Supplementary Information

Synthesis and characterization of bioactive isoxazole and 1,3,4-oxadiazole heterocycle containing scaffolds

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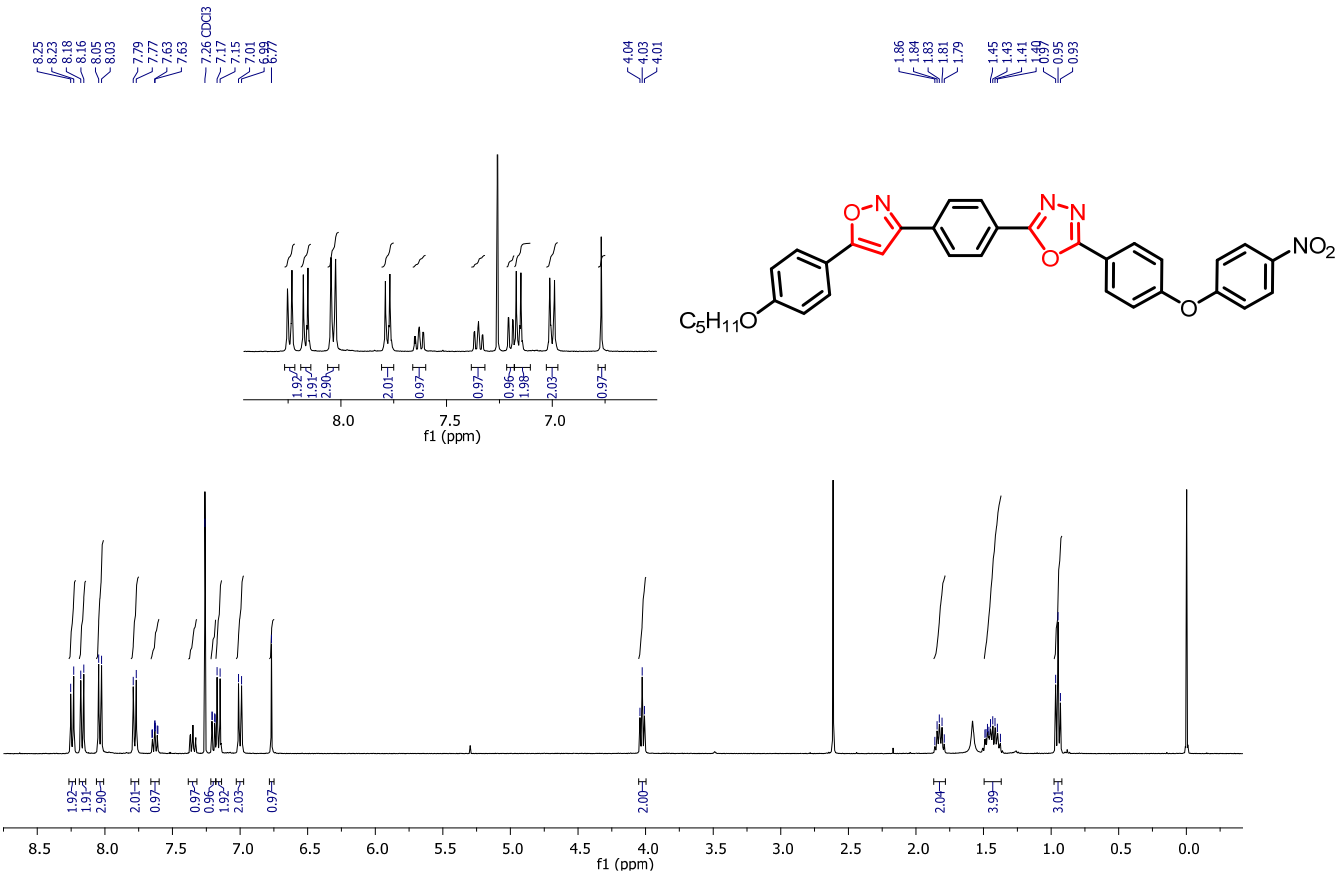
General Information

Intermediated B benzhydrezide derivative was prepared in the lab as per the literature report.[1] Required reagents, solvents, and catalysts were procured from various chemical vendors Spectrochem, Avra chemicals, and S.D. fine chem., otherwise stated. Anhydrous solvent, when required were prepared according to standard drying methods. The melting point was recorded in the open capillary in Büchi Melting point B-545. ^{1}H and ^{13}C NMR spectra were recorded at 400 MHz and 101 MHz respectively, on bruker AV400 Avance using CDCl3 purchased from Merck as internal standard (CDCl3 at 7.27 ppm for ^{1}H and 77.00 ppm for ^{13}C) with reference to TMS. Chemical shifts (δ) are given in ppm. IR analysis was carried out on Perkin- Elmer and Shimadzu FTIR. Mass analysis was carried out in Shimadzu LCMS, showing the molecular ion peak. The activity was carried out at Microcare laboratory, Surat. The strains were procured from the Institute of Microbial Technology, Chandigarh.

