

Supplementary Material

(Diacetoxyiodo)benzene mediated metal-free C(*sp*²)-H phenylselenation of imidazo[1,2-*a*]pyridines and imidazo[2,1-*b*]thiazoles using diphenyl diselenide

Imran A. Opai, Prakash D. Shirsath, Amit H. Kalbandhe, and Nandkishor N. Karade*

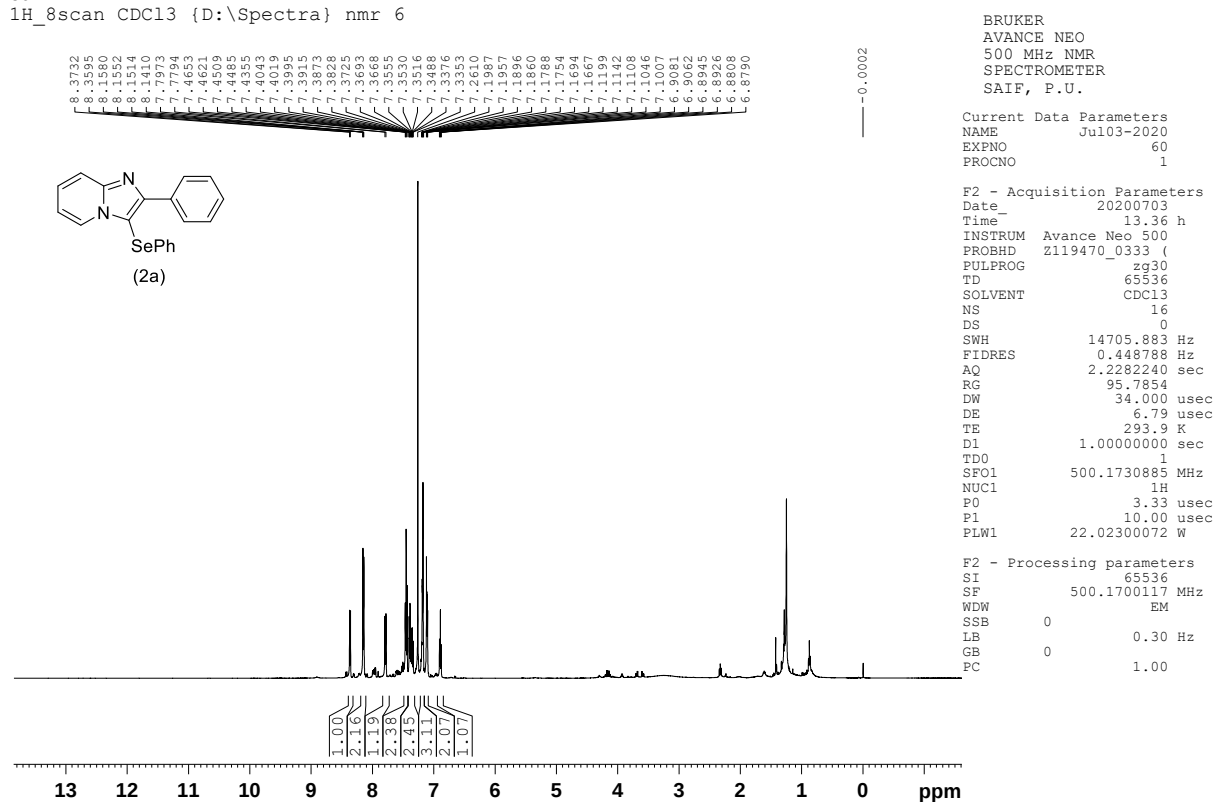
*Department of Chemistry, Rashtrasant Tukadoji Maharaj Nagpur University, Nagpur,
Maharashtra 440 033, India
Email: nnkarade@gmail.com*

Table of Contents

Copies of NMR (¹ H and ¹³ C) spectra.....	S2
--	----

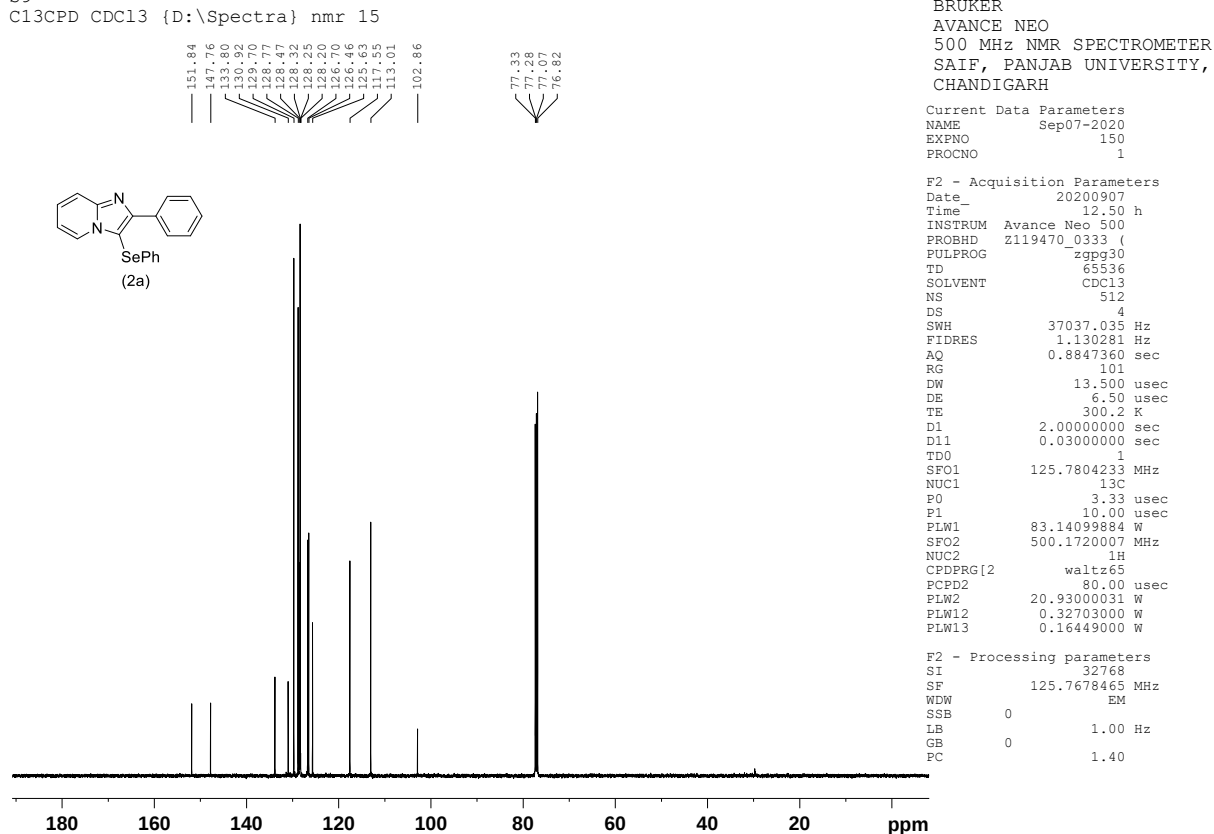
S9

1H_8scan CDC13 {D:\Spectra} nmr 6

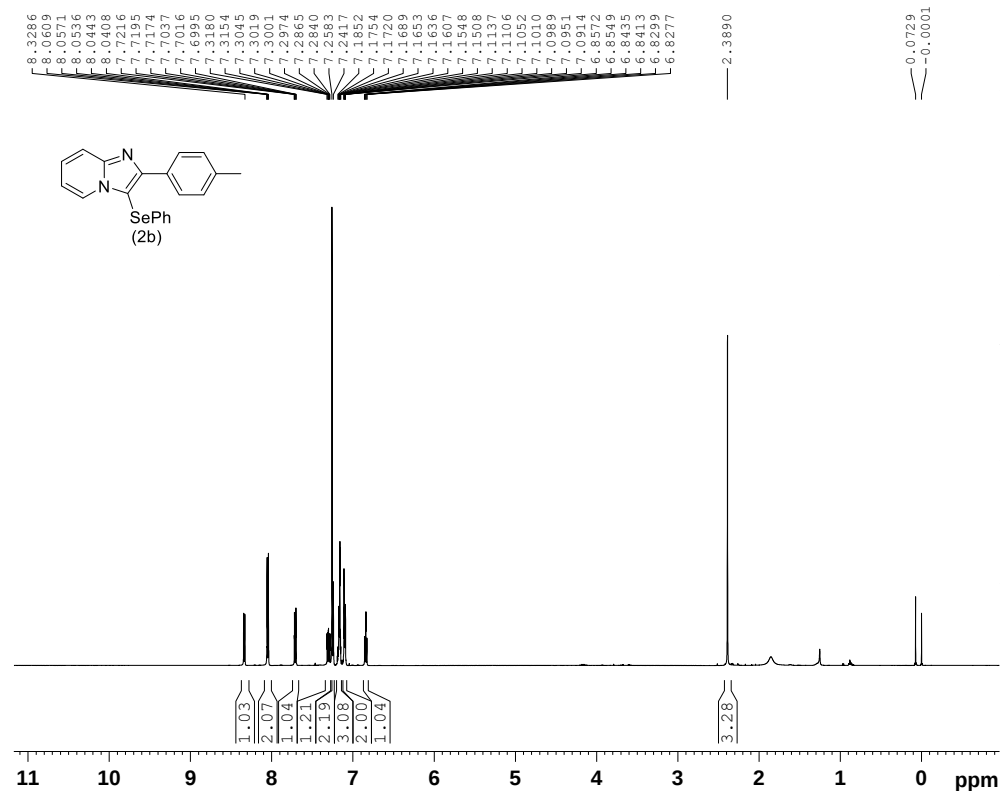


S9

C13CPD CDC13 {D:\Spectra} nmr 15



S6

¹H_8scan CDCl₃ {D:\Spectra} nmr 12

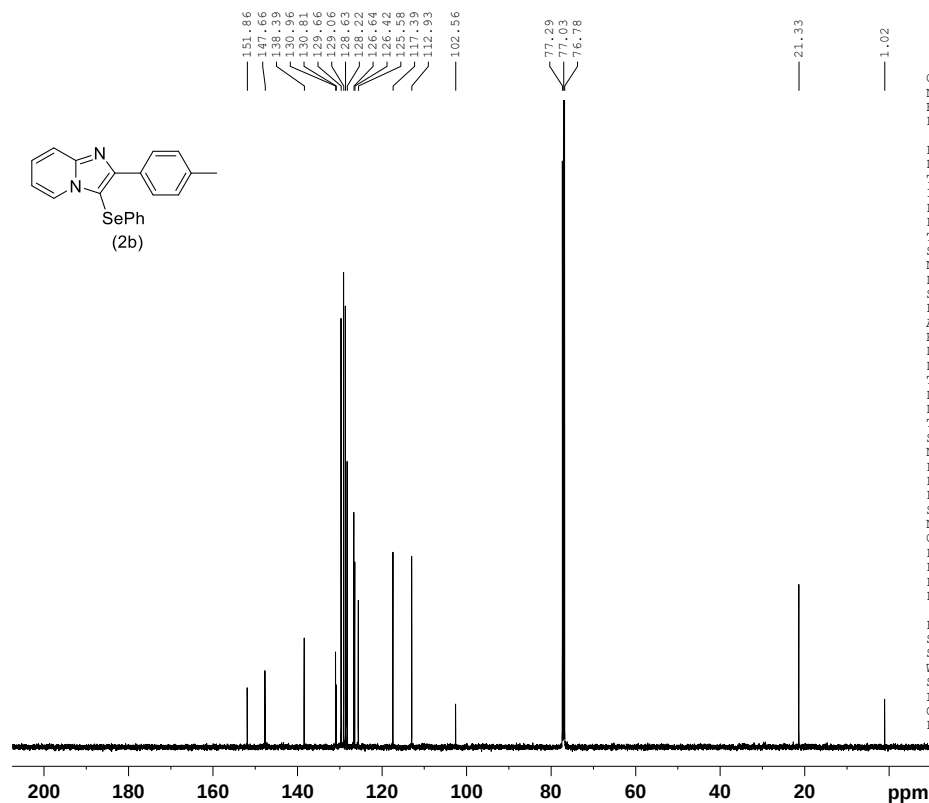
BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

Current Data Parameters
NAME Feb11-2020
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200211
Time_ 12.47 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 101
DW 34.000 usec
DE 6.79 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 22.02300072 W

F2 - Processing parameters
SI 65536
SF 500.1700129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S6

