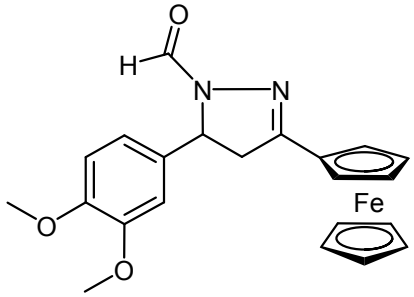
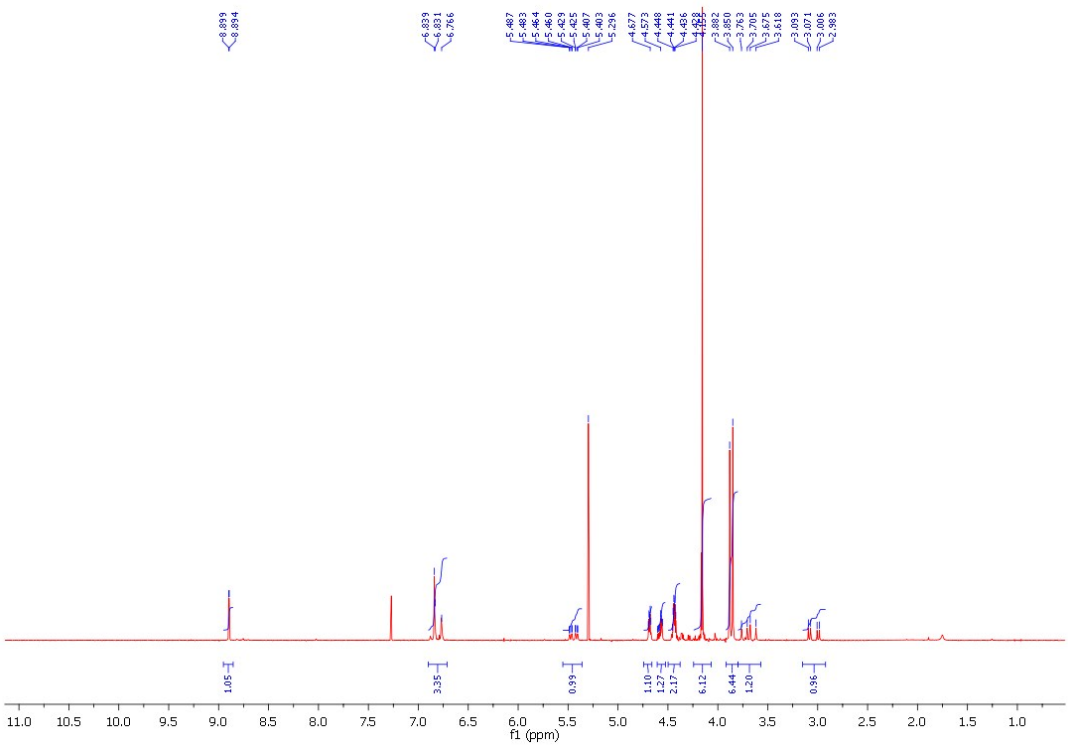
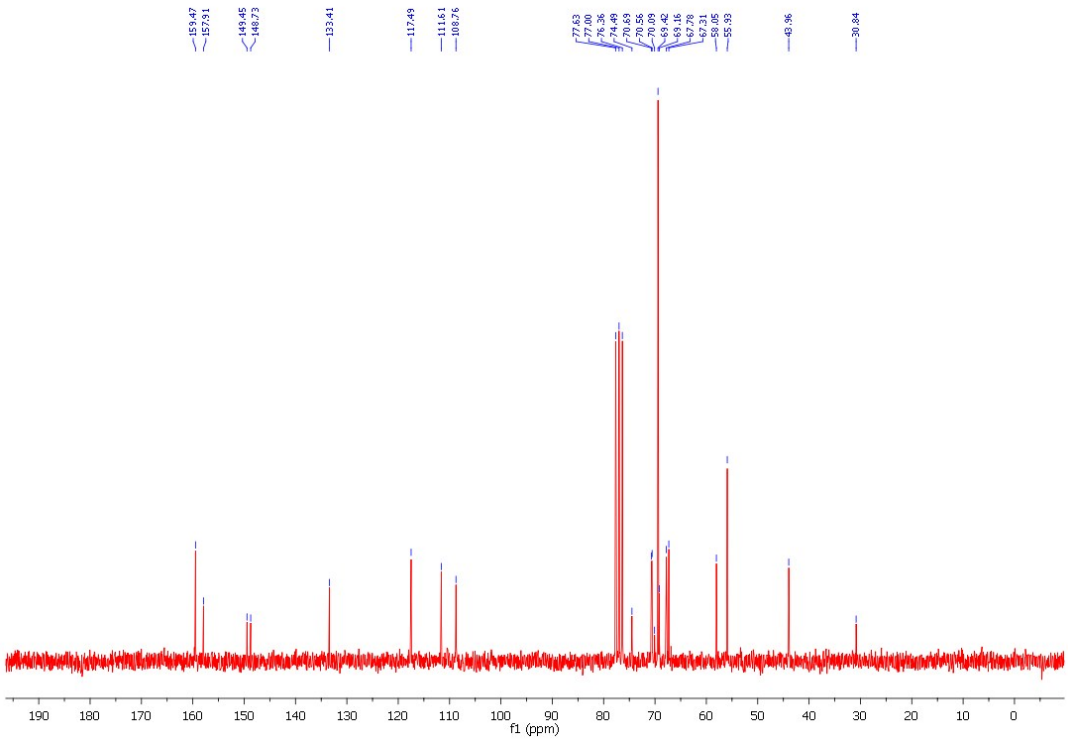
5-(3,4-dimethoxyphenyl)-3-ferrocenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde; **3a**



Orange oil; Yield 57%; IR (KBr): 2931, 1668, 1594, 1517, 1411, 1359, 1309, 1259, 1235, 1139, 1025, 819 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.04 (dd, *J*=17.6, 4.6Hz, 1H), 3.69 (dd, *J*=17.4, 11.4Hz, 1H), 3.87 (d, *J*=6.4Hz, 6H), 4.15 (s, 5H), 4.42-4.45 (m, 2H), 4.57 (dt, *J*=2.4, 1.4Hz, 1H), 4.68 (dt, *J*=2.6, 1.2Hz, 1H), 5.44 (dd, *J*=11.4, 4.4Hz, 1H), 6.77-6.84 (m, 3H), 8.89 (d, *J*=1.0Hz, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 30.8, 43.9, 55.9, 58, 67.3, 67.8, 69.2, 69.4, 70.6, 70.7, 74.5, 108.9, 111.6, 117.5, 133.4, 148.7, 149.4, 157.9, 159.5 (CO). **ESI-MS** (40 eV): *m/z* (%) = 418 (100%) $[M]^+$.

