Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Molecular hybrid design, synthesis and biological evaluation of N-phenyl sulfonamide linked N-acyl hydrazone derivatives functioning as COX-2 inhibitors: New anti-inflammatory, anti-oxidant and anti-bacterial agents

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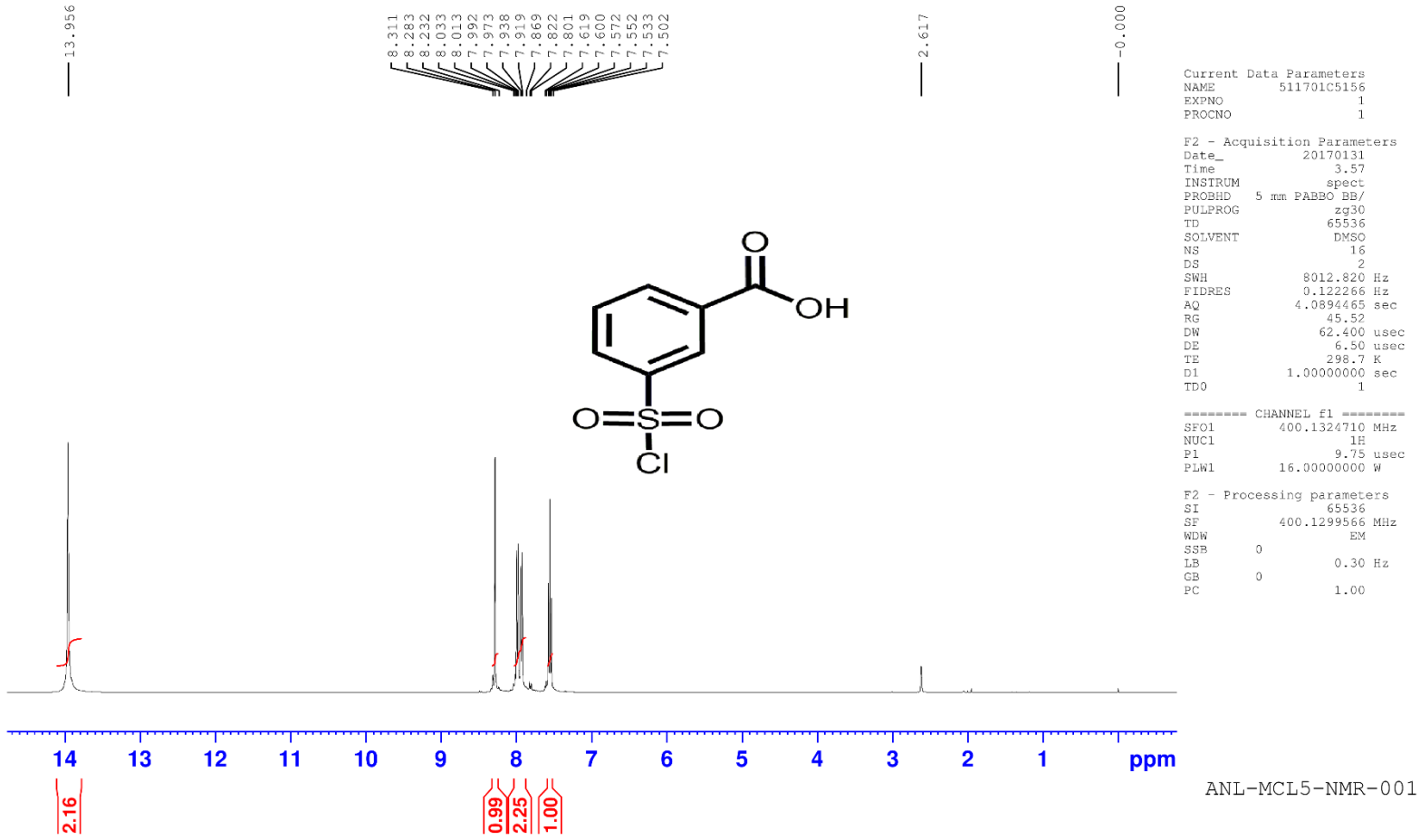
GVB-SK-INT-1

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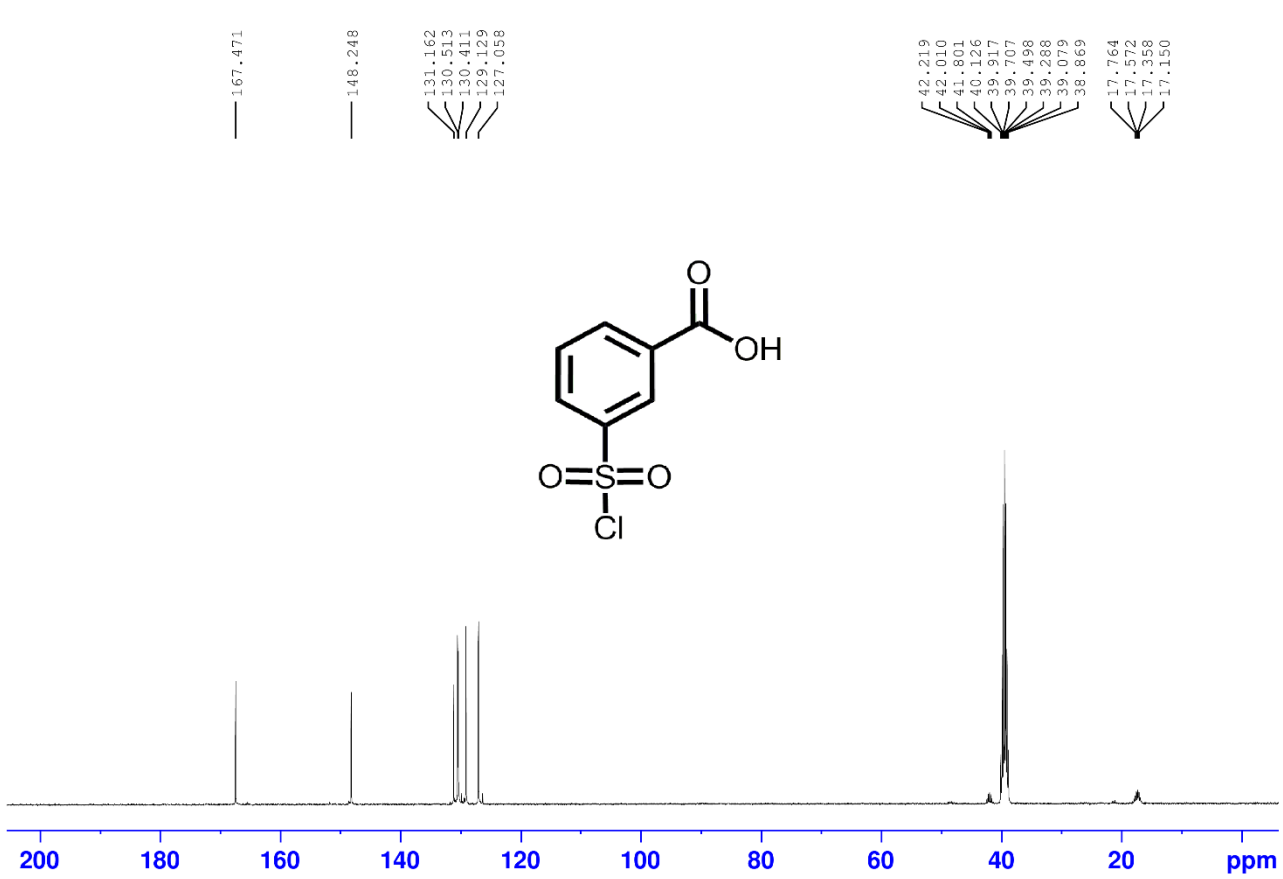
ANL-MCL5-NMR-001

^{1}H NMR of **Compound-B**

GVB-SK-INT-1

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TE                298.9 K
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TD0                    1

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NUC1                  13C
P1                  10.00 usec
PLW1          78.00000000 W

======== CHANNEL f2 ========
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NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          16.00000000 W
PLW12          0.18777999 W
PLW13          0.15210000 W

F2 - Processing parameters
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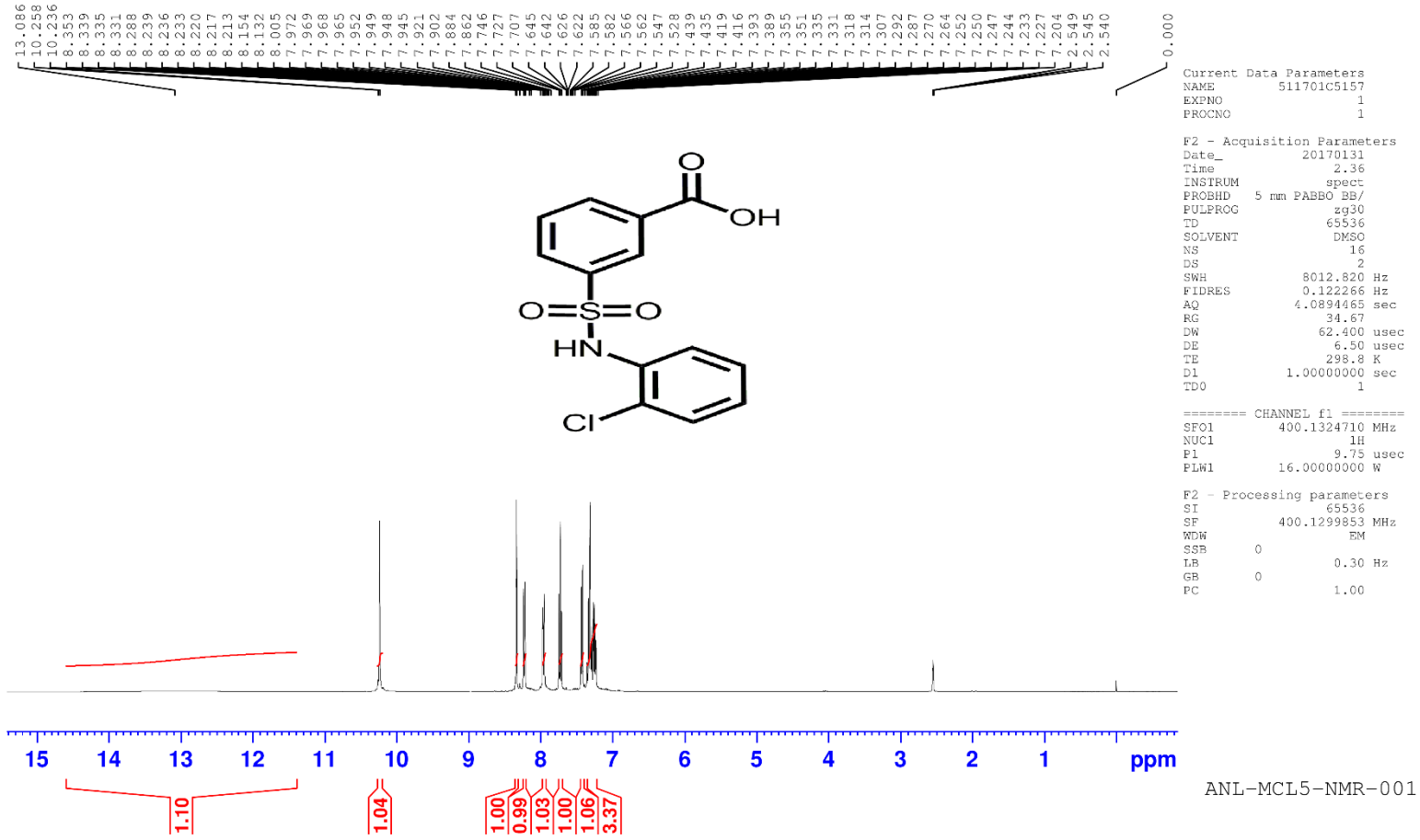
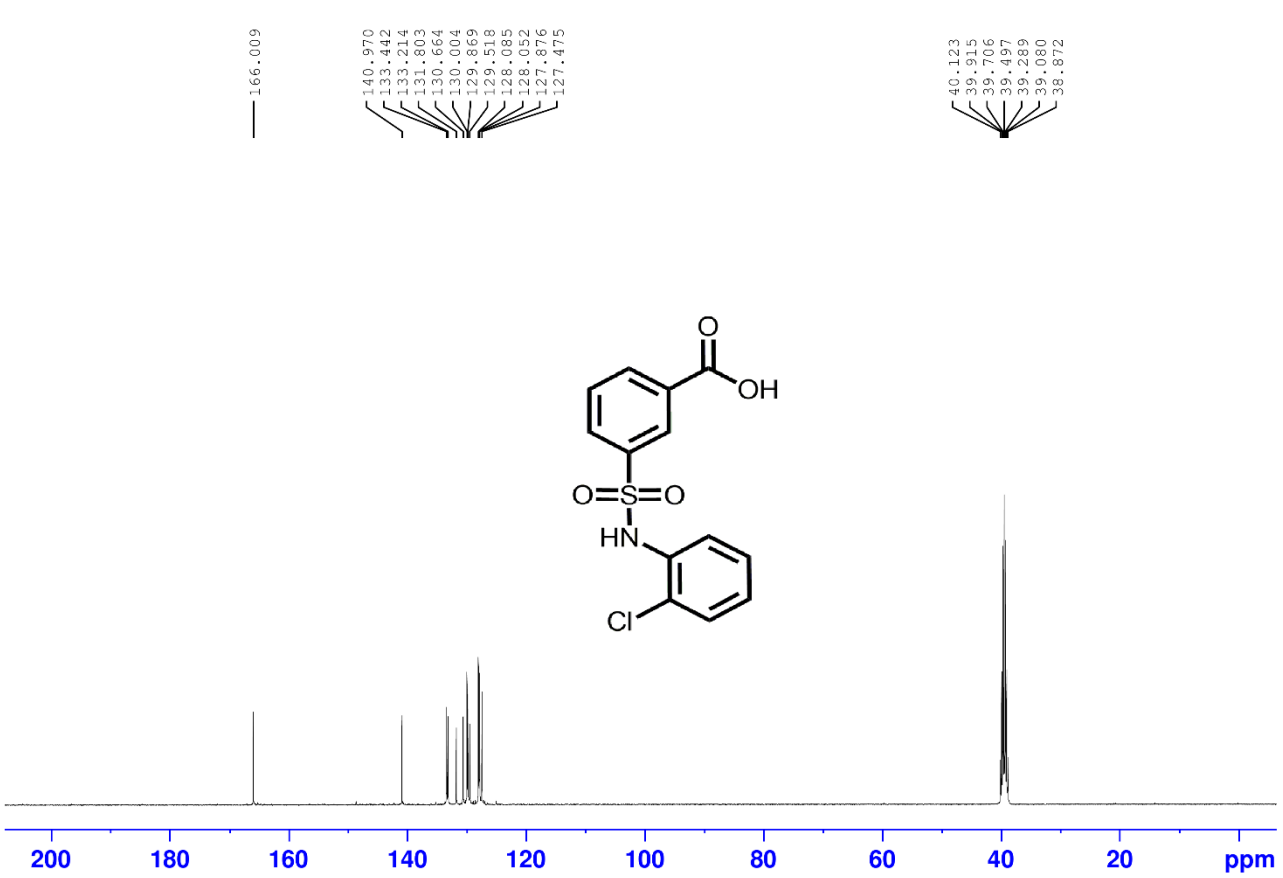
^{13}CNMR of **Compound-B**in DMSO-d_6



^{1}H NMR of **Compound-C**

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EXPNO                  2
PROCNO                 1

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PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
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SOLVENT             DMSO
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                 195.29
DW                 20.800 usec
DE                  6.50 usec
TE                 299.1 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                    1

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NUC1                  13C
P1                  10.00 usec
PLW1          78.00000000 W

======== CHANNEL f2 ========
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NUC2                  1H
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PCPD2              90.00 usec
PLW2          16.00000000 W
PLW12          0.18777999 W
PLW13          0.15210000 W

F2 - Processing parameters
SI                    32768
SF            100.6128108 MHz
WDW                     EM
SSB       0
LB                  2.00 Hz
GB        0
PC                  1.40
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ANL-MCL5-NMR-001

^{13}CNMR of **Compound-C** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

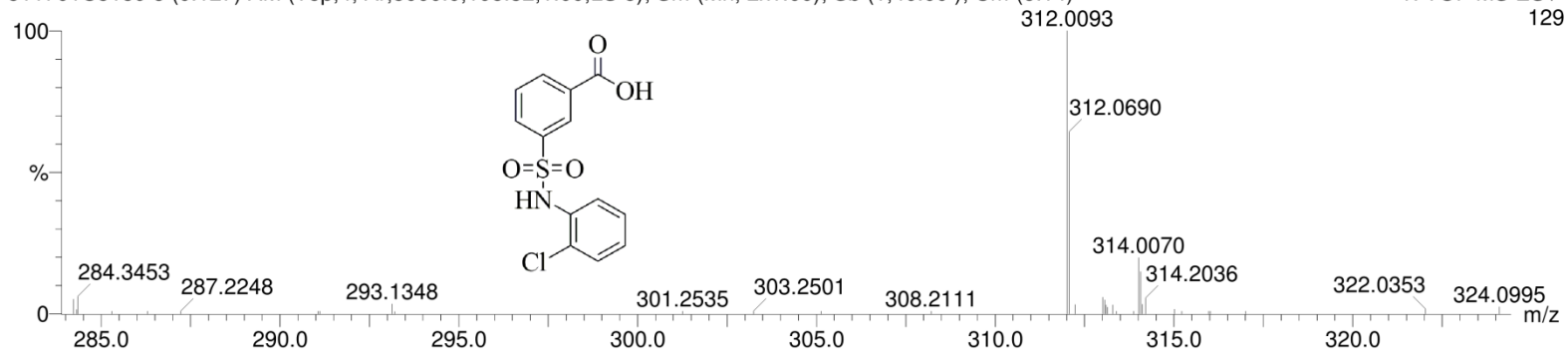
38 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-13 H: 0-11 N: 0-1 O: 0-4 S: 0-1 Cl: 0-1

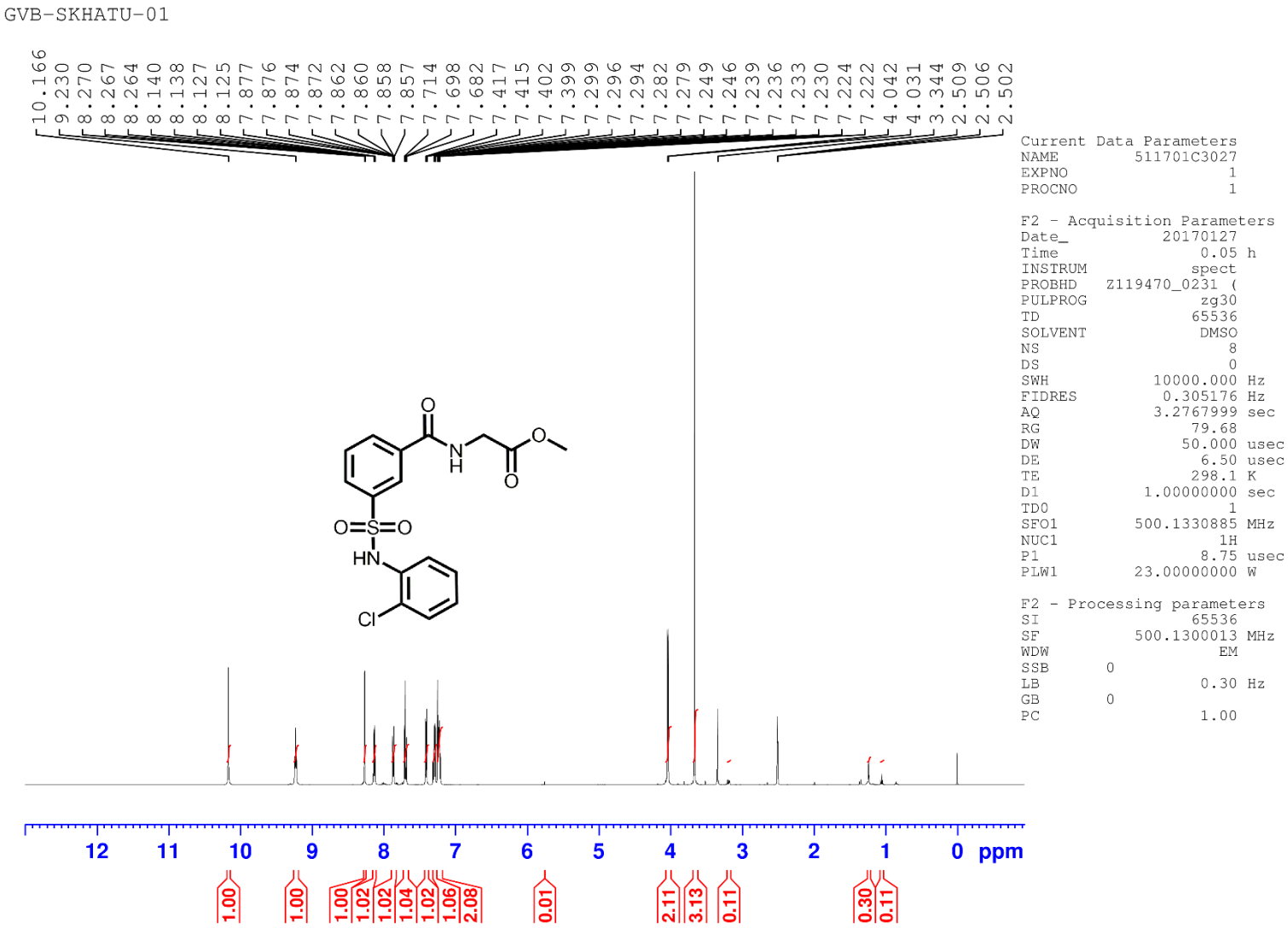
GVB-SK-INT-2

511701C5159 8 (0.127) AM (Top,4, Ar,5000.0,195.32,1.00,LS 5); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (6:14) 1: TOF MS ES+ 129



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
312.0093	312.0097	-0.4	-1.3	8.5	10.7	C13 H11 N O4 S Cl

HRMS of **Compound-C**



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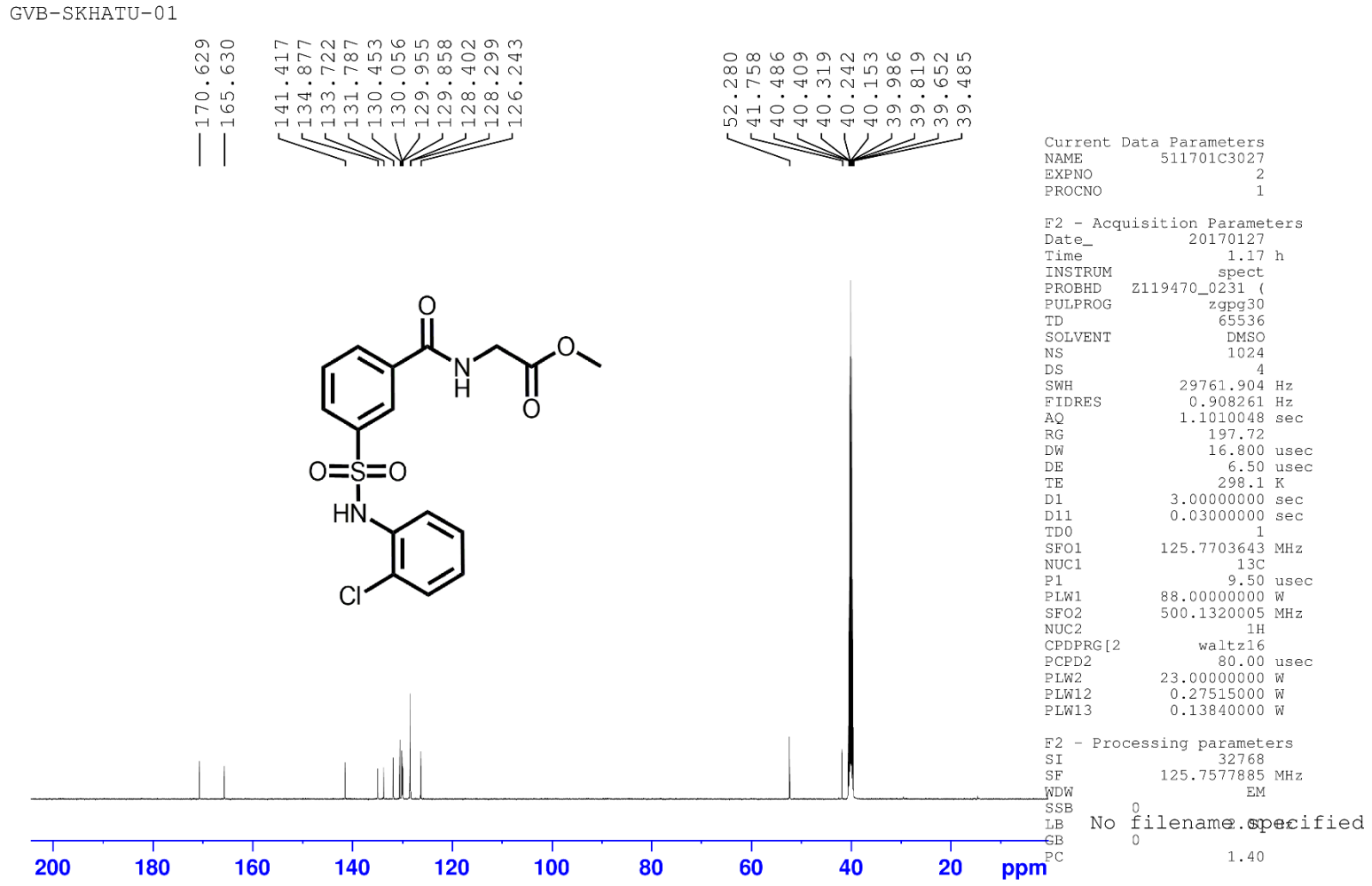


^{13}CNMR of **Compound-D** in DMSO-d_6

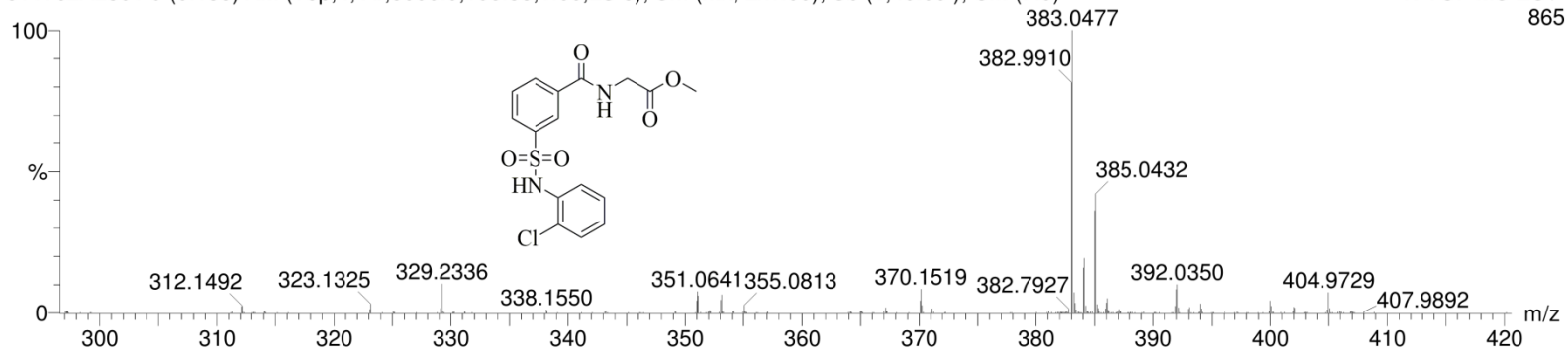
Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
70 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-16 H: 0-16 N: 0-2 O: 0-5 S: 0-1 Cl: 0-1

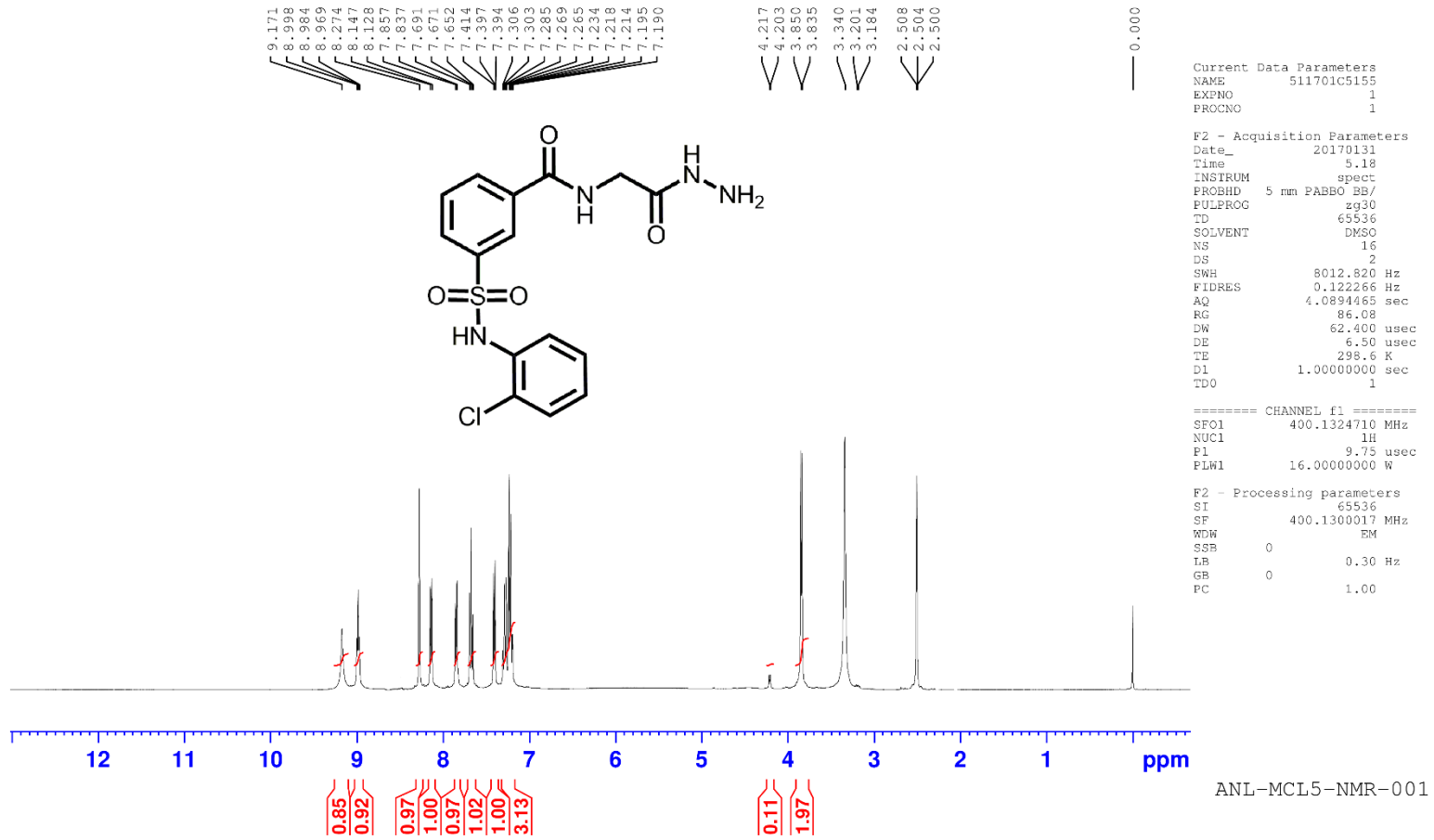
GVBSK-HATU-01
511702A2301 9 (0.135) AM (Top,4, Ar,5000.0,195.38,1.00,LS 5); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (7:9) 1: TOF MS ES+ 865



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
383.0477	383.0468	0.9	2.3	9.5	1.8	C16 H16 N2 O5 S Cl

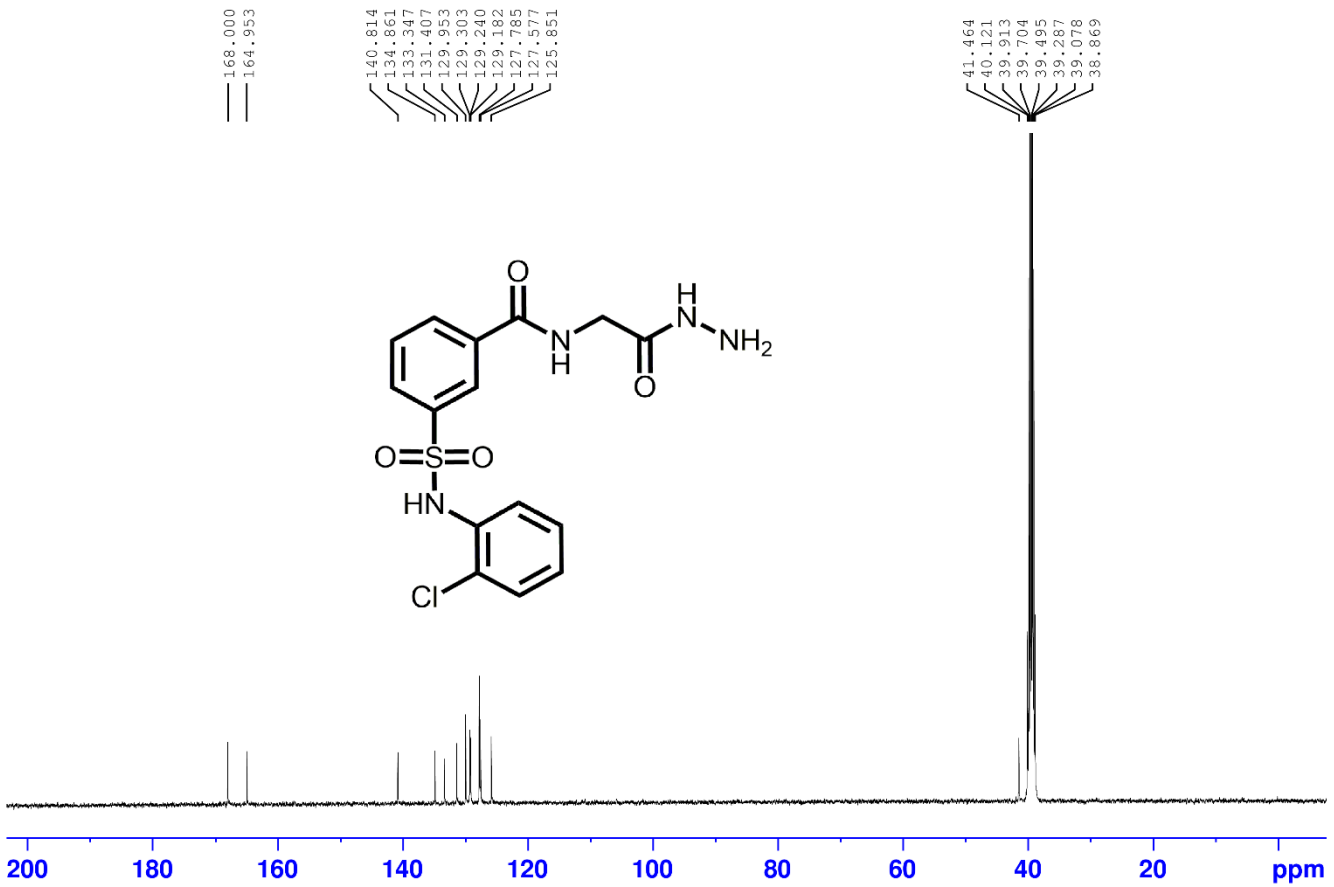
HRMS of **Compound-D**

GVB-SK-INT-4



^{1}H NMR of **Compound-E**

GVB-SK-INT-4

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TD                65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               195.29
DW               20.800 usec
DE                6.50 usec
TE               298.9 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
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NUC1                  13C
P1                10.00 usec
PLW1         78.00000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         16.00000000 W
PLW12         0.18777999 W
PLW13         0.15210000 W

F2 - Processing parameters
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WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

ANL-MCL5-NMR-001

^{13}CNMR of **Compound-E** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
98 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-16 N: 0-4 O: 0-4 S: 0-1 Cl: 0-1

GVB-SK-INT-4
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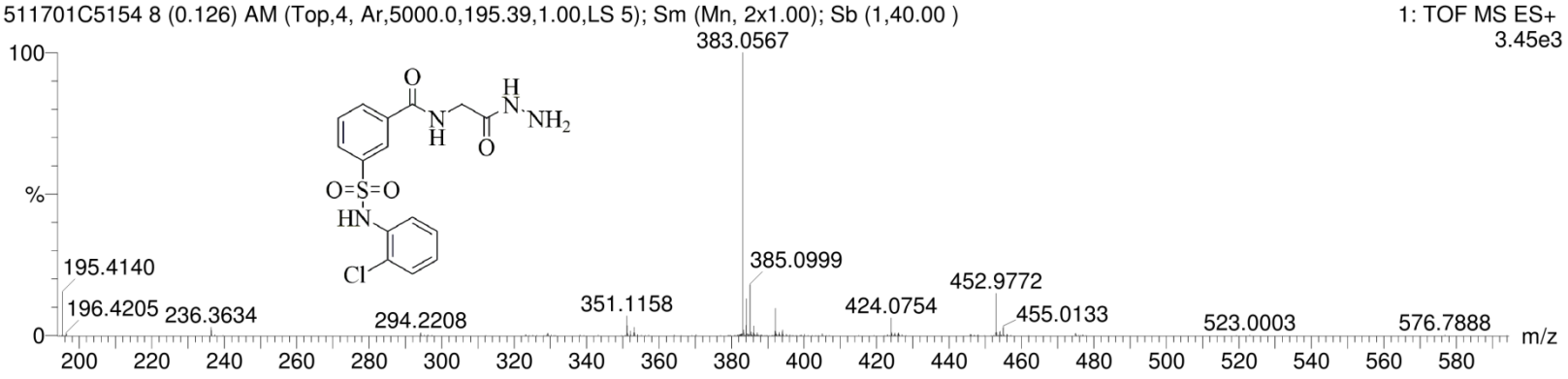
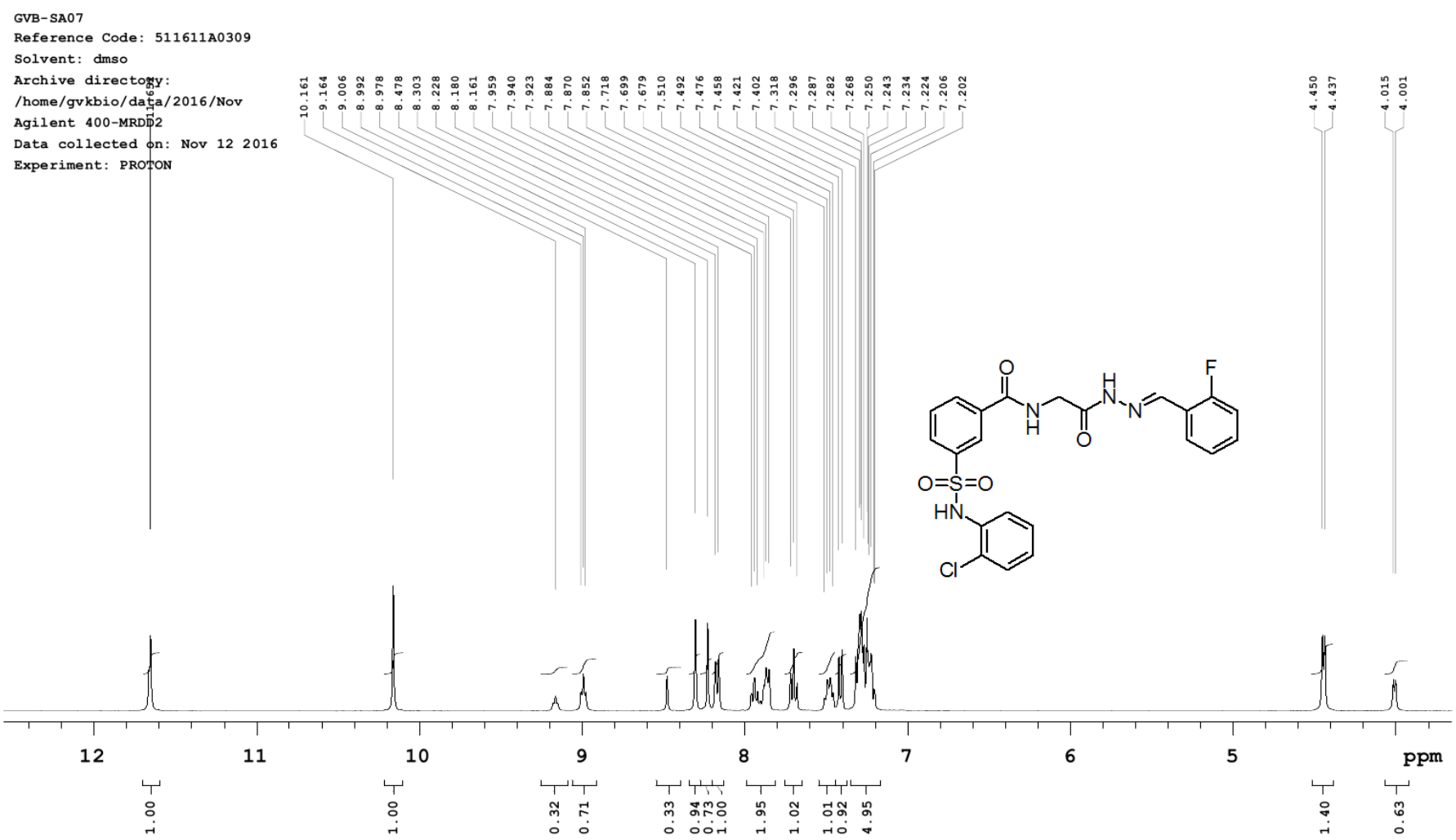
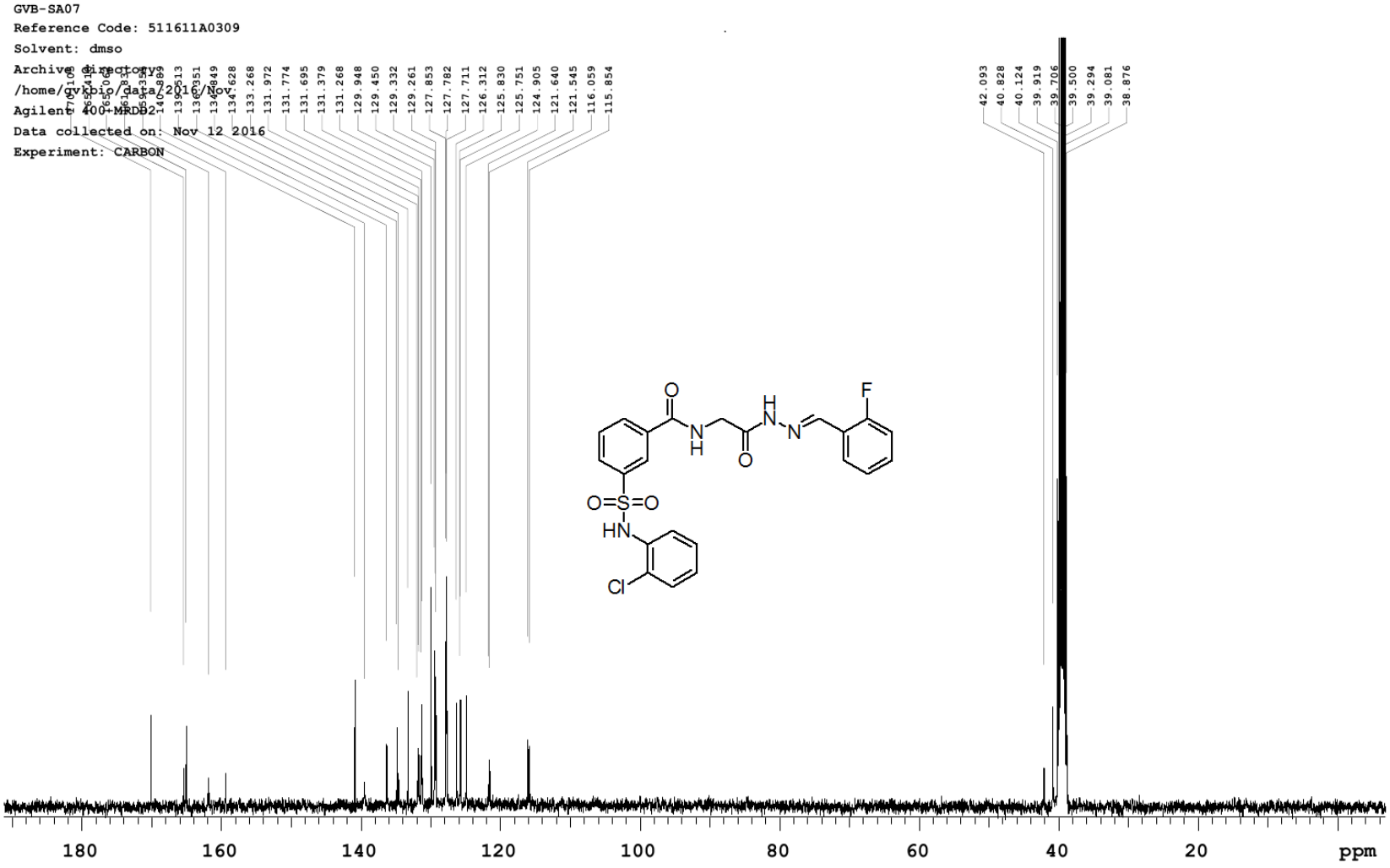


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
383.0567	383.0581	-1.4	-3.7	9.5	266.2	C15 H16 N4 O4 S Cl

HRMS of **Compound-E**



^{1}H NMR of **Compound-1a**



^{13}CNMR of **Compound-1a** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

178 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)

Elements Used:

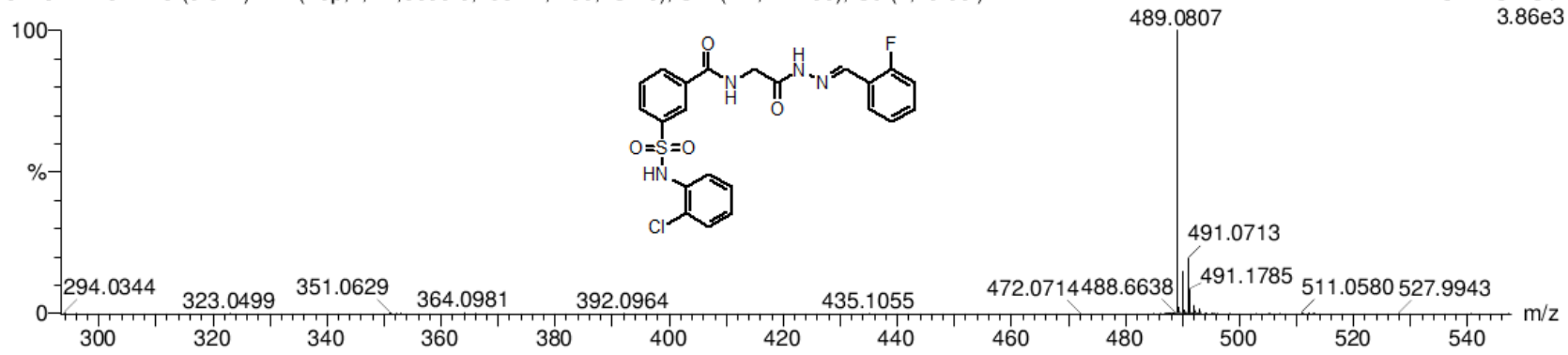
C: 0-23 H: 0-19 N: 0-4 O: 0-4 F: 0-1 S: 0-1 Cl: 0-1

GVB-SA07

511611B4321 23 (0.341) AM (Top,4, Ar,5000.0,195.14,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+

