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Supporting information

A one pot sequential five component domino reaction for expedient synthesis of polysubstituted pyrroles.

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General consideration

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.

General procedure for the synthesis of 2-(4-benzoyl-1, 2-diphenyl-1H-pyrrol-3-yl)-2-cyanoacetamide:

A 25 mL round bottom flask equipped with a magnetic stirrer was charged with acetophenone 1 (1.0 mmol), DMF-DMA **2** (1.0 mmol), the reaction mixture was heated on an oil bath at 100 °C for 1 h. after one hour the reaction colour was changed colourless to reddish-brown, then other reactants amine **3** (1.0 mmol), arylglyoxal **4** (1.0 mmol) and malanonitrile **5**(1.0 mmol) in methanol 5mL was added reaction system, the reaction was stirred 60-70 °C for 30 min. The completion of the reaction was monitored by TLC. After completion of the reaction, the mixture was cooled to room temperature and the solid product was filtered, washed with a small portion of cold ethanol to obtain pure product **6aa-au**. Analytical and spectroscopic data of the series of 2-(4-benzoyl-1, 2-diphenyl-1H-pyrrol-3-yl)-2-cyanoacetamide are given below.

*4.2.1 2-(4-benzoyl-2-(4-methoxyphenyl)-1-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (**6aa**).*

White solid, mp; 215-217 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.90 (d, *J* = 7.2 Hz, 2H), 7.67 (s, 1H), 7.58 (d, *J* = 6.6 Hz, 1H), 7.53-7.48 (m, 2H), 7.36 (s, 1H), 7.29 (broad, 3H), 7.20 (d, *J* = 7.5 Hz, 2H), 7.10 (broad, 2H), 6.86 (d, *J* = 7.8 Hz, 2H), 5.77 (s, 1H), 5.10 (s, 1H), 3.80 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.9, 167.3, 160.1, 139.5, 138.6, 136.9, 132.5, 132.2, 131.4, 129.3, 129.3, 128.5, 128.1, 125.8, 121.7, 120.7, 116.5, 114.1, 113.2, 55.3, 36.4 ppm. MS m/z 435.48 (M^++1). Anal. Calcd for $C_{27}H_{21}N_3O_3$: C, 74.47; H, 4.86; N, 9.65; found C, 74.41; H, 4.80; N, 9.58.

4.2.2 2-(4-benzoyl-1-(4-chlorophenyl)-2-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (***6ab***).

White solid, mp; 238-240 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.90 (d, *J* = 7.8 Hz, 2H), 7.61-7.58 (m, 2H), 7.54-7.48 (m, 3H), 7.38-7.36 (m, 4H), 7.29- 7.26 (m, 3H), 7.07 (d, *J* = 8.7 Hz, 2H), 6.84 (s, 1H), 5.08 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 190.9, 166.5, 139.0, 136.7, 136.2, 133.6, 132.0, 130.8, 130.7, 129.2, 128.9, 128.8, 128.5, 128.3, 128.2, 126.7, 121.6, 116.4, 113.7, 36.0 ppm. MS m/z 439.10 (M^++1). Anal. Calcd for $C_{26}H_{18}ClN_3O_2$: C, 70.99; H, 4.12; N, 9.55; found C, 70.92; H, 4.85; N, 9.48.

*4.2.3 2-(4-benzoyl-1, 2-bis(4-chlorophenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6ac**).*

White solid, mp; 186-188 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.89 (d, *J* = 8.7 Hz, 2H), 7.62-7.49 (m, 5H), 7.39 (s, 1H), 7.37-7.32 (m, 3H), 7.29-7.26 (m, 3H), 7.08 (d, *J* = 8.7 Hz, 2H), 5.08 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 190.6, 166.1, 138.9, 136.6, 136.0, 133.4, 131.7, 130.6, 129.0, 128.7, 128.6, 128.3, 128.1, 126.7, 121.4, 116.3, 113.6, 35.8 ppm. MS m/z 474.34 (M^++1). Anal. Calcd for $C_{26}H_{17}ClN_3O_2$: C, 65.84; H, 3.61; N, 8.86; found C, 65.79; H, 3.55; N, 8.80.

*4.2.4 2-(4-benzoyl-1-(3-chlorophenyl)-2-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (**6ad**).*

White solid, mp; 188-190 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.90 (d, *J* = 6.9 Hz, 2H), 7.60-7.49 (m, 5H), 7.37 (broad, 4H), 7.28-7.26 (m, 3H), 7.20 (d, *J* = 8.1 Hz, 1H), 6.91 (d, *J* = 7.2 Hz, 1H), 5.82 (s, 1H), 5.05 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.7, 166.9, 139.5, 139.3, 136.8, 135.0, 132.4, 131.1, 130.3, 129.4, 129.2, 128.9, 128.6, 128.4, 128.3, 125.8, 124.2, 122.1, 116.4, 114.0, 36.2 ppm.

MS m/z 439.10 (M^++1). Anal. Calcd for $C_{26}H_{18}ClN_3O_2$: C, 70.99; H, 4.12; N, 9.55; found C, 70.92; H, 4.06; N, 9.48.

*4.2.5 2-(1-(3-chlorophenyl)-4-(4-methoxybenzoyl)-2-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (**6ae**).*

White solid, mp; 170-173 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.93 (d, *J* = 8.7 Hz, 2H), 7.38-7.36 (m, 4H), 7.28-7.26 (m, 4H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.01 (d, *J* = 8.7 Hz, 2H), 6.91(d, *J* = 7.8 Hz, 1H), 5.79 (s, 1H), 5.04 (s, 1H), 3.90 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.7, 166.9, 139.5, 139.3, 136.8, 135.0, 132.4, 131.1, 130.3, 129.4, 129.2, 128.6, 128.4, 128.3, 125.8, 124.2, 122.1, 116.4, 114.0, 36.2 ppm. MS m/z 469.11 (M^++1). Anal. Calcd for $C_{27}H_{20}ClN_3O_3$: C, 69.01; H, 4.29; N, 8.94; found C, 69.01; H, 4.29; N, 8.94.

*4.2.6 2-(2-(4-bromophenyl)-1-(3-chlorophenyl)-4-(4-methoxybenzoyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6af**).*

White solid, mp; 176-178 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.92 (d, *J* = 8.7 Hz, 2H), 7.87 (s, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.35 (s, 1H), 7.31-7.16 (m, 5H), 7.01 (d, *J* = 8.7 Hz, 2H), 6.89 (d, *J* = 7.8, Hz, 1H), 5.83 (s, 1H), 5.08 (s, 1H), 3.90 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 190.5, 167.0, 163.5, 139.4, 135.2, 135.1, 132.7, 132.1, 131.8, 131.6, 130.5, 128.6, 127.3, 125.9, 124.3, 124.0, 122.4, 114.4, 114.0, 55.6, 36.2 ppm. MS m/z 547.02 (M^++1). Anal. Calcd for $C_{27}H_{19}BrClN_3O_3$: C, 59.09; H, 3.49; N, 7.66; found C, 59.01; H, 3.43; N, 7.60.

*4.2.7 2-(4-benzoyl-2-phenyl-1-(p-tolyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6ag**).*

White solid, mp; 225-227 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.89 (d, *J* = 7.8 Hz, 2H), 7.61-7.56 (m, 2H), 7.53-7.48 (m, 2H), 7.39-7.33 (m, 4H), 7.28-7.26 (m, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 6.97 (d, *J* = 8.4 Hz, 2H), 6.63 (s, 1H), 5.10 (s, 1H), 2.30 (s, 3H) ppm; ^{13}C NMR (75MHz, $CDCl_3$) δ: 191.1, 166.7, 139.1, 137.8, 136.3, 135.6, 131.8, 131.2, 130.7, 129.5, 128.8, 128.6, 128.5, 128.2, 128.2, 125.2, 121.1, 116.4, 113.1, 36.0, 20.7 ppm. MS m/z 419.16 (M^++1). Anal. Calcd for $C_{27}H_{21}N_3O_2$: C, 77.31; H, 5.05; N, 10.02; found C, 77.24; H, 4.99.; N, 9.95.

*4.2.8 2-cyano-2-(4-(4-methoxybenzoyl)-2-phenyl-1-(p-tolyl)-1H-pyrrol-3-yl)acetamide (**6ah**).*

White solid, mp; 148-150 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.93 (d, *J* = 8.7 Hz, 2H), 7.76 (s, 1H), 7.34-7.33 (m, 4H), 7.26 (broad, 2H), 7.07 (d, *J* = 8.1 Hz, 2H), 6.97 (t, *J* = 7.2 Hz, 4H), 5.78 (s, 1H), 5.06 (s, 1H), 3.89 (s, 3H), 2.31 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 190.6, 167.3, 153.2, 138.1, 136.5, 136.1, 132.0, 131.7, 131.2, 130.8, 129.9, 129.0, 128.8, 128.6, 125.5, 121.7, 116.5, 113.8, 113.4, 55.6, 36.4, 21.1 ppm. MS m/z 449.17 (M^++1). Anal. Calcd for $C_{28}H_{23}N_3O_3$: C, 74.82; H, 5.16; N, 9.35; found C, 74.75; H, 5.10.; N, 9.27.

*4.2.9 2-(2-(4-bromophenyl)-4-(4-methoxybenzoyl)-1-(p-tolyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6ai**).*

White solid, mp; 167-169 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.93 (d, *J* = 8.7 Hz, 2H), 7.81 (s, 1H), 7.35-7.33 (m, 5H), 7.28-7.26 (m, 1H), 7.07 (d, *J* = 8.1 Hz, 2H), 7.01-6.96 (m, 3H), 5.68 (s, 1H), 5.07 (s, 1H), 3.89 (s, 3H), 2.31 (s, 3H) ppm; 13C NMR (75 MHz, $CDCl_3$) δ: 190.6, 167.3, 163.2, 138.1, 136.6, 136.1, 132.0, 131.7, 131.2, 130.8, 129.9, 129.0, 128.9, 128.6, 125.6, 121.8, 113.8, 113.5, 55.6, 36.4, 21.1 ppm. MS m/z 527.08 (M^++1). Anal. Calcd for $C_{28}H_{22}BrN_3O_3$: C, 63.65; H, 4.20; N, 7.95; found C, 63.61; H, 4.15; N, 7.91.

*4.2.10 2-(4-benzoyl-1-(3,5-dichlorophenyl)-2-phenyl-1H-pyrrol-3-yl)-2-cyanoacetamide (**6aj**).*

White solid, mp; 163-165 °C; 1H NMR (300 MHz, $CDCl_3$) δ: 7.89 (d, *J* = 7.2 Hz, 2H), 7.62-7.28 (m, 11H), 6.99 (s, 2H), 5.94 (s, 1H), 5.037 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.5, 166.8, 140.0, 139.0, 136.7, 135.5, 132.4, 131.0, 130.7, 129.6, 129.2, 129.0, 128.6, 128.4, 127.8, 124.3, 122.3, 116.2, 114.2, 36.0 ppm. MS m/z 474.34 (M^++1). Anal. Calcd for $C_{26}H_{17}Cl_2N_3O_2$: C, 65.84; H, 3.61; N, 8.86; found C, 65.80; H, 3.56; N, 8.81.

*4.2.11 2-(4-benzoyl-2-(4-chlorophenyl)-1-(3-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6ak**).*

White solid, mp; 195-197 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.89(d, *J* = 7.5 Hz, 2H), 7.70 (s, 1H), 7.59 (d, J = 6.3 Hz, 1H), 7.54-7.49 (m, 2H), 7.38 (s, 1H), 7.34 (d, *J* = 8.4, 2H), 7.27-7.19 (m, 3H), 6.84 (d, *J*= 8.4 Hz, 1H), 6.67 (d, *J* = 7.8 Hz, 1H), 6.58 (s, 1H), 5.80 (s, 1H), 5.10 (s, 1H), 3.67 (s, 3H)

ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ:191.9, 167.0, 160.2, 139.4, 139.3, 135.5, 132.5, 132.3, 131.7, 130.2, 129.2, 129.0, 128.6, 127.2, 121.8, 118.0, 116.2, 114.0, 113.9, 111.9, 55.5, 36.2 ppm. MS m/z 469.11(M^++1). Anal. Calcd for $C_{27}H_{20}ClN_3O_3$: C, 69.01; H, 4.29; N, 8.94; found C, 68.97; H, 4.25; N, 8.89.

*4.2.12 2-(4-benzoyl-2-(4-chlorophenyl)-1-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6al**).*

White solid, mp; 203-205 °C; ^1H NMR (300 MHz, $CDCl_3$) δ: 7.89 (d, *J* = 7.2 Hz, 2H), 7.73 (s, 1H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.53–7.48 (m, 2H), 7.33 (s, 1H), 7.32 (d, *J* = 7.2 Hz, 2H), 7.26-7.22 (m, 2H), 7.01 (d, *J*= 8.9 Hz, 2H), 6.80 (d, *J* = 8.9 Hz, 2H), 5.82 (s, 1H), 5.11(s, 1H), 3.78 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.8, 167.3, 159.3, 139.3, 135.6, 135.2, 132.5, 132.3, 131.9, 131.0, 129.2, 128.8, 128.5, 127.0, 121.4, 116.2, 114.5, 113.4, 55.5, 36.2, 29.7 ppm. MS m/z 469.11 (M^++1). MS m/z 469.11(M^++1). Anal. Calcd for $C_{27}H_{20}ClN_3O_3$: C, 69.01; H, 4.29; N, 8.94; found C, 68.97; H, 4.26; N, 8.91.

*4.2.13 2-(4-benzoyl-2-(4-chlorophenyl)-1-(2-hydroxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6am**).*

Brown solid, mp; 155-157 °C; ^1H NMR (300 MHz, $CDCl_3$) δ: 7.84 (d, *J* = 7.2 Hz, 2H), 7.56-7.54 (m, 2H), 7.48–7.43 (m, 2H), 7.33 (s, 1H), 7.18 (broad, 5H), 7.09 (d, *J* = 7.8 Hz, 1H), 6.86-6.82 (m, 2H), 5.87 (s, 1H), 5.07 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.9, 168.2, 151.9, 139.0, 136.7, 135.1, 133.2, 132.3, 131.9, 130.6, 129.2, 128.7, 128.5, 127.0, 125.2, 121.2, 120.2, 117.4, 116.3, 112.2, 36.4 ppm. MS m/z 455.10 (M^++1). Anal. Calcd for $C_{26}H_{18}ClN_3O_3$: C, 68.50; H, 3.98; N, 9.22; found C, 68.46; H, 3.95; N, 9.18.

*4.2.14 2-(4-benzoyl-2-(4-chlorophenyl)-1-(4-hydroxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6an**).*

White solid, mp;148-150 °C; ^1H NMR (300 MHz, $CDCl_3$) δ: 7.85 (d, *J* = 7.2 Hz, 2H), 7.73 (s, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 2H), 7.28-7.23 (m, 3H), 7.17 (d, *J* = 8.1 Hz, 2H), 7.10 (s,

1H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.70 (d, J = 8.7 Hz, 2H), 5.94 (s, 1H), 5.13 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 192.0, 167.4, 156.3, 139.0, 135.6, 135.1, 132.3, 132.0, 130.3, 129.1,128.7, 128.4, 127.0, 121.1, 116.0, 112.9, 36.1 ppm. MS m/z 455.10 (M^++1). Anal. Calcd for $C_{26}H_{18}ClN_3O_3$: C, 68.50; H, 3.98; N, 9.22; found C, 68.47; H, 3.94; N, 9.17.

*4.2.15 2-(4-benzoyl-1-(4-hydroxyphenyl)-2-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6ao**).*

White solid, mp; 113-115 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.84 (d, *J* = 8.4 Hz, 2H), 7.54 (t, *J* = 7.2 Hz, 2H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.26 (s, 1H), 7.20 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.79 (d, *J* = 9.0 Hz, 2H), 6.69 (d, *J* = 8.7 Hz, 2H), 5.94 (s, 1H), 5.08 (s, 1H), 3.72 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 192.2, 167.9, 160.0, 156.2, 139.3, 137.1, 132.4, 132.3,132.3, 131.7, 131.0, 129.2, 128.5, 127.1, 121.1, 120.7, 116.0, 114.1, 112.5, 55.2, 36.6 ppm. MS m/z 451.15 (M^++1). Anal. Calcd for $C_{27}H_{21}N_3O_4$: C, 71.83; H, 4.69; N, 9.31; found C, 71.79; H, 4.65; N, 9.28.

*4.2.16 2-(4-benzoyl-1-(4-iodophenyl)-2-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6ap**).*

White solid, mp; 225-227 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.88 (d, *J* = 8.4 Hz, 2H), 7.63-7.57 (m, 4H), 7.53-7.48 (m, 2H), 7.32 (s, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 5.81 (s, 1H), 5.06 (s, 1H), 3.82 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.8, 167.1, 160.3, 139.3, 138.5, 138.3, 136.7, 132.5, 132.4, 130.9, 129.3, 128.6, 127.4, 122.0, 120.3, 116.4, 114.3, 113.7, 93.5, 55.3, 36.3 ppm. MS m/z 561.05 (M^++1). Anal. Calcd for $C_{27}H_{20}IN_3O_3$: C, 57.77; H, 3.59; N, 7.49; found C, 57.73; H, 3.56; N, 7.45.

*4.2.17 2-(4-benzoyl-1-(4-ethylphenyl)-2-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6aq**).*

White solid, mp; 167-169 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.89 (d, *J* = 7.5 Hz, 2H), 7.66 (s, 1H), 7.60-7.55 (m, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.33 (s, 1H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 2H), 6.99 (d, *J* = 7.8 Hz, 2H), 6.86 (d, *J* = 7.8 Hz, 2H), 5.95 (s, 1H), 5.11 (s, 1H), 3.88, (s, 3H), 2.61 (q, *J* = 7.5Hz, 2H), 1.17 (t, *J* = 7.5 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.2, 167.4, 160.0, 144.3, 139.5, 136.8, 136.2, 132.1, 131.6, 129.2, 128.6, 128.5, 125.6, 121.4, 120.8, 116.5, 114.1, 113.0,

55.3, 36.4, 28.4, 15.3 ppm. MS m/z 463.18 (M^++1). Anal. Calcd for $C_{29}H_{25}N_3O_3$: C, 75.14; H, 5.44; N, 9.07; found C, 75.10; H, 5.41; N, 9.03.

*4.2.18 2-(4-benzoyl-1-(4-fluorophenyl)-2-(4-methoxyphenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6ar**).*

White solid, mp; 168-170 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.89 (d, *J* = 7.5 Hz, 2H), 7.62-7.57 (m, 2H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.32 (s, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.10-7.06 (m, 2H), 7.01-6.96 (m, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 5.87 (s, 1H), 5.08 (s, 1H), 3.80 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.8, 167.1, 163.6, 160.3, 139.6, 137.0, 134.8, 132.6, 132.2, 131.2, 129.2, 128.6, 127.7, 127.6, 121.8, 120.5, 116.5, 116.2, 114.3, 113.5, 55.3, 36.3 ppm. MS m/z 453.14 (M^++1). Anal. Calcd for $C_{27}H_{20}FN_3O_3$: C, 71.51; H, 4.45; N, 4.19; found C, 71.47; H, 4.41; N, 4.14.

*4.2.19 2-(4-benzoyl-2-(4-chlorophenyl)-1-(4-fluorophenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6as**).*

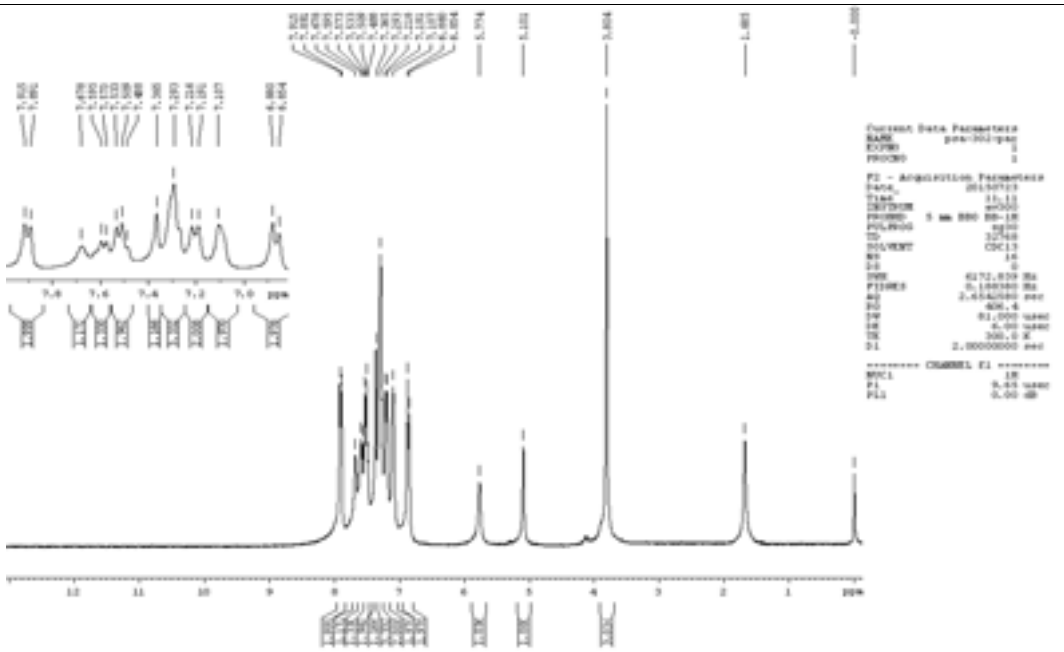
White solid, mp; 189-191 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.88 (d, *J* = 7.5 Hz, 2H), 7.62-7.57 (m, 2H), 7.52-7.47 (m, 2H), 7.35 (s, 1H), 7.32 (d, *J* = 8.7 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 7.11-7.06 (m, 2H), 7.01 (d, *J* = 7.8 Hz, 2H), 6.30 (s, 1H), 5.14 (s, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.7, 167.1, 163.6, 160.3, 139.1, 135.5, 135.5, 134.3, 134.2, 132.5, 132.4, 131.6, 129.2, 129.0, 128.5, 127.7, 127.6, 126.8, 121.7, 116.6, 116.3, 116.1, 113.9, 36.1 ppm. MS m/z 457.09 (M^++1). Anal. Calcd for $C_{26}H_{17}ClFN_3O_2$: C, 68.20; H, 3.74; N, 9.18; found C, 74.78; H, 5.12; N, 9.31.

