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Electronic Supplementary Information

A reusable multichannel anthraimidazoledione based receptor for Hg^{2+} and Cu^{2+} ions: Ultrasensitive, economical and facile detection of Hg^{2+} in real water sources through fluorescence readout

Manzoor Ahmad Wani, Neha Thakur, Mrituanjay D. Pandey* and Rampal Pandey*

Department of Chemistry, Dr. Harisingh Gour Central University, Sagar (MP), India

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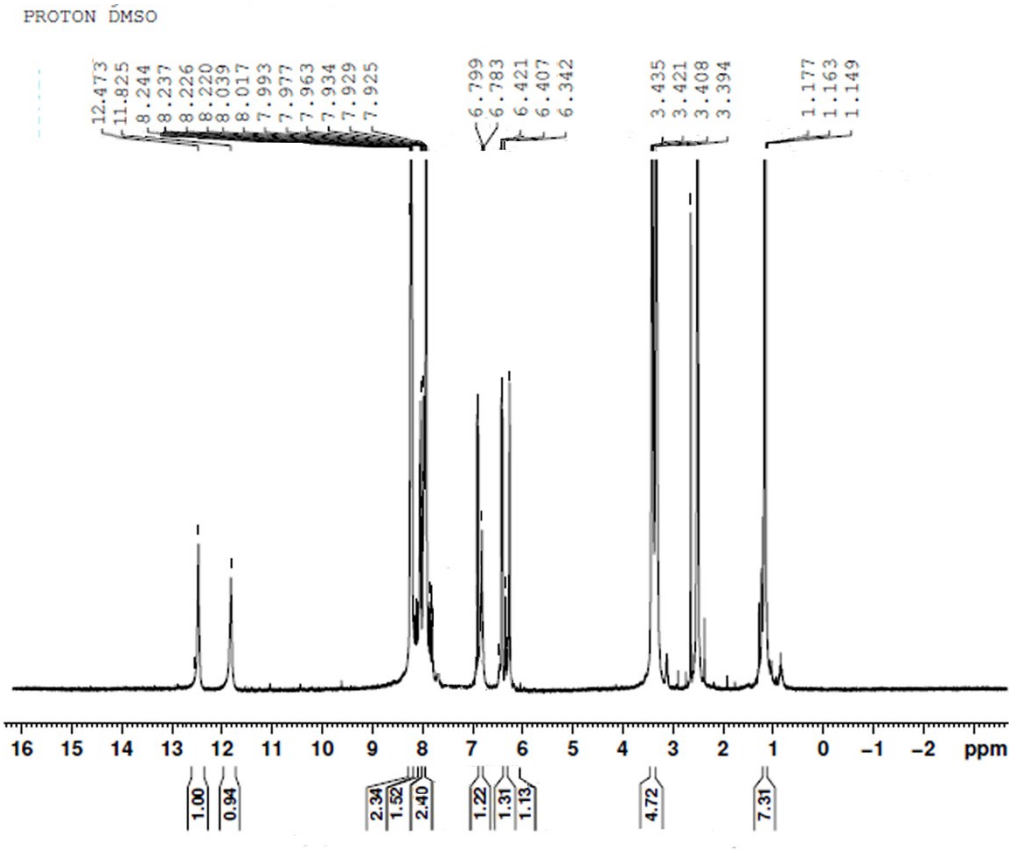


Fig. S1. ^{1}H NMR spectrum of **1** in dmso-d_6.

