Discovery of diazahexa/hepta cyclic cage-like systems compounds with broad-spectrum antifungal activity against human fungal pathogens

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Supporting information

Hexacyclic compound **5a**: Pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.86 (dd, *J*=14.6, 5.1 Hz, 1H), 3.01 (d, *J*=12.4 Hz, 1H), 3.15 (dd, *J*=13.9, 3.6 Hz, 1H), 3.40 (d, *J*=17.6 Hz, 1H), 3.68 (dd, *J*=17.6, 2.2 Hz, 1H), 4.21-4.35 (m, 3H), 6.30 (s, 1H), 6.37 (d, *J*=7.3 Hz, 1H), 6.43 (d, *J*=6.6 Hz, 1H), 7.03-7.62 (m, 19H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 37.8, 51.2, 53.0, 56.8, 62.0, 72.8, 90.3, 103.8, 120.9, 121.4, 125.5, 125.8, 127.1, 127.4, 127.8, 127.9, 128.4, 128.8, 128.9, 129.1, 129.6, 130.1, 130.4, 132.9, 133.9, 136.1, 136.4, 136.8, 138.9, 140.9, 196.7. MS (EI, 70 eV): *m/z* 560.7 (M^+); Anal. Calcd for $C_{39}H_{32}N_2O_2$: C, 83.54; H, 5.75; N, 5.00%; Found: C, 83.66; H, 5.84; N, 5.14%.

*Hexacyclic compound (***5b*)**:** Pale yellow solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.79-2.87 (m, 1H), 3.13 (d, *J*=12.2 Hz, 1H), 3.31 (d, *J*=11.0 Hz, 1H), 3.42 (d, *J*=17.6 Hz, 1H), 3.67 (d, *J*=17.6 Hz, 1H), 4.05-4.12 (m, 1H), 4.58 (d, *J*=10.2 Hz, 1H), 4.92 (d, *J*=9.5 Hz, 1H), 5.85 (brs, 1H, OH), 6.56 (s, 1H), 6.94-7.72 (m, 19H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 40.1, 52.2, 52.6, 57.3, 60.5, 65.6, 73.8, 90.7, 103.4, 121.3, 121.5, 123.8, 125.8, 126.5, 127.5, 127.7, 128.8, 129.1, 129.2, 129.7, 130.8, 132.5, 133.8, 134.4, 134.5, 135.1, 136.2, 136.5, 137.3, 138.9, 140.6, 171.3, 195.4 ppm; MS (EI, 70 eV): *m/z* 718.6 (M^+); Anal. Calcd for $C_{39}H_{30}Br_2N_2O_2$: C, 65.20; H, 4.21; N, 3.90%; Found: C, 65.33; H, 4.35; N, 3.81%.

Hexacyclic compounds **(5c):** Pale yellow solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.82-2.87 (m, 1H), 2.96 (d, *J* = 11.8 Hz, 1H), 3.12 (d, *J* = 11.8, 1H), 3.32 (d, *J* = 16.8 Hz, 1H), 3.62 (d, *J* = 16.8 Hz, 1H), 4.15-4.30 (m, 3H), 6.17 (s, 1H), 6.21-7.61 (m, 19H, Ar-H). ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 37.7, 50.5, 52.9, 56.6, 61.8, 72.6, 90.2, 103.8, 120.9, 121.4, 121.5, 122.9, 125.6, 125.9, 127.2, 128.1, 128.5, 129.0, 130.0, 130.4, 130.8, 130.9, 131.2, 131.9, 131.9, 132.7, 133.5, 134.7, 135.4, 135.7, 136.0, 136.1, 138.7,140.7, 196.4 ppm; MS (EI, 70 eV): *m/z* 718.9 (M^+); Anal. Calcd for $C_{39}H_{30}Br_2N_2O_2$: C, 65.20; H, 4.21; N, 3.90; Found: C, 65.31; H, 4.33; N, 3.83.

*Hexacyclic compound (***5d*)**:** Pale yellow solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.84 (dd, *J*=13.9, 6.6 Hz, 1H), 3.10 (dd, *J*=14.7, 3.6 Hz, 1H), 3.28 (d, *J*=12.5 Hz, 1H), 3.42 (d, *J*=17.6 Hz, 1H), 3.67 (dd, *J*=17.6, 2.2 Hz, 1H), 4.08-4.12 (m, 1H), 4.58 (d, *J*=11.7 Hz, 1H), 4.88 (d, *J*=11.0 Hz, 1H), 5.97 (d, *J*=7.3 Hz, 1H, NH), 6.55 (s, 1H), 6.89-7.74 (m, 19H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 39.4, 49.0, 52.5, 57.5, 73.8, 90.6, 103.5, 121.2, 121.4, 125.8, 126.5, 126.8, 126.9, 128.1, 128.7, 128.8, 129.3, 129.6, 130.7, 131.1, 132.5, 132.7, 134.0, 134.2, 134.8, 136.2, 136.8,

138.8, 140.5, 195.6 ppm; MS (EI, 70 eV): *m/z* 629.6 (M^+); Anal. Calcd for $C_{39}H_{30}Cl_2N_2O_2$: C, 74.40; H, 4.80; N, 4.45%; Found: C, 74.51; H, 4.95; N, 4.58%.

*Hexacyclic compound (**5e**)*: Pale yellow solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.82-2.86 (m, 1H), 3.06 (d, *J*=13.2 Hz, 1H), 3.21 (d, *J*=11.7 Hz, 1H), 3.35 (d, *J*=17.6, 1H), 3.63 (d, *J*=17.0 Hz, 1H), 4.06-4.10 (m, 1H), 4.51 (d, *J*=11.7 Hz, 1H), 4.78 (d, *J*=9.6 Hz, 1H), 5.89 (d, *J*=7.3 Hz, 1H, NH), 6.42 (s, 1H), 6.89-7.70 (m, 17H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 39.3, 52.4, 57.3, 60.5, 73.8, 90.5, 103.5, 121.3, 121.5, 125.8, 126.4, 126.5, 127.0, 127.2, 128.2, 128.8, 129.2, 129.4, 130.0, 130.6, 130.7, 130.9, 131.5, 133.4, 133.7, 134.6, 134.8, 136.1, 136.4, 136.9, 138.7, 140.2, 195.3ppm; MS (EI, 70 eV): *m/z* 698.5 (M^+); Anal. Calcd for $C_{39}H_{28}Cl_4N_2O_2$: C, 67.06; H, 4.04; N, 4.01%; Found: C, 67.19; H, 4.16; N, 4.13%.

*Hexacyclic compound (**5f**)*: Pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.85 (dd, *J*=13.9, 4.4 Hz, 1H), 2.97 (d, *J*=11.7 Hz, 1H), 3.13 (dd, *J*=13.9, 3.7 Hz, 1H), 3.34 (d, *J*=17.6 Hz, 1H), 3.64 (d, *J*=16.8 Hz, 1H), 4.17-4.28 (m, 3H), 6.19 (s, 1H), 6.28 (d, *J*=8.8 Hz, 2H), 6.38 (d, *J*=6.6 Hz, 1H), 7.01-7.61 (m, 16H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 37.7, 50.5, 53.1, 56.8, 61.9, 72.8, 90.4, 103.8, 120.9, 121.5, 125.6, 125.8, 127.2, 128.1, 128.2, 128,5, 129.0, 130.0, 130.4, 130.8, 132.3, 133.3, 133.6, 134.5, 135.2, 136.0, 138.8, 140.8, 196.6 ppm; MS (EI, 70 eV): *m/z* 629.6 (M^+); Anal. Calcd for $C_{39}H_{30}Cl_2N_2O_2$: C, 74.40; H, 4.80; N, 4.45%; Found: C, 74.54; H, 4.91; N, 4.58%.

*Hexacyclic compound (**5g**)*: Pale yellow solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.20 (s, 3H, CH_3), 2.39 (s, 3H, CH_3), 2.85 (dd, *J*=14.7, 5.2 Hz, 1H), 3.00 (d, *J*=11.7 Hz, 1H), 3.14 (dd, *J*=14.7, 3.7 Hz, 1H), 3.39 (d, *J* =17.6 Hz, 1H), 3.66 (d, *J*=16.8 Hz, 1H), 4.19 (d, *J*= 11.0 Hz, 1H), 4.25-4.33 (m, 2H), 6.09 (s, 1H), 6.17 (d, *J*=7.3 Hz, 1H), 6.26 (s, 1H), 6.43 (d, *J*=6.6 Hz, 1H), 6.88-7.61 16H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 21.3, 21.8, 37.9, 51.2, 53.0, 56.9, 62.0, 72.7, 90.4, 103.8, 120.9, 121.4, 125.4, 125.7, 125.8, 126.4, 127.0, 127.7, 127.9, 128.4, 128.6,128.9, 129.2, 130.1, 130.2, 130.5, 132.9, 133.9, 136.1, 136.3, 136.5, 136.7, 137.4, 138.3, 138.9, 141.0, 196.8 ppm; MS (EI, 70 eV): *m/z* 588.8 (M^+); Anal. Calcd for $C_{41}H_{36}N_2O_2$: C, 83.64; H, 6.16; N, 4.76%; Found: C, 83.55; H, 6.32; N, 4.85%.

