

Electronic Supporting Information (ESI)

**Three-Component Nanorotors Generated from Fusion of Complexes and  
Post-Fusion Metal-Metal Exchange**

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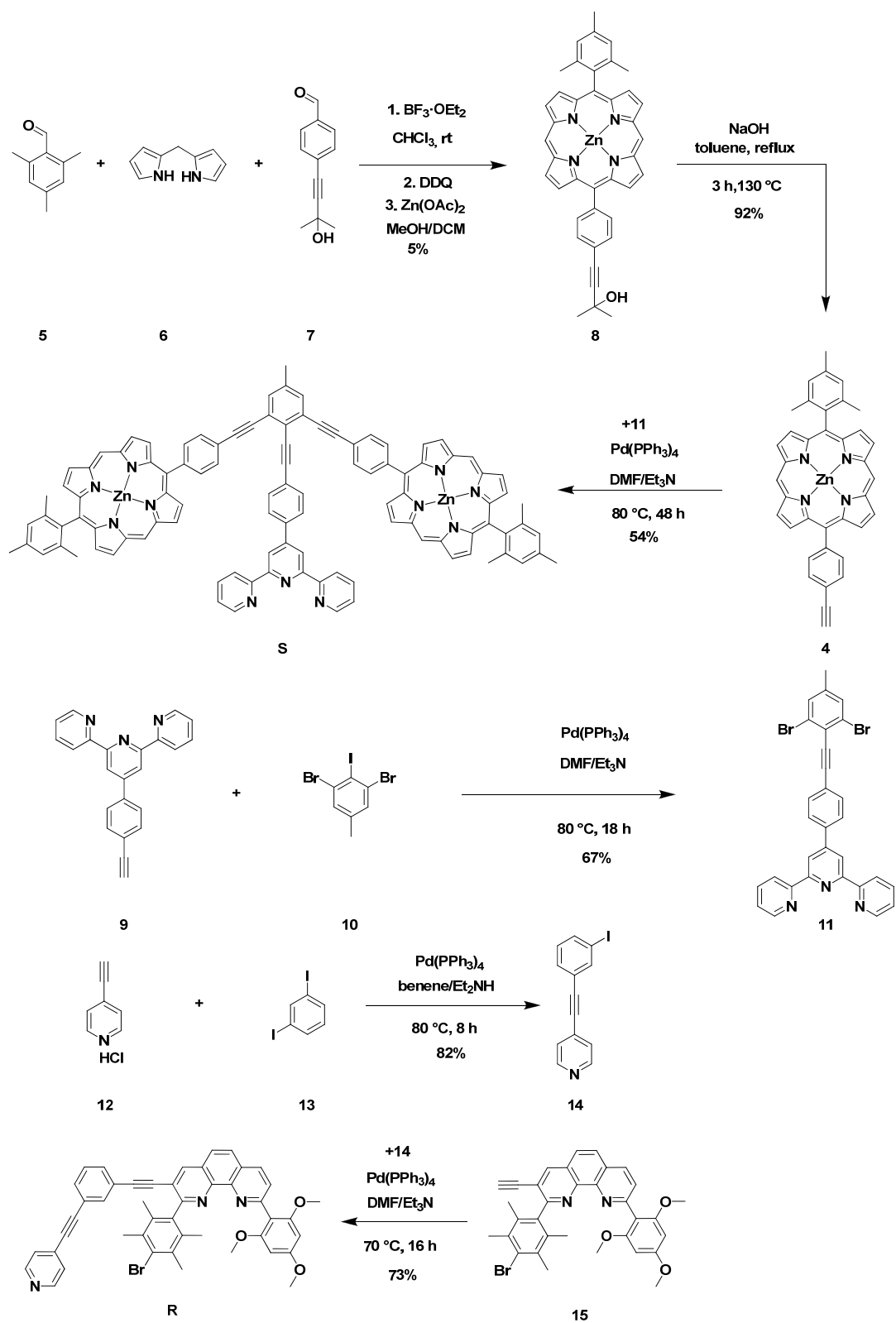
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## 1. Synthesis

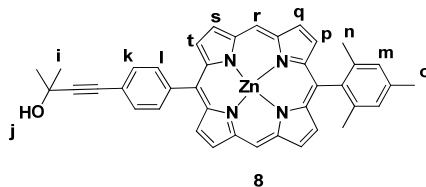
### General Remarks

All solvents were dried by distillation prior to use while commercial reagents (**1**, **3**, **5**, **10**, **12**, **13**, hexacyclen) were used without any further purification. Bruker Avance (400 MHz) and Varian (600 MHz) spectrometers were used to measure  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra using a deuterated solvent as the lock and residual protonated solvent as internal reference ( $\text{CDCl}_3$ :  $\delta_{\text{H}}$  7.26 ppm,  $\delta_{\text{C}}$  77.0 ppm;  $\text{CD}_2\text{Cl}_2$ :  $\delta_{\text{H}}$  5.32 ppm,  $\delta_{\text{C}}$  53.8 ppm, THF- $d_8$ :  $\delta_{\text{H}}$  1.72 ppm, 3.58 ppm,  $\delta_{\text{C}}$  25.3 ppm, 67.2 ppm). The following abbreviations were used to define NMR peak pattern: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, ddd = doublet of doublets of doublets, td = triplet of doublets, br = broad, m = multiplet. The coupling constant values are given in Hertz (Hz) and, wherever possible, assignment of protons is provided. The numbering of different carbons in different molecular skeletons does not necessarily follow IUPAC nomenclature rules; it was exclusively implemented for assigning NMR signals. All electrospray ionization (ESI-MS) spectra were recorded on a Thermo-Quest LCQ deca and the theoretical isotopic distributions of the mass signals were calculated using IsoPro 3.0 software. Melting points of compounds were measured on a BÜCHI 510 instrument and are not corrected. Infrared spectra were recorded on a Varian 1000 FT-IR instrument. Elemental analysis was performed using the EA-3000 CHNS analyzer. UV-vis spectra were recorded on a Cary Win 50 (298 K) spectrometer. Binding constants were determined through UV-vis titrations in combination with a 1:1 binding formula of two ligands or with SPECFIT/32TM global analysis system by Spectrum Software Associates (Marlborough, MA). Column chromatography was performed either on silica gel (60-400 mesh) or neutral alumina (Fluka, 0.05-0.15 mm, Brockmann Activity 1). Merck silica gel (60 F254) or neutral alumina (150 F254) sheets were used for thin layer chromatography (TLC). All rotor preparations were performed directly in the NMR tube using  $\text{CD}_2\text{Cl}_2$  as solvent. Compounds **6**,<sup>1</sup> **7**,<sup>2</sup> **9**,<sup>3</sup> **17**<sup>4</sup> were synthesized according to the literature known procedures.



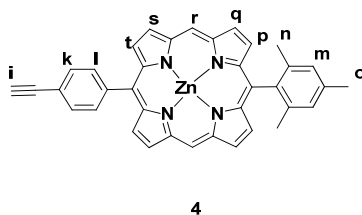
**Scheme S1.** Synthesis of stator **S** and rotator **R**.

**Zinc(II)-5-(4-(3-hydroxy-3-methylbut-1-ynyl)phenyl)-15-(2,4,6-trimethylphenyl)porphyrin (8)**



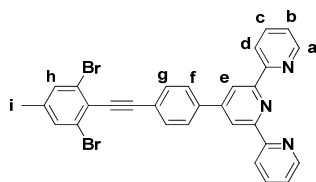
An ethereal solution of boron trifluoride (0.25 ml, 2.0 mmol) was added dropwise to a solution of mesitaldehyde (**5**) (1.02 g, 6.90 mmol), di(1*H*-pyrrol-2-yl)methane (**6**) (2.02 g, 13.8 mmol) and 4-(3-hydroxy-3-methylbut-1-ynyl) benzaldehyde (**7**) (1.30 g, 6.90 mmol) in 1.0 L of chloroform over 10 min. The resultant solution was allowed to stir at room temperature for 4 h in the dark. Then DDQ (2.04 g, 8.99 mmol) was added and stirring was continued for another 2 h. The solution was concentrated to 50 mL, then Zn(OAc)<sub>2</sub>·2H<sub>2</sub>O (1.50 g, 6.80 mmol) in 15 mL of CH<sub>3</sub>OH was added. After stirring the reaction mixture for 3 h, the solution was evaporated to dryness and the crude black product was purified by column chromatography (silica gel, CH<sub>2</sub>Cl<sub>2</sub>, *R<sub>f</sub>* = 0.2) providing 240 mg of **8** as a pink solid (369 μmol, 5%). **Mp** > 250 °C. **IR (KBr):**  $\bar{\nu}$  = 416, 570, 701, 719, 733, 783, 814, 832, 839, 852, 904, 995, 1058, 1141, 1157, 1209, 1282, 1309, 1349, 1391, 1433, 1479, 1503, 1519, 1545, 1620, 2220, 2940, 3079, 3442 cm<sup>-1</sup>. **<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):**  $\delta$  = 1.77 (s, 6H, i-H), 1.83 (s, 6H, n-H), 2.13 (s, 1H, j-H), 2.67 (s, 3H, o-H), 7.33 (s, 2H, m-H), 7.85 (d, <sup>3</sup>*J* = 8.4 Hz, 2H, k-H), 8.20 (d, <sup>3</sup>*J* = 8.4 Hz, 2H, l-H), 8.99 (d, <sup>3</sup>*J* = 4.5 Hz, 2H, p-H), 9.09 (d, <sup>3</sup>*J* = 4.5 Hz, 2H, t-H), 9.40 (d, <sup>3</sup>*J* = 4.5 Hz, 2H, q-H), 9.43 (d, <sup>3</sup>*J* = 4.5 Hz, 2H, s-H), 10.29 (s, 2H, r-H) ppm. **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 21.5, 21.7, 31.6, 65.8, 82.3, 94.7, 106.0, 118.6, 119.0, 121.9, 127.7, 129.9, 131.5, 131.8, 132.0, 132.3, 134.5, 137.6, 138.7, 139.3, 142.8, 149.4, 149.6, 149.7, 150.0 ppm. **Elemental analysis:** Calculated for C<sub>40</sub>H<sub>32</sub>N<sub>4</sub>OZn: C, 73.90; H, 4.96; N, 8.62. Found: C, 73.61; H, 5.09; N, 8.75.

**Zinc(II)-5-(4-ethynylphenyl)-15-(2,4,6-trimethylphenyl)porphyrin (4)**



NaOH granules (148 mg, 3.69 mmol) were added to a solution of porphyrin **8** (240 mg, 369  $\mu\text{mol}$ ) in toluene (30 mL), which was then refluxed for 3 h. The resulting reaction mixture was cooled, washed with water and evaporated to dryness furnishing a purple solid as crude product. The crude material was chromatographed (silica gel,  $\text{CH}_2\text{Cl}_2/\text{hexane} = 3:7$ ,  $R_f = 0.3$ ) to yield 200 mg of **4** as pink solid (338  $\mu\text{mol}$ , 92%). **Mp** > 250  $^\circ\text{C}$ . **IR (KBr):**  $\bar{\nu} = 410, 434, 507, 547, 564, 607, 633, 702, 720, 734, 784, 812, 832, 858, 906, 995, 1059, 1102, 1141, 1162, 1178, 1211, 1286, 1315, 1372, 1390, 1437, 1491, 1521, 1552, 1609, 1712, 1800, 2110, 2240, 2914, 3031, 3079 \text{ cm}^{-1}$ .  **$^1\text{H NMR (400 MHz, CDCl}_3\text{):$**   $\delta = 1.83$  (s, 6H, n-H), 2.67 (s, 3H, o-H), 3.34 (s, 1H, i-H), 7.33 (s, 2H, m-H), 7.93 (d,  $^3J = 8.4 \text{ Hz}$ , 2H, k-H), 8.23 (d,  $^3J = 8.4 \text{ Hz}$ , 2H, l-H), 8.99 (d,  $^3J = 4.5 \text{ Hz}$ , 2H, p-H), 9.10 (d,  $^3J = 4.5 \text{ Hz}$ , 2H, t-H), 9.40 (d,  $^3J = 4.5 \text{ Hz}$ , 2H, q-H), 9.44 (d,  $^3J = 4.5 \text{ Hz}$ , 2H, s-H), 10.29 (s, 2H, r-H) ppm.  **$^{13}\text{C NMR (100 MHz, CDCl}_3\text{):$**   $\delta = 21.5, 21.7, 78.0, 83.8, 106.0, 118.6, 118.8, 121.3, 127.7, 130.4, 131.5, 131.9, 132.0, 132.3, 134.5, 137.6, 138.7, 139.3, 143.4, 149.4, 149.6, 149.6, 150.0$  ppm. **Elemental analysis:** Calculated for  $\text{C}_{37}\text{H}_{26}\text{N}_4\text{Zn}$ : C, 75.06; H, 4.43; N, 9.46. Found: C, 75.16; H, 4.53; N, 9.67.

#### 4'-(4-((2,6-Dibromo-4-methylphenyl)ethynyl)phenyl)-2,2';6',2''-terpyridine (**11**)

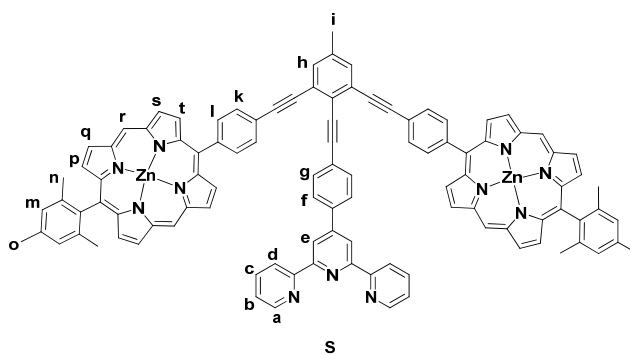


**11**

In an oven-dried 100 mL sealed tube, a mixture of 1,3-dibromo-2-iodo-5-methylbenzene (**10**) (676 mg, 1.80 mmol) and 4'-(4-ethynylphenyl)-2,2';6',2''-terpyridine (**9**) (200 mg, 600  $\mu\text{mol}$ ) were dissolved in dry DMF (20 mL) and  $\text{Et}_3\text{N}$  (20 mL) and degassed thoroughly. Then  $\text{Pd}(\text{PPh}_3)_4$  (70.0 mg, 60.0  $\mu\text{mol}$ ) was added and the mixture was refluxed at 80  $^\circ\text{C}$  for 18 h for completion of the coupling reaction. The reaction mixture was cooled down to room temperature and the solvents were removed. The residue was subjected to column chromatography (silica gel, ethyl acetate/hexane = 3:7,  $R_f = 0.3$ ) to afford 230 mg of compound **9** as brown solid (0.40 mmol, 67%). **Mp** = 216  $^\circ\text{C}$ . **IR (KBr):**  $\bar{\nu} = 528, 565, 577, 621, 653, 660, 696, 710, 734, 742, 791, 832, 848, 857, 893, 905, 990, 1037, 1075, 1087, 1109, 1121, 1191, 1263, 1387, 1411, 1442, 1460, 1466, 1516, 1538, 1565, 1584, 1602, 2223, 2920, 3052 \text{ cm}^{-1}$ .  **$^1\text{H NMR (400 MHz, CD}_2\text{Cl}_2\text{):$**   $\delta = 2.35$  (s, 3H, i-H), 7.39 (ddd,  $^3J = 7.8 \text{ Hz}$ ,  $^3J = 4.8 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 2H, b-H), 7.47 (s, 2H, h-H),

7.77 (d,  $^3J = 8.8$  Hz, 2H, g-H), 7.91 (td,  $^3J = 7.8$  Hz,  $^4J = 1.2$  Hz, 2H, c-H), 7.95 (d,  $^3J = 8.8$  Hz, 2H, f-H), 8.69 (ddd,  $^3J = 7.8$  Hz,  $^4J = 1.2$  Hz,  $^5J = 0.8$  Hz, 2H, d-H), 8.73 (ddd,  $^3J = 4.8$  Hz,  $^4J = 1.2$  Hz,  $^5J = 0.8$  Hz, 2H, a-H), 8.79 (s, 2H, e-H).  **$^{13}\text{C}$  NMR (100 MHz,  $\text{CD}_2\text{Cl}_2$ ):**  $\delta = 21.1, 89.2, 97.4, 118.9, 121.5, 123.8, 124.2, 124.4, 126.2, 127.7, 132.6, 132.6, 137.3, 139.4, 141.8, 149.5, 149.6, 156.3, 156.5$  ppm. **ESI-MS:**  $m/z$  (%) 582.3 (100) [**12** + H] $^+$ ; **Elemental analysis:** Calculated for  $\text{C}_{30}\text{H}_{19}\text{Br}_2\text{N}_3$ : C, 61.99; H, 3.29; N, 7.23. Found: C, 61.73; H, 3.24; N, 7.15.

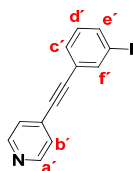
### Stator S



In an oven-dried 100 mL sealed tube, compounds **11** (100 mg, 172  $\mu\text{mol}$ ) and **4** (500 mg, 844  $\mu\text{mol}$ ) were dissolved in dry DMF (20 mL) and  $\text{Et}_3\text{N}$  (20 mL) and degassed thoroughly. Then  $\text{Pd}(\text{PPh}_3)_4$  (20.0 mg, 17.3  $\mu\text{mol}$ ) was added and the mixture was refluxed at 80  $^\circ\text{C}$  for 48 h for completion of the coupling reaction. The reaction mixture was cooled down to room temperature and the solvents were removed. The obtained residue was subjected to column chromatography (silica gel, ethyl acetate/ $\text{CH}_2\text{Cl}_2 = 3:7$ ,  $R_f = 0.2$ ) to afford 150 mg of compound **S** as brown solid (93.6  $\mu\text{mol}$ , 54%). **Mp:**  $> 250$   $^\circ\text{C}$ . **IR (KBr):**  $\bar{\nu} = 564, 608, 634, 702, 720, 734, 785, 813, 833, 858, 906, 995, 1059, 1142, 1212, 1287, 1315, 1391, 1439, 1496, 1521, 1608, 2227, 2915$   $\text{cm}^{-1}$ .  **$^1\text{H}$  NMR (400 MHz,  $\text{CD}_2\text{Cl}_2$ ):**  $\delta = 1.82$  (s, 12H, n-H), 2.62 (s, 3H, i-H), 2.70 (s, 6H, o-H), 7.11 (ddd,  $^3J = 8.0$  Hz,  $^3J = 5.0$  Hz,  $^4J = 1.2$  Hz, 2H, b-H), 7.38 (s, 4H, m-H), 7.70 (td,  $^3J = 8.0$  Hz,  $^4J = 1.2$  Hz, 2H, c-H), 7.73 (s, 2H, h-H), 8.11 (d,  $^3J = 8.4$  Hz, 2H, g/f-H), 8.15 (d,  $^3J = 8.4$  Hz, 2H, f/g-H), 8.19 (d,  $^3J = 8.0$  Hz, 4H, k-H), 8.33 (ddd,  $^3J = 5.0$  Hz,  $^4J = 1.2$  Hz,  $^5J = 0.8$  Hz, 2H, a-H), 8.38 (d,  $^3J = 8.0$  Hz, 4H, l-H), 8.47 (ddd,  $^3J = 8.0$  Hz,  $^4J = 1.2$  Hz,  $^5J = 0.8$  Hz, 2H, d-H),

8.75 (s, 2H, e-H), 8.95 (d,  $^3J = 4.4$  Hz, 4H, p-H), 9.23 (d,  $^3J = 4.4$  Hz, 4H, t-H), 9.43 (d,  $^3J = 4.4$  Hz, 4H, q-H), 9.51 (d,  $^3J = 4.4$  Hz, 4H, s-H), 10.28 (s, 4H, r-H).  **$^{13}\text{C}$  NMR (100 MHz,  $\text{d}_8\text{-THF}:\text{CD}_2\text{Cl}_2 = 8:2$ ):**  $\delta = 20.6, 21.0, 21.5, 89.2, 89.5, 94.3, 97.3, 105.6, 117.7, 118.4, 118.6, 120.9, 122.5, 124.0, 125.0, 125.6, 126.8, 127.7, 127.9, 130.1, 130.7, 131.7, 131.9, 132.1, 132.7, 132.7, 135.3, 136.7, 137.5, 138.9, 139.0, 139.3, 139.8, 144.5, 149.2, 149.3, 149.8, 149.8, 149.9, 149.9, 156.1, 156.4$  ppm. **ESI-MS:**  $m/z$  (%) 1604.7 (100)  $[\text{S} + \text{H}]^+$ . **Elemental analysis:** Calculated for  $\text{C}_{104}\text{H}_{69}\text{N}_{11}\text{Zn}_2 \cdot \text{H}_2\text{O}$ : C, 77.03; H, 4.41; N, 9.50. Found: C, 77.04; H, 4.15; N, 9.40.

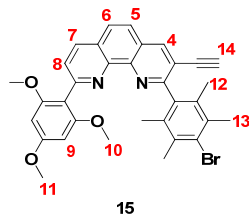
#### 4-((3-Iodophenyl)ethynyl)pyridine (**14**)



14

A solution of 4-ethynylpyridine hydrochloride (**12**) (280 mg, 2.01 mmol), 1,3-diiodobenzene (**13**) (825 mg, 2.50 mmol),  $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$  (140 mg, 199  $\mu\text{mol}$ ) and  $\text{CuI}$  (38.0 mg, 199  $\mu\text{mol}$ ), in benzene (60 mL) and  $\text{Et}_2\text{NH}$  (30 mL), was placed in a three-neck flask equipped with a condenser. The solution was refluxed for 8 h and then evaporated to dryness. The crude product was purified by column chromatography (silica gel,  $\text{CH}_2\text{Cl}_2$ ,  $R_f = 0.3$ ) providing 500 mg of **14** as white solid (1.64 mmol, 82%). **Mp** = 120  $^\circ\text{C}$ ; **IR (KBr):**  $\tilde{\nu} = 435, 471, 533, 539, 563, 656, 684, 725, 790, 816, 869, 895, 908, 991, 1059, 1089, 1145, 1207, 1311, 1394, 1402, 1413, 1466, 1486, 1529, 1544, 1551, 1589, 1686, 1795, 1936, 2220, 3052$   $\text{cm}^{-1}$ .  **$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):**  $\delta = 7.07$  (t,  $^3J = 8.0$  Hz, 1H, d'-H), 7.33 (d,  $^3J = 6.2$  Hz, 2H, b'-H), 7.48 (ddd,  $^3J = 8.0$  Hz,  $^4J = 1.6$  Hz,  $^4J = 1.2$  Hz, 1H, e'-H), 7.69 (ddd,  $^3J = 8.0$  Hz,  $^4J = 1.6$  Hz,  $^4J = 1.2$  Hz, 1H, c'-H), 7.88 (t,  $^3J = 1.6$  Hz, 1H, f'-H), 8.59 (d,  $^3J = 6.2$  Hz, 2H, a'-H), ppm.  **$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):**  $\delta = 87.7, 91.9, 93.7, 124.0, 125.4, 129.9, 130.8, 130.8, 138.1, 140.2, 149.7$  ppm. **ESI-MS:**  $m/z$  (%) 306.2 (100)  $[\text{15} + \text{H}]^+$ . **Elemental analysis:** Calculated for  $\text{C}_{13}\text{H}_8\text{IN}$ : C, 51.17; H, 2.64; N, 4.59. Found: C, 50.85; H, 2.49; N, 4.47.

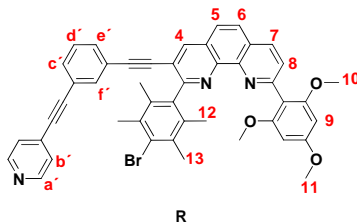
**2-(4-Bromo-2,3,5,6-tetramethylphenyl)-3-ethynyl-9-(2,4,6-trimethoxyphenyl)-1,10-phenanthroline (15).**



Under N<sub>2</sub> atmosphere a solution of *n*-BuLi (2.5 M) in *n*-hexane (1.72 mL, 4.30 mmol) was added dropwise to a solution of 2-bromo-1,3,5-trimethoxybenzene (1.06 g, 4.30 mmol) in dry Et<sub>2</sub>O (20 mL) over a period of 10 min at 0 °C. After stirring at room temperature for 6 h, 2-(4-bromo-2,3,5,6-tetramethylphenyl)-3-((trimethylsilyl)ethynyl)-1,10-phenanthroline (**17**) (700 mg, 1.44 mmol) was added under N<sub>2</sub> atmosphere. The resulting brown solution was stirred at room temperature for 12 h for completion of the reaction. The solution was neutralized with aqueous NH<sub>4</sub>Cl (100 mL) and extracted with dichloromethane (3 × 50 mL). The combined organic layer was then dried over anhydrous MgSO<sub>4</sub> and concentrated to yield a brown solid. The crude product was subsequently dissolved in 20 mL of THF-CH<sub>3</sub>OH (1:1) and treated with 2 N aqueous KOH solution (20 mL). The resulting solution was stirred for another 3 h and then extracted with dichloromethane (3 × 50 mL). The combined organic layer was concentrated to dryness and purified by column chromatography (silica gel, *n*-hexane/ethyl acetate = 7:3, *R<sub>f</sub>* = 0.2) to afford 420 mg of compound **15** as yellow solid (722 μmol, 50%). **Mp** > 250 °C; **IR (KBr):**  $\bar{\nu}$  = 529, 593, 613, 640, 665, 722, 759, 771, 811, 848, 896, 918, 948, 983, 1013, 1037, 1052, 1073, 1126, 1156, 1185, 1205, 1225, 1276, 1335, 1356, 1370, 1384, 1414, 1438, 1460, 1489, 1535, 1585, 1607, 2112, 2836, 2935, 2995, cm<sup>-1</sup>. **<sup>1</sup>H NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>):**  $\delta$  = 1.97 (s, 6H, 13-H), 2.46 (s, 6H, 12-H), 3.21 (s, 1H, 14-H), 3.68 (s, 6H, 10-H), 3.87 (s, 3H, 11-H), 6.26 (s, 2H, 9-H), 7.59 (d, <sup>3</sup>*J* = 8.2 Hz, 1H, 8-H), 7.83 (d, <sup>3</sup>*J* = 8.8 Hz, 1H, 5/6-H), 7.90 (d, <sup>3</sup>*J* = 8.8 Hz, 1H, 6/5-H), 8.27 (d, <sup>3</sup>*J* = 8.2 Hz, 1H, 7-H), 8.51 (s, 1H, 4-H) ppm. **<sup>13</sup>C NMR (100 MHz, CD<sub>2</sub>Cl<sub>2</sub>):**  $\delta$  = 18.5, 21.1, 55.8, 56.3, 80.6, 83.0, 91.3, 112.9, 118.8, 125.7, 127.1, 127.2, 127.8, 128.5, 129.4, 133.7, 134.3, 135.8, 139.5, 140.9, 145.7, 146.2, 156.2, 159.3, 162.0, 162.4 ppm; ESI-MS: *m/z* (%) 583.4 (100) [**12** + H]<sup>+</sup>. **Elemental analysis:** Calculated for C<sub>33</sub>H<sub>29</sub>BrN<sub>2</sub>O<sub>3</sub>: C, 68.16; H, 5.03; N, 4.82. Found: C, 67.93; H, 5.23; N, 4.75.

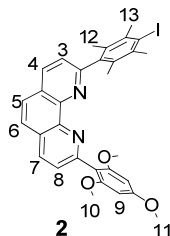


**2-(4-Bromo-2,3,5,6-tetramethylphenyl)-3-(((pyridin-4 yl-ethynyl)phen-3-yl)ethynyl)-9-(2,4,6-trimethoxyphenyl)-1,10-phenanthroline = rotator **R**.**



A N<sub>2</sub>-purged sealed tube was loaded with **14** (94.0 mg, 308 μmol), **15** (90.0 mg, 155 μmol), 20 mL of dry DMF, and 20 mL of dry Et<sub>3</sub>N. The solution was degassed thoroughly to remove oxygen. The catalyst, Pd(PPh<sub>3</sub>)<sub>4</sub> (20.0 mg, 17.3 μmol), was then added to the reaction mixture that was stirred at 70 °C for 16 hours to complete the coupling reaction. Solvents were removed from the reaction mixture under reduced pressure yielding a brown residue, which was purified by column chromatography (silica gel, CH<sub>2</sub>Cl<sub>2</sub>/ethyl acetate = 9:1, R<sub>f</sub> = 0.3) affording 83.0 mg of compound **R** as yellow solid (0.11 mmol, 73%). **Mp** > 220 °C. **IR (KBr):**  $\tilde{\nu}$  = 533, 613, 640, 663, 678, 773, 792, 821, 848, 887, 895, 919, 947, 988, 1015, 1049, 1072, 1132, 1159, 1207, 1226, 1277, 1334, 1384, 1412, 1432, 1460, 1490, 1535, 1588, 1596, 2211, 2836, 2935 cm<sup>-1</sup>. **<sup>1</sup>H NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>):**  $\delta$  = 2.02 (s, 6H, 12-H), 2.51 (s, 6H, 13-H), 3.70 (s, 6H, 10-H), 3.87 (s, 3H, 11-H), 6.26 (s, 2H, 9-H), 7.17 (ddd, <sup>3</sup>J = 7.8 Hz, <sup>4</sup>J = 1.6 Hz, <sup>4</sup>J = 1.2 Hz, 1H, e'/c'-H), 7.21 (t, <sup>3</sup>J = 1.2 Hz, 1H, f'-H), 7.33 (t, <sup>3</sup>J = 7.8 Hz, 1H, d'-H), 7.44 (d, <sup>3</sup>J = 6.0 Hz, 2H, b'-H), 7.50 (ddd, <sup>3</sup>J = 7.8 Hz, <sup>4</sup>J = 1.6 Hz, <sup>4</sup>J = 1.2 Hz, 1H, c'/e'-H), 7.59 (d, <sup>3</sup>J = 8.0 Hz, 1H, 8-H), 7.87 (d, <sup>3</sup>J = 8.8 Hz, 1H, 5/6-H), 7.92 (d, <sup>3</sup>J = 8.8 Hz, 1H, 6/5-H), 8.28 (d, <sup>3</sup>J = 8.0 Hz, 1H, 7-H), 8.51 (s, 1H, 4-H), 8.61 (d, <sup>3</sup>J = 6.0 Hz, 2H, a'-H) ppm. **<sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):**  $\delta$  = 18.6, 21.1, 55.9, 56.3, 87.6, 87.9, 91.3, 92.8, 94.5, 113.0, 119.7, 123.0, 123.6, 125.9, 125.9, 127.2, 127.3, 127.7, 128.4, 129.2, 129.4, 131.3, 132.1, 132.2, 133.8, 134.3, 135.1, 135.8, 138.9, 139.7, 145.5, 146.3, 150.3, 156.2, 159.3, 162.0, 162.7 ppm. **ESI-MS:** *m/z* (%) 760.4 (100) [**R** + H]<sup>+</sup>; **Elemental analysis:** Calculated for C<sub>46</sub>H<sub>36</sub>BrN<sub>3</sub>O<sub>3</sub>•0.4 H<sub>2</sub>O: C, 72.14; H, 4.84; N, 5.49. Found: C, 71.83; H, 4.78; N, 5.87.

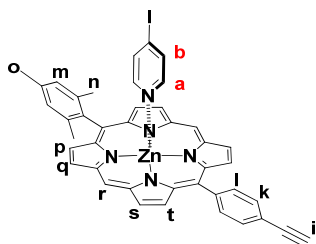
## Characterization of 2-(4-iodo-2,3,5,6-tetramethylphenyl)-9-(2,4,6-trimethoxyphenyl)-1,10-phenanthroline (**2**)



**Data for 2:** Mp > 200 °C. **IR (KBr):**  $\tilde{\nu}$  = 535, 610, 640, 690, 727, 751, 809, 848, 836, 909, 948, 1008, 1027, 1064, 1128, 1143, 1158, 1182, 1205, 1228, 1278, 1301, 1334, 1351, 1372, 1385, 1415, 1435, 1452, 1465, 1486, 1497, 1512, 1539, 1587, 1612, 2837, 2935, 3001 cm<sup>-1</sup>. **<sup>1</sup>H NMR (CD<sub>2</sub>Cl<sub>2</sub>, 400 MHz):**  $\delta$  = 2.00 (s, 6H, 13-H), 2.55 (s, 6H, 12-H), 3.68 (s, 6H, 10-H), 3.87 (s, 3H, 11-H), 6.26 (s, 3H, 9-H), 7.51 (d, <sup>3</sup>J = 8.0 Hz, 1H, 8-H), 7.58 (d, <sup>3</sup>J = 8.0 Hz, 1H, 3-H), 7.88 (s, 2H, 5+6-H), 8.33 (d, <sup>3</sup>J = 8.0 Hz, 1H, 7-H), 8.42 (d, <sup>3</sup>J = 8.0 Hz, 1H, 4-H) ppm. **<sup>13</sup>C NMR (100 MHz, CD<sub>2</sub>Cl<sub>2</sub>):**  $\delta$  = 19.6, 27.7, 55.8, 56.3, 91.2, 111.6, 113.1, 124.6, 126.4, 126.8, 126.9, 127.6, 128.0, 132.9, 135.8, 136.7, 138.0, 142.0, 146.5, 146.7, 155.7, 159.3, 161.2, 162.0. **ESI-MS:** *m/z* (%) 605.2 (100) [M + H]<sup>+</sup>. **Elemental analysis:** Calculated for C<sub>31</sub>H<sub>29</sub>IN<sub>2</sub>O<sub>3</sub>•0.8CH<sub>2</sub>Cl<sub>2</sub>: C, 56.80; H, 4.59; N, 4.17. Found: C, 56.89; H, 4.44; N, 4.15.

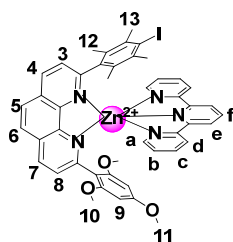
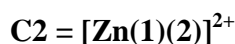
## 2. Synthesis and characterization of complexes:

### Complex C1 = [3•4]



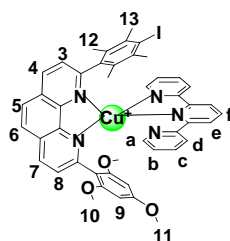
In an NMR tube, porphyrin **4** (0.456 mg, 0.770  $\mu$ mol) and 4-iodopyridine (**3**) (0.158 mg, 0.771  $\mu$ mol) were dissolved in 500  $\mu$ L of CD<sub>2</sub>Cl<sub>2</sub> and NMR spectra were recorded. Yield: quantitative; **Mp** > 200 °C; **IR (KBr):**  $\tilde{\nu}$  = 558, 614, 697, 721, 787, 809, 838, 886, 909, 995, 1057, 1121, 1143, 1158, 1182, 1209, 1228, 1288, 1313, 1374, 1395, 1437, 1522, 1559, 1612, 2137, 2915, 3051, 3079 cm<sup>-1</sup>. **<sup>1</sup>H NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>):**  $\delta$  = 1.77 (s, 6H, n-H), 2.66 (s, 3H, o-H), 3.02 (brs, 2H, a-H), 3.40 (s, 1H, i-H), 6.12 (d, <sup>3</sup>J = 5.6 Hz, 2H, b-H), 7.33 (s, 2H, m-H), 7.93 (d, <sup>3</sup>J =

8.0 Hz, 2H, k-H), 8.25 (d,  $^3J = 8.0$  Hz, 2H, l-H), 8.88 (d,  $^3J = 4.5$  Hz, 2H, p-H), 9.06 (d,  $^3J = 4.5$  Hz, 2H, t-H), 9.36 (d,  $^3J = 4.5$  Hz, 2H, q-H), 9.41 (d,  $^3J = 4.5$  Hz, 2H, s-H), 10.21 (s, 2H, r-H) ppm. **Elemental analysis:** Calculated for **C1** (C<sub>42</sub>H<sub>30</sub>IN<sub>5</sub>Zn): C, 63.29; H, 3.79; N, 8.79. Found: C, 63.43; H, 3.82; N, 8.91.



In an NMR tube, phenanthroline **2** (0.469 mg, 0.776  $\mu$ mol), terpyridine (**1**) (0.181 mg, 0.776  $\mu$ mol), and Zn(OTf)<sub>2</sub> (0.282 mg, 0.776  $\mu$ mol) were dissolved in 500  $\mu$ L of CD<sub>2</sub>Cl<sub>2</sub>:CD<sub>3</sub>CN = 10:1. After heating the sample at 50 °C for 2 h, NMR spectra were recorded showing exclusive formation of the zinc HETTAP complex (> 95%). **IR (KBr):**  $\tilde{\nu} = 580, 613, 637, 779, 1031, 1129, 1159, 1227, 1268, 1382, 1430, 1460, 1560, 1603, 2221, 2853, 2924$  cm<sup>-1</sup>. **<sup>1</sup>H NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>:CD<sub>3</sub>CN = 10:1)**  $\delta = 0.86$  (s, 6H, 13-H), 1.94 (s, 6H, 12-H), 2.91 (s, 6H, 10-H), 3.48 (s, 3H, 11-H), 5.58 (s, 2H, 9-H), 7.49 (ddd,  $^3J = 7.6$  Hz,  $^3J = 5.6$  Hz,  $^4J = 1.6$  Hz, 2H, b-H), 7.59 (ddd,  $^3J = 5.6$  Hz,  $^4J = 1.6$  Hz,  $^5J = 0.8$  Hz, 2H, a-H), 7.87 (d,  $^3J = 8.4$  Hz, 1H, 8-H), 8.08 (d,  $^3J = 8.4$  Hz, 1H, 3-H), 8.25 (td,  $^3J = 7.6$  Hz,  $^4J = 1.6$  Hz, 2H, c-H), 8.41 – 8.49 (m, 6H, d-, e-, 5- & 6-H), 8.59 (dd,  $^3J = 8.4$  Hz,  $^3J = 7.8$  Hz, 1H, f-H), 8.97 (d,  $^3J = 8.4$  Hz, 1H, 7-H), 9.00 (d,  $^3J = 8.4$  Hz, 1H, 4-H) ppm. **ESI-MS:** *m/z* (%) 450.8 (20) [**C2**], 1049.8 (100) [**C2** + OTf<sup>-</sup>]. **Elemental analysis:** Calculated for C<sub>48</sub>H<sub>40</sub>F<sub>6</sub>IN<sub>5</sub>O<sub>9</sub>S<sub>2</sub>Zn•0.7CH<sub>2</sub>Cl<sub>2</sub>: C, 46.39; H, 3.31; N, 5.55; S, 5.09. Found: C, 46.74; H, 2.92; N, 5.64; S, 5.27.

