

Supporting Information

Org. Commun. X:X (202X) XX-X

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

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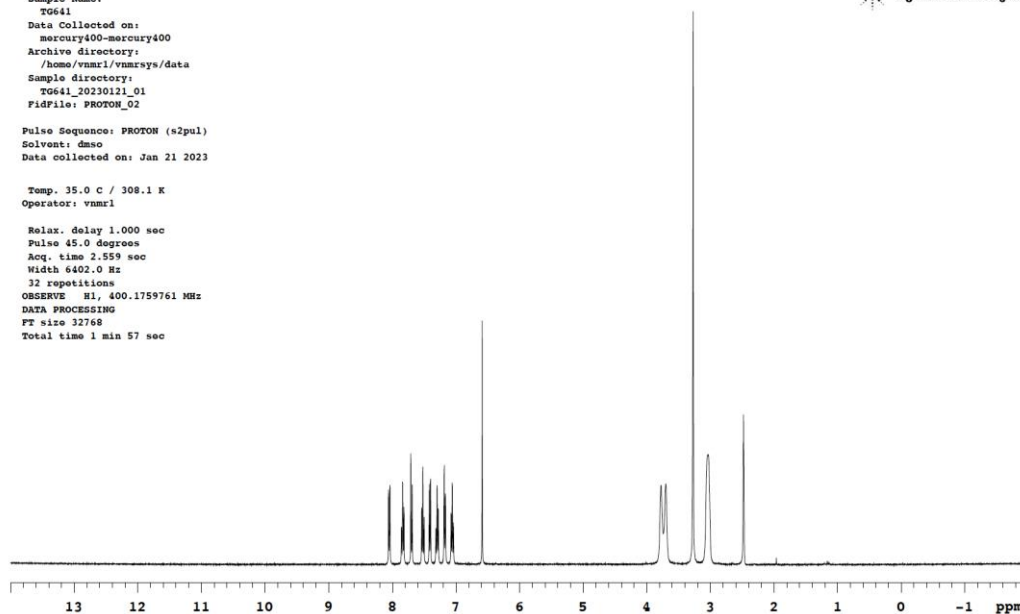
TG641

Sample Name:
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Data Collected on:
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Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
TG641_20230121_01
Fidfile: PROTON_02