C13CPD CDCl₃ {D:\Spectra} nmr 12

BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

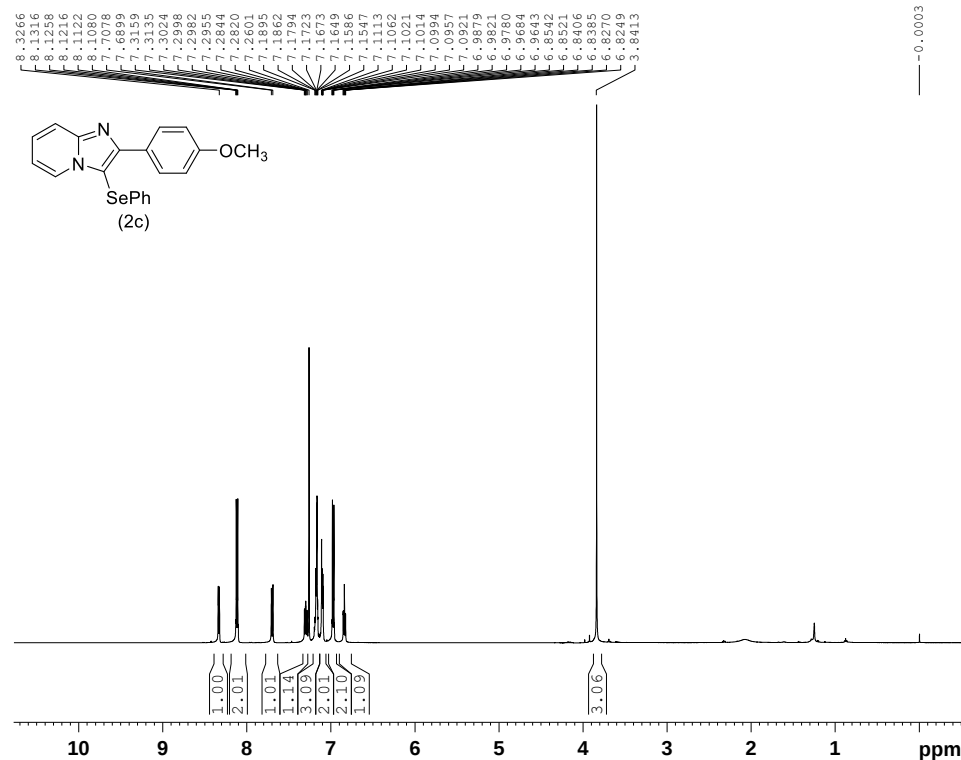
Current Data Parameters
NAME Jun17-2020
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200617
Time_ 14.41 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 512
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 79.56099701 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 22.02300072 W
PLW12 0.34411001 W
PLW13 0.17308000 W

F2 - Processing parameters
SI 32768
SF 125.7678481 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S3

1H_8scan CDC13 {D:\Spectra} nmr 5



BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

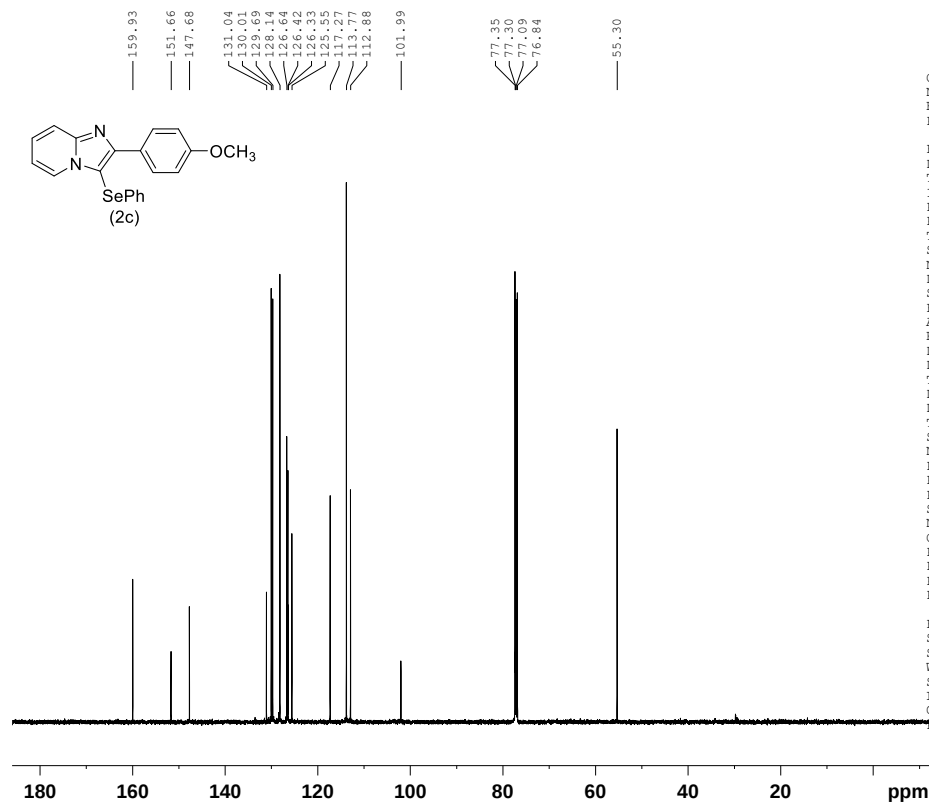
Current Data Parameters
NAME Jul03-2020
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200703
Time_ 13.32 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 ()
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 22.02300072 W

F2 - Processing parameters
SI 65536
SF 500.1700121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S-3

C13CPD CDC13 {D:\Spectra} nmr 6



BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

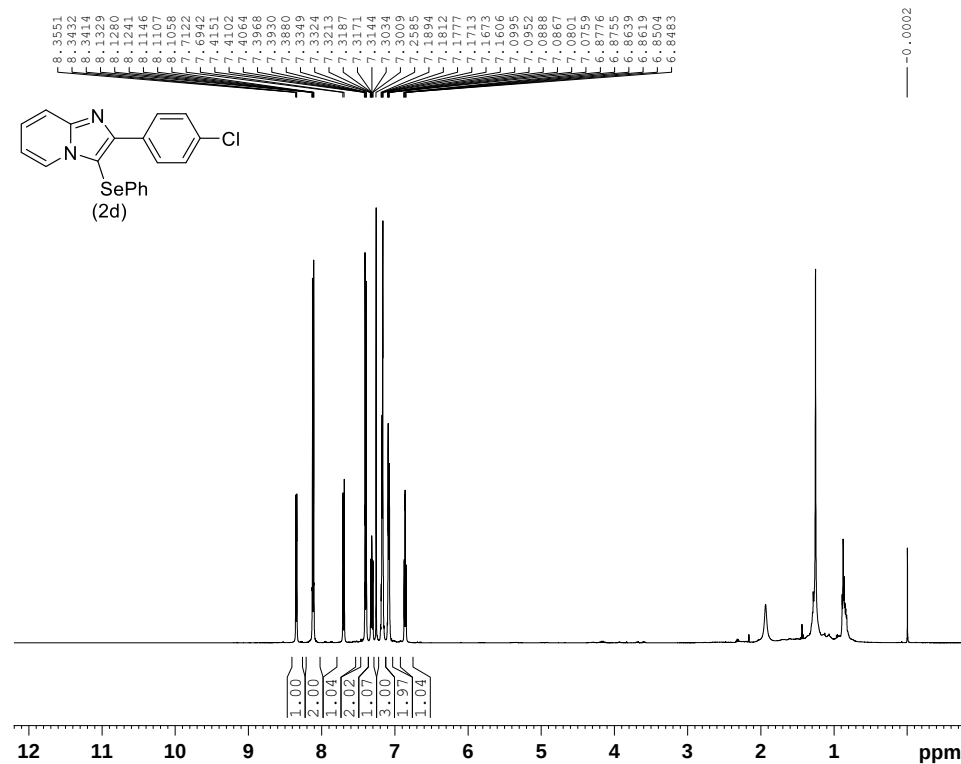
Current Data Parameters
NAME Jul13-2020
EXPNO 60
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200713
Time_ 13.35 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 ()
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7678465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S8

1H_8scan CDC13 {D:\Spectra} nmr 24



BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

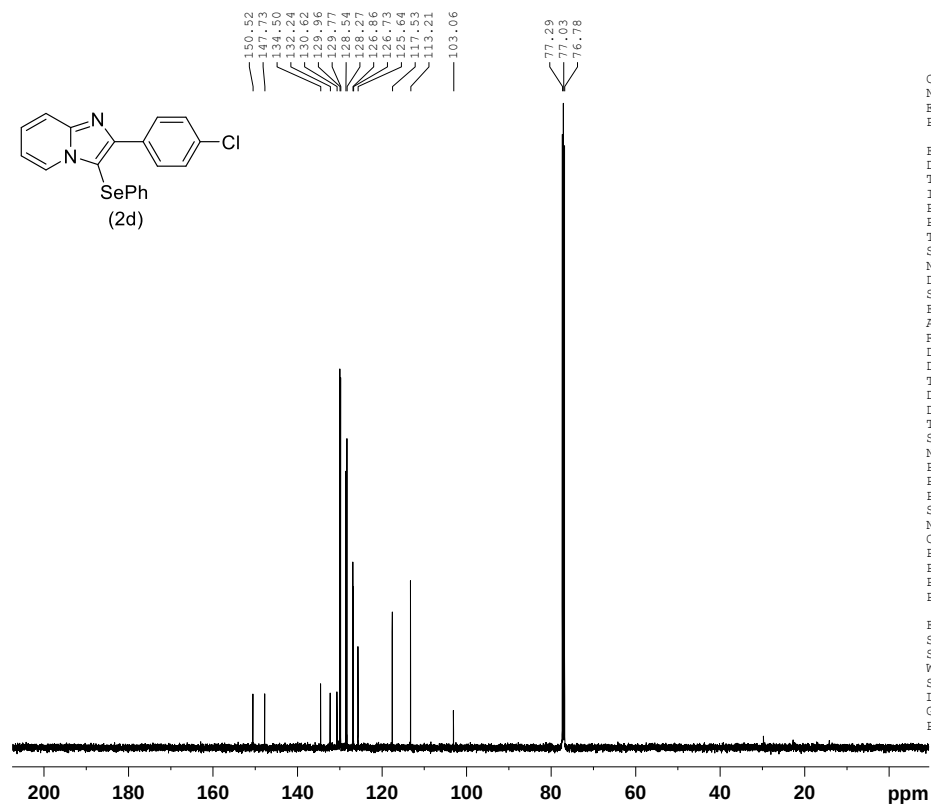
Current Data Parameters
NAME Mar06-2020
EXPNO 240
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200306
Time 12.23 h
INSTRUM Avance Neo 500
PROBHD 2119470_0333 (PULPROG zg30)
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 22.02300072 W

F2 - Processing parameters
SI 65536
SF 500.1700128 MHz
WDW EM
LB 0
GB 0.30 Hz
PC 1.00

S8

C13CPD CDC13 {D:\Spectra} nmr 14



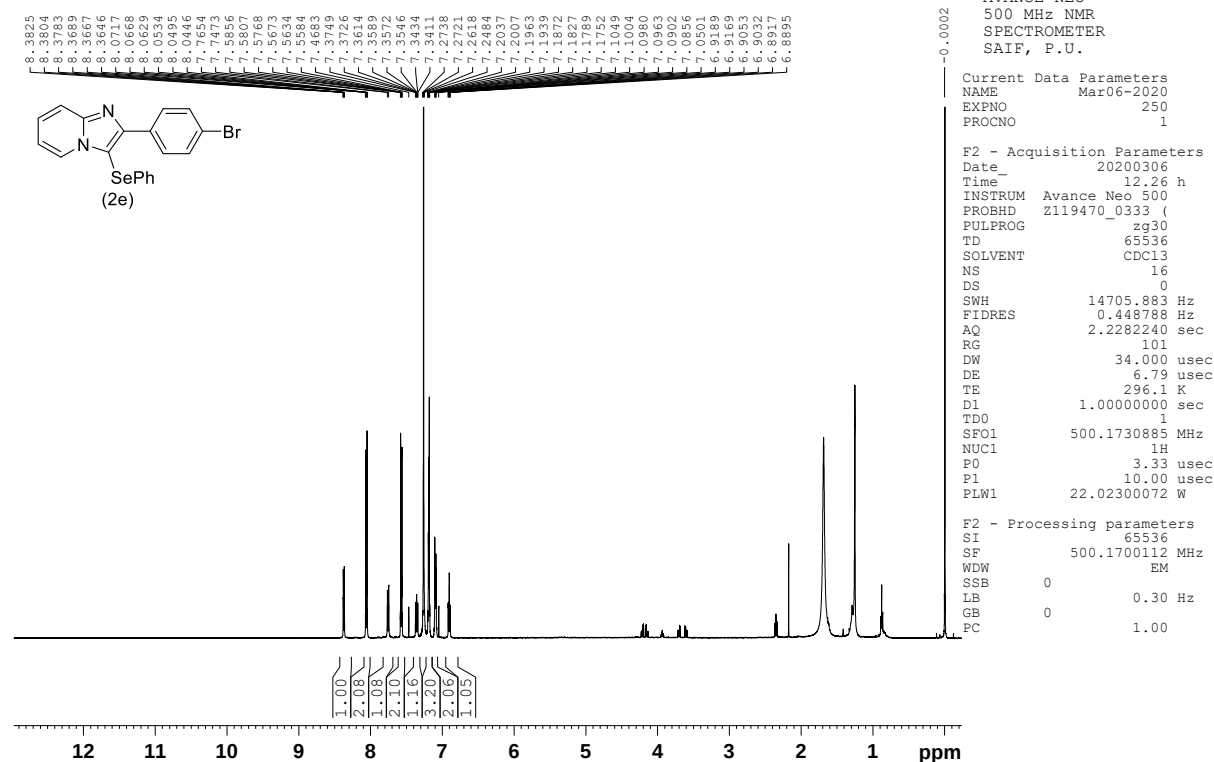
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun17-2020
EXPNO 140
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200617
Time 15.23 h
INSTRUM Avance Neo 500
PROBHD 2119470_0333 (PULPROG zgpg30)
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 79.56099701 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 22.02300072 W
PLW12 0.34411001 W
PLW13 0.17308000 W

