

## Supplementary Data

### Synthesis, Characterization, *In Vitro* and *In Silico* Studies of Novel Lophine Clubbed Acylthioureas

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**ABA Series**  
**(Lophine Clubbed Acylthioureas (8a-l))**

<b>Compound Code</b>	<b>Compound No.</b>
<b>ABA-1</b>	<b>8a</b>
<b>ABA-2</b>	<b>8b</b>
<b>ABA-3</b>	<b>8c</b>
<b>ABA-4</b>	<b>8d</b>
<b>ABA-5</b>	<b>8e</b>
<b>ABA-6</b>	<b>8f</b>
<b>ABA-7</b>	<b>8g</b>
<b>ABA-8</b>	<b>8h</b>
<b>ABA-9</b>	<b>8i</b>
<b>ABA-10</b>	<b>8j</b>
<b>ABA-11</b>	<b>8k</b>
<b>ABA-12</b>	<b>8l</b>

ABA 1

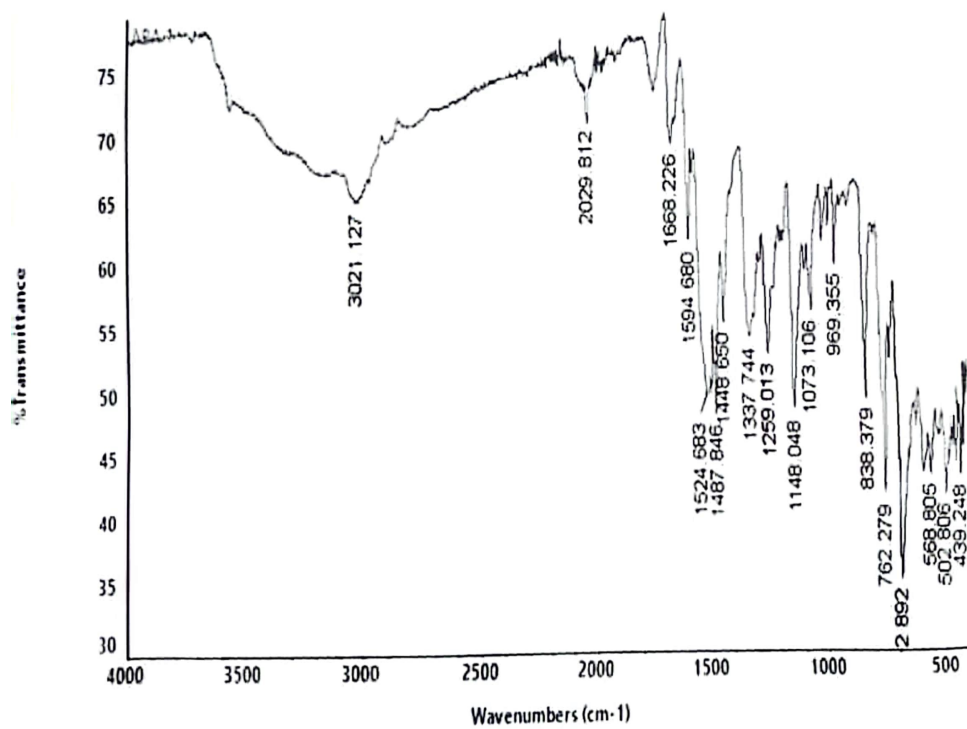
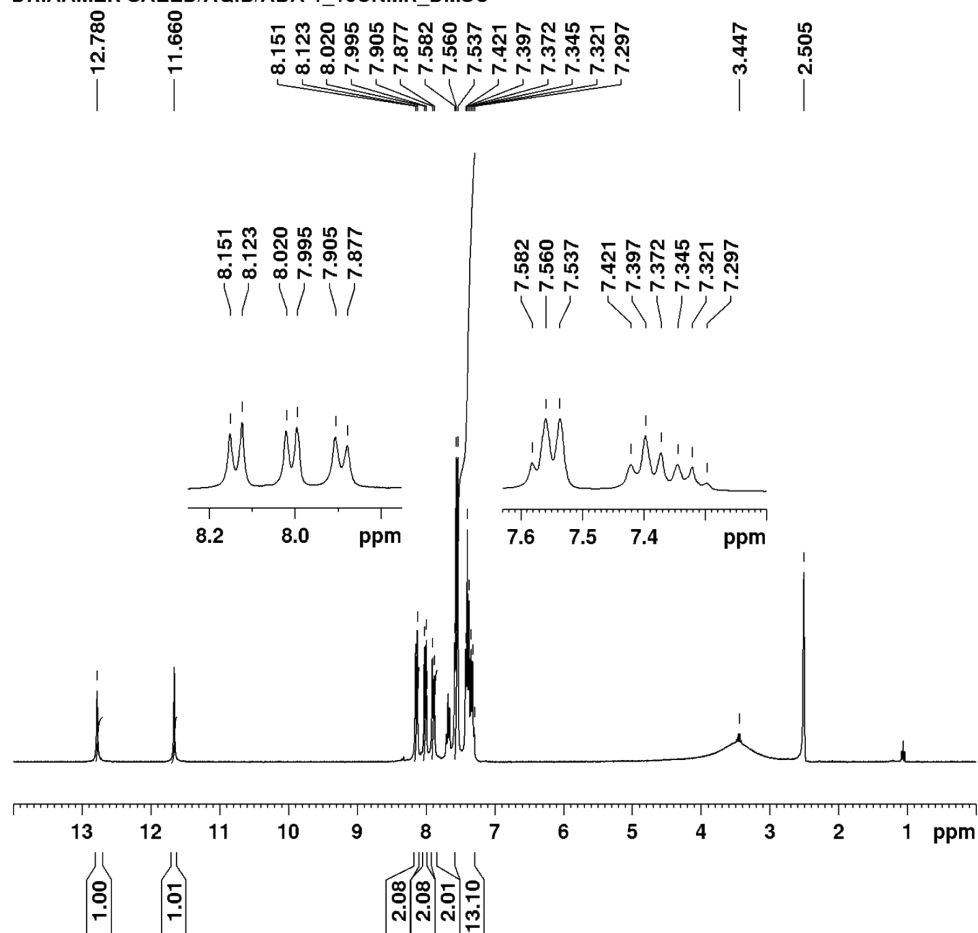


Figure S1. FTIR Spectrum of ABA-1.