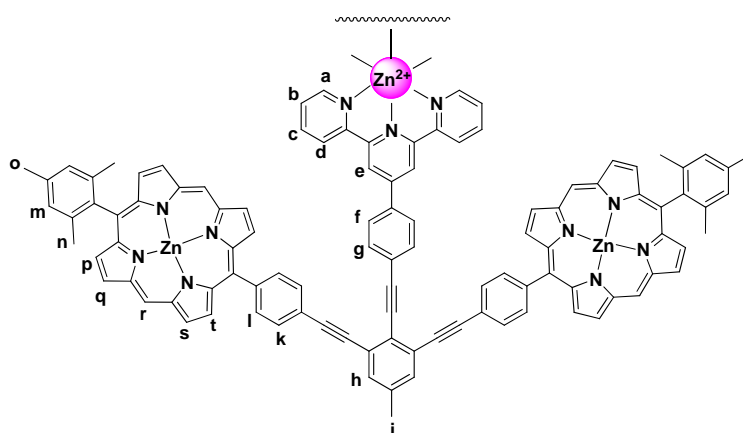
**Complex C3 = [Cu(1)(2)]<sup>+</sup>.**



In an NMR tube, phenanthroline **2** (0.469 mg, 0.776  $\mu\text{mol}$ ), terpyridine **1** (0.181 mg, 0.776  $\mu\text{mol}$ ), and  $[\text{Cu}(\text{CH}_3\text{CN})_4]\text{PF}_6$  (0.289 mg, 0.776  $\mu\text{mol}$ ) were dissolved in 500 of  $\mu\text{L}$   $\text{CD}_2\text{Cl}_2$ . NMR spectra were recorded showing quantitative formation of the copper(I) HETTAP complex.

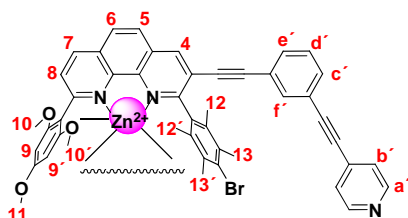
**IR (KBr):**  $\tilde{\nu} = 558, 610, 651, 768, 843, 949, 992, 1031, 1067, 1128, 1158, 1184, 1206, 1228, 1338, 1384, 1429, 1456, 1486, 1585, 1608, 2931 \text{ cm}^{-1}$ . **<sup>1</sup>H NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>)**  $\delta = 1.39$  (s, 6H, 13-H), 1.93 (s, 6H, 12-H), 3.21 (s, 6H, 10-H), 3.56 (s, 3H, 11-H), 5.65 (s, 2H, 9-H), 7.08 (ddd,  $^3J = 7.4 \text{ Hz}$ ,  $^3J = 5.6 \text{ Hz}$ ,  $^4J = 1.6 \text{ Hz}$ , 2H, b-H), 7.32 (td,  $^3J = 7.4 \text{ Hz}$ ,  $^4J = 1.6 \text{ Hz}$ , 2H, c-H), 7.62 (d,  $^3J = 8.4 \text{ Hz}$ , 1H, 8-H), 7.90 (d,  $^3J = 8.4 \text{ Hz}$ , 1H, 3-H), 8.01 (ddd,  $^3J = 5.6 \text{ Hz}$ ,  $^4J = 1.6 \text{ Hz}$ ,  $^5J = 0.8 \text{ Hz}$ , 2H, a-H), 8.04 – 8.18 (m, 7H, d-, e-, f-, 5- & 6-H), 8.49 (d,  $^3J = 8.4 \text{ Hz}$ , 1H, 7-H), 8.62 (d,  $^3J = 8.4 \text{ Hz}$ , 1H, 4-H) ppm. **<sup>13</sup>C NMR (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>)**  $\delta = 19.5, 27.2, 55.4, 55.7, 90.0, 110.0, 112.4, 121.5, 122.9, 124.8, 126.7, 126.7, 127.2, 127.8, 128.5, 129.5, 131.9, 136.5, 136.7, 137.0, 137.3, 137.9, 140.6, 143.8, 143.9, 148.6, 152.7, 152.8, 155.2, 158.6, 158.9, 162.4$ . **ESI-MS:**  $m/z$  (%) 900.1 (100) [**C3**]. **Elemental analysis:** Calculated for  $\text{C}_{46}\text{H}_{40}\text{CuF}_6\text{IN}_5\text{O}_3\text{P} \cdot 0.5\text{CH}_2\text{Cl}_2$ : C, 51.30; H, 3.80; N, 6.43. Found: C, 51.29; H, 3.63; N, 6.35.

**Complex C4 = [Zn(S)<sub>2</sub>]<sup>2+</sup>.**



In an NMR tube, stator **S** (0.706 mg, 0.440  $\mu\text{mol}$ ) was dissolved in 500  $\mu\text{L}$  of  $\text{CD}_2\text{Cl}_2$ , then  $\text{Zn}(\text{OTf})_2$  (80.0  $\mu\text{g}$ , 0.220  $\mu\text{mol}$ ) was added as a standard solution in  $\text{CD}_3\text{OD}$ . After 5 min of sonication, quantitative formation of complex **C4** was observed in ESI-MS and  $^1\text{H}$  NMR. **IR (KBr):**  $\bar{\nu} = 456, 527, 571, 638, 702, 727, 733, 789, 812, 833, 857, 997, 1015, 1030, 1066, 1213, 1281, 1340, 1392, 1437, 1495, 1528, 1547, 1606, 2219, 2923, 3016 \text{ cm}^{-1}$ .  **$^1\text{H}$  NMR (400 MHz,  $\text{CD}_2\text{Cl}_2:\text{CD}_3\text{OD} = 4:1$ ):**  $\delta = 1.76$  (s, 24H, n-H), 2.59 (s, 6H, i-H), 2.62 (s, 12H, o-H), 6.71 (ddd,  $^3J = 8.0 \text{ Hz}$ ,  $^3J = 5.4 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 4H, b-H), 7.19 (td,  $^3J = 8.0 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 4H, c-H), 7.27 (ddd,  $^3J = 5.4 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ ,  $^5J = 0.8 \text{ Hz}$ , 4H, a-H), 7.30 (s, 8H, m-H), 7.70 (s, 4H, h-H), 7.99 (d,  $^3J = 8.0 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ ,  $^5J = 0.8 \text{ Hz}$ , 4H, d-H), 8.08 (d,  $^3J = 8.6 \text{ Hz}$ , 4H, g/f-H), 8.11 (d,  $^3J = 8.0 \text{ Hz}$ , 8H, k-H), 8.18 (d,  $^3J = 8.6 \text{ Hz}$ , 4H, f/g-H), 8.33 (d,  $^3J = 8.0 \text{ Hz}$ , 8H, l-H), 8.57 (s, 4H, e-H), 8.84 (d,  $^3J = 4.6 \text{ Hz}$ , 8H, p-H), 9.12 (d,  $^3J = 4.6 \text{ Hz}$ , 8H, t-H), 9.27 (d,  $^3J = 4.6 \text{ Hz}$ , 8H, q-H), 9.39 (d,  $^3J = 4.6 \text{ Hz}$ , 8H, s-H), 10.13 (s, 8H, r-H) ppm. **ESI-MS:**  $m/z$  (%) 1637.1 (100) [**C4**]. **Elemental analysis:** Calculated for  $\text{C}_{210}\text{H}_{138}\text{F}_6\text{N}_{22}\text{O}_6\text{S}_2\text{Zn}_5 \cdot \text{CH}_2\text{Cl}_2$ : C, 69.34; H, 3.83; N, 8.43; S, 1.75. Found: C, 69.11; H, 3.65; N, 8.42; S, 1.47.

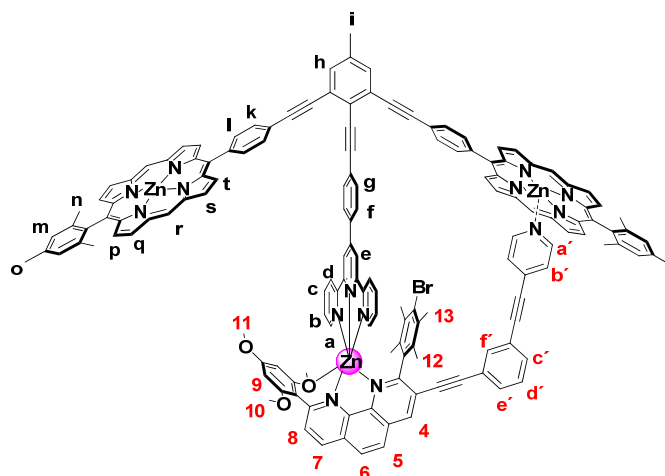
**Complex C5 =  $[\text{Zn}(\text{R})_2]^{2+}$**



In an NMR tube, rotator **R** (0.334 mg, 0.440  $\mu\text{mol}$ ) was dissolved in 500  $\mu\text{L}$  of  $\text{CD}_2\text{Cl}_2$ , then  $\text{Zn}(\text{OTf})_2$  (80.0  $\mu\text{g}$ , 0.220  $\mu\text{mol}$ ) was added as a standard solution in  $\text{CD}_3\text{CN}$ . After 5 min of sonication, exclusive formation (>95%) of complex **C5** was observed in ESI-MS and  $^1\text{H}$  NMR. **IR (KBr):**  $\bar{\nu} = 452, 613, 725, 819, 991, 1021, 1103, 1188, 1214, 1261, 1348, 1403, 1472, 1506, 1591, 1683, 2221, 2360, 2538, 2853, 2922 \text{ cm}^{-1}$ .  **$^1\text{H}$  NMR (400 MHz,  $\text{CD}_2\text{Cl}_2:\text{CH}_3\text{CN} = 4:1$ ):**  $\delta = 0.89$  (s, 6H, 13'-H), 1.62 (s, 6H, 13-H), 2.07 (s, 6H, 12'-H), 2.10 (s, 6H, 12-H), 2.75 (s, 6H, 10'-H), 3.80 (s, 6H, 11-H), 3.82 (s, 6H, 10-H), 5.51 (s, 2H, 9'-H), 6.30 (s, 2H, 9-H), 6.73 (t,  $^3J = 1.2 \text{ Hz}$ , 2H, f'-H), 6.93 (ddd,  $^3J = 7.8 \text{ Hz}$ ,  $^4J = 1.4 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 2H, c'/e'-H), 7.25 (td,  $^3J = 7.8 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 2H, d'-H), 7.39 (d,  $^3J = 6.0 \text{ Hz}$ , 4H, b'-H), 7.47 (ddd,  $^3J = 7.8 \text{ Hz}$ ,  $^4J = 1.4 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 2H, e'/c'-H), 8.17 (d,  $^3J = 8.6 \text{ Hz}$ , 2H, 8-H), 8.21 (d,  $^3J = 8.8 \text{ Hz}$ , 2H, 5/6-H), 8.24 (d,  $^3J = 8.8 \text{ Hz}$ , 2H, 6/5-H), 8.59 (d,  $^3J = 6.0 \text{ Hz}$ , 4H, a'-H), 8.64 (d,  $^3J = 8.6 \text{ Hz}$ , 2H, 7-H),

8.92 (s, 2H, 4-H) ppm. **ESI-MS:**  $m/z$  (%) 760.5 (20) [ $\mathbf{R}+\mathbf{H}^+$ ], 791.3 (100) [ $\mathbf{C5}$ ], 972.1 (20) [ $\mathbf{C5}-\mathbf{R}+\text{OTf}^-$ ]. **Elemental analysis:** Calculated for  $\text{C}_{94}\text{H}_{72}\text{Br}_2\text{F}_6\text{N}_6\text{O}_{12}\text{S}_2\text{Zn}\cdot 2\text{CH}_2\text{Cl}_2\cdot \text{H}_2\text{O}$ : C, 55.73; H, 3.80; N, 4.06; S, 3.10. Found: C, 55.80; H, 3.53; N, 3.86; S, 2.87.

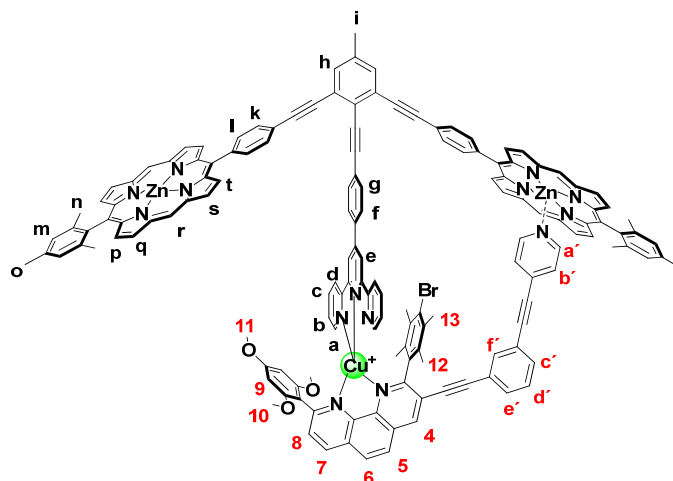
**Synthesis of nanorotor  $\mathbf{C6} = [\text{Zn}(\mathbf{S})(\mathbf{R})]^{2+}$  :**



Both complexes  $\mathbf{C4}$  and  $\mathbf{C5}$  (1:1) were dissolved in 5 mL of  $\text{CH}_3\text{OH} / \text{CH}_2\text{Cl}_2 / \text{CH}_3\text{CN}$  (1:2:1). The nanorotor  $\mathbf{C6}$  was prepared quantitatively after 3 min of mixing at room temperature (concluded from UV/Vis measurement, Figure S71). **Mp:**  $> 250$  °C. **IR (KBr):**  $\bar{\nu} = 413, 517, 571, 638, 702, 720, 733, 786, 812, 832, 851, 991, 1015, 1030, 1056, 1223, 1260, 1340, 1392, 1427, 1475, 1492, 1518, 1547, 1603, 1655, 2209, 2923$   $\text{cm}^{-1}$ .  **$^1\text{H NMR}$  (600 MHz,  $\text{CD}_2\text{Cl}_2$ ):**  $\delta = 0.71$  (s, 6H, 13-H), 1.64 (s, 6H, 12-H), 1.80 (s, 12H, n-H), 2.19 (d,  $^3J = 6.4$  Hz, 2H, a'-H), 2.61 (s, 3H, i-H), 2.66 (s, 6H, o-H), 2.69 (s, 3H, 11-H), 2.72 (s, 6H, 10-H), 5.17 (s, 2H, 9-H), 5.33 (merged with  $\text{CDHCl}_2$ , 2H, b'-H), 5.98 (s, 1H, f'-H), 6.94 (ddd,  $^3J = 7.8$  Hz,  $^4J = 1.4$  Hz,  $^4J = 1.2$  Hz, 1H, e'/c'-H), 7.03 (t,  $^3J = 7.8$  Hz, 1H, d'-H), 7.21 (ddd,  $^3J = 7.8$  Hz,  $^4J = 1.4$  Hz,  $^4J = 1.2$  Hz, 1H, c'/e'-H), 7.34 (s, 4H, m-H), 7.43 (ddd,  $^3J = 7.8$  Hz,  $^3J = 5.2$  Hz,  $^4J = 1.2$  Hz, 2H, b-H), 7.57 (ddd,  $^3J = 5.2$  Hz,  $^4J = 1.2$  Hz,  $^5J = 0.8$  Hz, 2H, a-H), 7.74 (s, 2H, h-H), 7.90 (d,  $^3J = 8.4$  Hz, 1H, 8-H), 8.09 (br, 2H, g/f-H), 8.14-8.17 (m, 6H, k-H + c-H), 8.28 (d,  $^3J = 8.8$  Hz, 1H, 5/6-H), 8.38 (d,  $^3J = 8.8$  Hz, 1H, 6/5-H), 8.39 (d,  $^3J = 8.0$  Hz, 4H, l-H), 8.47 (br, 2H, f/g-H), 8.55 (d,  $^3J = 8.0$  Hz,  $^4J = 1.2$  Hz,  $^5J = 0.8$  Hz, 2H, d-H), 8.83 (s, 1H, 4-H), 8.86 (d,  $^3J = 8.4$  Hz, 1H, 7-H), 8.91 (d,  $^3J = 4.4$  Hz, 4H, p-H), 8.97 (s, 2H, e-H), 9.18 (d,  $^3J = 4.4$  Hz, 4H, t-H), 9.37 (d,  $^3J = 4.4$  Hz, 4H, q-H), 9.45 (d,  $^3J = 4.4$  Hz, 4H, s-H), 10.25 (s, 4H, r-H) ppm. **ESI-MS:**  $m/z$  (%) 1213.2

(100)  $[[\text{Zn}(\text{S})(\text{R})]^{2+}]$ . **Elemental analysis:** Calculated for  $\text{C}_{152}\text{H}_{105}\text{BrF}_6\text{N}_{14}\text{O}_9\text{S}_2\text{Zn}_3 \cdot \text{CH}_2\text{Cl}_2 \cdot \text{H}_2\text{O}$ : C, 64.96; H, 3.88; N, 6.93; S, 2.27. Found: C, 65.29; H, 3.86; N, 6.59; S, 2.34.

**Synthesis of nanorotor  $\text{C7} = [\text{Cu}(\text{S})(\text{R})]^+$  :**



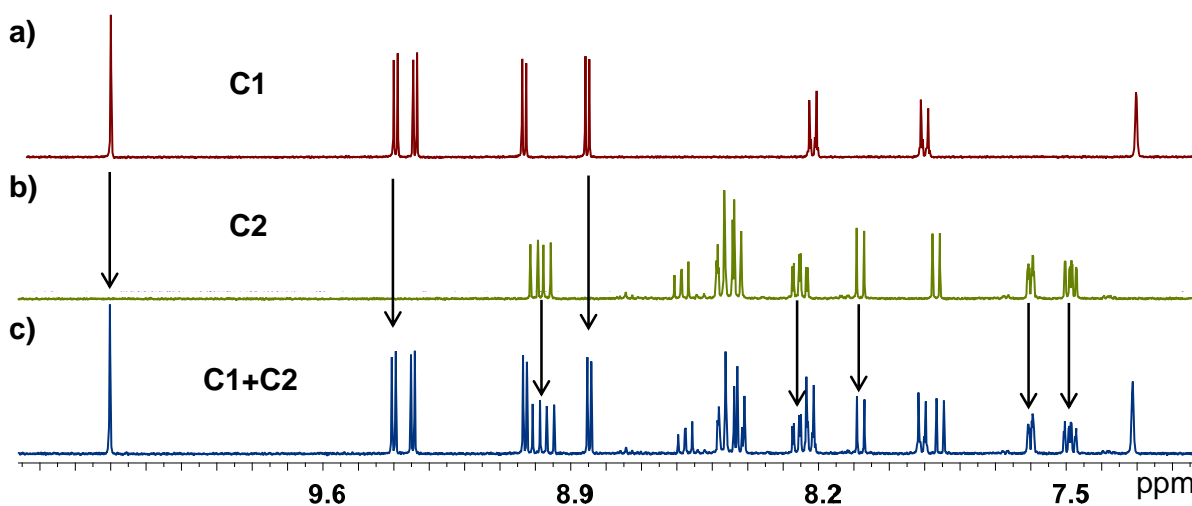
Complex **C6** was mixed with the separately prepared chelate complex,  $[\text{Cu}(\text{hexacyclen})]\text{PF}_6$  (0.88  $\mu\text{mol}$ ). The resulting solution was heated at 50  $^\circ\text{C}$  for 2 h. NMR and ESI-MS spectra confirm the quantitative formation of nanorotor  $[\text{Cu}(\text{S})(\text{R})]\text{PF}_6$ . **IR (KBr):**  $\tilde{\nu} = 417, 478, 523, 758, 663, 704, 726, 736, 787, 815, 832, 856, 996, 1024, 1037, 1066, 1158, 1236, 1346, 1389, 1435, 1486, 1506, 1536, 1605, 1684, 2216, 2936, 3012 \text{ cm}^{-1}$ .  **$^1\text{H}$  NMR (600 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta$  =** 1.10 (s, 6H, 13-H), 1.57 (s, 6H, 12-H), 1.80 (s, 12H, n-H), 2.18 (d,  $^3J = 6.6 \text{ Hz}$ , 2H, a'-H), 2.60 (s, 3H, i-H), 2.66 (s, 6H, o-H), 2.89 (s, 6H, 10-H), 2.93 (s, 3H, 11-H), 5.23 (s, 2H, 9-H), 5.39 (d,  $^3J = 6.6 \text{ Hz}$ , 2H, b'-H), 6.04 (t,  $^4J = 1.2 \text{ Hz}$ , 1H, f'-H), 6.95 (ddd,  $^3J = 7.8 \text{ Hz}$ ,  $^4J = 1.4 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 1H, e'/c'-H), 6.98 (ddd,  $^3J = 7.8$ ,  $^3J = 4.8 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 2H, b-H), 7.00 (td,  $^3J = 7.8 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 1H, d'-H), 7.17 (ddd,  $^3J = 7.8 \text{ Hz}$ ,  $^4J = 1.4 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 1H, c'/e'-H), 7.22 (td,  $^3J = 7.8 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ , 4H, c-H), 7.34 (s, 4H, m-H), 7.73 (s, 2H, h-H), 7.73 (d,  $^3J = 8.8 \text{ Hz}$ , 1H, 8-H), 7.90 (ddd,  $^3J = 4.8 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ ,  $^5J = 0.8 \text{ Hz}$ , 2H, a-H), 7.95 (d,  $^3J = 8.8 \text{ Hz}$ , 1H, 5/6-H), 7.97 (ddd,  $^3J = 7.8 \text{ Hz}$ ,  $^4J = 1.2 \text{ Hz}$ ,  $^5J = 0.8 \text{ Hz}$ , 2H, d-H), 8.01 (d,  $^3J = 8.0 \text{ Hz}$ , 2H, g/f-H), 8.08 (d,  $^3J = 8.8 \text{ Hz}$ , 1H, 6/5-H), 8.15 (d,  $^3J = 8.0 \text{ Hz}$ , 2H, k-H), 8.17 (d,  $^3J = 8.0 \text{ Hz}$ , 2H, f/g-H), 8.26 (s, 2H, e-H), 8.37 (d,  $^3J = 8.0 \text{ Hz}$ , 2H, l-H), 8.46 (s, 1H, 4-H), 8.51 (d,  $^3J = 8.8 \text{ Hz}$ , 1H, 7-H), 8.91 (d,  $^3J = 4.4 \text{ Hz}$ , 4H, p-H), 9.17 (d,  $^3J = 4.4 \text{ Hz}$ , 4H, t-H), 9.37 (d,  $^3J = 4.4 \text{ Hz}$ , 4H, q-H), 9.45 (d,  $^3J = 4.4 \text{ Hz}$ , 4H, s-H), 10.23 (s, 4H, r-H) ppm. **ESI-MS:**  $m/z$  (%) 2473.6 (100)

[Cu(S)(R)(CH<sub>3</sub>OH)(H<sub>2</sub>O)]<sup>+</sup>; **Elemental analysis:** Calculated for C<sub>150</sub>H<sub>105</sub>BrCuF<sub>6</sub>N<sub>14</sub>O<sub>3</sub>PZn<sub>2</sub>•4CH<sub>3</sub>OH: C, 68.53; H, 4.52; N, 7.27. Found: C, 68.28; H, 4.24; N, 6.91.

### 3. Model Study:

#### Model Study 1.

An equimolar (0.77 μmol) mixture of ligands **1**, **2**, **3**, **4** and Zn(OTf)<sub>2</sub> (1:1:1:1:1) was refluxed at 50 °C in 500 μL of CD<sub>2</sub>Cl<sub>2</sub>:CD<sub>3</sub>CN = 10:1 for 3 h. The <sup>1</sup>H NMR spectrum was compared with those of the individual complexes.

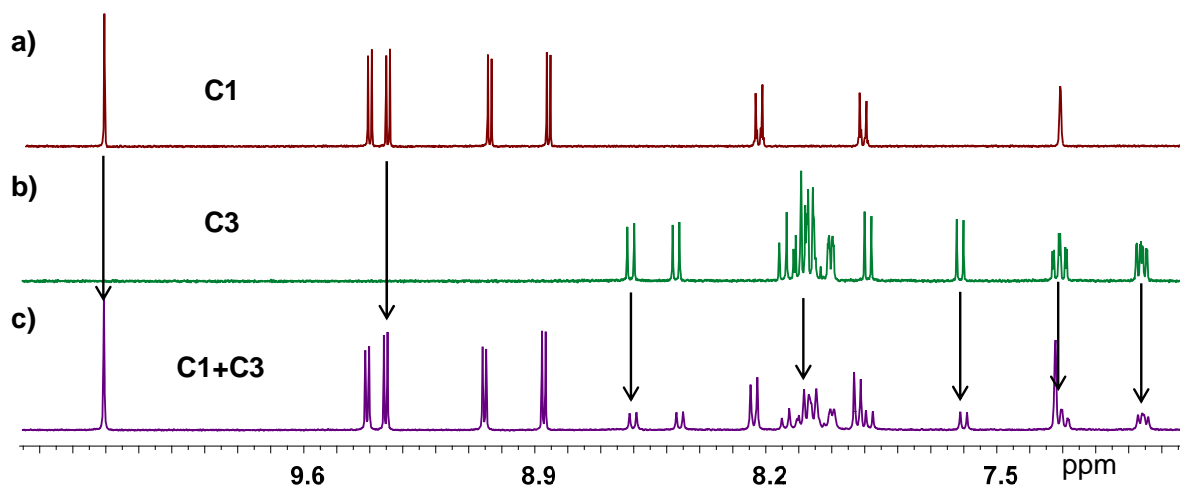


**Figure S1.** <sup>1</sup>H NMR (400 MHz, 298 K) Comparison of (C1 + C2) with individually prepared C1 and C2 in CD<sub>2</sub>Cl<sub>2</sub>:CD<sub>3</sub>CN = 10:1. Complexes C1 + C2 in a mixture (c) showed exactly the superposition of the two individual spectra indicating orthogonality among C1 (a) and C2 (b).

#### Model Study 2.

In an NMR tube ligands **1**, **2**, **3**, **4** and [Cu(CH<sub>3</sub>CN)]PF<sub>6</sub> (each 0.77 μmol) were placed and dissolved in 500 μL of CD<sub>2</sub>Cl<sub>2</sub>. The <sup>1</sup>H NMR spectrum was compared with those of the individual complexes.

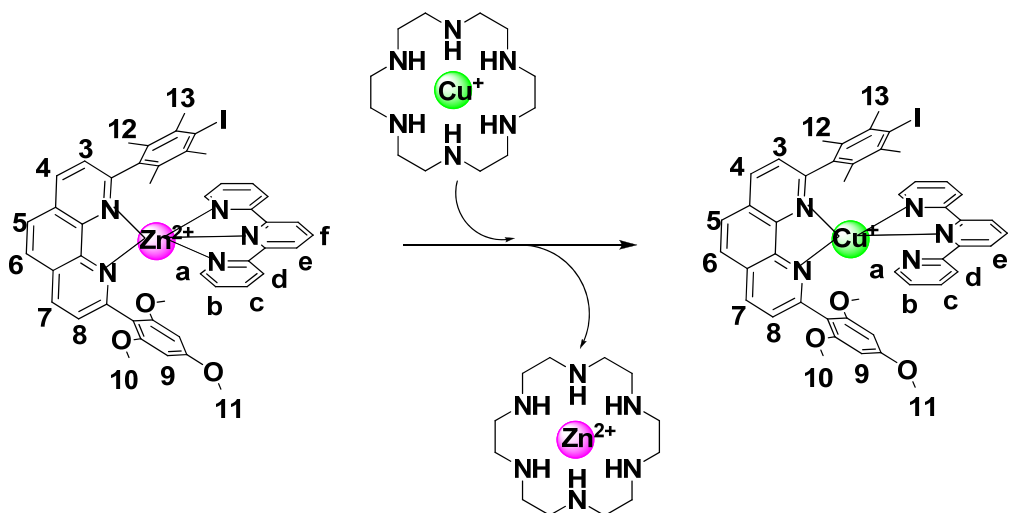


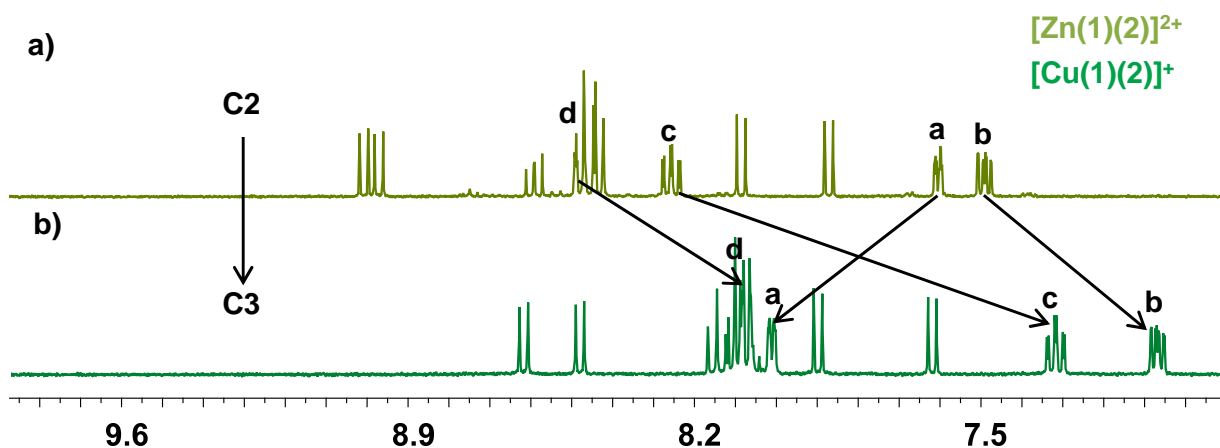


**Figure S2.**  $^1\text{H}$  NMR (400 MHz, 298 K) Comparison of (**C1** + **C3**) with individually prepared **C1** and **C3** in  $\text{CD}_2\text{Cl}_2\text{:CD}_3\text{CN} = 10:1$ . Complexes **C1** + **C3** in a mixture (**c**) showed exactly the superposition of the two individual spectra indicating orthogonality among **C1** (**a**) and **C3** (**b**).

### Model Study 3.

An equimolar amount ( $0.77\ \mu\text{mol}$ ) of  $[\text{Cu}(\text{hexacyclen})]\text{PF}_6$  was added to **C2** at room temperature. Immediately the color of the solution changed from yellow to deep brown.  $^1\text{H}$  NMR and ESI-MS investigations (Fig. S45) confirm complete metal exchange process.

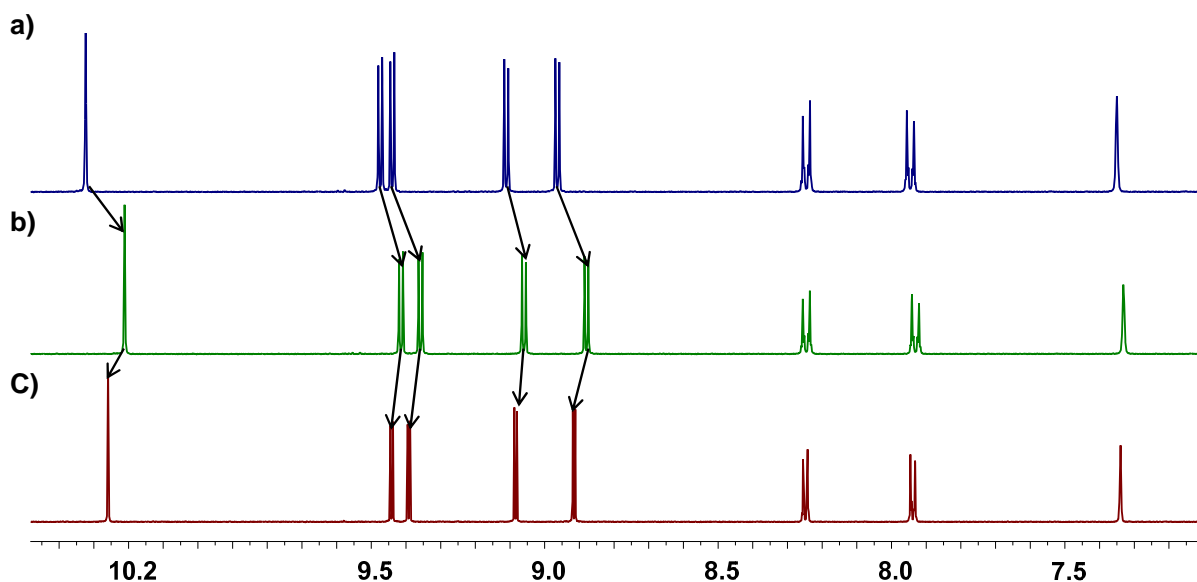




**Figure S3.** Comparison of partial  $^1\text{H}$  NMR after metal-metal exchange by  $[\text{Cu}(\text{hexacyclen})]\text{PF}_6$  in  $\text{CD}_2\text{Cl}_2:\text{CH}_3\text{CN} = 4:1$  (400 MHz, 298 K).

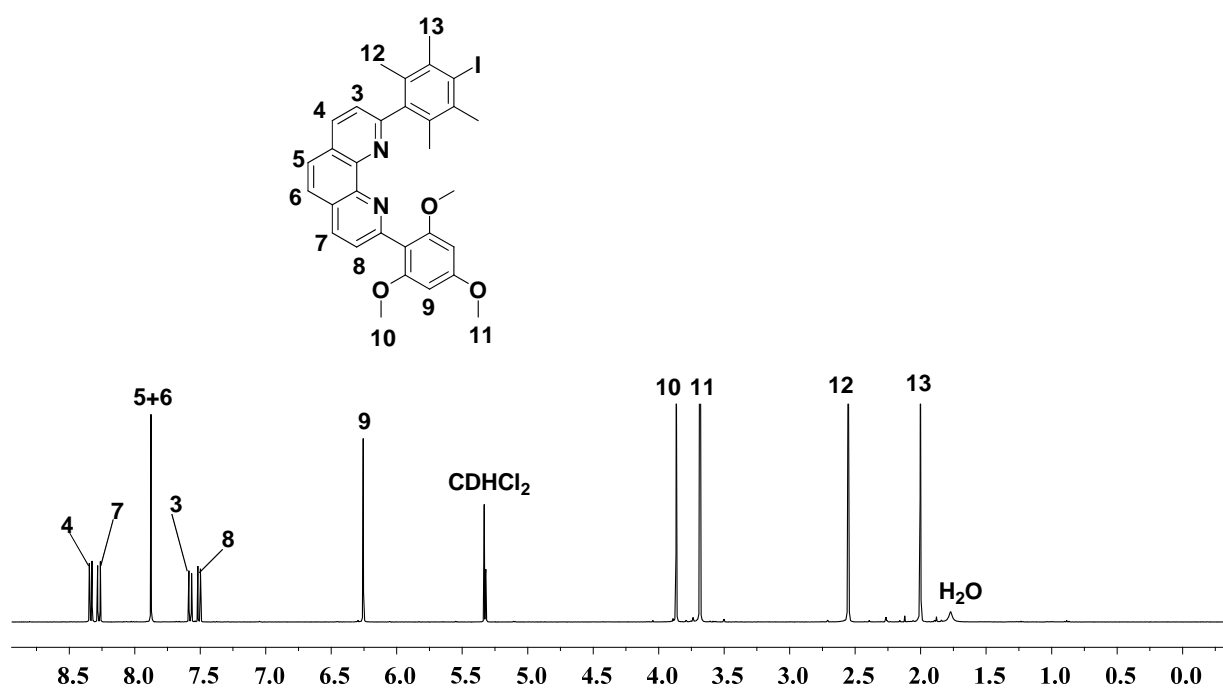
#### Model Study 4

Upon addition of 1 equivalent of **3** to **4** (both 0.77  $\mu\text{mol}$ ) a characteristic  $^1\text{H}$  NMR shift occurred from 10.32 to 10.21 ppm due to the  $\text{N}_{\text{py}} \rightarrow \text{ZnPor}$  interaction in **3•4**. Upon mixing of **3** (0.77  $\mu\text{mol}$ ) and **4** in (1:2) ratio the *meso*-proton signal shifted to 10.25 ppm suggesting fast exchange of 4-iodopyridine between different zinc porphyrins **4**.

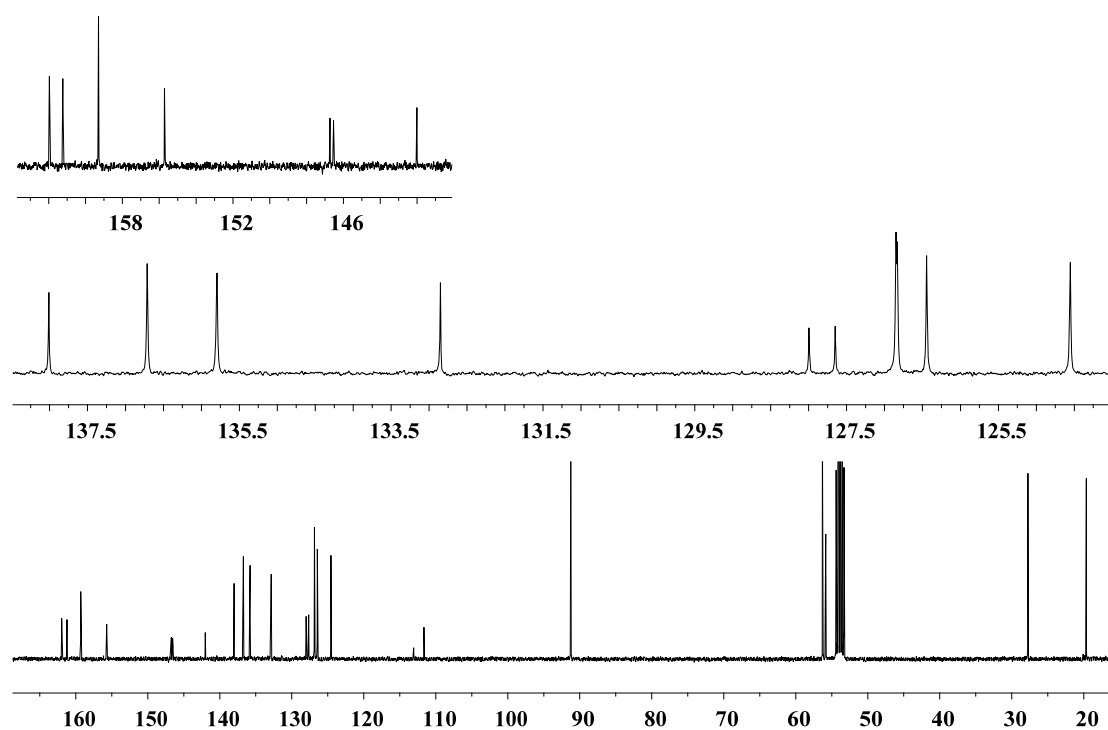


**Figure S4.** Comparison of partial  $^1\text{H}$  NMR (400 MHz, 298 K,  $\text{CD}_2\text{Cl}_2$ ) of (a) **4**, (b) **3•4**, and (c) **3** : **4** = 1:2.