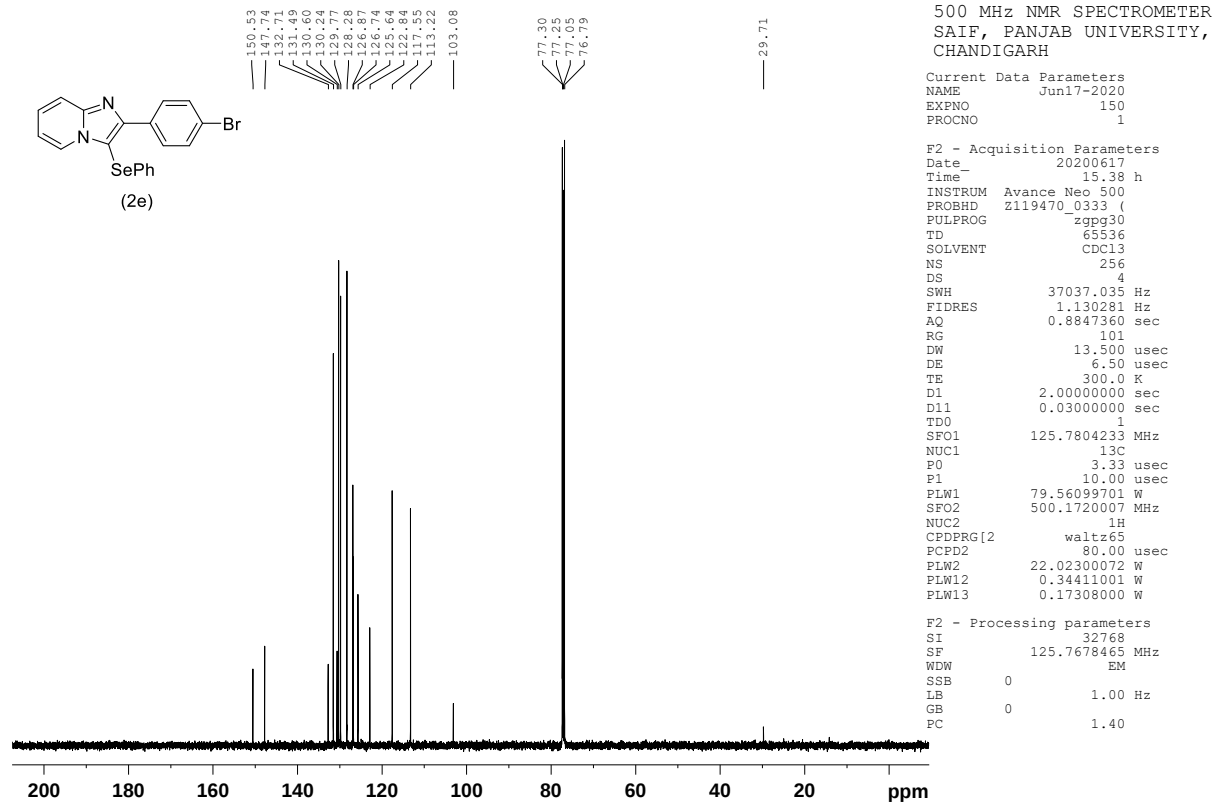
F2 - Processing parameters
SI 32768
SF 125.7678465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

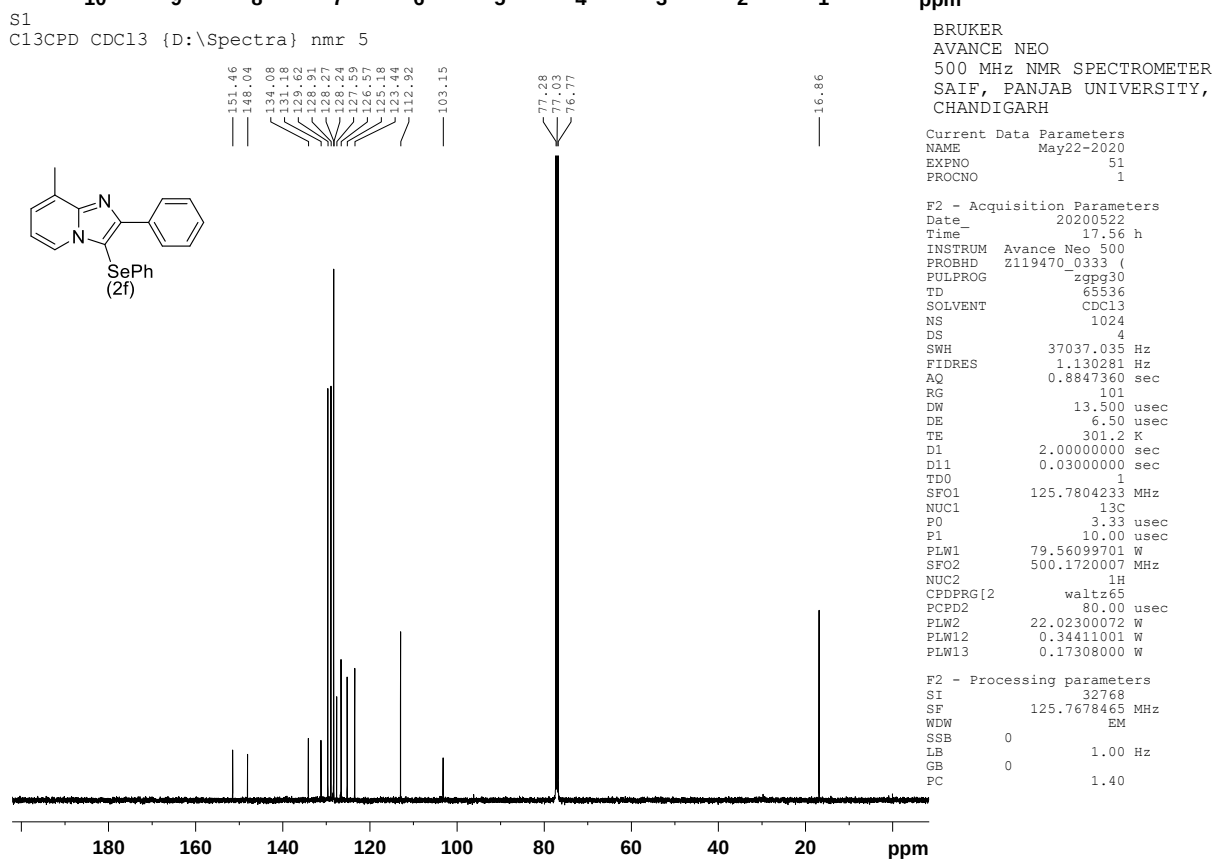
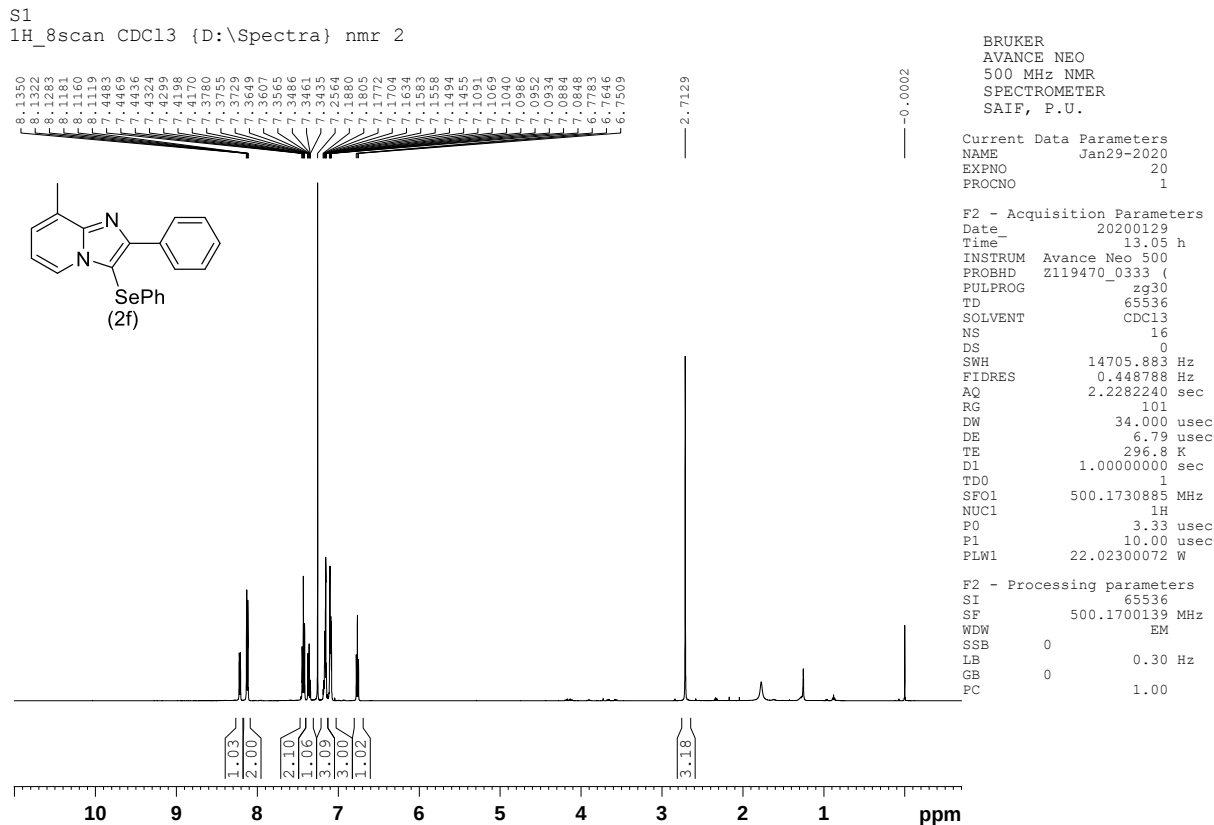
S12

¹H_8scan CDC13 {D:\Spectra} nmr 25

S12

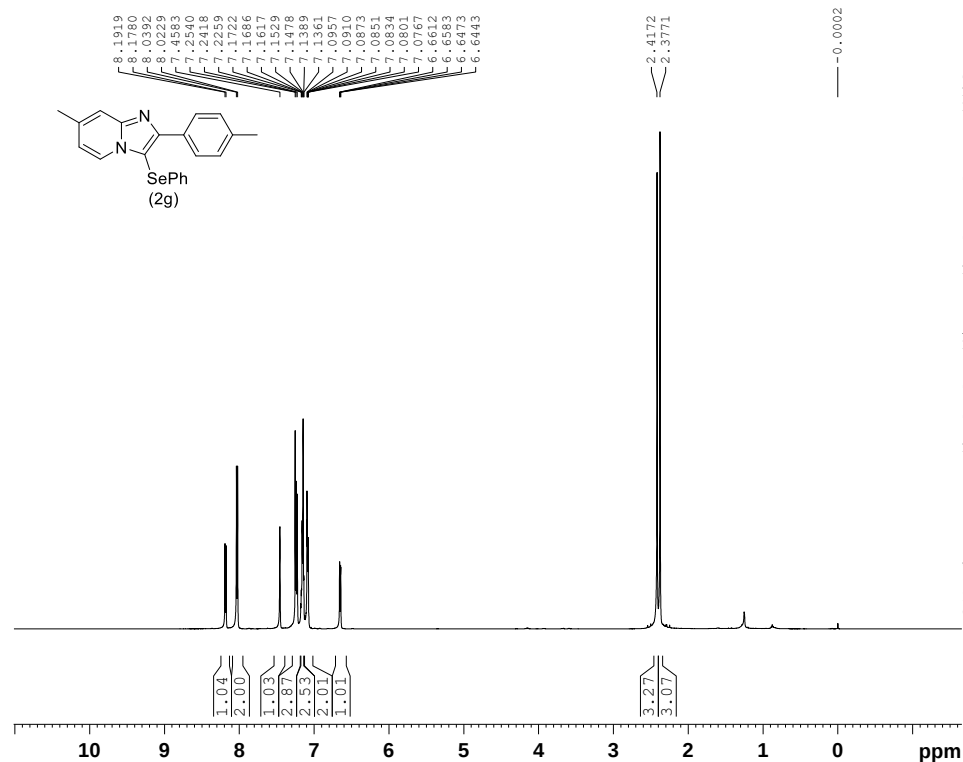
C13CPD CDC13 {D:\Spectra} nmr 15





S11

1H_8scan CDC13 {D:\Spectra} nmr 8



BRUKER
 AVANCE NEO
 500 MHz NMR
 SPECTROMETER
 SAIF, P.U.

