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Supporting information

Iodine -Mediated C-N and C-S bond formation: Regioselective synthesis of benzo [4,5]imidazo [2,1-*b*] thiazoles.

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1. General methods

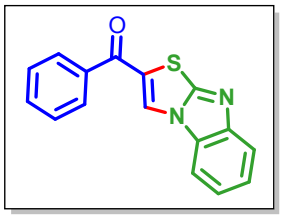
The melting points were measured in open capillary tubes and are uncorrected. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker (Avance) 300 MHz NMR instrument using TMS as internal standard either $CDCl_3$ or DMSO-d_6 as solvent. Chemical shifts are given in parts per million (δ-scale) and the coupling constants are given in hertz (Hz). Silica gel-G plates (Merck) were used for thin layer chromatography (TLC) analysis with a mixture of petroleum ether (60-80 °C) and ethyl acetate as eluent. The single crystal X-ray data were collected on BRUKER GADDS X-ray (three-circle) diffractometer with Mo Ka(k= 1.5418 A˚) radiation. Elemental analyses were performed on a vario EL III CHNS elemental analyzer. Mass spectra were recorded in LCQ Fleet mass spectrometer, Thermo Fisher Instruments Limited, US. Electrospray ionization mass spectrometry (ESI-MS) analysis was performed in the positive ion and negative ion mode on a liquid chromatography ion trap.

2. General experimental procedure for SA-1:

A mixture of 2-mercaptobenzimidazole 1 (1.0 equiv), (E)-1-(4-aryl)-3-(dimethylamino)-prop-2-en-1-one 2 (1.0 equiv), and iodine (1.0equiv) was added to 5 mL of acetic acid under open air at room temperature for 2 h. The completion of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was poured into water and workup with sodium thiosulfate and the solution was extracted with ethyl acetate. The combined organic phase was dried over Na_2SO_4 and then the solvent was removed. The crude sample was purified by column chromatography.

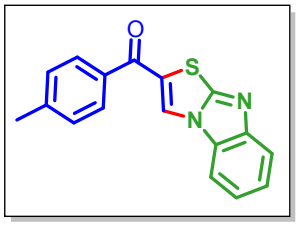
3. Spectral data

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(phenyl)methanone (SA-1)



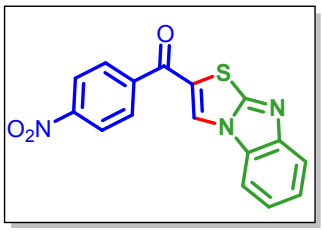
White solid, mp; 142-44 °C; 1H NMR (300 MHz, $CDCl_3$) δ: 8.22 (s, 1H), 7.86 (d, *J* = 8.1 Hz, 2H), 7.77 (d, *J* = 8.1 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 2H), 7.57 (t, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.28 (t, *J* = 7.2 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 187.2, 156.7, 148.6, 137.0, 133.1, 130.0, 129.5, 129.0, 128.7, 125.1, 122.0, 122.0, 119.7, 110.8 ppm. MS m/z 279.1 $(M+1)^+$. Anal. Calcd for $C_{16}H_{10}N_2O_2S$: C, 69.05; H, 3.62; N, 10.07; found C, 69.01; H, 3.59; N, 10.04.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(p-tolyl)methanone (SA-2)



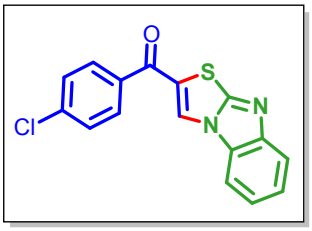
White solid, mp; 155-57 °C; 1H NMR (300 MHz, $CDCl_3$) *δ*: 8.21 (s, 1H), 7.77 (d, *J* = 8.1 Hz, 3H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.42-7.34 (m, 3H), 7.26 (t, *J* = 7.5 Hz, 1H), 2.47 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 186.8, 156.7, 148.5, 144.0, 134.3, 130.2, 129.7, 128.8, 125.0, 121.9, 119.6, 110.7, 21.79 ppm. MS m/z 292.3560 $(M)^+$. Anal. Calcd for $C_{17}H_{12}N_2OS$: C, 69.84; H, 4.14; N, 9.58; found C, 69.81; H, 4.11; N, 9.54.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(4-nitrophenyl)methanone (SA-3)

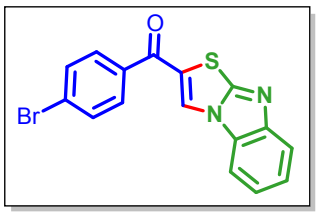


Yellow solid, mp; 190-92 °C; 1H NMR (300 MHz, $CDCl_3$) δ: 8.73 (s, 1H), 8.54 (d, *J* = 8.1 Hz, 2H), 8.28 (s, 1H), 8.23 (d, *J* = 8.1 Hz, 2H), 7.82 (m, 2H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.8 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 185.6, 150.7, 128.5, 124.7, 123.3, 121.5, 120.1, 119.7, 117.6, 116.6, 114.2, 105.1, 104.6 ppm. MS m/z 323.03 $(M+1)^+$. Anal. Calcd for $C_{16}H_9N_3O_3S$: C, 59.44; H, 2.81; N, 13.00; found C, 59.41; H, 2.78; N, 12.97**.**

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(4-chlorophenyl)methanone (SA-4)



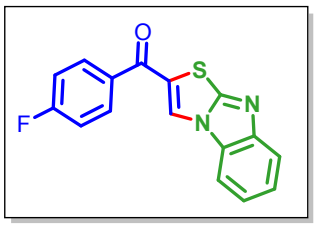
White solid, mp; 177-79 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.25 (s, 1H), 7.83-7.63 (m, 3H), 7.68 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.5 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 185.9, 156.6, 148.6, 139.5, 135.2, 130.0, 129.7, 129.5, 129.34, 125.4, 125.2, 122.1, 119.7, 110.8 ppm. MS m/z 313.18 $(M+1)^+$. Anal. Calcd for $C_{16}H_9ClN_2OS$: C, 61.44; H, 2.90; N, 8.96; found C, 61.41; H, 2.88; N, 8.93.



benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(4-bromophenyl)methanone (SA-5)

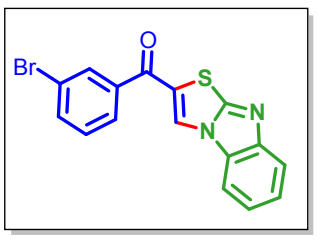
White solid, mp; 208-10 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.64 (s, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.62 (d, *J* = 8.7 Hz, 2H), 7.56-7.52 (m, 3H), 7.24 (t, *J* = 8.1 Hz, 1H) 7.10 (t, *J* = 8.1 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 185.6, 155.8, 147.2, 135.0, 131.7, 130.0, 129.2, 129.0, 127.4, 127.2, 124.7, 121.7, 118.5, 111.5 ppm. MS m/z 357.0 $(M+1)^+$. Anal. Calcd for $C_{16}H_9BrN_2OS$: C, 53.80; H, 2.54; N, 7.54; found C, 53.77; H, 2.51; N, 7.51.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(4-flurophenyl)methanone (SA-6)



White solid, mp; 180-82°C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.43 (s, 1H), 7.42-7.38 (m, 3H), 7.07 (d, *J* = 7.8 Hz, 1H) 6.79 (t, *J* = 7.8 Hz, 1H), 6.75 - 6.66 (m, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 184.2, 164.1 (d, $^1J_{C\text{-}F}$ =251.8 Hz), 155.0, 146.8, 131.9, 130.4 (d, $^3J_{C\text{-}F}$ = 9 Hz), 128.7, 127.9, 126.8, 123.7, 120.7, 117.6, 114.8 (d, $^2J_{C\text{-}F}$ = 21.8 Hz), 111.1 ppm. MS m/z 297.13 $(M+1)^+$. Anal.Calcd for $C_{16}H_9FN_2OS$: C, 64.85; H, 3.06; N, 9.45; found C, 64.81; H, 3.03; N, 9.41**.**

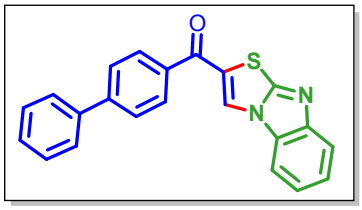
benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(3-bromophenyl)methanone (SA-7)



White solid, mp; 163-65 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.38 (s, 1H), 8.11(s, 1H), 7.91 (d, *J* = 7.8 Hz, 2H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.60 - 7.55 (m, 2H), 7.45 (t, *J* = 7.5 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 185.6, 138.8, 136.0, 131.6, 130.7, 129.8, 127.2, 125.6, 125.5, 123.3, 122.4, 119.8,

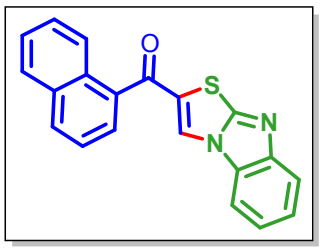
111.1 ppm. MS m/z 358.98 $(M+1)^+$. Anal. Calcd for $C_{16}H_9BrN_2OS$: C, 53.80; H, 2.54; N, 7.84; found C, 53.76; H, 2.51; N, 7.81.

[1,1'-biphenyl]-4-yl(benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl)methanone (SA-8)



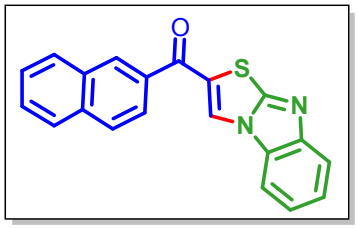
Brown solid, mp; 157-59 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.41 (s, 1H), 8.07 (d, *J* = 7.8 Hz, 2H), 7.92-7.87 (m, 3H), 7.83-7.73 (m, 3H), 7.64-7.51 (m, 4H), 7.43 (t, *J* = 7.5 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 186.9, 157.3, 148.9, 146.3, 139.9, 136.0, 130.6, 129.6, 129.4, 129.4, 128.8, 127.9, 127.6, 127.6, 125.4, 122.3, 120.0, 111.1 ppm. MS m/z 353.07 $(M-1)^-$. Anal. Calcd for $C_{22}H_{14}N_2OS$: C, 74.55; H, 3.98; N, 7.90; found C, 74.52; H, 3.95; N, 7.87.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(naphthalen-1-yl)methanone (SA-9)



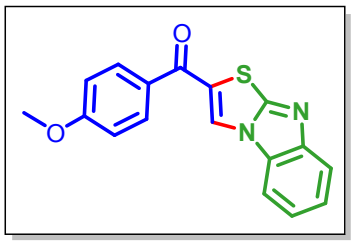
White solid, mp; 203-05 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.17 (s, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 7.95-7.93 (m, 1H), 7.83 (t, *J* = 7.5 Hz, 2H), 7.66 (m, 4H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 188.2, 134.4, 134.0, 133.0, 132.3, 130.4, 129.1, 128.6, 128.0, 127.3, 127.1, 126.6, 125.8, 125.1, 124.4, 122.7, 119.0, 111.2 ppm. MS m/z 329.11 $(M+1)^+$. Anal. Calcd for $C_{20}H_{12}N_2OS$: C, 73.15; H, 3.68; N, 8.53; found C, 73.12; H, 3.66; N, 8.50.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(naphthalen-2-yl)methanone (SA-10)



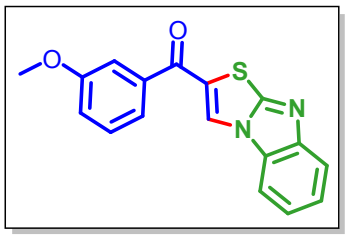
White solid, mp; 212-14 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.43 (s, 1H), 8.33 (s, 1H), 8.06-8.03 (m, 2H), 7.97 (t, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 7.8 Hz, 1H), 7.72-7.64 (m, 3H), 7.47 (t, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.8, 161.2, 152.7, 140.1, 138.9, 137.2, 135.2, 134.5, 133.7, 133.5, 132.6, 132.0, 129.8, 129.5, 126.8, 123.6, 117.2 ppm. MS m/z 329.09 $(M+1)^+$. Anal. Calcd for $C_{20}H_{12}N_2OS$: C, 73.15; H, 3.68; N, 8.53; found C, 73.11; H, 3.65; N, 8.50.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(4-methoxyphenyl)methanone (SA-11)



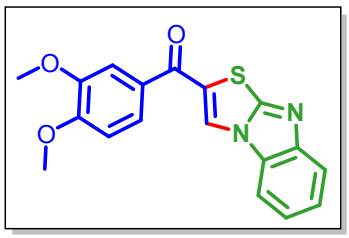
White solid, mp; 161-63 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.25 (s, 1H), 7.91(d, *J* = 8.4 Hz, 2H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 2H), 7.31 (t, *J* = 7.5 Hz, 1H), 3.92 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ:185.6, 163.7, 156.5, 148.4, 131.0, 130.2, 129.5, 124.9, 124.5, 121.9, 119.5, 114.2, 110.8, 55.6 ppm. MS m/z 309.13 $(M+1)^+$. Anal. Calcd for $C_{17}H_{12}N_2O_2S$: C, 66.22; H, 3.92; N, 9.08; found C, 66.18; H, 3.89; N, 9.04.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(3-methoxyphenyl)methanone (SA-12)

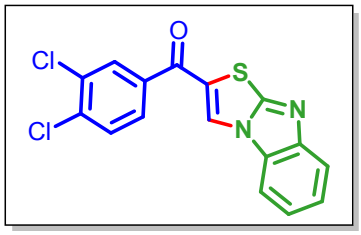


White solid, mp; 170-72 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.29 (s, 1H), 8.01 (s, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.44 (broad, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 3.97 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ:185.6, 153.6, 149.6, 130.0, 129.7, 125.0, 124.5, 123.2, 121.9, 119.7, 113.3, 110.7, 110.3, 56.2 ppm. Anal. Calcd for $C_{17}H_{12}N_2O_2S$: C, 66.22; H, 3.92; N, 9.08; found C, 66.18; H, 3.89; N, 9.04.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(3,4-dimethoxyphenyl)methanone (SA-13)



White solid, mp; 127-29 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.29 (s, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.44 (broad, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 4.00 (s, 3H), 3.97 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ:185.7, 156.8, 153.6, 149.7, 148.5, 130.1, 129.8, 129.6, 125.0, 124.5, 123.3, 122.0, 119.7, 111.3, 110.8, 110.3, 56.3, 56.3 ppm. MS m/z 339.30 $(M+1)^+$. Anal. Calcd for $C_{18}H_{14}N_2O_3S$: C, 63.89; H, 4.17; N, 8.28; found C, 63.86; H, 4.15; N, 8.25.

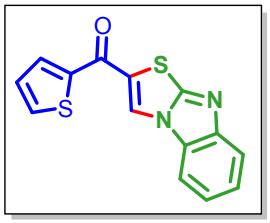


benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(3,4-dichlorophenyl)methanone (SA-14)

Yellow solid, mp; 127-29 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.26 (s, 1H), 7.96 (s, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.72

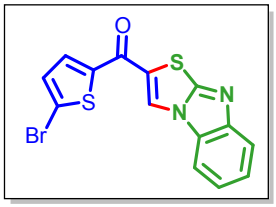
- 7.64 (m, 3H), 7.46 (t, J = 7.5 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 184.7, 156.6, 148.8, 137.8, 136.7, 133.9, 131.2, 130.6, 129.6, 129.4, 127.7, 125.6, 125.4, 122.3, 120.0, 110.9 ppm. Anal. Calcd for $C_{16}H_8Cl_2N_2OS$: C, 55.35; H, 2.32; N, 8.07; found C, 55.31; H, 2.30; N, 8.04.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(thiophen-2-yl)methanone (SA-15)



Yellow solid, mp; 185-87 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.52 (s, 1H), 7.96 (d, J = 3.9 Hz, 1H), 7.80 (t, J = 8.1 Hz, 2H), 7.74 (d, J = 7.8 Hz,1H), 7.44 (t, J = 7.8 Hz,1H), 7.35 (t, J = 7.8 Hz,1H), 7.28(m, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 177.6, 156.5, 148.6, 141.3, 134.2, 132.9, 129.6, 129.3, 128.5, 125.1, 123.8, 122.1, 119.7, 110.9 ppm. MS m/z 285.0 $(M+1)^+$. Anal. Calcd for $C_{14}H_8N_2OS_2$: C, 62.85; H, 3.23; N, 8.93; found C, 62.82; H, 3.20; N, 8.90.

benzo[4,5]imidazo[2,1-*b*]thiazol-2-yl(5-bromothiophen-2-yl)methanone (SA-16)



Yellow solid, mp; 178-80 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.47 (s, 1H), 8.89 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.69 (d, J = 4.2 Hz, 1H), 7.42 (t, J = 7.8 Hz, 1H), 7.31 (t, J = 7.8 Hz, 1H), 7.22 (d, J = 4.2 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 176.3, 156.3, 148.7, 142.9, 133.0, 131.6, 129.6, 128.5, 125.3, 123.8, 123.4, 122.2, 119.9, 110.9 ppm. MS m/z 364.9 $(M+1)^+$. Anal. Calcd for $C_{14}H_7BrN_2OS_2$: C, 46.29; H, 1.94; N, 7.71; found C, 46.26; H, 1.92; N, 7.68.

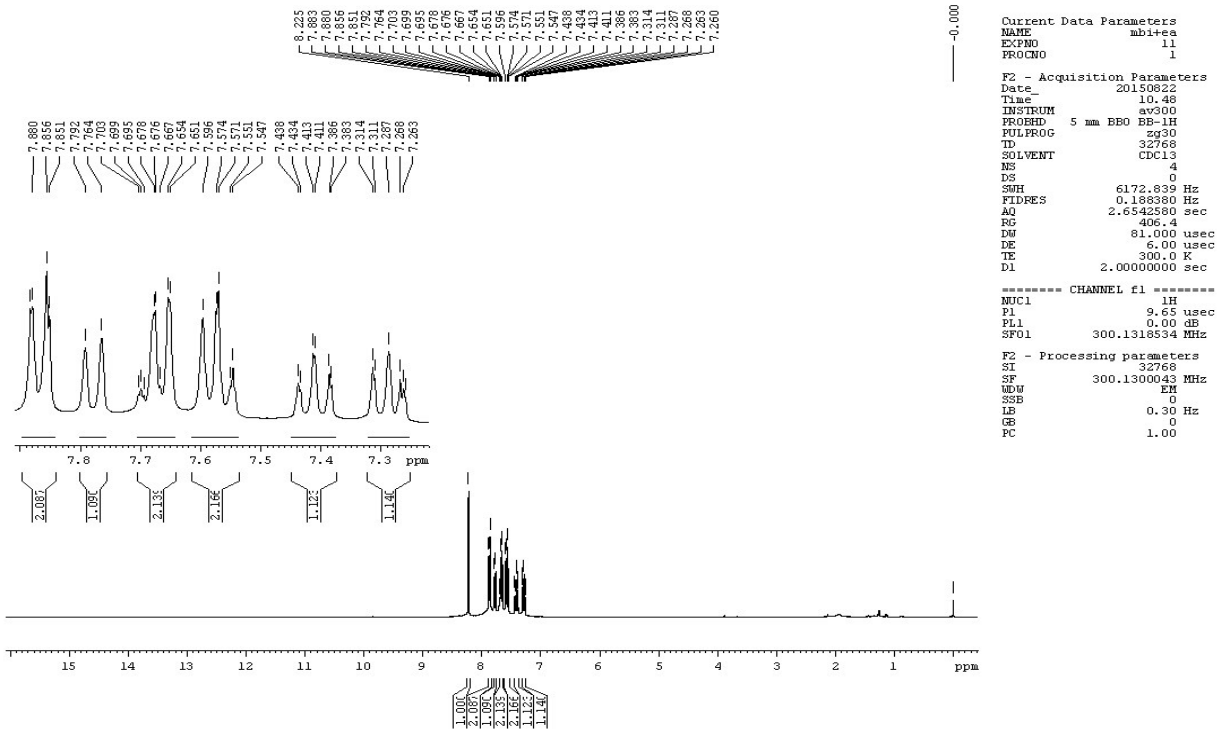


Figure S1.[1]H spectrum of **SA-1.**

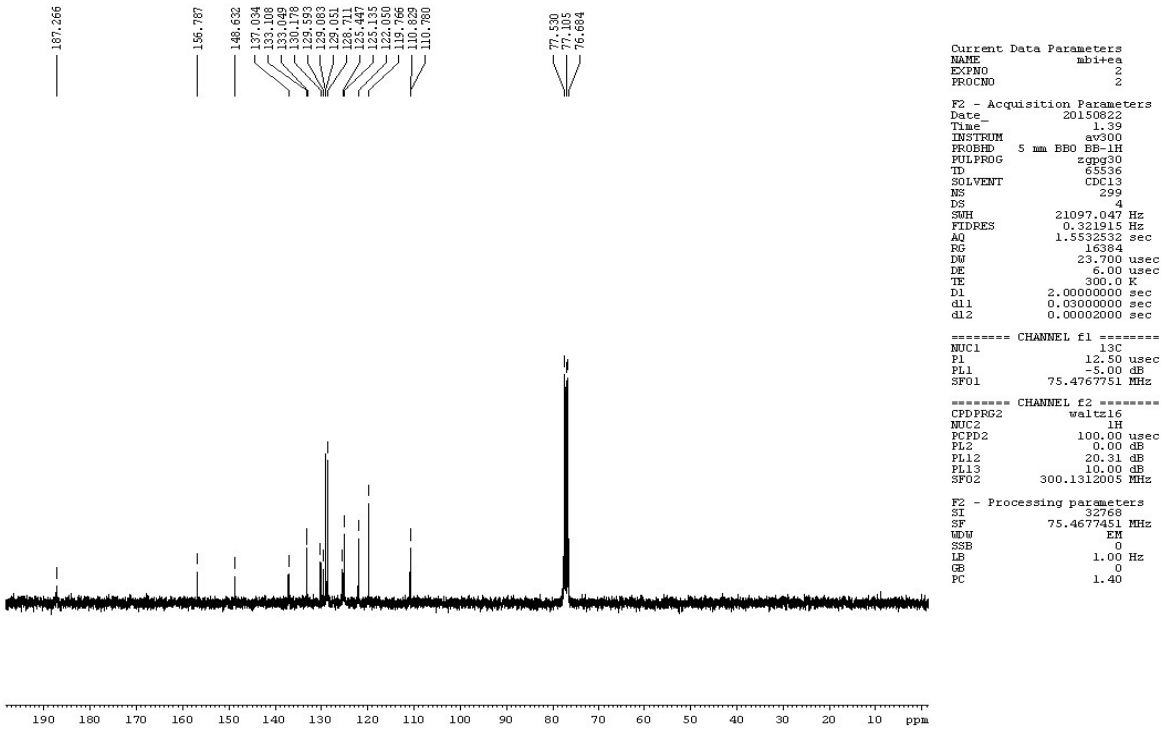
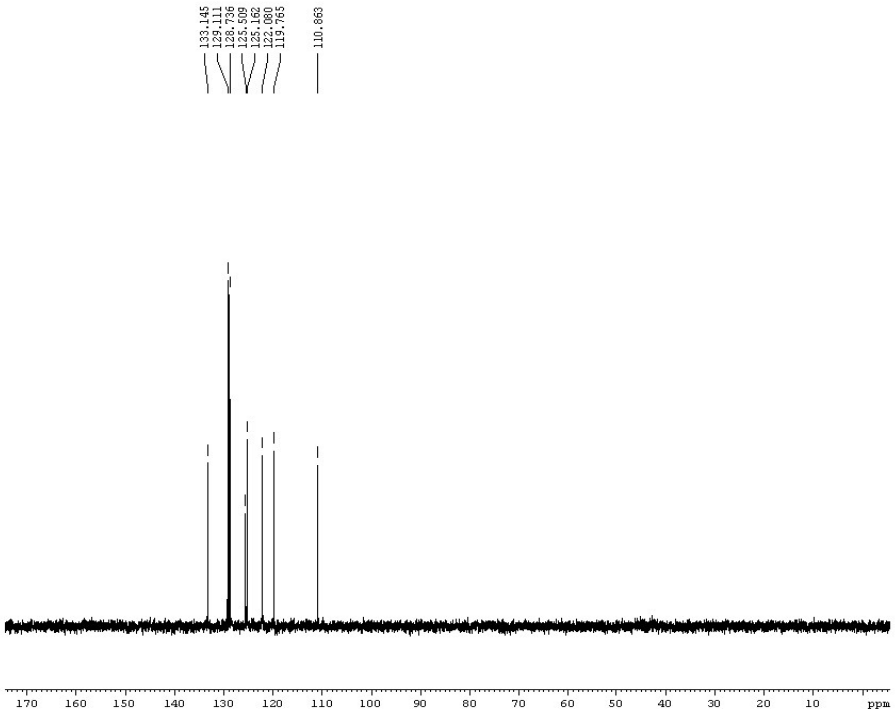


