

Supporting Information

Chemosensors

Synthesis and Spectrophotometric Studies of Heterocyclic Bay-substituted Naphthalenediimide Colorimetric pH Indicators

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Purifications & Techniques

Column chromatography was performed using sand (50-70 mesh), high purity grade silica gel (pore size 60 Å, 70-230 mesh, 63-200 µm) or aluminium oxide (pore size 60 Å, 50-200 µm). Thin-layer chromatography (TLC) was performed using silica gel on aluminium foils (pore size 60 Å) or aluminium oxide neutral (pore size 60 Å) from Sigma-Aldrich. NMR spectra were recorded in deuterated chloroform (99.8% atom D, 0.05% (v/v) TMS, Sigma-Aldrich) or (99.6 atom% stabilized with silver chip, TCI). FTIR spectra were measured with potassium bromide (99%, Fischer) dried in an oven at 200 °C and compressed with a handheld press into discs. Vanillin and caffeine analytical standards (Sigma-Aldrich) were used as melting point standards.

Instrumentation

Synthetic reactions were carried out in round-bottom flasks fitted with a reflux condenser on IKA C-MAG HP 7 hot plates equipped with a ETS-D5 temperature probe. A Stuart RE300D8 rotatory evaporator and water bath set was used for solvent removal under vacuum. Nuclear magnetic resonance (NMR) spectra were measured on a Bruker Avance III HD NMR spectrometer equipped with an Ascend 500 MHz superconducting magnet operating at 500.13 MHz and 125.76 MHz for ¹H and ¹³C respectively. Chemical shifts were calibrated versus TMS at 0.00 ppm or versus the solvent peak (CHCl₃/CDCl₃) set at 7.26 ppm and 77.00 ppm for ¹H and ¹³C, respectively. Data were acquired using a 5 mm PABBO probe and analysed using the software TopSpin version 3.2. Infra-red spectra were measured using a Shimadzu IR-Affinity1 spectrophotometer calibrated against a polystyrene film standard at 1601 cm⁻¹. Spectra were interpreted using SpectraGraph V1.2. High resolution mass spectrometry were measured by Medac Ltd. using a Waters LC premier instrument. Melting points were measured on a Stuart SMP11 melting point apparatus and are corrected. Naked eye emission was observed with a UVGL-58 handheld lamp with two wavelength settings at 254 nm and 365 nm.

Ultraviolet-visible absorbance and steady-state emission spectra were recorded on JASCO V-650 and Jasco FP-8300 spectrophotometers connect to a desktop computer at room temperature. Solutions were contained within 3.0 mL Suprasil quartz cuvettes (QS-101-10-40) with a 1.0 cm path length. For the fluorescence experiments, dilute solutions with an optical

density (OD) below 0.10 were used at the excitation wavelengths of 472 nm and 470 nm to avoid reabsorption effects. Excitation and emission slit widths were set at 2.5 nm. Anthracene used as the fluorescence quantum yield standard ($\Phi_F = 0.27$ in EtOH).

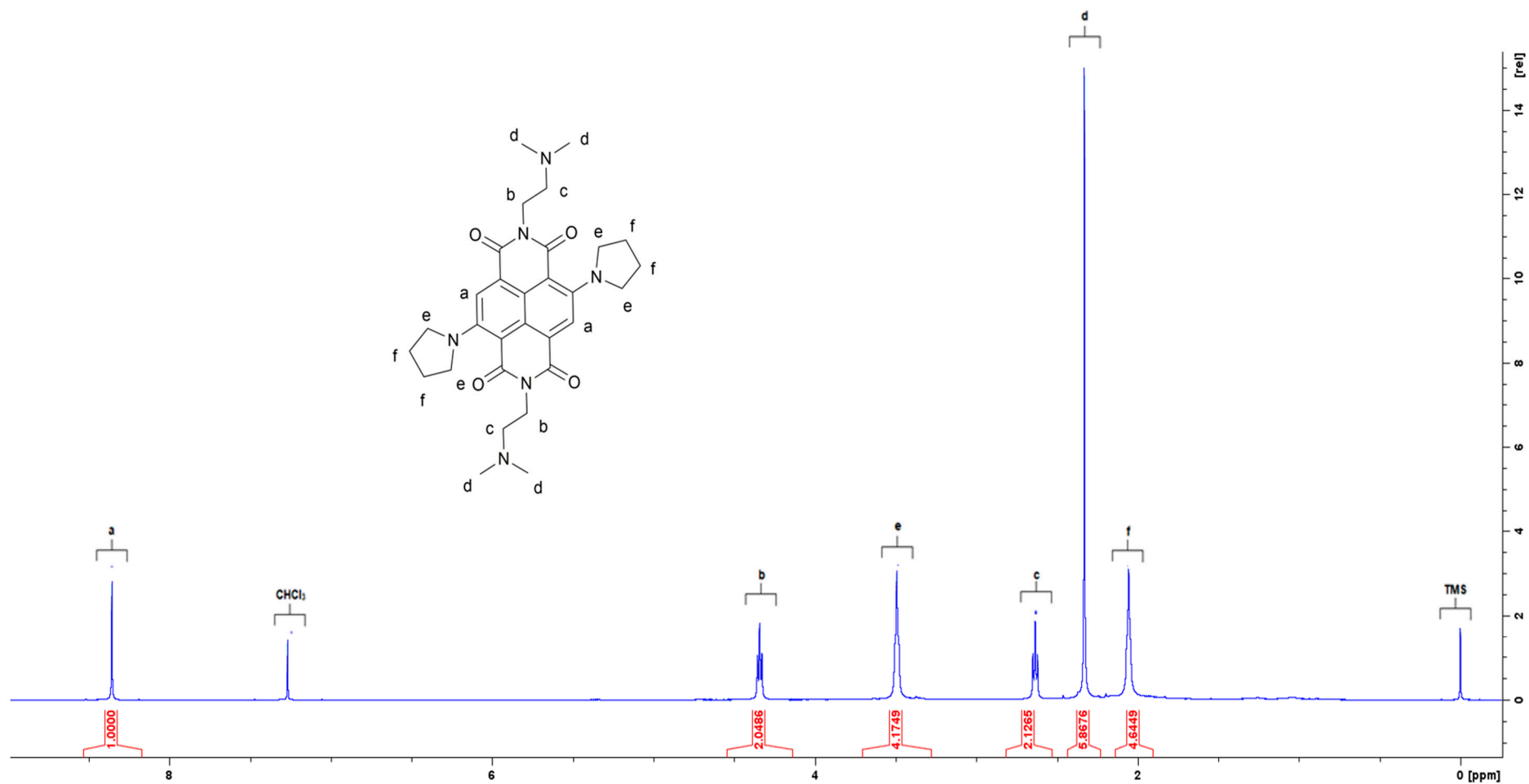


Figure S1 ^1H NMR spectrum of **1** in CDCl_3 with 0.03% TMS.