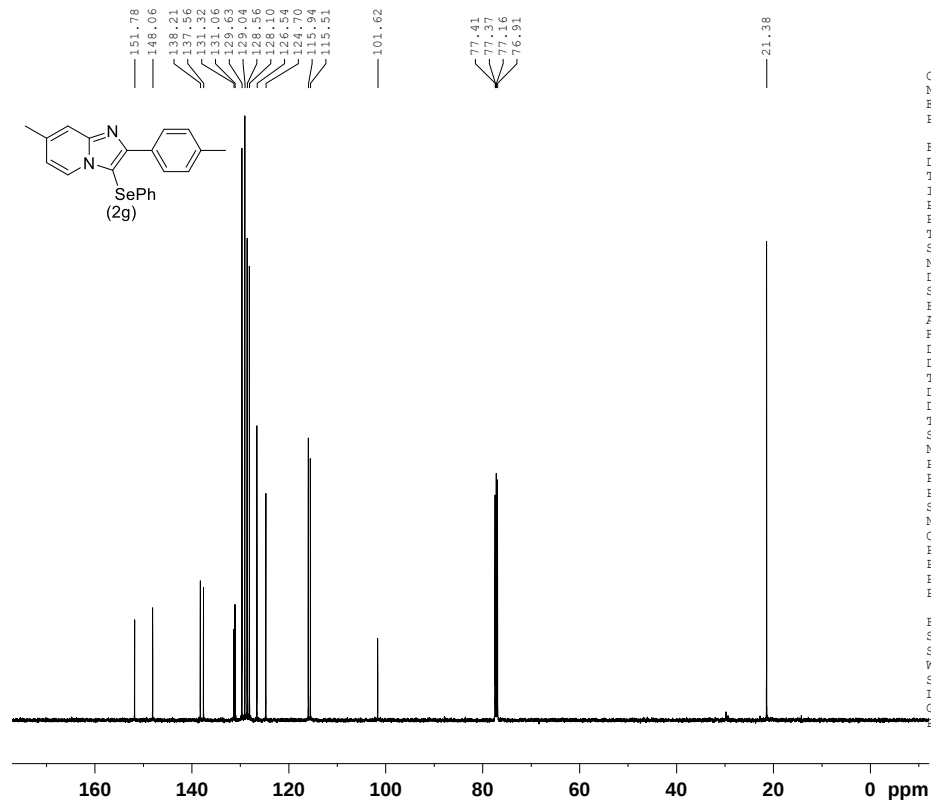
Current Data Parameters
 NAME Jul03-2020
 EXPNO 80
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200703
 Time_ 13.41 h
 INSTRUM Avance Neo 500
 PROBHD Z119470_0333 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 14705.883 Hz
 FIDRES 0.448788 Hz
 AQ 2.2282240 sec
 RG 95.7854
 DW 34.000 usec
 DE 6.79 usec
 TE 293.9 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1730885 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 22.02300072 W

F2 - Processing parameters
 SI 65536
 SF 500.1700152 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S-11

C13CPD CDC13 {D:\Spectra} nmr 9



BRUKER
 AVANCE NEO
 500 MHz NMR SPECTROMETER
 SAIF, PANJAB UNIVERSITY,
 CHANDIGARH

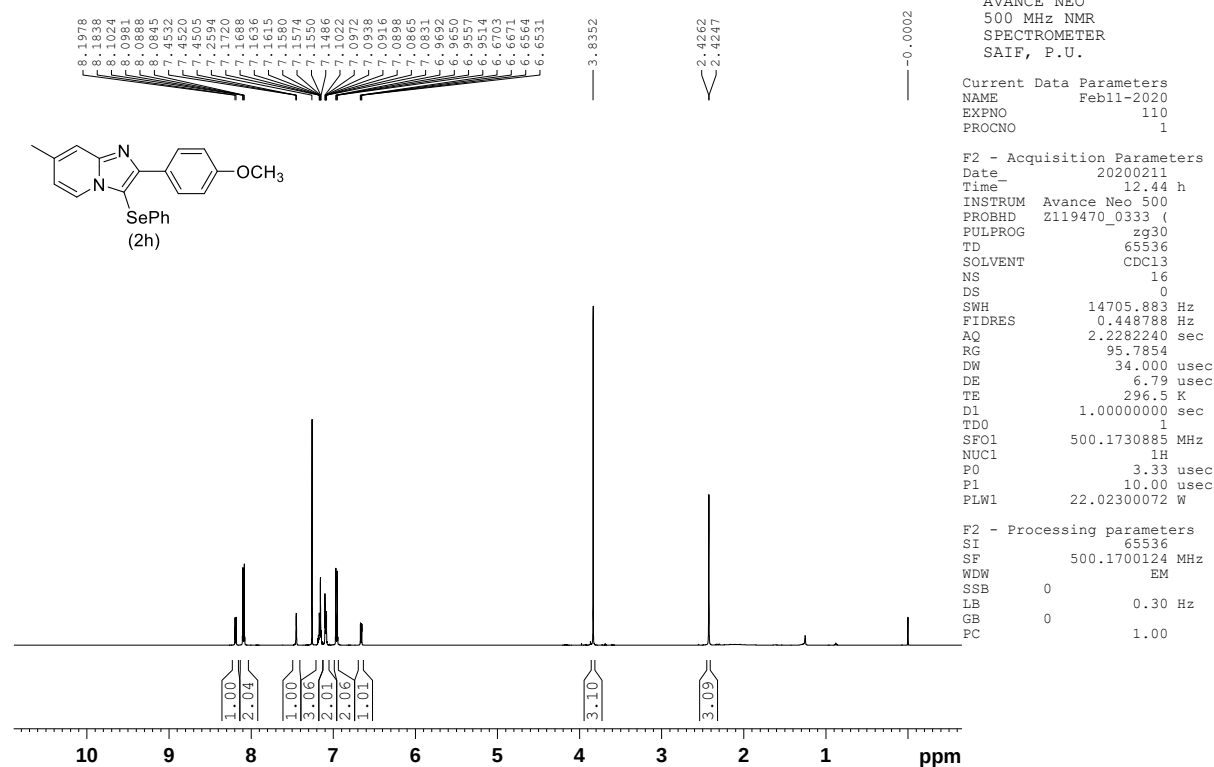
Current Data Parameters
 NAME Jul13-2020
 EXPNO 90
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200713
 Time_ 14.26 h
 INSTRUM Avance Neo 500
 PROBHD Z119470_0333 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 200
 DS 4
 SWH 37037.035 Hz
 FIDRES 1.130281 Hz
 AQ 0.8847360 sec
 RG 101
 DW 13.500 usec
 DE 6.50 usec
 TE 296.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7804233 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 83.14099884 W
 SFO2 500.1720007 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 80.00 usec
 PLW2 20.93000031 W
 PLW12 0.32703000 W
 PLW13 0.16449000 W

F2 - Processing parameters
 SI 32768
 SF 125.7678465 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