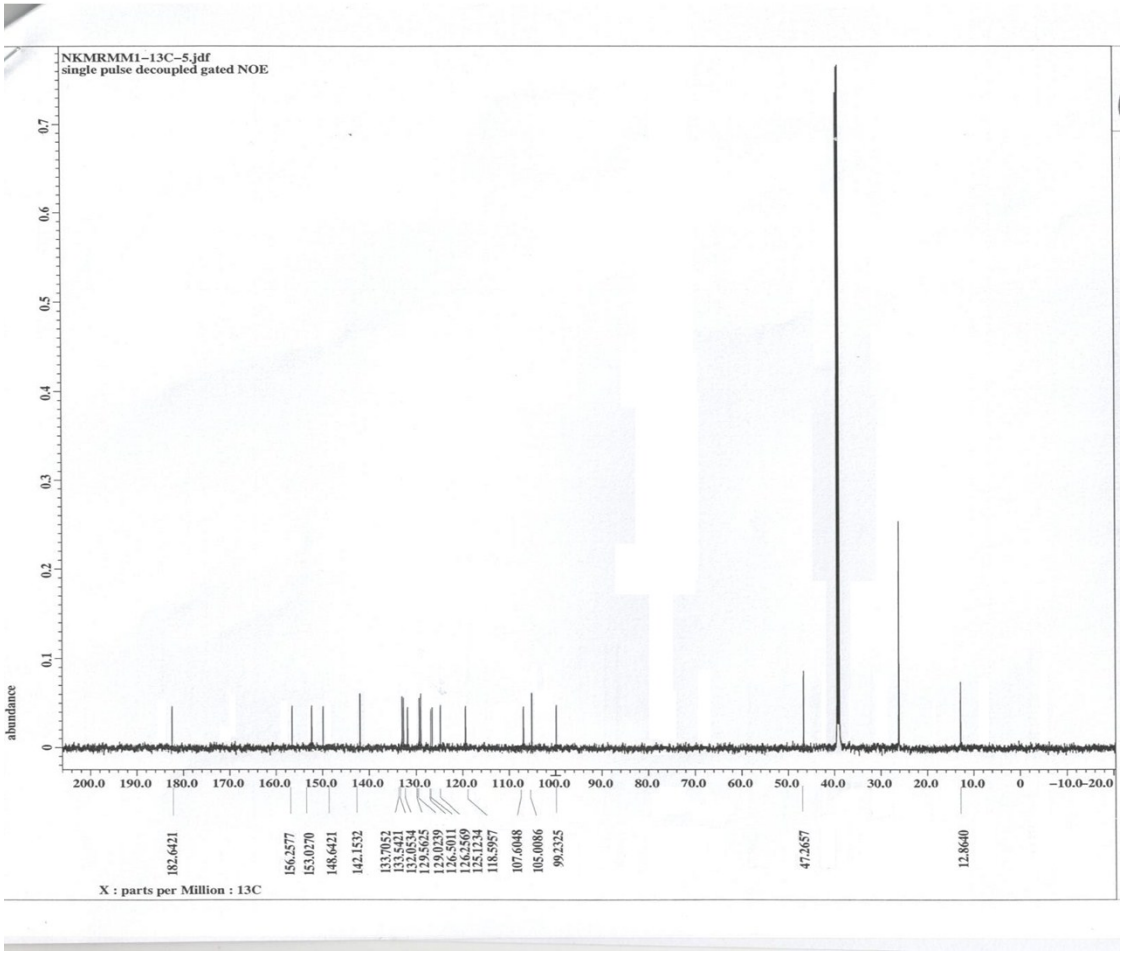


Fig. S2. ^{13}C NMR spectrum of **1** in dmso-d_6.

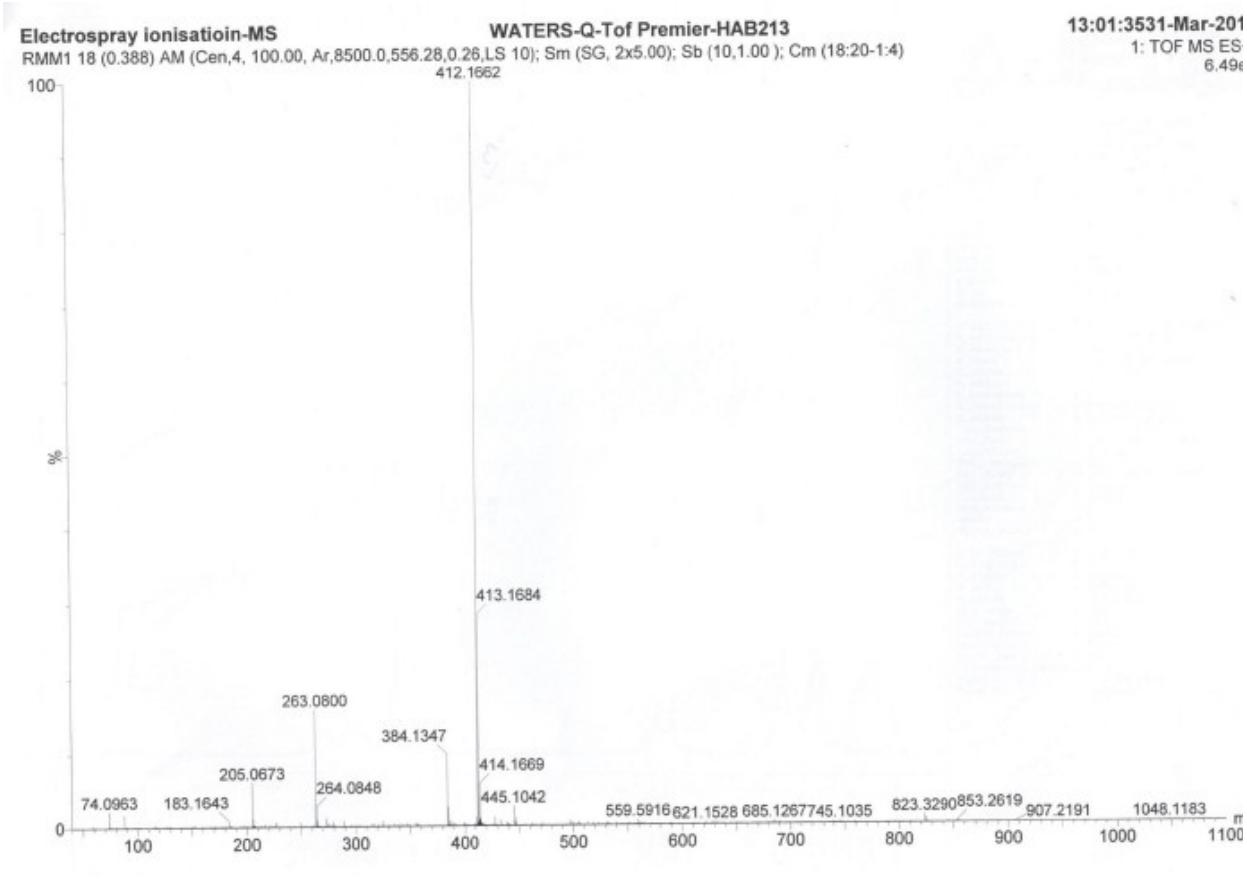


Fig. S3 ESI-MS spectrum of **1**.

