

## Supporting Information

### One-pot facile synthesis of 4-amino-1,8-naphthalimide derived Tröger's base supramolecular scaffolds *via* a nucleophilic displacement approach

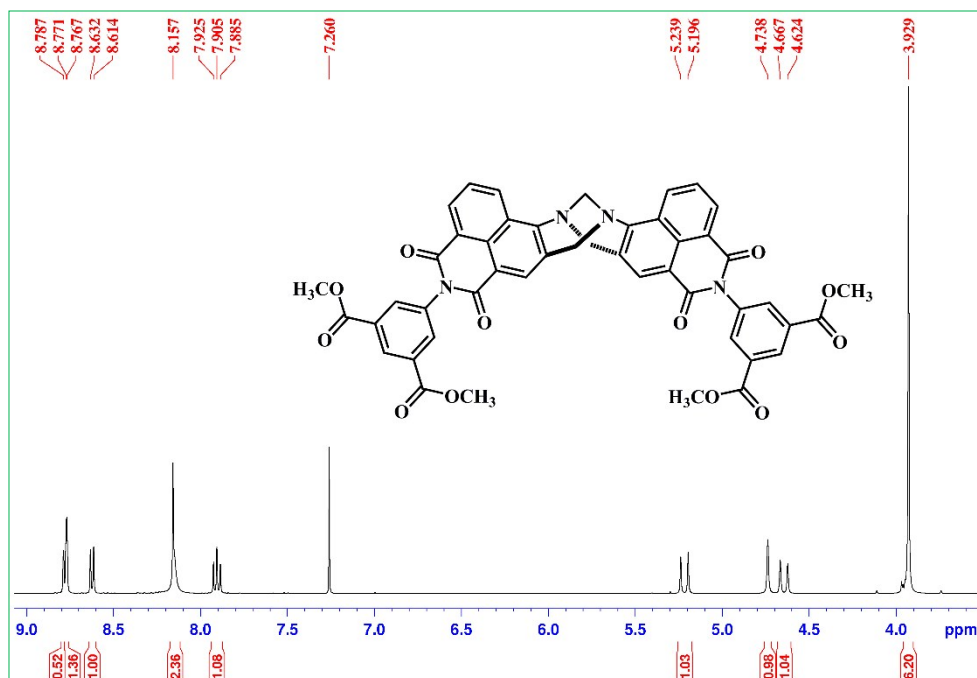
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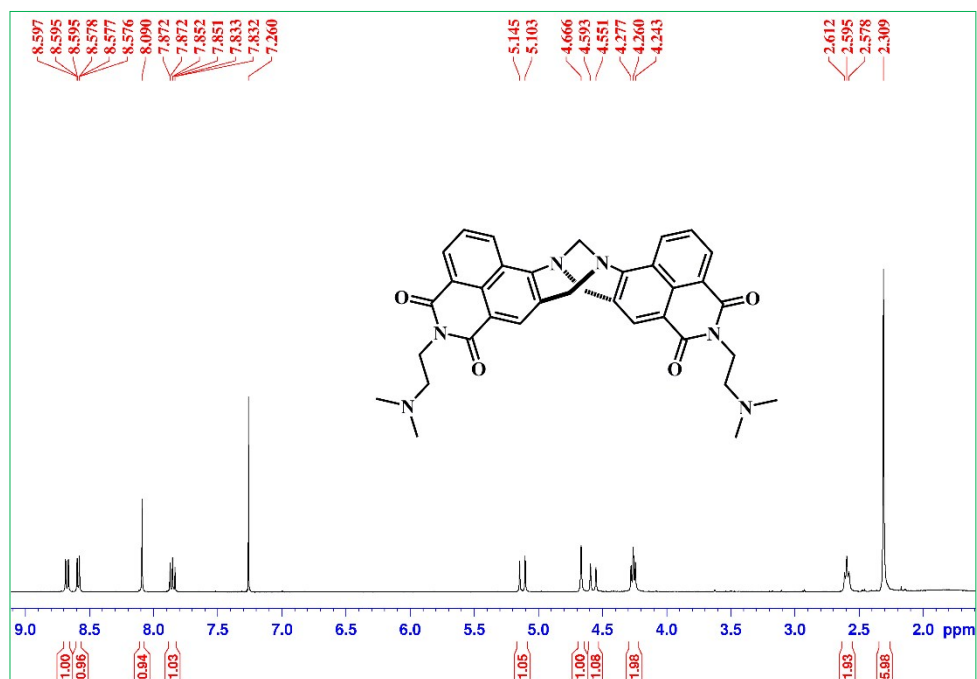
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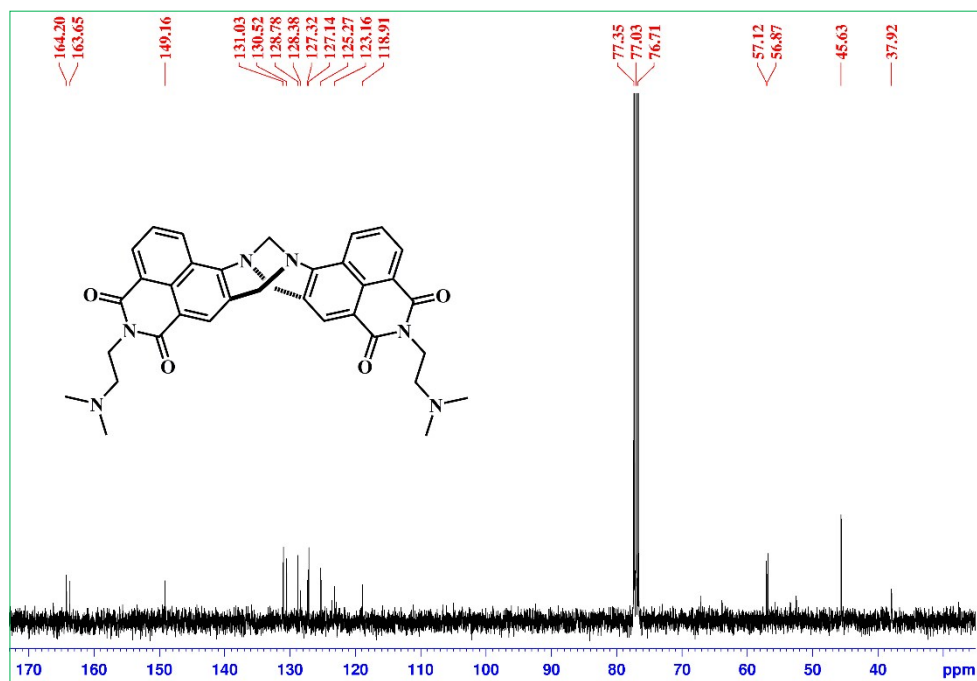
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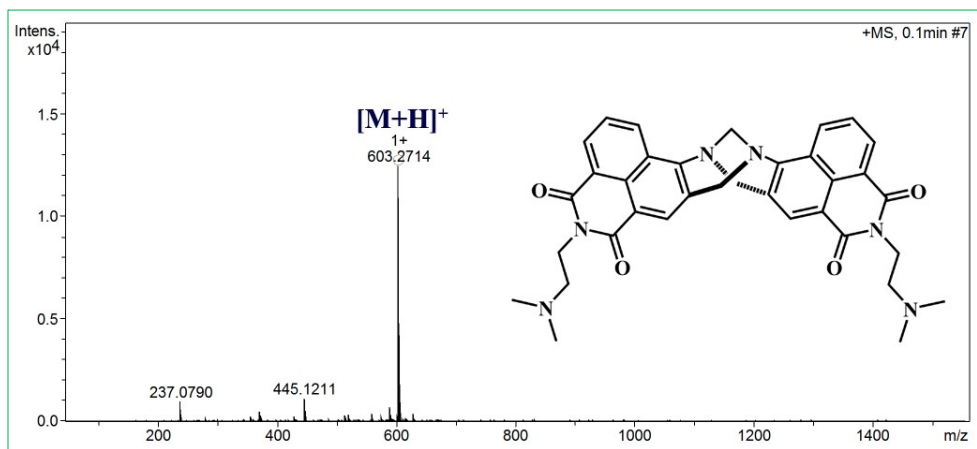
**Fig. S1.** <sup>1</sup>H NMR spectrum of **TB-1** (400 MHz, CDCl<sub>3</sub>).



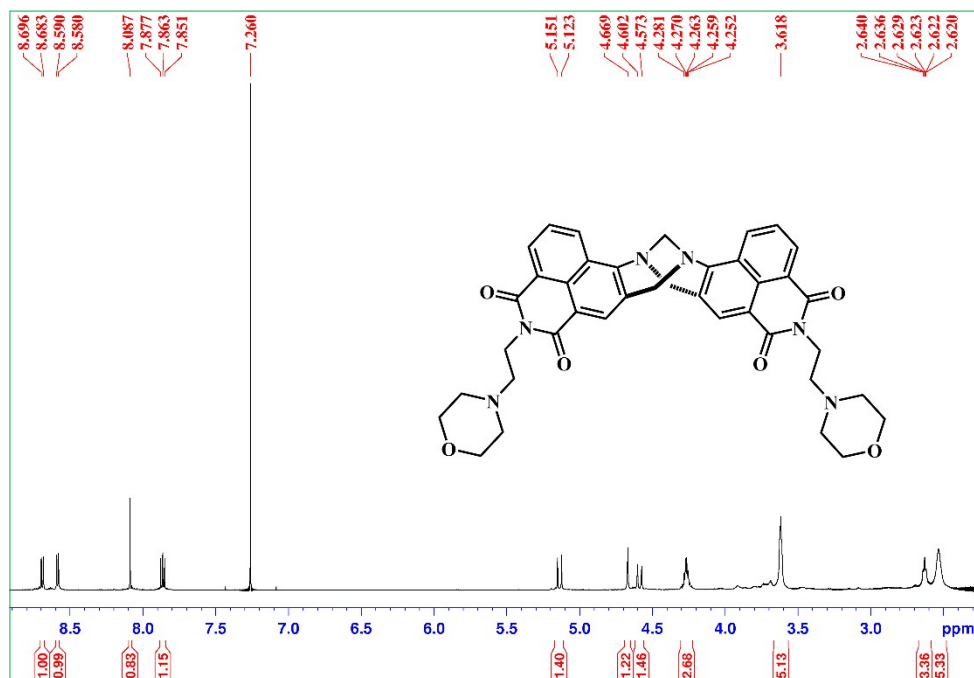
**Fig. S2.** <sup>1</sup>H NMR spectrum of **TB-2a** (400 MHz, CDCl<sub>3</sub>).



