

Supplementary Materials

Development of Halogenated-Chalcones Bearing with Dimethoxy Phenyl Head as Monoamine Oxidase-B Inhibitors

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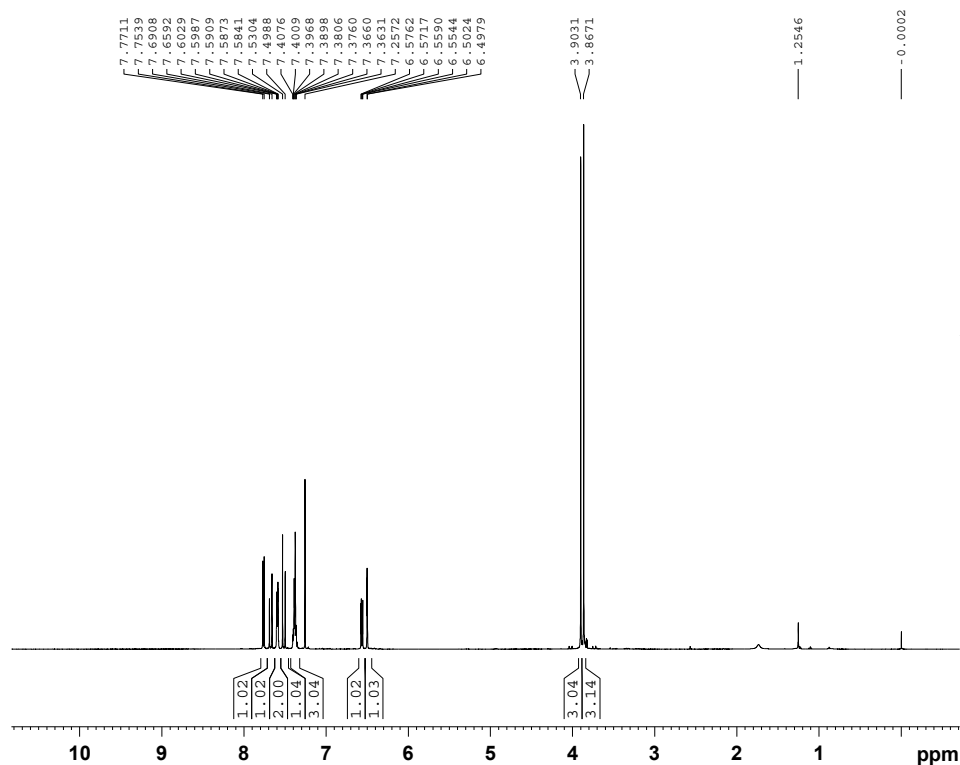
† These authors contributed equally to this work.

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Figure S1. ¹H-NMR spectra

D1
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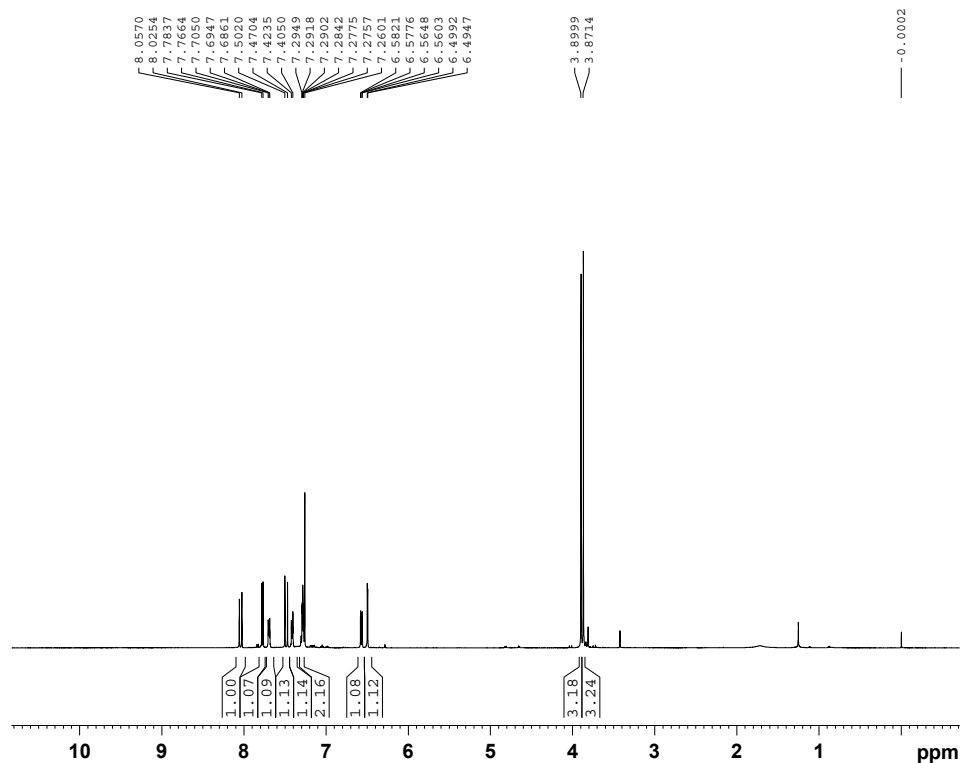
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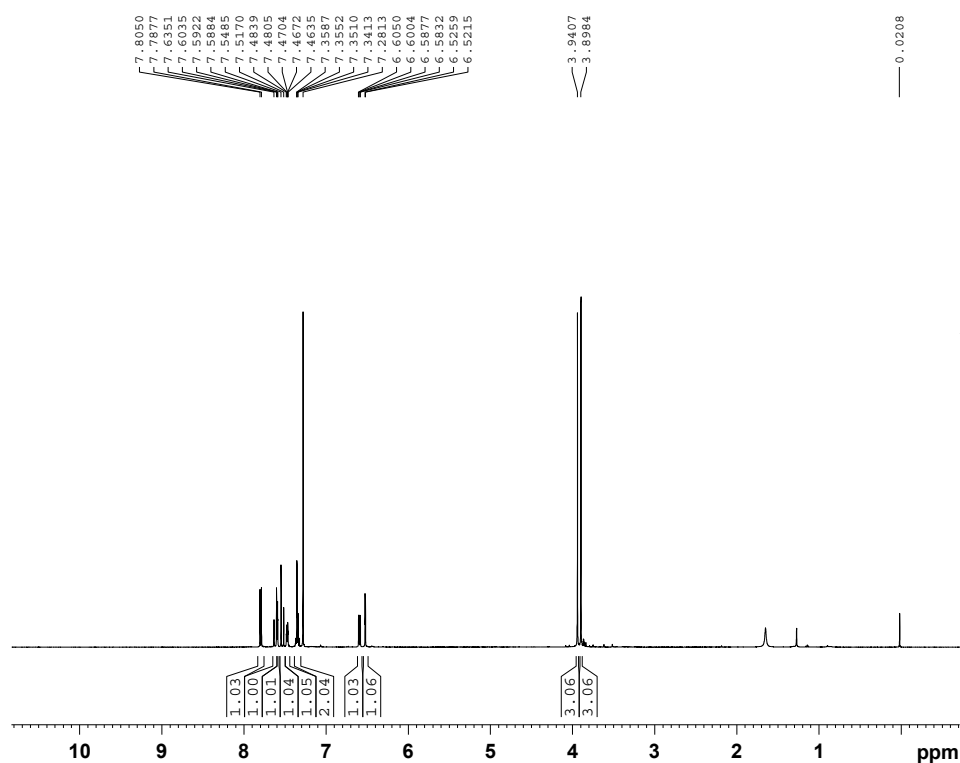
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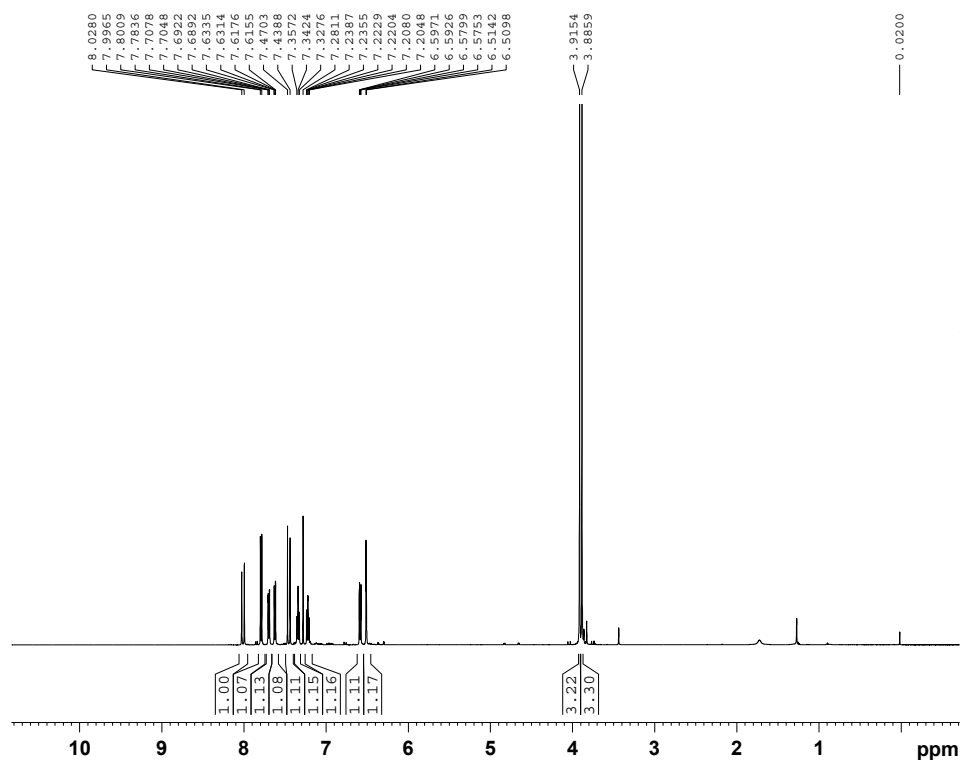
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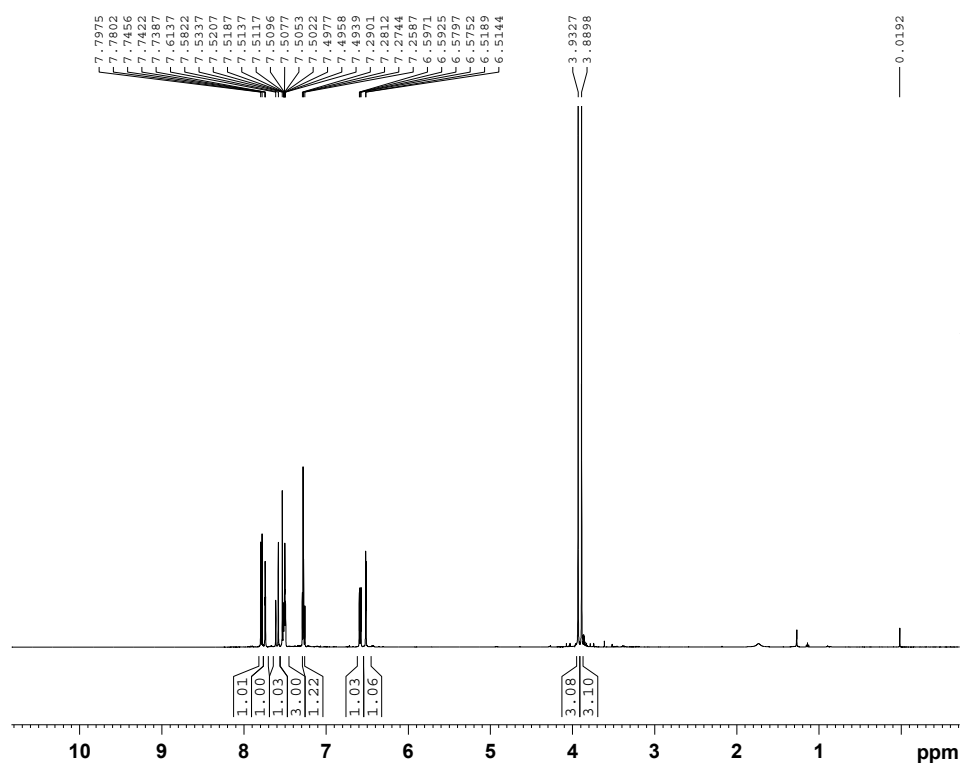
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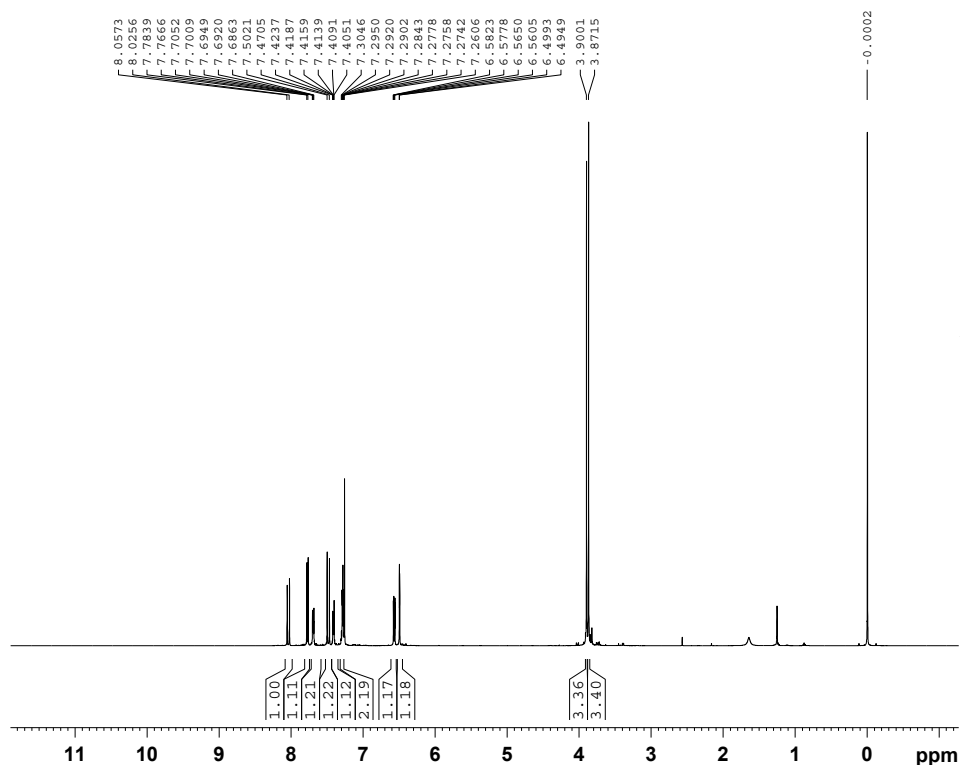
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SAIF, P.U.

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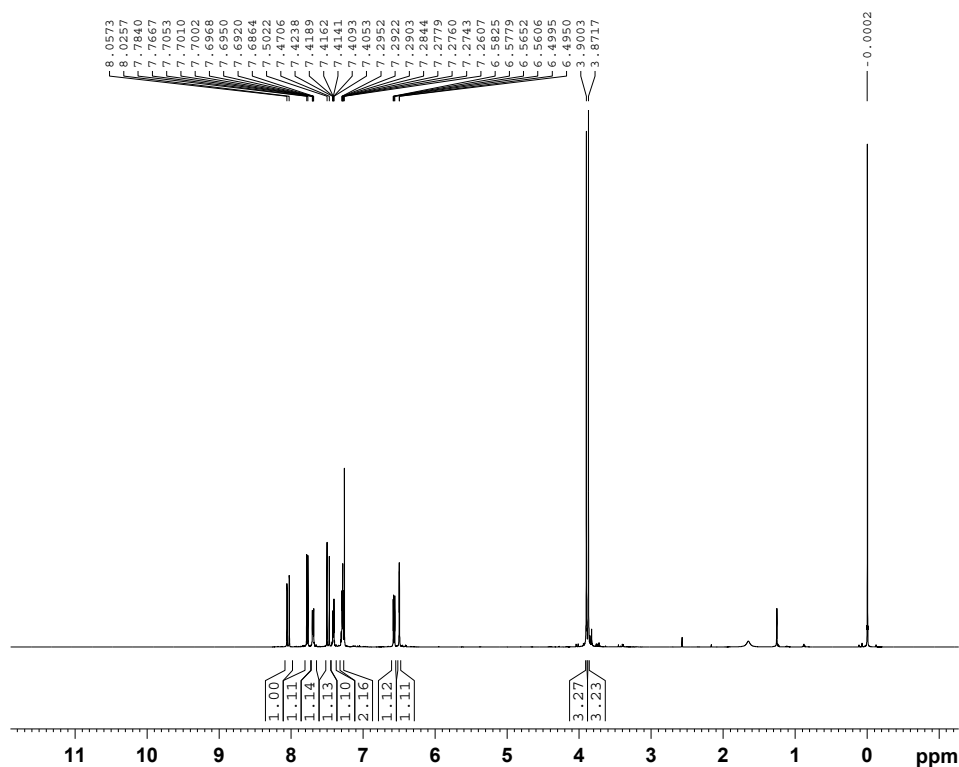
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SAIF, P.U.