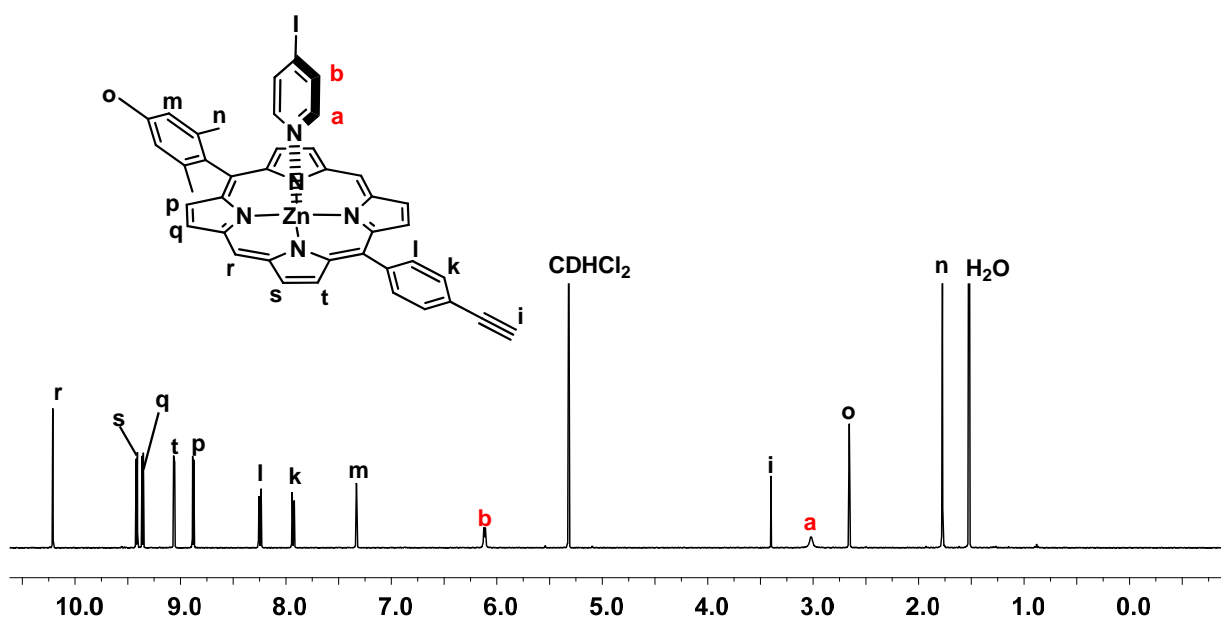
#### 4. NMR Spectra: $^1\text{H}$ , $^{13}\text{C}$ , $^1\text{H}$ - $^1\text{H}$ COSY, $^1\text{H}$ - $^1\text{H}$ NOESY



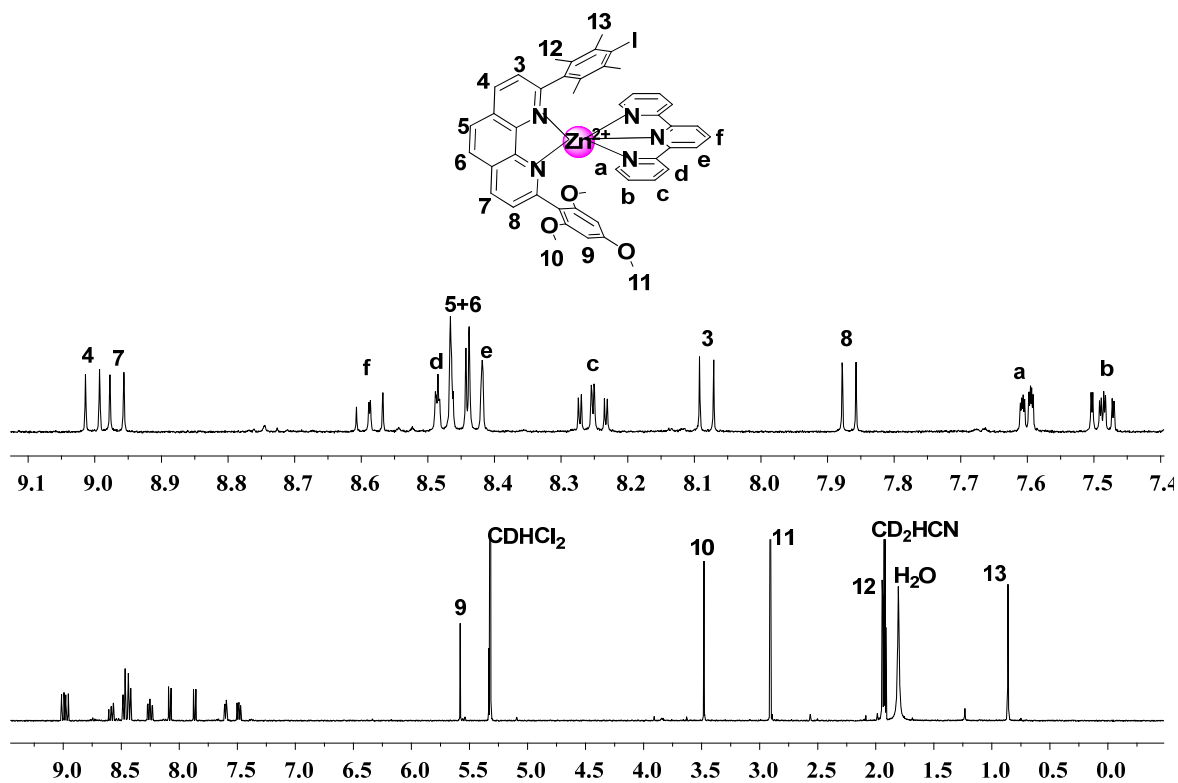
**Figure S5.**  $^1\text{H}$  NMR spectrum of **2** in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



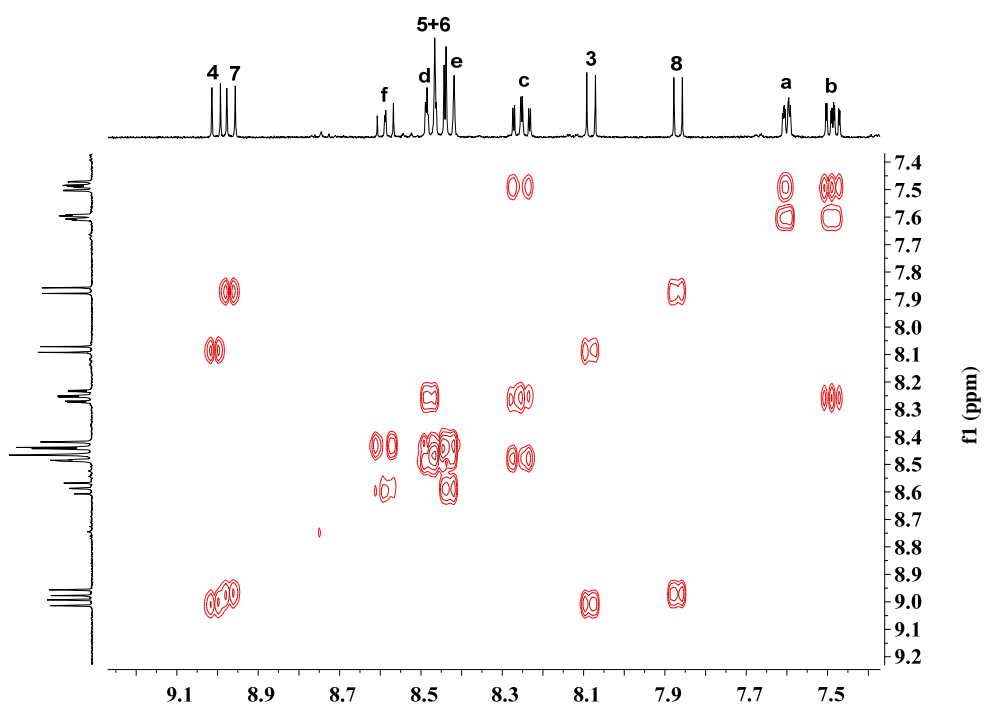
**Figure S6.**  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{CD}_2\text{Cl}_2$  (100 MHz, 298 K).



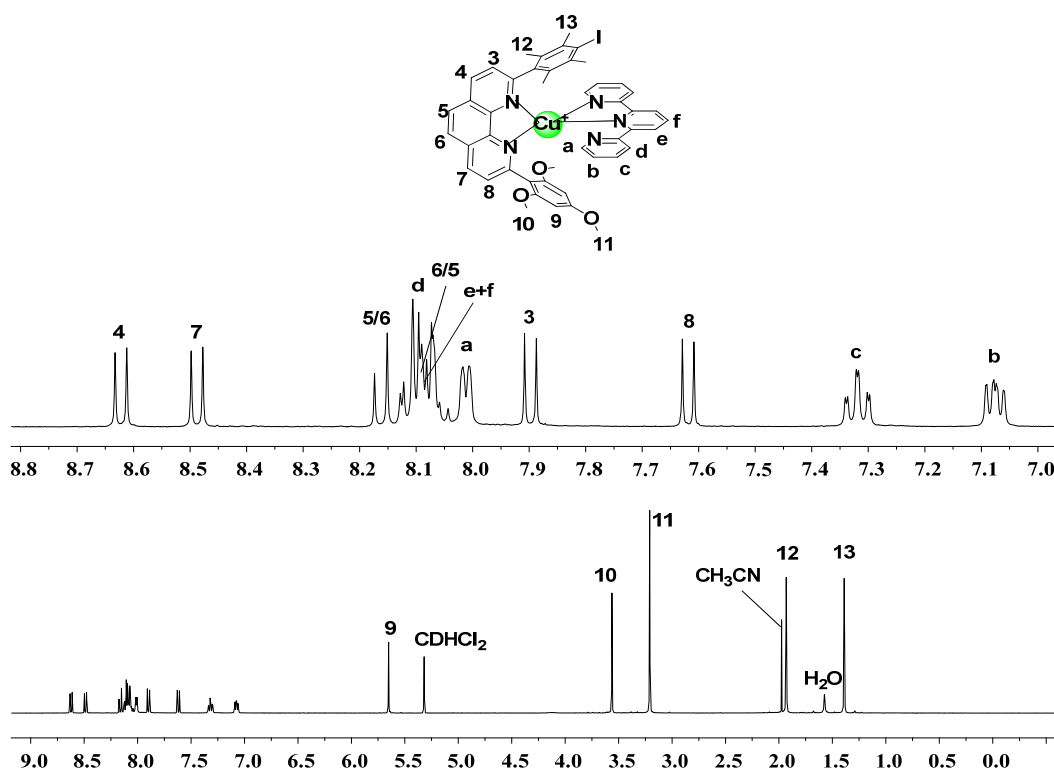
**Figure S7.**  $^1\text{H}$  NMR spectrum of C1 (**3•4**) in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



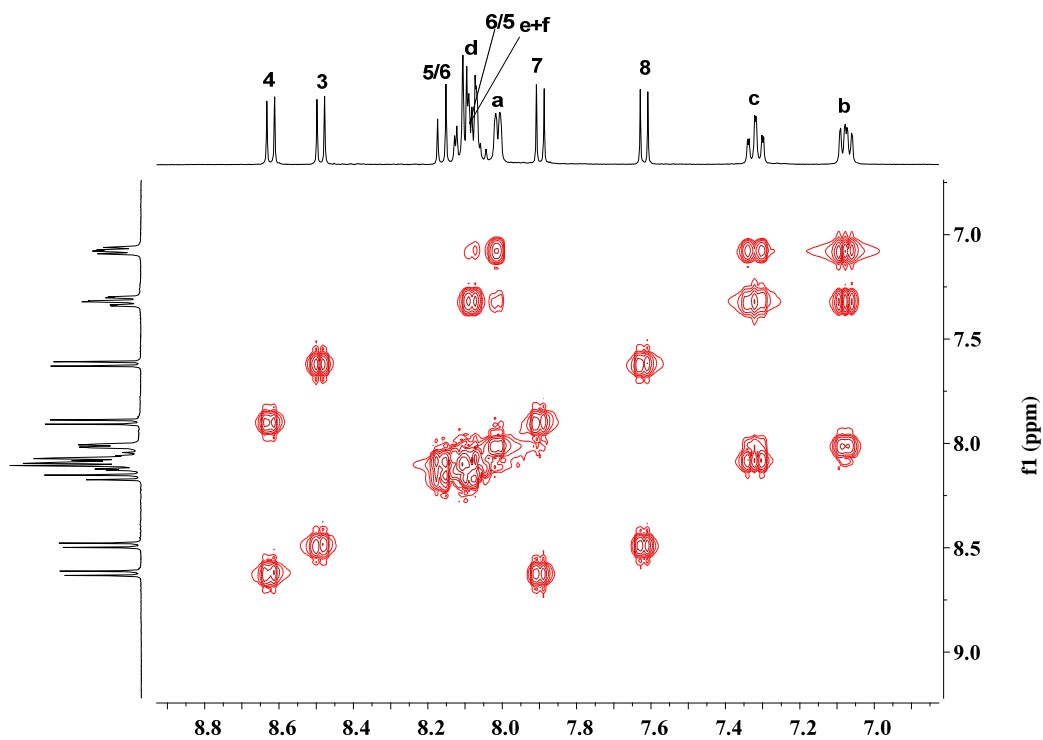
**Figure S8.**  $^1\text{H}$  NMR spectrum of C2 in  $\text{CD}_2\text{Cl}_2:\text{CD}_3\text{CN}$  (9:1) (400 MHz, 298 K). Corresponding homoleptic complexes are present in minor amounts (<5 %).



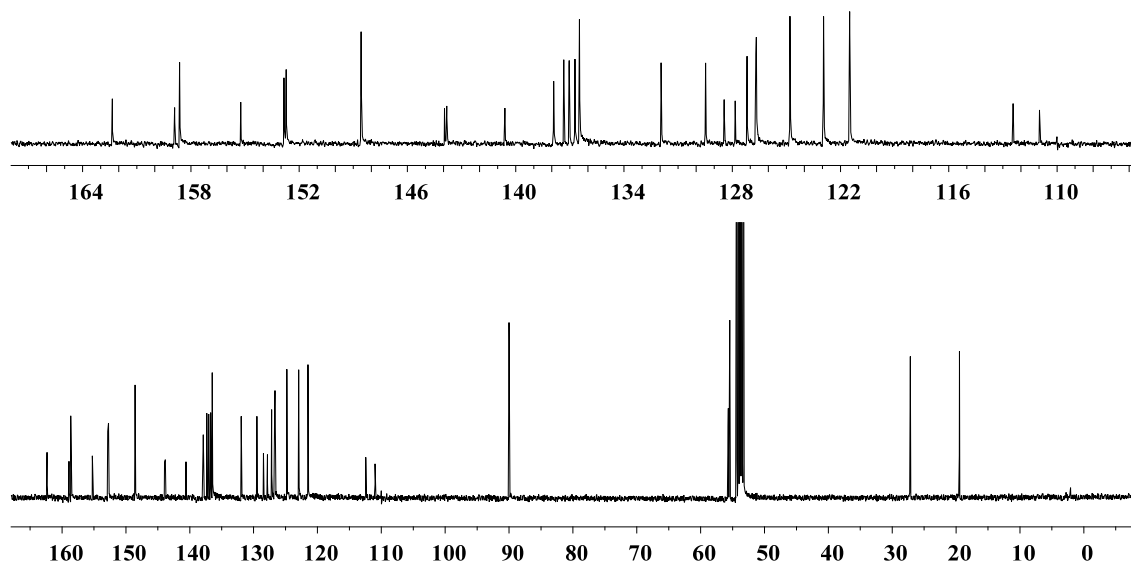
**Figure S9.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **C2** in  $\text{CD}_2\text{Cl}_2:\text{CD}_3\text{CN}$  (9:1) (400 MHz, 298 K).



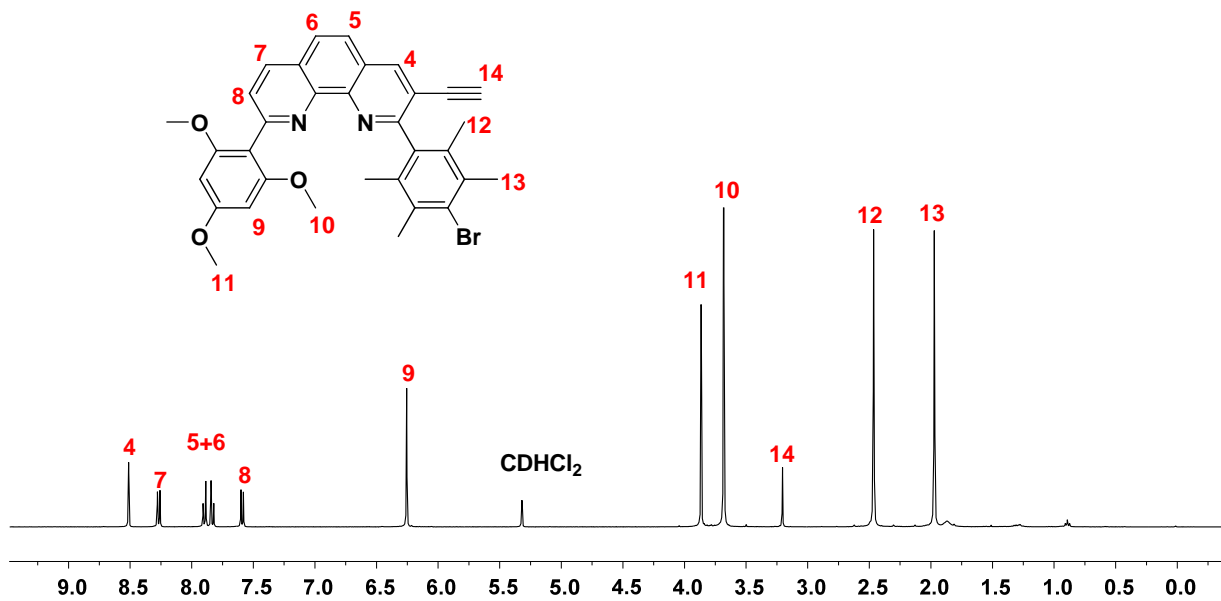
**Figure S10.**  $^1\text{H}$  NMR spectrum of **C3** in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



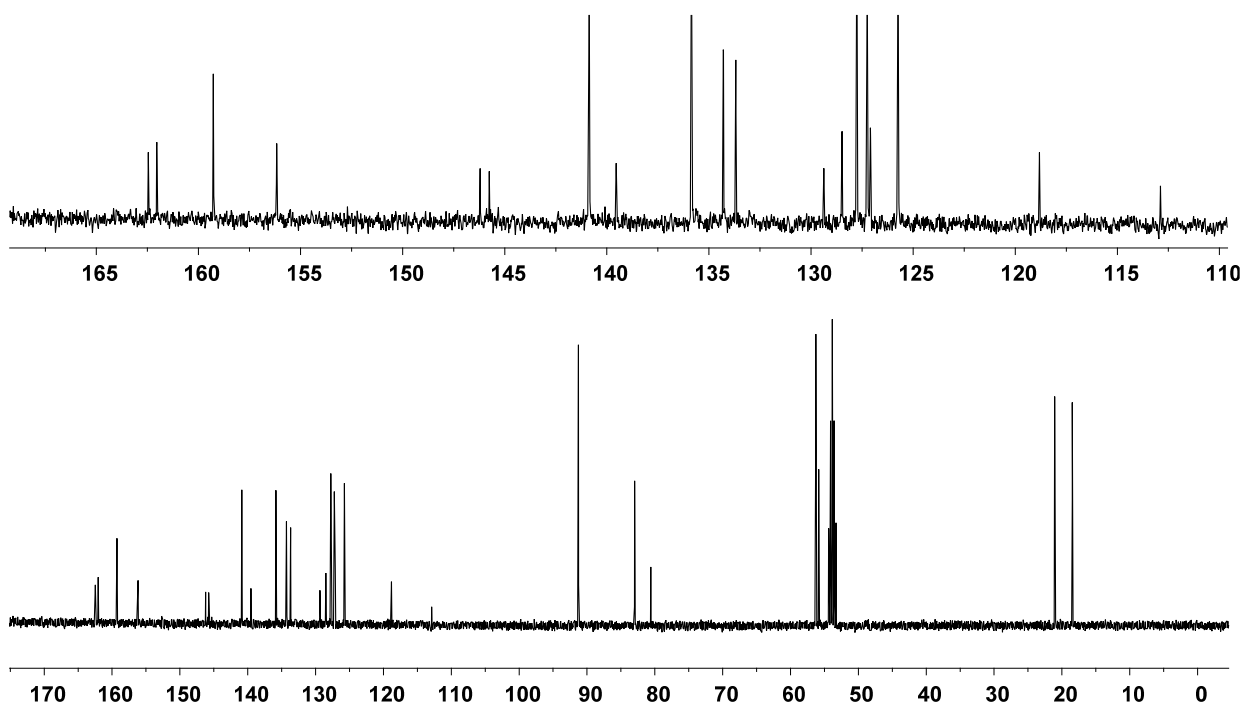
**Figure S11.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of C3 in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



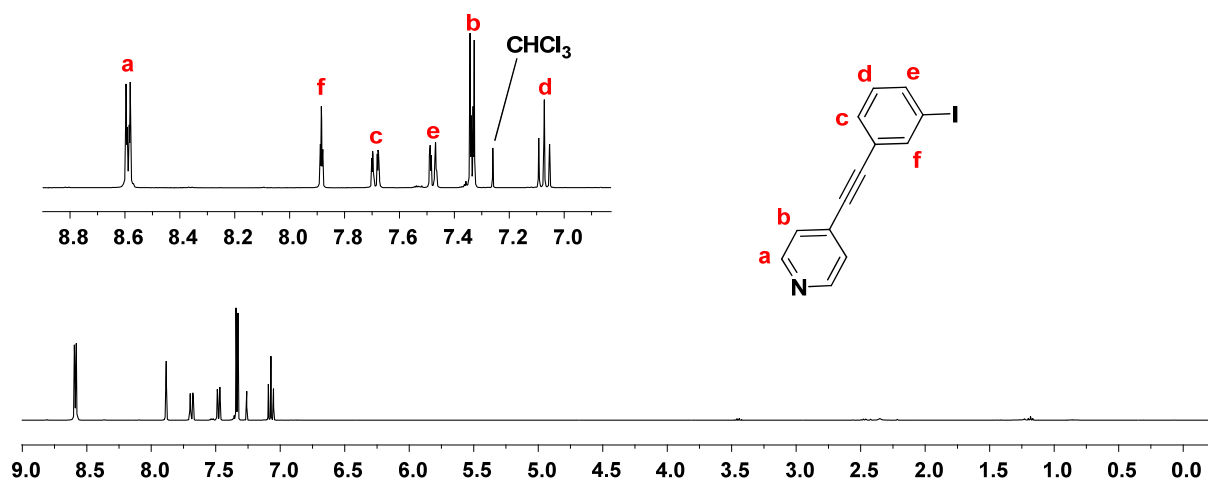
**Figure S12.**  $^{13}\text{C}$  NMR spectrum of C3 in  $\text{CD}_2\text{Cl}_2$  (100 MHz, 298 K).



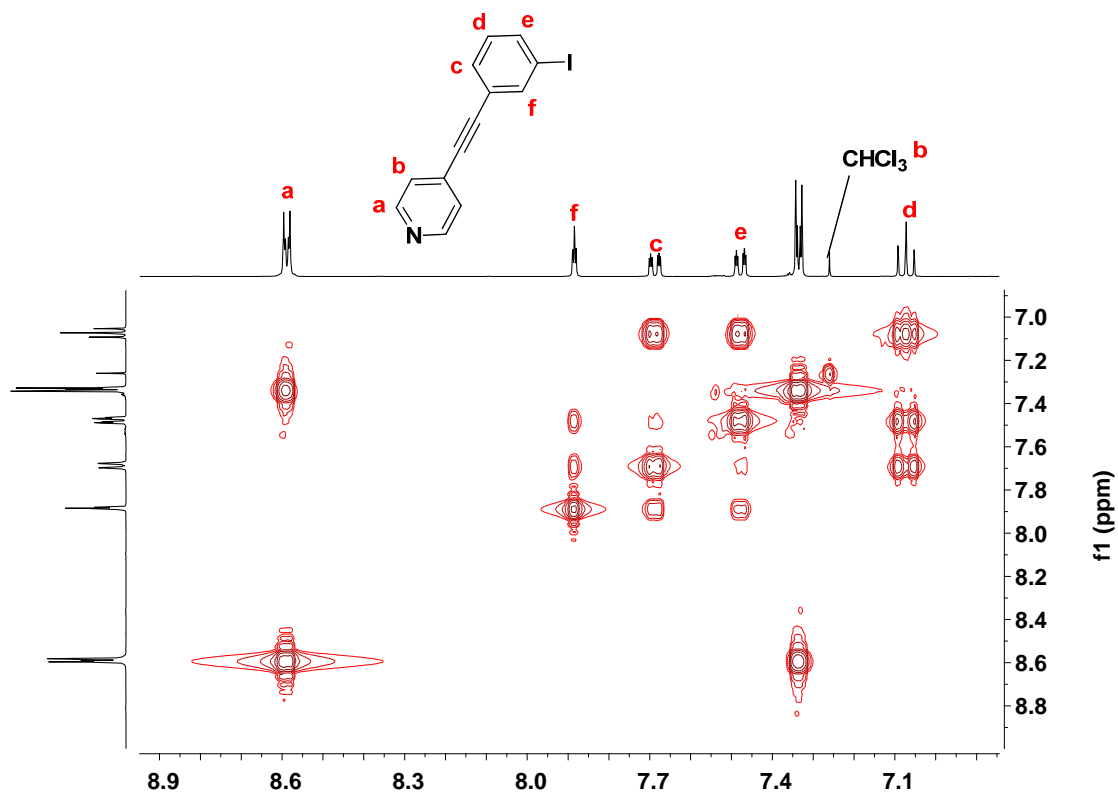
**Figure S13.**  $^1\text{H}$  NMR spectrum of **15** in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



**Figure S14.**  $^{13}\text{C}$  NMR spectrum of **15** in  $\text{CD}_2\text{Cl}_2$  (100 MHz, 298 K).

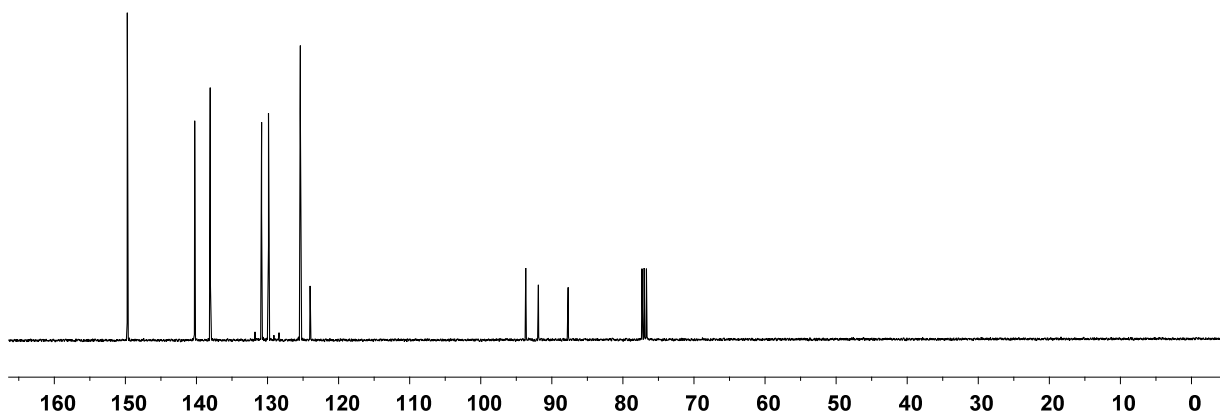


**Figure 15.**  $^1\text{H}$  NMR spectrum of **14** in  $\text{CDCl}_3$  (400 MHz, 298 K).

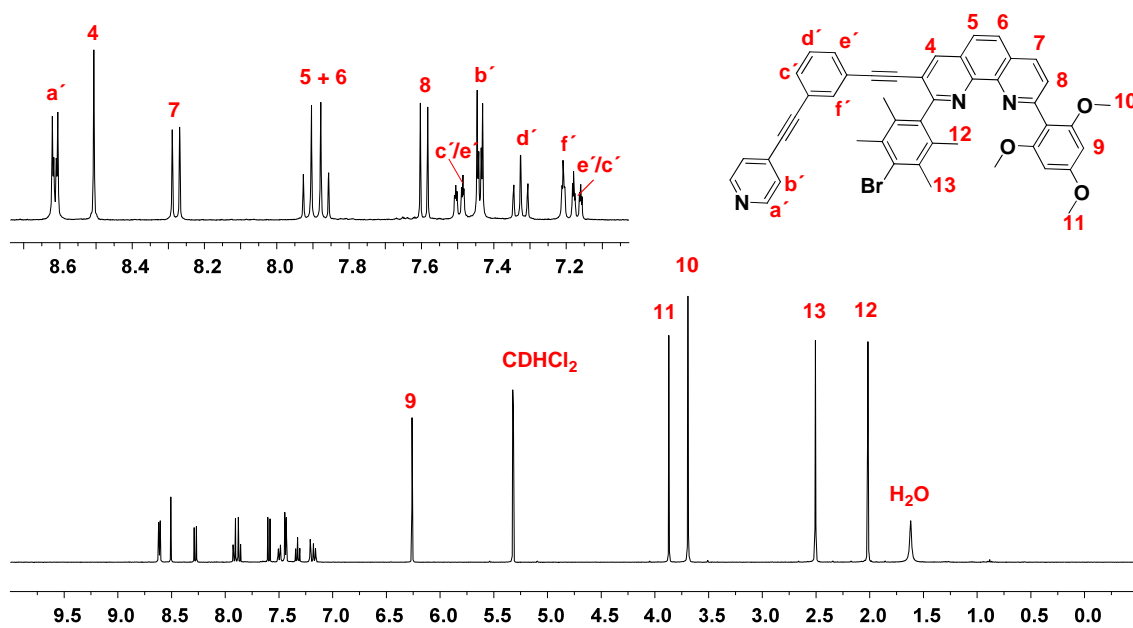


**Figure 16.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **14** in  $\text{CDCl}_3$  (400 MHz, 298 K).

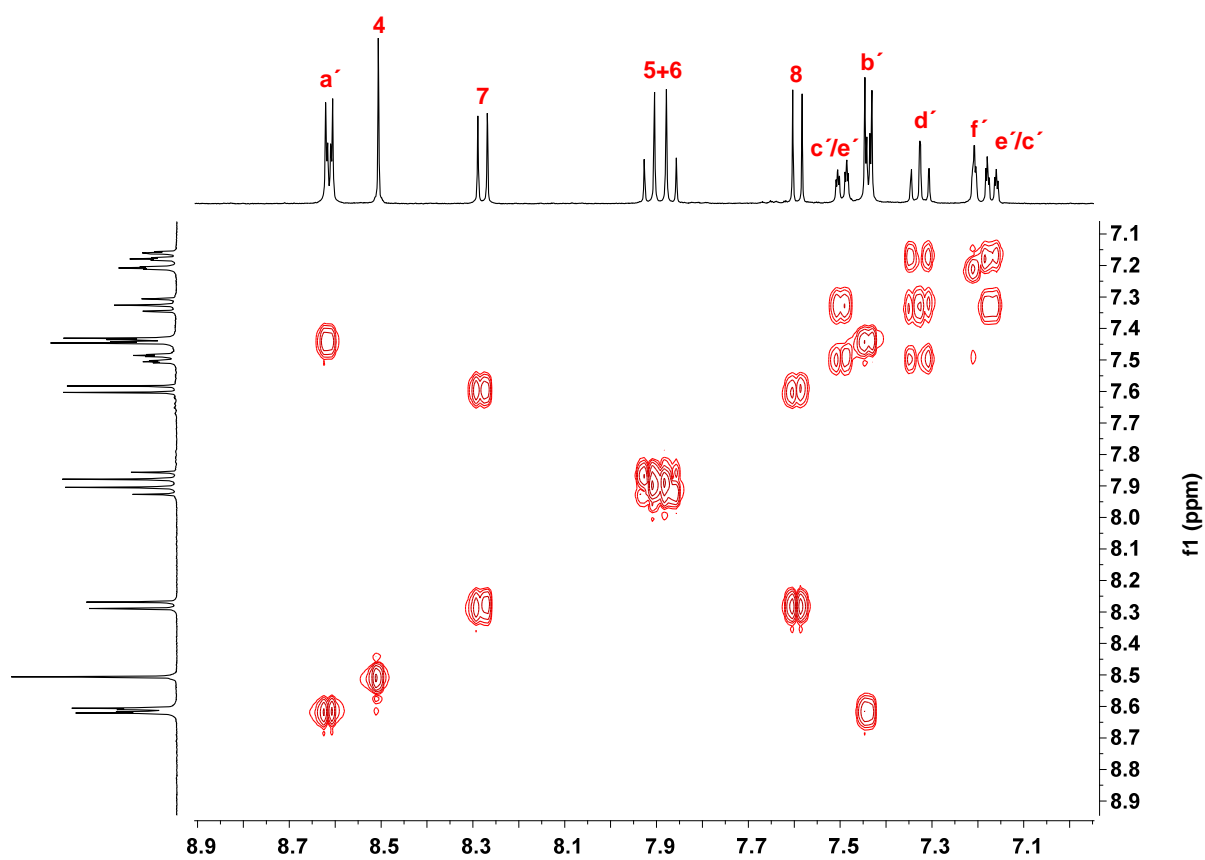




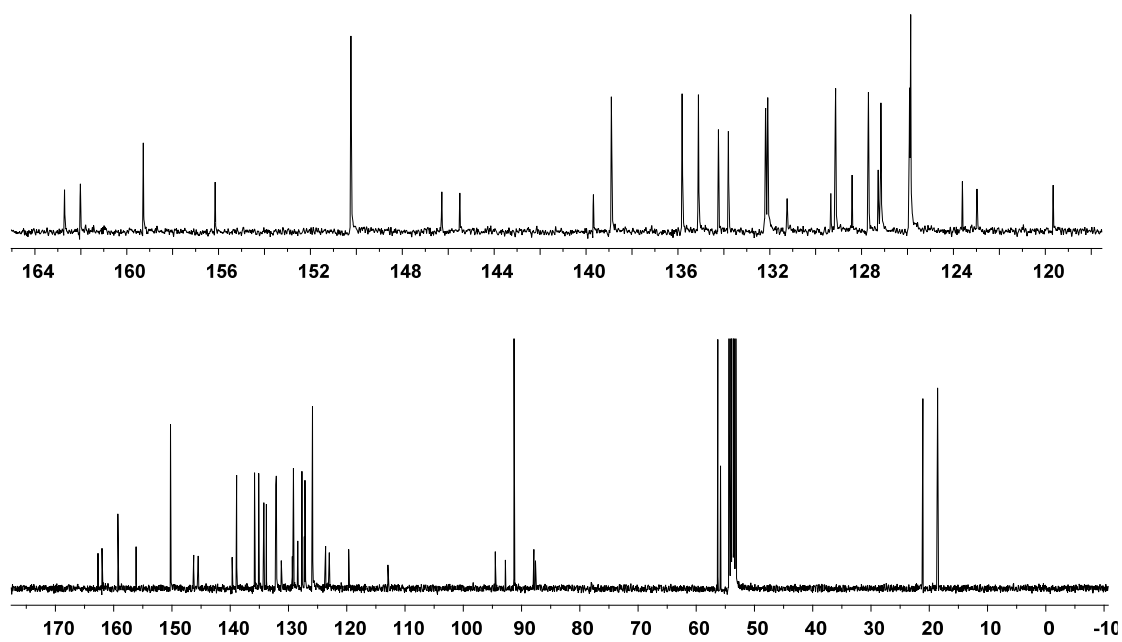
**Figure 17.**  $^{13}\text{C}$  NMR spectrum of **14** in  $\text{CDCl}_3$  (100 MHz, 298 K).



