Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Evaluation of PIC and EDTA coupled Acetamidobenzoxazolone probes as specific marker for 18 kDa protein (TSPO)

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➢ **Characterization of bis(pyridin-2-ylmethyl)amine (2)**

Physical state and Yield: yellow oil, 72 %

$\mathbf{R_f}$ = 0.3 (20 % MeOH in $CHCl_3$)

IR (KBr) ν_{max}: 3394, 2361, 1593, 1435, 769 cm^{-1}

^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.48 (2H, d, *J* = 4.4 Hz), 7.76-7.72 (2H, m), 7.45 (2H, d, *J* = 7.6 Hz), 7.25-7.21 (2H, m), 3.82 (4H, s) and 3.76 (1H, brs)

^{13}C NMR (DMSO-d_6, 100.6 MHz): δ 160.10, 148.80, 136.50, 121.94, 121.83 and 54.02

HR-ESI-TOF-MS: *m/z* 200.1185 ($[M+H]^+$), calcd. for $[C_{12}H_{13}N+H]^+$ 200.1182

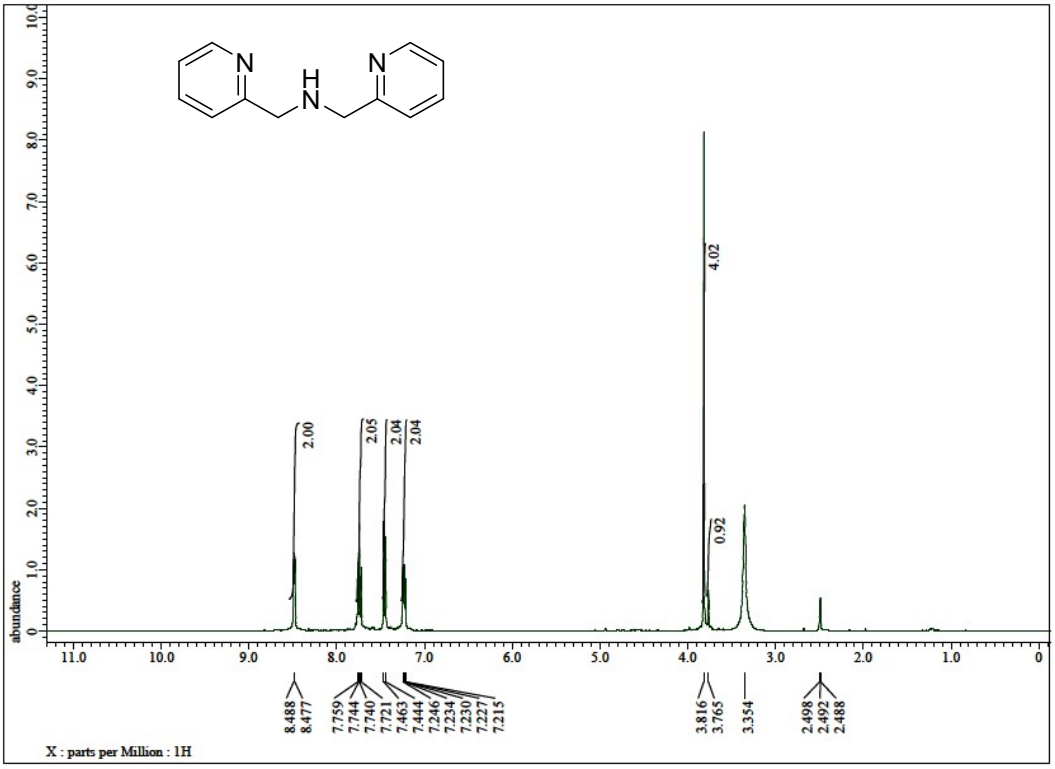

Figure 1: ^{1}H NMR spectrum of compound **2** (DMSO- d_6, 400 MHz)