*4.2.20 2-(4-benzoyl-1-benzyl-2-(4-chlorophenyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6at**).*

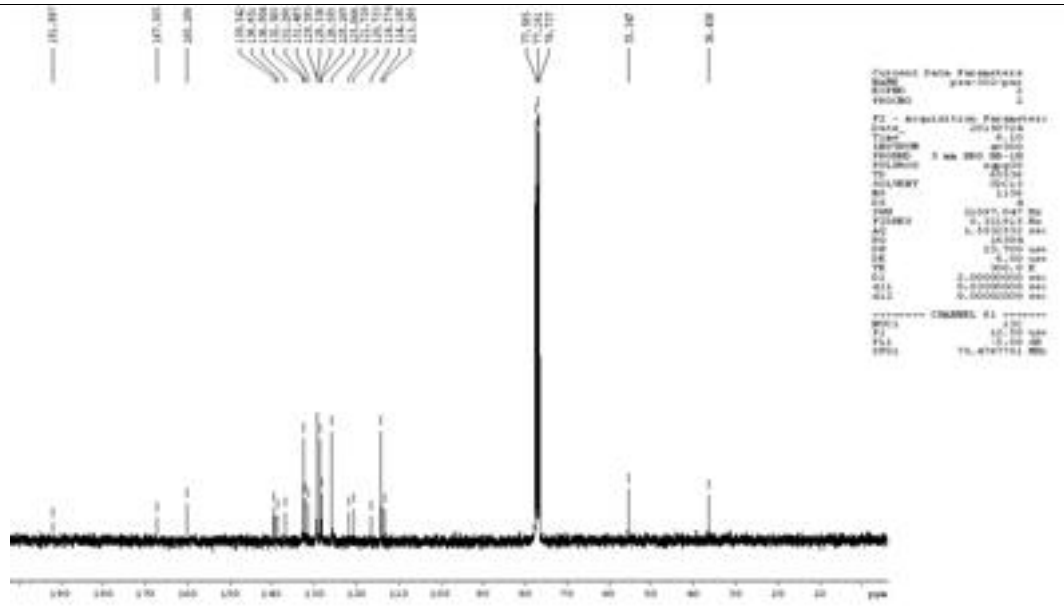
White solid, mp;213-215 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.82 (d, *J* = 7.8 Hz, 2H), 7.67 (s, 1H), 7.61-7.56 (m, 1H), 7.49 (d, *J* = 7.8 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 3H), 7.32-7.26 (m, 4H), 7.21 (s, 1H), 6.90 (m, 2H), 5.58 (s, 1H), 5.08 (s, 1H), 4.95 (s, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 191.4, 166.7, 139.1, 135.8, 135.7, 135.3, 132.6, 132.1, 130.7, 129.1, 128.8, 128.3, 128.0, 126.7, 126.6, 120.6, 116.1, 113.2, 51.4, 35.9 ppm. MS m/z 453.92 (M^++1). Anal. Calcd for $C_{27}H_{20}ClN_3O_2$: C, 71.44; H, 4.44; N, 9.26; found C, 71.40; H, 4.41; N, 9.22.

*4.2.21 2-(4-(5-bromothiophene-2-carbonyl)-2-phenyl-1-(p-tolyl)-1H-pyrrol-3-yl)-2-cyanoacetamide (**6au**).*

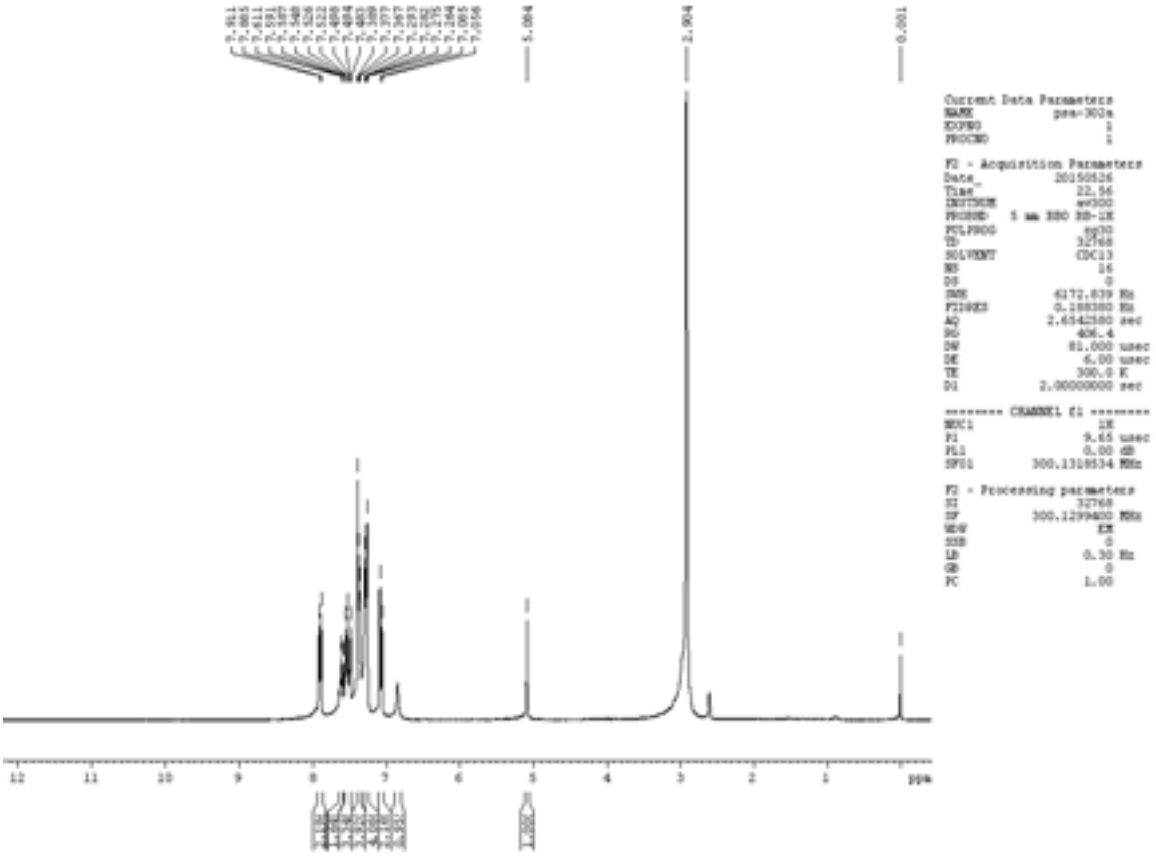
White solid, mp; 163-165 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.66-7.65 (m, 2H), 7.52 (s, 1H), 7.35-7.33 (m, 3H), 7.24-7.19 (m, 3H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.92 (s, 1H), 4.98 (s, 1H), 2.33 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ: 180.3, 166.3, 145.5, 137.9, 135.6, 132.7, 130.9, 130.7, 129.6, 129.1, 128.7, 128.5, 128.2, 125.3, 120.5, 116.3, 113.2, 36.0, 20.7 ppm. MS m/z 504.40 (M^{+}+1). Anal. Calcd for $C_{25}H_{18}BrN_3O_2S$: C, 59.53; H, 3.60; N, 8.33; found C, 59.48; H, 3.57; N, 8.29.



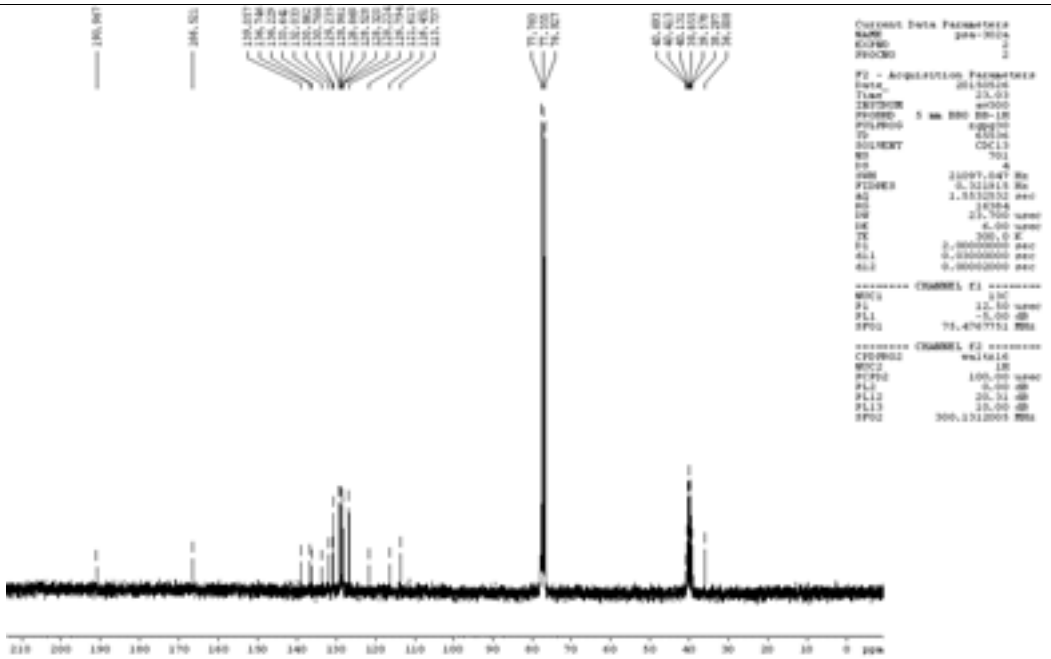
^{1}H spectrum of **6aa**.



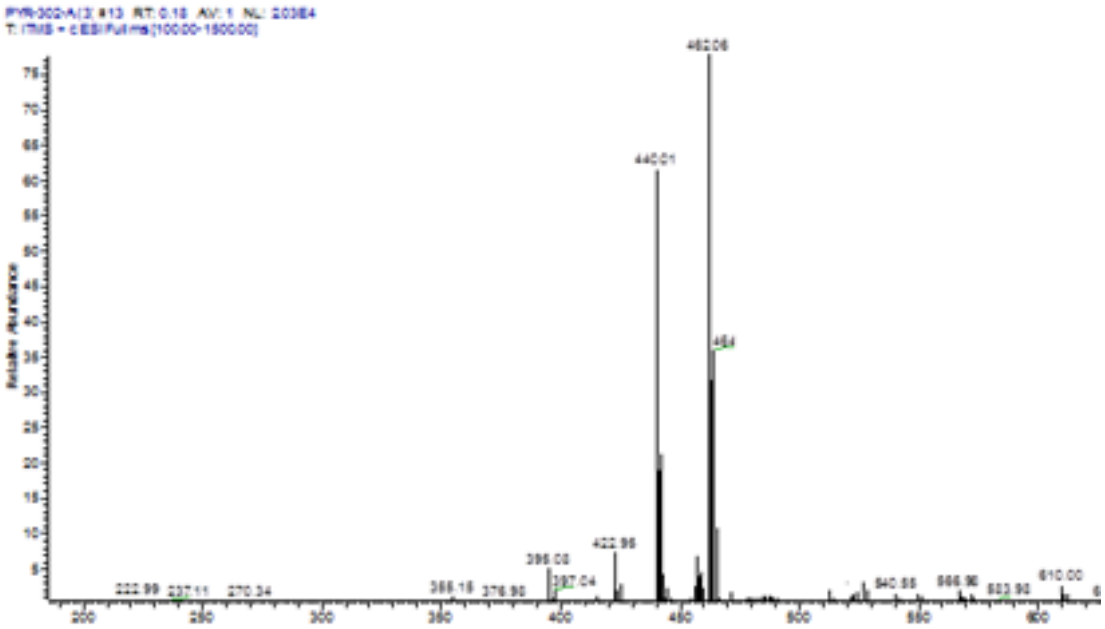
^{13}C NMR Spectrum of **6aa**.



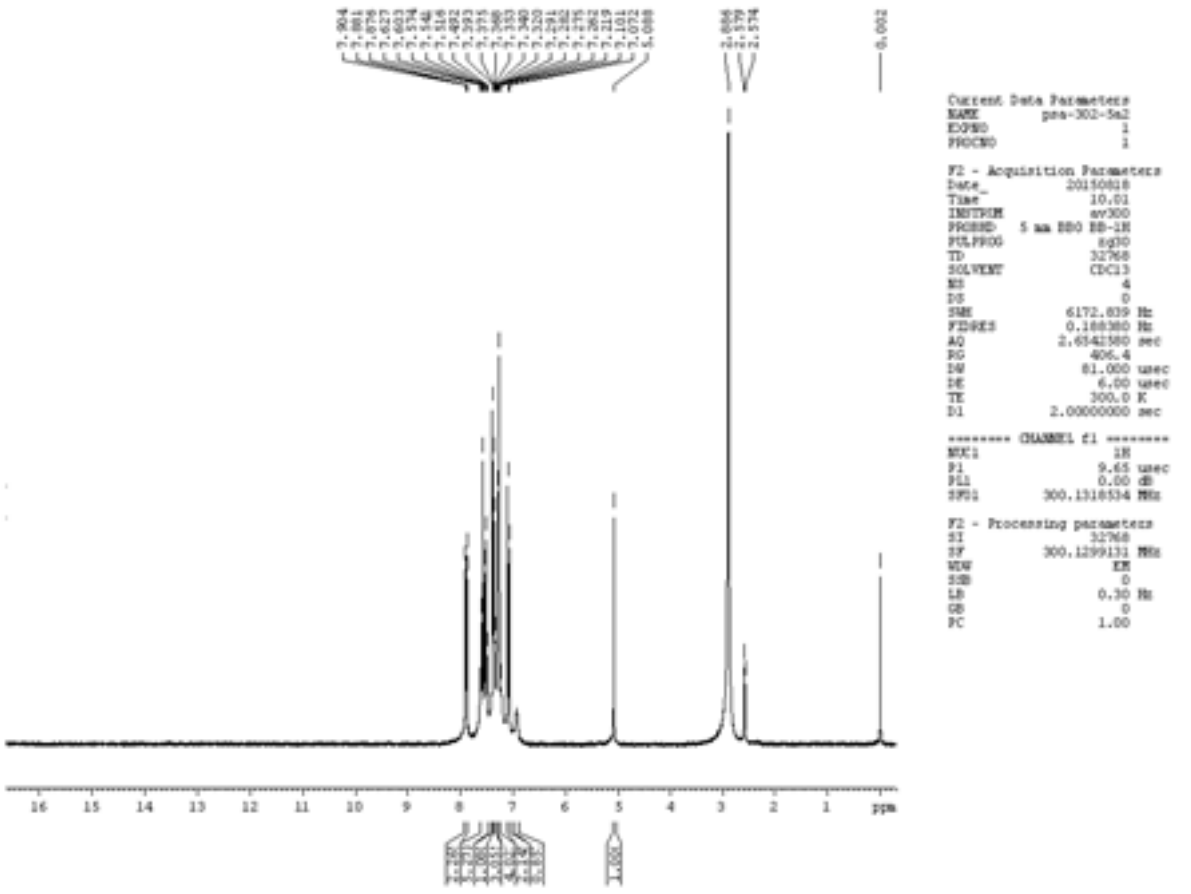
^{1}H spectrum of **6ab**.



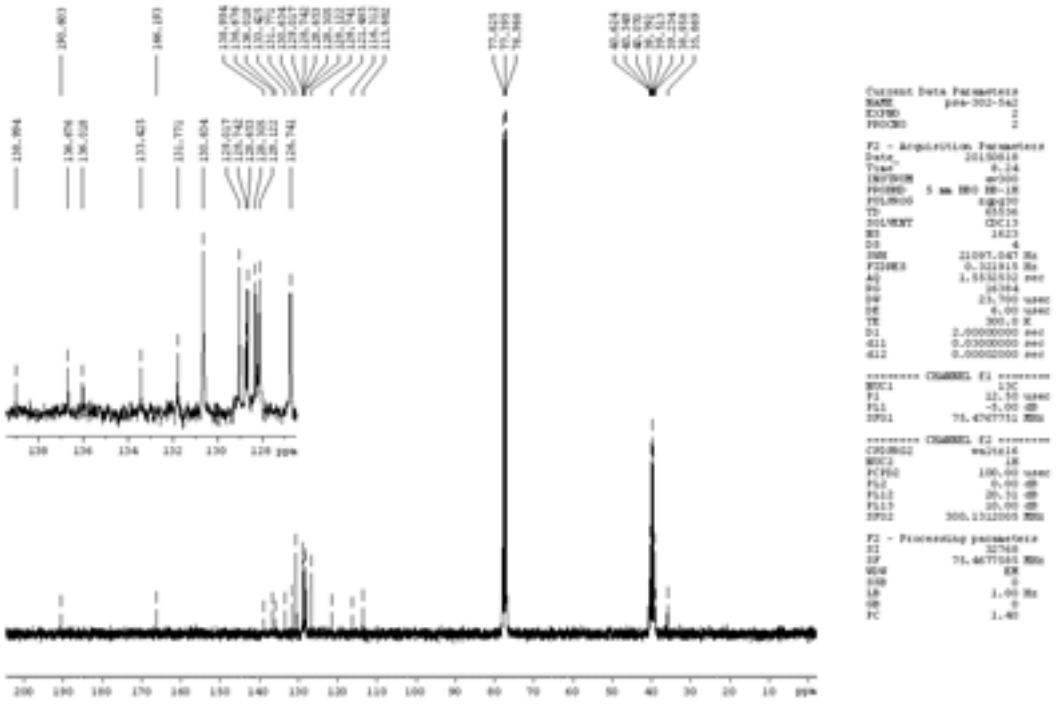
^{13}C NMR Spectrum of **6ab**.



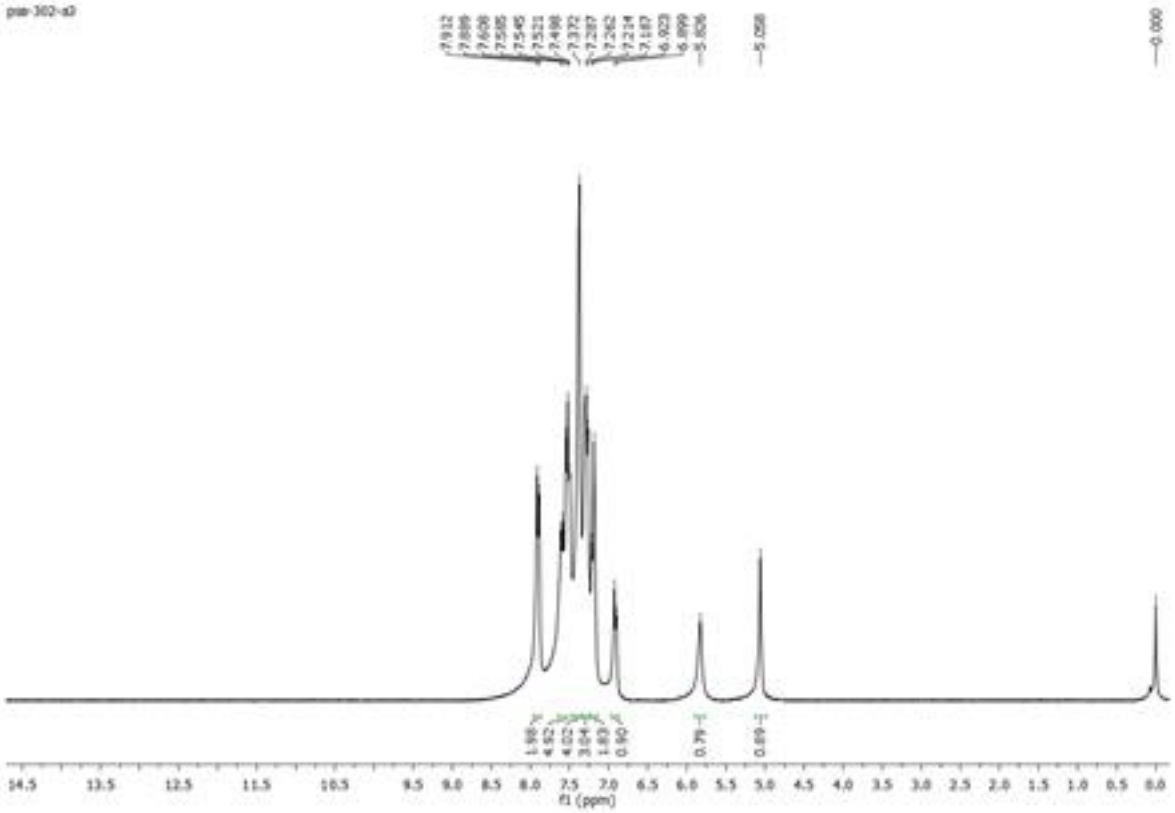
ESI-MASS Spectrum of **6ab**.