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P1 10.00 usec
PLW1 20.93000031 W

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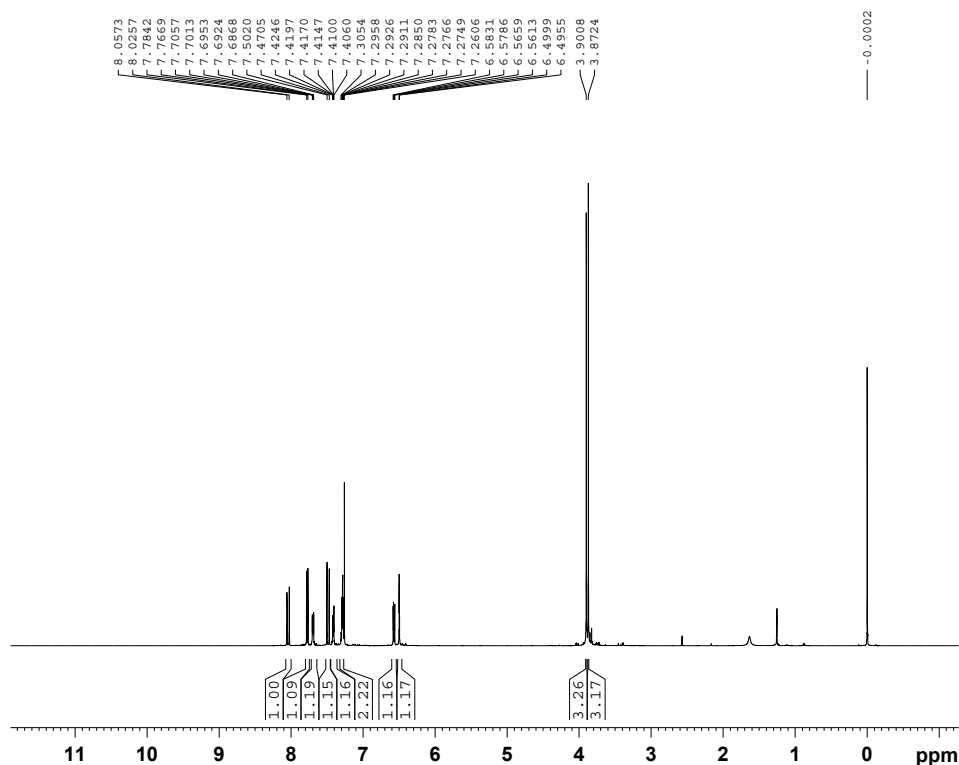
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SAIF, P.U.

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PROCNO 1

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SOLVENT CDCl3
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AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 300.1 K
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SFO1 500.1730885 MHz
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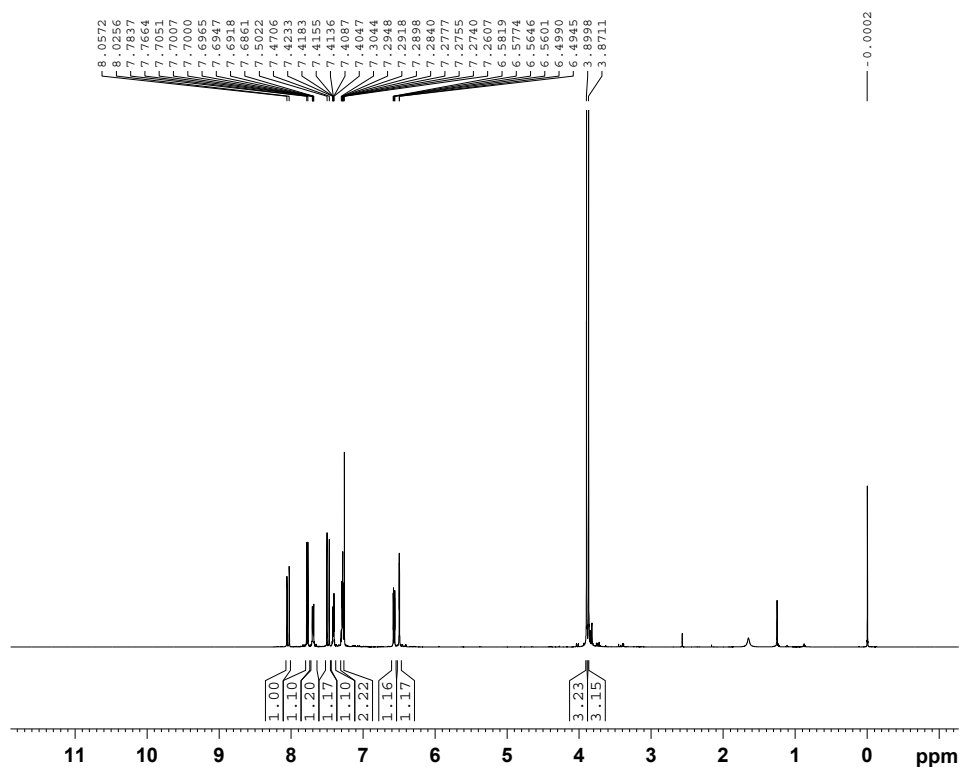
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SPECTROMETER
SAIF, P.U.

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SOLVENT CDCl3
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DE 6.79 usec
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SFO1 500.1730885 MHz
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P1 10.00 usec
PLW1 20.93000031 W

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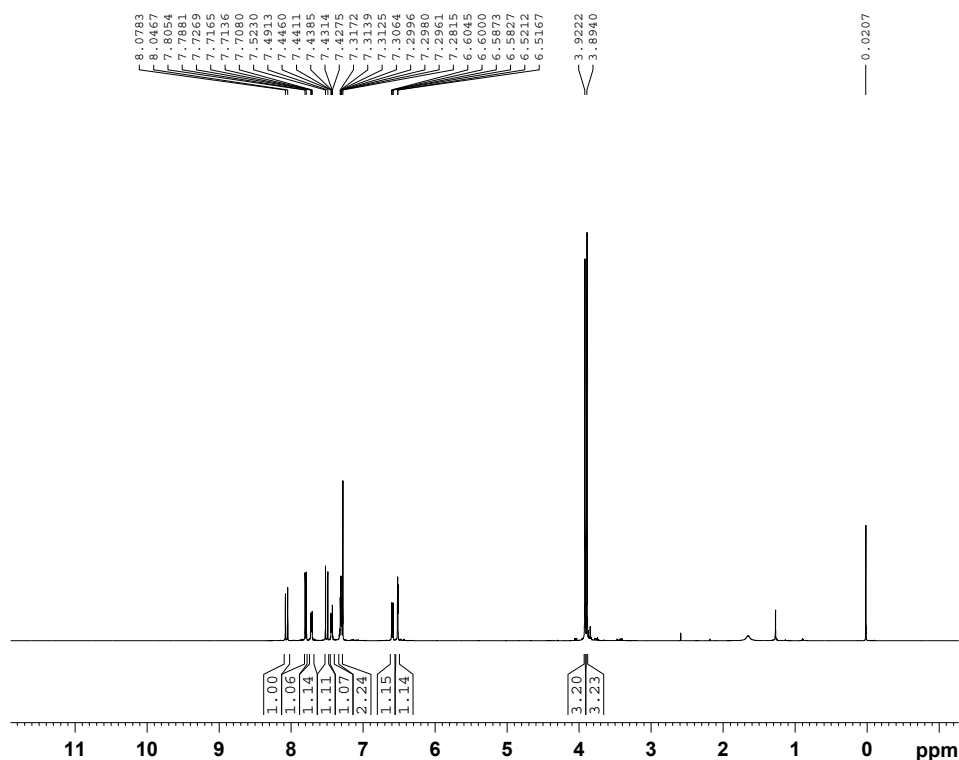
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SAIF, P.U.

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AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
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P1 10.00 usec
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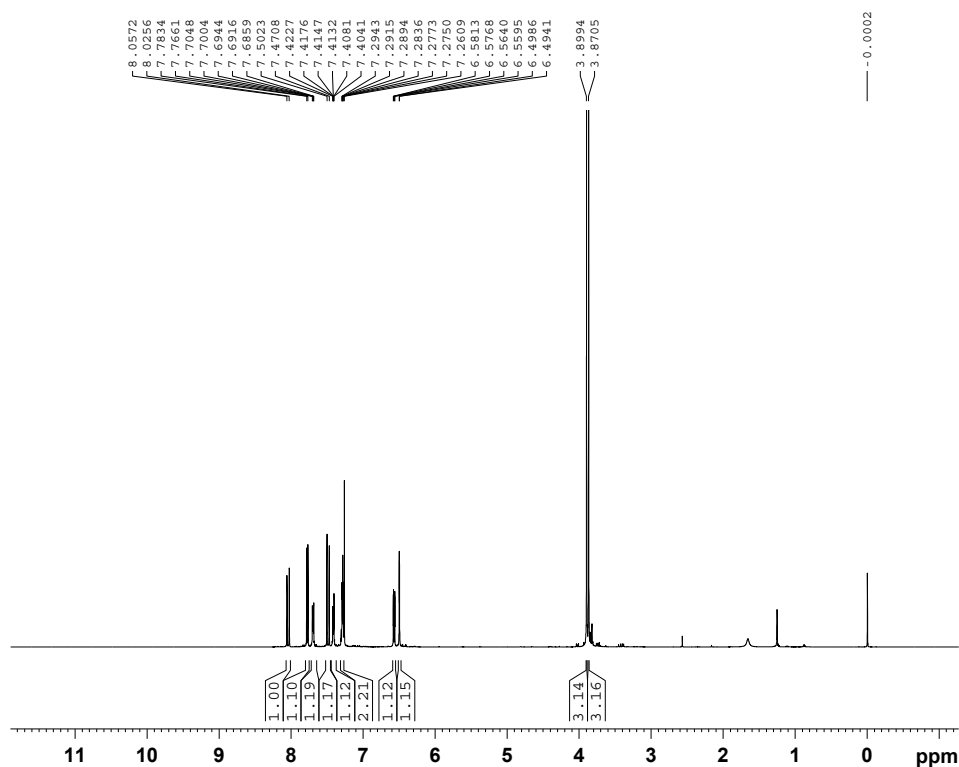
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SPECTROMETER
SAIF, P.U.

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AQ 2.2282240 sec
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DE 6.79 usec
TE 300.1 K
D1 1.00000000 sec
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SFO1 500.1730885 MHz
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P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
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PC 1.00

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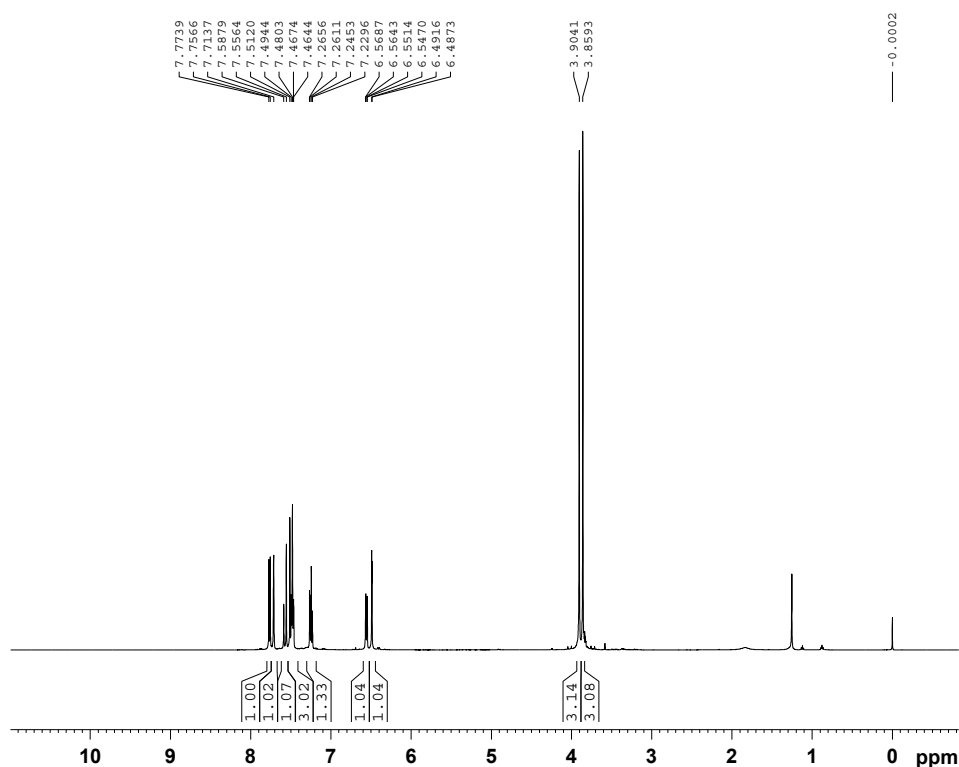
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SAIF, P.U.

Current Data Parameters
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PULPROG zg30
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SOLVENT CDCl3
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FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 300.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
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P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

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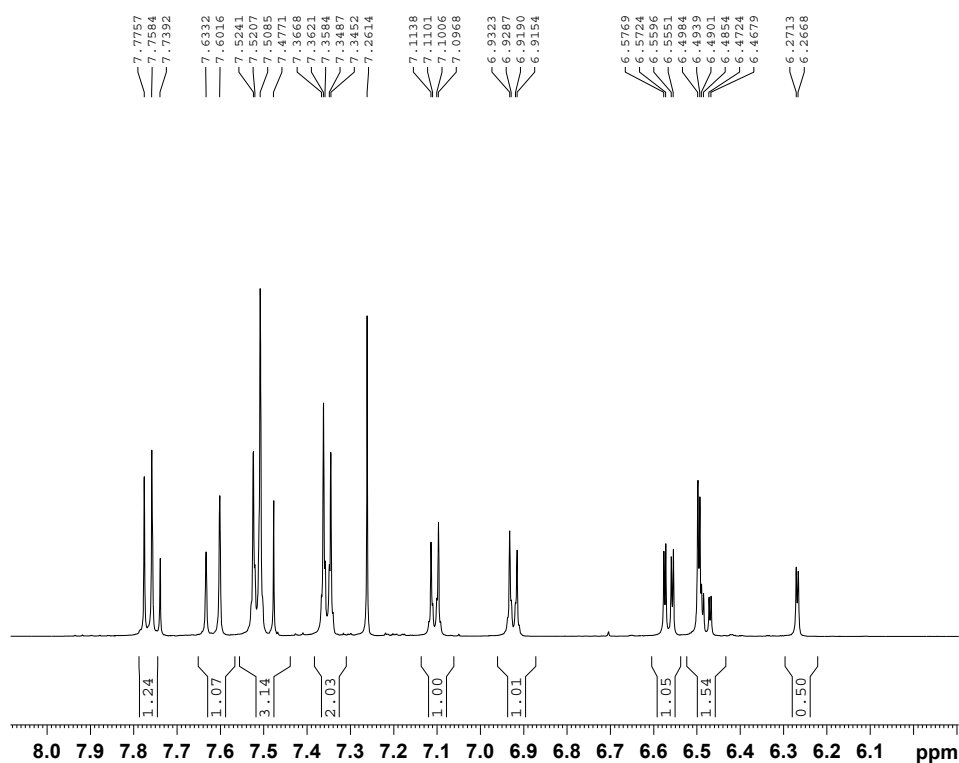
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SPECTROMETER
SAIF, P.U.

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P1 10.00 usec
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PC 1.00

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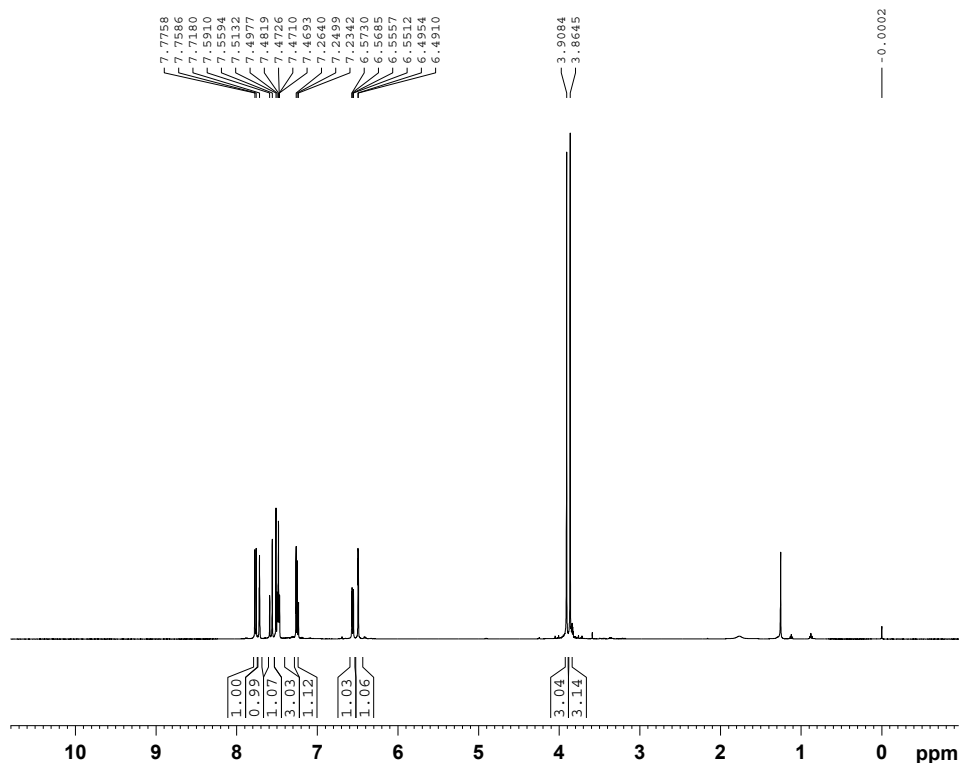
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SAIF, P.U.

