

**Facile Synthesis of D- π -A structured Dyes and their applications towards cost effective
fabrication of solar cell as well as sensing of hazardous Hg (II)**

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Supporting Information S1

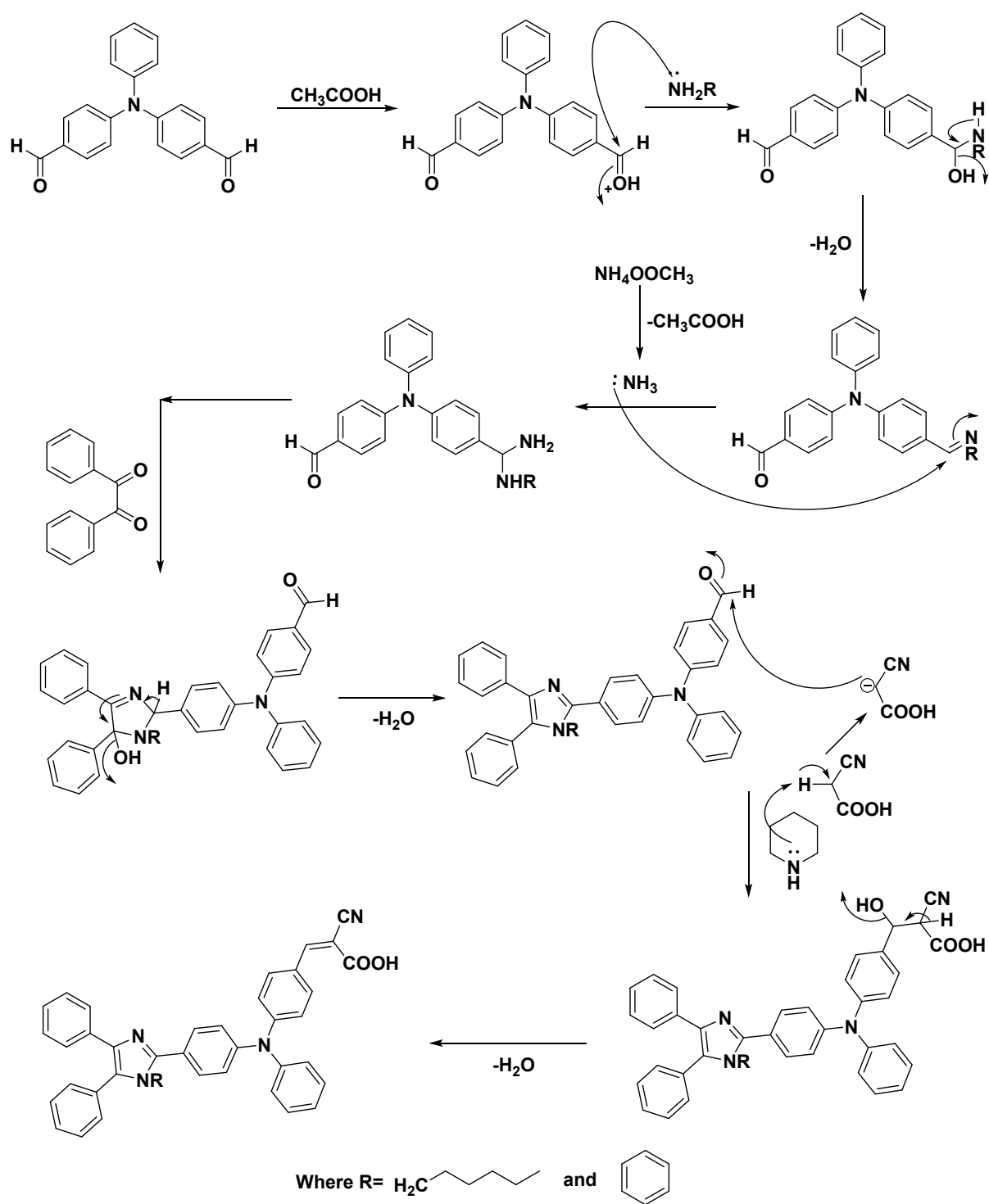


Fig S1. Plausible mechanism for the synthesis of compound 1 and 2