Structure determination. Suitable dark pink single crystals of **1** were collected and its structural analysis was carried out on a Bruker SMART APEX CCD Diffractometer with Mo Kα radiation (λ = 0.710 73 Å). The scaling and integration of intensity of reflections were made by using the program SMART (version 6.45) while as the absorption corrections done by using 'multi-scan' program. The crystal structures were solved by direct methods and refined by full matrix least squares against F^2 (SHELXL 97, 2012).[1] The refinement of non-hydrogen atoms was done with anisotropic thermal parameters and their positions were geometrically fixed isotropically.[2] The important parameters related to the crystal structure of **1** have been given in Table 1. Crystallographic details for **1** have been deposited with the CCDC No. 1501310 which can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html (or from the

CCDC, 12 Union Road, Cambridge CB21EZ, UK; Fax: +44-1223-336033; E-mail: deposit@ccdc.cam.ac.uk).

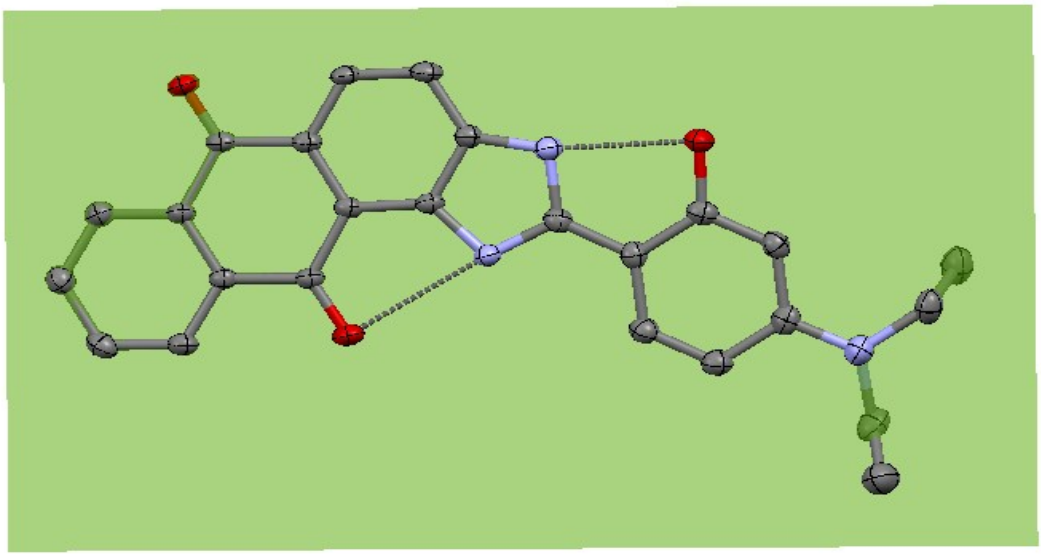


Fig. S4 Highly planar structure of **1** shown by a crystallographic plane containing all the atoms

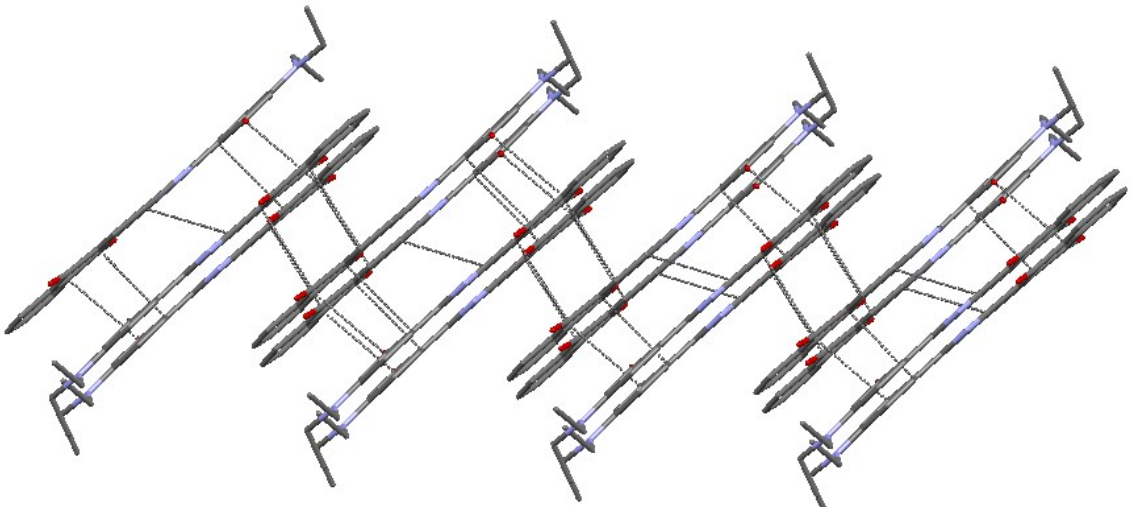
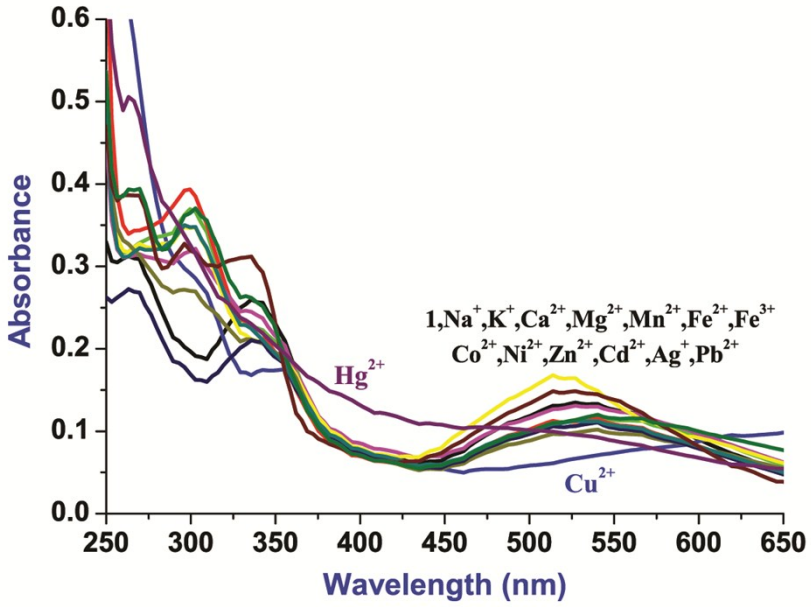
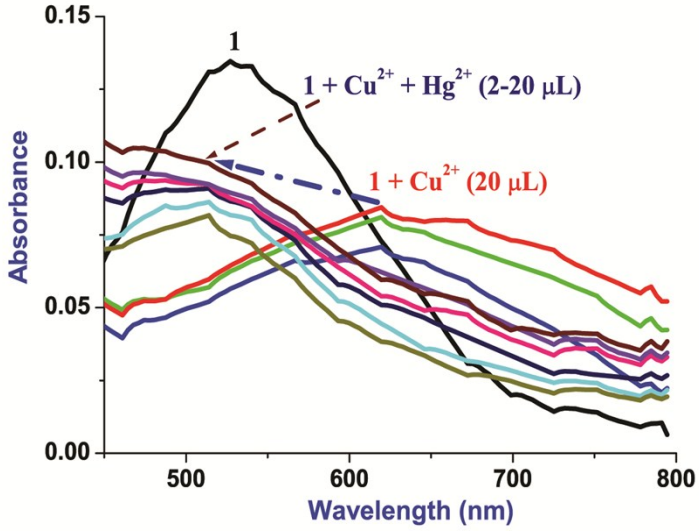