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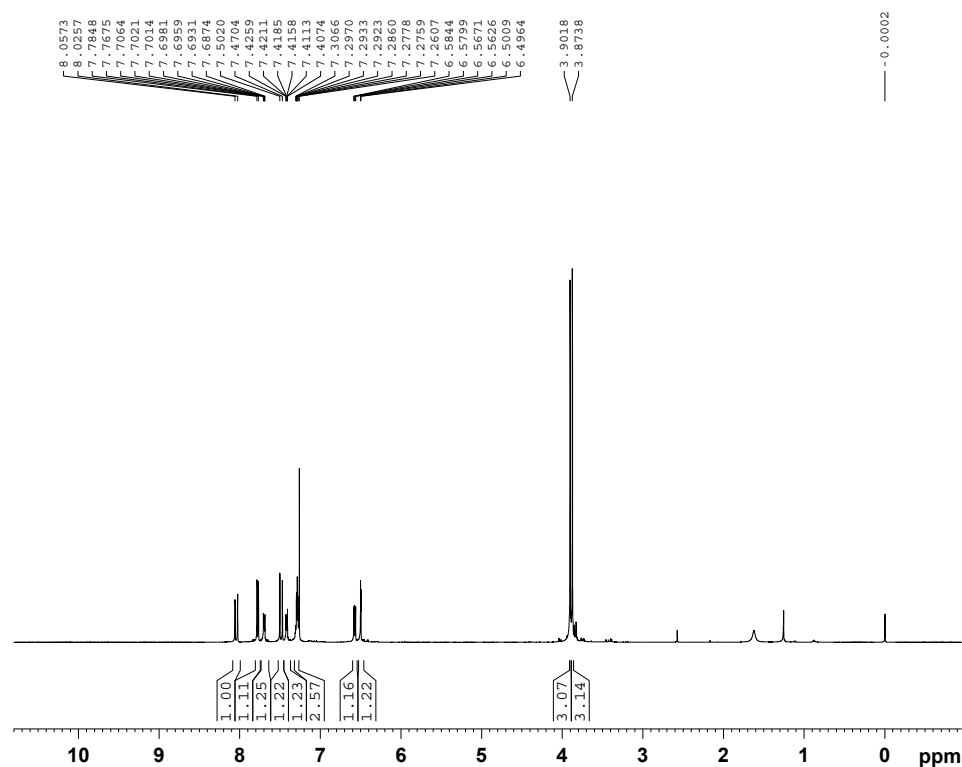
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SAIF, P.U.

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P1 10.00 usec
PLW1 20.93000031 W

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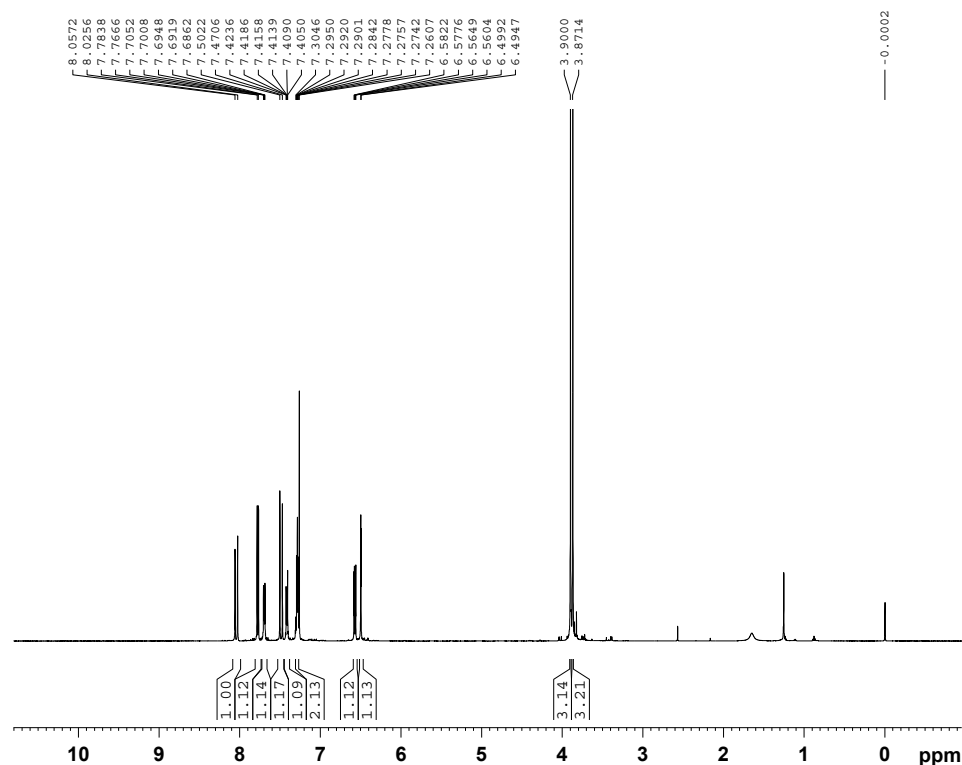
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SAIF, P.U.

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SOLVENT CDCl3
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FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 101
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DE 6.79 usec
TE 300.1 K
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SFO1 500.1730885 MHz
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P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

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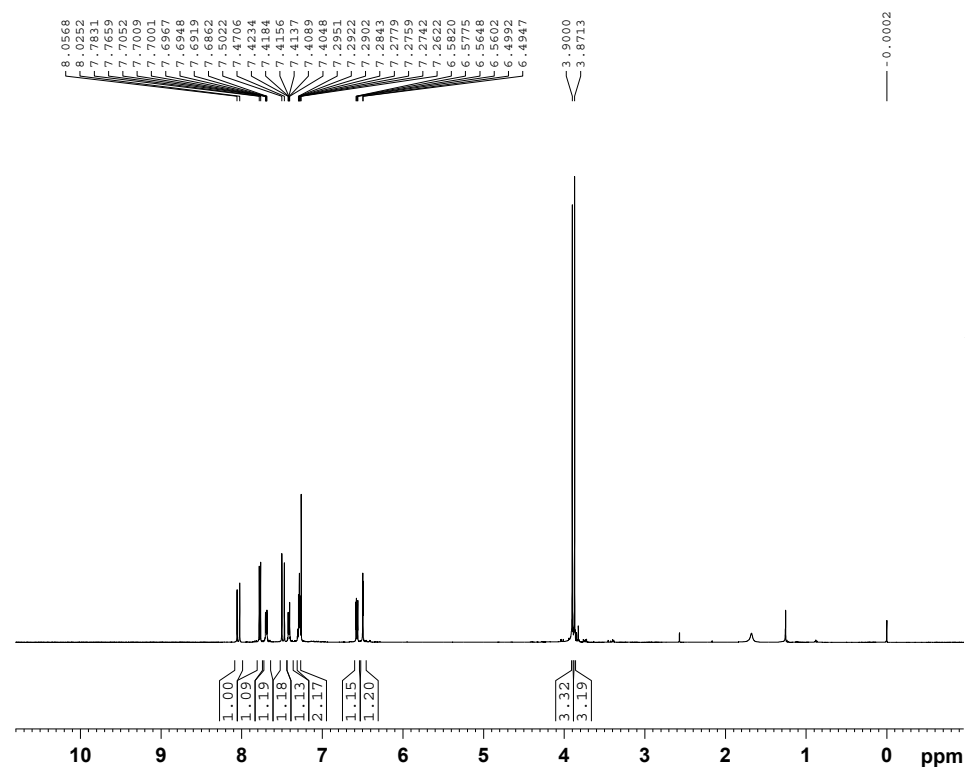
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SPECTROMETER
SAIF, P.U.

Current Data Parameters
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PROCNO 1

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SOLVENT CDCl3
NS 16
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SWH 14705.883 Hz
FIDRES 0.448788 Hz
AQ 2.2282240 sec
RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1730885 MHz
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P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

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

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BRUKER
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SPECTROMETER
SAIF, P.U.

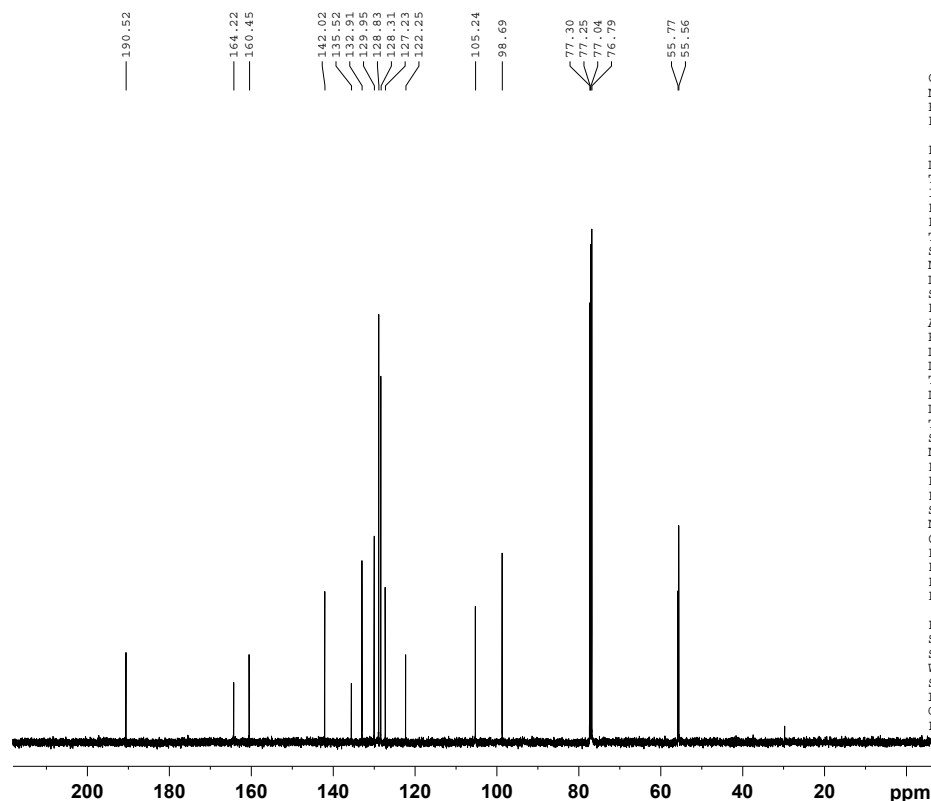
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RG 95.7854
DW 34.000 usec
DE 6.79 usec
TE 300.2 K
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TD0 1
SFO1 500.1730885 MHz
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P0 3.33 usec
P1 10.00 usec
PLW1 20.93000031 W

F2 - Processing parameters
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PC 1.00

Figure S2. ^{13}C -NMR spectra

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C13CPD CDC13 {D:\Spectra} nmr 13



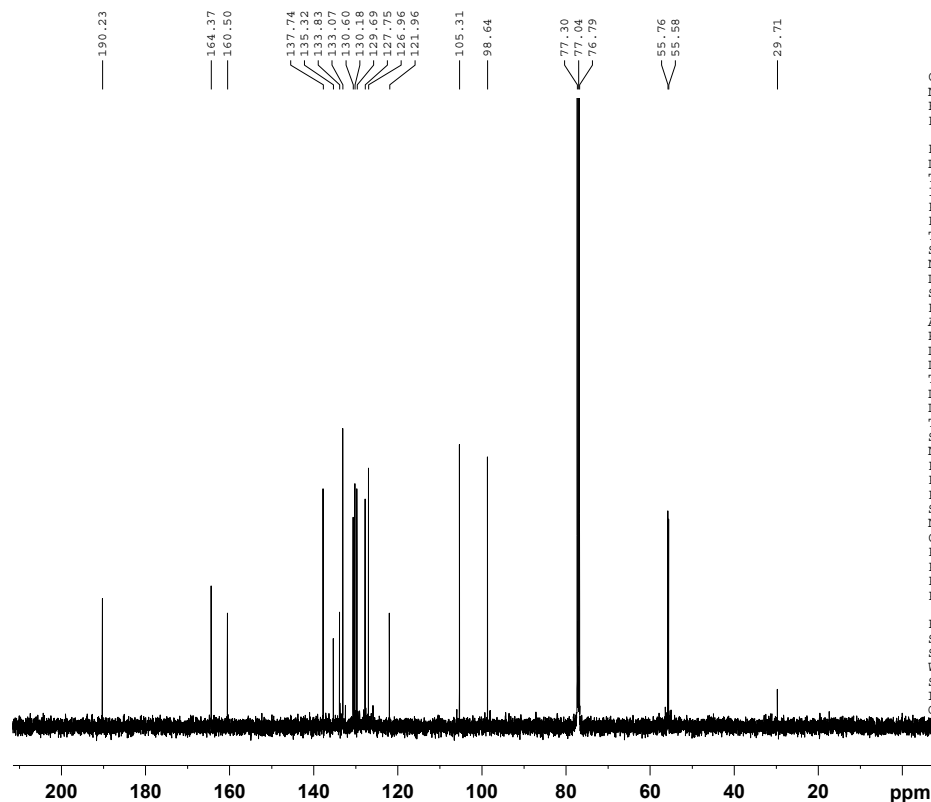
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AVANCE NEO
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SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
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EXPNO 131
PROCNO 1

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TE 300.1 K
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D11 0.03000000 sec
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SFO1 125.7804233 MHz
NUC1 13C
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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

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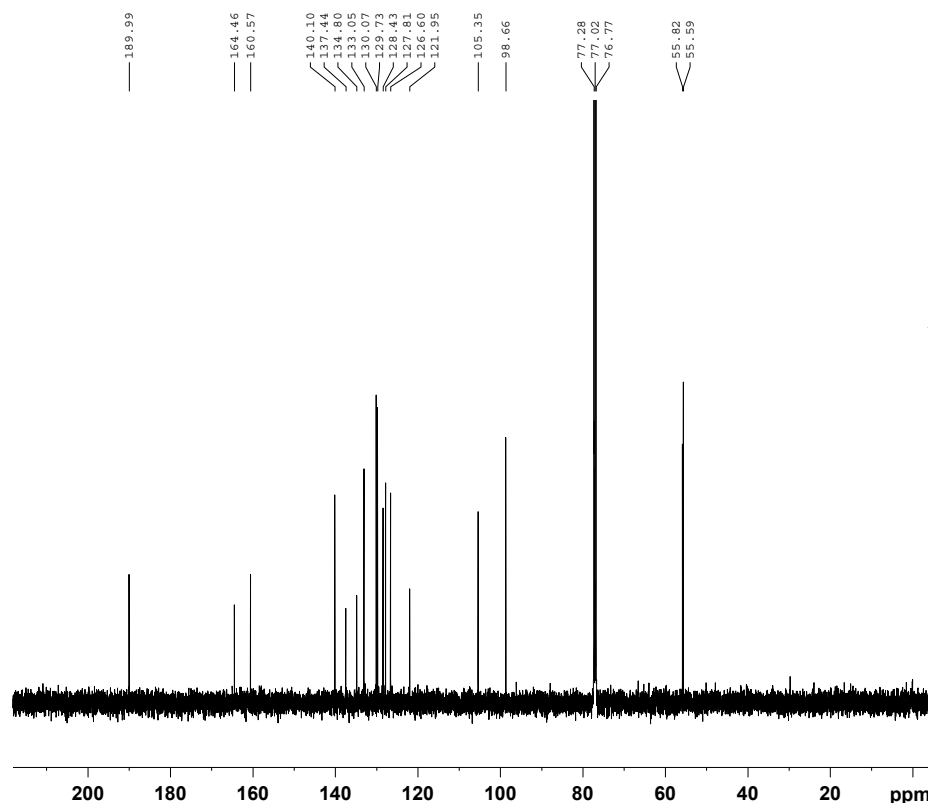
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AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

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PROCNO 1

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SOLVENT CDC13
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TE 298.6 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

D3
C13CPD CDC13 {D:\Spectra} nmr 15



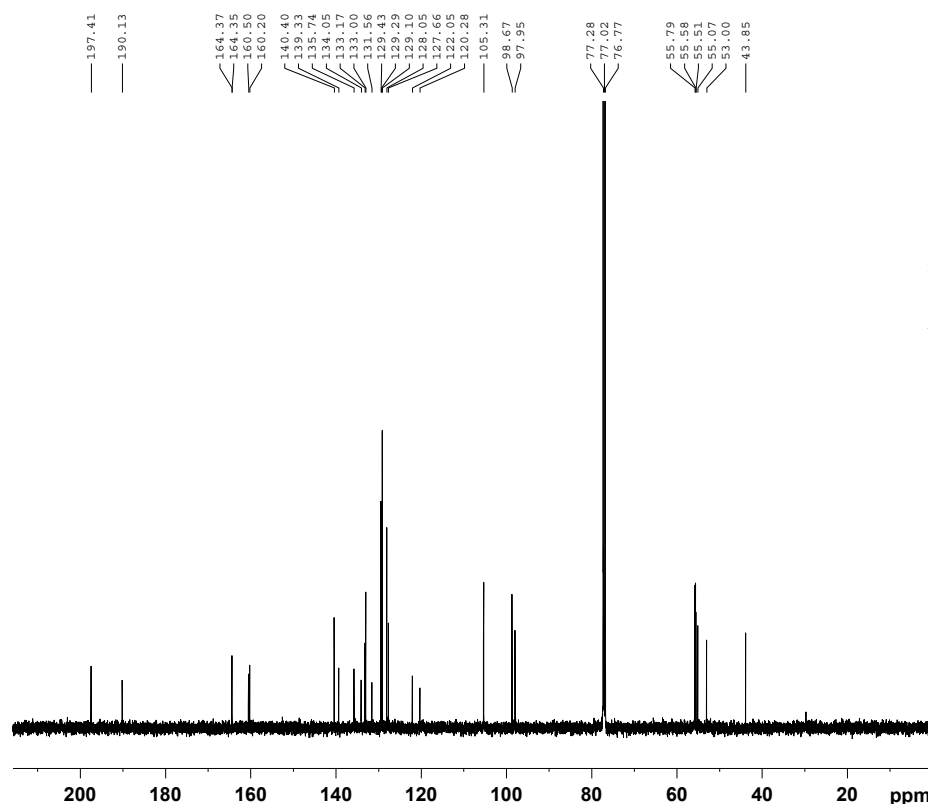
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Dec15-2020
EXPNO 152
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201215
Time_ 17.14 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 240
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 298.8 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