*Hexacyclic compound (**5h**)*: Pale yellow solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.21 (s, 3H, CH_3), 2.35 (s, 3H, CH_3), 2.85 (dd, *J*=14.7, 5.1 Hz, 1H), 3.00 (d, *J*=12.5 Hz, 1H), 3.15 (dd, *J*=14.7, 3.7 Hz, 1H), 3.40 (d, *J* =17.6 Hz, 1H), 3.70 (d, *J*=17.6 Hz, 1H), 4.20-4.32 (m, 3H), 6.32 (d, *J*=7.3 Hz, 2H), 6.42 (d, *J*=6.6 Hz, 1H), 6.86 (d, *J*=8.1 Hz, 2H), 7.16-7.59 (m, 15H, Ar-H) ppm; ^{13}C NMR

(100 MHz, $CDCl_3$) δ_C: 21.2, 21.4, 37.8, 50.8, 52.9, 56.5, 61.9, 72.5, 90.1, 103.8, 121.0, 121.4, 125.6, 125.7, 127.0, 127.9, 128.4, 128.7, 128.9, 129.5, 129.8, 130.1, 130.4, 131.2, 131.8, 133.7, 136.1, 136.3, 136.5, 137.0, 138.8, 140.9, 196.6 ppm; MS (EI, 70 eV): *m/z* 588.7 (M^+); Anal. Calcd for $C_{41}H_{36}N_2O_2$: C, 83.64; H, 6.16; N, 4.76%; Found: C, 83.56; H, 6.28; N, 4.87%.

*Hexacyclic compound (***5i***)*: Pale yellow solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.85 (dd, *J*=14.7, 5.1 Hz, 1H), 3.00 (d, *J*=12.5 Hz, 1H), 3.14 (dd, *J*=14.0, 3.7 Hz, 1H), 3.40 (d, *J*=17.6 Hz, 1H), 3.71 (s, 3H, OCH_3), 3.73 (m, 1H), 3.81 (s, 3H, OCH_3), 4.19-4.28 (m, 3H), 6.29 (s, 1H), 6.42-6.45 (m, 2H), 6.58 (d, *J*=8.8 Hz, 2H), 6.92 (d, *J*=8.8 Hz, 2H), 7.16-7.60 (m, 13H, Ar-H) ppm;^{13}C NMR (100 MHz, $CDCl_3$): δ_C 37.8, 50.4, 53.2, 55.3, 55.4, 56.7, 62.0, 72.4, 90.2, 103.8, 113.4, 114.2, 120.9, 121.3, 125.5, 125.6, 126.8, 127.0, 127.9, 128.4, 128.8, 128.9, 130.0, 130.4, 131.8, 135.9, 136.1, 136.6, 139.0, 141.1, 158.8, 159.8, 196.8 ppm; MS (EI, 70 eV): *m/z* 620.9 (M^+); Anal. Calcd for $C_{41}H_{36}N_2O_4$: C, 79.33; H, 5.85; N, 4.51%; Found: C, 79.45; H, 5.76; N, 4.68%.

*Hexacyclic compound (***5j***)*: Pale yellow solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.91-2.98 (m, 1H), 3.12 (dd, *J*=14.0, 3.7 Hz, 1H), 3.26 (d, *J*=16.9 Hz, 1H), 3.63 (d, *J*=17.6 Hz, 1H), 4.09-4.12 (m, 1H), 4.28-4.39 (m, 3H), 6.15 (s, 1H), 6.50 (d, *J*=6.6 Hz, 1H), 6.63 (d, *J*=7.4 Hz, 1H), 7.02-8.41 (m, 17H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 38.1, 50.9, 52.8, 56.8, 60.5, 61.9, 73.1, 90.3, 103.9, 121.0, 121.6, 122.5, 122.9, 123.8, 124.1, 125.6, 126.2, 127.3, 128.1, 128.7, 128.9, 129.1, 129.7, 129.9, 130.5, 133.1, 134.4, 135.2, 135.3, 135.6, 135.8, 136.0, 138.4, 138.9, 140.4, 147.6, 148.6, 196.3 ppm; MS (EI, 70 eV): *m/z* 650.7 (M^+); Anal. Calcd for $C_{39}H_{30}N_4O_6$: C, 71.99; H, 4.65; N, 8.61%; Found: C, 71.87; H, 4.75; N, 8.78%.

Heptacyclic compound **6a**: Colorless crystals. ^{1}H NMR (300 MHz, $CDCl_3$) δ_H: 2.62 (d, *J*=13.2, 6.3 Hz, 1H), 2.89-2.94 (m, 1H), 3.04 (d, *J*=12.6 Hz, 1H), 3.19 (d, *J*=17.4 Hz, 1H), 3.62 (dd, *J*=17.4, 2.7 Hz 1H), 3.95 (d, *J*=7.2 Hz, 1H), 4.11 (d, *J*=7.5 Hz, 1H), 4.14-4.17 (m, 2H), 4.32 (dd, *J*=12.6, 2.4 Hz, 1H), 6.30 (m, *J*=6.0 Hz, 2H), 6.42 (s, 1H), 6.96-7.61 (m, 19H, Ar-H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ_C: 41.6, 50.7, 52.4, 57.5, 70.3, 70.6, 87.4, 95.8, 100.1, 116.2, 121.9, 122.3, 125.1, 126.3, 126.4, 127.4, 127.6, 127.8, 128.1, 128.4, 128.6, 128.8, 129.3, 129.4, 130.1, 130.4, 133.6, 134.0, 134.5, 136.7, 136.9, 138.7, 139.3, 195.9 ppm; MS (EI, 70 eV): *m/z* 572.8 (M^+); Anal. Calcd for $C_{40}H_{32}N_2O_2$: C, 83.89; H, 5.63; N, 4.89%; Found: C, 83.75; H, 5.54; N, 4.98%.

*Heptacyclic compound (***6b***)*: White solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.65-2.71 (m, 1H), 2.95 (d, *J*=13.2 Hz, 1H), 3.08 (d, *J*=12.4 Hz, 1H), 3.20 (d, *J*=17.6 Hz, 1H), 3.64 (dd, *J*= 17.6, 2.2 Hz 1H), 4.03 (d, *J*=8.1 Hz, 1H), 4.11 (d, *J*=7.4 Hz, 1H), 4.14-4.21 (m, 2H), 4.34 (d, *J*=11.0 Hz, 1H),

6.22 (d, *J*=8.8 Hz, 2H), 6.37 (s, 1H), 7.08-7.68 (m, 17H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 41.5, 50.1, 52.4, 57.5, 60.5, 70.1, 70.5, 87.4, 95.8, 116.3, 121.5, 122.1, 122.3, 122.9, 125.3, 126.5, 127.9, 128.2, 128.9, 130.1, 130.9, 131.2, 131.8, 132.8, 134.3, 135.6, 135.7, 138.3, 138.7, 139.1, 195.7 ppm; MS (EI, 70 eV): *m/z* 730.5 (M^+); Anal. Calcd for $C_{40}H_{30}Br_2N_2O_2$: C, 65.77; H, 4.14; N, 3.83%; Found: C, 65.89; H, 4.25; N, 3.74%.

*Heptacyclic compound (***6c***)*: White solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.71-2.77 (m, 1H), 2.87 (m, 1H), 3.24 (d, *J*=17.6 Hz, 1H), 3.39 (d, *J*=12.5 Hz, 1H), 3.64 (dd, *J*=17.6, 2.2 Hz, 1H), 3.93-4.01 (m, 3H), 4.71 (d, *J*=11.8 Hz, 1H), 4.98 (d, *J*=11.0 Hz, 1H), 6.68 (s, 1H), 6.86 (t, *J*=7.3 Hz, 1H), 6.98-7.77 (m, 18H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 42.3, 47.3, 51.7, 57.8, 71.6, 73.0, 87.2, 95.8, 115.7, 122.0, 122.5, 125.6, 125.9, 126.3, 126.6, 126.9, 127.9, 128.3, 128.6, 128.9, 129.3, 129.4, 129.7, 130.7, 130.9, 132.7, 133.5, 133.7, 134.5, 134.9, 135.1, 136.6, 138.7, 138.9, 139.0, 194.7 ppm; MS (EI, 70 eV): *m/z* 641.7 (M^+); Anal. Calcd for $C_{40}H_{30}Cl_2N_2O_2$: C, 74.88; H, 4.71; N, 4.37%; Found: C, 74.95; H, 4.83; N, 4.48%.