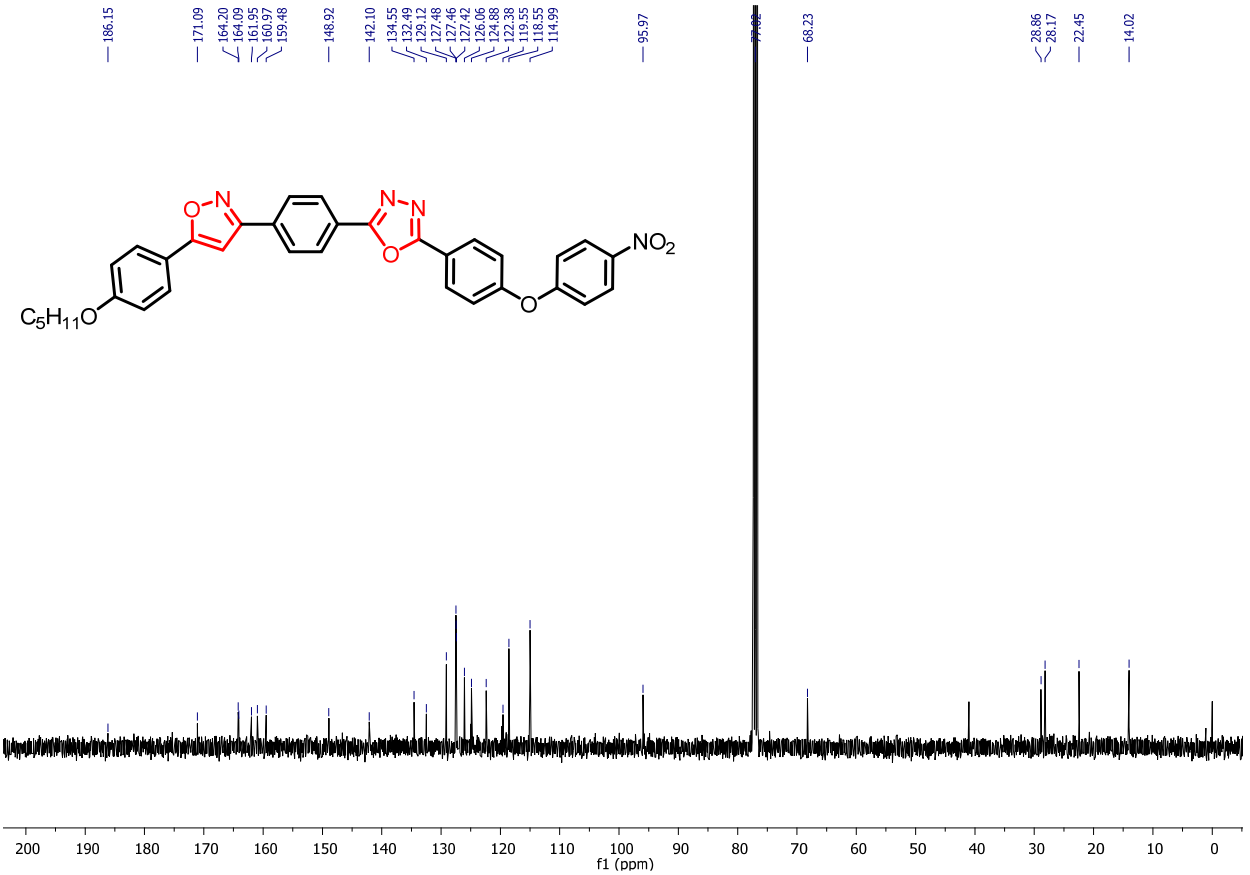
Reference

[1]Ohigashi, A., Kanda, A., Tsuboi, H., Hashimoto, N.; *Org. Process Res. Dev.***2005**, *9*, 179-184



