

## Supporting Information

### An Easy Access to Multi-State Redox-Active, Push-Pull Naphthalenediimides: Panchromatic Radical Anions and Supramolecular Networks

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## Experimental

**General:** Chemicals were sourced either from Sigma-Aldrich, or TCI chemicals, India and were used as received. Thin layer chromatography (TLC) was carried out on aluminium plates coated with silica gel mixed with fluorescent indicator and was sourced from Merck, Germany. NMR ( $^1\text{H}$ ,  $^{13}\text{C}$ ) spectra were recorded on a Bruker 500 MHz spectrometer in  $\text{CDCl}_3$  or  $\text{DMSO-}d_6$  with TMS as a standard. Spin multiplicities are reported as a singlet (s), doublet (d), and triplet (t) with coupling constants (J) given in Hz, or multiplet (m). ESI-HRMS spectral data were obtained using a waters make ESI-MS model Synapt G2 high definition mass spectrometry. Absorption studies were performed on a JASCO V-670 UV-vis-NIR Spectrophotometer. All the spectroscopic experiments were carried out in UV Grade solvents which was sourced from Spectrochem, India. The FTIR spectra were recorded with a Perkin–Elmer FTIR 2000 or spectrum–two spectrometer.

**Cyclic and Differential Pulse Voltammetry (CV/DPV):** CV and DPV were carried out using a computer controlled potentiostat (CHI 650C) and a standard three electrode arrangement that consisted of both platinum working and auxiliary electrodes and saturated calomel (SCE) as reference electrode.<sup>1</sup> All electrochemical measurements were carried out in Ar-purged DCM with  $n\text{-Bu}_4\text{NPF}_6$  as the supporting electrolyte. CV studies of the molecules 1-8 were performed in degassed DCM under Ar atmosphere and the scan rate for the measurements was typically 200-300 mV/s. DPV was carried out keeping peak amplitude 50 mV, peak width 0.01 sec, pulse period 0.05 sec and increment E at 20 mV.

**Theoretical calculations:** The ground-state geometry optimization was carried out applying the density functional theory (DFT) with the Becke three-parameter<sup>2</sup> hybrid exchange functional in concurrence with the Lee-Yang-Parr gradient-corrected correlation function (B3LYP functional)<sup>3</sup> with the 6-311G++(d,p) basis set as implemented in Gaussian 09W.<sup>4</sup> All the geometries were optimized without any constrain. To reduce the calculation time axial group ( $\text{C}_4\text{H}_9$ ) of all molecules has been replaced by methyl group.

**X-ray Crystallography:** The data for 6 was collected on Bruker Kappa Apex-CCD diffractometer equipped with graphite monochromatic  $\text{Mo-K}\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ).<sup>5</sup> The frames were collected at 298 K. The data was processed with XCalibur S Saint,<sup>6</sup> and empirical absorption corrections were applied by using the spherical harmonic incorporated in the

SCALE3 ABSPACK scaling algorithm.<sup>5</sup> The structures were solved by direct methods using SIR-92<sup>7</sup> and refined by full-matrix least-squares refinement techniques on  $F^2$  by using SHELXL-2018<sup>8</sup> in the WinGX module.<sup>9</sup> All hydrogen atoms were fixed at the calculated positions were refined isotropically.

## Synthesis

*Ethyl-4-((2,7-dibutyl-9-(dimethylamino)-1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[lmn][3,8]phenanthrolin-4-yl)amino)benzoate (1)*. A mixture of N,N-dibutyl-2,3-dibromo-naphthalene-1,4,5,8-tetracarboxylic acid bisimide (NDI-Br<sub>2</sub>) (0.1g, 0.19 mmol) and Ethyl-4-aminobenzoate (0.3g, 0.56 mmol) was dissolved in DMF (10 ml) and stirred at 80°C for 10 h. The temperature of the resulting red color reaction mixture was further increased to 140 °C and stirred for another 1h. To this hot anhy. K<sub>2</sub>CO<sub>3</sub> (1g) was added and reaction mixture was again stirred for another 1h resulting in the purple color solution. The reaction was stopped and allowed to attain room temperature. The residual solvent was removed under reduced pressure followed by addition of water. The compound was extracted from aqueous layer by CHCl<sub>3</sub> and washed with water several times. The organic layer was dried using rotatory evaporator and the resultant solid was purified by silica column chromatography (100-200 mesh) with CHCl<sub>3</sub>/Hexane as an eluent. Yield: 0.02 g (19.0 %). M. P. > 250°C. ESI-HRMS (CHCl<sub>3</sub>, m/z): calcd. 585.2708 For **1** + H<sup>+</sup>; found 585.2785 (obs.). Anal. Calc. for C<sub>33</sub>H<sub>36</sub>N<sub>4</sub>O<sub>6</sub>: C, 67.79; H, 6.21; N, 9.58. Found: C, 67.65; H, 6.38; N, 9.14. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ (ppm) = 11.35 (s, 1H), 8.70 (s, 1H), 8.51 (s, 1H), 8.153 (d, 2H), 7.43 (d, 2H), 4.43 (q, 2H), 4.26-4.18 (m, 4H), 3.20 (s, 6H), 1.78-1.70 (m, 4H), 1.57 (s, 3H), 1.52-1.43 (m, 4H), 1.04 (t, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ (ppm) = 131.51, 121.65, 44.14, 40.75, 30.37, 30.18, 20.43, 20.37, 13.85. FTIR spectrum (Zn-Se ATR, selected peaks, cm<sup>-1</sup>): 3190 (-NH), 1724 (-COOEt), 1682 and 1638 (C=O). Absorption spectrum [ $\lambda_{\max}$ , nm, DCM ( $\epsilon \times 10^2$ , M<sup>-1</sup>cm<sup>-1</sup>): 598 (649), 340 (935), 330 (979).

*Ethyl-3-((2,7-dibutyl-9-(dimethylamino)-1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[lmn][3,8]phenanthrolin-4-yl)amino)benzoate (2)*. A synthetic procedure similar to **1** was followed using following reagents (0.1g, 0.19 mmol) and Dimethyl 5-aminoisophthalate (0.3g, 0.56 mmol) and anhy. K<sub>2</sub>CO<sub>3</sub> (1g). Yield: 0.02g (18.0 %). M. P. 170°C. ESI-HRMS (CHCl<sub>3</sub>, m/z): calcd. 585.2708 for **2** + H<sup>+</sup>; found 585.2793 (obs.). Anal. Calc. for C<sub>33</sub>H<sub>36</sub>N<sub>4</sub>O<sub>6</sub>: C, 67.79; H, 6.21; N, 9.58. Found: C, 67.15; H, 6.98; N, 9.84. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ (ppm) = 11.24 (s, 1H), 8.49 (d, 2H), 8.03 (s, 1H), 7.97 (d,

1H), 7.62-7.54 (m, 2H), 4.41 (t, 2H), 4.26-4.16 (m, 4H), 3.19 (s, 6H), 1.78-1.68 (m, 4H), 1.52-1.42 (m, 7H), 1.02 (t, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ (ppm) = 166.43, 166.29, 165.85, 162.90, 162.51, 146.92, 139.02, 132.49, 129.94, 128.14, 126.87, 125.92, 125.28, 124.33, 122.30, 120.26, 119.61, 61.31, 59.53, 44.13, 40.71, 38.16, 31.94, 30.35, 22.70, 20.43, 14.32. FTIR spectrum (Zn-Se ATR, selected peaks, cm<sup>-1</sup>): 3248 (-NH), 1722 (-COOEt), 1685 and 1632 (C=O). Absorption spectrum [ $\lambda_{\max}$ , nm, DCM ( $\epsilon \times 10^2$ , M<sup>-1</sup>cm<sup>-1</sup>): 598 (1092), 366 (649), 347 (644).

*dimethyl5-((2,7-dibutyl-9-(dimethylamino)-1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[lmn][3,8]phenanthroline-4-yl)amino)isophthalate (3)*. A synthetic procedure similar to **1** was followed using following reagents (0.1g, 0.19 mmol) and Ethyl-3-aminobenzoate (0.4g, 1.89 mmol) and anhy. K<sub>2</sub>CO<sub>3</sub> (1g). Yield: 0.02g (20.0 %). M. P. 227°C. ESI-HRMS (CHCl<sub>3</sub>, m/z): calcd 629.2606 for **3** + H<sup>+</sup>; found 629.2651 (obs.) Anal. Calc. for C<sub>34</sub>H<sub>36</sub>N<sub>4</sub>O<sub>8</sub>: C, 64.96; H, 5.77; N, 8.91. Found: C, 64.25; H, 5.42; N, 9.14. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ (ppm) = 11.27 (s, 1H), 8.57 (s, 1H), 8.52 (s, 1H), 8.45 (s, 1H), 8.24 (s, 2H), 4.25-4.10 (d, 4H), 3.99 (s, 6H), 3.20 (s, 6H), 2.07-2.05 (m, 4H), 1.51-1.44 (m, 4H), 1.03-0.908 (m, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ (ppm) = 165.61, 147.96, 132.43, 128.43, 119.28, 52.63, 44.16, 29.72, 20.37, 13.86. FTIR spectrum (Zn-Se ATR, selected peaks, cm<sup>-1</sup>): 3190 (-NH), 1726 (-COOMe), 1687 and 1643 (C=O). Absorption spectrum [ $\lambda_{\max}$ , nm, DCM ( $\epsilon \times 10^2$ , M<sup>-1</sup>cm<sup>-1</sup>): 594 (551), 366 (310), 349 (315).

*Diethyl-4,4'-((2,7-dibutyl-1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[lmn][3,8]phenanthroline-4,9-diyl)bis(azanediyl))dibenzoate (4)*. A mixture of N,N-dibutyl-2,3-dibromo-naphthalene-1,4,5,8-tetracarboxylic acid bisimide (NDI-Br<sub>2</sub>) (0.1g, 0.19 mmol) and Ethyl-4-aminobenzoate (0.3g, 0.56 mmol) was dissolved in DMSO (10 ml) and stirred at 140°C for 10 h. To this hot anhy. K<sub>2</sub>CO<sub>3</sub> (1g) was added and stirred for another 2h. The reaction was stopped and allowed to attain room temperature. Further, water was added to the reaction mixture resulting in the formation of blue color precipitates. Solid compound was filtered and washed with methanol few times followed by air drying. The resultant solid was purified by silica column chromatography (100-200 mesh) with CHCl<sub>3</sub>/Hexane as an eluent. Yield: 0.03g (20.0 %). ESI-HRMS (CHCl<sub>3</sub>, m/z): calcd. 705.2919 for **4** + H<sup>+</sup>; found 705.2907 (obs.). Anal. Calc. for C<sub>40</sub>H<sub>40</sub>N<sub>4</sub>O<sub>8</sub>: C, 68.17; H, 5.72; N, 7.95. Found: C, 68.15; H, 5.81; N, 7.44. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ (ppm) = 11.25 (s, 2H), 8.612 (s, 2H), 8.06 (d, 4H), 7.33 (d, 4H), 4.34 (d, 4H), 4.09 (s, 4H), 1.64 (s, 4H), 1.50 (s, 4H), 1.35 (s, 6H), 0.91 (s, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ (ppm) 166.21,

165.88, 162.35, 145.82, 131.53, 127.01, 125.86, 122.57, 121.90, 120.82, 61.03, 40.51, 30.11, 20.42, 14.38, 13.81. Absorption spectrum [ $\lambda_{\max}$ , nm, DCM ( $\epsilon \times 10^2$ ,  $M^{-1}cm^{-1}$ ): 602 (553), 370 (410), 346 (1175).

*2,7-dibutyl-4,9-bis(dimethylamino)benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetraone* (**5**). A solution of N,N-dibutyl-2,3-dibromo-naphthalene-1,4,5,8-tetracarboxylic acid bisimide (NDI-Br<sub>2</sub>) (0.1g) in DMF (10 ml) was stirred at 80°C for 10 h. The temperature was raised to 140 °C followed by addition of anhy. K<sub>2</sub>CO<sub>3</sub> (1g). The reaction was allowed to stir for 24h. The reaction was stopped and reaction workup was performed similar to **1** to afford blue color compound. Yield: 0.006g (8%). ESI-HRMS (CHCl<sub>3</sub>, m/z): calcd. 465.2496 for **5** + H<sup>+</sup>; found 465.2403 (obs.). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, 298 K, TMS):  $\delta$  (ppm) = 8.46 (s, 2H), 4.22 (t, 4H), 3.19 (s, 12H), 1.73 (t, 4H), 1.46 (t, 4H), 1.01 (s, 6H). Absorption spectrum [ $\lambda_{\max}$ , nm, DCM ( $\epsilon \times 10^2$ ,  $M^{-1}cm^{-1}$ ): 619 (869), 365 (513), 344 (406).

*4-((2,7-dibutyl-9-(dimethylamino)-1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[lmn][3,8]phenanthroline-4-yl)amino)benzoic acid* (**6**). To the solution of **1** (0.05 g) in THF/H<sub>2</sub>O (1:1) was added NaOH (10 equiv.) followed by refluxing for 10h. The reaction was stopped and THF was removed under the reduced pressure. The solution was cooled and neutralized using 2N HCl solution while continuous monitoring using pH paper. The blue precipitates were formed at the pH of around 4. The compound was filtered and washed with water 3-4 times. Yield: 0.04g (90.0 %). M. P > 250°C. ESI-HRMS (DMF, m/z): calcd 557.2395 for **6** + H<sup>+</sup>; found 557.2345 (obs.). Anal. Calc. for C<sub>31</sub>H<sub>32</sub>N<sub>4</sub>O<sub>6</sub>: C, 66.89; H, 5.79; N, 10.07. Found: C, 67.20; H, 5.48; N, 9.84. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, 298 K, TMS):  $\delta$  (ppm) = 12.88 (s, 1H), 11.05 (d, 1H), 8.37 (dd, 2H), 8.02 (t, 2H), 7.52 (s, 2H), 4.05 (t, 2H), 3.32 (s, 6H), 1.61 (q, 4H), 1.36 (q, 4H), 0.96 (t, 6H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, 298 K, TMS):  $\delta$  (ppm) = 167.17, 165.90, 162.42, 160.99, 151.27, 144.13, 143.51, 131.58, 126.79, 126.05, 124.05, 123.51, 121.62, 106.35, 104.53, 79.65, 43.93, 30.20, 20.30, 14.16. . FTIR spectrum (Zn-Se ATR, selected peaks, cm<sup>-1</sup>): 3587 (-COOH), 3153 (-NH), 1685 and 1632 (C=O). Absorption Spectrum [ $\lambda_{\max}$ , nm, DCM ( $\epsilon \times 10^2$ ,  $M^{-1}cm^{-1}$ ): 598 (861), 367 (684), 338 (1318).

*3-((2,7-dibutyl-9-(dimethylamino)-1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[lmn][3,8]phenanthroline-4-yl)amino)benzoic acid* (**7**). Compound **7** was synthesized in the similar manner to that of **6** using **2** (0.05 g) as a starting material. Yield: 0.04g (92.0 %). M. P > 250°C. ESI-HRMS (DMF, m/z): calcd. 557.2395 for **7** + H<sup>+</sup>; found 557.2301 (obs.). Anal. Calc. for C<sub>31</sub>H<sub>32</sub>N<sub>4</sub>O<sub>6</sub>: C, 66.89; H, 5.79; N, 10.07. Found: C, 66.49; H,

5.18; N, 9.77. <sup>1</sup>H NMR (500 MHz, d<sub>6</sub>-DMSO, 298 K, TMS): δ (ppm) = 11.17 (t, 1H), 8.37 (t, 1H), 7.97 (s, 1H), 7.90 (s, 1H), 7.58 (s, 2H), 4.13 (dd, 4H), 3.16 (s, 6H), 1.68 (dd, 4H), 1.43 (m, 4H), 1.25 (t, 6H). FTIR spectrum (Zn-Se ATR, selected peaks, cm<sup>-1</sup>): 3542 (-COOH), 3235 (-NH), 1685 and 1640 (C=O). Absorption spectrum [ $\lambda_{\max}$ , nm, DCM ( $\epsilon \times 10^2$ , M<sup>-1</sup>cm<sup>-1</sup>)]: 604 (144), 370 (40), 350 (60).

5-((2,7-dibutyl-9-(dimethylamino)-1,3,6,8-tetraoxo-1,2,3,6,7,8-hexahydrobenzo[*lmn*][3,8]phenanthroline-4-yl)amino)isophthalic acid (**8**). Compound **8** was synthesized in the similar manner to that of **6** using **3** (0.05 g) as a starting material. Yield: 0.04g (90.0 %). M. P > 250°C. ESI-HRMS (DMF, m/z): calcd. 601.2293 for **8** + H<sup>+</sup>; found 601.2271 (obs.). Anal. Calc. for C<sub>32</sub>H<sub>32</sub>N<sub>4</sub>O<sub>8</sub>: C, 63.99; H, 5.37; N, 9.33. Found: C, 64.15; H, 5.15; N, 9.10. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, 298 K, TMS): δ (ppm) = 11.02 (s, 1H), 8.31 (s, 2H), 8.20 (s, 1H), 8.07 (s, 1H), 3.73 (dd, 4H), 3.04 (s, 6H), 1.60 (dd, 4H), 1.38 (dd, 4H), 0.98 (t, 6H). FTIR spectrum (Zn-Se ATR, selected peaks, cm<sup>-1</sup>): 3564 (-COOH), 3248 (-NH), 1680 and 1640 (C=O). Absorption spectrum [ $\lambda_{\max}$ , nm, DCM ( $\epsilon \times 10^2$ , M<sup>-1</sup>cm<sup>-1</sup>)]: 595 (591), 366 (340), 349 (350).

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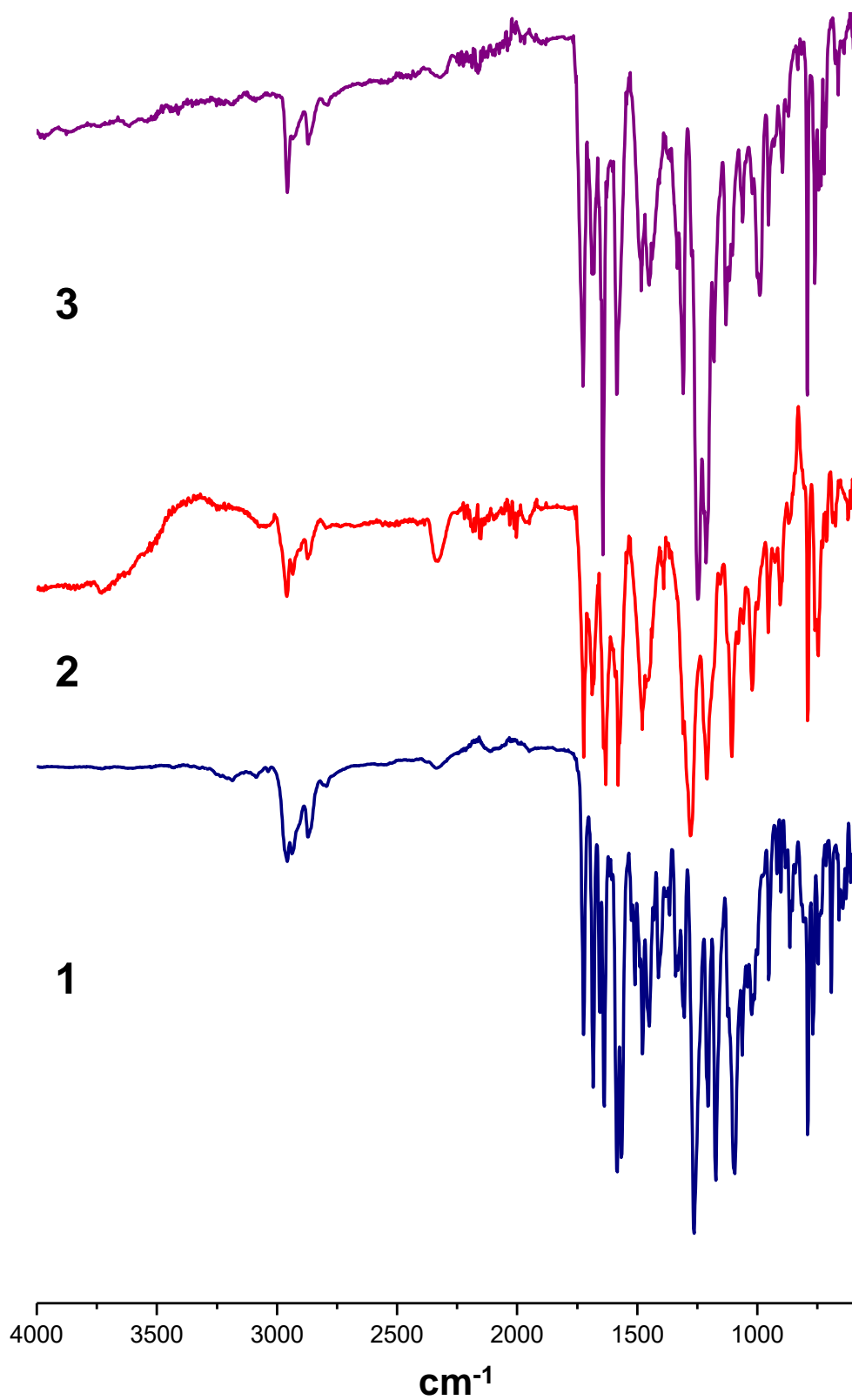


Figure S1. FT-IR spectra of **1** (blue traces), **2** (red traces) and **3** (purple traces).

