Electronic Supplementary Material (ESI) for RSC Medicinal Chemistry.

Design, synthesis, and anticancer assessment of structural analogues of (E)-1-((3,4,5-trimethoxybenzylidene)amino)-4-(3,4,5-trimethoxyphenyl)imidazo[1,2-*a*]quinoxaline-2-carbonitrile (6b), an imidazo[1,2-*a*]quinoxaline-based non-covalent EGFR Inhibitor

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2. Department of Human Genetics and Molecular Medicine, Central University of Punjab, Bathinda- 151401 Punjab, India

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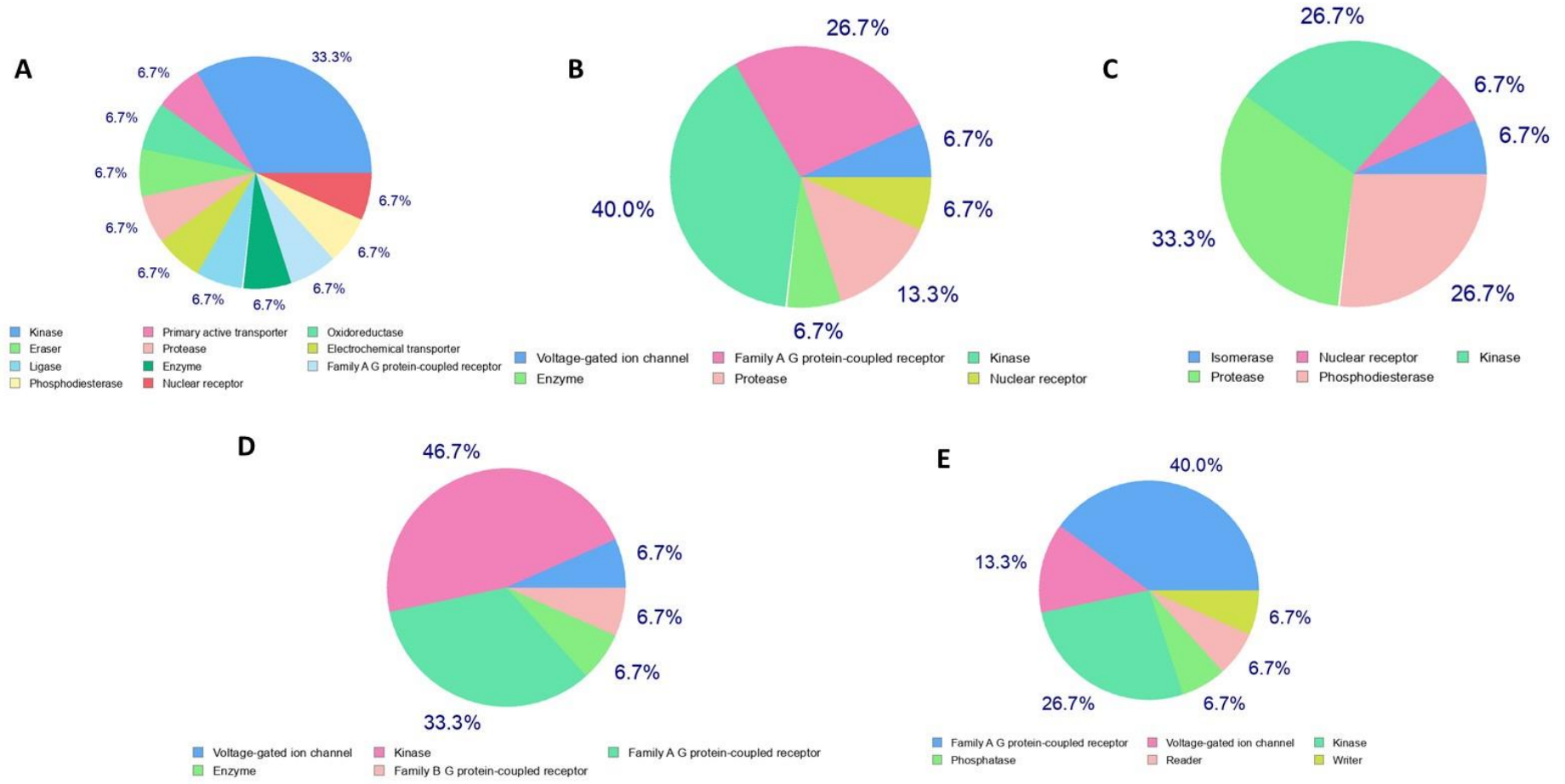


Figure S1. Pie chart of possible target prediction by Swiss Target Prediction tool **(**http://www.swisstargetprediction.ch/**)** of synthetics **(A)** 5a **(B)** 5e **(C)** 5h**, (D)** 5l and **(E)** 5o

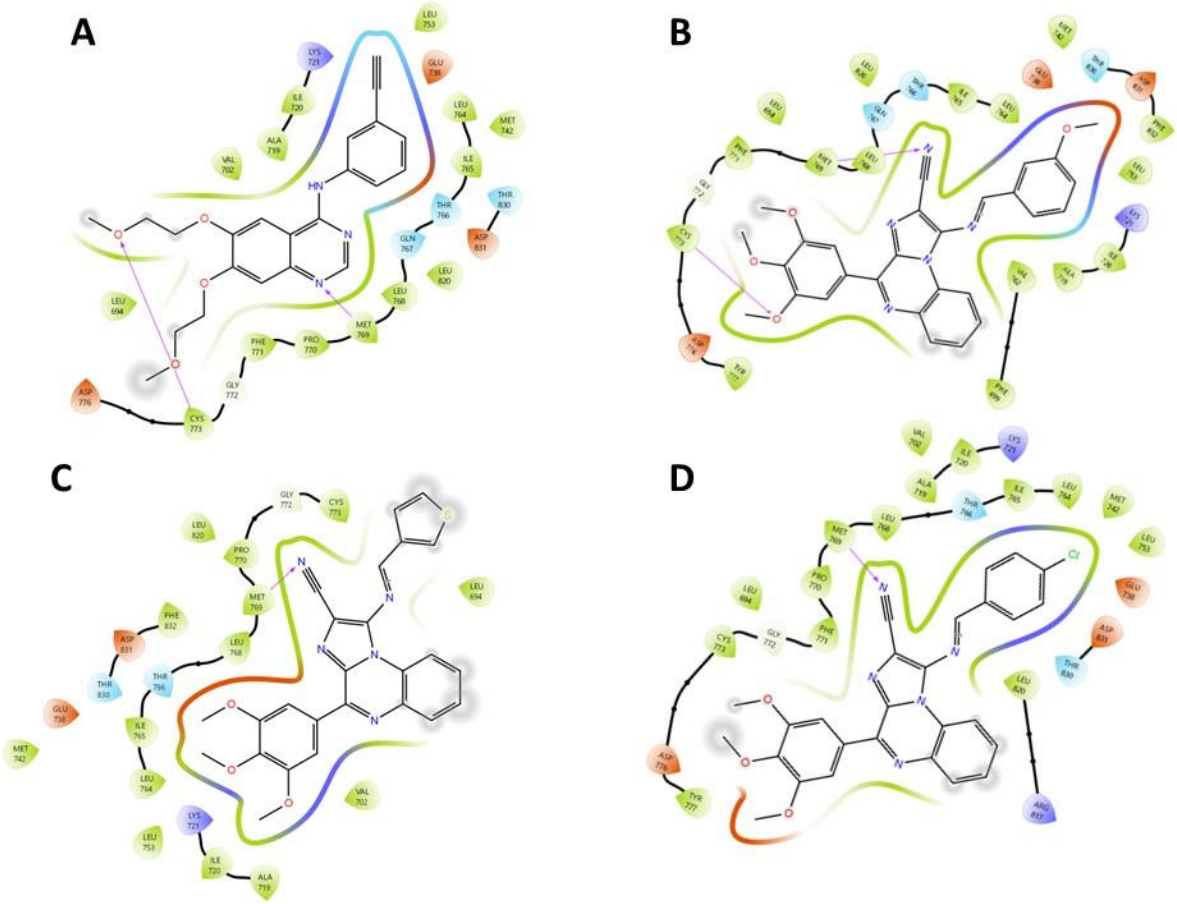


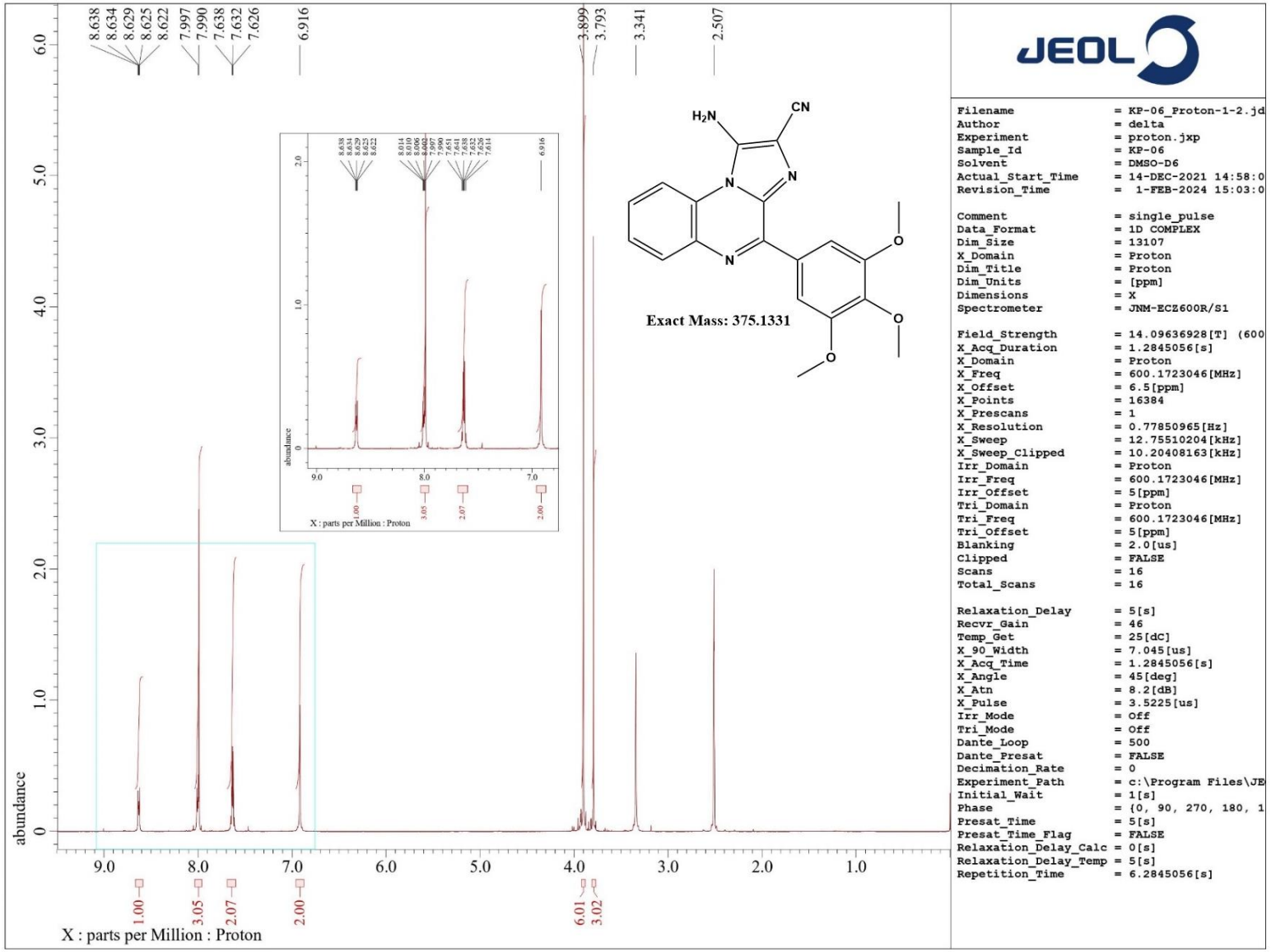
Figure S2. 2D interactions of **6b** (A), **5a** (B) and **5v** (C) in the binding pocket of $EGFR_{WT}$ (PDB:1M17)

Table S1: Antiproliferative potential of target compounds

S.No.	Compound Code	IC_{50} (µM)		
		A549	**MCF7**	**MDA-MB-231**
1.	**Erlotinib**	4,68	>10	>10
2.	**MRP-1**	21.15	10.97±0.08	13.8±0.04
3.	**5a**	3.53±0.03	13.58±0.10	5.77±0.03
4.	**5b**	15.49±0.09	15.86±0.08	15.58±0.08
5.	**5c**	15.18±0.04	10.82±0.23	15.18±0.05
6.	**5d**	>25	4.16±0.16	13.23±0.09
7.	**5e**	4.43±0.08	3.82±0.14	5.94±0.04
8.	**5f**	11.01±0.06	15.47±0.13	9.48±0.06
9.	**5g**	14.12±0.09	9.89±0.23	14.72±0.02
10.	**5h**	3.25±0.02	9.99±0.15	11.36±0.04
11.	**5i**	5.05±0.10	15.545±0.24	12.91±0.06
12.	**5j**	8.65±0.06	12.558±0.13	19.47±0.03
13.	**5k**	>25	17.42±0.07	24.66±0.04
14.	**5l**	1.34±0.04	14.30±0.30	>25
15.	**5m**	11.67±0.13	17.69±0.26	16.3±0.18
16.	**5n**	15.03±0.22	15.68±0.54	22.41±0.12
17.	**5o**	4.27±0.14	23.85±0.24	8.661±0.11
18.	**5p**	>25	8.99±0.12	>25
19.	**5q**	16.49±0.39	13.14±0.43	8.88±0.14
20.	**5r**	>25	20.28±0.05	>25
21.	**5s**	14.79±0.11	>25	8.76±0.06
22.	**5t**	19.96±0.32	27.68±0.33	21.47±0.30
23.	**5u**	15.35±0.16	>25	21.01±0.39
24.	**5v**	10.38±0.19	11.66±0.08	15.14±0.09
25.	**5w**	24.3±0.10	19.48±0.15	21.42±0.12
26.	**5x**	13.17±0.14	24.04±0.12	6.41±0.13
27.	**5y**	9.95±0.08	11.24±0.06	14.74±0.1
28.	**5z**	18.6±0.29	>25	17.65±0.19
29.	**5aa**	>25	>25	>25

30.	**5ab**	16.44±0.08	19.15±0.1	>25
31.	**5ac**	>25	18.94±0.07	>25

Spectral data of compound MRP-1

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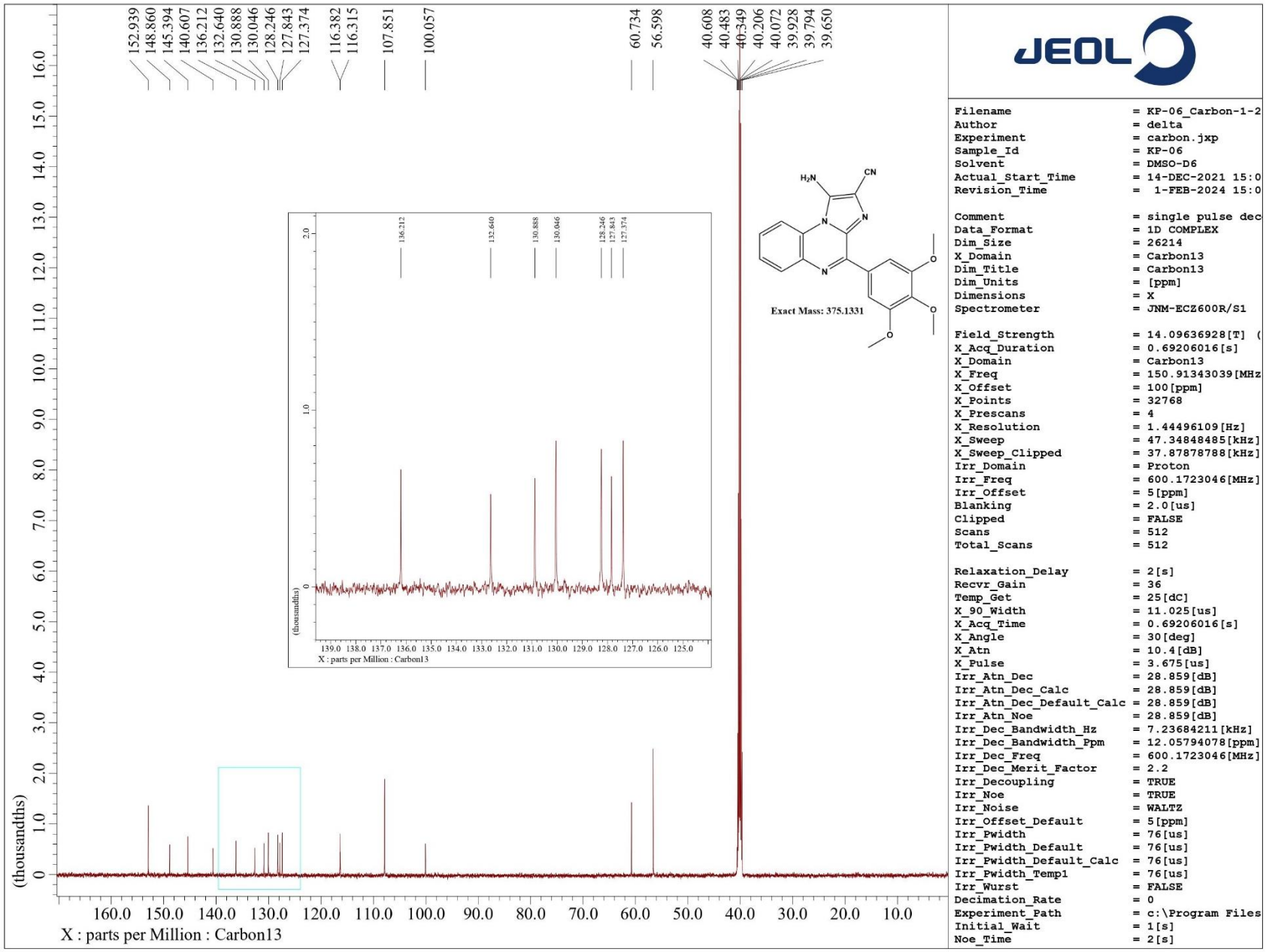
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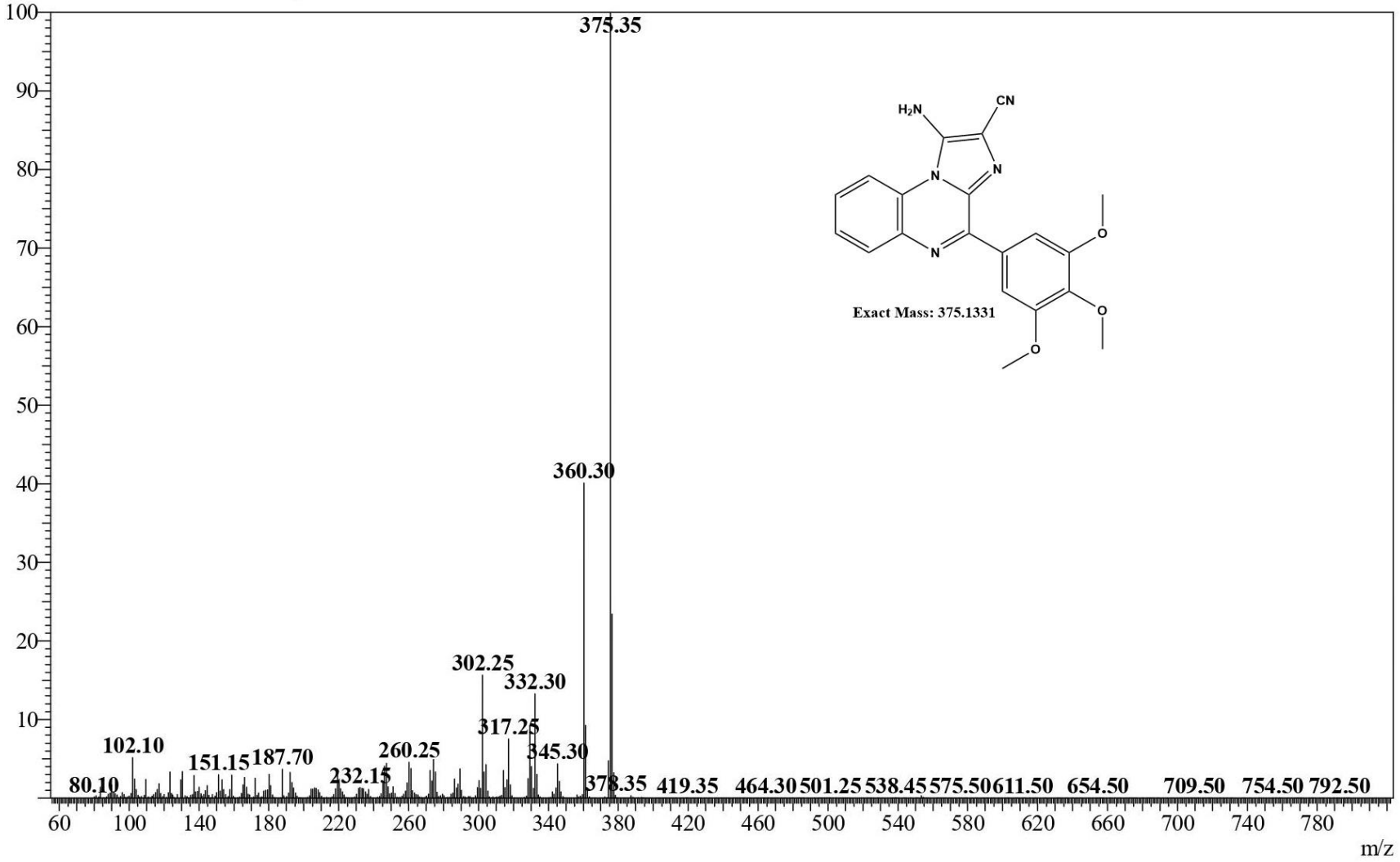
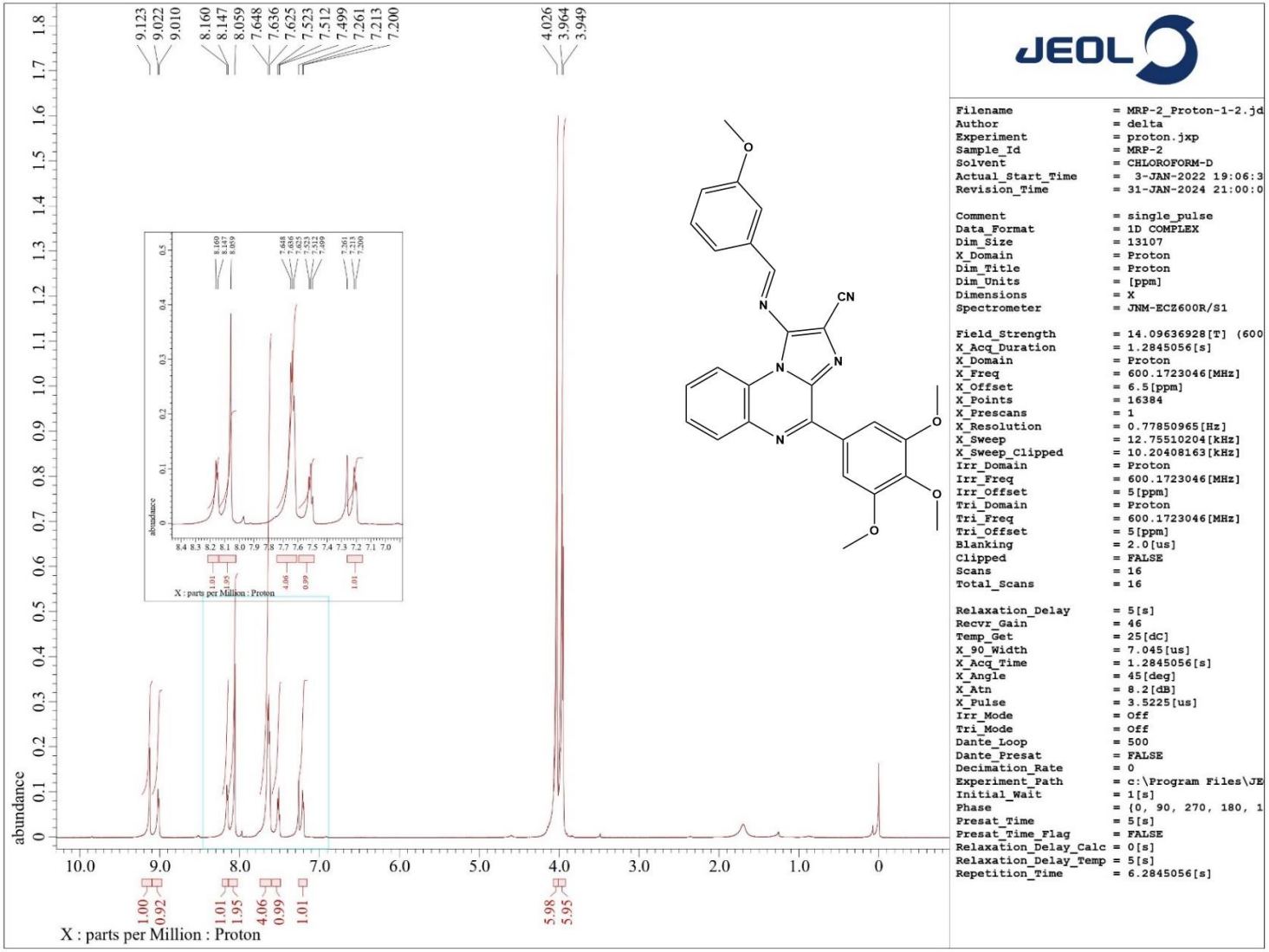


Spectral data of compound 5a

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X_Points                = 16384
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Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2.0[us]
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Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 25[dC]
X_90_Width              = 7.045[us]
X_Acq_Time              = 1.2845056[s]
X_Angle                 = 45[deg]
X_Atn                   = 8.2[dB]
X_Pulse                 = 3.5225[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
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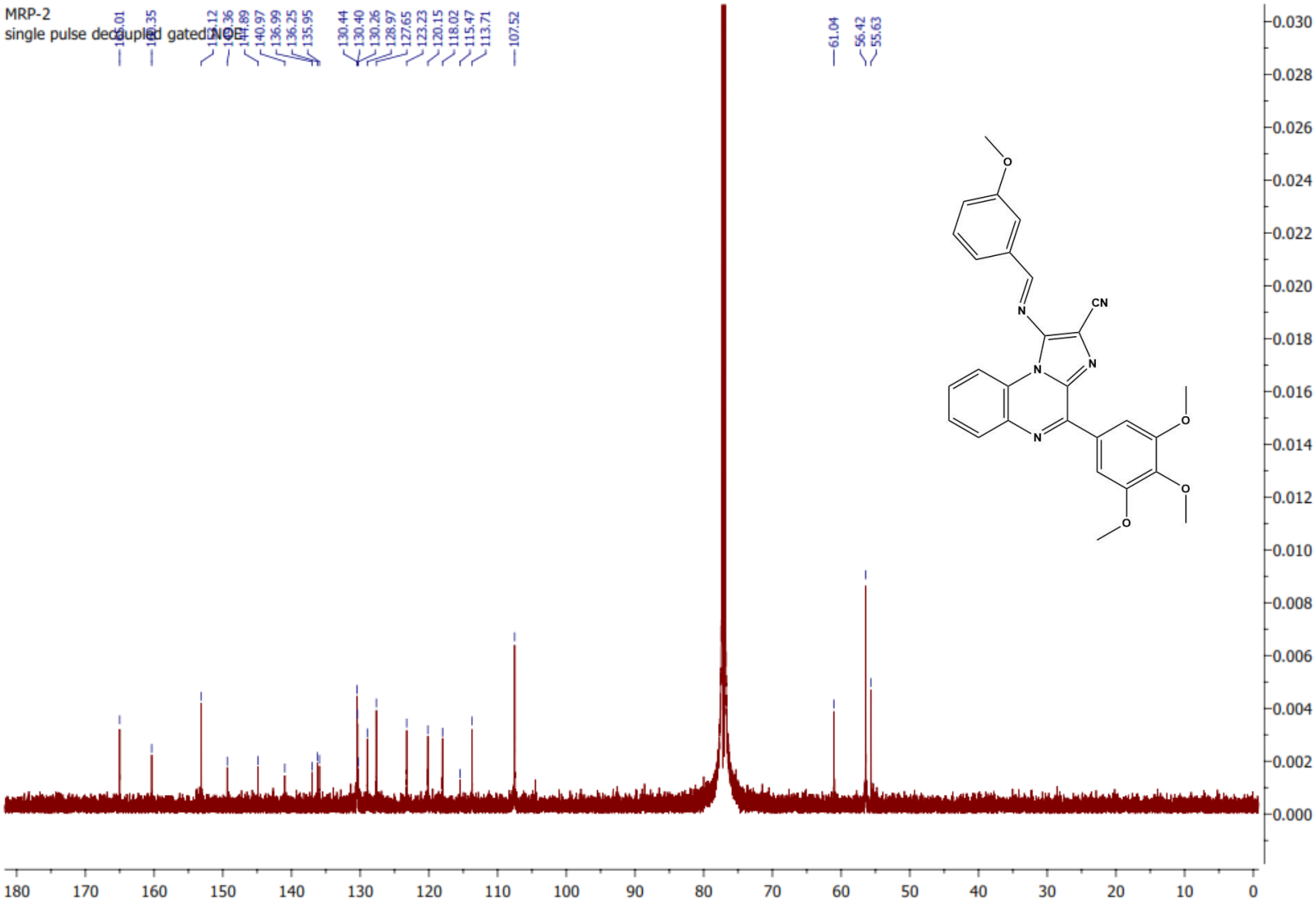
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N
O
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120
110
100
90
80
70
60
50
40
30
20
10
0

Elemental Composition Report

Single Mass Analysis

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Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
1608 formula(e) evaluated with 9 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-10 Br: 0-2

Sample Name : MRP_2
Test Name :
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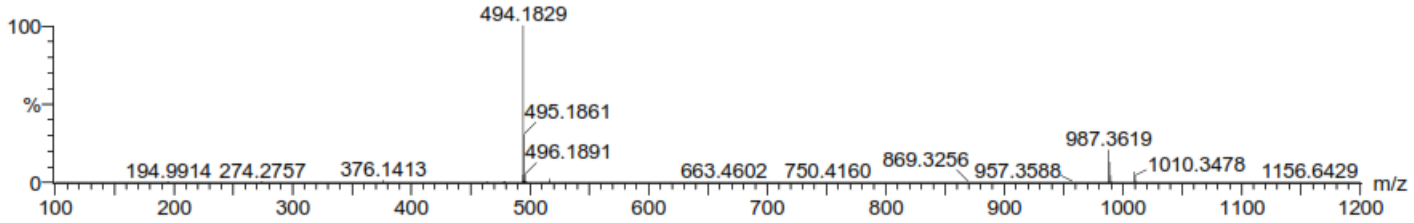
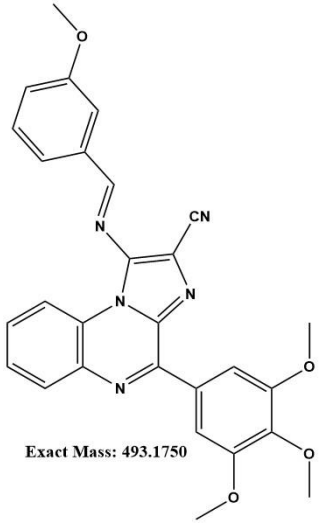
IITRPR

XEVO G2-XS QTOF

1: TOF MS ES+
1.87e+007





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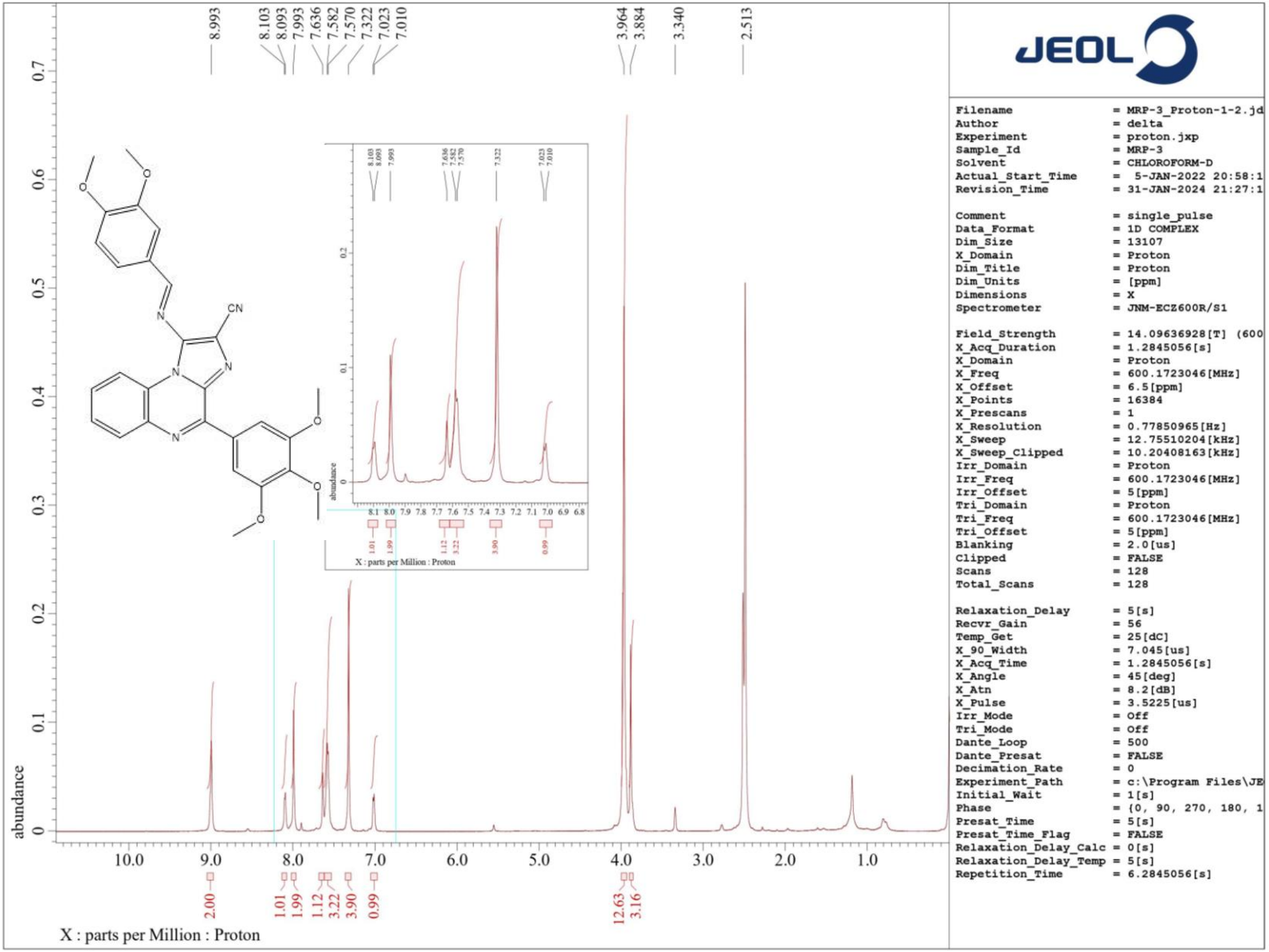
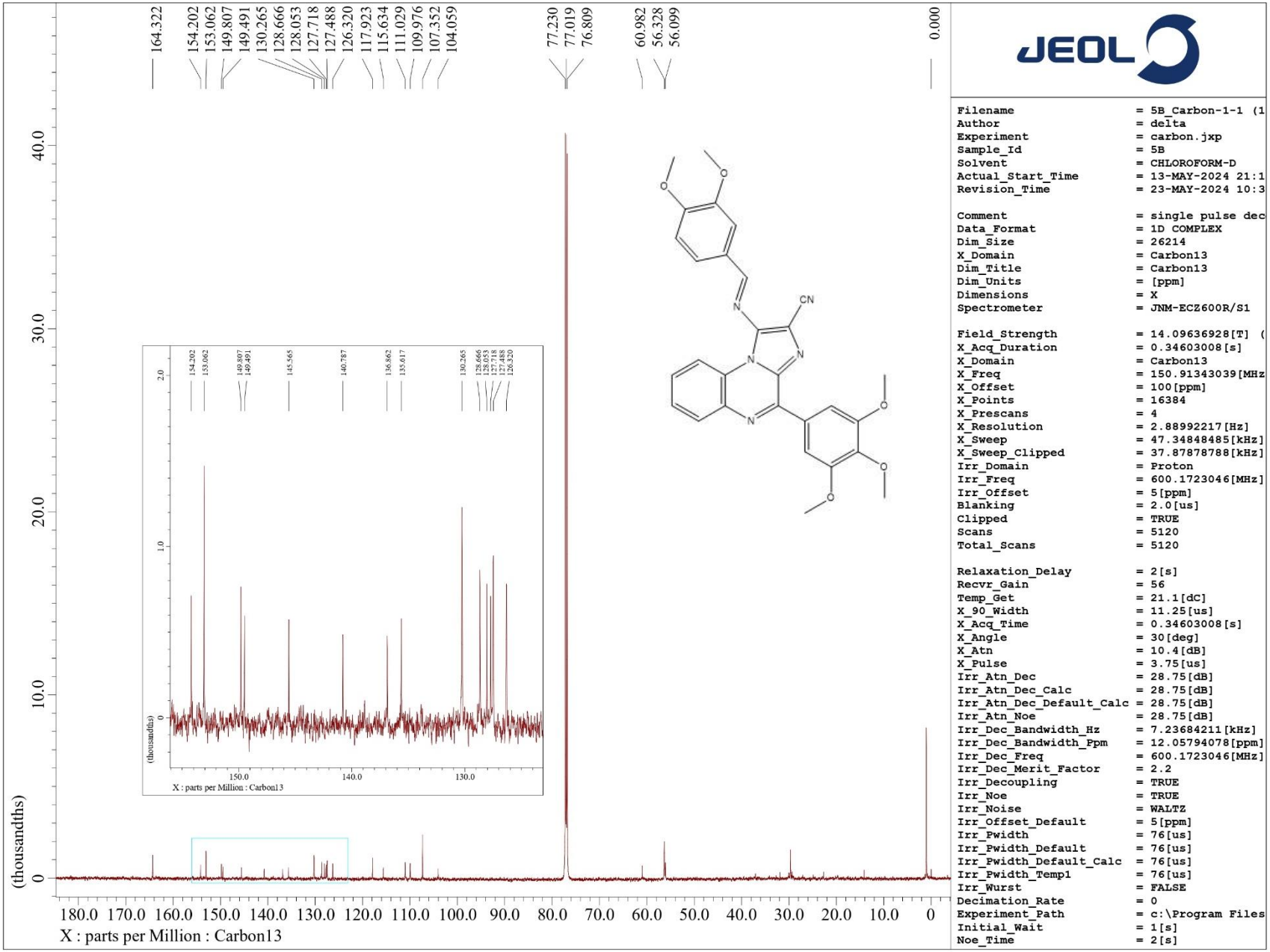
Spectral data of compound 5b

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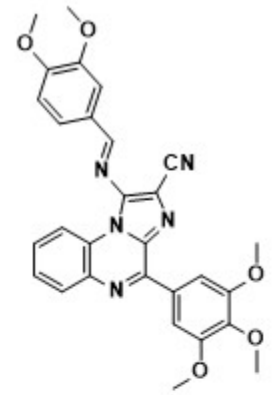
Elemental Composition Report



m/z: 523.1856 (100.0%)

Single Mass Analysis

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Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
1737 formula(e) evaluated with 13 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-10 Br: 0-2

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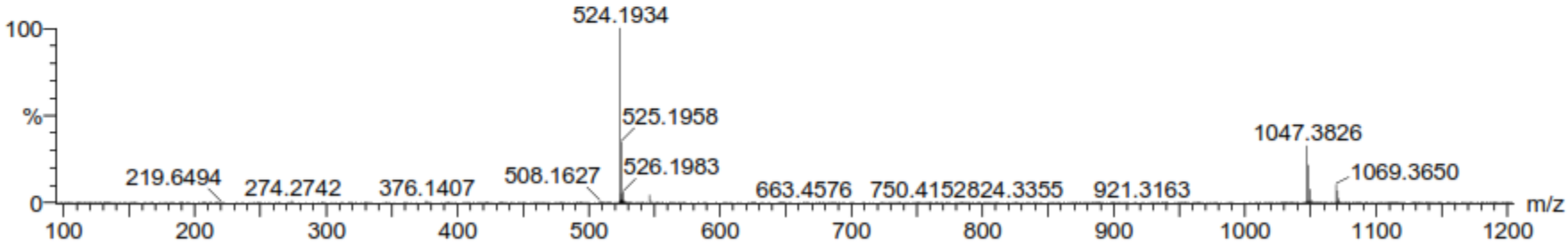
Test Name :
23032022_MRP_3 8 (0.186) 1: TOF MS ES+
3.27e+007



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Maximum:		2.0	10.0	50.0				
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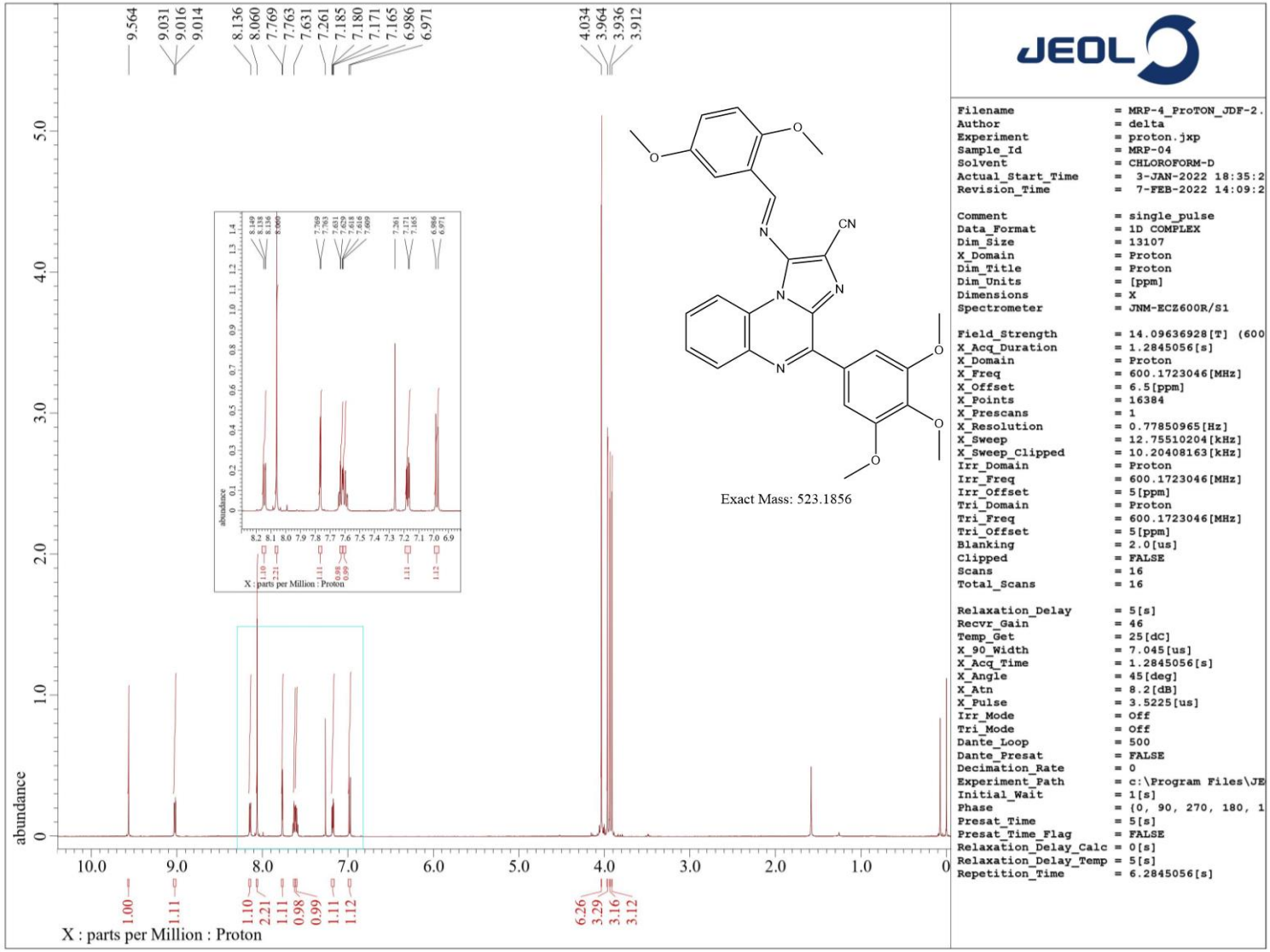
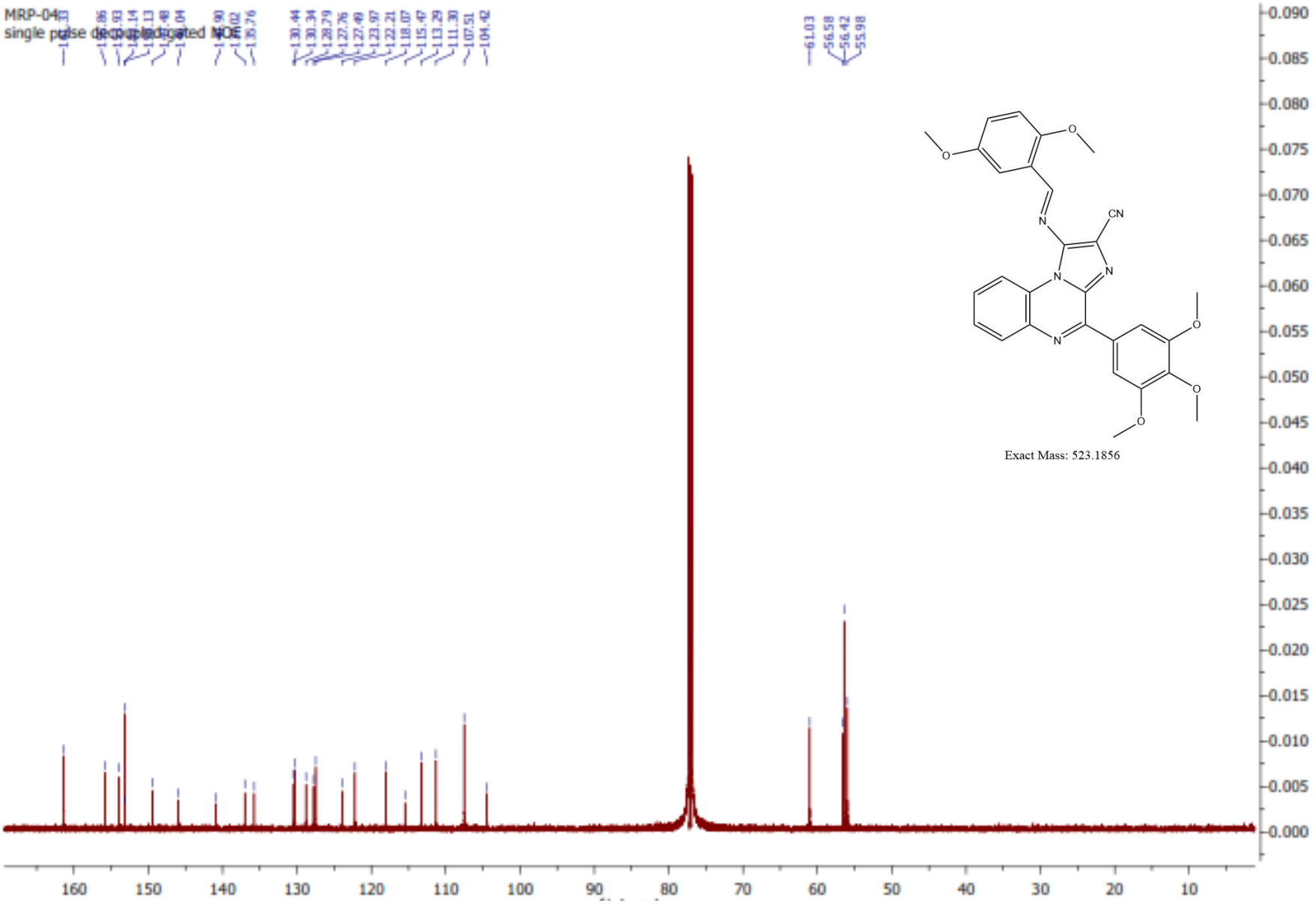
Spectral data of compound 5c




