

Supporting Information

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Synthesis of some piperazine/piperidine amides of chromone-2-carboxylic acid as potential soluble epoxide hydrolase (sEH) inhibitors

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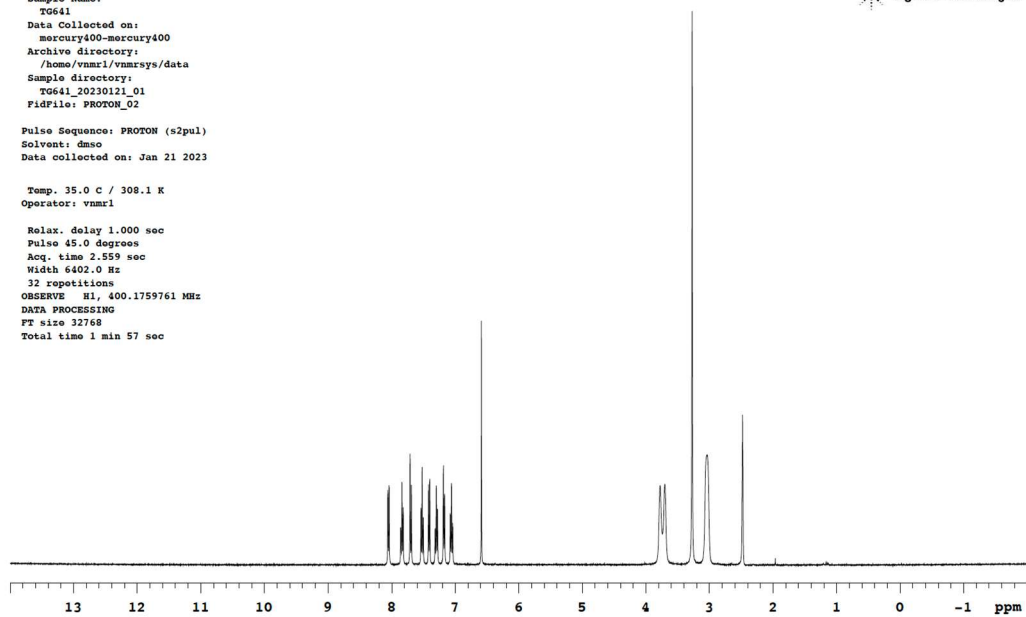
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TG641



Sample Name:
TG641
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
TG641_20230121_01
Fidfile: PROTON_01
Pulse Sequence: PROTON (s2pul)
Solvent: dmsd
Data collected on: Jan 21 2023
Temp. 35.0 C / 308.1 K
Operator: vnmr1
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
32 repetitions
OBSERVE H1, 400.1759761 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec



PROTON_01 -- TG641 --

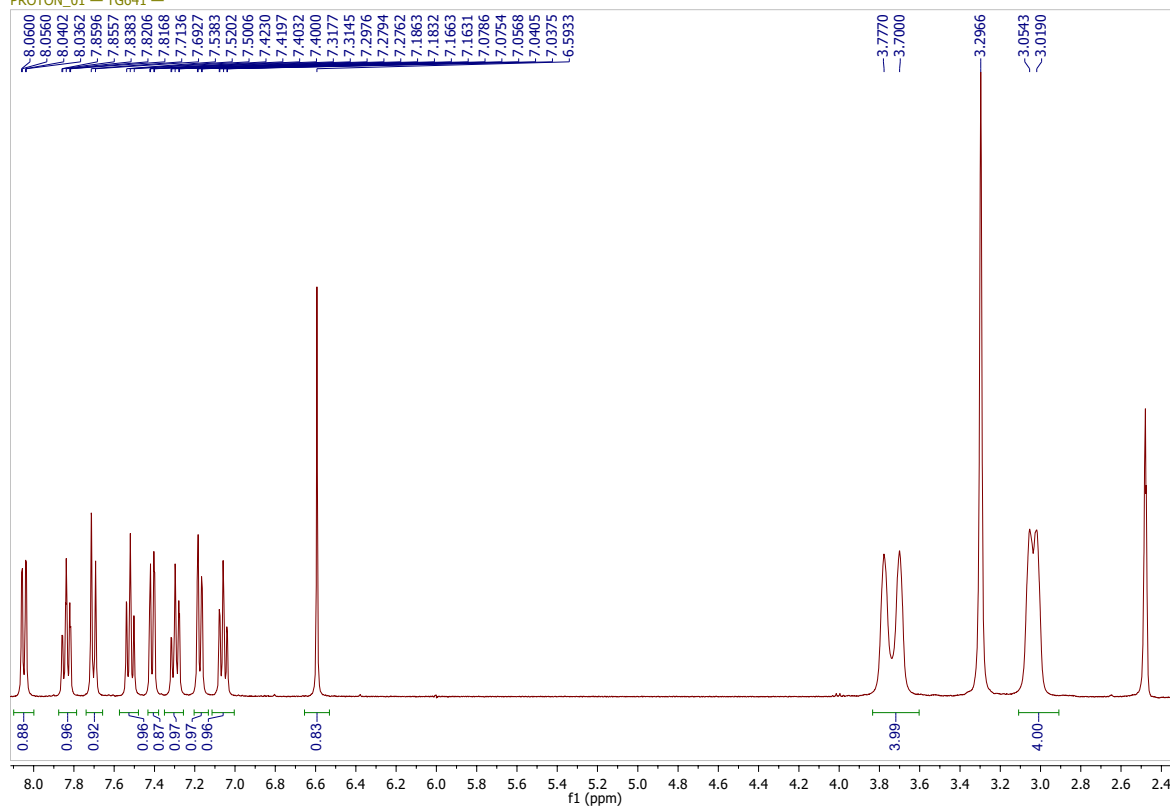


Figure S1: $^1\text{H-NMR}$ spectrum of **2**

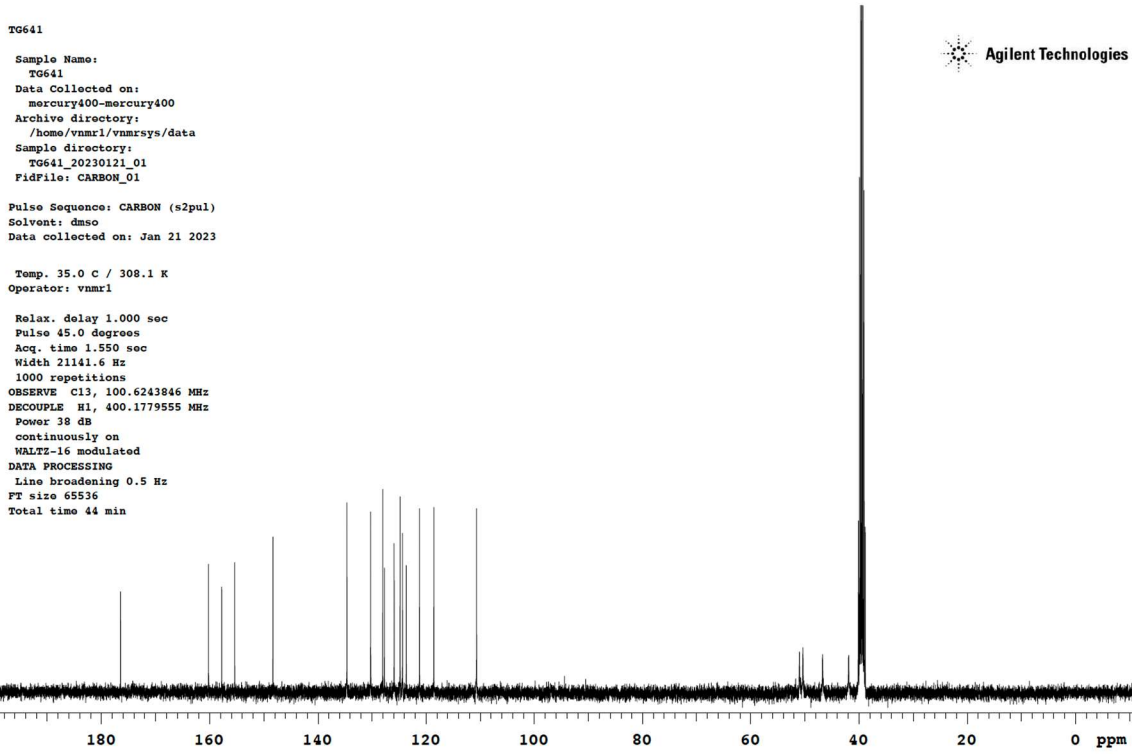


Figure S2: ¹³C-NMR spectrum of 2

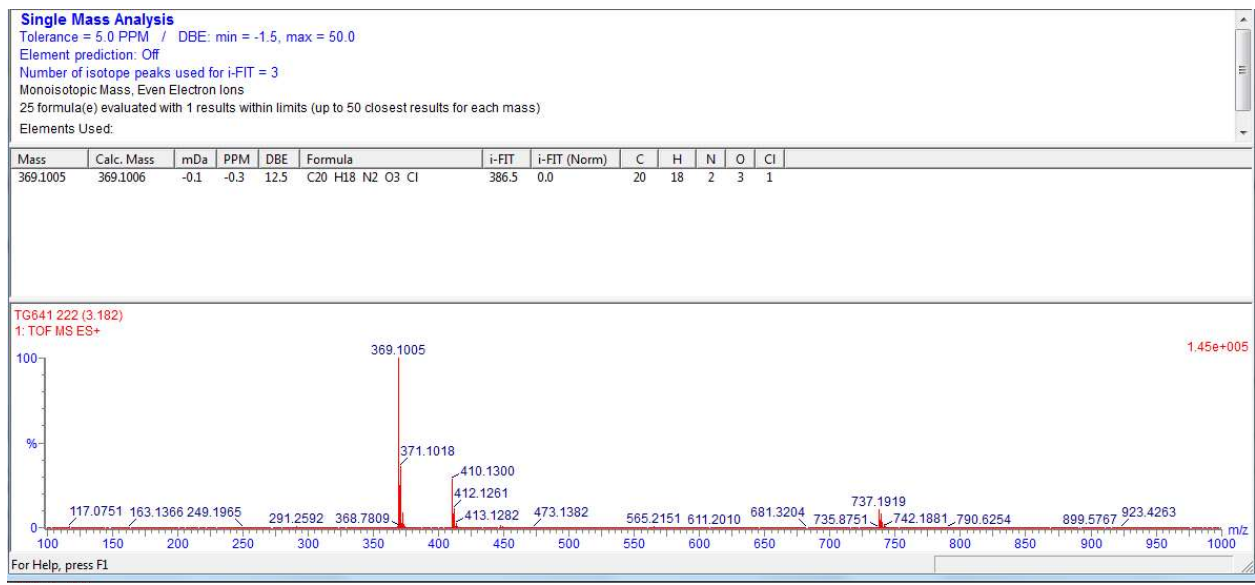
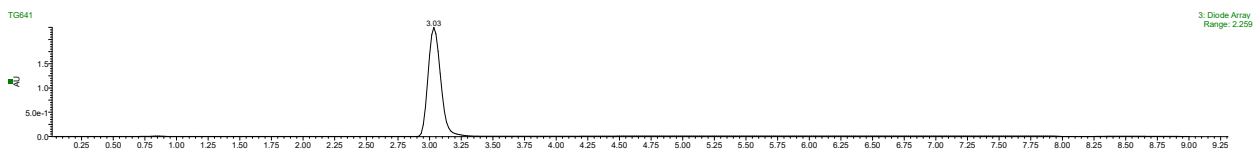


Figure S3: HRMS spectrum of compound 2

TG643

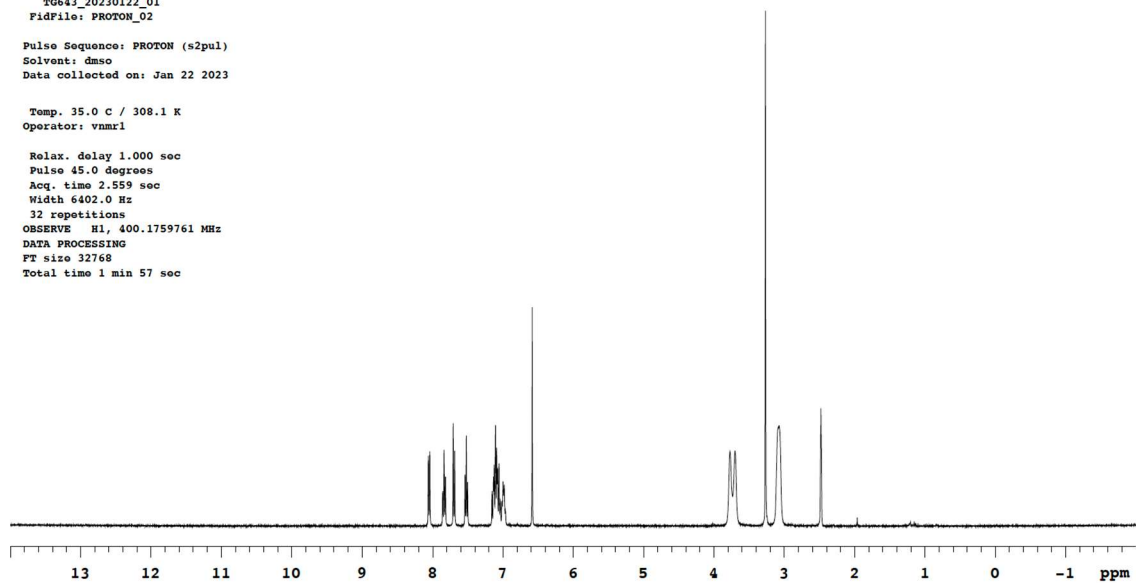


Sample Name:
TG643
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
TG643_20230122_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: dmsc
Data collected on: Jan 22 2023

Temp. 35.0 C / 308.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
32 repetitions
OBSERVE H1, 400.1759761 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec



PROTON_01 — TG643 —

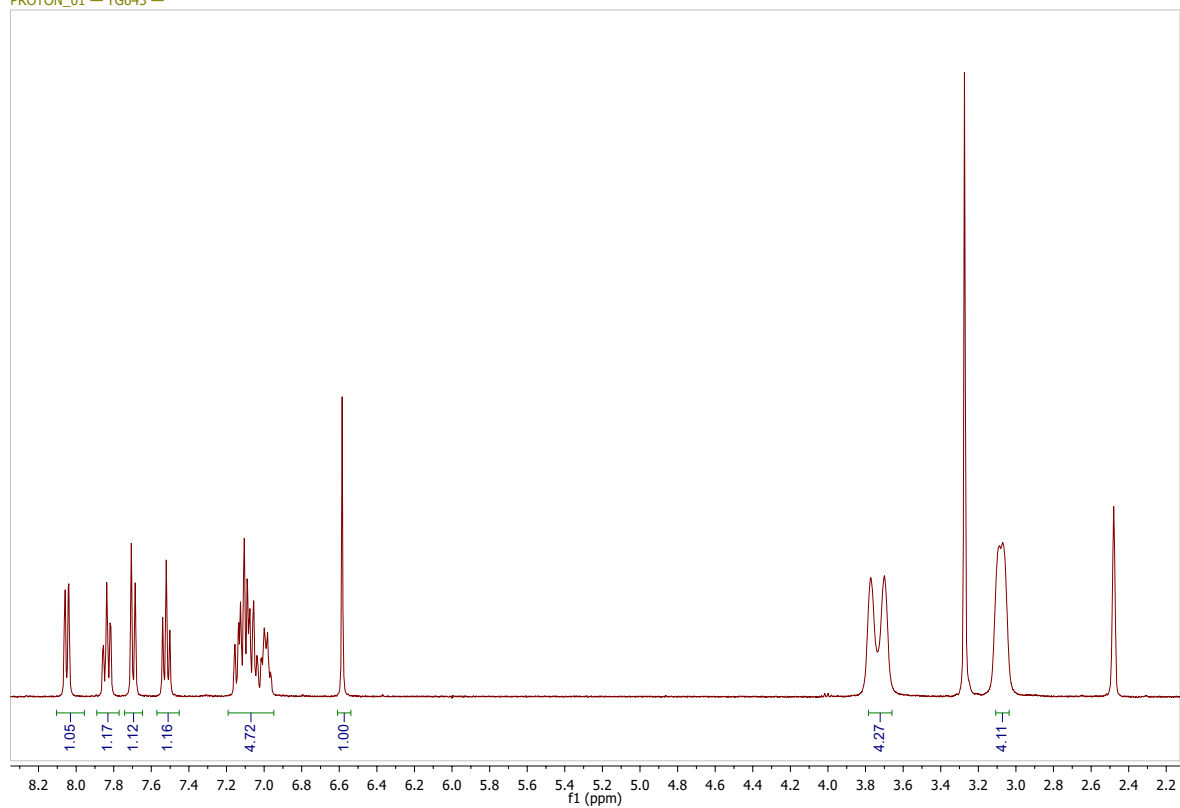


Figure S4: $^1\text{H-NMR}$ spectrum of **3**

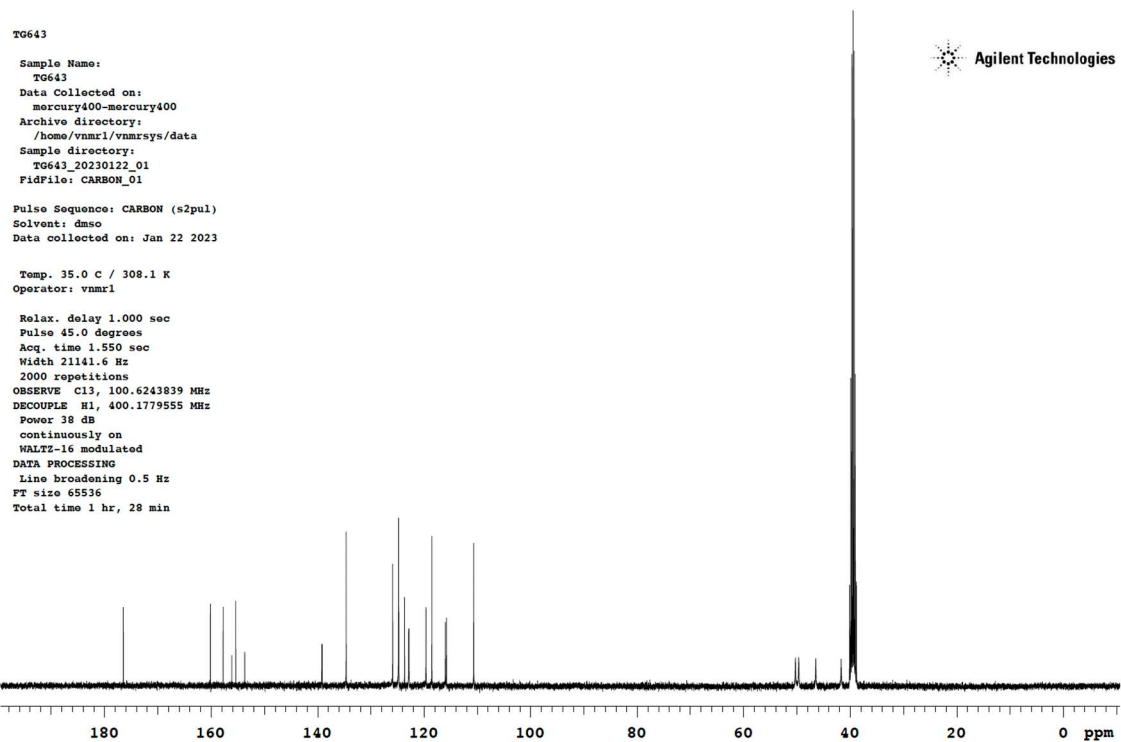


Figure S5: ^{13}C -NMR spectrum of **3**

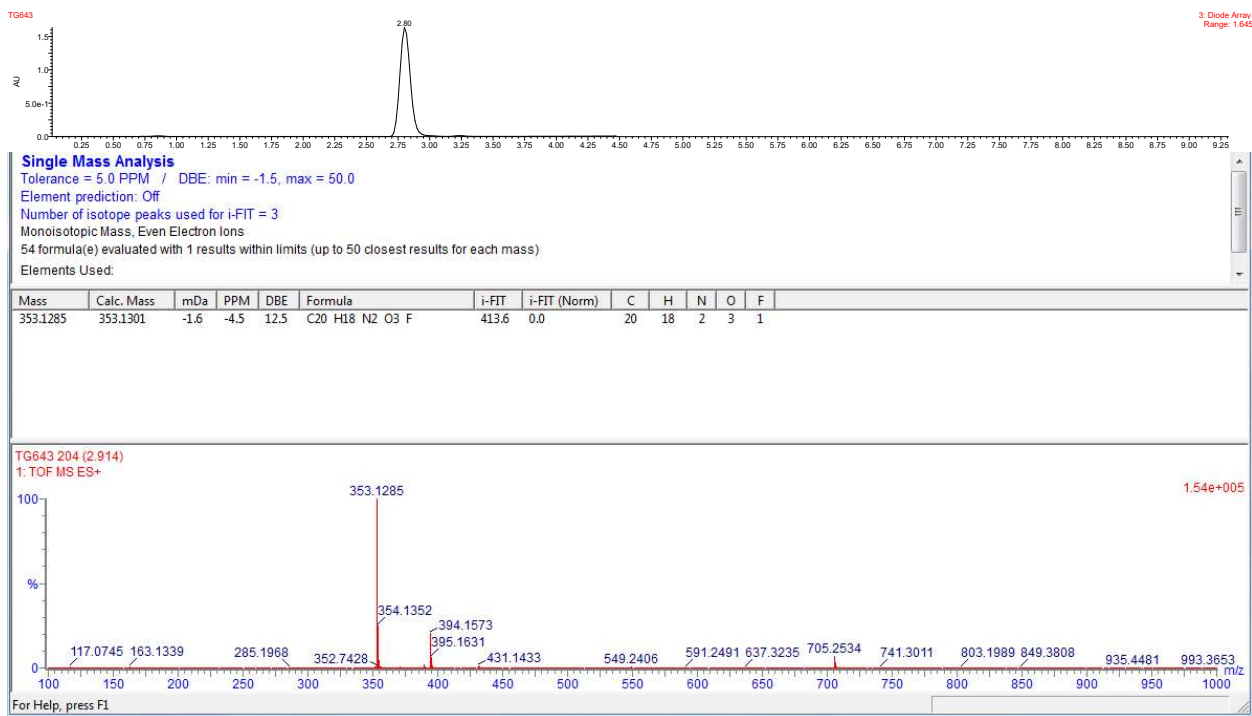


Figure S6: HRMS spectrum of compound **3**

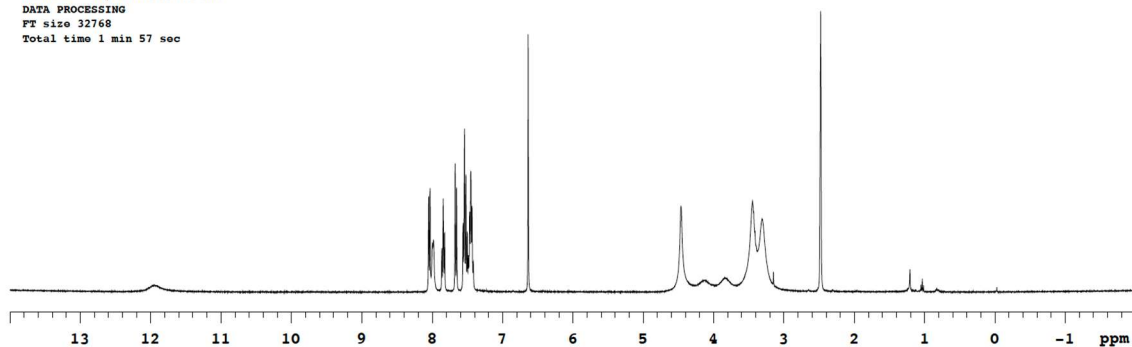
TG642



Sample Name:
TG642
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
TG642_20230121_01
FidFile: PROTON_02
Pulse Sequence: PROTON (s2pul)
Solvent: dms0
Data collected on: Jan 21 2023

Temp. 35.0 C / 308.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
32 repetitions
OBSERVE H1, 400.1759761 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec



PROTON_01 -- TG642 --

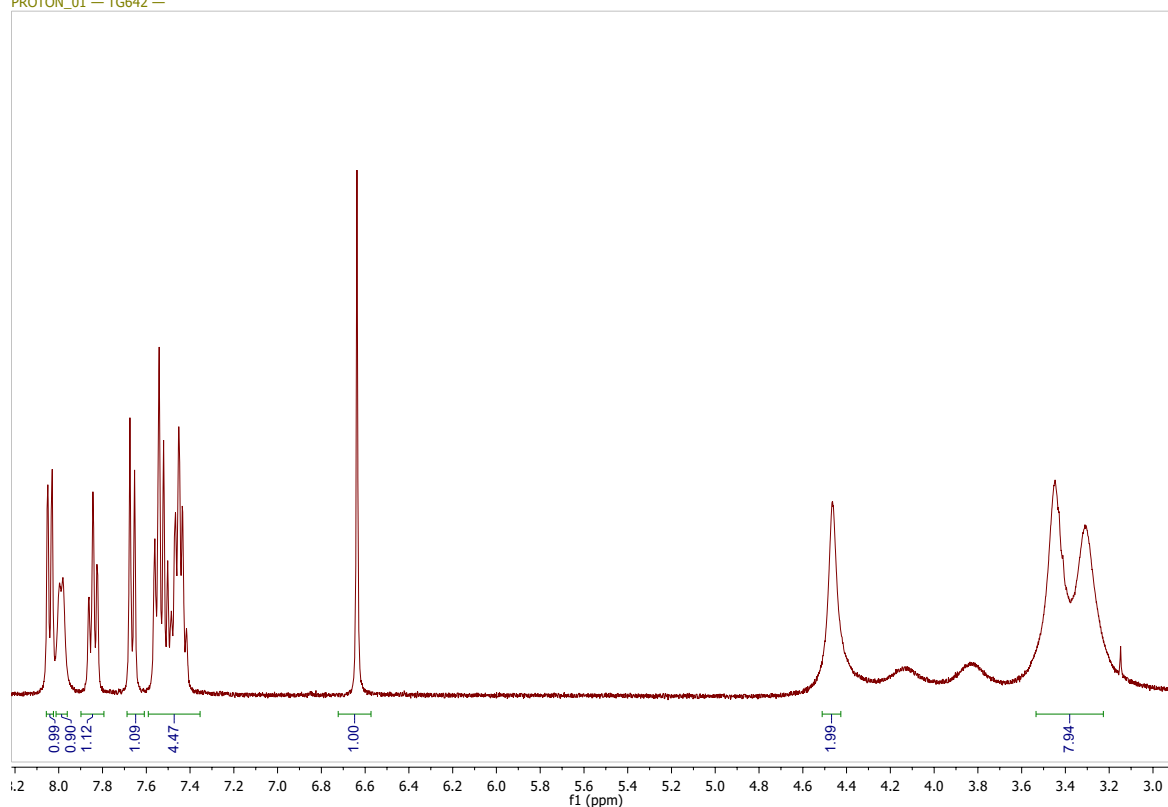


Figure S7: ¹H-NMR spectrum of **4**

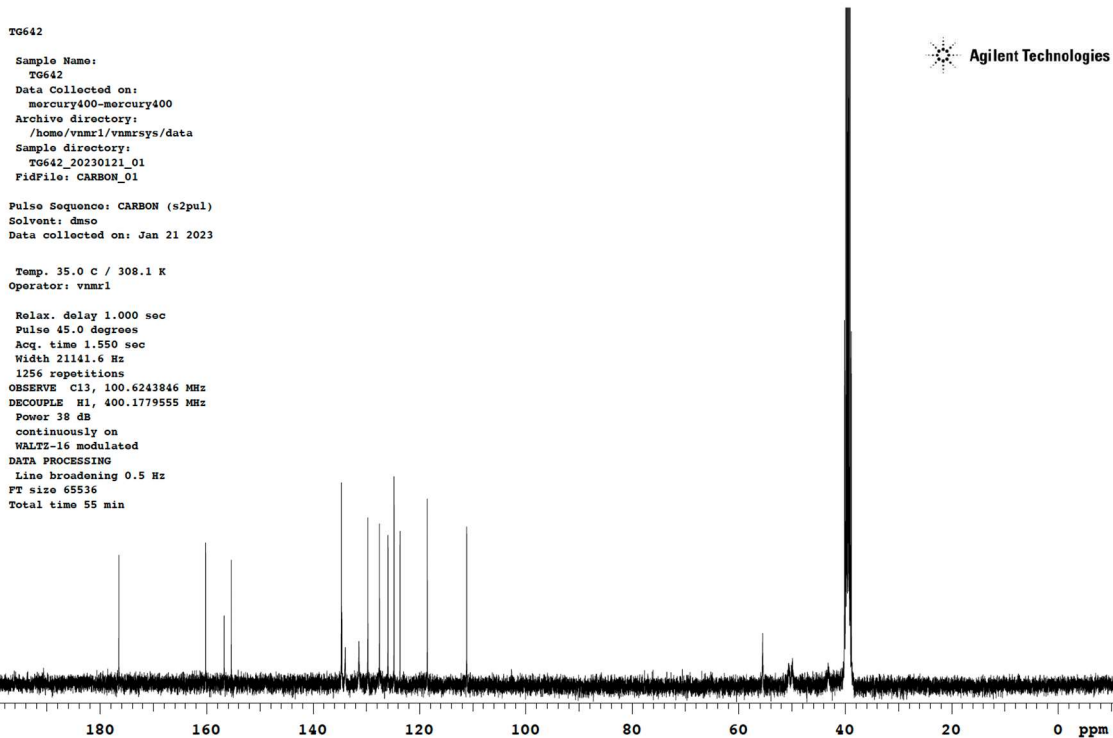


Figure S8: ^{13}C -NMR spectrum of 4

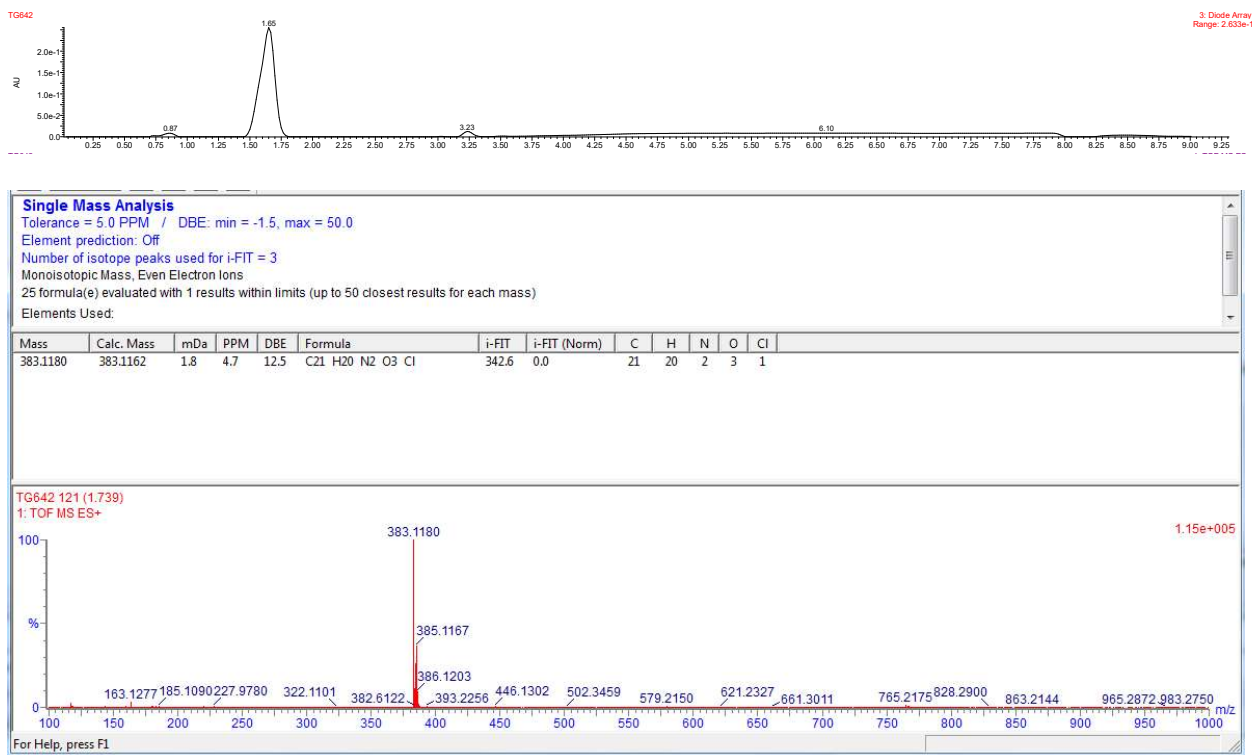


Figure S9: HRMS spectrum of 4

TG644

Sample Name:
TG644
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
TG644_20230122_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: dmsc
Data collected on: Jan 22 2023



Temp. 35.0 C / 308.1 K
Operator: vnmr1

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.559 sec
Width 6402.0 Hz
32 repetitions
OBSERVE H1, 400.1759761 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 57 sec

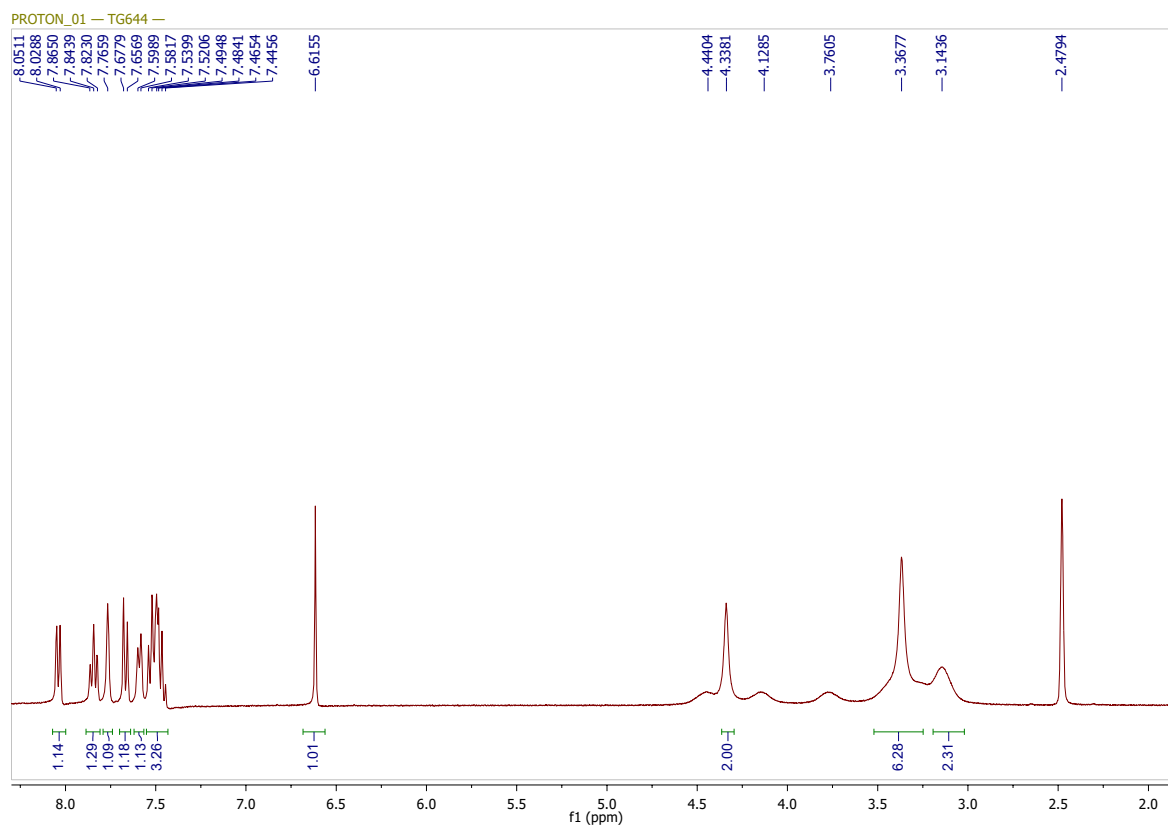
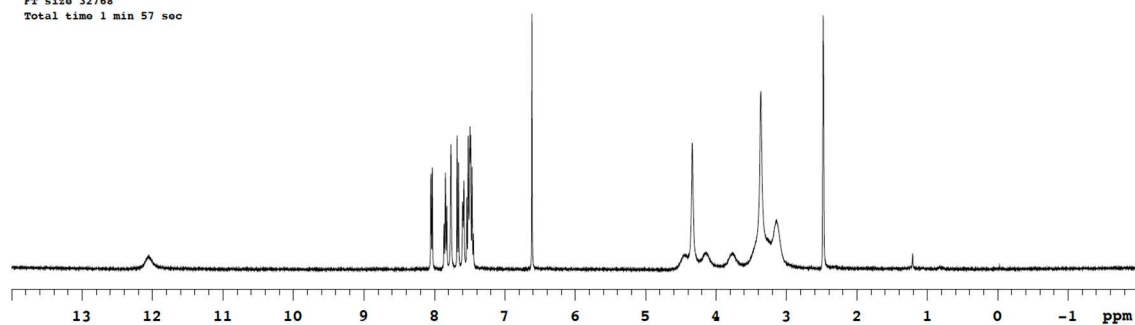


Figure S10: $^1\text{H-NMR}$ spectrum of **5**

TG644

Sample Name:
TG644

Data Collected on:
mercury400-mercury400

Archive directory:
/home/vnmr1/vnmrsys/data

Sample directory:
TG644_20230122_01

FidFile: current

Pulse Sequence: CARBON (s2pul)

Solvent: dmsc

Data collected on: Jan 22 2023

Temp. 35.0 C / 308.1 K

Operator: vnmr1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.550 sec

Width 21141.6 Hz

1984 repetitions

OBSERVE C13, 100.6243846 MHz

DECOUPLE H1, 400.1779555 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 28 min

