Supporting Information

Organic & Biomolecular Chemistry

Proof of Principle of a Three-Input AND-INHIBIT-OR Combinatorial Logic Gate Array

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Experimental

Instrumentation

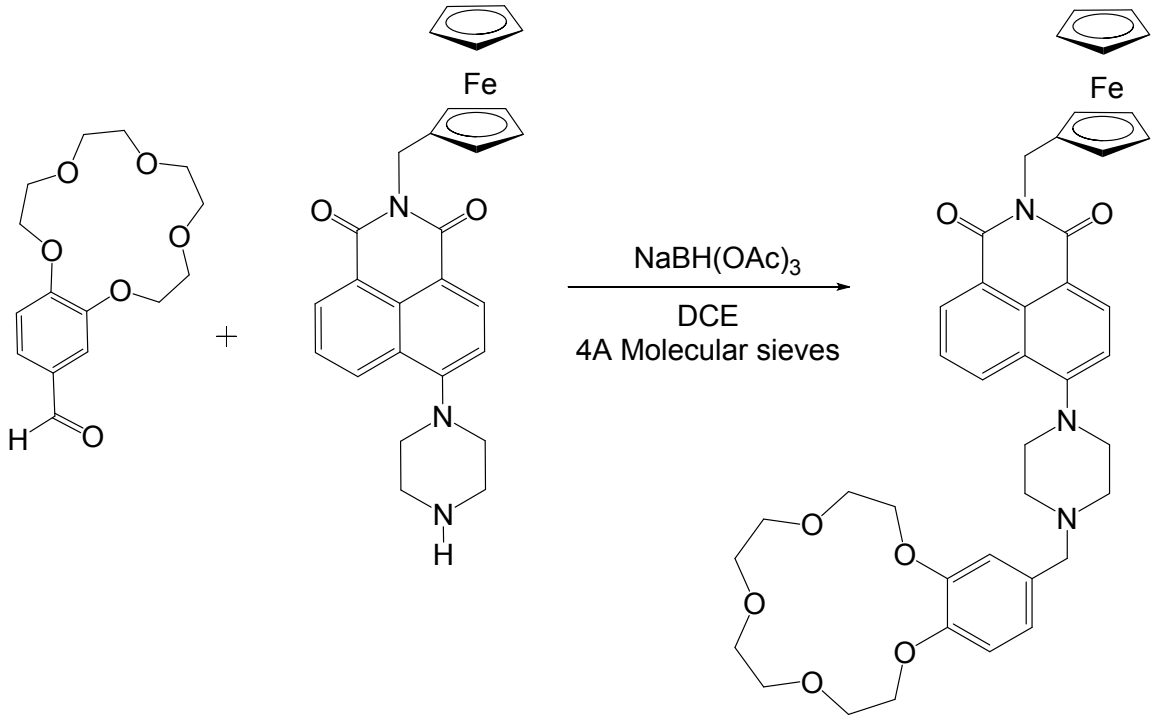
^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III HD NMR spectrometer equipped with an Ascend 500 11.75 Tesla Superconducting Magnet, operating at a frequency of 500.13 MHz for ^{1}H NMR and 125.76 MHz for ^{13}C NMR and with a multinuclear 5 mm PABBO Probe. Data were acquired and processed via Topspin Software, ver. 3.2. Chemical shifts for ^{1}H NMR were recorded in ppm downfield from TMS set at δ = 0.00 ppm and ^{13}C NMR spectra were referenced to the solvent triplet signal of $CDCl_3$ at δ = 77.00 ppm. Infra-red spectra were recorded on a Shimadzu IR-affinity 1 FT-IR spectrometer calibrated against polystyrene at 1602 cm^{-1} as KBr disks. Electrospray time-of-flight (ES-TOF) spectra were performed on a Waters LC Premier instrument.

UV-visible absorption spectra were recorded on a Jasco V-650 spectrophotometer connected to a desktop computer. The instrumentation parameters were set to medium response, bandwidth of 2 nm and scan speed of 200 nm min^{-1}. Samples were scanned over the range of 350-600 nm. All spectra were background corrected for the solvent by scanning the appropriate blank solvent prior to beginning the experiments. Fluorimetric studies were conducted using a Jasco FP-8300 spectrophotometer with a 10 mm path length quartz cuvette. The excitation and emission slits were set at 2.5 and 5.0 nm, respectively. The emission range was 400-650 nm, unless otherwise stated.