DR.AAMER SAEED/AQIB/ABA-1\_13CNMR\_DMSO



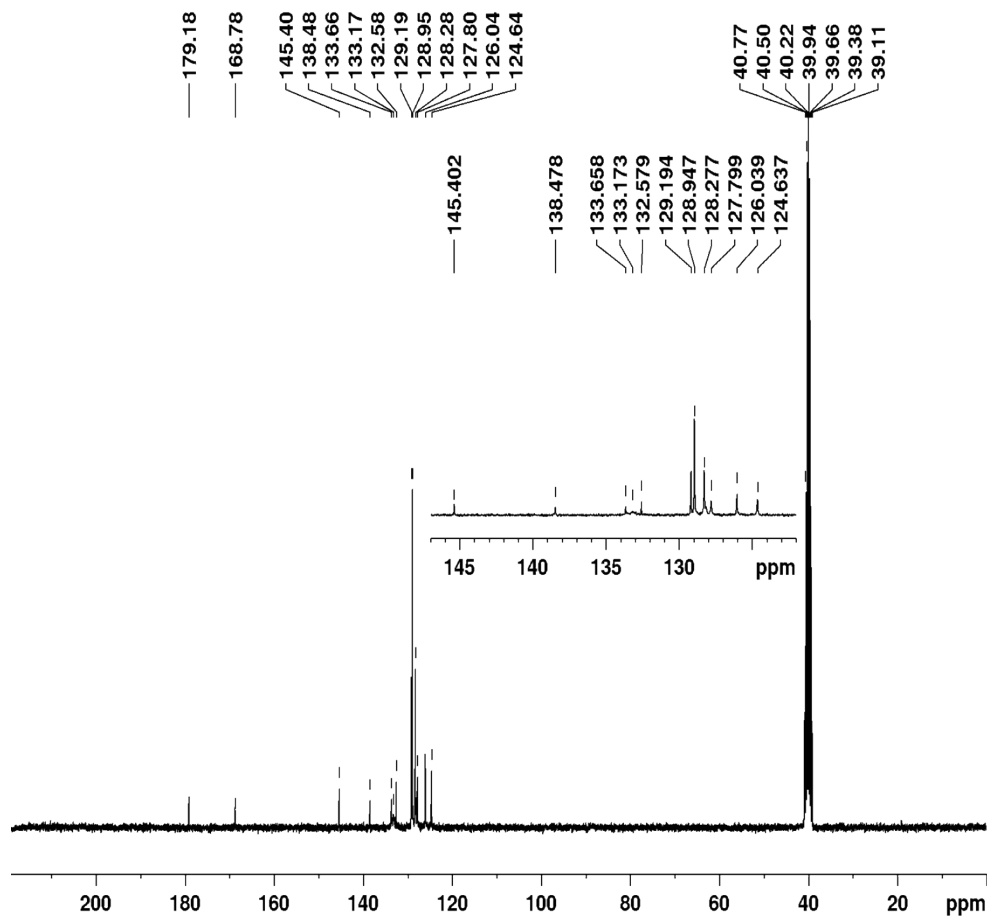
Current Data Parameters  
NAME ABA-1\_1HNMR\_DMSO  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231006  
Time 16.30  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 0  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084159 sec  
RG 203.2  
DW 81.000 usec  
DE 6.00 usec  
TE 293.3 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.00 usec  
PL1 2.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S2. <sup>1</sup>H-NMR Spectrum of ABA-1.



Current Data Parameters  
 NAME ABA-1\_13CNMR\_DMSO  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20231006  
 Time 16.22  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 35968  
 SOLVENT DMSO  
 NS 1024  
 DS 0  
 SWH 17985.611 Hz  
 FIDRES 0.500045 Hz  
 AQ 0.9999104 sec  
 RG 2048  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 293.8 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.88999998 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 6.00 usec  
 PL1 -5.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 20.98 dB  
 PL13 20.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Figure S3. <sup>13</sup>C-NMR Spectrum of ABA-1.

ABA 2

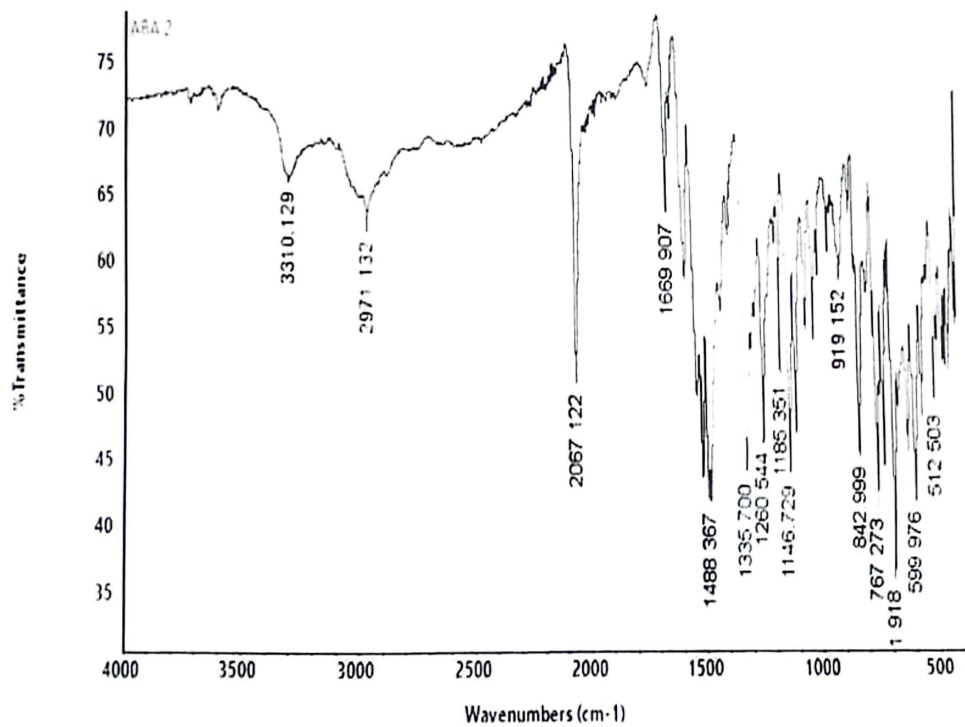
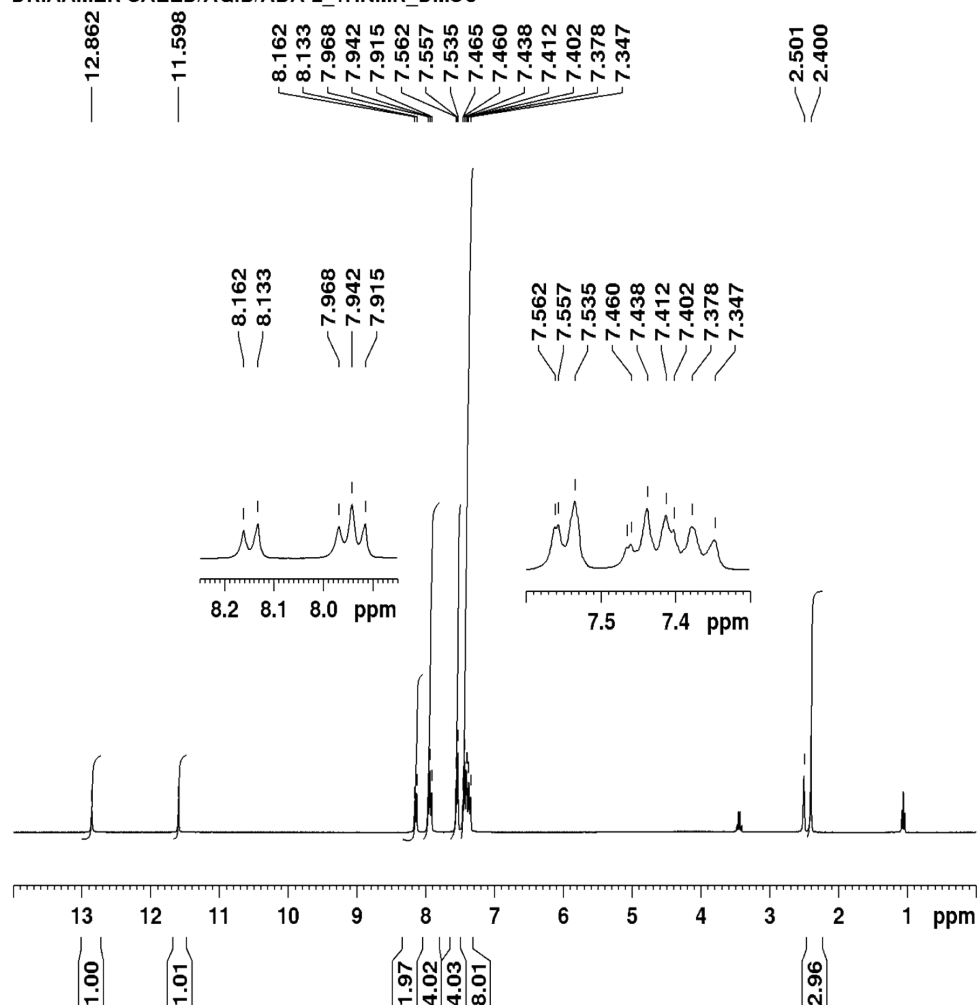


Figure S4. FTIR Spectrum of ABA-2.