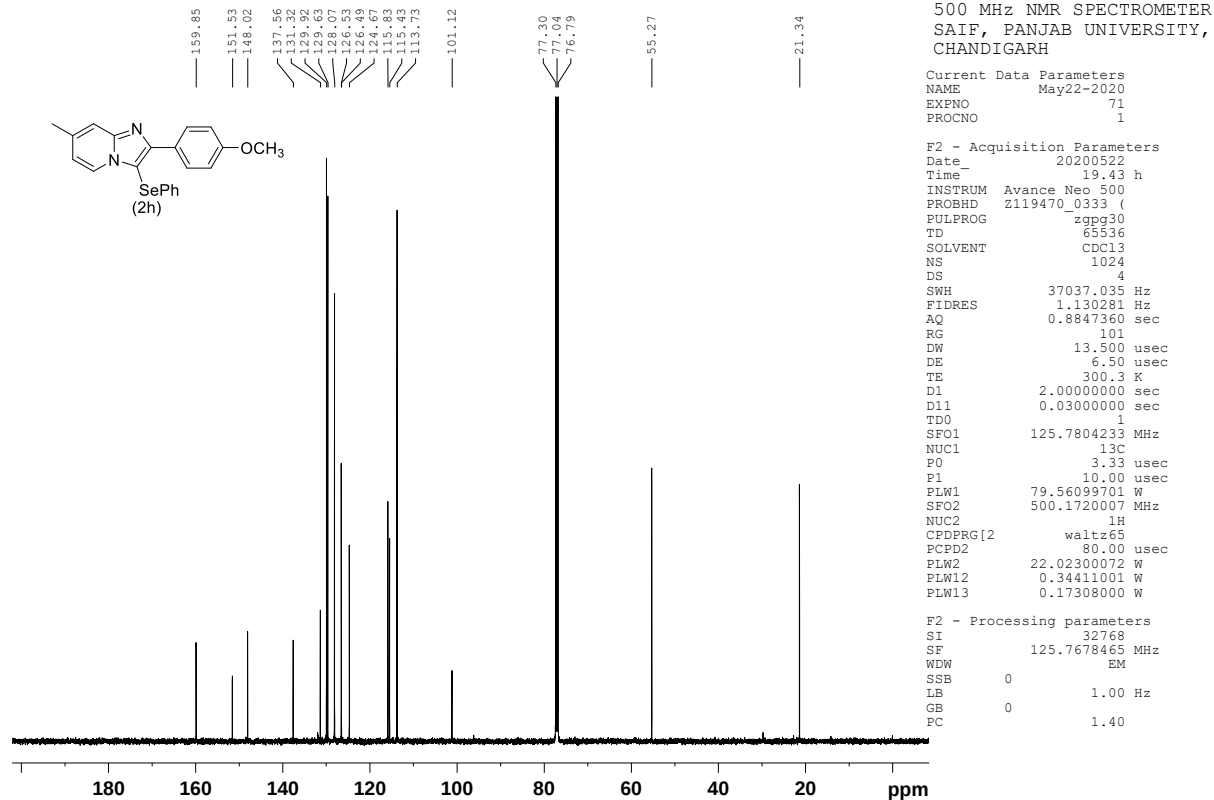
S4

1H_8scan CDC13 {D:\Spectra} nmr 11



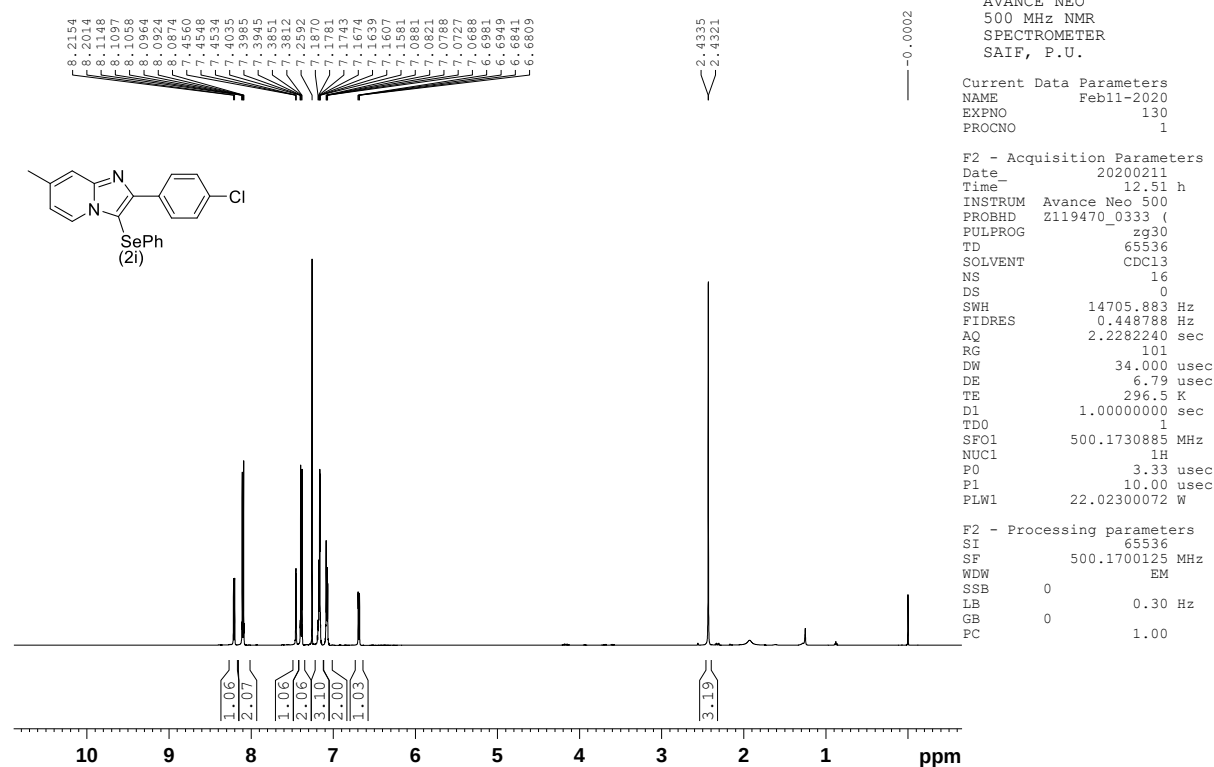
S4

C13CPD CDC13 {D:\Spectra} nmr 7



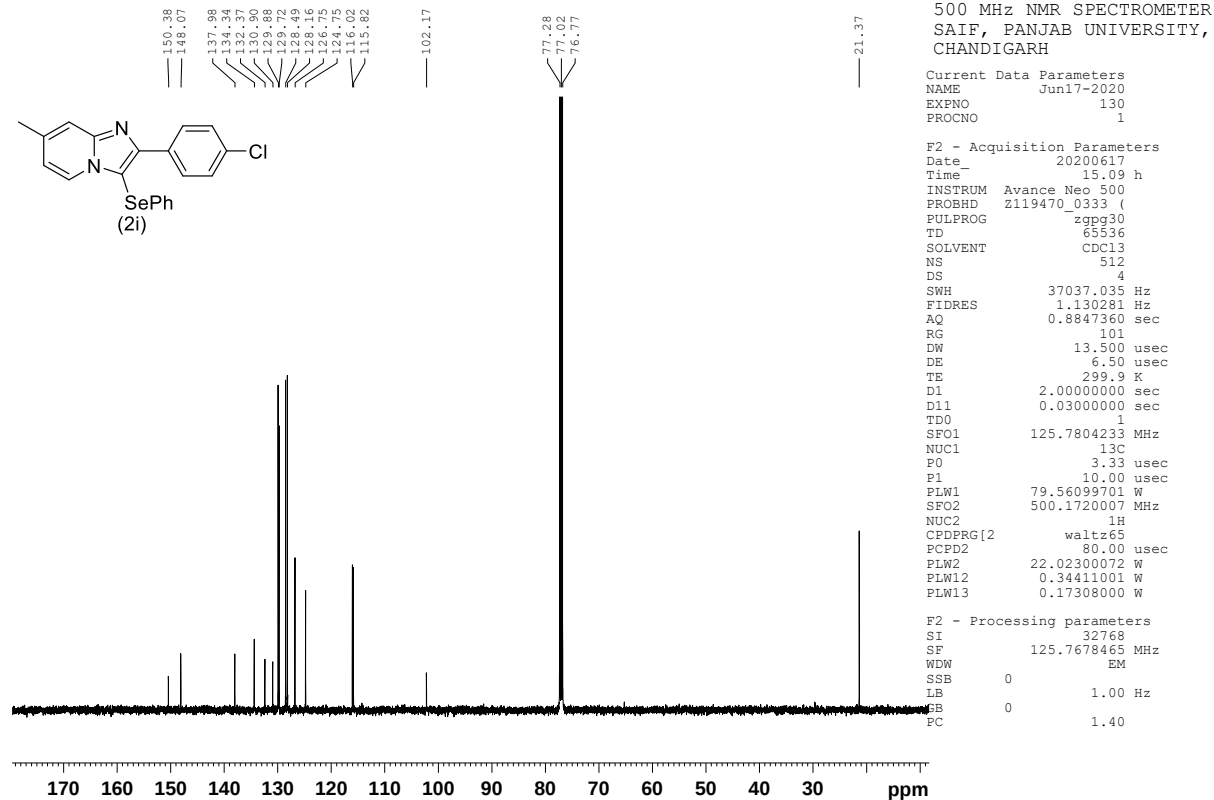
S7

1H_8scan CDC13 {D:\Spectra} nmr 13



S7

C13CPD CDC13 {D:\Spectra} nmr 13



Chemical structure of compound (2) is shown as an inset: 2-(4-methylphenyl)-4-phenyl-1H-imidazole-5-selenophene. The SePh group is labeled.

¹³C NMR spectrum (CDCl₃) of compound (2) showing chemical shifts (ppm):

- 151.65
- 146.80
- 133.91
- 131.30
- 129.69
- 129.64
- 128.67
- 128.50
- 128.30
- 128.04
- 126.57
- 123.33
- 122.84
- 116.87
- 102.31
- 77.36
- 77.10
- 76.85
- 18.42

```

BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME          Jul13-2020
EXPNO         80
PROCNO        1

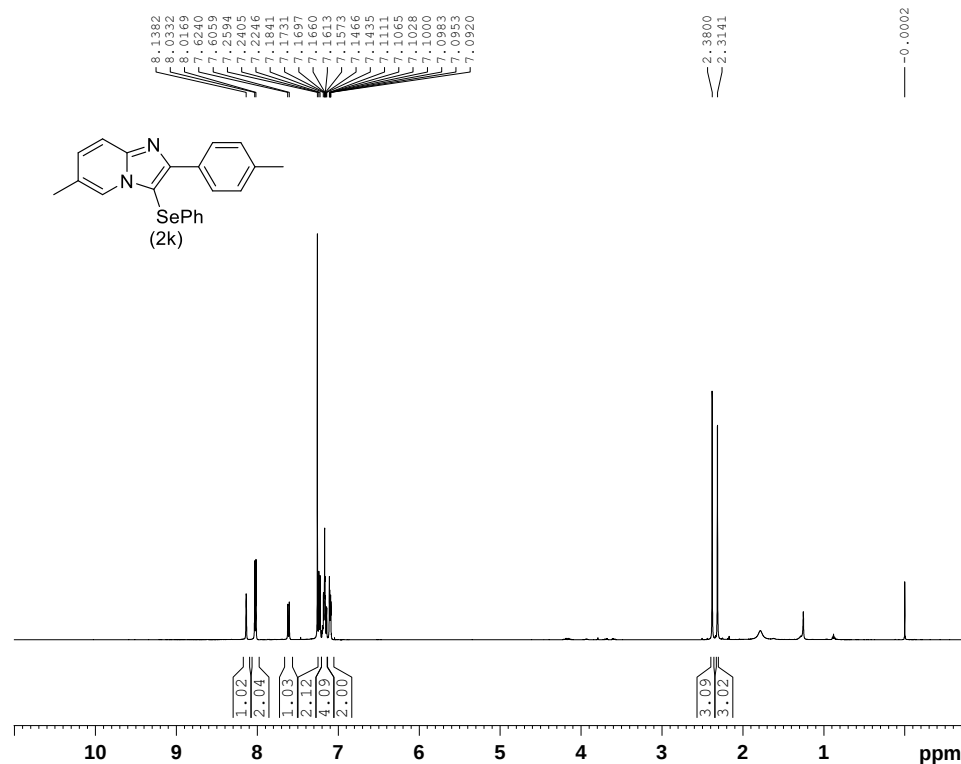
F2 - Acquisition Parameters
Date_         20200713
Time_         14.15 h
INSTRUM       Avance Neo 500
PROBHD        Z119470_0333 (
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            200
DS            4
SWH           37037.035 Hz
FIDRES        1.130281 Hz
AQ            0.8847360 sec
RG            101
WV           13.500 usec
DE            6.50 usec
TE            296.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1
SF01          125.7804233 MHz
NUC1          13C
P0            3.33 usec
P1            10.00 usec
PLW1          83.14099884 W
SF02          500.1720007 MHz
NUC2          1H
CPDPRG2       waltz65
PCPD2         80.00 usec
PLW2          20.93000031 W
PLW12         0.32703000 W
PLW13         0.16449000 W

F2 - Processing parameters
SI            32768
SF            125.7678465 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB           0
PC            1.40

```

S2

1H_8scan CDC13 {D:\Spectra} nmr 3



BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

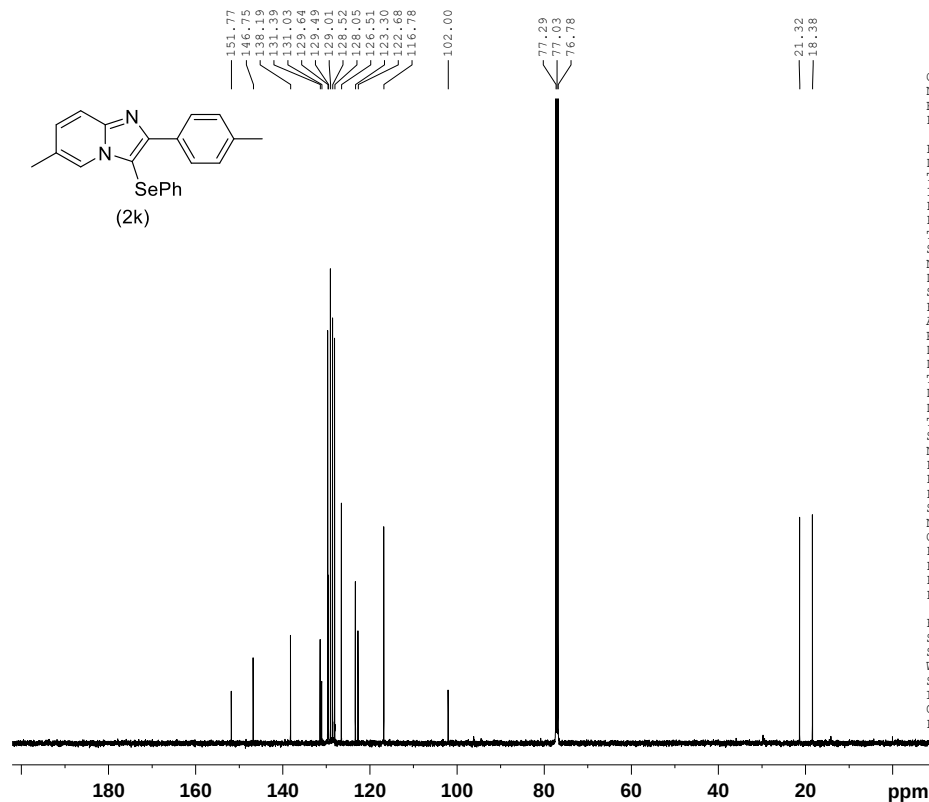
Current Data Parameters
NAME Jan29-2020
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200129
Time_ 13.08 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (PULPROG zg30)
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 101
DW 34.000 usec
DE 6.79 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 22.02300072 W

F2 - Processing parameters
SI 65536
SF 500.1700125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S2

C13CPD CDC13 {D:\Spectra} nmr 6



BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

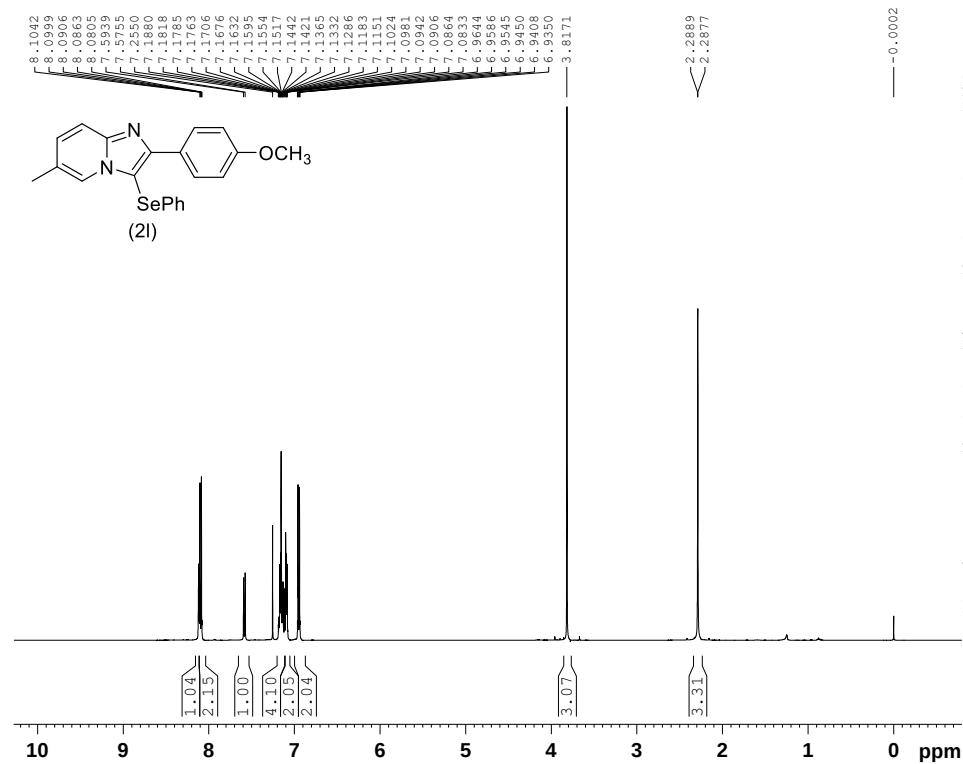
Current Data Parameters
NAME May22-2020
EXPNO 61
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200522
Time_ 18.50 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (PULPROG zgpg30)
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 79.56099701 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 22.02300072 W
PLW12 0.34411001 W
PLW13 0.17308000 W

F2 - Processing parameters
SI 32768
SF 125.7678465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S5

1H_8scan CDC13 {D:\Spectra} nmr 23



BRUKER
 AVANCE NEO
 500 MHz NMR
 SPECTROMETER
 SAIF, P.U.