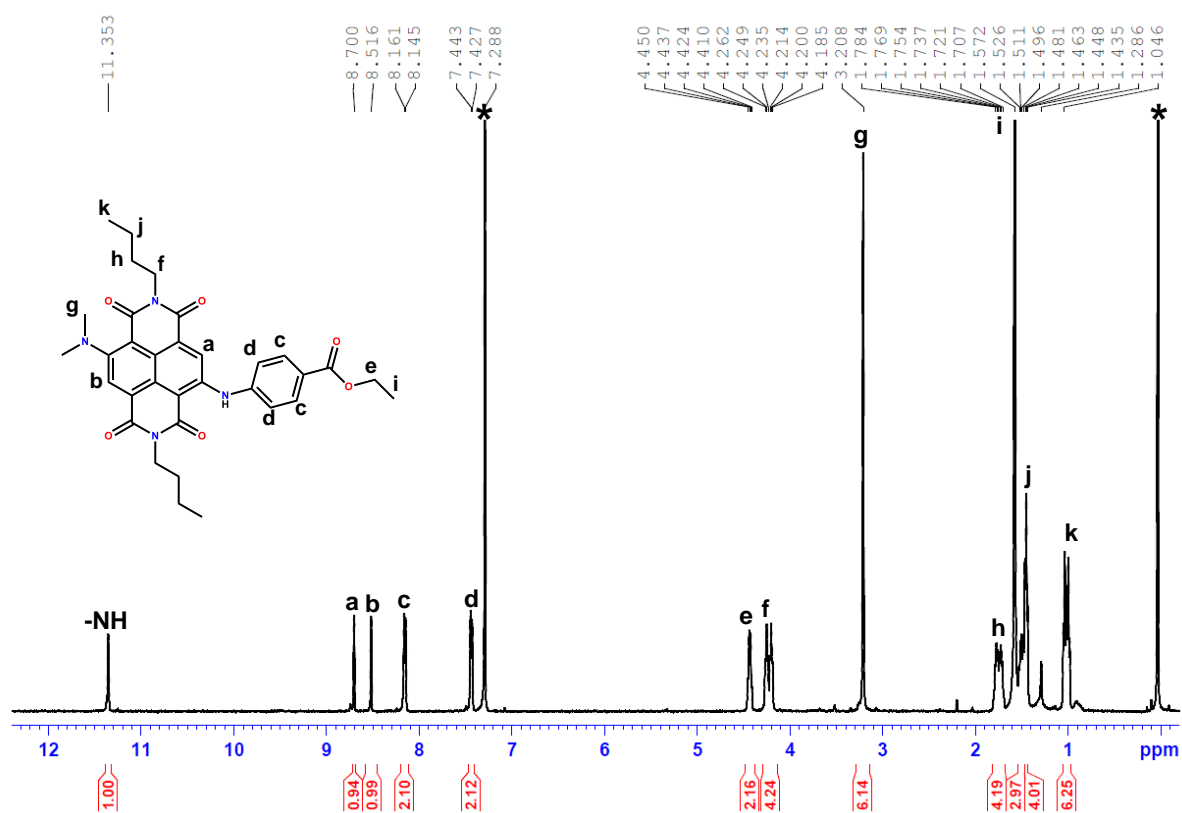


Figure S2. 500 MHz <sup>1</sup>H NMR spectrum of **1** in CDCl<sub>3</sub> at room temperature. \* represents residual solvent, TMS and H<sub>2</sub>O peaks.



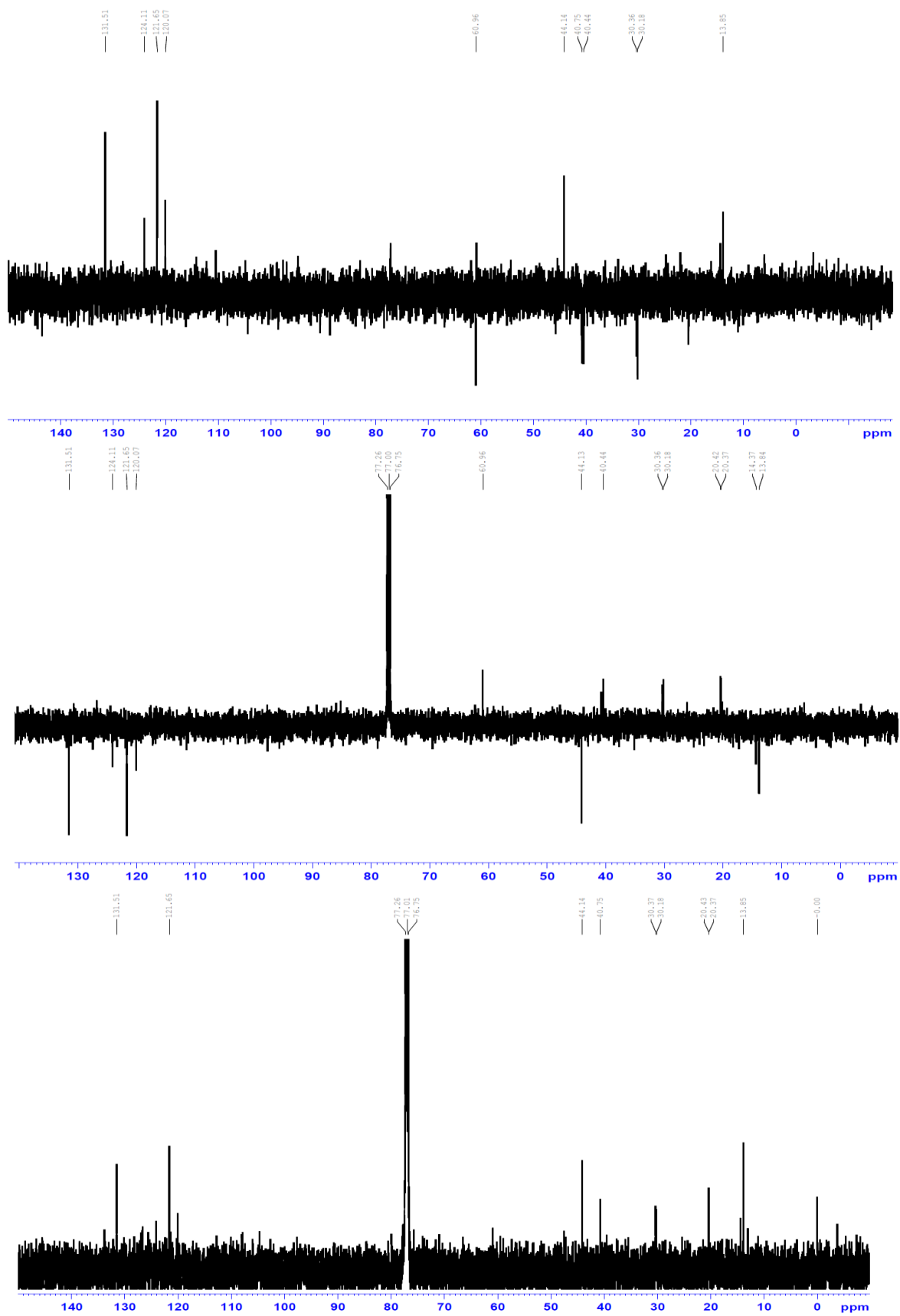


Figure S3. 125 MHz  $^{13}\text{C}$  (bottom), APT (middle) and DEPT 135 (top) spectra of **1** in  $\text{CDCl}_3$  at room temperature. \* represents residual solvent peak.

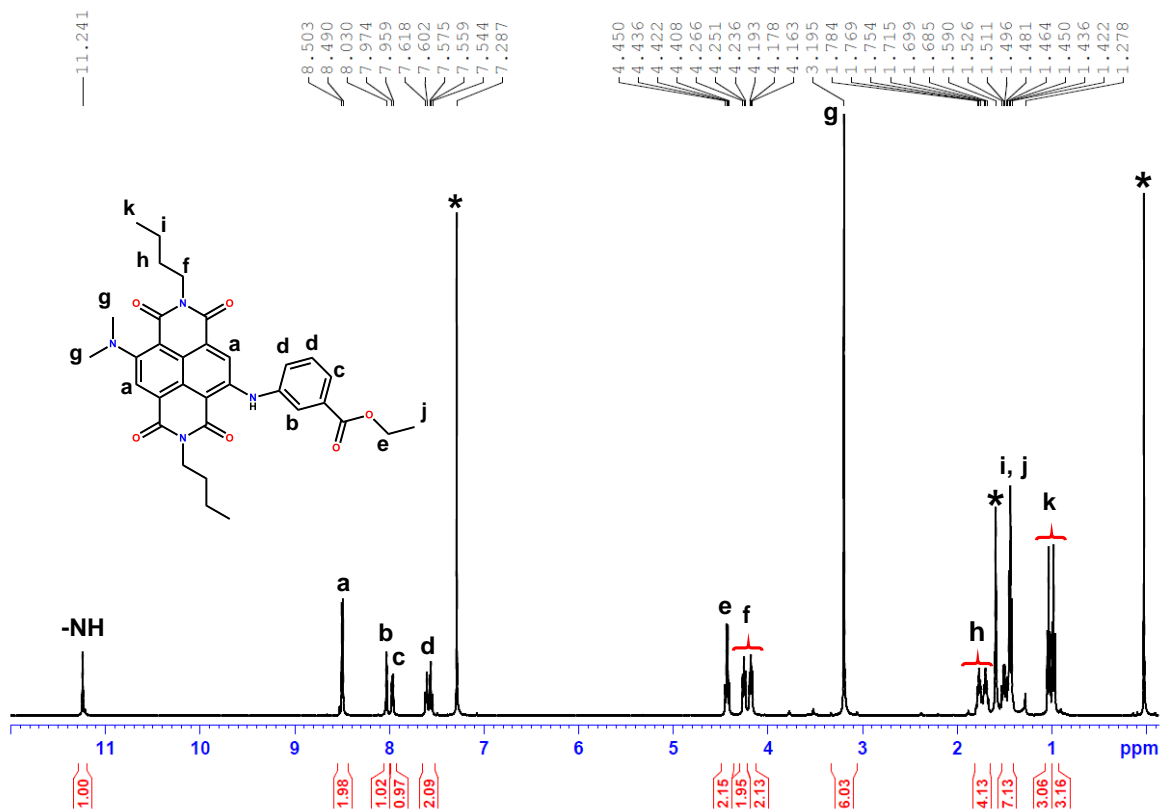


Figure S4. 500 MHz <sup>1</sup>H NMR spectrum of **2** in CDCl<sub>3</sub> at room temperature. \* represents residual solvent, TMS and H<sub>2</sub>O peaks.

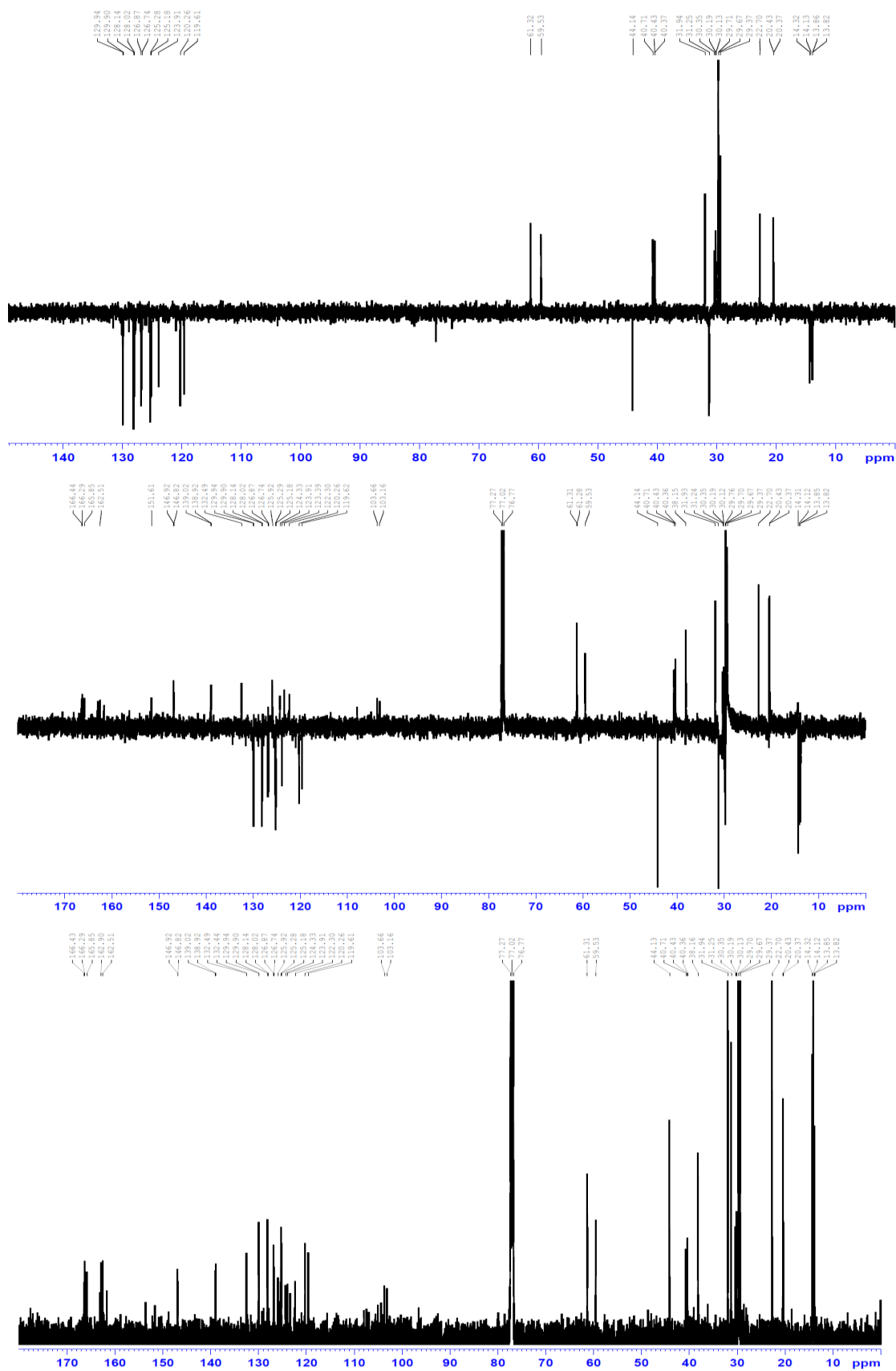


Figure S5. 125 MHz  $^{13}\text{C}$  (bottom), APT (middle) and DEPT 135 (top) spectra of **2** in  $\text{CDCl}_3$  at room temperature. \* represents residual solvent peak.

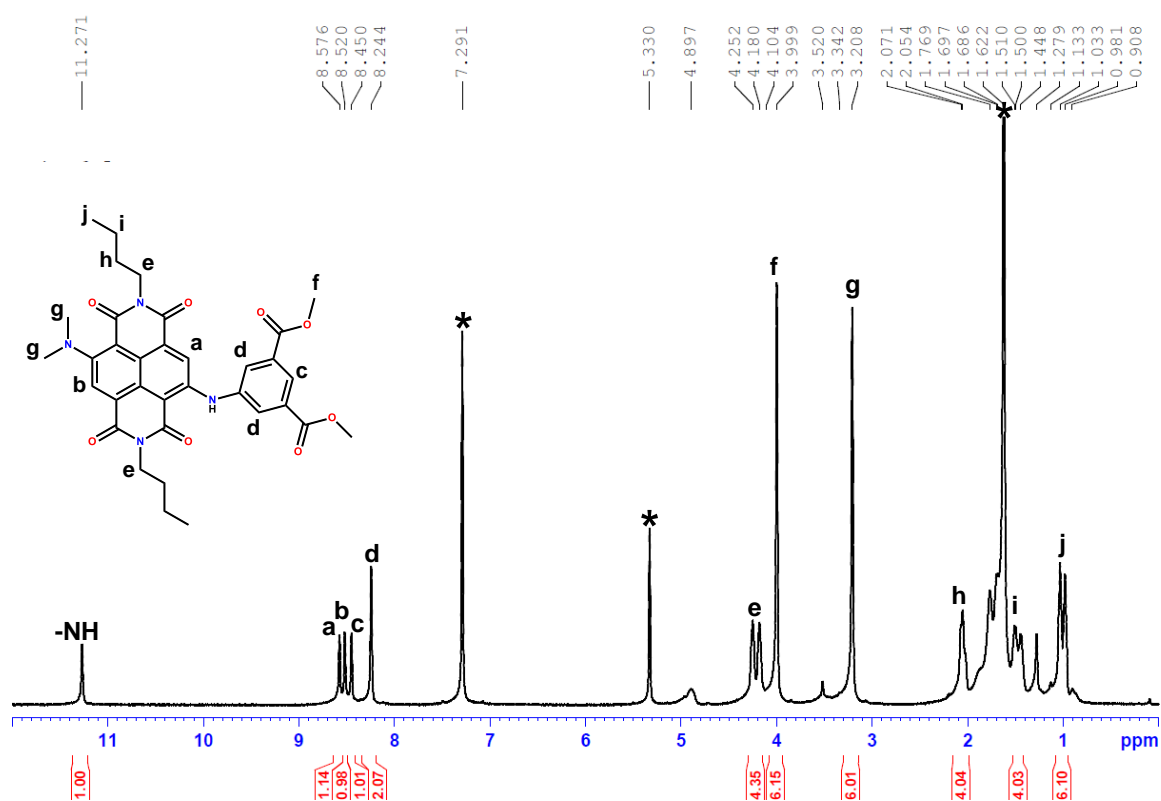


Figure S6. 500 MHz  $^1\text{H}$  NMR spectrum of **3** in  $\text{CDCl}_3$  at room temperature. \* represents residual solvent, TMS and  $\text{H}_2\text{O}$  peaks.

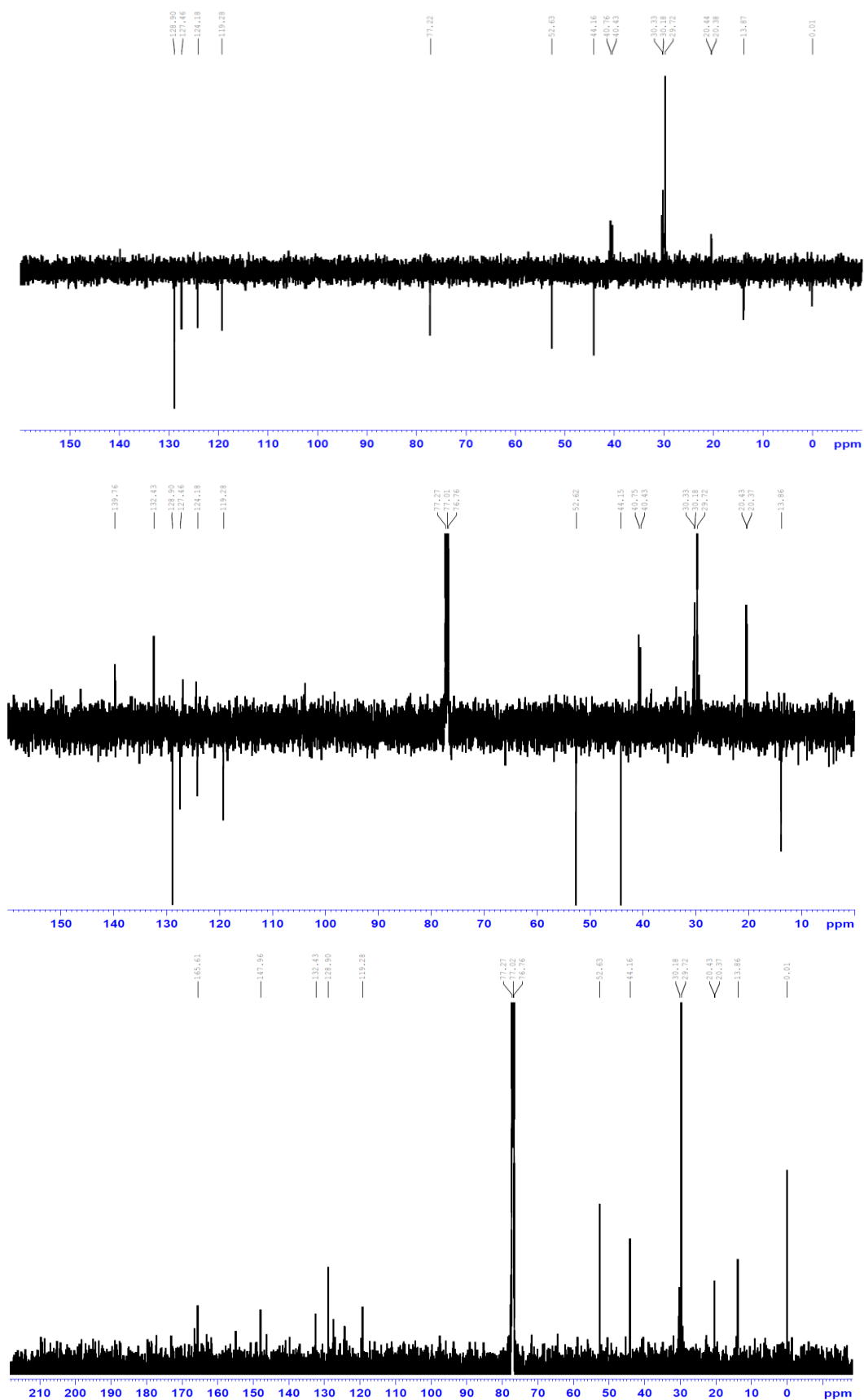


Figure S7. 125 MHz  $^{13}\text{C}$  (bottom), APT (middle) and DEPT 135 (top) spectra of **3** in  $\text{CDCl}_3$  at room temperature. \* represents residual solvent peak.

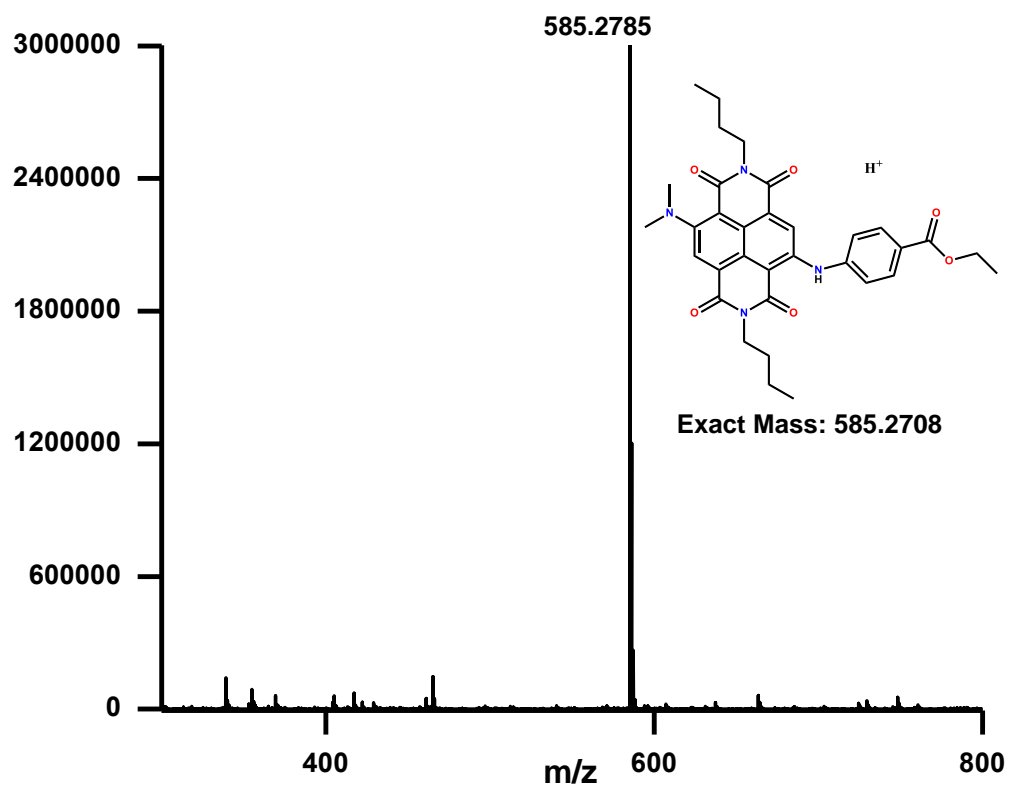


Figure S8. ESI-HRMS of **1** in  $\text{CHCl}_3$ .