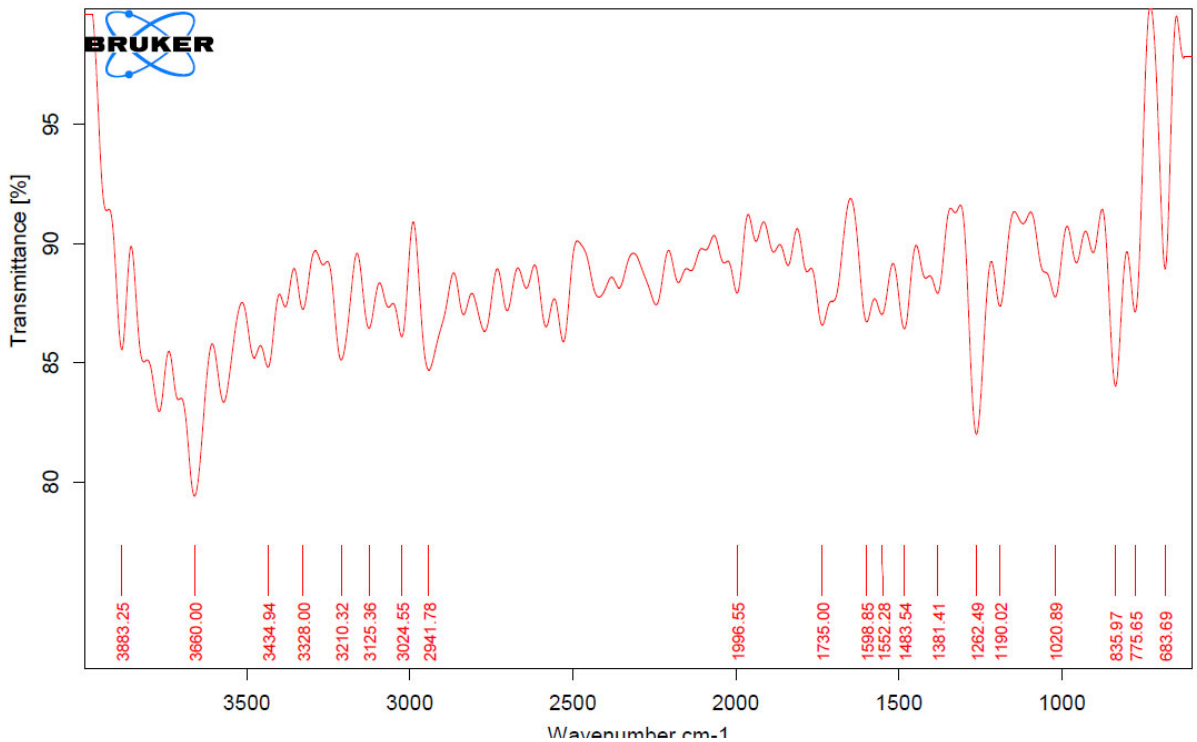
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.5 Hz, 2H), 8.17 (d, *J* = 8.9 Hz, 2H), 8.04 (d, *J* = 8.5 Hz, 3H), 7.78 (d, *J* = 8.8 Hz, 2H), 7.63 (ddd, *J* = 8.3, 7.5, 1.7 Hz, 1H), 7.39 – 7.32 (m, 1H), 7.20 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.16 (d, *J* = 8.9 Hz, 2H), 7.00 (d, *J* = 8.9 Hz, 2H), 6.77 (s, 1H), 4.03 (t, *J* = 6.6 Hz, 2H), 1.87 – 1.78 (m, 2H), 1.52 – 1.35 (m, 4H), 0.95 (t, *J* = 7.1 Hz, 3H).

