Processing parameters
SI 65536
SF 500.3000101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.93
0.96
0.92
0.68
1.25
1.55
1.91
0.84
2.14
3.33
2.55

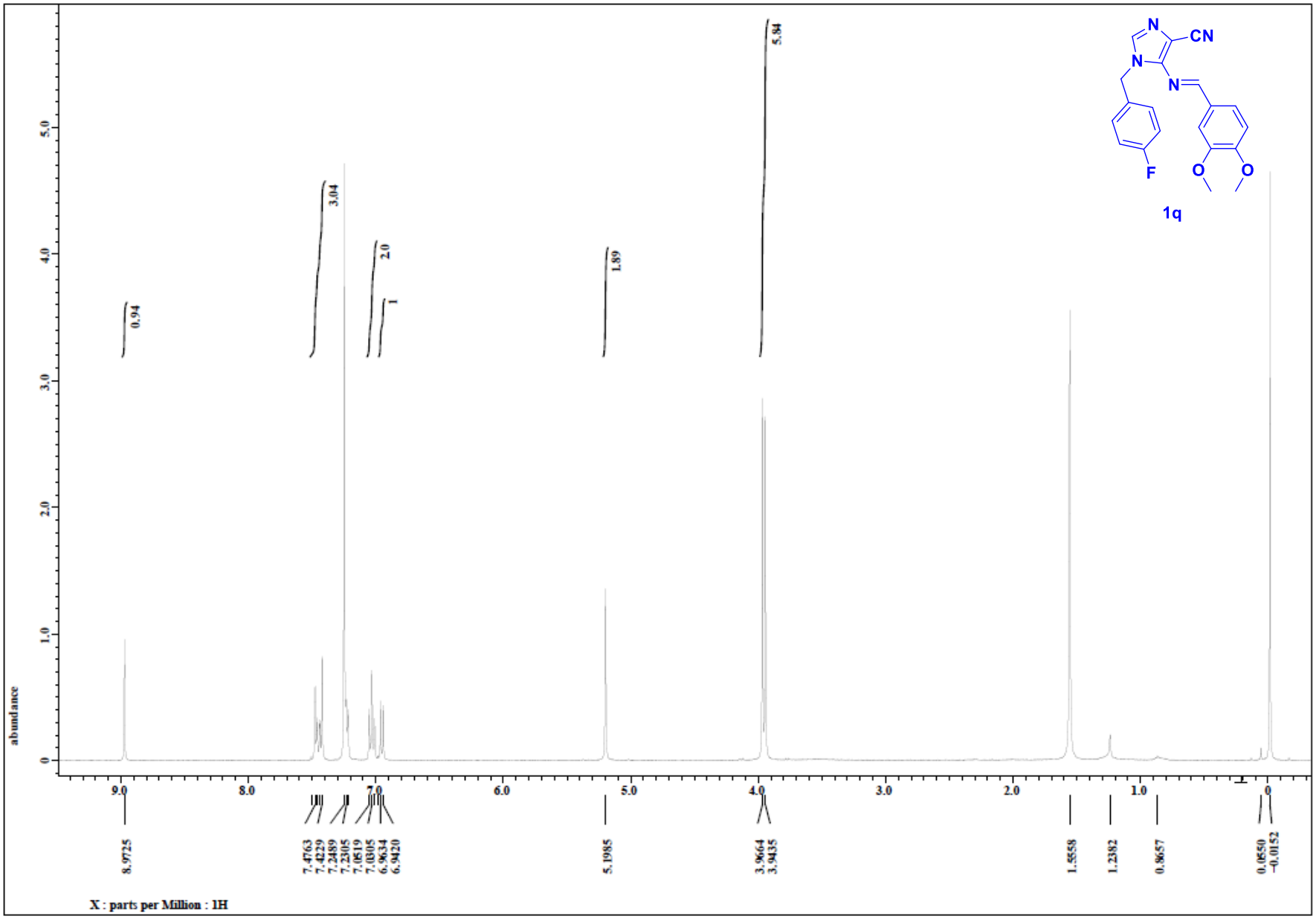
SA-11



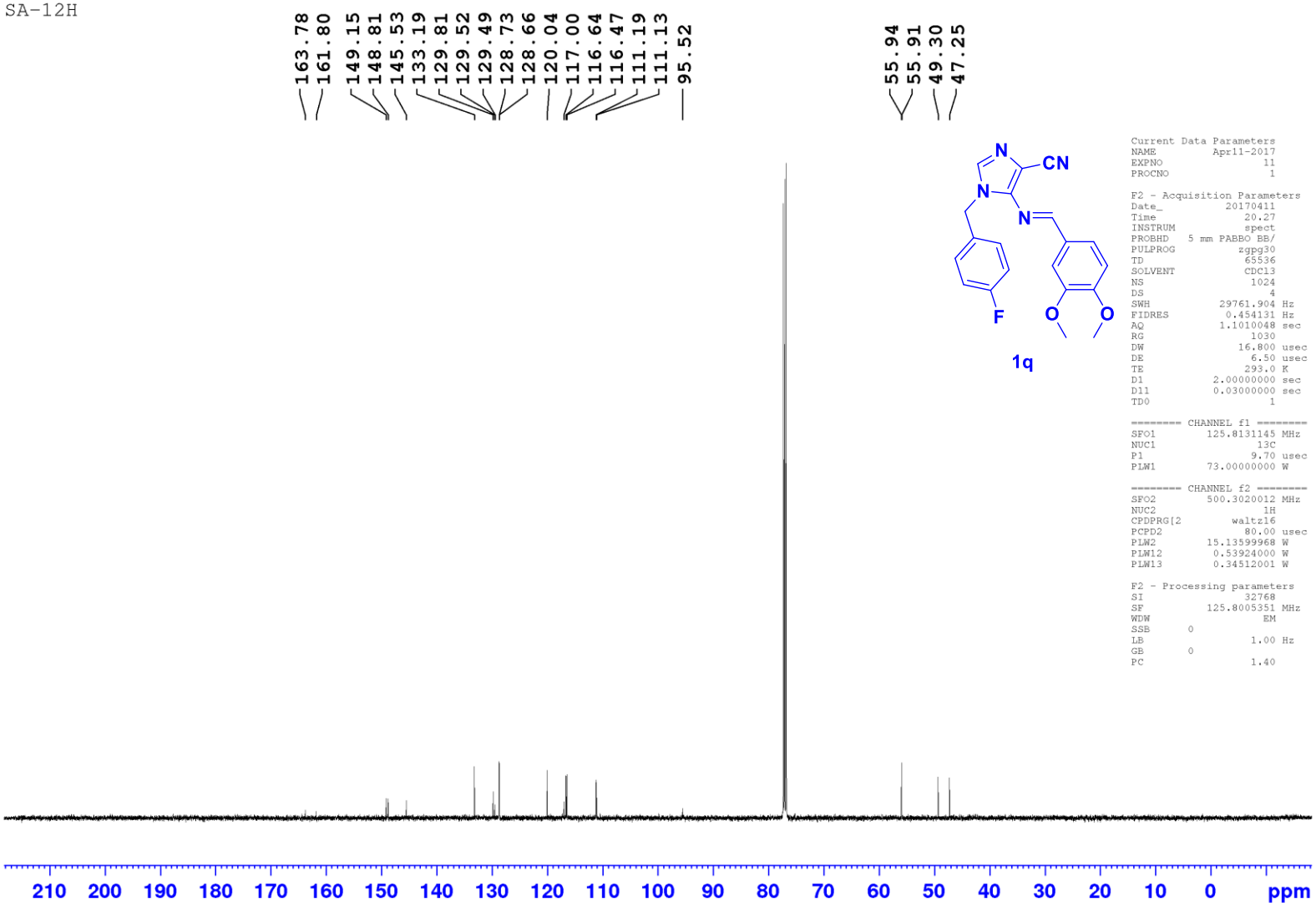

```
Current Data Parameters
NAME                 Apr15-2017
EXPNO                       111
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20170415
Time                      17.23
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         357
DS                           4
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                    1.1010048 sec
RG                        2050
DW                      16.800 usec
DE                       6.50 usec
TE                      294.9 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1                125.8131145 MHz
NUC1                        13C
P1                        9.70 usec
PLW1                73.00000000 W

======== CHANNEL f2 ========
SFO2                500.3020012 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    80.00 usec
PLW2                15.13599968 W
PLW12                0.53924000 W
PLW13                0.34512001 W

F2 - Processing parameters
SI                          32768
SF                  125.8005351 MHz
WDW                            EM
SSB                 0
LB                        1.00 Hz
GB                  0
PC                        1.40
```

Line#:2 R.Time:5.600(Scan#:821)
MassPeaks:564
RawMode:Averaged 5.595-5.605(820-822) BasePeak:109(3565792)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity




1q
abundance
X : parts per Million : 1H
0.94
3.04
2.0
1
1.89
5.84
8.9725
7.4763
7.4229
7.2489
7.2305
7.0619
7.0305
6.9634
6.9420
5.1985
3.9664
3.9435
1.5559
1.2382
0.8657
0.0550
-0.0152

SA-12H


163.78
161.80
149.15
148.81
145.53
133.19
129.81
129.52
129.49
128.73
128.66
120.04
117.00
116.64
116.47
111.19
111.13
95.52
55.94
55.91
49.30
47.25
N
CN
N
N
F
O
O
1q
Current Data Parameters
NAME Apr11-2017
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170411
Time 20.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 1030
DW 16.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.8131145 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
======== CHANNEL f2 ========
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.34512001 W
F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Elemental Composition Report

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

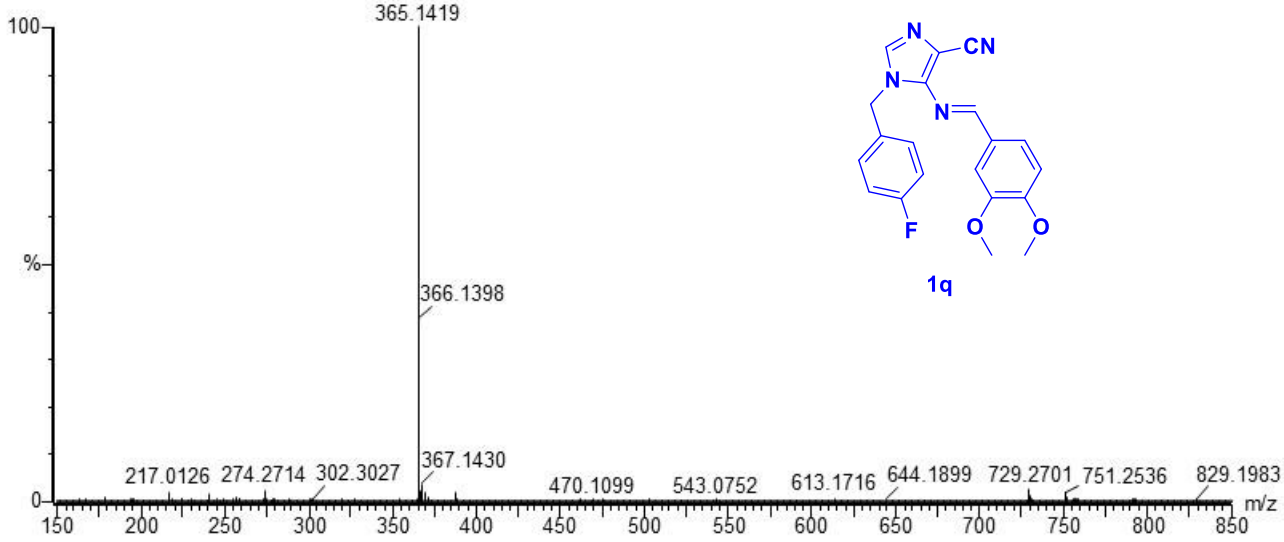
Monoisotopic Mass, Even Electron Ions
43 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-22 H: 11-30 N: 0-5 O: 0-3 F: 0-1

Sample Name : SA-12
Test Name : HRMS-1
160120-SA-12 17 (0.174)

IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
4.61e+007

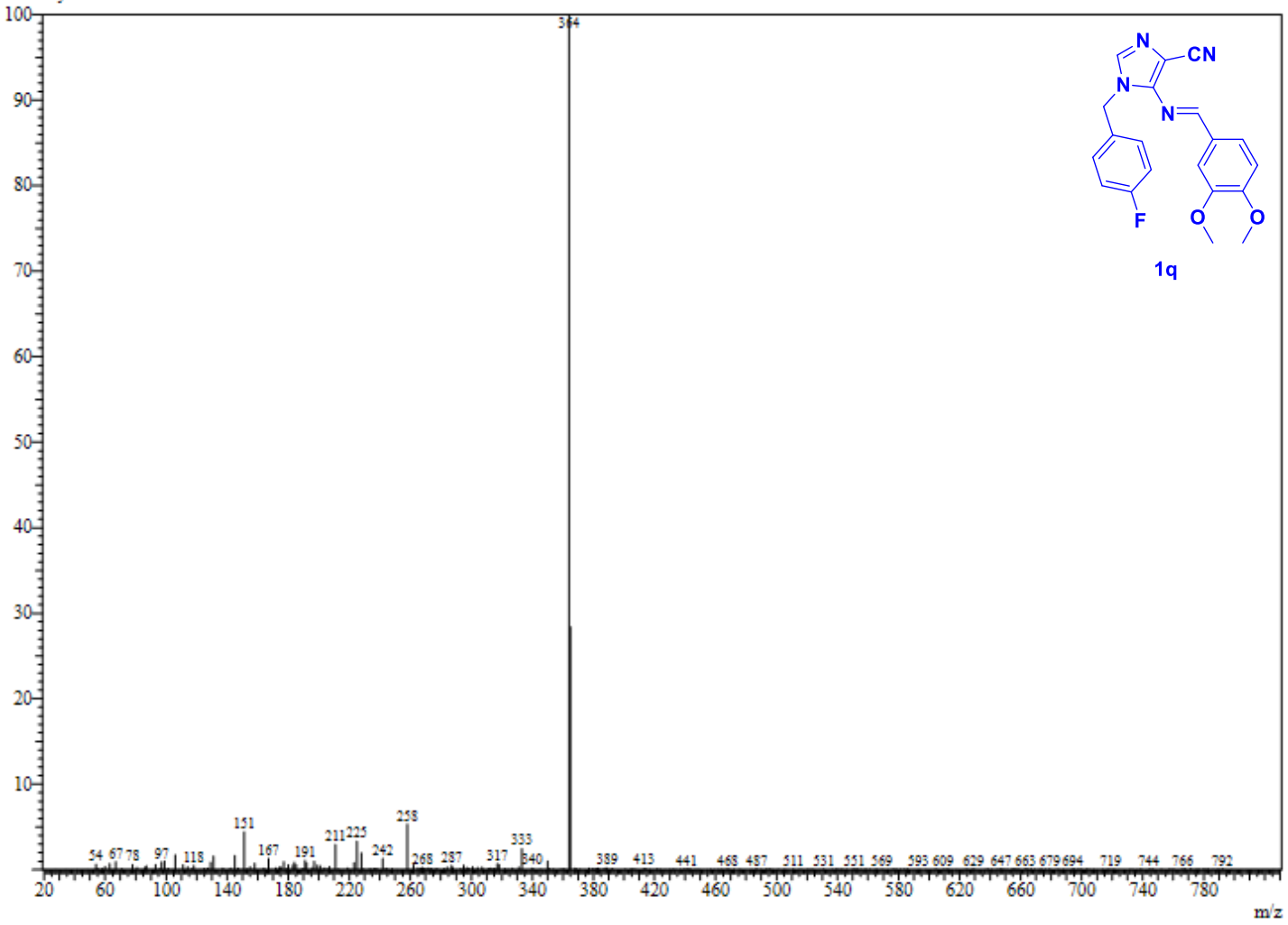


1q

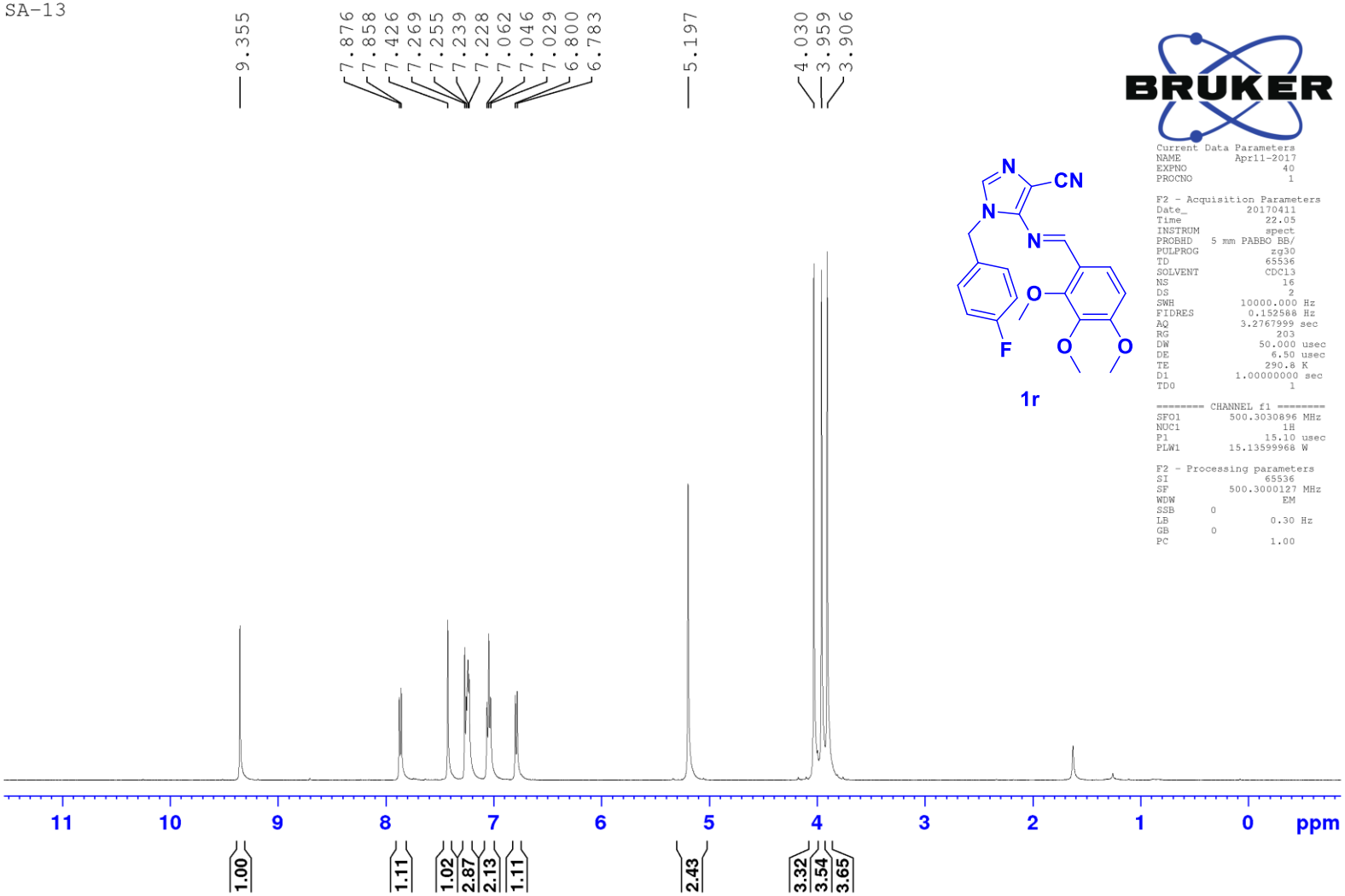
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
365.1419	365.1414	0.5	1.4	13.5	2169.2	n/a	n/a	C20 H18 N4 O2 F

Spectrum

Line#:1 R.Time:6.395(Scan#:980)
MassPeaks:305
RawMode:Averaged 6.395-6.400(980-981) BasePeak:364(14417)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity



SA-13



1r

BRUKER

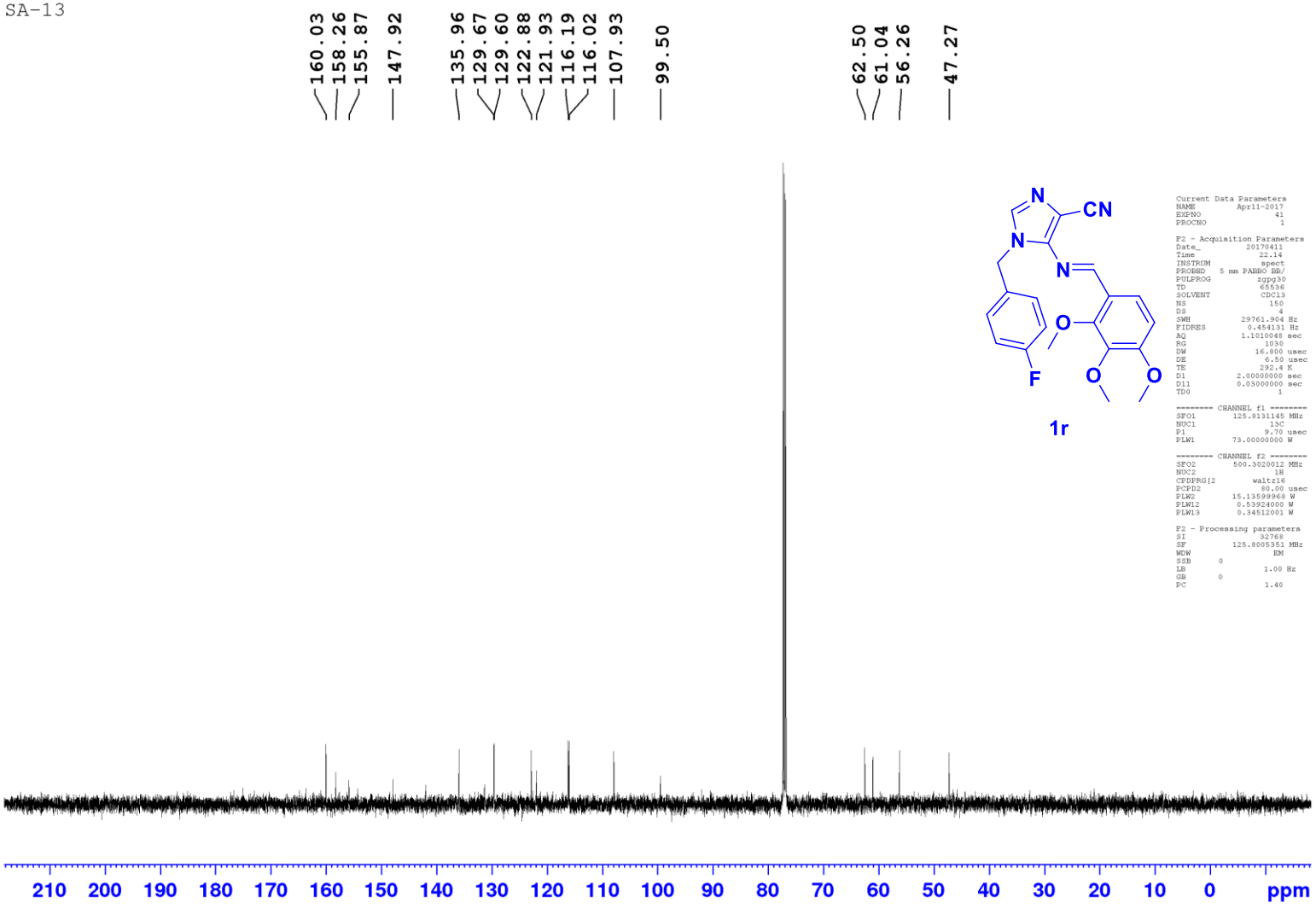
Current Data Parameters
NAME Apr11-2017
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170411
Time 22.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 290.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 500.3030896 MHz
NUC1 1H
P1 15.10 usec
PLW1 15.13599968 W

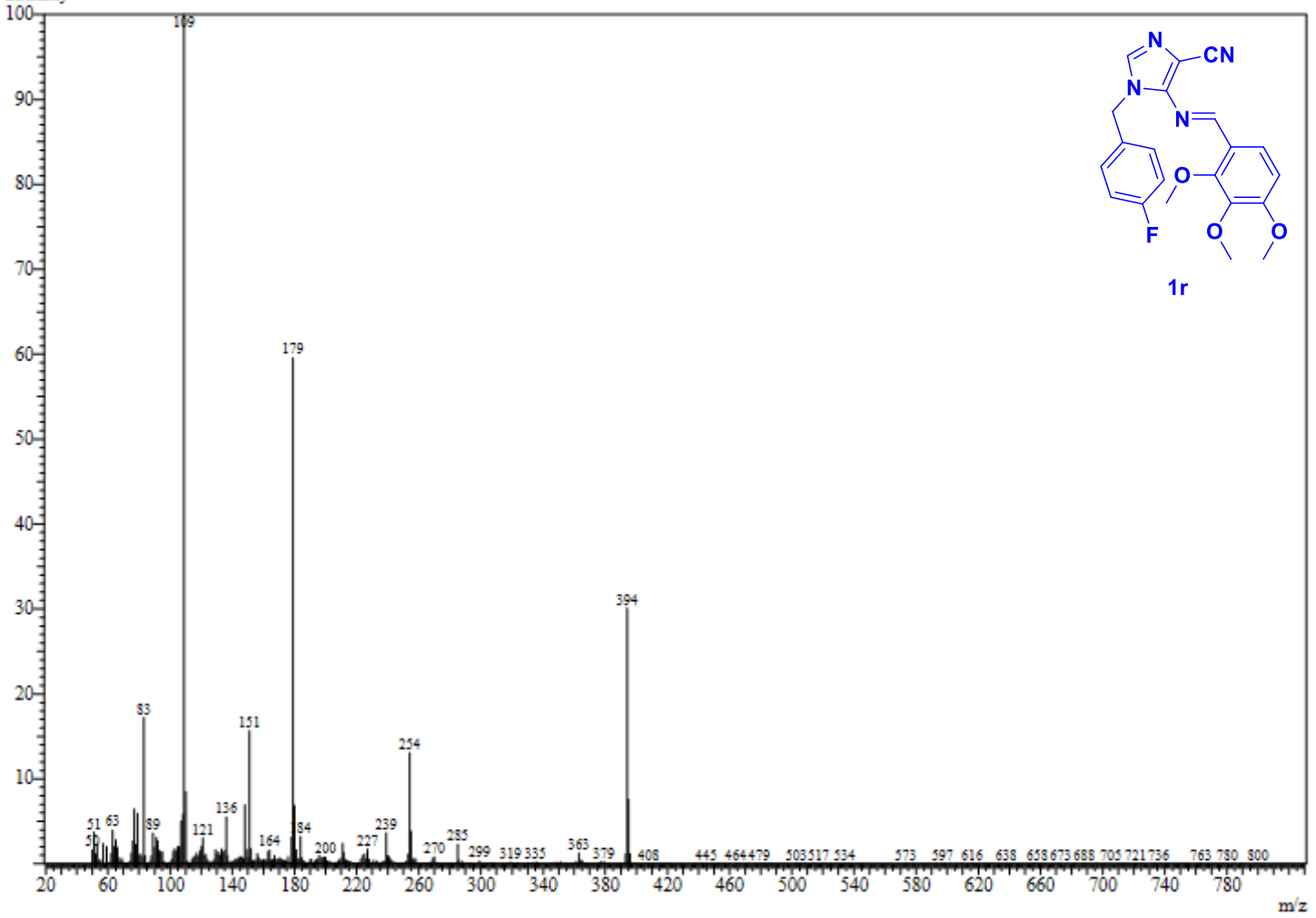
F2 - Processing parameters
SI 65536
SF 500.3000127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

SA-13

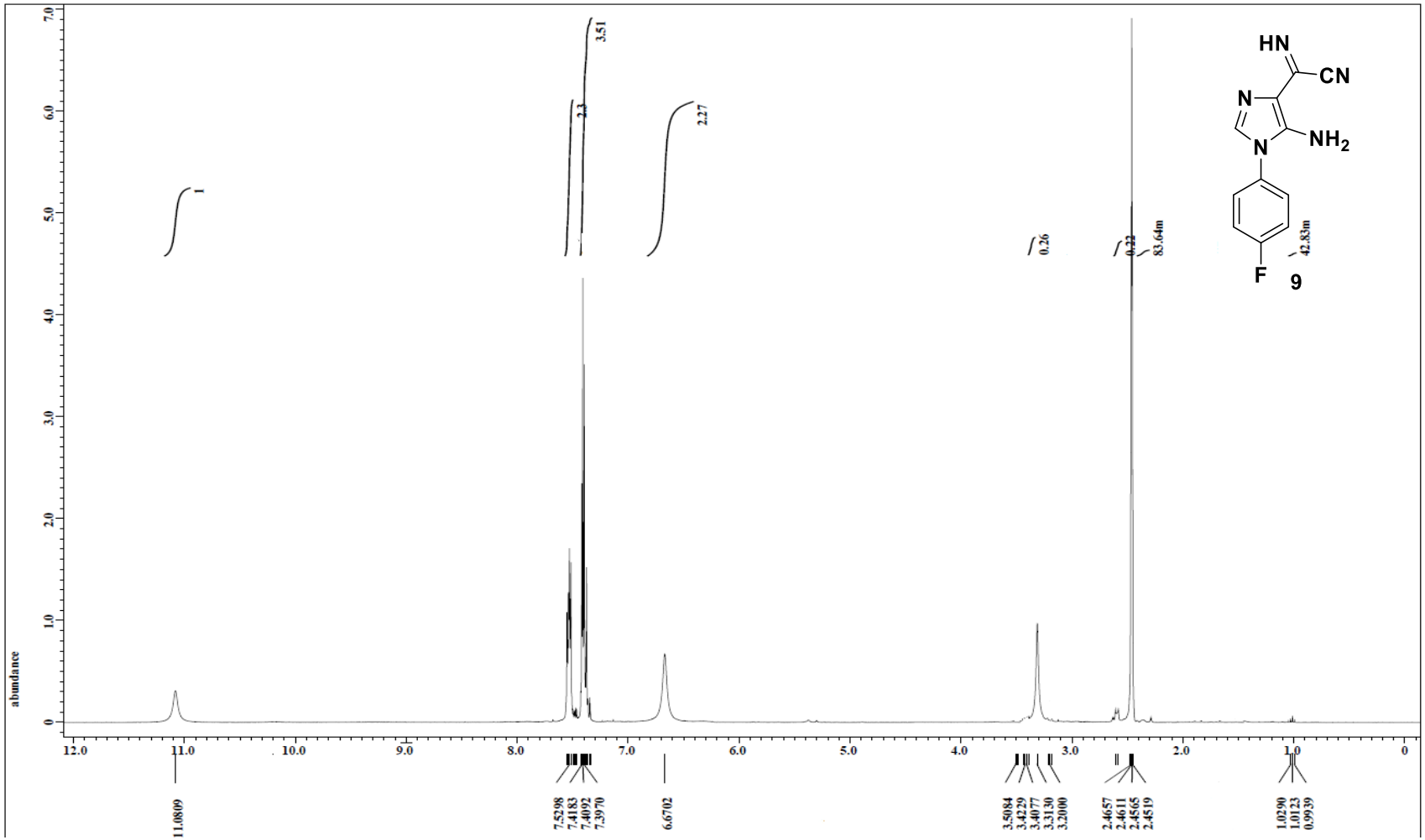

160.03
158.26
155.87
147.92
135.96
129.67
129.60
122.88
121.93
116.19
116.02
107.93
99.50
62.50
61.04
56.26
47.27
N
CN
N
N
O
F
O
O
1r
Current Data Parameters
NAME Apr11-2017
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170411
Time 22.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 150
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 1030
DW 16.800 usec
DE 6.50 usec
TE 292.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 125.8131145 MHz
NUC1 13C
P1 9.70 usec
PLW1 73.00000000 W
======== CHANNEL f2 ========
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.13599968 W
PLW12 0.53924000 W
PLW13 0.34512001 W
F2 - Processing parameters
SI 32768
SF 125.8005351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

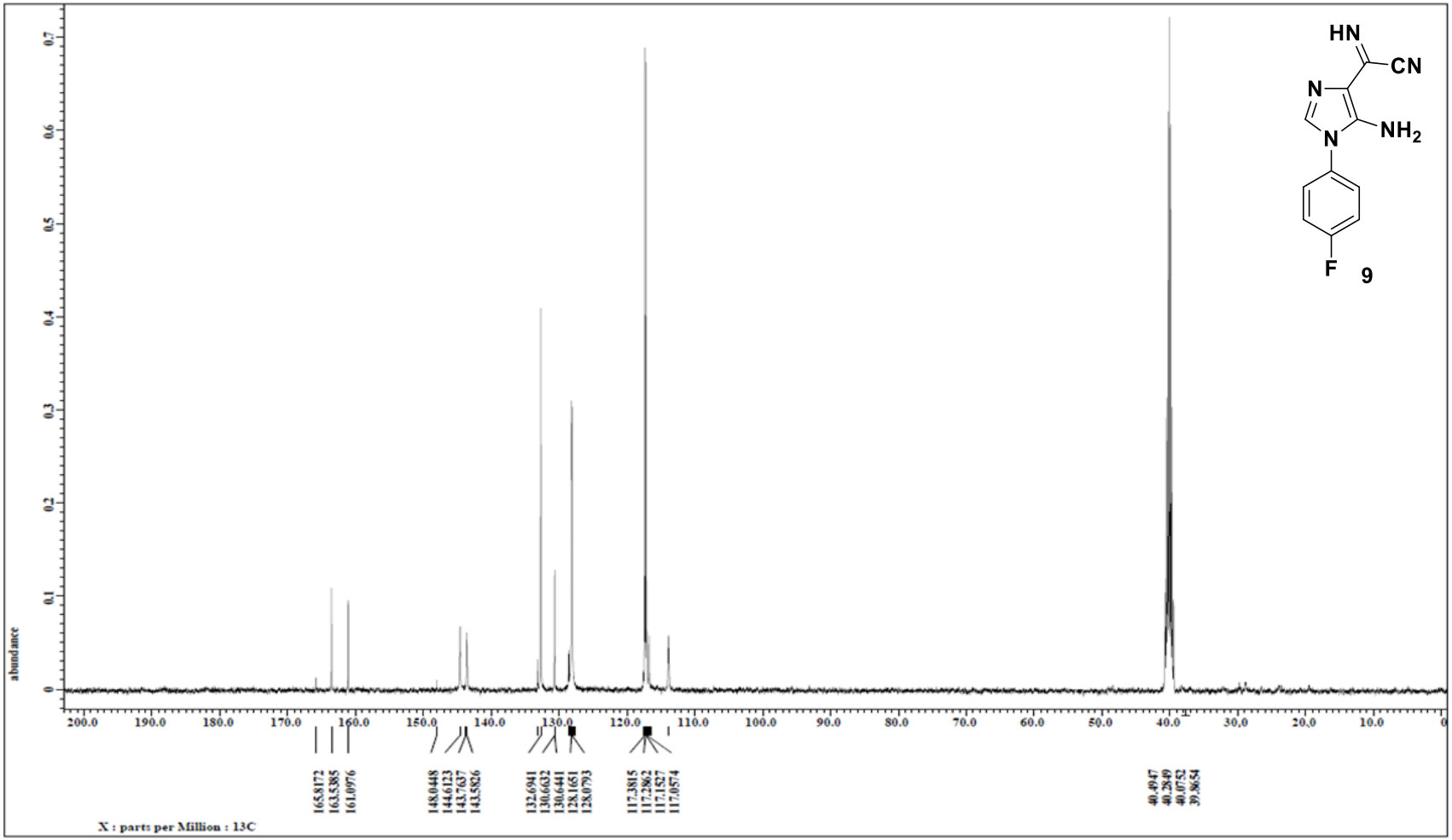
Spectrum

Line#:1 R.Time:6.410(Scan#:983)
MassPeaks:589
RawMode:Averaged 6.405-6.415(982-984) BasePeak:109(6930995)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity



Series 2


HN
CN
N
NH2
N
F
9
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
11.0809
7.5298
7.4183
7.4092
7.3970
6.6702
3.5084
3.4229
3.4077
3.3130
3.2000
2.4657
2.4611
2.4565
2.4519
1.0290
1.0123
0.9939


HN
CN
N
NH2
N
F
9
abundance
X : parts per Million : 13C
165.8172
163.5385
161.0976
148.0448
144.6123
143.7637
143.5826
132.6941
130.6632
130.6441
128.1651
128.0793
117.3815
117.2862
117.1527
117.0574
40.4947
40.2849
40.0752
39.8654

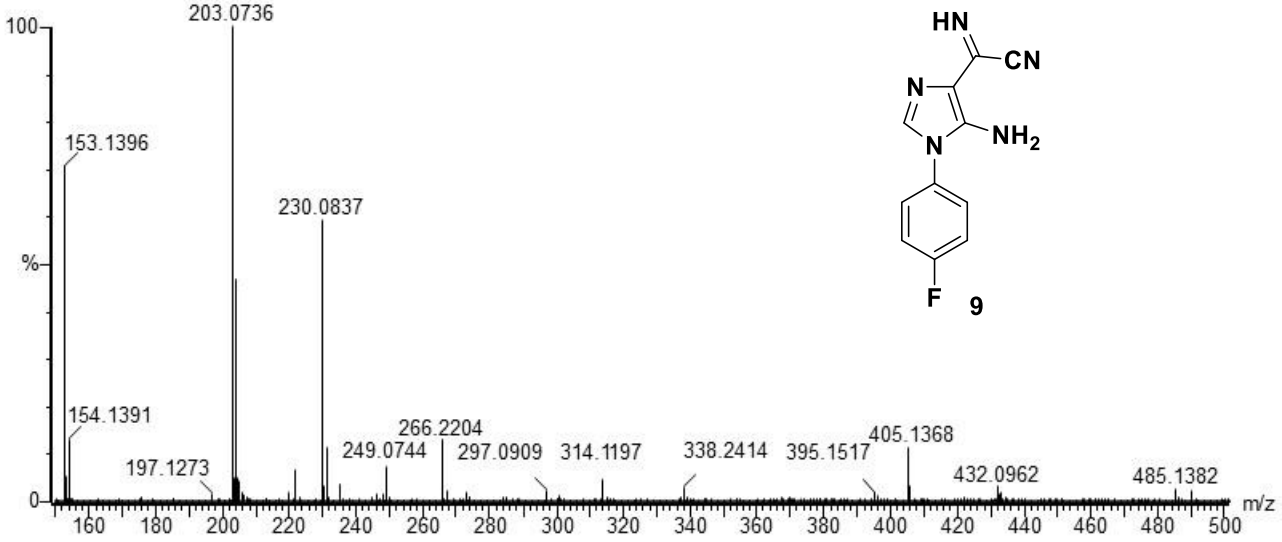
Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
65 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-22 H: 8-25 N: 0-5 O: 0-3 F: 0-1

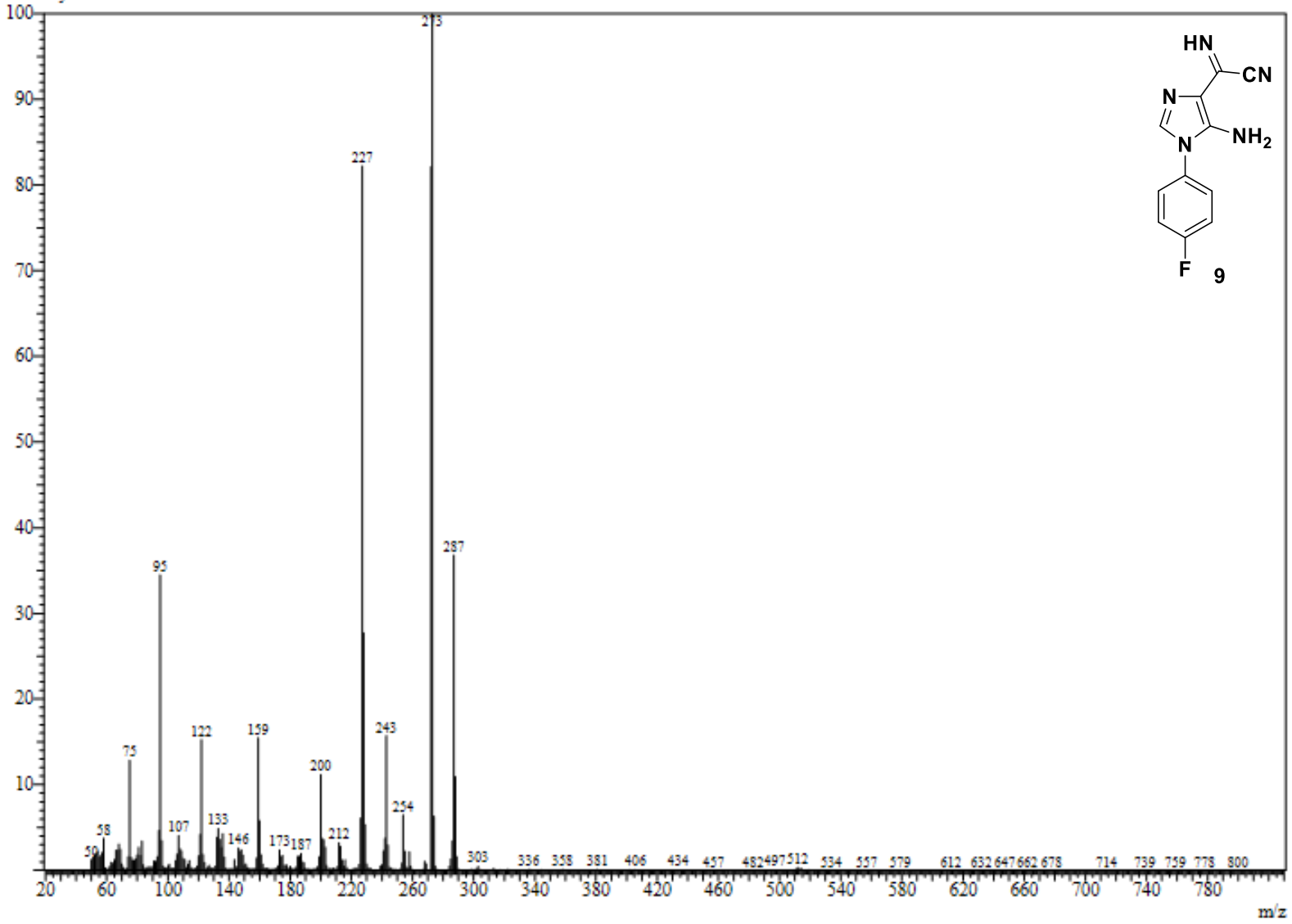
Sample Name : Int-2 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
160120-Int-2 12 (0.131) 1: TOF MS ES+
1.59e+008

