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Supplementary Information

Synthesis, Urease Inhibition, Antioxidant and Antibacterial Studies of Some 4-Amino-5-aryl-3*H*-1,2,4-triazole-3-thiones and their 3,6-Disubstituted 1,2,4-Triazolo[3,4-*b*]1,3,4-thiadiazole Derivatives

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Characterization data

3-(4-Methoxyphenyl)propanehydrazide (**3a**)

Yield 85%; mp 82-84 °C; R_f = 0.19 (petroleum ether-ethyl acetate, 8:2); IR ν_{max}/cm^{-1} 3296 (NH_2), 3204 (NH), 1637 (C=O), 1525, 1491, 1451 (C=C), 1238(C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.96 (s, 1H, N*H*), 7.1 (d, 2H, *J* 8.4 Hz, Ar-*H*), 6.83 (d, 2H, *J* 8.4 Hz, Ar-*H*), 4.16 (s, 2H, broad, NH_2), 3.70 (s, 3H, OCH_3), 2.75 (t, 2H, *J* 7.5 Hz, CH_2), 2.29 (t, 2H, *J* 7.5 Hz, CH_2); ^{13}C NMR (75 MHz, DMSO-d_6) δ 171.33 (C=O), {157.98, 133.54, 129.58, 114.15} (Ar-*C*), 55.40 (OCH_3), 35.89 (CH_2), 30.63 (CH_2); Analysis calcd. for $C_{10}H_{14}N_2O_2$: C, 61.84; H, 7.27; N, 14.42; Found: C, 59.66; H, 6.49; N, 15.41.

2-(2-Methoxyphenyl)acetohydrazide (**3b**)

Yield 85-89%; mp 121-122 °C; R_f = 0.21 (petroleum ether-ethyl acetate, 8:2); IR ν_{max}/cm^{-1} 3312 (NH_2), 3210 (NH), 1626 (C=O), 1597 (C=C), 1249 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.26 (s, 1H, N*H*), 7.48-7.40 (m, 2H, Ar-*H*), 7.19-7.08 (m, 2H, Ar-*H*), 4.46 (s, broad, 2H, NH_2), 3.96 (s, 3H, OCH_3), 3.51 (s, 2H, CH_2C=O); ^{13}C NMR (75 MHz, DMSO-d_6) δ 170.36 (C=O), {130.92, 128.64, 124.93, 120.77, 114.31, 111.31} (Ar-*C*), 55.81 (OCH_3), 35.22 (CH_2); Analysis calcd for $C_9H_{12}N_2O_2$: C, 59.99; H, 6.71; N, 15.55; Found: C, 59.65; H, 6.50; N, 15.43.

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2-(3-Methoxyphenyl)acetohydrazide (**3c**)

Yield 82%; mp 83-85 °C; R_f = 0.20 (petroleum ether-ethyl acetate, 8:2); IR ν_{max}/cm^{-1}); 3308, 3214 (NH_2), 3181 (NH), 1617 (C=O), 1593, 1491 (C=C), 1248 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.20 (s, 1H, N*H*), 7.20 (t, 1H, *J* 8.1 Hz, Ar-*H*), 6.84-6.772 (m, 3H, Ar-*H*), 4.45 (s, 2H, broad, NH_2), 3.73 (s, 3H, OCH_3), 3.31 (s, 2H, CH_2C=O); ^{13}C NMR (75 MHz, DMSO-d_6) δ 169.89 (C=O), {138.17, 129.62, 121.67, 115.16, 112.21, 114.34} (Ar-*C*), 55.40 (OCH_3), 40.98 (CH_2); Analysis calcd. for $C_9H_{12}N_2O_2$: C, 59.99; H, 6.71; N, 15.55; Found: C, 59.68; H, 6.56; N, 15.35.

2-(4-Methoxyphenyl)acetohydrazide (**3d**)

Yield 86%; mp 126-127 °C; R_f = 0.21 (petroleum ether-ethyl acetate, 8:2); IR ν_{max}/cm^{-1}); 3338, 3302 (NH_2), 3205 (NH), 1610 (C=O), 1507, 1440 (C=C), 1234 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.16 (s, 1H, N*H*), 7.18 (d, 2H, *J* 8.7 Hz, Ar-*H*), 6.85 (d, 2H, *J* 8.7 Hz, Ar-*H*), 4.21 (s, 2H, broad, NH_2), 3.71 (s, 3H, OCH_3), 3.27 (s, 2H, CH_2C=O); ^{13}C NMR (75 MHz, DMSO-d_6) δ 170.38 (C=O), {158.37, 130.82, 128.64, 114.06} (Ar-*C*), 55.47 (OCH_3), 40.51 (CH_2); Analysis calcd. for $C_9H_{12}N_2O_2$: C, 59.99; H, 6.71; N, 15.55; Found: C, 59.69; H, 6.58; N, 15.49.

2-(2,5-Dimethoxyphenyl)acetohydrazide (**3e**)

Yield 82%; mp 145-147 °C; R_f = 0.22 (petroleum ether-ethyl acetate, 8:2); IR ν_{max}/cm^{-1} 3298 (NH_2), 3205

(NH), 1625 (C=O), 1561, 1448 (C=C), 1233 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 9.09 (s, 1H, N*H*), 7.02 (d, 1H, *J* 2.1 Hz, Ar-*H*), 6.74 (d, 1H, *J* 8.7 Hz, Ar-*H*), 6.65 (d, 2H, *J* 8.7 Hz, Ar-*H*), 4.26 (s, 2H, broad, NH_2), 3.74 (s, 3H, OCH_3), 3.72 (s, 3H, OCH_3), 3.36 (s, 2H, CH_2C=O); ^{13}C NMR (75 MHz, DMSO-d_6) δ 169.45 (C=O), {159.32, 134.78, 132.48, 130.76, 128.43, 111.16} (Ar-*C*), 55.87 (OCH_3), 55.65 (OCH_3) 41.78 (CH_2); Analysis calcd. for $C_9H_{12}N_2O_2$: C, 57.13; H, 6.71; N, 13.33; Found: C, 57.01; H, 6.65; N, 13.20.

4-Amino-3-(4-methoxyphenethyl)-1*H*-1,2,4-triazole-5(4*H*)-thione (**5a**)

Yield 58%; mp 203-205 °C; R_f = 0.21 (petroleum ether-ethyl acetate, 6:3); IR ν_{max}/cm^{-1} 3249 (NH_2), 3153 (NH), 2931, 2831 (C-H) 1631 (C=N), 1611, 1568, 1509 (C=C), 1243 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 13.44 (s, 1H, N*H*), 7.14 (dd, 2H, *J* 8.7, 3.0 Hz, Ar-*H*), 6.84 (dd, 2H, *J* 8.7, 3 Hz, Ar-*H*), 5.58 (s, 2H, NH_2), 3.71 (s, 2H, OCH_3), 2.89 (t, 2H, *J* 7.8 Hz, CH_2), 2.56 (t, 2H, *J* 7.8 Hz, CH_2); ^{13}C NMR (75 MHz, DMSO-d_6) δ 166.21 (C=S), 158.63 (C=N), {157.81, 134.22, 129.31, 114.31} (Ar-C), 55.56 (OCH_3), 27.25 and 26.54 (CH_2); EI-MS *m/z* (rel. abund. %), 250 ($M^{+\cdot}$, 31), 121 (100), 91 (9), 77 (11), 65 (4); Analysis calcd. for $C_{11}H_{14}N_4OS$: C, 52.78; H, 5.64; N, 22.38; S, 12.81; Found: C, 52.55; H, 5.61; N, 22.19; S, 12.65.

4-Amino-3-(2-methoxybenzyl)-1*H*-1,2,4-triazole-5(4*H*)-thione (**5b**)

Yield 62%; mp 159-160 °C; R_f = 0.24 (petroleum ether-ethyl acetate, 6:3); IR ν_{max}/cm^{-1} 3327 (NH_2), 3105 (NH), 2949, 2835 (C-H), 1638 (C=N), 1570, 1490 (C=C), 1242(C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 13.47 (s, 1H, N*H*), 7.26 (dt, 1H, *J* 9, 1.5 Hz, Ar-*H*), 7.10 (dd, 1H, *J* 7.5, 1.5 Hz, Ar-*H*), 6.99 (d, 1H, *J* 7.8 Hz, Ar-*H*), 6.87 (dt, 1H, *J* 7.5, 0.9 Hz, Ar-*H*), 5.55 (s, 2H, NH_2), 3.95 (s, 2H, CH_2), 3.76 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 166.21 (C=S), 157.35 (C=N), {151.51, 130.39, 128.79, 123.66, 120.73, 111.26} (Ar-C), 55.89 (OCH_3), 25.24 (CH_2); EI-MS *m/z* (rel. abund. %), 236 ($M^{+\cdot}$, 89), 221 (100), 205 (30), 188 (18), 147 (14), 121 (21), 91 (39), 77 (24), 65 (13); Analysis calcd. for $C_{10}H_{12}N_4OS$: C, 50.83; H, 5.12; N, 23.71; S, 13.57; Found: C, 50.71; H, 5.01; N, 23.59; S, 13.45.

4-Amino-3-(3-methoxybenzyl)-1*H*-1,2,4-triazole-5(4*H*)-thione (**5c**)

Yield 55%; mp 125-126 °C; R_f = 0.23 (petroleum ether-ethyl acetate, 6:3); IR ν_{max}/cm^{-1} 3309 (NH_2), 3149 (NH), 3035, 2930, 2829 (C-H), 1628 (C=N), 1583, 1559, 1478 (C=C), 1256 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 13.55 (s, 1H, N*H*), 7.22 (t, 1H, *J* 7.5 Hz, Ar-*H*), 6.82 (m, 3H, Ar-H), 5.57 (s, 2H, NH_2), 3.99 (s, 2H, CH_2), 3.73 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 166.49 (C=S), 159.75 (C=N), {151.77, 137.45, 129.99, 121.46, 115.02, 112.67} (Ar-C), 55.43 (OCH_3), 30.59 (CH_2); EI-MS *m/z* (rel. abund. %), 236 ($M^{+\cdot}$, 100), 220 (78), 161 (10), 146 (14), 121 (29), 91 (7), 77 (9), 51 (4); Analysis calcd. for $C_{10}H_{12}N_4OS$: C, 50.83; H, 5.12; N, 23.71; S, 13.57; Found: C, 50.78; H, 5.07; N, 23.56; S, 13.45.

4-Amino-3-(4-methoxybenzyl)-1*H*-1,2,4-triazole-5(4*H*)-thione (**5d**)

Yield 65%; mp 204-206 °C; R_f = 0.25 (petroleum ether-ethyl acetate, 6:3); IR ν_{max}/cm^{-1} 3290 (NH_2), 3201 (NH), 2919, 2836 (C-H), 1645 (C=N), 1609, 1561, 1509 (C=C), 1247 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 13.52 (s, 1H, N*H*), 7.21 (d, 2H, *J* 8.7 Hz, Ar-*H*), 6.87 (d, 2H, *J* 8.7 Hz, Ar-*H*), 5.54 (s, 2H, NH_2), 3.94 (s, 2H, CH_2), 3.71 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 166.39 (C=S), 158.58 (C=N), {152.16, 130.41, 127.73, 114.33} (Ar-C), 55.55 (OCH_3), 29.79 (CH_2); EI-MS *m/z* (rel. abund. %), 236 ($M^{+\cdot}$, 100), 220 (18), 193 (17), 161 (9), 121 (21), 91 (11), 77 (12), 51 (4); Analysis calcd. for $C_{10}H_{12}N_4OS$: C, 50.83; H, 5.12; N, 23.71; S, 13.57; Found: C, 50.67; H, 5.07; N, 23.61; S, 13.43.

4-Amino-3-(2,5-dimethoxybenzyl)-1*H*-1,2,4-triazole-5(4*H*)-thione (**5e**)

Yield 60%; mp 189-191 °C; R_f = 0.25 (petroleum ether-ethyl acetate, 6:3); IR ν_{max}/cm^{-1} 3302 (NH_2), 3197 (NH), 3082, 2921, 2835 (C-H), 1641 (C=N), 1568, 1502, 1479 (C=C), 1221 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 13.71 (s, 1H, N*H*), 6.98 (s, 1H, Ar-*H*), 6.67 (d, 1H, *J* 7.5 Hz, Ar-*H*), 6.58 (d, 1H, *J* 7.5 Hz, Ar-*H*), 5.59 (s, 2H, NH_2), 3.91 (s, 2H, CH_2), 3.71 and 3.68 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 168.21 (C=S), 160.35 (C=N), {157.51, 151.32, 141.45, 134.66, 121.25, 114.20} (Ar-C), 55.89 and 54.67 (OCH_3), 25.29 (CH_2); EI-MS *m/z* (rel. abund. %), 266 ($M^{+\cdot}$, 100), 251 (68), 235 (36), 218 (81), 177 (18), 162 (29), 121 (16), 91 (18), 77 (17), 65 (18); Analysis calcd. for $C_{11}H_{14}N_4O_2S$: C, 49.61; H, 5.30; N, 21.04; S, 12.04; Found: C, 49.49; H, 5.25; N, 20.91; S, 12.00.

6-(4-Chlorophenyl)-3-(4-methoxyphenethyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6a**)

Yield 65%; mp 133-134 °C; R_f = 0.21 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3073 (sp^2 C-H),

2954, 2919, 2850 (sp^3 C-H), 1596 (C=N), 1509, 1568 (C=C), 1241 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.96 (td, 2H, *J* 8.7, 2.7 Hz, Ar-*H*), 7.69 (td, 2H, *J* 8.7, 2.7 Hz, Ar-*H*), 7.15 (dd, 2H, *J* 8.1, 1.8 Hz, Ar-*H*), 6.81 (dd, 2H, *J* 8.1, 1.8 Hz, Ar-*H*), 3.67 (s, 3H, OCH_3), 3.32 (t, 2H, *J* 7.5 Hz, CH_2), 3.09 (t, 2H, *J* 7.5 Hz, CH_2); ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.20, 158.20 (C=N), {147.62, 137.90, 132.44, 130.20, 129.85, 129.32, 128.36, 114.19} (Ar-C), 55.39 (OCH_3), 31.67 and 26.99 (CH_2); EI-MS *m/z* (rel. abund. %), 370 ($M^{+\cdot}$, 31), 372 (M + 2, 11), 339 (3), 232 (7), 155 (9), 132 (12), 121 (100), 91 (9), 77 (8); Analysis calcd. for $C_{18}H_{15}ClN_4OS$: C, 58.30; H, 4.08; N, 15.11; S, 8.65; Found: C, 58.19; H, 4.01; N, 15.04; S, 8.51.

6-(2,5-Difluorophenyl)-3-(4-methoxyphenethyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6b**)

Yield 63%; mp 160-162 °C; R_f = 0.22 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3033 (sp^2 C-H), 2954, 2917, 2849 (sp^3 C-H), 1612 (C=N), 1509, 1457 (C=C), 1242 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.83-7.87 (m, 1H, Ar-*H*), 7.64-7.60 (m, 2H, Ar-*H*), 7.15 (d, 2H, *J* 8.7 Hz, Ar-*H*), 6.81 (d, 2H, *J* 8.7 Hz, Ar-*H*), 3.67 (s, 3H, OCH_3), 3.31 (t, 2H, *J* 7.8 Hz, CH_2), 3.09 (t, 2H, *J* 7.8 Hz, CH_2); ^{13}C NMR (75 MHz, DMSO-d_6) δ 158.99, 158.20 (C=N), {154.75, 153.57, 147.51, 132.46, 129.89, 119.73, 118.77, 118.65, 115.60, 114.16} (Ar-C), 55.40 (OCH_3), 31.70 and 27.01 (CH_2); EI-MS *m/z* (rel. abund. %), 372 ($M^{+\cdot}$, 72), 232 (5), 157 (8), 134 (12), 121 (100), 91 (7), 77 (8); Analysis calcd. for $C_{18}H_{14}F_2N_4OS$: C, 58.06; H, 3.79; N, 15.05; S, 8.61; Found: C, 58.01; H, 3.65; N, 14.95; S, 8.56.

6-(4-Chlorophenyl)-3-(2-methoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6c**)

Yield 68%; mp 180-181 °C; R_f: 0.22 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3057, 3022 (sp^2 C-H), 2962, 2918, 2849 (sp^3 C-H), 1594 (C=N), 1491, 1464 (C=C), 1244 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.30-7.20 (m, 2H, Ar-H), 7.01 (d, 2H, *J* 7.5 Hz, Ar-*H*), 6.90 (t, 1H, *J* 7.5 Hz, Ar-*H*), 7.94 (td, 2H, *J* 8.7, 2.4 Hz, Ar-*H*), 7.68 (td, 2H, *J* 8.7, 2.4 Hz, Ar-*H*), 4.37 (s, 2H, CH_2), 3.77 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.40, 157.40 (C=N), {152.96, 146.82, 146.82, 137.91, 130.46, 130.23, 129.27, 129.00, 128.38, 123.86, 120.82, 111.39} (Ar-H), 56.01 (OCH_3), 25.38 (CH_2); EI-MS *m/z* (rel. abund. %), 356 ($M^{+\cdot}$, 58), 358 (M +2, 18), 341 (7), 325 (100), 267 (11), 250 (61), 155 (38), 137 (10), 116 (16), 91 (25), 77 (15), 65 (7), 51 (8); Analysis calcd. for $C_{17}H_{13}ClN_4OS$: C, 57.22; H, 3.67; N, 15.70; S, 8.99; Found: C, 57.16; H, 3.61; N, 15.61; S, 8.85.

6-(2,5-Difluorophenyl)-3-(2-methoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6d**)

Yield 58%; mp 178-180 °C; R_f = 0.21 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3065 (sp^2 C-H), 2918, 2849 (sp^3 C-H), 1590 (C=N), 1493, 1456, 1426 (C=C), 1246 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.30-7.23 (m, 2H, Ar-*H*), 7.02 (d, 1H, *J* 8.1 Hz, Ar-*H*), 6.91 (t, 2H, *J* 7.2 Hz, Ar-*H*), 7.87-7.81 (m, 1H, Ar-*H*), 7.64-7.59 (m, 2H, Ar-*H*), 4.39 (s, 2H, CH_2), 3.77 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 159.26, 158.02 (C=N), {154.76, 146.70, 130.62, 123.79, 120.80, 118.82, 118.80, 118.52, 115.27, 114.93, 111.38} (Ar-C), 55.97 (OCH_3), 25.39 (CH_2); EI-MS *m/z* (rel. abund. %), 358 ($M^{+\cdot}$, 67), 327 (100), 269 (7), 252 (73), 204 (12), 157 (42), 116 (17), 104 (9), 91 (24), 77 (16), 51 (7); Analysis calcd. for $C_{17}H_{12}F_2N_4OS$: C, 56.98; H, 3.38; N, 15.63; S, 8.95; Found: C, 56.82; H, 3.31; N, 15.51; S, 8.81.

6-(4-Chlorophenyl)-3-(3-methoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6e**)

Yield 65%; mp 133-134 °C; R_f = 0.21 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3046 (sp^2 C-H), 3005, 2918, 2838 (sp^3 C-H), 1594 (C=N), 1512, 1465 (C=C), 1245 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.45 (d, 2H, *J* 7.5 Hz, Ar-*H*), 7.03 (d, 2H, *J* 7.5 Hz, Ar-*H*), 6.98 (t, 1H, *J* 1.2 Hz, Ar-*H*), 6.81-6.79 (m, 3H, Ar-*H*), 4.32 (s, 2H, CH_2), 3.81 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 166.33, 160.34 (C=N), {143.33, 137.27, 131.61, 129.66, 129.31, 121.86, 115.76, 113.56} (Ar-C), 55.81 (OCH_3), 29.01 (CH_2); EI-MS *m/z* (rel. abund. %), 356 ($M^{+\cdot}$, 100), 358 (M + 2, 36), 325 (44), 321 (12), 245 (32), 111 (56), 91 (14), 77 (28), 51 (16); Analysis calcd. for $C_{17}H_{13}ClN_4OS$: C, 57.22; H, 3.67; N, 15.70; S, 8.99; Found: C, 57.14; H, 3.59; N, 15.58; S, 8.88.

6-(2,5-Difluorophenyl)-3-(3-methoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6f**)

Yield 71%; mp 170-172 °C; R_f = 0.23 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3066 (sp^2 C-H), 2916, 2835 (sp^3 C-H), 1613 (C=N), 1509, 1458 (C=C), 1249 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.91-7.86 (m, 2H, Ar-H), 7.63-7.59 (m, 2H, Ar-H), 7.32 (d, 1H, *J* 1.5 Hz, Ar-H), 7.11 (d, 2H, *J* 8.5 Hz, Ar-H), 6.99 (t, 1H, *J* 7.5 Hz, Ar-H), 4.38 (s, 2H, CH_2), 3.70 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 158.70 (C=N), {147.43, 130.41, 127.77, 121.84, 119.63, 119.43, 115.34, 114.98, 114.46} (Ar-C), 55.49 (OCH_3), 29.95 (CH_2); EI-MS *m/z* (rel. abund. %), 356 ($M^{+\cdot}$, 100), 327 (57), 242 (43), 157 (23), 116 (14),

91 (24), 77 (13), 51 (08); Analysis calcd. for $C_{17}H_{12}F_2N_4OS$: C, 56.98; H, 3.38; N, 15.63; S, 8.95; Found: C, 56.87; H, 3.31; N, 15.55; S, 8.86.

6-(4-Chlorophenyl)-3-(4-methoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6g**)

Yield 61%; mp 180-182 °C; R_f = 0.19 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3076 (sp^2 C-H), 2996, 2850 (sp^3 C-H), 1608 (C=N), 1581, 1510, 1459 (C=C), 1443 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.95 (d, 2H, *J* 8.1 Hz, Ar-*H*), 7.68 (d, 2H, *J* 8.1 Hz, Ar-*H*), 7.29 (d, 2H, *J* 8.1 Hz, Ar-*H*), 6.88 (d, 2H, *J* 8.1 Hz, Ar-*H*), 4.37 (s, 2H, CH_2), 3.36 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) 165.55, 158.69 (C=N), {147.47, 137.94, 130.32, 130.23, 129.29, 128.31, 127.83, 114.84} (Ar-C), 55.50 (OCH$_3$), 31.16 (CH$_2$); EI-MS *m/z* (rel. abund. %), 356 (M$^{+\cdot}$, 100), 358 (M + 2, 34), 314 (8), 323 (9), 219 (19), 204 (24), 186 (38), 155 (39), 146 (35), 121 (40), 102 (9), 77 (18), 51 (8); Analysis calcd. for $C_{17}H_{13}ClN_4OS$: C, 57.22; H, 3.67; N, 15.70; S, 8.99; Found: C, 57.10; H, 3.65; N, 15.58; S, 8.01.

6-(2,5-Difluorophenyl)-3-(4-methoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6h**)

Yield 59%; mp 148-150 °C; R_f = 0.22 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3056 (sp^2 C-H), 2952, 2865 (sp^3 C-H), 1603 (C=N), 1596, 1552, 1450 (C=C), 1245 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.91-7.86 (m, 1H, Ar-*H*), 7.60 (dt, 2H, *J* 6.9, 4.8 Hz, Ar-*H*), 7.31 (d, 2H, *J* 8.4 Hz, Ar-*H*), 6.88 (d, 2H, *J* 8.7 Hz, Ar-*H*), 4.38 (s, 2H, CH_2), 3.70 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 158.70 (C=N), {147.43, 130.41, 127.77, 121.84, 119.63, 119.43, 115.34, 114.98, 114.46} (Ar-C), 55.49 (OCH$_3$), 29.95 (CH$_2$); EI-MS *m/z* (rel. abund. %), 358 (M$^{+\cdot}$,100), 327 (35), 219 (12), 157 (42), 146 (24), 104 (9), 91 (24), 77 (16), 51 (7); Analysis calcd. for $C_{17}H_{12}F_2N_4OS$: C, 56.98; H, 3.38; N, 15.63; S, 8.95; Found: C, 56.88; H, 3.35; N, 15.53; S, 8.91.

6-(2,5-Difluorophenyl)-3-(2,5-dimethoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6i**)

Yield 69%; mp 177-179 °C; R_f = 0.21 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3078 (sp^2 C-H), 2995, 2918, 2849, 2834 (sp^3 C-H), 1603 (C=N), 1507, 1455, 1424 (C=C), 1267 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 6.95-6.89 (m, 2H, Ar-*H*), 7.88-7.86 (m, 1H, Ar-*H*), 7.66-7.61 (m, 2H, Ar-*H*), 6.85-6.81 (m, 2H, Ar-*H*), 4.37 (s, 2H, CH_2), 3.71 (s, 3H, OCH_3), 3.68 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.74 (C=N), {153.44, 151.63, 124.85, 117.12, 113.02, 112.45} (Ar-H), 55.45 and 54.98 (OCH$_3$), 28.45 (CH$_2$); EI-MS *m/z* (rel. abund. %), 388 (M$^{+\cdot}$,100), 373 (33), 357 (98), 252 (86), 239 (9), 218 (9), 157 (36), 139 (17), 119 (10), 91 (12), 77 (11), 65 (12); Analysis calcd. for $C_{18}H_{14}F_2N_4O_2S$: C, 55.66; H, 3.63; N, 14.43; S, 8.26; Found: C, 55.56; H, 3.54; N, 14.31; S, 8.19.

3-(2,5-Dimethoxybenzyl)-6-(3-methoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6j**)

Yield 75%; mp 150-152 °C; R_f = 0.22 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3038 (sp^2 C-H), 2996, 2917, 2834 (sp^3 C-H), 1607 (C=N), 1506, 1469 (C=C), 1251 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.29 (t, 1H, *J* 7.8 Hz, Ar-*H*), 6.96-6.87 (m, 4H, Ar-*H*), 6.83-6.76 (m, 2H, Ar-*H*), 4.39 (s, 2H, CH_2), 4.28 (s, 2H, CH_2), 3.74 (s, 3H, OCH_3), 3.68 (s, 3H, OCH_3), 3.65 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 170.05, 160.01 (C=N), {153.53, 153.43, 151.50, 146.16, 137.26, 130.52, 125.09, 121.72, 115.70, 113.54, 112.83, 112.45} (Ar-H), 56.38, 55.80 and 55.49 (OCH$_3$), 37.52 (CH$_2$), 25.35 (CH$_2$); EI-MS *m/z* (rel. abund. %), 396 (M$^{+\cdot}$, 95), 381 (26), 365 (100), 260 (67), 162 (23), 147 (18), 133 (10), 121 (51), 105 (4), 91 (20), 77 (18), 65 (11), 51 (5), 28 (6); Analysis calcd. for $C_{20}H_{20}N_4O_3S$: C, 60.59; H, 5.08; N, 14.13; S, 8.09; Found: C, 60.45; H, 5.01; N, 14.01; S, 8.01.

6-(4-Bromophenyl)-3-(2,5-dimethoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6k**)

Yield 52%; mp 190-192 °C; R_f = 0.23 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3069 (sp^2 C-H), 2963, 2917, 2833 (sp^3 C-H), 1589 (C=N), 1497, 1465 (C=C), 1269 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.89 (dd, 2H, *J* 6.6, 2.1 Hz, Ar-*H*), 7.83 (dd, 2H, *J* 6.6, 2.1 Hz, Ar-*H*), 6.93 (d, 1H, *J* 8.4 Hz, Ar-*H*), 6.86-6.80 (m, 2H, Ar-*H*), 4.35 (s, 2H, CH_2), 3.71 (s, 3H, OCH_3), 3.67 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.58 (C=N), {153.44, 151.57, 146.73, 133.18, 129.35, 128.73, 126.56, 124.95, 116.93, 112.94, 112.46} (Ar-H), 56.44 and 55.99 (OCH$_3$), 25.41 (CH$_2$); EI-MS *m/z* (rel. abund. %), 430 (M$^{+\cdot}$,82), 432 (M + 2, 87), 415 (30), 401 (100), 296 (83), 234 (24), 218 (28), 201 (32), 181 (21), 162 (69), 148 (32), 133 (21), 120 (31), 102 (42), 77 (22), 65 (24), 51 (14), 39 (6); Analysis calcd. for $C_{18}H_{15}BrN_4O_2S$: C, 50.13; H, 3.51; N, 12.99; S, 7.43; Found: C, 50.02; H, 3.47; N, 12.91; S, 7.38.

3-(2,5-Dimethoxybenzyl)-6-(3,4-dimethoxyphenyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6l**)

Yield 51%; mp 185-186 °C; R_f = 0.19 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3058 (sp^2 C-H),

2959, 2917, 2839 (sp^3 C-H), 1589 (C=N), 1503, 1462 (C=C), 1270 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.49(dd, 1H, *J* 8.4, 2.1 Hz, Ar-*H*), 7.38 (d, 1H, *J* 2.1 Hz, Ar-*H*), 7.15 (d, 1H, *J* 8.4 Hz, Ar-*H*), 6.94 (d, 1H, *J* 8.4 Hz, Ar-*H*), 6.89 (d, 1H, *J* 3 Hz, Ar-*H*), 6.82 (dd, 1H, *J* 7.8, 3 Hz, Ar-*H*), 4.35 (s, 2H, CH_2), 3.87 (s, 3H, OCH_3), 3.86 (s, 3H, OCH_3), 3.72 (s, 3H, OCH_3), 3.67 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 160.5 (C=N), {153.42, 153.06, 151.64, 149.68, 124.95, 121.77, 112.91, 112.45} (Ar-H), 57.65, 56.24, 56.11 and 55.89 (OCH_3); EI-MS *m/z* (rel. abund. %), 412 ($M^{+\cdot}$, 100), 397 (19), 381 (93), 323 (18), 276 (78), 218 (21), 177 (32), 163 (34), 148 (26), 137 (11), 120 (13), 92 (9), 77 (11), 65 (13); Analysis calcd. for $C_{20}H_{20}N_4O_4S$: C, 58.24; H, 4.89; N, 13.58; S, 7.77; Found: C, 58.10; H, 4.85; N, 13.50; S, 7.69.

6-(4-Chlorophenyl)-3-(2,5-dimethoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6m**)

Yield 56%; mp 188-189 °C; R_f = 0.18 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3062 (sp^2 C-H), 2999, 2960, 2917, 2832 (sp^3 C-H), 1604 (C=N), 1558, 1498, 1465 (C=C), 1269 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.95 (d, 2H, *J* 8.1 Hz, Ar-*H*), 7.52 (d, 2H, *J* 8.1 Hz, Ar-*H*), 6.95-6.86 (m, 2H, Ar-*H*), 6.76 (d, 1H, *J* 8.2 Hz, Ar-*H*), 4.35 (s, 2H, CH_2), 3.76 (s, 3H, OCH_3), 3.75 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.42 (C=N), {153.45, 151.58, 137.92, 130.26, 129.25, 128.38, 124.96, 116.93, 112.94, 112.47} (Ar-H), 56.49 and 55.80 (OCH_3), 25.41 (CH_2); EI-MS *m/z* (rel. abund. %), 386 ($M^{+\cdot}$, 93), 388 (M + 2, 37), 371 (32), 355 (100), 250 (85), 234 (11), 218 (20), 178 (16), 162 (43), 148 (22), 137 (23), 119 (17), 102 (12), 91 (15), 77 (14), 65 (16), 51 (8); Analysis calcd. for $C_{18}H_{15}ClN_4O_2S$: C, 55.88; H, 3.91; N, 14.48; S, 8.29; Found: C, 55.78; H, 3.88; N, 14.35; S, 8.19.

6-(2-Chlorophenyl)-3-(2,5-dimethoxybenzyl)-[1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazole (**6n**)

Yield 65%; mp 145-146 °C; R_f = 0.24 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3088 (sp^2 C-H), 2959, 2916, 2835 (sp^3 C-H), 1591 (C=N), 1498, 1424 (C=C), 1277 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.98 (dd, 1H, *J* 7.8, 1.5 Hz, Ar-*H*), 7.75 (dd, 1H, *J* 8.4, 1.2 Hz, Ar-*H*), 7.71-7.57 (m, 2H, Ar-*H*), 6.93 (d, 1H, *J* 8.7 Hz, Ar-*H*), 6.87 (d, 1H, *J* 3 Hz, Ar-*H*), 6.82 (dd, 1H, *J* 9, 3.3 Hz, Ar-*H*), 4.37 (s, 2H, CH_2), 3.70 (s, 3H, OCH_3), 3.67 (s, 3H, OCH_3); ^{13}C NMR (75 MHz, DMSO-d_6) δ 165.52 (C=N), {153.45, 151.60, 134.09, 132.19, 131.97, 131.51, 128.67, 127.93, 124.90, 117.07, 112.95, 112.46} (Ar-H), 56.47 and 55.81 (OCH_3), 25.49 (CH_2); EI-MS *m/z* (rel. abund. %), 386 ($M^{+\cdot}$, 92), 388 (M + 2, 36), 371 (30), 355 (100), 250 (84), 234 (11), 218 (19), 205 (7), 178 (18), 162 (40), 148 (23), 137 (15), 119 (13), 102 (12), 91 (16), 77 (15), 65 (16), 51 (7), 39 (4); Analysis calcd. for $C_{18}H_{15}ClN_4O_2S$: C, 55.88; H, 3.91; N, 14.48; S, 8.29; Found: C, 55.75; H, 3.84; N, 14.40; S, 8.24.

3-(2,5-Dimethoxybenzyl)-6-*o*-tolyl-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole (**6o**)

Yield 72%; mp 159-160 °C; R_f = 0.21 (petroleum ether-ethyl acetate, 5:5); IR ν_{max}/cm^{-1} 3066 (sp^2 C-H), 2956, 2918, 2849 (sp^3 C-H), 1608 (C=N), 1497, 1464 (C=C), 1271 (C-O); ^{1}H NMR (300 MHz, DMSO-d_6) δ 7.67 (d, 1H, *J* 8.1 Hz, Ar-*H*), 7.41-7.36 (m, 2H, Ar-*H*), 7.28 (d, 1H, *J* 8.1 Hz, Ar-H), 6.90-6.71 (m, 3H, Ar-H), 4.37 (s, 2H, CH_2), 3.78 (s, 3H, OCH_3), 3.76 (s, 3H, OCH_3), 2.51 (s, 3H, CH_3); ^{13}C NMR (75 MHz, DMSO-d_6) 164.27 (C=N), {154.40, 151.61, 134.29, 132.11, 131.17, 131.51, 128.67, 127.93, 124.90, 117.07, 112.95, 112.46} (Ar-H), 56.76 and 55.45 (OCH_3), 25.49 (CH_2), 22.15 (CH_3); EI-MS *m/z* (rel. abund. %), 366 ($M^{+\cdot}$, 88), 351 (25), 335 (100), 277 (9), 230 (75), 218 (16), 162 (20), 148 (12), 135 (30), 116 (8), 91 (18), 77 (7), 65 (11); Analysis calcd. for $C_{19}H_{18}NOS$: C, 62.28; H, 4.95; N, 15.29; S, 8.75; Found: C, 62.21; H, 4.87; N, 15.21; S, 8.65.