MRP-04
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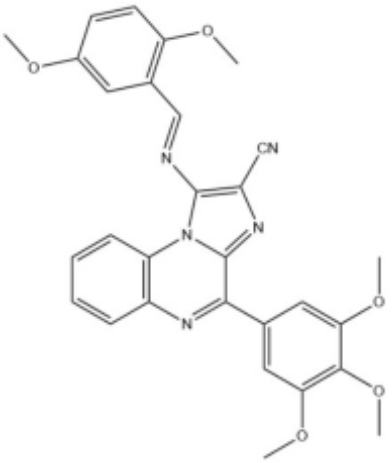
CN
N
O
Exact Mass: 523.1856

Elemental Composition Report



Exact Mass: 523.1856

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
1737 formula(e) evaluated with 13 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-10 Br: 0-2

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Test Name :
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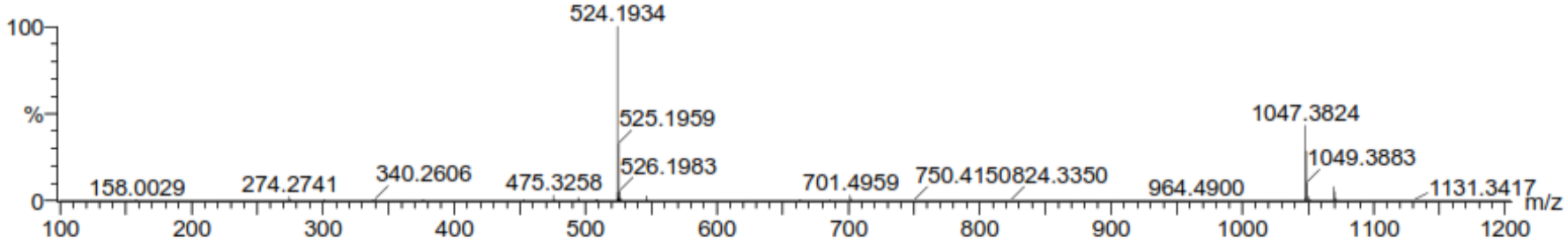
1.41e+007



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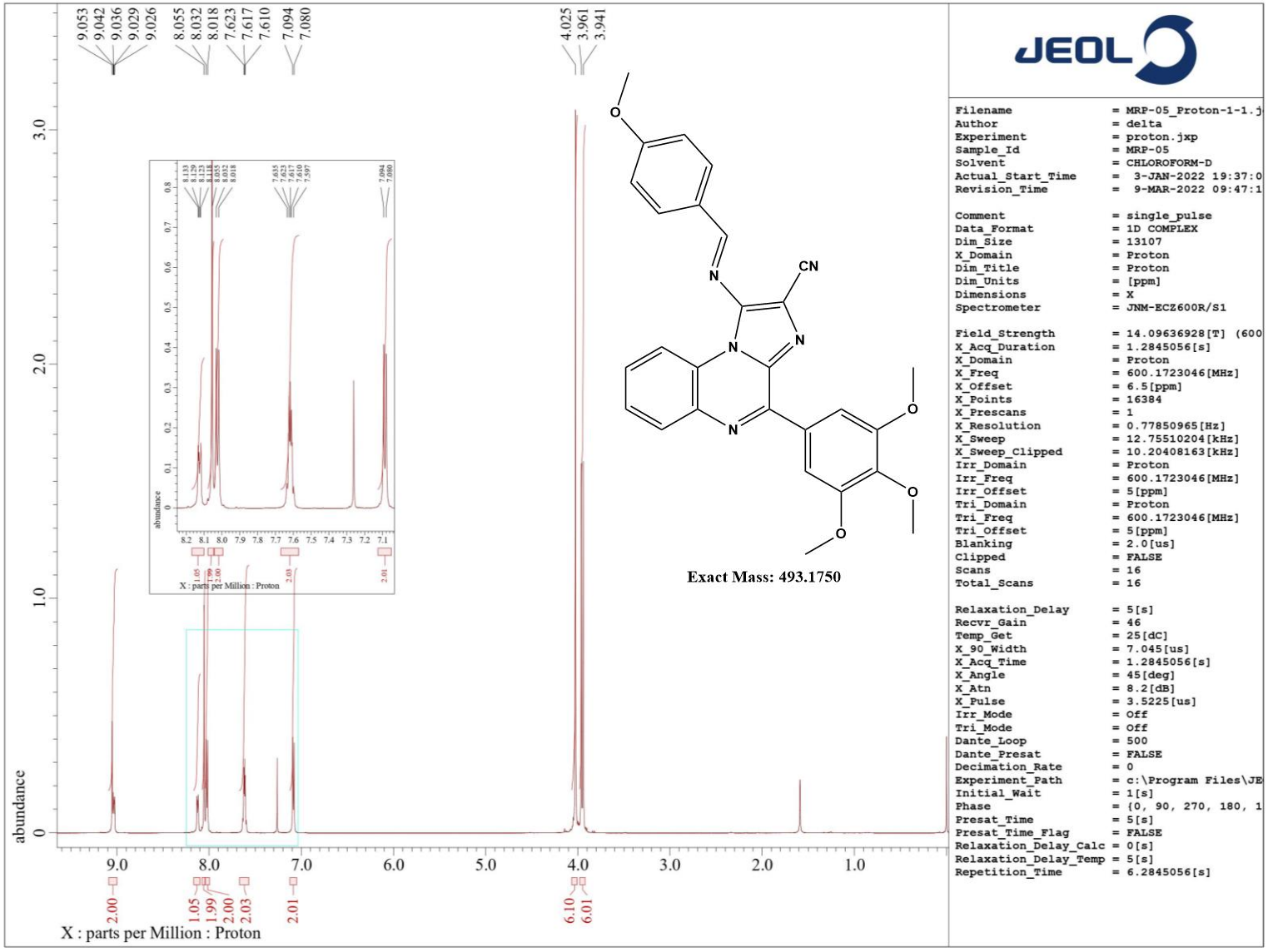
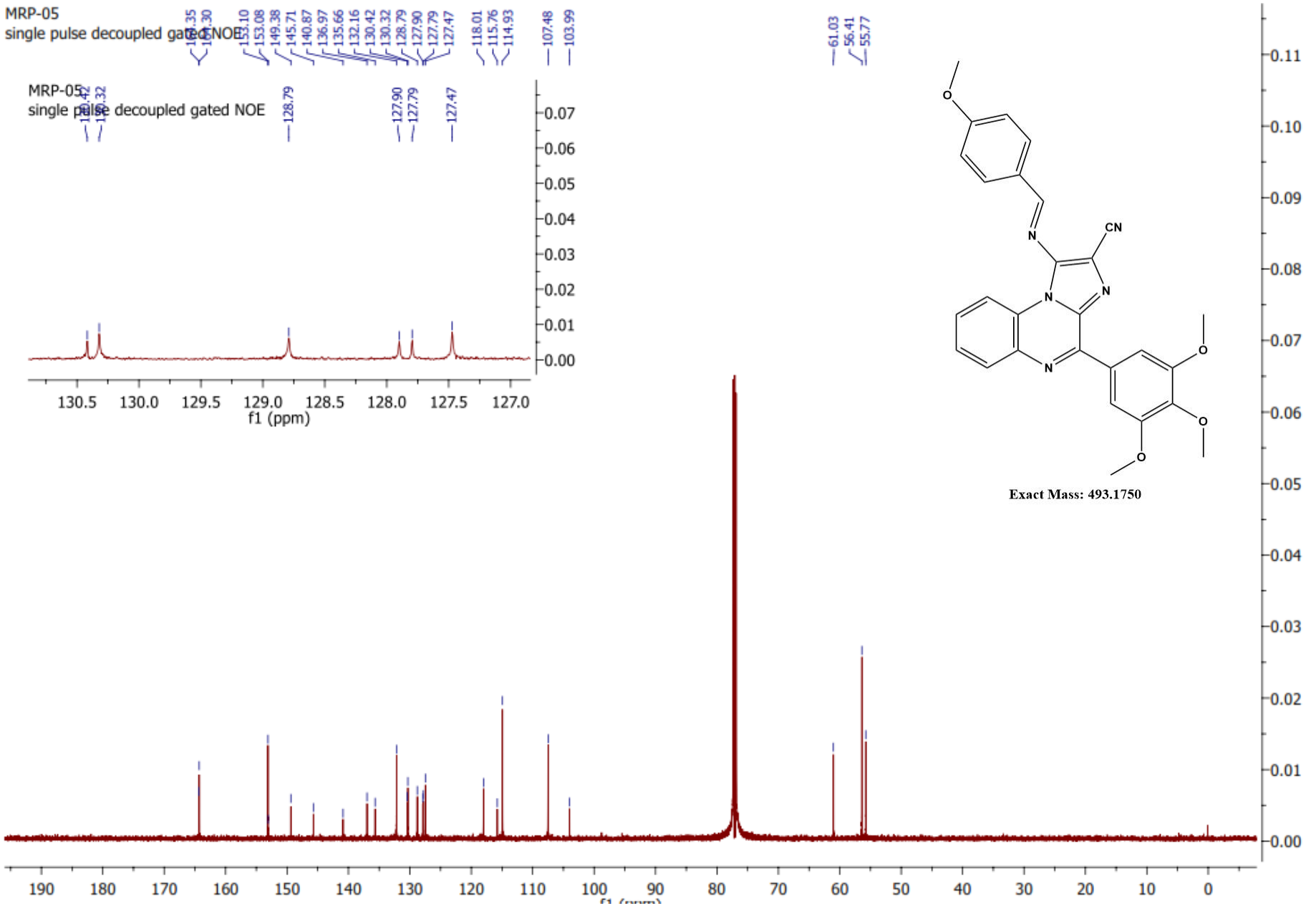
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
524.1934	524.1934	0.0	0.0	19.5	1205.6	n/a	n/a	C29 H26 N5 O5

Spectral data of compound 5d




```
Filename              = MRP-05_Proton-1-1.j
Author                = delta
Experiment            = proton.jxp
Sample_Id             = MRP-05
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  3-JAN-2022 19:37:0
Revision_Time         =  9-MAR-2022 09:47:1

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S1

Field_Strength        = 14.09636928[T] (600
X_Acq_Duration        = 1.2845056[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 6.5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.77850965[Hz]
X_Sweep               = 12.75510204[kHz]
X_Sweep_Clipped       = 10.20408163[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2.0[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 46
Temp_Get              = 25[dC]
X_90_Width            = 7.045[us]
X_Acq_Time            = 1.2845056[s]
X_Angle               = 45[deg]
X_Atn                 = 8.2[dB]
X_Pulse               = 3.5225[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JE
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 1
Presat_Time           = 5[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time       = 6.2845056[s]
```

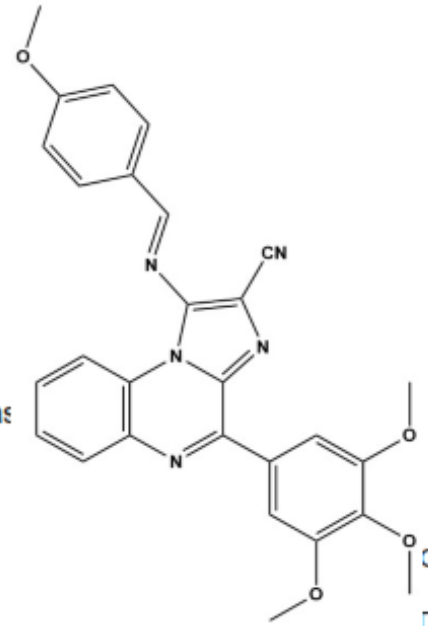

MRP-05
single pulse decoupled gated NOE
MRP-05
single pulse decoupled gated NOE
f1 (ppm)
Exact Mass: 493.1750

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
1608 formula(e) evaluated with 9 results within limits (up to 1 closest results for each mas
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-10 Br: 0-2



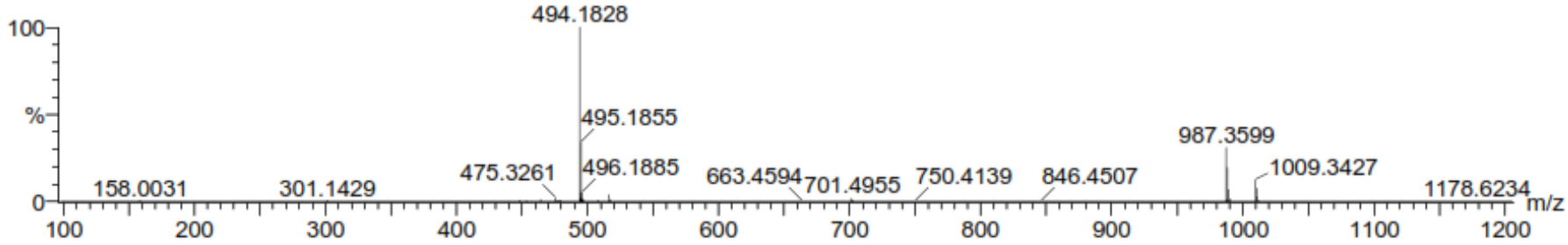
Exact Mass: 493.1750

Sample Name : MRP_5
Test Name :
23032022_MRP_5 11 (0.249)

IITRPR

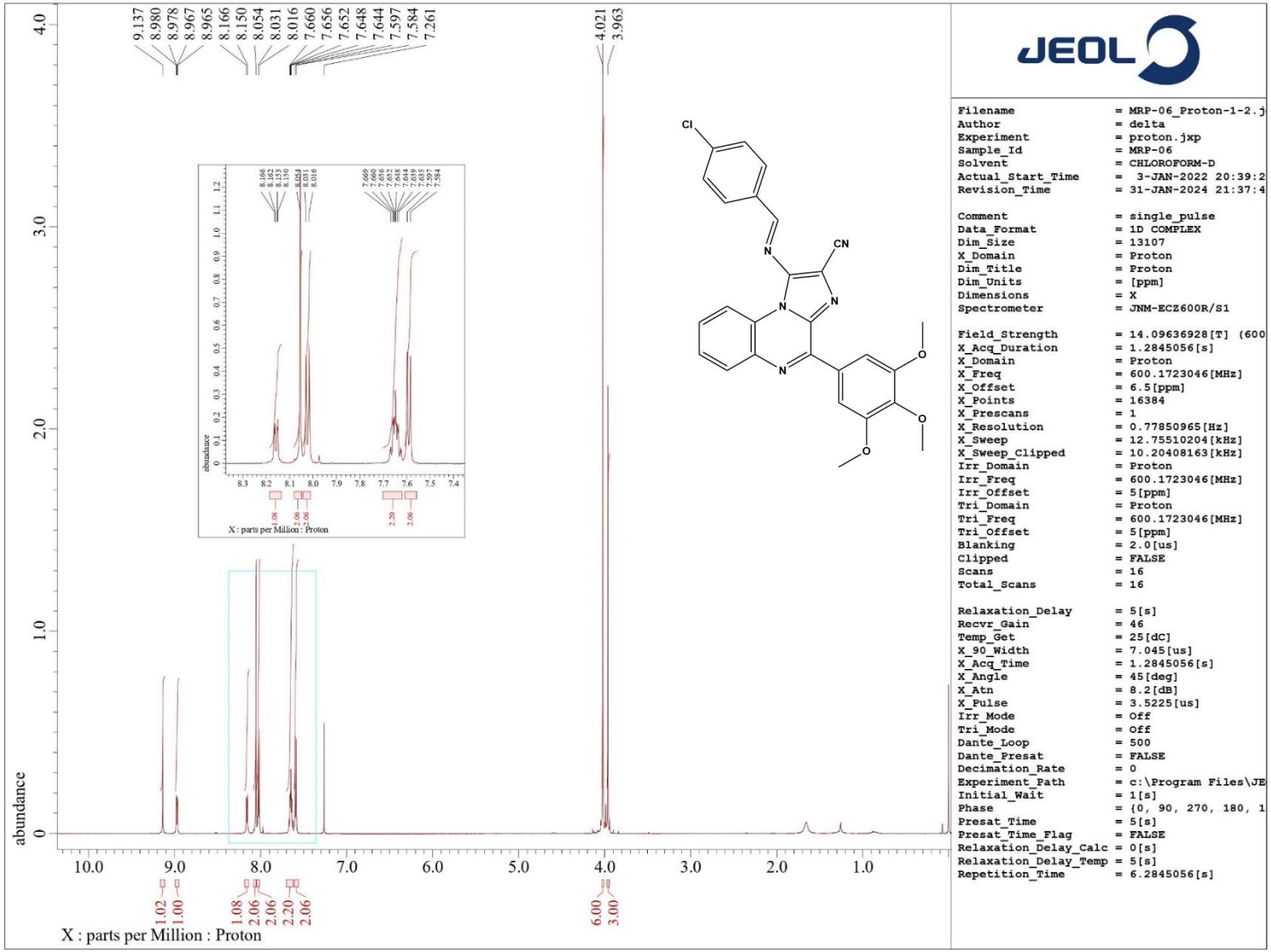
G2-XS QTOF

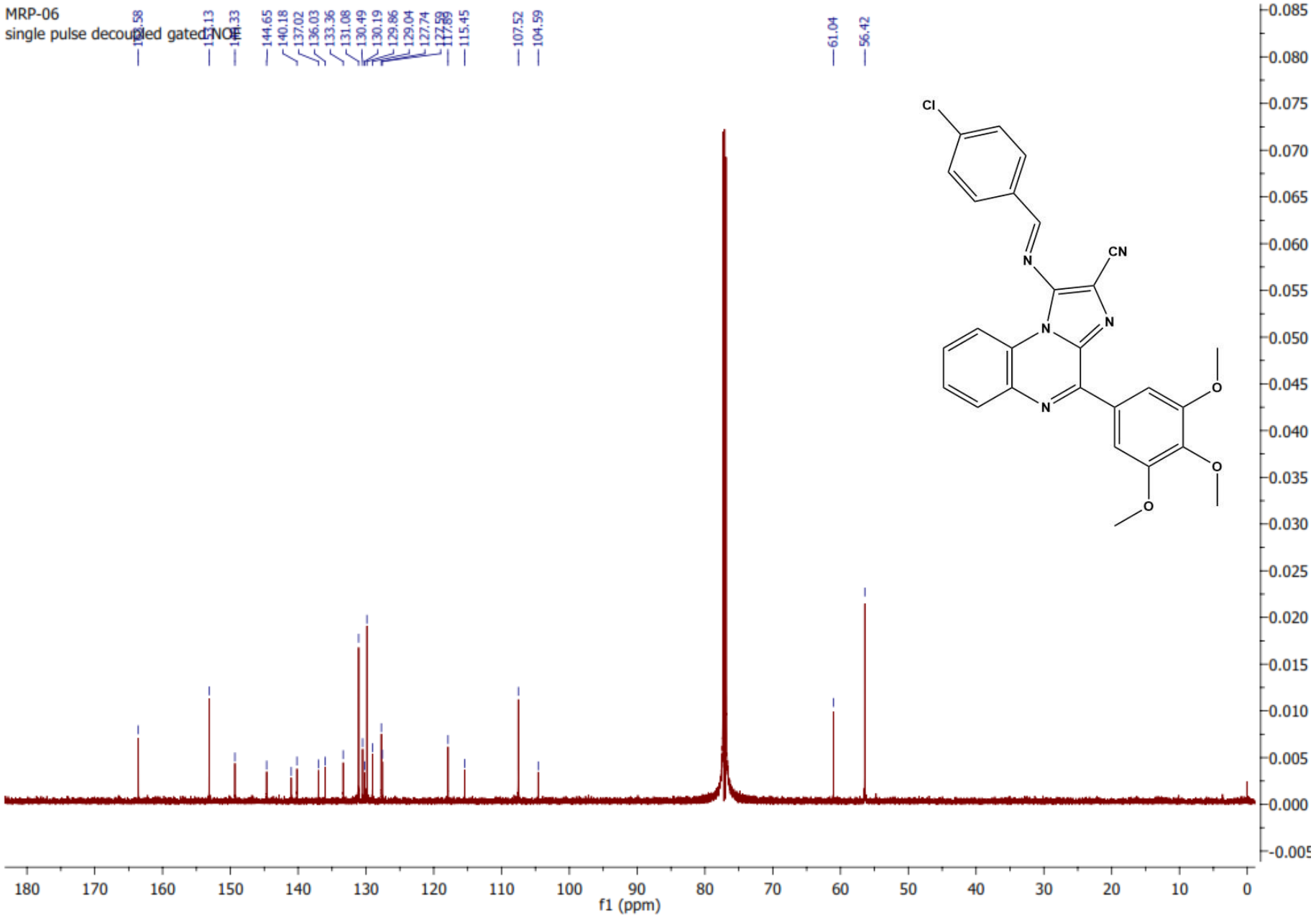
TOF MS ES+
1.90e+007



Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
494.1828	494.1828	0.0	0.0	19.5	1345.7	n/a	n/a	C28 H24 N5 O4

Spectral data of compound 5e



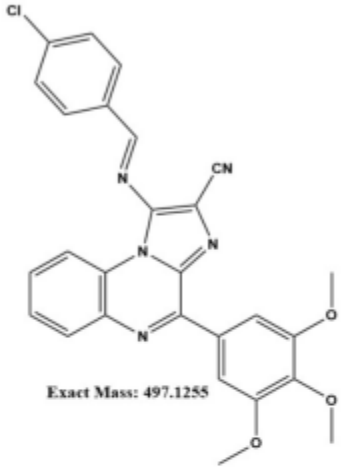

MRP-06
single pulse decoupled gated NOE
158.13
144.65
140.18
137.02
136.03
133.36
131.08
130.49
130.19
129.86
129.04
127.74
115.45
107.52
104.59
61.04
56.42
Cl
N
CN
N
N
N
O
O
O
f1 (ppm)

Elemental Composition Report

Single Mass Analysis

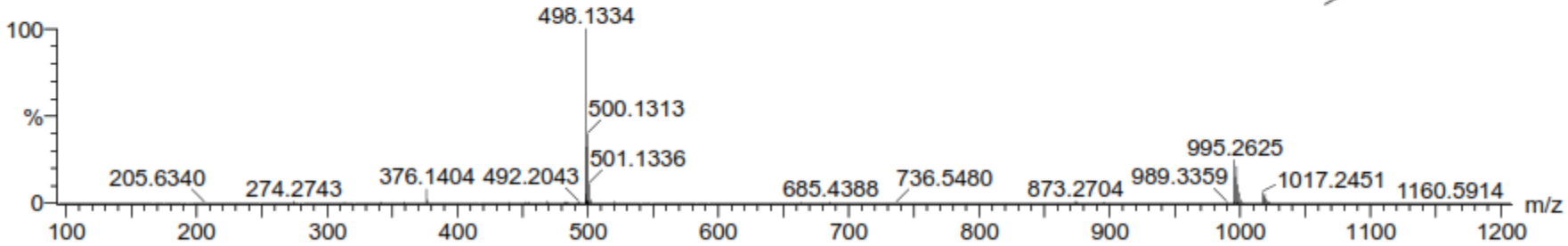
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
1822 formula(e) evaluated with 17 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 0-10 O: 0-10 Cl: 0-2



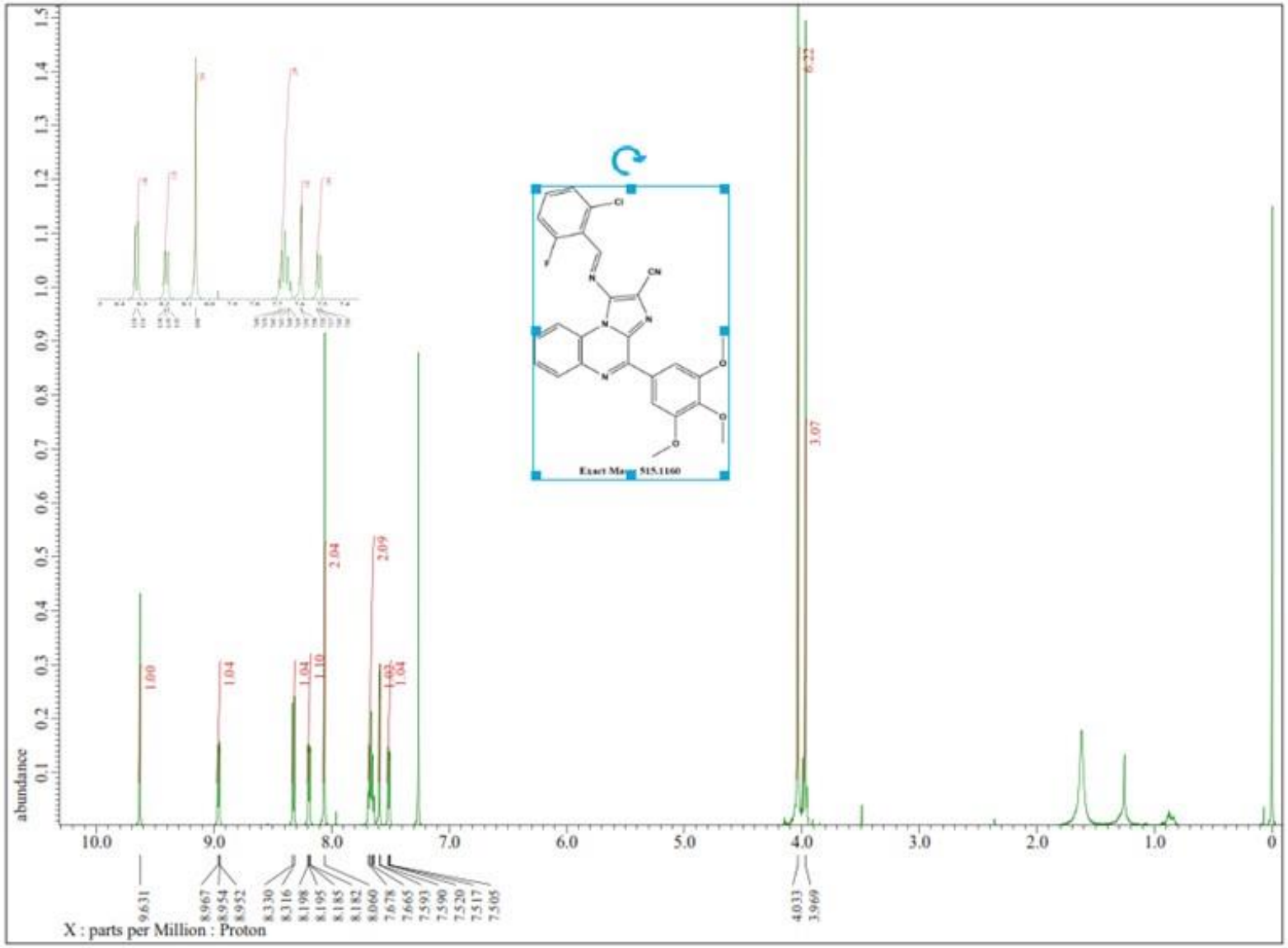
Sample Name : MRP_6 IITRPR
Test Name :
23032022_MRP_6 8 (0.186)

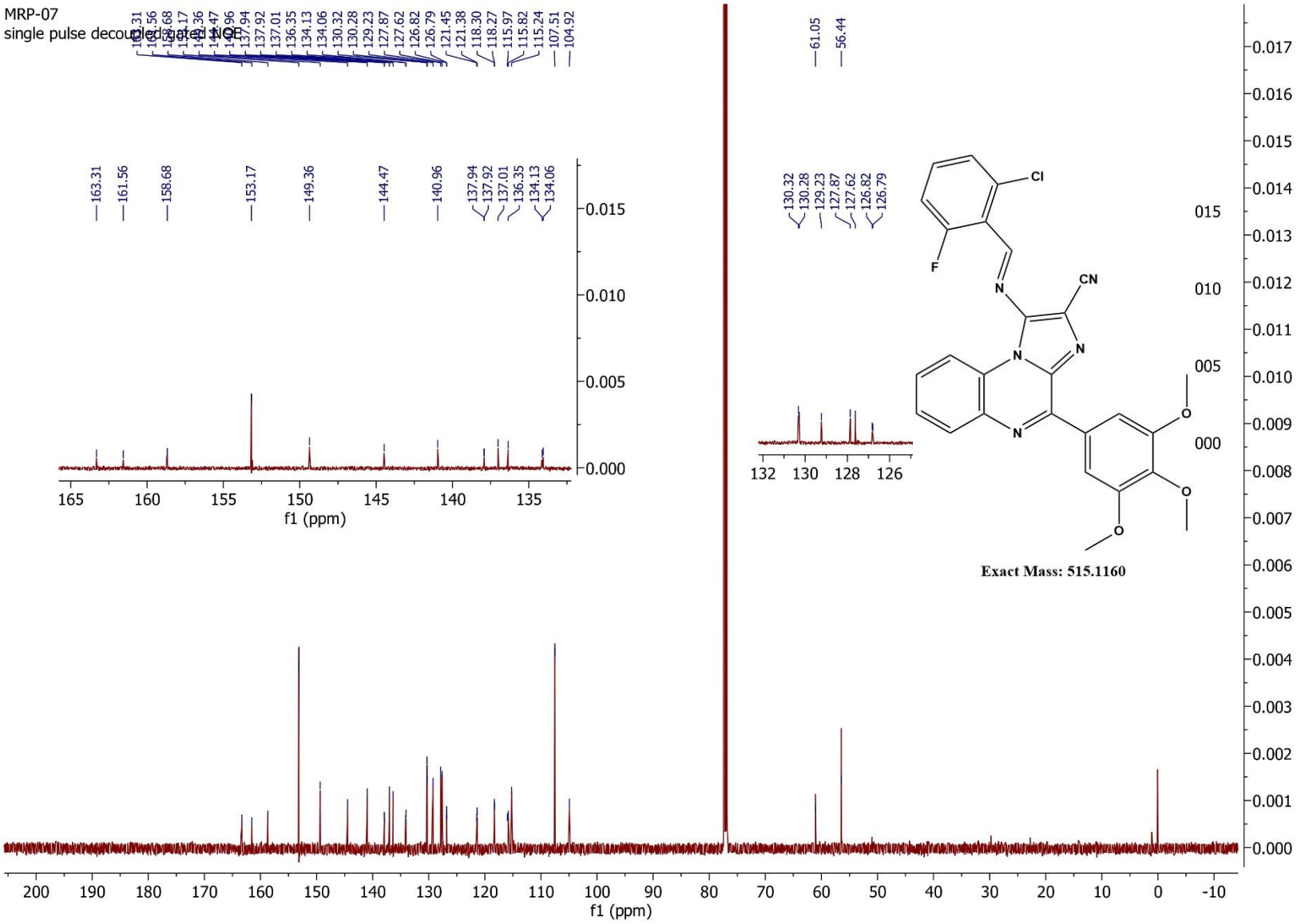
32-XS QTOF
OF MS ES+
4.38e+007



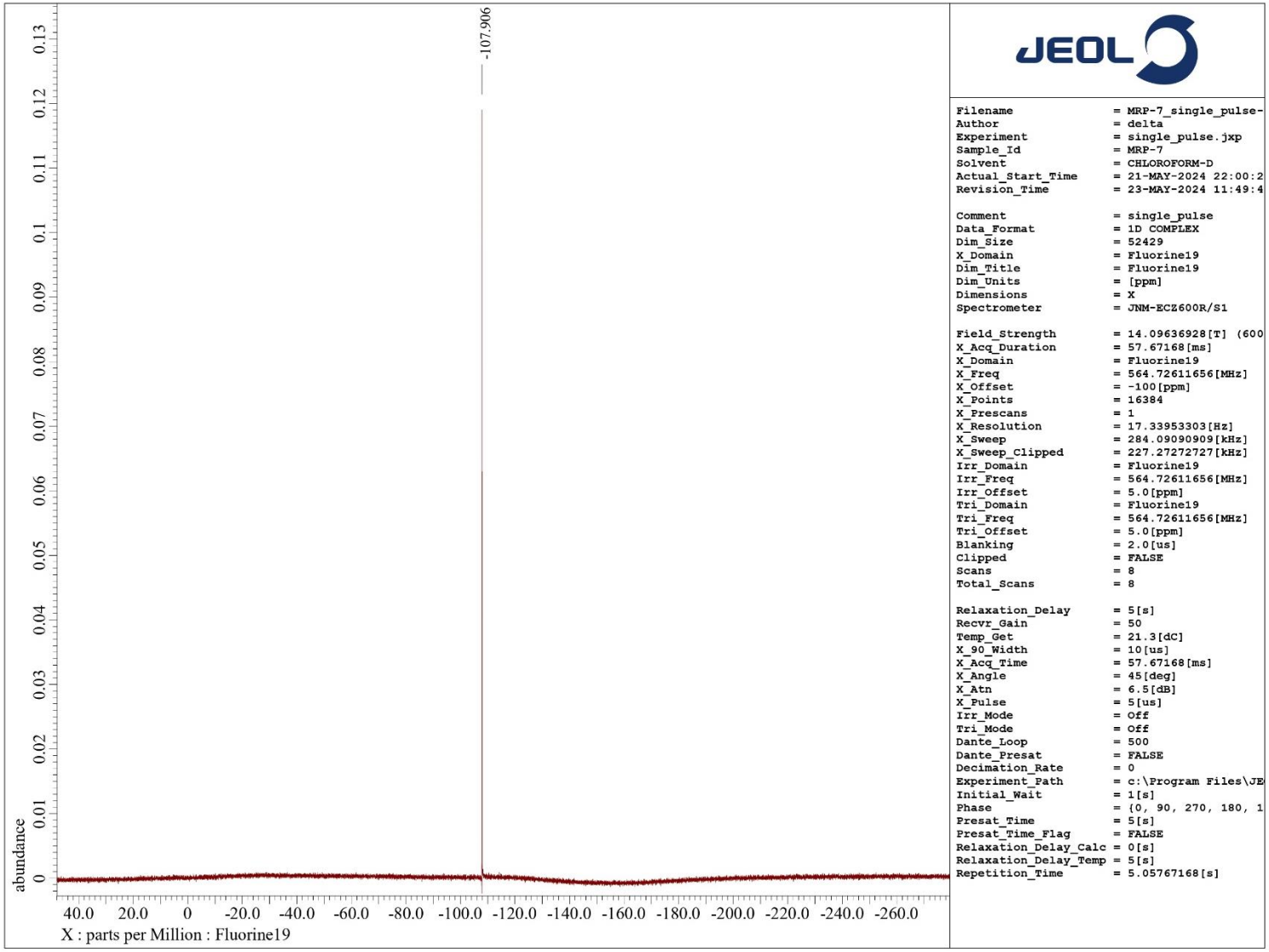
Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
498.1334	498.1333	0.1	0.2	19.5	1373.8	n/a	n/a	C27 H21 N5 O3 Cl

Spectral data of compound 5f




MRP-07
single pulse decoupled gated NOE
163.31
161.56
158.68
153.17
149.36
144.47
140.96
137.94
137.92
137.01
136.35
134.13
134.06
130.32
130.28
129.23
127.87
127.62
126.82
126.79
121.45
121.38
118.30
118.27
115.97
115.82
115.24
107.51
104.92
61.05
56.44
f1 (ppm)
Cl
F
CN
N
O
Exact Mass: 515.1160

^{19}F NMR

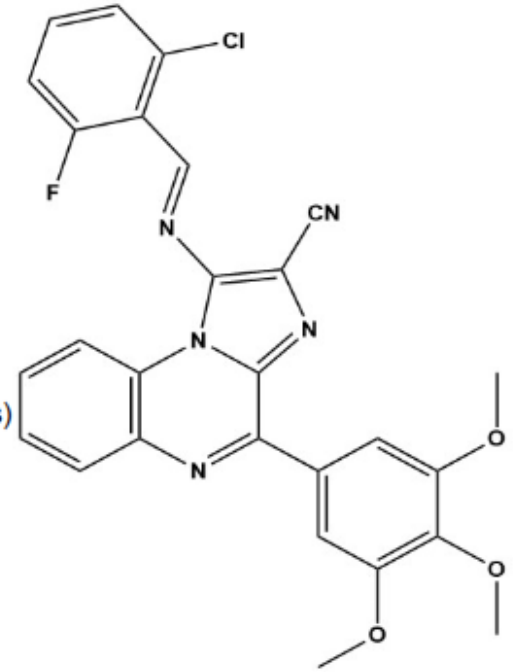

-107.906
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
40.0 20.0 0 -20.0 -40.0 -60.0 -80.0 -100.0 -120.0 -140.0 -160.0 -180.0 -200.0 -220.0 -240.0 -260.0
X : parts per Million : Fluorine19
JEOL
Filename = MRP-7_single_pulse-
Author = delta
Experiment = single_pulse.jxp
Sample_Id = MRP-7
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-MAY-2024 22:00:2
Revision_Time = 23-MAY-2024 11:49:4
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 52429
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T] (600
X_Acq_Duration = 57.67168[ms]
X_Domain = Fluorine19
X_Freq = 564.72611656[MHz]
X_Offset = -100[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 17.33953303[Hz]
X_Sweep = 284.09090909[kHz]
X_Sweep_Clipped = 227.27272727[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 564.72611656[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 564.72611656[MHz]
Tri_Offset = 5.0[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 50
Temp_Get = 21.3[dC]
X_90_Width = 10[us]
X_Acq_Time = 57.67168[ms]
X_Angle = 45[deg]
X_Atn = 6.5[dB]
X_Pulse = 5[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 1
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.05767168[s]

Elemental Composition Report

Single Mass Analysis

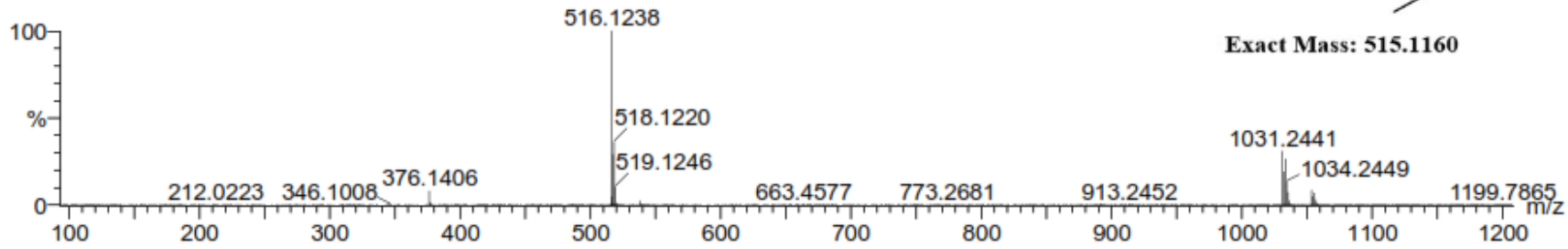
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
4359 formula(e) evaluated with 54 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 Cl: 0-2 F: 0-4



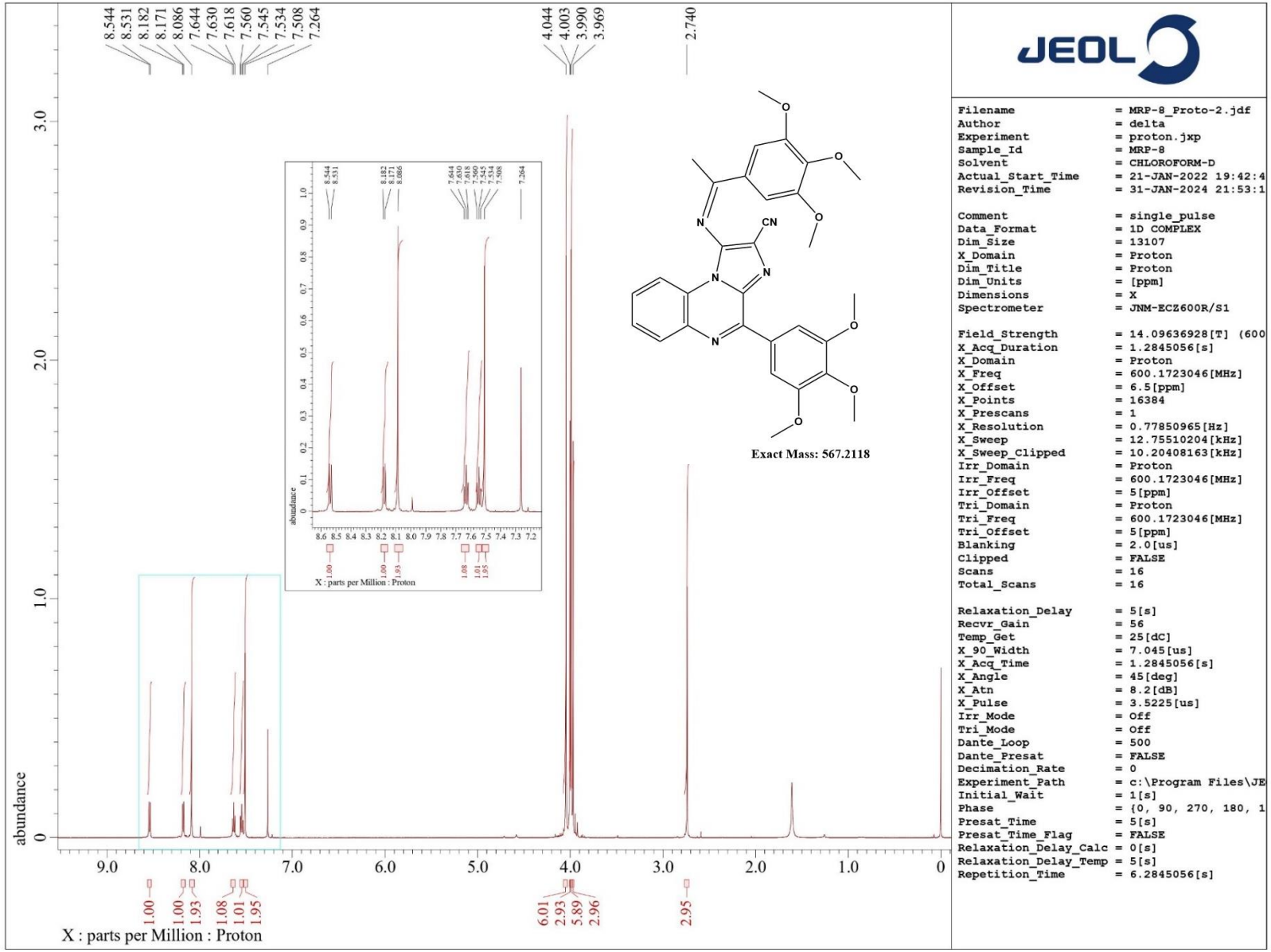
Exact Mass: 515.1160

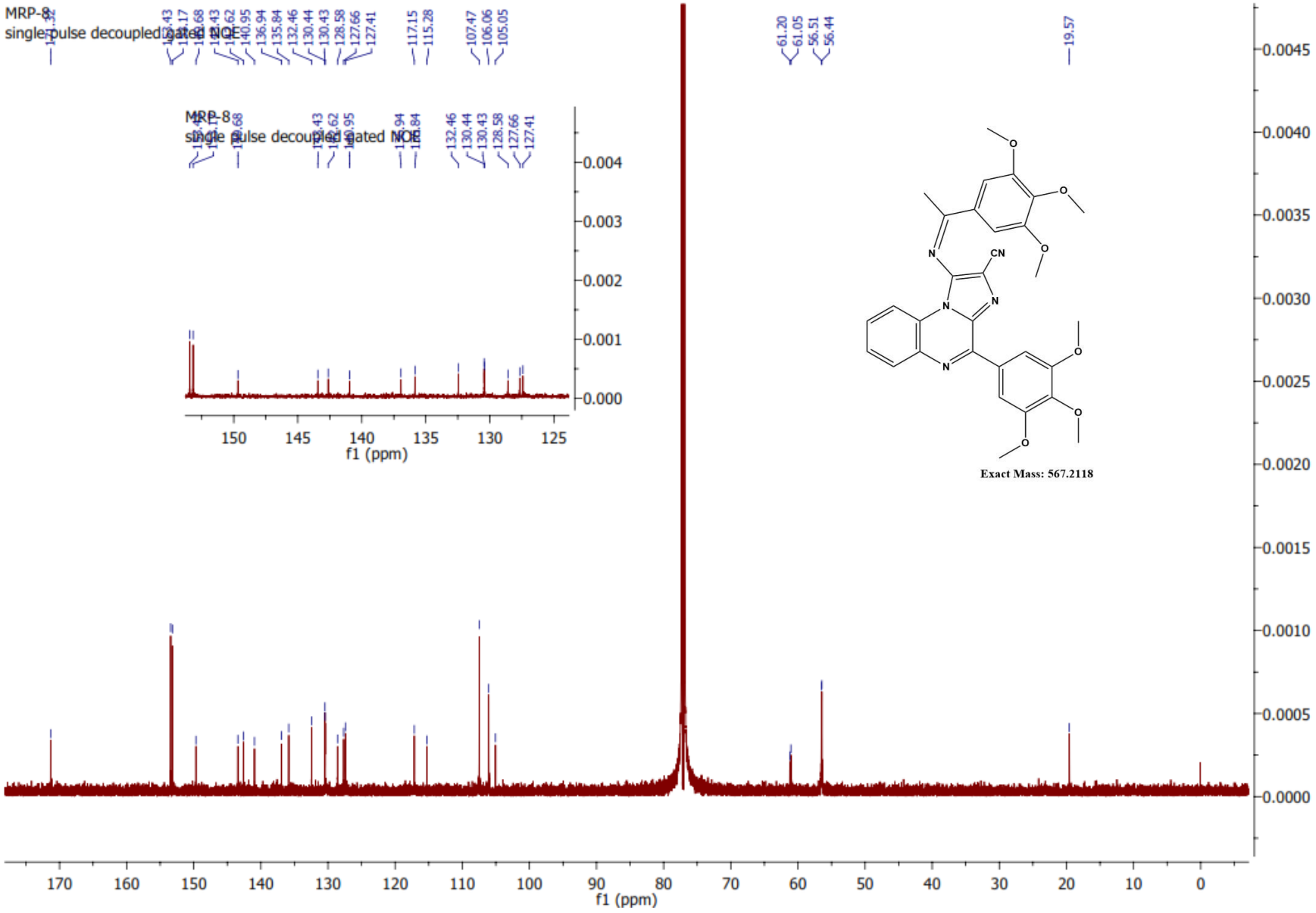
Sample Name : MRP_7 IITRPR
Test Name :
23032022_MRP_7 9 (0.203)



Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
516.1238	516.1239	-0.1	-0.2	19.5	602.6	n/a	n/a	C27 H20 N5 O3 Cl F

Spectral data of compound 5g




MRP-8
single pulse decoupled gated NOE
MRP-8
single pulse decoupled gated NOE
f1 (ppm)
f1 (ppm)
Exact Mass: 567.2118