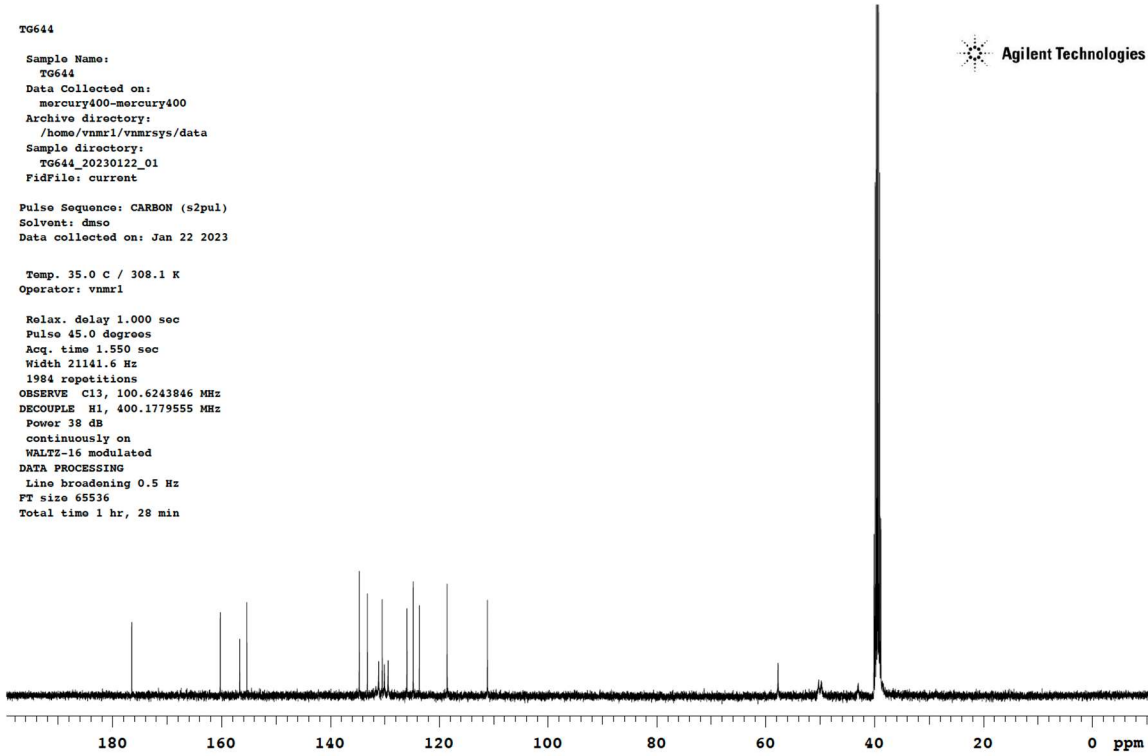


Figure S11: ¹³C-NMR spectrum of 5

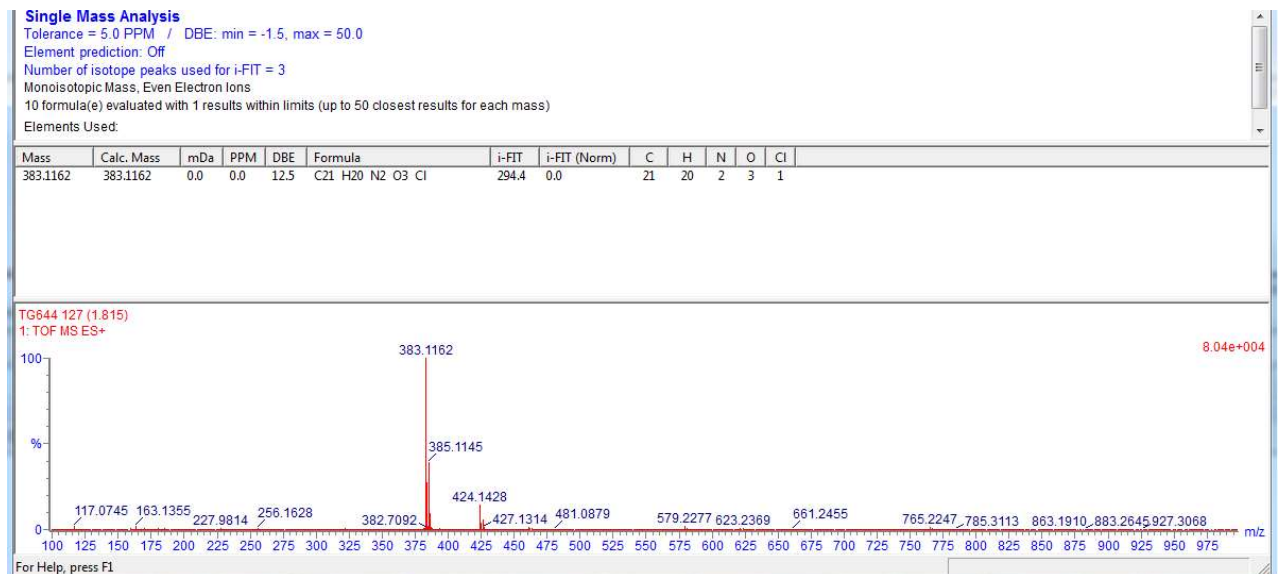
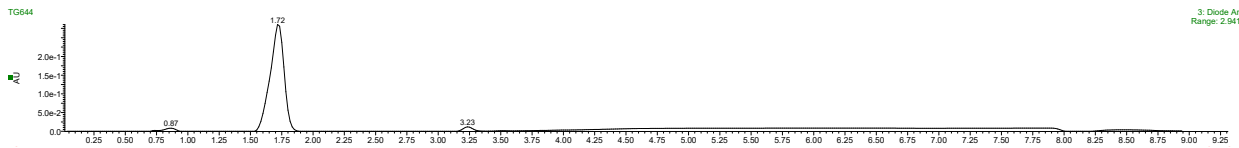


Figure S12. HRMS spectrum of 5



Current Data Parameters
NAME TG613
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220728
Time 10:46 h
INSTRUM Avance
PROBHD Z151574_0038 ()
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330883 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.04299927 W

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

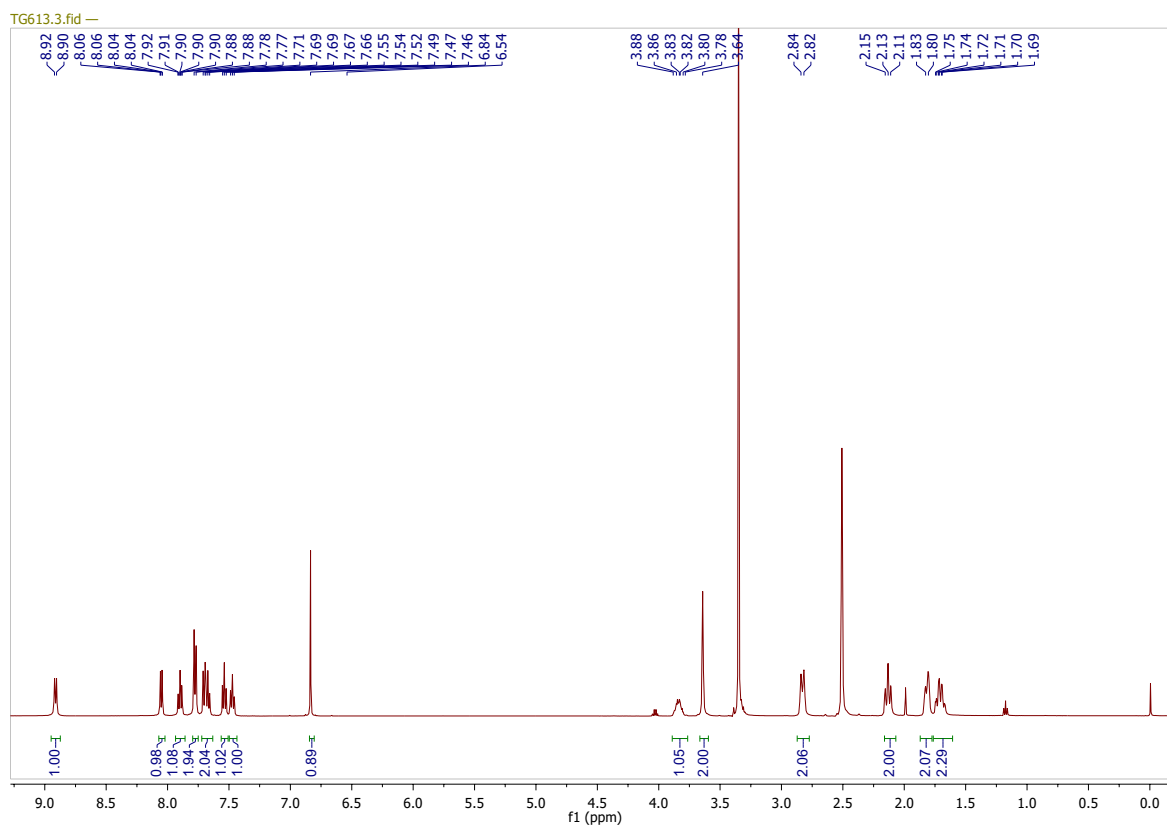
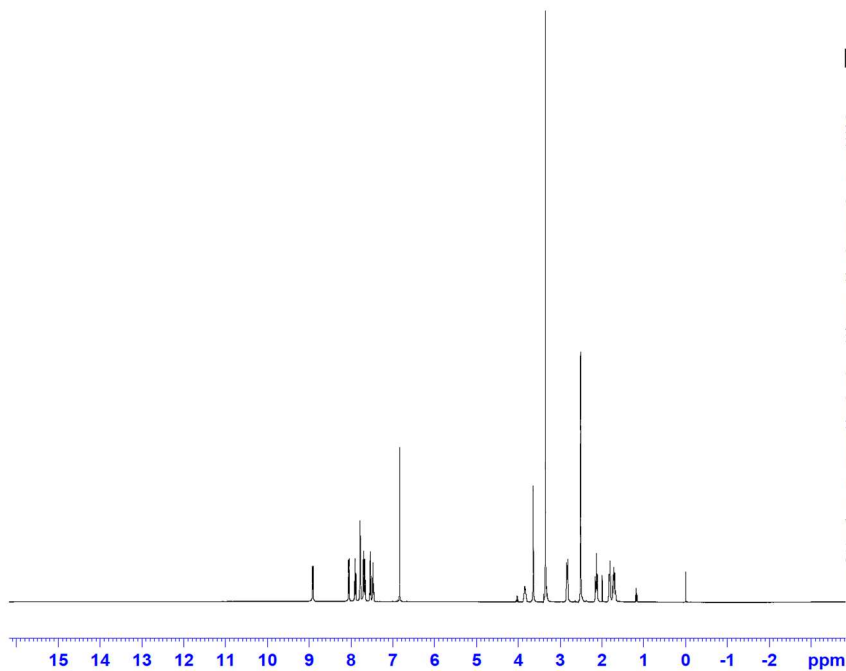