*Heptacyclic compound (***6d***)*: White solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.69 (dd, *J*=13.2, 5.7 Hz, 1H), 2.95 (d, *J*=13.9 Hz, 1H), 3.08 (d, *J*=12.5 Hz, 1H), 3.21 (d, *J*=17.6 Hz, 1H), 3.64 (d, *J*=17.6 Hz, 1H), 4.03 (d, *J*=7.3 Hz, 1H), 4.17-4.22 (m, 3H), 4.93-5.0 (m, 1H), 6.29 (d, *J*=8.8 Hz, 1H), 6.39 (s, 1H), 7.00-7.67 (m, 18H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ_C 41.8, 52.5, 57.4, 60.7, 70.2, 70.5, 87.4, 95.6, 116.2, 121.4, 122.3, 125.4, 126.5, 128.2, 128.9, 130.1, 130.6, 130.7, 131.2, 131.9, 132.6, 134.1, 135.1, 135.6, 138.2, 138.6, 139.1, 195.8 ppm; MS (EI, 70 eV): *m/z* 641.8 (M^+); Anal. Calcd for $C_{40}H_{30}Cl_2N_2O_2$: C, 74.88; H, 4.71; N, 4.37%; Found: C, 74.97; H, 4.65; N, 4.46%.

*Heptacyclic compound (***6e***)*: White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.16 (s, 3H, CH_3), 2.42 (s, 3H, CH_3), 2.66-2.71 (m, 1H), 2.98 (d, *J*=13.2 Hz, 1H), 3.12 (d, *J*=12.4 Hz, 1H), 3.28 (d, *J*=17.6 Hz, 1H), 3.63-3.69 (dd, *J*=17.6, 2.2 Hz 1H), 4.02 (d, *J*=7.4 Hz, 1H), 4.17 (d, *J*=7.3 Hz, 1H), 4.21-4.24 (m, 2H), 4.40 (d, *J*=12.5 Hz, 1H), 6.10 (s, 1H), 6.19 (d, *J*=7.4 Hz, 1H), 6.47 (s, 1H), 6.88-7.69 (m, 18H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 21.3, 21.8, 41.7, 50.8, 52.5, 57.7, 70.5, 70.7, 87.4, 95.9, 116.3, 121.9, 122.3, 125.1, 125.9, 126.4, 127.7, 127.8, 128.1, 128.2, 128.5, 129.2, 130.2, 130.5, 133.7, 134.1, 134.6, 136.7, 137.1, 137.5, 138.2, 138.7, 138.8, 139.5, 196.0 ppm; MS (EI, 70 eV): *m/z* 600.9 (M^+); Anal. Calcd for $C_{42}H_{36}N_2O_2$: C, 83.97; H, 6.04; N, 4.66%; Found: C, 83.86; H, 6.17; N, 4.78%.

*Heptacyclic compound (***6f***)*: White solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.21 (s, 3H, CH_3), 2.36 (s, 3H, CH_3), 2.67 (dd, *J*=13.2, 5.84 Hz, 1H), 2.98 (d, *J*=12.5 Hz, 1H), 3.10 (d, *J*=12.4 Hz, 1H), 3.27 (d, *J*=17.6 Hz, 1H), 3.71 (d, *J*=17.6 Hz 1H), 4.01 (d, *J*=7.3 Hz, 1H), 4.14 (m, 3H), 4.37 (d, *J*=11.8 Hz, 1H), 6.34 (d, *J*=8.1 Hz, 1H), 6.52 (s, 1H), 6.86 (d, *J*=8.1 Hz, 1H), 7.10-7.65 (m, 17H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 21.2, 21.3, 41.7, 50.4, 52.5, 57.4, 70.4, 70.5, 87.5, 95.8, 116.3, 121.9, 122.4, 125.1, 126.3, 126.5, 127.7, 128.2, 128.7, 128.9, 129.1, 129.4, 129.8, 130.2, 130.4, 131.3, 132.6, 133.7, 137.0, 138.7, 138.8, 139.5, 196.0 ppm; MS (EI, 70 eV): *m/z* 600.8 (M^+); Anal. Calcd for $C_{42}H_{36}N_2O_2$: C, 83.97; H, 6.04; N, 4.66%; Found: C, 83.85; H, 6.15; N, 4.74%.

*Heptacyclic compound (***6g***)*: White solid.^{1}H NMR (400 MHz, $CDCl_3$) δ_H: 2.68 (dd, *J*=13.2, 7.3 Hz, 1H), 2.97 (d, *J*=13.2 Hz, 1H), 3.10 (d, *J*=12.5 Hz, 1H), 3.26 (d, *J*=16.8 Hz, 1H), 3.71 (s, 3H, OCH_3), 3.72-3.76 (m, 1H), 3.82 (s, 3H, OCH_3), 4.01 (d, *J*=7.3 Hz, 1H), 4.15-4.19 (m, 3H), 4.34 (d, *J*=11.8 Hz, 1H), 6.47 (d, *J*=8.8 Hz, 1H), 6.52 (s, 1H), 6.59 (d, *J*=8.8 Hz, 1H), 6.93 (d, *J*=8.8 Hz, 1H), 7.09-7.64 (m, 16H, Ar-H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ_C: 41.6, 49.9, 52.5, 55.3, 57.3, 70.4, 70.5, 87.5, 95.7, 113.5, 114.1, 116.3, 121.9, 122.3, 125.1, 126.3, 126.5, 126.8, 127.7, 128.2, 128.8, 128.9, 130.1, 130.2, 131.2, 131.8, 134.5, 136.8, 138.7, 138.8, 139.5, 158.8, 159.9, 196.0 ppm; MS (EI, 70 eV): *m/z* 632.9 (M^+); Anal. Calcd for $C_{42}H_{36}N_2O_4$: C, 79.72; H, 5.73; N, 4.43%; Found: C, 79.83; H, 5.61; N, 4.58%.