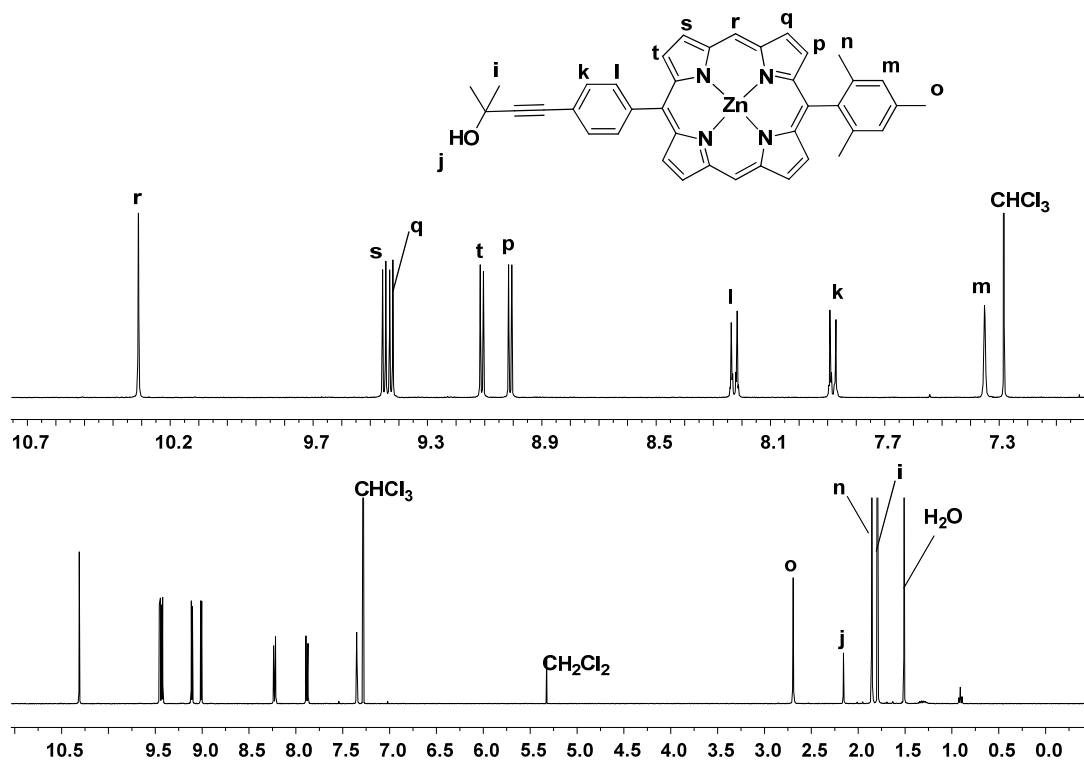
**Figure S18.**  $^1\text{H}$  NMR spectrum of **R** in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



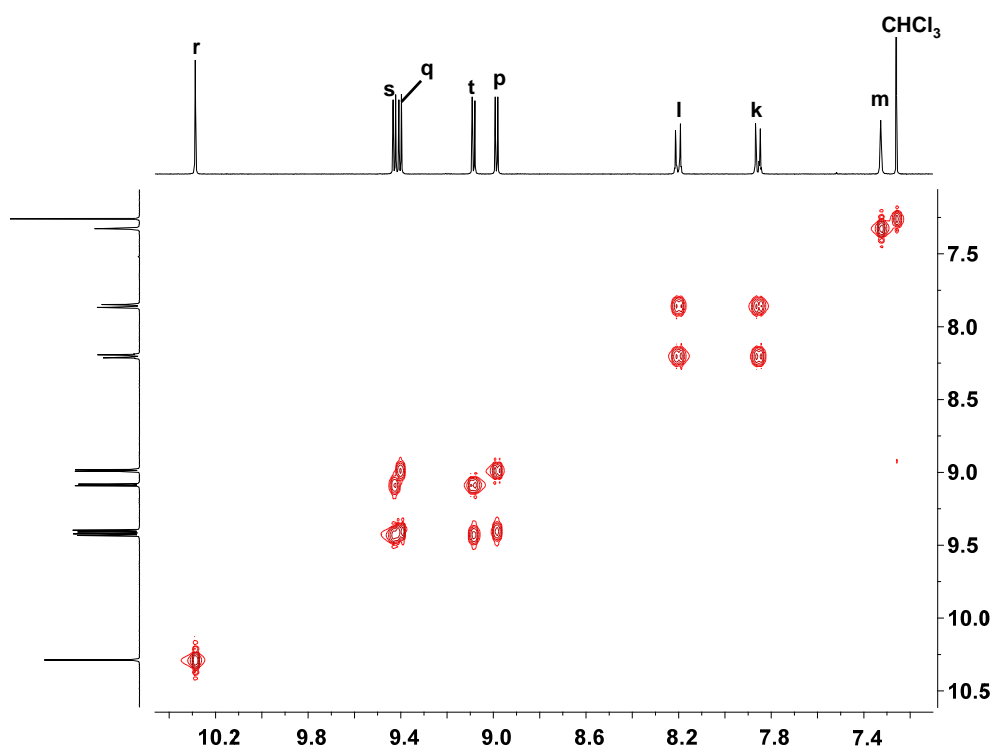
**Figure S19.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **R** in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



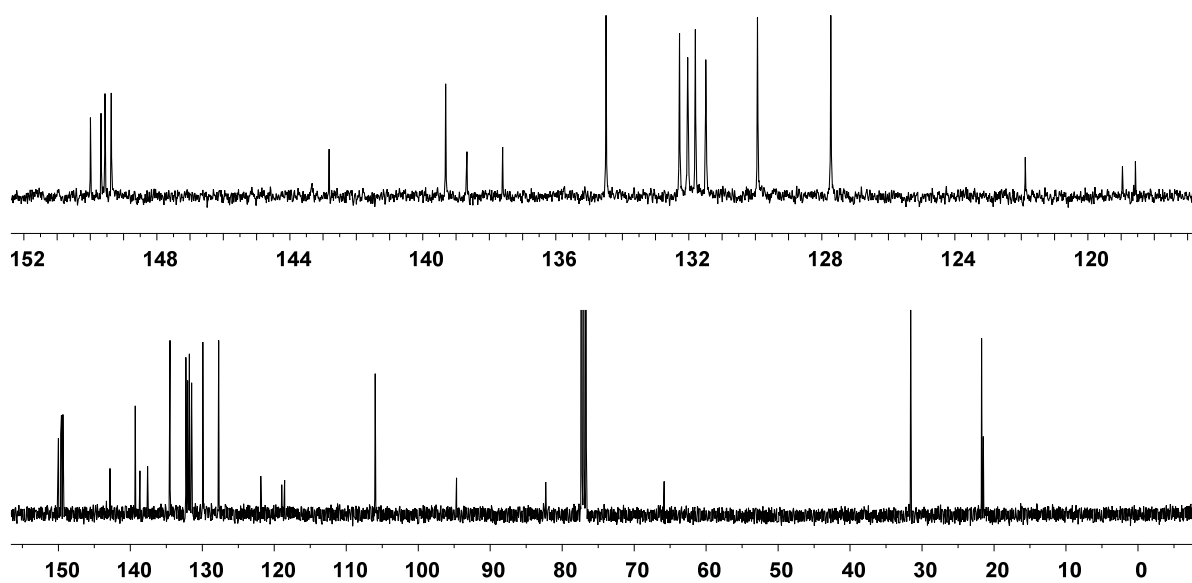
**Figure S20.**  $^{13}\text{C}$  NMR spectrum of **R** in  $\text{CD}_2\text{Cl}_2$  (100 MHz, 298 K).



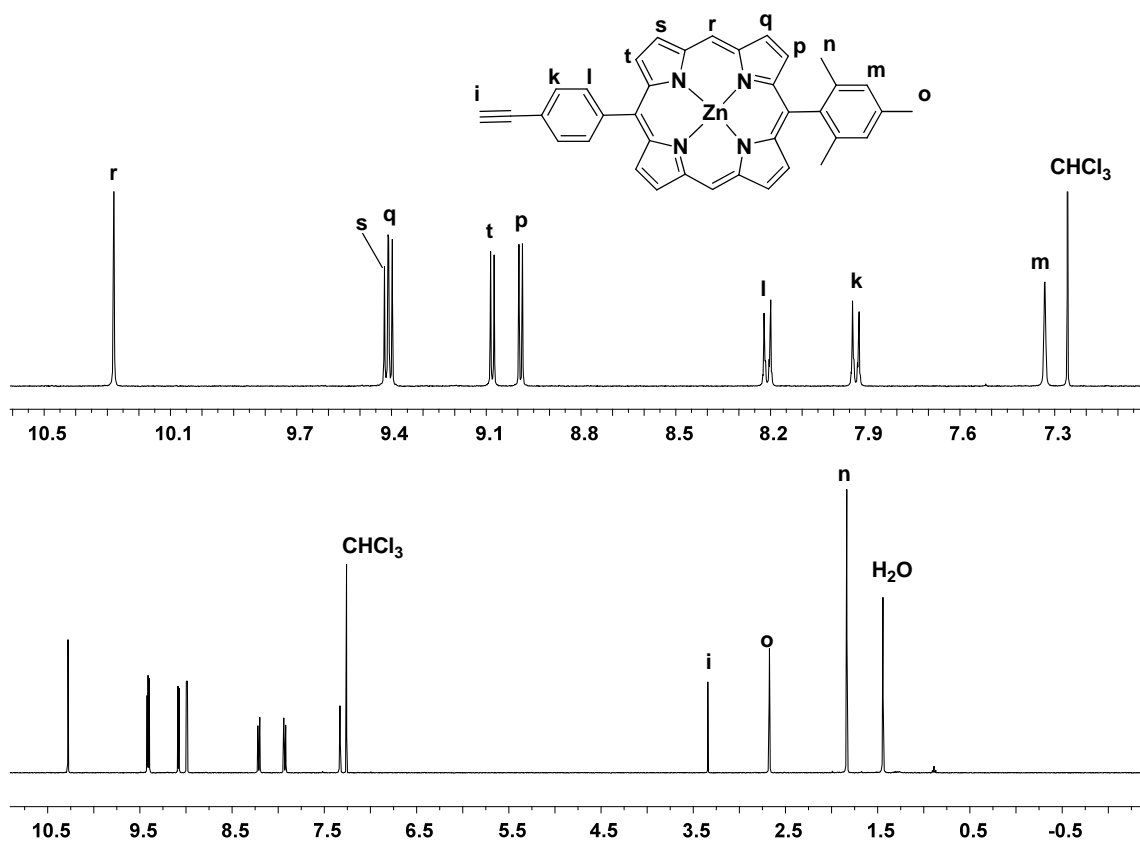
**Figure S21.**  $^1\text{H}$  NMR spectrum of **8** in  $\text{CDCl}_3$  (400 MHz, 298 K).



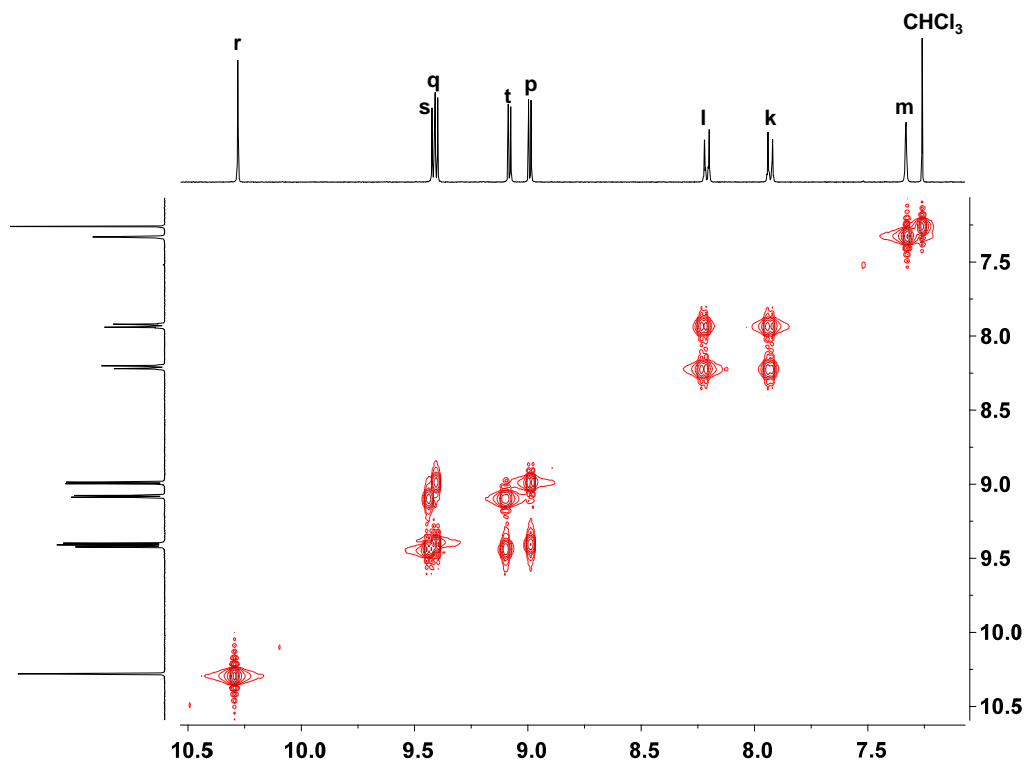
**Figure S22.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **8** in  $\text{CDCl}_3$  (400 MHz, 298 K).



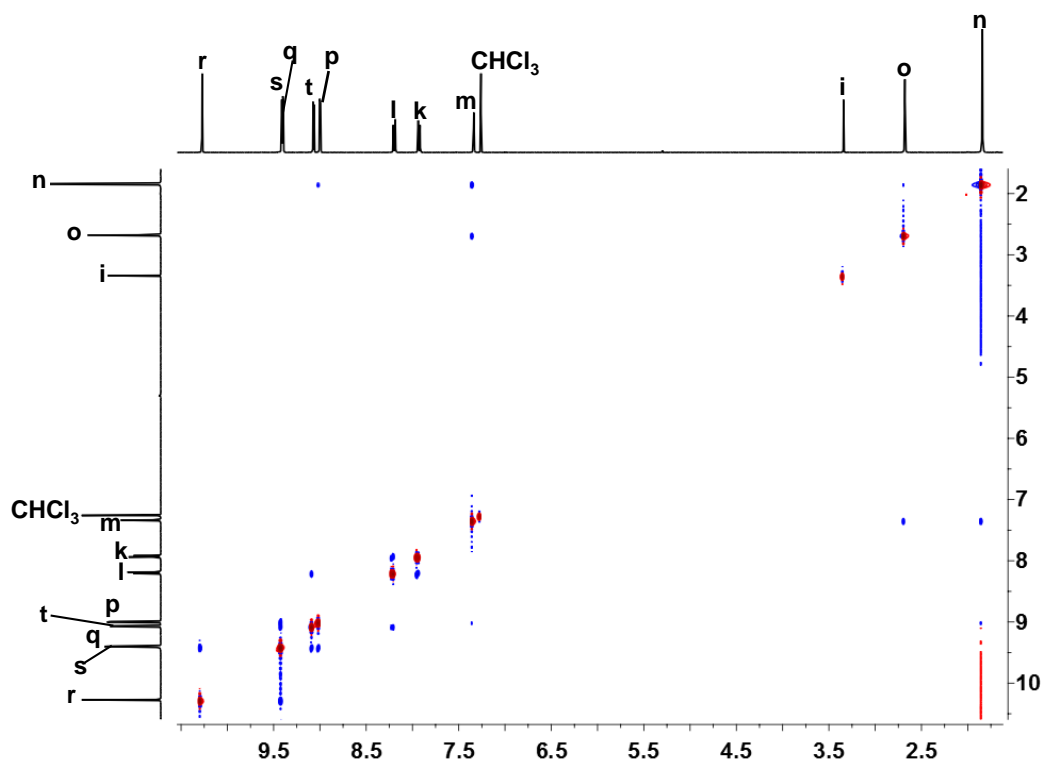
**Figure S23.**  $^{13}\text{C}$  NMR spectrum of **8** in  $\text{CDCl}_3$  (100 MHz, 298 K).



**Figure S24.**  $^1\text{H}$  NMR spectrum of **4** in  $\text{CDCl}_3$  (400 MHz, 298 K).



**Figure S25.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4** in  $\text{CDCl}_3$  (400 MHz, 298 K).



**Figure S26.**  $^1\text{H}$ - $^1\text{H}$  NOESY spectrum of **4** in  $\text{CDCl}_3$  (400 MHz, 298 K).

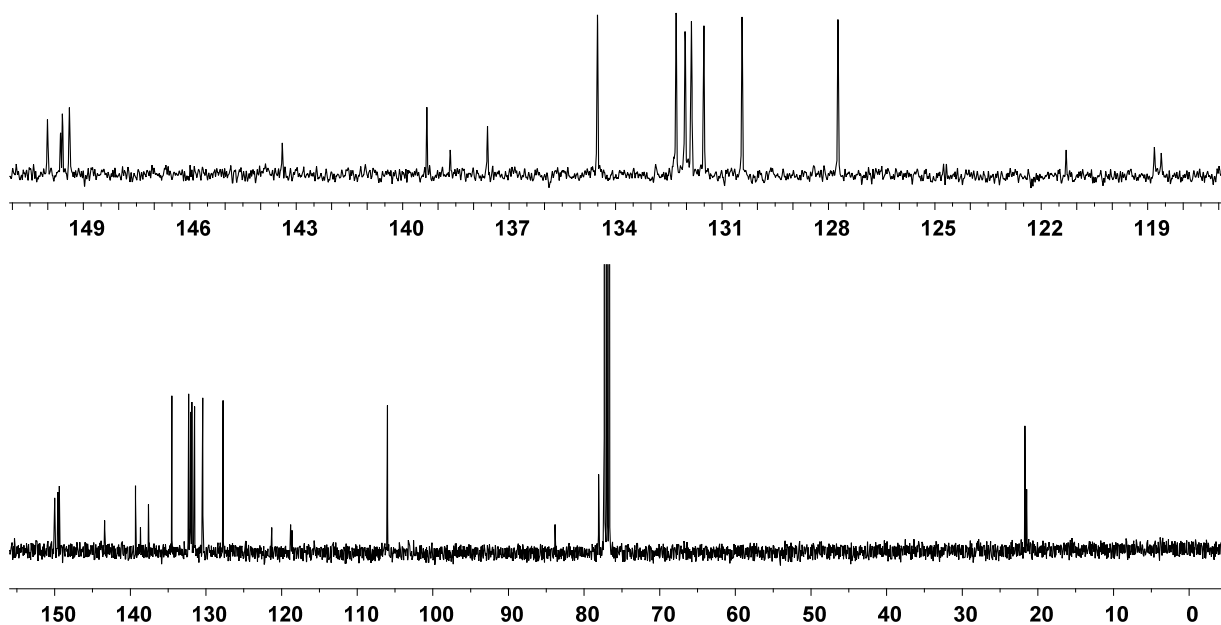


Figure S27.  $^{13}\text{C}$  NMR spectrum of **4** in  $\text{CDCl}_3$  (100 MHz, 298 K).

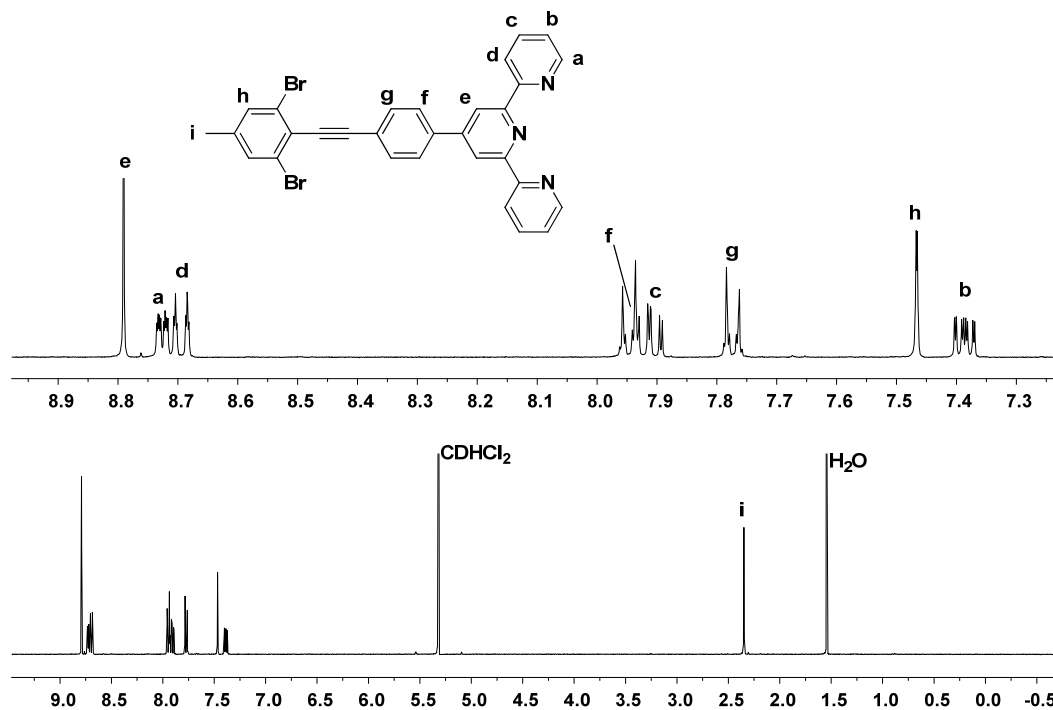
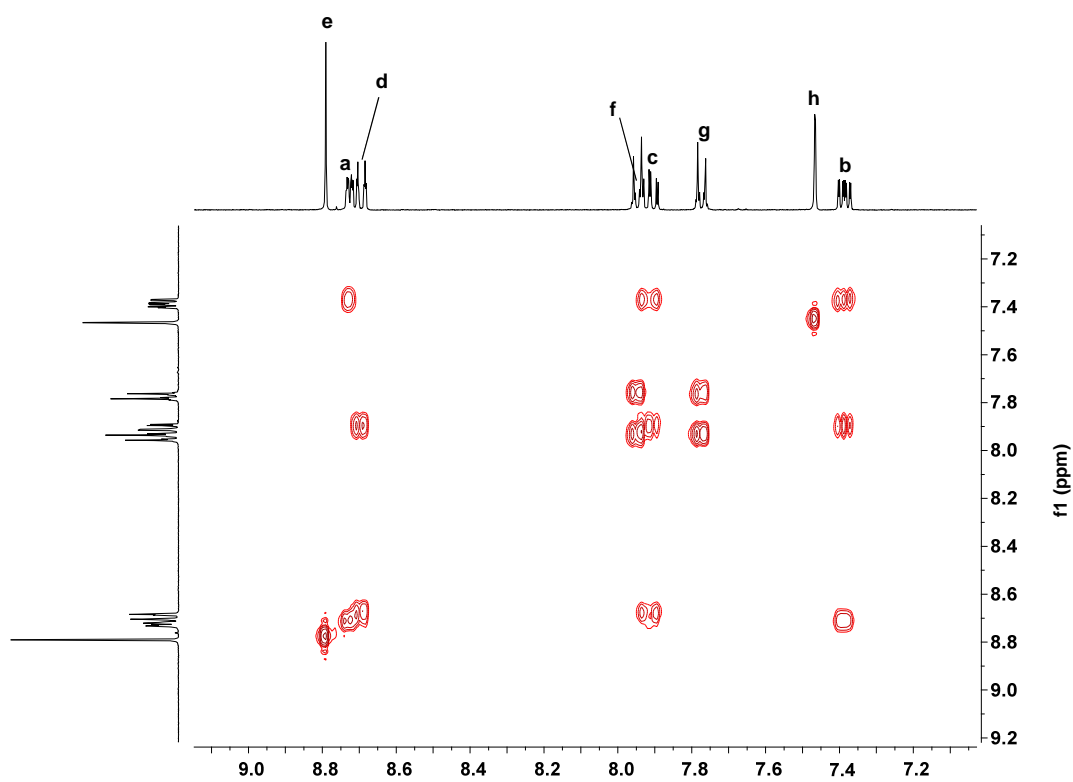
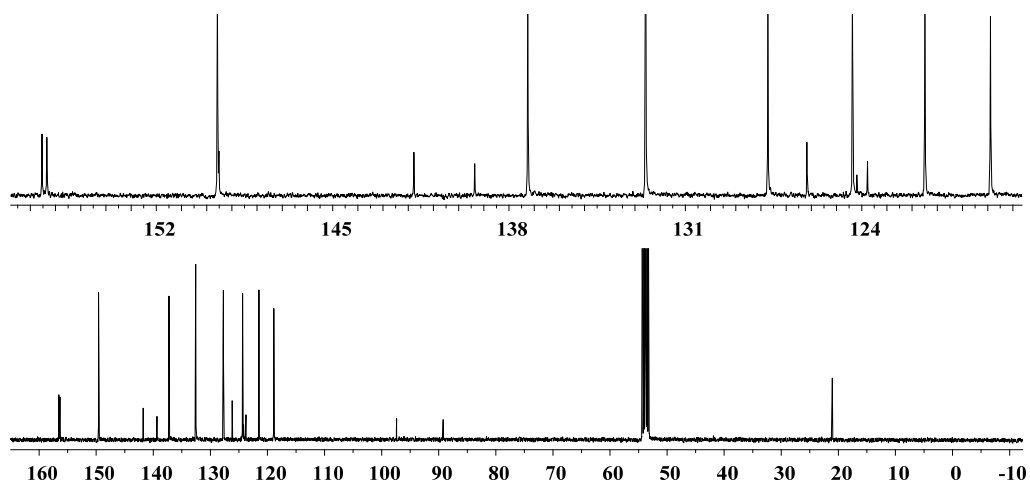


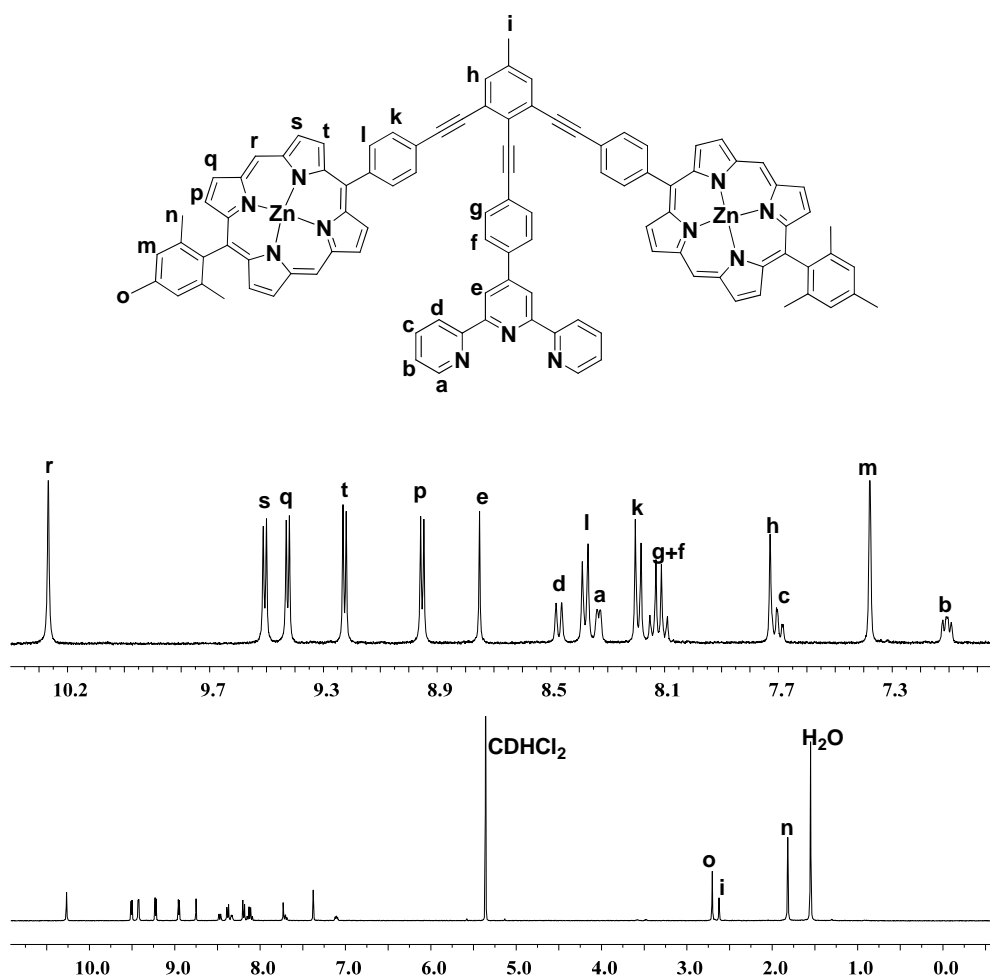
Figure S28.  $^1\text{H}$  NMR spectrum of **11** in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



**Figure S29.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **11** in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).

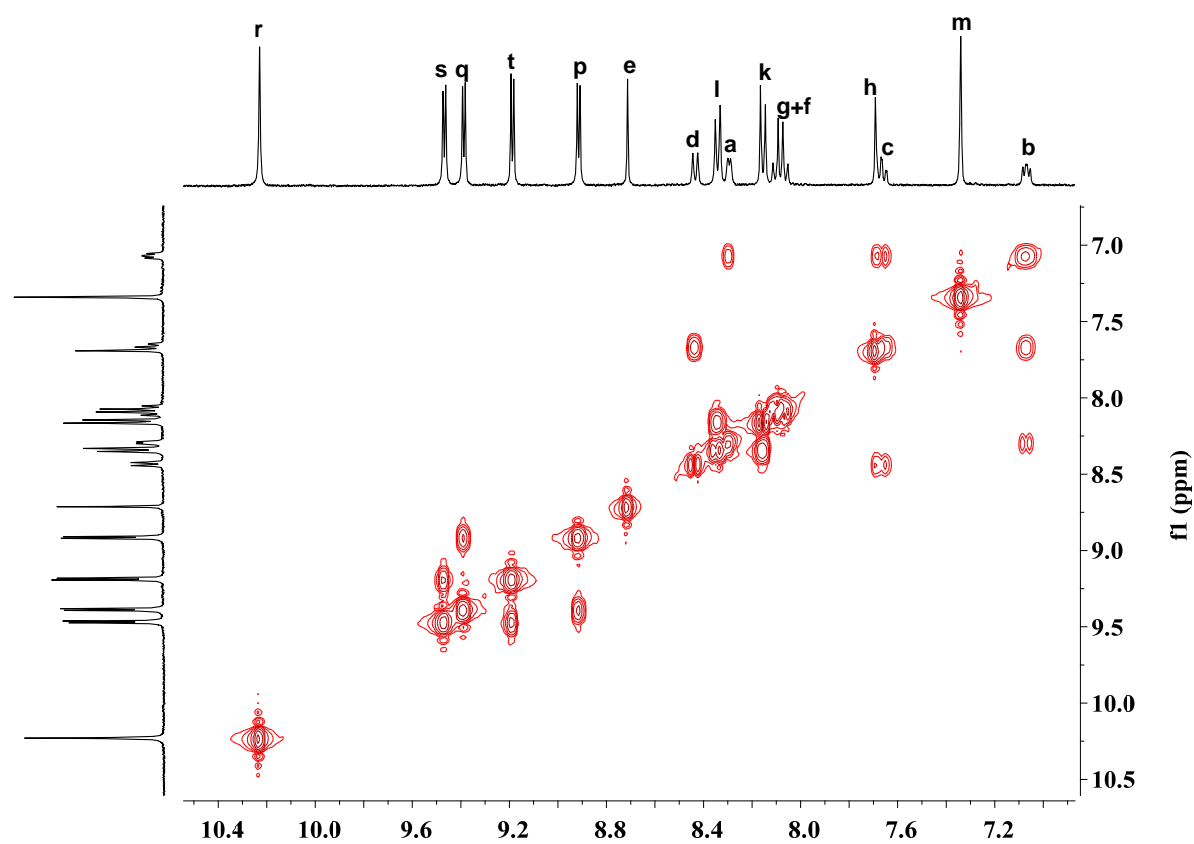


**Figure S30.**  $^{13}\text{C}$  NMR spectrum of **11** in  $\text{CD}_2\text{Cl}_2$  (100 MHz, 298 K).

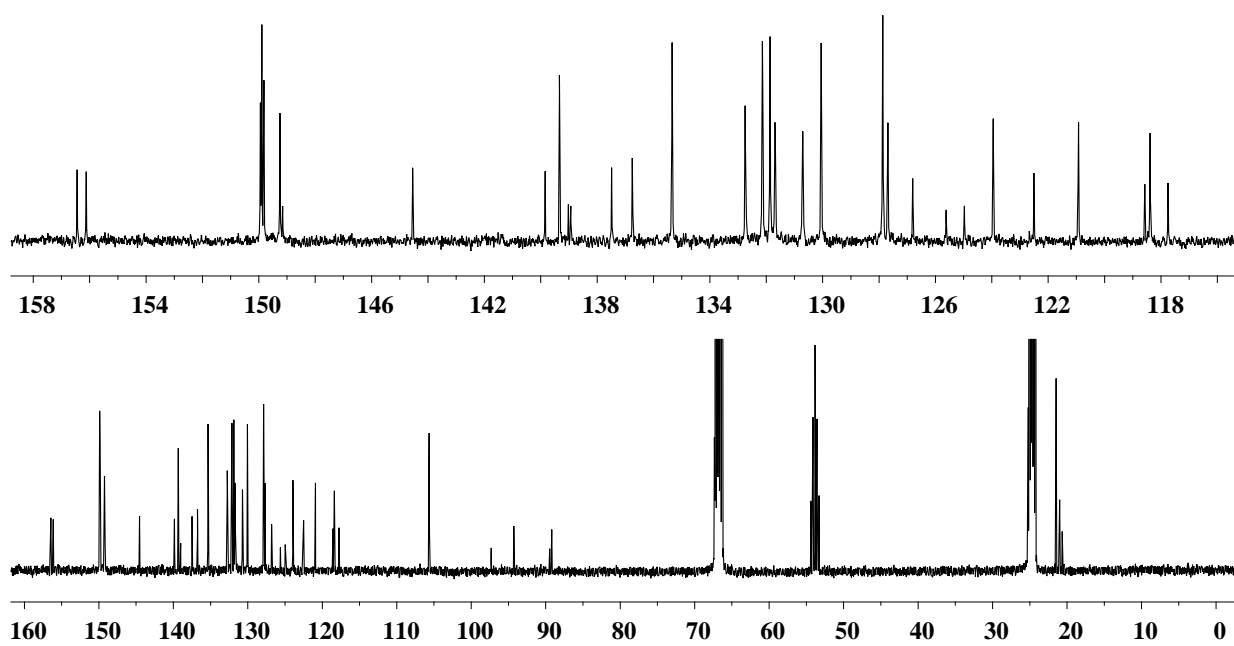


**Figure S31.**  $^1\text{H}$  NMR spectrum of **S** in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).





**Figure S32.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **S** in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



**Figure S33.**  $^{13}\text{C}$  NMR spectrum of **S** in  $\text{THF-d}_8:\text{CD}_2\text{Cl}_2$  (9:1) (100 MHz, 298 K).

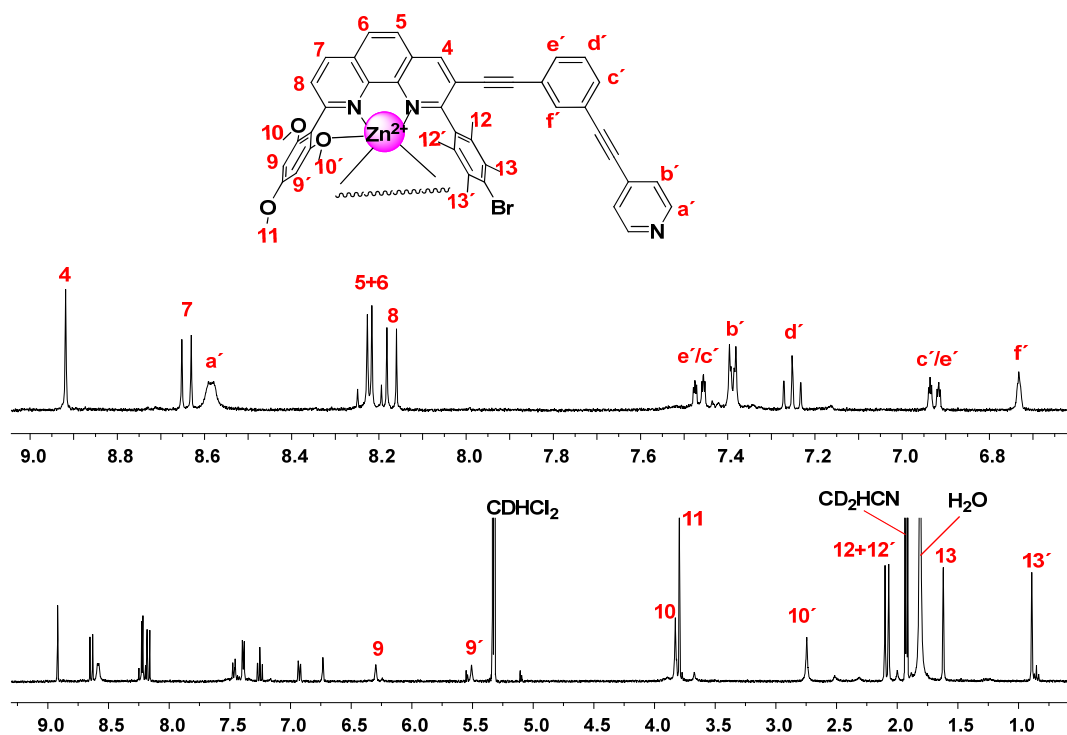


Figure S34.  $^1\text{H}$  NMR spectrum of  $[\text{Zn}(\text{R})_2]^{2+}$  in  $\text{CD}_2\text{Cl}_2:\text{CD}_3\text{CN}$  (8:2) (400 MHz, 298 K).