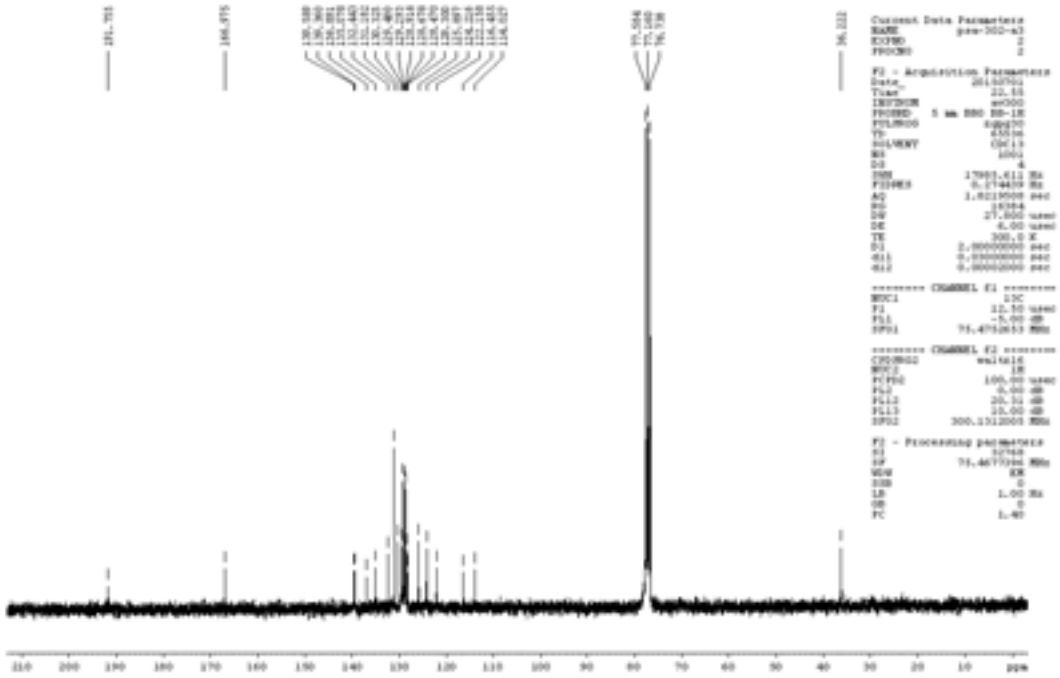
^{1}H spectrum of **6ac**.



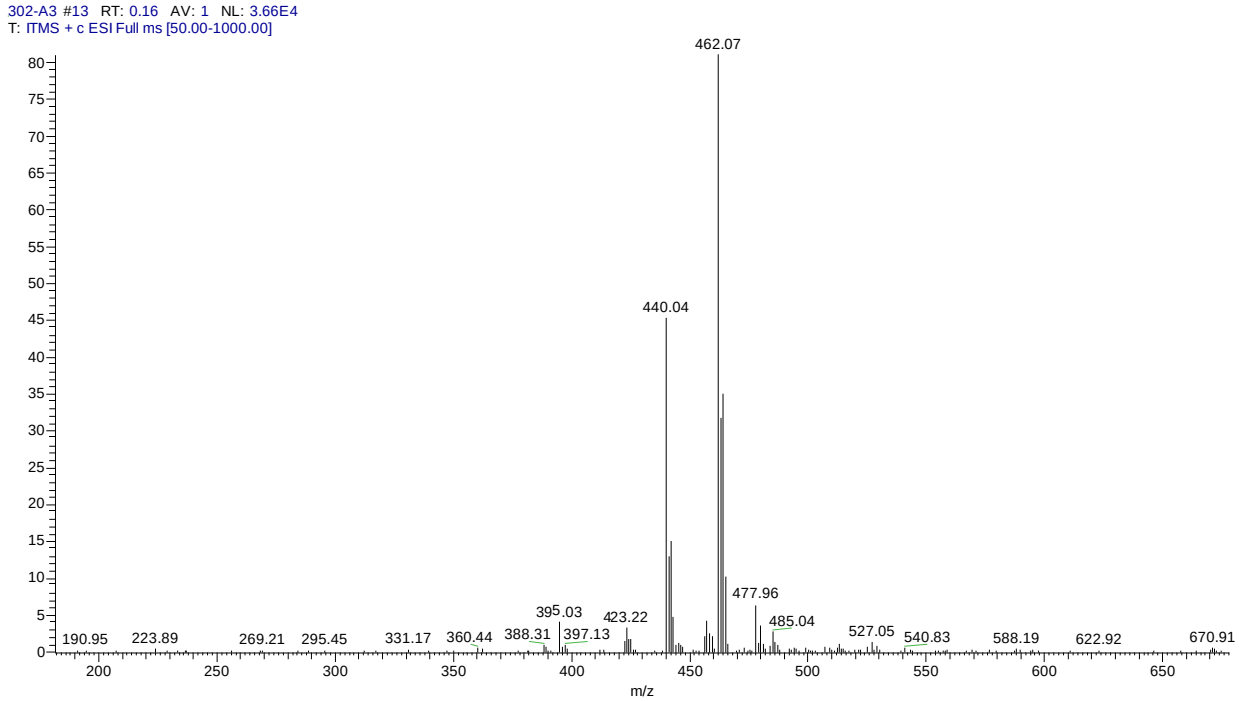
^{13}C NMR Spectrum of **6ac**.



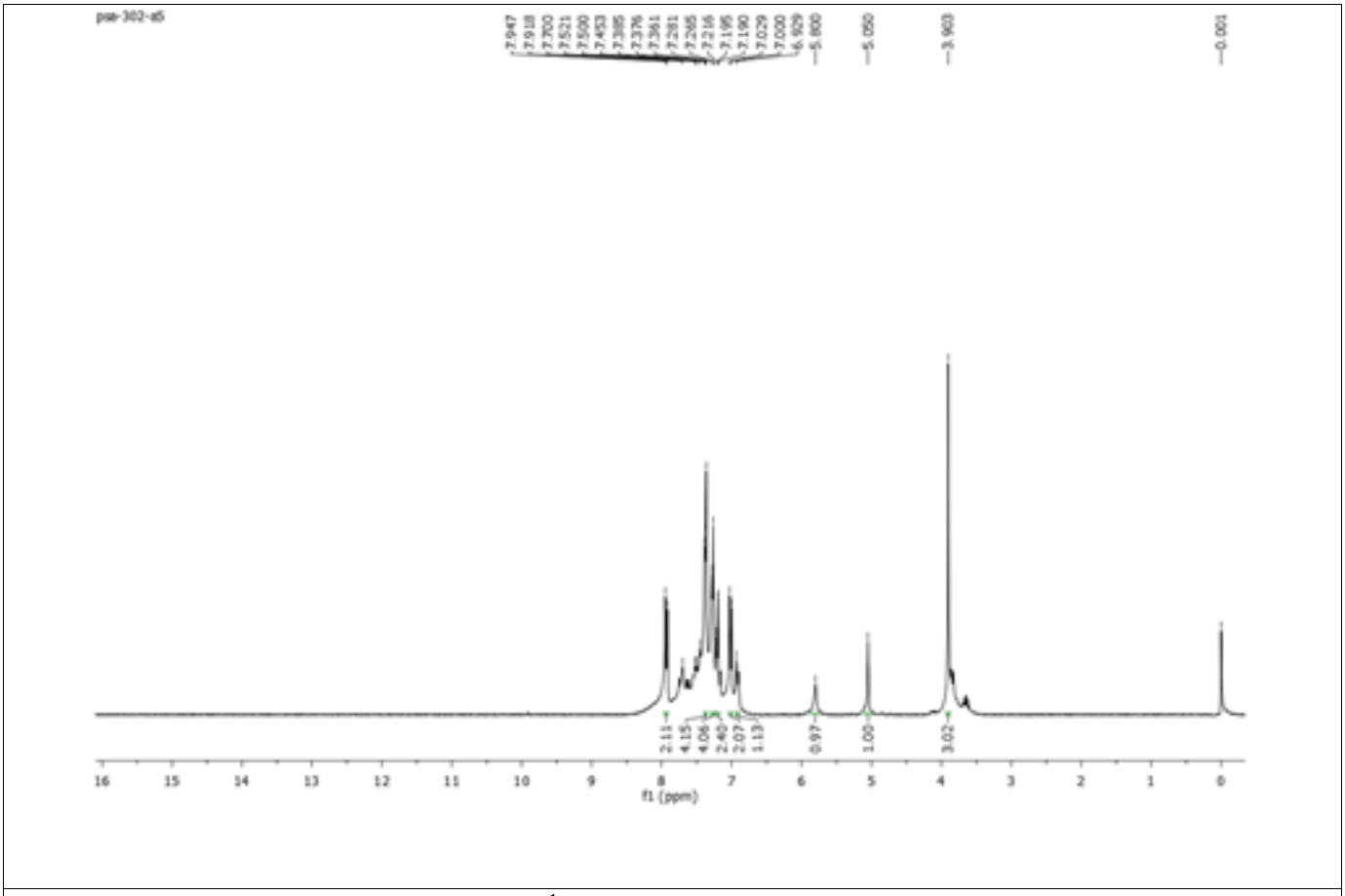
^{1}H spectrum of **6ad**.



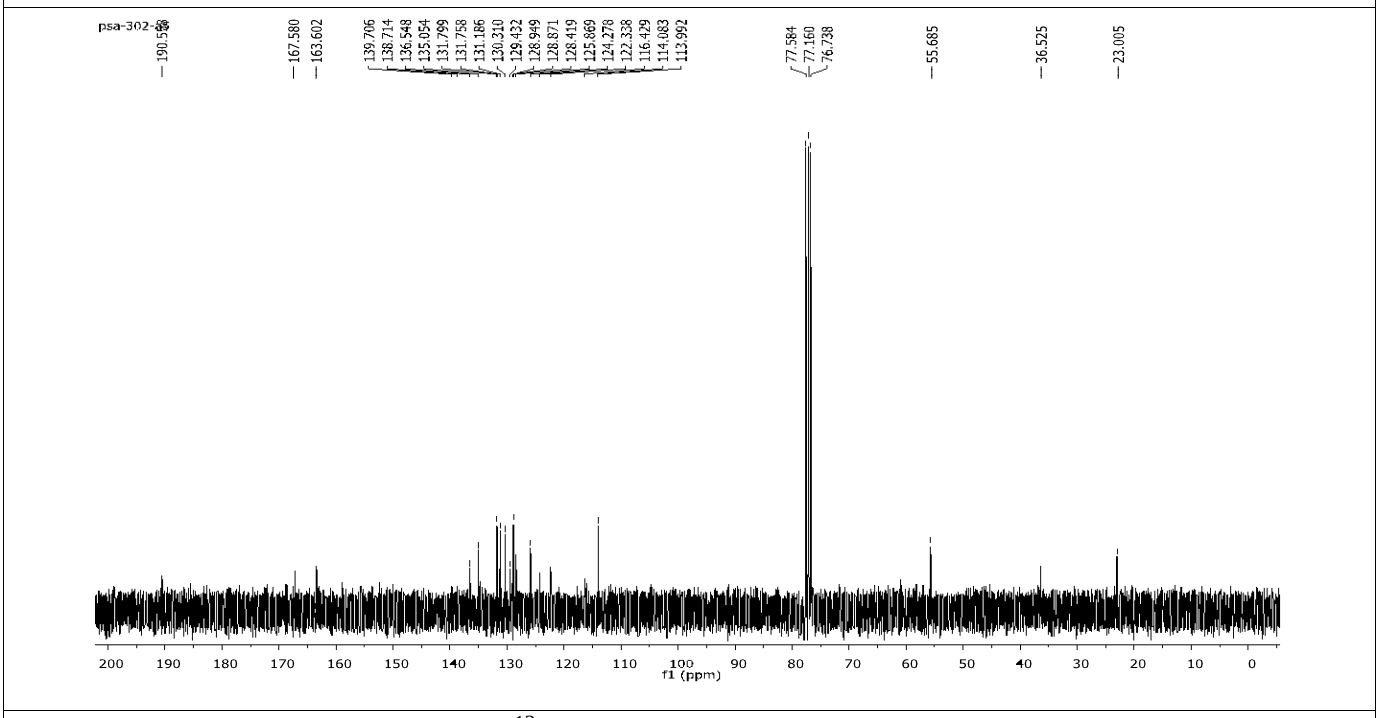
^{13}C NMR Spectrum of **6ad**.



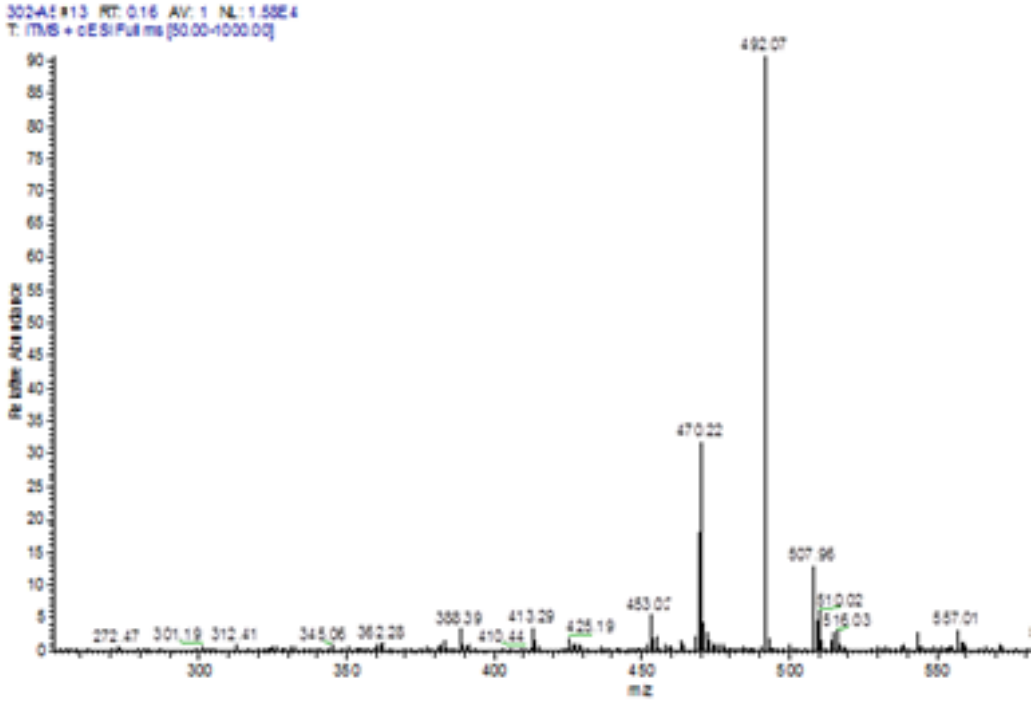
ESI-MASS Spectrum of **6ad.**



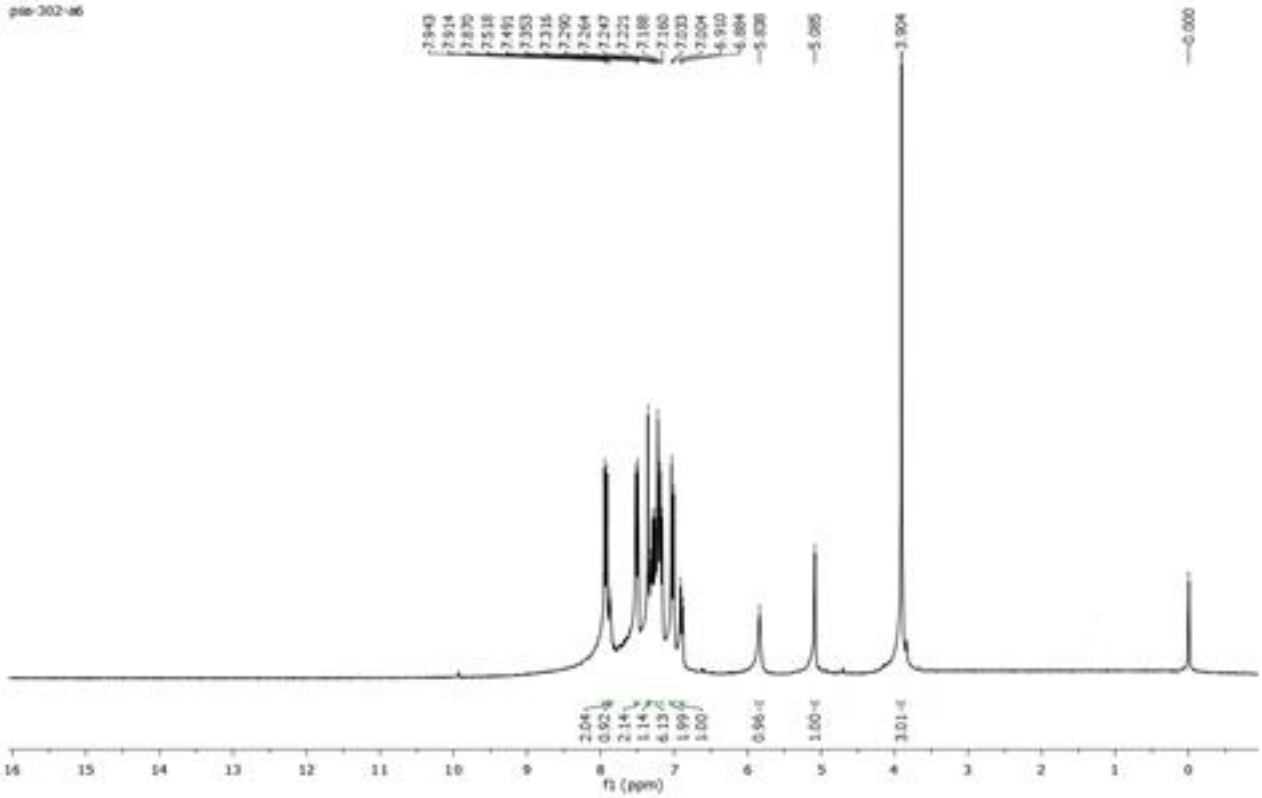
^{1}H spectrum of **6ae**.



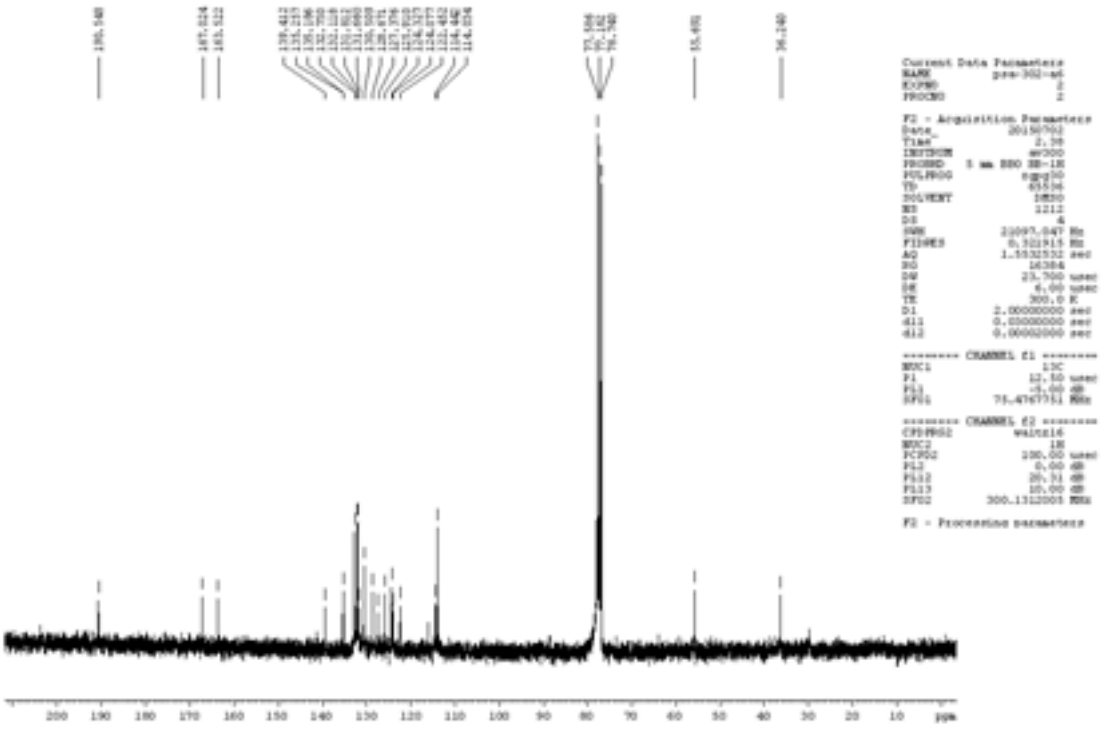
^{13}C NMR Spectrum of **6ae**.