3.86e3



Minimum:				-1.5		
Maximum:		5.0	10000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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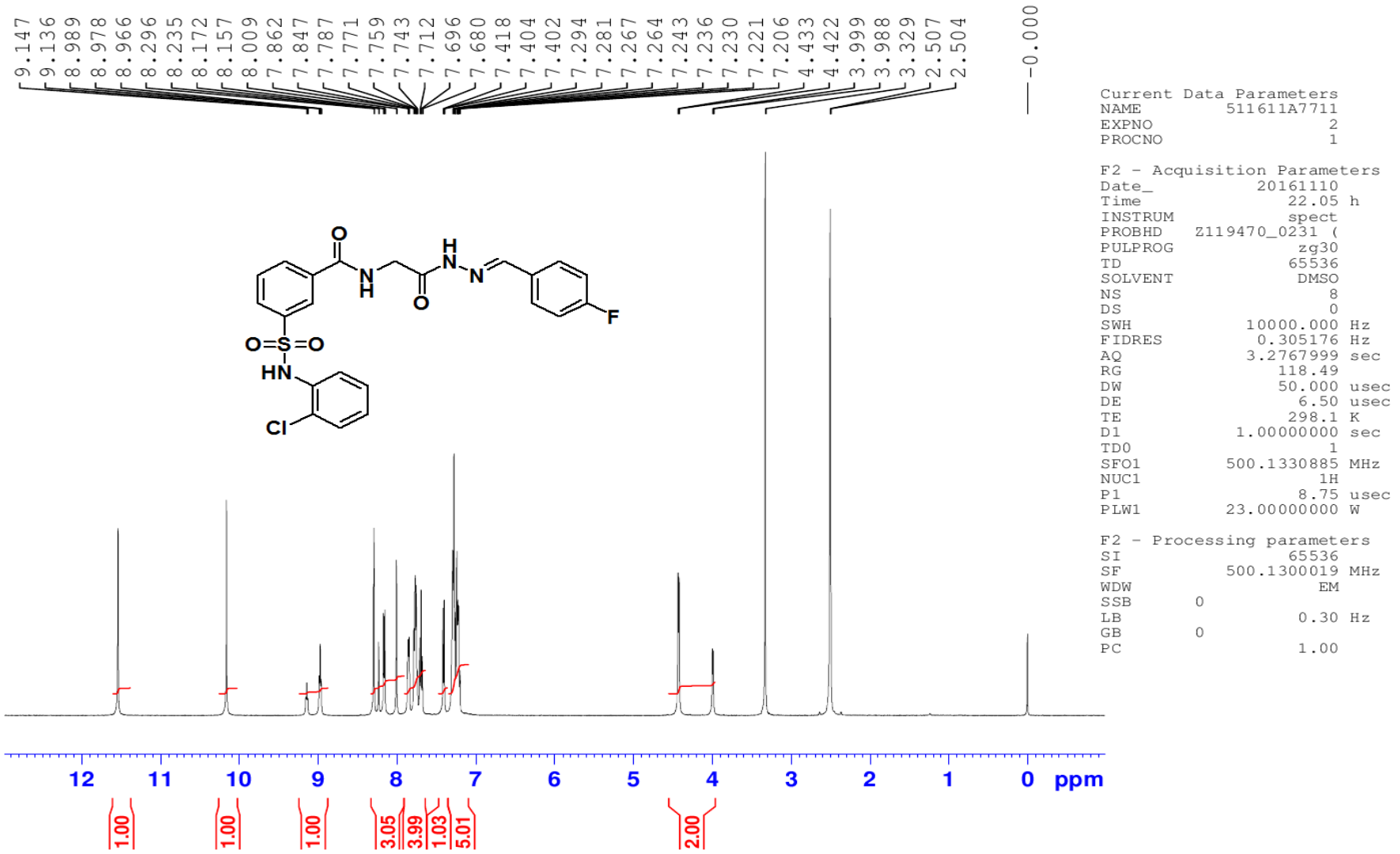
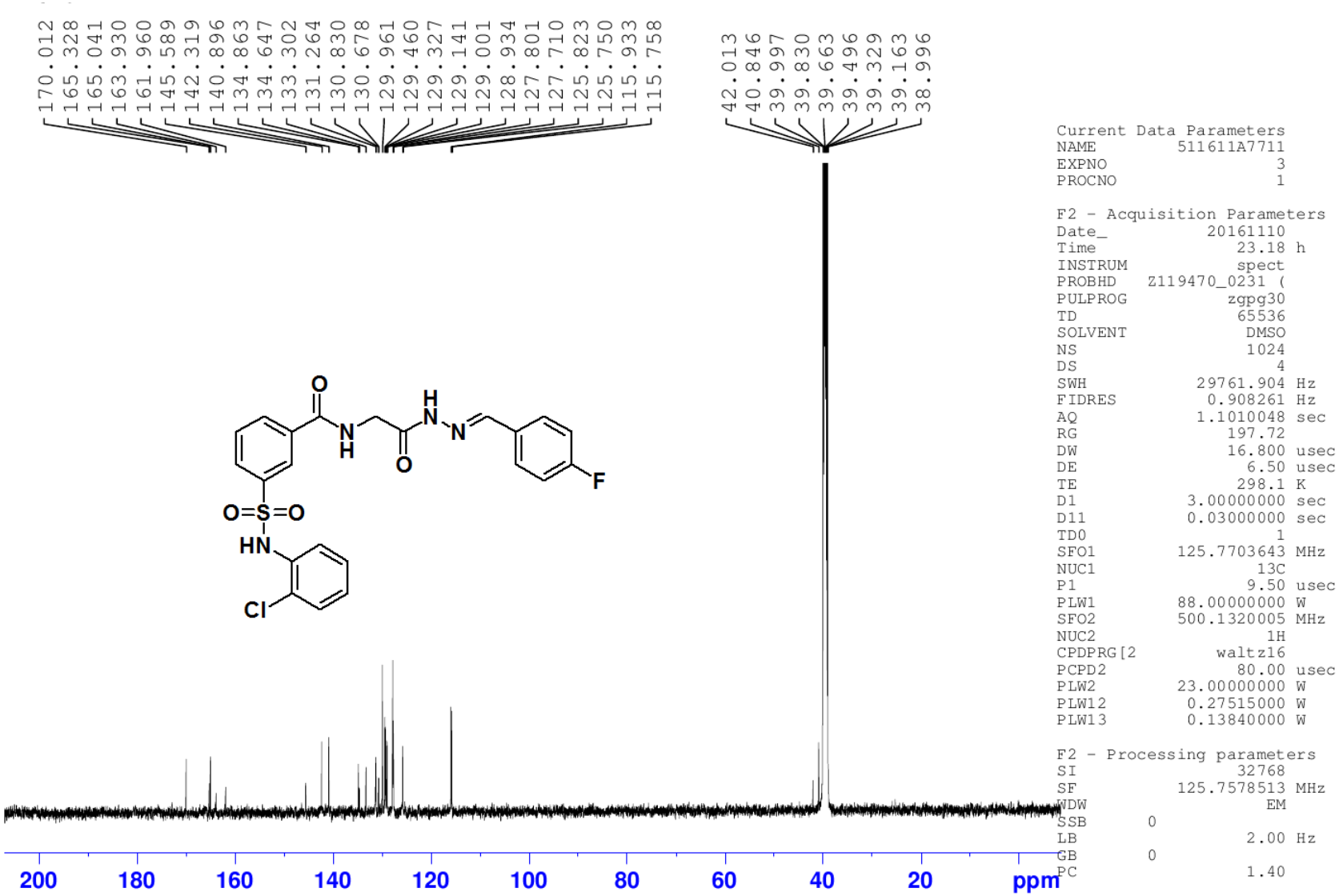
HRMS of **Compound-1a**



^{1}H NMR of **Compound-1b**

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SOLVENT             DMSO
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DS                     4
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FIDRES          0.908261 Hz
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RG                197.72
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TE                298.1 K
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NUC2                1H
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PCPD2             80.00 usec
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PLW13         0.13840000 W

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^{13}CNMR of **Compound-1b** in DMSO-d_6

Elemental Composition Report

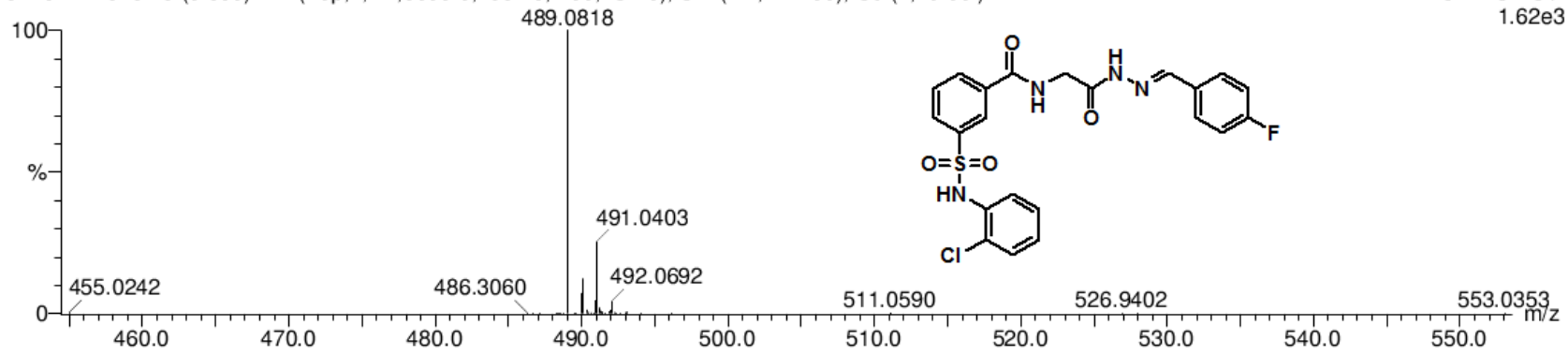
Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
190 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-22 H: 0-19 N: 0-4 O: 0-4 F: 0-1 S: 0-1 Cl: 0-1

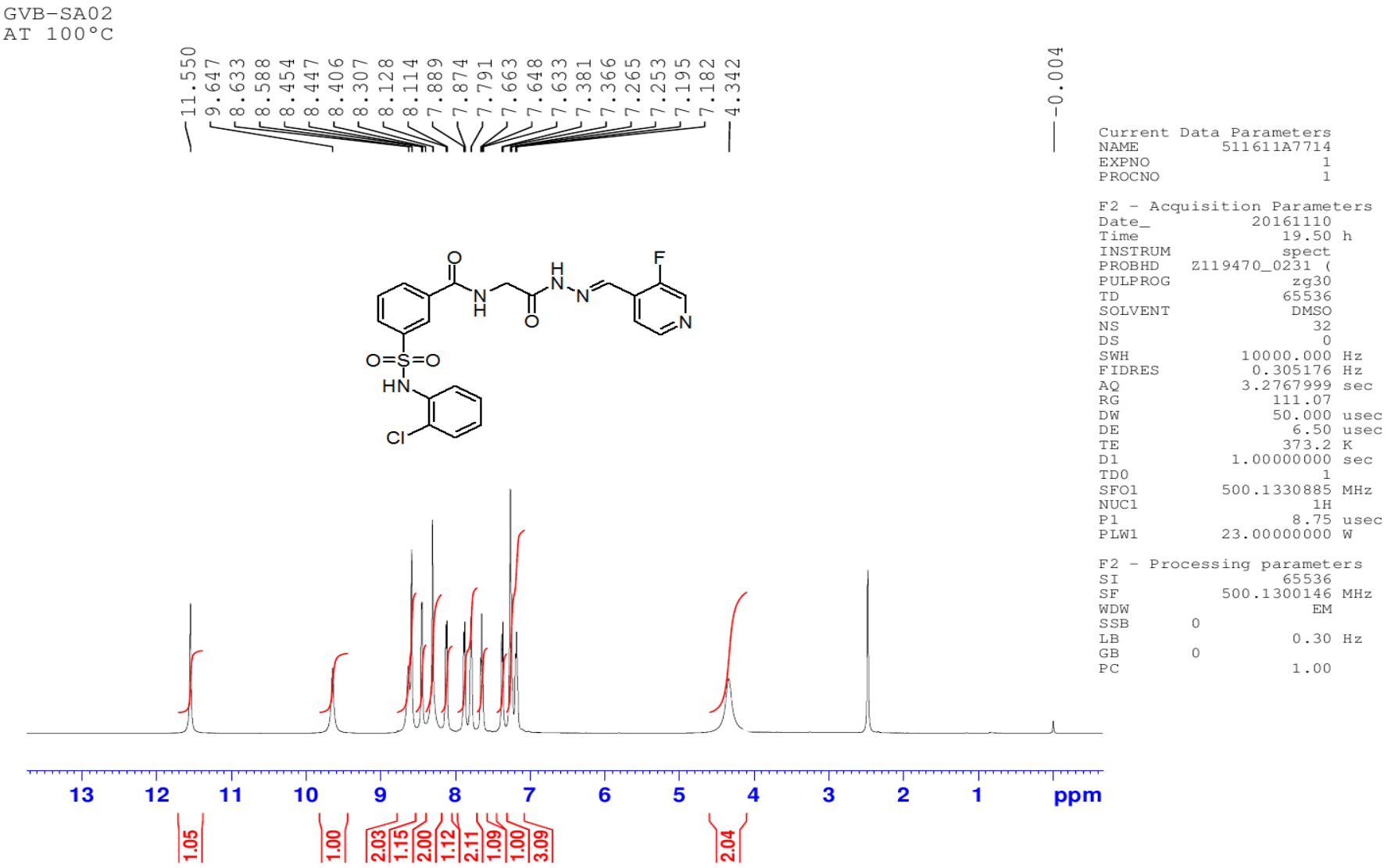
GVB-SA01
511611B4315 25 (0.360) AM (Top,4, Ar,5000.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
1.62e3

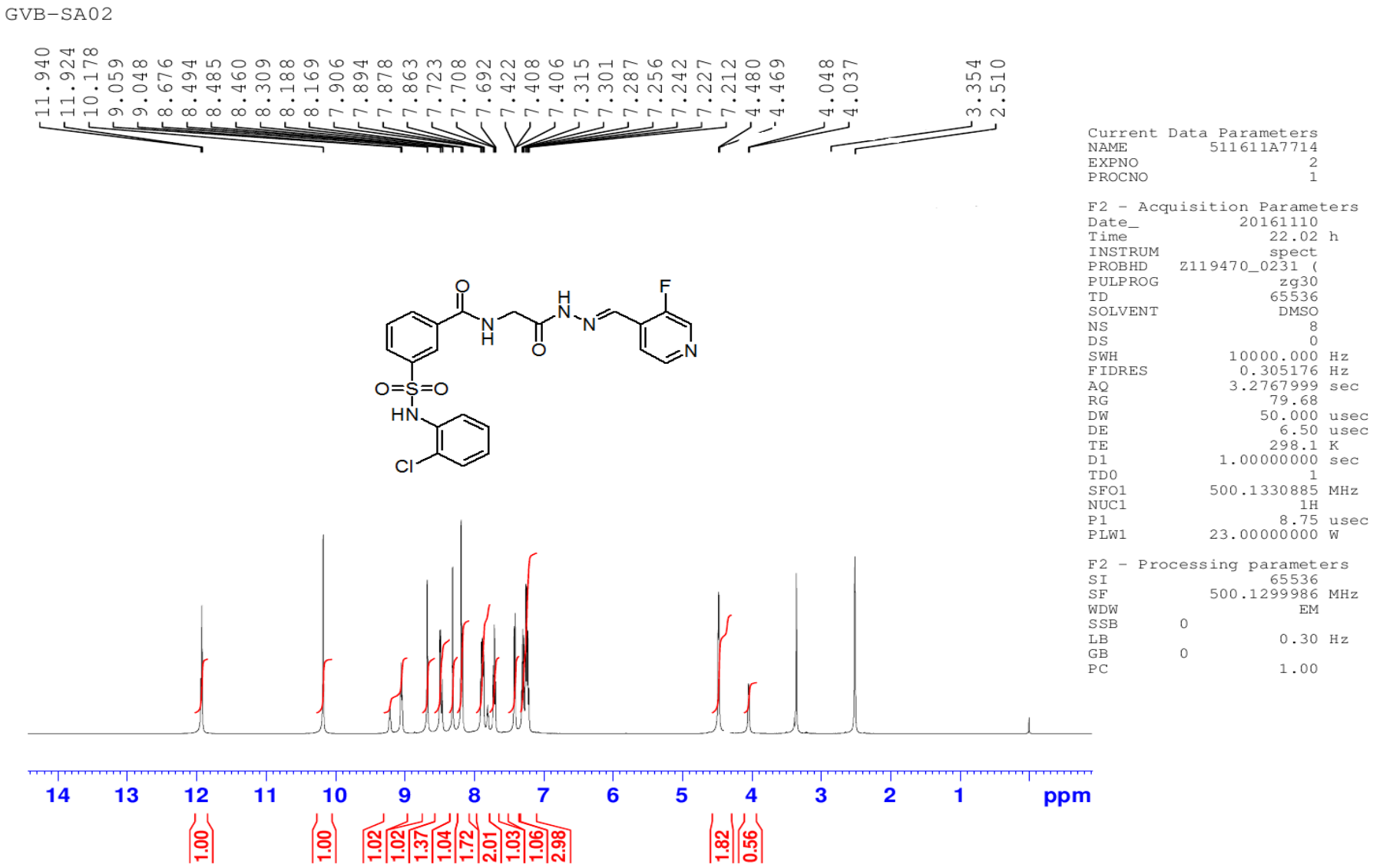


Minimum:				-1.5		
Maximum:		5.0	10000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
489.0818	489.0800	1.8	3.7	14.5	94405.7	C22 H19 N4 O4 F S Cl

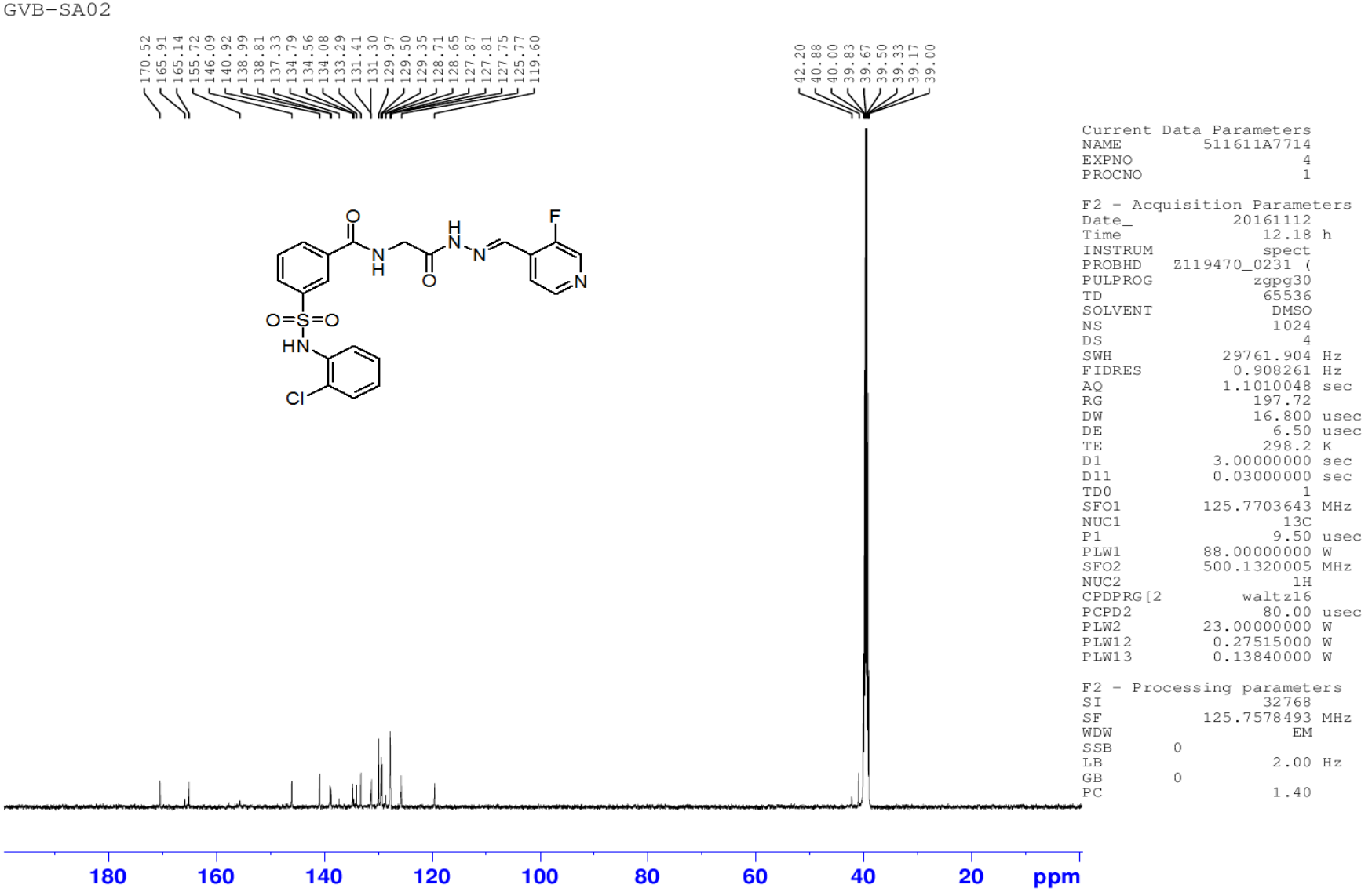
HRMS of **Compound-1b**



^{1}H NMR of **Compound-1c at 100^{o}C**



^{1}H NMR of **Compound-1c**



^{13}CNMR of **Compound-1c** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

230 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

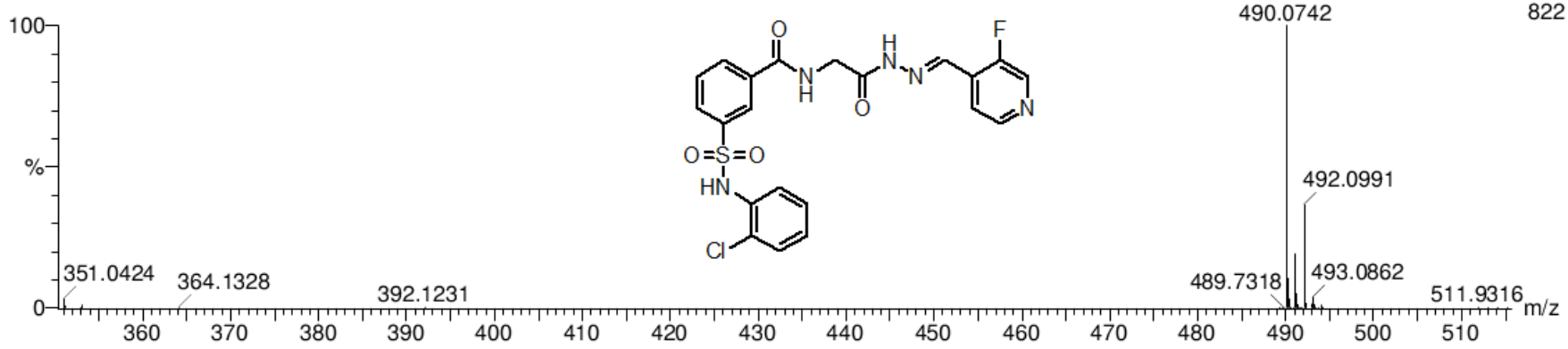
C: 0-21 H: 0-18 N: 0-5 O: 0-4 F: 0-1 S: 0-1 Cl: 0-1

GVB-SA02

511611B4316 23 (0.343) AM (Top,4, Ar,5000.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

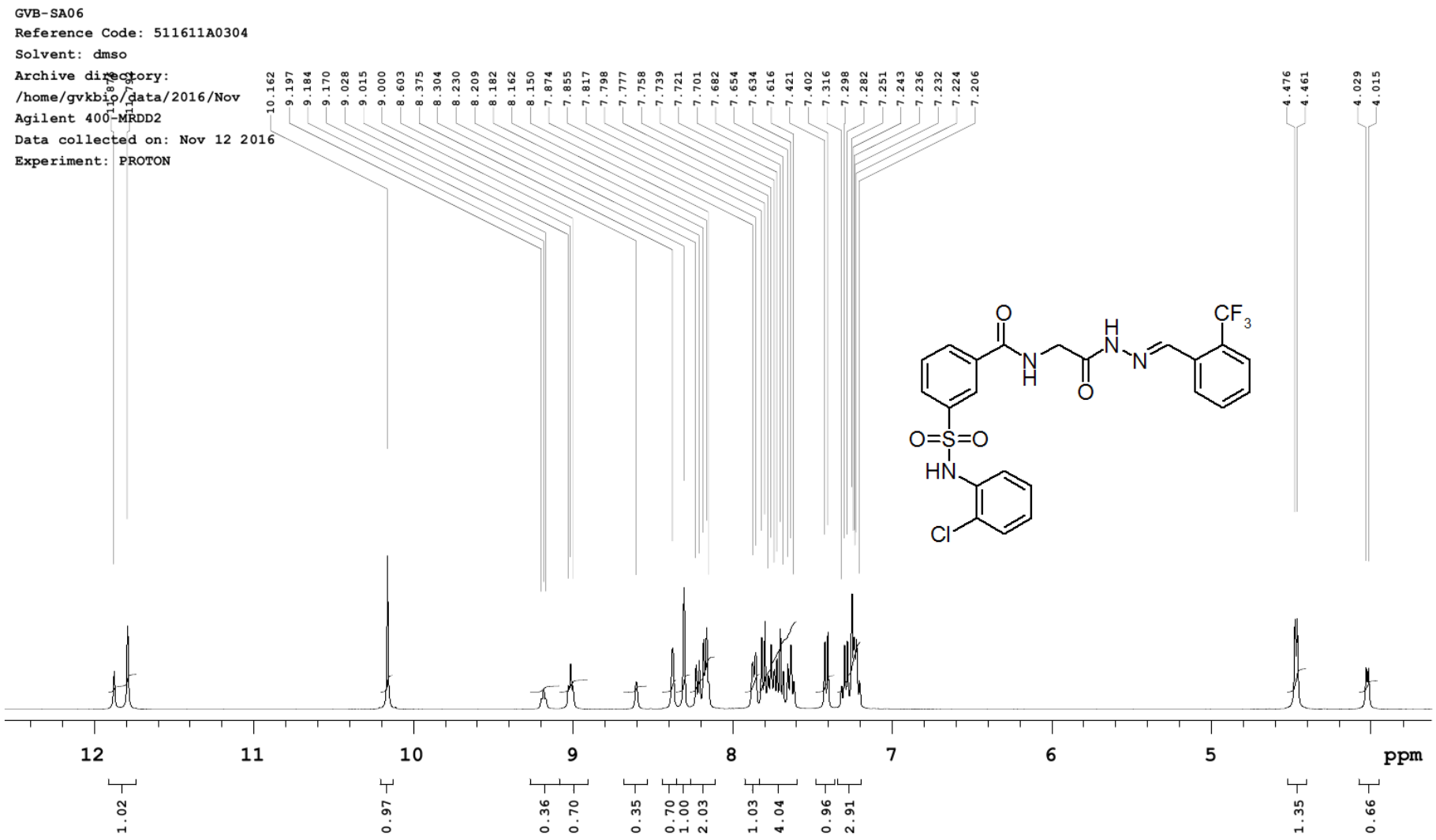
1: TOF MS ES+

822

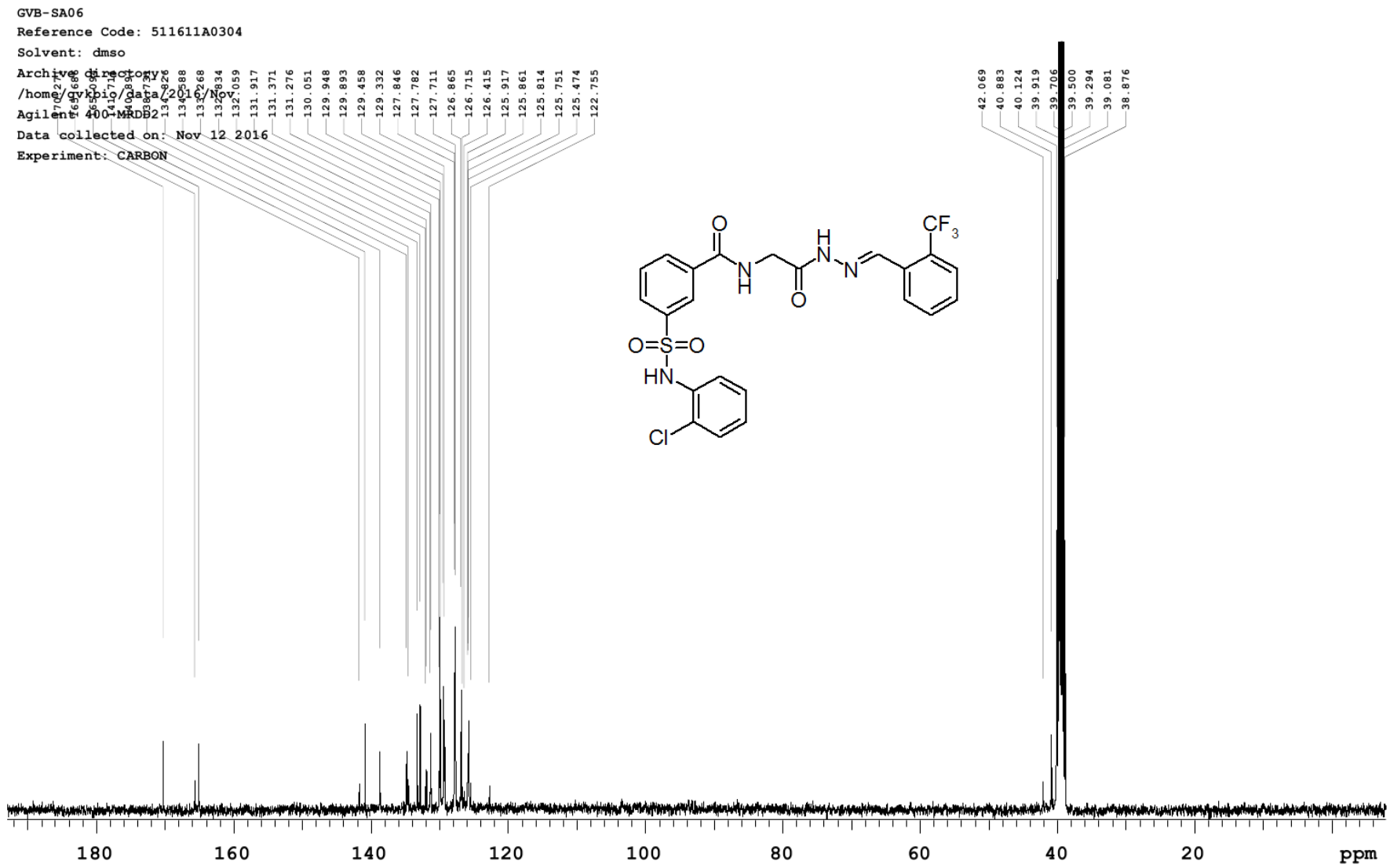


Minimum:				-1.5		
Maximum:		5.0	10000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
490.0742	490.0752	-1.0	-2.0	14.5	47774.1	C21 H18 N5 O4 F S Cl

HRMS of **Compound-1c**



^{1}H NMR of **Compound-1d** in DMSO-d_6



^{13}CNMR of **Compound-1d** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
389 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-19 N: 0-4 O: 0-4 F: 0-3 S: 0-1 Cl: 0-1

GVB-SA06
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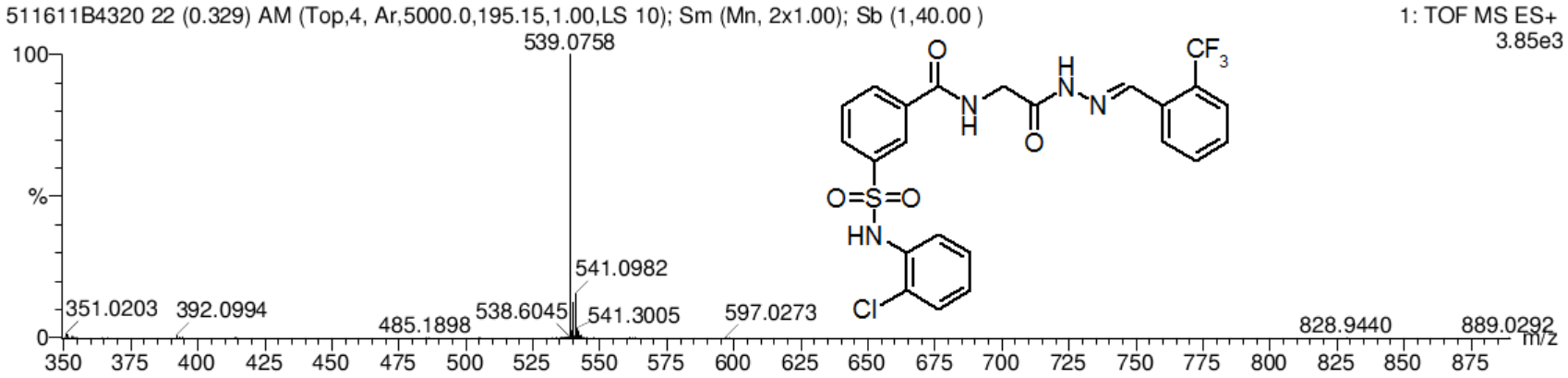
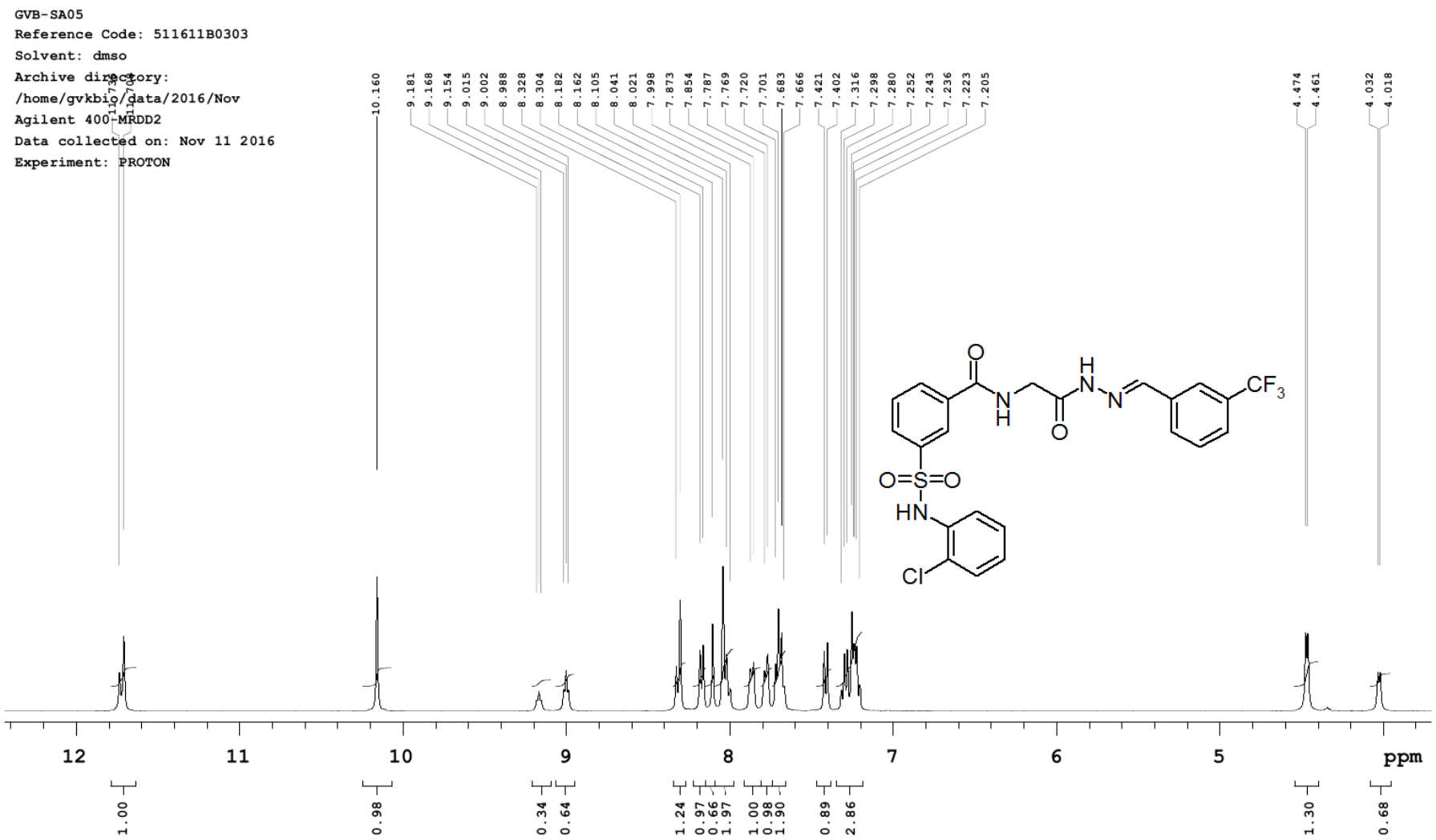
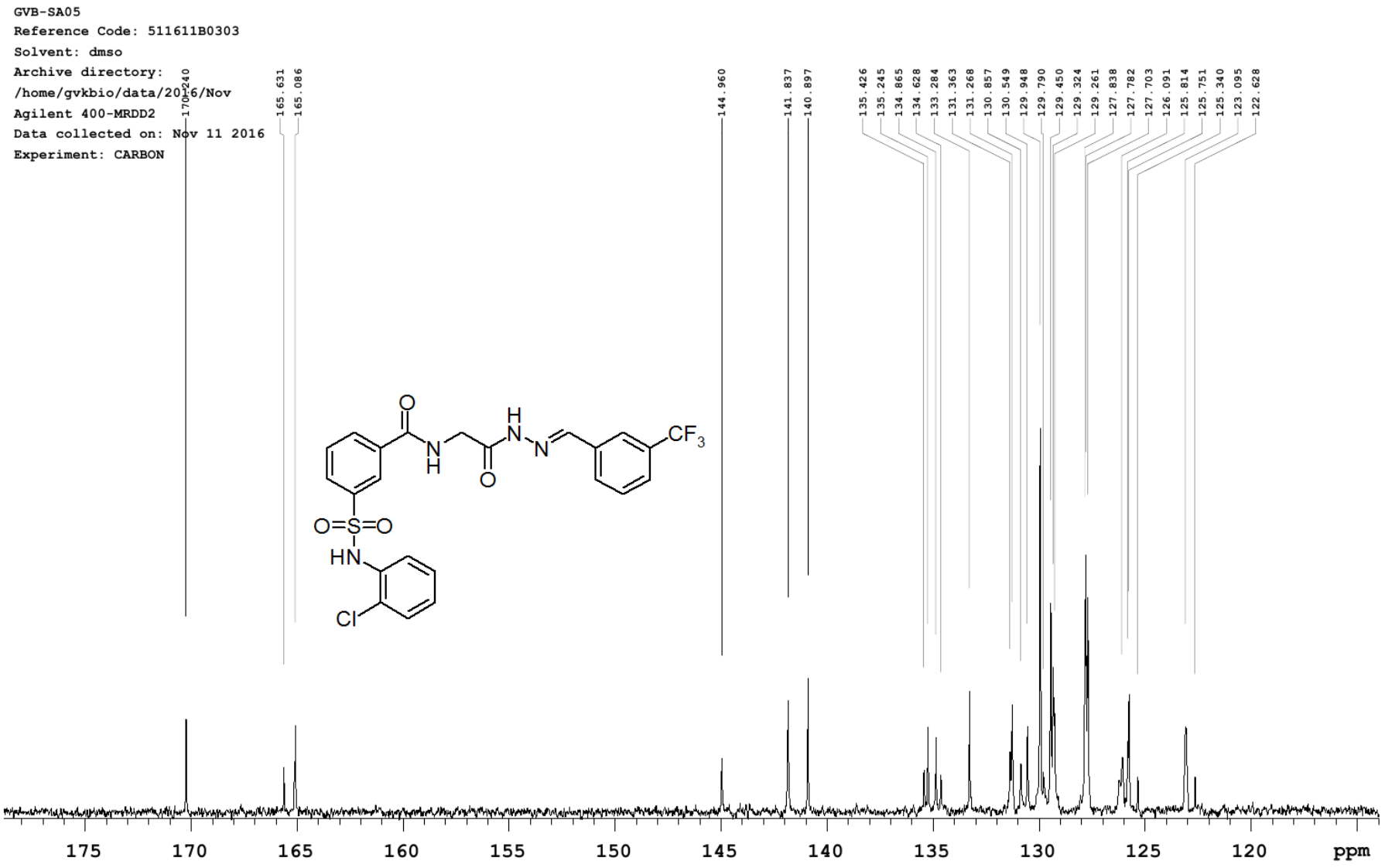


Minimum:				-1.5		
Maximum:		5.0	10000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
539.0758	539.0768	-1.0	-1.9	14.5	185151.5	C23 H19 N4 O4 F3 S Cl

HRMS of **Compound-1d**



^{1}H NMR of **Compound-1e** in DMSO-d_6



^{13}CNMR of **Compound-1e** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

389 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

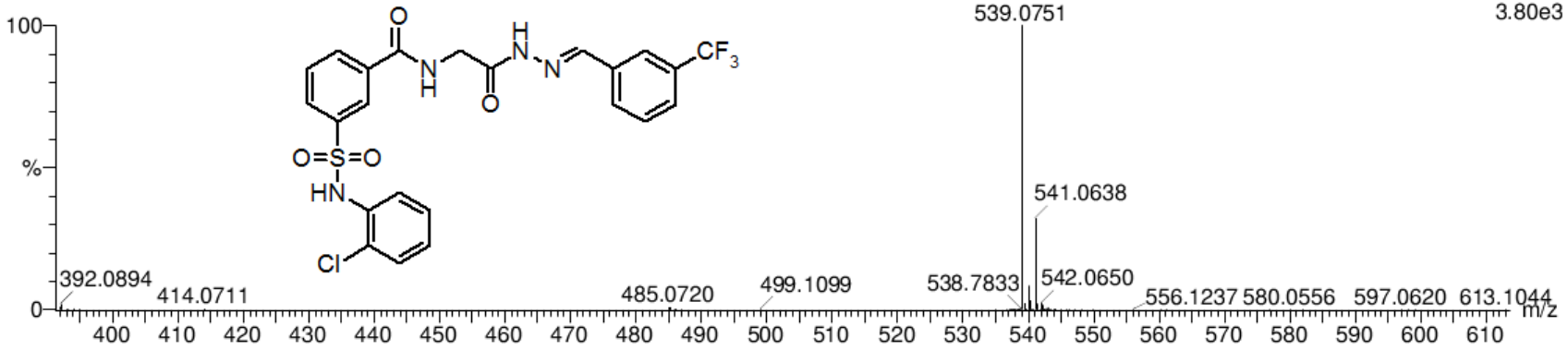
C: 0-23 H: 0-19 N: 0-4 O: 0-4 F: 0-3 S: 0-1 Cl: 0-1

GVB-SA05

511611B4319 22 (0.330) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

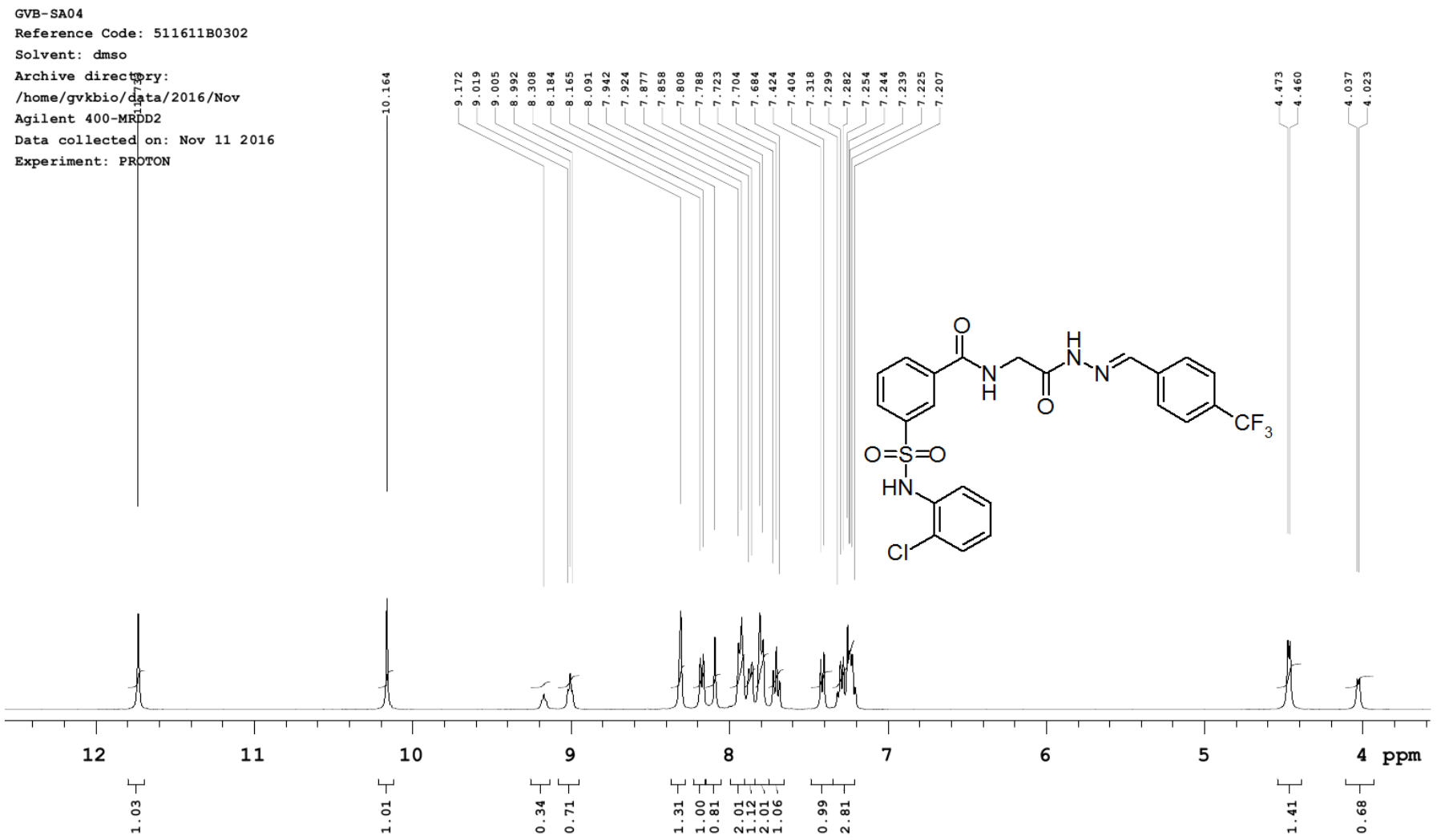
1: TOF MS ES+

3.80e3

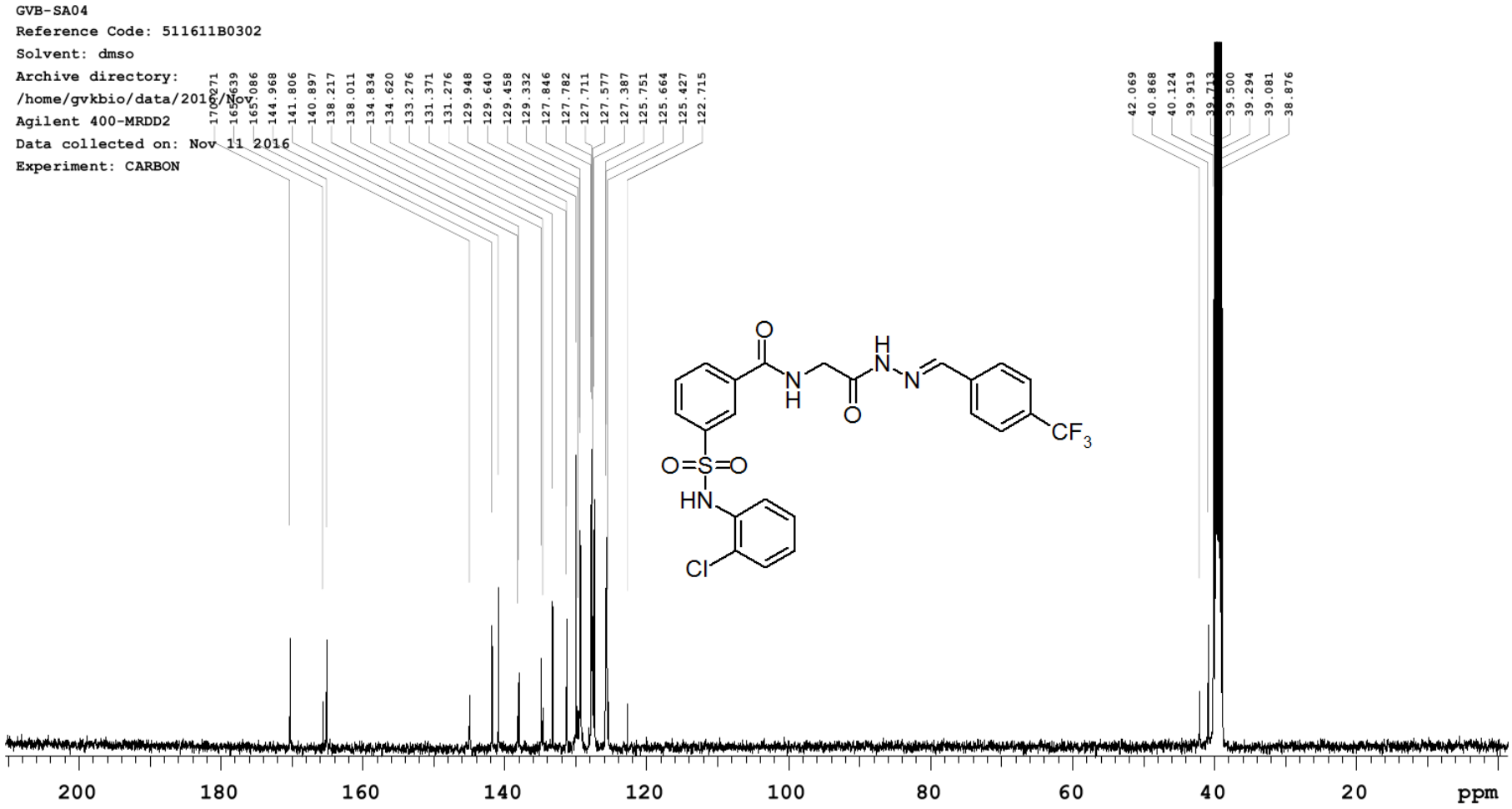


Minimum:				-1.5		
Maximum:		5.0	10000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
539.0751	539.0768	-1.7	-3.2	14.5	182666.4	C23 H19 N4 O4 F3 S Cl