DR.AAMER SAEED/AQIB/ABA-2\_1HNMR\_DMSO



Current Data Parameters  
NAME ABA-2\_1HNMR\_DMSO  
EXPNO 1  
PROCNO 1

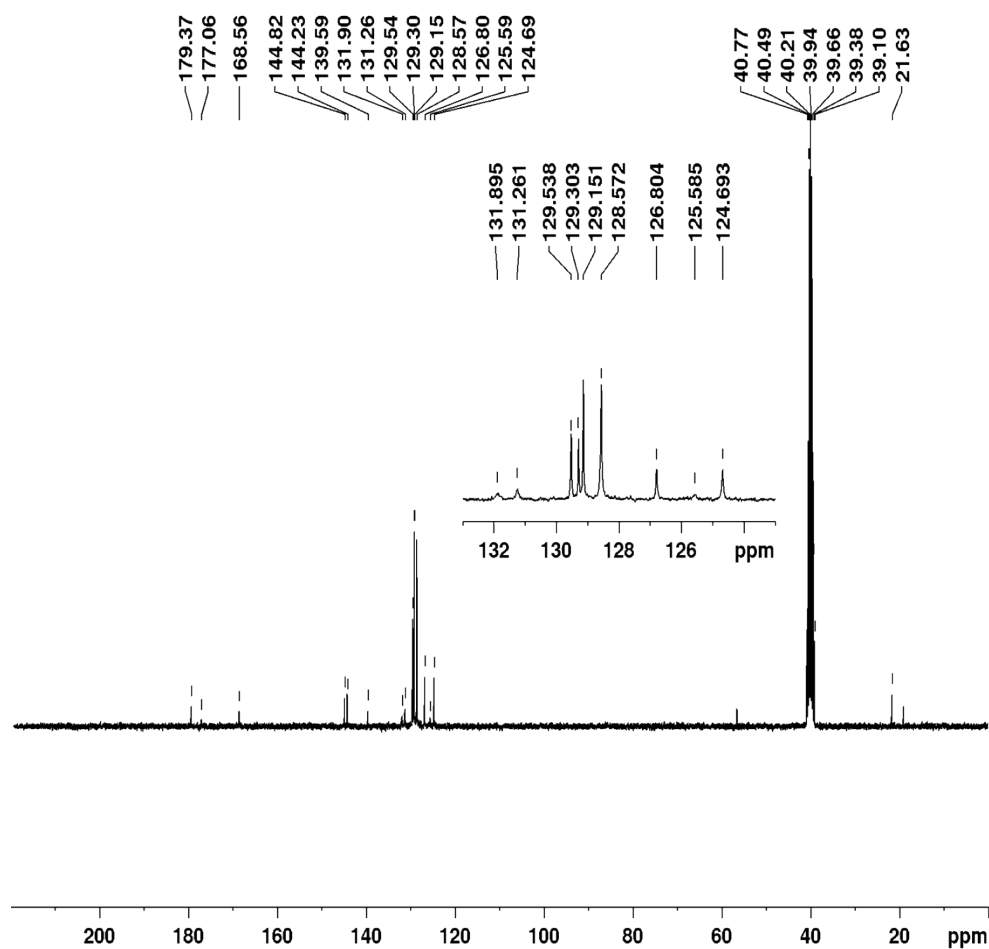
F2 - Acquisition Parameters  
Date\_ 20231020  
Time 15.13  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 0  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084159 sec  
RG 181  
DW 81.000 usec  
DE 6.00 usec  
TE 292.5 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.00 usec  
PL1 2.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S5. <sup>1</sup>H-NMR Spectrum of ABA-2.

DR.AAMER SAEED/AQIB/ABA-2\_13CNMR\_DMSO



Current Data Parameters  
NAME ABA-2\_13CNMR\_DMSO  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231020  
Time 14.05  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zgpg30  
TD 35968  
SOLVENT DMSO  
NS 1024  
DS 0  
SWH 17985.611 Hz  
FIDRES 0.500045 Hz  
AQ 0.9999104 sec  
RG 32768  
DW 27.800 usec  
DE 6.00 usec  
TE 293.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 6.00 usec  
PL1 -5.00 dB  
SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 2.00 dB  
PL12 20.98 dB  
PL13 20.00 dB  
SFO2 300.1312005 MHz

F2 - Processing parameters  
SI 32768  
SF 75.4677490 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Figure S6. <sup>13</sup>C-NMR Spectrum of ABA-2.

ABA 3

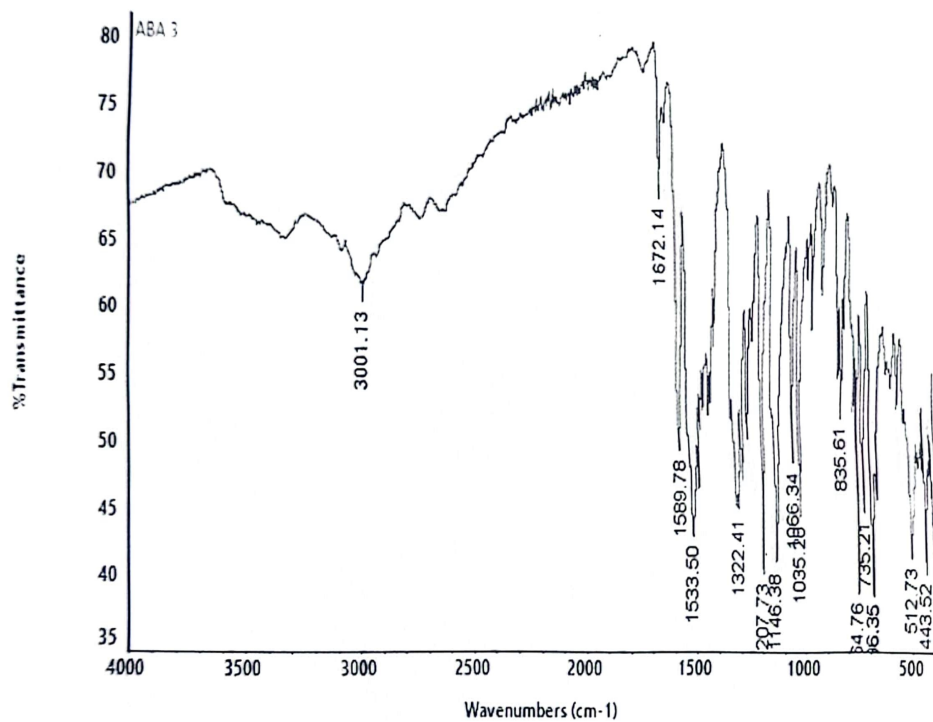
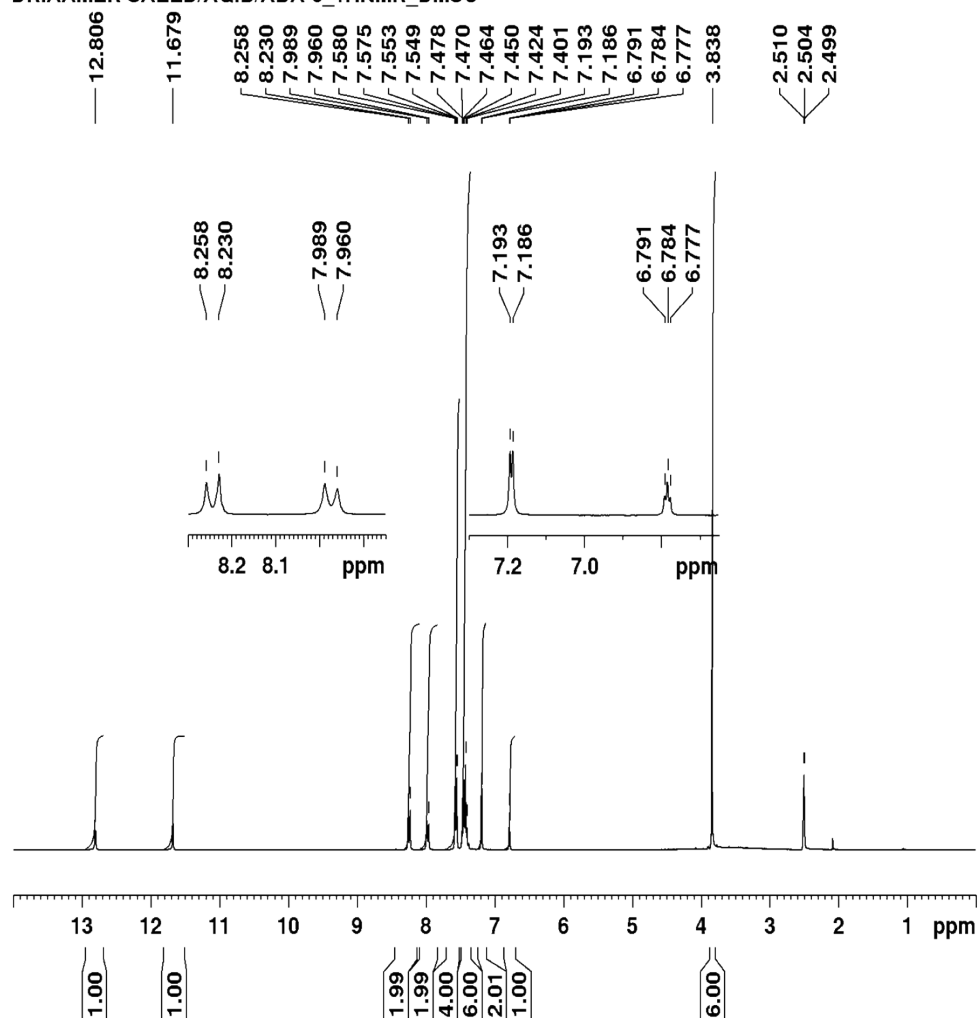