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

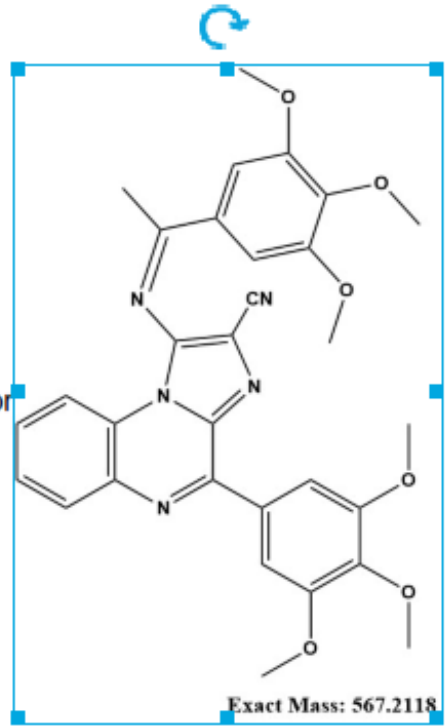
Monoisotopic Mass, Even Electron Ions
1111 formula(e) evaluated with 12 results within limits (up to 1 closest results for
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 Cl: 0-2

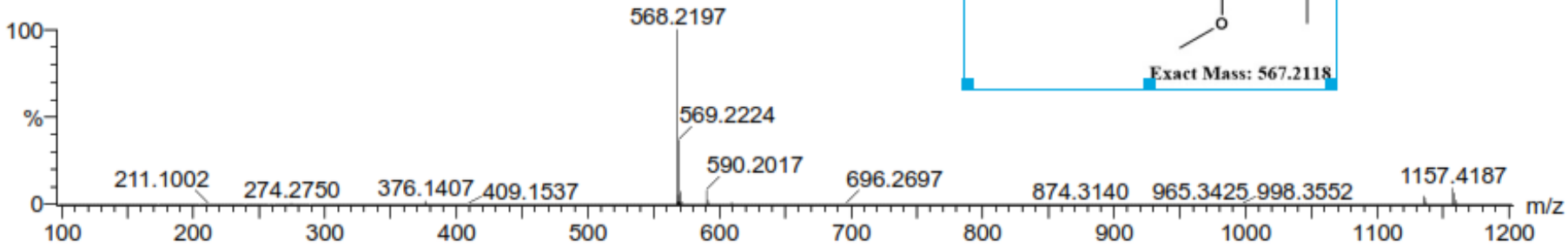
Sample Name : MRP_8
Test Name :
23032022_MRP_8 9 (0.203)

IITRPR

XEVO G2-XS QTOF

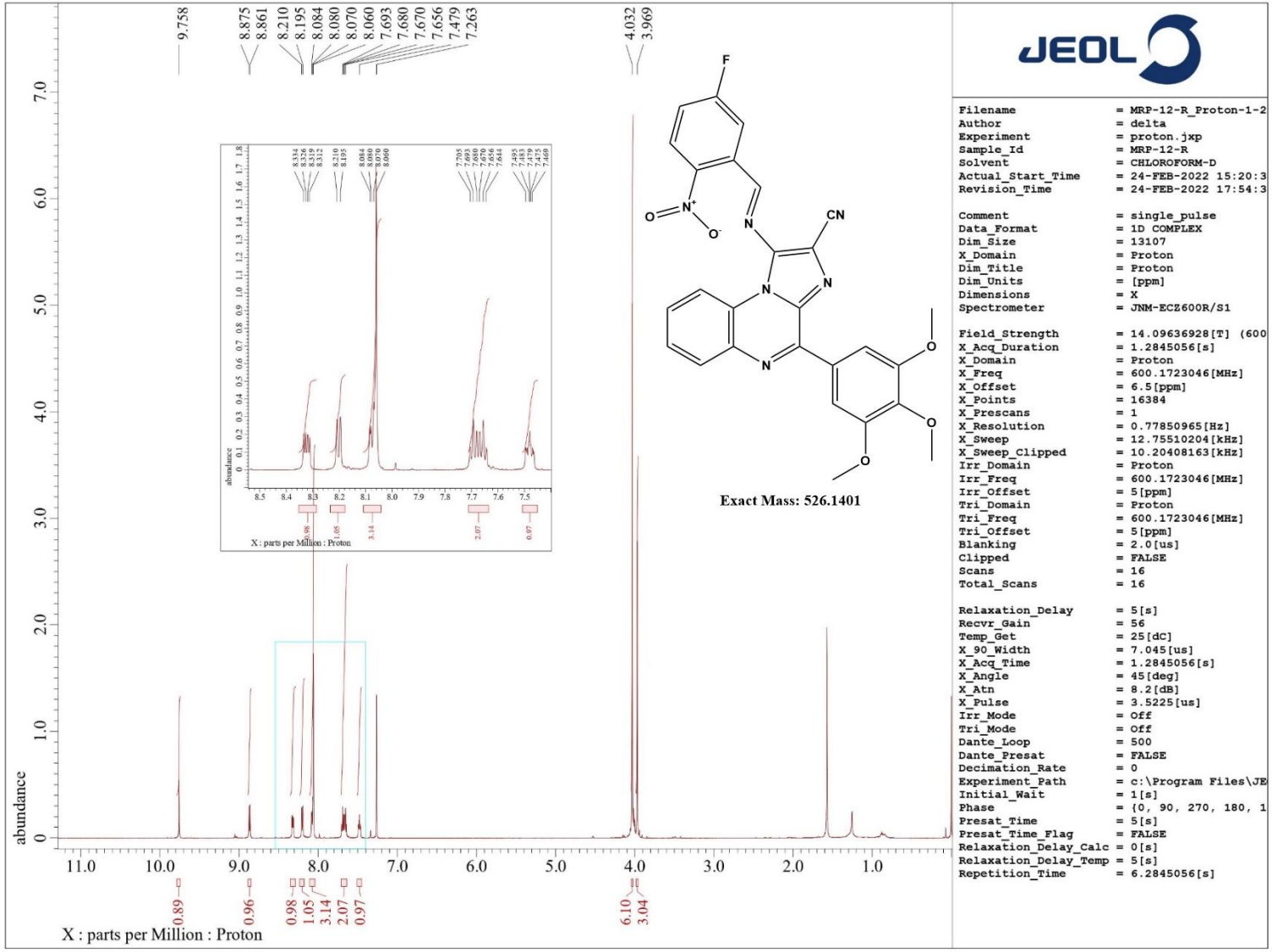
1: TOF MS ES+
4.67e+007



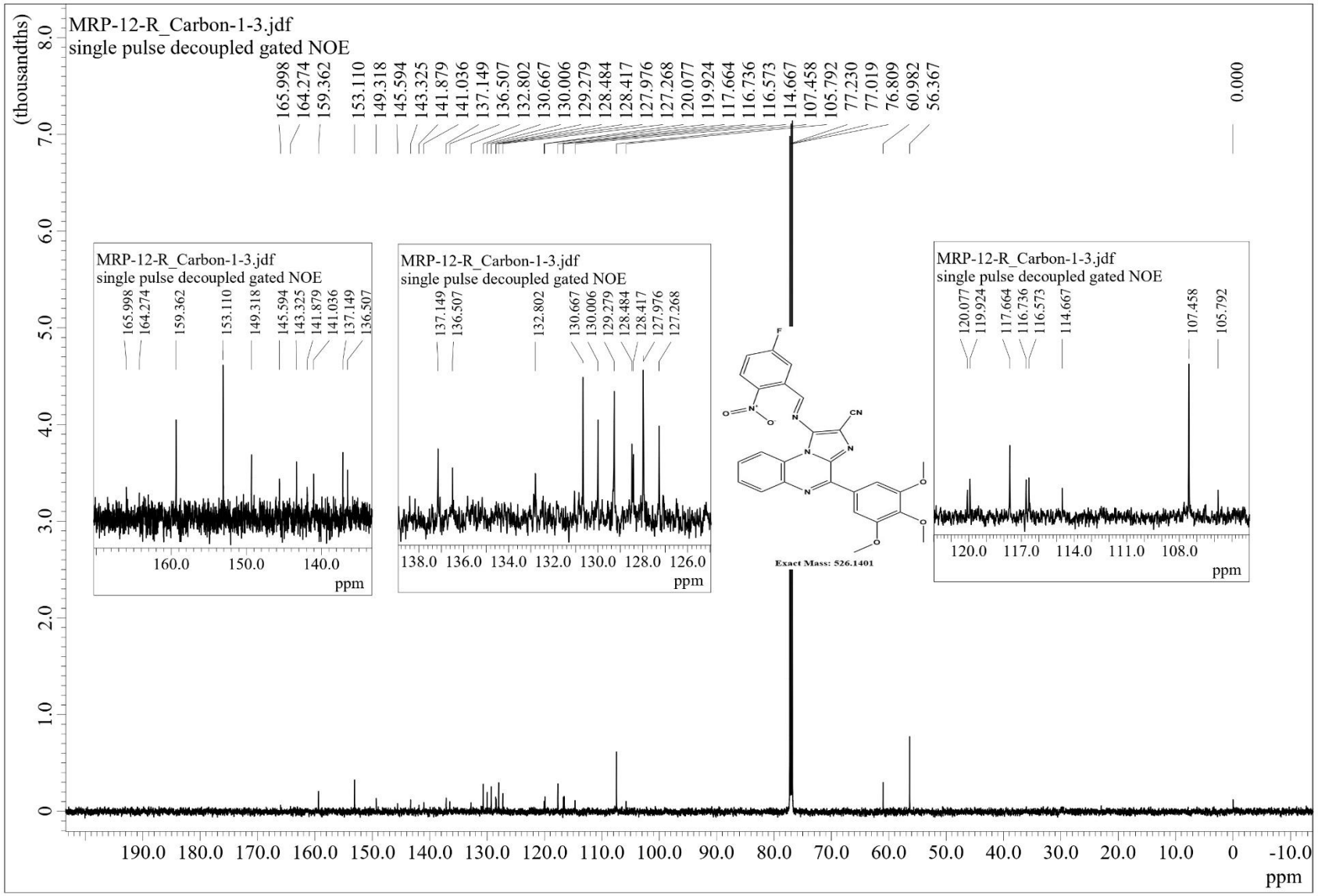


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
568.2197	568.2196	0.1	0.2	19.5	1270.6	n/a	n/a	C31 H30 N5 O6

Spectral data of compound 5h



Filename	= MRP-12-R_Proton-1-2
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MRP-12-R
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 24-FEB-2022 15:20:3
Revision_Time	= 24-FEB-2022 17:54:3
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S1
Field_Strength	= 14.09636928[T] (600
X_Acq_Duration	= 1.2845056[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 6.5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.77850965[Hz]
X_Sweep	= 12.75510204[kHz]
X_Sweep_Clipped	= 10.20408163[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 56
Temp_Get	= 25[dC]
X_90_Width	= 7.045[us]
X_Acq_Time	= 1.2845056[s]
X_Angle	= 45[deg]
X_Atn	= 8.2[dB]
X_Pulse	= 3.5225[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JE
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 1
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.2845056[s]

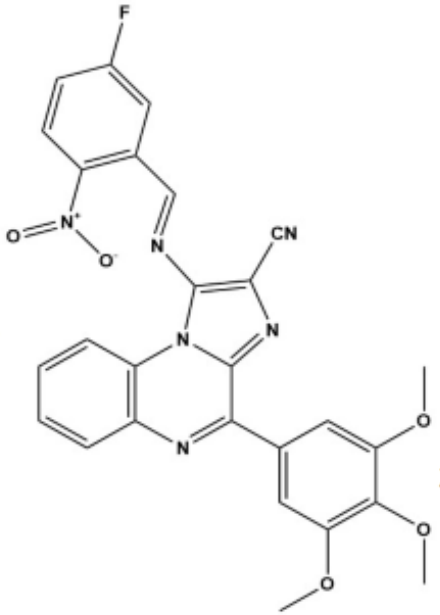

MRP-12-R_Carbon-1-3.jdf
single pulse decoupled gated NOE
(thousandths)
165.998 164.274 159.362 153.110 149.318 145.594 143.325 141.879 141.036 137.149 136.507 132.802 130.667 130.006 129.279 128.484 128.417 127.976 127.268 120.077 119.924 117.664 116.736 116.573 114.667 107.458 105.792 77.230 77.019 76.809 60.982 56.367 0.000
MRP-12-R_Carbon-1-3.jdf
single pulse decoupled gated NOE
165.998 164.274 159.362 153.110 149.318 145.594 143.325 141.879 141.036 137.149 136.507
160.0 150.0 140.0
ppm
MRP-12-R_Carbon-1-3.jdf
single pulse decoupled gated NOE
137.149 136.507 132.802 130.667 130.006 129.279 128.484 128.417 127.976 127.268
138.0 136.0 134.0 132.0 130.0 128.0 126.0
ppm
MRP-12-R_Carbon-1-3.jdf
single pulse decoupled gated NOE
120.077 119.924 117.664 116.736 116.573 114.667 107.458 105.792
120.0 117.0 114.0 111.0 108.0
ppm
Exact Mass: 526.1401
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 -10.0
ppm

Elemental Composition Report

Single Mass Analysis

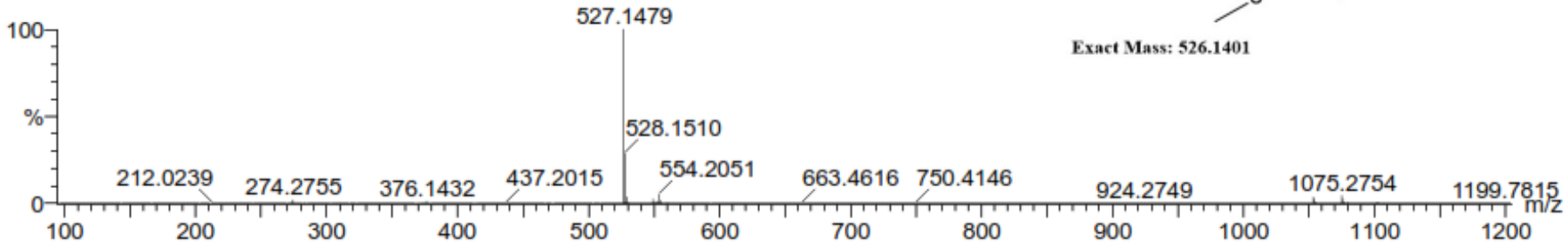
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
4495 formula(e) evaluated with 55 results within limits (up to 1 closest results for
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 Cl: 0-2 F: 0-4



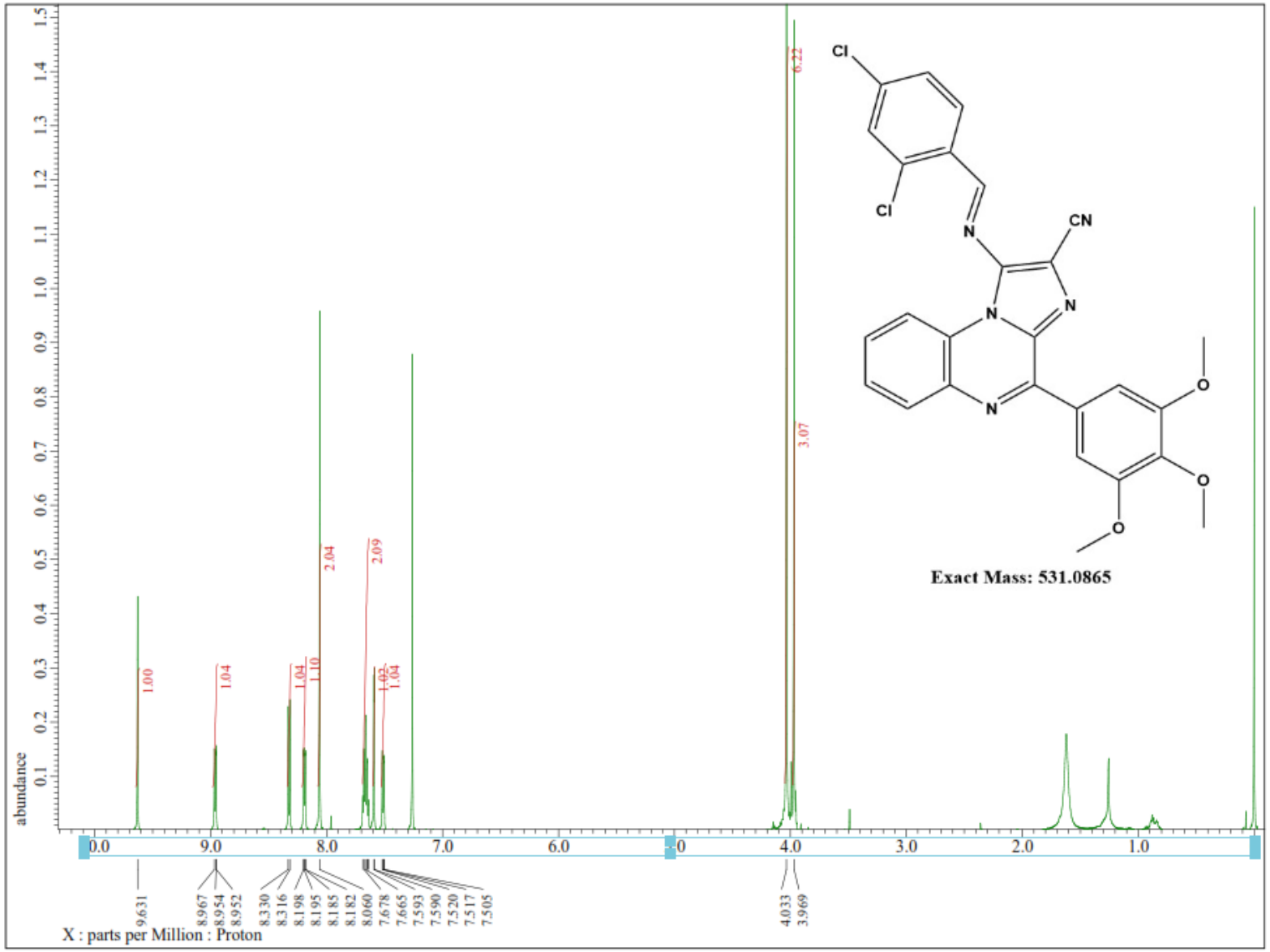
Exact Mass: 526.1401

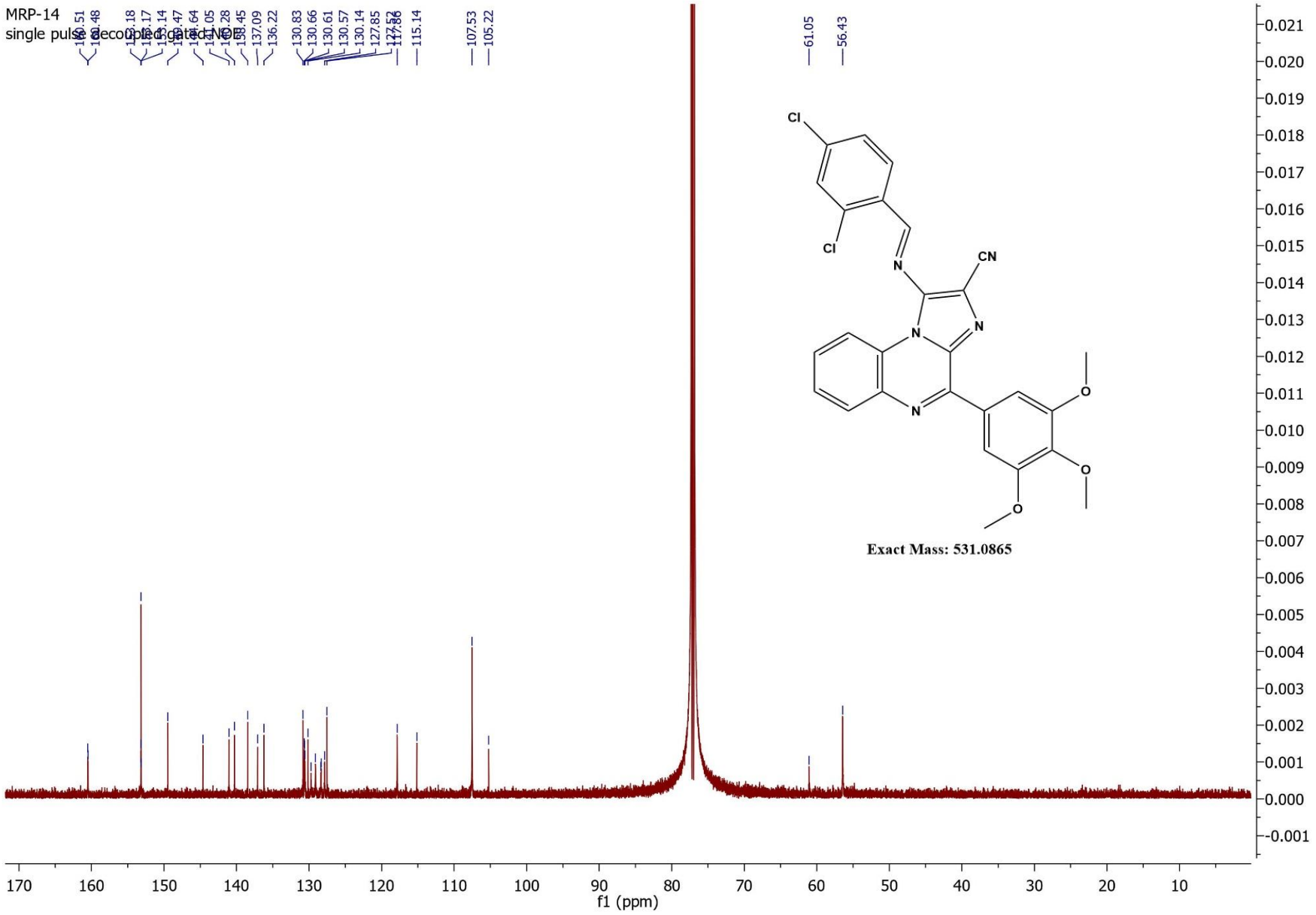
Sample Name : MRP_12R IITRPR XEVO G2-XS QTOF
Test Name :
23032022_MRP_12R 10 (0.232) 1: TOF MS ES+
6.21e+006



Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
527.1479	527.1479	0.0	0.0	20.5	649.1	n/a	n/a	C27 H20 N6 O5 F

Spectral data of compound 5i




MRP-14
single pulse decoupled gated NOE
163.51
160.48
152.18
151.17
151.14
147.47
144.64
144.05
140.28
138.45
137.09
136.22
130.83
130.66
130.61
130.57
130.14
127.85
117.86
115.14
107.53
105.22
61.05
56.43
Cl
Cl
N
CN
N
N
N
O
O
O
Exact Mass: 531.0865
0.021
0.020
0.019
0.018
0.017
0.016
0.015
0.014
0.013
0.012
0.011
0.010
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0.000
-0.001
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

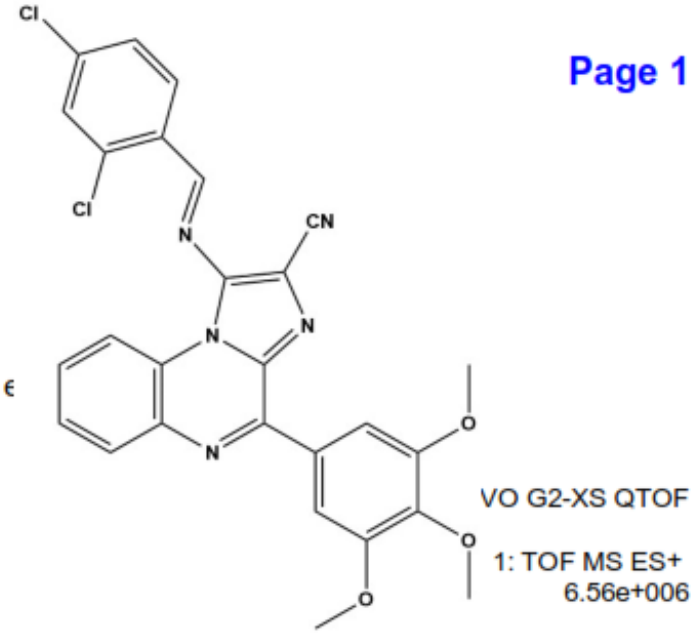
Elemental Composition Report

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

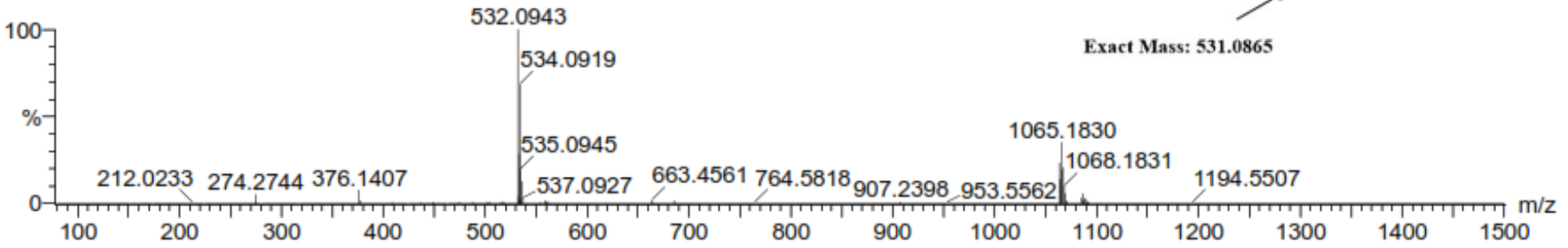
Monoisotopic Mass, Even Electron Ions
4549 formula(e) evaluated with 56 results within limits (up to 1 closest results for e
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 F: 0-4 Cl: 0-2

Sample Name : MRP_14 IITRPR
Test Name :
23032022_MRP_14 8 (0.186)



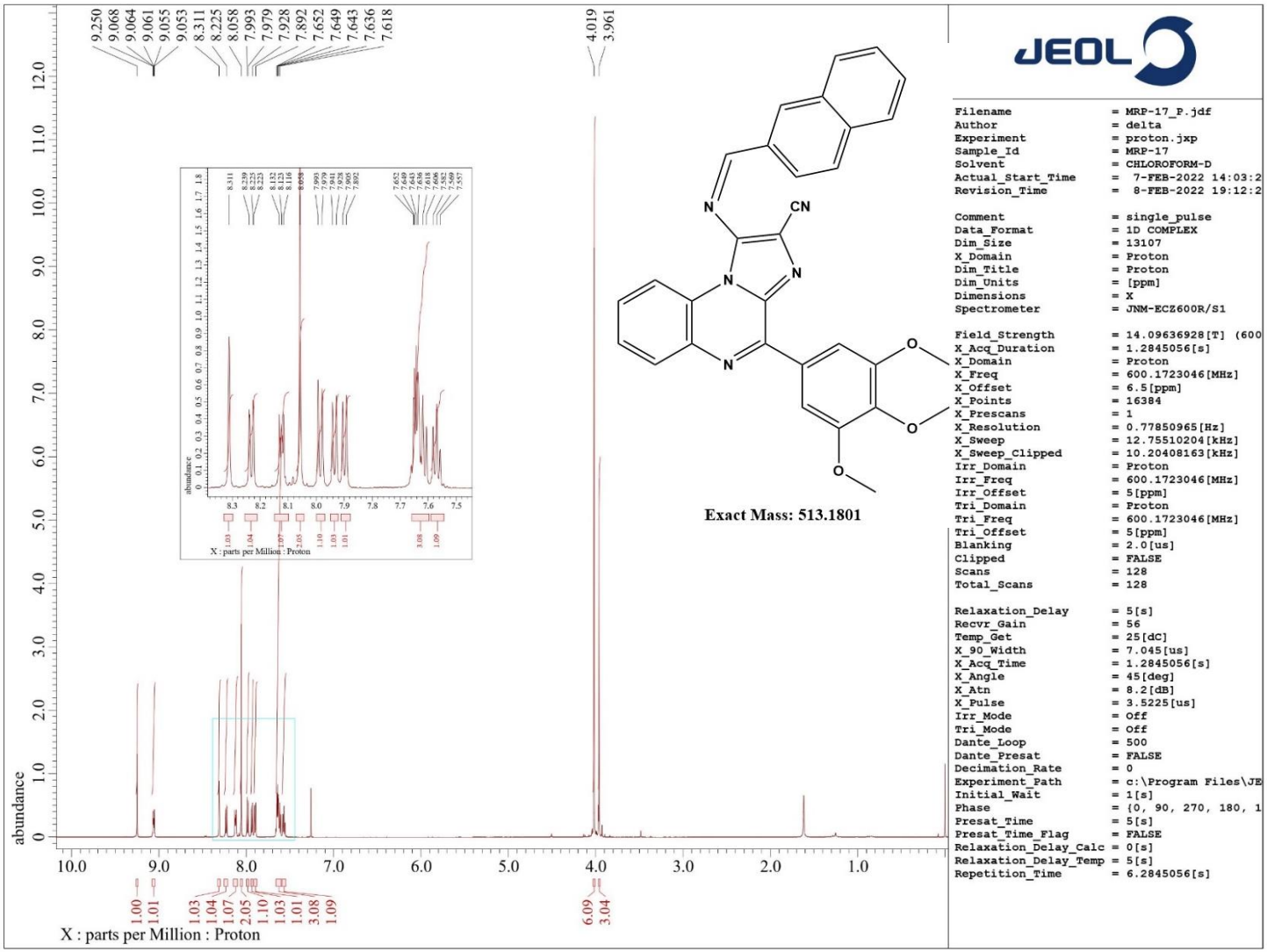
VO G2-XS QTOF
1: TOF MS ES+
6.56e+006

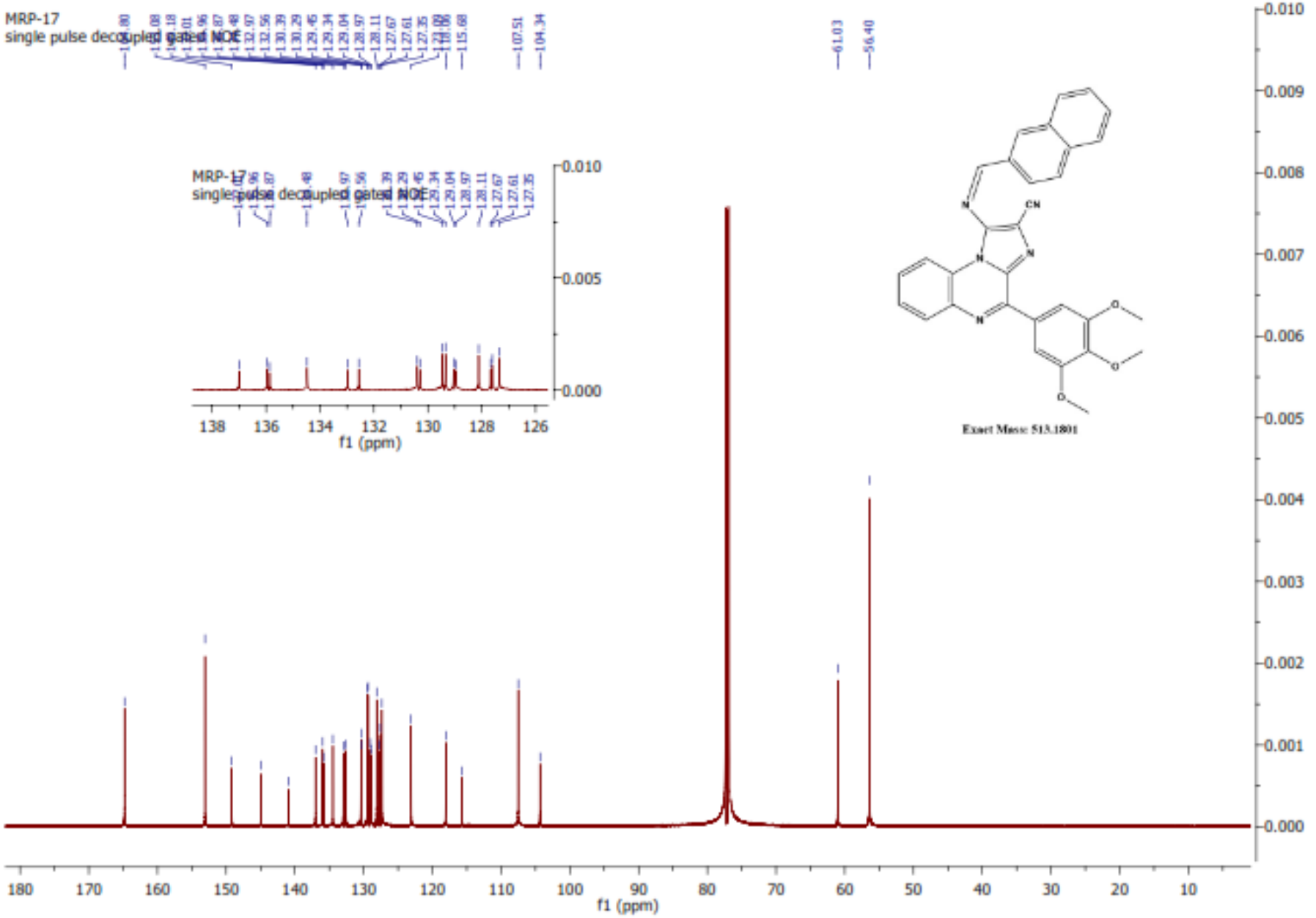
Exact Mass: 531.0865



Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
532.0943	532.0943	0.0	0.0	19.5	752.0	n/a	n/a	C27 H20 N5 O3 Cl2

Spectral data of compound 5j




MRP-17
single pulse decoupled gated NOE
MRP-17
single pulse decoupled gated NOE
f1 (ppm)
f1 (ppm)
Exact Mass: 513.1801

Elemental Composition Report

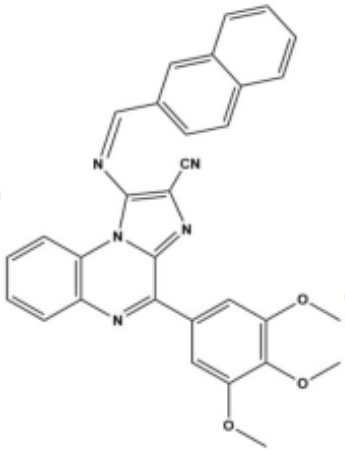
Single Mass Analysis

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
357 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10

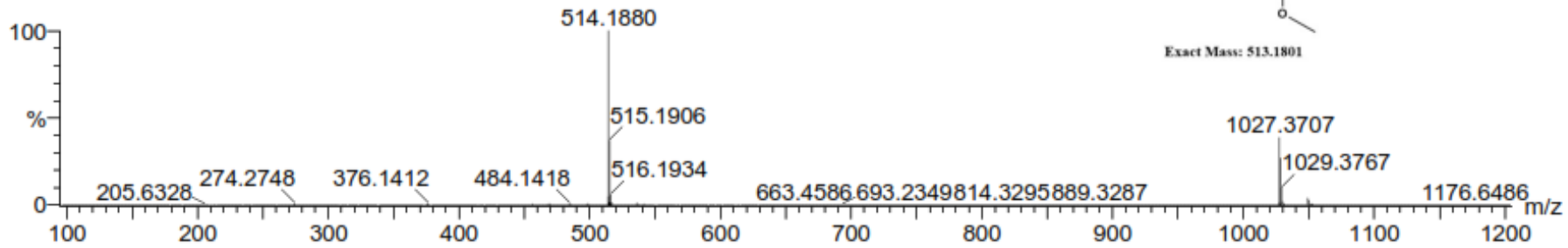
Sample Name : MRP_17
Test Name :
23032022_MRP_17 8 (0.186)

IITRPR



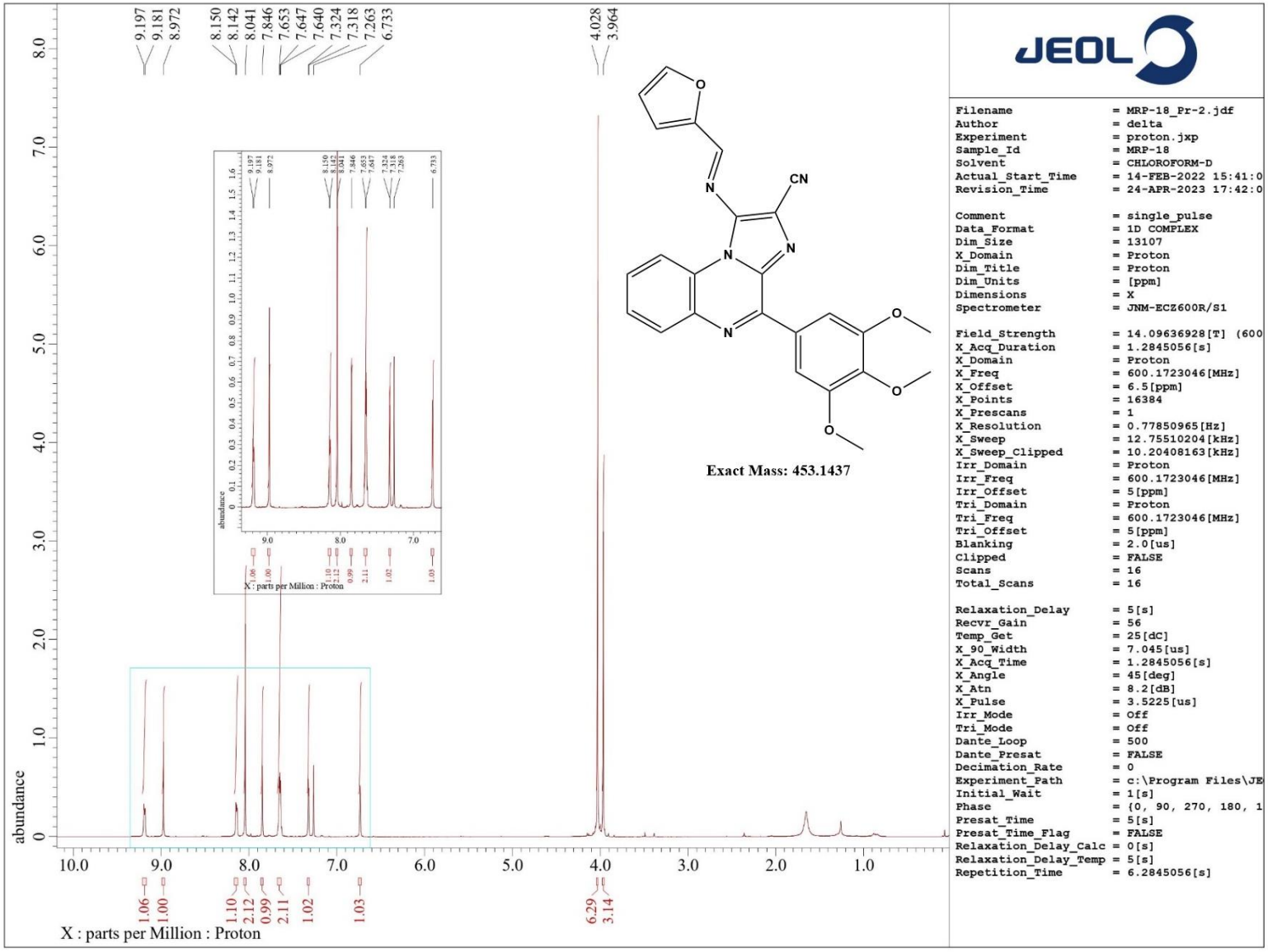
VO G2-XS QTOF

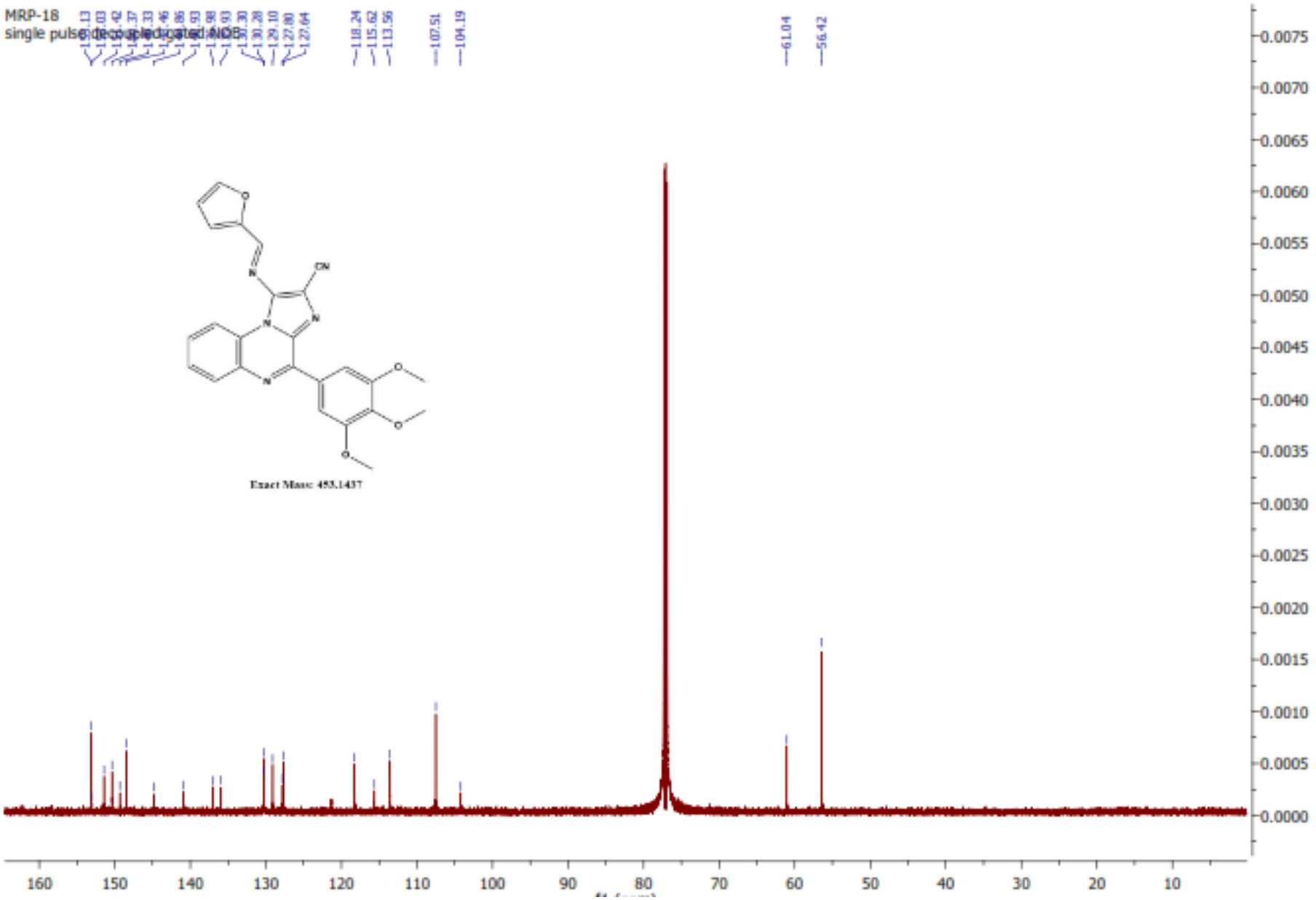
1: TOF MS ES+
5.00e+007



Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
514.1880	514.1879	0.1	0.2	22.5	1323.5	n/a	n/a	C31 H24 N5 O3

Spectral data of compound 5k



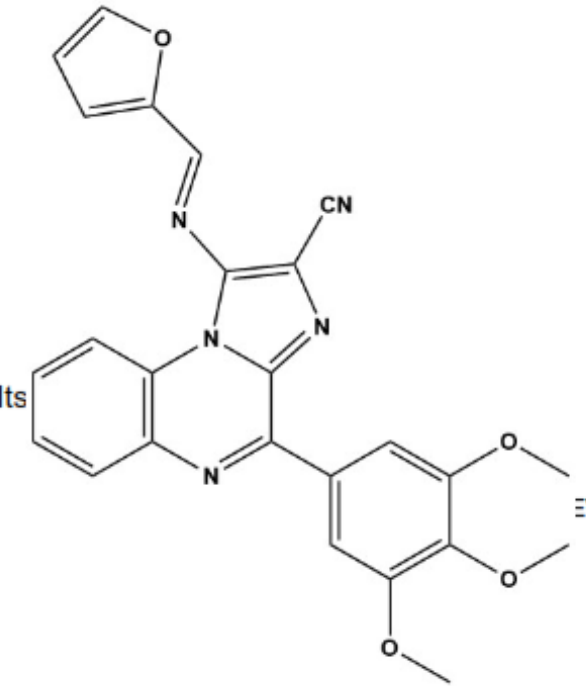

MRP-18
single pulse decoupled gated NOE
118.24
115.62
113.56
107.51
104.19
61.04
56.42
Exact Mass: 453.1437
0.0075
0.0070
0.0065
0.0060
0.0055
0.0050
0.0045
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

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
314 formula(e) evaluated with 3 results within limits (up to 1 closest results
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10



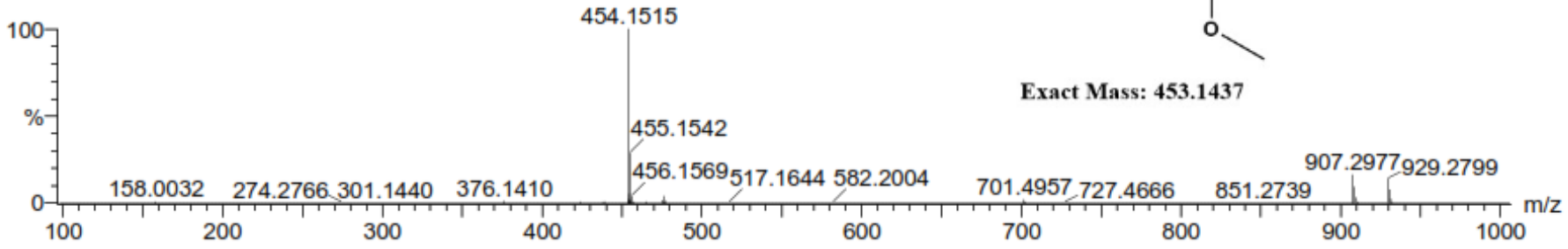
Exact Mass: 453.1437

Sample Name : MRP_18
Test Name :
23032022_MRP_18 12 (0.265)