HRMS of **Compound-1e**



^{1}H NMR of **Compound-1f** in DMSO-d_6



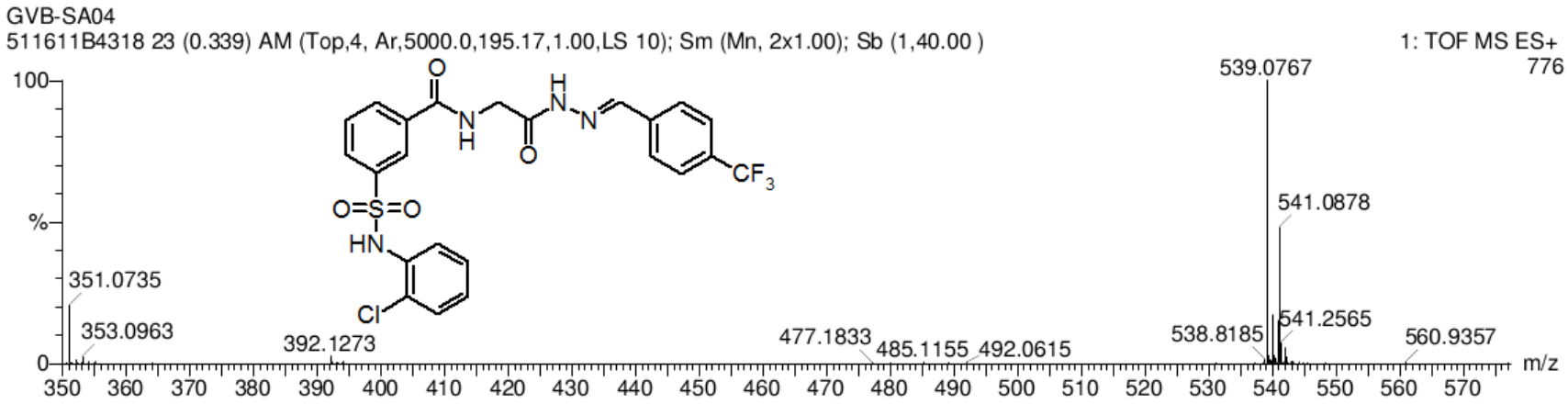
^{13}CNMR of **Compound-1f** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

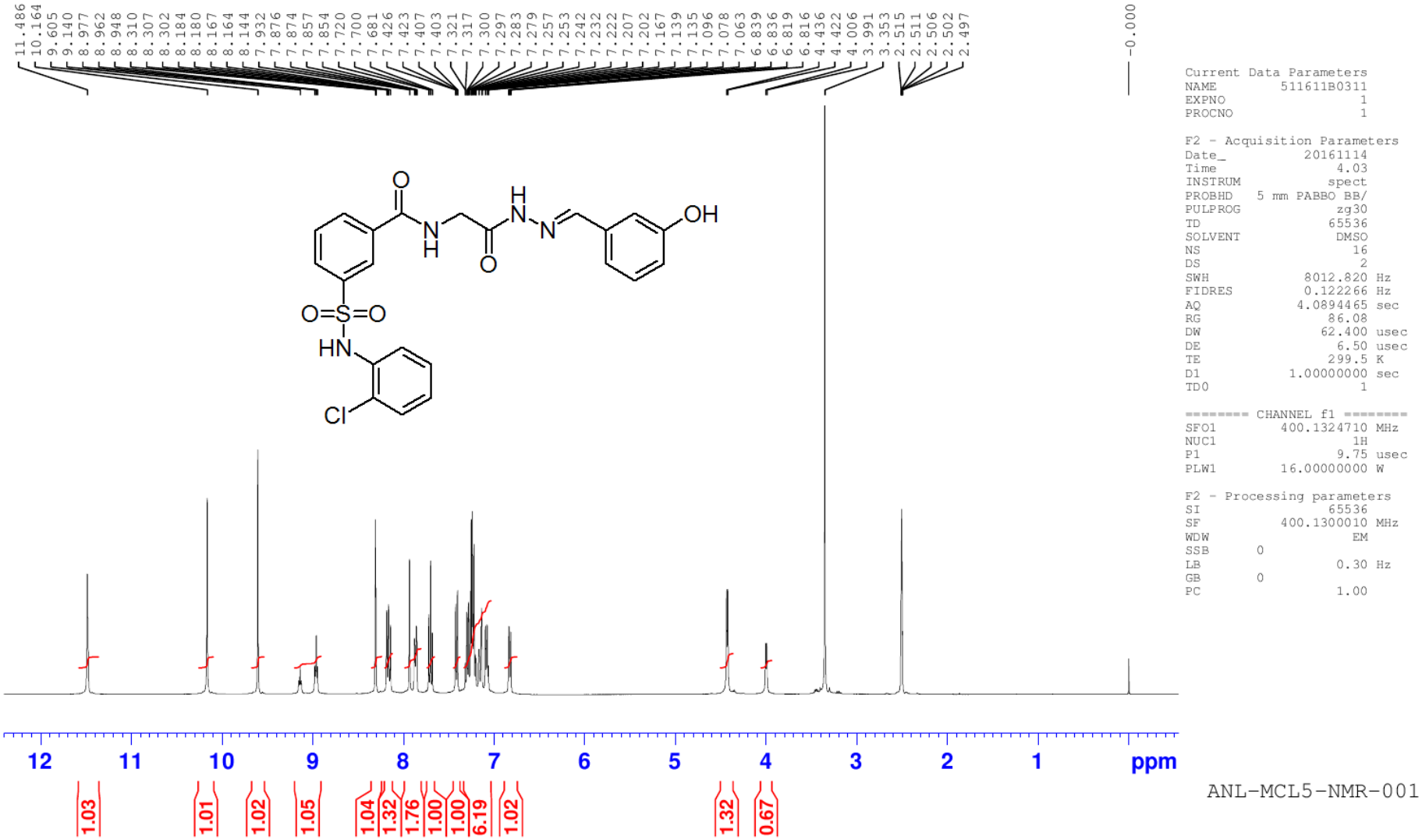
Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
389 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-19 N: 0-4 O: 0-4 S: 0-1 Cl: 0-1 F: 0-3



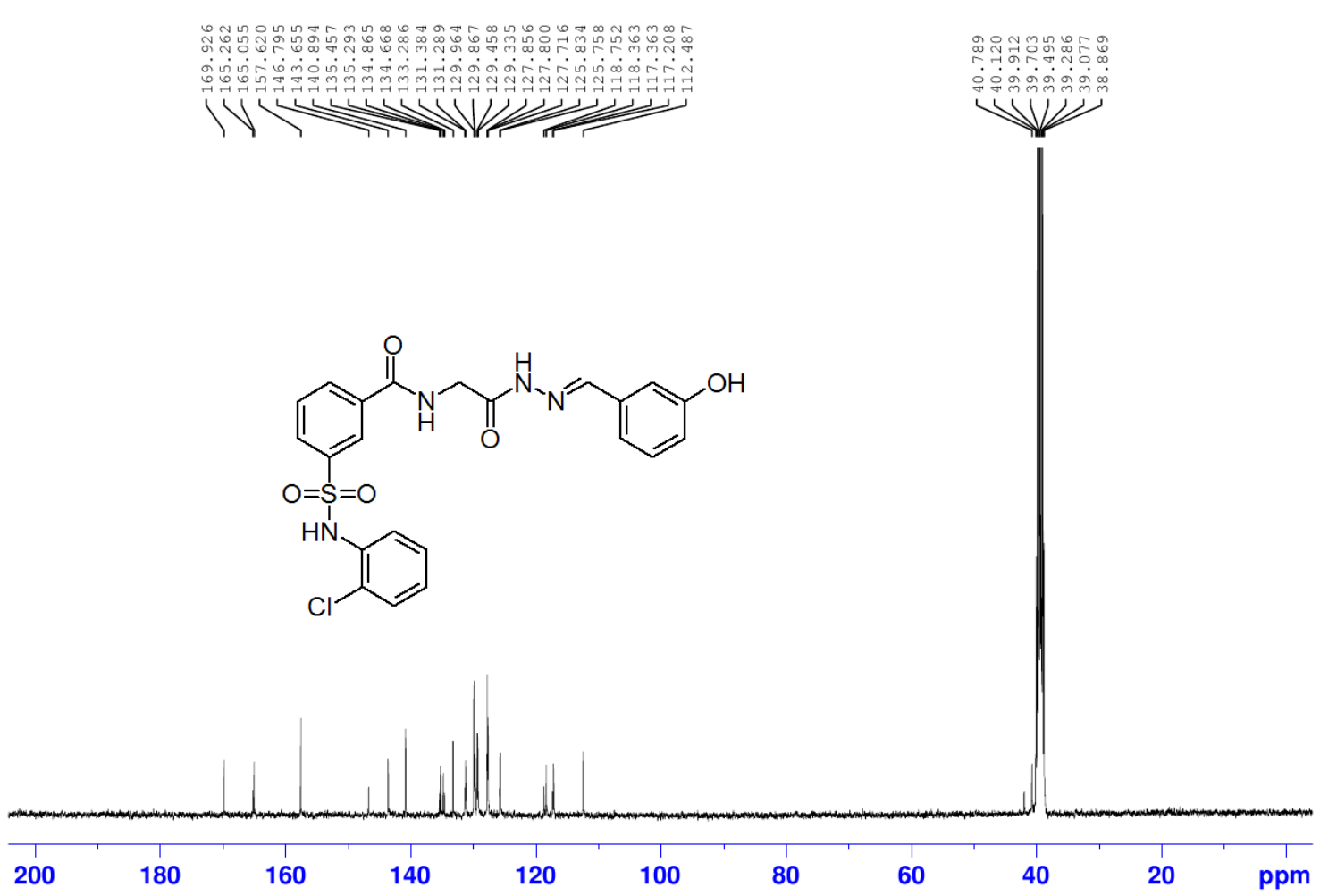
Minimum:				-1.5		
Maximum:		5.0	10000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
539.0767	539.0768	-0.1	-0.2	14.5	37263.6	C23 H19 N4 O4 S Cl F3

HRMS of **Compound-1f**



^{1}H NMR of **Compound-1g** in DMSO-d_6

GVB-SA08

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EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
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PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                195.29
DW                20.800 usec
DE                 6.50 usec
TE                299.6 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                 13C
P1                 10.00 usec
PLW1          78.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          16.00000000 W
PLW12          0.18777999 W
PLW13          0.15210000 W

F2 - Processing parameters
SI                  32768
SF            100.6128186 MHz
WDW                    EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

^{13}CNMR of **Compound-1g** in DMSO-d_6

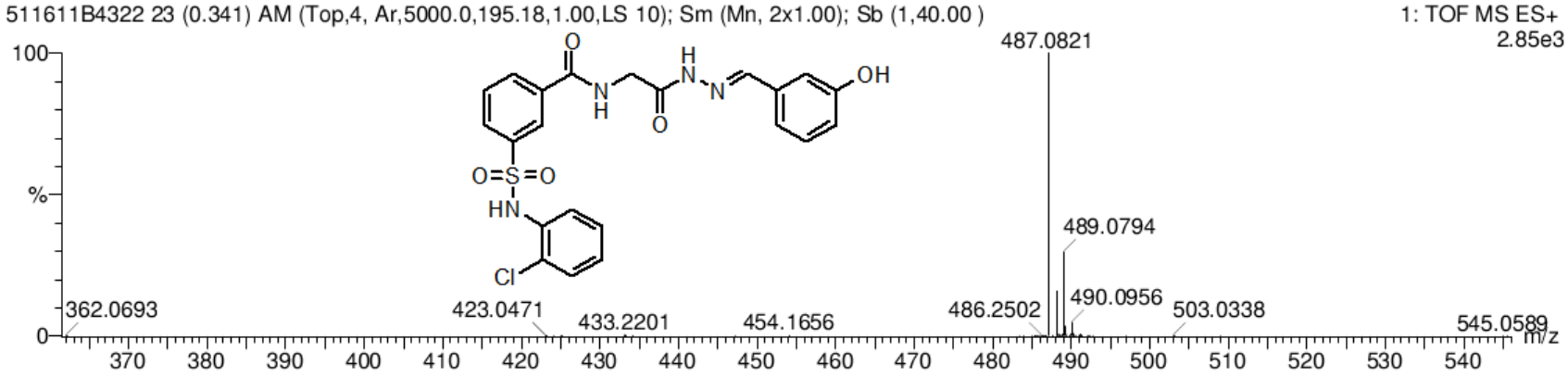
Elemental Composition Report

Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

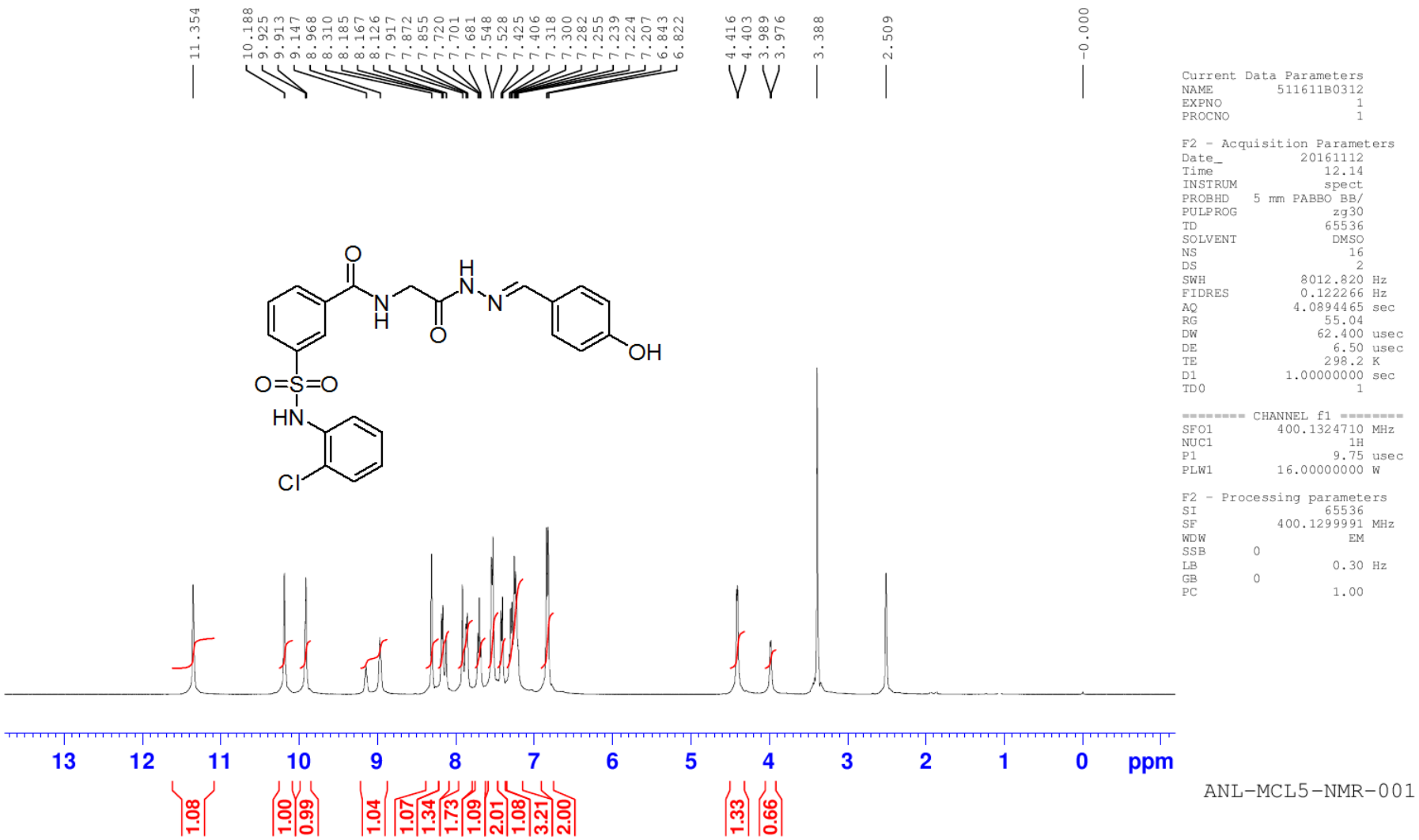
Monoisotopic Mass, Even Electron Ions
106 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-20 N: 0-4 O: 0-5 S: 0-1 Cl: 0-1

GVB-SA08
511611B4322 23 (0.341) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

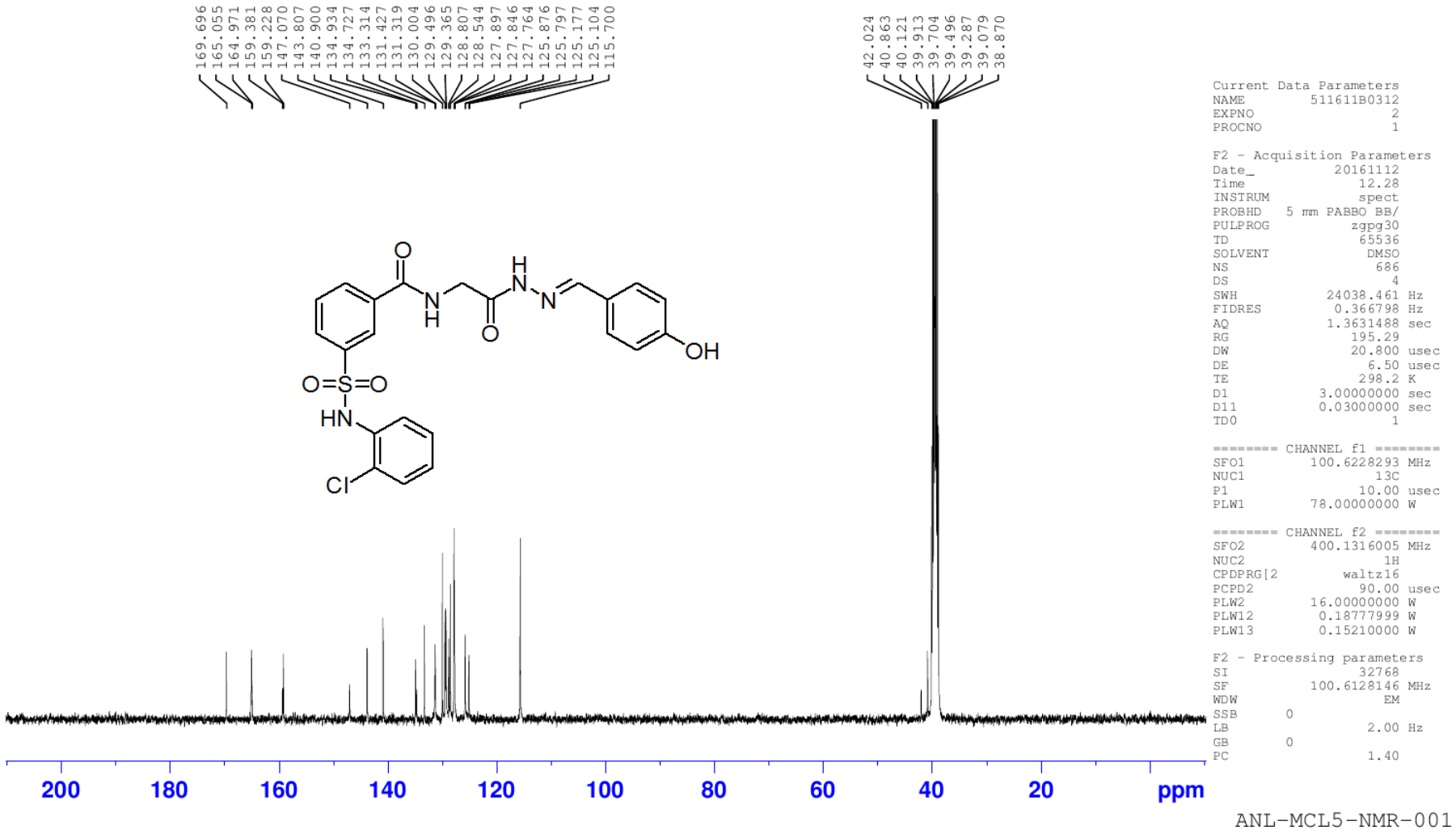


Minimum:				-1.5		
Maximum:		5.0	10000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
487.0821	487.0843	-2.2	-4.5	14.5	168119.6	C22 H20 N4 O5 S Cl

HRMS of **Compound-1g**



^{1}H NMR of **Compound-1h** in DMSO-d_6



^{13}CNMR of **Compound-1h** in DMSO-d_6

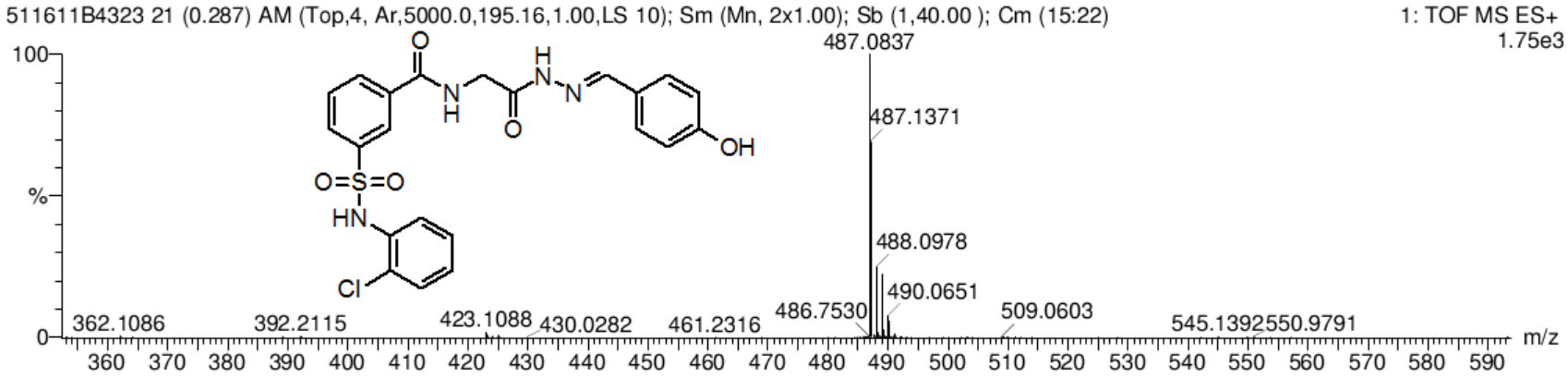
Elemental Composition Report

Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

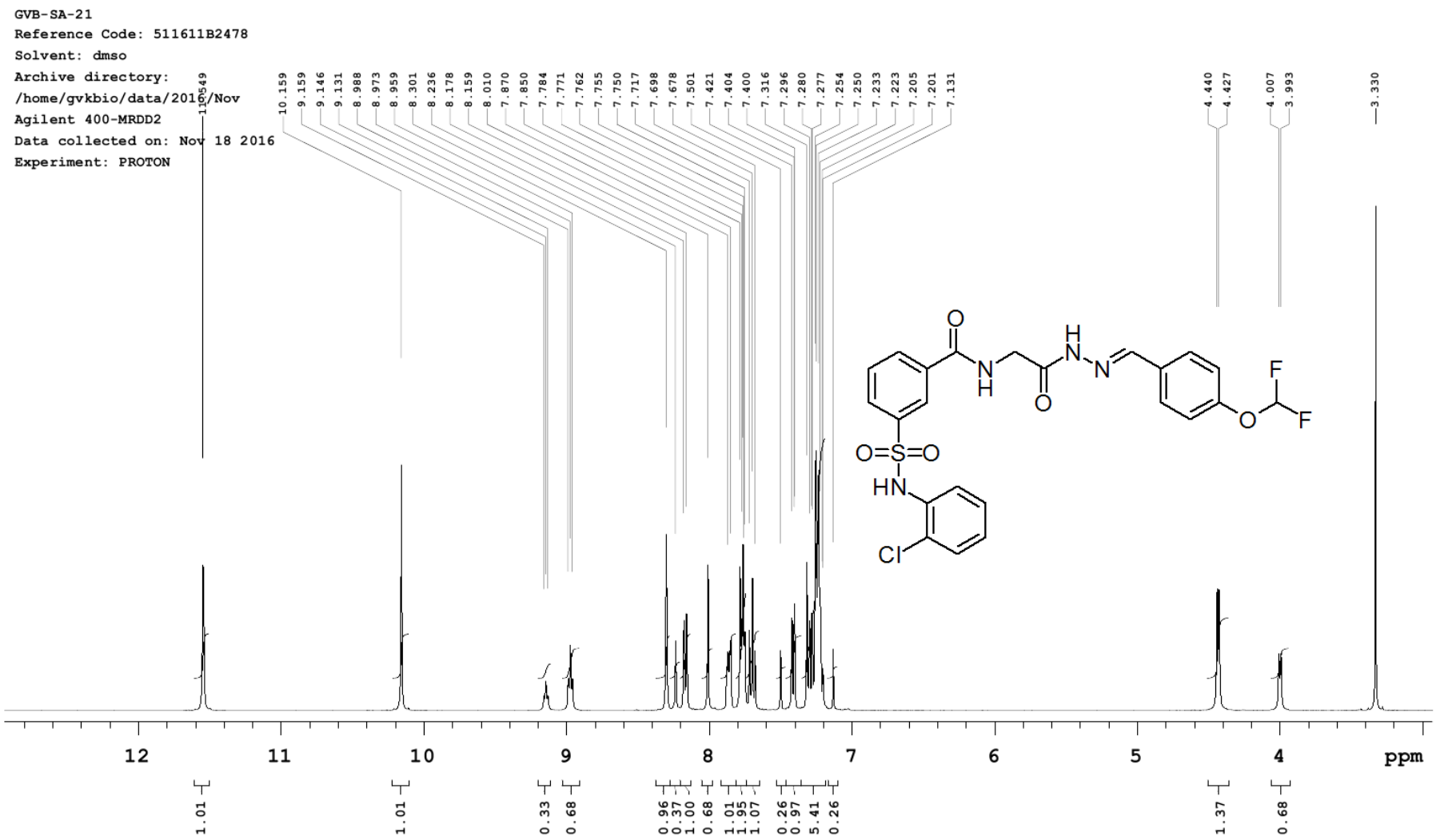
Monoisotopic Mass, Even Electron Ions
106 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-20 N: 0-4 O: 0-5 S: 0-1 Cl: 0-1

GVB-SA09
511611B4323 21 (0.287) AM (Top,4, Ar,5000.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (15:22)

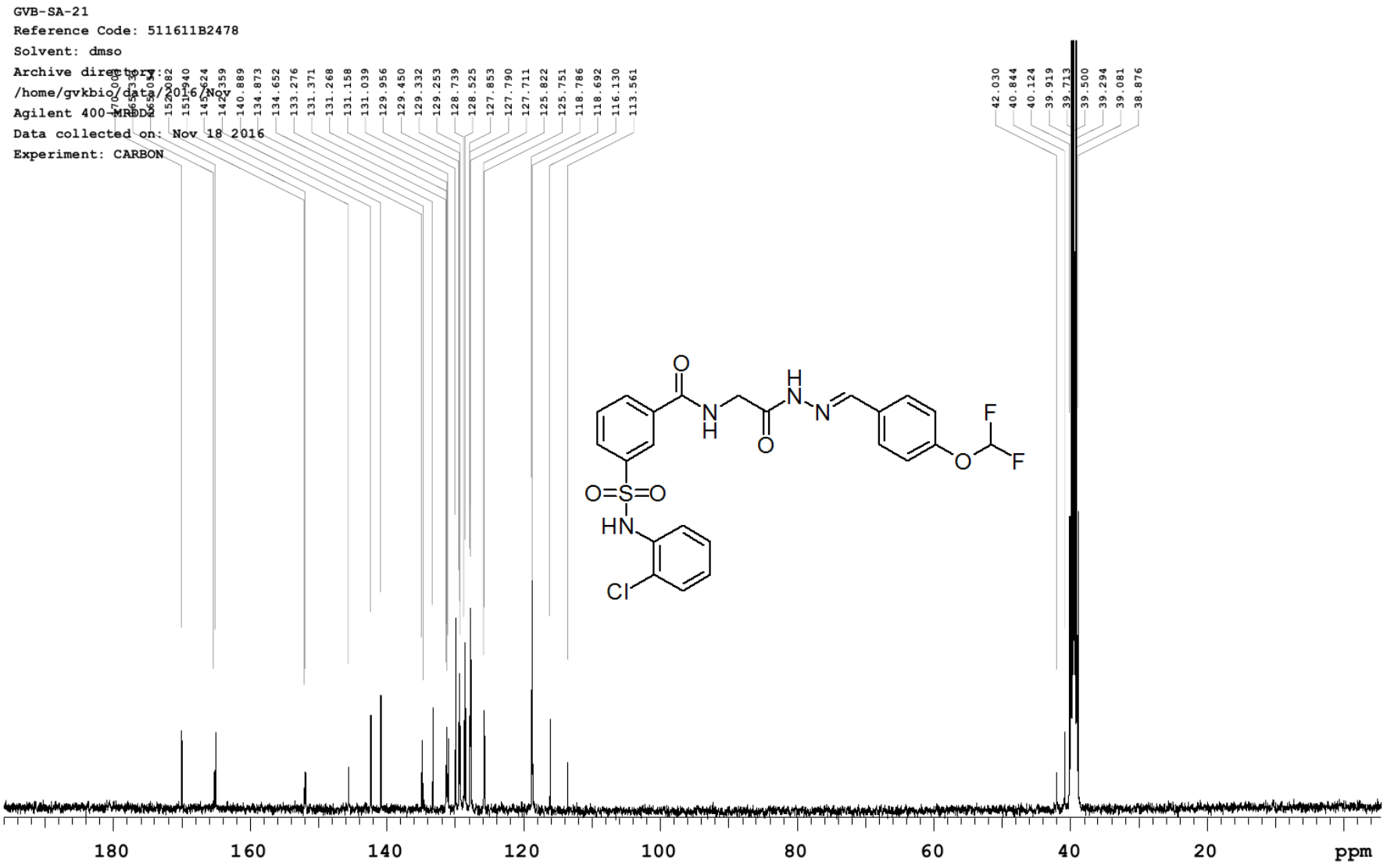


Minimum:				-1.5		
Maximum:		5.0	10000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
487.0837	487.0843	-0.6	-1.2	14.5	102982.1	C22 H20 N4 O5 S Cl

HRMS of **Compound-1h**



^{1}H NMR of **Compound-1i** in DMSO-d_6



^{13}CNMR of **Compound-1i** in DMSO-d_6

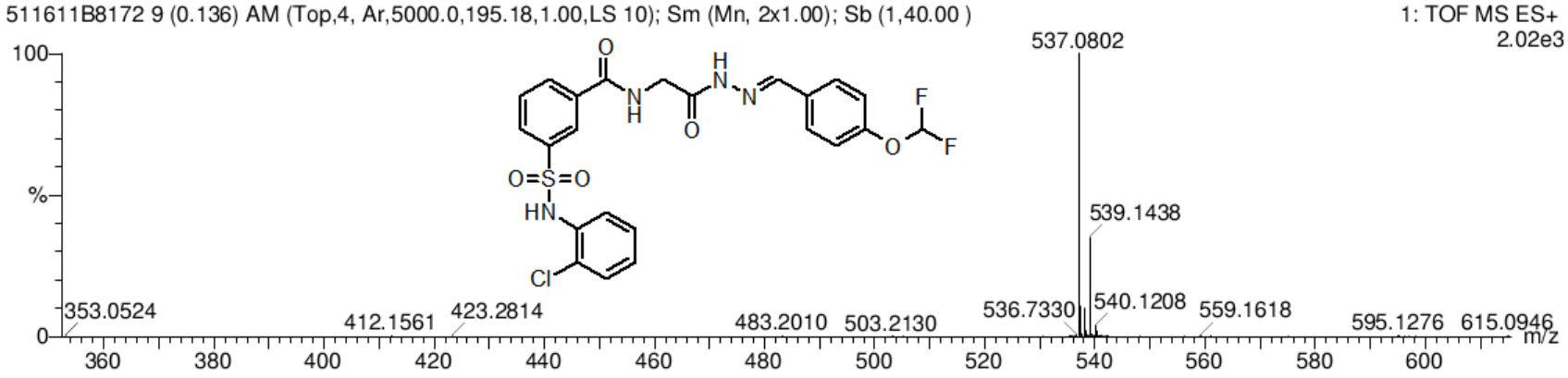
Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

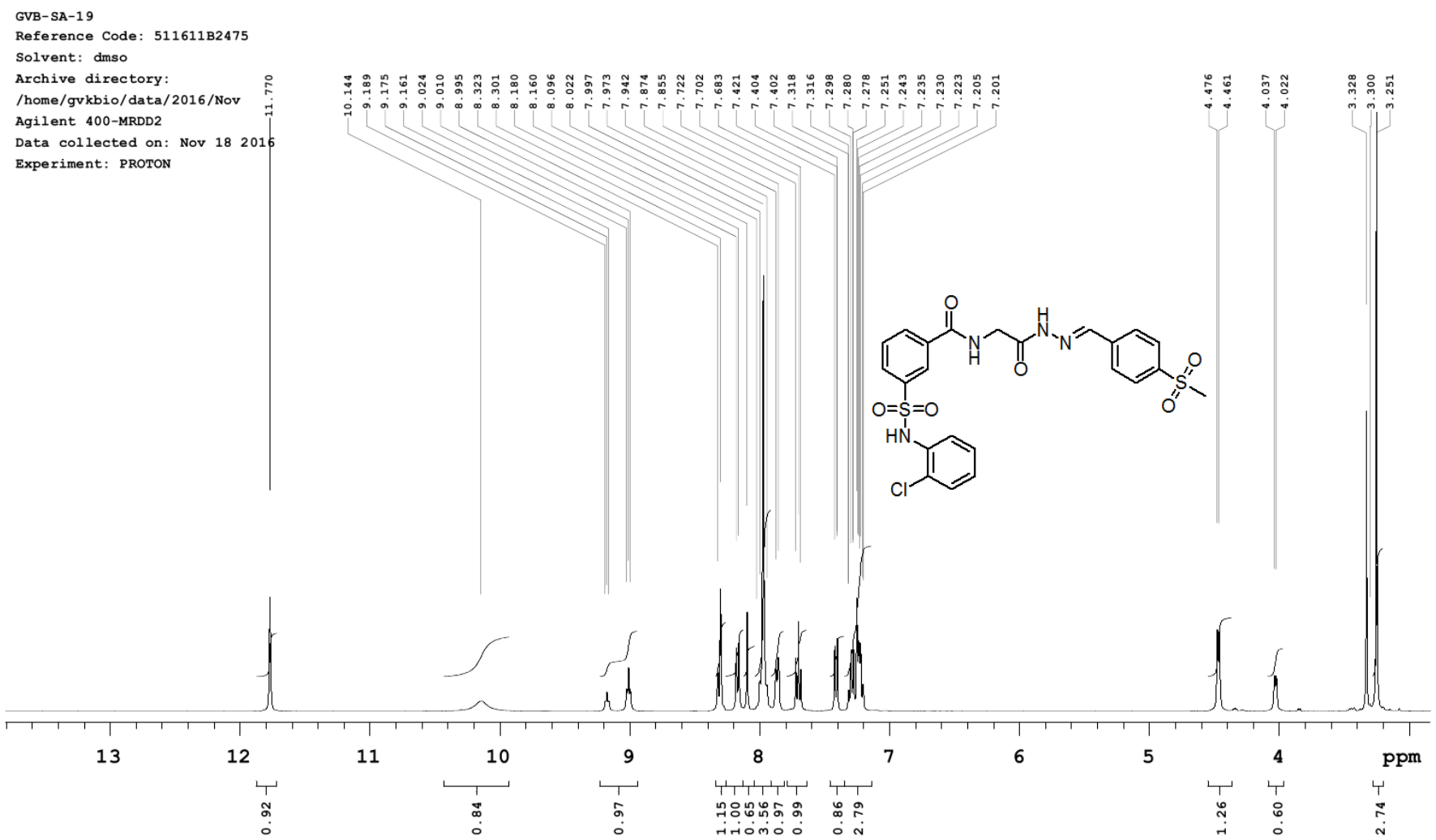
Monoisotopic Mass, Even Electron Ions
335 formula(e) evaluated with 2 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-24 H: 0-20 N: 0-4 O: 0-5 S: 0-1 Cl: 0-1 F: 0-2

GVB-SA21
511611B8172 9 (0.136) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

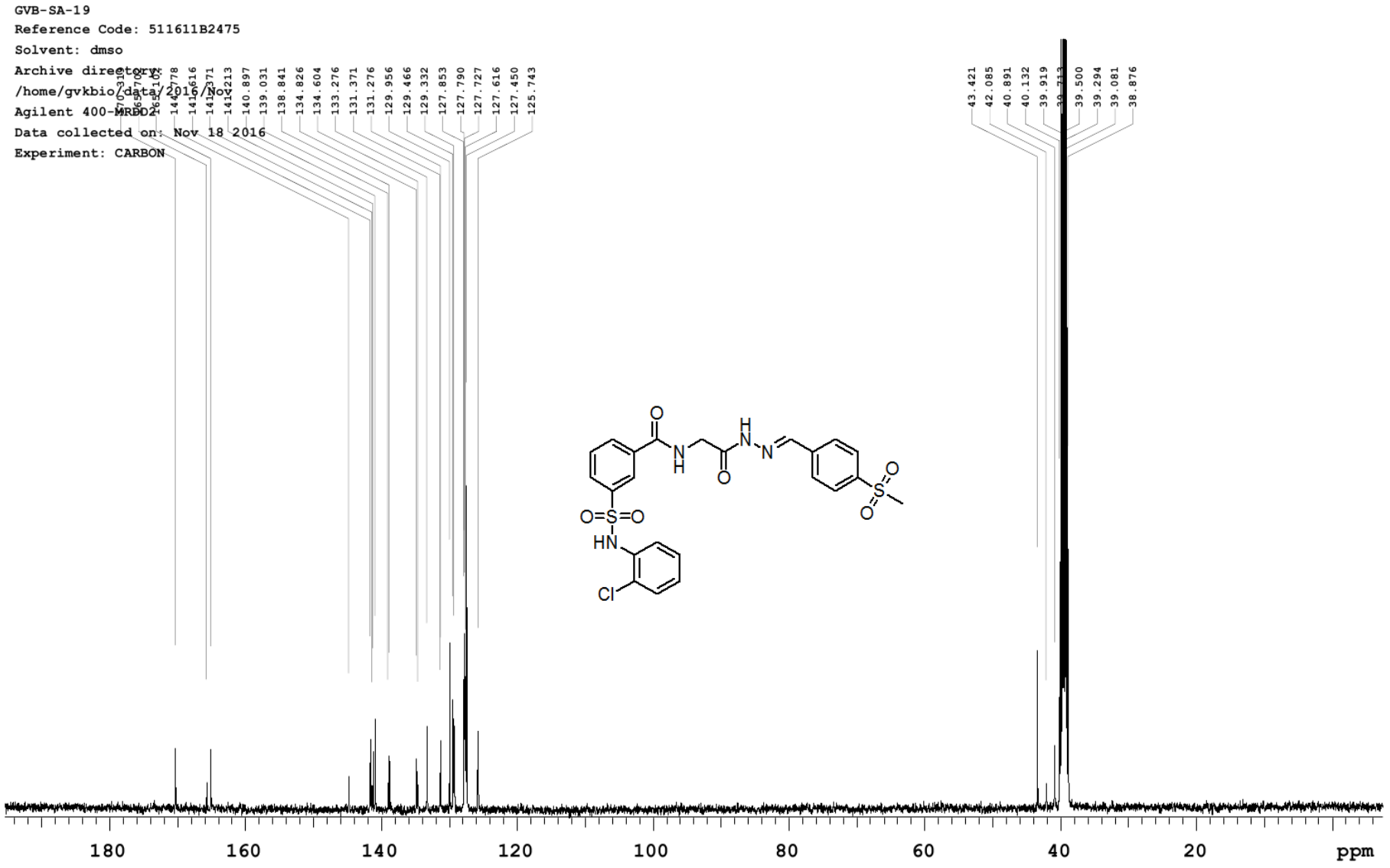


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
537.0802	537.0811	-0.9	-1.7	14.5	232.2	C23 H20 N4 O5 S Cl F2

HRMS of **Compound-1i**



^{1}H NMR of **Compound-1j** in DMSO-d_6



^{13}CNMR of **Compound-1j** in DMSO-d_6

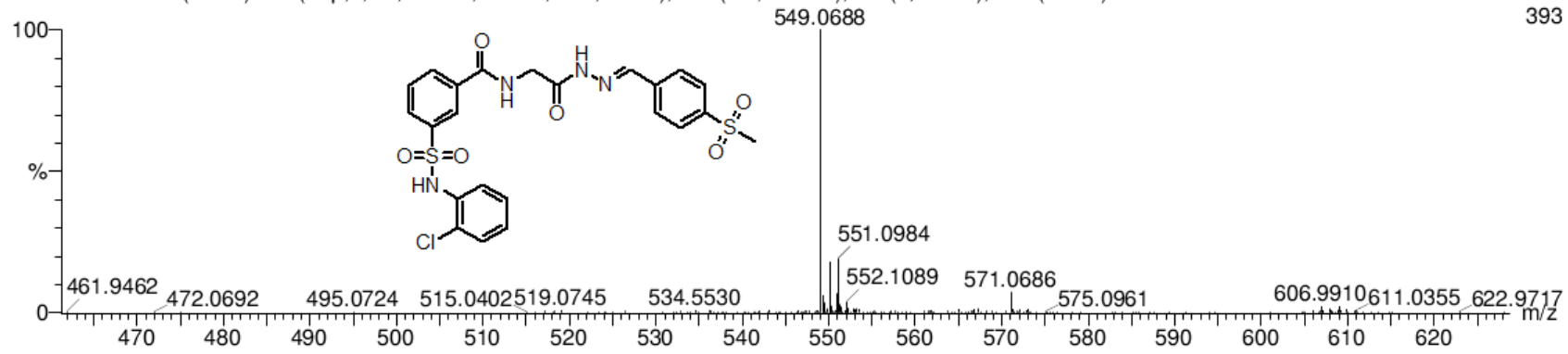
Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

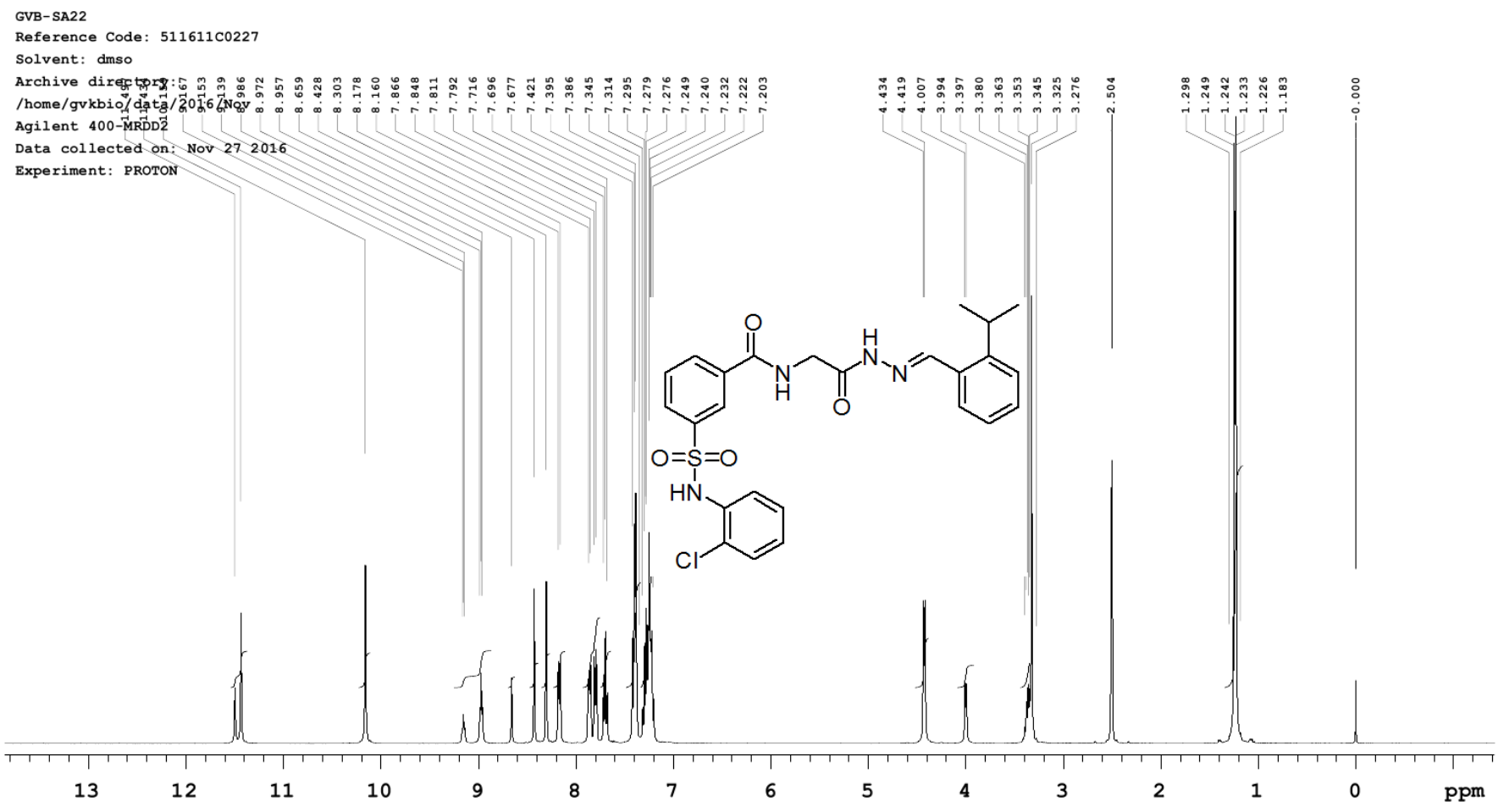
Monoisotopic Mass, Even Electron Ions
203 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-23 H: 0-22 N: 0-4 O: 0-6 S: 0-2 Cl: 0-1

GVB-SA19
511611B8169 56 (0.800) AM (Top,4, Ar,5000.0,195.15,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00); Cm (28:56) 1: TOF MS ES+
393