Figure S2.^{13}C spectrum of **SA-1.**




```
Current Data Parameters
NAME                  mbi+ea
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20150822
Time                   1.27
INSTRUM                av300
PROBHD    5 mm BBO BB-1H
PULPROG             dept135
TD                    65536
SOLVENT               CDCl3
NS                      151
DS                        4
SWH               17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                    16384
DW                  27.800 usec
DE                   6.00 usec
TE                  300.0 K
CNST2         145.0000000
D1              2.00000000 sec
d2              0.00344828 sec
d12             0.00002000 sec
DELTA           0.00001592 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  12.50 usec
p2                  25.00 usec
PL1                 -5.00 dB
SF01           75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
P3                   9.65 usec
p4                  19.30 usec
PCPD2              100.00 usec
PL2                  0.00 dB
PL12                20.31 dB
SF02         300.1312005 MHz

F2 - Processing parameters
SI                    32768
SF             75.4677445 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Figure S3.DEPT-135 spectrum of **SA-1.**

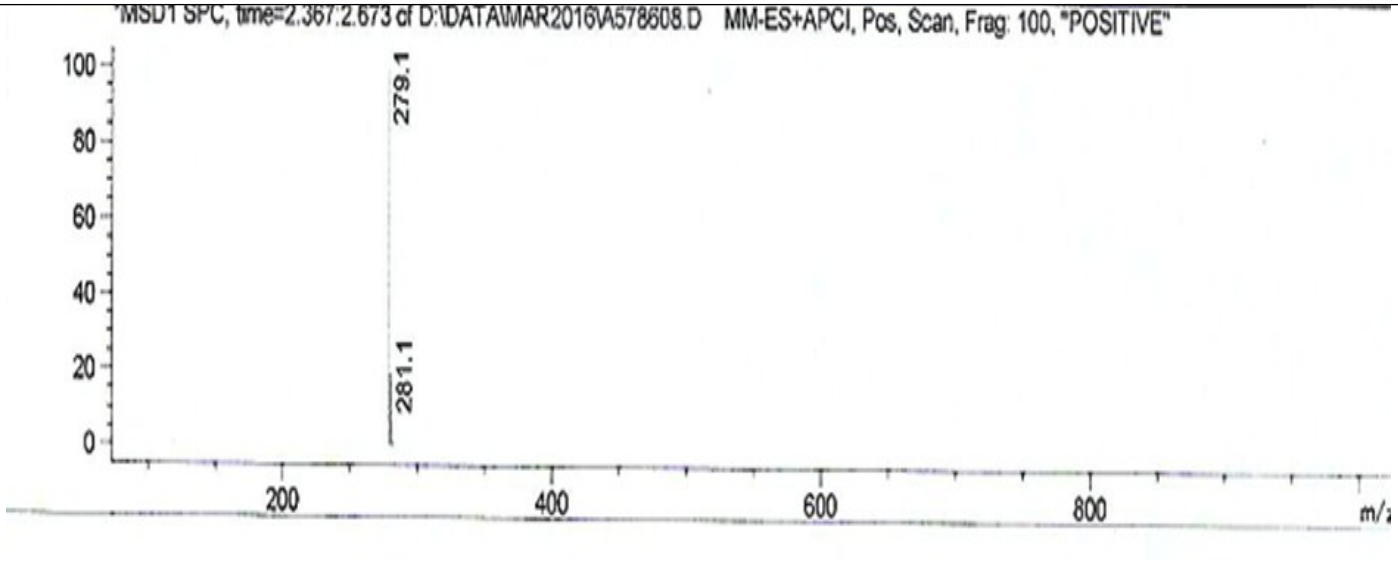


Figure S4. ESI-MASS Spectrum of **SA-1.**

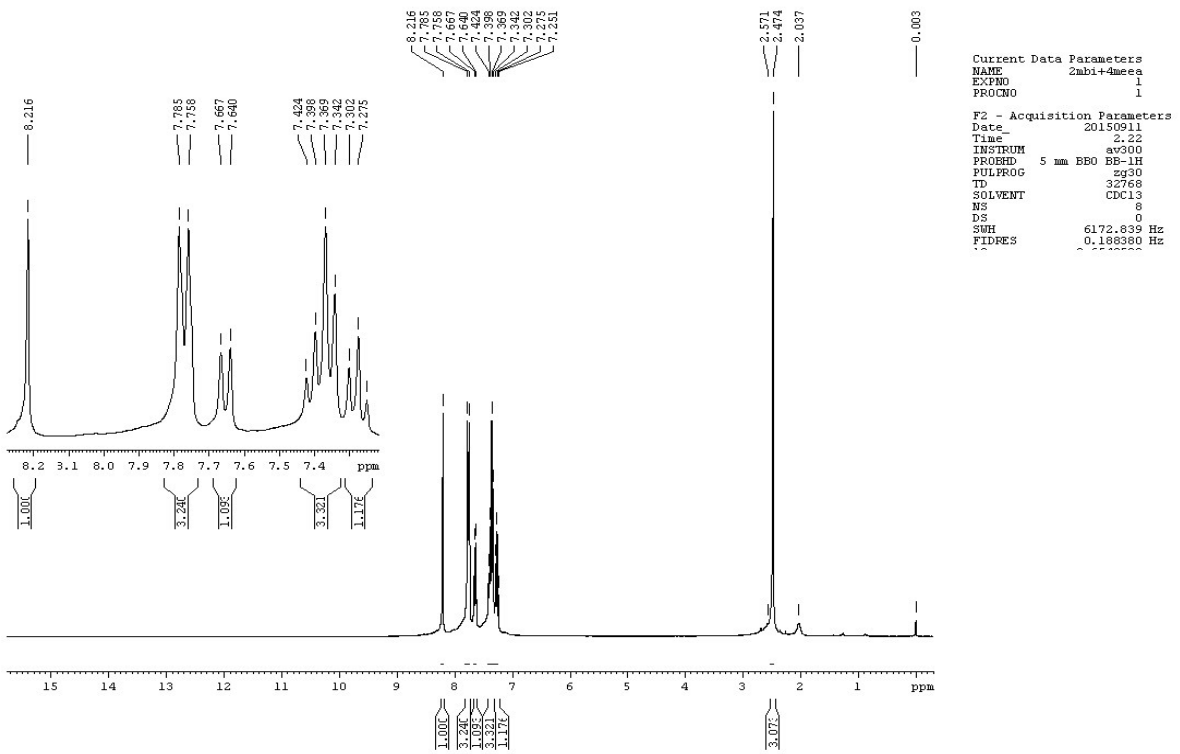


Figure S5.[1]H spectrum of **SA-2.**

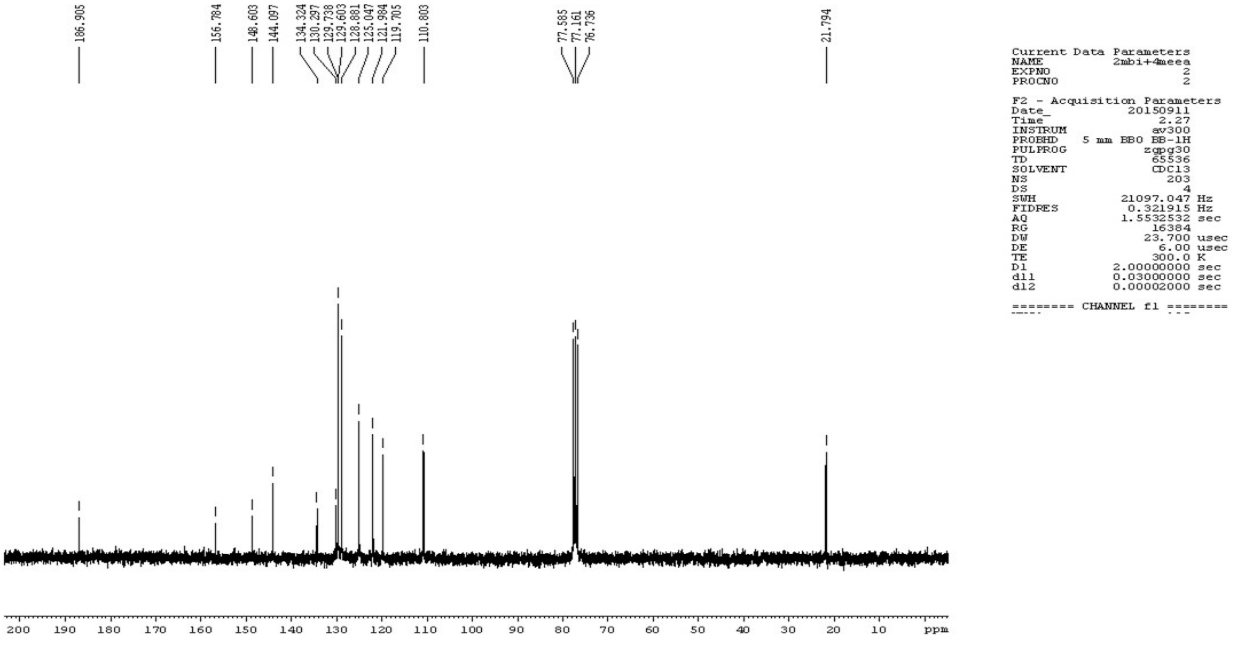


Figure S6.[13]C spectrum of **SA-2.**

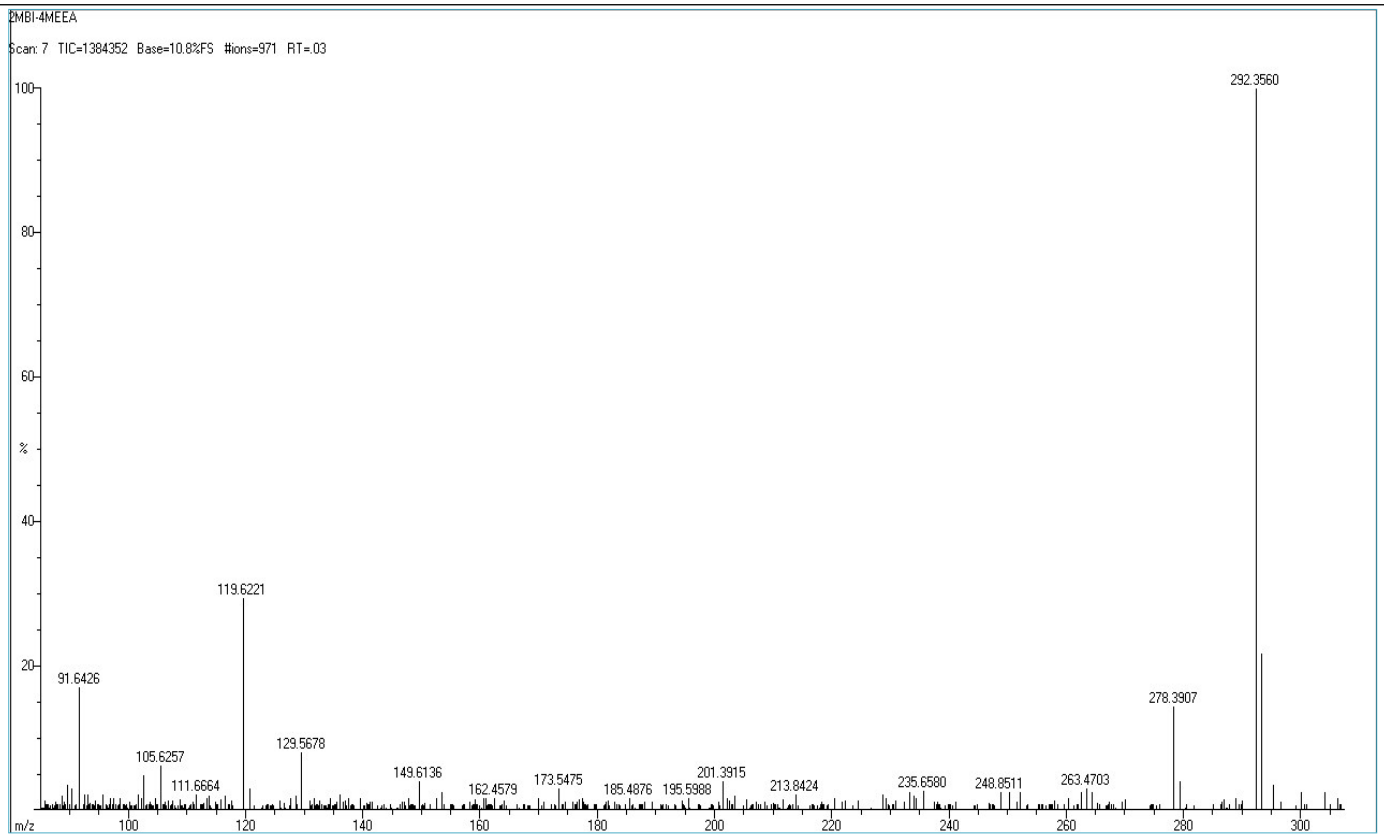


Figure S7.HRM spectrum of **SA-2.**

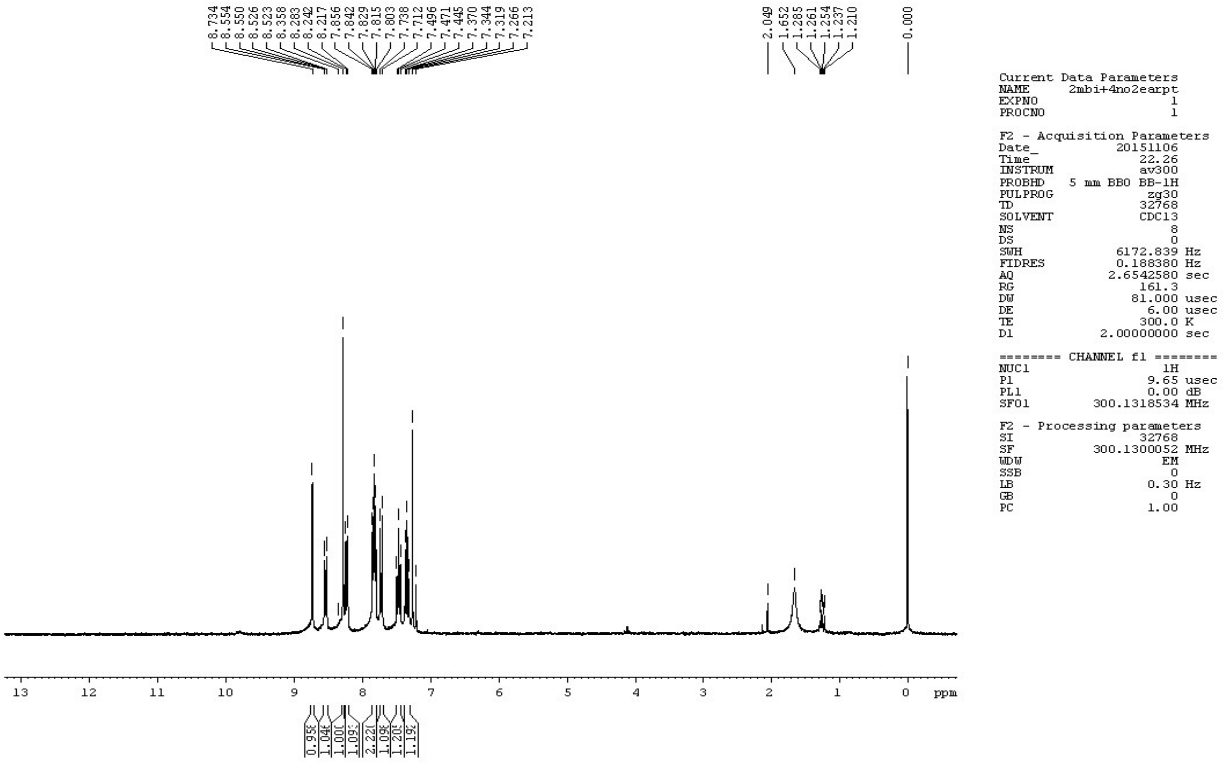


Figure S8.[1]H spectrum of **SA-3.**

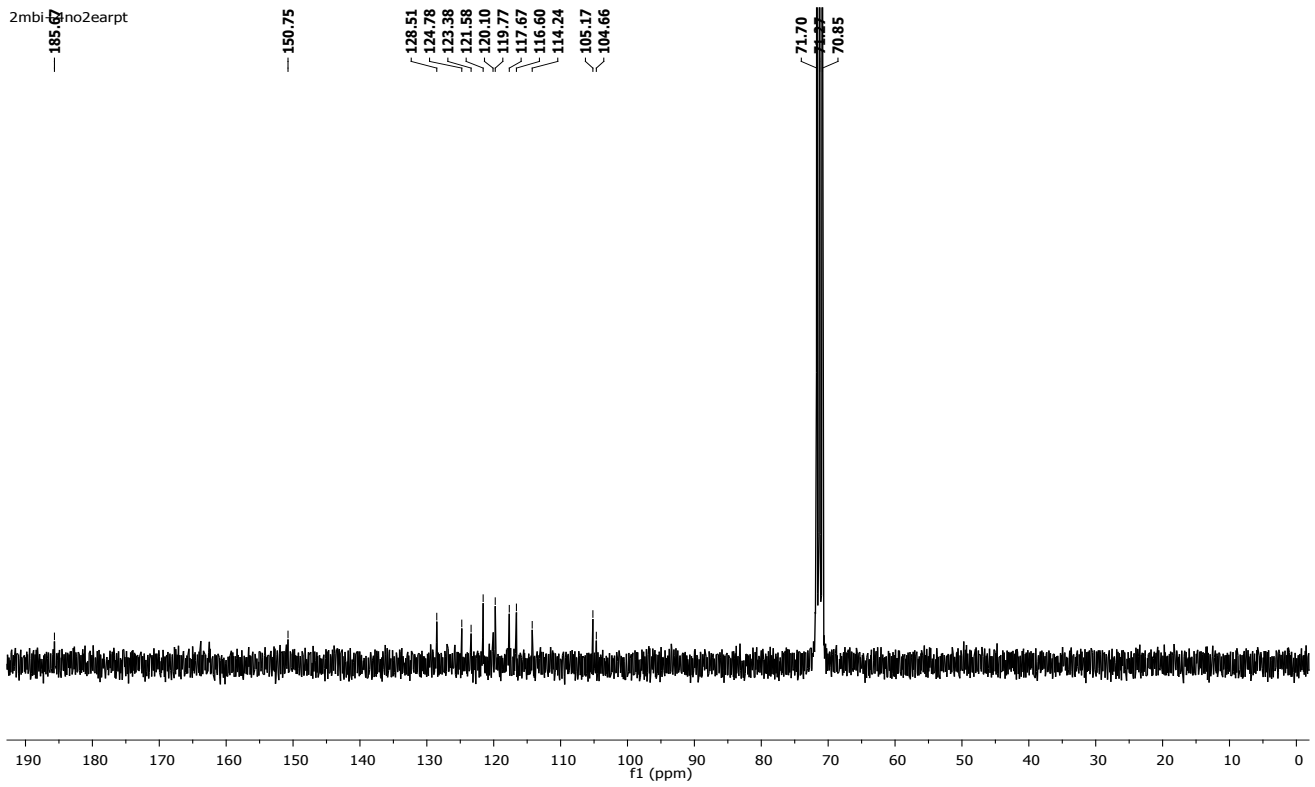


Figure S9.[13]C spectrum of **SA-3.**

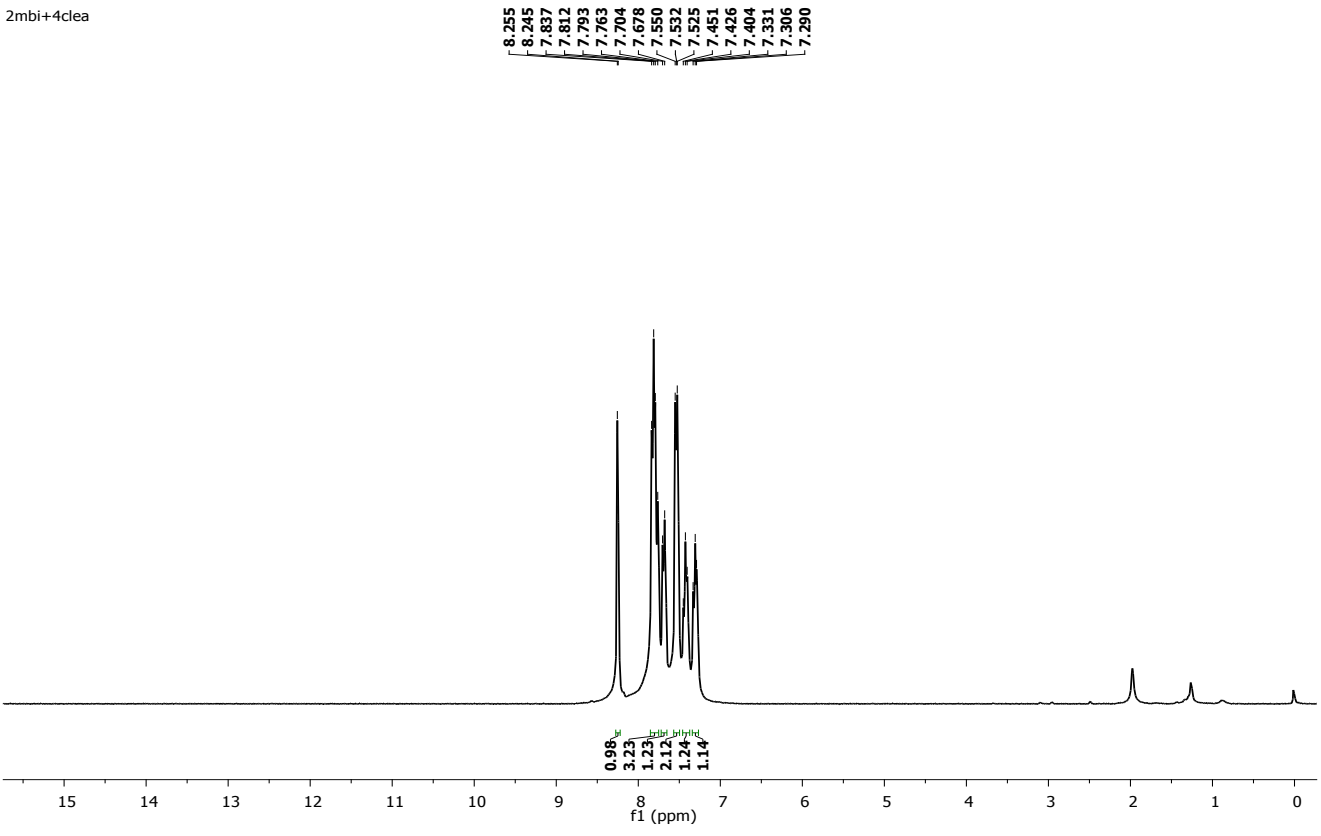
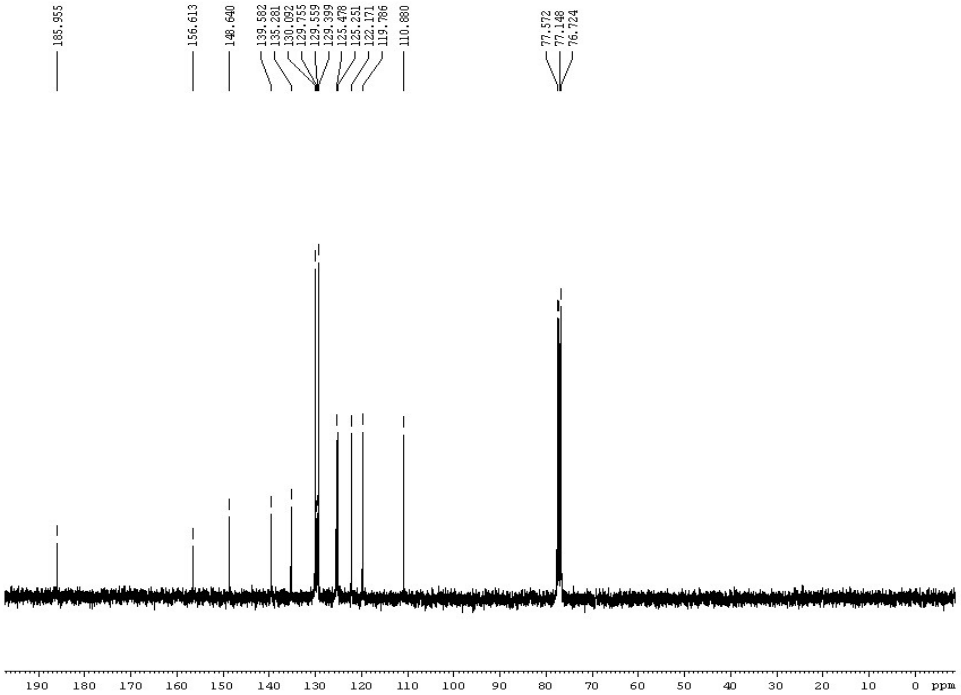


Figure S10.[1]H spectrum of **SA-4.**