D4
C13CPD CDC13 {D:\Spectra} nmr 16



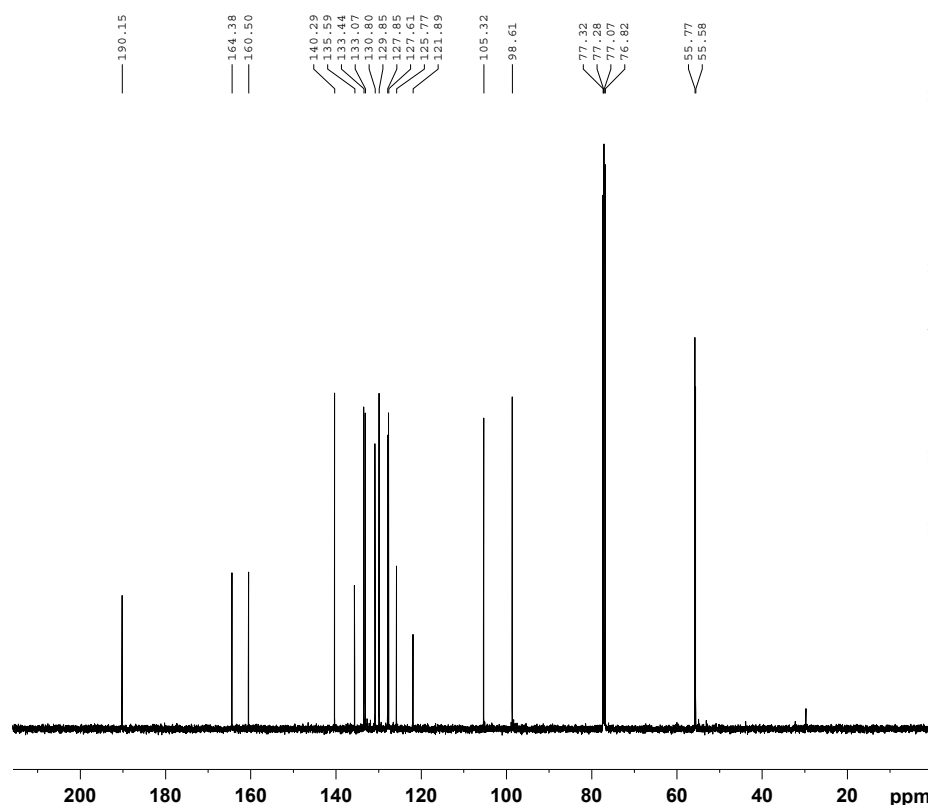
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Dec15-2020
EXPNO 161
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201215
Time_ 17.45 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 298.6 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

D5
C13CPD CDC13 {D:\Spectra} nmr 17



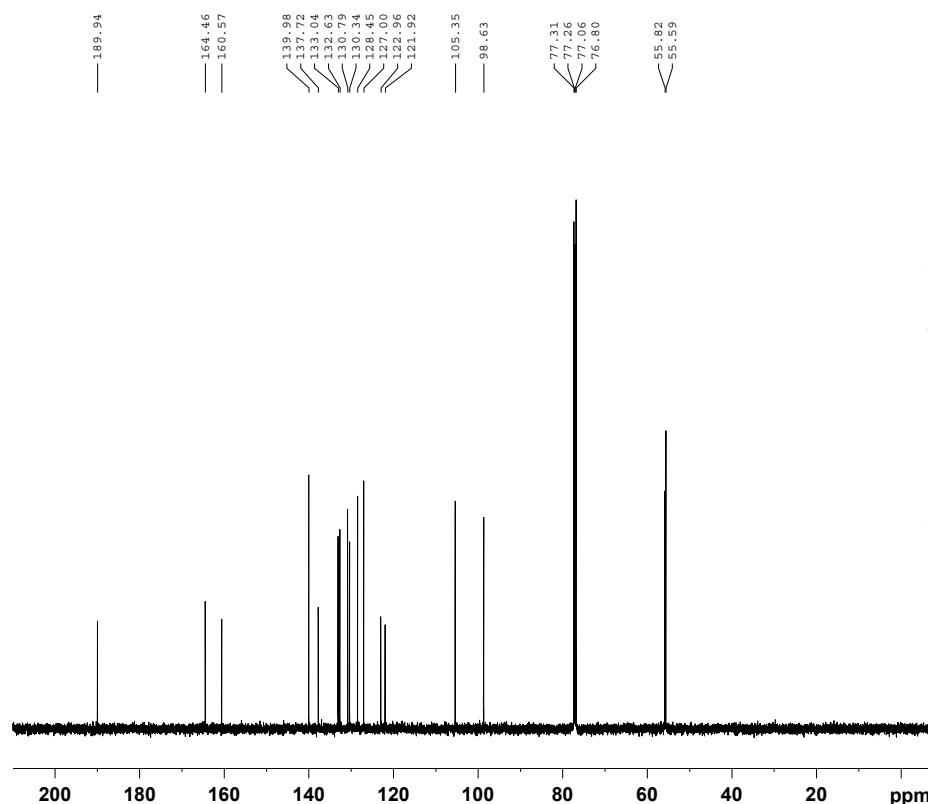
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Dec15-2020
EXPNO 171
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201216
Time 9.53 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 170
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 297.8 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

D6
C13CPD CDC13 {D:\Spectra} nmr 18



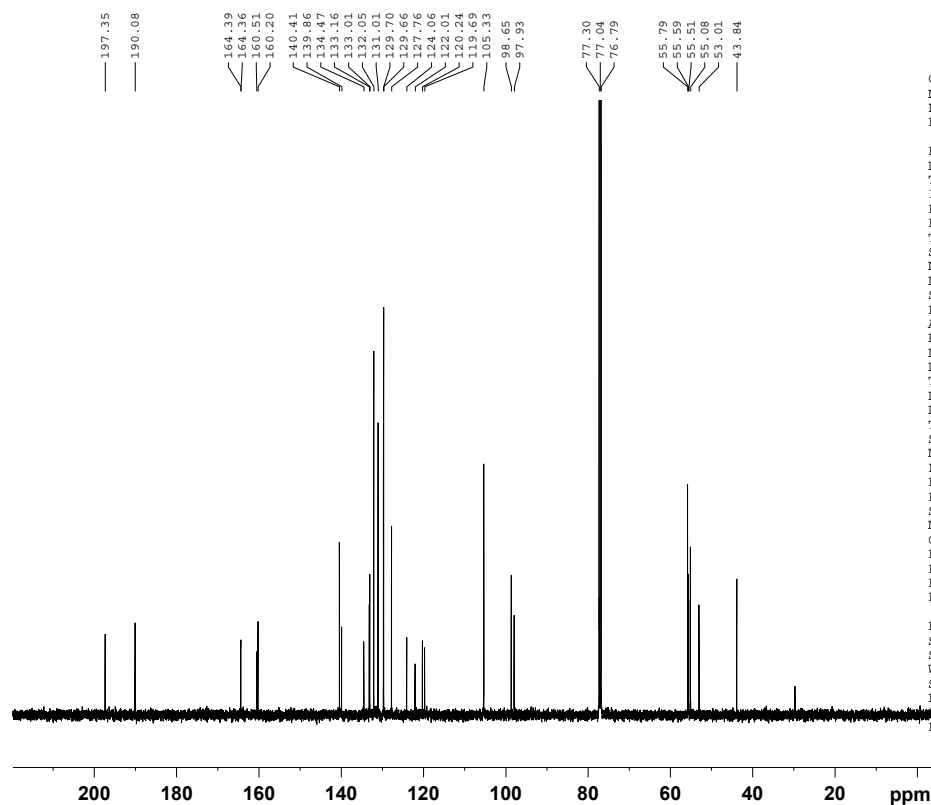
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Dec15-2020
EXPNO 181
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201216
Time 10.00 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 84
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 297.8 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

D7
C13CPD CDC13 {D:\Spectra} nmr 19



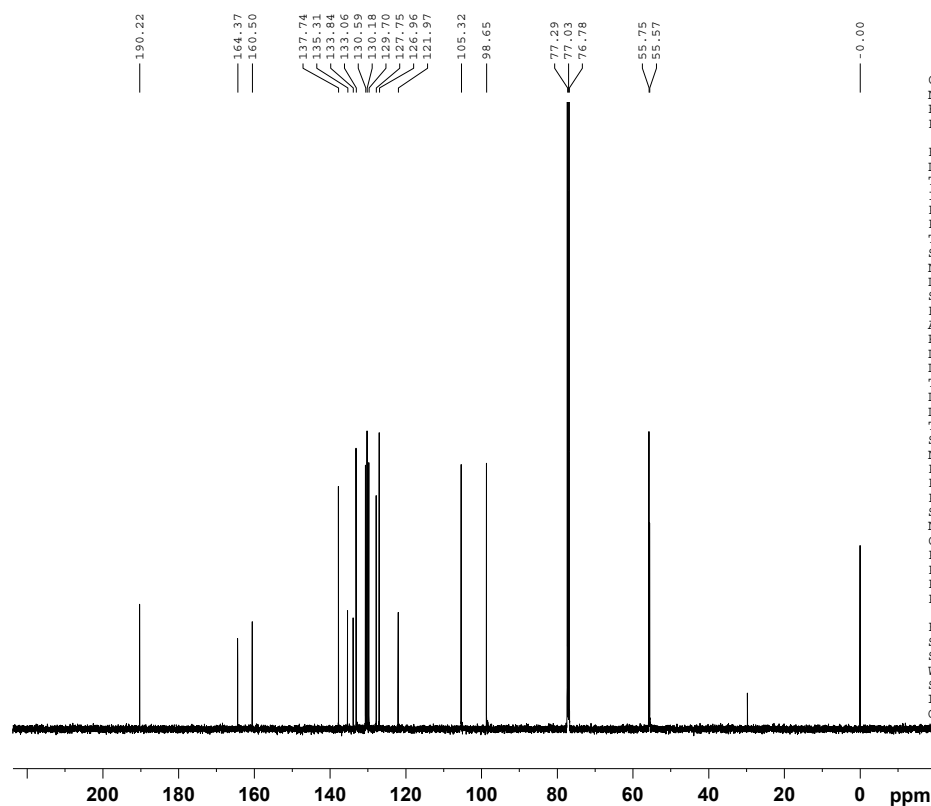
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Dec15-2020
EXPNO 191
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201216
Time 10.13 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 202
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 297.7 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

D8
C13CPD CDC13 {D:\Spectra} nmr 24



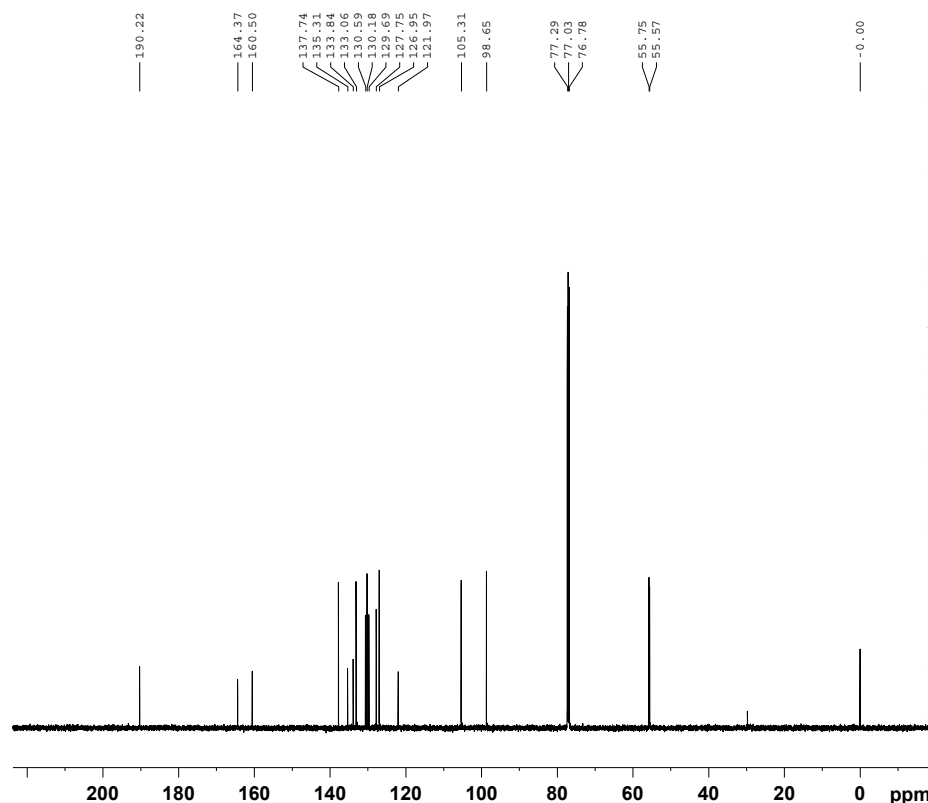
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 241
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220621
Time 16.13 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 300.6 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 125.7678466 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

D9
C13CPD CDC13 {D:\Spectra} nmr 25



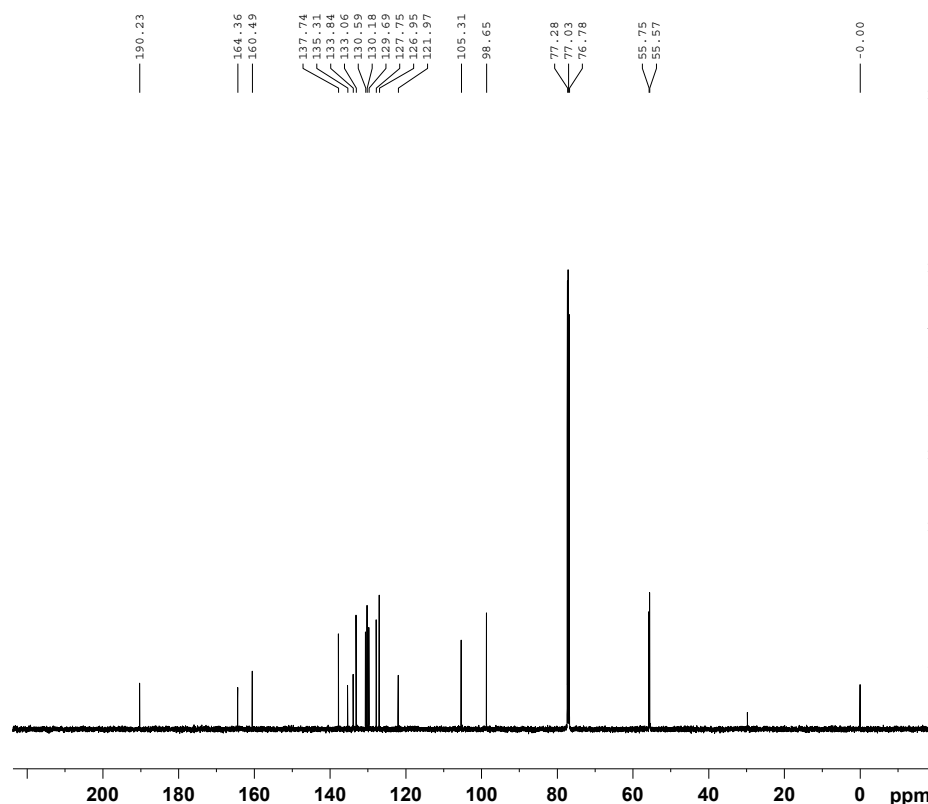
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 251
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220621
Time 16.29 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 265
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 300.3 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
CPDPRG2 waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7678468 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

D10
C13CPD CDC13 {D:\Spectra} nmr 26



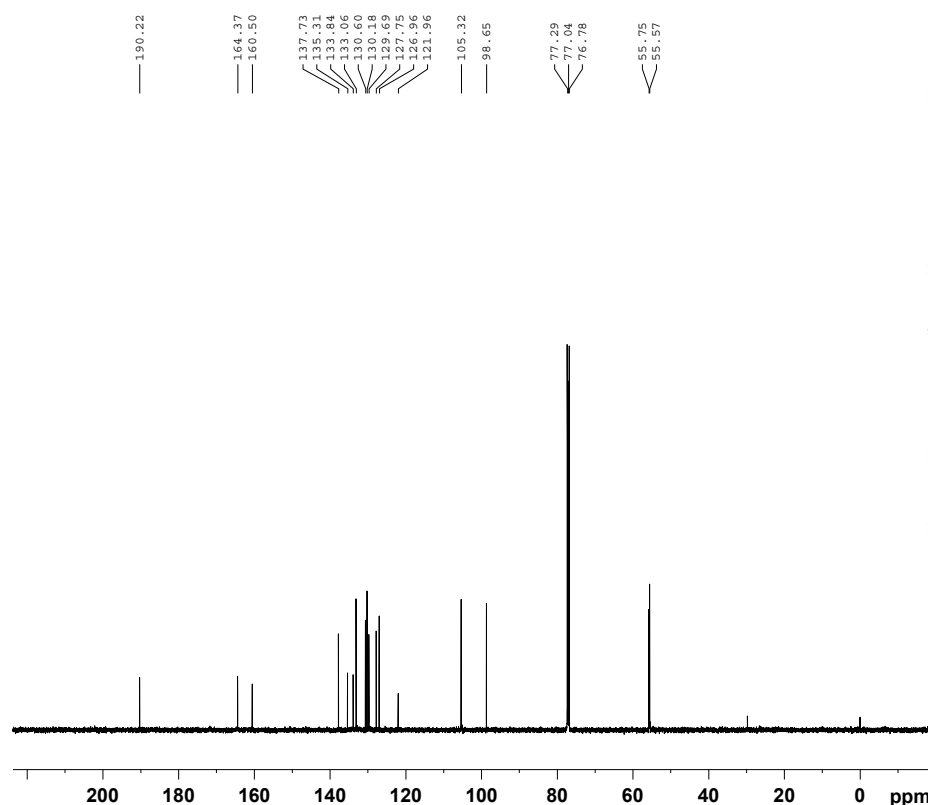
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 261
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220621
Time 16.45 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 261
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 300.3 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
CPDPRG2 waltz65
PCPD2 80.00 usec
PLW2 20.93000031 W
PLW12 0.32703000 W
PLW13 0.16449000 W