IITRPR

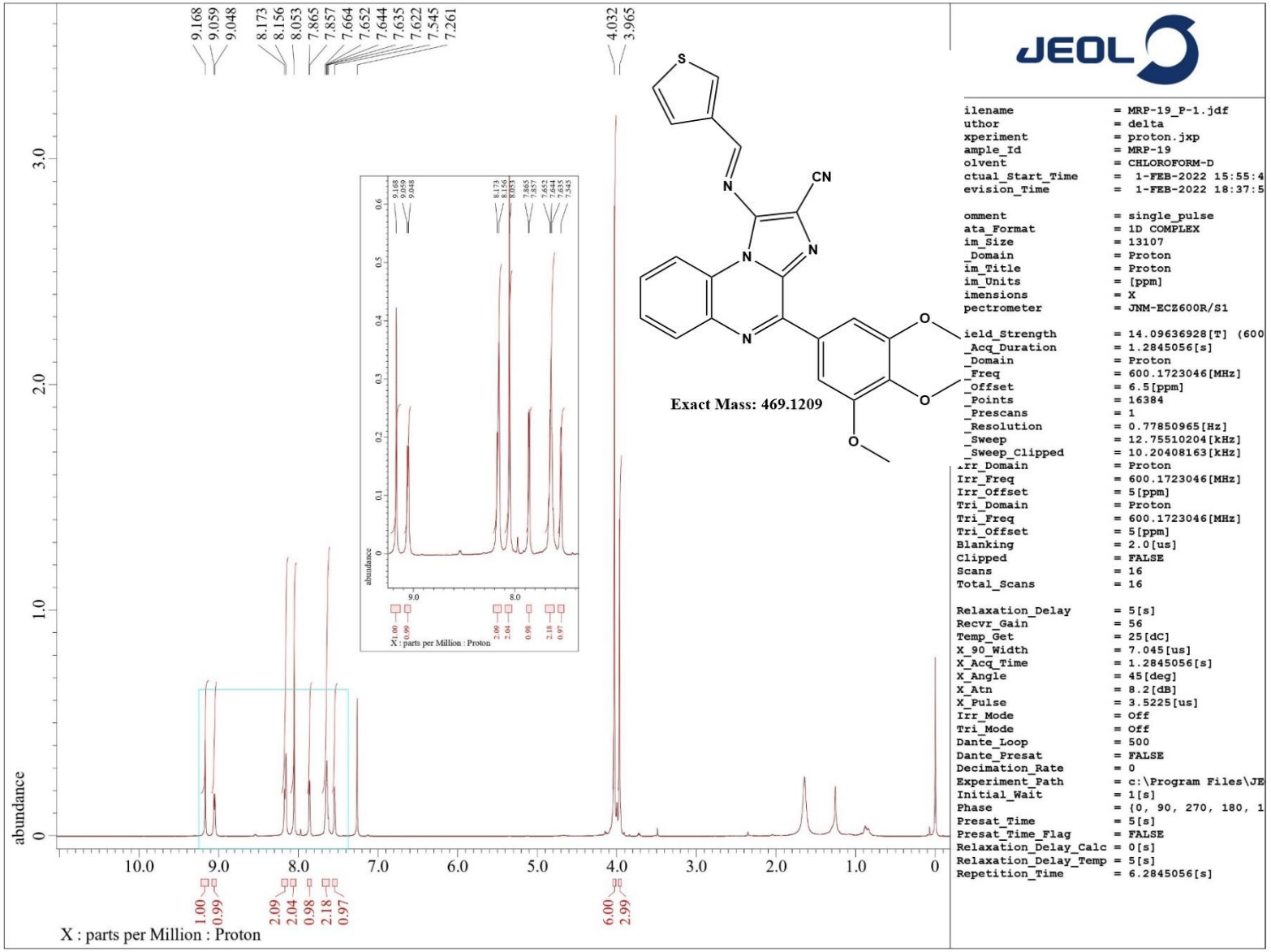
EVO G2-XS QTOF

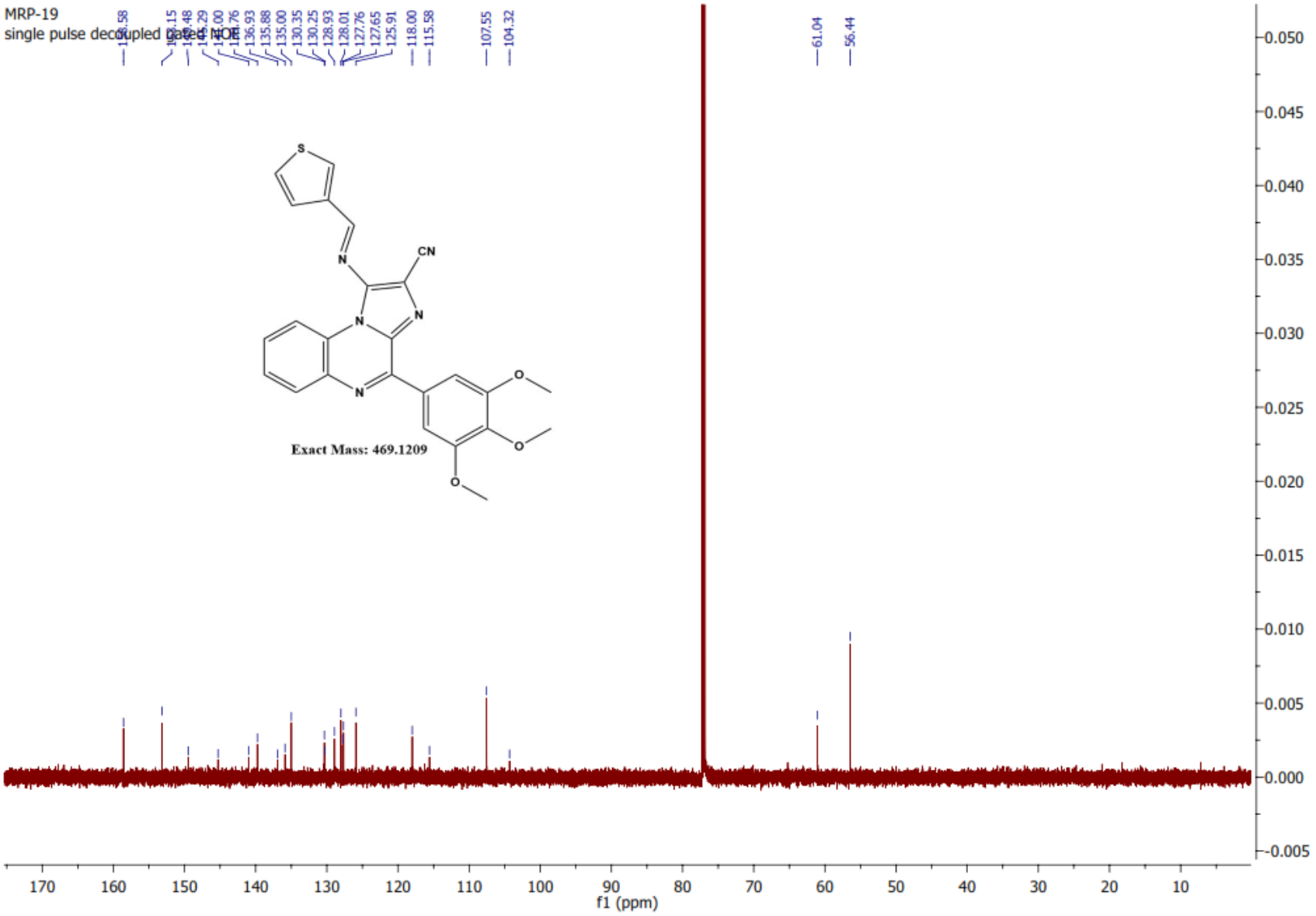
1: TOF MS ES+
1.71e+007



Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
454.1515	454.1515	0.0	0.0	18.5	1331.2	n/a	n/a	C25 H20 N5 O4

Spectral data of compound 5l




MRP-19
single pulse decoupled gated NOE
158.58
151.15
149.48
147.29
147.00
141.76
136.93
135.88
135.00
130.35
130.25
128.93
128.01
127.76
127.65
125.91
118.00
115.58
107.55
104.32
61.04
56.44
S
N
CN
N
N
N
O
O
O
Exact Mass: 469.1209
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
-0.005
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

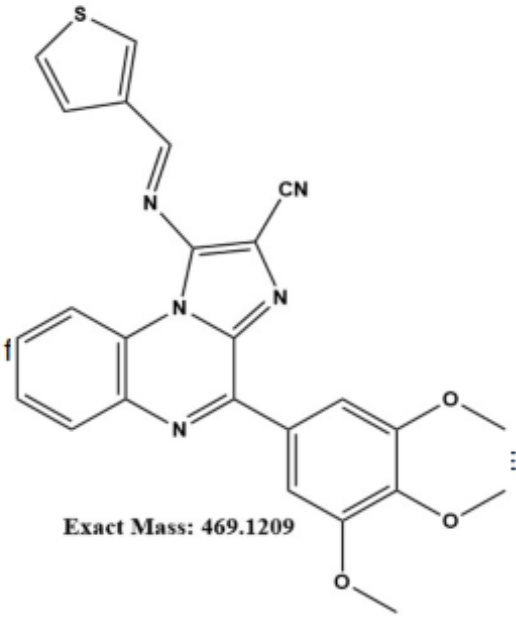
Elemental Composition Report

Single Mass Analysis

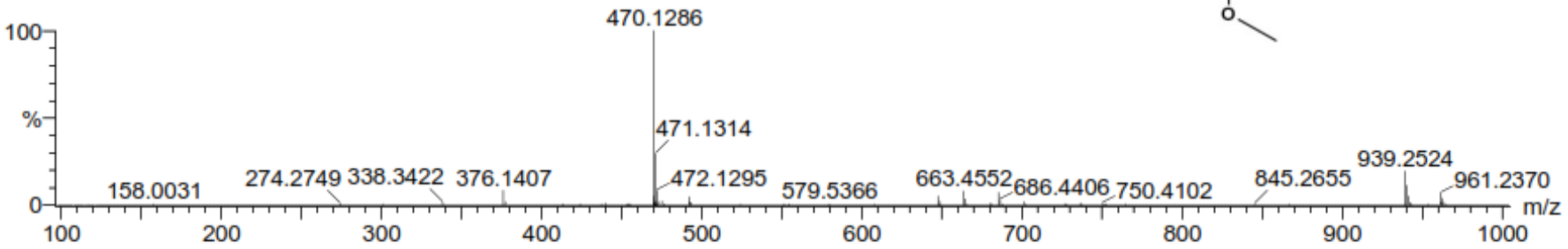
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
1141 formula(e) evaluated with 13 results within limits (up to 1 closest results f
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 S: 0-3

Sample Name : MRP_19 IITRPR :VO G2-XS QTOF
Test Name :
23032022_MRP_19 9 (0.203)

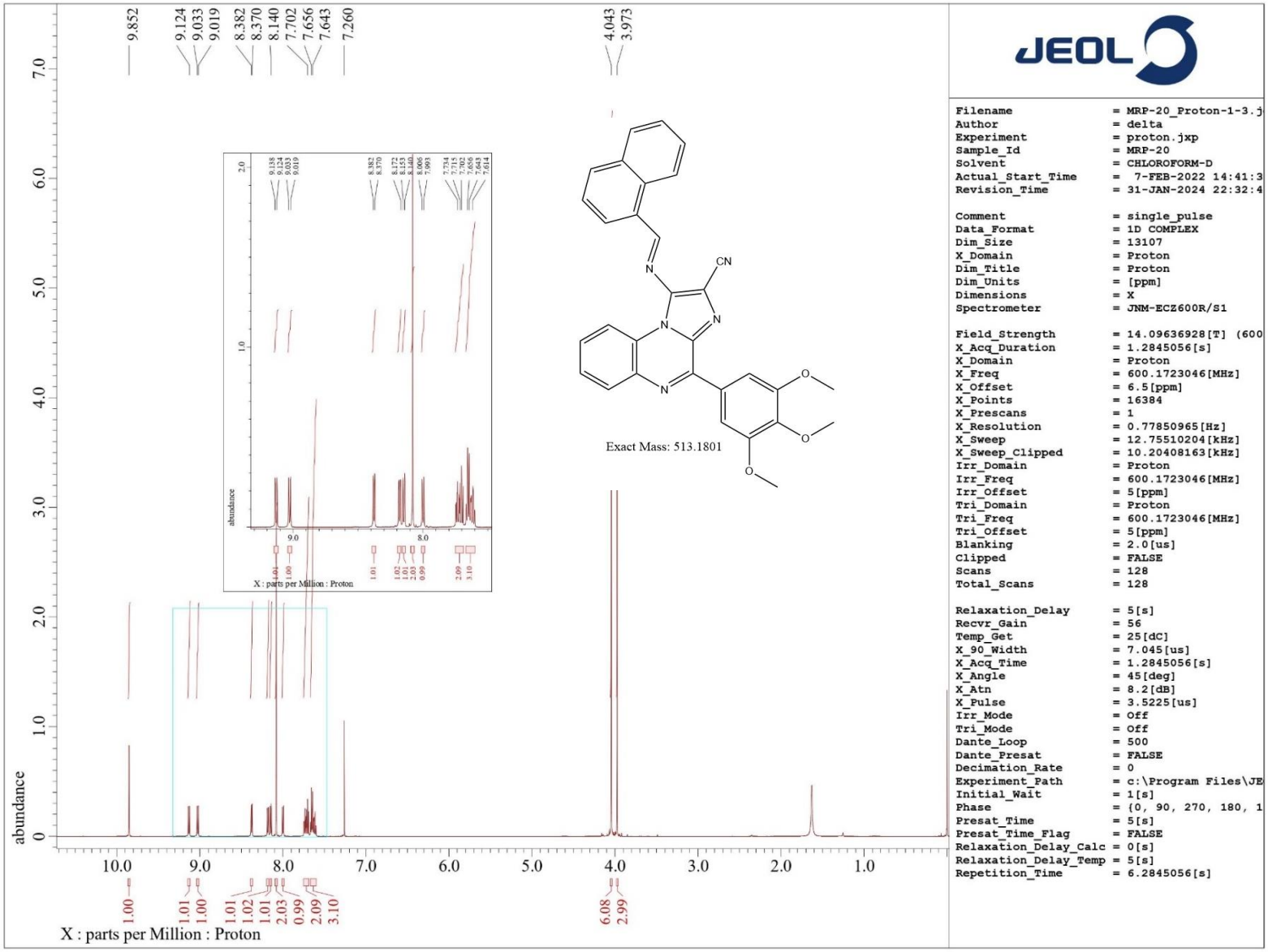


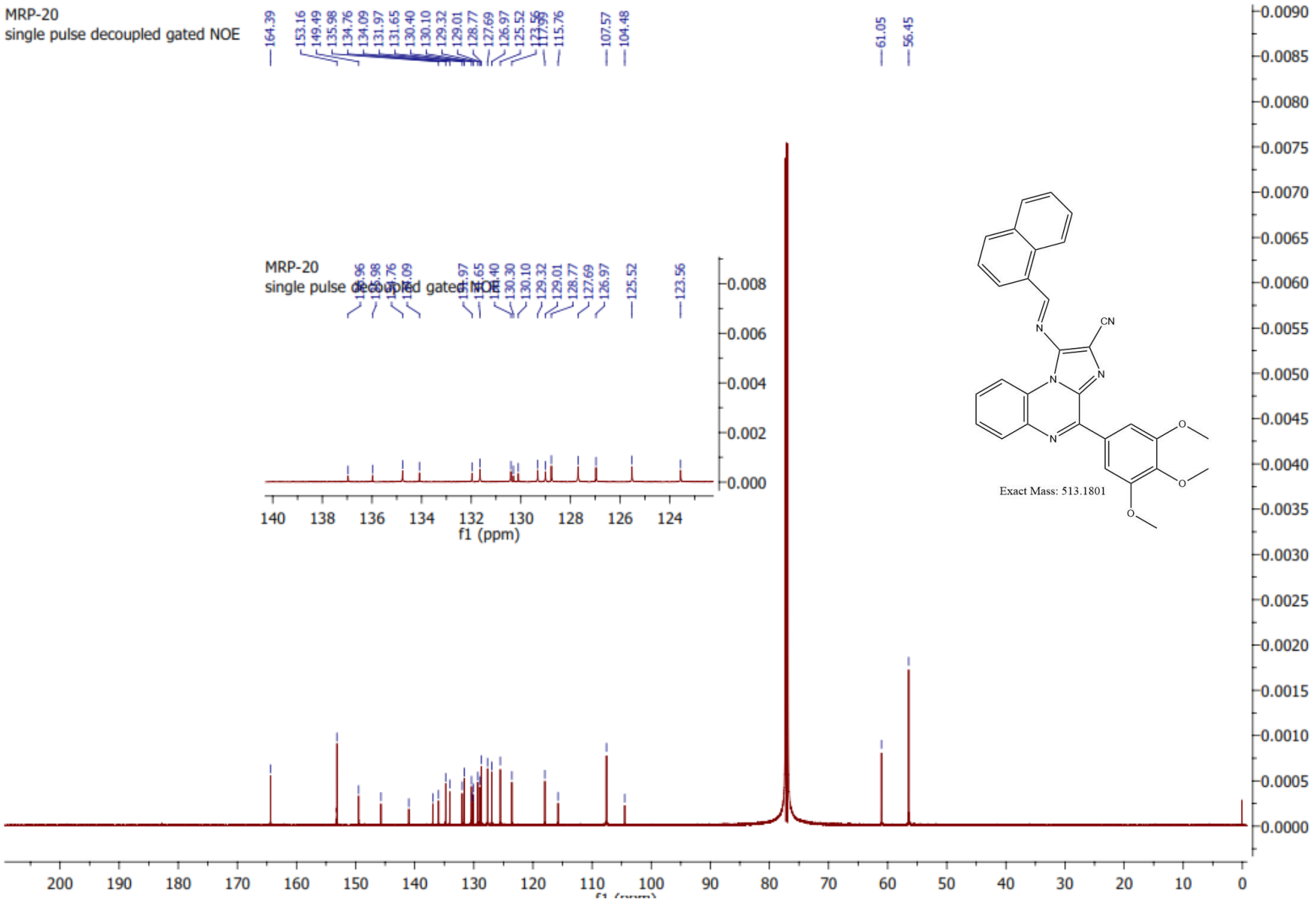
1: TOF MS ES+
1.65e+007



Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
470.1286	470.1287	-0.1	-0.2	18.5	1391.3	n/a	n/a	C25 H20 N5 O3 S

Spectral data of compound 5m



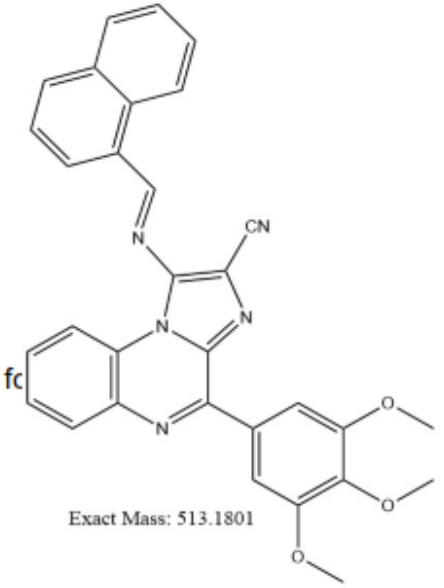

MRP-20
single pulse decoupled gated NOE
164.39
153.16
149.49
135.98
134.76
134.09
131.97
131.65
130.40
130.10
129.32
129.01
128.77
127.69
126.97
125.52
115.76
107.57
104.48
61.05
56.45
MRP-20
single pulse decoupled gated NOE
125.52
123.56
f1 (ppm)
CN
Exact Mass: 513.1801
f1 (ppm)

Elemental Composition Report

Single Mass Analysis

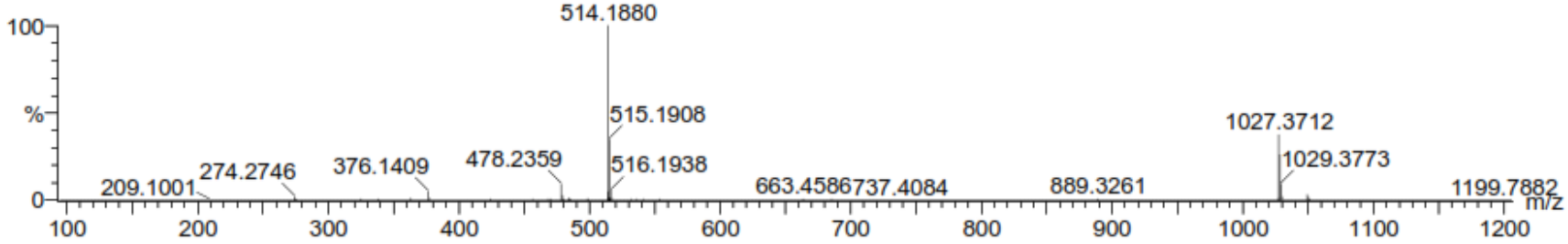
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
1279 formula(e) evaluated with 13 results within limits (up to 1 closest results fc
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 S: 0-3



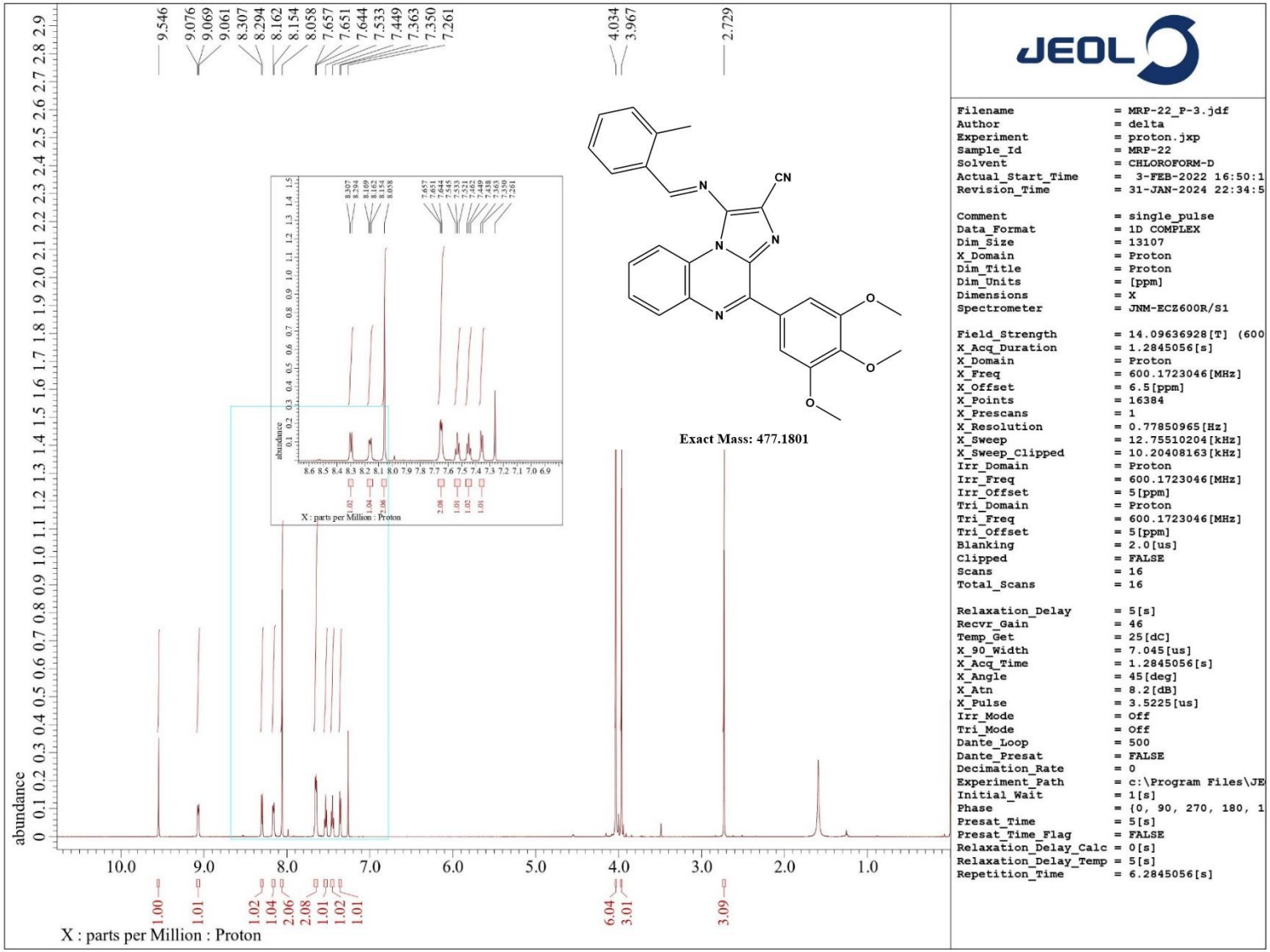
Exact Mass: 513.1801

Sample Name : MRP_20 IITRPR XEVO G2-XS QTOF
Test Name :
23032022_MRP_20 8 (0.186) 1: TOF MS ES+
4.63e+007



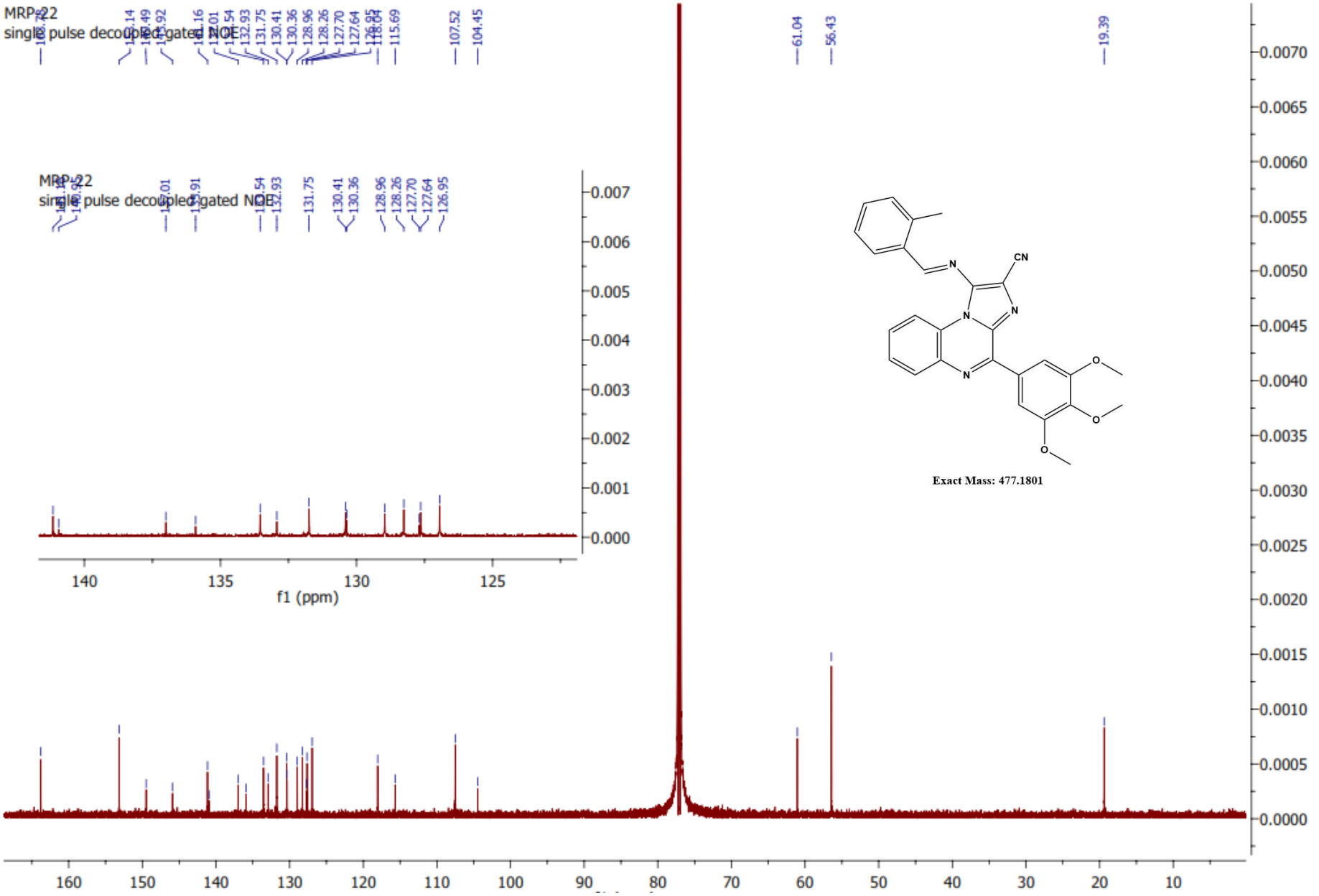
Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
514.1880	514.1879	0.1	0.2	22.5	1491.4	n/a	n/a	C31 H24 N5 O3

Spectral data of compound 5n

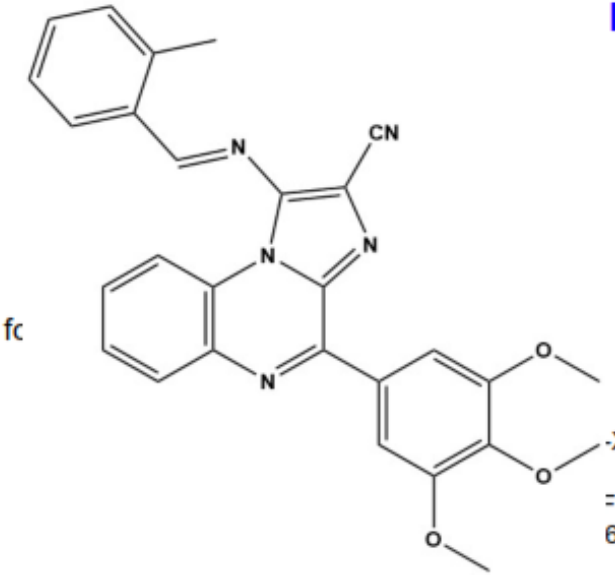


JEOL

Filename	= MRP-22_P-3.jdf
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MRP-22
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-FEB-2022 16:50:1
Revision_Time	= 31-JAN-2024 22:34:5
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S1
Field_Strength	= 14.09636928[T] (600
X_Acq_Duration	= 1.2845056[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 6.5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.77850965[Hz]
X_Sweep	= 12.75510204[kHz]
X_Sweep_Clipped	= 10.20408163[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 25[dC]
X_90_Width	= 7.045[us]
X_Acq_Time	= 1.2845056[s]
X_Angle	= 45[deg]
X_Atn	= 8.2[dB]
X_Pulse	= 3.5225[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JE
Initial_Wait	= 1[s]
Phase	= (0, 90, 270, 180, 1
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.2845056[s]


MRP-22
single pulse decoupled gated NOE
MRP-22
single pulse decoupled gated NOE
f1 (ppm)
Exact Mass: 477.1801

Elemental Composition Report



Exact Mass: 477.1801

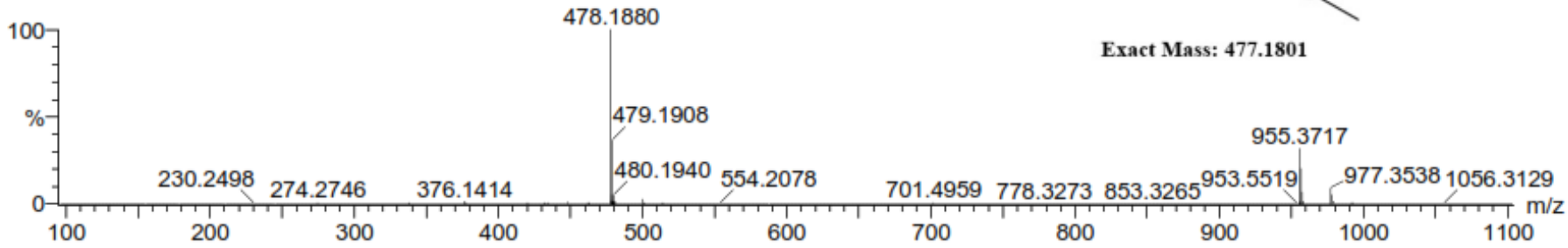
Single Mass Analysis

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
1169 formula(e) evaluated with 11 results within limits (up to 1 closest results fc
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 S: 0-3

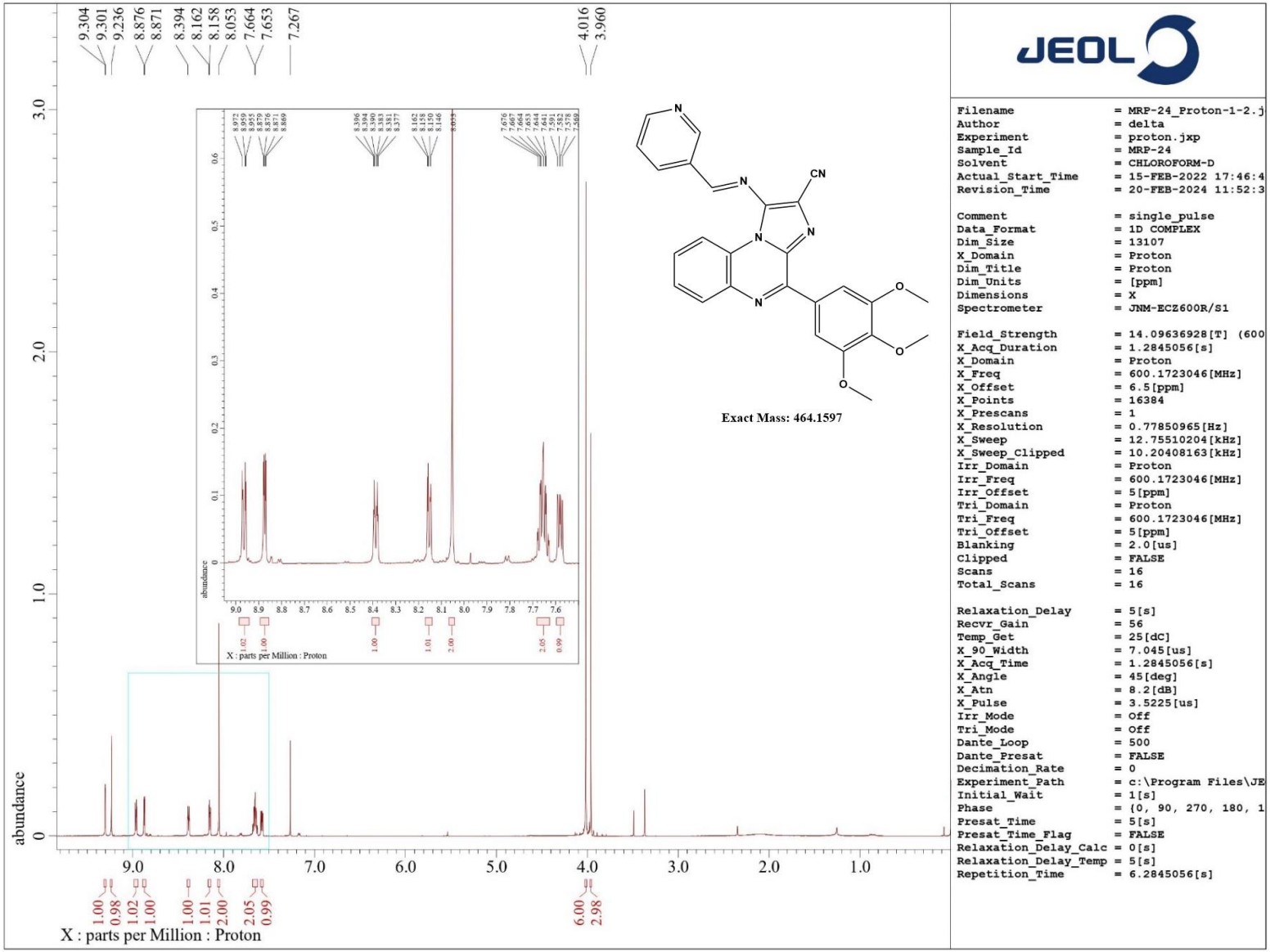
Sample Name : MRP_22 IITRPR
Test Name :
23032022_MRP_22 8 (0.186)

-XS QTOF
= MS ES+
6.51e+007

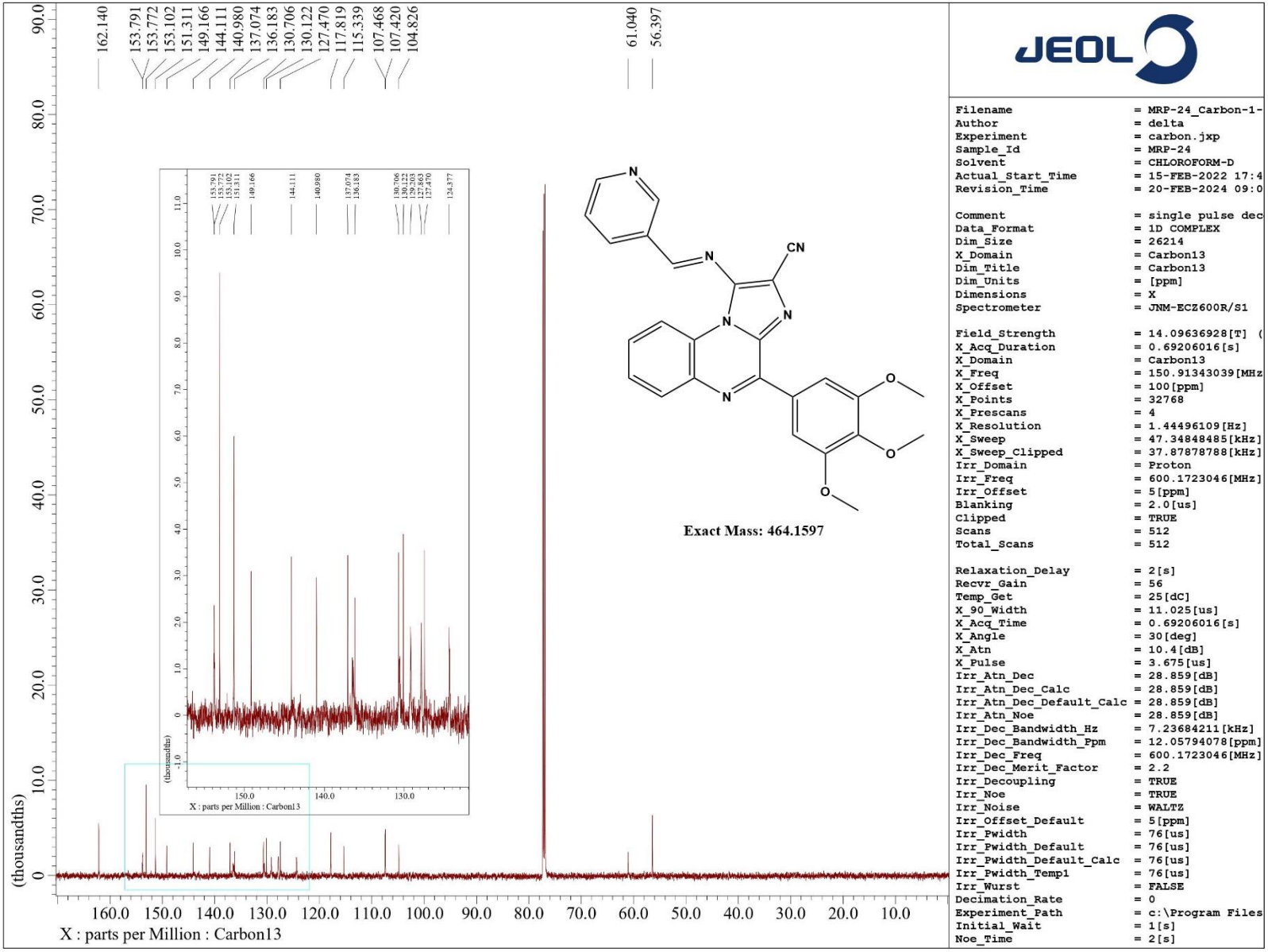


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
478.1880	478.1879	0.1	0.2	19.5	1467.9	n/a	n/a	C28 H24 N5 O3

Spectral data of compound 5o



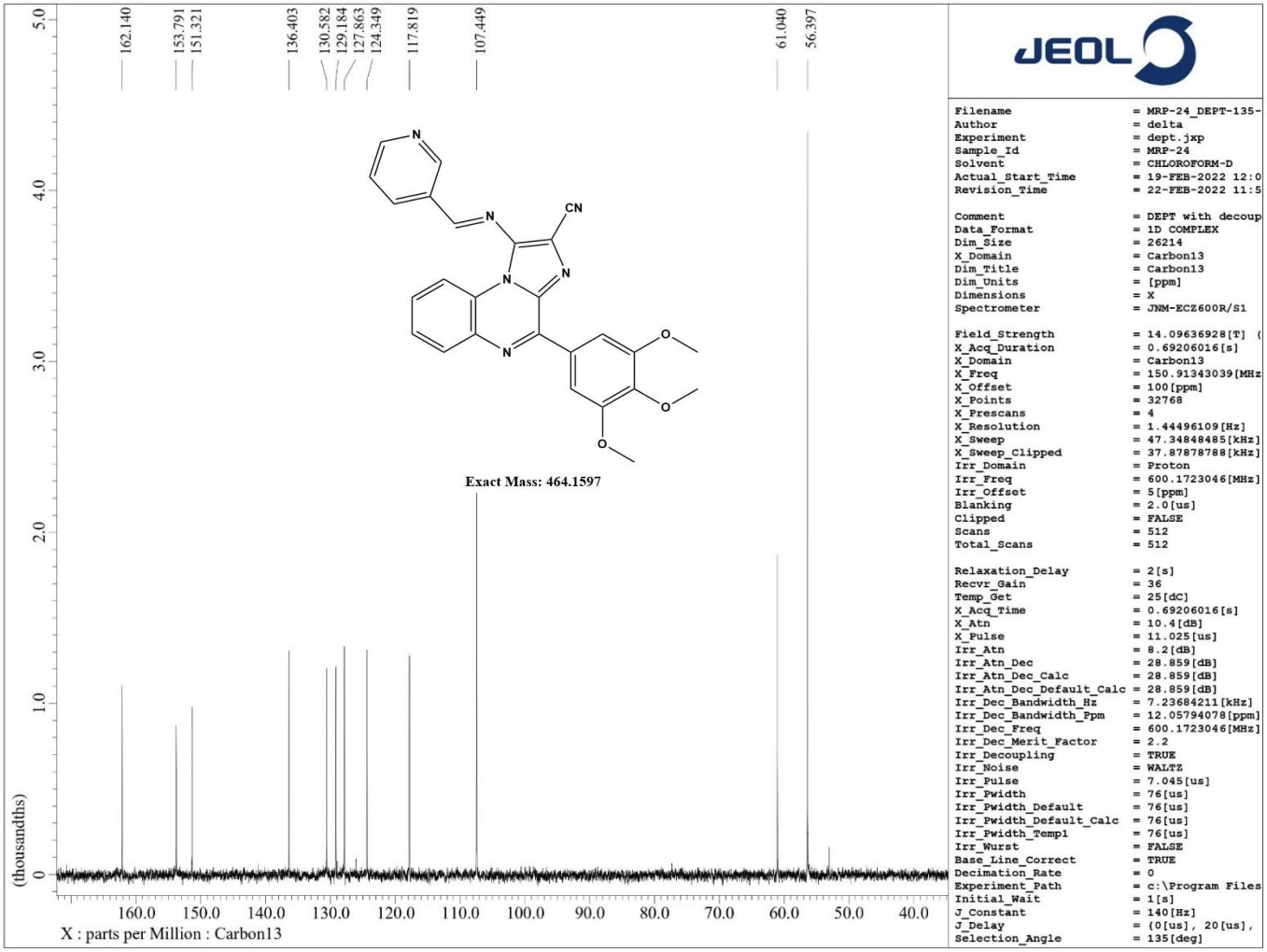

```
Filename              = MRP-24_Proton-1-2.j
Author                = delta
Experiment            = proton.jxp
Sample_Id             = MRP-24
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 15-FEB-2022 17:46:4
Revision_Time         = 20-FEB-2024 11:52:3

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S1

Field_Strength        = 14.09636928[T] (600
X_Acq_Duration        = 1.2845056[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 6.5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.77850965[Hz]
X_Sweep               = 12.75510204[kHz]
X_Sweep_Clipped       = 10.20408163[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2.0[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 25[dC]
X_90_Width            = 7.045[us]
X_Acq_Time            = 1.2845056[s]
X_Angle               = 45[deg]
X_Atn                 = 8.2[dB]
X_Pulse               = 3.5225[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JE
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 1
Presat_Time           = 5[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time       = 6.2845056[s]
```



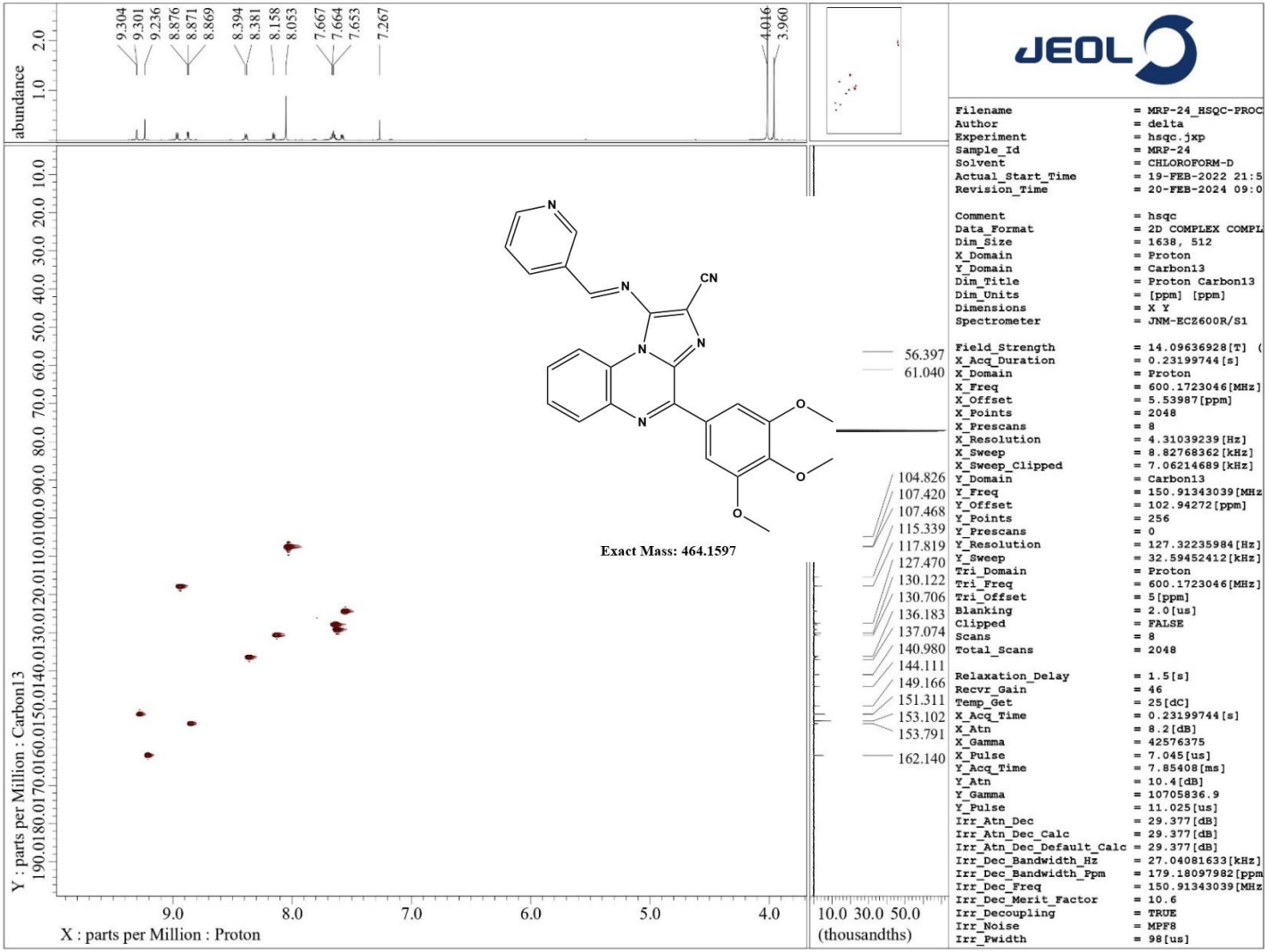
Filename	= MRP-24_Carbon-1-
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= MRP-24
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 15-FEB-2022 17:4
Revision_Time	= 20-FEB-2024 09:0
Comment	= single pulse dec
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S1
Field_Strength	= 14.09636928[T] (
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= TRUE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 25[dC]
X_90_Width	= 11.025[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 10.4[dB]
X_Pulse	= 3.675[us]
Irr_Atn_Dec	= 28.859[dB]
Irr_Atn_Dec_Calc	= 28.859[dB]
Irr_Atn_Dec_Default_Calc	= 28.859[dB]
Irr_Atn_Noe	= 28.859[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files
Initial_Wait	= 1[s]
Noe_Time	= 2[s]

