Supporting Information

Copper-Induced Fluorescence Enhancement and Particle-Size Decrease of a C-6 Unsubstituted Tetrahydropyrimidine Racemate

Lan Huang, Jingru Su, Desheng Zhong, Ruiyuan Liu, Haibo Wang, Le Yu, Qiuhua Zhu,*

*Shuwen Liu**

School of Pharmaceutical Sciences, Southern Medical University, 1838 Guangzhou Avenue North, Guangzhou 510515, China

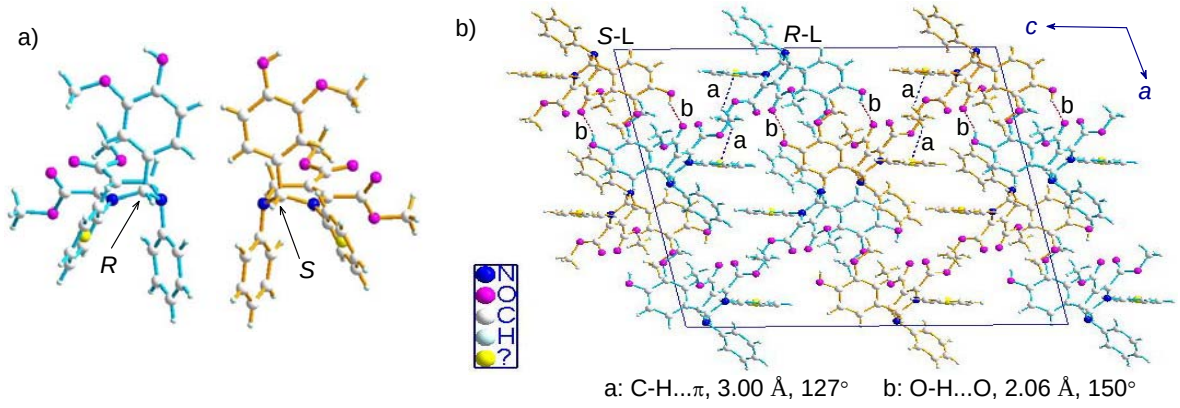

Figure S-1. Molecular conformation and stacking mode in a unit cell of THP-1. (a) Molecular conformation of THP-1 (CCDC 911650). (b) Molecular stacking mode (MSM) viewed down crystallographic *b*-axis.

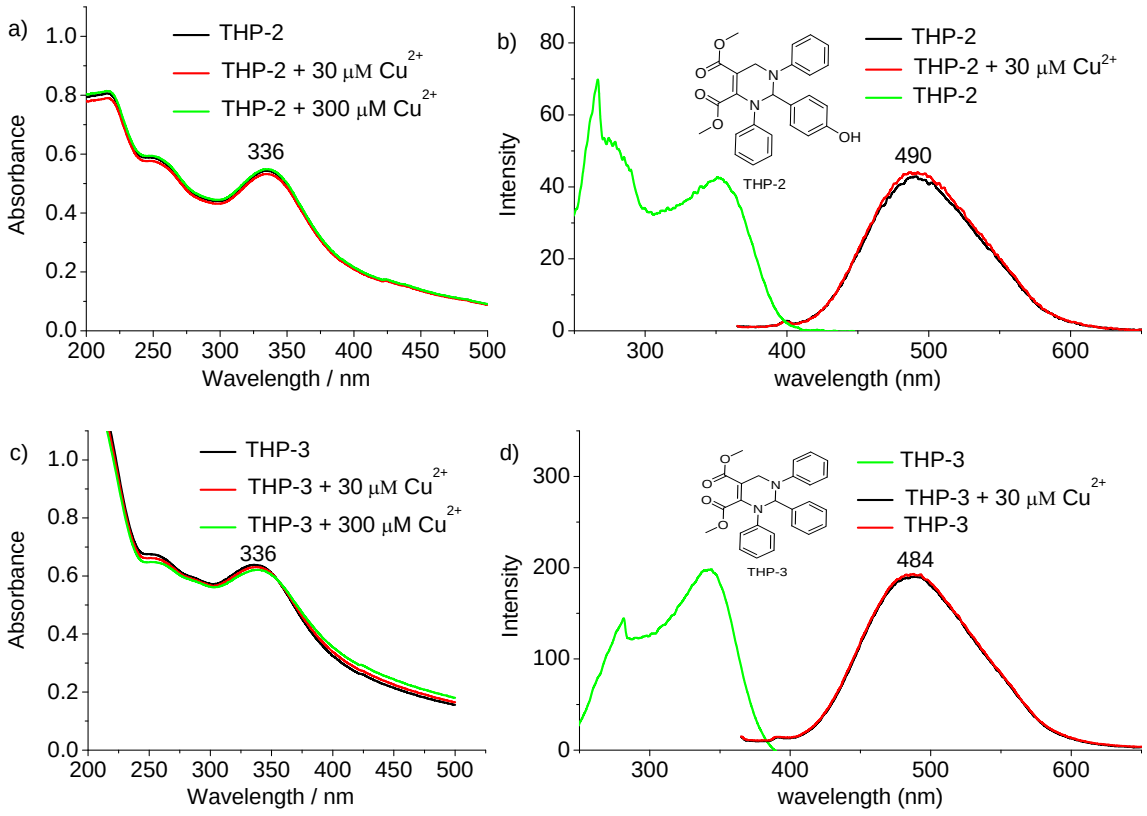

Figure S2. Influence of Cu^{2+} on the optical properties of THP-2 and THP-3 (30 μM) in ethanol–water (1:99, v/v) mixture. (a) Absorption, (b) excitation and emission spectra of THP-2 in the absence and presence of Cu^{2+} ion (30 and 300 μM). (c) absorption, (d) excitation and emission spectra of THP-3 in the absence and presence of Cu^{2+} ion (30 and 300 μM) (excitation at 350 nm, emission at corresponding maximum emission wavelength).