```
Current Data Parameters
NAME          2mbi+4clea
EXPNO                  2
PROCNO                 2

F2 - Acquisition Parameters
Date_           20150911
Time              2.18
INSTRUM           av300
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 332
DS                   4
SWH         21097.047 Hz
FIDRES       0.321915 Hz
AQ           1.5532532 sec
RG               16384
DW              23.700 usec
DE               6.00 usec
TE              300.0 K
D1           2.00000000 sec
```

Figure S11.^{13}C spectrum of **SA-4.**

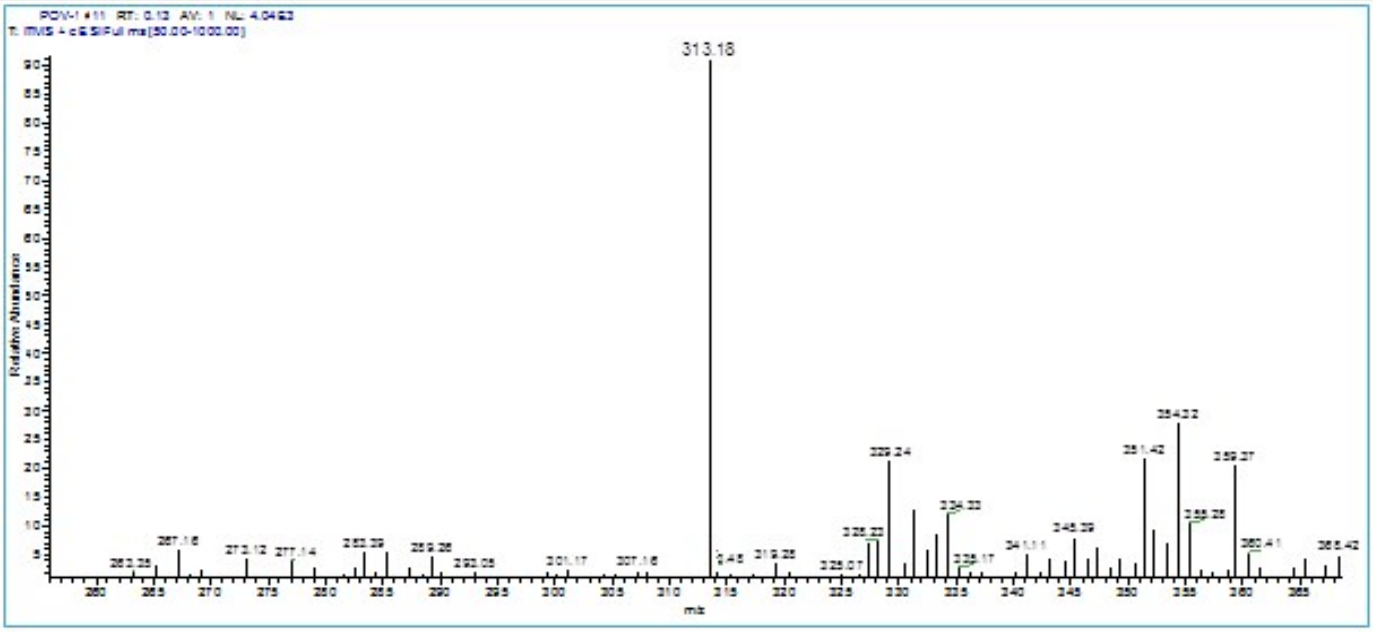
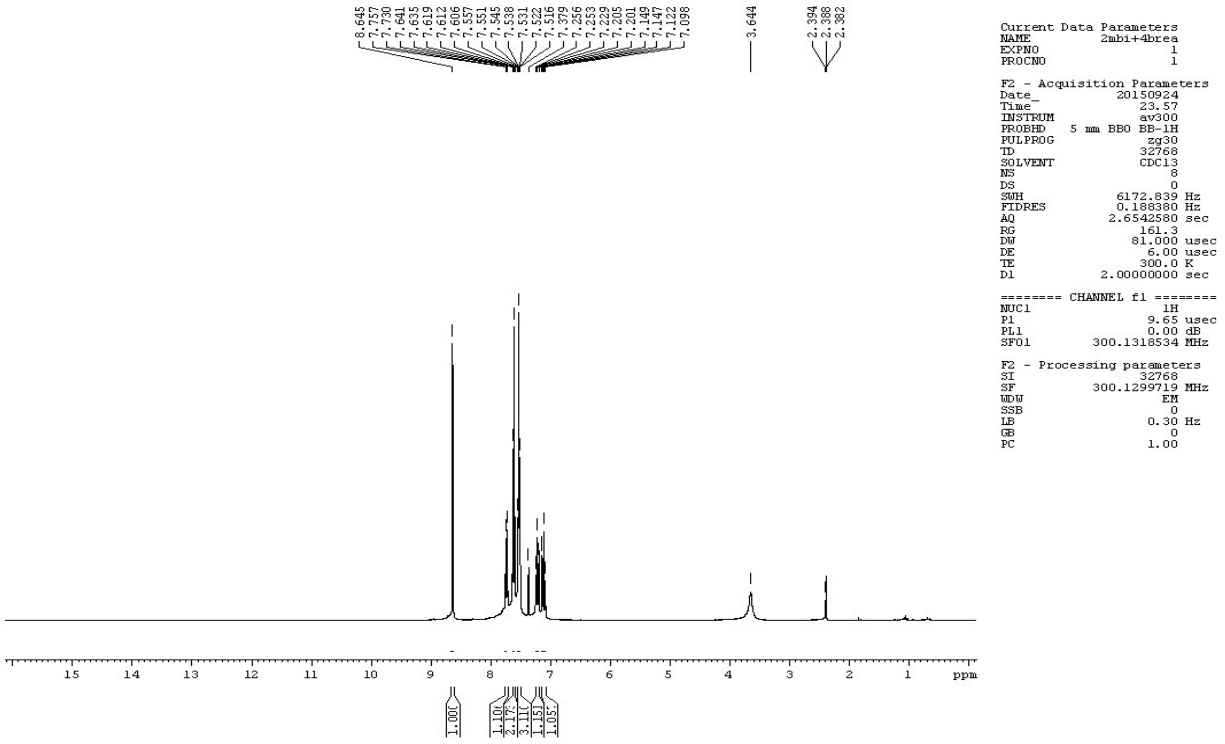


Figure S12.ESI-MASS Spectrum of **SA-4.**



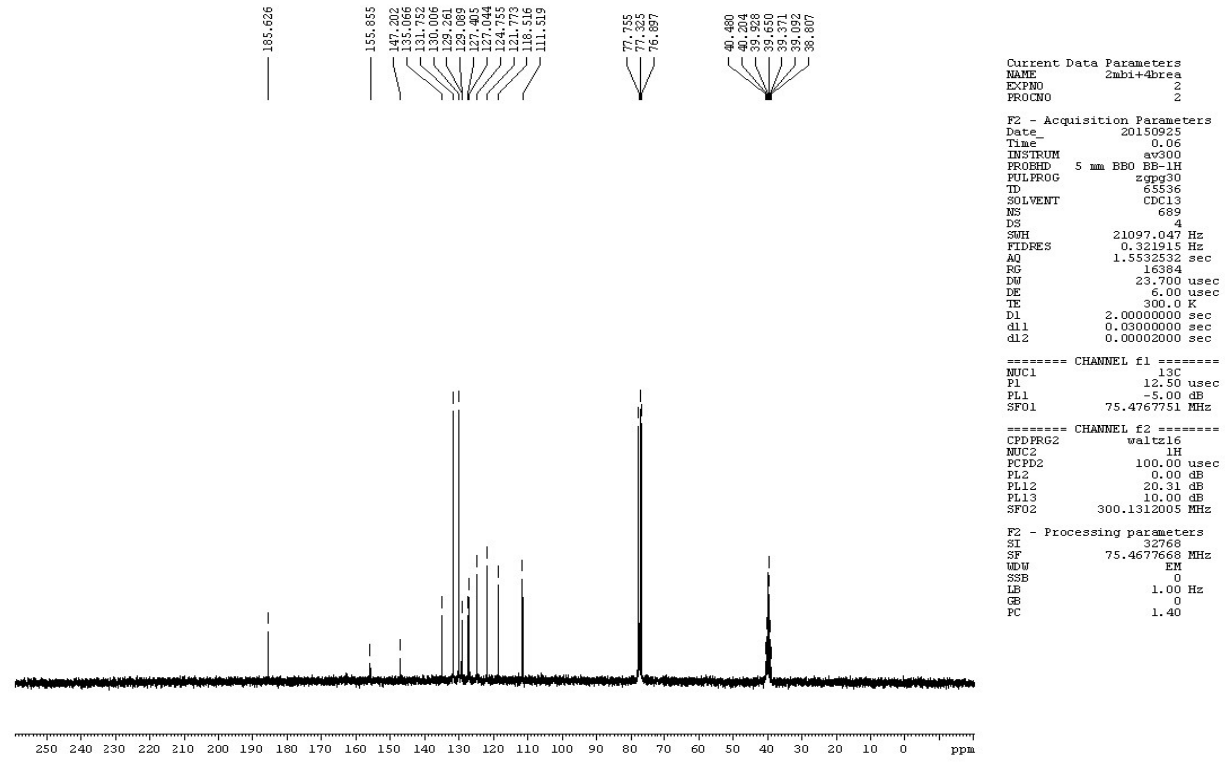

```
Current Data Parameters
NAME                  2mbi+4brea
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20150924
Time                      23.57
INSTRUM                   av300
PROBHD     5 mm BBO BB-1H
PULPROG                    zg30
TD                        32768
SOLVENT                   CDCl3
NS                             8
DS                             0
SWH                    6172.839 Hz
FIDRES                 0.188380 Hz
AQ                     2.6542580 sec
RG                         161.3
DW                        81.000 usec
DE                         6.00 usec
TE                        300.0 K
D1                     2.00000000 sec

======== CHANNEL f1 ========
NUC1                          1H
P1                          9.65 usec
PL1                         0.00 dB
SFO1                300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF                  300.1299719 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

Figure S13.[1]H spectrum of **SA-5.**




```
Current Data Parameters
NAME                  2mbi+4brea
EXPNO                          2
PROCNO                         2

F2 - Acquisition Parameters
Date_                  20150925
Time                       0.06
INSTRUM                   av300
PROBHD     5 mm BBO BB-1H
PULPROG                 zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                           689
DS                             4
SWH                   21097.047 Hz
FIDRES                 0.321915 Hz
AQ                     1.5532532 sec
RG                         16384
DW                        23.700 usec
DE                         6.00 usec
TE                        300.0 K
D1                     2.00000000 sec
d11                    0.03000000 sec
d12                    0.00002000 sec

======== CHANNEL f1 ========
NUC1                         13C
P1                         12.50 usec
PL1                        -5.00 dB
SFO1                75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                          1H
PCPD2                    100.00 usec
PL2                         0.00 dB
PL12                       20.31 dB
PL13                       10.00 dB
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF                  75.4677668 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```

Figure S14.[13]C spectrum of **SA-5.**

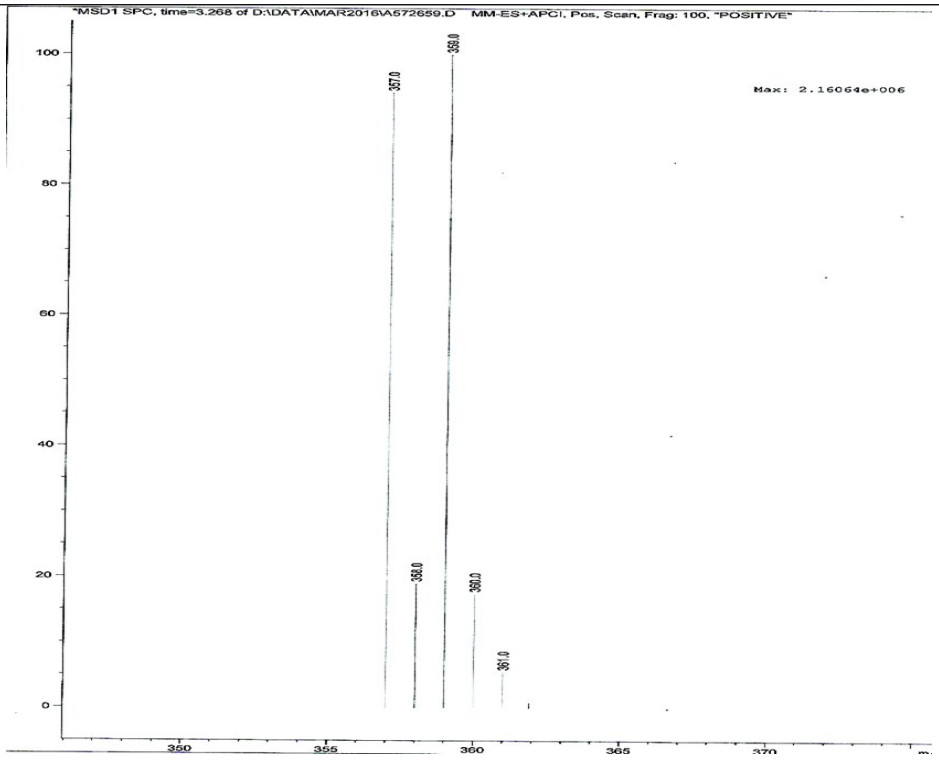


Figure S15.ESI-MASS Spectrum of **SA-5.**

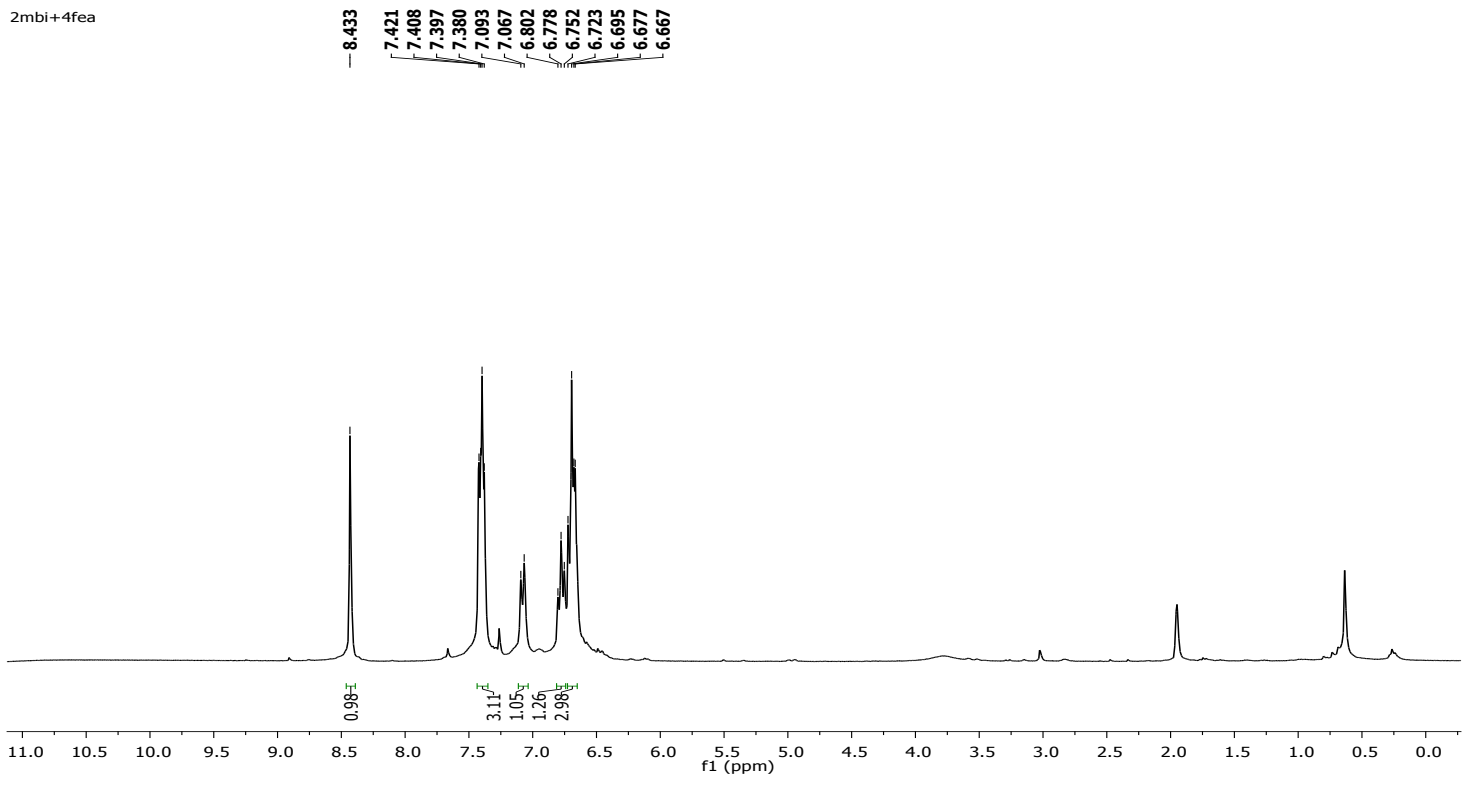
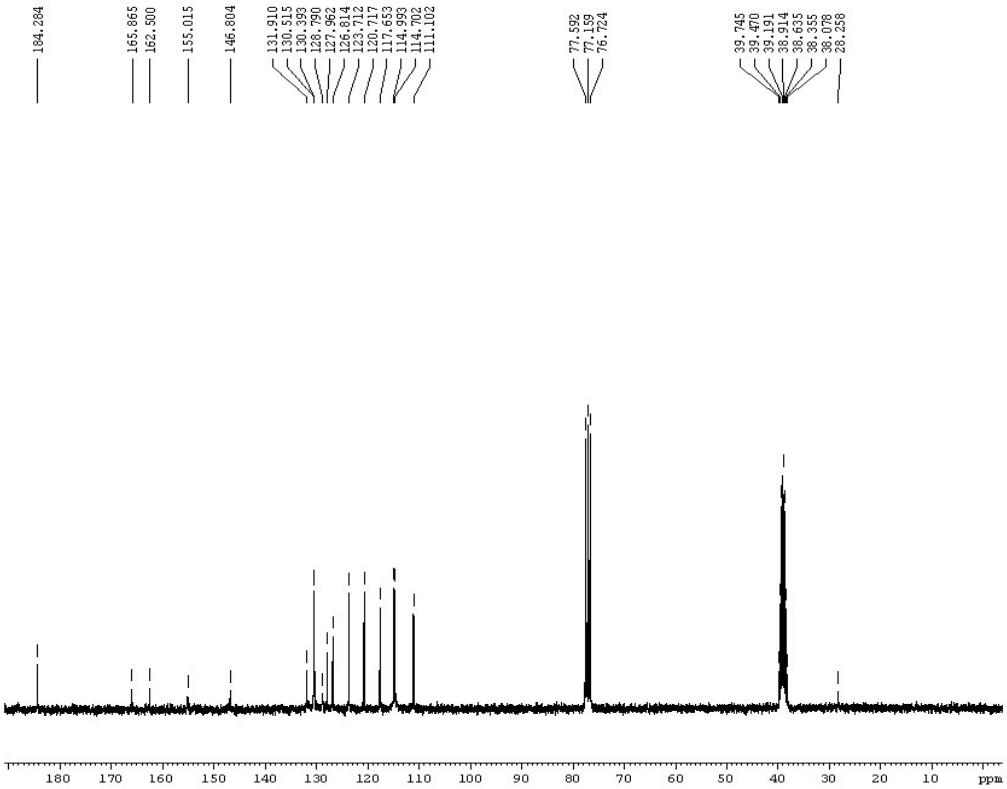


Figure S16.^{1}H spectrum of **SA-6.**




