

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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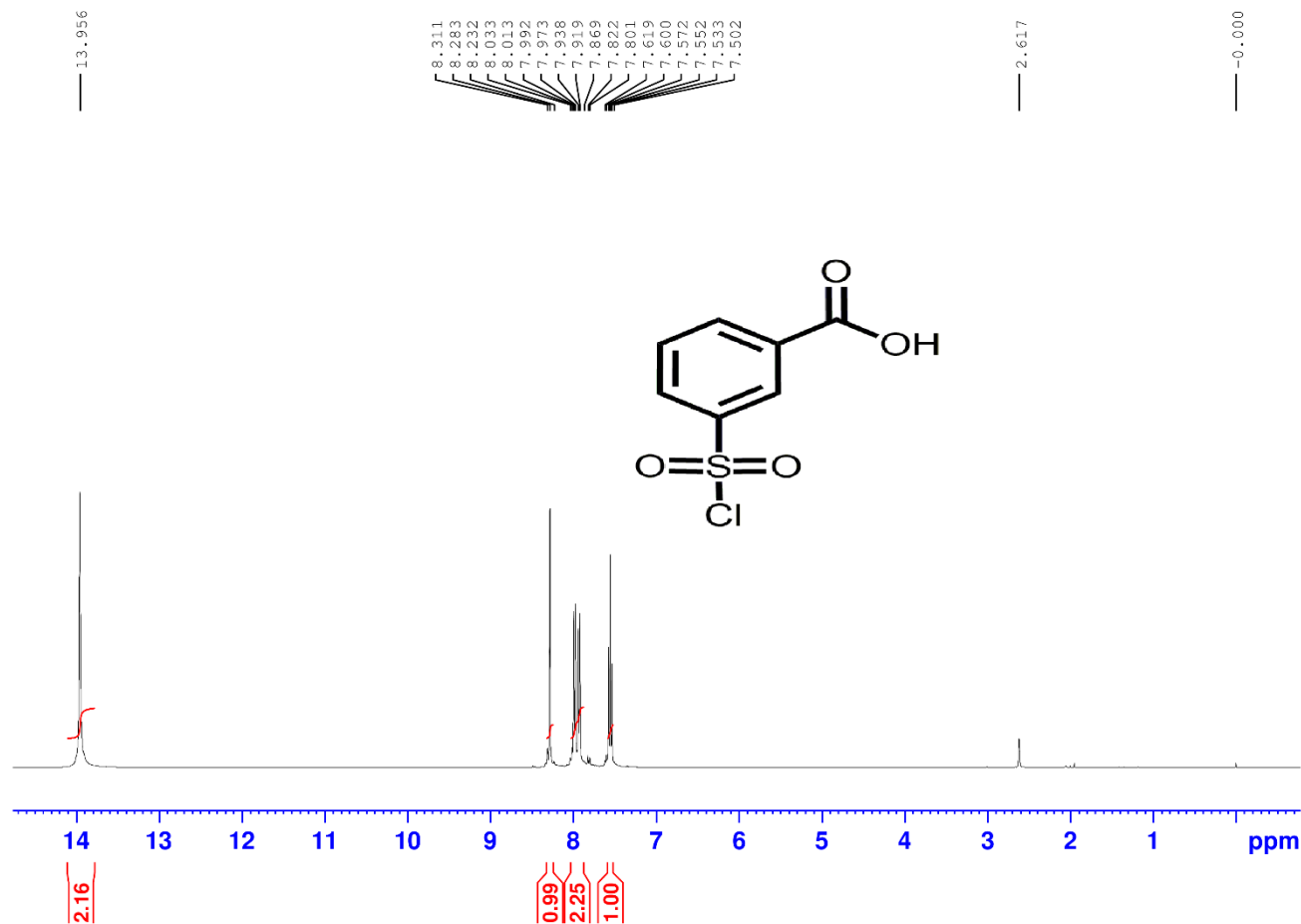
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502 102

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Pradesh, Bapatla, India, 522 101

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GVB-SK-INT-1



Current Data Parameters
 NAME 511701C5156
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170131
 Time 3.57
 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
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 RG 45.52
 DW 62.400 usec
 DE 6.50 usec
 TE 298.7 K
 D1 1.00000000 sec
 TD0 1

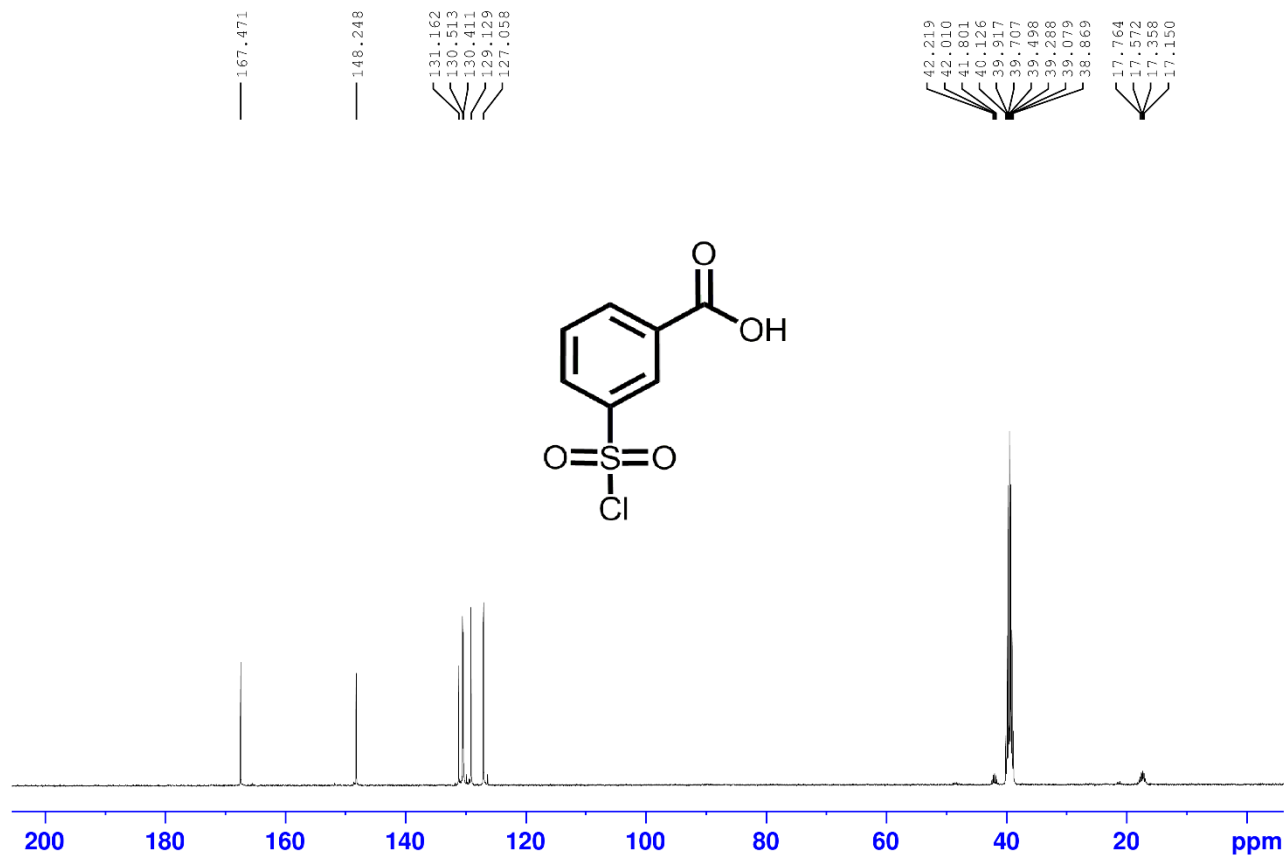
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 NUC1 1H
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 PLW1 16.00000000 W

F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ANL-MCL5-NMR-001

¹H NMR of Compound-B

GVB-SK-INT-1



Current Data Parameters
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EXPNO 2
PROCNO 1

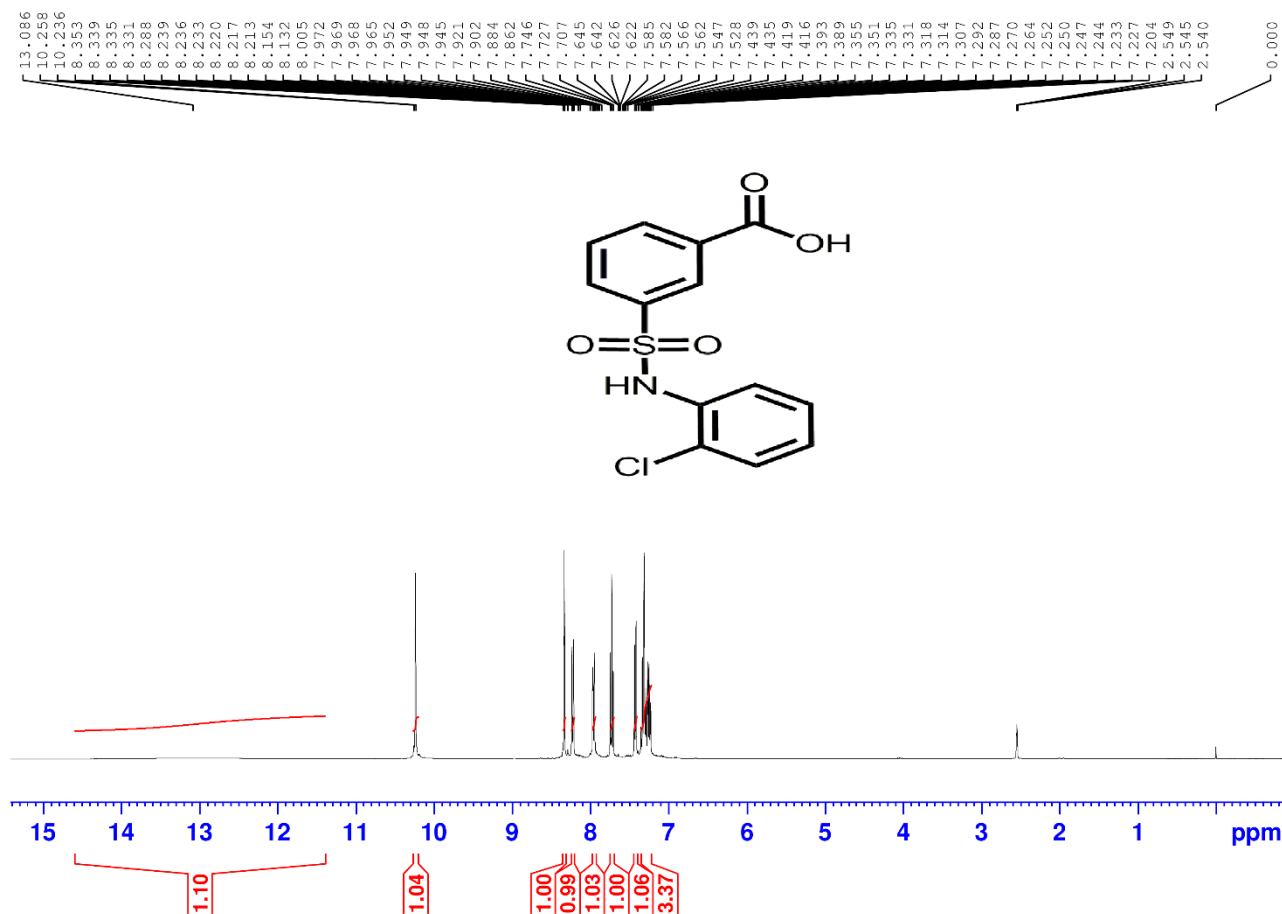
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Time 5.14
INSTRUM spect
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PULPROG zgpg30
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SOLVENT DMSO
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 195.29
DW 20.800 usec
DE 6.50 usec
TE 298.9 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
CPDPRG12 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.18777999 W
PLW13 0.15210000 W

F2 - Processing parameters
SI 32768
SF 100.6127420 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

¹³CNMR of Compound-Bin DMSO-d₆



Current Data Parameters
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EXPNO 1
PROCNO 1

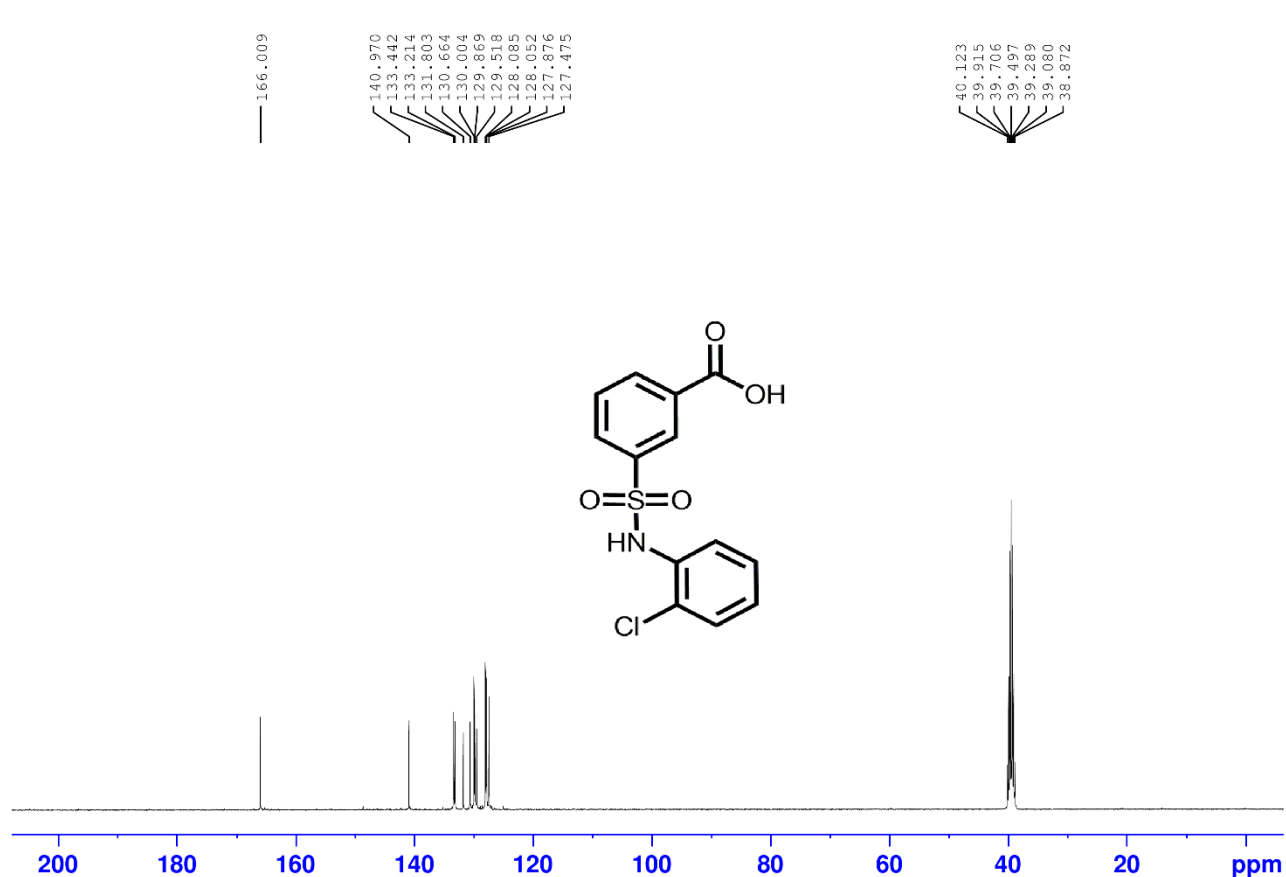
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Time 2.36
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 34.67
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1299853 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL5-NMR-001

¹H NMR of Compound-C



Current Data Parameters

NAMF 511701C5157

EXPNO 2

PROCNO 1

F2 - Acquisition Parameters

Date_ 20170131

Time 3.53

INSTRUM spect

PROBHD 5 mm PABBO BB/

PULPROG zgpg30

ID 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 299.1 K

D1 3.0000000 sec

D11 0.0300000 sec

TD0 1

===== CHANNEL f1 =====

SFO1 100.6228293 MHz

NUC1 13C

P1 10.00 usec

PLW1 78.0000000 W

===== CHANNEL f2 =====

SFO2 400.1316005 MHz

NUC2 1H

CPDPRG2 waltz16

PCPD2 90.00 usec

PLW2 16.0000000 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

ANL-MCL5-NMR-001

¹³CNMR of Compound-C in DMSO-d₆

Elemental Composition Report

Page 1

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)

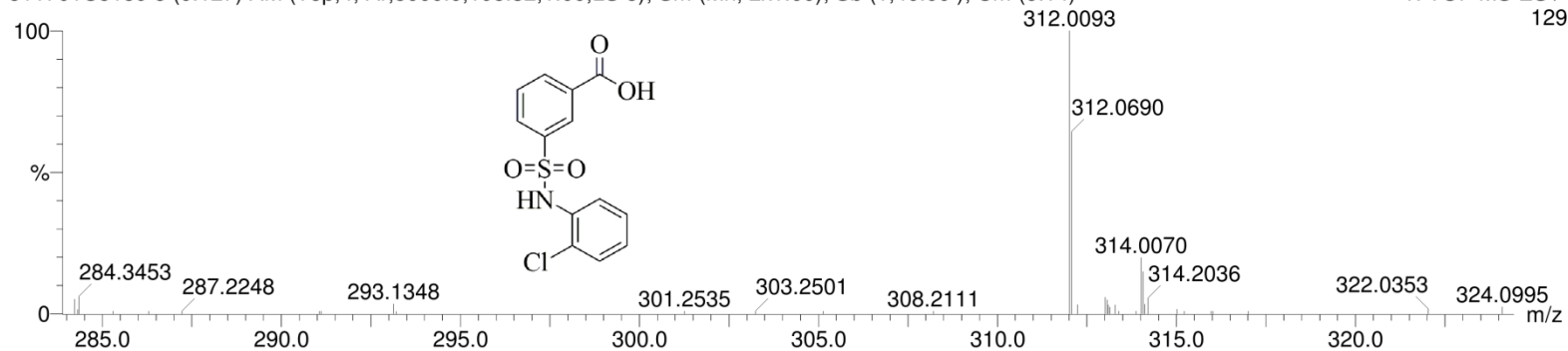
Elements Used:

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

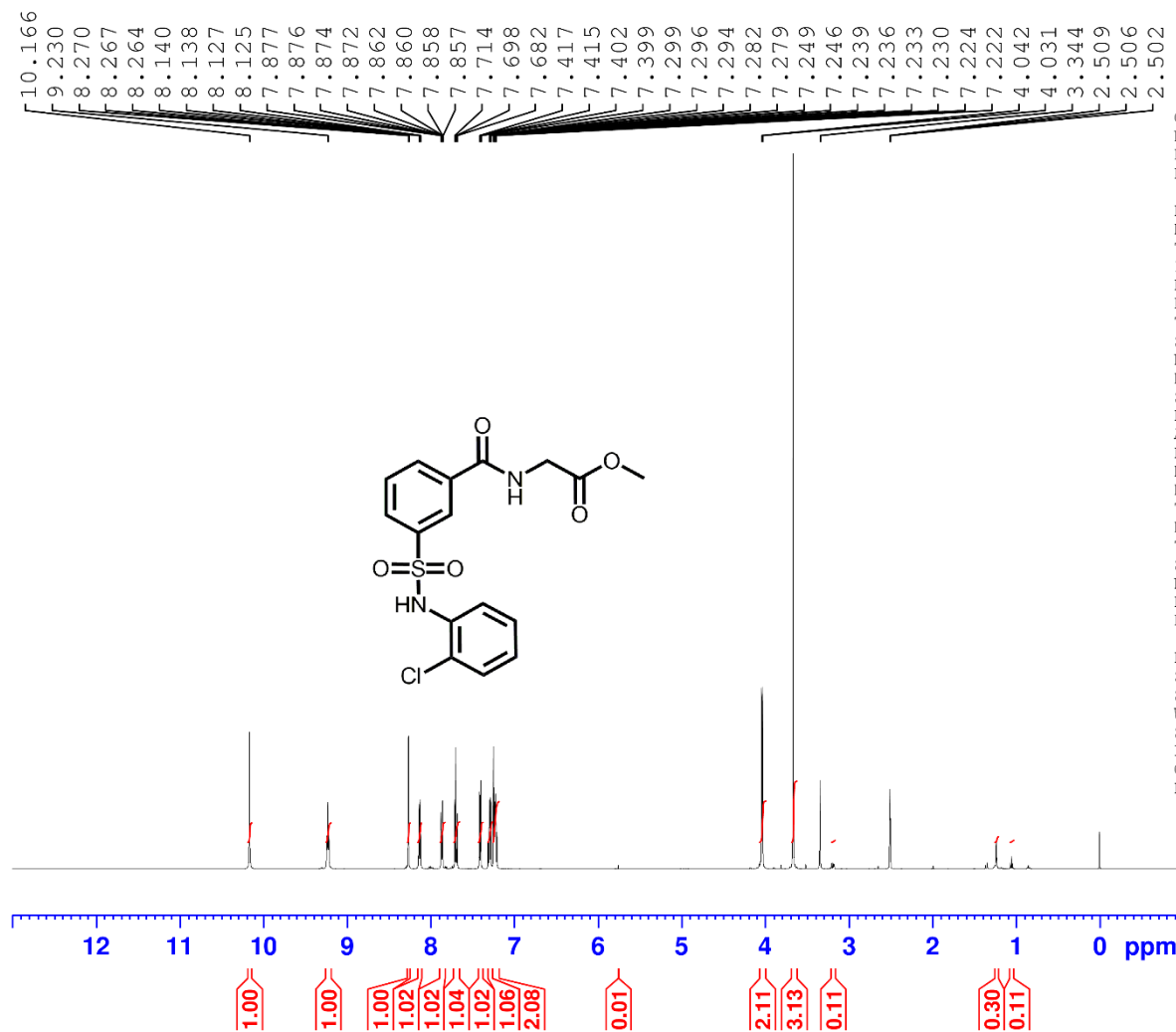


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SKHATU-01



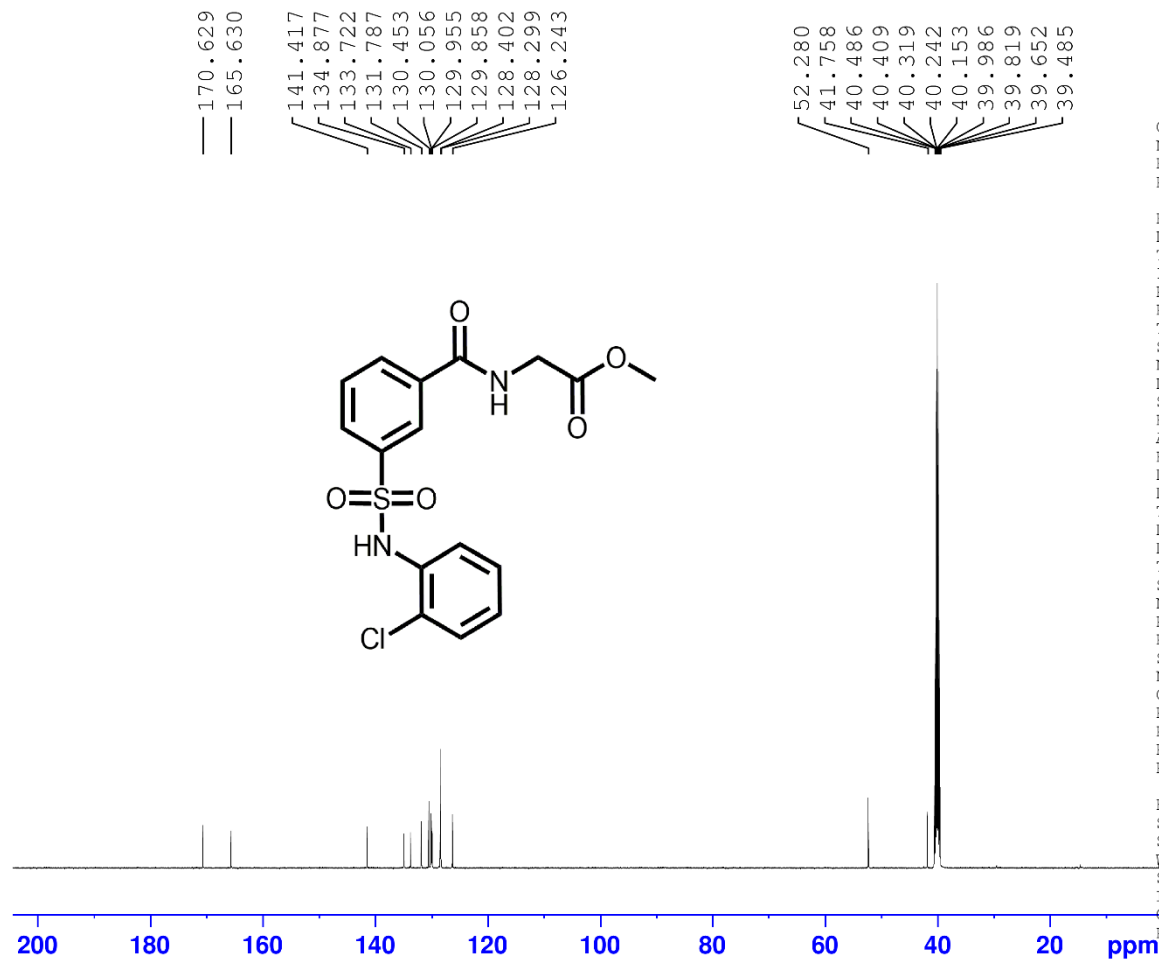
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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170127
 Time 0.05 h
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 PROBHD Z119470_0231 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 79.68
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1
 SF01 500.1330885 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 23.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300013 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of Compound-D

GVB-SKHATU-01



Current Data Parameters
NAME 511701C3027
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170127
Time_ 1.17 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W

F2 - Processing parameters
SI 32768
SF 125.7577885 MHz
WDW EM
SSB 0
LB No filename specified
GB 0
PC 1.40

¹³CNMR of Compound-D in DMSO-d₆

Elemental Composition Report

Page 1

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)

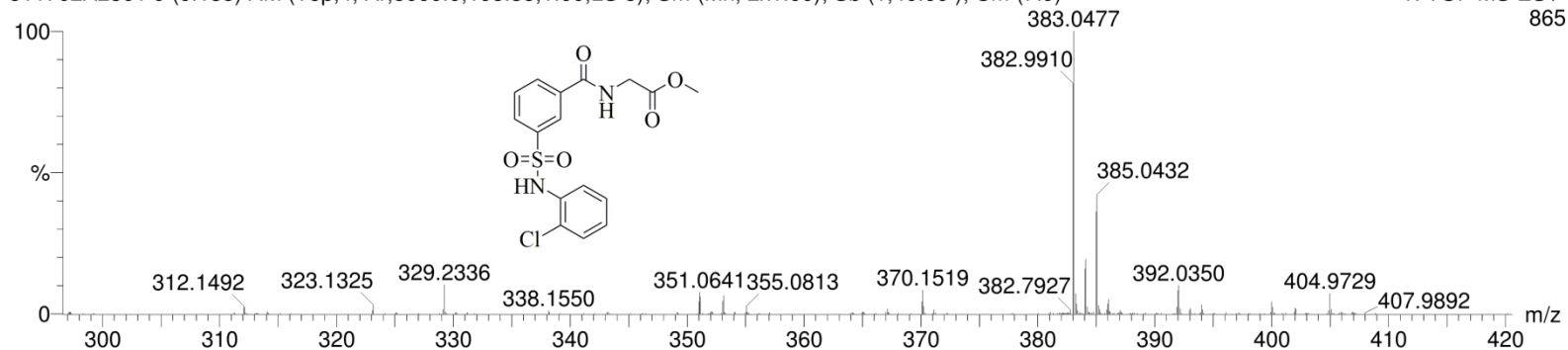
Elements Used:

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

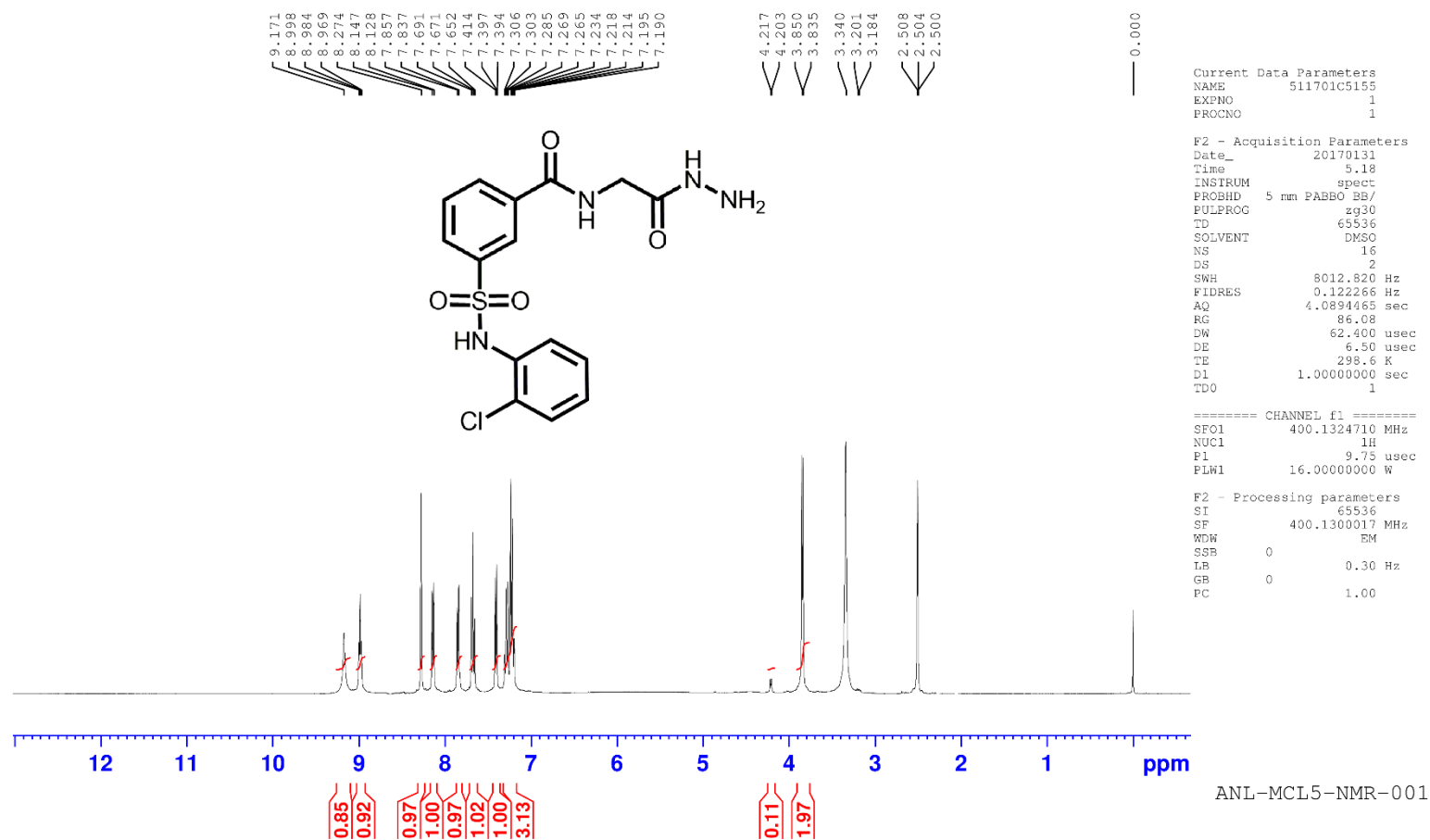


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

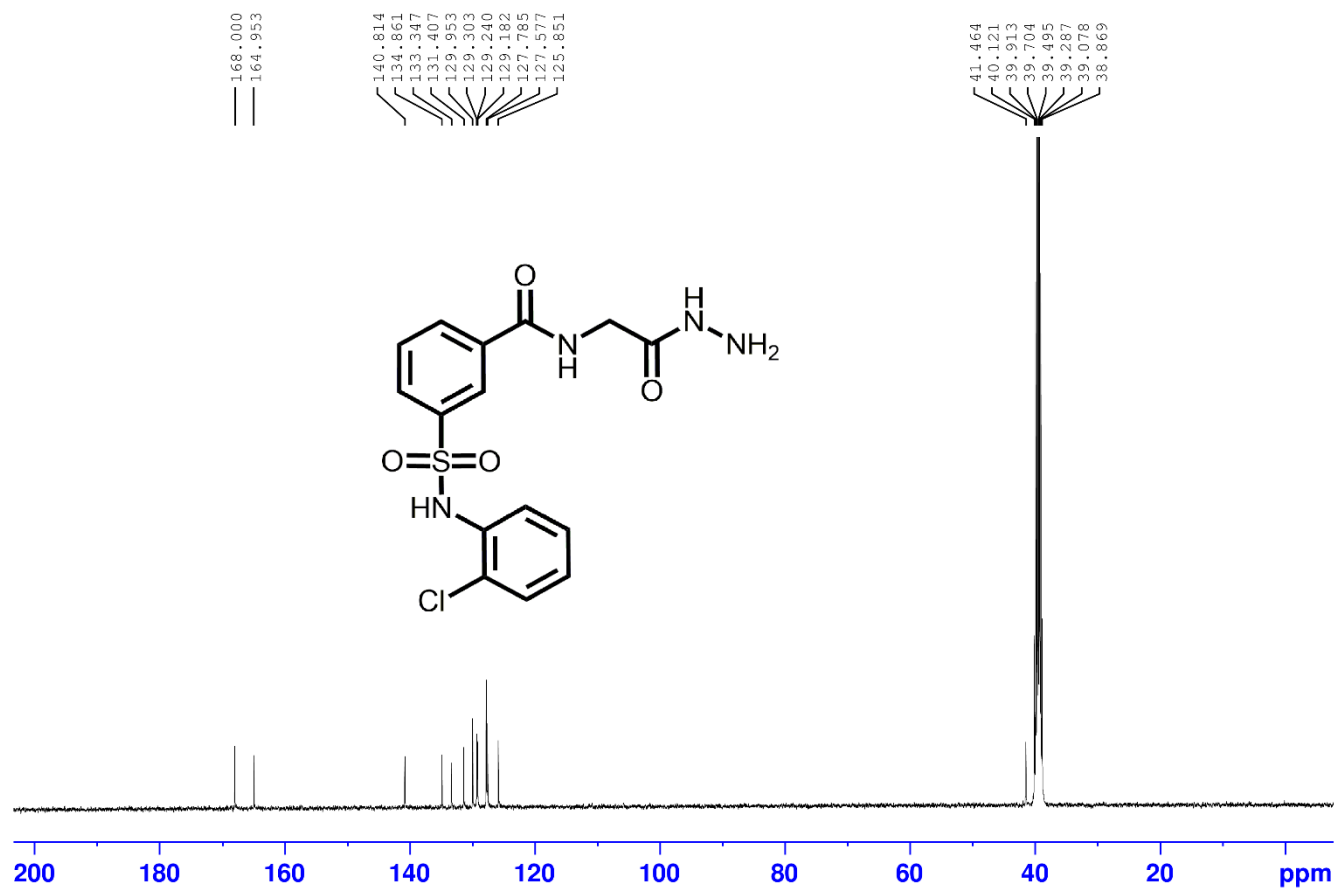
HRMS of Compound-D

GVB-SK-INT-4



¹H NMR of Compound-E

GVB-SK-INT-4



Current Data Parameters
NAME 511701C5155
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170131
Time 6.03
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 298.9 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
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.18777999 W
PLW13 0.15210000 W

F2 - Processing parameters
SI 32768
SF 100.6128182 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL5-NMR-001

¹³CNMR of Compound-E in DMSO-d₆

Elemental Composition Report

Page 1

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)

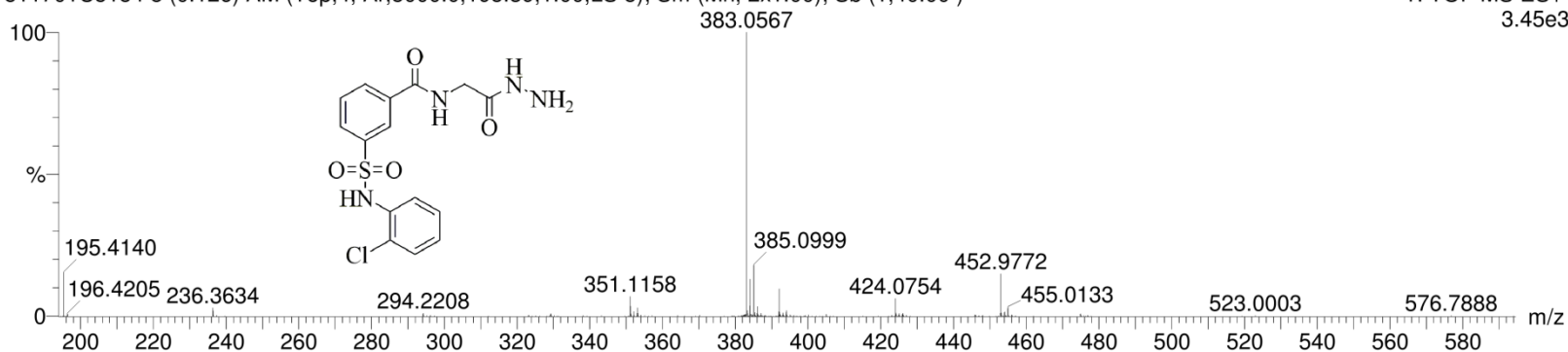
Elements Used:

C: 0-15 H: 0-16 N: 0-4 O: 0-4 S: 0-1 Cl: 0-1

GVB-SK-INT-4

511701C5154 8 (0.126) AM (Top,4, Ar,5000.0,195.39,1.00,LS 5); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
3.45e3

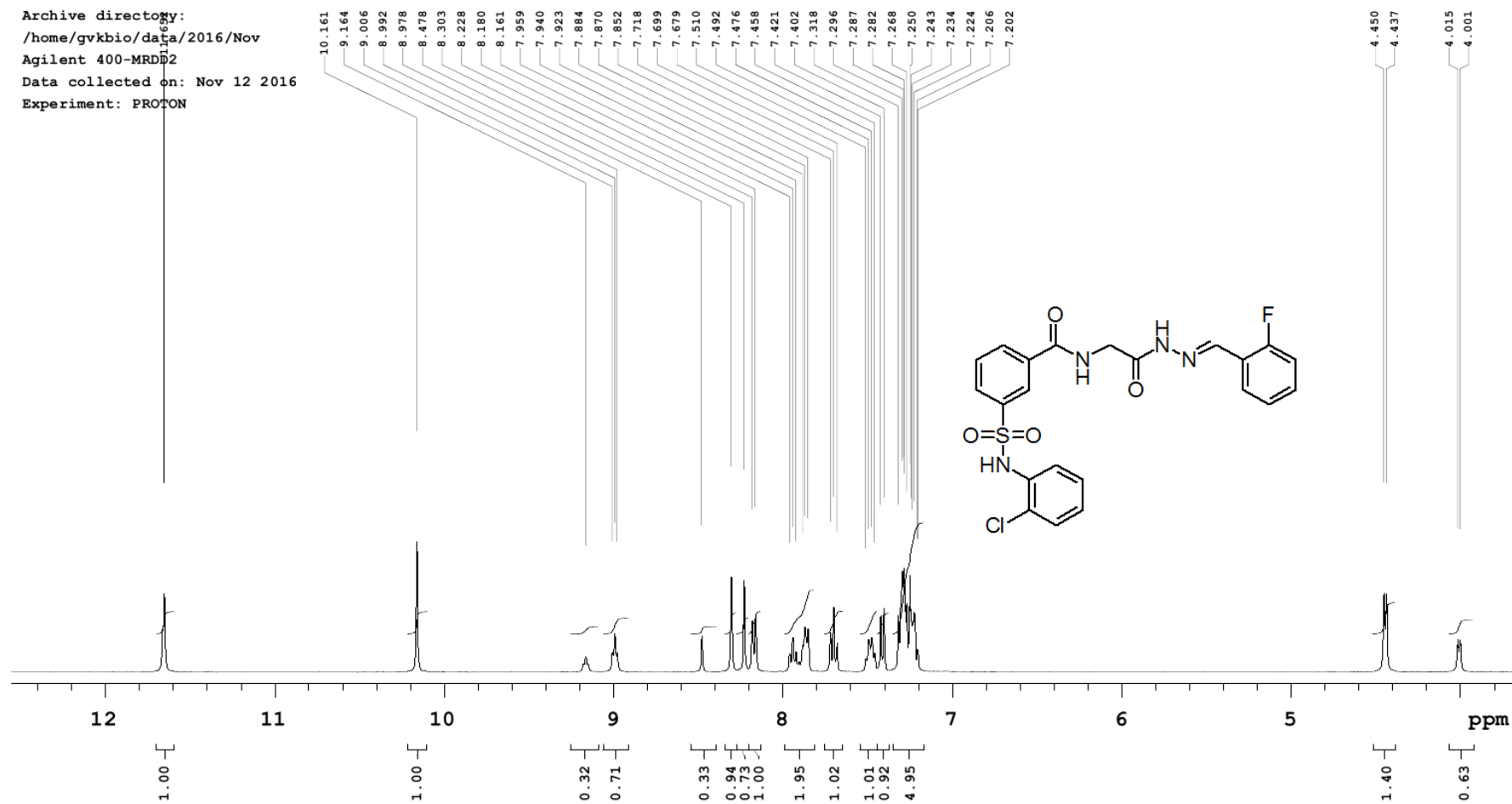


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
383.0567	383.0581	-1.4	-3.7	9.5	266.2	C15 H16 N4 O4 S Cl

HRMS of Compound-E

GVB-SA07
 Reference Code: 511611A0309
 Solvent: dmsd
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDE2
 Data collected on: Nov 12 2016
 Experiment: PROTON



¹H NMR of Compound-1a

Elemental Composition Report

Page 1

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

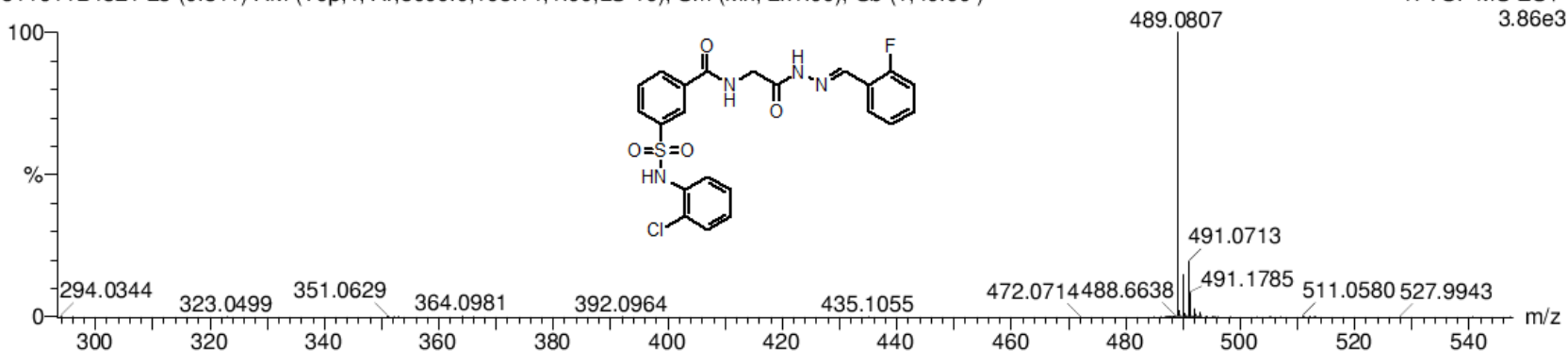
178 formula(e) evaluated with 2 results within limits (up to 1 closest results for each mass)

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

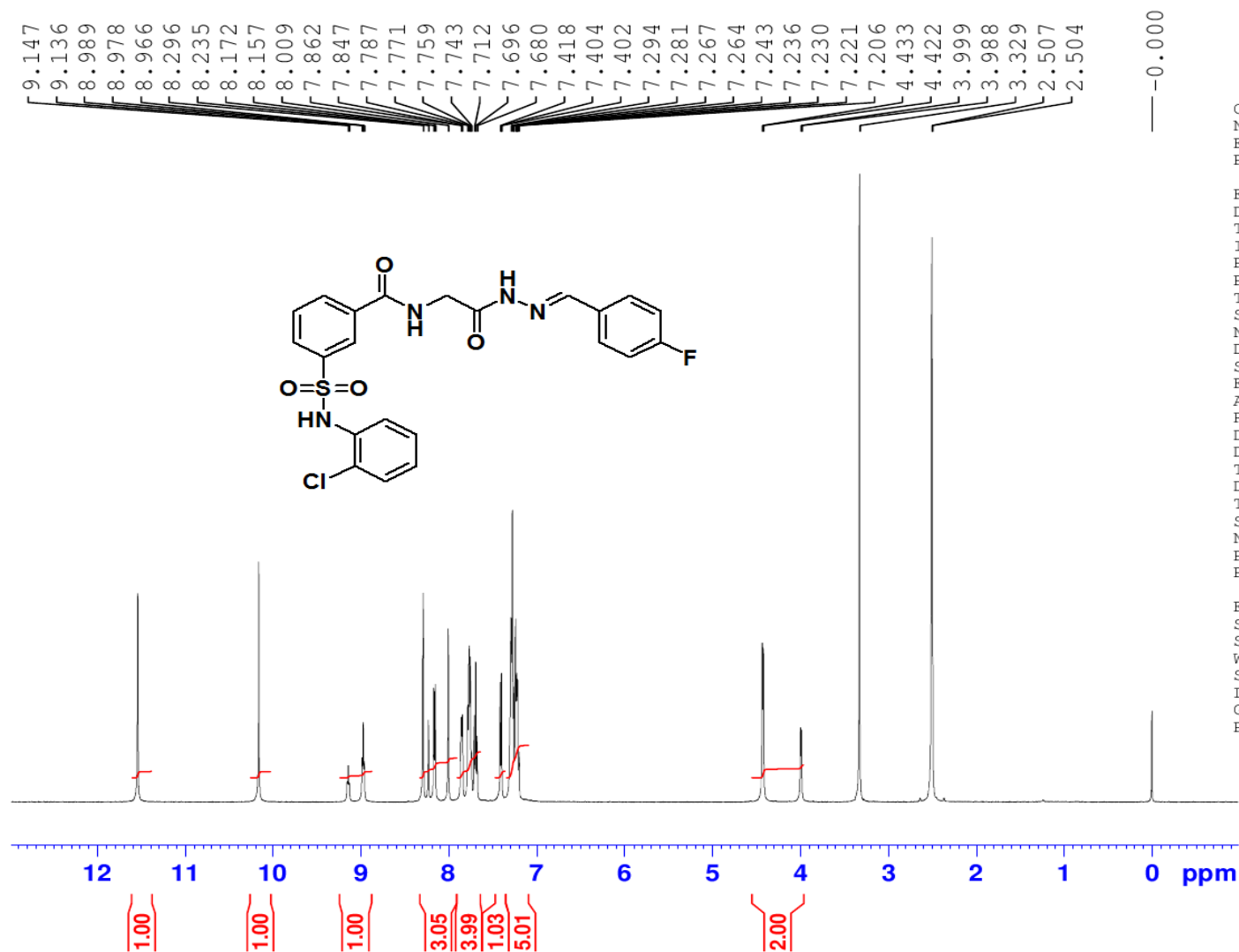
511611B4321 23 (0.341) AM (Top,4, Ar,5000.0,195.14,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)