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 —

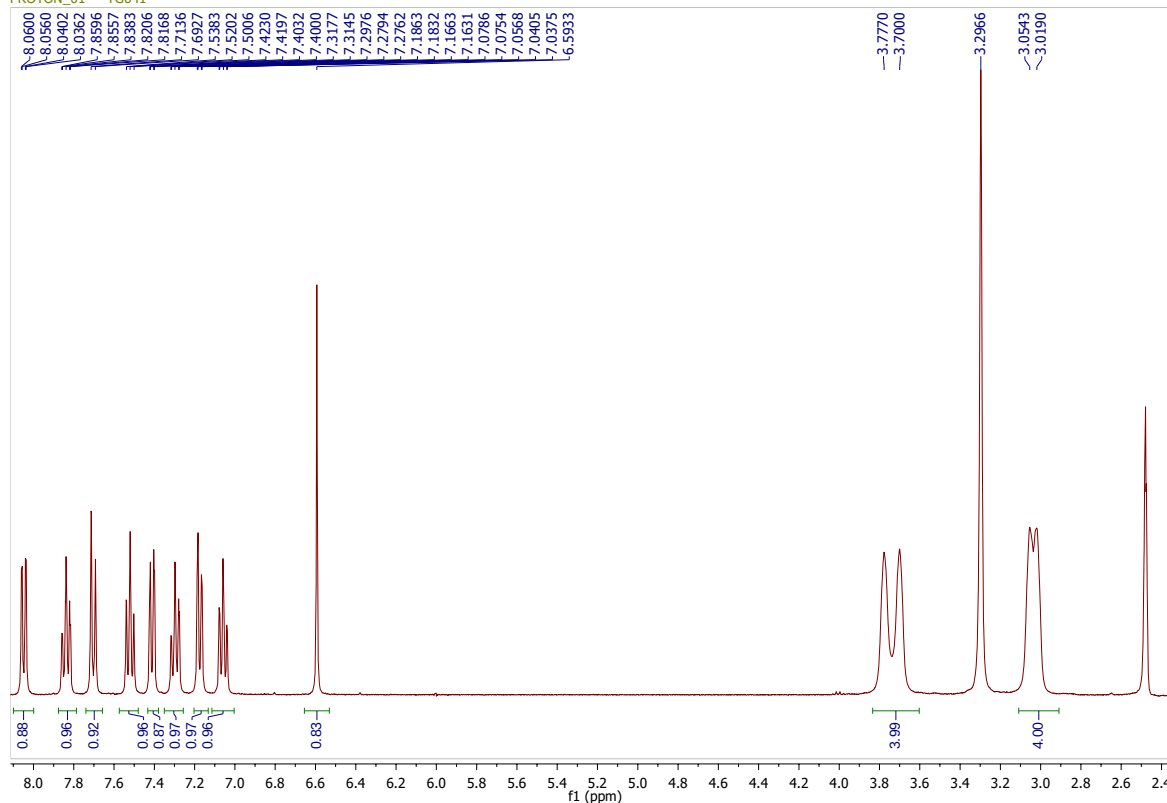


Figure S1: ^1H -NMR spectrum of **2**

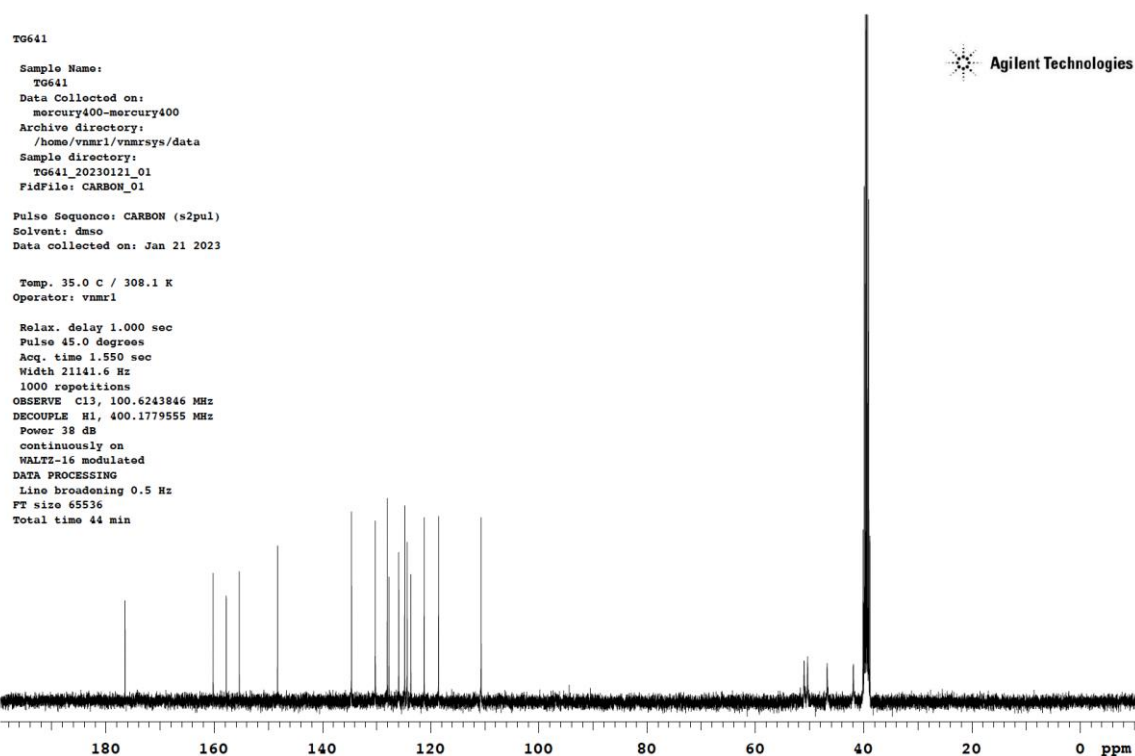


Figure S2: ^{13}C -NMR spectrum of 2

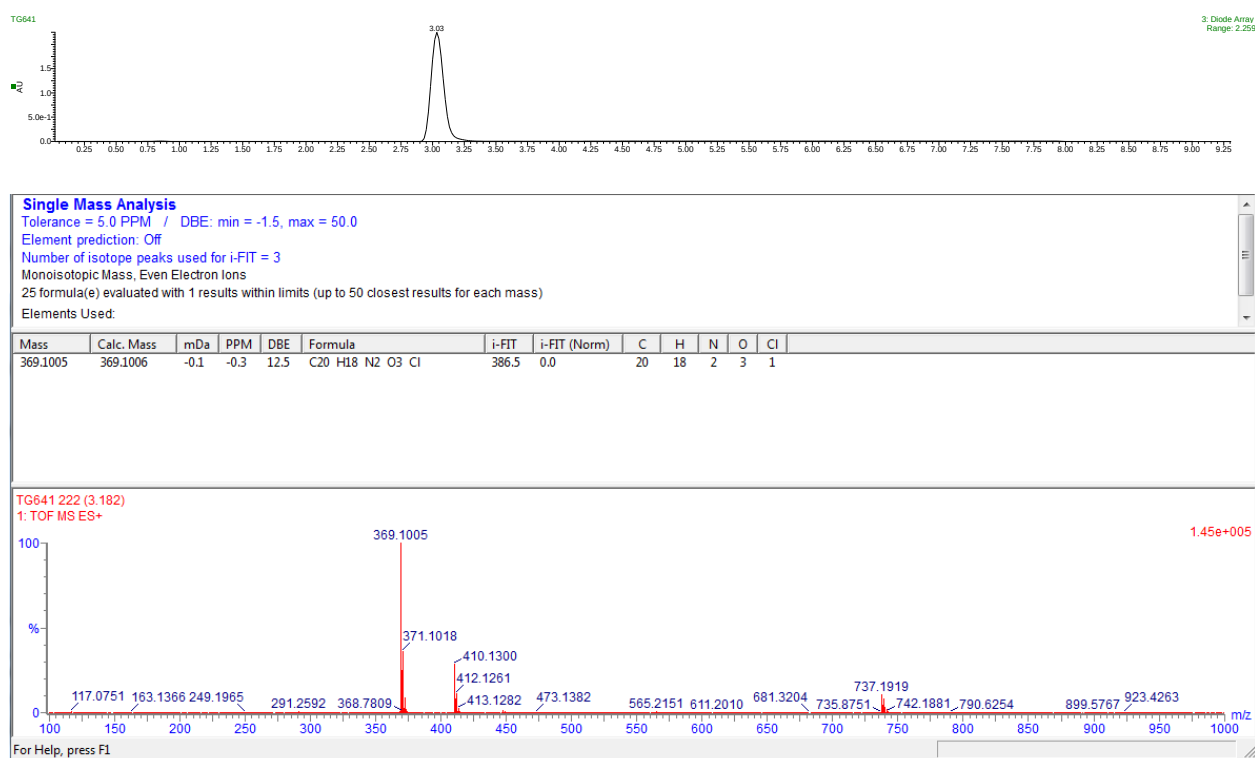


Figure S3: HRMS spectrum of compound 2

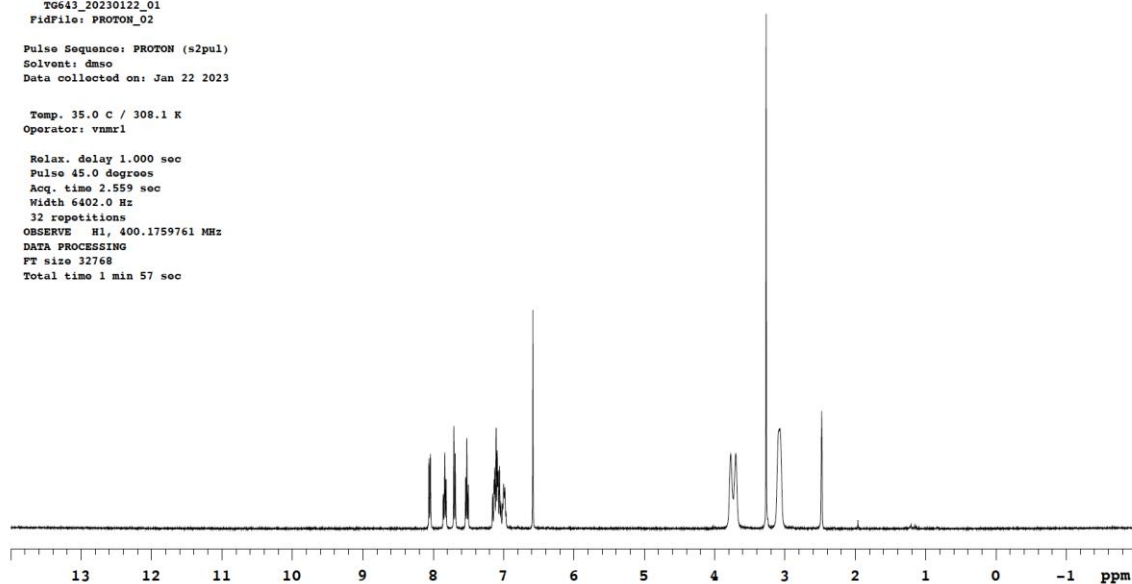
TG643

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

Pulse Sequence: PROTON (s2pul)
Solvent: dms
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 —