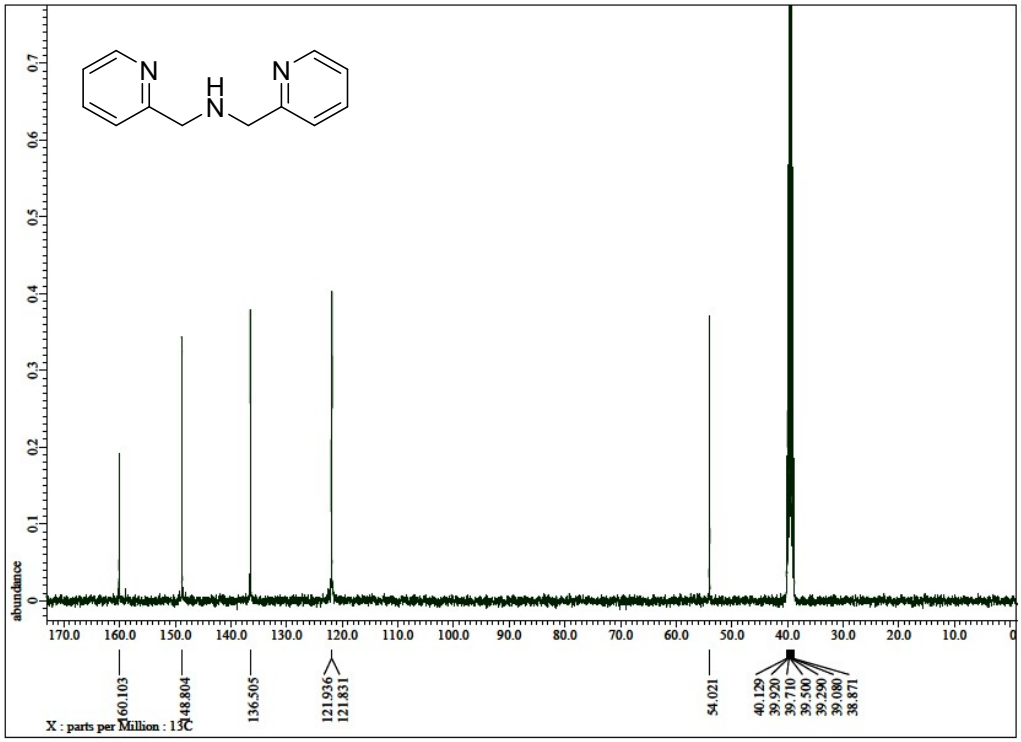

Figure 2: ^{13}C NMR spectrum of compound **2** (DMSO-d_6, 100.6 MHz)

- **Characterization of 2-(5-(2-bromoacetamido)-2-oxobenzo[d]oxazol3(2H)-yl)-N-methyl-N-phenylacetamide (4)**

Physical state and yield: Off white solid, 87%

R_f = 0.4 (10 % methanol in chloroform)

M. Pt.: 168-170

IR (thin film) ν_{max}: 3294, 2918, 1778, 1643, 1495, 1018, 701 cm^{-1}

^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.73 (1H, s), 7.60-7.45 (6H, m), 7.37 (1H, d, *J* = 8.4 Hz), 7.26 (1H, d, *J* = 8.4 Hz), 4.29 (2H, s), 3.99 (2H, s) and 3.20 (3H, s)

^{13}C NMR (DMSO-d_6, 100.6 MHz): δ 170.9, 164.9, 154.3, 142.0, 137.9, 134.8, 131.3, 130.2, 128.5, 127.4, 113.7, 109.6, 101.6, 61.9, 43.5 and 37.3

HR-ESI-TOF-MS: *m/z* 418.0387 ([M+H]$^+$), calcd. for [$C_{18}H_{16}BrN_3O_4$+H]$^+$ 418.0397.