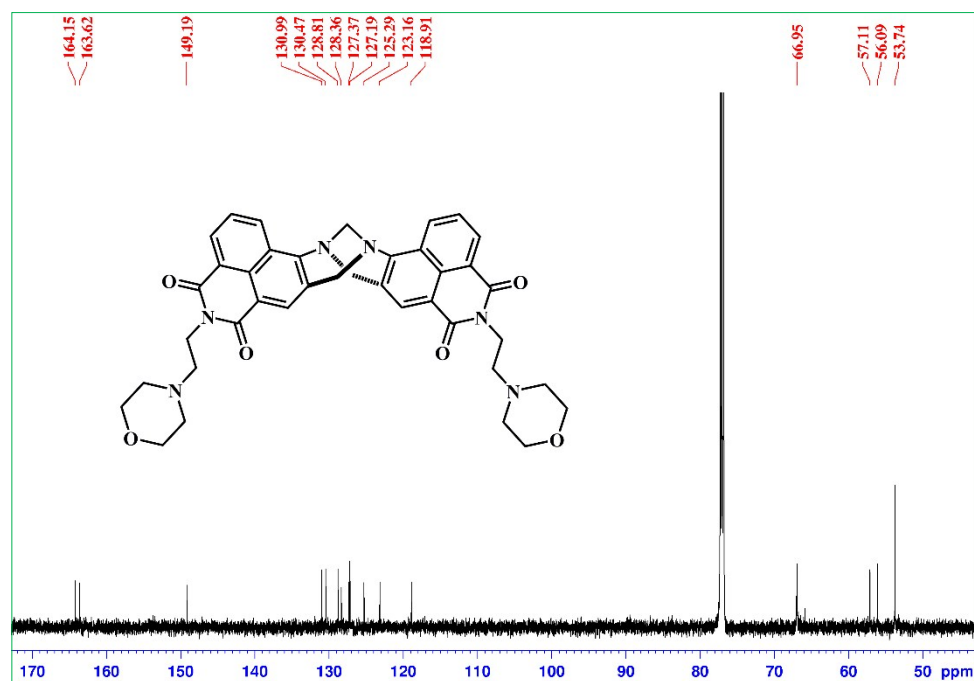
**Fig. S3.** <sup>13</sup>C NMR spectrum of TB-2a (100 MHz, CDCl<sub>3</sub>).



**Fig. S4.** HRMS spectrum of TB-2a.



**Fig. S5.** <sup>1</sup>H NMR spectrum of **TB-2b** (600 MHz, CDCl<sub>3</sub>).



**Fig. S6.** <sup>13</sup>C NMR spectrum of **TB-2b** (150 MHz, CDCl<sub>3</sub>).

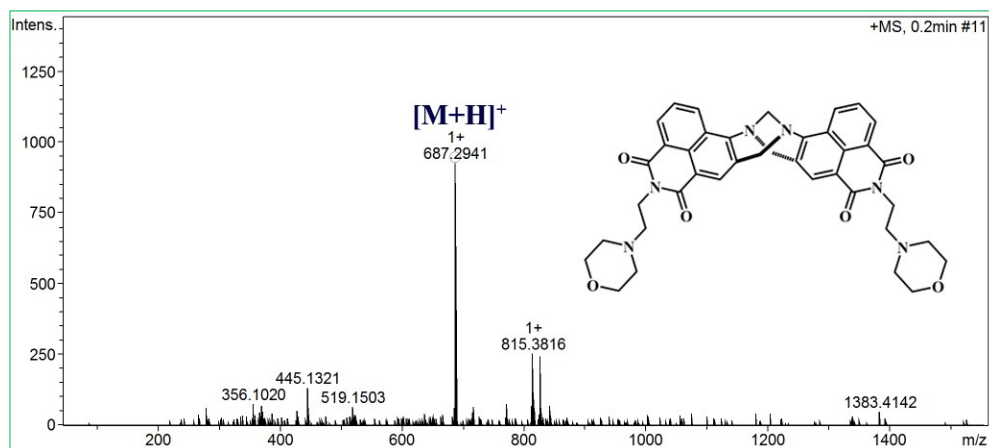


Fig. S7. HRMS spectrum of TB-2b.

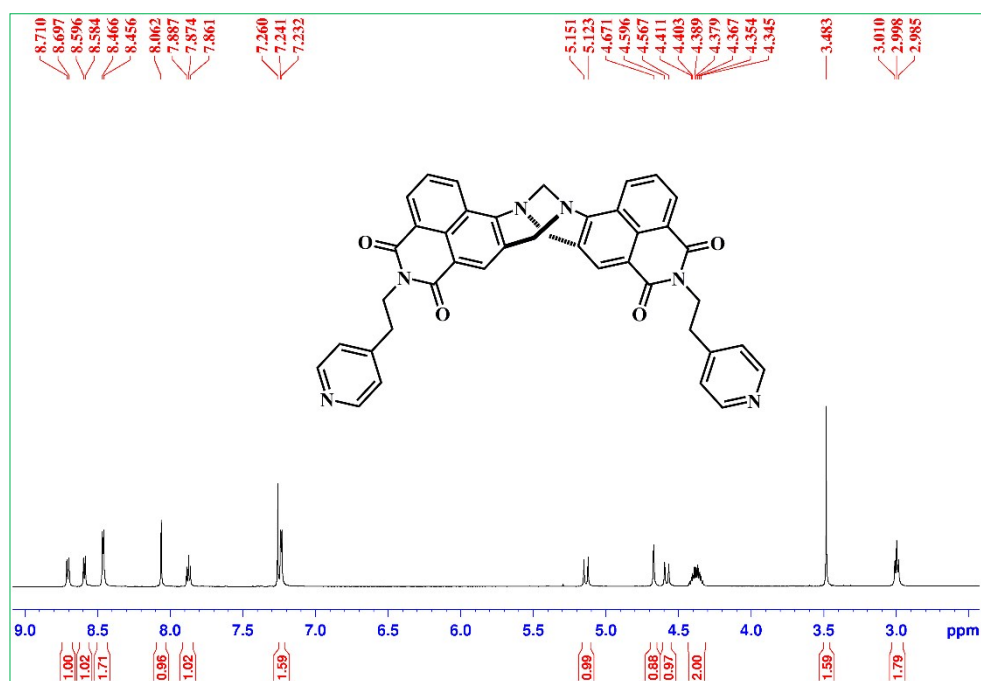
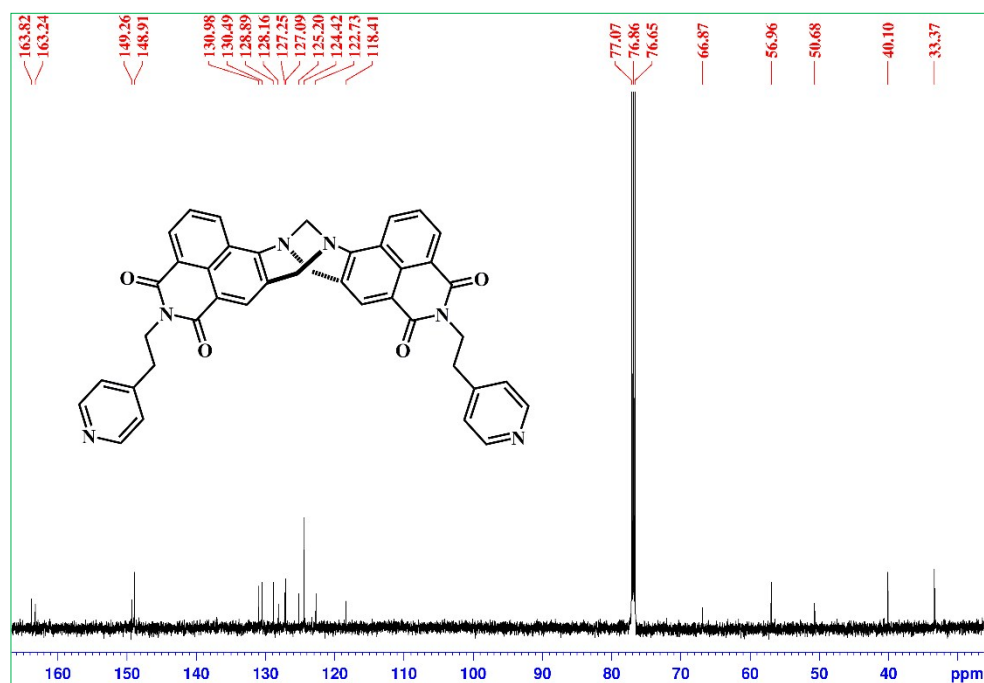
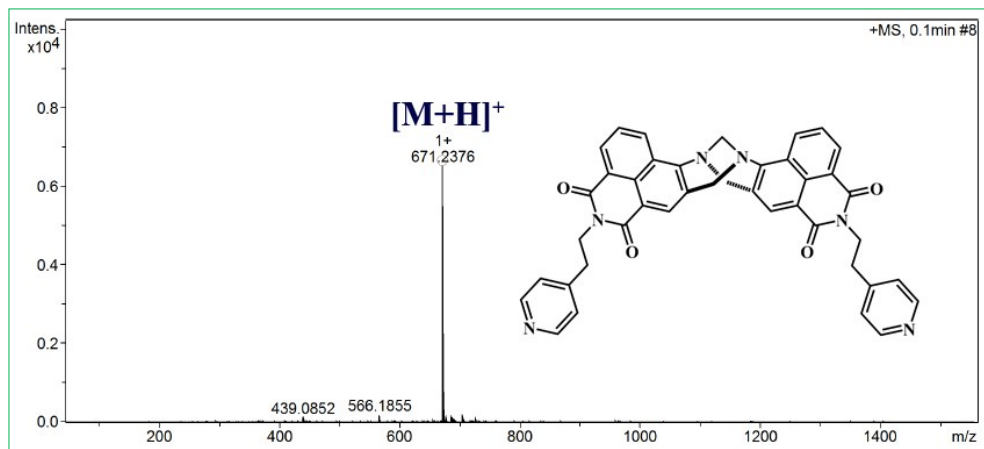


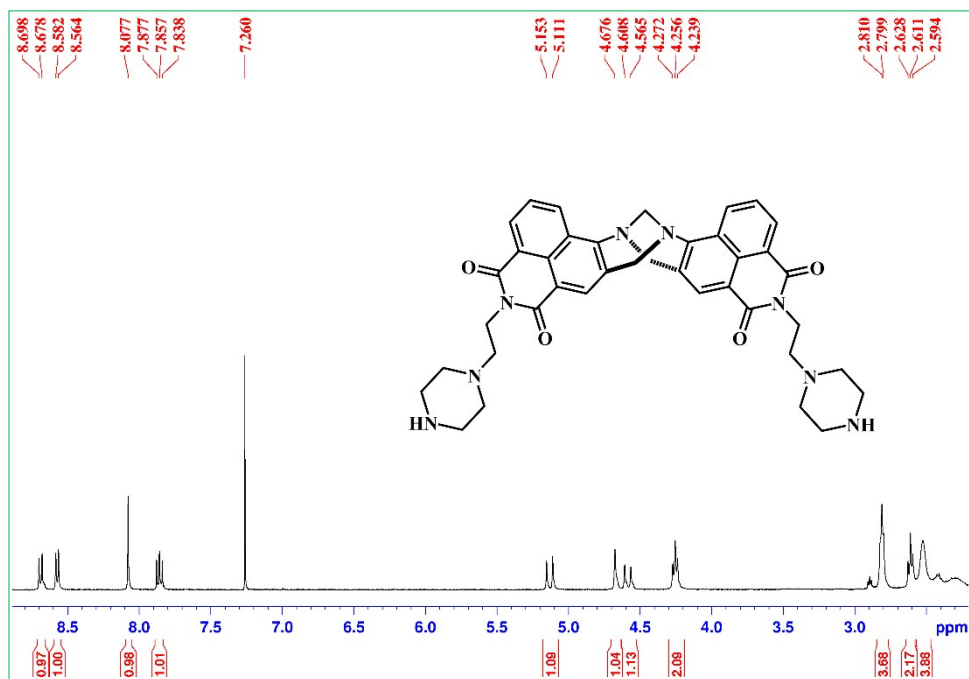
Fig. S8.  $^1\text{H}$  NMR spectrum of TB-2c (600 MHz,  $\text{CDCl}_3$ ).