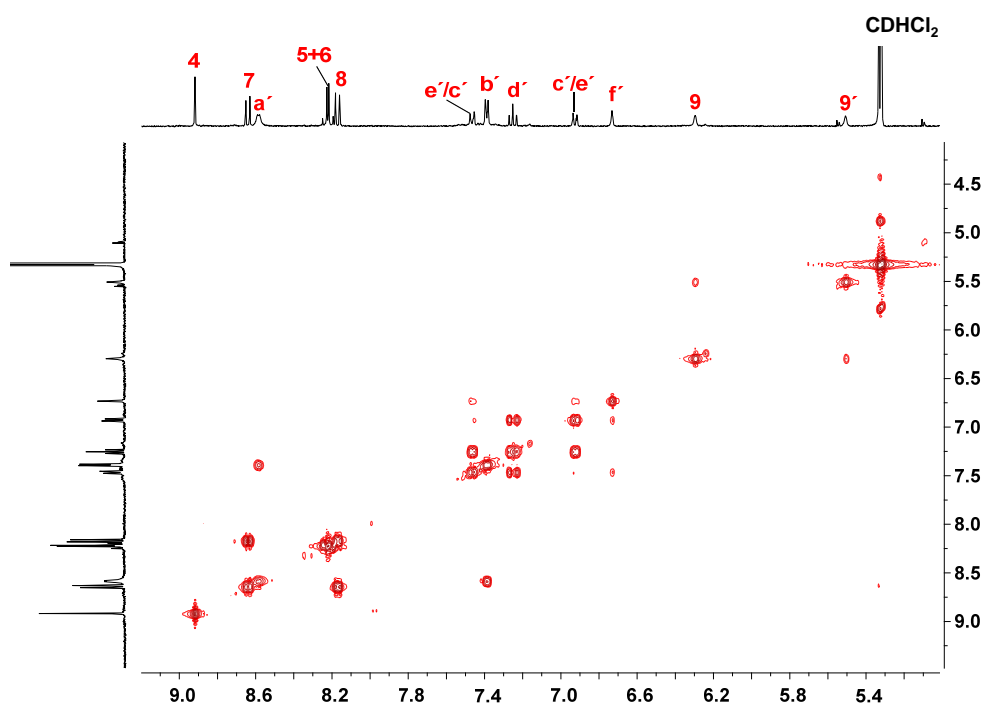
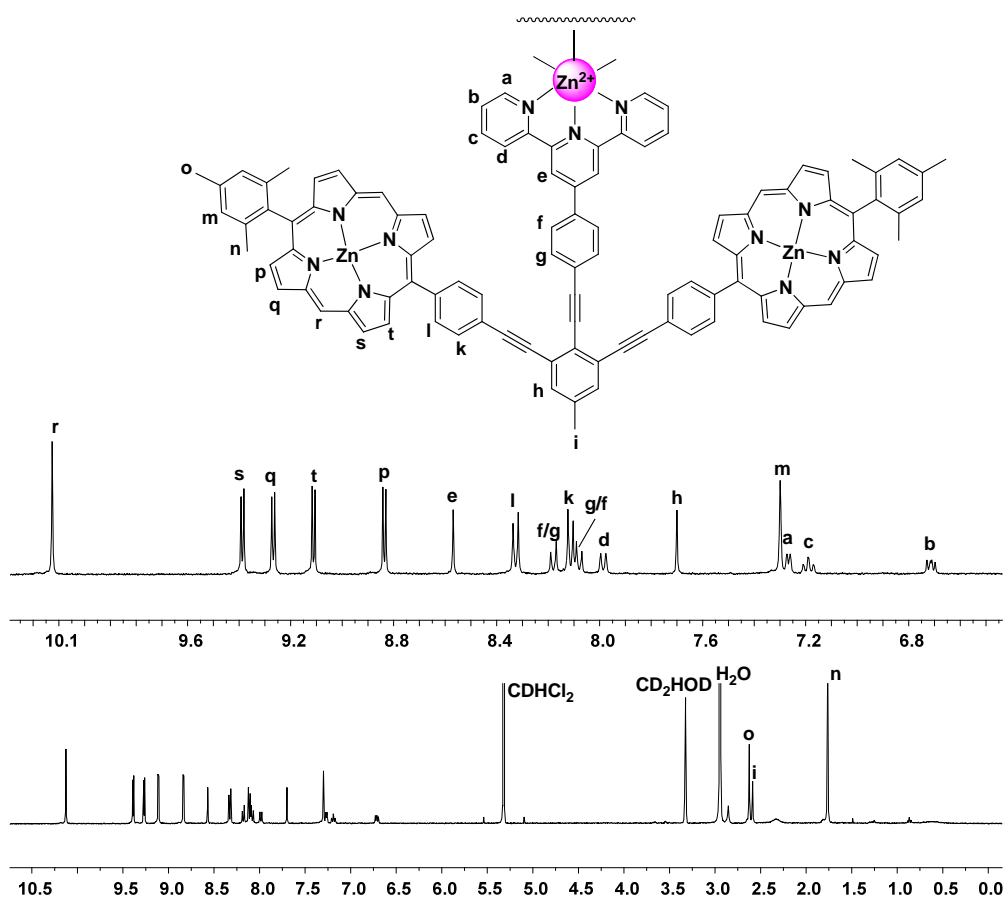
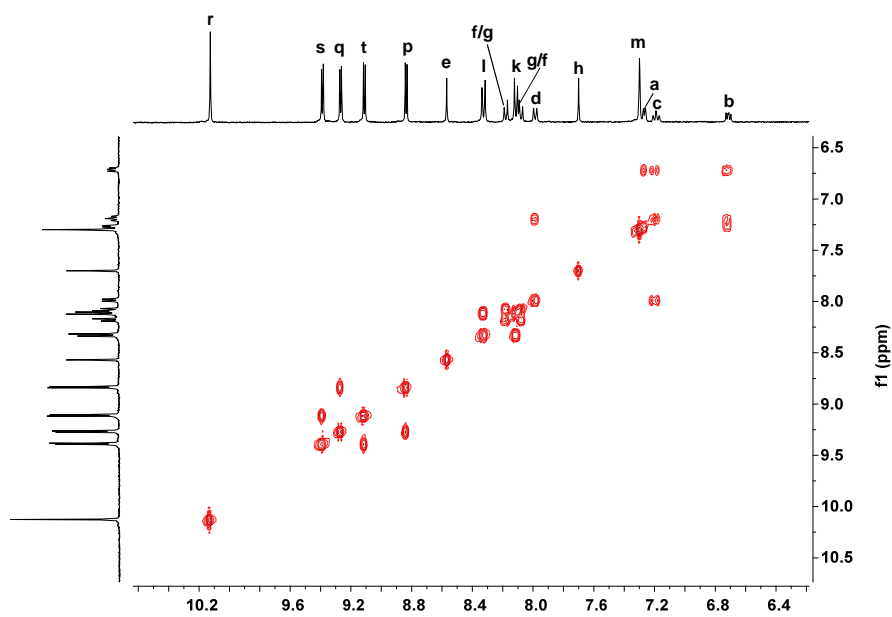


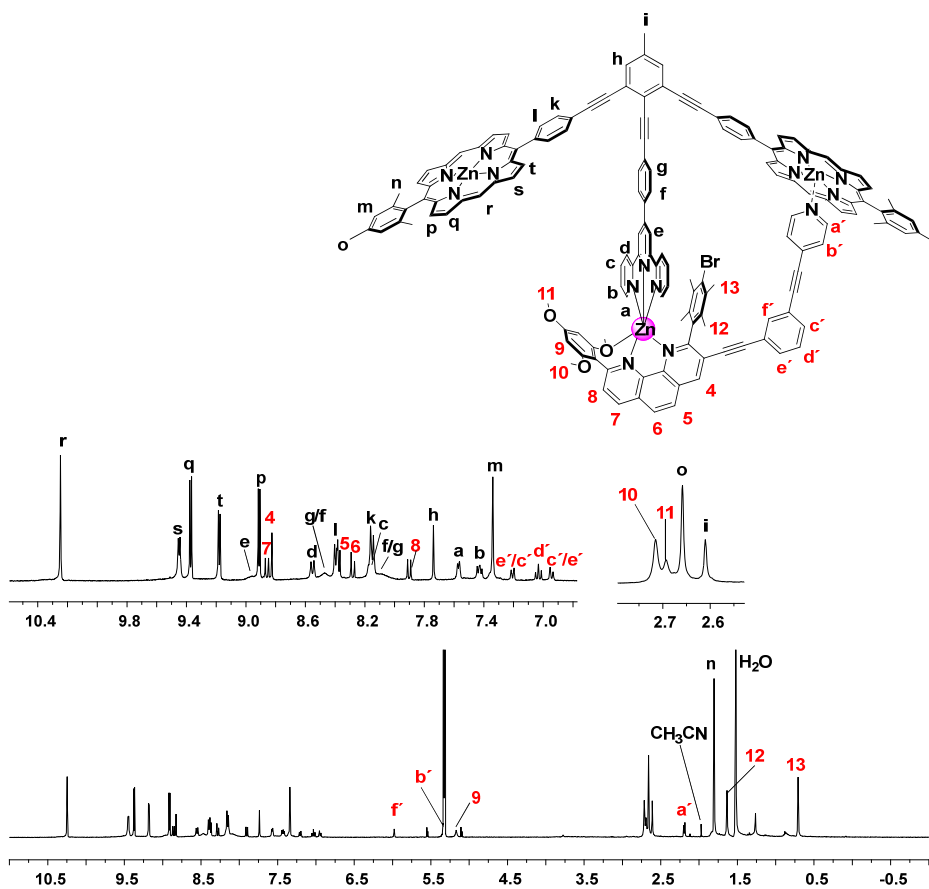
Figure S35.  $^1\text{H}-^1\text{H}$  COSY spectrum of  $[\text{Zn}(\text{R})_2]^{2+}$  in  $\text{CD}_2\text{Cl}_2:\text{CD}_3\text{CN}$  (8:2) (400 MHz, 298 K).



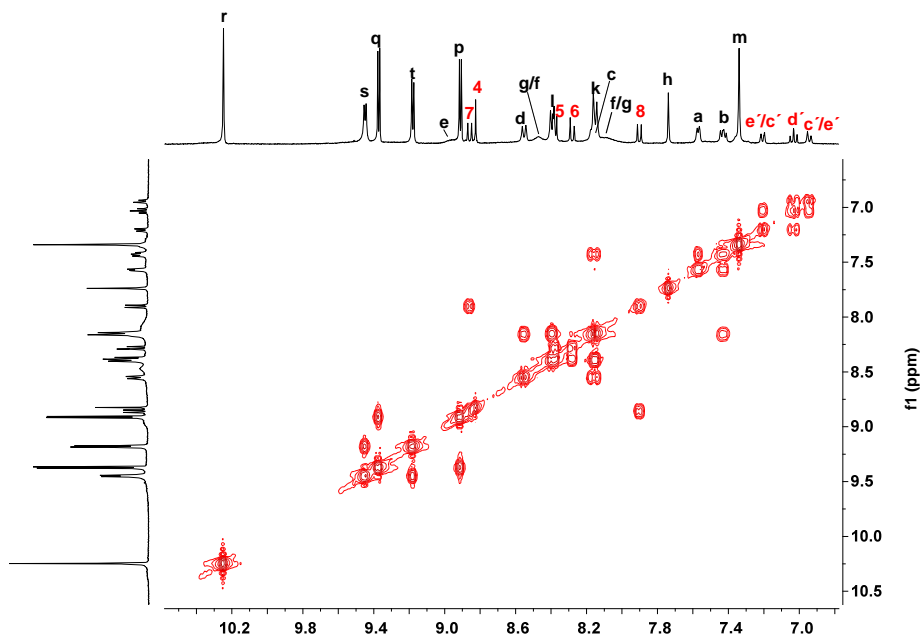
**Figure S36.**  $^1\text{H}$  NMR spectrum of  $[\text{Zn}(\text{S})_2]^{2+}$  in  $\text{CD}_2\text{Cl}_2$ :  $\text{CD}_3\text{OD}$  (8:2) (400 MHz, 298 K).



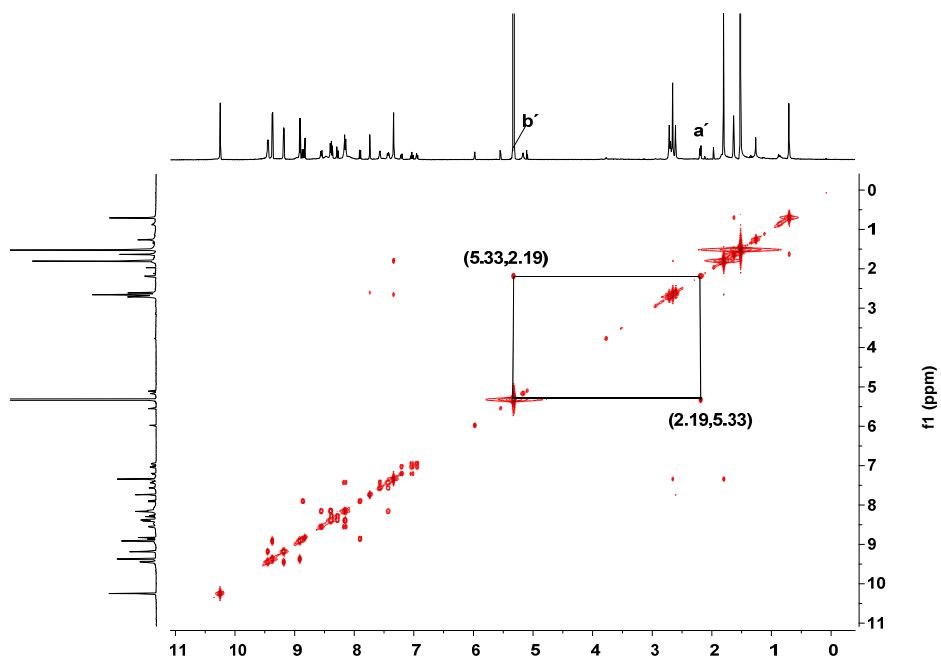
**Figure S37.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of  $[\text{Zn}(\text{S})_2]^{2+}$  in  $\text{CD}_2\text{Cl}_2$ :  $\text{CD}_3\text{OD}$  (8:2) (400 MHz, 298 K).



**Figure S38.**  $^1\text{H}$  NMR spectrum of  $[\text{Zn}(\text{S})(\text{R})]^{2+}$  in  $\text{CD}_2\text{Cl}_2$  (600 MHz, 298 K).



**Figure S39.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of  $[\text{Zn}(\text{S})(\text{R})]^{2+}$  in  $\text{CD}_2\text{Cl}_2$  (600 MHz, 298 K)



**Figure S40.** Full  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of  $[\text{Zn}(\text{S})(\mathbf{R})]^{2+}$  in  $\text{CD}_2\text{Cl}_2$  (600 MHz, 298 K). Pyridyl proton  $\text{b}'\text{-H}$  is merged with residual solvent signal ( $\text{CDHCl}_2$ ) at 5.33 ppm.

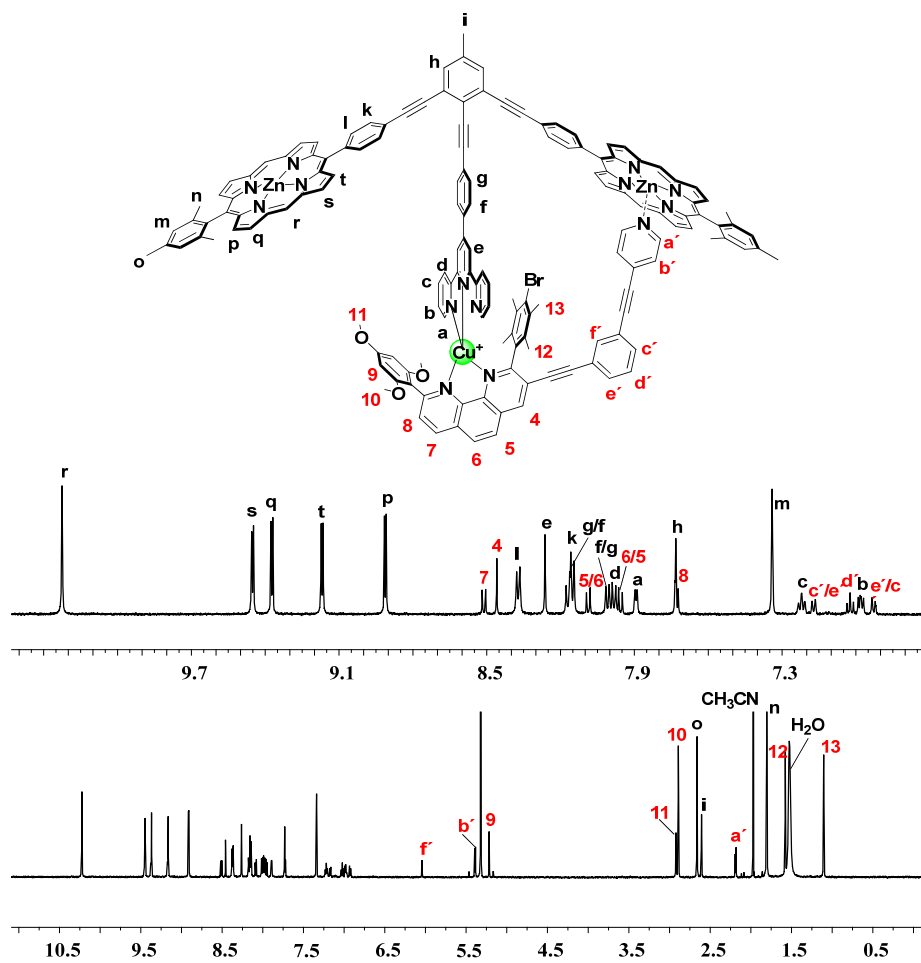


Figure S41.  $^1\text{H}$  NMR spectrum of  $[\text{Cu}(\text{S})(\text{R})]^+$  in  $\text{CD}_2\text{Cl}_2$  (600 MHz, 298 K).

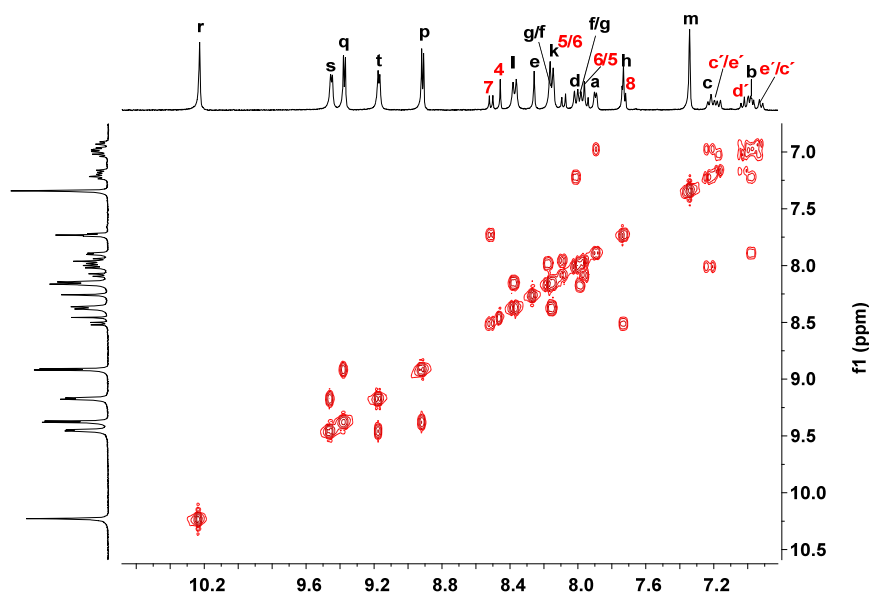
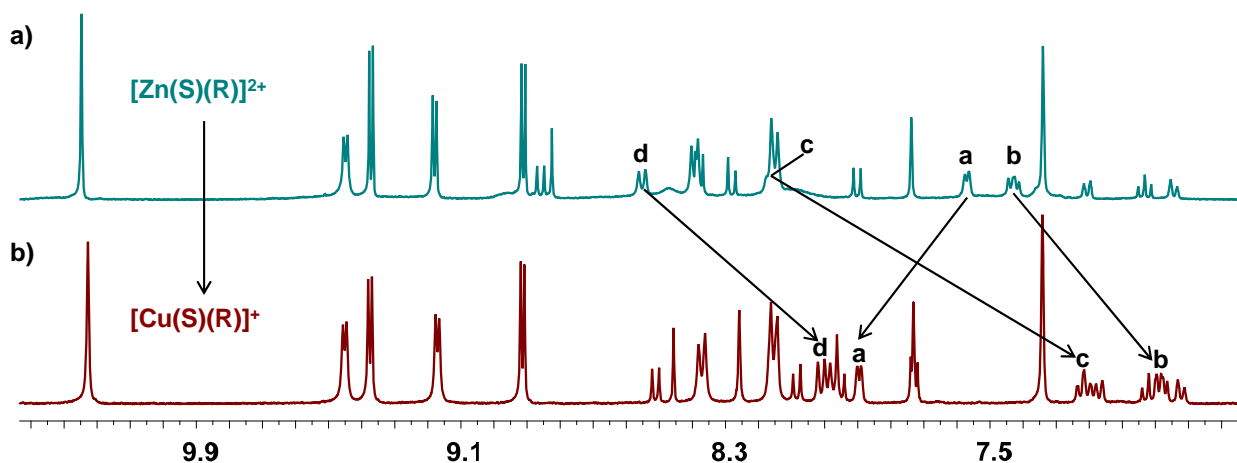
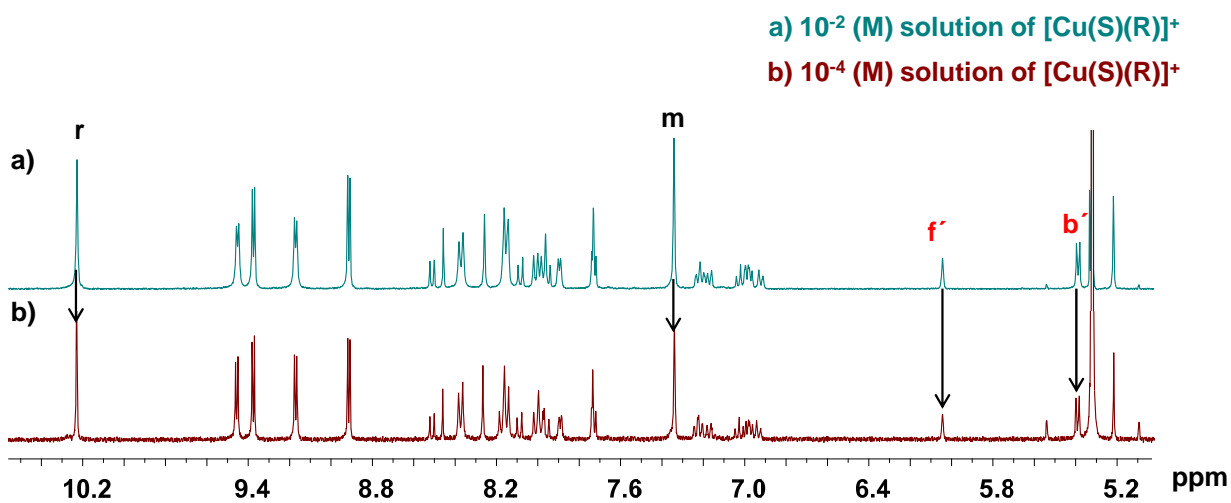


Figure S42.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of  $[\text{Cu}(\text{S})(\text{R})]^+$  in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).



**Figure S43.** Change in chemical shift in  $^1\text{H}$  NMR after metal-metal exchange by  $[\text{Cu}(\text{hexacyclen})]\text{PF}_6$  in  $\text{CD}_2\text{Cl}_2 : \text{CD}_3\text{CN} = 4:1$  (400 MHz, 298 K).



**Figure S44.** Comparison of  $^1\text{H}$  NMR spectra of  $[\text{Cu}(\text{S})(\text{R})]^+$  at two concentrations in  $\text{CD}_2\text{Cl}_2$  (400 MHz, 298 K).

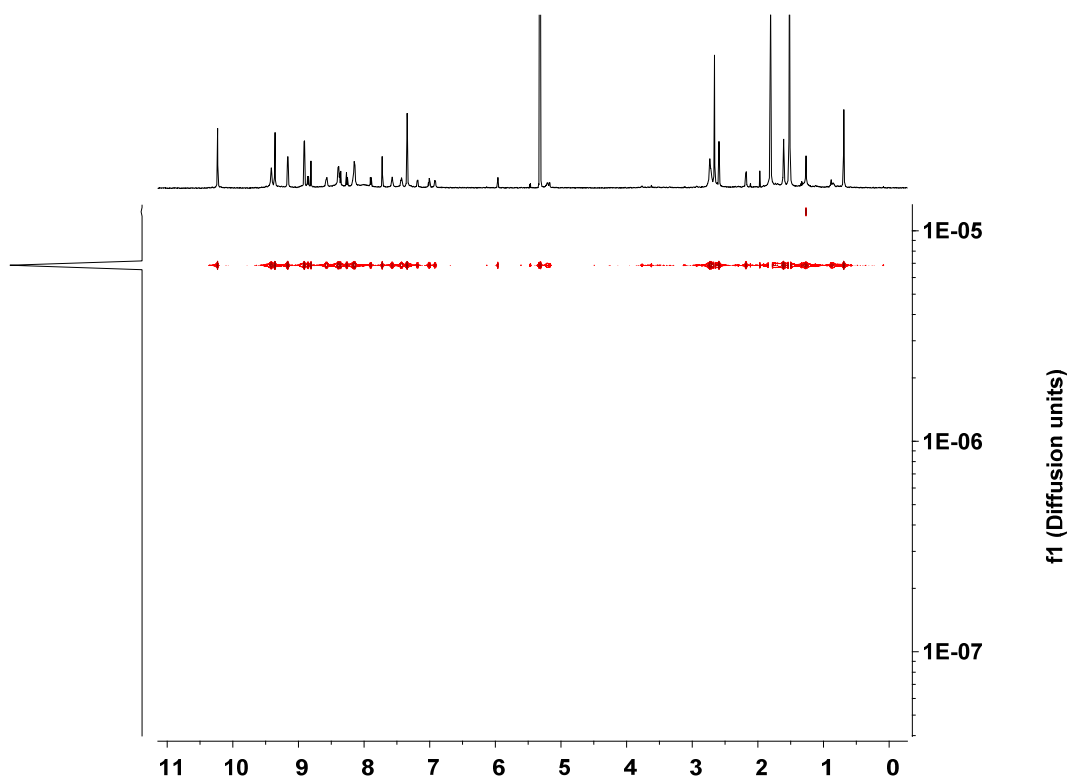
## 5. DOSY NMR spectra

### Calculation of hydrodynamic radius from:

- a) **DOSY**: The diffusion coefficient  $D$  for  $[\text{Zn}(\text{S})(\mathbf{R})]^{2+}$  and  $[\text{Cu}(\text{S})(\mathbf{R})]^+$  was obtained from their DOSY spectrum. The corresponding hydrodynamic radius was calculated by using the Stokes-Einstein equation

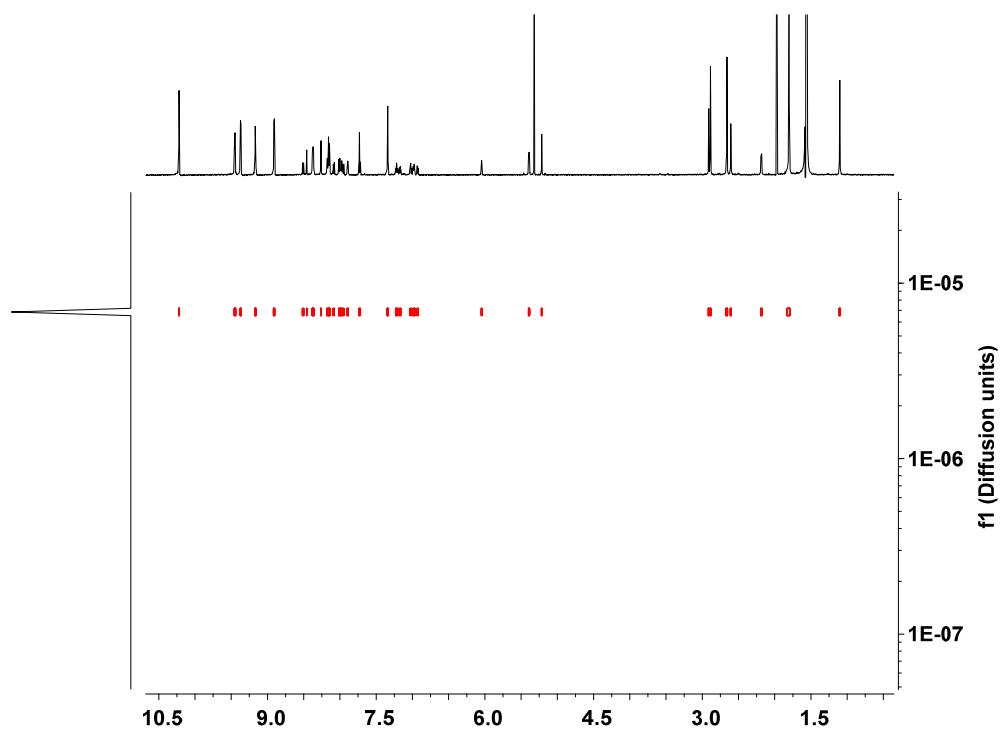
$$r = k_B T / 6\pi\eta D$$

- b) **Optimized structure**: Radius of  $[\text{Zn}(\text{S})(\mathbf{R})]^{2+}$  was calculated from their optimized structures at PM6 level. First a circle around the structure was considered and its radius approximated as hydrodynamic radius of the rotor. It is denoted as  $r_{\text{com}}$ .



**Figure S45.**  $^1\text{H}$ -DOSY NMR of  $[\text{Zn}(\text{S})(\mathbf{R})]^{2+}$  in  $\text{CD}_2\text{Cl}_2$  (600 MHz, 298K). Diffusion coefficient  $D = 4.35 \times 10^{-10} \text{ m}^2 \text{ s}^{-1}$ , Hydrodynamic radius  $r = 12.1 \text{ \AA}$  and the computed value  $r_{\text{com}} = 13.0 \text{ \AA}$ .



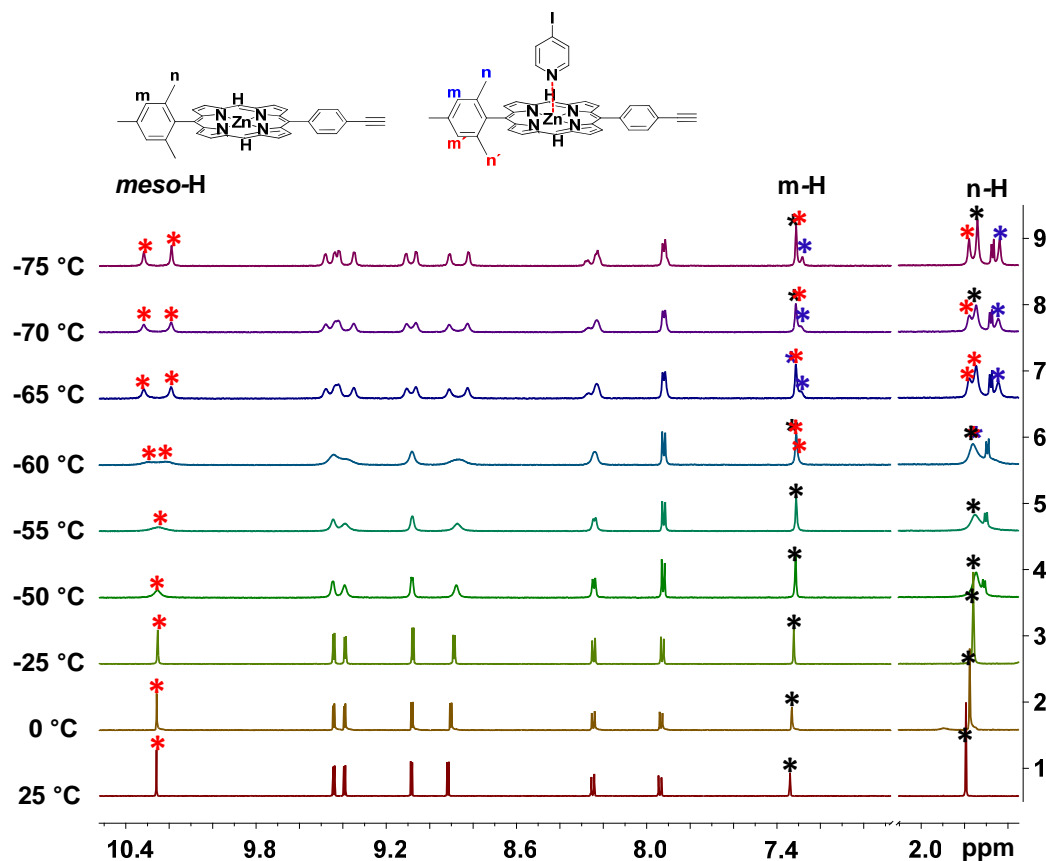


**Figure S46.** <sup>1</sup>H-DOSY NMR of [Cu(S)(R)]<sup>2+</sup> in CD<sub>2</sub>Cl<sub>2</sub> (600 MHz, 298K). Diffusion coefficient  $D = 4.61 \times 10^{-10}$  m<sup>2</sup> s<sup>-1</sup>, Hydrodynamic radius  $r = 11.5$  Å and the computed value  $r_{\text{com}} = 12.5$  Å.

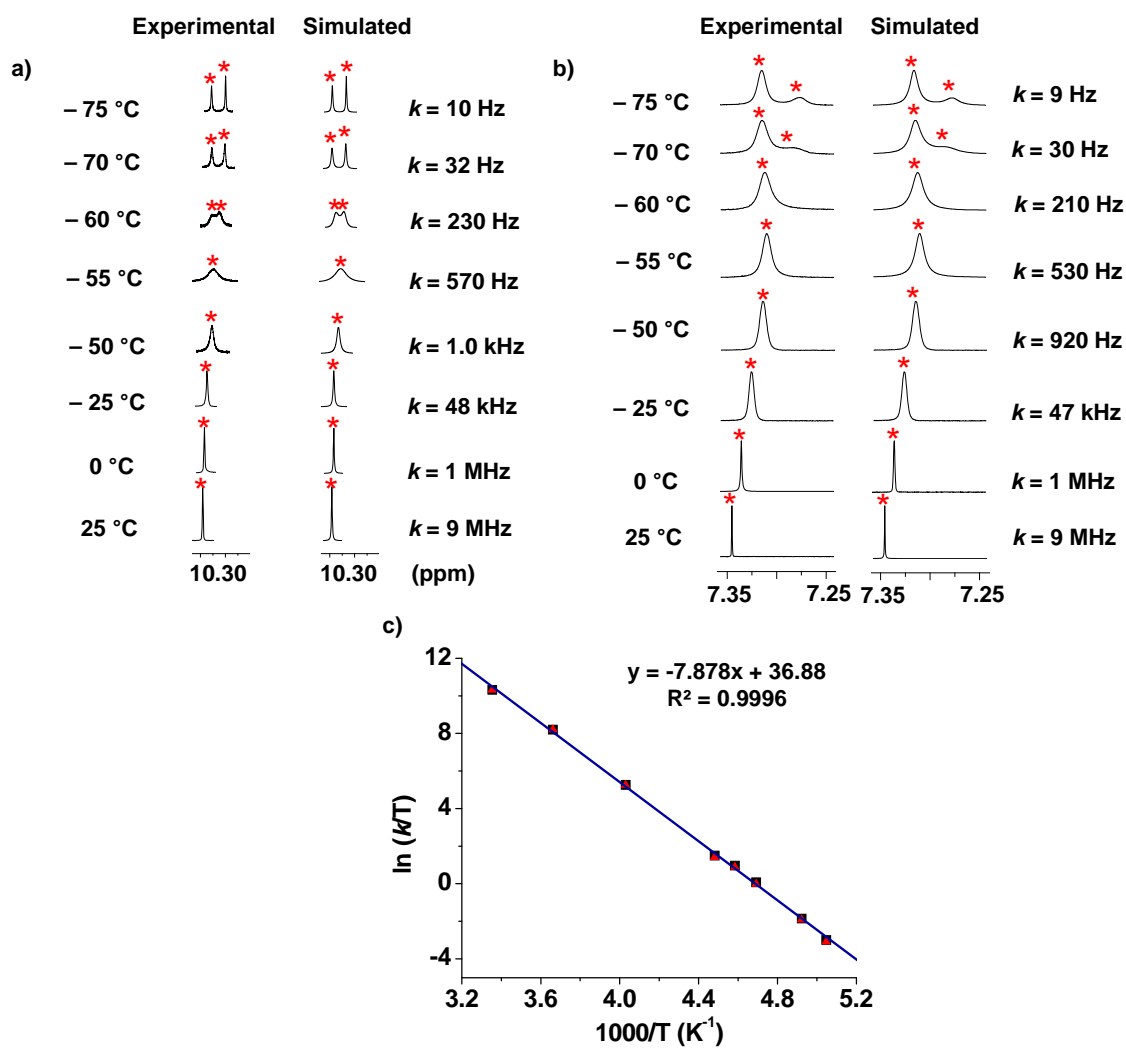
## 6. Variable temperature studies and determination of kinetic parameters

### Model complex **3•4**(1:2):

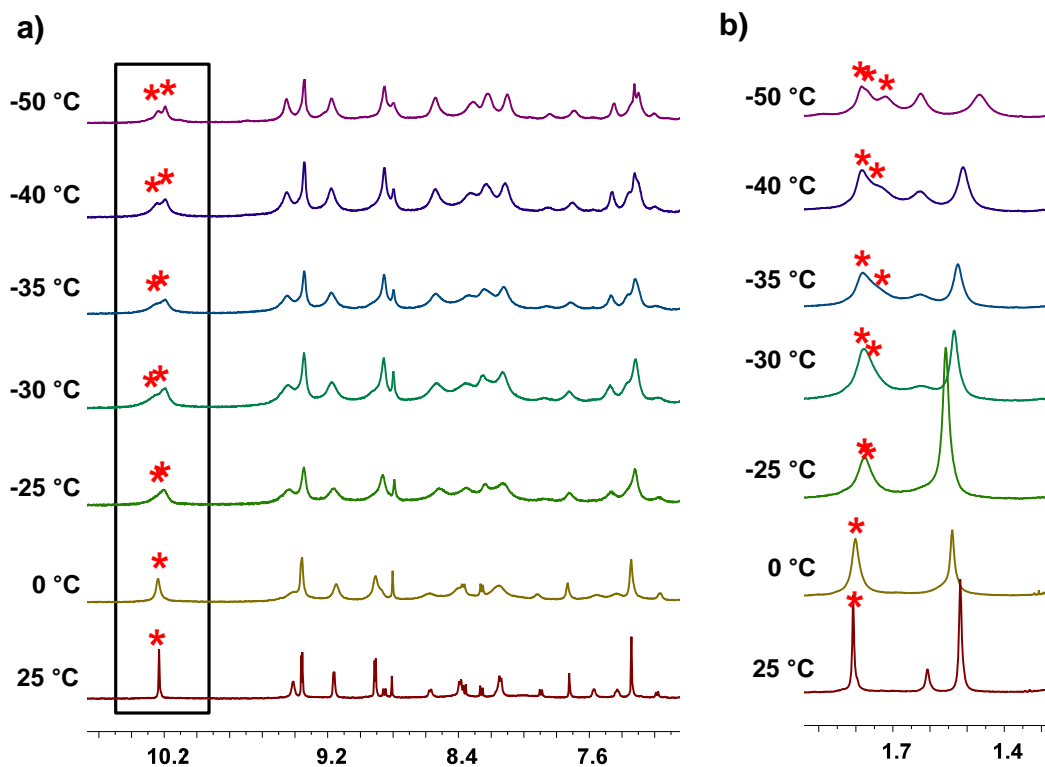
In an NMR tube, **4** (0.521 mg, 0.880  $\mu\text{mol}$ ) was dissolved in  $\text{CD}_2\text{Cl}_2$  and **3** (0.090mg, 0.439  $\mu\text{mol}$ ) was added. NMR spectra of the mixture were recorded at different temperature.