Fig. S1 — ^{1}H NMR spectrum of **8a**



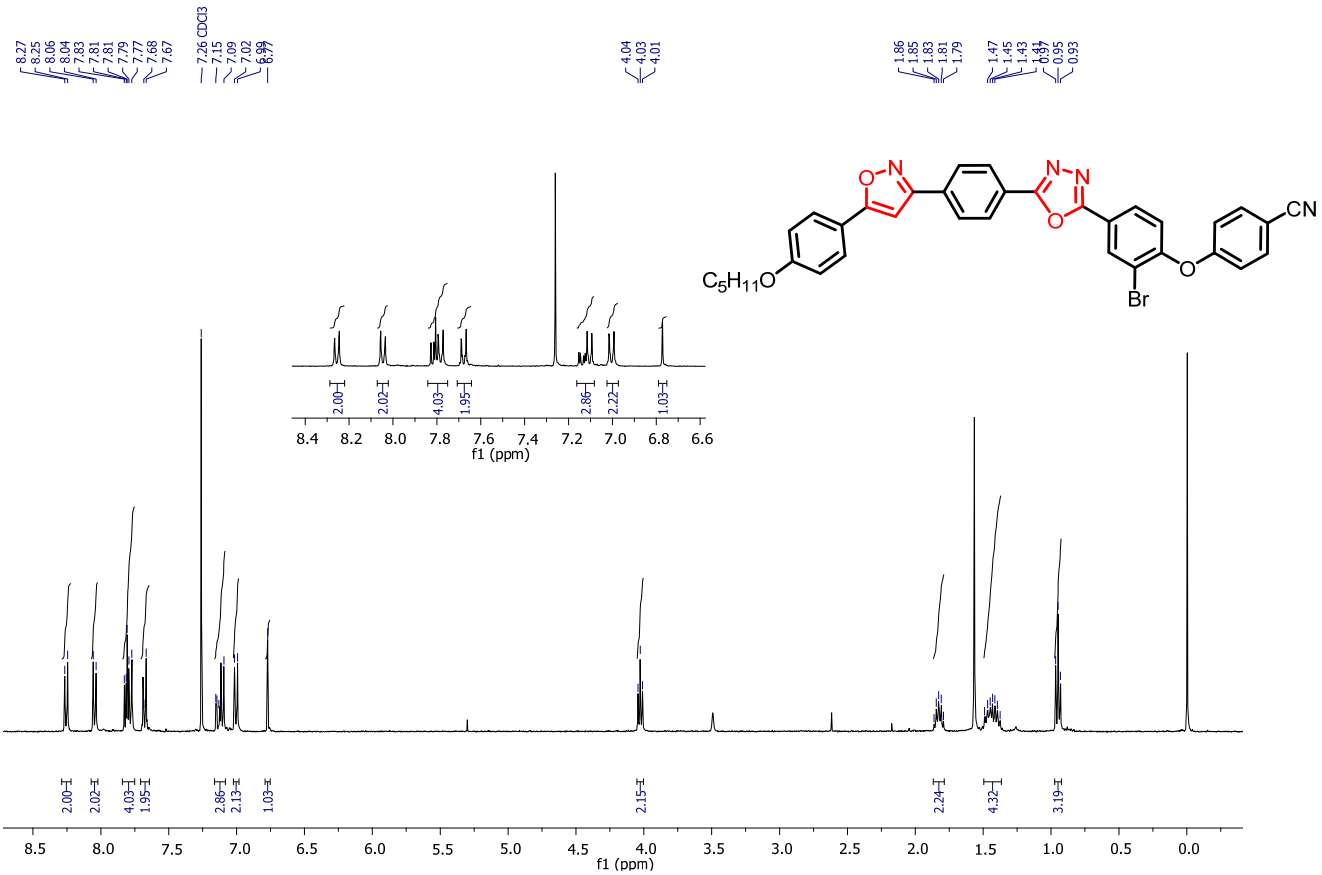
^{13}C NMR (101 MHz, $CDCl_3$) δ 186.15, 171.09, 164.20, 164.09, 161.95, 160.97, 159.48, 148.92, 142.10, 134.55, 132.49, 129.12, 127.48, 127.46, 127.42, 126.06, 124.88, 122.38, 119.55, 118.55, 114.99, 95.97, 68.23, 28.86, 28.17, 22.45, 14.02.