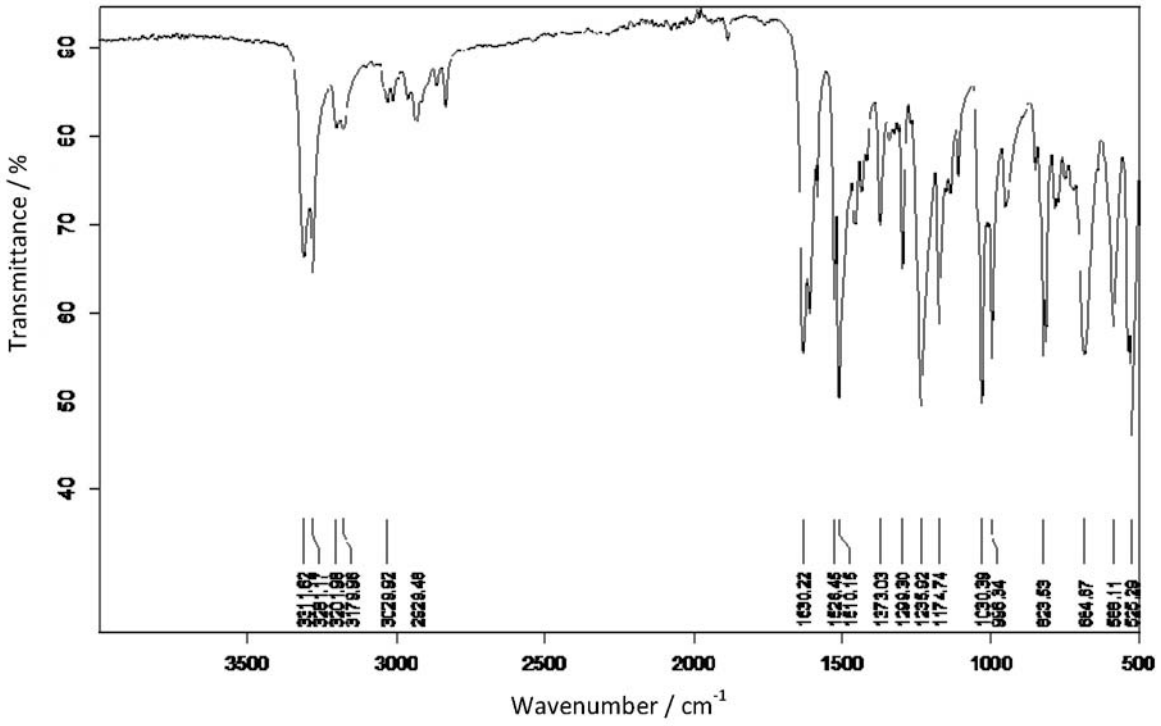

Figure S1. IR (neat) spectrum of **3a**.

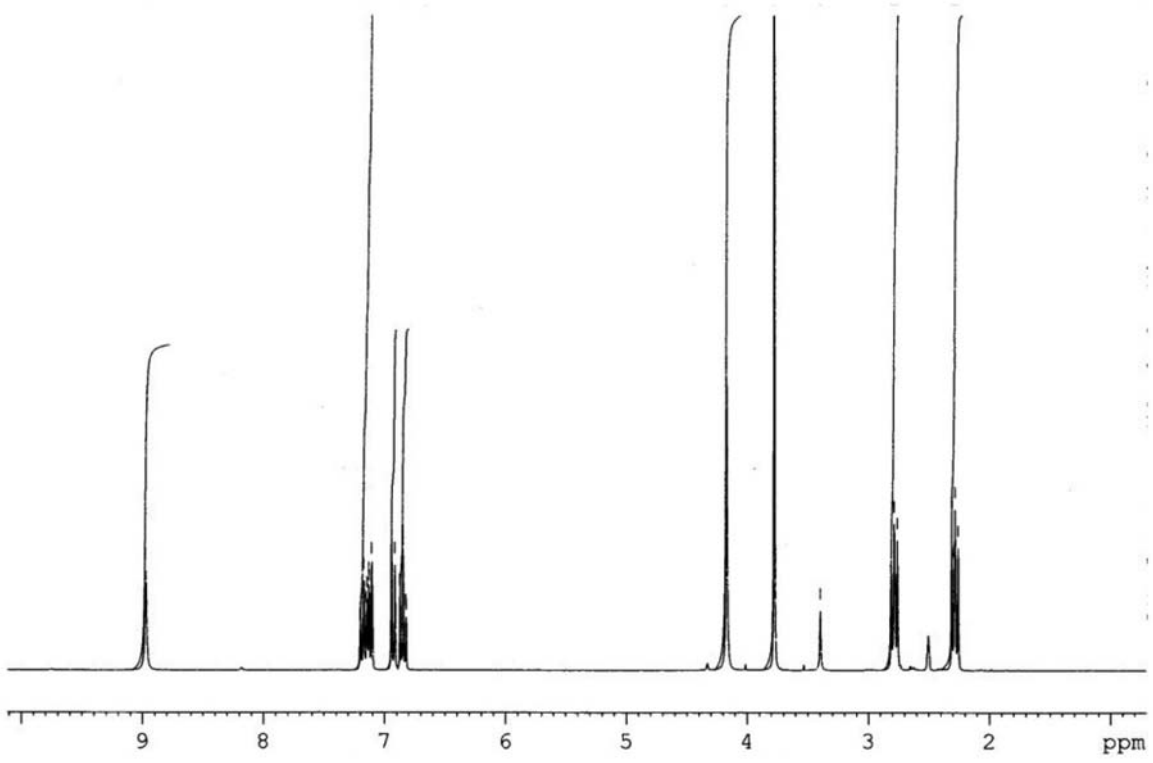

Figure S2. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **3a**.

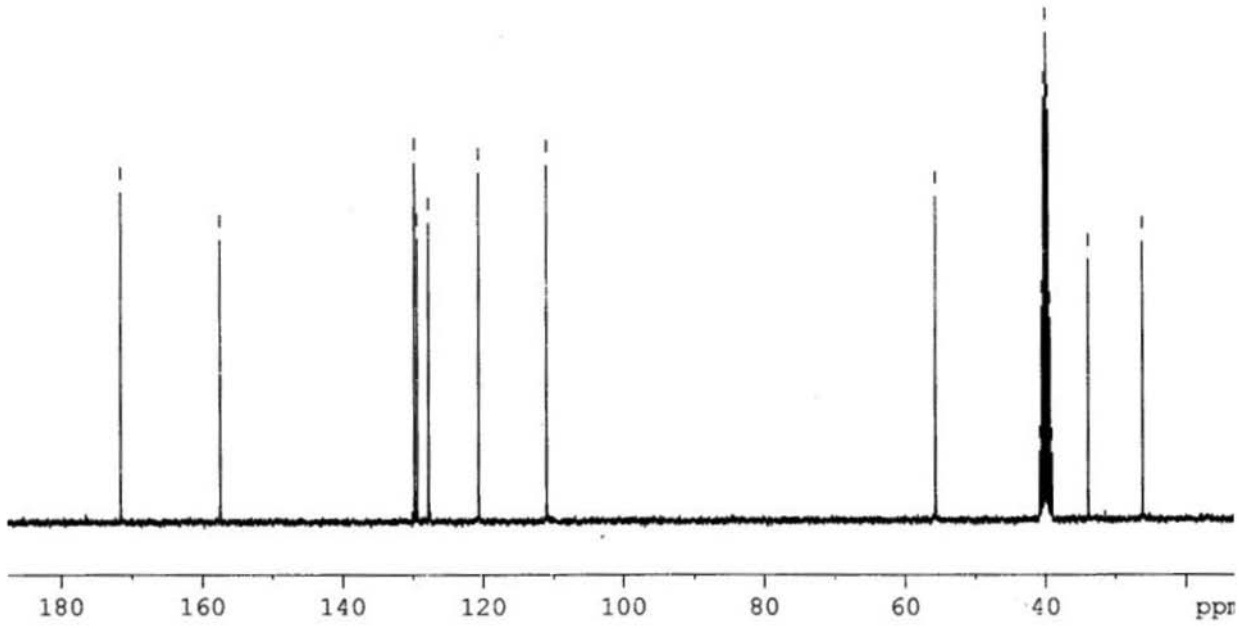

Figure S3. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **3a**.

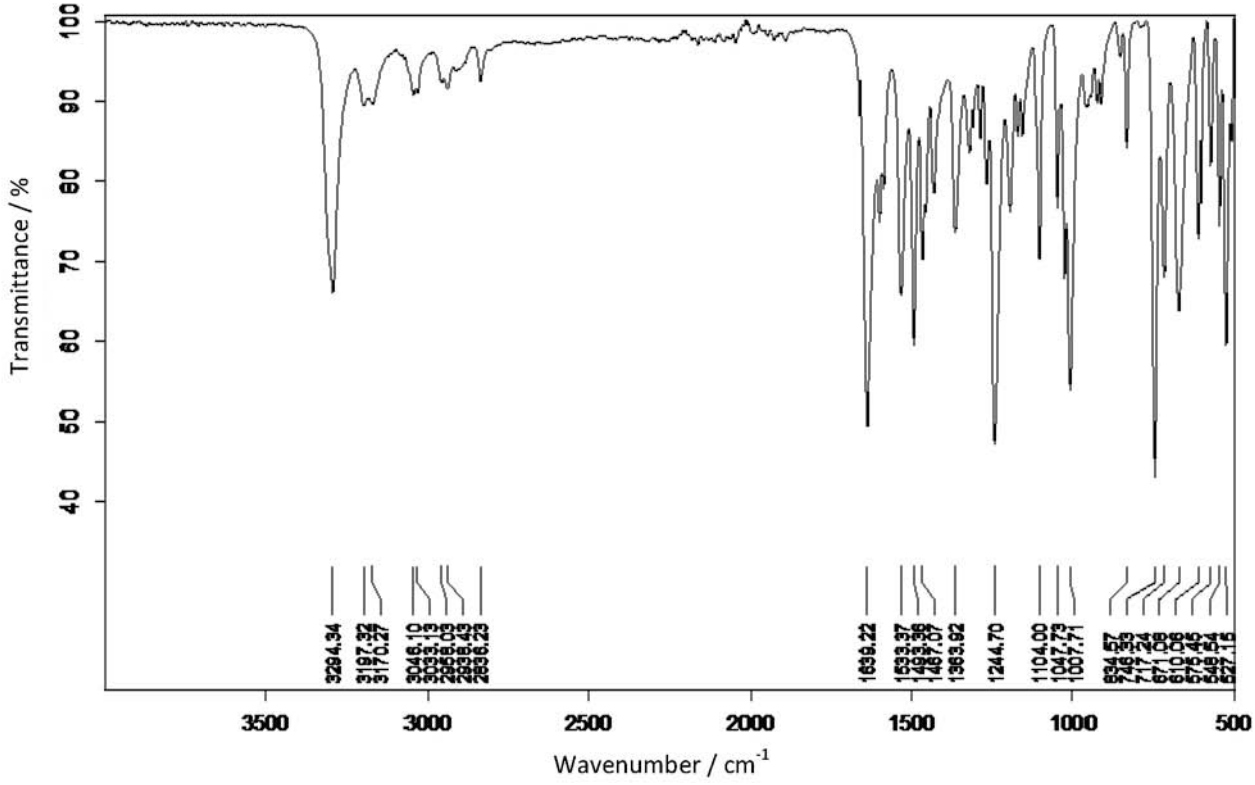

Figure S4. IR (neat) spectrum of **3b**.

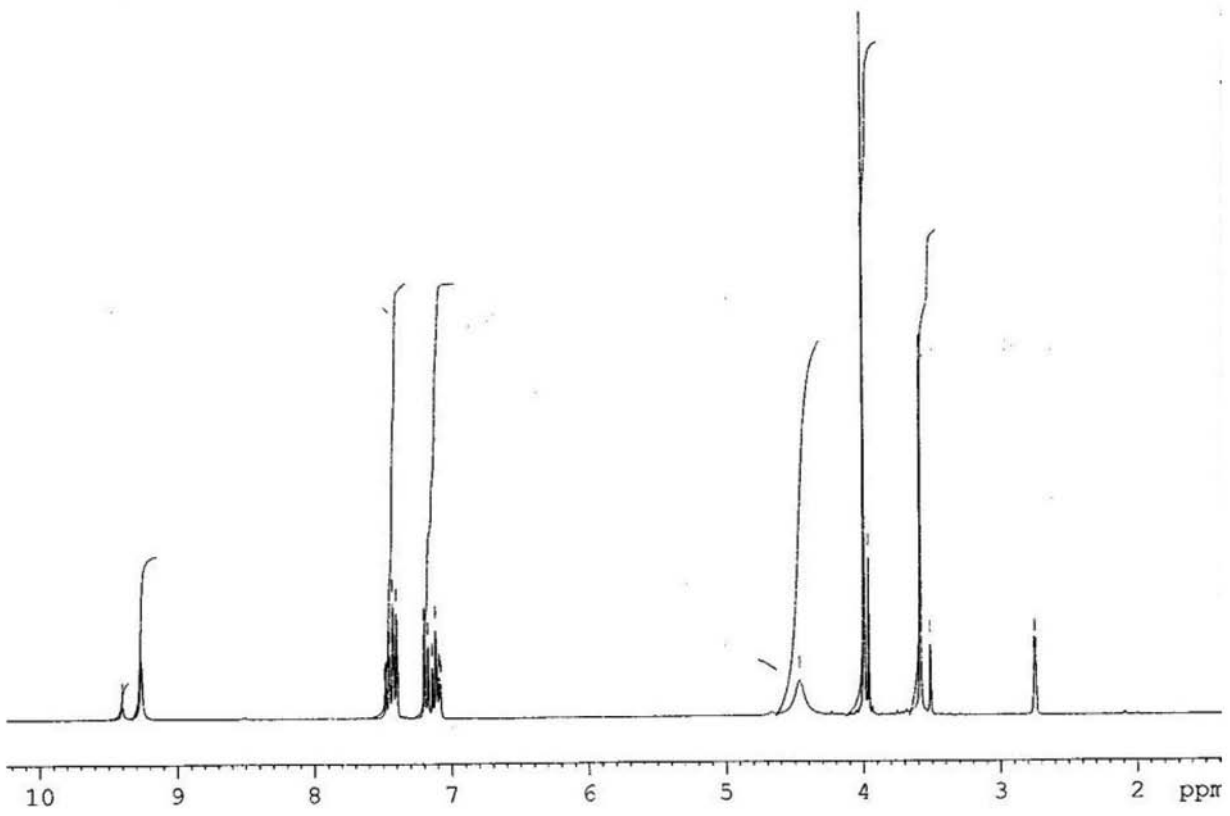

Figure S5. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **3b**.

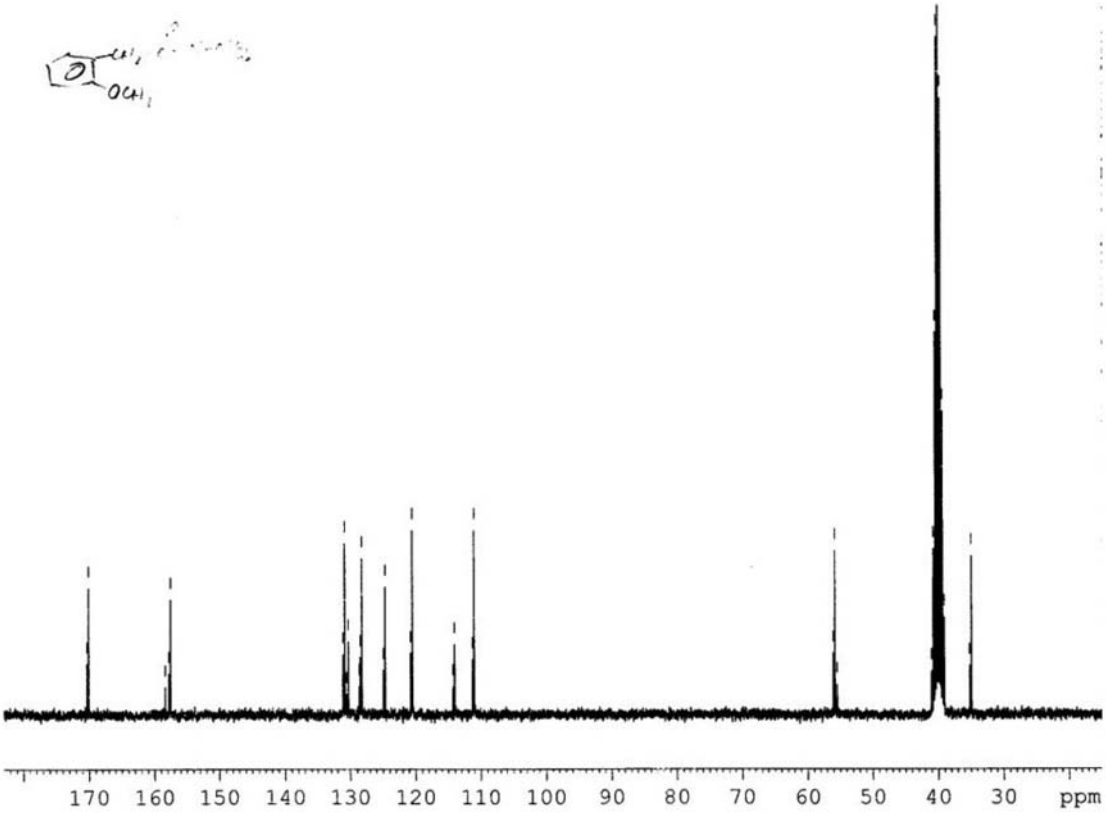

Figure S6. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **3b**.

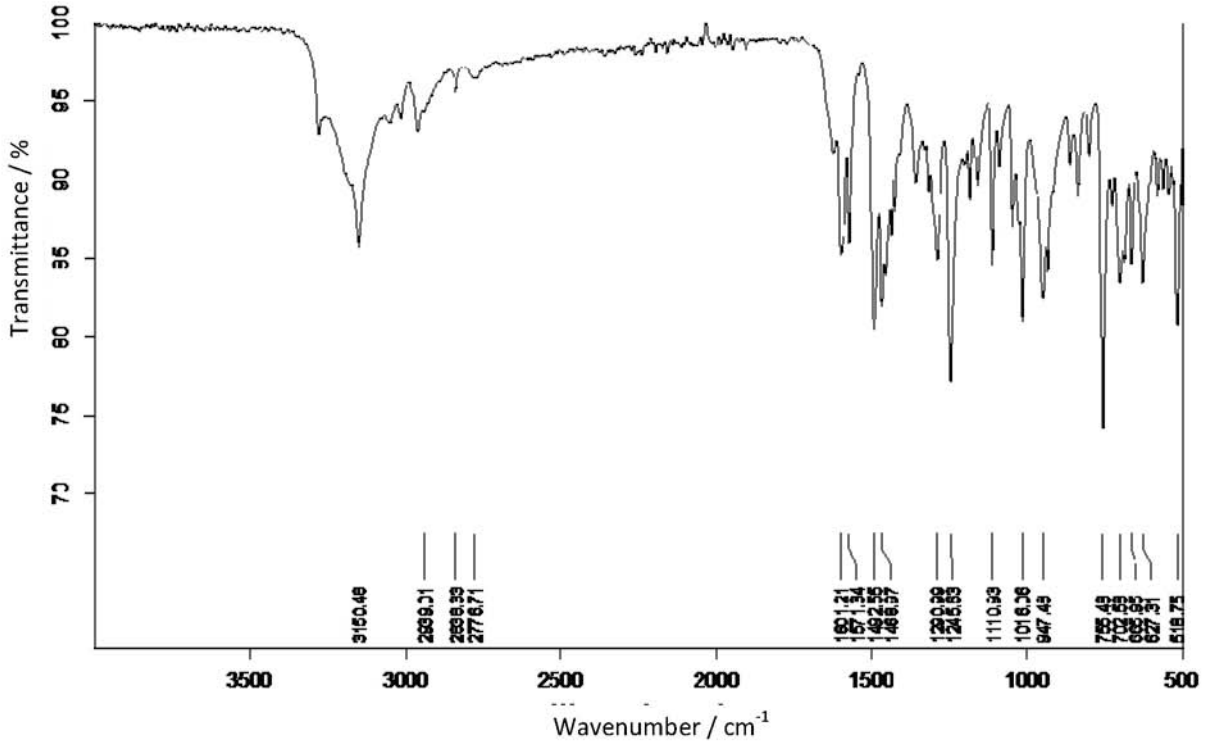

Figure S7. IR (neat) spectrum of **3c**.

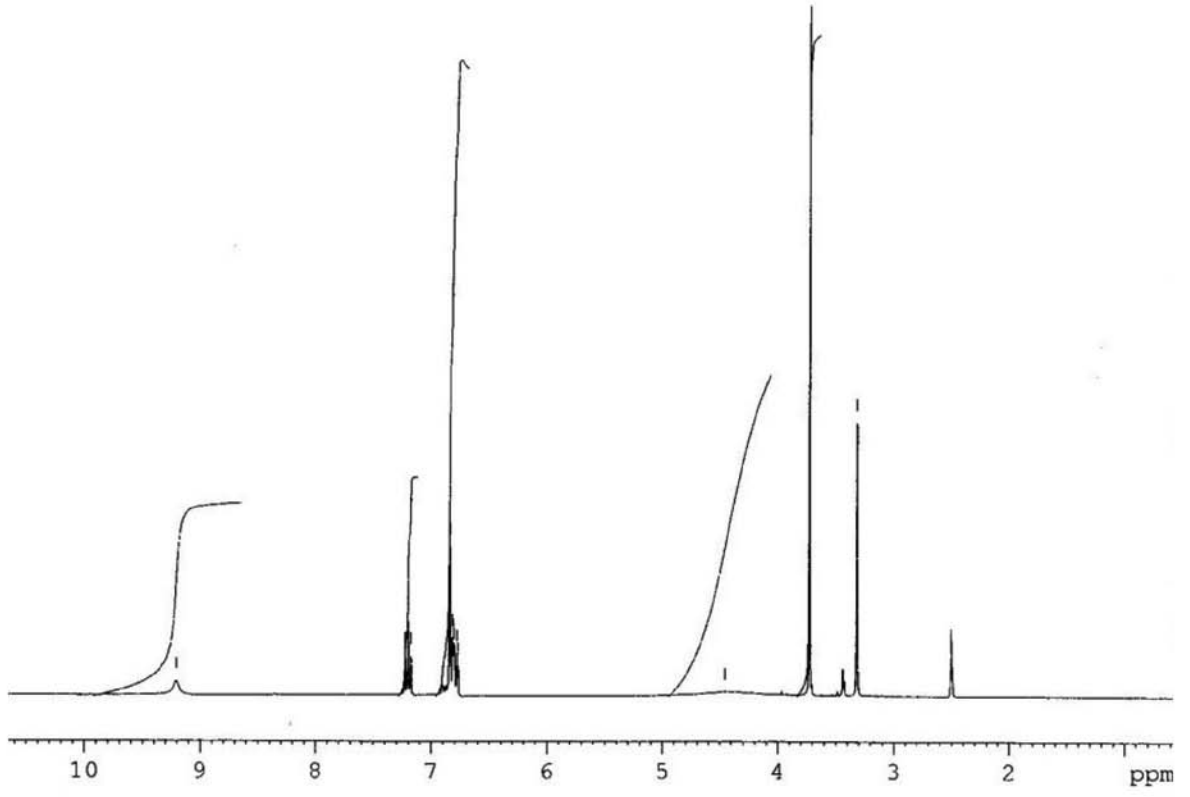

Figure S8. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **3c**.

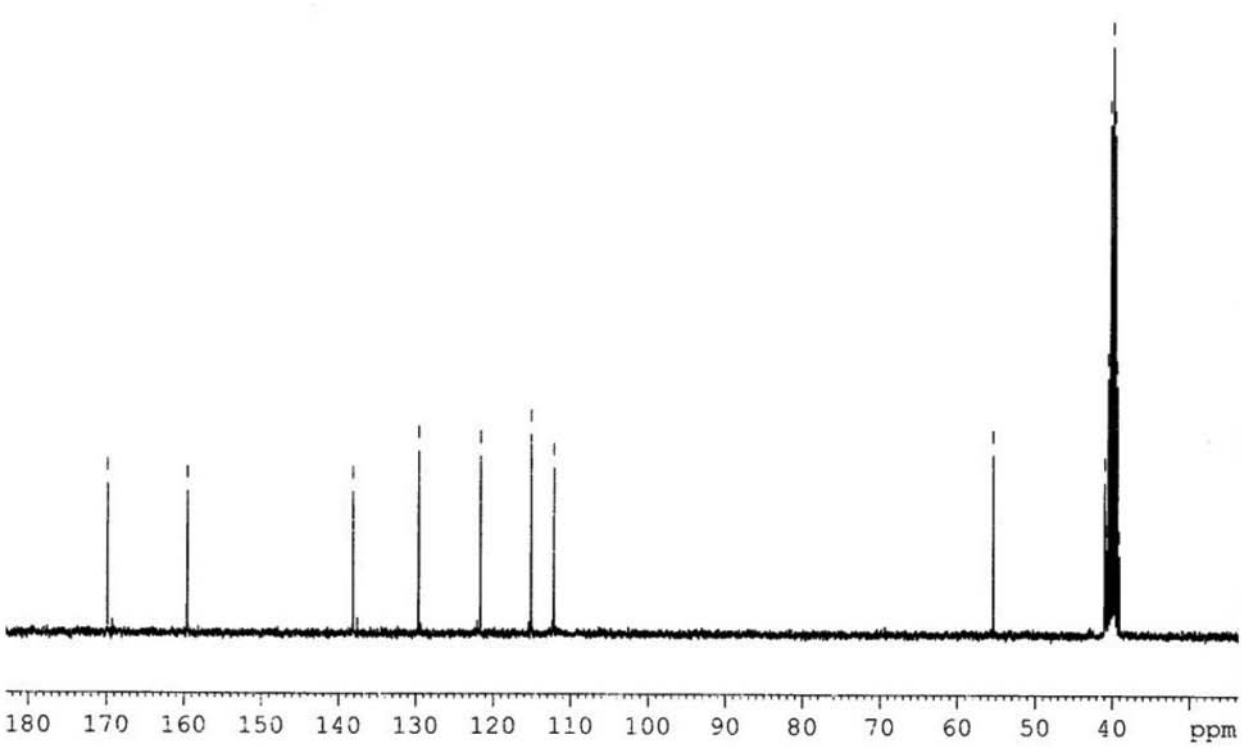

Figure S9. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **3c**.

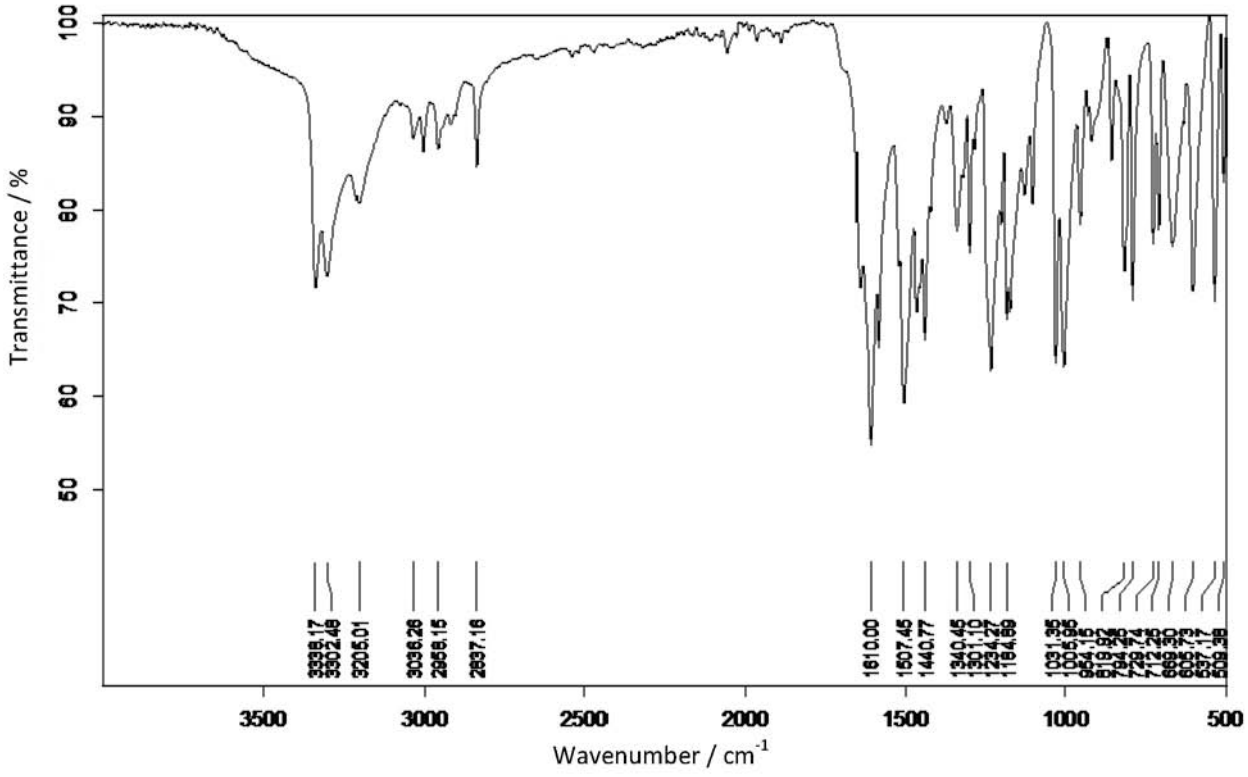

Figure S10. IR (neat) spectrum of **3d**.

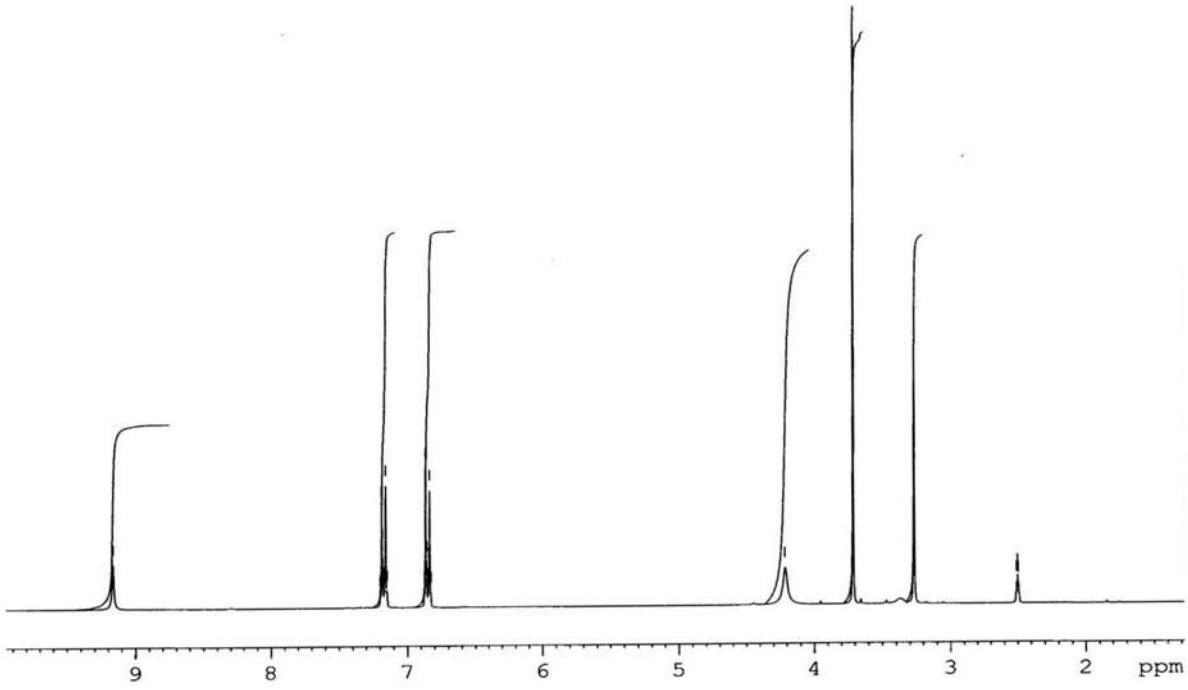

Figure S11. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **3d**.

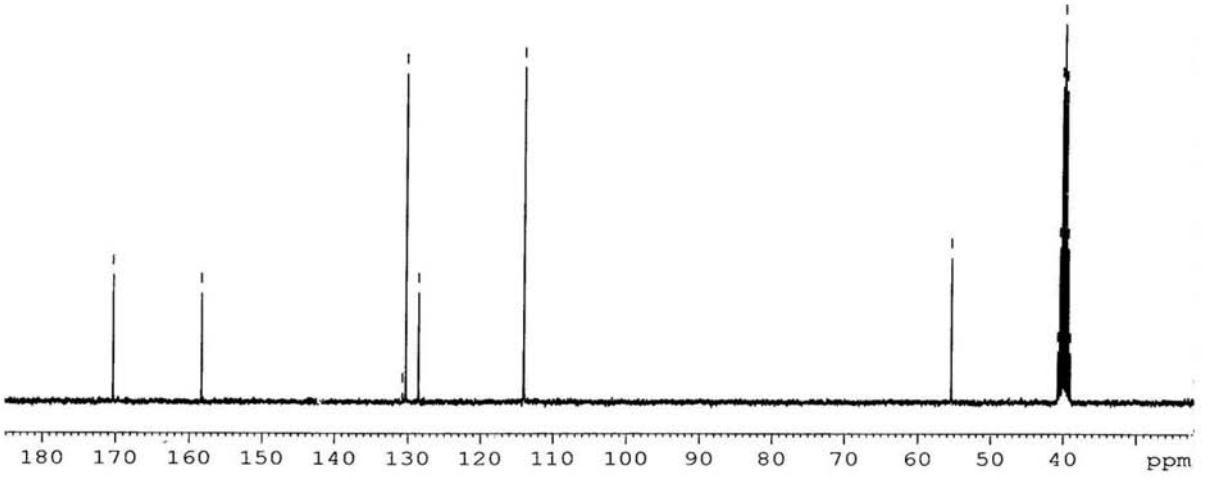

Figure S12. ^{13}C NMR (75 MHz, DMSO-d_6) specrum of **3d**.