```
Current Data Parameters
NAME                  2mbi+4fea
EXPNO                         2
PROCNO                        2

F2 - Acquisition Parameters
Date_                  20151019
Time                      23.15
INSTRUM                   av300
PROBHD    5 mm BBO BB-1H
PULPROG                zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                         1000
DS                            4
SWH                21097.047 Hz
FIDRES              0.321915 Hz
AQ                  1.5532532 sec
RG                        16384
DW                       23.700 usec
DE                        6.00 usec
TE                       300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
d12                0.00002000 sec

======== CHANNEL f1 ========
NUC1                        13C
P1                       12.50 usec
PL1                      -5.00 dB
SF01               75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                  100.00 usec
PL2                       0.00 dB
PL12                     20.31 dB
PL13                     10.00 dB
SF02              300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                 75.4682041 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```

Figure S17.^{13}C spectrum of **SA-6.**

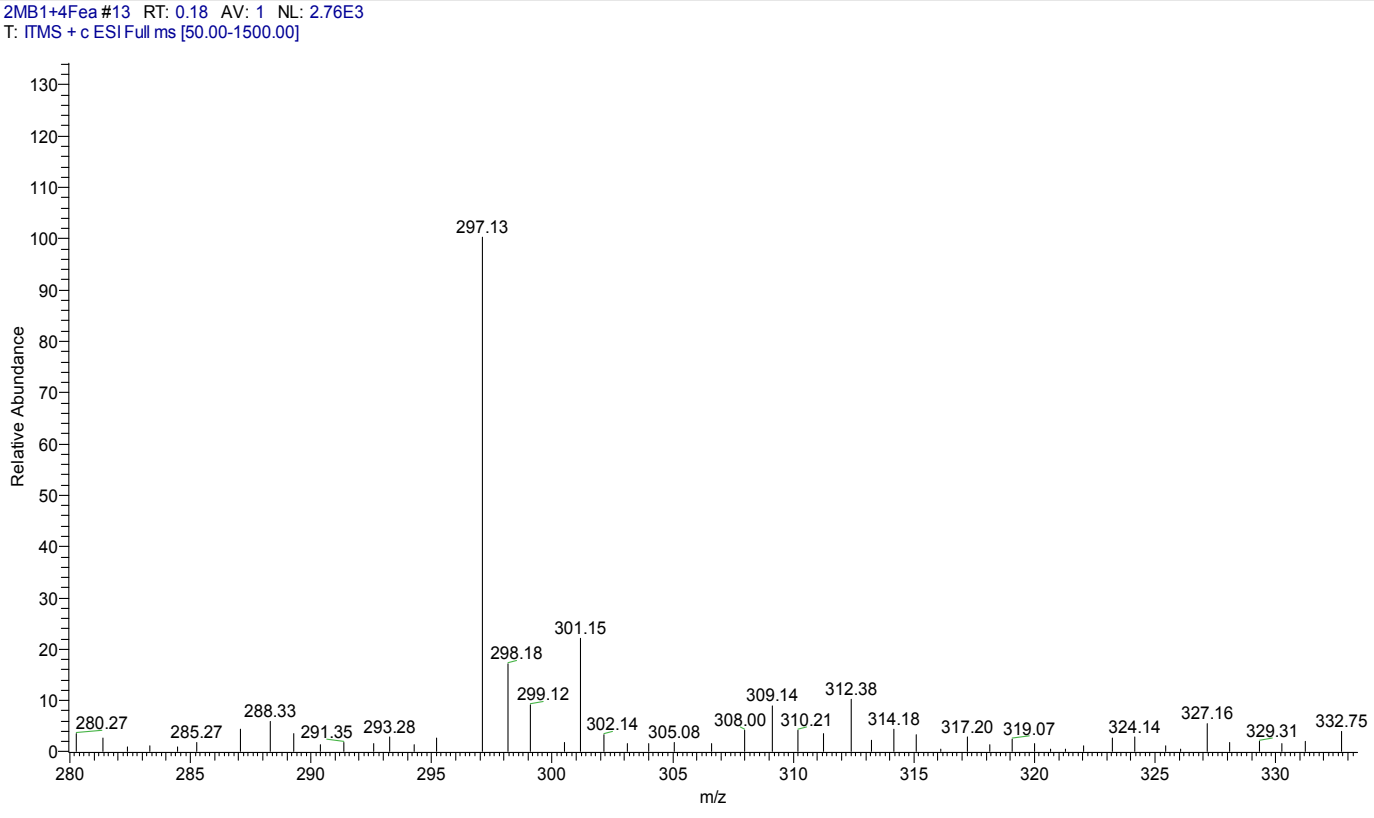


Figure S18.ESI-MASS Spectrum of **SA-6.**

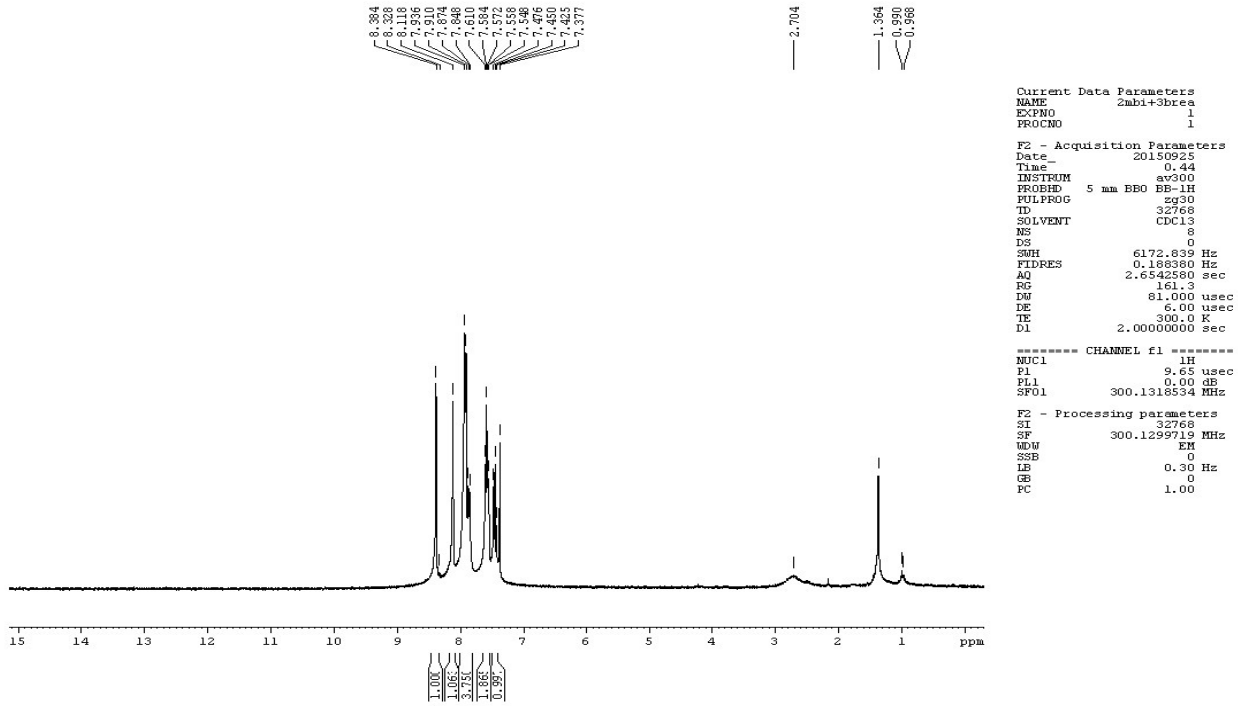


Figure S19.[1]H spectrum of **SA-7.**

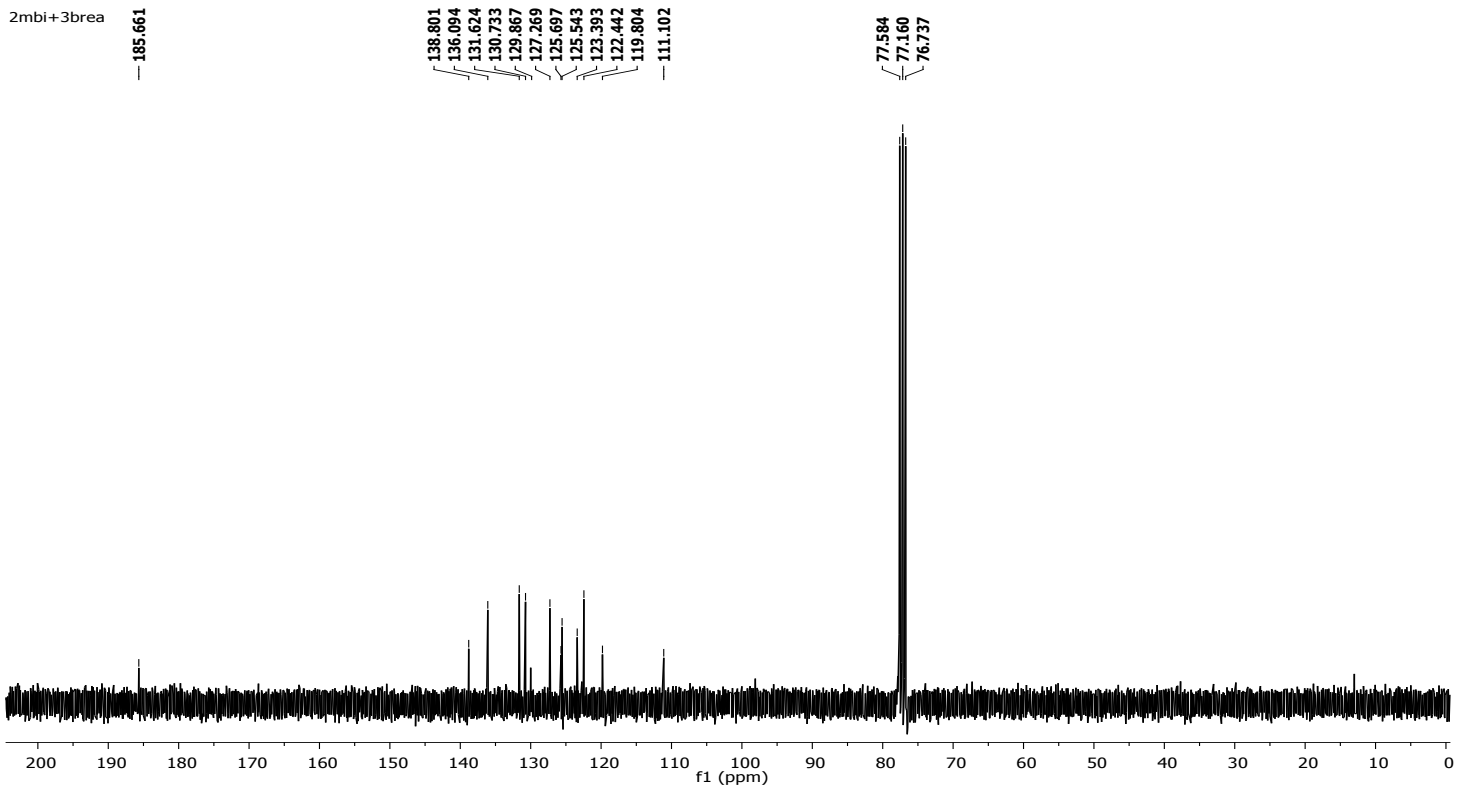


Figure S20.[13]C spectrum of **SA-7.**

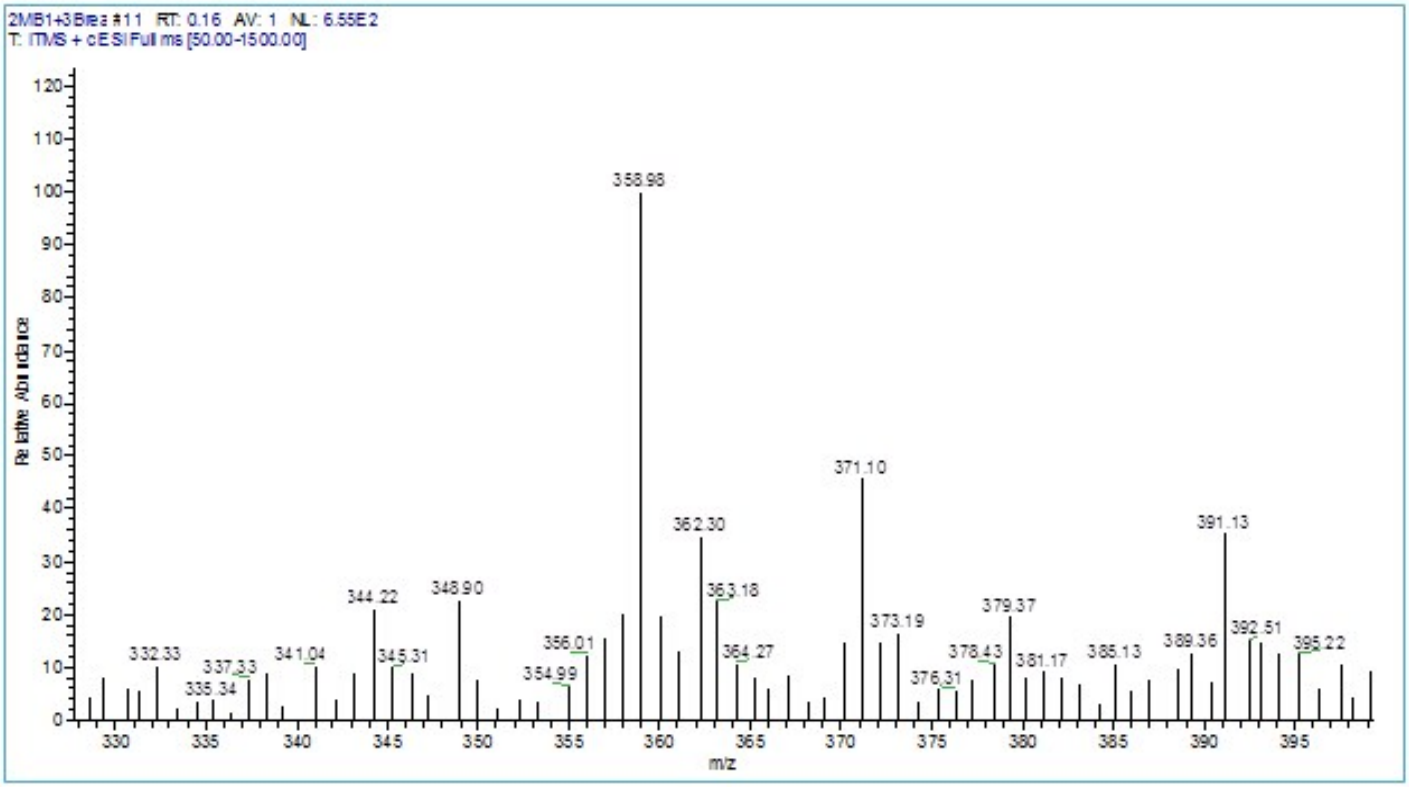


Figure S21.ESI-MASS Spectrum of SA-7.

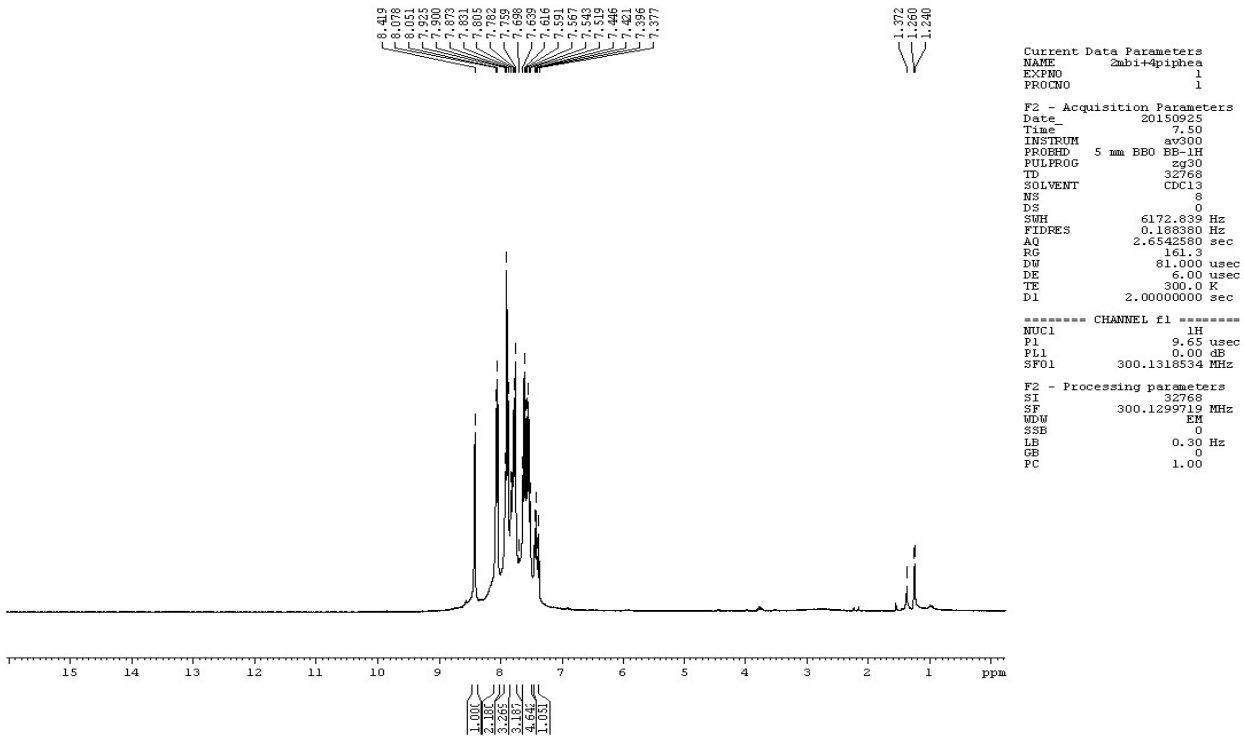
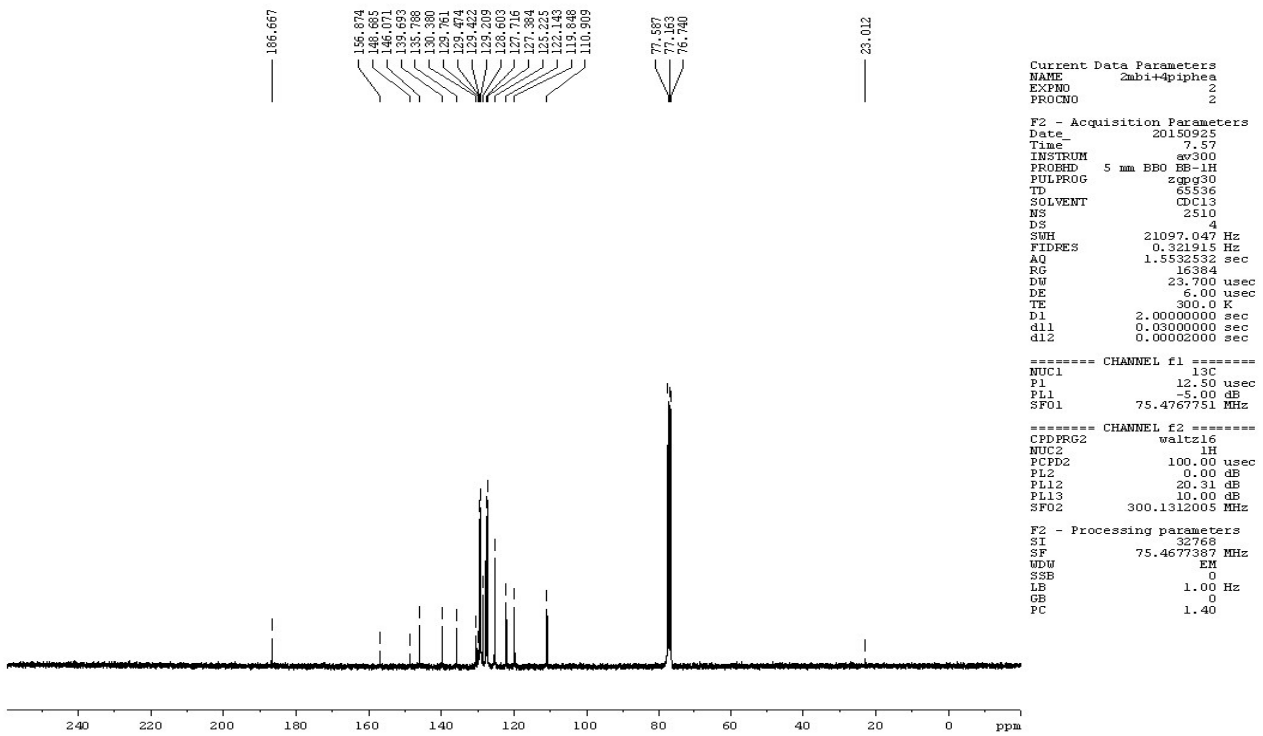