Minimum: -1.5
Maximum: 5.0 10000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
489.0807	489.0800	0.7	1.4	14.5	225054.8	C22 H19 N4 O4 F S Cl

HRMS of Compound-1a

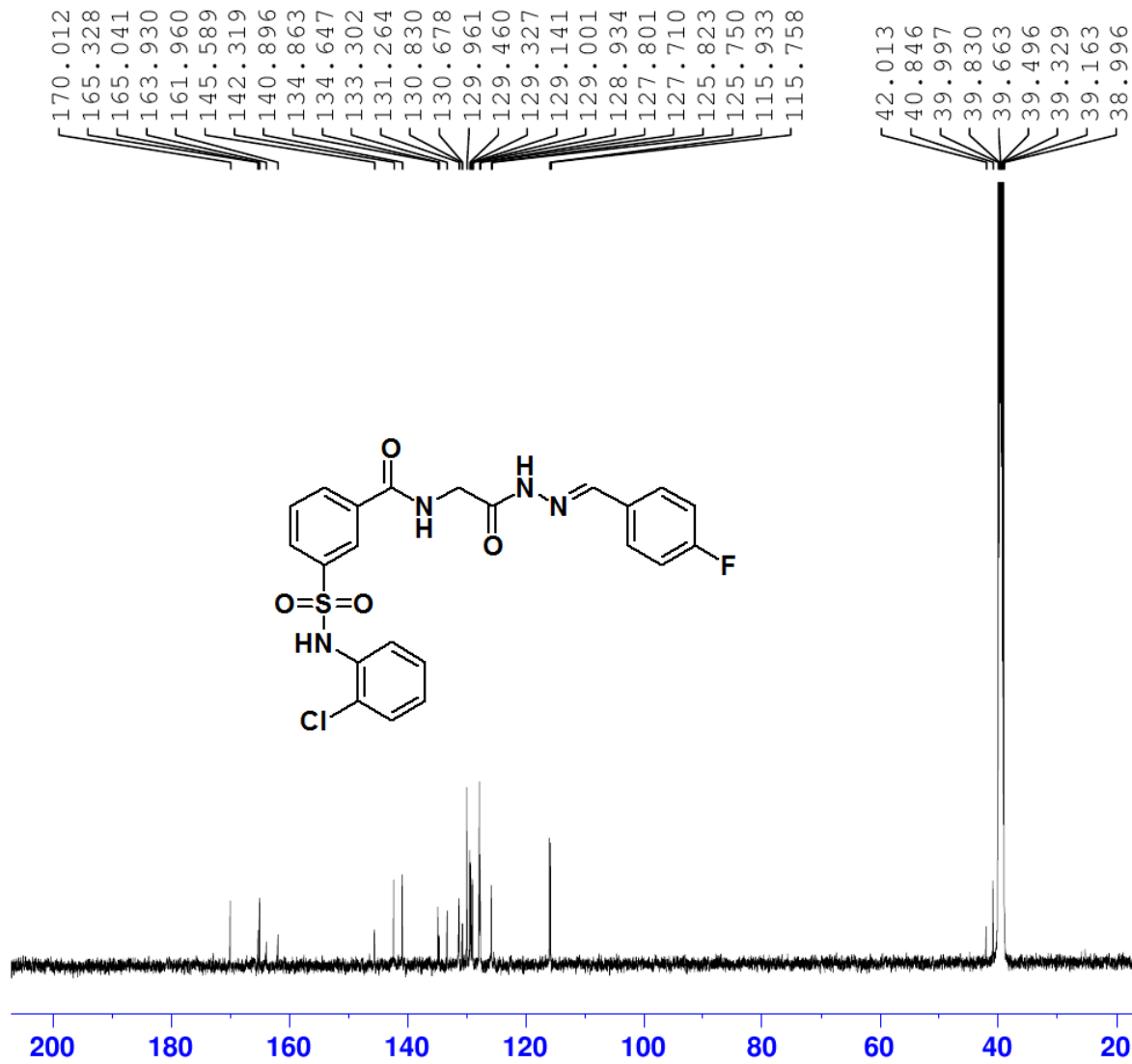


Current Data Parameters
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 PROCNO 1

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 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 118.49
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 23.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300019 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of Compound-1b



Current Data Parameters
NAME 511611A7711
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161110
Time 23.18 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W

F2 - Processing parameters
SI 32768
SF 125.7578513 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

¹³CNMR of **Compound-1b** in DMSO-d₆

Elemental Composition Report

Page 1

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)

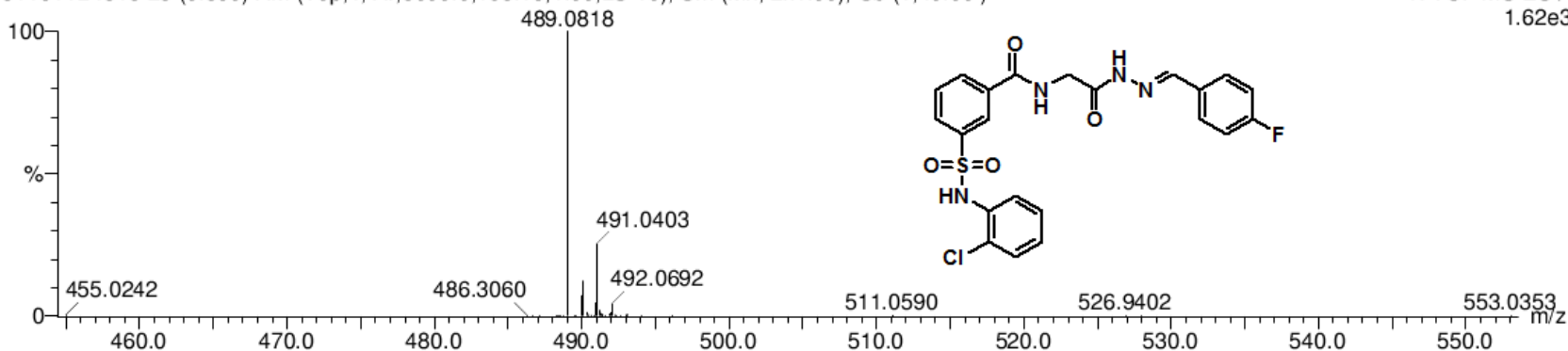
Elements Used:

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

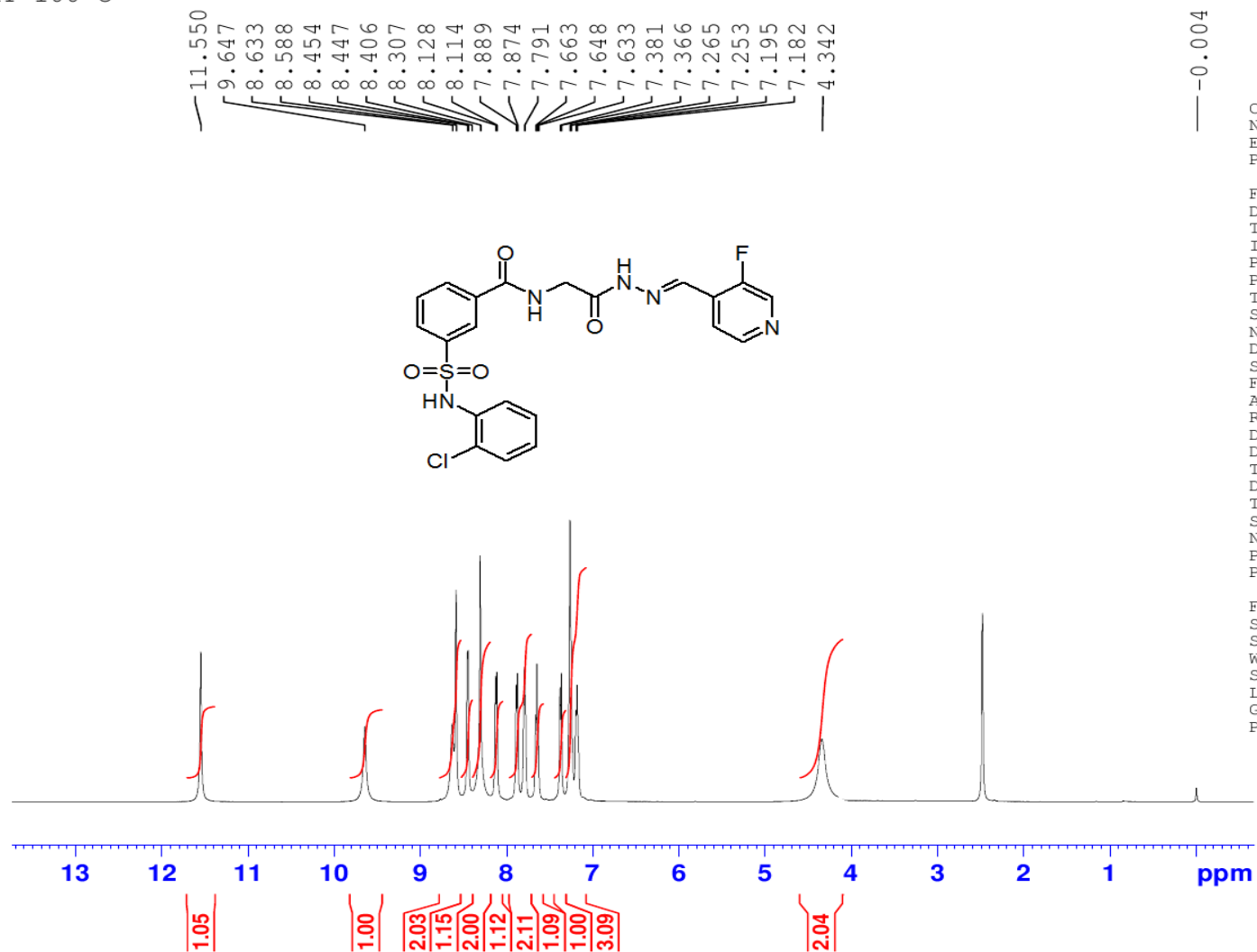


Minimum: -1.5
Maximum: 5.0 10000.0 50.0

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

GVB-SA02
AT 100°C



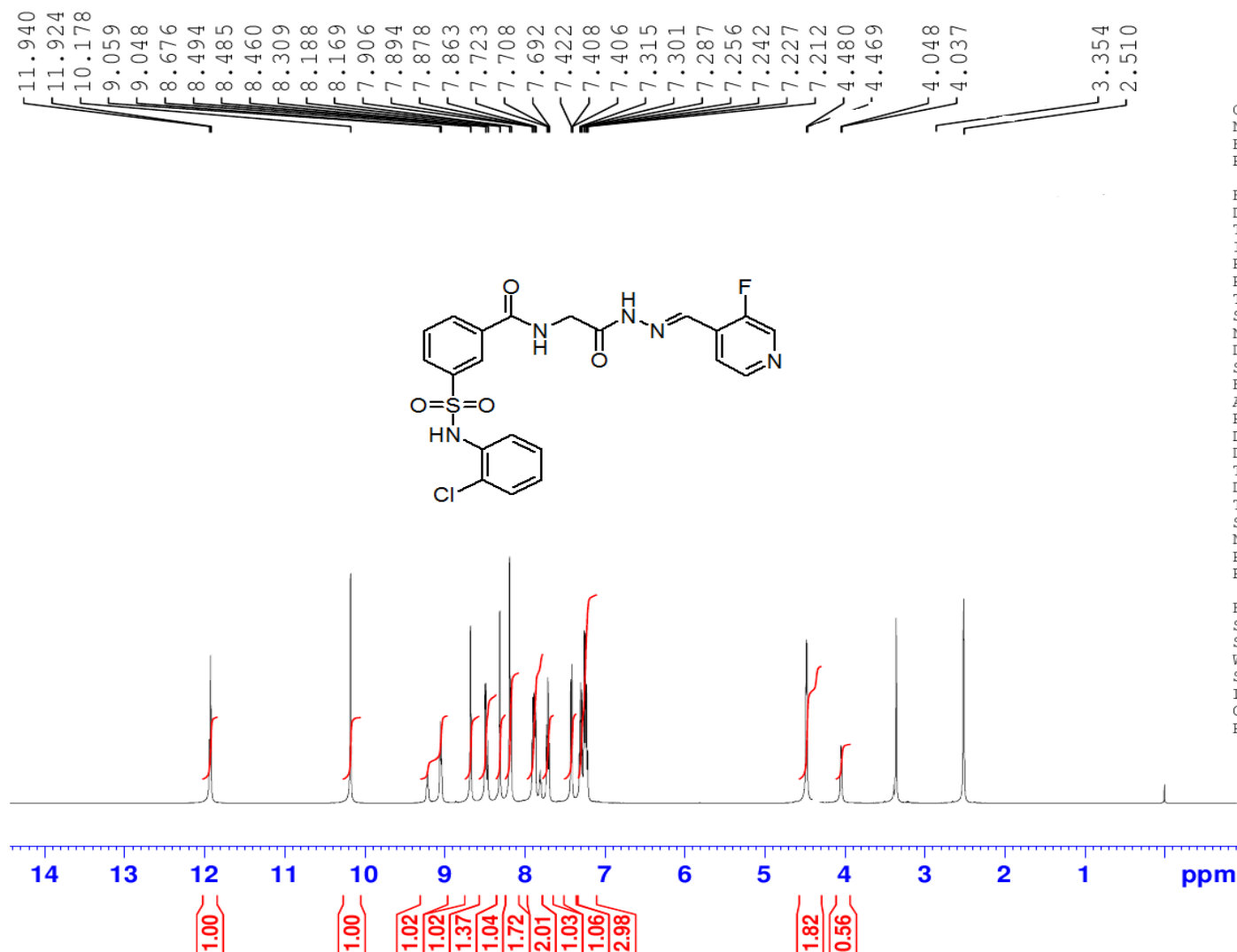
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EXPNO 1
PROCNO 1

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Date_ 20161110
Time 19.50 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 111.07
DW 50.000 usec
DE 6.50 usec
TE 373.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of Compound-1c at 100°C

GVB-SA02



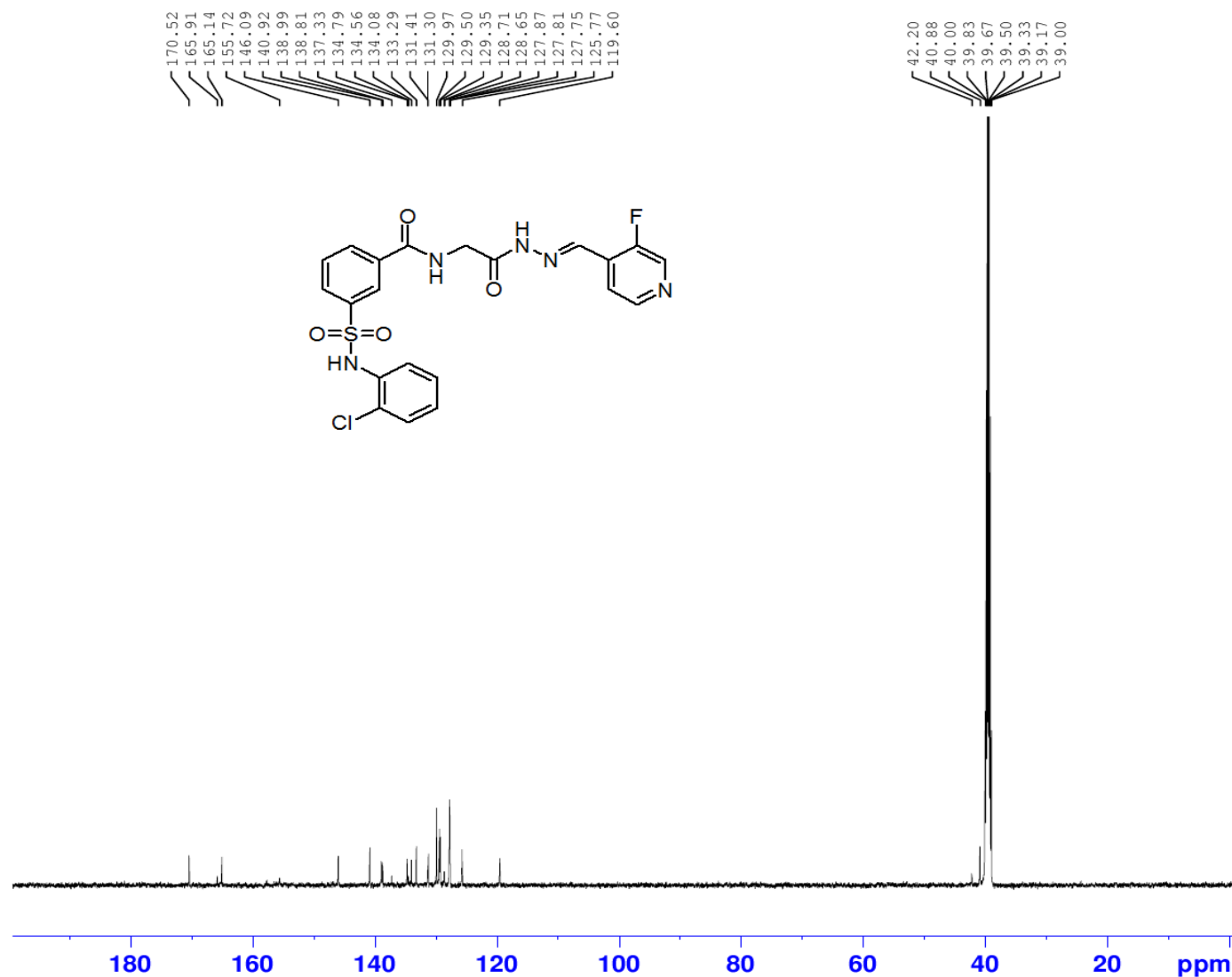
Current Data Parameters
 NAME 511611A7714
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161110
 Time 22.02 h
 INSTRUM spect
 PROBHD Z119470_0231 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 79.68
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 23.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1299986 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of Compound-1c

GVB-SA02



Current Data Parameters
 NAME 511611A7714
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161112
 Time 12.18 h
 INSTRUM spect
 PROBHD Z119470_0231 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 197.72
 DW 16.800 usec
 DE 6.50 usec
 TE 298.2 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 88.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 23.00000000 W
 PLW12 0.27515000 W
 PLW13 0.13840000 W

F2 - Processing parameters
 SI 32768
 SF 125.7578493 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

¹³CNMR of Compound-1c in DMSO-d₆

Elemental Composition Report

Page 1

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

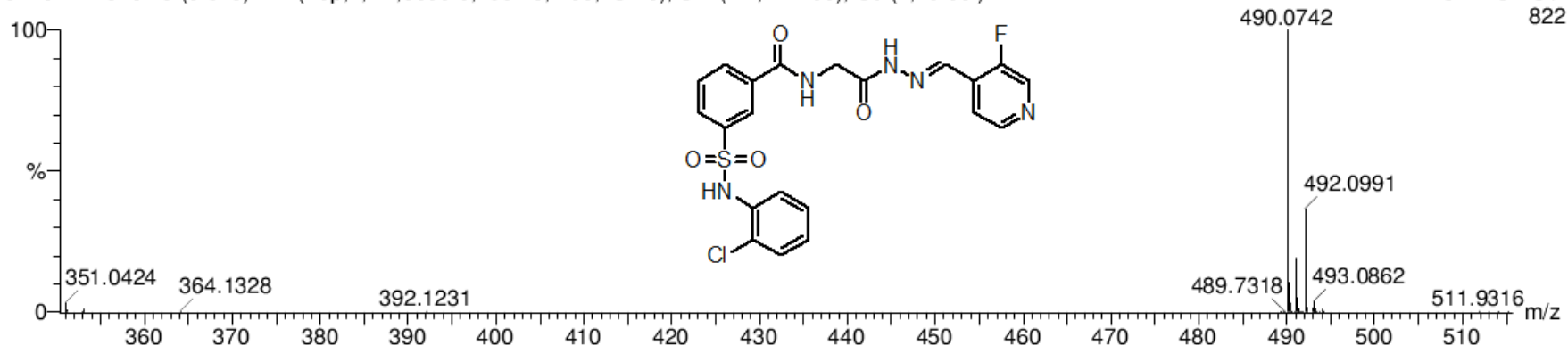
230 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

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)

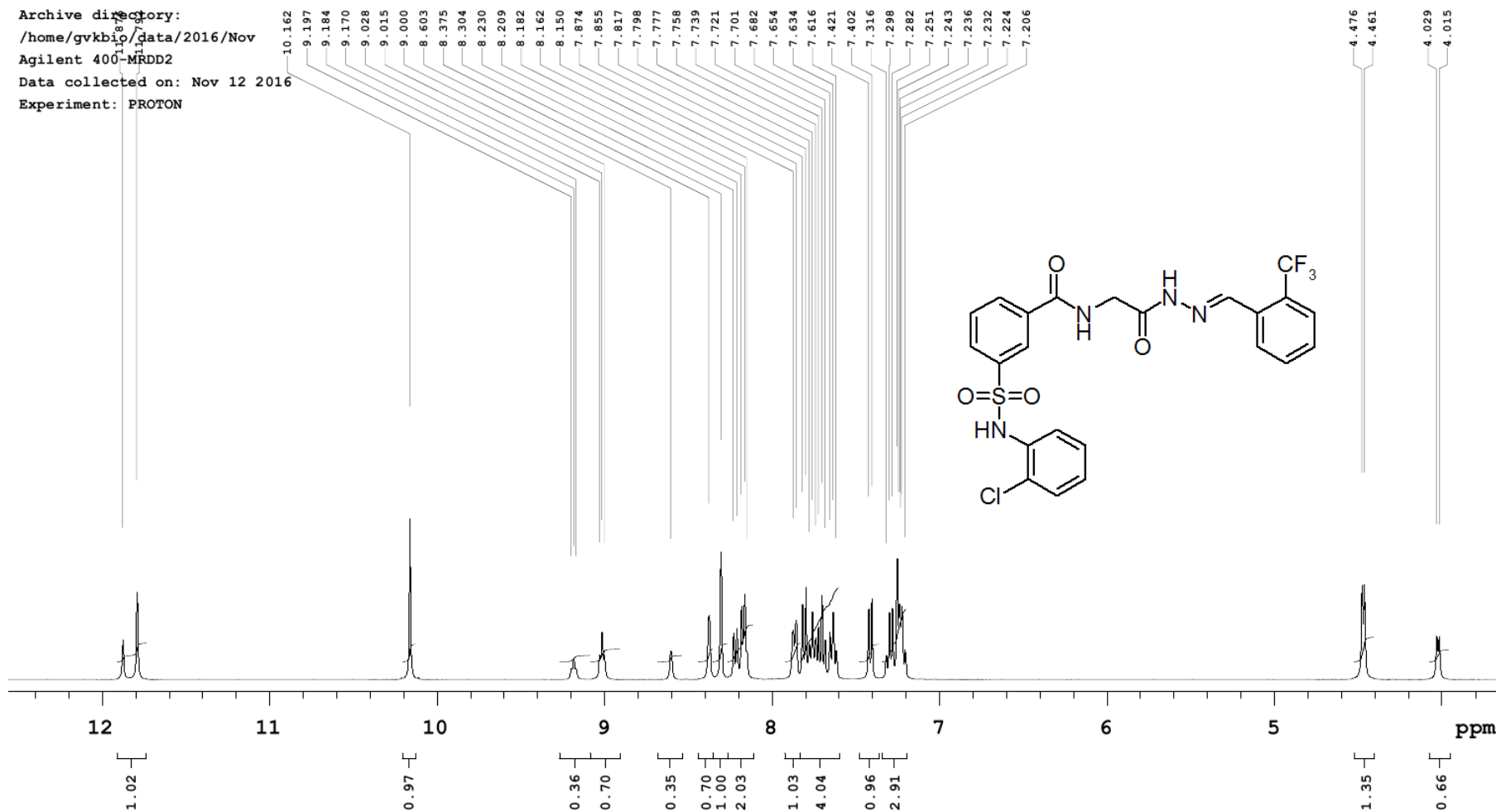


Minimum: -1.5
Maximum: 5.0 10000.0 50.0

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

GVB-SA06
 Reference Code: 511611A0304
 Solvent: dms
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 12 2016
 Experiment: PROTON



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

Elemental Composition Report

Page 1

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)

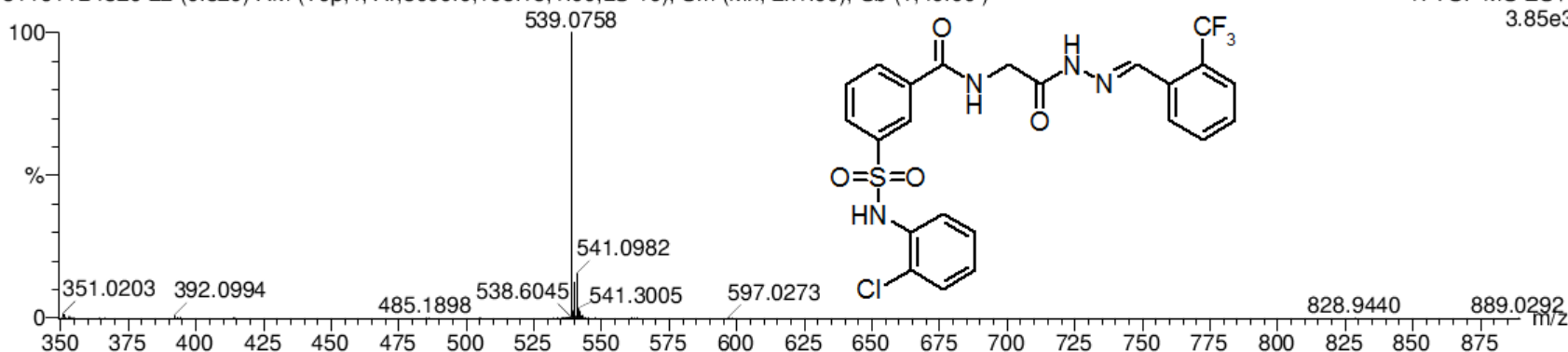
Elements Used:

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

GVB-SA06

511611B4320 22 (0.329) AM (Top,4, Ar,5000.0,195.15,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
3.85e3

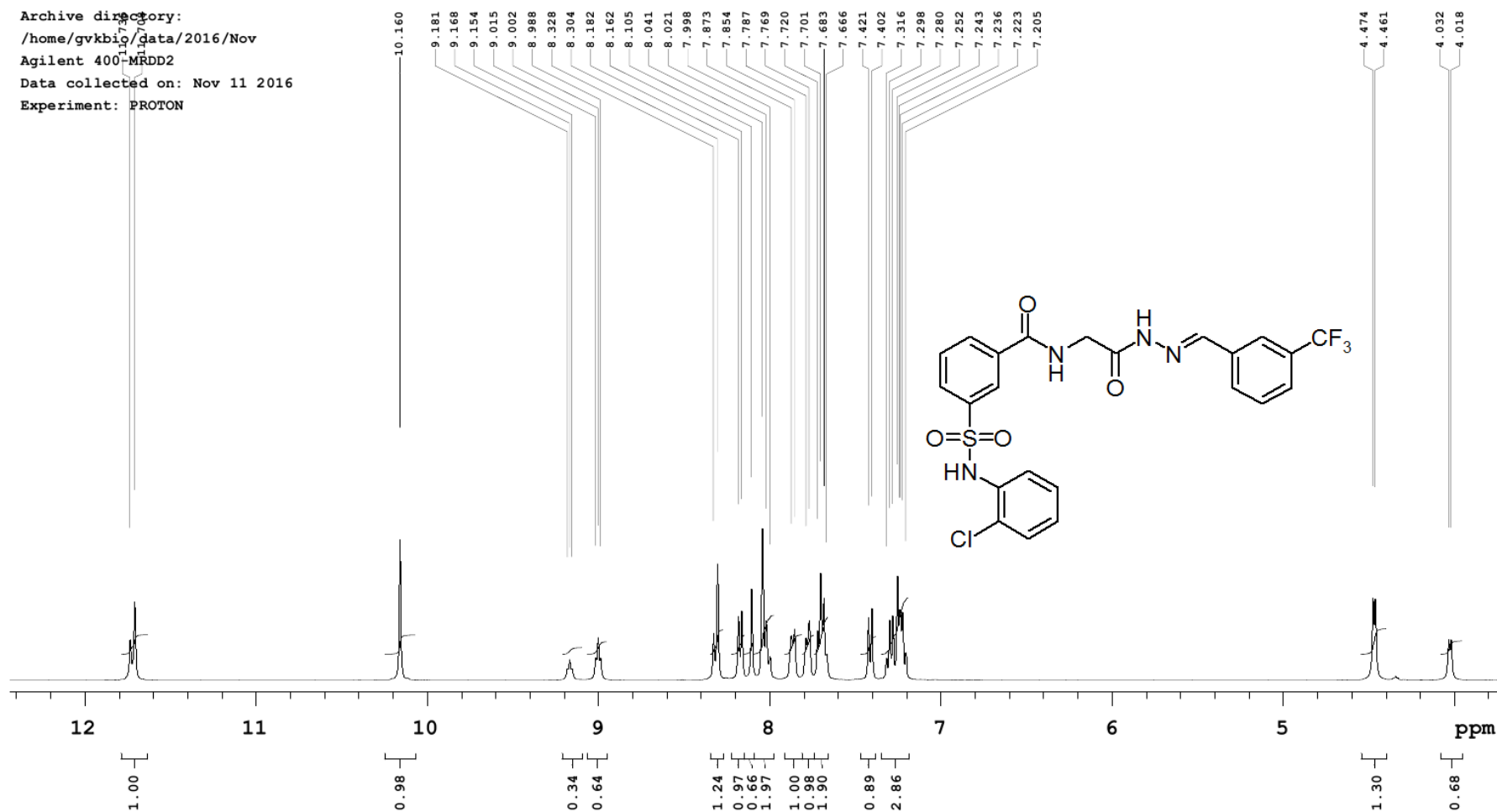


Minimum: -1.5
Maximum: 5.0 10000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
539.0758	539.0768	-1.0	-1.9	14.5	185151.5	C ₂₃ H ₁₉ N ₄ O ₄ F ₃ S Cl

HRMS of Compound-1d

GVB-SA05
 Reference Code: 511611B0303
 Solvent: dmsd
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 11 2016
 Experiment: PROTON



¹H NMR of **Compound-1e** in DMSO-d₆

GVB-SA05

Reference Code: 511611B0303

Solvent: dms

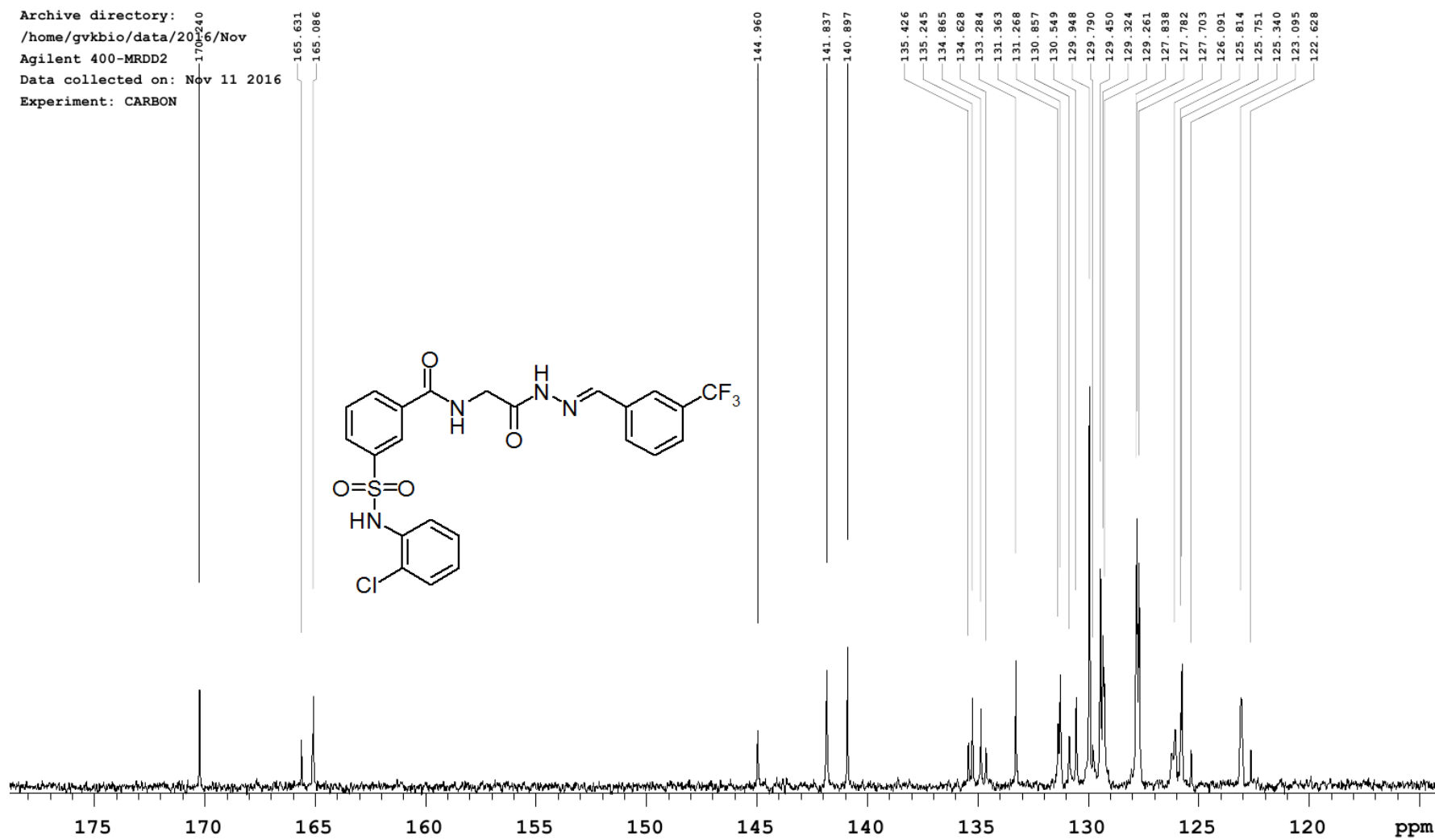
Archive directory:

/home/gvkbio/data/2016/Nov

Agilent 400-MRDD2

Data collected on: Nov 11 2016

Experiment: CARBON



¹³CNMR of **Compound-1e** in DMSO-d₆

Elemental Composition Report

Page 1

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)

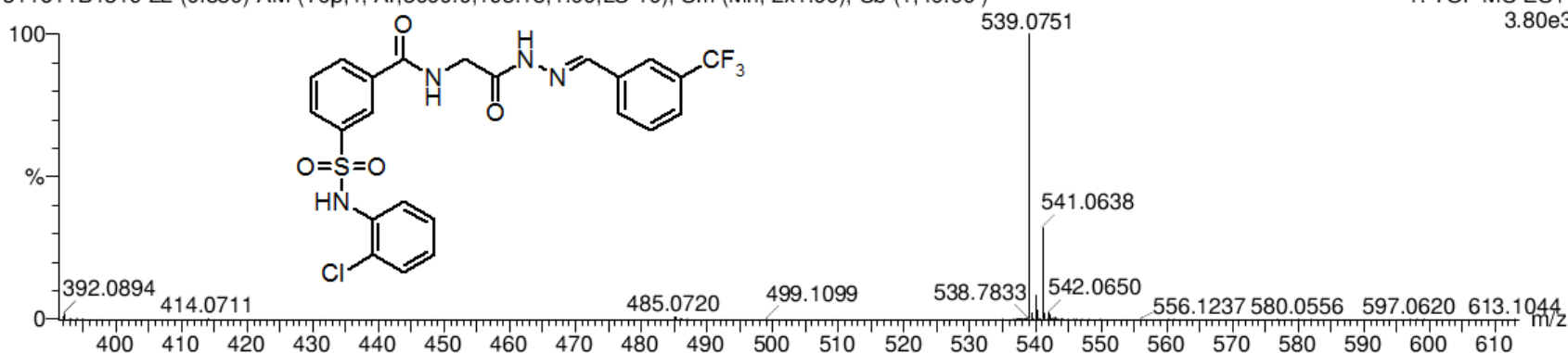
Elements Used:

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

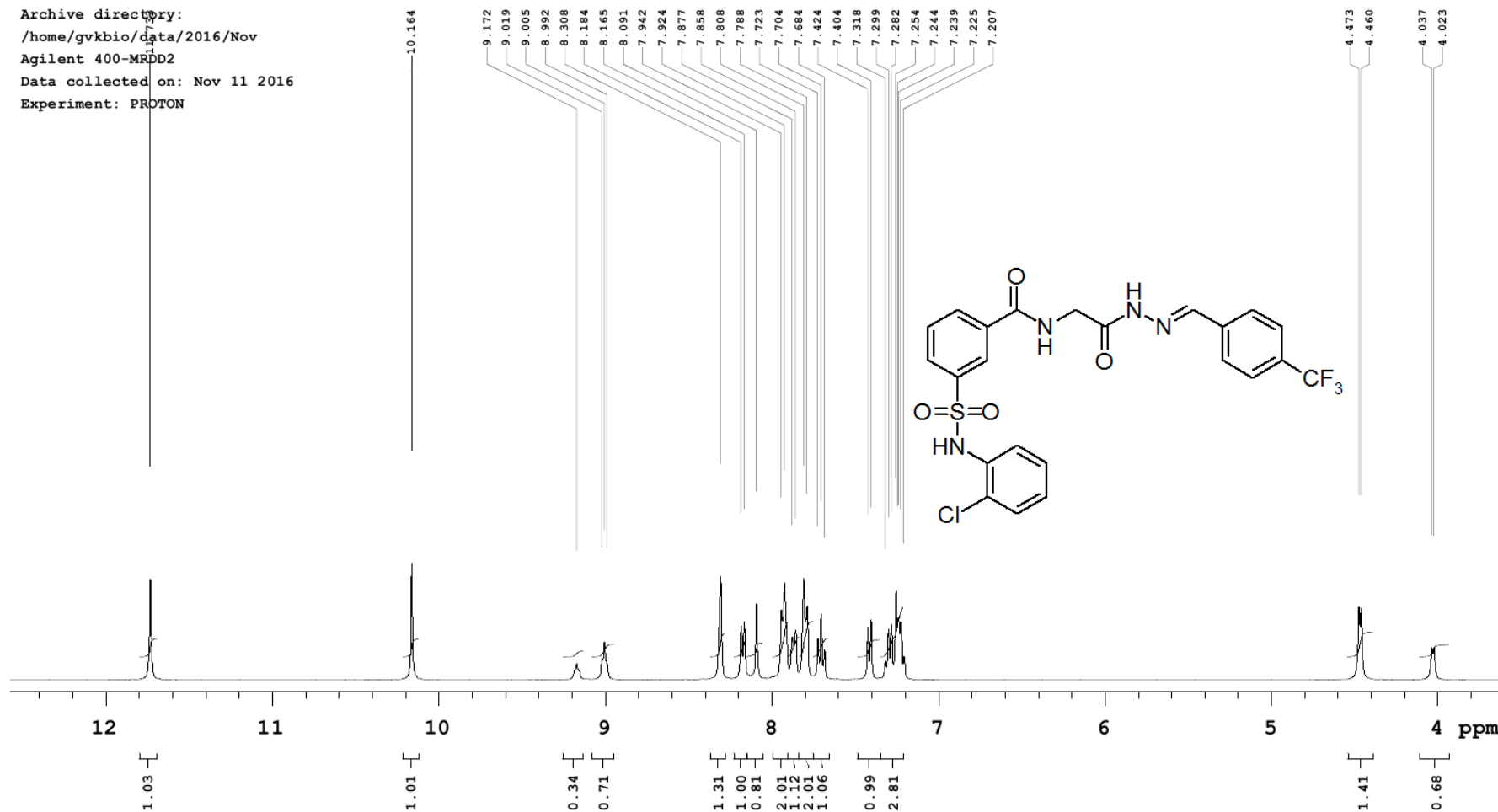


Minimum: -1.5
Maximum: 5.0 10000.0 50.0

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

GVB-SA04
 Reference Code: 511611B0302
 Solvent: dmsc
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 11 2016
 Experiment: PROTON



¹H NMR of **Compound-1f** in DMSO-d₆

GVB-SA04

Reference Code: 511611B0302

Solvent: dms

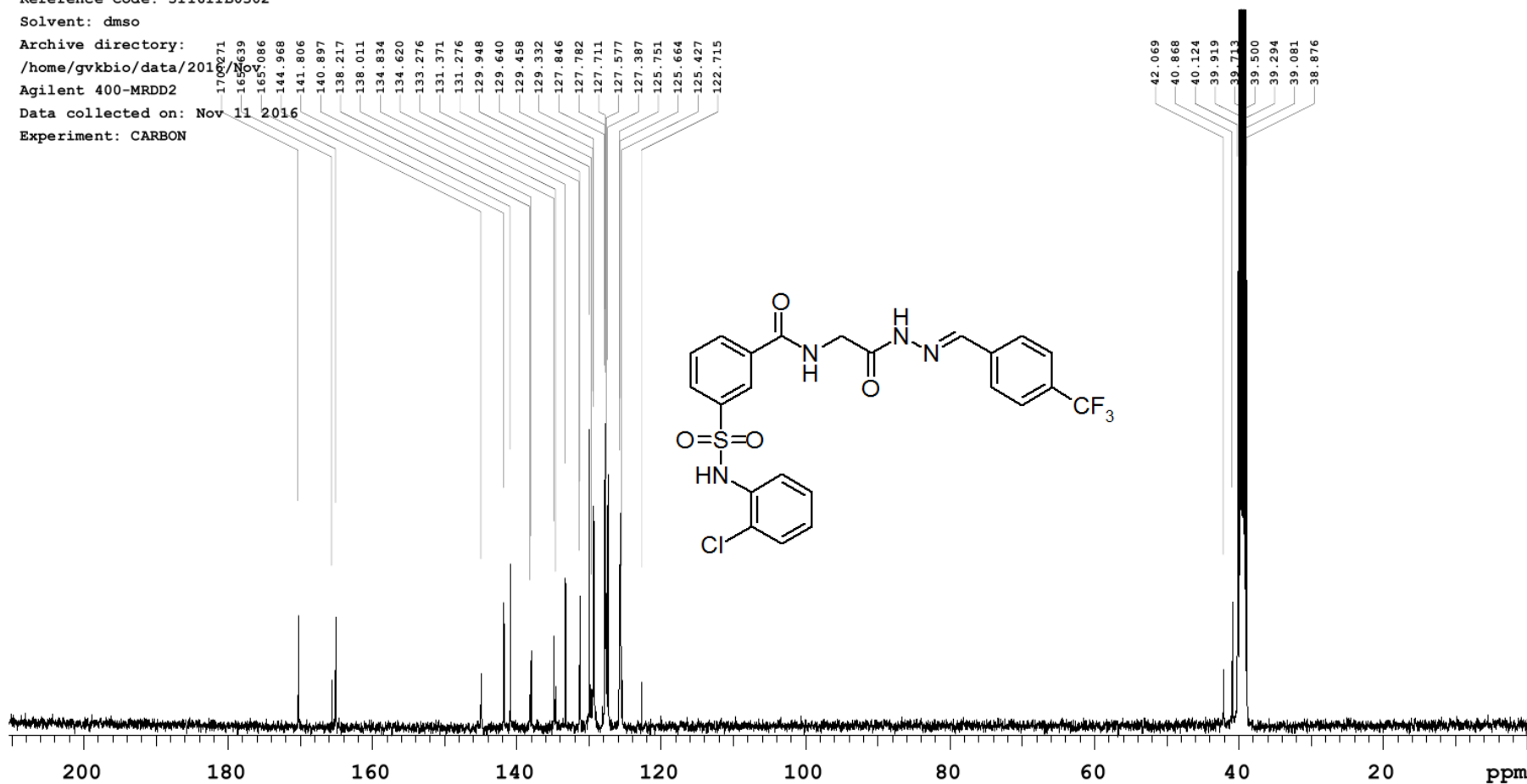
Archive directory:

/home/gvkbio/data/2016

Agilent 400-MRDD2

Data collected on: Nov 11 2016

Experiment: CARBON



¹³CNMR of Compound-1f in DMSO-d₆

Elemental Composition Report

Page 1

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

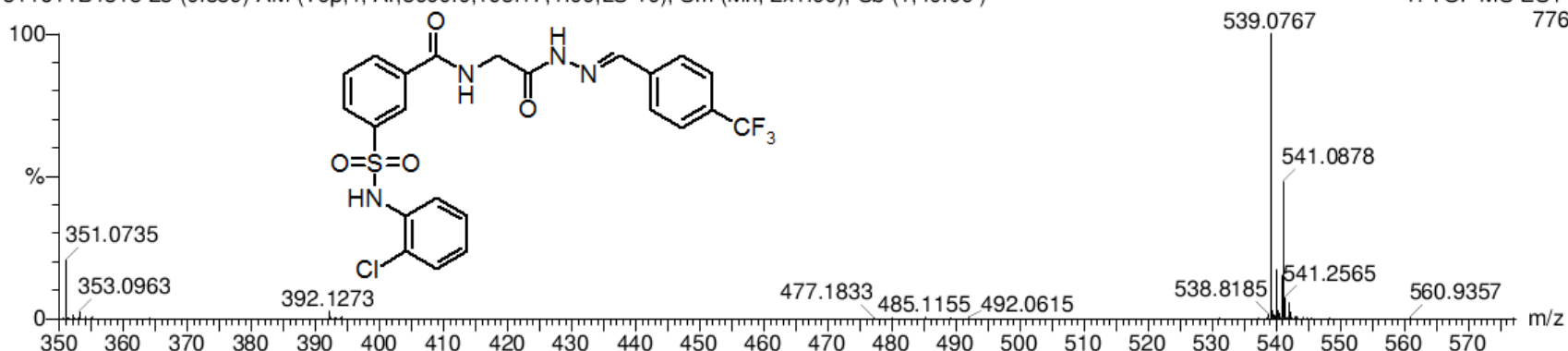
389 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