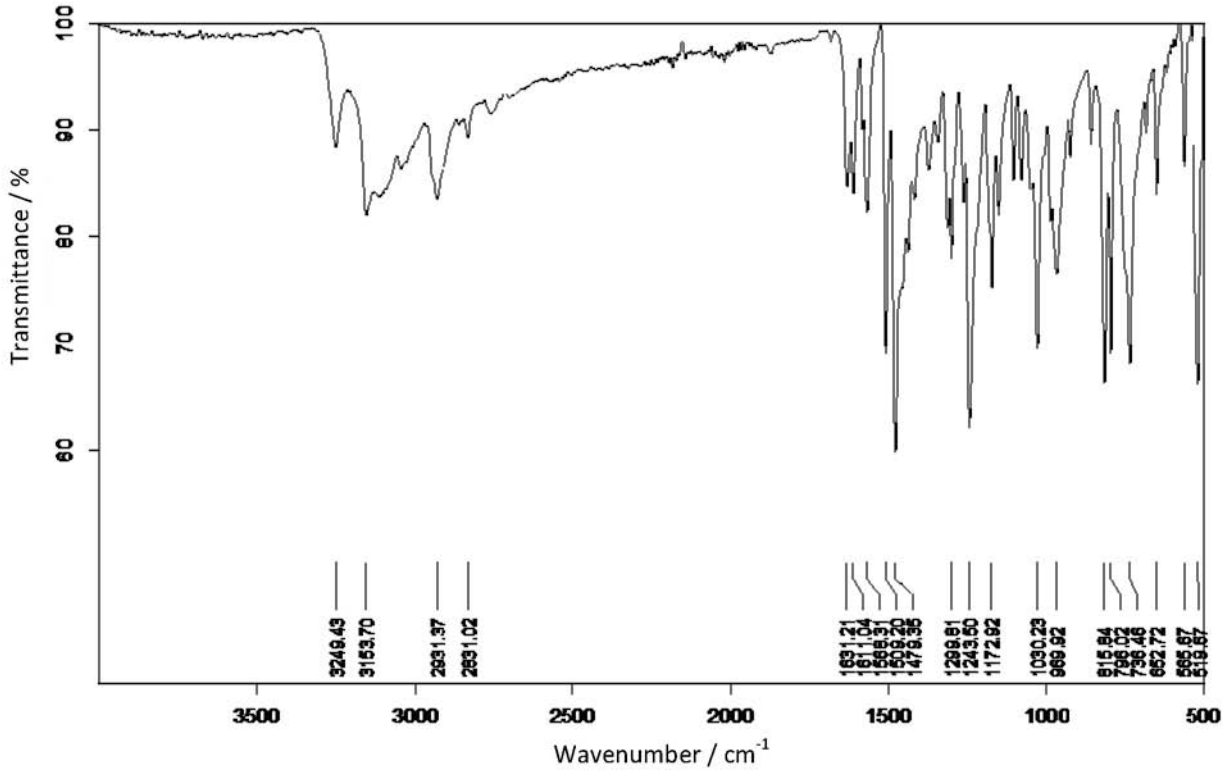

Figure S13. IR (neat) spectrum of **5a**.

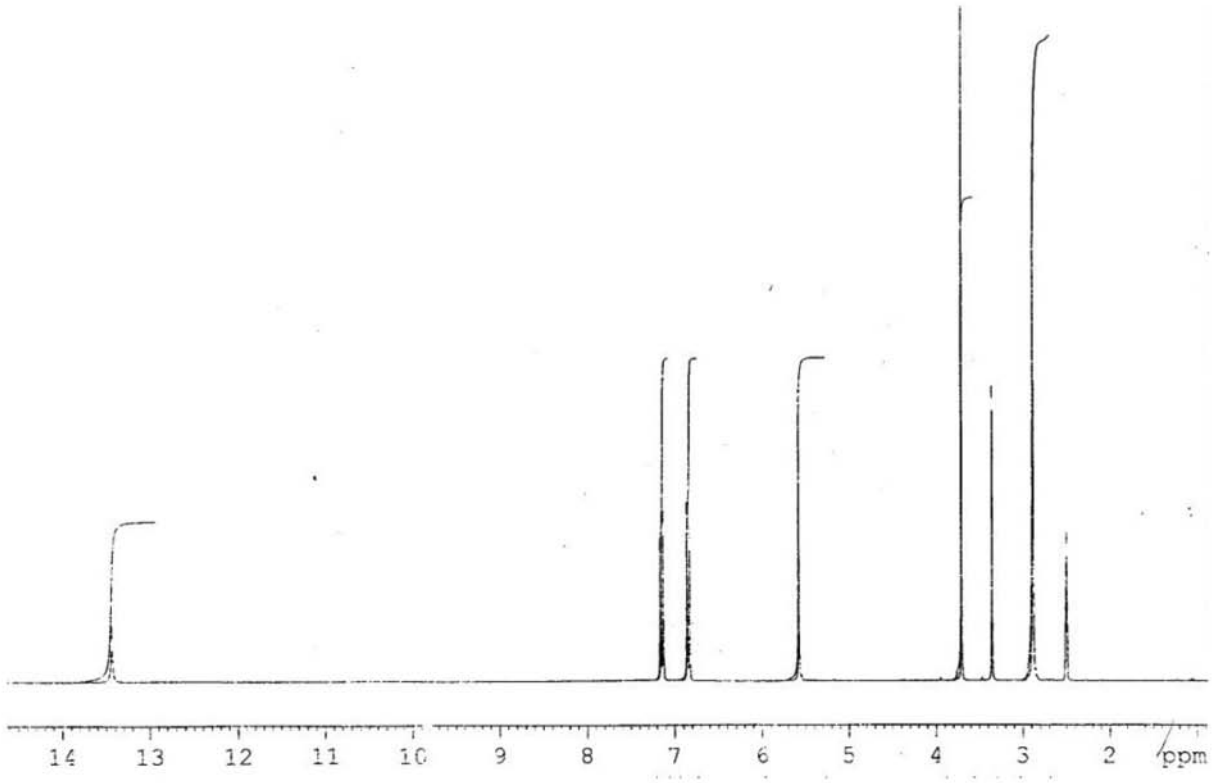

Figure S14. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **5a**.

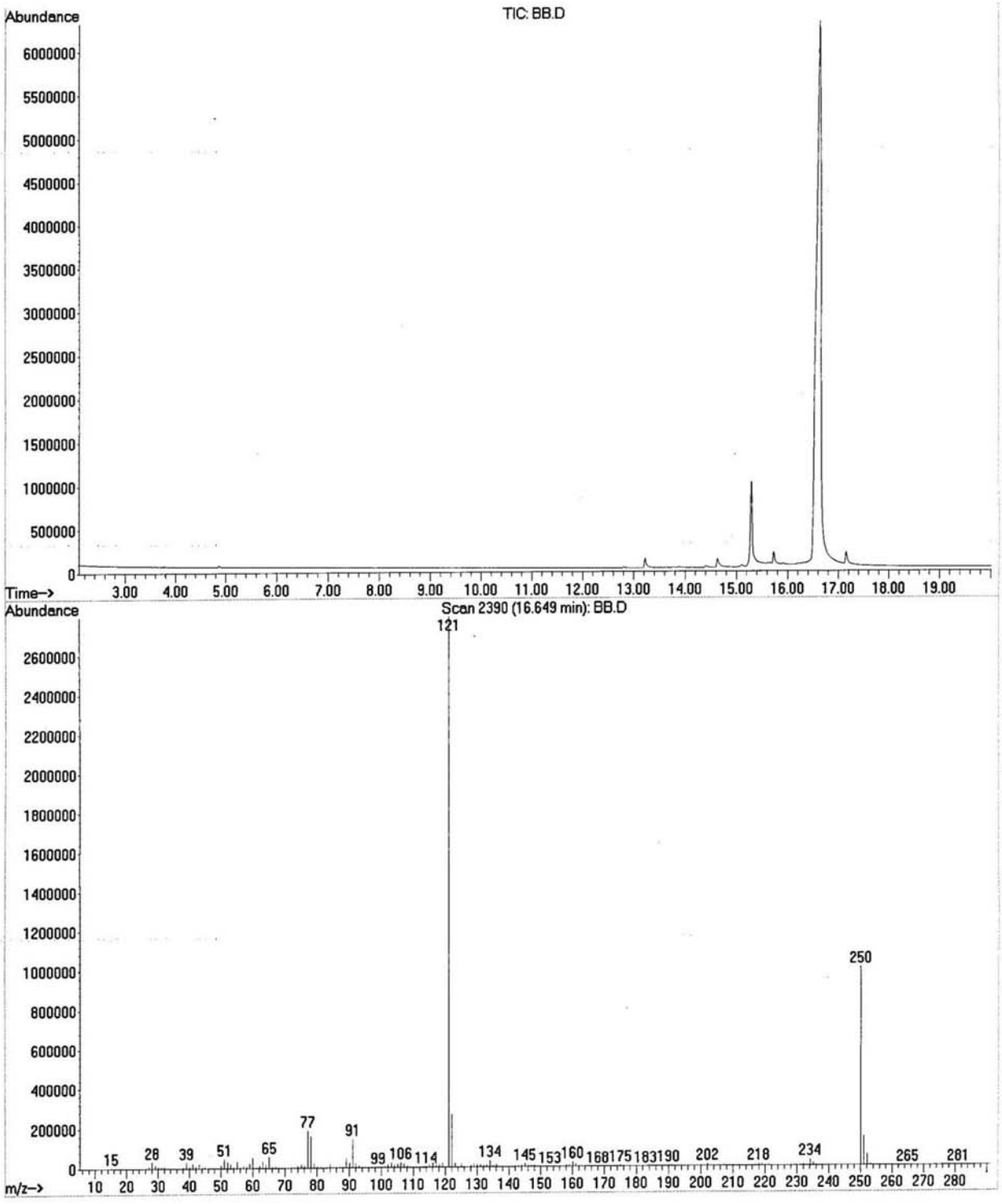

Figure S15. GC MS spectrum of **5a**.

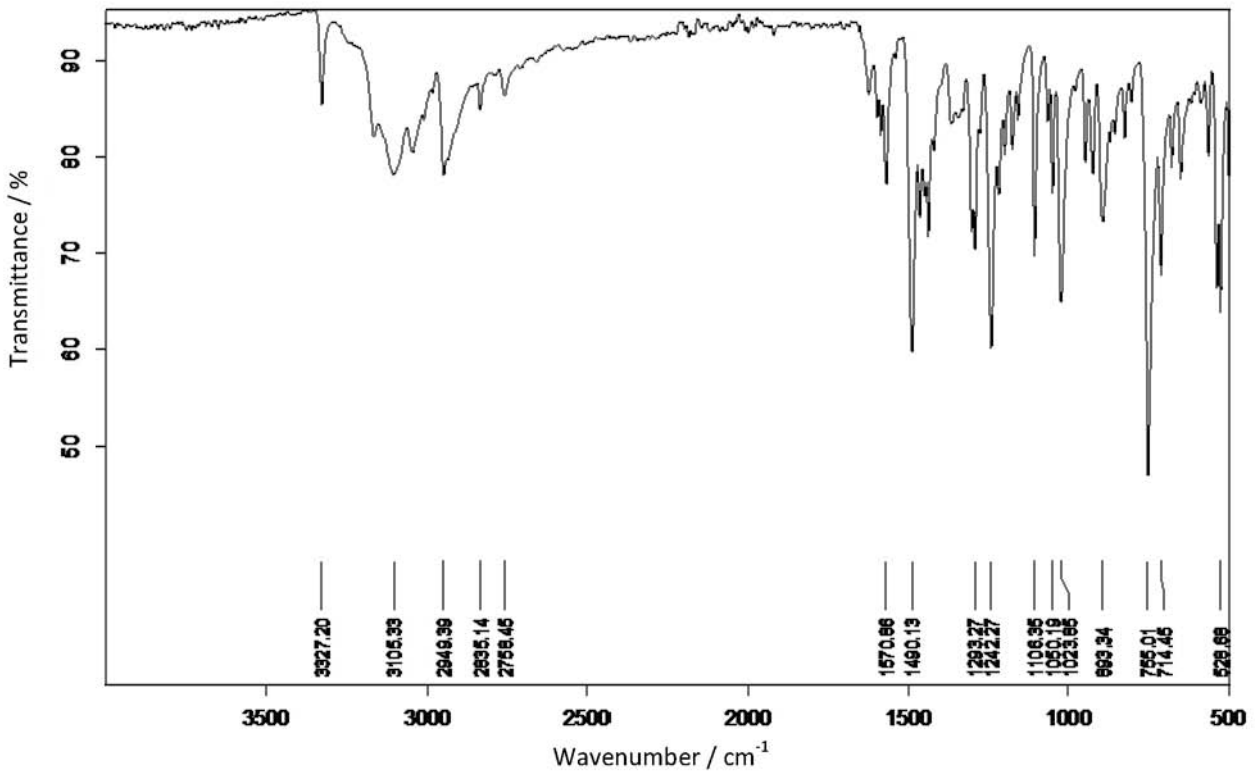

Figure S16. IR (neat) spectrum of **5b**.

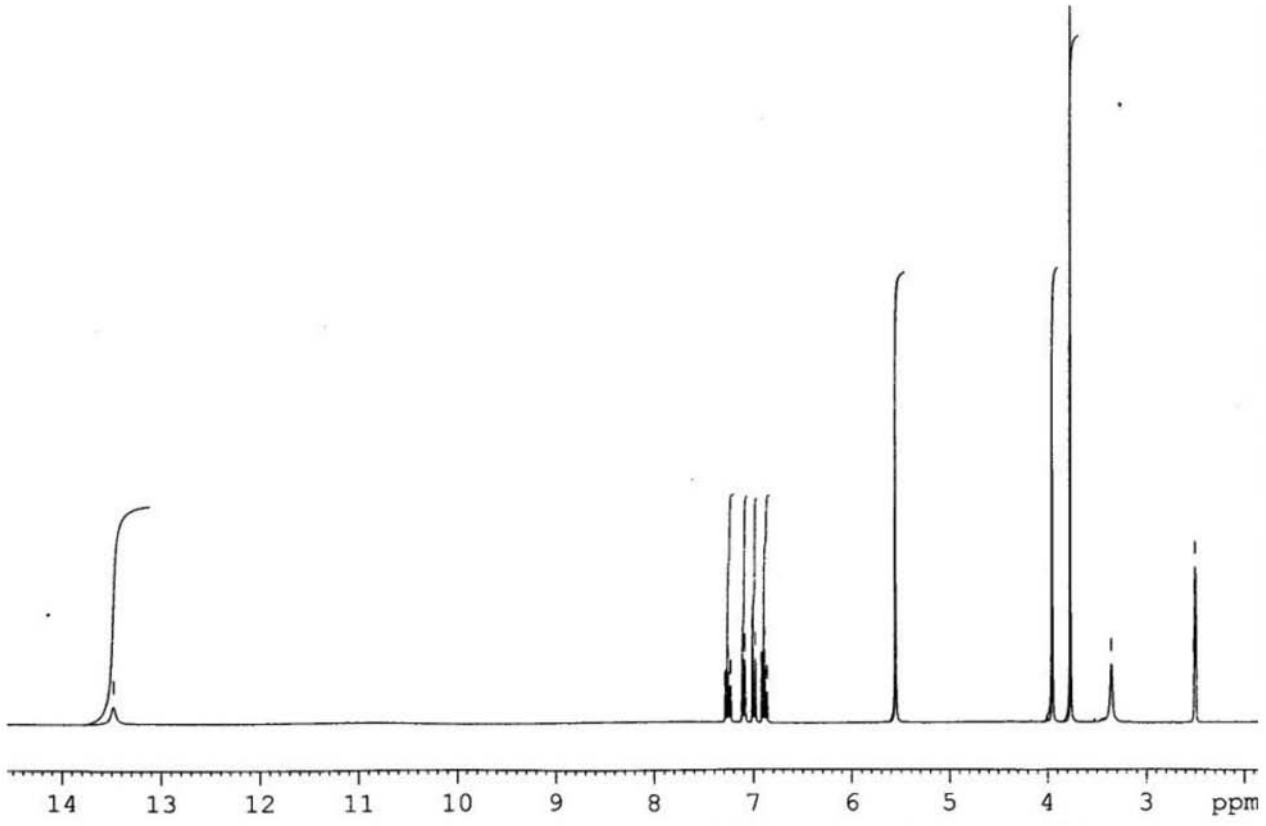

Figure S17. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **5b**.

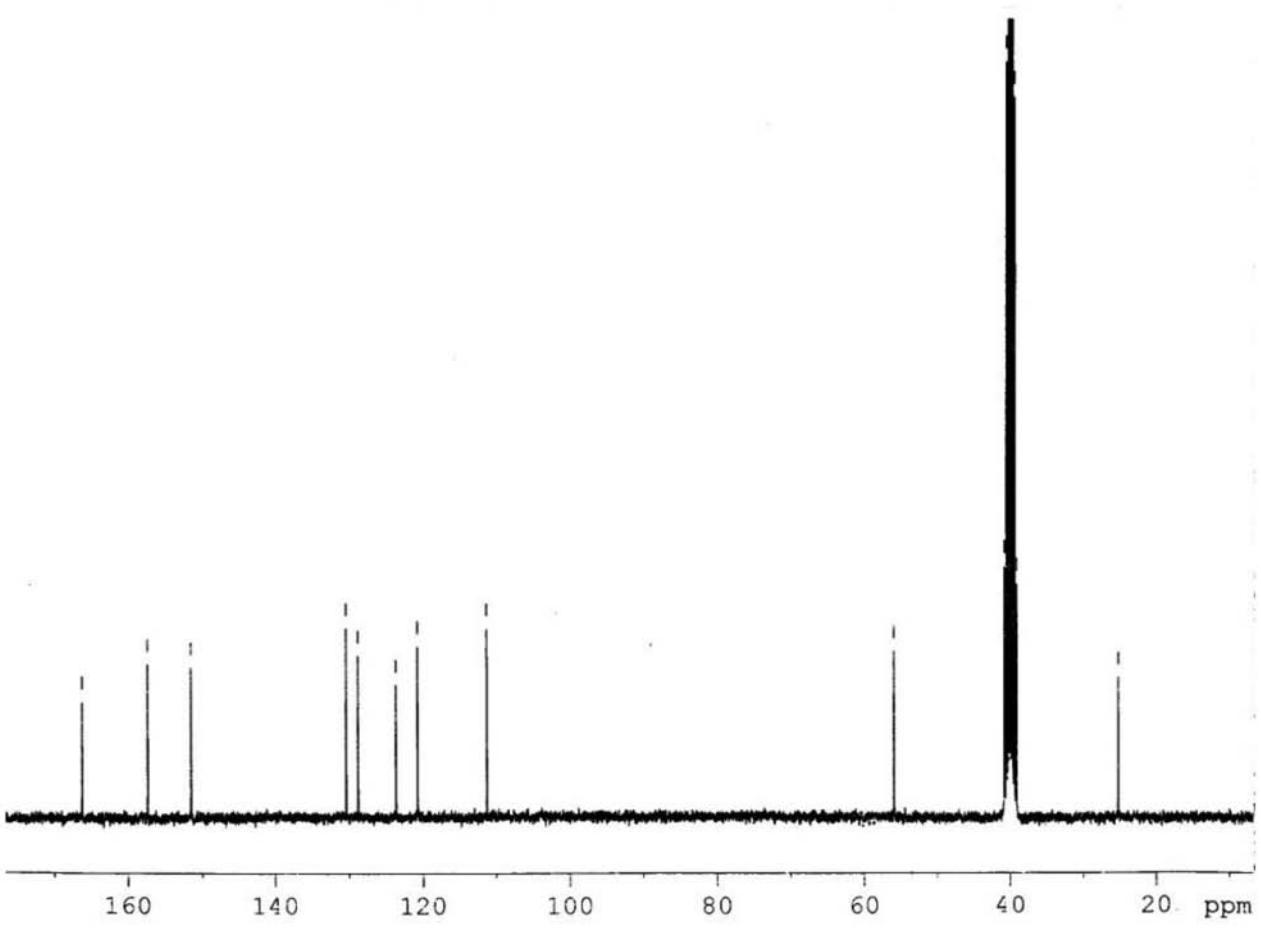

Figure S18. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **5b**.

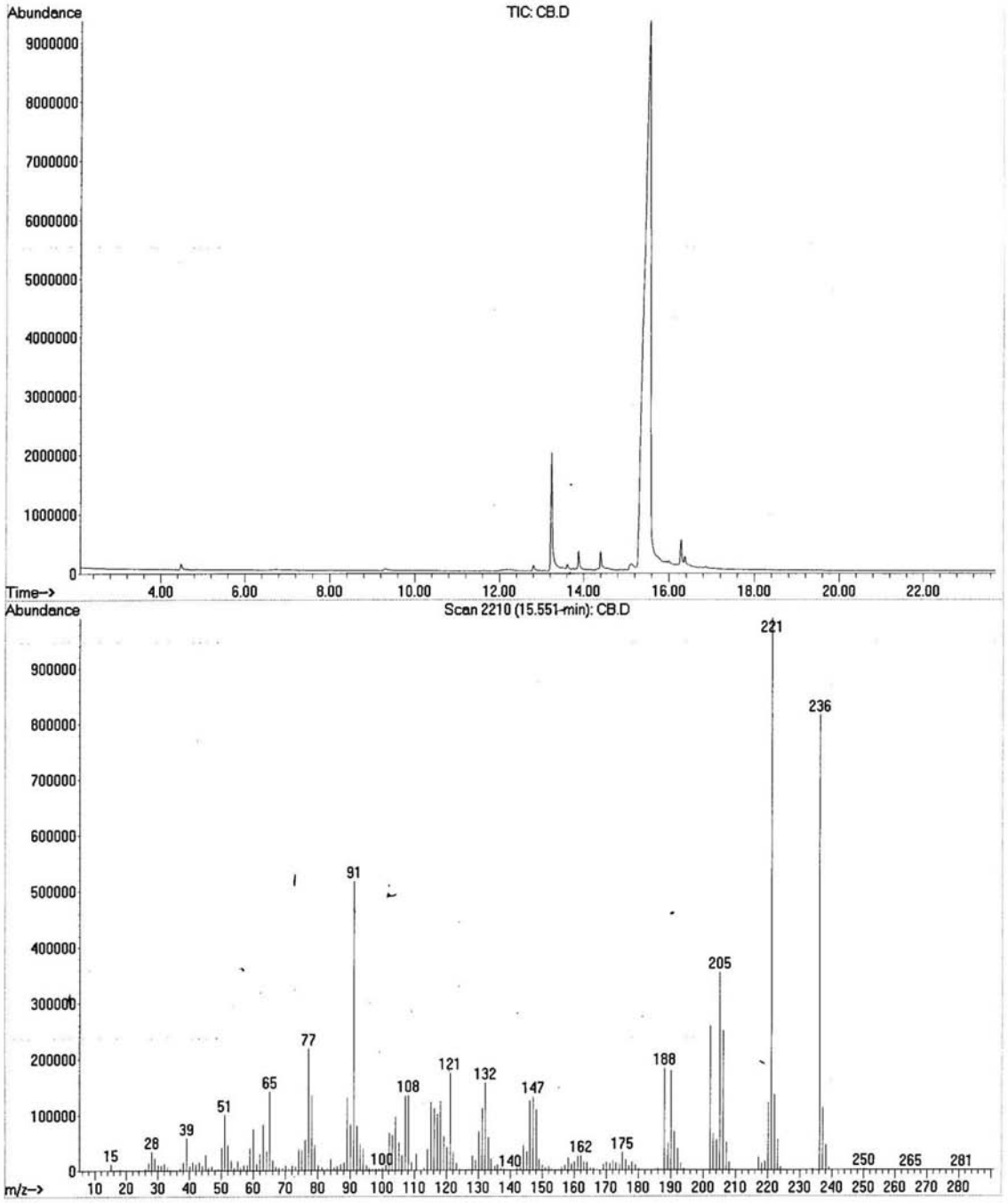

Figure S19. GC MS spectrum of **5b**.

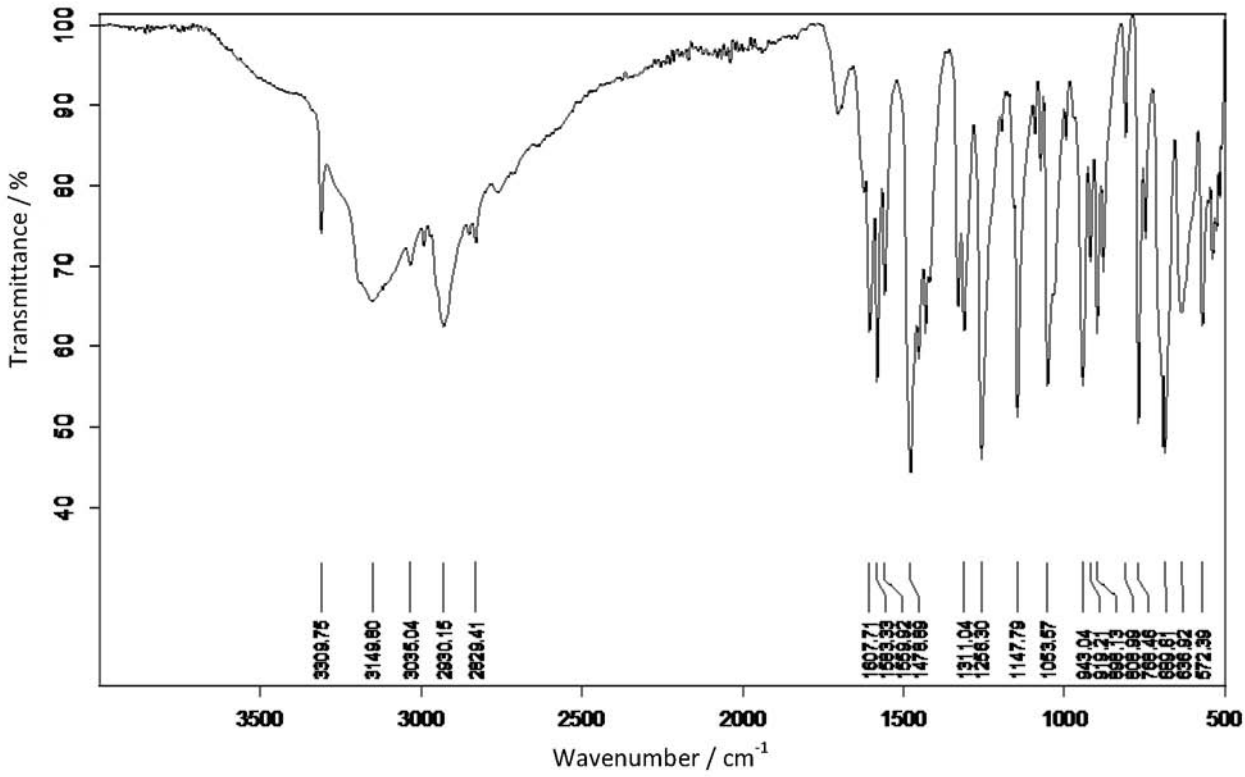

Figure S20. IR (neat) spectrum of **5c**.

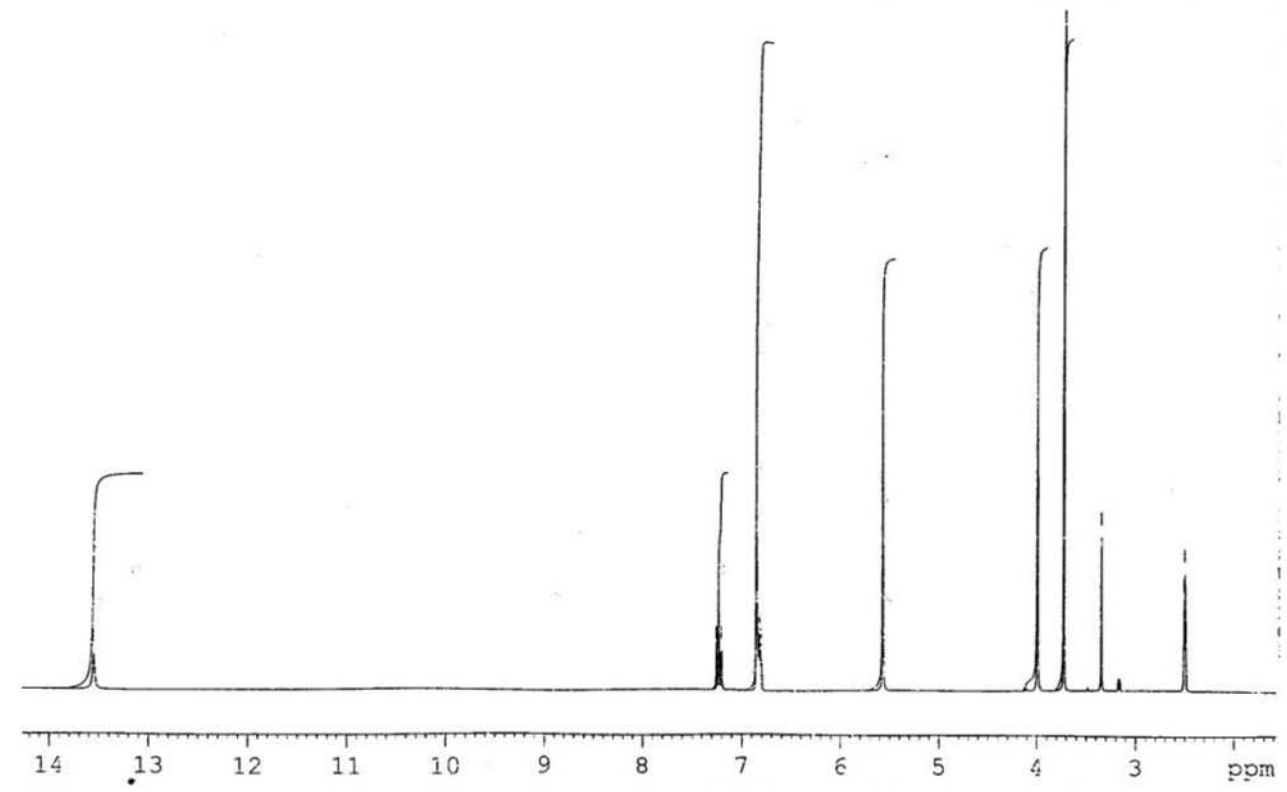

Figure S21. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **5c**.

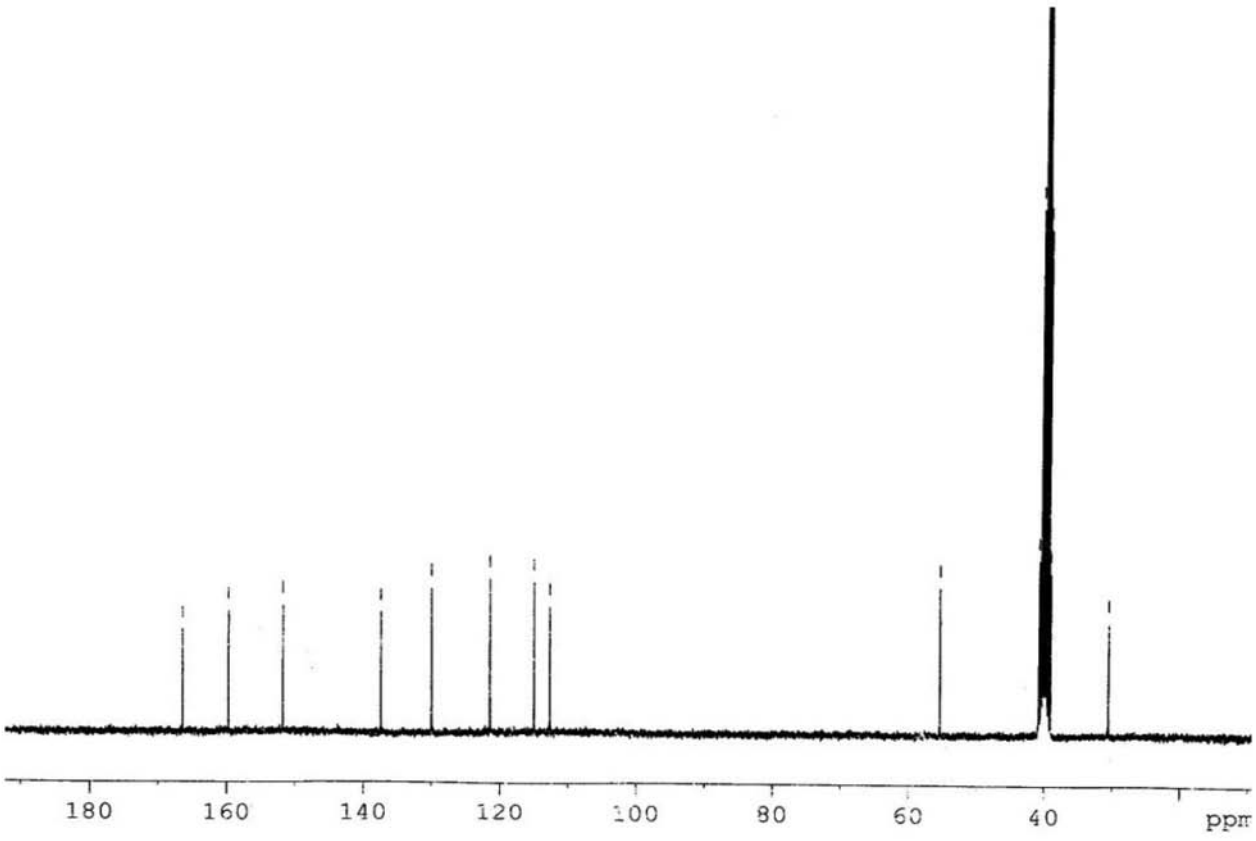

Figure S22. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **5c**.

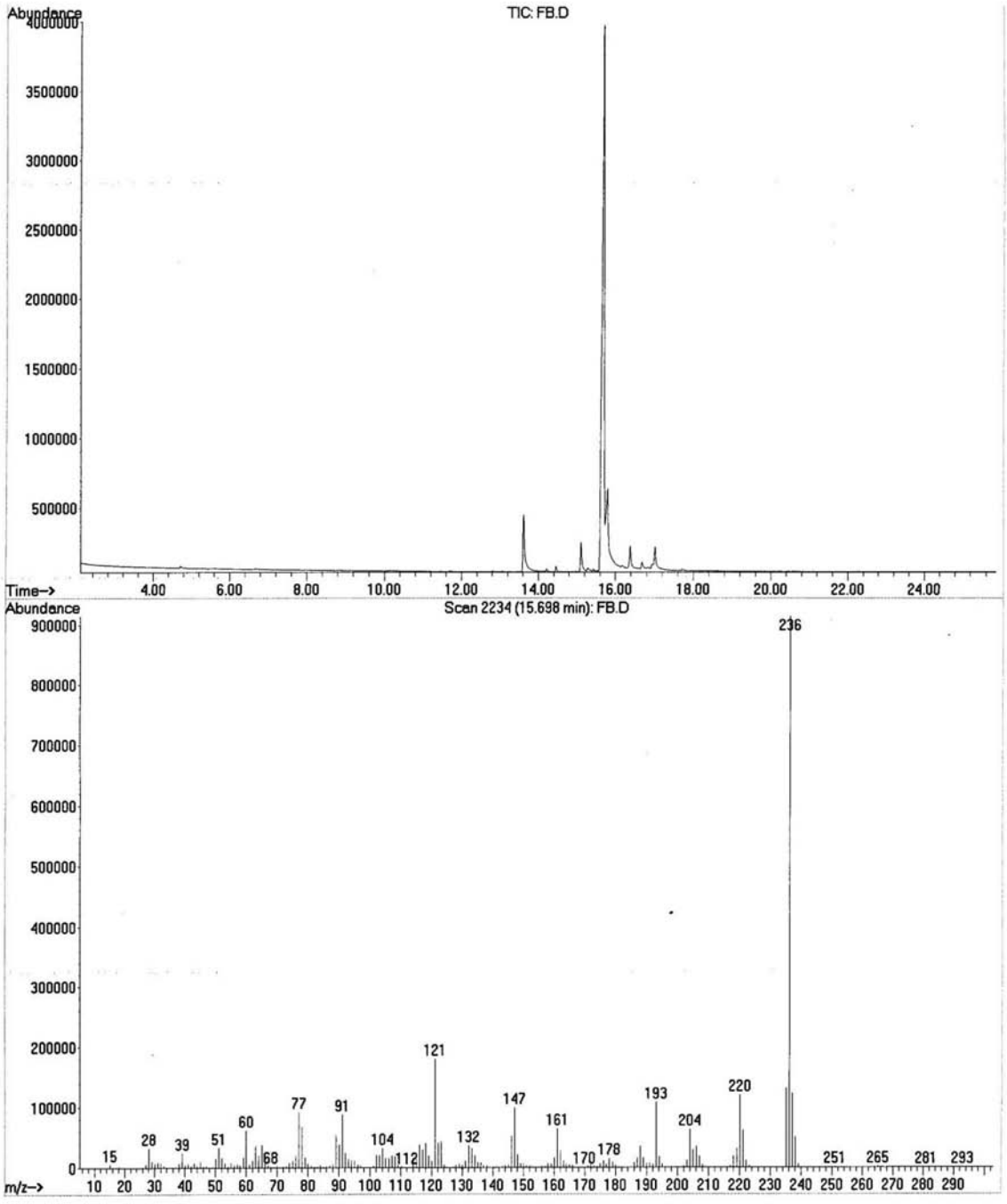

Figure S23. GC MS spectrum of **5c**.

