

Electronic Supplementary Information (ESI)

A terpyridine appended hexaarylbenzene fluorophore: synthesis, photophysical properties and application for colorimetric detection of Fe²⁺ in aqueous solution

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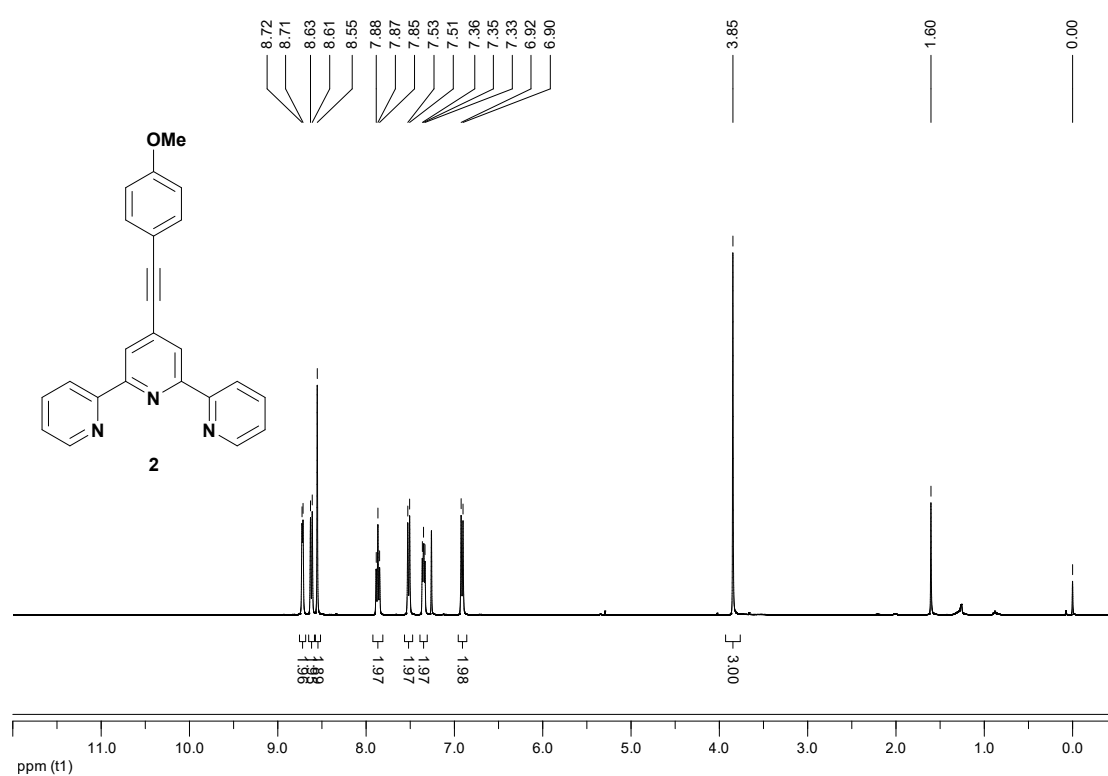


Fig. S1 ¹H NMR spectrum of **2** in CDCl₃.