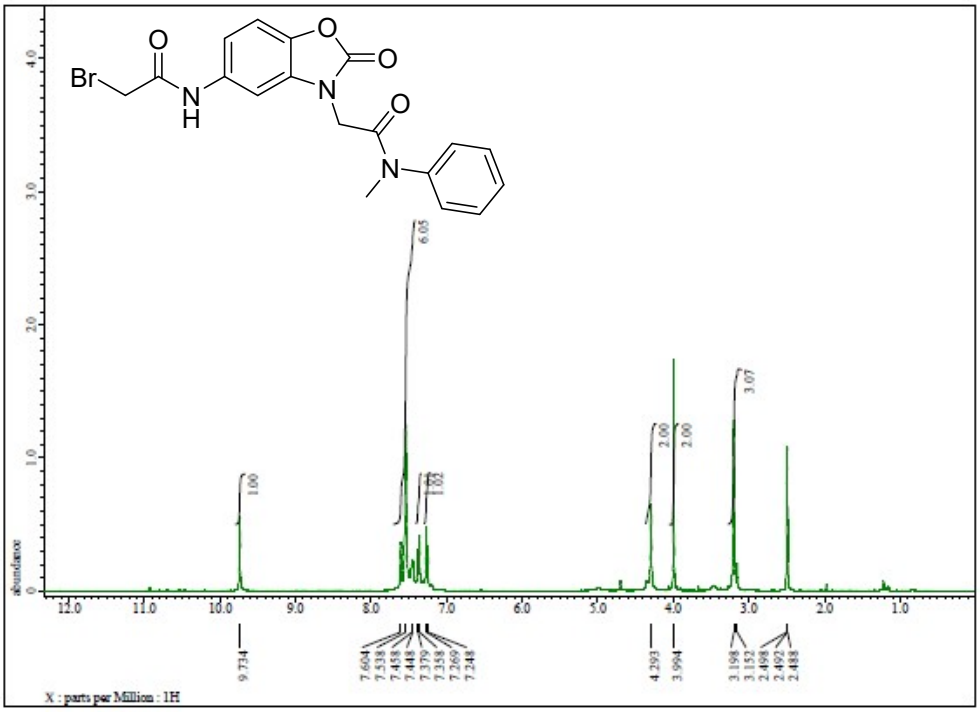

Figure 3: ^{1}H NMR spectrum of compound 4 (400 MHz, DMSO-d_6)

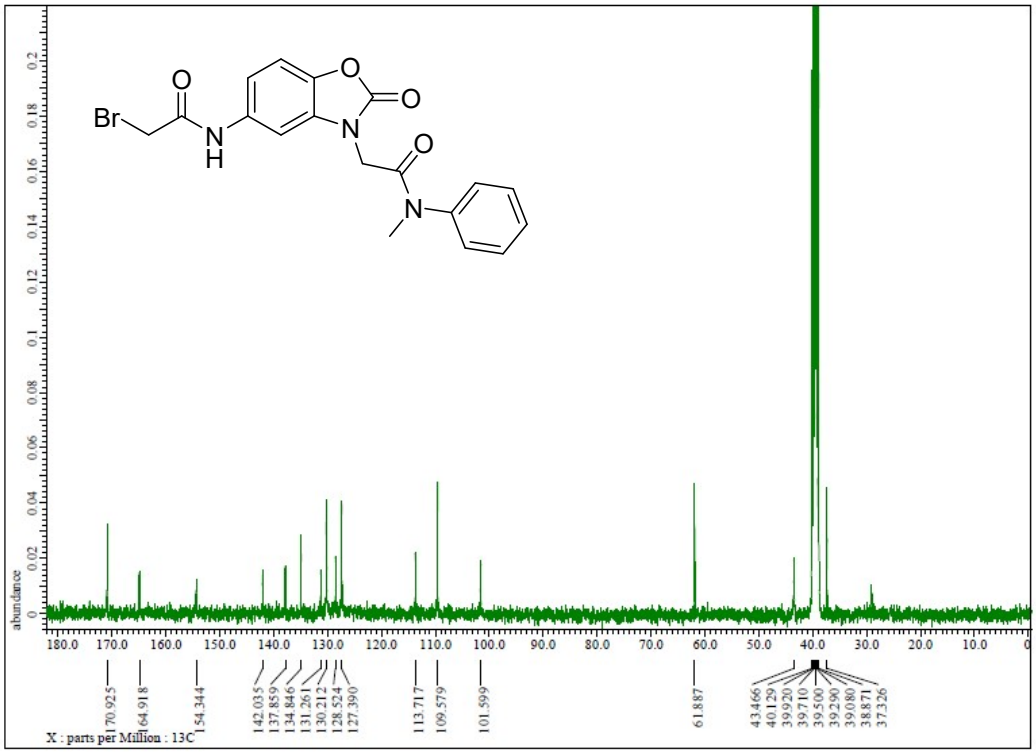

Figure 4: ^{13}C NMR spectrum of compound **4** (100.6 MHz, DMSO-d_6)

- **Characterization of 2-(5-(2-(bis(pyridin-2-ylmethyl)amino)acetamido)-2-oxobenzo[*d*]oxazol-3(2*H*)-yl)-*N*-methyl-*N*-phenylacetamide (5)**

Physical state and Yield: off-white solid (0.21 g, 54 %

R_f = 0.2 (20 % MeOH in $CHCl_3$)