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

GVB-SA04

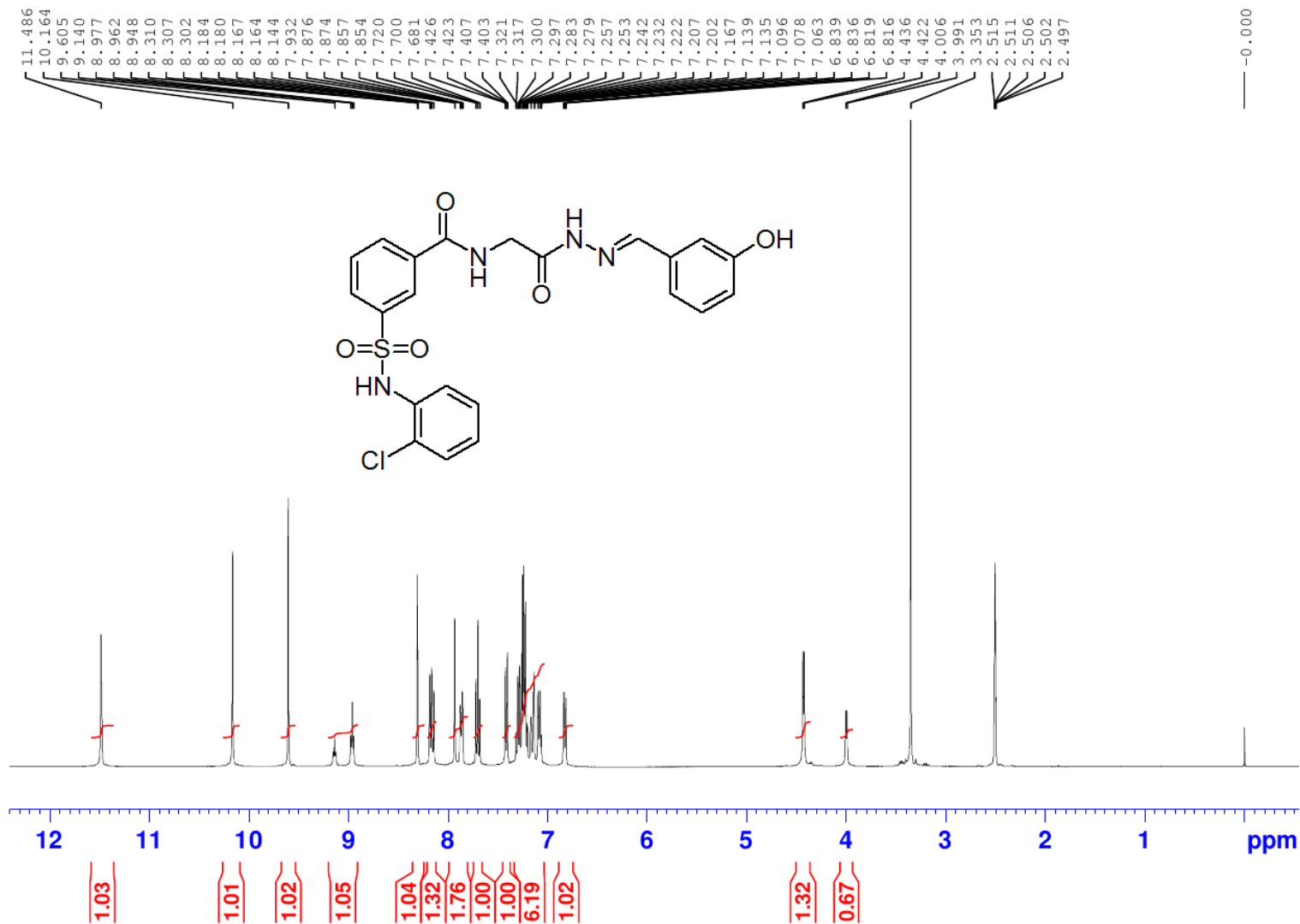
511611B4318 23 (0.339) AM (Top,4, Ar,5000.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)



Minimum: -1.5
Maximum: 5.0 10000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
539.0767	539.0768	-0.1	-0.2	14.5	37263.6	C23 H19 N4 O4 S Cl F3

HRMS of Compound-1f



Current Data Parameters
NAME 511611B0311
EXPNO 1
PROCNO 1

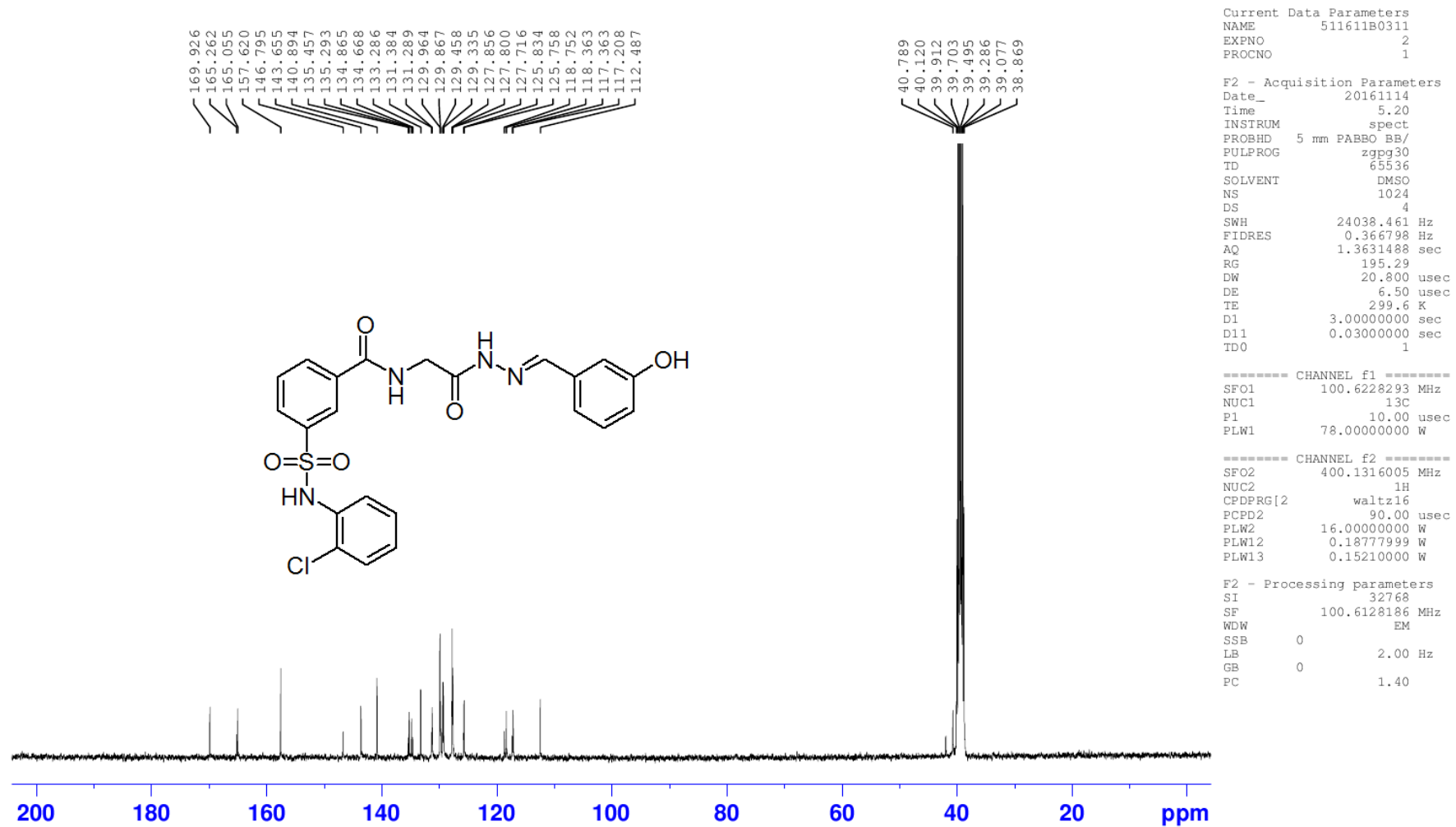
F2 - Acquisition Parameters
Date_ 20161114
Time 4.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 86.08
DW 62.400 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300010 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of **Compound-1g** in DMSO-d₆

GVB-SA08



¹³CNMR of **Compound-1g** in DMSO-*d*₆

Elemental Composition Report

Page 1

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)

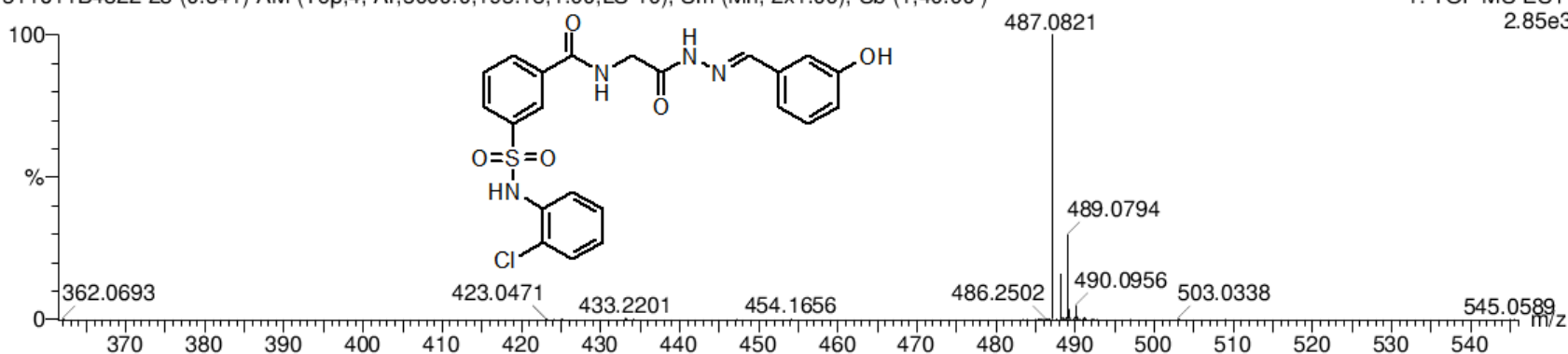
Elements Used:

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)

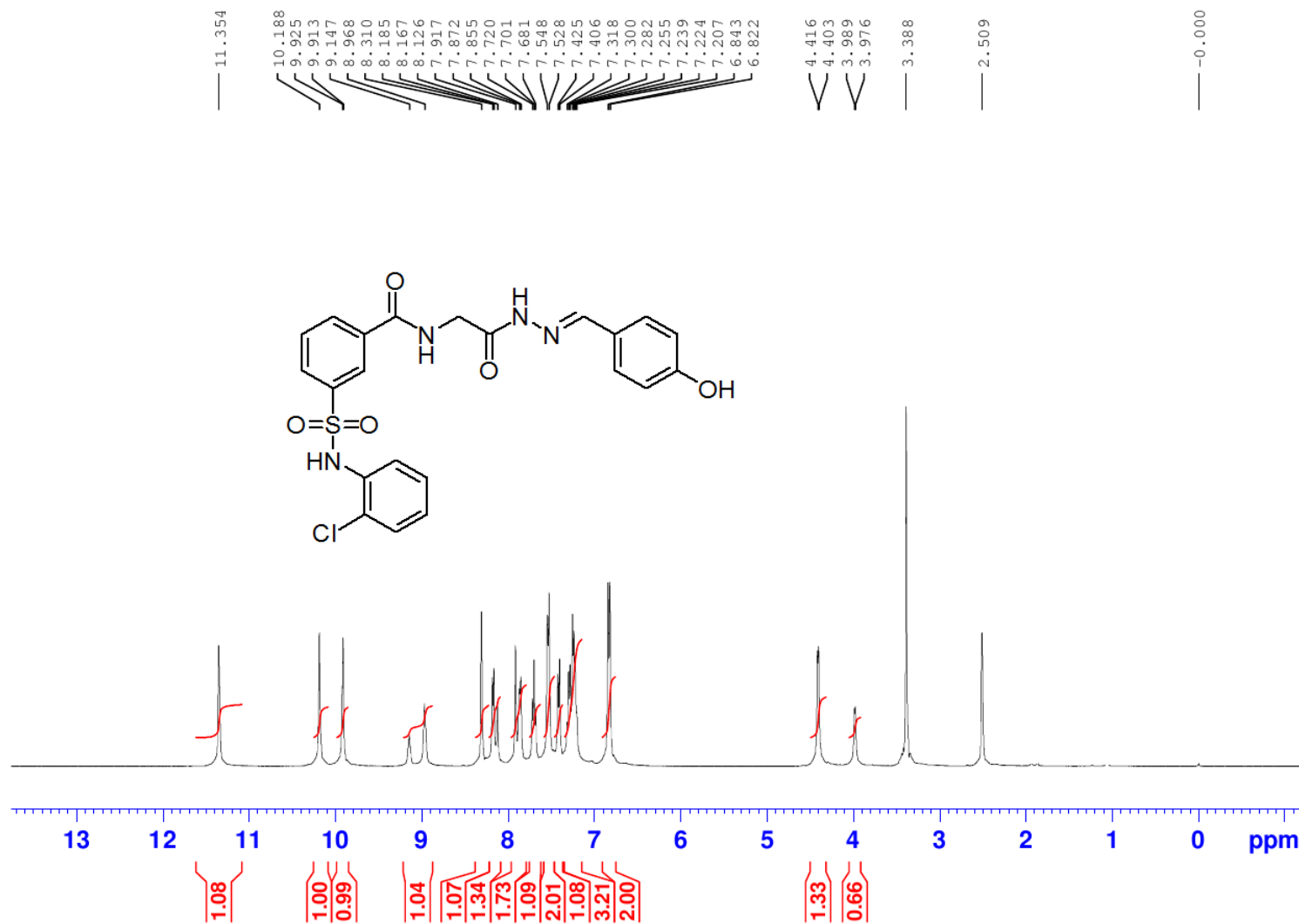
1: TOF MS ES+
2.85e3



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	C ₂₂ H ₂₀ N ₄ O ₅ S Cl

HRMS of Compound-1g



Current Data Parameters
NAME 511611B0312
EXPNO 1
PROCNO 1

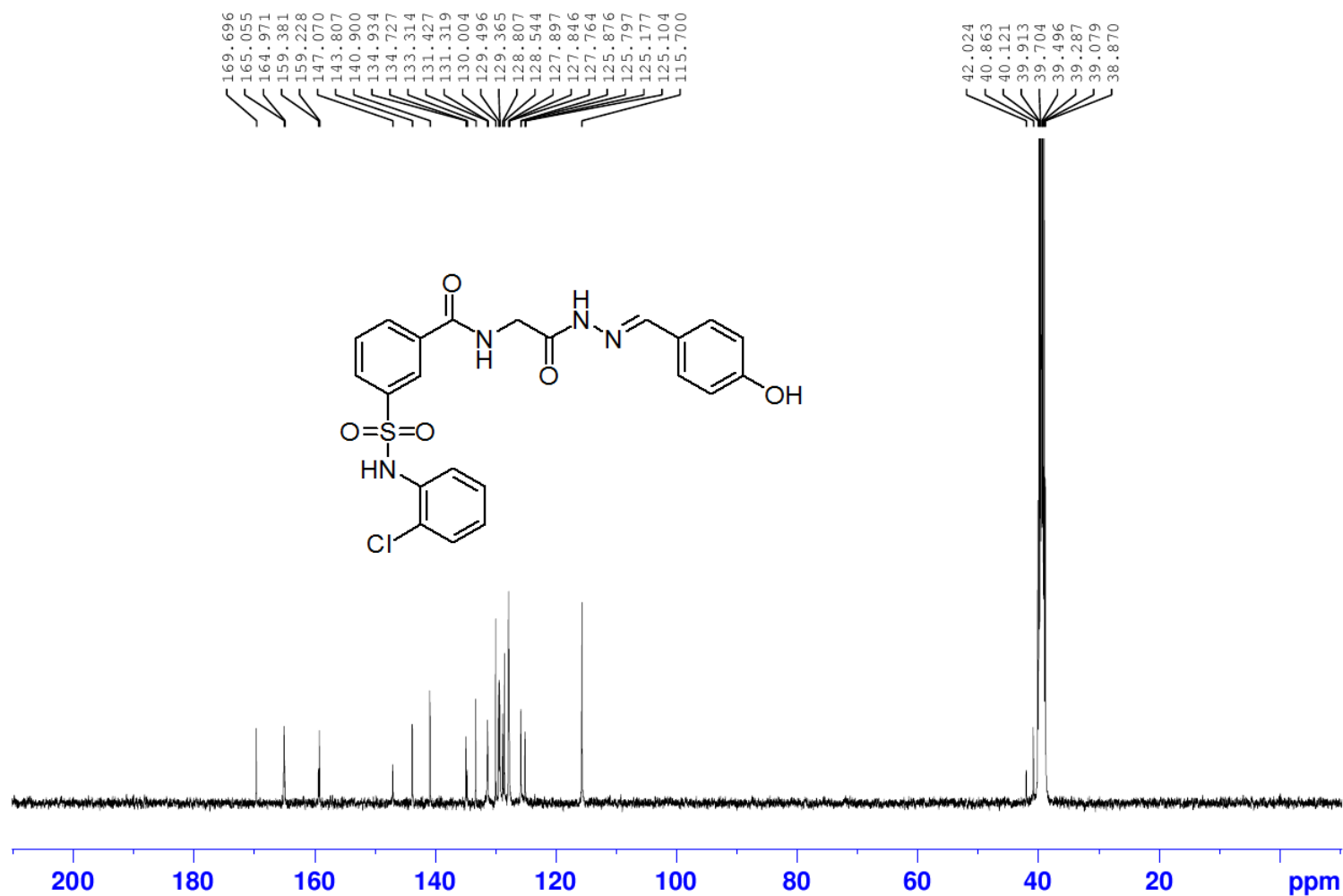
F2 - Acquisition Parameters
Date_ 20161112
Time 12.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 55.04
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1299991 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL5-NMR-001

¹H NMR of **Compound-1h** in DMSO-d₆



Current Data Parameters
 NAME 511611B0312
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161112
 Time 12.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 686
 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 298.2 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 100.6128146 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

ANL-MCL5-NMR-001

¹³CNMR of **Compound-1h** in DMSO-*d*₆

Elemental Composition Report

Page 1

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)

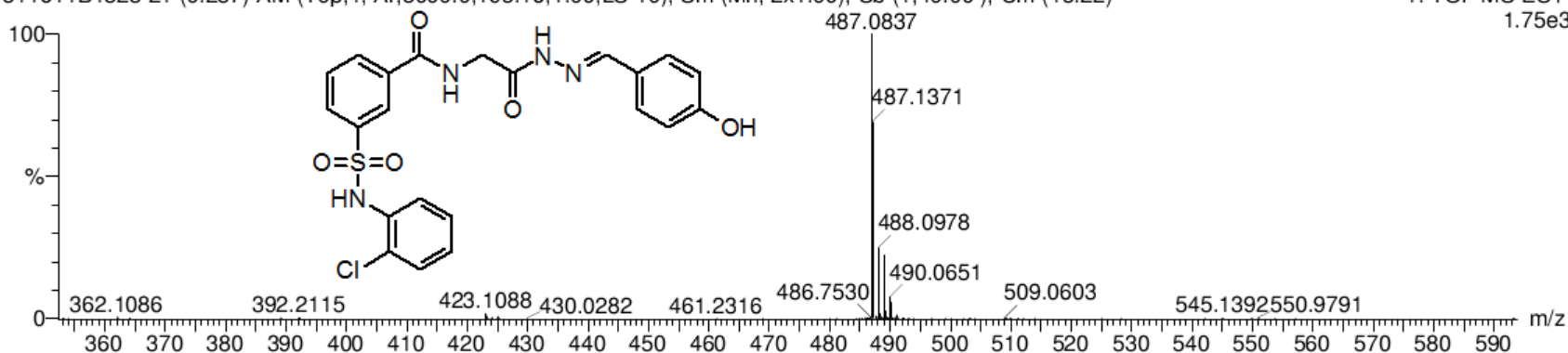
Elements Used:

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)

1: TOF MS ES+
1.75e3

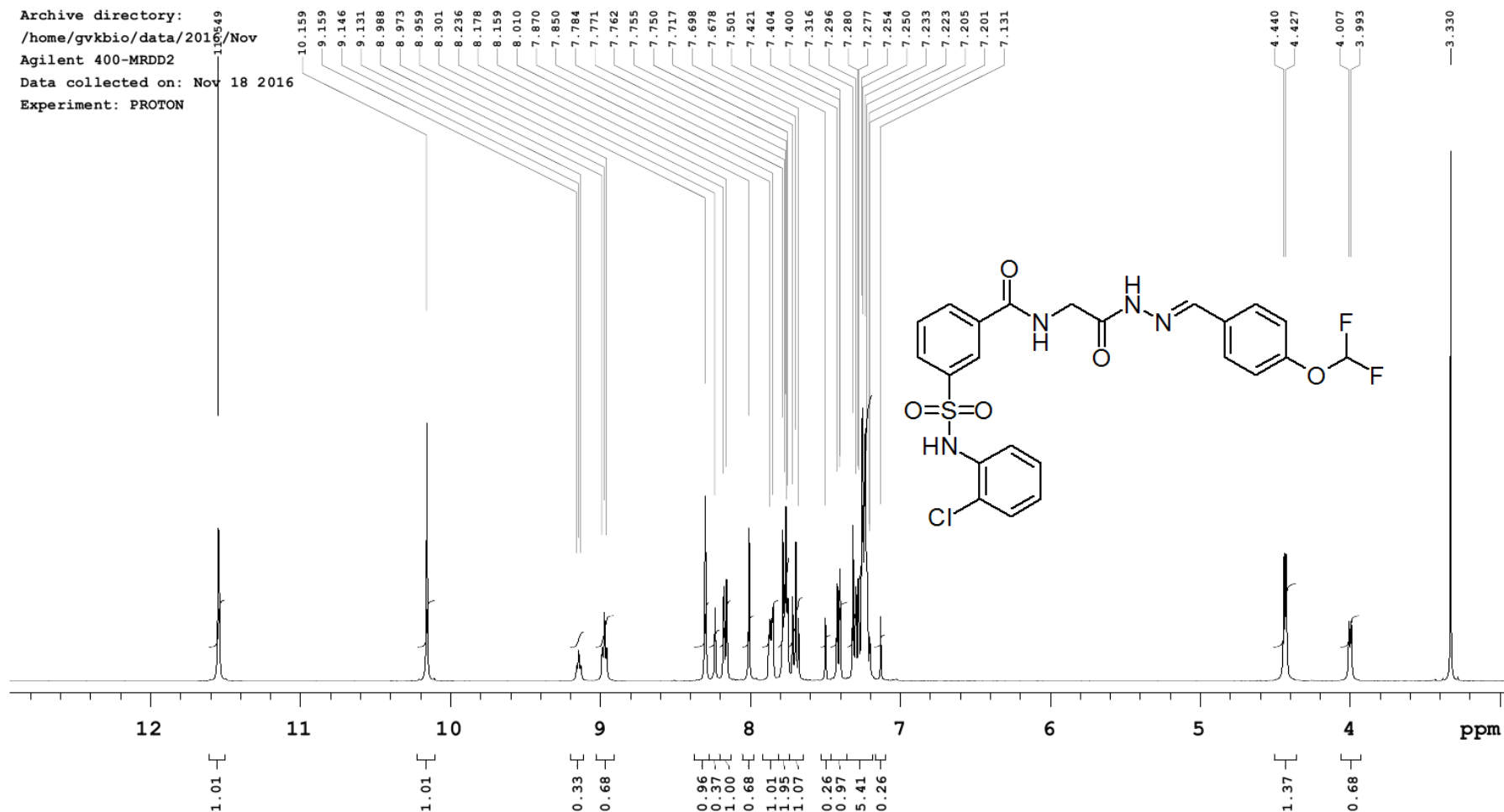


Minimum: -1.5
Maximum: 5.0 10000.0 50.0

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

GVB-SA-21
 Reference Code: 511611B2478
 Solvent: dmso
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 18 2016
 Experiment: PROTON



¹H NMR of **Compound-1i** in DMSO-d₆

GVB-SA-21

Reference Code: 511611B2478

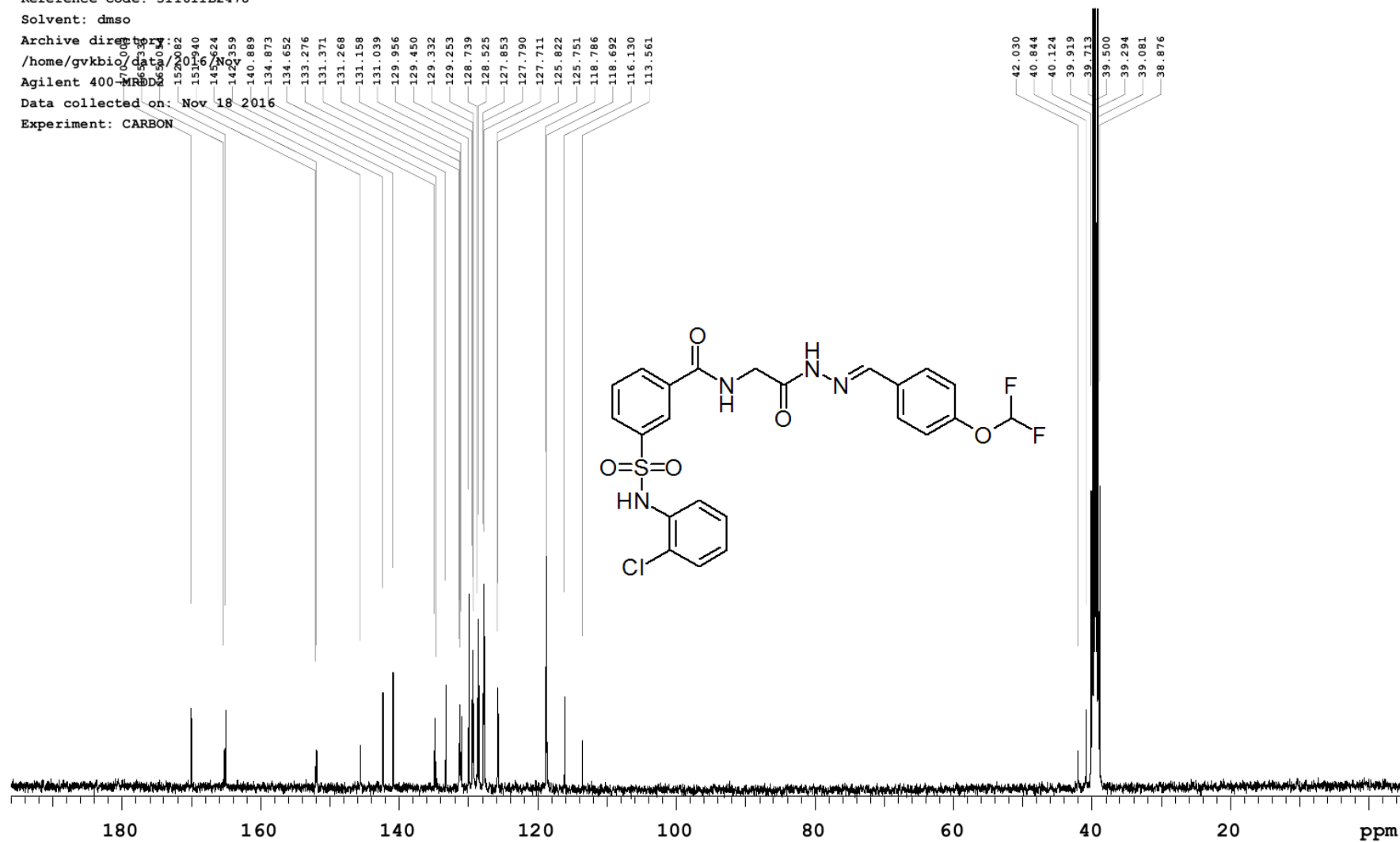
Solvent: dms

Archive directory:
/home/gvkbio/data/2016/Nov

Agilent 400-MRBD

Data collected on: Nov 18 2016

Experiment: CARBON



^{13}C NMR of Compound-1i in DMSO- d_6

Elemental Composition Report

Page 1

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)

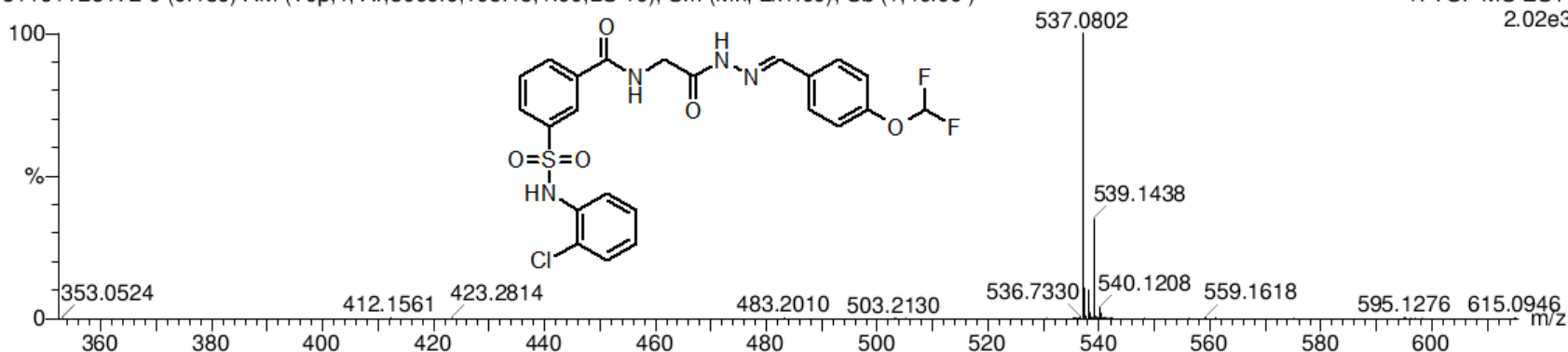
Elements Used:

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)

1: TOF MS ES+
2.02e3

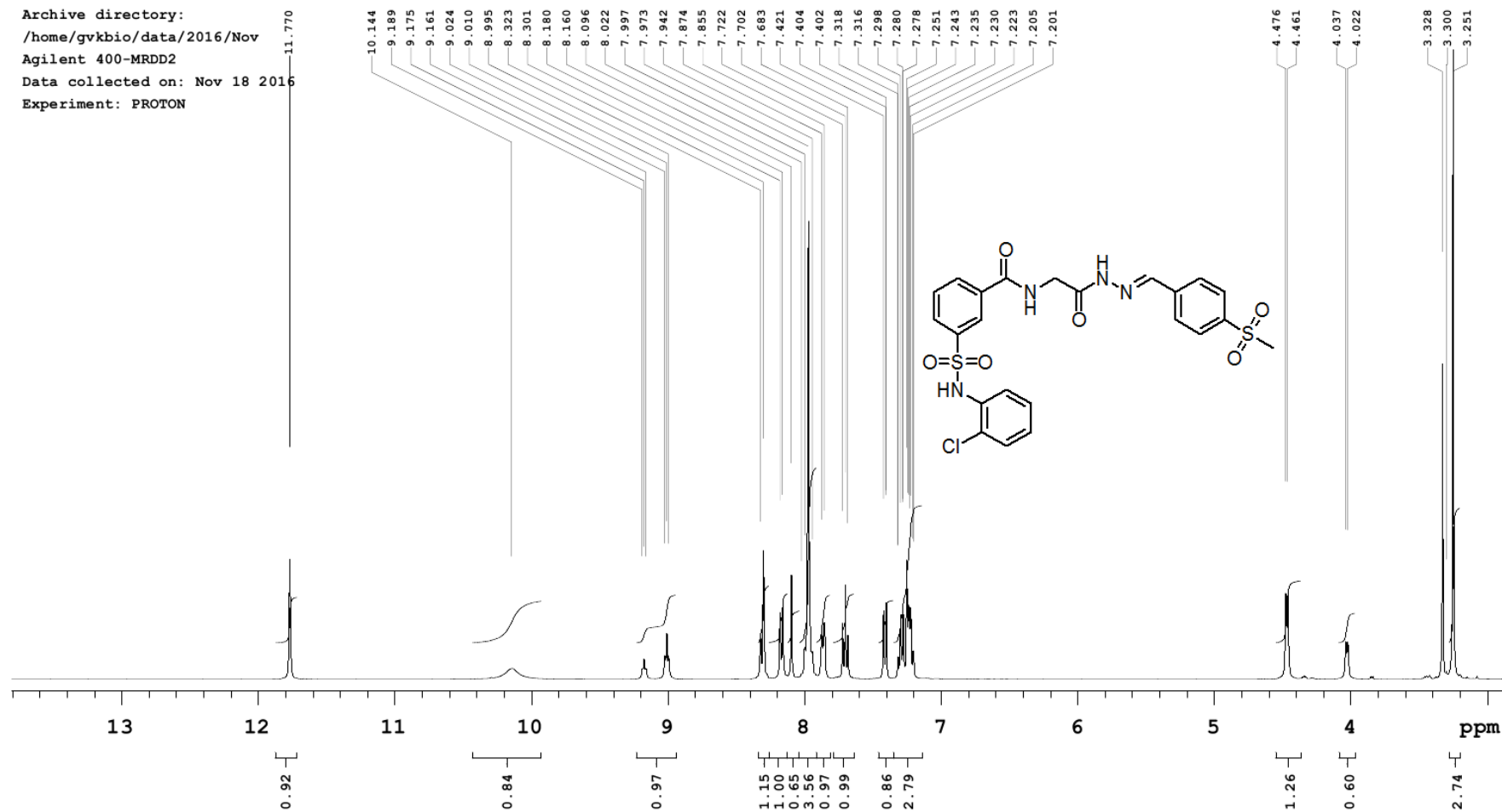


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SA-19
 Reference Code: 511611B2475
 Solvent: dmsc
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 18 2016
 Experiment: PROTON



¹H NMR of Compound-1j in DMSO-d₆

GVB-SA-19

Reference Code: 511611B2475

Solvent: dmsc

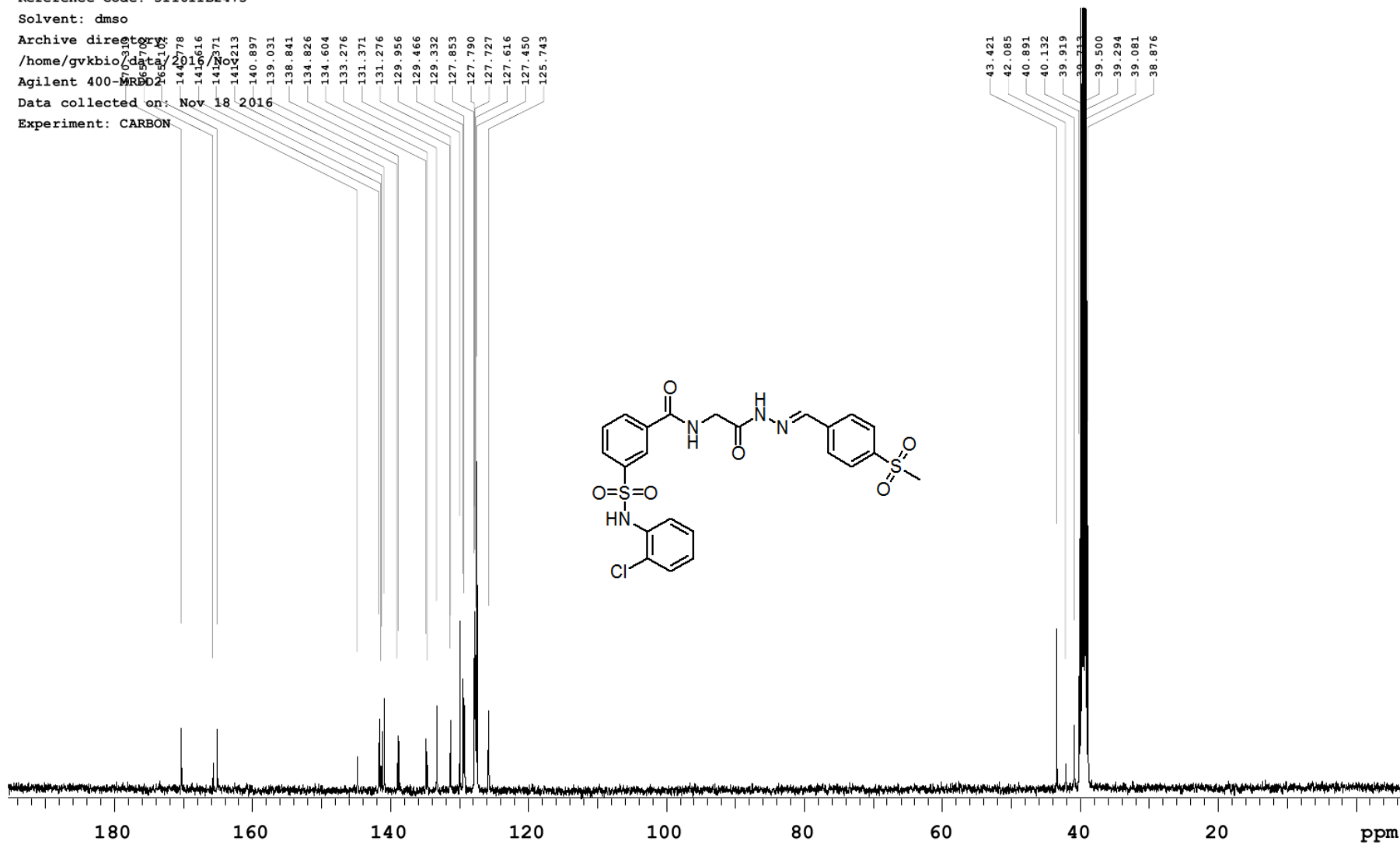
Archive directory

/home/gvkbio/data/2016/Nov

Agilent 400-MRBD

Data collected on: Nov 18 2016

Experiment: CARBON



¹³CNMR of Compound-1j in DMSO-d₆

Elemental Composition Report

Page 1

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)

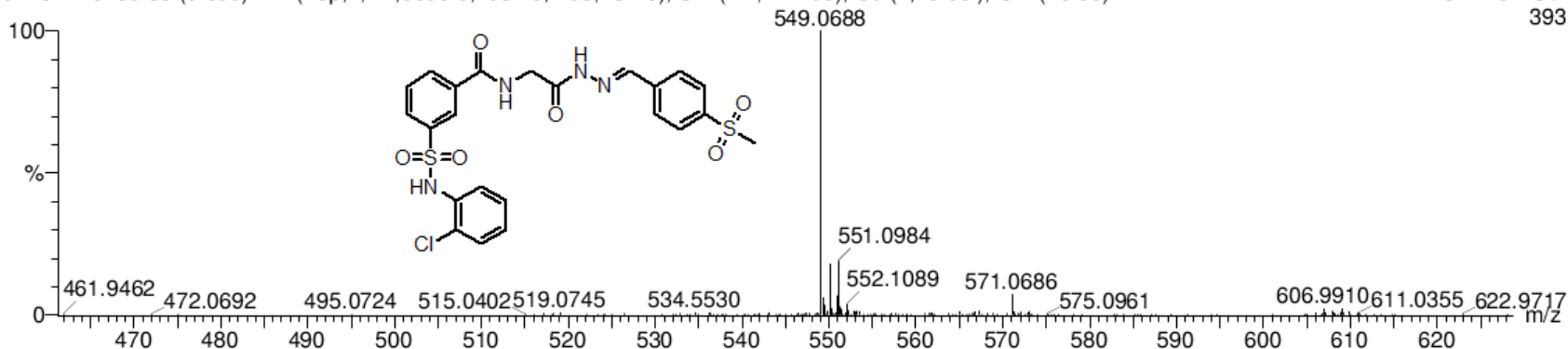
Elements Used:

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

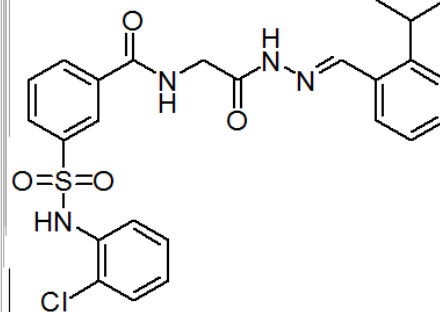


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

Experiment: PROTON



GVB-SA22

Reference Code: 511611C0227

Solvent: dms

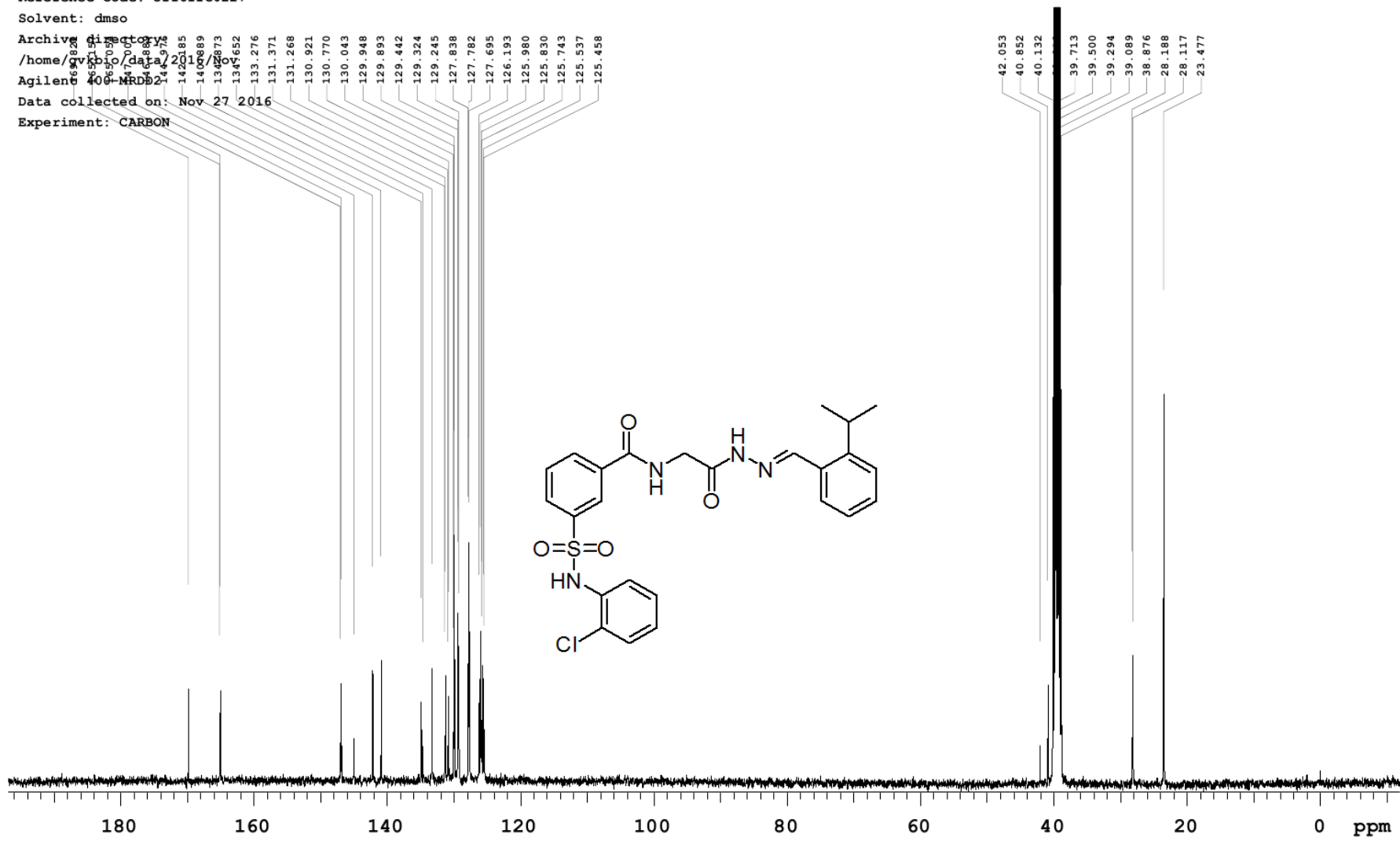
Archive directory

/home/gvbio/data/2016/Nov

Agilent 400-MRDS

Data collected on: Nov 27 2016

Experiment: CARBON



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

Elemental Composition Report

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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)

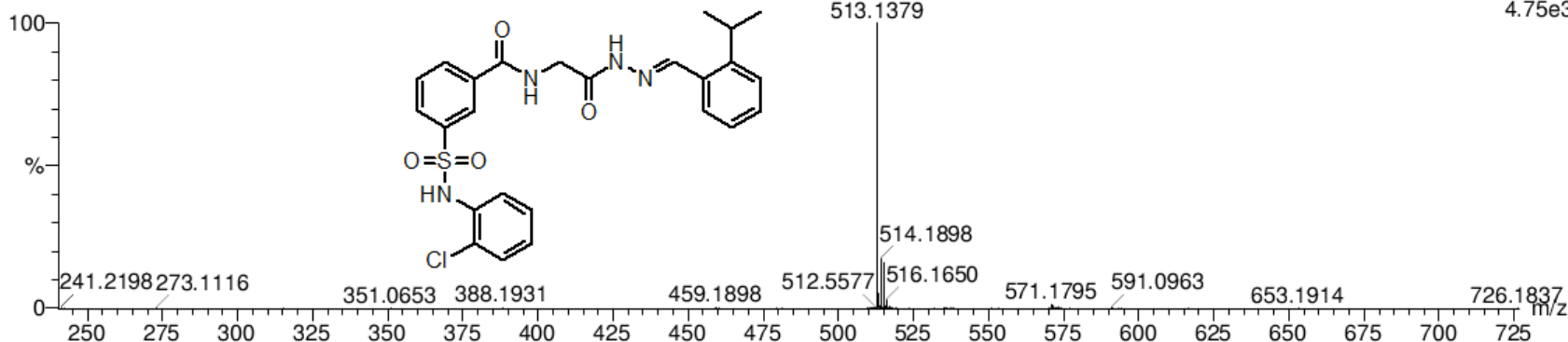
Elements Used:

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

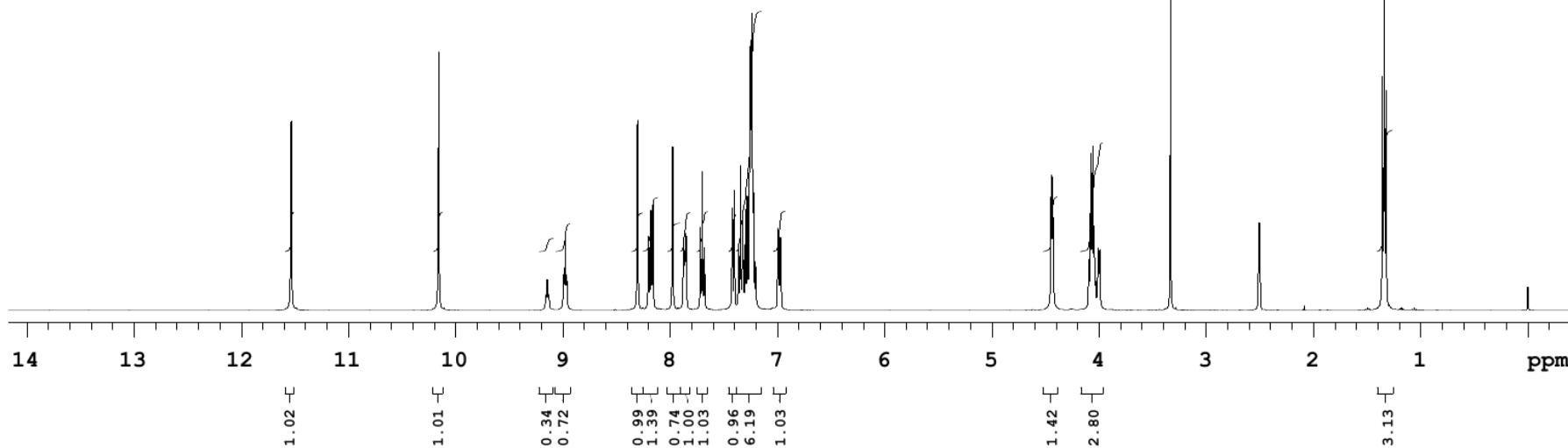
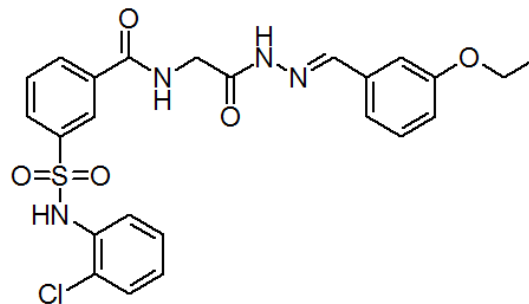


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
513.1379	513.1363	1.6	3.1	14.5	525.4	C ₂₅ H ₂₆ N ₄ O ₄ S Cl

HRMS of Compound-1k

GVB-SA-20
 Reference Code: 511611B2476
 Solvent: dmso
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 18 2016
 Experiment: PROTON



¹H NMR of **Compound-11** in DMSO-d₆

GVB-SA-20

Reference Code: 511611B2476

Solvent: dmso

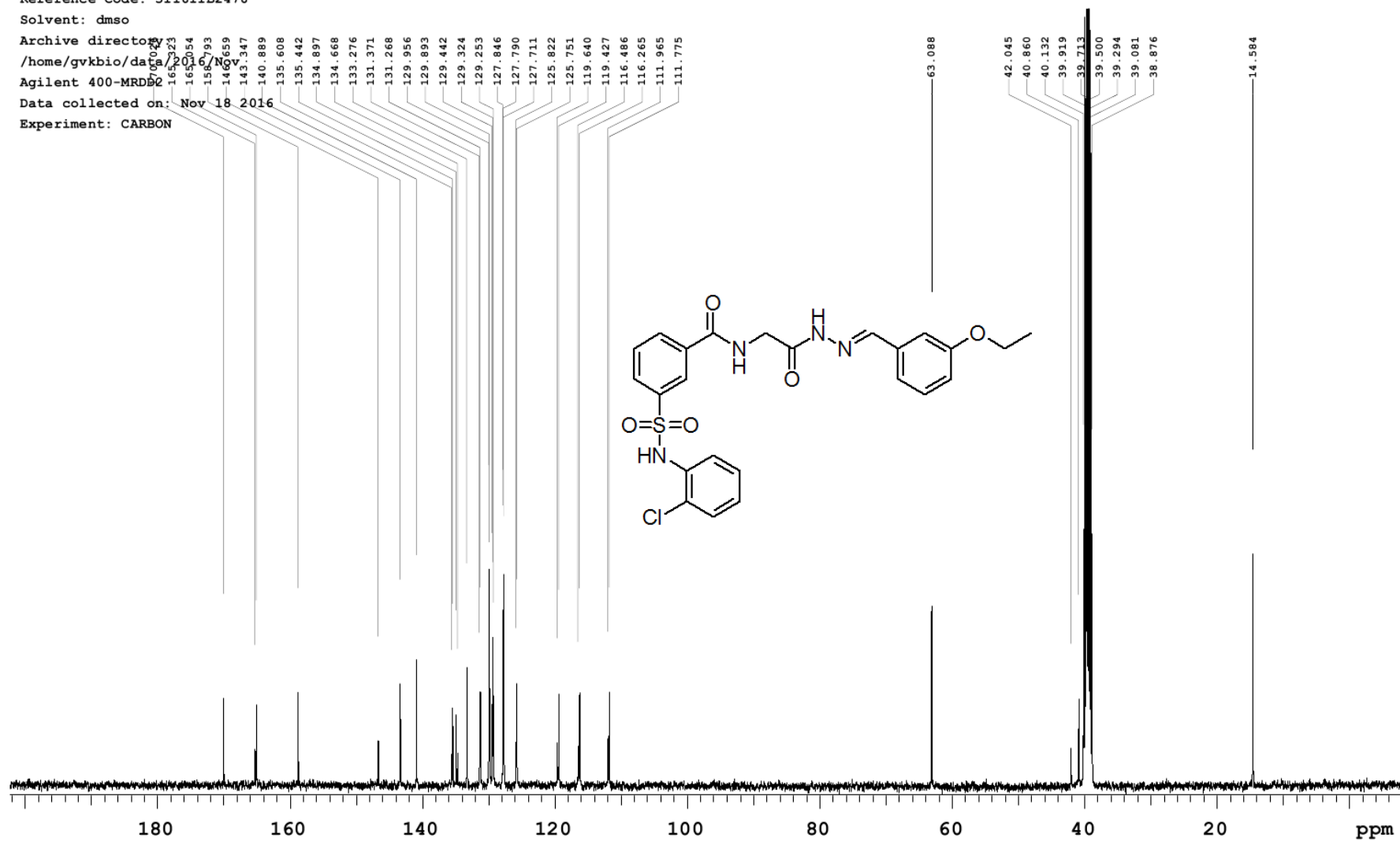
Archive directory

/home/gvkbio/data/2016/

Agilent 400-MRDS2

Data collected on: Nov 18 2016

Experiment: CARBON



^{13}C NMR of Compound-11 in DMSO- d_6

Elemental Composition Report

Page 1

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)

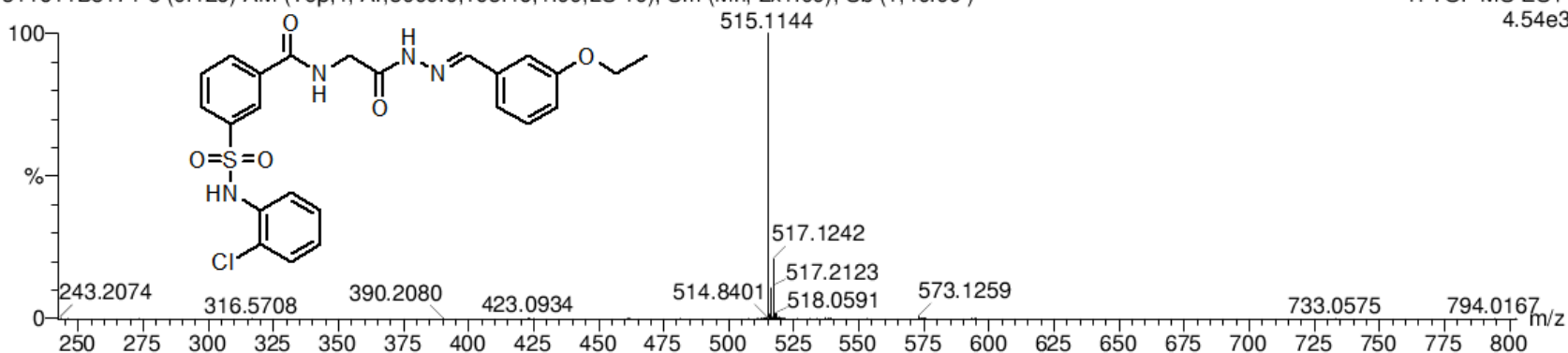
Elements Used:

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)

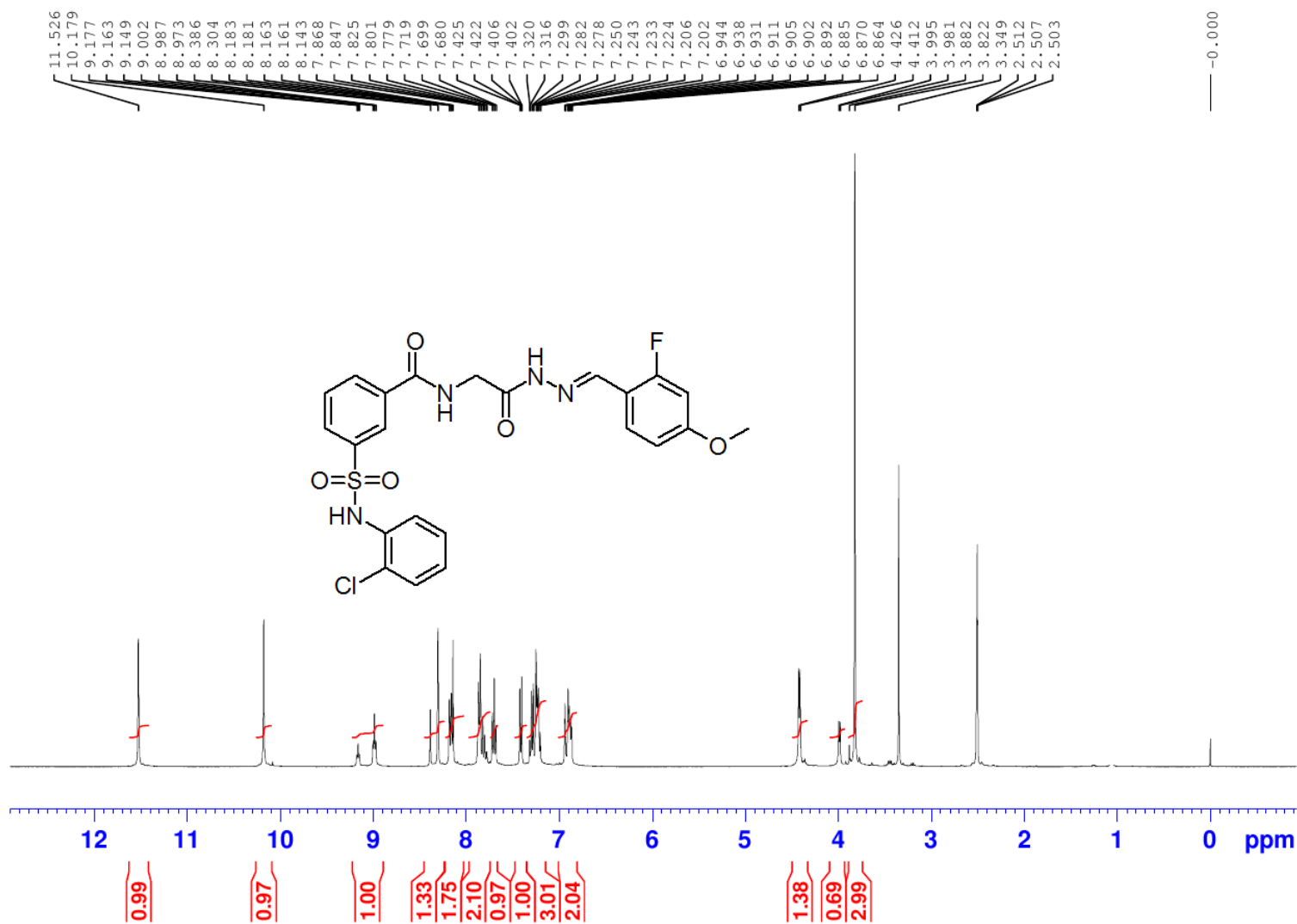
1: TOF MS ES+
4.54e3



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-11



Current Data Parameters
NAME 511611B2470
EXPNO 1
PROCNO 1

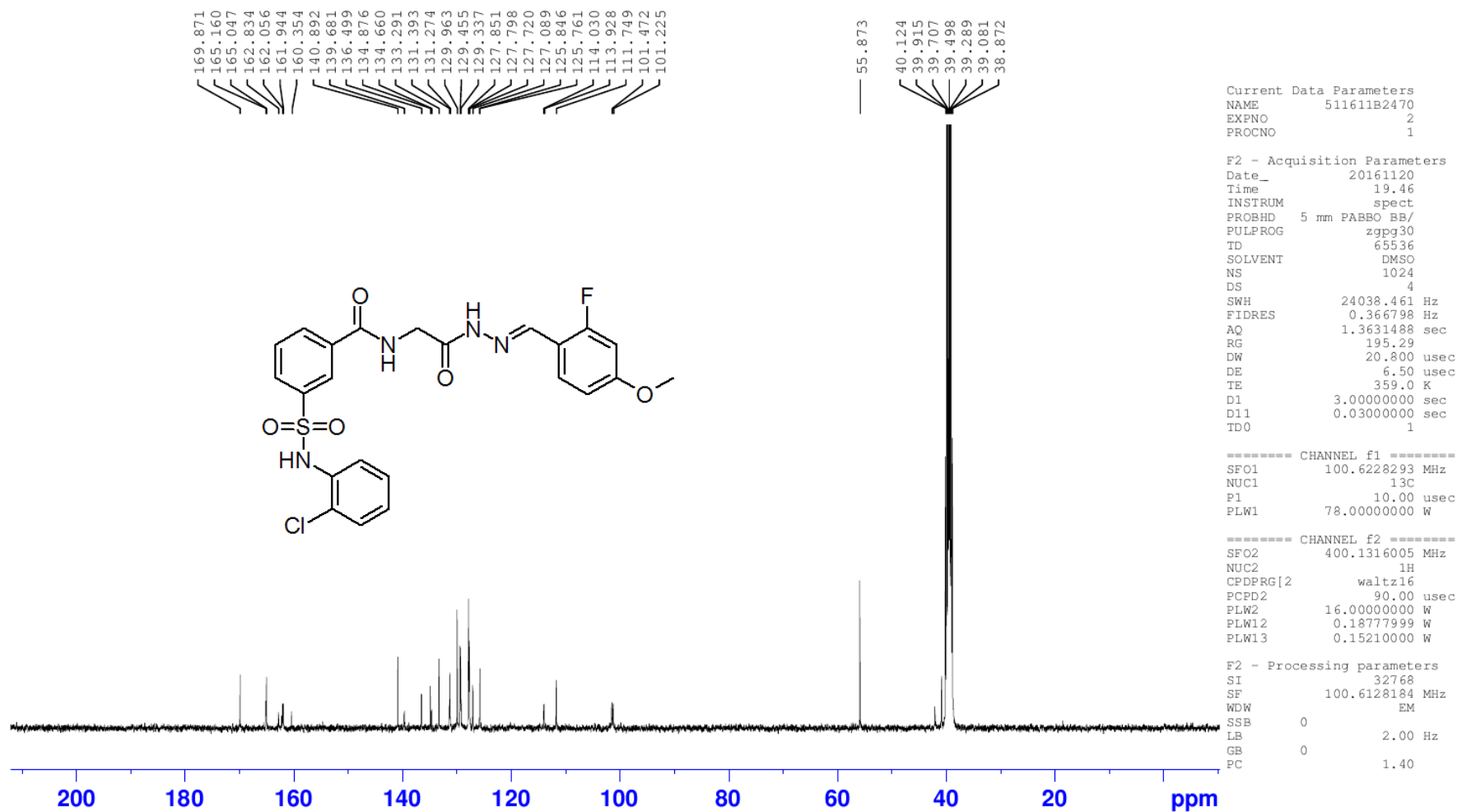
F2 - Acquisition Parameters
Date_ 20161120
Time 18.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 86.08
DW 62.400 usec
DE 6.50 usec
TE 359.7 K
D1 1.00000000 sec
TD0 1

===== 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

ANL-MCL5-NMR-001

¹H NMR of **Compound-1m** in DMSO-d₆



ANL-MCL5-NMR-001

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

Elemental Composition Report

Page 1

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)

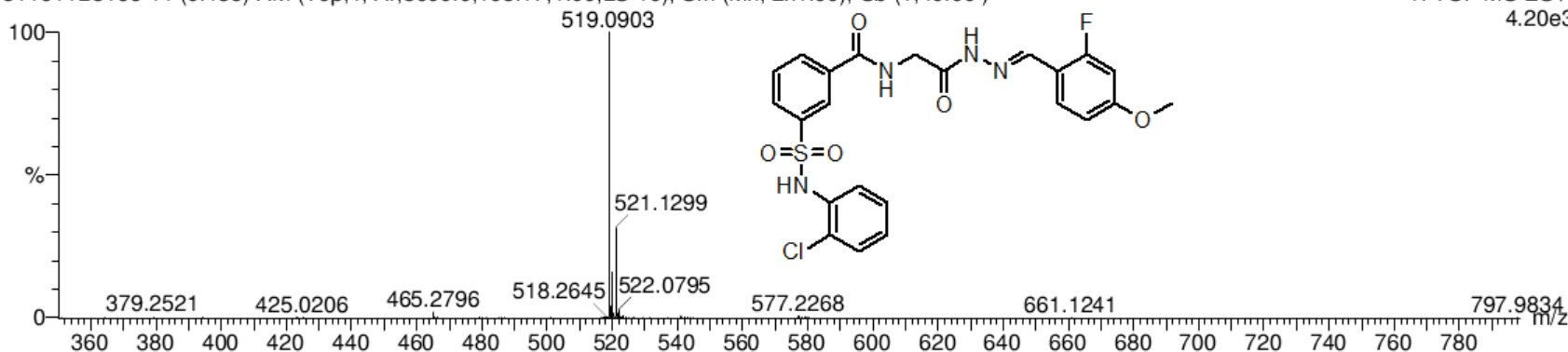
Elements Used:

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)

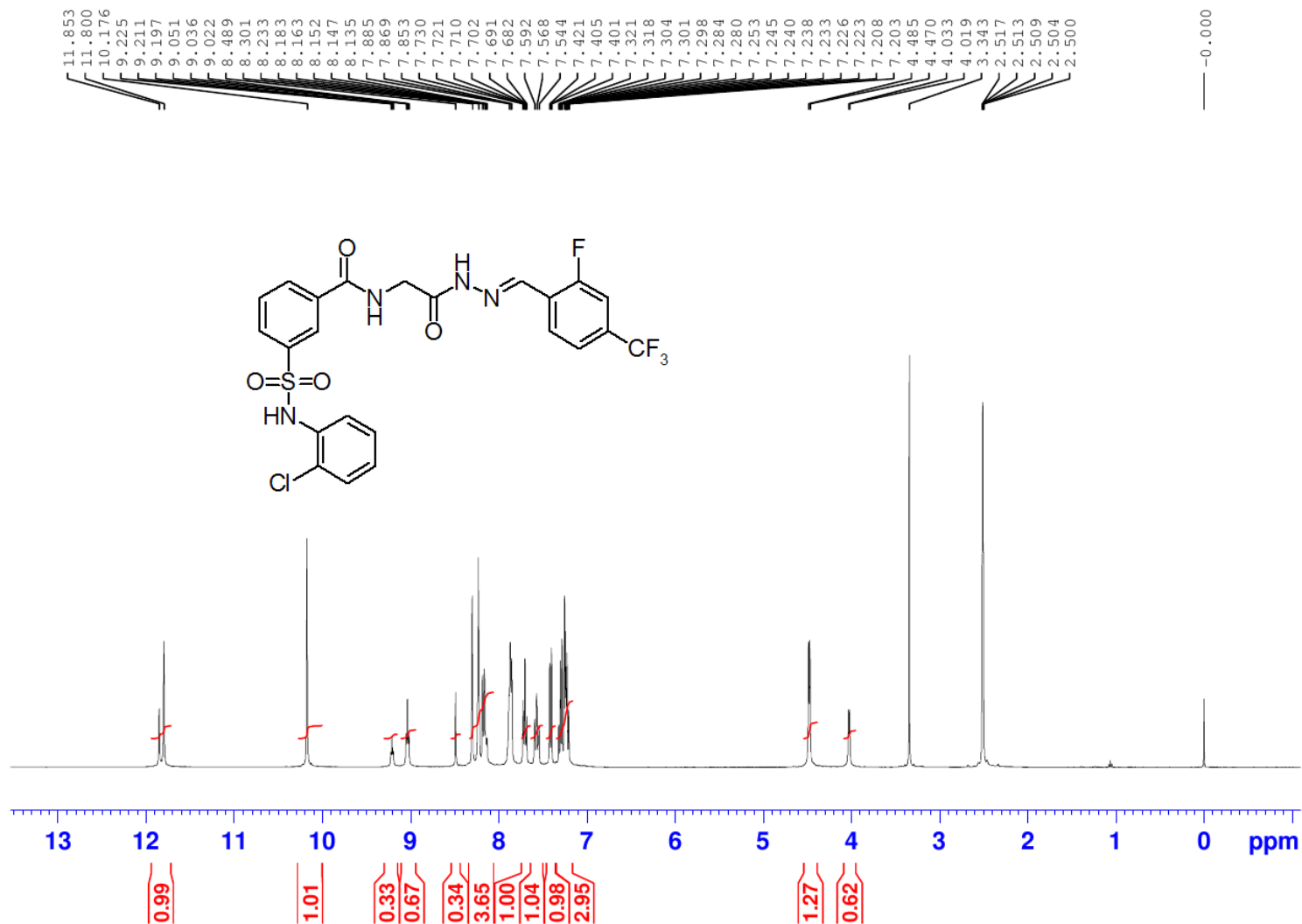
1: TOF MS ES+
4.20e3



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	C ₂₃ H ₂₁ N ₄ O ₅ F S Cl

HRMS of Compound-1m



Current Data Parameters
 NAME 511611B2473
 EXPNO 1
 PROCNO 1

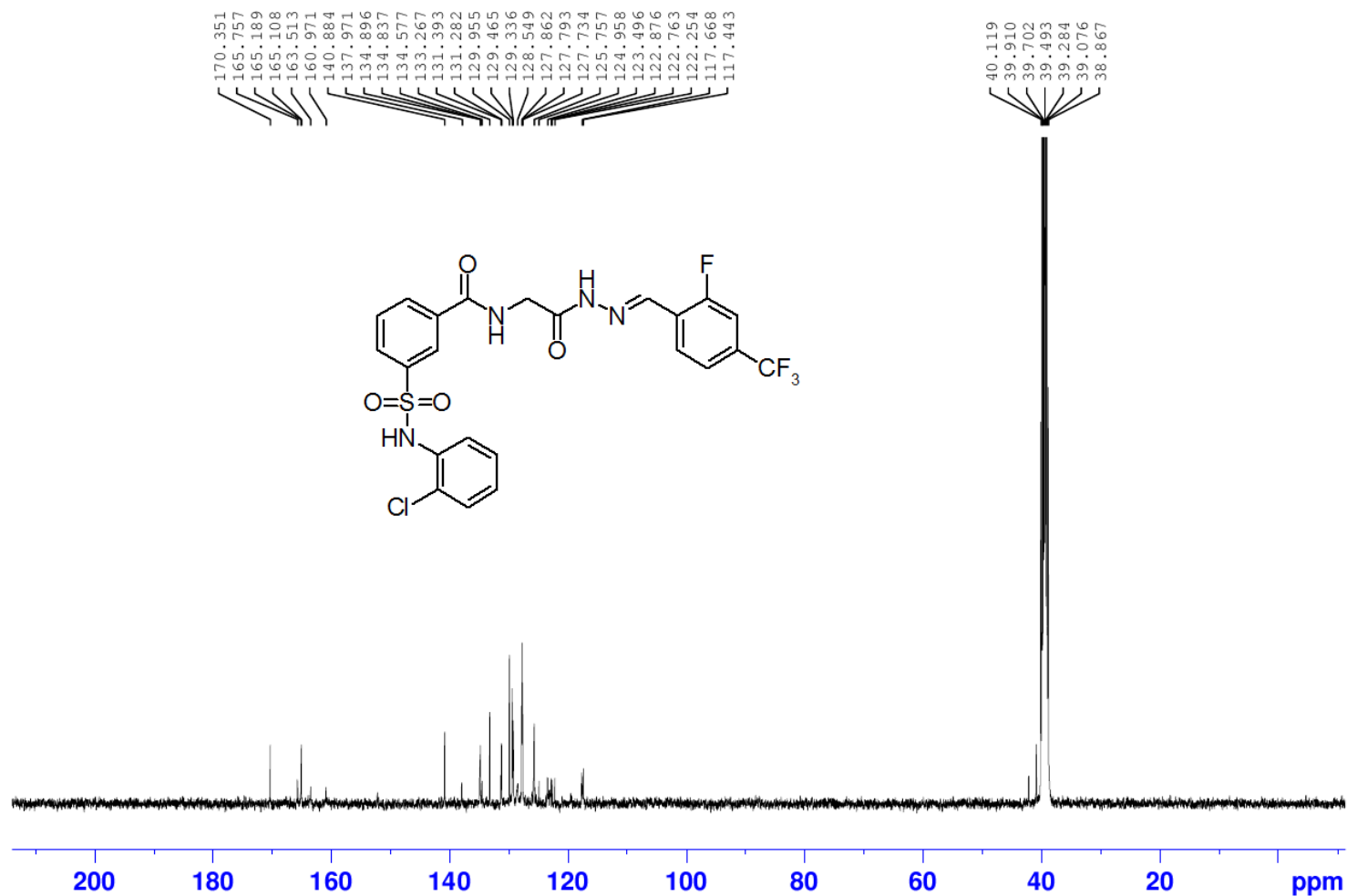
F2 - Acquisition Parameters
 Date_ 20161120
 Time 17.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 86.08
 DW 62.400 usec
 DE 6.50 usec
 TE 359.7 K
 D1 1.00000000 sec
 TD0 1

===== 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

ANL-MCL5-NMR-001

¹H NMR of **Compound-1n** in DMSO-d₆



Current Data Parameters
NAME 511611B2473
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161120
Time 18.25
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 360.7 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 100.6128185 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL5-NMR-001

¹³CNMR of **Compound-1n** in DMSO-d₆

Elemental Composition Report

Page 1

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)

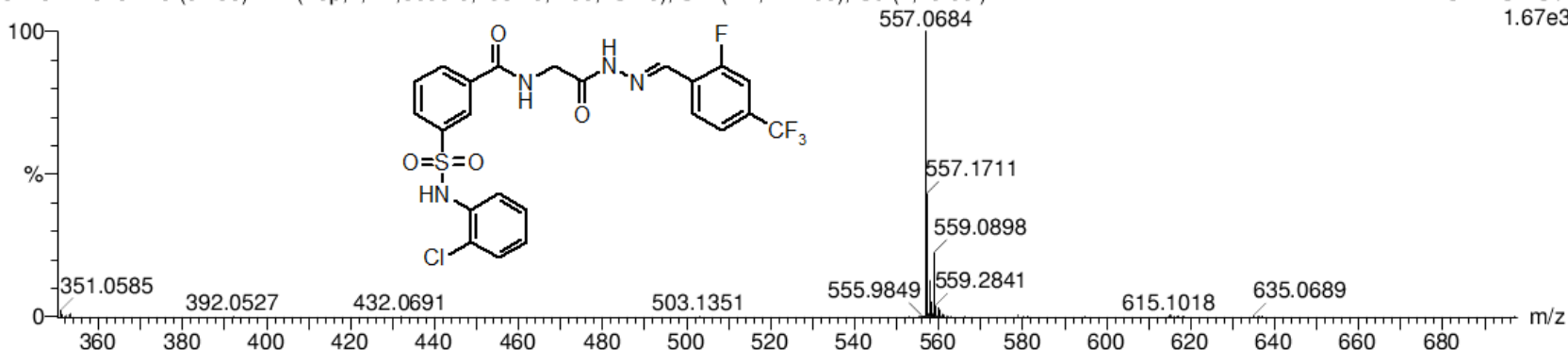
Elements Used:

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

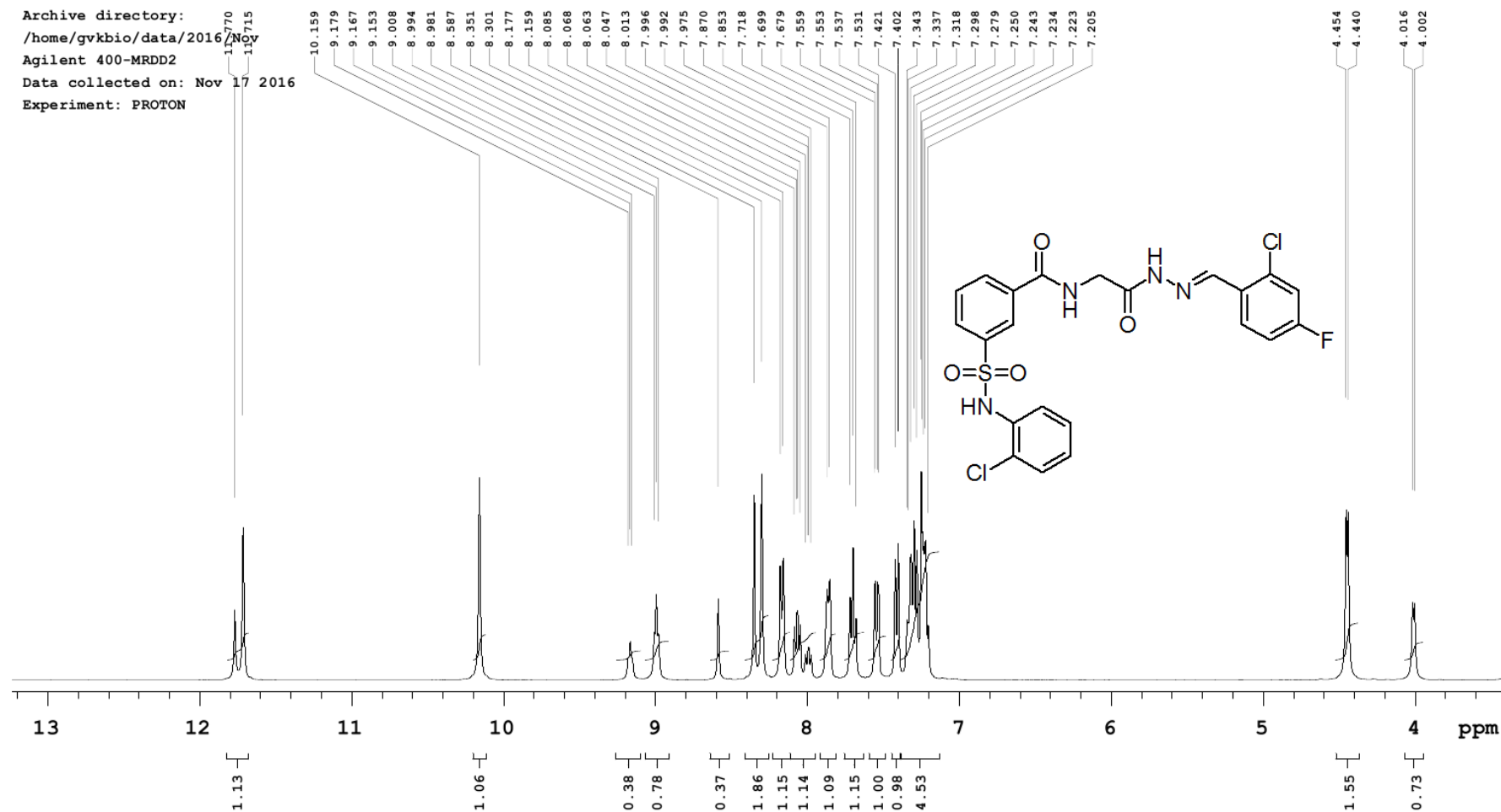


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SA15
 Reference Code: 511611B2469
 Solvent: dmsd
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 17 2016
 Experiment: PROTON



¹H NMR of **Compound-1o** in DMSO-d₆

GVB-SA-15

Reference Code: 511611B2469

Solvent: dms

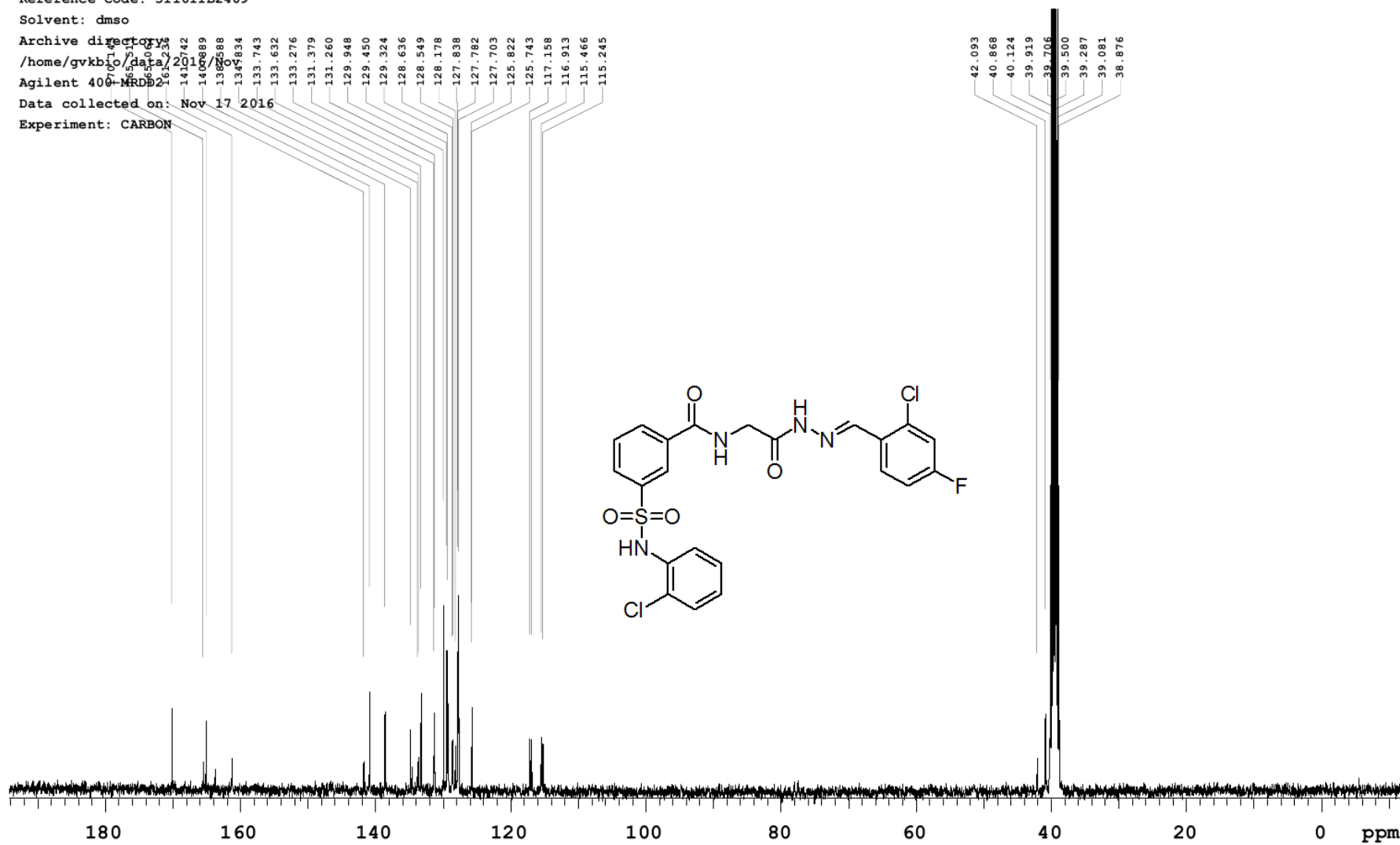
Archive directory

/home/gvkbio/data/2010/Nov

Agilent 400-MRDP

Data collected on: Nov 17 2016

Experiment: CARBON



^{13}C NMR of **Compound-1o** in $\text{DMSO-}d_6$

Elemental Composition Report

Page 1

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)

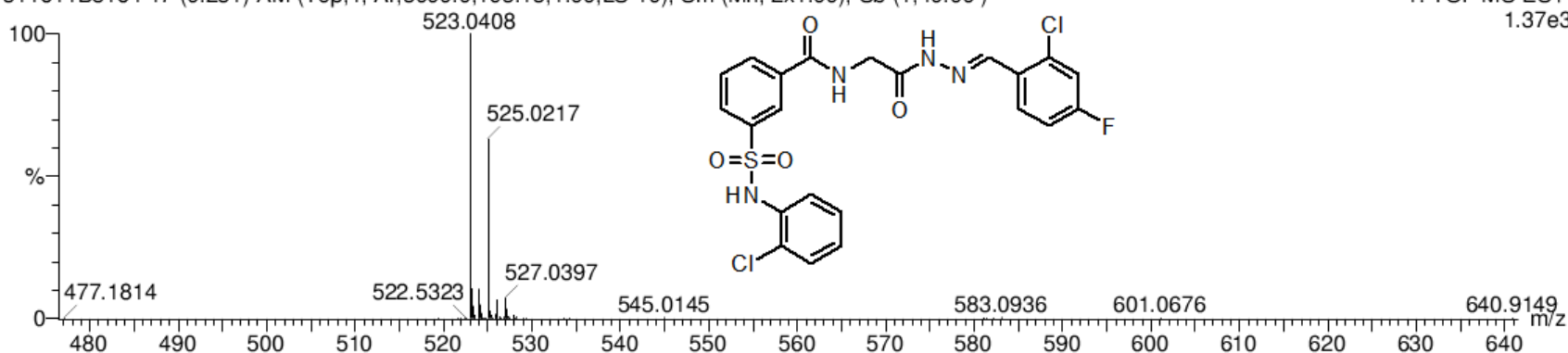
Elements Used:

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)

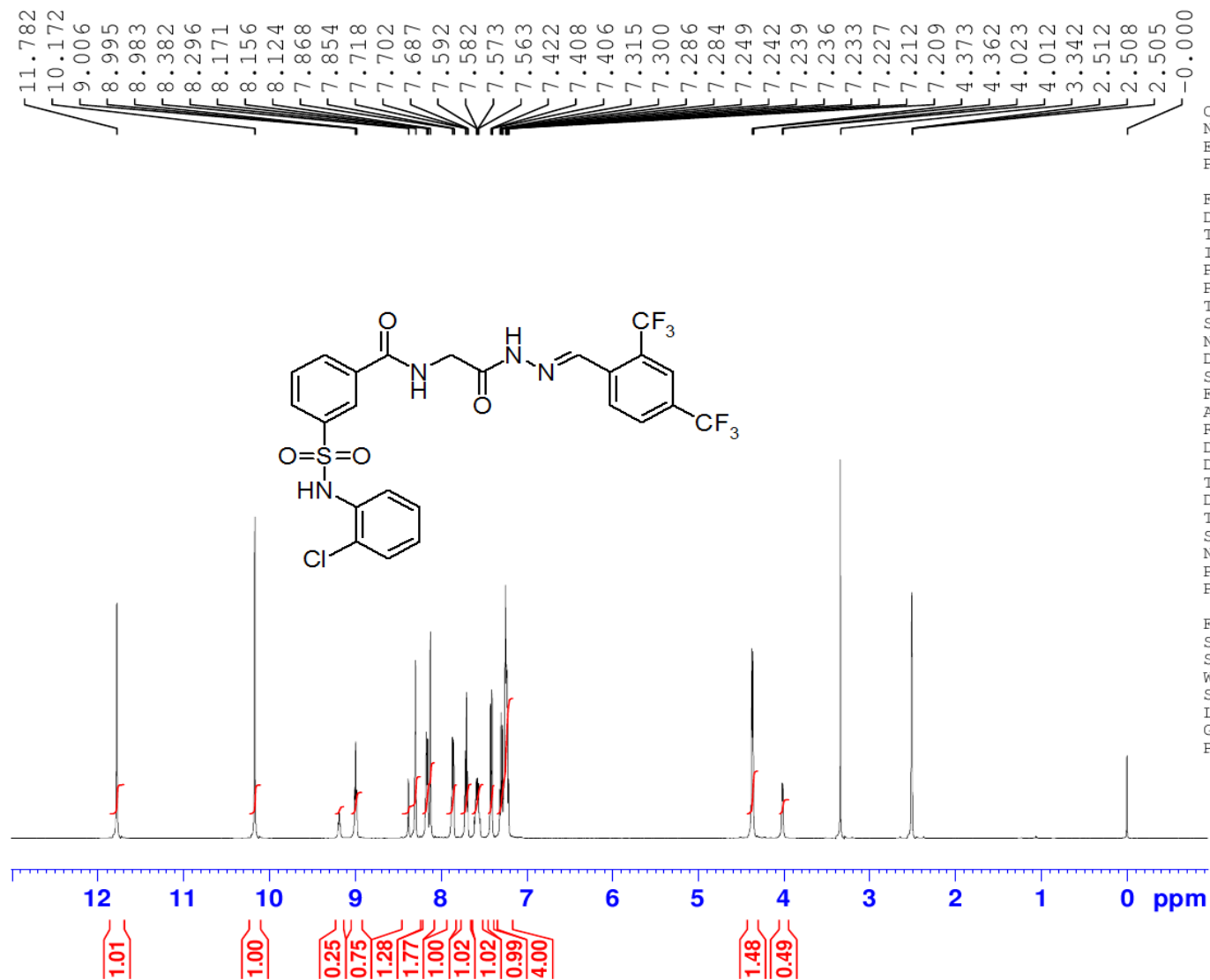
1: TOF MS ES+
1.37e3



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



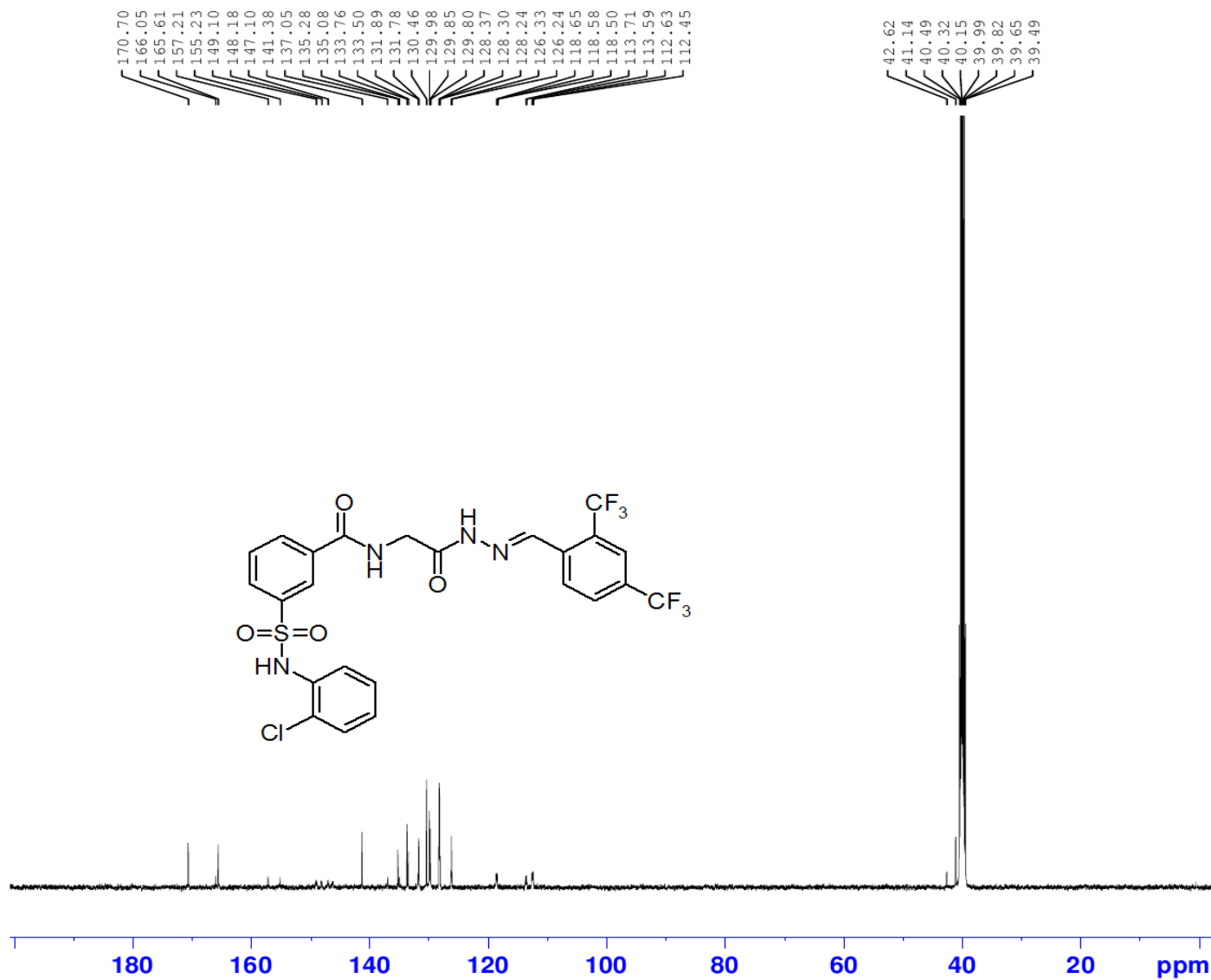
Current Data Parameters
 NAME 511611B1542
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161115
 Time 8.09 h
 INSTRUM spect
 PROBHD Z119470_0231 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 97.81
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 23.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300002 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of **Compound-1p** in DMSO-d₆