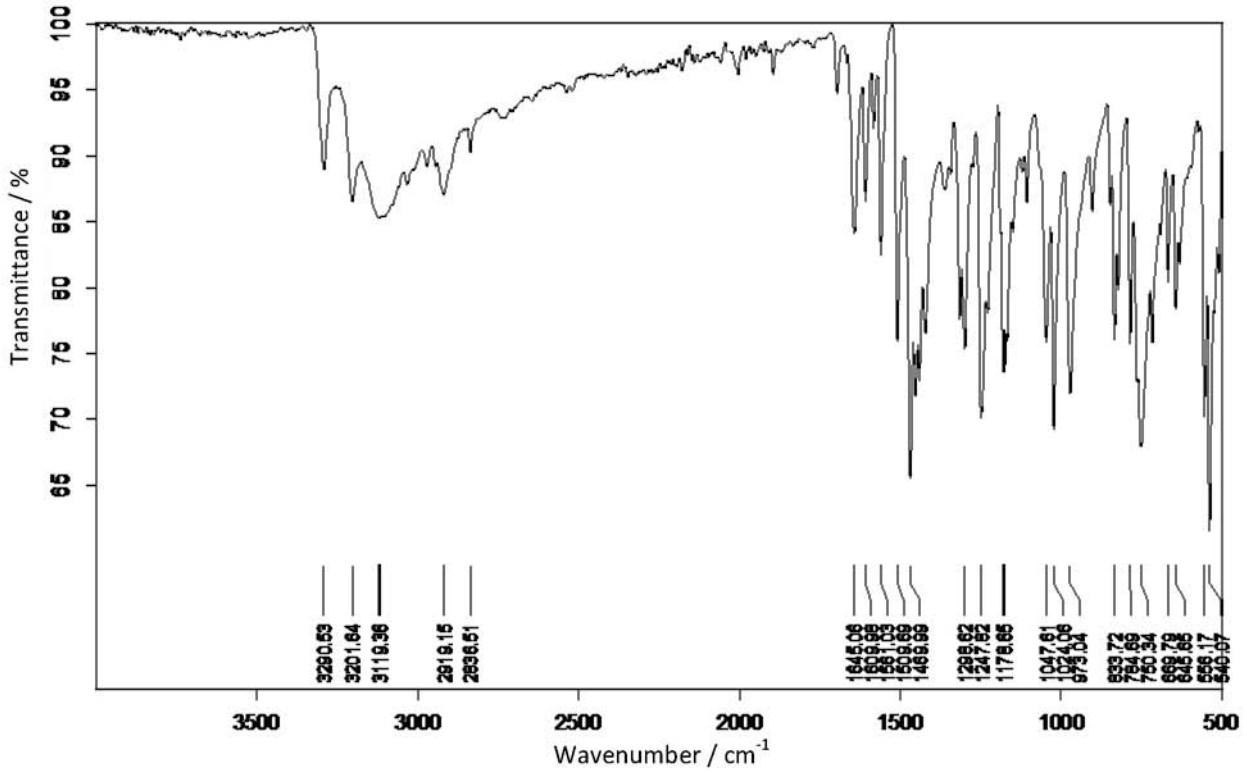

Figure S24. IR (neat) spectrum of **5d**.

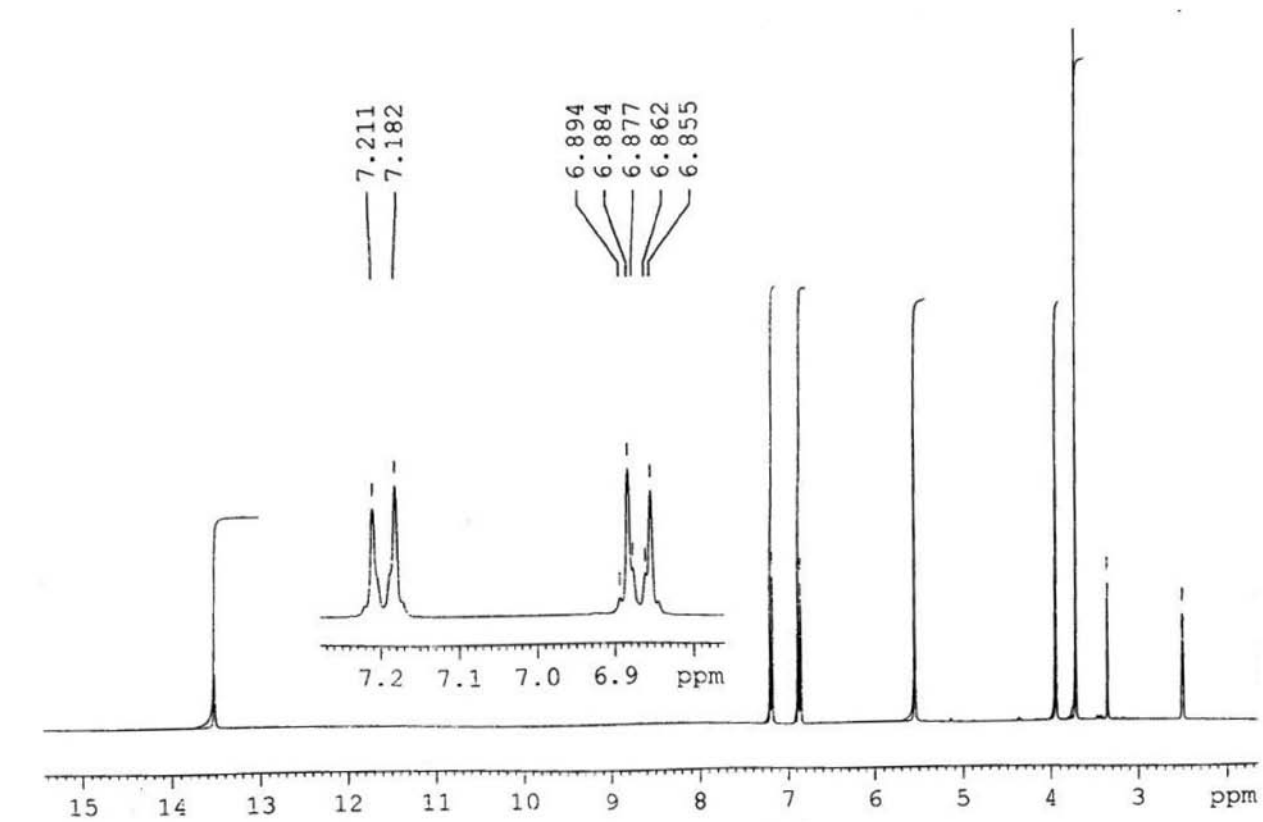

Figure S25. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **5d**.

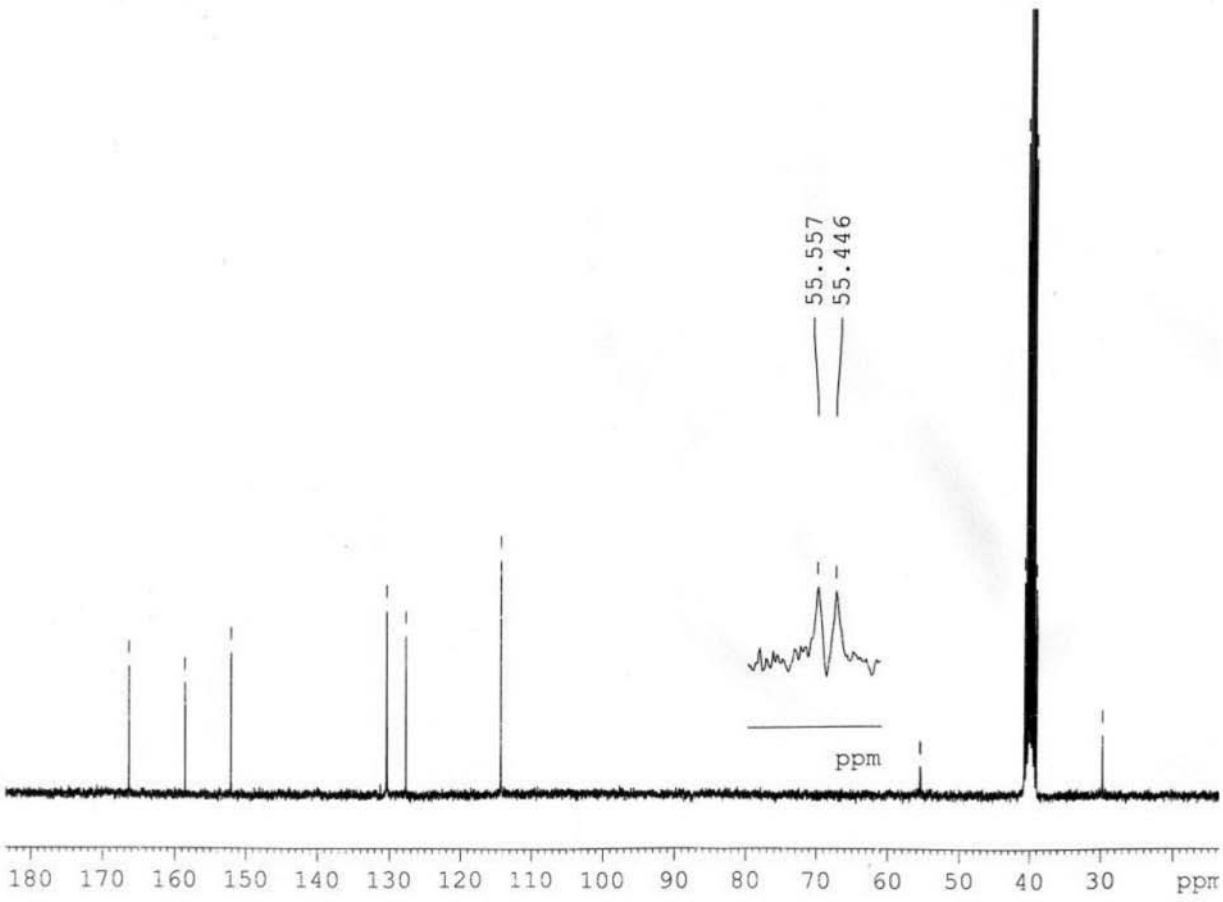

Figure S26. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **5d**.

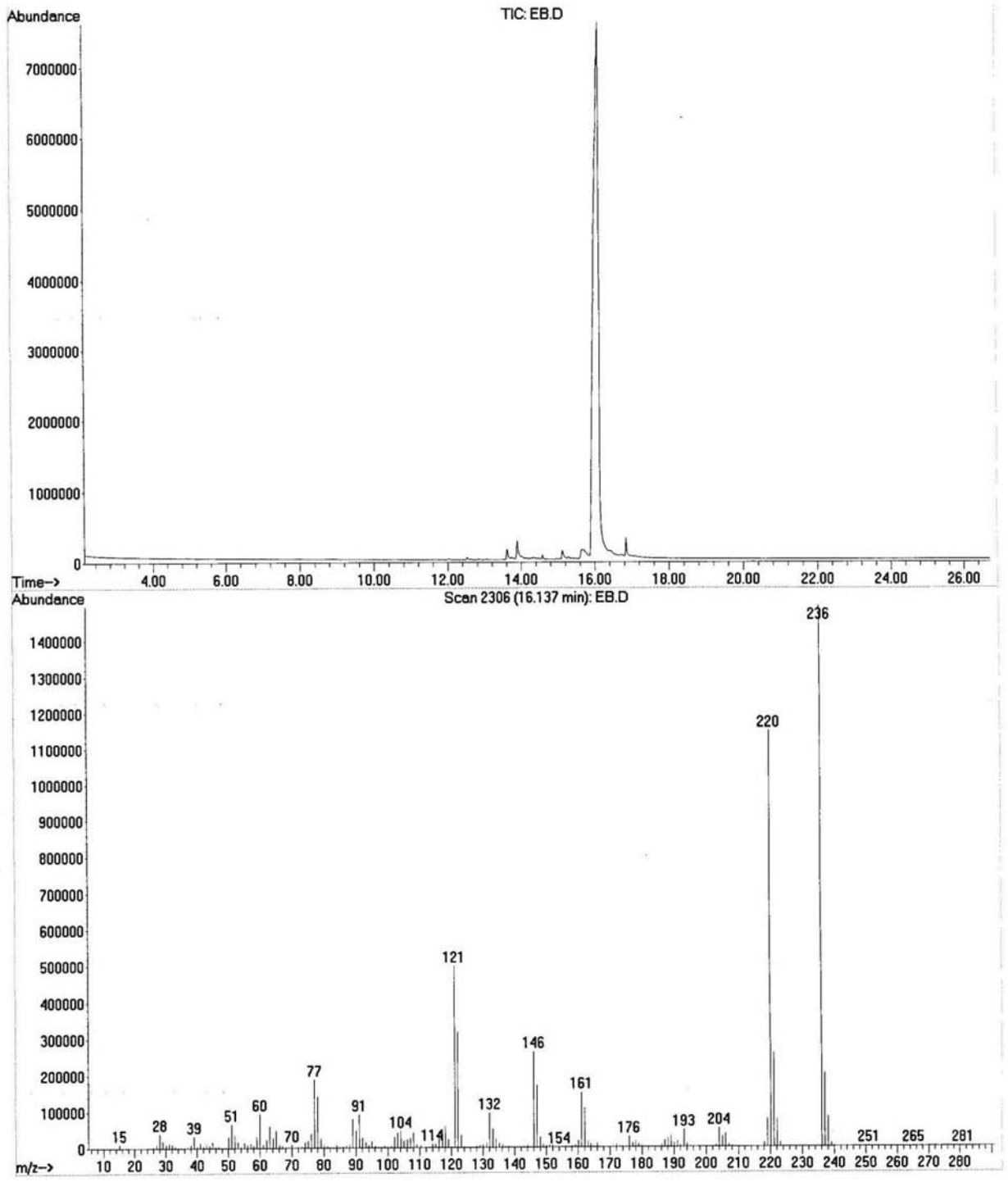

Figure S27. GC MS spectrum of **5d**.

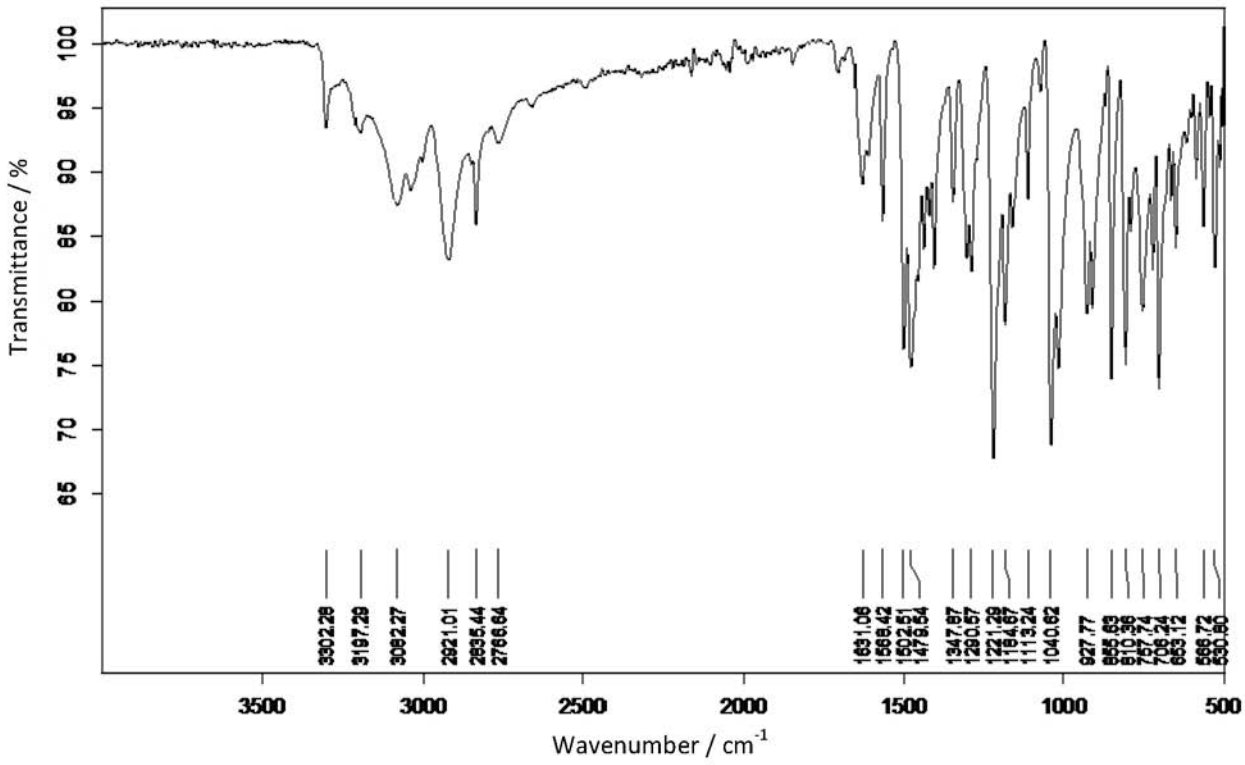

Figure S28. IR (neat) spectrum of **5e**.

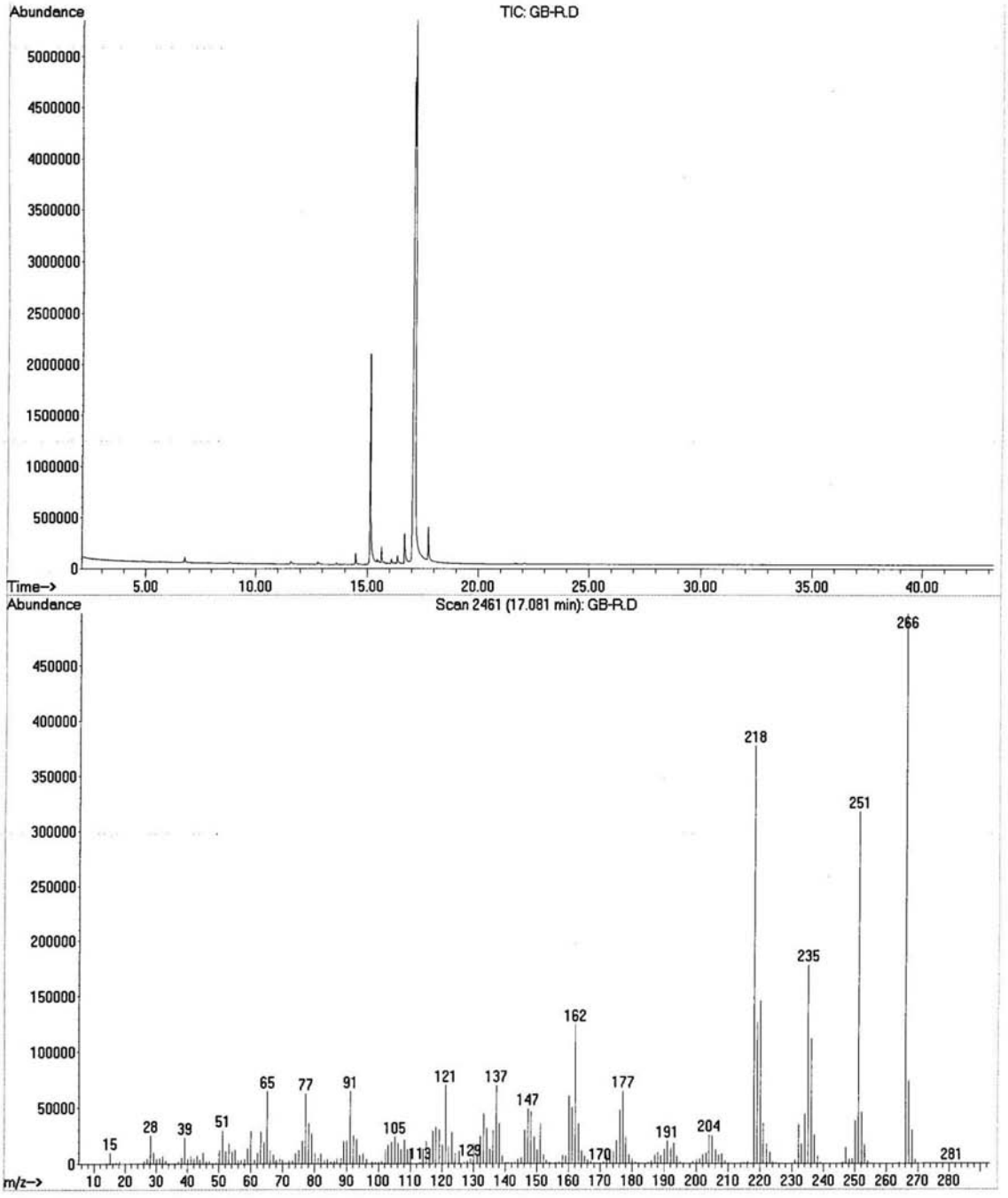

Figure S29. GC MS spectrum of **5e**.

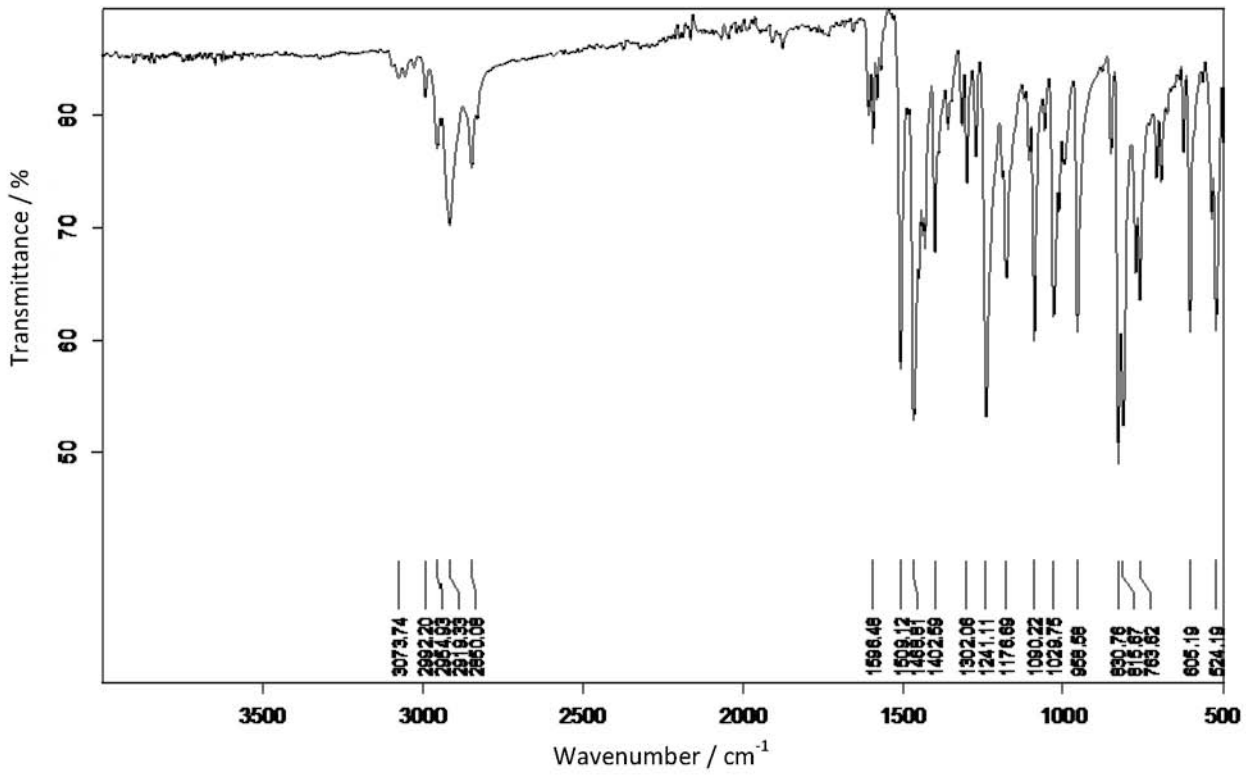

Figure S30. IR (neat) spectrum of **6a**.

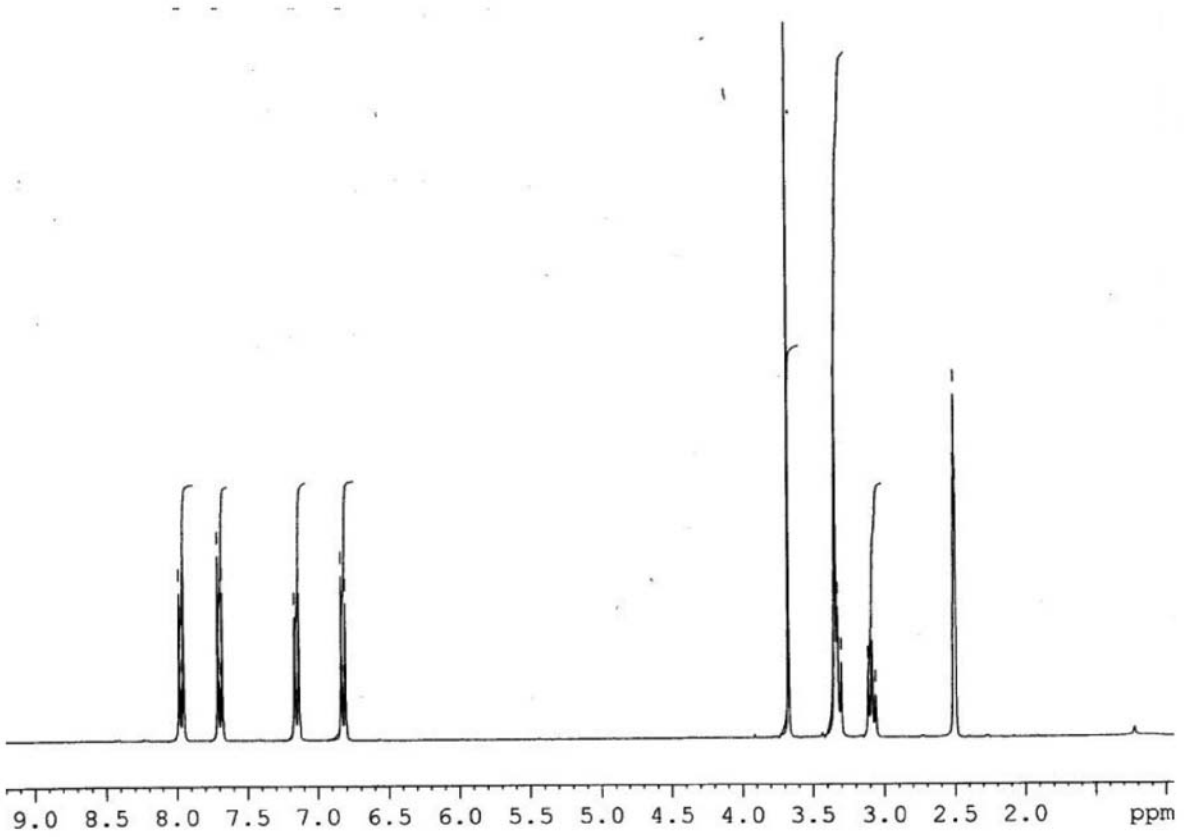

Figure S31. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6a**.

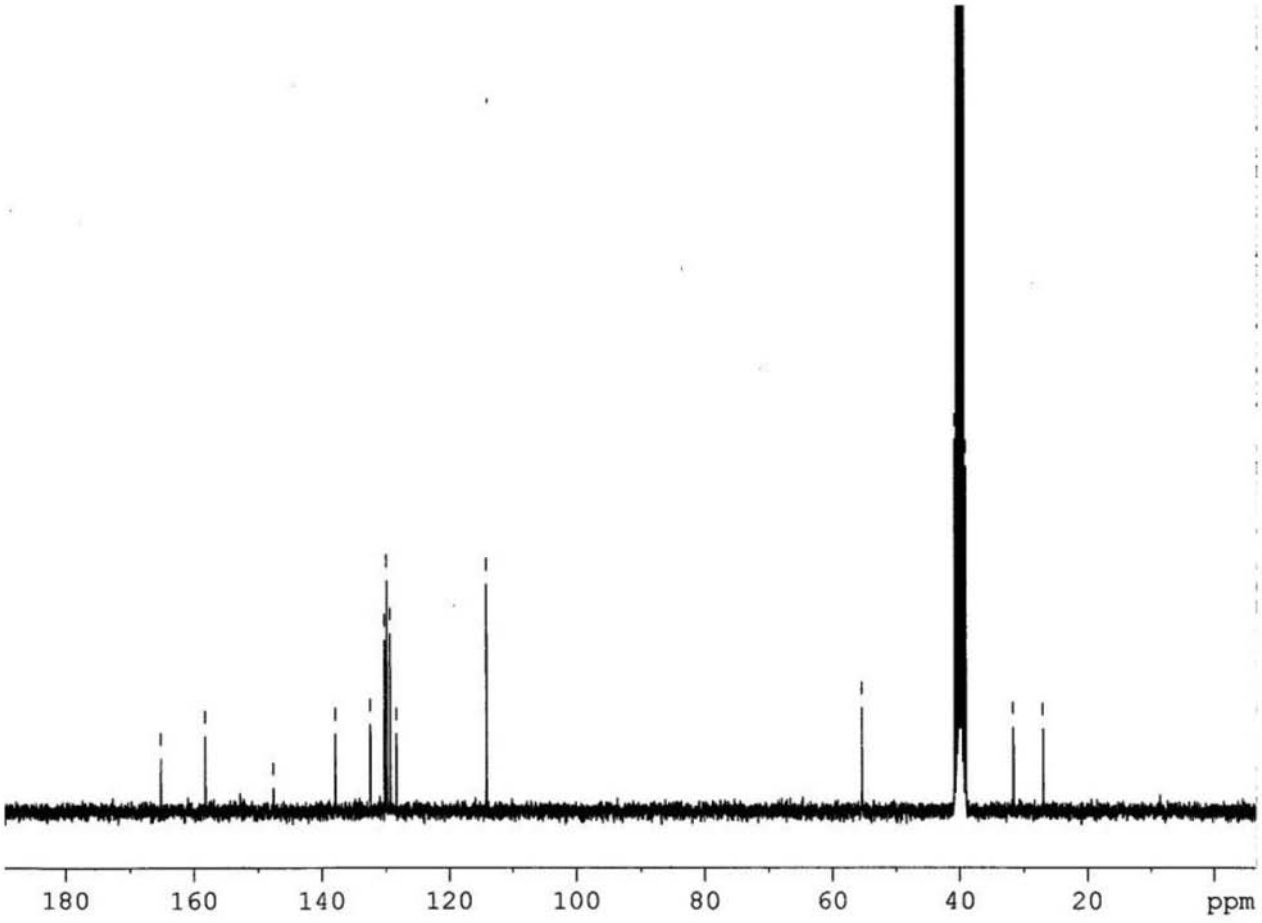

Figure S32. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6a**.

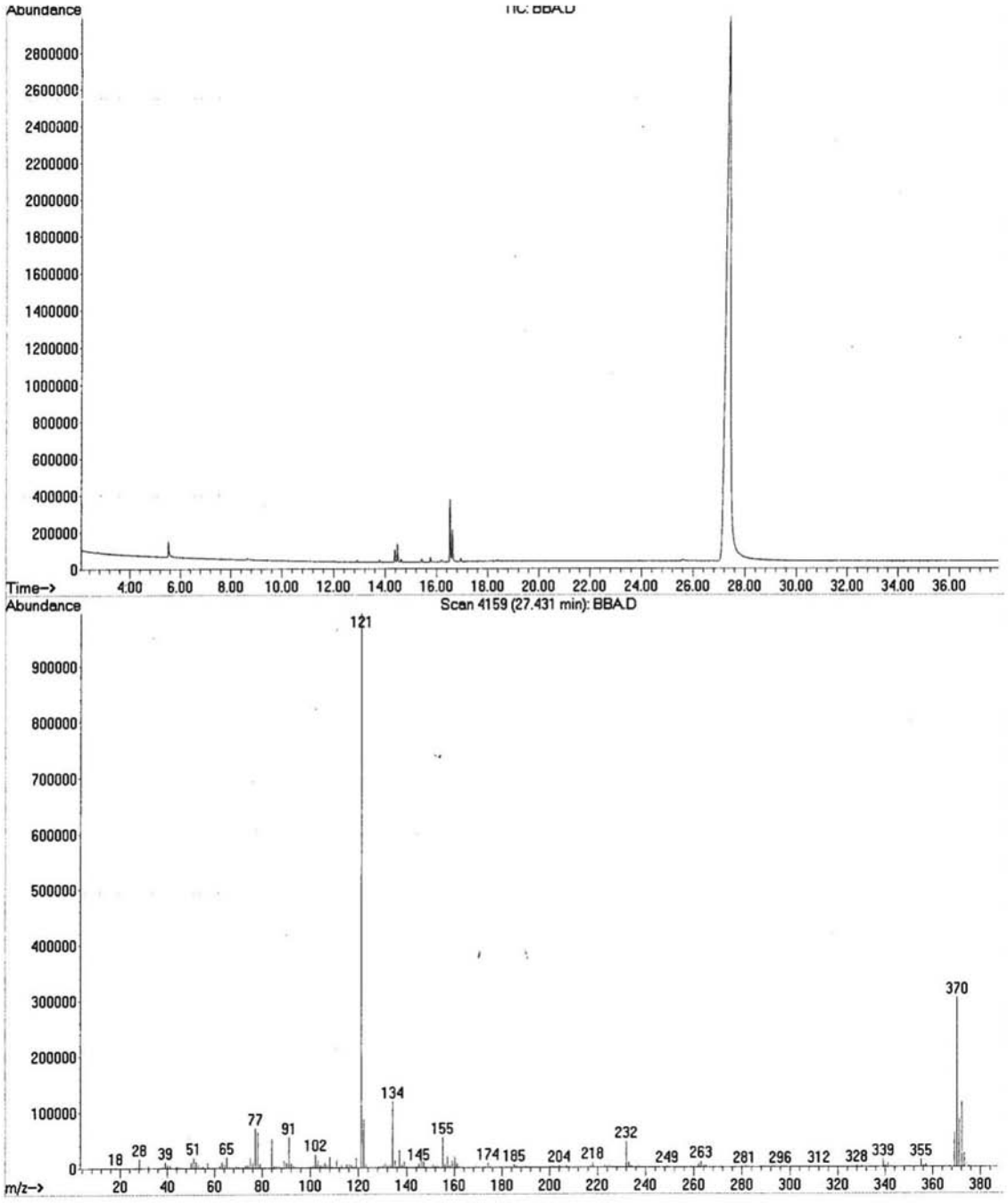

Figure S33. GC MS spectrum of **6a**.