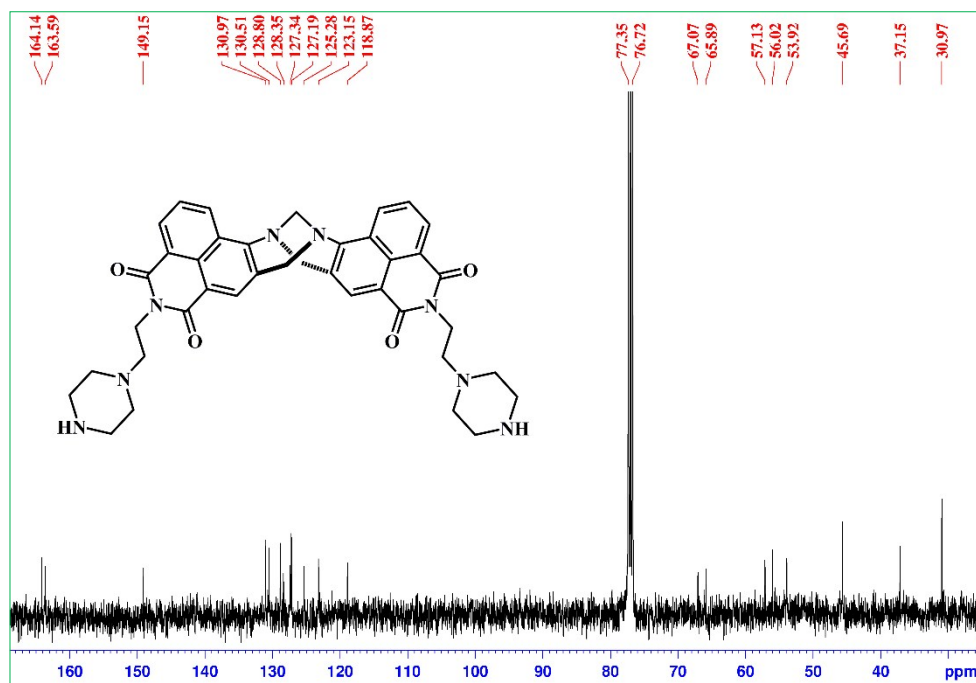
**Fig. S9.**  $^{13}\text{C}$  NMR spectrum of **TB-2c** (150 MHz,  $\text{CDCl}_3$ ).



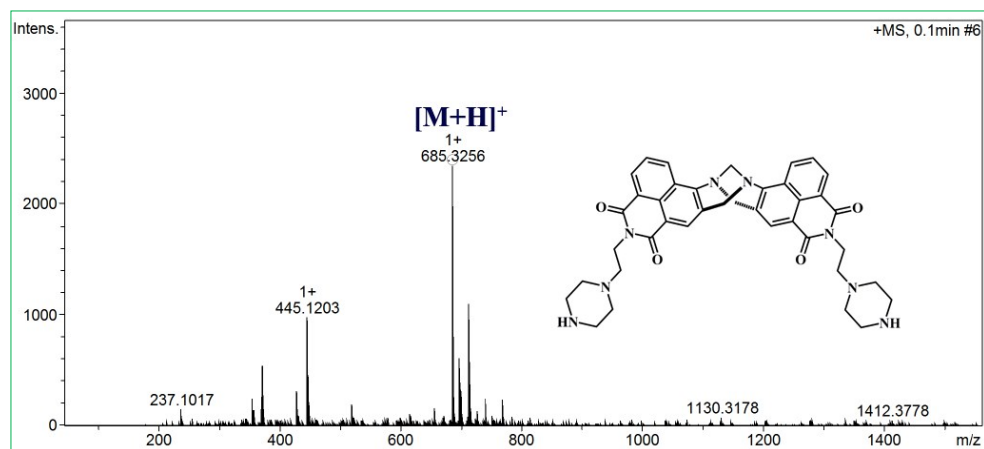
**Fig. S10.** HRMS spectrum of **TB-2c**.



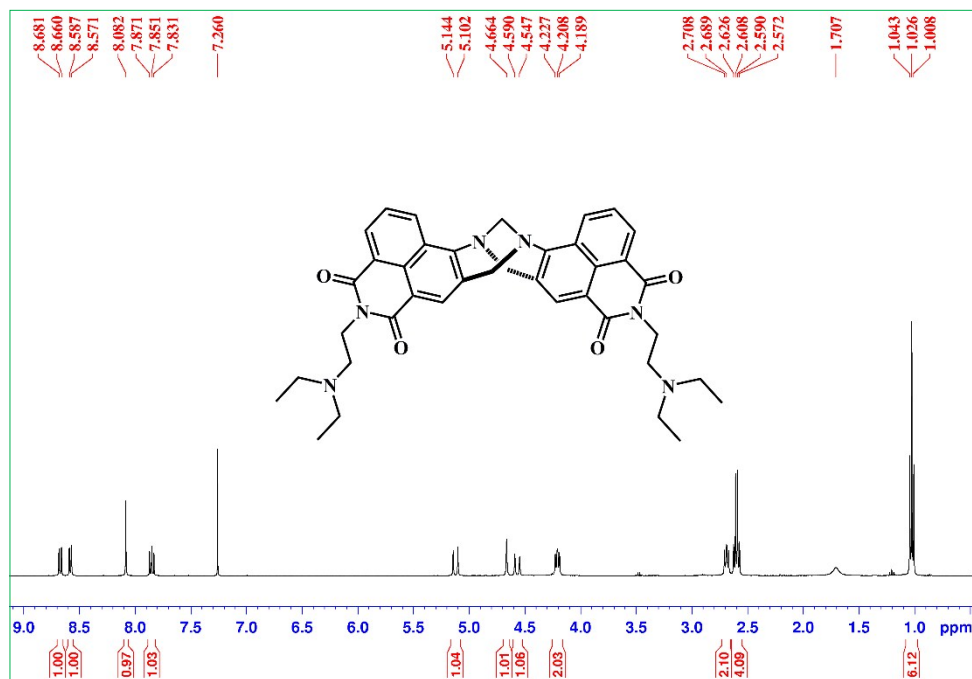
**Fig. S11.** <sup>1</sup>H NMR spectrum of **TB-2d** (400 MHz, CDCl<sub>3</sub>).



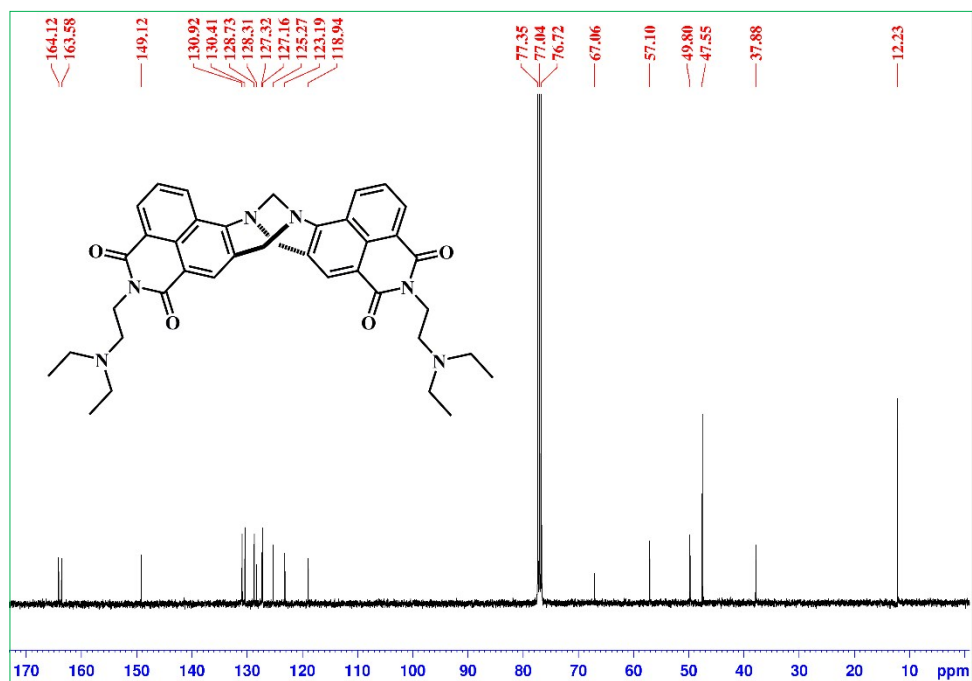
**Fig. S12.** <sup>13</sup>C NMR spectrum of **TB-2d** (100 MHz, CDCl<sub>3</sub>).



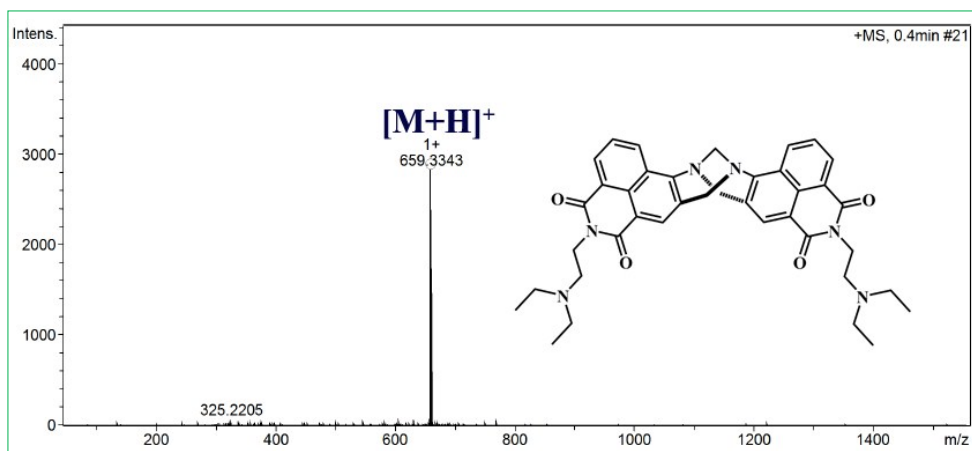
**Fig. S13.** HRMS spectrum of TB-2d.