Figure S7. FTIR Spectrum of ABA-3.

DR.AAMER SAEED/AQIB/ABA-3\_1HNMR\_DMSO



Current Data Parameters  
NAME ABA-3\_1HNMR\_DMSO  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231202  
Time 15.51  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 0  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084159 sec  
RG 287.4  
DW 81.000 usec  
DE 6.00 usec  
TE 294.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.00 usec  
PL1 2.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S8. <sup>1</sup>H-NMR Spectrum of ABA-3.

DR.AAMER SAEED/AQIB/ABA-3\_13CNMR\_DMSO

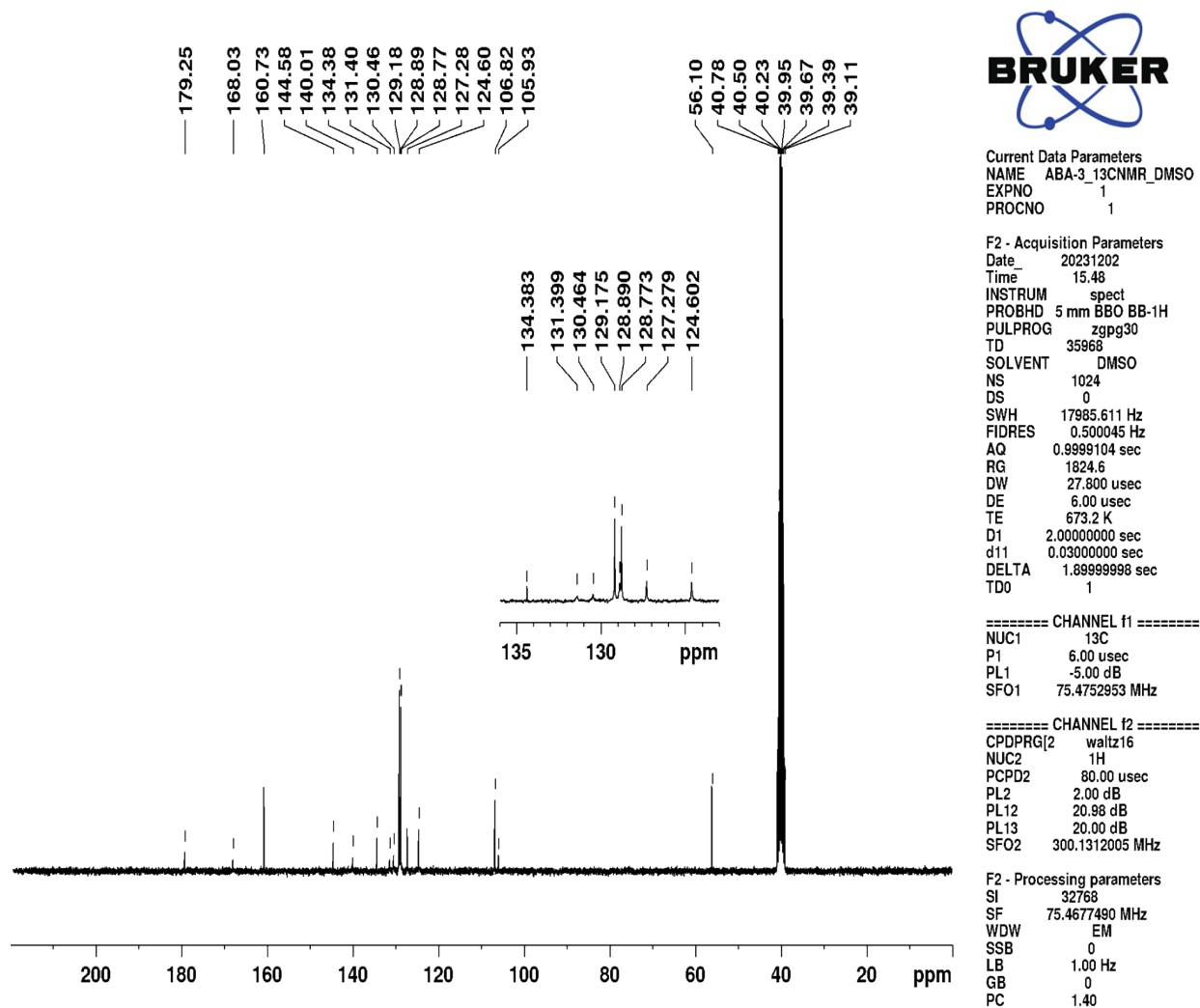


Figure S9. <sup>13</sup>C-NMR Spectrum of ABA-3.