F2 - Processing parameters
SI 32768
SF 125.7678467 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

D11
C13CPD CDC13 {D:\Spectra} nmr 27



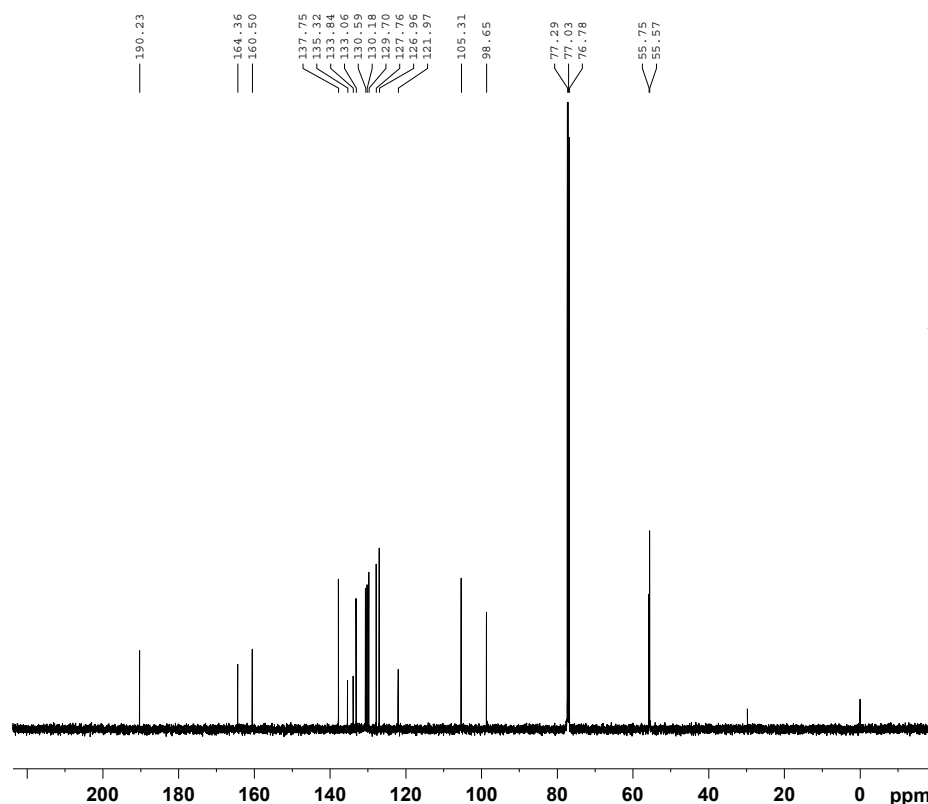
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 271
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220621
Time 16.59 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 224
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 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

D12
C13CPD CDC13 {D:\Spectra} nmr 28



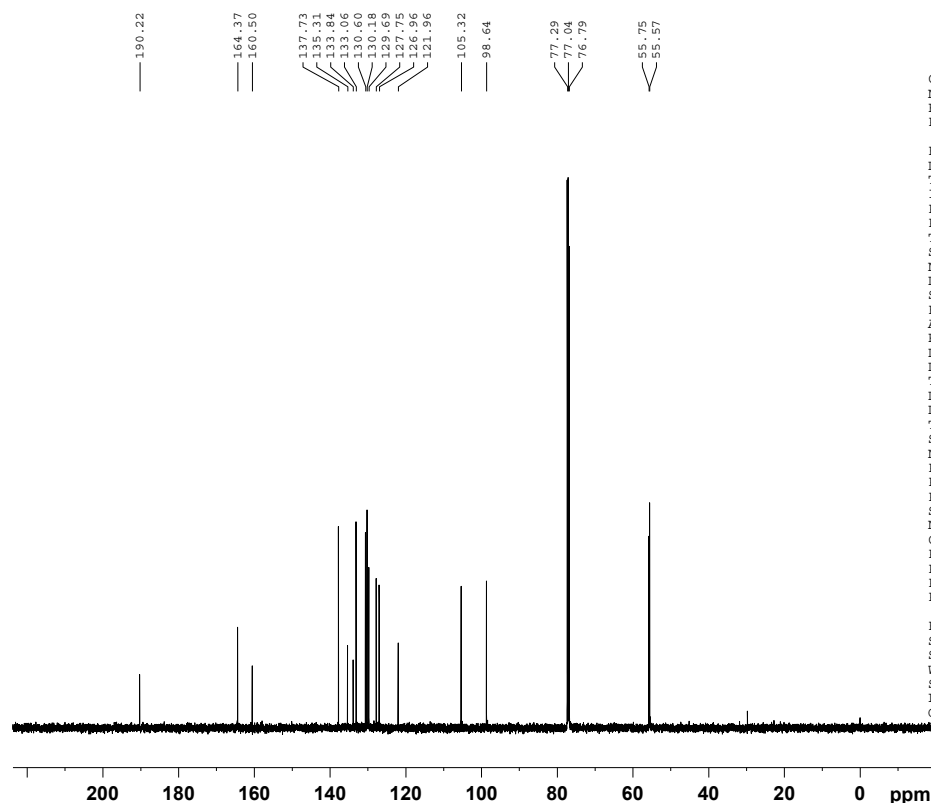
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 281
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220621
Time 17.12 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 205
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 300.3 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
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

D13
C13CPD CDC13 {D:\Spectra} nmr 29



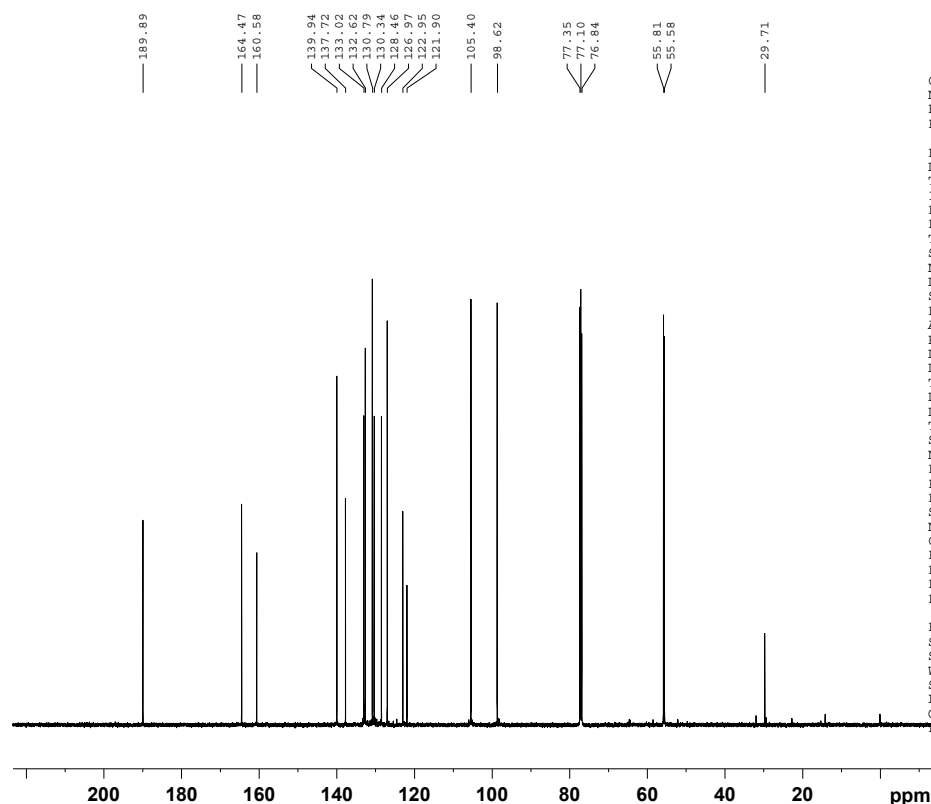
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 291
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220621
Time_ 17.23 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 156
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 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

D14
C13CPD CDC13 {D:\Spectra} nmr 30



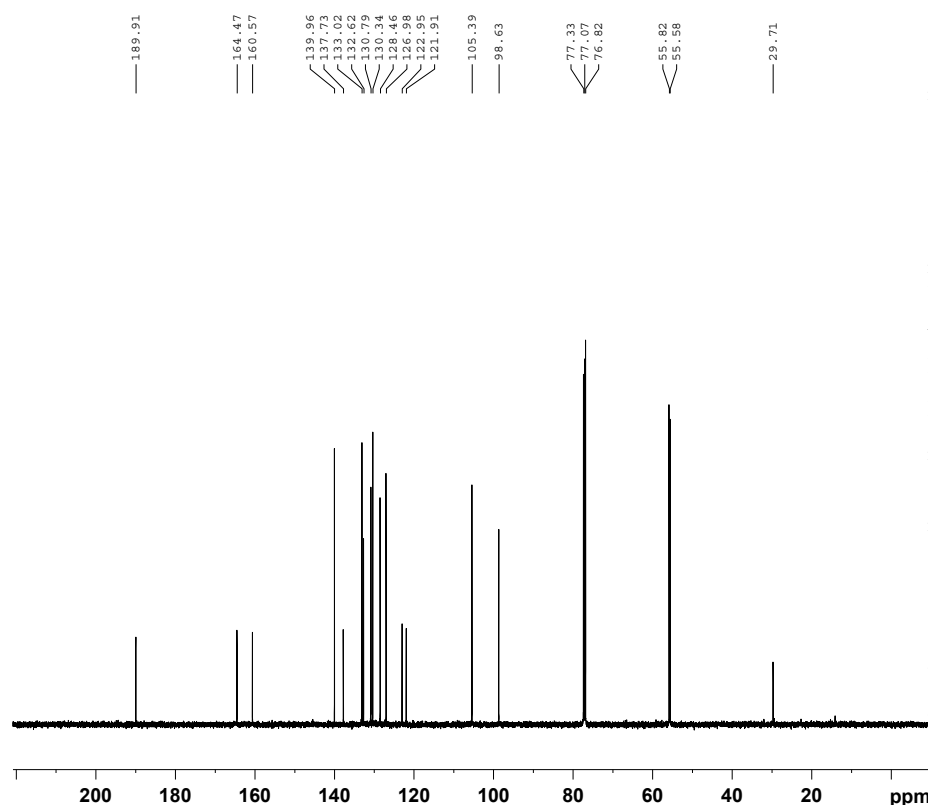
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 301
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220621
Time_ 17.52 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 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

D16
C13CPD CDC13 {D:\Spectra} nmr 32



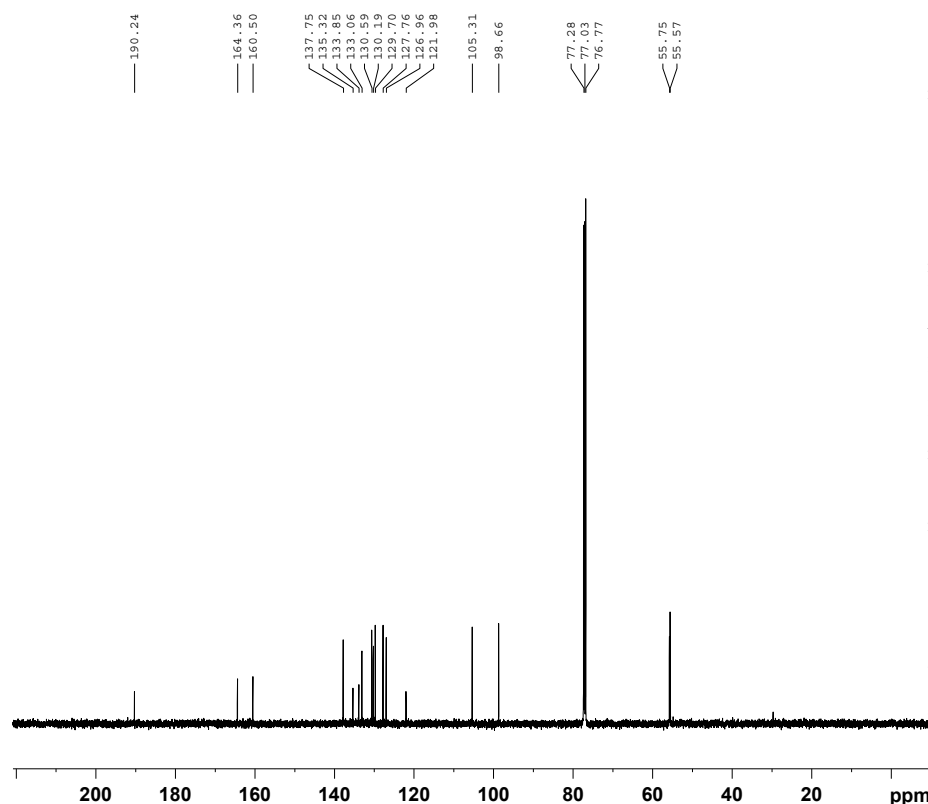
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 321
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220622
Time_ 10.51 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 156
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 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

D17
C13CPD CDC13 {D:\Spectra} nmr 33



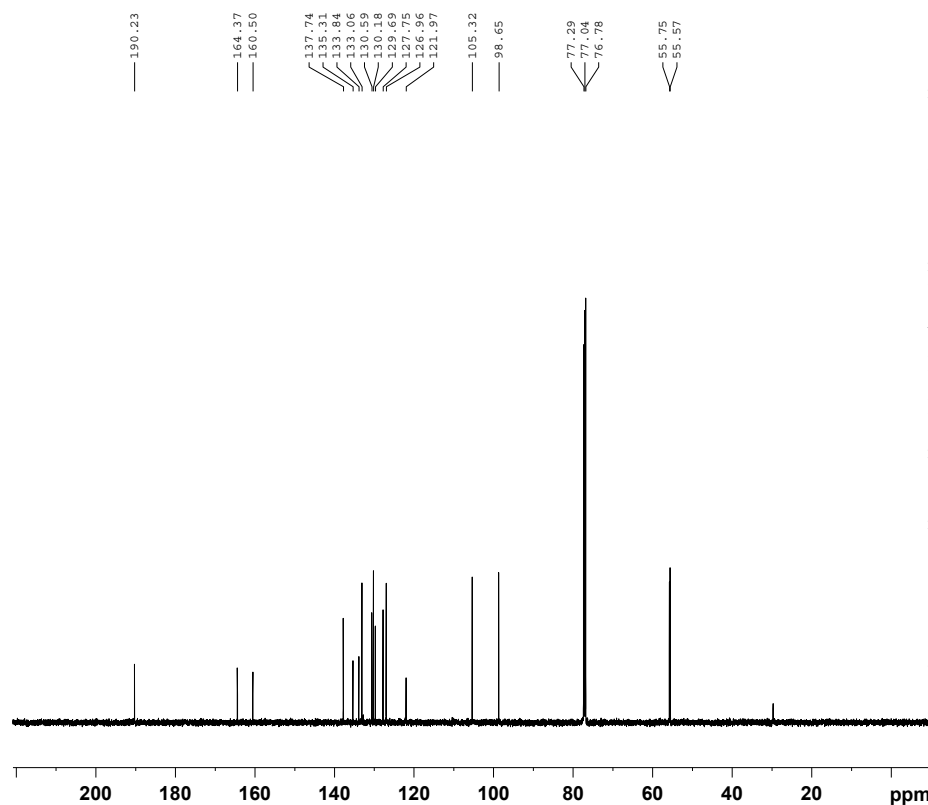
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 331
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220622
Time_ 11.07 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 270
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 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