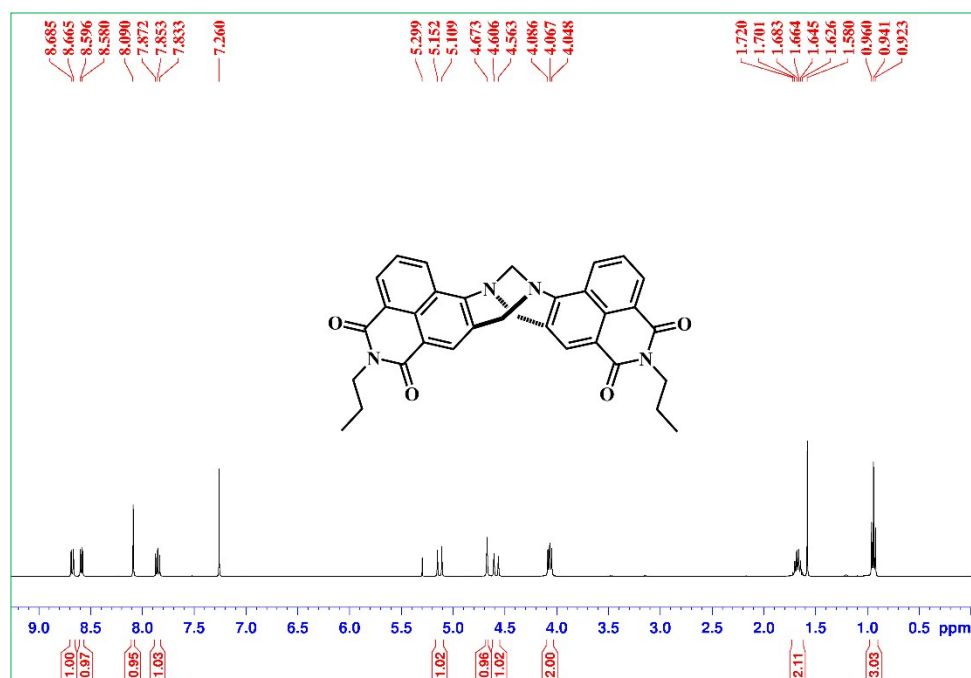
**Fig. S14.**  $^1\text{H}$  NMR spectrum of TB-2e (400 MHz,  $\text{CDCl}_3$ ).



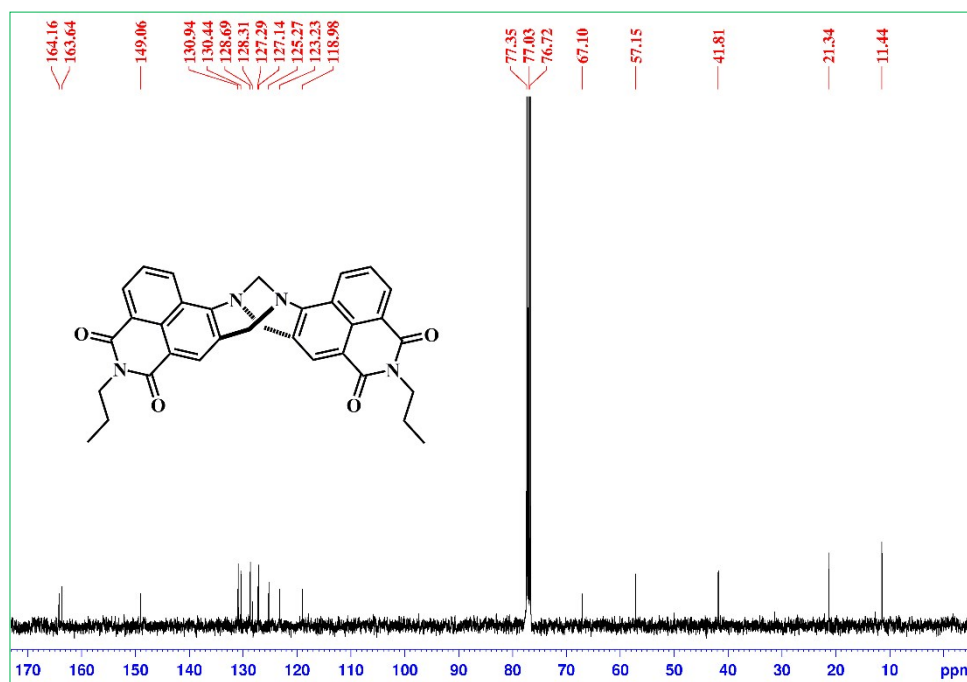
**Fig. S15.** <sup>13</sup>C NMR spectrum of TB-2e (100 MHz, CDCl<sub>3</sub>).



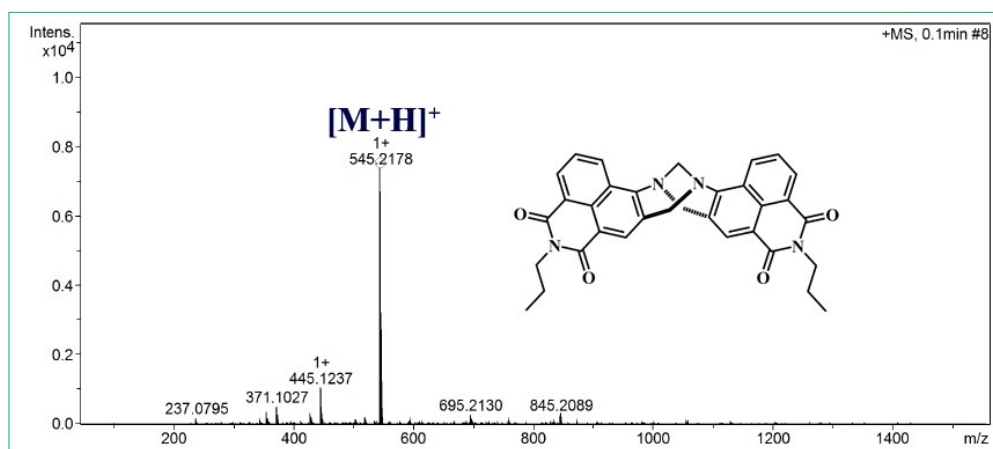
**Fig. S16.** HRMS spectrum of TB-2e.



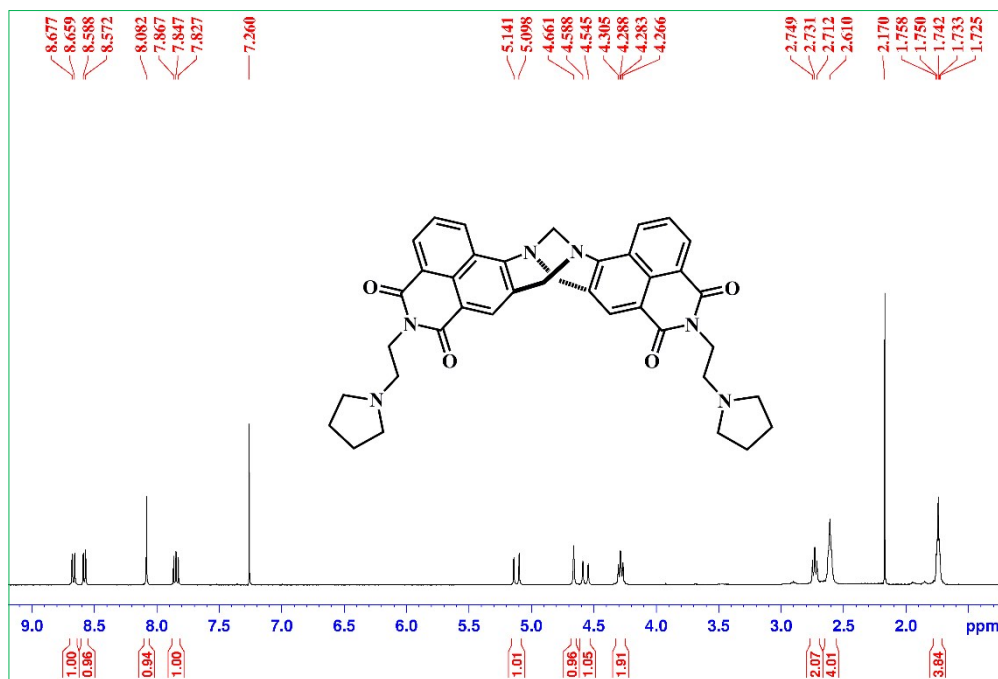
**Fig. S17.** <sup>1</sup>H NMR spectrum of TB-2f (400 MHz, CDCl<sub>3</sub>).



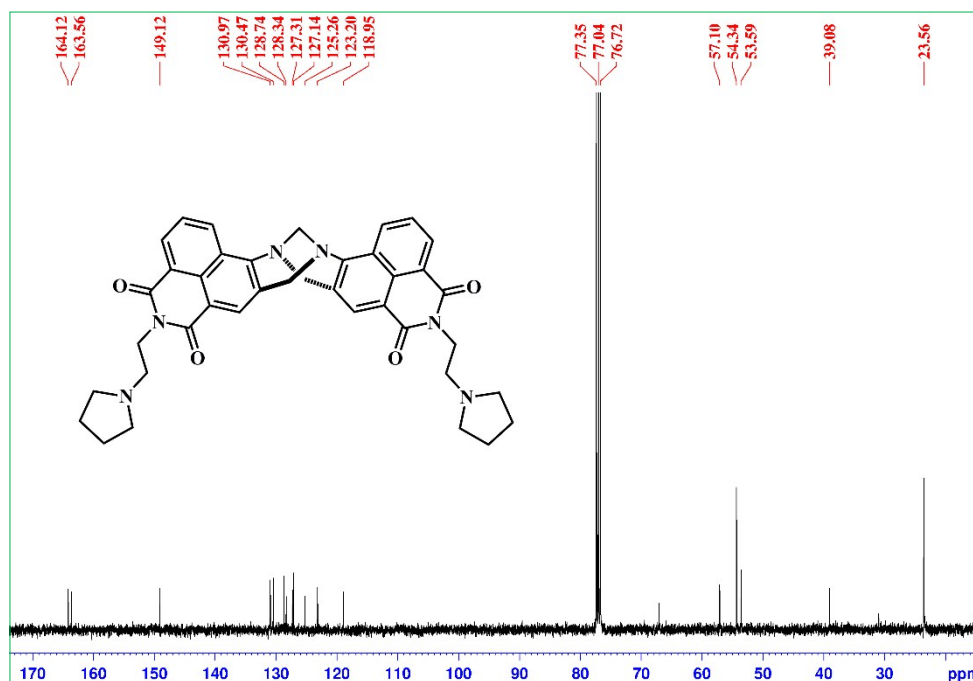
**Fig. S18.** <sup>13</sup>C NMR spectrum of TB-2f (100 MHz, CDCl<sub>3</sub>).



