Supporting Information

First Example of a Hexadentate Phthalocyanine Analogue Containing a Divalent Metal Center

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Measurements

Mass spectra were obtained by using a Thermo Scientific LTQ Orbitrap XL spectrometer. Magnetic susceptibility measurements were carried out on a Quantum Design MPMS LX7AC SQUID (superconducting quantum interference device) magnetometer. The diamagnetic susceptibility contributions were corrected by using the Pascal constants. ^{1}H NMR spectrum was obtained by employing a JEOL ECS-400 spectrometer.

Synthesis of 3

Phthalonitrile (1.0 g, 8.8 mmol) was added to dry methanol (40 mL) in which lithium metal (125 mg, 18 mmol) was dissolved at room temperature under an argon atmosphere. The mixture was heated at 70 °C with stirring for 10 min, followed by the addition of cadmium acetate dihydrate (430 mg, 1.6 mmol). After 2 h, the solvent was evaporated *in vacuo*. The residue was chromatographed (silica, CH_2Cl_2/MeOH = 100 : 3 (v/v)) to give **3** as an yellow solid (297 mg, 22%). Anal. calcd for $C_{48}H_{25}N_{13}Cd\cdot 1.8CH_2Cl_2\cdot 0.3H_2O$: C, 56.72; H, 2.79; N, 17.27%. Found: C, 56.77; H, 2.87; N, 17.07%; *m/z* (ESI-FT) 898.1481 $[M+H]^+$ (calcd for $[\mathbf{3}+H]^+$ 898.1475); δ_H (400 MHz, acetone-d_6) 7.53−7.56 (m, 10 H, ArH), 7.70 (dd, 2H, ArH), 7.76 (dd, 2H, ArH), 7.88 (dd, 2H, ArH), 7.96−8.00 (m, 4 H, ArH), 8.03 (dd, 2H, ArH), 8.38 (d, 2H, ArH).

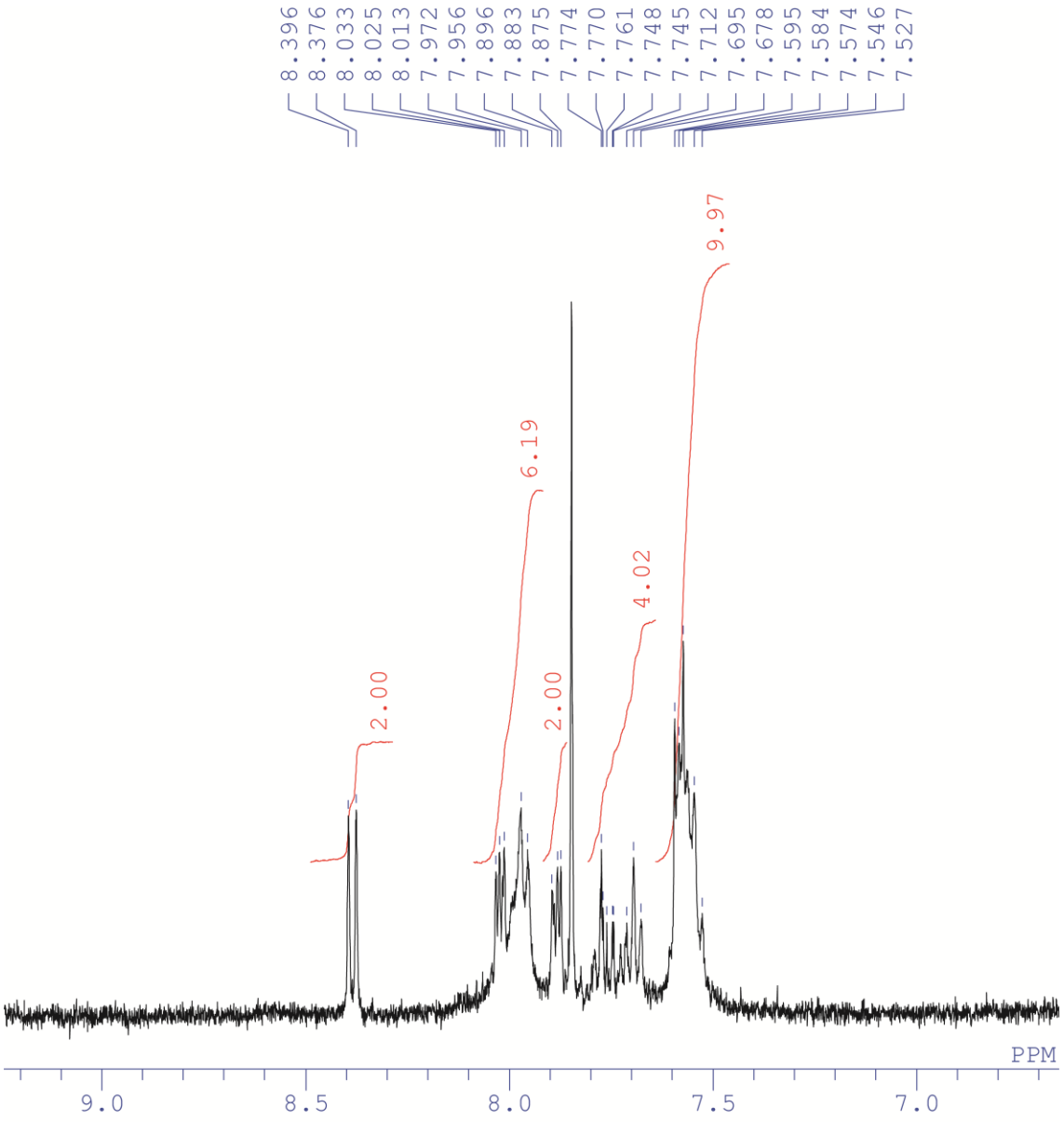

Figure S1 ^{1}H NMR spectrum of **3** in acetone-d_6. The singlet signal at 7.82 ppm is due to trace amount of remaining $CDCl_3$. No signals arising from the NH site were observed.