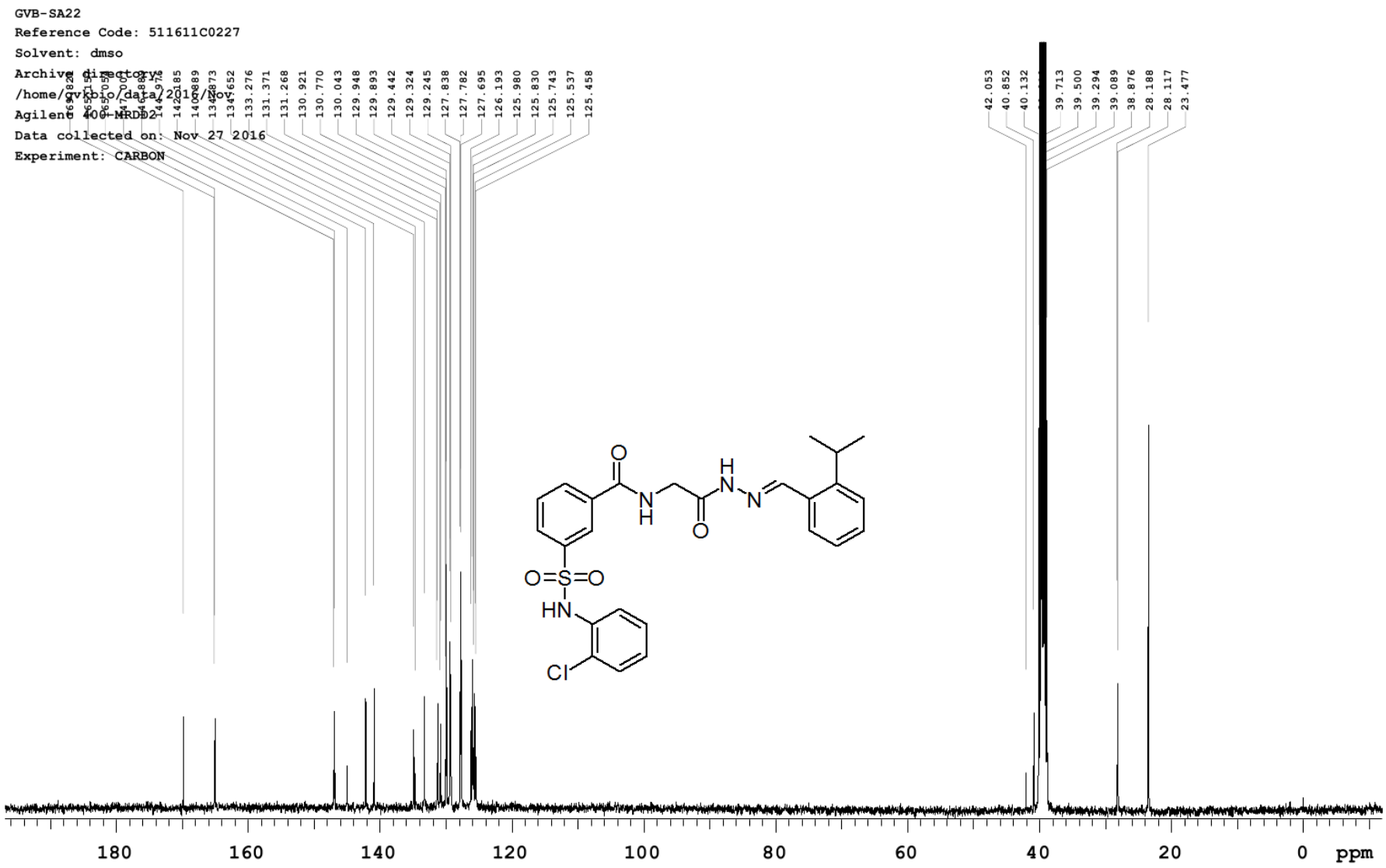


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
549.0688	549.0669	1.9	3.5	14.5	37.2	C23 H22 N4 O6 S2 Cl

HRMS of **Compound-1j**



^{1}H NMR of **Compound-1k** in DMSO-d_6



^{13}CNMR of **Compound-1k** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

93 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

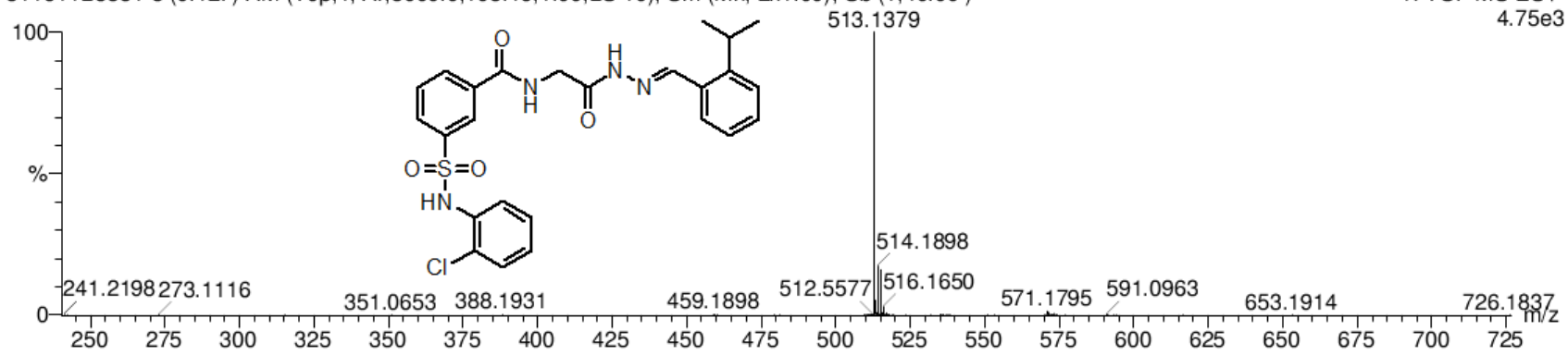
C: 0-25 H: 0-26 N: 0-4 O: 0-4 S: 0-1 Cl: 0-1

GVB-SA22

511611B8551 8 (0.127) AM (Top,4, Ar,5000.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

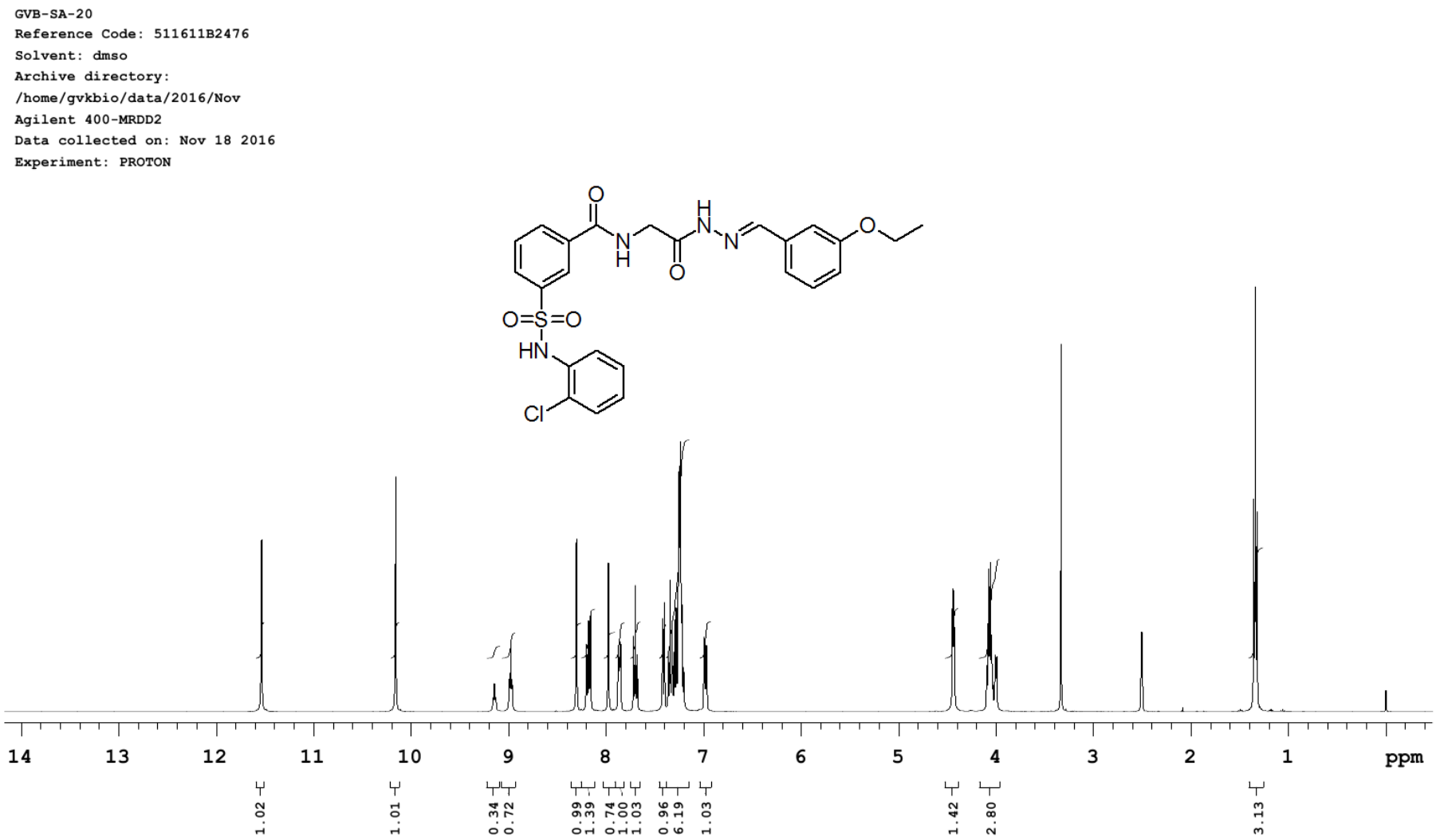
1: TOF MS ES+

4.75e3



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
513.1379	513.1363	1.6	3.1	14.5	525.4	C25 H26 N4 O4 S Cl

HRMS of **Compound-1k**



^{1}H NMR of **Compound-1l** in DMSO-d_6

^{13}CNMR of **Compound-1l** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

161 formula(e) evaluated with 7 results within limits (up to 1 best isotopic matches for each mass)

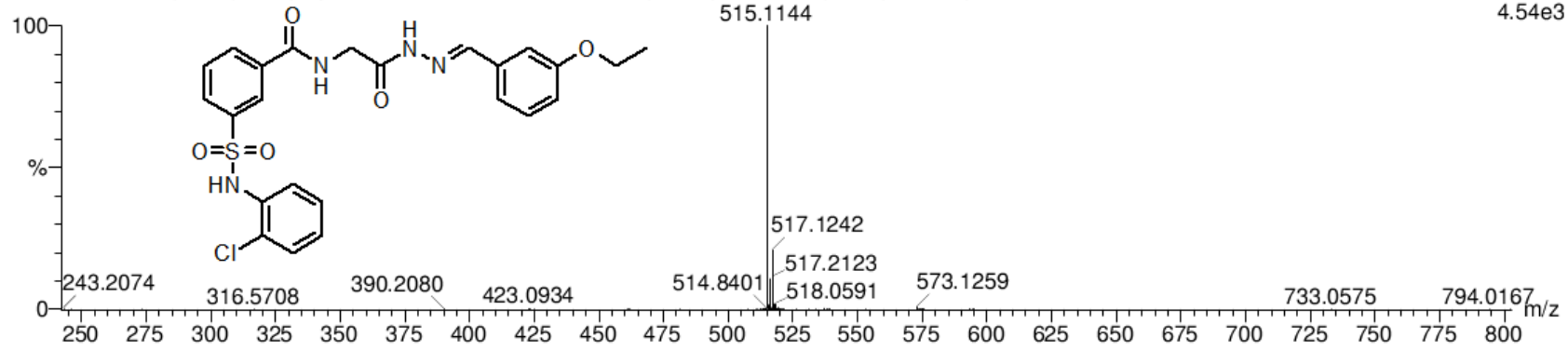
Elements Used:

C: 0-24 H: 0-24 N: 0-4 O: 0-5 S: 0-2 Cl: 0-1

GVB-SA20

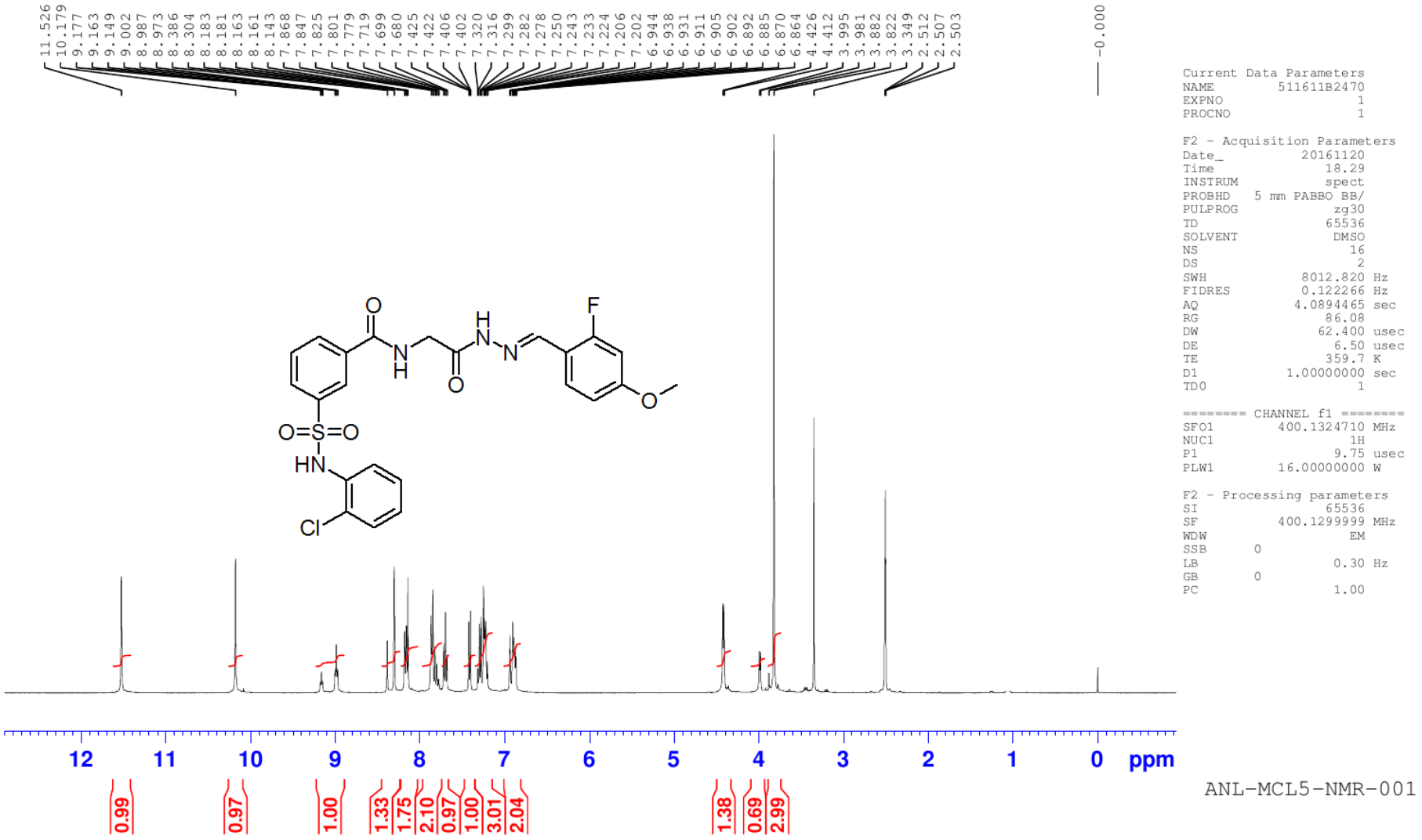
511611B8171 8 (0.126) AM (Top,4, Ar,5000.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
4.54e3



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
515.1144	515.1156	-1.2	-2.3	14.5	481.0	C24 H24 N4 O5 S Cl

HRMS of **Compound-1l**

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PROCNO                 1

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Time               18.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  86.08
DW                 62.400 usec
DE                  6.50 usec
TE                 359.7 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                   9.75 usec
PLW1        16.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.1299999 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
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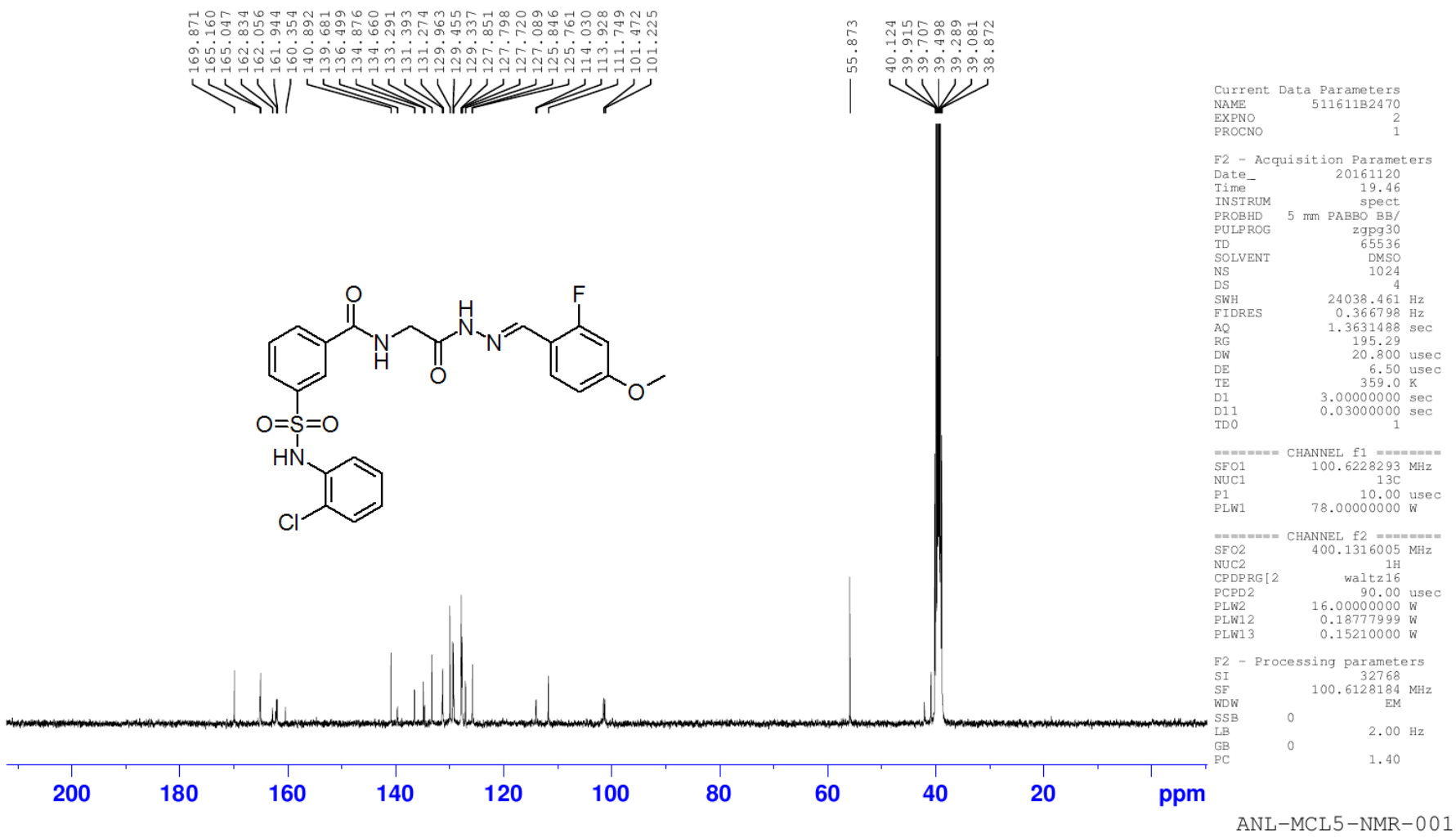
ANL-MCL5-NMR-001

^{1}H NMR of **Compound-1m** in DMSO-d_6



^{13}CNMR of **Compound-1m** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

230 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

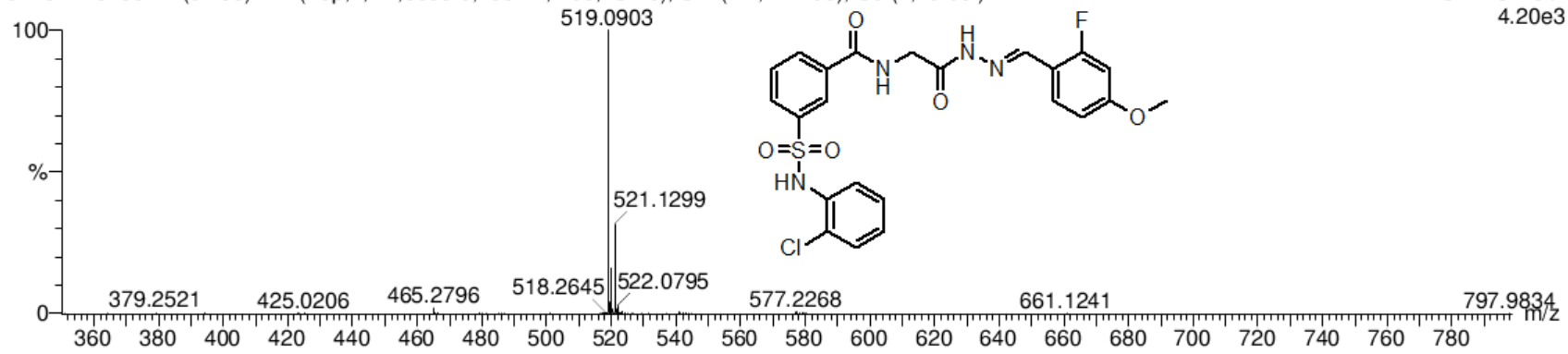
Elements Used:

C: 0-23 H: 0-21 N: 0-4 O: 0-5 F: 0-1 S: 0-1 Cl: 0-1

GVB-SA16

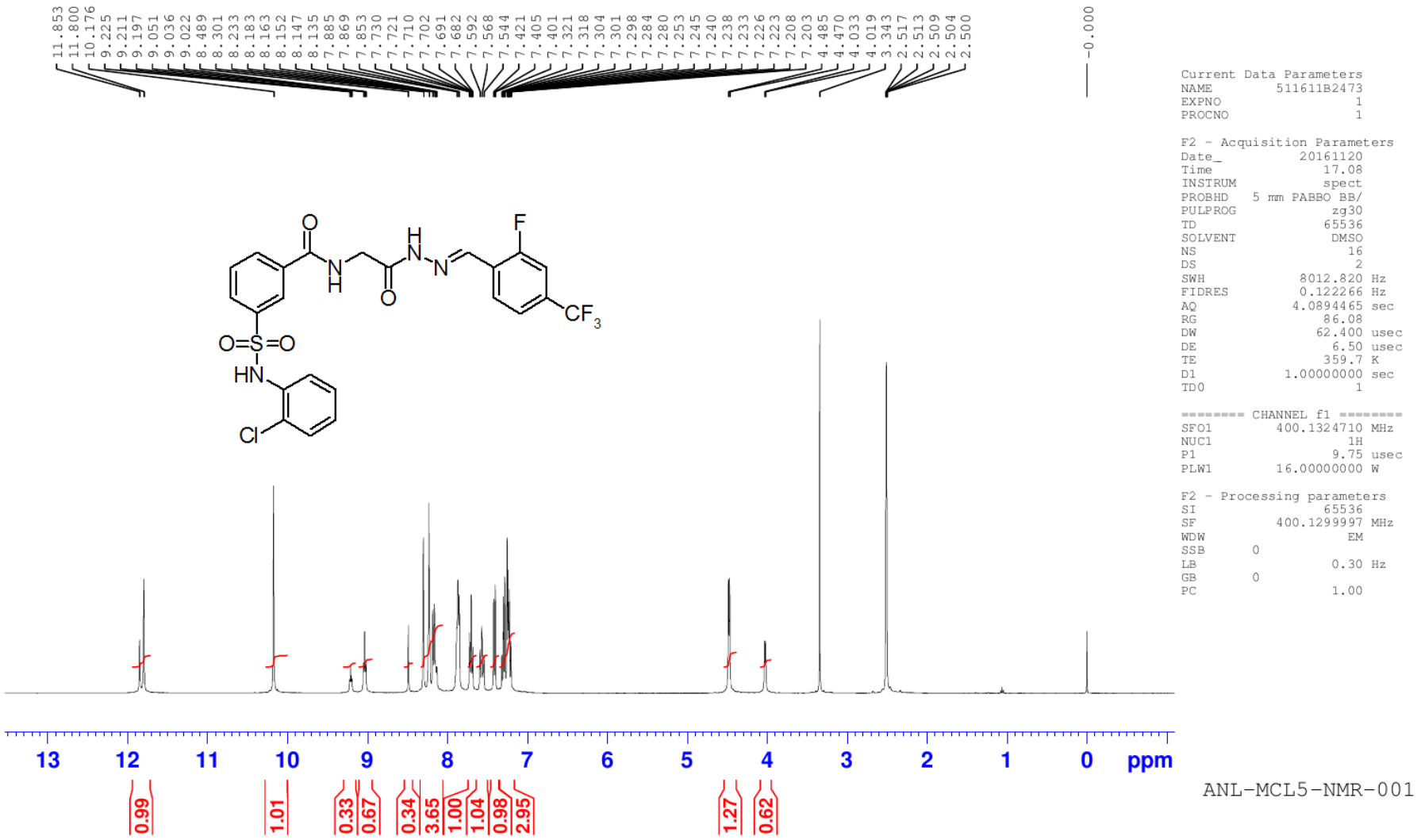
511611B8166 14 (0.186) AM (Top,4, Ar,5000.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
4.20e3



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
519.0903	519.0905	-0.2	-0.4	14.5	174.9	C23 H21 N4 O5 F S Cl

HRMS of **Compound-1m**

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EXPNO                   1
PROCNO                  1

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Time                17.08
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  86.08
DW                 62.400 usec
DE                  6.50 usec
TE                 359.7 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                   1H
P1                   9.75 usec
PLW1          16.00000000 W

F2 - Processing parameters
SI                  65536
SF            400.1299997 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
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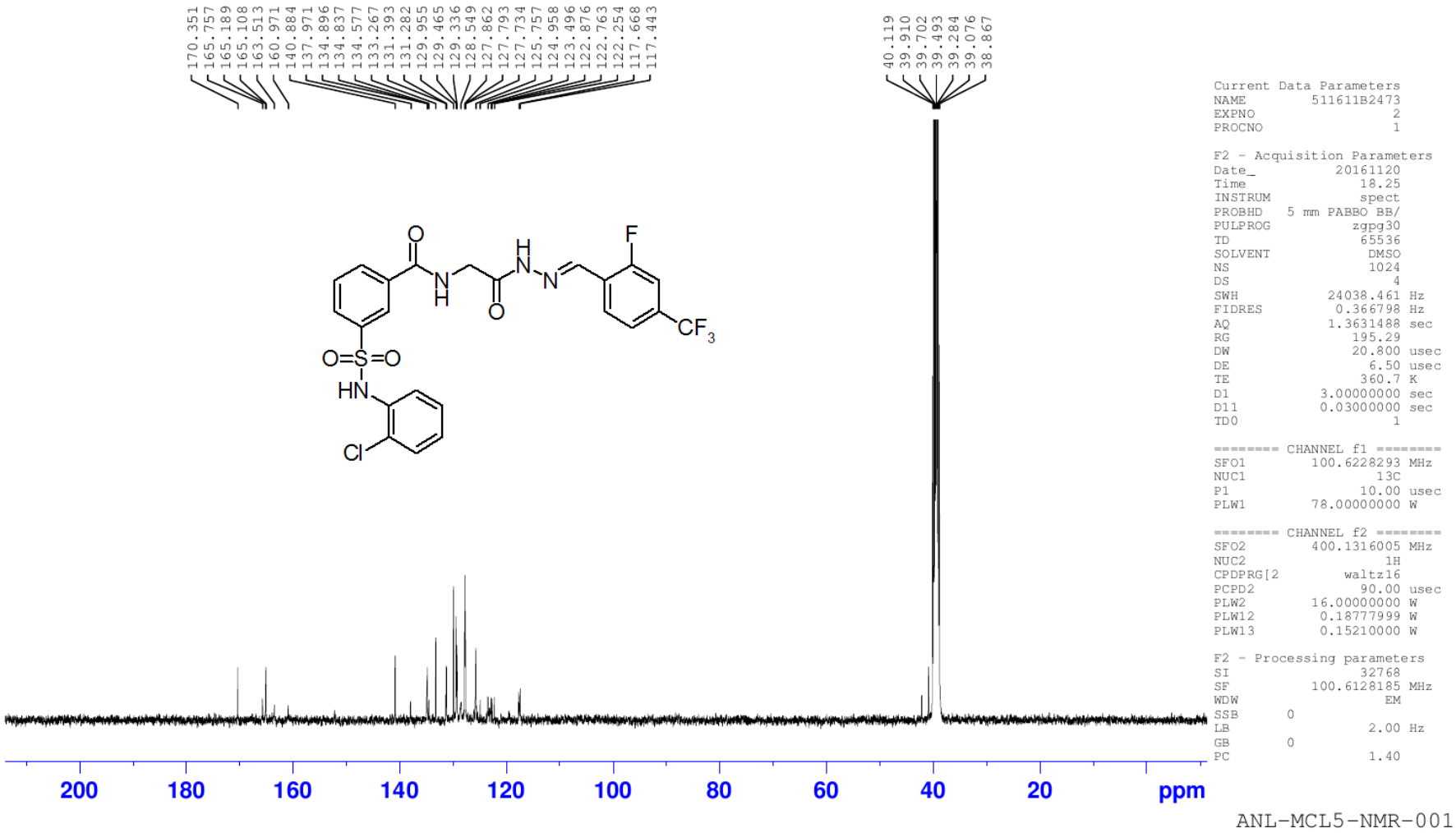
ANL-MCL5-NMR-001

^{1}H NMR of **Compound-1n** in DMSO-d_6



^{13}CNMR of **Compound-1n** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

489 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

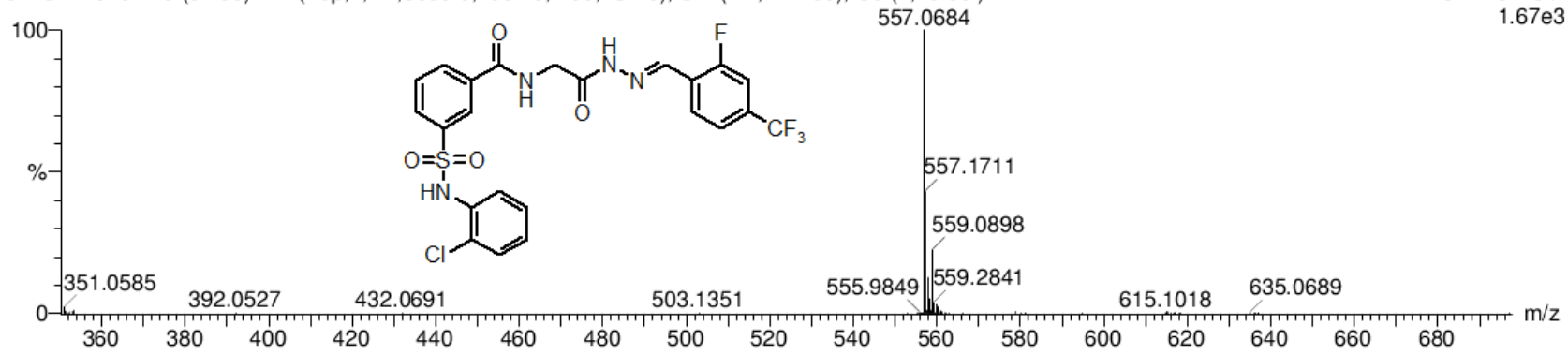
C: 0-23 H: 0-18 N: 0-4 O: 0-4 F: 0-4 S: 0-1 Cl: 0-1

GVB-SA17

511611B8167 16 (0.238) AM (Top,4, Ar,5000.0,195.20,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

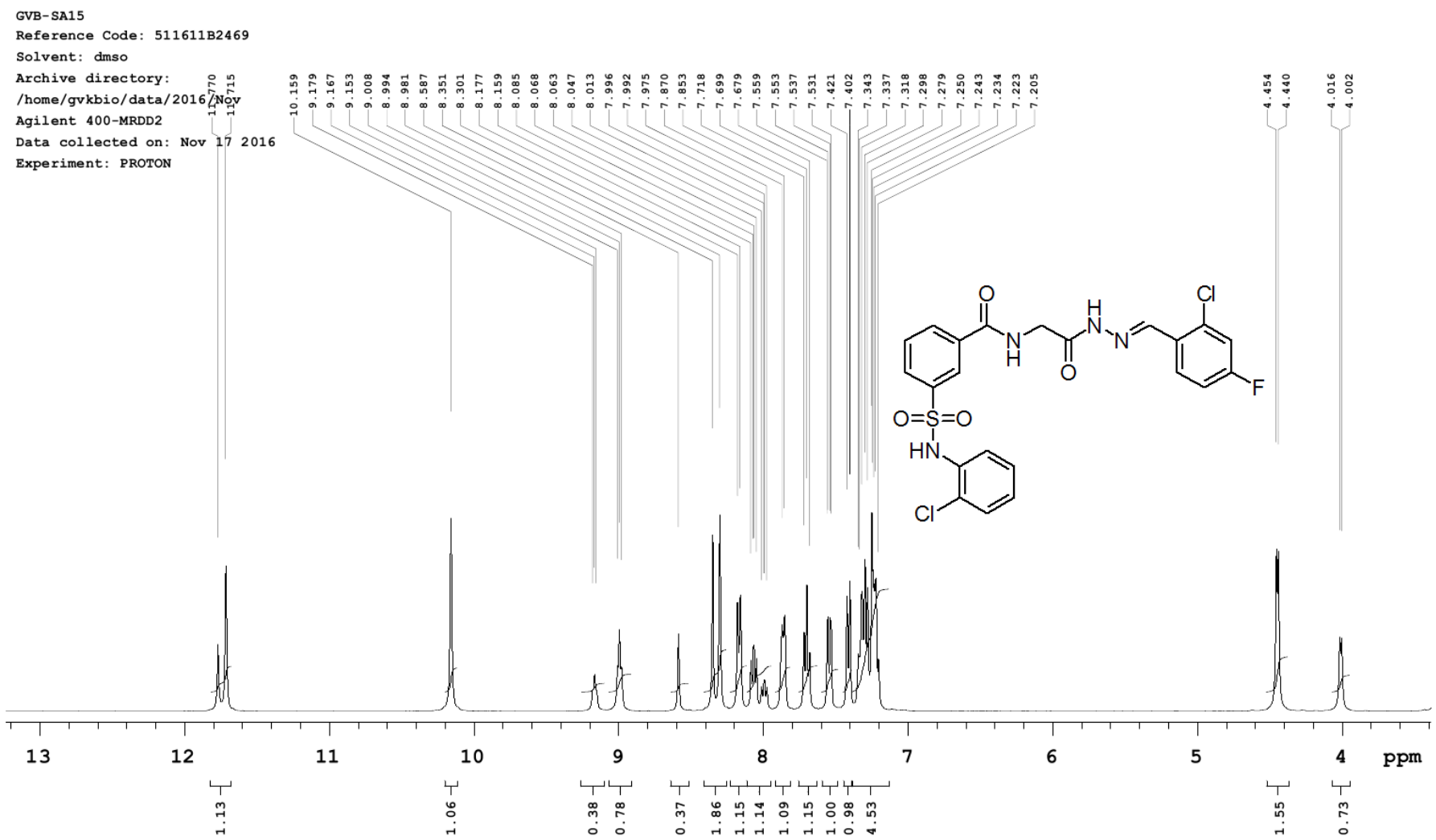
1: TOF MS ES+

1.67e3

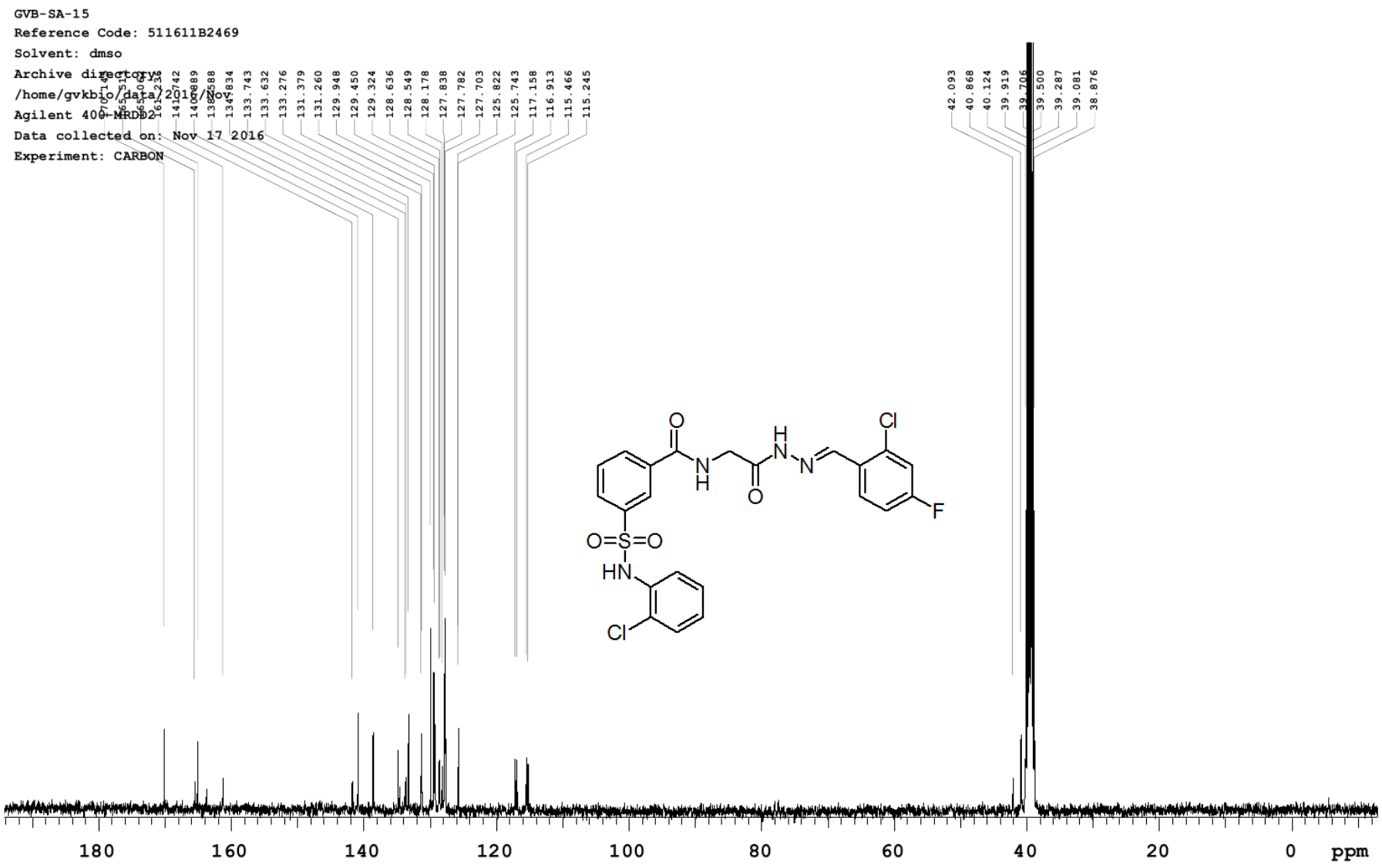


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
557.0684	557.0673	1.1	2.0	14.5	128.2	C23 H18 N4 O4 F4 S Cl

HRMS of **Compound-1n**



^{1}H NMR of **Compound-1o** in DMSO-d_6



^{13}CNMR of **Compound-1o** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

290 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

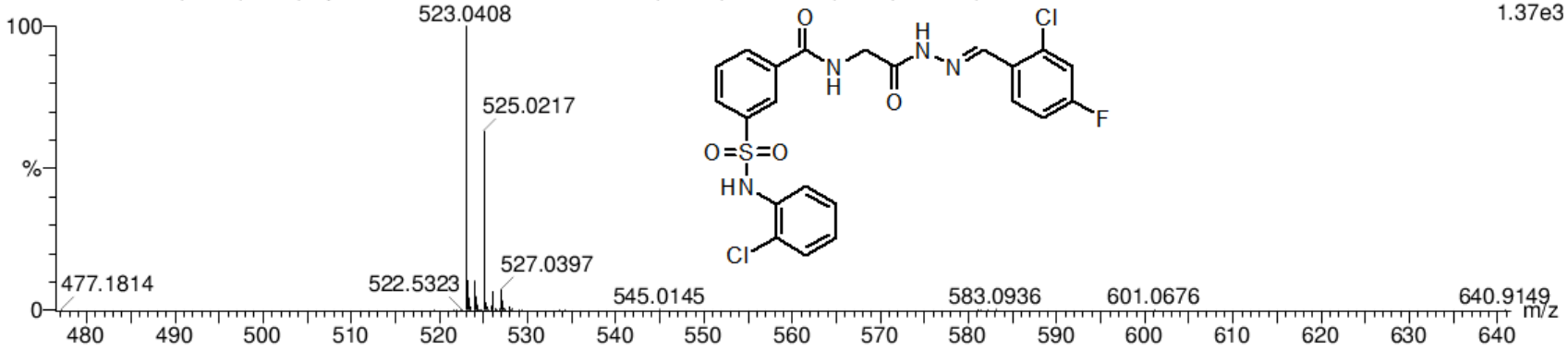
Elements Used:

C: 0-22 H: 0-18 N: 0-4 O: 0-4 F: 0-1 S: 0-1 Cl: 0-2

GVB-SA15

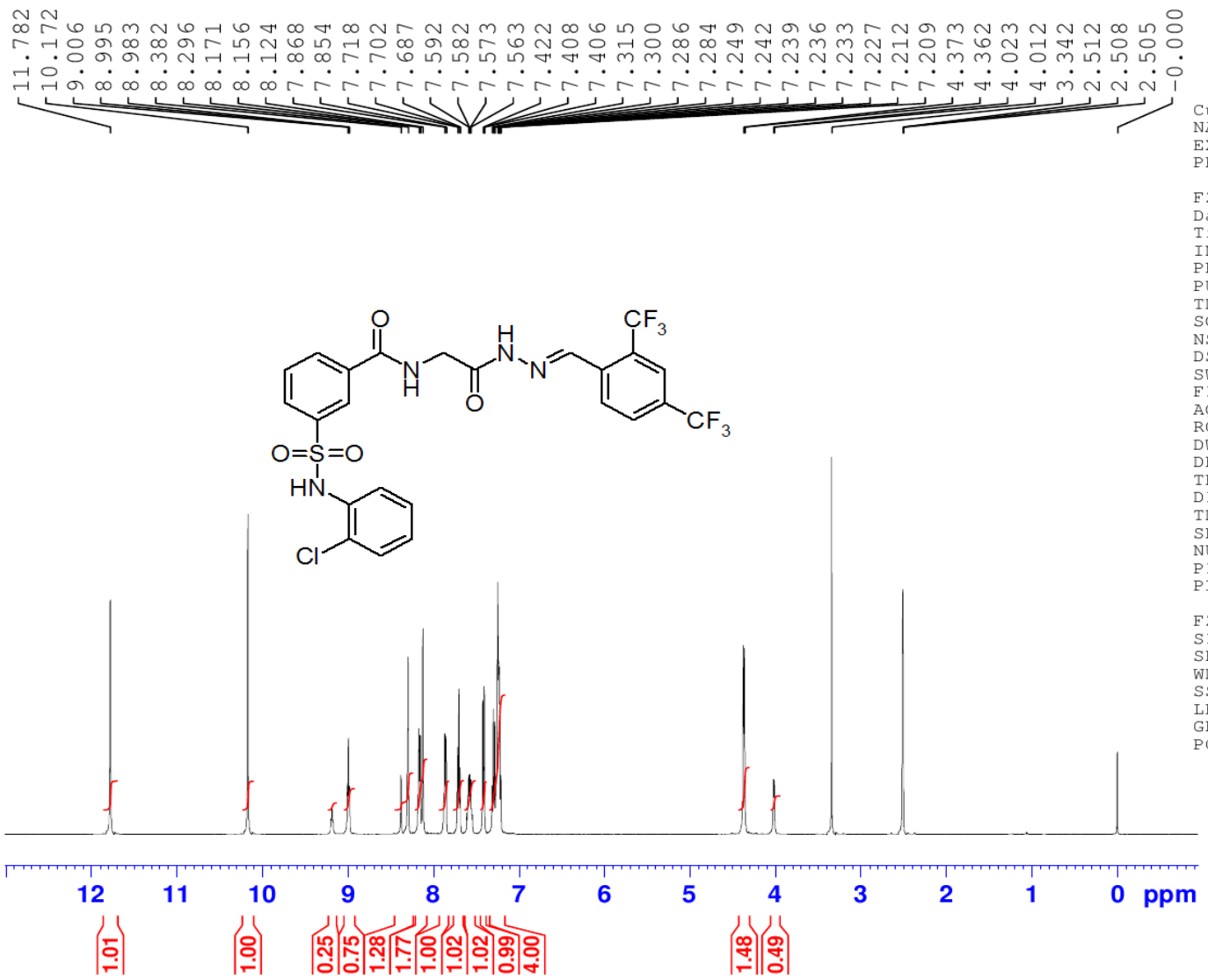
511611B8164 17 (0.251) AM (Top,4, Ar,5000.0,195.15,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
1.37e3

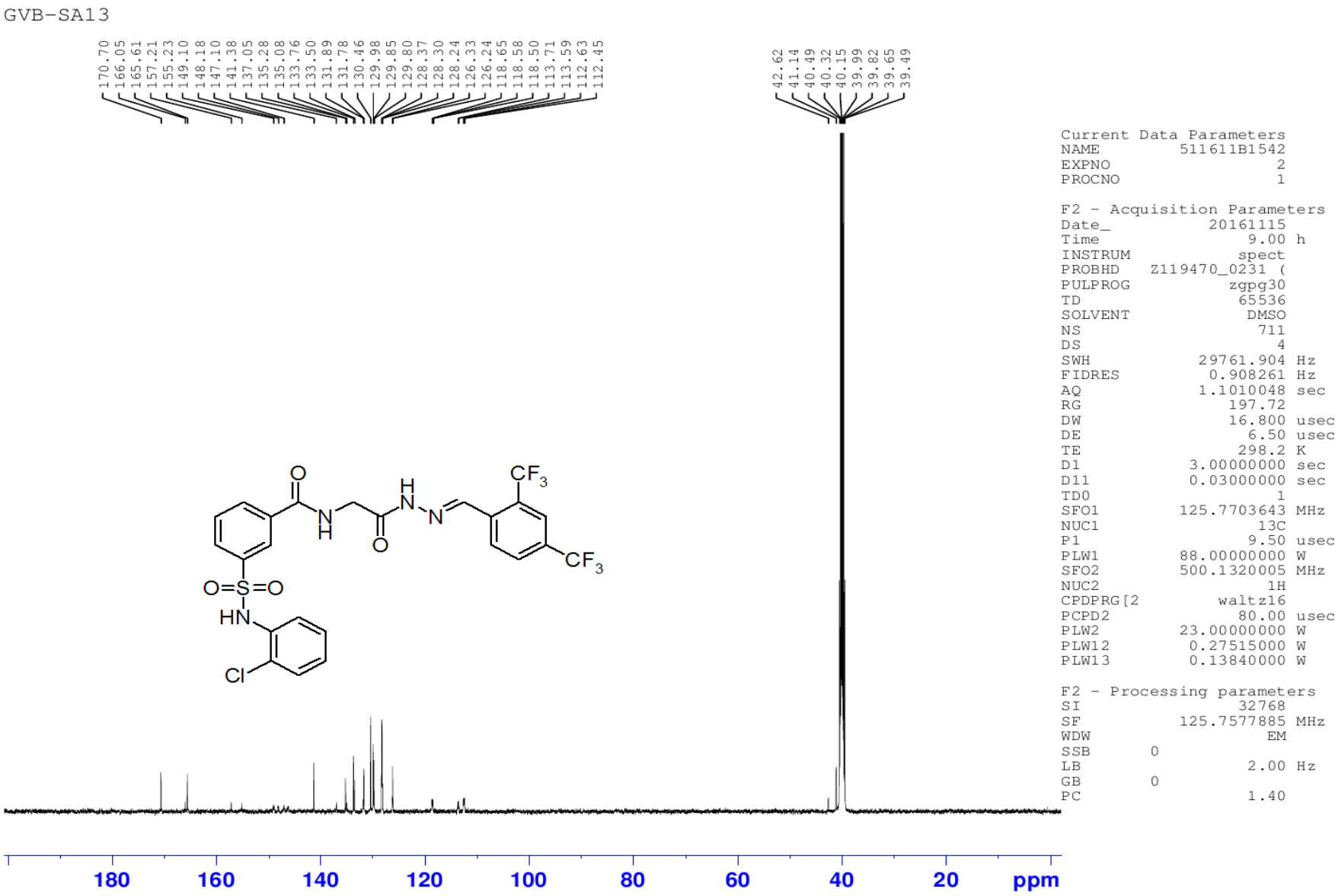


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
523.0408	523.0410	-0.2	-0.4	14.5	120.3	C22 H18 N4 O4 F S Cl2

HRMS of **Compound-1o**



^{1}H NMR of **Compound-1p** in DMSO-d_6



^{13}CNMR of **Compound-1p** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

689 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

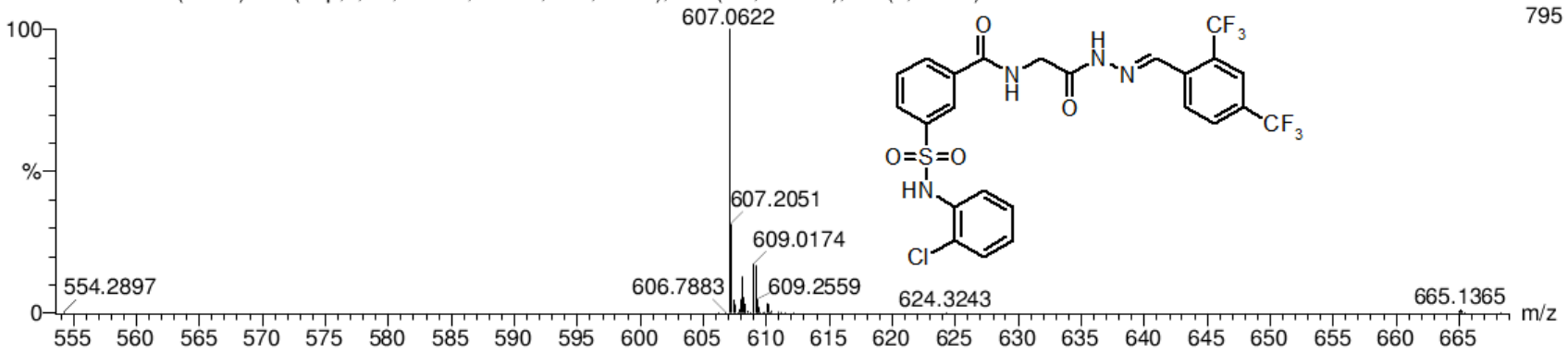
C: 0-24 H: 0-18 N: 0-4 O: 0-4 F: 0-6 S: 0-1 Cl: 0-1