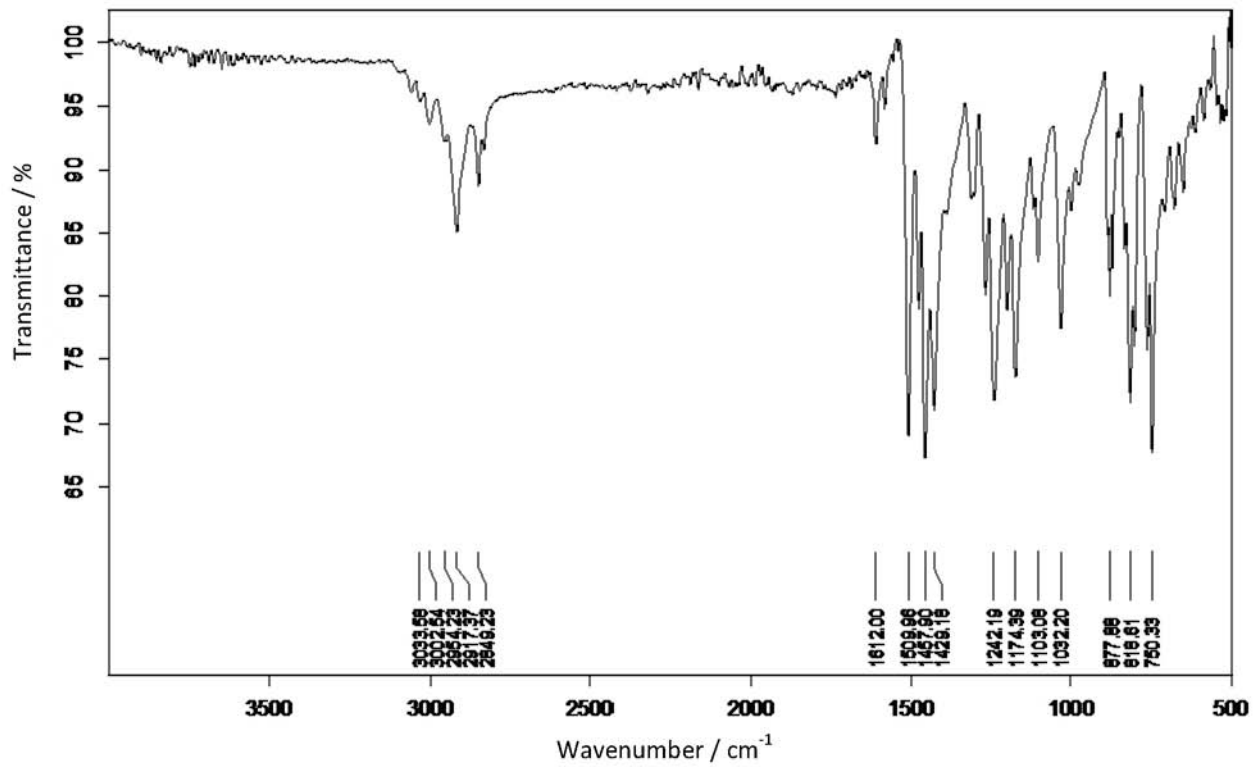

Figure S34. IR (neat) spectrum of **6b**.

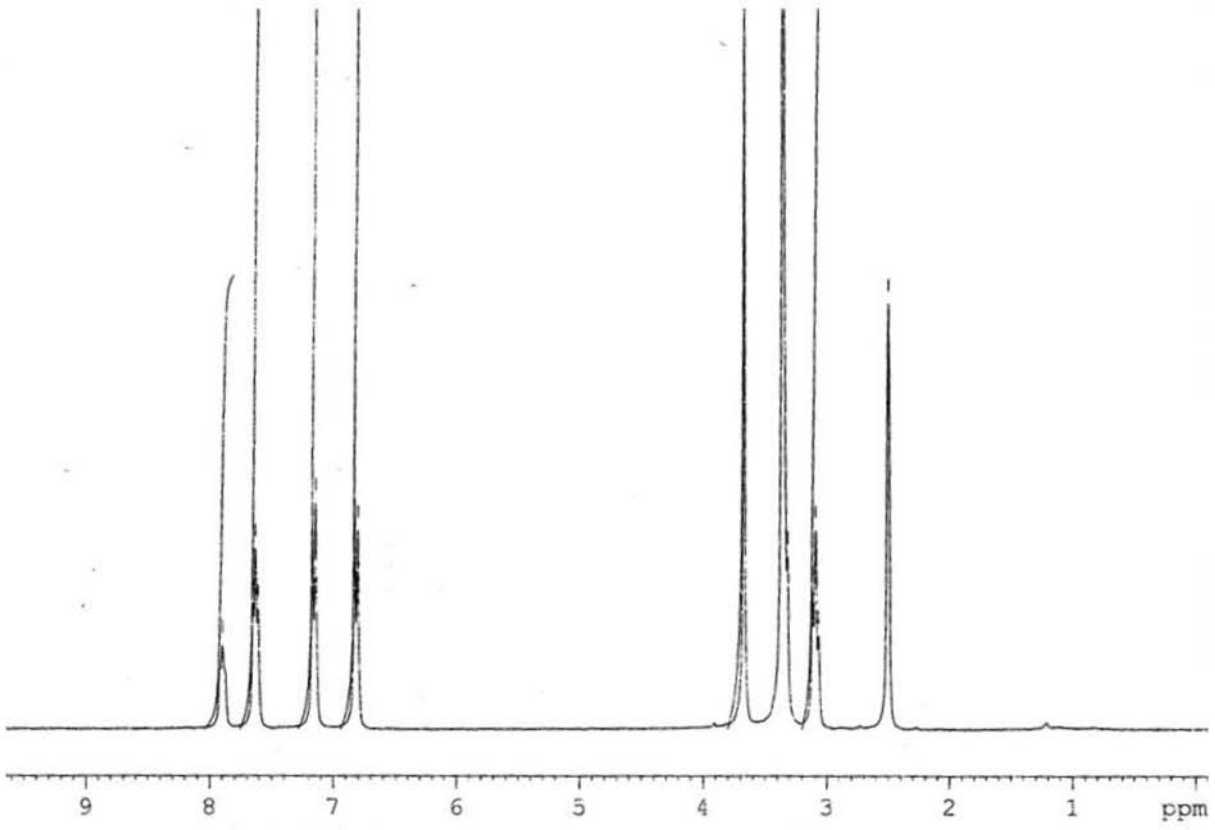

Figure S35. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6b**.

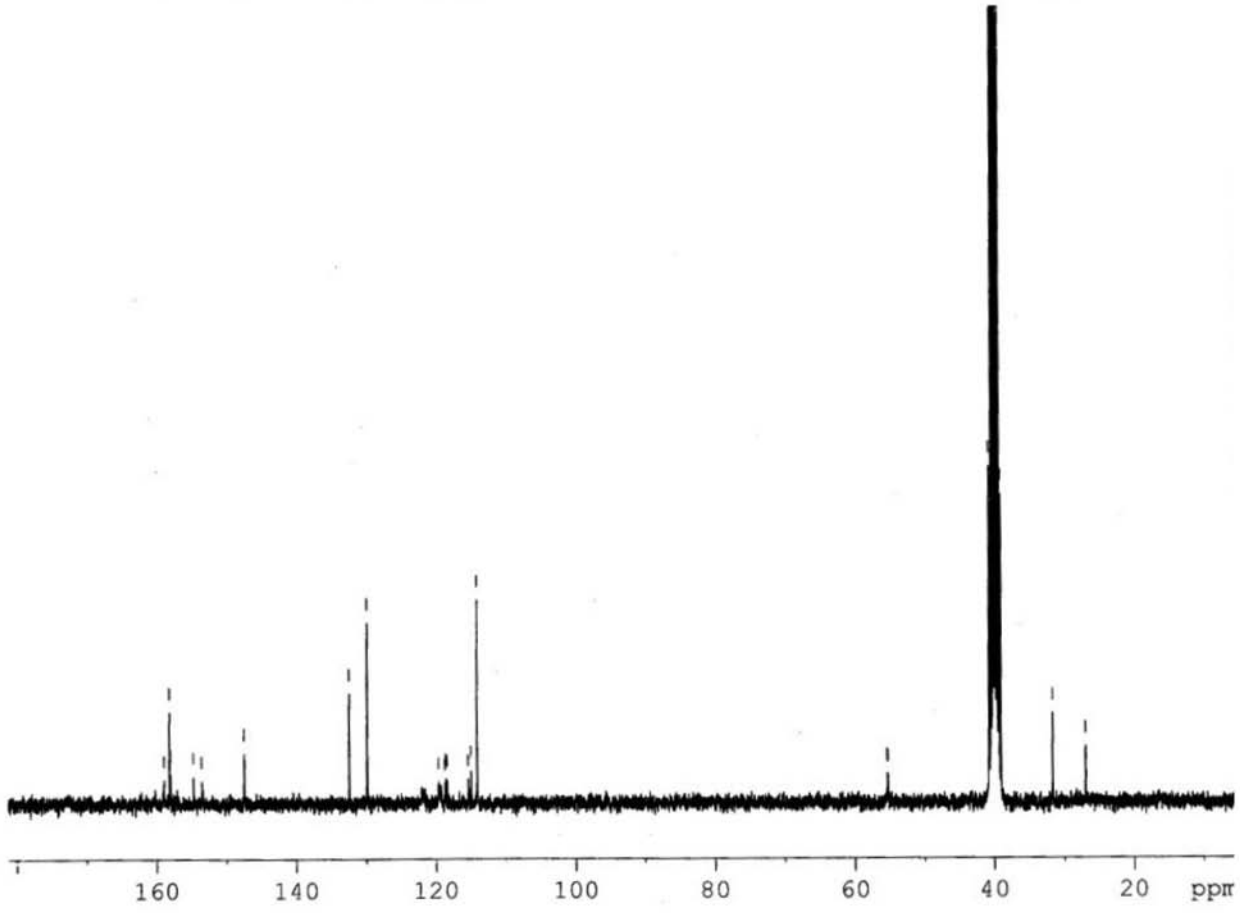

Figure S36. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6b**.

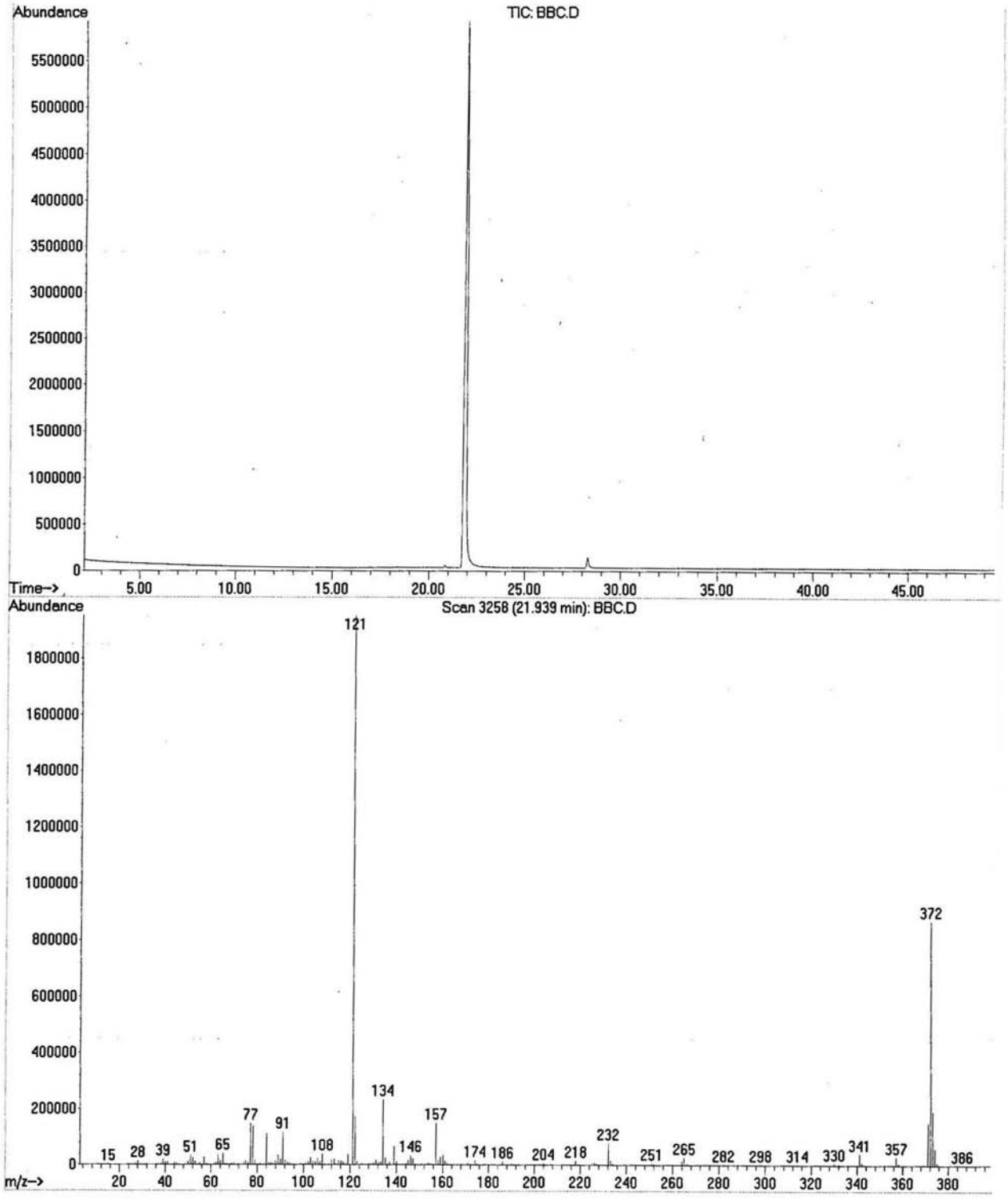

Figure S37. GC MS spectrum of **6b**.

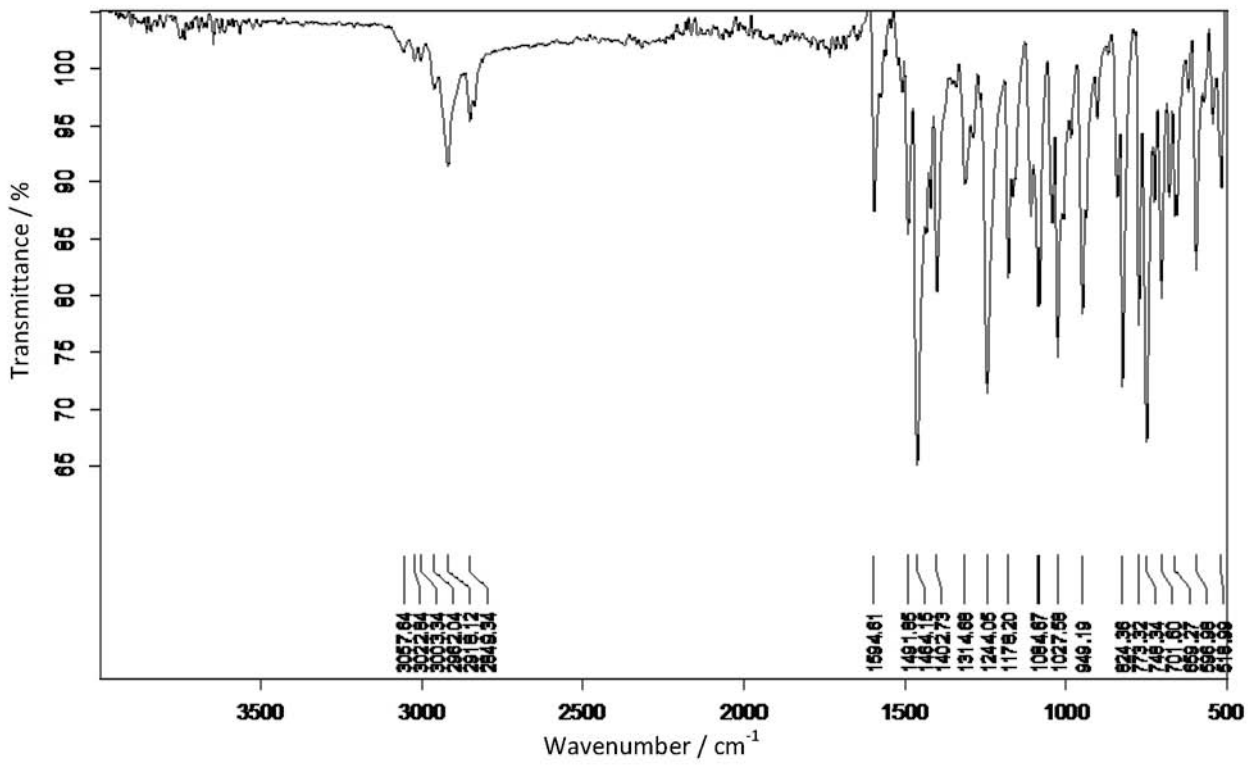

Figure S38. IR (neat) spectrum of **6c**.

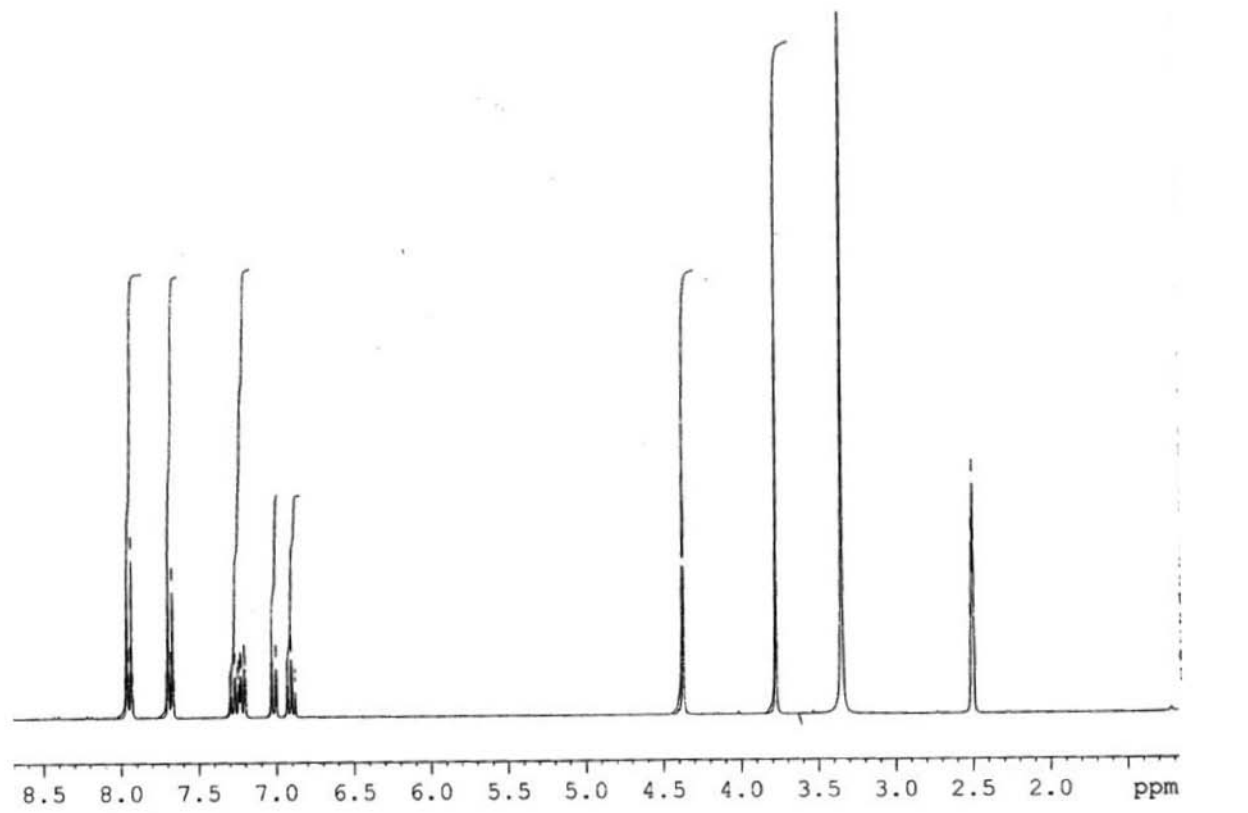

Figure S39. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6c**.

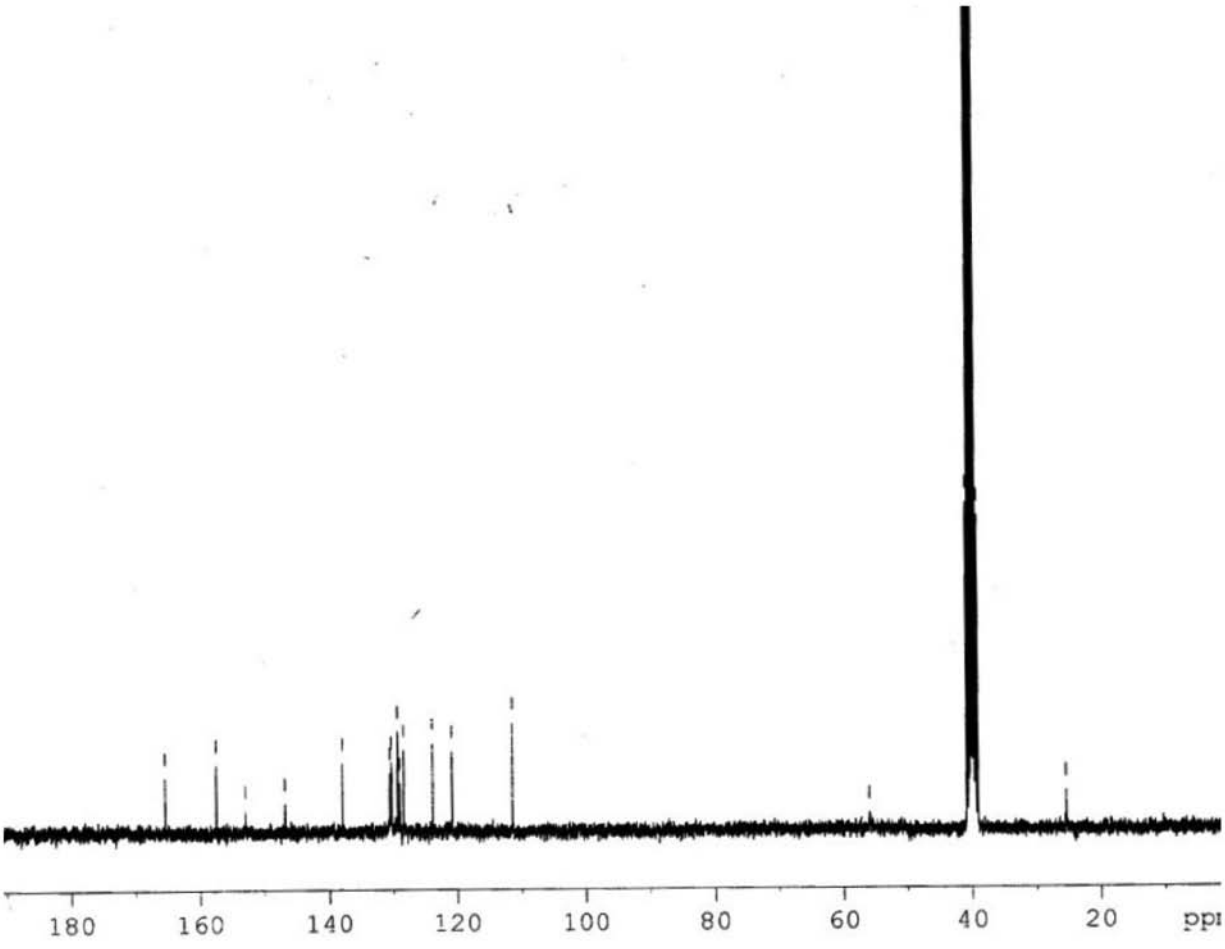

Figure S40. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6c**.

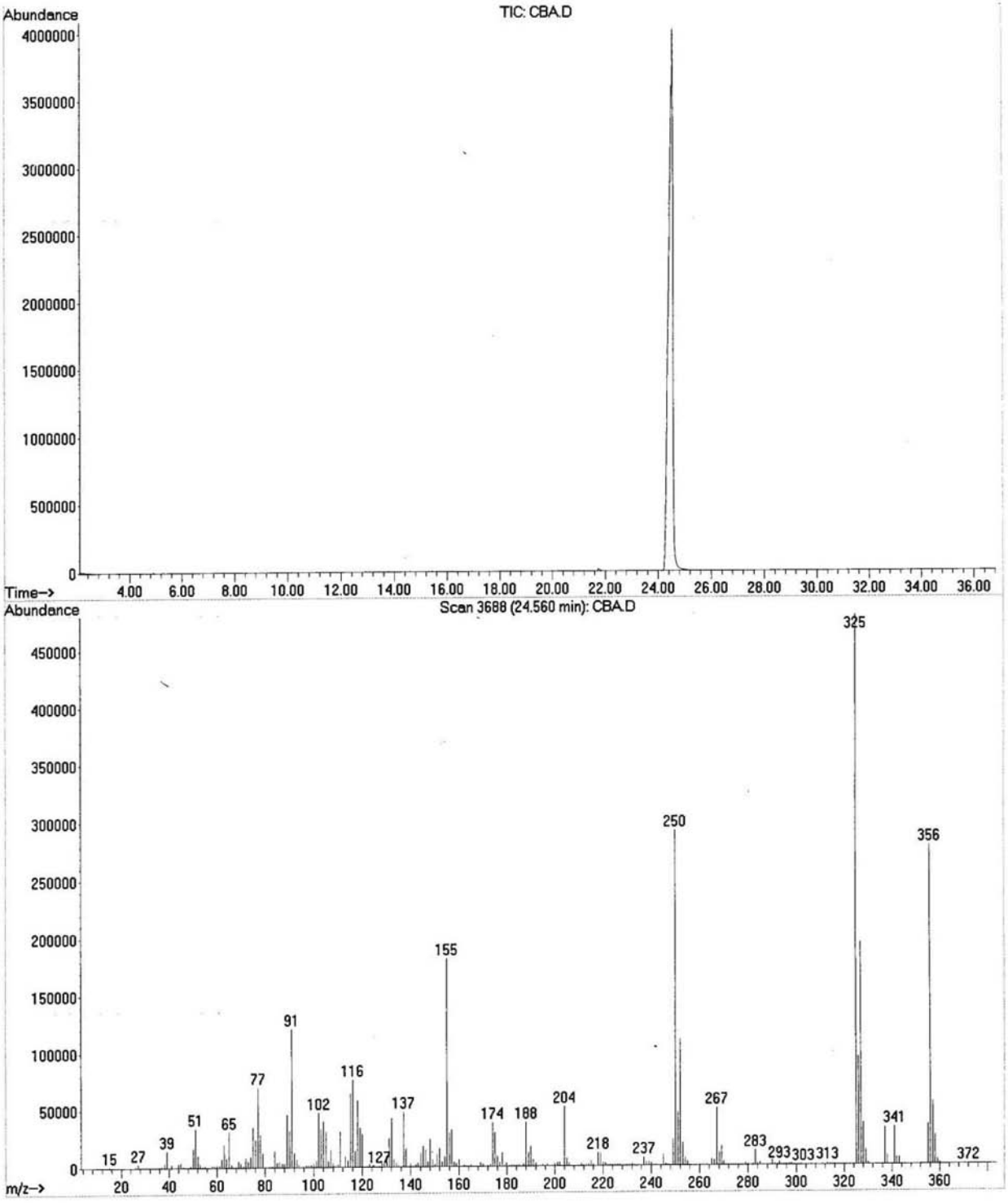

Figure S41. GC MS spectrum of **6c**.

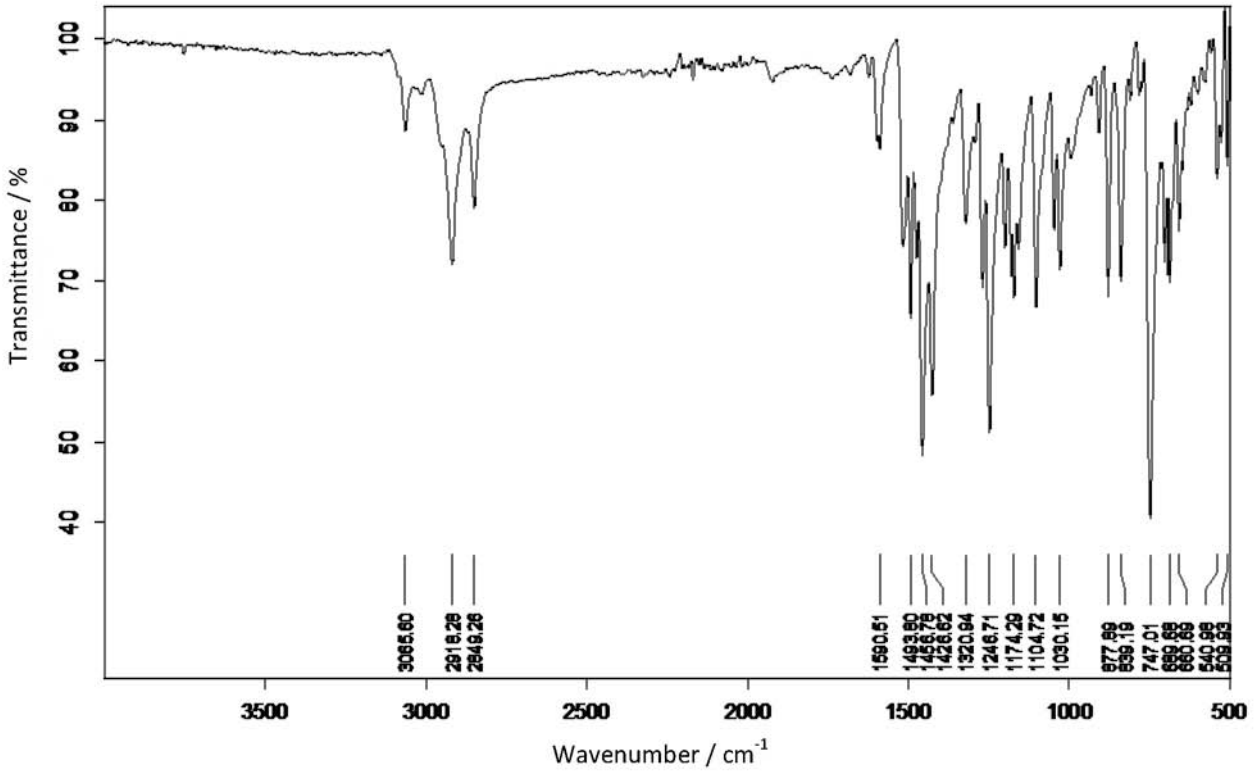

Figure S42. IR (neat) spectrum of **6d**.

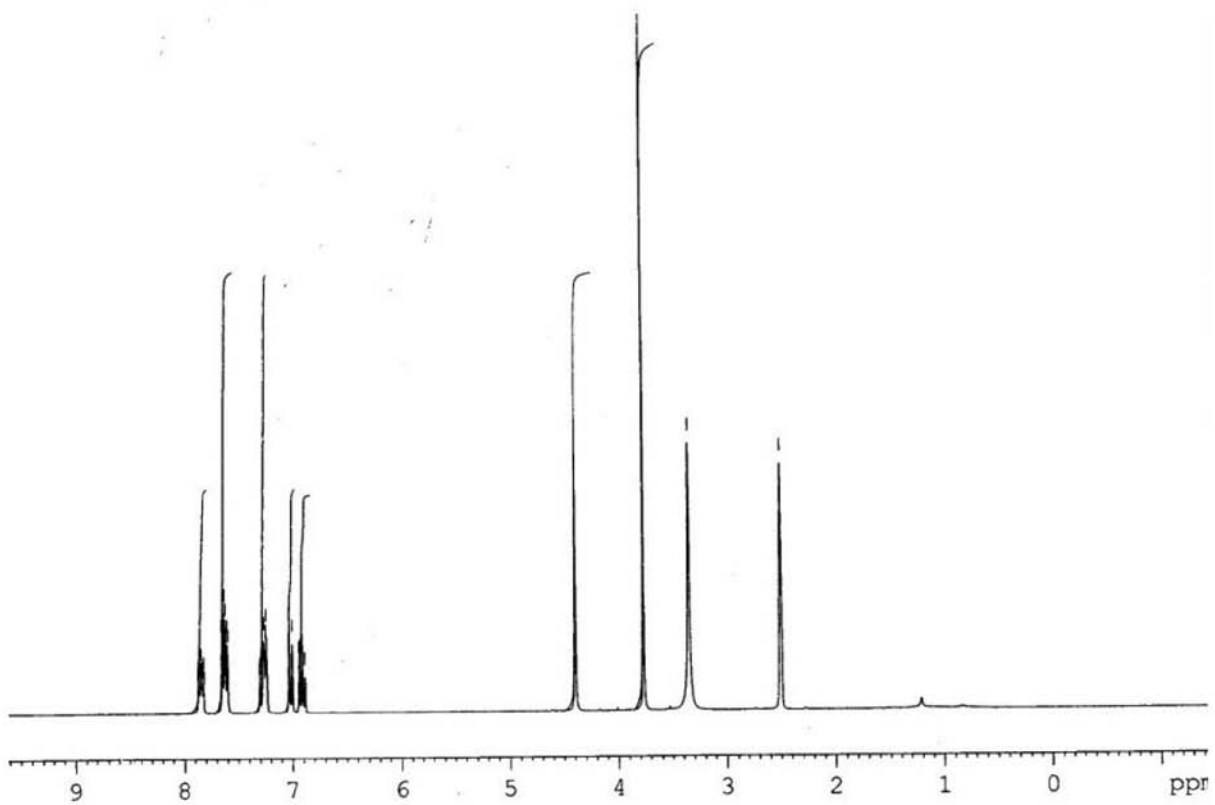

Figure S43. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6d**.