2D-Spectral data of compound 5o

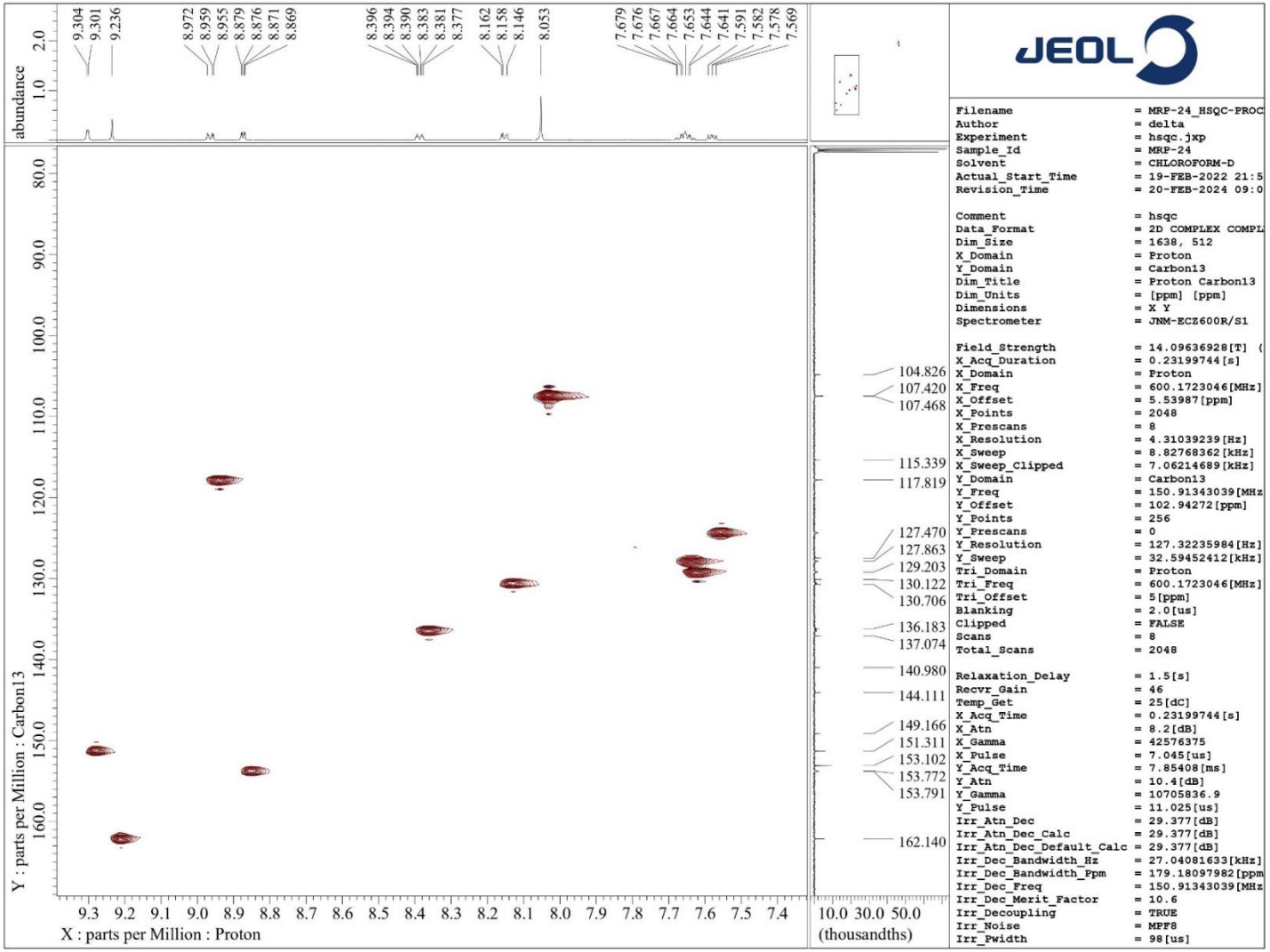
DEPT-135

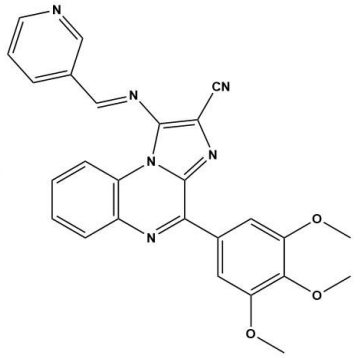


HSQC-1


9.304
9.301
9.236
8.876
8.871
8.869
8.394
8.381
8.158
8.053
7.667
7.664
7.653
7.267
4.016
3.960
abundance
Y : parts per Million : Carbon13
X : parts per Million : Proton
Exact Mass: 464.1597
56.397
61.040
104.826
107.420
107.468
115.339
117.819
127.470
130.122
130.706
136.183
137.074
140.980
144.111
149.166
151.311
153.102
153.791
162.140
(thousandths)
Filename = MRP-24_HSQC-PROC
Author = delta
Experiment = hsqc.jxp
Sample_Id = MRP-24
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2022 21:5
Revision_Time = 20-FEB-2024 09:0
Comment = hsqc
Data_Format = 2D COMPLEX COMPL
Dim_Size = 1638, 512
X_Domain = Proton
Y_Domain = Carbon13
Dim_Title = Proton Carbon13
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T]
X_Acq_Duration = 0.23199744[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5.53987[ppm]
X_Points = 2048
X_Prescans = 8
X_Resolution = 4.31039239[Hz]
X_Sweep = 8.82768362[kHz]
X_Sweep_Clipped = 7.06214689[kHz]
Y_Domain = Carbon13
Y_Freq = 150.91343039[MHz
Y_Offset = 102.94272[ppm]
Y_Points = 256
Y_Prescans = 0
Y_Resolution = 127.32235984[Hz]
Y_Sweep = 32.59452412[kHz]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 2048
Relaxation_Delay = 1.5[s]
Recvr_Gain = 46
Temp_Get = 25[dC]
X_Acq_Time = 0.23199744[s]
X_Atn = 8.2[dB]
X_Gamma = 42576375
X_Pulse = 7.045[us]
Y_Acq_Time = 7.85408[ms]
Y_Atn = 10.4[dB]
Y_Gamma = 10705836.9
Y_Pulse = 11.025[us]
Irr_Atn_Dec = 29.377[dB]
Irr_Atn_Dec_Calc = 29.377[dB]
Irr_Atn_Dec_Default_Calc = 29.377[dB]
Irr_Dec_Bandwidth_Hz = 27.04081633[kHz]
Irr_Dec_Bandwidth_Ppm = 179.18097982[ppm
Irr_Dec_Freq = 150.91343039[MHz
Irr_Dec_Merit_Factor = 10.6
Irr_Decoupling = TRUE
Irr_Noise = MPF8
Irr_Pwidth = 98[us]

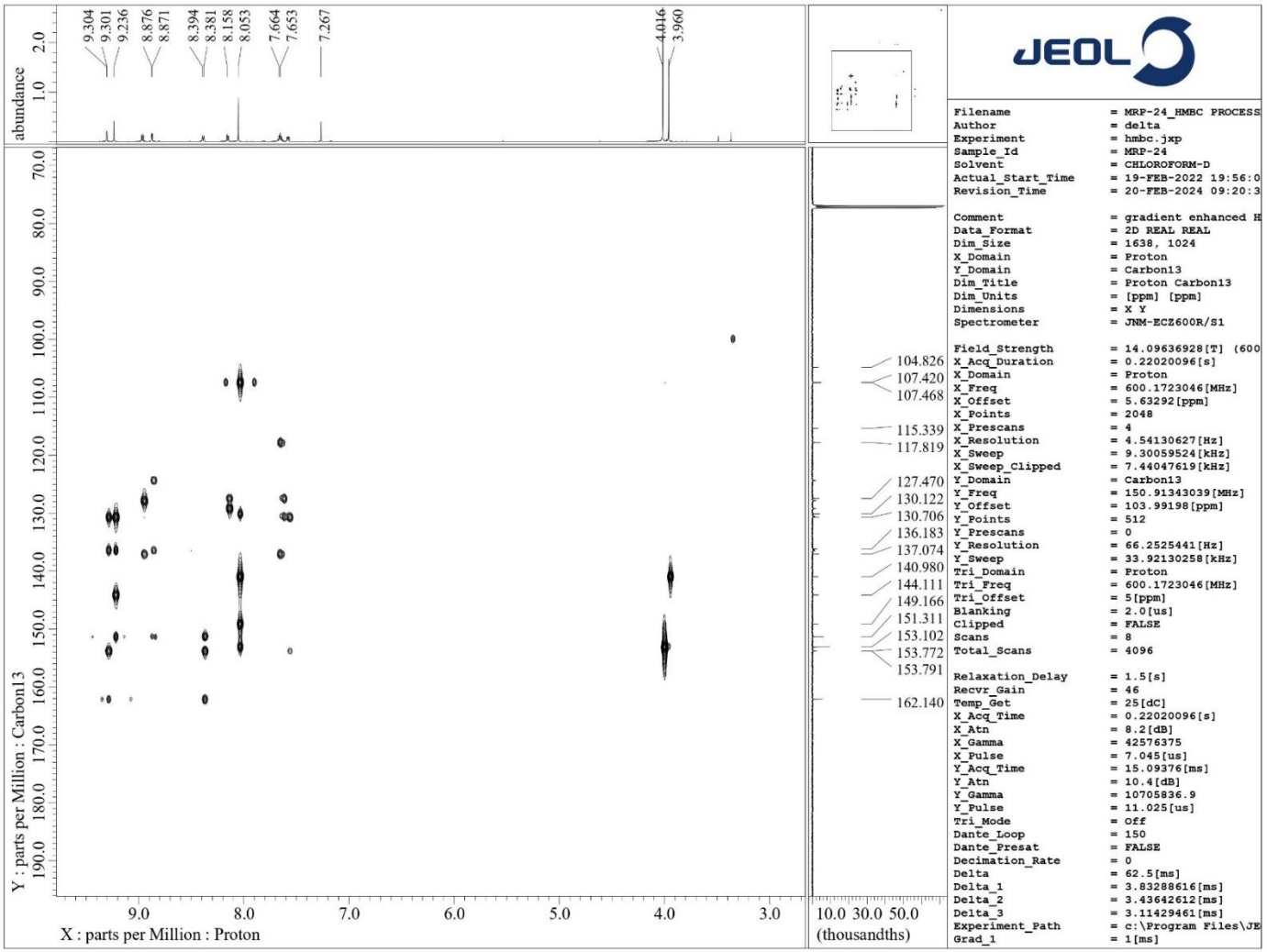
HSQC-2



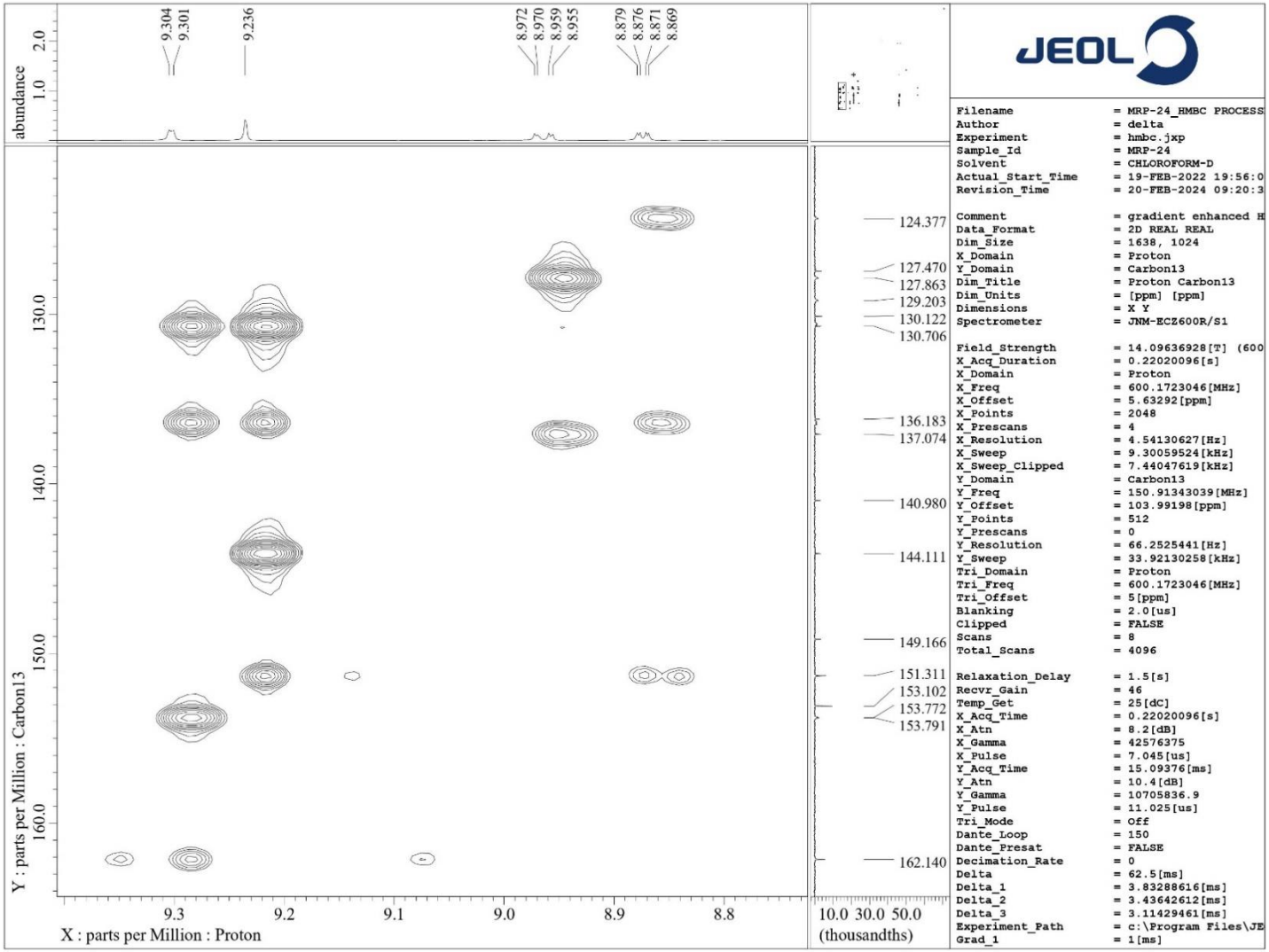


Exact Mass: 464.1597

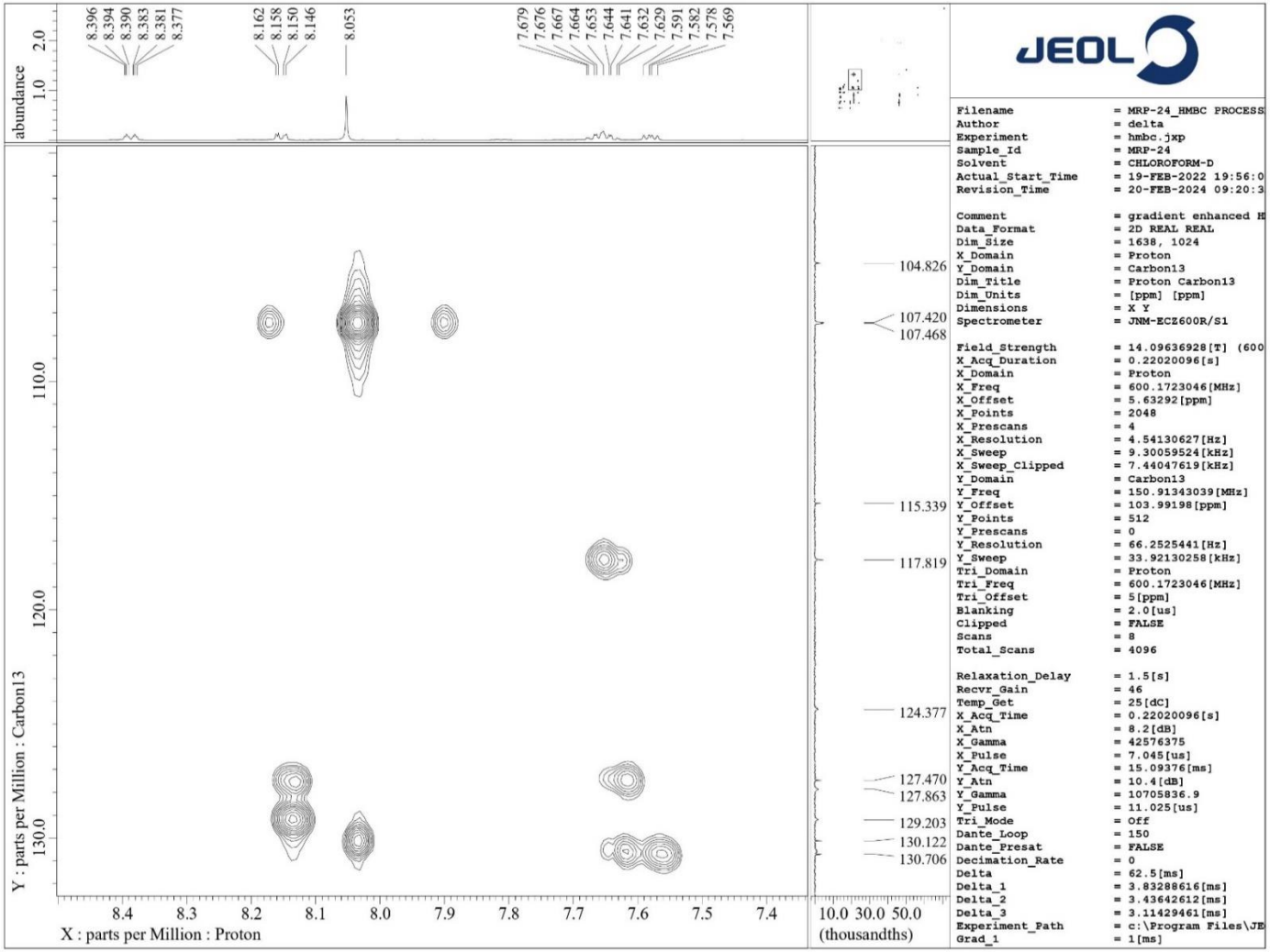
HMBC-1


9.304
9.301
9.236
8.876
8.871
8.394
8.381
8.158
8.053
7.664
7.653
7.267
4.016
3.960
abundance
Y : parts per Million : Carbon13
X : parts per Million : Proton
104.826
107.420
107.468
115.339
117.819
127.470
130.122
130.706
136.183
137.074
140.980
144.111
149.166
151.311
153.102
153.772
153.791
162.140
(thousandths)
Filename = MRP-24_HMBC PROCESS
Author = delta
Experiment = hmbc.jxp
Sample_Id = MRP-24
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2022 19:56:0
Revision_Time = 20-FEB-2024 09:20:3
Comment = gradient enhanced H
Data_Format = 2D REAL REAL
Dim_Size = 1638, 1024
X_Domain = Proton
Y_Domain = Carbon13
Dim_Title = Proton Carbon13
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T] (600
X_Acq_Duration = 0.22020096[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5.63292[ppm]
X_Points = 2048
X_Prescans = 4
X_Resolution = 4.54130627[Hz]
X_Sweep = 9.30059524[kHz]
X_Sweep_Clipped = 7.44047619[kHz]
Y_Domain = Carbon13
Y_Freq = 150.91343039[MHz]
Y_Offset = 103.99198[ppm]
Y_Points = 512
Y_Prescans = 0
Y_Resolution = 66.2525441[Hz]
Y_Sweep = 33.92130258[kHz]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 4096
Relaxation_Delay = 1.5[s]
Recvr_Gain = 46
Temp_Get = 25[dC]
X_Acq_Time = 0.22020096[s]
X_Atn = 8.2[dB]
X_Gamma = 42576375
X_Pulse = 7.045[us]
Y_Acq_Time = 15.09376[ms]
Y_Atn = 10.4[dB]
Y_Gamma = 10705836.9
Y_Pulse = 11.025[us]
Tri_Mode = Off
Dante_Loop = 150
Dante_Presat = FALSE
Decimation_Rate = 0
Delta = 62.5[ms]
Delta_1 = 3.83288616[ms]
Delta_2 = 3.43642612[ms]
Delta_3 = 3.11429461[ms]
Experiment_Path = c:\Program Files\JE
Grad_1 = 1[ms]

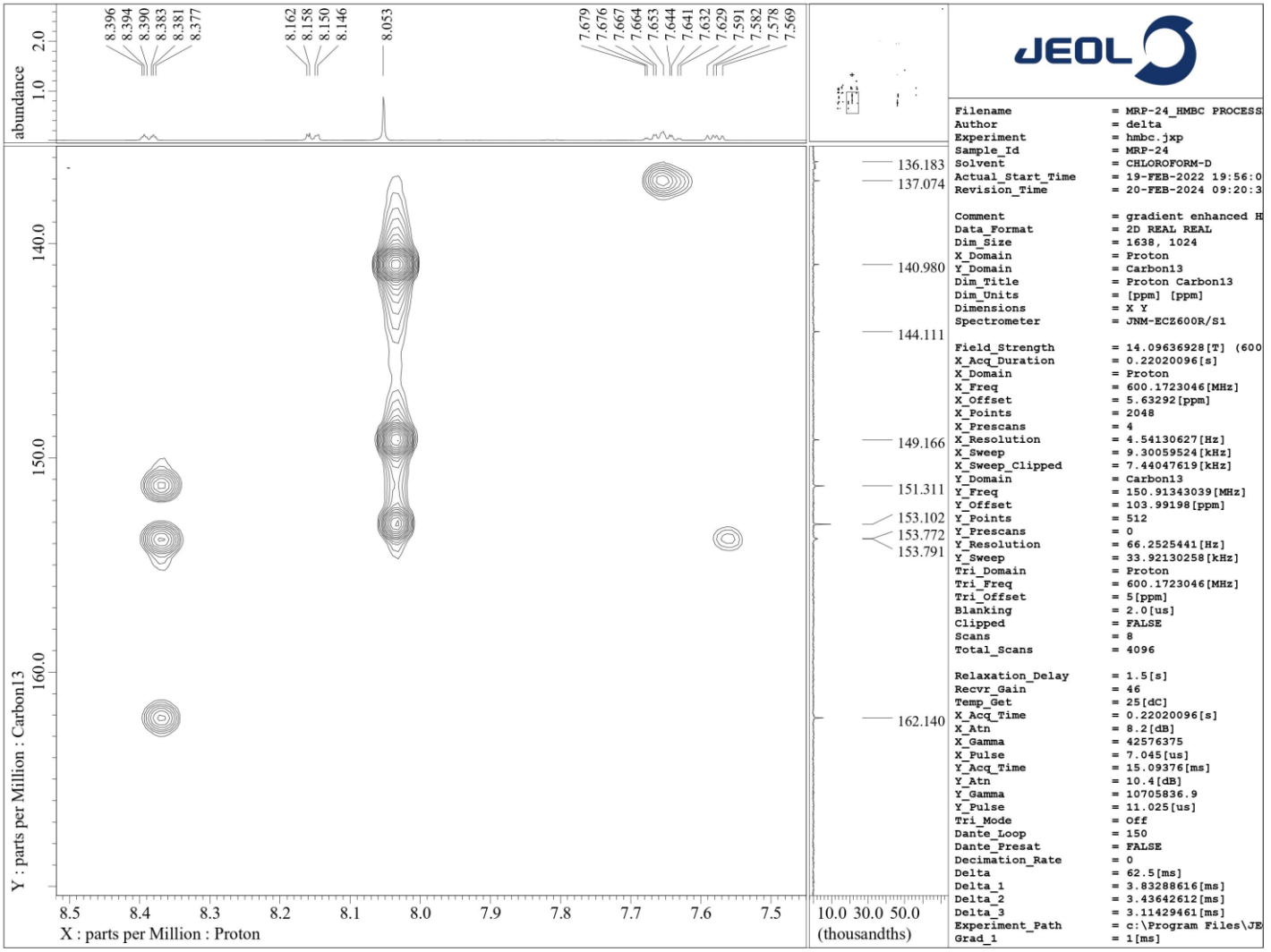
HMBC-2


abundance
9.304
9.301
9.236
8.972
8.970
8.959
8.955
8.879
8.876
8.871
8.869
Y : parts per Million : Carbon13
X : parts per Million : Proton
(thousandths)
124.377
127.470
127.863
129.203
130.122
130.706
136.183
137.074
140.980
144.111
149.166
151.311
153.102
153.772
153.791
162.140
Filename = MRP-24_HMBC PROCESS
Author = delta
Experiment = hmbc.jxp
Sample_Id = MRP-24
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2022 19:56:0
Revision_Time = 20-FEB-2024 09:20:3
Comment = gradient enhanced H
Data_Format = 2D REAL REAL
Dim_Size = 1638, 1024
X_Domain = Proton
Y_Domain = Carbon13
Dim_Title = Proton Carbon13
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T] (600
X_Acq_Duration = 0.22020096[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5.63292[ppm]
X_Points = 2048
X_Prescans = 4
X_Resolution = 4.54130627[Hz]
X_Sweep = 9.30059524[kHz]
X_Sweep_Clipped = 7.44047619[kHz]
Y_Domain = Carbon13
Y_Freq = 150.91343039[MHz]
Y_Offset = 103.99198[ppm]
Y_Points = 512
Y_Prescans = 0
Y_Resolution = 66.2525441[Hz]
Y_Sweep = 33.92130258[kHz]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 4096
Relaxation_Delay = 1.5[s]
Recvr_Gain = 46
Temp_Get = 25[dC]
X_Acq_Time = 0.22020096[s]
X_Atn = 8.2[dB]
X_Gamma = 42576375
X_Pulse = 7.045[us]
Y_Acq_Time = 15.09376[ms]
Y_Atn = 10.4[dB]
Y_Gamma = 10705836.9
Y_Pulse = 11.025[us]
Tri_Mode = Off
Dante_Loop = 150
Dante_Presat = FALSE
Decimation_Rate = 0
Delta = 62.5[ms]
Delta_1 = 3.83288616[ms]
Delta_2 = 3.43642612[ms]
Delta_3 = 3.11429461[ms]
Experiment_Path = c:\Program Files\JE
Grad_1 = 1[ms]

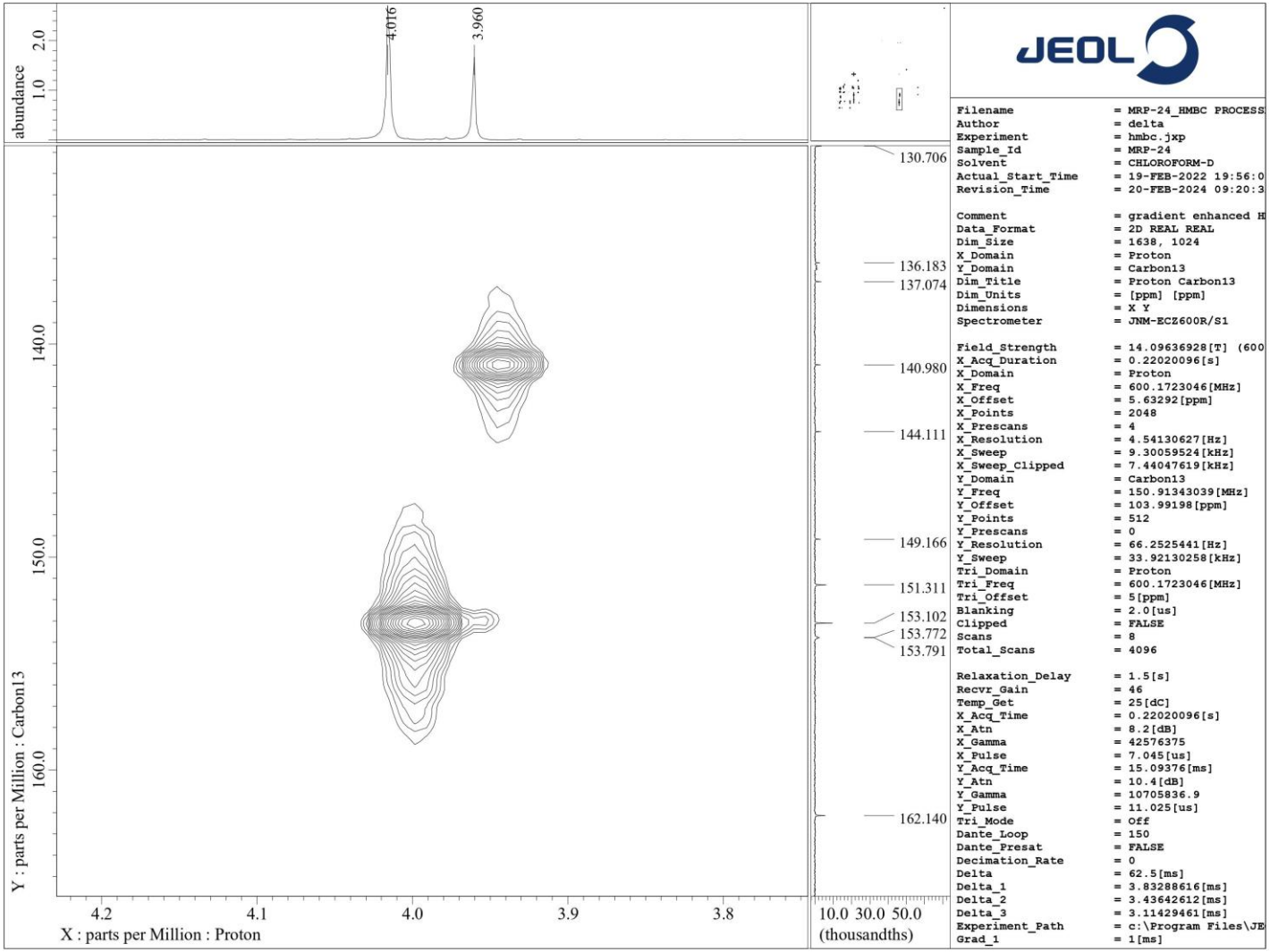
HMBC-3


8.396
8.394
8.390
8.383
8.381
8.377
8.162
8.158
8.150
8.146
8.053
7.679
7.676
7.667
7.664
7.653
7.644
7.641
7.632
7.629
7.591
7.582
7.578
7.569
abundance
2.0
1.0
110.0
120.0
130.0
Y : parts per Million : Carbon13
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
X : parts per Million : Proton
104.826
107.420
107.468
115.339
117.819
124.377
127.470
127.863
129.203
130.122
130.706
10.0 30.0 50.0
(thousandths)
JEOL
Filename = MRP-24_HMBC PROCESS
Author = delta
Experiment = hmbc.jxp
Sample_Id = MRP-24
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2022 19:56:0
Revision_Time = 20-FEB-2024 09:20:3
Comment = gradient enhanced H
Data_Format = 2D REAL REAL
Dim_Size = 1638, 1024
X_Domain = Proton
Y_Domain = Carbon13
Dim_Title = Proton Carbon13
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T] (600
X_Acq_Duration = 0.22020096[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5.63292[ppm]
X_Points = 2048
X_Prescans = 4
X_Resolution = 4.54130627[Hz]
X_Sweep = 9.30059524[kHz]
X_Sweep_Clipped = 7.44047619[kHz]
Y_Domain = Carbon13
Y_Freq = 150.91343039[MHz]
Y_Offset = 103.99198[ppm]
Y_Points = 512
Y_Prescans = 0
Y_Resolution = 66.2525441[Hz]
Y_Sweep = 33.92130258[kHz]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 4096
Relaxation_Delay = 1.5[s]
Recvr_Gain = 46
Temp_Get = 25[dC]
X_Acq_Time = 0.22020096[s]
X_Atn = 8.2[dB]
X_Gamma = 42576375
X_Pulse = 7.045[us]
Y_Acq_Time = 15.09376[ms]
Y_Atn = 10.4[dB]
Y_Gamma = 10705836.9
Y_Pulse = 11.025[us]
Tri_Mode = Off
Dante_Loop = 150
Dante_Presat = FALSE
Decimation_Rate = 0
Delta = 62.5[ms]
Delta_1 = 3.83288616[ms]
Delta_2 = 3.43642612[ms]
Delta_3 = 3.11429461[ms]
Experiment_Path = c:\Program Files\JE
Grad_1 = 1[ms]

HMBC-4


8.396
8.394
8.390
8.383
8.381
8.377
8.162
8.158
8.150
8.146
8.053
7.679
7.676
7.667
7.664
7.653
7.644
7.641
7.632
7.629
7.591
7.582
7.578
7.569
abundance
2.0
1.0
140.0
150.0
160.0
Y : parts per Million : Carbon13
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
X : parts per Million : Proton
136.183
137.074
140.980
144.111
149.166
151.311
153.102
153.772
153.791
162.140
10.0 30.0 50.0
(thousandths)
JEOL
Filename = MRP-24_HMBC PROCESS
Author = delta
Experiment = hmbc.jxp
Sample_Id = MRP-24
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2022 19:56:0
Revision_Time = 20-FEB-2024 09:20:3
Comment = gradient enhanced H
Data_Format = 2D REAL REAL
Dim_Size = 1638, 1024
X_Domain = Proton
Y_Domain = Carbon13
Dim_Title = Proton Carbon13
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T] (600
X_Acq_Duration = 0.22020096[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5.63292[ppm]
X_Points = 2048
X_Prescans = 4
X_Resolution = 4.54130627[Hz]
X_Sweep = 9.30059524[kHz]
X_Sweep_Clipped = 7.44047619[kHz]
Y_Domain = Carbon13
Y_Freq = 150.91343039[MHz]
Y_Offset = 103.99198[ppm]
Y_Points = 512
Y_Prescans = 0
Y_Resolution = 66.2525441[Hz]
Y_Sweep = 33.92130258[kHz]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 4096
Relaxation_Delay = 1.5[s]
Recvr_Gain = 46
Temp_Get = 25[dC]
X_Acq_Time = 0.22020096[s]
X_Atn = 8.2[dB]
X_Gamma = 42576375
X_Pulse = 7.045[us]
Y_Acq_Time = 15.09376[ms]
Y_Atn = 10.4[dB]
Y_Gamma = 10705836.9
Y_Pulse = 11.025[us]
Tri_Mode = Off
Dante_Loop = 150
Dante_Presat = FALSE
Decimation_Rate = 0
Delta = 62.5[ms]
Delta_1 = 3.83288616[ms]
Delta_2 = 3.43642612[ms]
Delta_3 = 3.11429461[ms]
Experiment_Path = c:\Program Files\JE
Grad_1 = 1[ms]

HMBC-5


4.016
3.960
abundance
2.0
1.0
140.0
150.0
160.0
Y : parts per Million : Carbon13
4.2
4.1
4.0
3.9
3.8
X : parts per Million : Proton
130.706
136.183
137.074
140.980
144.111
149.166
151.311
153.102
153.772
153.791
162.140
10.0 30.0 50.0
(thousandths)
JEOL
Filename = MRP-24_HMBC PROCESS
Author = delta
Experiment = hmbc.jxp
Sample_Id = MRP-24
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2022 19:56:0
Revision_Time = 20-FEB-2024 09:20:3
Comment = gradient enhanced H
Data_Format = 2D REAL REAL
Dim_Size = 1638, 1024
X_Domain = Proton
Y_Domain = Carbon13
Dim_Title = Proton Carbon13
Dim_Units = [ppm] [ppm]
Dimensions = X Y
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T] (600
X_Acq_Duration = 0.22020096[s]
X_Domain = Proton
X_Freq = 600.1723046[MHz]
X_Offset = 5.63292[ppm]
X_Points = 2048
X_Prescans = 4
X_Resolution = 4.54130627[Hz]
X_Sweep = 9.30059524[kHz]
X_Sweep_Clipped = 7.44047619[kHz]
Y_Domain = Carbon13
Y_Freq = 150.91343039[MHz]
Y_Offset = 103.99198[ppm]
Y_Points = 512
Y_Prescans = 0
Y_Resolution = 66.2525441[Hz]
Y_Sweep = 33.92130258[kHz]
Tri_Domain = Proton
Tri_Freq = 600.1723046[MHz]
Tri_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 8
Total_Scans = 4096
Relaxation_Delay = 1.5[s]
Recvr_Gain = 46
Temp_Get = 25[dC]
X_Acq_Time = 0.22020096[s]
X_Atn = 8.2[dB]
X_Gamma = 42576375
X_Pulse = 7.045[us]
Y_Acq_Time = 15.09376[ms]
Y_Atn = 10.4[dB]
Y_Gamma = 10705836.9
Y_Pulse = 11.025[us]
Tri_Mode = Off
Dante_Loop = 150
Dante_Presat = FALSE
Decimation_Rate = 0
Delta = 62.5[ms]
Delta_1 = 3.83288616[ms]
Delta_2 = 3.43642612[ms]
Delta_3 = 3.11429461[ms]
Experiment_Path = c:\Program Files\JE
Grad_1 = 1[ms]

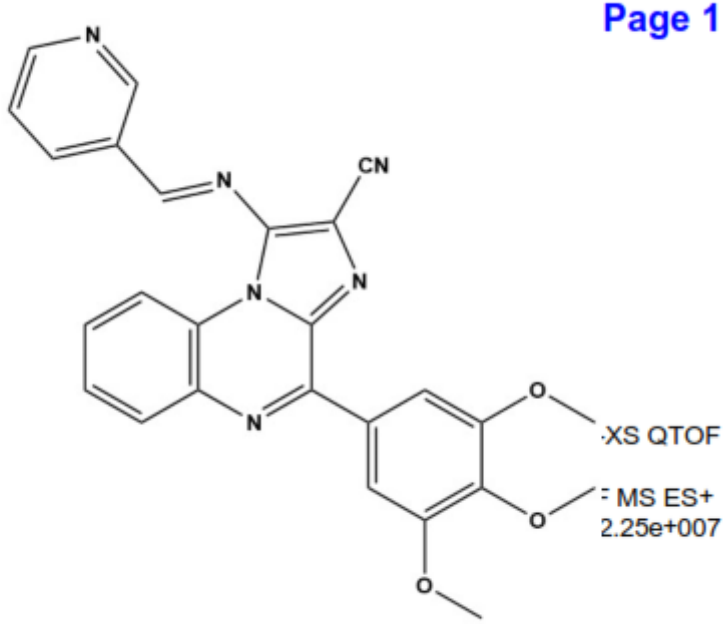
Elemental Composition Report

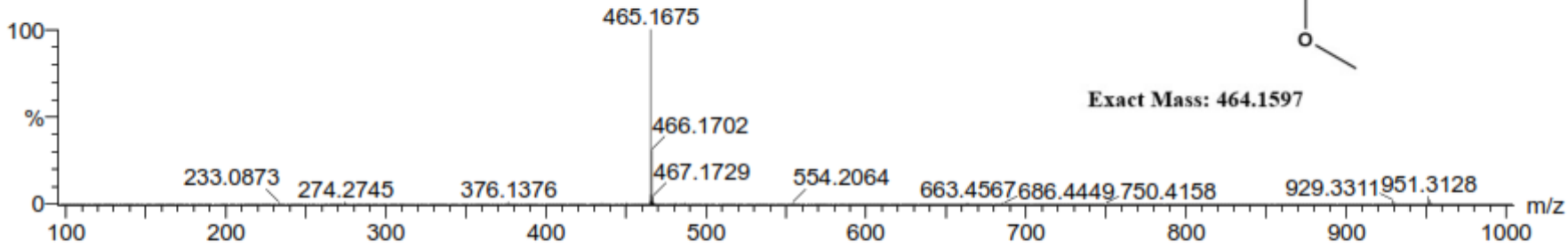
Single Mass Analysis

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
1149 formula(e) evaluated with 10 results within limits (up to 1 closest results
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 S: 0-3

Sample Name : MRP_24 IITRPR
Test Name :
23032022_MRP_24 8 (0.186)

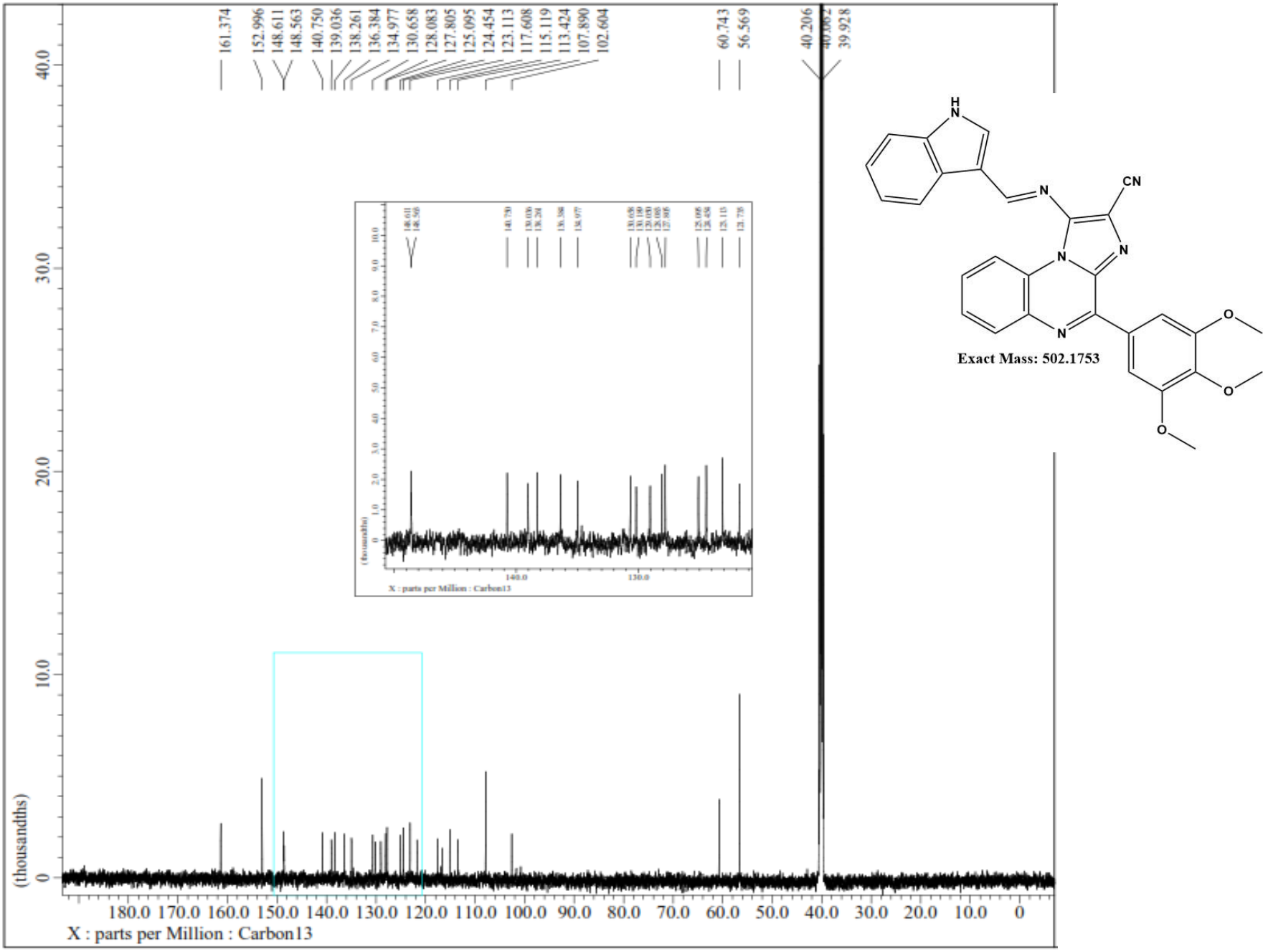




Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
465.1675	465.1675	0.0	0.0	19.5	1051.3	n/a	n/a	C26 H21 N6 O3

,

Spectral data of compound 5p


161.374
152.996
148.611
148.563
140.750
139.036
138.261
136.384
134.977
130.658
128.083
127.805
125.095
124.454
123.113
117.608
115.119
113.424
107.890
102.604
60.743
56.569
40.206
39.928
(thousandths)
X : parts per Million : Carbon13
Exact Mass: 502.1753

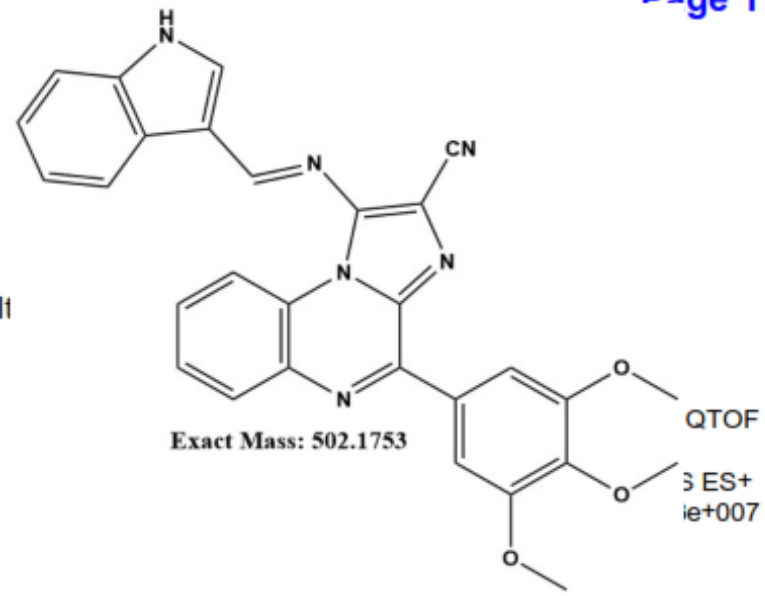
Elemental Composition Report

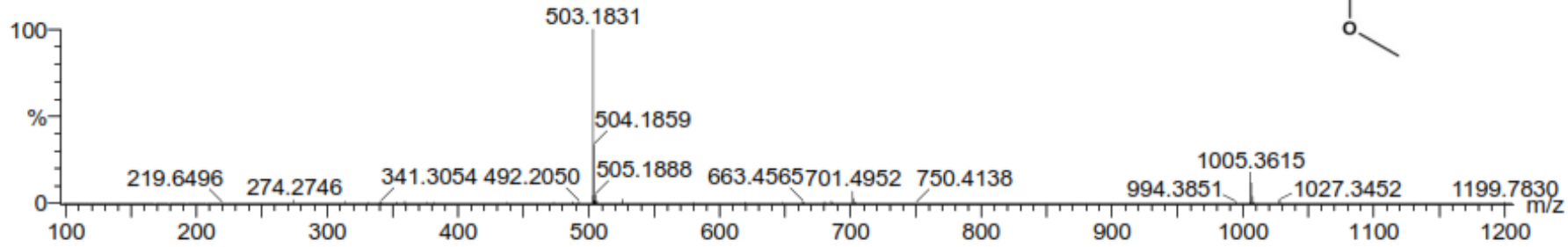
Single Mass Analysis

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
1268 formula(e) evaluated with 12 results within limits (up to 1 closest result
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 S: 0-3

