

Supporting information

Donor- π -Acceptor (D- π -A) Dyad for ratiometric detection of Hg²⁺ and PPI

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Table S1. Topological parameters Laplacian electron density ($\nabla^2\rho$), potential energy density [V(r)], Lagrangian kinetic energy G(r), total energy density [H(r)], hydrogen bonding energy [E_{HB}(kJmol⁻¹)] at a bond critical pint of non-covalent interactions (D \cdots HA) for dyad **1**.PPI adduct at B3LYP/6-31G**.

Figure S8. Calibration curve for variable concentration of Hg²⁺ ions.

Figure S9. Reports of analysis Hg²⁺ ions two water samples though AAS.

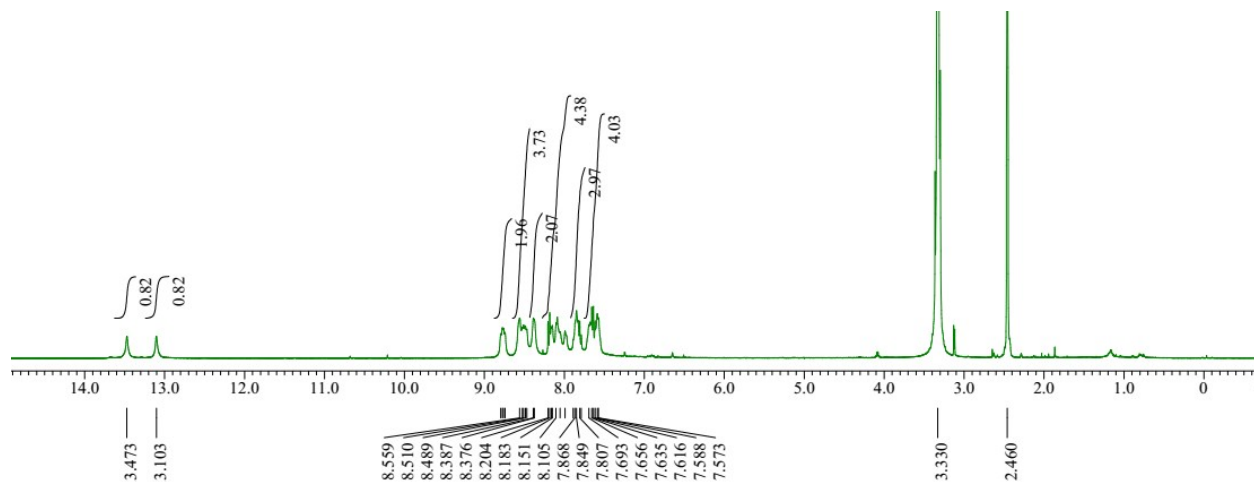


Figure S1. ^1H NMR of dyad 1

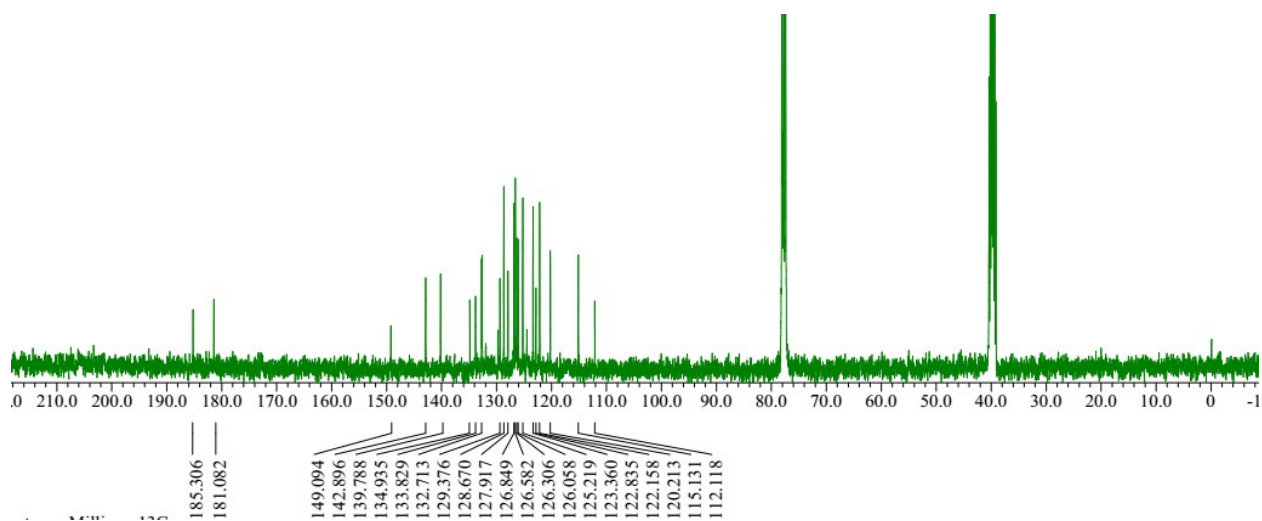


Figure S2. ^{13}C NMR of dyad 1

WATERS, Q-TOF MICROMASS (ESI-MS)

RUHI RR-507 26 (0.603) Cm (26:48)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH

TOF MS ES+
1.42e3

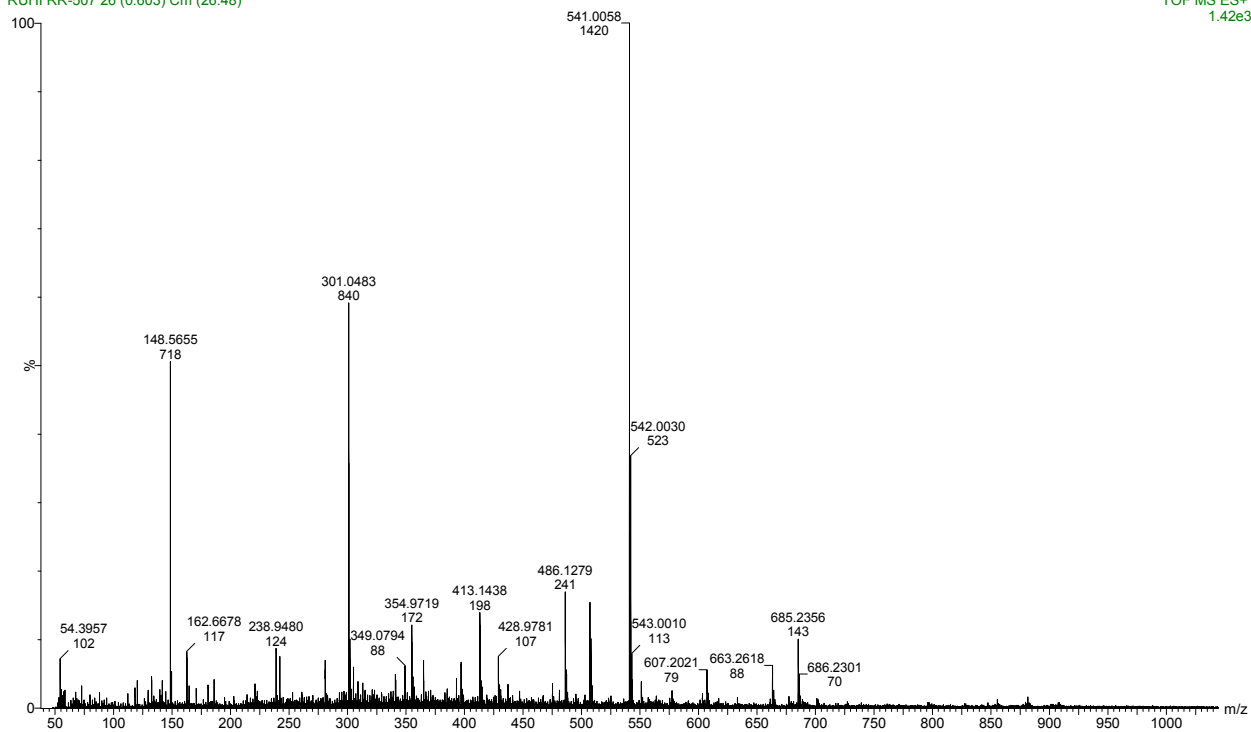


Figure S3. Mass spectrum of dyad 1

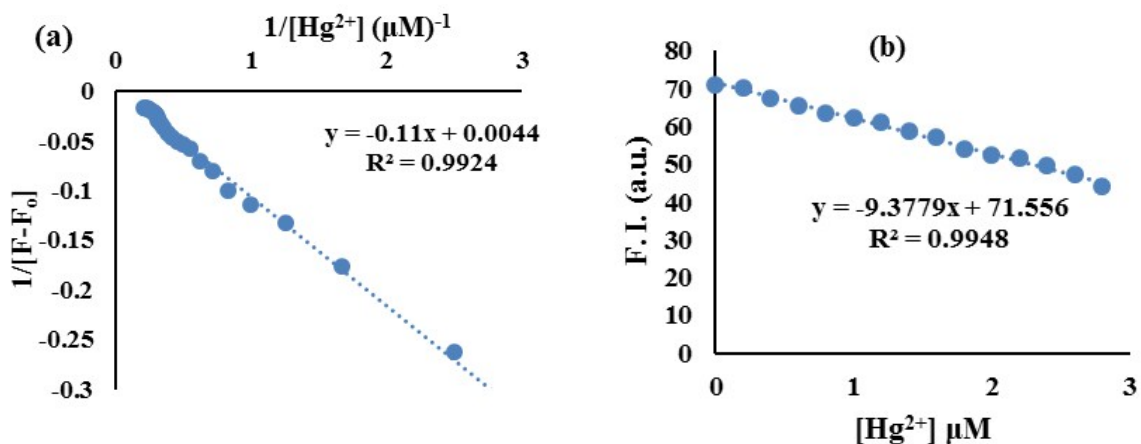


Figure S4. (a) Benesi-Hildebrand plot for stability constant and (b) calibration curve for lowest detection limit for of complex.