Synthesis: *N*-ferrocenylmethyl-4-(piperazine-4′-benzo-15-crown-5)-1,8-naphthalimide **1**

4′-Formylbenzo-15-crown-5 (0.215 g, 0.730 mmol), 3 (0.118 g, 0.250 mmol), sodium triacetoxyborohydride (0.237 g, 1.12 mmol) and glacial acetic acid (0.053 g/ 50 μL, 0.88 mmol) were mixed in 20 mL of 1,2-dichloroethane (DCE).[1] The reaction was carried out at room temperature for 5 days in the presence of 4 Å molecular sieves. The reaction mixture was filtered and then washed with copious amount of water to remove Na^{+} cations from the crown ether. The product was extracted with dichloromethane and dried using activated molecular sieves size 4 Å. Excess solvent was removed by rotary evaporator and the desired product was purified via recrystallisation using 1:1 (*v/v*)

acetone/ethanol. A yellow solid was collected in 12% yield. R_f = 0.61 (8:1 (*v*/*v*) CH_2Cl_2/MeOH); m.p. = 137-141 °C; ^{1}H NMR ($CDCl_3$, ppm): δ 8.55 (dd, 1H, *J* = 7.4, 1.1 Hz, Ar-*H*), 8.48 (d, 1H, *J* = 8.1 Hz, Ar-*H*), 8.37 (dd, 1H, *J* = 8.5, 1.1 Hz, Ar-*H*), 7.64 (dd, 1H, *J* = 7.9, 1.1 Hz, Ar-*H*), 7.17 (d, 1H, *J* = 8.1 Hz, Ar-*H*), 6.93 (d, 1H, *J* = 1.7 Hz, Ar(benzo)-*H*), 6.86 (dd, 1H, *J* = 8.1, 1.7 Hz, Ar(benzo)-*H*), 6.83 (d, 1H, *J* = 8.1 Hz, Ar(benzo)-*H*), 5.11 (s, 2H, -NC*H*$_2$Cp), 4.49 (t, 2H, *J* = 1.8 Hz, Cp), 4.20 (m, 5H, Cp), 4.17 (m, 2H, crown *H*s), 4.14 (m, 2H, crown *H*s), 4.06 (t, 2H, *J* = 1.8 Hz, Cp), 3.92 (m, 4H, crown *H*s), 3.76 (m, 8H, crown *H*s), 3.56 (s, 2H, Ar(benzo)-C*H*$_2$N), 3.26 (m, 4H, -N(C*H*$_2$CH$_2$)$_2$NCH$_2$), 2.73 (m, 4H, -N(CH$_2$C*H*$_2$)$_2$NCH$_2$); ^{13}C NMR ($CDCl_3$, ppm): δ 164.3, 163.8, 156.1, 149.2, 148.4, 132.6, 131.0, 130.9, 130.3, 129.9, 126.1, 125.5, 123.2, 122.0, 116.7, 114.9, 114.8, 113.7, 83.4, 71.1, 70.6, 70.4, 69.7, 69.2, 69.1, 68.6, 68.0, 62.7, 53.1, 53.0, 39.1; IR (KBr, cm^{-1}): 3450, 3089, 2926, 2870, 2814, 1692, 1684, 1656, 1647, 1590, 1506, 1456, 1385, 1372, 1334, 1243, 1136, 1103, 938, 785; HRMS (ES-ToF): Calculated $C_{42}H_{45}N_3O_7NaFe$ $[M+Na]^+$ 782.2505, found 782.2538.



Scheme S1: The synthesis of molecule **1** by reductive animation.