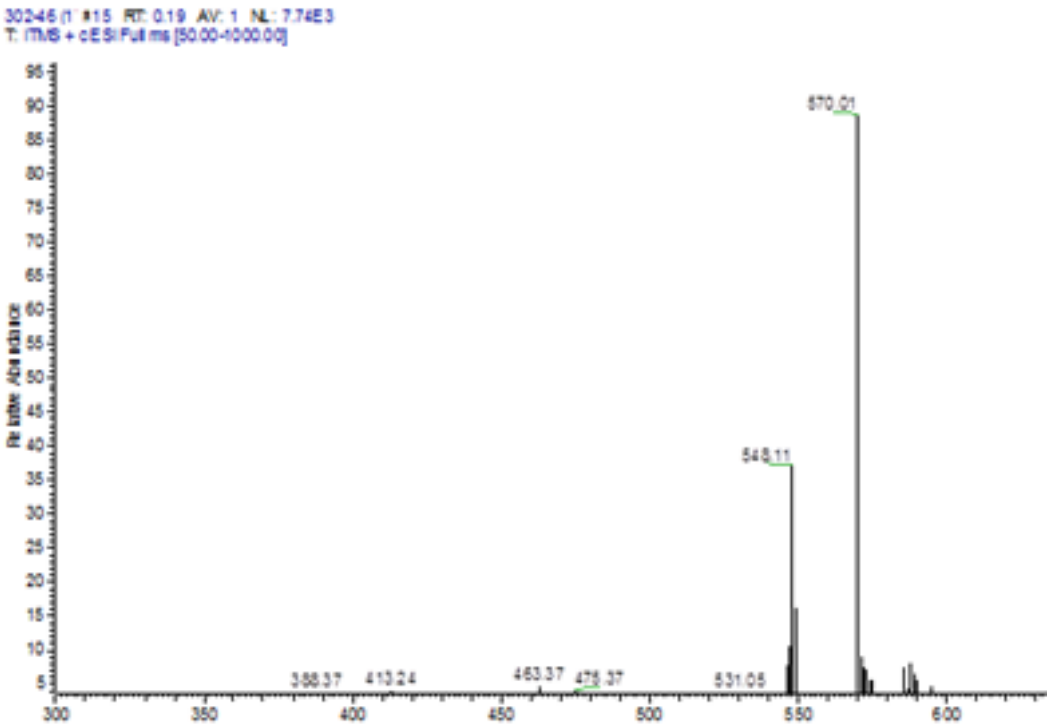
ESI-MASS Spectrum of **6ae.**



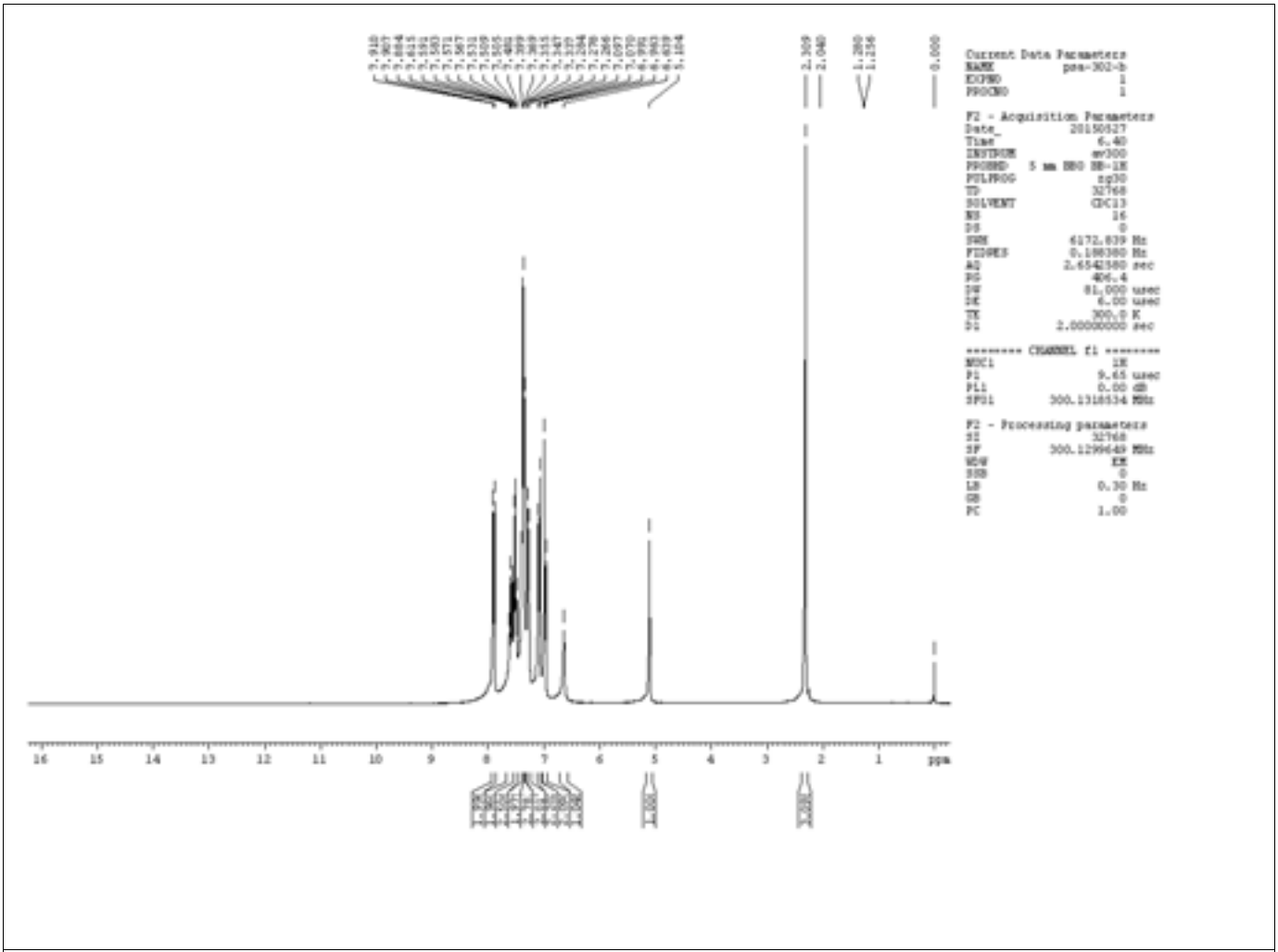
^{1}H NMR Spectrum of **6af**.



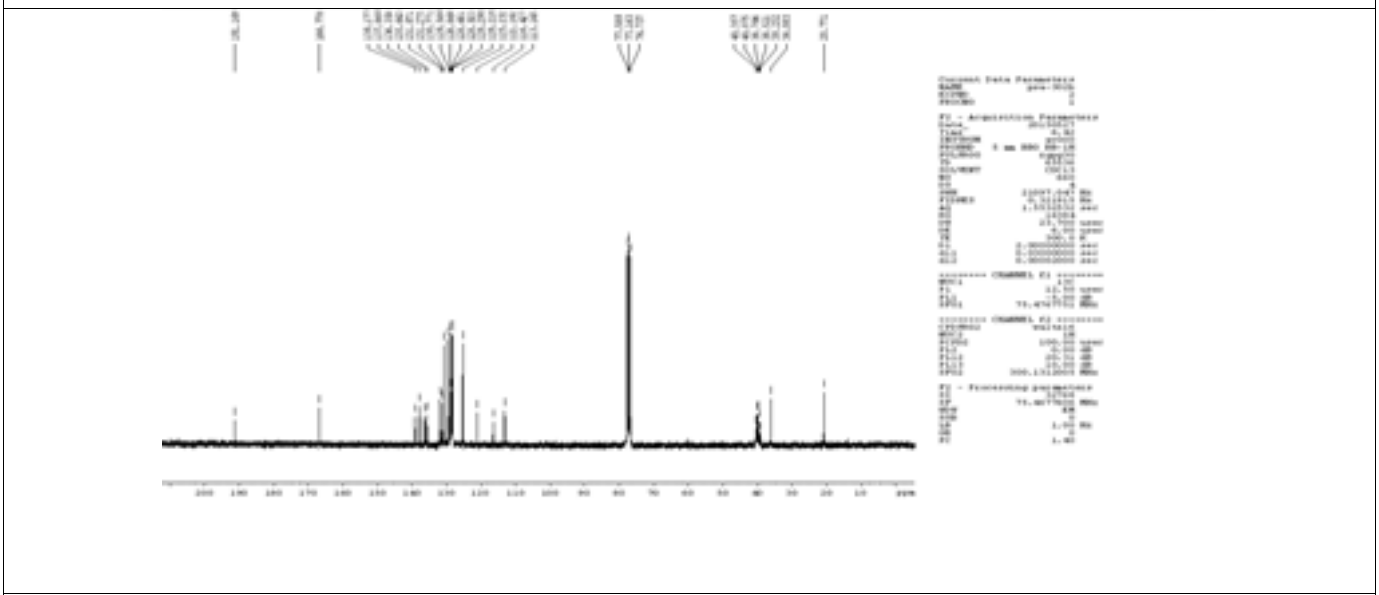
^{13}C NMR Spectrum of **6af**.



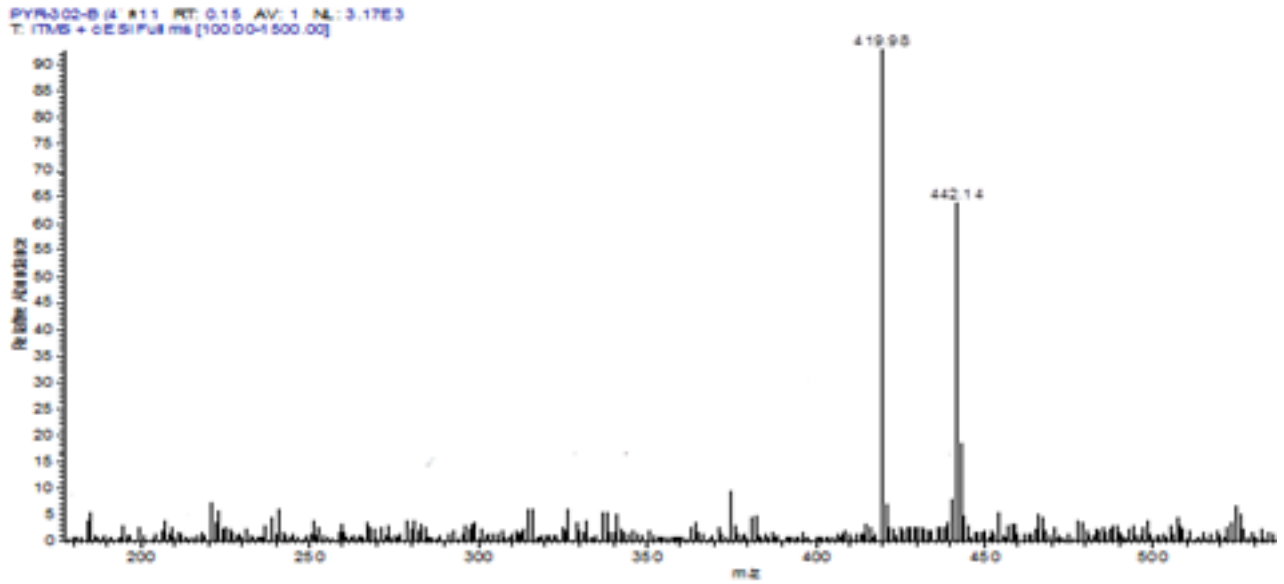
ESI-MASS Spectrum of **6af.**



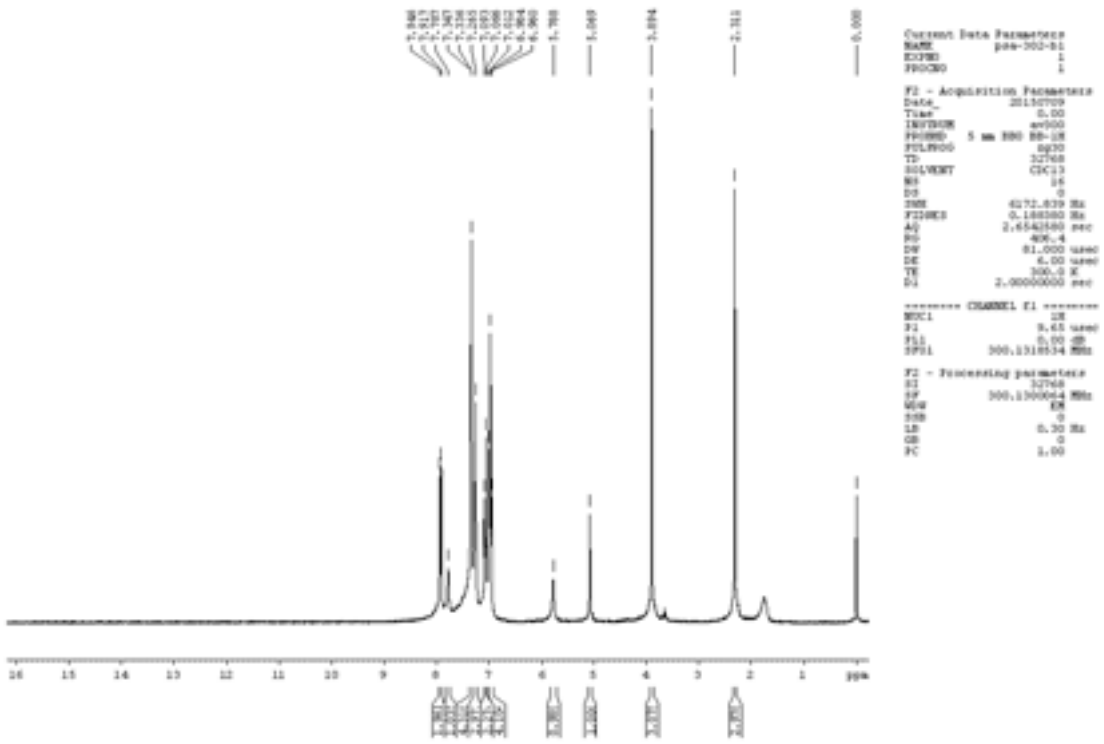
^{1}H NMR Spectrum of **6ag**.



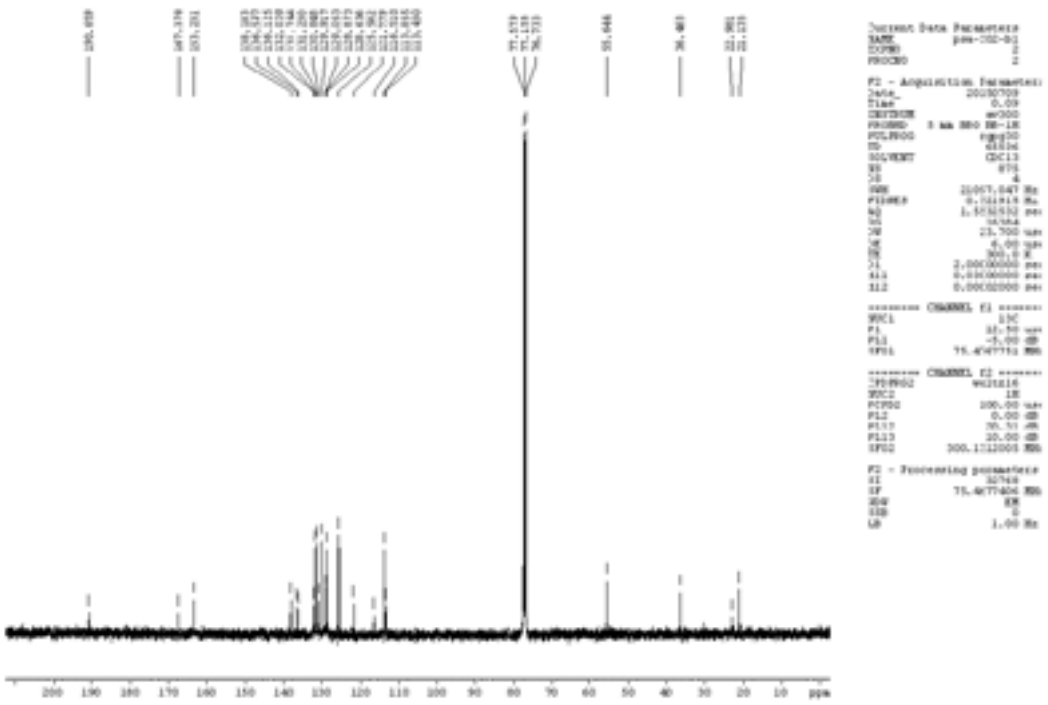
^{13}C NMR Spectrum of **6ag**.



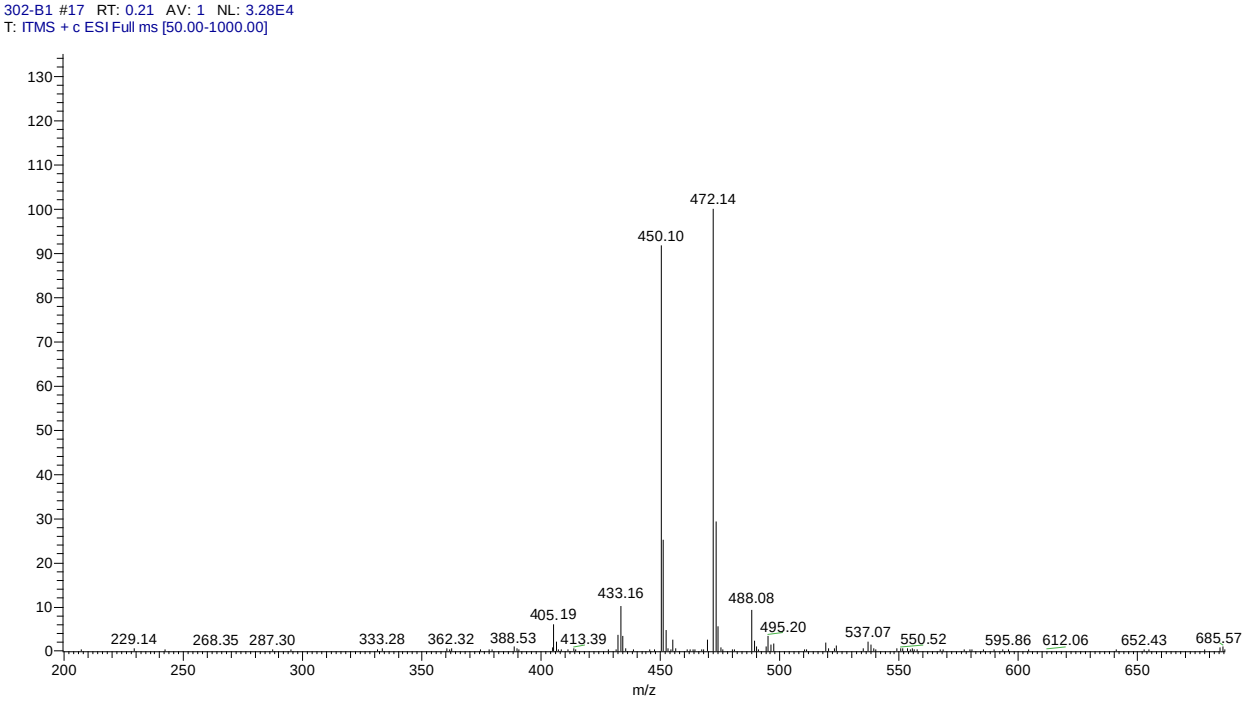
ESI-MASS Spectrum of **6ag**.



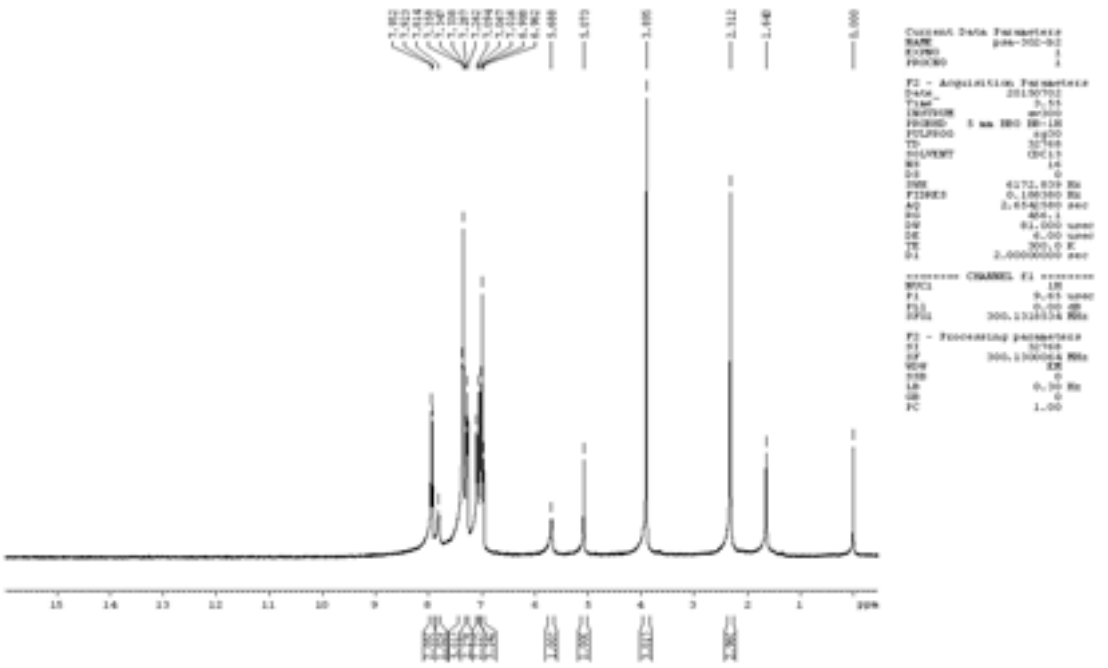
^{1}H NMR Spectrum of **6ah**.