Fig. S2 — ^{13}C NMR spectrum of **8a**



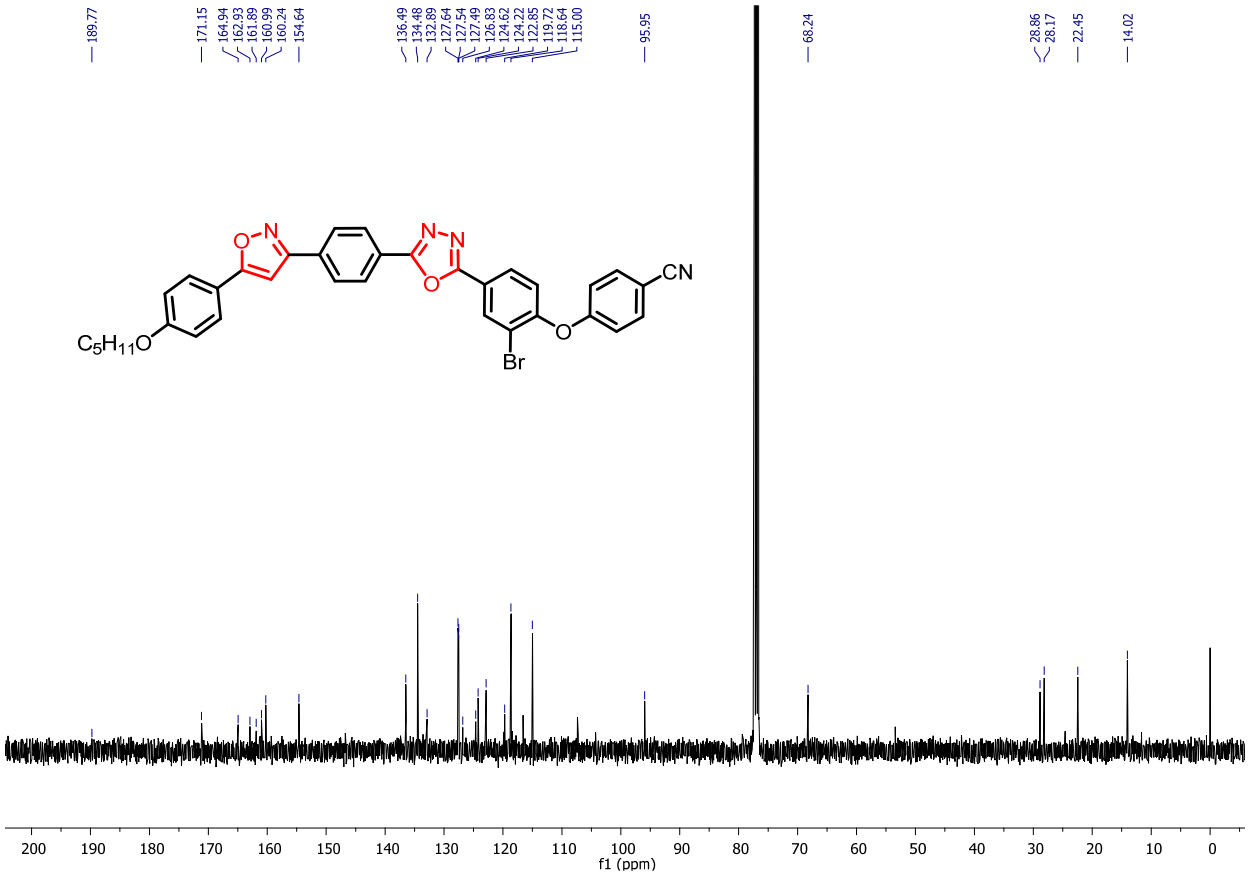
IR (KBr) cm^{-1}: 3883, 3660, 3435, 3328, 3210, 3125, 3025, 2942, 1997, 1735, 1599, 1552, 1484, 1381, 1262, 1190, 1021, 836, 776, 684;

Fig. S3 — IR spectrum of **8a**



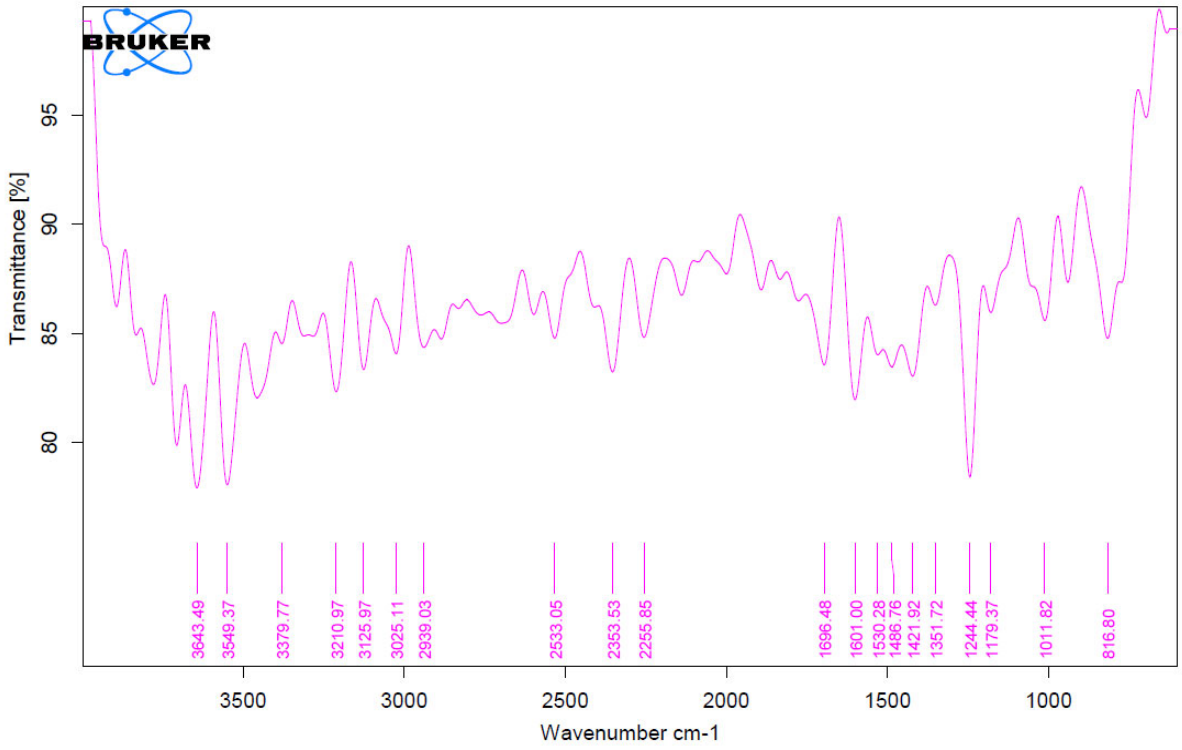
^{1}H NMR (400 MHz, CHLOROFORM-D) δ 8.26 (d, *J* = 8.3 Hz, 2H), 8.05 (d, *J* = 8.4 Hz, 2H), 7.84 – 7.75 (m, 4H), 7.68 (d, *J* = 7.0 Hz, 2H), 7.13 (dd, *J* = 14.8, 8.9 Hz, 3H), 7.00 (d, *J* = 8.8 Hz, 2H), 6.77 (s, 1H), 4.03 (t, *J* = 6.5 Hz, 2H), 1.87 – 1.77 (m, 2H), 1.50 – 1.36 (m, 4H), 0.95 (t, *J* = 7.1 Hz, 3H).