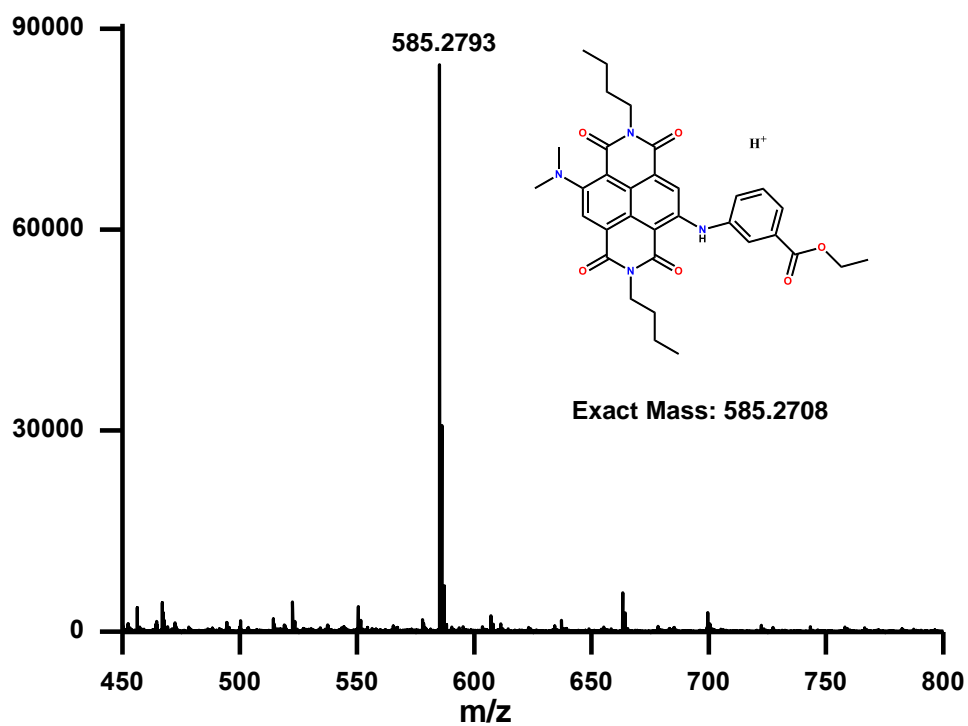


Figure S9. ESI-HRMS of **2** in  $\text{CHCl}_3$ .

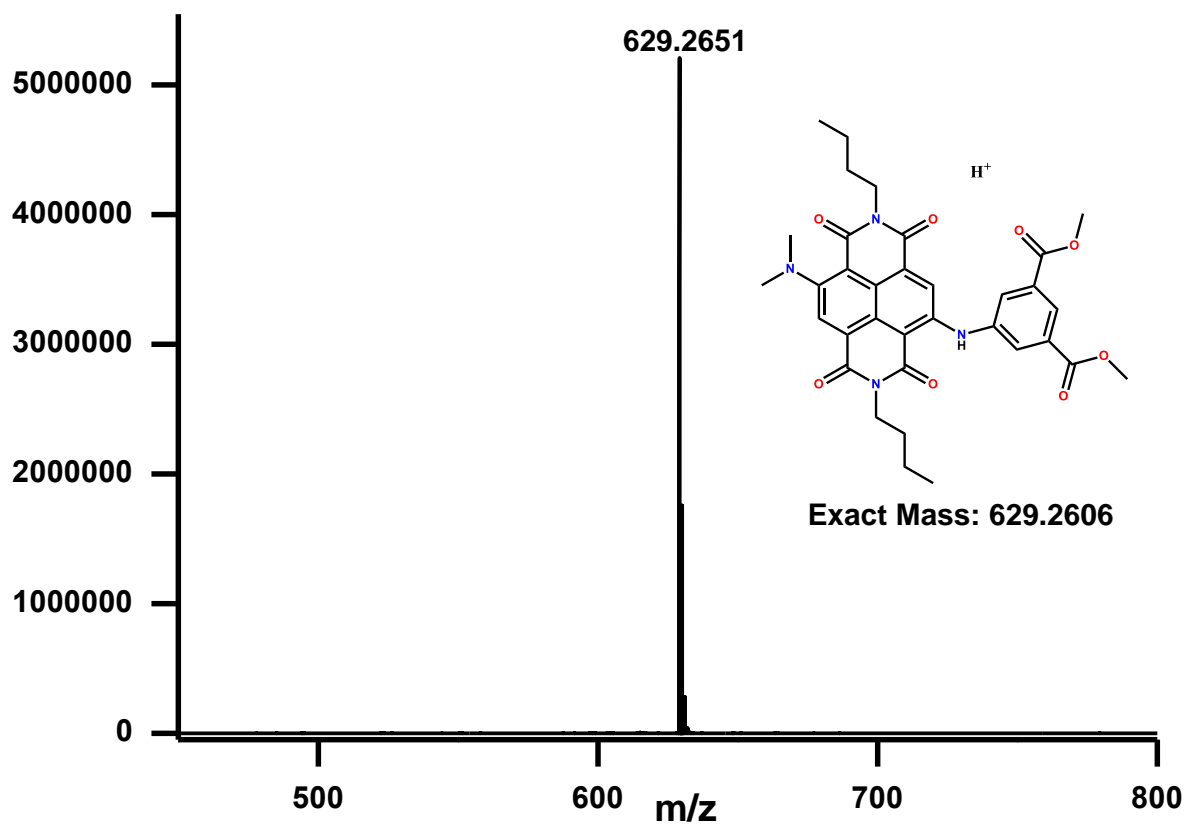


Figure S10. ESI-HRMS of **3** in CHCl<sub>3</sub>.

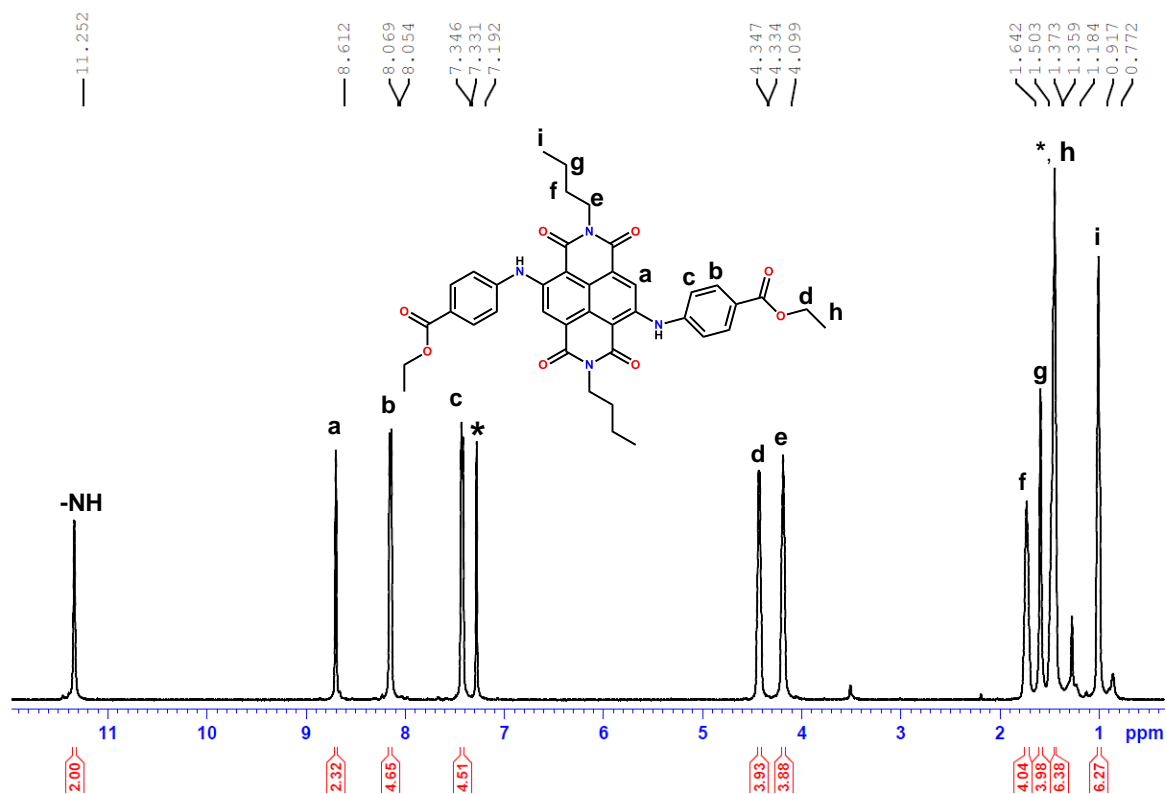


Figure S11. 500 MHz  $^1\text{H}$  NMR spectrum of **4** in  $\text{CDCl}_3$  at room temperature. \* represents residual solvent, TMS and  $\text{H}_2\text{O}$  peaks.

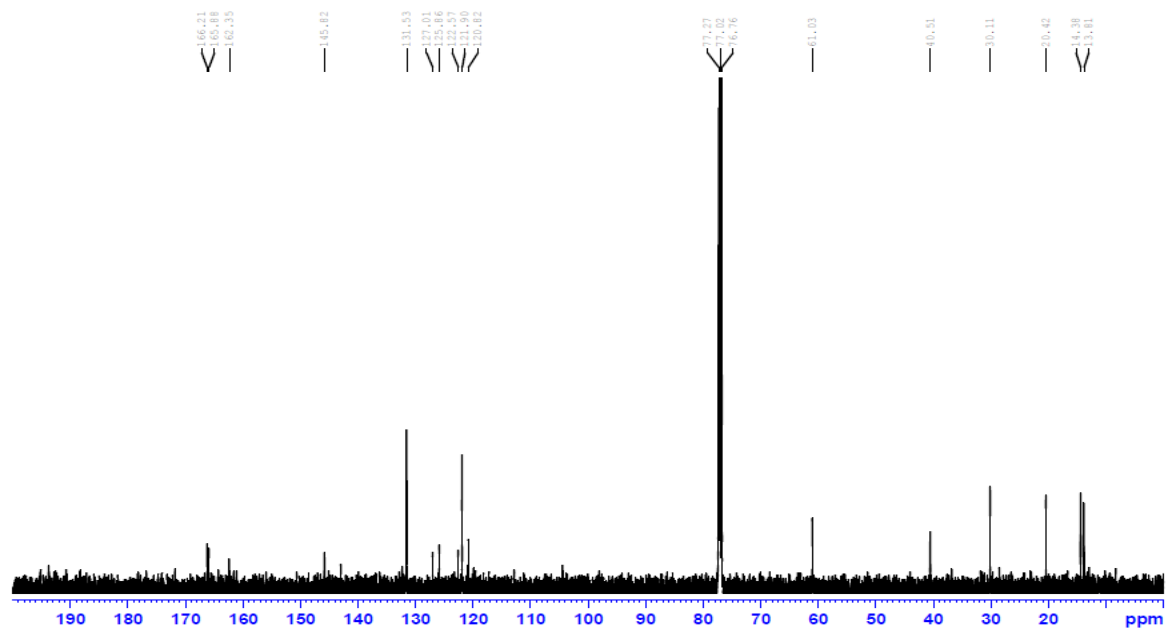


Figure S12. 125 MHz  $^{13}\text{C}$  (bottom) spectrum of **4** in  $\text{CDCl}_3$  at room temperature. \* represents residual solvent peak.



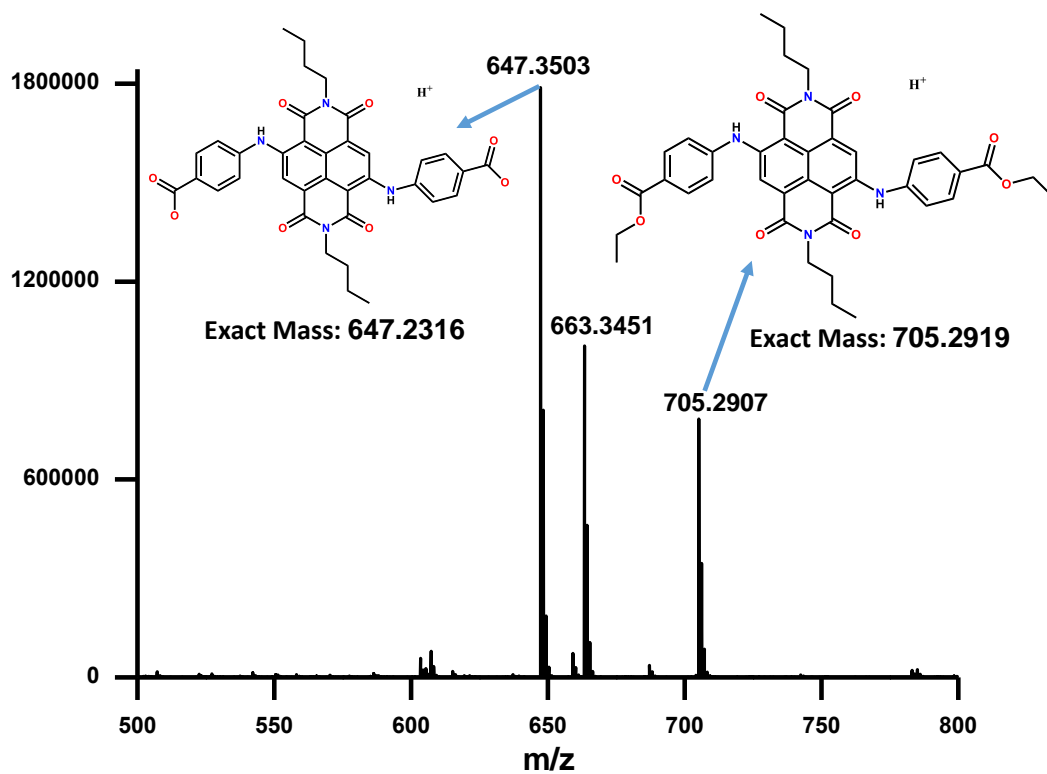


Figure S13. ESI-HRMS of **4** in  $\text{CHCl}_3$ .

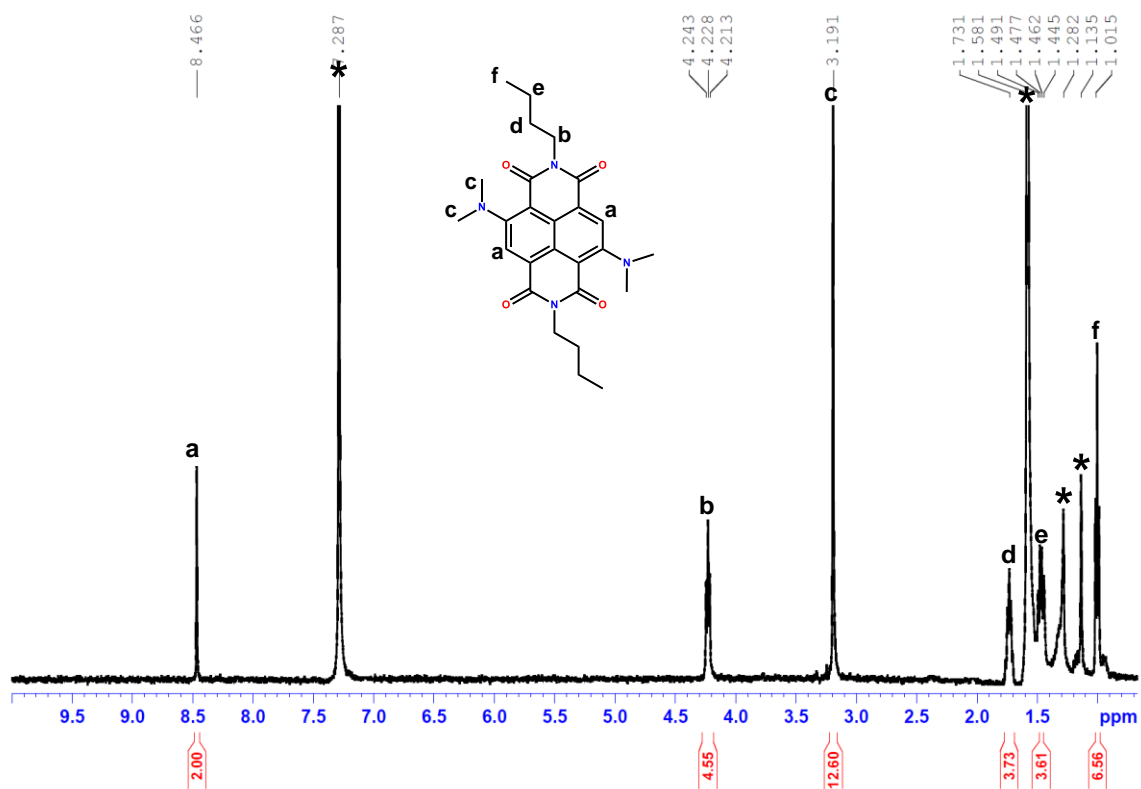


Figure S14. 125 MHz  $^{13}\text{C}$  (bottom) spectrum of **5** in  $\text{CDCl}_3$  at room temperature. \* represents residual solvent peak.

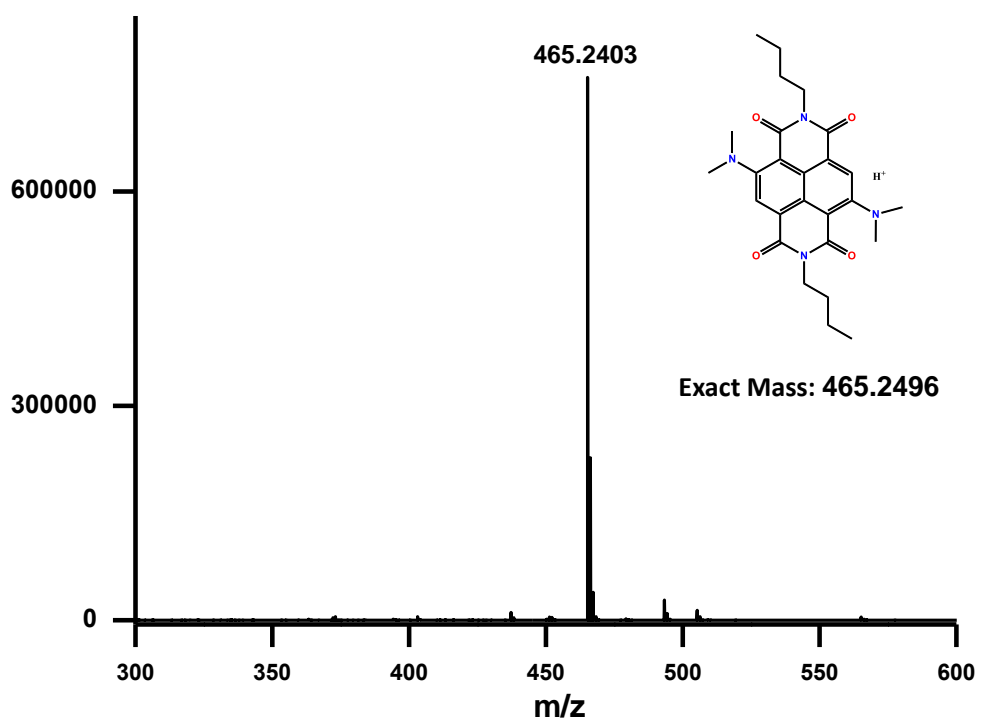


Figure S15. ESI-HRMS of **5** in  $\text{CHCl}_3$ .