Fig. S5 Intermolecular edge-to-edge π-π interactions in **1**



(a)



(b)

Fig. S6 (a) UV/vis spectra of **1** in presence of various metal ions. (b) UV/vis spectra showing selectivity of **1** toward Hg^{2+} over Cu^{2+}.

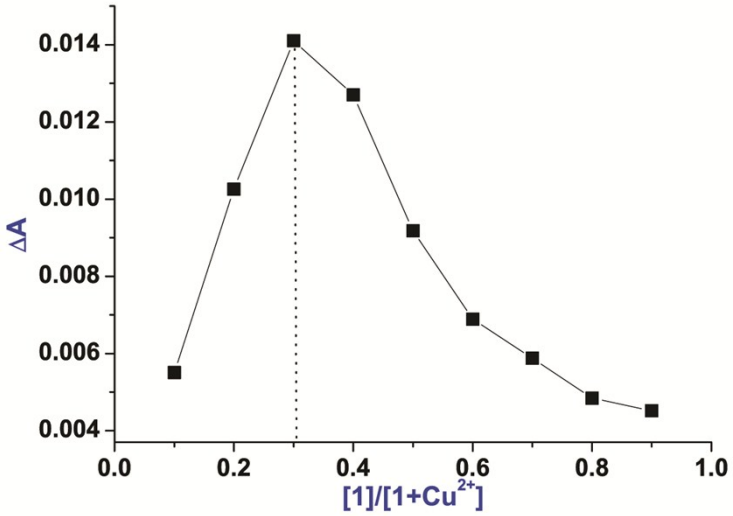


Fig. S7a Job's plot analysis showing (1:2) binding stochiometry between **1** and Cu^{2+} ion

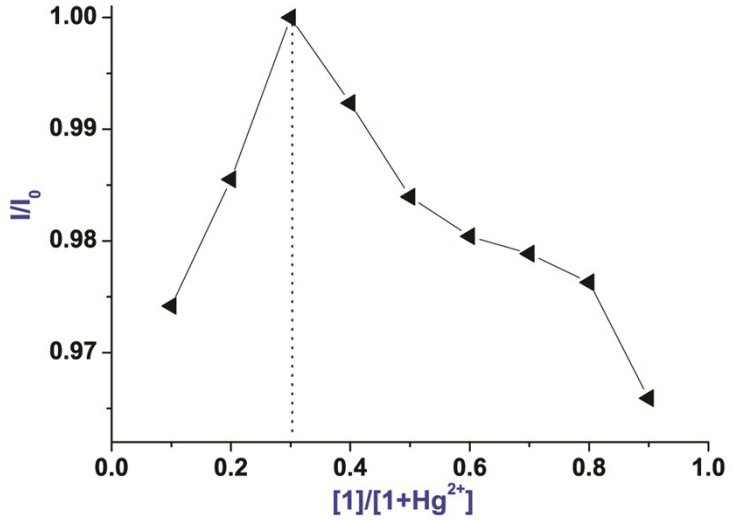


Fig. S7b Job's plot analysis showing (1:2) binding stochiometry between **1** and Hg^{2+} ion

