Supporting Information

A One-step Synthesized Acridine-based Fluorescent Chemosensor for Selective Detection of Copper (II) Ions and Living Cell Imaging

Qiuzi Dai ,[a,b,1] Haiyang Liu,[a,b,c,1] Chunmei Gao,[b,d] Wenlu Li,[a,b] Caizhen Zhu,[e] Chengdong Lin,[e] Ying Tan,[b] Zigao Yuan*[a,b] and Yuyang Jiang*[b,f]

[a] *Department of Chemistry, Tsinghua University, Beijing, 100084, PR China*

[b] *The Ministry-Province Jointly Constructed Base for State Key Lab-Shenzhen Key Laboratory of Chemical Biology, the Graduate School at Shenzhen, Tsinghua University, Shenzhen, Guangdong 518055, PR China*

[c] *Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Optoelectronic Engineering, Shenzhen University, Shenzhen, 518060, PR China*

[d] *College of Chemistry and Chemical Engineering, Shenzhen University, Shenzhen, 518060, PR China*

[e] *School of Chemistry and Environmental Engineering, Shenzhen University, Shenzhen, 518060, PR China*

[f] *Department of Pharmacology and Pharmaceutical Sciences, School of Medicine, Tsinghua University, Beijing, 100084, P. R. China*

[1] *The two authors contributed equally to the work.*

New Journal of Chemistry

* Corresponding author

Tel: +86-0755-26036017, Fax: +86-0755-26032094

E-mail addresses: yzg12@mails.tsinghua.edu.cn (Z. Yuan), jiangyy@sz.tsinghua.edu.cn (Y. Jiang).

1. ^{1}H NMR, ^{13}C NMR, and MS spectrum obtained for ACC

^{1}H NMR of ACC

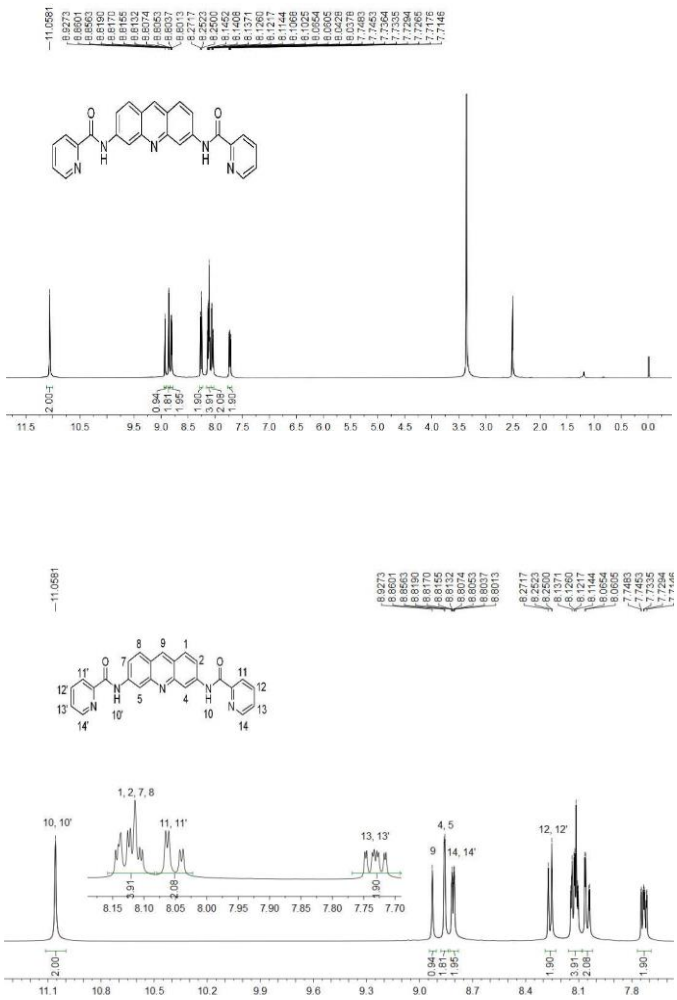

Figure S1. The above is the whole spectrum of ^{1}H NMR and the below is the partial spectrum.