Supporting Information S2

^1H NMR, ^{13}C NMR, Mass and HR-MS spectra of Compound (i), (ii), 1 and 2

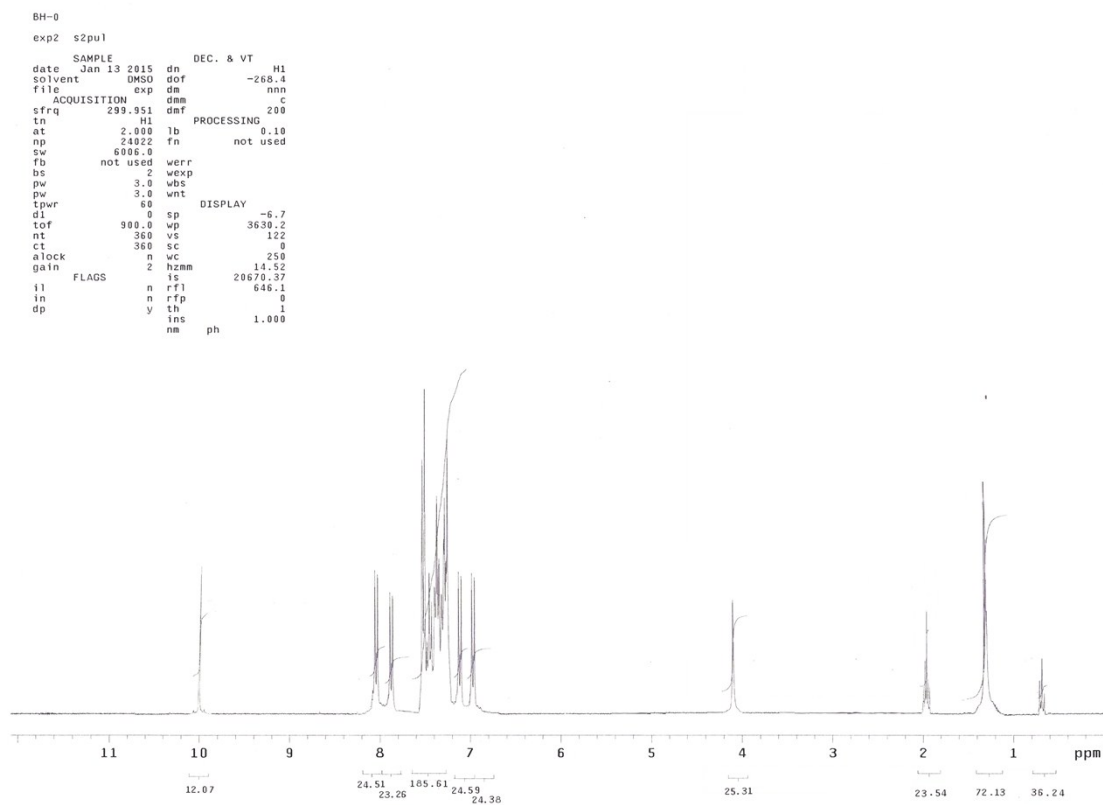


Fig S2.1. ^1H NMR of Compound (i) in DMSO- d_6

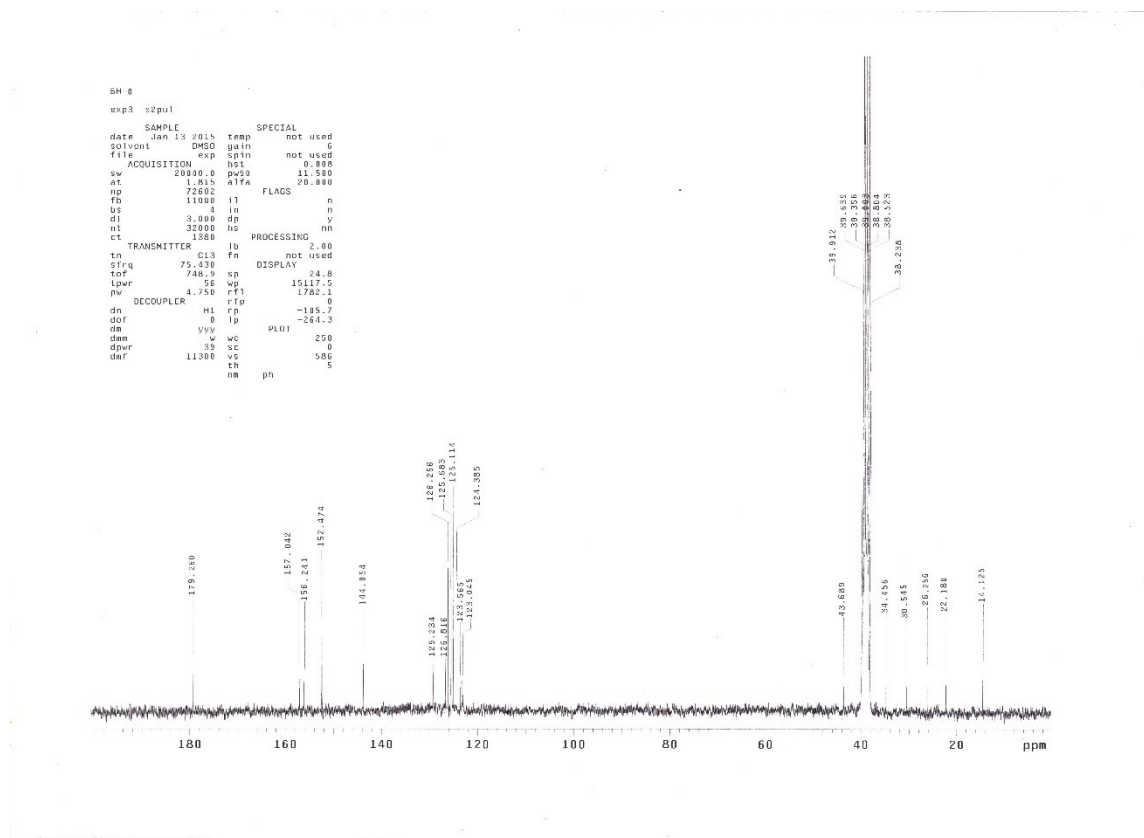


Fig S2.2. ^{13}C NMR of Compound (i) in $\text{DMSO}-d_6$

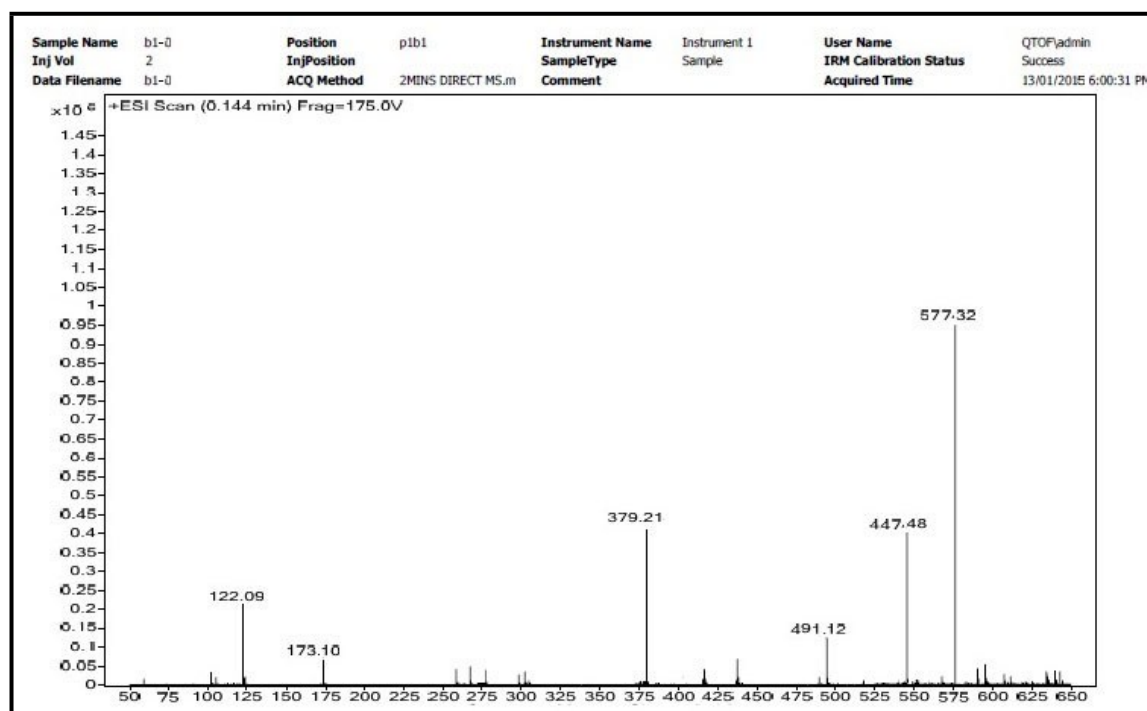


Fig S2.3. Mass Spectra of Compound (i)