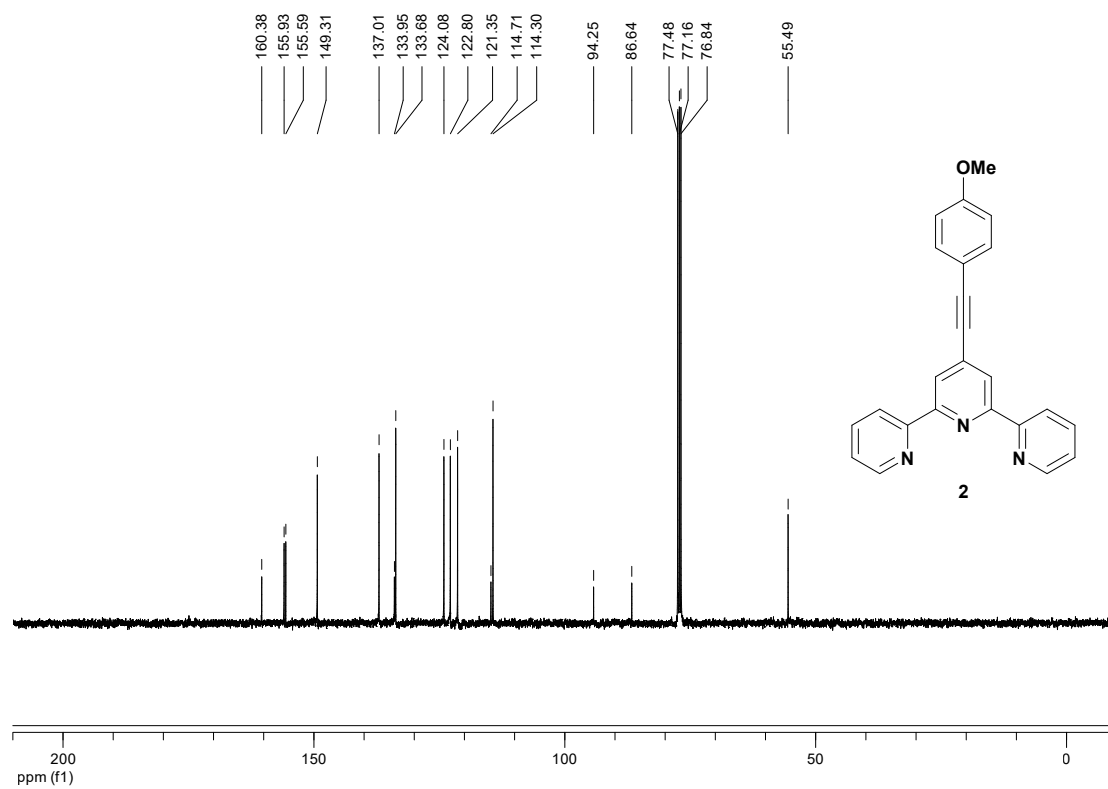
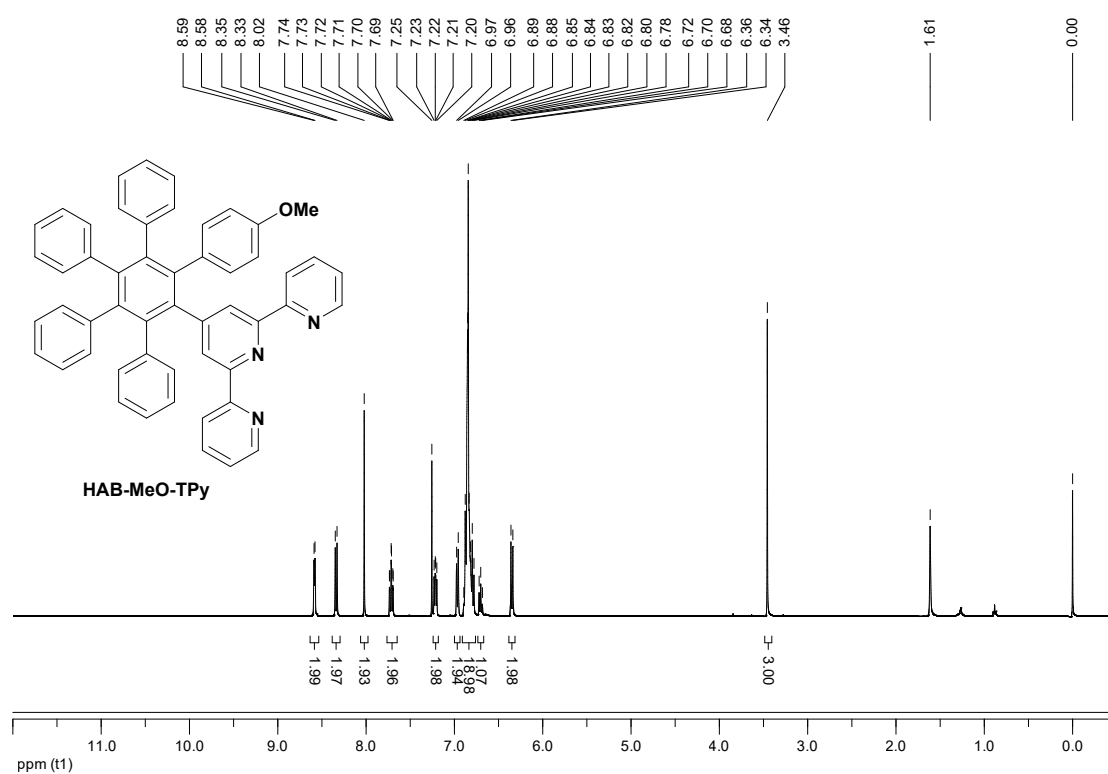


Fig. S2 ¹³C NMR spectrum of **2** in CDCl₃.