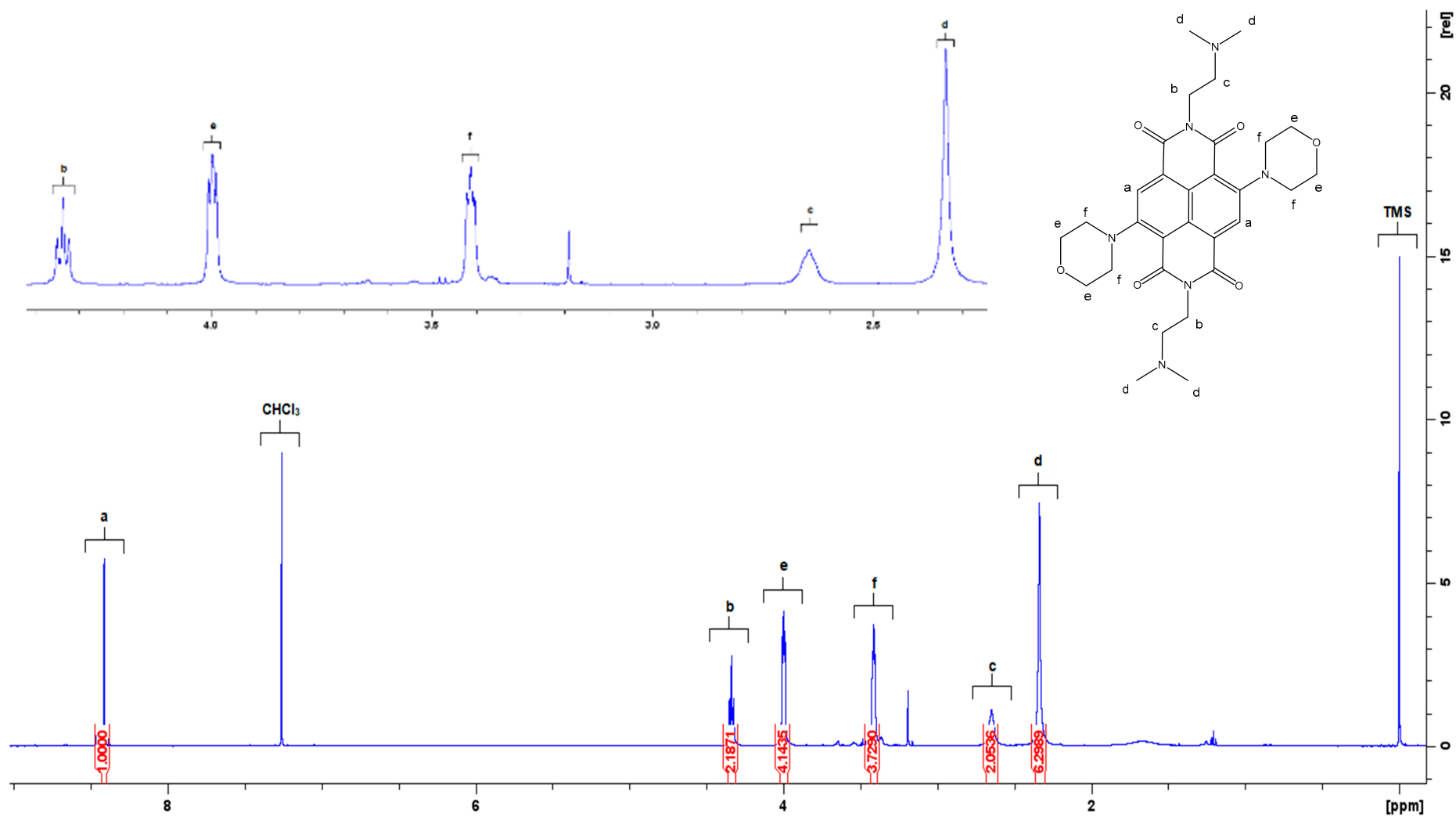


Figure S2 ^1H NMR spectrum of **2** in CDCl_3 with 0.03% TMS.

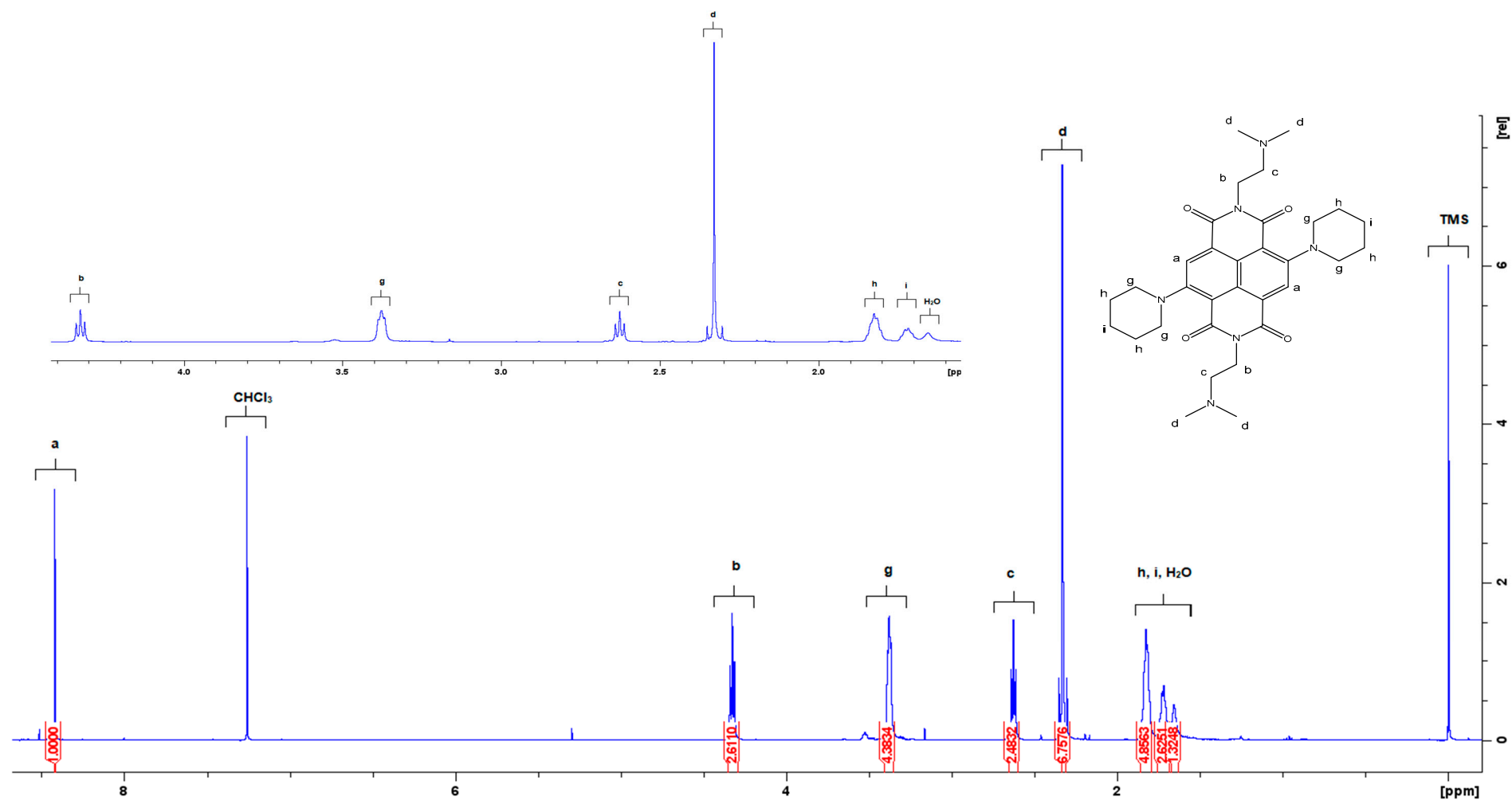


Figure S3 ^1H NMR spectrum of **3** in CDCl_3 with 0.03% TMS.

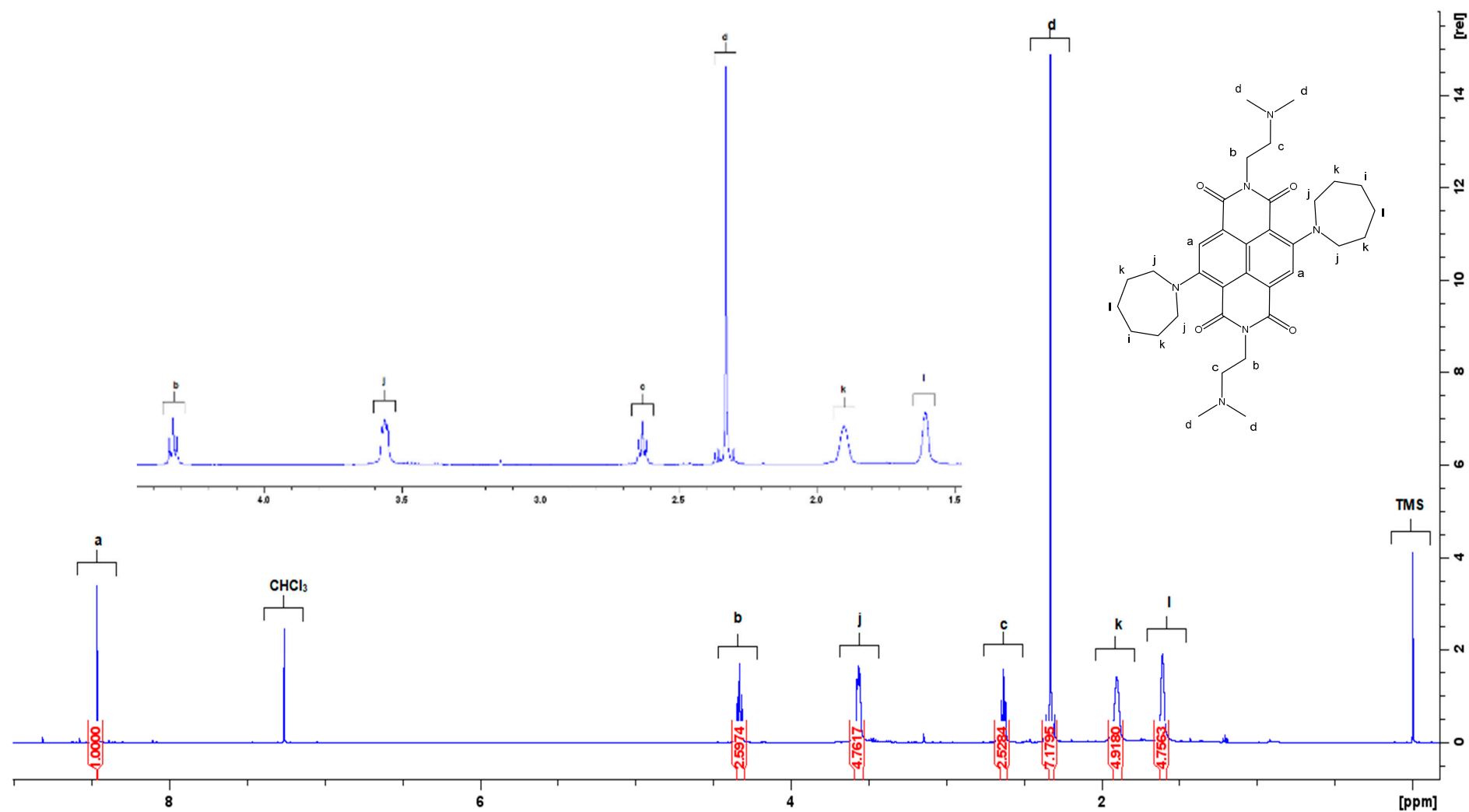


Figure S4 ^1H NMR spectrum of **4** in CDCl_3 with 0.03% TMS.