GVB-SA13



Current Data Parameters
 NAME 511611B1542
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161115
 Time 9.00 h
 INSTRUM spect
 PROBHD z119470_0231 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 711
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 197.72
 DW 16.800 usec
 DE 6.50 usec
 TE 298.2 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 88.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 23.00000000 W
 PLW12 0.27515000 W
 PLW13 0.13840000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

¹³CNMR of Compound-1p in DMSO-d₆

Elemental Composition Report

Page 1

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)

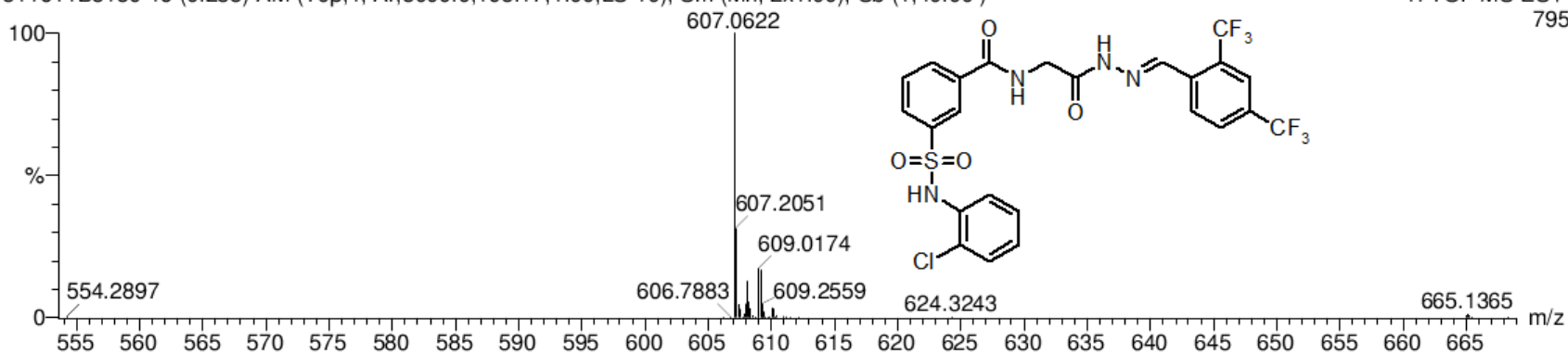
Elements Used:

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

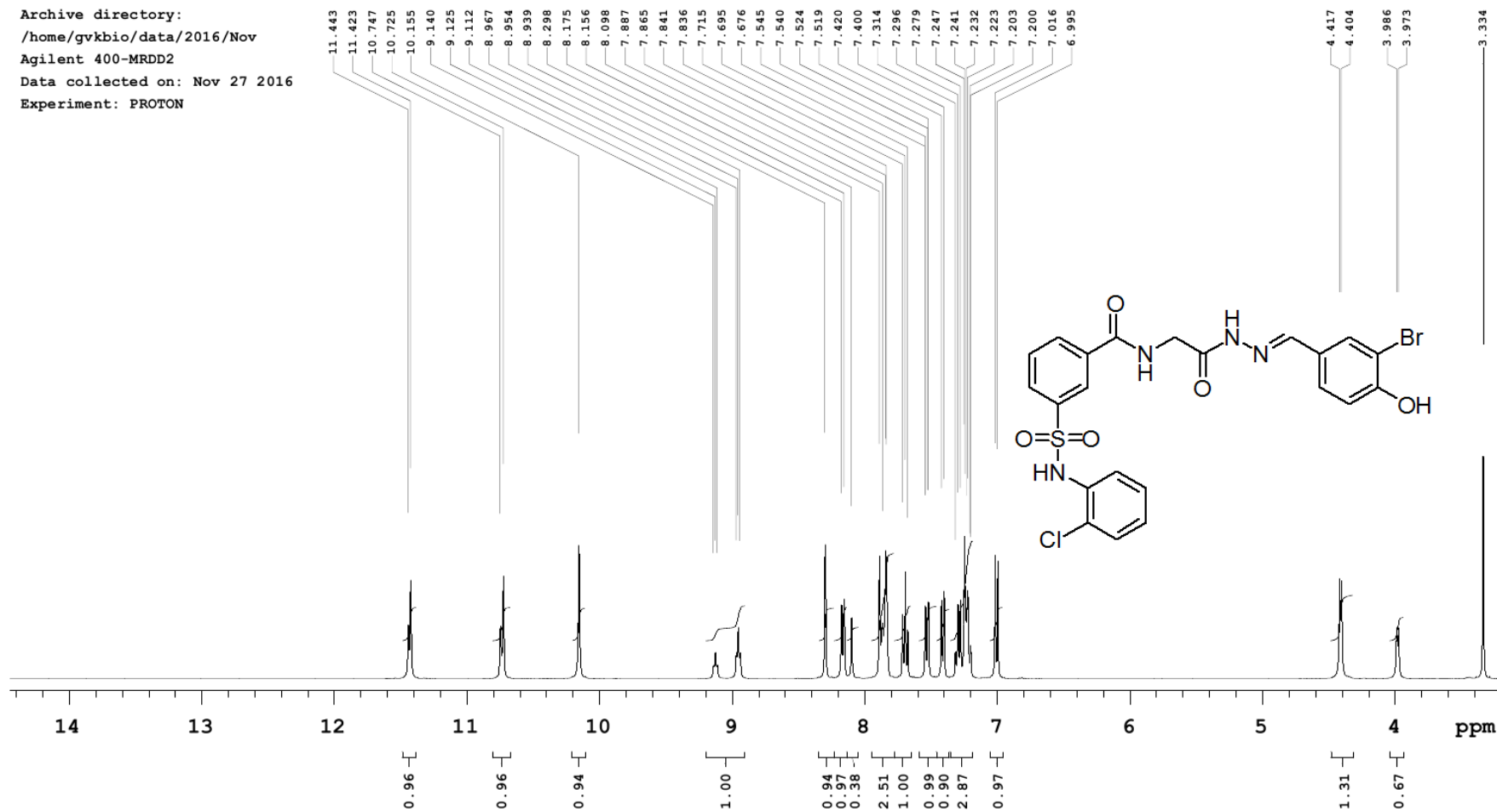


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
607.0622	607.0641	-1.9	-3.1	14.5	85.5	C ₂₄ H ₁₈ N ₄ O ₄ F ₆ S Cl

HRMS of Compound-1p

GVB-SA18
 Reference Code: 511611C0226
 Solvent: dmsc
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 27 2016
 Experiment: PROTON



¹H NMR of **Compound-1q** in DMSO-d₆

GVB-SA18

Reference Code: 511611C0226

Solvent: dms

Archive directory:

/home/gvkbio/data/2016

Agilent 400-MRDD2

Data collected on: Nov 27 2016

Experiment: CARBON



^{13}C NMR of Compound-1q in DMSO- d_6

Elemental Composition Report

Page 1

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)

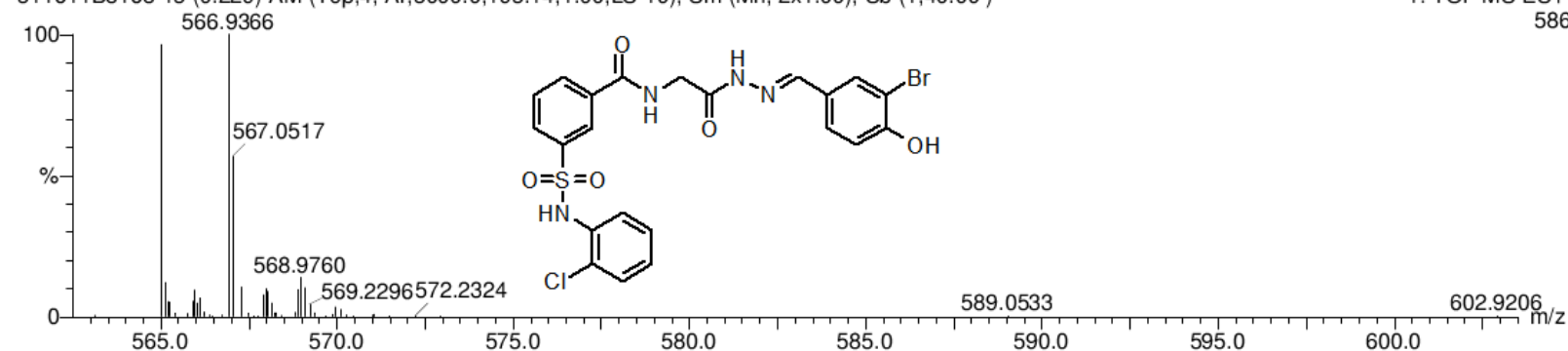
Elements Used:

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

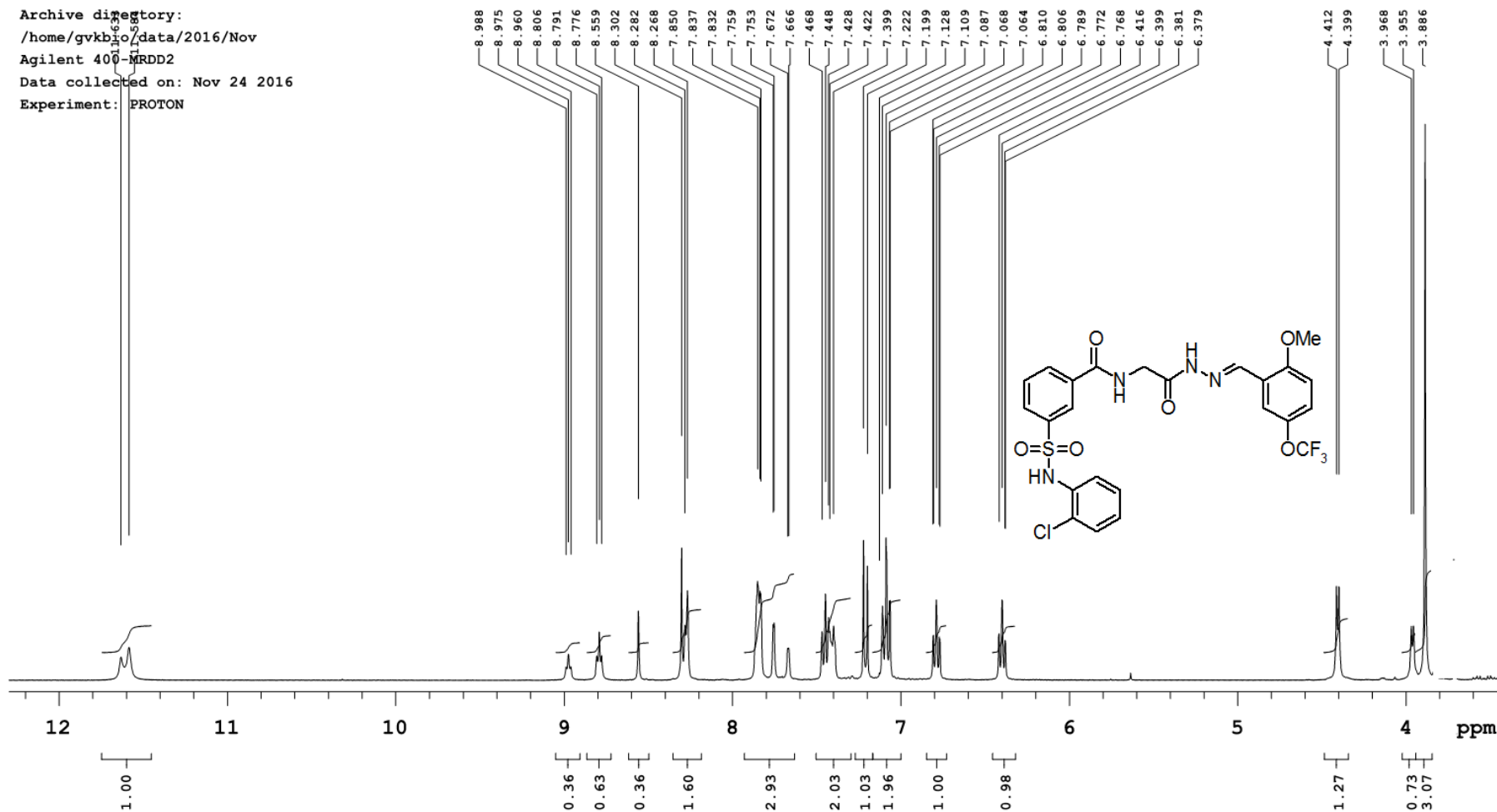


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SA11
 Reference Code: 511611C0225
 Solvent: dmsd
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 24 2016
 Experiment: PROTON



¹H NMR of **Compound-1r** in DMSO-d₆

GVB-SA11

Reference Code: 511611C0225

Solvent: dmsc

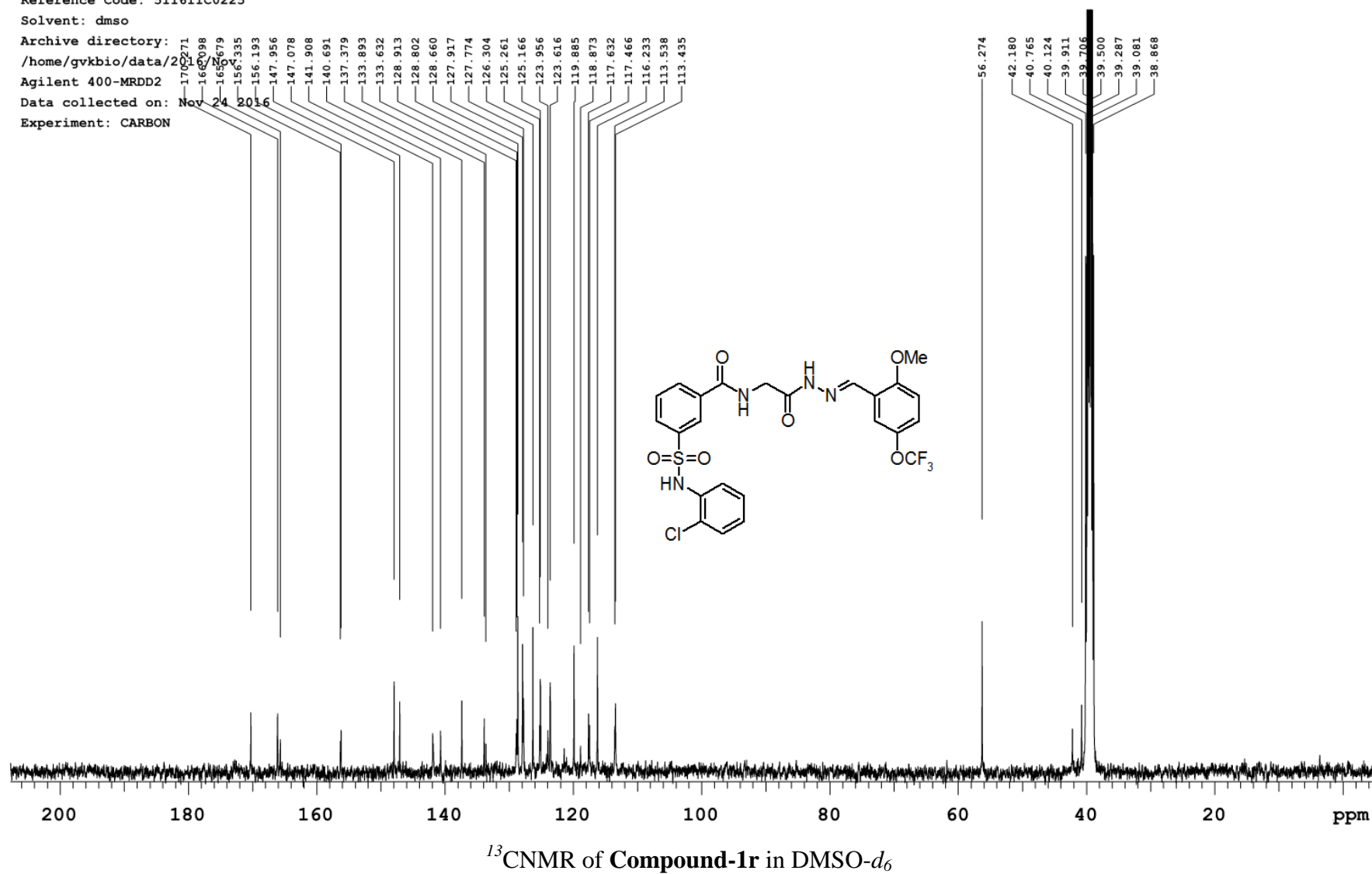
Archive directory:

/home/gvkbio/data/2016/Nov

Agilent 400-MRDD2

Data collected on: Nov 24 2016

Experiment: CARBON



Elemental Composition Report

Page 1

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)

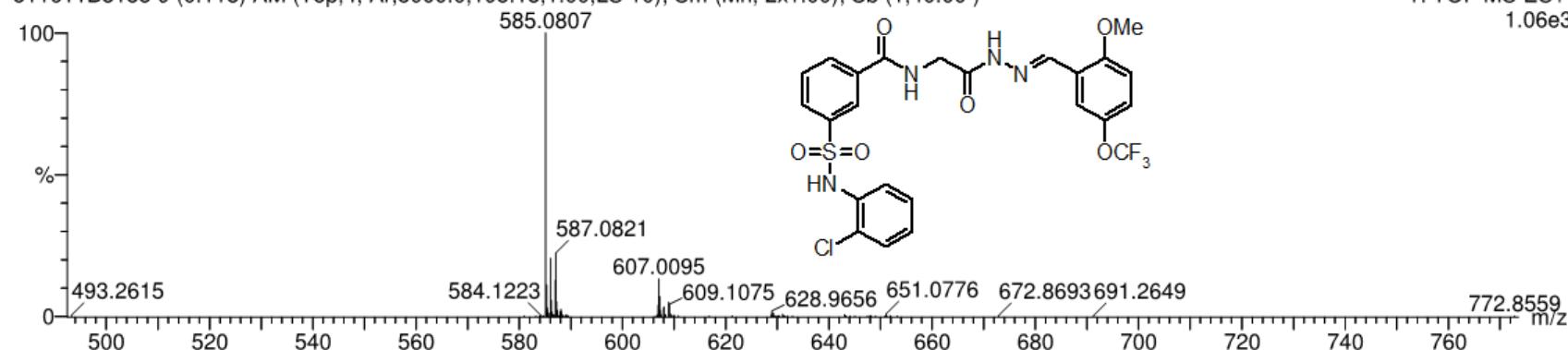
Elements Used:

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

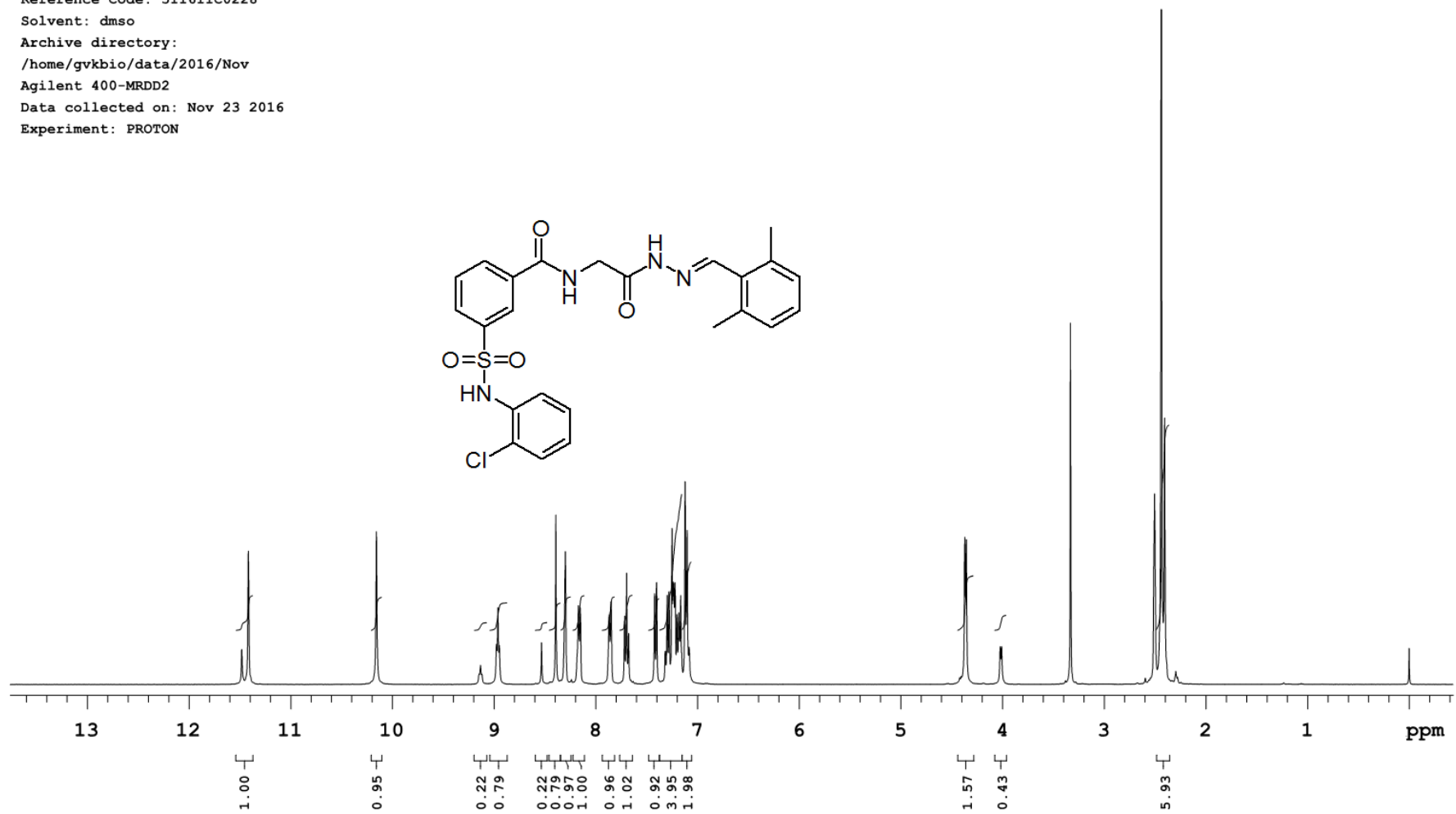


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SA23
Reference Code: 511611C0228
Solvent: dms
Archive directory:
/home/gvkbio/data/2016/Nov
Agilent 400-MRDD2
Data collected on: Nov 23 2016
Experiment: PROTON



¹H NMR of **Compound-1s** in DMSO-d₆

GVB-SA23

Reference Code: 511611C0228

Solvent: dmsc

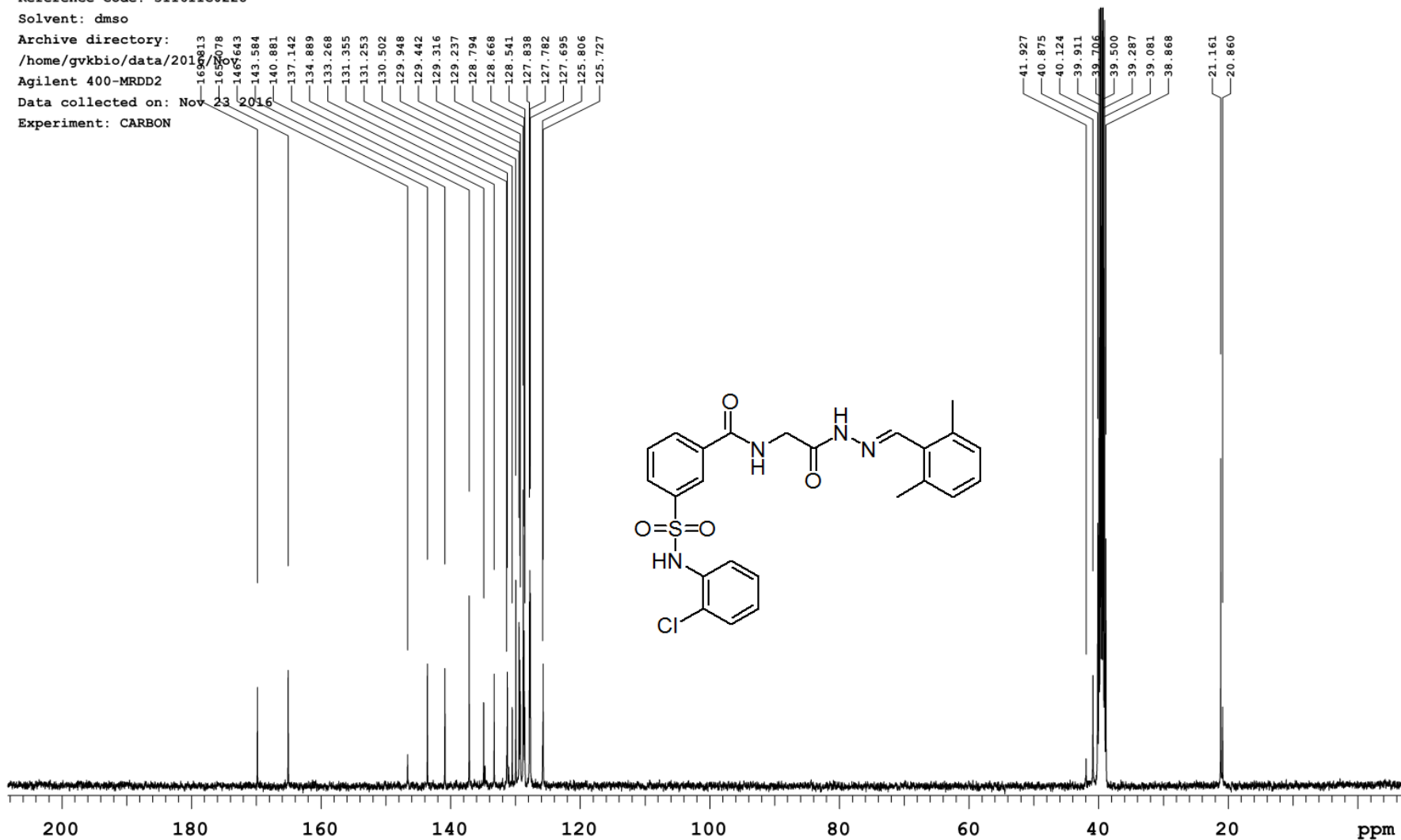
Archive directory:

/home/gvkbio/data/2016/Nov

Agilent 400-MRDD2

Data collected on: Nov 23 2016

Experiment: CARBON



¹³CNMR of **Compound-1s** in DMSO-*d*₆

Elemental Composition Report

Page 1

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)

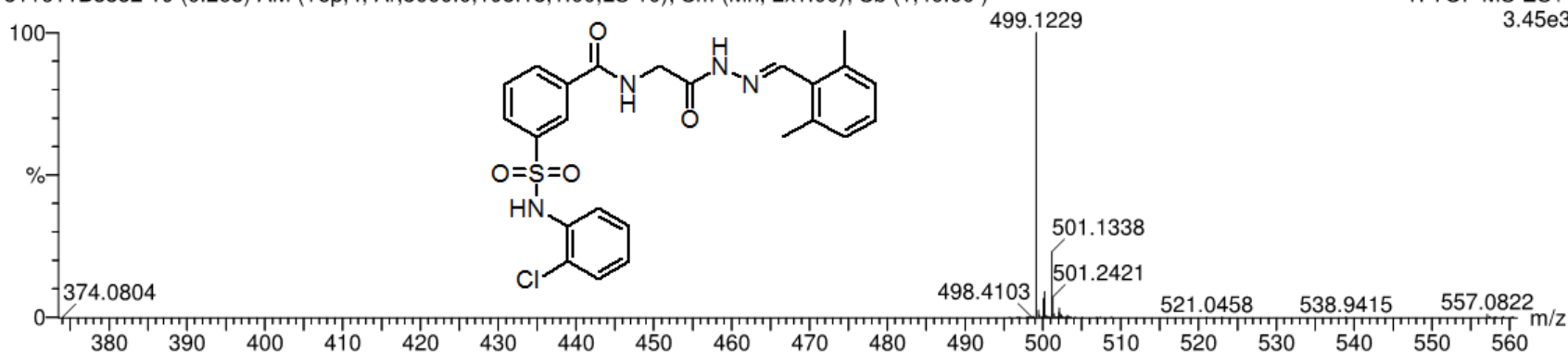
Elements Used:

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

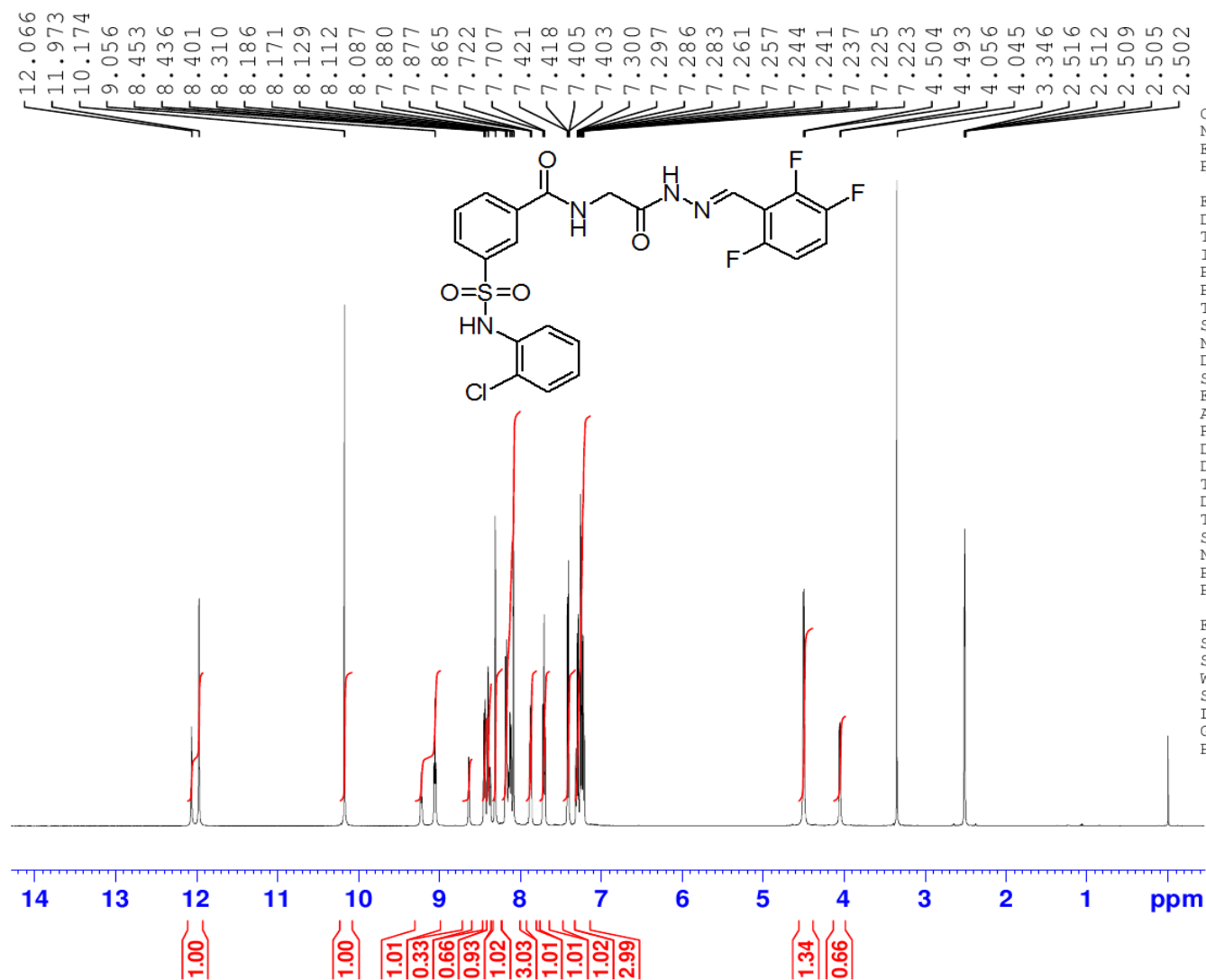


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SA12



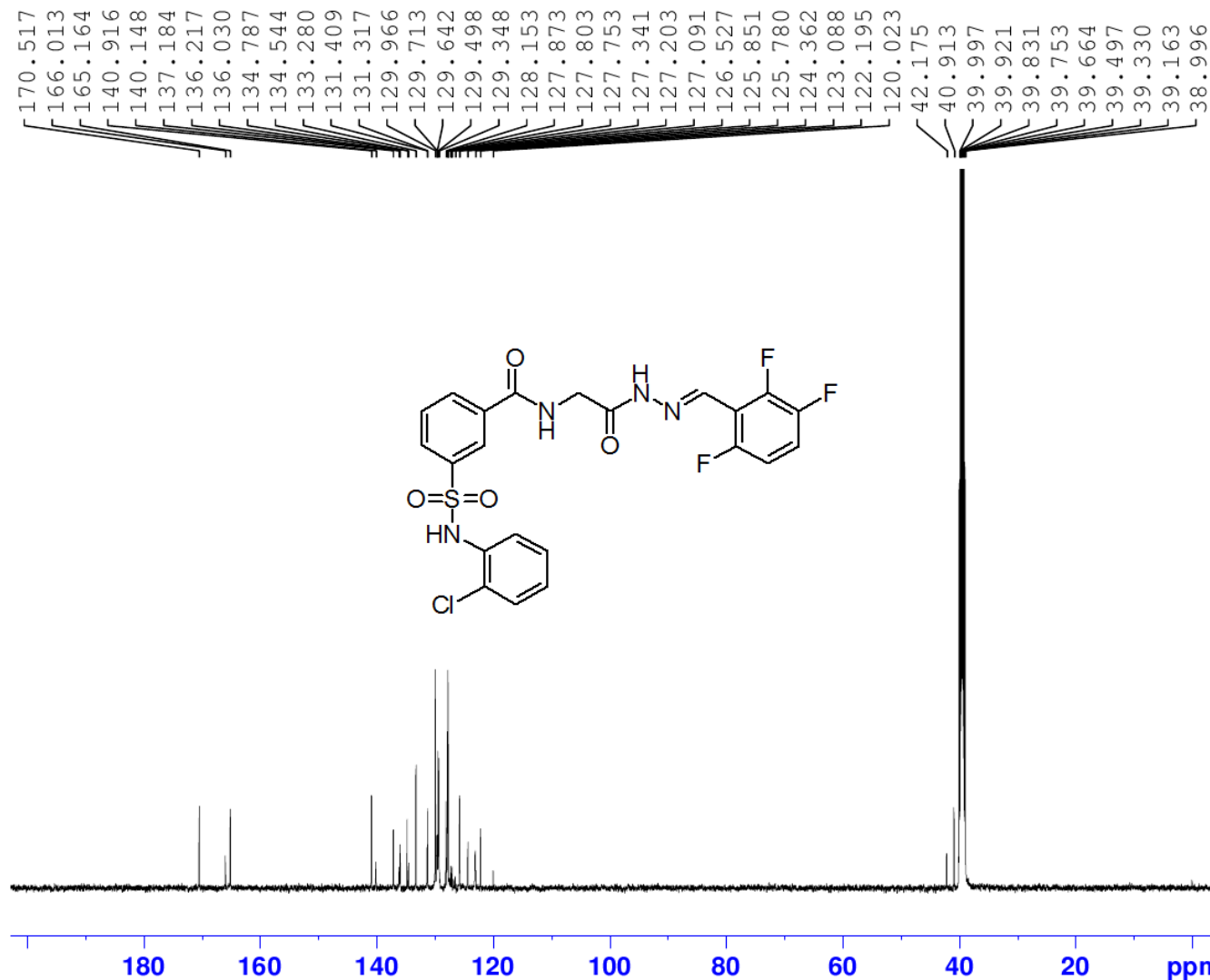
Current Data Parameters
 NAME 511611B1541
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161115
 Time 21.08 h
 INSTRUM spect
 PROBHD Z119470_0231 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 89.27
 DW 50.000 usec
 DE 6.50 usec
 TE 298.5 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 23.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of Compound-1t in DMSO-d₆

GVB-SA12



Current Data Parameters
 NAME 511611B1541
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161116
 Time 0.40 h
 INSTRUM spect
 PROBHD Z119470_0231
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 197.72
 DW 16.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 88.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 23.00000000 W
 PLW12 0.27515000 W
 PLW13 0.13840000 W

F2 - Processing parameters
 SI 32768
 SF 125.7578492 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

¹³CNMR of Compound-1t in DMSO-d₆

Elemental Composition Report

Page 1

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)

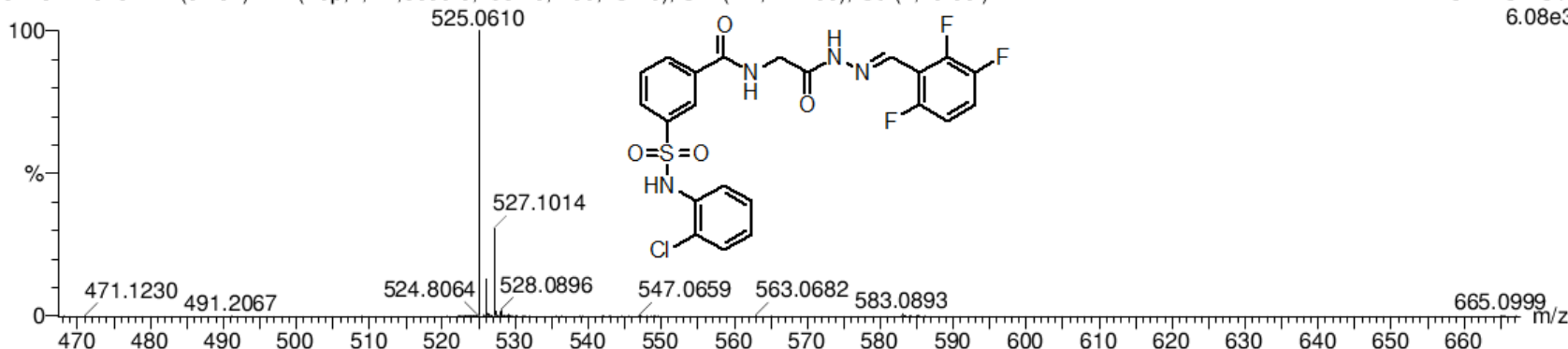
Elements Used:

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

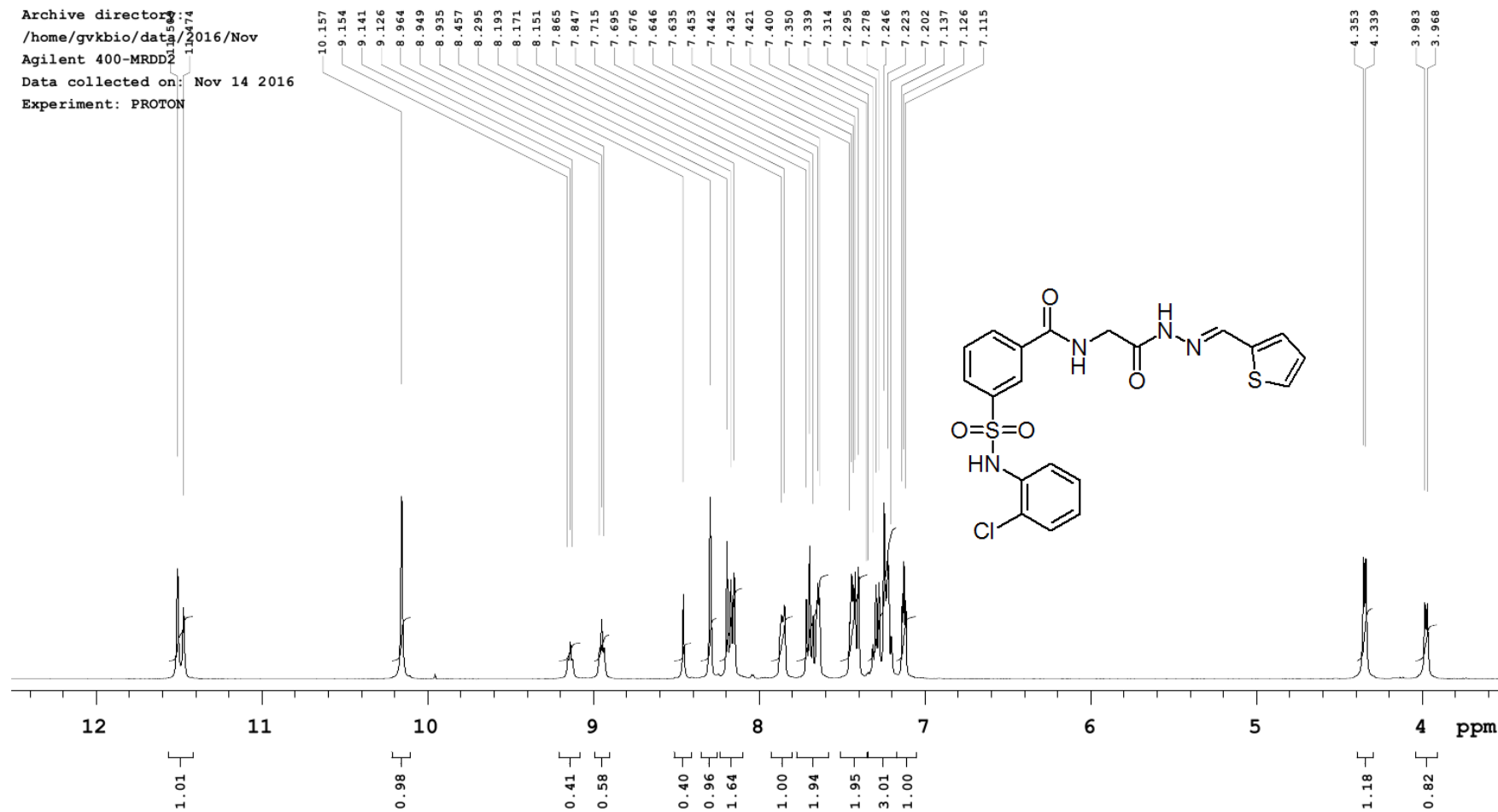


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SA03
 Reference Code: 511611A0300
 Solvent: dms
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD
 Data collected on: Nov 14 2016
 Experiment: PROTON



¹H NMR of **Compound-1u** in DMSO-d₆

GVB-SA03

Reference Code: 511611A0300

Solvent: dmsc

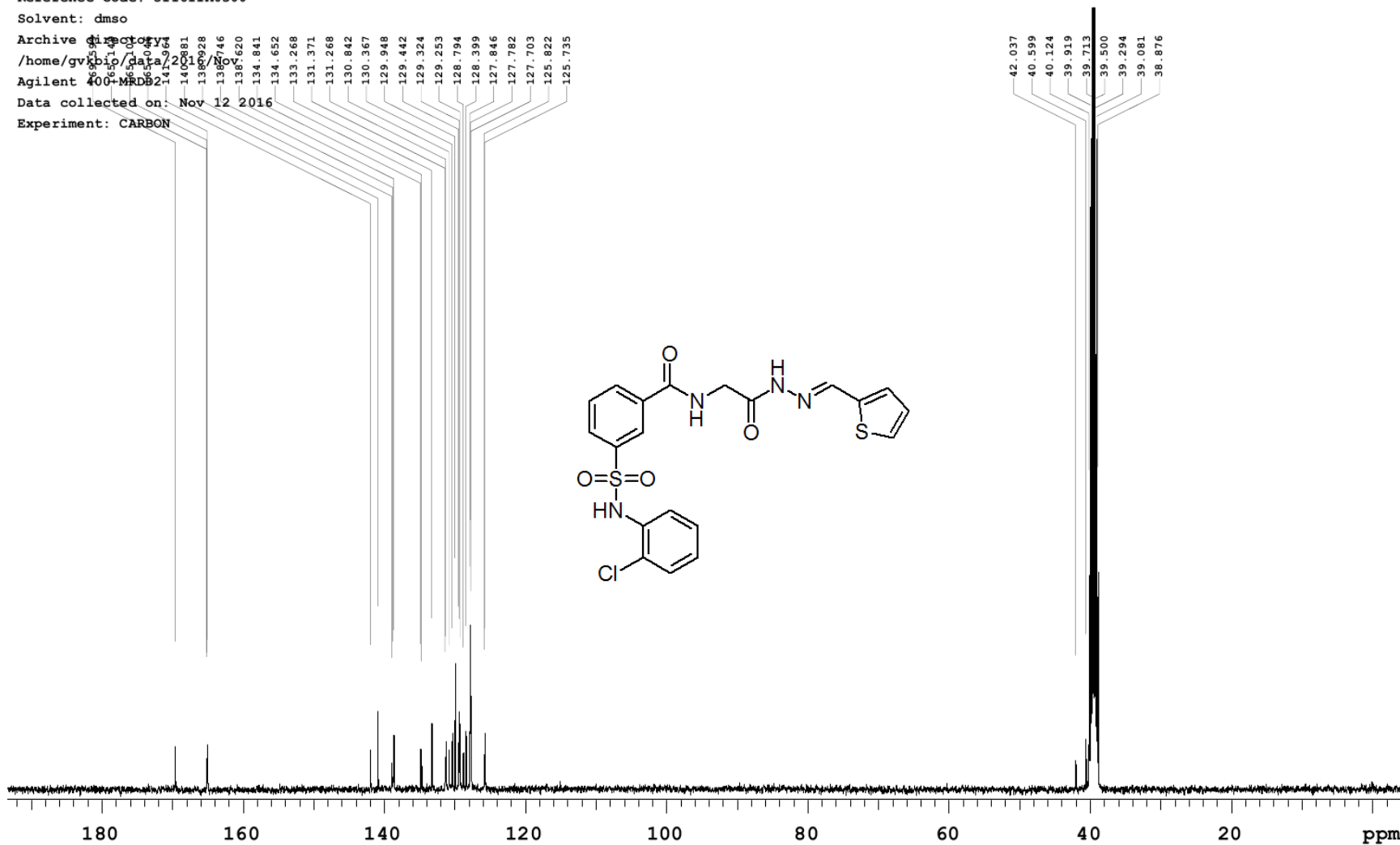
Archive directory

/home/gvxbip/data/2016/Nov

Agilent 400-MRDB2

Data collected on: Nov 12 2016

Experiment: CARBON



Elemental Composition Report

Page 1

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)