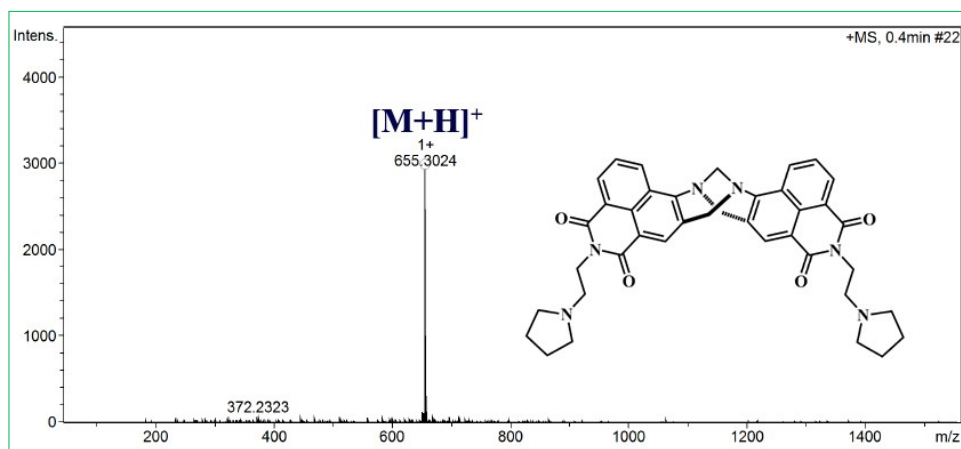
**Fig. S19.** HRMS spectrum of TB-2f.



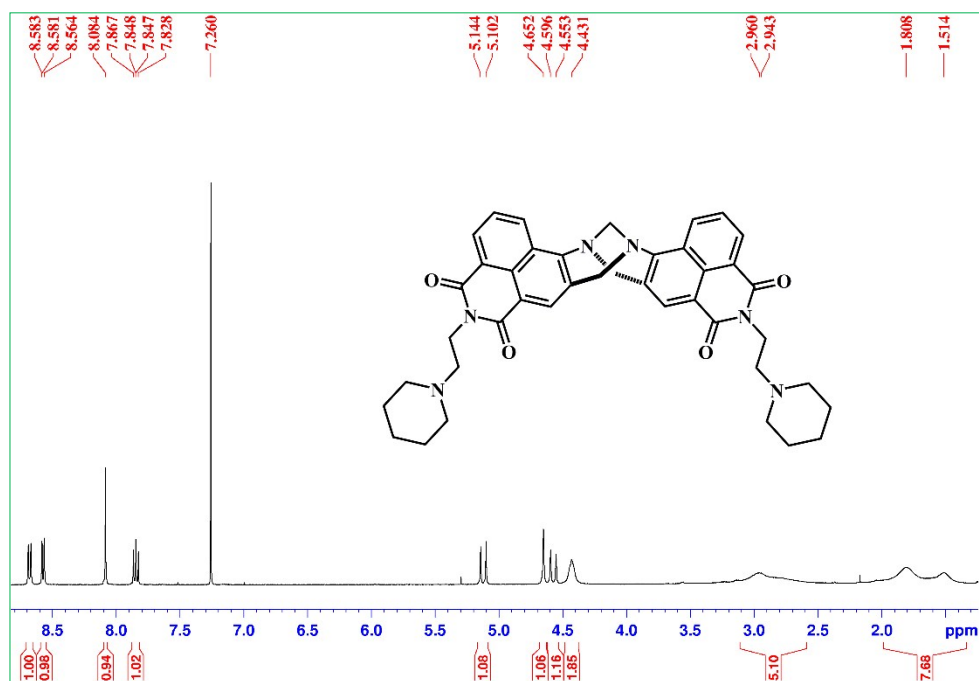
**Fig. S20.** <sup>1</sup>H NMR spectrum of TB-2g (400 MHz, CDCl<sub>3</sub>).



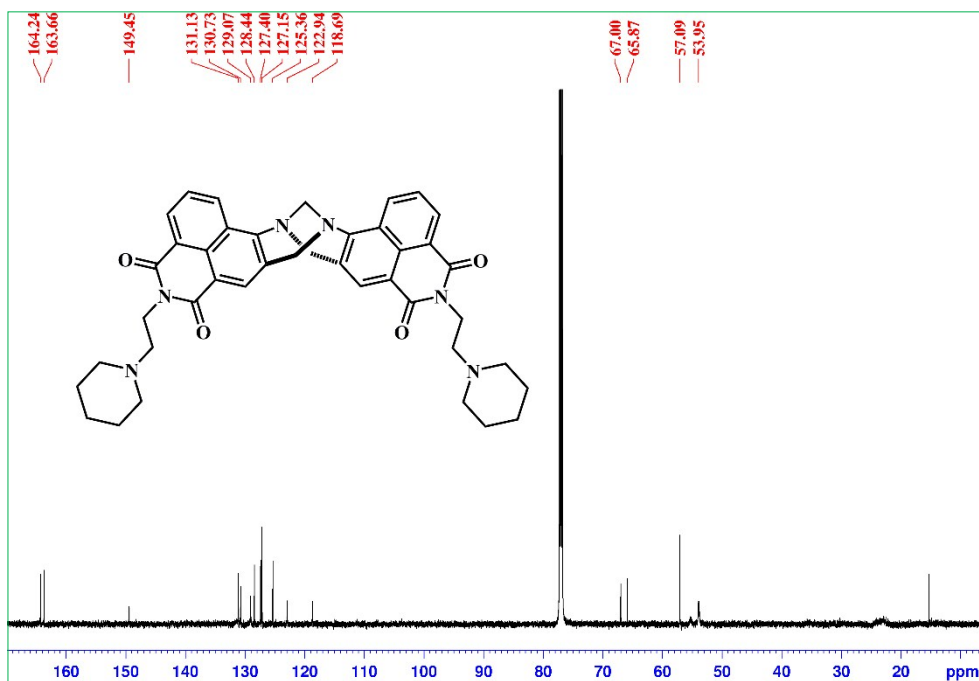
**Fig. S21.**  $^{13}\text{C}$  NMR spectrum of TB-2g (100 MHz,  $\text{CDCl}_3$ ).



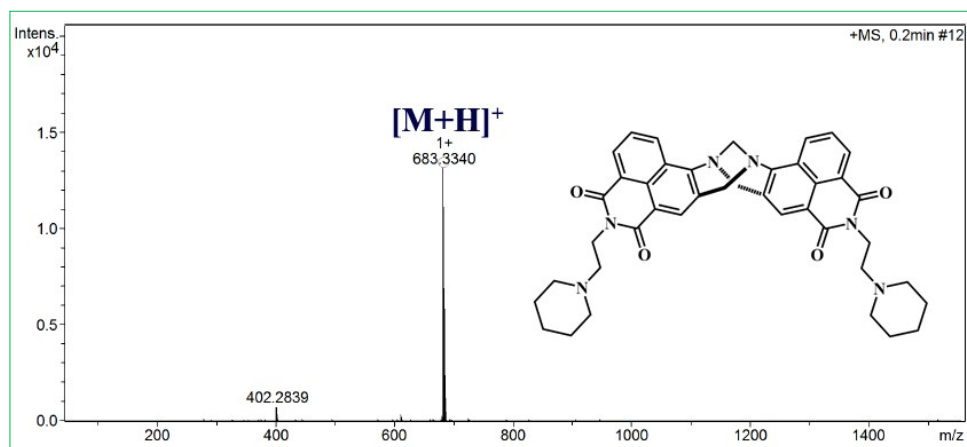
**Fig. S22.** HRMS spectrum of TB-2g.



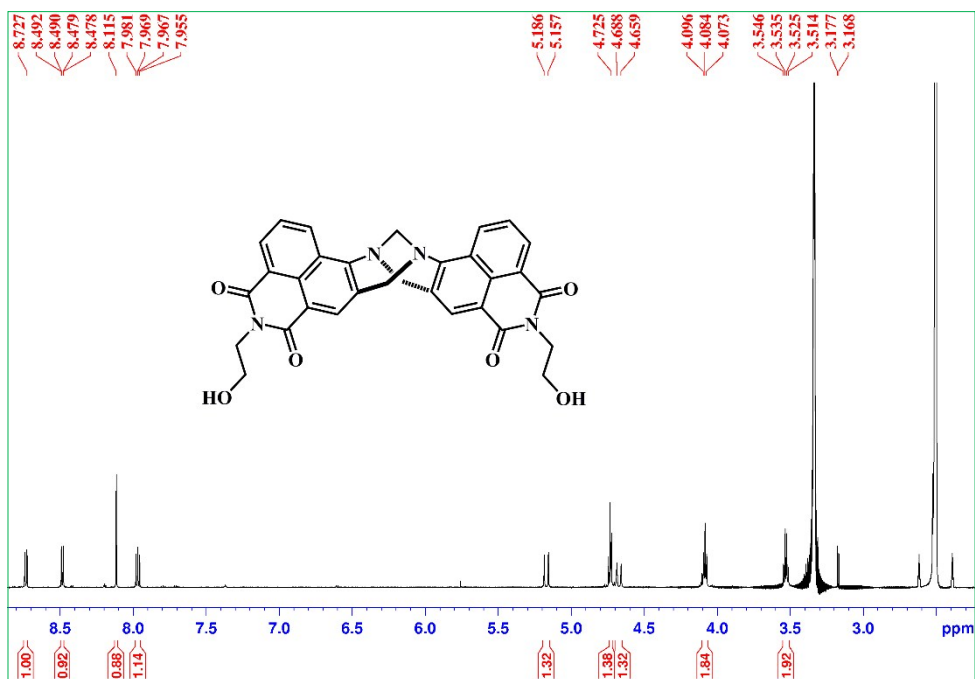
**Fig. S23.** <sup>1</sup>H NMR spectrum of **TB-2h** (400 MHz, CDCl<sub>3</sub>).