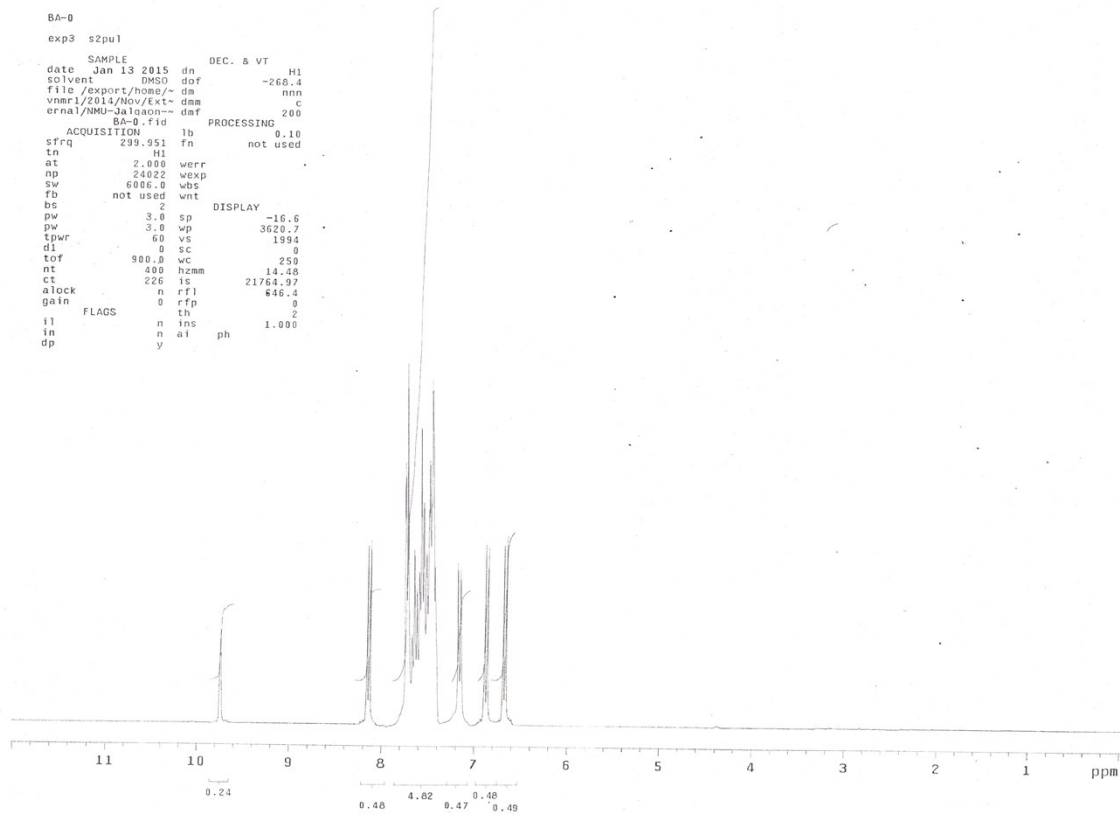


Fig S2.4. ^1H NMR of Compound (ii) in DMSO- d_6

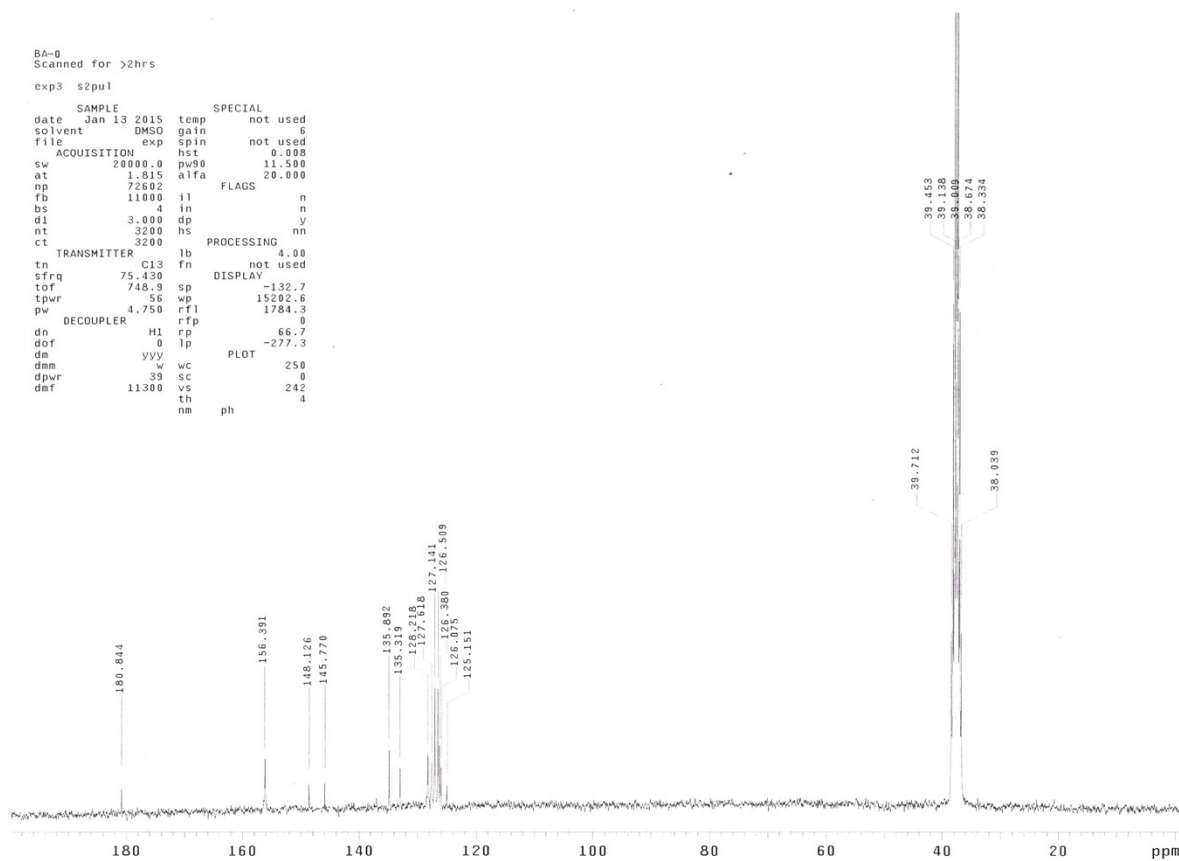