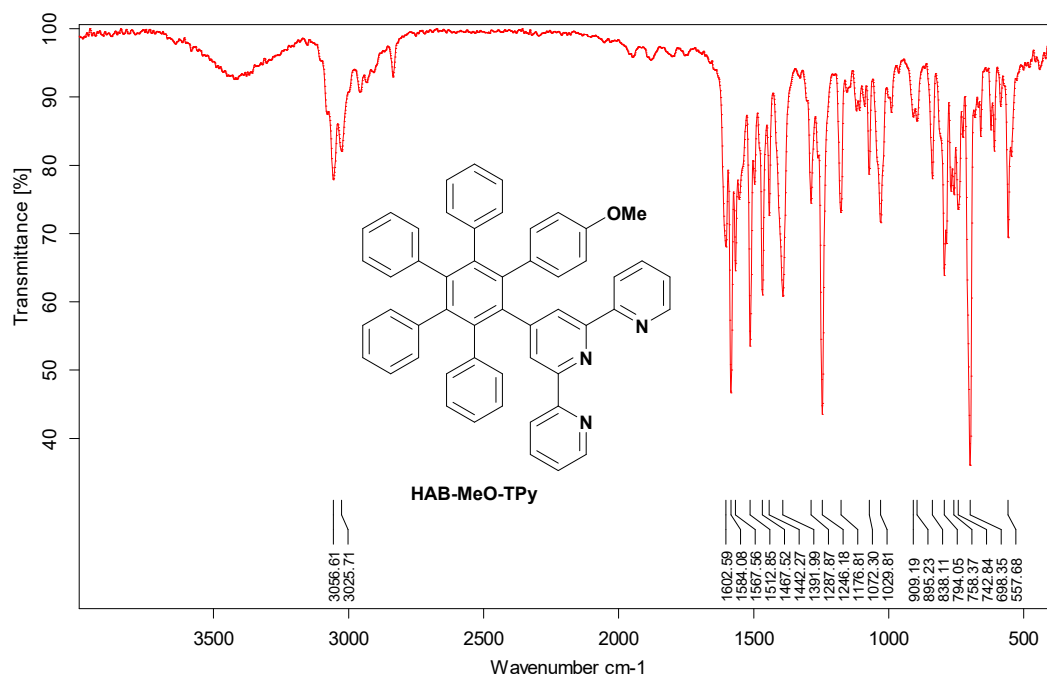


Fig. S5 FT-IR of HAB-MeO-TPy.

数据文件	10311205-S1.d	样品名称	10311205-S1
样品类型	Sample	位置	P1-A3
仪器名称	Instrument 1	用户名称	
采集方法	pos-1min-3000.m	采集时间	2022-11-04 15:59:22
IRM 校正状态	成功	数据方法	ZNZ-2022.m
注释			
设备类型	QuadrupoleTimeOfFlight	Sample Group	
Info.		Stream Name	LC 1
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0)		

化合物列表

化合物标签	RT	质量数	丰度	分子式	目标质量	误差 (ppm)
Cpd 1: C ₅₂ H ₃₇ N ₃ O	0.129	719.295	95938	C ₅₂ H ₃₇ N ₃ O	719.2937	1.83