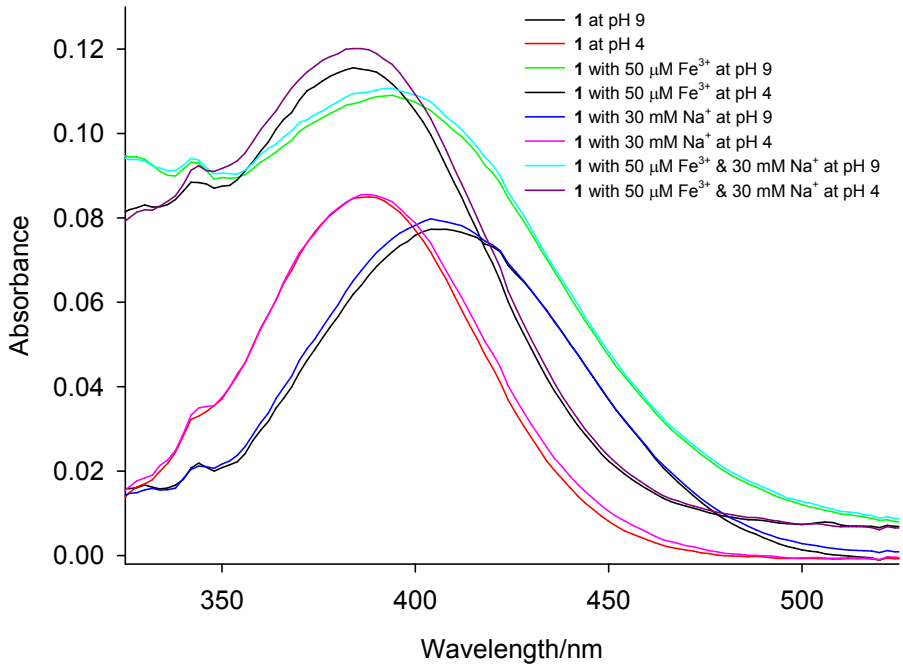


Fig. S1: UV-visible absorption spectra of 6 μM **1** in 1:1 (*v*/*v*) MeOH/H_2O for the eight inputs combinations H^+, Fe^{3+} and Na^+.