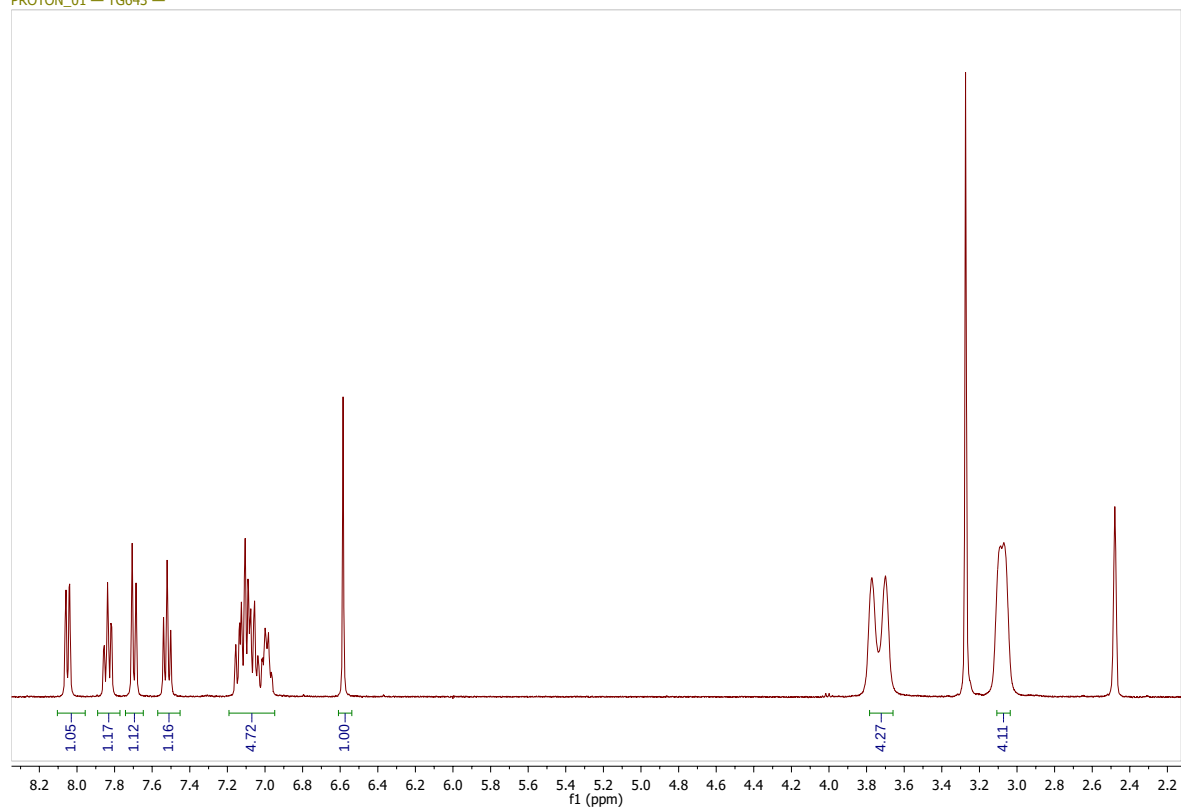


Figure S4: ¹H-NMR spectrum of **3**

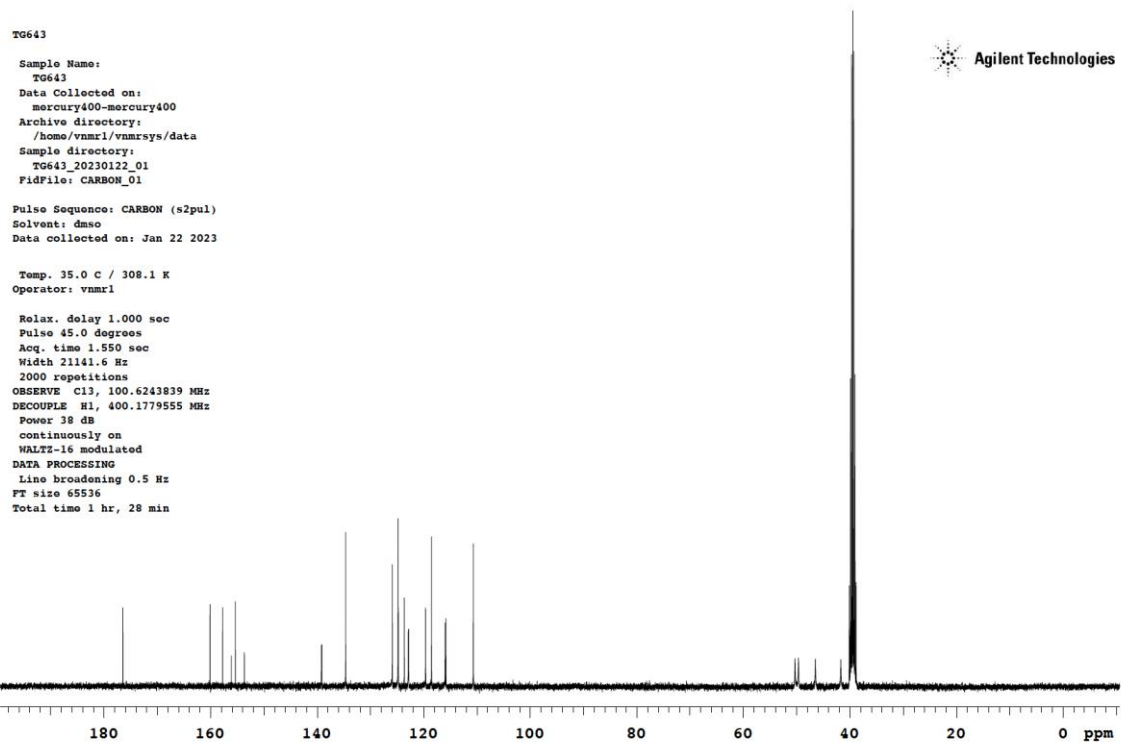


Figure S5: ^{13}C -NMR spectrum of 3

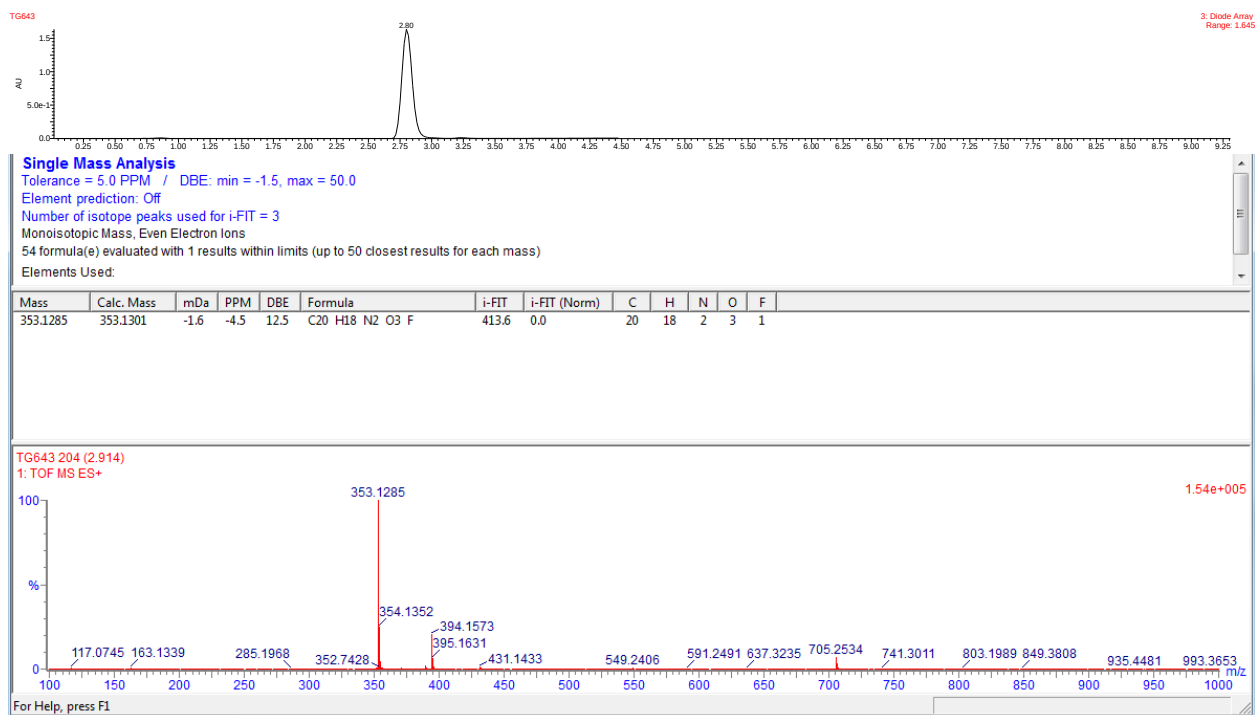


Figure S6: HRMS spectrum of compound 3

TG642

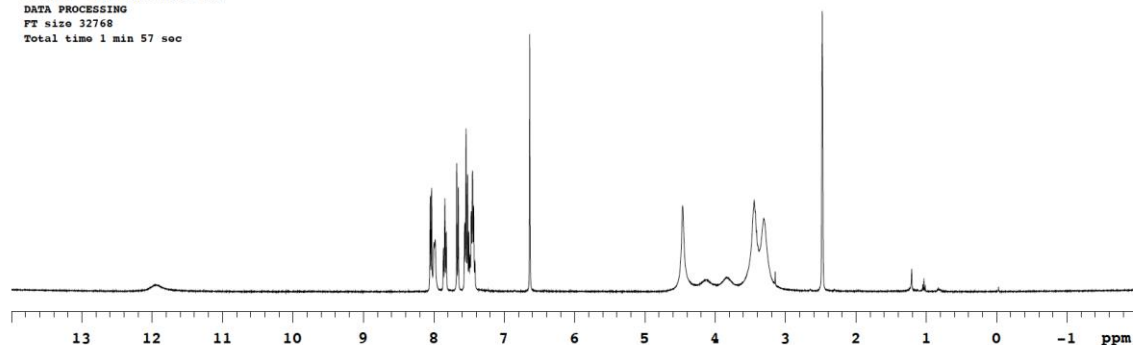


Sample Name:
TG642
Data Collected on:
mercury400-mercury400
Archive directory:
/home/vnmr1/vnmrsys/data
Sample directory:
TG642_20230121_01
FidFile: PROTON_02

Pulse Sequence: PROTON (s2pul)
Solvent: 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 — TG642 —