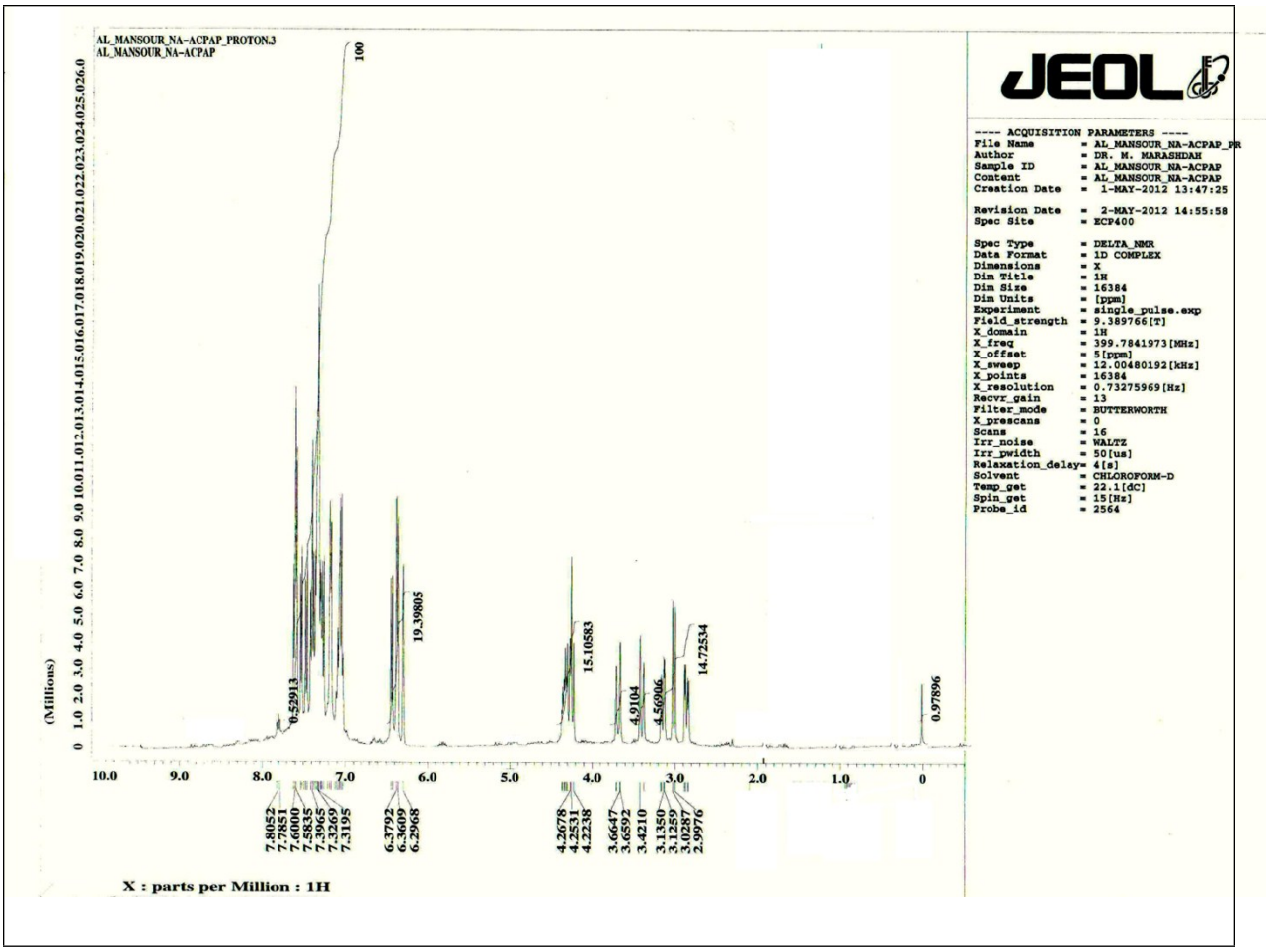

Figure 1. [1]H NMR spectrum of **5a**

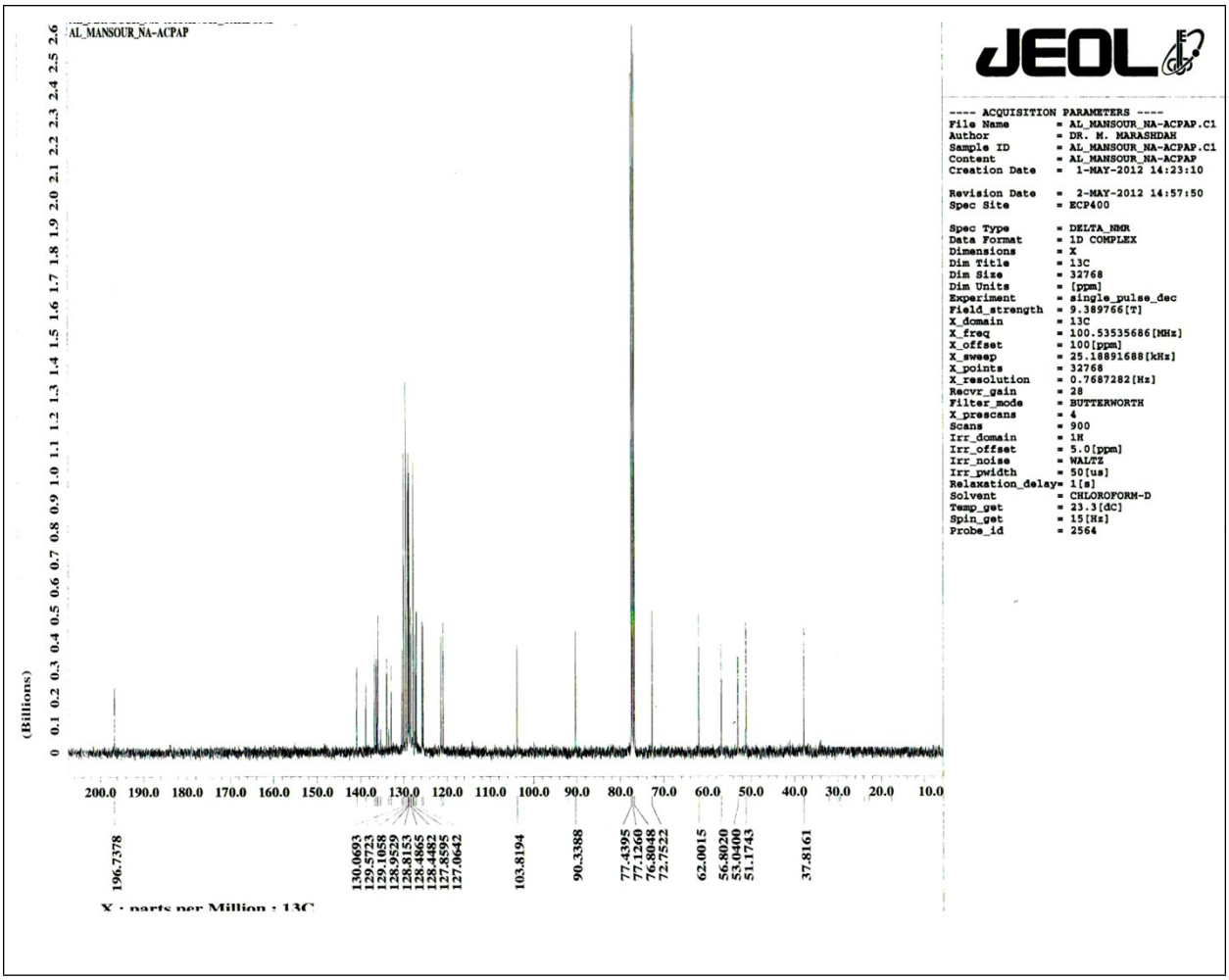

Figure 2. ^{13}C NMR spectrum of **5a**

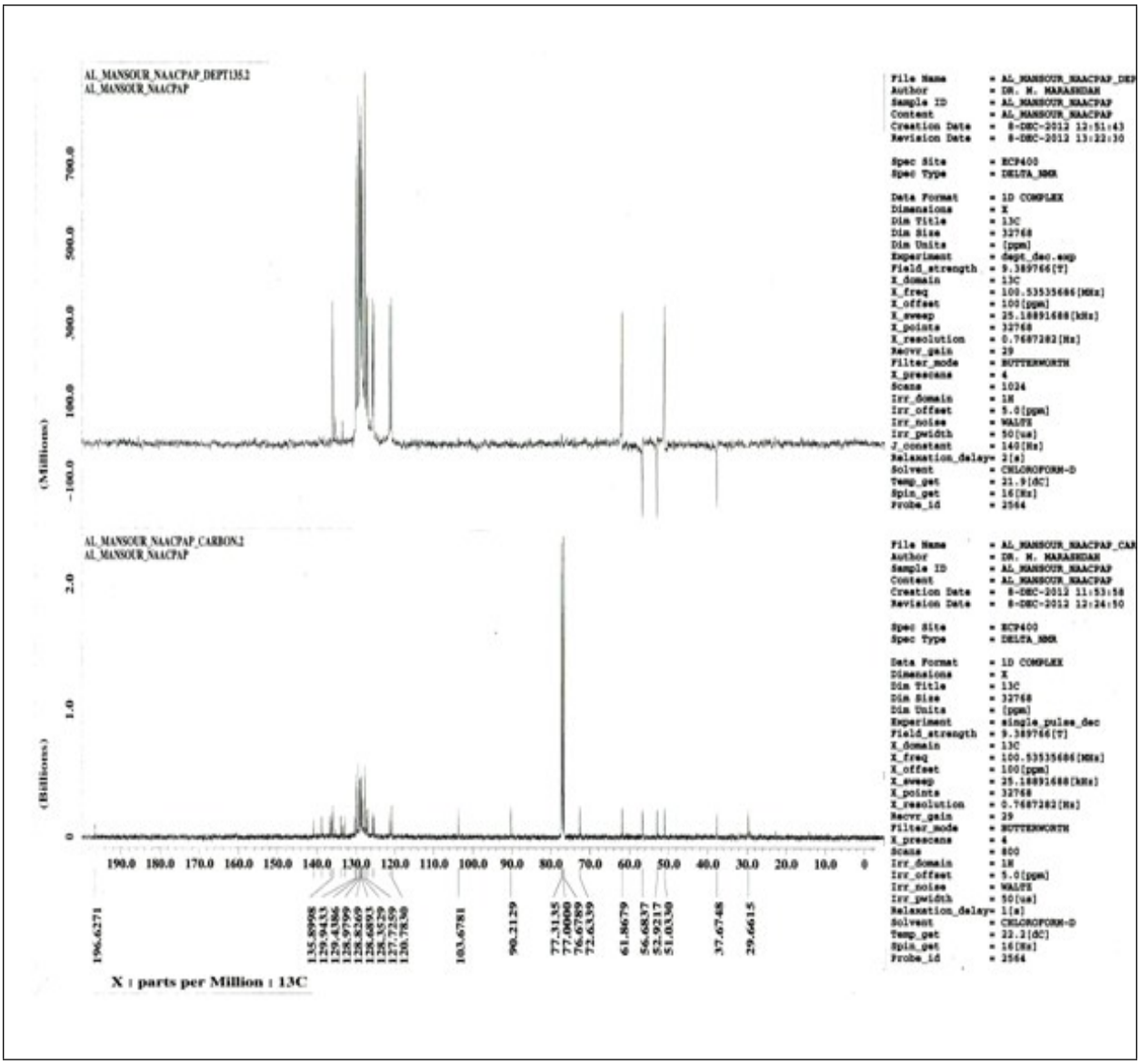