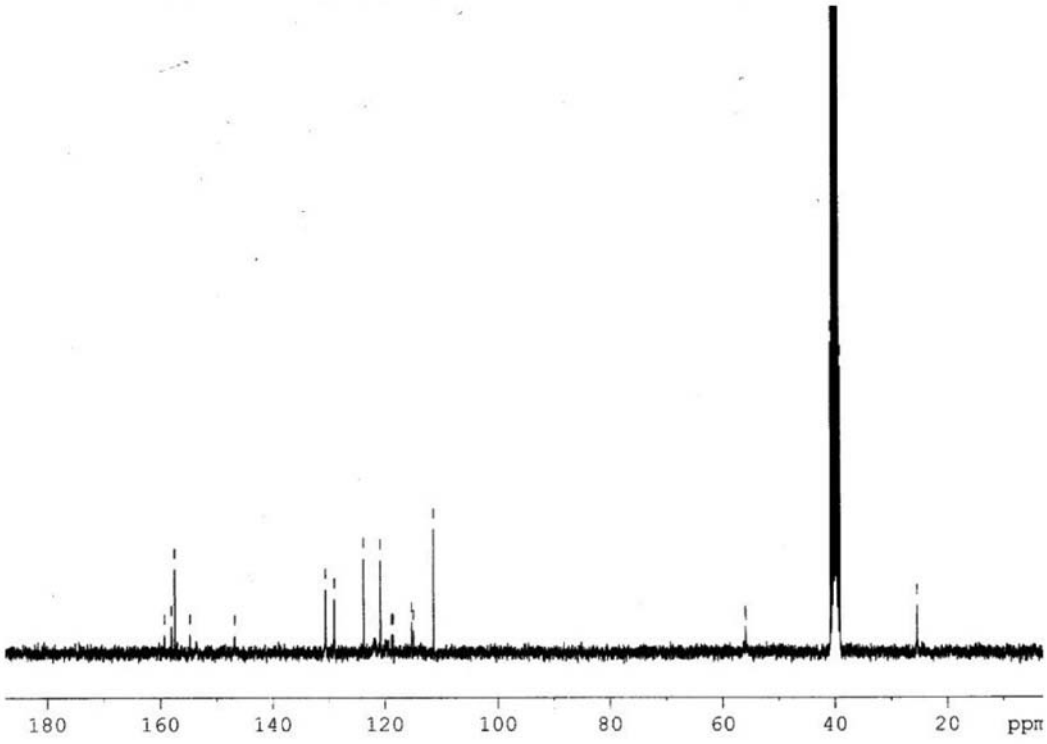

Figure S44. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6d**.

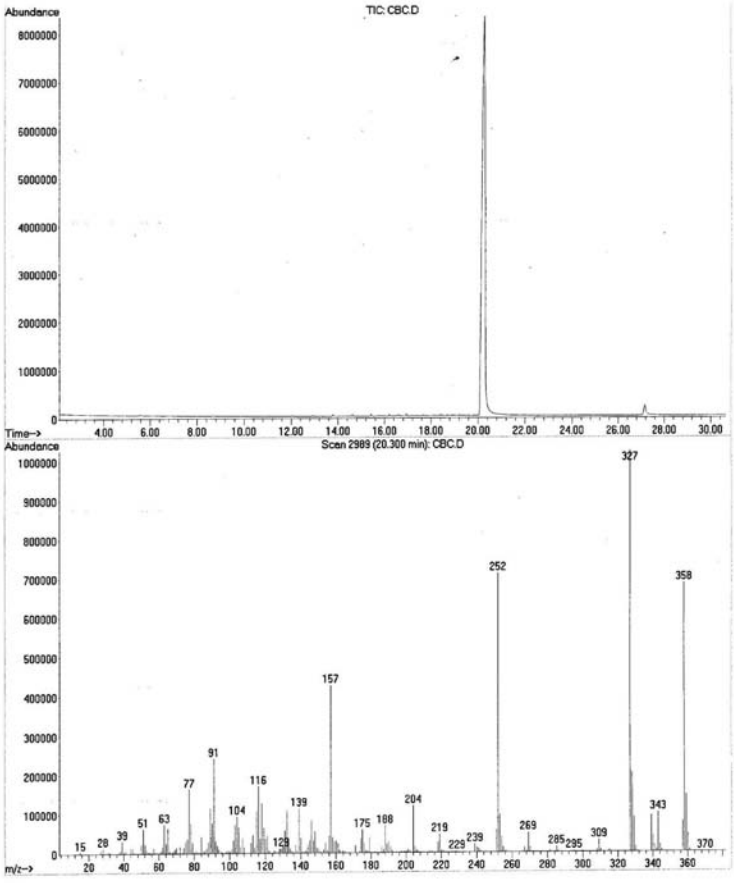

Figure S45. GC MS spectrum of **6d**.

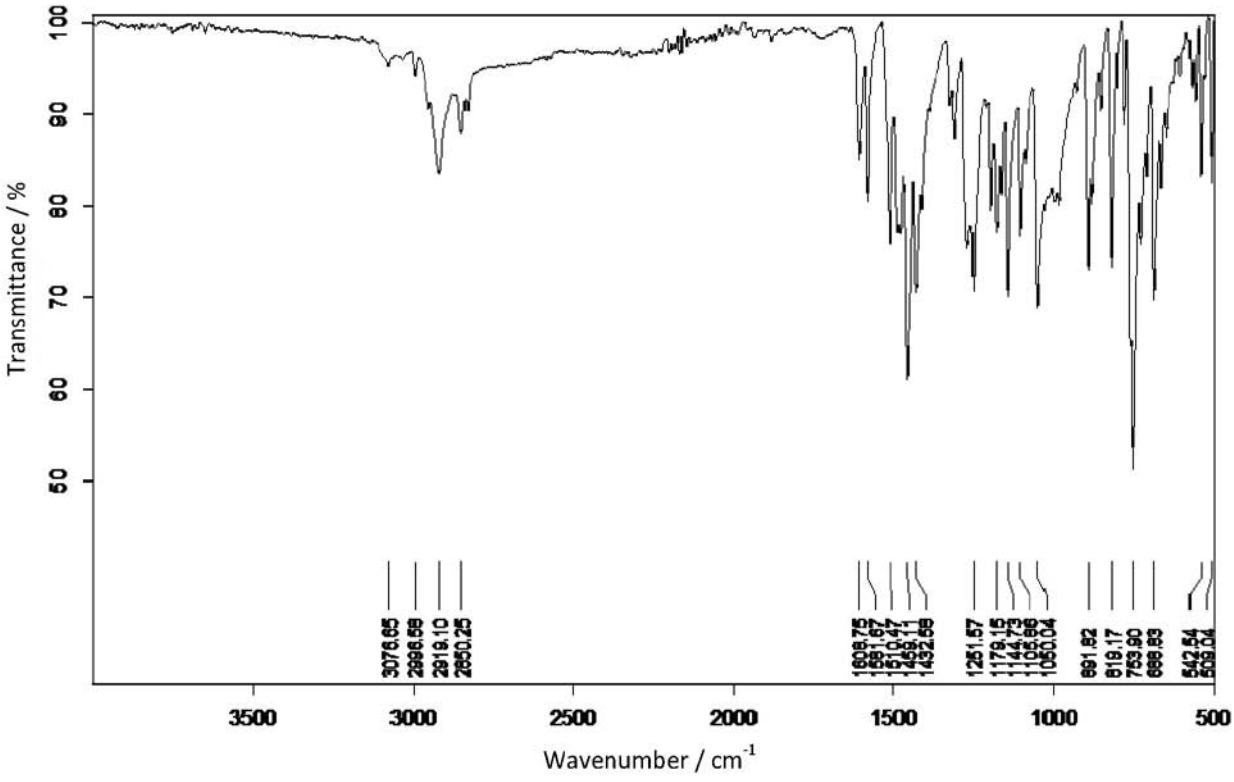

Figure S46. IR (neat) spectrum of **6e**.

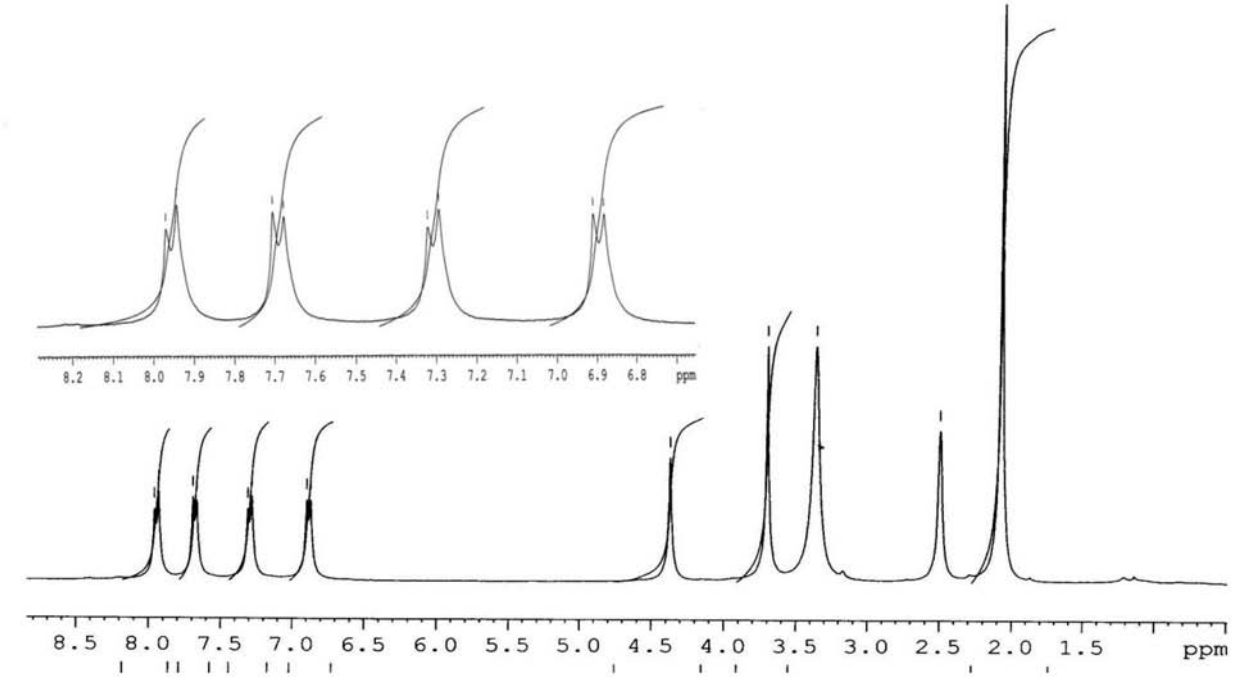

Figure S47. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6g**.

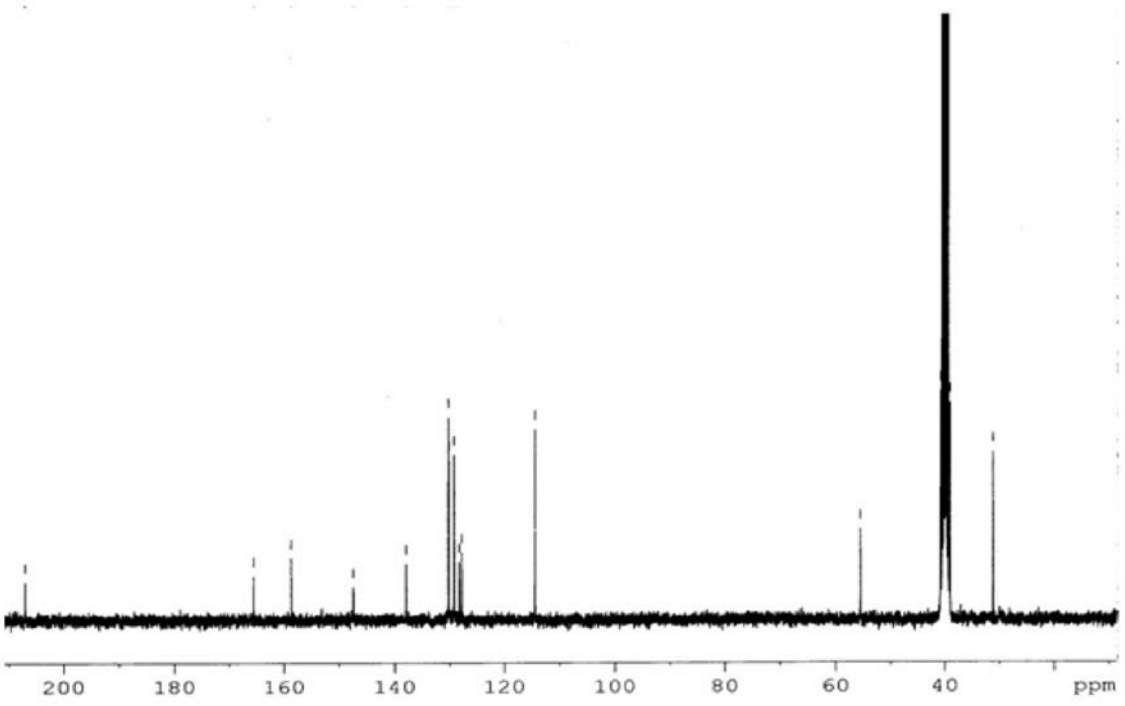

Figure S48. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6g**.

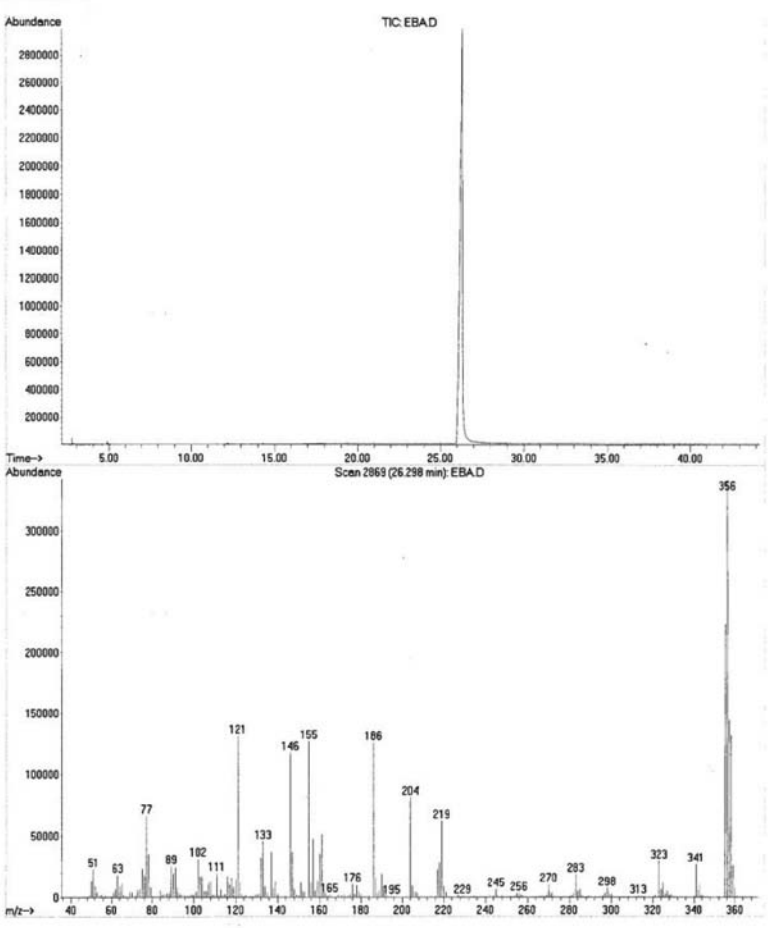

Figure S49. GC MS spectrum of **6g**.

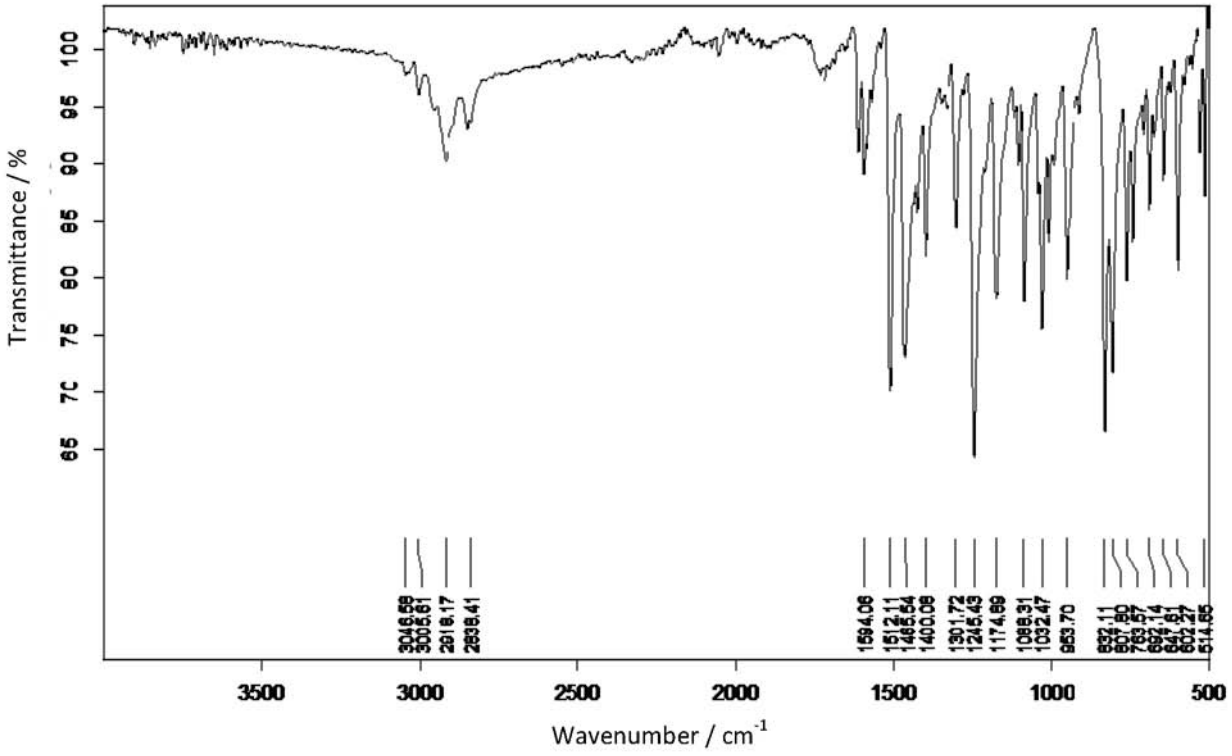

Figure S50. IR (neat) spectrum of **6h**.

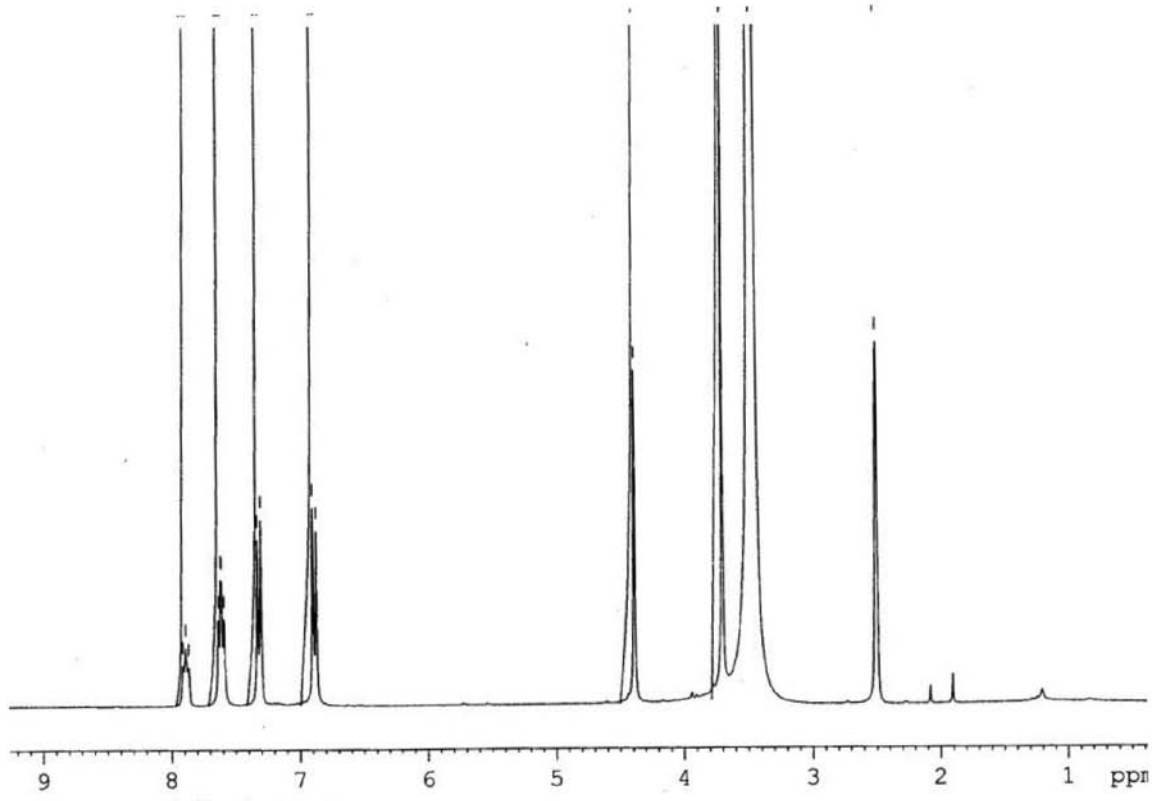

Figure S51. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6h**.

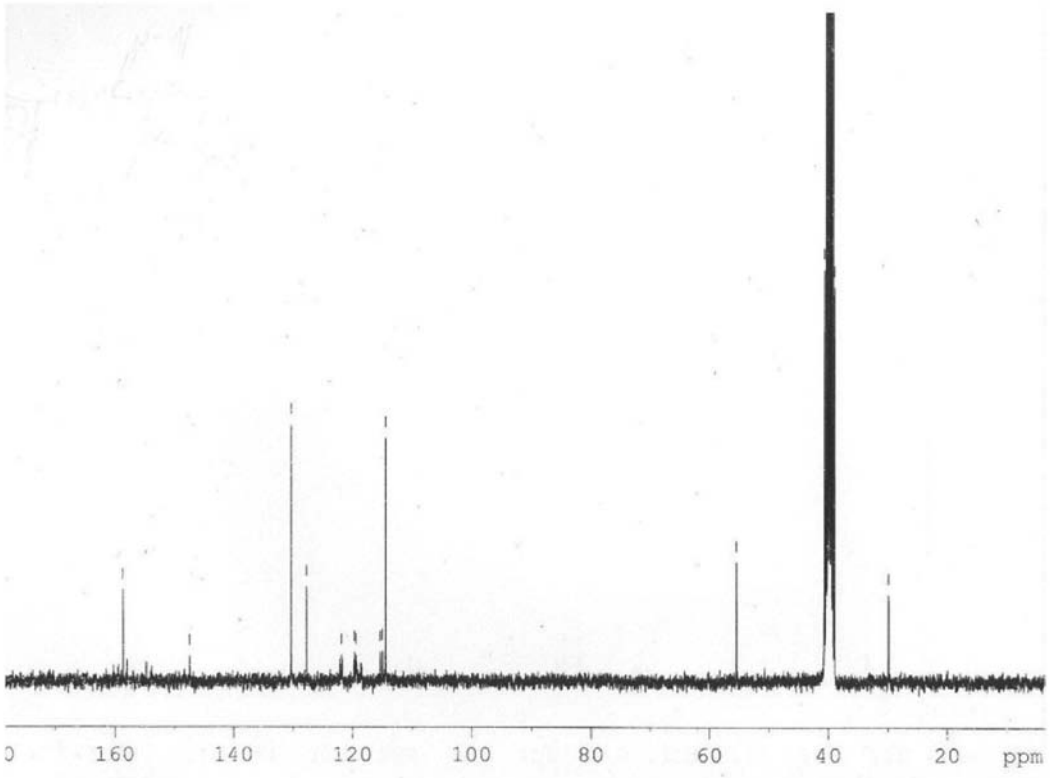

Figure S52. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6h**.

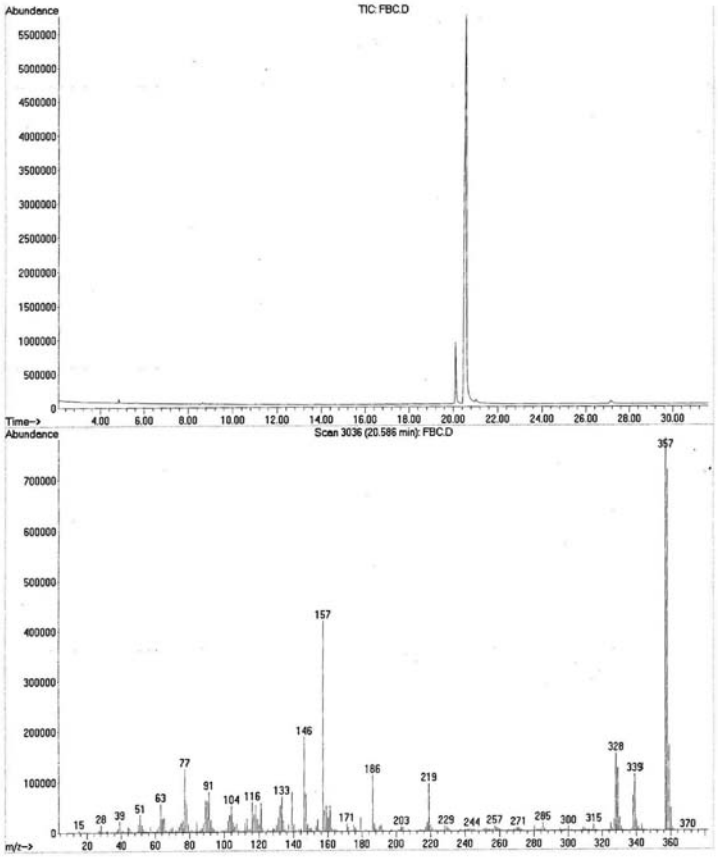

Figure S53. GC MS spectrum of **6h**.

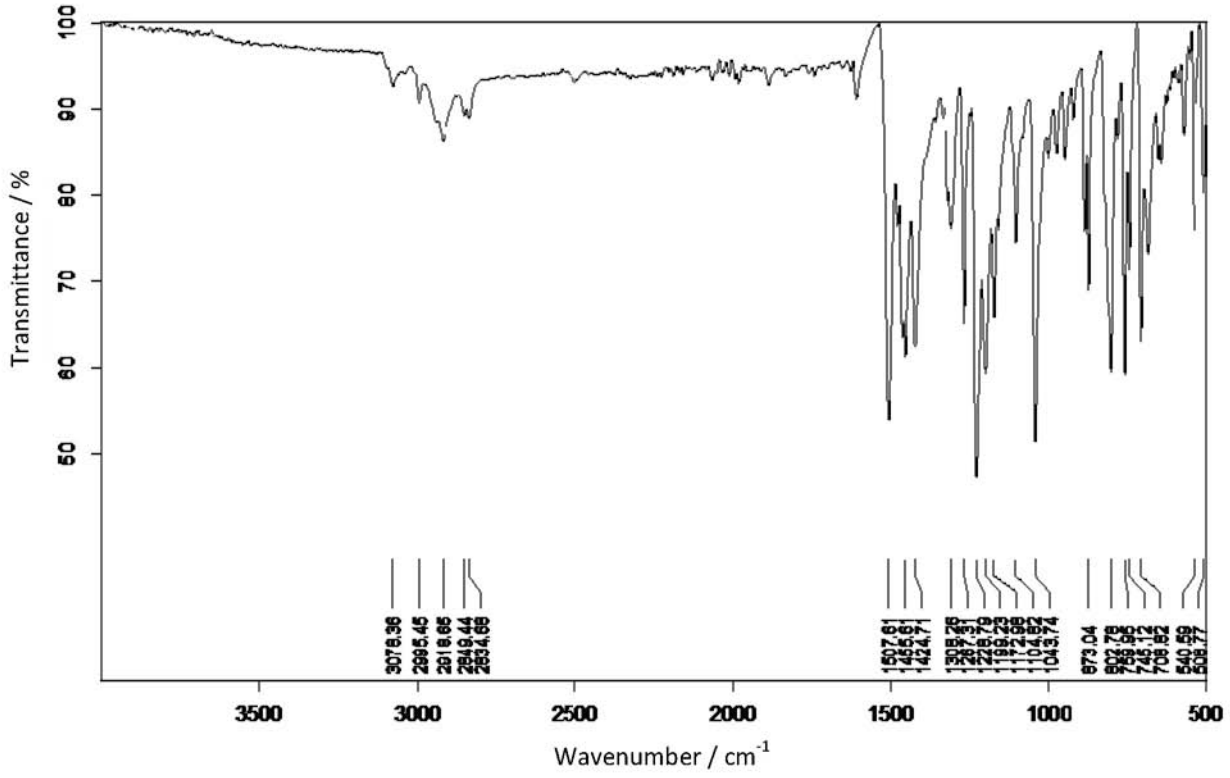

Figure S54. IR (neat) spectrum of **6i**.

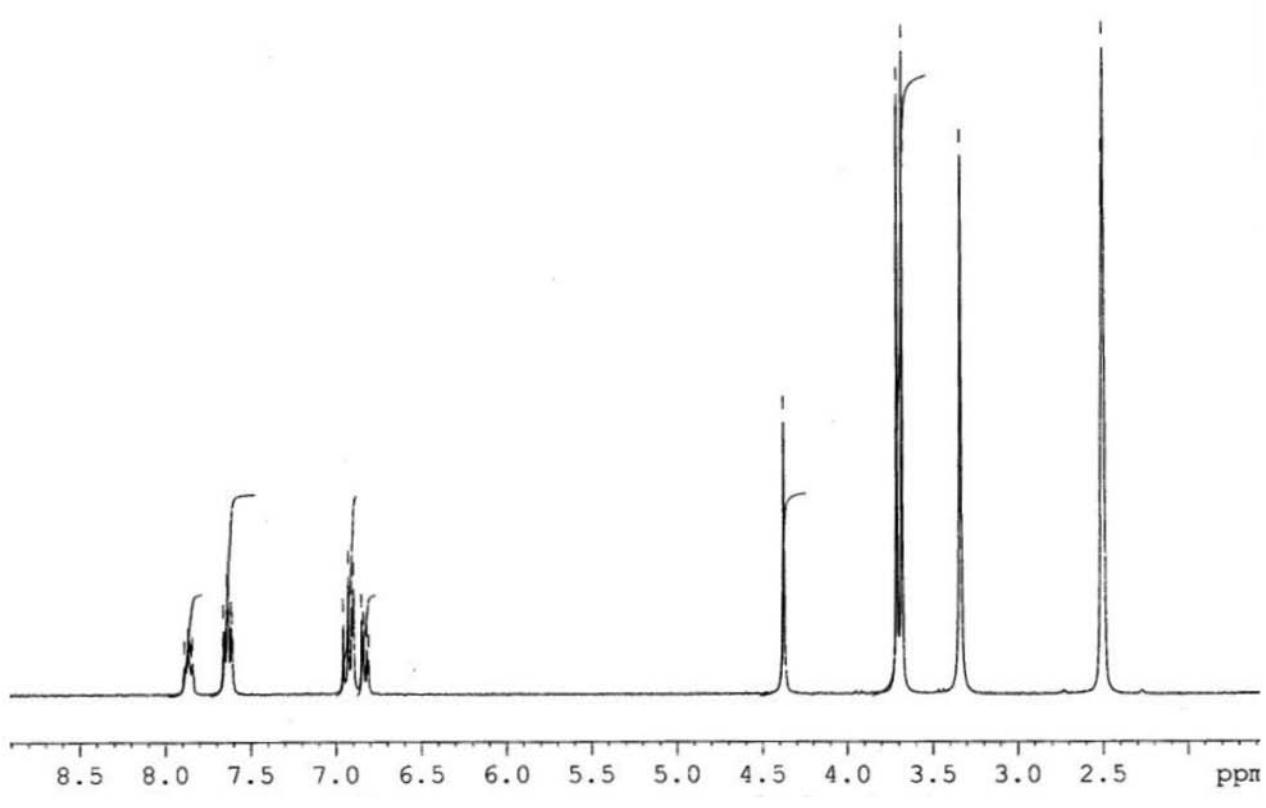

Figure S55. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6i**.

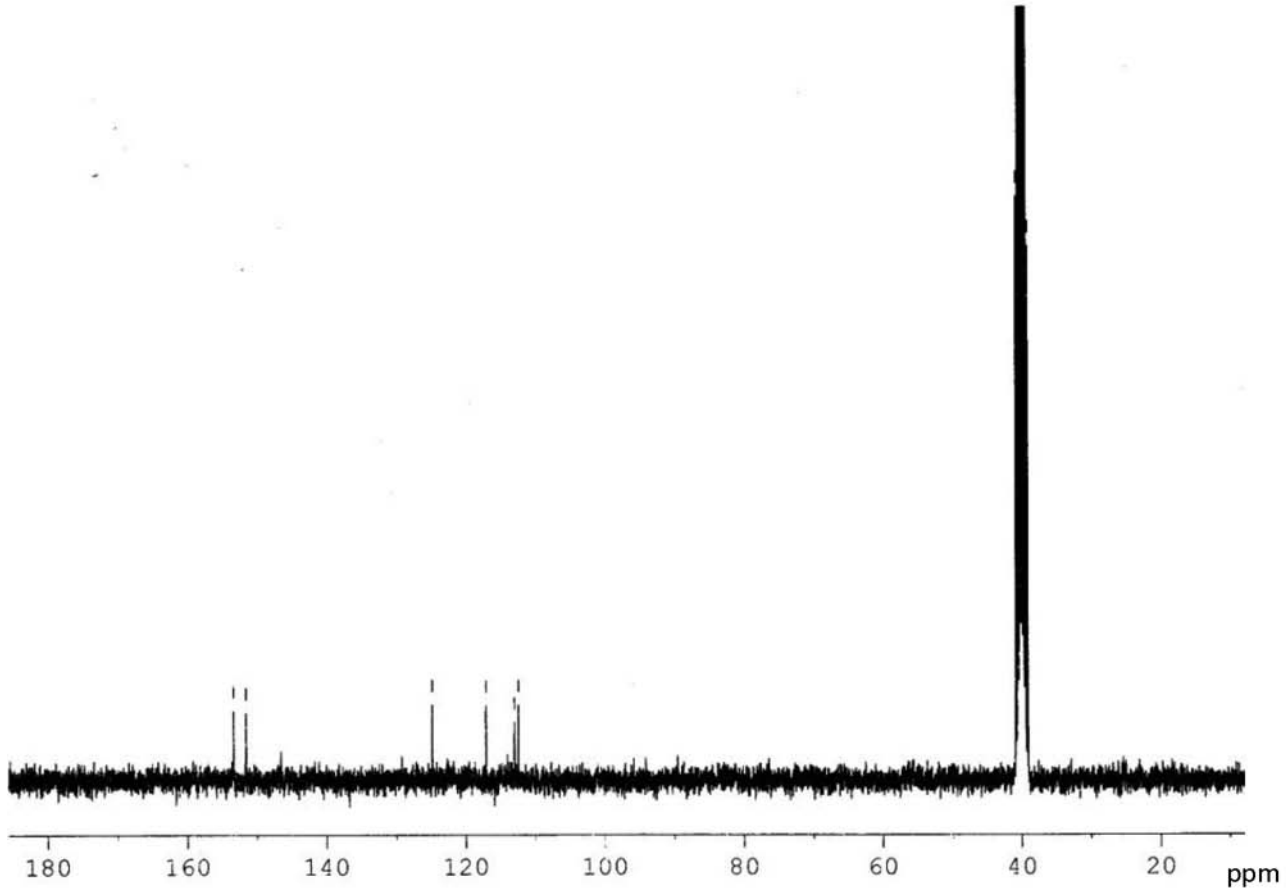

Figure S56. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6i**.