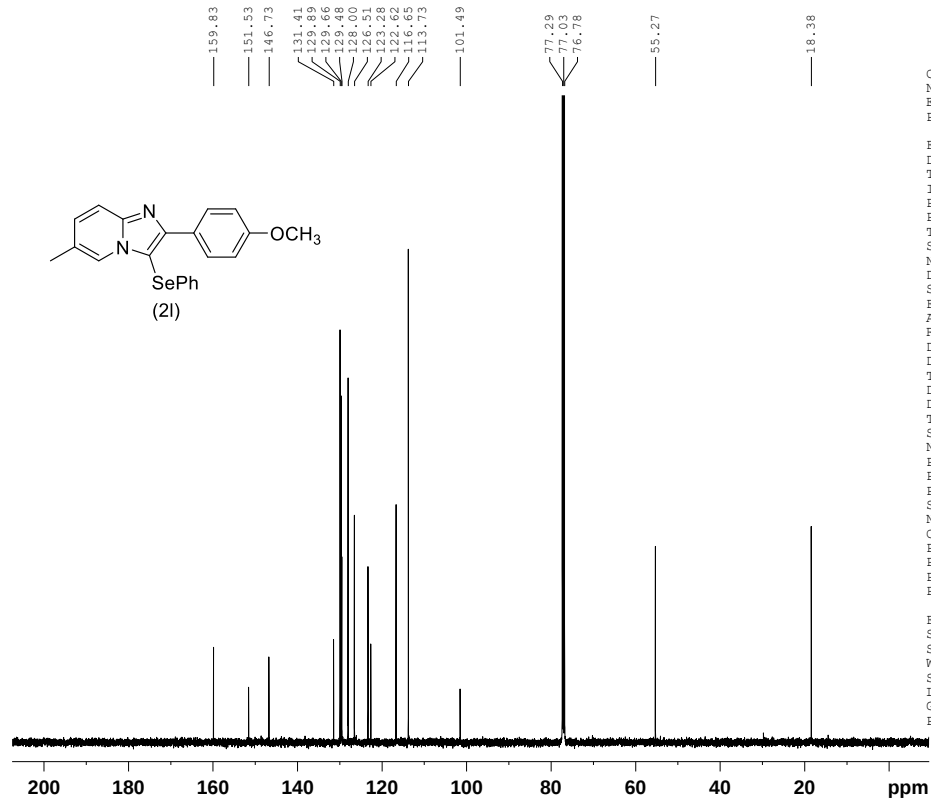
Current Data Parameters
 NAME Mar06-2020
 EXPNO 230
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200306
 Time_ 12.20 h
 INSTRUM Avance Neo 500
 PROBHD Z119470_0333 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 14705.883 Hz
 FIDRES 0.448788 Hz
 AQ 2.2282240 sec
 RG 65.313
 DW 34.000 usec
 DE 6.79 usec
 TE 296.0 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1730885 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 22.02300072 W

F2 - Processing parameters
 SI 65536
 SF 500.1700146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S5

C13CPD CDC13 {D:\Spectra} nmr 11



BRUKER
 AVANCE NEO
 500 MHz NMR SPECTROMETER
 SAIF, PANJAB UNIVERSITY,
 CHANDIGARH

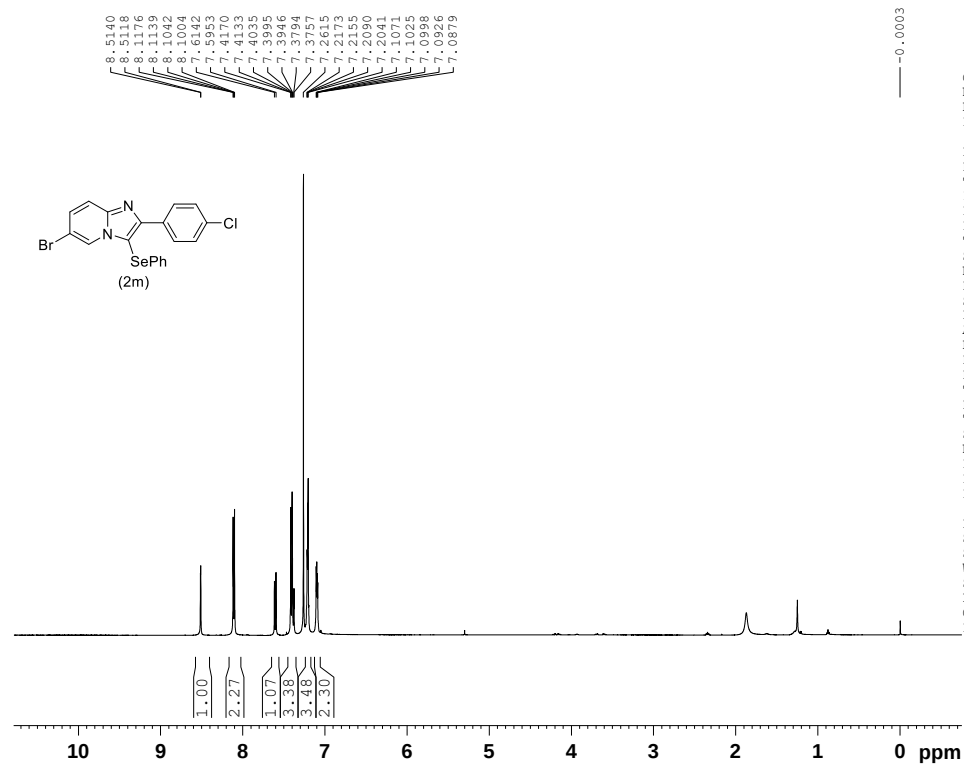
Current Data Parameters
 NAME Jun17-2020
 EXPNO 110
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200617
 Time_ 14.14 h
 INSTRUM Avance Neo 500
 PROBHD Z119470_0333 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 37037.035 Hz
 FIDRES 1.130281 Hz
 AQ 0.8847360 sec
 RG 101
 DW 13.500 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7804233 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 79.56099701 W
 SFO2 500.1720007 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 80.00 usec
 PLW2 22.02300072 W
 PLW12 0.34411001 W
 PLW13 0.17308000 W

F2 - Processing parameters
 SI 32768
 SF 125.7678465 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S15

1H_8scan CDC13 {D:\Spectra} nmr 10



BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

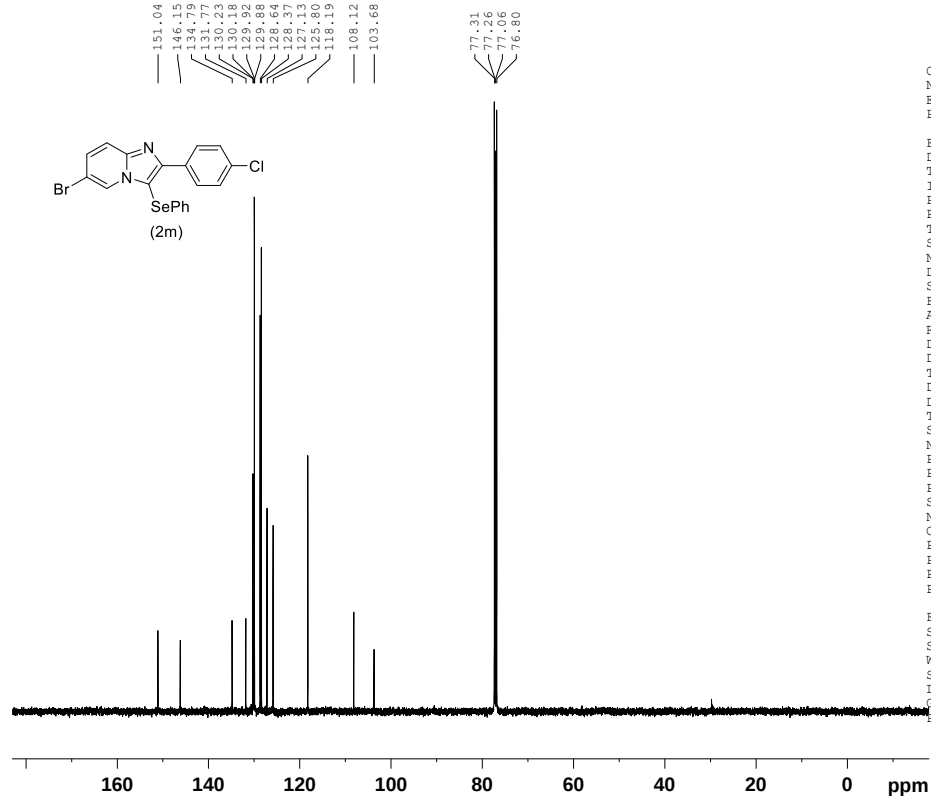
Current Data Parameters
NAME Jul03-2020
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200703
Time_ 13.47 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (PULPROG zg30)
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 101
DW 34.000 usec
DE 6.79 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 22.02300072 W

F2 - Processing parameters
SI 65536
SF 500.1700114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S-15

C13CPD CDC13 {D:\Spectra} nmr 11



BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

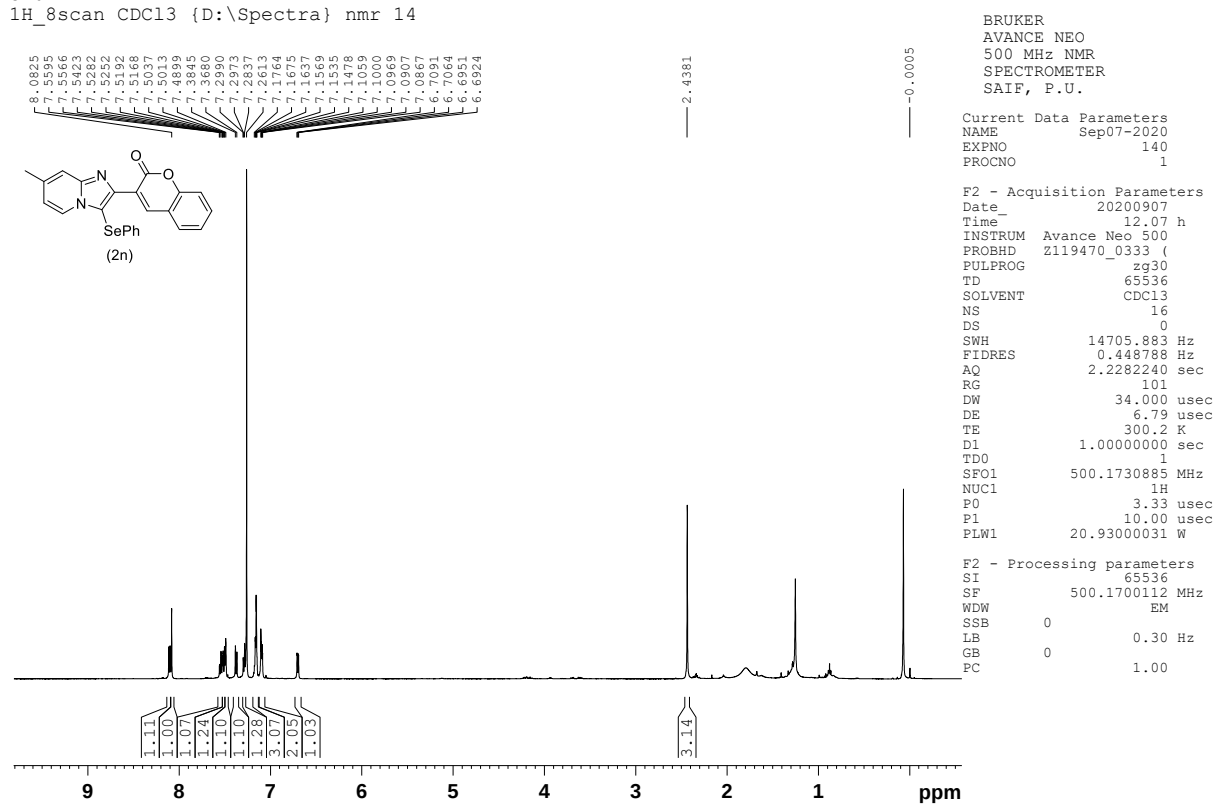
Current Data Parameters
NAME Jul13-2020
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200713
Time_ 14.55 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (PULPROG zgpg30)
TD 65536
SOLVENT CDC13
NS 300
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7678465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