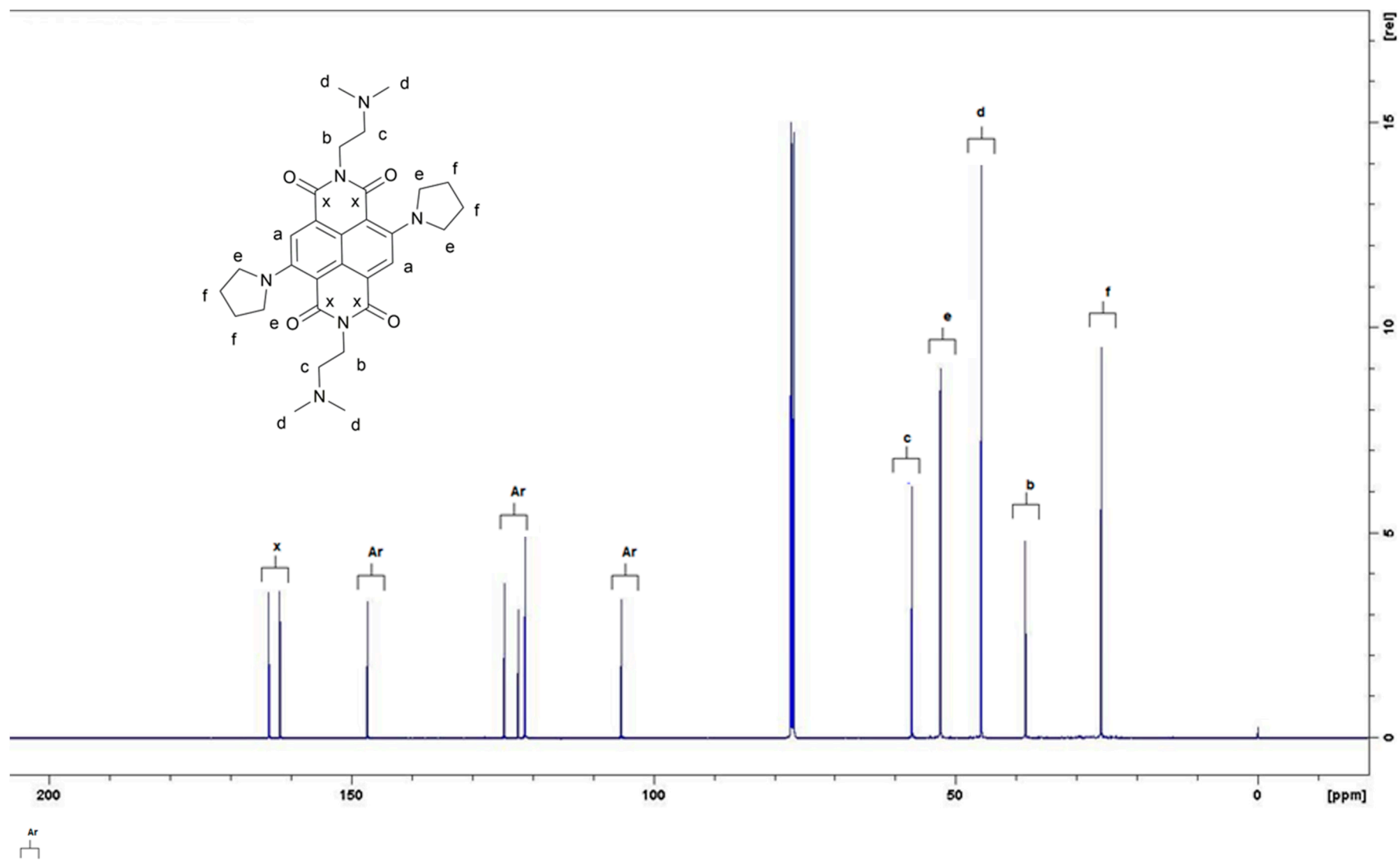


Figure S5 ¹³C NMR spectrum of **1** in CDCl₃ with 0.03% TMS.

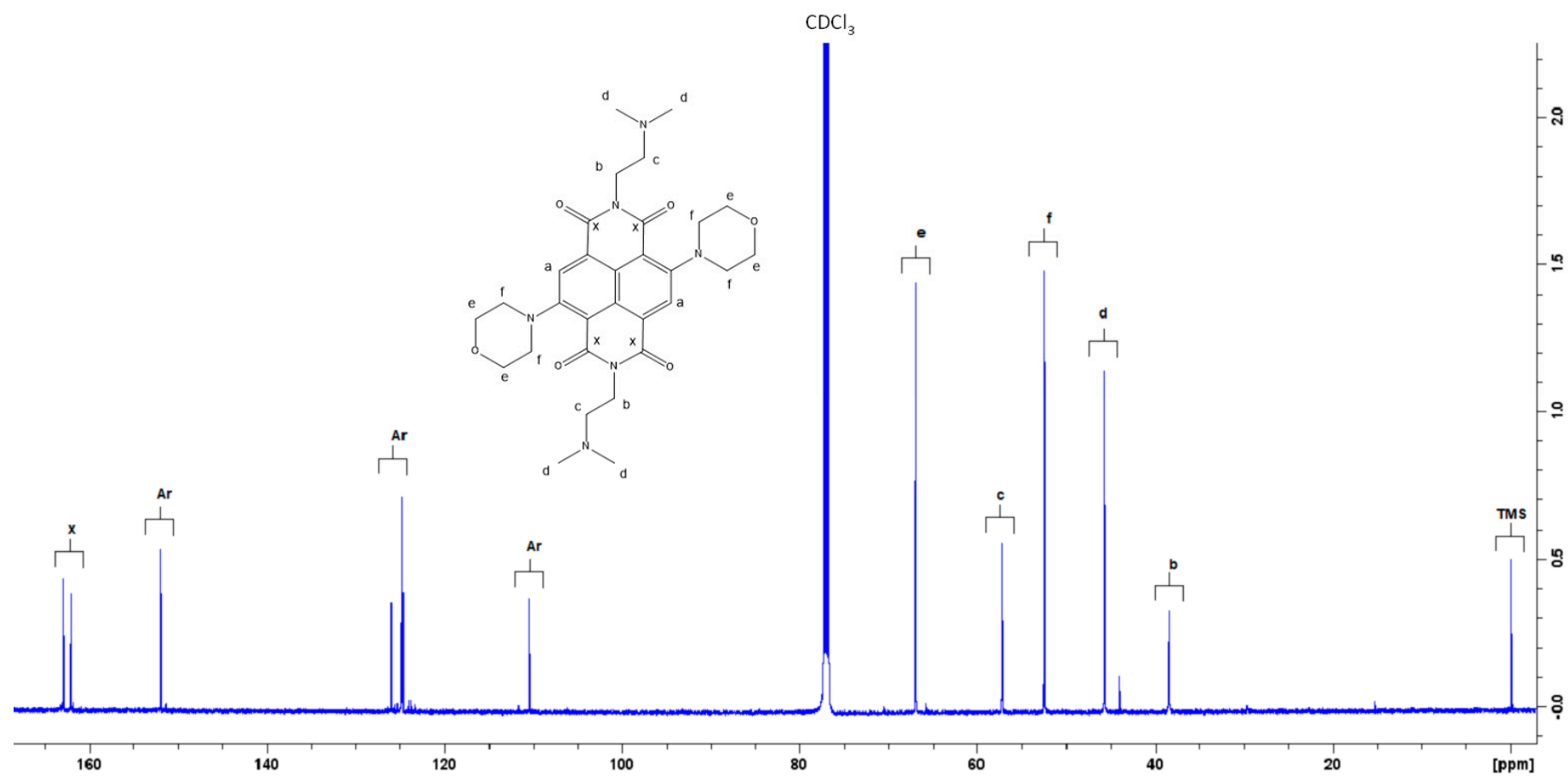


Figure S6 ^{13}C NMR spectrum of **2** in CDCl_3 with 0.03% TMS.