Fig S2.5. ^{13}C NMR of Compound (ii) in $\text{DMSO-}d_6$

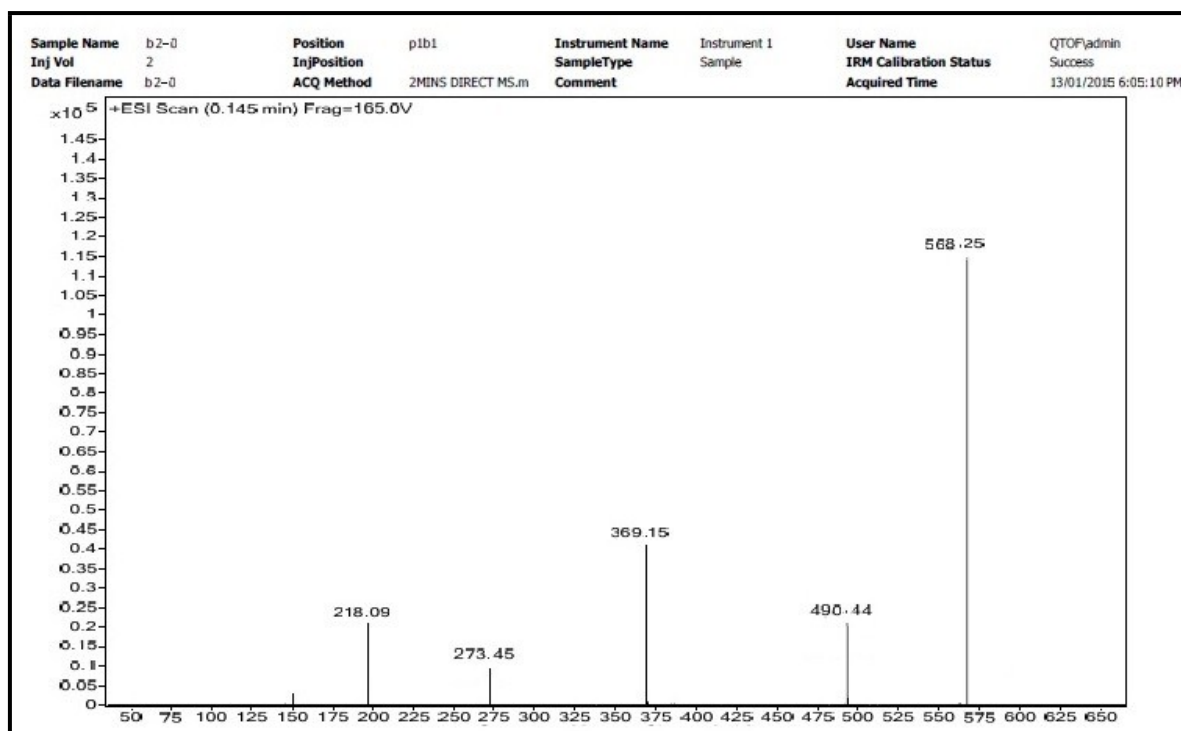


Fig S2.6. Mass spectra of Compound (ii)