Figure S13: $^1\text{H-NMR}$ spectrum of **7**

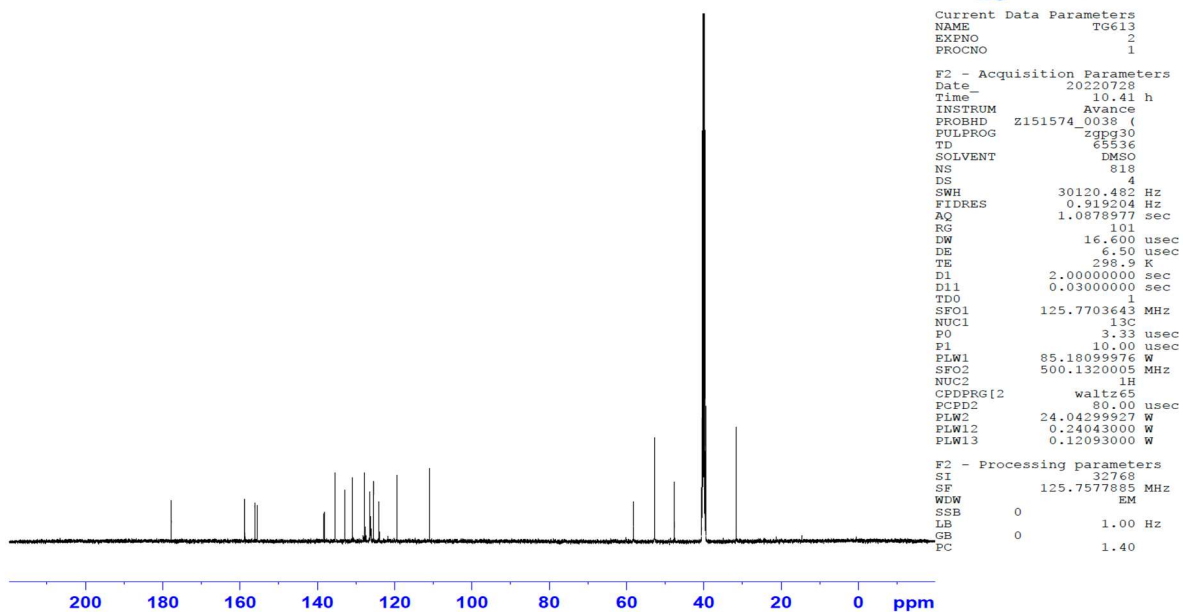
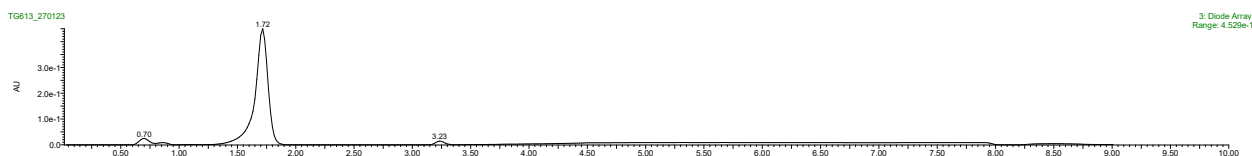


Figure S14: ^{13}C -NMR spectrum of 7



Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT (Norm)	C	H	N	O	F
431.1575	431.1583	-0.8	-1.9	12.5	C ₂₃ H ₂₂ N ₂ O ₃ F ₃	334.7	0.0	23	22	2	3	3

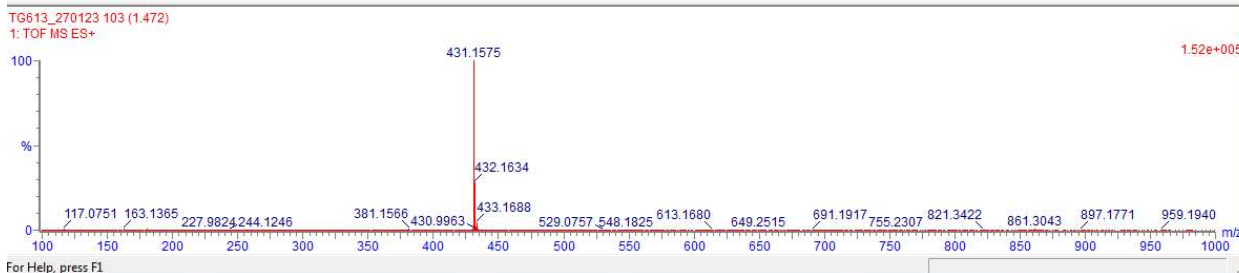


Figure S15: HRMS spectrum of 7



Current Data Parameters
NAME BY238
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220728
Time 12.58 h
INSTRUM Avance
PROBHD Z151574_0038 (z
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 32
DW 50.000 usec
DE 11.14 usec
TE 298.9 K
D1 1.00000000 sec
TDO 1
SFO1 500.1330883 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.04299927 W

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

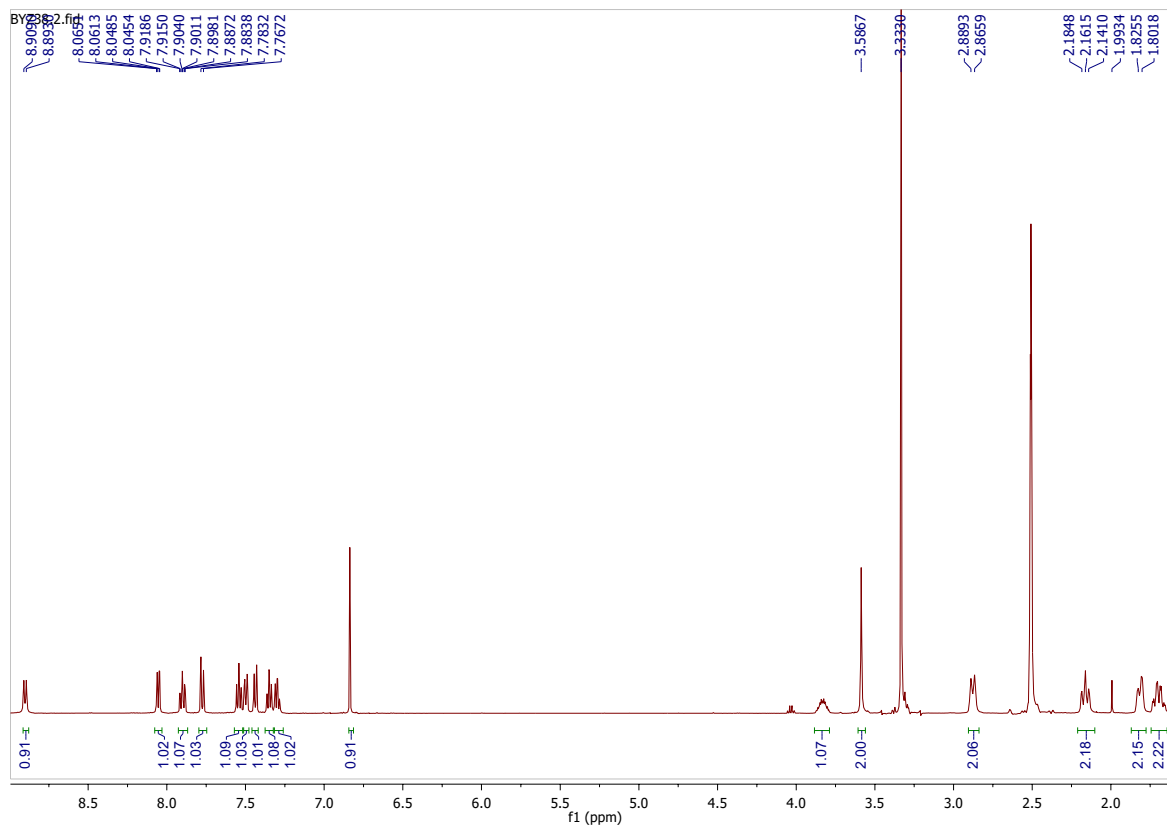
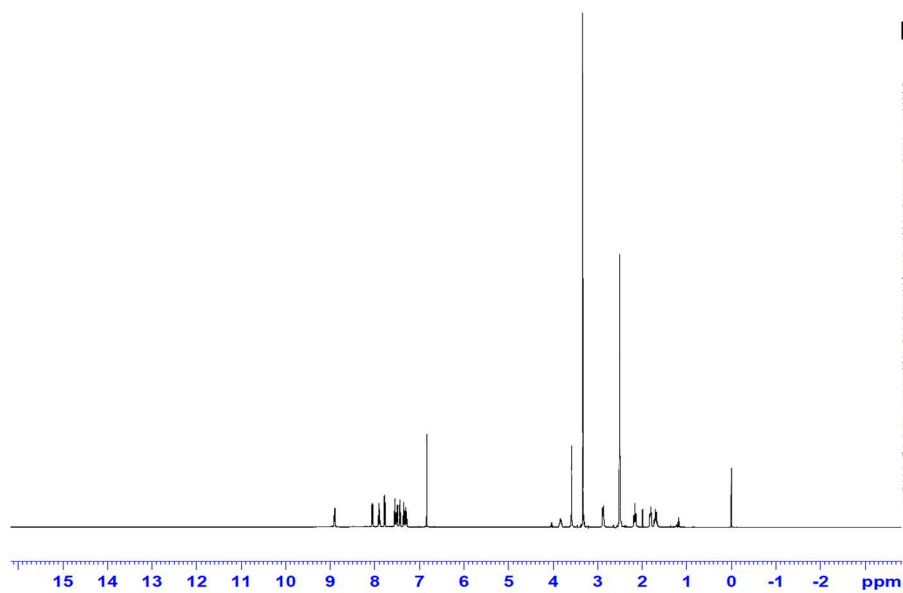