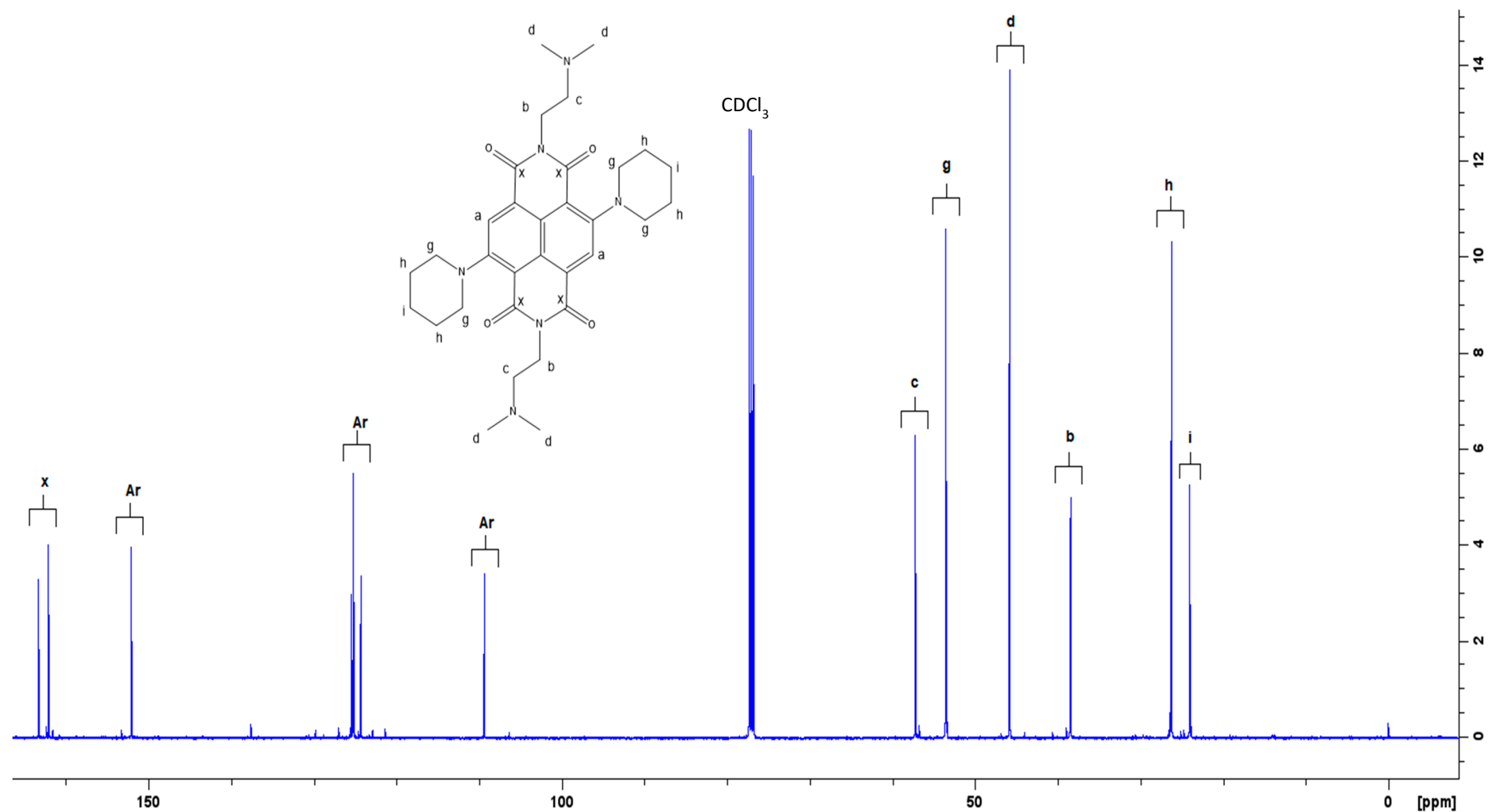


Figure S7 ^{13}C NMR spectrum of **3** in CDCl_3 with 0.03% TMS.

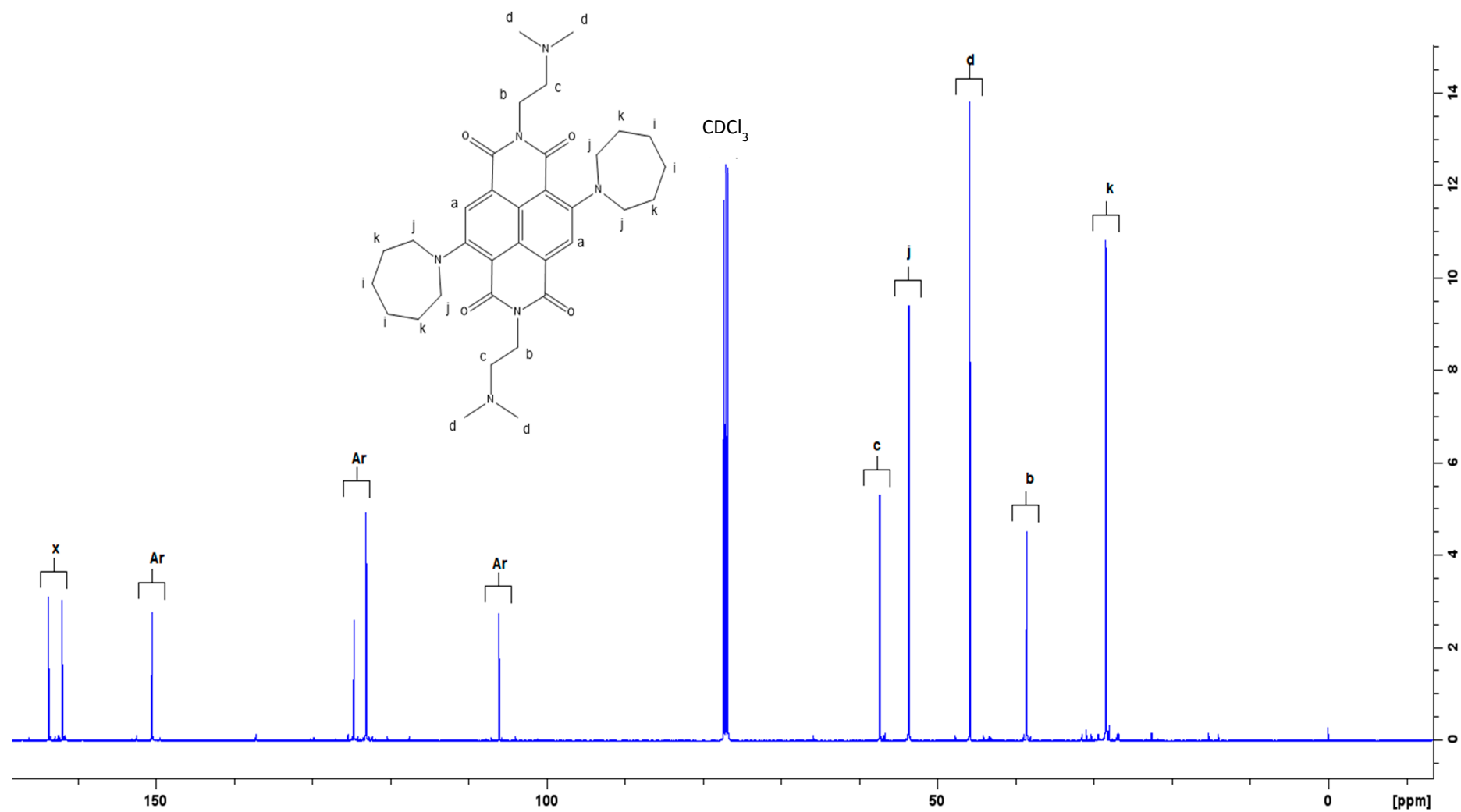


Figure S8 ^{13}C NMR spectrum of **4** in CDCl_3 with 0.03% TMS.