Figure S22.[1]H spectrum of **SA-8.**



Current Data Parameters
NAME 2mbi+4piphea
EXPNO 2
PROCNO 2

F2 - Acquisition Parameters
Date_ 20150925
Time 7.57
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2510
DS 4
SWH 21097.047 Hz
FIDRES 0.321915 Hz
AQ 1.5532532 sec
RG 16384
DW 23.700 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 12.50 usec
PL1 -5.00 dB
SFO1 75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 20.31 dB
PL13 10.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677387 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S23.^{13}C spectrum of **SA-8.**

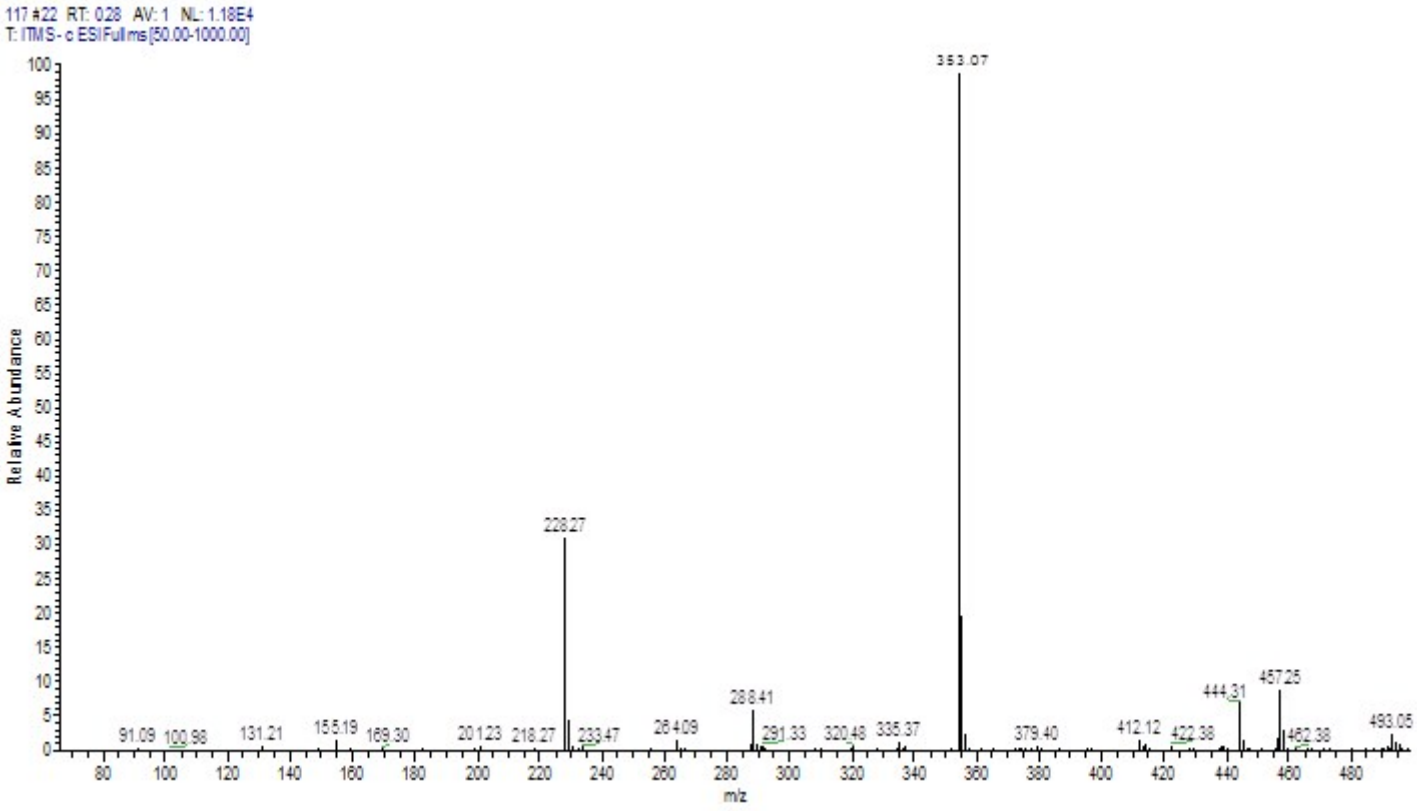


Figure S24.ESI-MASS Spectrum of **SA-8.**

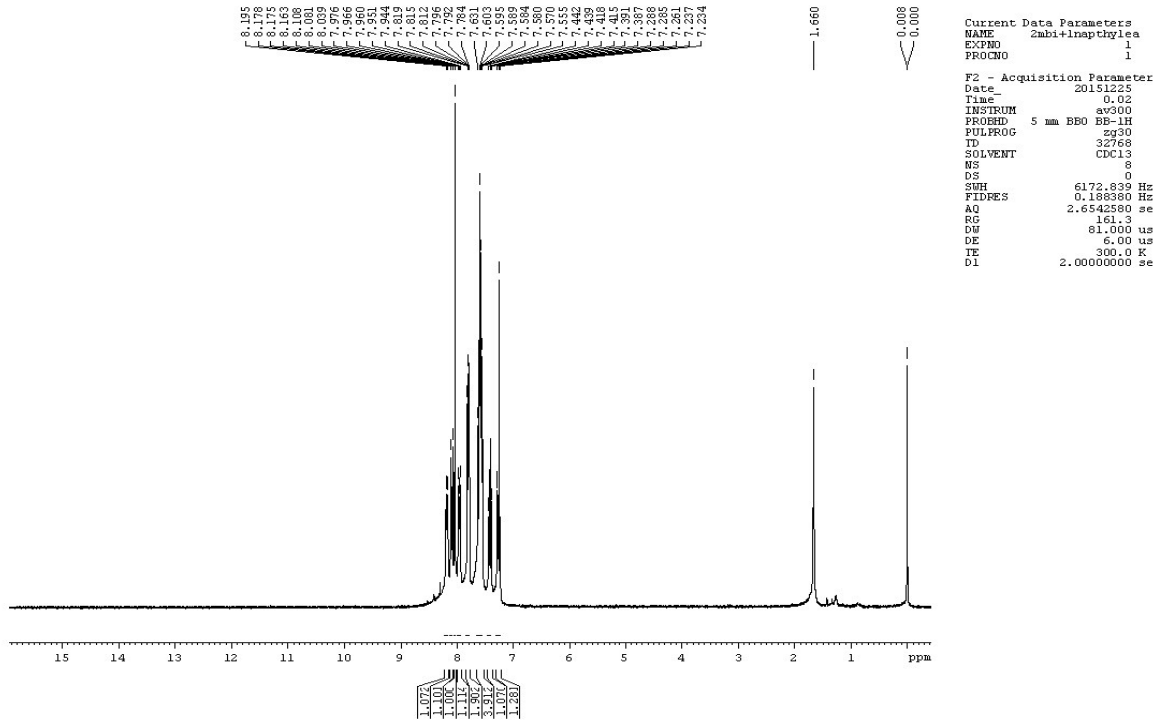


Figure S25.[1]H spectrum of **SA-9.**

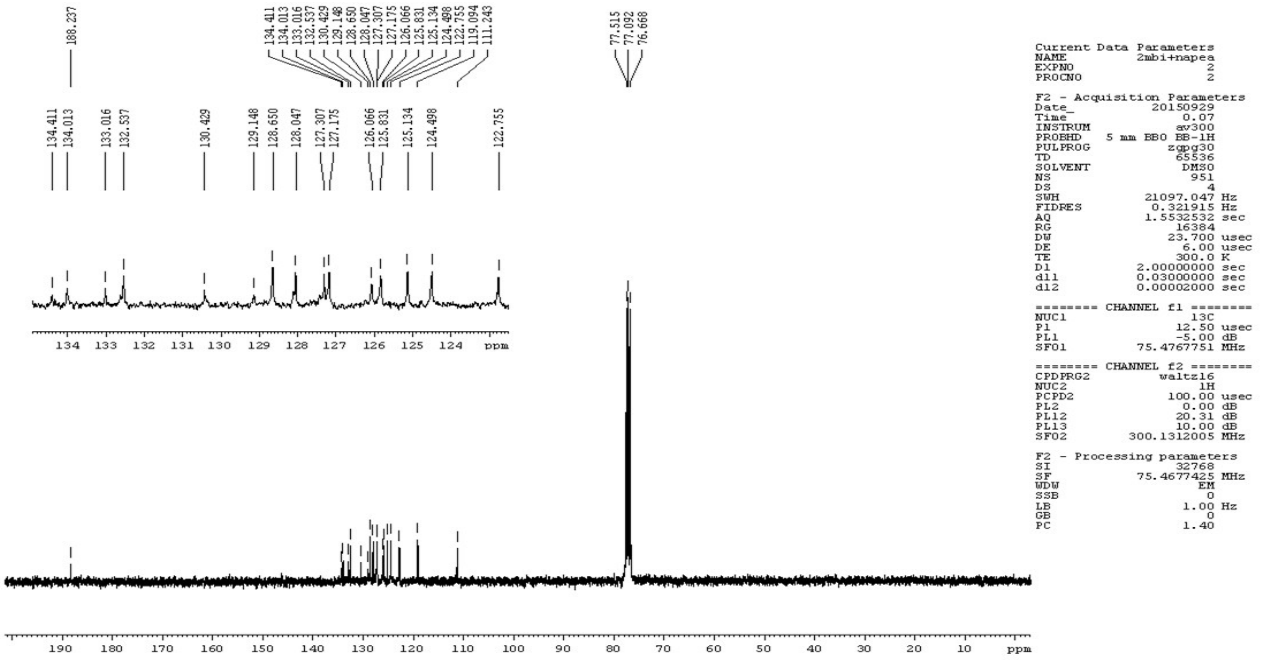


Figure S26.[13]C spectrum of **SA-9**.

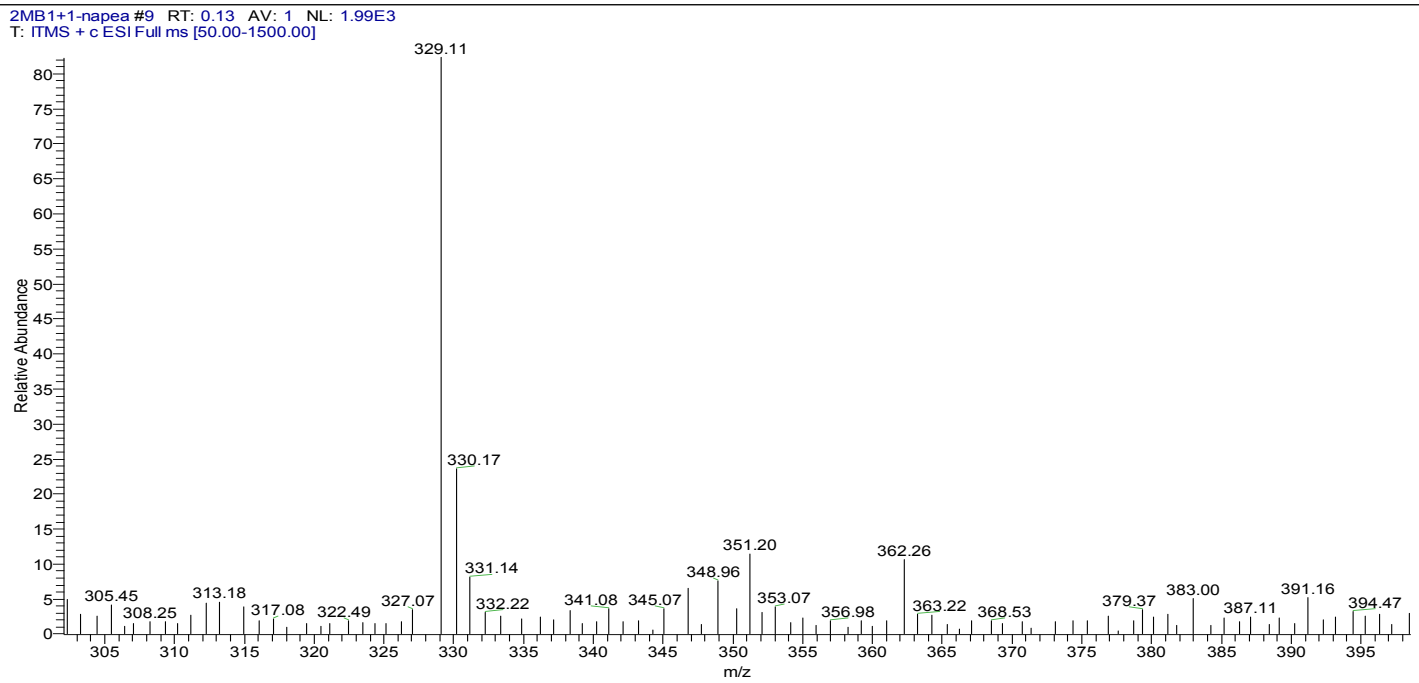


Figure S27.ESI-MASS Spectrum of **SA-9.**

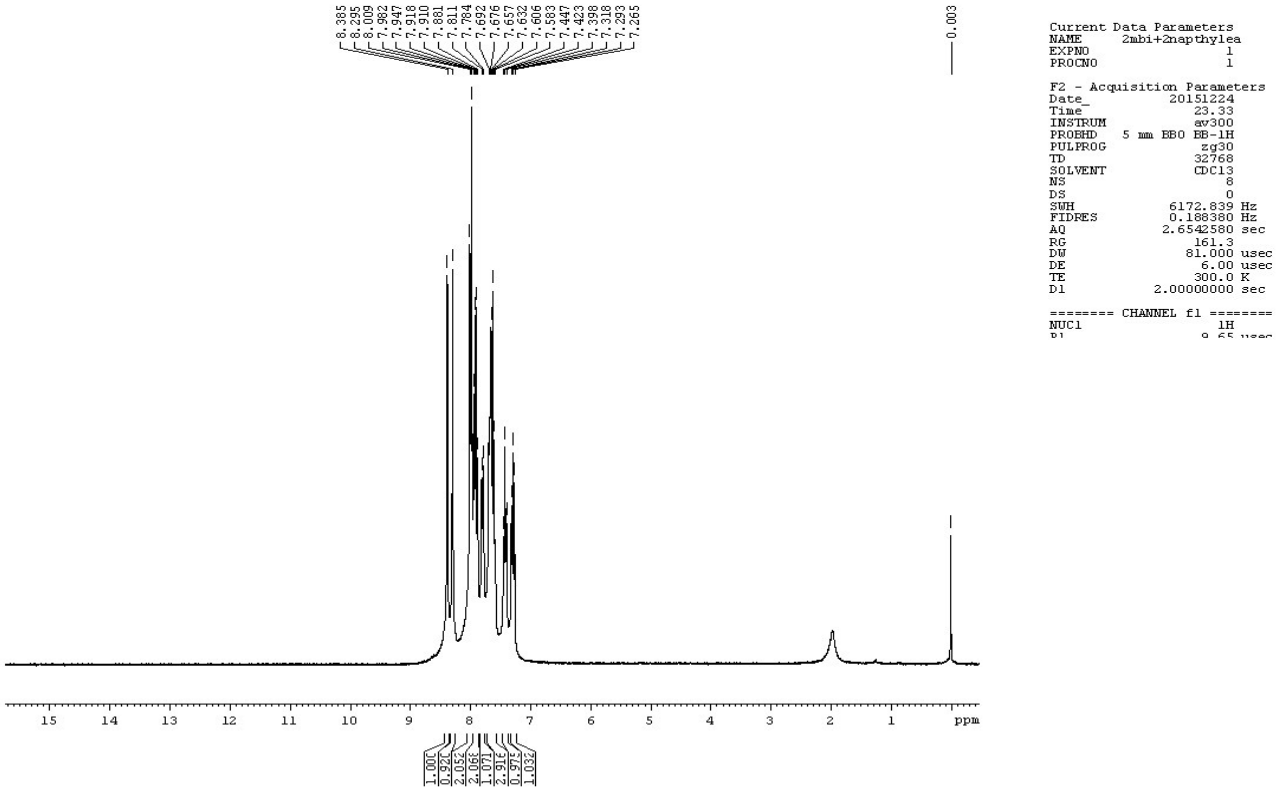
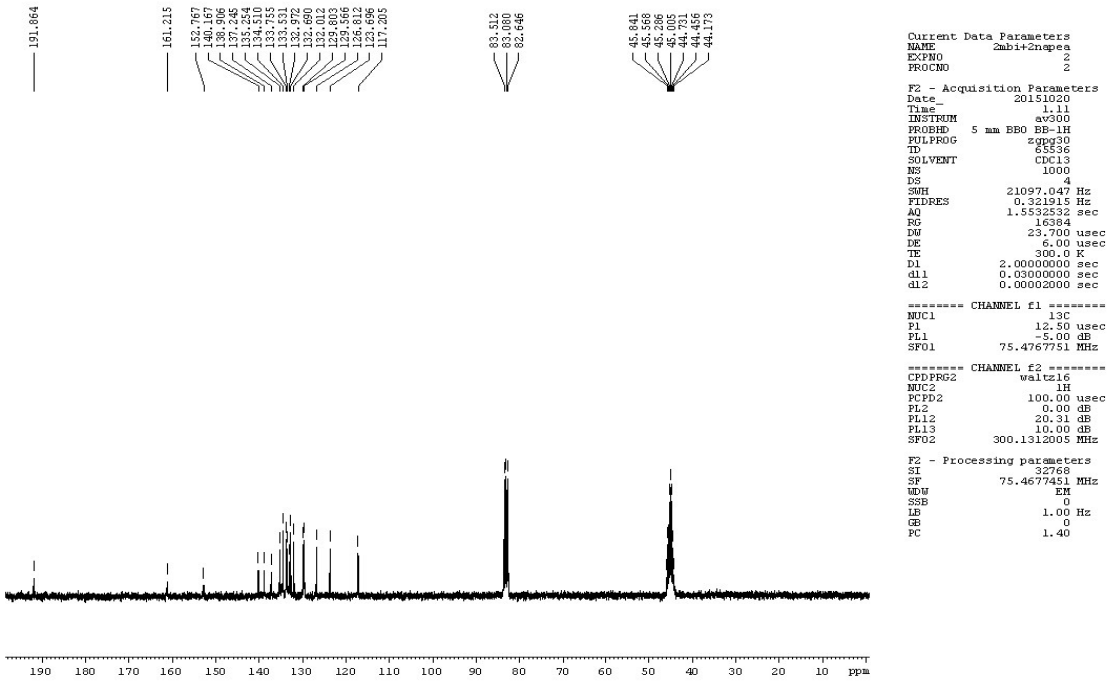