Figure S16: ^1H -NMR spectrum of **8**

BYZ-38

Sample Name:
BYZ-38

Data Collected on:
mercury400-mercury400

Archive directory:
/home/vnmr1/vnmrsys/data

Sample directory:
BYZ-38_20230120_01

FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)

Solvent: dmsc

Data collected on: Jan 20 2023

Temp. 33.0 C / 306.1 K

Operator: vnmr1

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.550 sec

Width 21141.6 Hz

2000 repetitions

OBSERVE C13, 100.6243826 MHz

DECOUPLE H1, 400.1779555 MHz

Power 38 db

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 28 min

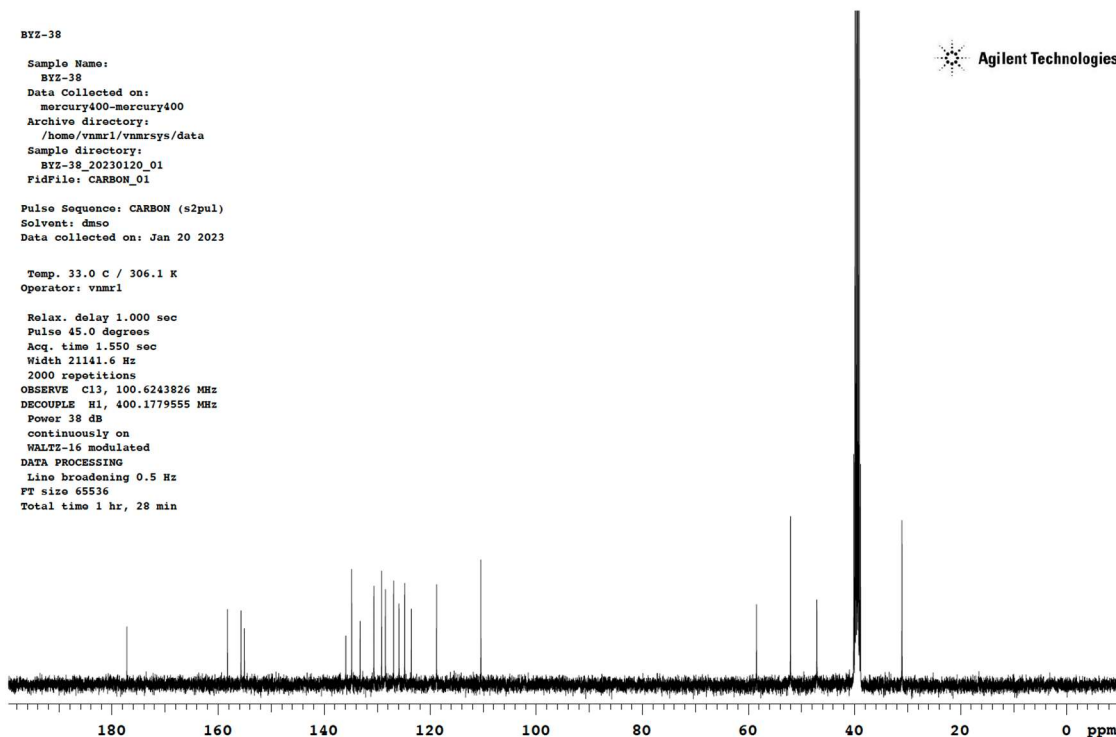


Figure S17: ¹³C-NMR spectrum of **8**

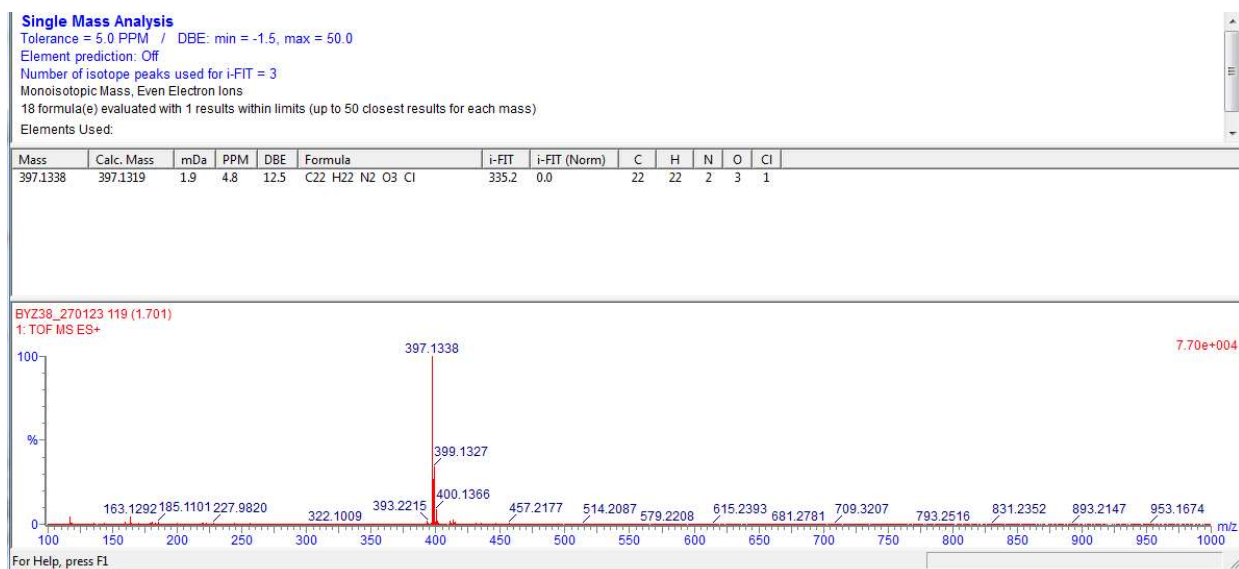
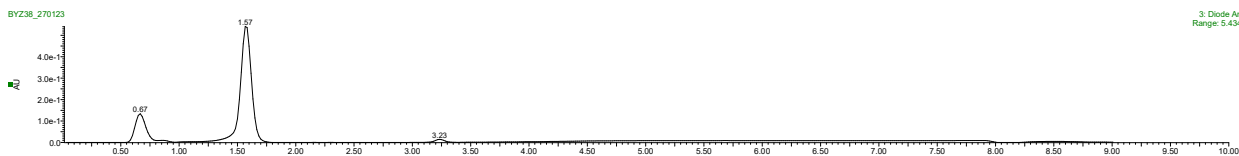


Figure S18: HRMS spectrum of **8**



Current Data Parameters
NAME TG616
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220728
Time 12.49 h
INSTRUM Avance
PROBHD Z151574_0038 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 101
DW 50.000 usec
DE 11.14 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330883 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 24.04299927 W