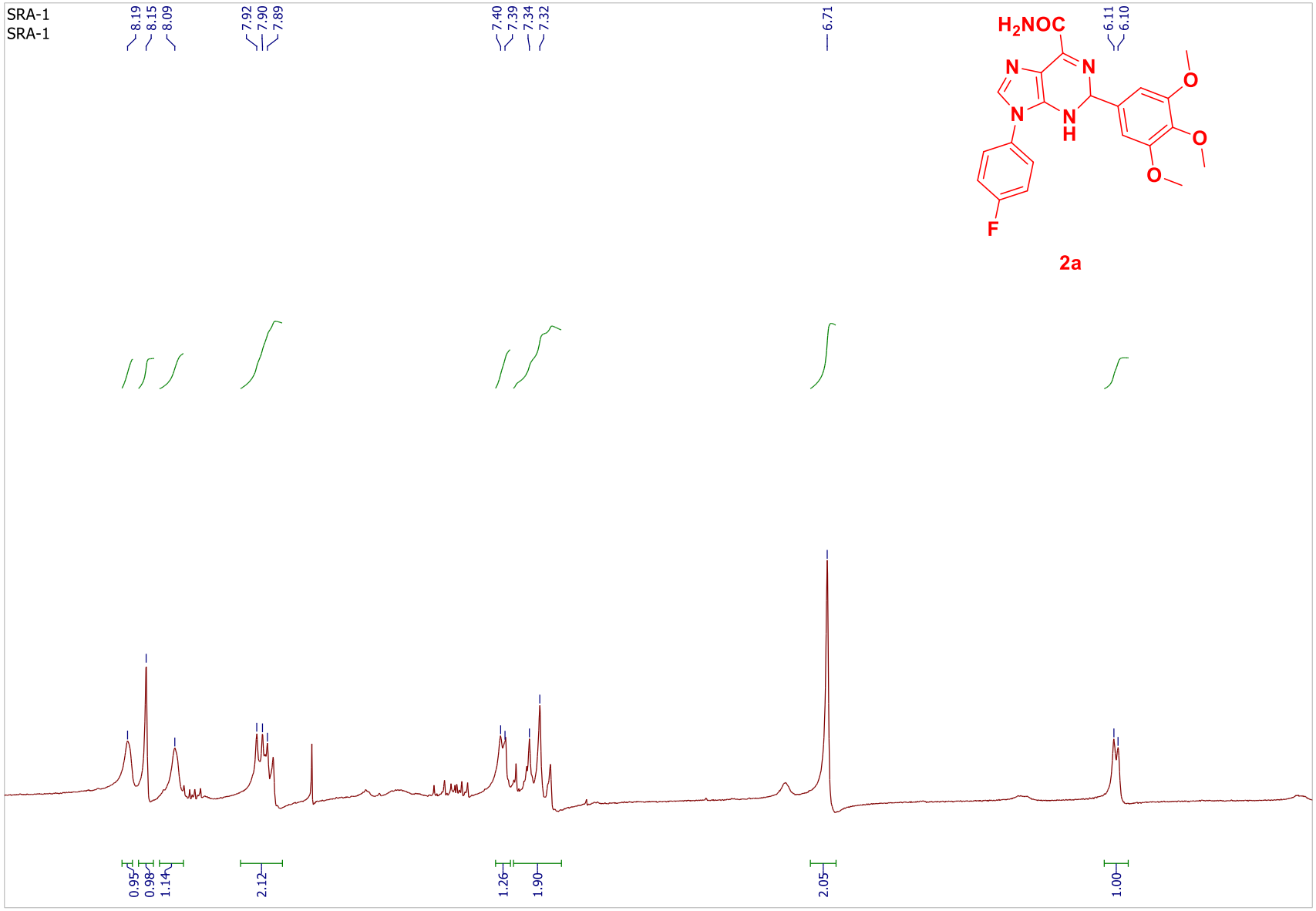


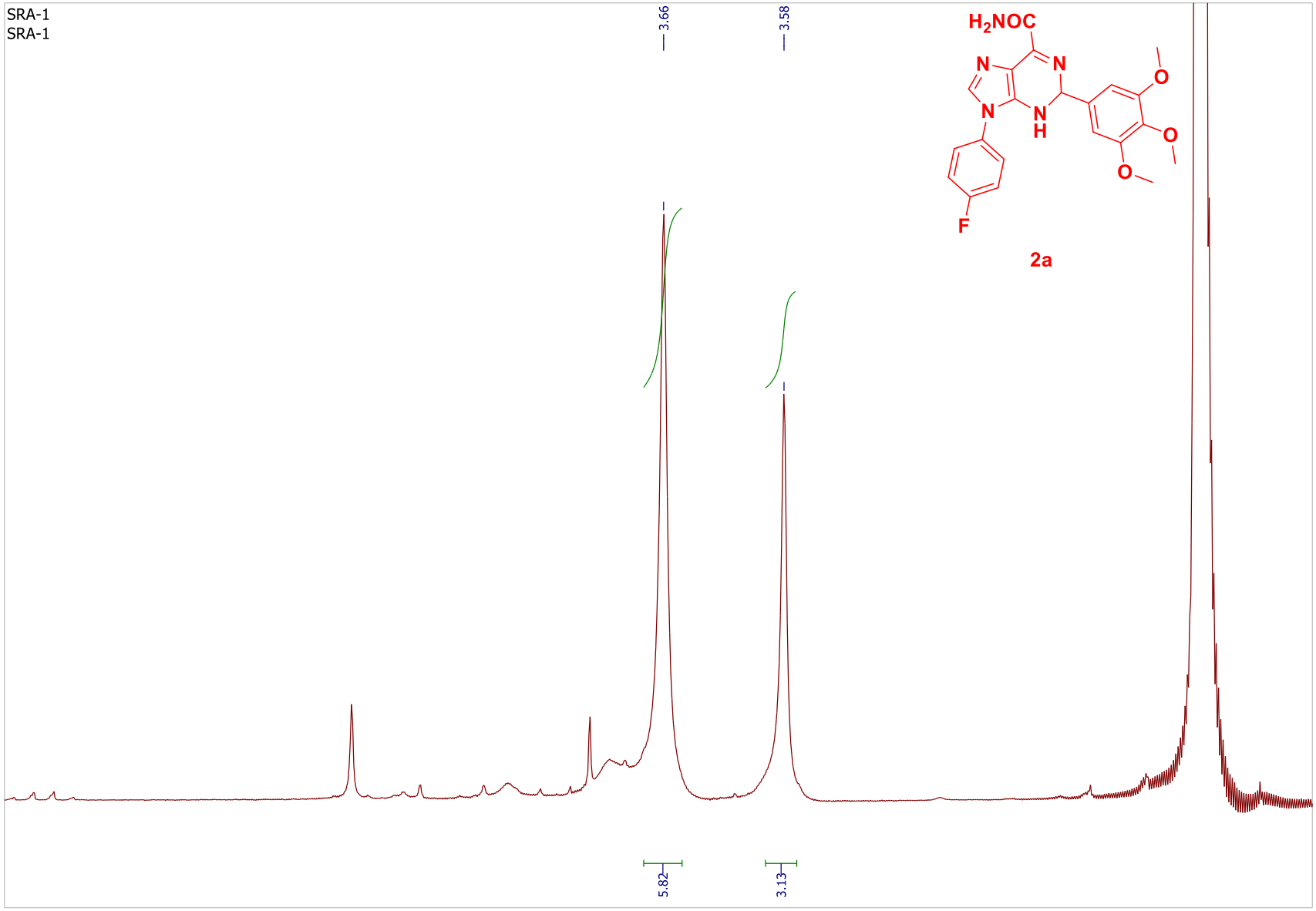
9

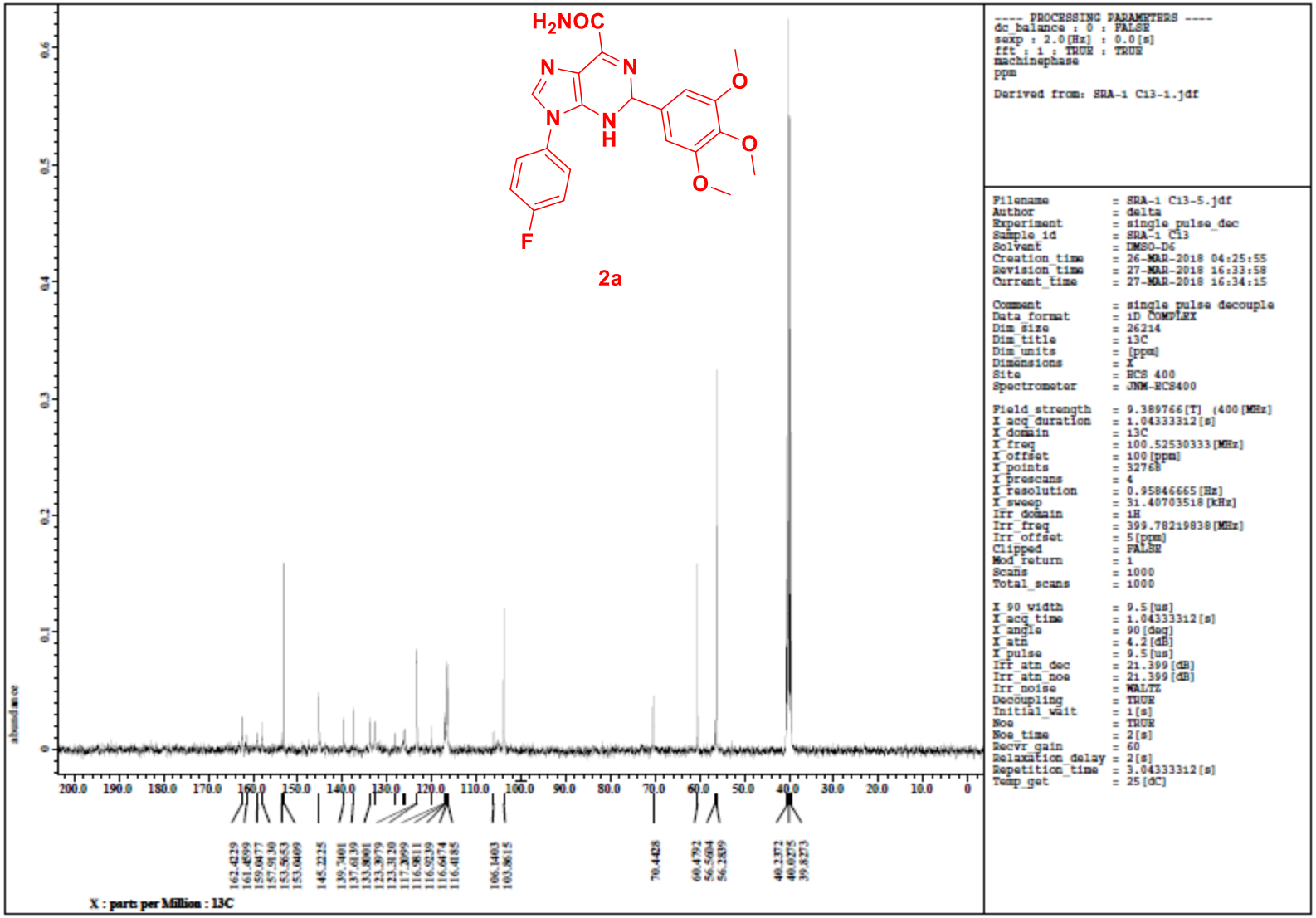
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
230.0837	230.0842	-0.5	-2.2	9.5	2053.6	n/a	n/a	C11 H9 N5 F

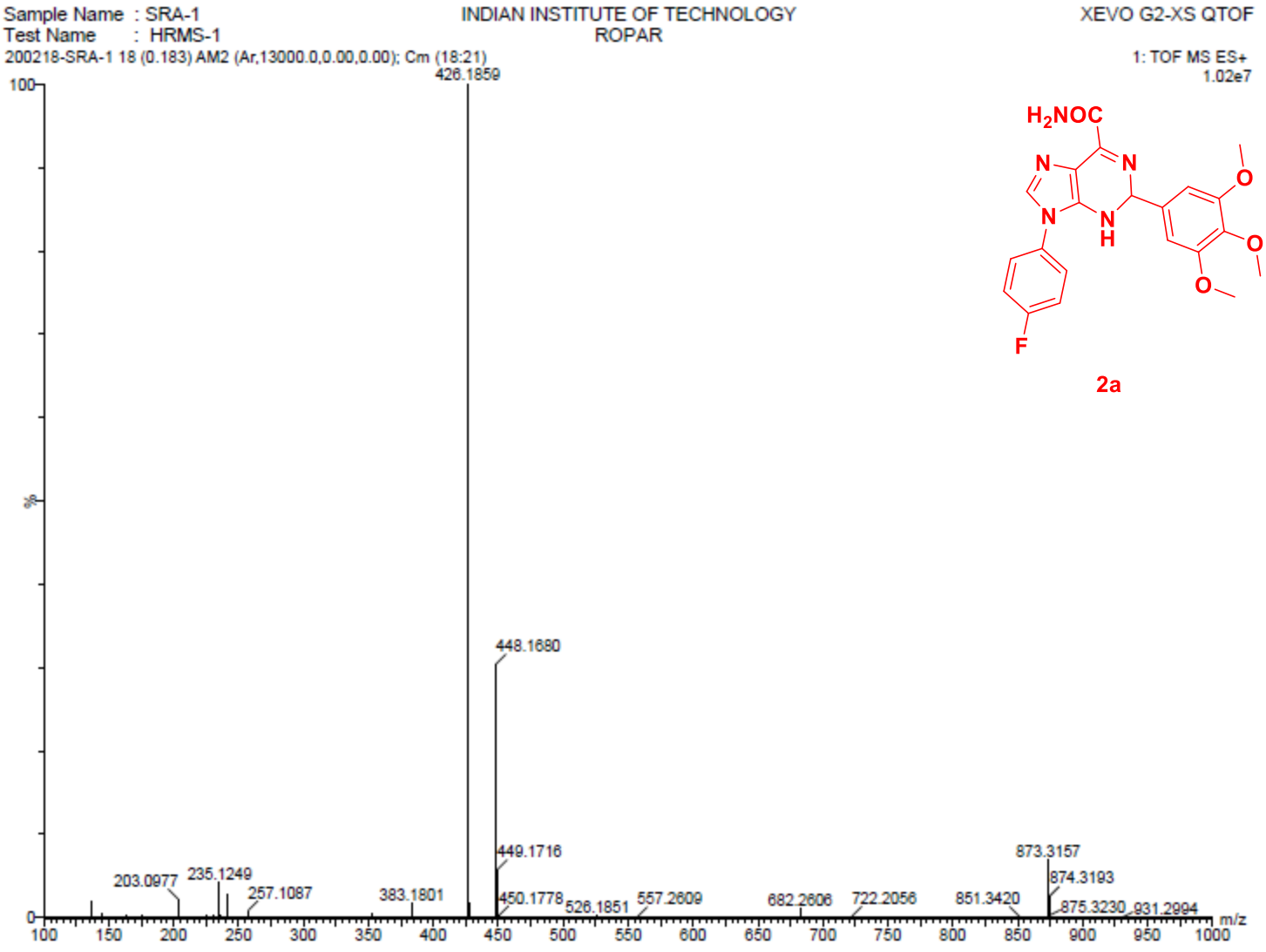
Line#:2 R.Time:5.775(Scan#:856)
MassPeaks:687
RawMode:Averaged 5.770-5.780(855-857) BasePeak:273(1487875)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity

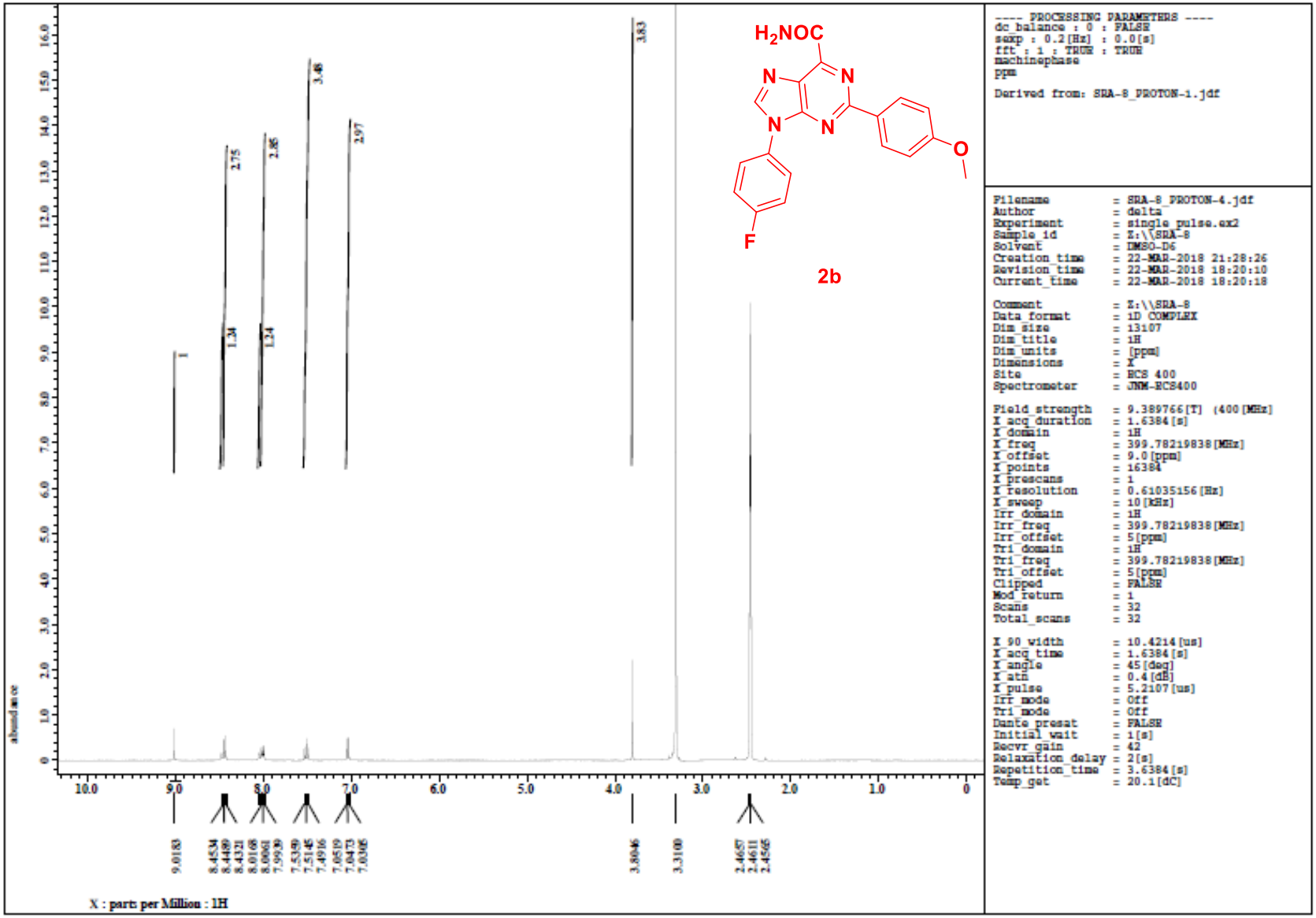



SRA-1
SRA-1
8.19
8.15
8.09
7.92
7.90
7.89
7.40
7.39
7.34
7.32
6.71
6.11
6.10
H_2NOC
N
N
N
N
H
O
O
O
F
2a
0.95
0.98
1.14
2.12
1.26
1.90
2.05
1.00


SRA-1
SRA-1
3.66
3.58
H2NOC
N
N
N
N
H
O
O
O
F
2a
5.82
3.13

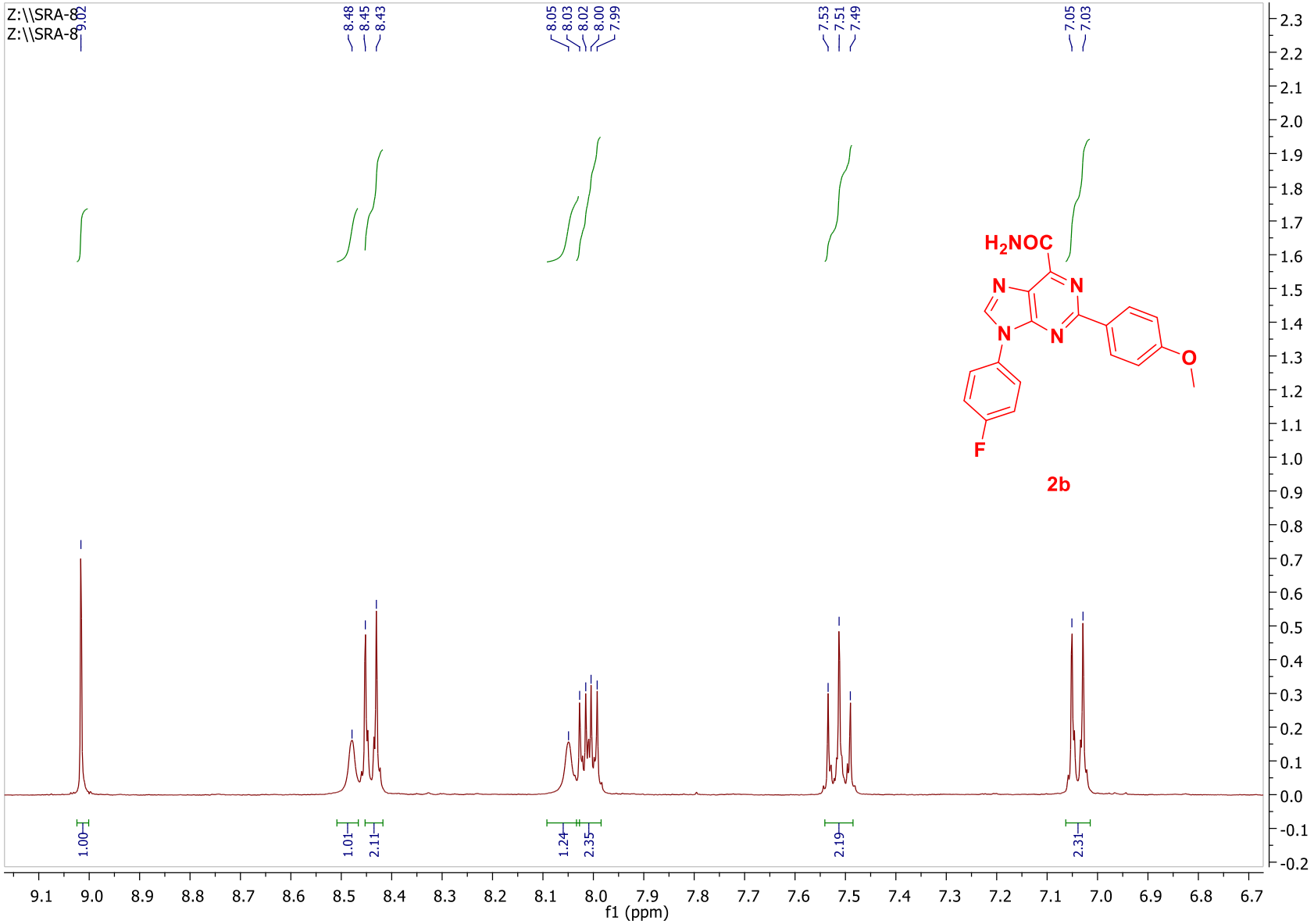

H2NOC
N
N
N
N
H
O
O
O
F
2a
abundance
0.6
0.5
0.4
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
162.4239
161.4599
159.0477
157.5830
153.5653
153.0469
145.2225
139.7401
137.6139
133.8001
123.3079
123.3120
117.2099
116.9811
116.9239
116.6474
116.4185
106.1403
103.8615
70.4428
60.4792
56.5604
56.2309
40.2372
40.0275
39.8273
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm
Derived from: SRA-1 C13-1.jdf
Filename = SRA-1 C13-5.jdf
Author = delta
Experiment = single_pulse_dec
Sample_id = SRA-1 C13
Solvent = DMSO-D6
Creation_time = 26-MAR-2018 04:25:55
Revision_time = 27-MAR-2018 16:33:58
Current_time = 27-MAR-2018 16:34:15
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = 13C
Dim_units = [ppm]
Dimensions = X
Site = NCS 400
Spectrometer = JNM-NCS400
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 1.04333312[s]
X_domain = 13C
X_freq = 100.52530333[MHz]
X_offset = 100[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95846665[Hz]
X_sweep = 31.40703518[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Scans = 1000
Total_scans = 1000
X_90_width = 9.5[us]
X_acq_time = 1.04333312[s]
X_angle = 90[deg]
X_atn = 4.2[dB]
X_pulse = 9.5[us]
Irr_atn_dec = 21.399[dB]
Irr_atn_noe = 21.399[dB]
Irr_noise = WALTZ
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 60
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
Temp_get = 25[dC]