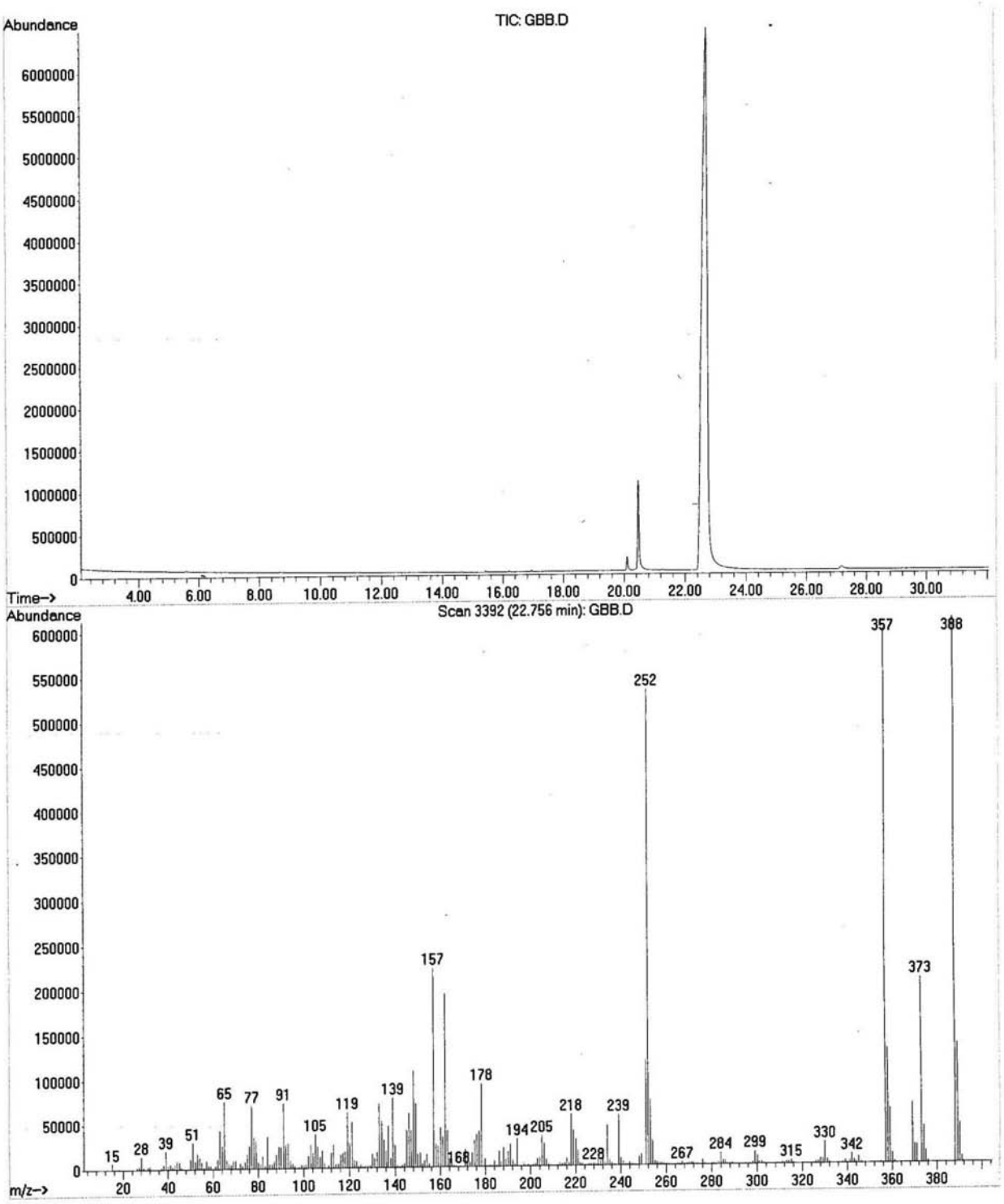

Figure S57. GC MS spectrum of **6i**.

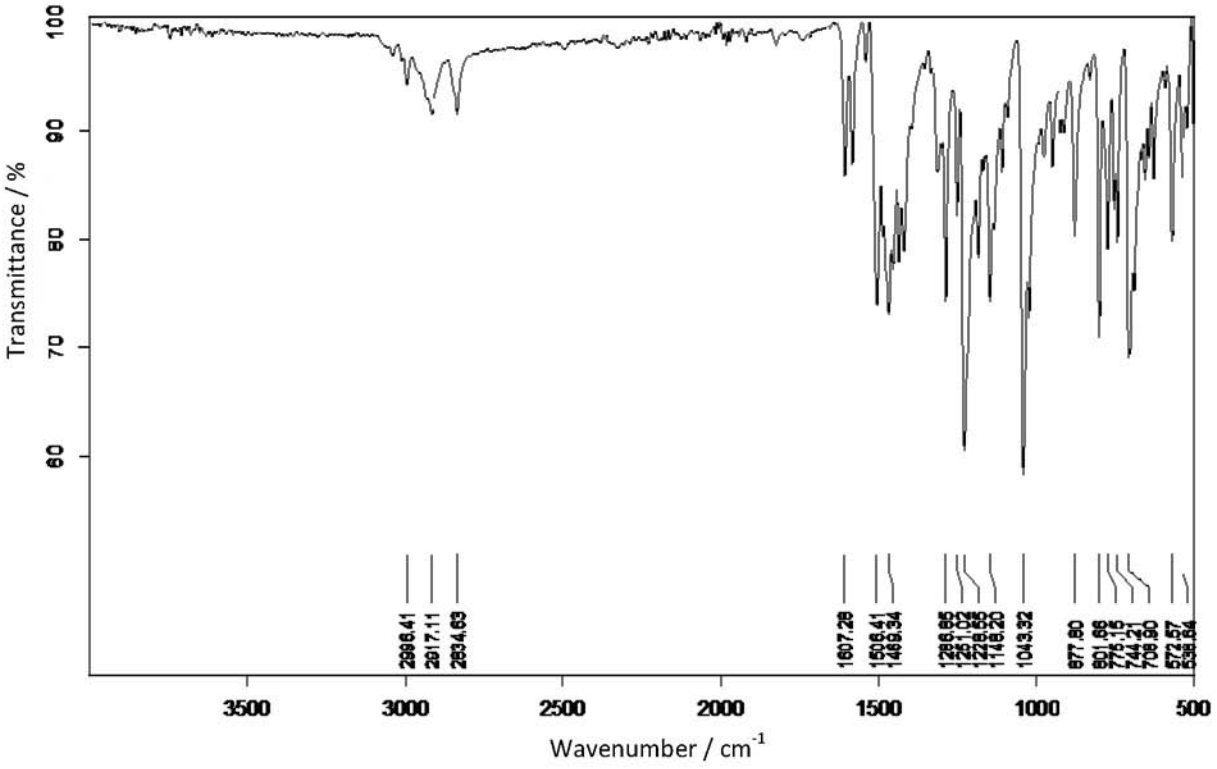

Figure S58. IR (neat) spectrum of **6j**.

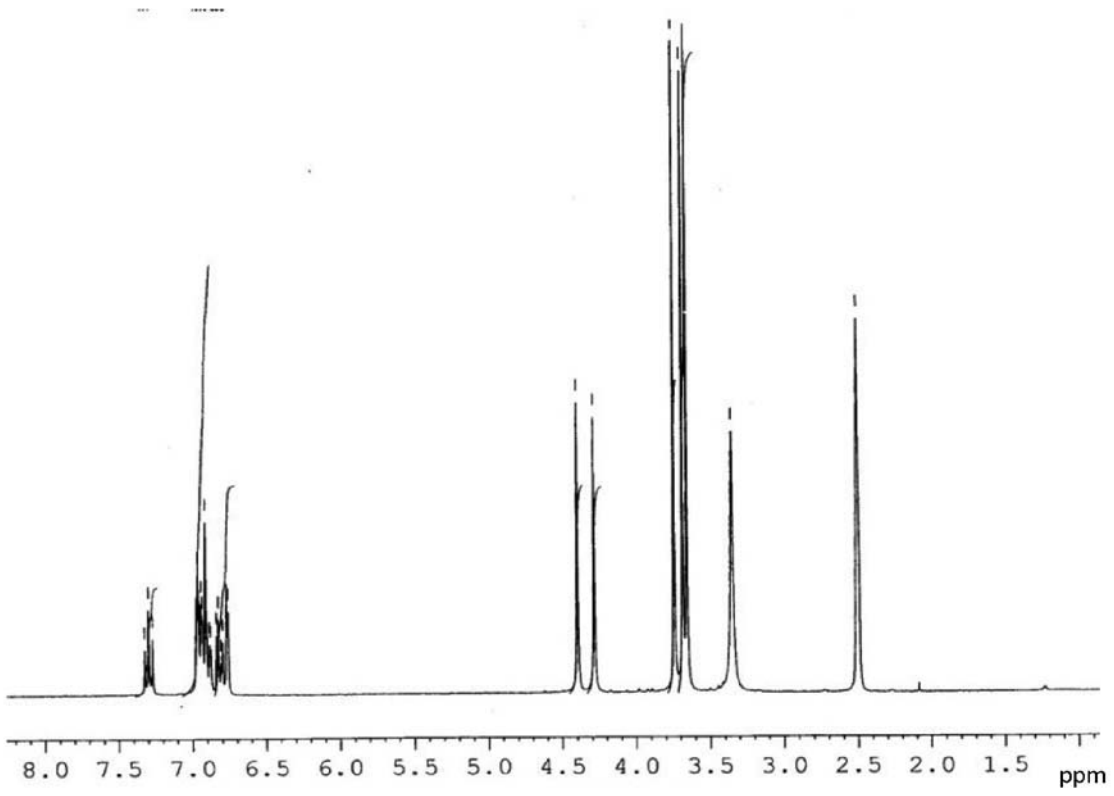

Figure S59. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6j**.

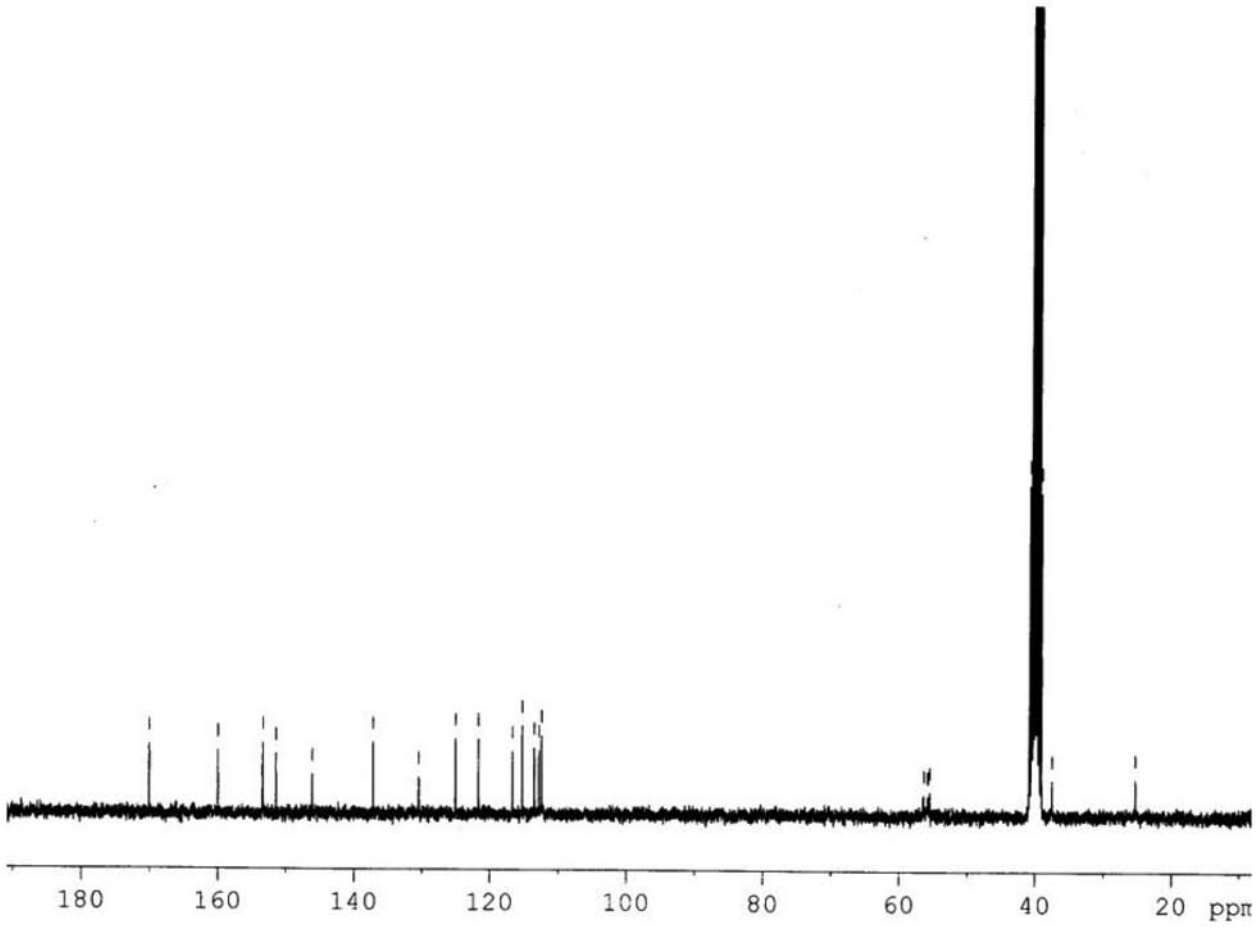

Figure S60. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6j**.

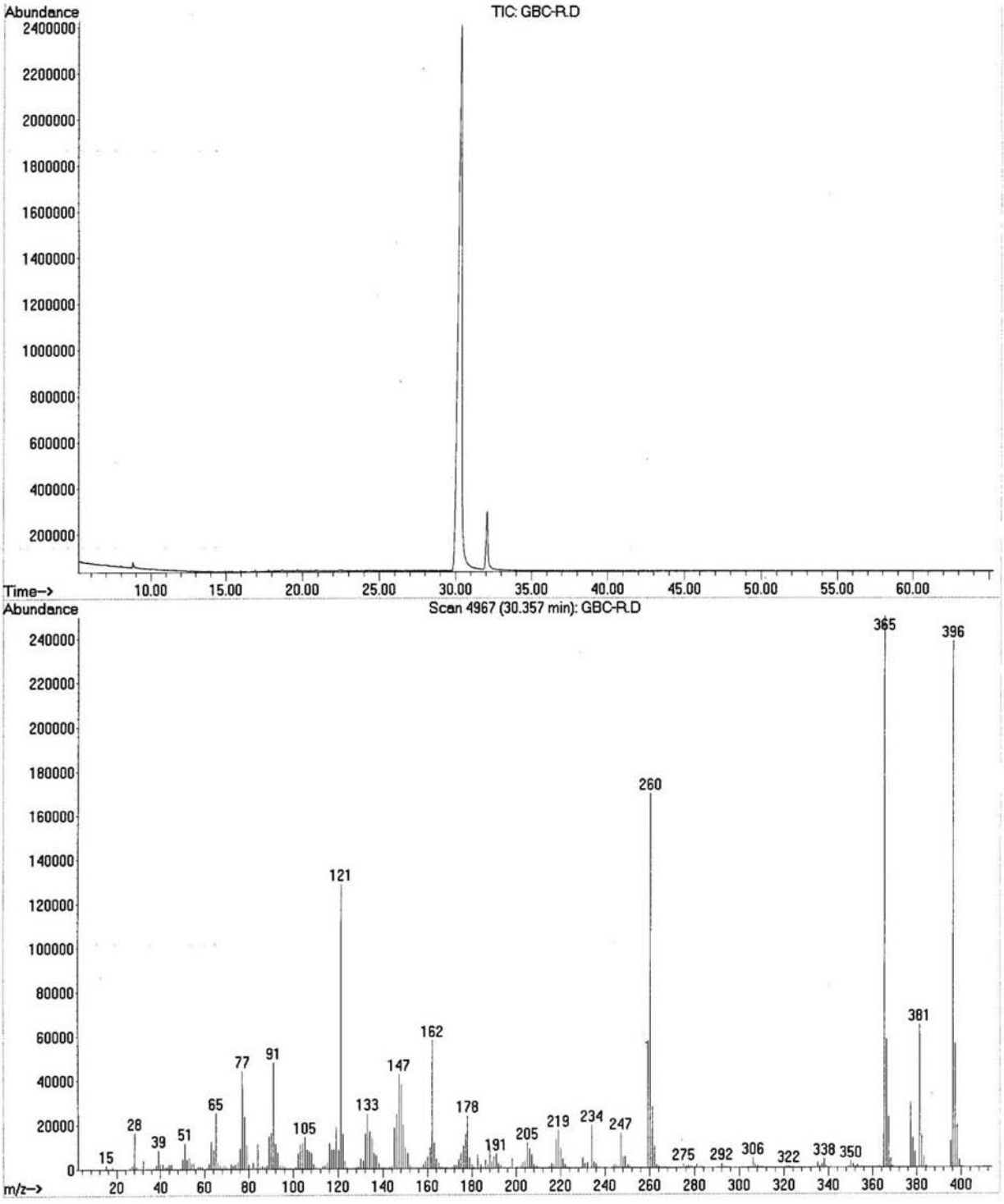

Figure S61. GC MS spectrum of **6j**.

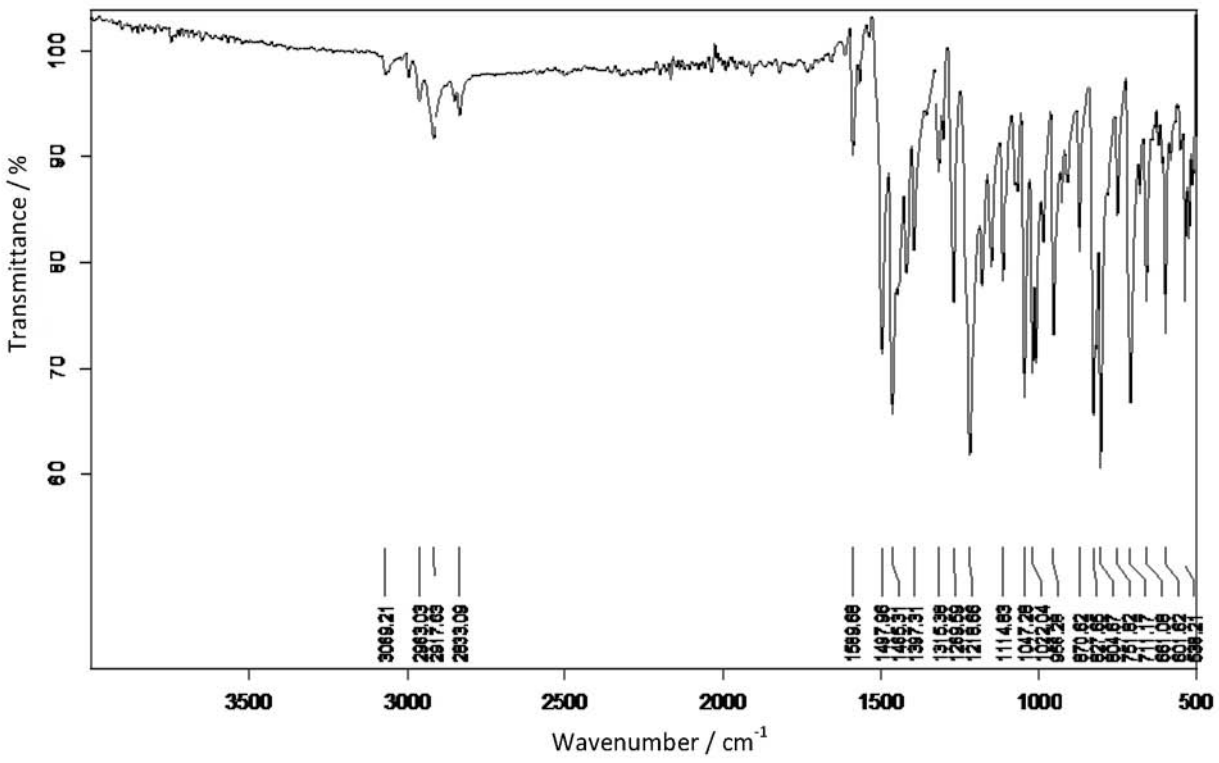

Figure S62. IR (neat) spectrum of **6k**.

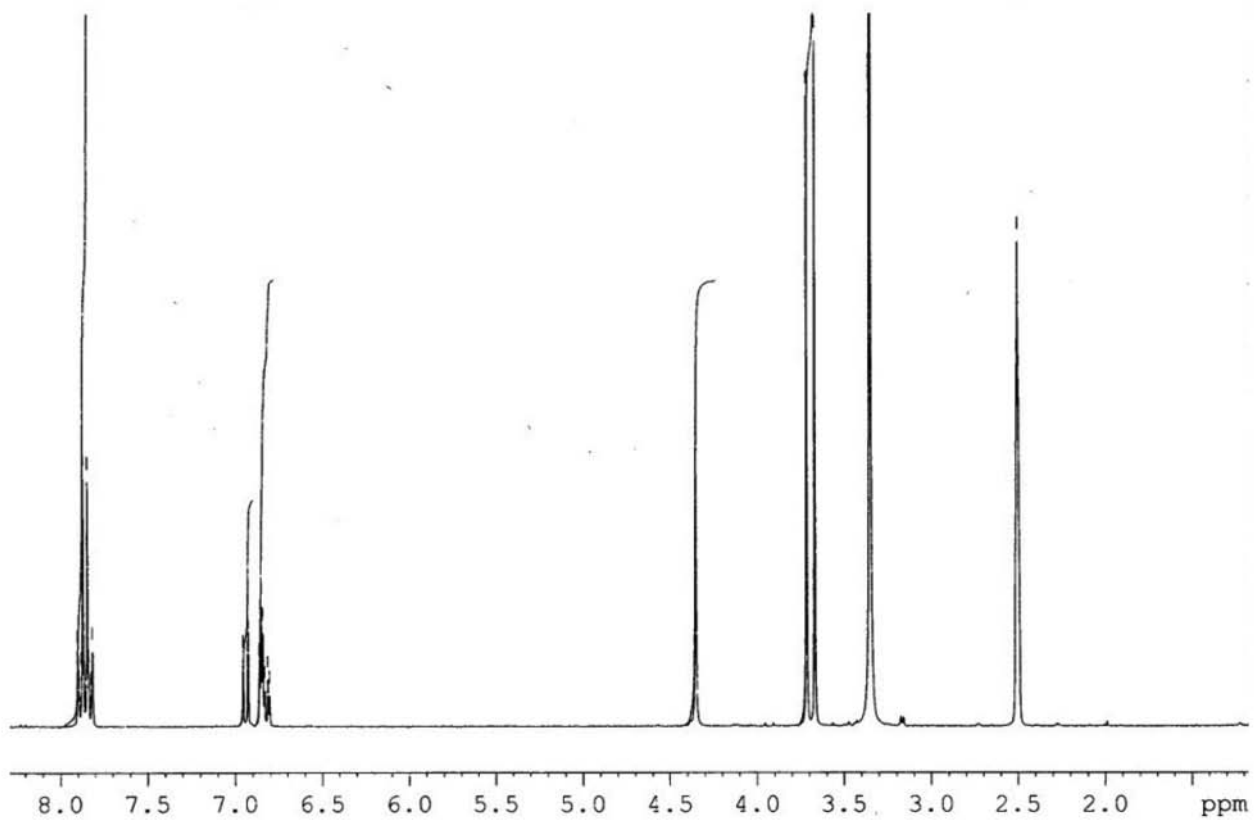

Figure S63. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6k**.

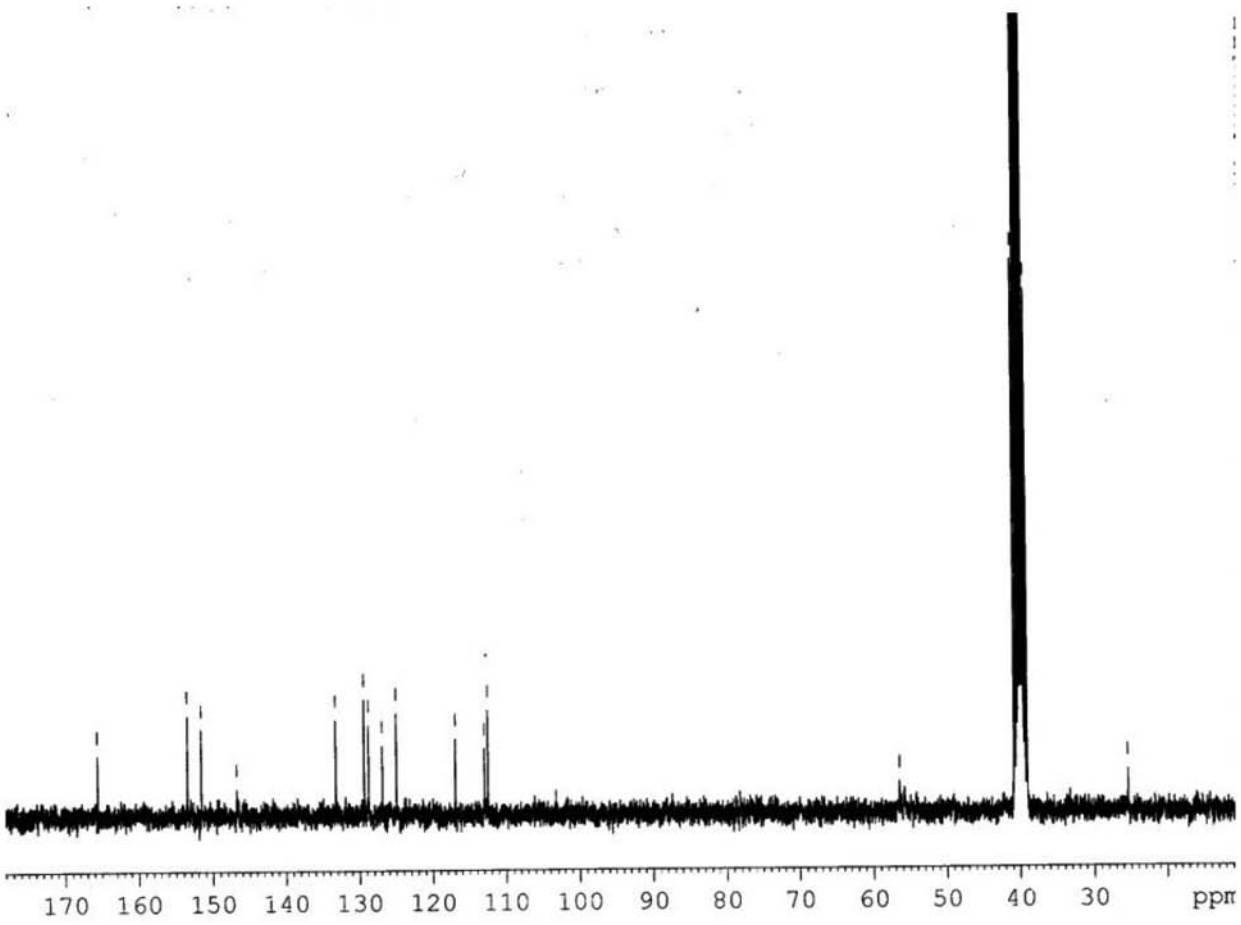

Figure S64. [13] C NMR (75 MHz, DMSO-d_6) spectrum of **6k**.

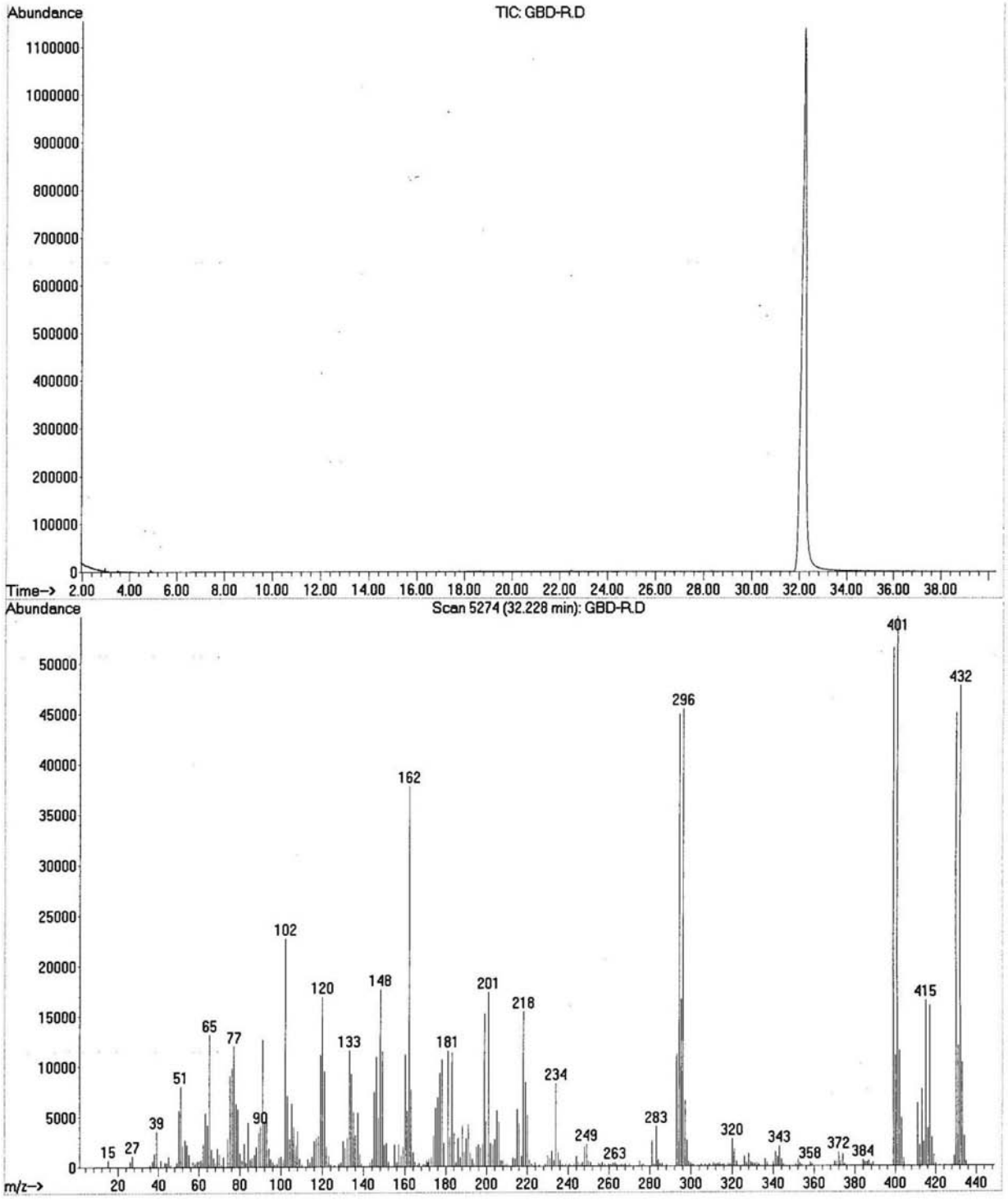

Figure S65. GC MS spectrum of **6k**.

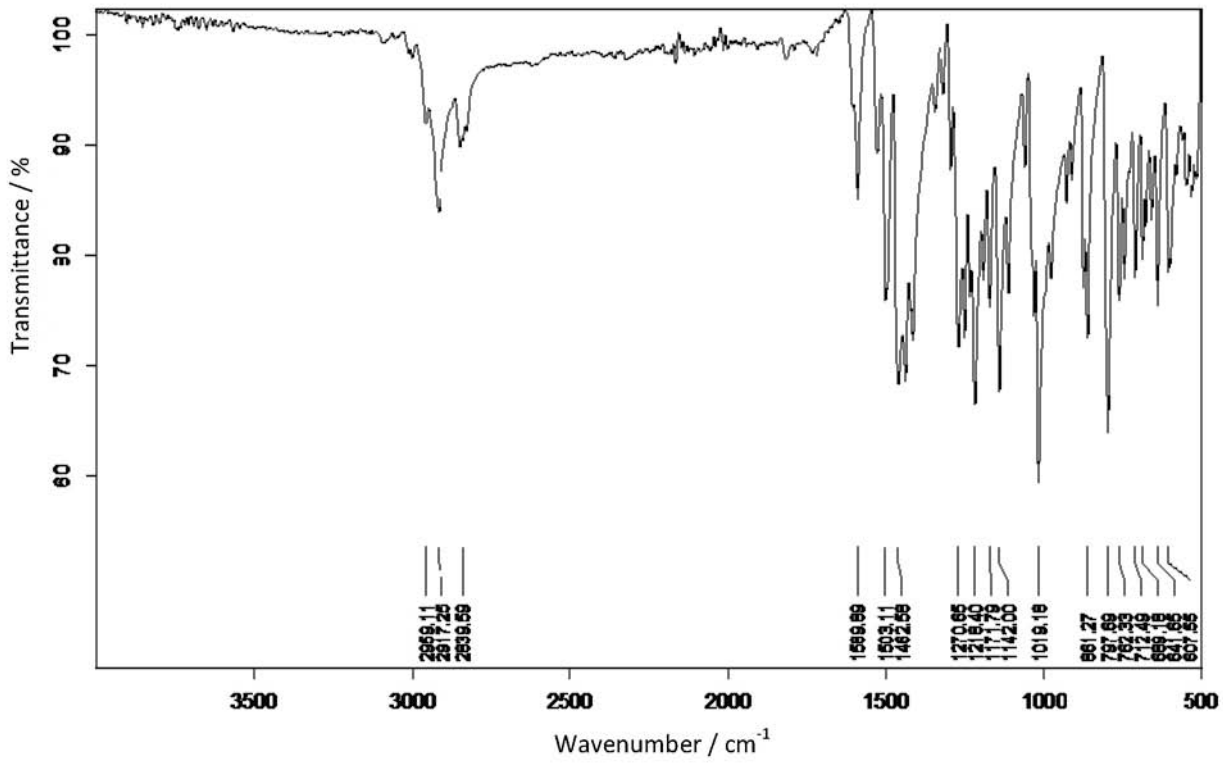

Figure S66. IR (neat) spectrum of **6l**.