^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.70 (1H, brs), 8.57 (2H, d, *J* = 4.4 Hz), 7.77 (2H, t, *J* = 7.6 Hz), 7.61 (1H, s), 7.53 (2H, s), 7.53 (2H, s),7.45 (2H, d, *J* = 7.6 Hz), 7.29 (5H, s), 4.35 (2H, s), 3.94 (4H, s), 3.47 (2H, s) and 3.21 (3H, s)

^{13}C NMR (DMSO-d_6, 100.6 MHz): δ 169.2, 165.0, 158.2, 154.3, 149.0, 142.0, 137.7, 136.9, 135.2, 131.4, 130.2, 128.5, 127.4, 123.2, 122.6, 113.1, 109.7, 101.1, 59.3, 57.7, 43.5 and 37.3

HR-ESI-TOF-MS: *m/z* 537.2256 ($[M+H]^+$), calcd. for $[C_{30}H_{28}N_6O_4+H]^+$ 537.2245.

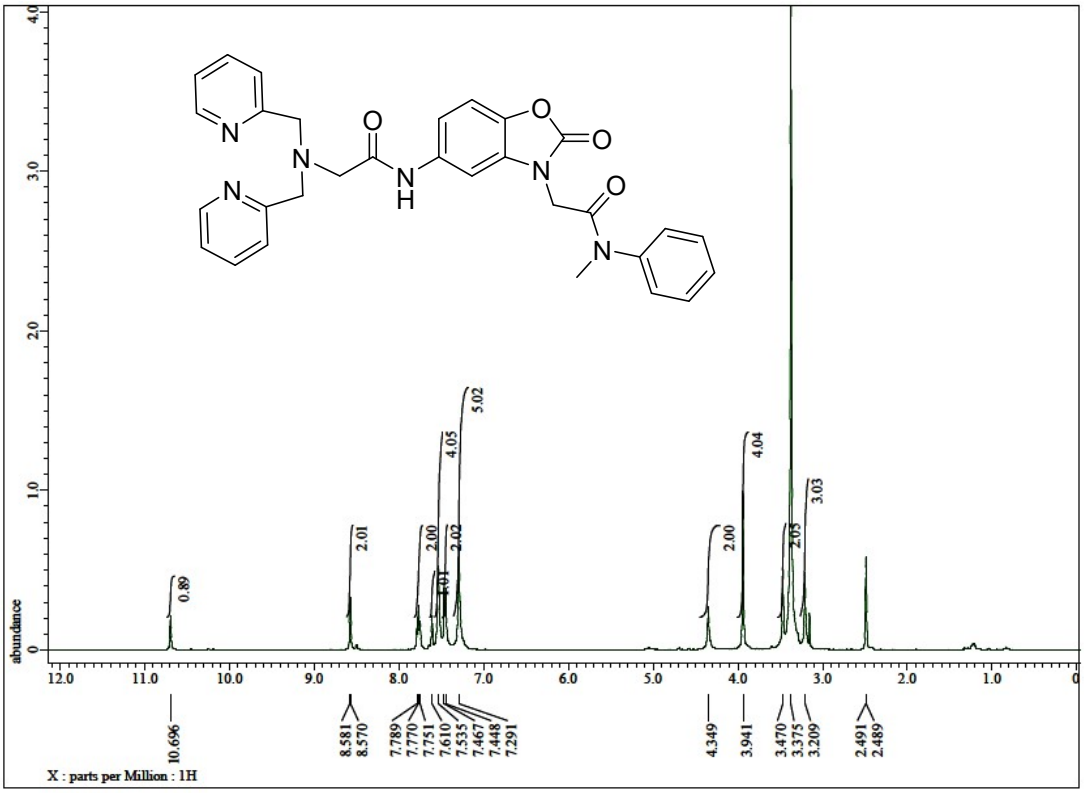

Figure 5: ^{1}H NMR spectrum of compound **5** (DMSO-d_6, 400 MHz)