MS 缩放的质谱图

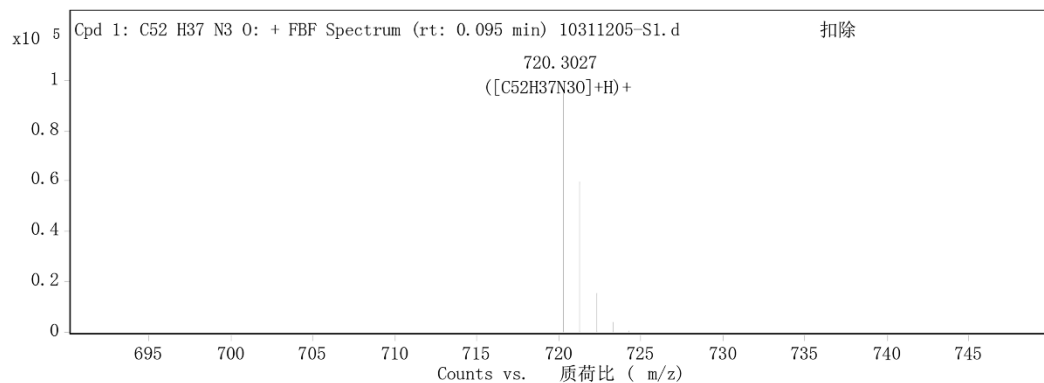


Fig. S6 HRMS of HAB-MeO-TPy.

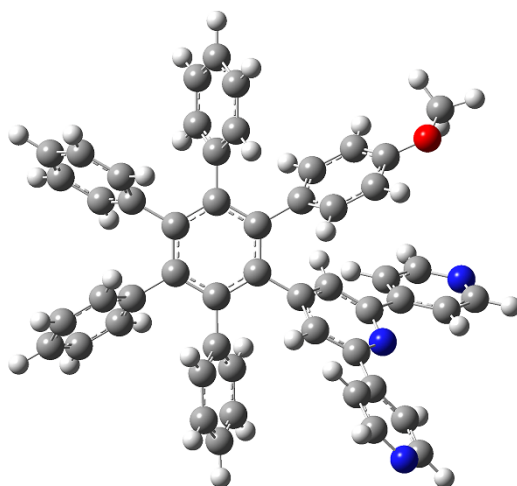


Fig. S7 Optimized molecular configuration of **HAB-MeO-TPy** calculated for the ground state.

Table S1 Photophysical data of **HAB-MeO-TPy** in various solvents

Solvent	$\lambda_{\text{abs}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	$\Phi_{\text{F}}/\%$
Cyclohexane	278	372	0.07
THF	278	398	2.08
CH ₂ Cl ₂	280	406	3.63
CH ₃ CN	276	418	4.11
DMSO	279	422	8.83

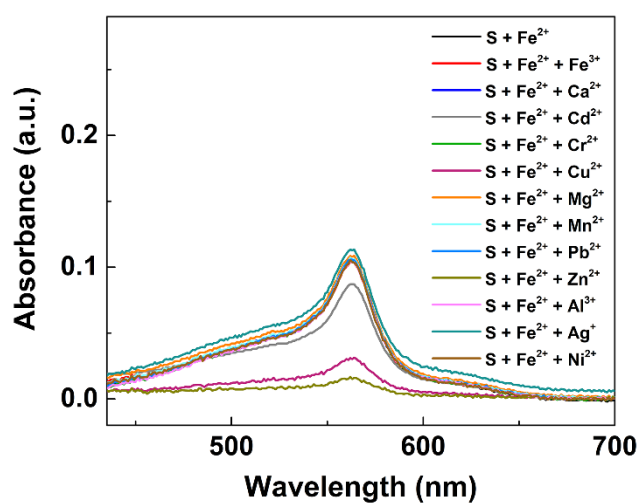


Fig. S8 UV-vis absorption spectra of **HAB-MeO-TPy** (abbreviated as **S**, 10 μM) upon addition of various metal ions (10 μM) mixed with Fe^{2+} (10 μM).