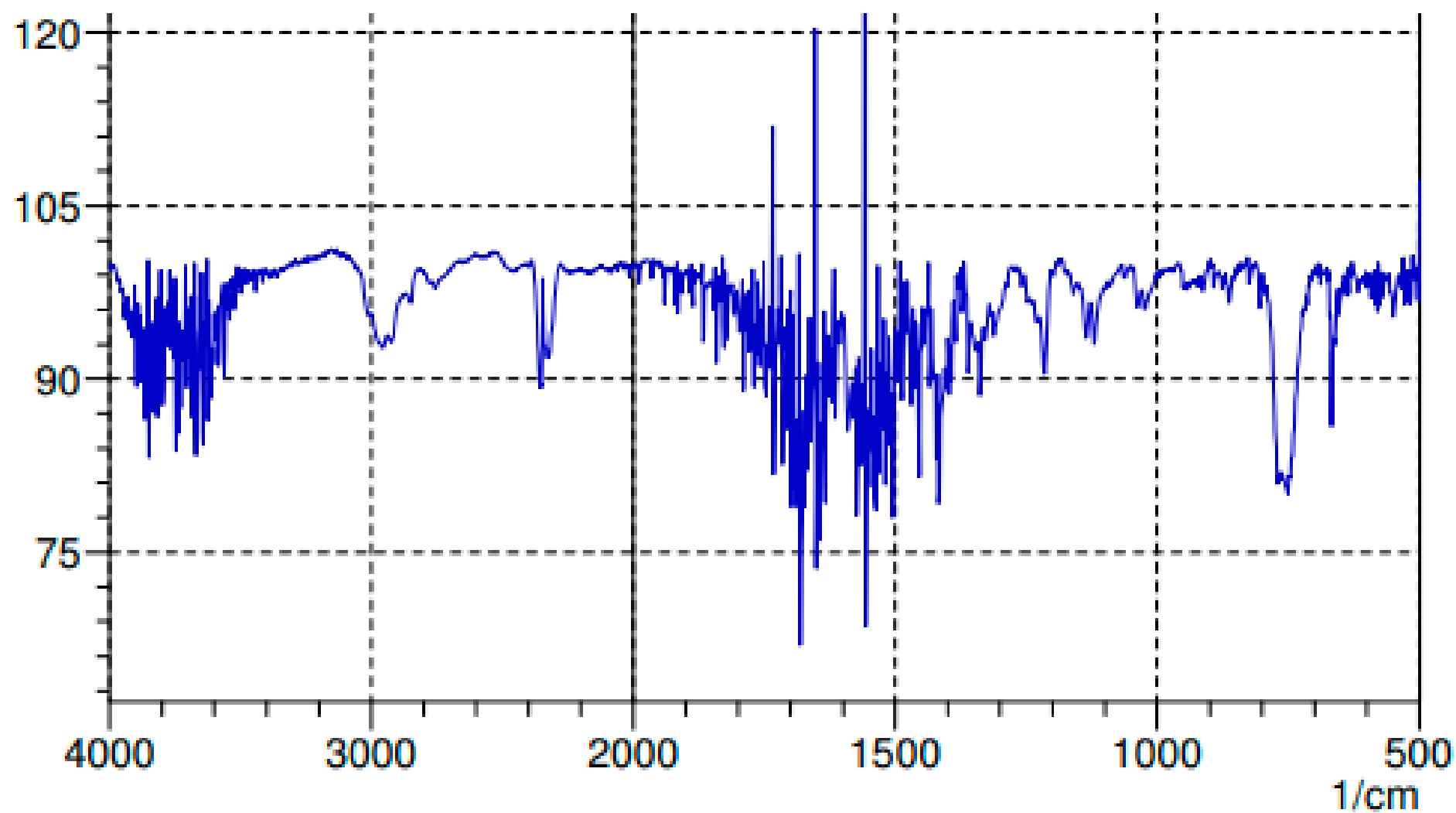


Figure S9 IR spectra of **1** obtained between NaCl plates.

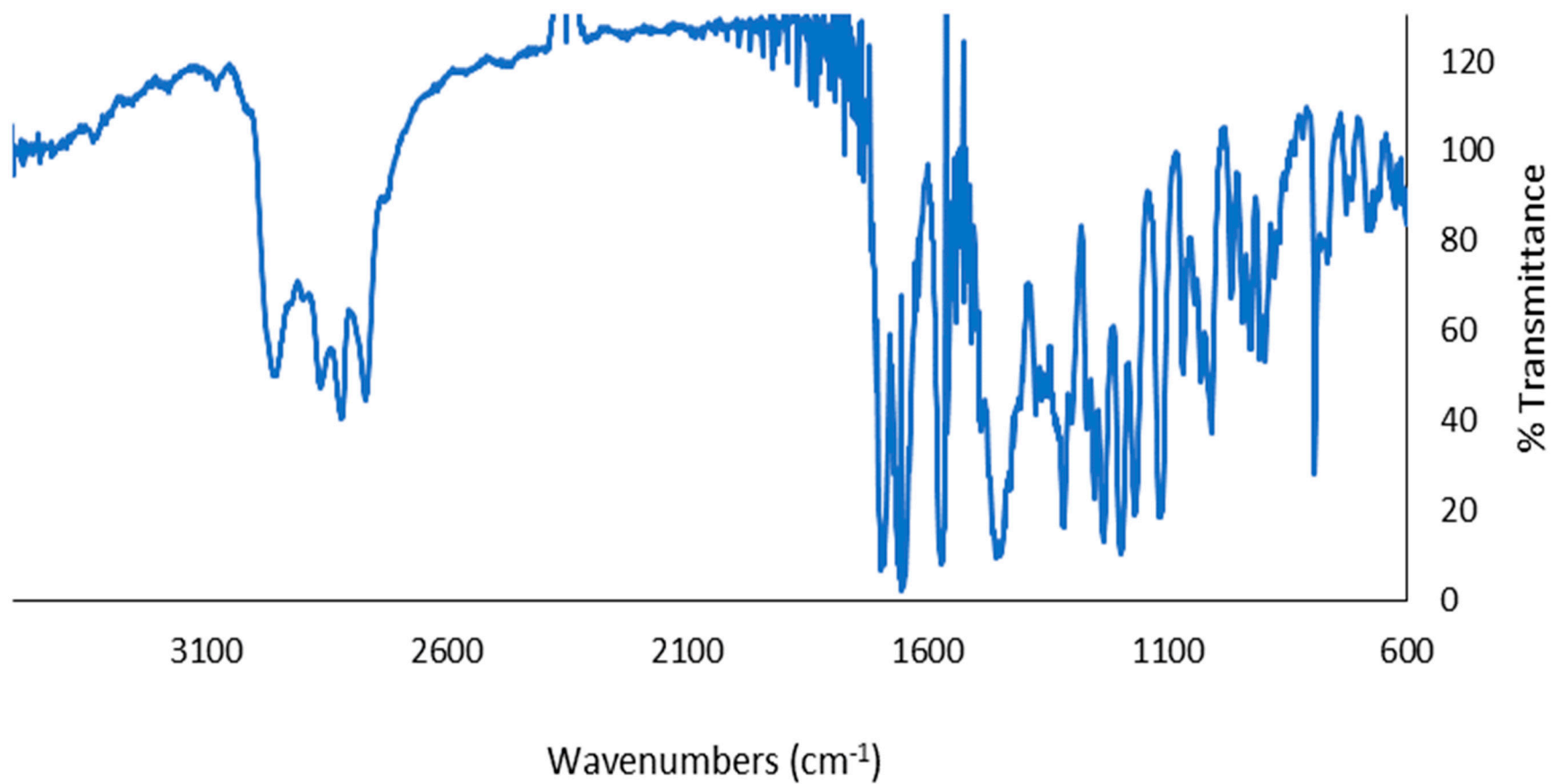


Figure S10 IR spectra of **2** obtained as a KBr disc.

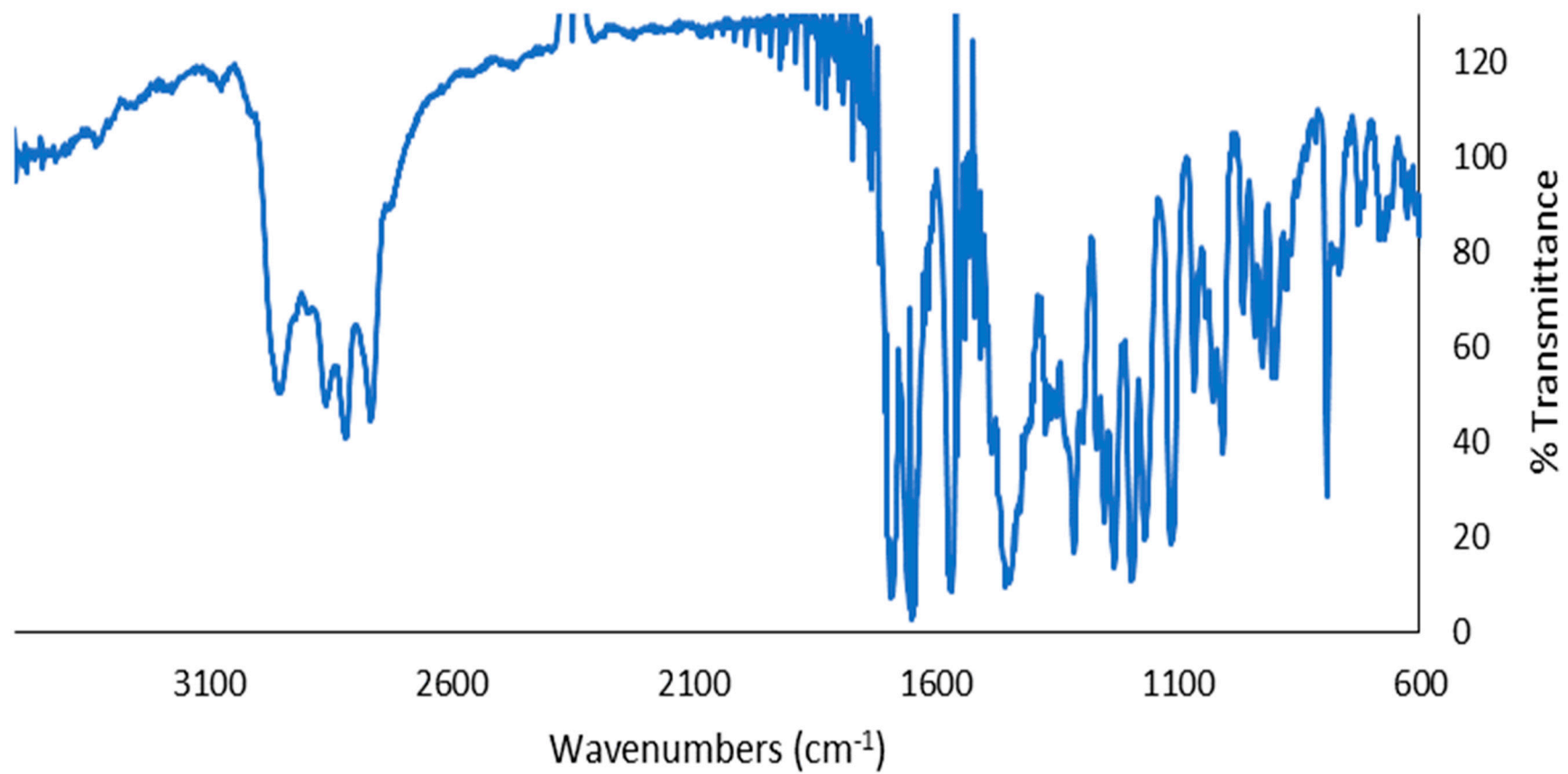


Figure S11 IR spectra of **3** obtained as a KBr disc.