Figure 3. DEPT-135 spectrum of **5a**

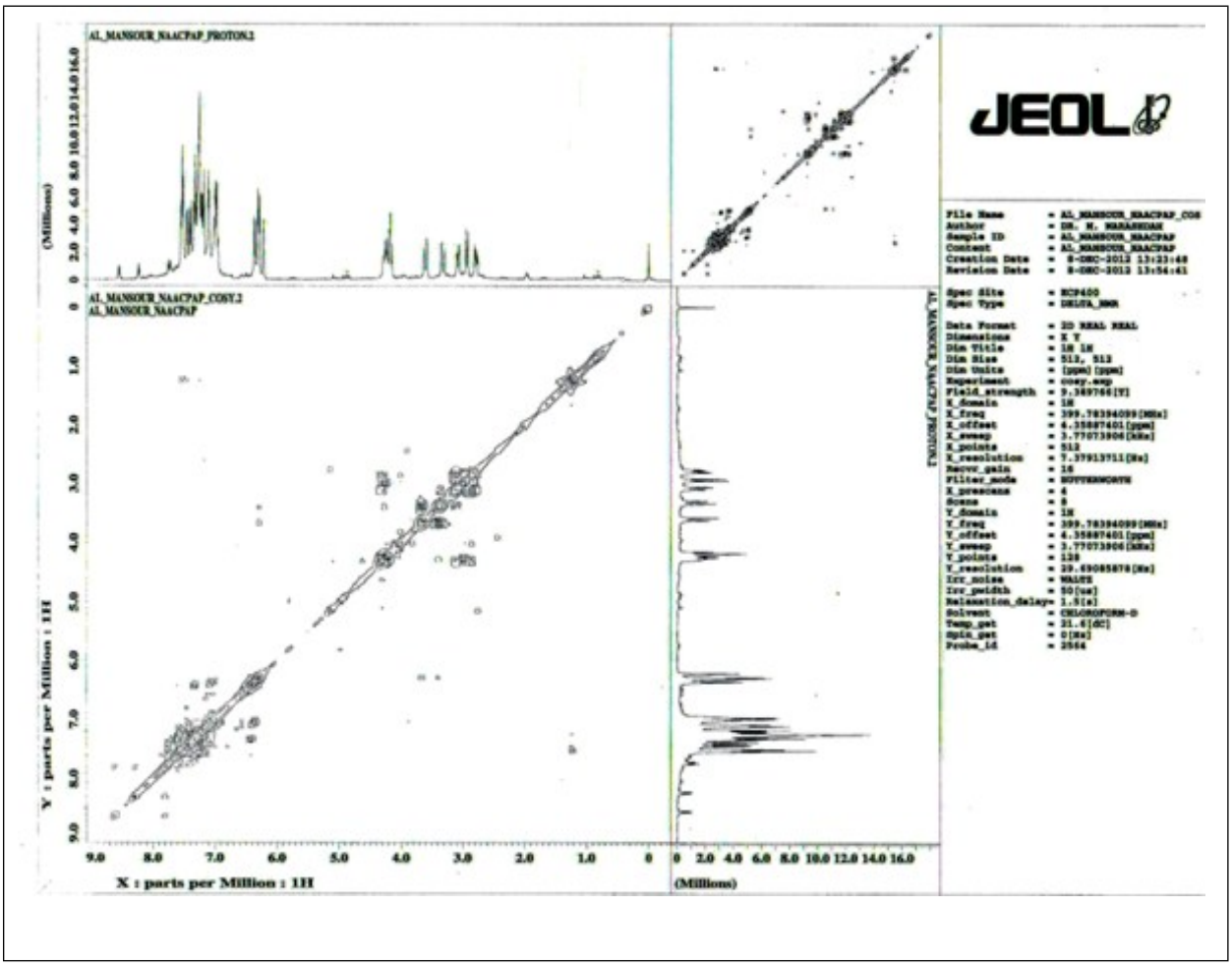

Figure 4. $^{1}H,^{1}H$-COSY spectrum of **5a**

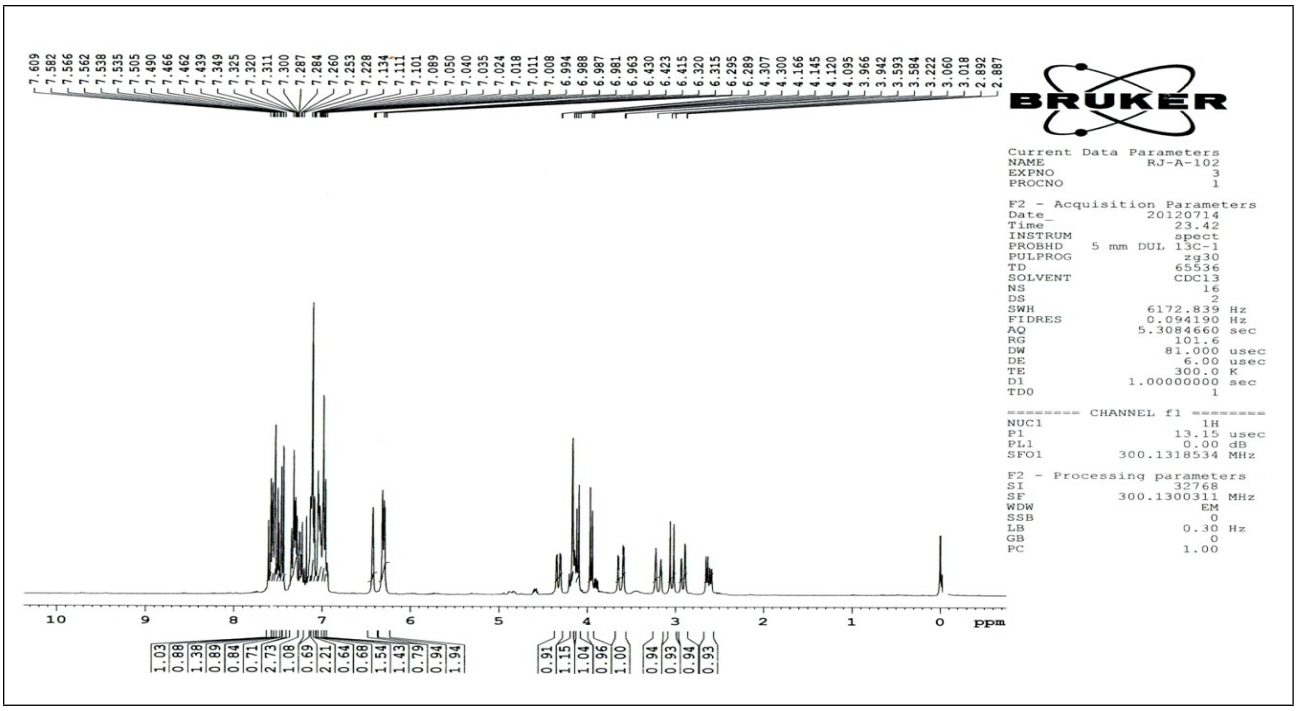

Figure 5. [1]H NMR spectrum of **6a**

