

Novel Polyhydroquinoline Hydrazide Linked Schiff's Base Derivatives: Multistep Synthesis, Antimicrobial and Calcium Channel Blocking Activities

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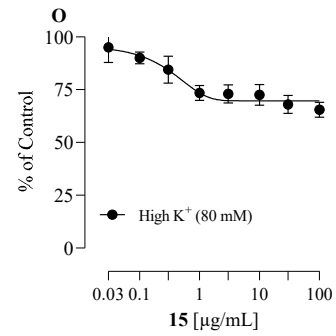
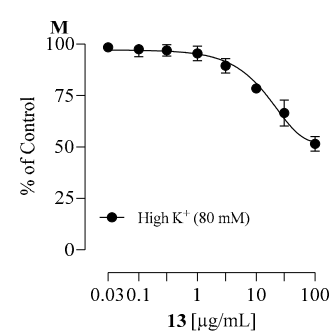
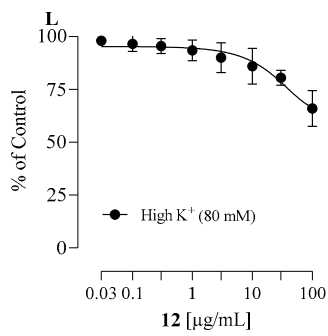
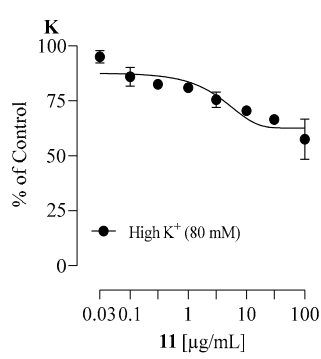
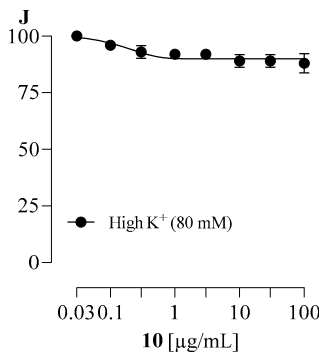
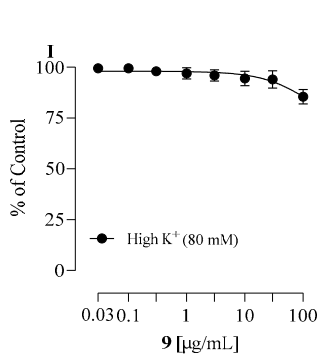
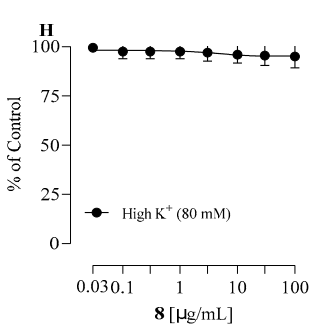
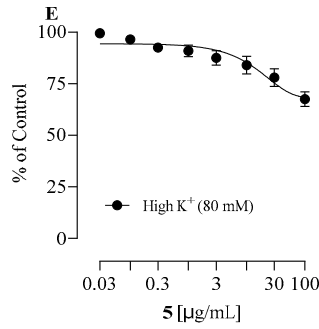
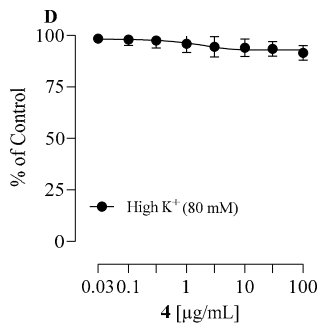
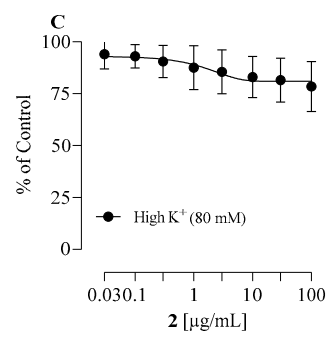
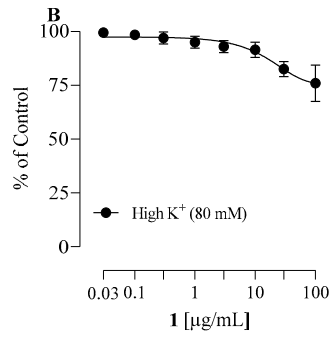
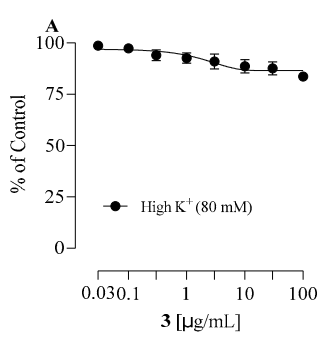
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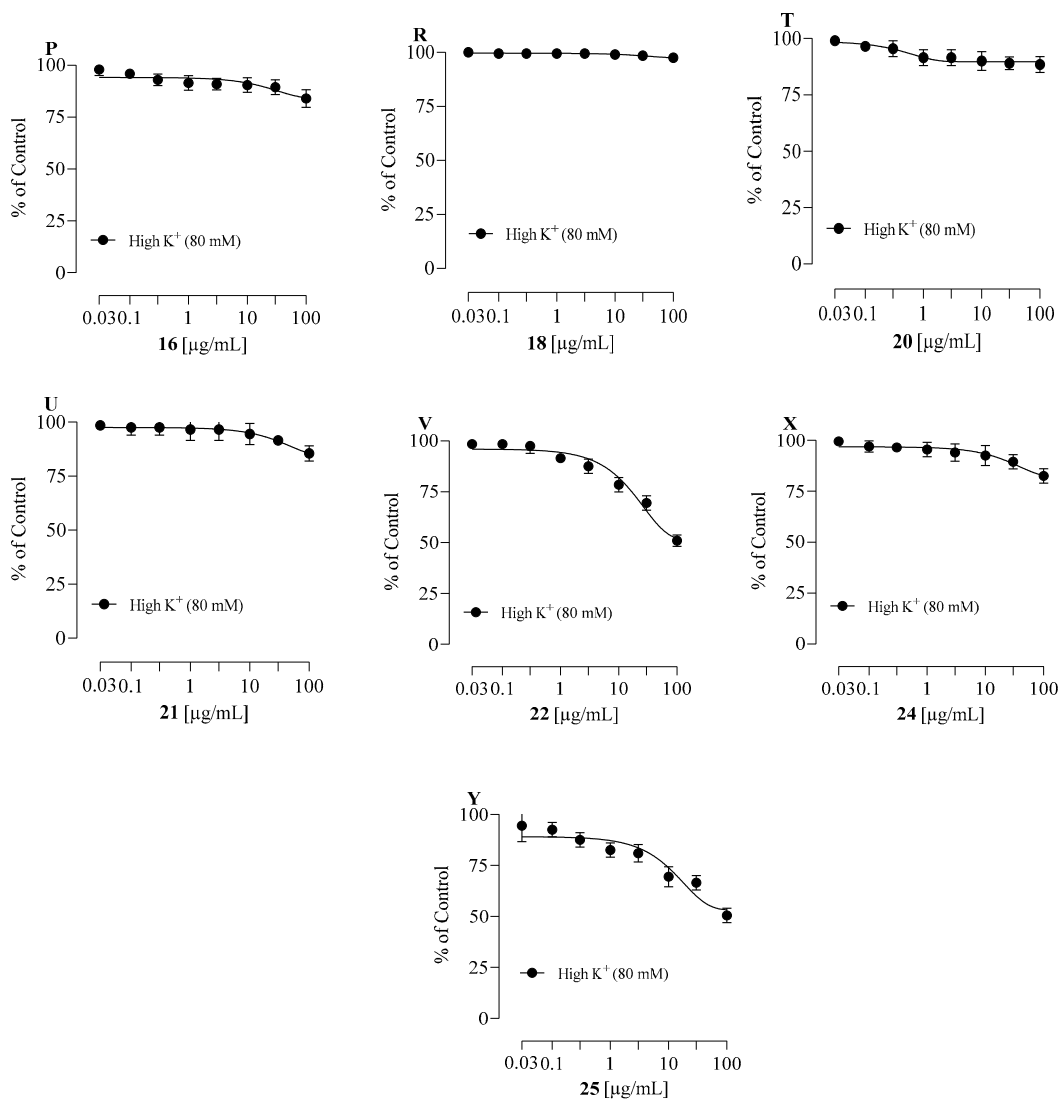


Figure S1: The effect of synthesized compounds against high K^+ (80 mM) induced contraction ($n = 3-5$), values represented as mean \pm SEM using two-way ANOVA.

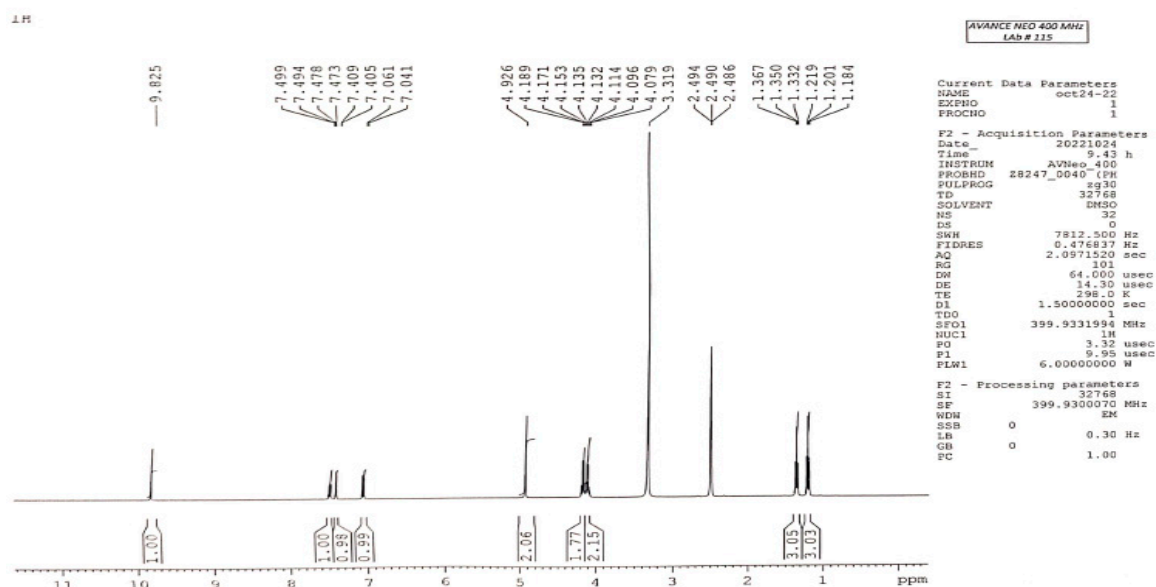
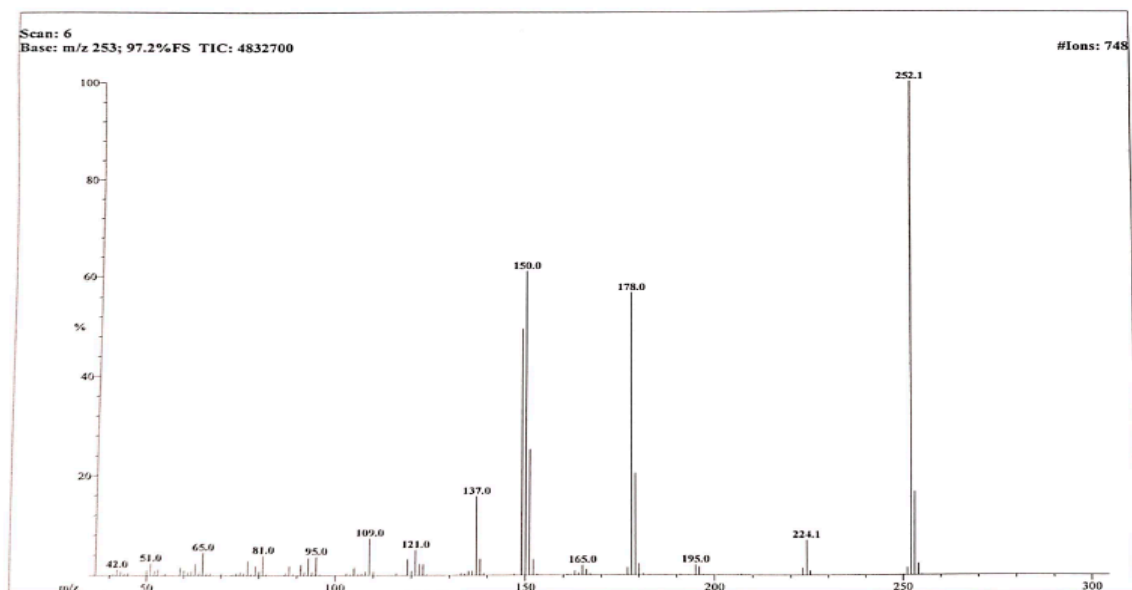
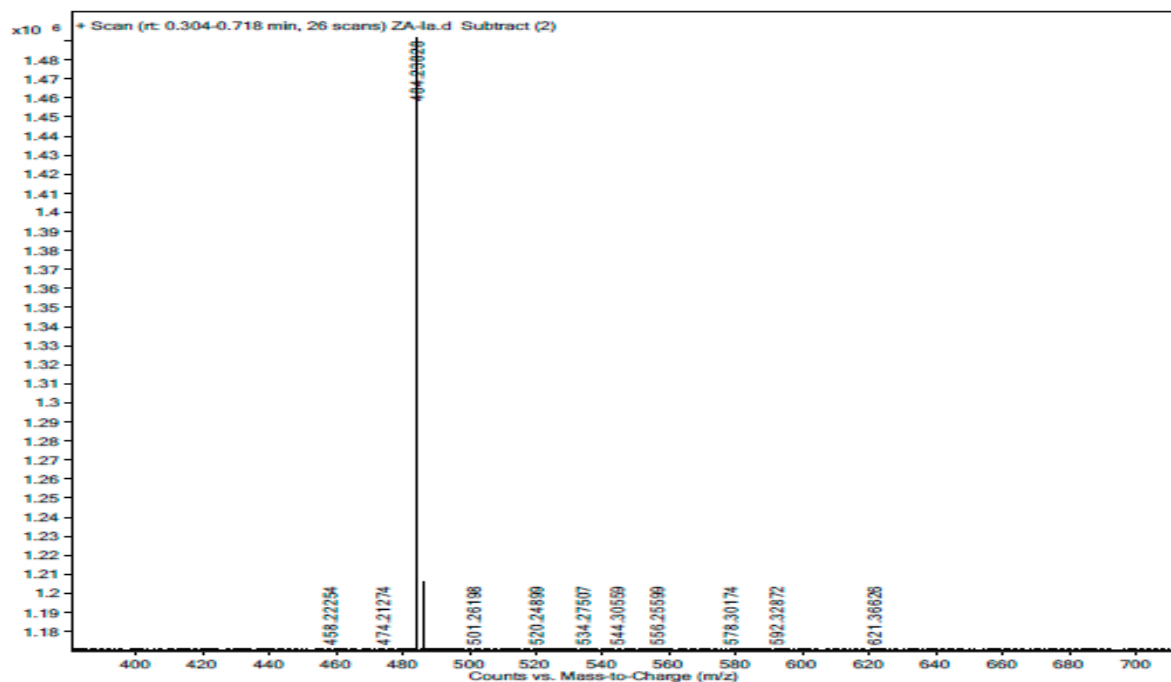
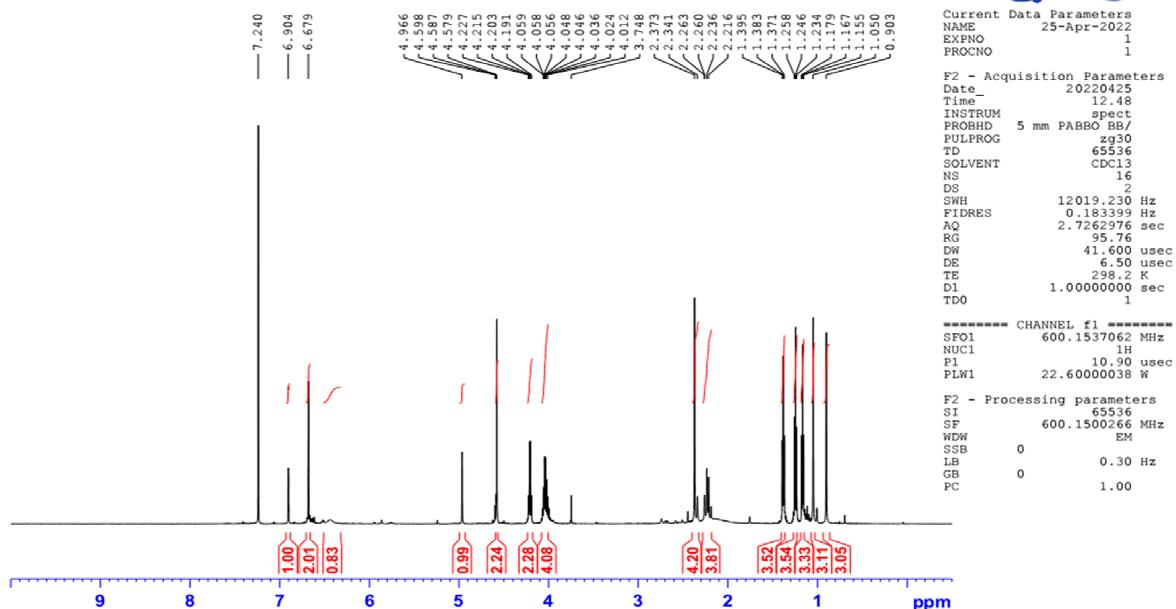


Figure S2: ^1H -NMR and ^{13}C -NMR spectra of ethyl-2-(2-ethoxy-4-formylphenoxy)acetate



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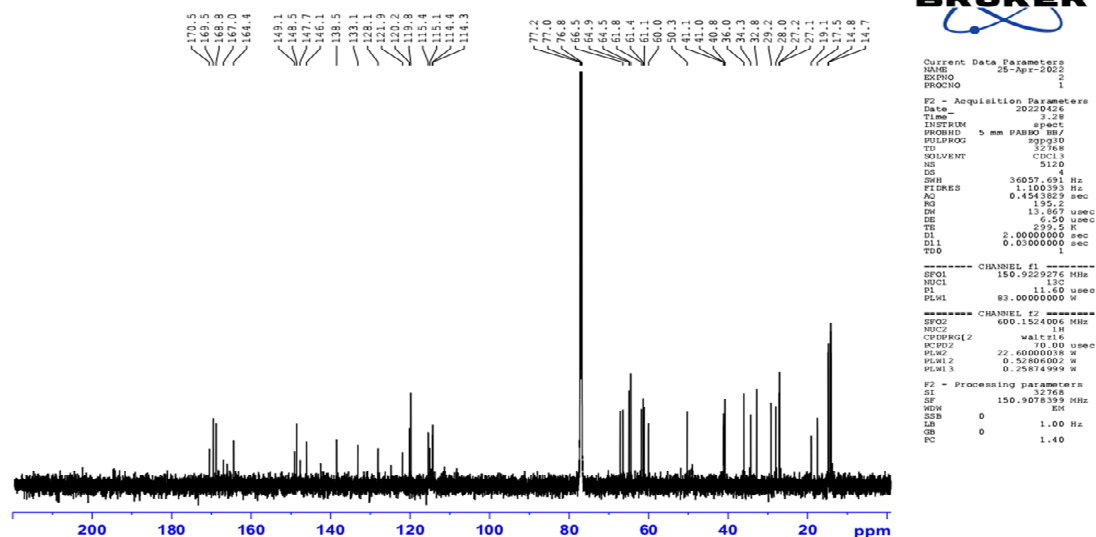
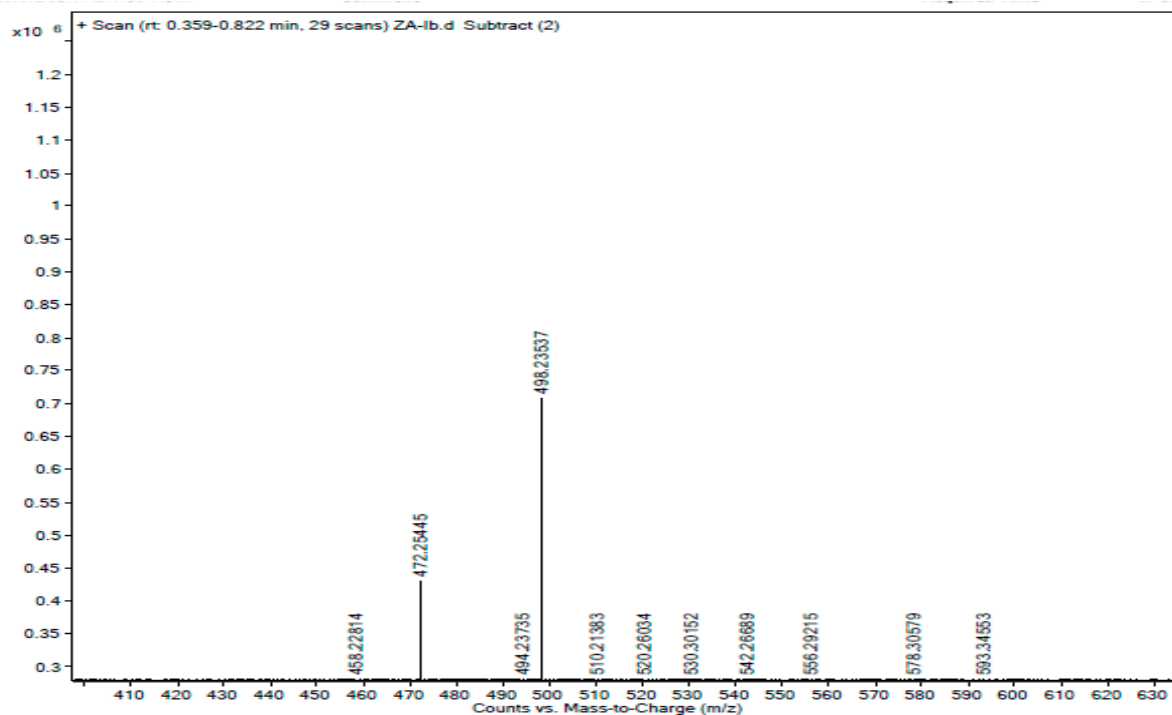
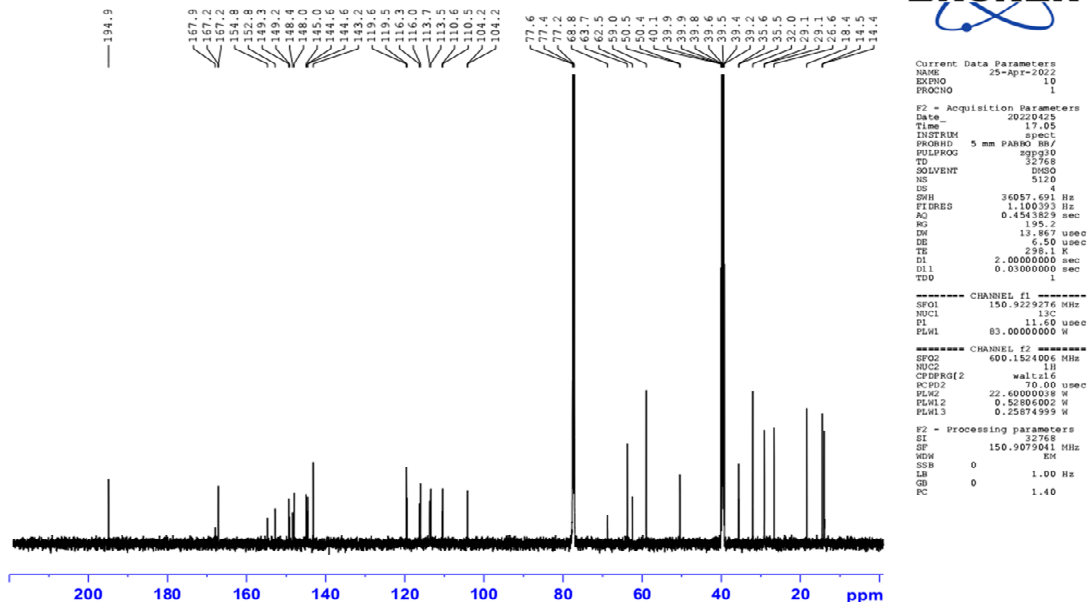
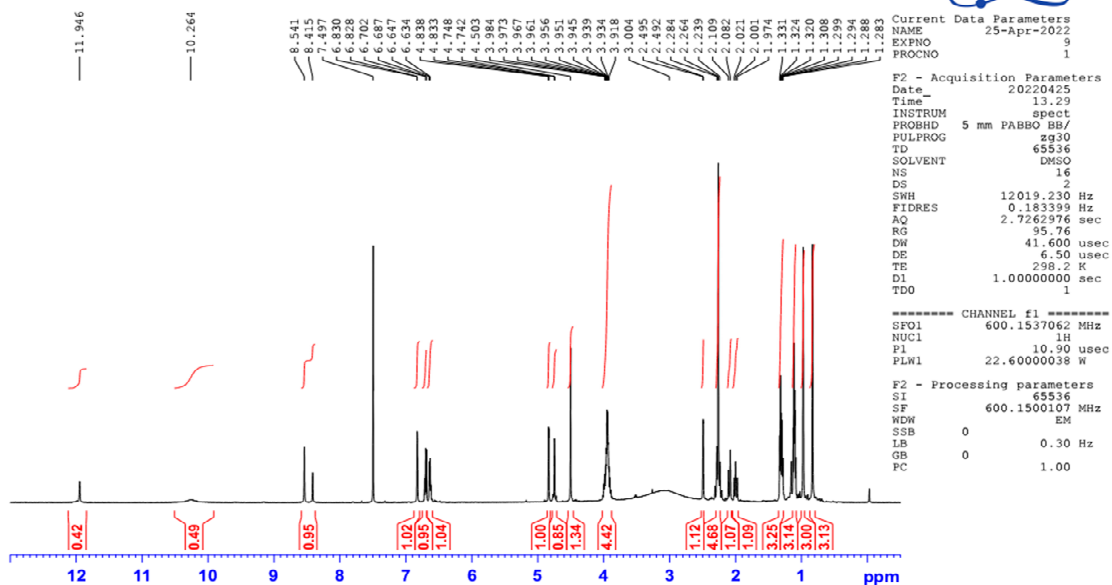
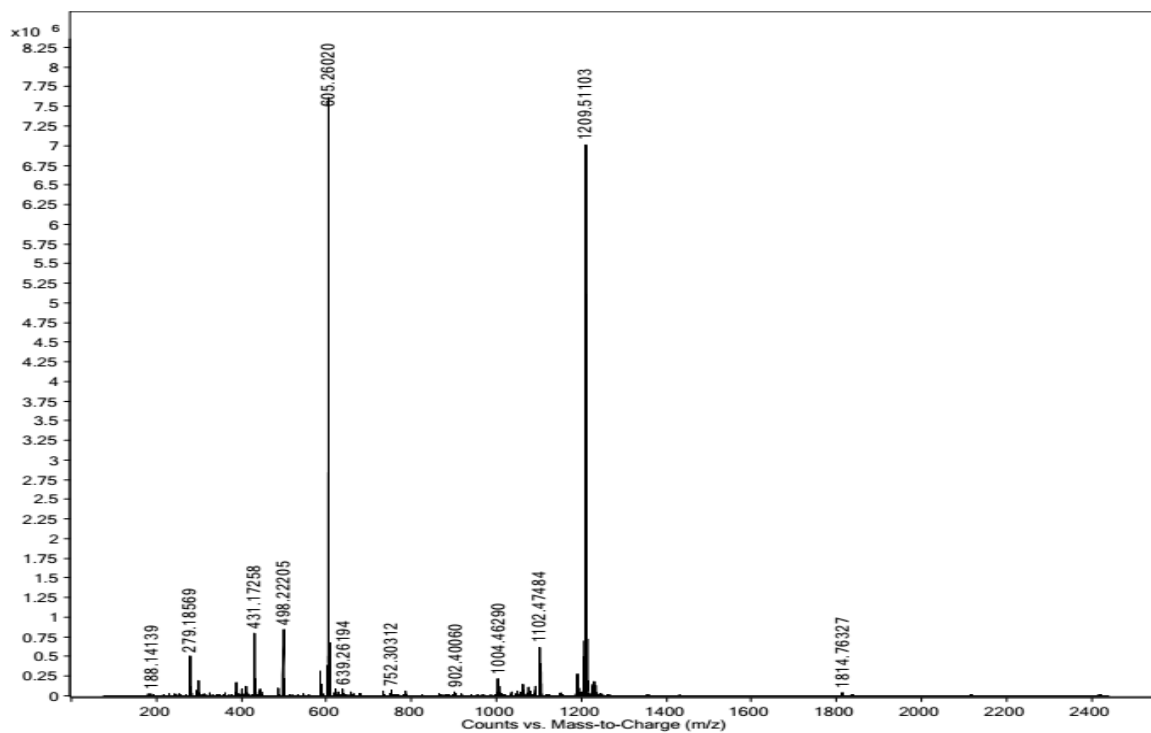