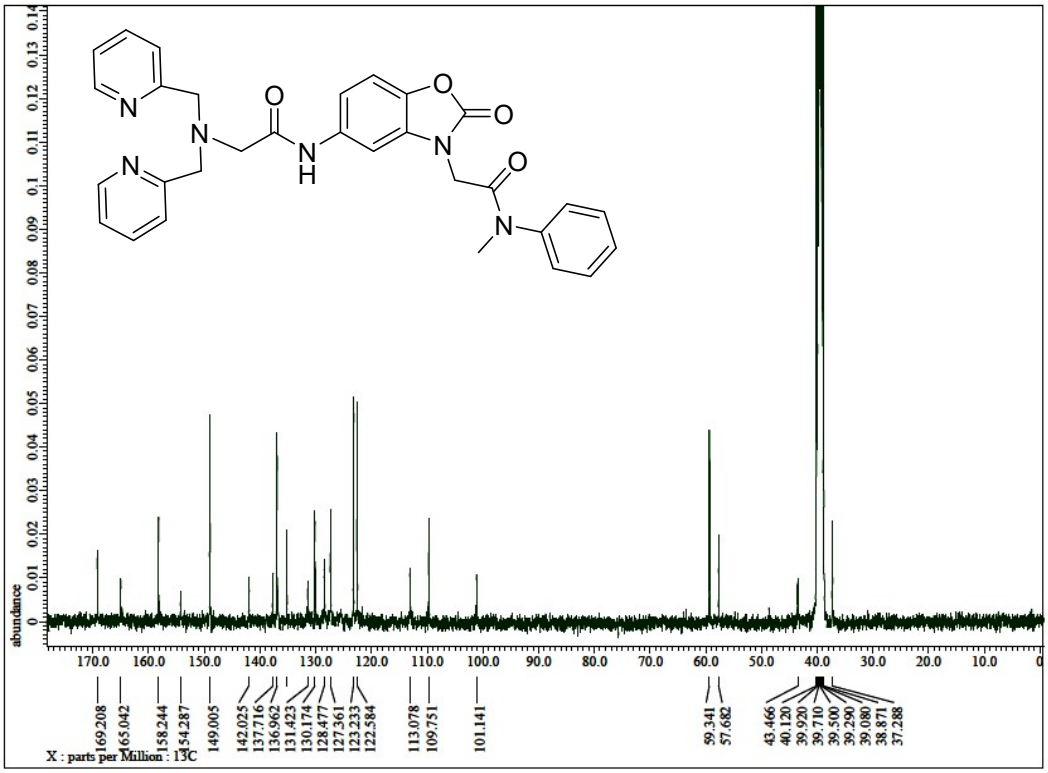

Figure 6: ^{13}C NMR spectrum of compound **5** (DMSO-d_6, 100.6 MHz)

- **Characterization of 2,2'-(ethane-1,2-diylbis((2-((3-(2-(methyl(phenyl)amino)-2-oxoethyl)-2-oxo-2,3-dihydrobenzo[d]oxazol-5-yl)amino)-2-oxoethyl)azanediyl)) diacetic acid (6)**

Physical state and Yield: white solid (0.28 g, 85 %)

IR (KBr) ν_{max}: 3286, 2982, 1774, 1660, 1491, 1389, 1229, 697 cm^{-1}

^{1}H NMR (DMSO-d_6, 400 MHz): δ 10.24 (2H, brs), 8.30 (1H, s), 7.94 (1H, s), 7.57-7.43 (12H, m), 7.28-7.19 (4H, m), 4.28 (4H, s), 3.53 (10H, s), 3.17 (4H, s) and 2.88 (4H, s)

^{13}C NMR (DMSO-d_6, 100.6 MHz): δ 172.83, 172.05, 169.51, 164.89, 162.32, 154.25, 141.98, 137.89, 135.20, 131.23, 130.11, 128.60, 127.29, 113.10, 109.54, 100.10, 79.32, 64.94, 57.10, 55.37, 54.61, 52.15, 43.36, 37.21 and 35.81

HR-ESI-TOF-MS: *m/z* 851.2946 ([M+H]$^+$), calcd. for [$C_{42}H_{42}N_8O_{12}$+H]$^+$ 851.2995