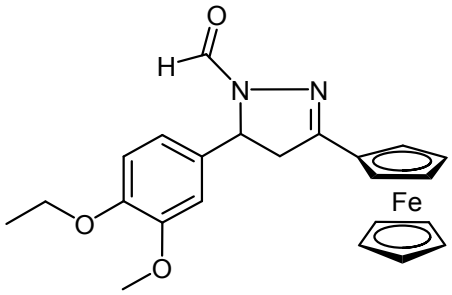


^{1}H NMR spectrum of compound **3a**

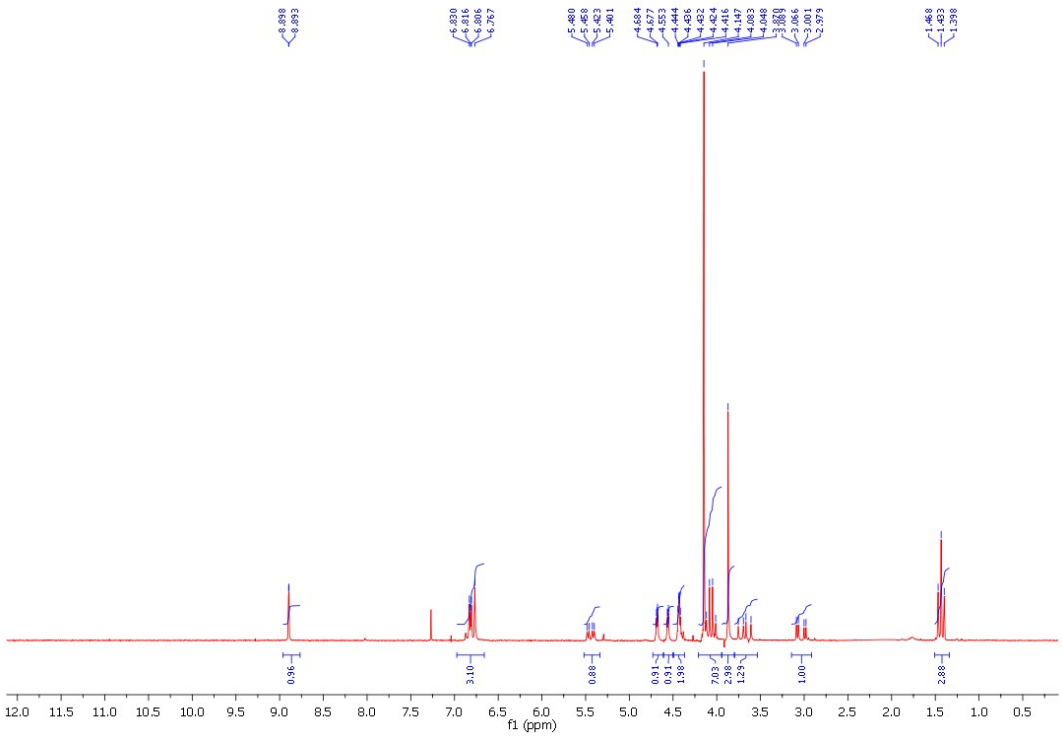


^{13}C NMR spectrum of compound **3a**

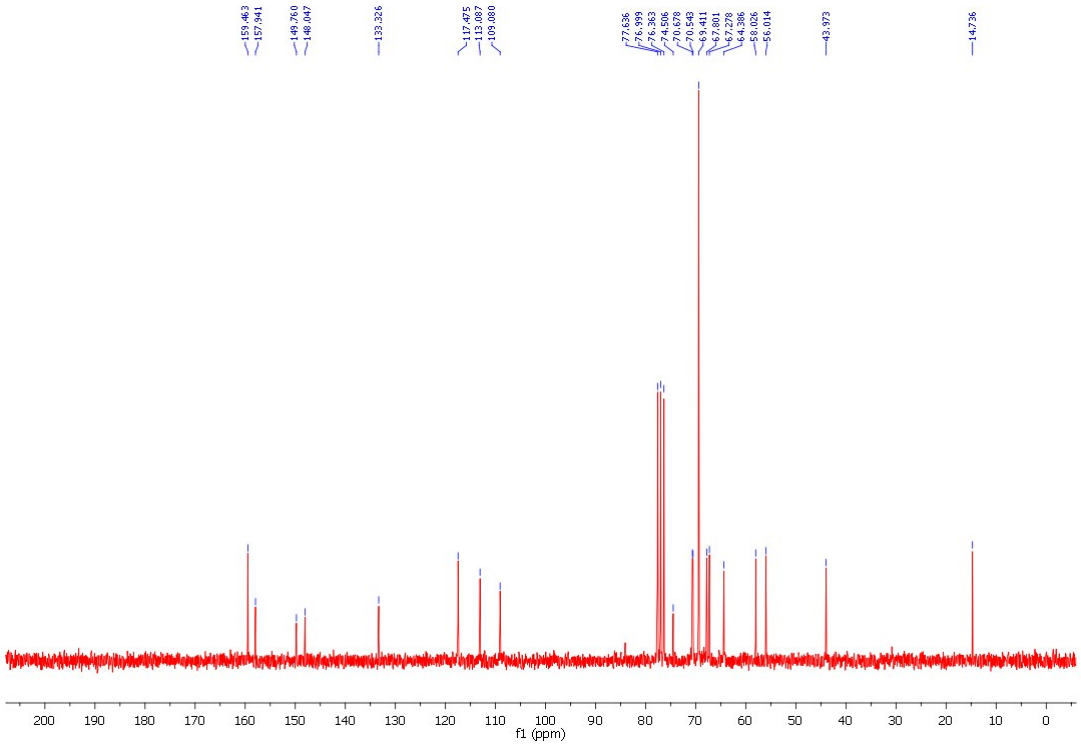
5-(4-etoxy-3-methoxyphenyl)-3-ferrocenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde; **3b**



Orange oil; Yield 63%; IR (KBr): 2929, 1671, 1594, 1516, 1415, 1360, 1308, 1259, 1233, 1140, 1121, 1034, 825 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$): δ 1.43 (t, *J*=7.0Hz, 3H), 3.03 (dd, *J*=17.4, 4.4Hz, 1H), 3.68 (dd, *J*=17.4, 11.6, 1H), 3.87 (s, 3H), 4.06 (q, *J*=7.0Hz, 2H), 4.15 (s, 5H), 4.42-4.44 (m, 2H), 4.56 (dt, *J*=2.6, 1.4Hz, 1H), 4.68 (dt, *J*=2.6, 1.2Hz, 1H), 5.44 (dd, *J*=11.4, 4.4Hz, 1H), 6.77-6.83 (m, 3H), 8.89 (d, *J*=1.0Hz, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 14.7, 43.9, 56, 58, 64.4, 67.3, 67.8, 69.4, 70.5, 70.7, 74.5, 84.1, 109.1, 113.1, 117.5, 133.3, 148, 149.8, 157.9, 159.5 (CO). **ESI-MS** (40 eV): *m/z* (%) = 432 (100%) $[M]^+$.