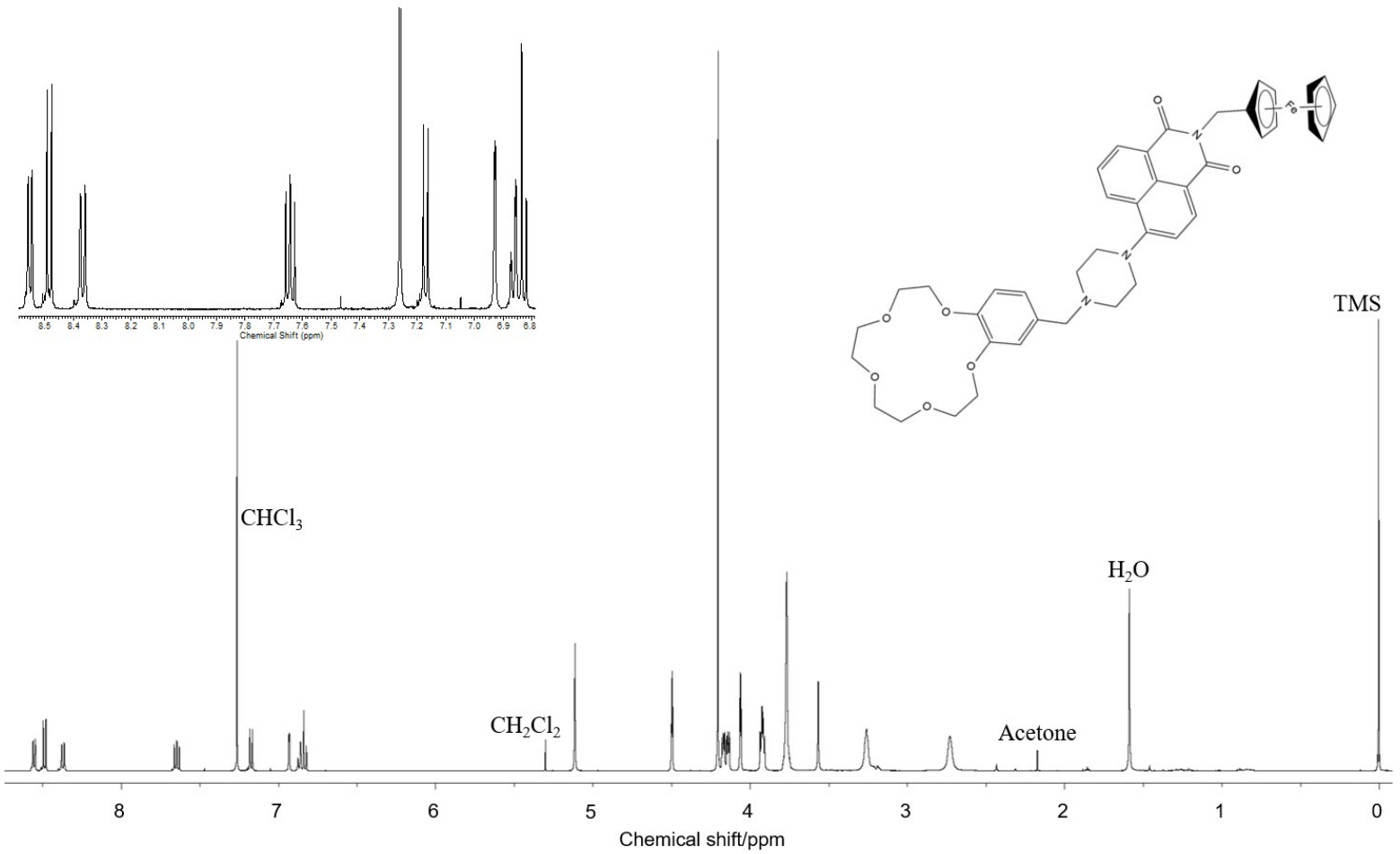


Fig. S2: ^{1}H NMR spectrum of **1** in $CDCl_3$ at 500 MHz.