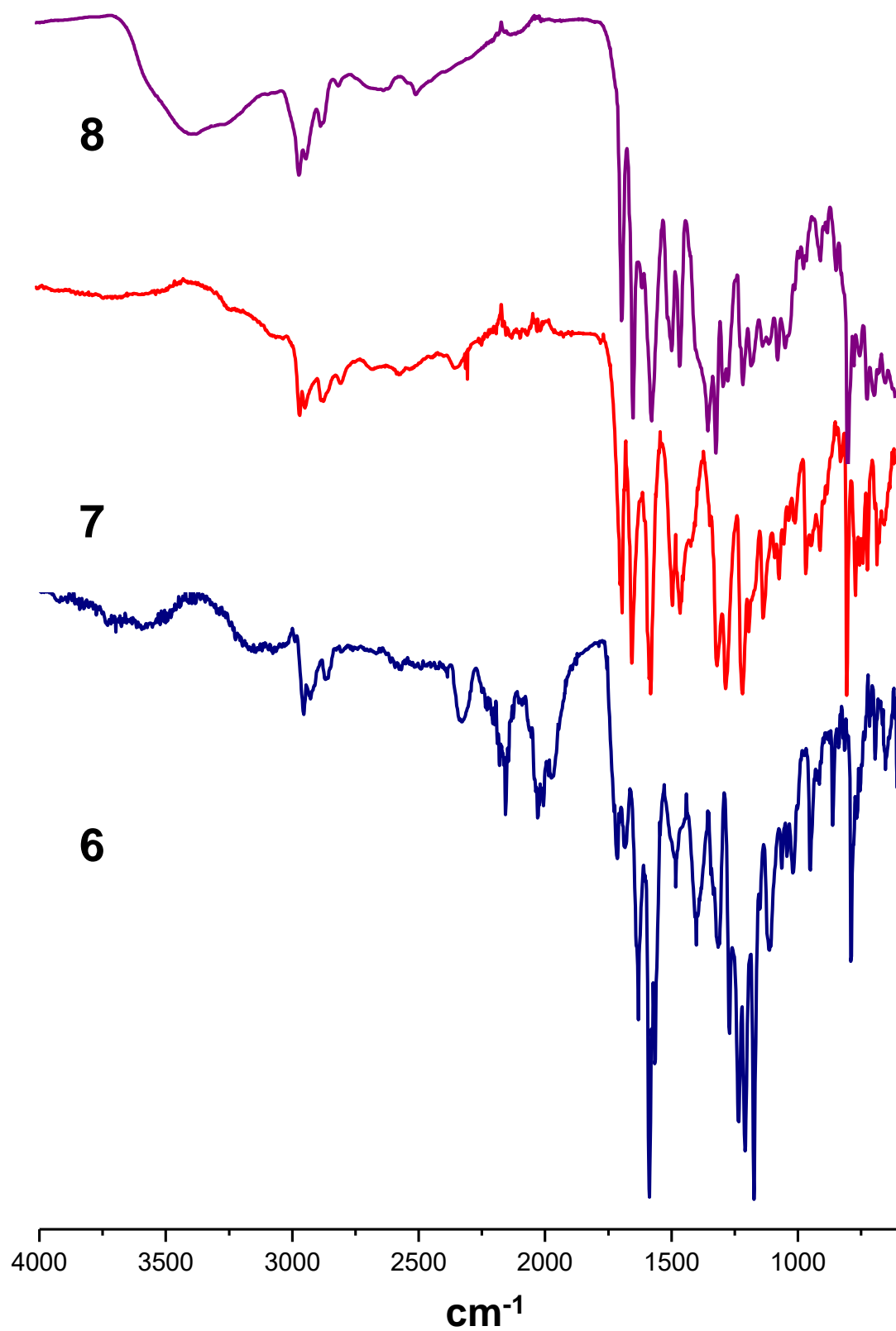


Figure S16. FTIR spectra of **6** (blue traces), **7** (red traces) and **8** (purple traces).

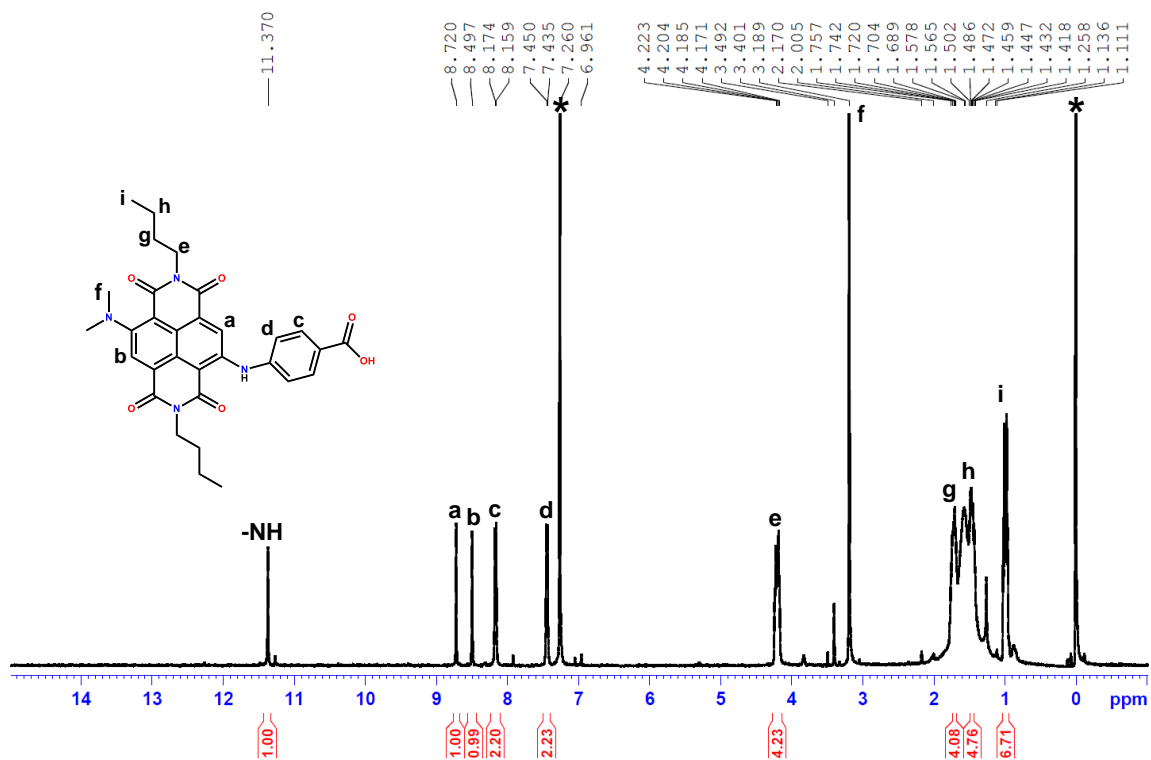


Figure S17. 500 MHz <sup>1</sup>H NMR spectrum of **6** in CDCl<sub>3</sub> at room temperature. \* represents residual solvent, H<sub>2</sub>O peaks.

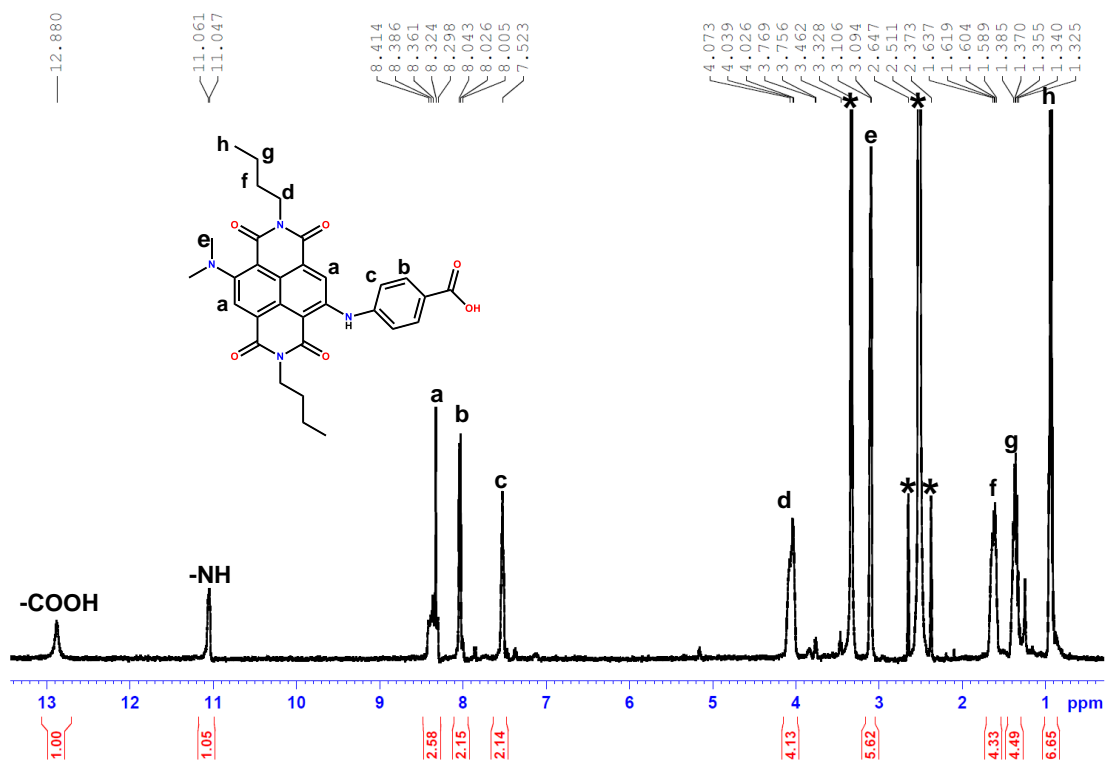


Figure S18. 500 MHz <sup>1</sup>H NMR spectrum of **6** in d<sub>6</sub>-DMSO at room temperature. \* represents residual solvent and H<sub>2</sub>O peaks.



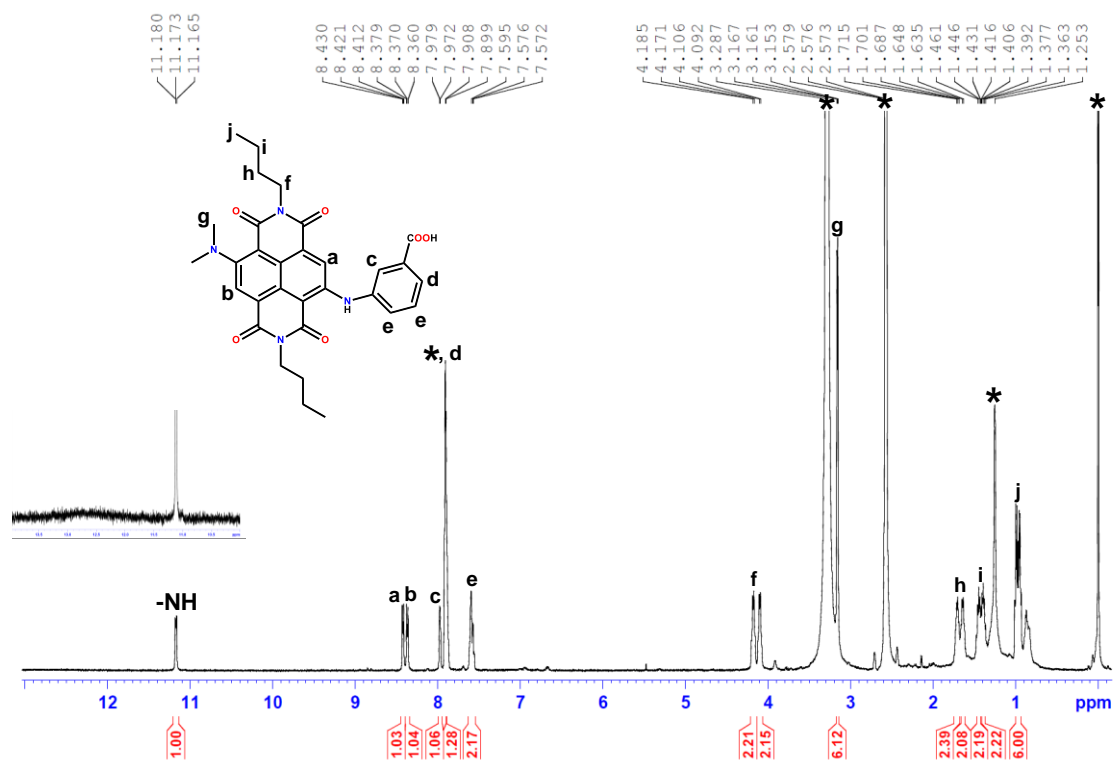


Figure S20. 500 MHz  $^1\text{H}$  NMR spectrum of **7** in  $d_6$ -DMSO at room temperature. \* represents residual solvent and  $\text{H}_2\text{O}$  peaks.

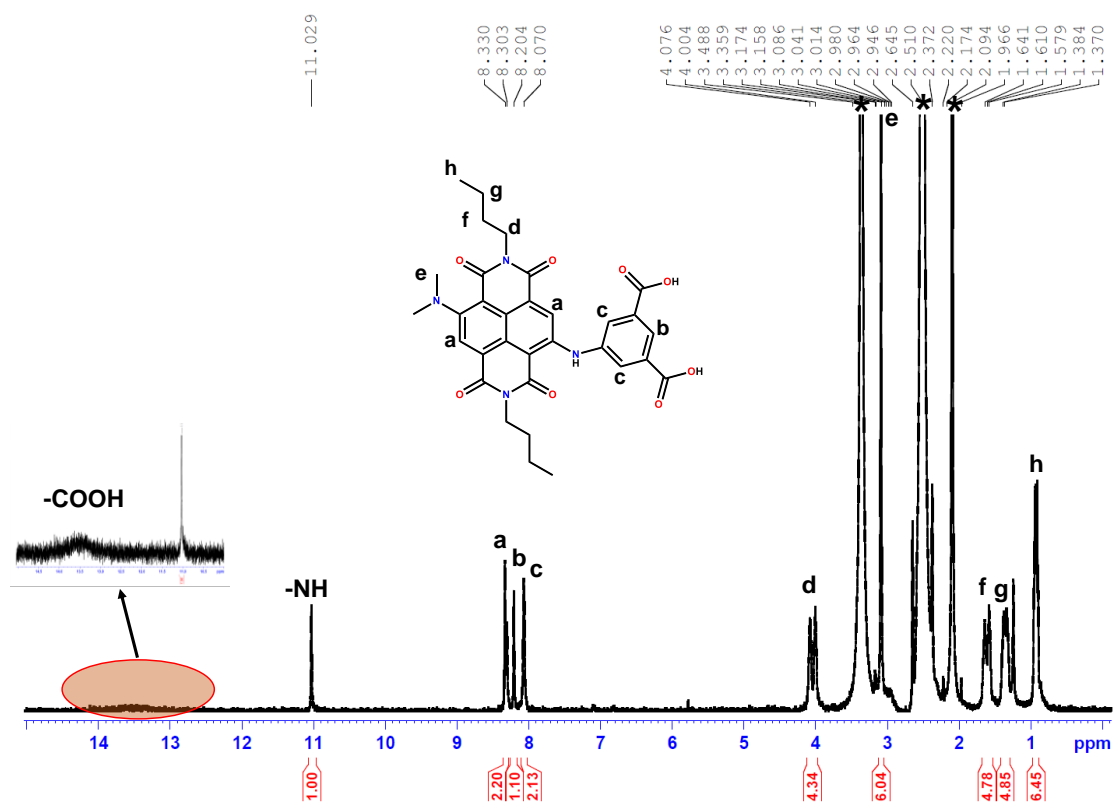


Figure S21. 500 MHz  $^1\text{H}$  NMR spectrum of **8** in  $d_6$ -DMSO at room temperature. \* represents residual solvent and  $\text{H}_2\text{O}$  peaks.

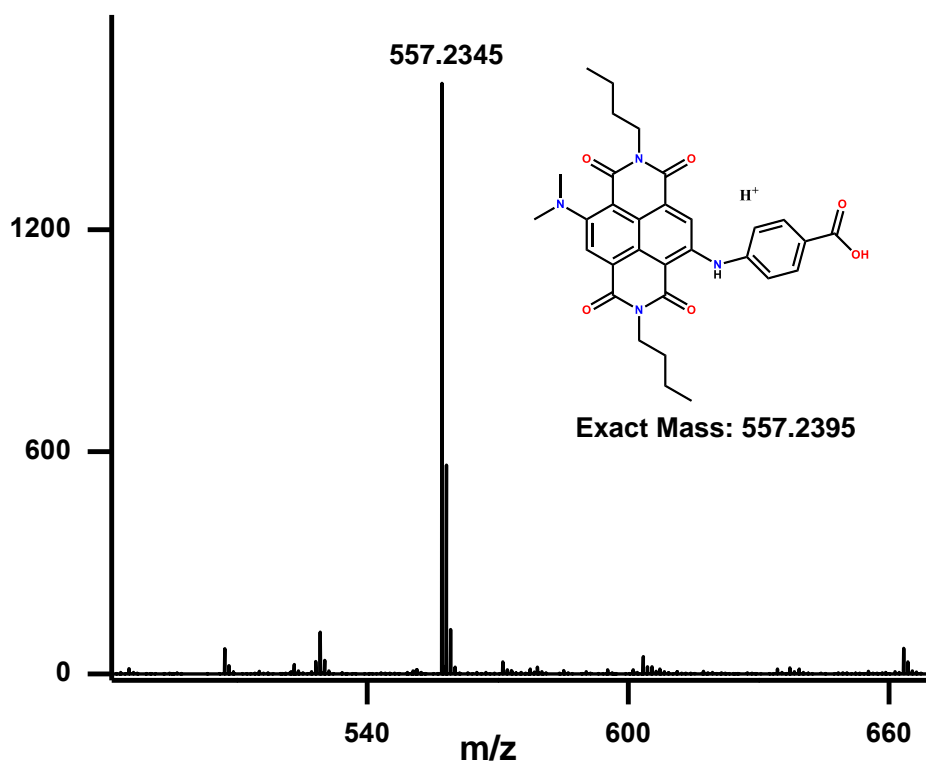


Figure S22. ESI-HRMS of **6** in DMF.

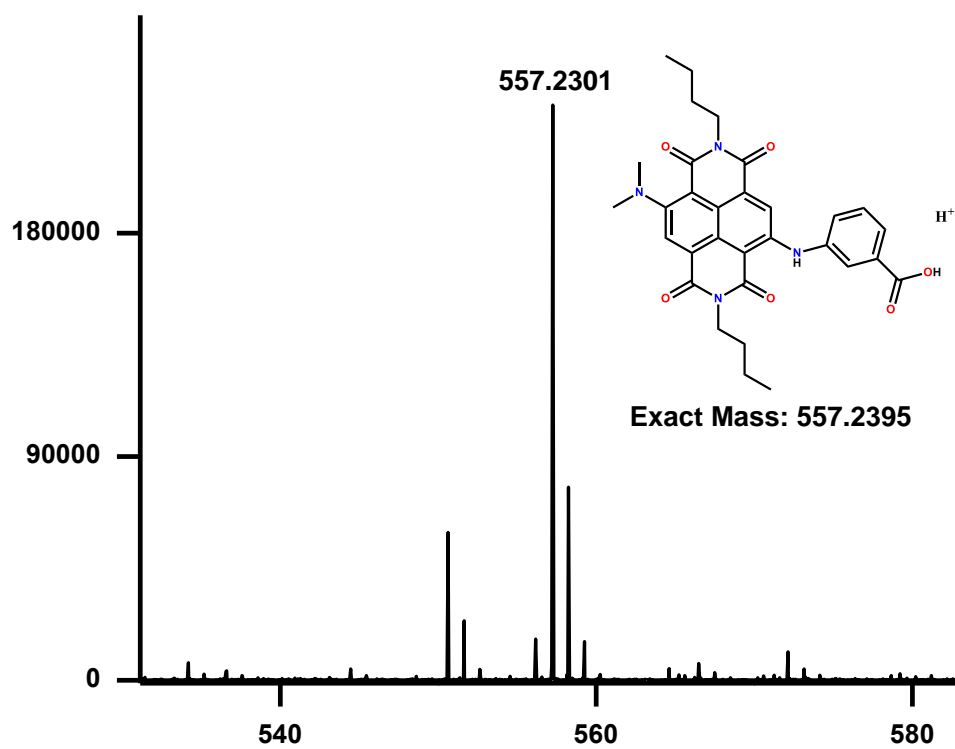


Figure S23. ESI-HRMS of **7** in DMF.

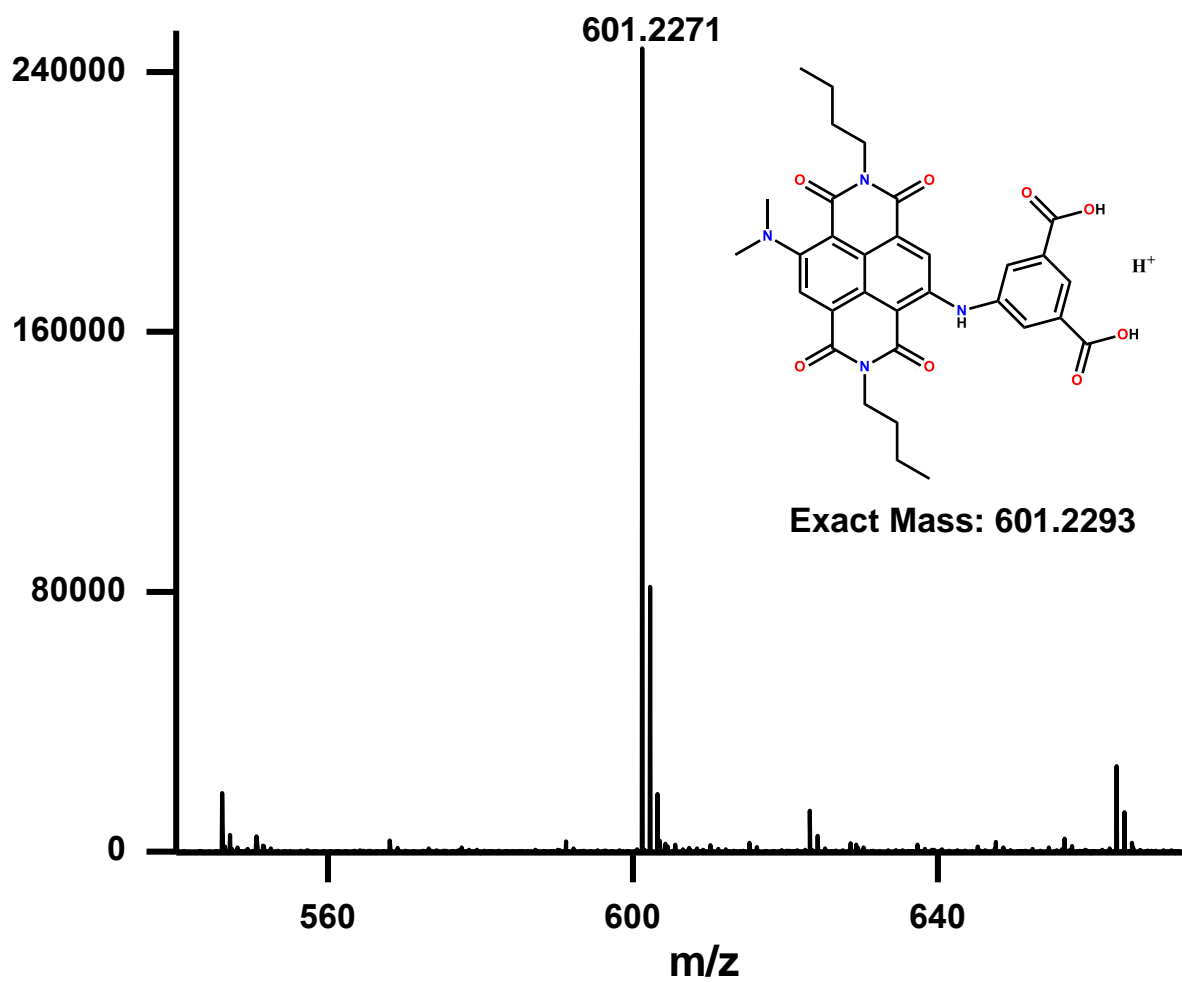


Figure S24. ESI-HRMS of **8** in DMF.