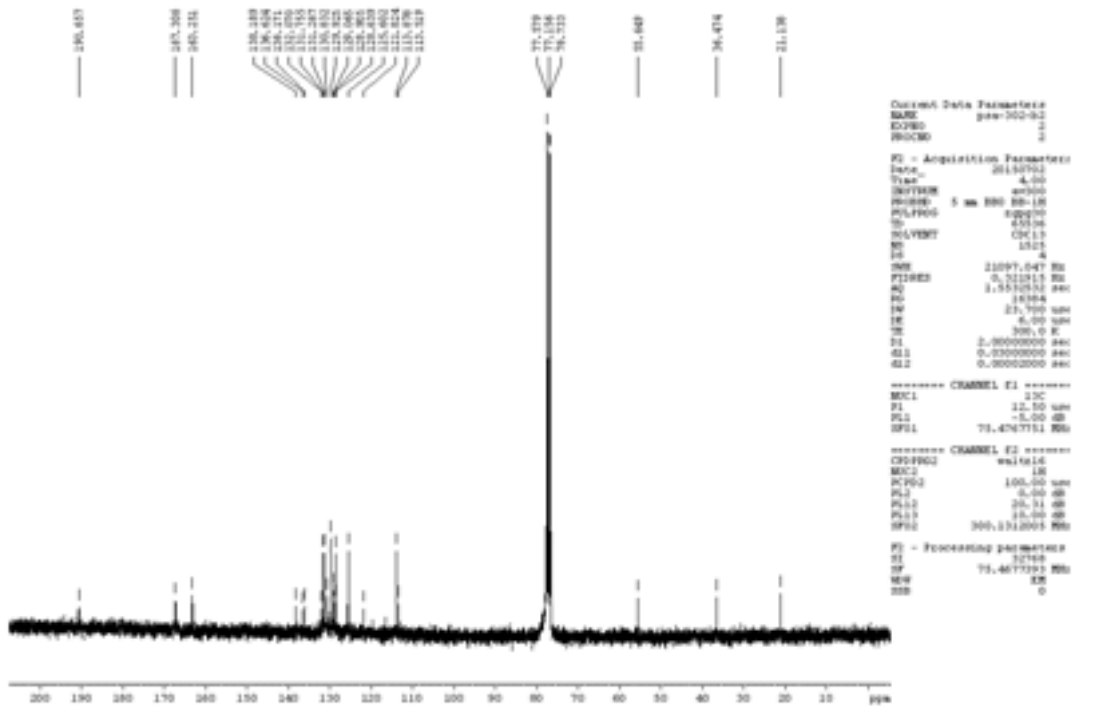
^{13}C NMR Spectrum of **6ah**.



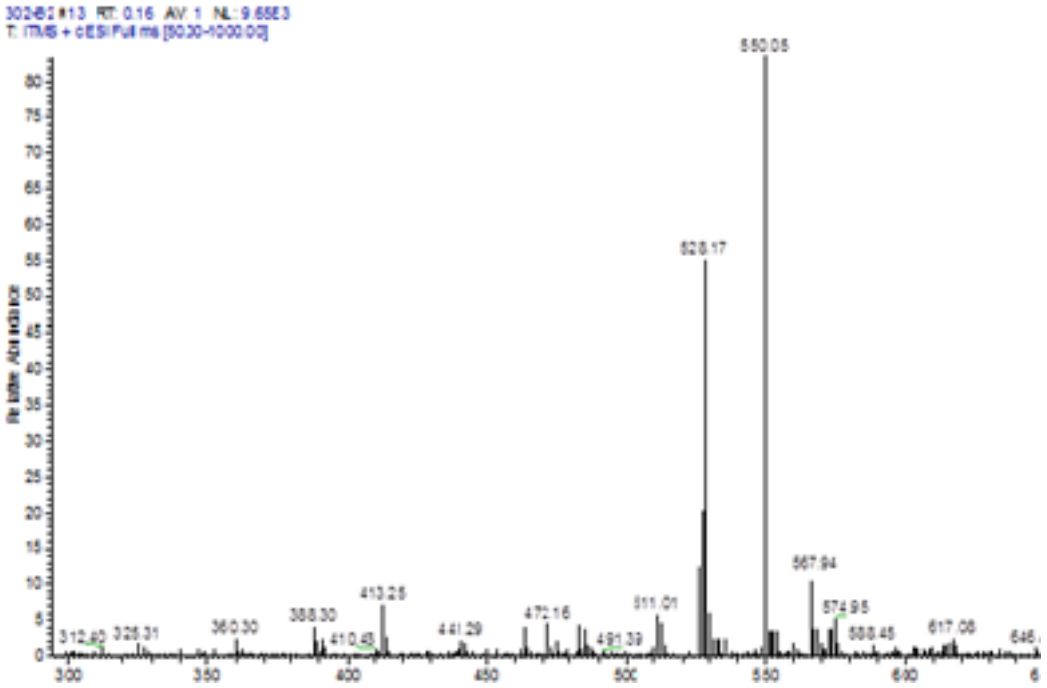
ESI-MASS Spectrum of **6ah.**



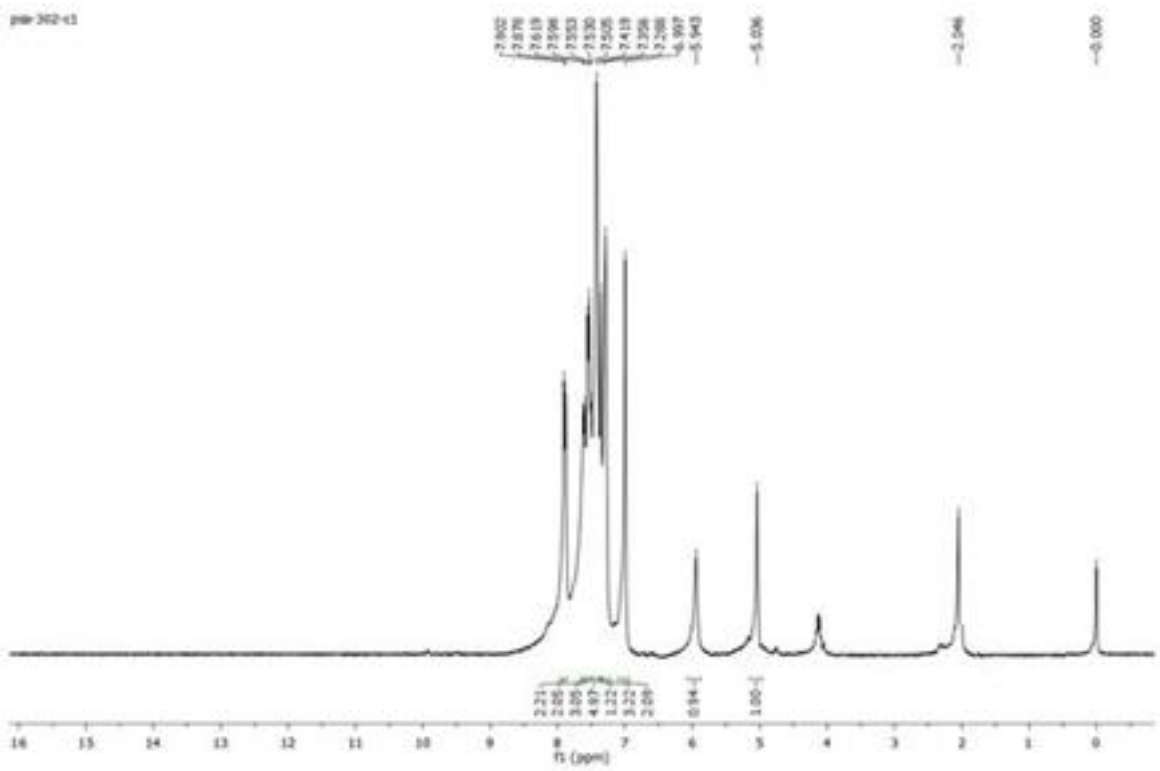
^{1}H NMR Spectrum of **6ai**.



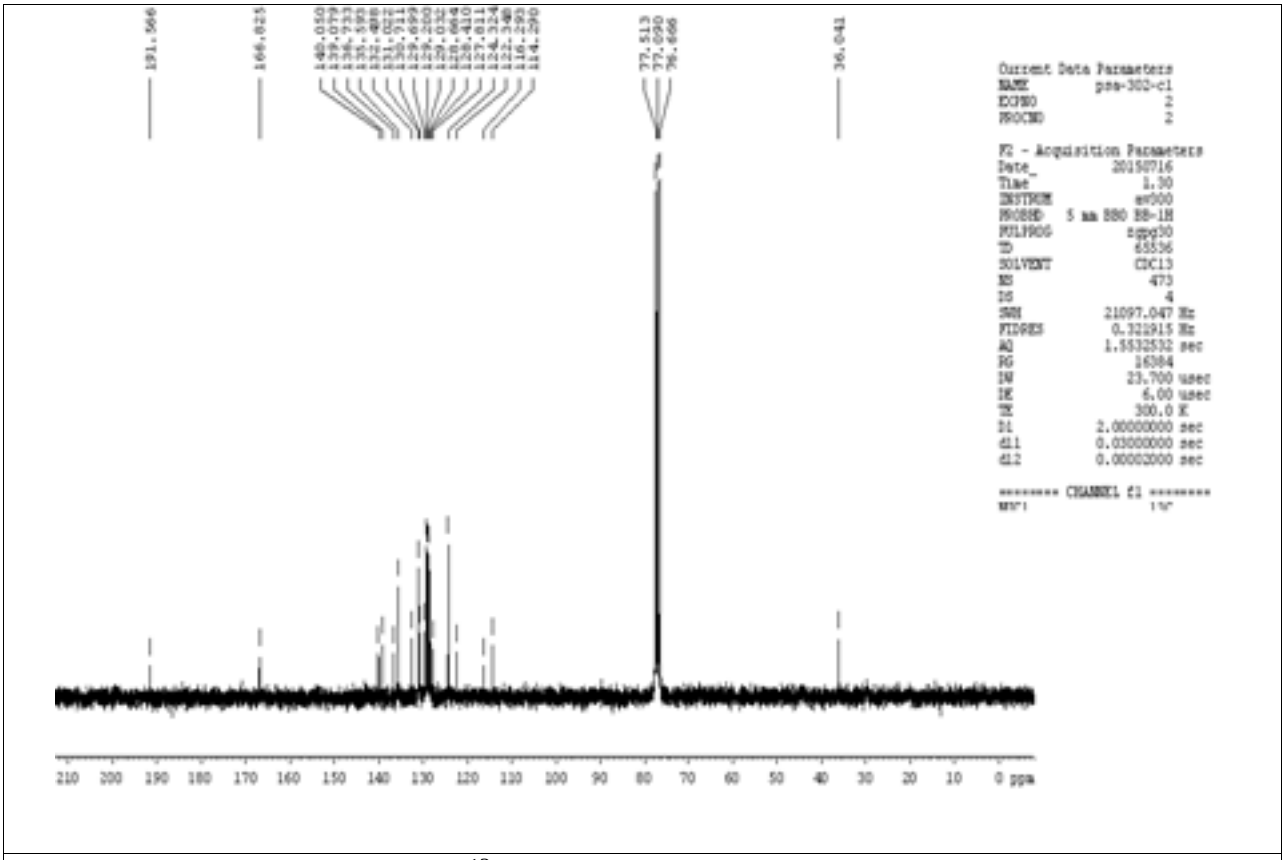
^{13}C NMR Spectrum of **6ai**.



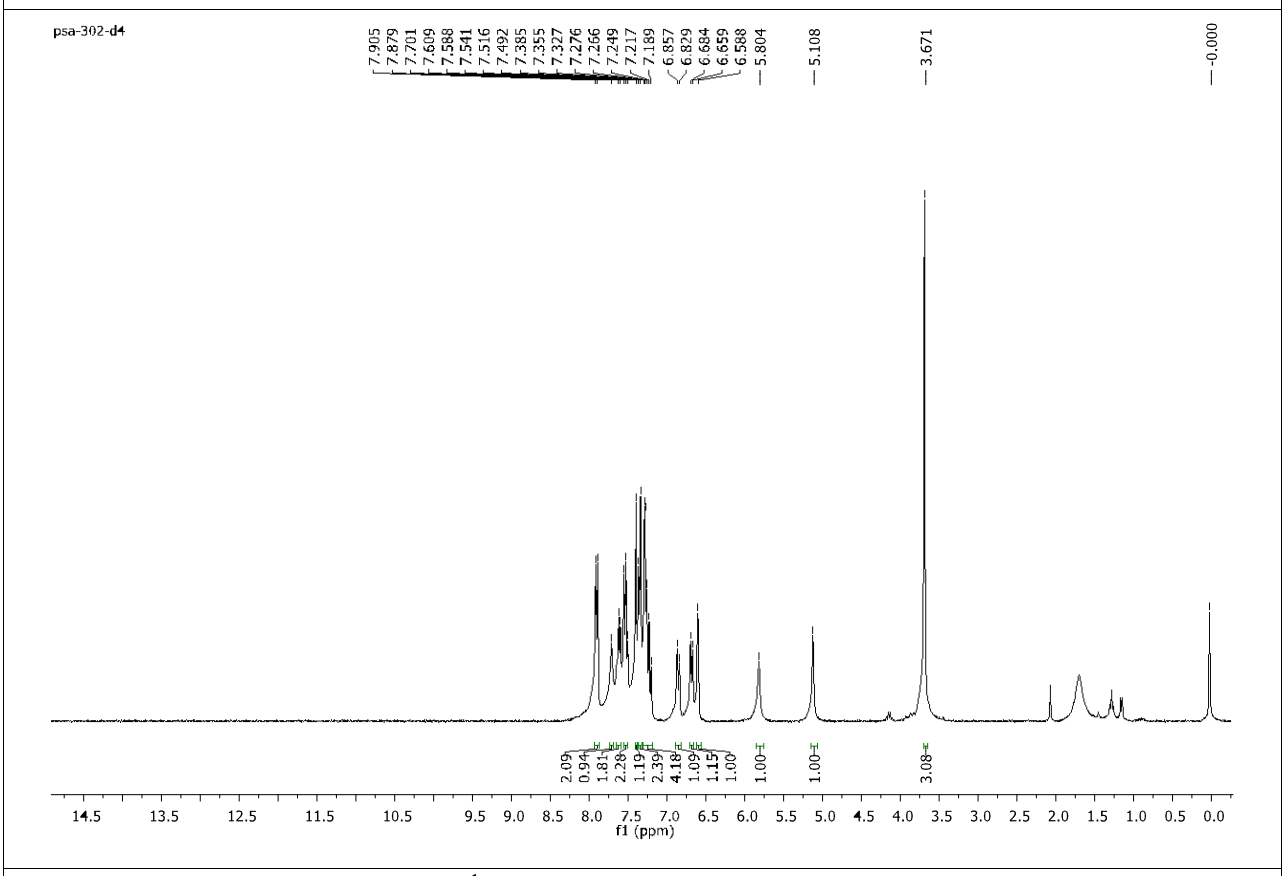
ESI-MASS Spectrum of **6ai.**



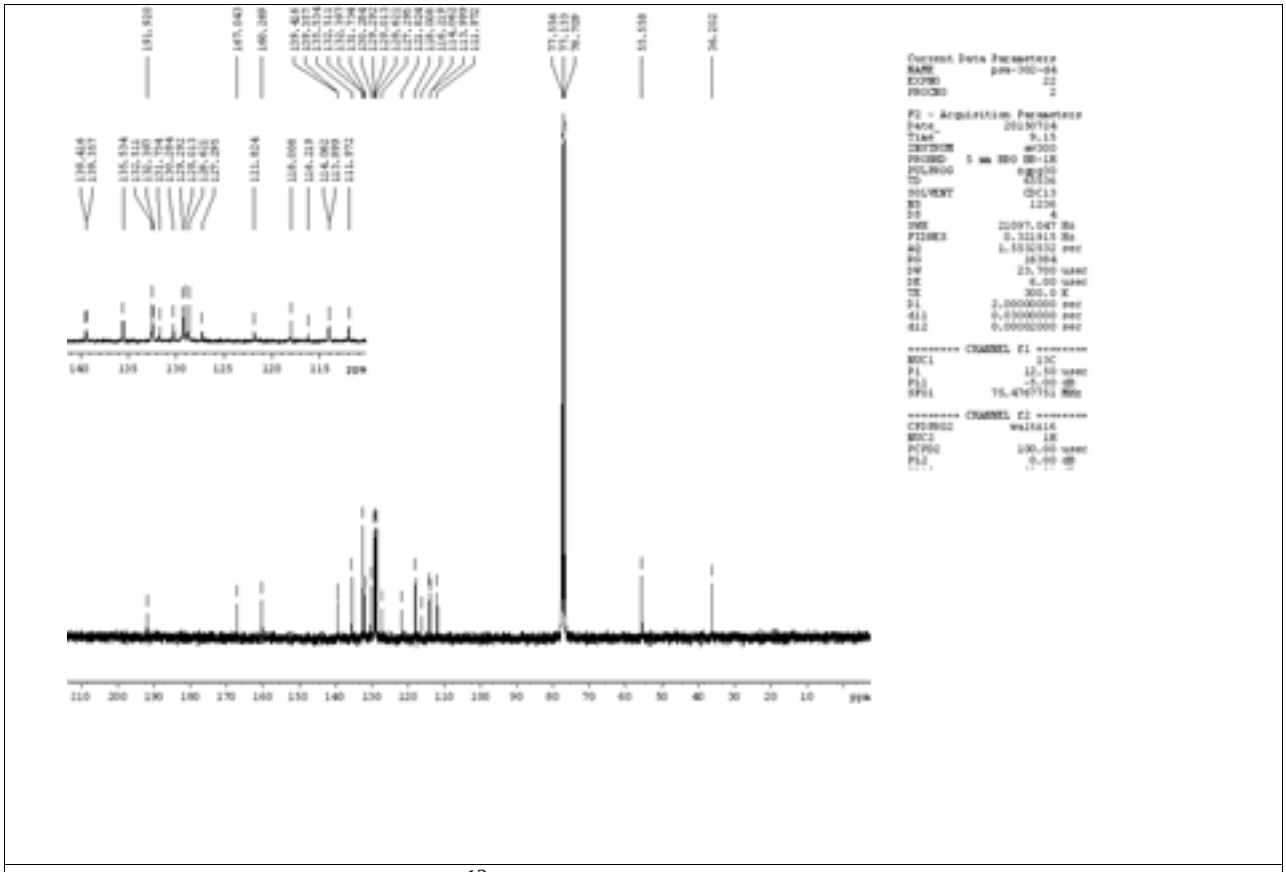
^{1}H NMR Spectrum of **6aj**.



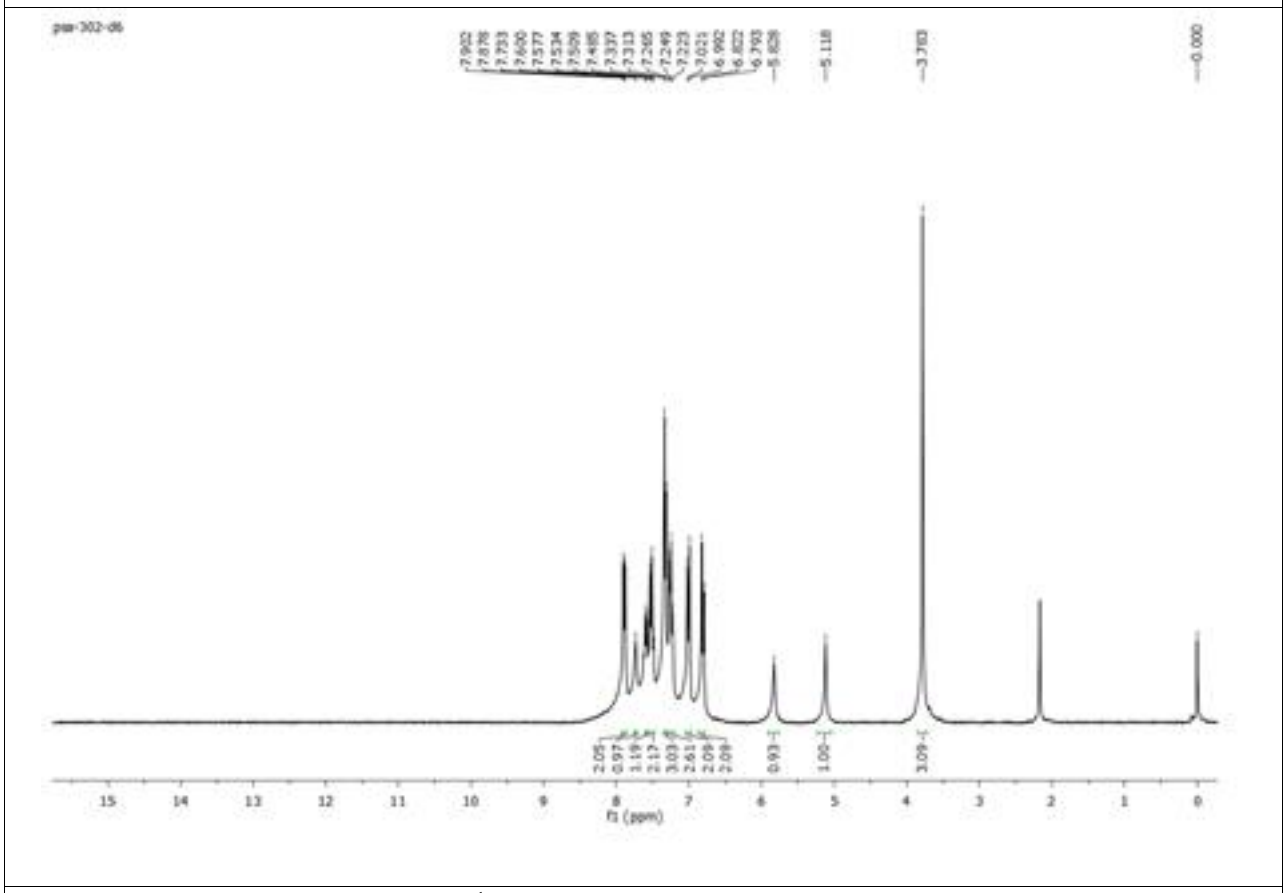
^{13}C NMR Spectrum of **6aj**.