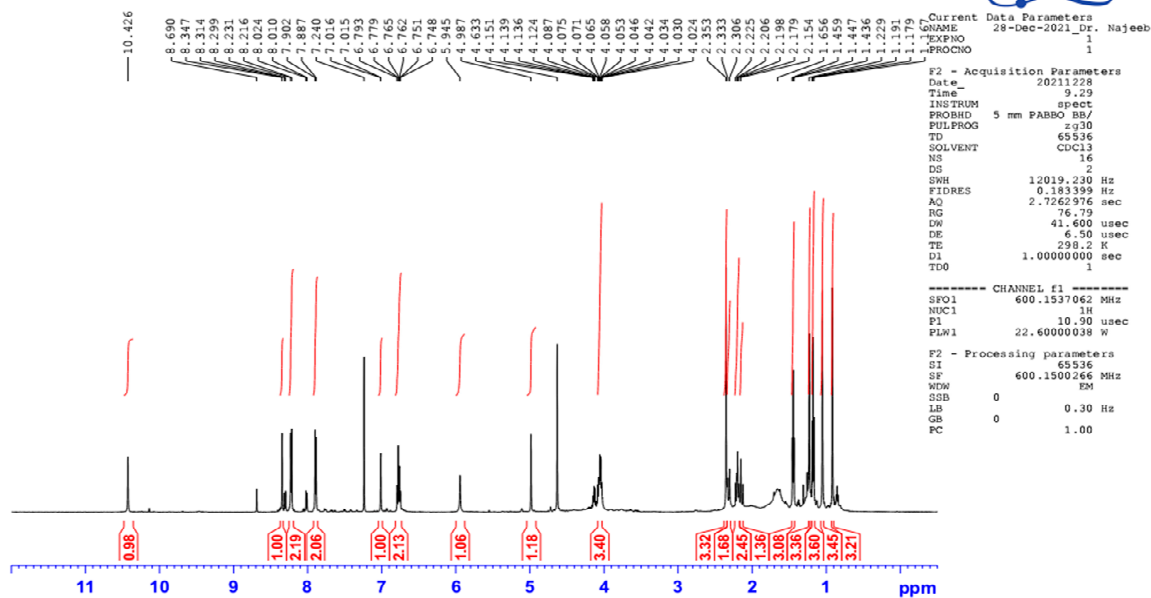
Figure S3: ^1H -NMR and ^{13}C -NMR spectra of compound 1







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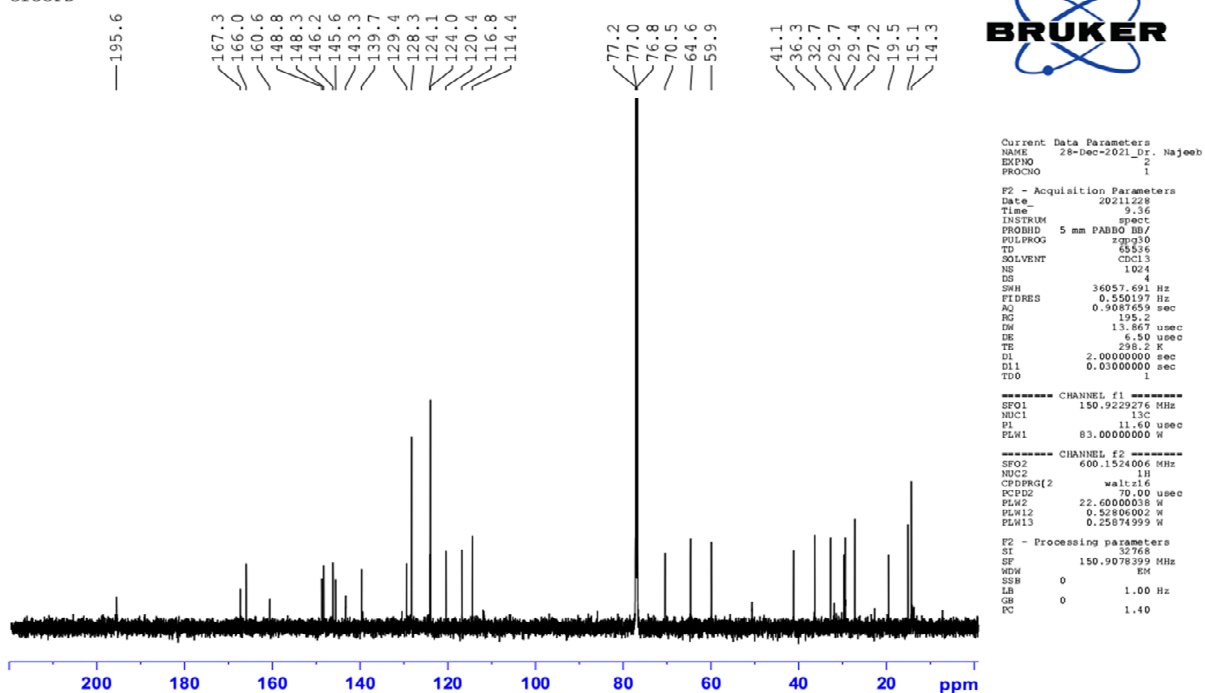
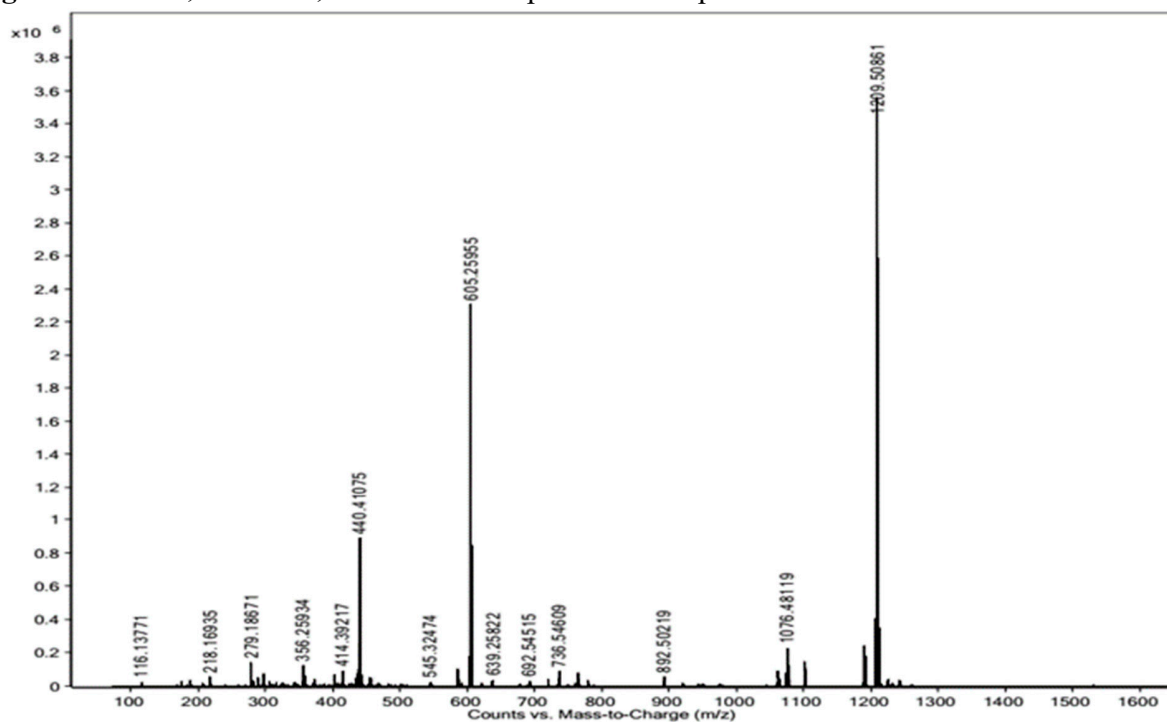
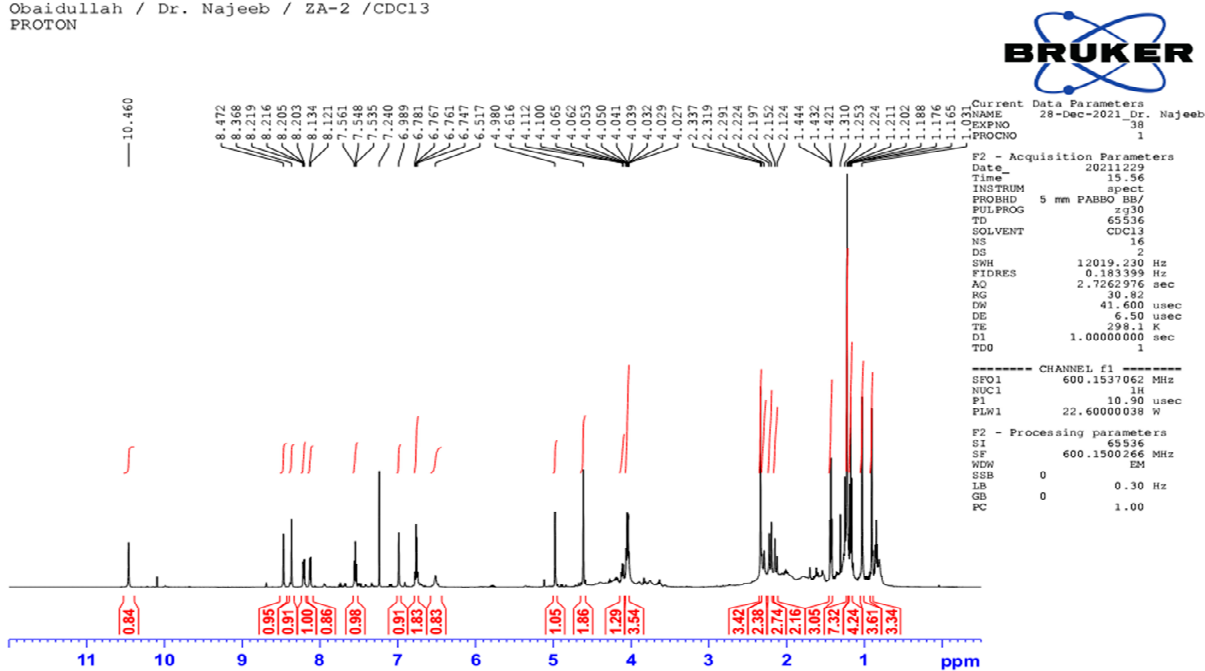


Figure S5: Mass, ¹H-NMR, and ¹³C-NMR spectra of compound **3**



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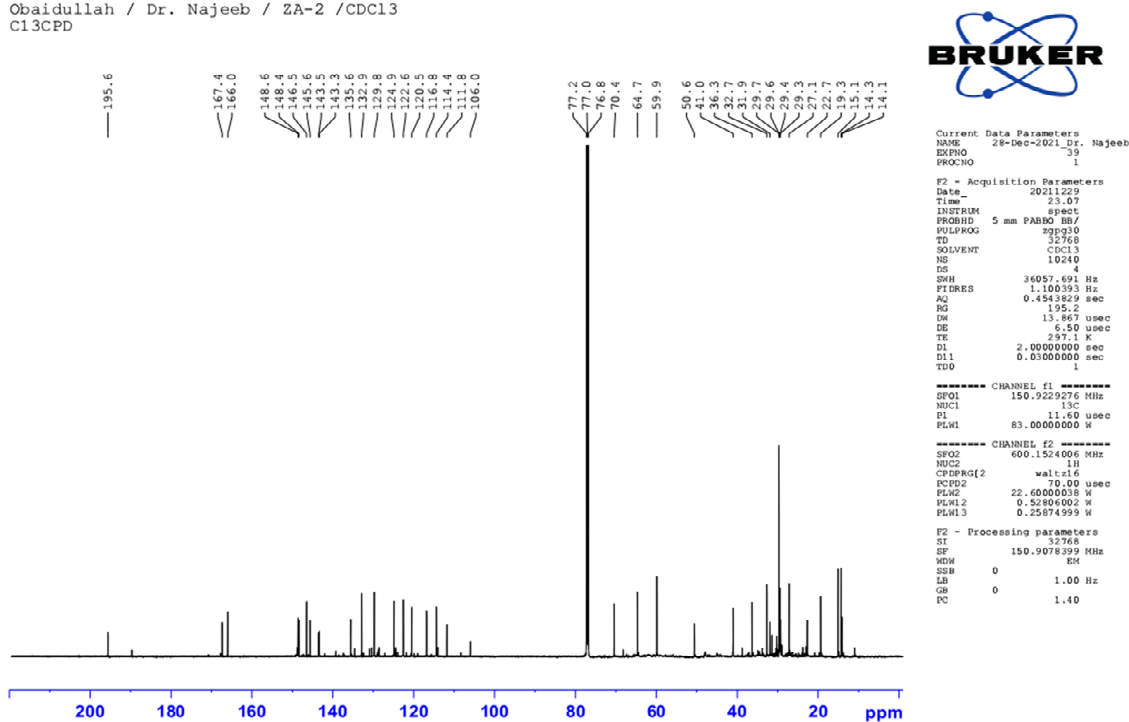
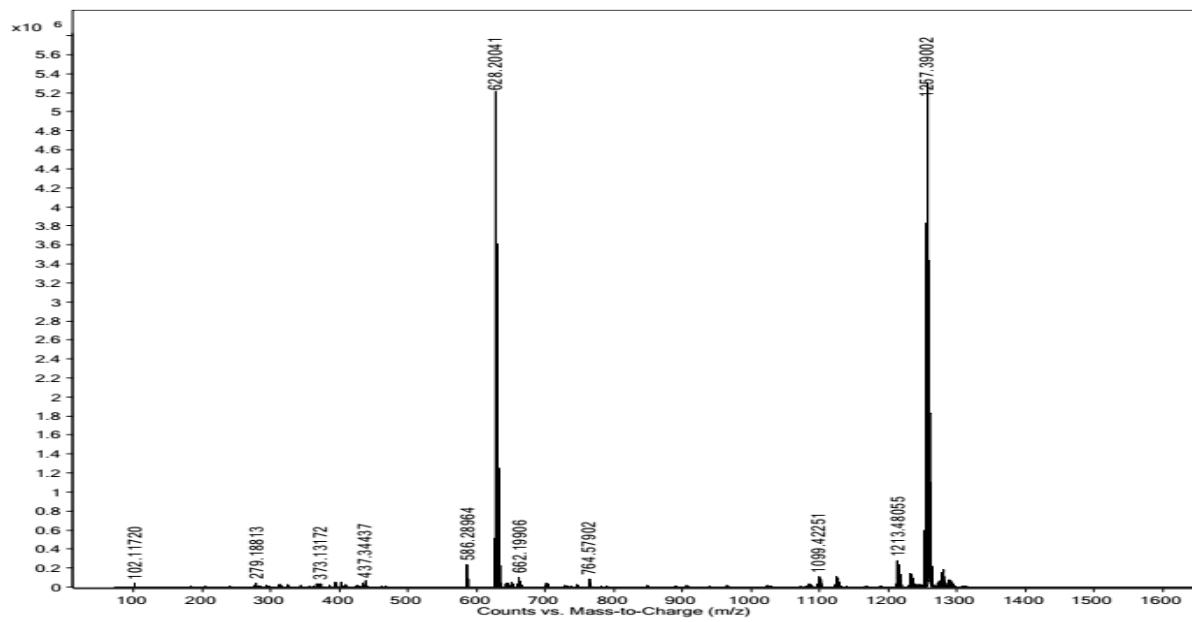
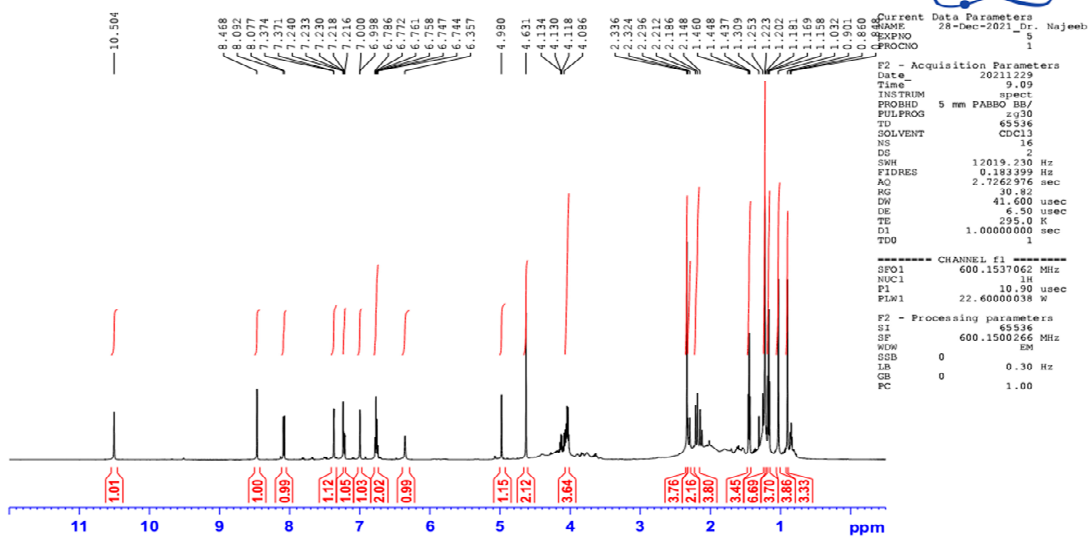