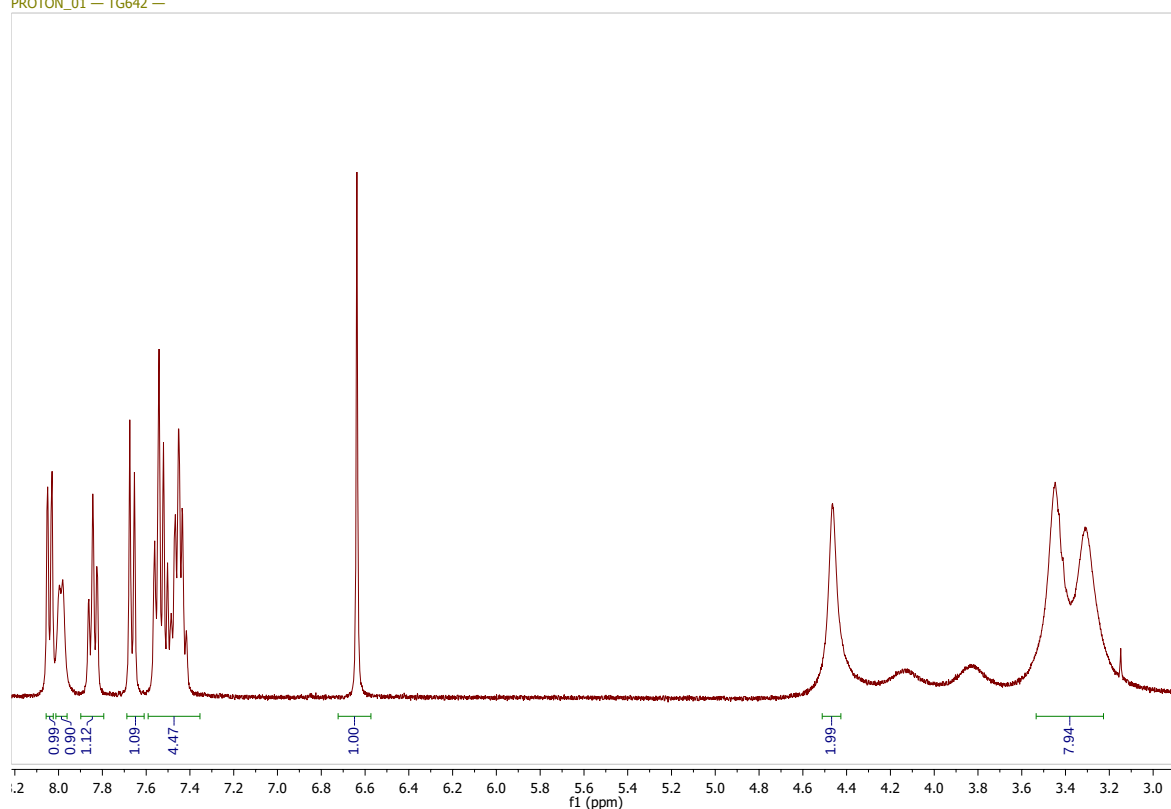


Figure S7: ^1H -NMR spectrum of **4**

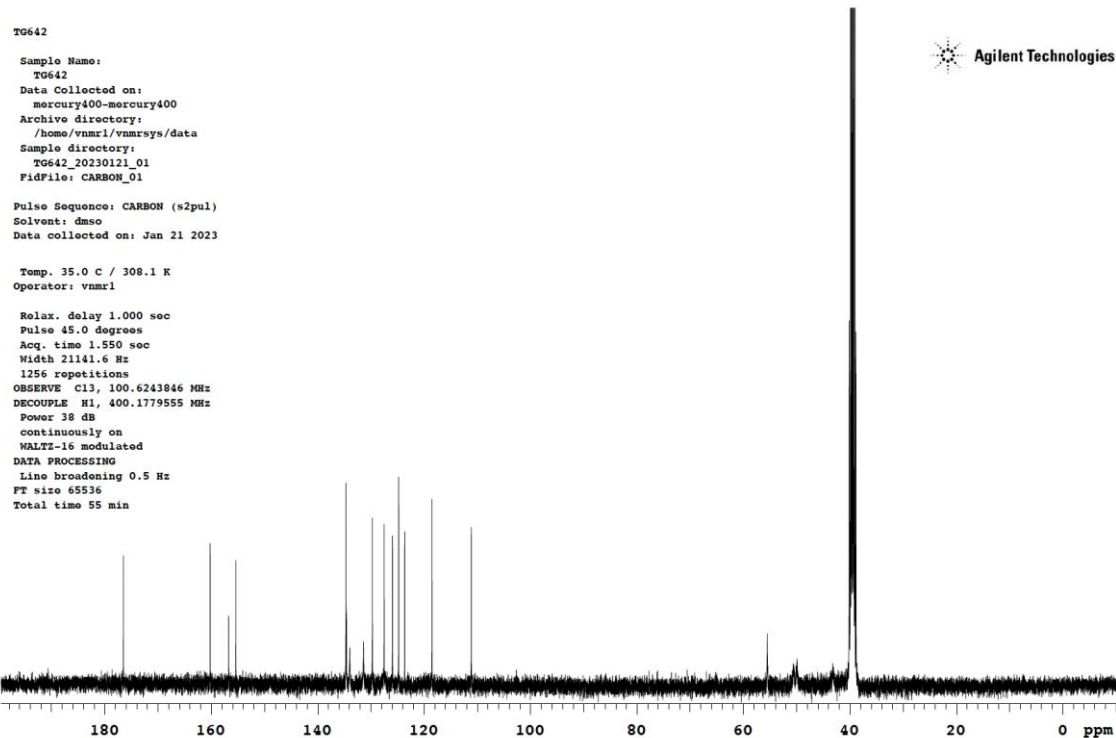


Figure S8: ^{13}C -NMR spectrum of **4**

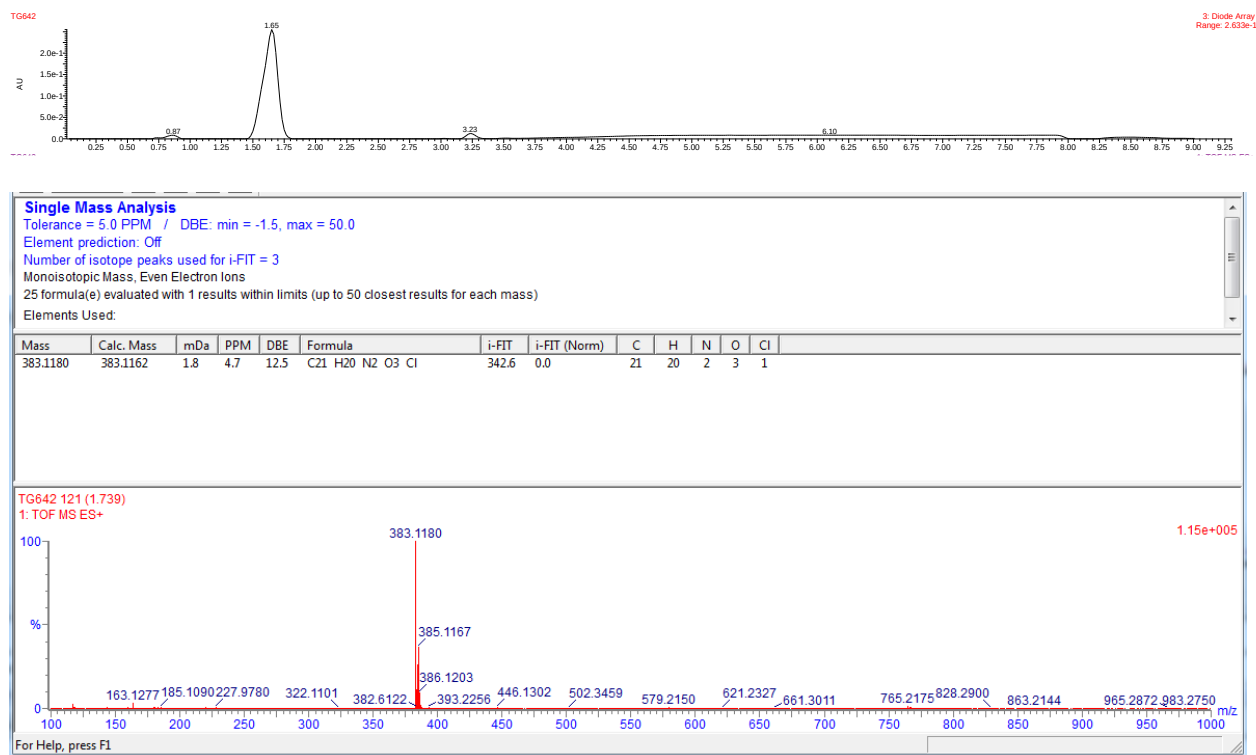


Figure S9: HRMS spectrum of **4**

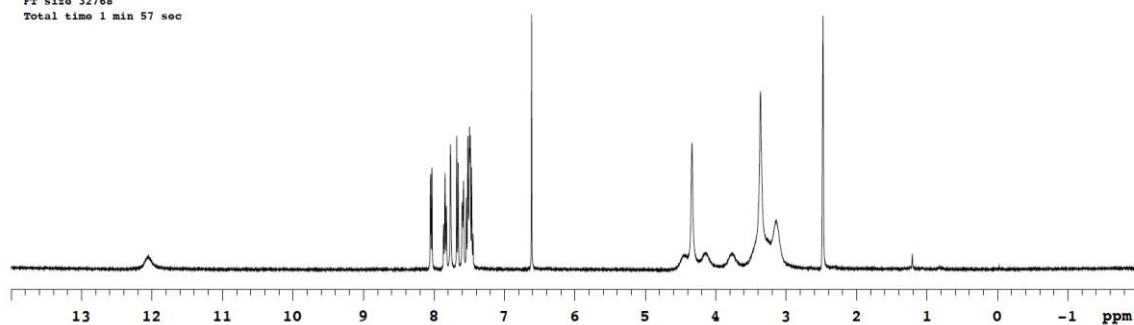
TG644

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



PROTON_01 — TG644 —

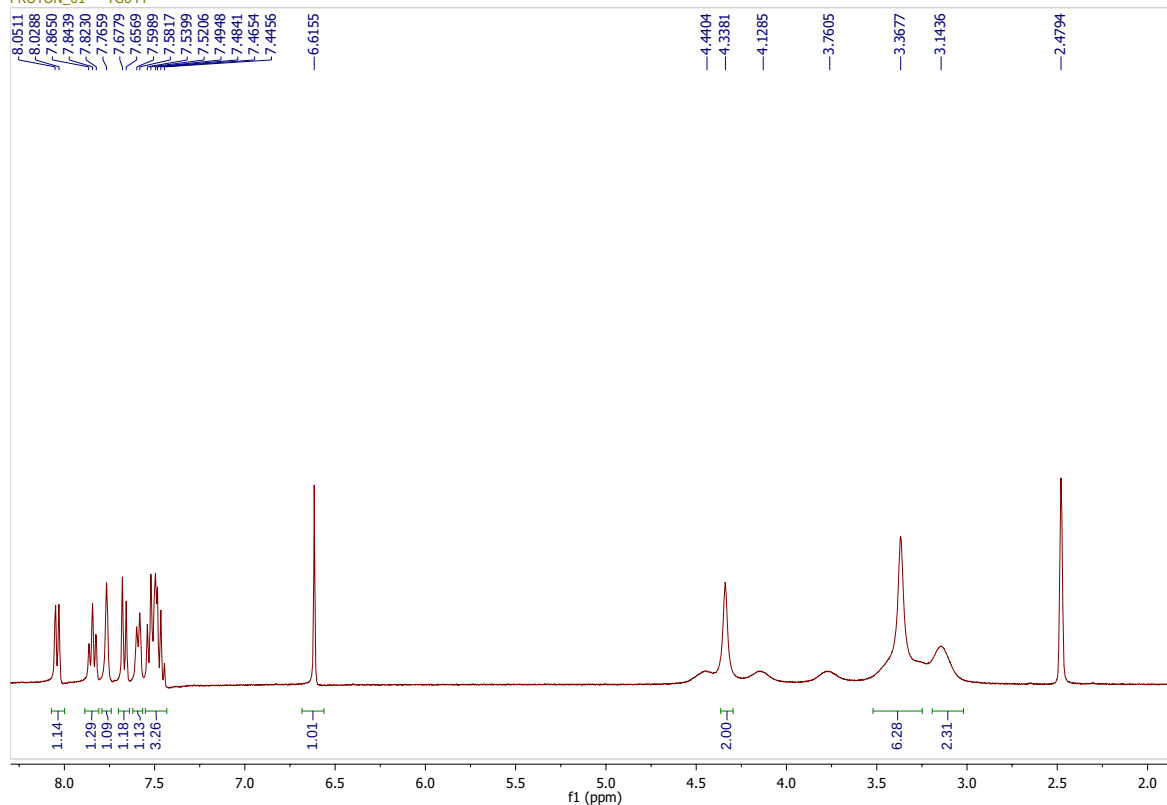


Figure S10: ^1H -NMR spectrum of **5**

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
MALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 28 min