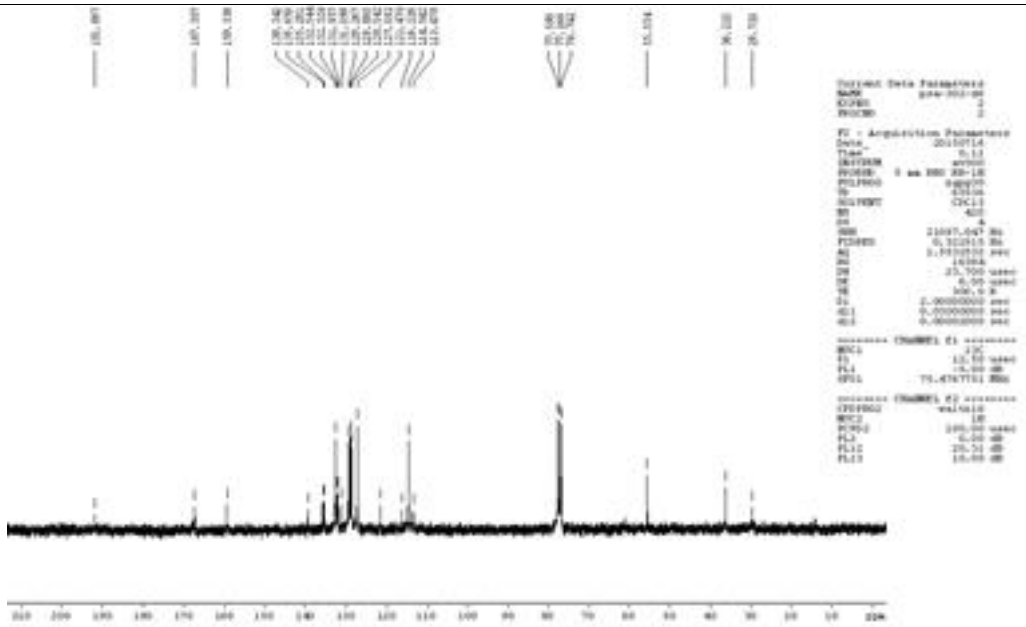
^{1}H NMR Spectrum of **6ak**.



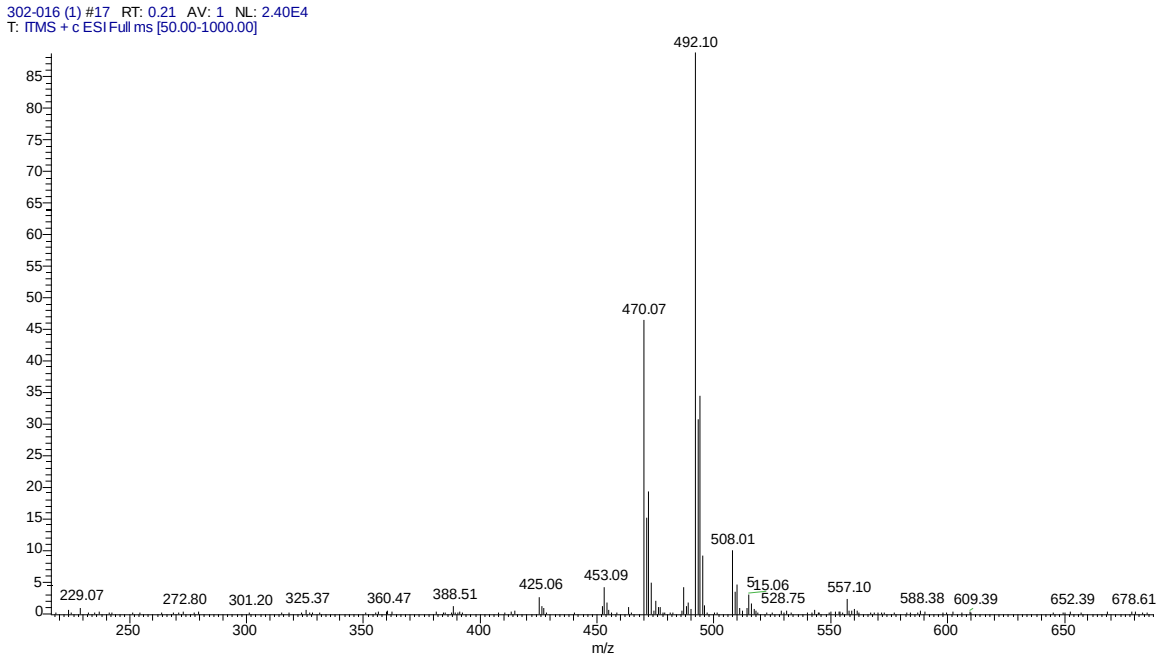
^{13}C NMR Spectrum of **6ak**.



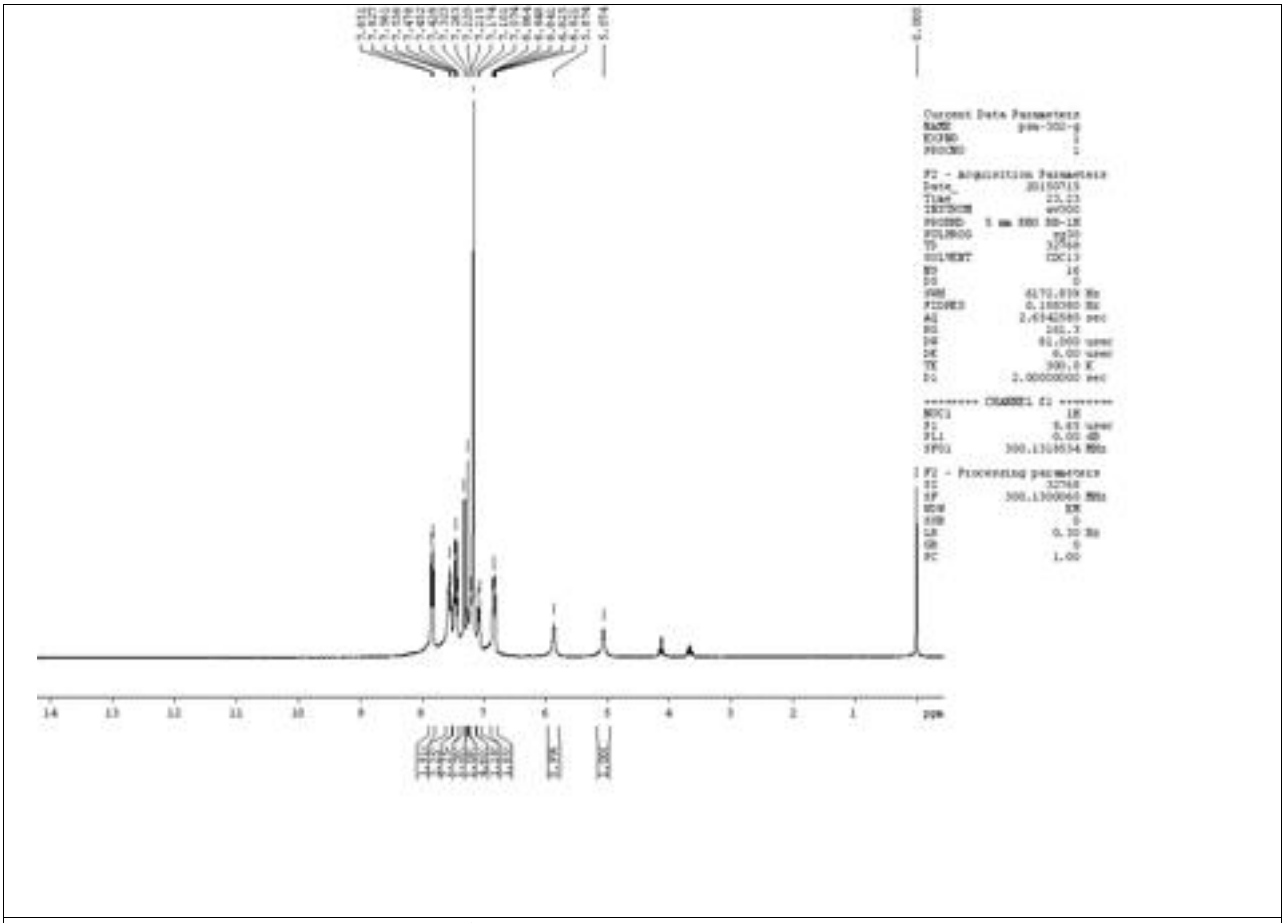
^{1}H NMR Spectrum of **6al**.



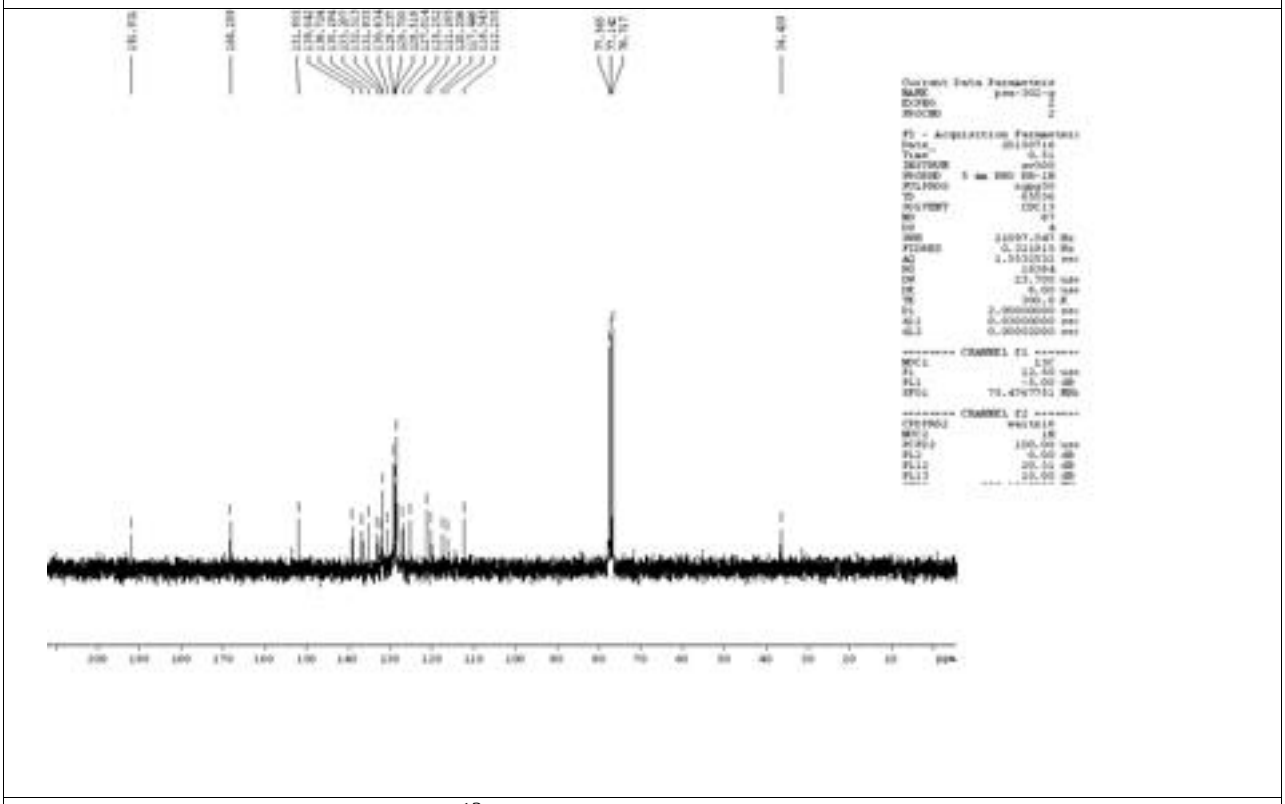
^{13}C NMR Spectrum of **6al**.



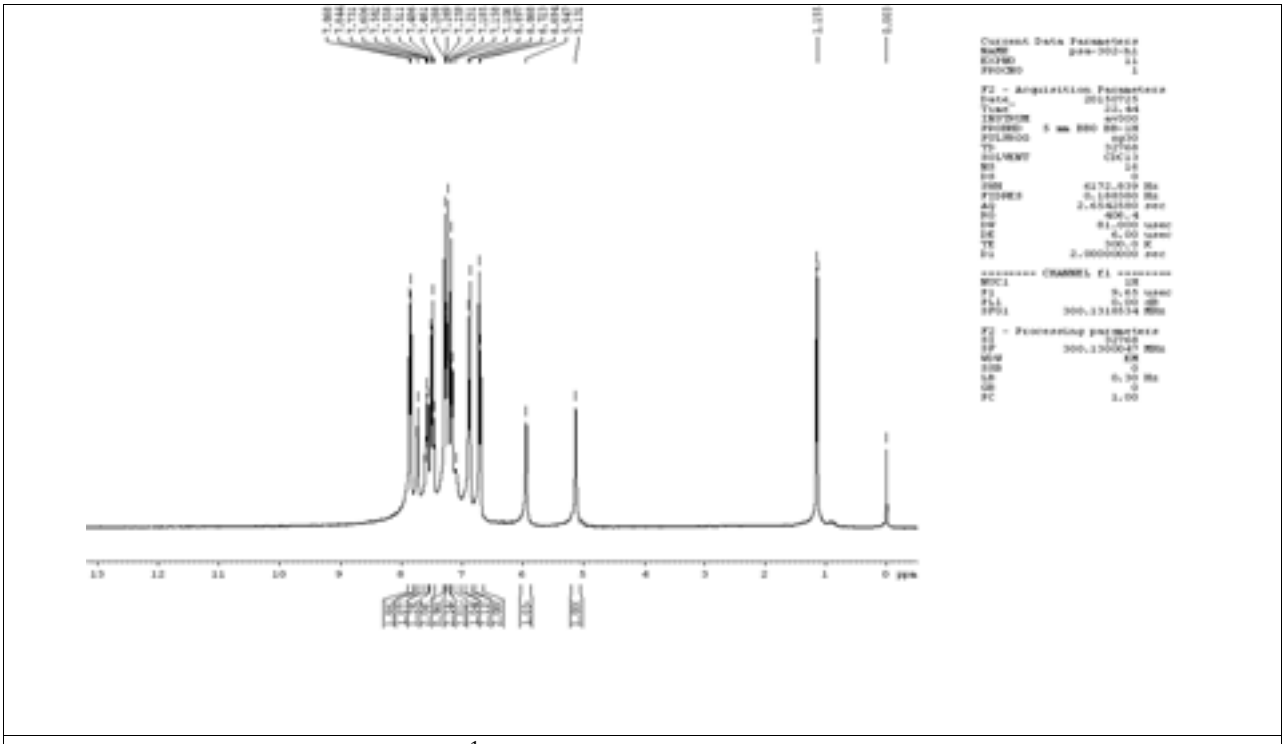
ESI-MASS Spectrum of **6al.**



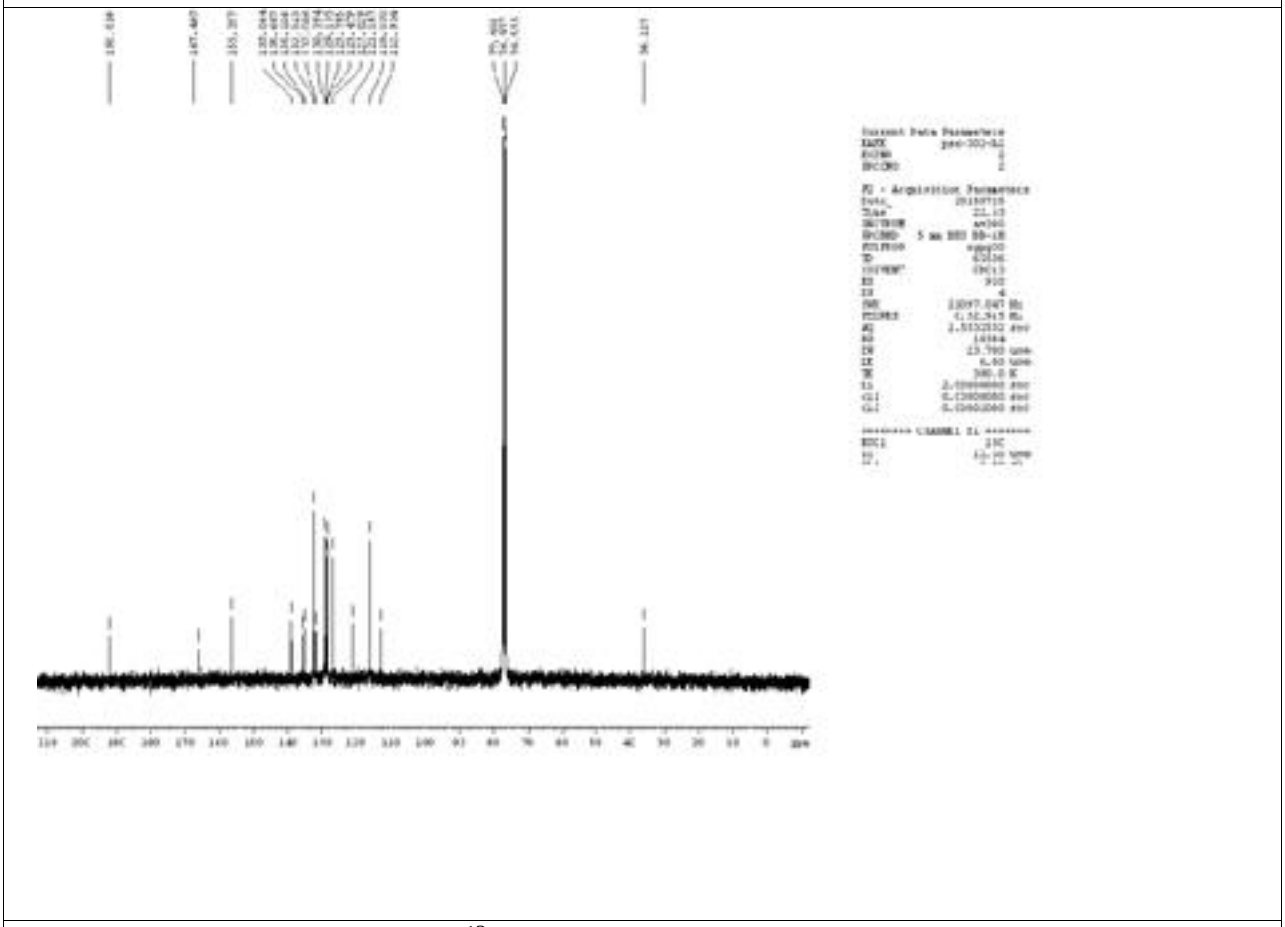
^{1}H NMR Spectrum of **6am**.



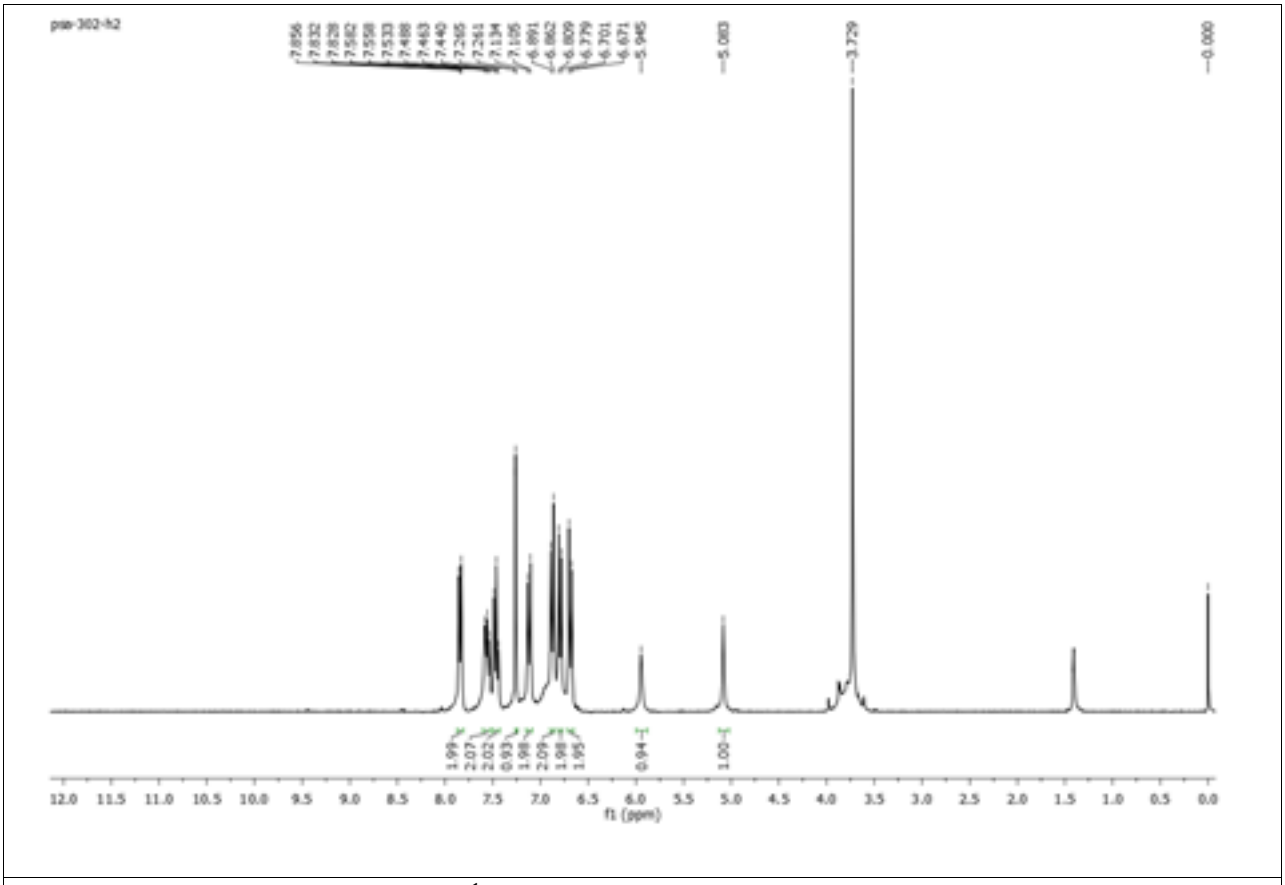
^{13}C NMR Spectrum of **6am**.