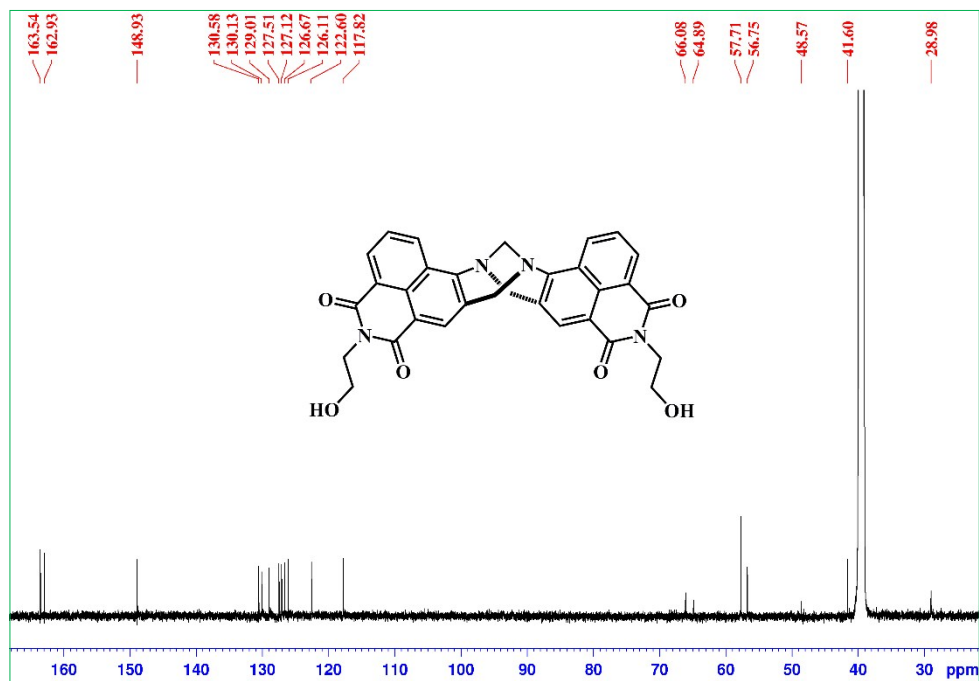
**Fig. S24.** <sup>13</sup>C NMR spectrum of **TB-2h** (100 MHz, CDCl<sub>3</sub>).



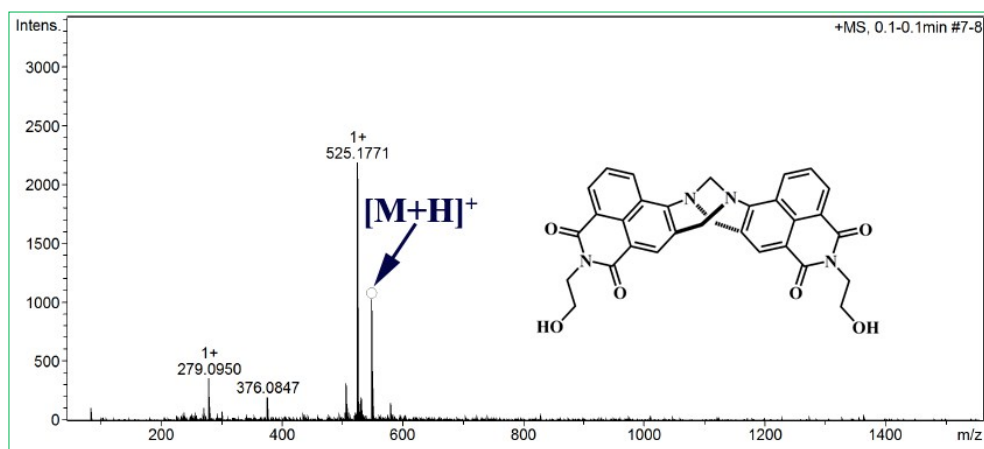
**Fig. S25.** HRMS spectrum of **TB-2h**.



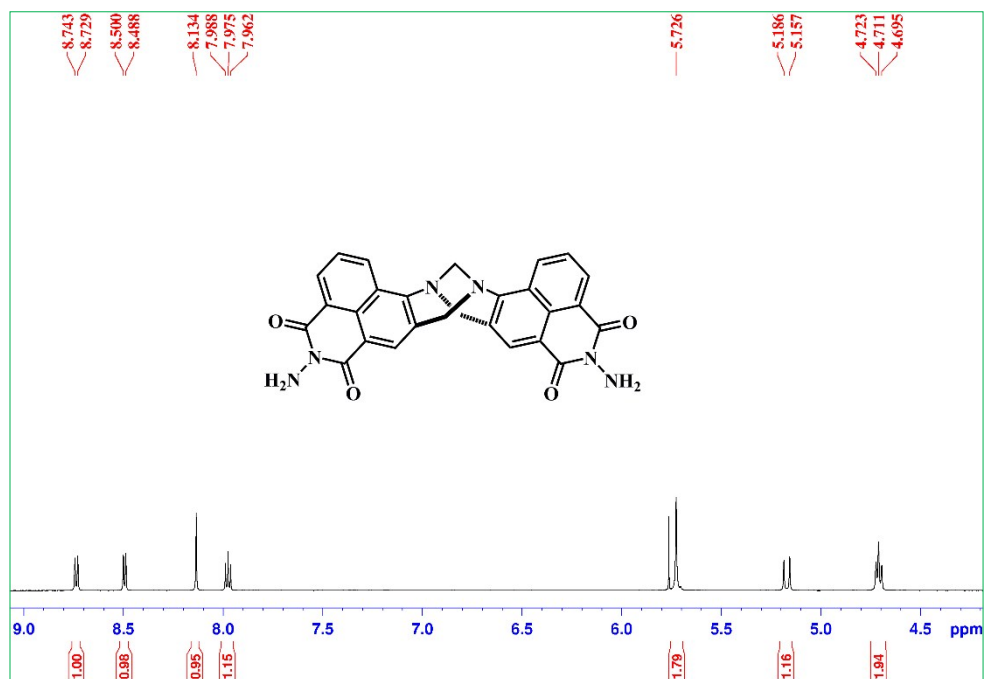
**Fig. S26.** <sup>1</sup>H NMR spectrum of **TB-2i** (600 MHz, DMSO-d<sub>6</sub>).



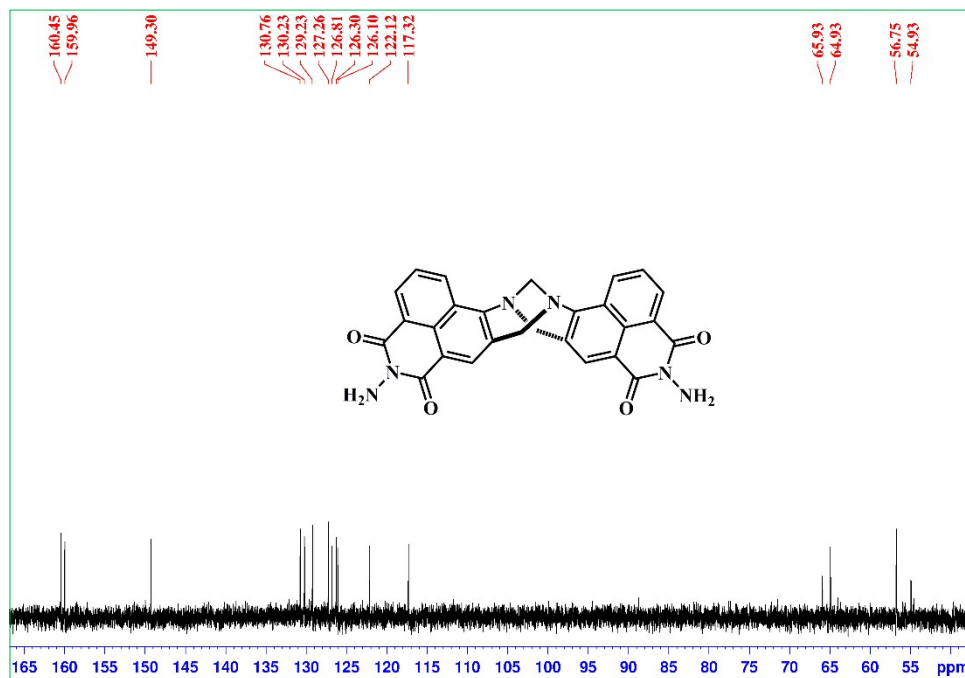
**Fig. S27.** <sup>13</sup>C NMR spectrum of **TB-2i** (150 MHz, DMSO-d<sub>6</sub>).



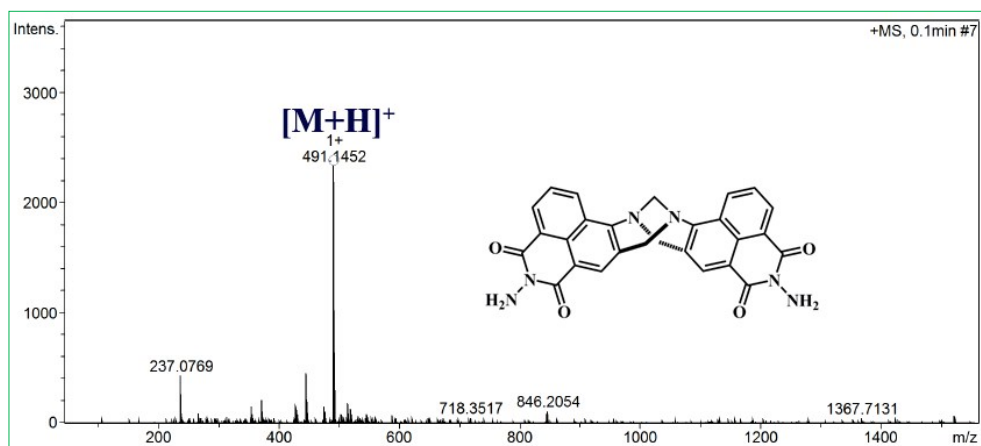
**Fig. S28.** HRMS spectrum of **TB-2i**.