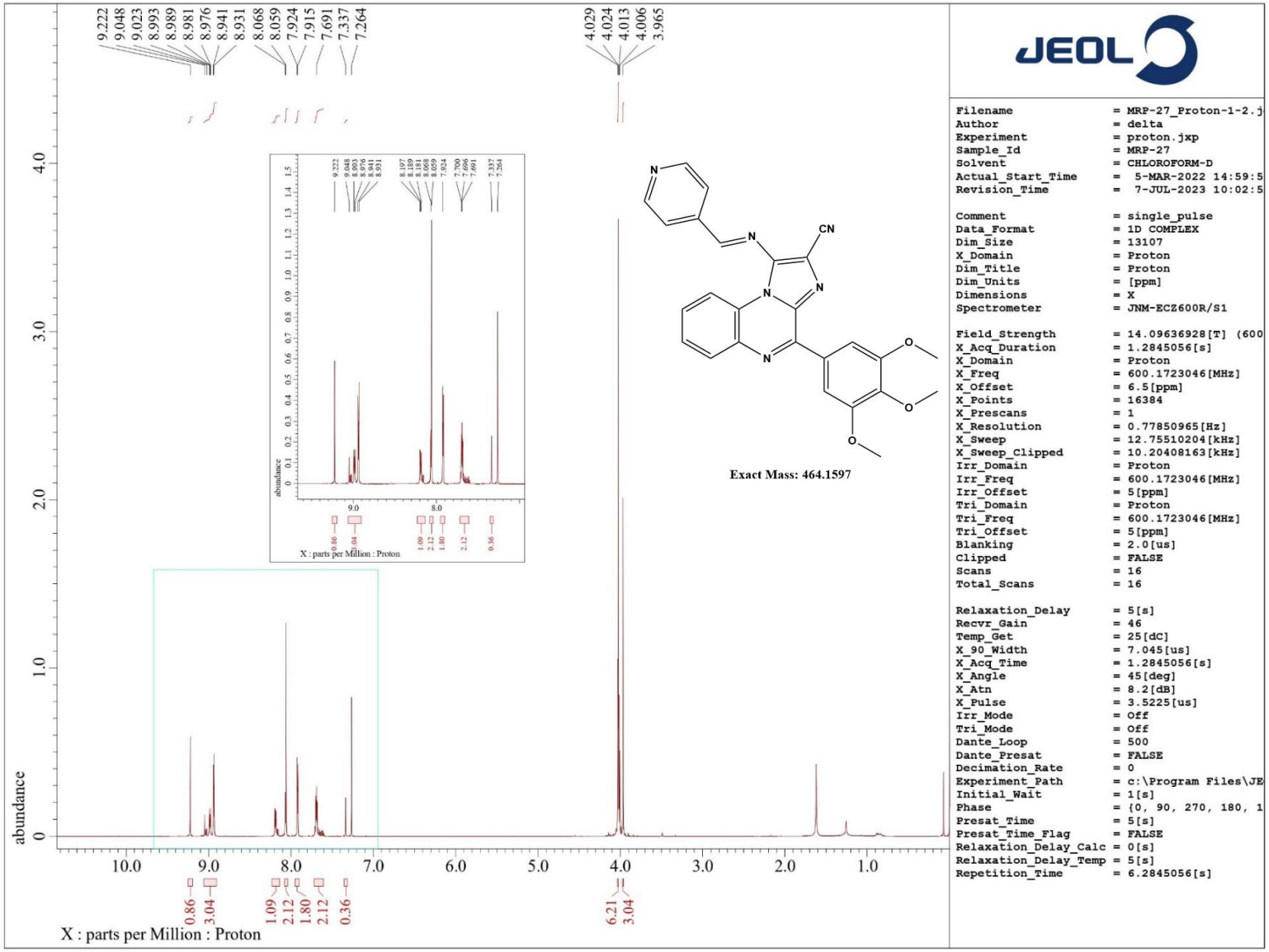
Sample Name : MRP_23 IITRPR
Test Name :
23032022_MRP_26 8 (0.186)





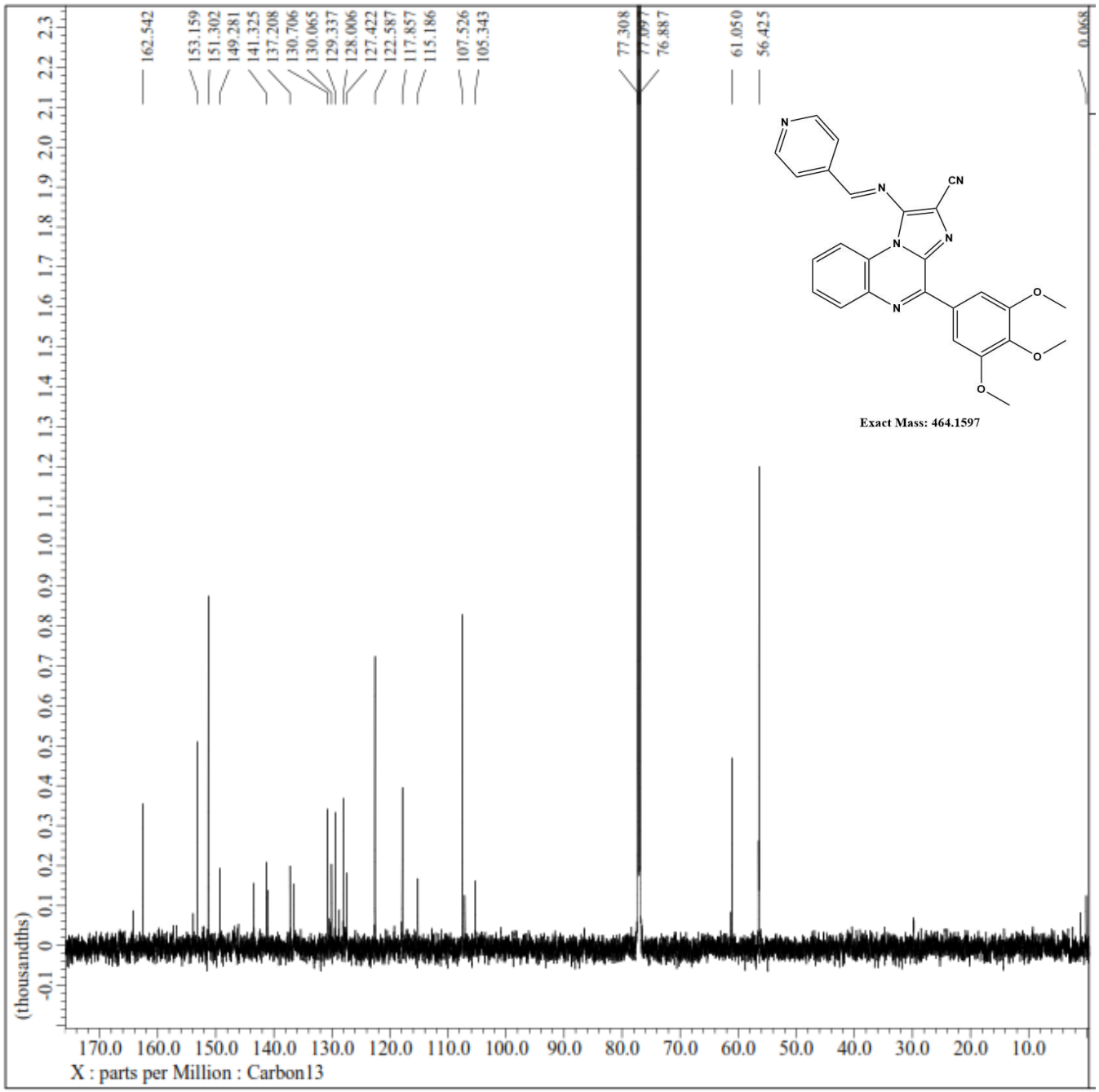
Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
503.1831	503.1832	-0.1	-0.2	21.5	1153.5	n/a	n/a	C29 H23 N6 O3

Spectral data of compound 5q



JEOL

Filename	= MRP-27_Proton-1-2.j
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MRP-27
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 5-MAR-2022 14:59:5
Revision_Time	= 7-JUL-2023 10:02:5
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S1
Field_Strength	= 14.09636928[T] (600
X_Acq_Duration	= 1.2845056[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 6.5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.77850965[Hz]
X_Sweep	= 12.75510204[kHz]
X_Sweep_Clipped	= 10.20408163[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 25[dC]
X_90_Width	= 7.045[us]
X_Acq_Time	= 1.2845056[s]
X_Angle	= 45[deg]
X_Atn	= 8.2[dB]
X_Pulse	= 3.5225[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JE
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 1
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.2845056[s]

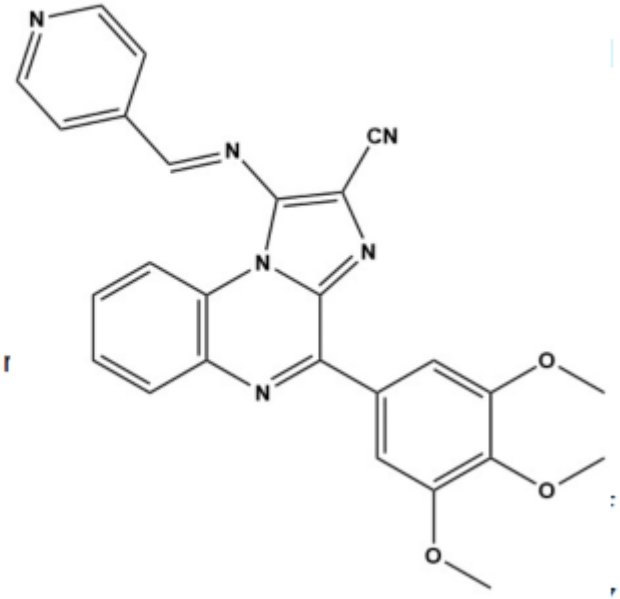

162.542
153.159
151.302
149.281
141.325
137.208
130.706
130.065
129.337
128.006
127.422
122.587
117.857
115.186
107.526
105.343
77.308
77.097
76.887
61.050
56.425
0.068
N
N
CN
N
N
N
O
O
O
Exact Mass: 464.1597
(thousandths)
-0.1 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3
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
X : parts per Million : Carbon13

Elemental Composition Report

Single Mass Analysis

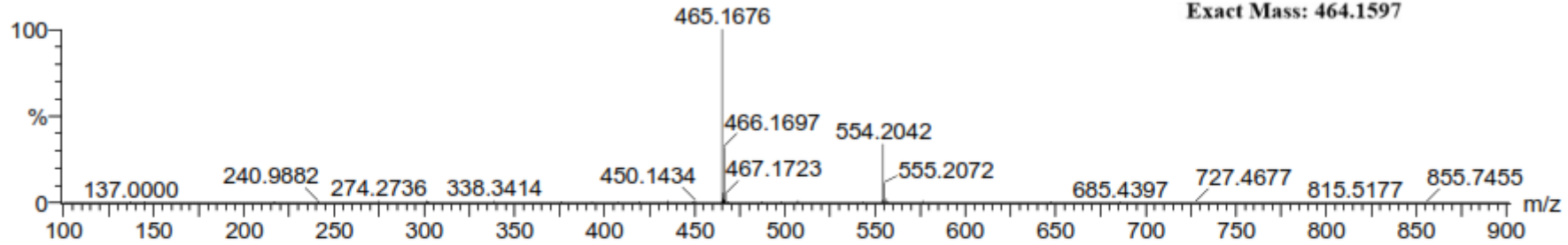
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
1430 formula(e) evaluated with 7 results within limits (up to 1 closest results for each r
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10 Br: 0-2



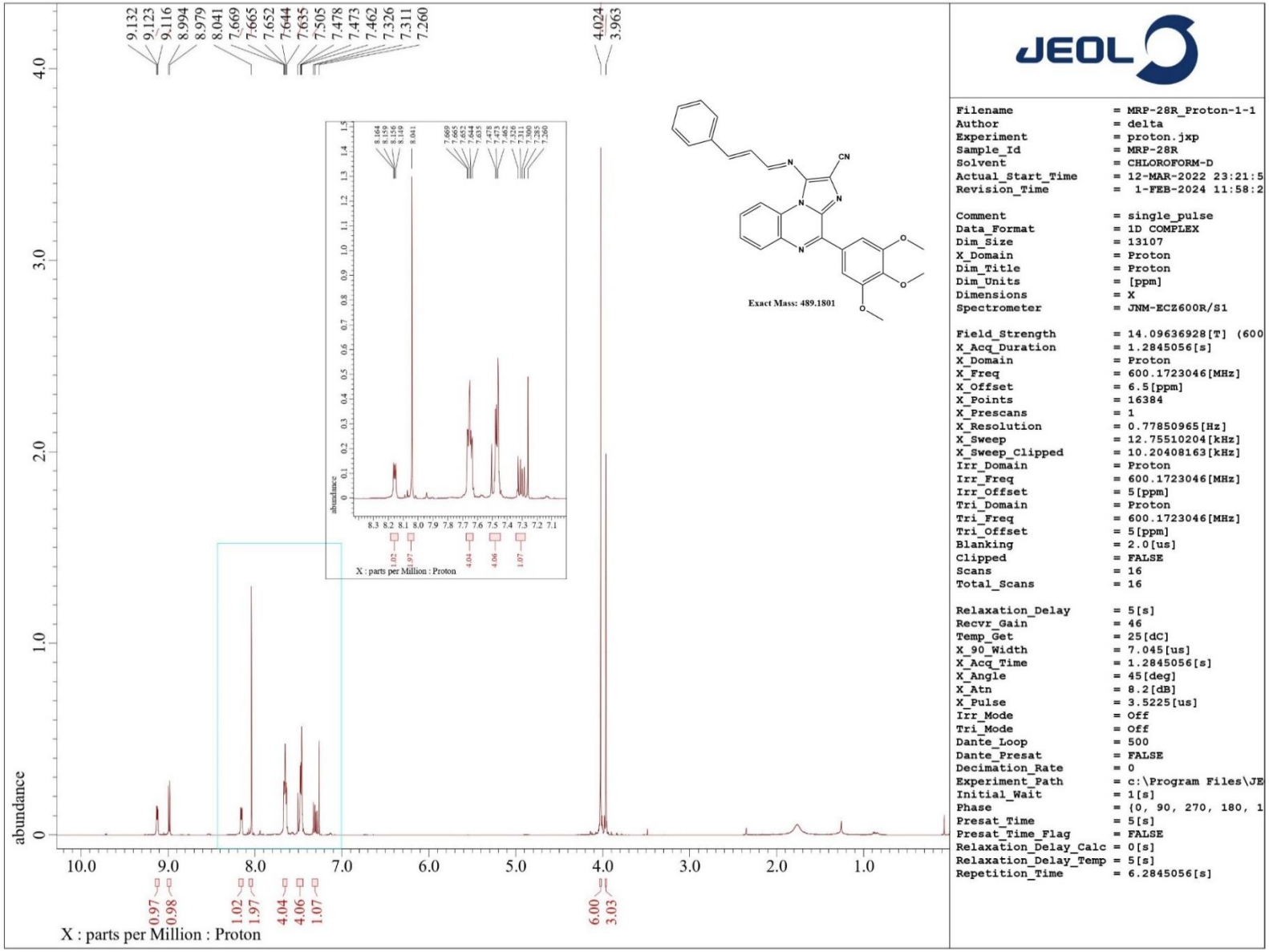
Exact Mass: 464.1597

Sample Name : MRP_27 IITRPR
Test Name :
260522_MRP_27 17 (0.197)

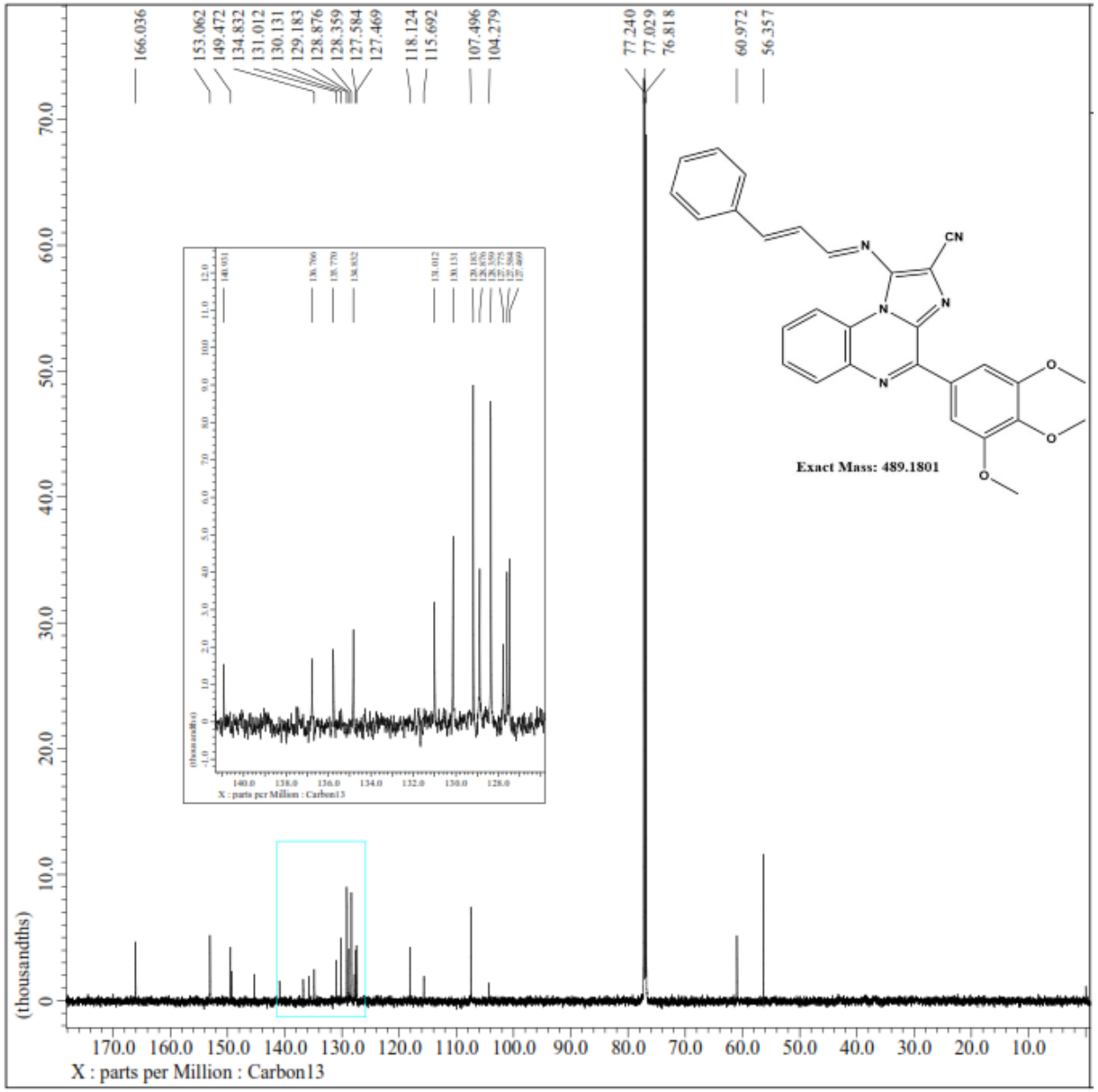


Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
465.1676	465.1675	0.1	0.2	19.5	1354.9	n/a	n/a	C26 H21 N6 O3

Spectral data of compound 5r



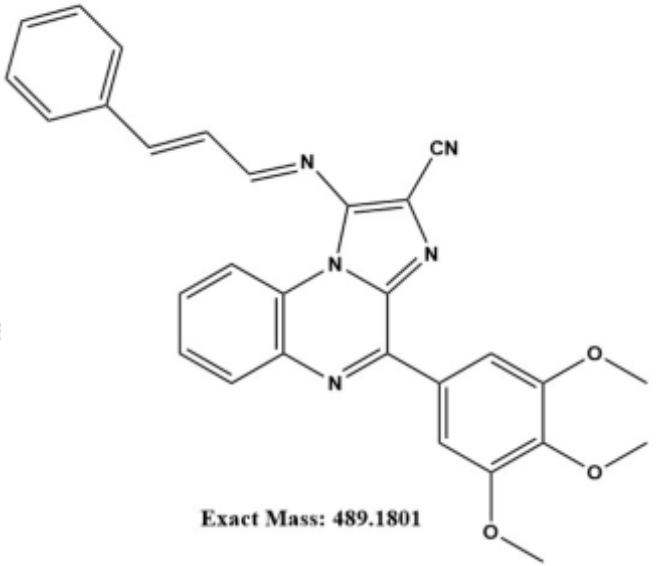
Filename	= MRP-28R_Proton-1-1
Author	= delta
Experiment	= proton.jxp
Sample_Id	= MRP-28R
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 12-MAR-2022 23:21:5
Revision_Time	= 1-FEB-2024 11:58:2
Comment	= single_pulse
Data_Format	= 1D COMPLEX
Dim_Size	= 13107
X_Domain	= Proton
Dim_Title	= Proton
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S1
Field_Strength	= 14.09636928[T] (600
X_Acq_Duration	= 1.2845056[s]
X_Domain	= Proton
X_Freq	= 600.1723046[MHz]
X_Offset	= 6.5[ppm]
X_Points	= 16384
X_Prescans	= 1
X_Resolution	= 0.77850965[Hz]
X_Sweep	= 12.75510204[kHz]
X_Sweep_Clipped	= 10.20408163[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Tri_Domain	= Proton
Tri_Freq	= 600.1723046[MHz]
Tri_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= FALSE
Scans	= 16
Total_Scans	= 16
Relaxation_Delay	= 5[s]
Recvr_Gain	= 46
Temp_Get	= 25[dC]
X_90_Width	= 7.045[us]
X_Acq_Time	= 1.2845056[s]
X_Angle	= 45[deg]
X_Atn	= 8.2[dB]
X_Pulse	= 3.5225[us]
Irr_Mode	= Off
Tri_Mode	= Off
Dante_Loop	= 500
Dante_Presat	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files\JE
Initial_Wait	= 1[s]
Phase	= {0, 90, 270, 180, 1
Presat_Time	= 5[s]
Presat_Time_Flag	= FALSE
Relaxation_Delay_Calc	= 0[s]
Relaxation_Delay_Temp	= 5[s]
Repetition_Time	= 6.2845056[s]


166.036
153.062
149.472
134.832
131.012
130.131
129.183
128.876
128.359
127.584
127.469
118.124
115.692
107.496
104.279
77.240
77.029
76.818
60.972
56.357
CN
N
O
Exact Mass: 489.1801
(thousandths)
X : parts per Million : Carbon13

Elemental Composition Report

Single Mass Analysis

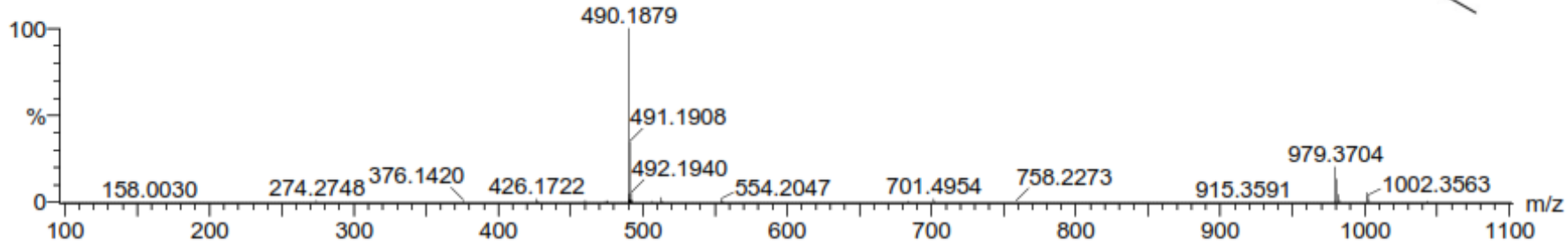
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5



Exact Mass: 489.1801

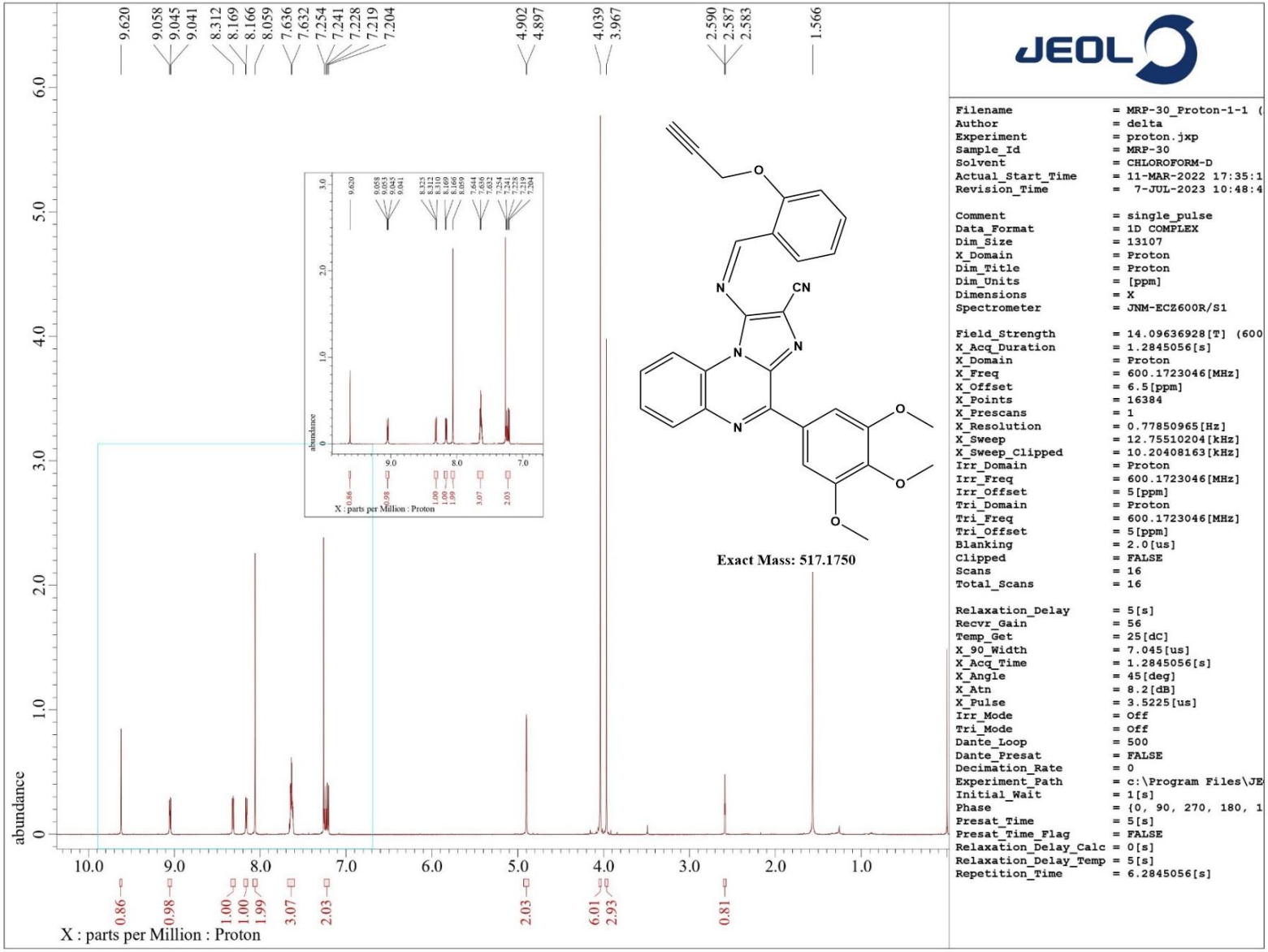
Monoisotopic Mass, Even Electron Ions
1206 formula(e) evaluated with 11 results within limits (up to 1 closest results for ea
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 S: 0-3

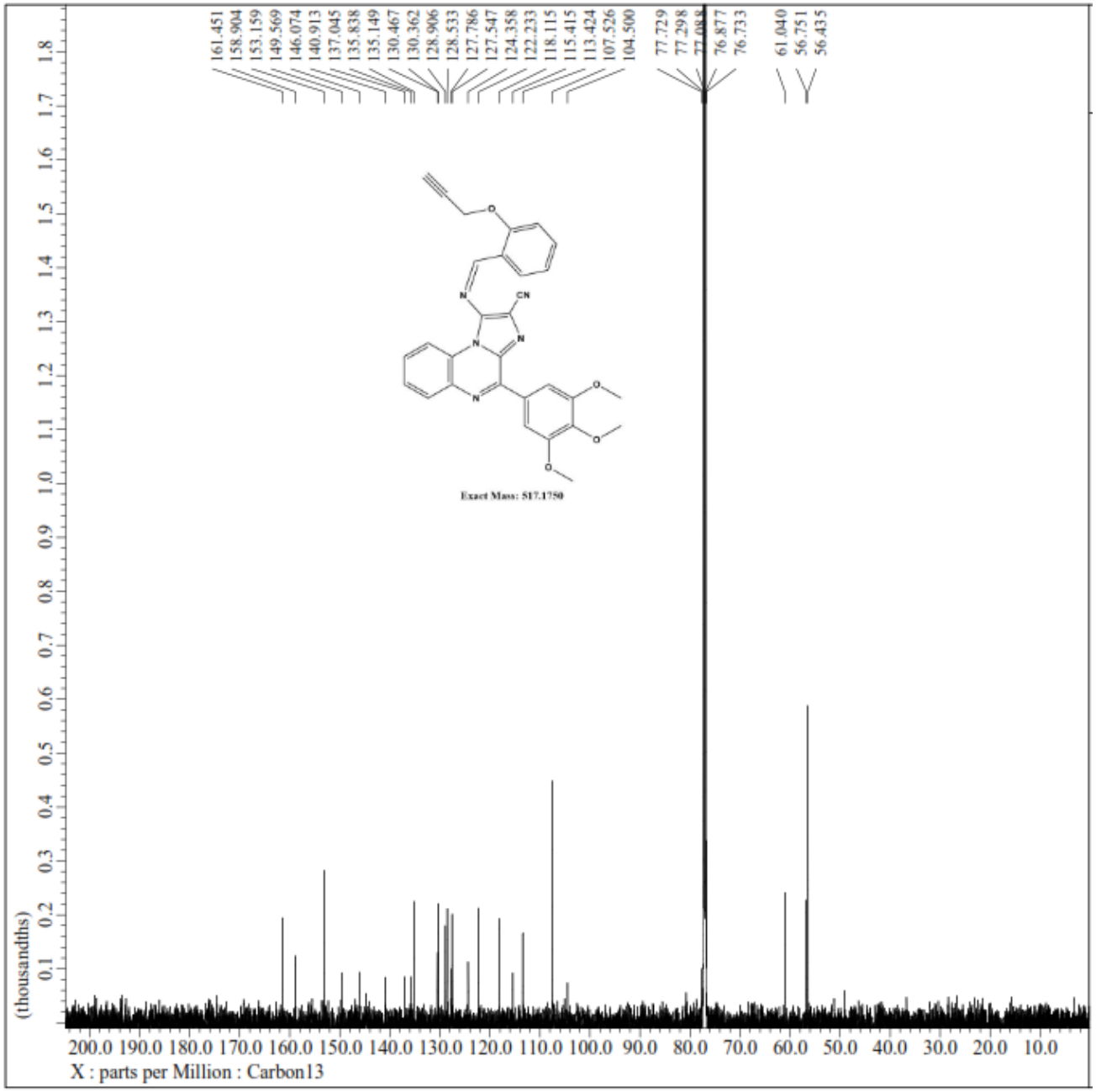
Sample Name : MRP_26 IITRPR
Test Name :
23032022_MRP_28 8 (0.186)



Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
490.1879	490.1879	0.0	0.0	20.5	1461.4	n/a	n/a	C29 H24 N5 O3

Spectral data of compound 5s




161.451
158.904
153.159
149.569
146.074
140.913
137.045
135.838
135.149
130.467
130.362
128.906
128.533
127.786
127.547
124.358
122.233
118.115
115.415
113.424
107.526
104.500
77.729
77.298
77.083
76.877
76.733
61.040
56.751
56.435
CN
Exact Mass: 517.1750
(thousandths)
X : parts per Million : Carbon13

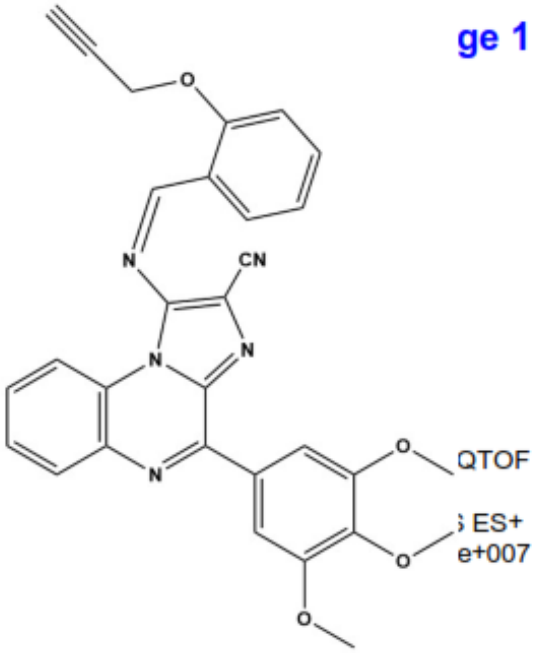
Elemental Composition Report

Single Mass Analysis

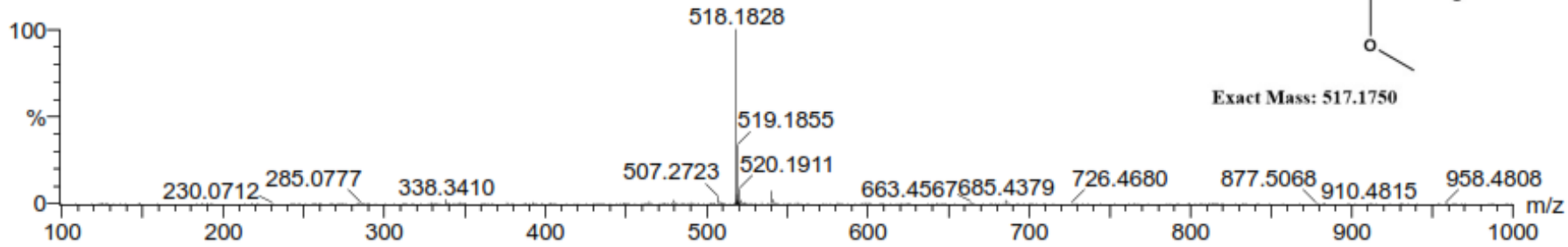
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions
673 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10

Sample Name : MRP_30 IITRPR
Test Name :
260522_MRP_30 17 (0.197)

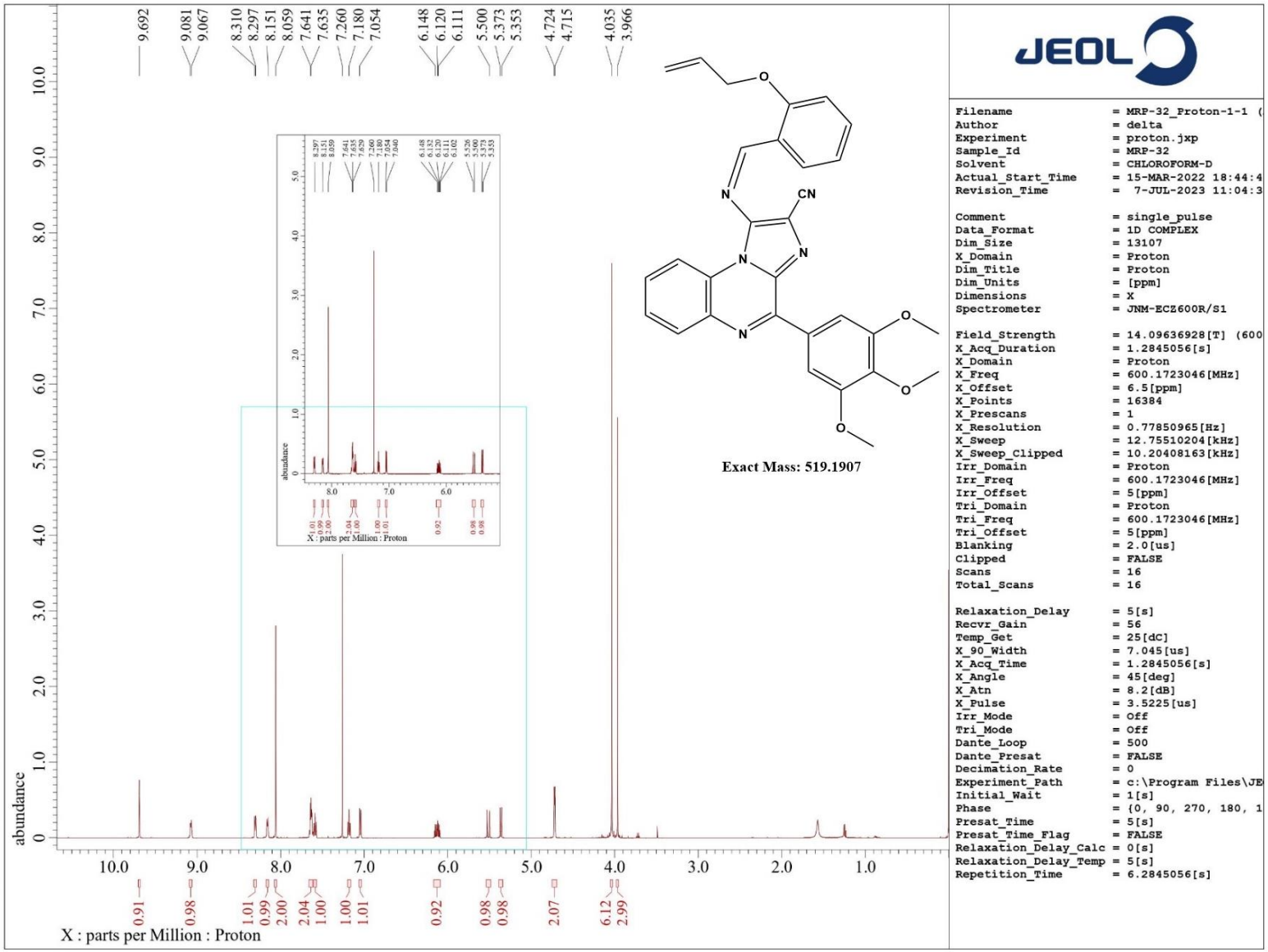


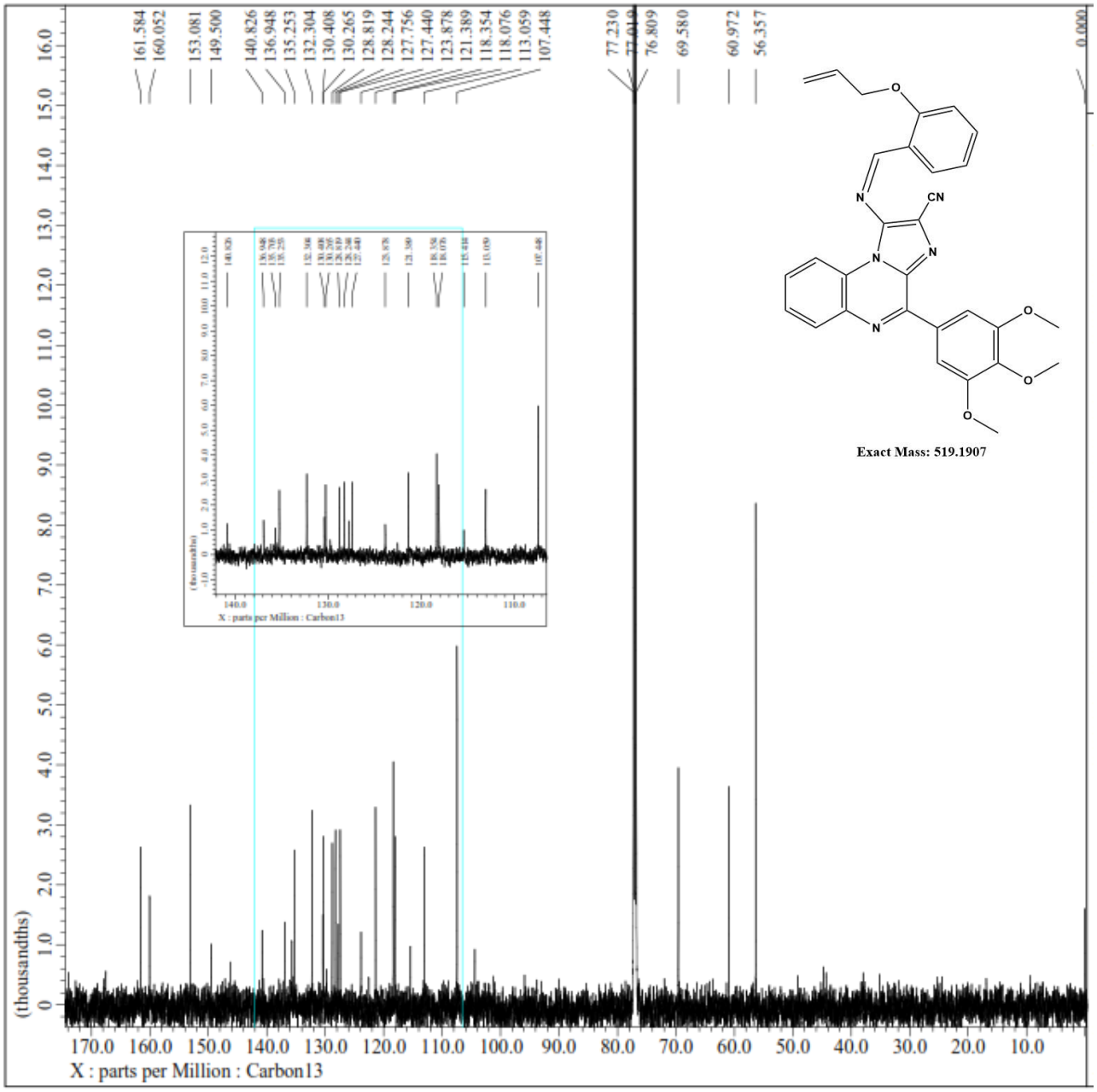
Exact Mass: 517.1750



Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
518.1828	518.1828	0.0	0.0	21.5	439.5	n/a	n/a	C30 H24 N5 O4

Spectral data of compound 5t




161.584
160.052
153.081
149.500
140.826
136.948
135.253
132.304
130.408
130.265
128.819
128.244
127.756
127.440
123.878
121.389
118.354
118.076
113.059
107.448
77.230
77.019
76.809
69.580
60.972
56.357
0.000
CN
N
O
Exact Mass: 519.1907
(thousandths)
X : parts per Million : Carbon13

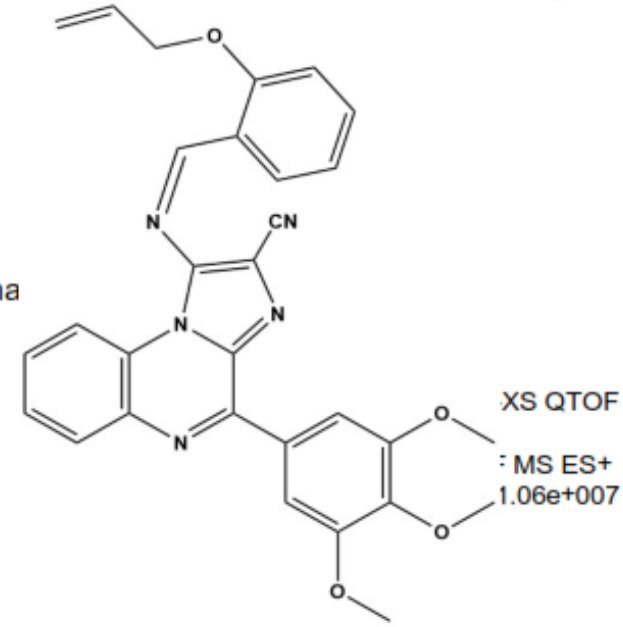
Elemental Composition Report

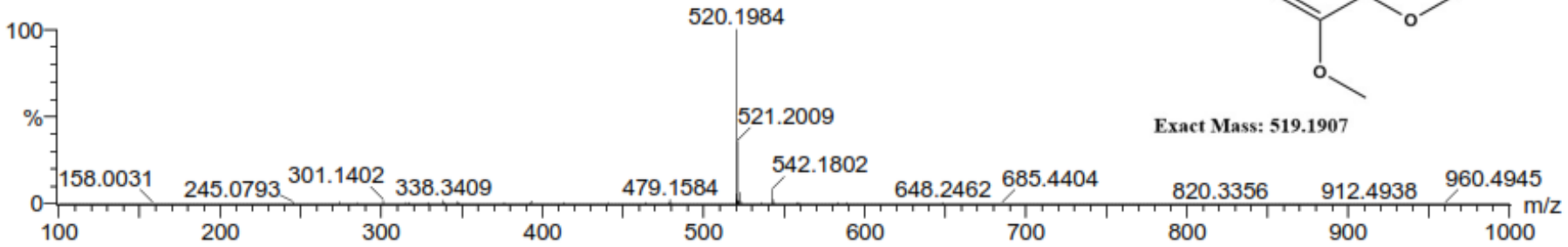
Single Mass Analysis

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
675 formula(e) evaluated with 3 results within limits (up to 1 closest results for each ma
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10

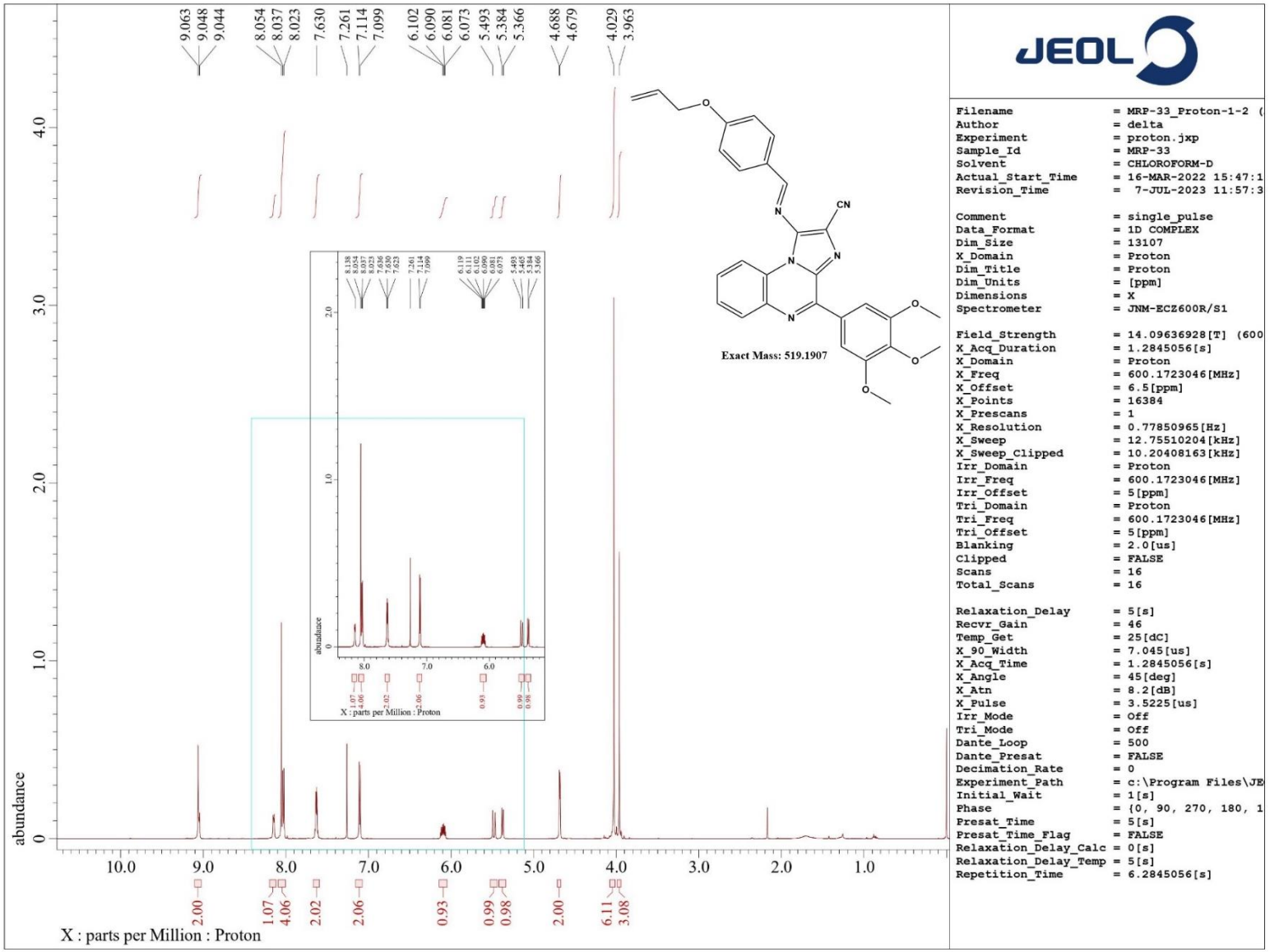
Sample Name : MRP_32 IITRPR XS QTOF
Test Name :
260522_MRP_32 20 (0.223) : MS ES+
1.06e+007





Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
520.1984	520.1985	-0.1	-0.2	20.5	1203.9	n/a	n/a	C30 H26 N5 O4

Spectral data of compound 5u

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Filename              = MRP-33_Proton-1-2 (
Author                = delta
Experiment            = proton.jxp
Sample_Id             = MRP-33
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 16-MAR-2022 15:47:1
Revision_Time         =  7-JUL-2023 11:57:3

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S1

Field_Strength        = 14.09636928[T] (600
X_Acq_Duration        = 1.2845056[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 6.5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.77850965[Hz]
X_Sweep               = 12.75510204[kHz]
X_Sweep_Clipped       = 10.20408163[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2.0[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 46
Temp_Get              = 25[dC]
X_90_Width            = 7.045[us]
X_Acq_Time            = 1.2845056[s]
X_Angle               = 45[deg]
X_Atn                 = 8.2[dB]
X_Pulse               = 3.5225[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JE
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 1
Presat_Time           = 5[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time       = 6.2845056[s]
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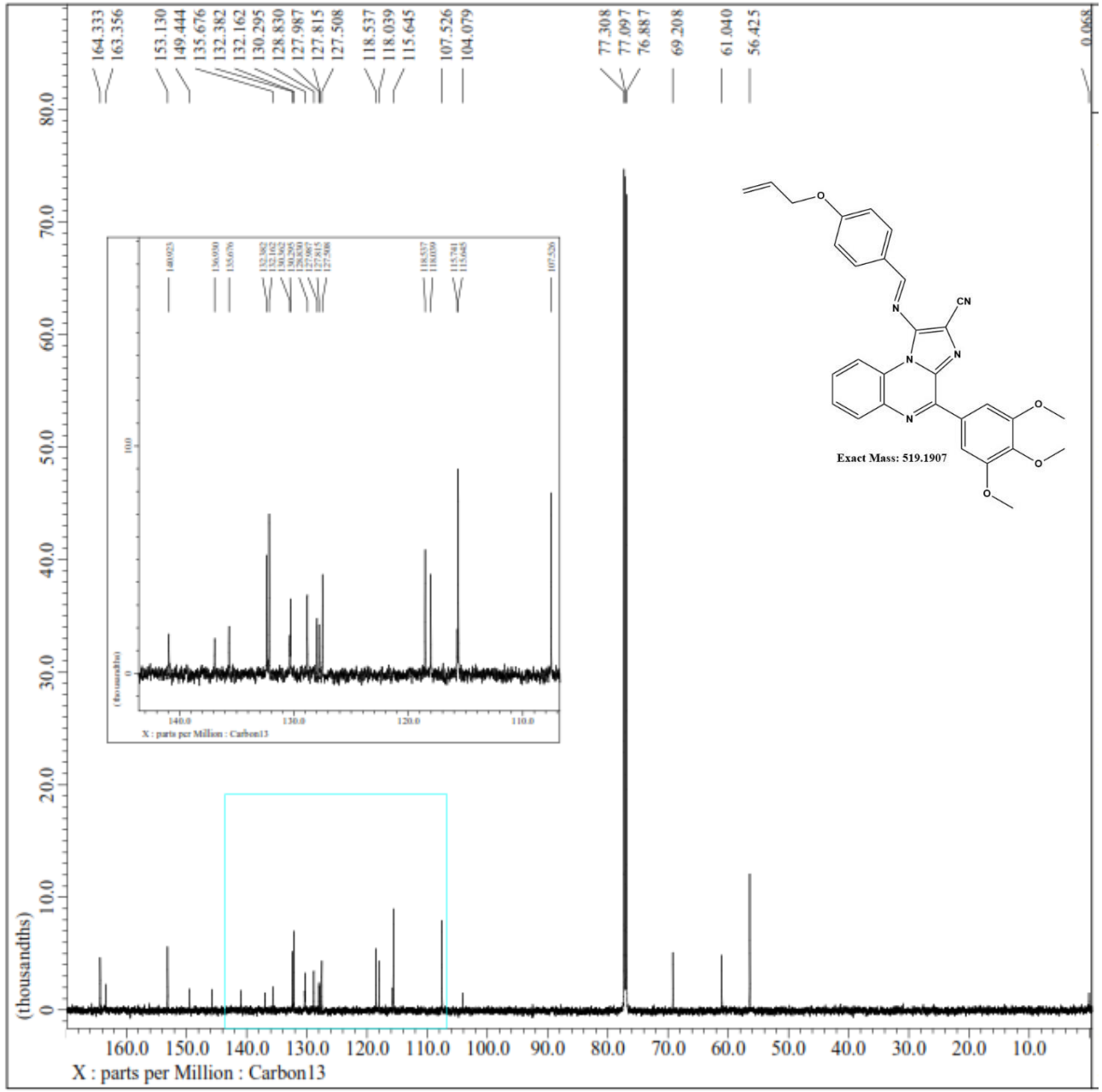

164.333
163.356
153.130
149.444
135.676
132.382
132.162
130.295
128.830
127.987
127.815
127.508
118.537
118.039
115.645
107.526
104.079
77.308
77.097
76.887
69.208
61.040
56.425
0.068
(thousandths)
X : parts per Million : Carbon13
Exact Mass: 519.1907
CN
O
N

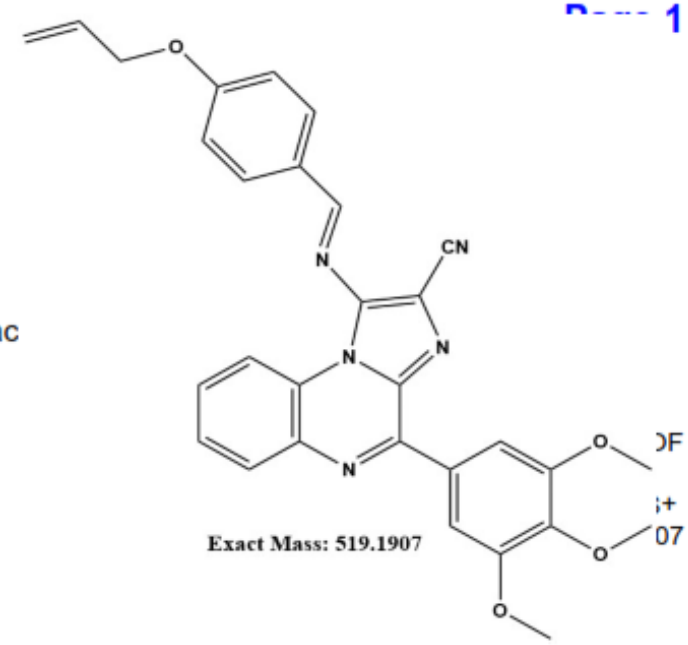
Elemental Composition Report

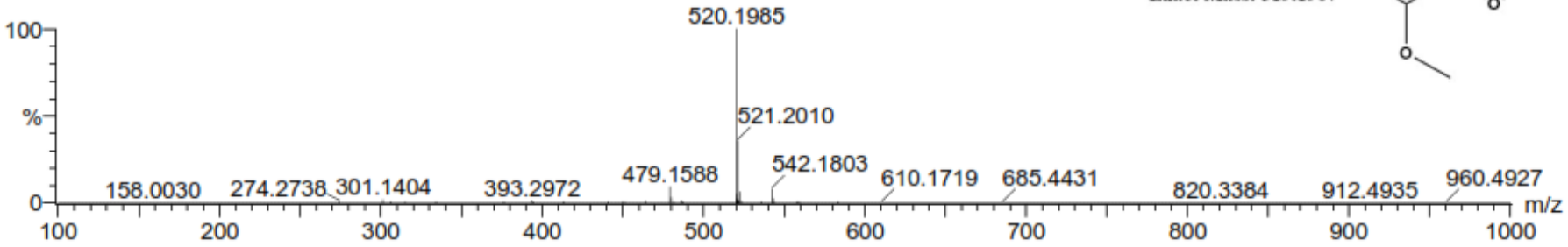
Single Mass Analysis

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
675 formula(e) evaluated with 3 results within limits (up to 1 closest results for eac
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10

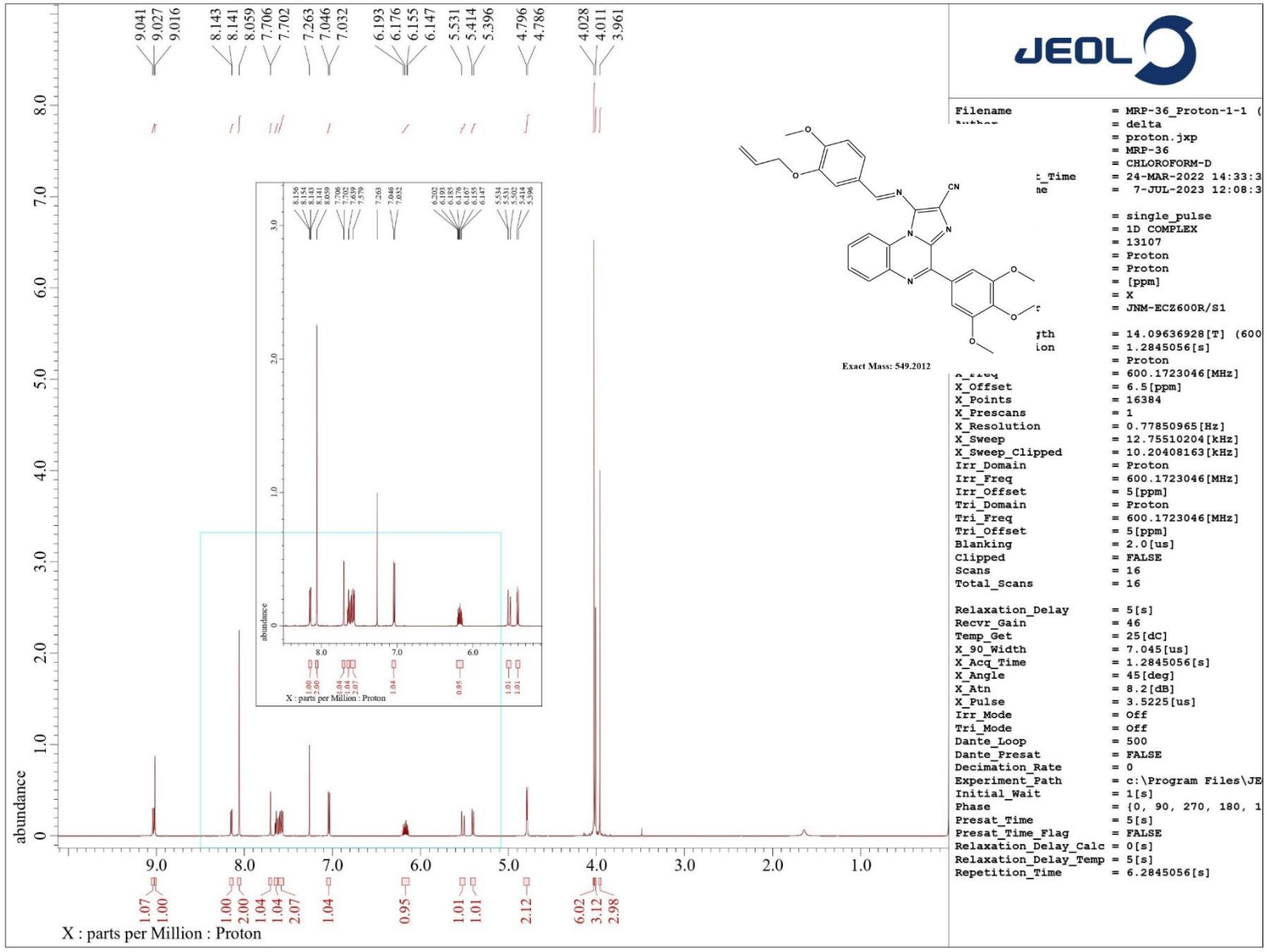
Sample Name : 260522_MRP_33 IITRPR
Test Name :
260522_MRP_33 23 (0.248)

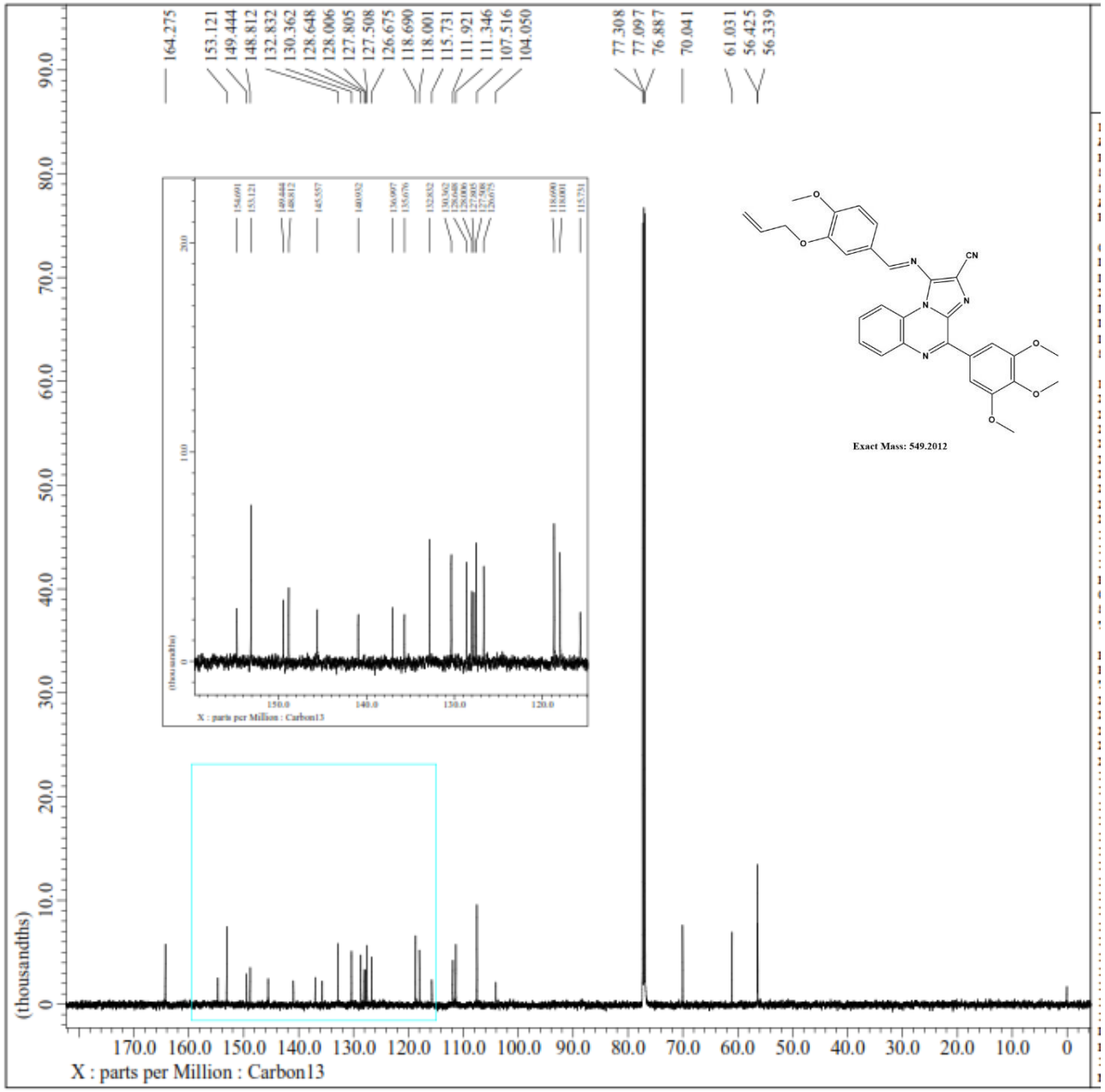




Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
520.1985	520.1985	0.0	0.0	20.5	1215.6	n/a	n/a	C30 H26 N5 O4

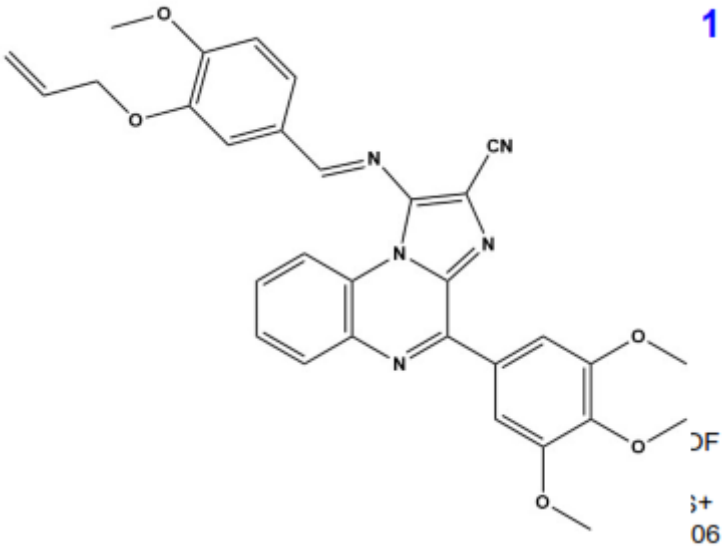
Spectral data of compound 5v




164.275
153.121
149.444
148.812
132.832
130.362
128.648
128.006
127.805
127.508
126.675
118.690
118.001
115.731
111.921
111.346
107.516
104.050
77.308
77.097
76.887
70.041
61.031
56.425
56.339
Exact Mass: 549.2012
(thousandths)
X : parts per Million : Carbon13

Elemental Composition Report

1



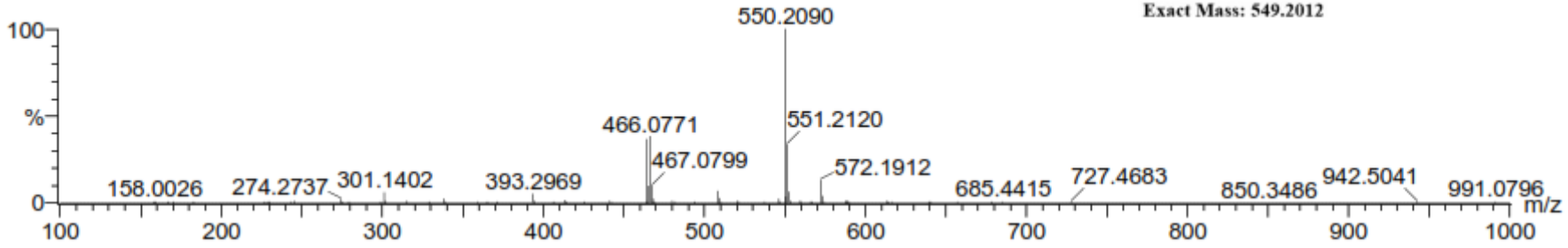
Exact Mass: 549.2012

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

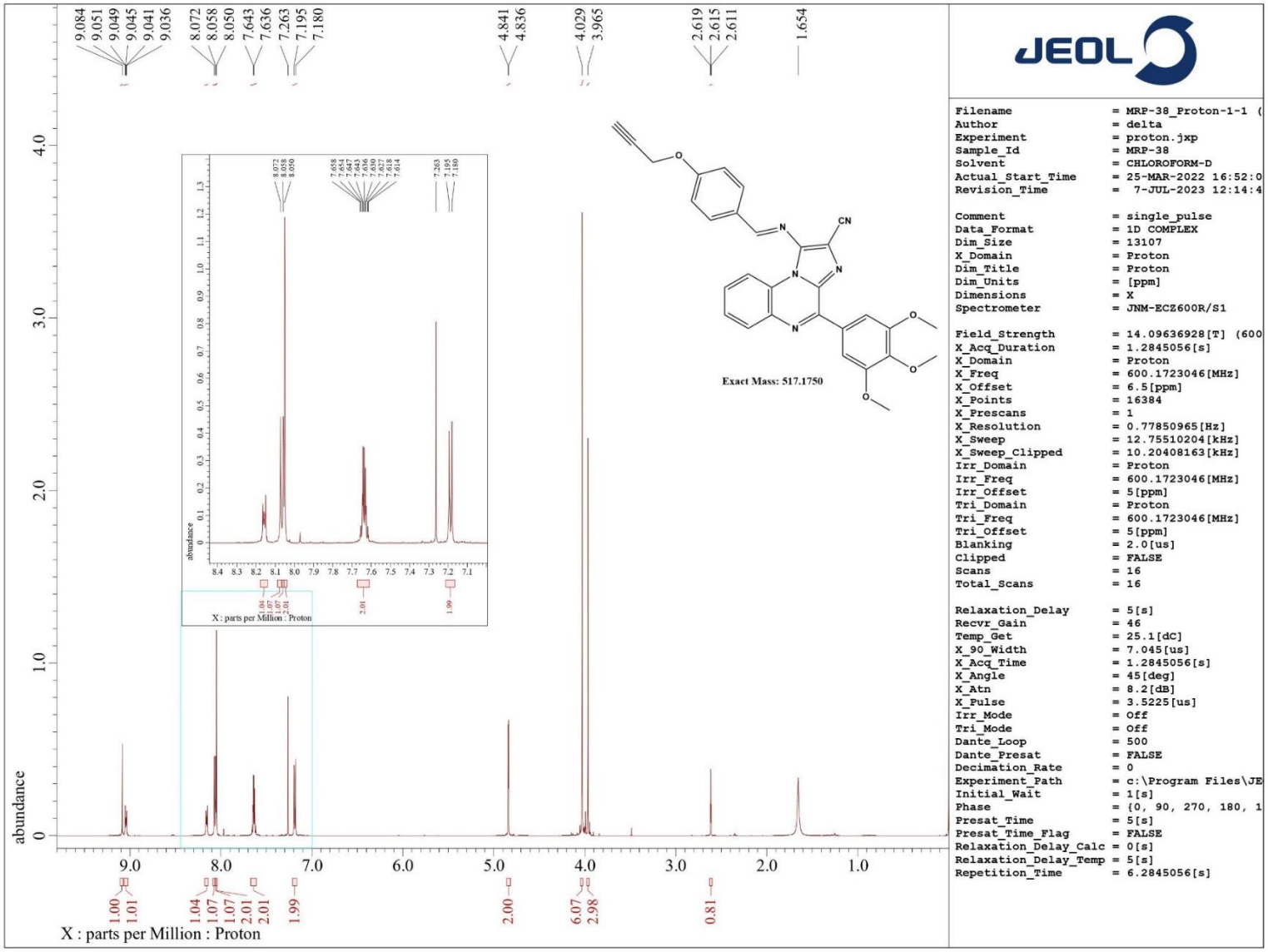
Monoisotopic Mass, Even Electron Ions
721 formula(e) evaluated with 3 results within limits (up to 1 closest results fo
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10

Sample Name : 260522_MRP_36 IITRPR
Test Name :
260522_MRP_36 24 (0.257)



Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
550.2090	550.2090	0.0	0.0	20.5	1050.6	n/a	n/a	C31 H28 N5 O5

Spectral data of compound 5w

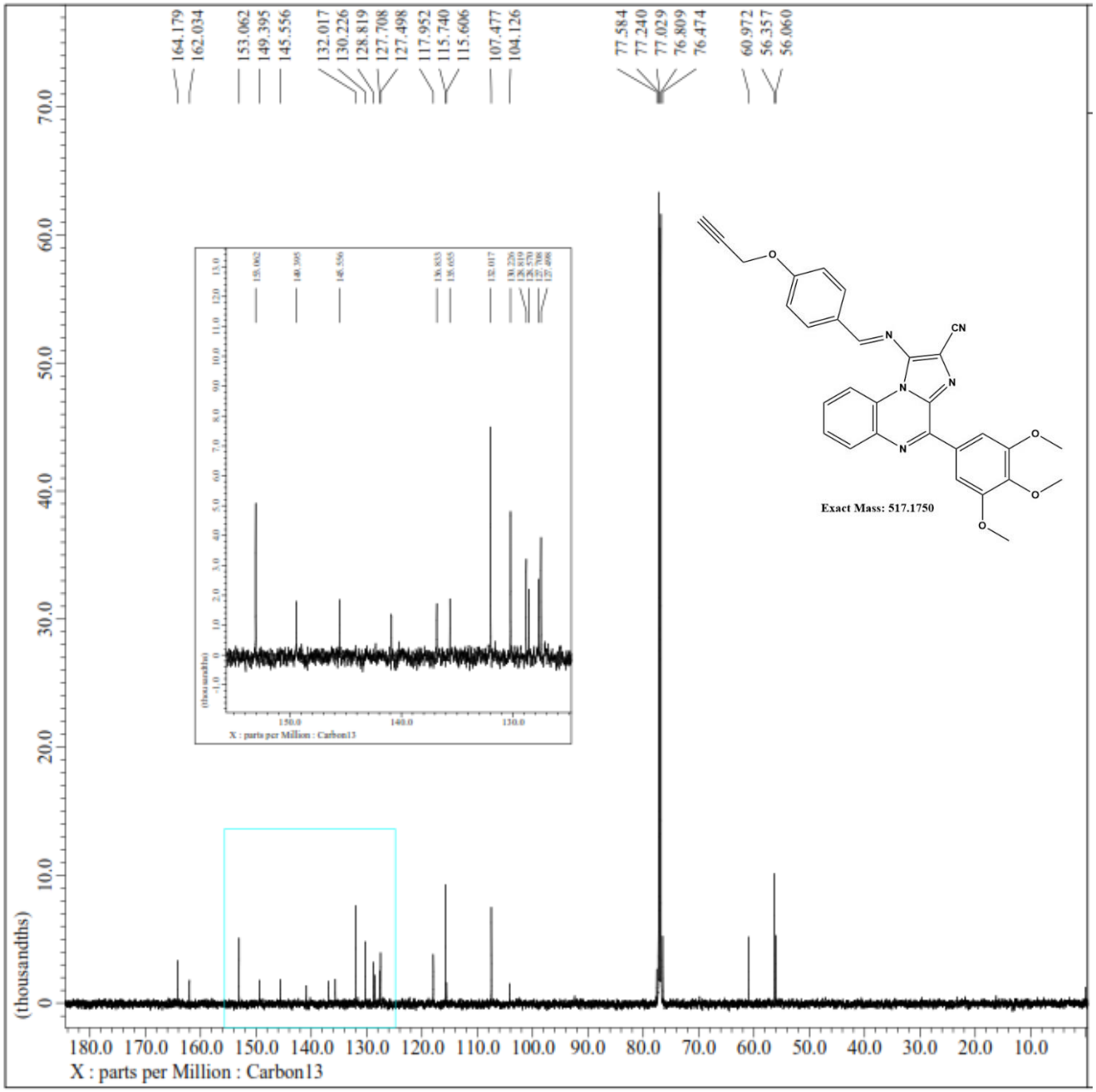



```
Filename              = MRP-38_Proton-1-1 (
Author                = delta
Experiment            = proton.jxp
Sample_Id             = MRP-38
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-MAR-2022 16:52:0
Revision_Time         =  7-JUL-2023 12:14:4

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S1

Field_Strength        = 14.09636928[T] (600
X_Acq_Duration        = 1.2845056[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 6.5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.77850965[Hz]
X_Sweep               = 12.75510204[kHz]
X_Sweep_Clipped       = 10.20408163[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2.0[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 46
Temp_Get              = 25.1[dC]
X_90_Width            = 7.045[us]
X_Acq_Time            = 1.2845056[s]
X_Angle               = 45[deg]
X_Atn                 = 8.2[dB]
X_Pulse               = 3.5225[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JE
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 1
Presat_Time           = 5[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time       = 6.2845056[s]
```

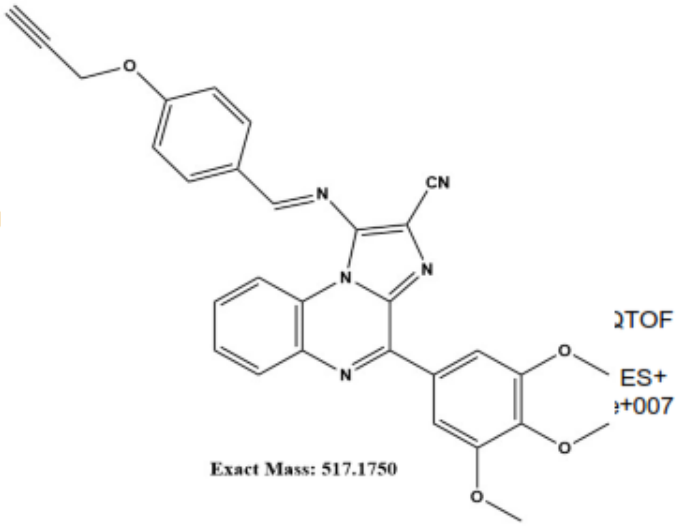

164.179
162.034
153.062
149.395
145.556
132.017
130.226
128.819
127.708
127.498
117.952
115.740
115.606
107.477
104.126
77.584
77.240
77.029
76.809
76.474
60.972
56.357
56.060
(thousandths)
X : parts per Million : Carbon13
Exact Mass: 517.1750

Elemental Composition Report

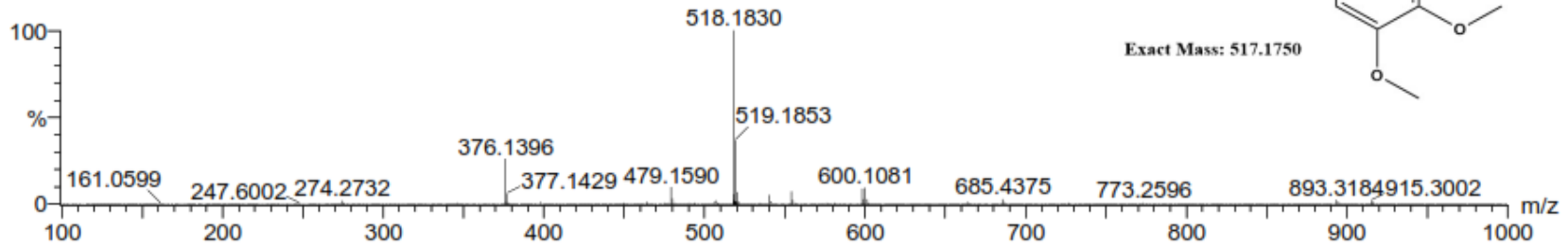
Single Mass Analysis

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
673 formula(e) evaluated with 3 results within limits (up to 1 closest results fo
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10

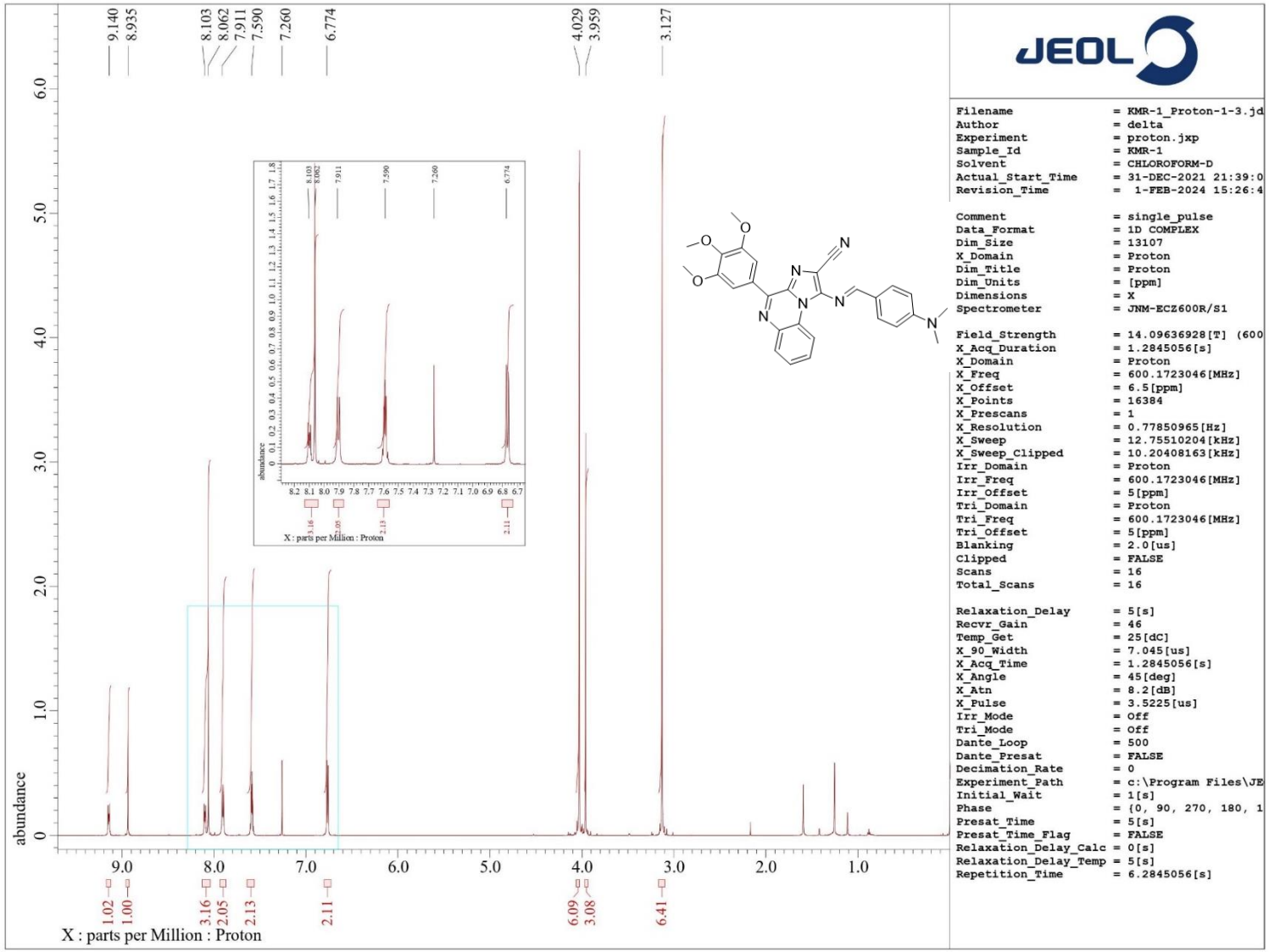


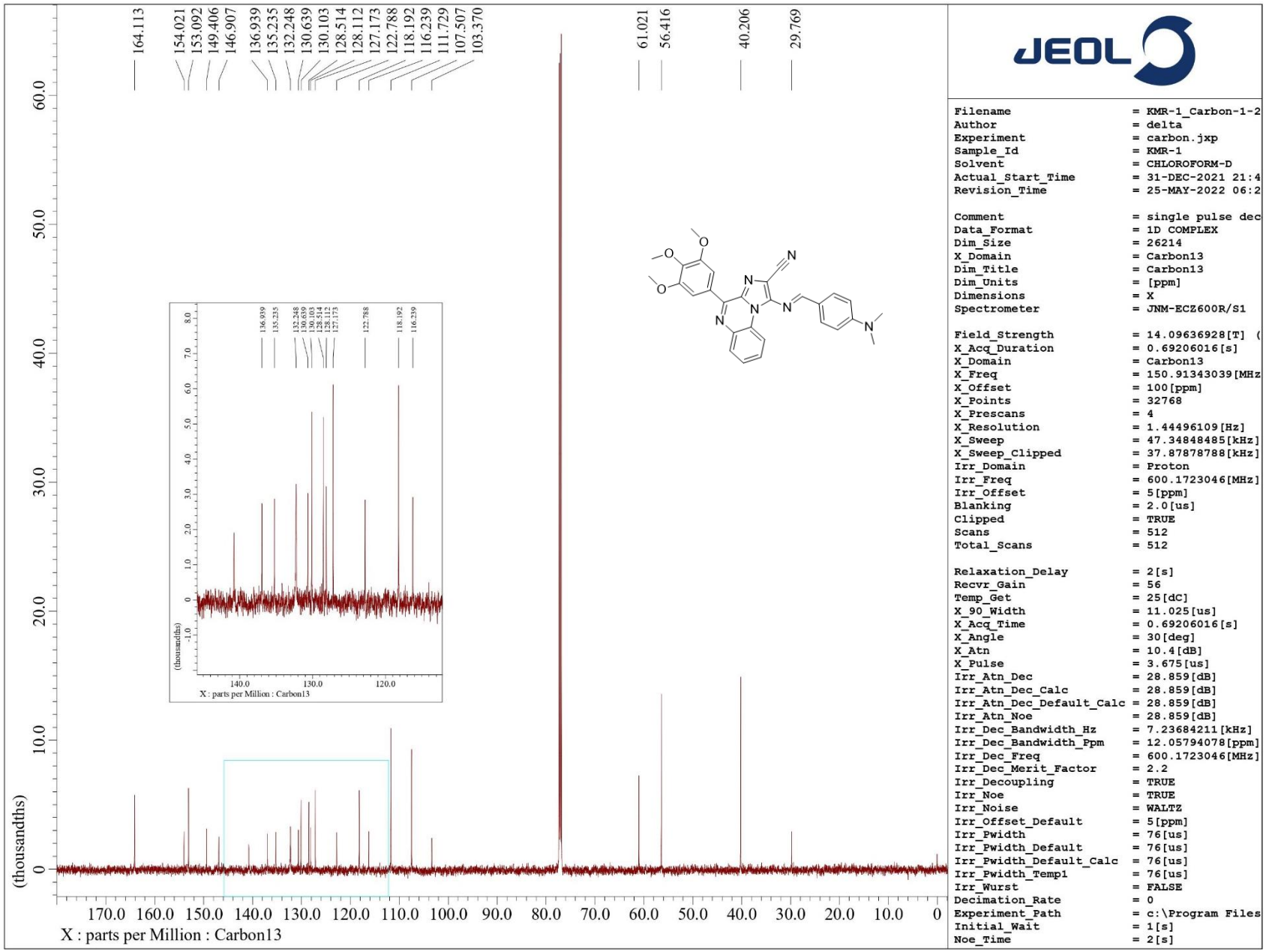
Sample Name : 260522_MRP_38 IITRPR QTOF
Test Name :
260522_MRP_38 16 (0.177) ES+
+007



Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
518.1830	518.1828	0.2	0.4	21.5	767.7	n/a	n/a	C30 H24 N5 O4

SPECTRAL DATA OF 5x

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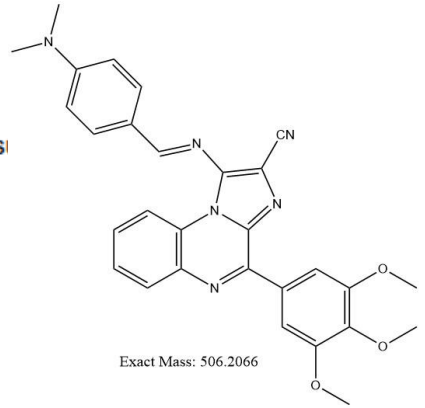
154.021
153.092
149.406
146.907
136.939
135.235
132.248
130.639
130.103
128.514
128.112
127.173
122.788
118.192
116.239
111.729
107.507
103.370
61.021
56.416
40.206
29.769
(thousandths)
X : parts per Million : Carbon13
Filename = KMR-1_Carbon-1-2
Author = delta
Experiment = carbon.jxp
Sample_Id = KMR-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-DEC-2021 21:4
Revision_Time = 25-MAY-2022 06:2
Comment = single pulse dec
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T] (
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = TRUE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 25[dC]
X_90_Width = 11.025[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 10.4[dB]
X_Pulse = 3.675[us]
Irr_Atn_Dec = 28.859[dB]
Irr_Atn_Dec_Calc = 28.859[dB]
Irr_Atn_Dec_Default_Calc = 28.859[dB]
Irr_Atn_Noe = 28.859[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files
Initial_Wait = 1[s]
Noe_Time = 2[s]

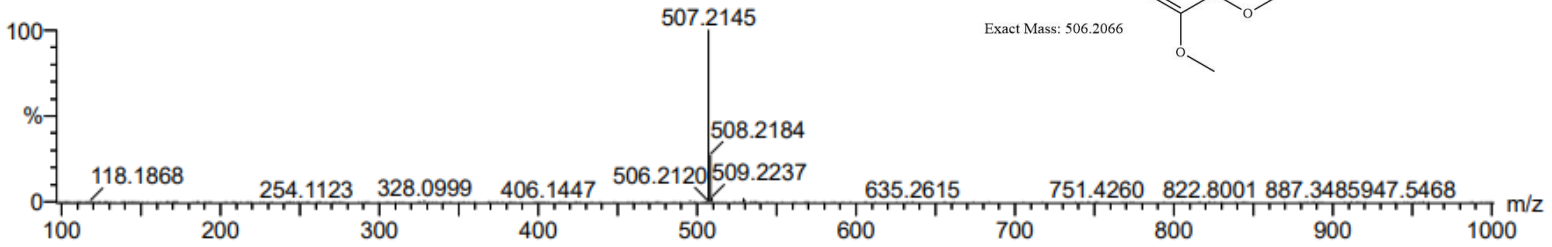
Single Mass Analysis

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
1281 formula(e) evaluated with 11 results within limits (up to 1 closest resu
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 S: 0-3

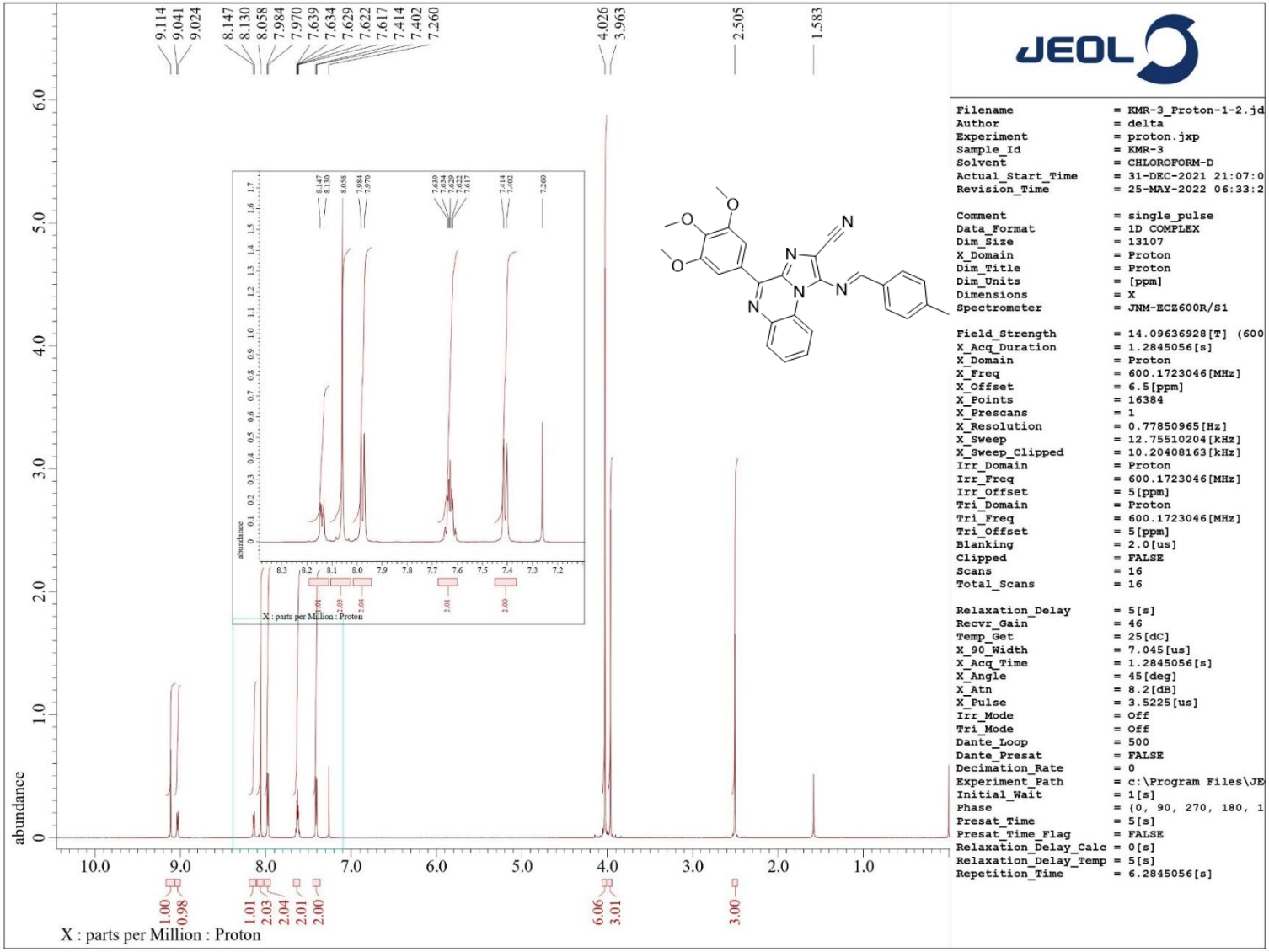
Sample Name : KMR_1 IITRPR XEVO G2-XS QTOF
Test Name :
23032022_KMR_1 12 (0.265) 1: TOF MS ES+
6.25e+005