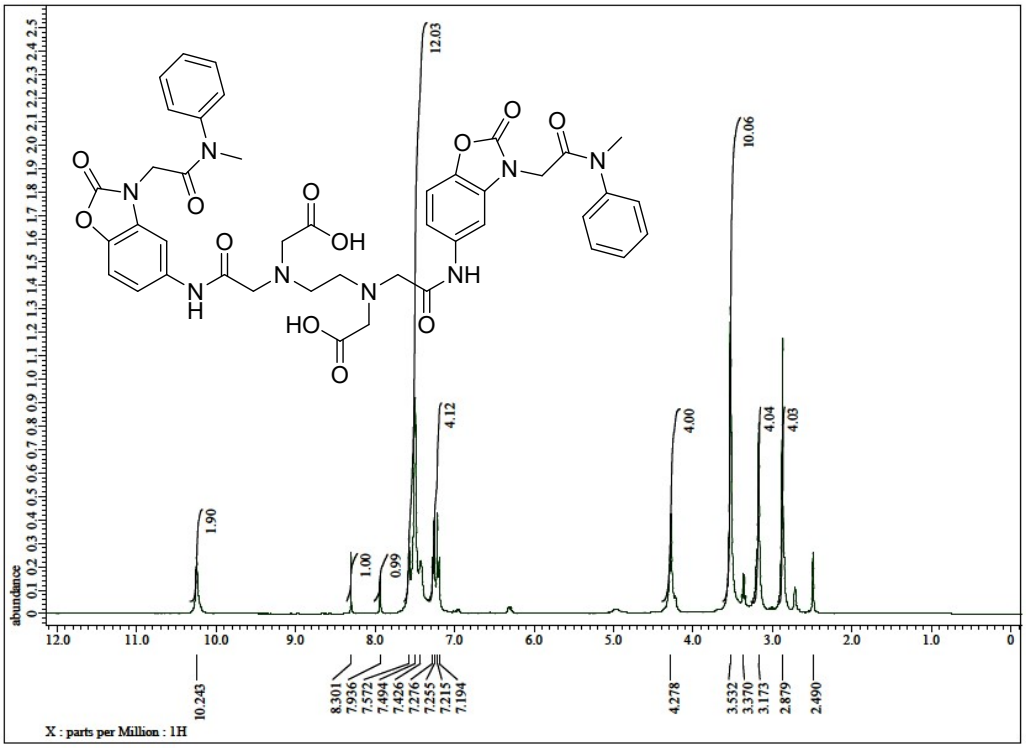

Figure 7: ^{1}H NMR spectrum of compound **6** (DMSO-d_6, 400 MHz)

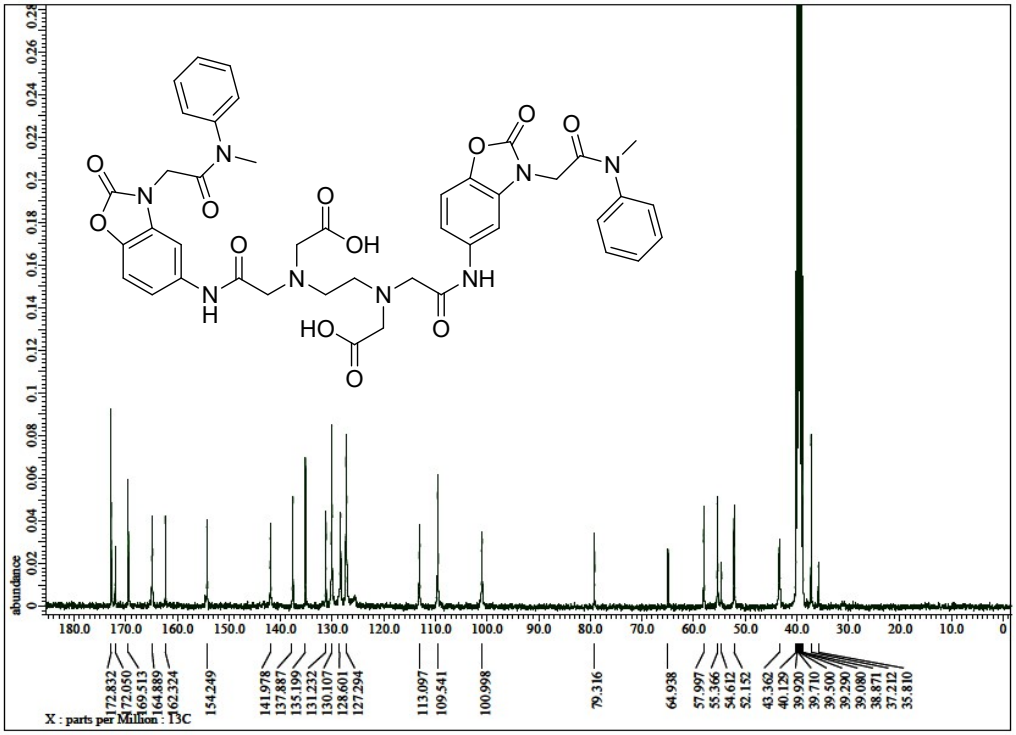

Figure 8: ^{13}C NMR spectrum of compound **6** (DMSO-d_6, 100.6 MHz)