ABA 4

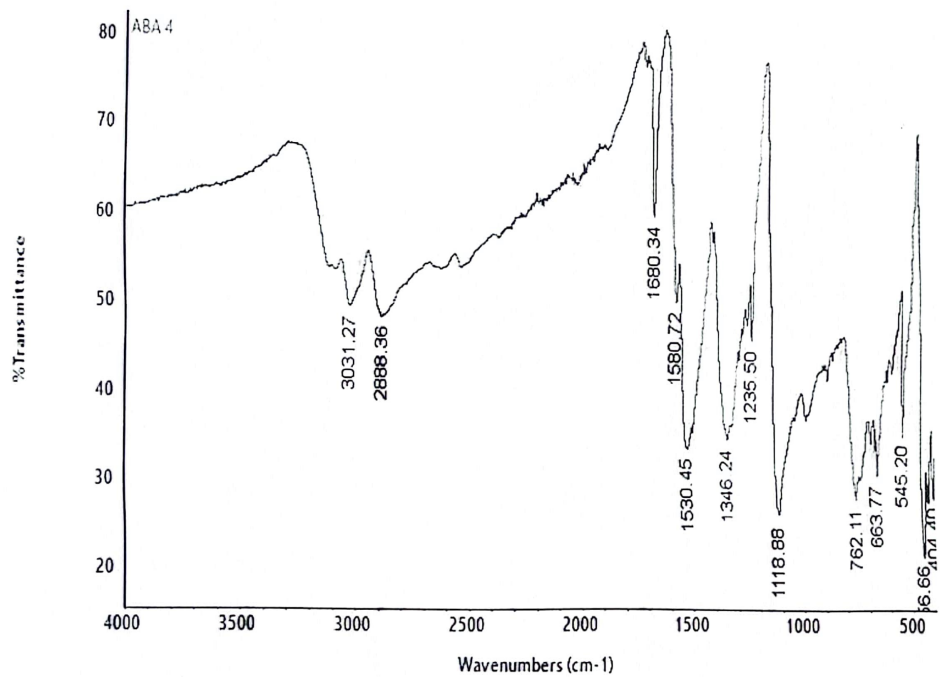
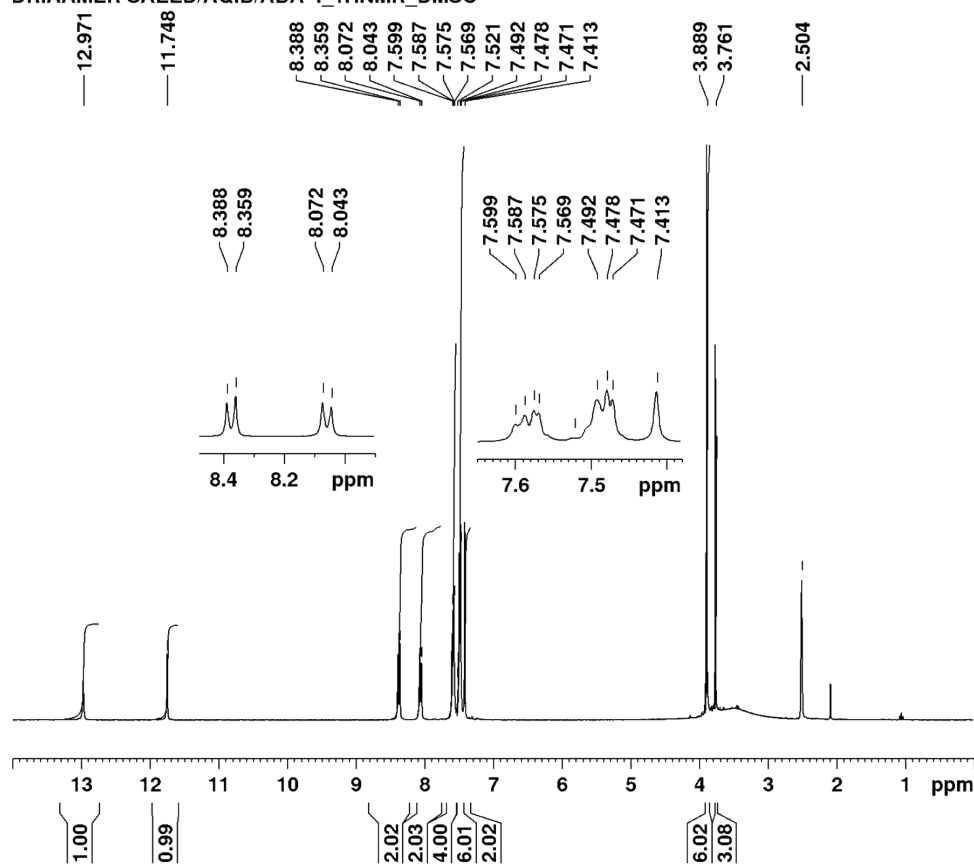


Figure S10. FTIR Spectrum of ABA-4.

DR.AAMER SAEED/AQIB/ABA-4\_1HNMR\_DMSO



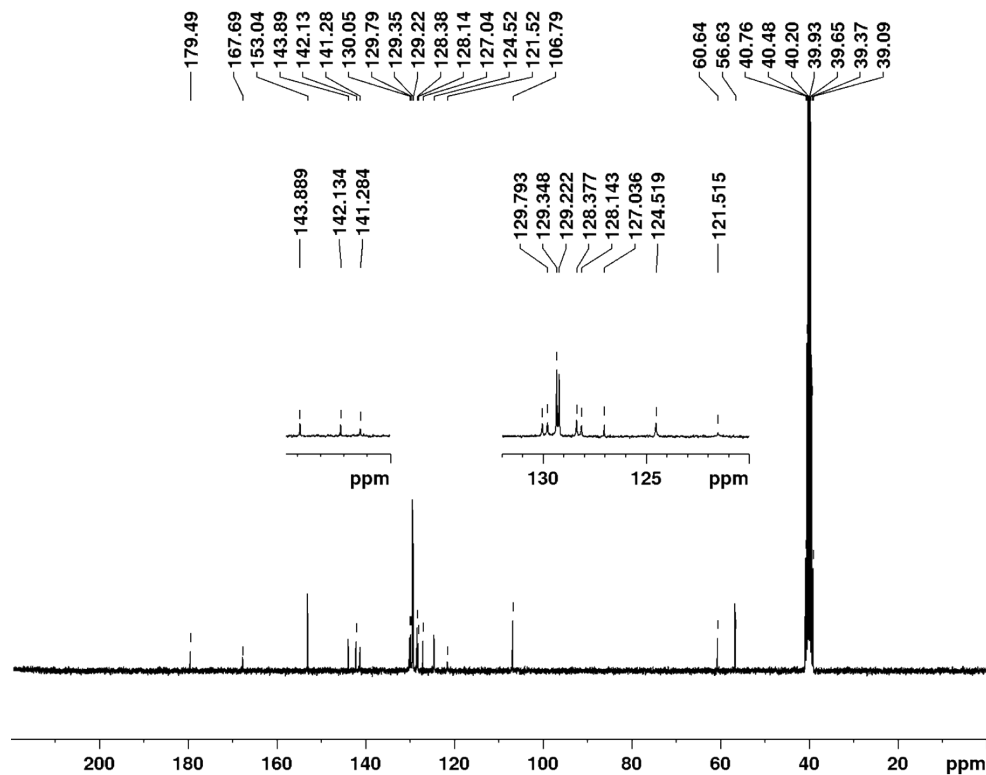
Current Data Parameters  
NAME ABA-4\_1HNMR\_DMSO  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20231119  
Time 12.05  
INSTRUM spect  
PROBHD 5 mm BBO BB-1H  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 8  
DS 0  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
AQ 5.3084159 sec  
RG 181  
DW 81.000 usec  
DE 6.00 usec  
TE 293.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.00 usec  
PL1 2.00 dB  
SFO1 300.1318534 MHz

F2 - Processing parameters  
SI 32768  
SF 300.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Figure S11. <sup>1</sup>H-NMR Spectrum of ABA-4.