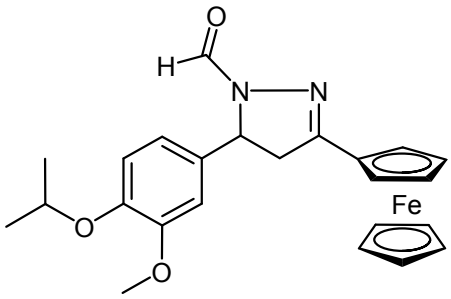


^{1}H NMR spectrum of compound **3b**

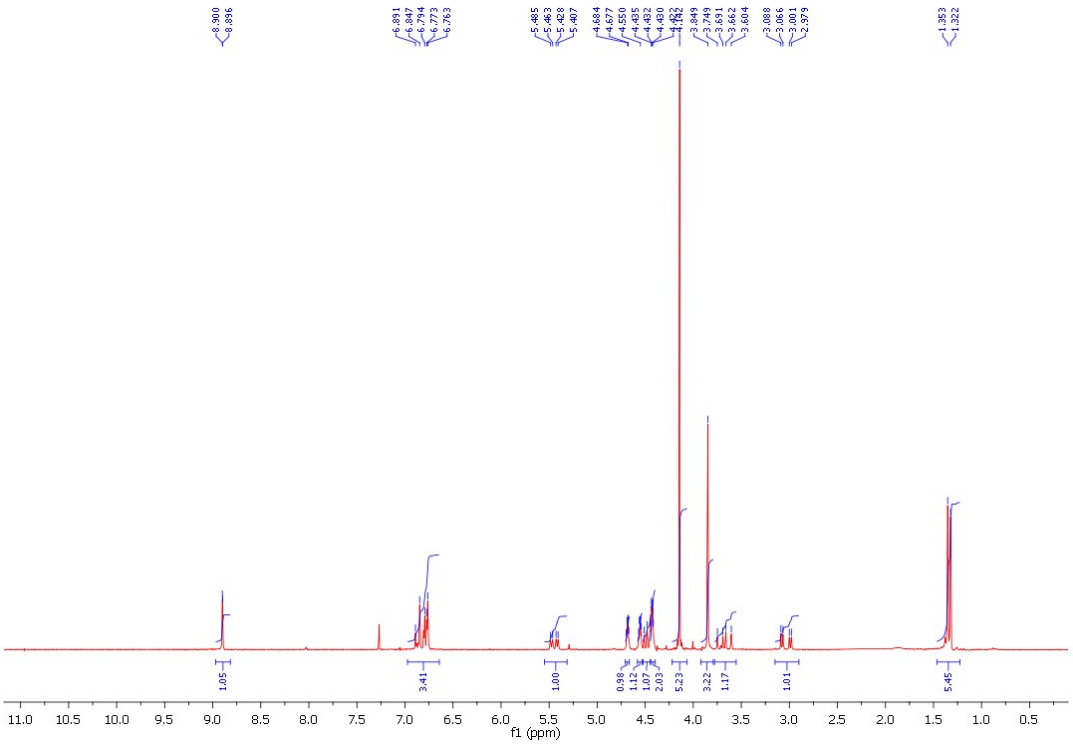


^{13}C NMR spectrum of compound **3b**

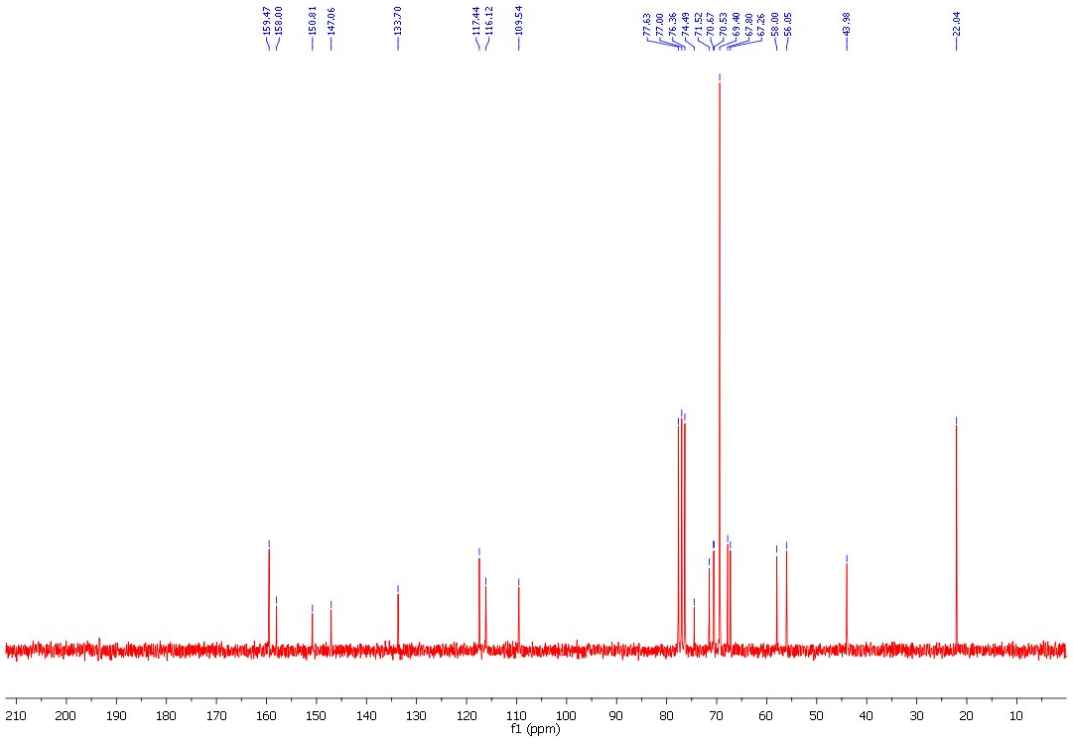
*5-(4-isopropoxy-3-methoxyphenyl)-3-ferrocenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde;***3c**



Light orange; mp 55-57ºC; Yield 54%; IR (KBr): 3086, 2973, 2926, 1671, 1591, 1512, 1412, 1359, 1307, 1258, 1231, 1138, 1106, 1032, 821 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$): δ 1.34 (d, *J*=6.2Hz, 6H), 3.03 (dd, *J*=17.4, 4.4Hz, 1H), 3.68 (dd, *J*=17.4, 11.6, 1H), 3.85 (s, 3H), 4.14 (s, 5H), 4.41-4.43 (m, 2H), 4.44-4.51 (m, 1H), 4.56 (dt, *J*=2.6, 1.4Hz, 1H), 4.69 (dt, *J*=2.6, 1.2Hz, 1H), 5.44 (dd, *J*=11.2, 4.2Hz, 1H), 6.79-6.89 (m, 3H), 8.93 (d, *J*=0.8Hz, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 22, 43.9, 56, 58, 67.3, 67.8, 69.4, 70.5, 70.7, 71.5, 74.5, 109.5, 116.1, 117.4, 133.7, 147.1, 150.8, 158, 159.5 (CO). **ESI-MS** (40 eV): *m/z* (%) = 446 (100%) $[M]^+$.