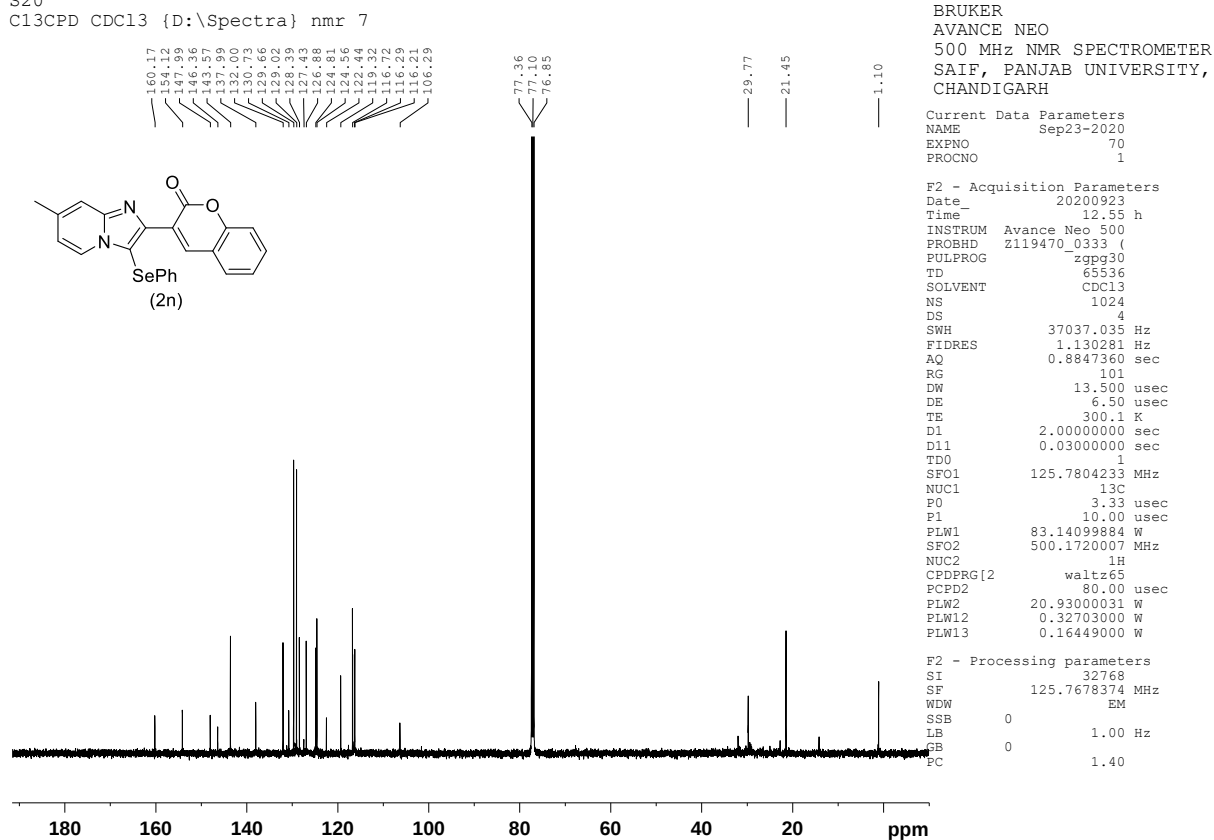
S20

1H_8scan CDC13 {D:\Spectra} nmr 14

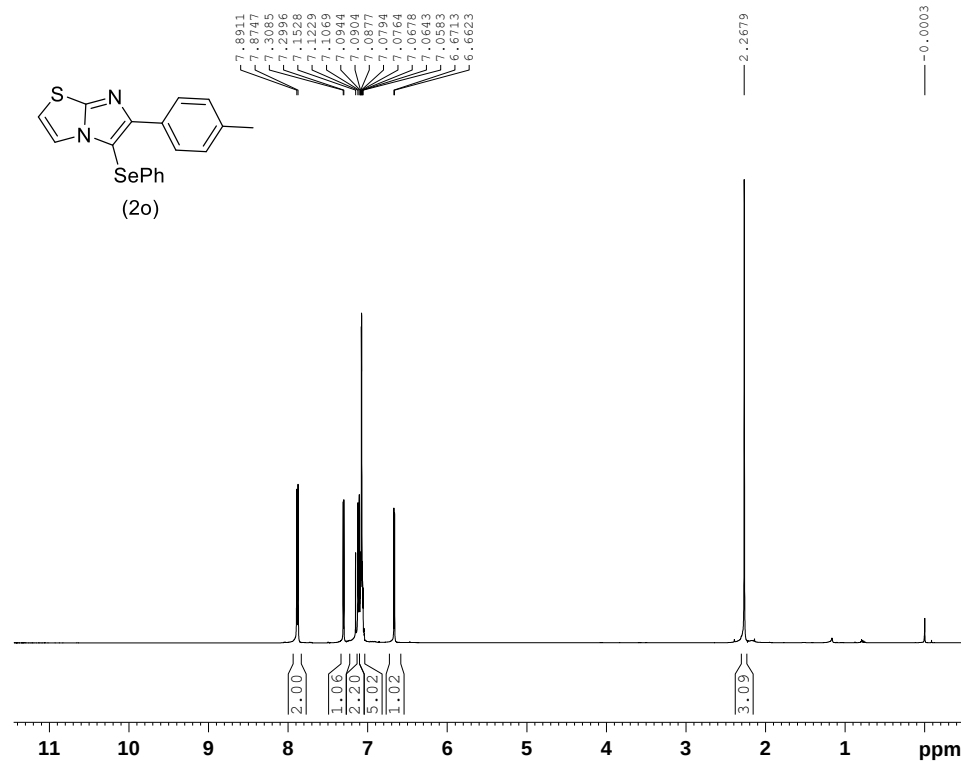


S20

C13CPD CDC13 {D:\Spectra} nmr 7



S19

¹H_8scan CDC13 {D:\Spectra} nmr 12

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

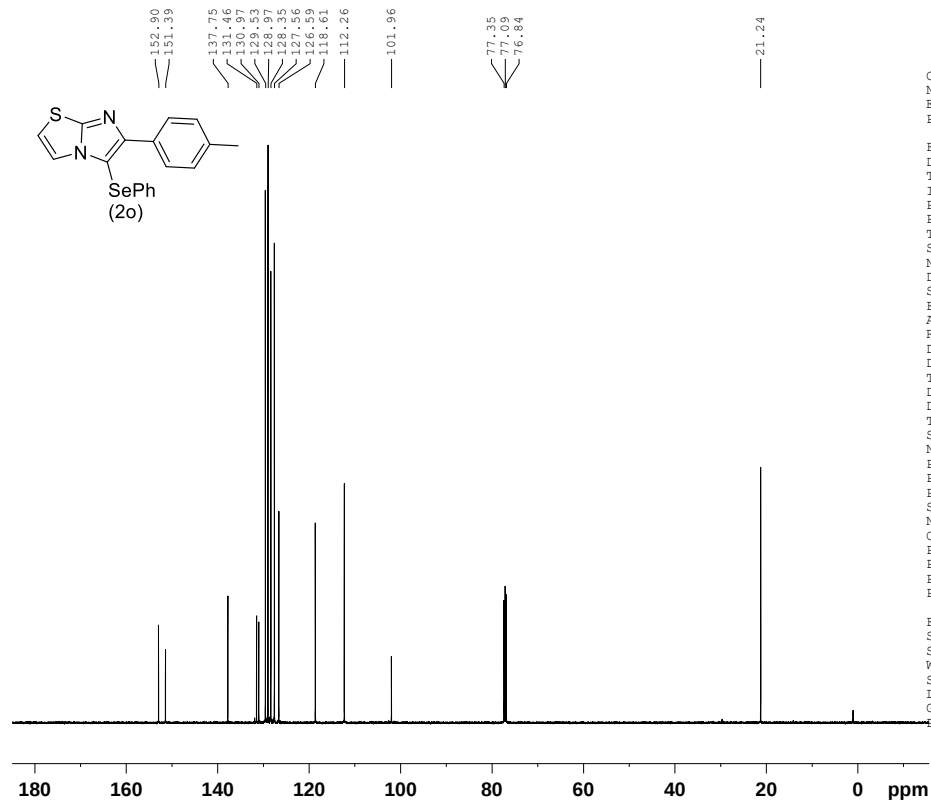
Current Data Parameters
NAME Jul03-2020
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200703
Time_ 13.53 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 ()
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 45.3677
DW 34.000 usec
DE 6.79 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 22.02300072 W

F2 - Processing parameters
SI 65536
SF 500.1700657 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S-19

C13CPD CDC13 {D:\Spectra} nmr 13



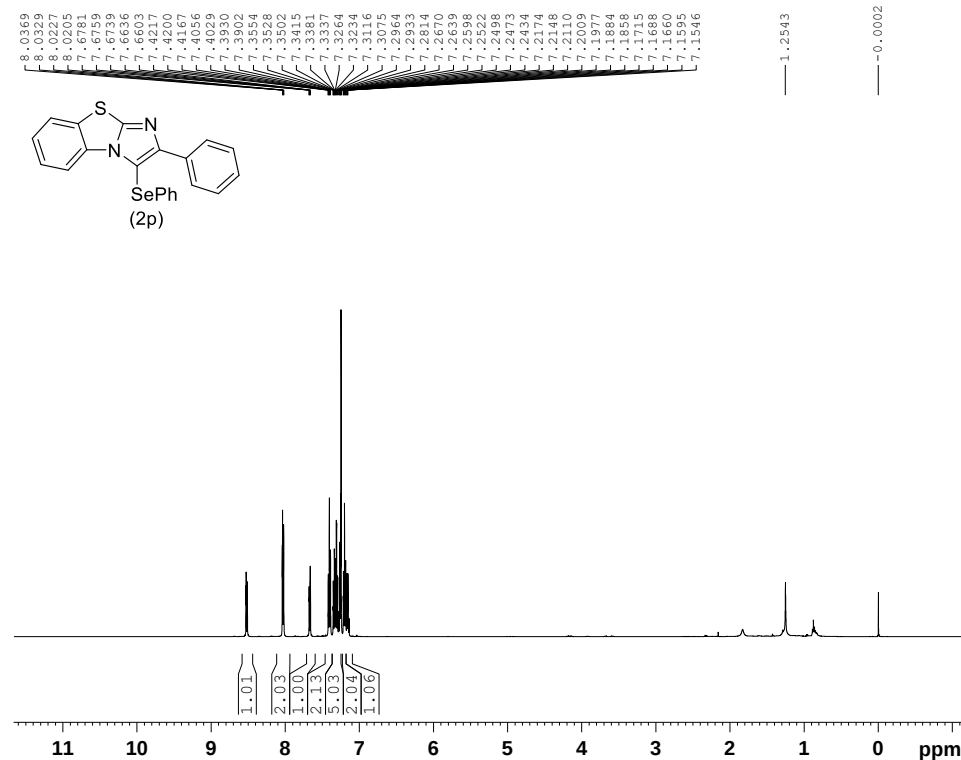
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jul13-2020
EXPNO 130
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200713
Time_ 15.35 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 ()
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 200
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 83.14099884 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7678650 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S13

¹H_8scan CDC13 {D:\Spectra} nmr 26

BRUKER
AVANCE NEO
500 MHz NMR
SPECTROMETER
SAIF, P.U.

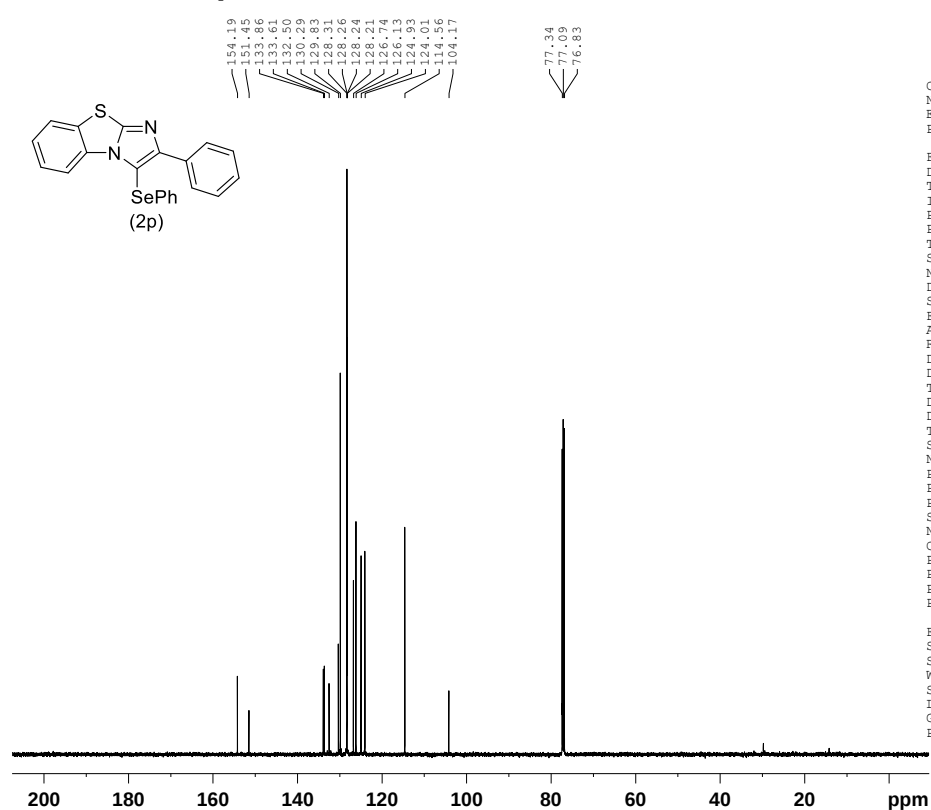
Current Data Parameters
NAME Mar06-2020
EXPNO 260
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200306
Time_ 12.29 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 22.02300072 W

F2 - Processing parameters
SI 65536
SF 500.1700185 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S13