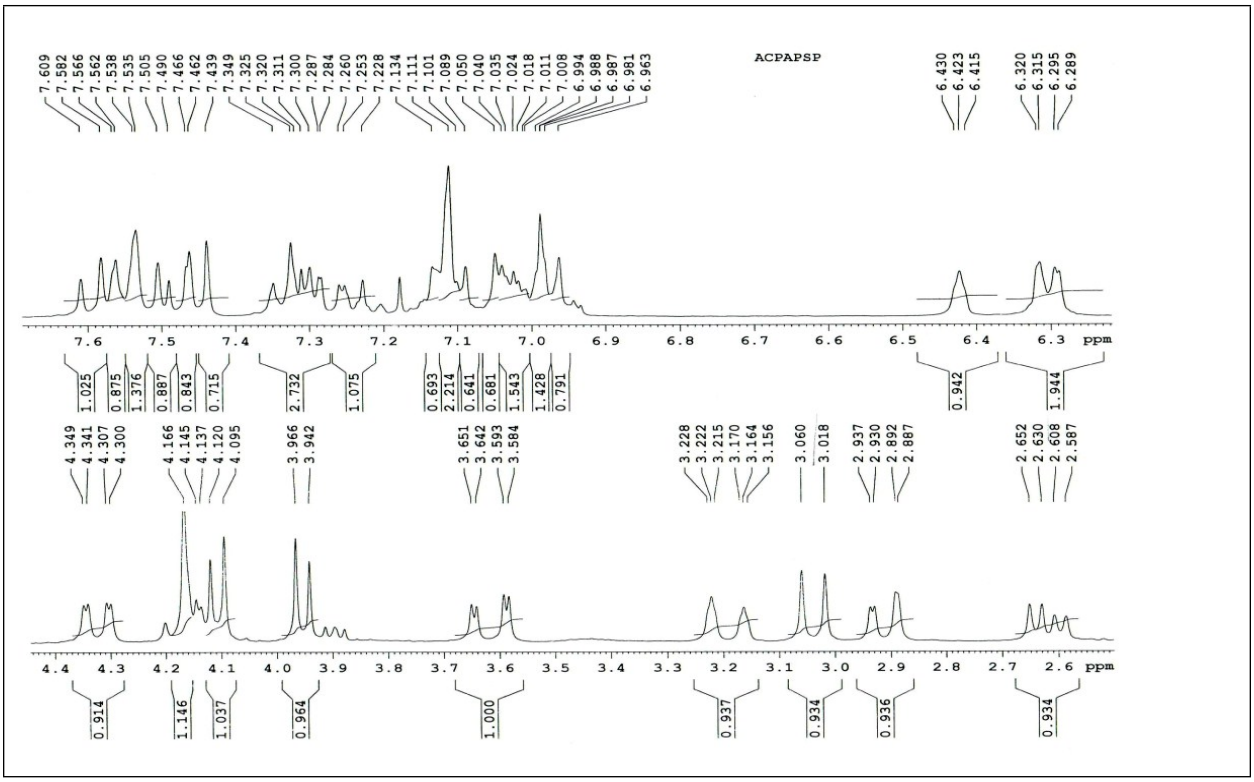

Figure 6. Expanded [1]H NMR spectrum of **6a**

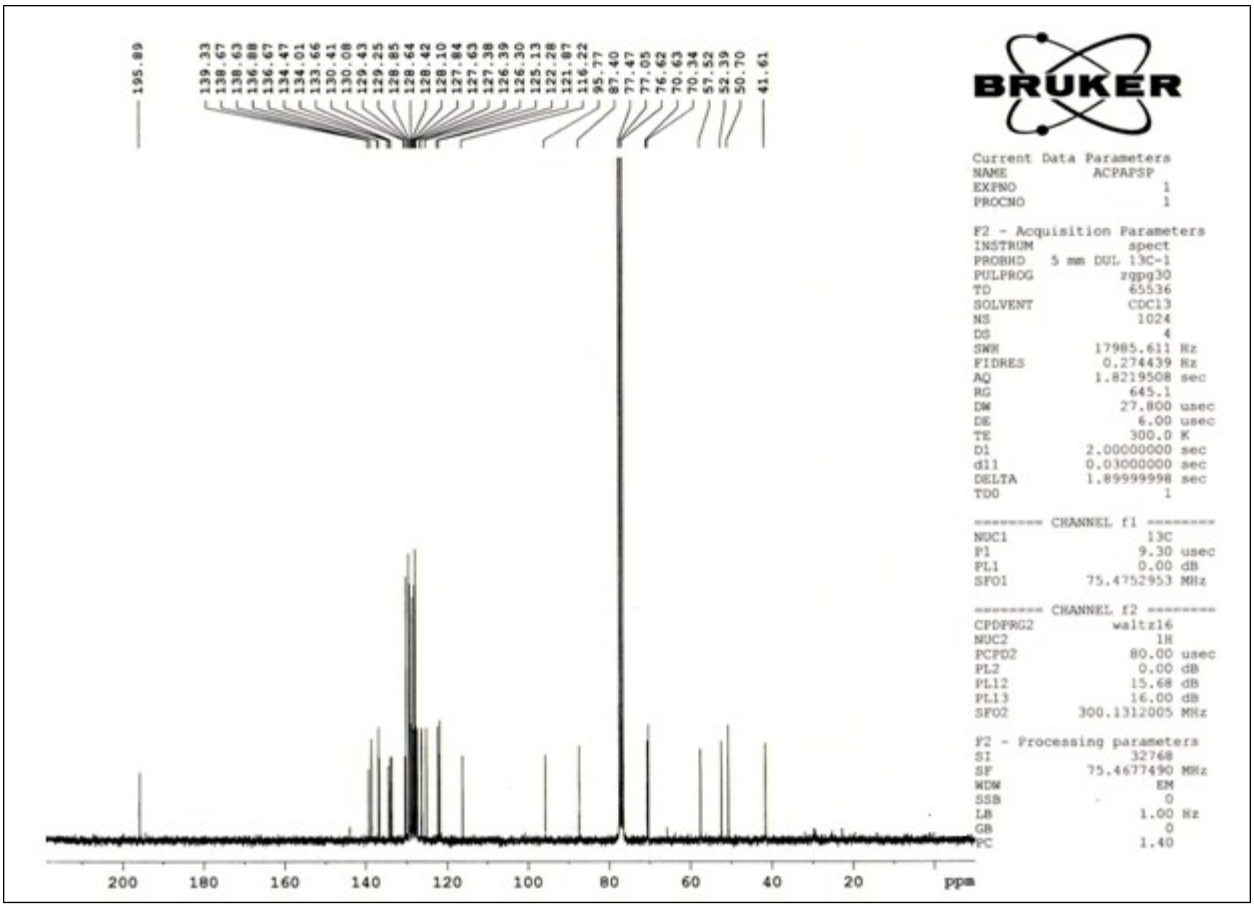

Figure 7. ^{13}C NMR spectrum of **6a**

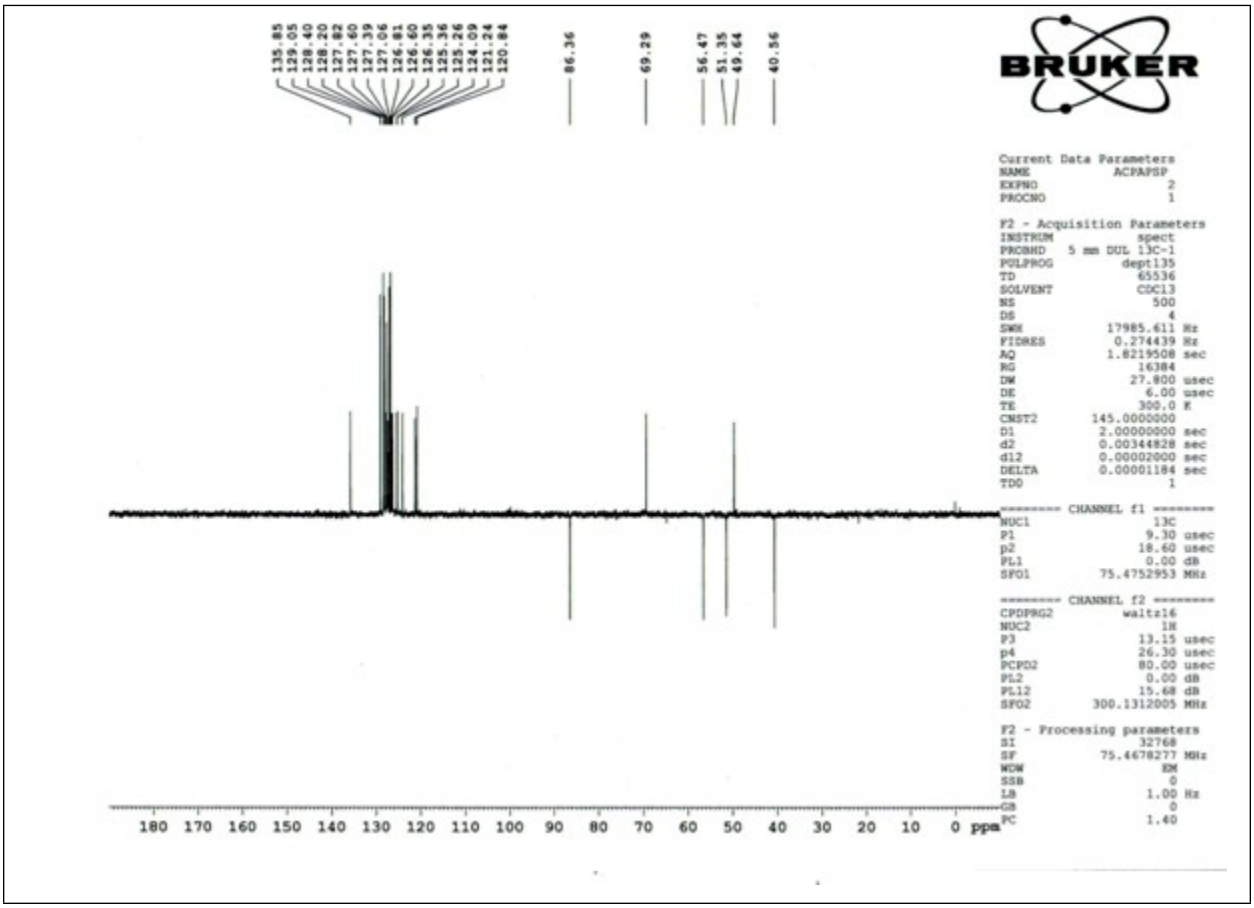