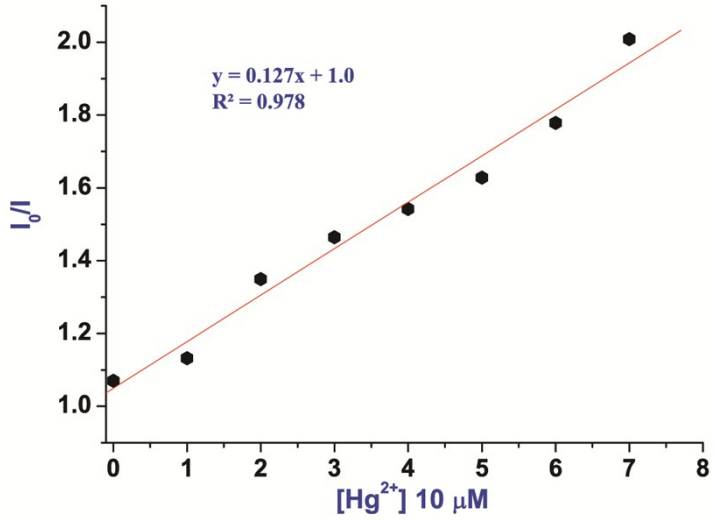


Fig. S8 Stern-Volmer plot for quenching of fluorescence of **1** in presence of Hg^{2+} ion

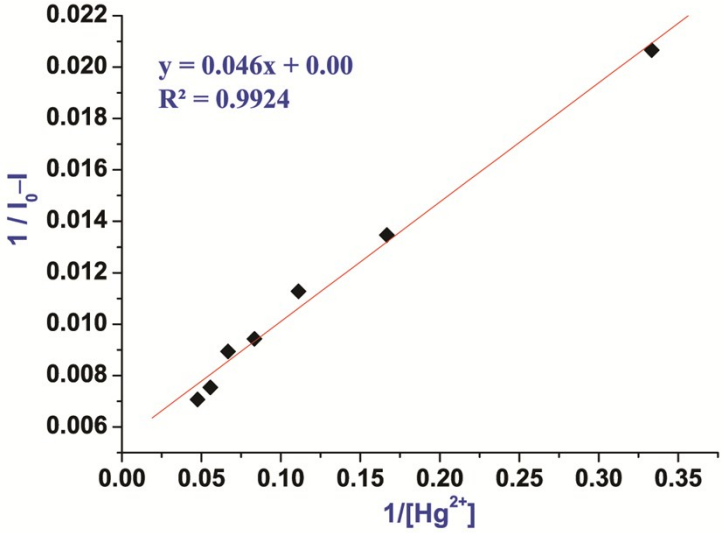


Fig. S9 Benesi-Hildebrand plot for binding of **1** with Hg^{2+} ion

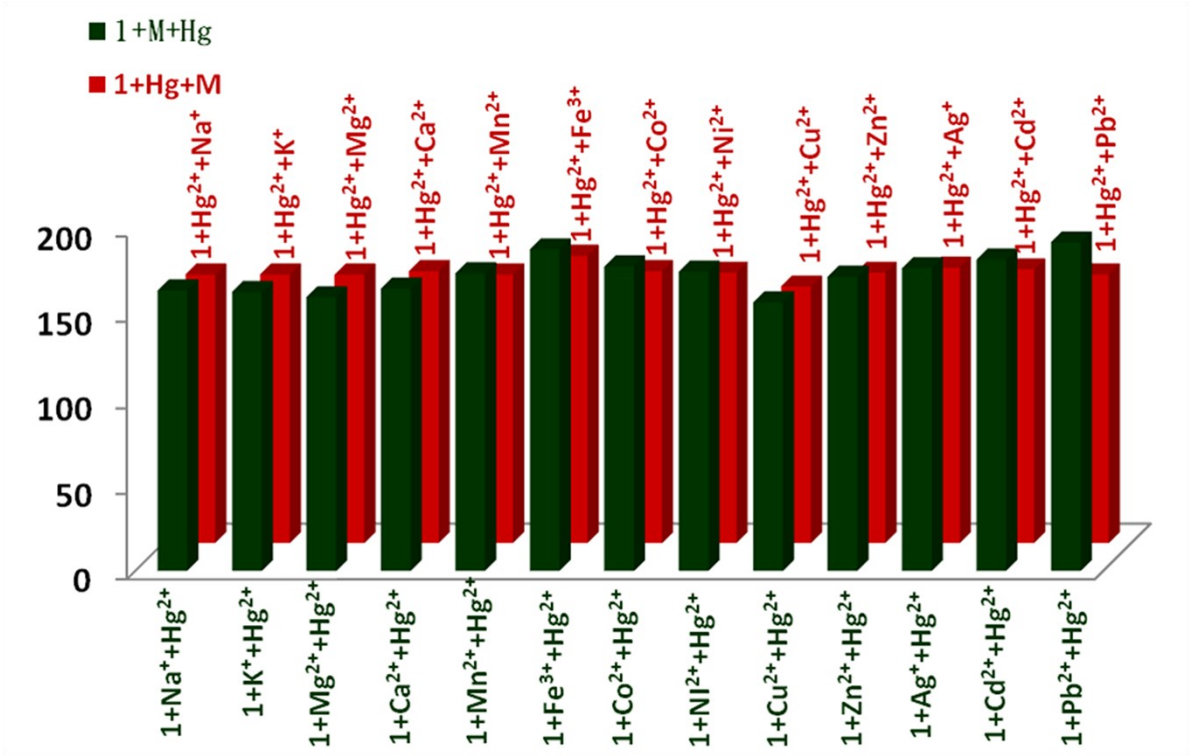


Fig. S10 Bar diagram showing interference of various cations in binding of **1** with Hg^{2+} in dual way (addition of metal ions to the solution of **1**+Hg^{2+}; addition of Hg^{2+} to the 1+M_n^{n+}).