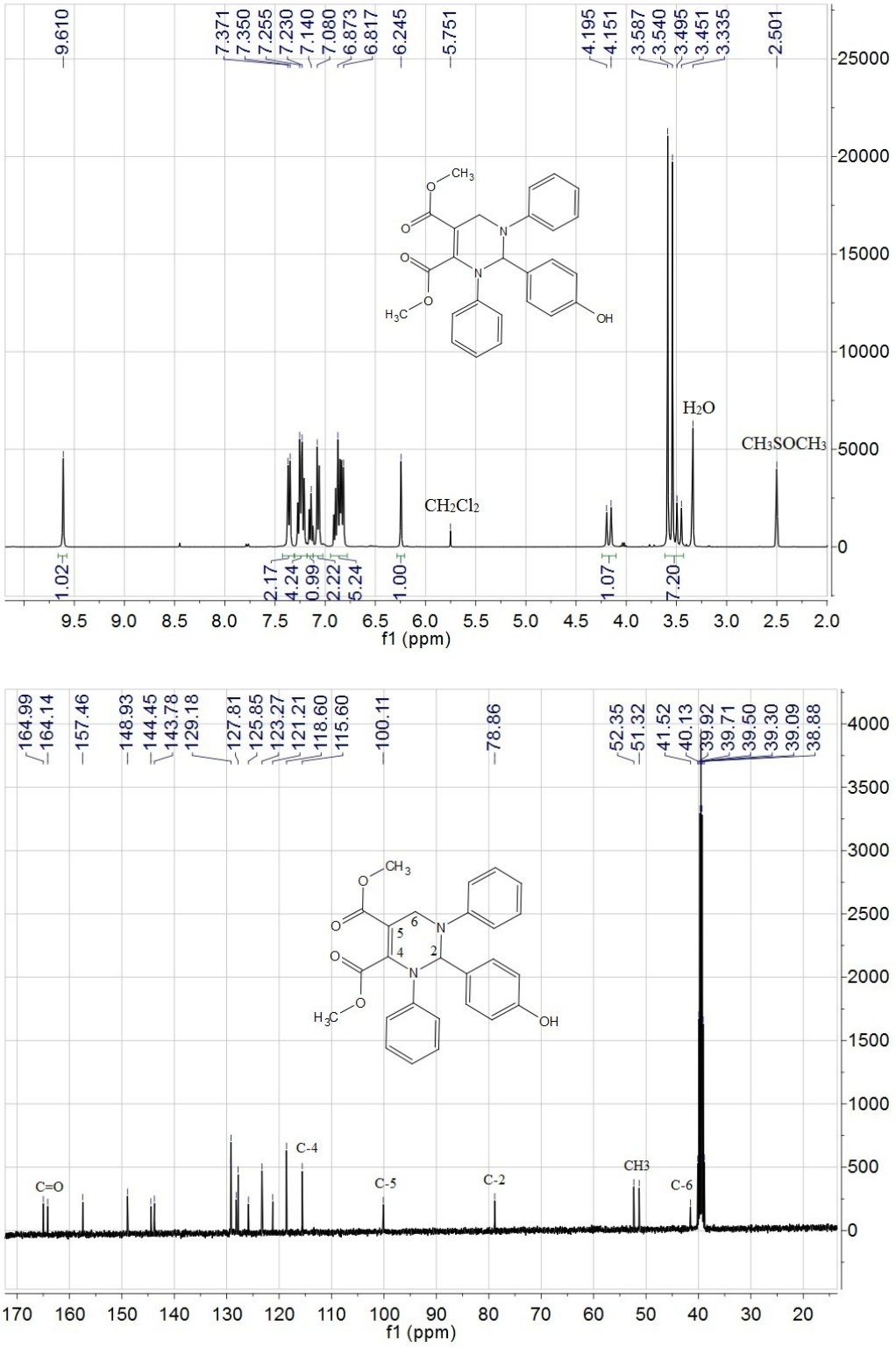

Figure S3 Copies of ^{1}H (400MHz, DMSO) and ^{13}C NMR (101Hz, DMSO) spectra of THP-2

The characterization data of THP-2

THP-2 were synthesized by the 5CR reported in our recent work.[1] 31% yield, light yellow solid, mp = 164.1– 64.8 ^{o}C; ^{1}H NMR (400 MHz, DMSO): δ = 9.61 (s, 1H, OH), 7.37–6.82 (m, 14H, Ph), 6.24 (s, 1H, N-CH-N), 4.17 (d, J = 17.6 Hz, 1H, CH_2), 3.59 (s, 3H, OCH_3), 3.54 (s, 3H, OCH_3), 3.52 (d, J = 17.6 Hz, 1H, CH_2) ppm; ^{13}C NMR (101 MHz, DMSO): δ = 164.99 (CO), 164.14 (CO), 157.46 (Ph-OH), 148.93, 144.45, 143.78, 129.21, 129.18, 127.81, 125.85, 123.27, 121.21, 118.60, 115.60 (C-4), 100.11 (C-5), 78.86 (C-2: NCN), 52.35 (CH_3O), 51.32 (CH_3O), 41.52 (C-6: CH_2).

References

[1] Q. Zhu, L. Huang, Z. Chen, S. Zheng, L. Lv, Z. Zhu, D. Cao, H. Jiang, S. Liu, A new series of C-6 unsubstituted tetrahydropyrimidines: Convenient one-pot chemoselective synthesis, aggregation-induced and size-independent emission characteristics. *Chem. Eur. J.* **2013**, *19*, 1268 – 1280.