D18
C13CPD CDCl3 {D:\Spectra} nmr 34



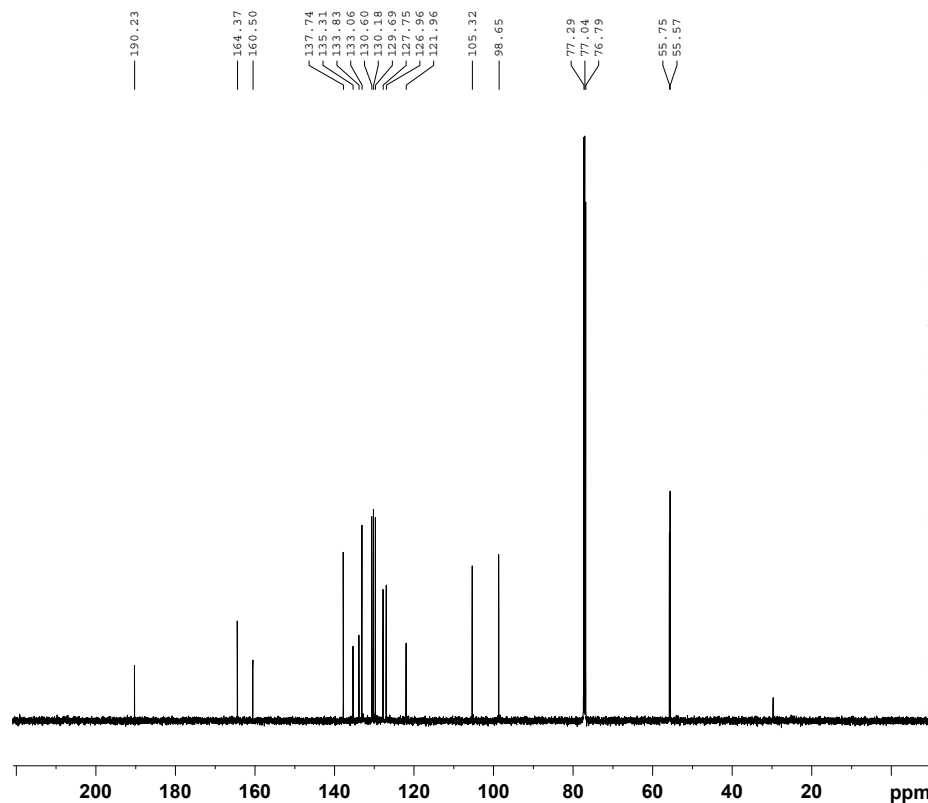
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 341
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220622
Time 11.59 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 176
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 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

D20
C13CPD CDCl3 {D:\Spectra} nmr 36



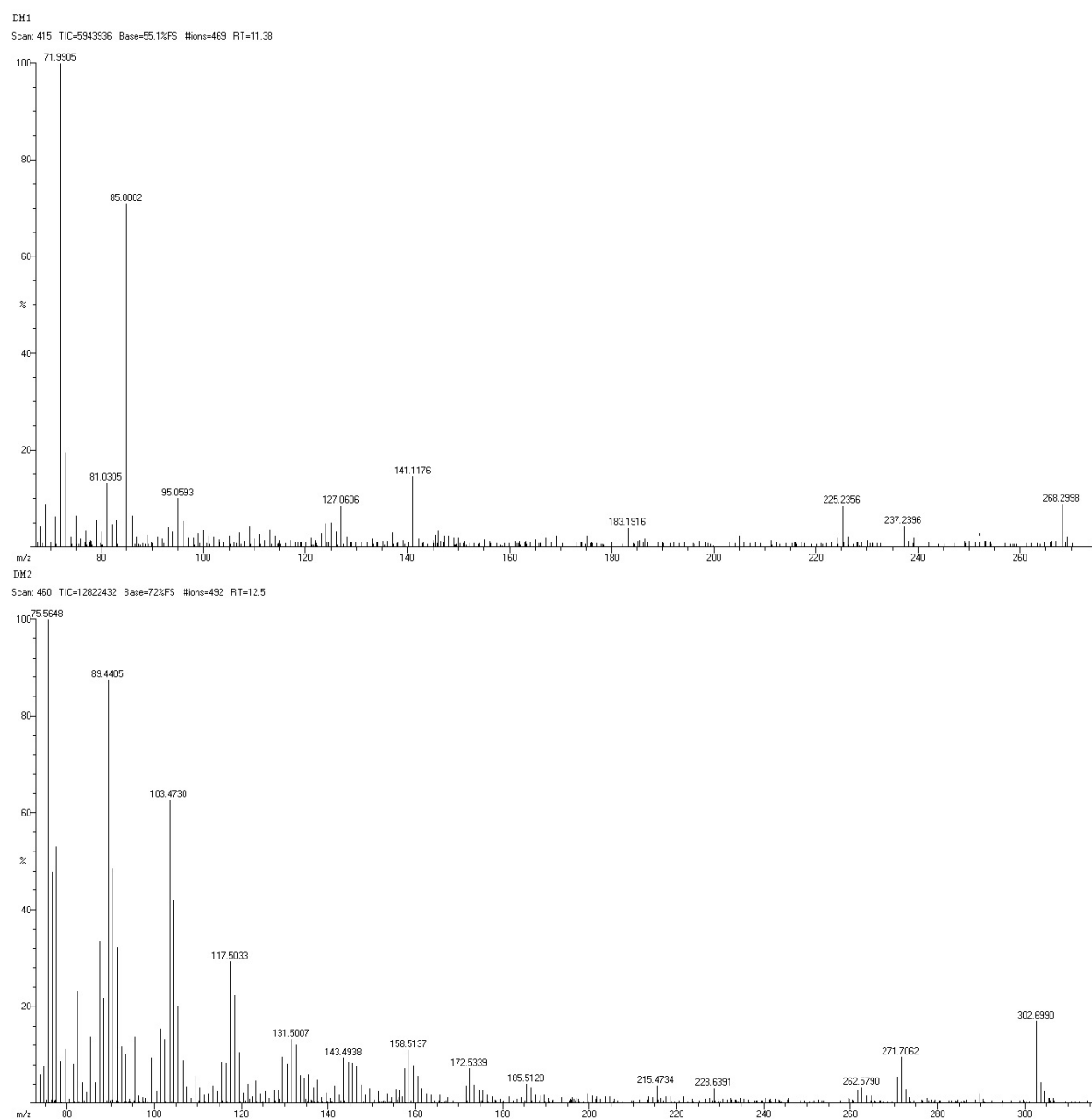
BRUKER
AVANCE NEO
500 MHz NMR SPECTROMETER
SAIF, PANJAB UNIVERSITY,
CHANDIGARH

Current Data Parameters
NAME Jun21-2022
EXPNO 361
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220622
Time 12.40 h
INSTRUM Avance Neo 500
PROBHD Z119470_0333 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 240
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 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

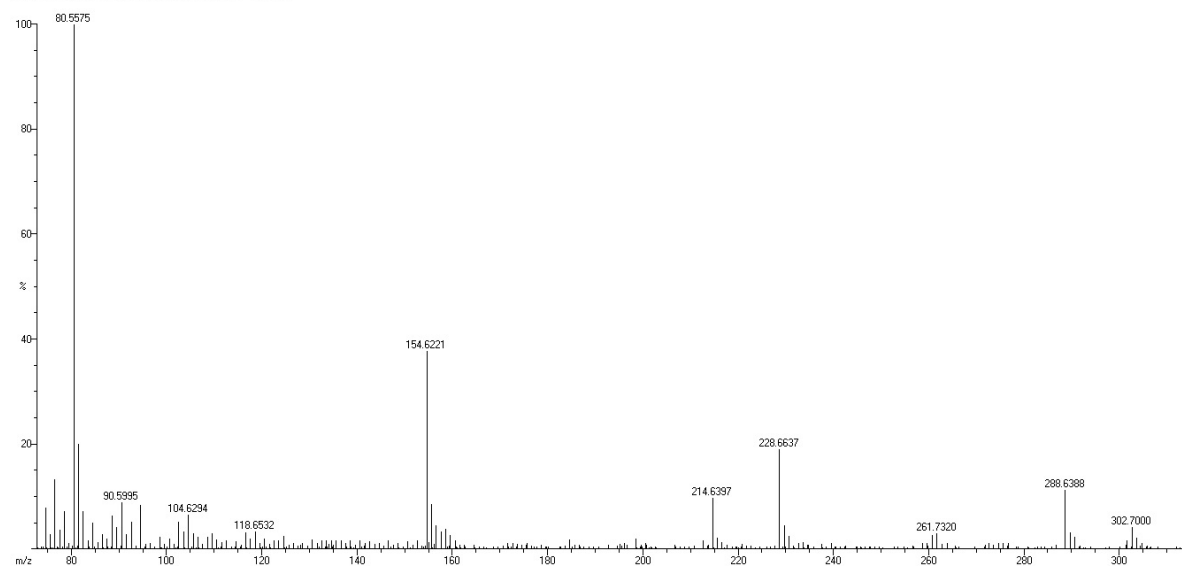
F2 - Processing parameters
SI 32768
SF 125.7678465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S3. MASS Spectra