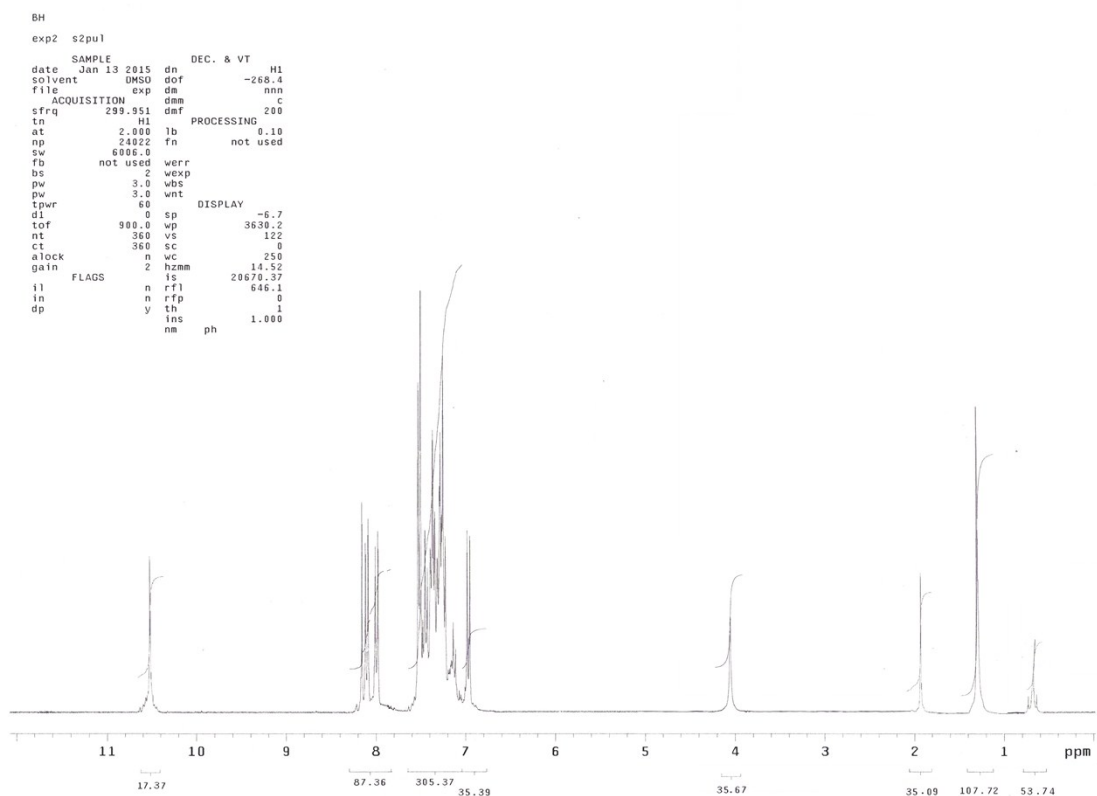


Fig S2.7. ^1H NMR of Compound 1 in $\text{DMSO-}d_6$

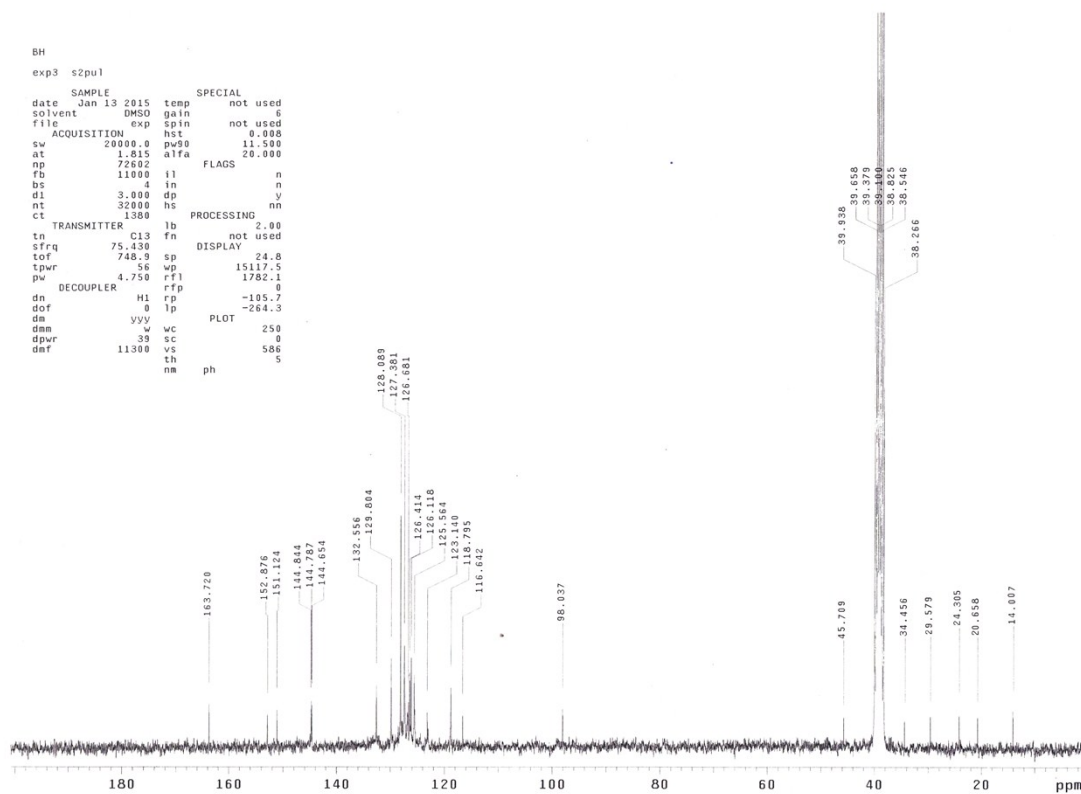


Fig S2.8. ^{13}C NMR of Compound 1 in $\text{DMSO-}d_6$

Qualitative Compound Report

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Sample Type Sample
Instrument Name Instrument 1
Acq Method 2MINS DIRECT MS.m
IRM Calibration Status Success
Comment

Sample Name BH
Position P104
User Name QTOF/admin
Acquired Time 10/21/2014 4:23:02 PM
DA Method default.m

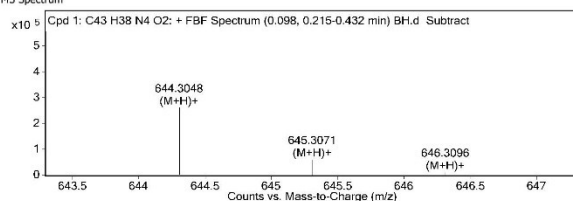
Sample Group Info.
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (85125.1)

Compound Table

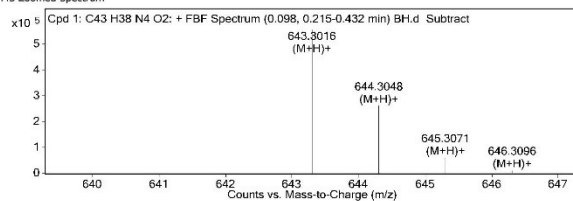
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C43 H38 N4 O2	0.181	642.2942	554002	C43 H38 N4 O2	642.2995	-8.16	C43 H38 N4 O2	C43 H38 N4 O2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C43 H38 N4 O2	643.3016	0.181	Find By Formula	642.2942

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
643.3016	1	554002.25	C43H38N4O2	(M+H)+
644.3048	1	258993.88	C43H38N4O2	(M+H)+
645.3071	1	58283.33	C43H38N4O2	(M+H)+
646.3096	1	9516.68	C43H38N4O2	(M+H)+
647.3114	1	1168.8	C43H38N4O2	(M+H)+