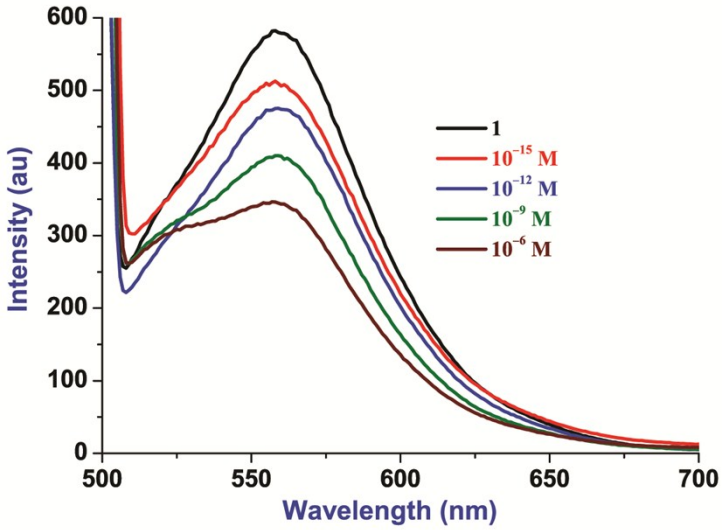


Fig. S11a Sensitivity of **1** toward Hg^{2+} from femtomolar to micromolar level

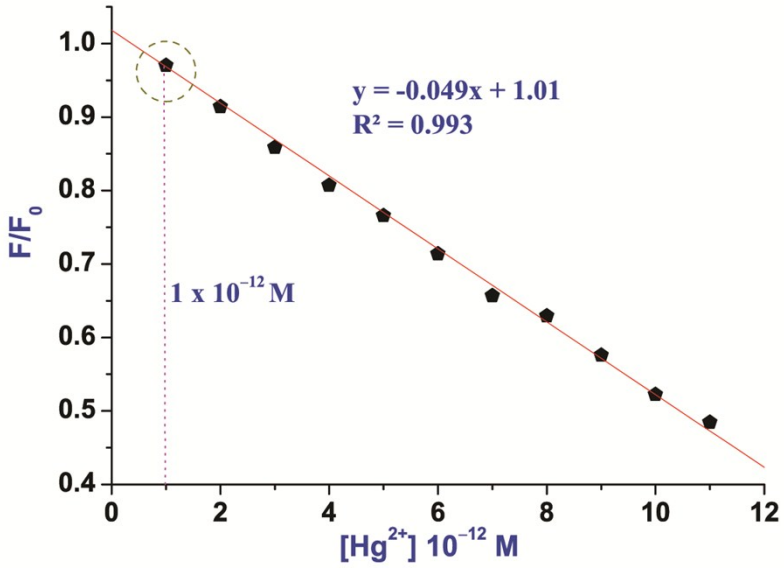


Fig. S11b Linear fluorescence quenching response of **1** towards picomolar (PM) Hg^{2+} having LOD of 1.0 PM.