GVB-SA13

511611B8159 16 (0.238) AM (Top,4, Ar,5000.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

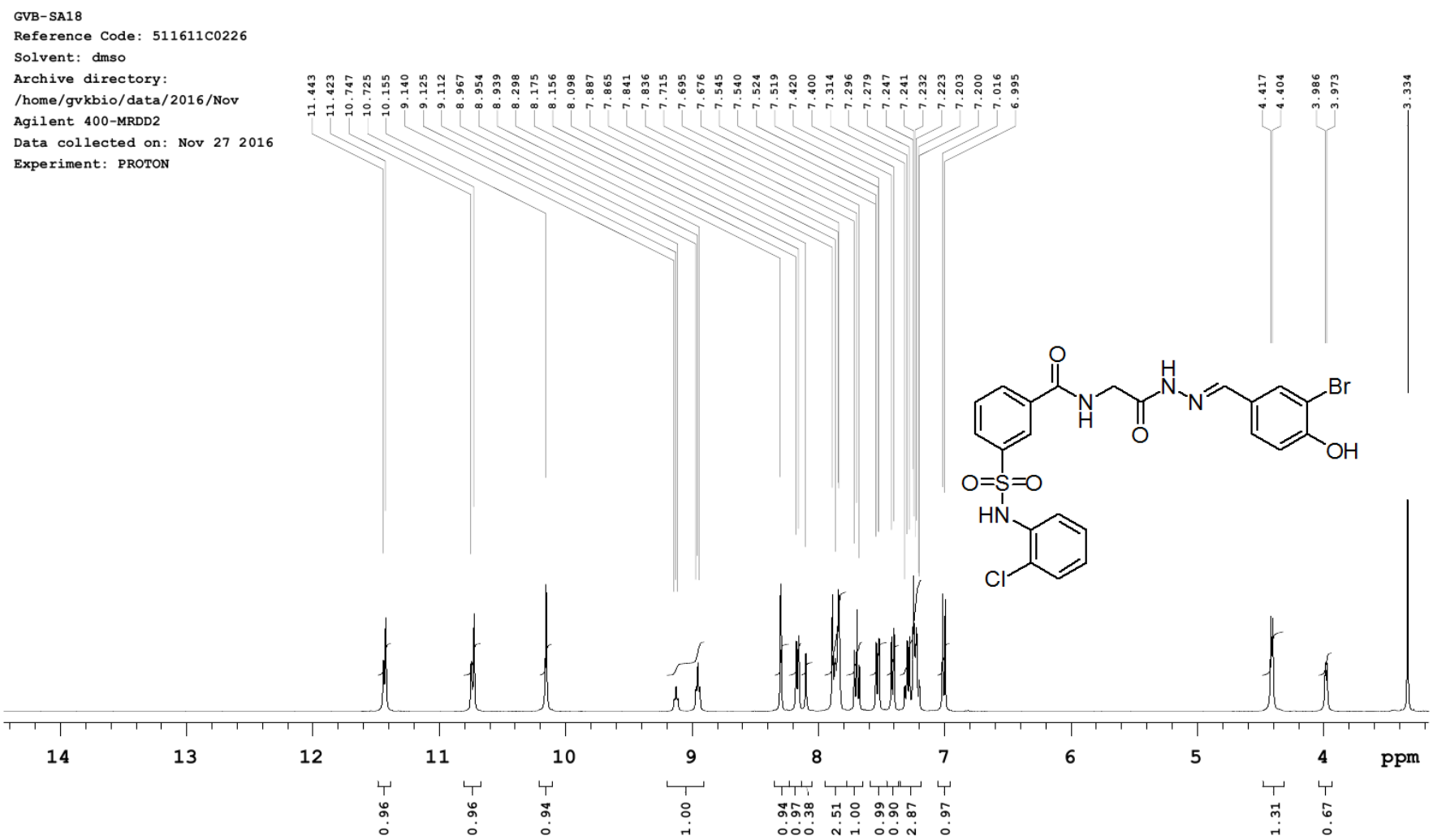
1: TOF MS ES+

795

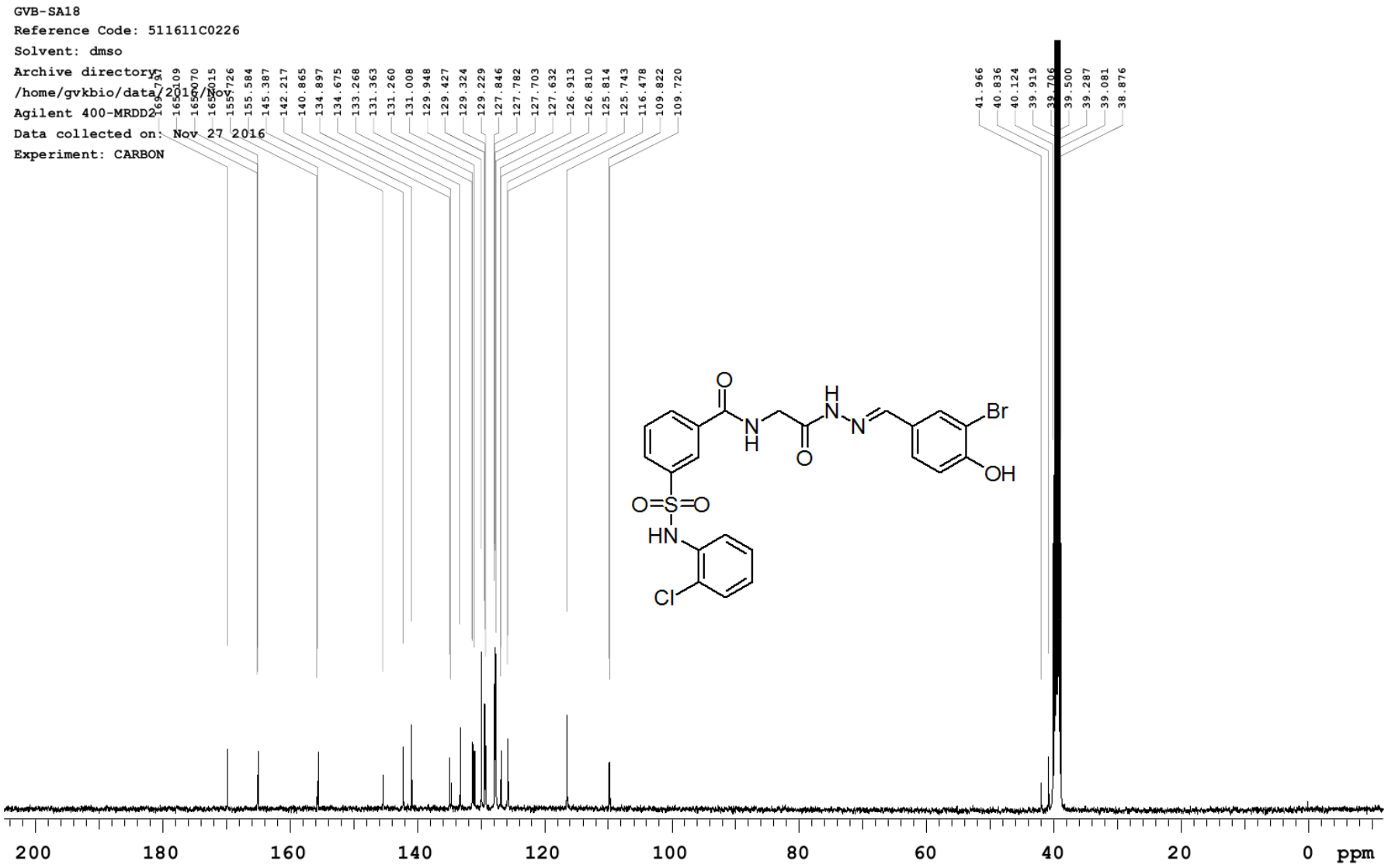


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
607.0622	607.0641	-1.9	-3.1	14.5	85.5	C24 H18 N4 O4 F6 S Cl

HRMS of **Compound-1p**



^{1}H NMR of **Compound-1q** in DMSO-d_6



^{13}CNMR of **Compound-1q** in DMSO-d_6

Elemental Composition Report

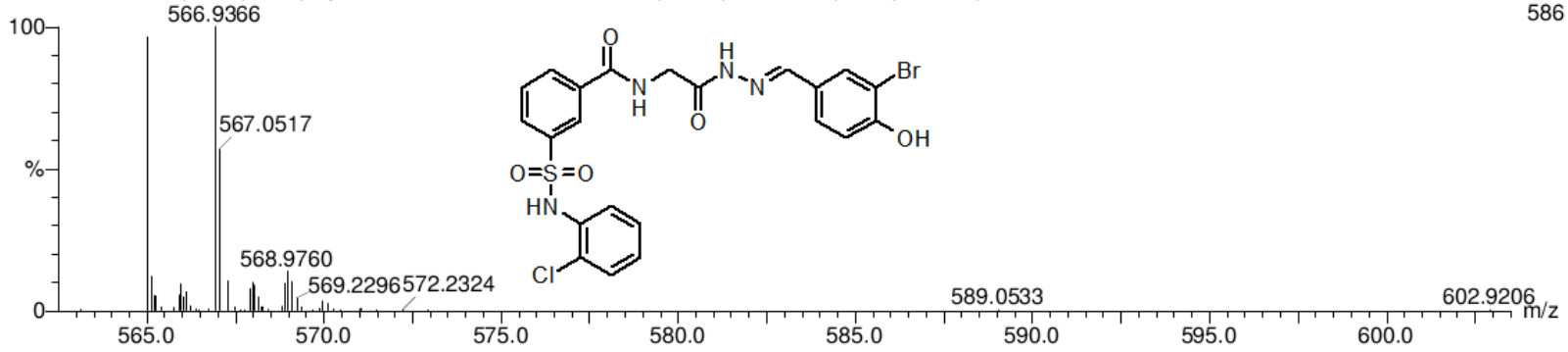
Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
233 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-19 N: 0-4 O: 0-5 S: 0-1 Cl: 0-1 Br: 0-1

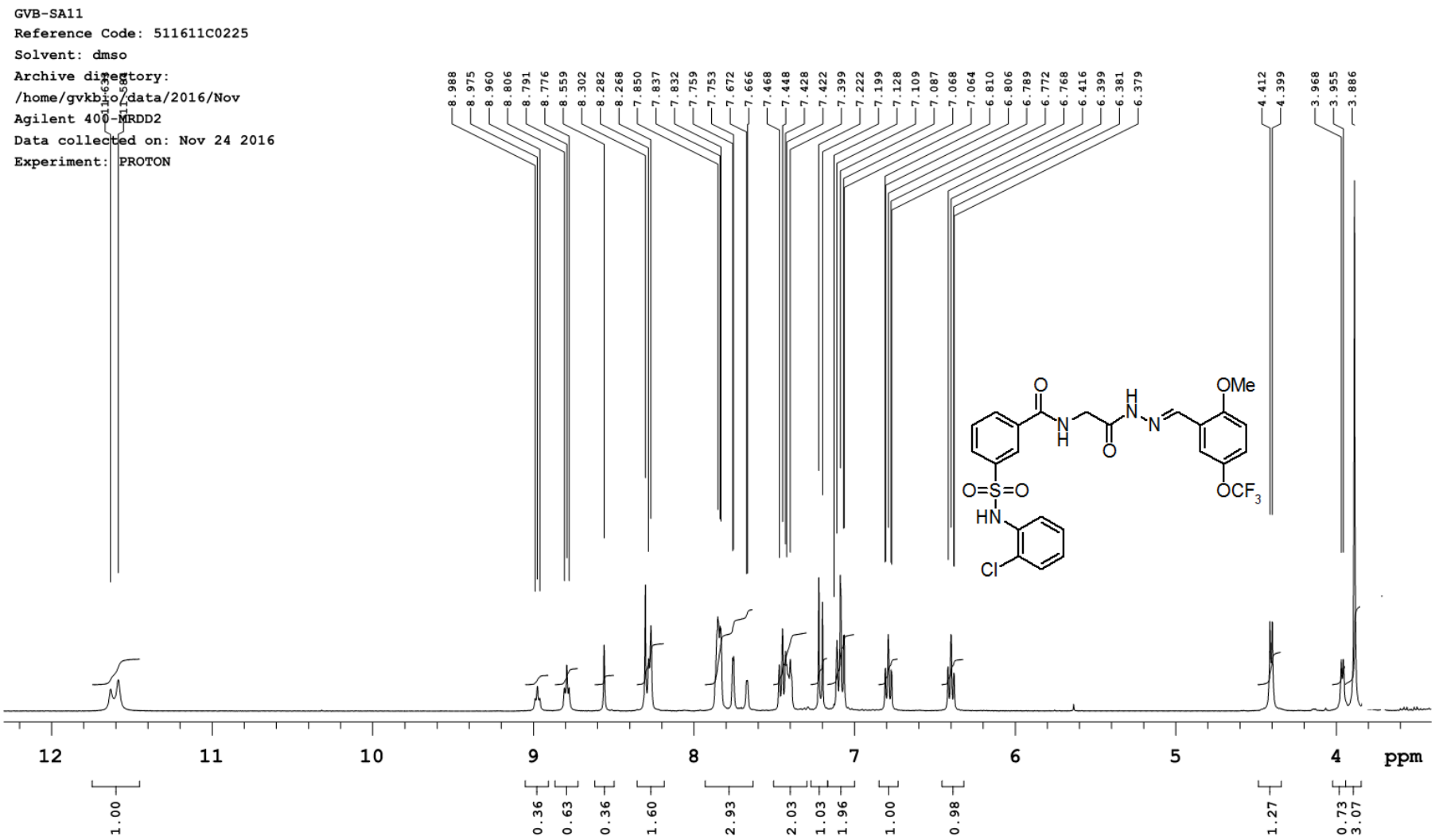
GVB-SA18
511611B8168 15 (0.229) AM (Top,4, Ar,5000.0,195.14,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
586

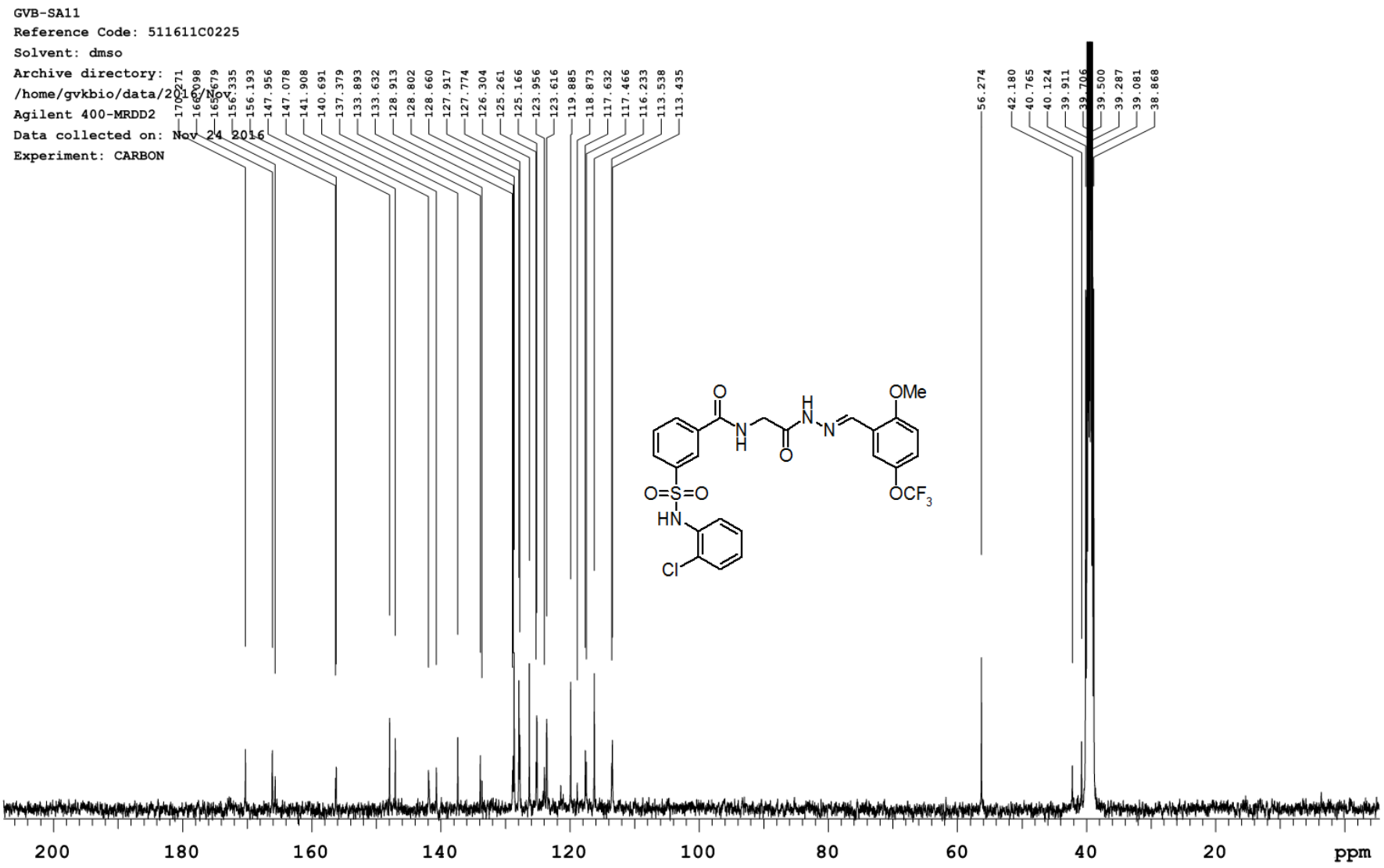


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
564.9930	564.9948	-1.8	-3.2	14.5	4654.9	C22 H19 N4 O5 S Cl Br

HRMS of **Compound-1q**



^{1}H NMR of **Compound-1r** in DMSO-d_6



^{13}CNMR of **Compound-1r** in DMSO-d_6

Elemental Composition Report

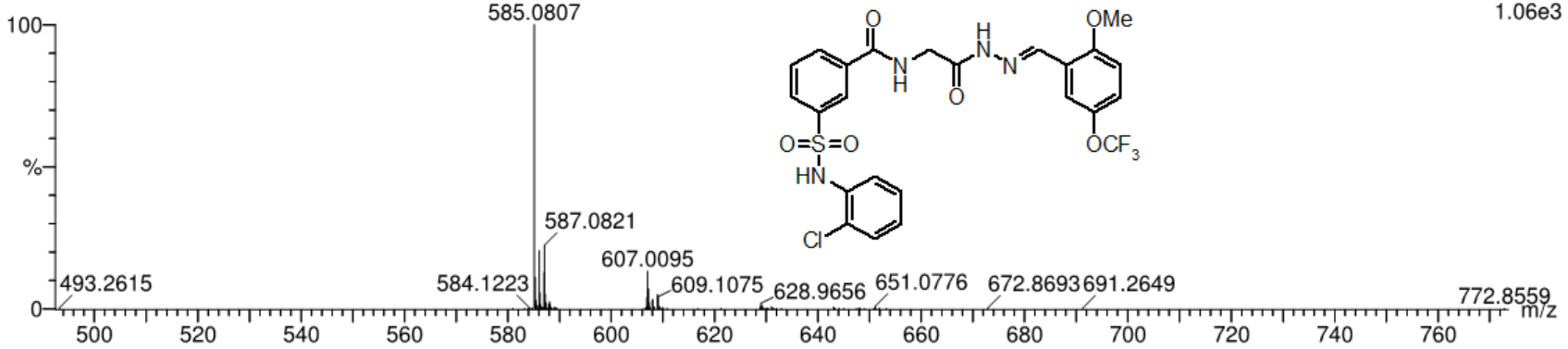
Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
549 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-24 H: 0-21 N: 0-4 O: 0-6 F: 0-3 S: 0-1 Cl: 0-1

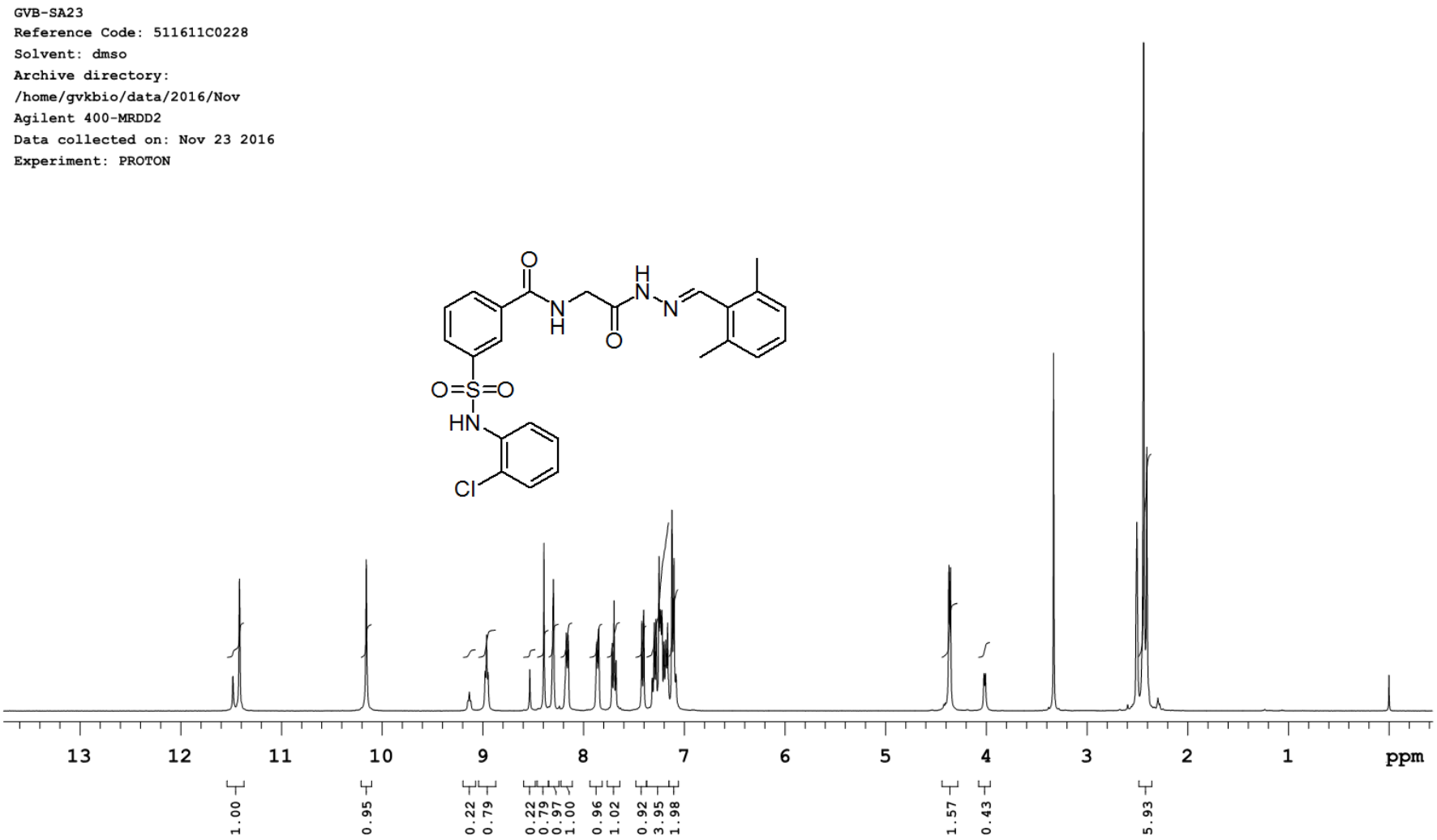
GVB-SA11
511611B8155 9 (0.118) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
1.06e3

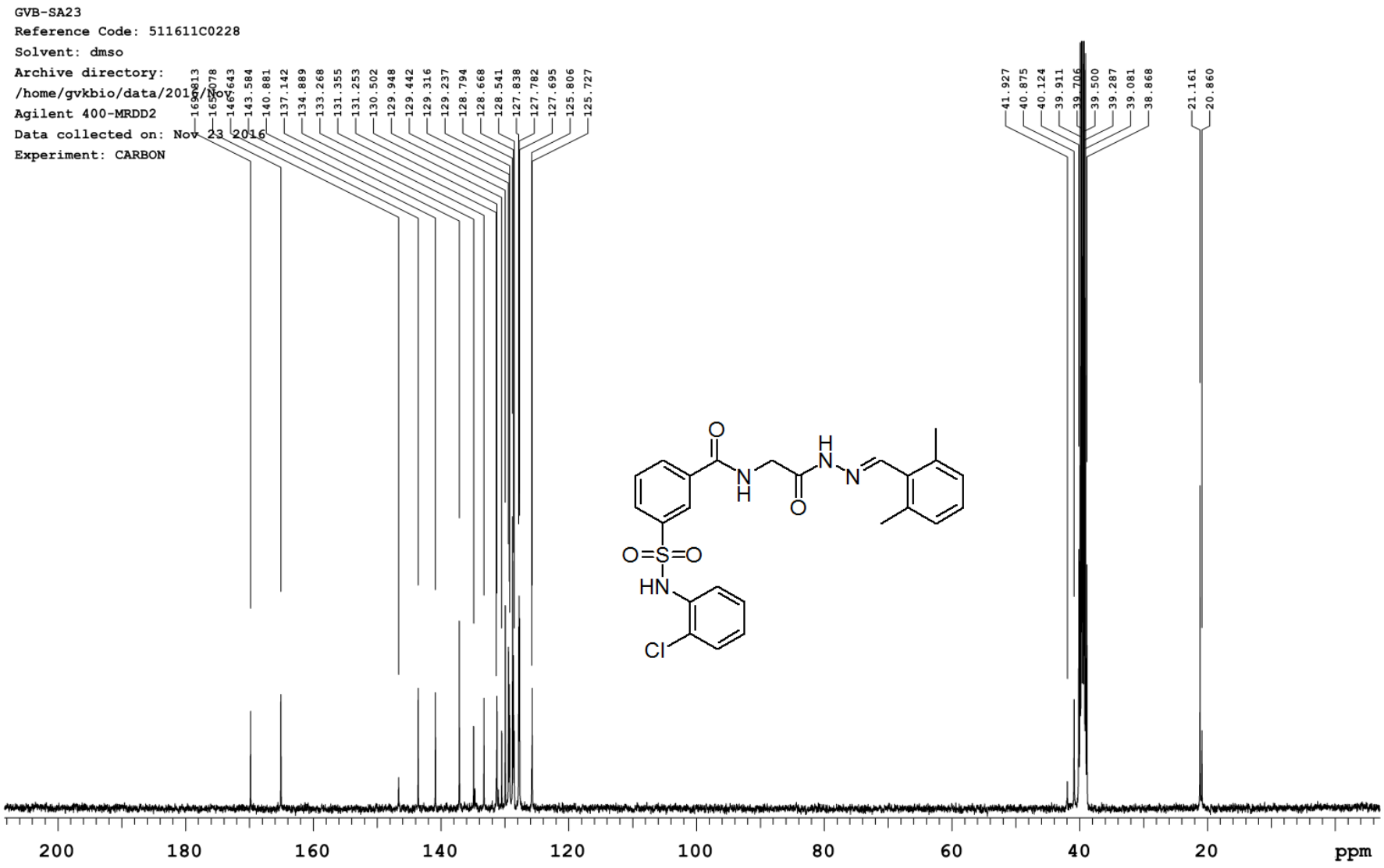


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
585.0807	585.0822	-1.5	-2.6	14.5	54.1	C24 H21 N4 O6 F3 S Cl

HRMS of **Compound-1r**



^{1}H NMR of **Compound-1s** in DMSO-d_6



^{13}CNMR of **Compound-1s** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

87 formula(e) evaluated with 2 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

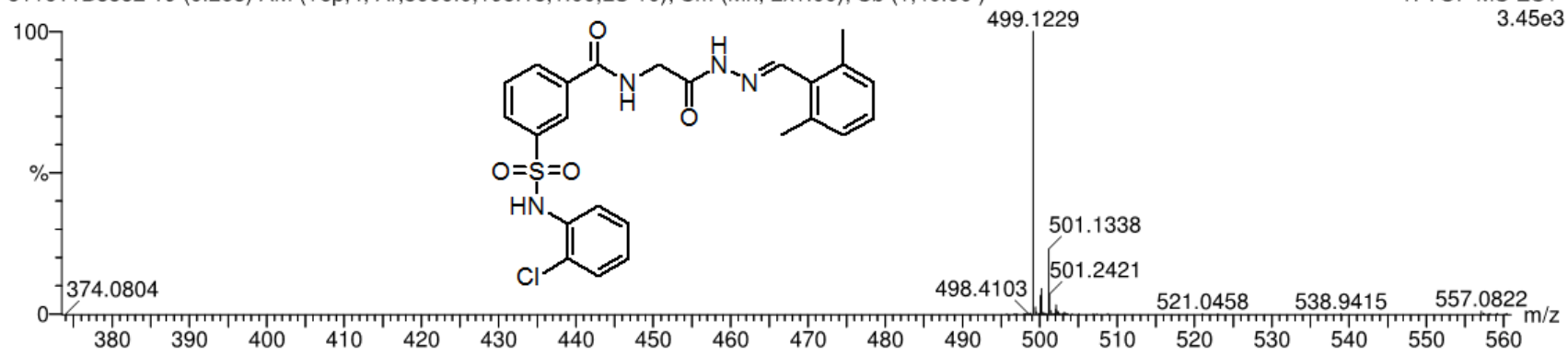
C: 0-25 H: 0-26 N: 0-4 O: 0-4 S: 0-1 Cl: 0-1

GVB-SA23

511611B8552 19 (0.268) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

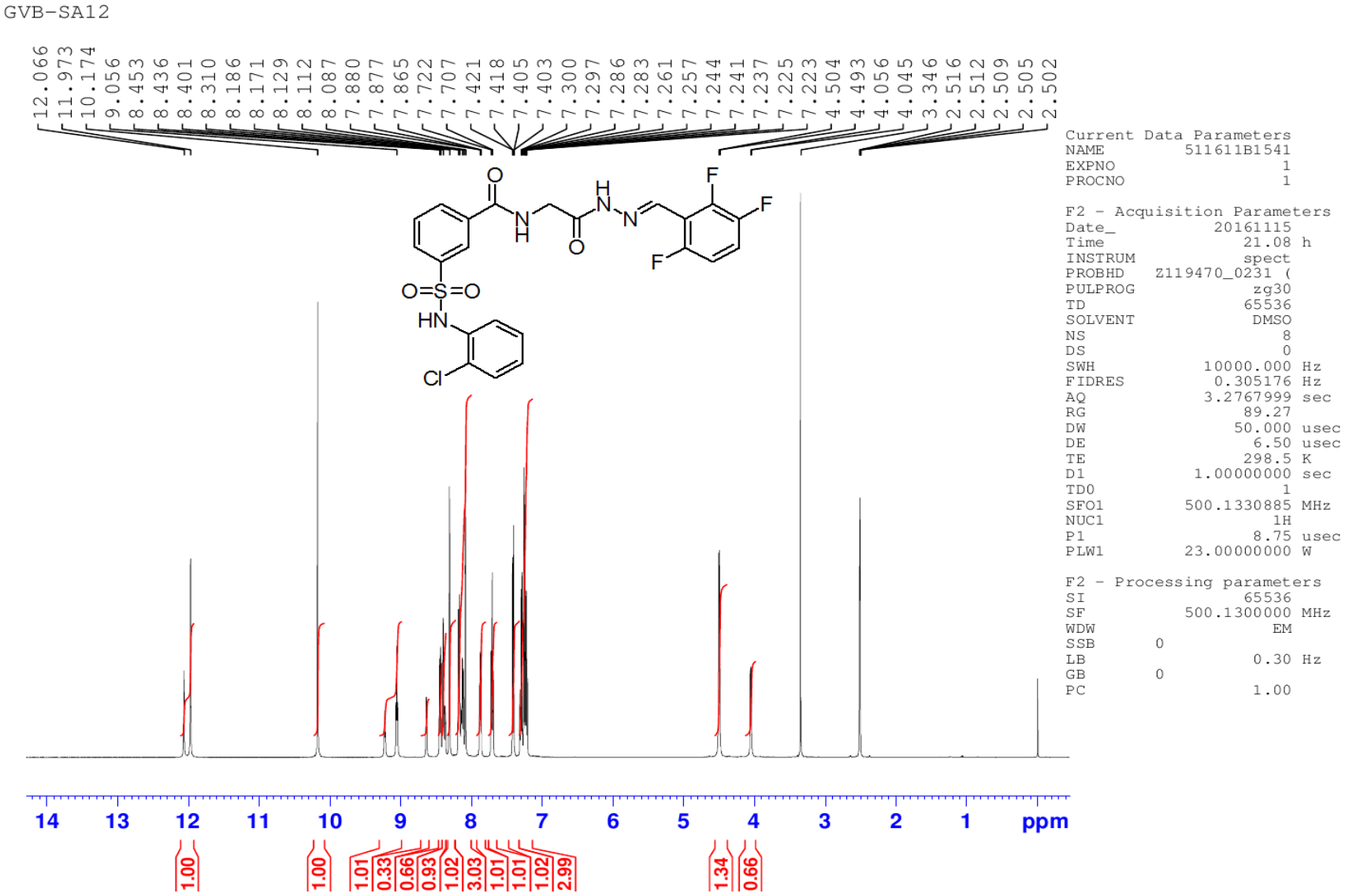
1: TOF MS ES+

3.45e3

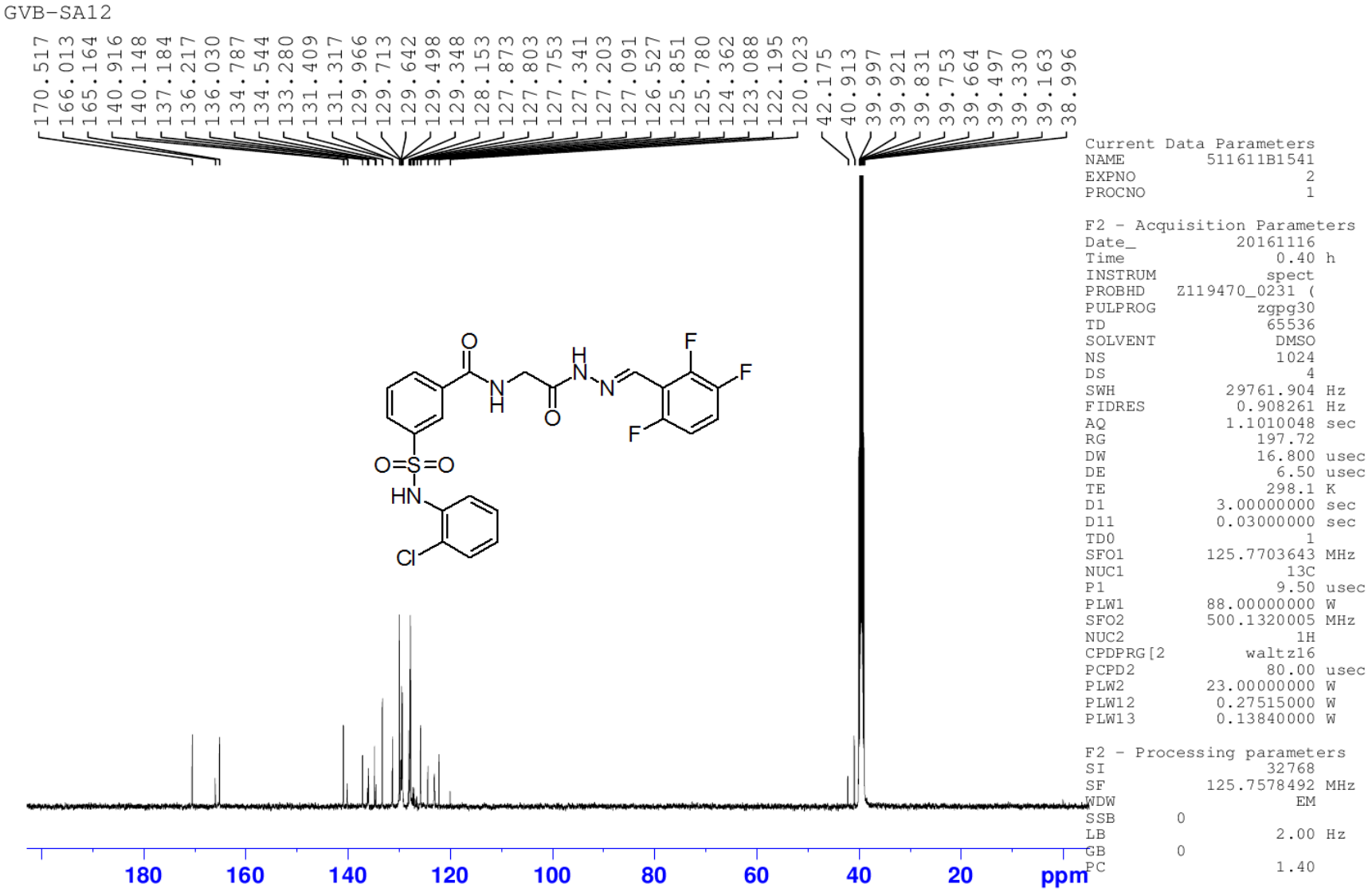


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
499.1229	499.1207	2.2	4.4	14.5	440.4	C24 H24 N4 O4 S Cl

HRMS of **Compound-1s**



^{1}H NMR of **Compound-1t** in DMSO-d_6



^{13}CNMR of **Compound-1t** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

389 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

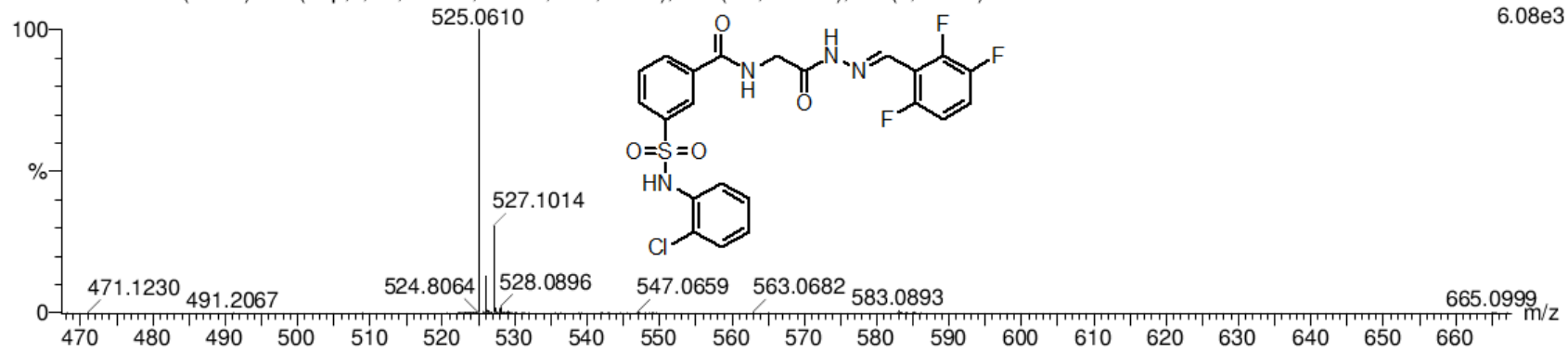
C: 0-22 H: 0-17 N: 0-4 O: 0-4 F: 0-3 S: 0-1 Cl: 0-1

GVB-SA12

511611B8157 12 (0.164) AM (Top,4, Ar,5000.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

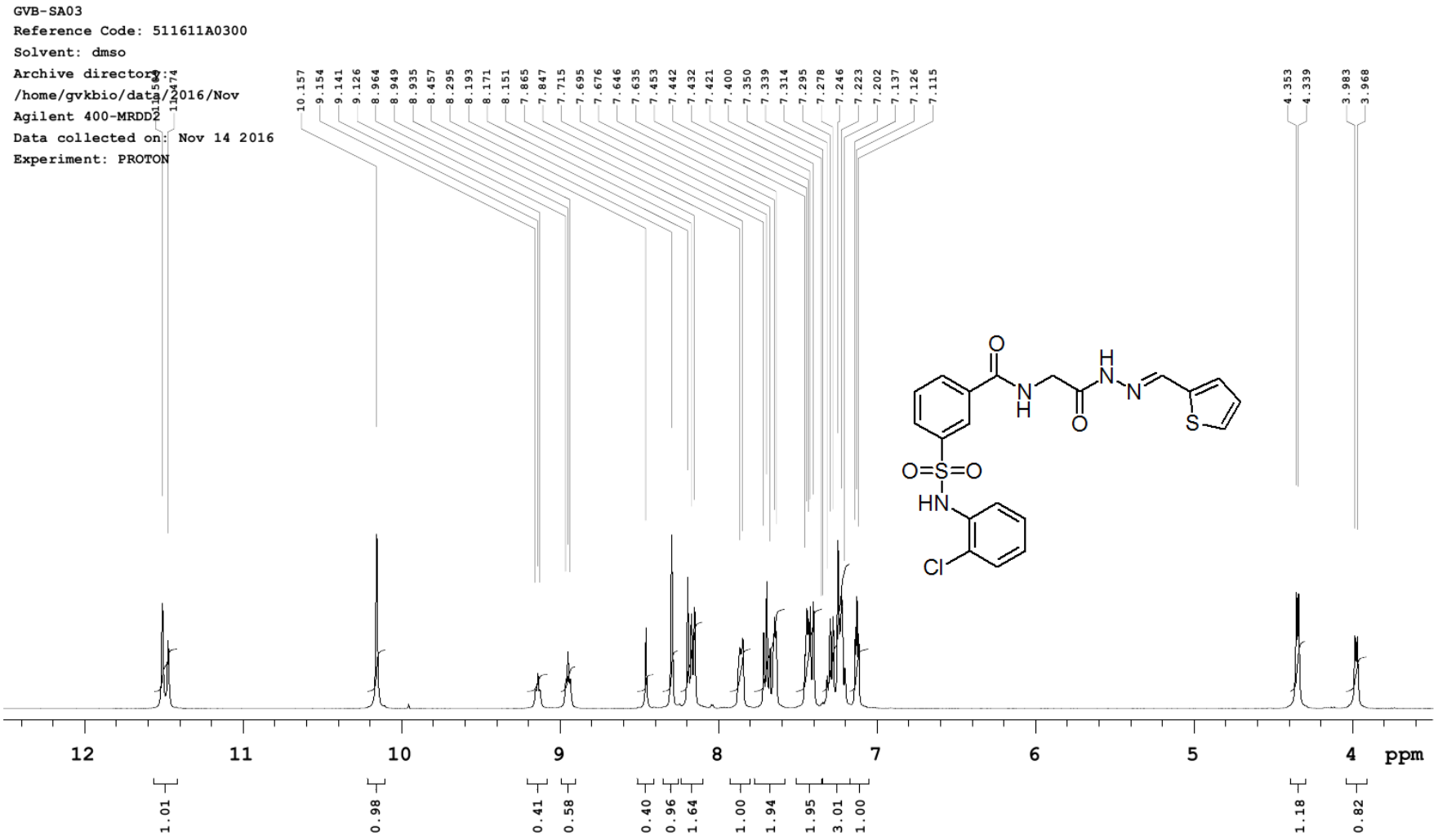
1: TOF MS ES+

6.08e3

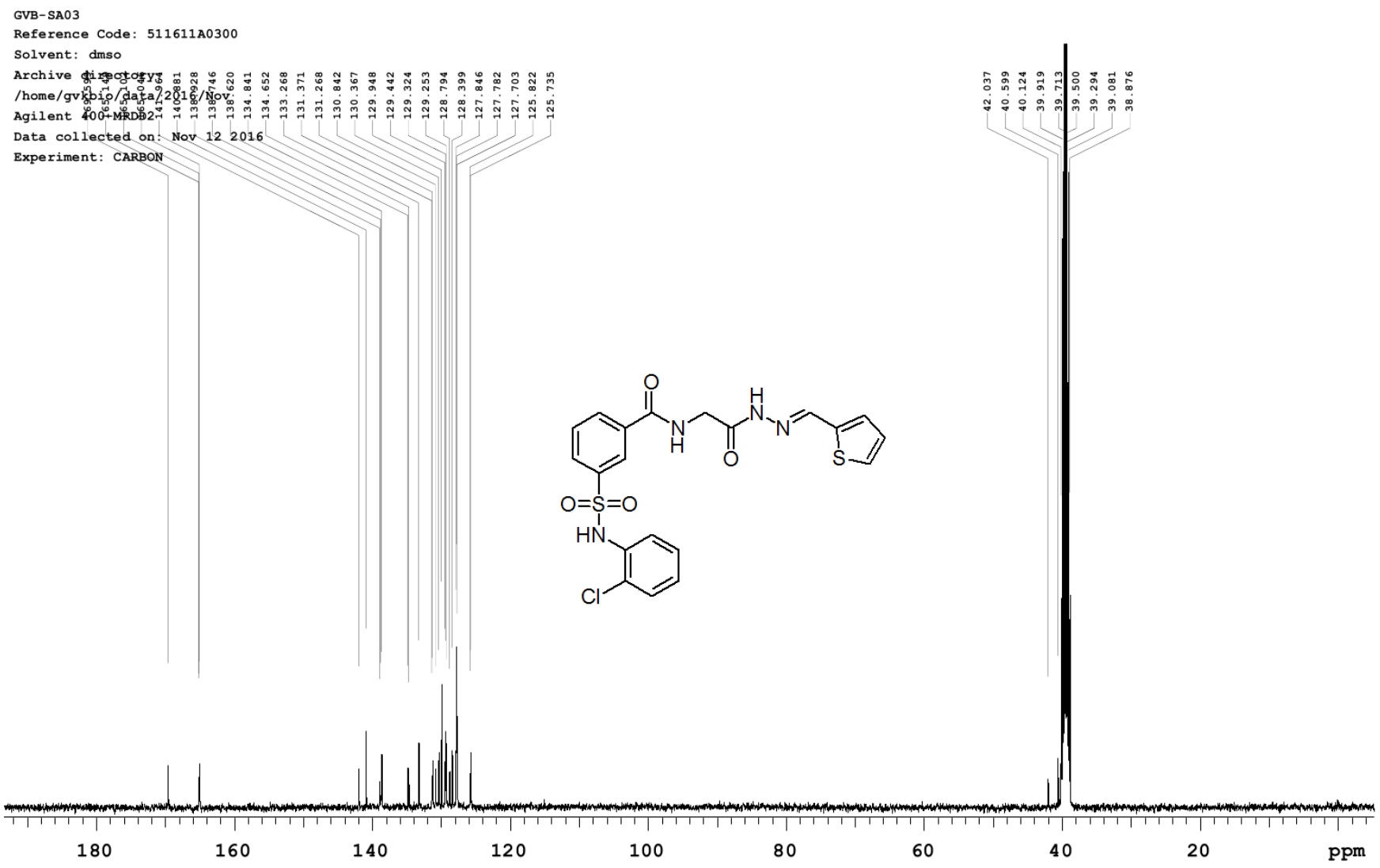


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
525.0610	525.0611	-0.1	-0.2	14.5	349.2	C22 H17 N4 O4 F3 S Cl

HRMS of **Compound-1t**



^{1}H NMR of **Compound-1u** in DMSO-d_6



^{13}CNMR of **Compound-1u** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 10000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

143 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

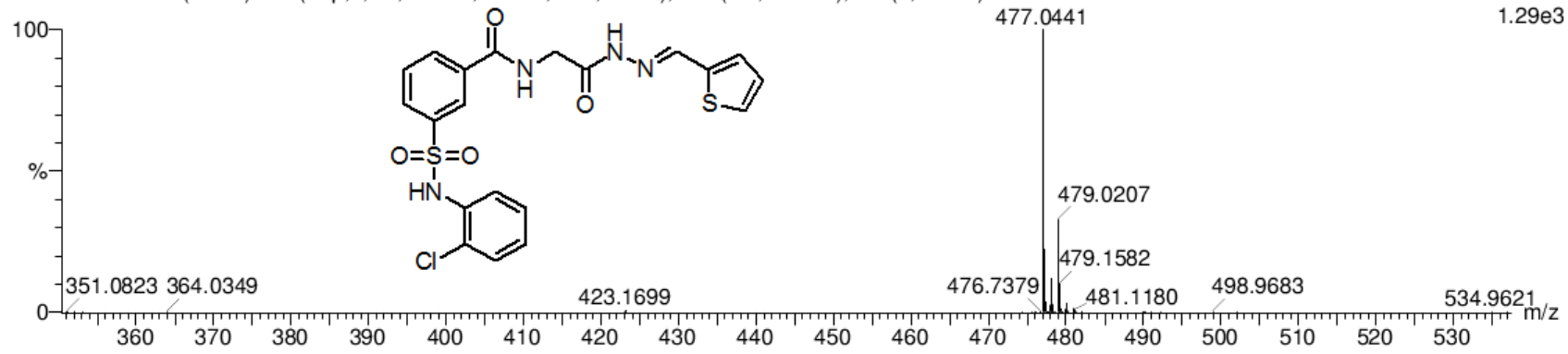
C: 0-20 H: 0-18 N: 0-4 O: 0-4 S: 0-2 Cl: 0-1