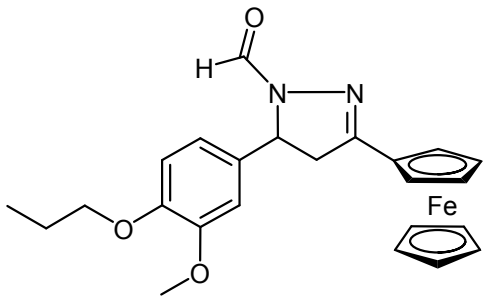
^{1}H NMR spectrum of compound **3c**



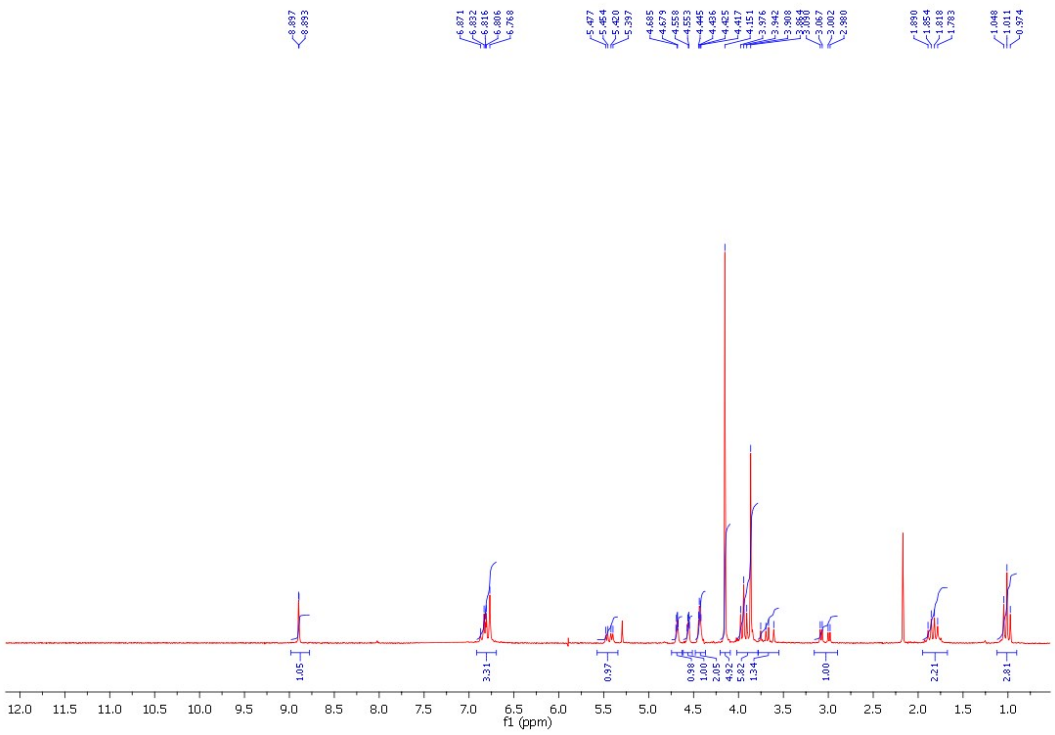
^{13}C NMR spectrum of compound **3c**

5-(3-methoxy-4-propoxyphenyl)-3-ferrocenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde;