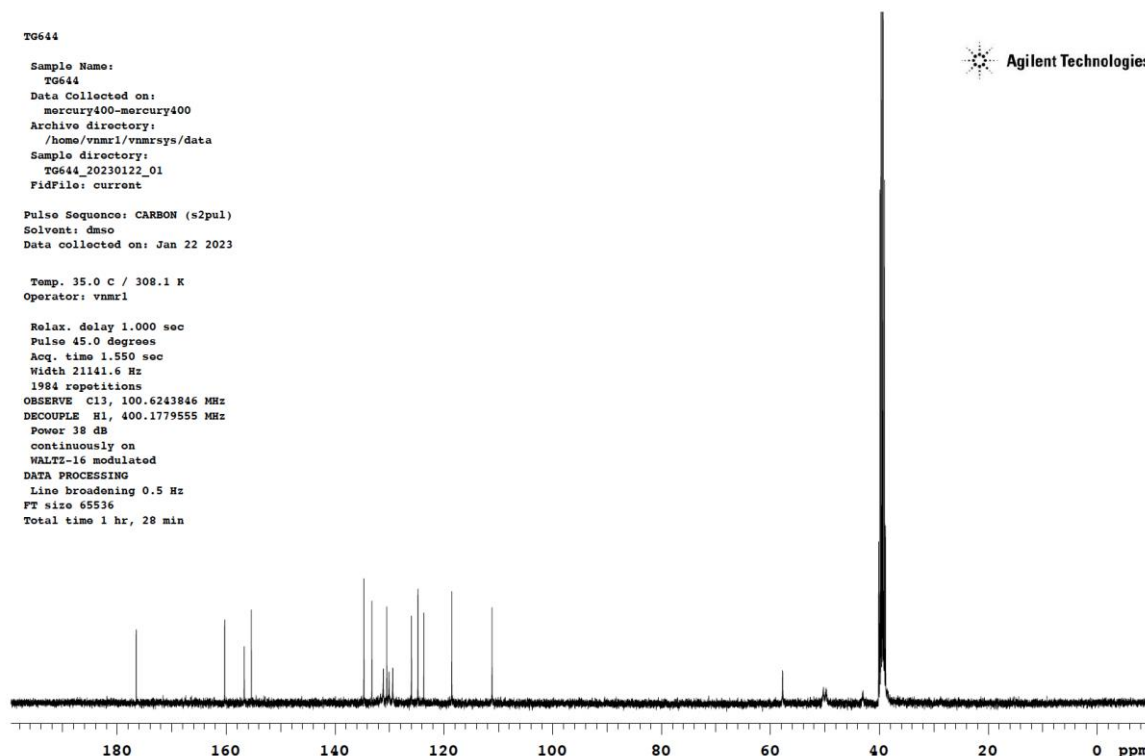
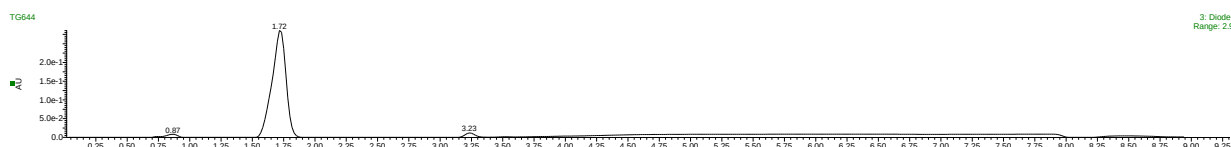


Figure S11: ^{13}C -NMR spectrum of 5



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

10 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	Cl
383.1162	383.1162	0.0	0.0	12.5	C ₂₁ H ₂₀ N ₂ O ₃ Cl	294.4	0.0	21	20	2	3	1

TG644 127 (1.815)

1: TOF MS ES+

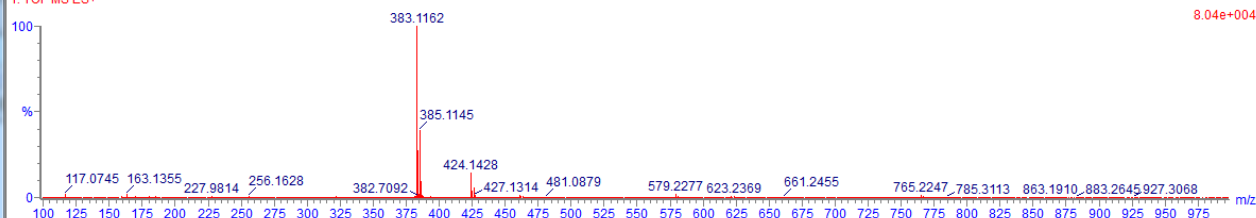


Figure S12. HRMS spectrum of 5

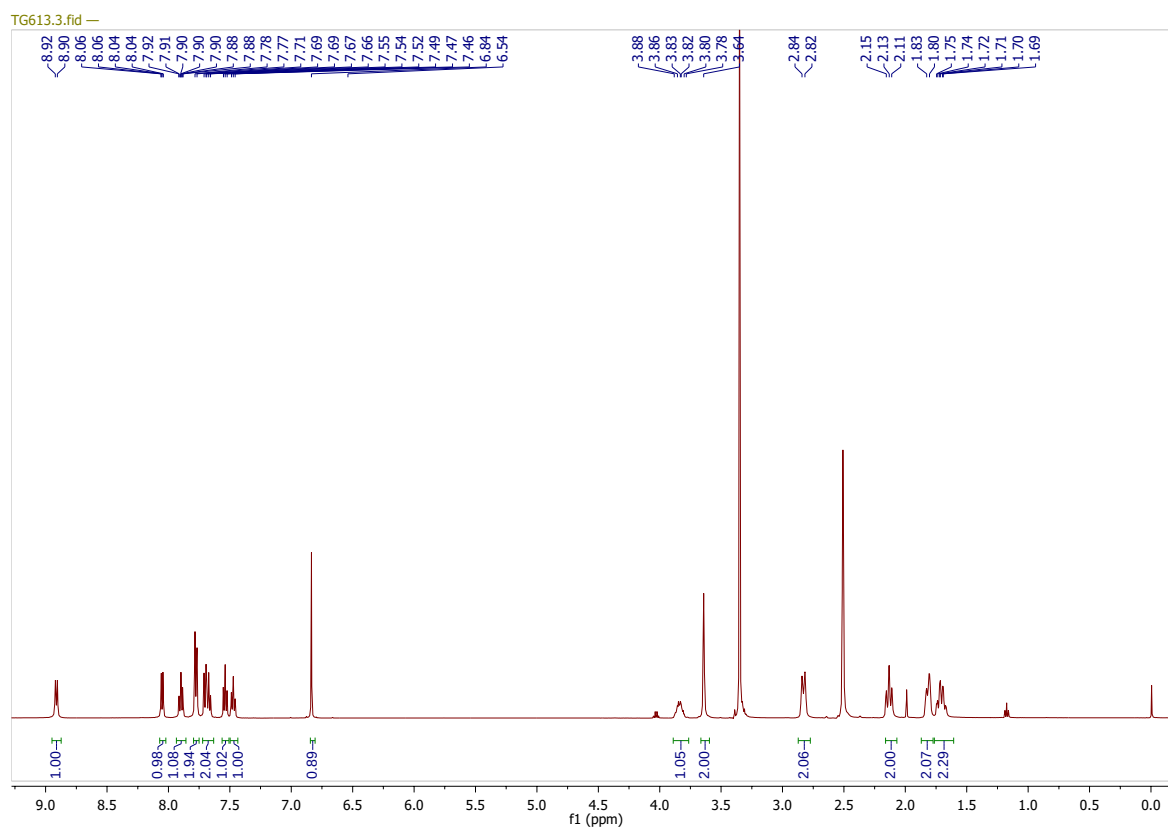
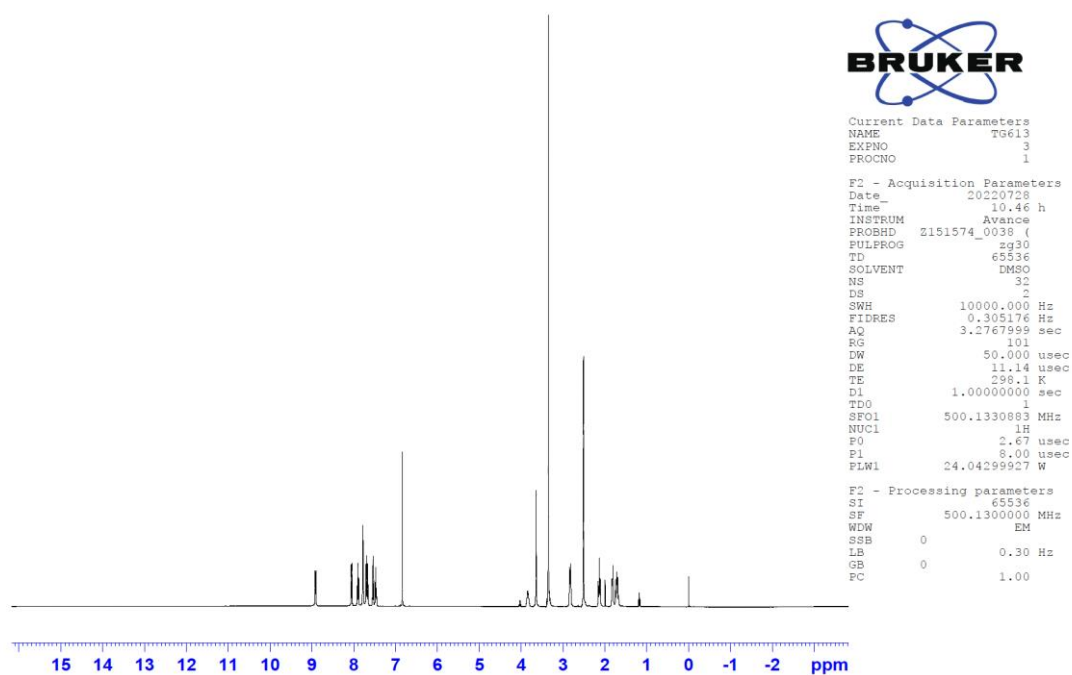