Figure S28.^{1}H spectrum of **SA-10.**




```
Current Data Parameters
NAME          2mbi+2napea
EXPNO                   2
PROCNO                  2

F2 - Acquisition Parameters
Date_          20151020
Time_              1.11
INSTRUM           av300
PROBHD   5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                1000
DS                   4
SWH          21097.047 Hz
FIDRES        0.321915 Hz
AQ            1.5532532 sec
RG               16384
DW              23.700 usec
DE               6.00 usec
TE              300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
d12          0.00002000 sec

======== CHANNEL f1 ========
NUC1              13C
P1              12.50 usec
PL1             -5.00 dB
SF01       75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2       waltz16
NUC2              1H
PCPD2          100.00 usec
PL2              0.00 dB
PL12            20.31 dB
PL13            10.00 dB
SF02       300.1312005 MHz

F2 - Processing parameters
SI               32768
SF         75.4677451 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

Figure S29.^{13}C spectrum of **SA-10.**

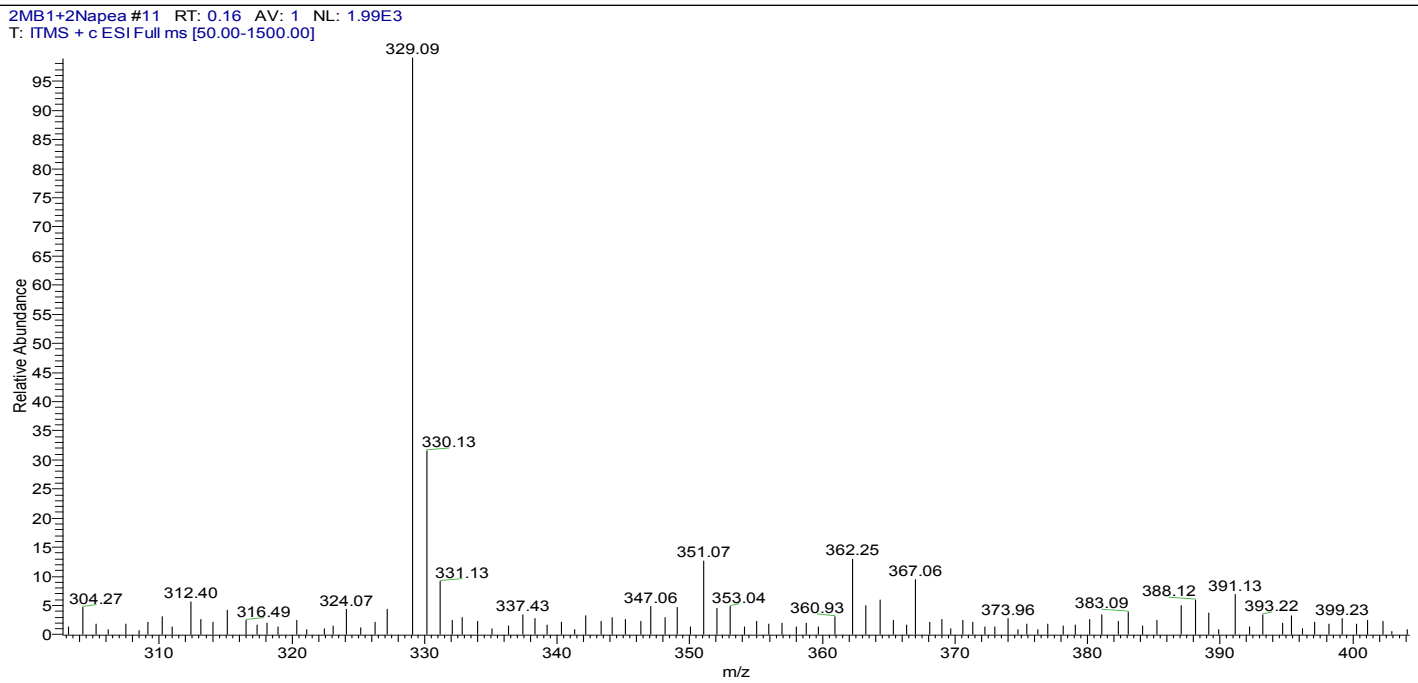


Figure S30.ESI-MASS Spectrum of **SA-10.**

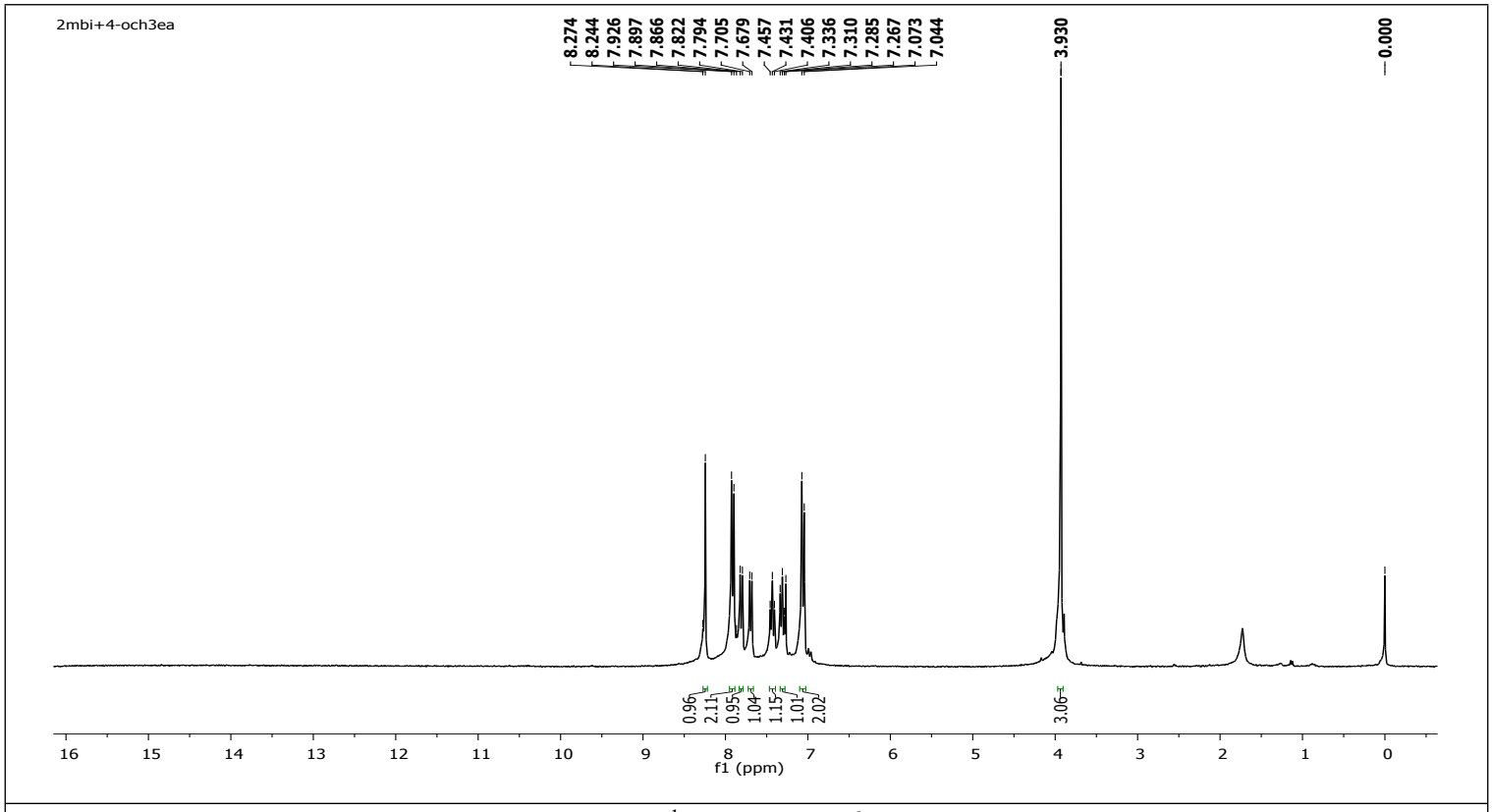


Figure S31.[1]H spectrum of **SA-11.**

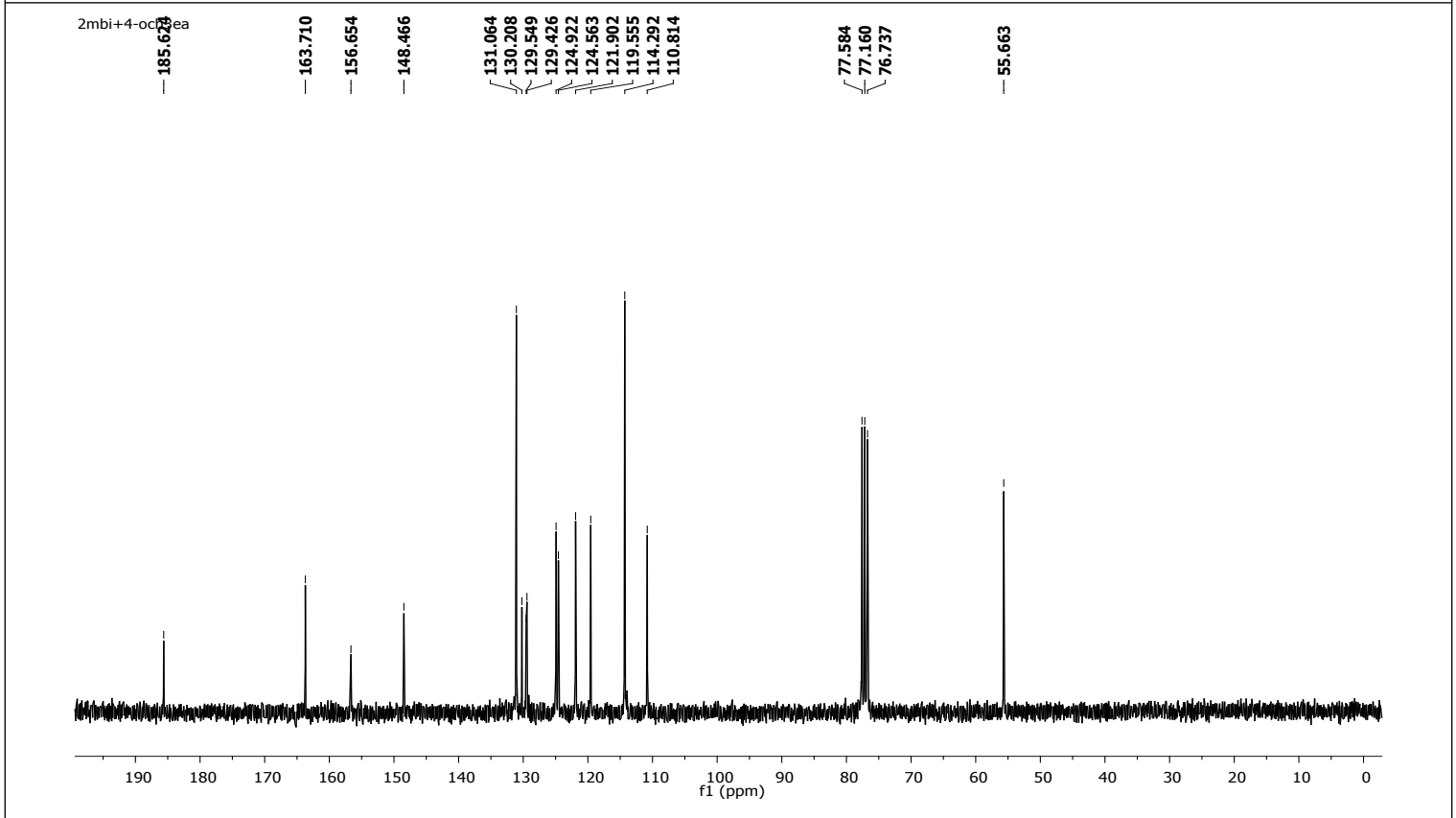


Figure S32.[13]C spectrum of **SA-11.**

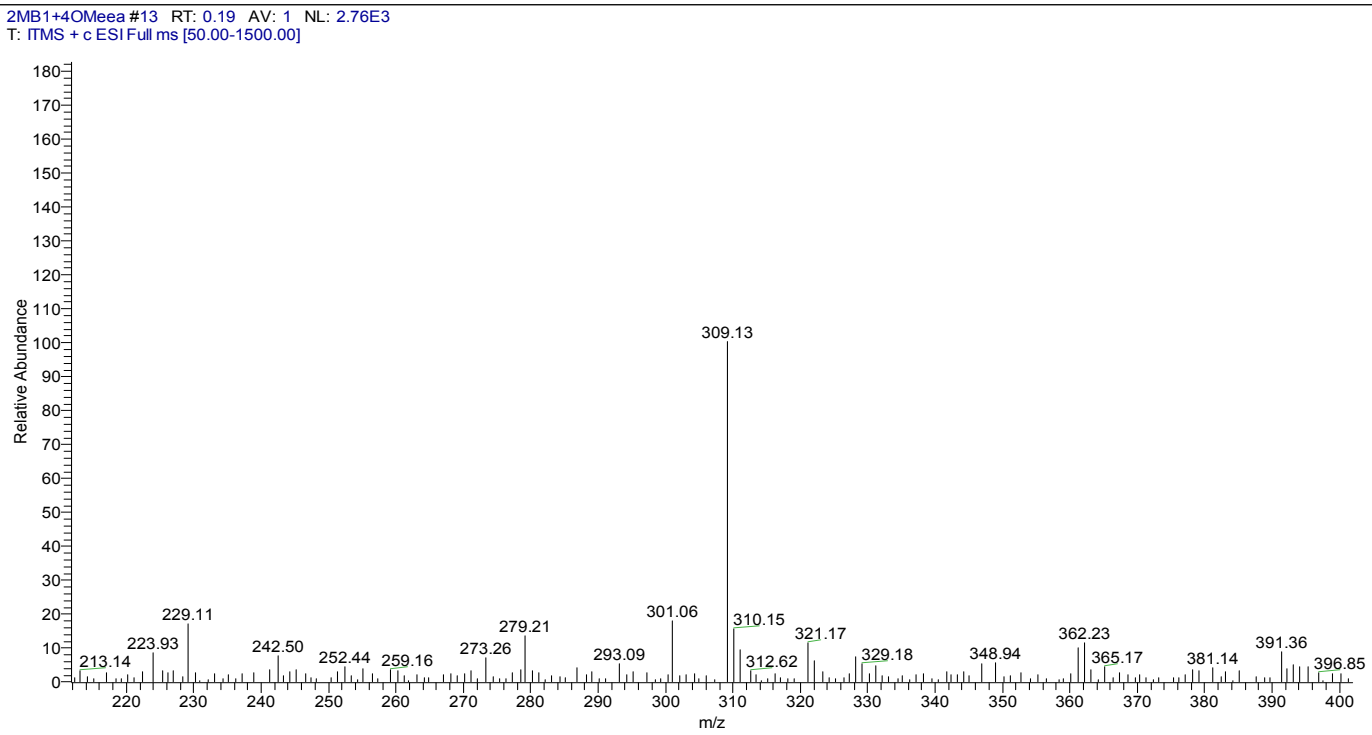


Figure S33.ESI-MASS Spectrum of **SA-11.**

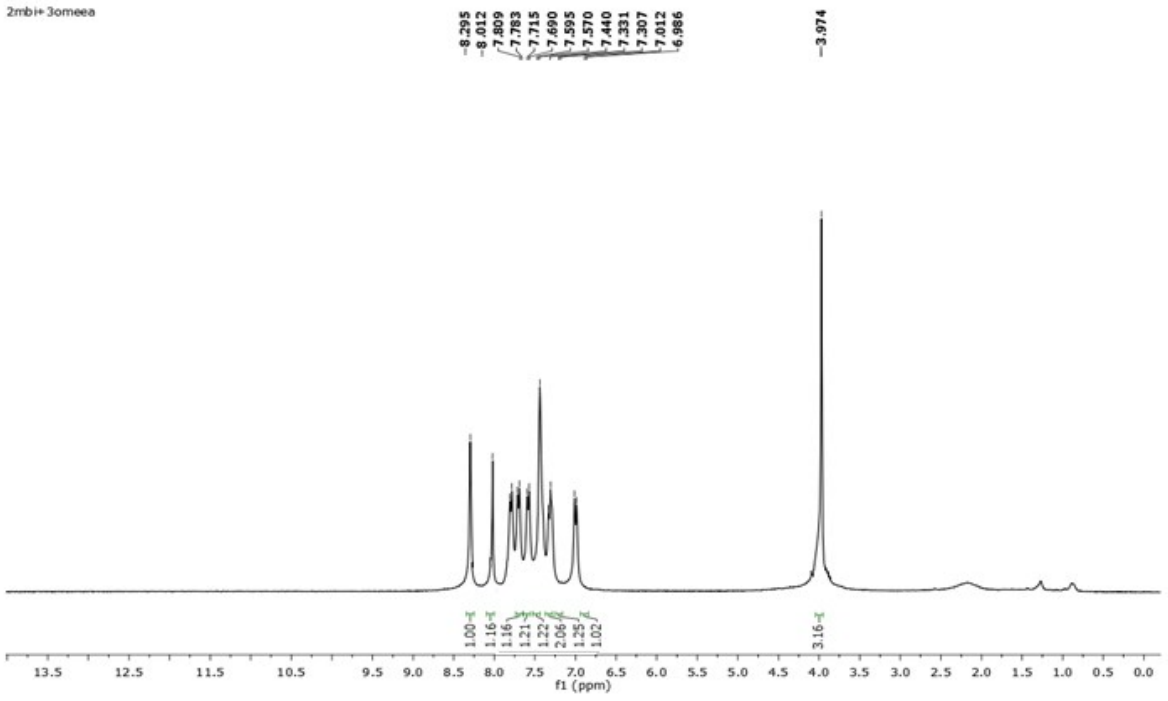
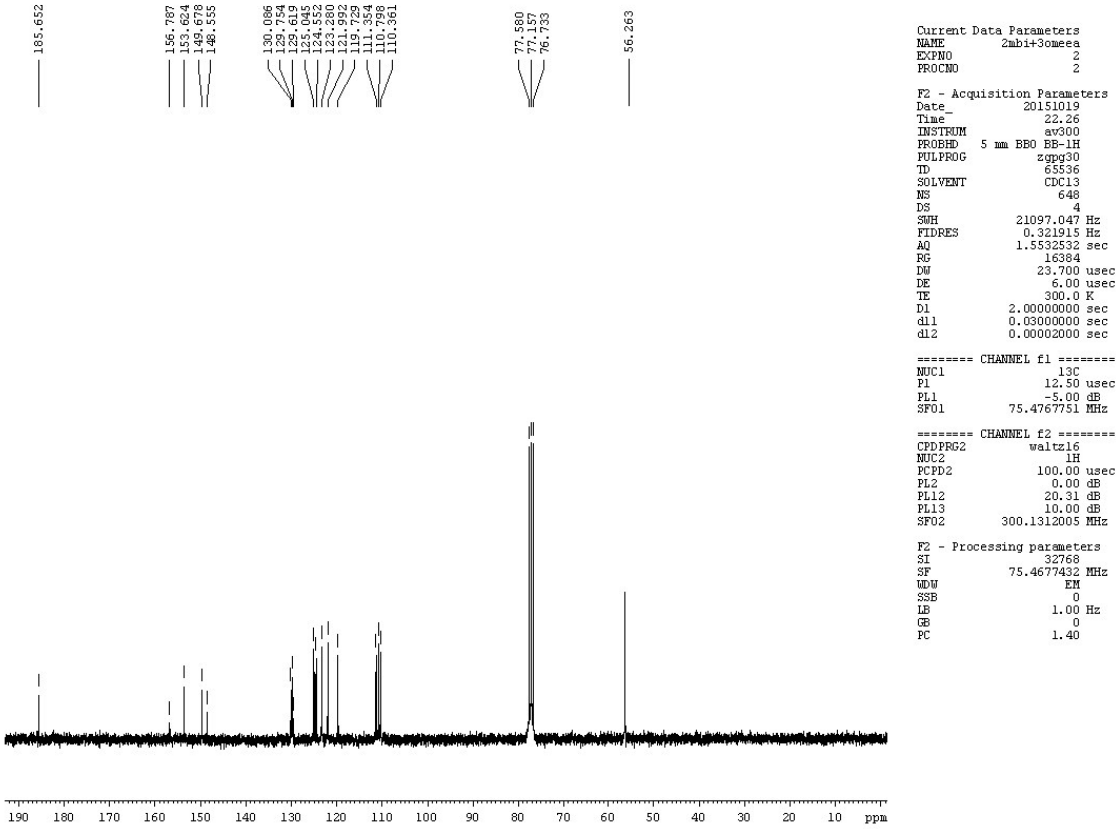


Figure S34.^{1}H spectrum of **SA-12.**




```
Current Data Parameters
NAME          2mbi+3omeea
EXPNO                   2
PROCNO                  2

F2 - Acquisition Parameters
Date_            20151019
Time                22.26
INSTRUM             av300
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  648
DS                    4
SWH           21097.047 Hz
FIDRES         0.321915 Hz
AQ             1.5532532 sec
RG                16384
DW               23.700 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                12.50 usec
PL1               -5.00 dB
SFO1         75.4767751 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           100.00 usec
PL2               0.00 dB
PL12             20.31 dB
PL13             10.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677432 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Figure S35.[13]C spectrum of **SA-12.**