dyad 1.Hg²⁺

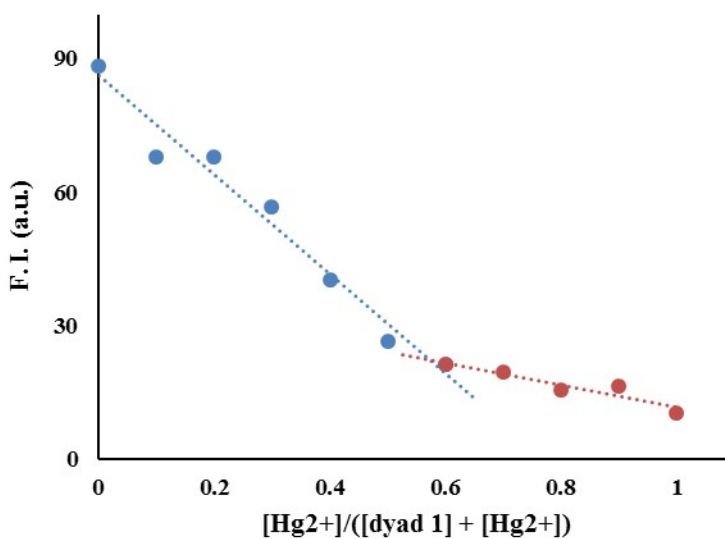


Figure S5. Job

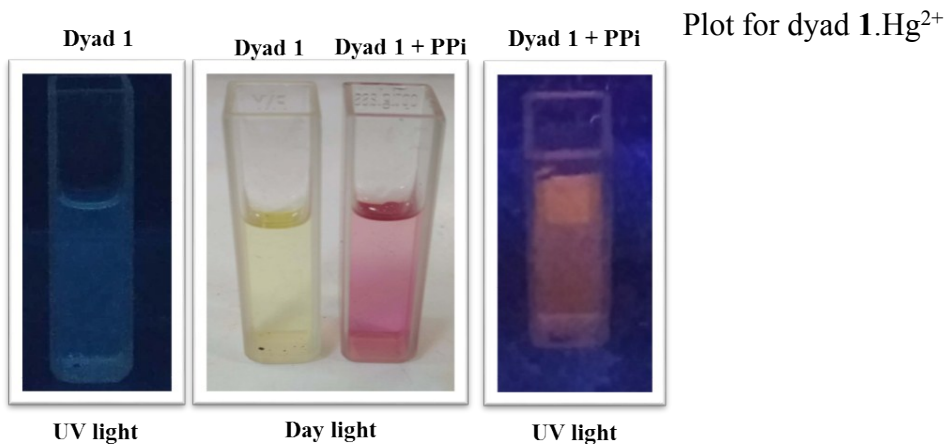


Figure S6. Colour changes of dyad 1 for PPI in daylight and under UV light.

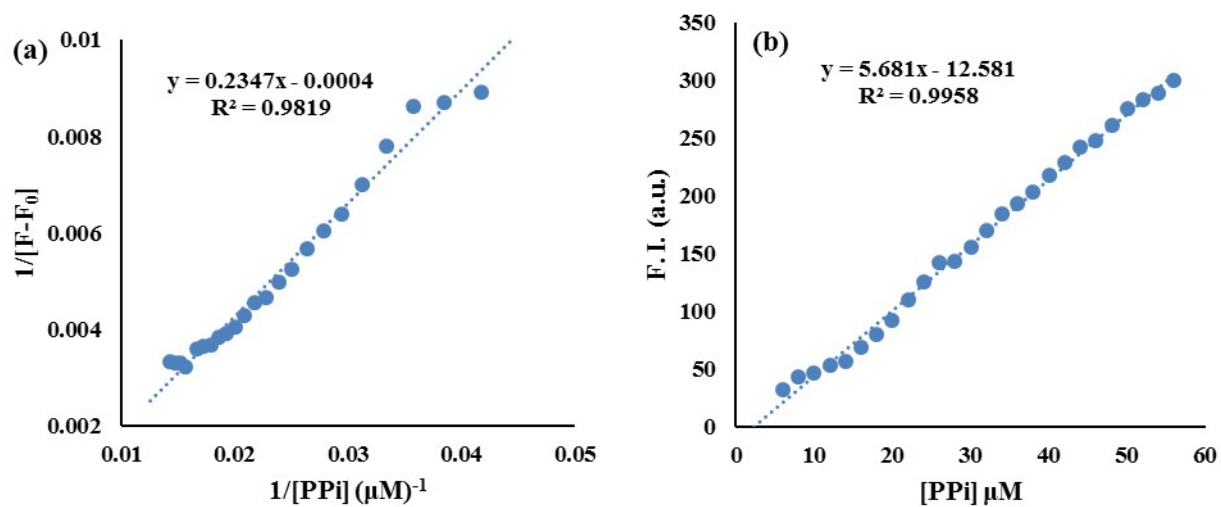


Figure S7. (a) Benesi-Hildebrand plot for stability constant and (b) calibration curve for lowest detection limit for dyad 1.PPI adduct.