Fig. S4 — ^{1}H NMR spectrum of **8b**



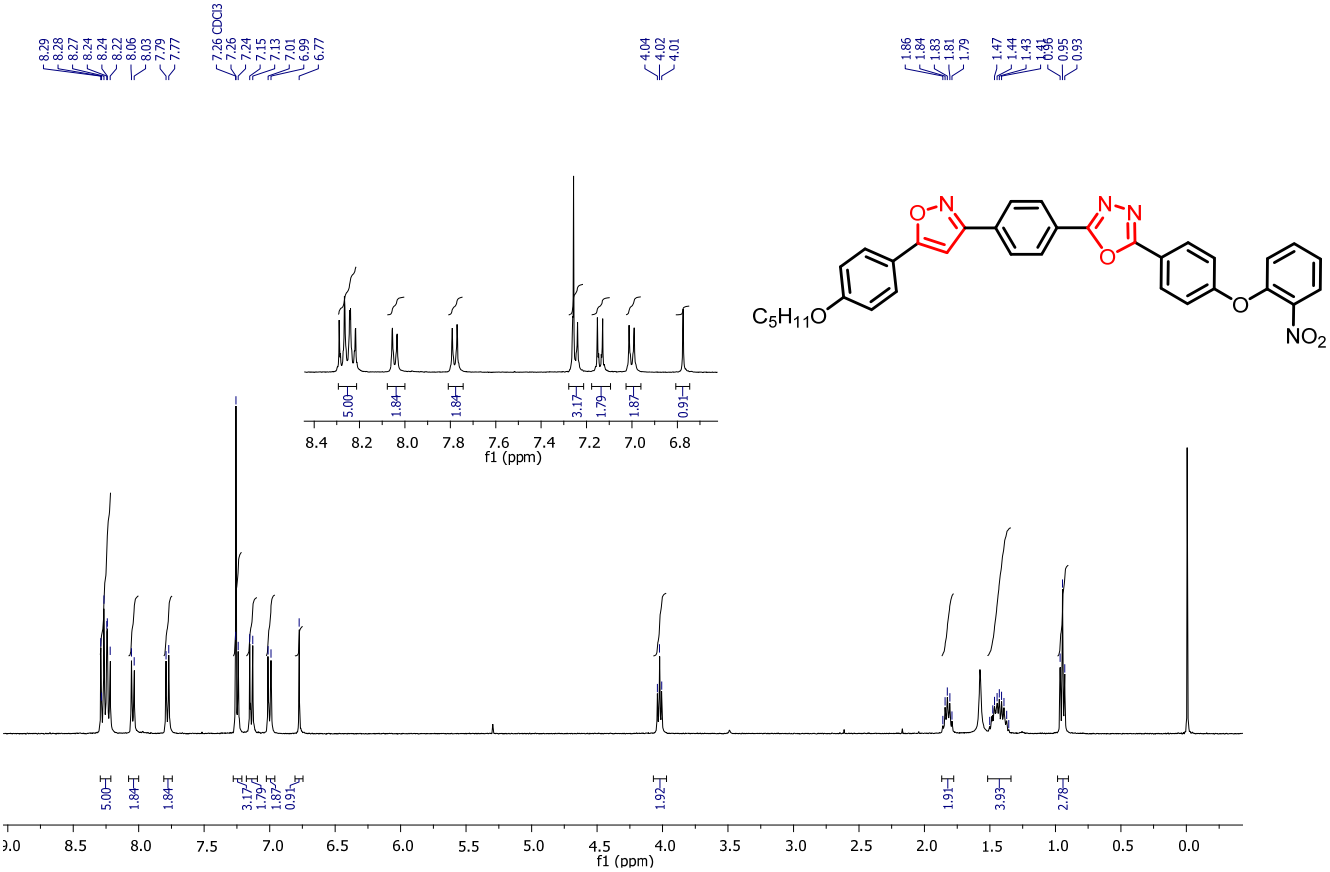
^{13}C NMR (101 MHz, $CDCl_3$) δ 189.77, 171.15, 164.94, 162.93, 161.89, 160.99, 160.24, 154.64, 136.49, 134.48, 132.89, 127.64, 127.54, 127.49, 126.83, 124.62, 124.22, 122.85, 119.72, 118.64, 115.00, 95.95, 68.24, 28.86, 28.17, 22.45, 14.02.