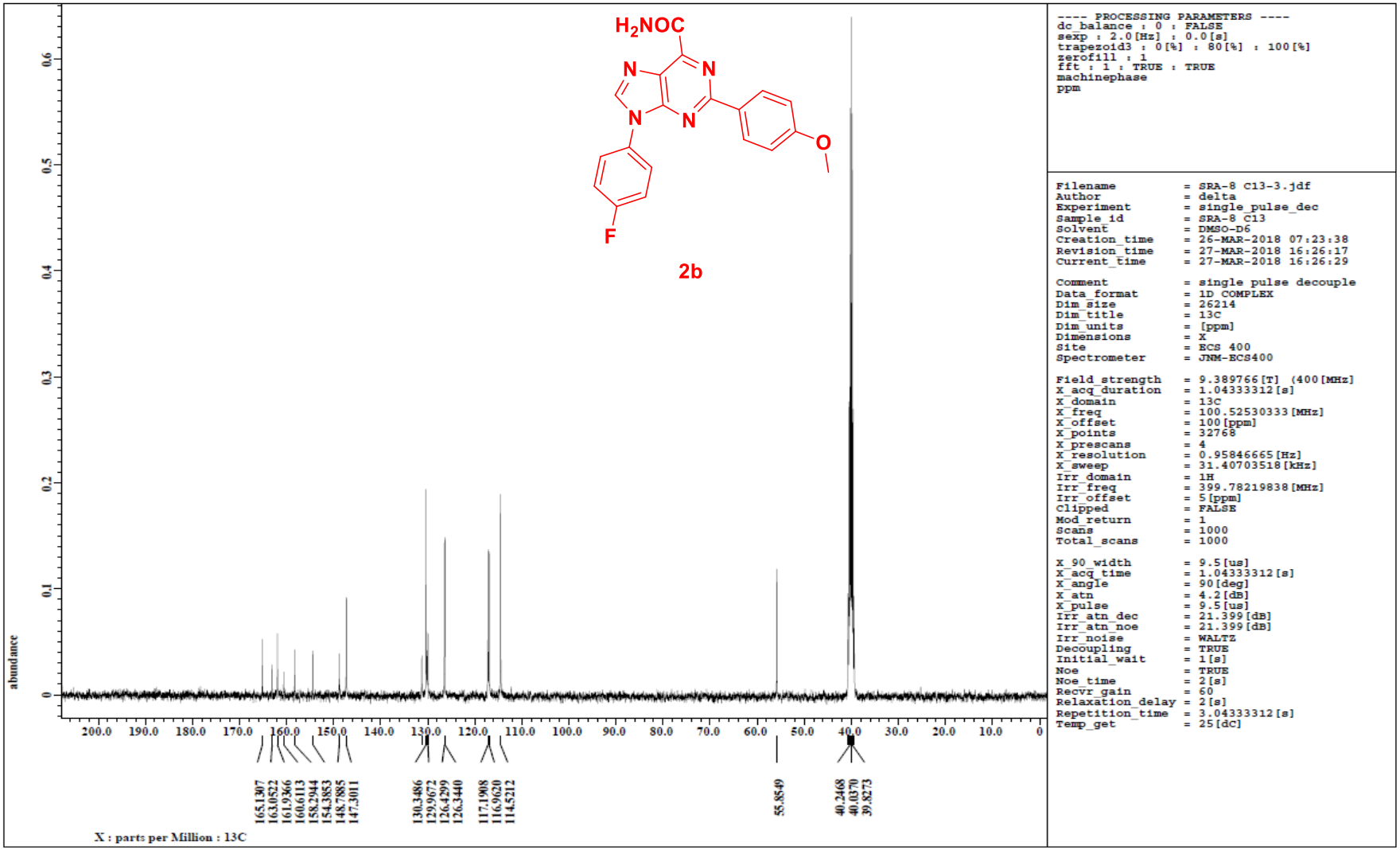

Sample Name : SRA-1
Test Name : HRMS-1
INDIAN INSTITUTE OF TECHNOLOGY
ROPAR
XEVO G2-XS QTOF
200218-SRA-1 18 (0.183) AM2 (Ar,13000.0,0.00,0.00); Cm (18:21)
1: TOF MS ES+
1.02e7
426.1859
448.1680
449.1716
873.3157
874.3193
203.0977
235.1249
257.1087
383.1801
450.1778
526.1851
557.2609
682.2606
722.2056
851.3420
875.3230
931.2994
%
m/z
H2NOC
F
2a




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: SRA-8_PROTON-1.jdf
```

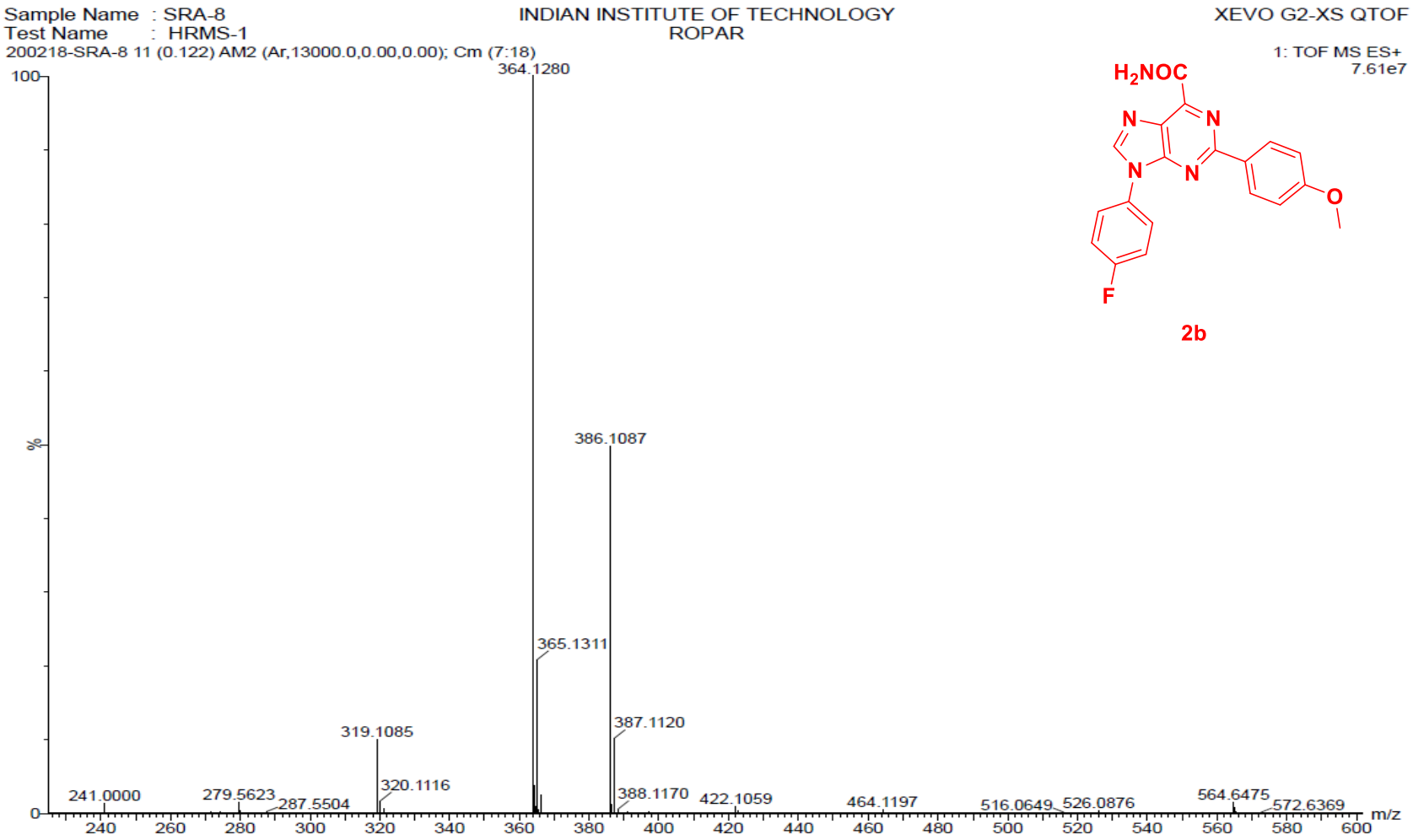
Filename	= SRA-8_PROTON-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= Z:\\SRA-8
Solvent	= DMSO-D6
Creation_time	= 22-MAR-2018 21:28:26
Revision_time	= 22-MAR-2018 18:20:10
Current_time	= 22-MAR-2018 18:20:18
Comment	= Z:\\SRA-8
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= NCS 400
Spectrometer	= JNM-EC8400
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 1.6384[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 9.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.61035156[Hz]
X_sweep	= 10[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 32
Total_scans	= 32
X_90_width	= 10.4214[us]
X_acq_time	= 1.6384[s]
X_angle	= 45[deg]
X_atn	= 0.4[dB]
X_pulse	= 5.2107[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 42
Relaxation_delay	= 2[s]
Repetition_time	= 3.6384[s]
Temp_get	= 20.1[dC]

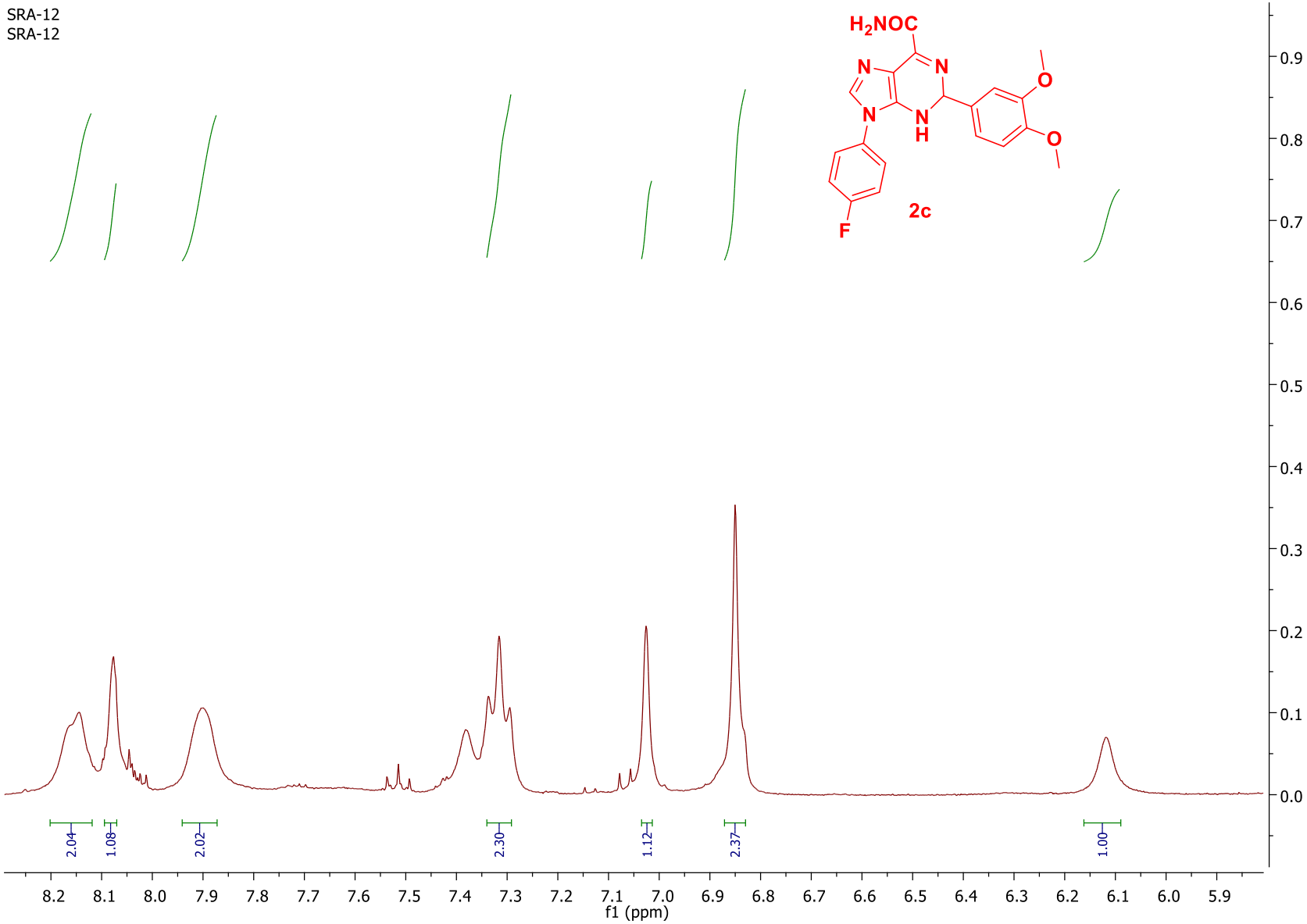

Z:\\SRA-8
Z:\\SRA-8
9.02
8.48
8.45
8.43
8.05
8.03
8.02
8.00
7.99
7.53
7.51
7.49
7.05
7.03
H2NOC
N
N
N
N
O
F
2b
1.00
1.01
2.11
1.24
2.35
2.19
2.31
f1 (ppm)

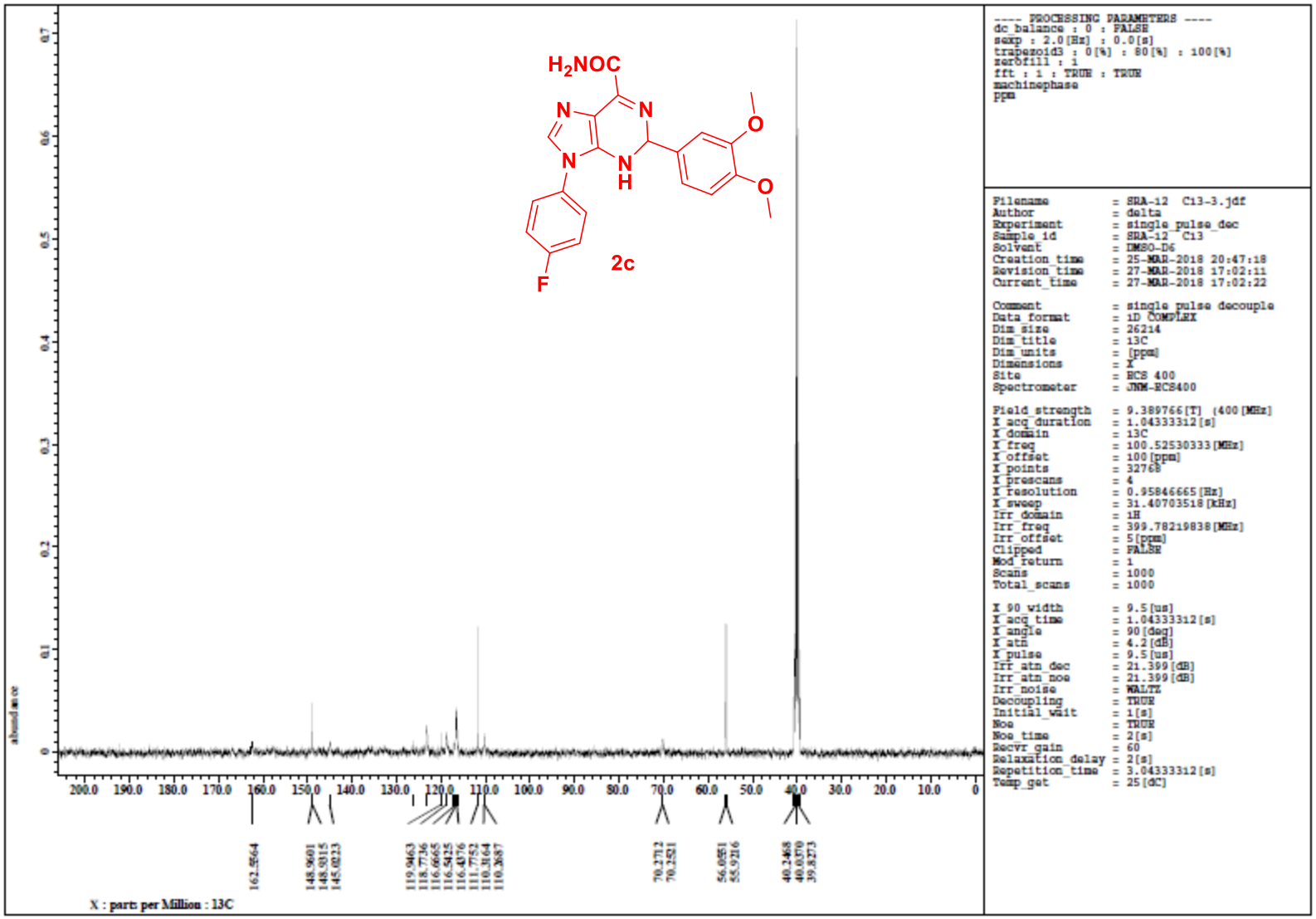


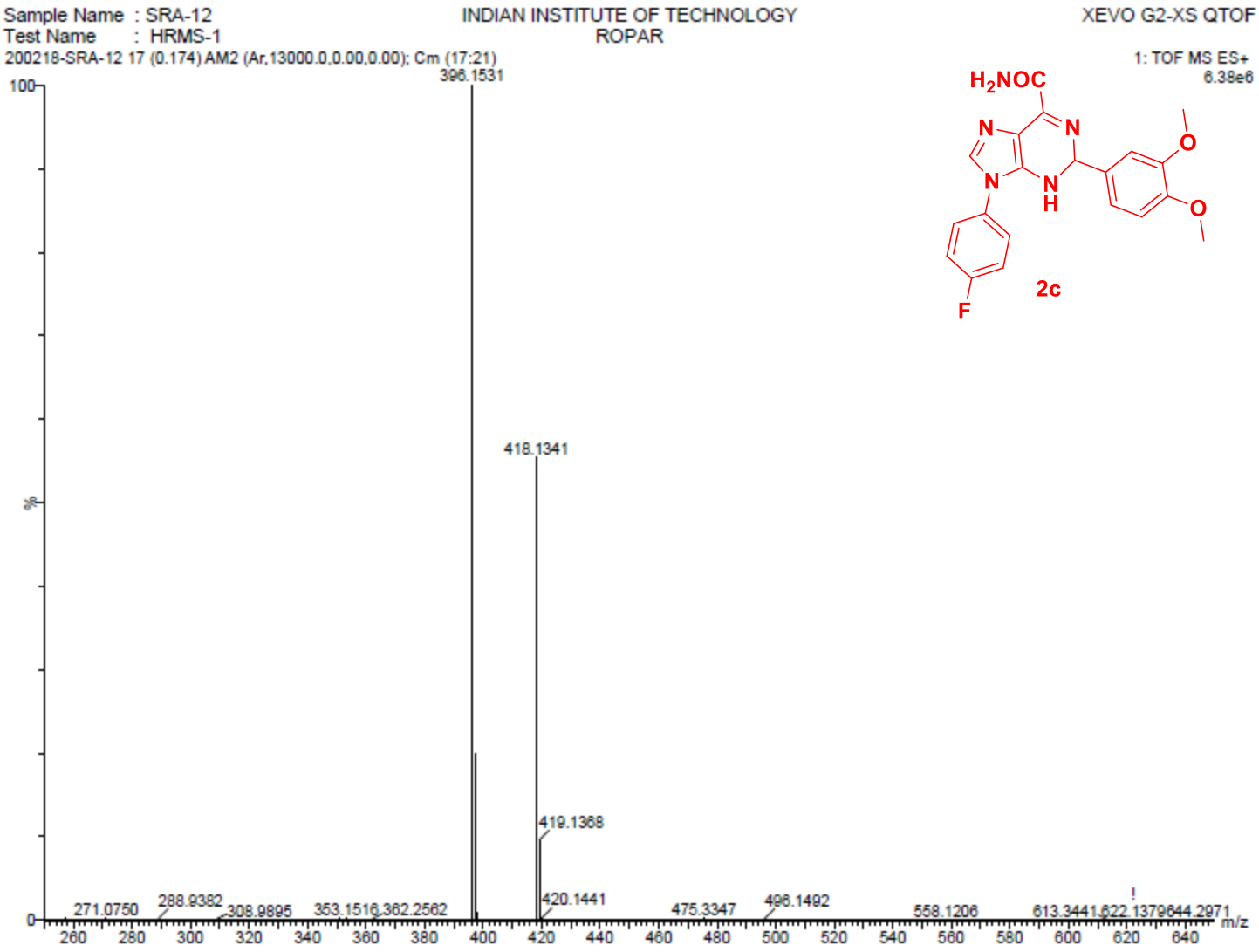

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

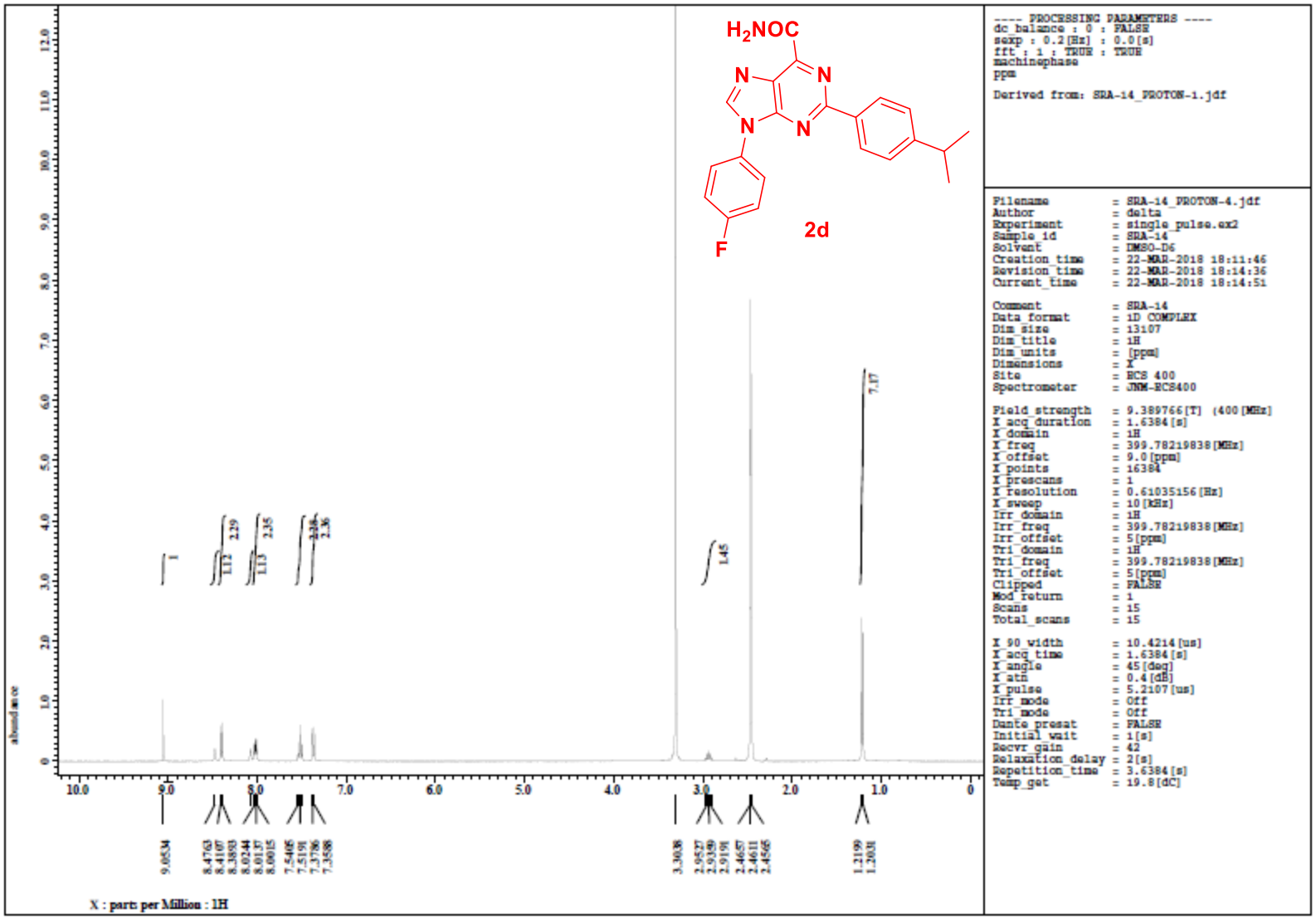
```
Filename          = SRA-8 C13-3.jdf
Author            = delta
Experiment        = single_pulse_dec
Sample_id         = SRA-8 C13
Solvent           = DMSO-D6
Creation_time     = 26-MAR-2018 07:23:38
Revision_time     = 27-MAR-2018 16:26:17
Current_time      = 27-MAR-2018 16:26:29