--- End Of Report ---

Fig S2.9. HRMS of Compound 1

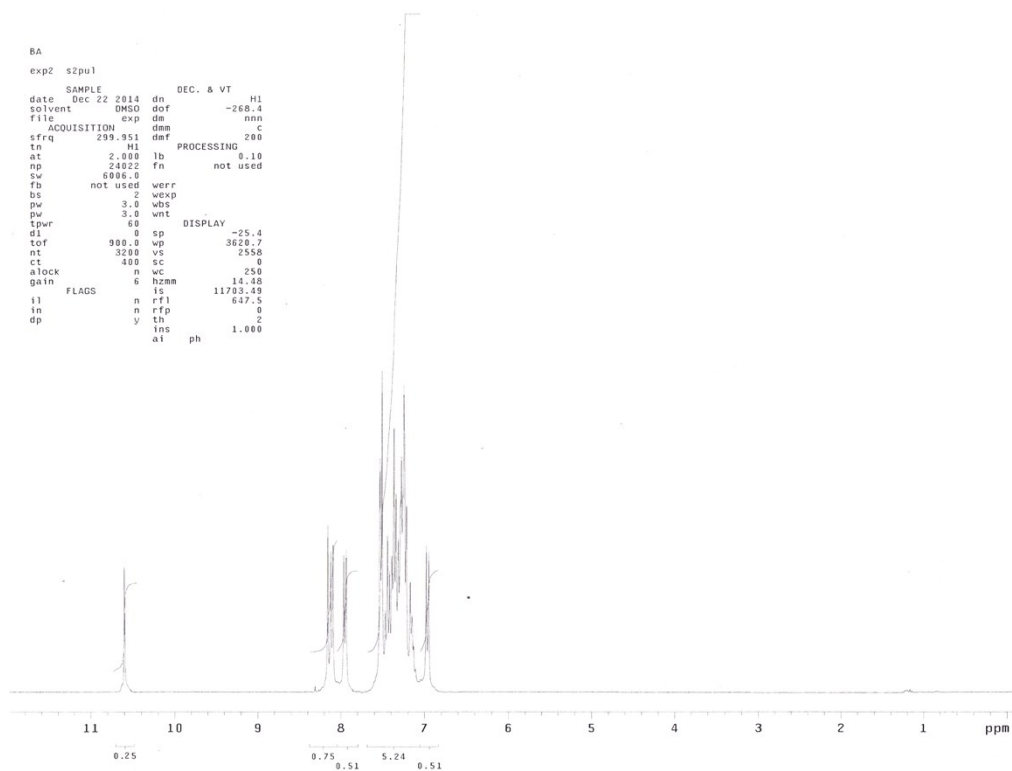


Fig S2.10. ^1H NMR of Compound 2 in $\text{DMSO-}d_6$

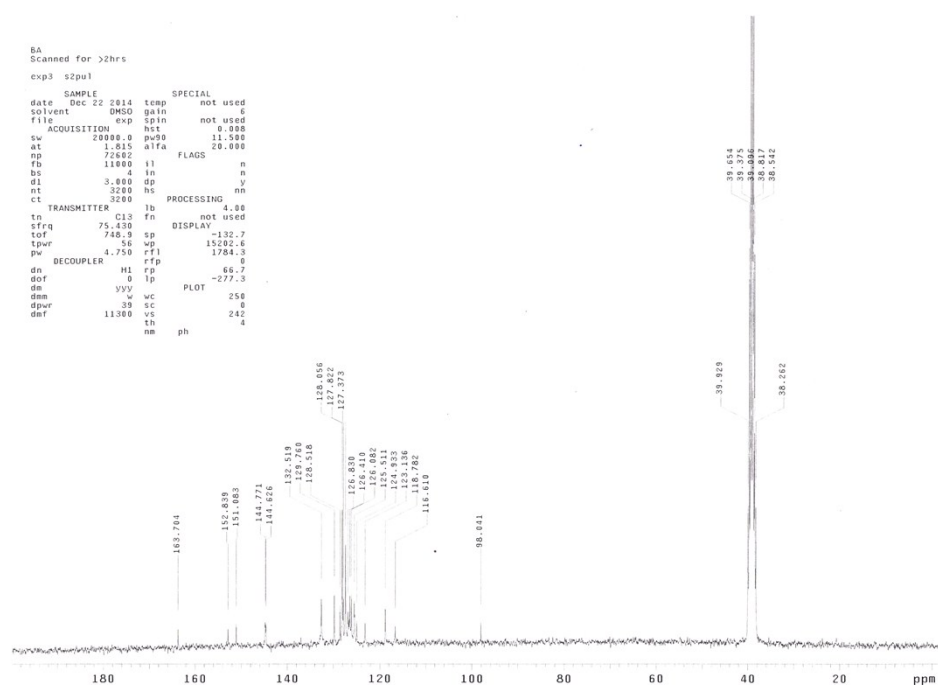


Fig S2.11. ^{13}C NMR of Compound 2 in $\text{DMSO-}d_6$

Qualitative Compound Report

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IRM Calibration Status	Success	DA Method	default.m
Comment			

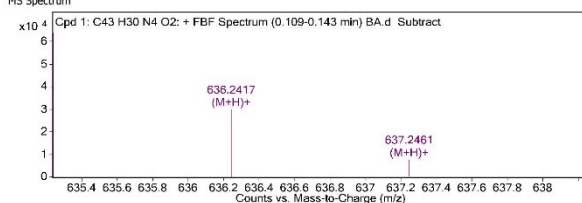
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Version	Q-TOF B.05.01 (85125.1)		

Compound Table

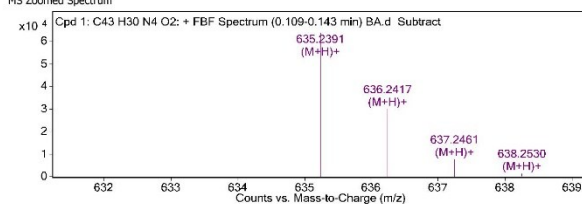
Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)	MFG Formula	DB Formula
Cpd 1: C43 H30 N4 O2	0.143	634.2317	63713	C43 H30 N4 O2	634.2369	-8.1	C43 H30 N4 O2	C43 H30 N4 O2

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: C43 H30 N4 O2	635.2391	0.143	Find By Formula	634.2317

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
635.2391	1	63713.08	C43H30N4O2	(M+H)+
636.2417	1	29894.95	C43H30N4O2	(M+H)+
637.2461	1	7575.06	C43H30N4O2	(M+H)+
638.2530	1	1378.42	C43H30N4O2	(M+H)+

--- End Of Report ---

Fig S2.12. HRMS of Compound 2

Supporting Information S3

Optical band gaps (E_g^{opt})