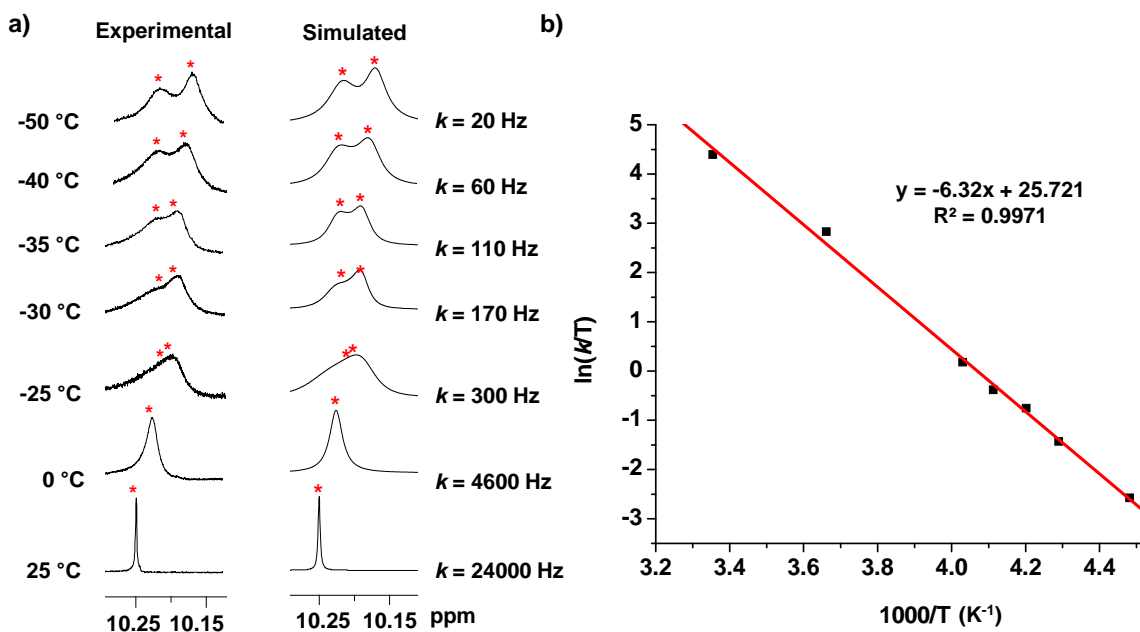
**Figure S47.** Partial  $^1\text{H}$  VT-NMR ( $\text{CD}_2\text{Cl}_2$ , 600 MHz) of **3•4**(1:2) shows the splitting of *meso*-H, *m*-H, and *n*-H (red asterisk marked) in aromatic and aliphatic region. Upon lowering the temperature *meso*-H splits into two sets in 1:1 ratio. Signal at 10.32 ppm corresponds to **3•4**, and the free porphyrin **4** shows a singlet at 10.19 ppm. In contrast, *m*-H splits into two sets at 1:3 ratio. Signal at 7.28 ppm corresponds to one *m*-H of **3•4** and the other is merged with two *m*-H of **4** at 7.31 ppm. Similarly, upon lowering the temperature protons *n*-H split into three sets in 1:2:1 ratio. Singlet at 1.74 ppm corresponds to free **4**, while the signals for the coordinated porphyrin arise at 1.78 and 1.64 ppm. Broadening and splitting of other aromatic protons is also observed.



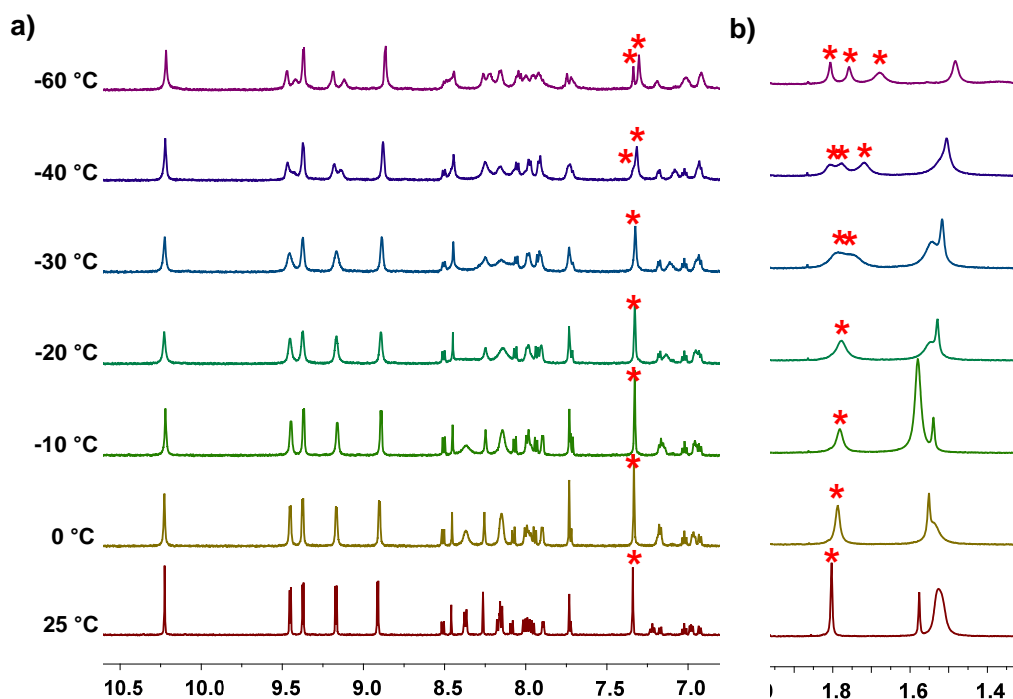
**Figure S48.** Partial  $^1\text{H}$  VT-NMR spectra ( $\text{CD}_2\text{Cl}_2$ , 600 MHz) of **3•4**(1:2) at different temperatures showing experimental and theoretical splitting of (a) *meso*-H and (b) *m*-H with corresponding rate constants. (c) Eyring plot for the exchange process.



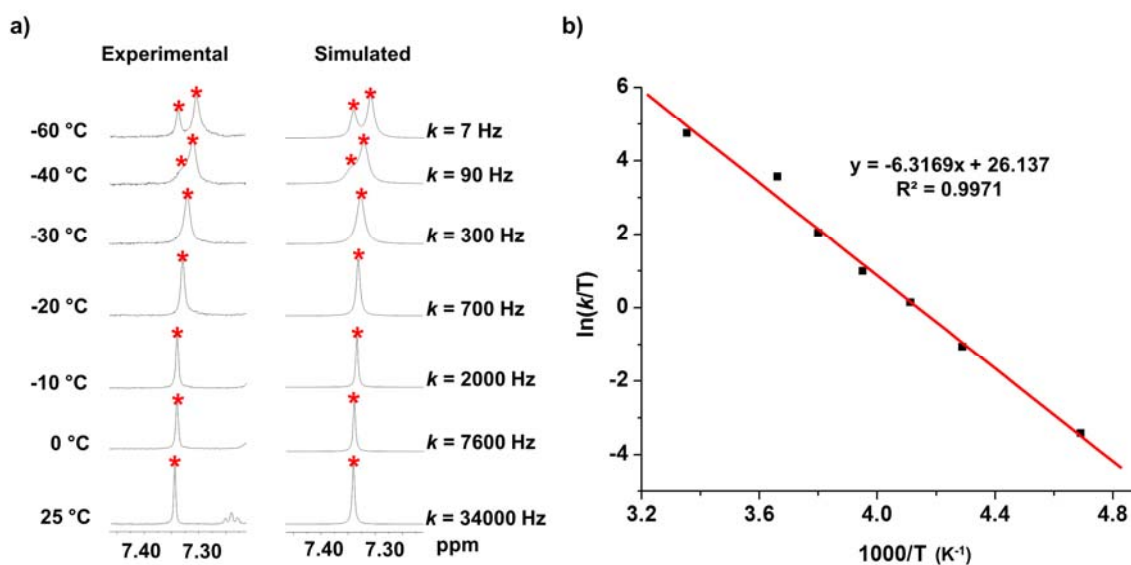
**Figure S49.** Partial  $^1\text{H}$  VT-NMR ( $\text{CD}_2\text{Cl}_2$ , 600 MHz) of  $[\text{Zn}(\text{S})(\text{R})]^{2+}$  with (a) aromatic and (b) aliphatic region showing the splitting of r-H, and n-H (red asterisk marked).



**Figure S50.** Partial  $^1\text{H}$  VT-NMR of  $[\text{Zn}(\text{S})(\text{R})]^{2+}$  ( $\text{CD}_2\text{Cl}_2$ , 600 MHz) at different temperatures showing experimental and theoretical splitting of r-H with corresponding rate constants. (b) Eyring plot for rotational dynamics in  $[\text{Zn}(\text{S})(\text{R})]^{2+}$ .



**Figure S51.** Partial  $^1\text{H}$  VT-NMR ( $\text{CD}_2\text{Cl}_2$ , 600 MHz) of  $[\text{Cu}(\text{S})(\text{R})]^+$  with (a) aromatic and (b) aliphatic region showing the splitting of m-H, and n-H (red asterisk marked). The splitting pattern is similar as in the model exchange process (Figure S43). In contrast, protons r-H are not well separated upon lowering the temperature.



**Figure S52.** Partial  $^1\text{H}$  VT-NMR of  $[\text{Cu}(\text{S})(\text{R})]^+$  ( $\text{CD}_2\text{Cl}_2$ , 600 MHz) at different temperatures showing experimental and theoretical splitting of m-H with corresponding rate constants. (b) Eyring plot for rotational dynamics in  $[\text{Cu}(\text{S})(\text{R})]^+$ .

## 7. ESI-MS Spectra:

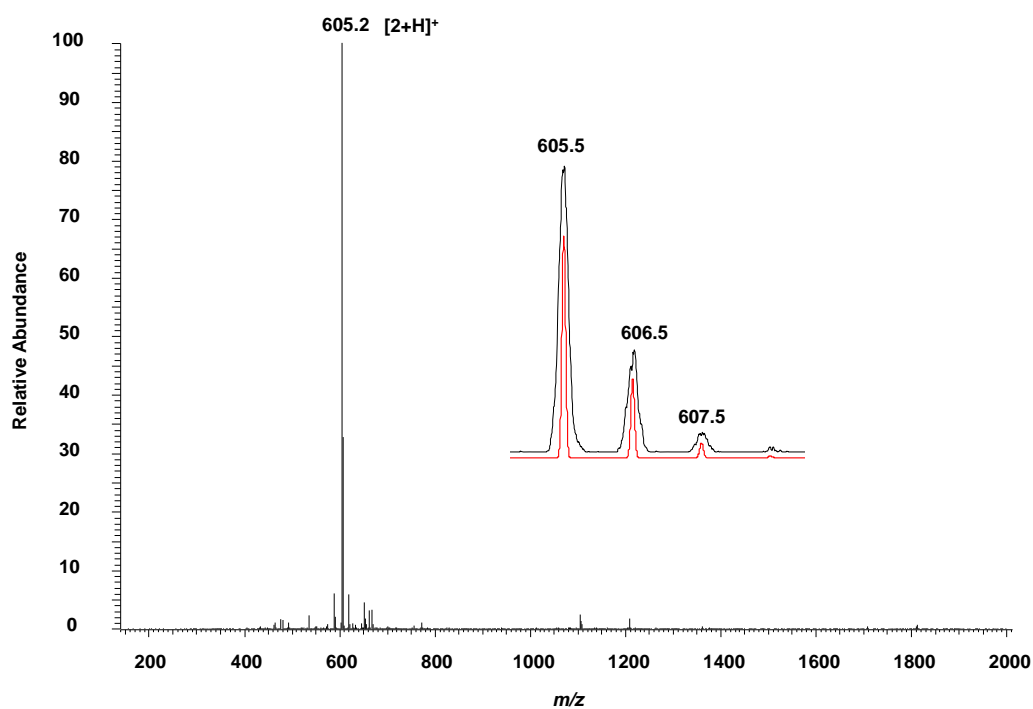


Figure S53. ESI-MS of compound 2 after protonation.

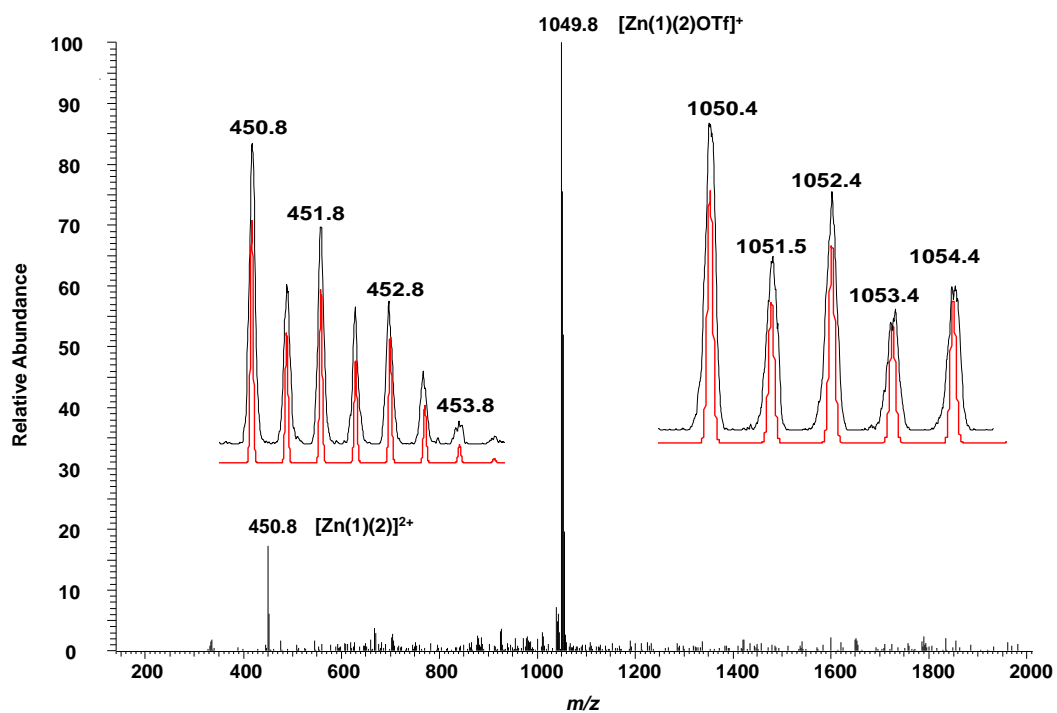


Figure S54. ESI-MS of C2.

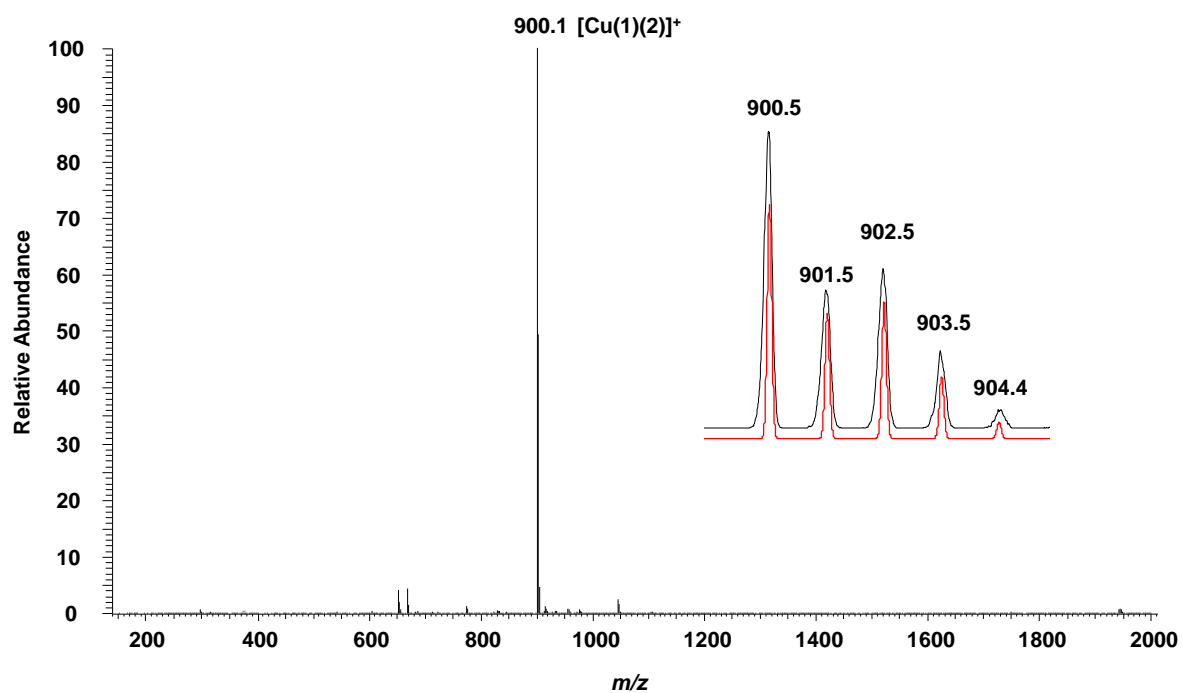


Figure S55. ESI-MS of C3.

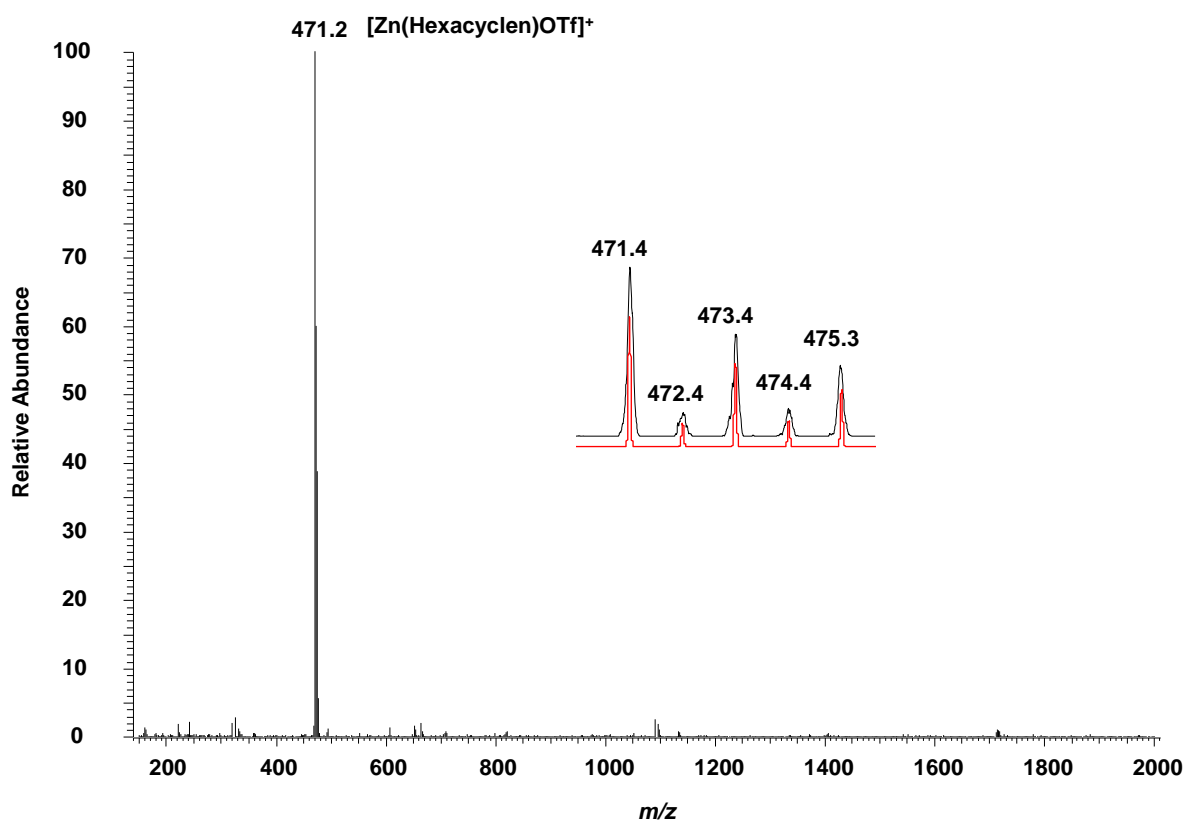
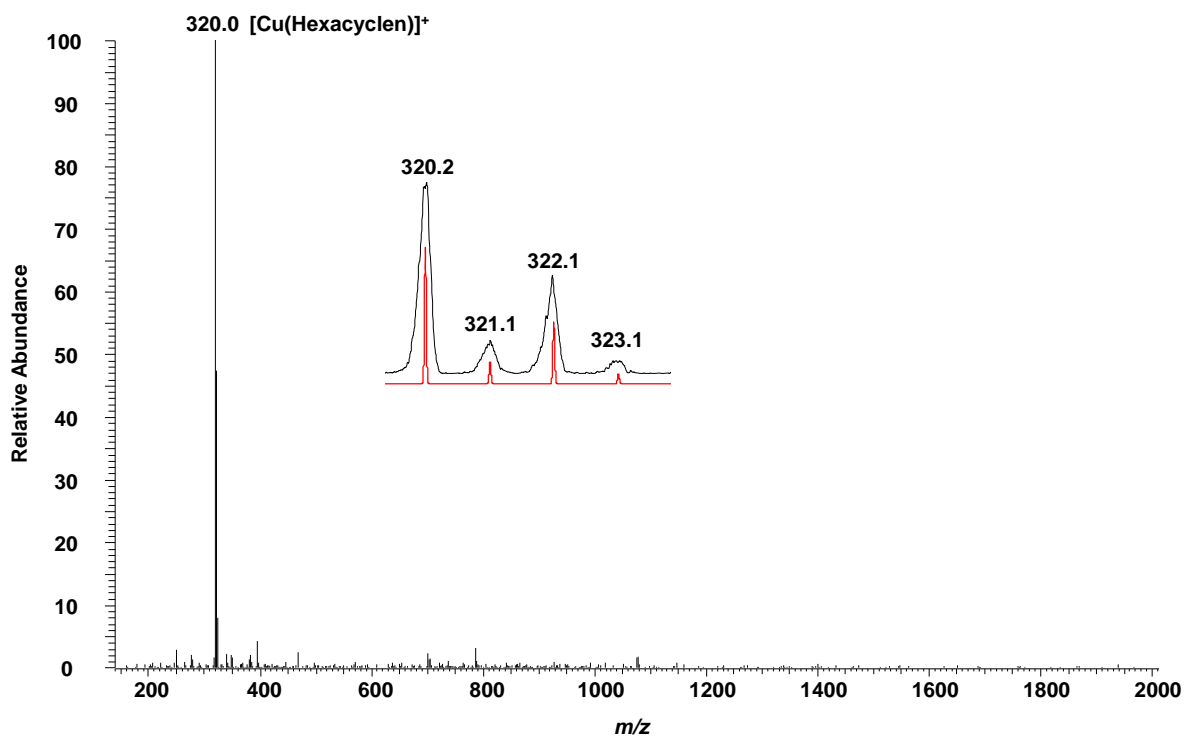
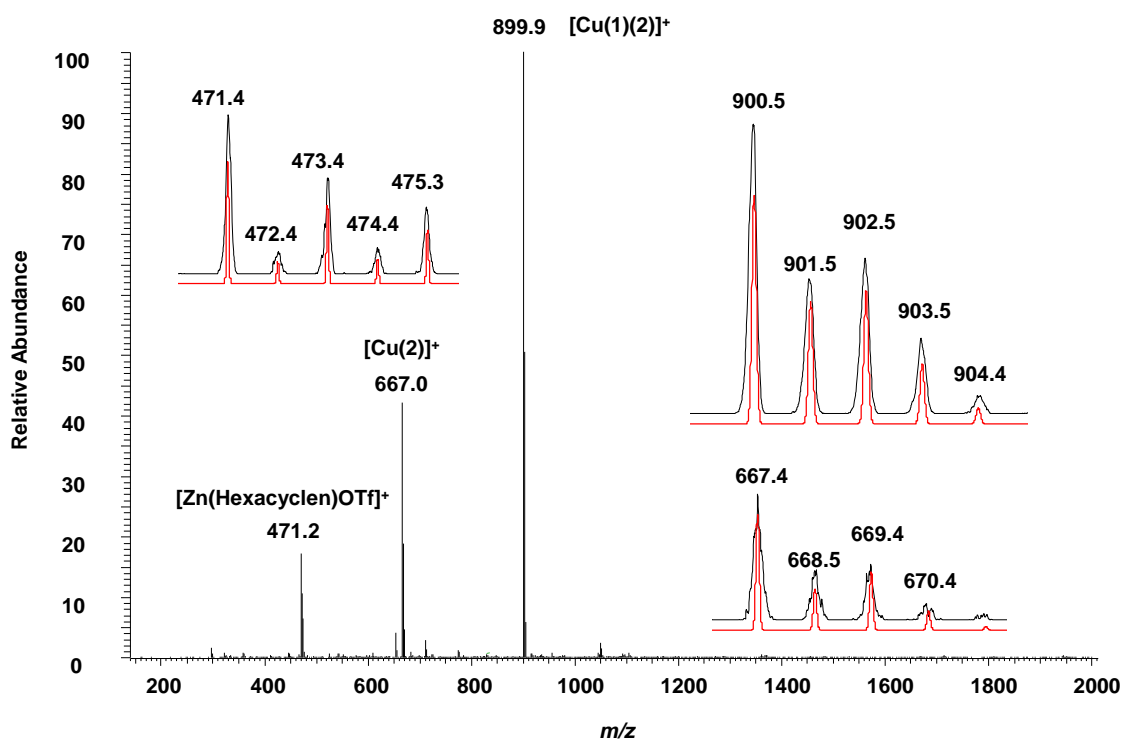


Figure S56. ESI-MS of  $[\text{Zn}(\text{hexacyclen})\text{OTf}]^+$ .



**Figure 57.** ESI-MS of  $[\text{Cu}(\text{hexacyclen})]^+$ .



**Figure S58.** ESI MS investigation for metal-metal exchange process, furnishing **C3** and  $[\text{Zn}(\text{hexacyclen})\text{OTf}]^{2+}$  from **C2** after treating with  $[\text{Cu}(\text{hexacyclen})]^+$ .



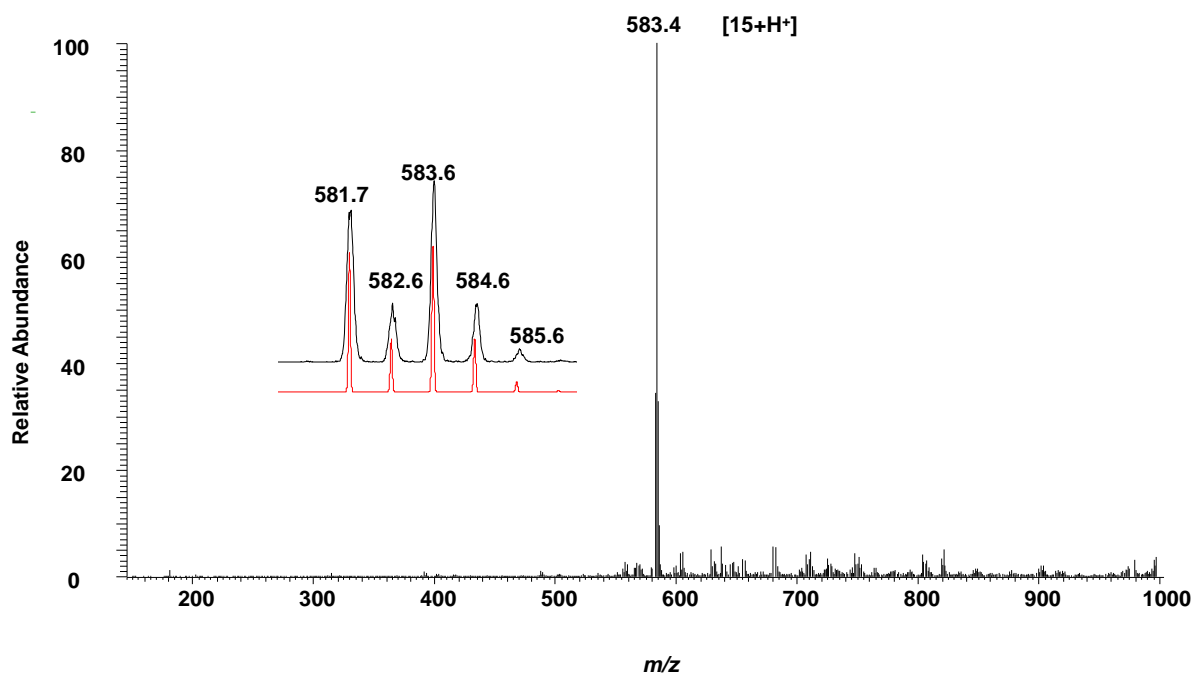


Figure S59. ESI-MS of compound 15 after protonation.

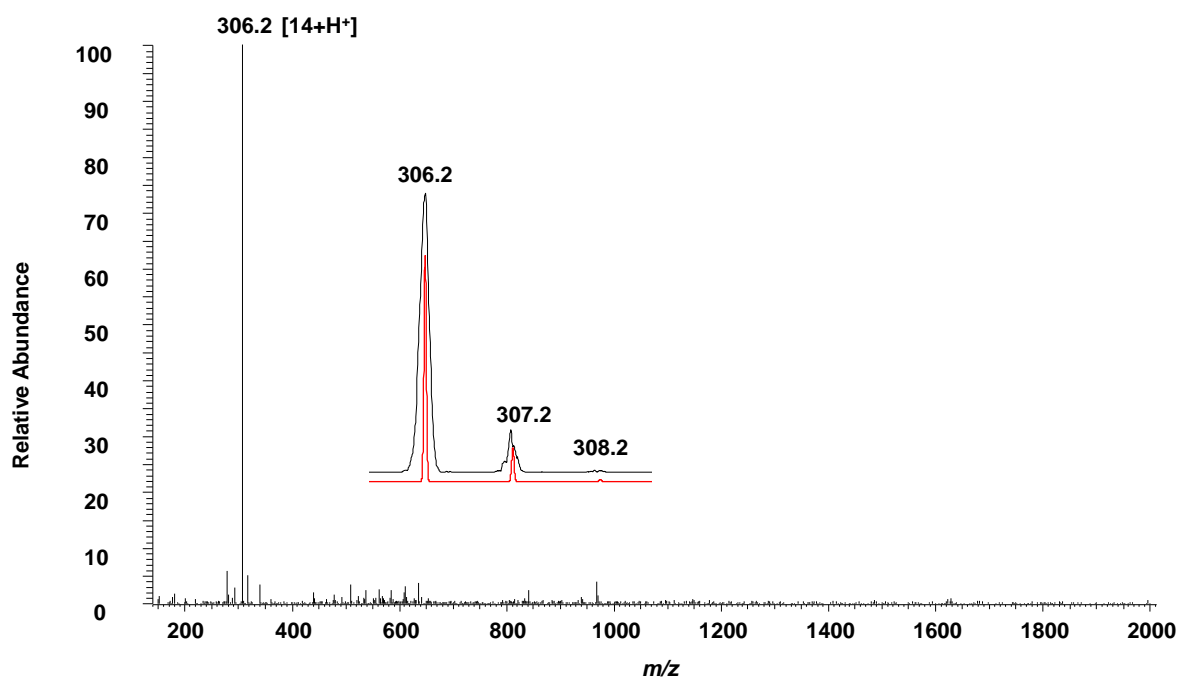
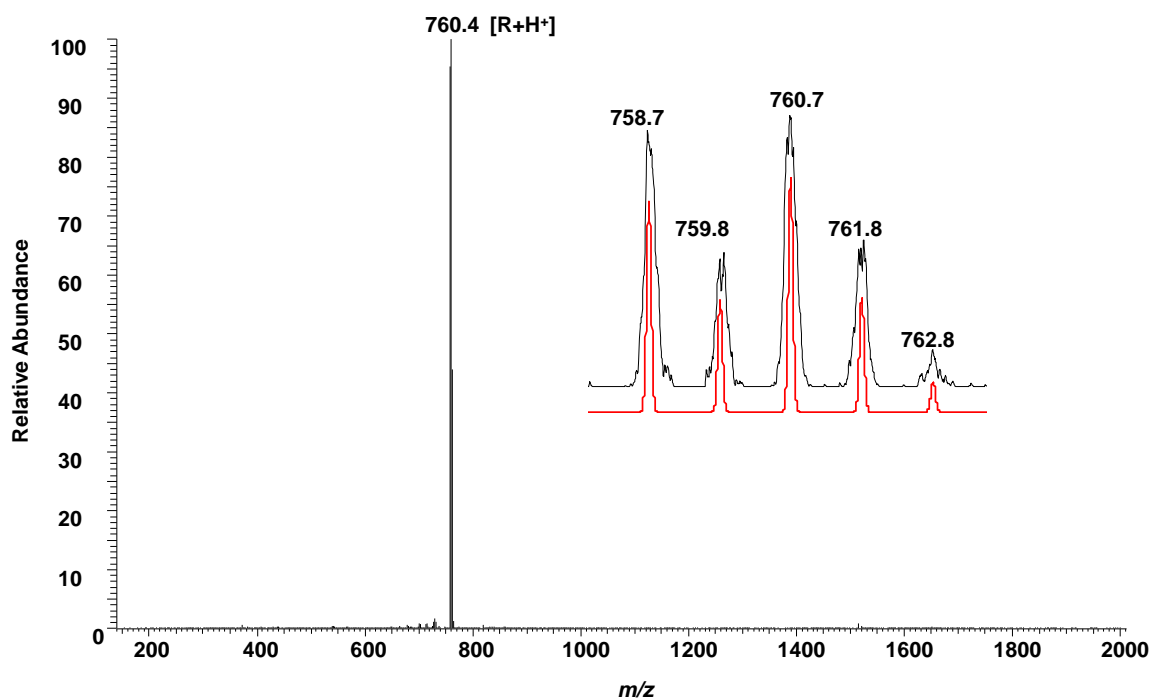
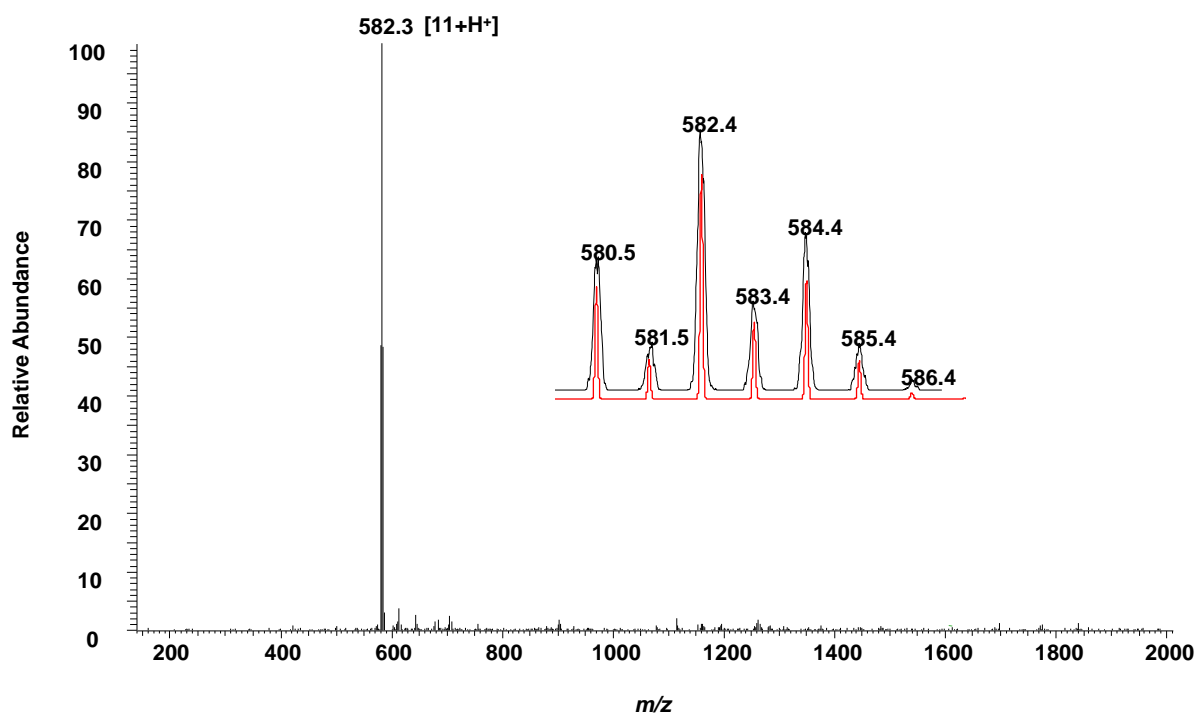


Figure S60. ESI-MS of compound 14 after protonation.



**Figure S61.** ESI-MS of compound **R** after protonation.



**Figure S62.** ESI-MS of compound **11** after protonation.

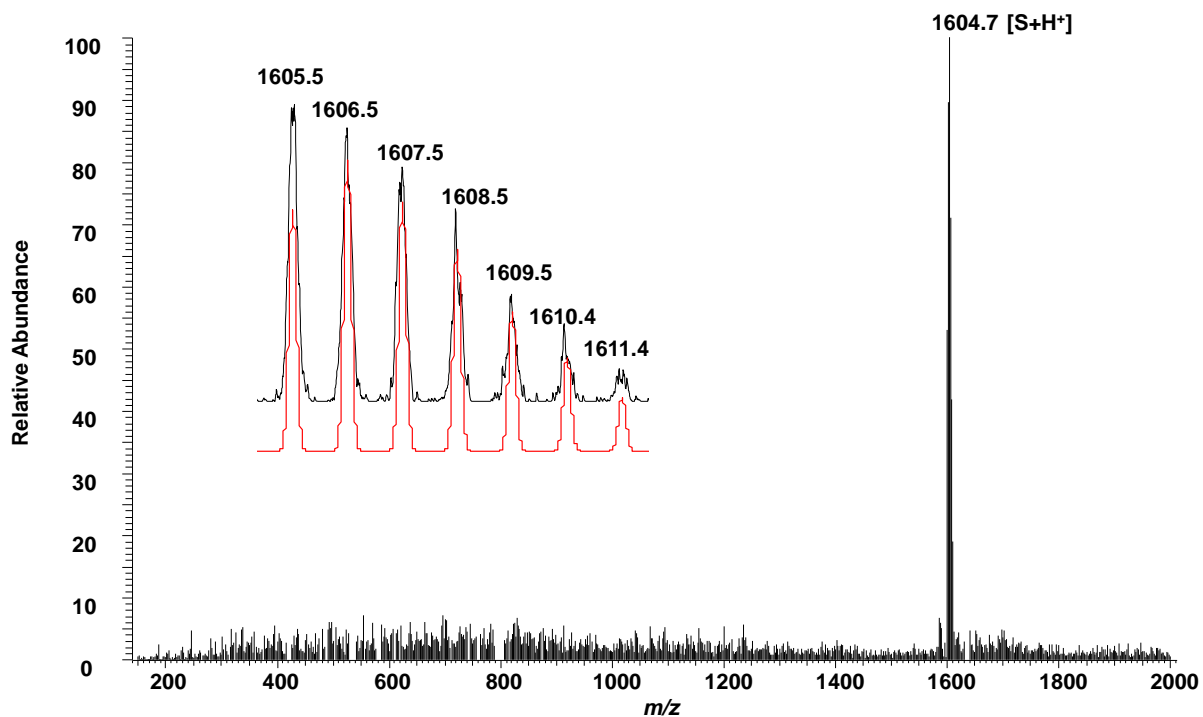


Figure S63. ESI-MS of compound S after protonation.