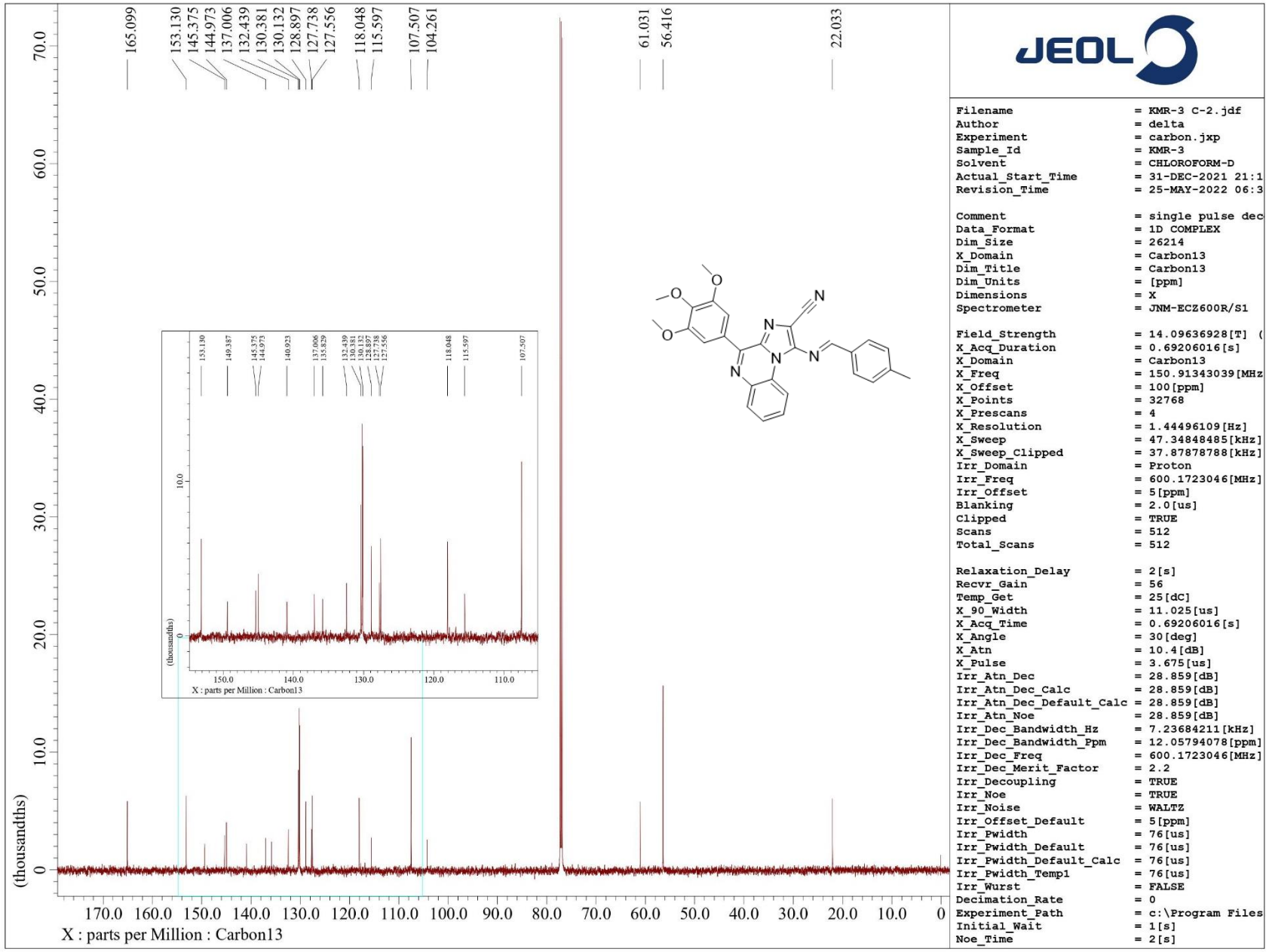




Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
507.2145	507.2145	0.0	0.0	19.5	50.4	n/a	n/a	C29 H27 N6 O3

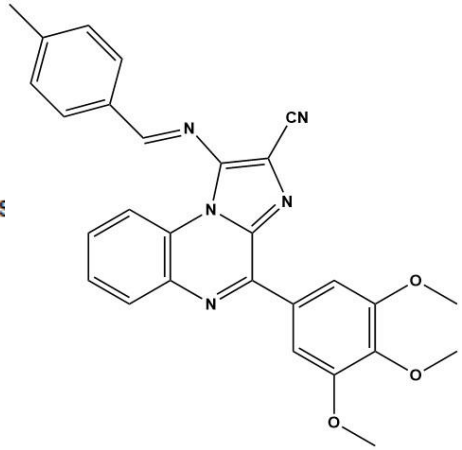
SPECTRAL DATA OF 5y




165.099
153.130
145.375
144.973
137.006
132.439
130.381
130.132
128.897
127.738
127.556
118.048
115.597
107.507
104.261
61.031
56.416
22.033
(thousandths)
X : parts per Million : Carbon13
Filename = KMR-3 C-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = KMR-3
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-DEC-2021 21:1
Revision_Time = 25-MAY-2022 06:3
Comment = single pulse dec
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T] (
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = TRUE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 25[dC]
X_90_Width = 11.025[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 10.4[dB]
X_Pulse = 3.675[us]
Irr_Atn_Dec = 28.859[dB]
Irr_Atn_Dec_Calc = 28.859[dB]
Irr_Atn_Dec_Default_Calc = 28.859[dB]
Irr_Atn_Noe = 28.859[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files
Initial_Wait = 1[s]
Noe_Time = 2[s]

Single Mass Analysis

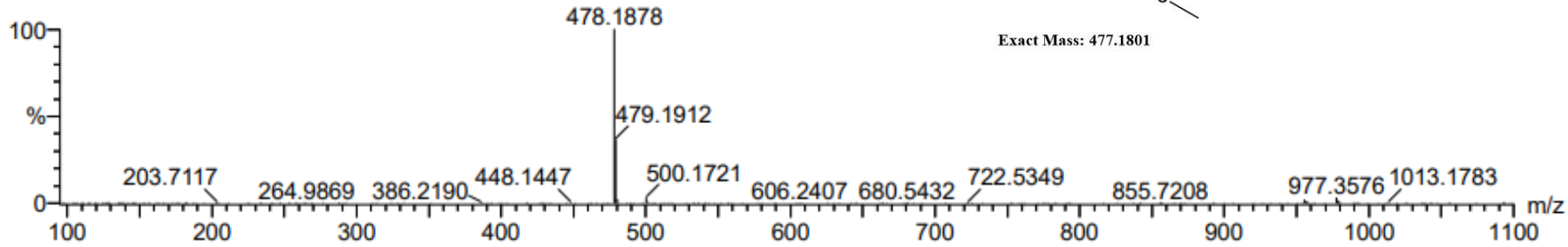
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 5



Exact Mass: 477.1801

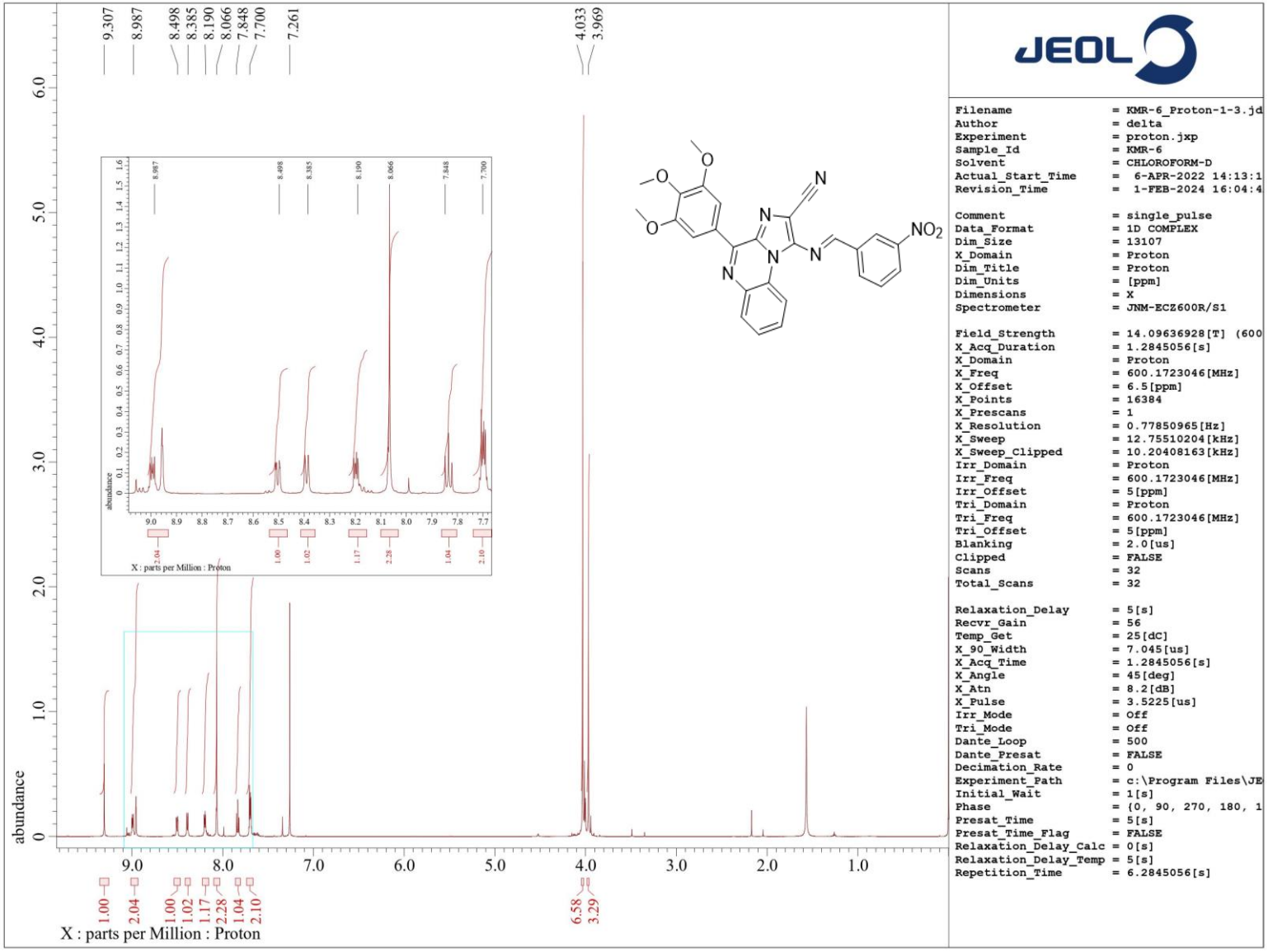
Monoisotopic Mass, Even Electron Ions
1169 formula(e) evaluated with 11 results within limits (up to 1 closest res
Elements Used:
C: 0-50 H: 0-100 N: 5-10 O: 0-10 S: 0-3

Sample Name : KMR_3 IITRPR XEVO G2-XS QTOF
Test Name :
23032022_KMR_3 19 (0.418) 1: TOF MS ES+
1.37e+006

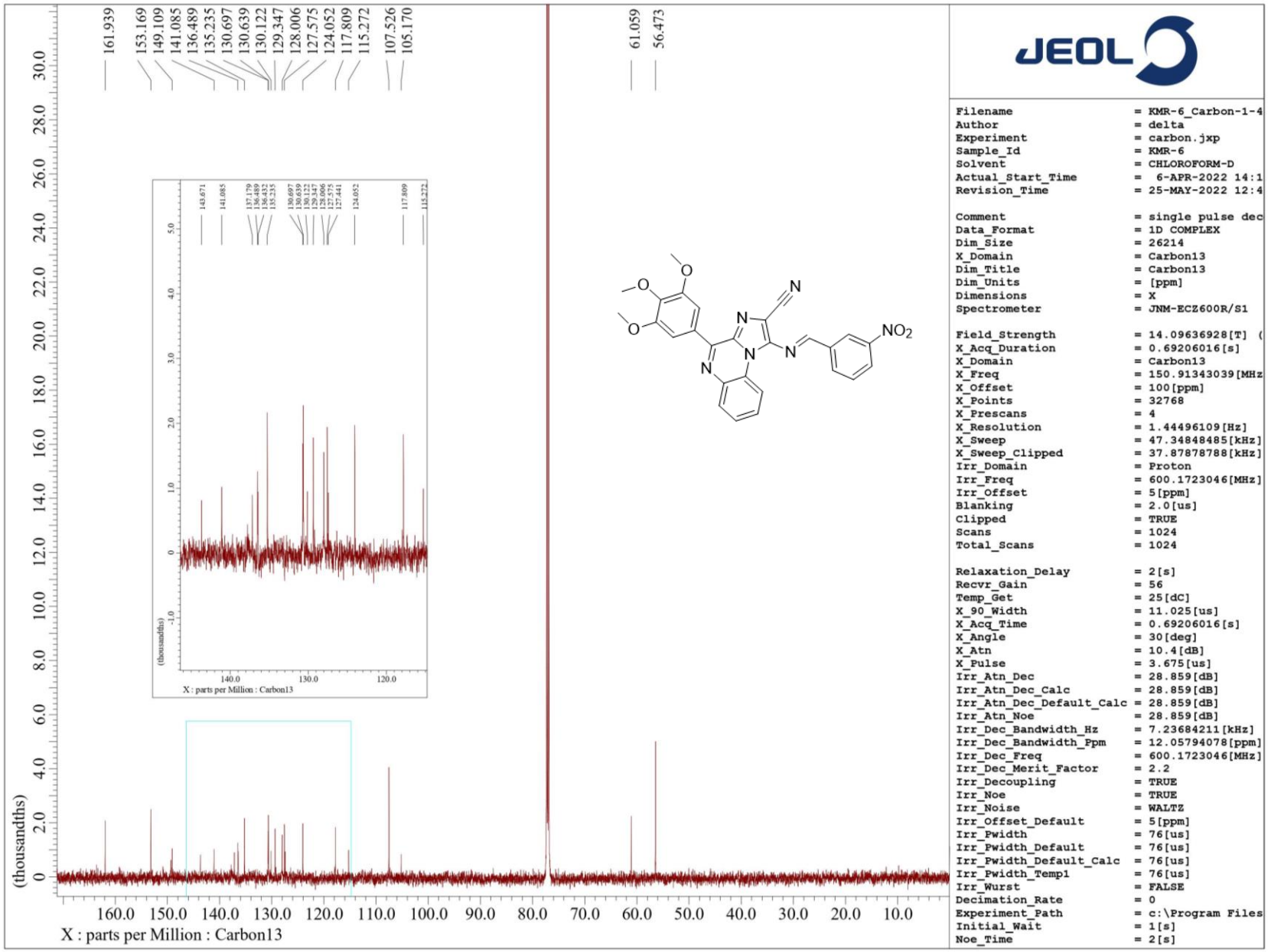


Minimum:				-1.5				
Maximum:		2.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
478.1878	478.1879	-0.1	-0.2	19.5	64.6	n/a	n/a	C28 H24 N5 O3

SPECTRAL DATA OF 5z



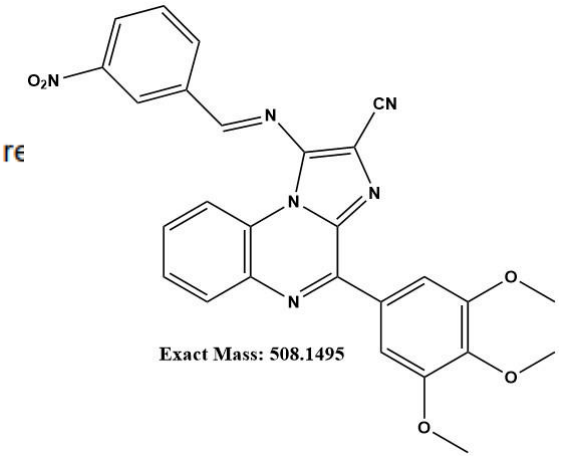

```
Filename              = KMR-6_Proton-1-3.jd
Author                = delta
Experiment            = proton.jxp
Sample_Id             = KMR-6
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  6-APR-2022 14:13:1
Revision_Time         =  1-FEB-2024 16:04:4

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S1

Field_Strength        = 14.09636928[T] (600
X_Acq_Duration        = 1.2845056[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 6.5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.77850965[Hz]
X_Sweep               = 12.75510204[kHz]
X_Sweep_Clipped       = 10.20408163[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2.0[us]
Clipped               = FALSE
Scans                 = 32
Total_Scans           = 32

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 25[dC]
X_90_Width            = 7.045[us]
X_Acq_Time            = 1.2845056[s]
X_Angle               = 45[deg]
X_Atn                 = 8.2[dB]
X_Pulse               = 3.5225[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JE
Initial_Wait          = 1[s]
Phase                 = (0, 90, 270, 180, 1
Presat_Time           = 5[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time       = 6.2845056[s]
```


161.939
153.169
149.109
141.085
136.489
135.235
130.697
130.639
130.122
129.347
128.006
127.575
124.052
117.809
115.272
107.526
105.170
61.059
56.473
(thousandths)
X : parts per Million : Carbon13
Filename = KMR-6_Carbon-1-4
Author = delta
Experiment = carbon.jxp
Sample_Id = KMR-6
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-APR-2022 14:1
Revision_Time = 25-MAY-2022 12:4
Comment = single pulse dec
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T]
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = TRUE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 25[dC]
X_90_Width = 11.025[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 10.4[dB]
X_Pulse = 3.675[us]
Irr_Atn_Dec = 28.859[dB]
Irr_Atn_Dec_Calc = 28.859[dB]
Irr_Atn_Dec_Default_Calc = 28.859[dB]
Irr_Atn_Noe = 28.859[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files
Initial_Wait = 1[s]
Noe_Time = 2[s]

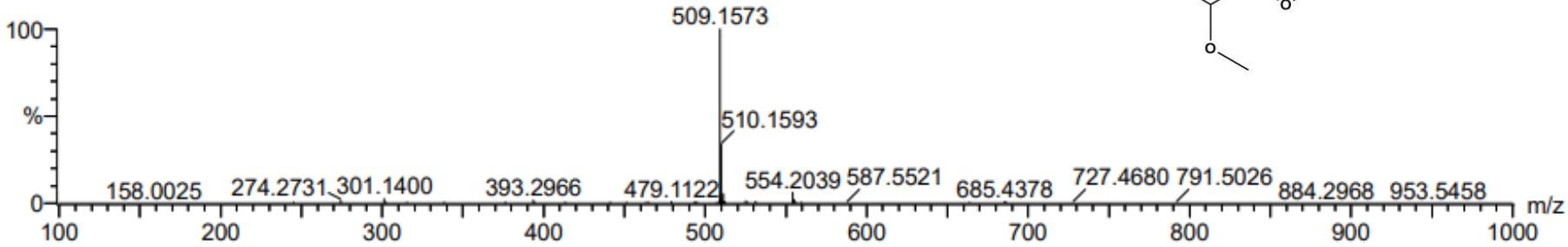
Single Mass Analysis

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
1869 formula(e) evaluated with 10 results within limits (up to 1 closest re
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10 S: 0-2

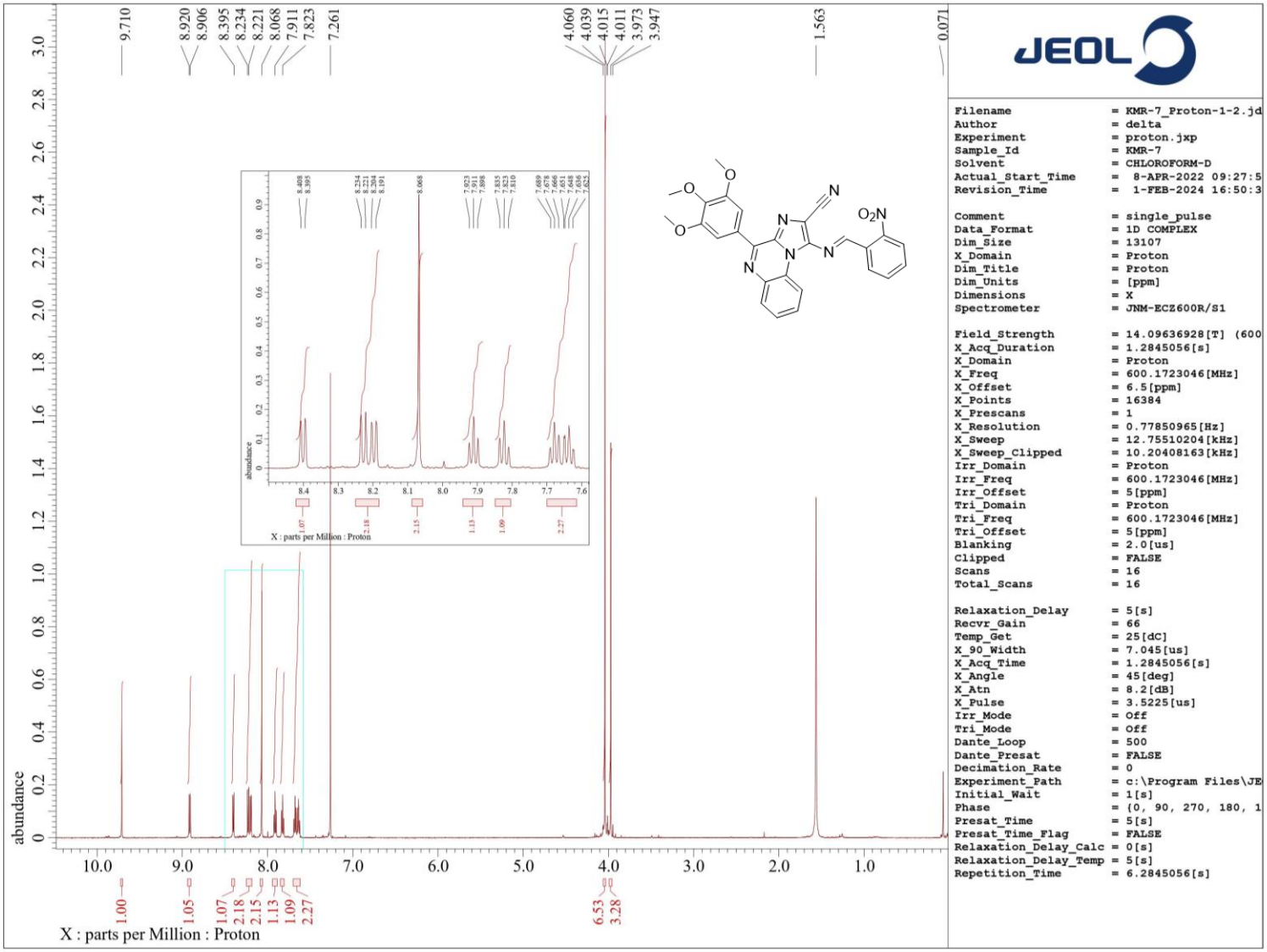


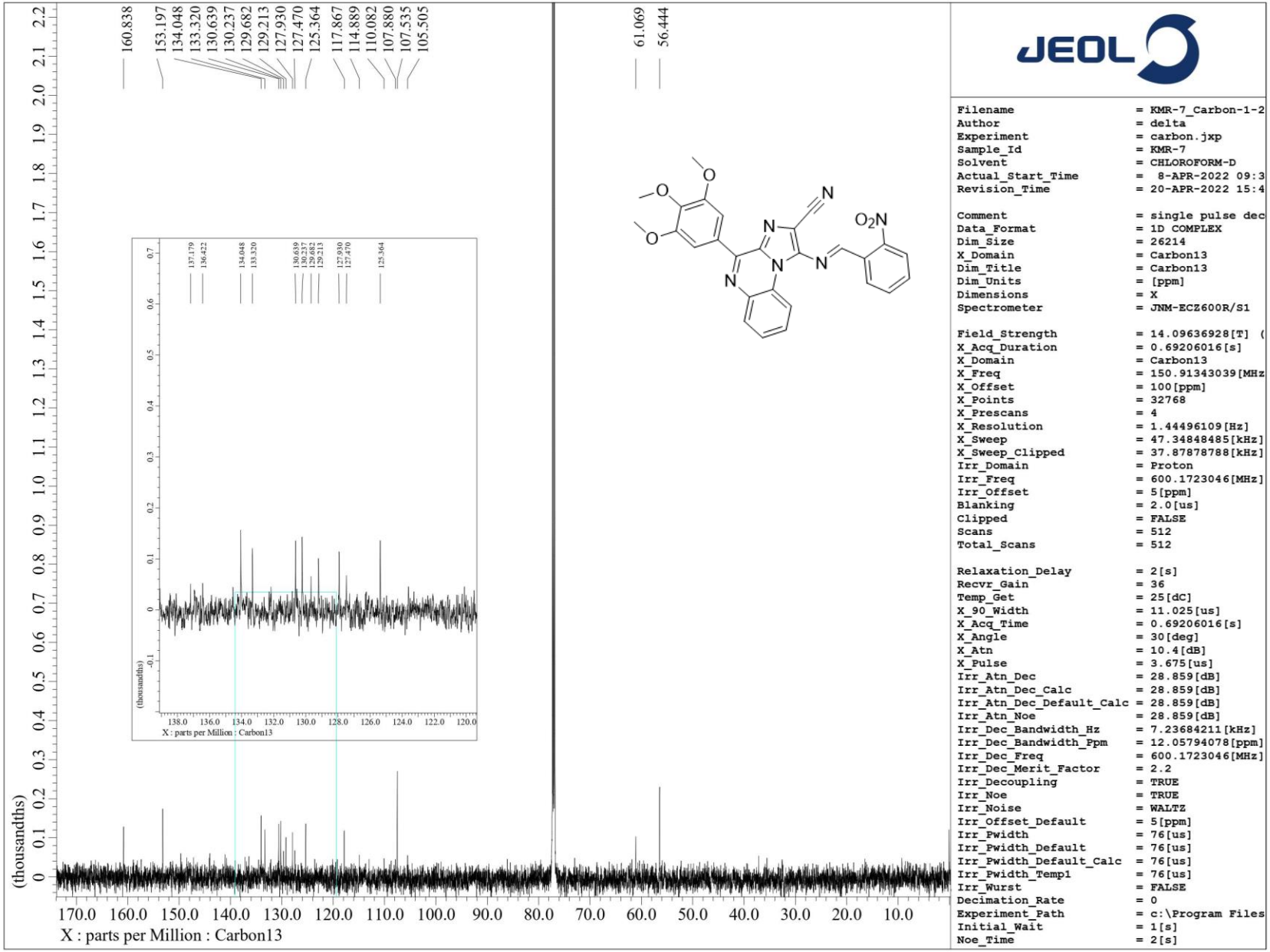
Sample Name : KMR_6 IITRPR XEVO G2-XS QTOF
Test Name :
260522_KMR_6 17 (0.197) 1: TOF MS ES+
1.09e+007



Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
509.1573	509.1573	0.0	0.0	20.5	1298.2	n/a	n/a	C27 H21 N6 O5

SPECTRAL DATA OF 5aa



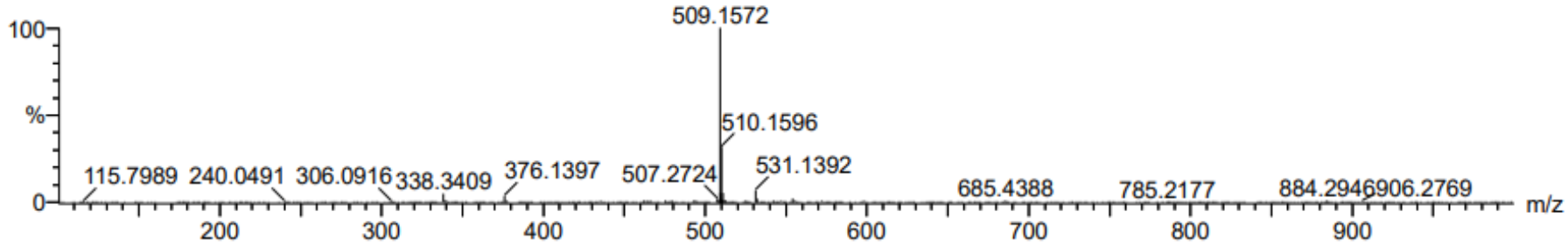

160.838
153.197
134.048
133.320
130.639
130.237
129.682
129.213
127.930
127.470
125.364
117.867
114.889
110.082
107.880
107.535
105.505
61.069
56.444
(thousandths)
X : parts per Million : Carbon13
Filename = KMR-7_Carbon-1-2
Author = delta
Experiment = carbon.jxp
Sample_Id = KMR-7
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-APR-2022 09:3
Revision_Time = 20-APR-2022 15:4
Comment = single pulse dec
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ600R/S1
Field_Strength = 14.09636928[T]
X_Acq_Duration = 0.69206016[s]
X_Domain = Carbon13
X_Freq = 150.91343039[MHz
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.44496109[Hz]
X_Sweep = 47.34848485[kHz]
X_Sweep_Clipped = 37.87878788[kHz]
Irr_Domain = Proton
Irr_Freq = 600.1723046[MHz]
Irr_Offset = 5[ppm]
Blanking = 2.0[us]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2[s]
Recvr_Gain = 36
Temp_Get = 25[dC]
X_90_Width = 11.025[us]
X_Acq_Time = 0.69206016[s]
X_Angle = 30[deg]
X_Atn = 10.4[dB]
X_Pulse = 3.675[us]
Irr_Atn_Dec = 28.859[dB]
Irr_Atn_Dec_Calc = 28.859[dB]
Irr_Atn_Dec_Default_Calc = 28.859[dB]
Irr_Atn_Noe = 28.859[dB]
Irr_Dec_Bandwidth_Hz = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm = 12.05794078[ppm]
Irr_Dec_Freq = 600.1723046[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 76[us]
Irr_Pwidth_Default = 76[us]
Irr_Pwidth_Default_Calc = 76[us]
Irr_Pwidth_Temp1 = 76[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files
Initial_Wait = 1[s]
Noe_Time = 2[s]

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

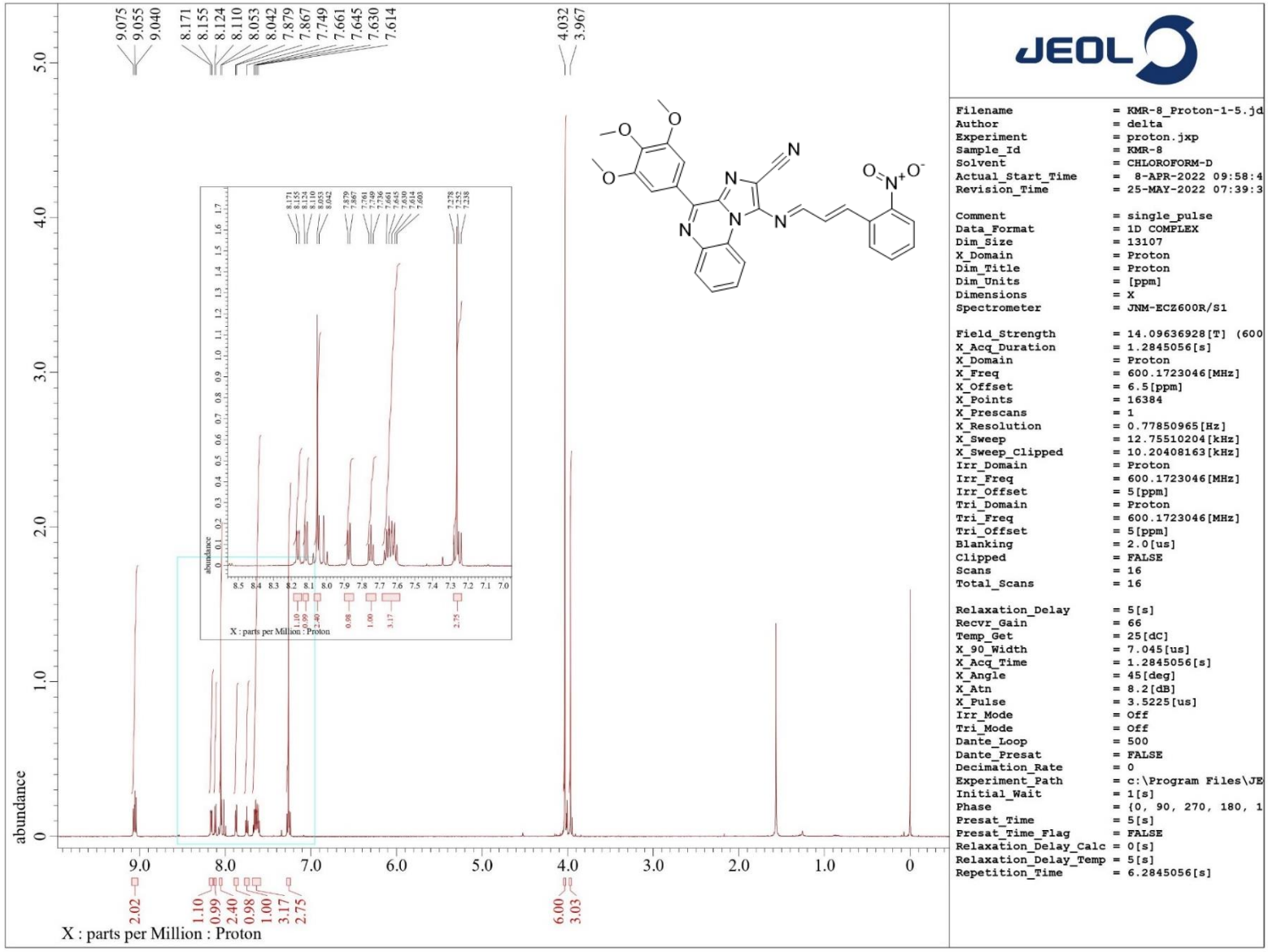
Monoisotopic Mass, Even Electron Ions
1869 formula(e) evaluated with 10 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10 S: 0-2

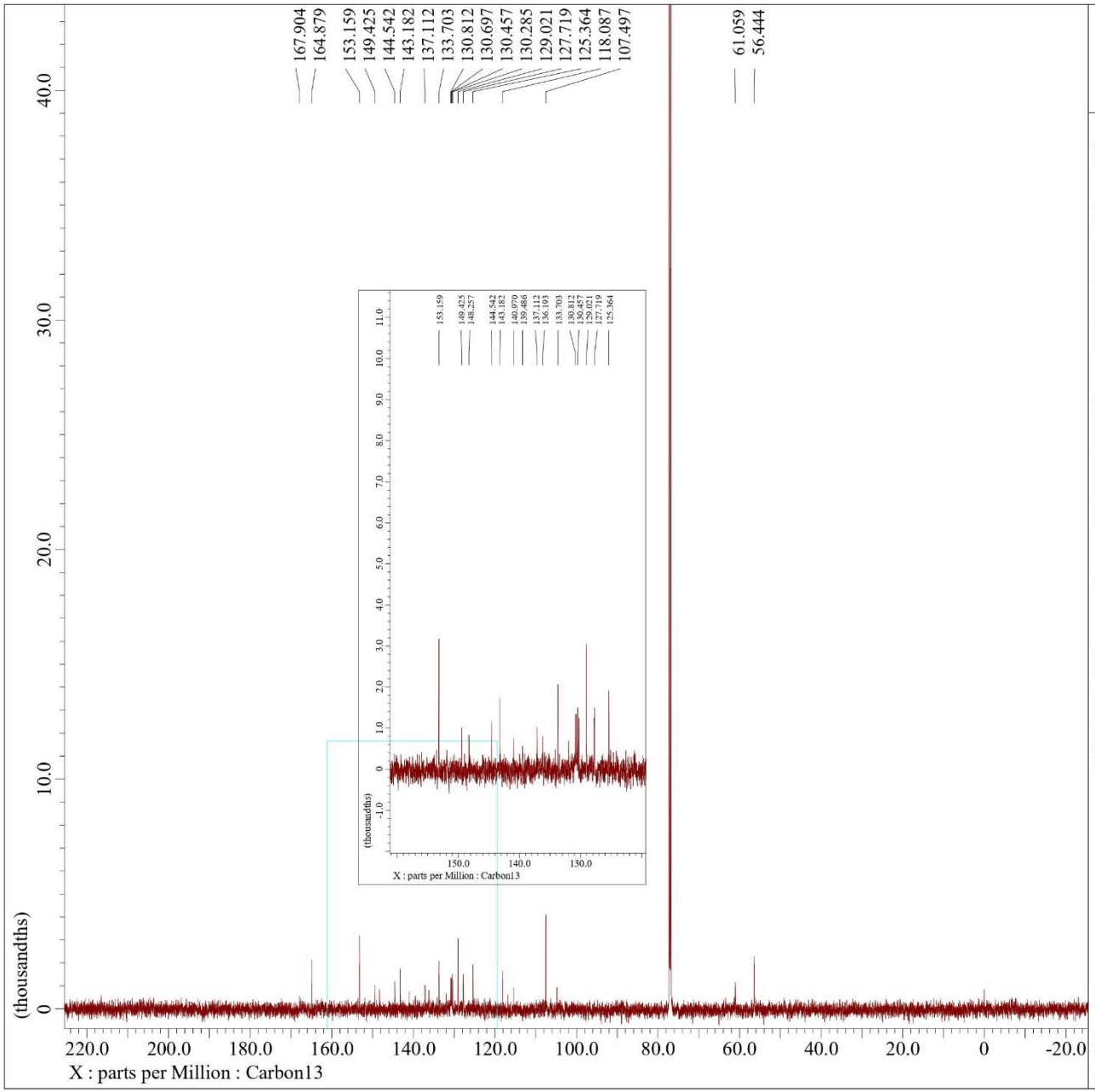
Sample Name : KMR_7 IITRPR XEVO G2-XS QTOF
Test Name :
260522_KMR_7 16 (0.177) 1: TOF MS ES+
2.14e+007



Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
509.1572	509.1573	-0.1	-0.2	20.5	673.0	n/a	n/a	C27 H21 N6 O5

SPECTRAL DATA OF 5ab

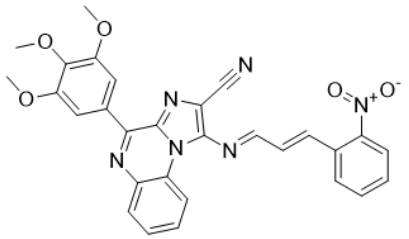




Filename	= KMR-8_Carbon NMR
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= KMR-8
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 8-APR-2022 10:0
Revision_Time	= 18-MAY-2022 12:1
Comment	= single pulse dec
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon13
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Spectrometer	= JNM-ECZ600R/S1
Field_Strength	= 14.09636928[T] (
X_Acq_Duration	= 0.69206016[s]
X_Domain	= Carbon13
X_Freq	= 150.91343039[MHz
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.44496109[Hz]
X_Sweep	= 47.34848485[kHz]
X_Sweep_Clipped	= 37.87878788[kHz]
Irr_Domain	= Proton
Irr_Freq	= 600.1723046[MHz]
Irr_Offset	= 5[ppm]
Blanking	= 2.0[us]
Clipped	= TRUE
Scans	= 512
Total_Scans	= 512
Relaxation_Delay	= 2[s]
Recvr_Gain	= 56
Temp_Get	= 25[dC]
X_90_Width	= 11.025[us]
X_Acq_Time	= 0.69206016[s]
X_Angle	= 30[deg]
X_Atn	= 10.4[dB]
X_Pulse	= 3.675[us]
Irr_Atn_Dec	= 28.859[dB]
Irr_Atn_Dec_Calc	= 28.859[dB]
Irr_Atn_Dec_Default_Calc	= 28.859[dB]
Irr_Atn_Noe	= 28.859[dB]
Irr_Dec_Bandwidth_Hz	= 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm	= 12.05794078[ppm]
Irr_Dec_Freq	= 600.1723046[MHz]
Irr_Dec_Merit_Factor	= 2.2
Irr_Decoupling	= TRUE
Irr_Noe	= TRUE
Irr_Noise	= WALTZ
Irr_Offset_Default	= 5[ppm]
Irr_Pwidth	= 76[us]
Irr_Pwidth_Default	= 76[us]
Irr_Pwidth_Default_Calc	= 76[us]
Irr_Pwidth_Temp1	= 76[us]
Irr_Wurst	= FALSE
Decimation_Rate	= 0
Experiment_Path	= c:\Program Files
Initial_Wait	= 1[s]
Noe_Time	= 2[s]

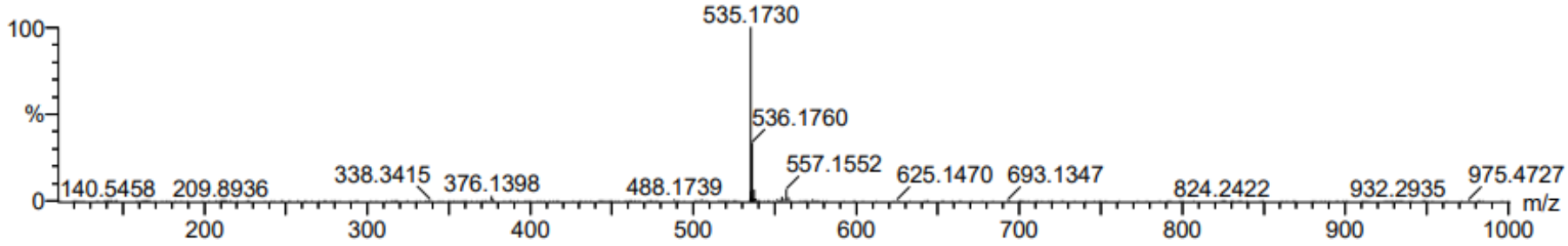
Single Mass Analysis

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



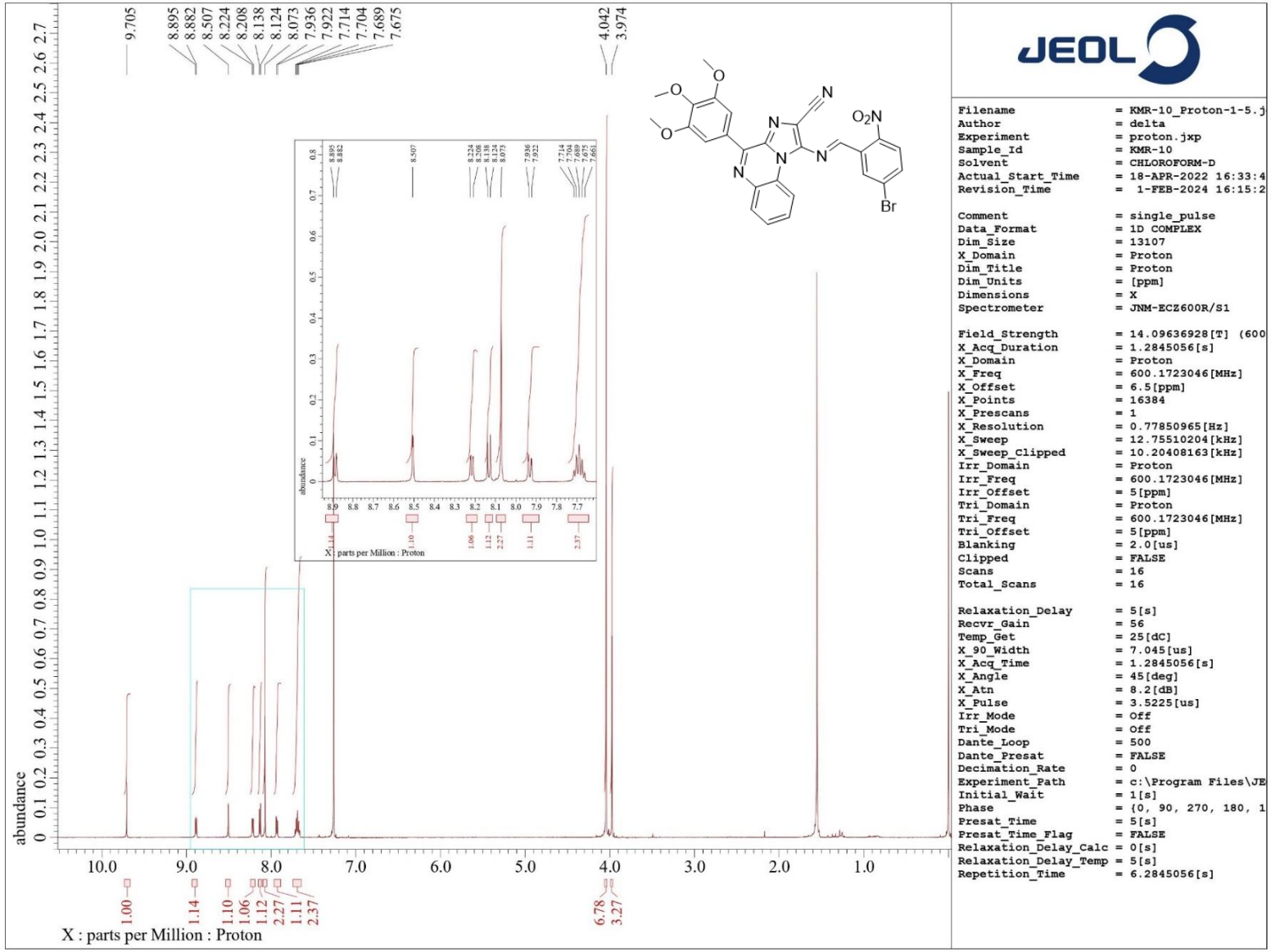
Monoisotopic Mass, Even Electron Ions
1975 formula(e) evaluated with 10 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10 S: 0-2

Sample Name : KMR_8 IITRPR XEVO G2-XS QTOF
Test Name :
260522_KMR_8 19 (0.214) 1: TOF MS ES+
1.44e+007



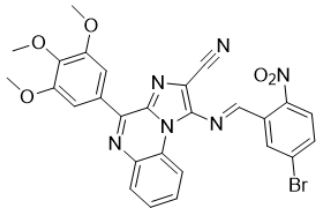
Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
535.1730	535.1730	0.0	0.0	21.5	451.5	n/a	n/a	C29 H23 N6 O5

SPECTRAL DATA OF 5ac




```
Filename              = KMR-10_Proton-1-5.j
Author                = delta
Experiment            = proton.jxp
Sample_Id             = KMR-10
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 18-APR-2022 16:33:4
Revision_Time         =  1-FEB-2024 16:15:2

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
X_Domain              = Proton
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ600R/S1

Field_Strength        = 14.09636928[T] (600
X_Acq_Duration        = 1.2845056[s]
X_Domain              = Proton
X_Freq                = 600.1723046[MHz]
X_Offset              = 6.5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.77850965[Hz]
X_Sweep               = 12.75510204[kHz]
X_Sweep_clipped       = 10.20408163[kHz]
Irr_Domain            = Proton
Irr_Freq              = 600.1723046[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 600.1723046[MHz]
Tri_Offset            = 5[ppm]
Blanking              = 2.0[us]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 25[dC]
X_90_Width            = 7.045[us]
X_Acq_Time            = 1.2845056[s]
X_Angle               = 45[deg]
X_Atn                 = 8.2[dB]
X_Pulse               = 3.5225[us]
Irr_Mode              = Off
Tri_Mode              = Off
Dante_Loop            = 500
Dante_Presat          = FALSE
Decimation_Rate       = 0
Experiment_Path       = c:\Program Files\JE
Initial_Wait          = 1[s]
Phase                 = {0, 90, 270, 180, 1
Presat_Time           = 5[s]
Presat_Time_Flag      = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time       = 6.2845056[s]
```

Elemental Composition Report

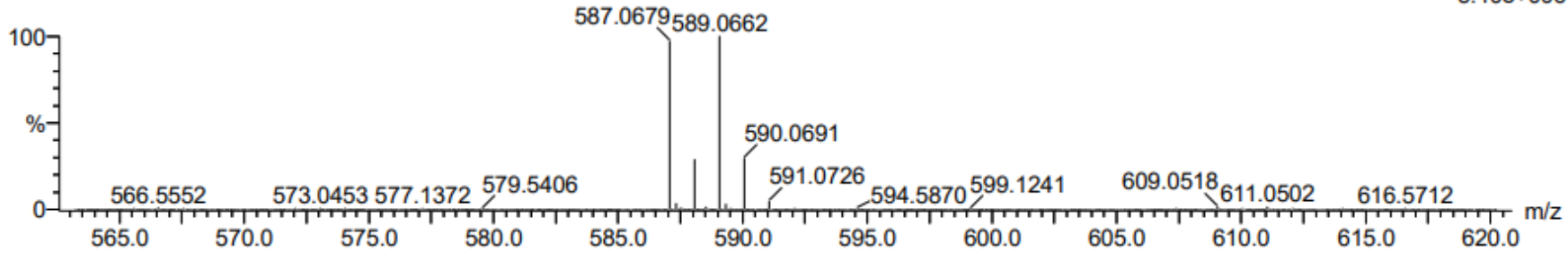


Single Mass Analysis

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
5463 formula(e) evaluated with 36 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 1-60 H: 1-100 N: 0-10 O: 0-10 S: 0-2 Br: 0-2

Sample Name : KMR_10 IITRPR XEVO G2-XS QTOF
Test Name :
260522_KMR_10 16 (0.177) 1: TOF MS ES+
3.40e+006



Minimum:				-1.5				
Maximum:		2.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
587.0679	587.0679	0.0	0.0	20.5	1171.3	n/a	n/a	C27 H20 N6 O5 Br