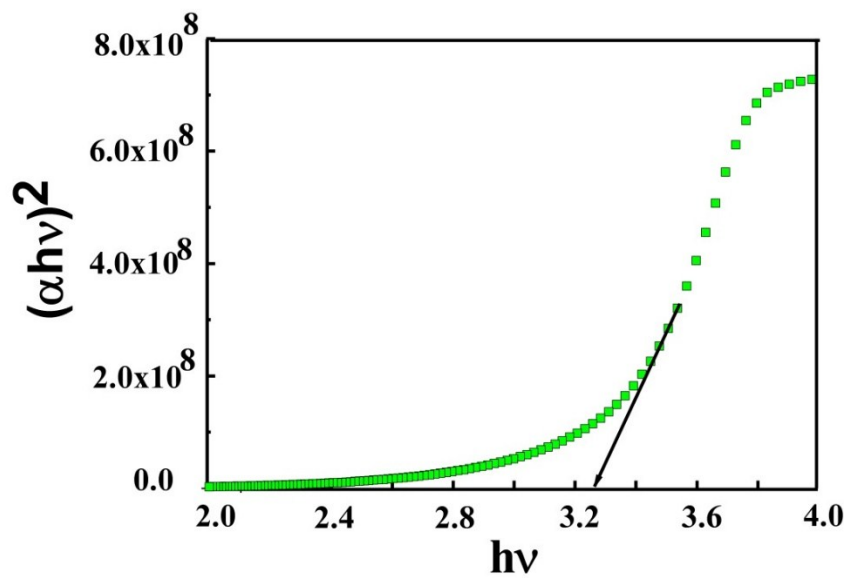


Fig S3.1. Optical Band gap of TiO_2

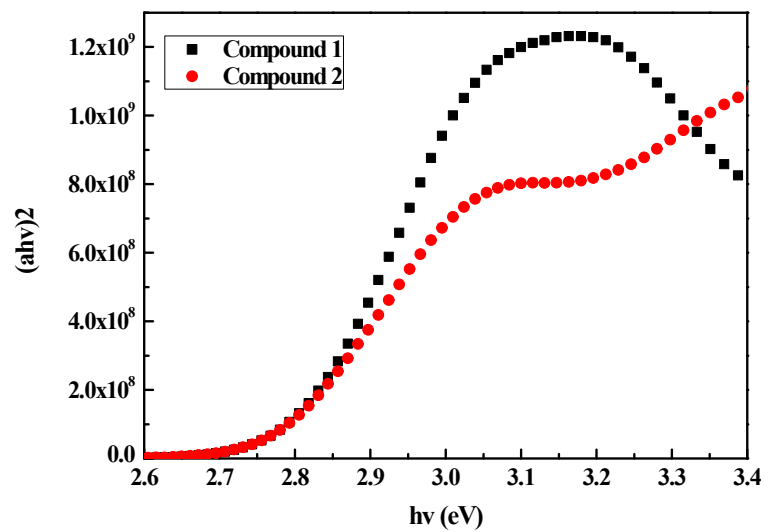


Fig S3.2. Optical Band gap of Compound 1 and compound 2

Supporting Information S4

^1H -NMR titration

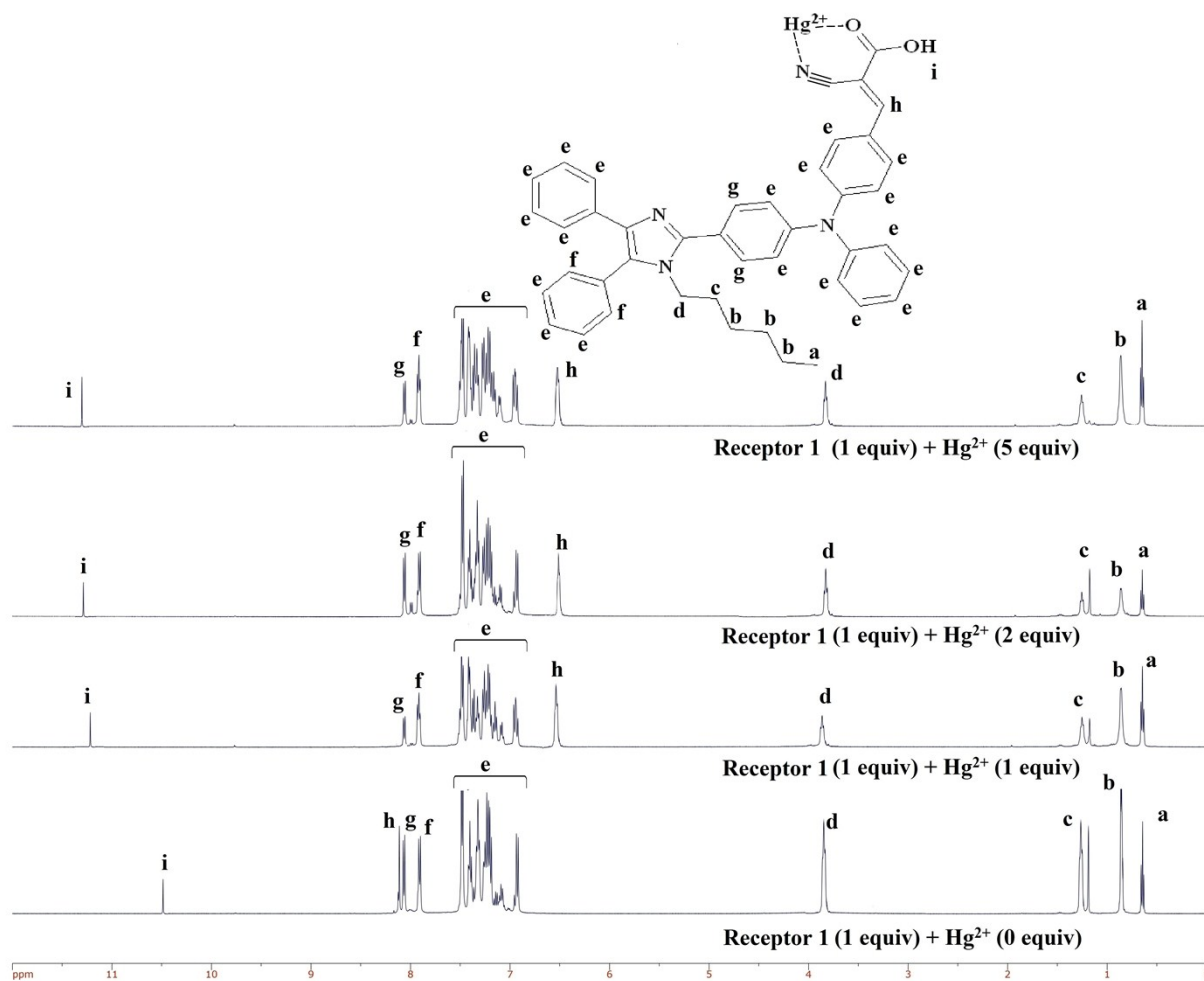


Fig S4.1. ^1H -NMR spectra of Receptor 1 upon the addition of 0,1,2,5 equiv of $\text{Hg}(\text{II})$ in $\text{DMSO}-d_6$