GVB-SA03

511611B4317 25 (0.362) AM (Top,4, Ar,5000.0,195.15,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

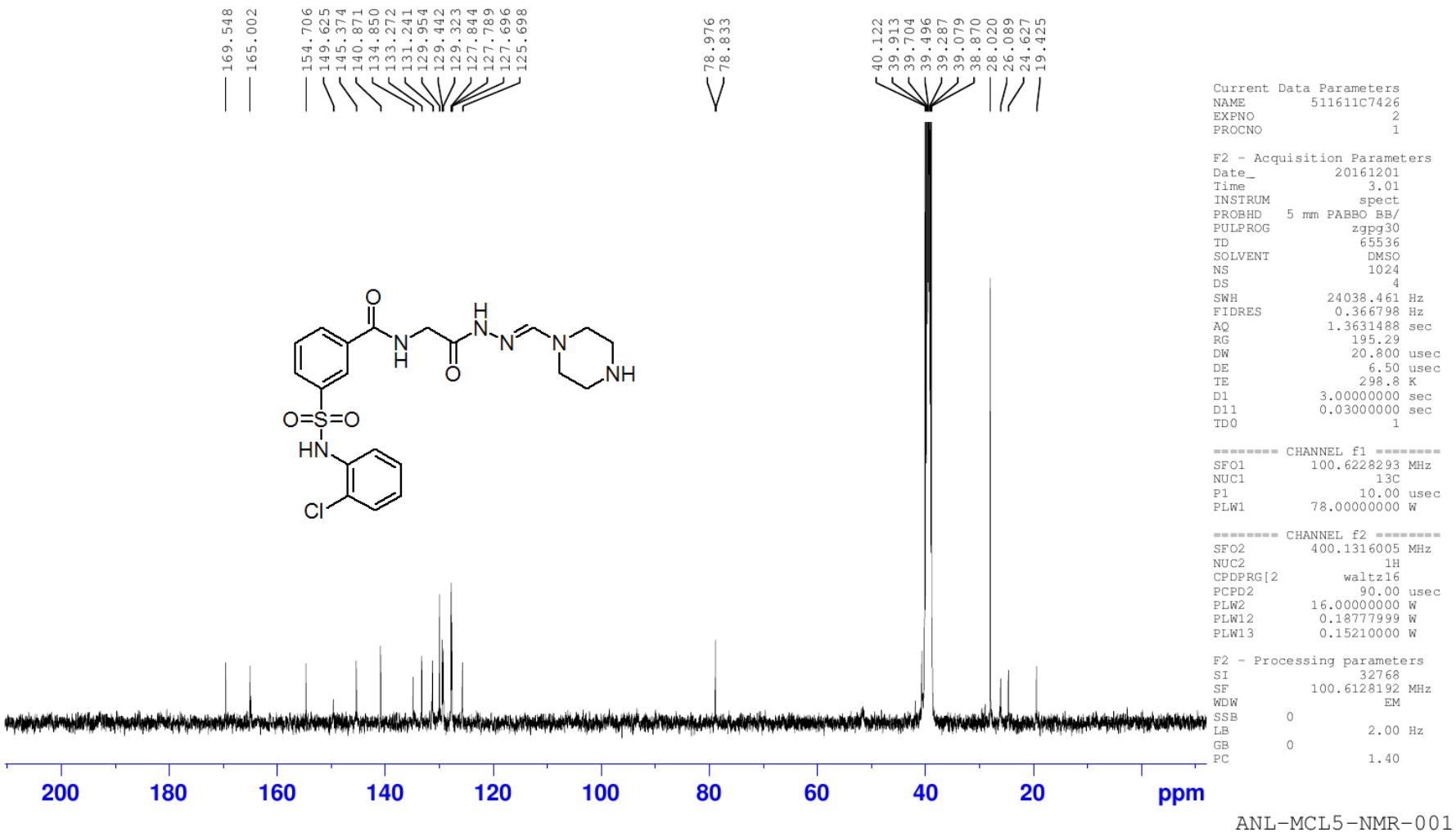
1: TOF MS ES+

1.29e3



Minimum:				-1.5		
Maximum:		5.0	10000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
477.0441	477.0458	-1.7	-3.6	13.5	78957.8	C20 H18 N4 O4 S2 Cl

HRMS of **Compound-1u**



^{13}CNMR of **Compound-1v** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

133 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

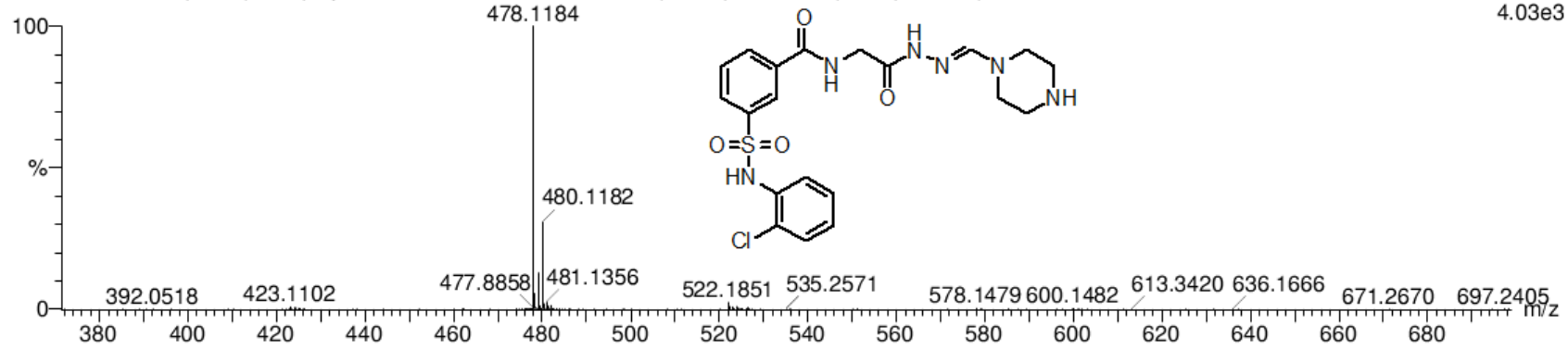
C: 0-20 H: 0-23 N: 0-6 O: 0-4 S: 0-1 Cl: 0-1

GVB-SA10

511611B8154 12 (0.143) AM (Top,4, Ar,5000.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

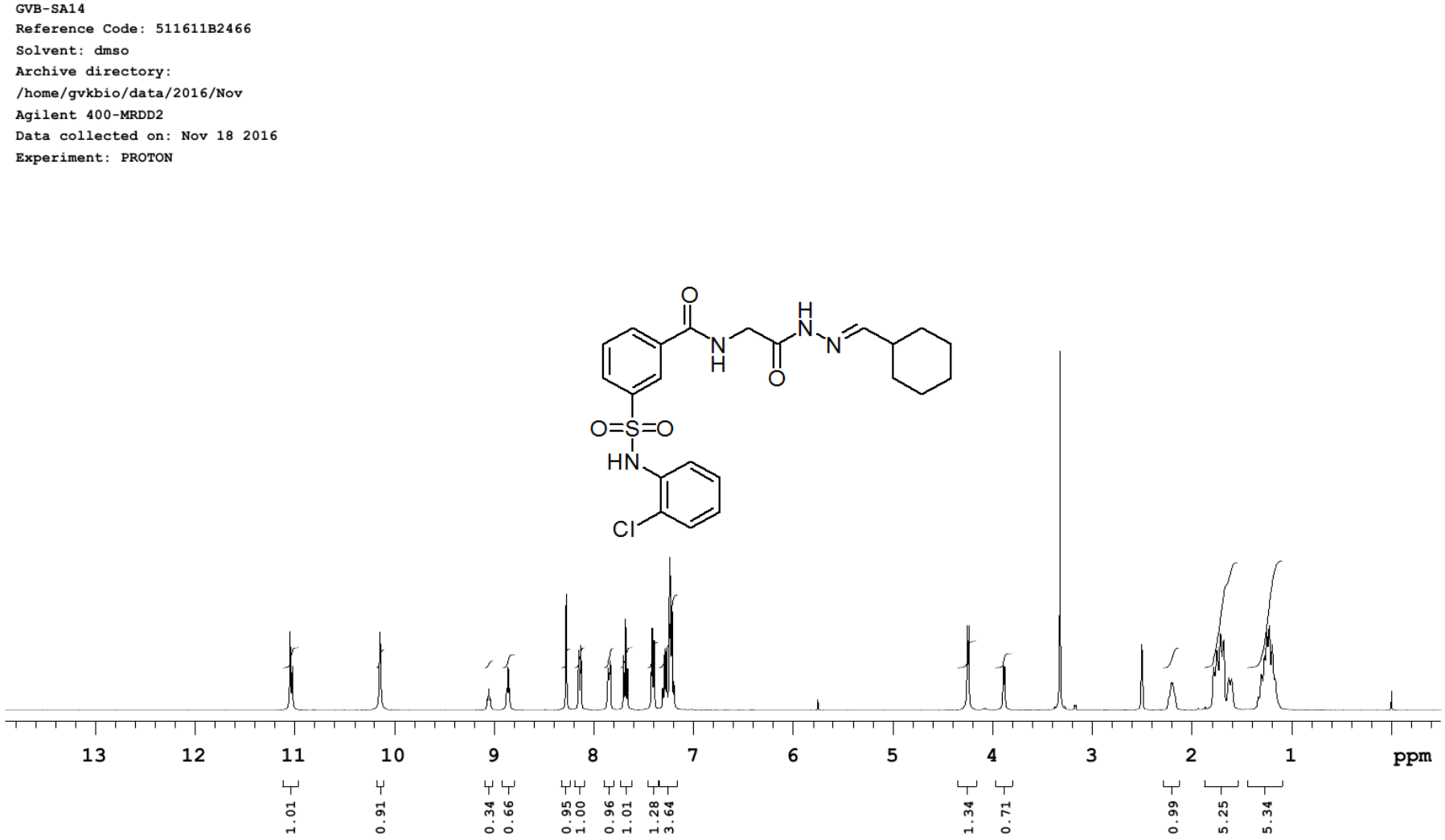
1: TOF MS ES+

4.03e3

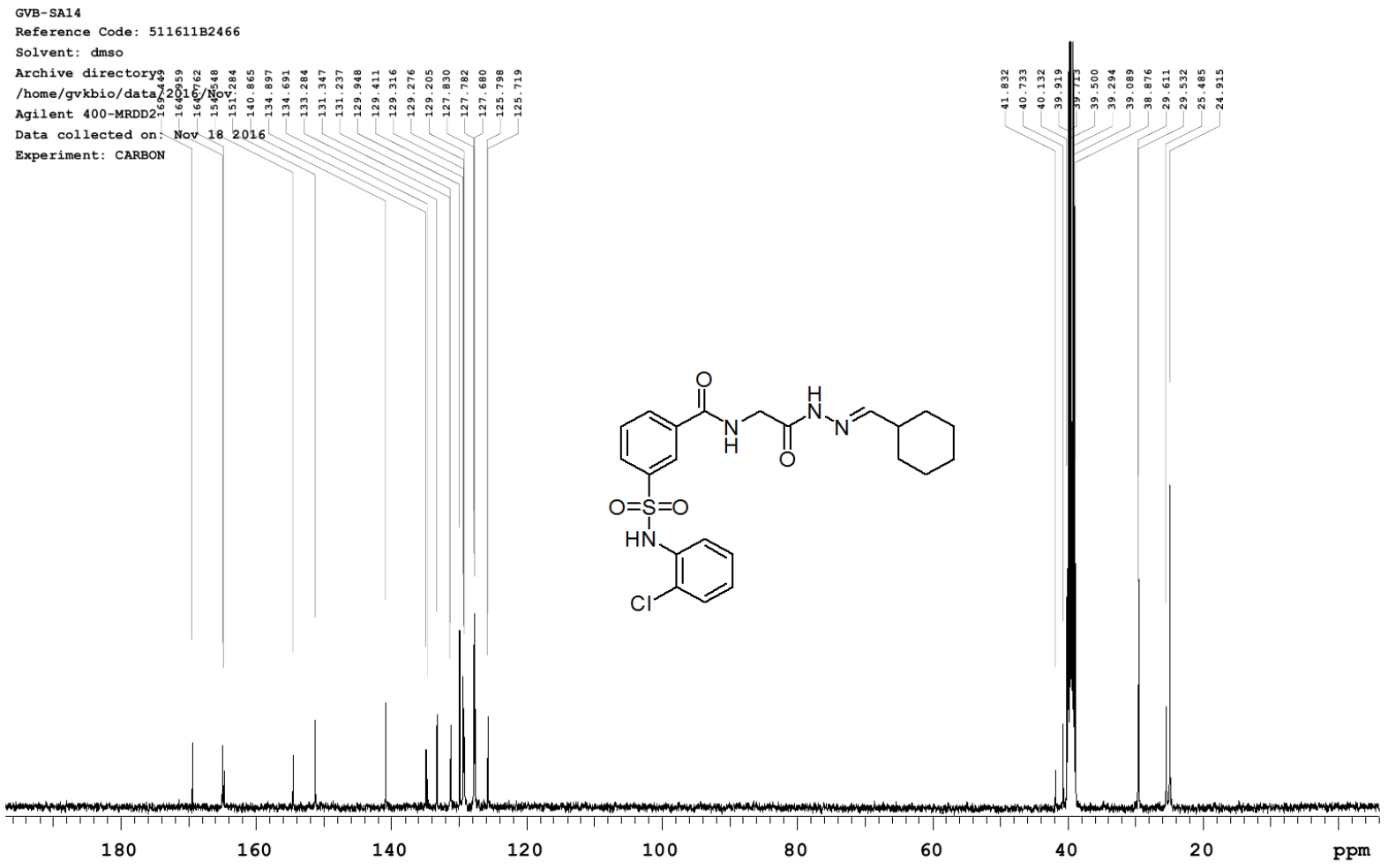


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
478.1184	478.1190	-0.6	-1.3	12.0	181.7	C20 H23 N6 O4 S Cl

HRMS of **Compound-1v**



^{1}H NMR of **Compound-1w** in DMSO-d_6



^{13}CNMR of **Compound-1w** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

94 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

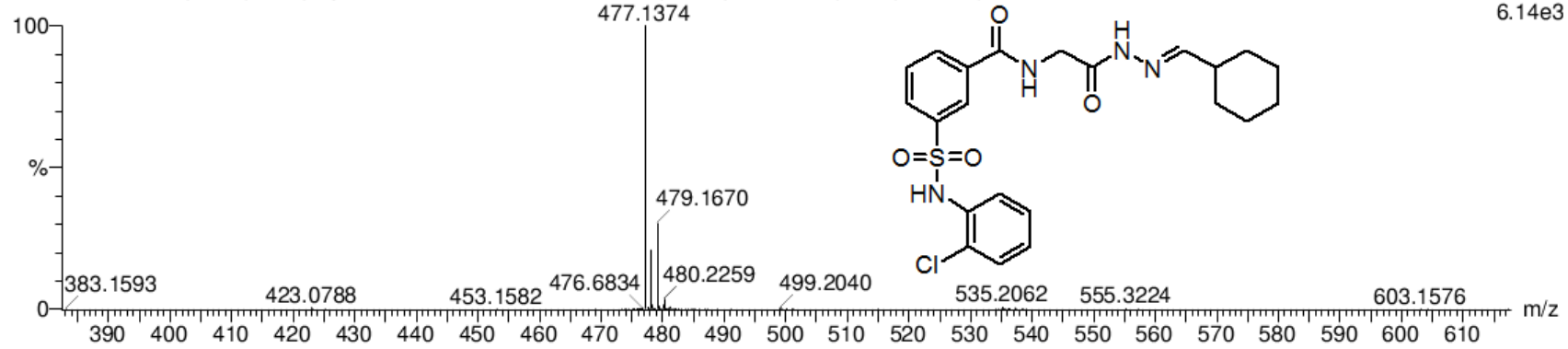
Elements Used:

C: 0-22 H: 0-26 N: 0-4 O: 0-4 S: 0-1 Cl: 0-1

GVB-SA14

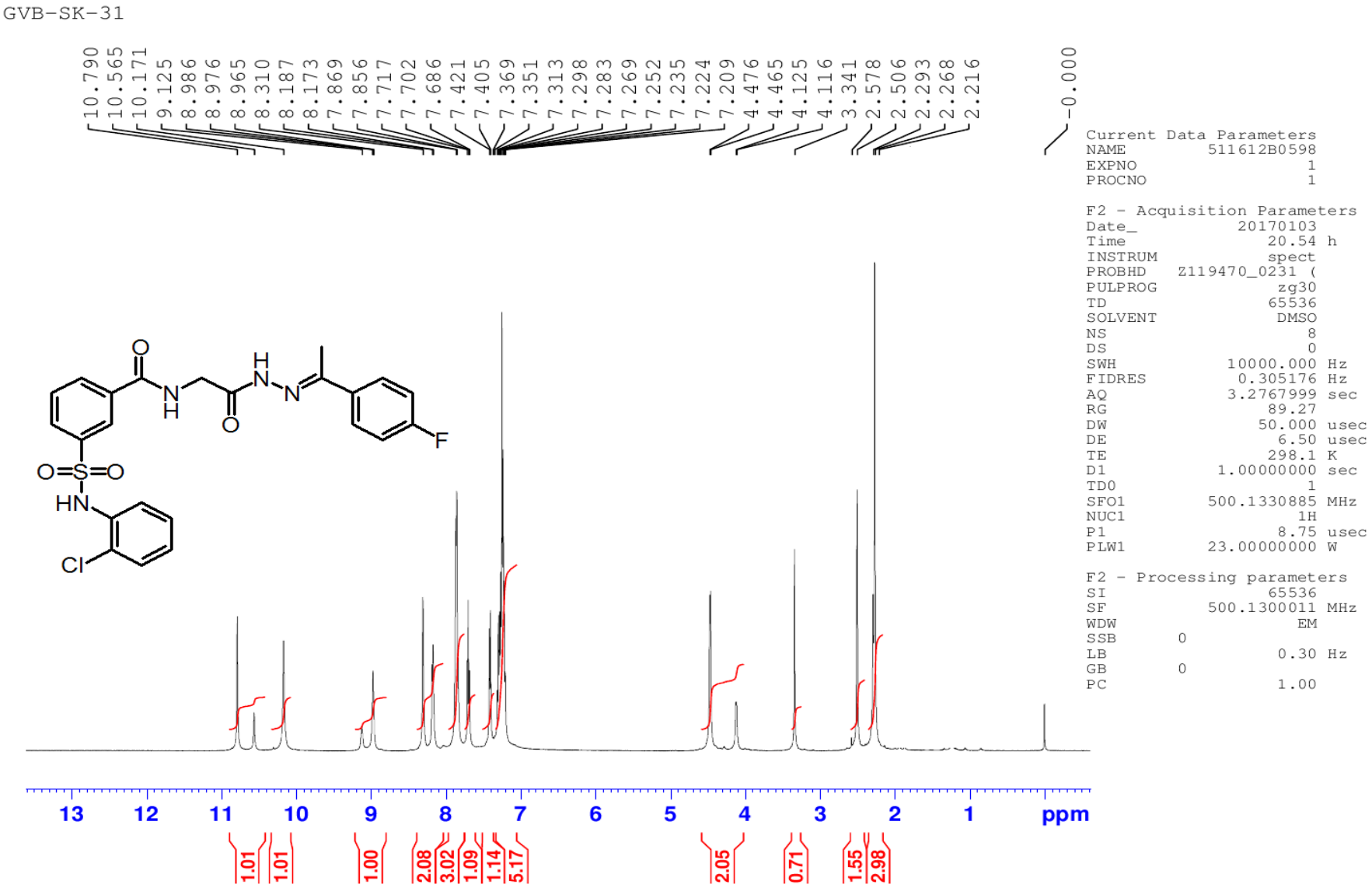
511611B8161 15 (0.228) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
6.14e3

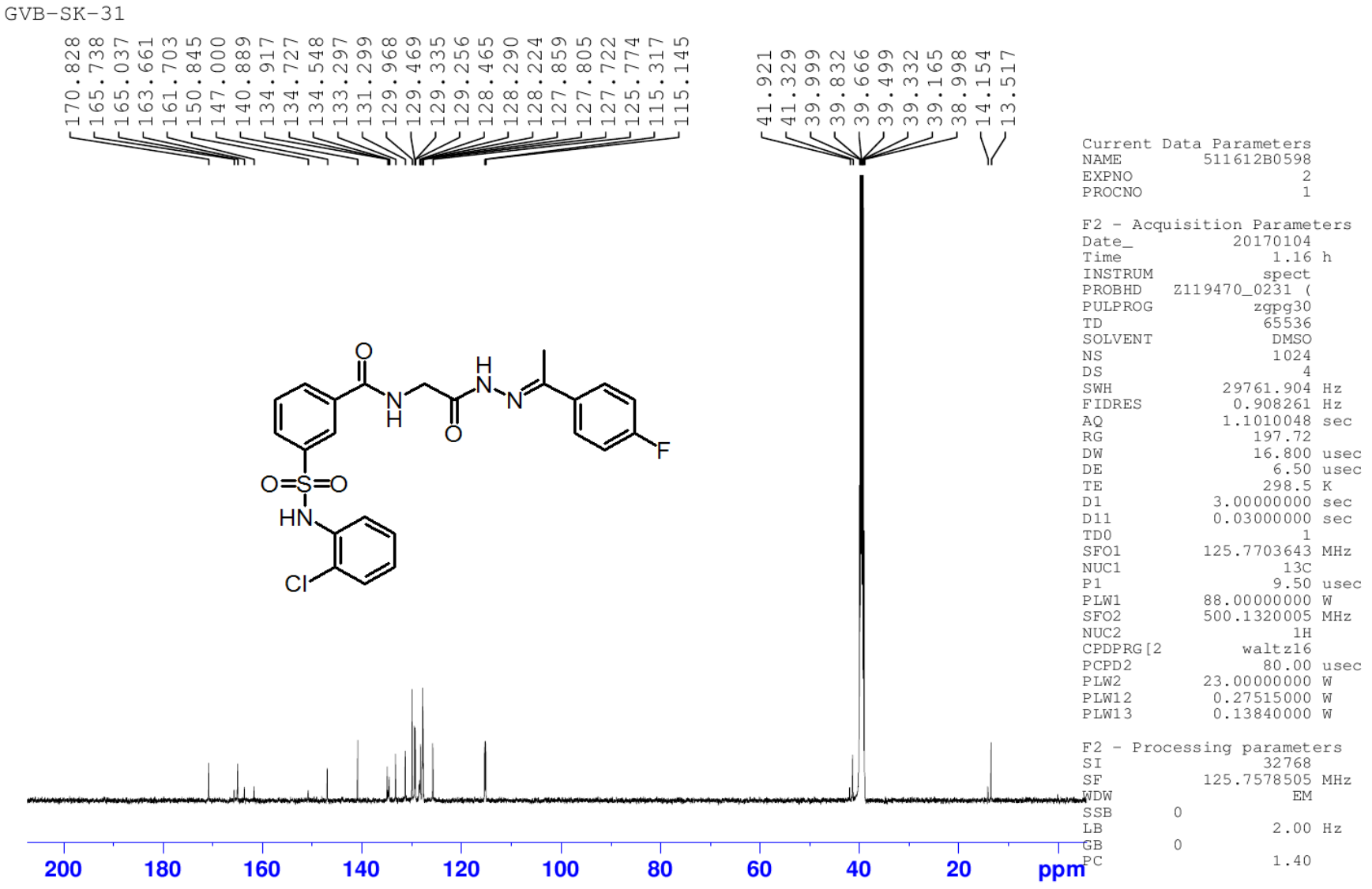


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
477.1374	477.1363	1.1	2.3	11.5	132.3	C22 H26 N4 O4 S Cl

HRMS of **Compound-1w**



^{1}H NMR of **Compound-2a** in DMSO-d_6



^{13}CNMR of **Compound-2a** in DMSO-d_6

Elemental Composition Report

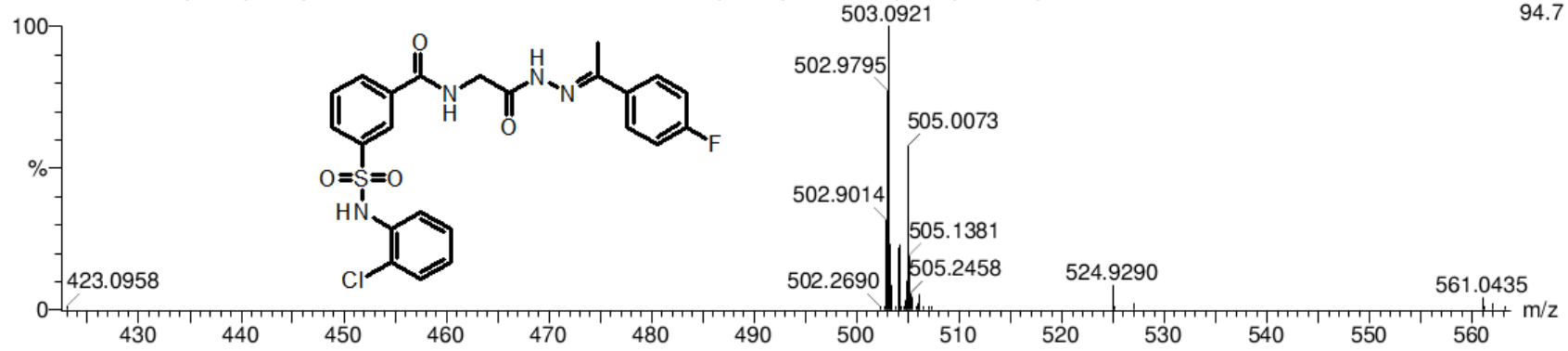
Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
190 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-21 N: 0-4 O: 0-4 F: 0-1 S: 0-1 Cl: 0-1

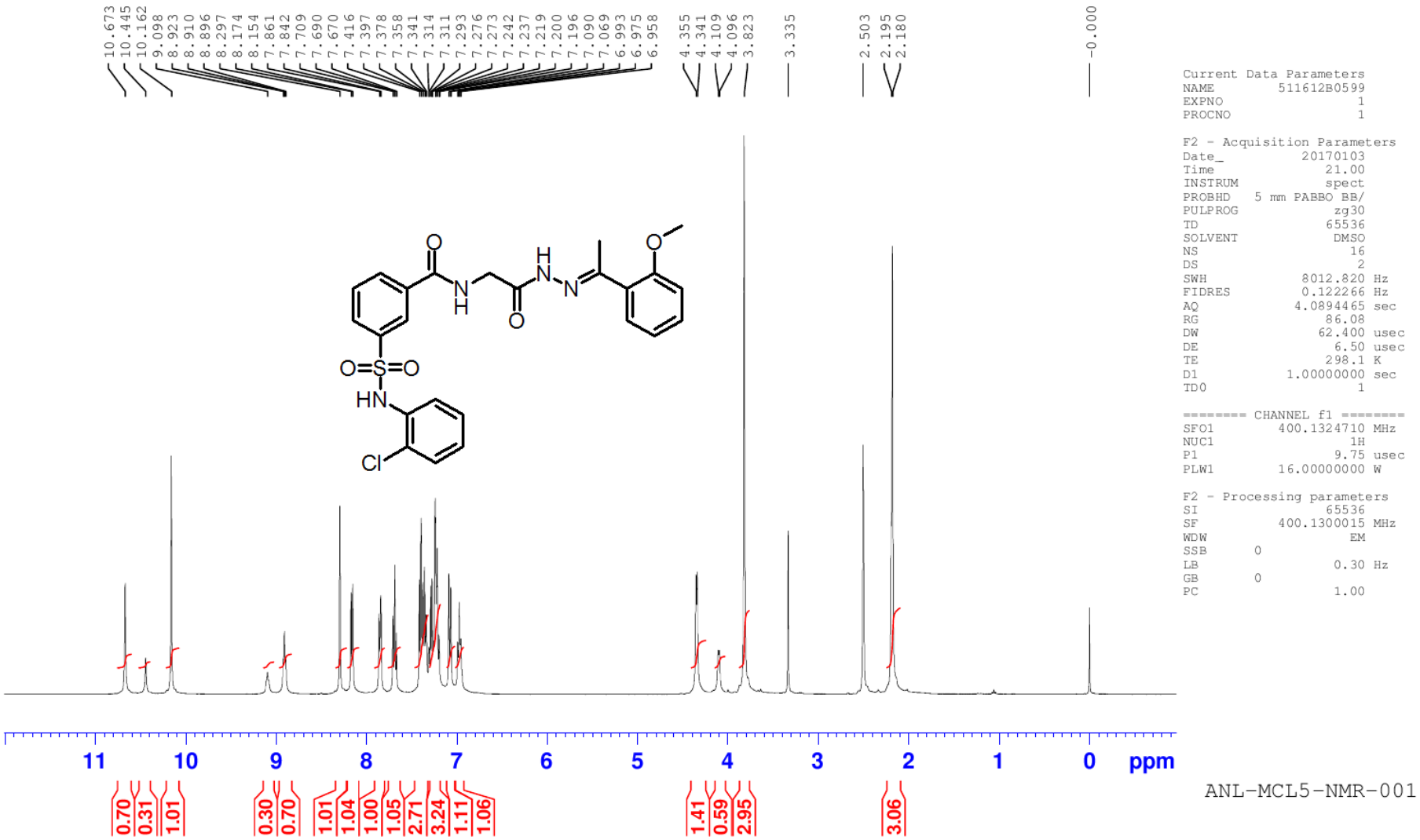
SAMPLE CODE:COMPOUND-31
511701A5143 61 (0.882) AM (Cen,4, 80.00, Ar,5000.0,195.13,1.00,LS 5); Sm (SG, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
94.7



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
503.0921	503.0956	-3.5	-7.0	14.5	7.9	C23 H21 N4 O4 F S Cl

HRMS of **Compound-2a**

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PROCNO                  1

F2 - Acquisition Parameters
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PULPROG              zg30
TD                  65536
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NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ              4.0894465 sec
RG                  86.08
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DE                 6.50 usec
TE                298.1 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
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NUC1                    1H
P1                   9.75 usec
PLW1          16.00000000 W

F2 - Processing parameters
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GB        0
PC                  1.00
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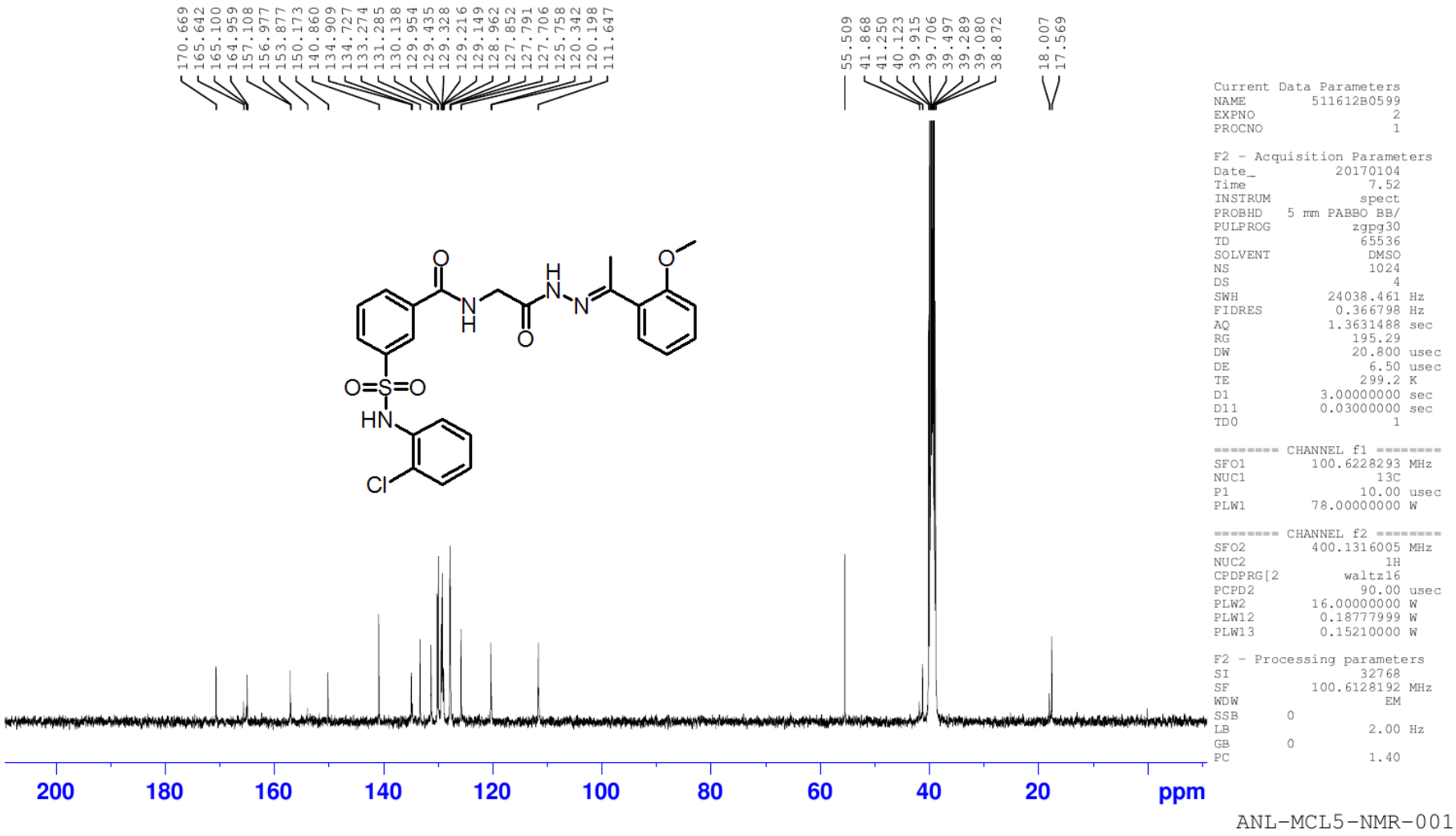
ANL-MCL5-NMR-001

^{1}H NMR of **Compound-2b** in DMSO-d_6



^{13}CNMR of **Compound-2b** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

199 formula(e) evaluated with 69 results within limits (up to 1 closest results for each mass)

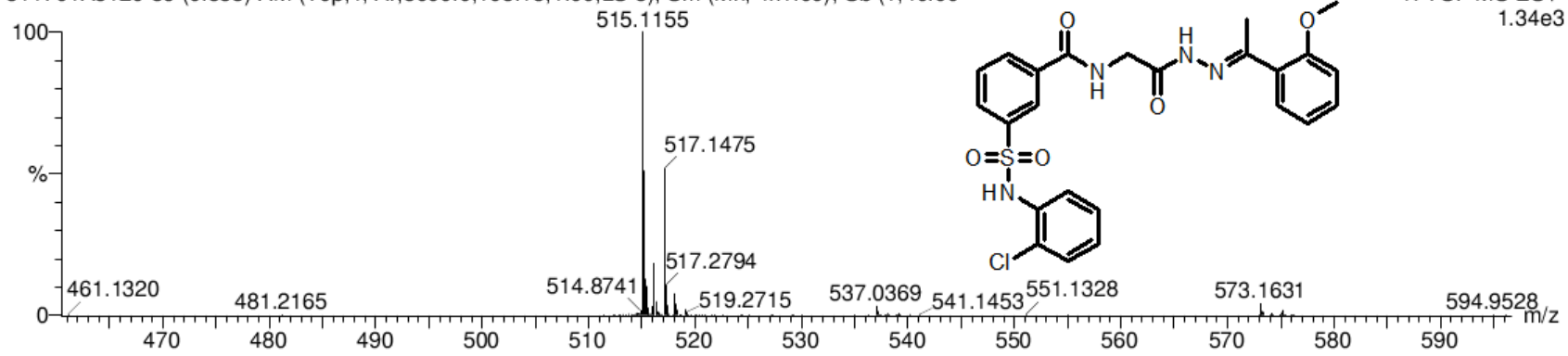
Elements Used:

C: 0-29 H: 0-25 N: 0-4 O: 0-5 F: 0-1 S: 0-1 Cl: 0-1

SAMPLE CODE:COMPOUND-32

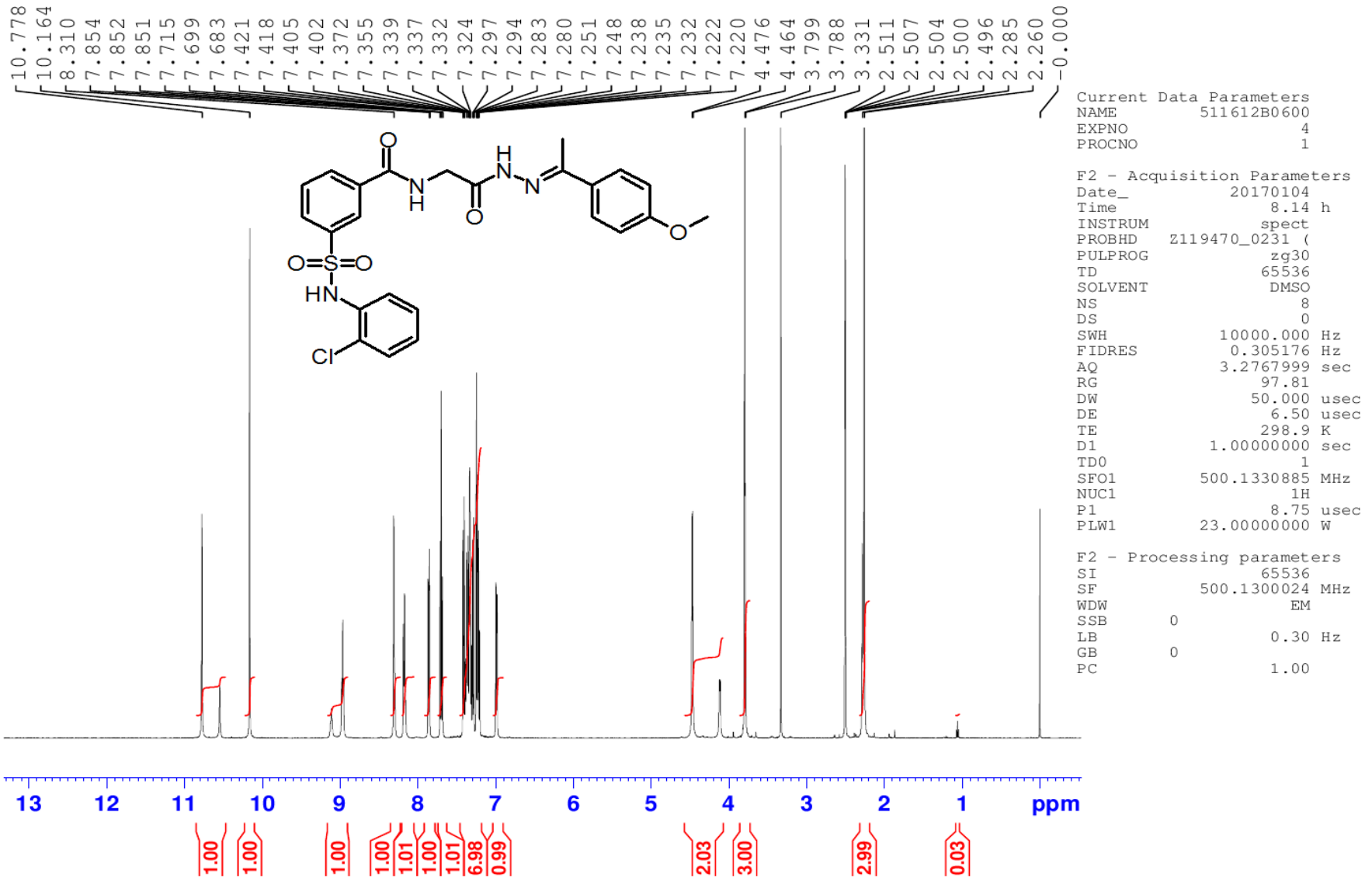
511701A5129 36 (0.533) AM (Top,4, Ar,5000.0,195.18,1.00,LS 5); Sm (Mn, 1x1.00); Sb (1,40.00 `

1: TOF MS ES+
1.34e3

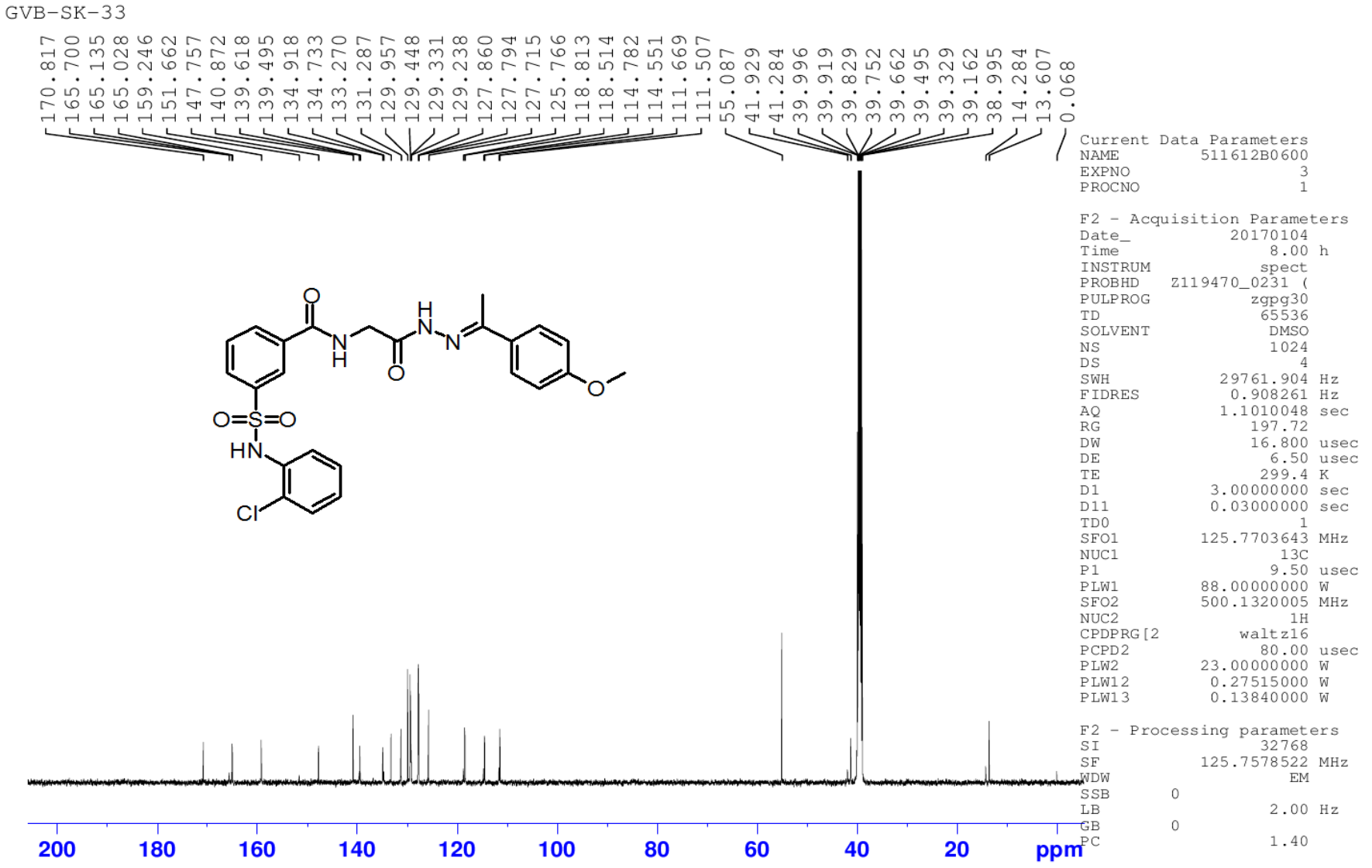


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
515.1155	515.1156	-0.1	-0.2	14.5	69.2	C24 H24 N4 O5 S Cl

HRMS of **Compound-2b**



^{1}H NMR of **Compound-2c** in DMSO-d_6



^{13}CNMR of **Compound-2c** in DMSO-d_6

Elemental Composition Report

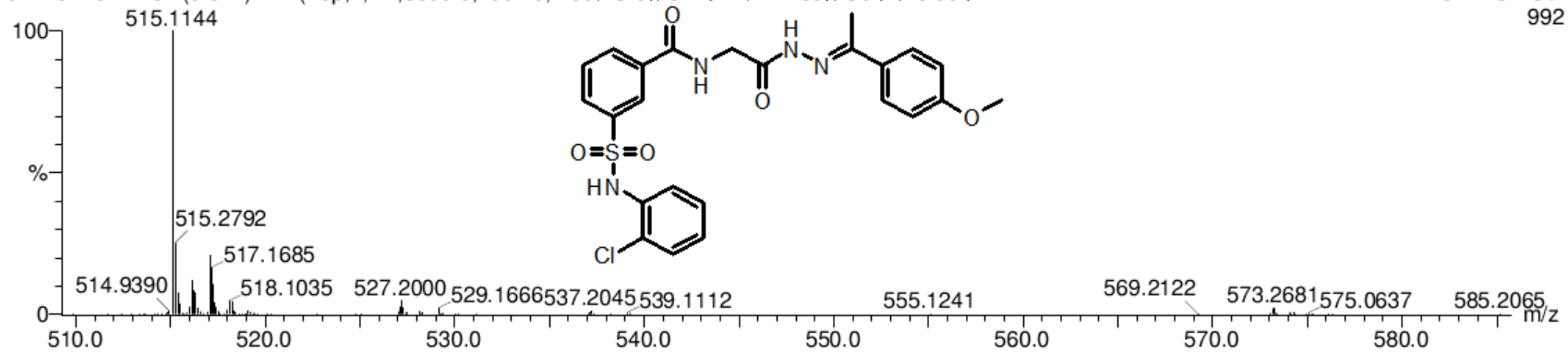
Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
113 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-24 H: 0-24 N: 0-4 O: 0-5 S: 0-1 Cl: 0-1

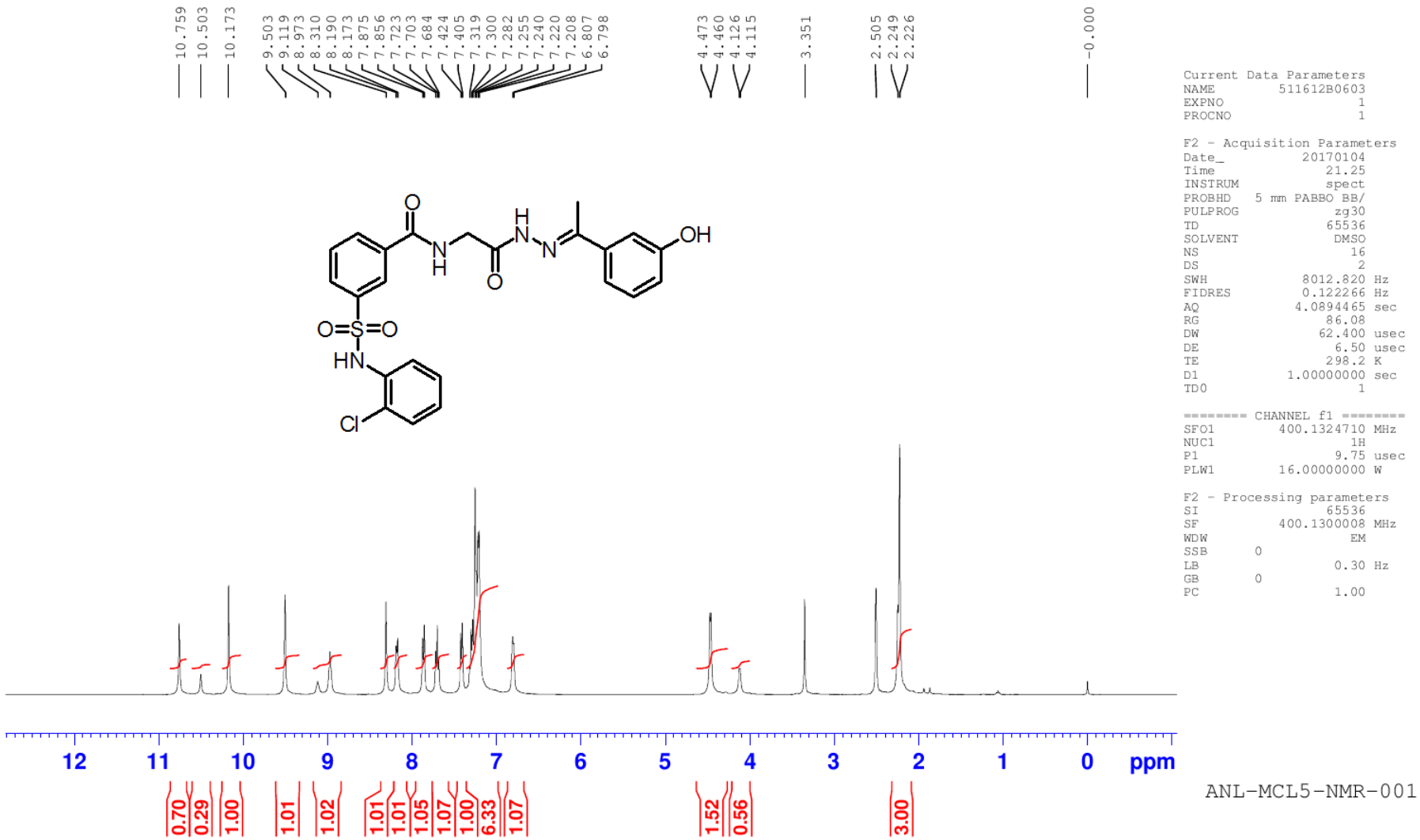
SAMPLE CODE:COMPOUND-33
511701A5142 37 (0.544) AM (Top,4, Ar,5000.0,195.18,1.00,LS 5); Sm (Mn, 1x1.00); Sb (1,40.00)