Figure 8. DEPT spectrum of **6a**

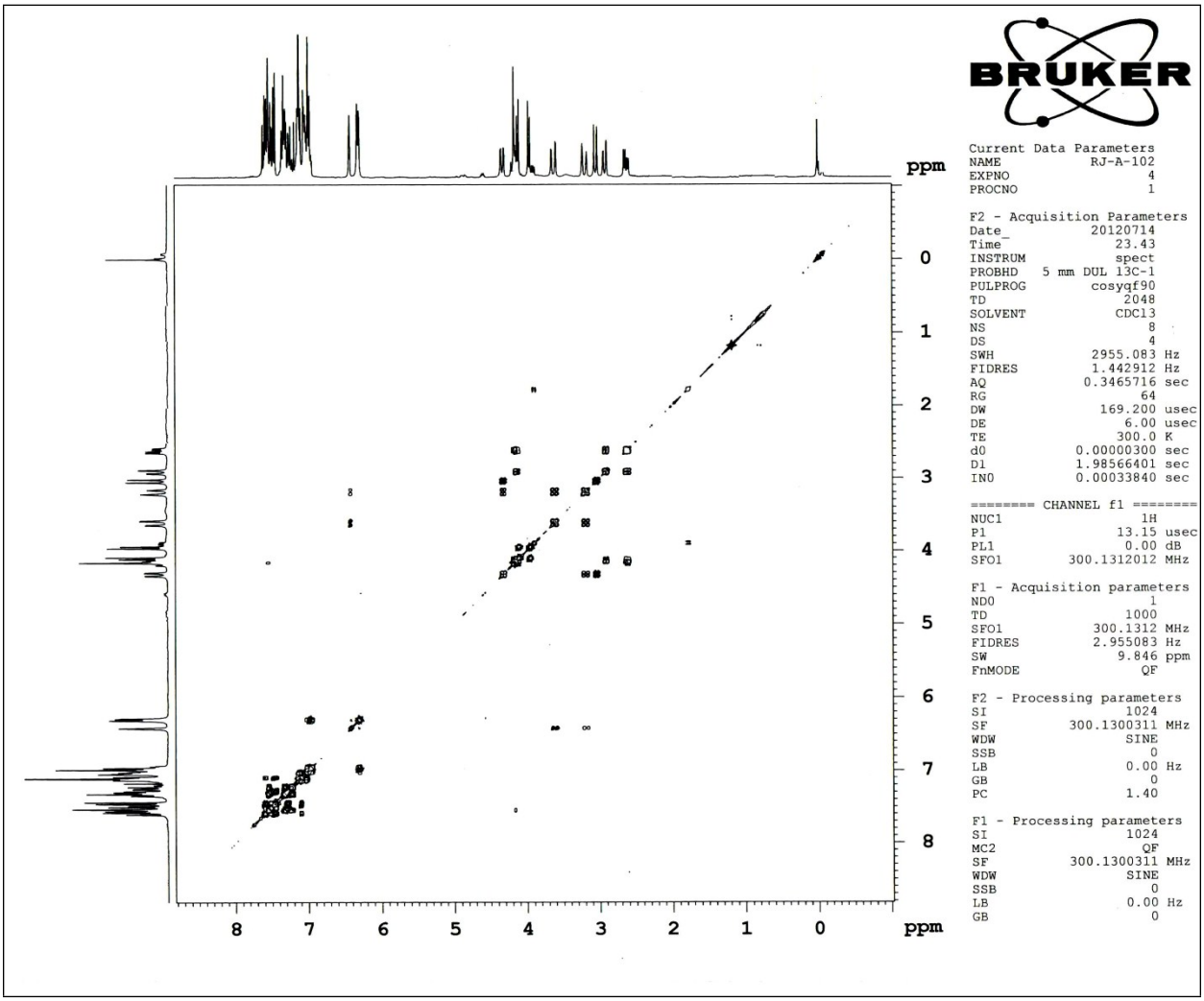

Figure 9. ^{1}H, ^{1}H-COSY spectrum of **6a**

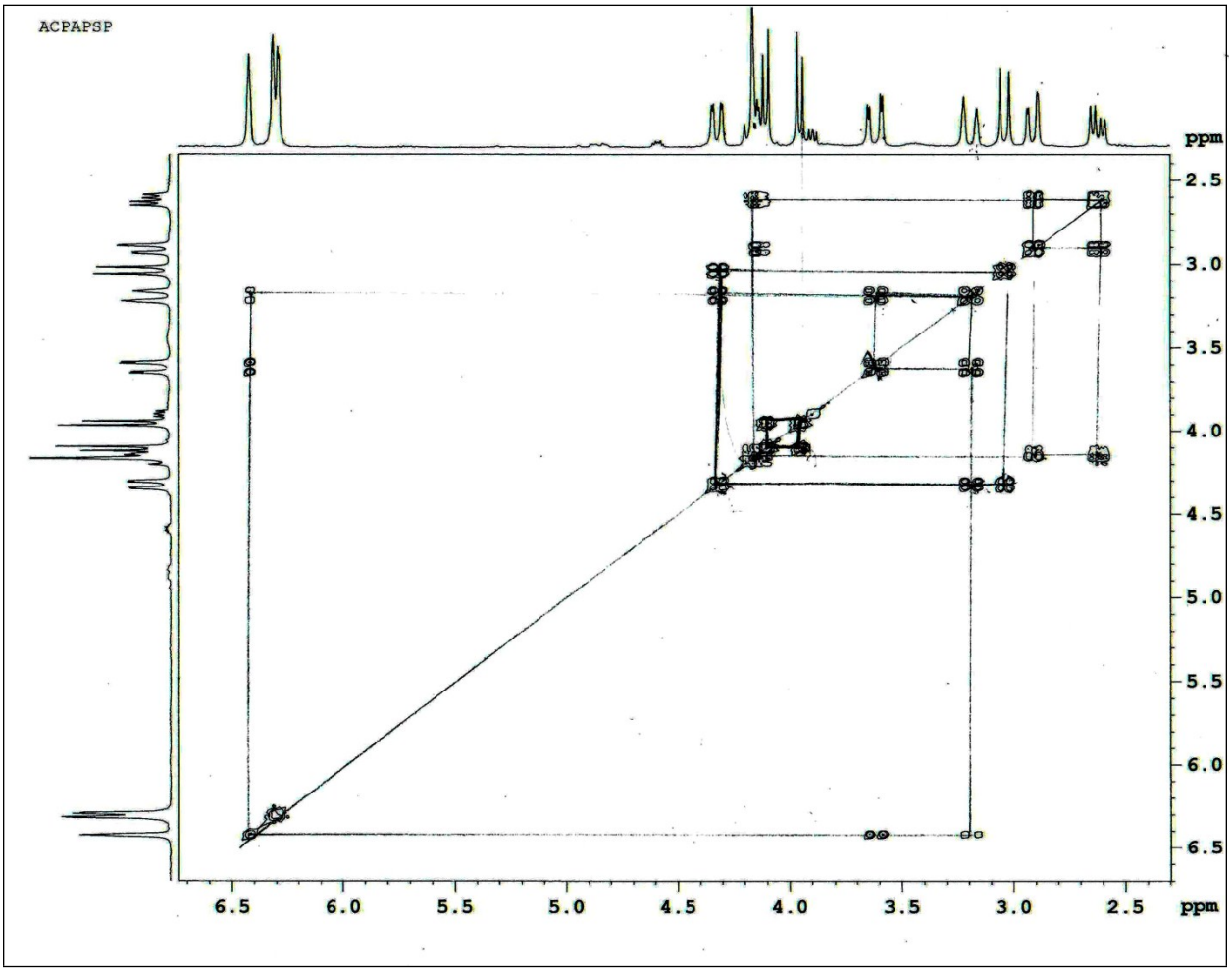