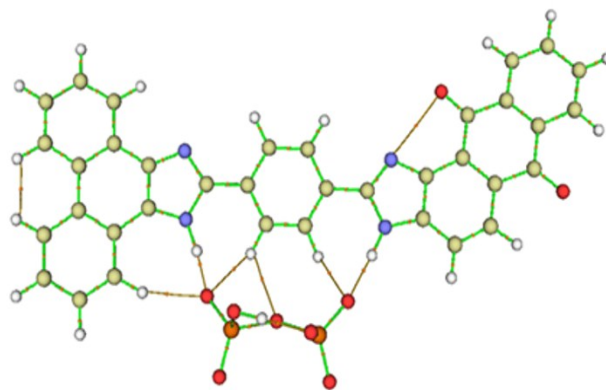


Figure S8. The molecular graph of dyad 1.PPi, with bond critical points and bond paths at interaction of dyad 1 towards PPi ions

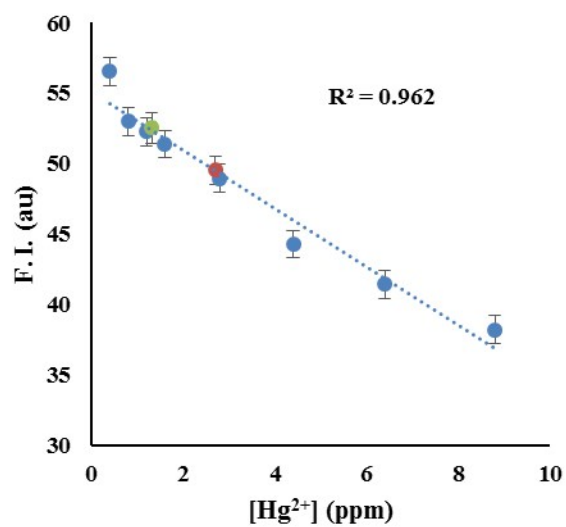


Figure S9. Calibration curve for variable concentration of Hg²⁺ ions.



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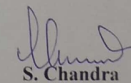
TEST REPORT

Test Report No.:	NN/18-19/047	Date:	23.05.2018
Service No.	NN/18-19/047 (01)	Customer's Ref.	Sample Submitted by Mr. Gulshan Kumar dtd 22.05.2018
Customer's name and address:			
M/s School of Chemistry and Biochemistry TIET Patiala. Kind Attn. Dr. Vijay Luxmi			
Sample Description	Liquid Sample (Research Sample)		
Condition of the sample received	O.K.		
Customer's sample identification No. (if any)	-		
Quantity/number of samples	One		
Sampling Procedure (if any)	--		
Test parameters	Mercury		
Standard/Specification/Method followed	Atomic Absorption Spectrometer		
Deviations (if any)	--		
Documents constituting this report (if any)	--		
Date of Receipt of Job	Date of Completion of Job	Total Number of Pages	
22.05.2018	23.05.2018	1	

TEST RESULTS

S. No.	Parameter	Test Method	Unit	Results	
				Readings	Average
1.	Mercury as Hg	Atomic Absorption Spectrometer	mg/l	i) 1.381	1.367
				ii) 1.337	
				iii) 1.382	

.....end of the report.....


S. Chandra

Head, SAI Labs
(Authorized Signatory)

- Note:
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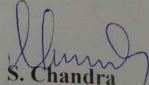
TEST REPORT

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Customer's name and address:			
M/s School of Chemistry and Biochemistry TIET Patiala. Kind Attn. Dr. Vijay Luxmi			
Sample Description	Liquid Sample (Research Sample)		
Condition of the sample received	O.K.		
Customer's sample identification No. (if any)	-		
Quantity/number of samples	One		
Sampling Procedure (if any)	--		
Test parameters	Mercury		
Standard/Specification/Method followed	Atomic Absorption Spectrometer		
Deviations (if any)	--		
Documents constituting this report (if any)			
Date of Receipt of Job		Date of Completion of Job	Total Number of Pages
09.05.2018		09.05.2018	1

TEST RESULTS

S. No.	Parameter	Test Method	Unit	Results	
				Readings	Average
1.	Mercury as Hg	Atomic Absorption Spectrometer	mg/l	i) 2.705	2.76
				ii) 2.716	
				iii) 2.848	

.....end of the report.....


S. Chandra
Head, SAI Labs
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Figure S10. Reports of analysis Hg^{2+} ions two water samples though AAS.