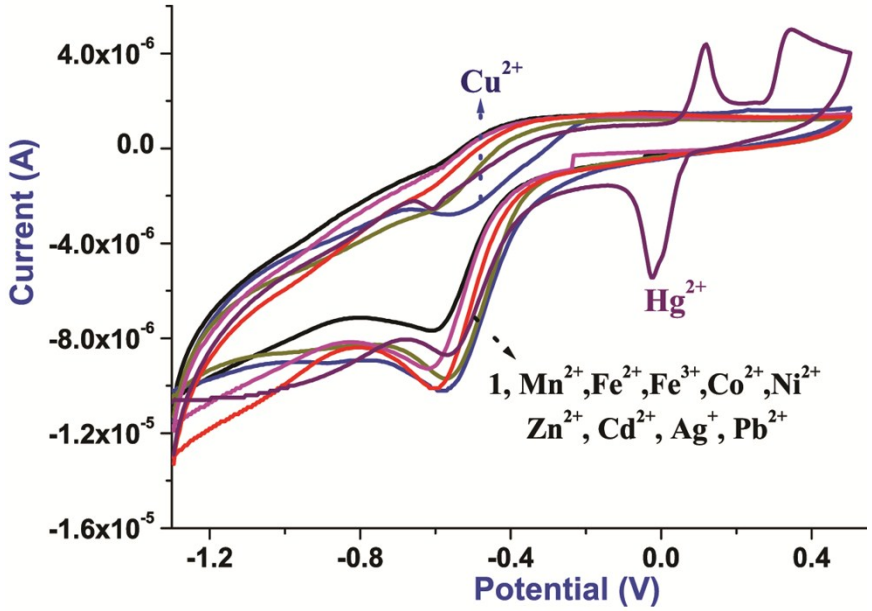


Fig. S12 Electrochemical response of **1** toward various metal ions

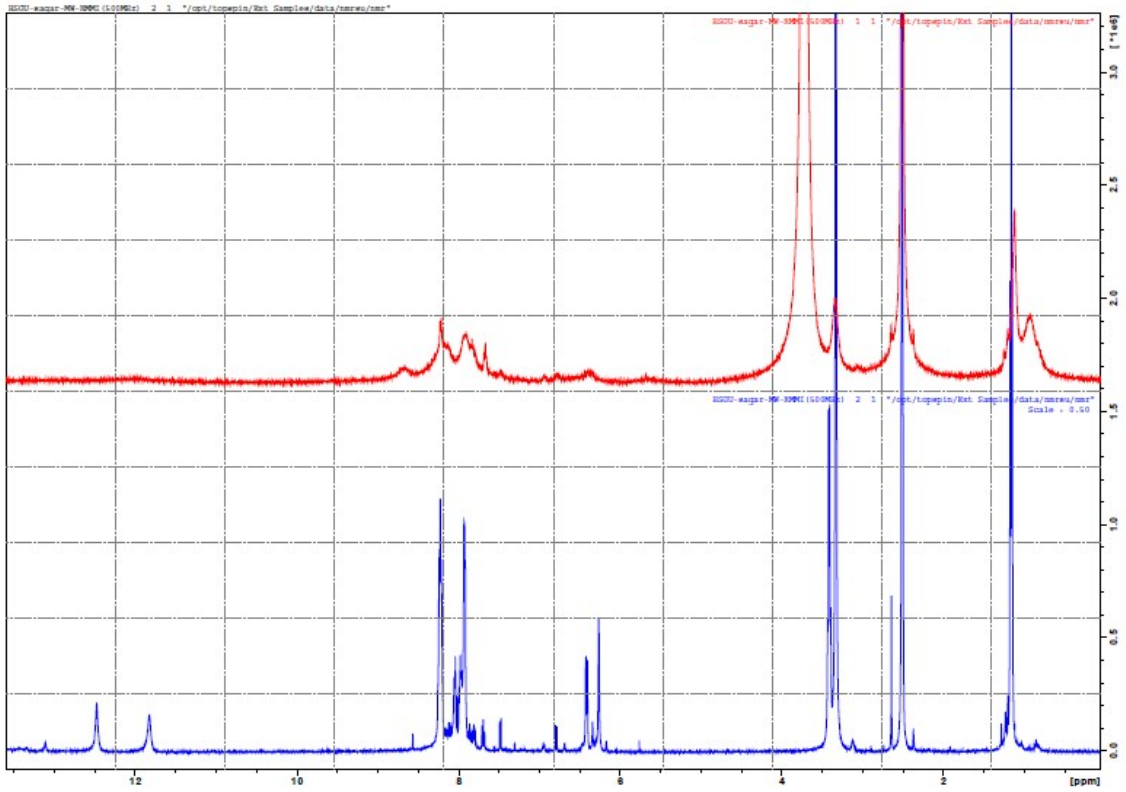


Fig. S13 ^{1}H NMR titration spectra of **1** (bottom) in presence of Cu^{2+} (1.0 equiv)