Figure S13: ^1H -NMR spectrum of **7**

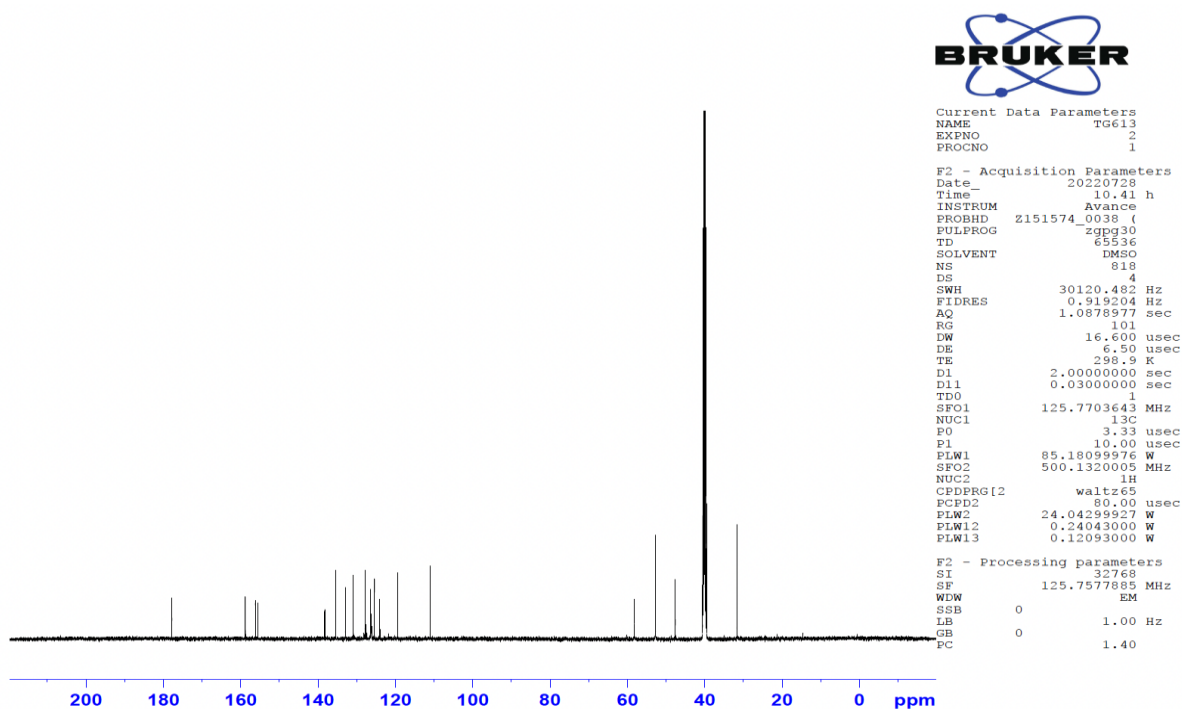


Figure S14: ^{13}C -NMR spectrum of 7

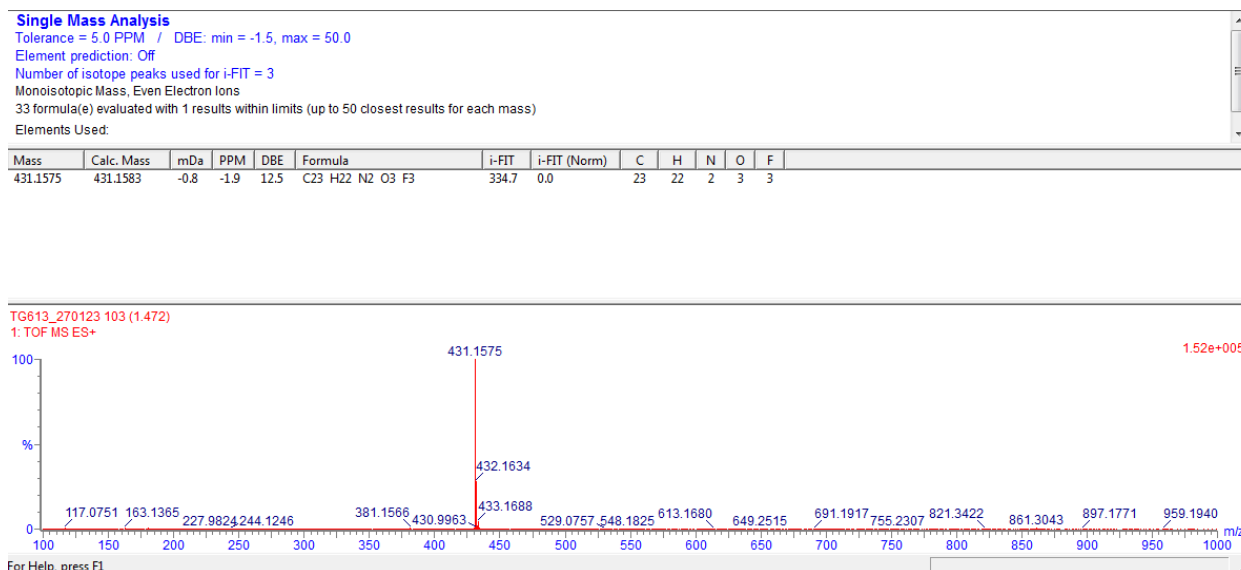
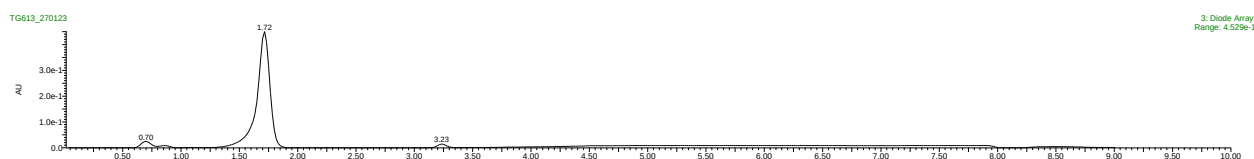


Figure S15: HRMS spectrum of 7

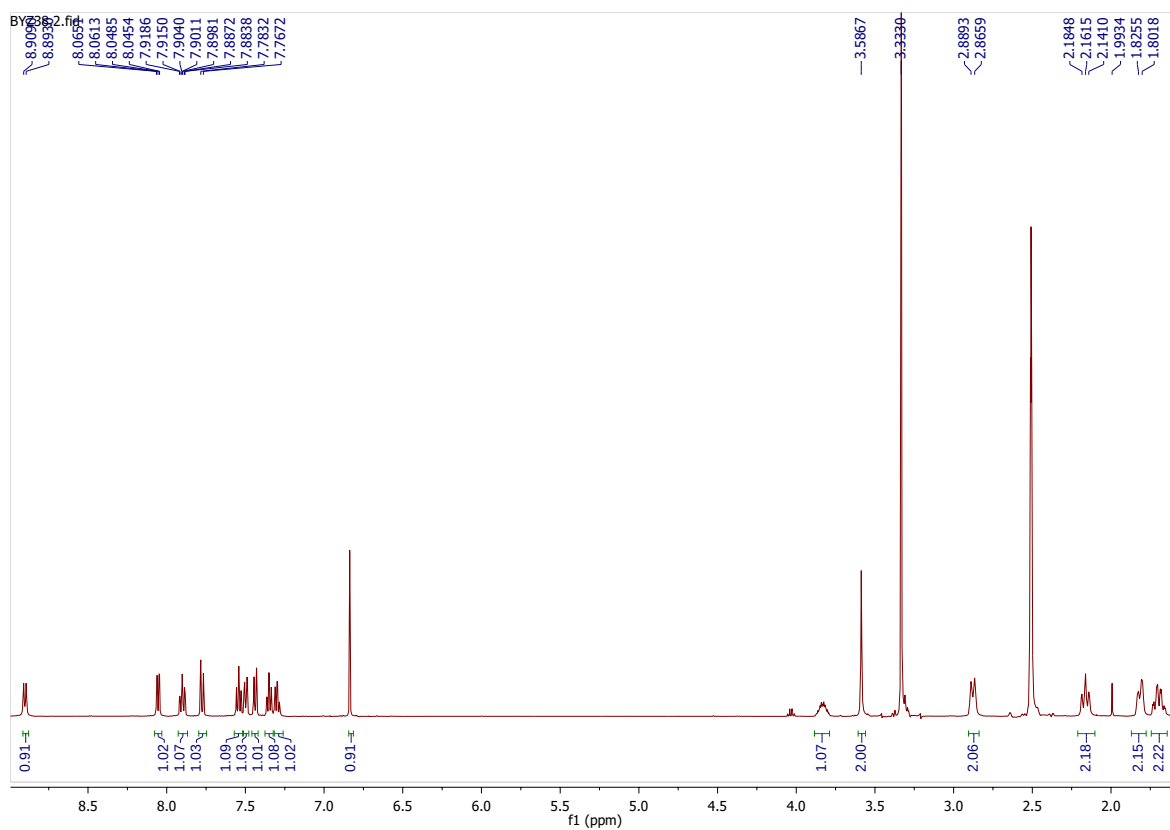
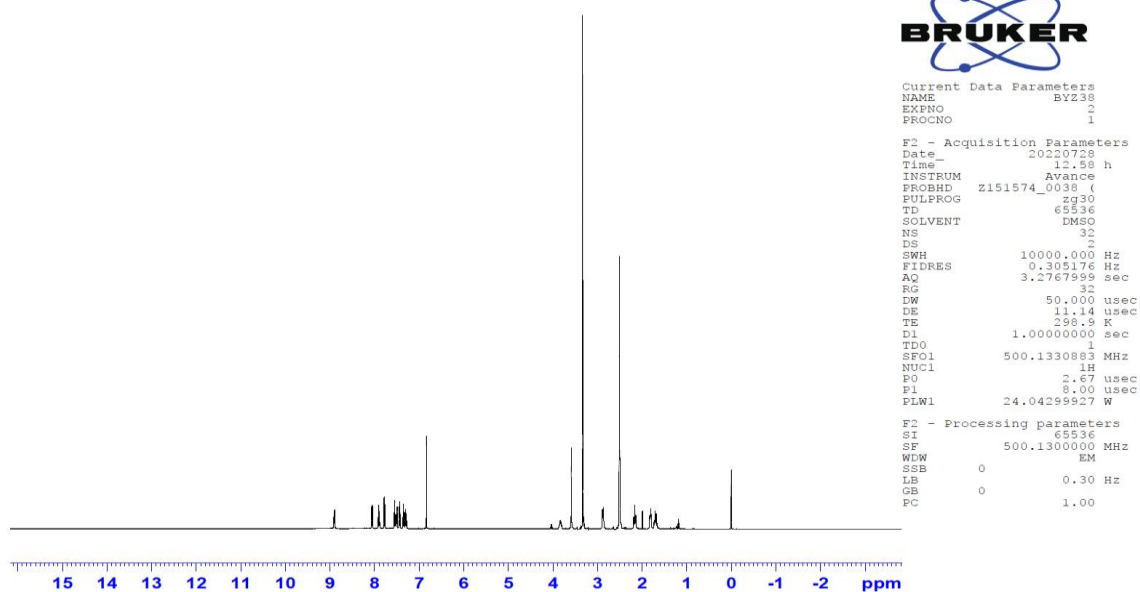