C13CPD CDC13 {D:\Spectra} nmr 16



BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

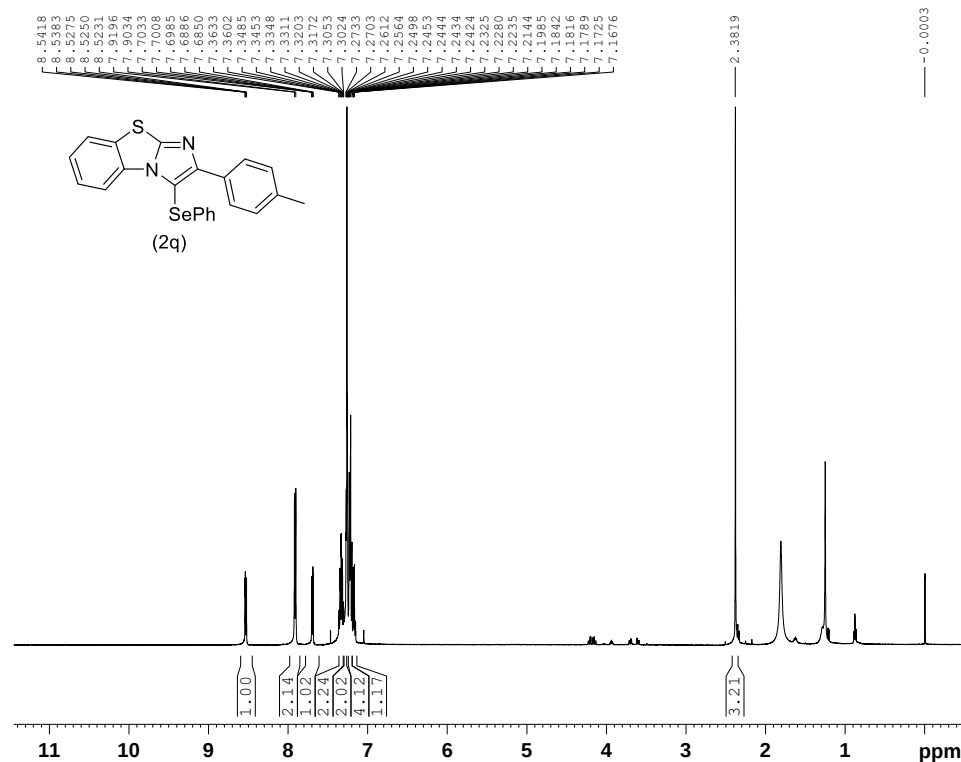
Current Data Parameters
NAME Jun17-2020
EXPNO 160
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200617
Time_ 15.56 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 315
DS 4
SWH 37037.035 Hz
FIDRES 1.130281 Hz
AQ 0.8847360 sec
RG 101
DW 13.500 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7804233 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 79.56099701 W
SFO2 500.1720007 MHz
NUC2 1H
CPDPRG2 waltz65
PCPD2 80.00 usec
PLW2 22.02300072 W
PLW12 0.34411001 W
PLW13 0.17308000 W

F2 - Processing parameters
SI 32768
SF 125.7678465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S16

1H_8scan CDC13 {D:\Spectra} nmr 11



BRUKER
 AVANCE NEO
 500 MHz NMR
 SPECTROMETER
 SAIF, P.U.

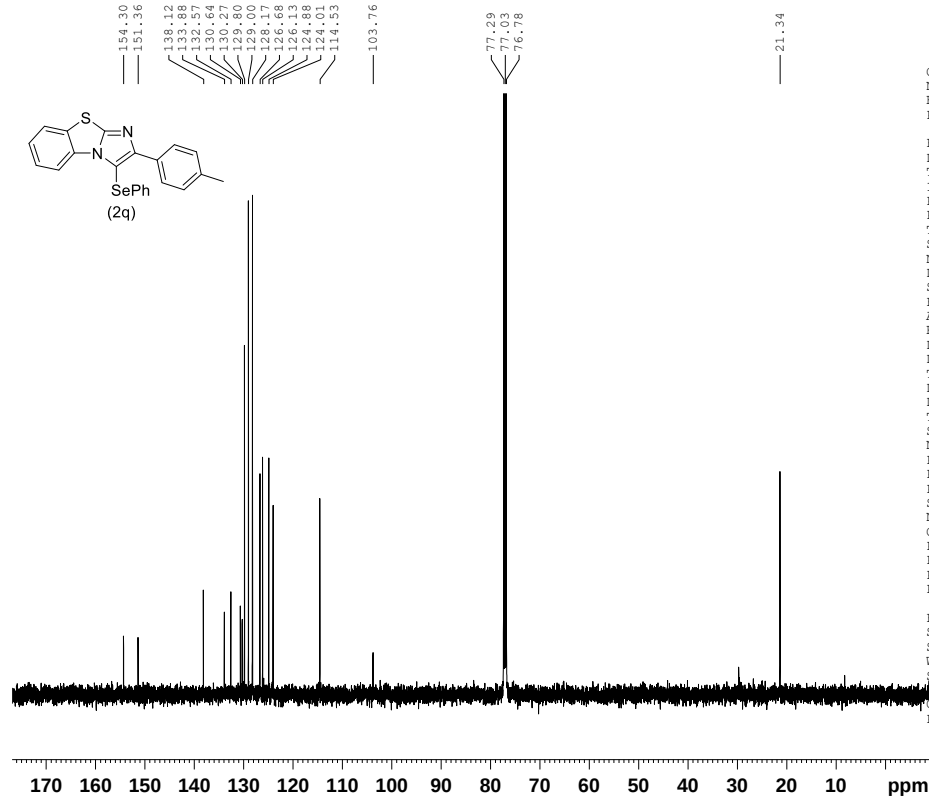
Current Data Parameters
 NAME Jul03-2020
 EXPNO 110
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200703
 Time_ 13.50 h
 INSTRUM Avance Neo 500
 PROBHD Z119470_0333 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 14705.883 Hz
 FIDRES 0.448788 Hz
 AQ 2.2282240 sec
 RG 101
 DW 34.000 usec
 DE 6.79 usec
 TE 293.9 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1730885 MHz
 NUC1 1H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 22.02300072 W

F2 - Processing parameters
 SI 65536
 SF 500.1700115 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S-16

C13CPD CDC13 {D:\Spectra} nmr 12



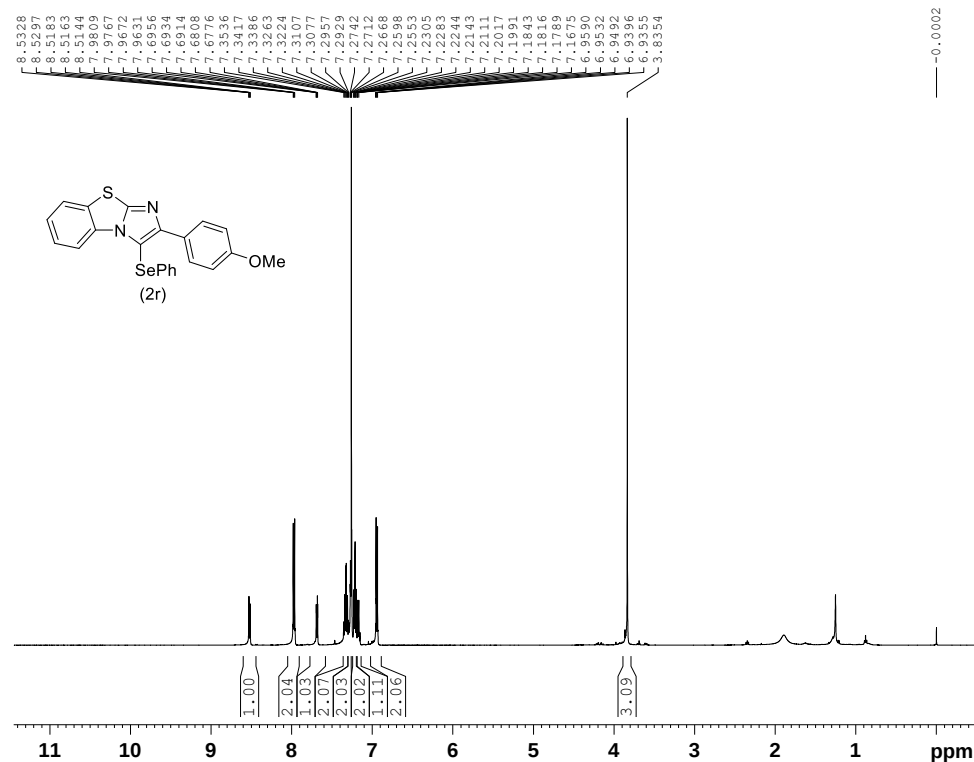
BRUKER
 AVANCE NEO
 500 MHz NMR SPECTROMETER
 SAIF, PANJAB UNIVERSITY,
 CHANDIGARH

Current Data Parameters
 NAME Jul13-2020
 EXPNO 120
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200713
 Time_ 15.23 h
 INSTRUM Avance Neo 500
 PROBHD Z119470_0333 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 37037.035 Hz
 FIDRES 1.130281 Hz
 AQ 0.8847360 sec
 RG 101
 DW 13.500 usec
 DE 6.50 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7804233 MHz
 NUC1 13C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 83.14099884 W
 SFO2 500.1720007 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 80.00 usec
 PLW2 20.93000031 W
 PLW12 0.32703000 W
 PLW13 0.16449000 W

F2 - Processing parameters
 SI 32768
 SF 125.7678465 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S14

¹H_8scan CDC13 {D:\Spectra} nmr 9

BRUKER
 AVANCE NEO
 500 MHz NMR
 SPECTROMETER
 SAIF, P.U.

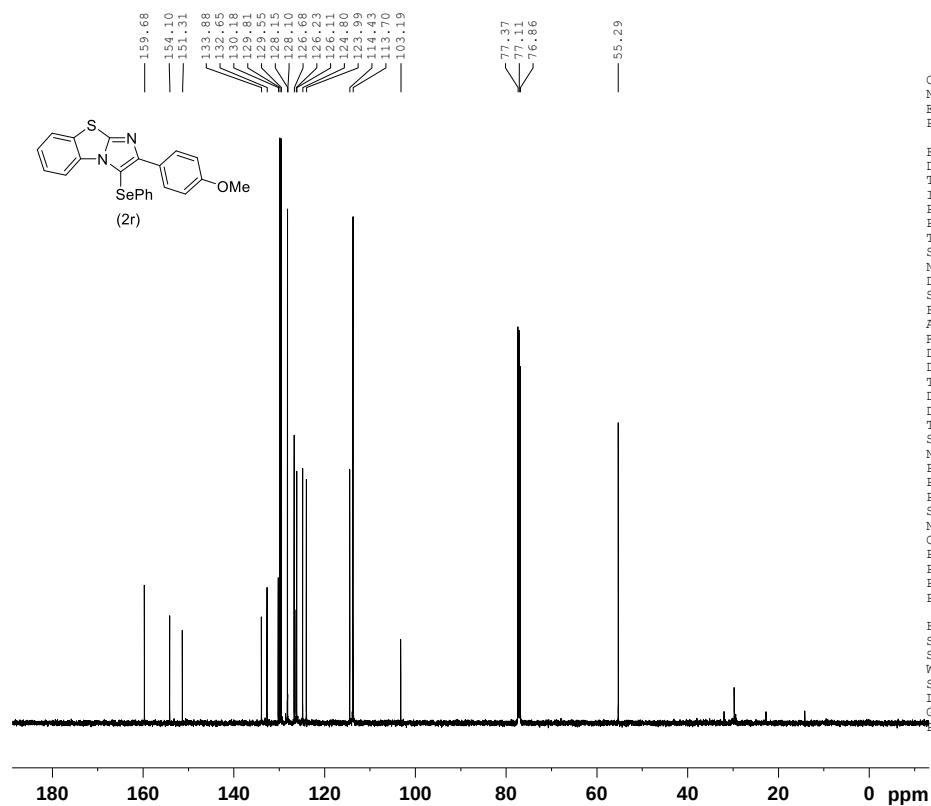
Current Data Parameters
 NAME Jul03-2020
 EXPNO 90
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200703
 Time 13.44 h
 INSTRUM Avance Neo 500
 PROBHD Z119470_0333 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 0
 SWH 14705.883 Hz
 FIDRES 0.448788 Hz
 AQ 2.2282240 sec
 RG 101
 DW 34.000 usec
 DE 6.79 usec
 TE 293.9 K
 D1 1.00000000 sec
 TD0 1
 SFO1 500.1730885 MHz
 NUC1 ¹H
 P0 3.33 usec
 P1 10.00 usec
 PLW1 22.02300072 W

F2 - Processing parameters
 SI 65536
 SF 500.1700123 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S-14

C13CPD CDC13 {D:\Spectra} nmr 10



BRUKER
 AVANCE NEO
 500 MHz NMR SPECTROMETER
 SAIF, PANJAB UNIVERSITY,
 CHANDIGARH

Current Data Parameters
 NAME Jul13-2020
 EXPNO 100
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200713
 Time 14.38 h
 INSTRUM Avance Neo 500
 PROBHD Z119470_0333 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 200
 DS 4
 SWH 37037.035 Hz
 FIDRES 1.130281 Hz
 AQ 0.8847360 sec
 RG 101
 DW 13.500 usec
 DE 6.50 usec
 TE 296.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7804233 MHz
 NUC1 ¹³C
 P0 3.33 usec
 P1 10.00 usec
 PLW1 83.14099884 W
 SFO2 500.1720007 MHz
 NUC2 ¹H
 CPDPRG2 waltz65
 PCPD2 80.00 usec
 PLW2 20.93000031 W
 PLW12 0.32703000 W
 PLW13 0.16449000 W

F2 - Processing parameters
 SI 32768
 SF 125.7678465 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40