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECS 400
Spectrometer      = JNM-ECS400

Field_strength    = 9.389766[T] (400[MHz]
X_acq_duration    = 1.04333312[s]
X_domain          = 13C
X_freq            = 100.52530333[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.95846665[Hz]
X_sweep           = 31.40703518[kHz]
Irr_domain        = 1H
Irr_freq          = 399.78219838[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1000
Total_scans       = 1000

X_90_width        = 9.5[us]
X_acq_time        = 1.04333312[s]
X_angle           = 90[deg]
X_atn             = 4.2[dB]
X_pulse           = 9.5[us]
Irr_atn_dec       = 21.399[dB]
Irr_atn_noe       = 21.399[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 3.04333312[s]
Temp_get          = 25[dC]
```


Sample Name : SRA-8
Test Name : HRMS-1
200218-SRA-8 11 (0.122) AM2 (Ar,13000.0,0.00,0.00); Cm (7:18)
INDIAN INSTITUTE OF TECHNOLOGY
ROPAR
XEVO G2-XS QTOF
1: TOF MS ES+
7.61e7
100
%
0
364.1280
386.1087
365.1311
387.1120
319.1085
320.1116
388.1170
241.0000
279.5623
287.5504
422.1059
464.1197
516.0649
526.0876
564.6475
572.6369
m/z
240
260
280
300
320
340
360
380
400
420
440
460
480
500
520
540
560
580
600
H2NOC
N
N
N
N
O
F
2b


SRA-12
SRA-12
H2NOC
N
N
N
N
H
O
O
F
2c
2.04
1.08
2.02
2.30
1.12
2.37
1.00
f1 (ppm)

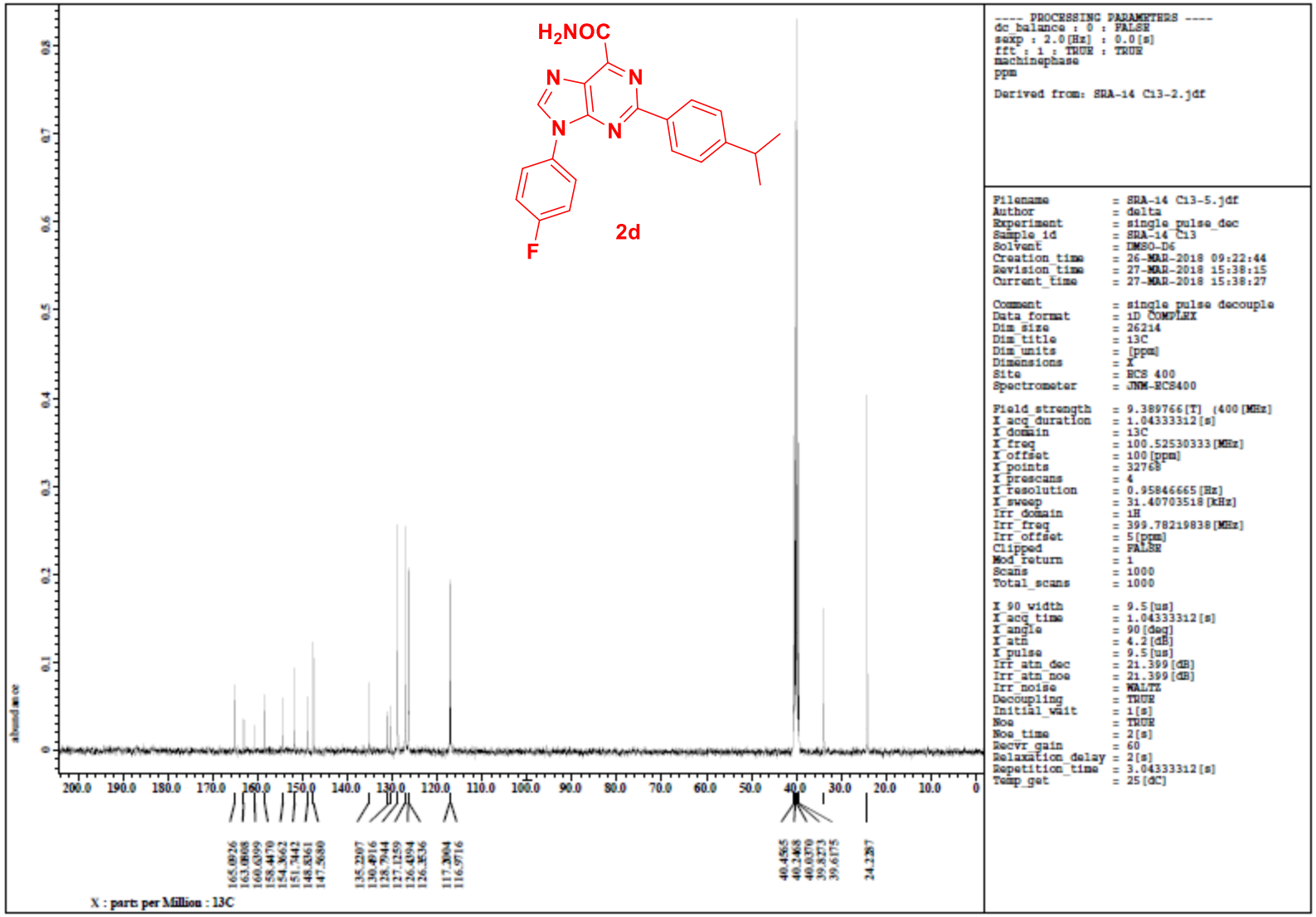

H2NOC
N
N
N
N
H
O
O
F
2c
abundance
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
162.5564
148.9601
148.0315
145.6823
119.9463
118.7736
116.6665
116.5425
116.4376
111.7752
110.3664
110.3687
70.3712
70.2521
56.6851
55.9216
40.2468
40.0570
39.8273
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
Filename = SRA-12 C13-3.jdf
Author = delta
Experiment = single pulse dec
Sample id = SRA-12 C13
Solvent = DMSO-D6
Creation time = 25-MAR-2018 20:47:18
Revision time = 27-MAR-2018 17:02:11
Current time = 27-MAR-2018 17:02:22
Comment = single pulse decouple
Data format = 1D COMPLEX
Dim size = 26214
Dim title = 13C
Dim units = [ppm]
Dimensions = X
Site = NCS 400
Spectrometer = JNM-ECS400
Field strength = 9.389766[T] (400[MHz]
X acq duration = 1.04333312[s]
X domain = 13C
X freq = 100.52530333[MHz]
X offset = 100[ppm]
X points = 32768
X prescans = 4
X resolution = 0.95846665[Hz]
X sweep = 31.40703518[kHz]
Irr domain = 1H
Irr freq = 399.78219838[MHz]
Irr offset = 5[ppm]
Clipped = FALSE
Mod return = 1
Scans = 1000
Total scans = 1000
X 90 width = 9.5[us]
X acq time = 1.04333312[s]
X angle = 90[deg]
X atn = 4.2[dB]
X pulse = 9.5[us]
Irr atn dec = 21.399[dB]
Irr atn noe = 21.399[dB]
Irr noise = WALTZ
Decoupling = TRUE
Initial wait = 1[s]
Noe = TRUE
Noe time = 2[s]
Recvr gain = 60
Relaxation delay = 2[s]
Repetition time = 3.04333312[s]
Temp get = 25[dC]


Sample Name : SRA-12
Test Name : HRMS-1
INDIAN INSTITUTE OF TECHNOLOGY
ROPAR
XEVO G2-XS QTOF
200218-SRA-12 17 (0.174) AM2 (Ar,13000.0,0.00,0.00); Cm (17:21)
1: TOF MS ES+
6.38e6
396.1531
418.1341
419.1368
420.1441
271.0750
288.9382
308.9895
353.1516
362.2562
475.3347
496.1492
558.1206
613.3441
622.1379
644.2971
%
m/z
H2NOC
2c
F




```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: SRA-14_PROTON-1.jdf
```

Filename	= SRA-14_PROTON-4.jdf
Author	= delta
Experiment	= single_pulse.ex2
Sample_id	= SRA-14
Solvent	= DMSO-D6
Creation_time	= 22-MAR-2018 18:11:46
Revision_time	= 22-MAR-2018 18:14:36
Current_time	= 22-MAR-2018 18:14:51
Comment	= SRA-14
Data_format	= 1D COMPLEX
Dim_size	= 13107
Dim_title	= 1H
Dim_units	= [ppm]
Dimensions	= X
Site	= NCS 400
Spectrometer	= JNM-ECS400
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 1.6384[s]
X_domain	= 1H
X_freq	= 399.78219838[MHz]
X_offset	= 9.0[ppm]
X_points	= 16384
X_prescans	= 1
X_resolution	= 0.61035156[Hz]
X_sweep	= 10[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Tri_domain	= 1H
Tri_freq	= 399.78219838[MHz]
Tri_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 15
Total_scans	= 15
X_90_width	= 10.4214[us]
X_acq_time	= 1.6384[s]
X_angle	= 45[deg]
X_atn	= 0.4[dB]
X_pulse	= 5.2107[us]
Irr_mode	= Off
Tri_mode	= Off
Dante_presat	= FALSE
Initial_wait	= 1[s]
Recvr_gain	= 42
Relaxation_delay	= 2[s]
Repetition_time	= 3.6384[s]
Temp_get	= 19.8[dC]




```
----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
sexp : 2.0[Hz] : 0.0[s]
fft : 1 : TRUE : TRUE
machinephase
ppm