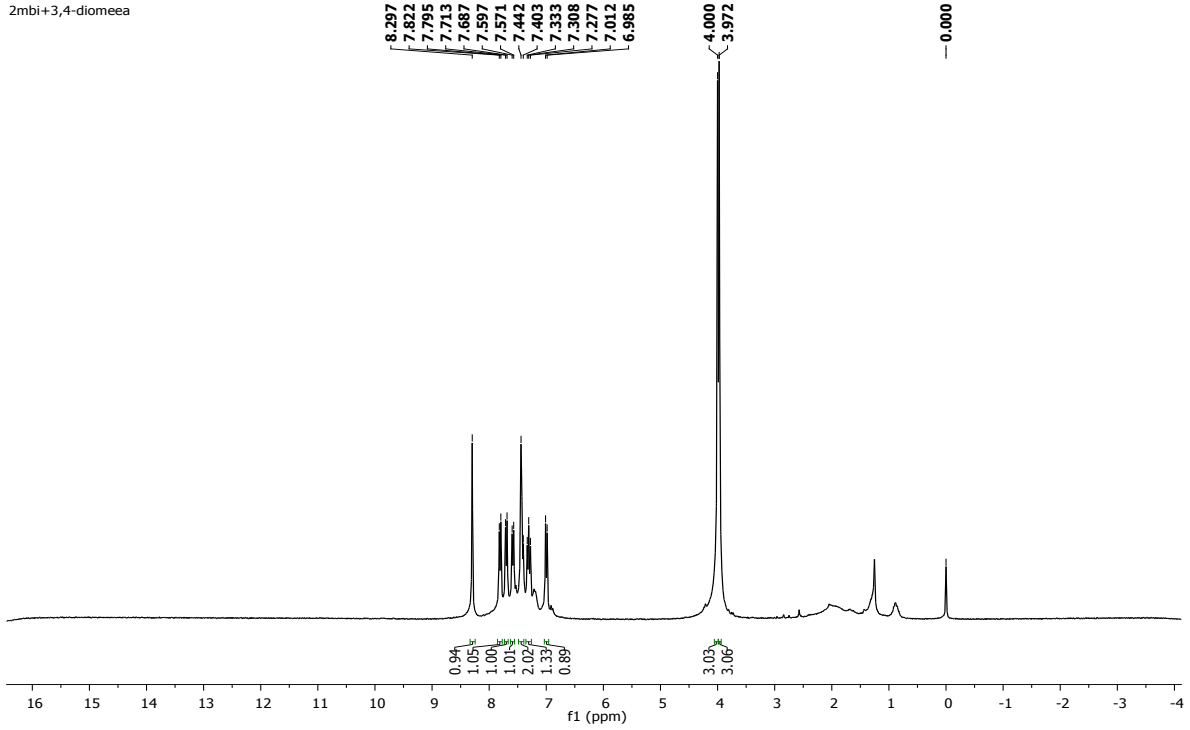


Figure S36.[1]H spectrum of **SA-13.**

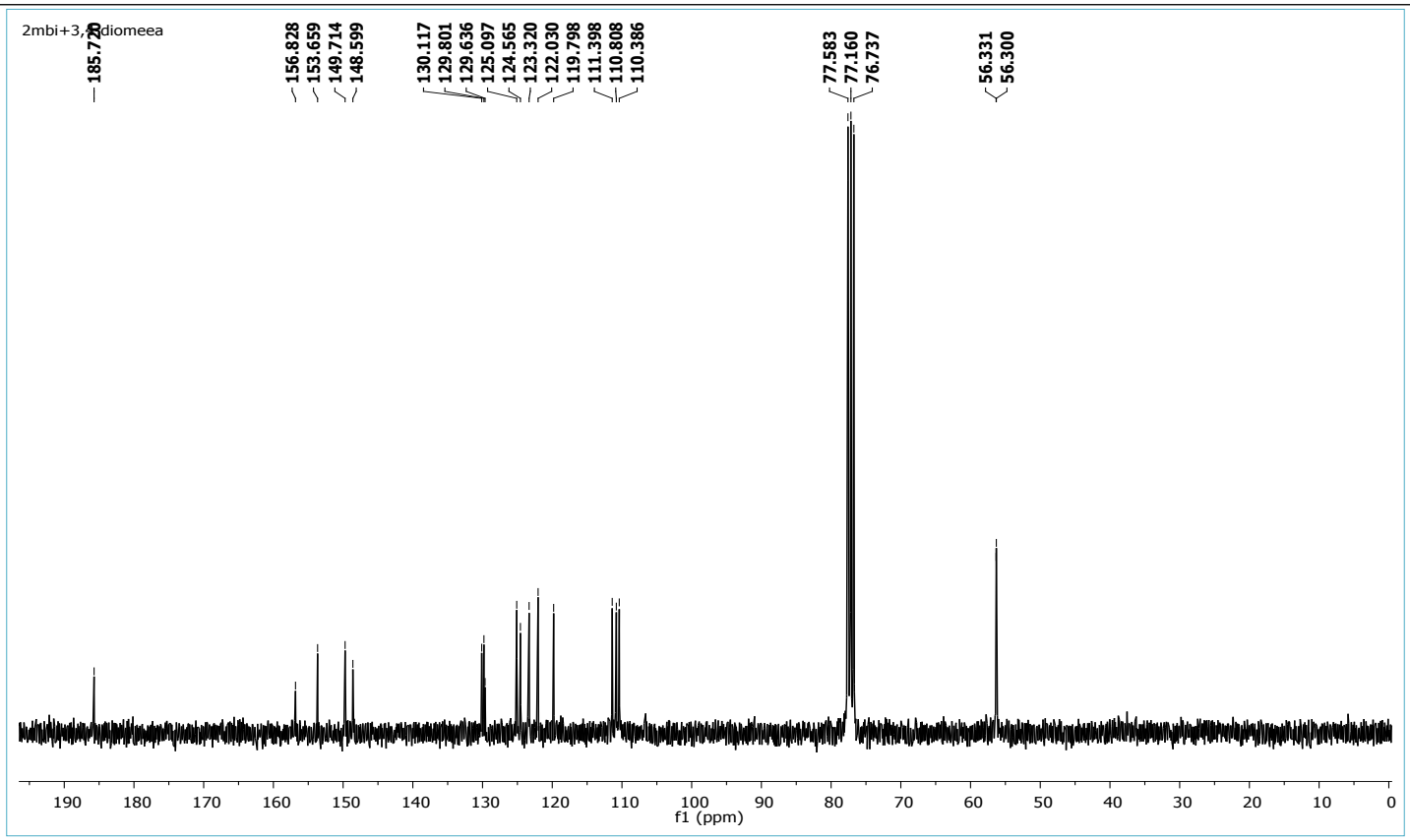


Figure S37.^{13}C spectrum of **SA-13.**

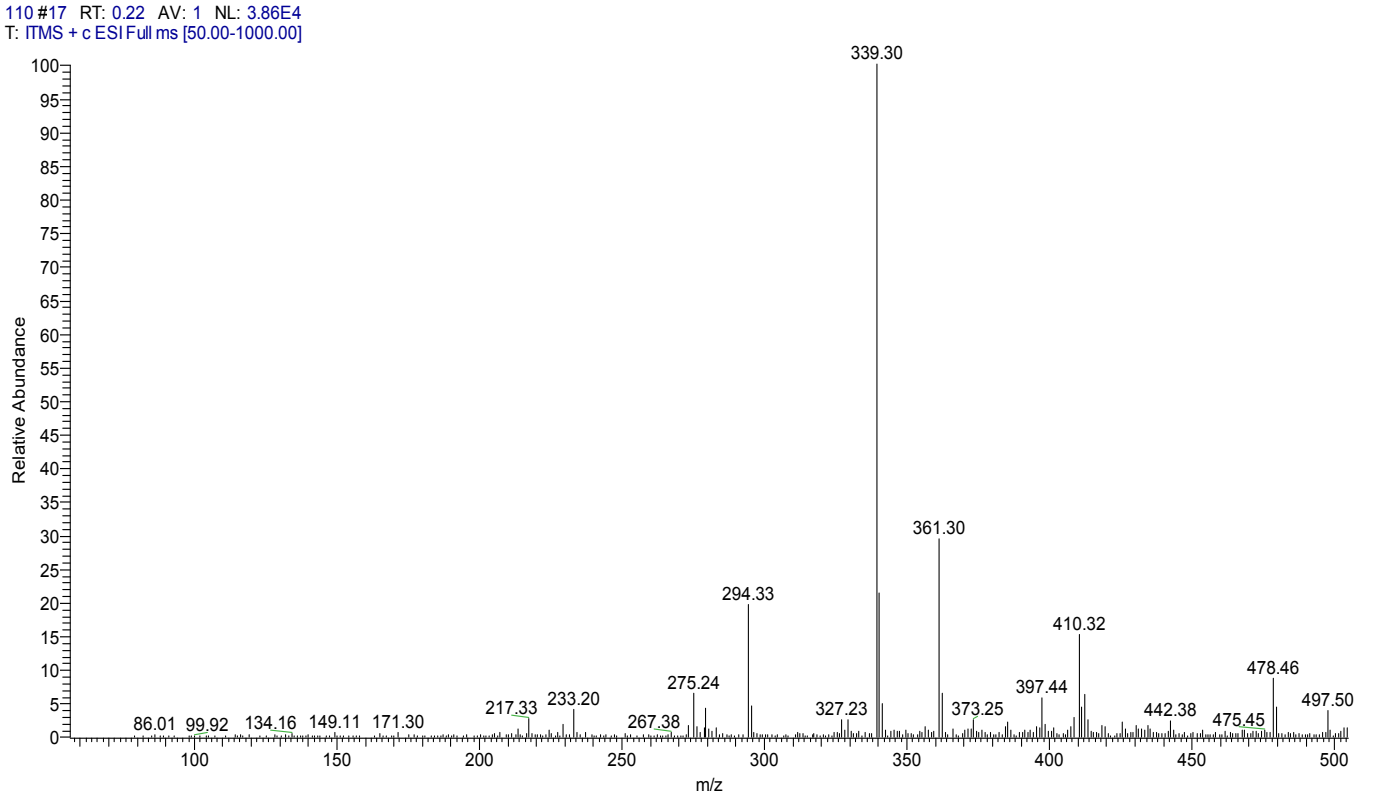
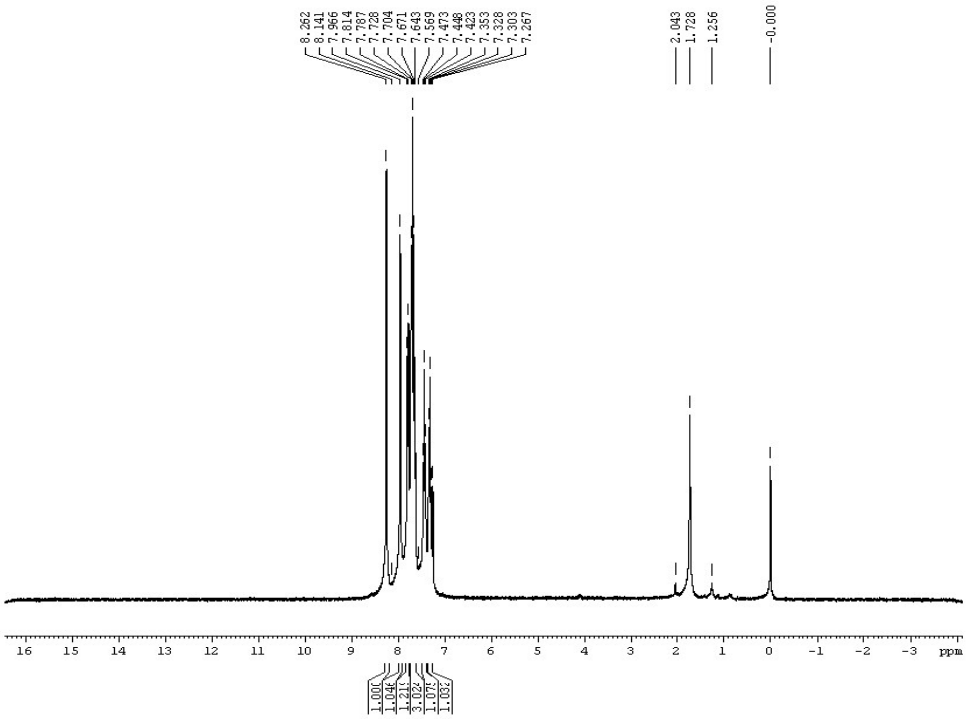


Figure S38.ESI-MASS Spectrum of **SA-13.**



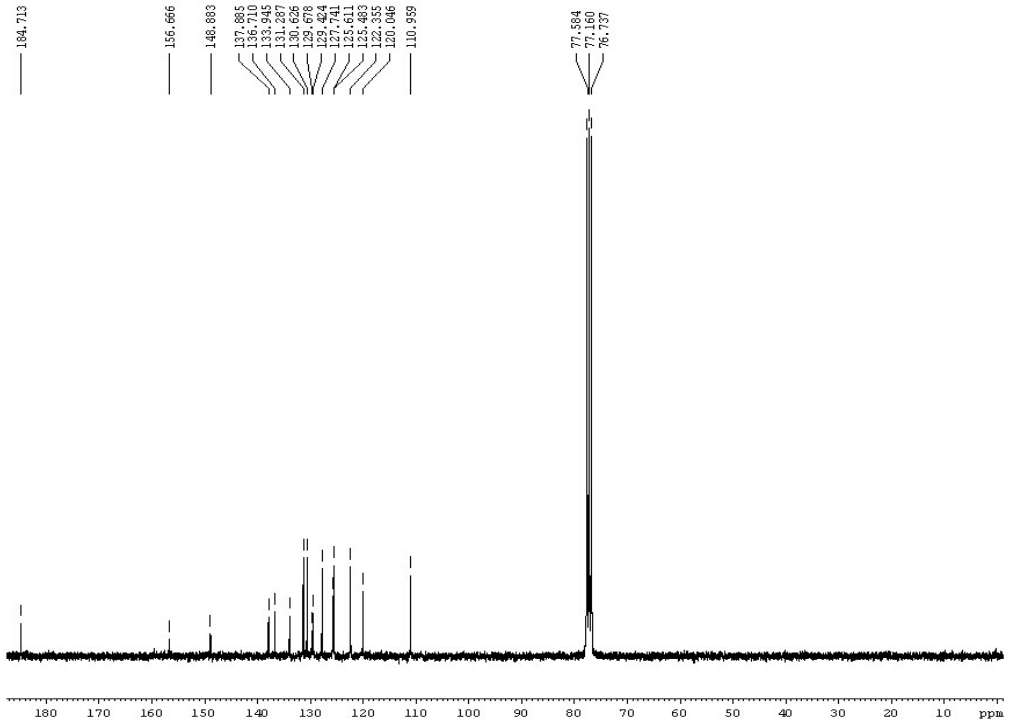

```
Current Data Parameters
NAME       2mbi+3,4diclearpt
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20151107
Time                   0.10
INSTRUM                av300
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        8
DS                        0
SWH                6172.839 Hz
FIDRES            0.188380 Hz
AQ                2.6542580 sec
RG                     161.3
DW                  81.000 usec
DE                   6.00 usec
TE                   300.0 K
D1                2.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     9.65 usec
PL1                    0.00 dB
SF01          300.1318534 MHz

F2 - Processing parameters
SI                        32768
SF               300.1300060 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

Figure S39.[1]H spectrum of **SA-14.**