1: TOF MS ES+
992



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
515.1144	515.1156	-1.2	-2.3	14.5	92.6	C24 H24 N4 O5 S Cl

HRMS of **Compound-2c**

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EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
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Time               21.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 86.08
DW                62.400 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.75 usec
PLW1        16.00000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300008 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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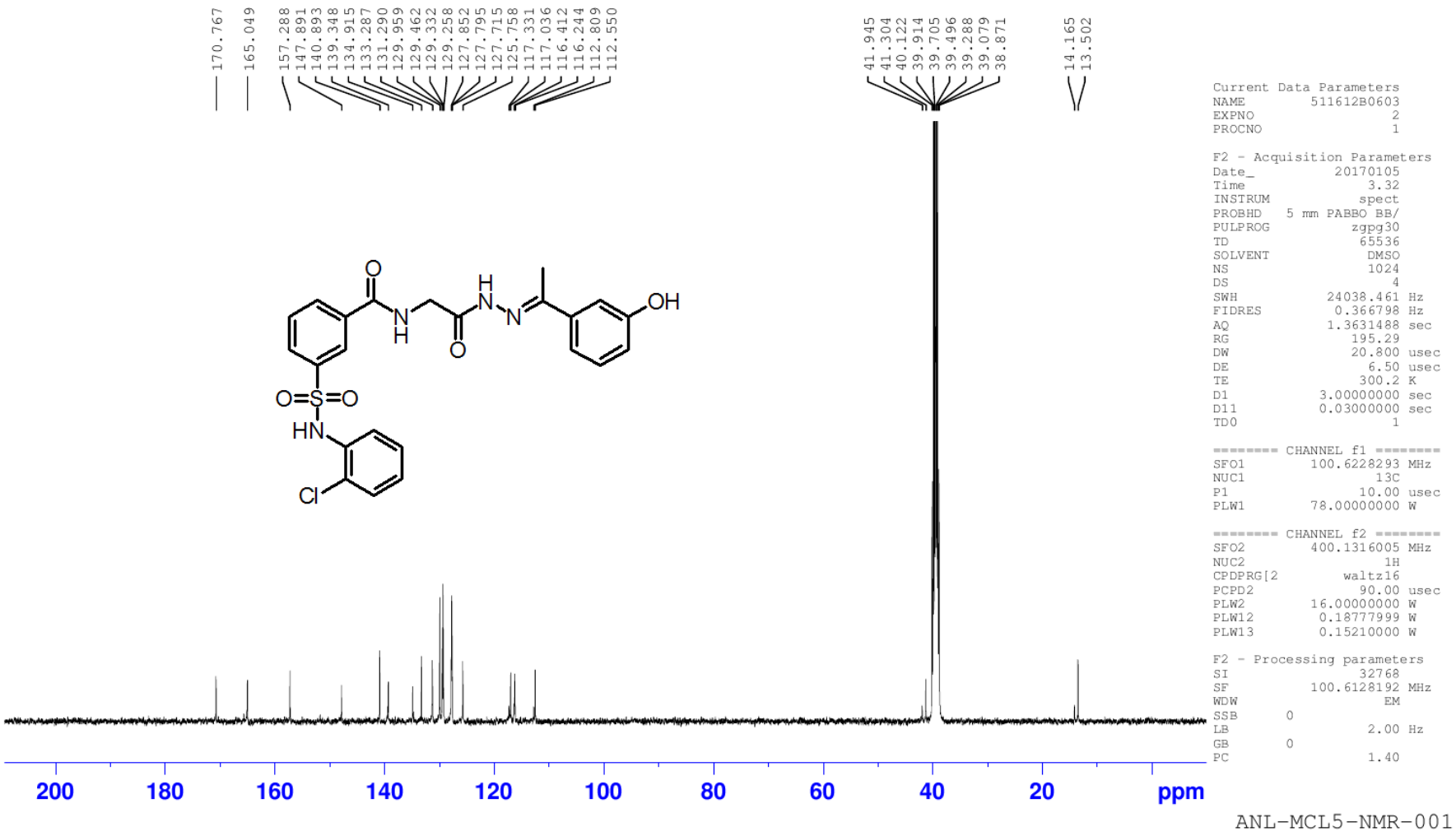
ANL-MCL5-NMR-001

^{1}H NMR of **Compound-2d** in DMSO-d_6



^{13}CNMR of **Compound-2d** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

221 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)

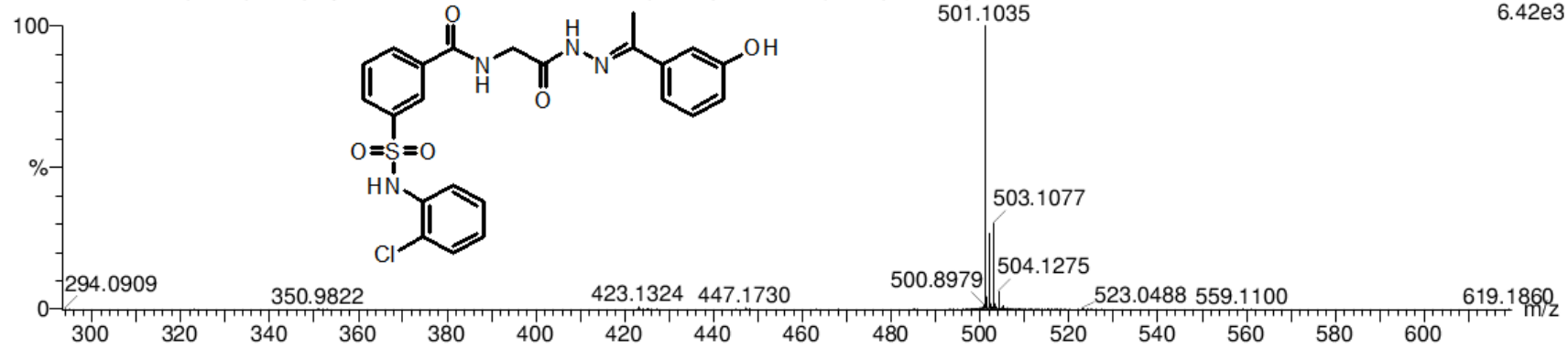
Elements Used:

C: 0-23 H: 0-22 N: 0-4 O: 0-5 F: 0-1 S: 0-1 Cl: 0-1

SAMPLE CODE:COMPOUND-36

511701A5132 18 (0.259) AM (Top,4, Ar,5000.0,195.16,1.00,LS 5); Sm (Mn, 1x1.00); Sb (1,40.00)

1: TOF MS ES+
6.42e3



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
501.1035	501.0999	3.6	7.2	14.5	91.8	C23 H22 N4 O5 S Cl

HRMS of **Compound-2d**

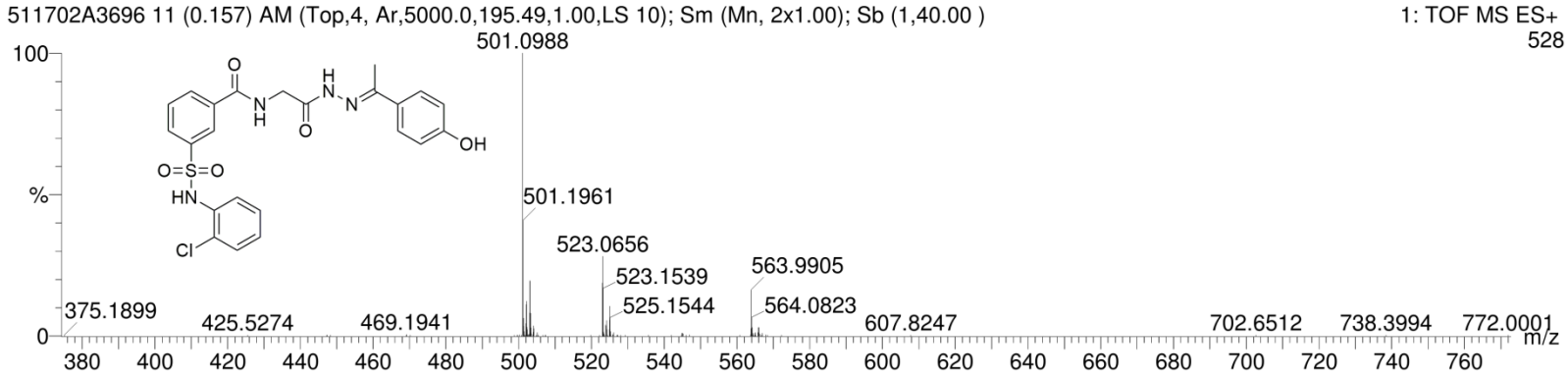
Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

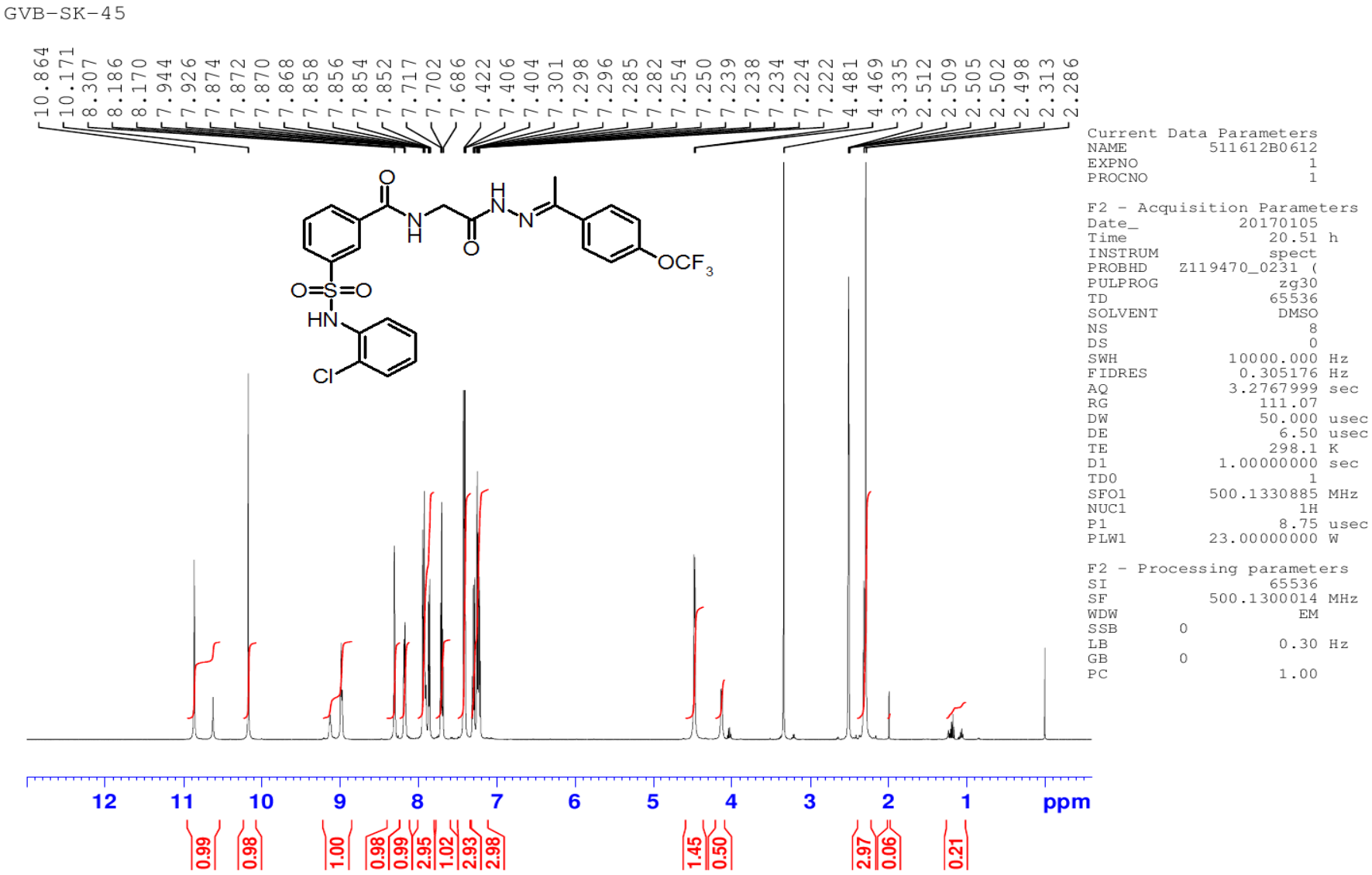
Monoisotopic Mass, Even Electron Ions
113 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-22 N: 0-4 O: 0-5 S: 0-1 Cl: 0-1

GVB-SK44-01
511702A3696 11 (0.157) AM (Top,4, Ar,5000.0,195.49,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

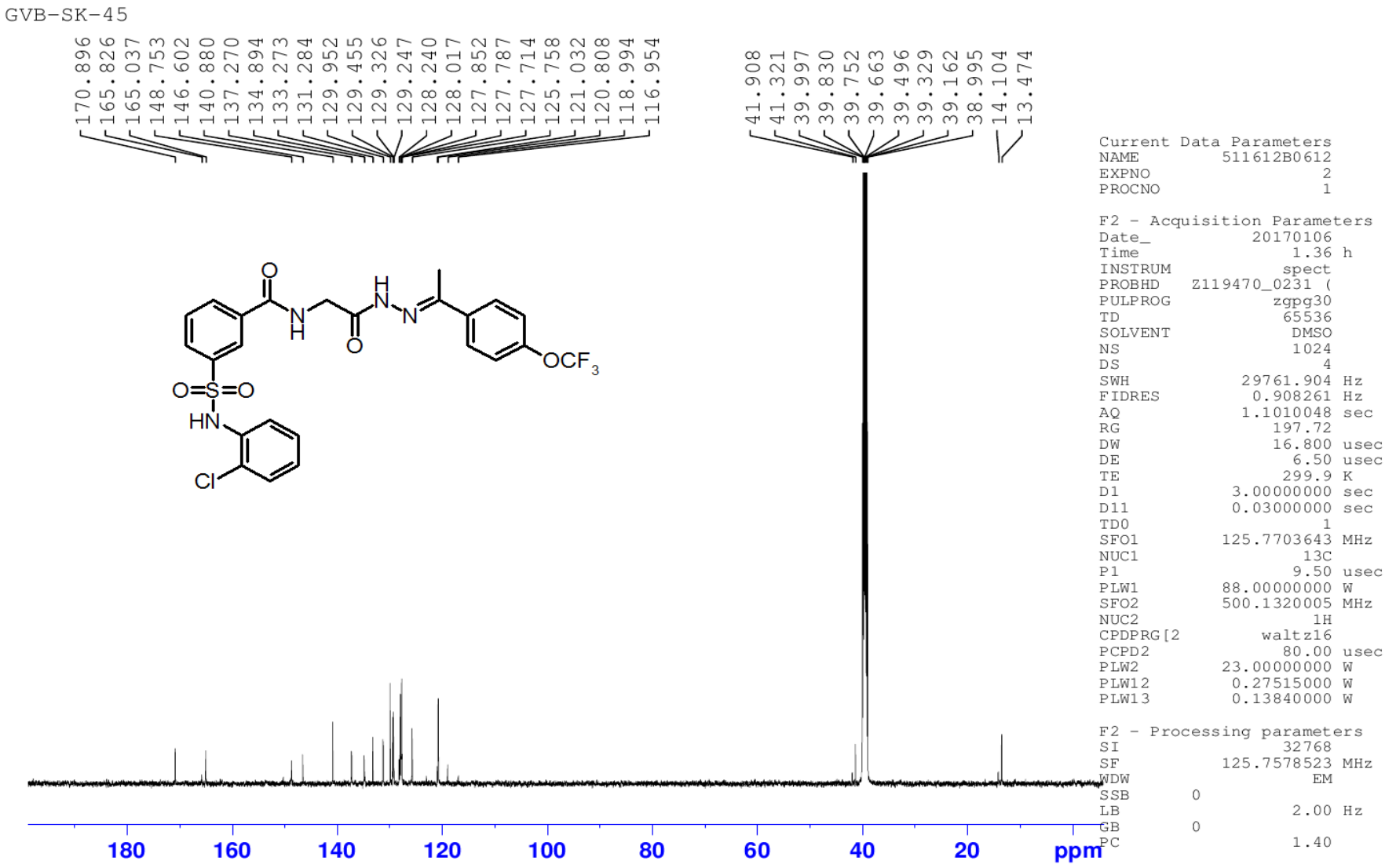


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
501.0988	501.0999	-1.1	-2.2	14.5	50.9	C23 H22 N4 O5 S Cl

HRMS of **Compound-2e**



^{1}H NMR of **Compound-2f** in DMSO-d_6



^{13}CNMR of **Compound-2f** in DMSO-d_6

Elemental Composition Report

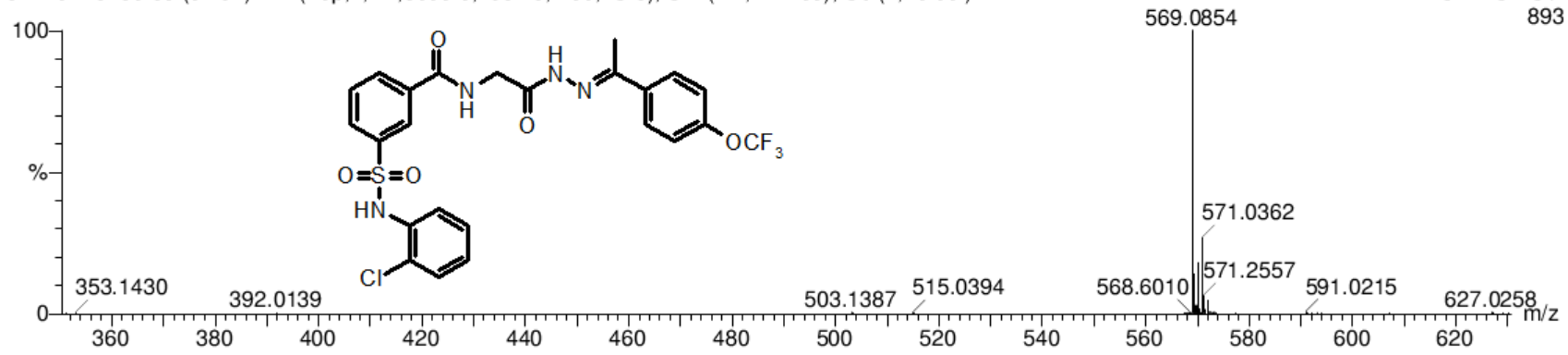
Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
469 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-24 H: 0-30 N: 0-4 O: 0-5 S: 0-1 Cl: 0-1 F: 0-3

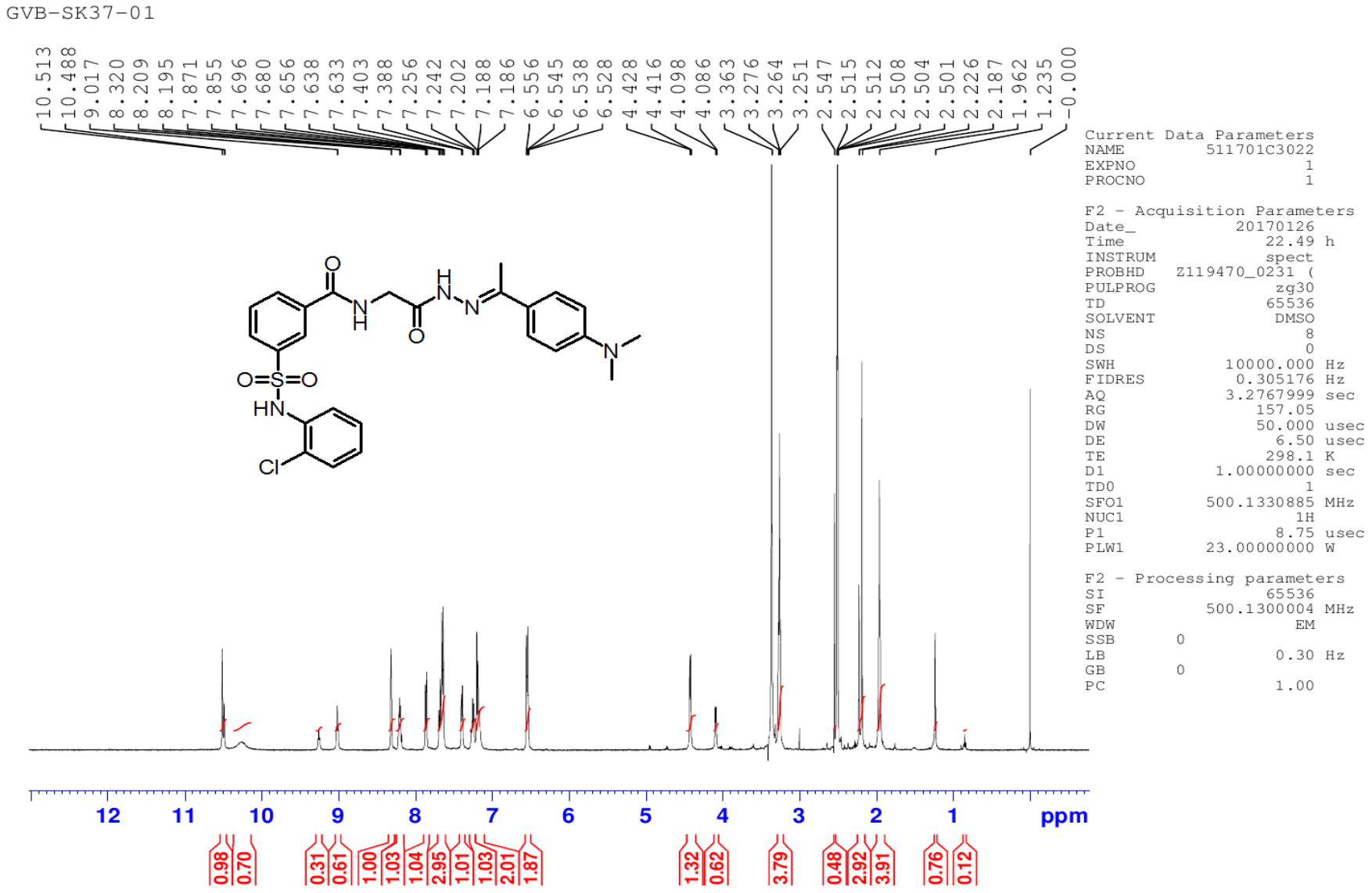
SAMPLE CODE:COMPOUND-45
511701A5130 56 (0.797) AM (Top,4, Ar,5000.0,195.15,1.00,LS 5); Sm (Mn, 1x1.00); Sb (1,40.00)

1: TOF MS ES+
893

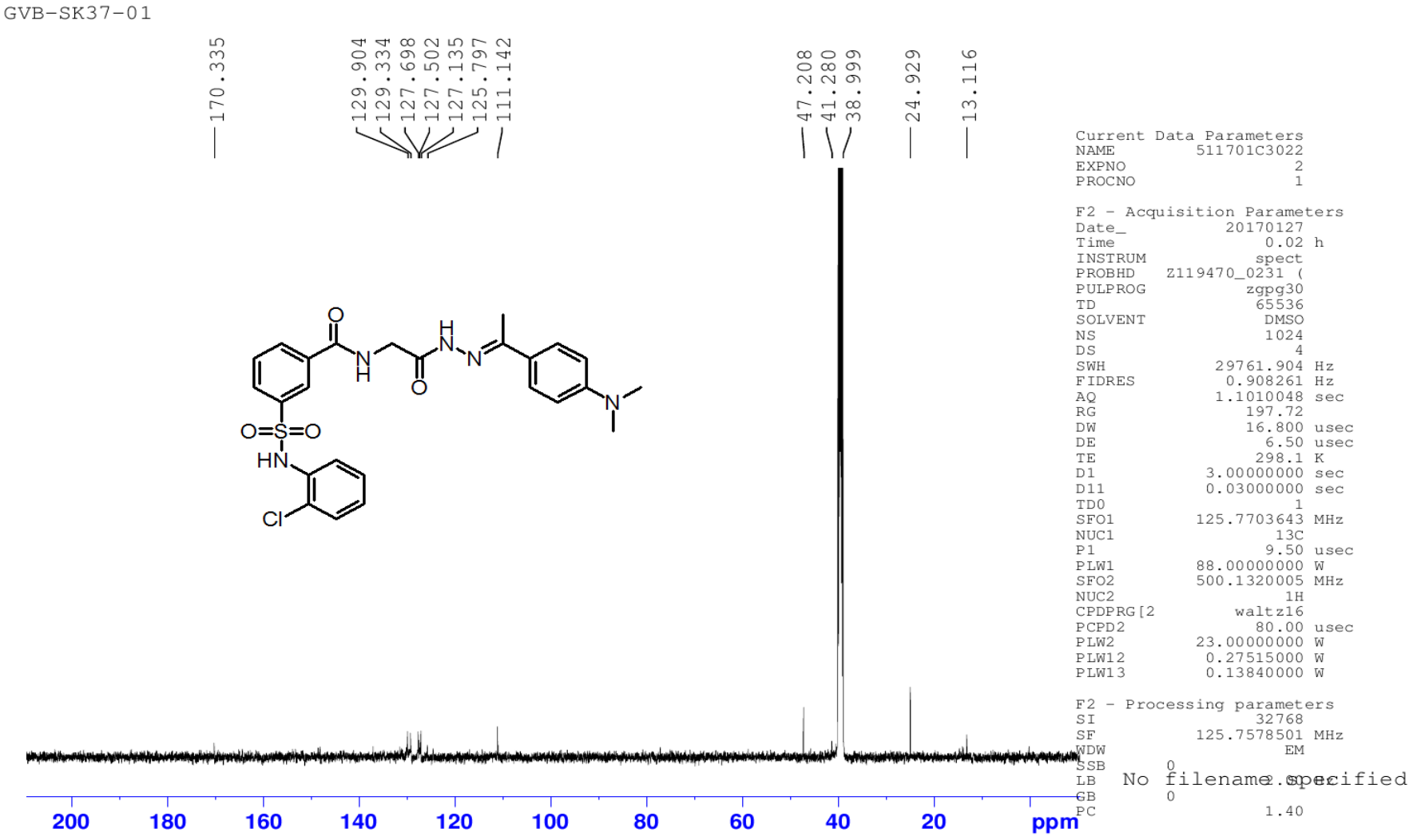


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
569.0854	569.0873	-1.9	-3.3	14.5	38.7	C24 H21 N4 O5 S Cl F3

HRMS of **Compound-2f**



^{1}H NMR of **Compound-2g** in DMSO-d_6



^{13}CNMR of **Compound-2g** in DMSO-d_6

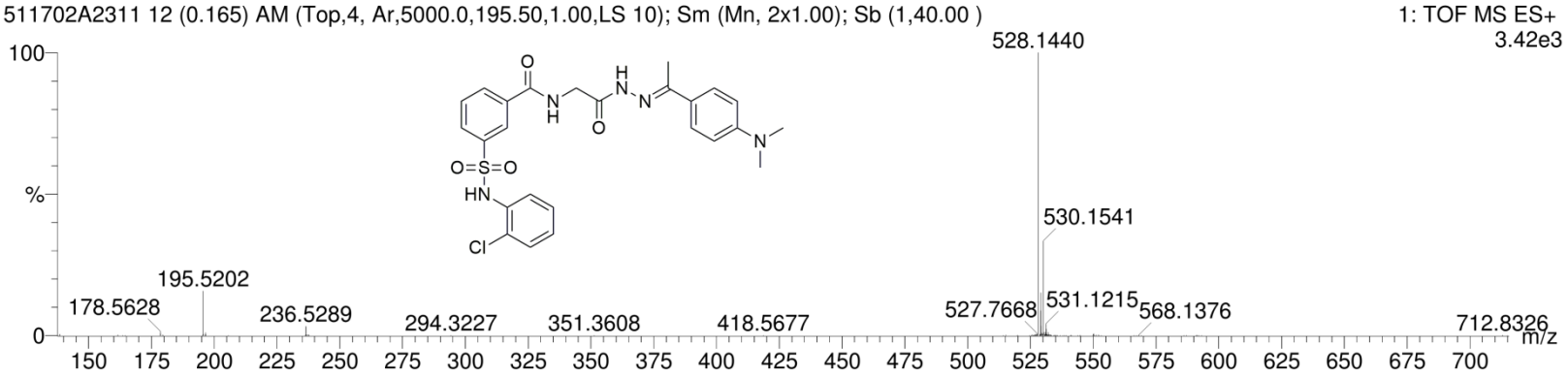
Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

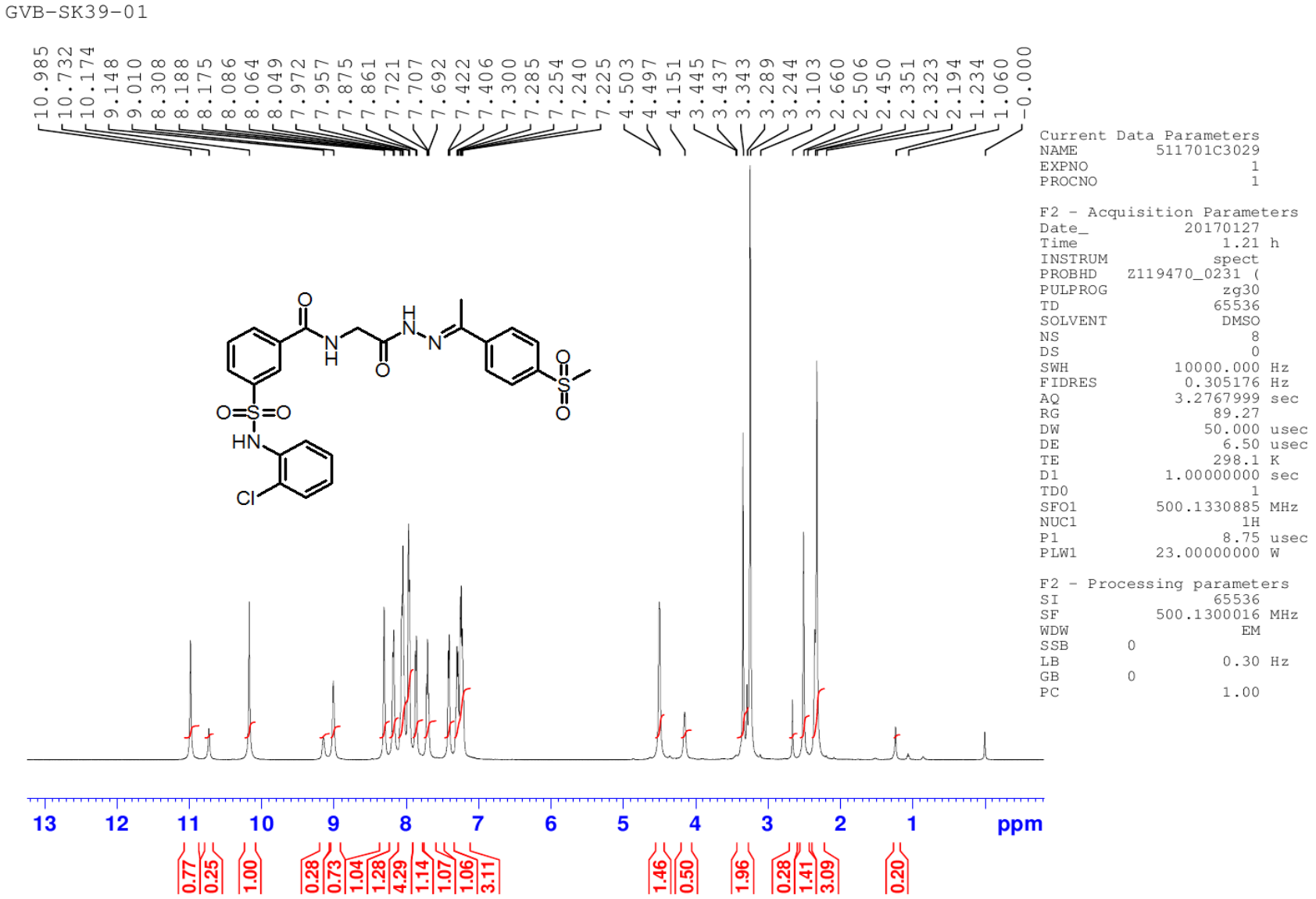
Monoisotopic Mass, Even Electron Ions
113 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-25 H: 0-27 N: 0-5 O: 0-4 S: 0-1 Cl: 0-1

GVB-SK37
511702A2311 12 (0.165) AM (Top,4, Ar,5000.0,195.50,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

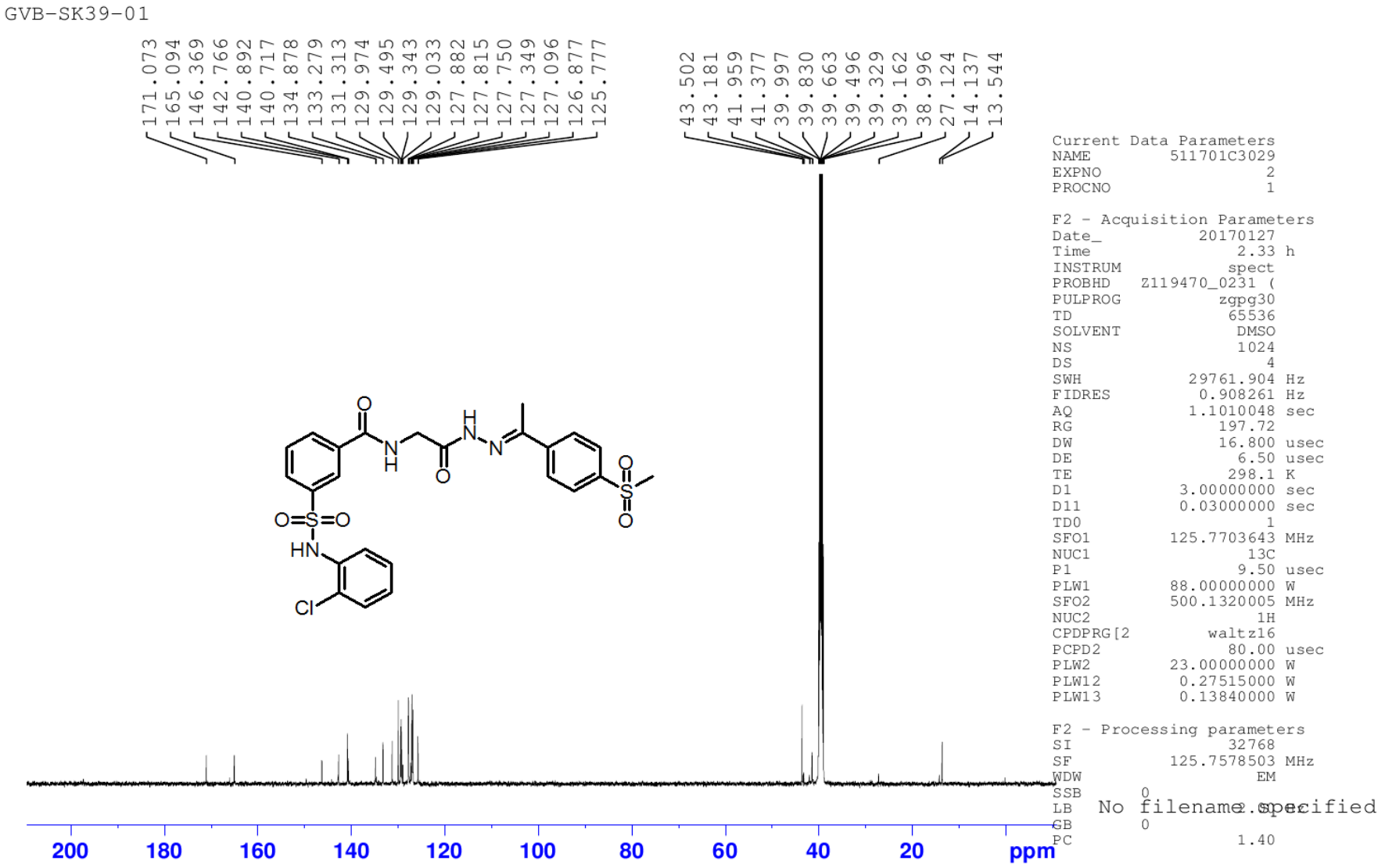


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
528.1440	528.1472	-3.2	-6.1	14.5	196.0	C25 H27 N5 O4 S Cl

HRMS of **Compound-2g**



^{1}H NMR of **Compound-2h** in DMSO-d_6



^{13}CNMR of **Compound-2h** in DMSO-d_6

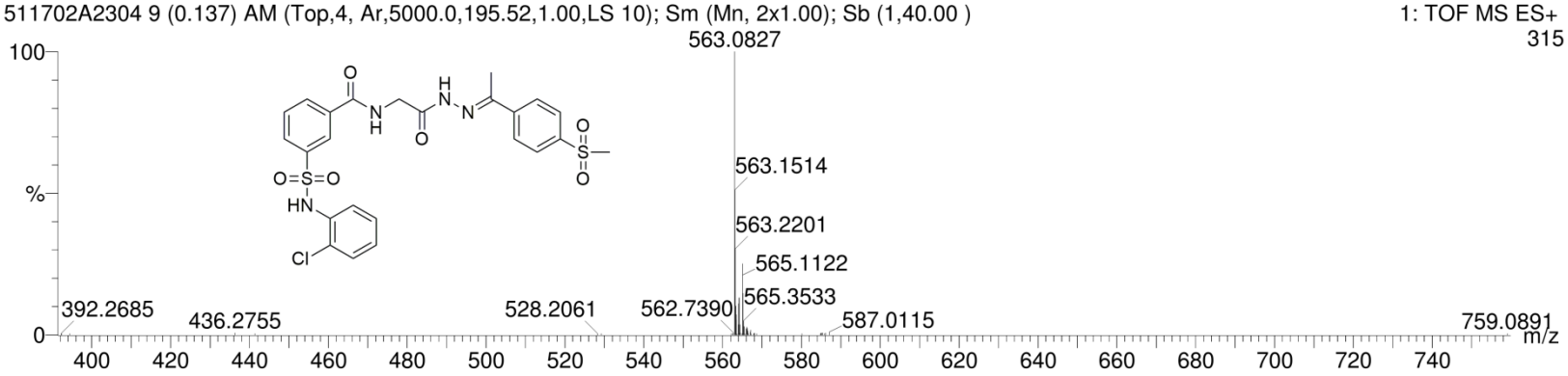
Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

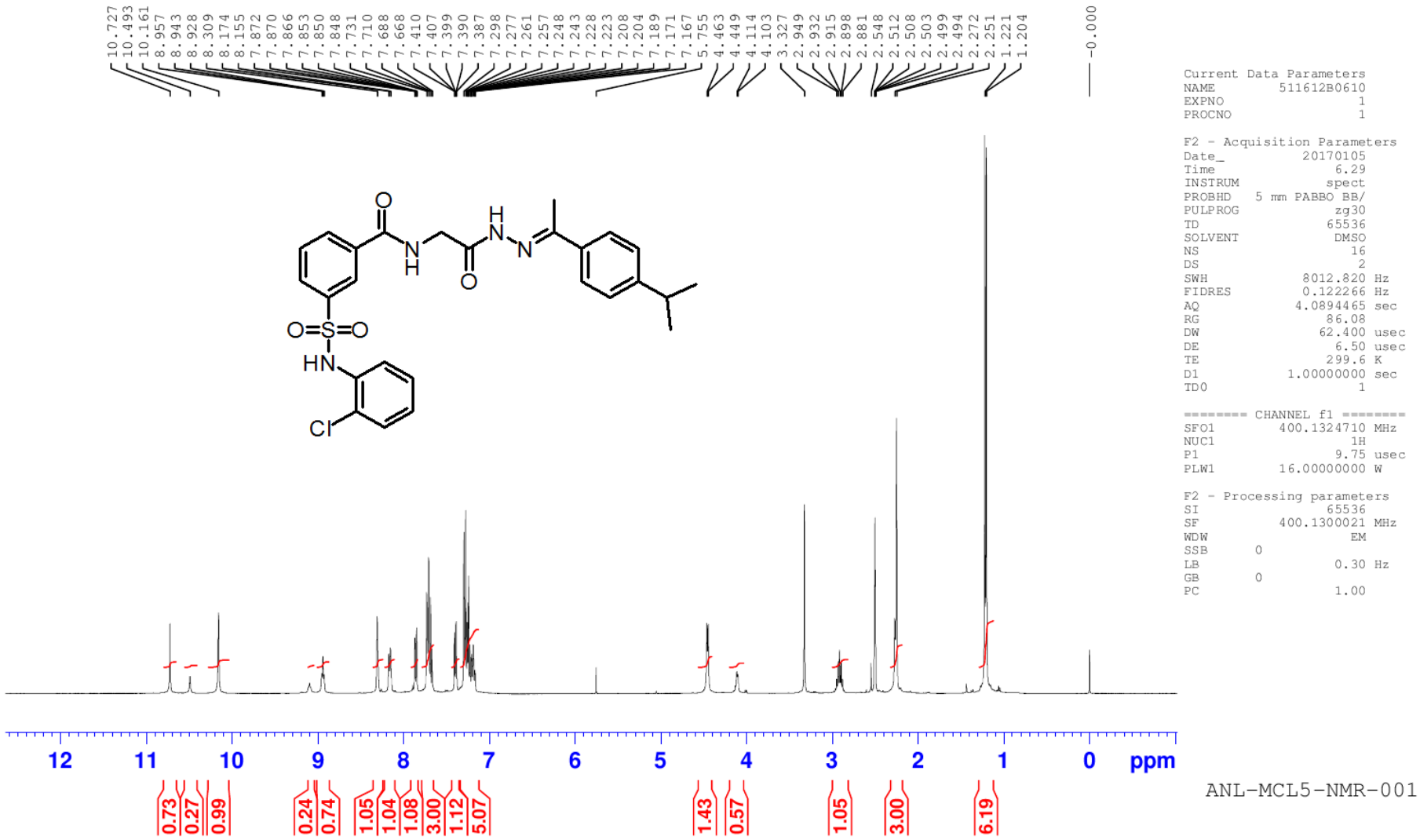
Monoisotopic Mass, Even Electron Ions
203 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-24 H: 0-24 N: 0-4 O: 0-6 S: 0-2 Cl: 0-1

GVB-SK39-01
511702A2304 9 (0.137) AM (Top,4, Ar,5000.0,195.52,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
563.0827	563.0826	0.1	0.2	14.5	26.5	C24 H24 N4 O6 S2 Cl

HRMS of **Compound-2h**

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EXPNO                   1
PROCNO                  1

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Time                6.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 86.08
DW                62.400 usec
DE                 6.50 usec
TE                299.6 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                  9.75 usec
PLW1         16.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300021 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
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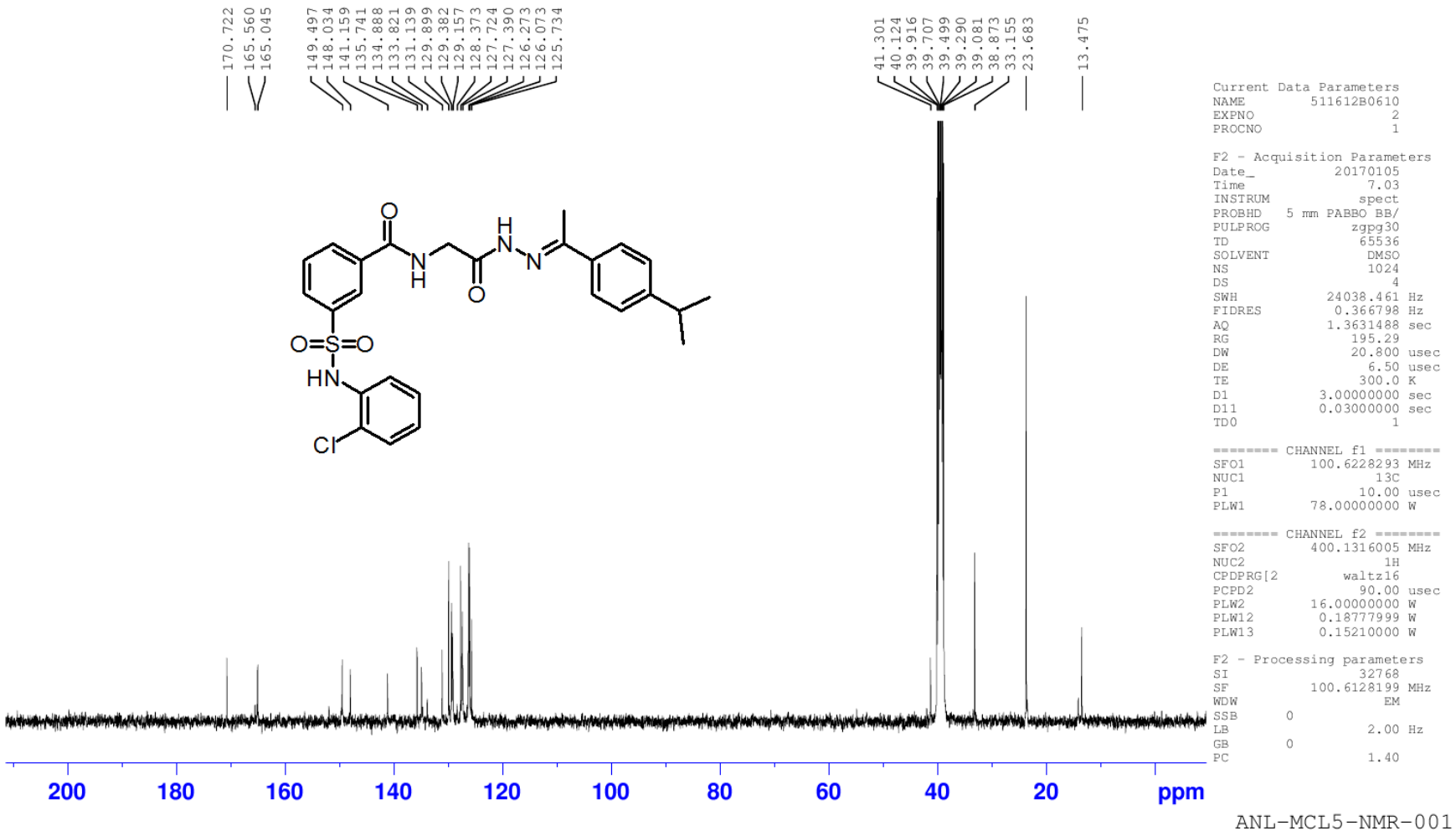
ANL-MCL5-NMR-001