Derived from: SRA-14 C13-2.jdf
```

Filename	= SRA-14 C13-5.jdf
Author	= delta
Experiment	= single_pulse_dec
Sample_id	= SRA-14 C13
Solvent	= DMSO-D6
Creation_time	= 26-MAR-2018 09:22:44
Revision_time	= 27-MAR-2018 15:38:15
Current_time	= 27-MAR-2018 15:38:27
Comment	= single pulse decouple
Data_format	= 1D COMPLEX
Dim_size	= 26214
Dim_title	= 13C
Dim_units	= [ppm]
Dimensions	= X
Site	= RCS 400
Spectrometer	= JNM-RC8400
Field_strength	= 9.389766[T] (400[MHz]
X_acq_duration	= 1.04333312[s]
X_domain	= 13C
X_freq	= 100.52530333[MHz]
X_offset	= 100[ppm]
X_points	= 32768
X_prescans	= 4
X_resolution	= 0.95846665[Hz]
X_sweep	= 31.40703518[kHz]
Irr_domain	= 1H
Irr_freq	= 399.78219838[MHz]
Irr_offset	= 5[ppm]
Clipped	= FALSE
Mod_return	= 1
Scans	= 1000
Total_scans	= 1000
X_90_width	= 9.5[us]
X_acq_time	= 1.04333312[s]
X_angle	= 90[deg]
X_atn	= 4.2[dB]
X_pulse	= 9.5[us]
Irr_atn_dec	= 21.399[dB]
Irr_atn_noe	= 21.399[dB]
Irr_noise	= WALTZ
Decoupling	= TRUE
Initial_wait	= 1[s]
Noe	= TRUE
Noe_time	= 2[s]
Recvr_gain	= 60
Relaxation_delay	= 2[s]
Repetition_time	= 3.04333312[s]
Temp_get	= 25[dC]

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

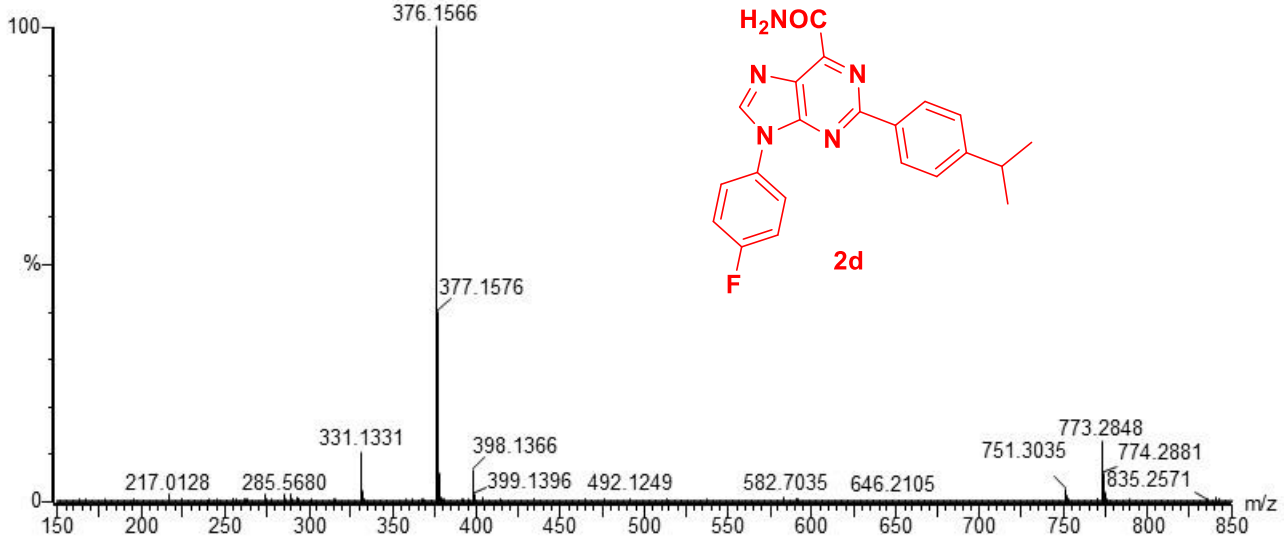
Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 9-22 H: 6-25 N: 0-5 O: 0-3 F: 0-1

Sample Name : SRA-14
Test Name : HRMS-1
160120-SRA-14 16 (0.165)

IITRPR

XEVO G2-XS QTOF

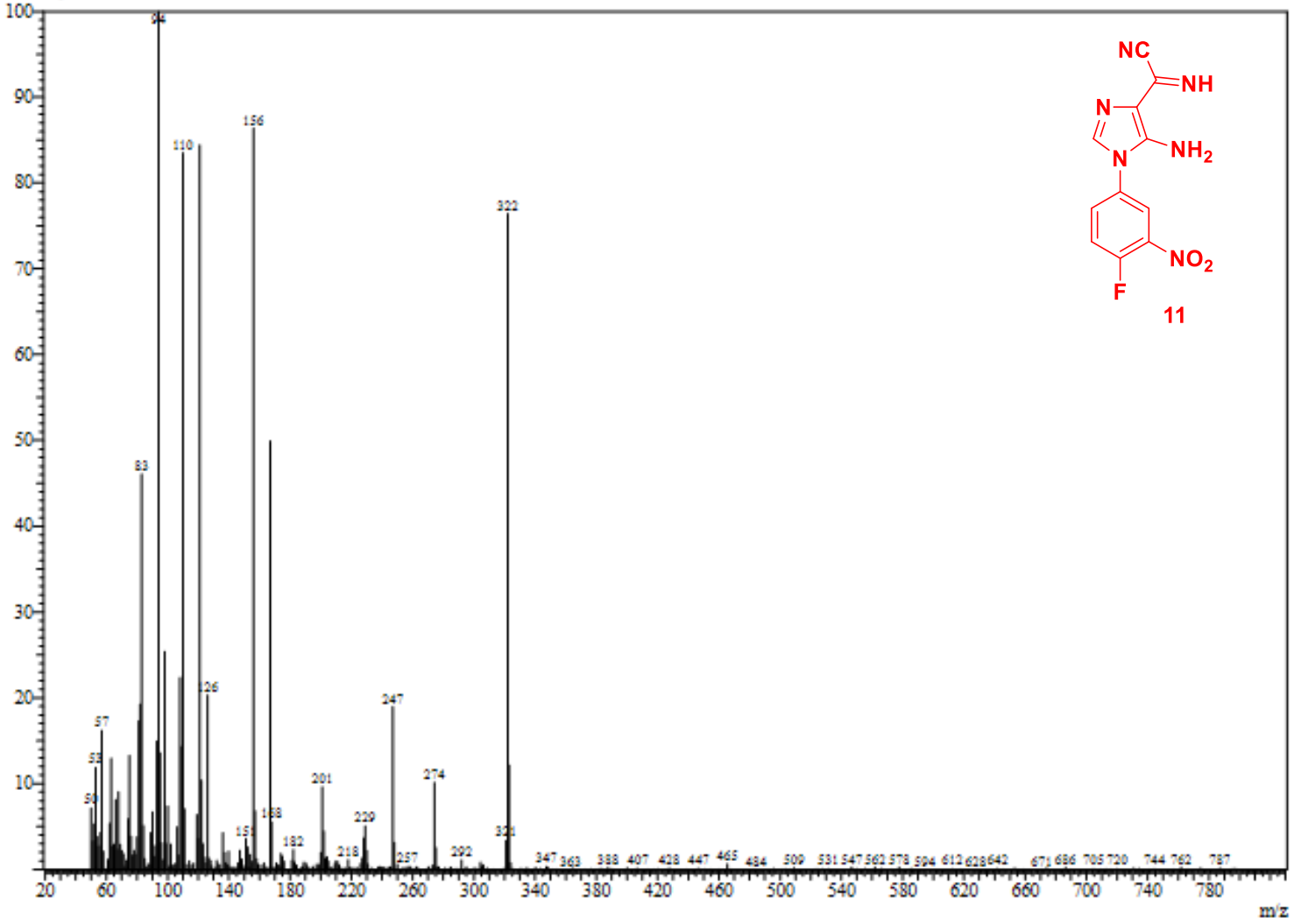
1: TOF MS ES+
4.43e+007



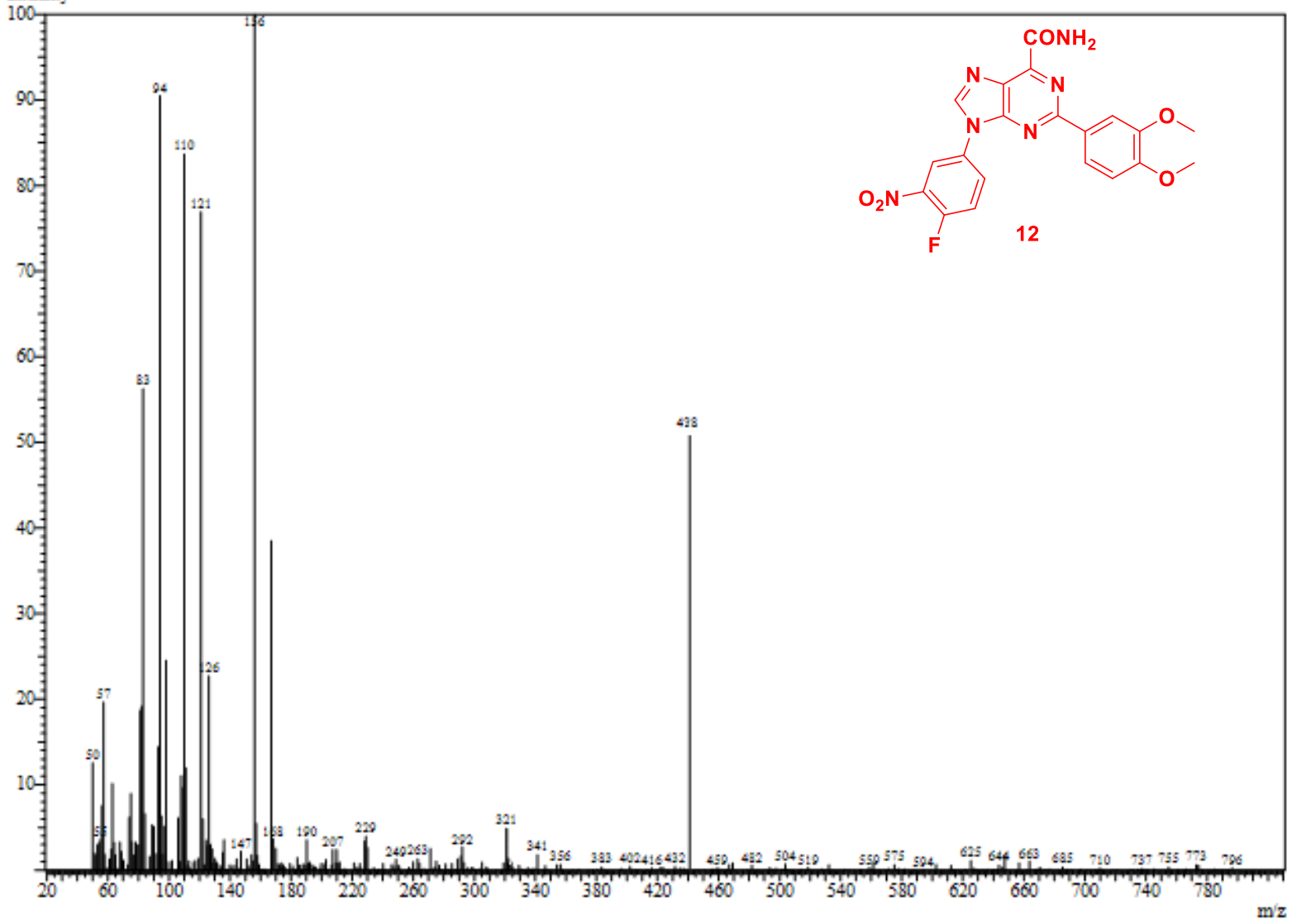
2d

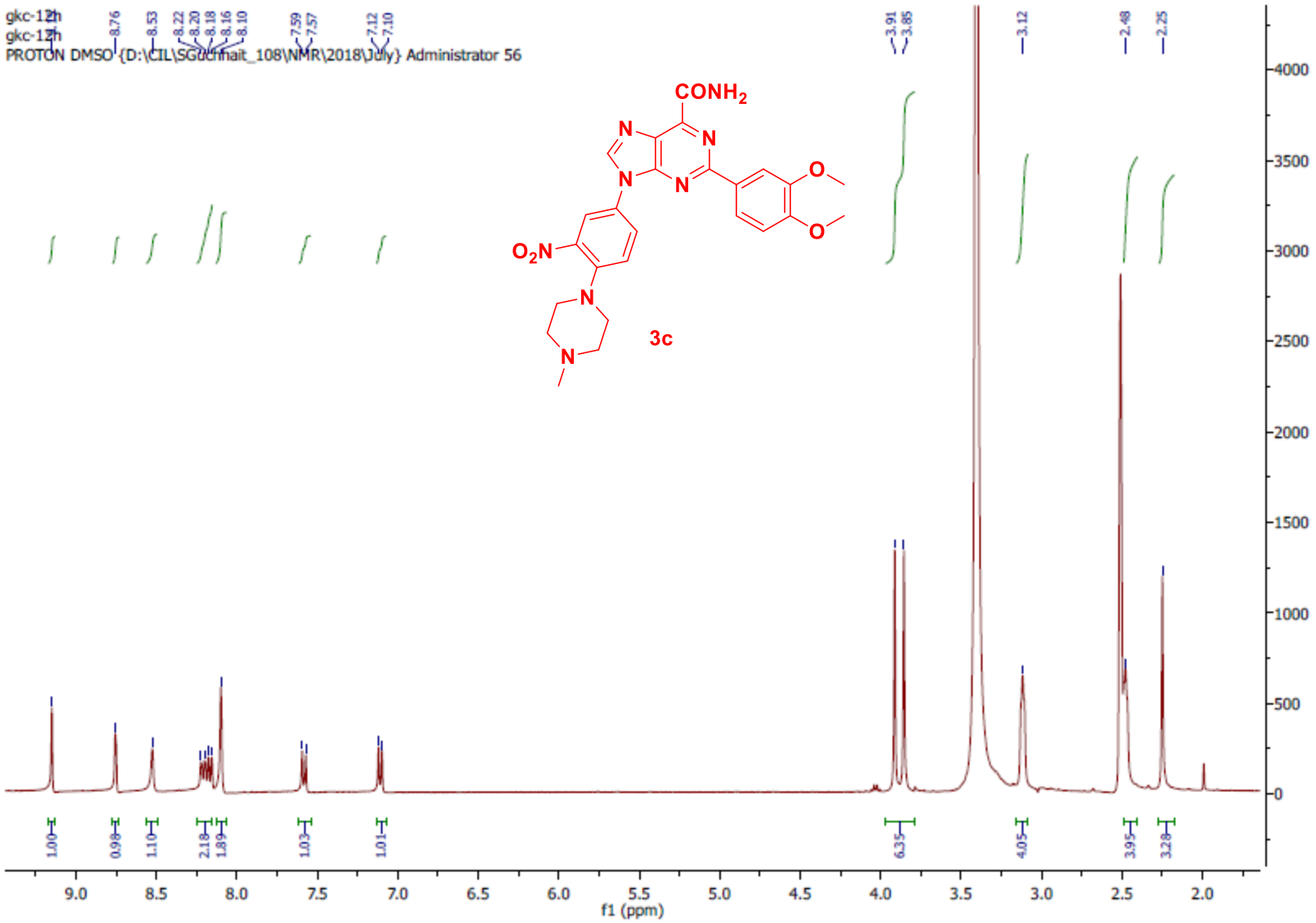
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
376.1566	376.1574	-0.8	-2.1	14.5	1626.0	n/a	n/a	C21 H19 N5 O F

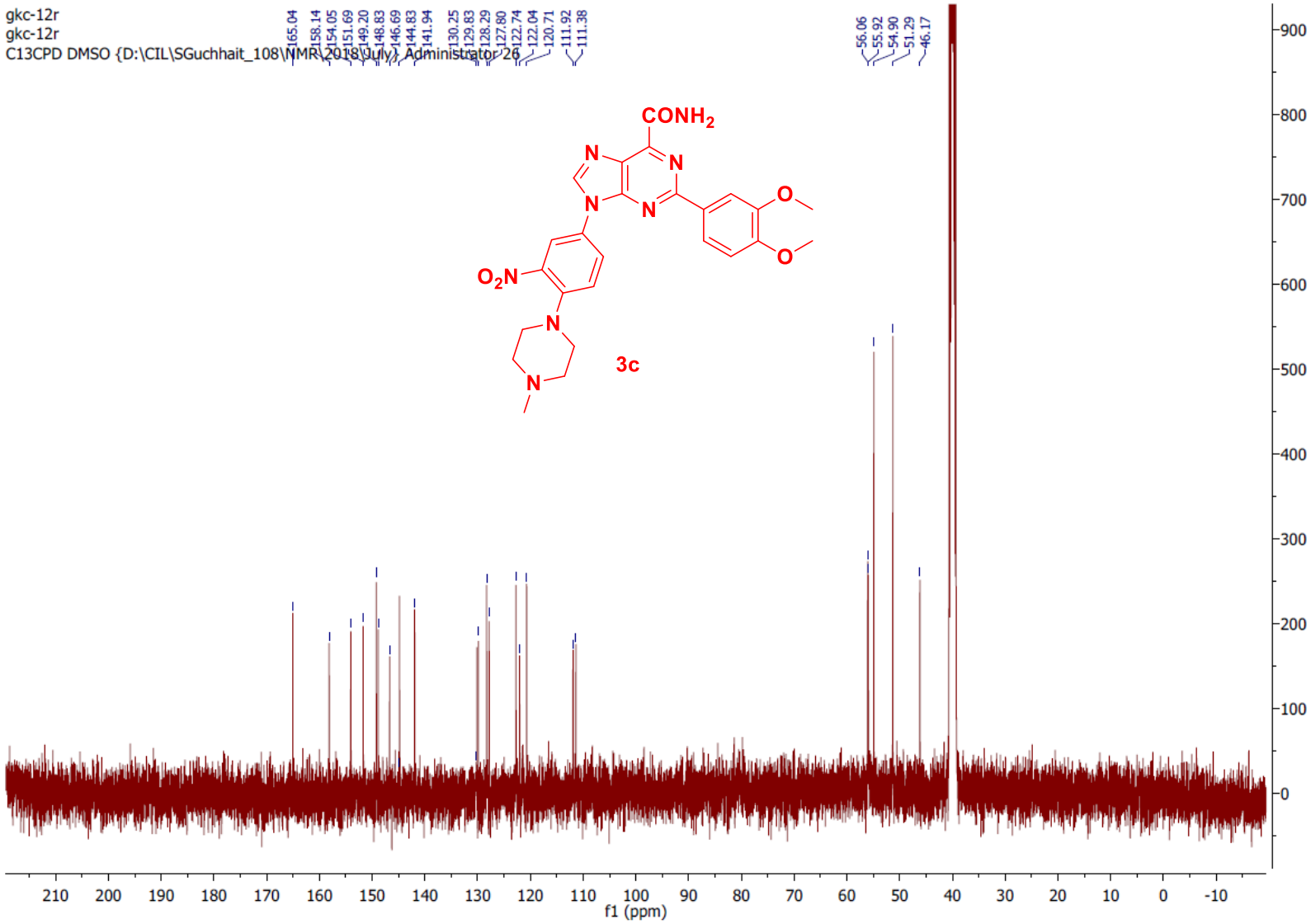
Line#:2 R.Time:7.485(Scan#:1198)
MassPeaks:487
RawMode:Averaged 7.480-7.490(1197-1199) BasePeak:94(1695199)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity

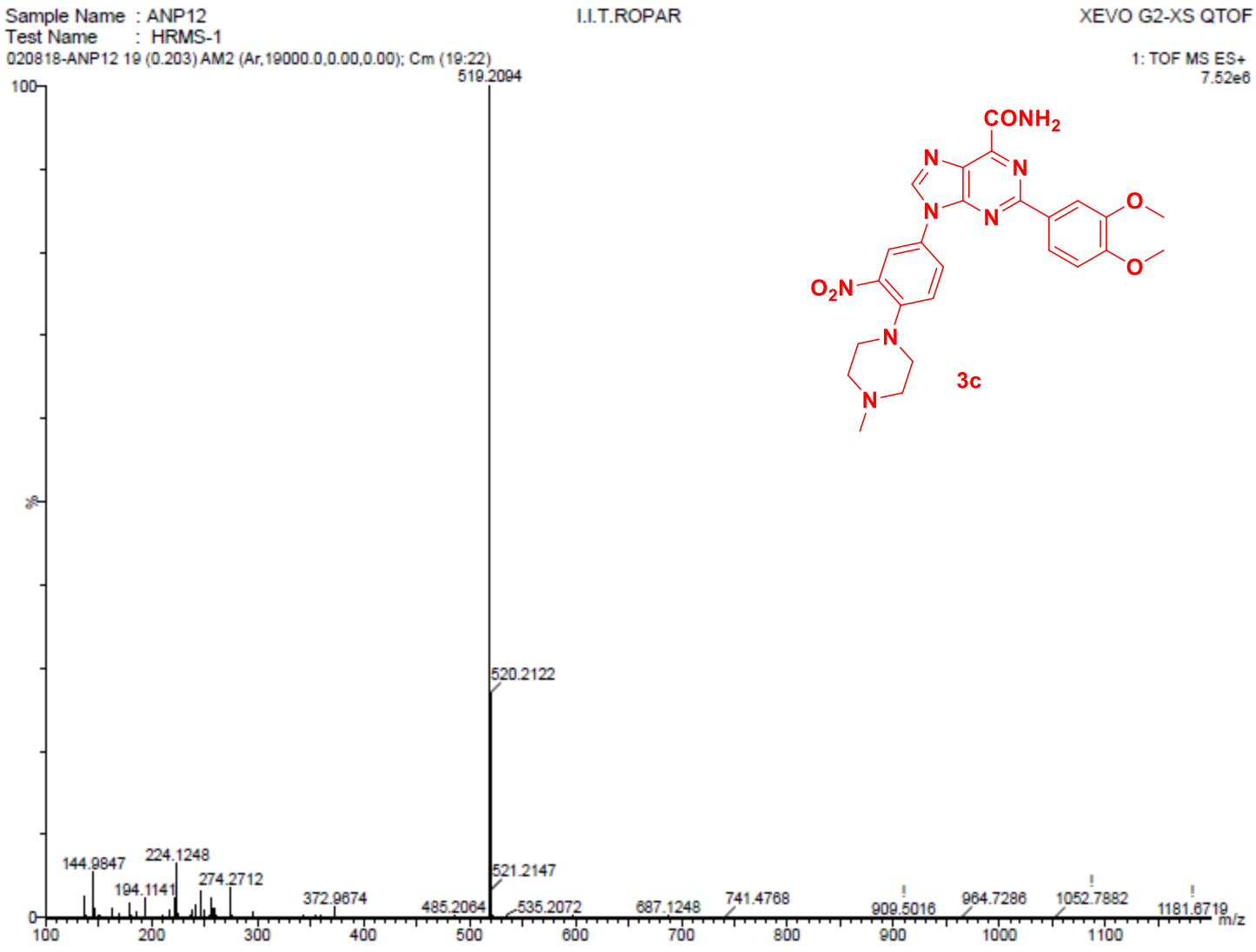


Line#:1 R.Time:6.935(Scan#:1088)
MassPeaks:431
RawMode:Averaged 6.930-6.940(1087-1089) BasePeak:156(346019)
BG Mode:Calc. from Peak Group 1 - Event 1
intensity




gkc-12h
gkc-12h
PROTON DMSO {D:\CIL\SGuchhait_108\NMR\2018\July} Administrator 56
8.76
8.53
8.22
8.20
8.18
8.16
8.10
7.59
7.57
7.12
7.10
3.91
3.85
3.12
2.48
2.25
CONH2
O2N
3c
1.00
0.98
1.10
2.18
1.89
1.03
1.01
6.35
4.05
3.95
3.28
f1 (ppm)


gkc-12r
gkc-12r
C13CPD DMSO {D:\CIL\SGuchhait_108\NMR\2018\July} Administrator 26
165.04
158.14
154.05
151.69
149.20
148.83
146.69
144.83
141.94
130.25
129.83
128.29
127.80
122.74
122.04
120.71
111.92
111.38
56.06
55.92
54.90
51.29
46.17
CONH2
O2N
3c
f1 (ppm)


Sample Name : ANP12
Test Name : HRMS-1
020818-ANP12 19 (0.203) AM2 (Ar,19000.0,0.00,0.00); Cm (19:22)
I.I.T.ROPAR
XEVO G2-XS QTOF
1: TOF MS ES+
7.52e6
519.2094
520.2122