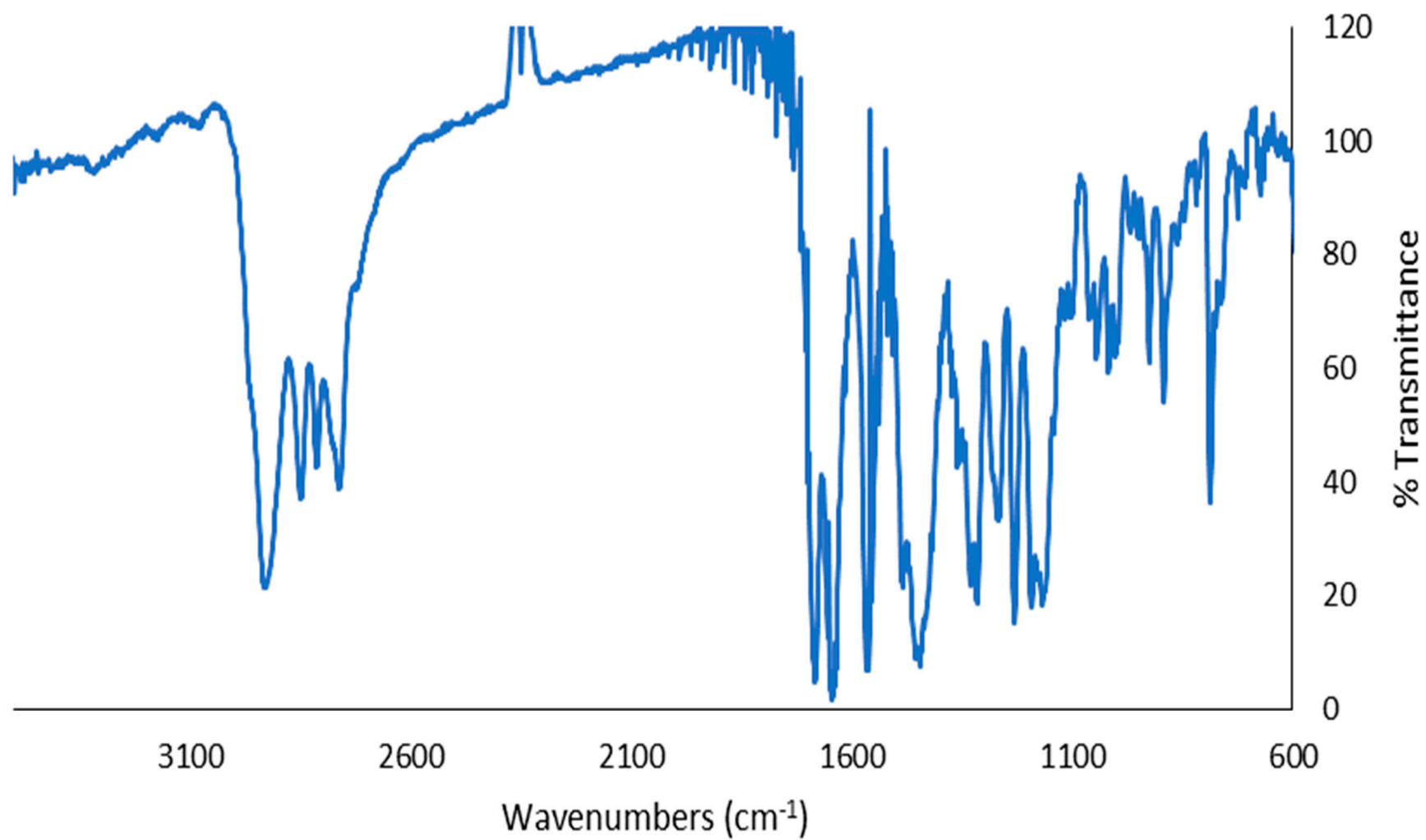


Figure S12 IR spectra of **4** obtained as a KBr disc.

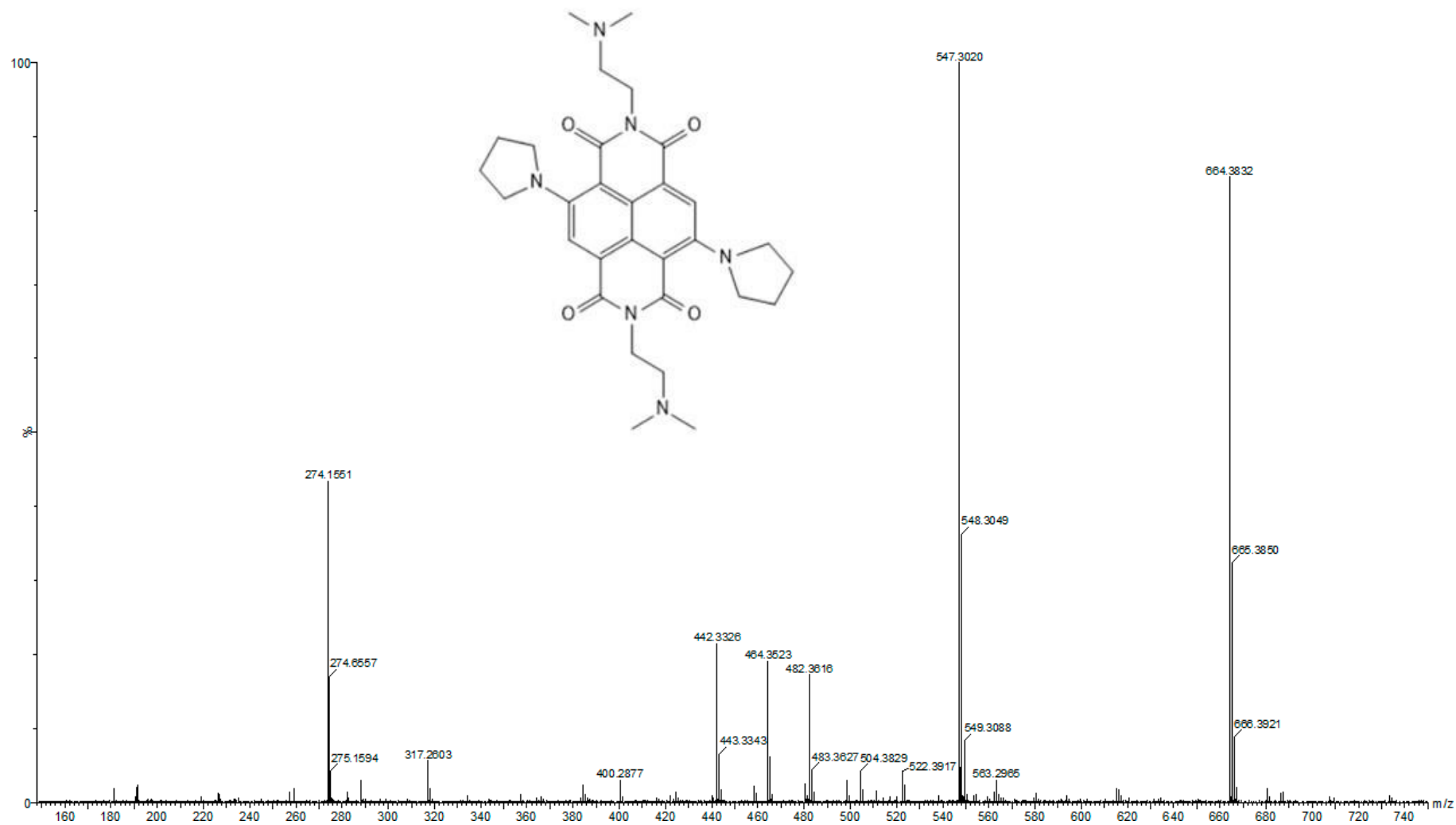


Figure S13 High-resolution mass spectrum of **1** by ESI-TOF.