Current Data Parameters  
 NAME ABA-4\_13CNMR\_DMSO  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20231119  
 Time 11.58  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 35968  
 SOLVENT DMSO  
 NS 1024  
 DS 0  
 SWH 17985.611 Hz  
 FIDRES 0.500045 Hz  
 AQ 0.9999104 sec  
 RG 32768  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 293.5 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 DELTA 1.8999998 sec  
 TD0 1

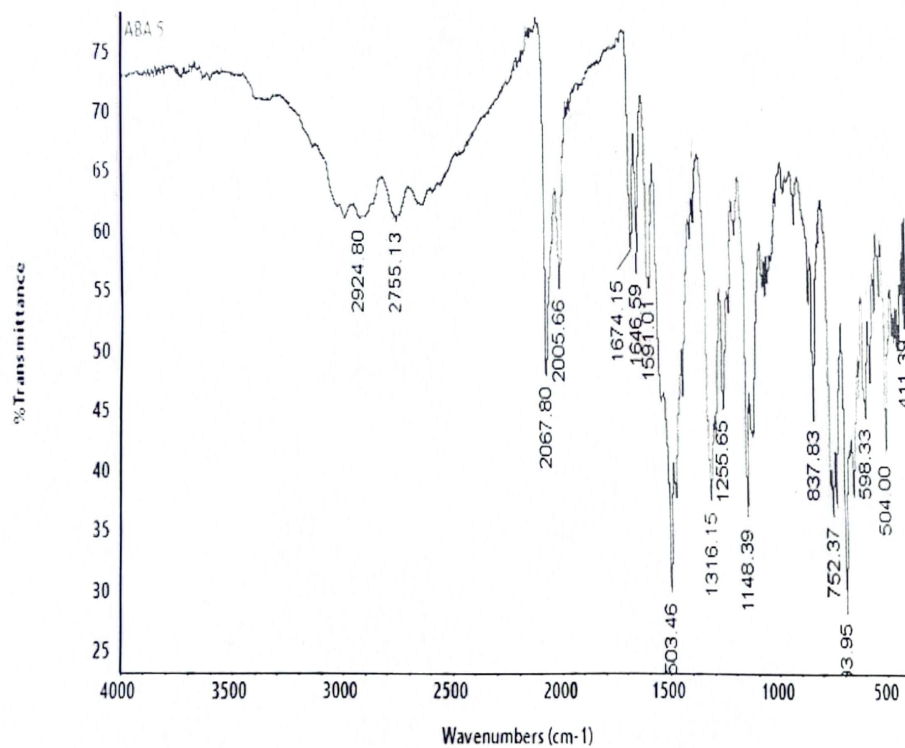
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 6.00 usec  
 PL1 -5.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 20.98 dB  
 PL13 20.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

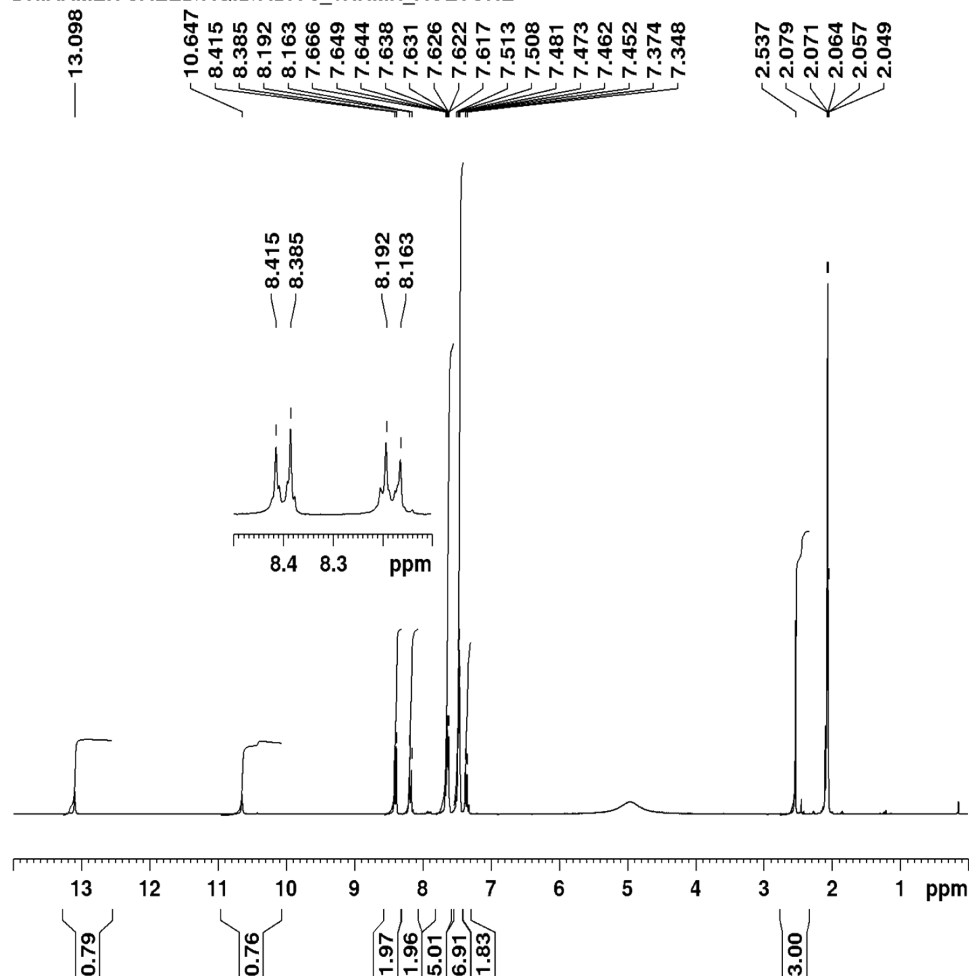
Figure S12. <sup>13</sup>C-NMR Spectrum of ABA-4.

ABA 5



**Figure S13.** FTIR Spectrum of ABA-5.

DR.AAMER SAEED/AQIB/ABA-5\_1HNMR\_ACETONE



Current Data Parameters  
 NAME ABA-5\_1HNMR\_ACETONE  
 EXPNO 1  
 PROCNO 1

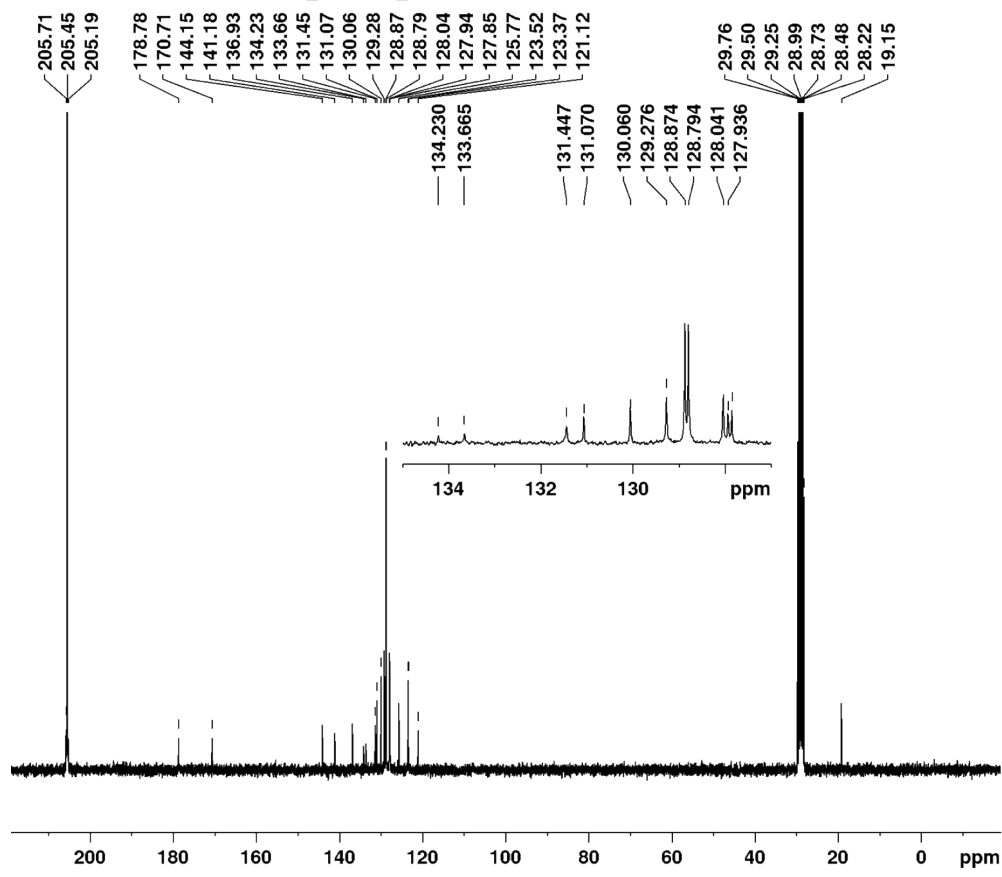
F2 - Acquisition Parameters  
 Date\_ 20231212  
 Time 16.06  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 65536  
 SOLVENT Acetone  
 NS 8  
 DS 0  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084159 sec  
 RG 362  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 292.7 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 9.00 usec  
 PL1 2.00 dB  
 SFO1 300.1316534 MHz

F2 - Processing parameters  
 SI 32768  
 SF 300.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Figure S14. <sup>1</sup>H-NMR Spectrum of ABA-5.