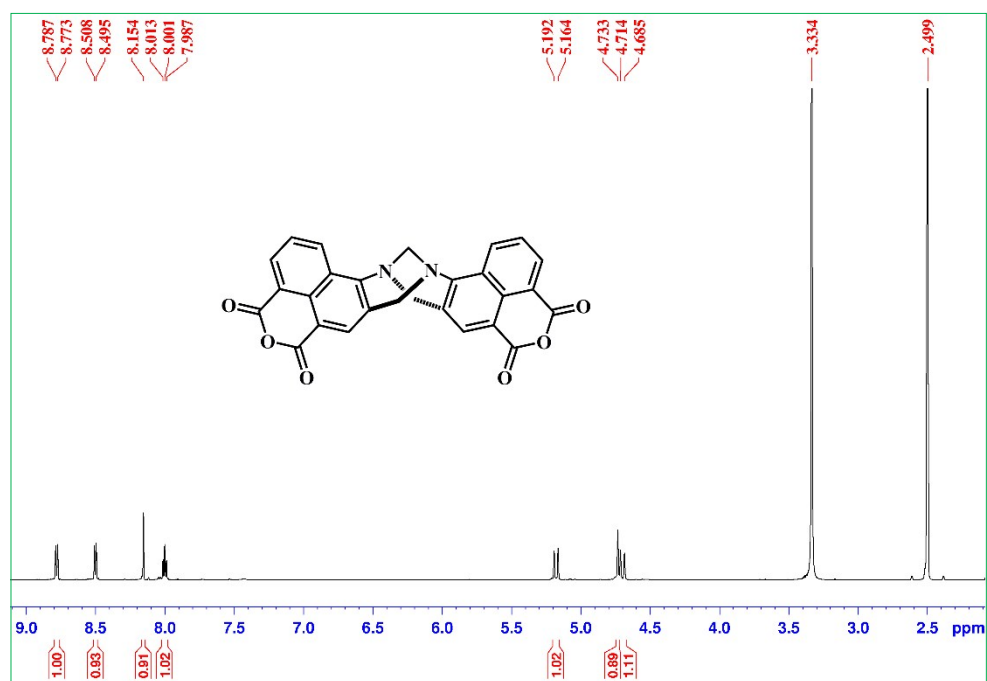
**Fig. S29.** <sup>1</sup>H NMR spectrum of TB-2j (600 MHz, DMSO-d<sub>6</sub>).



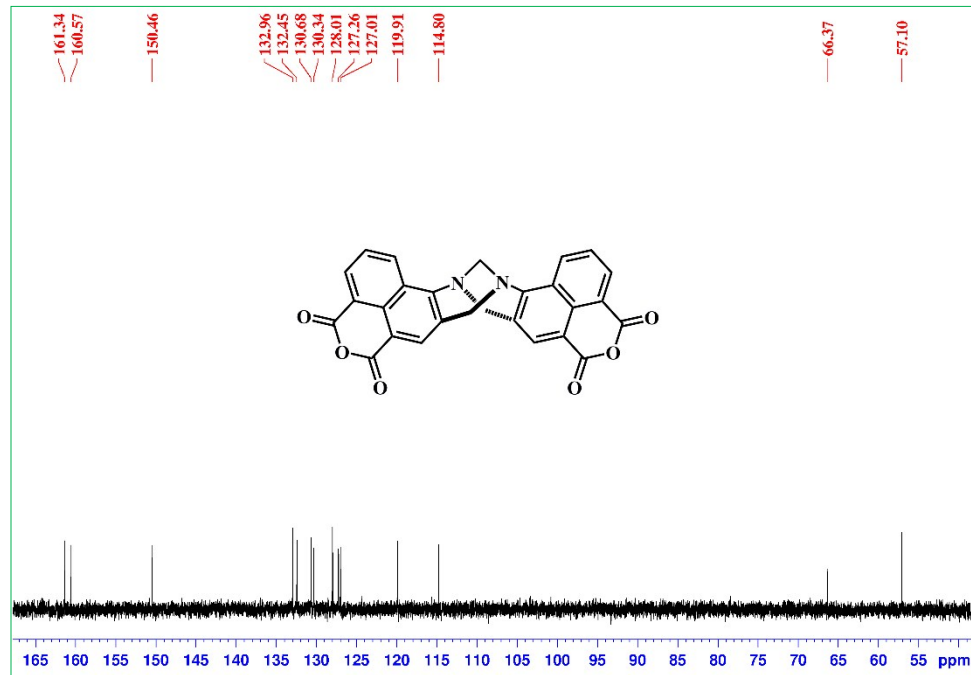
**Fig. S30.** <sup>13</sup>C NMR spectrum of TB-2j (150 MHz, DMSO-d<sub>6</sub>).



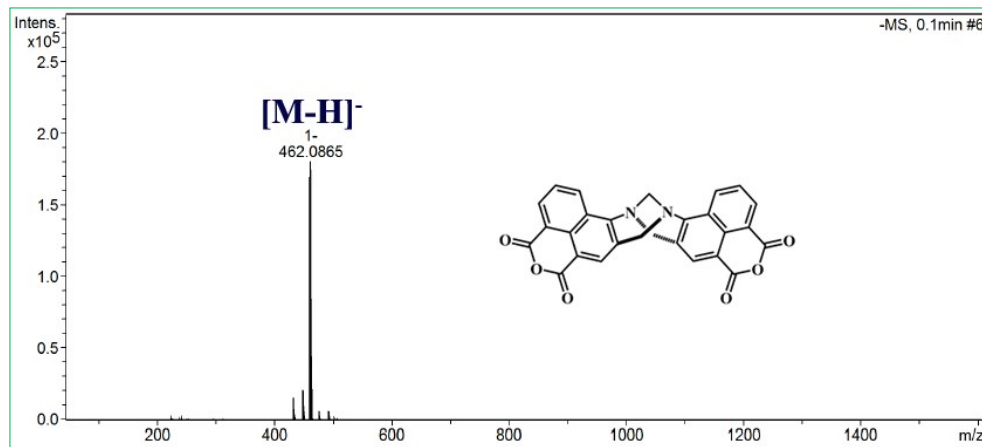
**Fig. S31.** HRMS spectrum of TB-2j.



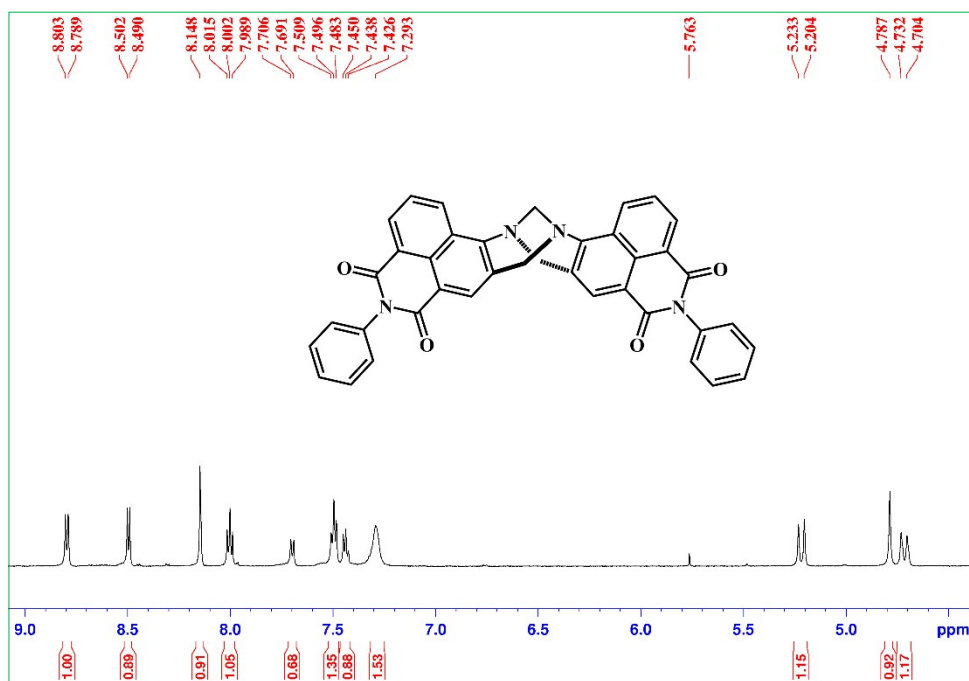
**Fig. S32.**  $^1\text{H}$  NMR spectrum of TB-2k (600 MHz, DMSO- $d_6$ ).



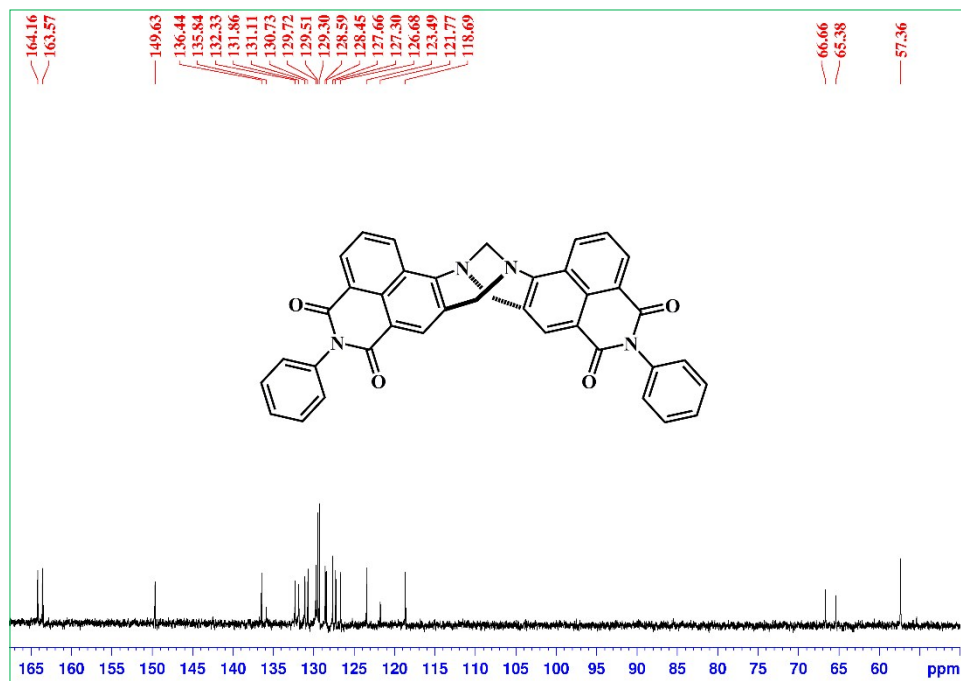
**Fig. S33.** <sup>13</sup>C NMR spectrum of **TB-2k** (150 MHz, DMSO-d<sub>6</sub>).



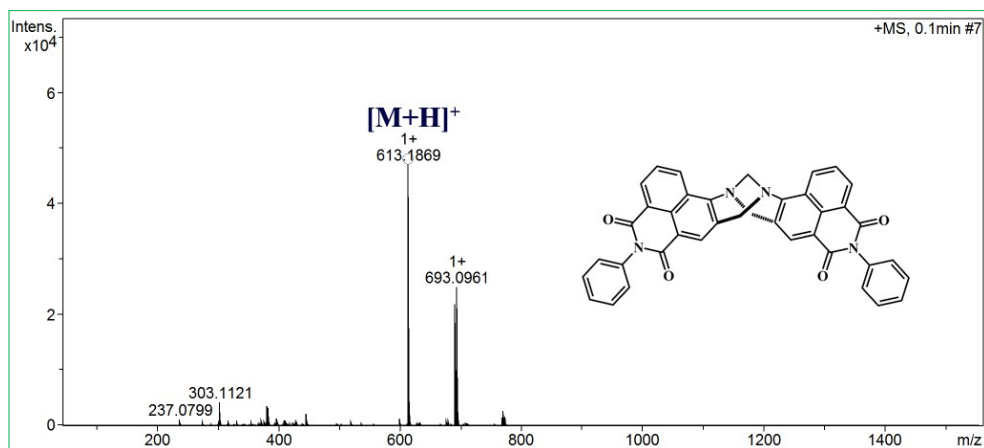
**Fig. S34.** HRMS spectrum of **TB-2k**.