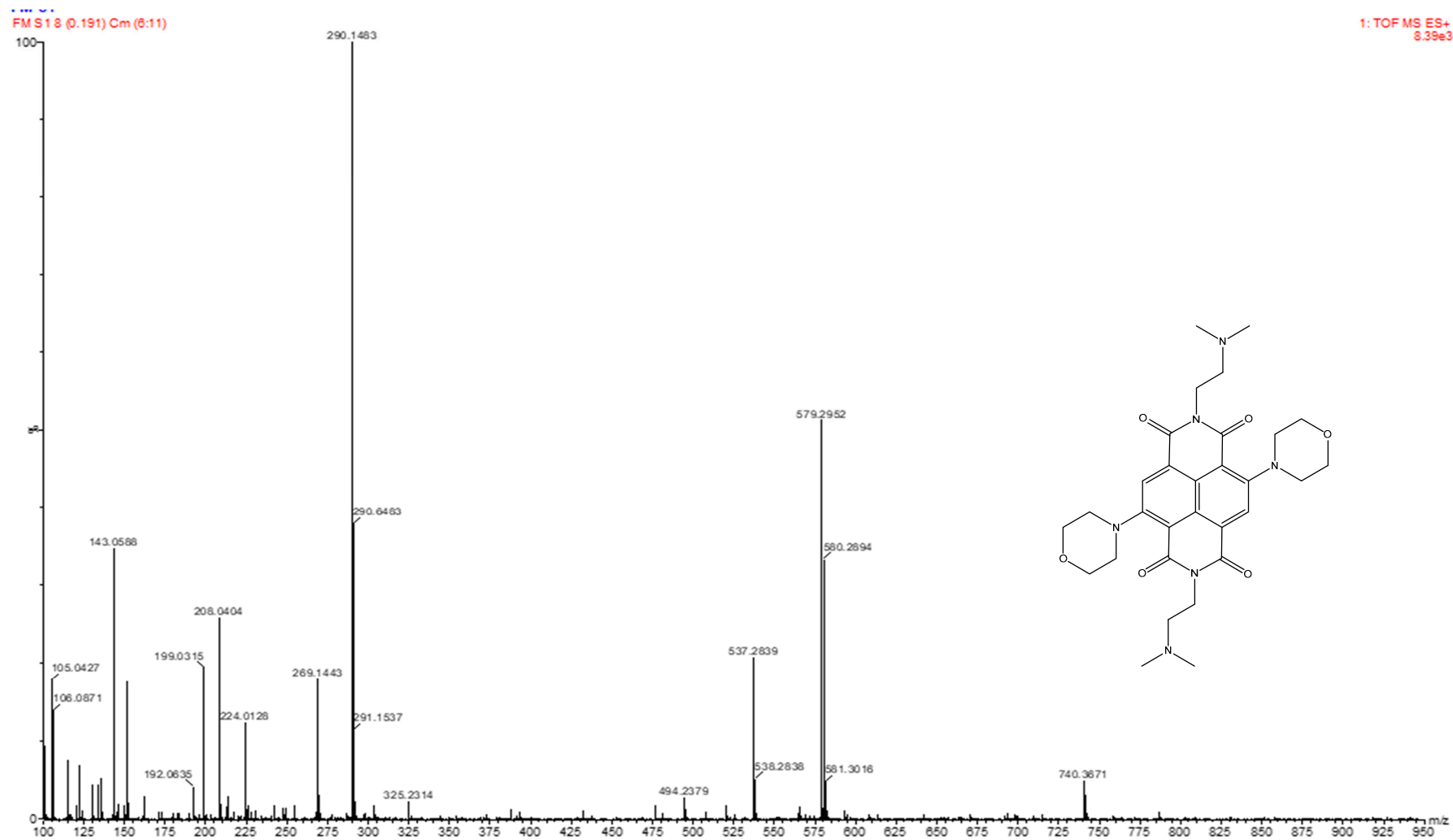


Figure S14 High-resolution mass spectrum of **2** by ESI-TOF.

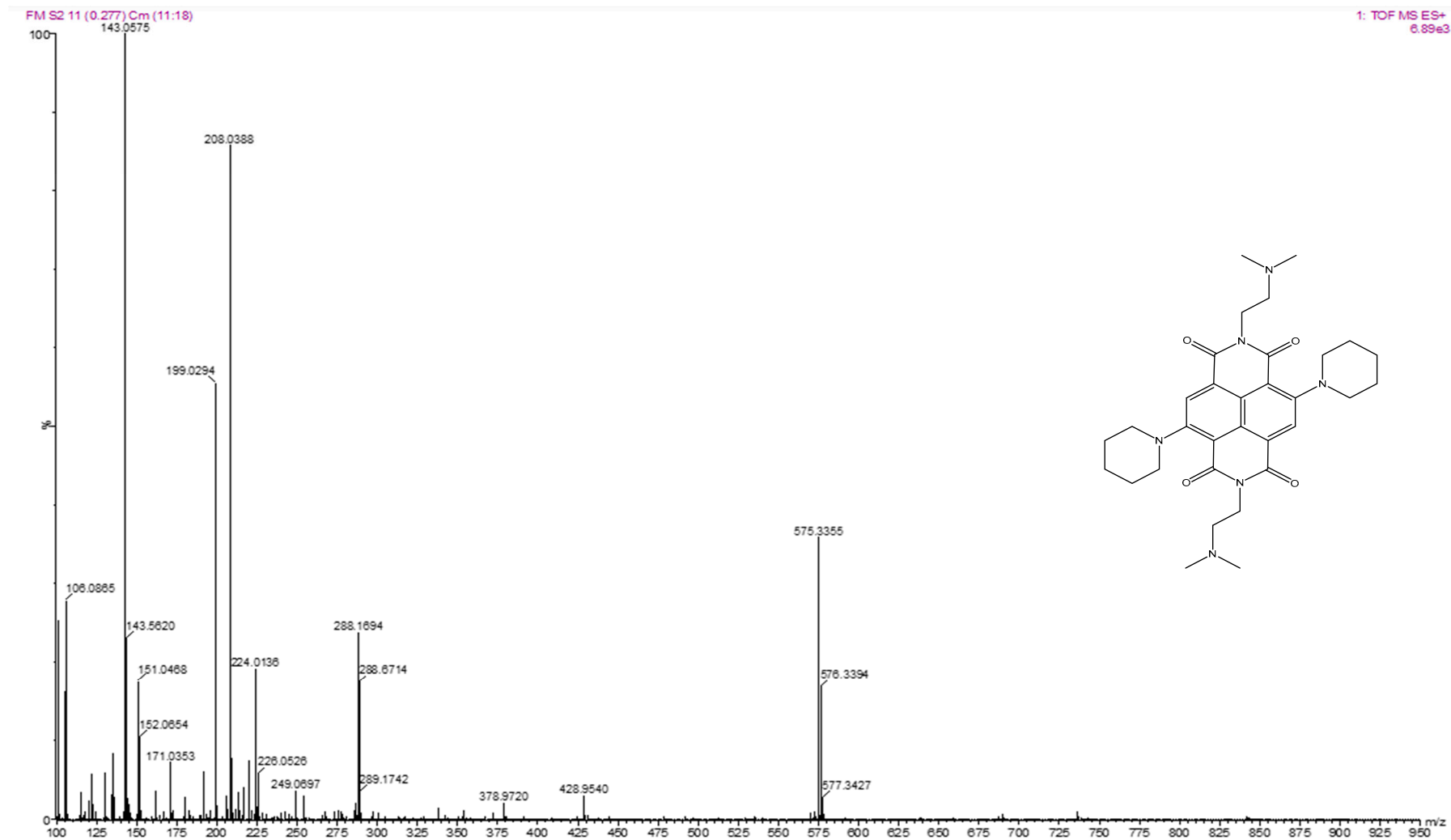


Figure S15 High-resolution mass spectrum of **3** by ESI-TOF.