DR.AAMER SAEED/AQIB/ABA-5 <sup>13</sup>CNMR\_ACETONE



Current Data Parameters  
 NAME ABA-5 <sup>13</sup>CNMR\_ACETONE  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20231212  
 Time 15.59  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 35968  
 SOLVENT Acetone  
 NS 1024  
 DS 0  
 SWH 17985.611 Hz  
 FIDRES 0.500045 Hz  
 AQ 0.9999104 sec  
 RG 8192  
 DW 27.900 usec  
 DE 6.00 usec  
 TE 293.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TDO 1

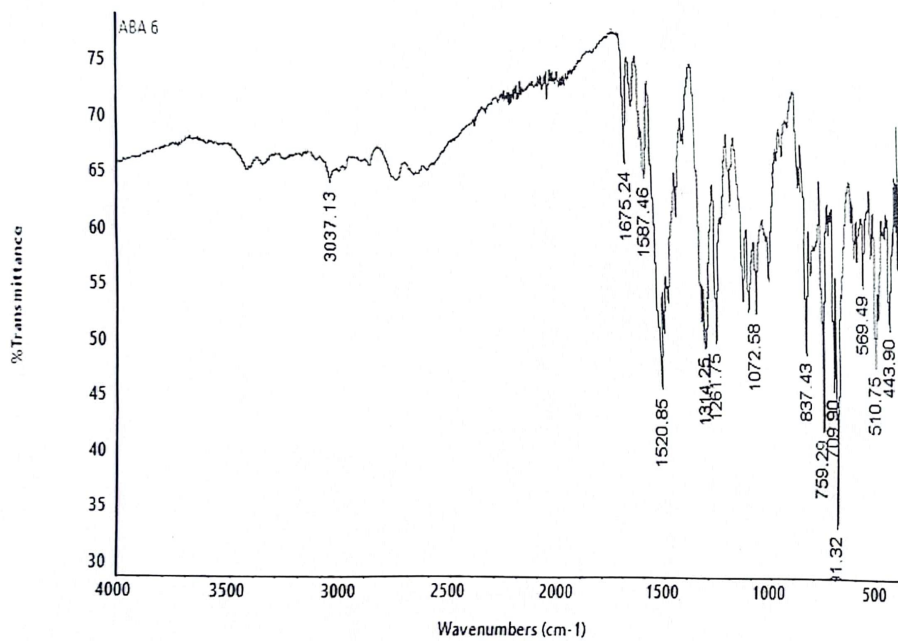
===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 6.00 usec  
 PL1 -5.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 80.00 usec  
 PL2 2.00 dB  
 PL12 20.96 dB  
 PL13 20.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

Figure S15. <sup>13</sup>C-NMR Spectrum of ABA-5.

ABA 6



**Figure S16.** FTIR Spectrum of ABA-6.

ABA 7

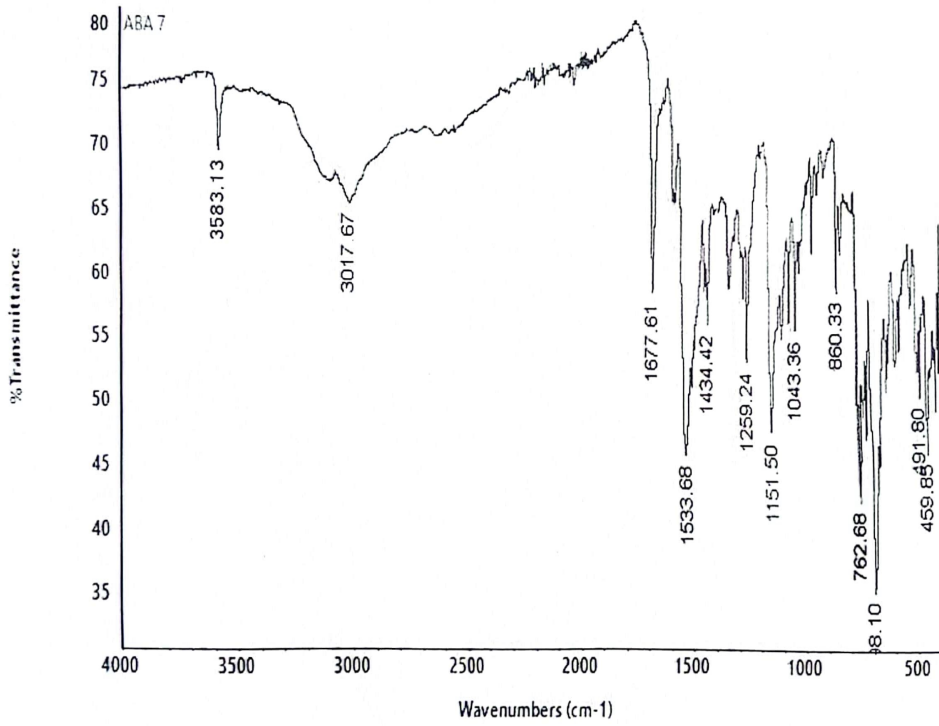
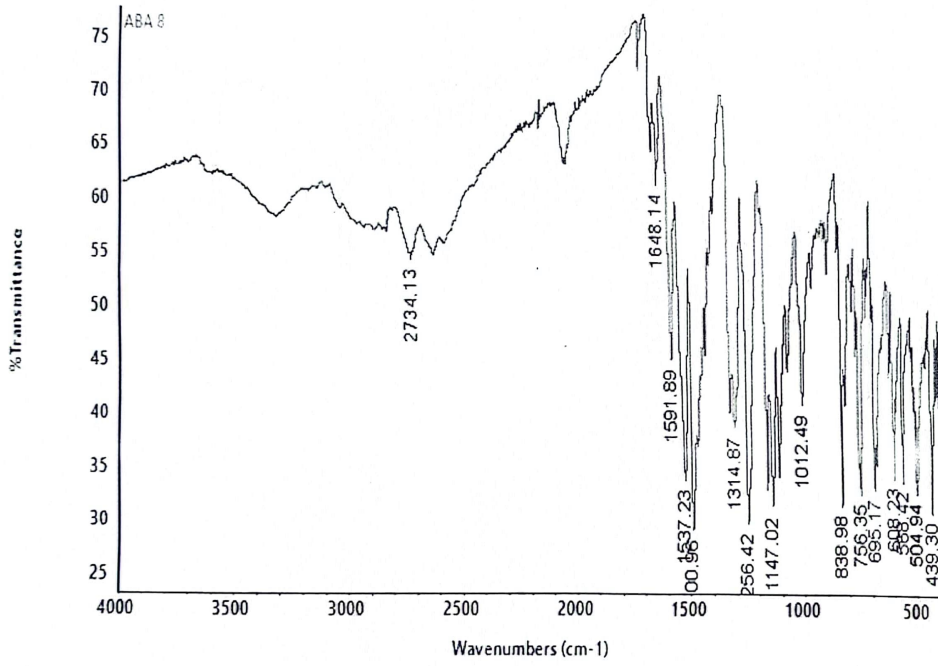


Figure S17. FTIR

ABA 8



Spectrum of ABA-7.