```
Current Data Parameters
NAME       2mbi+3,4diclearpt
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_               20151107
Time                   0.57
INSTRUM                av300
PROBHD    5 mm BBO BB-1H
PULPROG            zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     3000
DS                        4
SWH               17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                    32768
DW                  27.800 usec
DE                   6.00 usec
TE                   300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
d12               0.00002000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                    12.50 usec
PL1                   -5.00 dB
SF01          75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                100.00 usec
PL2                    0.00 dB
PL12                  20.31 dB
PL13                  10.00 dB
SF02          300.1312005 MHz
```

Figure S40.[13]C spectrum of **SA-14.**

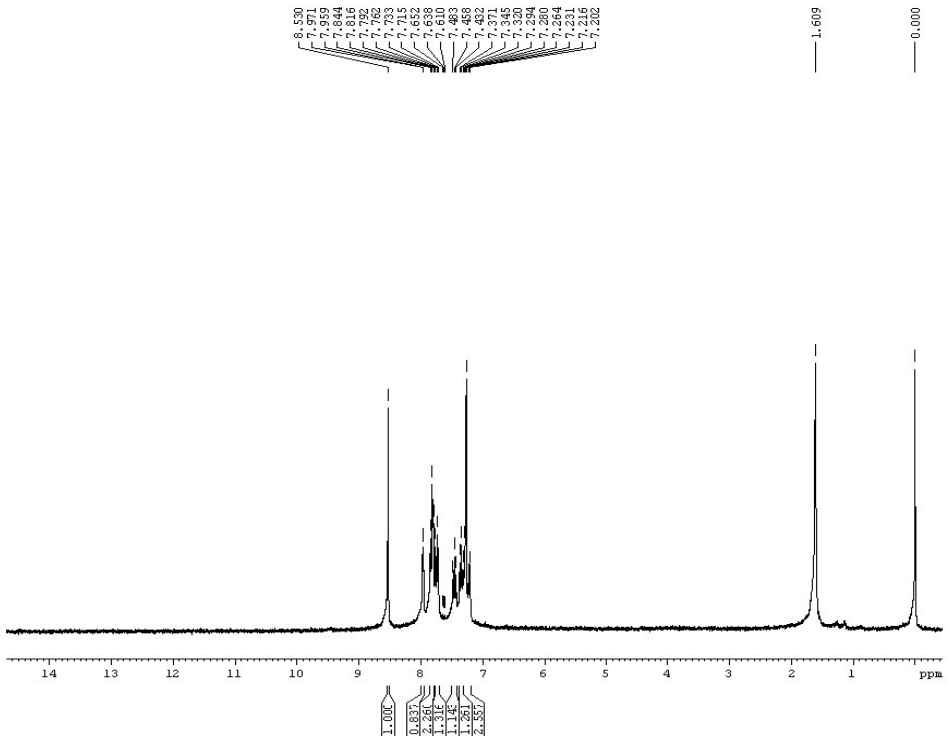


Figure S41.[1]H spectrum of **SA-15**.

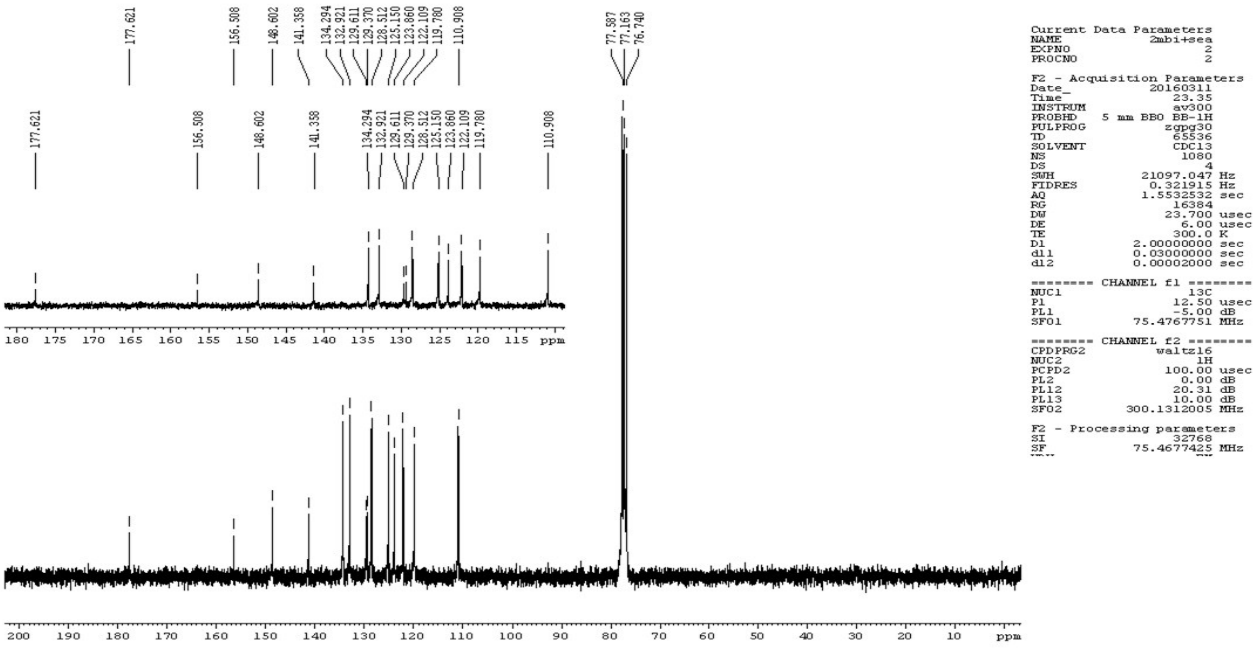


Figure S42.[13]C spectrum of **SA-15**.

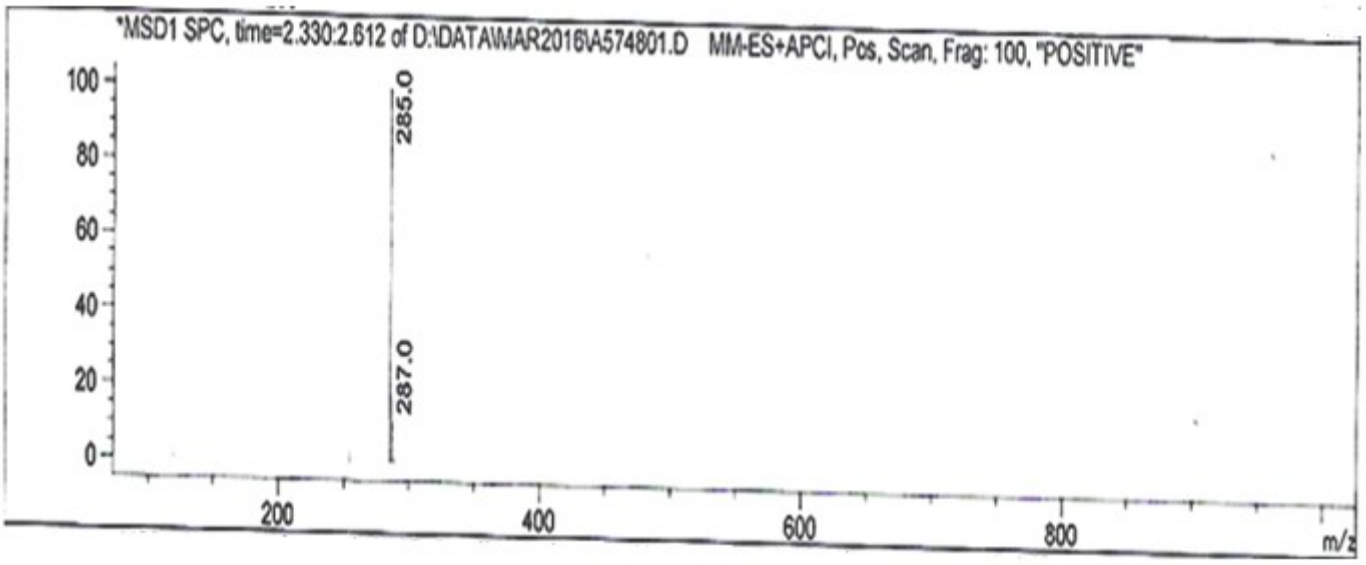


Figure S43.ESI-MASS Spectrum of **SA-15.**

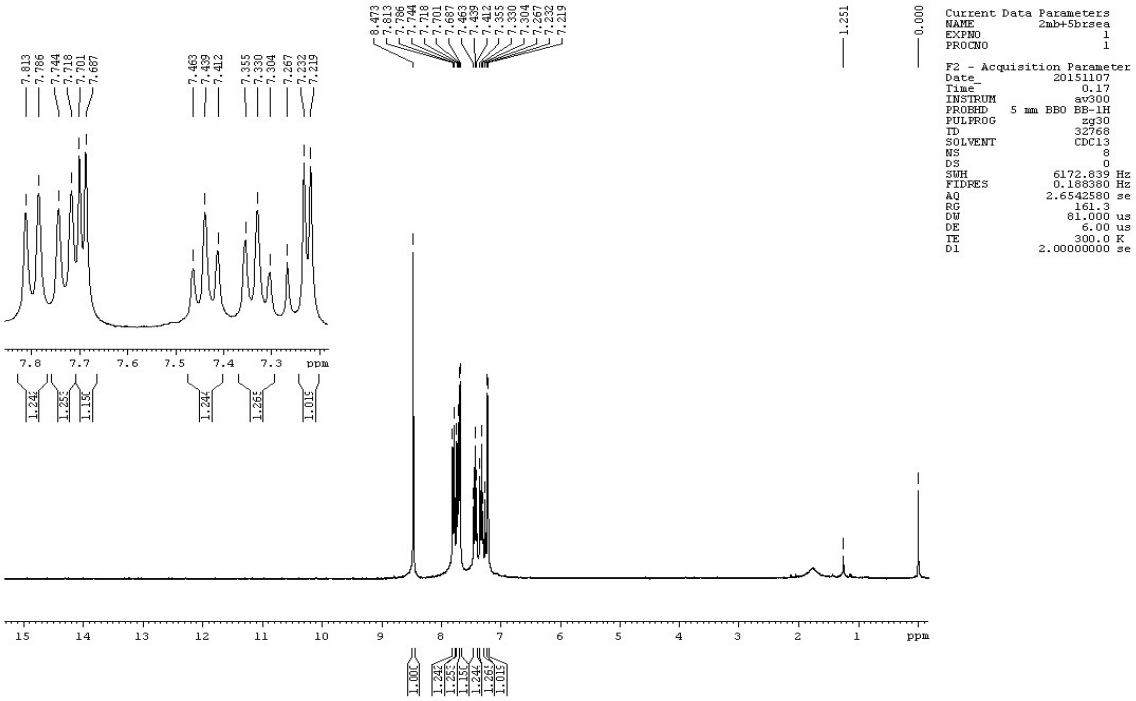


Figure S44.[1]H spectrum of **SA-16**.

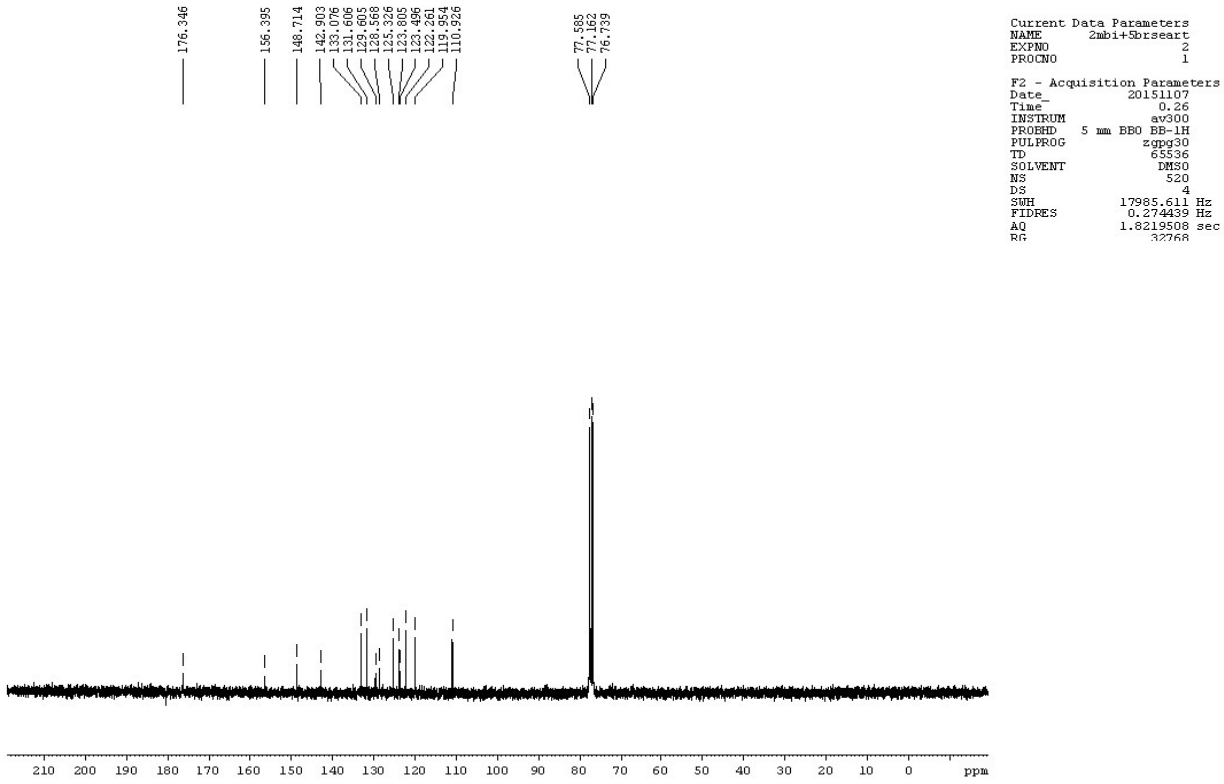


Figure S45.^{13}C spectrum of **SA-16**.

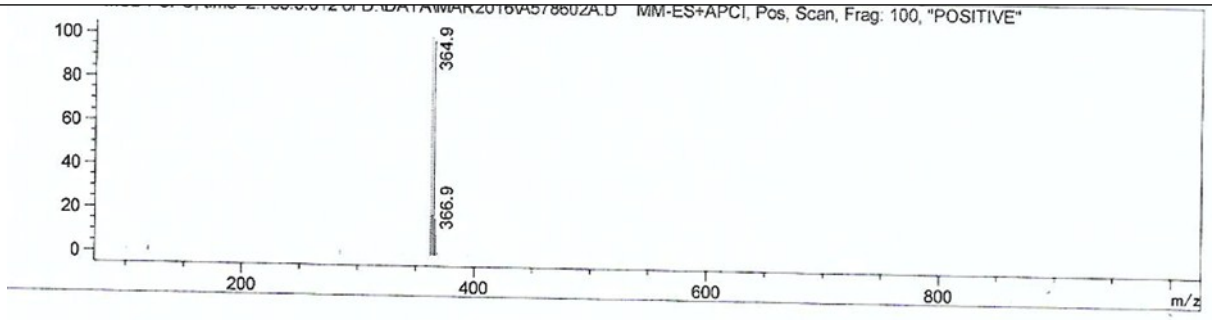


Figure S46.ESI-MASS Spectrum of **SA-16.**

4. Crystal Data:

1. Compound SA-2

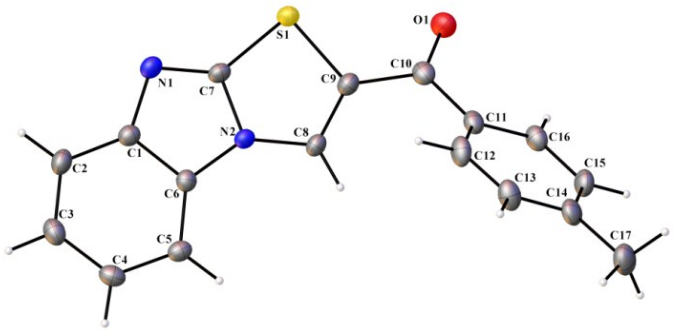


Figure.S47 ORTEP diagram of SA-2.

Table S1. Crystal data and structure refinement for PTB_151206_A1_MB1plus.

Identification code	mb1plus	
Empirical formula	C17 H12 N2 O S	
Formula weight	292.35	
Temperature	110.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 9.940(3) Å	α= 90°.
	b = 12.584(4) Å	β= 112.959(3)°.
	c = 11.973(4) Å	γ = 90°.
Volume	1379.0(7) $Å^3$	
Z	4	
Density (calculated)	1.408 Mg/m^3	
Absorption coefficient	0.234 mm^{-1}	
F(000)	608	
Crystal size	0.54 x 0.52 x 0.51 mm^3	
Theta range for data collection	2.271 to 27.585°.	
Index ranges	-12<=h<=12, -16<=k<=16, -15<=l<=15	
Reflections collected	15518	
Independent reflections	3174 [R(int) = 0.0560]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5972	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3174 / 0 / 192
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0389, wR2 = 0.0837
R indices (all data)	R1 = 0.0524, wR2 = 0.0905
Extinction coefficient	0.0276(19)
Largest diff. peak and hole	0.406 and -0.300 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for PTB_151206_A1_MB1plus. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	6291(1)	3722(1)	8437(1)	22(1)
O(1)	3001(1)	3985(1)	7536(1)	31(1)
N(1)	8923(2)	2833(1)	8517(1)	21(1)
N(2)	6872(1)	2747(1)	6799(1)	18(1)
C(1)	9194(2)	2288(1)	7603(1)	19(1)
C(2)	10481(2)	1816(1)	7644(2)	24(1)
C(3)	10456(2)	1320(1)	6605(2)	25(1)
C(4)	9191(2)	1277(1)	5542(2)	22(1)
C(5)	7895(2)	1724(1)	5482(1)	20(1)
C(6)	7939(2)	2228(1)	6526(1)	17(1)
C(7)	7534(2)	3071(1)	7992(1)	18(1)
C(8)	5426(2)	3020(1)	6221(1)	18(1)
C(9)	4929(2)	3551(1)	6965(1)	20(1)
C(10)	3410(2)	3865(1)	6701(2)	22(1)
C(11)	2403(2)	4012(1)	5411(2)	20(1)
C(12)	2877(2)	4418(1)	4547(2)	25(1)
C(13)	1908(2)	4575(1)	3364(2)	26(1)
C(14)	437(2)	4323(1)	2998(2)	24(1)
C(15)	-33(2)	3914(1)	3867(2)	25(1)
C(16)	923(2)	3770(1)	5056(2)	22(1)
C(17)	-614(2)	4507(2)	1707(2)	33(1)

Table S3. Bond lengths [Å] and angles [°] for PTB_151206_A1_MB1plus.

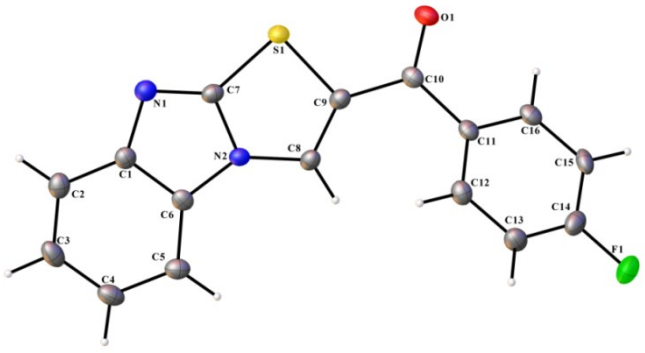
S(1)-C(7)	1.7306(17)
S(1)-C(9)	1.7675(17)
O(1)-C(10)	1.226(2)
N(1)-C(1)	1.404(2)
N(1)-C(7)	1.309(2)
N(2)-C(6)	1.389(2)
N(2)-C(7)	1.381(2)
N(2)-C(8)	1.373(2)
C(1)-C(2)	1.394(2)
C(1)-C(6)	1.403(2)
C(2)-H(2)	0.9500
C(2)-C(3)	1.383(2)
C(3)-H(3)	0.9500
C(3)-C(4)	1.398(2)
C(4)-H(4)	0.9500
C(4)-C(5)	1.382(2)
C(5)-H(5)	0.9500
C(5)-C(6)	1.387(2)
C(8)-H(8)	0.9500
C(8)-C(9)	1.351(2)
C(9)-C(10)	1.471(2)
C(10)-C(11)	1.488(2)
C(11)-C(12)	1.391(2)
C(11)-C(16)	1.397(2)
C(12)-H(12)	0.9500
C(12)-C(13)	1.381(2)
C(13)-H(13)	0.9500
C(13)-C(14)	1.390(2)
C(14)-C(15)	1.395(2)
C(14)-C(17)	1.508(2)
C(15)-H(15)	0.9500
C(15)-C(16)	1.380(2)
C(16)-H(16)	0.9500
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800

C(7)-S(1)-C(9)	89.80(8)
C(7)-N(1)-C(1)	103.02(13)
C(7)-N(2)-C(6)	106.40(13)
C(8)-N(2)-C(6)	138.13(14)
C(8)-N(2)-C(7)	115.47(13)
C(2)-C(1)-N(1)	129.30(15)
C(2)-C(1)-C(6)	118.96(15)
C(6)-C(1)-N(1)	111.73(14)
C(1)-C(2)-H(2)	121.1
C(3)-C(2)-C(1)	117.78(15)
C(3)-C(2)-H(2)	121.1
C(2)-C(3)-H(3)	119.0
C(2)-C(3)-C(4)	122.07(16)
C(4)-C(3)-H(3)	119.0
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-C(3)	121.36(15)
C(5)-C(4)-H(4)	119.3
C(4)-C(5)-H(5)	122.0
C(4)-C(5)-C(6)	115.97(15)
C(6)-C(5)-H(5)	122.0
N(2)-C(6)-C(1)	104.23(13)
C(5)-C(6)-N(2)	131.91(15)
C(5)-C(6)-C(1)	123.85(15)
N(1)-C(7)-S(1)	134.98(13)
N(1)-C(7)-N(2)	114.62(14)
N(2)-C(7)-S(1)	110.40(11)
N(2)-C(8)-H(8)	124.1
C(9)-C(8)-N(2)	111.81(14)
C(9)-C(8)-H(8)	124.1
C(8)-C(9)-S(1)	112.51(12)
C(8)-C(9)-C(10)	126.86(15)
C(10)-C(9)-S(1)	120.26(12)
O(1)-C(10)-C(9)	119.80(15)
O(1)-C(10)-C(11)	121.87(15)
C(9)-C(10)-C(11)	118.32(14)
C(12)-C(11)-C(10)	122.17(15)
C(12)-C(11)-C(16)	118.37(16)

C(16)-C(11)-C(10)	119.43(15)
C(11)-C(12)-H(12)	119.6
C(13)-C(12)-C(11)	120.88(16)
C(13)-C(12)-H(12)	119.6
C(12)-C(13)-H(13)	119.4
C(12)-C(13)-C(14)	121.15(16)
C(14)-C(13)-H(13)	119.4
C(13)-C(14)-C(15)	117.80(16)
C(13)-C(14)-C(17)	120.76(16)
C(15)-C(14)-C(17)	121.42(16)
C(14)-C(15)-H(15)	119.3
C(16)-C(15)-C(14)	121.41(16)
C(16)-C(15)-H(15)	119.3
C(11)-C(16)-H(16)	119.8
C(15)-C(16)-C(11)	120.37(16)
C(15)-C(16)-H(16)	119.8
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5

Symmetry transformations used to generate equivalent atoms:

2. Compound SA-6



FigureS48. ORTEP diagram of SA-6.

Table S4. Crystal data and structure refinement for PTB_151206_A1_2MB14Fea.

Identification code	2mb14fea	
Empirical formula	C16 H9 F N2 O S	
Formula weight	296.31	
Temperature	110.15 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.3722(18) Å	α= 90°.
	b = 11.278(3) Å	β= 90°.
	c = 17.837(5) Å	γ = 90°.
Volume	1281.8(6) $Å^3$	
Z	4	
Density (calculated)	1.535 Mg/m^3	
Absorption coefficient	0.264 mm^{-1}	
F(000)	608	
Crystal size	0.57 x 0.48 x 0.46 mm^3	
Theta range for data collection	2.136 to 27.563°.	
Index ranges	-8<=h<=8, -14<=k<=14, -23<=l<=23	
Reflections collected	14858	
Independent reflections	2957 [R(int) = 0.0463]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6640	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2957 / 0 / 190	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0362, wR2 = 0.0737	
R indices (all data)	R1 = 0.0420, wR2 = 0.0770	
Absolute structure parameter	0.01(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.210 and -0.278 $e.Å^{-3}$	

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for PTB_151206_A1_2MB14Fea. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	9153(1)	8505(1)	3722(1)	18(1)
F(1)	-1811(3)	8690(2)	1384(1)	33(1)
O(1)	6502(3)	10245(2)	2974(1)	22(1)
N(1)	10345(3)	6568(2)	4603(1)	19(1)
N(2)	7037(3)	6688(2)	4141(1)	15(1)
C(1)	9141(5)	5591(2)	4835(1)	18(1)
C(2)	9722(5)	4640(2)	5286(2)	21(1)
C(3)	8226(5)	3786(2)	5438(2)	24(1)
C(4)	6195(5)	3852(2)	5143(2)	23(1)
C(5)	5580(5)	4785(2)	4691(1)	20(1)
C(6)	7085(4)	5644(2)	4556(1)	16(1)
C(7)	9017(4)	7175(2)	4205(1)	17(1)
C(8)	5655(4)	7320(2)	3708(1)	17(1)
C(9)	6545(4)	8310(2)	3421(1)	17(1)
C(10)	5631(4)	9281(2)	2984(1)	17(1)
C(11)	3649(4)	9085(2)	2560(1)	17(1)
C(12)	3148(5)	7993(2)	2241(2)	20(1)
C(13)	1319(5)	7860(2)	1834(2)	23(1)
C(14)	26(5)	8821(3)	1760(2)	23(1)
C(15)	472(4)	9921(2)	2057(2)	21(1)
C(16)	2308(5)	10047(2)	2456(1)	18(1)

Table S6. Bond lengths [Å] and angles [°] for PTB_151206_A1_2MB14Fea.

S(1)-C(7)	1.731(3)
S(1)-C(9)	1.760(3)
F(1)-C(14)	1.357(3)
O(1)-C(10)	1.221(3)
N(1)-C(1)	1.405(3)
N(1)-C(7)	1.300(3)
N(2)-C(6)	1.391(3)
N(2)-C(7)	1.382(3)
N(2)-C(8)	1.371(3)
C(1)-C(2)	1.391(4)
C(1)-C(6)	1.402(4)
C(2)-H(2)	0.9500
C(2)-C(3)	1.383(4)
C(3)-H(3)	0.9500
C(3)-C(4)	1.398(4)
C(4)-H(4)	0.9500
C(4)-C(5)	1.383(4)
C(5)-H(5)	0.9500
C(5)-C(6)	1.384(4)
C(8)-H(8)	0.9500
C(8)-C(9)	1.352(4)
C(9)-C(10)	1.466(4)
C(10)-C(11)	1.488(4)
C(11)-C(12)	1.393(4)
C(11)-C(16)	1.394(4)
C(12)-H(12)	0.9500
C(12)-C(13)	1.382(4)
C(13)-H(13)	0.9500
C(13)-C(14)	1.368(4)
C(14)-C(15)	1.378(4)
C(15)-H(15)	0.9500
C(15)-C(16)	1.377(4)
C(16)-H(16)	0.9500
C(7)-S(1)-C(9)	89.76(13)
C(7)-N(1)-C(1)	102.6(2)

C(7)-N(2)-C(6)	105.8(2)
C(8)-N(2)-C(6)	139.0(2)
C(8)-N(2)-C(7)	115.2(2)
C(2)-C(1)-N(1)	129.0(3)
C(2)-C(1)-C(6)	119.1(3)
C(6)-C(1)-N(1)	111.9(2)
C(1)-C(2)-H(2)	121.1
C(3)-C(2)-C(1)	117.8(3)
C(3)-C(2)-H(2)	121.1
C(2)-C(3)-H(3)	119.1
C(2)-C(3)-C(4)	121.8(3)
C(4)-C(3)-H(3)	119.1
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-C(3)	121.5(3)
C(5)-C(4)-H(4)	119.3
C(4)-C(5)-H(5)	122.0
C(4)-C(5)-C(6)	116.0(3)
C(6)-C(5)-H(5)	122.0
N(2)-C(6)-C(1)	104.2(2)
C(5)-C(6)-N(2)	132.0(3)
C(5)-C(6)-C(1)	123.8(3)
N(1)-C(7)-S(1)	134.1(2)
N(1)-C(7)-N(2)	115.4(2)
N(2)-C(7)-S(1)	110.48(19)
N(2)-C(8)-H(8)	124.0
C(9)-C(8)-N(2)	111.9(2)
C(9)-C(8)-H(8)	124.0
C(8)-C(9)-S(1)	112.6(2)
C(8)-C(9)-C(10)	130.7(3)
C(10)-C(9)-S(1)	116.3(2)
O(1)-C(10)-C(9)	119.5(3)
O(1)-C(10)-C(11)	120.7(2)
C(9)-C(10)-C(11)	119.8(2)
C(12)-C(11)-C(10)	122.2(2)
C(12)-C(11)-C(16)	119.5(3)
C(16)-C(11)-C(10)	118.2(2)
C(11)-C(12)-H(12)	119.9
C(13)-C(12)-C(11)	120.3(3)

C(13)-C(12)-H(12)	119.9
C(12)-C(13)-H(13)	120.9
C(14)-C(13)-C(12)	118.2(3)
C(14)-C(13)-H(13)	120.9
F(1)-C(14)-C(13)	118.8(3)
F(1)-C(14)-C(15)	117.7(3)
C(13)-C(14)-C(15)	123.5(3)
C(14)-C(15)-H(15)	121.1
C(16)-C(15)-C(14)	117.8(3)
C(16)-C(15)-H(15)	121.1
C(11)-C(16)-H(16)	119.7
C(15)-C(16)-C(11)	120.6(3)
C(15)-C(16)-H(16)	119.7

Symmetry transformations used to generate equivalent atoms