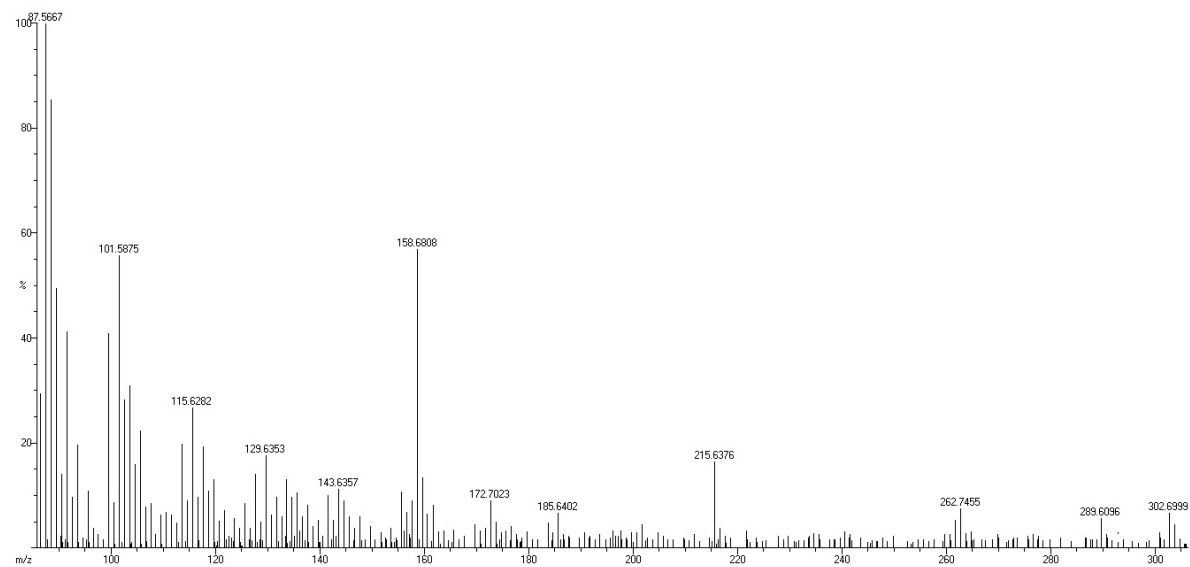
DM3

Scan: 466 TIC=7903072 Base=89.5%FS Hions=520 RT=12.67



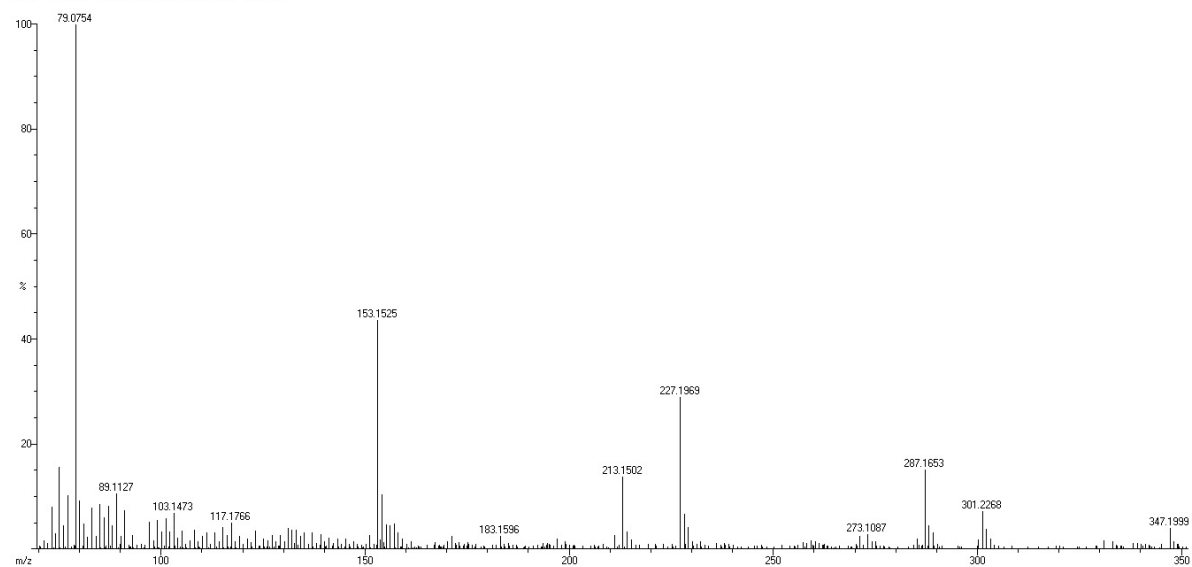
DM4

Scan: 496 TIC=8188048 Base=31.6%FS Hions=476 RT=13.42



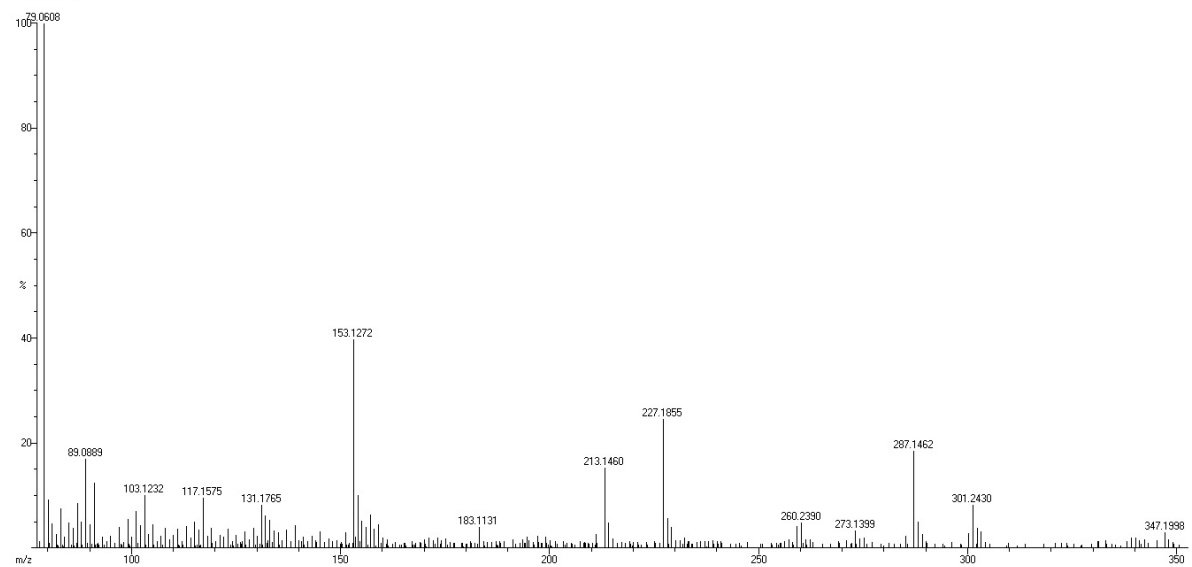
DM5

Scan: 504 TIC=8003024 Base=76%FS #Ions=512 RT=13.62



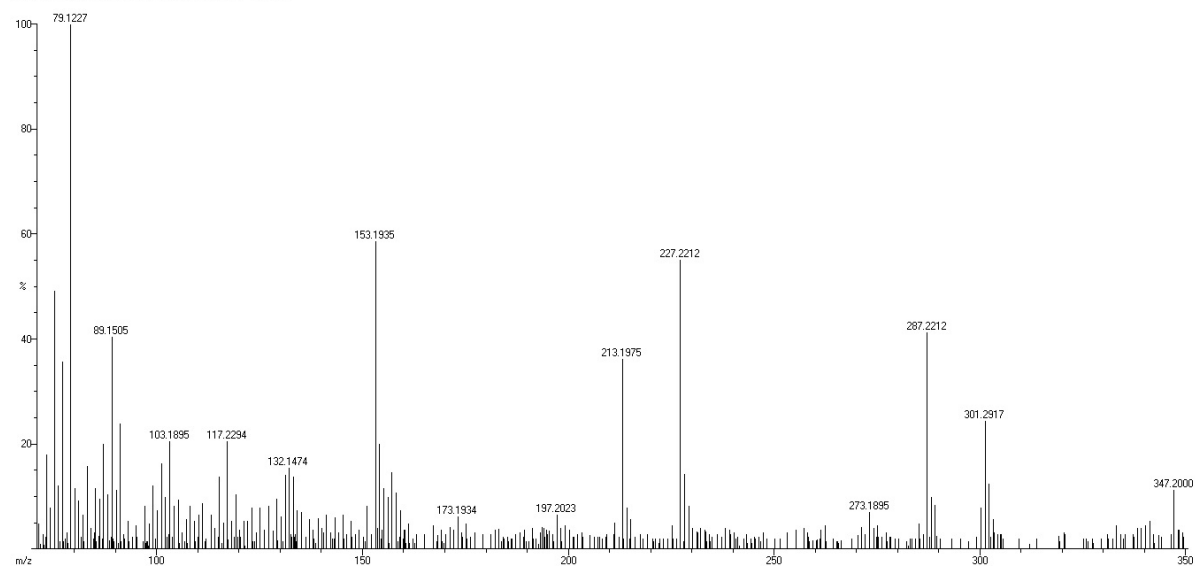
DM6

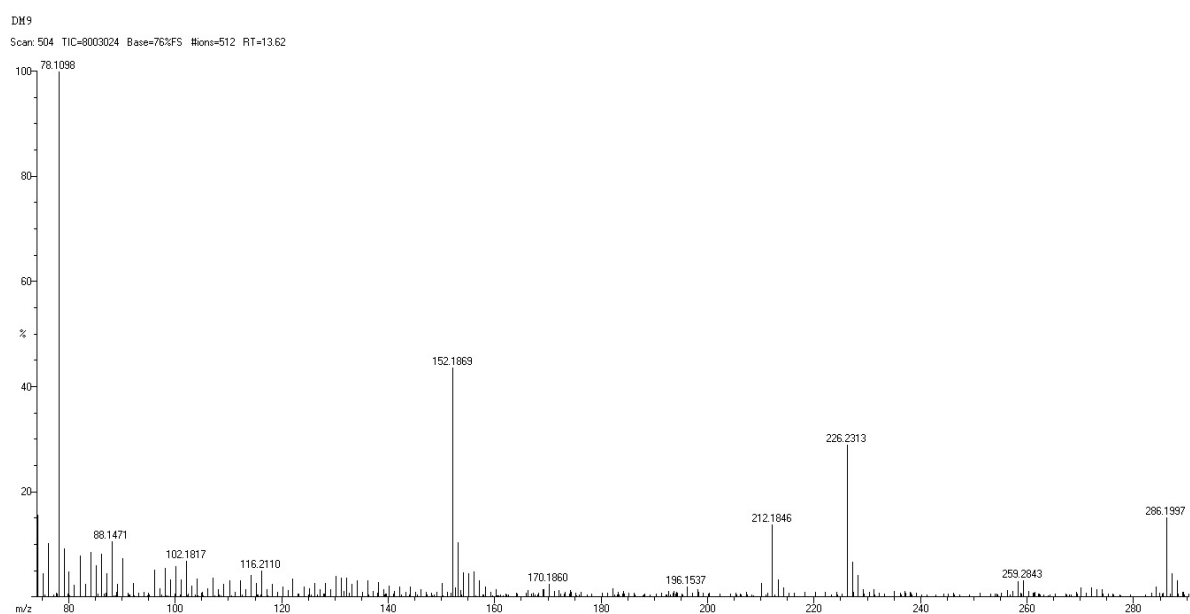
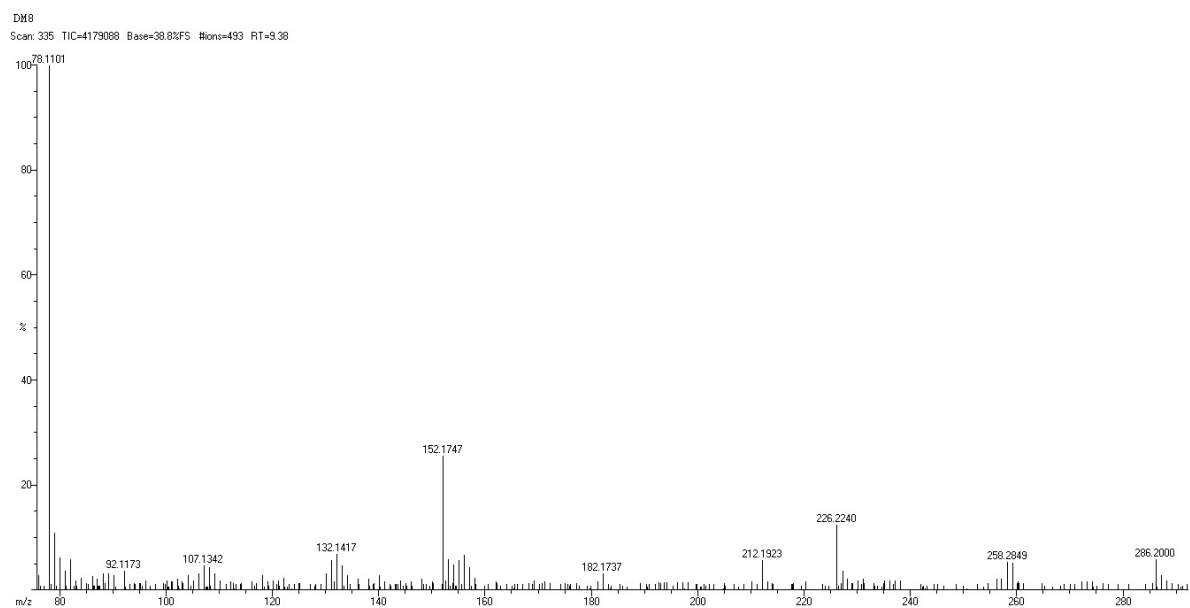
Scan: 549 TIC=7095940 Base=56.1%FS #Ions=516 RT=14.73



DM7

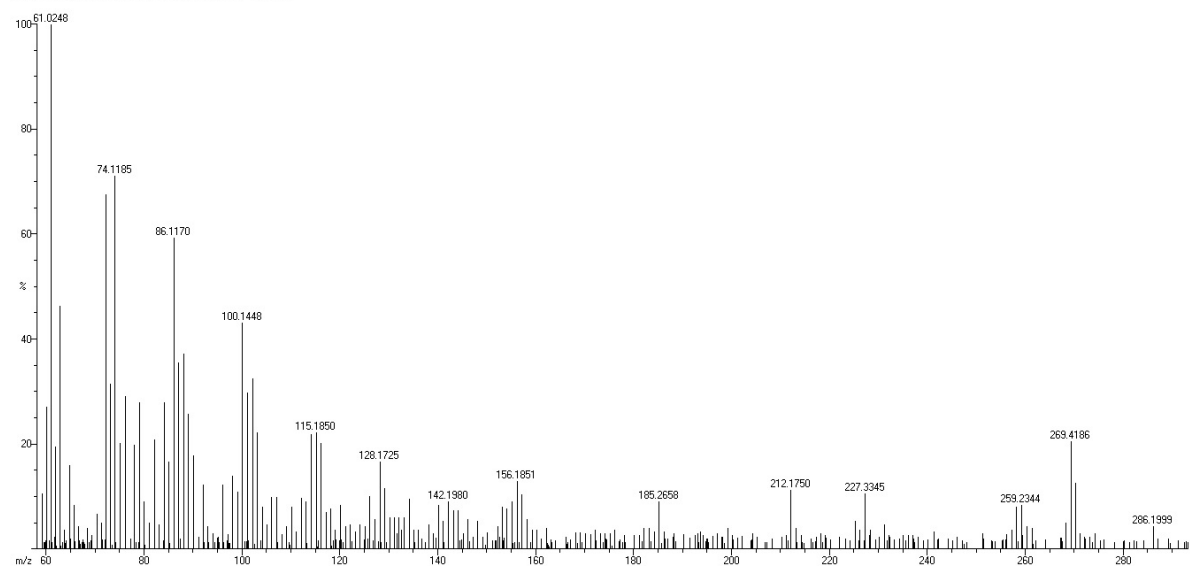
Scan: 609 TIC=8551136 Base=23.1%FS #Ions=522 RT=16.25