521.2147
144.9847
194.1141
224.1248
274.2712
372.9674
485.2064
535.2072
687.1248
741.4768
909.5016
964.7286
1052.7882
1181.6719
CONH2
O2N
3c
%
m/z

Molecular docking of 3c in HER-2 and other proteins

We performed molecular docking of most potent compound 3c into the HER-2 kinase and other related proteins such as CDK-2, 4, 6, ERα and PR and results were compared with their positive controls (Table S1). The Figure S1 represents the 3D binding pose of the lapatinib (positive control) and the compound 3c in the active site of the HER-2 (PDB: 3RCD). The laptinib occupied more surface are of 521.59 $Å^2$ of binding cavity of HER-2 protein than compound 3c (471.50 $Å^2$). This could be due to the presence of an extra flurophenyl ring in lapatanib structure which increases the surface area of lapatinib by 50 $Å^2$ and supports the crucial π- π interaction with PHE891 (Figure S1). Moreover, it was observed that lapatinib binding to active site was favoured by the hydrophobic interaction (LEU796, MET 801 and PHE891) and salt bridge interaction (ASP808) whereas compound 3c showed only one hydrophobic interaction (MET801), one polar interaction (GLN799) and one salt bridge interaction with LYS753 and hence lapatinib showed better dock score (-12.39) than our compound 3c (-6.08).

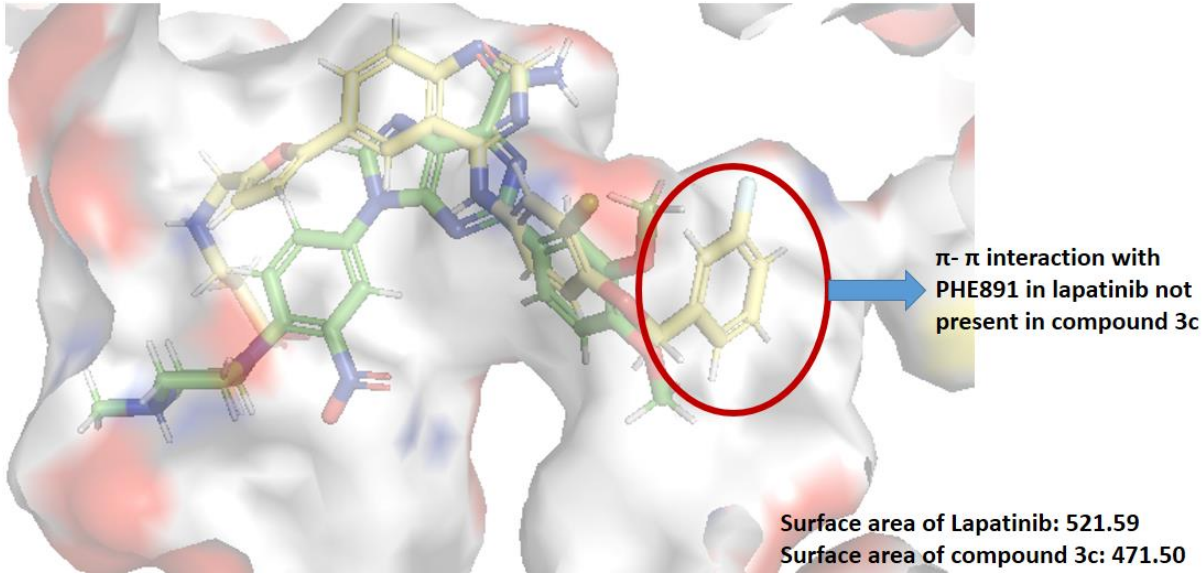
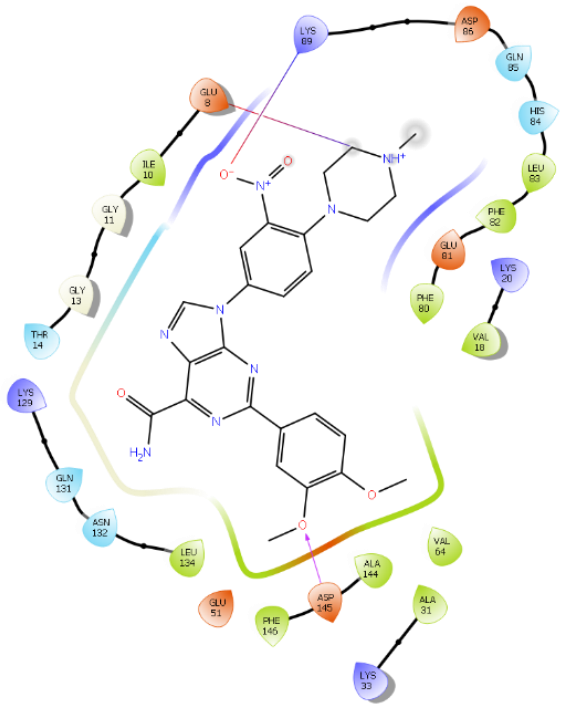
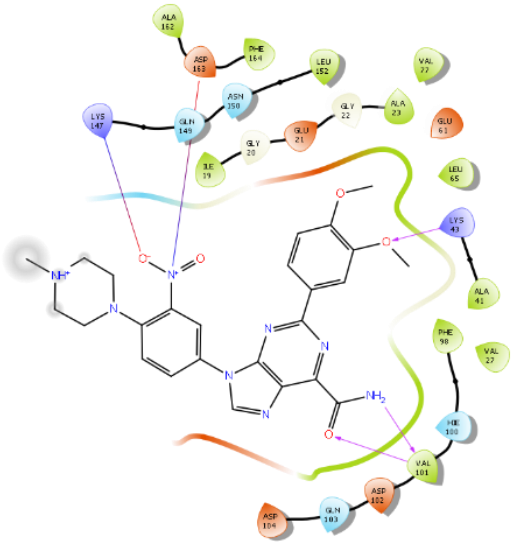


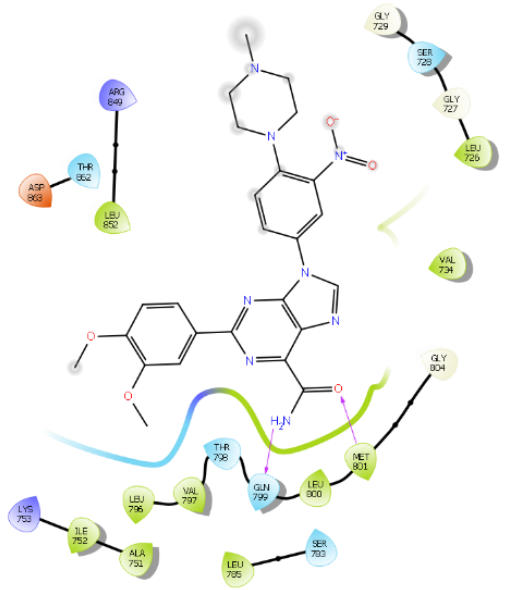
Figure S1: Represents the structure of lapatinib (yellow) and compound **3c** (green) in HER-2 protein (PDB: 3RCD) with important flurophenyl ring in lapatinib that increases surface area of lapatinib by 50 $Å^2$ and supports π- π interaction with PHE891.

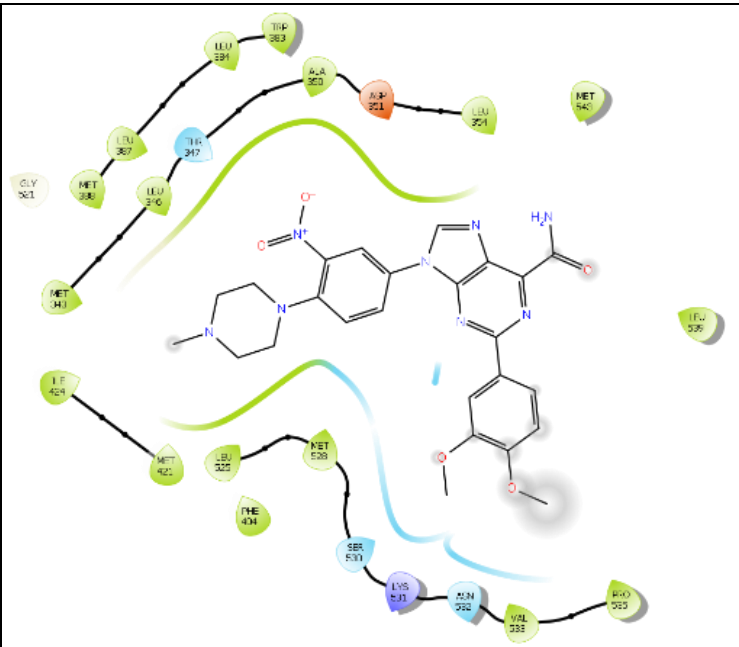
Similarly, docking results of compound **3c** were not favourable with other proteins as well (CDK-2, 4, 6, ERα and PR). We already mentioned in the manuscript that **3c** did not inhibit Cyclin dependant kinases (CDKs) under in vitro condition which could be due to poor binding and docking scores (Table S1). Compound 3c could not even enter binding cavity of some PR. Therefore, EGDR inhibition could seem to be one of the major anticancer mechanisms.

Table S1: Docking of compound 3c into other proteins

Protein	**ID**	**Positive Control (Dock Score)**	**Dock Score (Compound 3c)**	**2D interaction with 3c**
CDK2	**5L2W**	**Dinacicilib** **(-13.46)**	**-5.47**	
CDK4	**2W9Z**	**Pablocicilib**	**No co-crystallized ligand**	----------

		(NA)		
CDK6	**2EUF**	**Pablocicilib** **(-10.46)**	**-6.82**	

HER2	**3RCD**	**Lapatinib** **(-12.39)**	**-6.03**	

ERα	**5W9C**	**Tamoxifen** **(-12.75)**	**-2.78**	
PR	**2W8Y**	**Mifepristone (NA)**	**Not entered in cavity**	**-------**