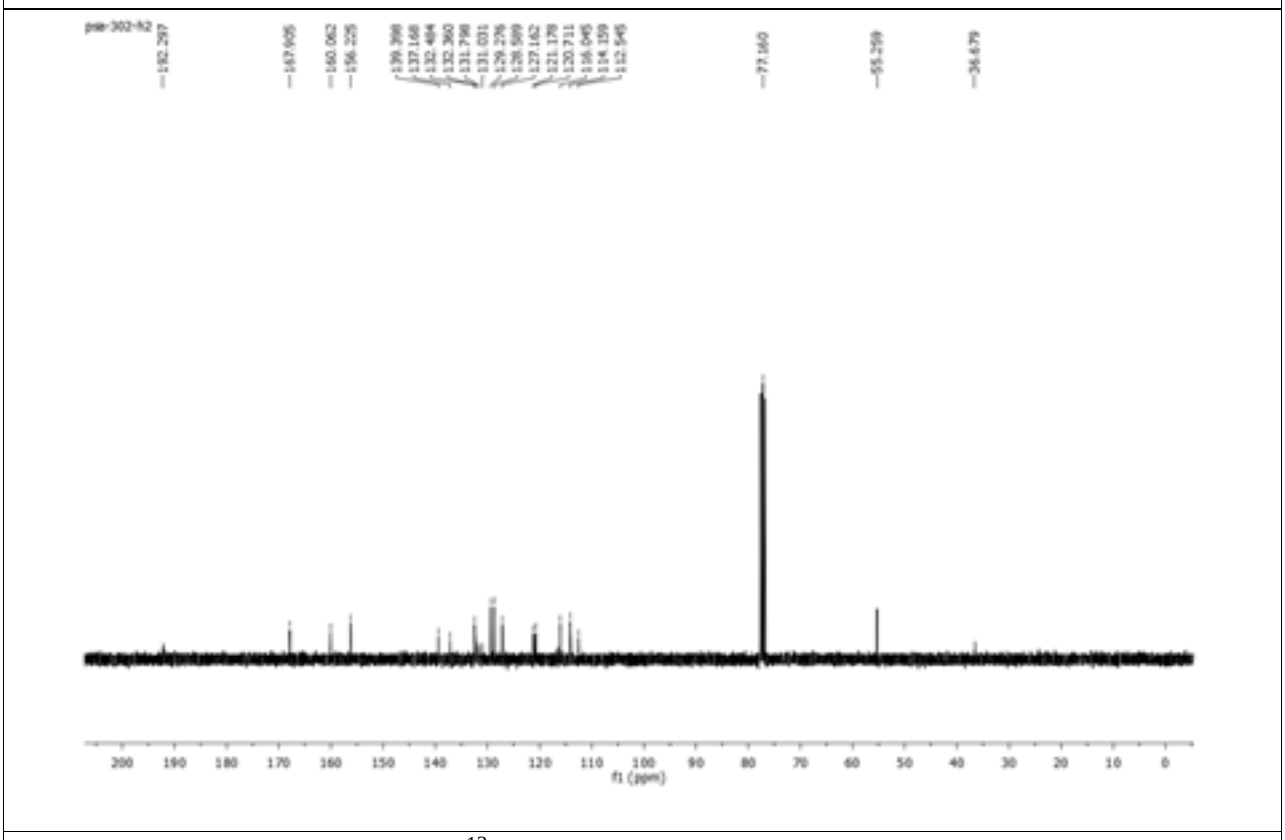
^{1}H NMR Spectrum of **6an**.



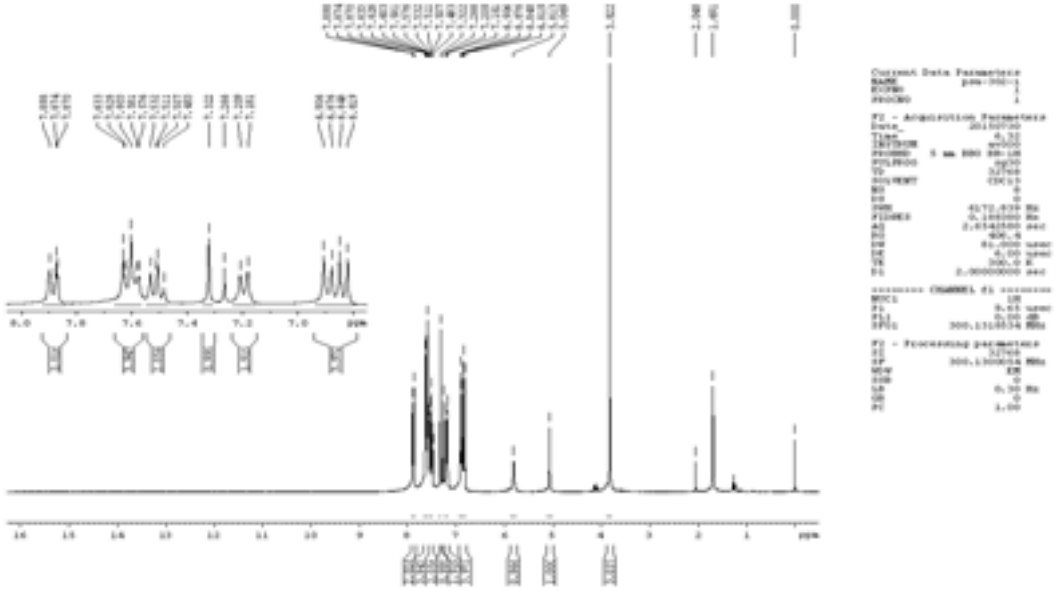
^{13}C NMR Spectrum of **6an**.



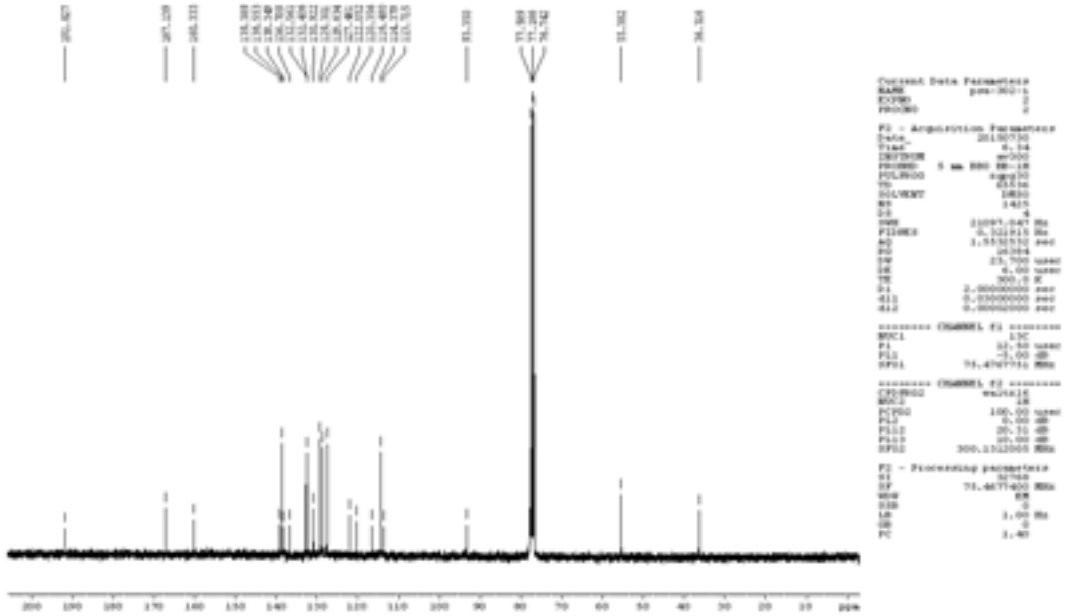
^{1}H NMR Spectrum of **6ao**.



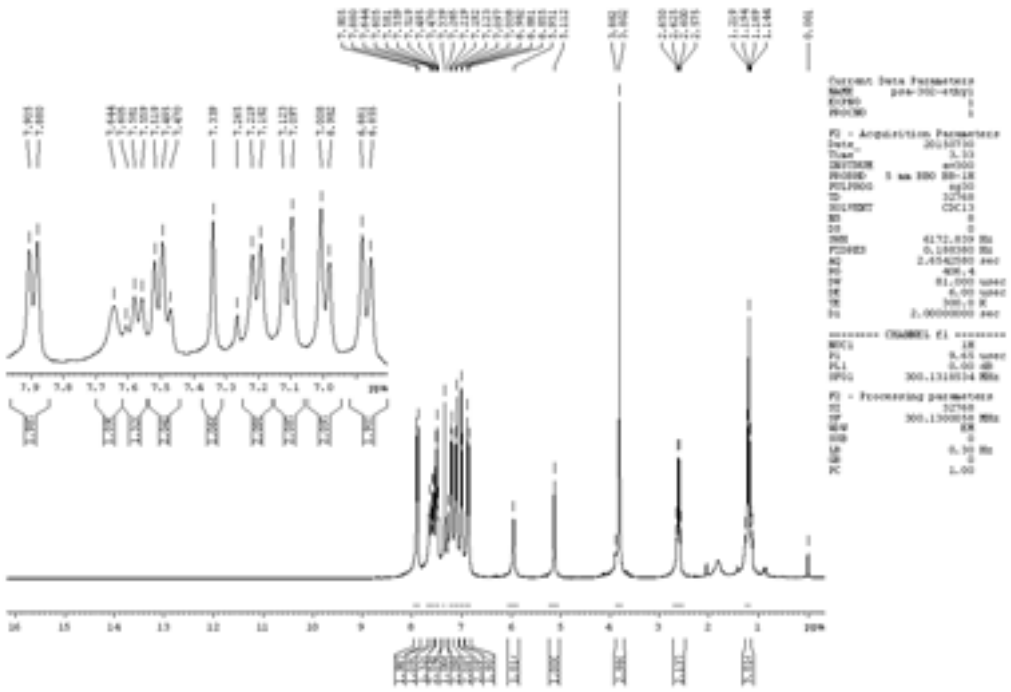
^{13}C NMR Spectrum of **6ao**.



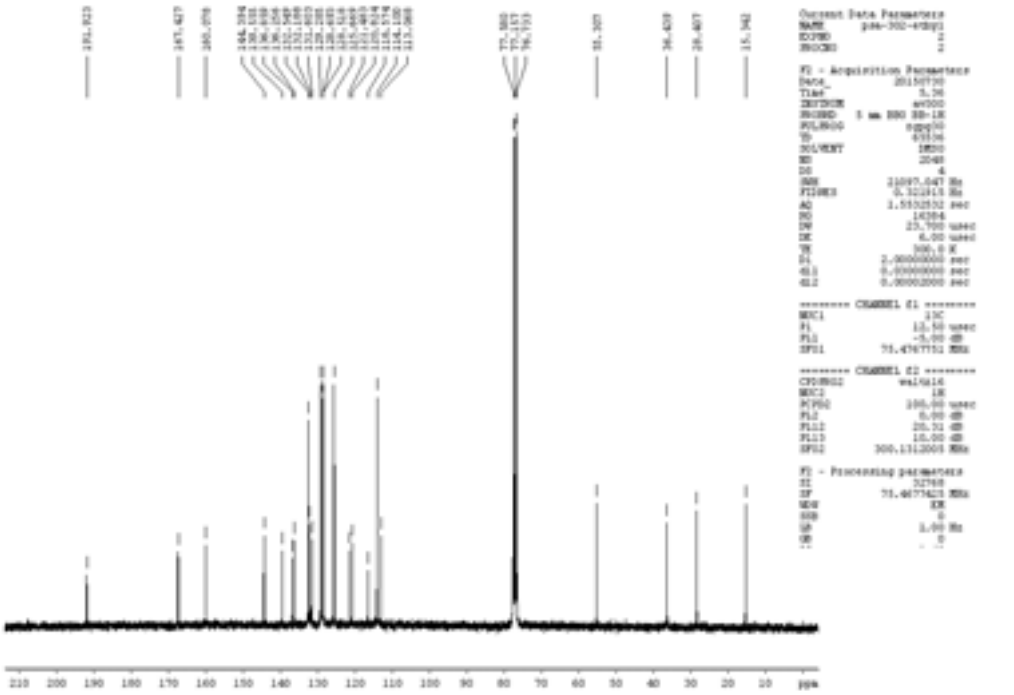
^{1}H NMR Spectrum of **6ap**.



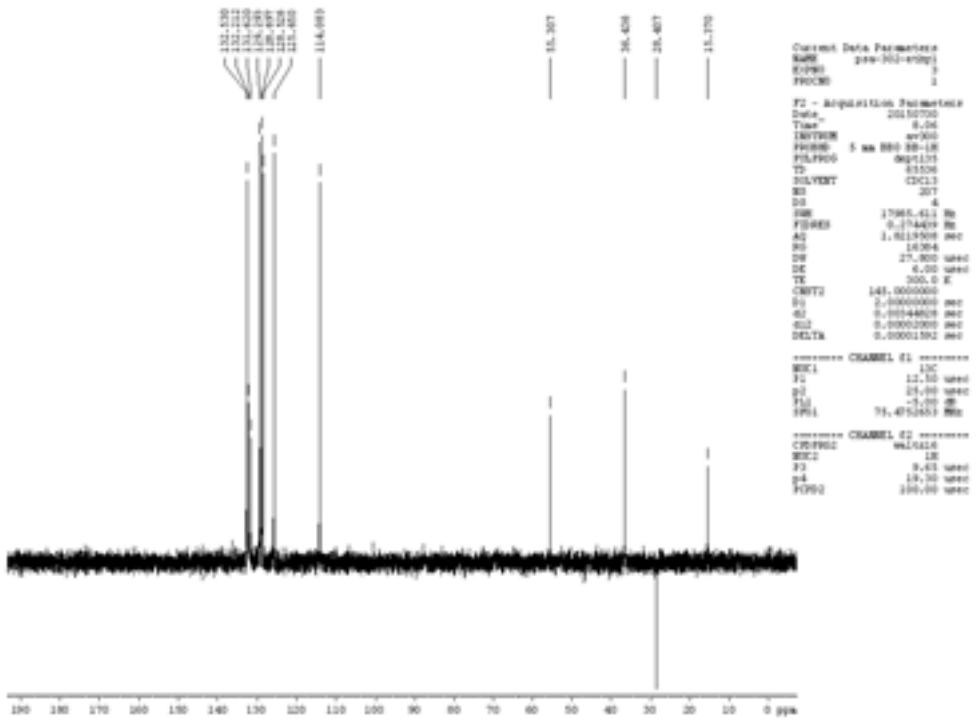
^{13}C NMR Spectrum of **6ap**.



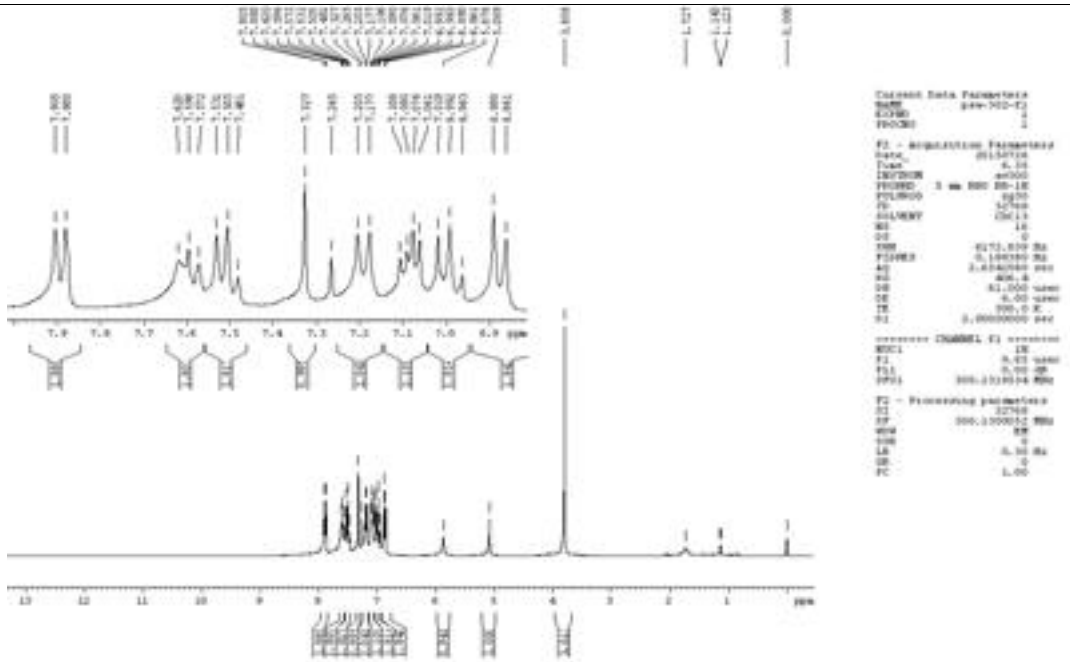
^{1}H NMR Spectrum of **6aq**.



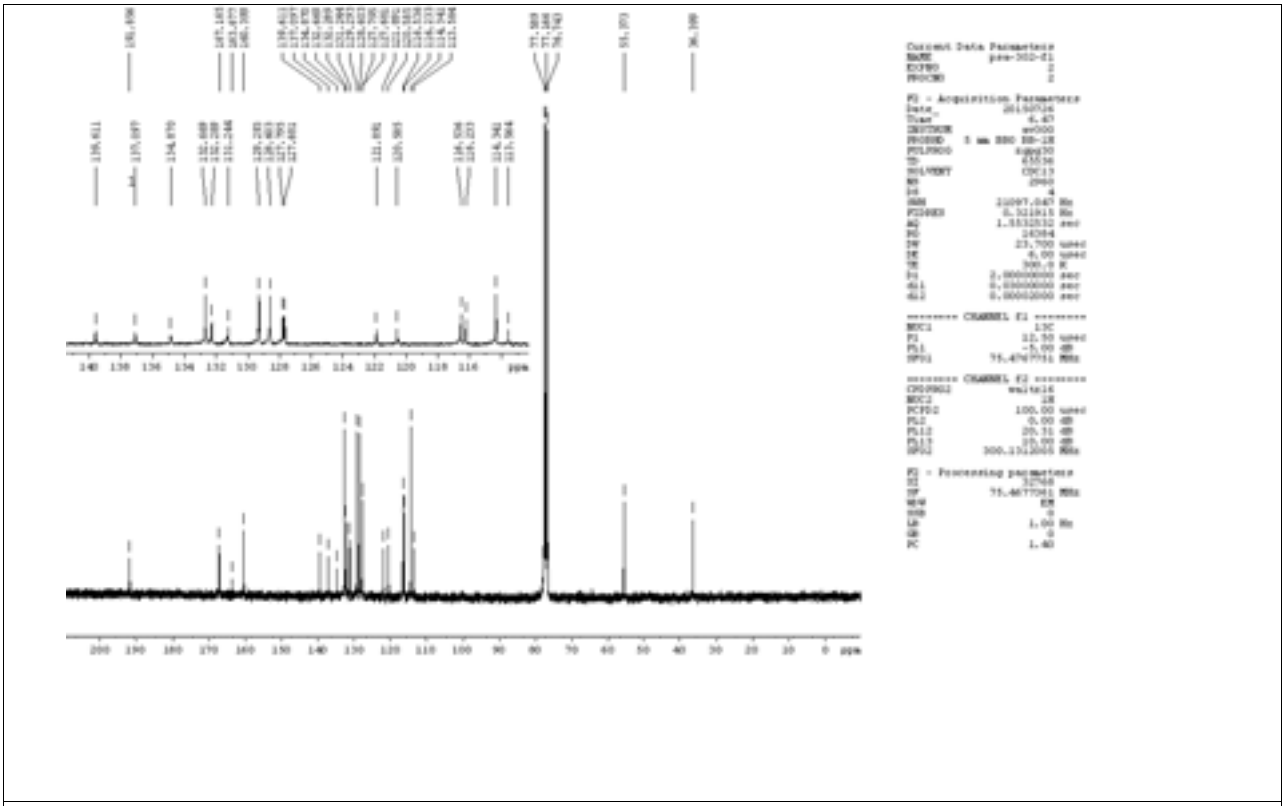
^{13}C NMR Spectrum of **6aq**.