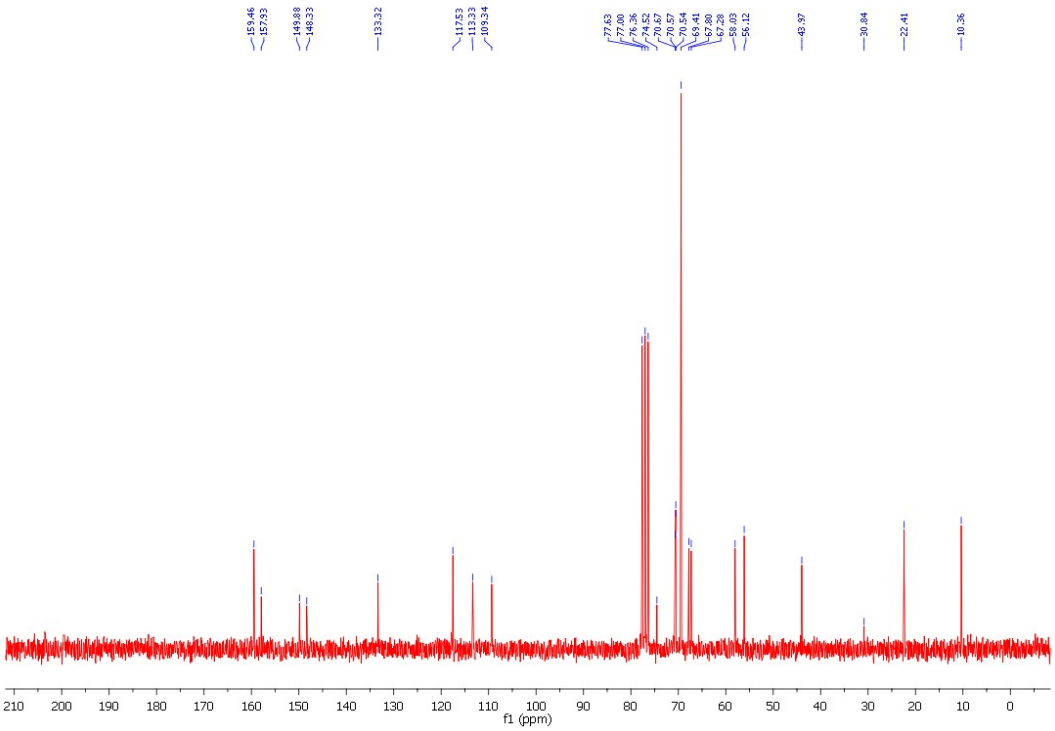
3d



Light orange; mp 52-54ºC; Yield 64%; IR (KBr): 2935, 2874, 1671, 1515, 1410, 1358, 1308, 1259, 1139, 1034, 818 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$): δ 1.01 (t, *J*=7.4Hz, 3H), 1.78-1.89 (m, 2H), 3.03 (dd, *J*=17.4, 4.4Hz, 1H), 3.68 (dd, *J*=17.6, 11.6, 1H), 3.86 (s, 3H), 3.94 (t, *J*=6.8Hz, 2H), 4.15 (s, 5H), 4.42-4.44 (m, 2H), 4.56 (dt, *J*=2.4, 1.4Hz, 1H), 4.68 (dt, *J*=2.4, 1.2Hz, 1H), 5.44 (dd, *J*=11.4, 4.6Hz, 1H), 6.77-6.87 (m, 3H), 8.89 (d, *J*=0.8Hz, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 10.4, 22.4, 30.8, 43.9, 56.1, 58, 67.3, 67.8, 69.4, 70.5, 70.6, 70.7, 74.5, 109.3, 113.3, 117.5, 133.3, 148.3, 149.9, 157.9, 159.5 (CO). **ESI-MS** (40 eV): *m/z* (%) = 446 (100%) $[M]^+$.

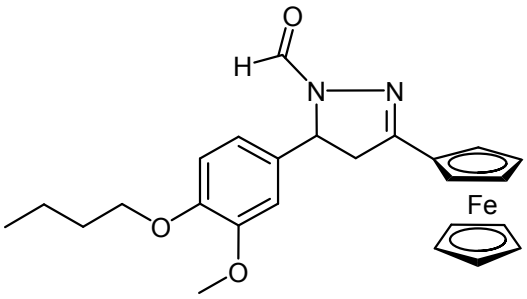


^{1}H NMR spectrum of compound **3d**

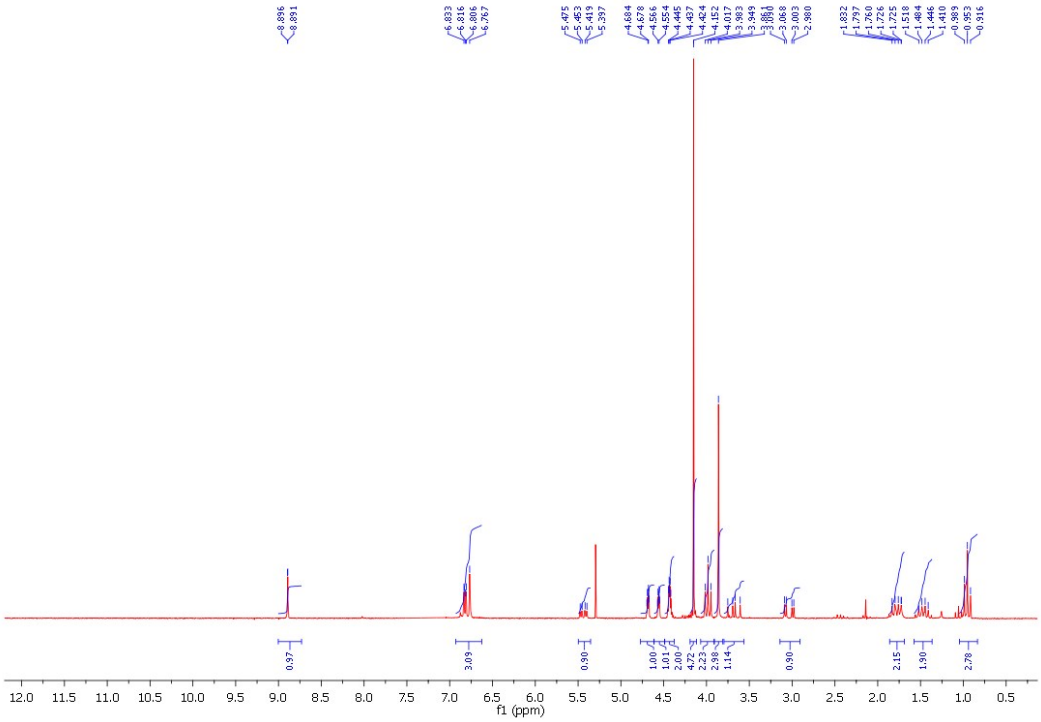


^{13}C NMR spectrum of compound **3d**

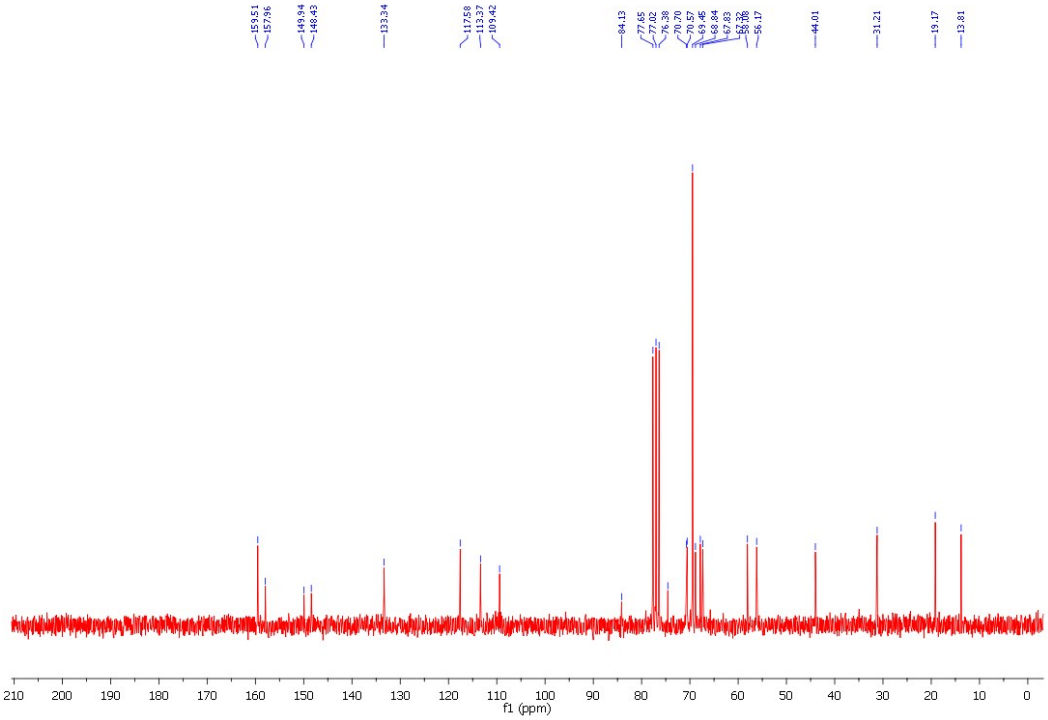
5-(4-butoxy-3-methoxyphenyl)-3-ferrocenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde; **3e**