Figure S6: Mass, ¹H-NMR, and ¹³C-NMR spectra of compound 4



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C13CPD

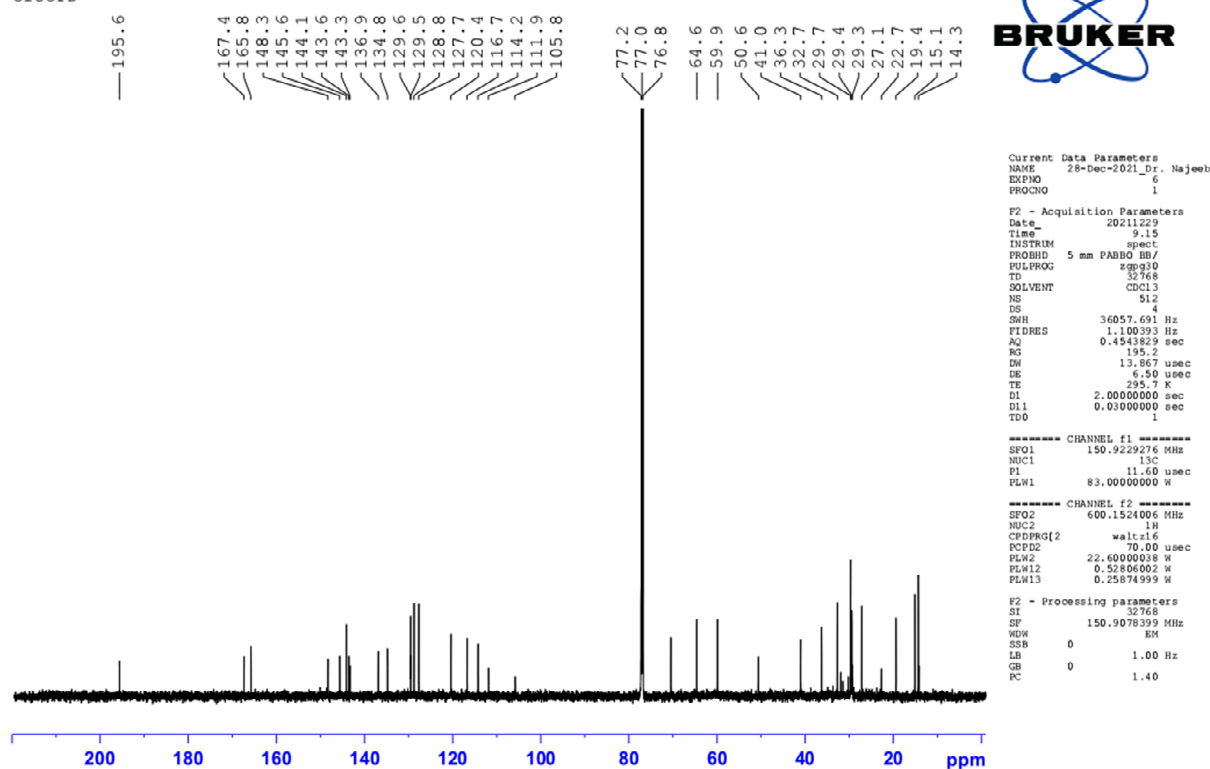
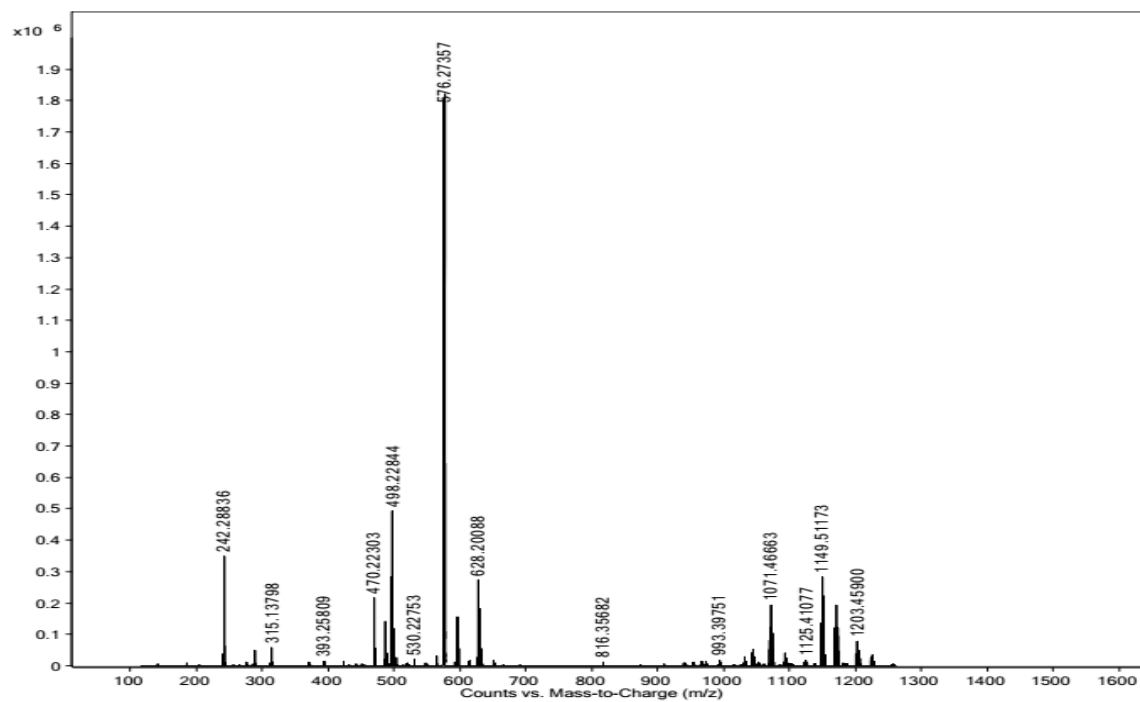
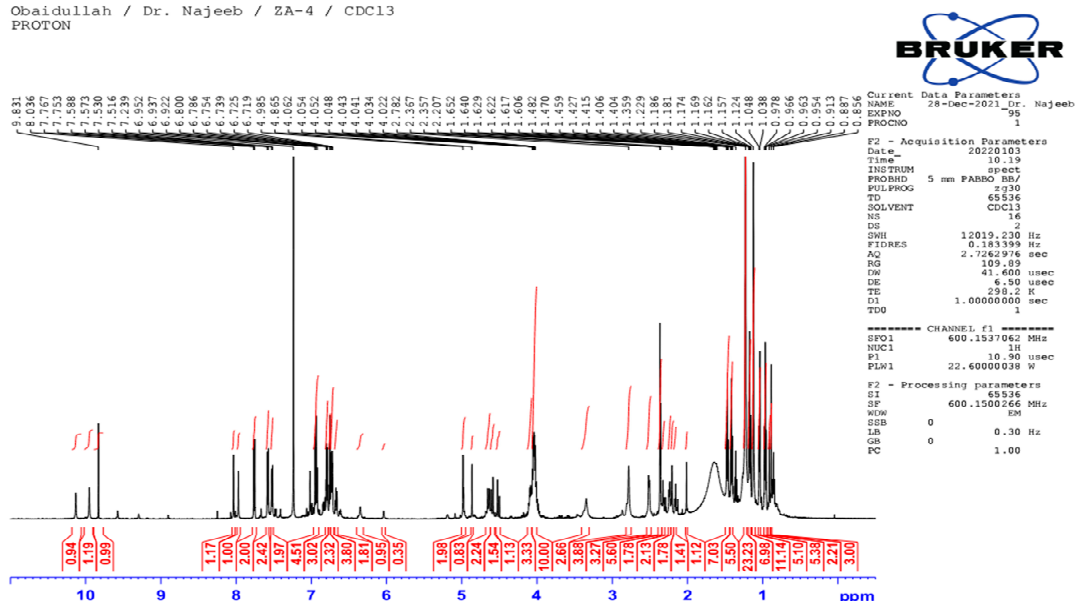


Figure S7: Mass, ¹H- and ¹³C-NMR spectra of compound **5**



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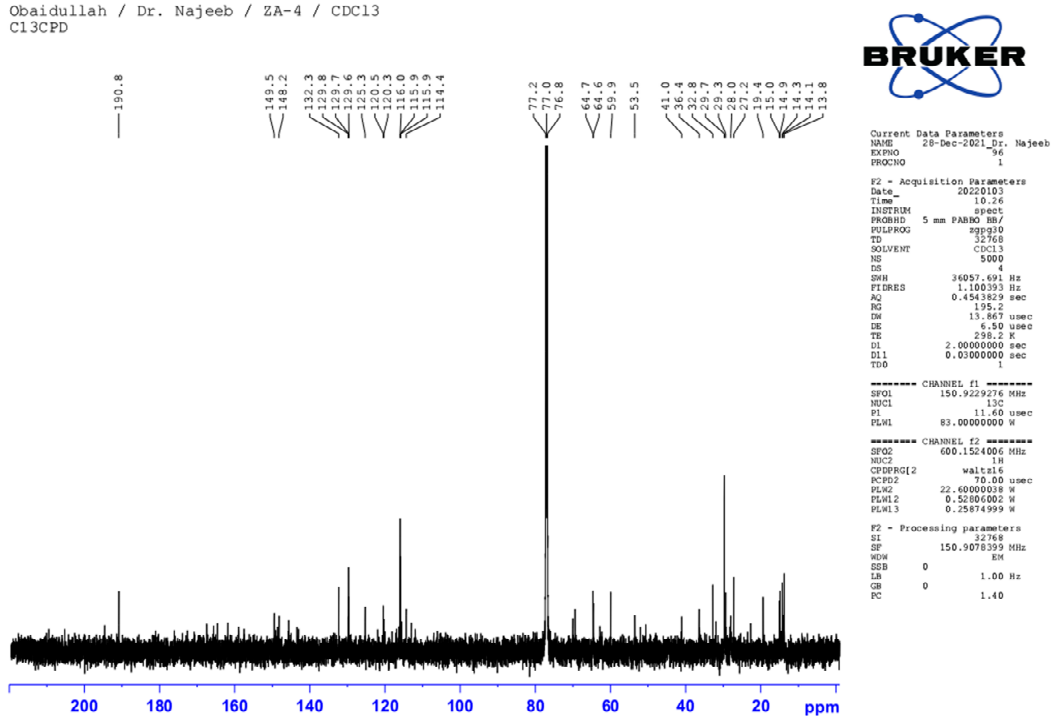
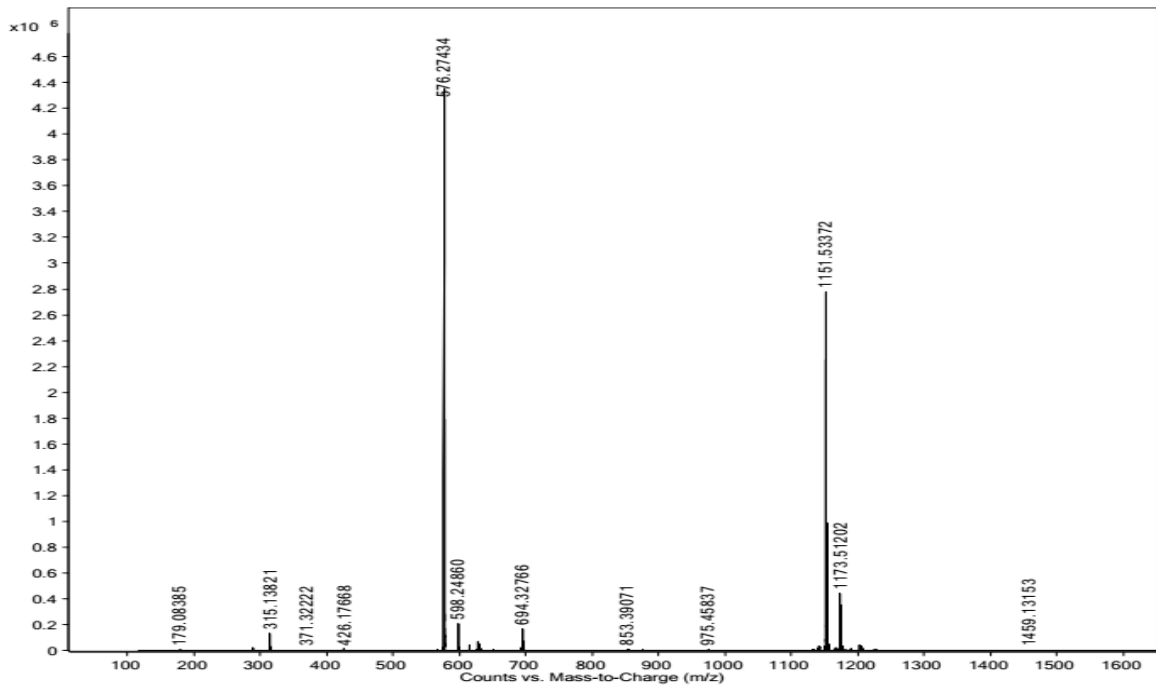
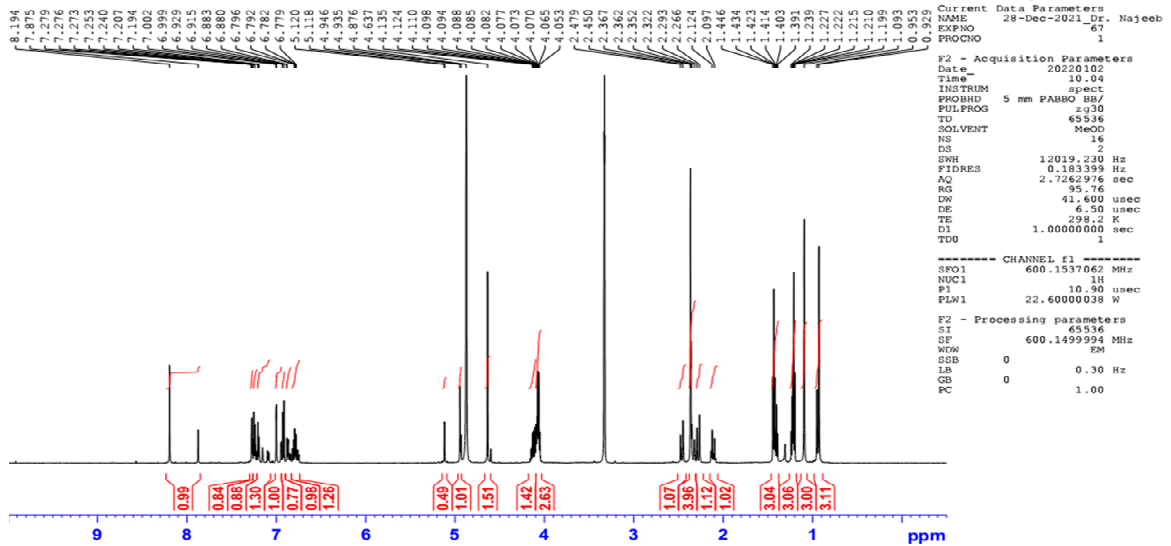


Figure S8: Mass, ^1H - and ^{13}C -NMR spectra of compound 6



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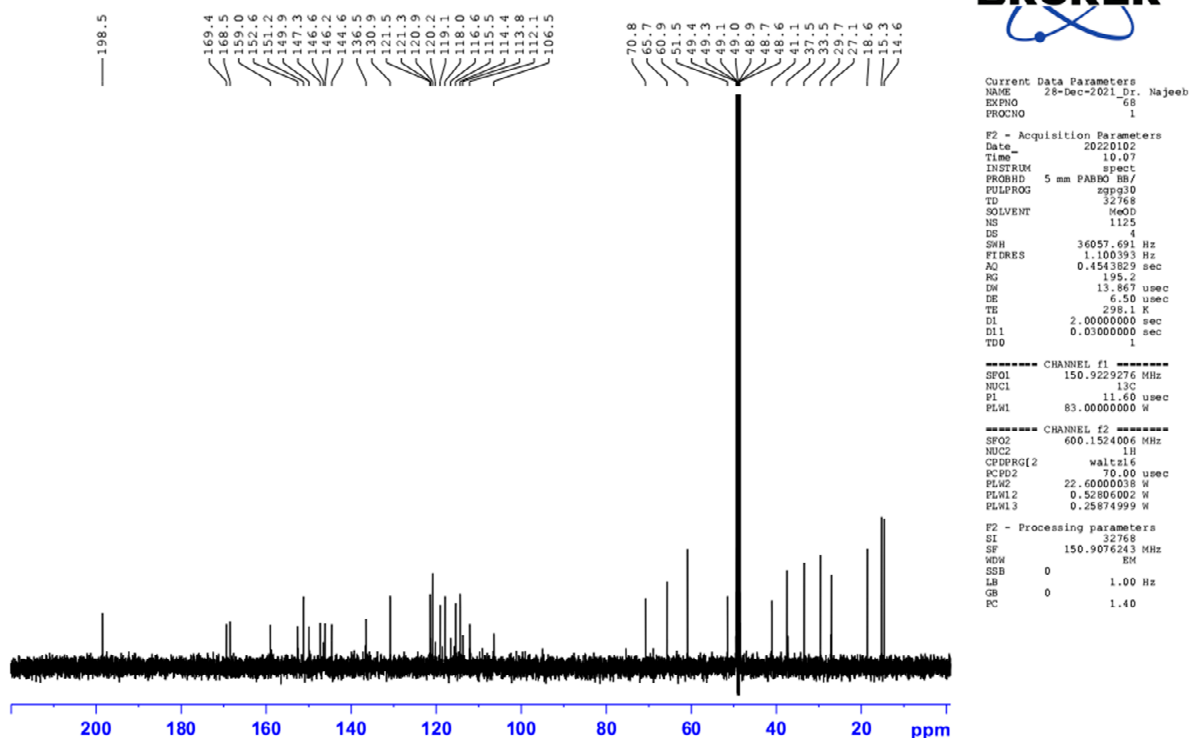
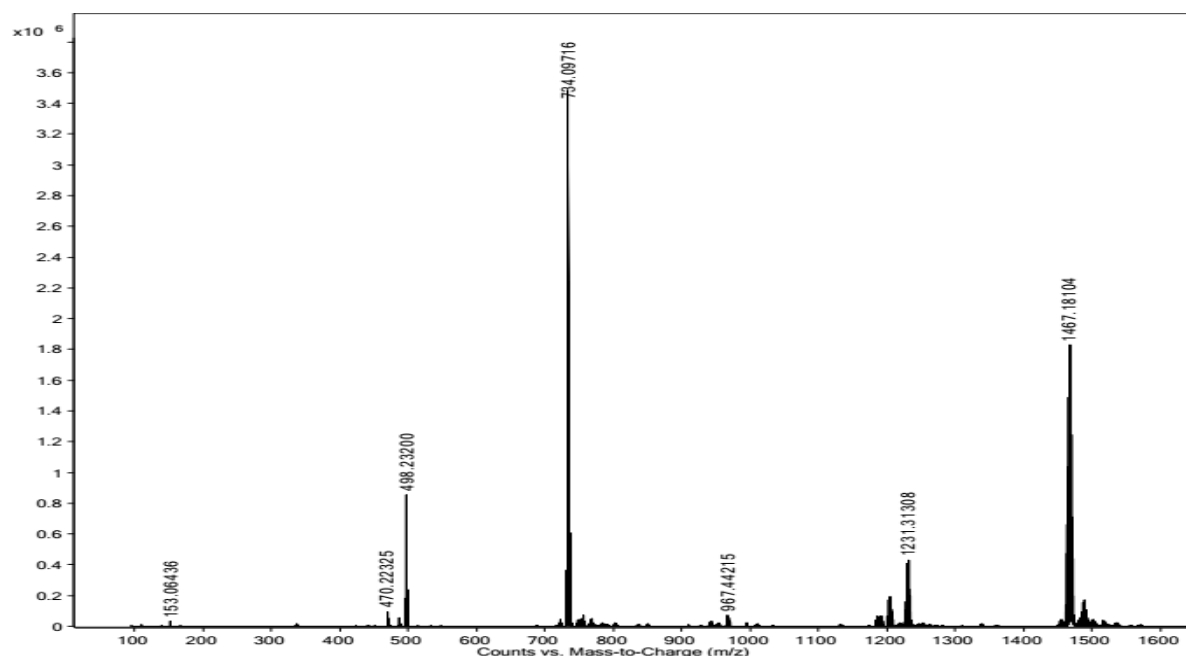
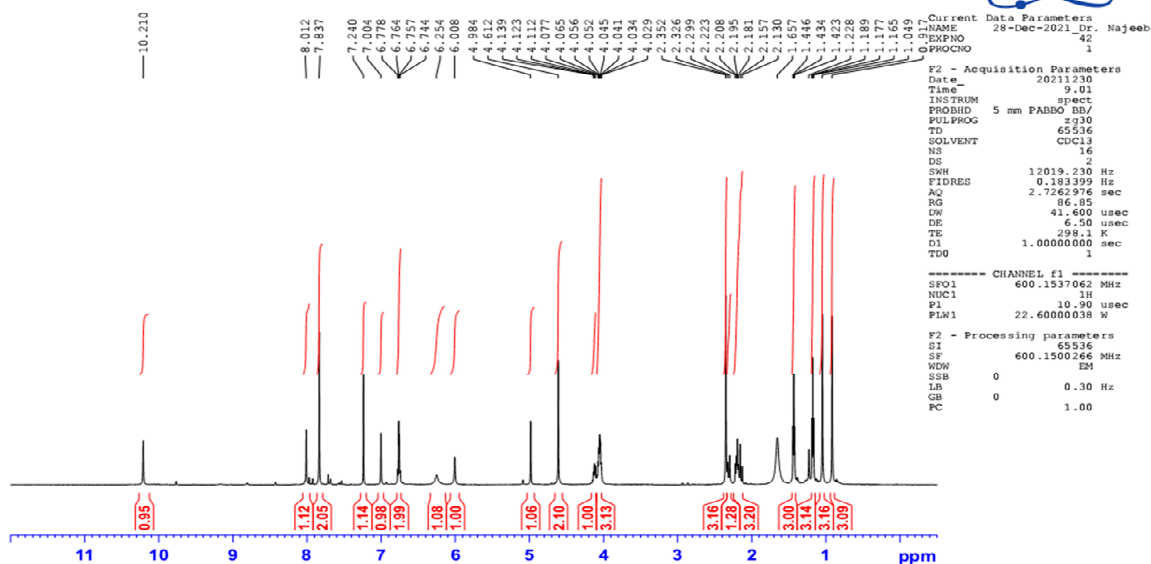


Figure S9: Mass, ^1H - and ^{13}C -NMR spectra of compound 7



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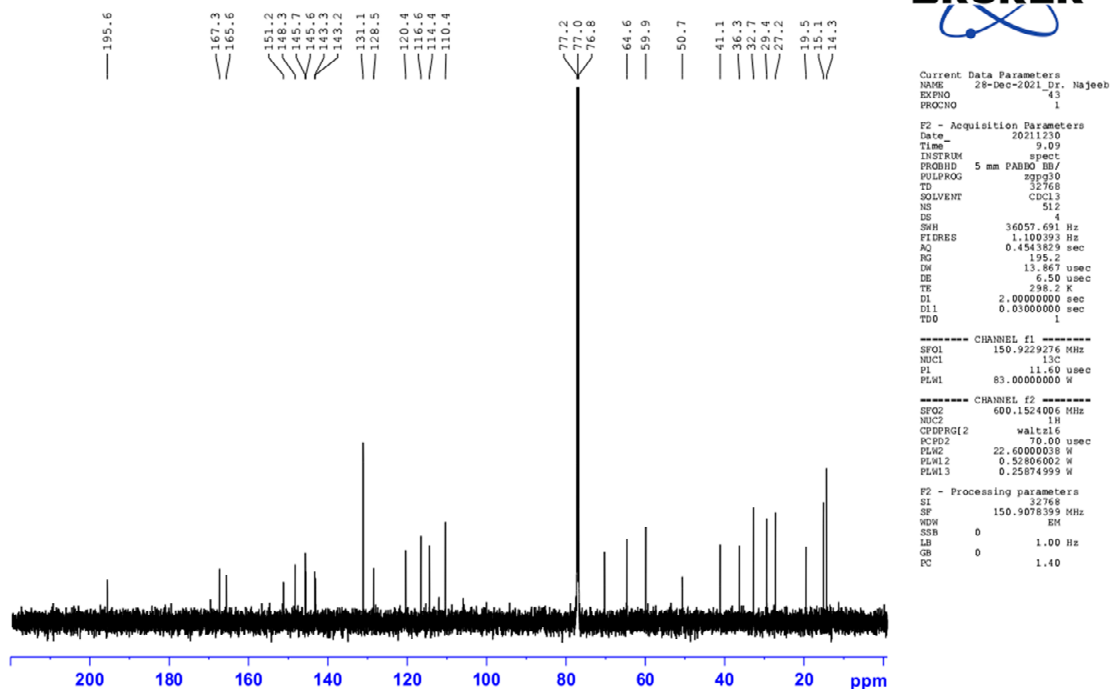