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

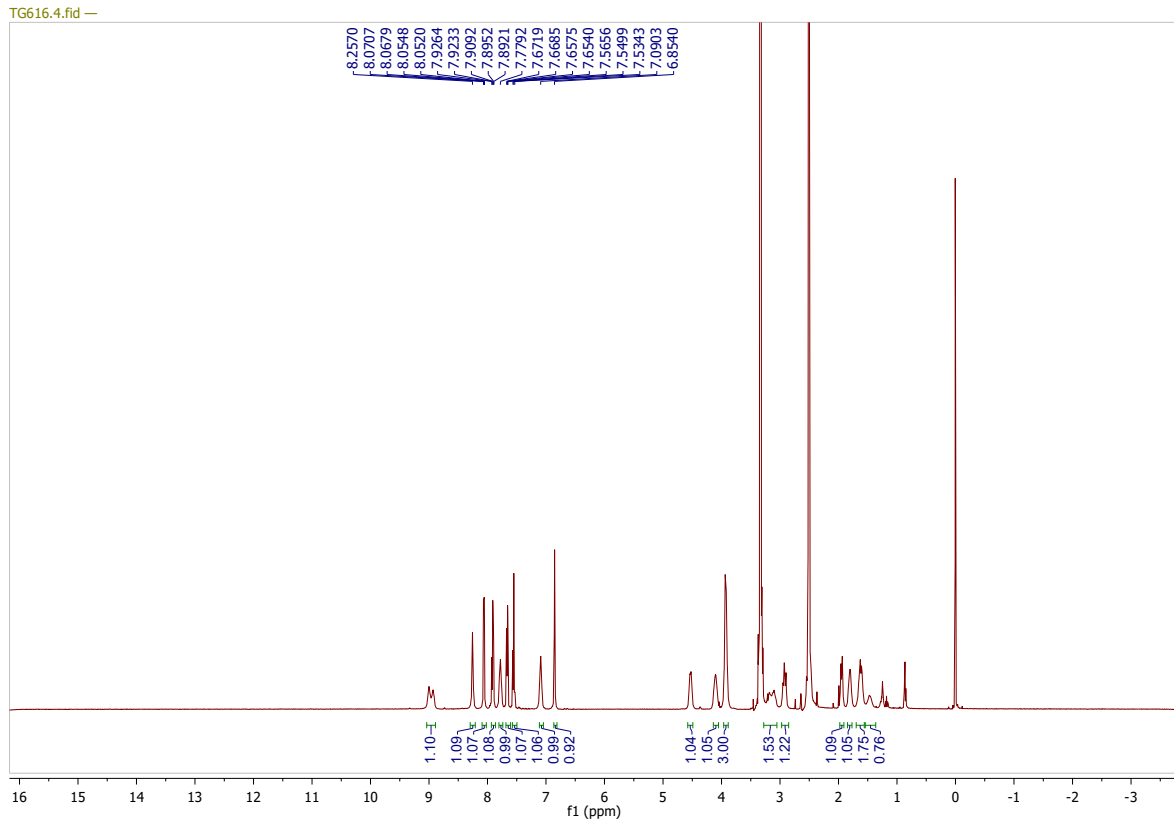
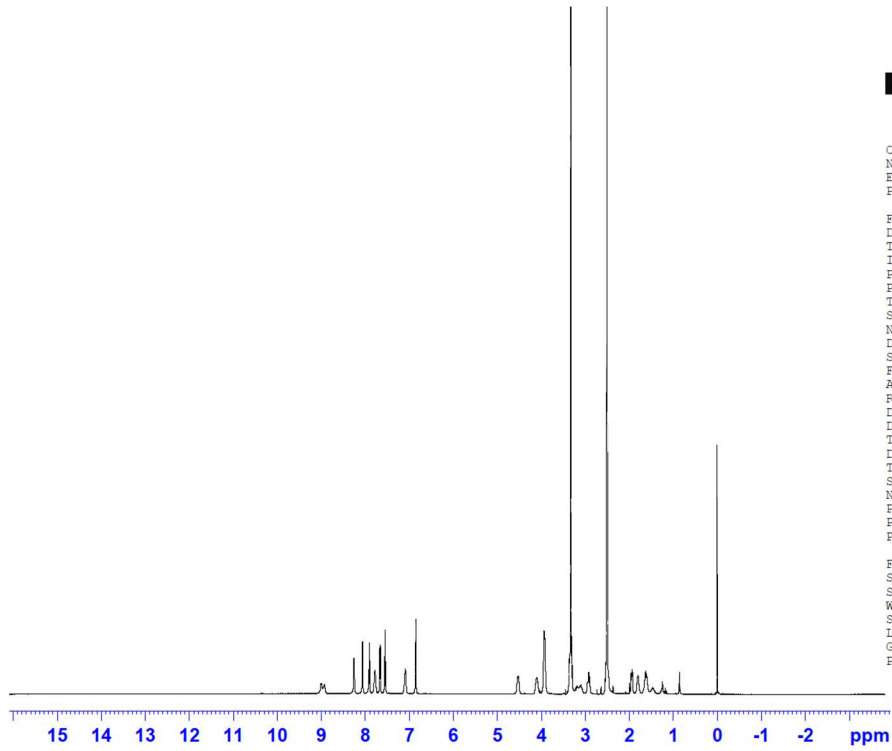


Figure S19: ^1H -NMR spectrum of **9**

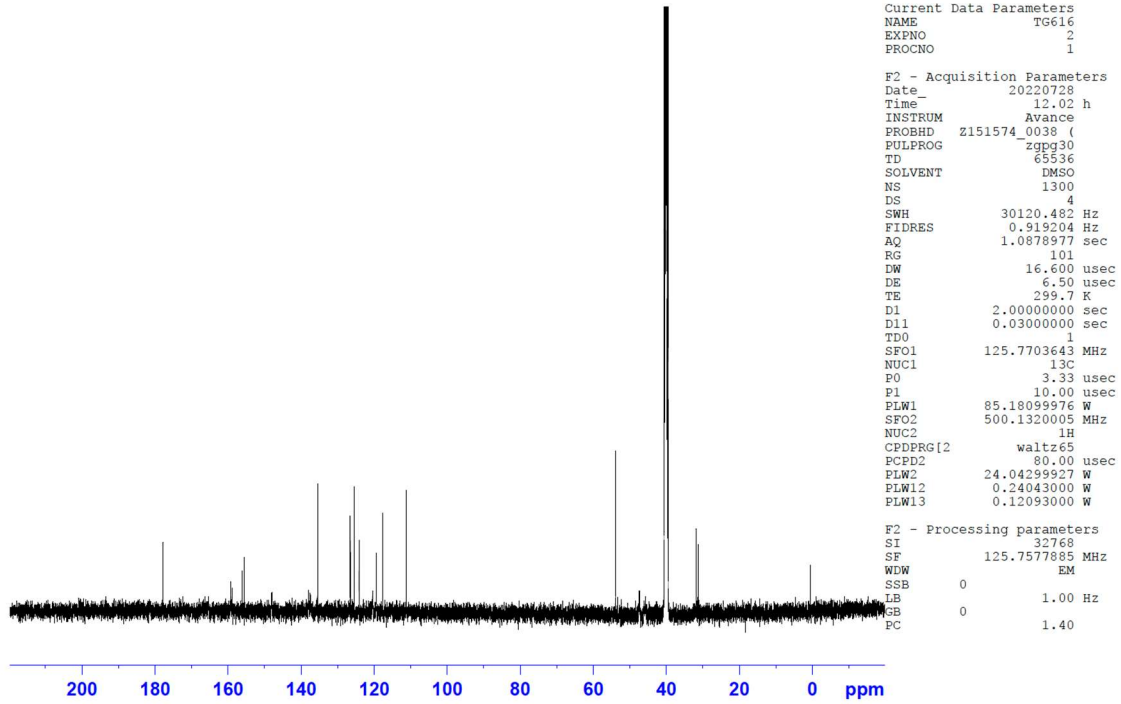


Figure S20: ¹³C-NMR spectrum of 9

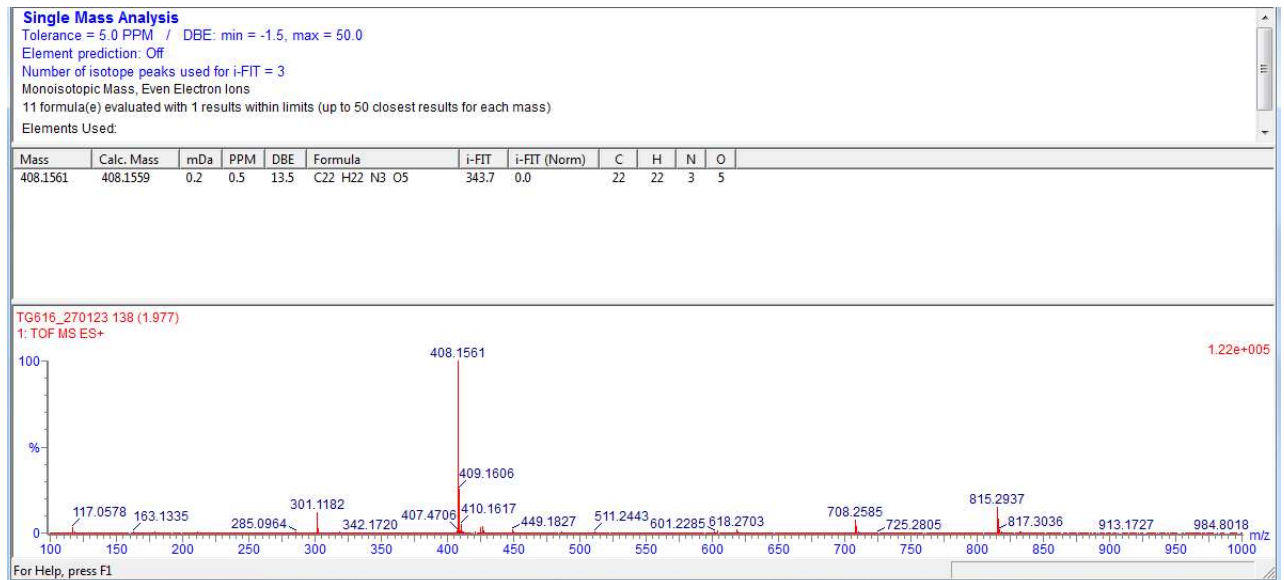
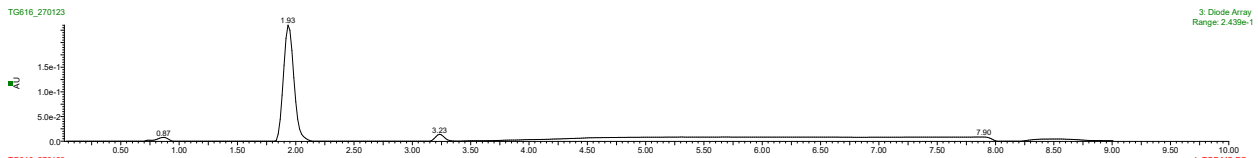


Figure S21: HRMS spectrum of 9