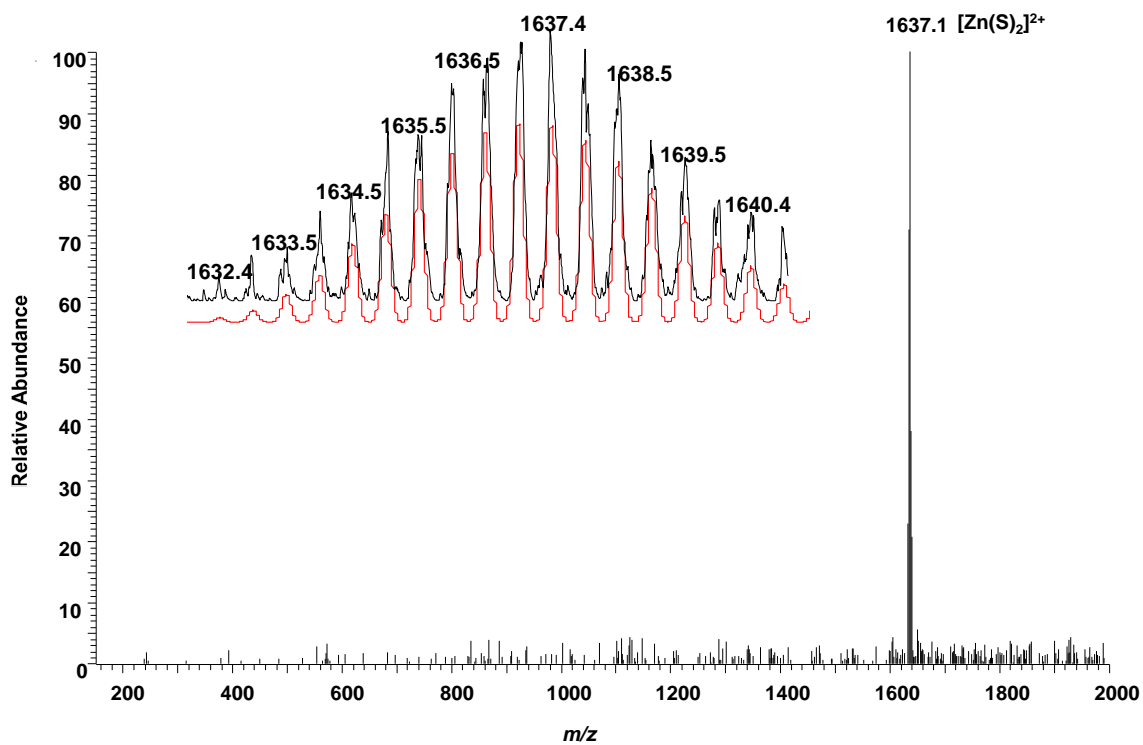


Figure S64. ESI-MS of  $[Zn(S)_2]^{2+}$ .

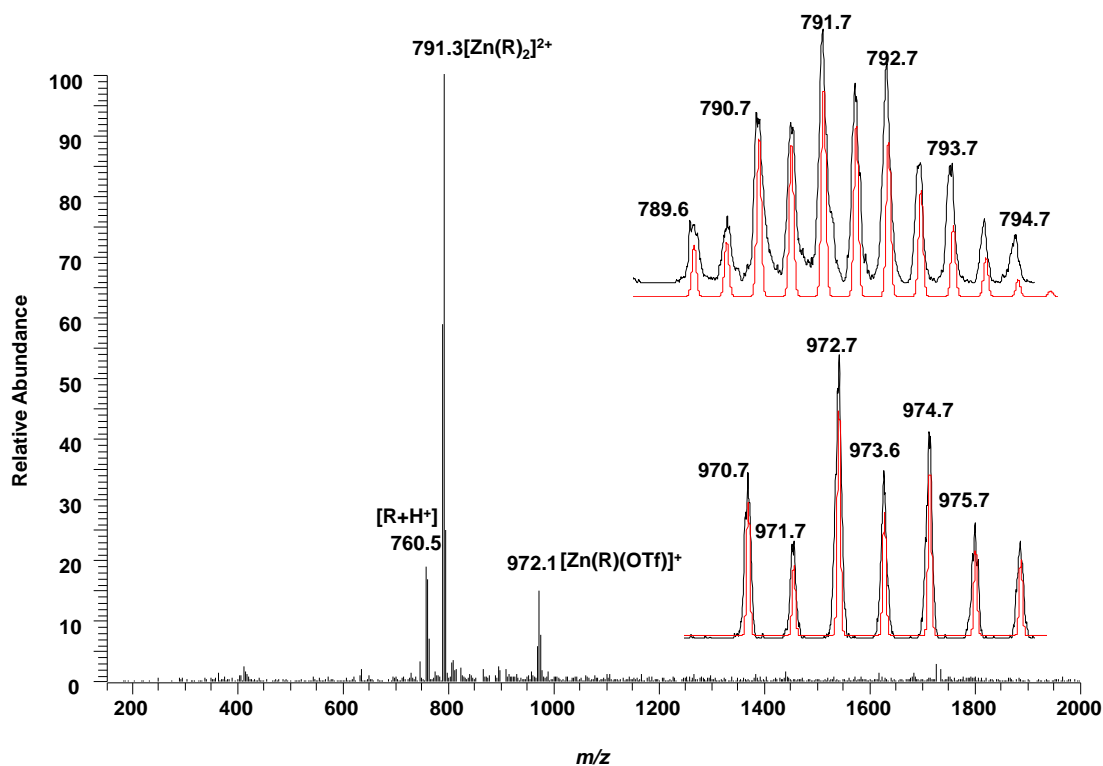


Figure S65. ESI-MS of  $[\text{Zn}(\text{R})_2]^{2+}$ .

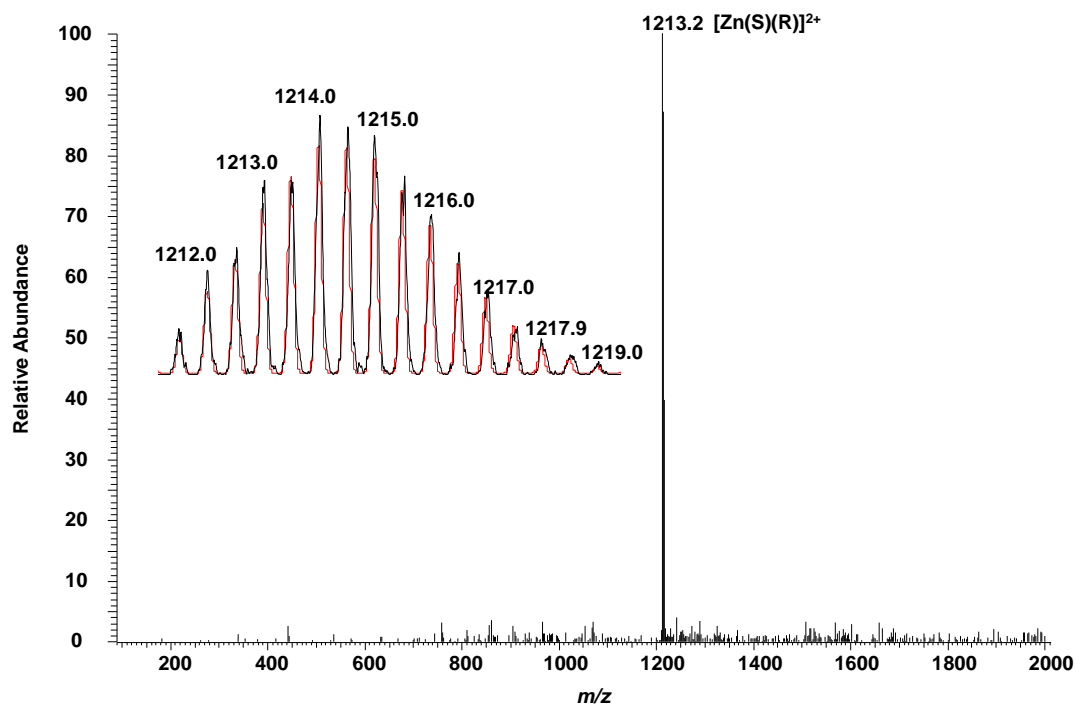
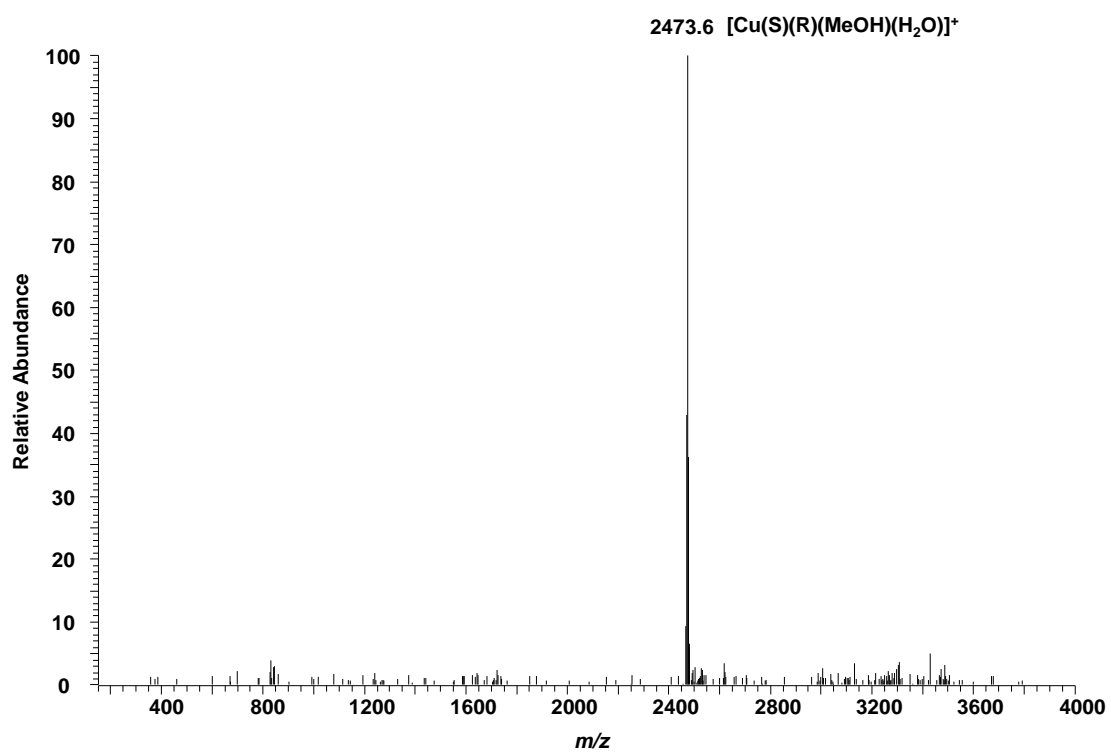


Figure S66. ESI-MS of nanorotor  $[\text{Zn}(\text{R})(\text{S})]^{2+}$ .

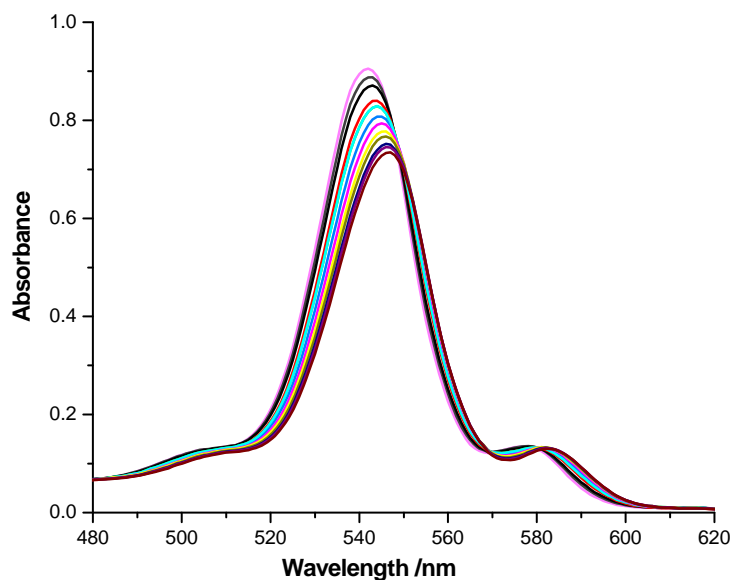


**Figure S67.** ESI-MS of nanorotor  $[\text{Cu}(\mathbf{R})(\mathbf{S})]^+$ .

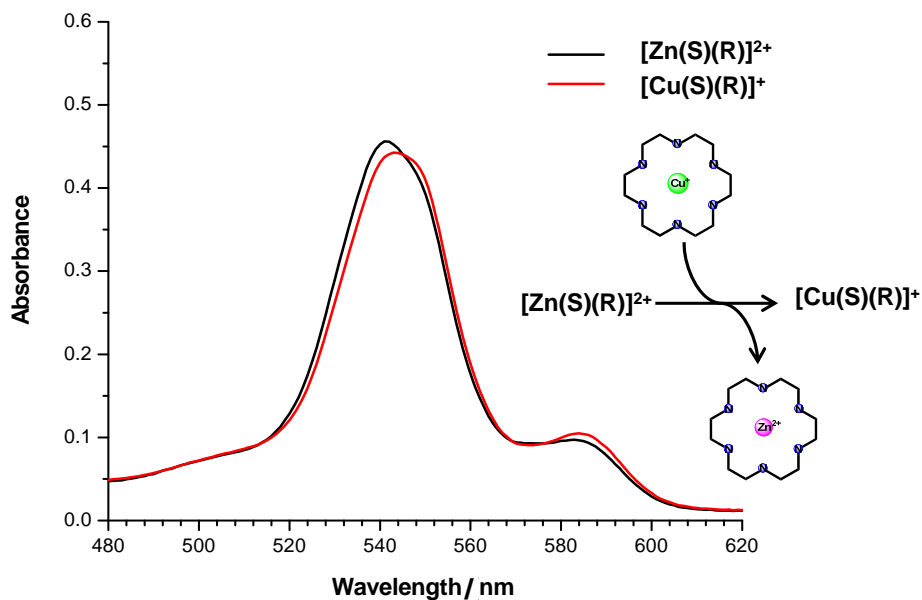
## 8. UV-Vis data

### Measurement of Binding Constant:

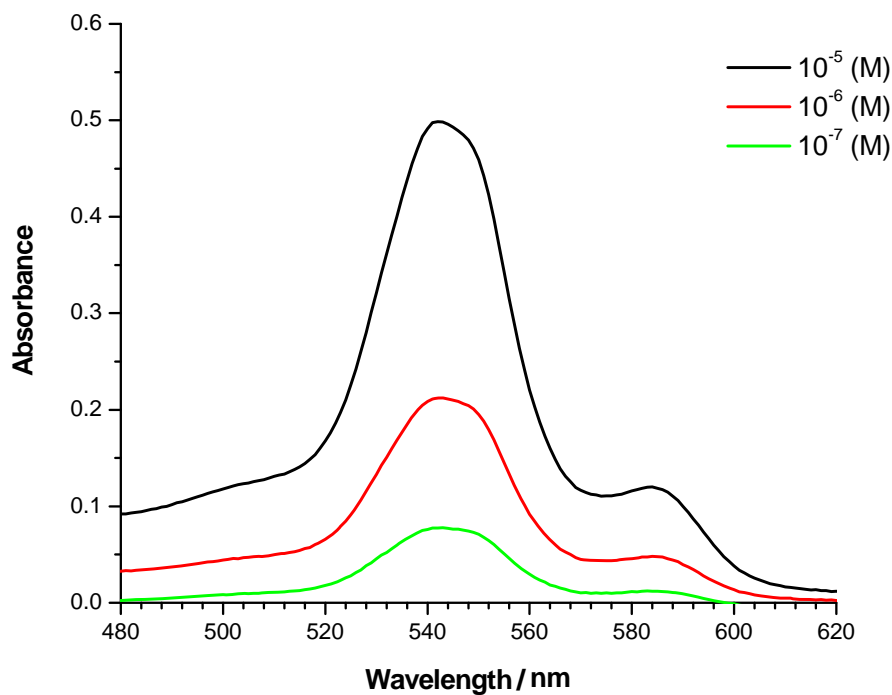
A UV-Vis titration was used to measure binding constant of complex **C1**



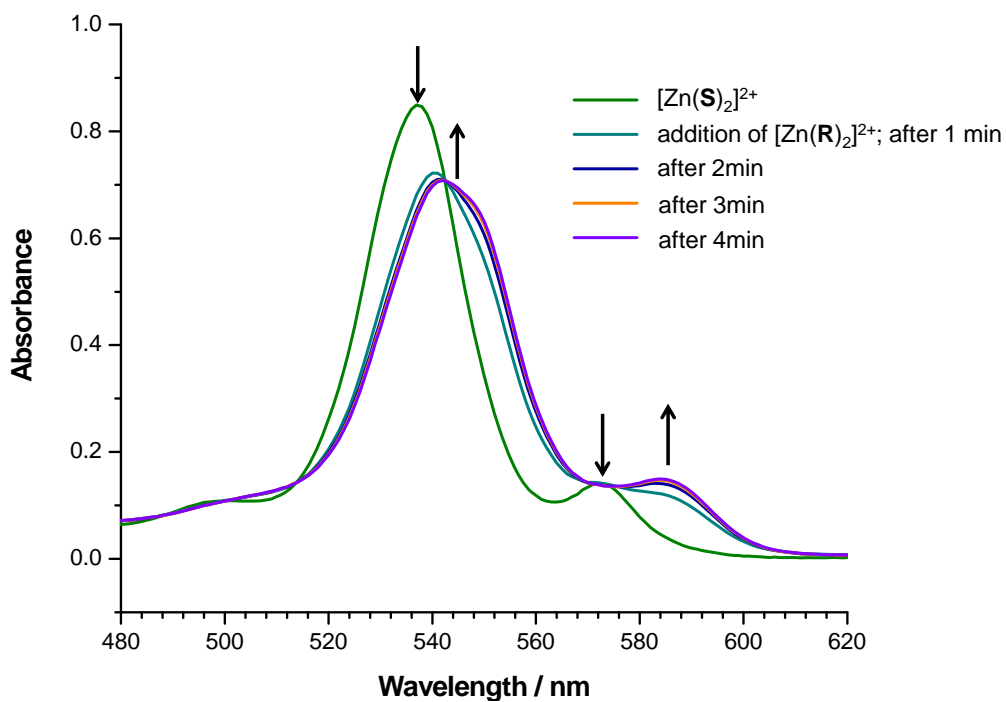
**Figure S68.** UV-vis titration of porphyrin **4** ( $1.2 \times 10^{-5}$  M) vs. **3** ( $1.1 \times 10^{-3}$  M) in  $\text{CH}_2\text{Cl}_2$  at 298 K. The binding constant was determined as  $\log K = 4.45 \pm 0.04$  using SPECFIT software.



**Figure S69.** Change in UV-vis from  $[\text{Zn}(\text{S})(\text{R})]^{2+}$  ( $10^{-5}$  M) to  $[\text{Cu}(\text{S})(\text{R})]^+$  after metal-metal exchange.

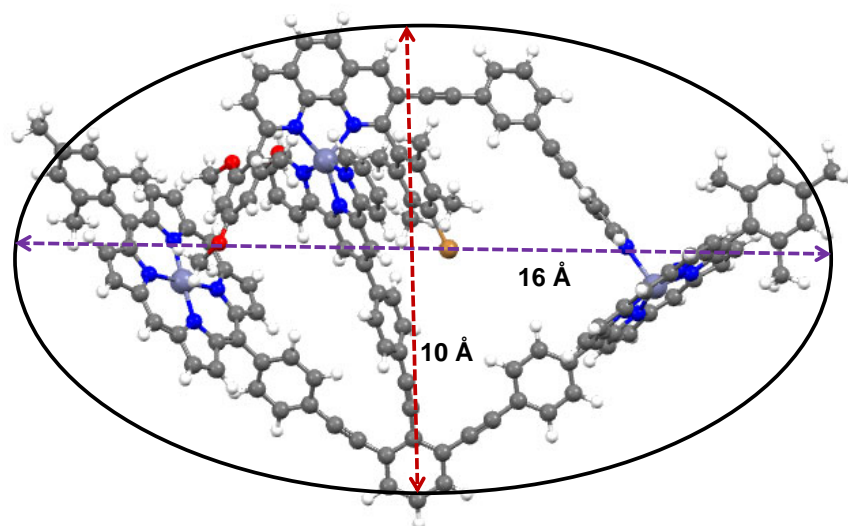


**Figure S70.** Change in UV-vis of nanorotor  $[\text{Cu}(\text{S})(\text{R})]^+$  at different concentrations.

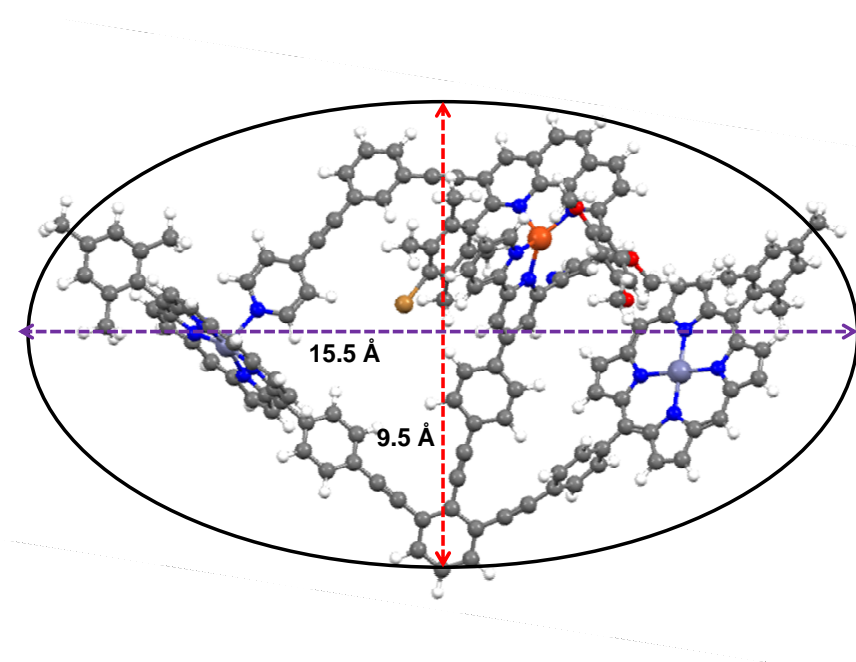


**Figure S71.** UV-vis spectra of fusion experiment, addition of  $[\text{Zn}(\text{R})_2]^{2+}$  ( $10^{-3}$  M) to  $[\text{Zn}(\text{S})_2]^{2+}$  ( $10^{-5}$  M), taken in 1-min intervals. The fusion process is fast and completed after 3 min.

## 9. Computational Results:

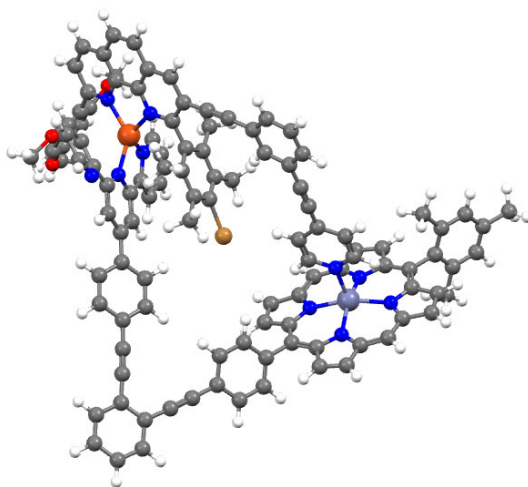


**Figure S72.** Hydrodynamic radius of  $[\text{Zn}(\text{S})(\text{R})]^{2+}$  from computed structure calculated using PM6 level. Radius  $r_{\text{com}} = (16+10)/2 = 13.0 \text{ \AA}$ .



**Figure S73.** Hydrodynamic radius of  $[\text{Cu}(\text{S})(\text{R})]^{+}$  from computed structure calculated using PM6 level. Radius  $r_{\text{com}} = (15.5+9.5)/2 = 12.5 \text{ \AA}$ .





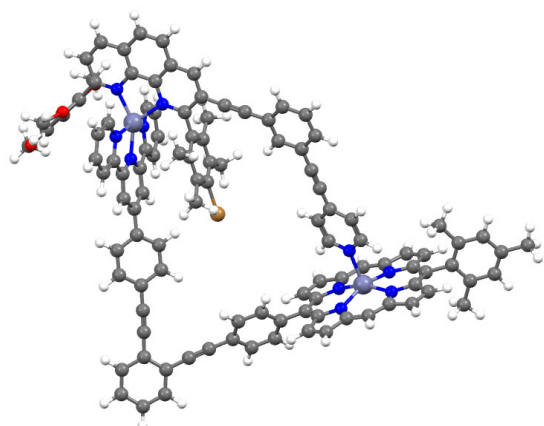
**Figure S74.** Perspective view of partial supramolecular nanorotor  $[\text{Cu}(\mathbf{S})(\mathbf{R})]^+$  obtained as energy minimized structure, calculated using Gaussian 09 at B3LYP/6-31G (d) level.

The x, y, z cartesian coordinates:

C	1.601956000	10.275534000	-0.371600000	C	-4.461837000	0.799936000	1.090030000
C	2.199924000	11.552533000	-0.419428000	H	-2.926440000	2.176079000	1.713221000
C	0.037720000	12.600754000	-0.732262000	C	-5.731392000	1.410174000	-0.787526000
C	-0.576877000	11.350658000	-0.685359000	H	-5.259273000	3.258551000	-1.731905000
C	0.181367000	10.174210000	-0.503013000	C	-6.835372000	1.149411000	-1.745859000
H	3.276935000	11.625528000	-0.318738000	C	-7.931544000	0.335816000	-1.428279000
H	-0.562955000	13.493038000	-0.872065000	C	-8.947995000	0.172728000	-2.375486000
C	-0.473458000	8.912411000	-0.440185000	H	-7.995990000	-0.122266000	-0.451829000
C	-1.051746000	7.838520000	-0.375204000	C	-7.725750000	1.628368000	-3.844558000
C	1.429583000	12.701045000	-0.596593000	C	-8.845022000	0.820923000	-3.610334000
C	-1.758149000	6.606620000	-0.299964000	H	-9.810818000	-0.443130000	-2.144834000
C	-3.140281000	6.557271000	-0.597707000	H	-7.605427000	2.161670000	-4.781376000
C	-1.110659000	5.404758000	0.072203000	H	-9.612739000	0.716573000	-4.368407000
C	-3.841931000	5.359869000	-0.517930000	C	-4.234993000	-0.193031000	2.159167000
H	-3.651011000	7.470293000	-0.881904000	C	-3.450497000	0.050177000	3.296469000
C	-1.818927000	4.208213000	0.154338000	C	-4.725820000	-2.356931000	2.930332000
H	-0.049311000	5.424150000	0.292235000	C	-3.296830000	-0.950857000	4.255533000
C	-3.199545000	4.165255000	-0.132062000	H	-2.975792000	1.011505000	3.442693000
H	-4.906766000	5.354596000	-0.726817000	C	-3.947919000	-2.177511000	4.071351000
H	-1.289760000	3.290133000	0.393970000	H	-5.272458000	-3.274211000	2.753630000
C	-3.968557000	2.907655000	-0.020185000	H	-2.688157000	-0.774049000	5.135014000
C	-3.710843000	1.972412000	0.996768000	H	-3.854289000	-2.977102000	4.796527000
C	-5.007877000	2.600439000	-0.911494000	N	-5.456893000	0.497557000	0.191806000

N	-4.860779000	-1.394693000	1.985164000	H	7.299143000	-1.816935000	-1.966450000
N	-6.743716000	1.795626000	-2.937733000	H	4.249459000	0.034291000	0.118803000
C	-6.855567000	-3.335072000	-1.553087000	N	5.832512000	-0.867865000	-0.855522000
C	-4.657624000	-2.709188000	-2.132735000	C	2.400967000	9.111884000	-0.204910000
C	-6.988298000	-4.161348000	-2.697293000	C	3.069587000	8.099555000	-0.071600000
C	-7.915098000	-3.271064000	-0.587910000	C	3.797245000	6.884527000	0.076468000
C	-4.715691000	-3.536767000	-3.305583000	C	5.133751000	6.871590000	0.532028000
C	-5.893118000	-4.238631000	-3.578890000	C	3.179178000	5.650427000	-0.227202000
C	-8.204824000	-4.904130000	-2.889836000	C	5.820469000	5.667048000	0.684328000
C	-9.084324000	-4.051571000	-0.778802000	H	5.620633000	7.810202000	0.773294000
H	-5.950033000	-4.867584000	-4.460296000	C	3.870705000	4.453080000	-0.066849000
C	-9.209247000	-4.854314000	-1.964676000	H	2.161470000	5.650106000	-0.602861000
H	-8.299967000	-5.520306000	-3.777712000	C	5.202823000	4.435458000	0.392416000
C	-10.068487000	-4.004886000	0.235359000	H	6.843013000	5.672891000	1.046567000
C	-8.665703000	-2.464312000	1.486409000	H	3.385212000	3.513448000	-0.309658000
H	-10.117335000	-5.431603000	-2.104657000	C	5.918602000	3.131762000	0.560089000
H	-10.979778000	-4.584109000	0.128709000	C	7.017591000	2.862976000	-0.280404000
C	-9.848191000	-3.232531000	1.360624000	C	5.436422000	2.256332000	1.556178000
H	-10.575847000	-3.196010000	2.161208000	N	7.752196000	1.687813000	-0.289645000
N	-5.710656000	-2.614353000	-1.296441000	C	7.556899000	3.772888000	-1.283235000
N	-7.727947000	-2.465937000	0.513874000	N	5.904092000	0.973417000	1.797245000
C	-3.572846000	-3.652214000	-4.139533000	C	4.410203000	2.580926000	2.536195000
C	-2.548133000	-3.731918000	-4.796697000	Zn	7.255900000	-0.121875000	0.635720000
C	-1.266543000	-3.756237000	-5.419849000	C	8.737811000	1.837567000	-1.250814000
C	-1.048298000	-4.310486000	-6.699518000	C	8.620160000	3.144511000	-1.868536000
C	-0.178995000	-3.212824000	-4.709940000	H	7.173752000	4.756543000	-1.503561000
C	0.238195000	-4.316011000	-7.244392000	C	5.215191000	0.491344000	2.899991000
H	-1.881712000	-4.730074000	-7.251502000	C	4.277141000	1.494951000	3.359317000
C	1.118893000	-3.228879000	-5.251764000	H	3.891528000	3.524376000	2.602941000
H	-0.342046000	-2.786793000	-3.727083000	N	9.042230000	-0.944042000	-0.056174000
H	0.401568000	-4.741172000	-8.228636000	N	7.251963000	-1.620932000	2.088701000
C	1.318777000	-3.786333000	-6.533836000	C	9.698381000	0.882302000	-1.585301000
H	2.315897000	-3.801586000	-6.958840000	H	9.266413000	3.522656000	-2.647942000
C	2.189186000	-2.702942000	-4.470359000	C	5.407885000	-0.758563000	3.489817000
C	3.027409000	-2.256464000	-3.705625000	H	3.626529000	1.389130000	4.216241000
C	3.977324000	-1.766807000	-2.766182000	C	9.858634000	-0.387131000	-1.027341000
C	5.351377000	-2.069545000	-2.882986000	C	9.579341000	-2.185364000	0.257477000
C	3.564890000	-0.983484000	-1.665762000	C	6.345312000	-1.727573000	3.129281000
C	6.238307000	-1.605928000	-1.916134000	C	8.019513000	-2.775935000	2.105277000
H	5.711962000	-2.663522000	-3.713701000	H	10.413691000	1.166016000	-2.351748000
C	4.517212000	-0.563107000	-0.743035000	H	4.777630000	-0.991531000	4.343459000
H	2.528468000	-0.701464000	-1.528346000	C	10.924686000	-1.314182000	-1.355363000

C	10.754648000	-2.420103000	-0.567649000	C	-7.955976000	-1.594622000	5.125389000
C	9.097837000	-3.062797000	1.246833000	C	-8.197182000	-0.215324000	5.121458000
C	6.537409000	-2.991621000	3.814821000	H	-8.750644000	1.516514000	4.002242000
C	7.564538000	-3.639114000	3.185761000	H	-7.673569000	-2.105460000	6.033509000
H	11.706275000	-1.128787000	-2.078510000	Br	0.399768000	0.548647000	-0.464187000
H	11.369129000	-3.306122000	-0.526724000	C	-0.544935000	-2.253456000	0.738328000
C	9.812452000	-4.376526000	1.430013000	H	-0.076892000	-3.206309000	0.459878000
H	5.968758000	-3.325229000	4.671443000	H	0.247490000	-1.546853000	0.973929000
H	7.991553000	-4.599782000	3.429019000	H	-1.123712000	-2.435755000	1.651464000
C	9.391984000	-5.518894000	0.708980000	C	-2.842751000	-3.786515000	-0.086114000
C	10.903083000	-4.474598000	2.327566000	H	-3.722893000	-4.284790000	-0.493440000
C	10.066327000	-6.734809000	0.895497000	H	-1.991302000	-4.467202000	-0.208757000
C	8.226128000	-5.448041000	-0.255367000	H	-2.999542000	-3.667641000	0.992384000
C	11.549669000	-5.709787000	2.484753000	C	-1.538676000	1.181932000	-2.914151000
C	11.377602000	-3.272437000	3.116856000	H	-2.254691000	1.995114000	-2.739530000
C	11.150256000	-6.851056000	1.776094000	H	-0.552017000	1.538082000	-2.625960000
H	9.735243000	-7.609248000	0.340641000	H	-1.533524000	0.984312000	-3.991541000
H	7.305550000	-5.129191000	0.248172000	C	-3.931377000	-0.266249000	-3.625550000
H	8.414912000	-4.726690000	-1.059940000	H	-4.206521000	0.783826000	-3.483251000
H	8.041124000	-6.424226000	-0.714289000	H	-3.397701000	-0.336061000	-4.582008000
H	12.384110000	-5.779253000	3.178010000	H	-4.860254000	-0.828651000	-3.727617000
H	11.716597000	-2.465408000	2.456450000	O	-8.101224000	0.587652000	6.242913000
H	10.576244000	-2.855988000	3.738082000	O	-7.853959000	-3.666480000	3.812899000
H	12.209907000	-3.542625000	3.773703000	O	-9.087557000	0.298490000	1.562281000
C	11.883766000	-8.164387000	1.939564000	C	-7.785650000	-0.012522000	7.530366000
H	12.290682000	-8.272746000	2.950717000	H	-7.797283000	0.815109000	8.237457000
H	11.225330000	-9.018007000	1.746124000	H	-8.540019000	-0.754149000	7.815413000
H	12.727956000	-8.239297000	1.240349000	H	-6.792088000	-0.474918000	7.518330000
H	1.911582000	13.672286000	-0.631232000	C	-7.675583000	-4.455261000	5.024065000
C	-3.410375000	-1.957743000	-1.781653000	H	-7.610978000	-5.487164000	4.682200000
C	-2.569658000	-2.458393000	-0.761841000	H	-6.751348000	-4.179994000	5.544489000
C	-3.074737000	-0.781413000	-2.488405000	H	-8.529929000	-4.338991000	5.699166000
C	-1.420265000	-1.726887000	-0.375464000	C	-9.469072000	1.706365000	1.542175000
C	-1.908386000	-0.058730000	-2.136049000	H	-8.623385000	2.346392000	1.813703000
C	-1.142937000	-0.538433000	-1.064512000	H	-9.765219000	1.902471000	0.513264000
C	-8.445554000	-1.660633000	2.719138000	H	-10.309955000	1.889844000	2.218473000
C	-8.689367000	-0.272324000	2.763037000	H	-1.653355000	11.265772000	-0.785572000
C	-8.086578000	-2.296984000	3.919185000	Cu	-5.972144000	-1.460842000	0.3393410
C	-8.561925000	0.454457000	3.945855000				



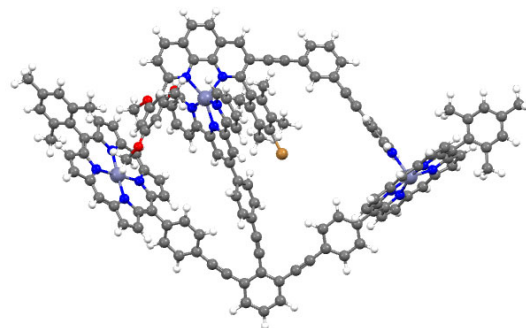
**Figure S75.** Perspective view of partial supramolecular nanorotor  $[\text{Zn}(\text{S})(\text{R})]^{2+}$  obtained from energy minimized structure, calculated using Gaussian 09 at B3LYP/6-31G (d) level

The x, y, z cartesian coordinates:

C	1.351384000	9.821790000	-0.694802000
C	1.975541000	11.087837000	-0.681642000
C	-0.140482000	12.186746000	-1.122370000
C	-0.781405000	10.950668000	-1.134103000
C	-0.059051000	9.755530000	-0.917651000
H	3.044905000	11.137593000	-0.511784000
H	-0.710868000	13.093802000	-1.289089000
C	-0.752261000	8.515910000	-0.894806000
C	-1.387210000	7.472460000	-0.848848000
C	1.241513000	12.254149000	-0.891228000
C	-2.163315000	6.289174000	-0.769913000
C	-3.528140000	6.301251000	-1.151743000
C	-1.607135000	5.072129000	-0.303325000
C	-4.305110000	5.154366000	-1.047164000
H	-3.963855000	7.224359000	-1.516114000
C	-2.391021000	3.929609000	-0.181628000
H	-0.554049000	5.041039000	-0.047804000
C	-3.757698000	3.958149000	-0.537466000
H	-5.356467000	5.196883000	-1.315954000
H	-1.932722000	2.984696000	0.092620000
C	-4.593031000	2.758474000	-0.368926000
C	-4.541642000	2.005254000	0.825212000
C	-5.472067000	2.321071000	-1.383979000
C	-5.339086000	0.872170000	0.968732000
H	-3.898197000	2.342690000	1.626770000
C	-6.198698000	1.144211000	-1.213953000
H	-5.525799000	2.881699000	-2.307805000
C	-7.072071000	0.536922000	-2.242425000
C	-7.343135000	1.128479000	-3.483801000
C	-8.166868000	0.462432000	-4.394699000
H	-6.921321000	2.091311000	-3.741824000
C	-8.415851000	-1.304592000	-2.786258000
C	-8.713685000	-0.777491000	-4.043339000
H	-8.378784000	0.904611000	-5.361480000
H	-8.831962000	-2.249401000	-2.462372000
H	-9.354655000	-1.322481000	-4.725358000
C	-5.453099000	0.065454000	2.202820000
C	-4.840703000	0.403257000	3.416882000
C	-6.449720000	-1.820037000	3.190053000
C	-5.046973000	-0.406428000	4.537138000
H	-4.223140000	1.288637000	3.495341000
C	-5.866764000	-1.536752000	4.426105000
H	-7.107019000	-2.668574000	3.056747000
H	-4.580670000	-0.154882000	5.482956000
H	-6.048767000	-2.183596000	5.275406000
N	-6.118488000	0.442417000	-0.056180000
N	-6.246251000	-1.043018000	2.104265000
N	-7.610339000	-0.670997000	-1.908163000
C	-7.129584000	-4.199812000	-0.458517000
C	-4.877974000	-3.538982000	-0.767939000
C	-6.861380000	-5.523629000	-0.889670000
C	-8.454925000	-3.844989000	-0.020107000
C	-4.534030000	-4.858647000	-1.225657000
C	-5.543168000	-5.826116000	-1.285814000
C	-7.922647000	-6.494442000	-0.893918000
C	-9.476830000	-4.828564000	-0.020545000
H	-5.300298000	-6.826684000	-1.625867000
C	-9.179164000	-6.159600000	-0.473757000
H	-7.702720000	-7.501293000	-1.231363000
C	-10.757110000	-4.433099000	0.438813000
C	-9.907328000	-2.193582000	0.840563000
H	-9.974434000	-6.897089000	-0.471815000
H	-11.566180000	-5.155855000	0.454284000
C	-10.965582000	-3.135584000	0.866077000