Figure S10: Mass, ¹H- and ¹³C-NMR spectra of compound 8



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C13CPD

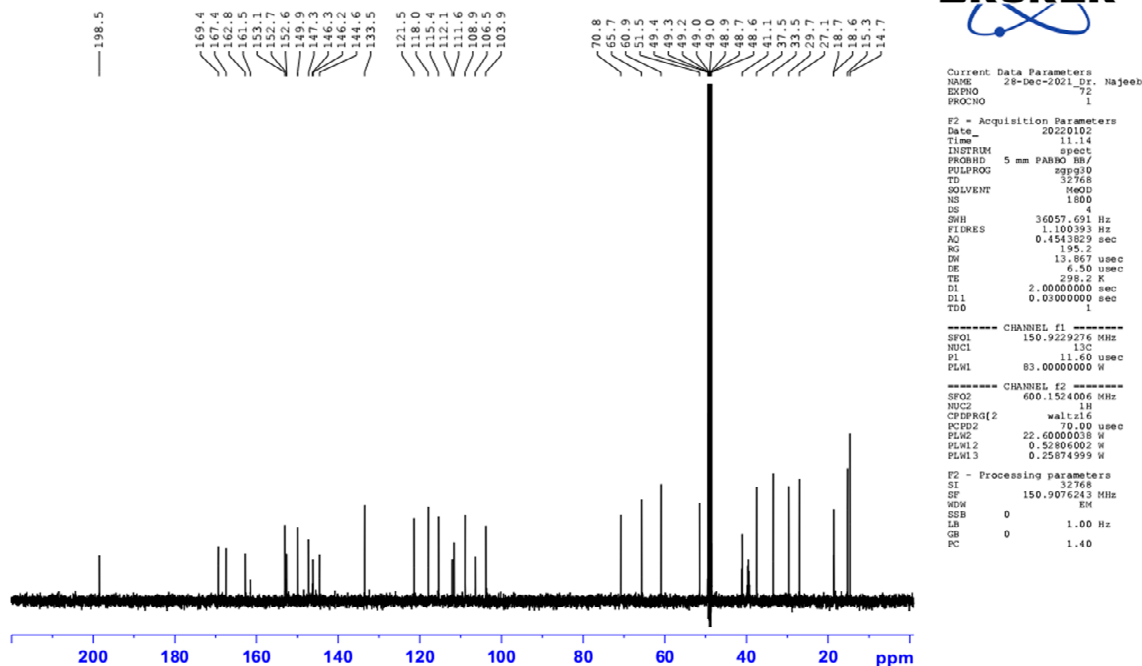
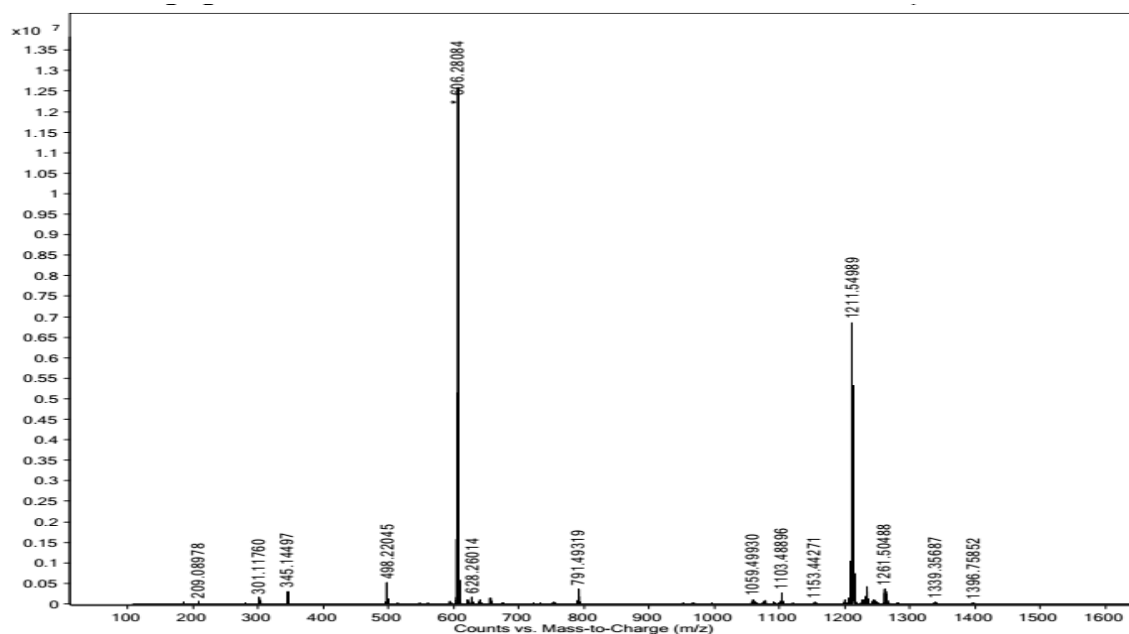
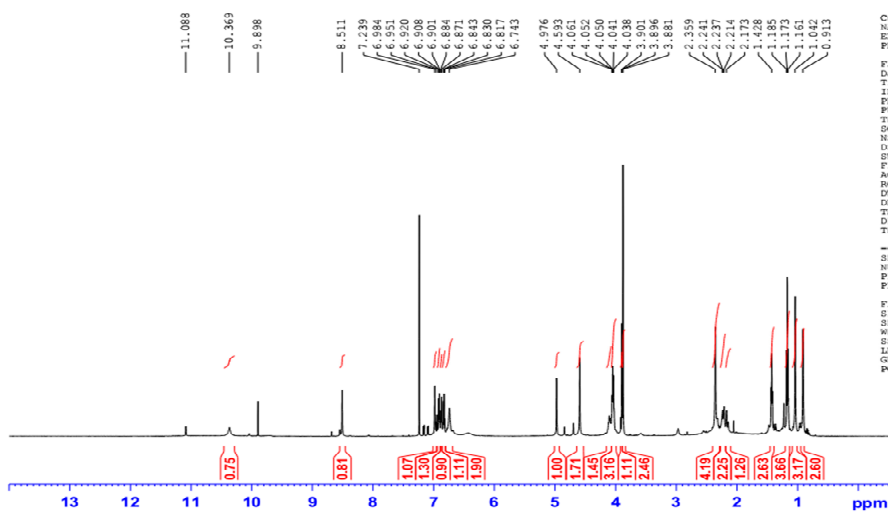


Figure S11: Mass, ^1H - and ^{13}C -NMR spectra of compound 9



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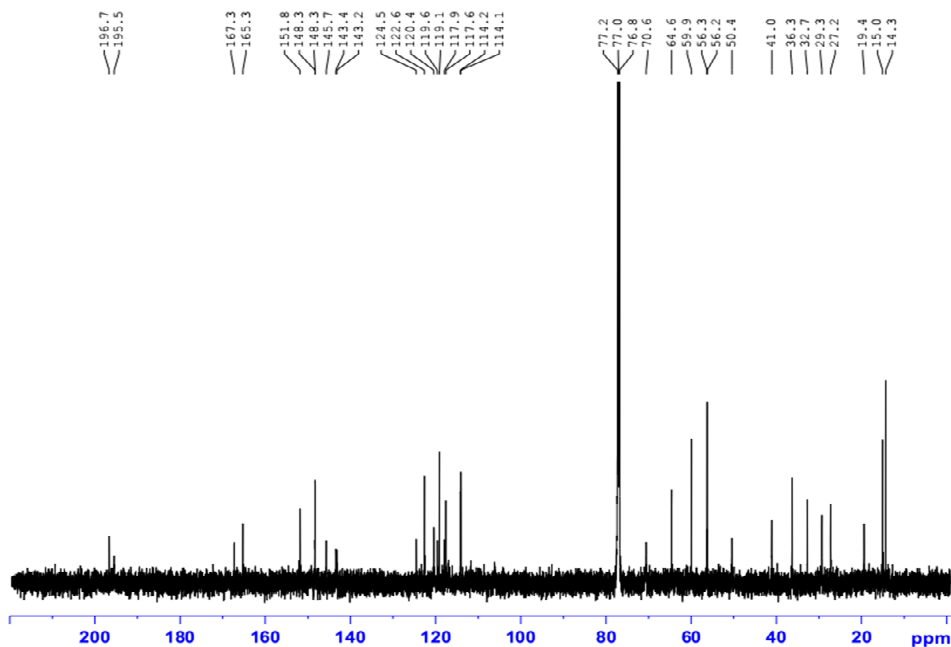
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C13CPD



BRUKER

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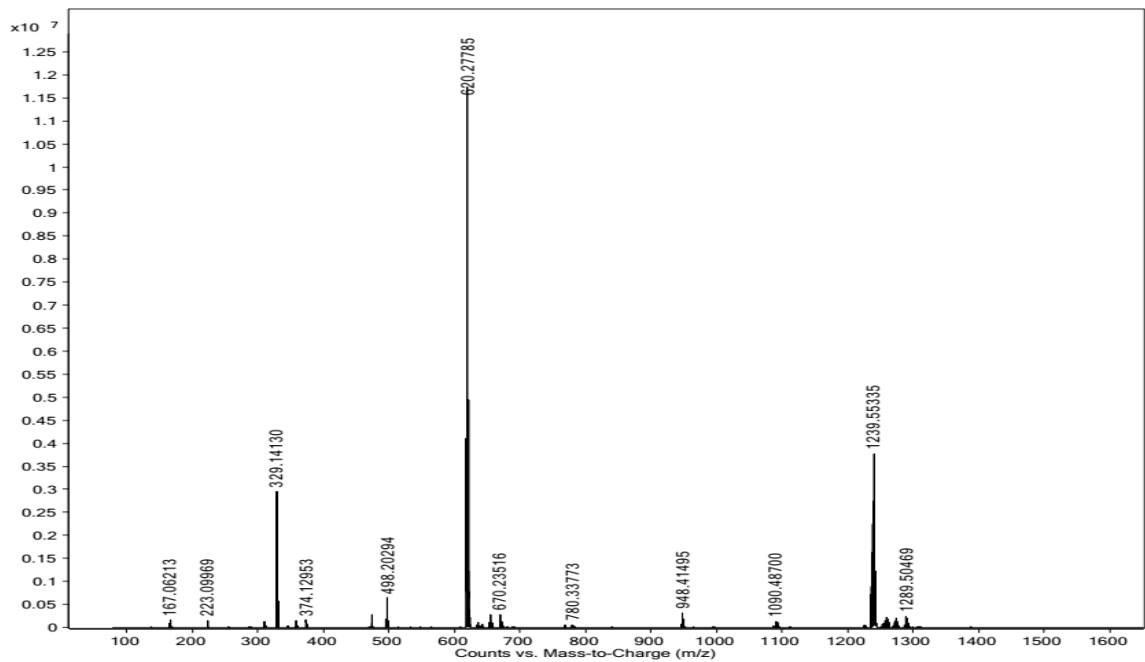
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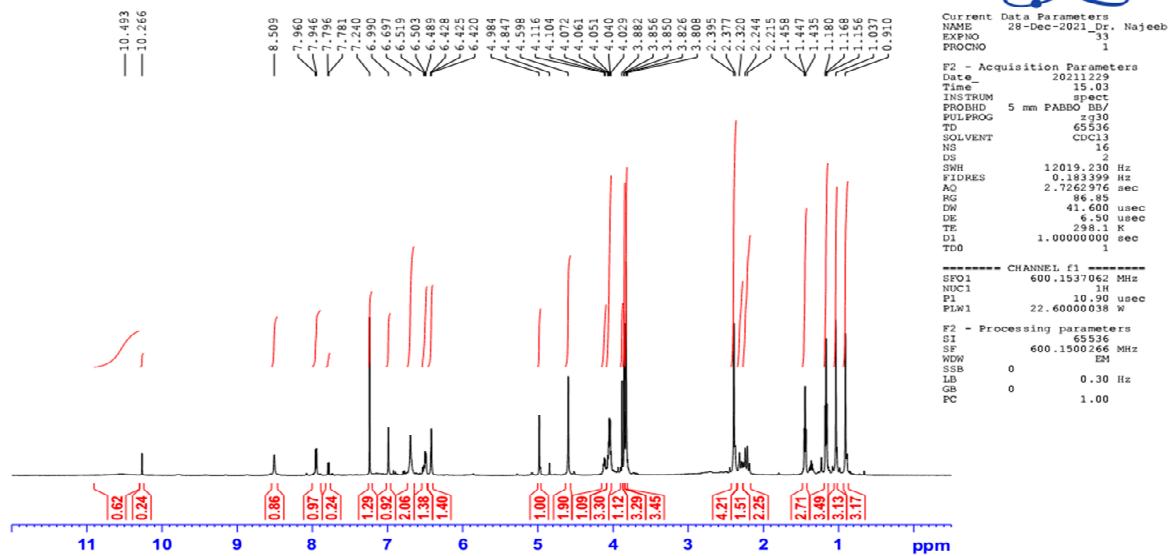
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Figure S12: Mass, ^1H - and ^{13}C -NMR spectra of compound 10



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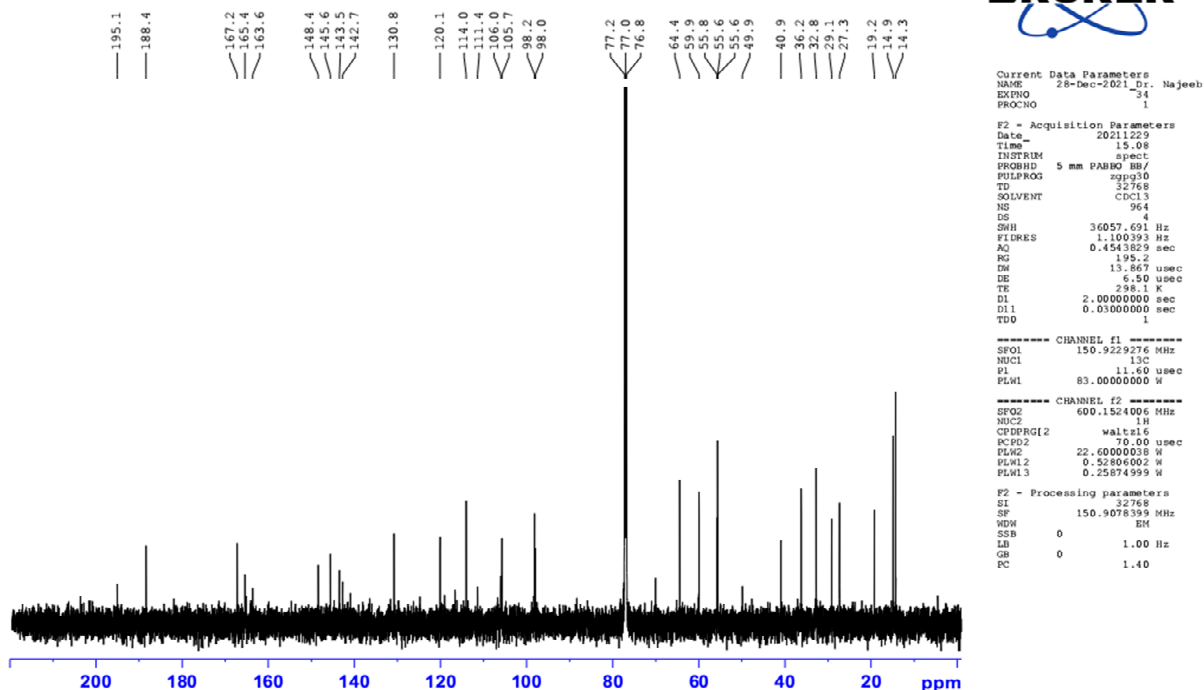
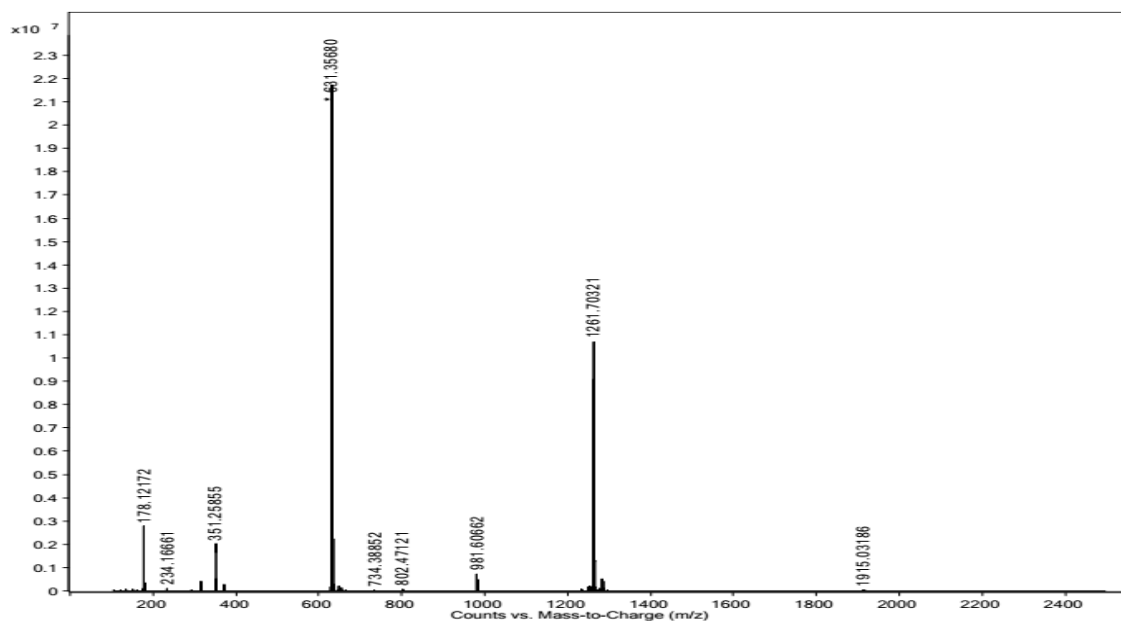
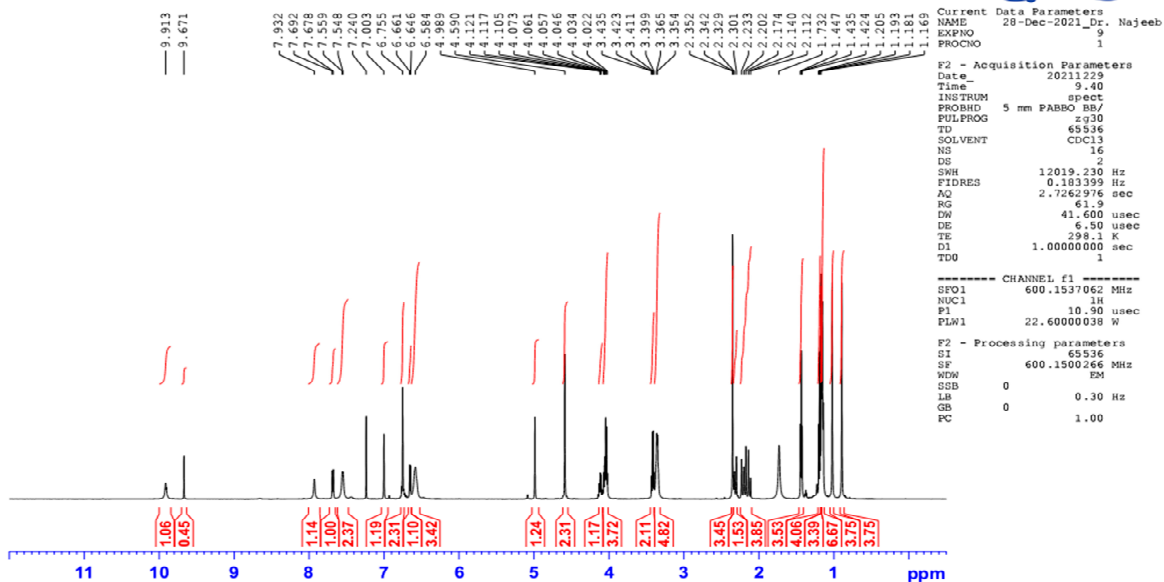


Figure S13: Mass, ¹H- and ¹³C-NMR spectra of compound 11



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PROTON



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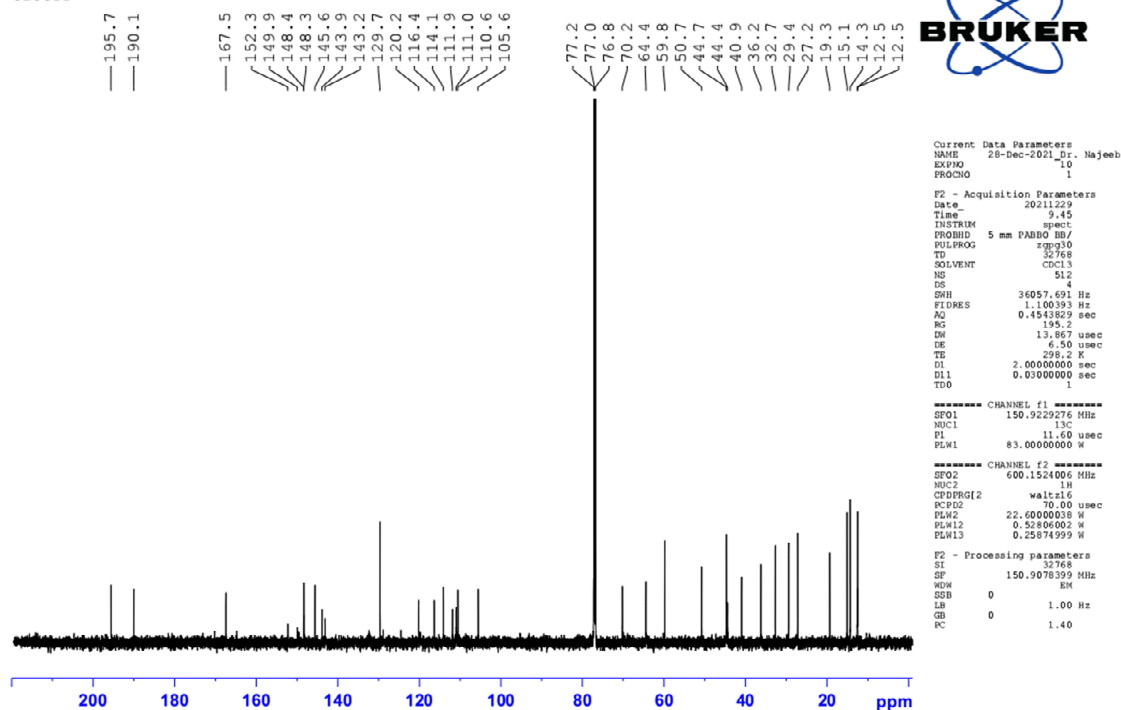
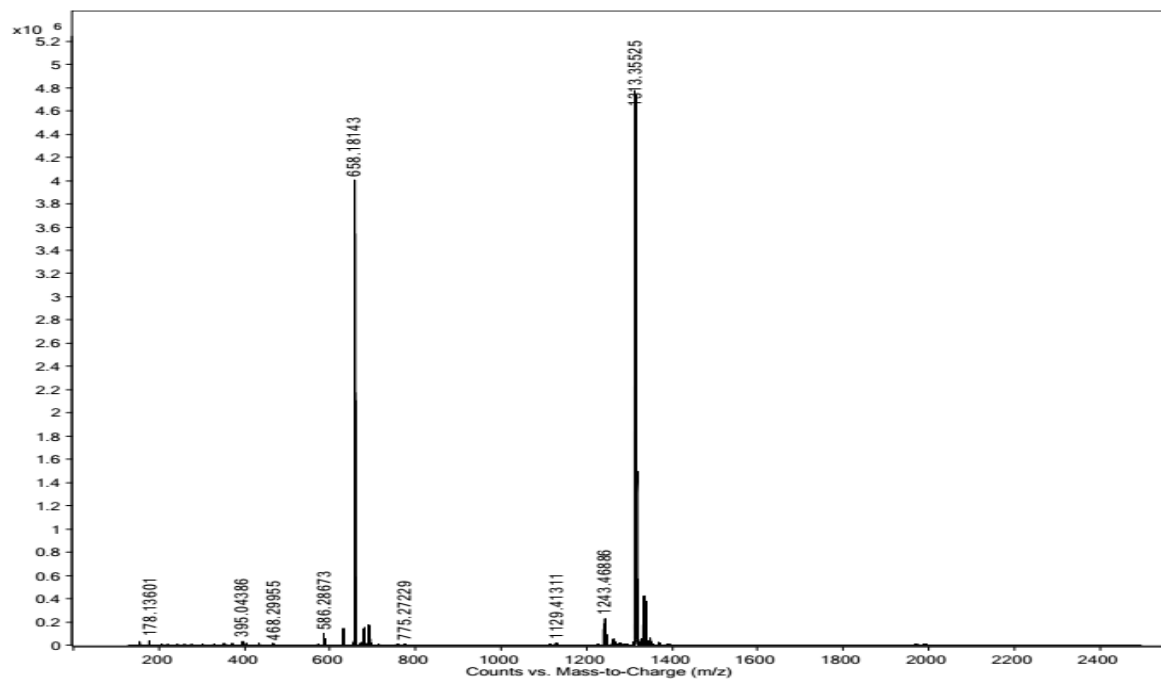
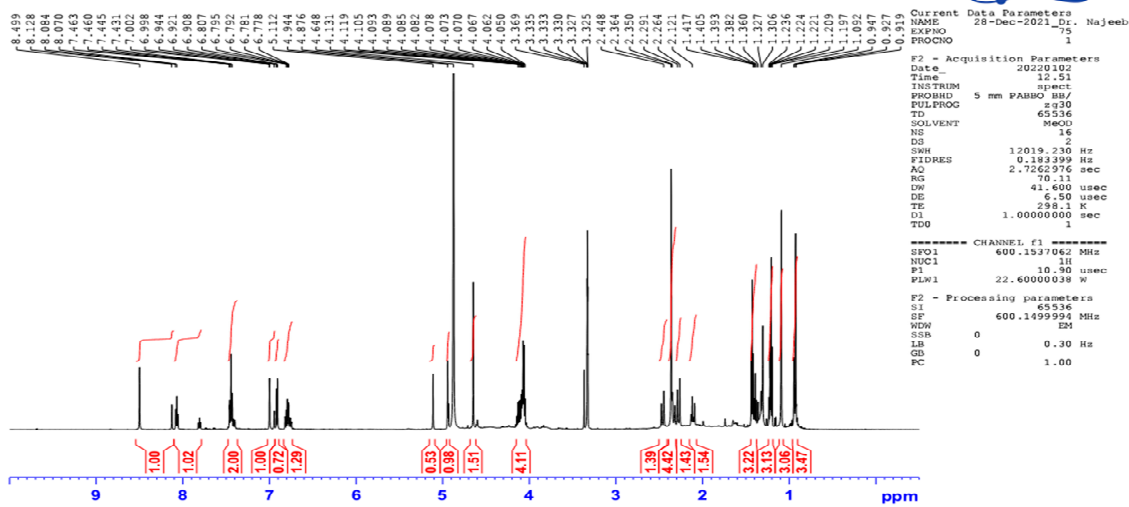