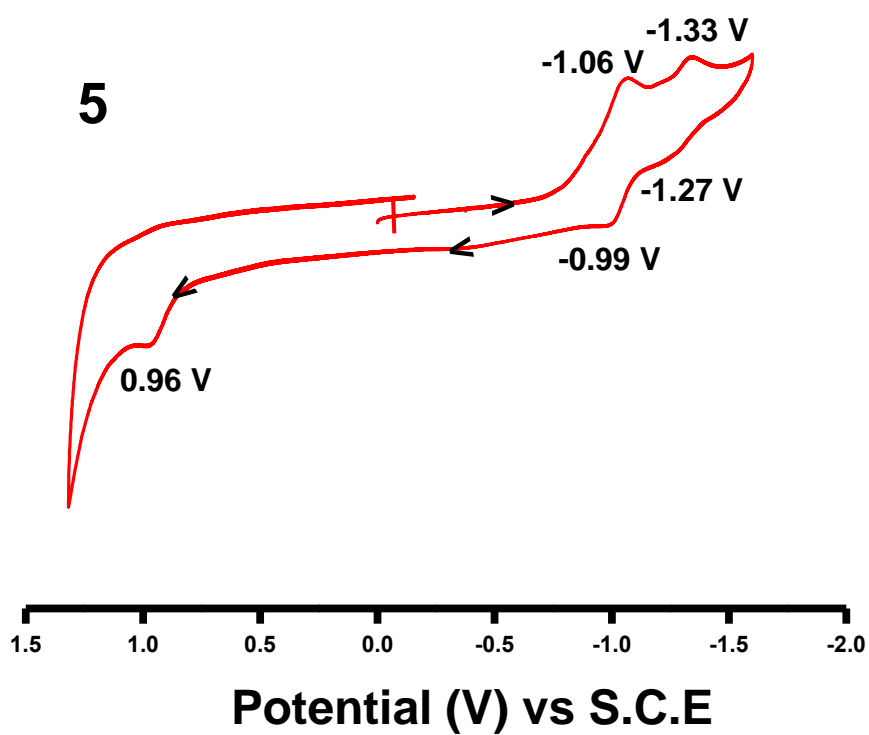
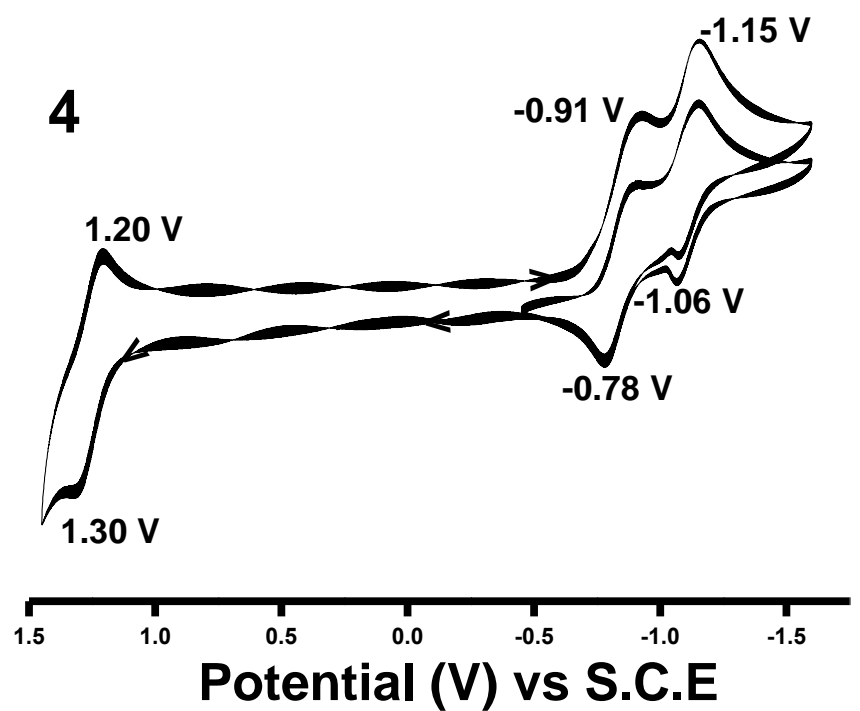


Figure S25. Cyclic voltammogram of **4** and **5**. Condition: 1 mM solution of **4** and **5** in DCM; 0.1 M Bu<sub>4</sub>NPF<sub>6</sub> at 298 K; scan rate, 200mV/s.

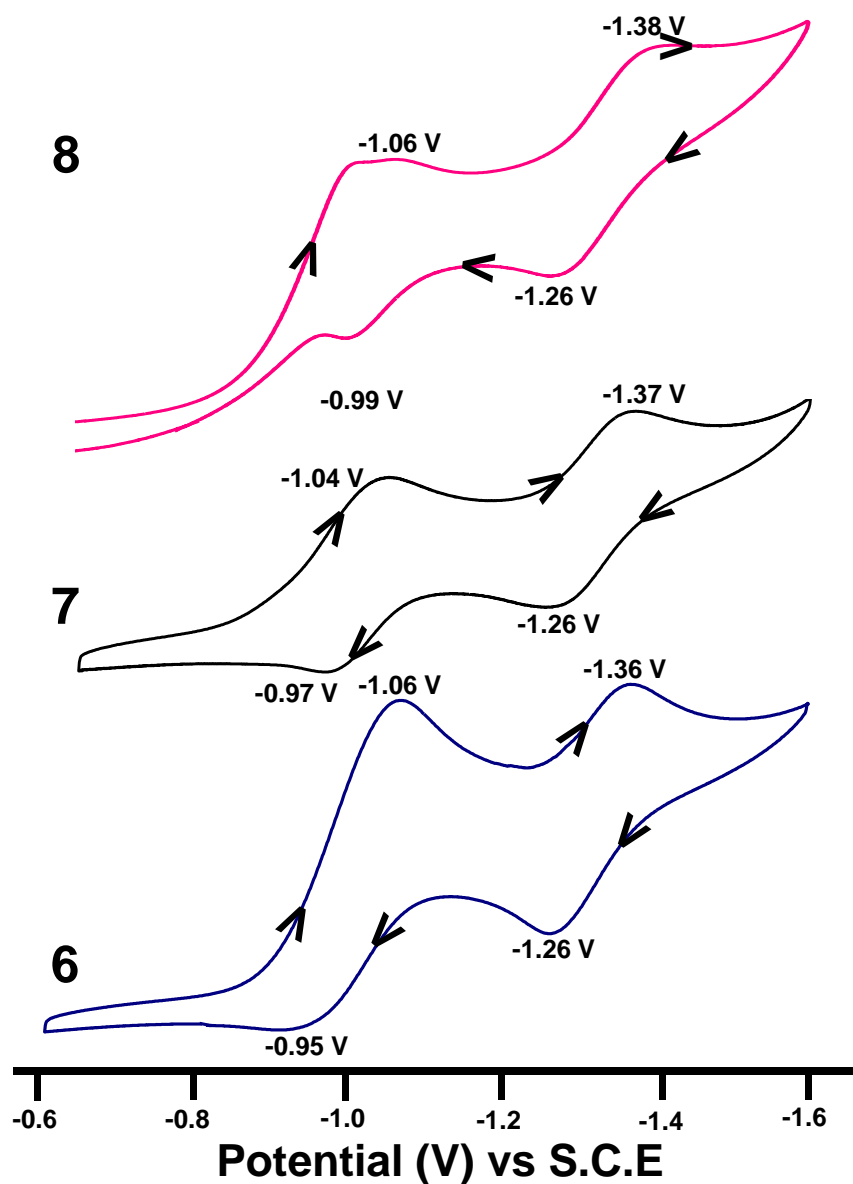


Figure S26. Cyclic voltammogram of **6-8**. Condition: 1 mM solution of **6-8** in DCM; 0.1 M  $\text{Bu}_4\text{NPF}_6$  at 298 K; scan rate, 200mV/s.

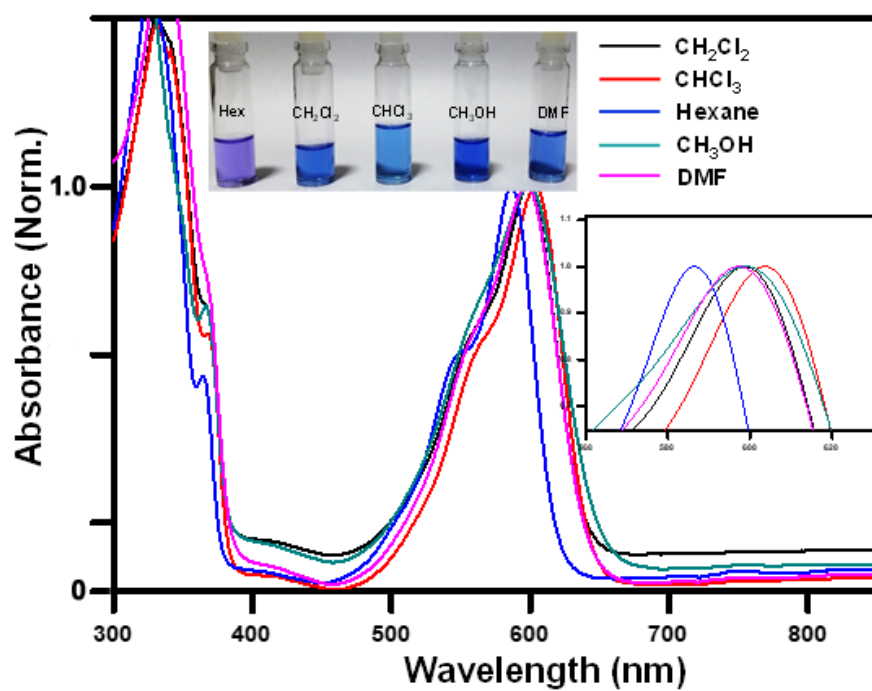


Figure S27. Normalized Uv-Vis absorption spectra of 1 in different solvents.

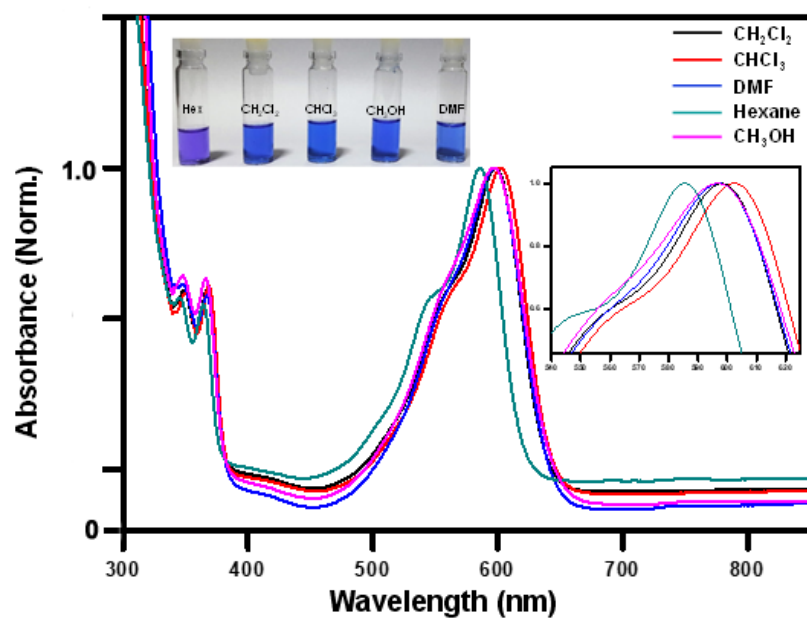


Figure S28. Normalized Uv-Vis absorption spectra of **2** in different solvents.

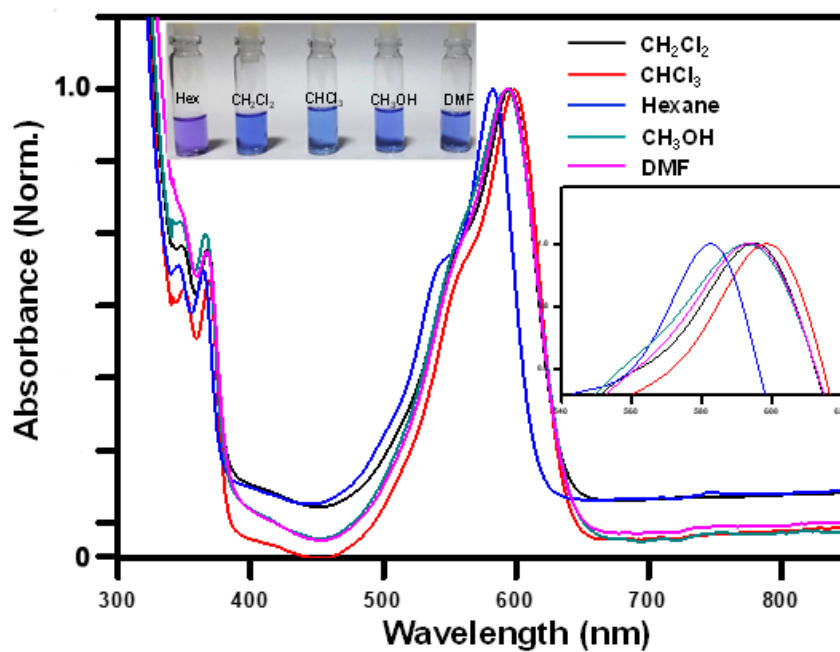


Figure S29. Normalized Uv-Vis absorption spectra of **3** in different solvents.

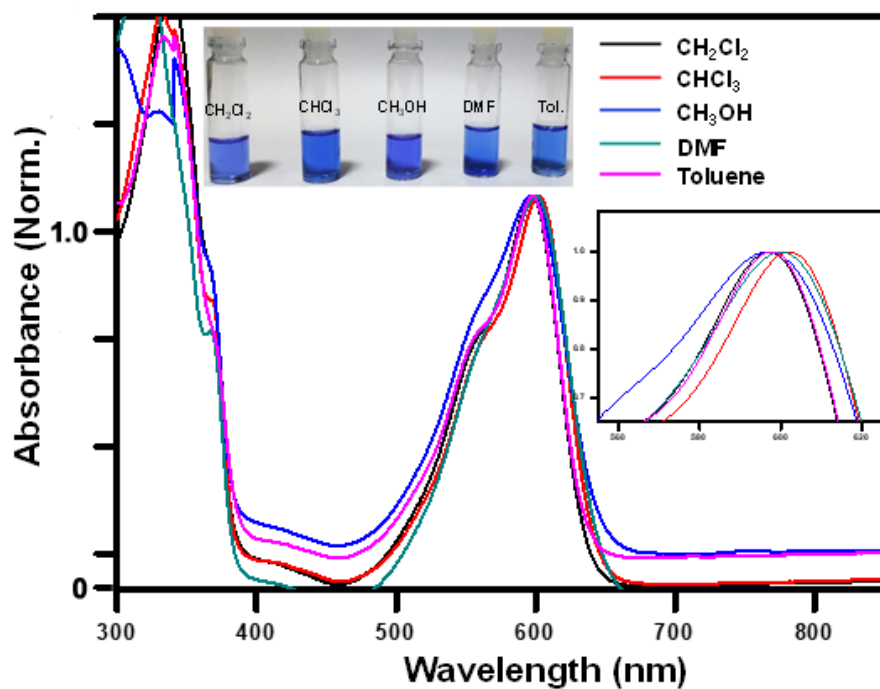


Figure S30. Normalized Uv-Vis absorption spectra of **6** in different solvents.

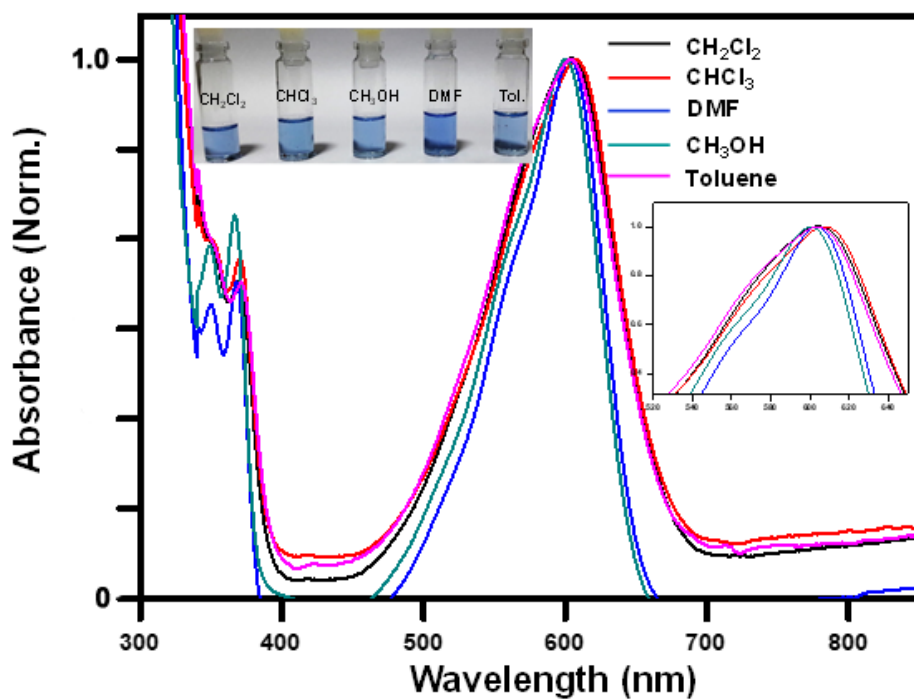


Figure S31. Normalized Uv-Vis absorption spectra of **7** in different solvents.

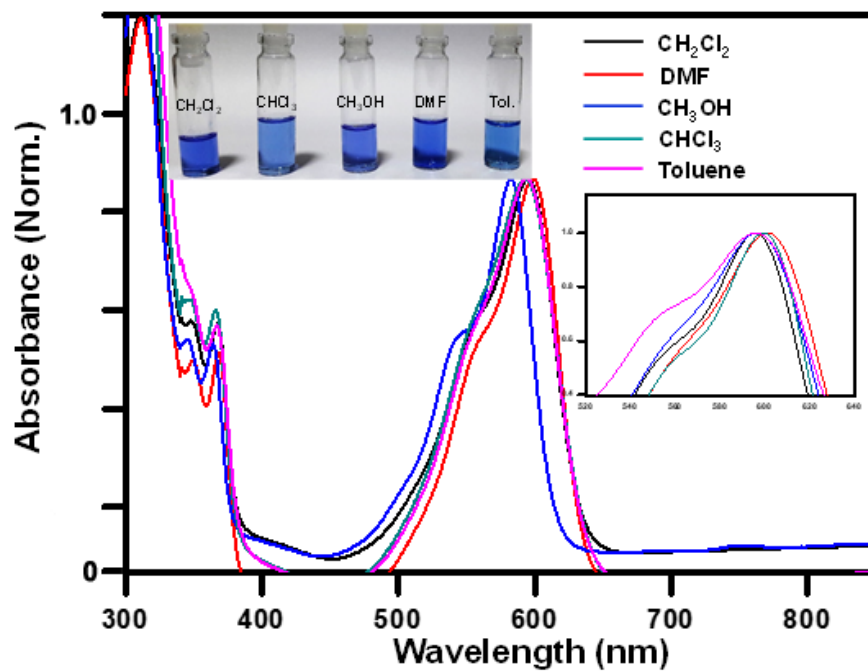


Figure S32. Normalized Uv-Vis absorption spectra of **8** in different solvents.

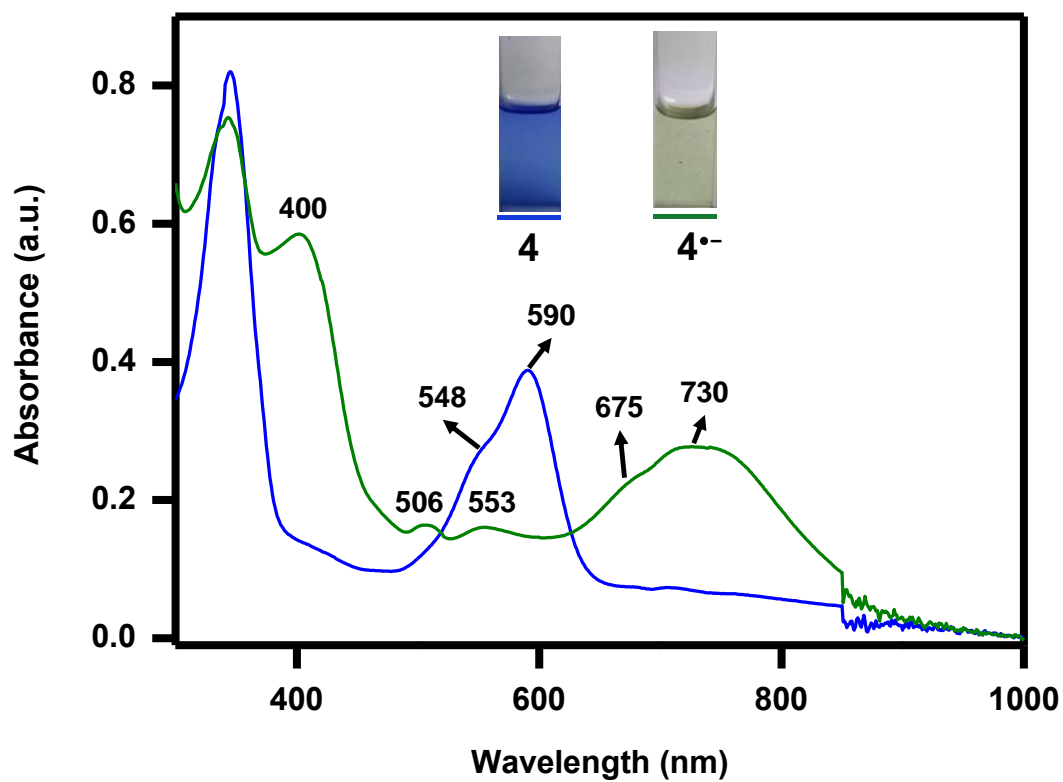


Figure S33. Uv-Vis-NIR spectra of **4** and **4<sup>•-</sup>** in DMF after the addition of 1M Na<sub>2</sub>S solution in Methanol. (All the solutions were prepared under ambient conditions).