Figure S16: ^1H -NMR spectrum of **8**

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

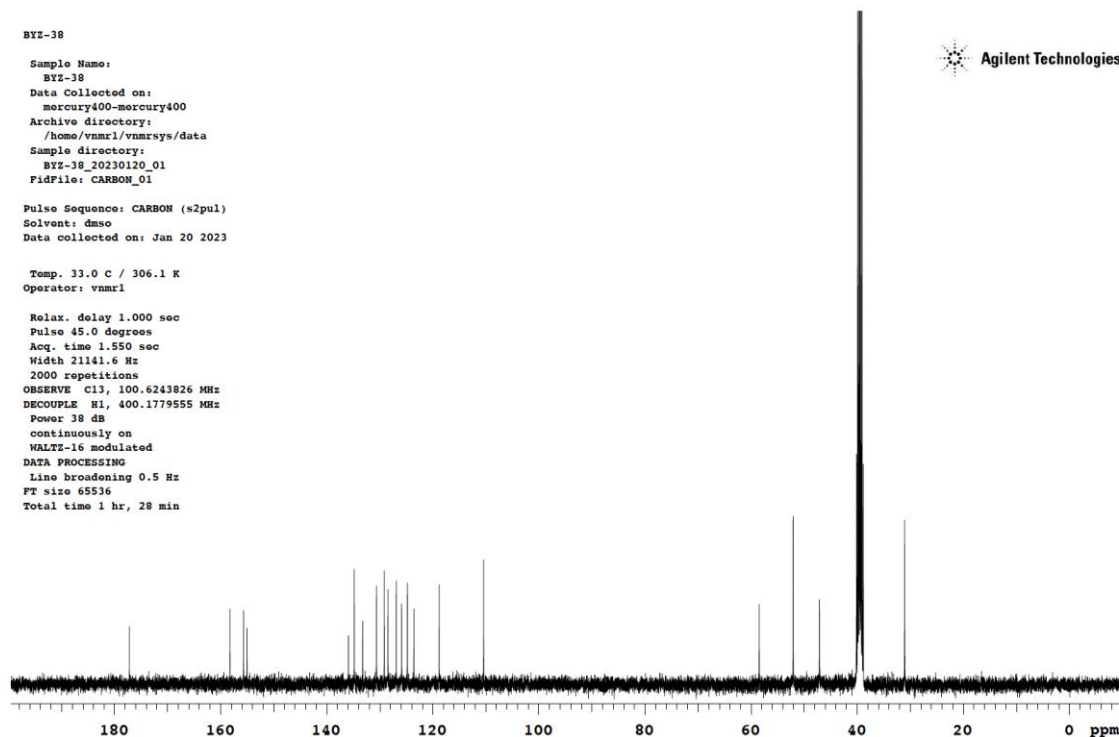
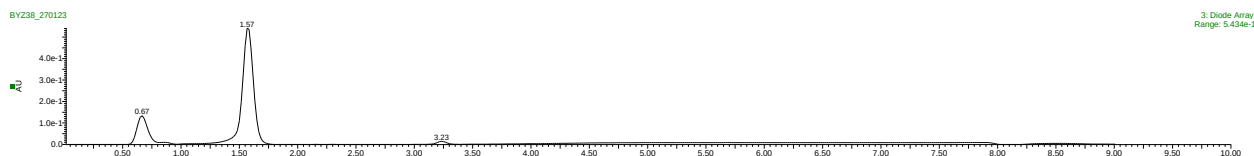


Figure S17: ^{13}C -NMR spectrum of **8**



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

18 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	Cl
397.1338	397.1319	1.9	4.8	12.5	C22 H22 N2 O3 Cl	335.2	0.0	22	22	2	3	1