Figure S14: Mass, ¹H- and ¹³C-NMR spectra of compound 12



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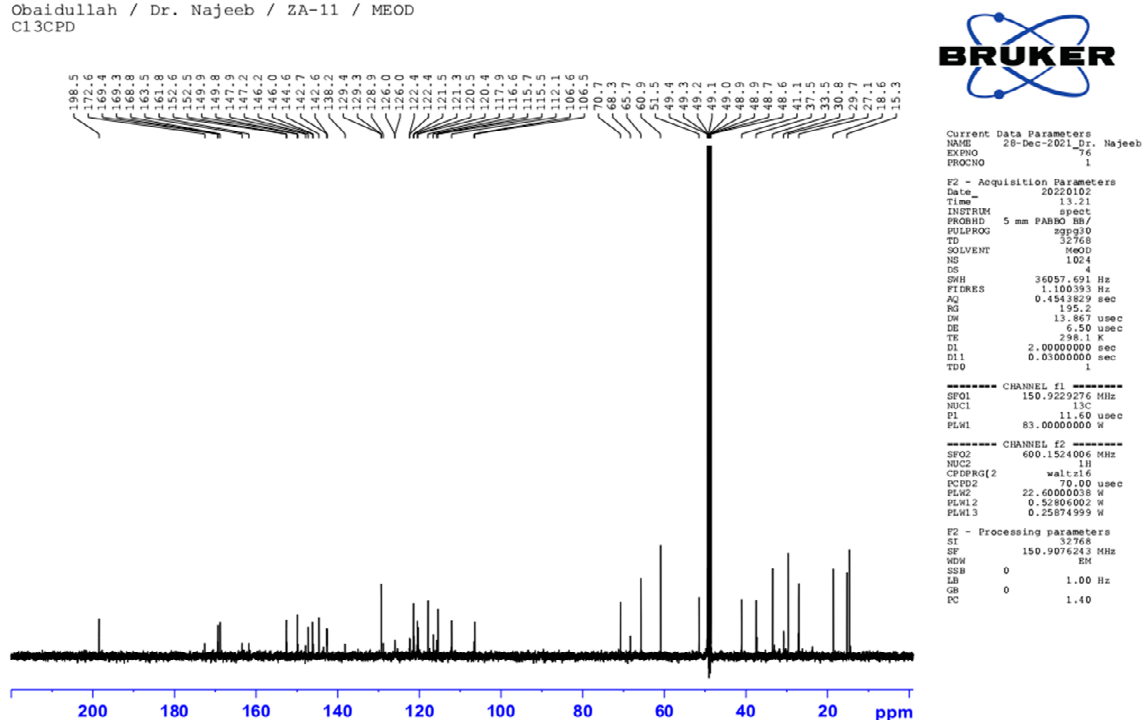
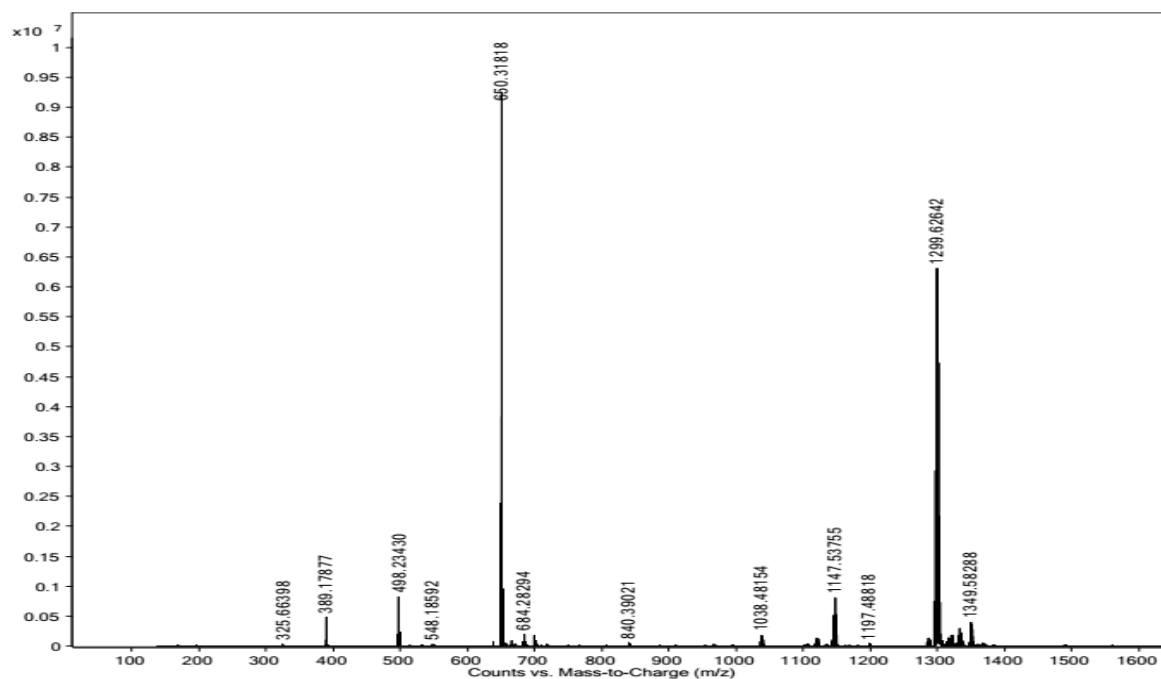
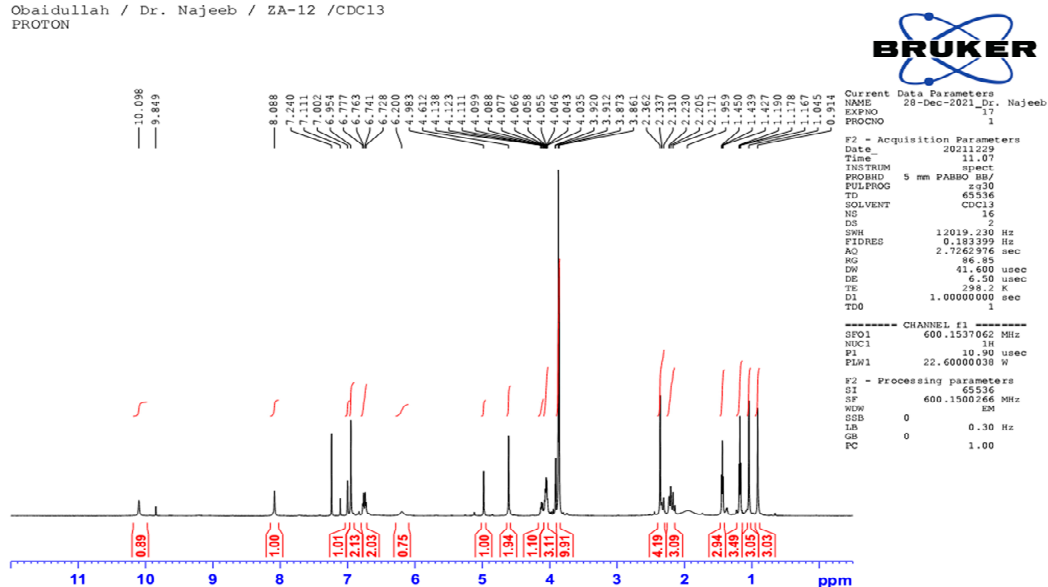


Figure S15: Mass, ^1H - and ^{13}C -NMR spectra of compound 13



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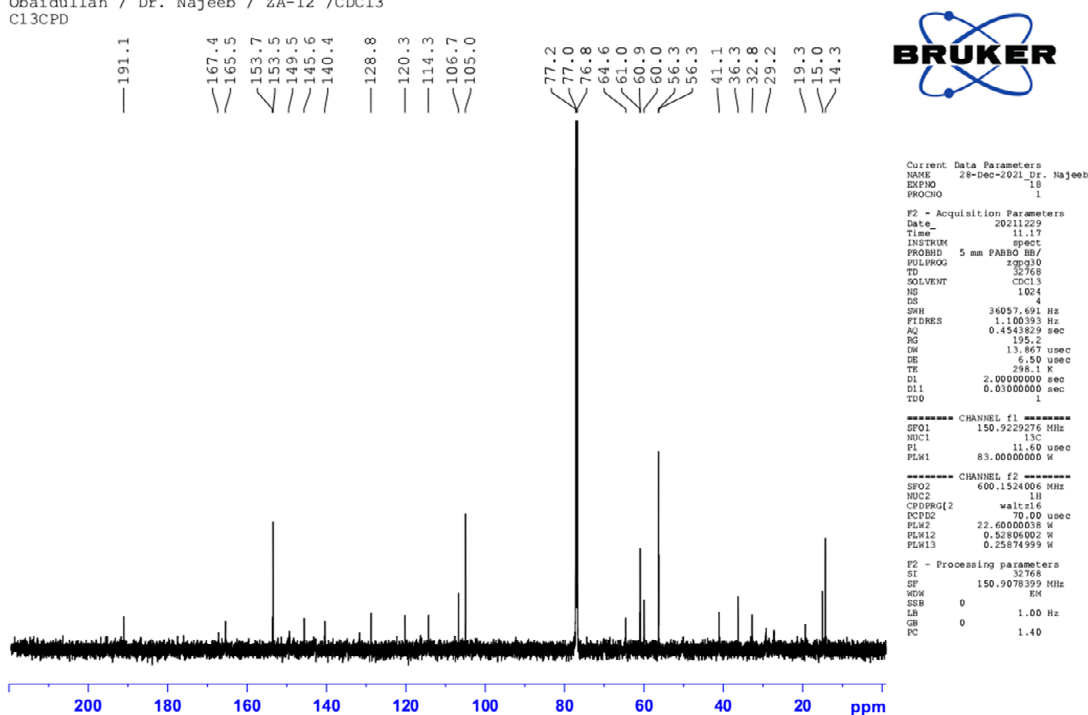
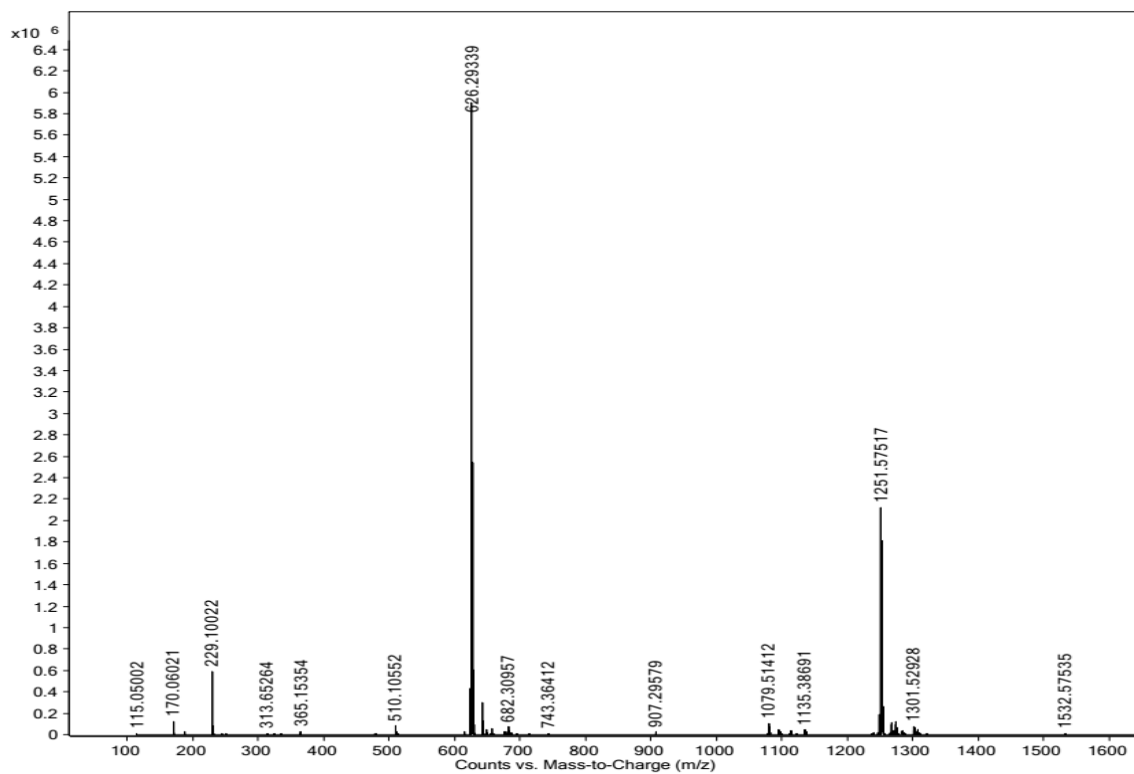
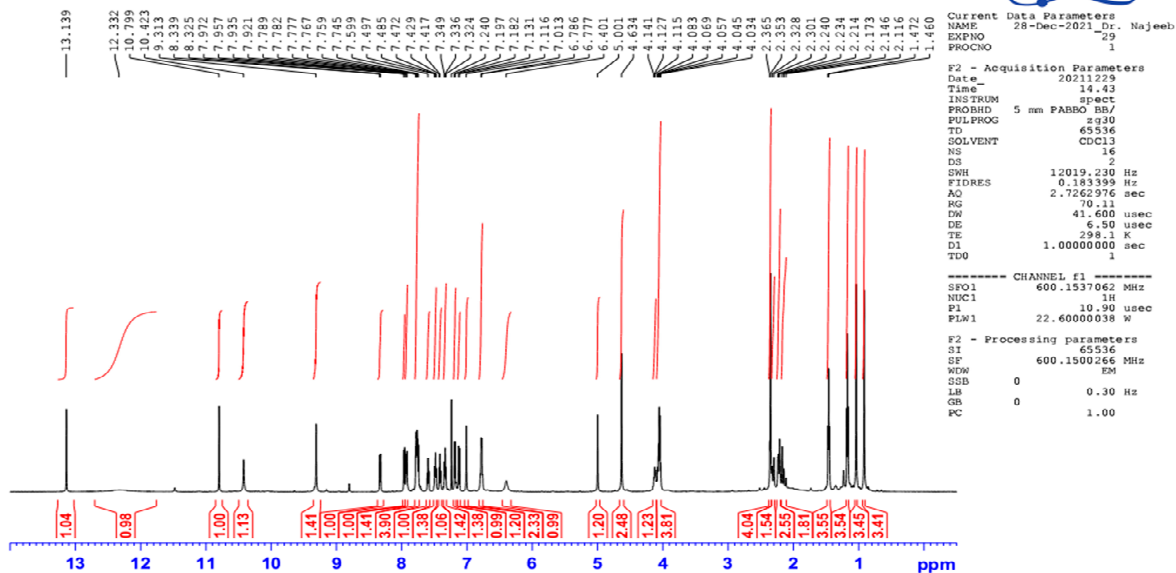


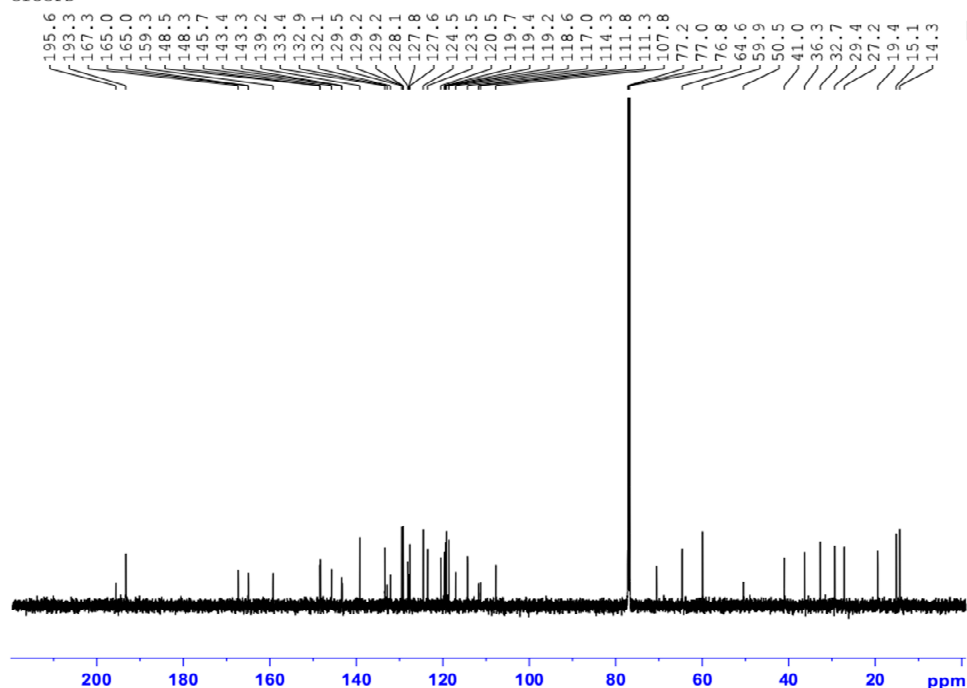
Figure S16: Mass, ¹H- and ¹³C-NMR spectra of compound 14



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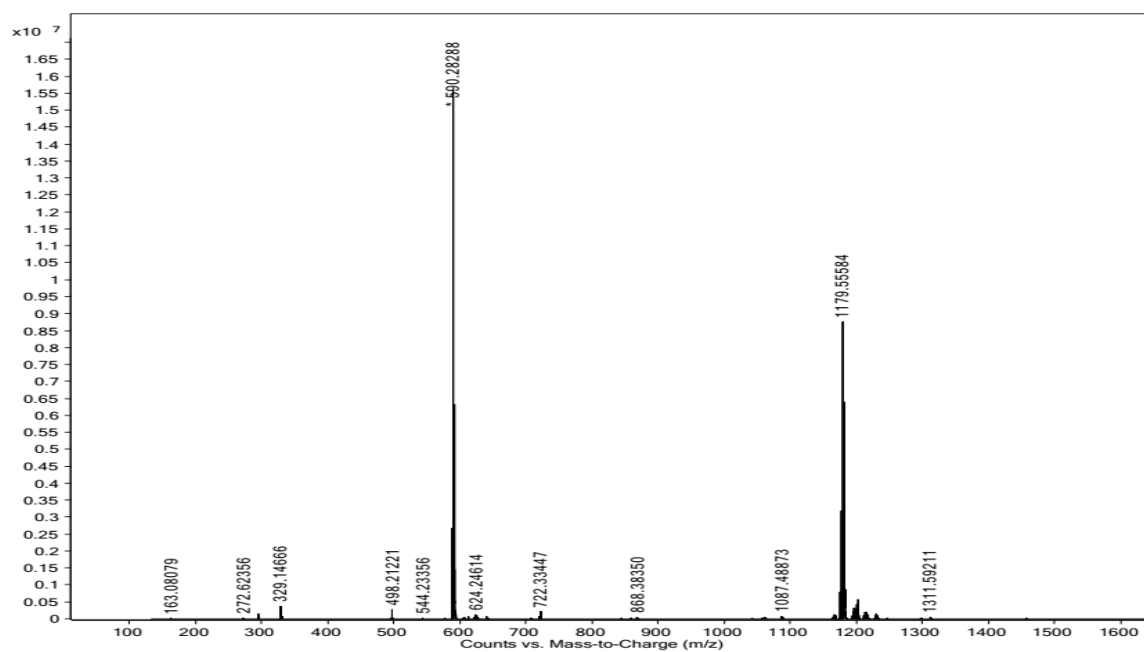
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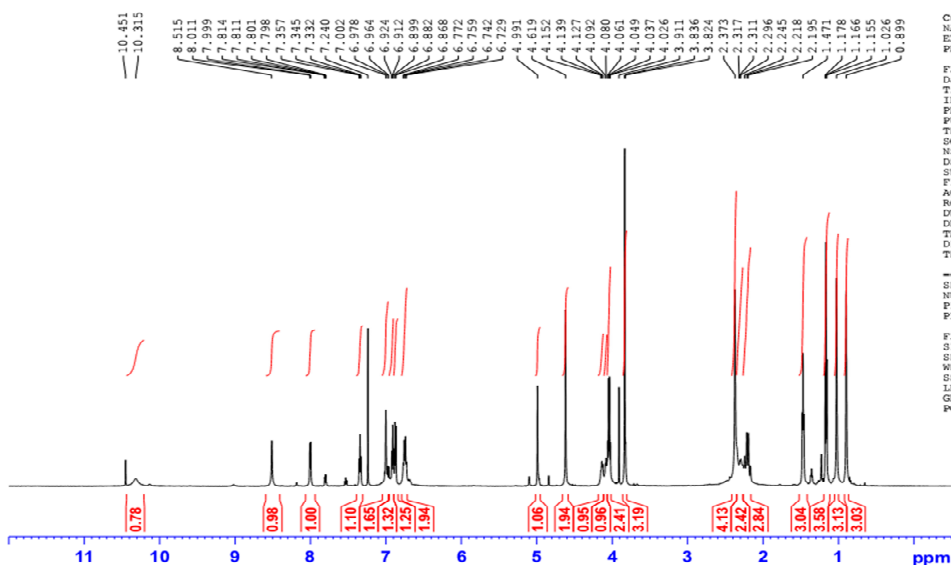
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Figure S17: Mass, ¹H- and ¹³C-NMR spectra of compound 15



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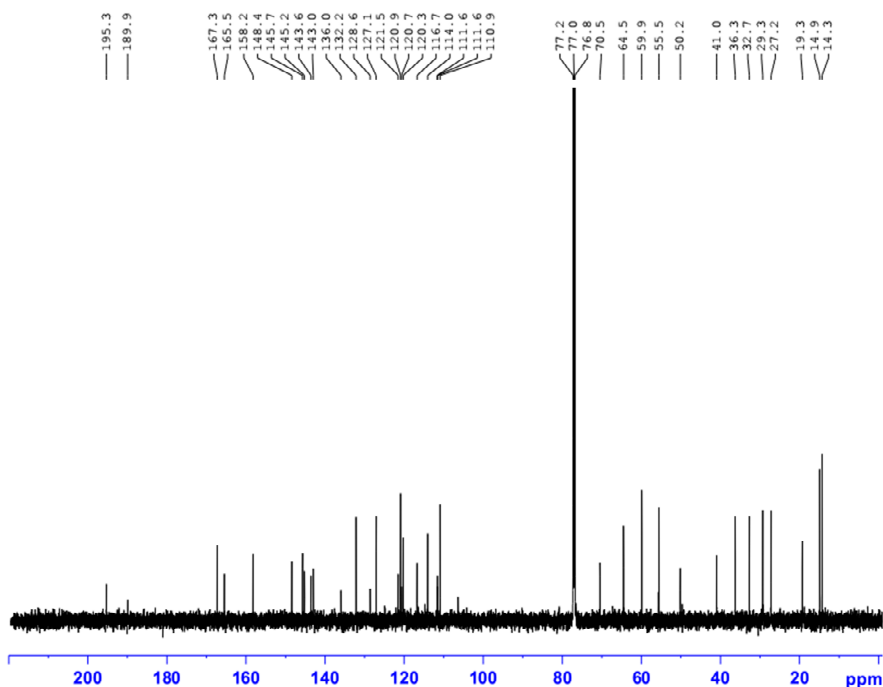
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C13CPD



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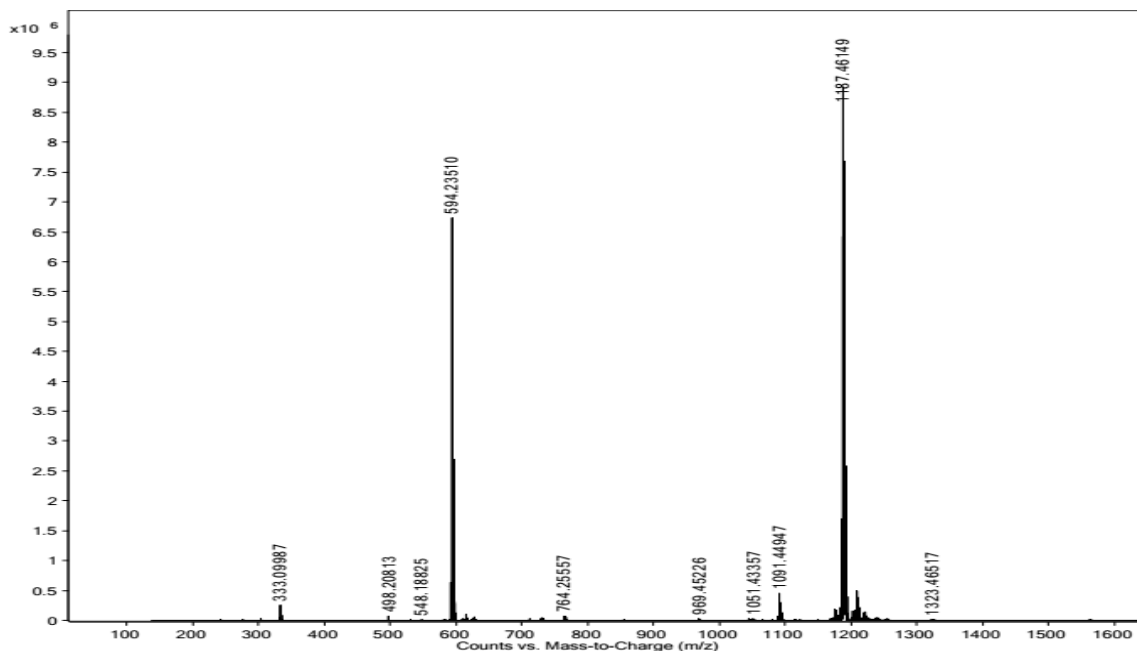
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P1 11.60 usec
PLW1 83.00000000 W