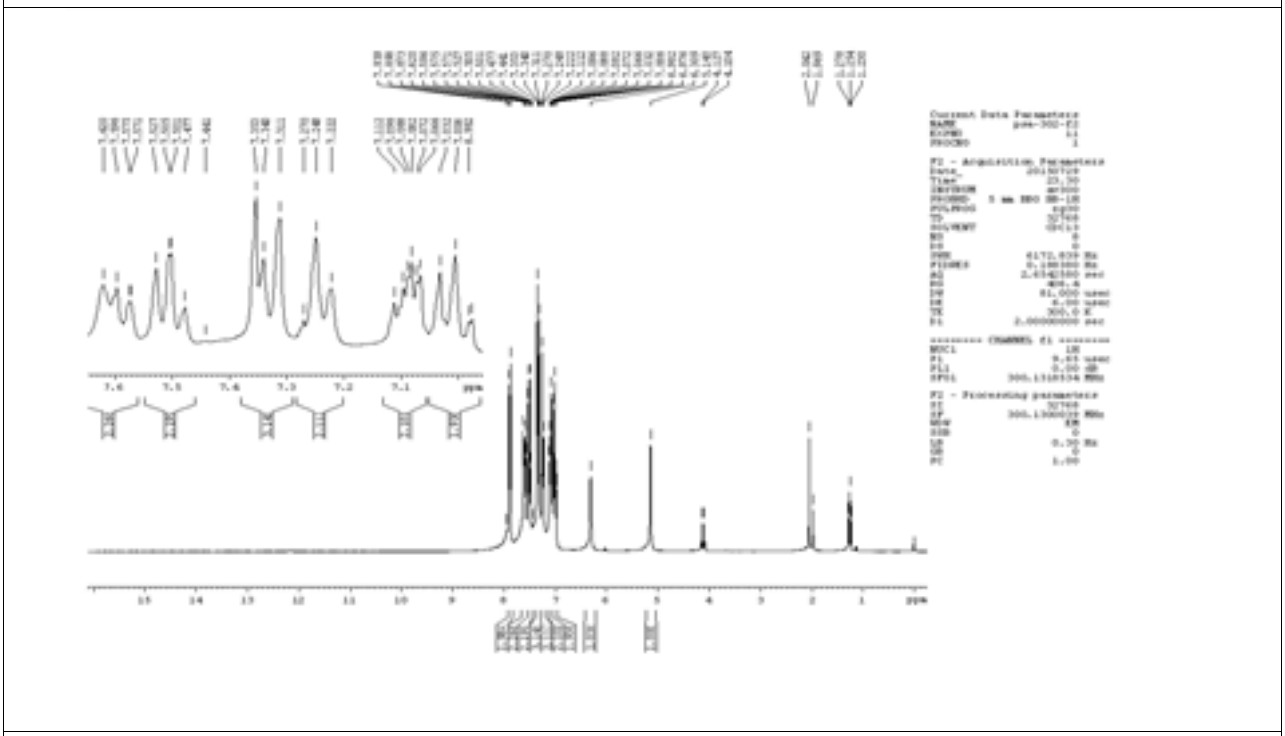
DEPT-135 NMR Spectrum of **6aq**.



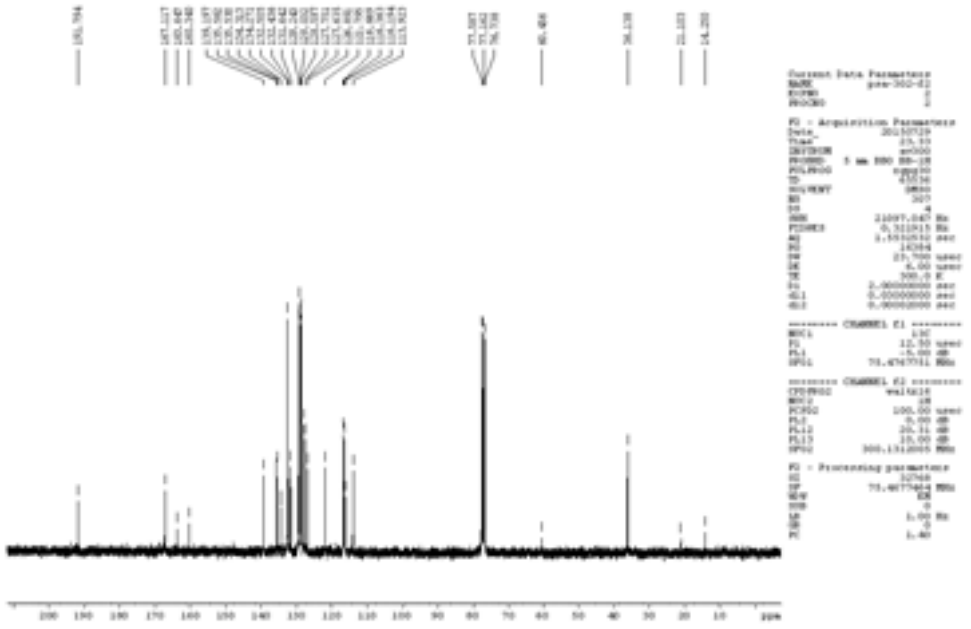
^{1}H NMR Spectrum of **6ar**.



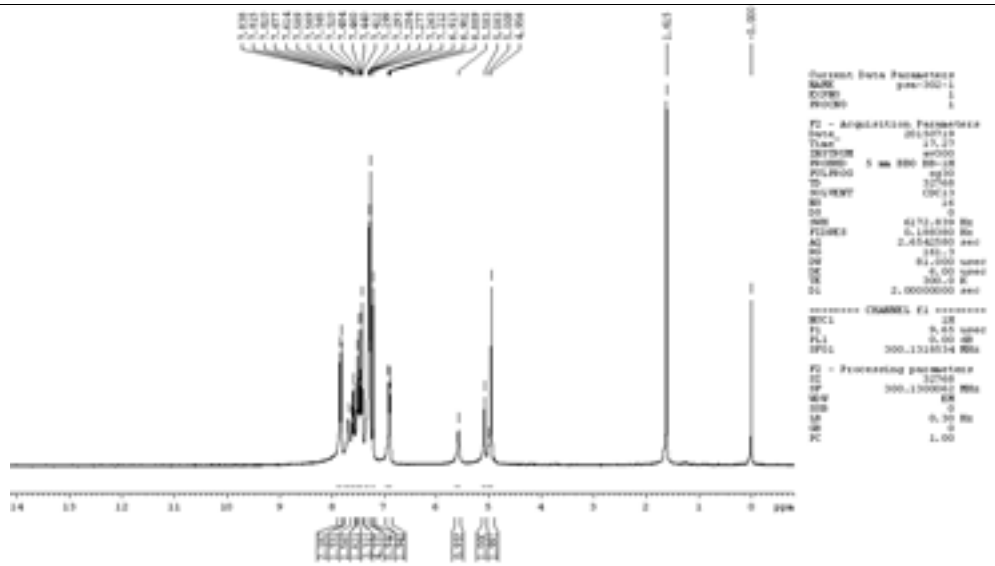
^{13}C NMR Spectrum of **6ar**.



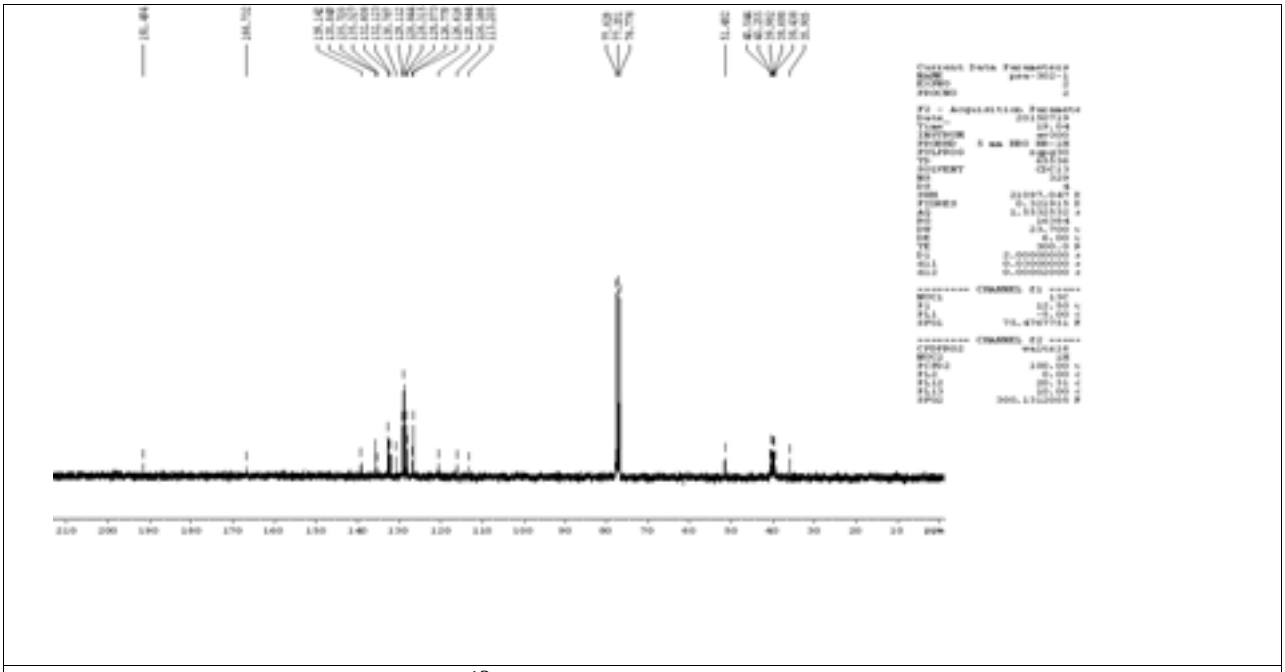
^{1}H NMR Spectrum of **6as**.



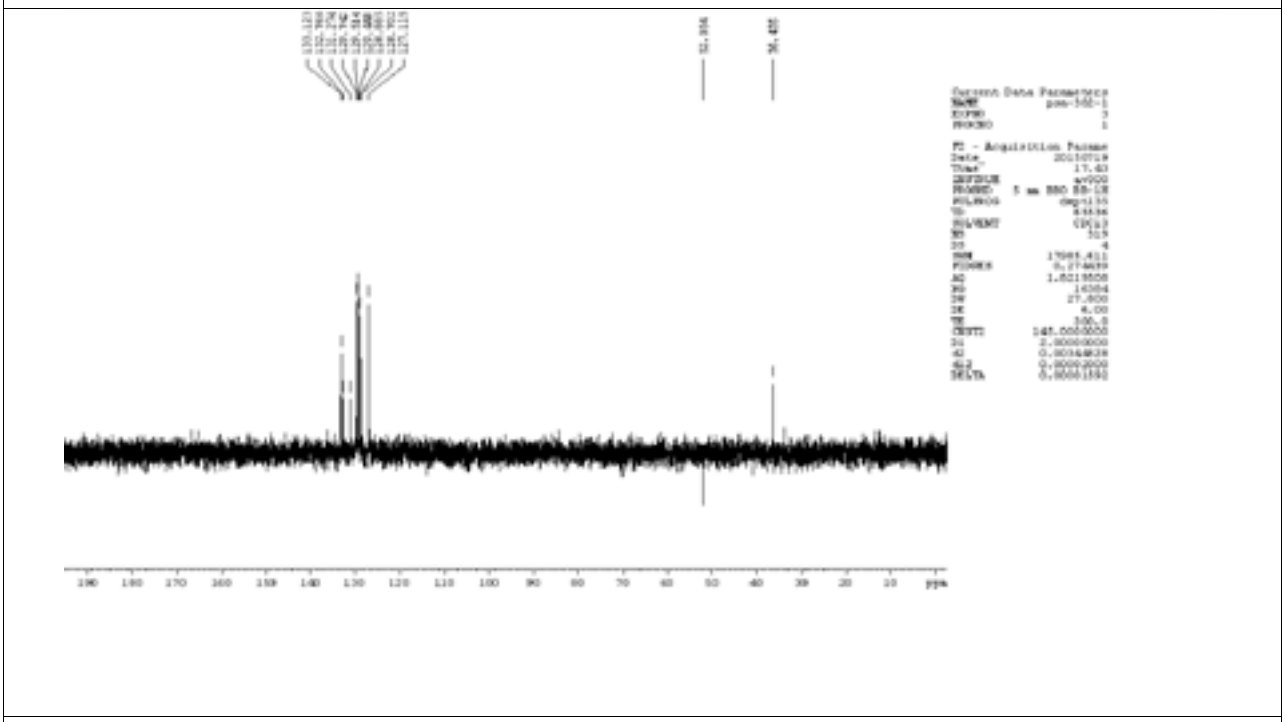
^{13}C NMR Spectrum of **6as**.



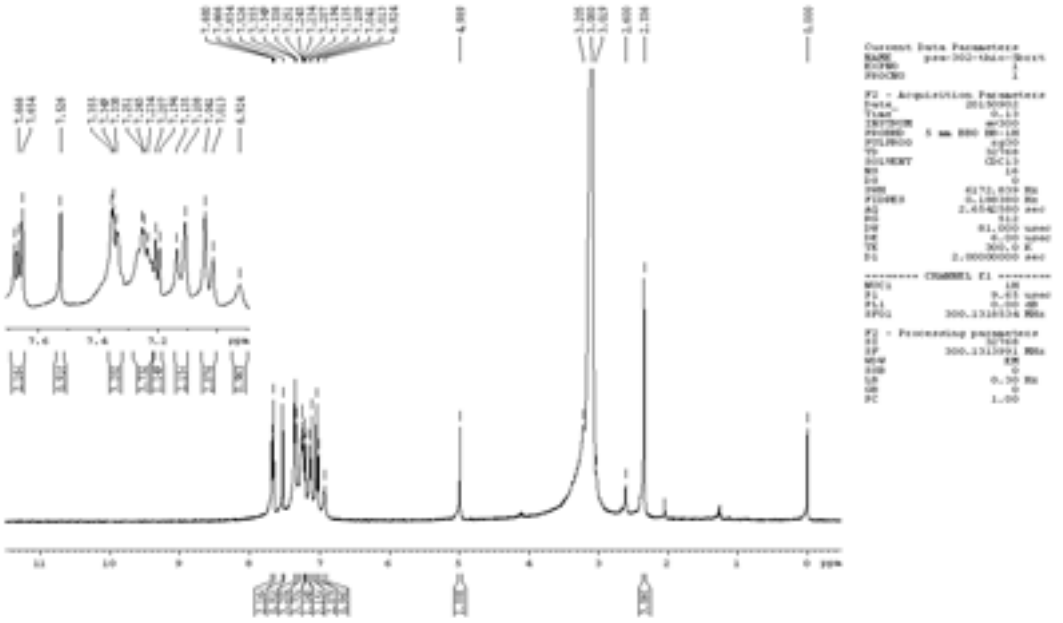
^{1}H NMR Spectrum of **6at**.



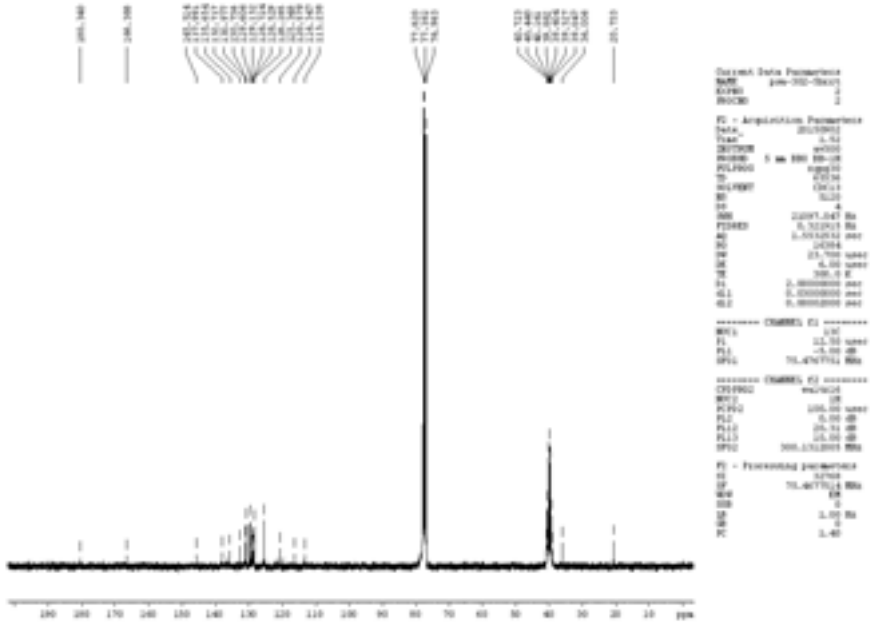
^{13}C NMR Spectrum of **6at**.



DEPT-135 NMR Spectrum of **6at**.



^{1}H NMR Spectrum of **6au**.



^{13}C NMR Spectrum of **6au**

1. **Data Collection**

A Leica MZ 75 microscope was used to identify a suitable colorless block with very well defined faces with dimensions (max, intermediate, and min) 0.08 x 0.02 x 0.02 mm^3 from a representative sample of crystals of the same habit. The crystal mounted on a nylon loop was then placed in a cold nitrogen stream (Oxford) maintained at 110 K.

A BRUKER GADDS X-ray (three-circle) diffractometer was employed for crystal screening, unit cell determination, and data collection. The goniometer was controlled using the FRAMBO software, v.4.1.05.[1] The sample was optically centered with the aid of a video camera such that no translations were observed as the crystal was rotated through all positions. The detector was set at 5.0 cm from the crystal sample. The X-ray radiation employed was generated from a Cu sealed X-ray tube (K_α = 1.5418 Å with a potential of 40 kV and a current of 40 mA) fitted with a graphite monochromator in the parallel mode (175 mm collimator with 0.5 mm pinholes).

180 data frames were taken at widths of 0.5°. These reflections were used to determine the unit cell using Cell_Now.[2] The unit cell was verified by examination of the *h k l* overlays on several frames of data. No super-cell or erroneous reflections were observed.

After careful examination of the unit cell, an extended data collection procedure (11 sets) was initiated using omega and phi scans.

Data Reduction, Structure Solution, and Refinement

Integrated intensity information for each reflection was obtained by reduction of the data frames with APEX2.[3] The integration method employed a three dimensional profiling algorithm and all data were corrected for Lorentz and polarization factors, as well as for crystal decay effects. Finally the data was merged and scaled to produce a suitable data set. SADABS[4] was employed to correct the data for absorption effects.

Systematic reflection conditions and statistical tests indicated the space group *C*2/*c*. A solution was obtained readily using XT/XS.[3,5] Hydrogen atoms were placed in idealized positions and were refined

using riding model. All non-hydrogen atoms were refined with anisotropic thermal parameters. The structure was refined (weighted least squares refinement on F^2) to convergence.[5,6] Platon[#] was used to verify the absence of additional symmetry. Platon,[#] though, indicated presence of voids of volume 517.4 Å^3, corresponding to 23 e^- per unit cell; the residual electron density map did not indicate any possible solvents. Upon SQUEEZE, the reliability factor did not decrease significantly indicating no possible contents in the voids.

OLEX2 was employed for the structure plots.[6]

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[1] FRAMBO v. 4.1.05 "Program for Data Collection on Area Detectors" BRUKER-Nonius Inc., 5465 East Cheryl Parkway, Madison, WI 53711-5373 USA

[2] Sheldrick, G. M. "Cell_Now (version 2008/1): Program for Obtaining Unit Cell Constants from Single Crystal Data": University of Göttingen, Germany

[3] APEX2 "Program for Data Collection and Integration on Area Detectors" BRUKER AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711-5373 USA

[4] Sheldrick, G.M. "SADABS: Program for Absorption Correction for Data from Area Detector Frames", University of Göttingen.

[5] Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122; Sheldrick, G. M. (2015), Acta Cryst. A71, 3-8. XT, XS, BRUKER AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711-5373 USA.

[6] Dolomanov, O. V, Bourhis, L. J., Gildea, R. J., Howard, J. A. K., and Puschmann, H. "OLEX2: A Complete Structure Solution, Refinement and Analysis Program", *J. Appl. Cryst.* **2009**, *42*, 339-341.

[#] Spek, A. L., "PLATON - A Multipurpose Crystallographic Tool" *J. Appl. Cryst.* **2003**, *36*, 7-13.; Spek, A. L., Utrecht University, Utrecht, The Netherlands **2008**.

Table 1. Crystal data and structure refinement for PTB_150921_G_5AM.

Identification code	psa5am	
Empirical formula	C27 H20 Cl N3 O3	
Formula weight	469.91	
Temperature	110.0 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 29.0413(17) Å	α= 90°.
	b = 12.5389(6) Å	β= 92.096(4)°.
	c = 13.3299(6) Å	γ = 90°.
Volume	4850.8(4) $Å^3$	
Z	8	
Density (calculated)	1.287 Mg/m^3	
Absorption coefficient	1.668 mm^{-1}	
F(000)	1952	
Crystal size	0.08 x 0.02 x 0.02 mm^3	
Theta range for data collection	3.045 to 60.568°.	
Index ranges	-32<=h<=32, -13<=k<=13, -15<=l<=15	
Reflections collected	25107	
Independent reflections	3533 [R(int) = 0.0525]	
Completeness to theta = 67.679°	80.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7519 and 0.6553	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3533 / 0 / 308	
Goodness-of-fit on F^2	1.096	
Final R indices [I>2sigma(I)]	R1 = 0.0343, wR2 = 0.0853	
R indices (all data)	R1 = 0.0427, wR2 = 0.0888	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.213 and -0.342 $e.Å^{-3}$	