**Figure S18.** FTIR Spectrum of ABA-8.

ABA 9

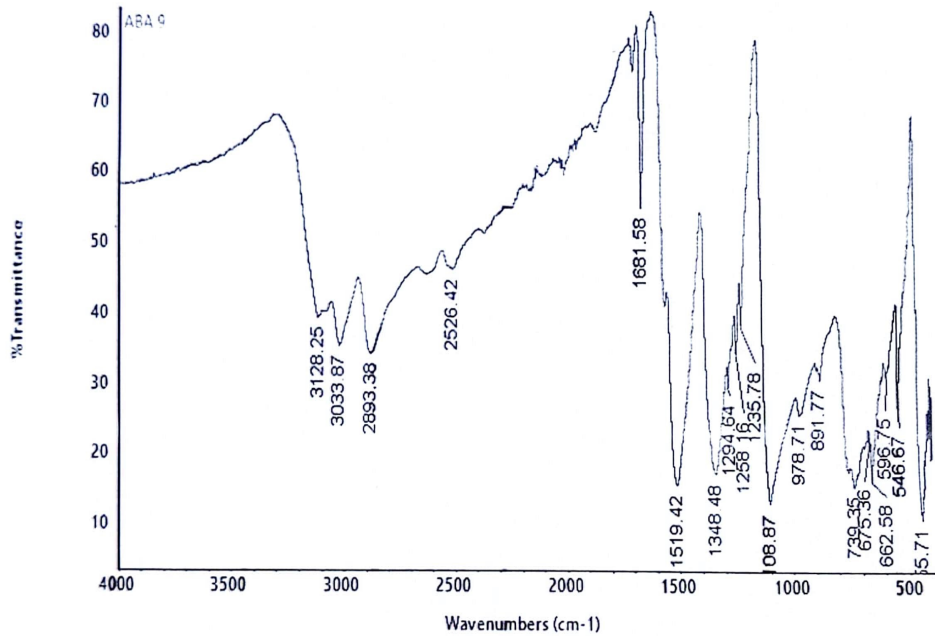


Figure S19. FTIR Spectrum of ABA-9.

ABA 10

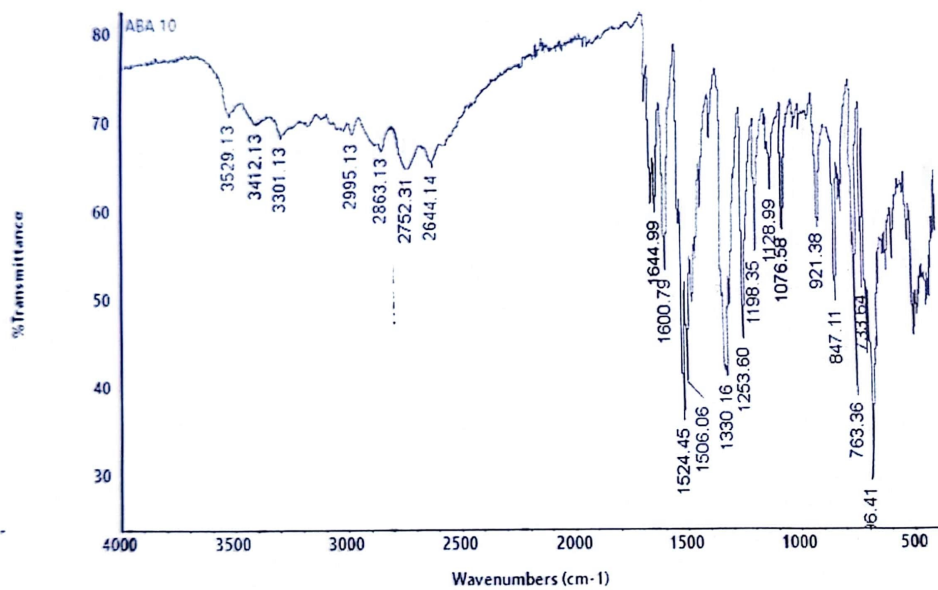
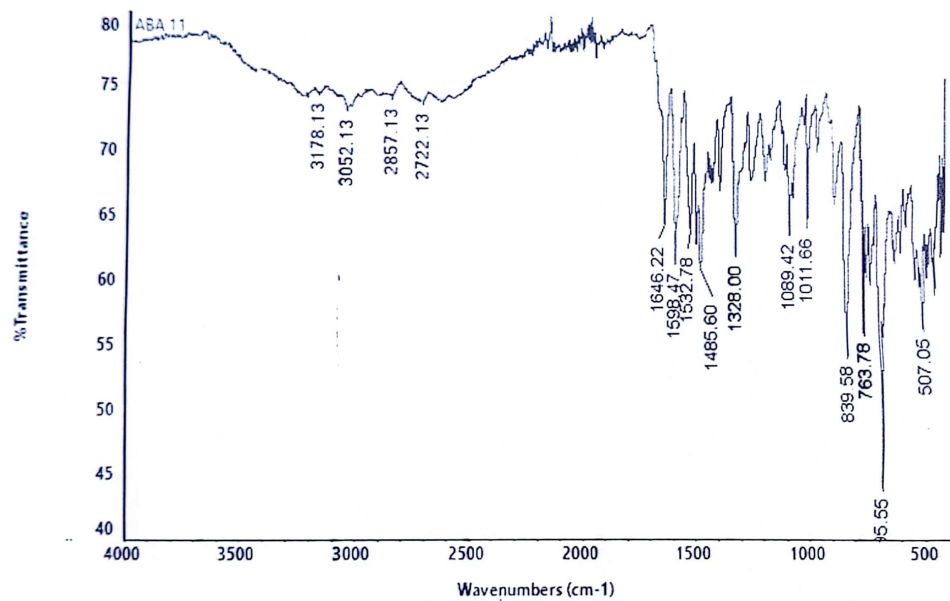


Figure S20. FTIR Spectrum of ABA-10.

ABA 11



**Figure S21.** FTIR Spectrum of ABA-11.

ABA 12

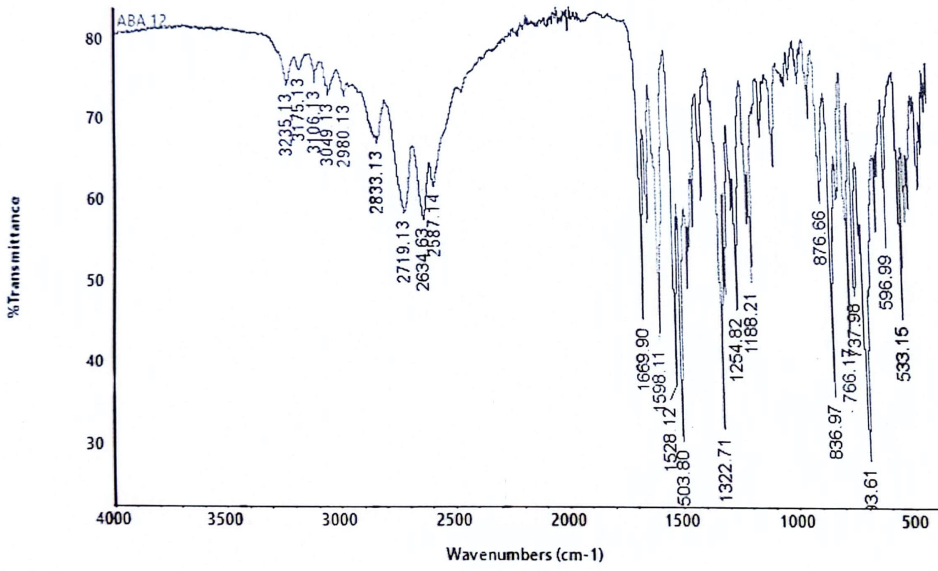


Figure S22. FTIR Spectrum of ABA-12.