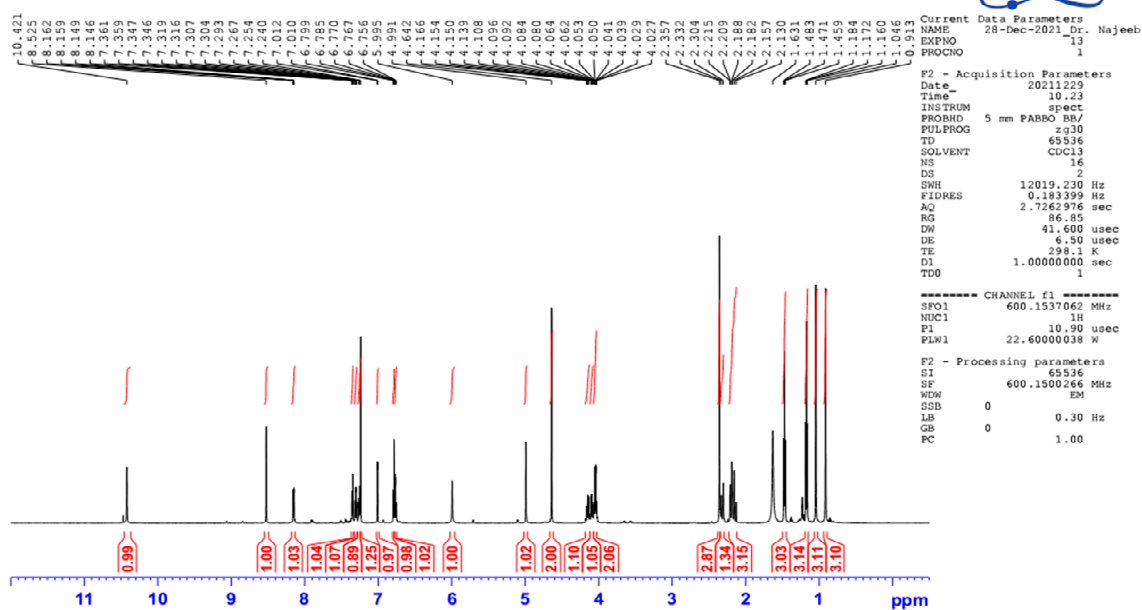
----- CHANNEL f2 -----
SFO2 600.1524006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 22.60000038 W
PLW12 0.52806002 W
PLW13 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9078399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

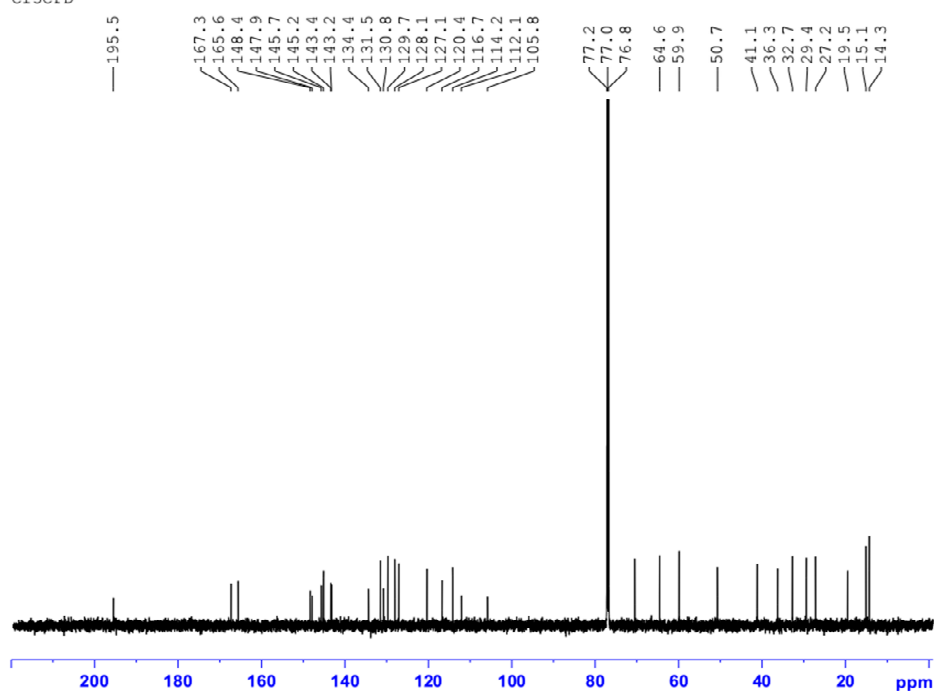
Figure S18: Mass, ^1H - and ^{13}C -NMR spectra of compound 16



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Current Data Parameters
NAME 28-Dec-2021 Dr. Najeeb
EXPNO 14
PROCNO 1

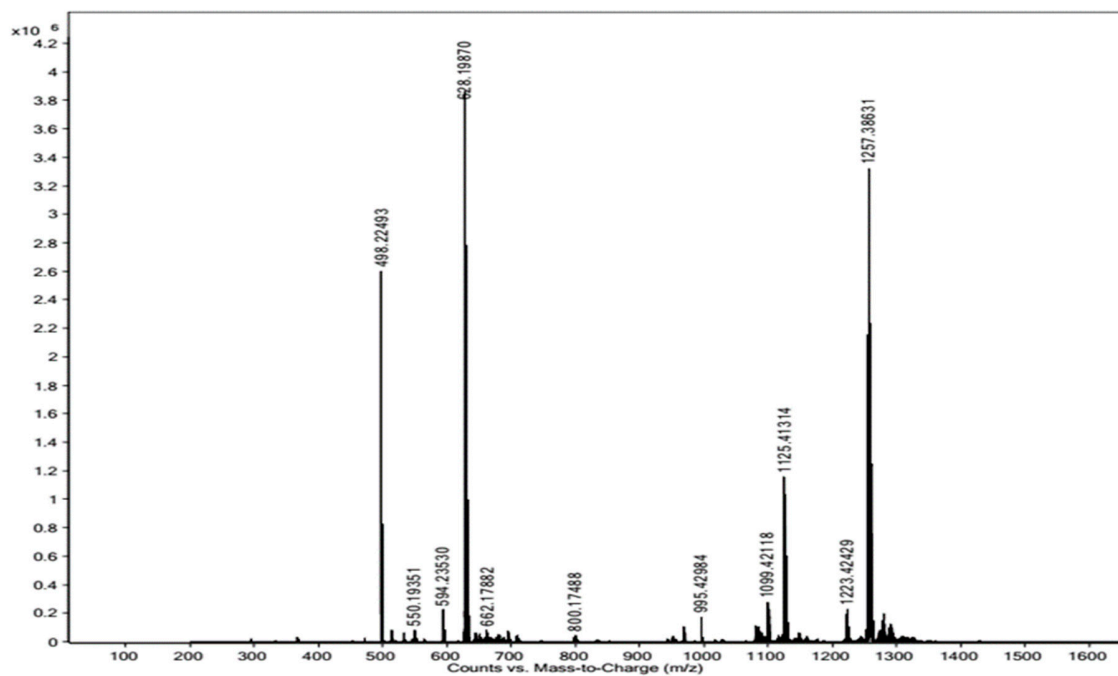
F2 - Acquisition Parameters
Date 20211229
Time 10.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 512
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 195.2
DM 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDD 1

----- CHANNEL f1 -----
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.00000000 W

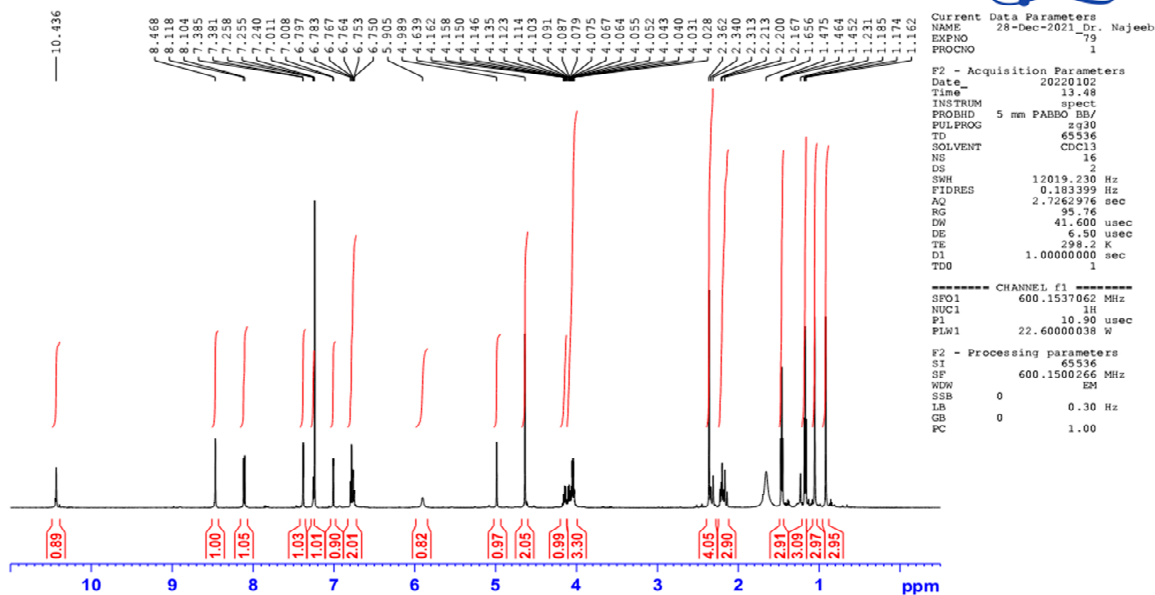
----- CHANNEL f2 -----
SFO2 600.1524006 MHz
NUC2 1H
CPRPG2 waltz16
PCPD 70.00 usec
PLW2 22.60000038 W
PLW12 0.52886602 W
PLW13 0.23876599 W

F2 - Processing parameters
SI 32768
SF 150.9078399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S19: Mass, ¹H- and ¹³C-NMR spectra of compound 17



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PROTON



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C13CPD

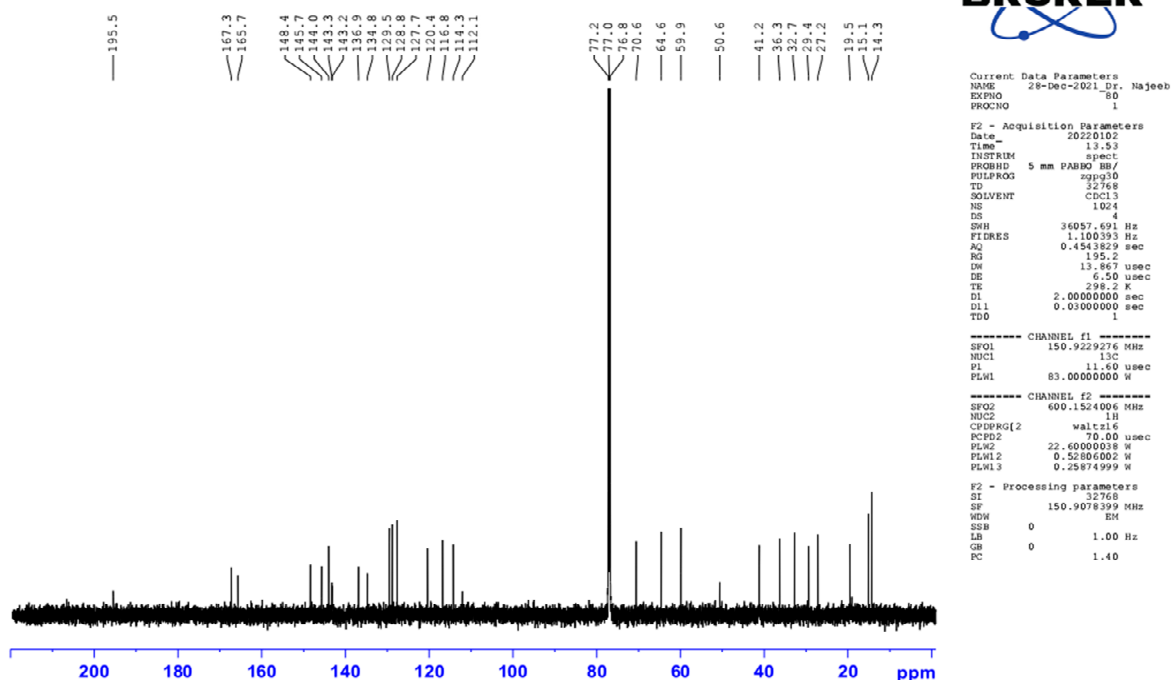
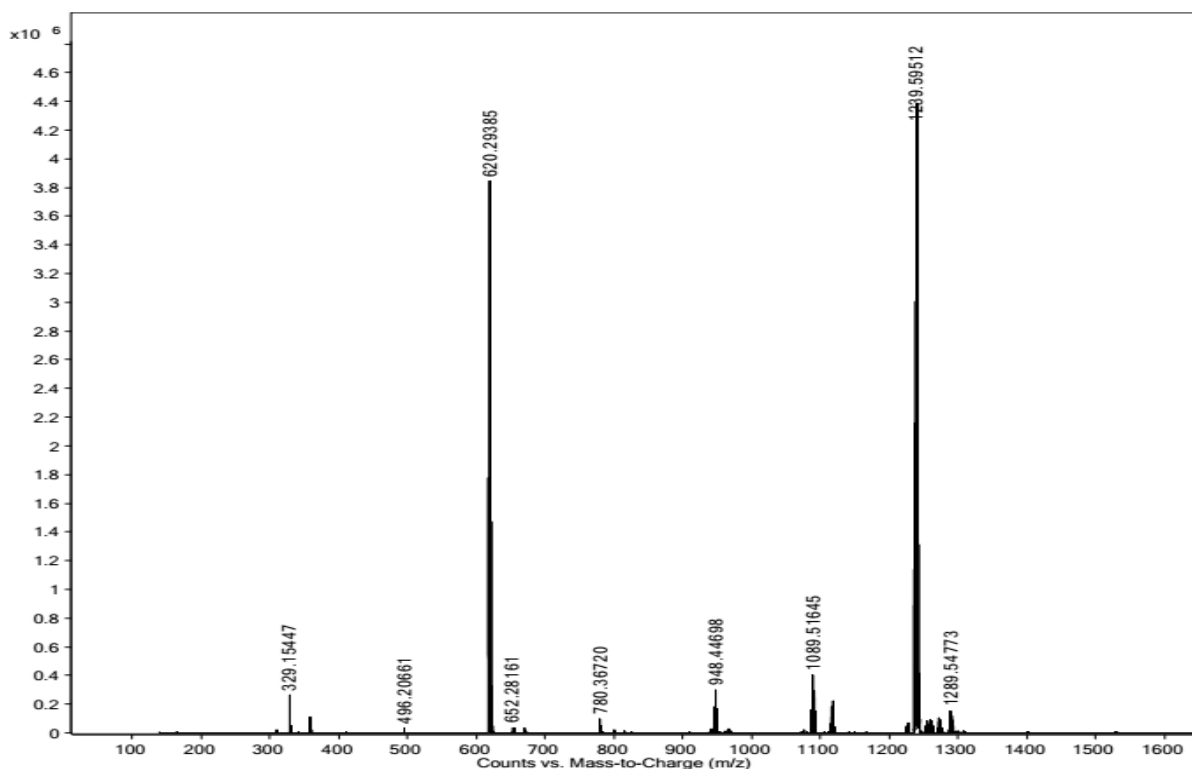
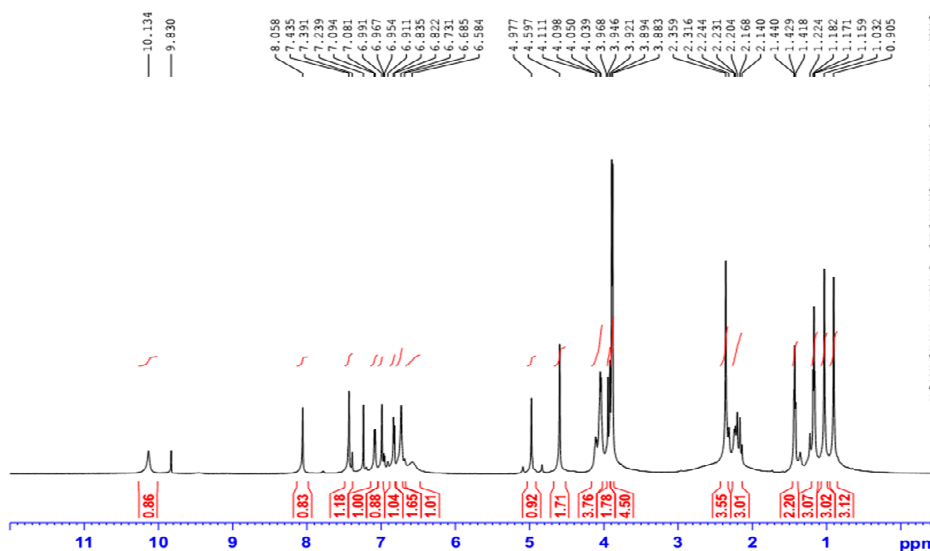


Figure S20: Mass, ¹H- and ¹³C-NMR spectra of compound 18



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PROTON



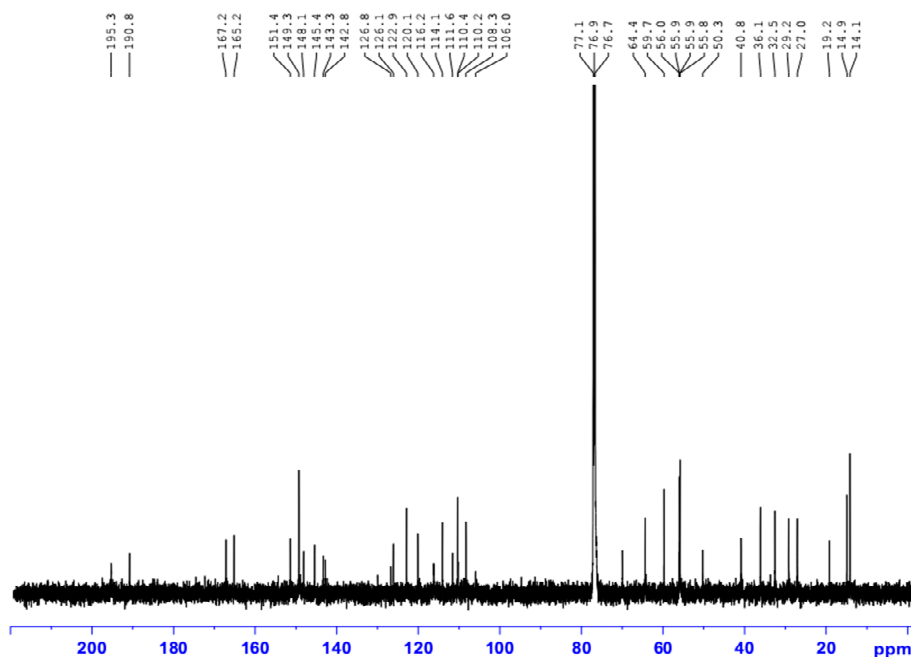
Current Data Parameters
NAME 28-Dec-2021_Dr. Najeeb
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211230
Time 10.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.103399 Hz
AQ 2.7262976 sec
RG 70.11
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.1537062 MHz
NUC1 1H
P1 10.50 usec
PLW1 22.60000038 W

F2 - Processing parameters
SI 65536
SF 600.1500266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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Cl3CPD



Current Data Parameters
NAME 28-Dec-2021 Dr. Najeeb
EXPNO 51
PROCNO 1

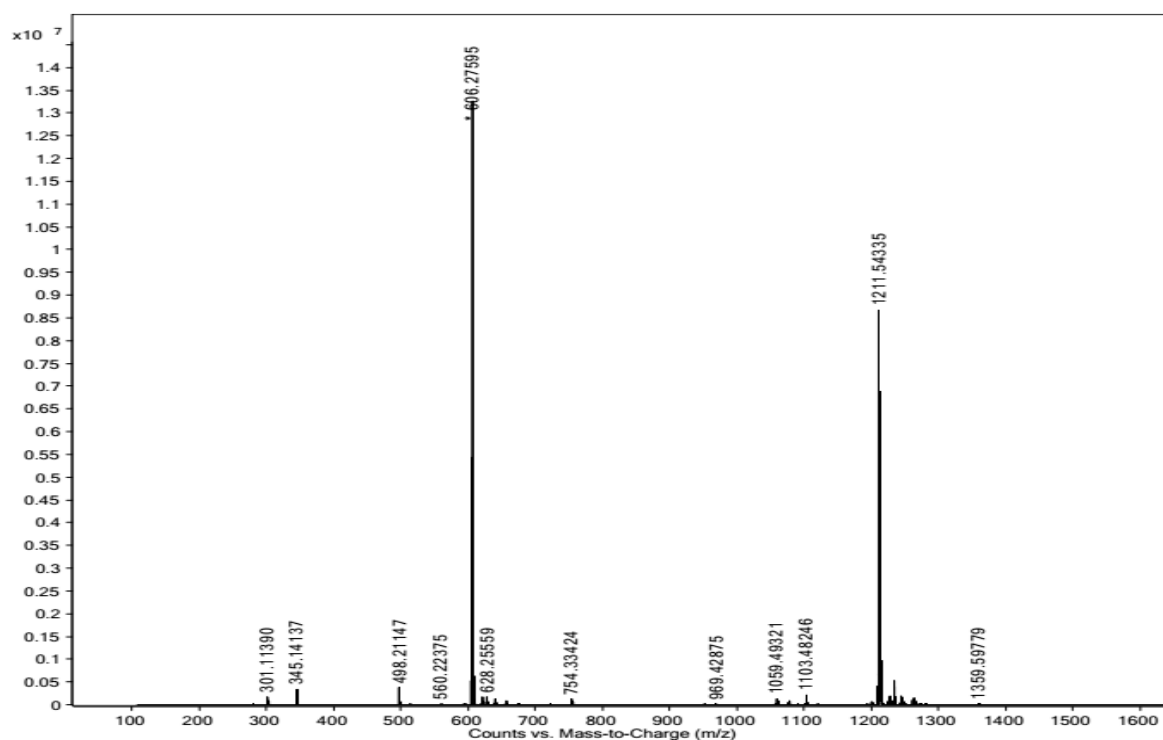
F2 - Acquisition Parameters
Date_ 20211230
Time 10.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 756
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 195.2
DM 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.00000000 W

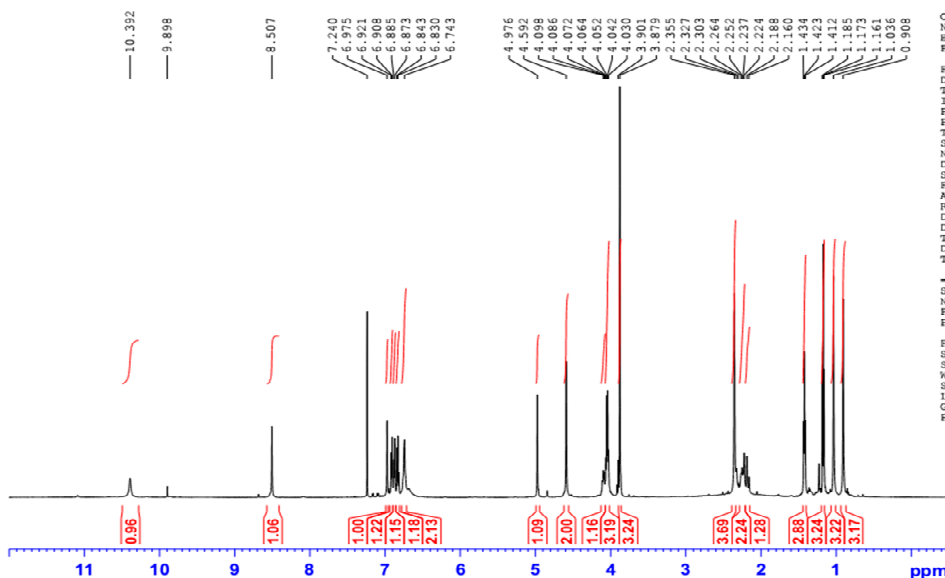
----- CHANNEL f2 -----
SFO2 600.1524006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 22.60000038 W
PLW12 0.34060002 W
PLW13 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9078641 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S21: Mass, ^1H - and ^{13}C -NMR spectra of compound 19