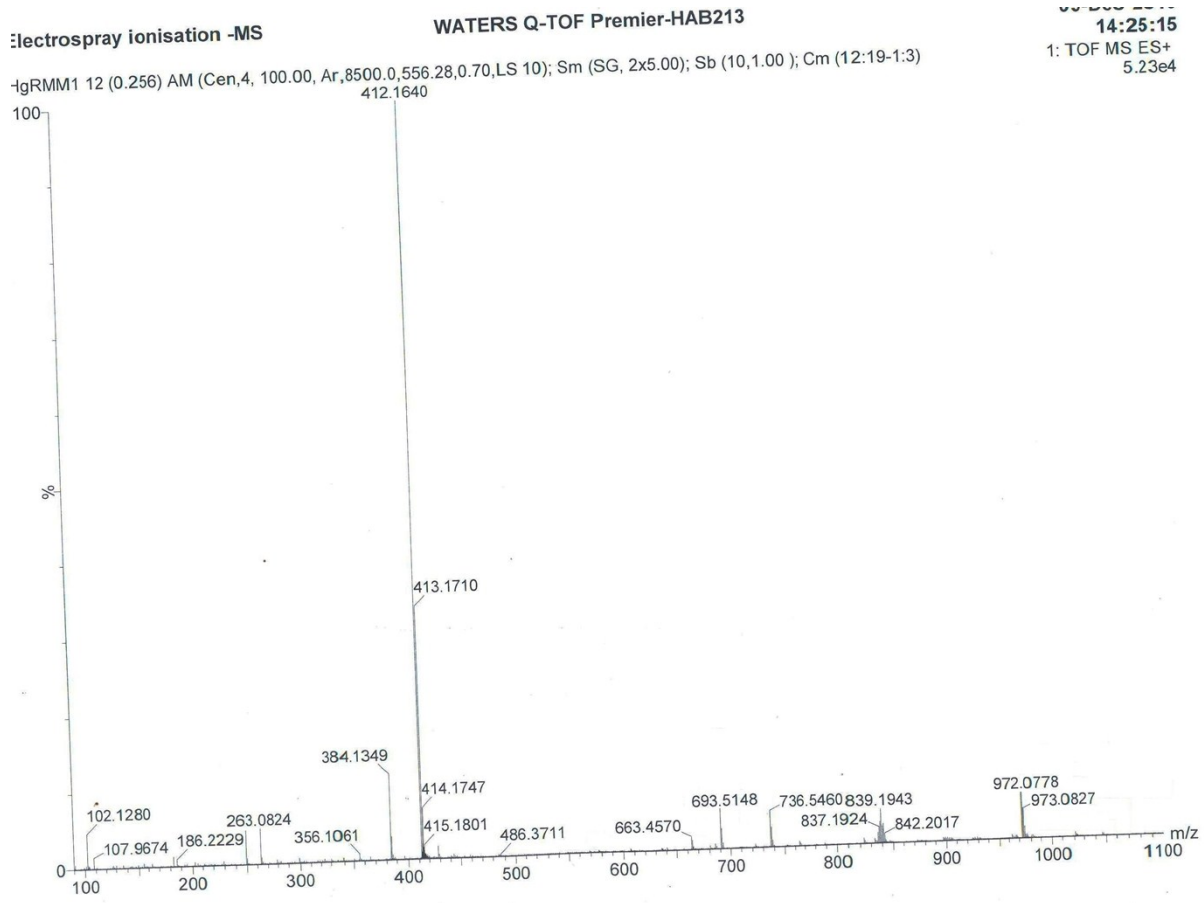


Fig. S14a ESI-MS spectrum of **1** + Hg^{2+} complex

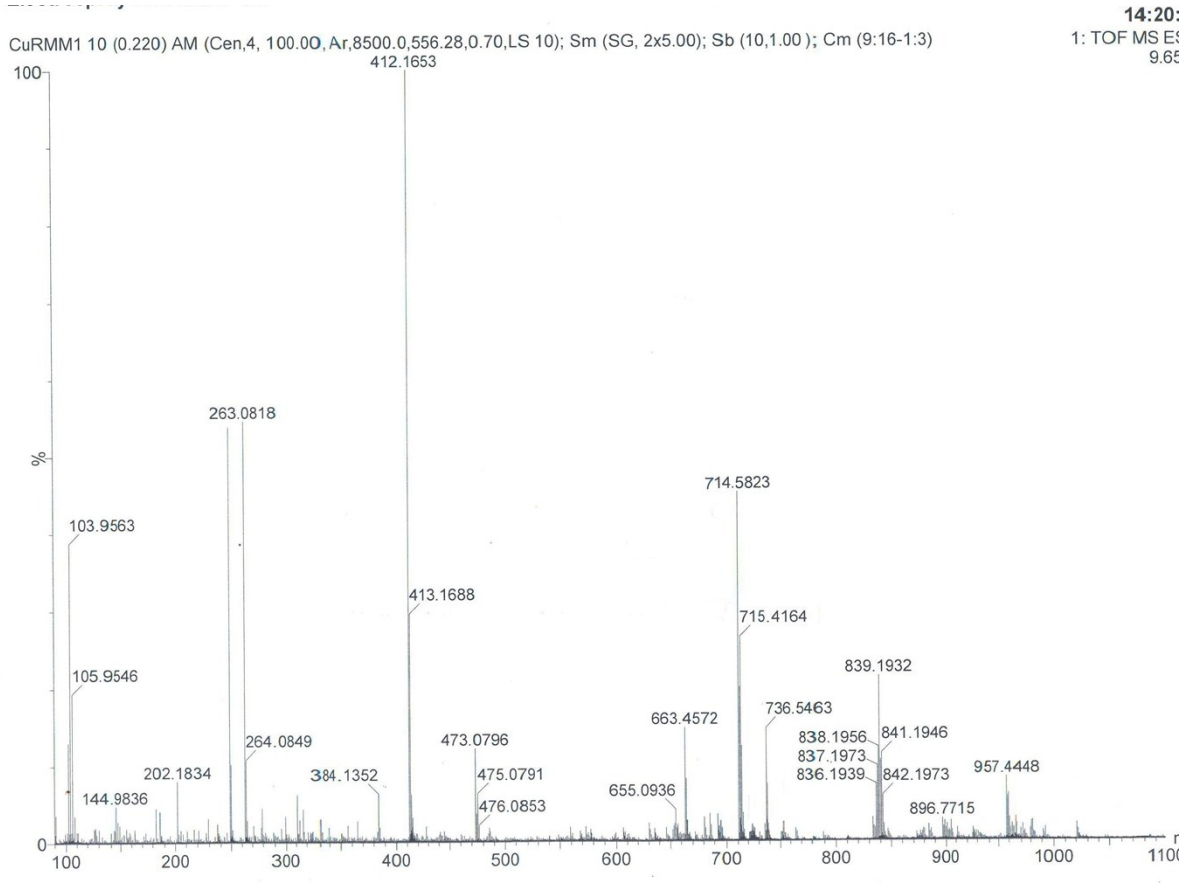


Fig. S14b ESI-MS spectrum of **1** + Cu^{2+}

References:

1 (a) G. M. Sheldrick, *SHELXL-97, Program for X-ray Crystal Structure Refinement*; Göttingen University: Göottingen, Germany, 1997; (b) R.W.W. Hooft, L.H. Straver, A.L. Spek, J. Appl. Cryst. 2008, **41**, 96. (c) A. L. Spek, Private communication, 2012.

2 (a) A. L. Spek, *PLATON, A Multipurpose Crystallographic Tools* Utrecht University, Utrecht, The Netherlands, 2000; (b) A. L. Spek, *Acta Crystallogr. A,* 1990, **46**, C31.