^{13}C NMR of ACC

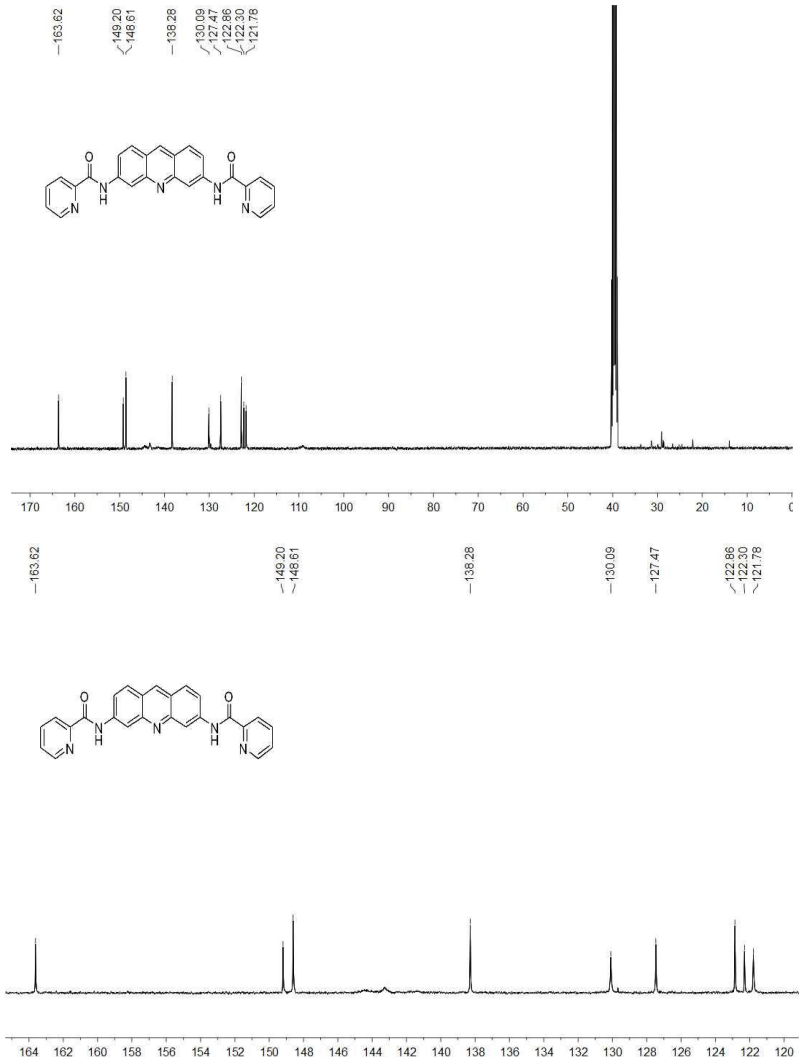

Figure S2. The above is the whole spectrum of ^{13}C NMR and the below is the partial spectrum.