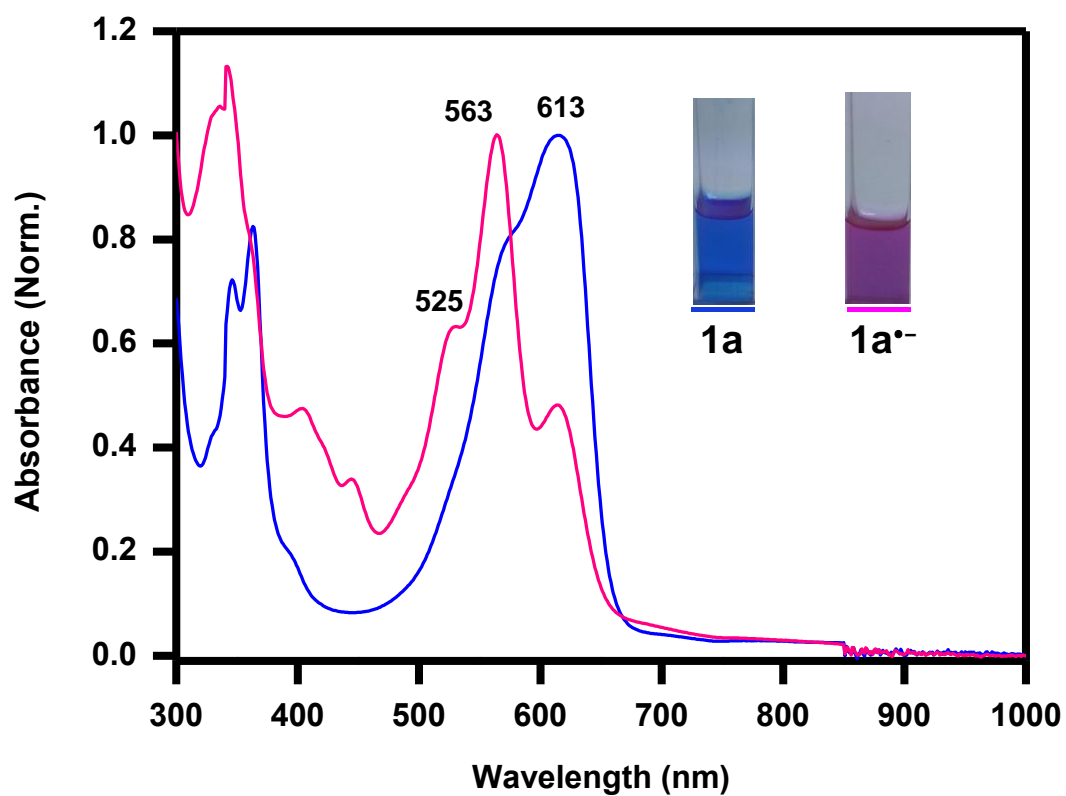


Figure S34. Uv-Vis-NIR spectra of **1a** and **1a<sup>-</sup>** in DMF after the addition of 1M Na<sub>2</sub>S solution in Methanol. (All the solutions were prepared under ambient conditions).



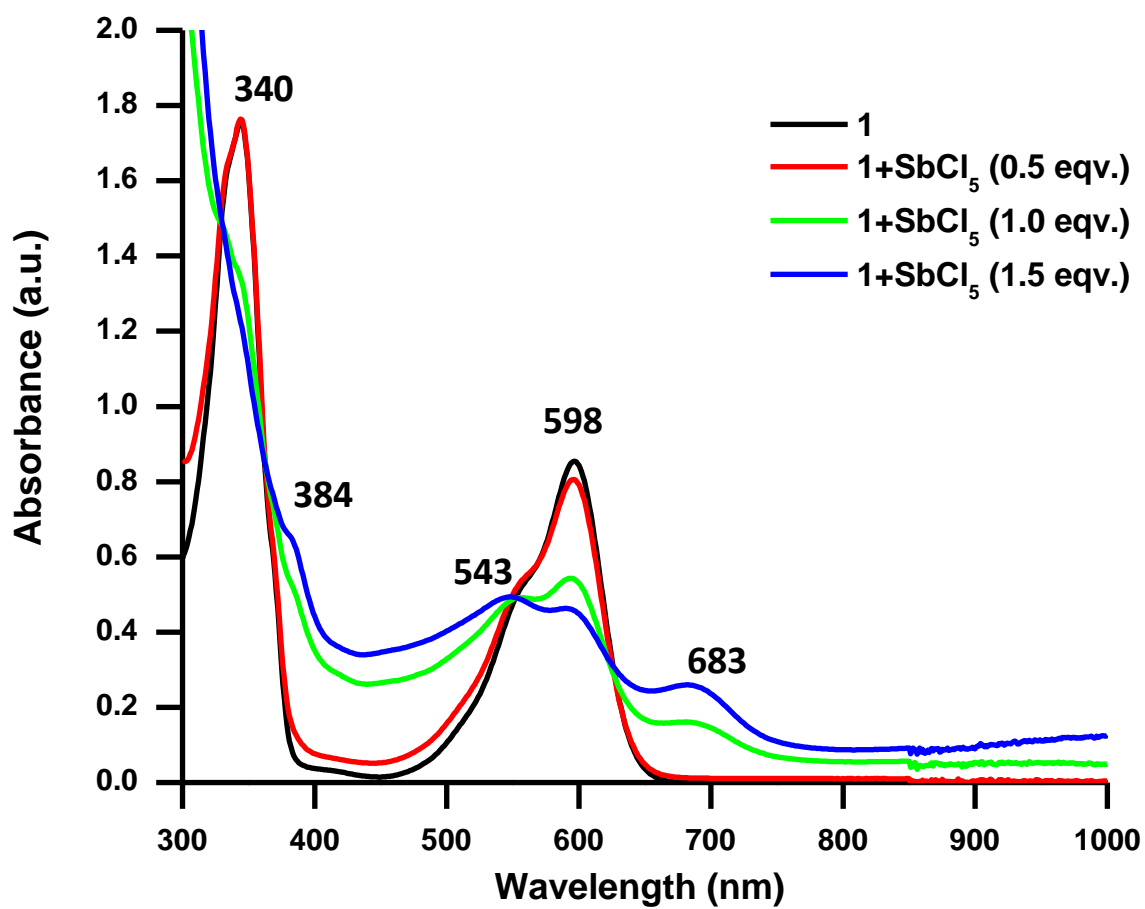


Figure S35. Changes in the Uv-Vis-NIR spectra of **1** before and after addition of SbCl<sub>5</sub> in DCM. (All the solutions were prepared under ambient conditions).

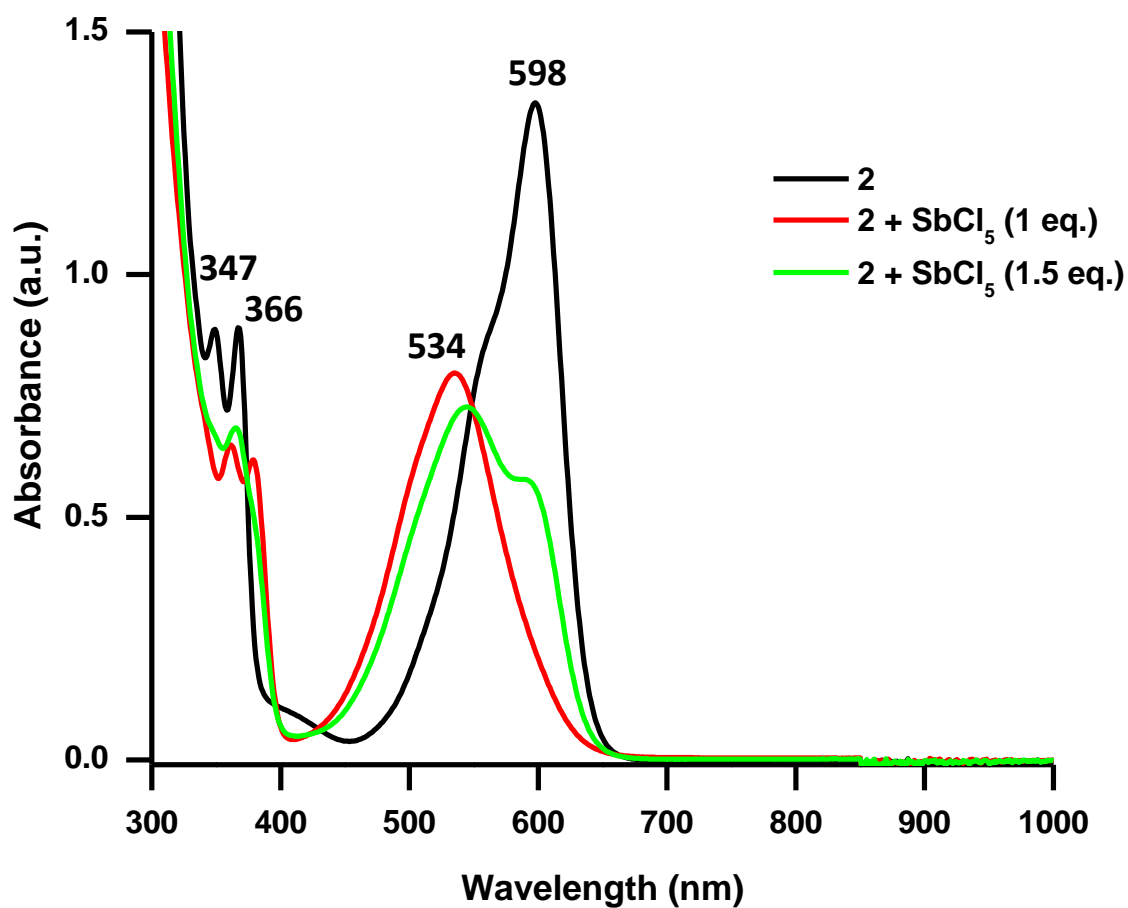


Figure S36. Changes in the Uv-Vis-NIR spectra of **2** before and after addition of SbCl<sub>5</sub> in DCM. (All the solutions were prepared under ambient conditions).

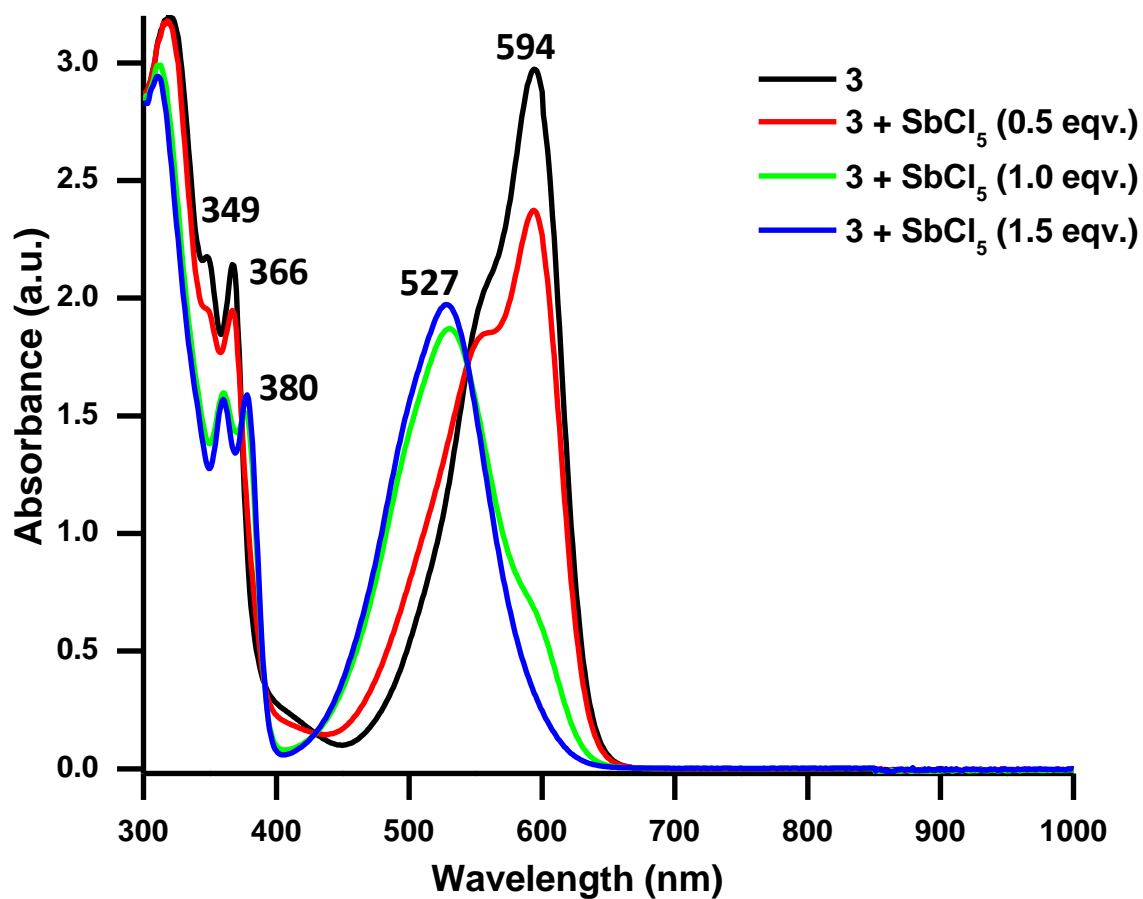


Figure S37. Changes in the Uv-Vis-NIR spectra of **3** before and after addition of SbCl<sub>5</sub> in DCM. (All the solutions were prepared under ambient conditions).

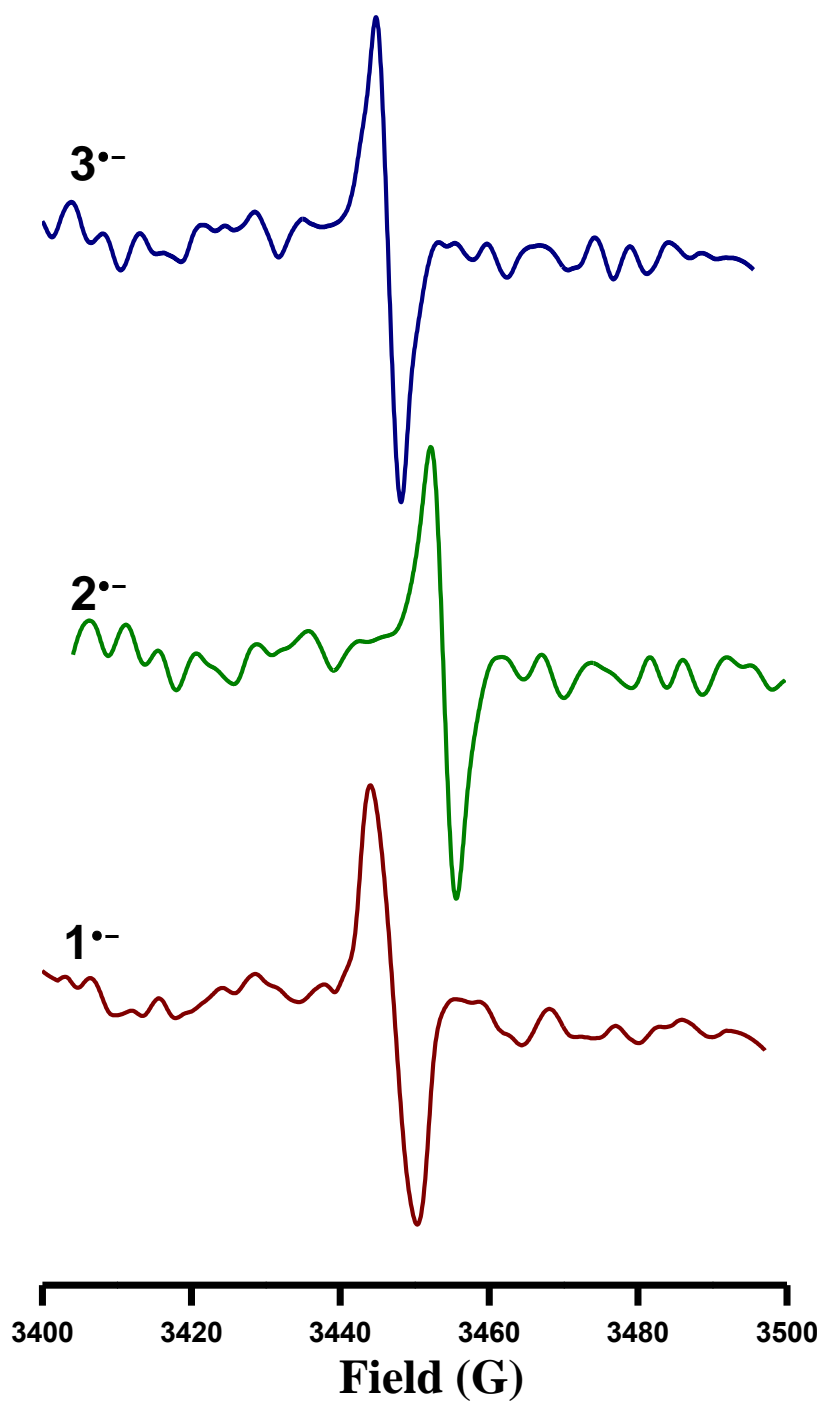


Figure S38. ESR spectra of  $1^{\bullet-}$ ,  $2^{\bullet-}$  and  $3^{\bullet-}$  in DMF. All solutions were prepared under ambient conditions.

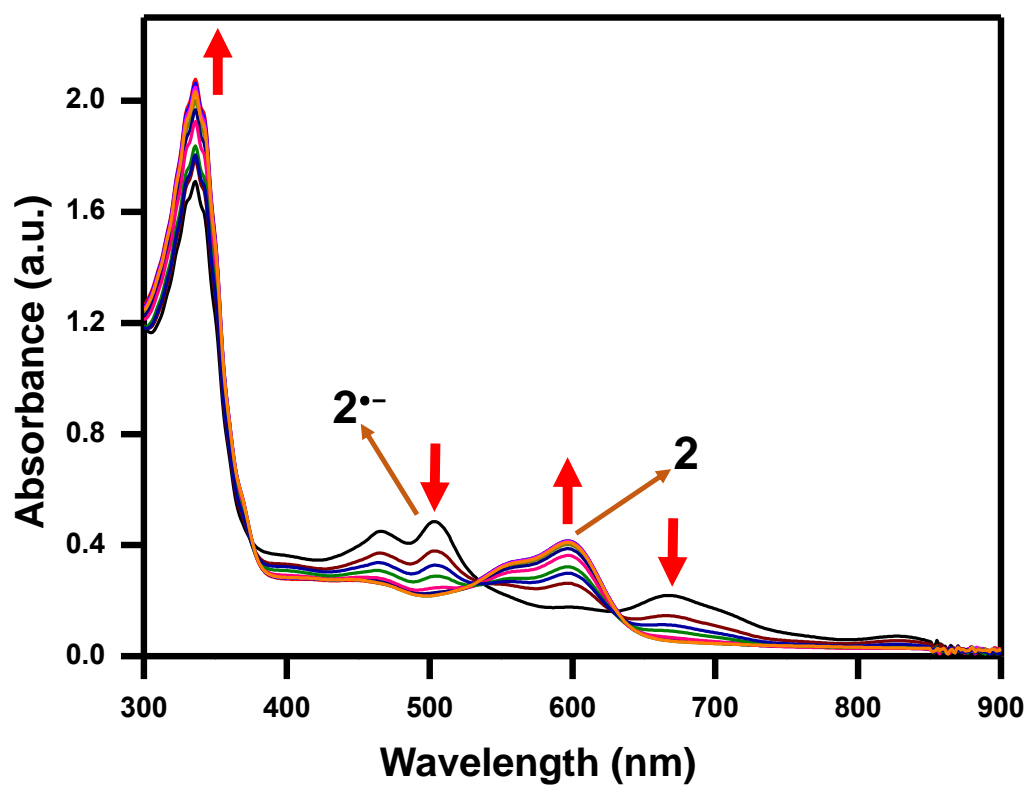


Figure S39. Time dependent Uv-Vis spectra of  $2^{\bullet-}$  in DMF displaying the reversible changes in absorption from  $2^{\bullet-} \rightarrow 2$ .

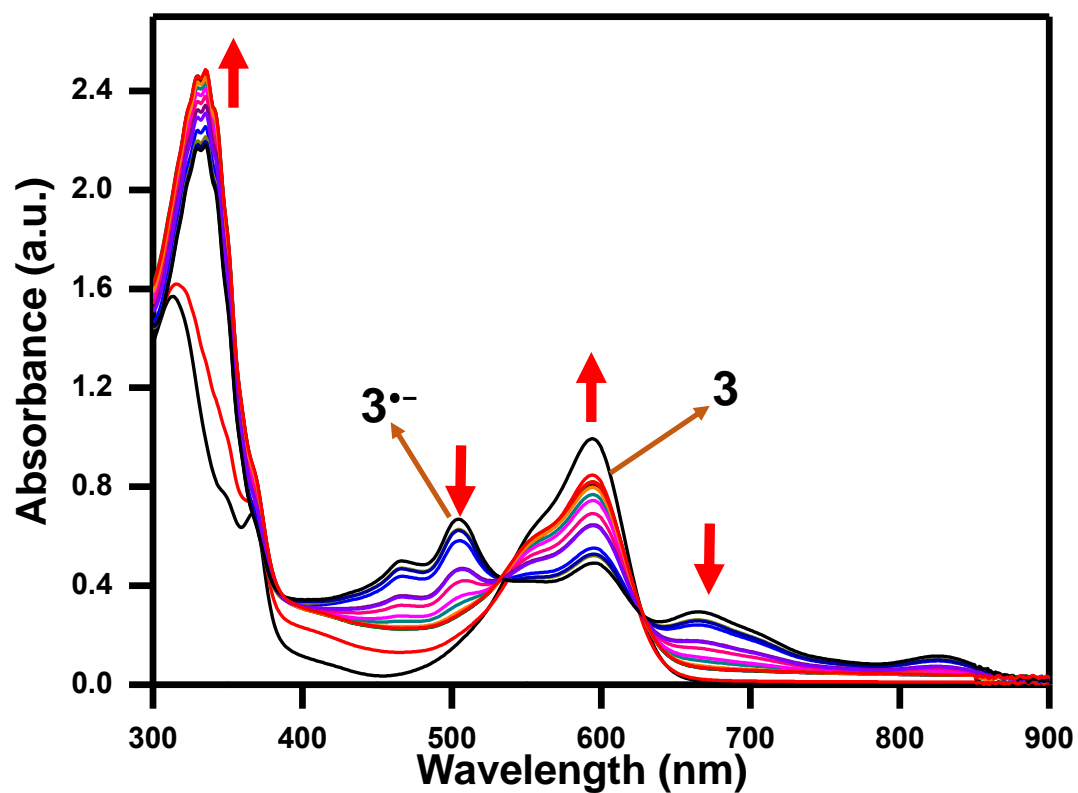


Figure S40. Time dependent Uv-Vis spectra of  $3^{\bullet-}$  in DMF displaying the reversible changes in absorption from  $3^{\bullet-} \rightarrow 3$ .