Figure 10. Expanded ^{1}H, ^{1}H-COSY spectrum of **6a**

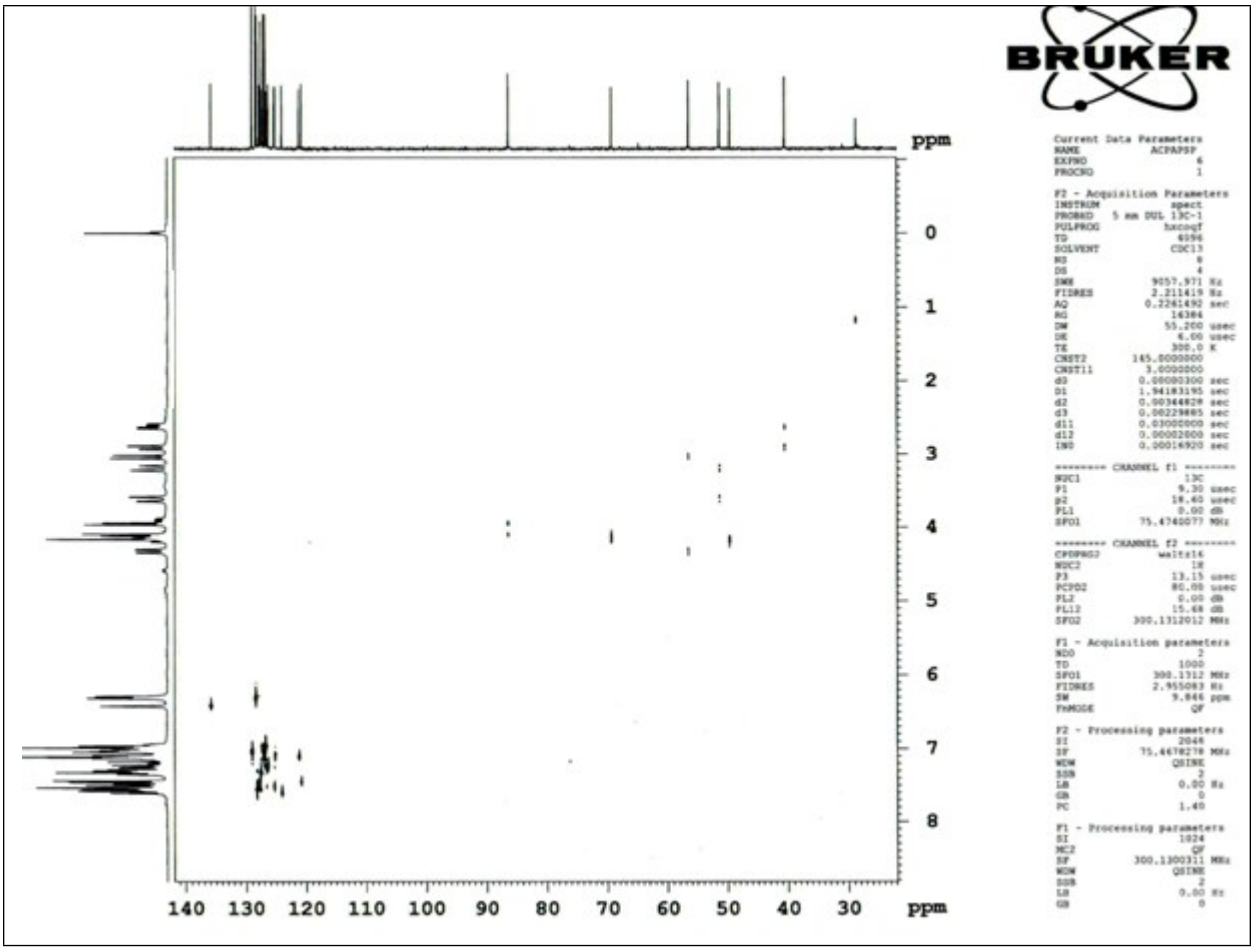

Figure 11. C,H-COSY spectrum of **6a**

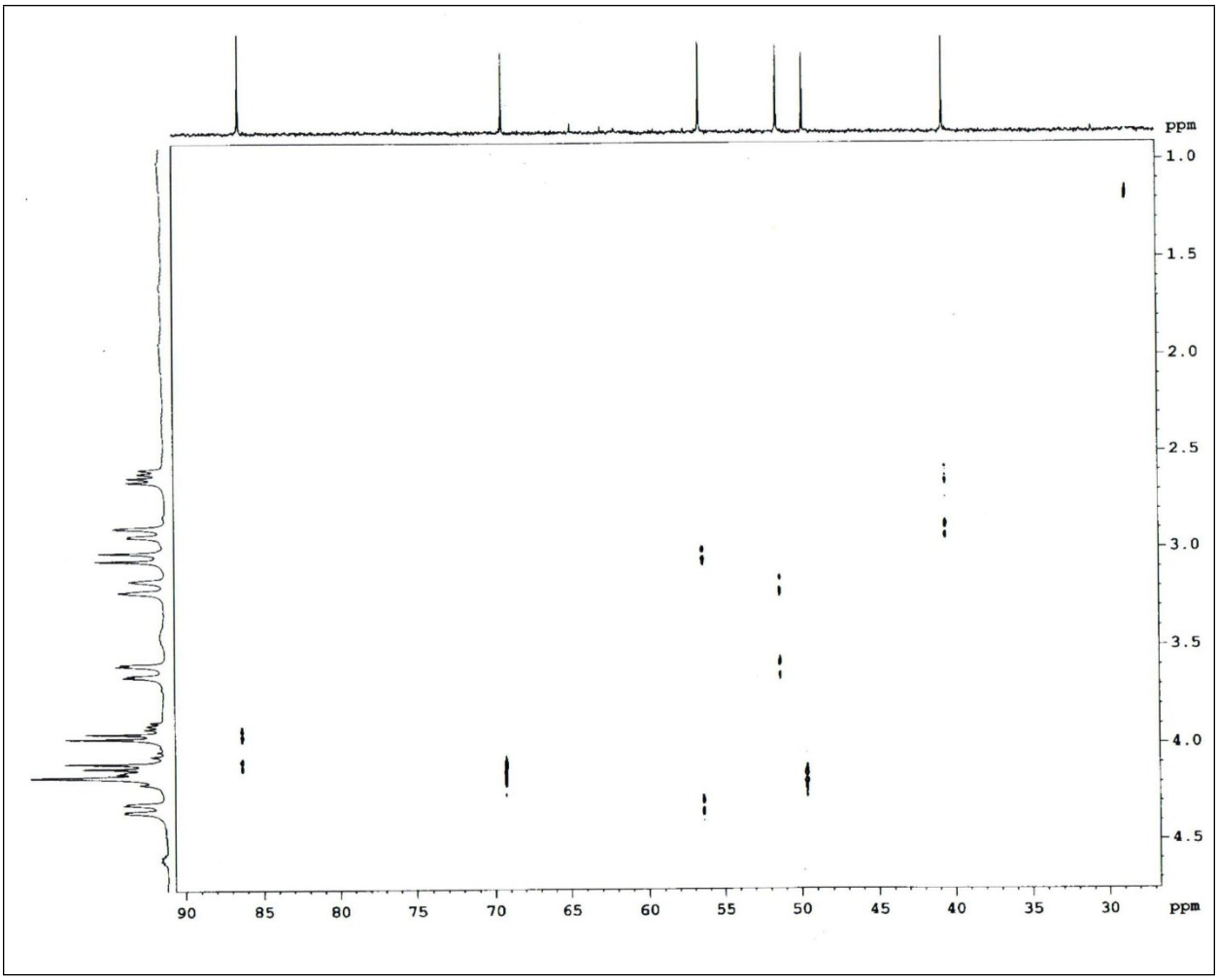

Figure 12. Expansion C, H-COSY spectrum of **6a**