ESI mass spectra of ACC

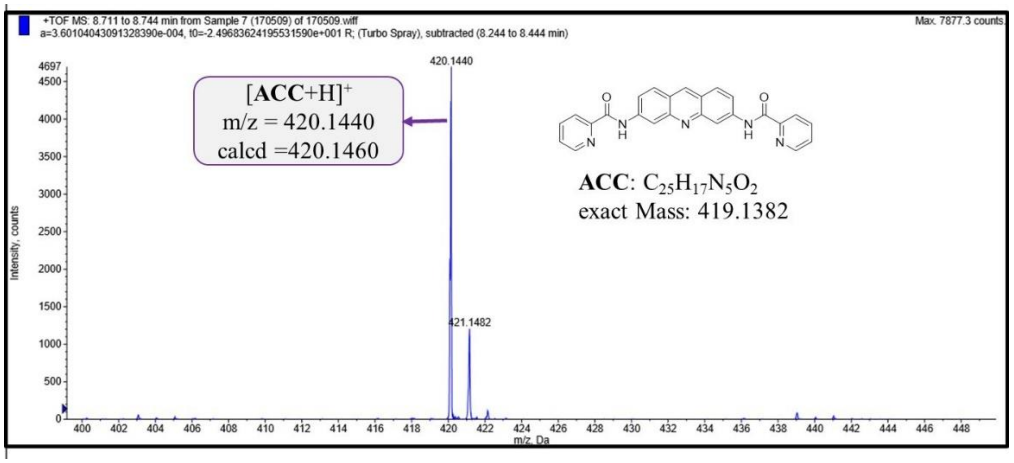

Figure S3. ESI mass spectra of **ACC**

2. pH analysis

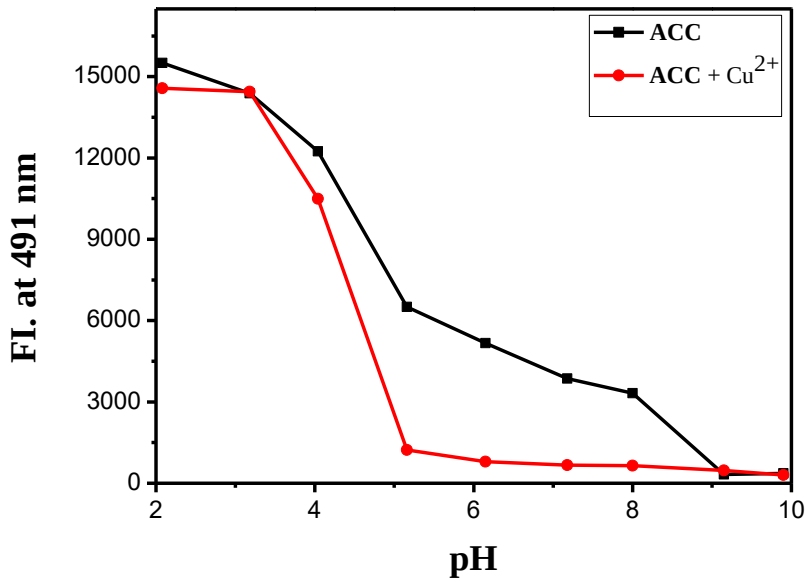

Figure S4. Fluorescence intensity recorded for chemosensor **ACC** (10 μM) at various pH values in the absence or presence of 3 equiv. Cu^{2+} (λ_{ex} = 370 nm, λ_{em} = 491 nm).

3. MTT analysis

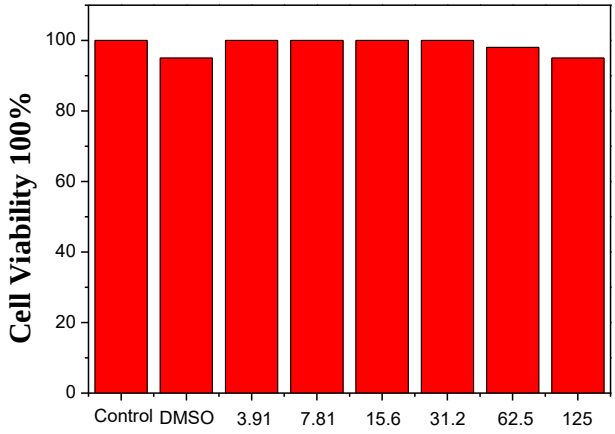

Figure S5. MTT assay of QLBA on HeLa cells (with **ACC** 3.91, 7.81, 15.6, 31.2, 62.5, 125 μM) for 48 h (DMSO denotes: Only 0.5% DMSO).

4. Calculation of the limit of detection

The limit of detection (*LOD*) was calculated based on the fluorescence titration according to the following equation (Eq. S1) [1,2], where "k" is the standard deviation of the blank solution and "s" is the slope of the calibration curve in Figure S6. To determine "s", the emission intensity of **ACC** in HEPES buffer (pH 7.2) without any metal ions was measured 10 times, respectively.

$$LOD = 3 \times k/S \quad \textbf{(Eq. S1)}$$

5. Calculation of the association constant

The association constant (Ka) of **ACC**-Cu^{2+} was obtained from nonlinear curve fitting of the fluorescence titration data according to the Benesie-Hildebrand equation (Eq.S2) [3-4], where F_0, F, F_{min} are the fluorescence intensity of **ACC** in the absence of Cu^{2+}, at a certain concentration of Cu^{2+} cation, and the minimum fluorescence intensity of **ACC**-Cu^{2+} in the linear range, [M] is the Cu^{2+} concentration, and n is the binding stoichiometry.

$$\log[(F_0\text{-}F)/(F\text{-}F_{min})] = n \log[M] + \log Ka \quad \textbf{(Eq.S2)}$$

6. Reference

[1] A. Barba-Bon, A. M. Costero, S. Gil, M. Parra, J .Soto and R. Martínez-Máñez, *Chem. Commun.*, 2012, **48**, 3000-3002.

[2] T. Mistri, R. Alam, M. Dolai, S. K. Mandal, A. R. Khuda-Bukhshb and M. Ali, *Org. Biomol. Chem.*, 2013, **11**, 1563-1569.

[3] H. A. benesi and J. H. Hildebrand, *J.Am. Chem. Soc.*,1949, **71**, 2703-2710.

[4] C. H. Zhang, B. Z. Gao, Q. Y. Zhang, G. M. Zhang, S. M. Shuang and C. Dong, *Talanta.*, 2016, **154**, 278-283.