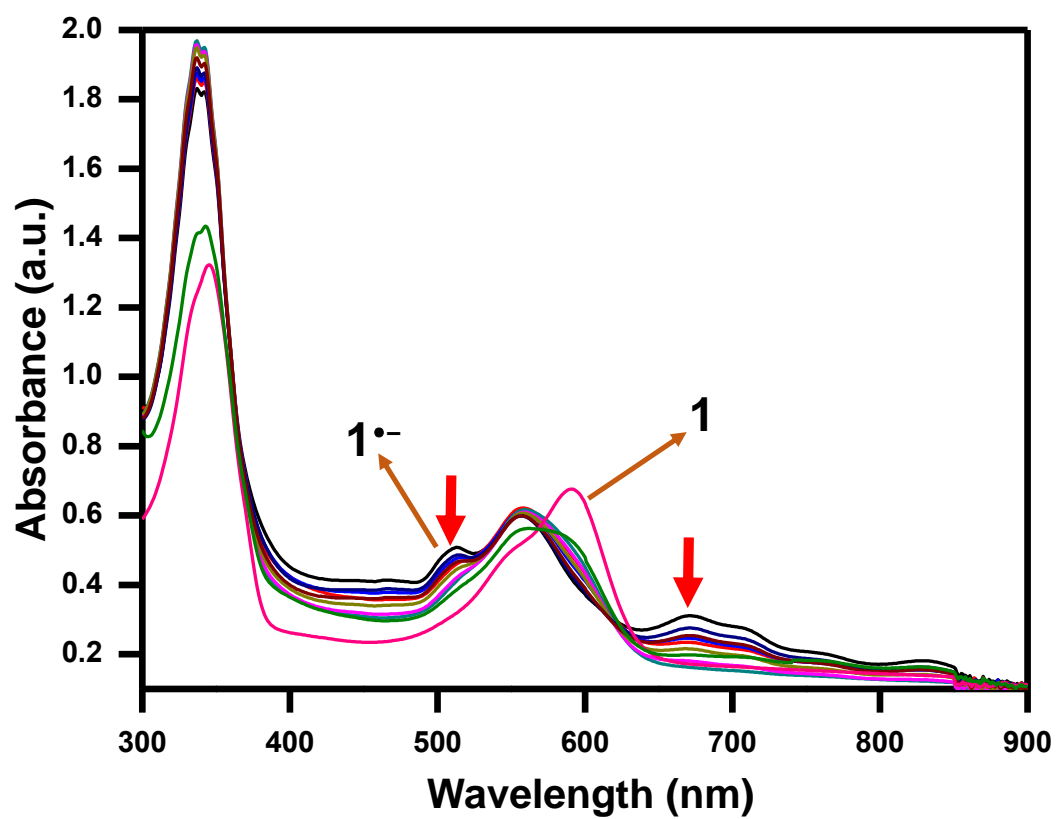


Figure S41. Time dependent Uv-Vis spectra of  $1^{\bullet-}$  in DMF displaying the changes in absorption profile.

Table S1. Crystal data and structural refinement parameters for **6**.

Compound	<b>6</b>
Formula	C <sub>32</sub> H <sub>33</sub> Cl <sub>3</sub> N <sub>4</sub> O <sub>6</sub>
Formula Wt.	675.97
T (K)	295(2) K
System	Monoclinic
Space group	P 2 <sub>1</sub> /n
a (Å)	15.0200 (10)
b (Å)	10.8841 (7)
c (Å)	20.8248 (13)
α (°)	90
β (°)	108.162 (2)
γ (°)	90
V (Å <sup>3</sup> )	3234.8 (4)
Z	4
ρ <sub>calc</sub> (mg/m <sup>3</sup> )	1.388
μ (mm <sup>-1</sup> )	0.333
F (000)	1408
Goodness-of-fit (GOF) on F <sup>2</sup>	1.085
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0726, wR <sub>2</sub> = 0.2272
R indices (all data)	R <sub>1</sub> = 0.0969, wR <sub>2</sub> = 0.2449
CCDC	1899200

Table S2. Spin density distribution data for **1<sup>•-</sup>**, **2<sup>•-</sup>** and **3<sup>•-</sup>** obtained from DFT calculations.

Atoms	<b>1<sup>•-</sup></b>	<b>2<sup>•-</sup></b>	Atoms	<b>3<sup>•-</sup></b>
C1	0.035813	0.041703	C1	0.039845
C2	0.053894	0.056104	C2	0.053355
C3	-0.031419	-0.027557	C3	-0.032685
C4	0.089365	0.081287	C4	0.087590
C5	0.038115	0.044032	C5	0.041365
C6	0.007084	0.003880	C6	0.004891
C7	-0.017503	-0.019722	C7	-0.015703
C8	0.041520	0.041946	C8	0.041274
C9	0.184899	0.182802	C9	0.183616
C10	0.051707	0.051701	C10	0.052417
C11	0.052891	0.051424	C11	0.051303
C12	0.064218	0.051532	C12	0.058166
C13	0.039450	0.032373	C13	0.034434
C14	0.111043	0.134226	C14	0.122599
O17	0.058522	0.060139	O17	0.059715
O18	0.059510	0.063902	O18	0.062304
O19	0.076883	0.073369	O19	0.074919
O20	0.064424	0.062609	O20	0.063178
C21	0.001039	0.001069	C21	0.001080
C25	-0.000121	-0.000030	C25	-0.000065
N29	-0.020229	-0.021649	N29	-0.021019
N30	-0.030060	-0.029158	N30	-0.029635
N31	0.020696	0.030412	N31	0.026548
N32	0.038967	0.035707	N32	0.037003
C34	-0.006173	-0.003441	C34	-0.002660
C35	0.009052	0.003954	C35	0.002948
C36	0.006032	0.006981	C36	0.011743
C37	0.004377	0.002432	C37	0.002147
C39	-0.002209	-0.001091	C39	-0.001950
C41	0.010009	0.006406	C41	0.008500
C42	-0.004563	-0.004437	C42	-0.004629
C46	0.002021	0.002239	C46	0.002282
C52	-0.000432	0.000368	C50	0.000845
O53	0.000601	-0.000145	O51	-0.000217
O54	-----	-0.000104	O52	-0.000112
C55	-----	-0.000053	C53	-0.000728
C58	-----	0.000036	O54	-0.000215
O52	0.002137	-----	O55	-0.000010
C54	-0.000076	-----	C57	0.000011
C57	-0.000018	-----	C61	0.000262



Table S3. Weak interaction table for compound **6**.

Atoms	D...A	D-H...A	∠ D-H...A
N3-H3...O3	2.642	2.070	137
C28-H28...O4	3.289	2.402	159
C30-H30C...O2	2.744	1.964	137
C30-H30b...O3	3.368	2.564	141
O6-H1...O5	2.618	2.151	116

**DFT calculations**

Opt: B3LYP/6-311++g(d,p)

scf=(cpcm, solvent=dichloromethane) geom=connectivity scf=xqc

[1]

**Calculation Type** FOPT  
**Calculation Method** RB3LYP  
**Basis Set** 6-311++G(d,p)  
**Charge** 0  
**Spin** Singlet  
**Energy (RB3LYP)** -1714.27401793 a.u.  
**RMS Gradient Norm** 0.00001476 a.u.  
**Imaginary Freq** -----  
**Dipole Moment** 5.5696 Debye  
**Point Group** C1

Symbol	X	Y	Z
C	3.57433	-2.61088	-0.22806
C	3.55517	-1.16139	0.02871
C	2.28807	-0.51813	0.05338
C	1.08628	-1.26893	0.13237
C	1.12762	-2.75109	0.17941
C	4.7417	-0.37692	0.07892
C	2.16711	0.89177	-0.00288
C	3.36324	1.64469	-0.11604
C	4.59243	1.03123	-0.07925
C	3.3181	3.12089	-0.23118

C	0.85219	2.99531	-0.02583
C	0.90305	1.53249	0.01817
C	-0.28143	0.75528	0.0919
C	-0.14296	-0.65406	0.16669
H	-1.017	-1.27929	0.27263
H	5.46448	1.66739	-0.11519
O	0.12304	-3.43133	0.34624
O	4.5526	-3.22446	-0.63502
O	-0.19771	3.64108	0.06199
O	4.32472	3.80389	-0.35934
C	1.9408	5.16657	-0.25598
H	2.9342	5.56583	-0.42953
H	1.27445	5.44157	-1.07249
H	1.53647	5.55999	0.67688
C	2.45359	-4.78894	-0.16408
H	2.56086	-5.06768	-1.21393
H	3.31694	-5.15584	0.38686
H	1.53875	-5.21387	0.23583
N	2.37387	-3.32724	-0.02706
N	2.05005	3.70162	-0.17817
N	-1.51534	1.35154	0.13739
N	5.9911	-0.88456	0.30842
H	-1.4739	2.3642	0.24159
C	-2.78627	0.77146	-0.01079
C	-3.04693	-0.27838	-0.90523
C	-3.84933	1.3241	0.72152
C	-4.33472	-0.7784	-1.03303
H	-2.25278	-0.68363	-1.5183
C	-5.13589	0.82761	0.57978
H	-3.65284	2.13863	1.40919
C	-5.39391	-0.23872	-0.29208
C	7.18751	-0.10702	-0.00773

H	7.06462	0.42979	-0.9477
H	7.4442	0.60628	0.7857
H	8.02158	-0.79936	-0.12712
C	6.22328	-2.00852	1.21111
H	6.52764	-2.9091	0.67443
H	7.00875	-1.72441	1.91747
H	5.32108	-2.23312	1.77856
H	-4.5352	-1.58586	-1.72575
C	-6.74795	-0.81848	-0.46952
O	-7.00461	-1.74708	-1.21089
O	-7.67483	-0.20847	0.28647
C	-9.03023	-0.71598	0.18342
H	-9.35022	-0.63691	-0.85852
H	-9.02409	-1.77374	0.45836
C	-9.90108	0.10569	1.10855
H	-9.89433	1.16042	0.82219
H	-10.93147	-0.25656	1.05377
H	-9.56413	0.02129	2.14481
H	-5.94404	1.25799	1.15693

[2]

<b>Calculation Type</b>	<b>FOPT</b>
<b>Calculation Method</b>	<b>RB3LYP</b>
<b>Basis Set</b>	<b>6-311++G(d,p)</b>
<b>Charge</b>	<b>0</b>
<b>Spin</b>	<b>Singlet</b>
<b>Energy (RB3LYP)</b>	<b>-1714.27219007 a.u.</b>
<b>RMS Gradient Norm</b>	<b>0.00000501 a.u.</b>
<b>Imaginary Freq</b>	<b>-----</b>
<b>Dipole Moment</b>	<b>5.2785 Debye</b>
<b>Point Group</b>	<b>C1</b>

Symbol	X	Y	Z
C	3.3408	-2.30776	-0.17184
C	3.06206	-0.88193	0.06444

C	1.70525	-0.46254	0.01322
C	0.64486	-1.40629	0.02887
C	0.93291	-2.86037	0.09078
C	4.09512	0.09118	0.17012
C	1.35132	0.90685	-0.05987
C	2.40785	1.85089	-0.11424
C	3.71947	1.45369	-0.00731
C	2.12043	3.29834	-0.24354
C	-0.29658	2.75751	-0.17175
C	-0.00213	1.32512	-0.1131
C	-1.04108	0.35829	-0.10459
C	-0.67008	-1.00822	-0.01351
H	-1.43148	-1.77239	0.0426
H	4.47236	2.22792	-0.00253
O	0.04946	-3.70125	0.20258
O	4.43155	-2.74802	-0.5116
O	-1.44346	3.21755	-0.14828
O	3.00303	4.14194	-0.32214
C	0.42158	5.08174	-0.36106
H	1.34132	5.64308	-0.48496
H	-0.23633	5.24042	-1.21446
H	-0.09339	5.40098	0.54521
C	2.60388	-4.64406	-0.14651
H	2.82271	-4.90191	-1.18428
H	3.48082	-4.85794	0.46083
H	1.75128	-5.21782	0.20171
N	2.26895	-3.2171	-0.0326
N	0.77194	3.65638	-0.26433
N	-2.3578	0.73108	-0.143
N	5.39812	-0.20094	0.4689
H	-2.50287	1.73514	-0.05366
C	-3.49278	-0.07326	-0.37632

C	-3.51137	-1.09501	-1.33597
C	-4.66352	0.22027	0.33082
C	-4.67476	-1.82845	-1.55659
H	-2.6275	-1.30175	-1.92581
C	-5.83328	-0.50515	0.08986
H	-4.65706	1.01189	1.06845
C	-5.83763	-1.54196	-0.8501
C	6.46387	0.7638	0.20609
H	6.30165	1.27205	-0.74378
H	6.55943	1.51071	1.00452
H	7.40595	0.219	0.13473
C	5.76439	-1.26854	1.39517
H	6.24277	-2.10731	0.88582
H	6.45185	-0.85637	2.13972
H	4.88235	-1.63912	1.91593
H	-4.67353	-2.6162	-2.30047
H	-6.74728	-2.10214	-1.02241
C	-7.09376	-0.21086	0.8236
O	-8.13323	-0.82	0.68054
O	-6.97912	0.8223	1.68541
C	-8.24595	1.00445	2.32326
H	-8.98881	1.22346	1.58495
H	-8.51452	0.10969	2.84497
C	-8.15453	2.17317	3.32192
H	-7.87855	3.06635	2.80138
H	-9.10449	2.31435	3.79367
H	-7.41703	1.95085	4.0646

[3]

<b>Calculation Type</b>	<b>FOPT</b>
<b>Calculation Method</b>	<b>RB3LYP</b>
<b>Basis Set</b>	<b>6-311++G(d,p)</b>
<b>Charge</b>	<b>0</b>
<b>Spin</b>	<b>Singlet</b>
<b>Energy (RB3LYP)</b>	<b>-1902.89101569 a.u.</b>
<b>RMS Gradient Norm</b>	<b>0.00000867 a.u.</b>
<b>Imaginary Freq</b>	<b>-----</b>
<b>Dipole Moment</b>	<b>8.0797 Debye</b>
<b>Point Group</b>	<b>C1</b>

Symbol	X	Y	Z
C	3.3408	-2.30776	-0.17184
C	3.06206	-0.88193	0.06444
C	1.70525	-0.46254	0.01322
C	0.64486	-1.40629	0.02887
C	0.93291	-2.86037	0.09078
C	4.09512	0.09118	0.17012
C	1.35132	0.90685	-0.05987
C	2.40785	1.85089	-0.11424
C	3.71947	1.45369	-0.00731
C	2.12043	3.29834	-0.24354
C	-0.29658	2.75751	-0.17175
C	-0.00213	1.32512	-0.1131
C	-1.04108	0.35829	-0.10459
C	-0.67008	-1.00822	-0.01351
H	-1.43148	-1.77239	0.0426
H	4.47236	2.22792	-0.00253
O	0.04946	-3.70125	0.20258
O	4.43155	-2.74802	-0.5116
O	-1.44346	3.21755	-0.14828
O	3.00303	4.14194	-0.32214
C	0.42158	5.08174	-0.36106
H	1.34132	5.64308	-0.48496

H	-0.23633	5.24042	-1.21446
H	-0.09339	5.40098	0.54521
C	2.60388	-4.64406	-0.14651
H	2.82271	-4.90191	-1.18428
H	3.48082	-4.85794	0.46083
H	1.75128	-5.21782	0.20171
N	2.26895	-3.2171	-0.0326
N	0.77194	3.65638	-0.26433
N	-2.3578	0.73108	-0.143
N	5.39812	-0.20094	0.4689
H	-2.50287	1.73514	-0.05366
C	-3.49278	-0.07326	-0.37632
C	-3.51137	-1.09501	-1.33597
C	-4.66352	0.22027	0.33082
C	-4.67476	-1.82845	-1.55659
H	-2.6275	-1.30175	-1.92581
C	-5.83328	-0.50515	0.08986
H	-4.65706	1.01189	1.06845
C	-5.83763	-1.54196	-0.8501
C	6.46387	0.7638	0.20609
H	6.30165	1.27205	-0.74378
H	6.55943	1.51071	1.00452
H	7.40595	0.219	0.13473
C	5.76439	-1.26854	1.39517
H	6.24277	-2.10731	0.88582
H	6.45185	-0.85637	2.13972
H	4.88235	-1.63912	1.91593
C	-7.12155	-0.16266	0.861
O	-8.24033	-0.67069	0.79926
O	-6.94377	0.8643	1.72999
C	-4.67301	-2.94812	-2.61391
O	-5.57512	-3.70746	-2.96486

O	-3.46809	-3.07774	-3.22447
H	-6.72809	-2.1093	-1.02363
C	-8.1599	1.1516	2.42524
H	-7.99891	1.96142	3.10581
H	-8.91795	1.42321	1.72062
H	-8.47283	0.28515	2.96951
C	-3.50684	-4.12519	-4.19722
H	-2.55776	-4.19266	-4.6867
H	-3.72512	-5.05394	-3.71277
H	-4.26664	-3.91274	-4.92004

[4]

<b>Calculation Type</b>	<b>FOPT</b>
<b>Calculation Method</b>	<b>RB3LYP</b>
<b>Basis Set</b>	<b>6-311++G(d,p)</b>
<b>Charge</b>	<b>0</b>
<b>Spin</b>	<b>Singlet</b>
<b>Energy (RB3LYP)</b>	<b>-2134.04381438 a.u.</b>
<b>RMS Gradient Norm</b>	<b>0.00000413 a.u.</b>
<b>Imaginary Freq</b>	<b>-----</b>
<b>Dipole Moment</b>	<b>0.0008 Debye</b>
<b>Point Group</b>	<b>C1</b>

Symbol	X	Y	Z
C	2.08857	-0.91126	-1.3646
C	1.68954	0.42553	-0.86752
C	0.32576	0.63658	-0.5363
C	-0.58921	-0.44803	-0.48516
C	-0.13631	-1.83452	-0.76741
C	2.58281	1.5155	-0.83013
C	-0.1777	1.9283	-0.23865
C	0.72632	3.01627	-0.29884
C	2.0569	2.80347	-0.58016
C	0.27032	4.39864	-0.02804
C	-1.99379	3.49348	0.40501



C	-1.54317	2.13783	0.08161
C	-2.44046	1.0397	0.09003
C	-1.91151	-0.25242	-0.17713
H	-2.55091	-1.12056	-0.11654
H	2.72586	3.65589	-0.58001
O	-0.87841	-2.79937	-0.65744
O	3.18368	-1.04913	-1.90553
O	-3.14775	3.75791	0.75787
O	1.02048	5.36212	-0.08924
C	-1.58476	5.88858	0.62161
H	-0.76856	6.5913	0.49408
H	-2.40444	6.13615	-0.05208
H	-1.95024	5.91756	1.64781
C	1.64677	-3.30401	-1.60754
H	1.69228	-3.37194	-2.69574
H	2.6413	-3.47464	-1.20127
H	0.94688	-4.03829	-1.22284
N	1.1783	-1.97062	-1.19881
N	-1.07523	4.54362	0.31105
N	-3.76204	1.21032	0.39707
N	3.95734	1.45078	-1.04978
H	-3.98002	2.14471	0.74234
C	-4.83887	0.32426	0.22658
C	-4.93767	-0.56087	-0.858
C	-5.89344	0.39297	1.15112
C	-6.05169	-1.37756	-0.98805
H	-4.16509	-0.58897	-1.61467
C	-7.00916	-0.41775	1.00788
H	-5.82428	1.08052	1.98621
C	-7.0972	-1.32248	-0.05895
H	-7.81156	-0.3583	1.73093
H	-6.12819	-2.05684	-1.82771

C	-8.26652	-2.22105	-0.24942
O	-8.37223	-3.02085	-1.1603
O	-9.20501	-2.05798	0.6981
C	-10.39191	-2.89304	0.6057
H	-10.87471	-2.70052	-0.35438
H	-10.08043	-3.93909	0.62922
C	-11.29039	-2.54288	1.77268
H	-11.58901	-1.49273	1.73849
H	-12.19364	-3.15667	1.73003
H	-10.79114	-2.7354	2.72496
H	4.33739	0.73174	-1.63162
C	4.84868	2.43949	-0.42618
C	5.33517	3.51082	-1.17588
C	5.20799	2.30669	0.91501
C	6.18132	4.44871	-0.58462
H	5.05233	3.61481	-2.23344
C	6.0536	3.24533	1.50687
H	4.82451	1.46247	1.50608
C	6.5404	4.31617	0.75729
H	6.56533	5.29283	-1.17564
H	6.33641	3.14059	2.56448
C	7.47465	5.35198	1.40987
O	7.90531	5.41615	2.56051
O	7.85334	6.32316	0.54106
C	8.71825	7.26363	1.18321
H	9.59255	6.75934	1.53844
H	8.20624	7.71369	2.00795
C	9.12825	8.3545	0.17647
H	9.81267	9.03162	0.64333
H	9.59821	7.89978	-0.67044
H	8.25872	8.89002	-0.14296

[5]

<b>Calculation Type</b>	<b>FOPT</b>
<b>Calculation Method</b>	<b>RB3LYP</b>
<b>Basis Set</b>	<b>6-311++G(d,p)</b>
<b>Charge</b>	<b>0</b>
<b>Spin</b>	<b>Singlet</b>
<b>Energy (RB3LYP)</b>	<b>-1294.50436157 a.u.</b>
<b>RMS Gradient Norm</b>	<b>0.00000427 a.u.</b>
<b>Imaginary Freq</b>	<b>-----</b>
<b>Dipole Moment</b>	<b>3.7599 Debye</b>
<b>Point Group</b>	<b>C1</b>

