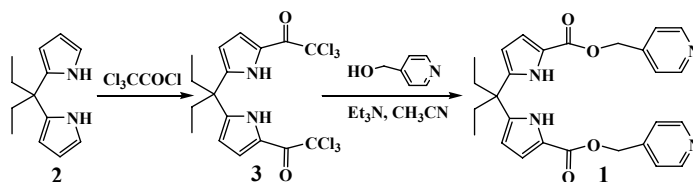


Hydrogen bonds assisting helical self-assembly and [n]catenane constructing

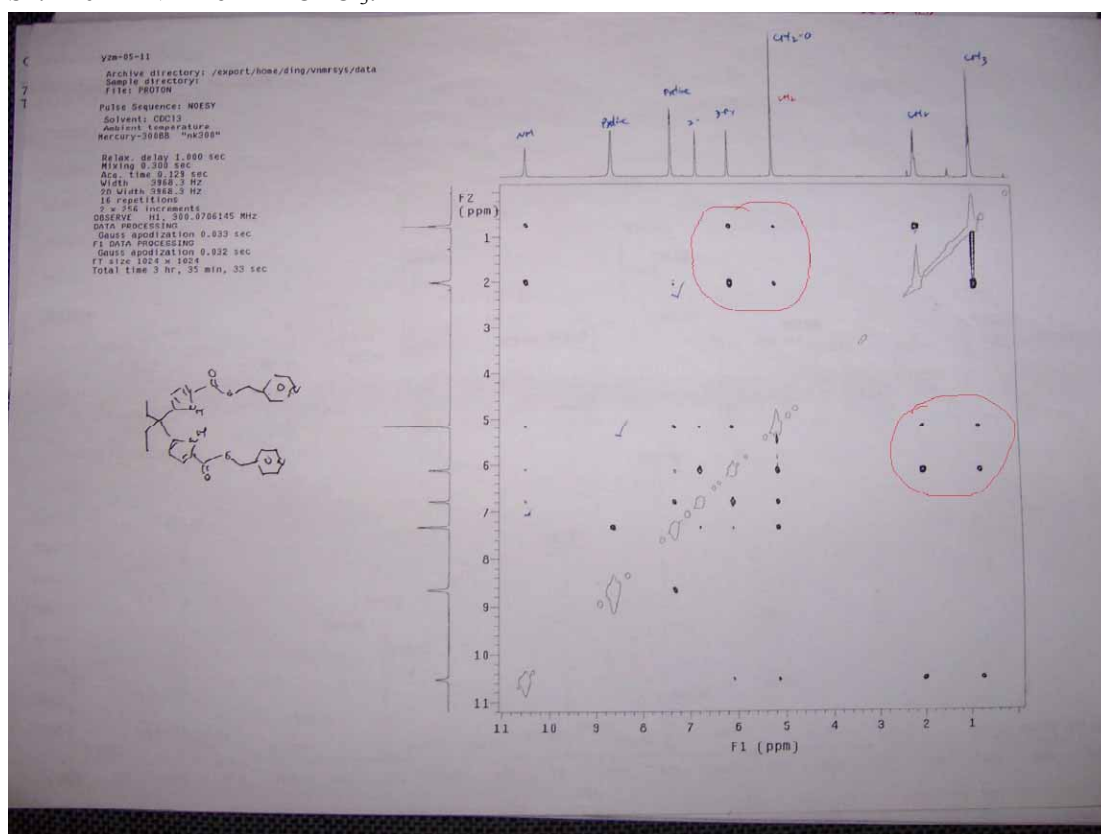
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S1. The synthesis of ligand **1**.



4-hydroxymethylpyridine (545 mg, 5 mmol), **3** (980 mg, 2 mmol) and triethylamine (0.5 mL) were added to acetonitrile (20 mL), and then the mixture was refluxed for 48h. The solution was evaporated under reduced pressure and the residue was purified by column chromatography on silica gel with ethyl acetate, affording the title compound (white powder, 610 mg, 65%), mp=163°. Spectroscopic data for **1**: ^1H NMR (300MHz, CDCl_3); δ 0.73 (t, 6H, $J=5.4$ Hz, $-\text{CH}_3$), 1.99 (q, 4H, $J=5.4$ Hz, $-\text{CH}_2-$), 5.16 (s, 4H, $-\text{CH}_2-$), 6.09 (s, 2H, PyCH), 6.77 (s, 2H, PyCH), 7.31 (d, 4H, $J=4.2$ Hz), 8.63 (d, 4H, $J=4.2$, Hz), 10.28 (s, 2H, NH); ^{13}C NMR (300MHz, CDCl_3); δ 8.8, 30.9, 45.2, 64.0, 109.1, 115.9, 121.1, 121.9, 143.1, 145.4, 150.2, 161.3; ESI-MS: 473($\text{M}+1^+$). Elemental analysis: $\text{C}_{27}\text{H}_{27}\text{N}_4\text{O}_4$: Calcd: C, 68.63; H, 5.97; N, 11.86. Found: C, 68.77; H, 6.01; N, 11.75.

S2: The 2D NMR of **1** in CDCl₃.



S3: The 2D NMR of **1** in DMSO.