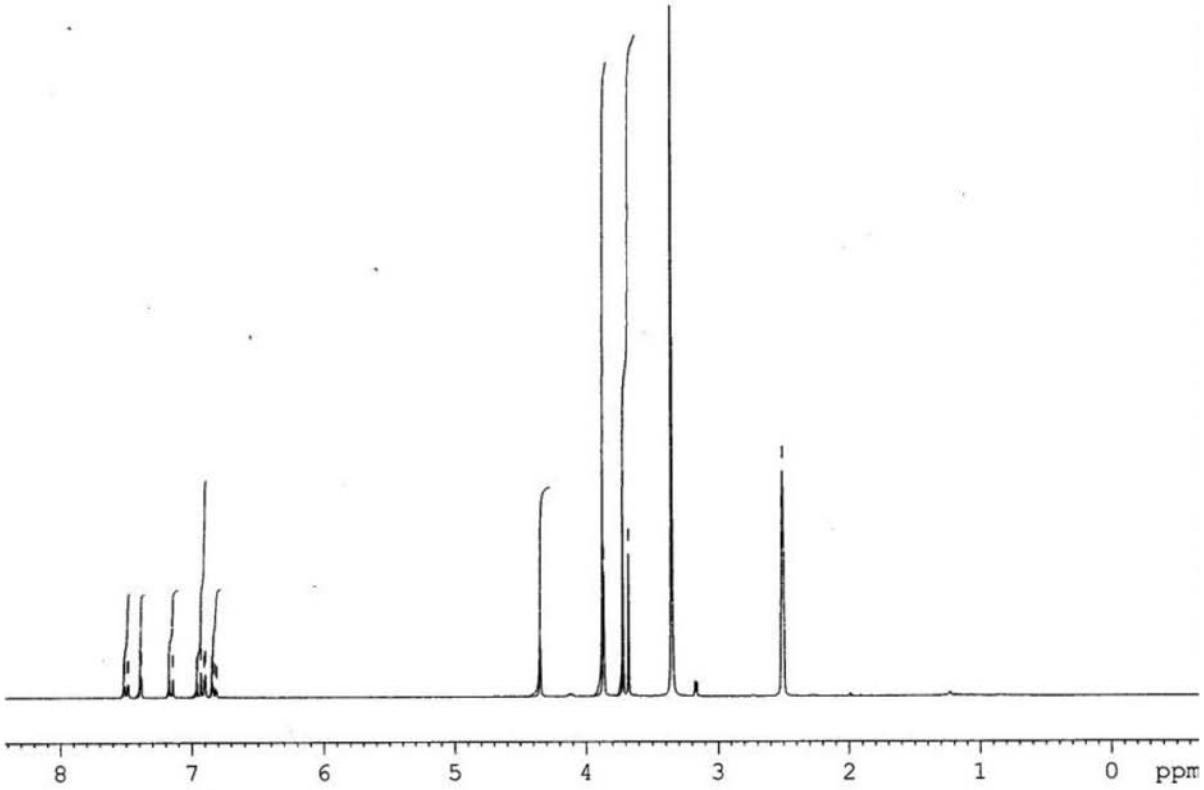

Figure S67. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6l**.

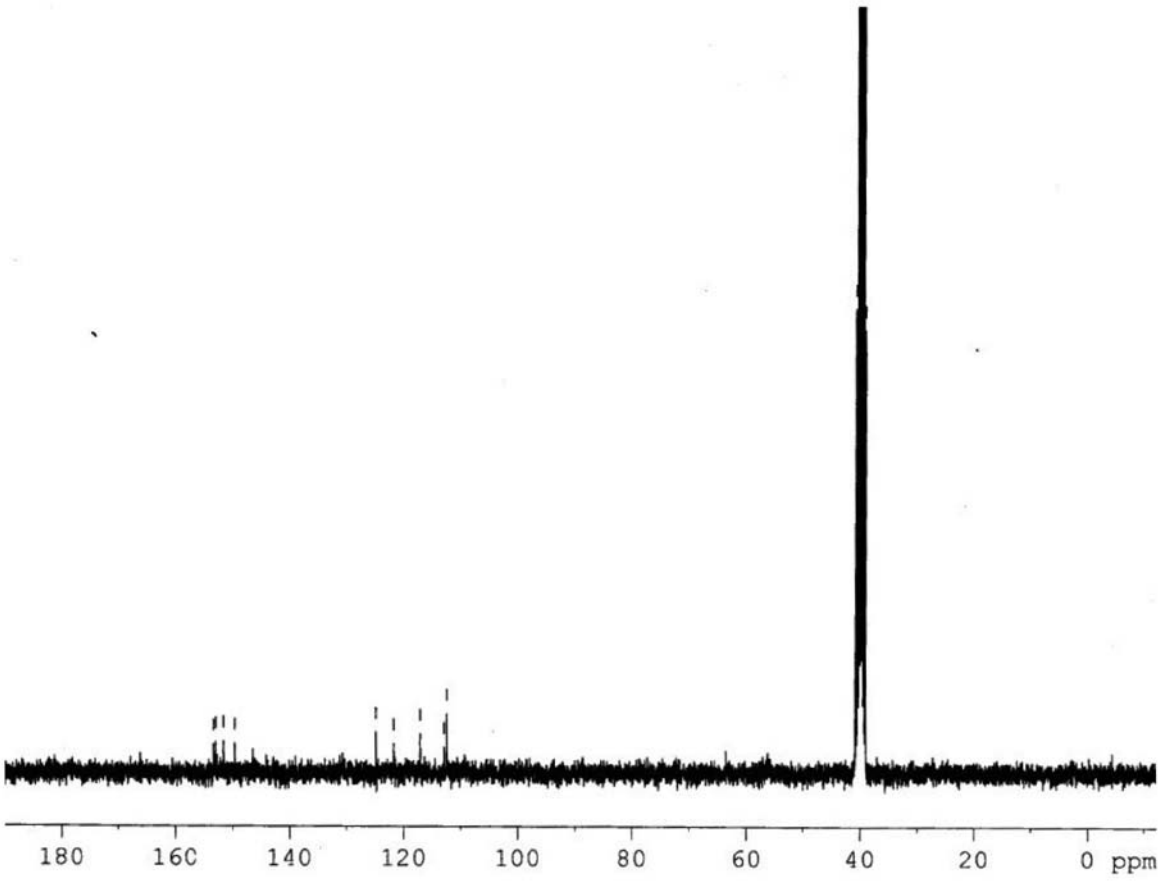

Figure S68. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6l**.

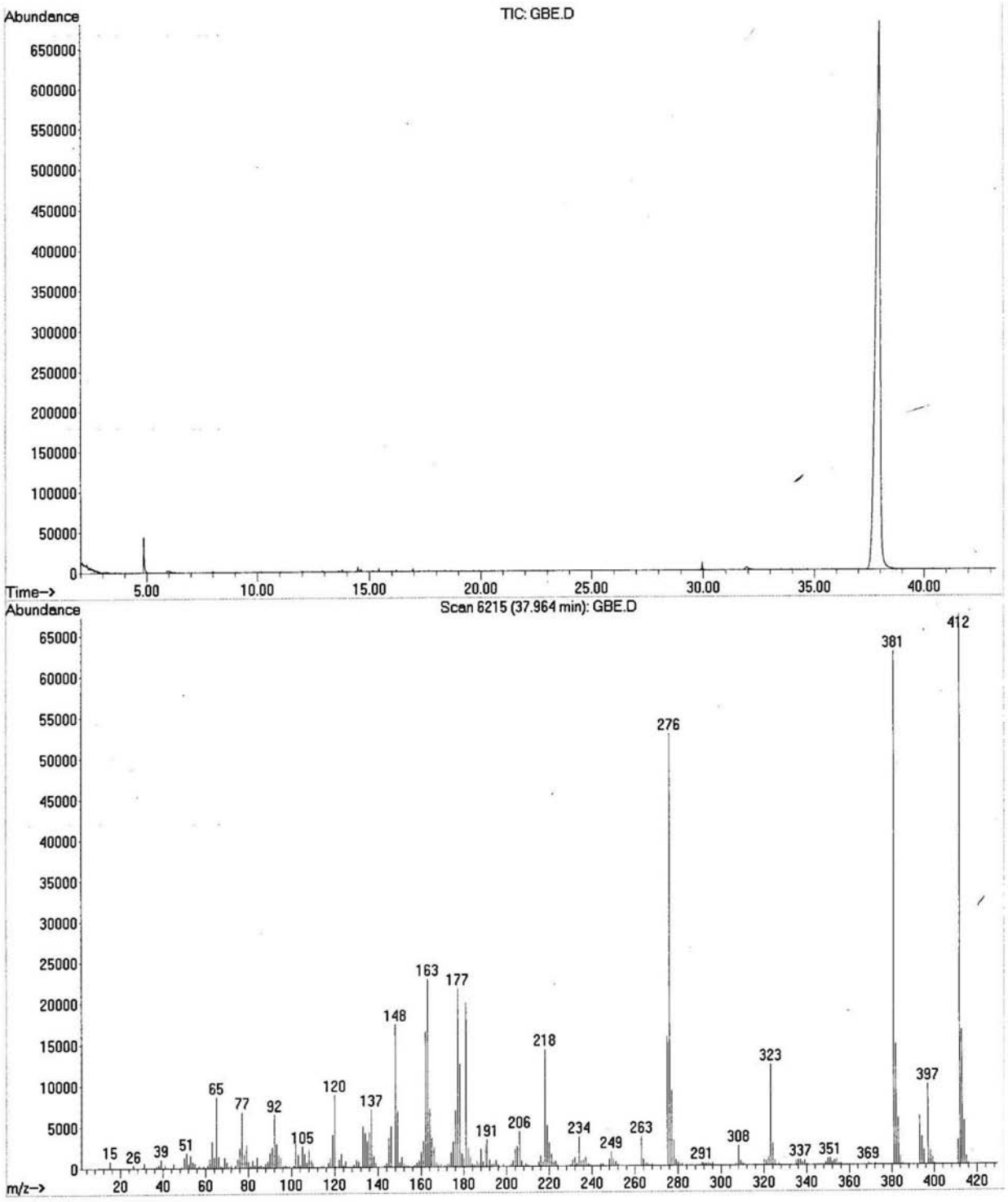

Figure S69. GC MS spectrum of **6l.**

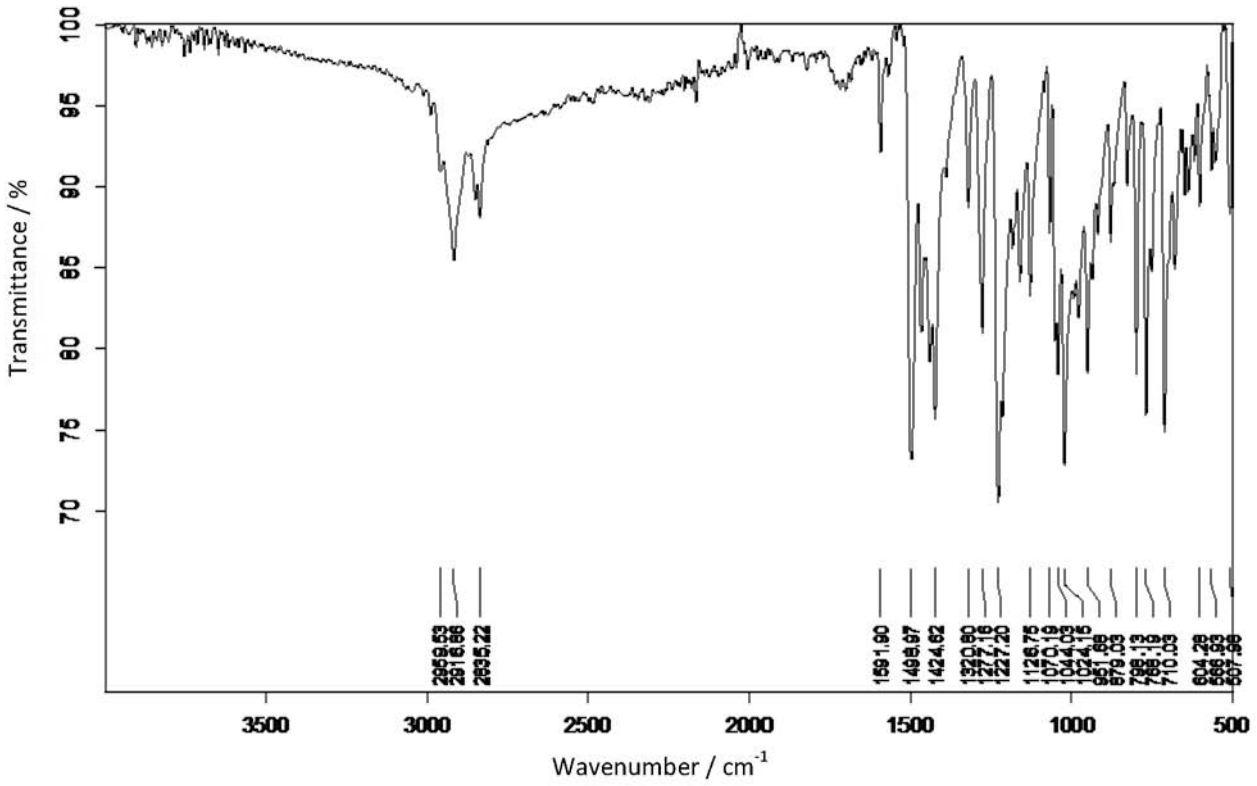

Figure S70. IR (neat) spectrum of **6n**.

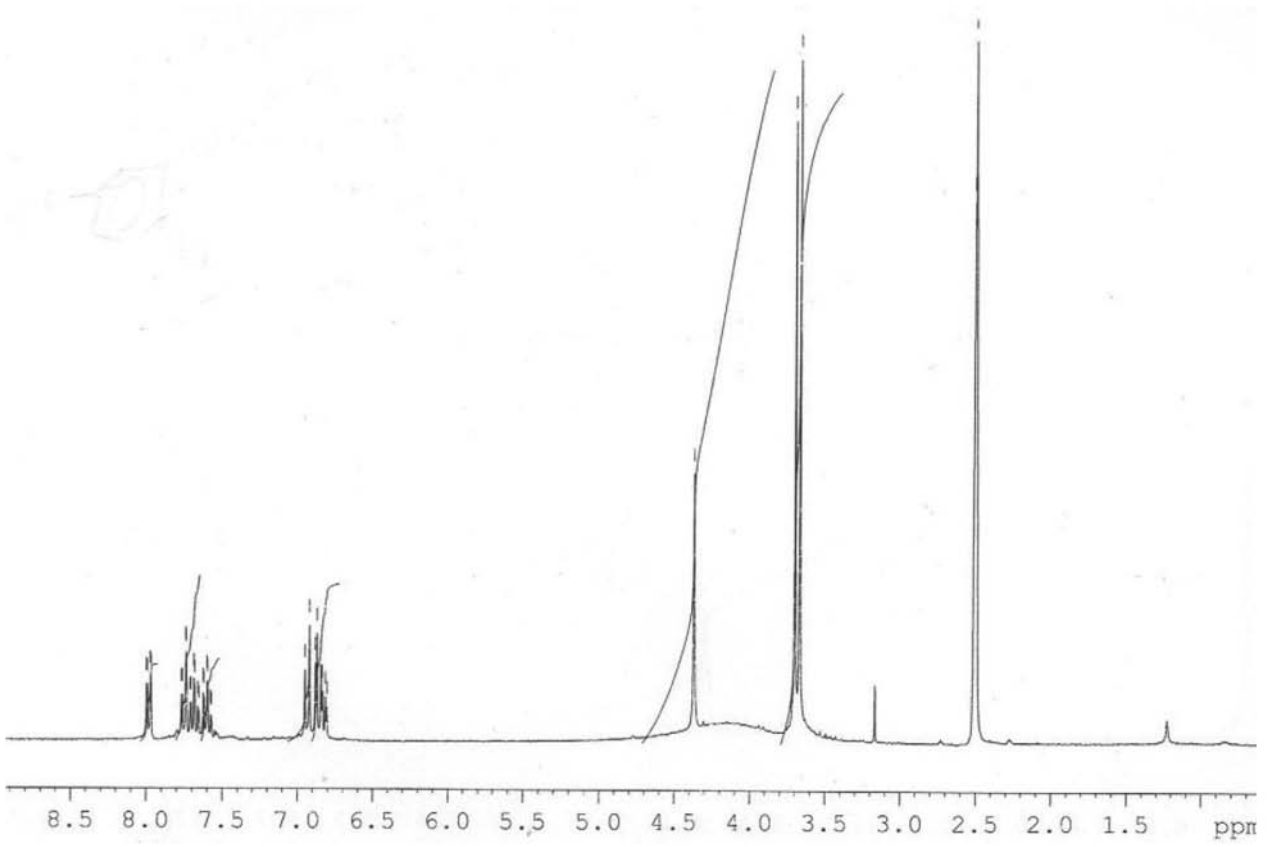

Figure S71. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6n**.

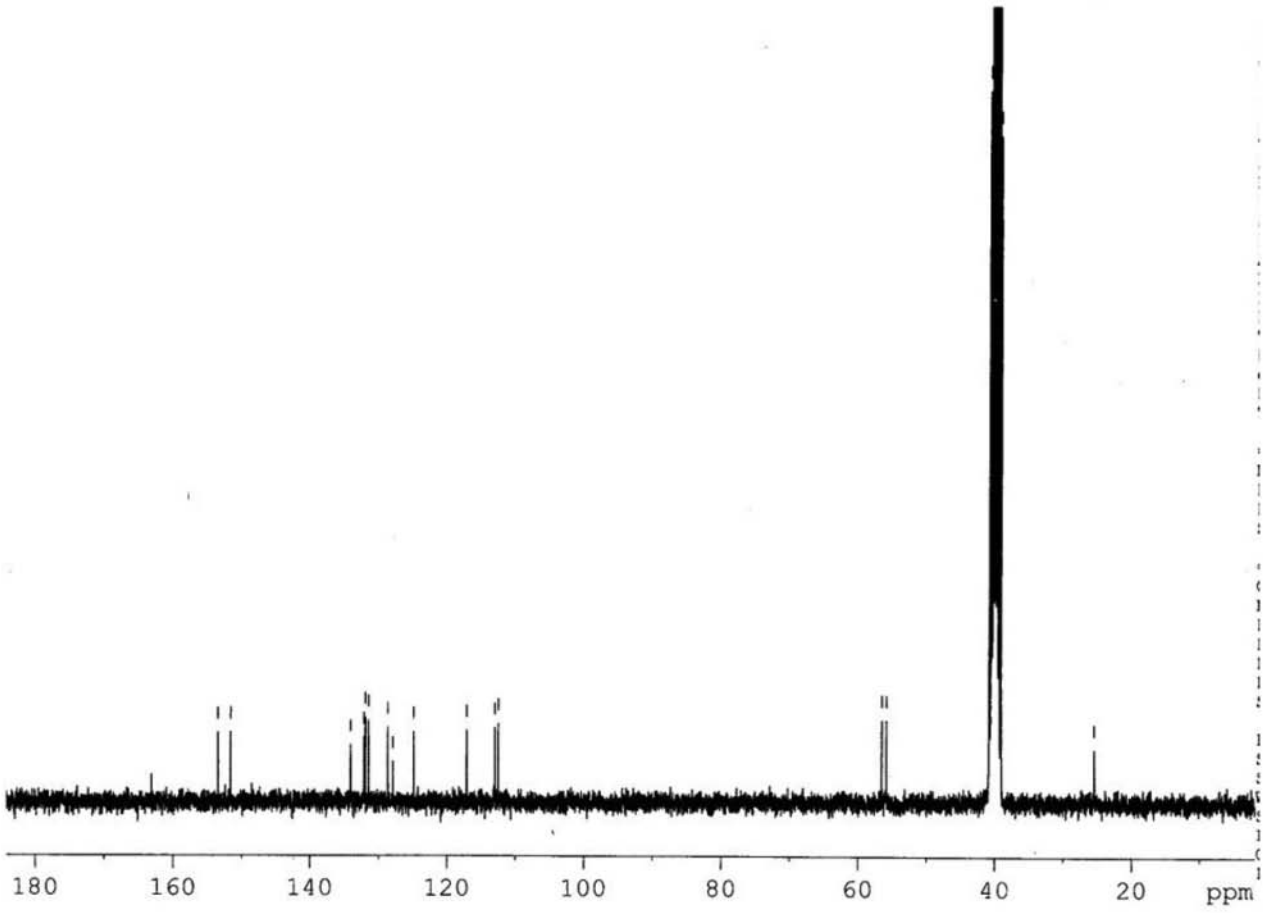

Figure S72. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of **6n**.

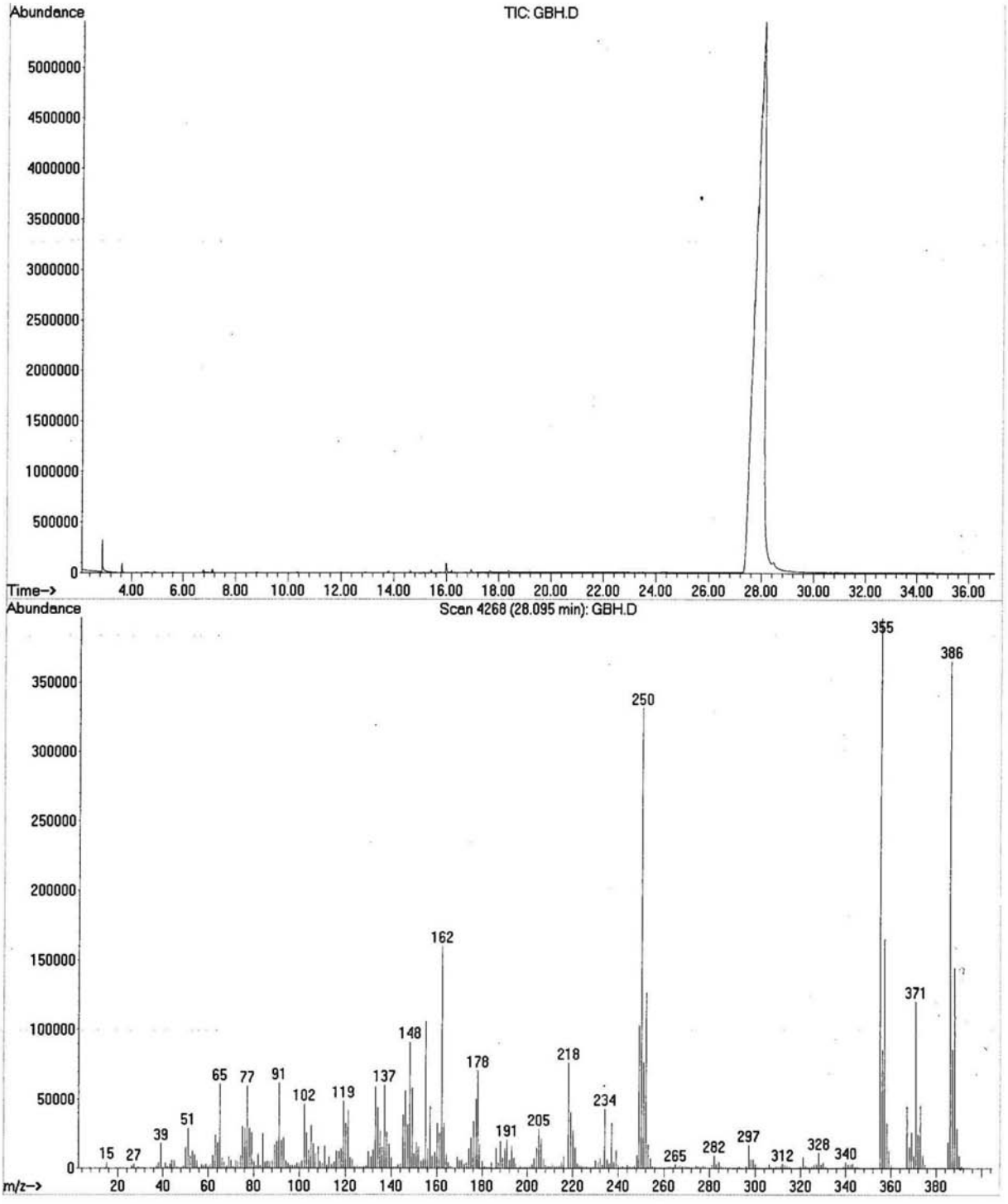

Figure S73. GC MS spectrum of **6n**.

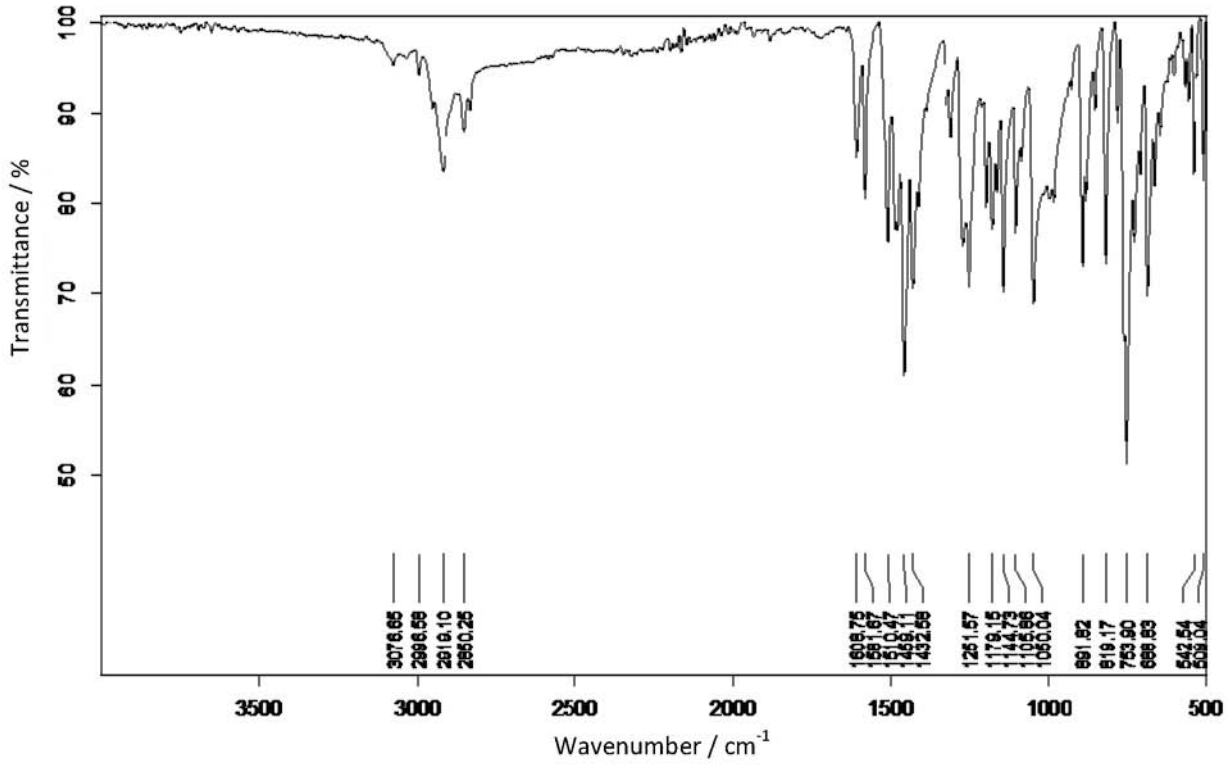

Figure S74. IR (neat) spectrum of **6o**.

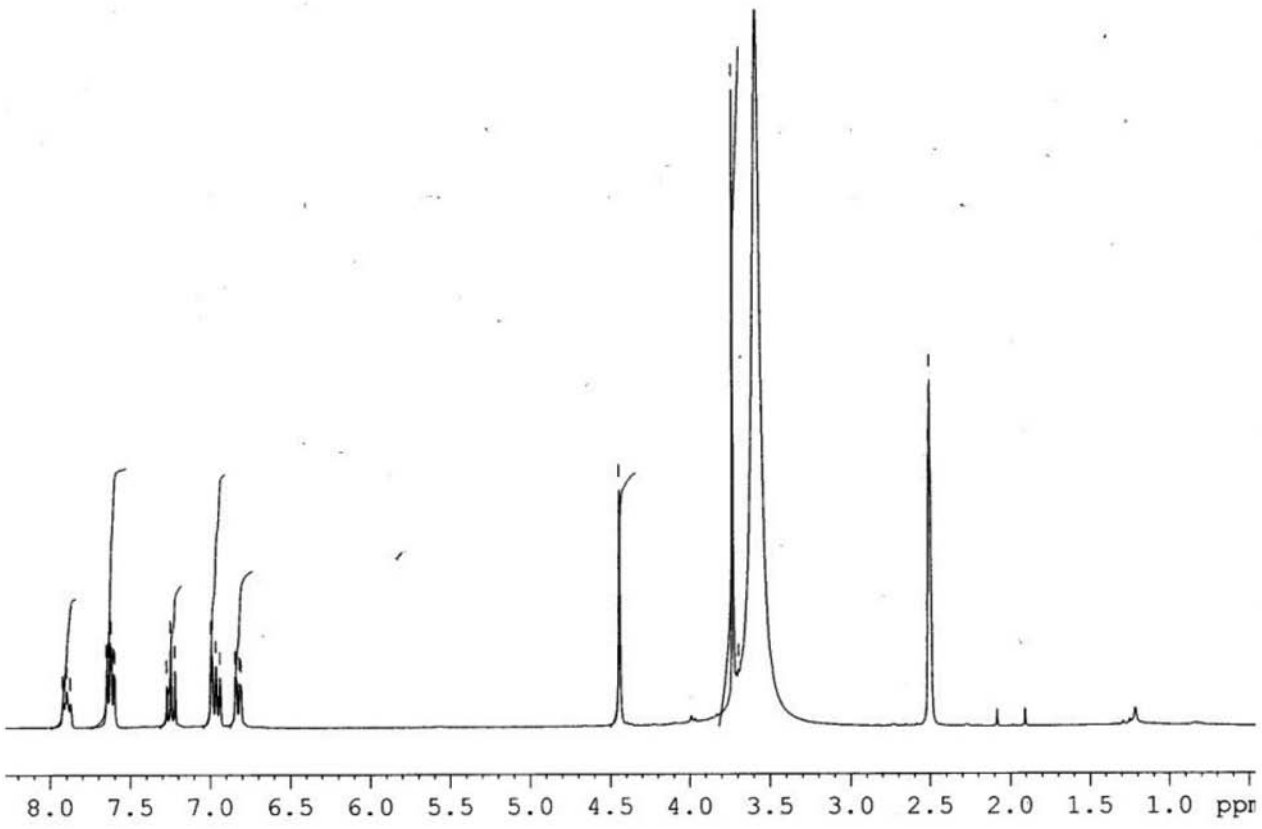

Figure S75. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of **6o**.

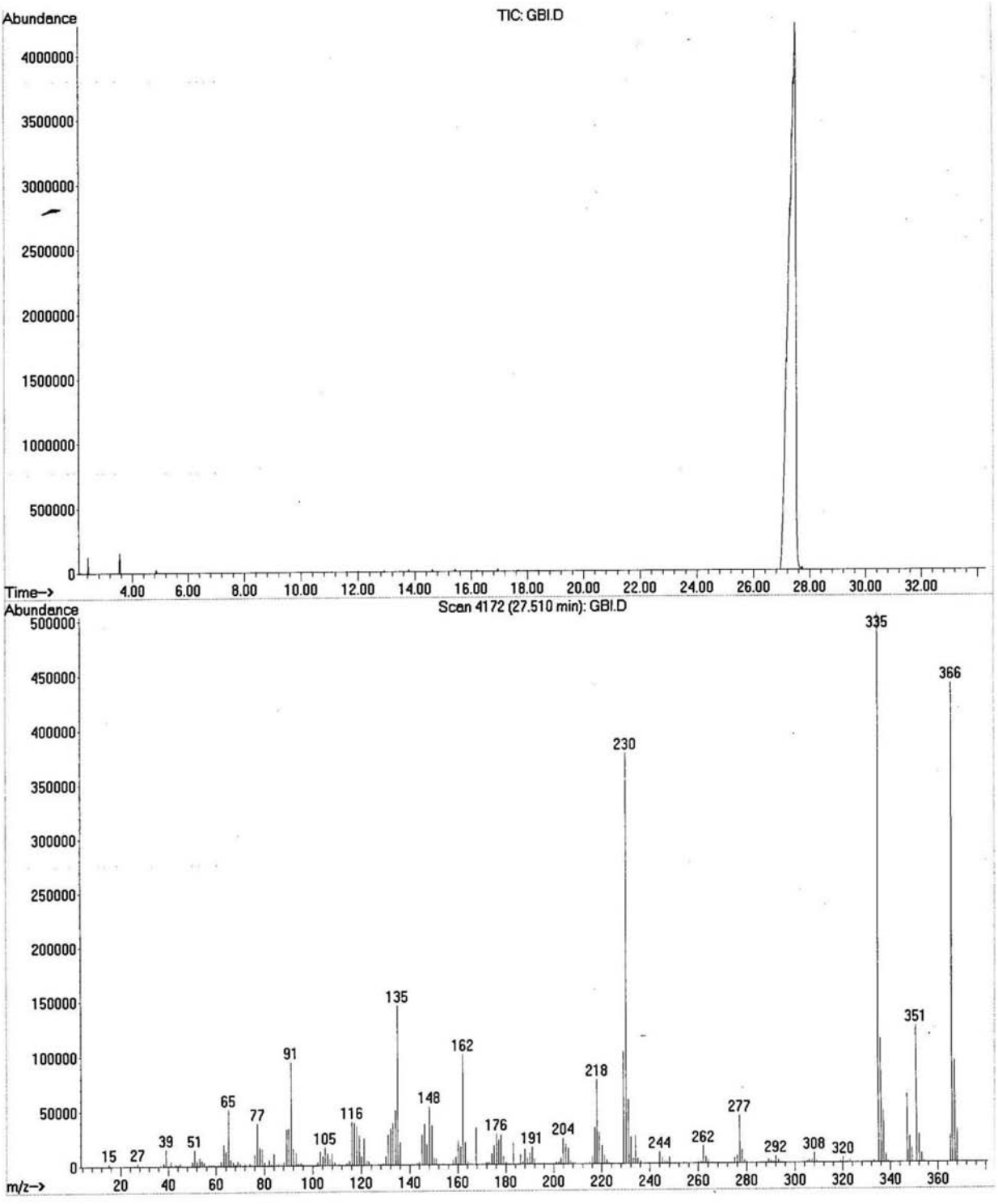

Figure S76. GC MS spectrum of **6o**.