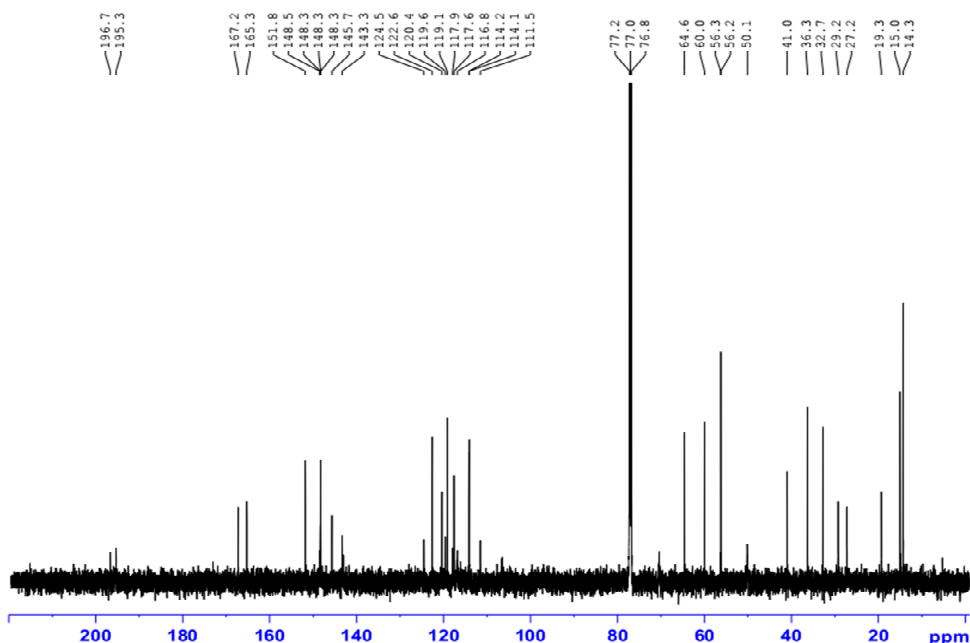


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PROTON



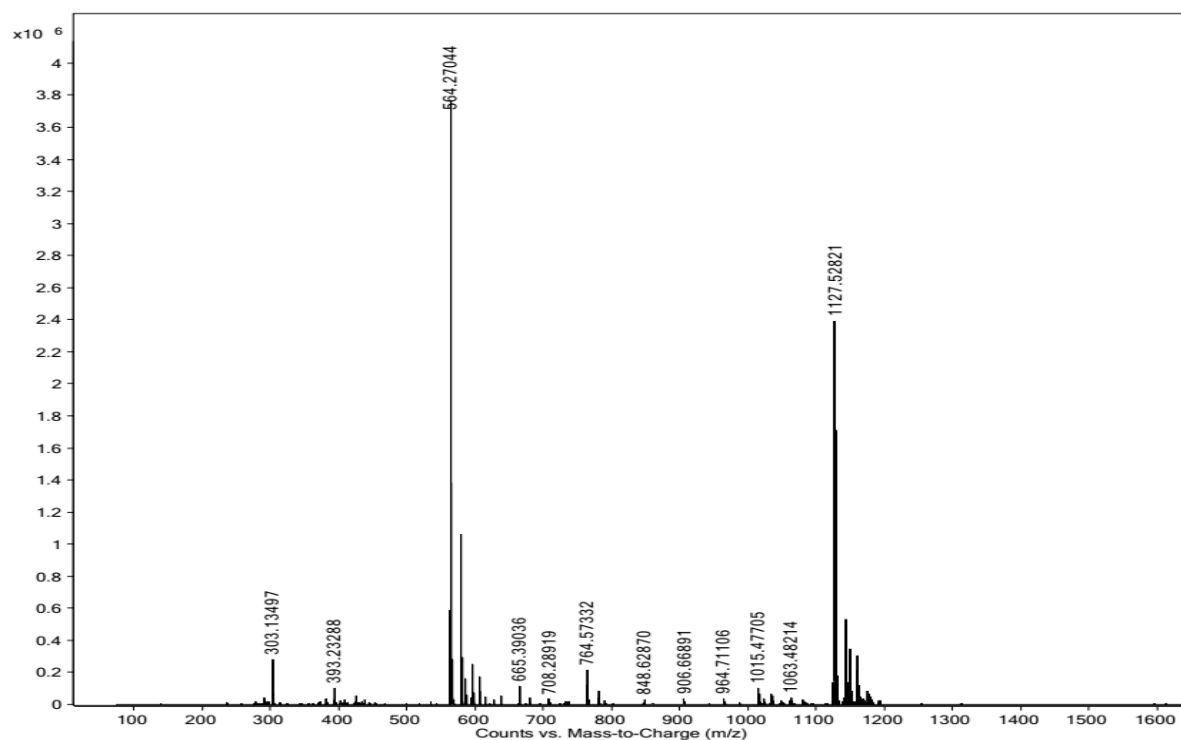
Current Data Parameters
NAME 28-Dec-2021 Dr. Najeeb
EXPNO 46
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211230
Time 9.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 76.79
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
----- CHANNEL f1 -----
SFO1 600.1537062 MHz
NUC1 ¹H
P1 10.30 usec
PLW1 22.60000038 W
F2 - Processing parameters
SI 65536
SF 600.1500266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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C13CPD



Current Data Parameters
NAME 28-Dec-2021 Dr. Najeeb
EXPNO 47
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211230
Time 9.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4541829 sec
RG 195.2
DW 15.967 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
----- CHANNEL f1 -----
SFO1 150.9229276 MHz
NUC1 ¹³C
P1 11.60 usec
PLW1 83.00000000 W
----- CHANNEL f2 -----
SFO2 600.1524006 MHz
NUC2 ¹H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 22.60000038 W
PLW12 0.52806002 W
PLW13 0.25874368 W
F2 - Processing parameters
SI 32768
SF 150.9078399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S22: Mass, ¹H-NMR and ¹³C-NMR spectra of compound 20



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PROTON

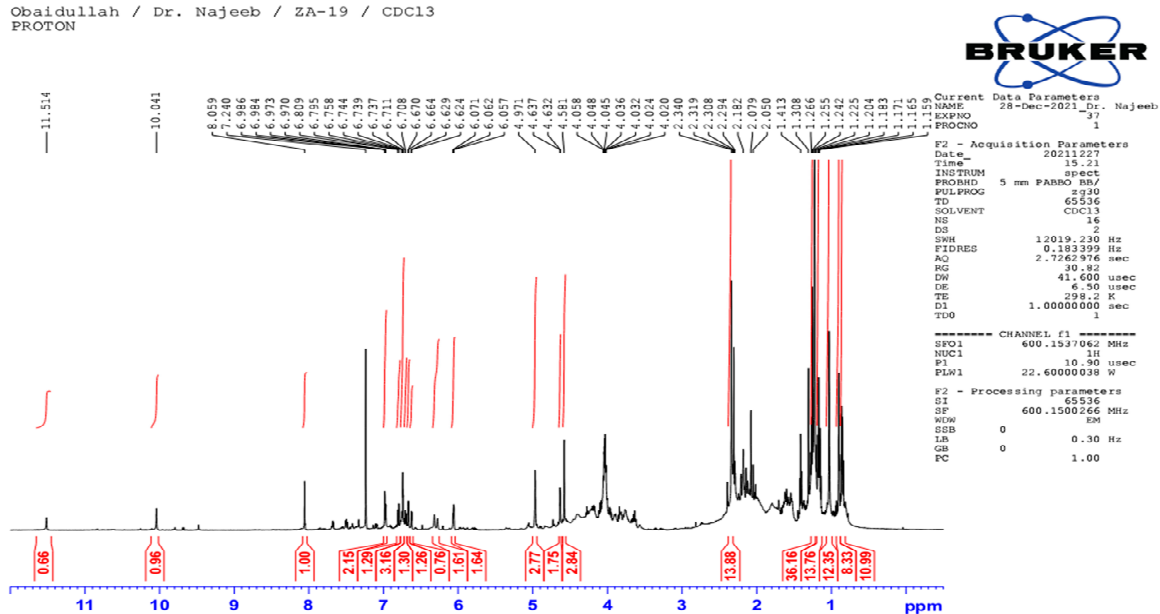
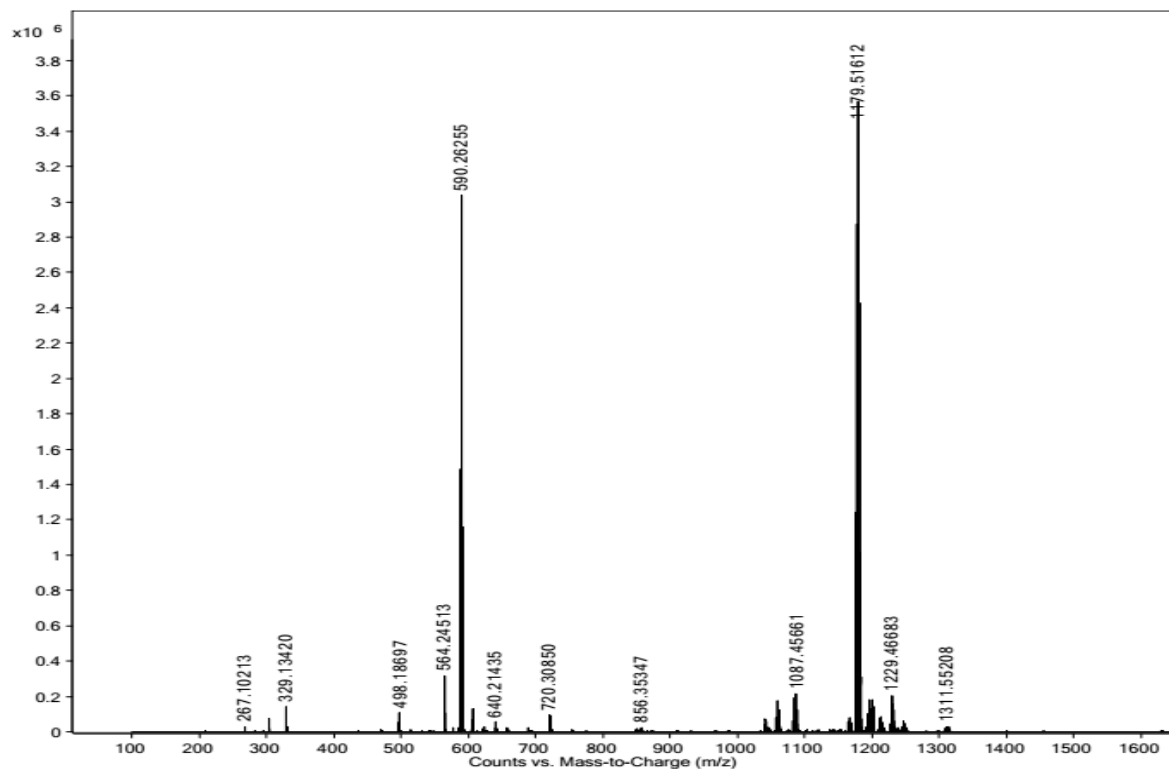
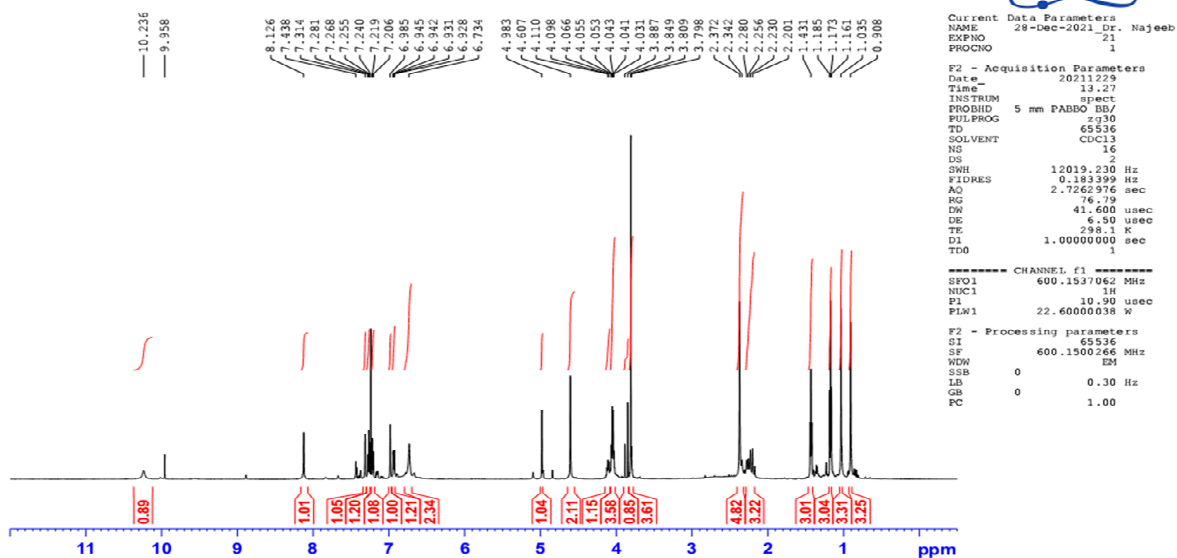


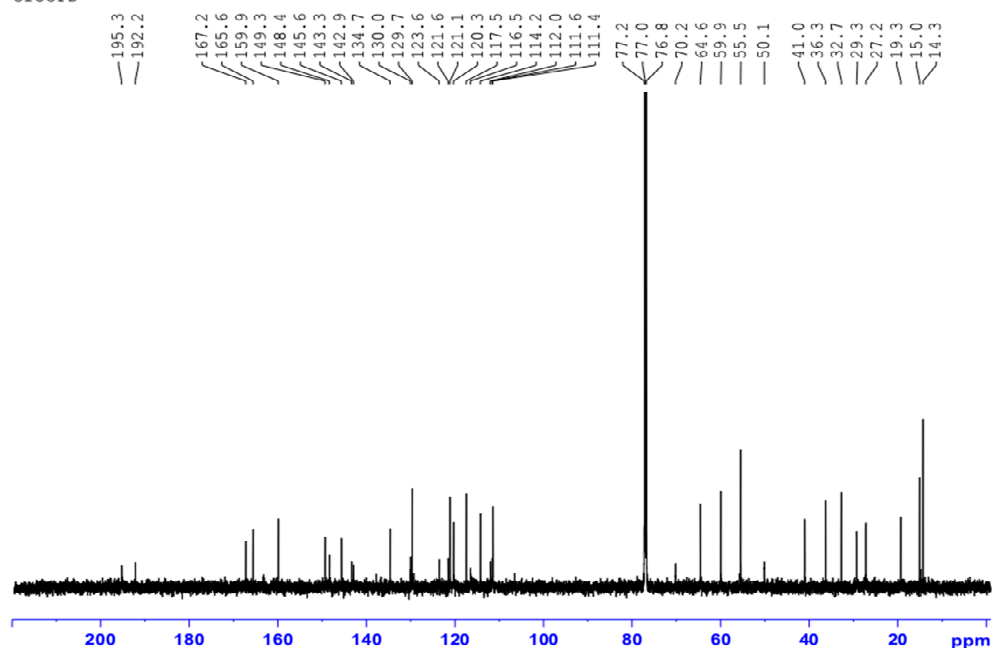
Figure S23: Mass and ¹H-NMR spectra of compound **21**



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PROTON



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C13CPD



Current Data Parameters
NAME 28-Dec-2021 Dr. Najeeb
EXPNO 1
PROCNO 1

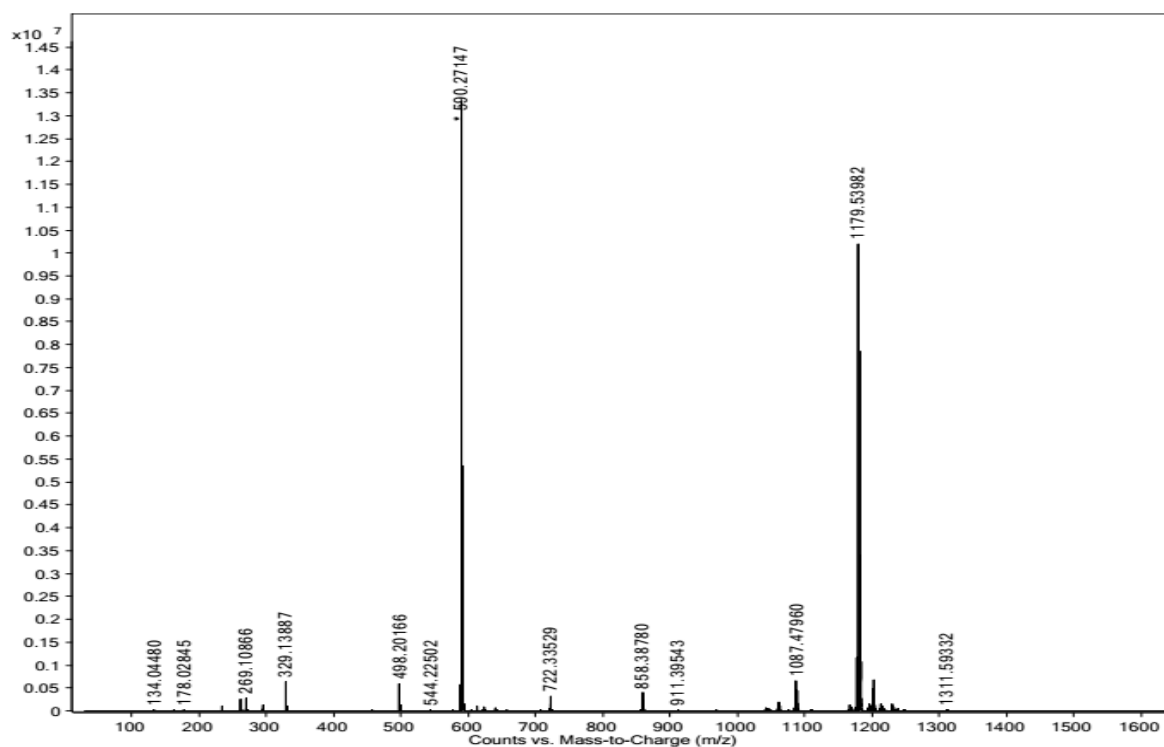
F2 - Acquisition Parameters
Date_ 20211229
Time_ 13.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 195.2
DM 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.00000000 W

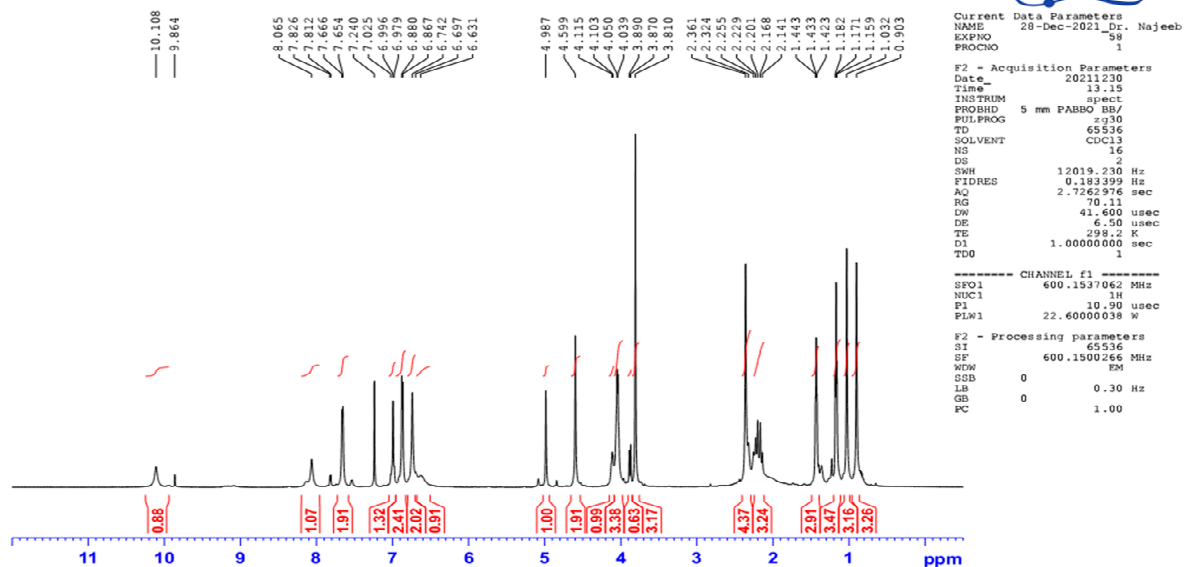
===== CHANNEL f2 =====
SFO2 600.1524006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 22.60000038 W
PLW12 0.52800002 W
PLW13 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9070399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S24: Mass, ^1H - and ^{13}C -NMR spectra of compound 22



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PROTON



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C13CPD

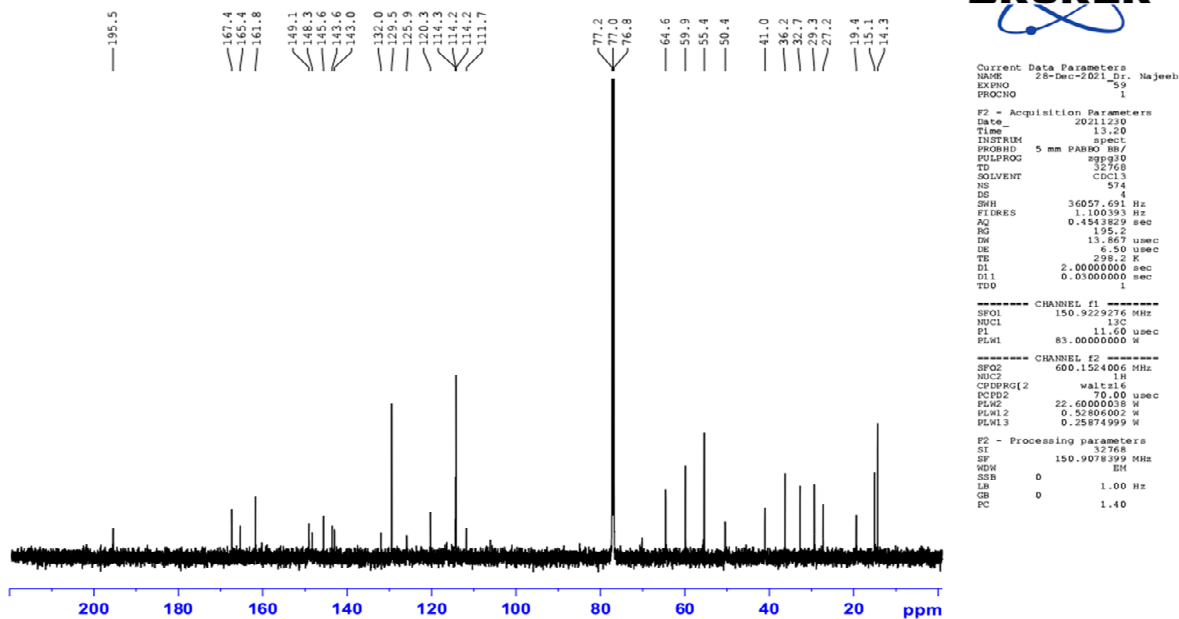
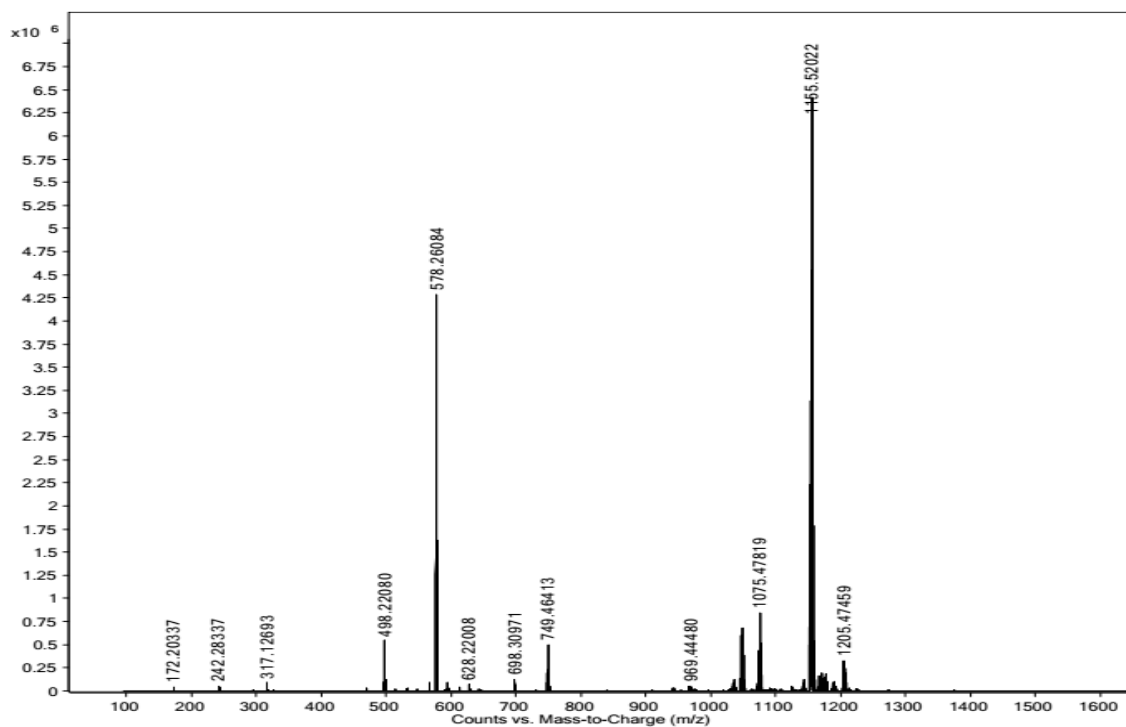
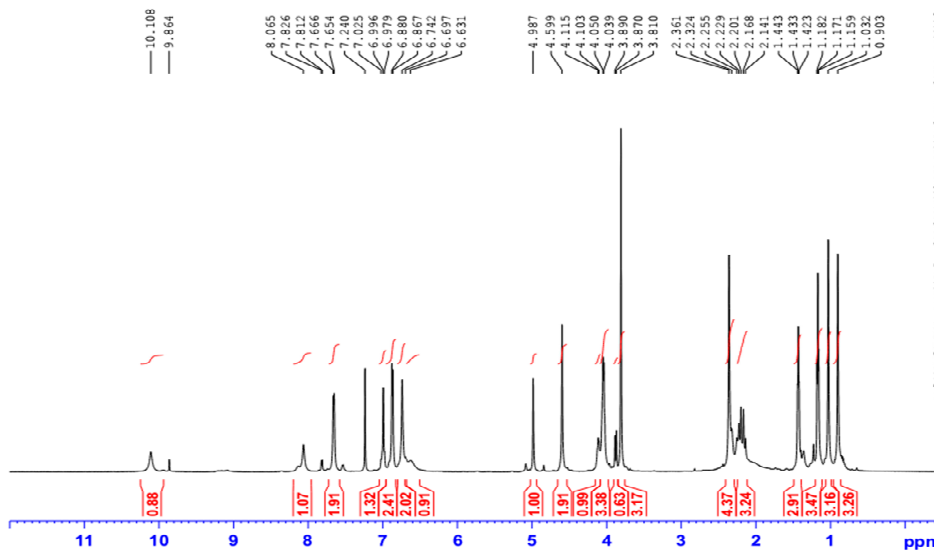