Orange oil; Yield 77%; IR (KBr): 2930, 2873, 1672, 1516, 1411, 1358, 1308, 1259, 1234, 1139, 1029, 824 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$): δ 0.95 (t, *J*=7.4Hz, 3H), 1.41-1.52 (m, 2H), 1.72-1.83 (m, 2H), 3.03 (dd, *J*=17.6, 4.6Hz, 1H), 3.68 (dd, *J*=17.6, 11.6, 1H), 3.86 (s, 3H), 3.98 (t, *J*=6.8Hz, 2H), 4.15 (s, 5H), 4.42-4.44 (m, 2H), 4.56 (dt, *J*=2.4, 1.4Hz, 1H), 4.68 (dt, *J*=2.6, 1.4Hz, 1H), 5.44 (dd, *J*=11.2, 4.4Hz, 1H), 6.77-6.83 (m, 3H), 8.89 (d, *J*=1.0Hz, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 13.8, 19.2, 31.2, 44, 56.2, 58.1, 67.3, 67.8, 68.8, 69.4, 70.6, 70.7, 74.6, 84.1, 109.4, 113.4, 117.6, 133.3, 148.4, 149.9, 157.9, 159.5 (CO). **ESI-MS** (40 eV): *m/z* (%) = 460 (100%) $[M]^+$.



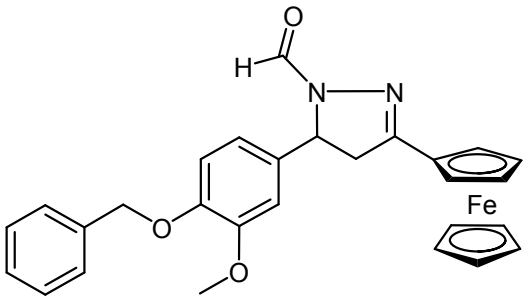
^{1}H NMR spectrum of compound **3e**



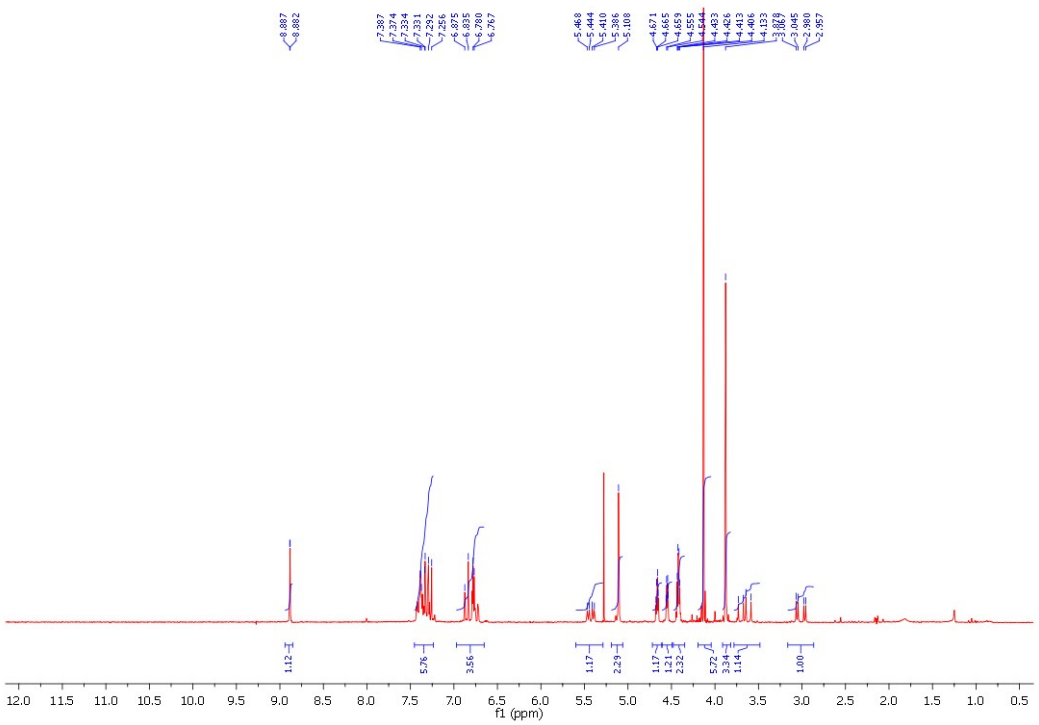
^{13}C NMR spectrum of compound **3e**

5-(4-benzyloxy-3-methoxyphenyl)-3-ferrocenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde;