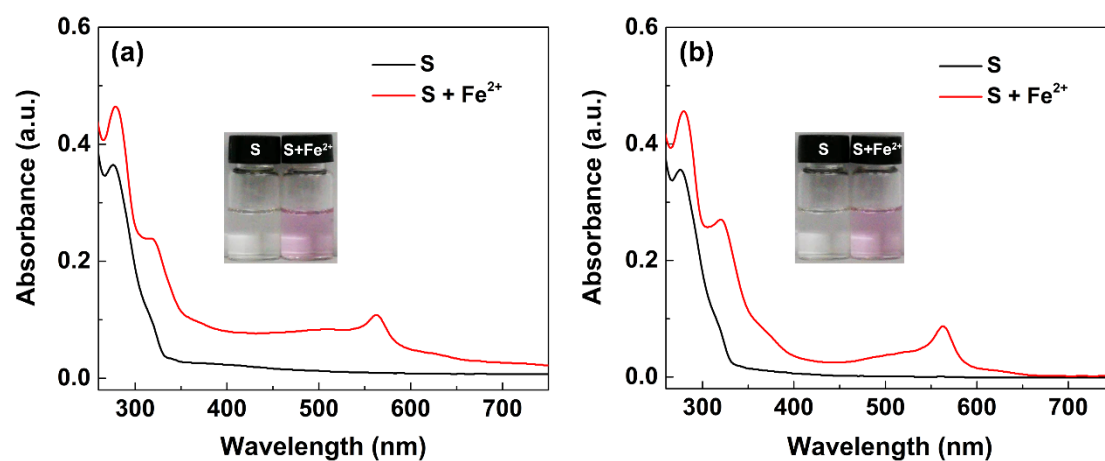


Fig. S9 UV-vis absorption spectra of **HAB-MeO-TPy** (abbreviated as **S**, 10 μ M) in the absence and presence of Fe^{2+} (1.0 equiv.) in CH_3CN /water solution (9/1, v/v) using (a) tap water and (b) pond water.

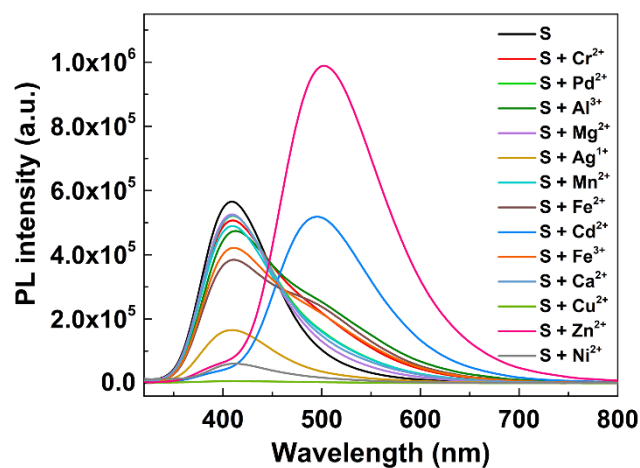


Fig. S10 Fluorescence spectra of **HAB-MeO-TPy** (abbreviated as **S**, 10 μ M) in the absence and presence of various metal ions (4.0 equiv.) in THF/water solution (9/1, v/v).

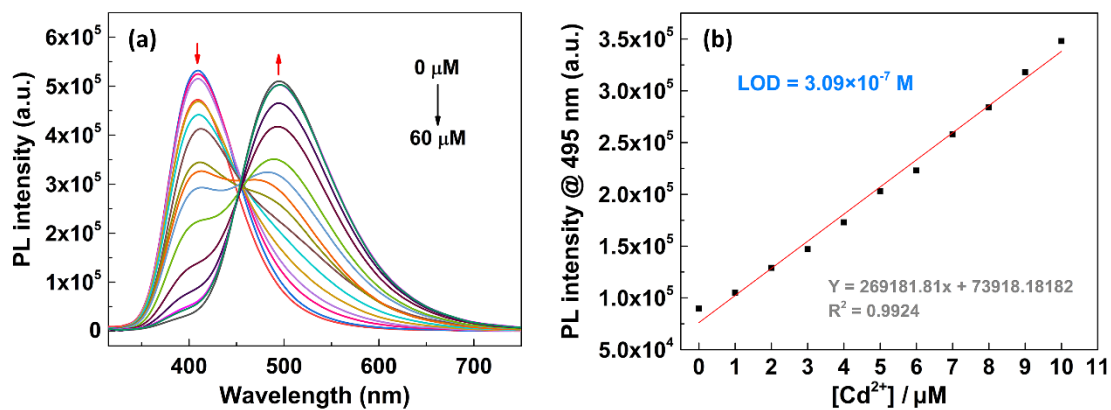


Fig. S11 (a) Fluorescence spectra of **HAB-MeO-TPy** (10 μM) upon addition of Cd²⁺ with different concentrations (0-60 μM) in THF/water solution (9/1, v/v). (b) Fitted calibration curve between the fluorescence intensity of **HAB-MeO-TPy** at 495 nm and the Cd²⁺ concentration (0-10 μM).