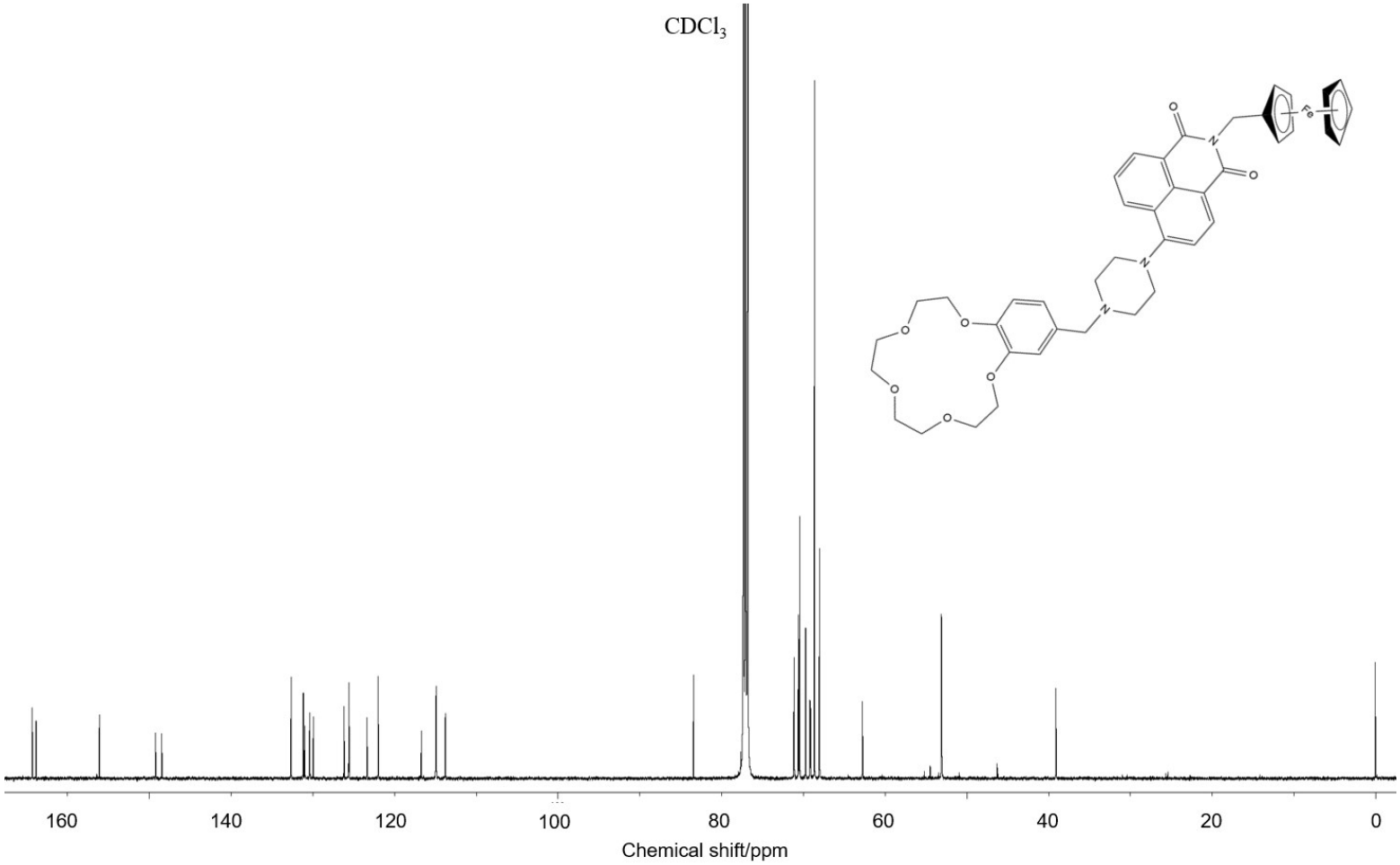


Fig. S3: ^{13}C NMR spectrum of **1** in $CDCl_3$ at 125 MHz.

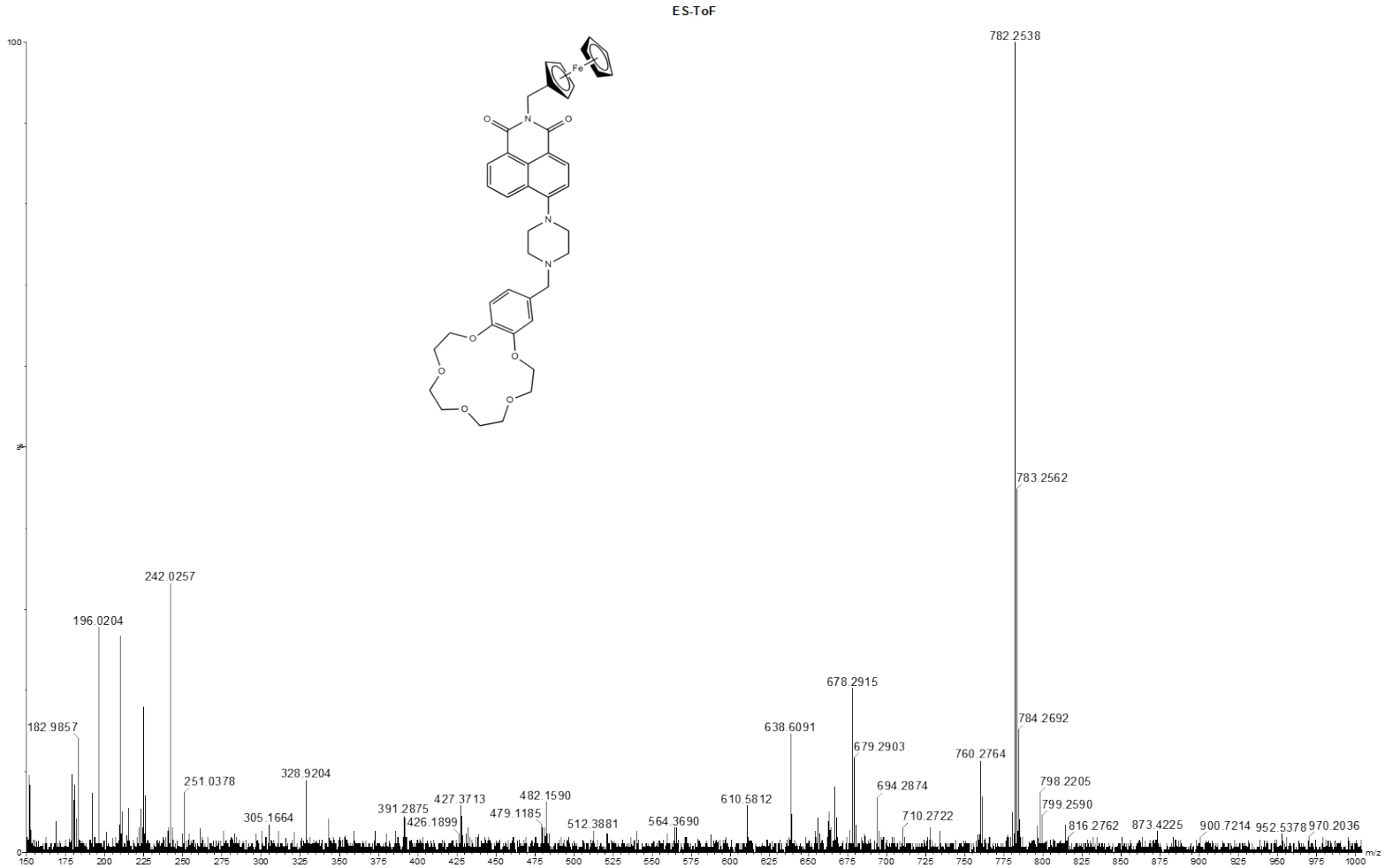


Fig. S4: High resolution MS of **1** by electrospray time-of-flight mass technique.