Fig. S5 — ^{13}C NMR spectrum of **8b**



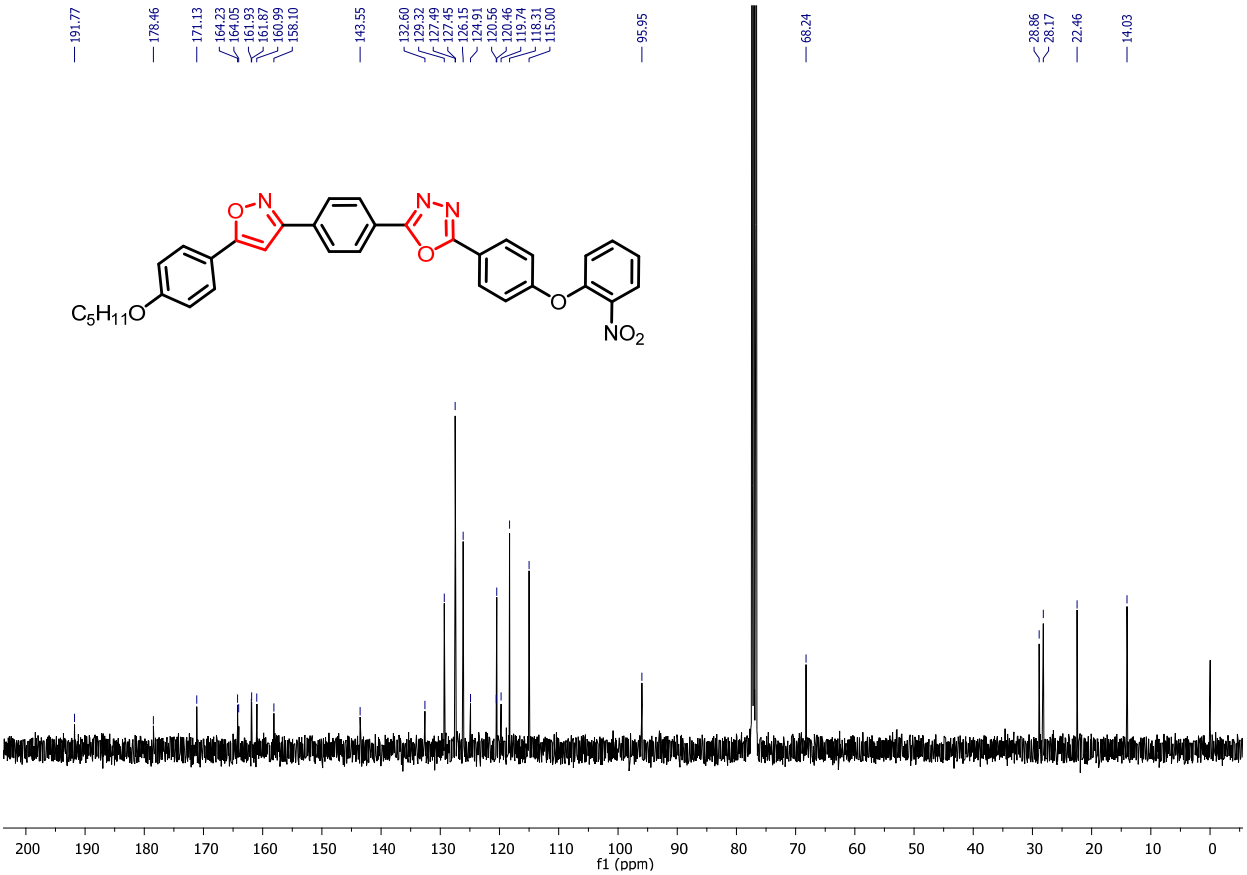
IR (KBr) cm^{-1}: 3643, 3549, 3380, 3211, 3126, 3025, 2939, 2533, 2354, 2256, 1696, 1601, 1530, 1487, 1422, 1352, 1244, 1179, 1012, 817;