^{1}H NMR of **Compound-2i** in DMSO-d_6



Current Data Parameters
NAME 511612B0610
EXPNO 2
PROCNO 1

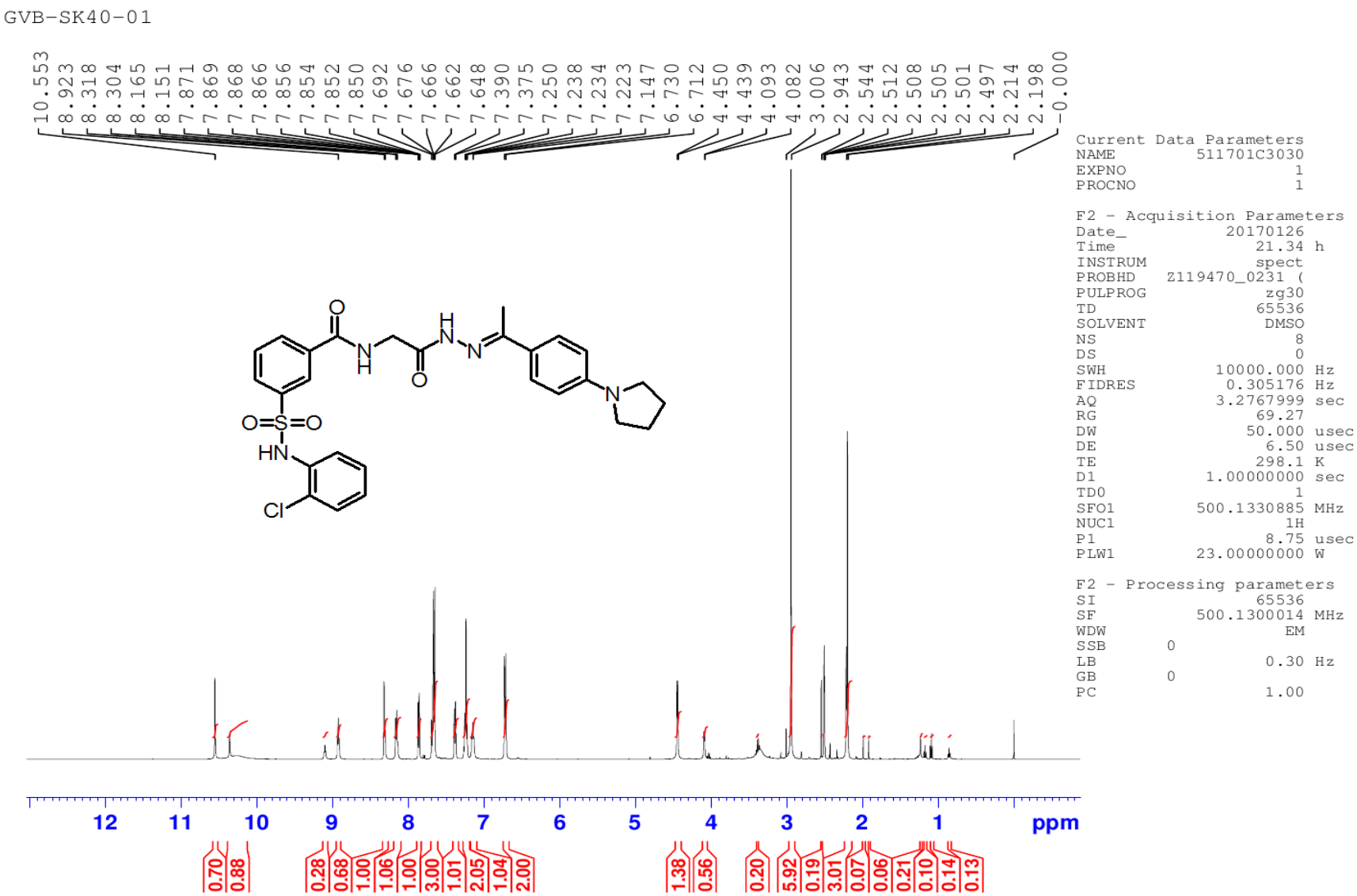
F2 - Acquisition Parameters
Date_ 20170105
Time 7.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 195.29
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 78.00000000 W

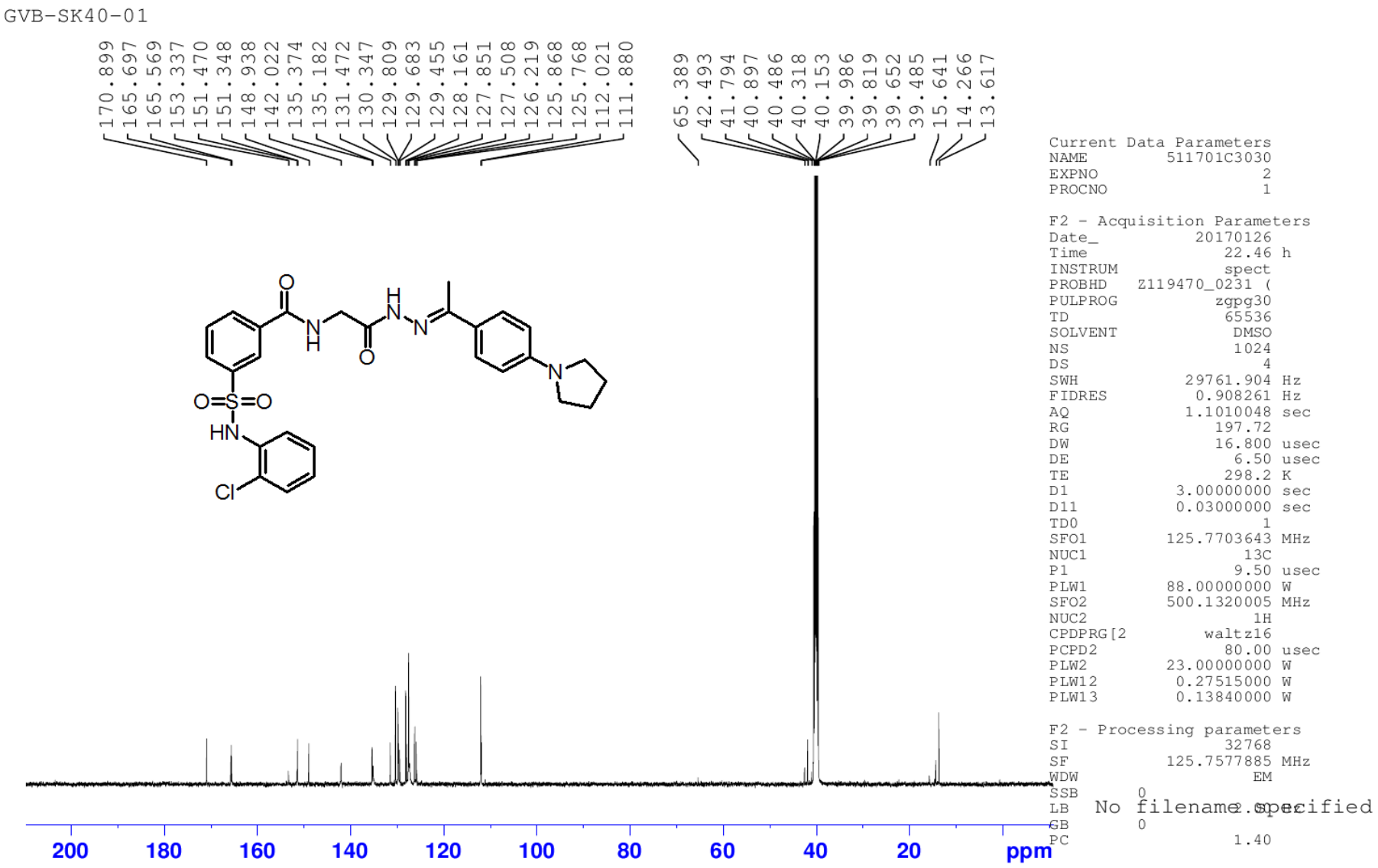
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.18777999 W
PLW13 0.15210000 W

F2 - Processing parameters
SI 32768
SF 100.6128199 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

^{13}CNMR of **Compound-2i** in DMSO-d_6



^{1}H NMR of **Compound-2j** in DMSO-d_6



^{13}CNMR of **Compound-2j** in DMSO-d_6

Elemental Composition Report

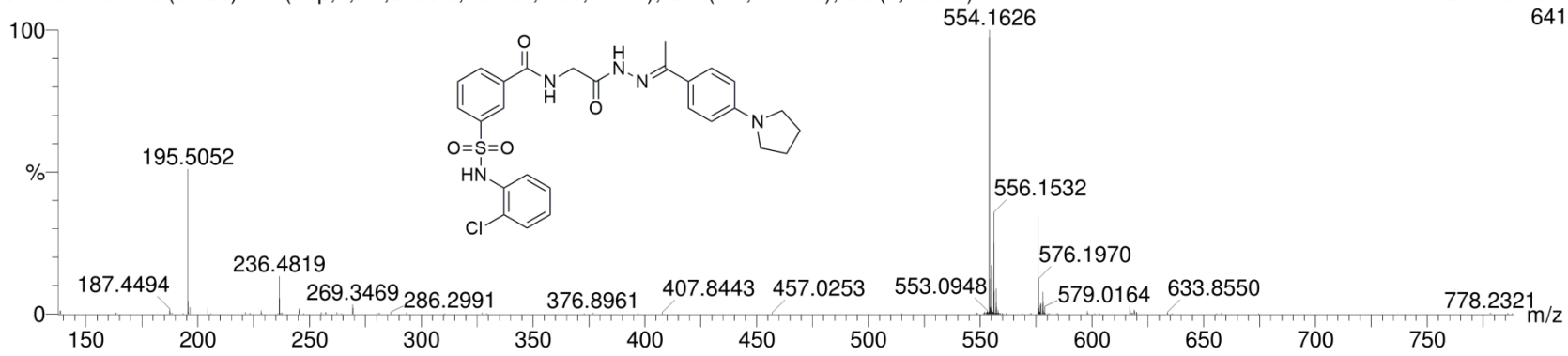
Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
113 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-27 H: 0-29 N: 0-5 O: 0-4 S: 0-1 Cl: 0-1

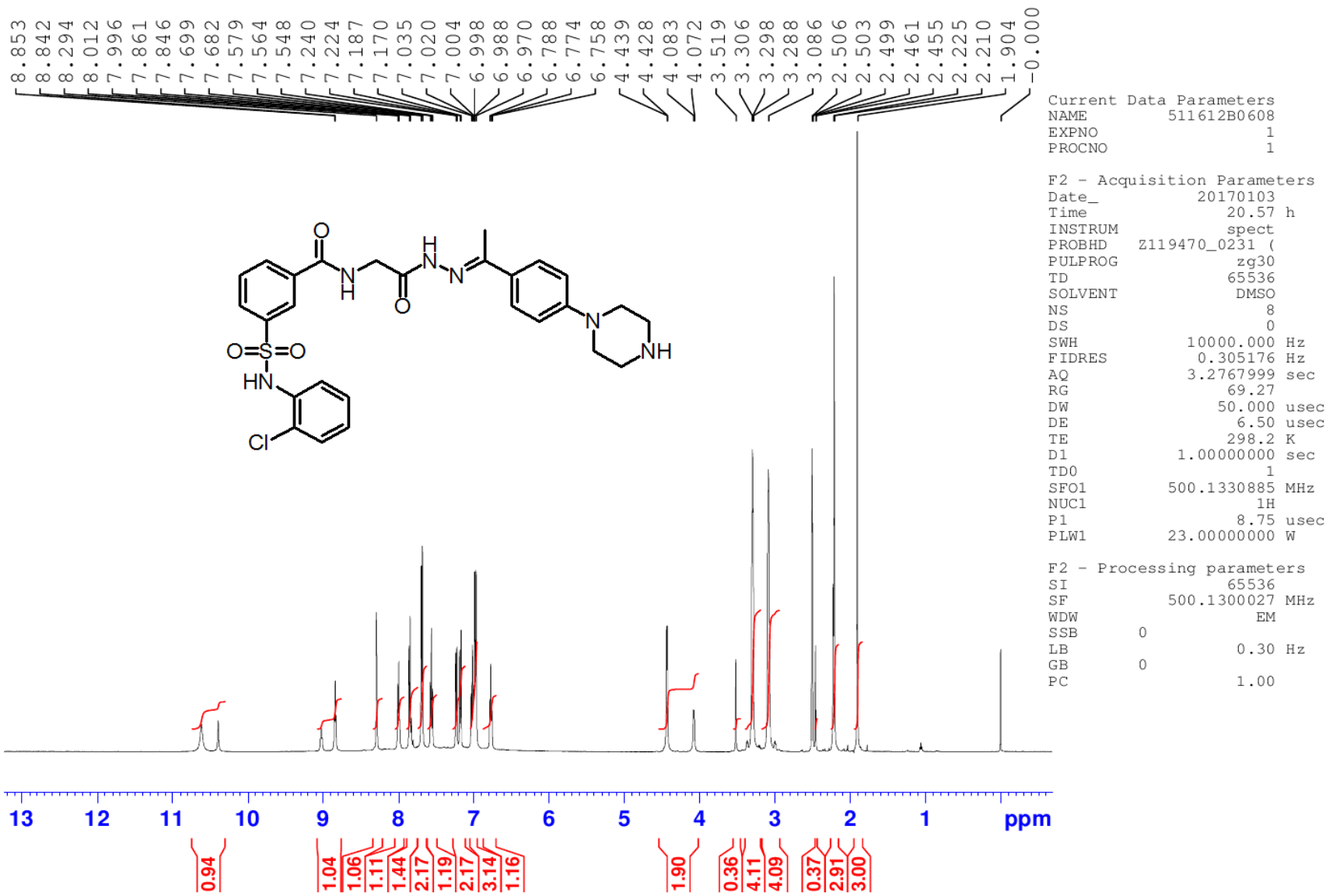
GVB-SK40
511702A2314 9 (0.136) AM (Top,4, Ar,5000.0,195.51,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
641

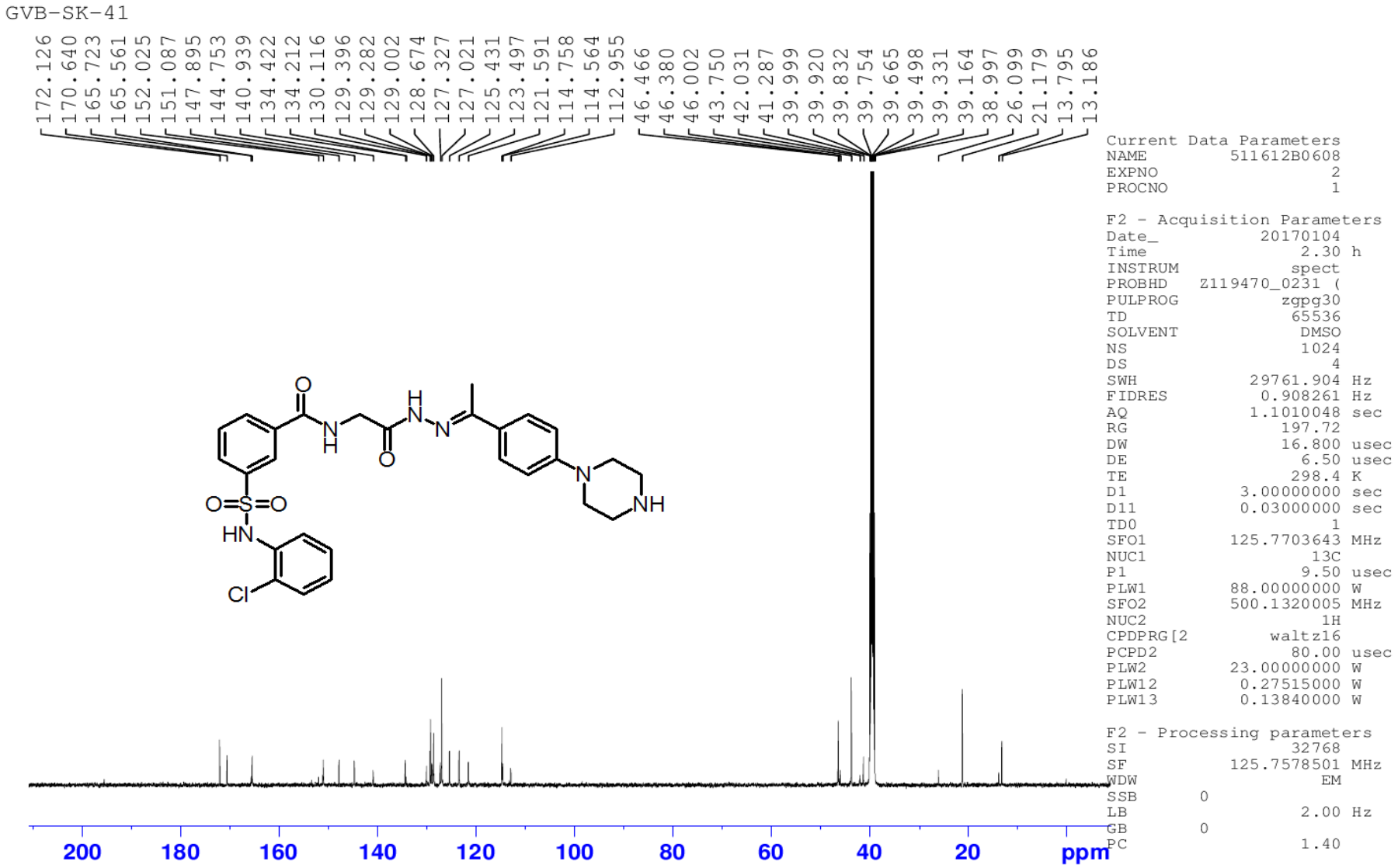


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
554.1626	554.1629	-0.3	-0.5	15.5	31.4	C27 H29 N5 O4 S Cl

HRMS of **Compound-2J**



^{1}H NMR of **Compound-2k** in DMSO-d_6



^{13}CNMR of **Compound-2k** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

133 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

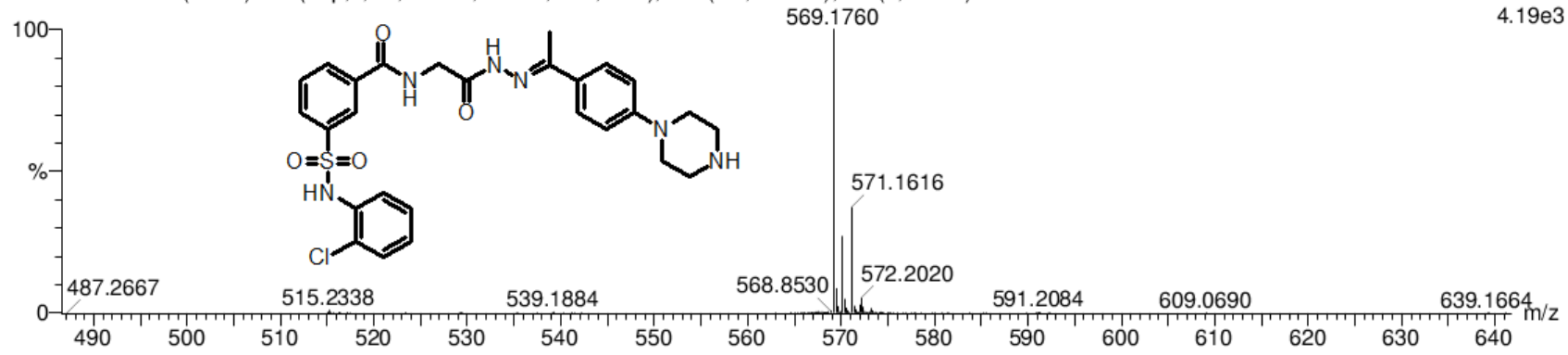
Elements Used:

C: 0-27 H: 0-30 N: 0-6 O: 0-4 S: 0-1 Cl: 0-1

SAMPLE CODE:COMPOUND-41

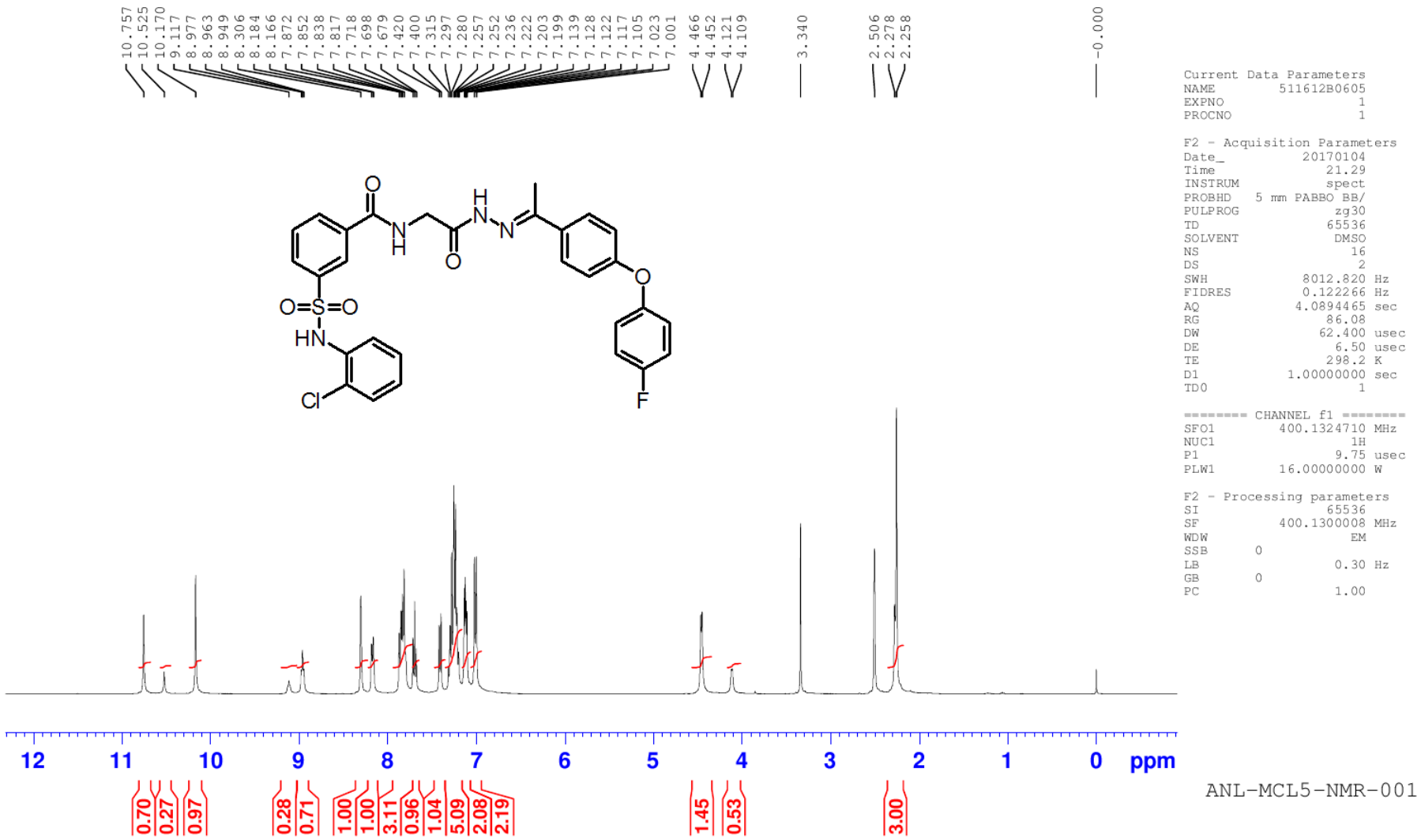
511701A5134 32 (0.462) AM (Top,4, Ar,5000.0,195.17,1.00,LS 5); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
4.19e3

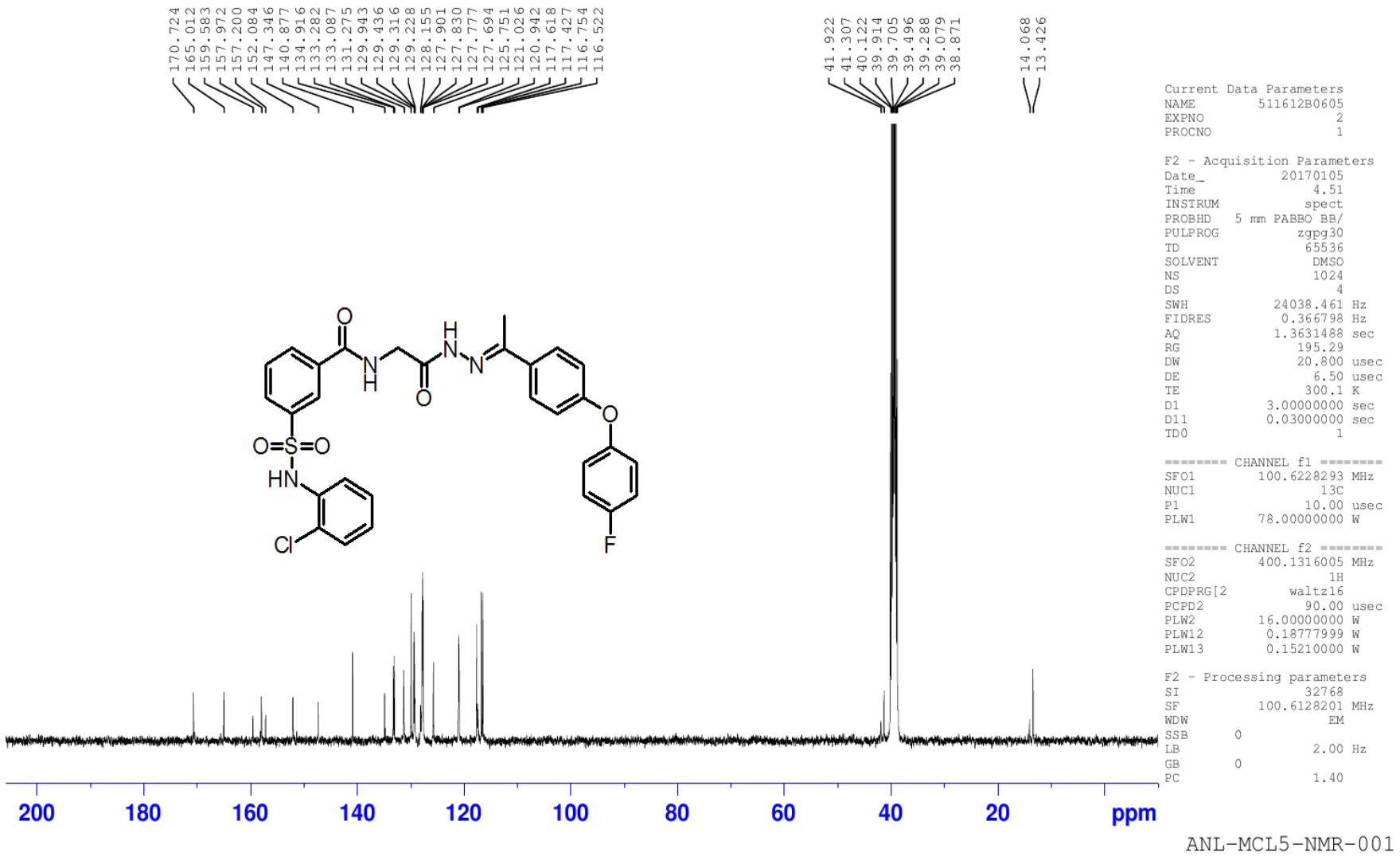


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
569.1760	569.1738	2.2	3.9	15.5	30.6	C27 H30 N6 O4 S Cl

HRMS of **Compound-2K**



^{1}H NMR of **Compound-2m** in DMSO-d_6



^{13}CNMR of **Compound-2m** in DMSO-d_6

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

226 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

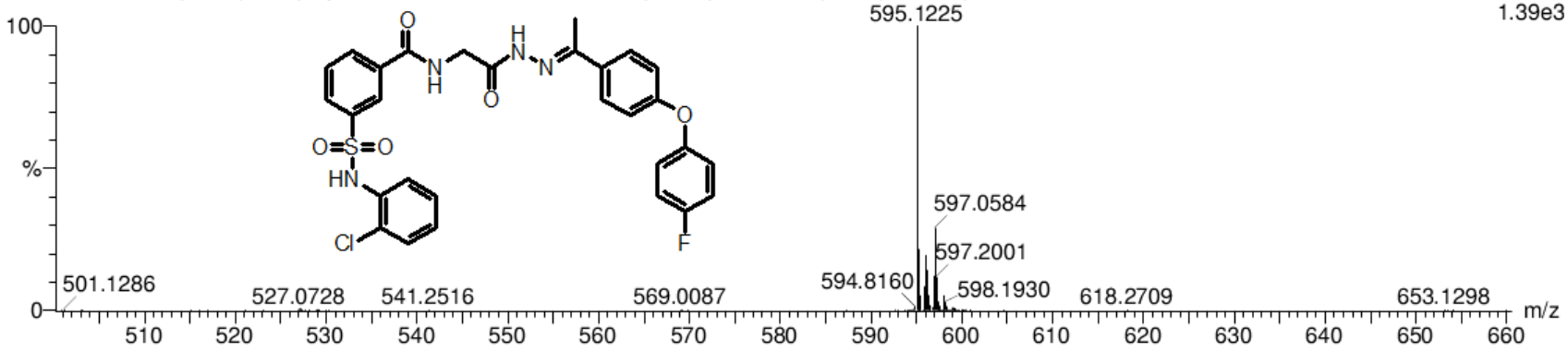
C: 0-29 H: 0-25 N: 0-4 O: 0-5 F: 0-1 S: 0-1 Cl: 0-1

SAMPLE CODE:COMPOUND-38

511701A5149 28 (0.392) AM (Top,4, Ar,5000.0,195.13,1.00,LS 5); Sm (Mn, 1x1.00); Sb (1,40.00)

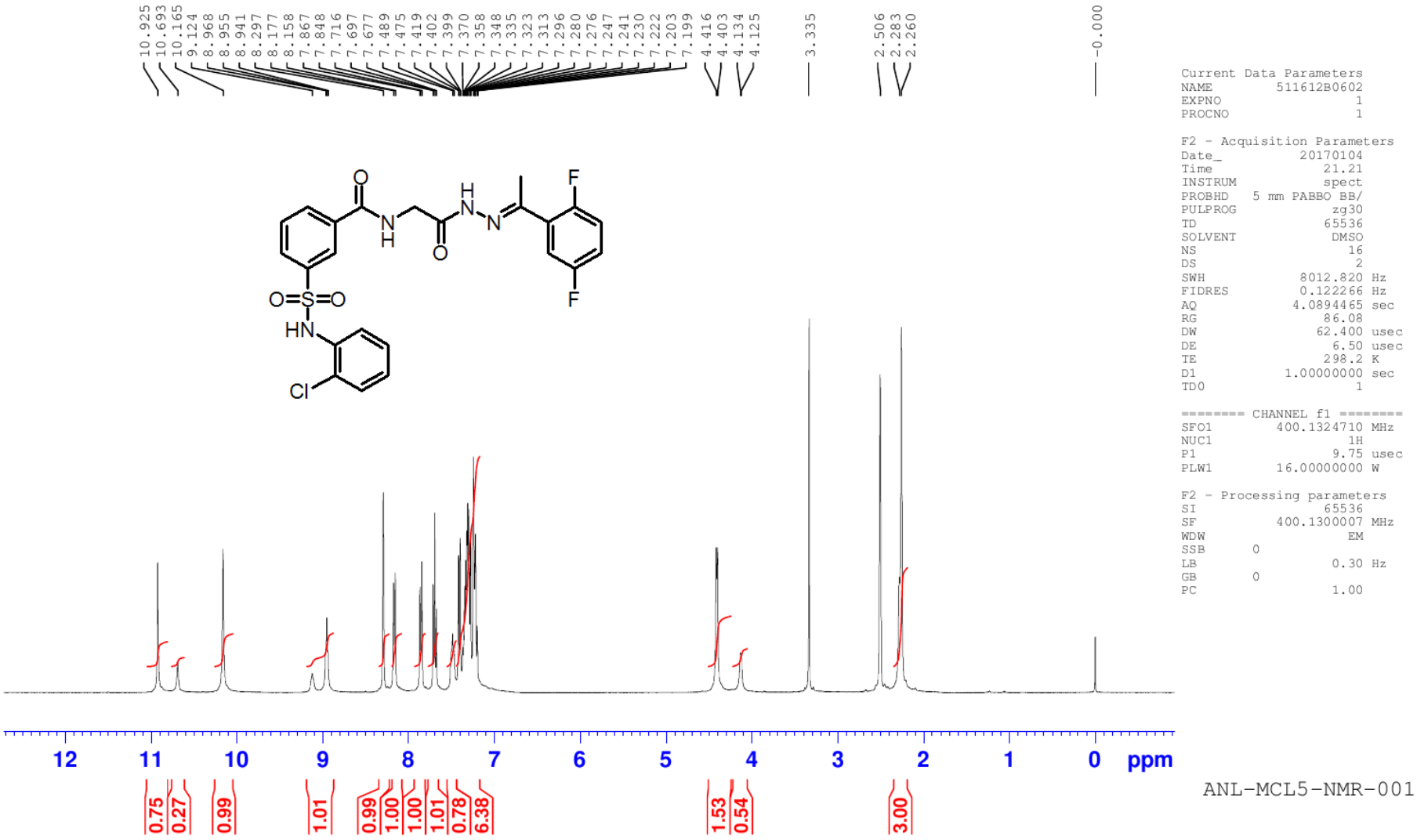
1: TOF MS ES+

1.39e3

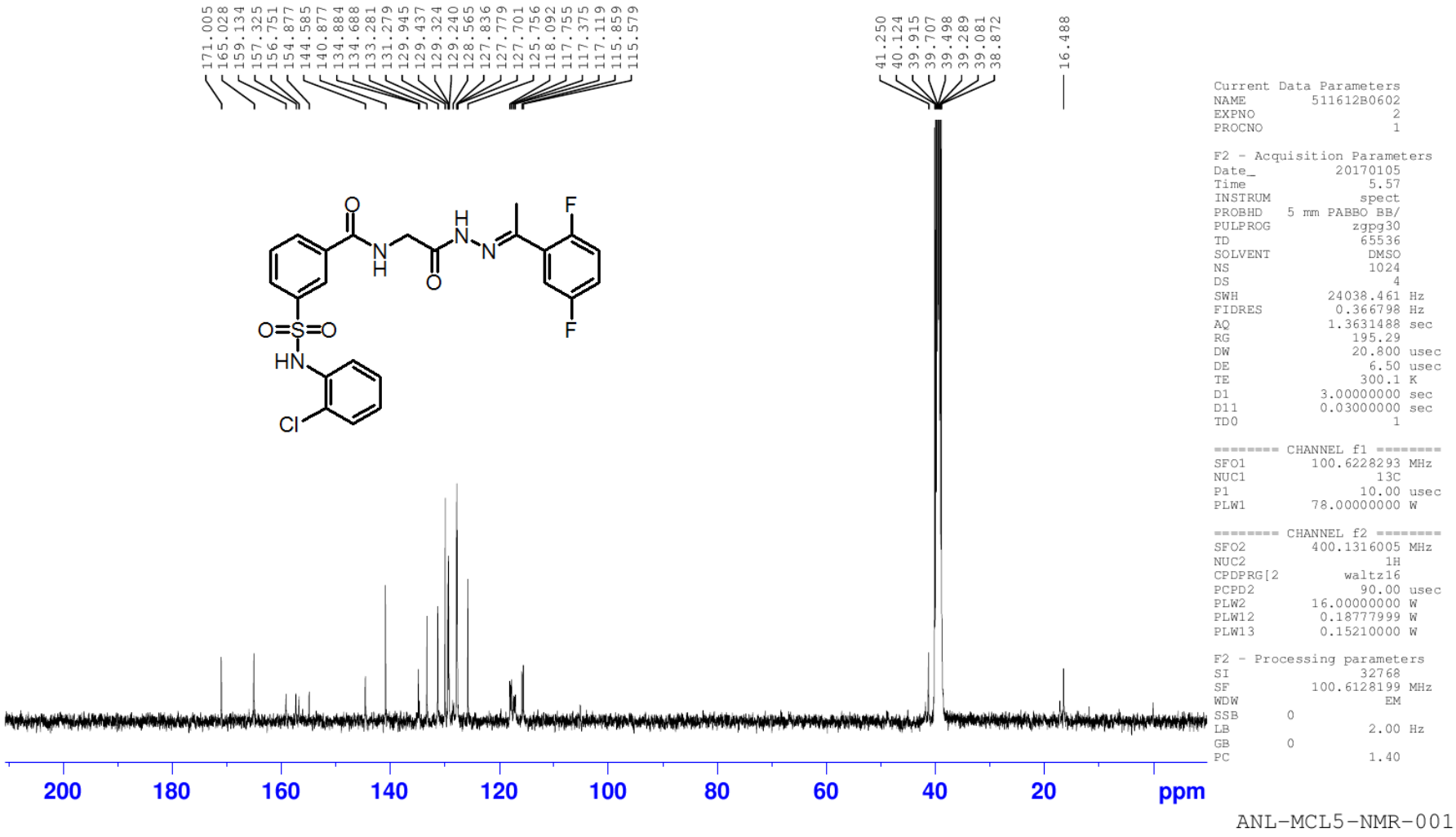


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
595.1225	595.1218	0.7	1.2	18.5	78.0	C29 H25 N4 O5 F S Cl

HRMS of **Compound-2m**



^{1}H NMR of **Compound-2n** in DMSO-d_6



^{13}CNMR of **Compound-2n** in DMSO-d_6

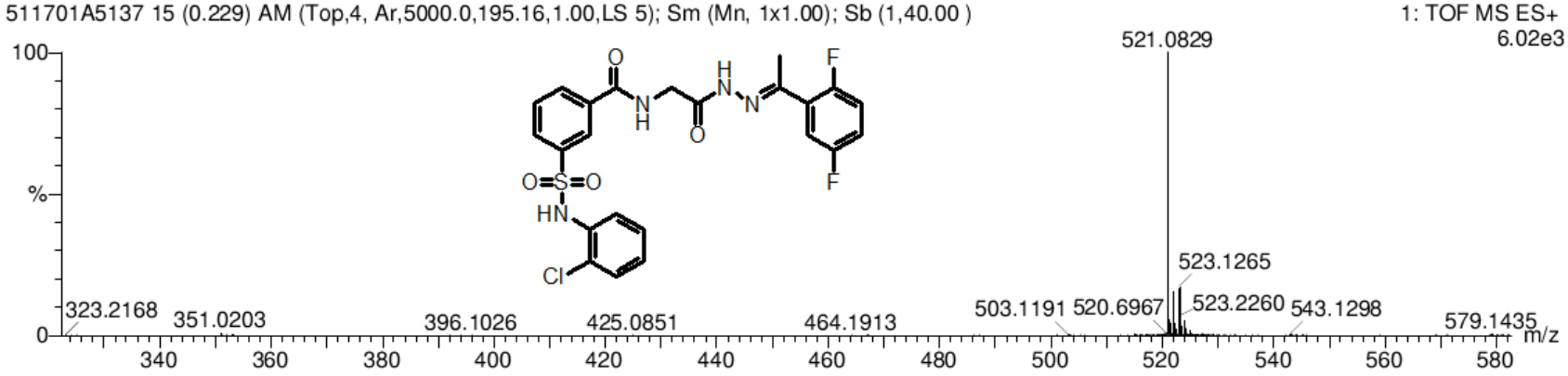
Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

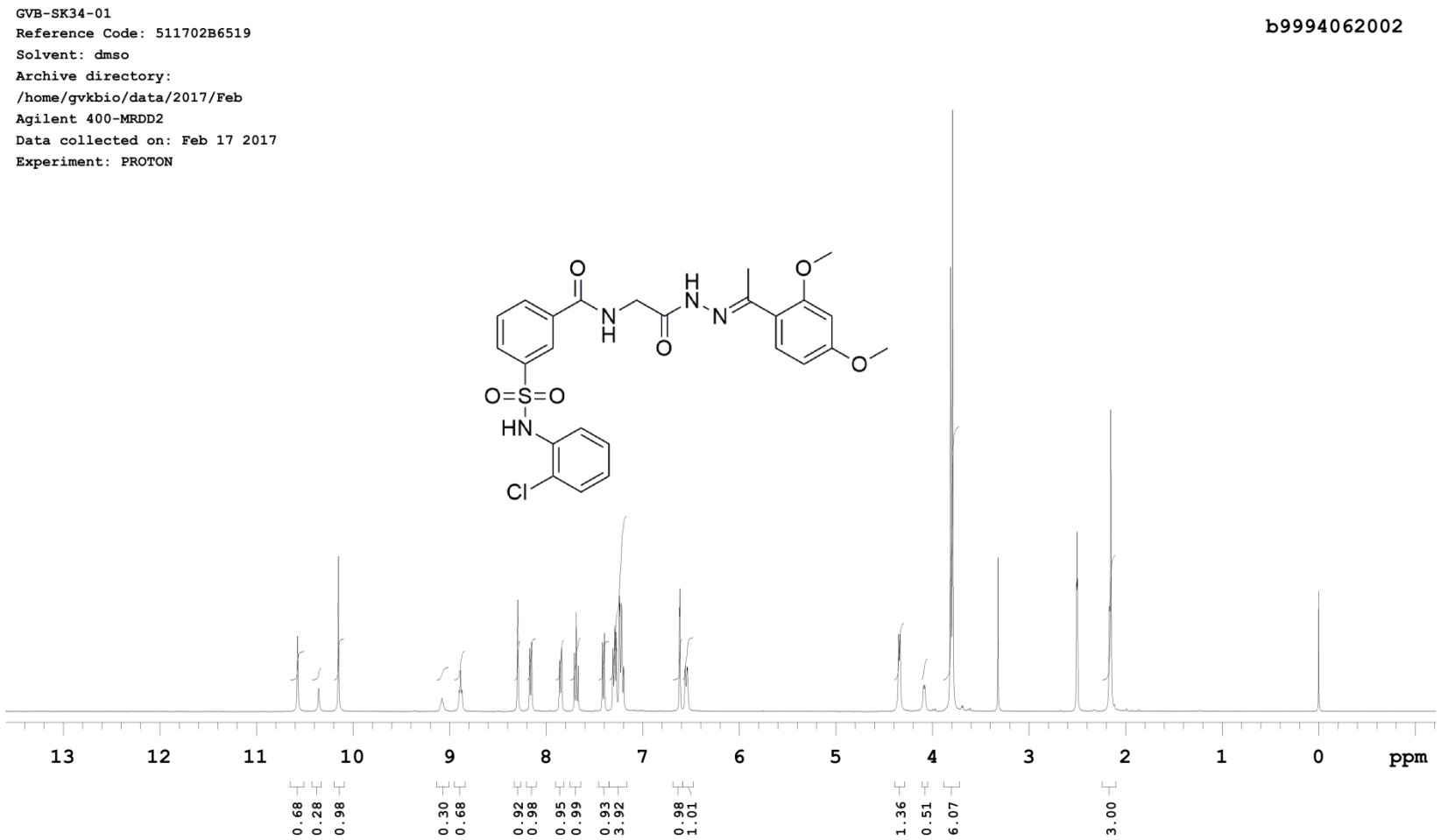
Monoisotopic Mass, Even Electron Ions
337 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-20 N: 0-4 O: 0-5 S: 0-1 Cl: 0-1 F: 0-2

SAMPLE CODE:COMPOUND-35
511701A5137 15 (0.229) AM (Top,4, Ar,5000.0,195.16,1.00,LS 5); Sm (Mn, 1x1.00); Sb (1,40.00)

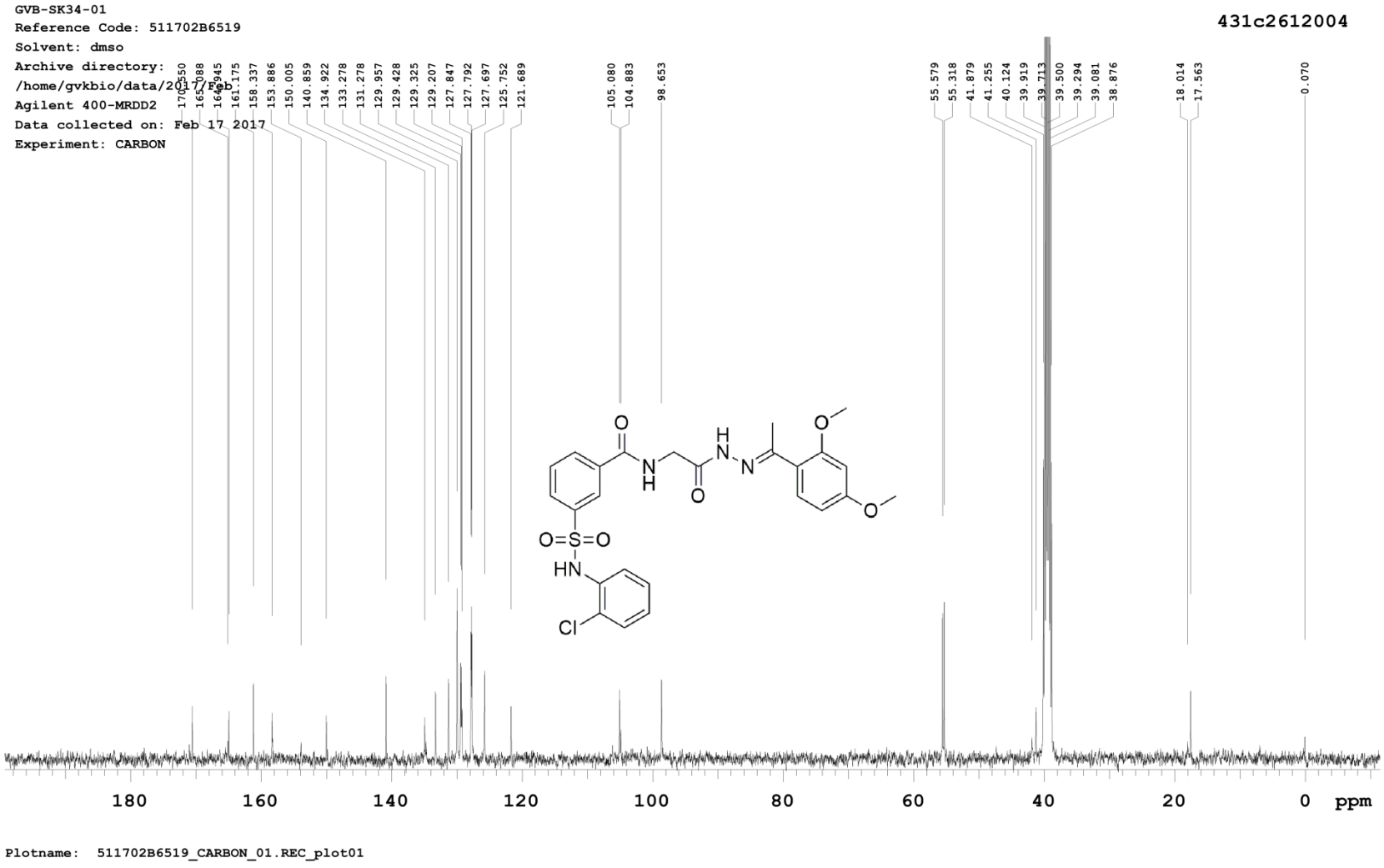


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
521.0829	521.0862	-3.3	-6.3	14.5	579.7	C23 H20 N4 O4 S Cl F2

HRMS of **Compound-2n**



^{1}H NMR of **Compound-2o** in DMSO-d_6



^{13}CNMR of **Compound-2o** in DMSO-d_6

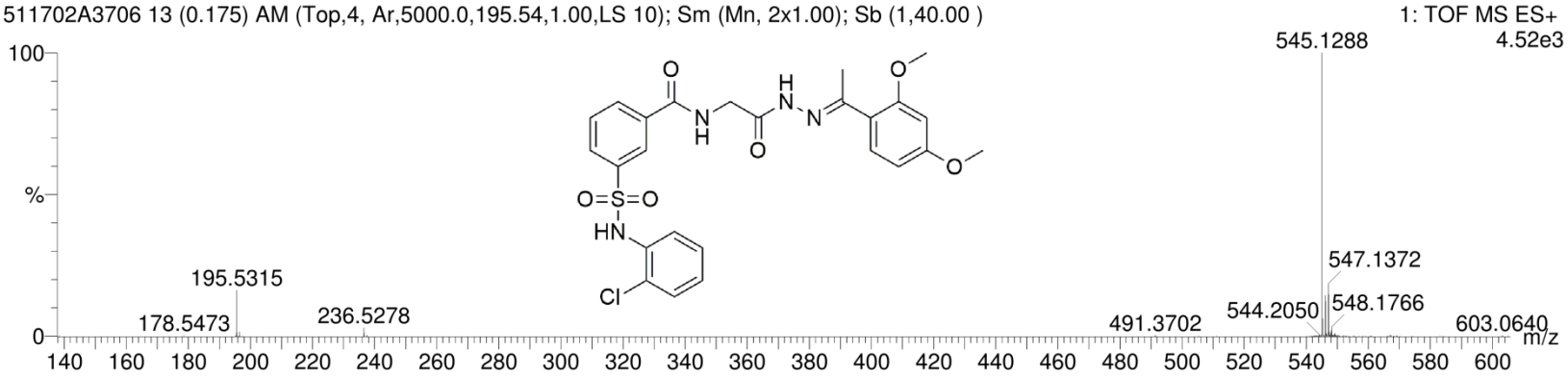
Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
133 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-25 H: 0-26 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1

GVB-SK34-01
511702A3706 13 (0.175) AM (Top,4, Ar,5000.0,195.54,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
545.1288	545.1262	2.6	4.8	14.5	427.1	C25 H26 N4 O6 S Cl

HRMS of **Compound-2o**