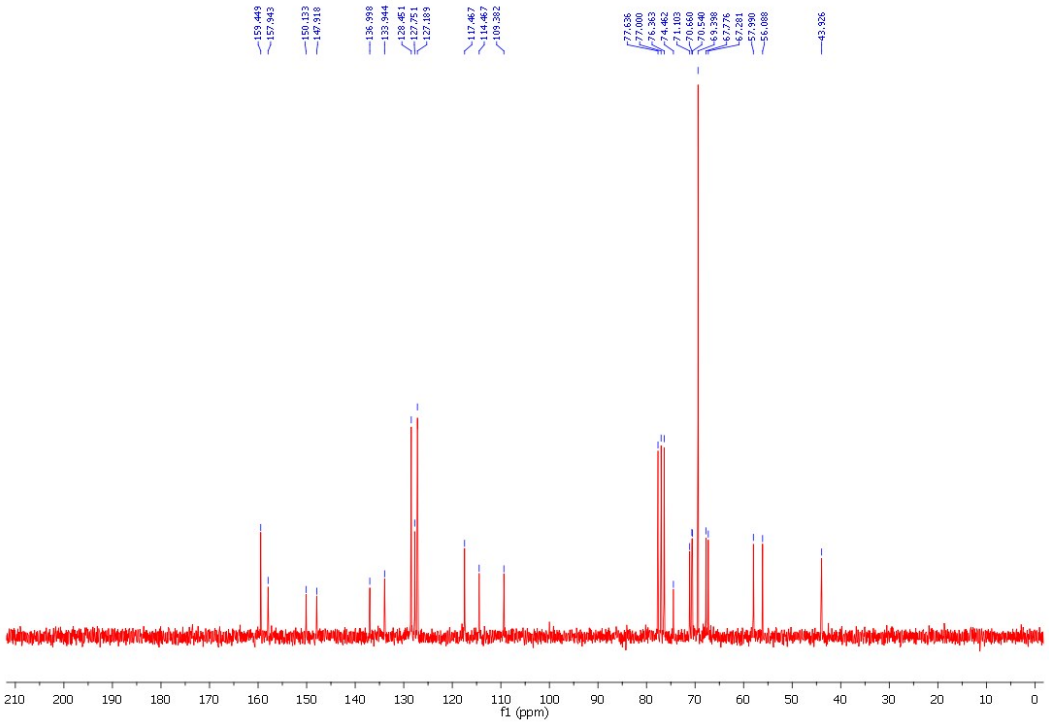
3f



Light orange; mp 149-150ºC; Yield 88%; IR (KBr): 3089, 2924, 2858, 1664, 1601, 1514, 1416, 1358, 1310, 1256, 1229, 1169, 1137, 1014 cm^{-1}; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.01 (dd, *J*=17.6, 4.6Hz, 1H), 3.66 (dd, *J*=17.6, 11.6Hz, 1H), 3.88 (s, 3H), 4.13 (s, 5H), 4.41-4.43 (m, 2H), 4.55 (dt, *J*=2.4, 1.4Hz, 1H), 4.66 (dt, *J*=2.4, 1.2Hz, 1H), 5.11 (s, 2H), 5.43 (dd, *J*=11.6, 4.8Hz, 1H), 6.77-6.87 (m, 3H), 7.26-7.39 (m, 5H), 8.88 (d, *J*=1.0Hz, 1H); ^{13}C NMR: δ 43.9, 56.1, 57.9, 67.3, 67.8, 69.4, 70.5, 70.7, 71.1, 74.5, 109.4, 114.5, 117.5, 127.2, 127.7, 128.4, 133.9, 136.9, 147.9, 150.1, 157.9, 159.4 (CO). **ESI-MS** (40 eV): *m/z* (%) = 494 (100%) $[M]^+$.



^{1}H NMR spectrum of compound **3f**



^{13}C NMR spectrum of compound **3f**

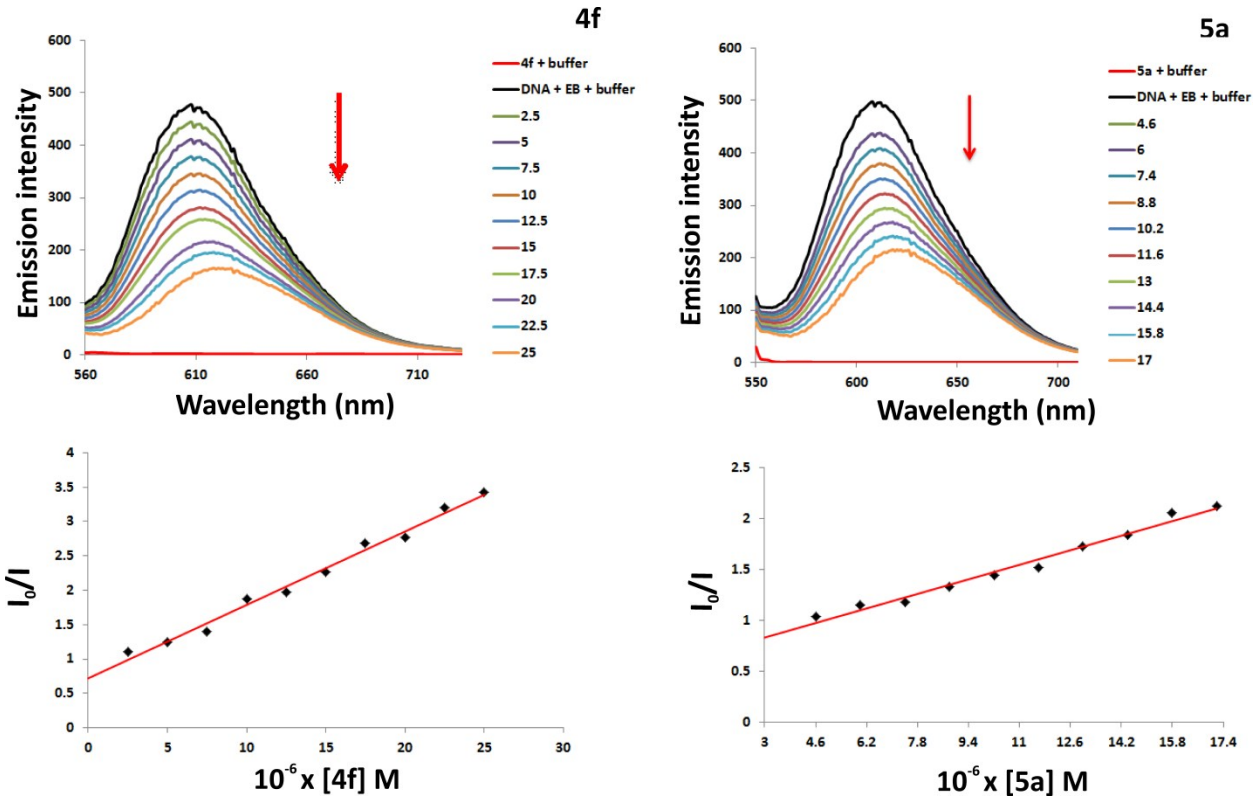


Fig. S1 Top: emission spectra of EB bound to DNA in the absence (black lines) and presence of compounds **4f** and **5a**. The red lines denote solutions: buffer + quencher. [EB] = 25 μM, [DNA] = 25 μM; [**4f**] = 0–25 μM and [**5a**]= 0–17.2 μM; pH = 7.4; λ_{ex} = 520 nm. Bottom: Stern-Volmer plots of I_0/I versus [Q].