Figure S25: Mass, ^1H - and ^{13}C -NMR spectra of compound 23



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PROTON



Current Data Parameters
NAME 28-Dec-2021 Dr. Najeeb
EXPNO 58
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211230
Time 13.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7462976 sec
RG 70.11
RW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.1537062 MHz
NUC1 1H
P1 10.90 usec
PLW1 22.60000038 W

F2 - Processing parameters
SI 65536
SF 600.1500466 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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Cl3CPD

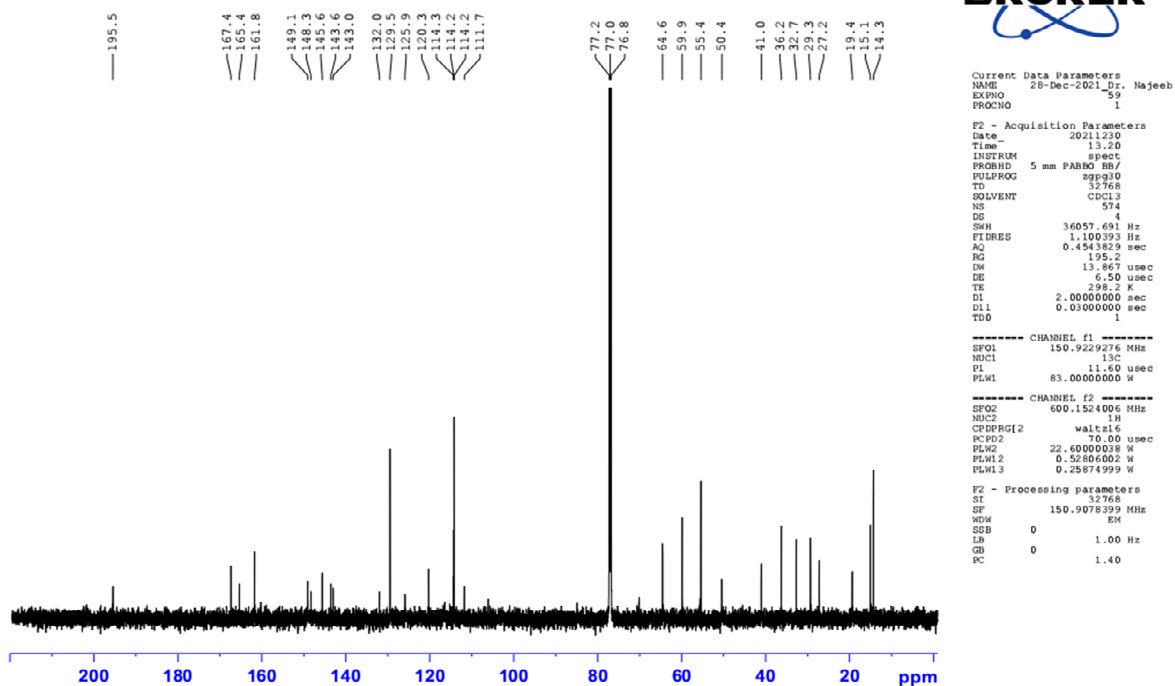
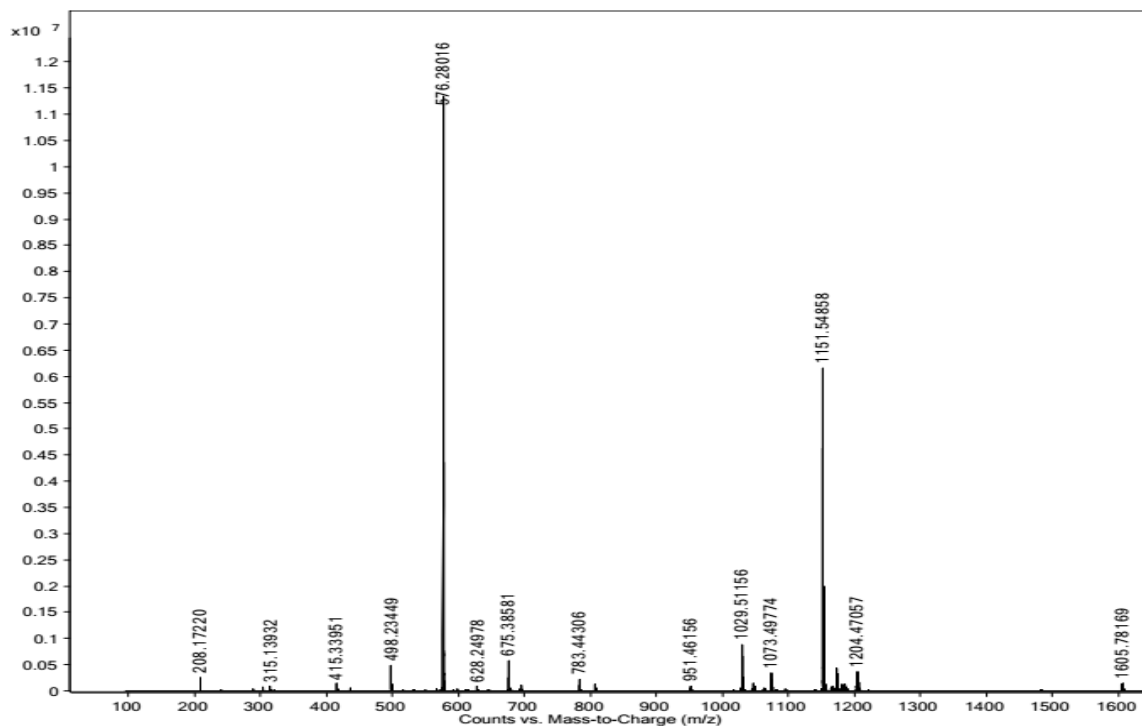
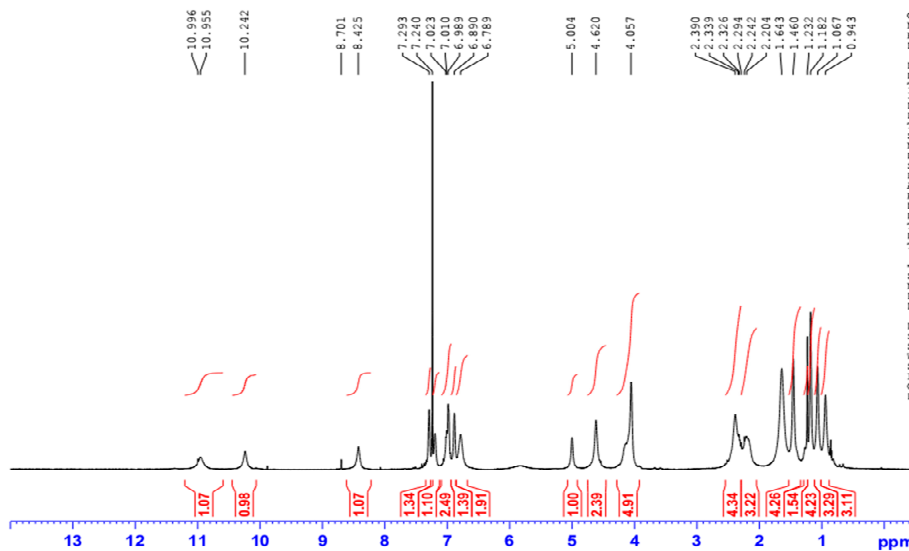


Figure S26: Mass, ^1H - and ^{13}C -NMR spectra of compound 24



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PROTON



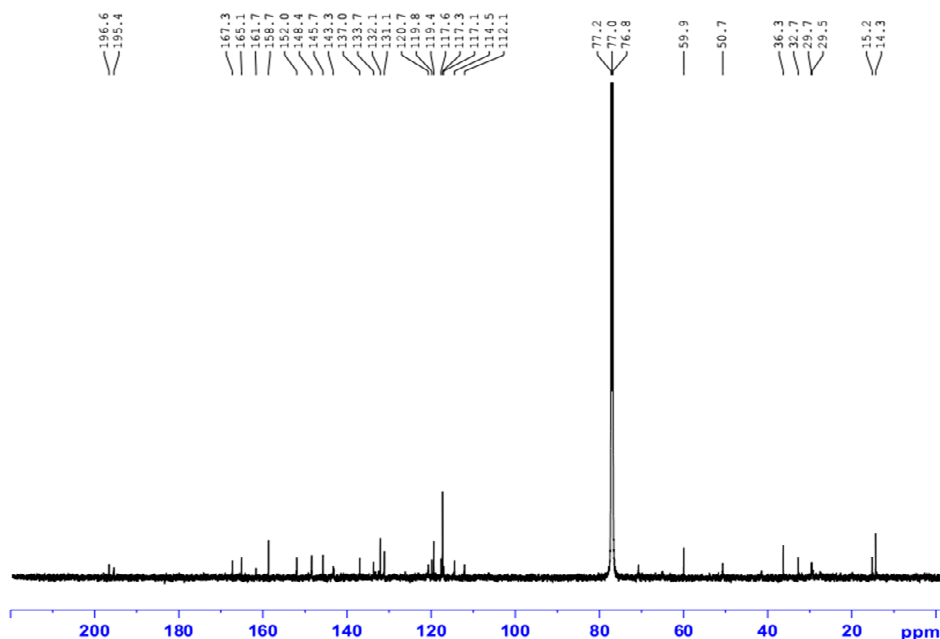
Current Data Parameters
NAME 28-Dec-2021_Dr. Najeeb
EXPNO 83
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220102
Time 14.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 95.76
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.1537062 MHz
NUC1 1H
P1 10.90 usec
PLW1 22.60000038 W

F2 - Processing parameters
SI 65536
SF 600.1500266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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C13CPD



Current Data Parameters
NAME 28-Dec-2021_Dr. Najeeb
EXPNO 84
PROCNO 1

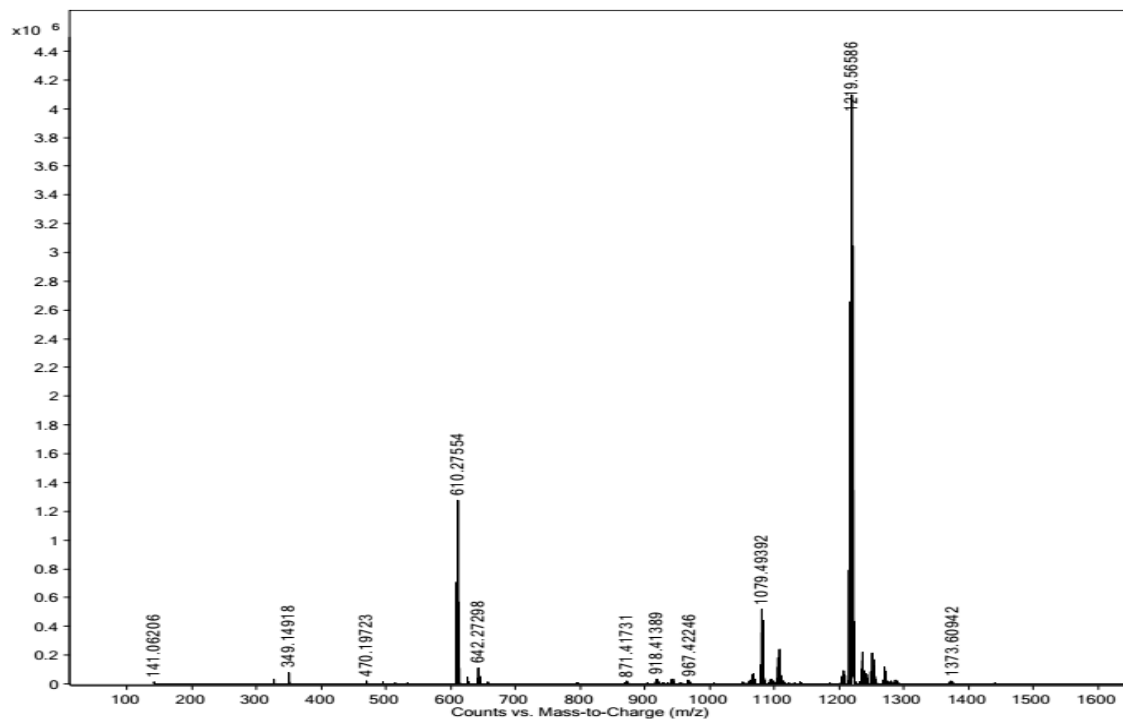
F2 - Acquisition Parameters
Date_ 20220103
Time 8.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 19727
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 195.2
DW 13.867 usec
DE 6.50 usec
TE 297.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.00000000 W

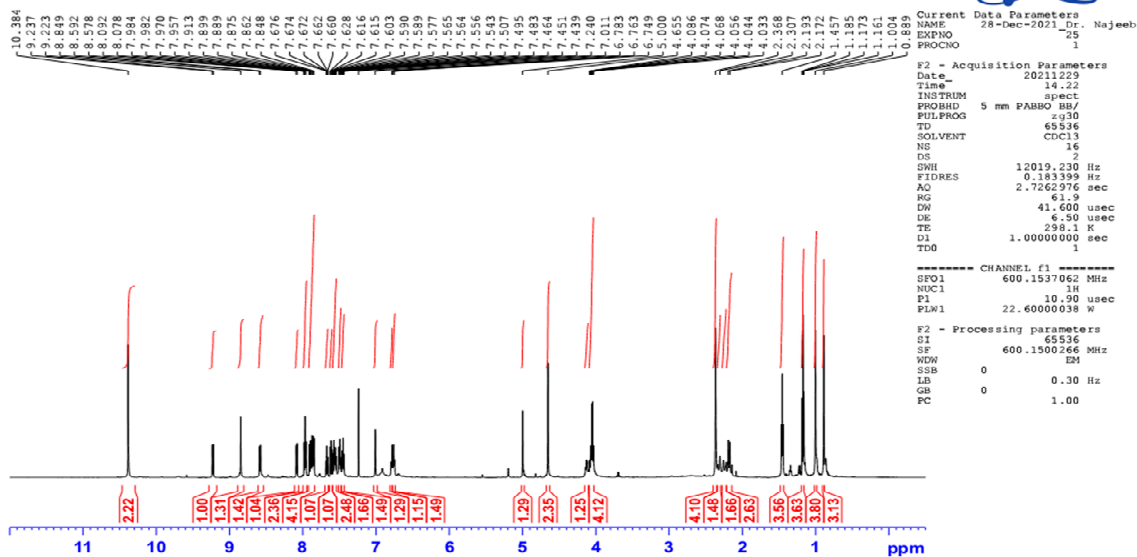
----- CHANNEL f2 -----
SFO2 600.1524006 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 70.00 usec
PLW2 22.60000038 W
PLW12 0.52806002 W
PLW13 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9078399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

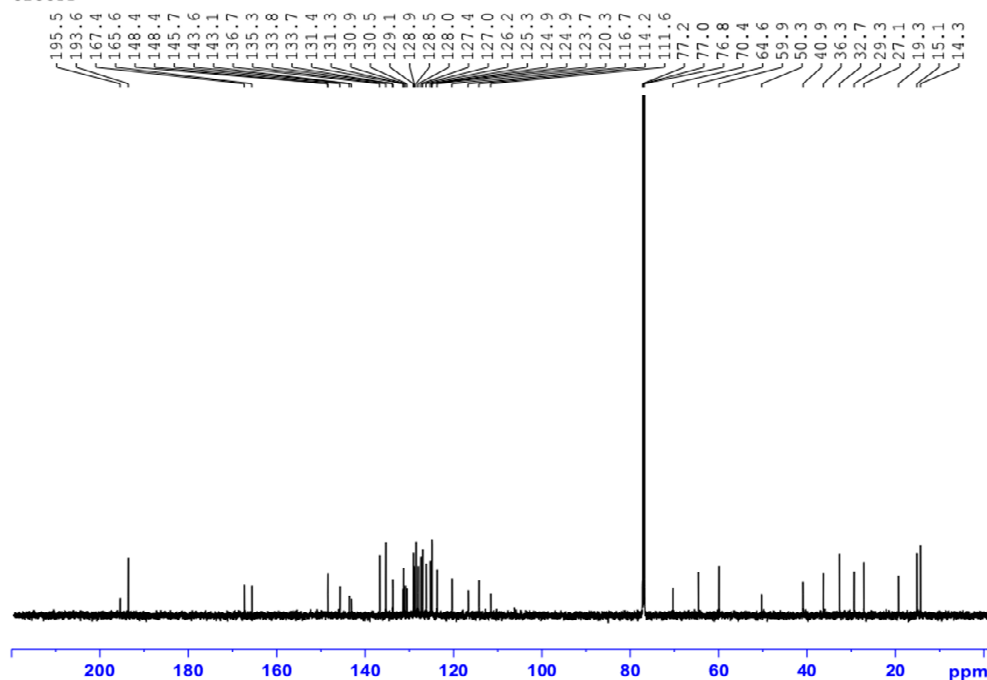
Figure S27: Mass, ¹H- and ¹³C-NMR spectra of compound 25



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PROTON



Obaidullah / Dr. Najeeb / ZA-24 / CDC13
C13CPD



Current Data Parameters
NAME 28-Dec-2021_Dr. Najeeb
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211229
Time 14.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 318
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 195.2
DM 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

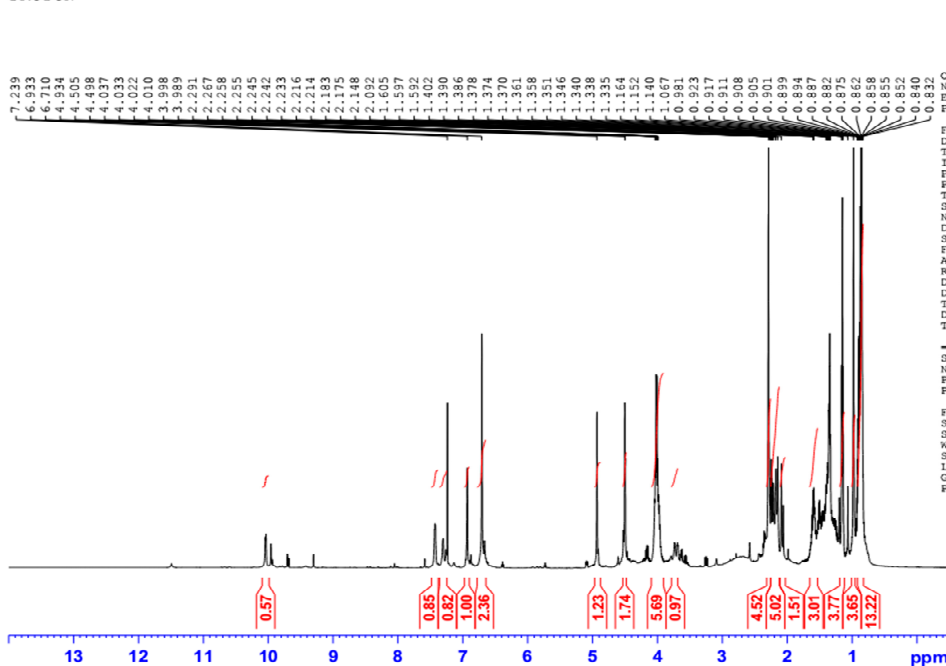
----- CHANNEL f1 -----
SFO1 150.922976 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.00000000 W

----- CHANNEL f2 -----
SFO2 600.1524006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 22.60000003 W
PLW12 0.52806002 W
PLW13 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9078399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S28: Mass, ^1H - and ^{13}C -NMR spectra of compound 26

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PROTON



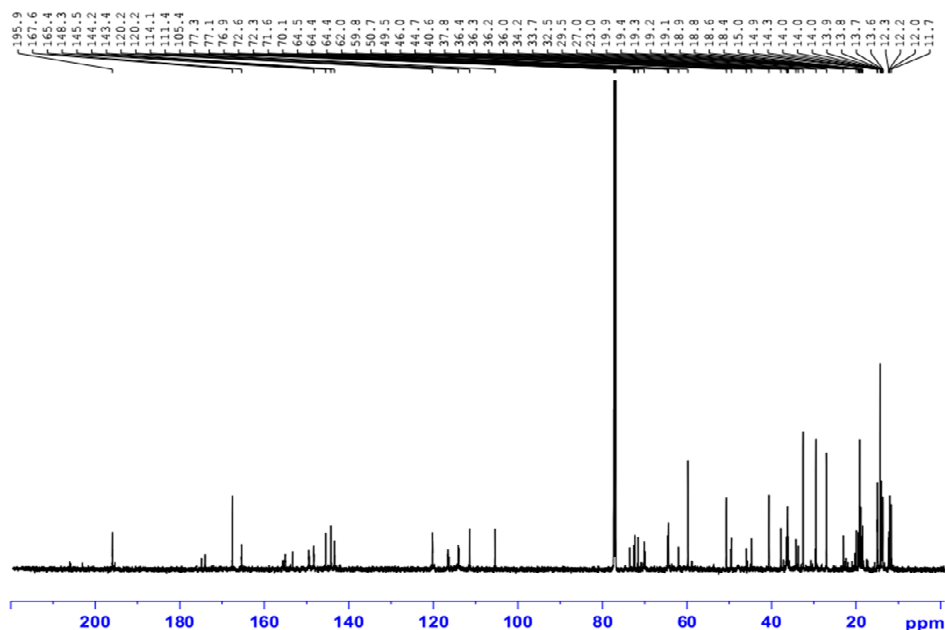
Current Data Parameters
NAME 28-Dec-2021_Dr. Najeeb
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220103
Time 8.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 15.5
DM 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.1537062 MHz
NUC1 1H
P1 10.90 usec
PLW1 22.60000038 W

F2 - Processing parameters
SI 65536
SF 600.1500266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Obaidullah / Dr. Najeeb / ZA-25 / CDC13
C13CPD



Current Data Parameters
NAME 28-Dec-2021 Dr. Najeeb
EXPNO 88
PROCNO 1

F2 - Acquisition Parameters
Date 20220103
Time 8.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 756
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 195.2
DM 13.867 usec
DE 6.90 usec
TE 298.4 K
D1 2.0000000 sec
D11 0.0300000 sec
TDD 1

===== CHANNEL f1 =====
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.00000000 W

===== CHANNEL f2 =====
SFO2 600.1524006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 22.60000038 W
PLW12 0.52806002 W
PLW13 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9078329 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S29. HR-ESI-MS, ^1H - and ^{13}C -NMR spectra of compounds **27**