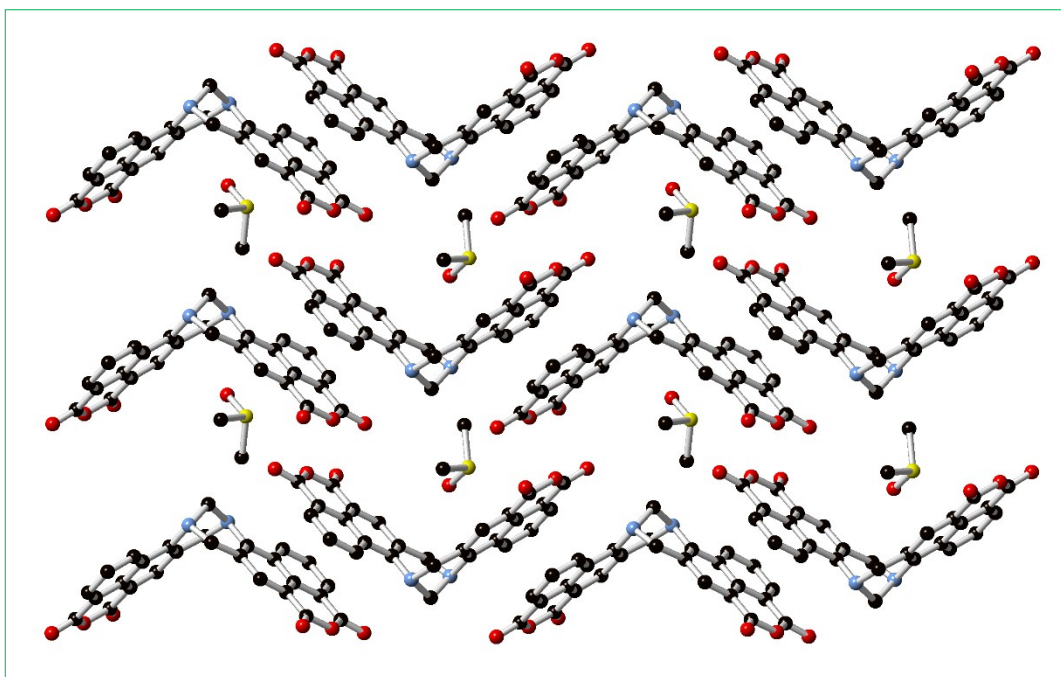
**Fig. S35.**  $^1\text{H}$  NMR spectrum of TB-3 (600 MHz, DMSO- $\text{d}_6$ ).



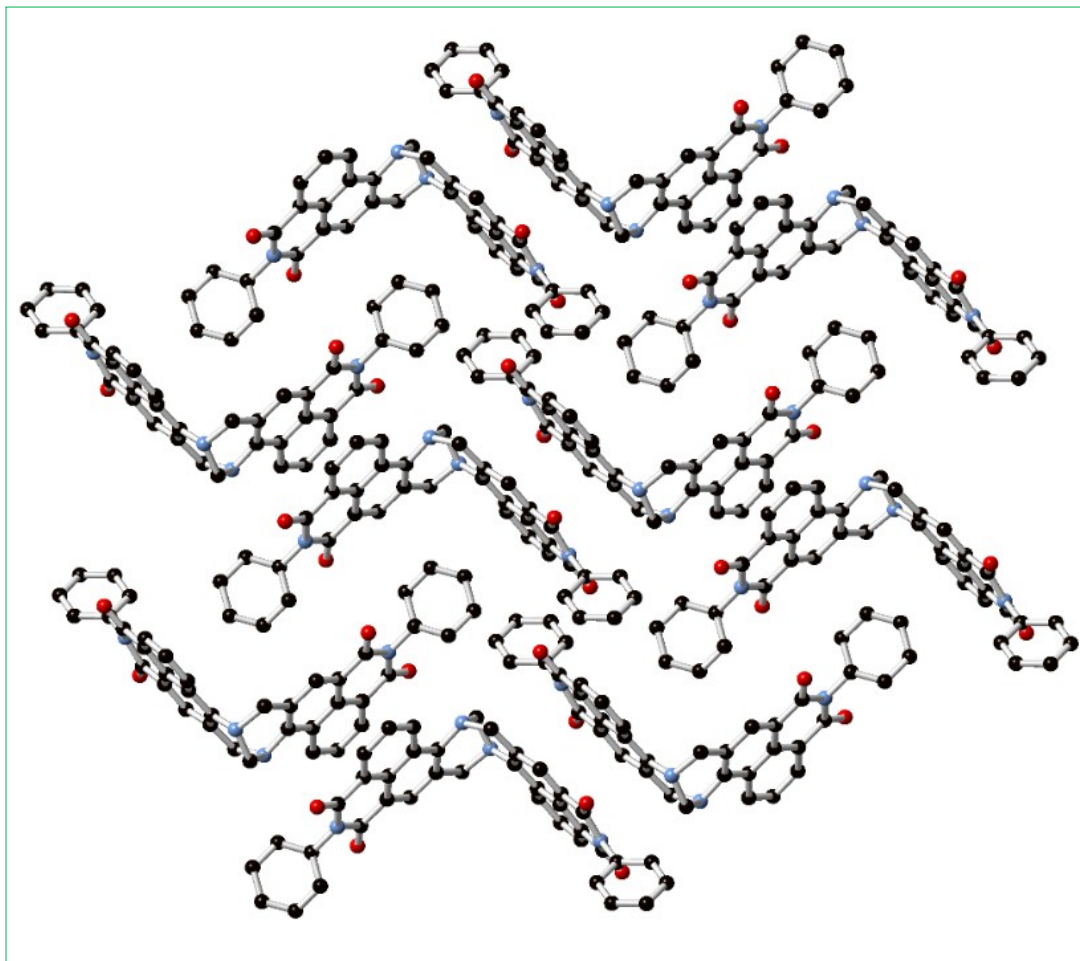
**Fig. S36.**  $^{13}\text{C}$  NMR spectrum of TB-3 (150 MHz, DMSO- $\text{d}_6$ ).



**Fig. S37.** HRMS spectrum of TB-3.



**Fig. S38.** Extended structure of TB-2k viewed parallel to the crystallographic  $a$ -axis. Hydrogen atoms and lattice solvent disorder are omitted for clarity.



**Fig. S39.** Extended structure of **TB-3** viewed parallel to the crystallographic *c*-axis. Hydrogen atoms and lattice solvent disorder are omitted for clarity.

**Table S1.** Crystallographic data and refinement parameters of **TB-2k** and **TB-3**.

| Identification code                                          | <b>TB-2k.2(CH<sub>3</sub>)<sub>2</sub>SO</b>                                 | <b>TB-3.CH<sub>2</sub>Cl<sub>2</sub></b>                                      |
|--------------------------------------------------------------|------------------------------------------------------------------------------|-------------------------------------------------------------------------------|
| Empirical formula                                            | C <sub>31</sub> H <sub>26</sub> N <sub>2</sub> O <sub>8</sub> S <sub>2</sub> | C <sub>40</sub> H <sub>26</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>4</sub> |
| Formula weight                                               | 618.66                                                                       | 697.55                                                                        |
| Temperature/K                                                | 100(2)                                                                       | 100.15                                                                        |
| Crystal system                                               | monoclinic                                                                   | triclinic                                                                     |
| Space group                                                  | <i>C2/c</i>                                                                  | <i>P</i> -1                                                                   |
| <i>a</i> /Å                                                  | 17.102(7)                                                                    | 10.406(2)                                                                     |
| <i>b</i> /Å                                                  | 8.688(3)                                                                     | 11.383(3)                                                                     |
| <i>c</i> /Å                                                  | 18.461(8)                                                                    | 13.621(3)                                                                     |
| $\alpha$ /°                                                  | 90                                                                           | 83.448(9)                                                                     |
| $\beta$ /°                                                   | 98.011(7)                                                                    | 87.082(1)                                                                     |
| $\gamma$ /°                                                  | 90                                                                           | 78.674(10)                                                                    |
| Volume/Å <sup>3</sup>                                        | 2716.3(19)                                                                   | 1571.0(6)                                                                     |
| <i>Z</i>                                                     | 4                                                                            | 2                                                                             |
| $\rho_{\text{calc}}$ g/cm <sup>3</sup>                       | 1.513                                                                        | 1.475                                                                         |
| $\mu$ /mm <sup>-1</sup>                                      | 2.286                                                                        | 0.260                                                                         |
| <i>F</i> (000)                                               | 1288                                                                         | 720.0                                                                         |
| Crystal size/mm <sup>3</sup>                                 | 0.32 × 0.07 × 0.03                                                           | 0.39 × 0.32 × 0.21                                                            |
| Radiation/ $\lambda$                                         | Cu K $\alpha$ ( $\lambda$ = 1.54178)                                         | Mo K $\alpha$ ( $\lambda$ = 0.71075)                                          |
| 2 $\Theta$ range for data collection/°                       | 4.84 to 68.28                                                                | 4.878 to 50.994                                                               |
| Reflections collected                                        | 2481                                                                         | 12875                                                                         |
| Data/restraints/parameters                                   | 2481/18/249                                                                  | 5827/0/451                                                                    |
| Data completeness                                            | 0.994                                                                        | 0.995                                                                         |
| S on <i>F</i> <sup>2</sup> (all data)                        | 1.031                                                                        | 1.048                                                                         |
| Final <i>R</i> indexes [ <i>I</i> ≥ 2 $\sigma$ ( <i>I</i> )] | <i>R</i> <sub>1</sub> = 0.0543, <i>wR</i> <sub>2</sub> = 0.1450              | <i>R</i> <sub>1</sub> = 0.0577, <i>wR</i> <sub>2</sub> = 0.1644               |
| Final <i>R</i> indexes [all data]                            | <i>R</i> <sub>1</sub> = 0.0660, <i>wR</i> <sub>2</sub> = 0.1584              | <i>R</i> <sub>1</sub> = 0.0644, <i>wR</i> <sub>2</sub> = 0.1702               |
| CCDC                                                         | 1563998                                                                      | 1564000                                                                       |