Symbol	X	Y	Z
C	3.3408	-2.30776	-0.17184
C	3.06206	-0.88193	0.06444
C	1.70525	-0.46254	0.01322
C	0.64486	-1.40629	0.02887
C	0.93291	-2.86037	0.09078
C	4.09512	0.09118	0.17012
C	1.35132	0.90685	-0.05987
C	2.40785	1.85089	-0.11424
C	3.71947	1.45369	-0.00731
C	2.12043	3.29834	-0.24354
C	-0.29658	2.75751	-0.17175
C	-0.00213	1.32512	-0.1131
C	-1.04108	0.35829	-0.10459
C	-0.67008	-1.00822	-0.01351
H	-1.43148	-1.77239	0.0426
H	4.47236	2.22792	-0.00253
O	0.04946	-3.70125	0.20258
O	4.43155	-2.74802	-0.5116
O	-1.44346	3.21755	-0.14828
O	3.00303	4.14194	-0.32214
C	0.42158	5.08174	-0.36106

H	1.34132	5.64308	-0.48496
H	-0.23633	5.24042	-1.21446
H	-0.09339	5.40098	0.54521
C	2.60388	-4.64406	-0.14651
H	2.82271	-4.90191	-1.18428
H	3.48082	-4.85794	0.46083
H	1.75128	-5.21782	0.20171
N	2.26895	-3.2171	-0.0326
N	0.77194	3.65638	-0.26433
N	-2.3578	0.73108	-0.143
N	5.39812	-0.20094	0.4689
C	-3.49278	-0.07326	-0.37632
C	6.46387	0.7638	0.20609
H	6.30165	1.27205	-0.74378
H	6.55943	1.51071	1.00452
H	7.40595	0.219	0.13473
C	5.76439	-1.26854	1.39517
H	6.24277	-2.10731	0.88582
H	6.45185	-0.85637	2.13972
H	4.88235	-1.63912	1.91593
H	-3.26104	-1.09232	-0.14673
H	-4.2985	0.25798	0.24496
H	-3.77977	0.0044	-1.40419
C	-2.5672	2.18037	-0.01404
H	-1.99669	2.55108	0.81179
H	-2.25172	2.6677	-0.91286
H	-3.60561	2.37724	0.15283

[6]

<b>Calculation Type</b>	<b>FOPT</b>	
<b>Calculation Method</b>	<b>RB3LYP</b>	
<b>Basis Set</b>	<b>6-311++G(d,p)</b>	
<b>Charge</b>	<b>0</b>	
<b>Spin</b>	<b>Singlet</b>	
<b>Energy (RB3LYP)</b>	<b>-1635.63571809</b>	<b>a.u.</b>
<b>RMS Gradient Norm</b>	<b>0.00000957</b>	<b>a.u.</b>
<b>Imaginary Freq</b>	<b>-----</b>	
<b>Dipole Moment</b>	<b>6.6581</b>	<b>Debye</b>
<b>Point Group</b>	<b>C1</b>	

Symbol	X	Y	Z
C	2.14971	-1.24134	-1.0129
C	1.72648	0.1441	-0.70204
C	0.34424	0.39155	-0.47429
C	-0.58368	-0.68081	-0.36555
C	-0.13458	-2.09294	-0.49787
C	2.62522	1.2347	-0.74226
C	-0.16884	1.70826	-0.34206
C	0.7448	2.78459	-0.46905
C	2.08781	2.54379	-0.65646
C	0.28668	4.19096	-0.36977
C	-2.01061	3.33658	0.03473
C	-1.54838	1.95205	-0.11388
C	-2.4533	0.86133	-0.02728
C	-1.92099	-0.45456	-0.14112
H	-2.56163	-1.32013	-0.034
H	2.74996	3.40297	-0.70913
O	-0.8973	-3.03814	-0.35007
O	3.26712	-1.53138	-1.41759
O	-3.18427	3.64198	0.28895
O	1.04662	5.1421	-0.49116
C	-1.59359	5.73844	0.01588
H	-0.75969	6.41738	-0.14108
H	-2.37813	5.91339	-0.72246

H	-2.02118	5.87689	1.01068
C	1.69081	-3.63565	-1.08269
H	1.97249	-3.74768	-2.13191
H	2.57256	-3.82719	-0.46953
H	0.88636	-4.32107	-0.82933
N	1.20674	-2.27135	-0.83444
N	-1.0799	4.36897	-0.12002
N	-3.78353	1.07915	0.20193
N	4.0061	1.15933	-0.8954
H	-3.99805	2.06031	0.39765
C	-4.8564	0.16928	0.13567
C	-4.95345	-0.82086	-0.85312
C	-5.90324	0.31923	1.0533
C	-6.06535	-1.66909	-0.89
H	-4.18297	-0.92417	-1.60626
C	-7.02269	-0.5161	0.99834
H	-5.85786	1.08221	1.82335
C	-7.10448	-1.52288	0.03349
C	4.59523	2.39833	-1.42333
H	3.90631	2.86138	-2.09851
H	4.80529	3.06634	-0.6143
H	5.50292	2.16912	-1.94147
C	4.98379	0.30911	-0.20105
H	5.38642	-0.40561	-0.88805
H	5.77479	0.91744	0.18516
H	4.50183	-0.20338	0.60515
H	-7.82074	-0.38369	1.69868
H	-6.12092	-2.43747	-1.63256
C	-8.31884	-2.46722	-0.0383
O	-8.55559	-3.3957	-0.80994
O	-9.24199	-2.19229	0.91754
H	-9.99569	-2.801	0.84998

[7]

<b>Calculation Type</b>	<b>FOPT</b>
<b>Calculation Method</b>	<b>RB3LYP</b>
<b>Basis Set</b>	<b>6-311++G(d,p)</b>
<b>Charge</b>	<b>0</b>
<b>Spin Singlet</b>	<b>Singlet</b>
<b>Energy (RB3LYP)</b>	<b>-1635.63351651 a.u.</b>
<b>RMS Gradient Norm</b>	<b>0.00000249 a.u.</b>
<b>Imaginary Freq</b>	<b>-----</b>
<b>Dipole Moment</b>	<b>5.2576 Debye</b>
<b>Point Group C1</b>	<b>C1</b>

Symbol	X	Y	Z
C	2.14971	-1.24134	-1.0129
C	1.72648	0.1441	-0.70204
C	0.34424	0.39155	-0.47429
C	-0.58368	-0.68081	-0.36555
C	-0.13458	-2.09294	-0.49787
C	2.62522	1.2347	-0.74226
C	-0.16884	1.70826	-0.34206
C	0.7448	2.78459	-0.46905
C	2.08781	2.54379	-0.65646
C	0.28668	4.19096	-0.36977
C	-2.01061	3.33658	0.03473
C	-1.54838	1.95205	-0.11388
C	-2.4533	0.86133	-0.02728
C	-1.92099	-0.45456	-0.14112
H	-2.56163	-1.32013	-0.034
H	2.74996	3.40297	-0.70913
O	-0.8973	-3.03814	-0.35007
O	3.26712	-1.53138	-1.41759
O	-3.18427	3.64198	0.28895
O	1.04662	5.1421	-0.49116
C	-1.59359	5.73844	0.01588
H	-0.75969	6.41738	-0.14108
H	-2.37813	5.91339	-0.72246

H	-2.02118	5.87689	1.01068
C	1.69081	-3.63565	-1.08269
H	1.97249	-3.74768	-2.13191
H	2.57256	-3.82719	-0.46953
H	0.88636	-4.32107	-0.82933
N	1.20674	-2.27135	-0.83444
N	-1.0799	4.36897	-0.12002
N	-3.78353	1.07915	0.20193
N	4.0061	1.15933	-0.8954
H	-3.99805	2.06031	0.39765
C	-4.8564	0.16928	0.13567
C	-4.95345	-0.82086	-0.85312
C	-5.90324	0.31923	1.0533
C	-6.06535	-1.66909	-0.89
H	-4.18297	-0.92417	-1.60626
C	-7.02269	-0.5161	0.99834
H	-5.85786	1.08221	1.82335
C	-7.10448	-1.52288	0.03349
C	4.59523	2.39833	-1.42333
H	3.90631	2.86138	-2.09851
H	4.80529	3.06634	-0.6143
H	5.50292	2.16912	-1.94147
C	4.98379	0.30911	-0.20105
H	5.38642	-0.40561	-0.88805
H	5.77479	0.91744	0.18516
H	4.50183	-0.20338	0.60515
H	-6.12092	-2.43747	-1.63256
H	-7.95257	-2.17451	0.00169
C	-8.17129	-0.32553	2.0063
O	-9.22837	-0.94294	2.12851
O	-7.9333	0.69236	2.87157
H	-8.67149	0.79076	3.49491



[8]

<b>Calculation Type</b>	<b>FOPT</b>
<b>Calculation Method</b>	<b>RB3LYP</b>
<b>Basis Set</b>	<b>6-311++G(d,p)</b>
<b>Charge</b>	<b>0</b>
<b>Spin Singlet</b>	<b>Singlet</b>
<b>Energy (RB3LYP)</b>	<b>-1824.27231009 a.u.</b>
<b>RMS Gradient Norm</b>	<b>0.00001238 a.u.</b>
<b>Imaginary Freq</b>	<b>-----</b>
<b>Dipole Moment</b>	<b>5.4482 Debye</b>
<b>Point Group</b>	<b>C1</b>

Symbol	X	Y	Z
C	2.14971	-1.24134	-1.0129
C	1.72648	0.1441	-0.70204
C	0.34424	0.39155	-0.47429
C	-0.58368	-0.68081	-0.36555
C	-0.13458	-2.09294	-0.49787
C	2.62522	1.2347	-0.74226
C	-0.16884	1.70826	-0.34206
C	0.7448	2.78459	-0.46905
C	2.08781	2.54379	-0.65646
C	0.28668	4.19096	-0.36977
C	-2.01061	3.33658	0.03473
C	-1.54838	1.95205	-0.11388
C	-2.4533	0.86133	-0.02728
C	-1.92099	-0.45456	-0.14112
H	-2.56163	-1.32013	-0.034
H	2.74996	3.40297	-0.70913
O	-0.8973	-3.03814	-0.35007
O	3.26712	-1.53138	-1.41759
O	-3.18427	3.64198	0.28895
O	1.04662	5.1421	-0.49116
C	-1.59359	5.73844	0.01588
H	-0.75969	6.41738	-0.14108
H	-2.37813	5.91339	-0.72246

H	-2.02118	5.87689	1.01068
C	1.69081	-3.63565	-1.08269
H	1.97249	-3.74768	-2.13191
H	2.57256	-3.82719	-0.46953
H	0.88636	-4.32107	-0.82933
N	1.20674	-2.27135	-0.83444
N	-1.0799	4.36897	-0.12002
N	-3.78353	1.07915	0.20193
N	4.0061	1.15933	-0.8954
H	-3.99805	2.06031	0.39765
C	-4.8564	0.16928	0.13567
C	-4.95345	-0.82086	-0.85312
C	-5.90324	0.31923	1.0533
C	-6.06535	-1.66909	-0.89
H	-4.18297	-0.92417	-1.60626
C	-7.02269	-0.5161	0.99834
H	-5.85786	1.08221	1.82335
C	-7.10448	-1.52288	0.03349
H	-7.95807	-2.18667	-0.01697
C	-8.09562	-0.29334	2.00966
O	-8.06528	0.56619	2.86671
O	-9.12858	-1.1572	1.8794
H	-9.7627	-0.92648	2.57842
C	-6.19642	-2.73965	-1.91975
O	-7.13369	-3.50593	-2.00099
O	-5.14723	-2.77856	-2.77593
H	-5.32824	-3.50919	-3.39013
C	4.59523	2.39833	-1.42333
H	3.90631	2.86138	-2.09851
H	4.80529	3.06634	-0.6143
H	5.50292	2.16912	-1.94147
C	4.98379	0.30911	-0.20105

H	5.38642	-0.40561	-0.88805
H	5.77479	0.91744	0.18516
H	4.50183	-0.20338	0.60515

[1]<sup>-</sup>

<b>Calculation Type</b>	<b>FOPT</b>
<b>Calculation Method</b>	<b>UB3LYP</b>
<b>Basis Set</b>	<b>6-311++G(d,p)</b>
<b>Charge</b>	<b>-1</b>
<b>Spin</b>	<b>Doublet</b>
<b>Energy (UB3LYP)</b>	<b>-1714.40294500 a.u.</b>
<b>RMS Gradient Norm</b>	<b>0.00000477 a.u.</b>
<b>Imaginary Freq</b>	<b>-----</b>
<b>Dipole Moment</b>	<b>6.7128 Debye</b>
<b>Point Group</b>	<b>C1</b>

Symbol	X	Y	Z
C	3.62427	-2.58315	-0.2318
C	3.58475	-1.13302	0.01704
C	2.30699	-0.51306	0.07088
C	1.1224	-1.28552	0.18507
C	1.1933	-2.76611	0.24489
C	4.75754	-0.32712	0.03305
C	2.15858	0.89427	0.0117
C	3.33778	1.66795	-0.13755
C	4.57833	1.07741	-0.13035
C	3.26264	3.14223	-0.26186
C	0.80686	2.97452	0.01876
C	0.88393	1.5115	0.06134
C	-0.28379	0.71198	0.16087
C	-0.11735	-0.69303	0.2435
H	-0.9758	-1.33369	0.37963
H	5.43713	1.72908	-0.19516
O	0.2072	-3.46363	0.44668
O	4.6029	-3.18025	-0.66197

O	-0.24978	3.60281	0.14119
O	4.25209	3.84206	-0.42585
C	1.84898	5.16335	-0.25151
H	2.83001	5.57955	-0.4532
H	1.15597	5.42412	-1.05035
H	1.46317	5.55201	0.69106
C	2.54723	-4.78162	-0.12002
H	2.61939	-5.06759	-1.17099
H	3.43822	-5.12659	0.40005
H	1.65701	-5.2208	0.31825
N	2.44409	-3.32059	0.00819
N	1.98648	3.70067	-0.17299
N	-1.52876	1.28697	0.22833
N	6.02022	-0.81086	0.23532
H	-1.49887	2.29818	0.34946
C	-2.7925	0.70818	0.05228
C	-3.0362	-0.37183	-0.81197
C	-3.87692	1.29676	0.72606
C	-4.32461	-0.86258	-0.96576
H	-2.23079	-0.80654	-1.38817
C	-5.16275	0.80796	0.55833
H	-3.69751	2.13522	1.3893
C	-5.4031	-0.28759	-0.28297
C	7.19586	-0.01456	-0.11191
H	7.04308	0.51428	-1.05201
H	7.45741	0.70762	0.67166
H	8.03875	-0.69321	-0.24591
C	6.29282	-1.93409	1.12751
H	6.59349	-2.82922	0.5797
H	7.09405	-1.64117	1.81202
H	5.40988	-2.172	1.71948
H	-4.5085	-1.69237	-1.63673

C	-6.75991	-0.85643	-0.48609
O	-7.00302	-1.80807	-1.20501
O	-7.70558	-0.20592	0.21428
C	-9.07105	-0.68839	0.09027
H	-9.36171	-0.63688	-0.96081
H	-9.09729	-1.73439	0.40191
C	-9.94692	0.1847	0.96362
H	-9.90727	1.22807	0.64266
H	-10.98284	-0.15606	0.89174
H	-9.64012	0.12744	2.01043
H	-5.98458	1.26949	1.08932

[2]<sup>-</sup>

<b>Calculation Type</b>	<b>FOPT</b>		
<b>Calculation Method</b>	<b>UB3LYP</b>		
<b>Basis Set</b>	<b>6-311++G(d,p)</b>		
<b>Charge</b>	<b>-1</b>		
<b>Spin</b>	<b>Doublet</b>		
<b>Energy (UB3LYP)</b>	<b>-1714.39952025 a.u.</b>		
<b>RMS Gradient Norm</b>	<b>0.00000538 a.u.</b>		
<b>Imaginary Freq</b>	<b>-----</b>		
<b>Dipole Moment</b>	<b>6.6069 Debye</b>		
<b>Point Group</b>	<b>C1</b>		
Symbol	X	Y	Z
C	4.00442	-2.1572	0.06911
C	3.60867	-0.74615	0.20454
C	2.23557	-0.43079	0.01851
C	1.24518	-1.44793	0.00322
C	1.62735	-2.87158	0.17187
C	4.55863	0.30498	0.34107
C	1.7954	0.90283	-0.16437
C	2.78539	1.91774	-0.18794
C	4.1069	1.62469	0.0523
C	2.41107	3.33093	-0.42746

C	0.03941	2.61794	-0.51956
C	0.42569	1.21686	-0.35176
C	-0.54187	0.17797	-0.36761
C	-0.0857	-1.15104	-0.16839
H	-0.79401	-1.96553	-0.13013
H	4.80151	2.4514	0.07322
O	0.79829	-3.76838	0.26376
O	5.14759	-2.53201	-0.15902
O	-1.13419	2.99359	-0.61707
O	3.23702	4.23179	-0.48542
C	0.60941	4.97495	-0.79012
H	1.49529	5.5959	-0.8675
H	0.02169	5.03905	-1.70496
H	-0.00619	5.30245	0.04782
C	3.43134	-4.53749	0.16415
H	3.75346	-4.8293	-0.83705
H	4.26694	-4.65672	0.85061
H	2.59397	-5.15422	0.4738
N	2.9905	-3.13495	0.17236
N	1.04779	3.5868	-0.57913
N	-1.87232	0.45182	-0.53074
N	5.84649	0.12557	0.7668
H	-2.09071	1.44633	-0.51418
C	-2.93446	-0.44364	-0.77942
C	-2.82218	-1.52284	-1.66642
C	-4.16608	-0.18583	-0.16821
C	-3.92002	-2.3452	-1.90821
H	-1.88924	-1.70658	-2.18398
C	-5.26923	-1.00222	-0.42921
H	-4.25955	0.6501	0.51238
C	-5.14309	-2.09388	-1.29521
C	6.86006	1.15594	0.55013

H	6.75483	1.6026	-0.43795
H	6.82201	1.94649	1.31038
H	7.84146	0.68298	0.59815
C	6.20244	-0.87092	1.77268
H	6.77822	-1.69529	1.34754
H	6.79361	-0.37853	2.5503
H	5.3053	-1.27987	2.23579
H	-3.81981	-3.17725	-2.59509
H	-6.00141	-2.72514	-1.48437
C	-6.59726	-0.75118	0.20701
O	-7.57351	-1.45529	0.0395
O	-6.60014	0.34052	0.98595
C	-7.84861	0.67619	1.65402
H	-8.62164	0.80336	0.89391
H	-8.13095	-0.16144	2.29468
C	-7.61747	1.94474	2.44672
H	-7.33009	2.77068	1.79223
H	-8.54113	2.22158	2.96113
H	-6.83718	1.80345	3.19793

[3]•-

<b>Calculation Type</b>	<b>FOPT</b>		
<b>Calculation Method</b>	<b>UB3LYP</b>		
<b>Basis Set</b>	<b>6-311++G(d,p)</b>		
<b>Charge</b>	<b>-1</b>		
<b>Spin</b>	<b>Doublet</b>		
<b>Energy (UB3LYP)</b>	<b>-1903.01938622 a.u.</b>		
<b>RMS Gradient Norm</b>	<b>0.00000540 a.u.</b>		
<b>Imaginary Freq</b>	<b>-----</b>		
<b>Dipole Moment</b>	<b>3.9512 Debye</b>		
<b>Point Group</b>	<b>C1</b>		
Symbol	X	Y	Z
C	-3.82553	-2.29949	-0.48227
C	-3.69693	-0.83773	-0.36681

C	-2.38488	-0.30217	-0.25813
C	-1.2433	-1.09567	-0.54267
C	-1.39606	-2.51195	-0.95686
C	-4.82109	0.0177	-0.19468
C	-2.15816	1.03804	0.14002
C	-3.29391	1.82416	0.46045
C	-4.56585	1.32859	0.30227
C	-3.13685	3.2193	0.93381
C	-0.68837	2.97094	0.64914
C	-0.84959	1.57102	0.25091
C	0.27291	0.74982	-0.02819
C	0.02877	-0.58342	-0.44468
H	0.85334	-1.22631	-0.716
H	-5.38762	1.99676	0.51343
O	-0.44553	-3.20037	-1.30673
O	-4.84756	-2.92275	-0.22513
O	0.40693	3.54101	0.69959
O	-4.0884	3.91985	1.24981
C	-1.60906	5.09211	1.42609
H	-2.56854	5.50776	1.71416
H	-0.92069	5.10922	2.27002
H	-1.17946	5.67163	0.60882
C	-2.87373	-4.46684	-1.11373
H	-3.0079	-4.99196	-0.16635
H	-3.75941	-4.61759	-1.72728
H	-1.99169	-4.84463	-1.62043
N	-2.6826	-3.02803	-0.87972
N	-1.82901	3.70296	0.99485
N	1.54968	1.24079	0.0602
N	-6.10558	-0.32729	-0.51471
H	1.59144	2.24693	0.21428
C	2.76594	0.53146	0.07512



C	2.91884	-0.69157	0.73708
C	3.87833	1.12137	-0.53689
C	4.16216	-1.32987	0.75624
H	2.08513	-1.14018	1.25763
C	5.12431	0.49243	-0.49655
H	3.76767	2.06968	-1.04584
C	5.26619	-0.74072	0.1406
C	-7.24125	0.42432	0.01574
H	-7.07186	0.70161	1.05562
H	-7.45598	1.32752	-0.5695
H	-8.12063	-0.21996	-0.01705
C	-6.42322	-1.17237	-1.66215
H	-6.78989	-2.15492	-1.3589
H	-7.18885	-0.6675	-2.25854
H	-5.542	-1.31065	-2.28726
C	6.33084	1.09852	-1.13692
O	7.42848	0.58116	-1.14287
O	6.06948	2.2839	-1.70749
C	4.35688	-2.64089	1.44709
O	5.41682	-3.22927	1.50072
O	3.22693	-3.10121	2.00419
H	6.228	-1.23404	0.16206
C	7.17697	2.94903	-2.35429
H	6.76652	3.87669	-2.74444
H	7.96764	3.15287	-1.63224
H	7.56622	2.33131	-3.16357
C	3.31444	-4.36767	2.69393
H	2.31357	-4.55837	3.07219
H	3.61867	-5.15259	2.00156
H	4.02898	-4.30147	3.51431