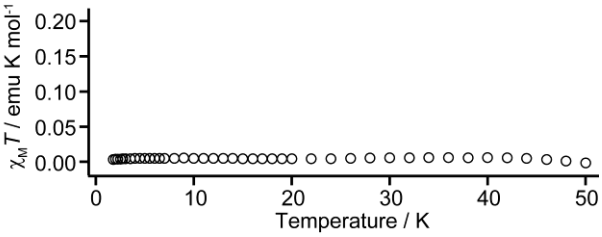

Figure S2 Magnetic susceptibility of **3**.

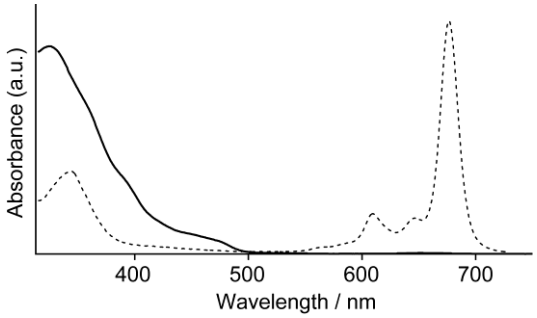

Figure S3 Electronic absorption spectra of **3** in CH_2Cl_2 (5% MeOH) (solid line) and CuPc in trichlorobenzene for comparison purpose (dashed line).

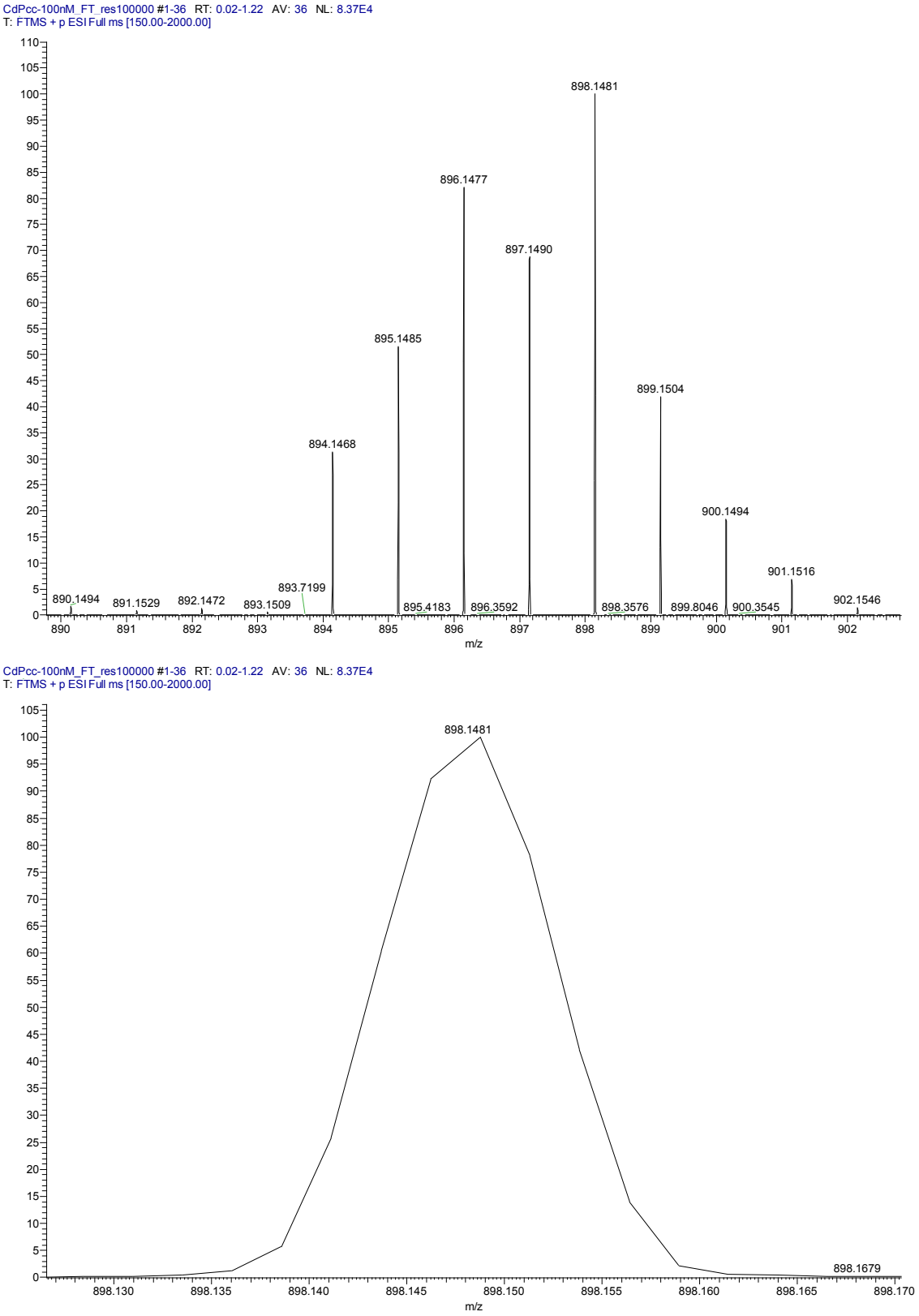

Figure S4 Enlarged views of ESI-Orbitrap FT mass spectrum of **3**