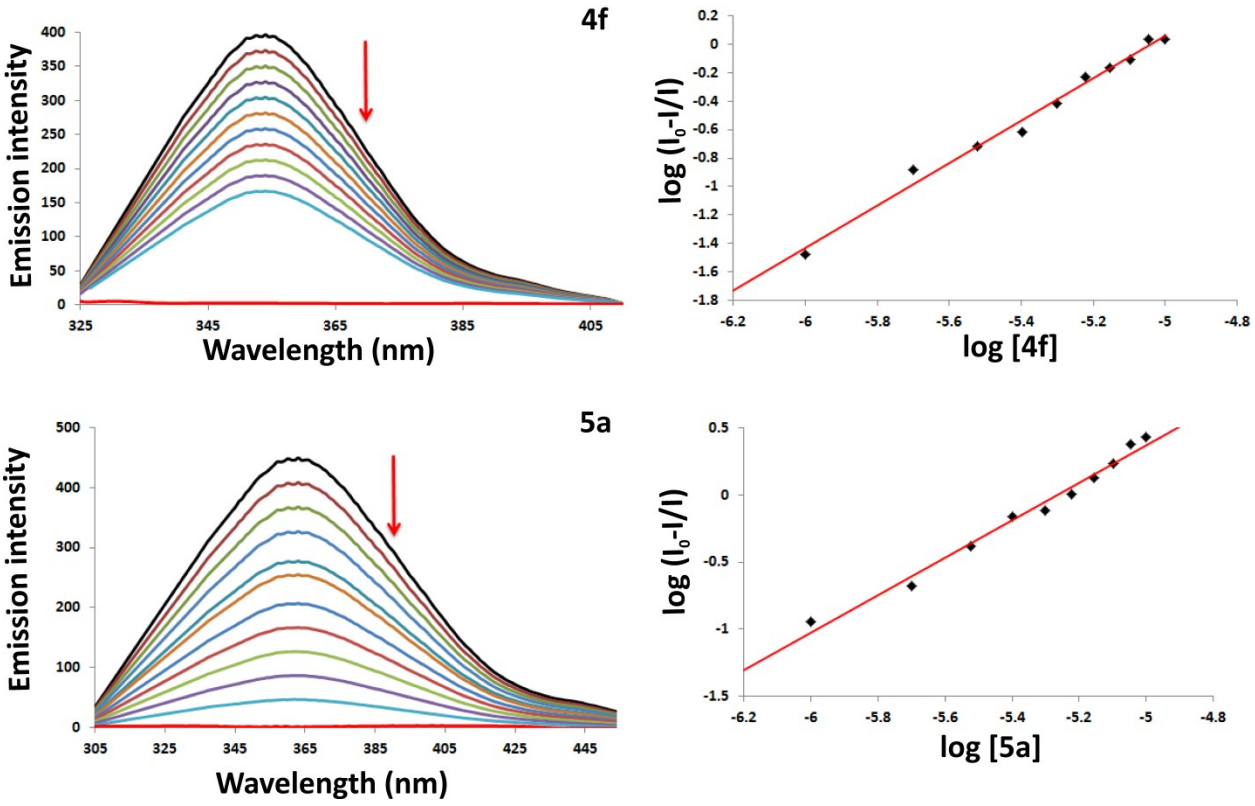
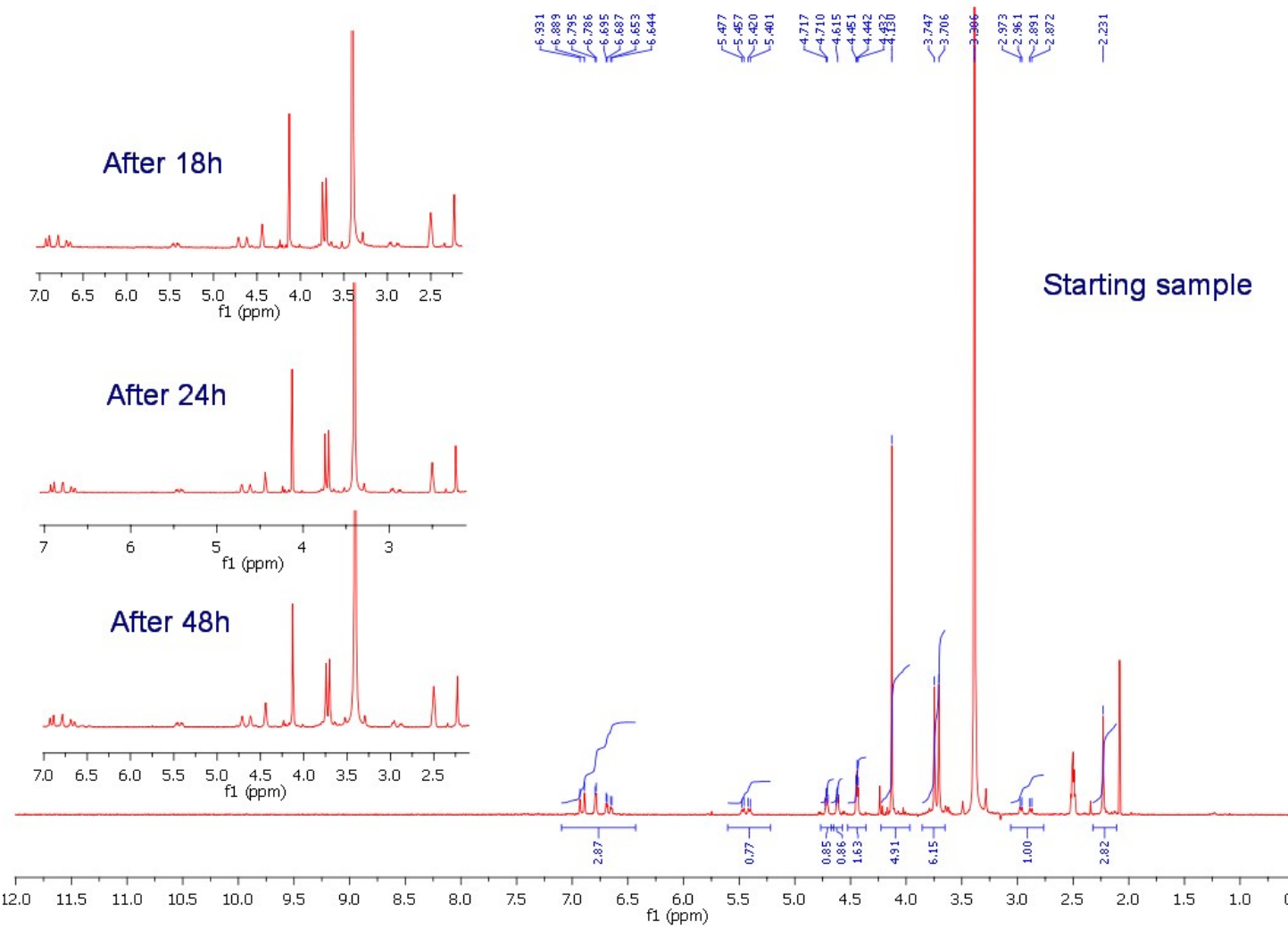


Fig. S2 Emission spectra of BSA in the absence (black lines) and presence of compounds **4f** and **5a**. The red lines denote solutions: buffer + quencher. [BSA] = 1.2 μM; [**4f**] and [**5a**] = 0.0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0 and 10.0 μM; pH = 7.4; λ_{ex} = 295 nm. Plots of log[(I_0-I/I)] versus log[Q].



Spectra of compound **4a** (the main reason for choosing this compound as representative compound is very good activity compared with others) were recorded in DMSO-d_6; NMR experiments were performed after 18, 24 and 48 hours.

No changes were observed in the spectra, which mean that compounds are stable in polar solvent.