Fig. S6 — IR spectrum of **8b**



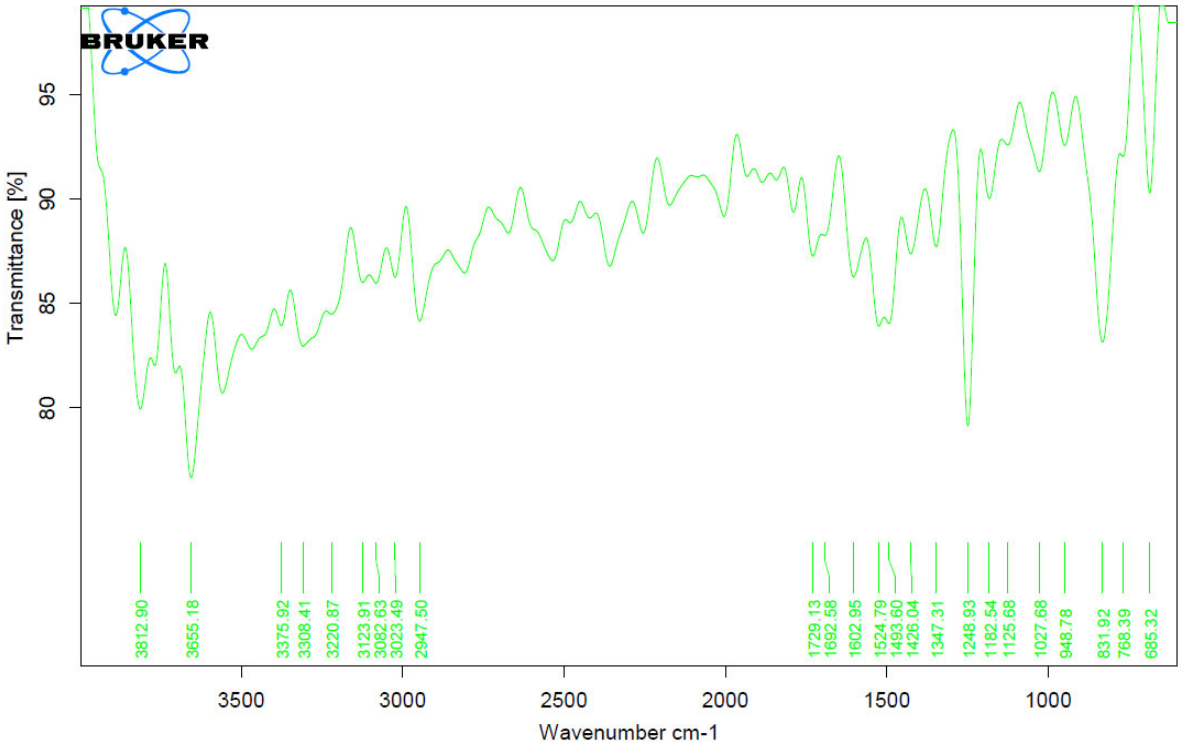
^{1}H NMR (400 MHz, CHLOROFORM-D) δ 8.30 – 8.21 (m, 5H), 8.04 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 8.5 Hz, 2H), 7.28 – 7.21 (m, 3H), 7.14 (d, *J* = 9.1 Hz, 2H), 7.00 (d, *J* = 8.9 Hz, 2H), 6.77 (s, 1H), 4.02 (t, *J* = 6.5 Hz, 2H), 1.86 – 1.77 (m, 2H), 1.50 – 1.35 (m, 4H), 0.95 (t, *J* = 7.1 Hz, 3H).

Fig. S7 — ^{1}H NMR spectrum of **8c**



^{13}C NMR (101 MHz, $CDCl_3$) δ 191.77, 178.46, 171.13, 164.23, 164.05, 161.93, 161.87, 160.99, 158.10, 143.55, 132.60, 129.32, 127.49, 127.45, 126.15, 124.91, 120.56, 120.46, 119.74, 118.31, 115.00, 95.95, 68.24, 28.86, 28.17, 22.46, 14.03.

Fig. S8 — ^{13}C NMR spectrum of **8c**



IR (KBr) cm^{-1}: 3813, 3655, 3376, 3308, 3221, 3124, 3083, 3023, 2948, 1729, 1693, 1603, 1525, 1494, 1426, 1347, 1249, 1183, 1126, 1028, 949, 832, 768, 685;

Fig. S9 — IR spectrum of **8c**