H	-11.934892000	-2.815079000	1.224635000	N	8.025627000	1.735458000	-1.104264000
N	-6.143585000	-3.242134000	-0.424475000	C	7.107081000	3.498492000	-2.294717000
N	-8.685917000	-2.555657000	0.398528000	N	7.352881000	1.455560000	1.674131000
C	-3.201482000	-5.169418000	-1.592432000	C	5.835702000	2.934921000	2.609252000
C	-2.059357000	-5.471013000	-1.902717000	Zn	8.394430000	0.246951000	0.316326000
C	-0.720571000	-5.812875000	-2.248560000	C	8.554080000	1.756539000	-2.385023000
C	-0.441026000	-7.011836000	-2.943680000	C	7.976579000	2.856146000	-3.131539000
C	0.338700000	-4.956411000	-1.888466000	H	6.526628000	4.382186000	-2.506241000
C	0.876397000	-7.336035000	-3.269697000	C	7.207969000	1.178613000	3.025487000
H	-1.254648000	-7.672522000	-3.220421000	C	6.255477000	2.098974000	3.608975000
C	1.668661000	-5.286873000	-2.209088000	H	5.128170000	3.744856000	2.687658000
H	0.129093000	-4.036548000	-1.355192000	N	9.946109000	-0.486669000	-0.867884000
H	1.087851000	-8.254892000	-3.804905000	N	9.285978000	-0.750711000	1.915006000
C	1.926028000	-6.488459000	-2.908715000	C	9.522651000	0.881871000	-2.879744000
H	2.948596000	-6.746017000	-3.159295000	H	8.227456000	3.113185000	-4.150768000
C	2.736038000	-4.423855000	-1.823340000	C	7.892180000	0.184026000	3.726593000
C	3.646835000	-3.688663000	-1.481583000	H	5.960088000	2.109780000	4.648644000
C	4.706099000	-2.829610000	-1.072025000	C	10.181479000	-0.135963000	-2.186945000
C	6.043371000	-3.087548000	-1.442348000	C	10.860875000	-1.481591000	-0.548956000
C	4.451006000	-1.690872000	-0.277249000	C	8.859215000	-0.691502000	3.230017000
C	7.046814000	-2.221047000	-1.018437000	C	10.276502000	-1.719985000	1.860239000
H	6.287368000	-3.948965000	-2.051503000	H	9.827758000	1.036932000	-3.910468000
C	5.510978000	-0.877045000	0.108443000	H	7.669694000	0.103574000	4.786657000
H	3.439665000	-1.452758000	0.028924000	C	11.253715000	-0.950508000	-2.723875000
H	8.083687000	-2.376079000	-1.287619000	C	11.673080000	-1.778687000	-1.718229000
H	5.361515000	0.003077000	0.720625000	C	11.013829000	-2.082051000	0.715906000
N	6.790637000	-1.132422000	-0.254395000	C	9.592398000	-1.657169000	4.026106000
C	2.132533000	8.647748000	-0.508685000	C	10.465322000	-2.290615000	3.185567000
C	2.853153000	7.671268000	-0.373340000	H	11.643789000	-0.878329000	-3.729078000
C	3.718066000	6.547741000	-0.229563000	H	12.466833000	-2.508763000	-1.747802000
C	4.843976000	6.608790000	0.622170000	C	12.062696000	-3.152879000	0.863832000
C	3.486732000	5.355976000	-0.952189000	H	9.462904000	-1.812399000	5.087698000
C	5.701910000	5.517836000	0.744873000	H	11.181064000	-3.060281000	3.428734000
H	5.041555000	7.521054000	1.174265000	C	11.734421000	-4.505840000	0.619400000
C	4.356260000	4.273652000	-0.831263000	C	13.381748000	-2.805470000	1.248369000
H	2.630397000	5.297688000	-1.615976000	C	12.726275000	-5.488512000	0.763878000
C	5.478990000	4.329937000	0.019300000	C	10.335340000	-4.909810000	0.201558000
H	6.569989000	5.587554000	1.391318000	C	14.341465000	-3.818503000	1.379812000
H	4.171677000	3.368576000	-1.400833000	C	13.766355000	-1.365501000	1.517321000
C	6.413365000	3.167701000	0.134600000	C	14.035327000	-5.166975000	1.142847000
C	7.133414000	2.792030000	-1.020633000	H	12.467857000	-6.527319000	0.575720000
C	6.538884000	2.544584000	1.396122000	H	9.584209000	-4.571724000	0.925479000

H	10.066501000	-4.474507000	-0.769562000	C	-4.179460000	-1.828549000	-3.057352000
H	10.255352000	-5.997602000	0.114060000	H	-4.616184000	-0.890518000	-3.416221000
H	15.351819000	-3.546214000	1.674204000	H	-3.472033000	-2.167788000	-3.823161000
H	13.580040000	-0.727625000	0.645322000	H	-4.983233000	-2.565388000	-3.010818000
H	13.190496000	-0.941940000	2.348923000	O	-11.086230000	3.075373000	2.562940000
H	14.827683000	-1.288299000	1.770303000	O	-9.589446000	-1.500287000	3.489720000
C	15.093187000	-6.237817000	1.294533000	O	-10.801148000	-0.229440000	-0.894169000
H	15.491288000	-6.264639000	2.316595000	C	-11.043311000	3.493670000	3.960056000
H	14.692400000	-7.230306000	1.066787000	H	-11.368512000	4.532033000	3.950813000
H	15.942775000	-6.058491000	0.623929000	H	-11.729198000	2.895029000	4.568419000
H	1.744631000	13.214940000	-0.879147000	H	-10.025275000	3.426917000	4.358942000
C	-3.821678000	-2.485891000	-0.619830000	C	-9.715568000	-1.346810000	4.937339000
C	-3.133240000	-2.394294000	0.610817000	H	-9.478270000	-2.327062000	5.348149000
C	-3.490082000	-1.656093000	-1.716668000	H	-9.008029000	-0.602840000	5.317529000
C	-2.122442000	-1.416626000	0.776461000	H	-10.737596000	-1.068240000	5.211162000
C	-2.471517000	-0.686014000	-1.563815000	C	-11.526074000	0.645094000	-1.813984000
C	-1.835596000	-0.591326000	-0.317020000	H	-10.959134000	1.559547000	-2.015258000
C	-10.132714000	-0.798664000	1.302012000	H	-11.633676000	0.066102000	-2.729369000
C	-10.623772000	0.188040000	0.418562000	H	-12.512065000	0.897276000	-1.412499000
C	-10.011003000	-0.463854000	2.662062000	H	-1.850519000	10.889735000	-1.304848000
C	-10.925078000	1.472835000	0.862592000	Zn	-6.990287000	-1.395193000	0.102611000
C	-10.311486000	0.819546000	3.136224000				
C	-10.763695000	1.781624000	2.222180000				
H	-11.302858000	2.244837000	0.208027000				
H	-10.207063000	1.058459000	4.183876000				
Br	-0.419473000	0.762064000	-0.139461000				
C	-1.385120000	-1.317947000	2.090907000				
H	-0.814961000	-2.232139000	2.298059000				
H	-0.687908000	-0.483078000	2.078575000				
H	-2.076021000	-1.176409000	2.930371000				
C	-3.405918000	-3.355465000	1.749783000				
H	-2.529501000	-3.987093000	1.942508000				
H	-3.622518000	-2.826801000	2.684062000				
H	-4.246385000	-4.020065000	1.545390000				
C	-2.051819000	0.220625000	-2.698632000				
H	-2.265745000	1.270988000	-2.466610000				
H	-0.972306000	0.155266000	-2.868581000				
H	-2.551859000	-0.026977000	-3.634088000				
C	2.726800000	9.143610000	0.119161000				



**Figure S76.** Perspective view of supramolecular nanorotor  $[\text{Zn}(\text{S})(\text{R})]^{2+}$  obtained from energy minimized structure, calculated using PM6 level.

The x, y, z cartesian coordinates:

C	2.929968000	10.530007000	0.261264000
C	0.532636000	10.892992000	0.421901000
C	0.306753000	9.518474000	0.278853000

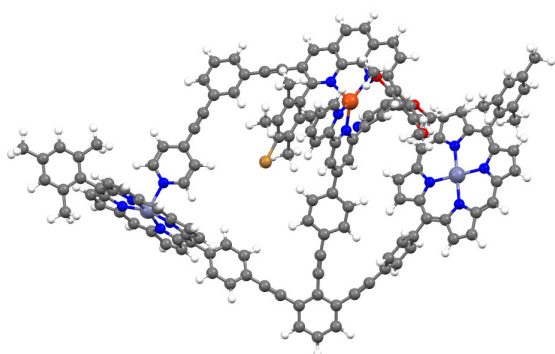
C	1.407811000	8.632299000	0.111114000	N	-4.416363000	-2.454249000	1.225218000
H	3.947765000	10.925085000	0.259247000	N	-2.760575000	-3.320905000	-2.544212000
H	-0.311042000	11.573103000	0.546163000	C	-3.290076000	-6.109727000	0.381571000
C	1.146552000	7.252174000	-0.061264000	C	-1.228659000	-5.006951000	0.748986000
C	0.843373000	6.088951000	-0.211539000	C	-2.825934000	-7.306961000	0.964892000
C	1.841616000	11.389489000	0.405666000	C	-4.639200000	-6.048743000	-0.172277000
C	0.386977000	4.761687000	-0.362532000	C	-0.692010000	-6.205428000	1.362186000
C	-0.268502000	4.374731000	-1.550443000	C	-1.496063000	-7.329699000	1.468526000
C	0.513864000	3.838364000	0.696987000	C	-3.705986000	-8.449772000	1.016223000
C	-0.847156000	3.112244000	-1.650347000	C	-5.465065000	-7.187845000	-0.117673000
H	-0.326420000	5.077632000	-2.384817000	H	-1.109283000	-8.244335000	1.933456000
C	-0.073290000	2.582164000	0.595541000	C	-4.964259000	-8.392782000	0.498598000
H	1.060500000	4.127033000	1.597166000	H	-3.328931000	-9.366477000	1.481677000
C	-0.783481000	2.221654000	-0.565065000	C	-6.771828000	-7.088564000	-0.686821000
H	-1.371166000	2.830507000	-2.563562000	C	-6.297611000	-4.773629000	-1.289619000
H	0.025672000	1.864071000	1.419301000	H	-5.628165000	-9.263205000	0.535657000
C	-1.485895000	0.931404000	-0.614843000	H	-7.436259000	-7.959423000	-0.658757000
C	-2.349031000	0.572777000	0.442637000	C	-7.173909000	-5.908486000	-1.260747000
C	-1.331736000	0.049184000	-1.704363000	H	-8.167782000	-5.798877000	-1.709485000
C	-3.005893000	-0.659452000	0.403286000	N	-2.493804000	-4.963584000	0.292421000
H	-2.503758000	1.267069000	1.273307000	N	-5.057329000	-4.844171000	-0.751965000
C	-2.012253000	-1.172141000	-1.693850000	C	0.635219000	-6.207521000	1.829715000
H	-0.670185000	0.322901000	-2.530531000	C	1.780895000	-6.214574000	2.225617000
C	-1.994643000	-2.190479000	-2.785427000	C	3.121221000	-6.226665000	2.683448000
C	-1.295973000	-2.013112000	-3.981966000	C	3.546495000	-7.222853000	3.583450000
C	-1.383661000	-3.002841000	-4.974359000	C	4.022064000	-5.245906000	2.231052000
H	-0.691558000	-1.118308000	-4.152096000	C	4.870447000	-7.233298000	4.028178000
C	-2.853270000	-4.256424000	-3.521497000	H	2.846191000	-7.982658000	3.931536000
C	-2.172476000	-4.126907000	-4.748204000	C	5.352375000	-5.269230000	2.681961000
H	-0.839445000	-2.881899000	-5.917814000	H	3.693906000	-4.473360000	1.535622000
H	-3.506990000	-5.124919000	-3.331351000	H	5.202513000	-8.005052000	4.727250000
H	-2.266823000	-4.907875000	-5.507674000	C	5.774498000	-6.266028000	3.584575000
C	-3.976149000	-1.155448000	1.421642000	H	6.810383000	-6.279579000	3.932893000
C	-4.438381000	-0.366432000	2.477472000	C	6.274227000	-4.293325000	2.226977000
C	-5.324959000	-2.960926000	2.095208000	C	7.070636000	-3.468106000	1.841682000
C	-5.373753000	-0.910243000	3.372924000	C	8.005891000	-2.501776000	1.389639000
H	-4.095052000	0.663970000	2.604159000	C	8.680450000	-1.676284000	2.304668000
C	-5.817795000	-2.215348000	3.184901000	C	8.273847000	-2.354941000	0.017847000
H	-5.685640000	-3.985588000	1.913777000	C	9.592479000	-0.728332000	1.820712000
H	-5.752206000	-0.304311000	4.203368000	H	8.504526000	-1.769071000	3.376363000
H	-6.547146000	-2.663786000	3.865697000	C	9.198332000	-1.385937000	-0.394046000
N	-2.813272000	-1.525899000	-0.639447000	H	7.780308000	-2.987818000	-0.717937000

H	10.138900000	-0.069317000	2.519641000	C	13.428779000	-1.722907000	-2.823413000
H	9.431190000	-1.253421000	-1.466265000	C	13.987712000	-1.191751000	-0.399649000
N	9.850896000	-0.573496000	0.488775000	C	14.172898000	0.300134000	2.901331000
C	3.823073000	8.258044000	0.004844000	C	14.655032000	-0.587630000	1.975820000
C	4.738828000	7.469390000	-0.069932000	H	12.363497000	-1.524442000	-4.743543000
C	5.780935000	6.514439000	-0.136622000	H	14.207132000	-2.443535000	-2.993212000
C	7.130340000	6.915419000	-0.152727000	C	15.122171000	-2.150335000	-0.467411000
C	5.457797000	5.143262000	-0.171613000	H	14.549709000	0.514586000	3.880139000
C	8.140363000	5.955778000	-0.190030000	H	15.502591000	-1.244486000	2.055392000
H	7.381731000	7.976306000	-0.136824000	C	14.938217000	-3.493685000	-0.085985000
C	6.471556000	4.189397000	-0.207871000	C	16.386137000	-1.710094000	-0.916600000
H	4.413690000	4.836071000	-0.165996000	C	16.013198000	-4.388621000	-0.151932000
C	7.821885000	4.586073000	-0.209971000	C	13.598707000	-3.958440000	0.387447000
H	9.187600000	6.262051000	-0.209607000	C	17.450765000	-2.616211000	-0.976697000
H	6.228750000	3.128976000	-0.228263000	C	16.580720000	-0.287766000	-1.322532000
C	8.885683000	3.564583000	-0.230123000	C	17.270210000	-3.954471000	-0.595832000
C	9.087819000	2.833413000	-1.418867000	H	15.872469000	-5.424962000	0.143190000
C	9.670920000	3.380700000	0.915240000	H	13.283112000	-3.400578000	1.282559000
N	9.968668000	1.811562000	-1.606220000	H	12.830542000	-3.793645000	-0.383539000
C	8.348666000	3.102105000	-2.694606000	H	13.583966000	-5.024584000	0.643652000
N	10.656064000	2.445533000	1.090653000	H	18.426648000	-2.280910000	-1.321084000
C	9.539522000	4.205975000	2.162898000	H	15.900316000	-0.009435000	-2.144207000
Zn	11.215045000	0.926403000	-0.204843000	H	16.362940000	0.400156000	-0.489561000
C	9.865711000	1.407146000	-2.984613000	H	17.601662000	-0.071581000	-1.661394000
C	8.813986000	2.243731000	-3.625856000	C	18.420806000	-4.903849000	-0.665850000
H	7.605574000	3.872869000	-2.784632000	H	19.243499000	-4.580686000	-0.010233000
C	11.213426000	2.653695000	2.397276000	H	18.154297000	-5.925587000	-0.366465000
C	10.459829000	3.768362000	3.044341000	H	18.829088000	-4.963097000	-1.685781000
H	8.818133000	4.996375000	2.264810000	H	2.010728000	12.463815000	0.512030000
N	12.100071000	-0.177273000	-1.703036000	Zn	-3.590661000	-3.436971000	-0.550252000
N	12.789416000	0.466731000	1.046845000	C	-0.996131000	8.960564000	0.311851000
C	10.607187000	0.459927000	-3.601815000	C	-2.056976000	8.378173000	0.343439000
H	8.538720000	2.144446000	-4.659074000	C	-3.231093000	7.586692000	0.368215000
C	12.246650000	1.980273000	2.950914000	C	-4.435678000	8.044835000	0.928955000
H	10.676203000	4.118785000	4.037010000	C	-3.157306000	6.281969000	-0.163988000
C	11.677009000	-0.291797000	-3.001005000	C	-5.547684000	7.200249000	0.975363000
C	13.201894000	-1.048446000	-1.561448000	H	-4.497597000	9.057325000	1.330962000
C	13.014461000	0.951027000	2.297798000	C	-4.268621000	5.445324000	-0.117657000
C	13.806415000	-0.497072000	0.793696000	H	-2.223114000	5.934469000	-0.606714000
H	10.427739000	0.245880000	-4.661313000	C	-5.466446000	5.898053000	0.461296000
H	12.576155000	2.236772000	3.963063000	H	-6.481241000	7.552964000	1.415597000
C	12.488213000	-1.258202000	-3.715171000	H	-4.214039000	4.440568000	-0.529859000



C	-6.623173000	4.974690000	0.523769000	C	-14.967926000	-2.593318000	0.745328000
C	-6.725174000	4.114583000	1.636225000	H	-13.795590000	-3.738210000	-0.659926000
C	-7.554089000	4.985053000	-0.507958000	H	-11.580646000	-1.423564000	-1.819320000
N	-7.648815000	3.122190000	1.809406000	H	-10.672067000	-2.076117000	-0.437904000
C	-5.810169000	4.169396000	2.816387000	H	-11.646603000	-3.151697000	-1.460447000
N	-8.635781000	4.131485000	-0.652203000	H	-15.911075000	-1.230160000	2.129468000
C	-7.530074000	5.957068000	-1.648565000	H	-13.247342000	0.874132000	2.968176000
C	-7.366259000	2.507311000	3.082761000	H	-14.077242000	1.669413000	1.624145000
C	-6.204876000	3.214192000	3.684277000	H	-15.011360000	0.835863000	2.868918000
H	-5.014419000	4.891258000	2.900322000	C	-16.088752000	-3.575460000	0.796064000
C	-9.329635000	4.543292000	-1.834838000	H	-17.003237000	-3.155824000	0.345965000
C	-8.592203000	5.697091000	-2.433160000	H	-15.872355000	-4.509842000	0.261878000
H	-6.769011000	6.714653000	-1.747408000	H	-16.345652000	-3.849065000	1.830801000
C	-8.025593000	1.458337000	3.623363000	C	-0.386331000	-3.795844000	0.580990000
H	-5.812397000	2.976784000	4.656388000	C	-0.361045000	-2.820538000	1.596022000
C	-10.453389000	3.986512000	-2.343718000	C	0.391675000	-3.674965000	-0.588454000
H	-8.916811000	6.192960000	-3.332500000	C	0.408747000	-1.651733000	1.405131000
C	-9.137558000	0.776943000	3.023098000	C	1.163432000	-2.509980000	-0.781303000
H	-7.735291000	1.095607000	4.615725000	C	1.133669000	-1.514893000	0.210278000
C	-11.153815000	2.880900000	-1.755953000	C	-6.723129000	-3.516654000	-1.903228000
H	-10.897903000	4.402499000	-3.254978000	C	-6.519315000	-3.264877000	-3.287535000
N	-9.745287000	1.127135000	1.833101000	C	-7.428136000	-2.528179000	-1.166709000
C	-9.797077000	-0.361920000	3.608681000	C	-6.958782000	-2.102563000	-3.904669000
N	-10.783582000	2.217717000	-0.626880000	C	-7.887320000	-1.346285000	-1.749600000
C	-12.370399000	2.299180000	-2.327158000	C	-7.649213000	-1.147345000	-3.120512000
Zn	-9.230895000	2.671925000	0.615514000	H	-6.813427000	-1.897510000	-4.961893000
C	-10.815519000	0.228654000	1.662057000	H	-8.419729000	-0.599676000	-1.166974000
C	-10.840098000	-0.696492000	2.764414000	Br	2.133088000	0.088801000	-0.076983000
H	-9.538704000	-0.815741000	4.542388000	C	0.478319000	-0.587233000	2.448253000
C	-11.754553000	1.179488000	-0.431889000	H	1.512567000	-0.464170000	2.819075000
C	-12.737488000	1.266585000	-1.514416000	H	0.163822000	0.400967000	2.061206000
H	-12.858684000	2.665607000	-3.210268000	H	-0.140898000	-0.804440000	3.332452000
C	-11.772189000	0.274575000	0.608940000	C	-1.113163000	-3.066659000	2.863009000
H	-11.564118000	-1.481732000	2.886977000	H	-0.680293000	-3.923083000	3.409236000
H	-13.587361000	0.609293000	-1.600083000	H	-1.066832000	-2.211049000	3.559004000
C	-12.871282000	-0.722044000	0.652092000	H	-2.173491000	-3.285679000	2.692189000
C	-12.802148000	-1.900567000	-0.117059000	C	2.010713000	-2.330231000	-1.996383000
C	-14.001095000	-0.477548000	1.465783000	H	1.738583000	-1.428640000	-2.564372000
C	-13.845918000	-2.829945000	-0.064317000	H	3.076594000	-2.218106000	-1.725351000
C	-11.620430000	-2.156269000	-0.998526000	H	1.959741000	-3.183124000	-2.691427000
C	-15.037420000	-1.416470000	1.505673000	C	0.410875000	-4.799356000	-1.572503000
C	-14.092955000	0.775977000	2.268228000	H	1.016548000	-4.571485000	-2.467139000

H	0.865054000	-5.700181000	-1.123846000
H	-0.590481000	-5.073721000	-1.923561000
O	-8.029049000	-0.063888000	-3.833382000
O	-7.602654000	-2.861002000	0.146469000
O	-5.847589000	-4.277658000	-3.925681000
C	-8.784376000	0.992773000	-3.171197000
H	-8.990754000	1.672749000	-4.011056000
H	-9.716419000	0.596502000	-2.754393000
H	-8.163083000	1.480747000	-2.414217000
C	-8.477058000	-2.023775000	0.959505000
H	-8.520004000	-2.579722000	1.903416000
H	-8.036950000	-1.030968000	1.094834000
H	-9.482434000	-1.962424000	0.502001000
C	-5.827167000	-4.265154000	-5.381734000
H	-5.202157000	-3.441690000	-5.737937000
H	-5.387009000	-5.243741000	-5.611443000
H	-6.847631000	-4.199588000	-5.7779580



**Figure S77.** Perspective view of supramolecular nanorotor  $[\text{Cu}(\text{S})(\text{R})]^+$  obtained from energy minimized structure, calculated using PM6 level.

The x, y, z cartesian coordinates:

C	-2.442369000	9.211799000	0.024245000
C	-2.693077000	10.597547000	0.029756000
C	-0.310942000	11.056488000	0.115501000
C	-0.038947000	9.682073000	0.108558000
C	-1.108098000	8.743760000	0.062657000
H	-3.723422000	10.955001000	0.000222000
H	0.511235000	11.771661000	0.151459000
C	-0.797290000	7.363621000	0.053006000

C	-0.448665000	6.204064000	0.042905000
C	-1.635269000	11.505183000	0.075323000
C	0.043810000	4.878121000	0.020846000
C	1.435705000	4.672473000	0.122719000
C	-0.818466000	3.773466000	-0.110671000
C	1.957189000	3.382277000	0.075043000
H	2.101606000	5.532117000	0.235158000
C	-0.290422000	2.483872000	-0.159216000
H	-1.895215000	3.933295000	-0.178450000
C	1.096699000	2.282303000	-0.077289000
H	3.035303000	3.230508000	0.144749000
H	-0.960833000	1.620596000	-0.244708000
C	1.659916000	0.920445000	-0.169032000
C	1.342834000	0.094484000	-1.262140000
C	2.532260000	0.429722000	0.809094000
C	1.903853000	-1.186517000	-1.337019000
H	0.672160000	0.461648000	-2.041513000
C	3.064374000	-0.867366000	0.674501000
H	2.789479000	1.035690000	1.682153000
C	4.005503000	-1.376508000	1.715663000
C	5.263967000	-1.908728000	1.395372000
C	6.096182000	-2.331448000	2.440883000
H	5.603815000	-1.988758000	0.357842000
C	4.387956000	-1.660051000	4.001593000
C	5.661585000	-2.208941000	3.760534000
H	7.081020000	-2.749285000	2.216044000
H	4.001474000	-1.541728000	5.022424000
H	6.288945000	-2.529995000	4.590584000
C	1.625970000	-2.086387000	-2.494003000
C	0.617684000	-1.820612000	-3.435648000
C	2.279052000	-4.018583000	-3.654243000
C	0.463622000	-2.689528000	-4.521649000
H	-0.041501000	-0.957575000	-3.320854000
C	1.305707000	-3.796636000	-4.642996000
H	2.967787000	-4.876669000	-3.707619000
H	-0.309067000	-2.497904000	-5.269467000
H	1.211204000	-4.479172000	-5.486119000
N	2.760363000	-1.686609000	-0.377938000
N	2.442412000	-3.190888000	-2.587182000
N	3.568542000	-1.247098000	3.005665000
C	3.288221000	-5.867588000	0.867622000
C	1.111222000	-4.987264000	0.906212000

C	2.966295000	-6.866382000	1.816014000	C	-4.431520000	7.499836000	-0.049281000
C	4.633716000	-5.832414000	0.294580000	C	-5.487460000	6.557228000	-0.082462000
C	0.701689000	-5.992917000	1.863804000	C	-6.636588000	6.800250000	-0.859170000
C	1.636902000	-6.910005000	2.314808000	C	-5.386914000	5.367475000	0.663897000
C	3.974122000	-7.810145000	2.236548000	C	-7.665259000	5.860907000	-0.892930000
C	5.582978000	-6.792334000	0.712214000	H	-6.718926000	7.724941000	-1.430101000
H	1.359234000	-7.672829000	3.046798000	C	-6.419486000	4.432378000	0.626754000
C	5.226500000	-7.772947000	1.708818000	H	-4.501697000	5.184830000	1.271574000
H	3.697390000	-8.553734000	2.986648000	C	-7.565001000	4.668208000	-0.154466000
C	6.873559000	-6.758011000	0.108858000	H	-8.560740000	6.048919000	-1.486301000
C	6.130698000	-4.881341000	-1.247531000	H	-6.345898000	3.513966000	1.205583000
H	5.992715000	-8.486112000	2.020609000	C	-8.651172000	3.670338000	-0.191074000
H	7.630492000	-7.480963000	0.421072000	C	-9.469008000	3.531983000	0.944689000
C	7.141424000	-5.824007000	-0.861121000	C	-8.861650000	2.939014000	-1.372232000
H	8.114093000	-5.774188000	-1.354267000	N	-10.477600000	2.629161000	1.117342000
N	2.368368000	-4.918444000	0.429140000	C	-9.353673000	4.396453000	2.165278000
N	4.910056000	-4.860158000	-0.666485000	N	-9.774991000	1.940760000	-1.557574000
C	-0.634278000	-6.028315000	2.316424000	C	-8.080998000	3.144554000	-2.636403000
C	-1.785247000	-6.051270000	2.691098000	Zn	-11.042742000	1.090734000	0.151073000
C	-3.137420000	-6.066548000	3.114972000	C	-11.063543000	2.884722000	2.406205000
C	-3.584401000	-7.039414000	4.029077000	C	-10.305014000	4.004520000	3.036285000
C	-4.029868000	-5.103739000	2.612426000	H	-8.624389000	5.181347000	2.254463000
C	-4.920791000	-7.046799000	4.435014000	C	-9.655268000	1.499272000	-2.920658000
H	-2.888572000	-7.783098000	4.417121000	C	-8.557926000	2.283233000	-3.557717000
C	-5.372189000	-5.121768000	3.027597000	H	-7.296660000	3.874047000	-2.723256000
H	-3.683391000	-4.349144000	1.904738000	N	-12.655379000	0.689007000	1.076279000
H	-5.267559000	-7.800759000	5.143953000	N	-11.933640000	-0.021374000	1.643995000
C	-5.817412000	-6.096880000	3.940872000	C	-12.123451000	2.247527000	2.950508000
H	-6.860446000	-6.106023000	4.260453000	H	-10.537614000	4.389695000	4.011924000
C	-6.276552000	-4.153009000	2.524373000	C	-10.406668000	0.556777000	3.531981000
C	-7.044639000	-3.323237000	2.093779000	H	-8.258929000	2.142773000	-4.579533000
C	-7.938245000	-2.345176000	1.591094000	C	-12.893168000	1.209571000	2.312237000
C	-9.301737000	-2.637932000	1.415922000	C	-13.679973000	-0.265311000	0.833501000
C	-7.474085000	-1.060099000	1.258946000	C	-11.503438000	-0.158423000	2.930489000
C	-10.152696000	-1.643351000	0.917292000	C	-13.060303000	-0.872544000	1.500837000
H	-9.695202000	-3.623264000	1.664000000	H	-12.467466000	2.534373000	3.949857000
C	-8.382364000	-0.113823000	0.769174000	H	-10.208027000	0.307734000	4.579355000
H	-6.423279000	-0.800514000	1.381304000	C	-14.066927000	0.589589000	2.912585000
H	-11.228388000	-1.848382000	0.769731000	C	-14.545942000	-0.317206000	2.000818000
H	-8.042342000	0.903897000	0.506817000	C	-13.861371000	-0.977005000	0.356413000
N	-9.708852000	-0.392180000	0.594947000	C	-12.328492000	-1.120353000	3.646375000
C	-3.519831000	8.295426000	-0.017054000	C	-13.283917000	-1.557971000	2.762335000

H	-14.454509000	0.829297000	3.880654000	H	-2.149692000	-2.834005000	-3.242920000
H	-15.401986000	-0.960735000	2.085939000	H	-2.182624000	-4.568856000	-2.887277000
C	-15.019978000	-1.908212000	0.421876000	C	-0.398962000	-5.575628000	-1.450064000
H	-12.190613000	-1.400494000	4.669325000	H	-0.609831000	-6.424357000	-0.780605000
H	-14.073460000	-2.266598000	2.930520000	H	-1.051249000	-5.701128000	-2.329834000
C	-14.874347000	-3.254722000	0.037484000	H	0.638358000	-5.677321000	-1.799154000
C	-16.271122000	-1.434390000	0.872982000	C	-1.277035000	-0.590959000	1.431947000
C	-15.973405000	-4.120573000	0.103636000	H	-1.085413000	0.302313000	0.809070000
C	-13.549872000	-3.757070000	0.442025000	H	-2.323523000	-0.531705000	1.769856000
C	-17.360395000	-2.311134000	0.933899000	H	-0.645795000	-0.485998000	2.329721000
C	-16.425924000	-0.007714000	1.280741000	C	0.595284000	-2.638033000	2.474720000
C	-17.216789000	-3.652999000	0.550726000	H	0.606747000	-1.586741000	2.812826000
H	-15.861122000	-5.159574000	0.193830000	H	0.109510000	-3.225803000	3.268772000
H	-12.771785000	-3.599634000	0.320505000	H	1.650295000	-2.944666000	2.434986000
H	-13.238904000	-3.224659000	1.353604000	O	7.694174000	-1.292429000	-5.311367000
H	-13.562754000	-4.828381000	0.678106000	O	5.390849000	-5.346249000	-3.837571000
H	-18.325647000	-1.949530000	1.280386000	O	7.485258000	-2.558560000	-0.745179000
H	-16.180586000	0.673778000	0.449325000	C	7.415112000	-1.499947000	-6.721704000
H	-15.739330000	0.248837000	2.104474000	H	7.901954000	-0.622359000	-7.172015000
H	-17.440870000	0.239102000	1.614490000	H	7.881969000	-2.426255000	-7.068031000
C	-18.393025000	-4.571381000	0.621646000	H	6.336740000	-1.484398000	-6.900747000
H	-18.800972000	-4.619392000	1.641975000	C	5.220533000	-5.862660000	-5.184624000
H	-18.152919000	-5.599522000	0.322155000	H	4.703460000	-6.813132000	-4.994505000
H	-19.206118000	-4.225972000	0.034041000	H	4.604478000	-5.181186000	-5.777149000
H	-1.841427000	12.576919000	0.080204000	H	6.196115000	-6.039336000	-5.649720000
C	0.112057000	-3.995044000	0.424211000	C	8.343969000	-1.443736000	-0.371811000
C	-0.616613000	-4.272048000	-0.750788000	H	7.899897000	-0.491996000	-0.675707000
C	-0.109486000	-2.823804000	1.172886000	H	8.367462000	-1.537223000	0.725497000
C	-1.540576000	-3.320195000	-1.229605000	H	9.353920000	-1.583260000	-0.790873000
C	-1.019413000	-1.857041000	0.686196000	Cu	3.367854000	-3.586123000	0.834975000
C	-1.686077000	-2.117797000	-0.518689000	C	1.287315000	9.182863000	0.145917000
C	6.451424000	-3.928338000	-2.321986000	C	2.373609000	8.650113000	0.177111000
C	7.201714000	-2.747556000	-2.067435000	C	3.581793000	7.912089000	0.218218000
C	6.117982000	-4.193901000	-3.670829000	C	4.385777000	7.907455000	1.372773000
C	7.601798000	-1.885612000	-3.087128000	C	3.928063000	7.100346000	-0.880446000
C	6.501288000	-3.357328000	-4.725632000	C	5.484073000	7.050822000	1.451553000
C	7.242951000	-2.207611000	-4.410403000	H	4.139252000	8.563857000	2.207781000
H	8.174645000	-0.981233000	-2.902157000	C	5.024029000	6.244292000	-0.795003000
H	6.234740000	-3.583997000	-5.748066000	H	3.326805000	7.135654000	-1.789476000
Br	-2.846105000	-0.765622000	-1.234528000	C	5.788811000	6.192898000	0.382584000
C	-2.357834000	-3.571300000	-2.453993000	H	6.103788000	7.037683000	2.348468000
H	-3.436763000	-3.511555000	-2.232794000	H	5.283305000	5.602472000	-1.636230000

C	6.885195000	5.206148000	0.499829000	C	13.322038000	1.691143000	0.748218000
C	8.073286000	5.418653000	-0.182936000	C	11.859728000	0.328265000	0.810913000
C	6.659333000	4.067006000	1.309895000	C	9.213313000	-0.813859000	3.051420000
N	9.168379000	4.568033000	-0.224616000	C	10.449414000	-1.001149000	2.457055000
C	8.361964000	6.639772000	-1.004594000	H	13.868487000	3.425630000	1.987934000
N	7.525722000	3.032258000	1.503423000	H	14.149675000	1.004065000	0.795591000
C	5.406717000	3.835741000	2.088111000	C	12.885943000	-0.744855000	0.851092000
C	10.147177000	5.196210000	1.053780000	H	8.729778000	-1.439180000	3.771286000
Zn	9.387758000	2.794336000	0.717304000	H	11.132187000	-1.818142000	2.597319000
C	9.598816000	6.507690000	-1.517770000	C	12.922617000	-1.727728000	0.158214000
H	7.654515000	7.445433000	-1.110522000	C	13.826549000	-0.778290000	1.903754000
C	6.885656000	2.118323000	2.419322000	C	13.888398000	-2.740280000	0.106599000
C	5.549226000	2.670355000	2.755571000	C	11.944674000	-1.686104000	1.287856000
H	4.579628000	4.524285000	2.082253000				
C	11.361376000	4.698765000	1.390313000				
N	11.226164000	2.559191000	0.133198000				
N	9.592245000	1.004764000	1.665187000				
H	10.153882000	7.178913000	2.149381000				
C	7.409497000	0.965619000	2.893108000				
H	4.864547000	2.181341000	3.425066000				
C	11.869094000	3.432003000	0.950883000				
H	12.022941000	5.280330000	2.039517000				
H	15.515043000	-1.822896000	2.747237000				
H	13.958973000	1.272995000	2.543765000				
H	12.825076000	0.294804000	3.481038000				
H	14.566872000	0.119299000	3.737461000				
C	15.859233000	-3.851093000	0.991451000				
H	15.885117000	-4.343554000	1.974465000				
H	15.703310000	-4.637390000	0.241594000				
H	16.863702000	-3.435289000	0.816152000				
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H	10.900624000	-1.690150000	0.922744000				
H	12.073013000	-0.768617000	1.884514000				
H	12.052286000	-2.534321000	1.975731000				
C	13.799948000	0.268486000	2.966582000				
C	14.821783000	-2.778666000	0.939065000				
C	14.786894000	-1.795516000	1.939167000				
C	12.106042000	1.435393000	0.033767000				
C	8.693514000	0.429287000	2.545151000				
C	10.685000000	0.124856000	1.594511000				
H	6.826124000	0.365472000	3.602805000				
C	13.182768000	2.906319000	1.347303000				

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