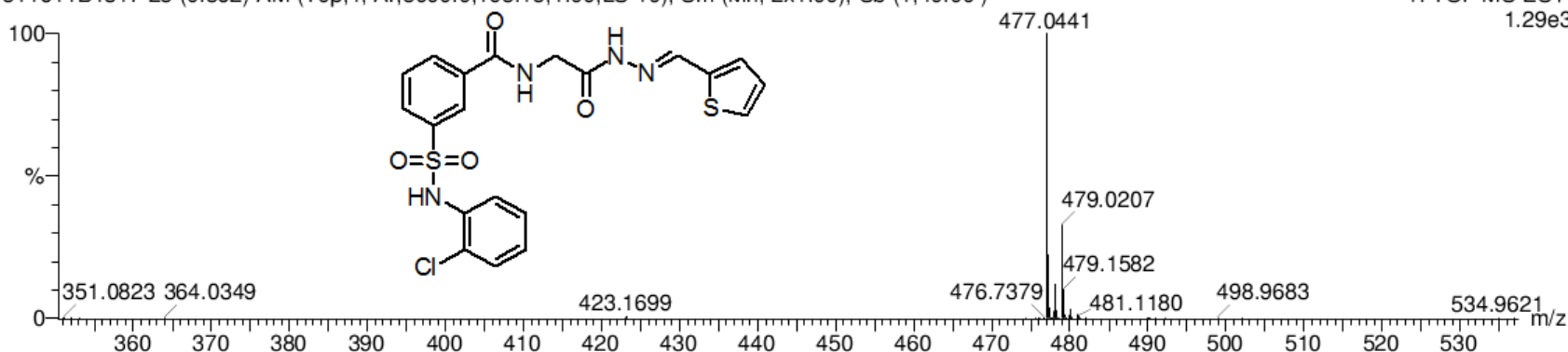
Elements Used:

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)

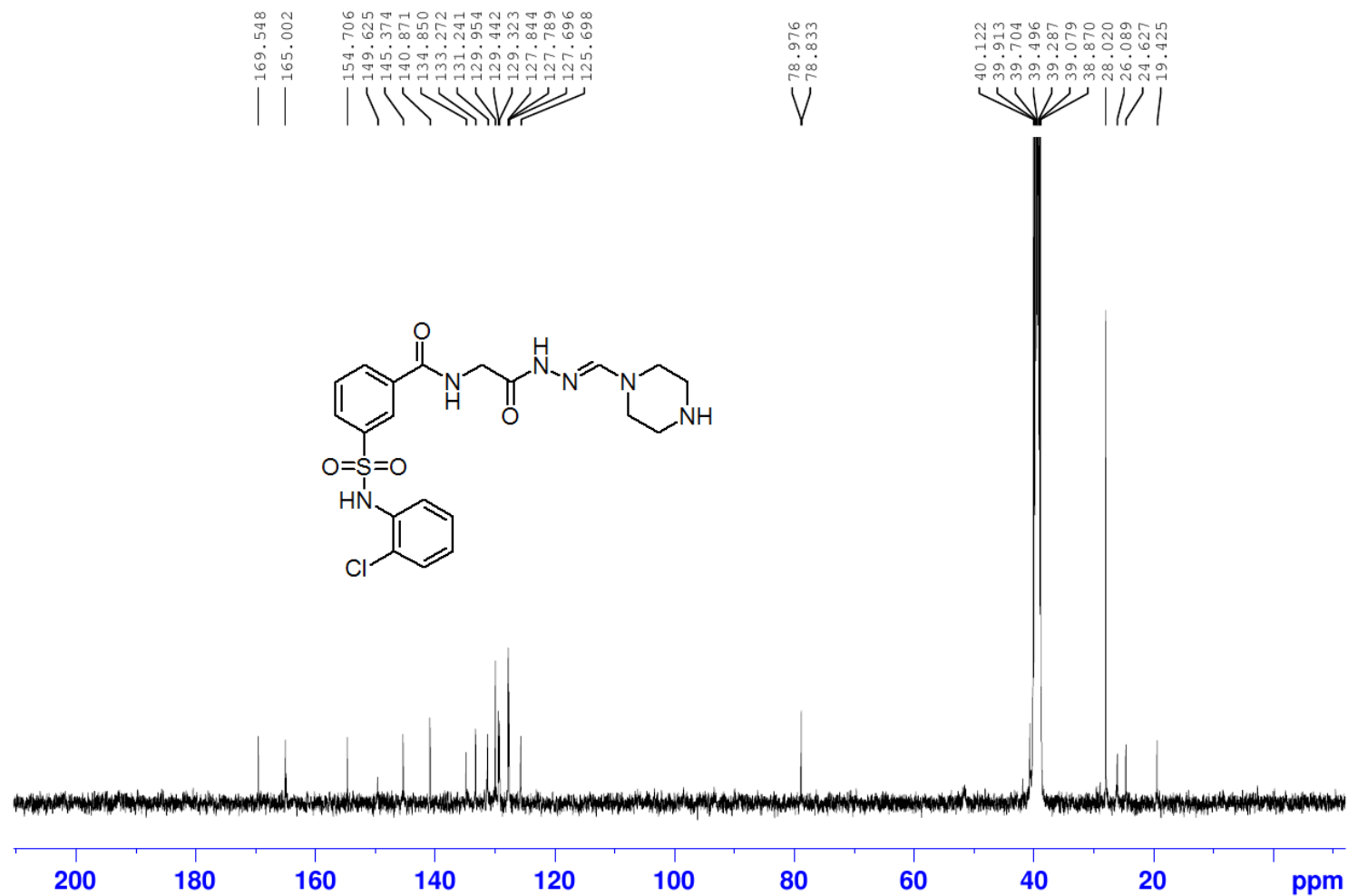
1: TOF MS ES+
1.29e3



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



Current Data Parameters
NAME 511611C7426
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161201
Time 3.01
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 298.8 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 100.6128192 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL5-NMR-001

¹³CNMR of Compound-1v in DMSO-*d*₆

Elemental Composition Report

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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)

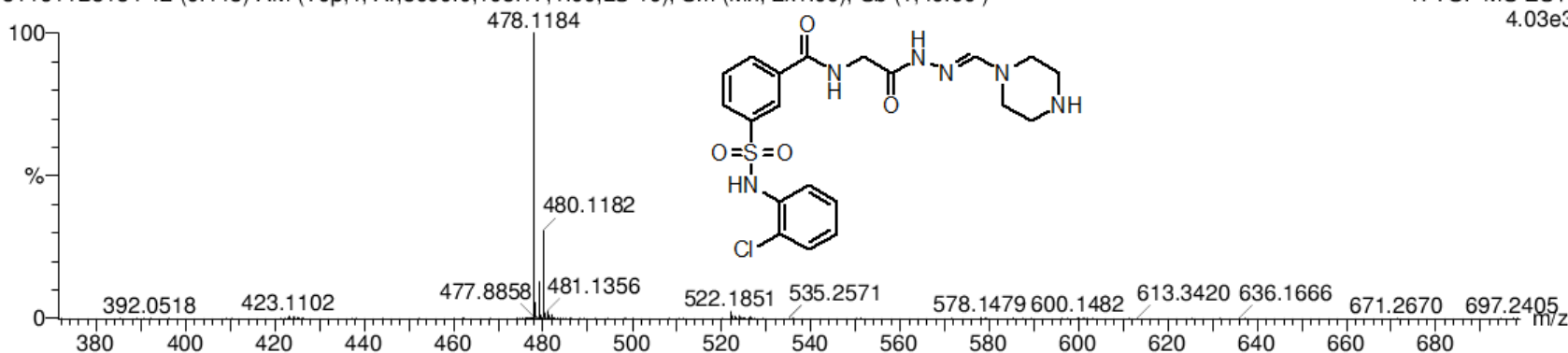
Elements Used:

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

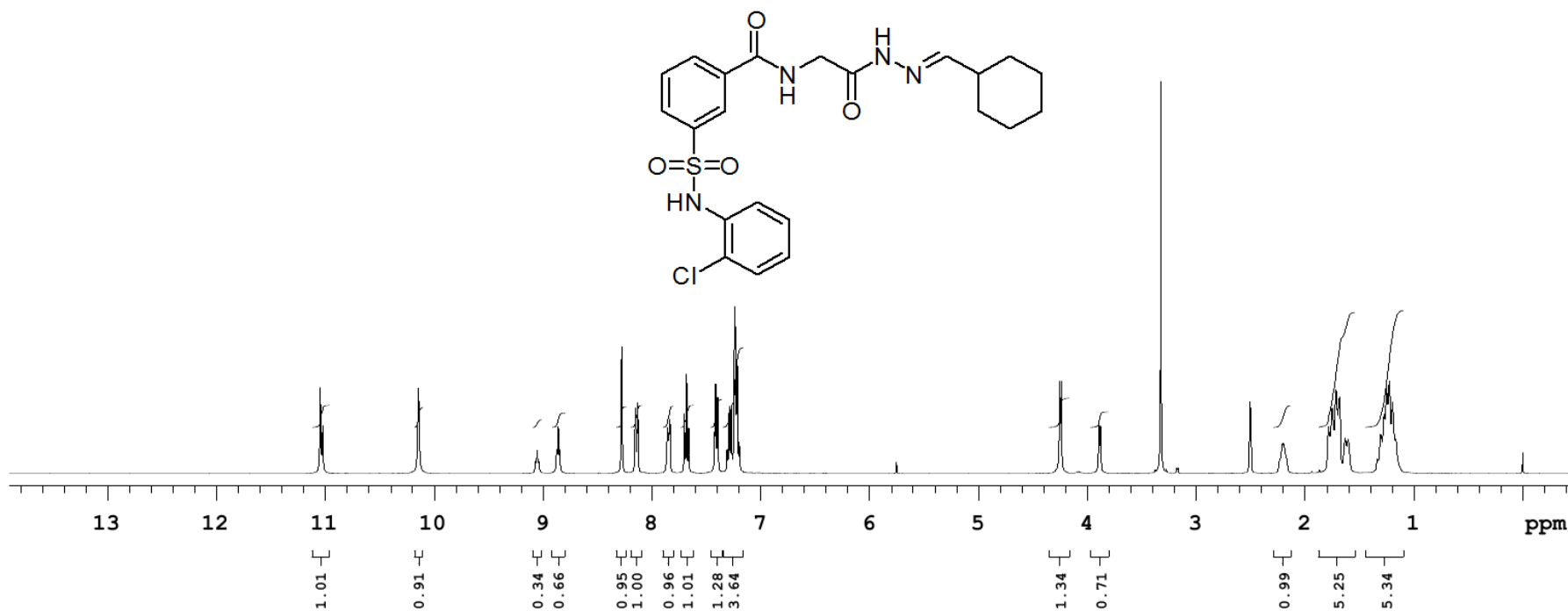


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

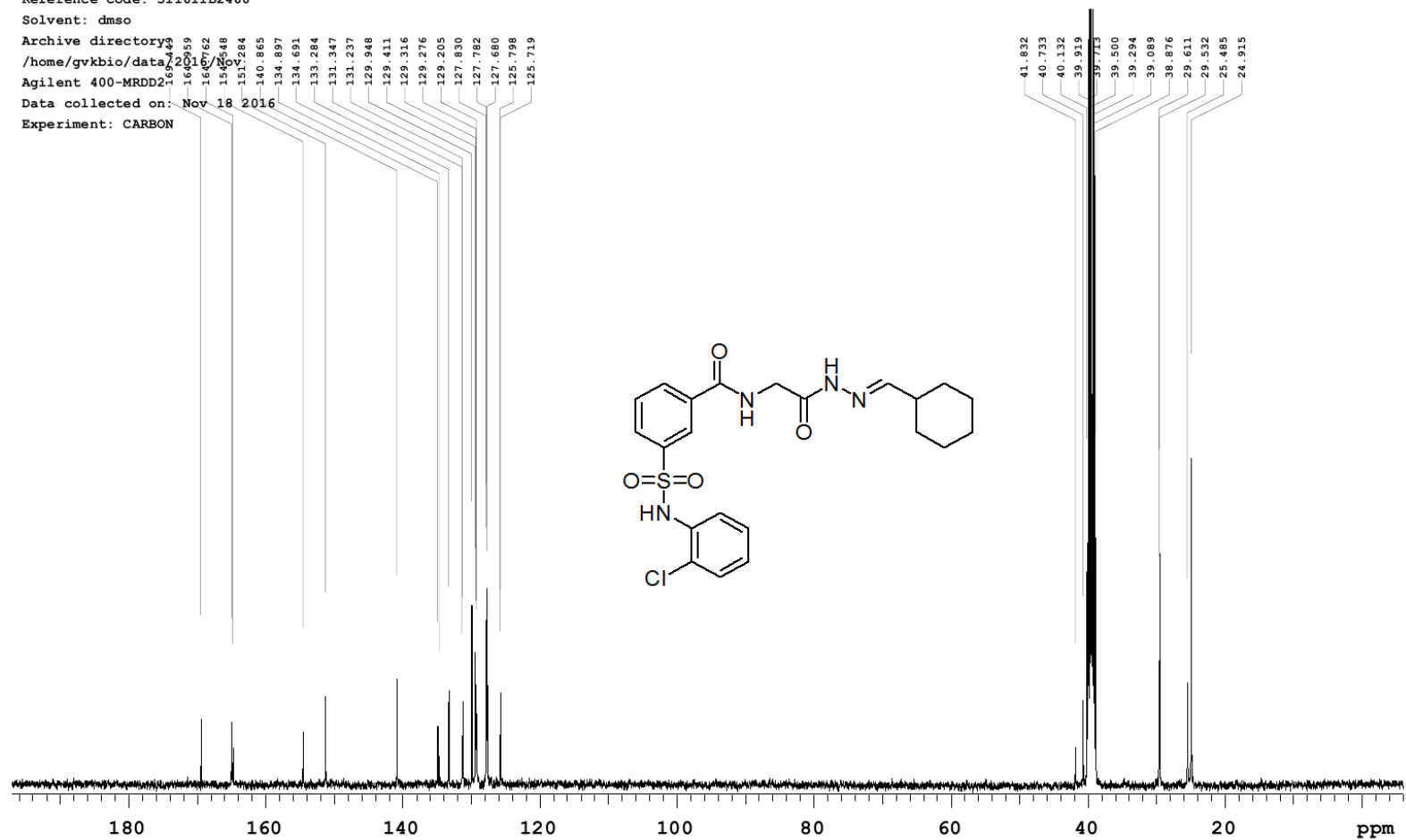
HRMS of Compound-1v

GVB-SA14
Reference Code: 511611B2466
Solvent: dms
Archive directory:
/home/gvkbio/data/2016/Nov
Agilent 400-MRDD2
Data collected on: Nov 18 2016
Experiment: PROTON



¹H NMR of **Compound-1w** in DMSO-d₆

GVB-SA14
 Reference Code: 511611B2466
 Solvent: dmsd
 Archive directory:
 /home/gvkbio/data/2016/Nov
 Agilent 400-MRDD2
 Data collected on: Nov 18 2016
 Experiment: CARBON



^{13}C NMR of **Compound-1w** in $\text{DMSO-}d_6$

Elemental Composition Report

Page 1

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)

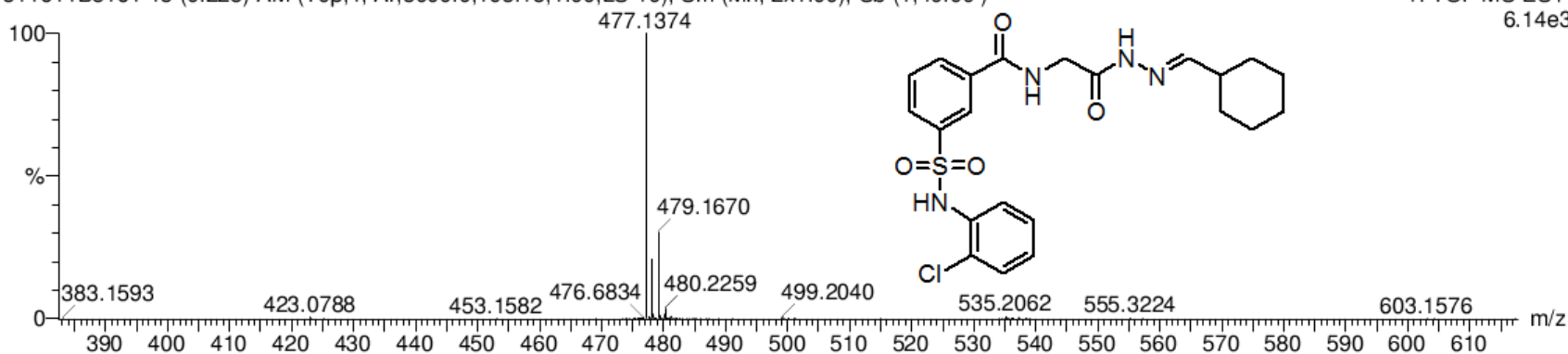
Elements Used:

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

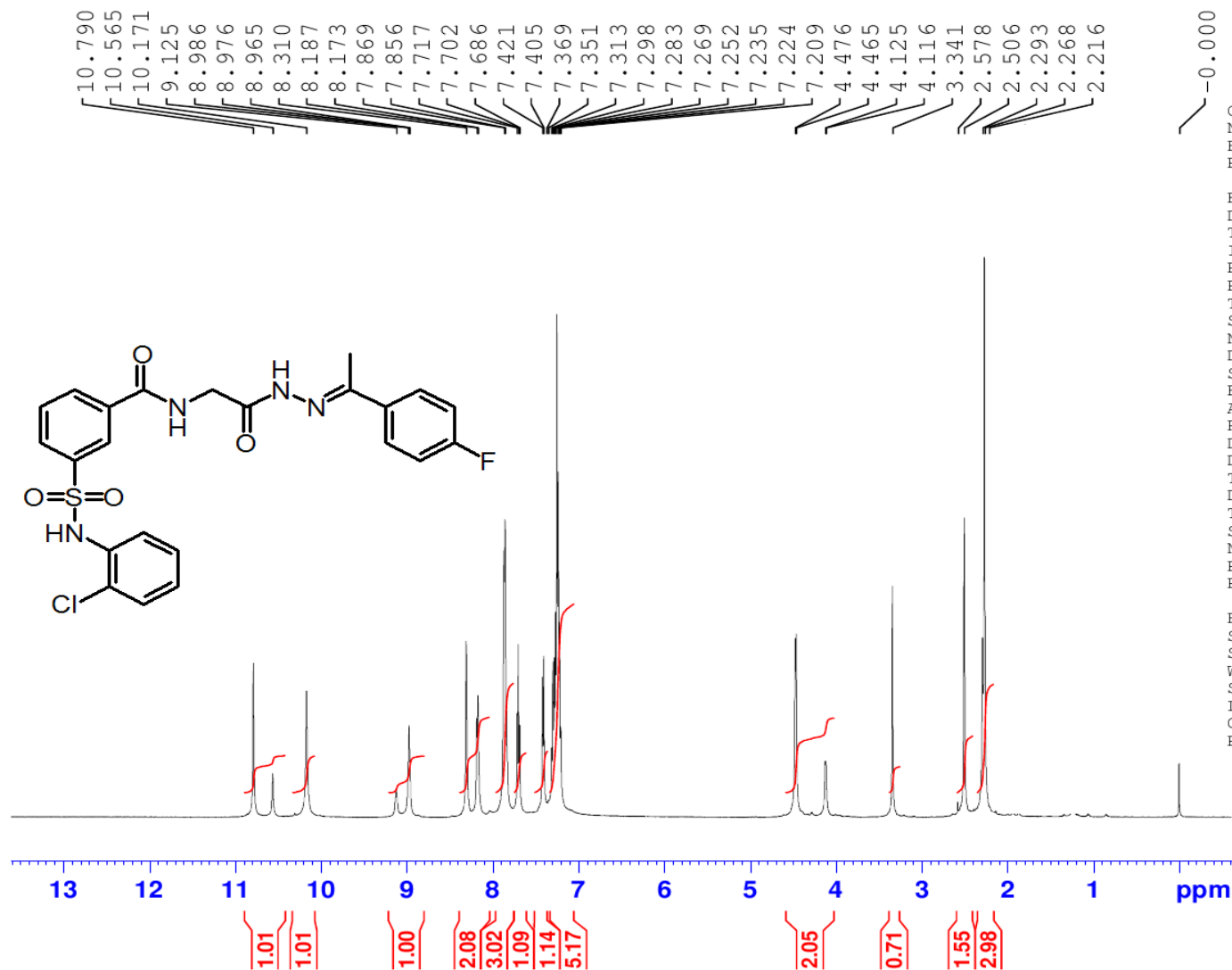


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SK-31



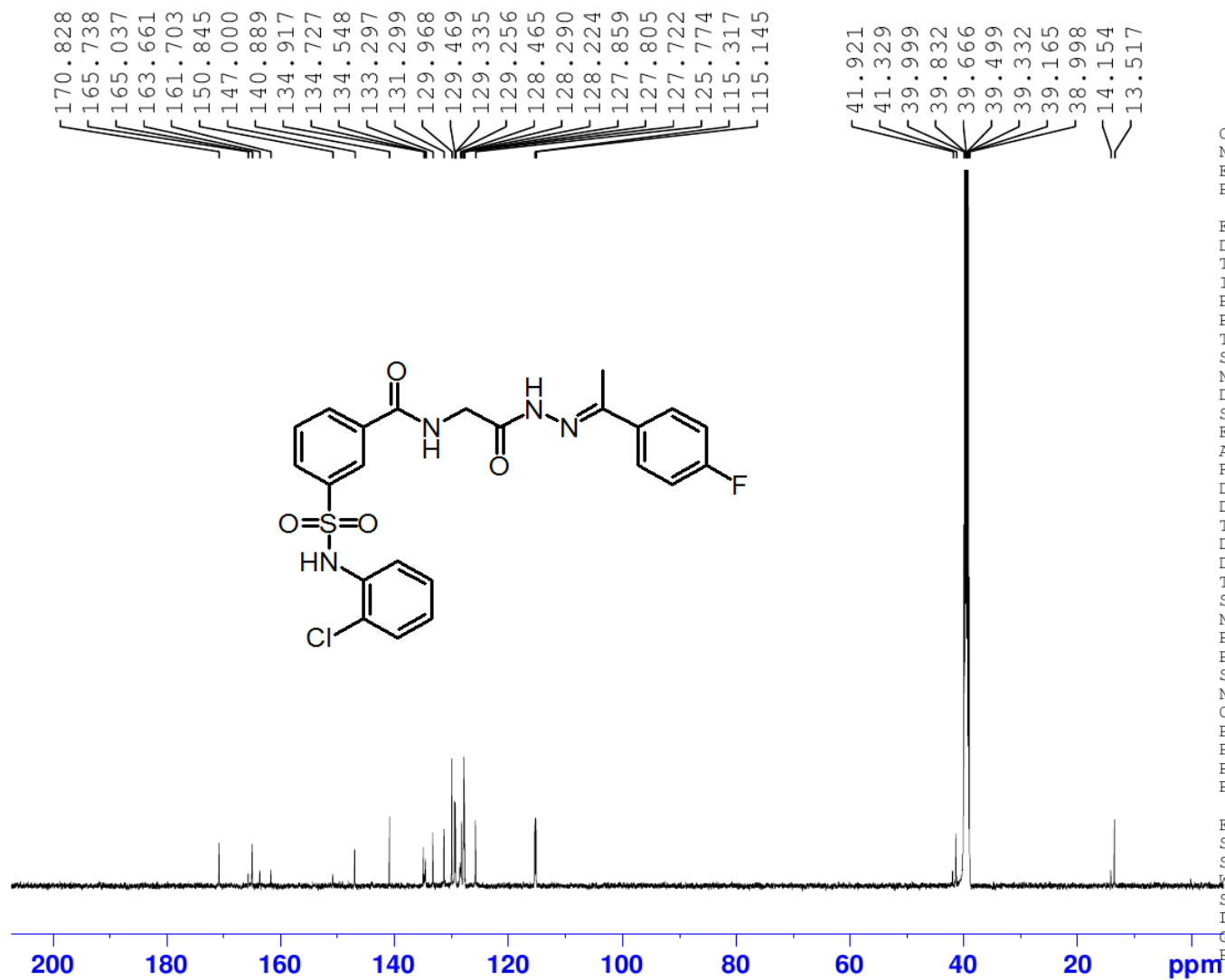
Current Data Parameters
 NAME 511612B0598
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170103
 Time 20.54 h
 INSTRUM spect
 PROBHD Z119470_0231
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 89.27
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 23.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300011 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of Compound-2a in DMSO-d₆

GVB-SK-31



Current Data Parameters
 NAME 511612B0598
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170104
 Time 1.16 h
 INSTRUM spect
 PROBHD z119470_0231 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 197.72
 DW 16.800 usec
 DE 6.50 usec
 TE 298.5 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 88.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 23.00000000 W
 PLW12 0.27515000 W
 PLW13 0.13840000 W

F2 - Processing parameters
 SI 32768
 SF 125.7578505 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

¹³CNMR of Compound-2a in DMSO-d₆

Elemental Composition Report

Page 1

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)

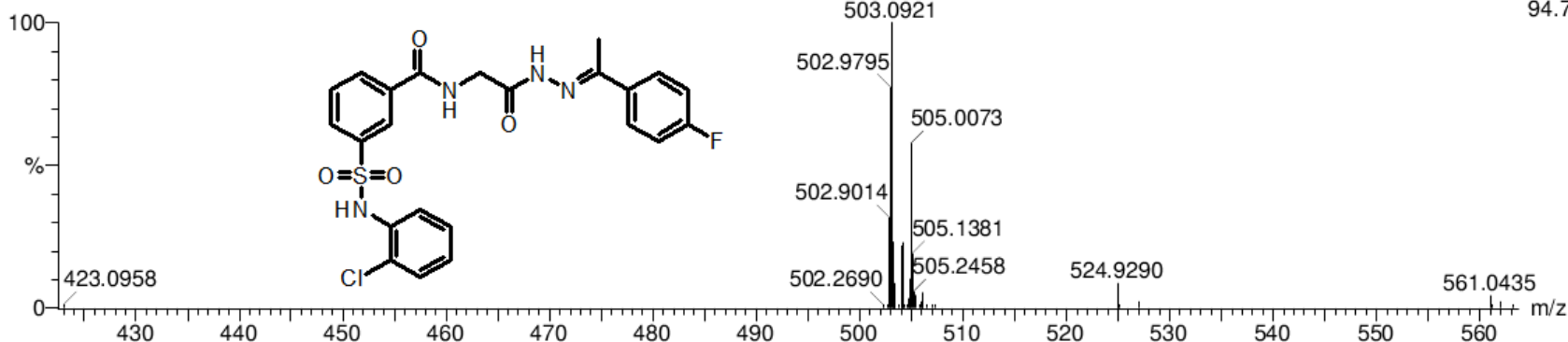
Elements Used:

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

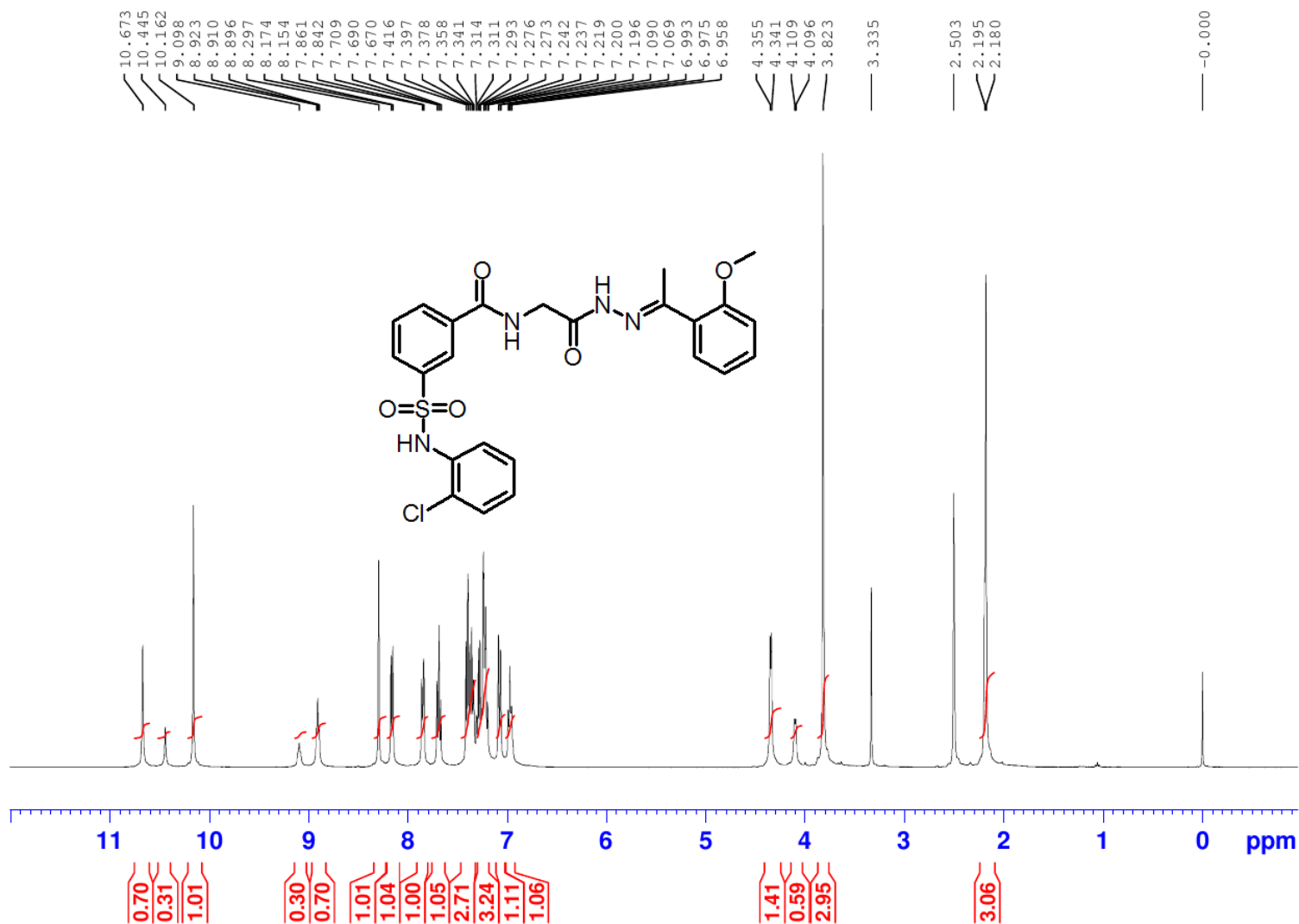


Minimum: -1.5

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



Current Data Parameters
NAME 511612B0599
EXPNO 1
PROCNO 1

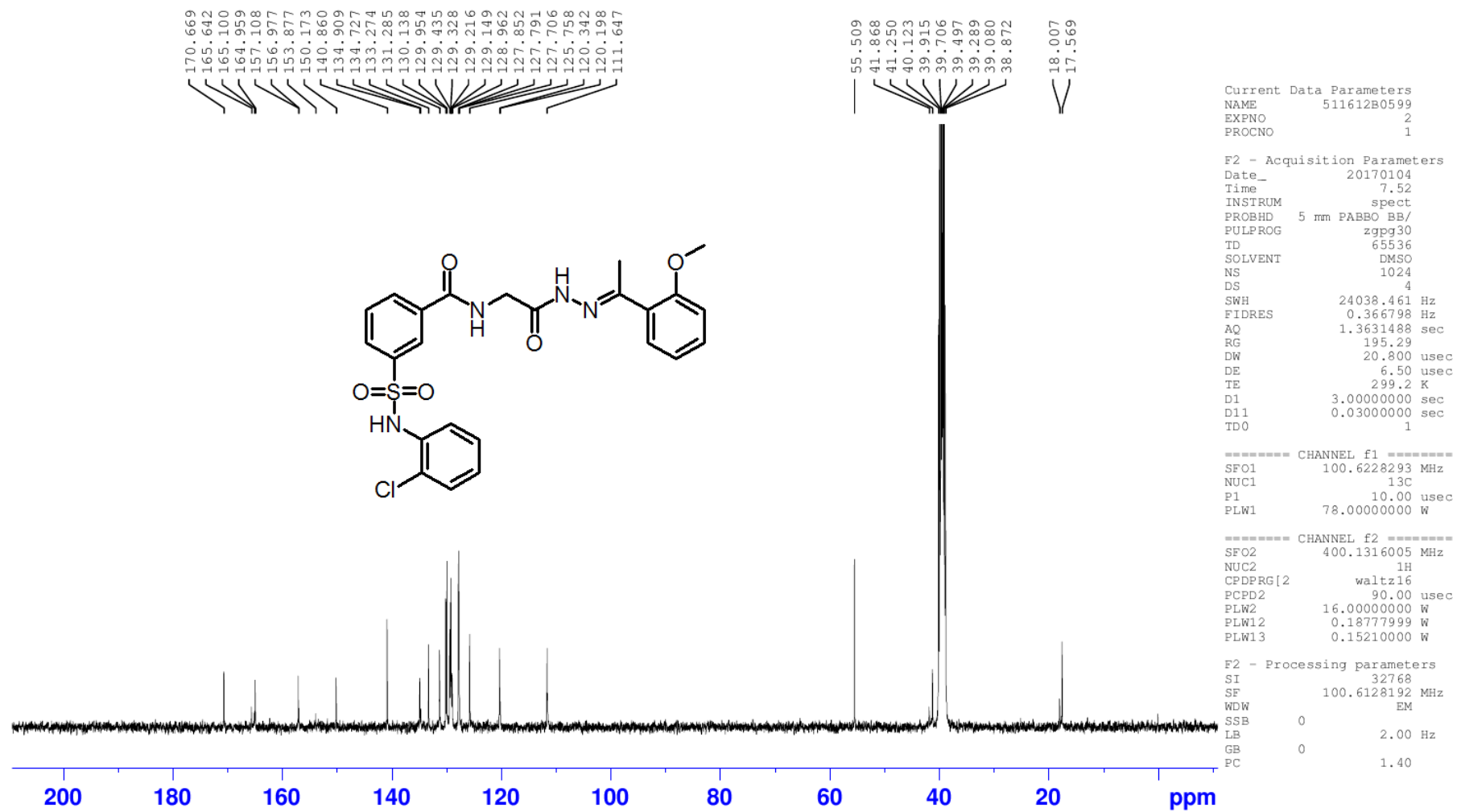
F2 - Acquisition Parameters
Date_ 20170103
Time 21.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 86.08
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300015 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL5-NMR-001

¹H NMR of **Compound-2b** in DMSO-d₆



ANL-MCL5-NMR-001

¹³CNMR of **Compound-2b** in DMSO-d₆

Elemental Composition Report

Page 1

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

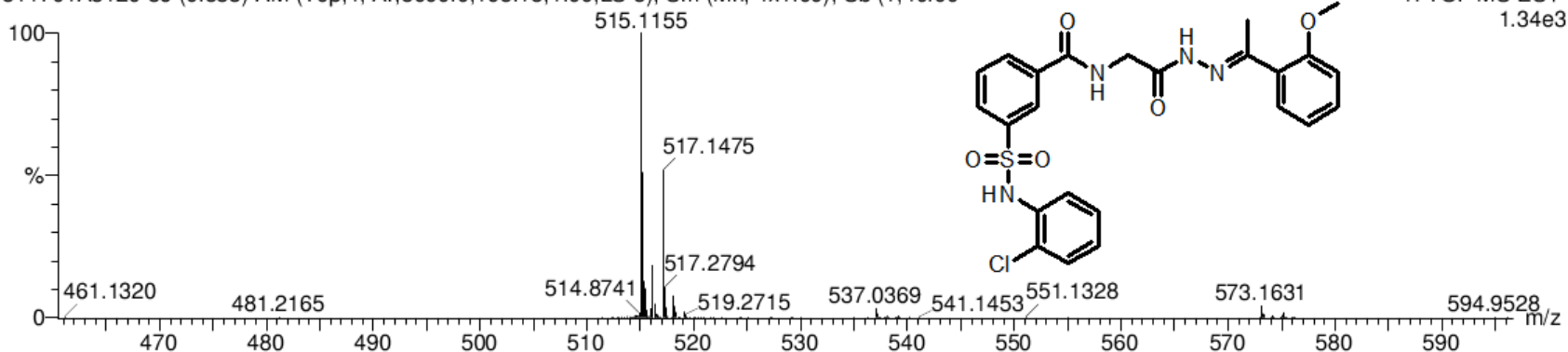
199 formula(e) evaluated with 69 results within limits (up to 1 closest results for each mass)

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

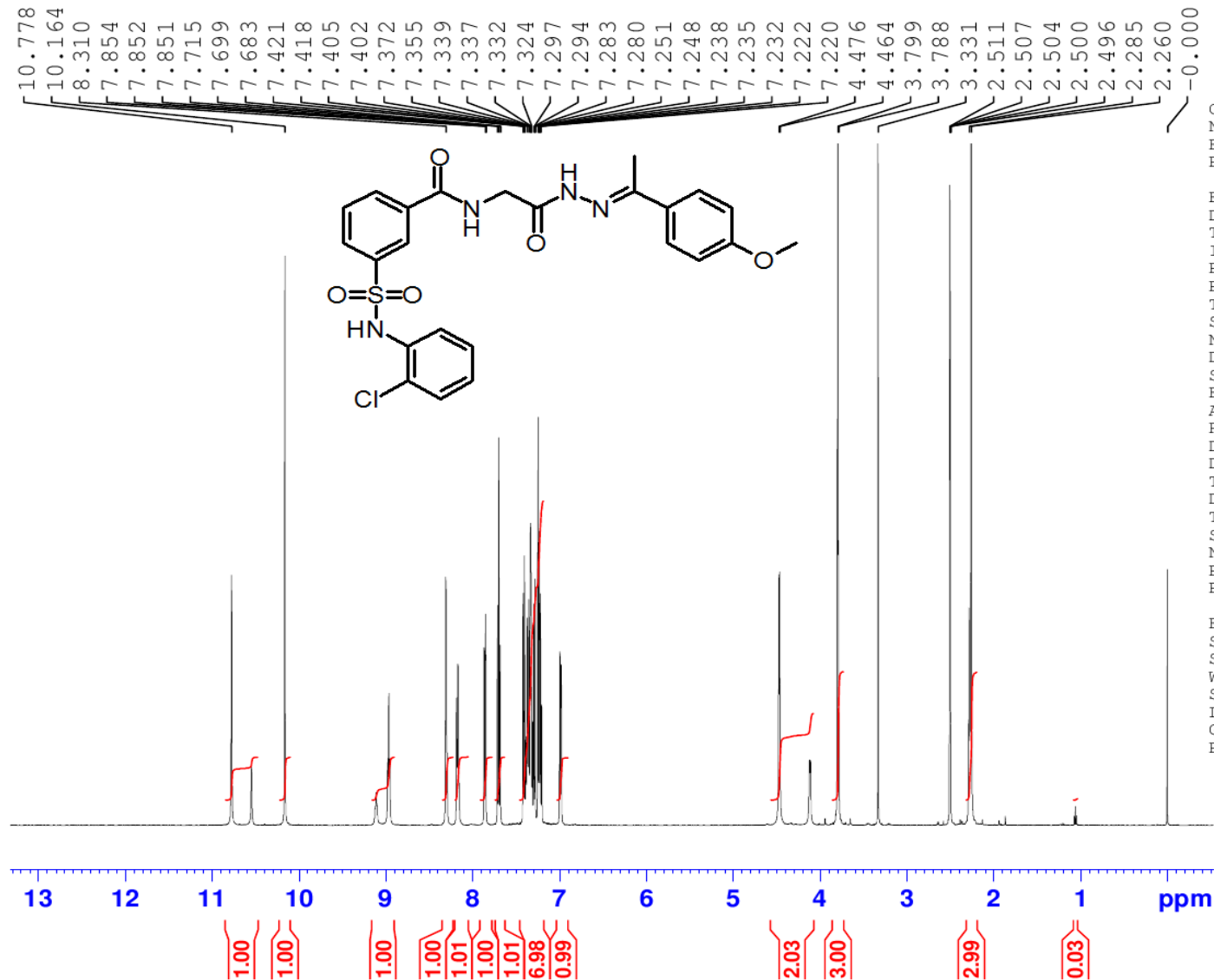
511701A5129 36 (0.533) AM (Top,4, Ar,5000.0,195.18,1.00,LS 5); Sm (Mn, 1x1.00); Sb (1,40.00)



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	C ₂₄ H ₂₄ N ₄ O ₅ S Cl

HRMS of Compound-2b



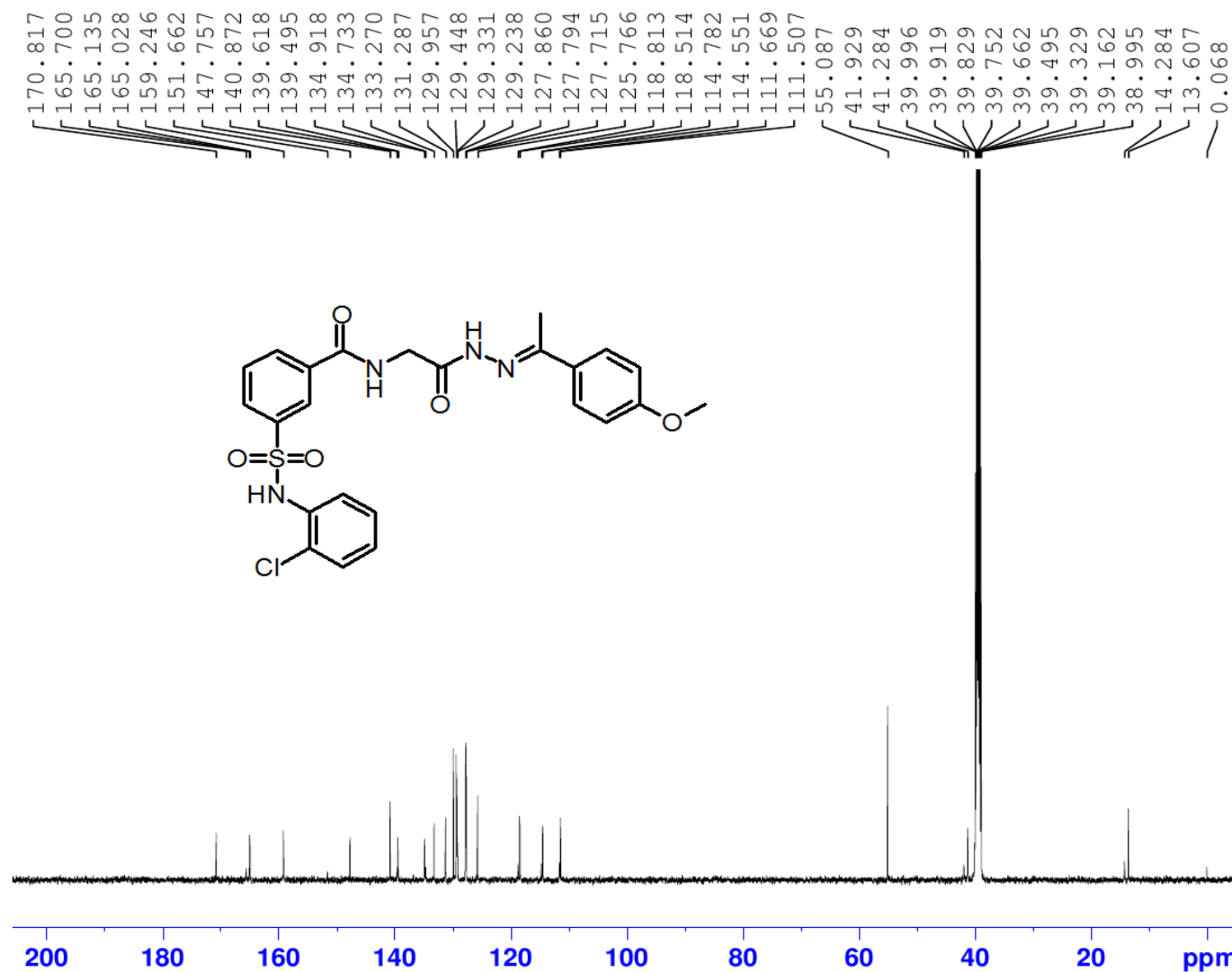
Current Data Parameters
 NAME 511612B0600
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170104
 Time 8.14 h
 INSTRUM spect
 PROBHD Z119470_0231 (zg30)
 PULPROG 65536
 TD 8
 SOLVENT DMSO
 NS 0
 DS 10000.000 Hz
 SWH 0.305176 Hz
 FIDRES 3.2767999 sec
 AQ 97.81
 RG 50.000 usec
 DW 6.50 usec
 DE 298.9 K
 TE 1.00000000 sec
 D1 1
 TD0 500.1330885 MHz
 SFO1 1H
 NUC1 8.75 usec
 P1 23.00000000 W
 PLW1

F2 - Processing parameters
 SI 65536
 SF 500.1300024 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of Compound-2c in DMSO-d₆

GVB-SK-33



Current Data Parameters
NAME 511612B0600
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170104
Time 8.00 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.4 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W

F2 - Processing parameters
SI 32768
SF 125.7578522 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

¹³CNMR of Compound-2c in DMSO-d₆

Elemental Composition Report

Page 1

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)

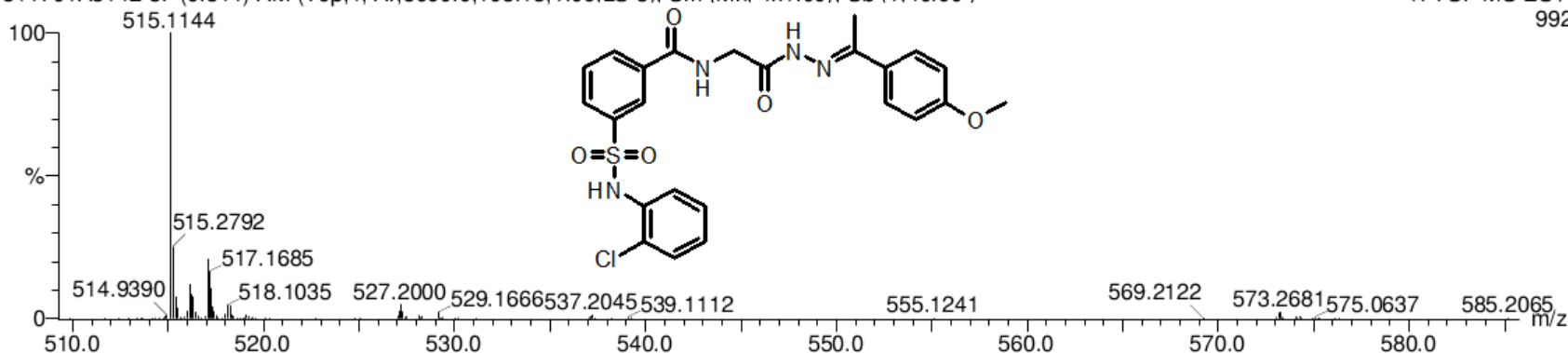
Elements Used:

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)

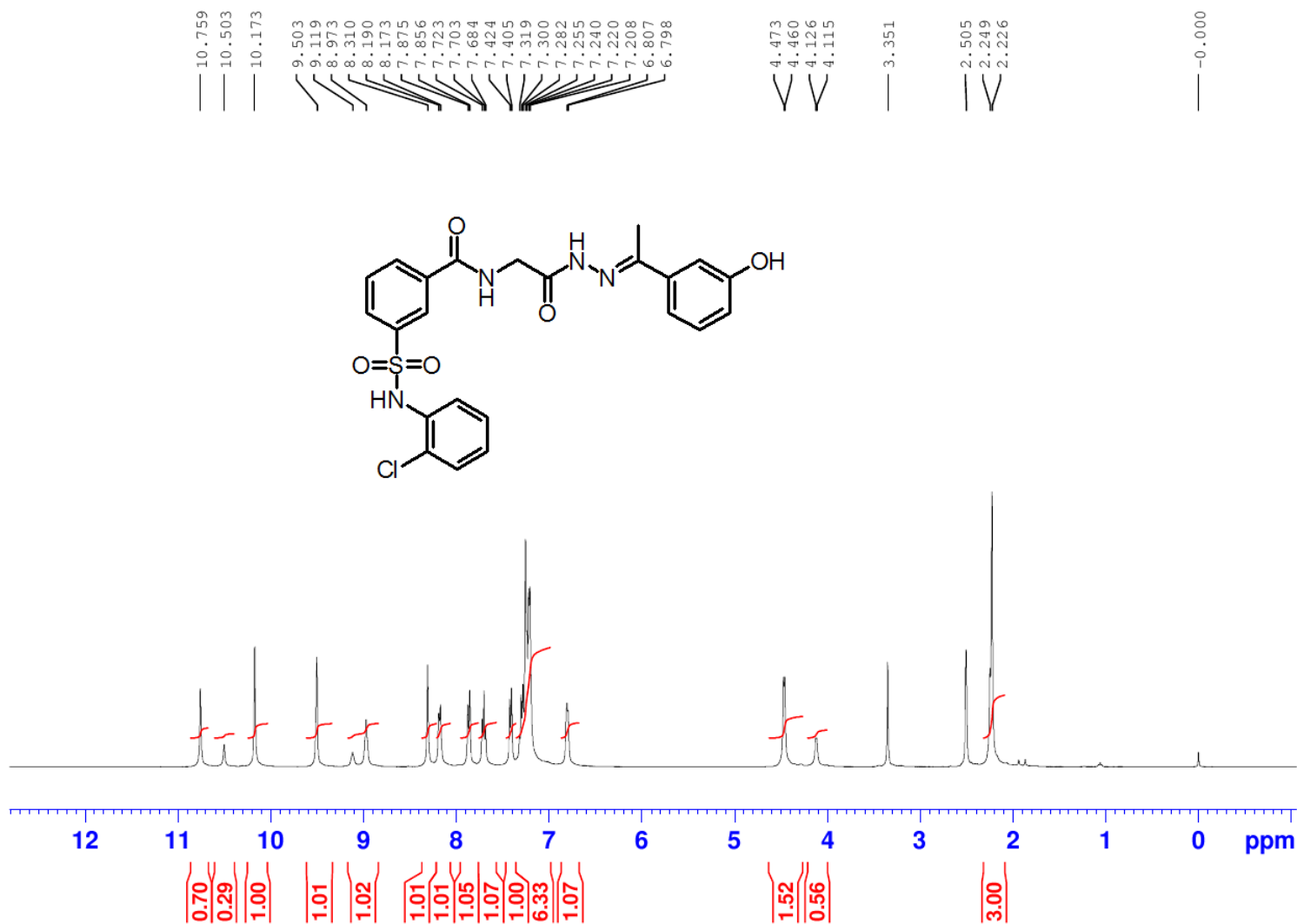
1: TOF MS ES+
992



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	C ₂₄ H ₂₄ N ₄ O ₅ S Cl

HRMS of Compound-2c



Current Data Parameters
 NAME 511612B0603
 EXPNO 1
 PROCNO 1

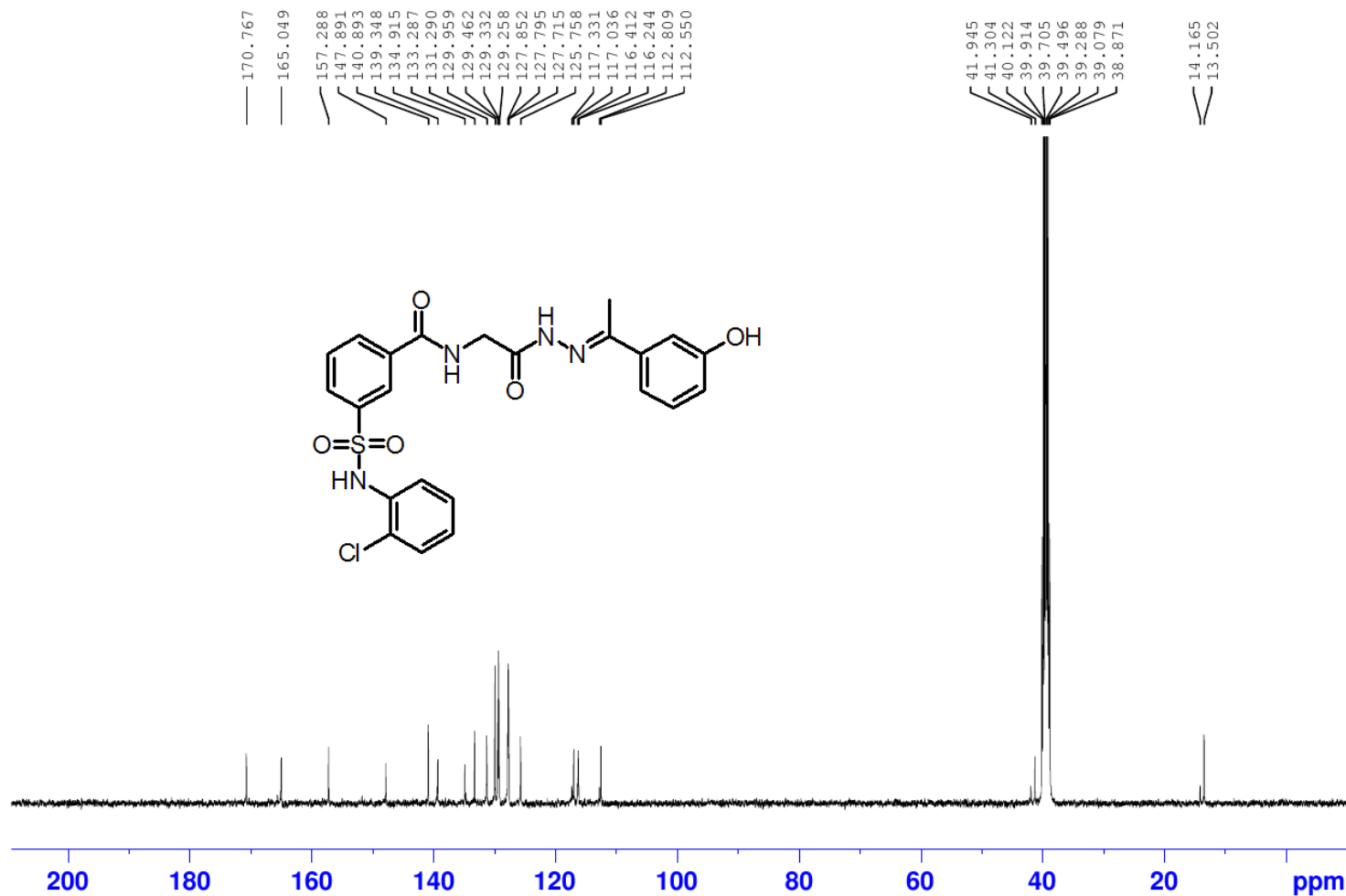
F2 - Acquisition Parameters
 Date_ 20170104
 Time 21.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 86.08
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== 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

ANL-MCL5-NMR-001

¹H NMR of **Compound-2d** in DMSO-d₆



Current Data Parameters
NAME 511612B0603
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170105
Time 3.32
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 300.2 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 100.6128192 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

ANL-MCL5-NMR-001

¹³CNMR of **Compound-2d** in DMSO-d₆

Elemental Composition Report

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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)

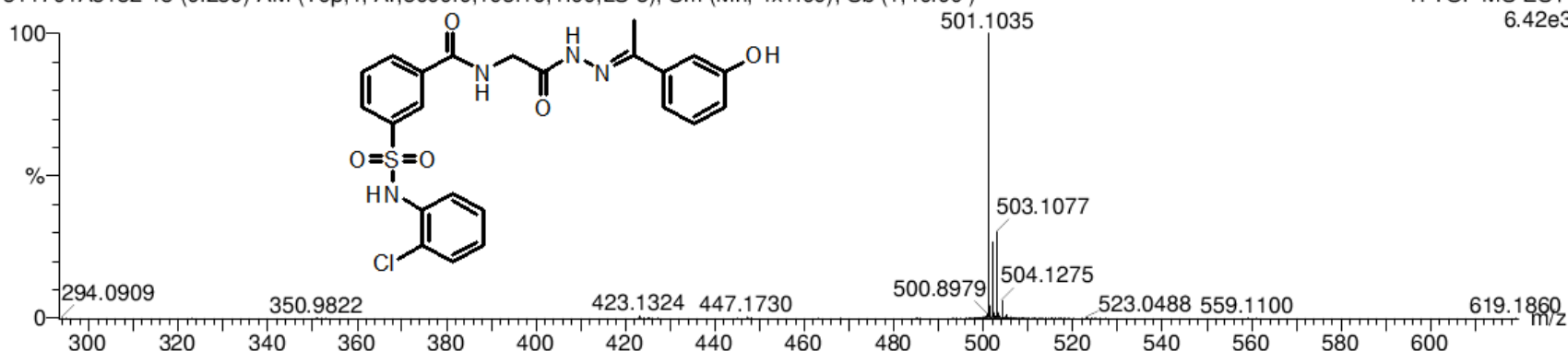
Elements Used:

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

Page 1

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)

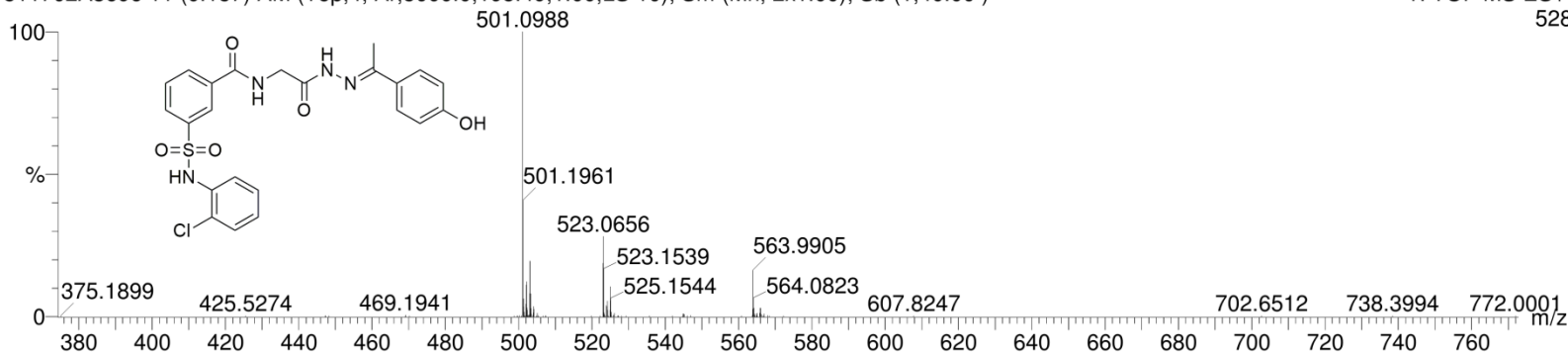
Elements Used:

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)

1: TOF MS ES+
528

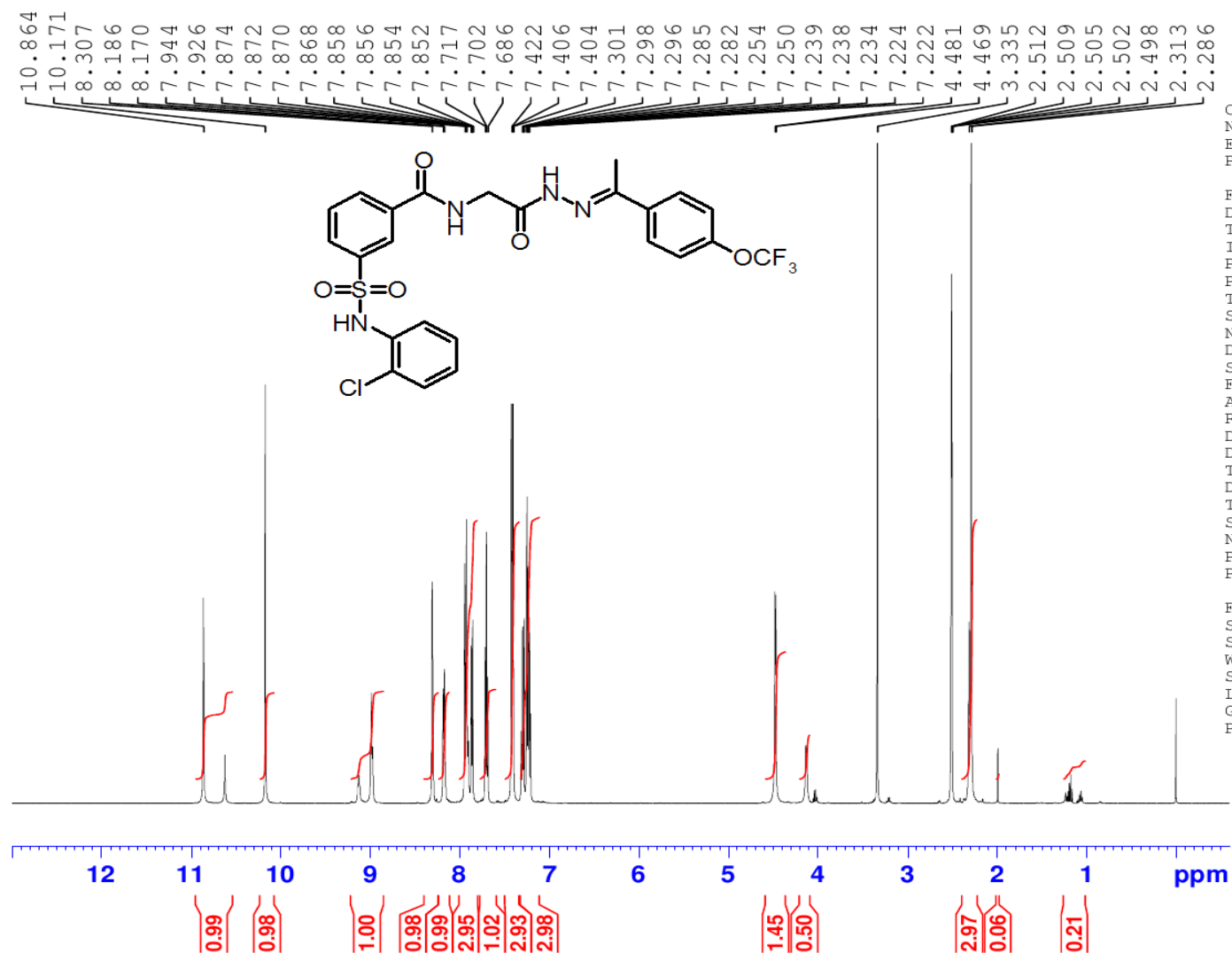


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SK-45



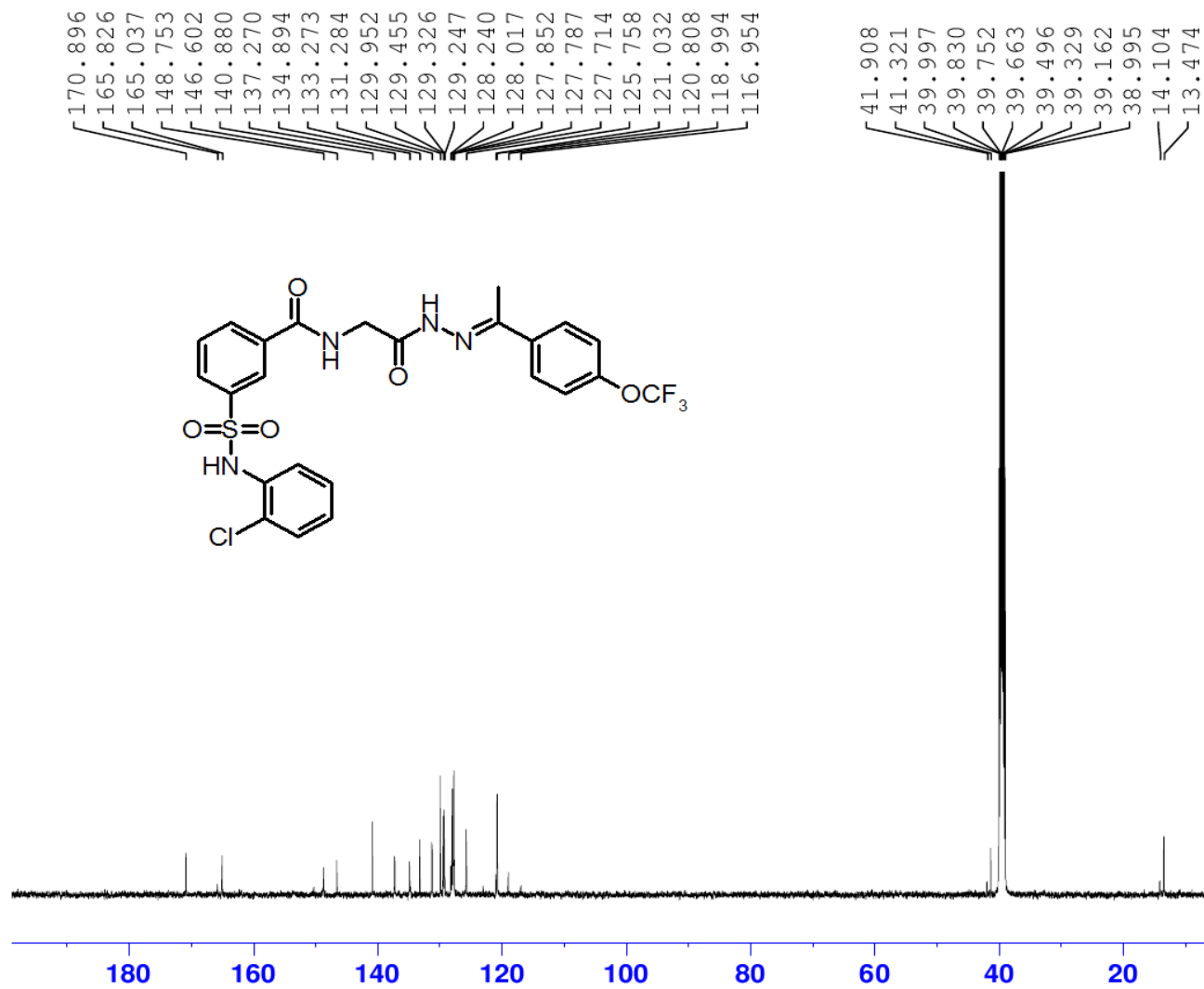
Current Data Parameters
NAME 511612B0612
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170105
Time 20.51 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 111.07
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300014 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of **Compound-2f** in DMSO-d₆

GVB-SK-45



Current Data Parameters
 NAME 511612B0612
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170106
 Time 1.36 h
 INSTRUM spect
 PROBHD z119470_0231 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 197.72
 DW 16.800 usec
 DE 6.50 usec
 TE 299.9 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 88.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 23.00000000 W
 PLW12 0.27515000 W
 PLW13 0.13840000 W

F2 - Processing parameters
 SI 32768
 SF 125.7578523 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

¹³CNMR of Compound-2f in DMSO-d₆

Elemental Composition Report

Page 1

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

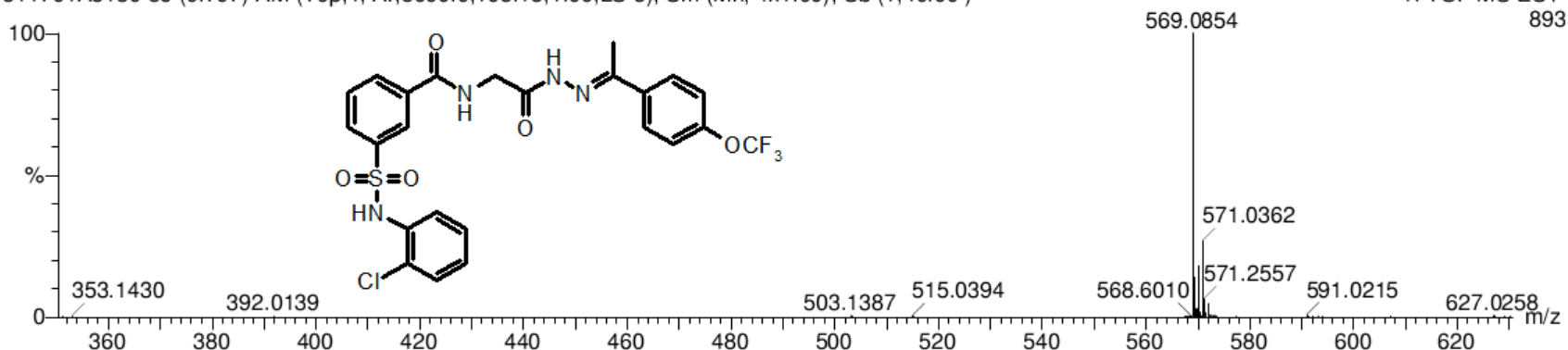
469 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

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)

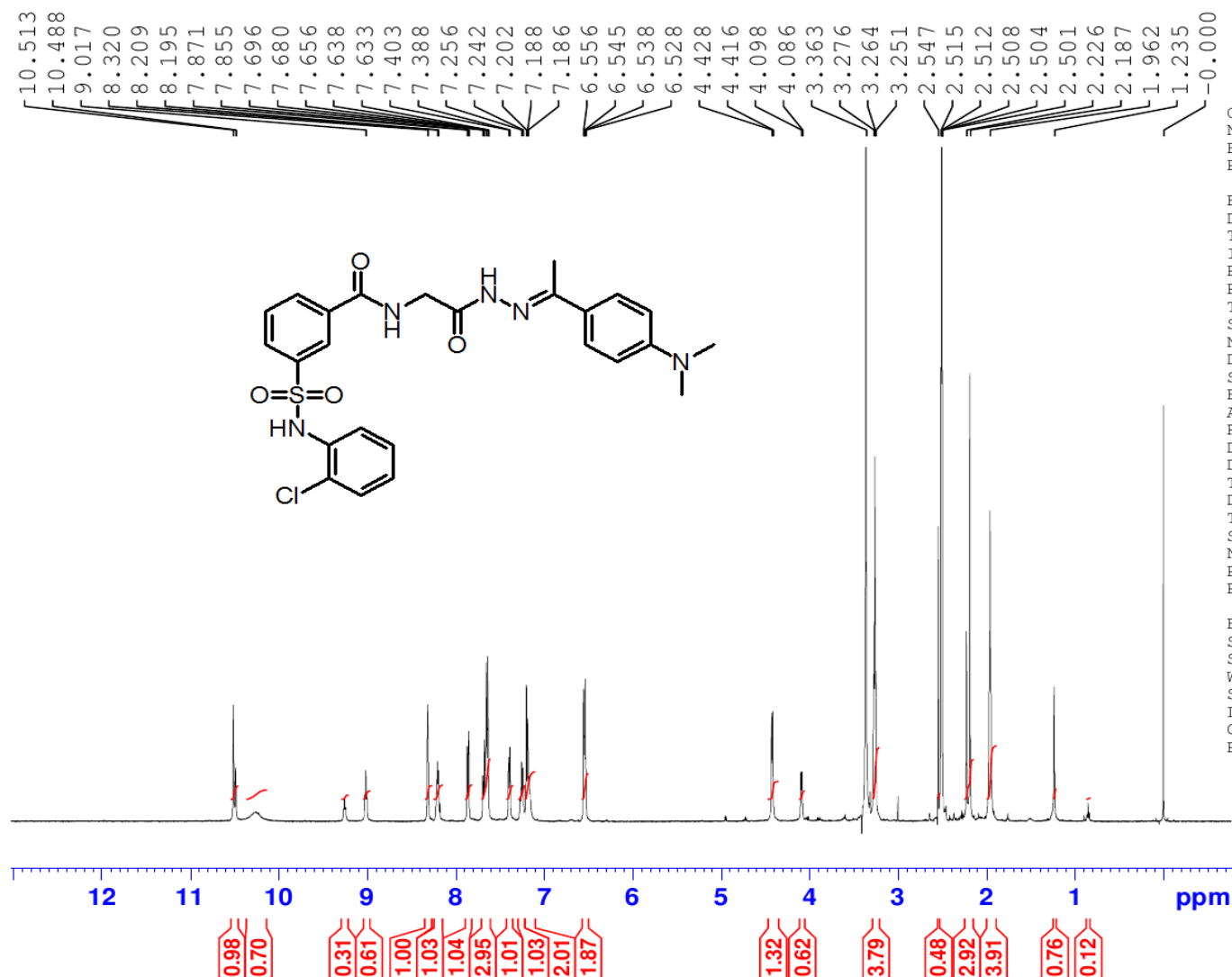


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
569.0854	569.0873	-1.9	-3.3	14.5	38.7	C ₂₄ H ₂₁ N ₄ O ₅ S Cl F ₃

HRMS of Compound-2f

GVB-SK37-01



Current Data Parameters
 NAME 511701C3022
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170126
 Time 22.49 h
 INSTRUM spect
 PROBHD z119470_0231 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 157.05
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 23.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300004 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of Compound-2g in DMSO-d₆

GVB-SK37-01



Current Data Parameters
 NAME 511701C3022
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170127
 Time 0.02 h
 INSTRUM spect
 PROBHD Z119470_0231 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 197.72
 DW 16.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 88.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 23.00000000 W
 PLW12 0.27515000 W
 PLW13 0.13840000 W

F2 - Processing parameters
 SI 32768
 SF 125.7578501 MHz
 WDW EM
 SSB 0
 LB No filename specified
 GB 0
 PC 1.40

¹³CNMR of Compound-2g in DMSO-d₆

Elemental Composition Report

Page 1

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)

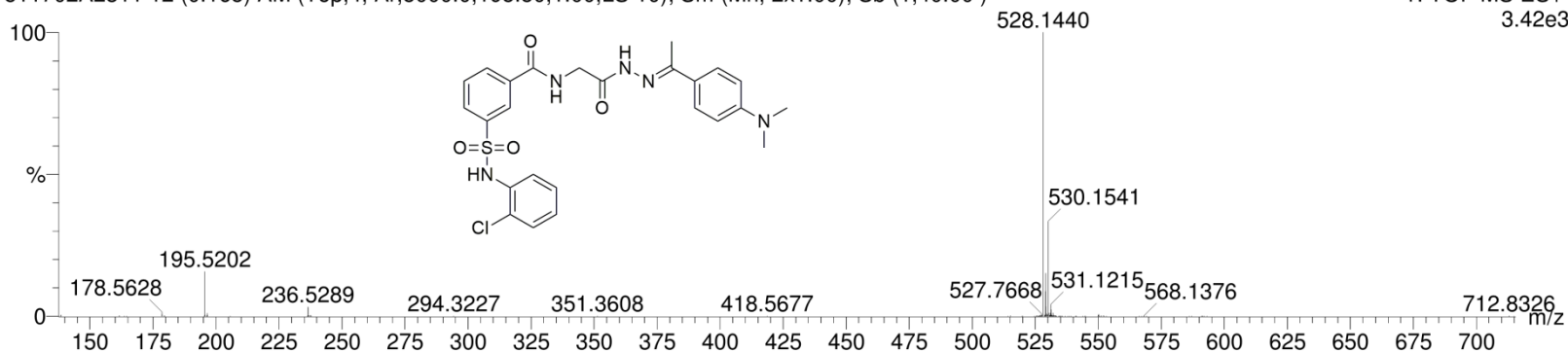
Elements Used:

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)

1: TOF MS ES+
3.42e3

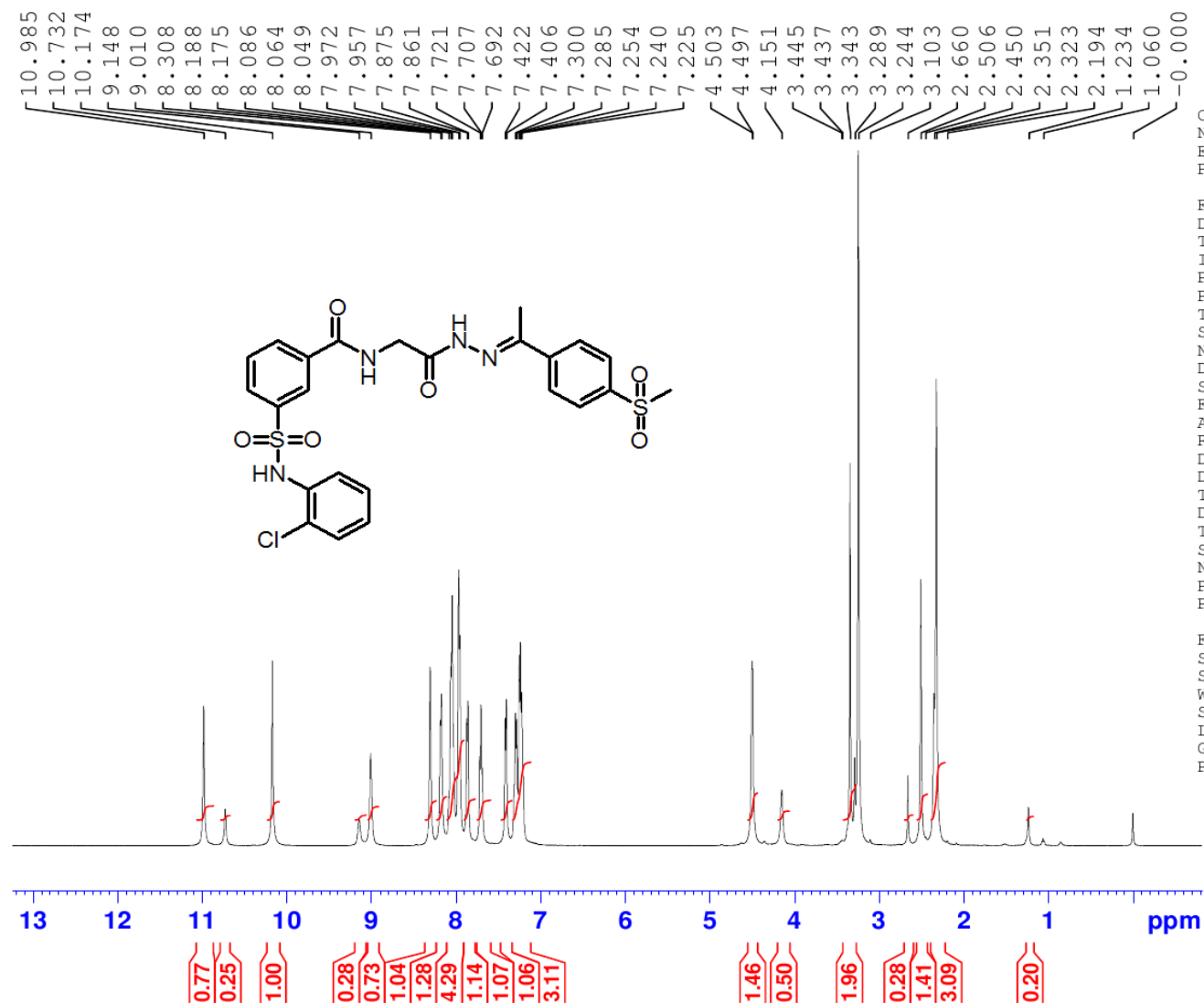


Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SK39-01



Current Data Parameters
 NAME 511701C3029
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170127
 Time 1.21 h
 INSTRUM spect
 PROBHD Z119470_0231 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 89.27
 DW 50.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 23.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300016 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of **Compound-2h** in DMSO-d₆

GVB-SK39-01



Current Data Parameters
 NAME 511701C3029
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20170127
 Time 2.33 h
 INSTRUM spect
 PROBHD Z119470_0231 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 197.72
 DW 16.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 88.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 23.00000000 W
 PLW12 0.27515000 W
 PLW13 0.13840000 W

F2 - Processing parameters

SI 32768
 SF 125.7578503 MHz
 WDW EM
 SSB 0
 LB No filename specified
 GB 0
 PC 1.40

¹³CNMR of **Compound-2h** in DMSO-d₆

Elemental Composition Report

Page 1

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)

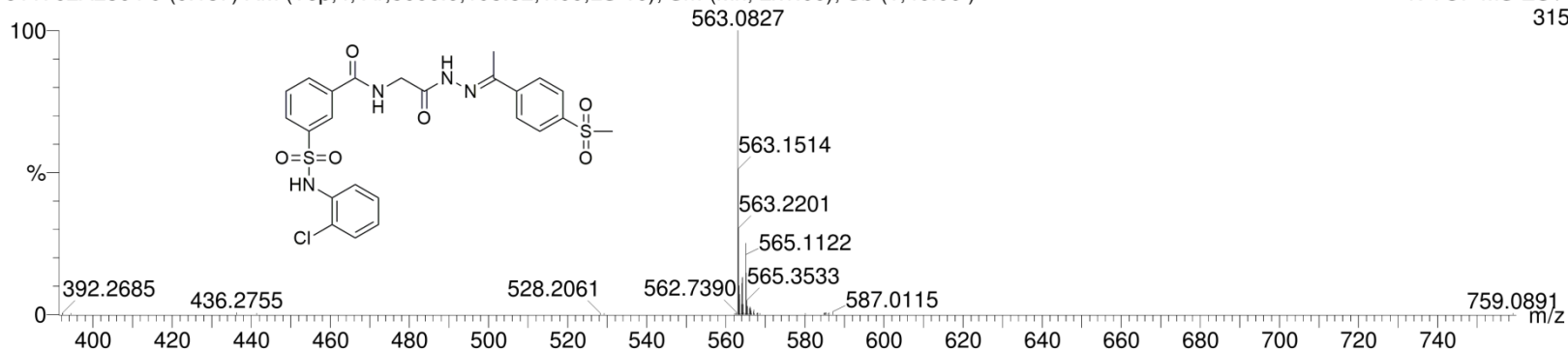
Elements Used:

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)

1: TOF MS ES+
315

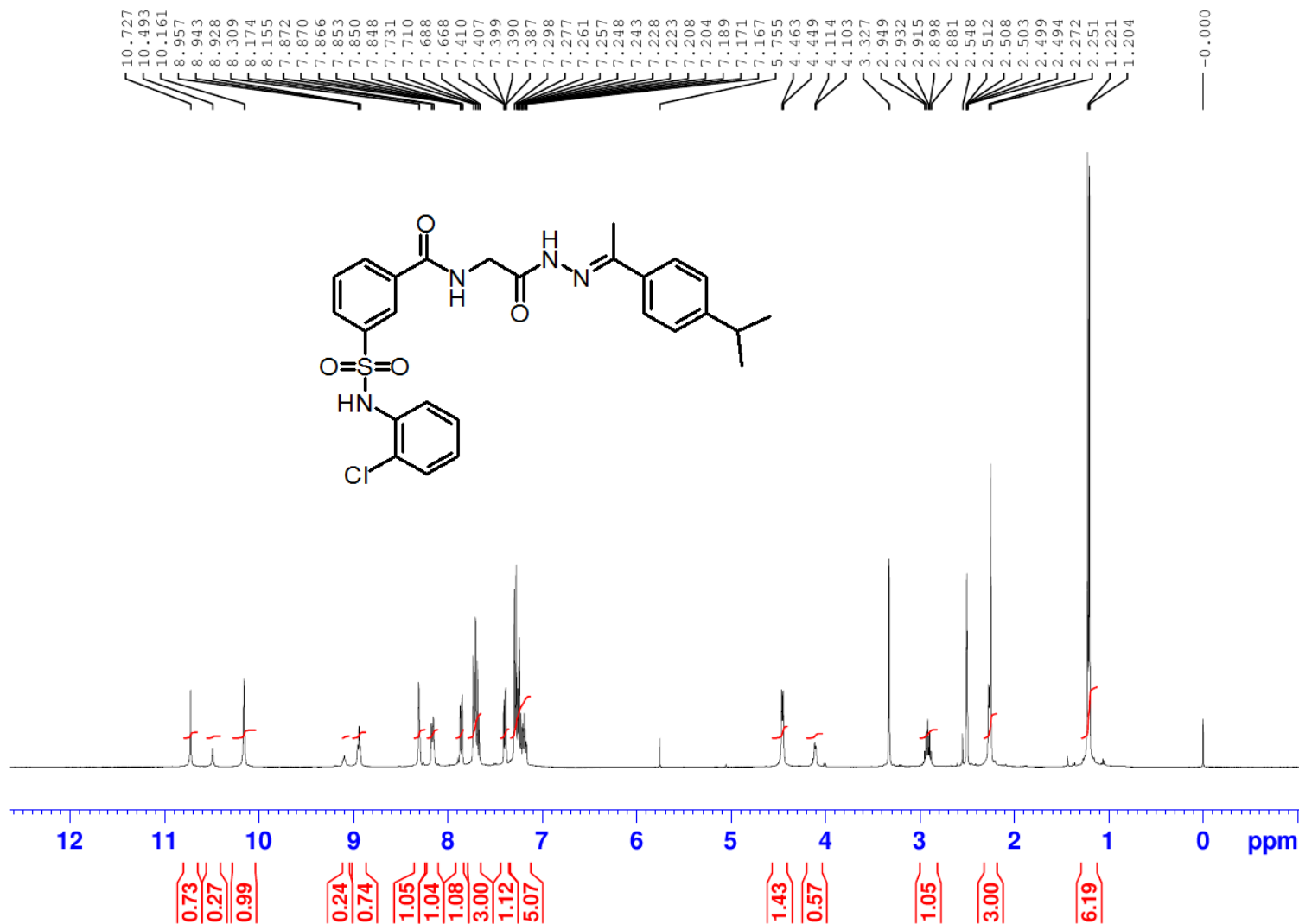


Minimum: -1.5

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



Current Data Parameters
NAME 511612B0610
EXPNO 1
PROCNO 1

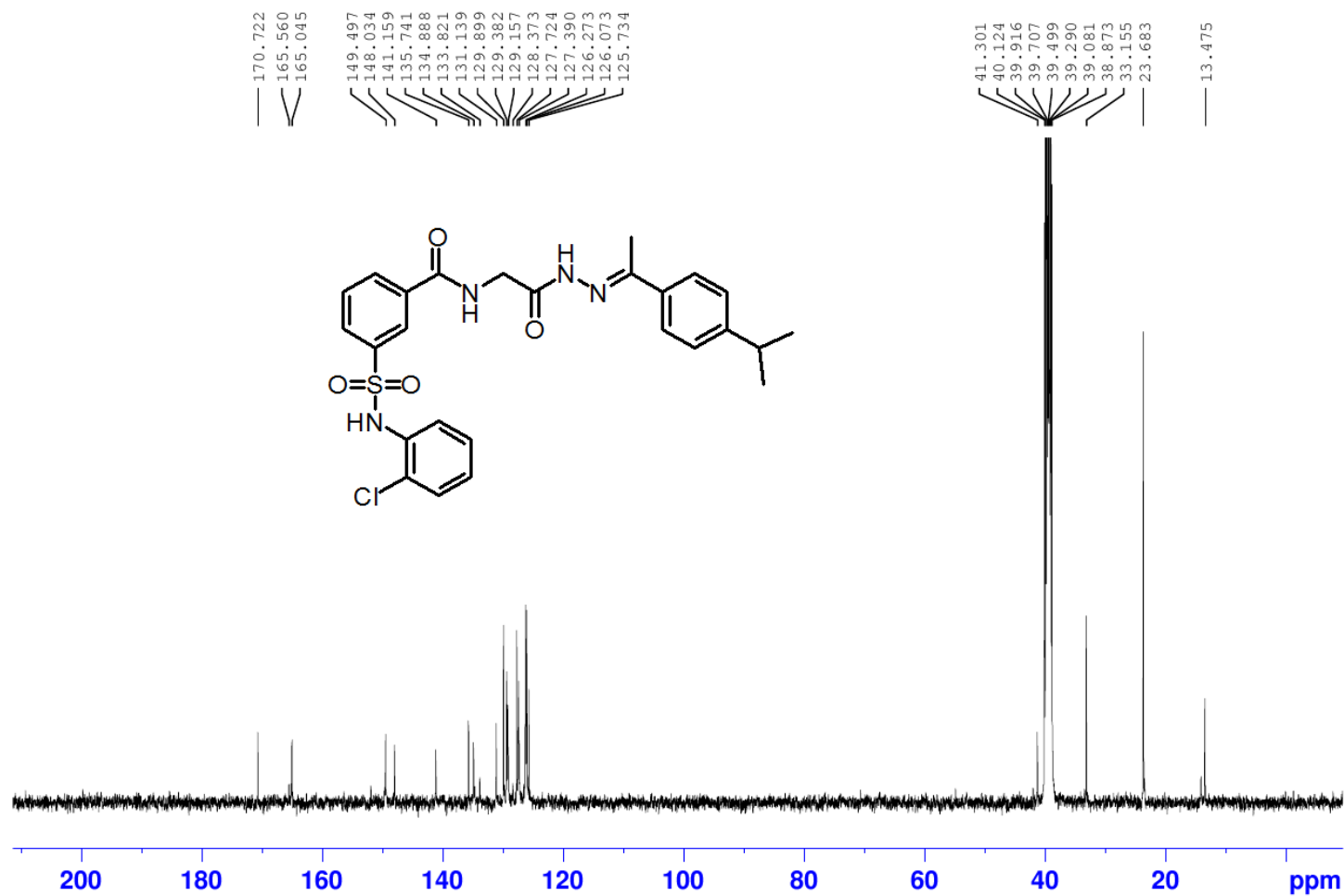
F2 - Acquisition Parameters
Date_ 20170105
Time 6.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 86.08
DW 62.400 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
TD0 1

===== 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

ANL-MCL5-NMR-001

¹H NMR of Compound-2i in DMSO-d₆



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

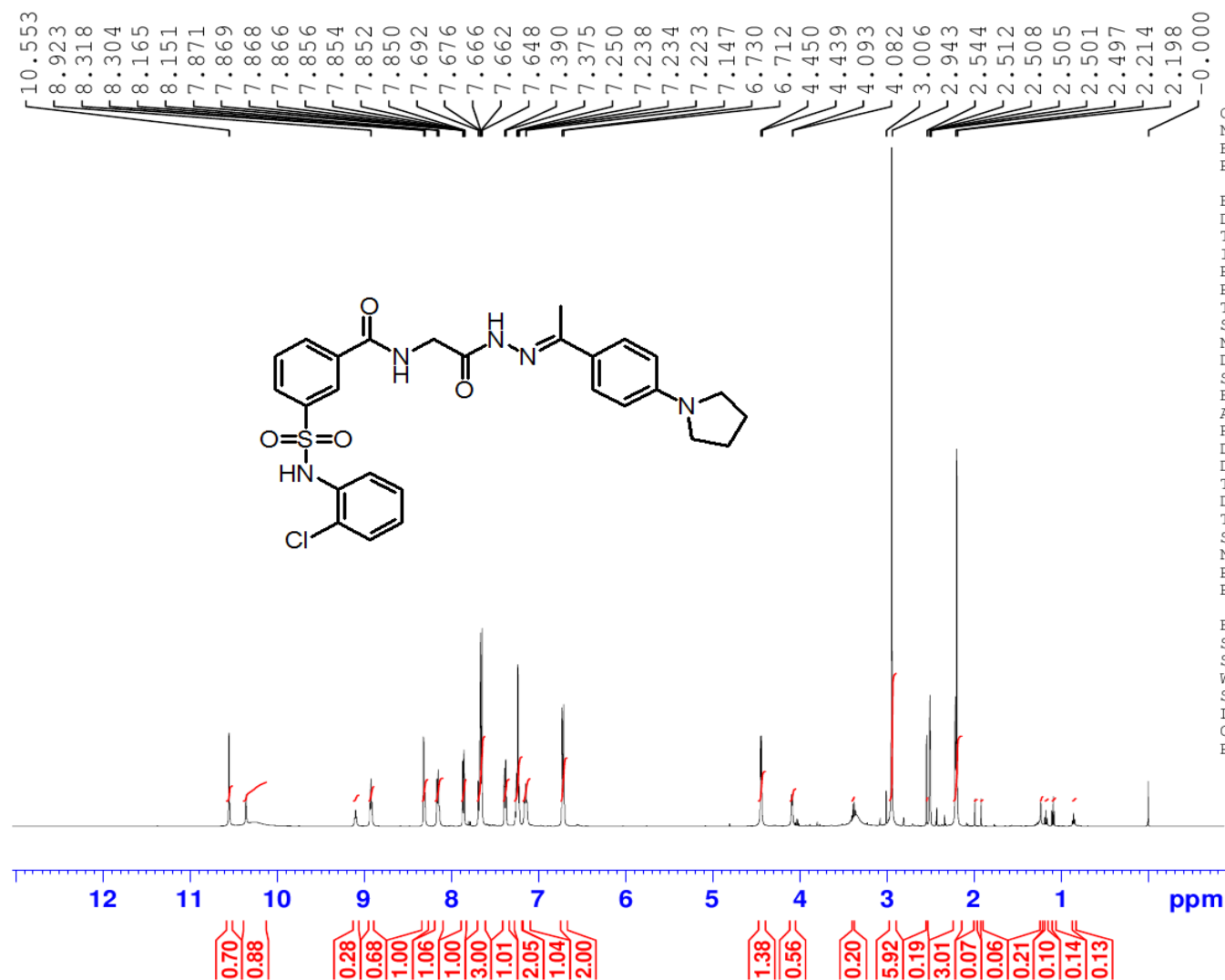
===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.18777999 W
PLW13 0.15210000 W