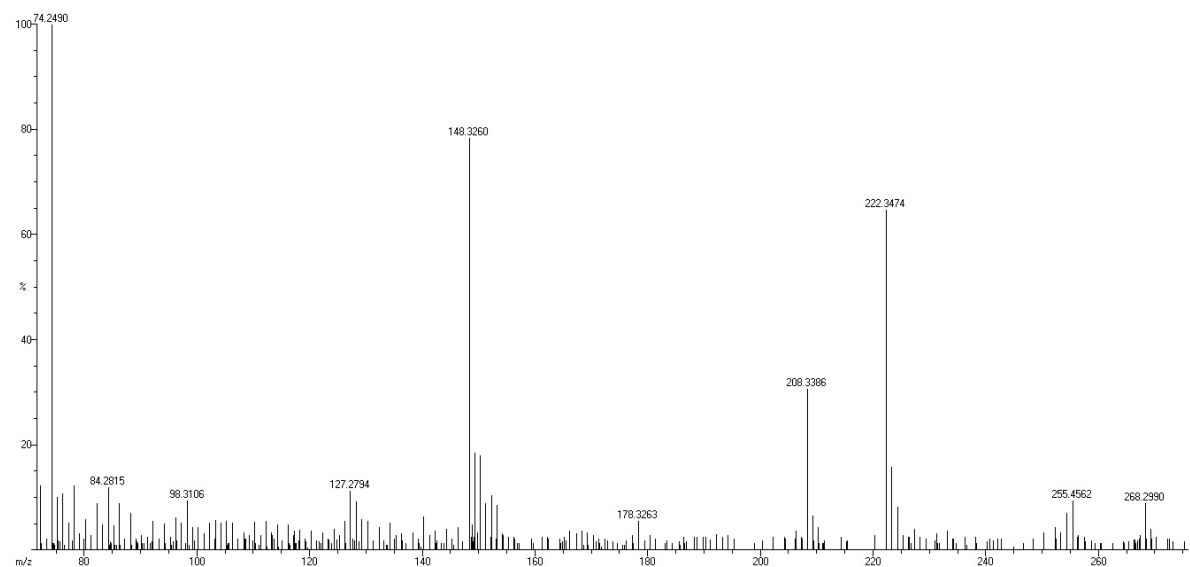
DM10

Scan: 462 TIC=7408880 Base=28.4%FS #Ions=480 RT=12.57



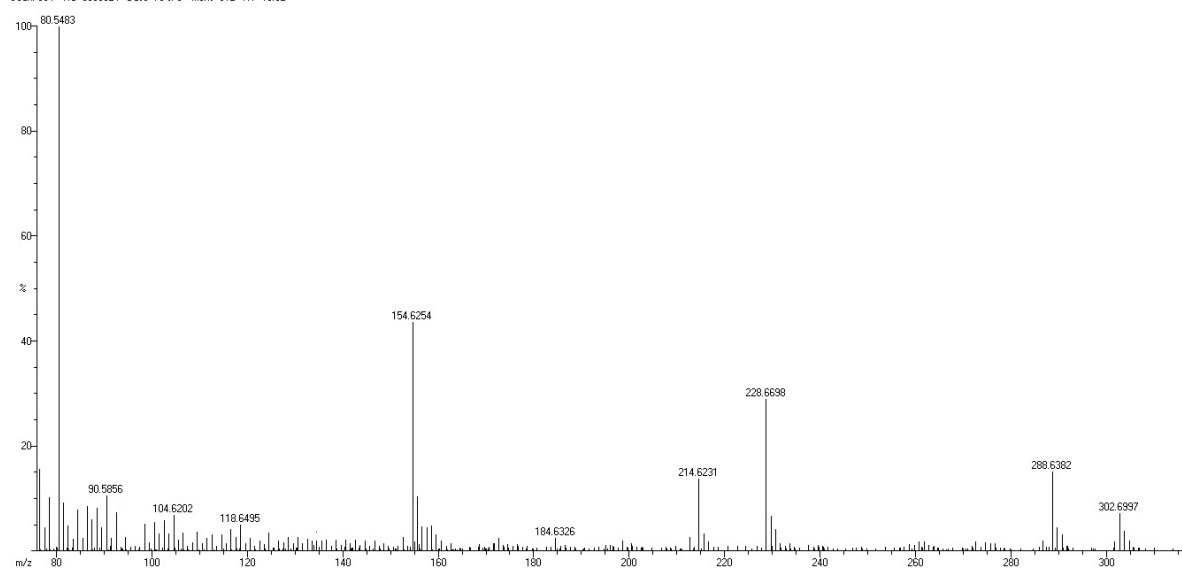
DM11

Scan: 427 TIC=5800144 Base=25.8%FS #Ions=485 RT=11.68



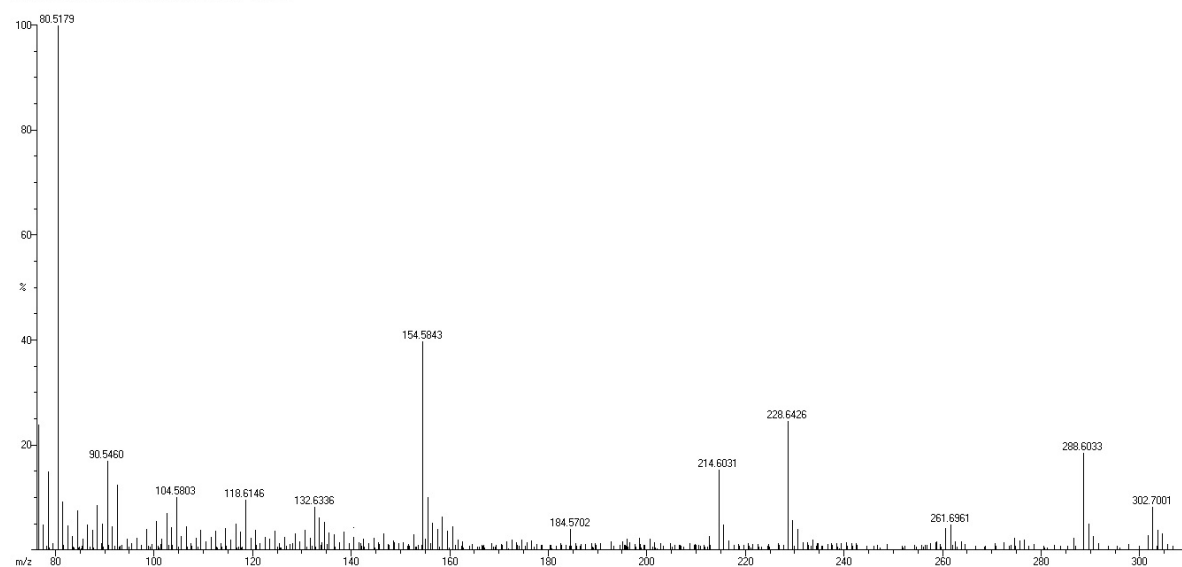
DM12

Scan: 504 TIC=8003024 Base=76%FS #Ions=512 RT=13.62



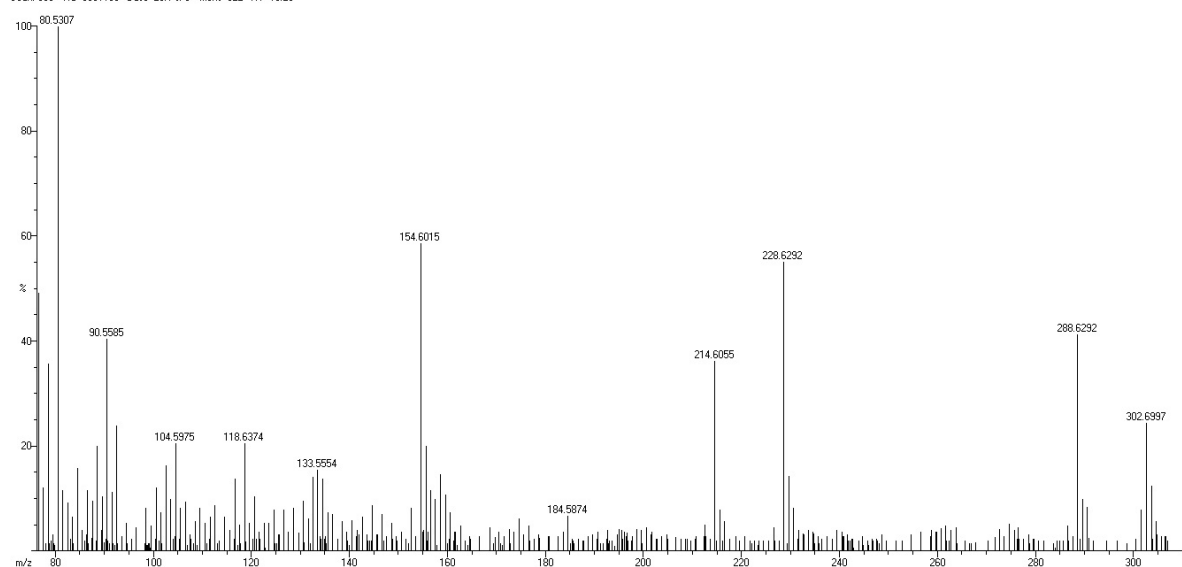
DM13

Scan: 549 TIC=7095940 Base=56.1%FS #Ions=516 RT=14.73

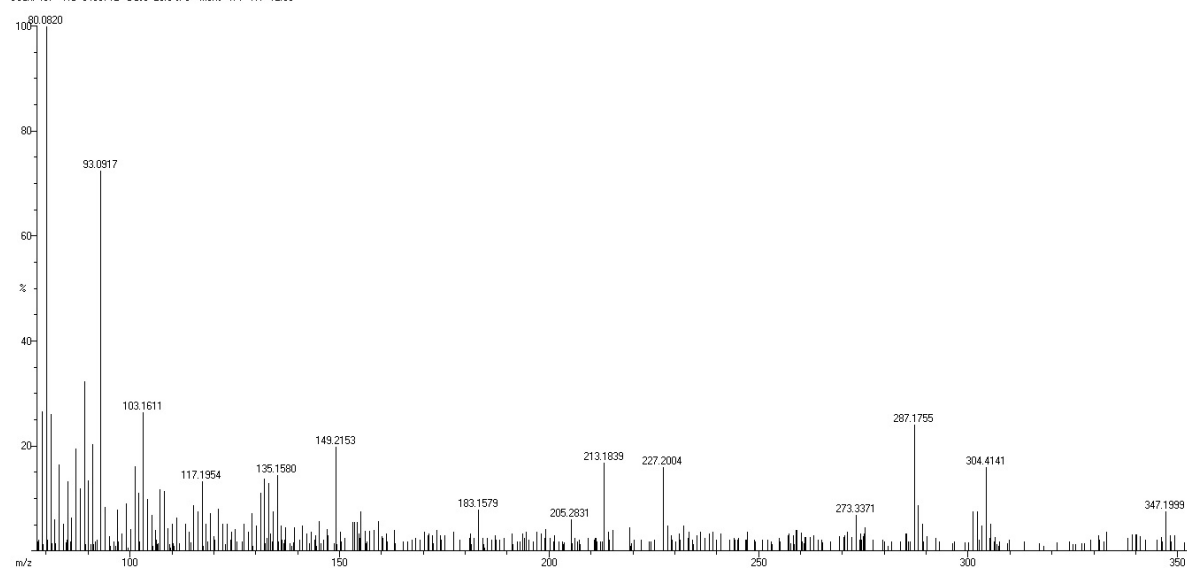


DM14

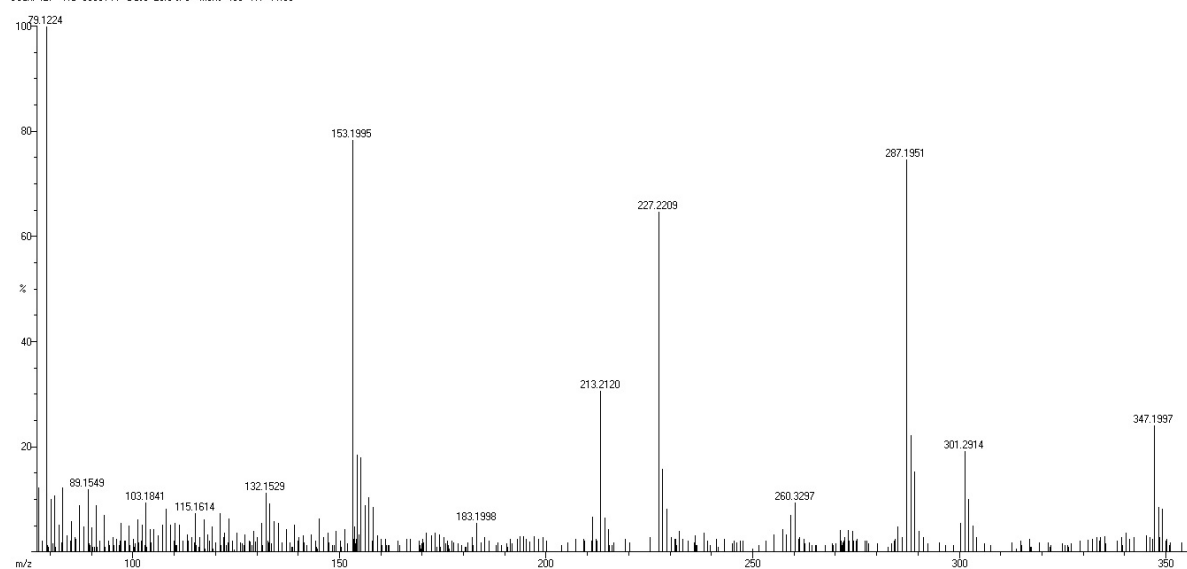
Scan: 609 TIC=6551136 Base=23.1%FS #Ions=522 RT=16.25



DM15
Scan: 467 TIC=6433712 Base=25.3%FS #Ions=471 RT=12.68

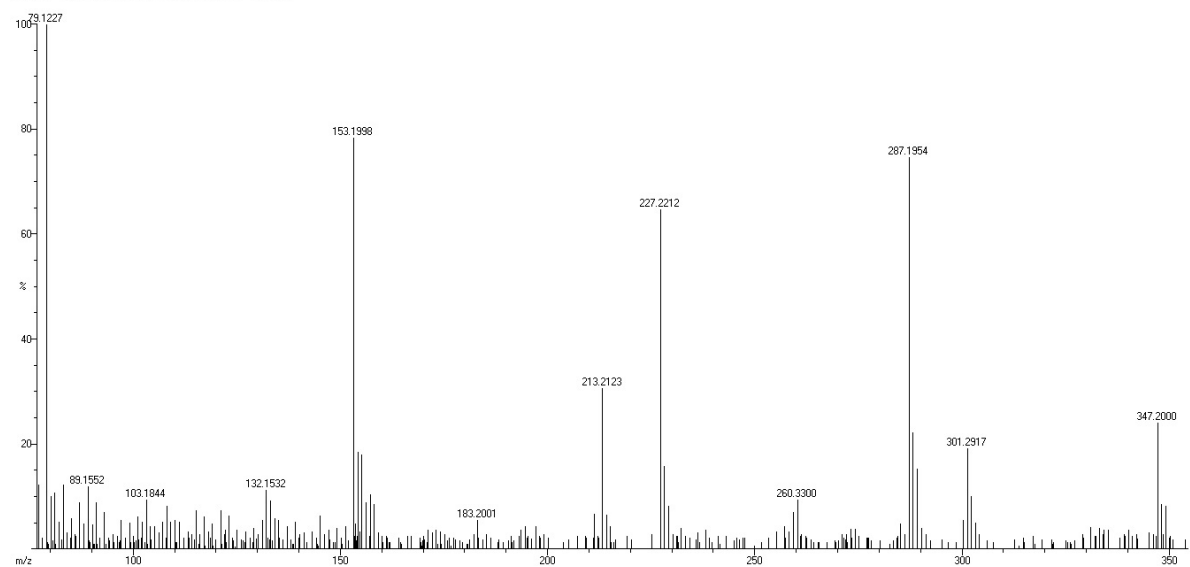


DM16
Scan: 427 TIC=5800144 Base=25.8%FS #Ions=485 RT=11.68



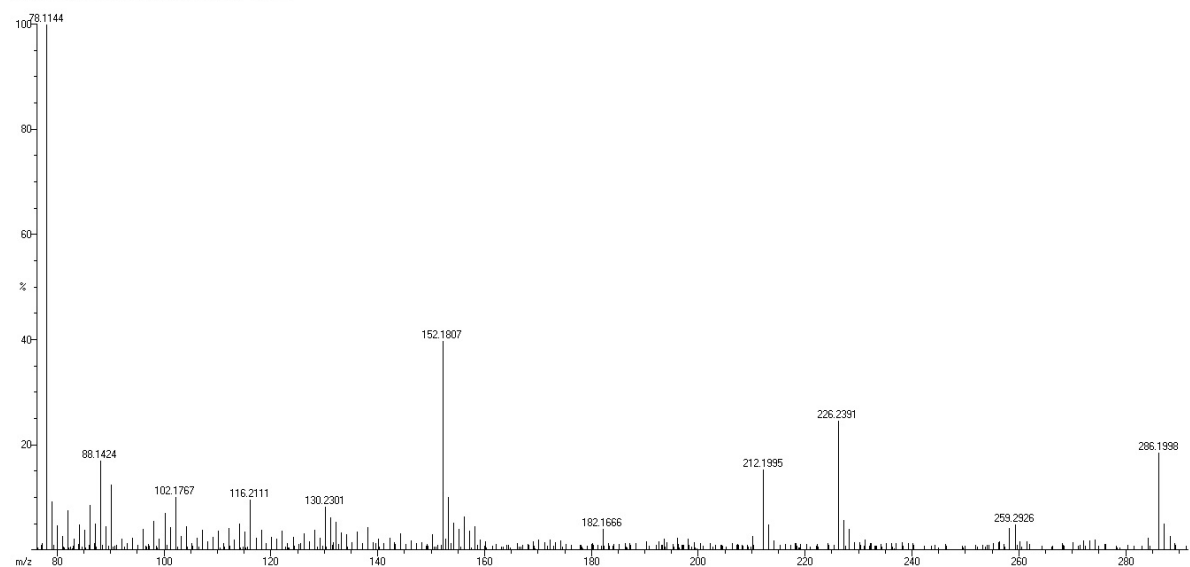
DM17

Scan: 427 TIC=5800144 Base=25.8%FS Hions=495 RT=11.68



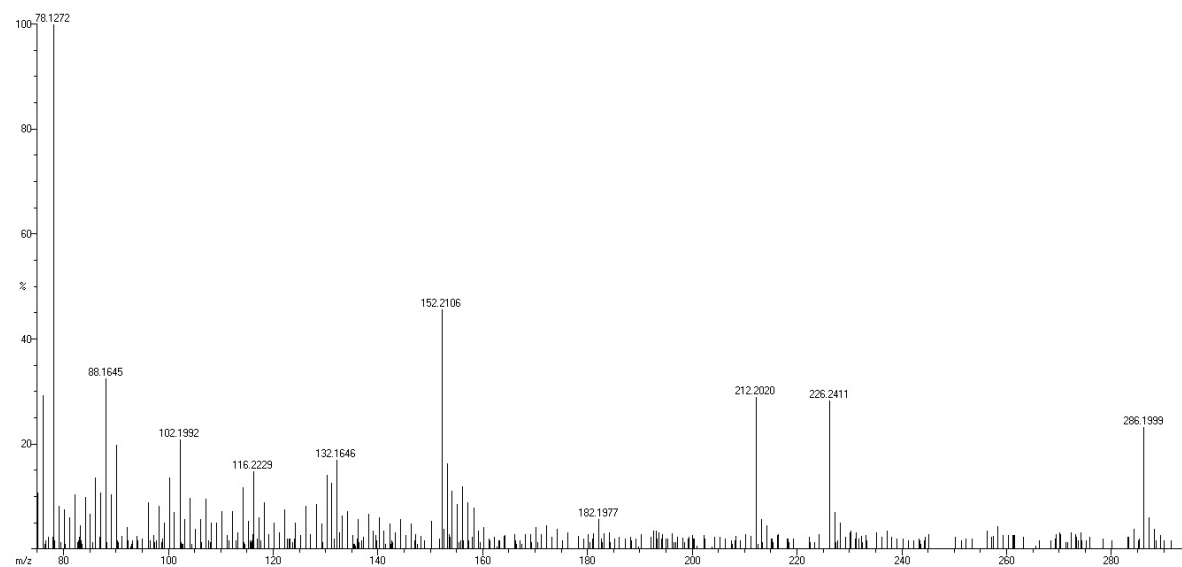
DM18

Scan: 549 TIC=7095840 Base=56.1%FS Hions=516 RT=14.73



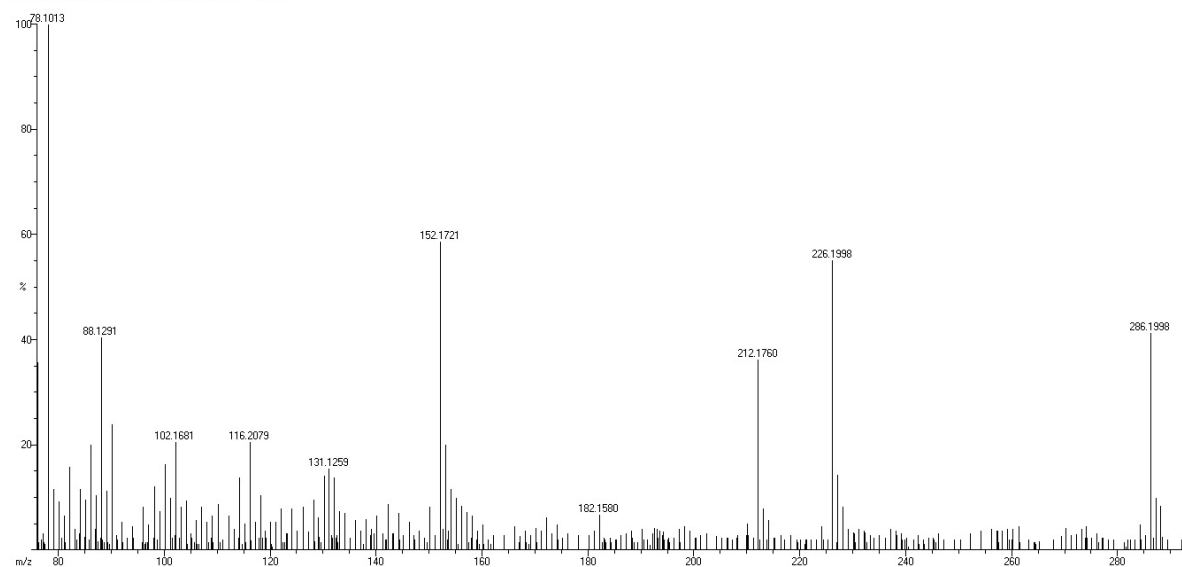
DM19

Scan: 608 TIC=6094944 Base=26.8%FS Hions=500 RT=16.22



DM20

Scan: 609 TIC=6551136 Base=23.1%FS Hions=522 RT=16.25



Text S1. Supplementary procedure for toxicity evaluation

Cell culture

The cell line of Vero (African green monkey kidney cells) was procured from NCCS (Pune, India) and was grown in liquid medium (DMEM) containing 100 ug/mL penicillin, 100 µg/mL streptomycin, and 10% Fetal Bovine Serum (FBS) and preserved under an atmosphere of 5% CO₂ at 37°C.

MTT Assay

The **DM2** was assayed for *in vitro* cytotoxicity by MTT assay using the cultured Vero cells. Briefly, the cultured Vero cells were produced by cell dissociation with trypsin (trypsinization), collectively in a 15 mL tube. At a density of 1×10⁵ cells/mL cells/well (200 µL), the cells were plated for 24-48 h at 37°C into 96-well tissue culture plate in DMEM medium containing 10 % FBS and 1% antibiotic solution. The wells were washed with sterile phosphate buffered saline (PBS) and further allowed to react with varying concentrations of the **DM2** in a serum free DMEM medium. The samples were triplicated and the cells were kept for incubation at 37°C for 24 h in a humidified 5% CO₂ incubator. MTT (20 µL of 5 mg/mL) was added into each well after the incubation and the cells were incubated for another 2-4 h. The end point was determined by the purple precipitation, which was clearly seen under an inverted microscope. At the end, the medium along with MTT (220 µL) were used for the aspiration of the wells and later washed with 1X PBS (200 µL). In order to dissolve formazan crystals, DMSO (100 µL) was added to the plate with shaking for 5 min. The absorbance at 570 nm was measured using a micro plate reader (Thermo Fisher Scientific, USA). The IC₅₀ value and the percentage cell viability was calculated using GraphPad Prism 8.0 software (USA).

Table S1. Inhibitions of AChE, BChE, and BACE-1 by DM series^a

Compounds	Residual activity at 10 μ M (%)		
	AChE	BChE	BACE-1
DM1	75.60 \pm 2.35	93.21 \pm 0.30	92.67 \pm 0.26
DM2	71.91 \pm 2.87	64.16 \pm 0.44	100.50 \pm 0.18
DM3	81.47 \pm 4.09	69.87 \pm 0.19	99.67 \pm 0.53
DM4	74.23 \pm 2.43	80.07 \pm 1.59	90.82 \pm 0.09
DM5	71.15 \pm 6.12	60.54 \pm 0.03	87.80 \pm 0.29
DM6	73.04 \pm 0.75	79.72 \pm 1.10	88.53 \pm 0.22
DM7	87.23 \pm 1.19	98.21 \pm 1.01	97.29 \pm 0.34
DM8	82.69 \pm 10.41	85.42 \pm 0.67	91.01 \pm 0.06
DM9	71.92 \pm 3.06	72.50 \pm 3.69	88.20 \pm 0.28
DM10	64.26 \pm 6.85	92.84 \pm 0.51	87.13 \pm 0.42
DM11	80.34 \pm 5.21	80.53 \pm 1.36	97.51 \pm 1.02
DM12	68.52 \pm 2.87	63.48 \pm 1.47	94.27 \pm 1.06
DM13	95.00 \pm 3.40	100.38 \pm 7.32	99.86 \pm 0.28
DM14	97.58 \pm 3.42	76.53 \pm 1.37	99.83 \pm 0.81
DM15	83.89 \pm 4.91	55.16 \pm 1.01	99.54 \pm 0.24
DM16	82.70 \pm 9.21	91.21 \pm 1.43	99.74 \pm 0.04
DM17	81.78 \pm 6.31	68.89 \pm 1.57	100.03 \pm 0.04
DM18	78.55 \pm 4.89	59.55 \pm 4.08	99.94 \pm 0.01
DM19	70.00 \pm 2.02	103.45 \pm 8.13	99.86 \pm 0.12
DM20	86.98 \pm 0.45	93.10 \pm 6.50	99.89 \pm 0.08
Donepezil ^b	0.010 \pm 0.002	0.180 \pm 0.004	-
Quercetin ^c	-	-	13.400 \pm 0.035

^a Results are the means \pm standard errors of duplicate or triplicate experiments.^b IC₅₀ of reference compounds for AChE and BChE.^c IC₅₀ of reference compound for BACE-1.

The AChE and BChE inhibitory activities were measured by continuous colorimetric determination method [64], in the presence of 0.5 mM acetylthiocholine iodide (ACTI) and butyrylthiocholine iodide (BTCl) as substrates, respectively, for 15 min at 412 nm using UV/Vis spectrophotometer (OPTIGEN POP, K LAB, Daejeon, Korea) [65,66]. After adding the substrate, 0.5 mM 5,5-dithiobis (2-nitrobenzoic acid) (DTNB) was added as the color development solution. The BACE-1 inhibitory activity was evaluated by β -secretase (BACE1) activity detection kit (Sigma-Aldrich, St. Louis, Mo, USA) using a fluorescence spectrometer (FS-2, Scinco, Seoul, Korea) [67].

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