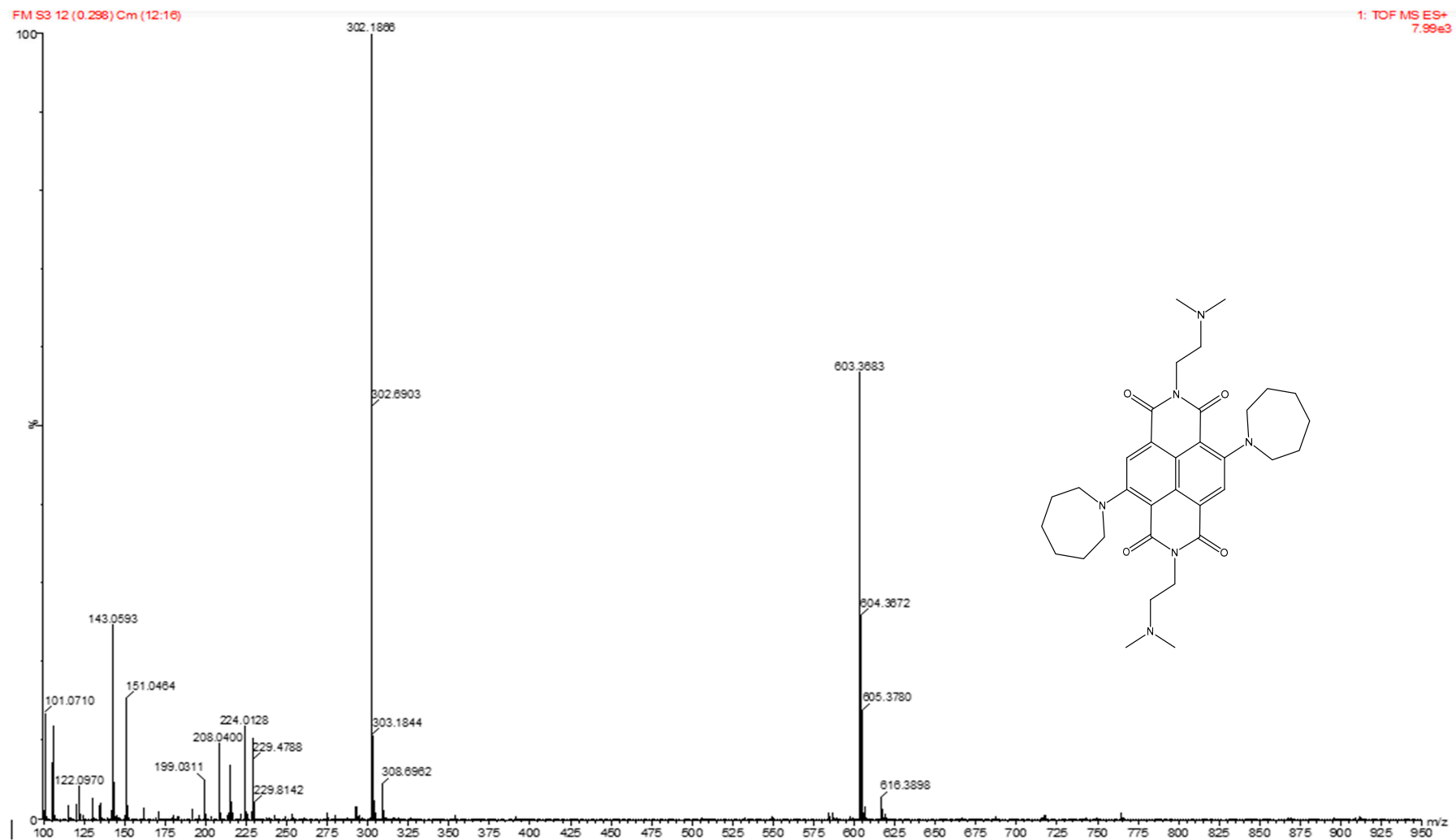


Figure S16 High-resolution mass spectrum of **4** by ESI-TOF.

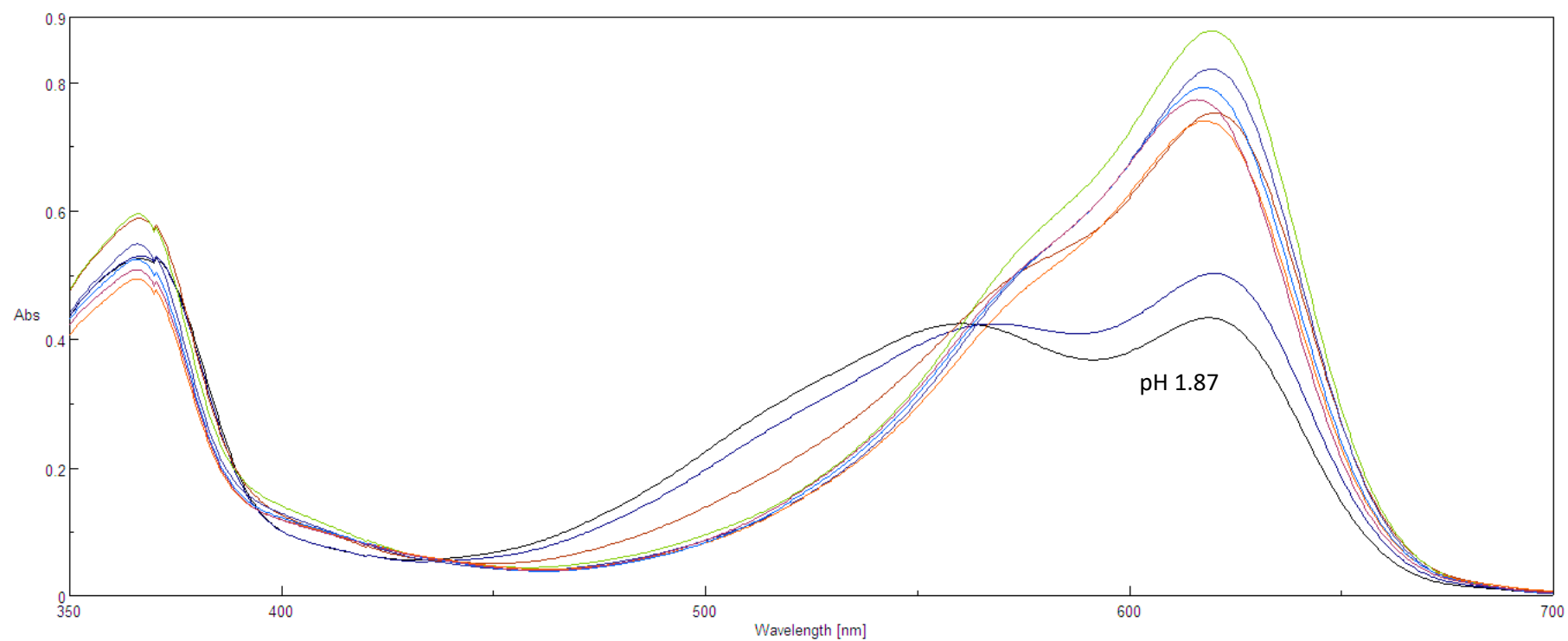


Figure S17 UV-vis absorbance spectra of 10^{-5} **1** in 1:1 MeOH/H₂O between pH 1.87 and pH 8.5.

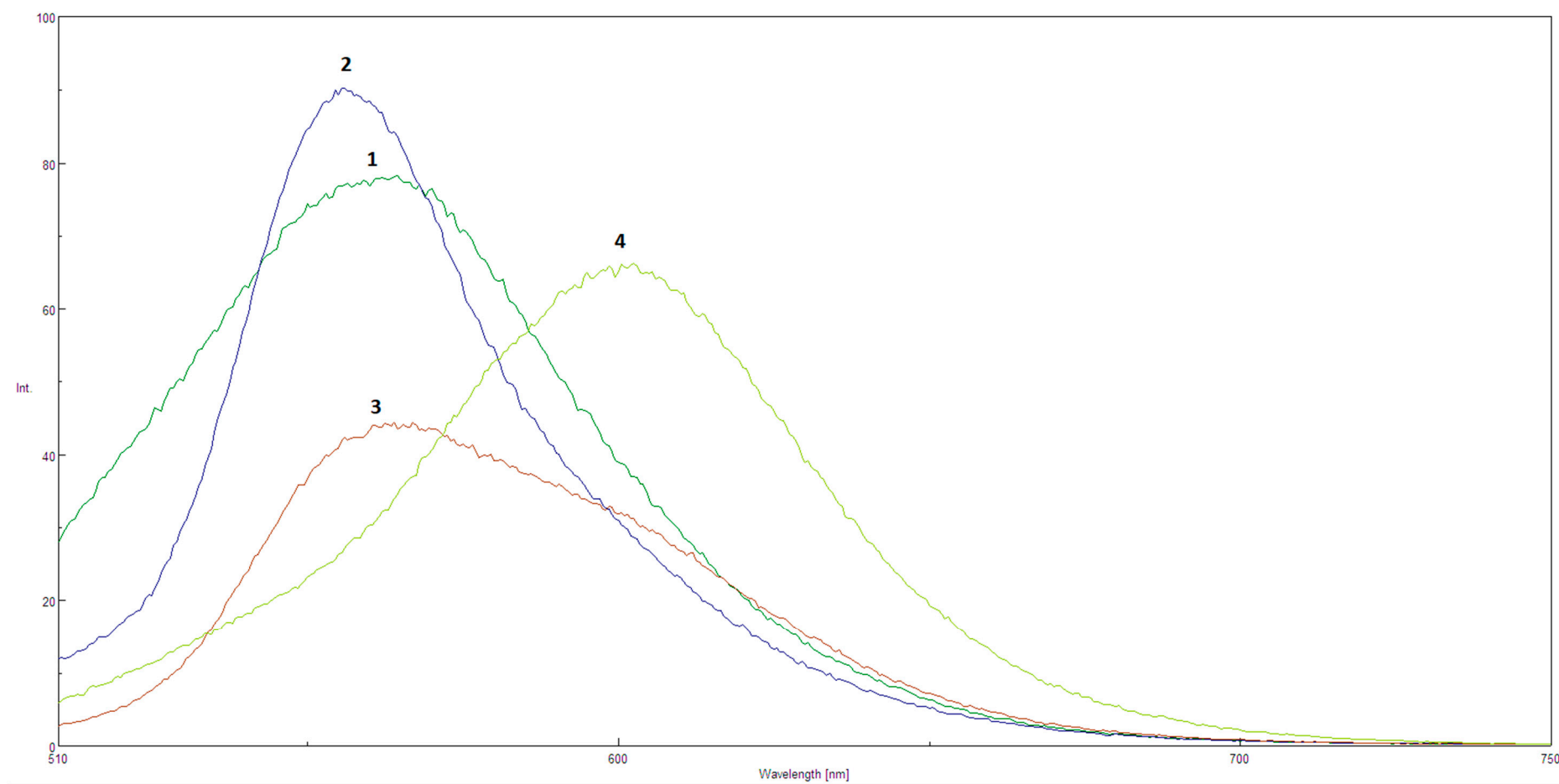


Figure S18 Emission spectra of 10^{-6} M **1-4** in 1:1 MeOH/H₂O excited at 500 nm.