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

ANL-MCL5-NMR-001

¹³CNMR of Compound-2i in DMSO-d₆

GVB-SK40-01



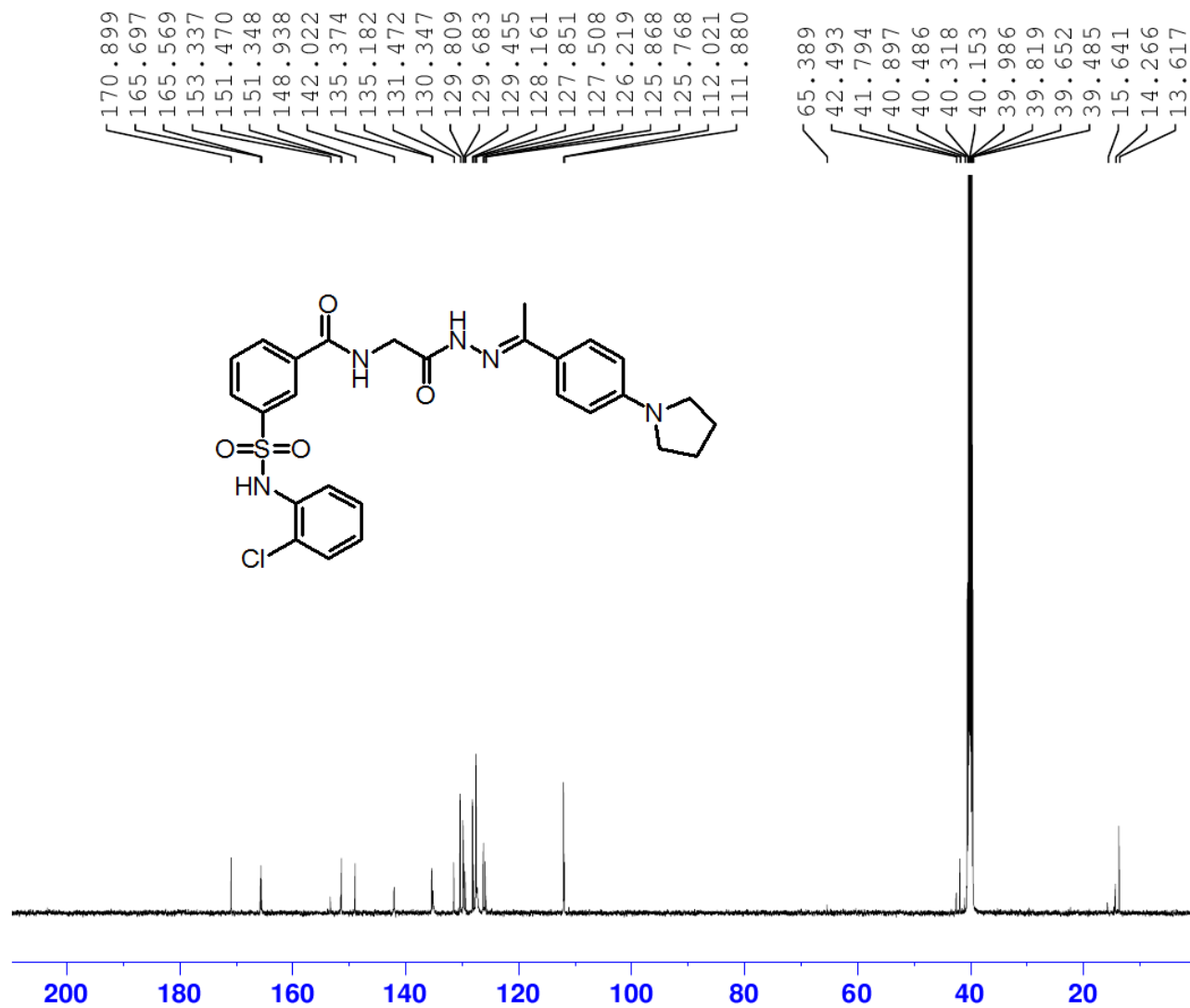
Current Data Parameters
NAME 511701C3030
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170126
Time 21.34 h
INSTRUM spect
PROBHD z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 69.27
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300014 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR of **Compound-2j** in DMSO-d₆

GVB-SK40-01



Current Data Parameters
 NAME 511701C3030
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170126
 Time 22.46 h
 INSTRUM spect
 PROBHD Z119470_0231 (
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 197.72
 DW 16.800 usec
 DE 6.50 usec
 TE 298.2 K
 D1 3.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7703643 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 88.00000000 W
 SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 23.00000000 W
 PLW12 0.27515000 W
 PLW13 0.13840000 W

F2 - Processing parameters
 SI 32768
 SF 125.7577885 MHz
 WDW EM
 SSB 0
 LB No filename specified
 GB 0
 PC 1.40

¹³CNMR of Compound-2j in DMSO-d₆

Elemental Composition Report

Page 1

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)

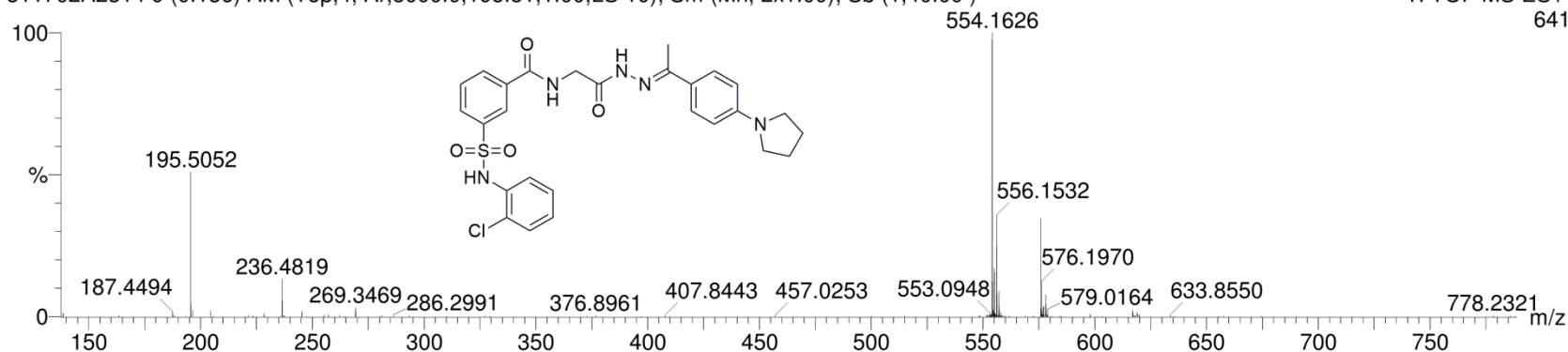
Elements Used:

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)

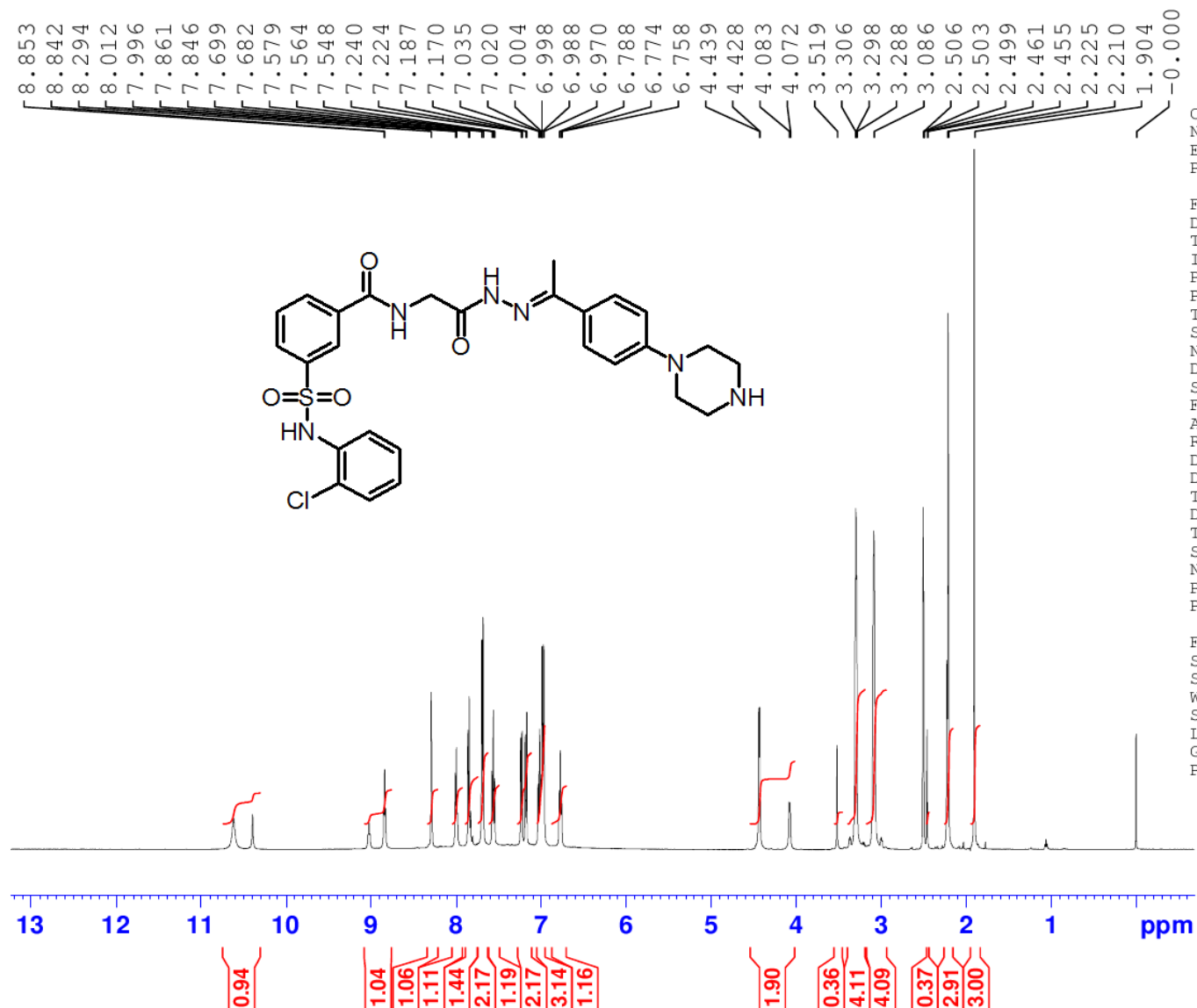
1: TOF MS ES+
641



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	C ₂₇ H ₂₉ N ₅ O ₄ S Cl

HRMS of Compound-2J



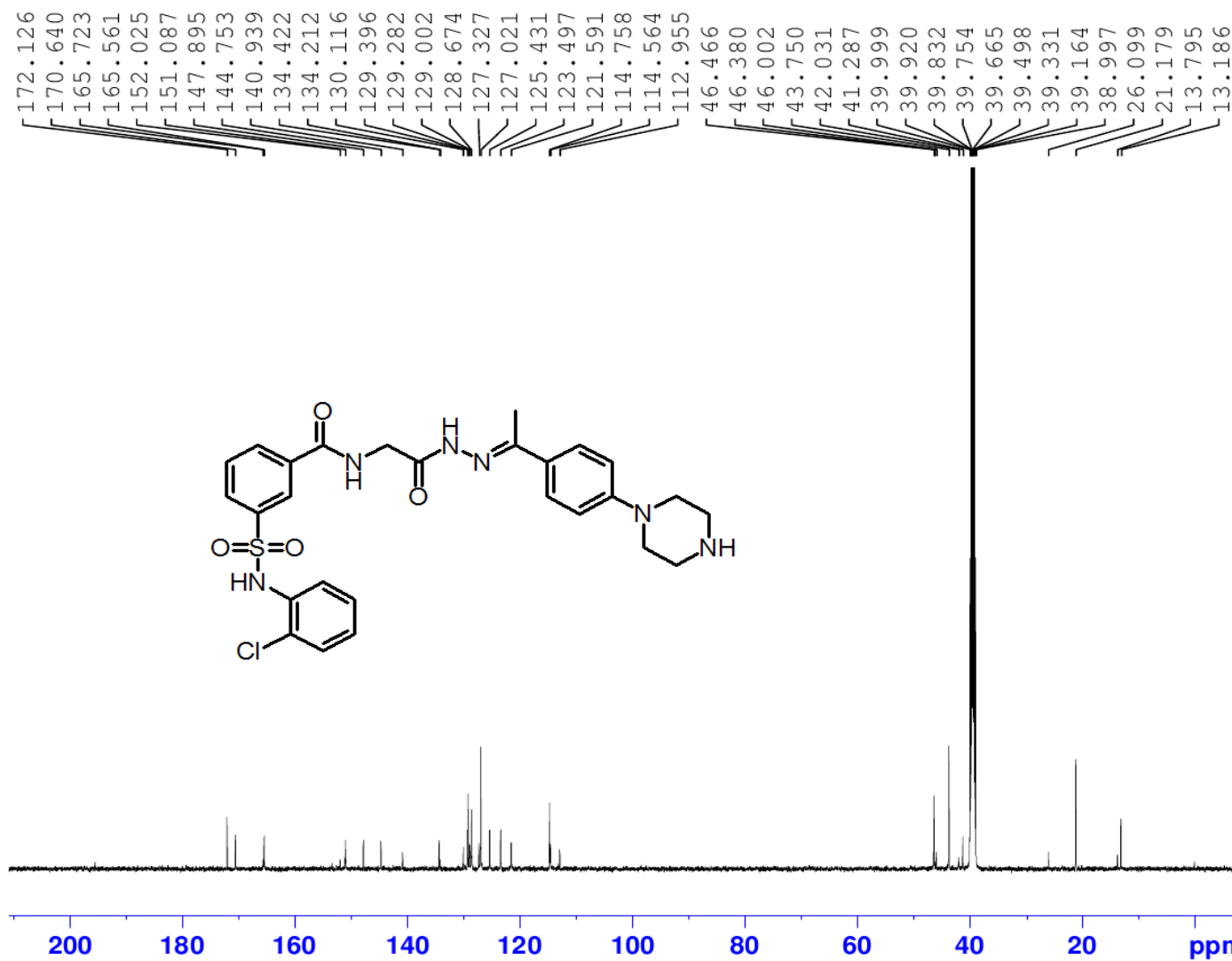
Current Data Parameters
 NAME 511612B0608
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170103
 Time 20.57 h
 INSTRUM spect
 PROBHD Z119470_0231 (
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.305176 Hz
 AQ 3.2767999 sec
 RG 69.27
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.75 usec
 PLW1 23.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.1300027 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H NMR of **Compound-2k** in DMSO-d₆

GVB-SK-41



Current Data Parameters
NAME 511612B0608
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170104
Time 2.30 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.4 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W

F2 - Processing parameters
SI 32768
SF 125.7578501 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

¹³CNMR of **Compound-2k** in DMSO-d₆

Elemental Composition Report

Page 1

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)

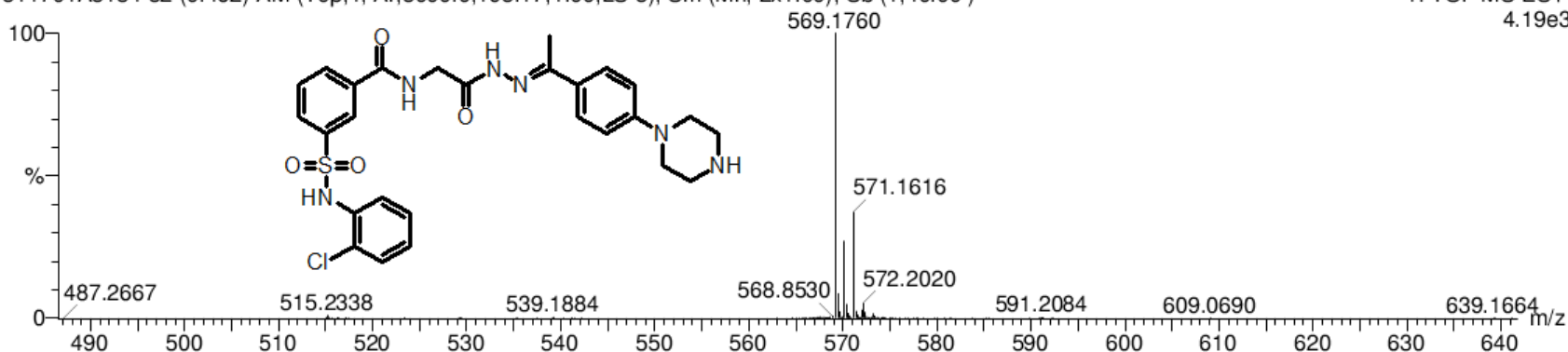
Elements Used:

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)

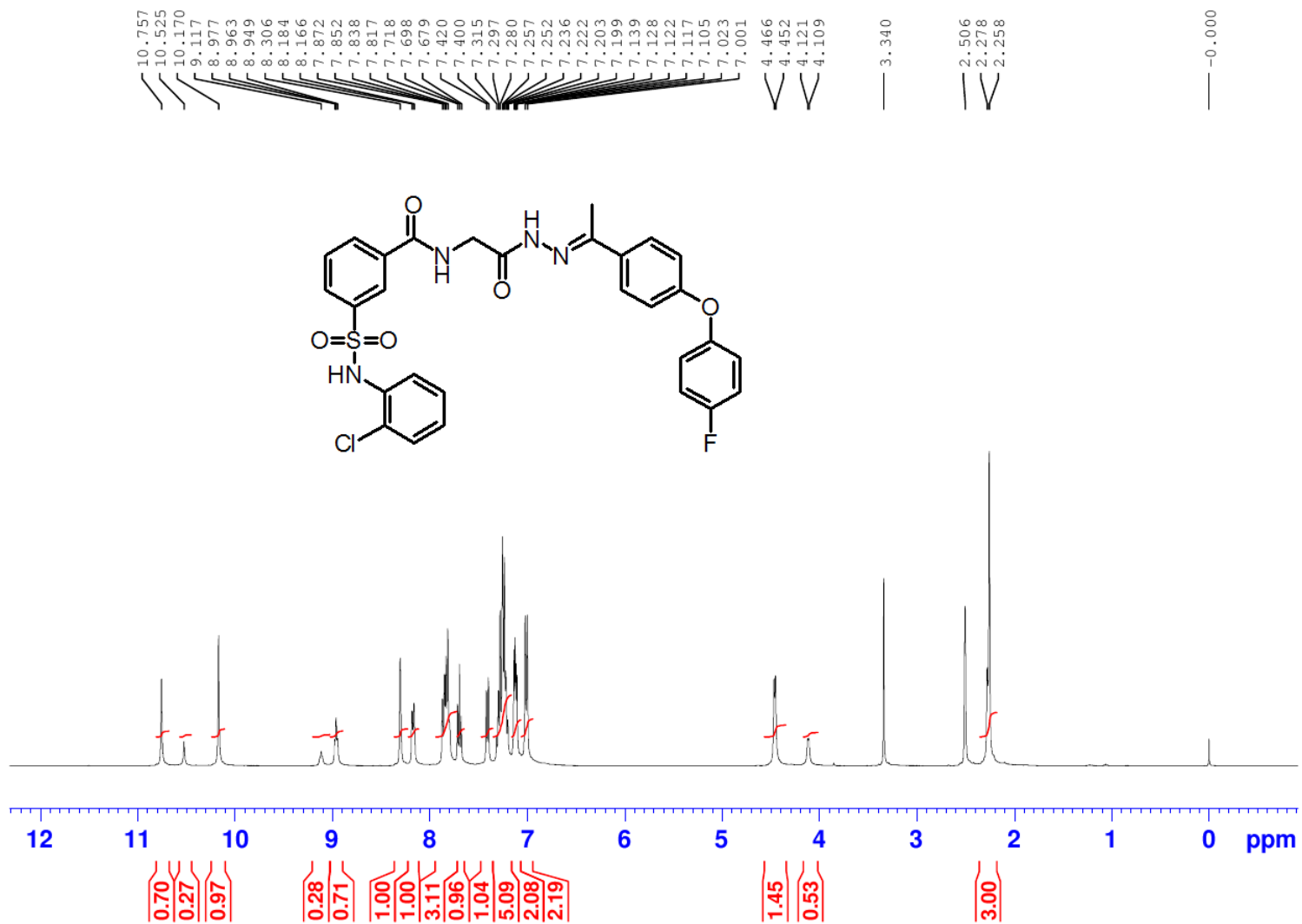
1: TOF MS ES+
4.19e3



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	C ₂₇ H ₃₀ N ₆ O ₄ S Cl

HRMS of Compound-2K



Current Data Parameters
 NAME 511612B0605
 EXPNO 1
 PROCNO 1

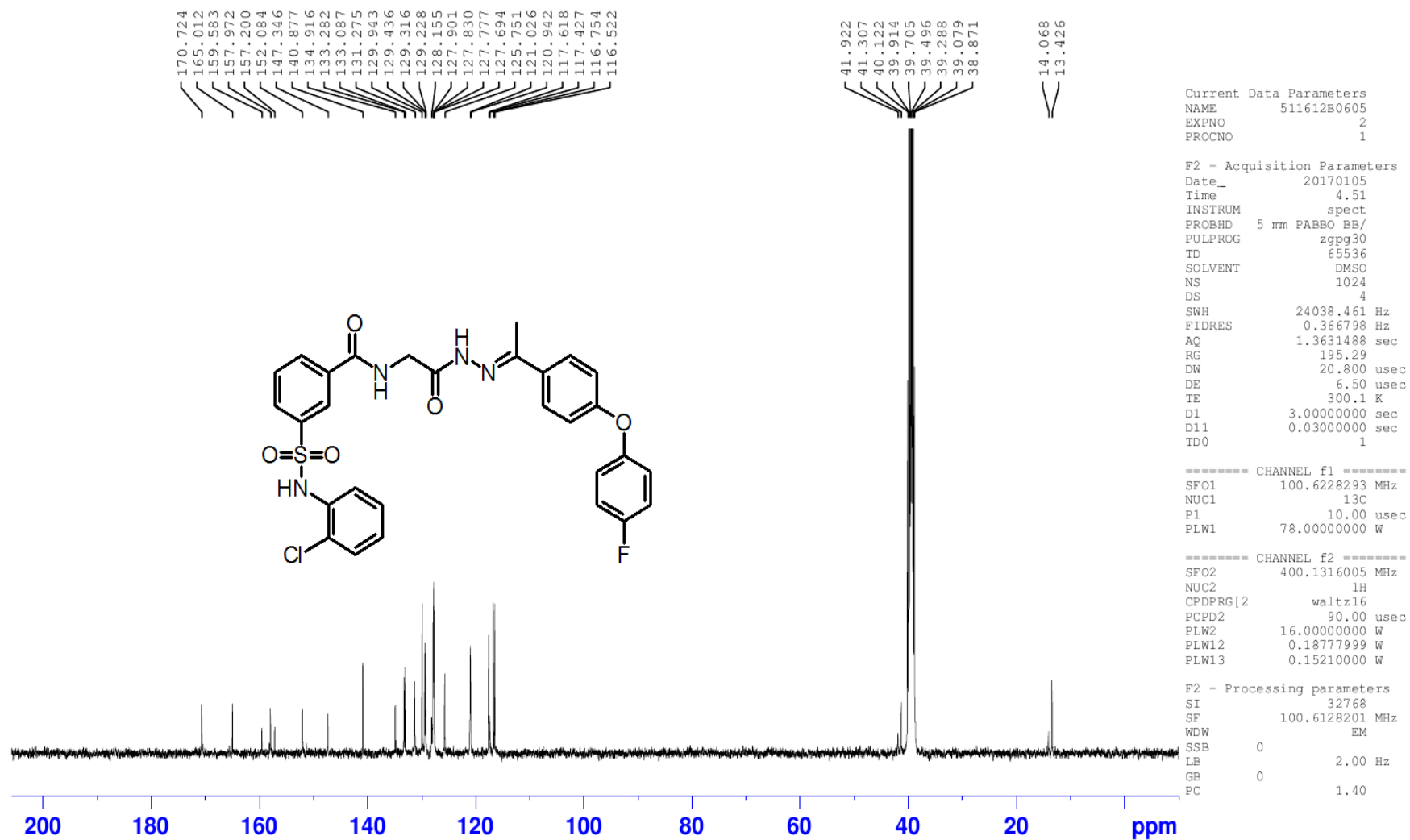
F2 - Acquisition Parameters
 Date_ 20170104
 Time 21.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 86.08
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== 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

ANL-MCL5-NMR-001

¹H NMR of **Compound-2m** in DMSO-d₆



ANL-MCL5-NMR-001

¹³CNMR of **Compound-2m** in DMSO-d₆

Elemental Composition Report

Page 1

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)

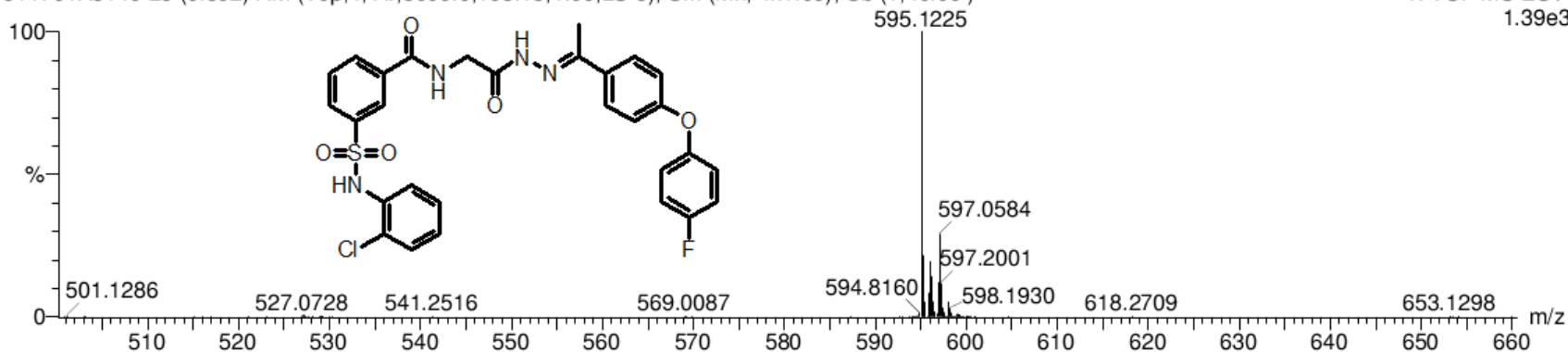
Elements Used:

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)

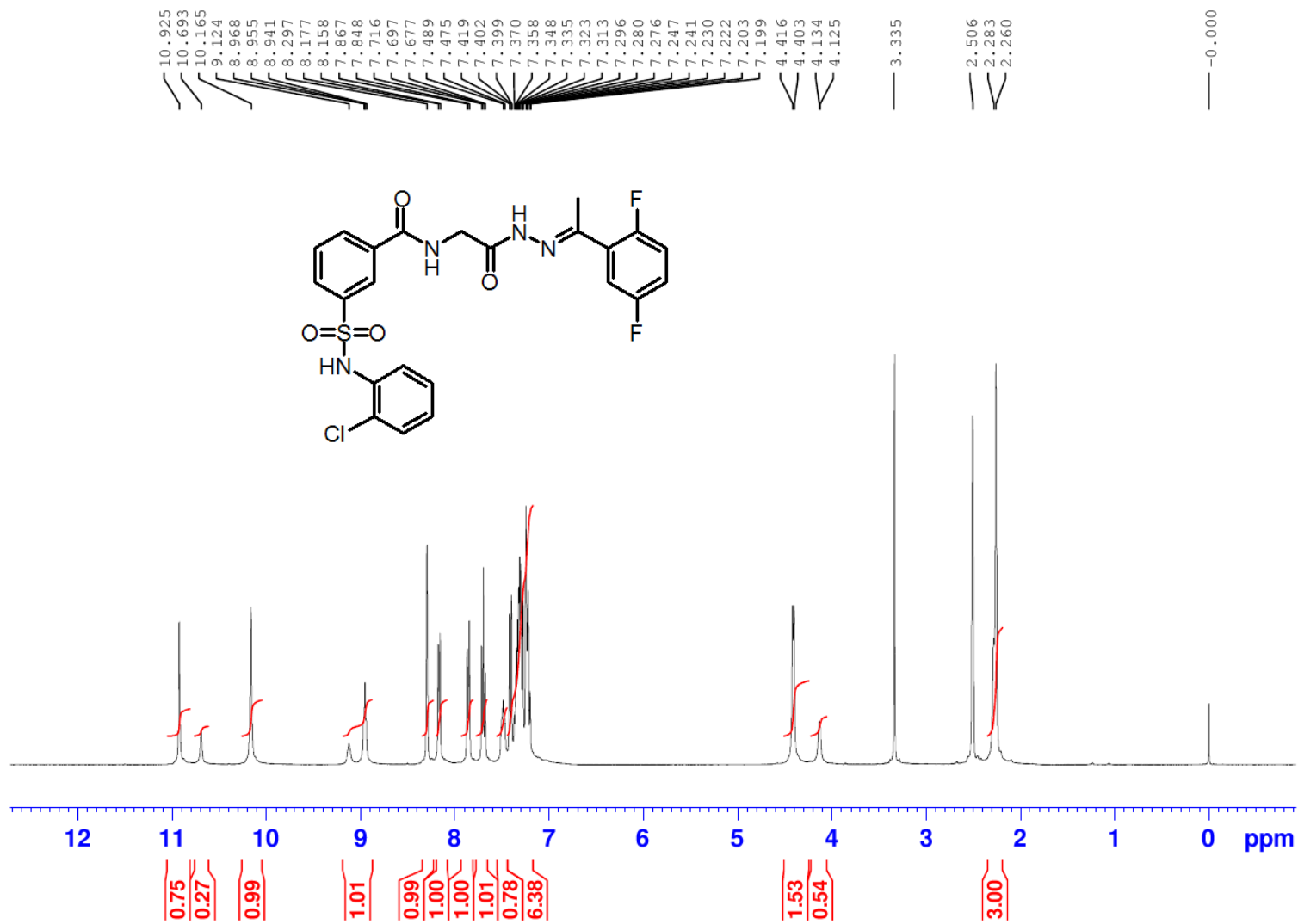
1: TOF MS ES+
1.39e3



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	C ₂₉ H ₂₅ N ₄ O ₅ F S Cl

HRMS of Compound-2m



Current Data Parameters
 NAME 511612B0602
 EXPNO 1
 PROCNO 1

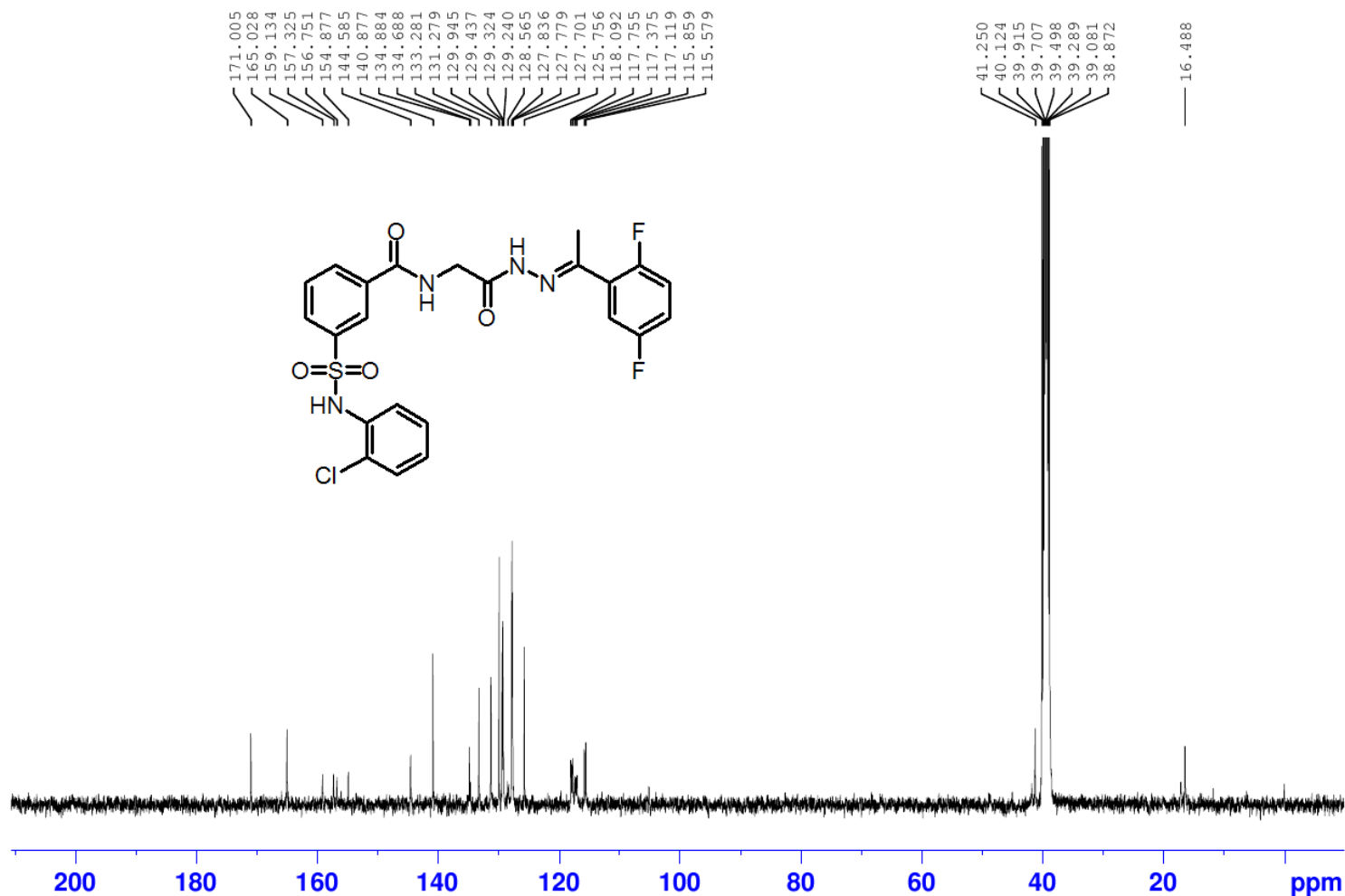
F2 - Acquisition Parameters
 Date_ 20170104
 Time 21.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 86.08
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 9.75 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300007 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ANL-MCL5-NMR-001

¹H NMR of **Compound-2n** in DMSO-d₆



Current Data Parameters
NAME 511612B0602
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170105
Time 5.57
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 300.1 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

ANL-MCL5-NMR-001

¹³CNMR of **Compound-2n** in DMSO-d₆

Elemental Composition Report

Page 1

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

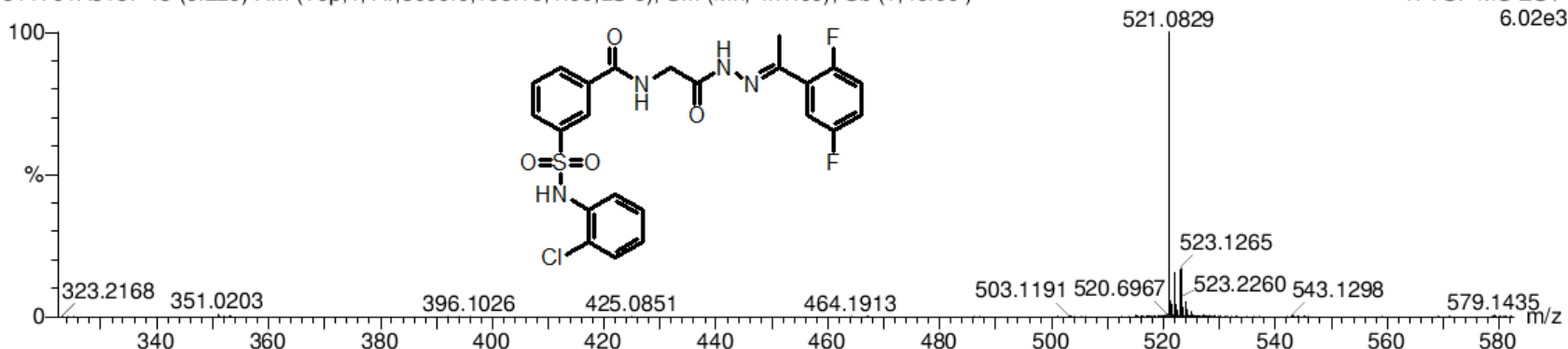
337 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)

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)



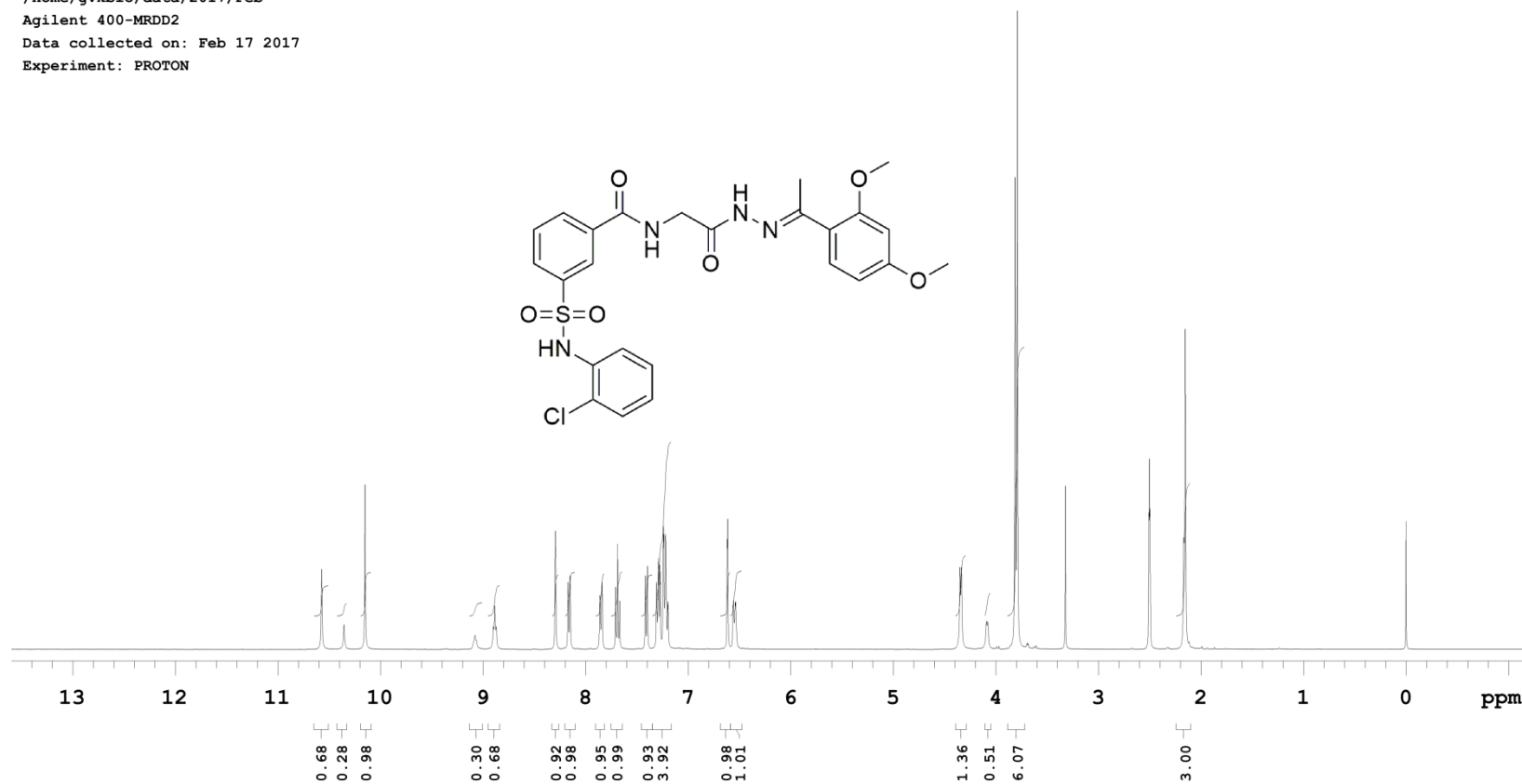
Minimum: -1.5
Maximum: 5.0 1000.0 50.0

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

GVB-SK34-01
Reference Code: 511702B6519
Solvent: dms
Archive directory:
/home/gvkbio/data/2017/Feb
Agilent 400-MRDD2
Data collected on: Feb 17 2017
Experiment: PROTON

b9994062002



¹H NMR of **Compound-2o** in DMSO-d₆

GVB-SK34-01

Reference Code: 511702B6519

Solvent: dms

Archive directory:

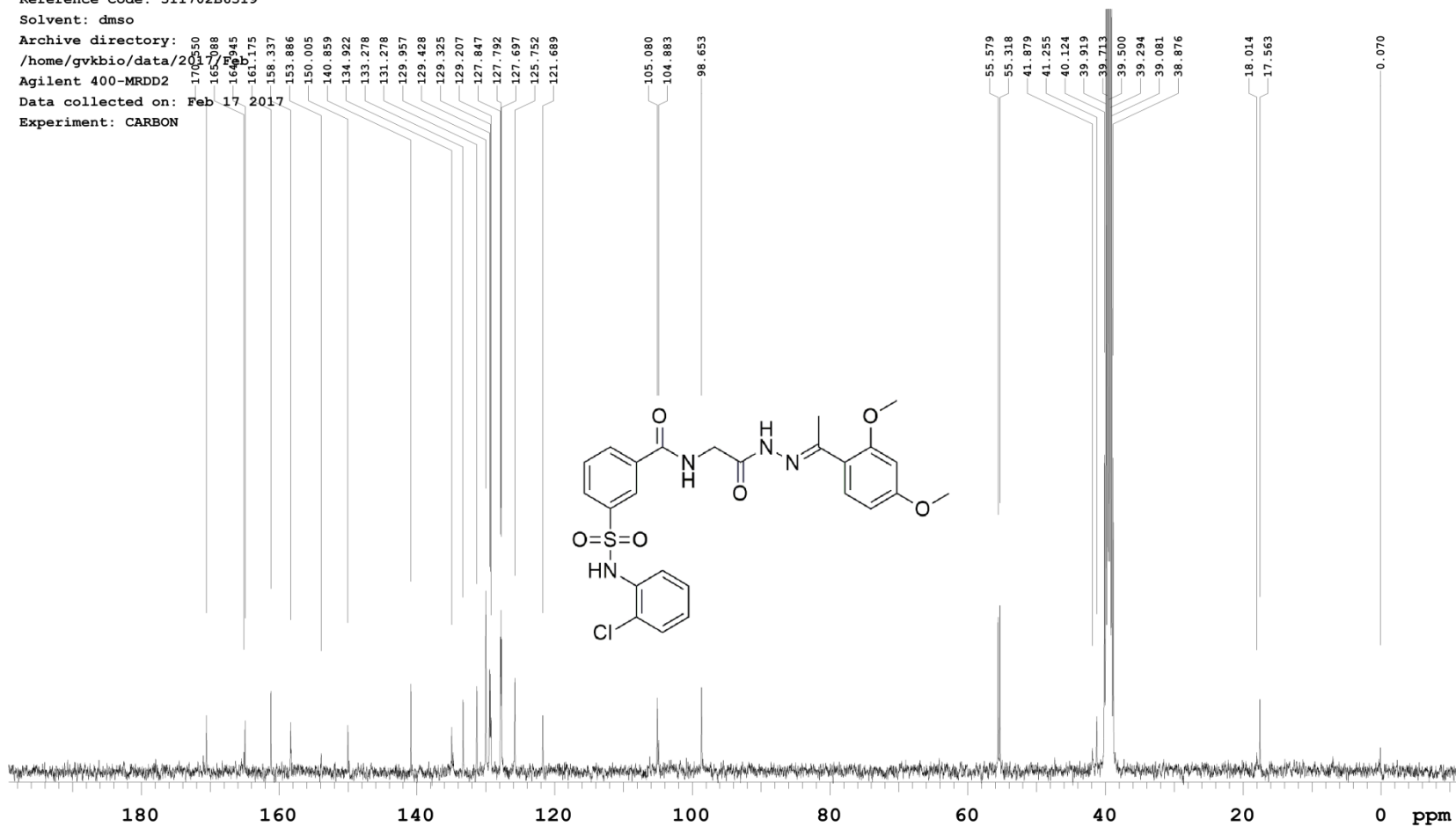
/home/gvkbic/data/2017/

Agilent 400-MRDD2

Data collected on: Feb 17 2017

Experiment: CARBON

431c2612004



Plotname: 511702B6519_CARBON_01.REC_plot01

¹³CNMR of **Compound-2o** in DMSO-d₆

Elemental Composition Report

Page 1

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

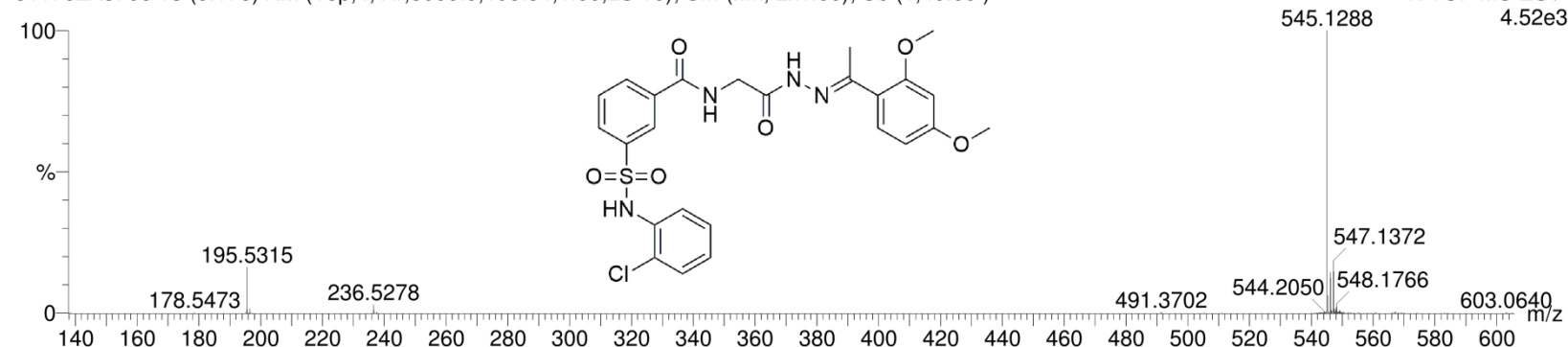
133 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

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