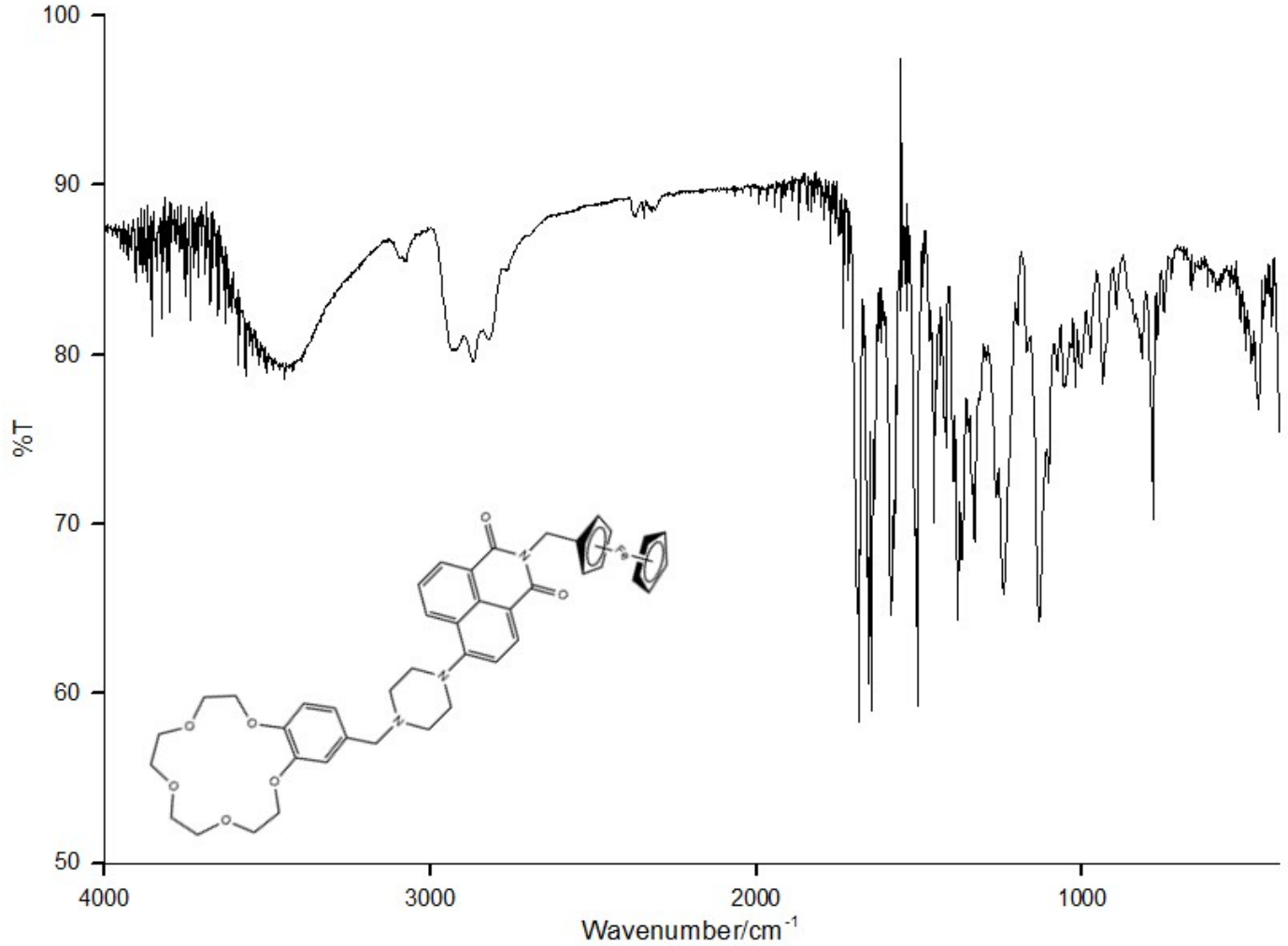


Fig. S5: IR spectrum of **1** (KBr disk).