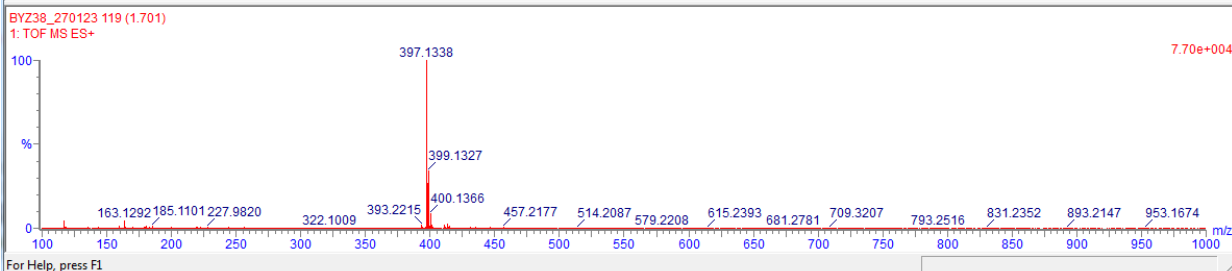


Figure S18: HRMS spectrum of **8**

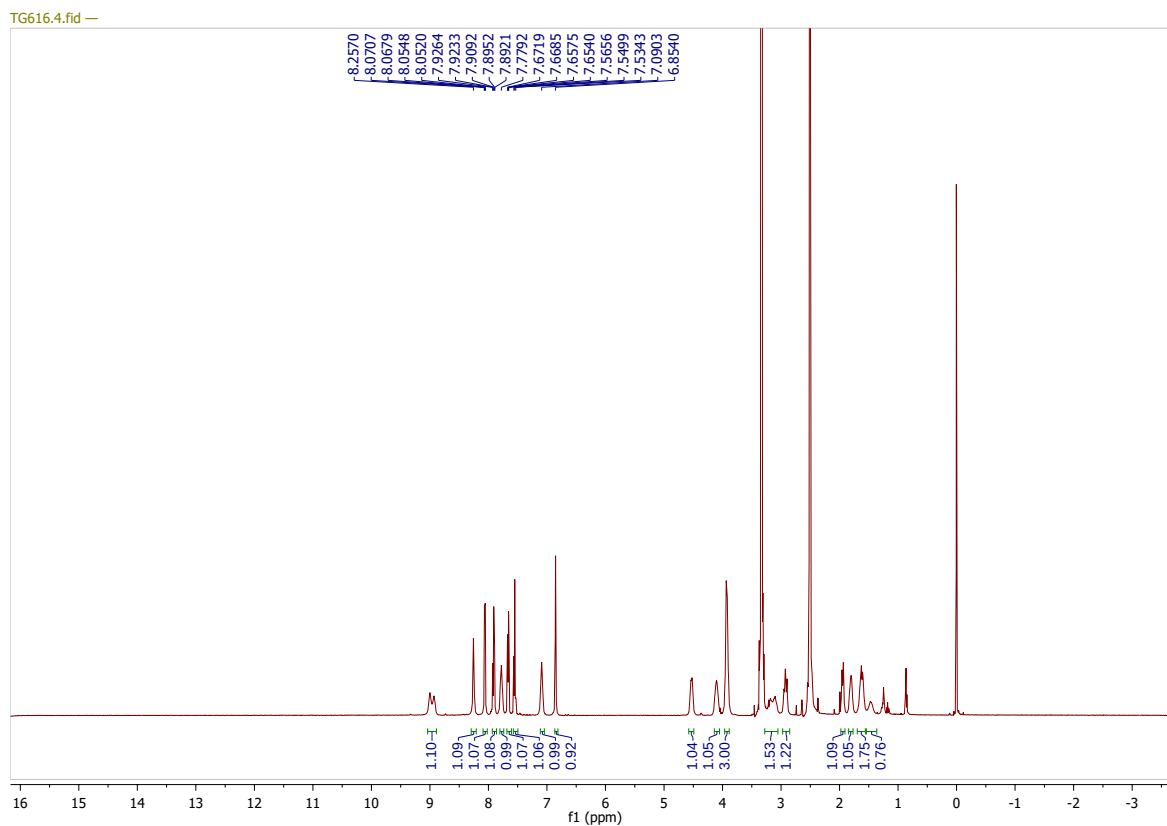
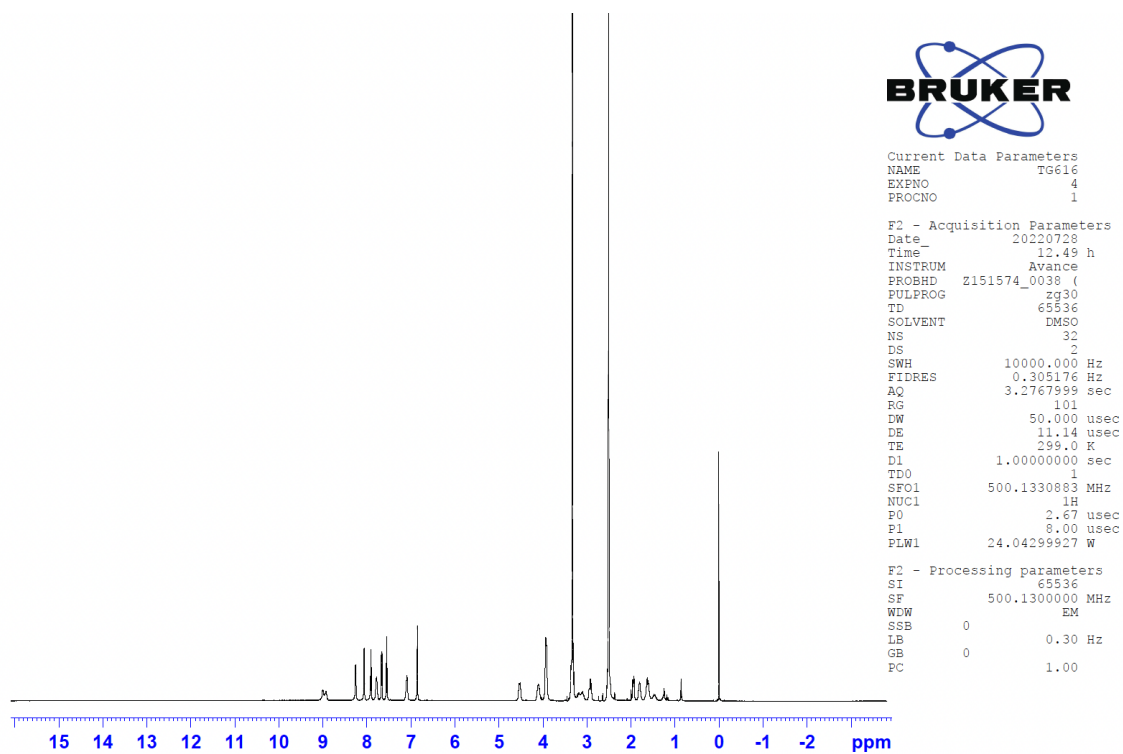
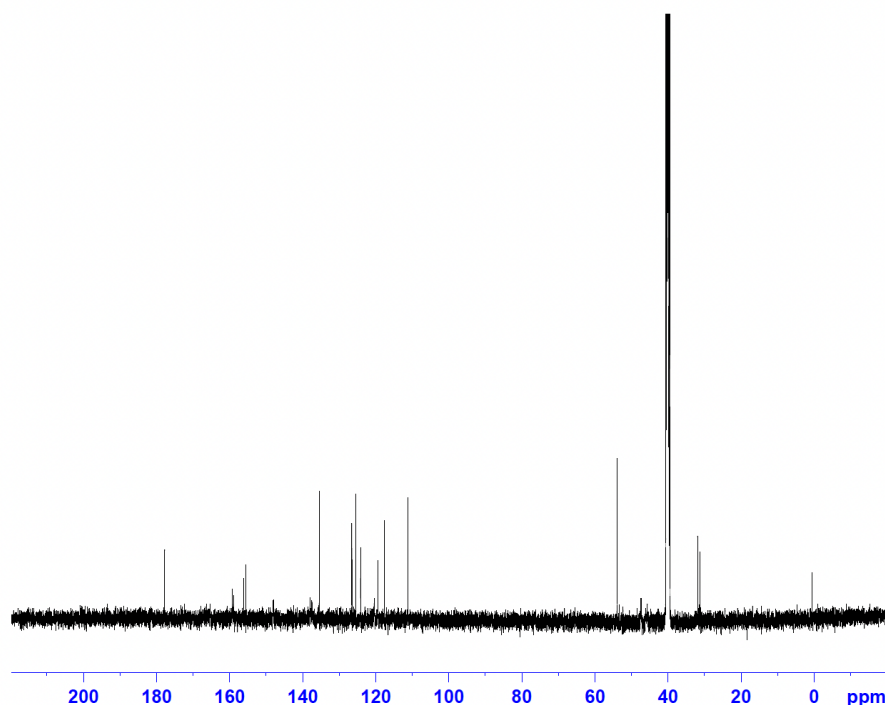


Figure S19: ^1H -NMR spectrum of **9**



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EXPNO 2
PROCNO 1

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Time 12:02 h
INSTRUM Avance
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1300
DS 4
SWH 30120.482 Hz
FIDRES 0.919204 Hz
AQ 1.0878977 sec
RG 101
DW 16.600 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 85.18099976 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 80.00 usec
PLW2 24.04299927 W
PLW12 0.24043000 W
PLW13 0.12093000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S20: ^{13}C -NMR spectrum of **9**

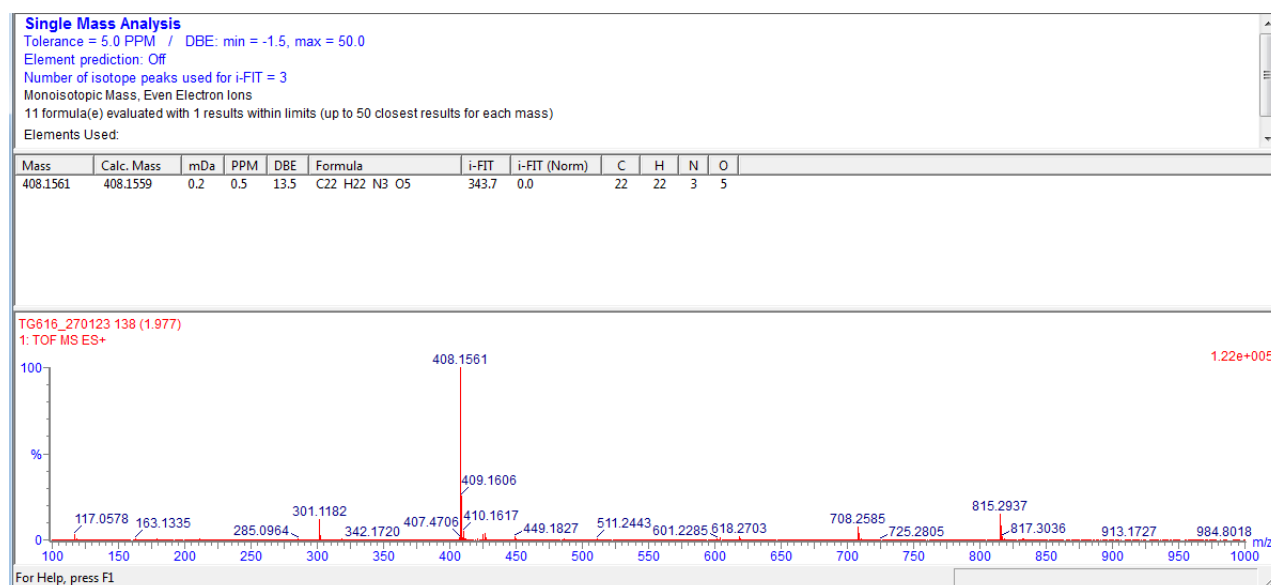
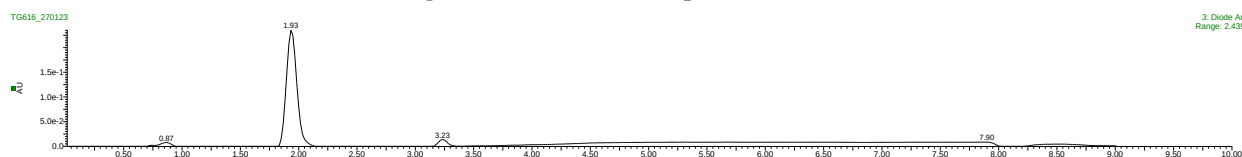


Figure S21: HRMS spectrum of **9**