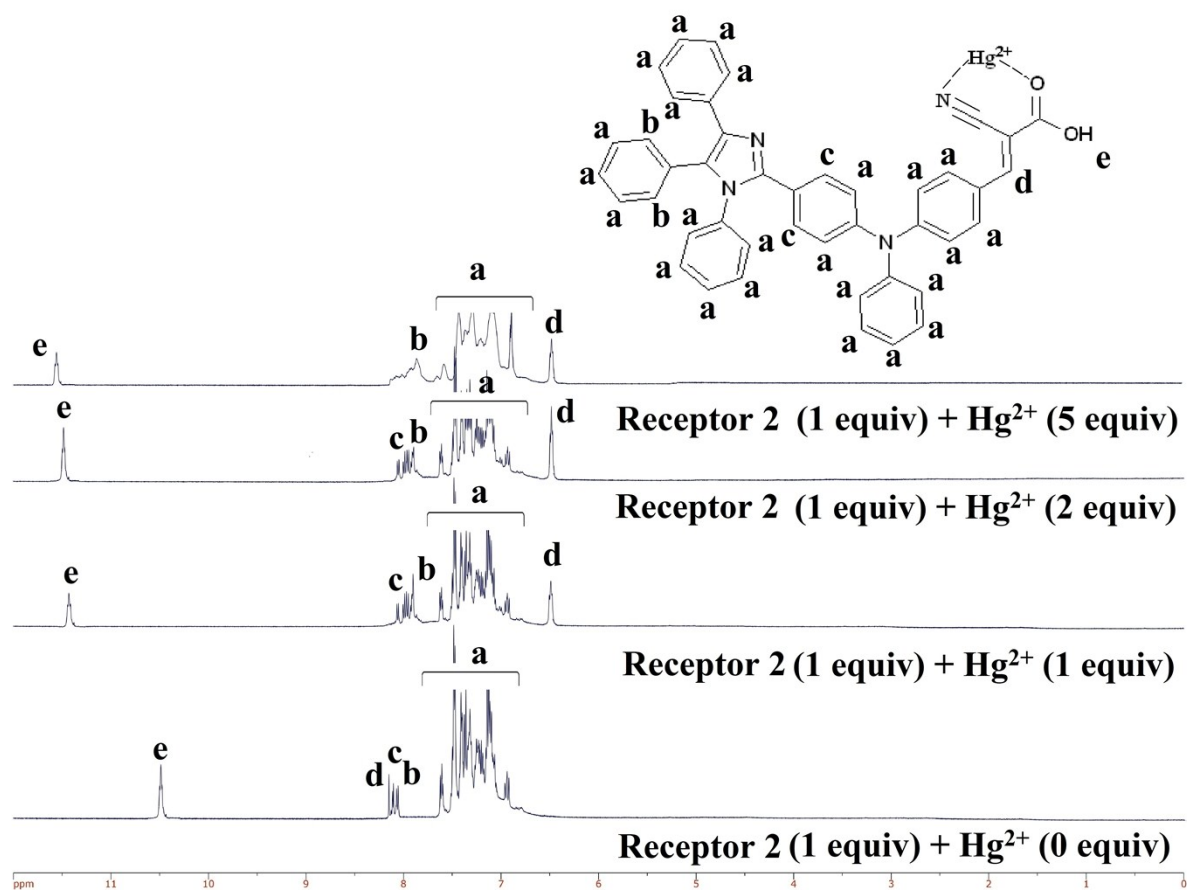


Fig S4.2. ¹H-NMR spectra of Receptor 2 upon the addition of 0,1,2,5 equiv of Hg (II) in DMSO-*d*₆

Supporting Information S5

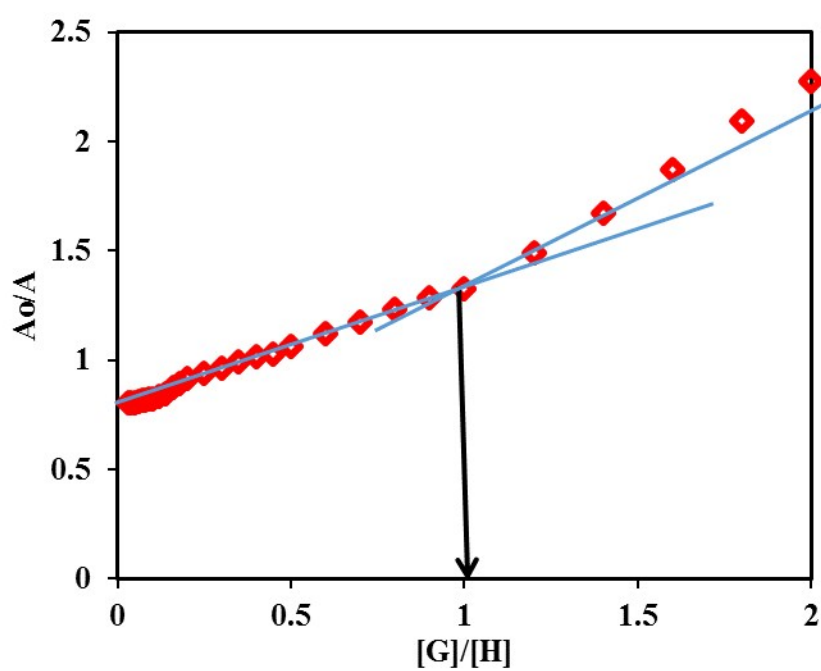


Fig S5.1. Mole ratio plot for Receptor 1. Hg(II)

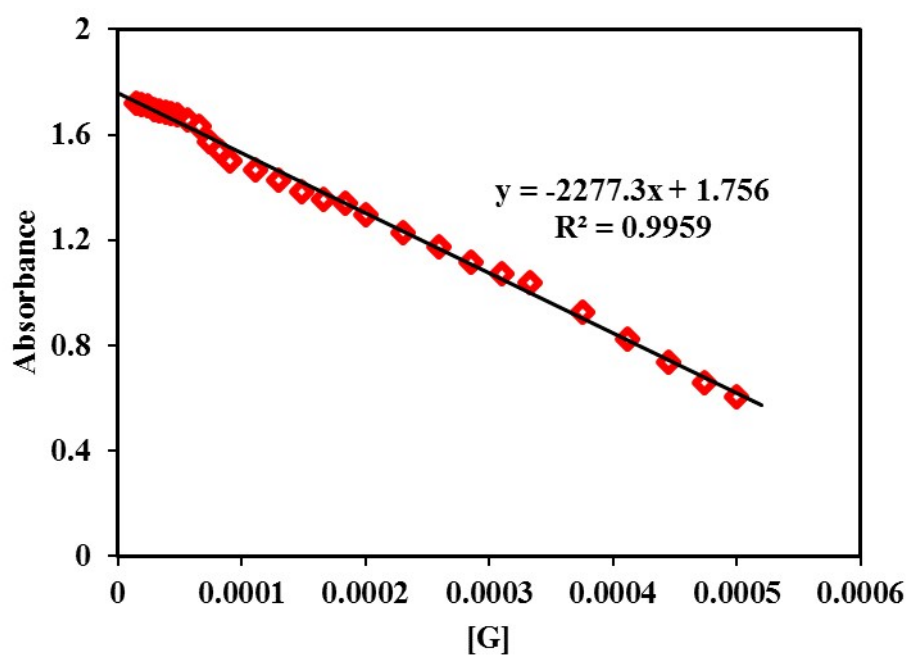


Fig S5.2. Normalized plot for Receptor 1. Hg(II)

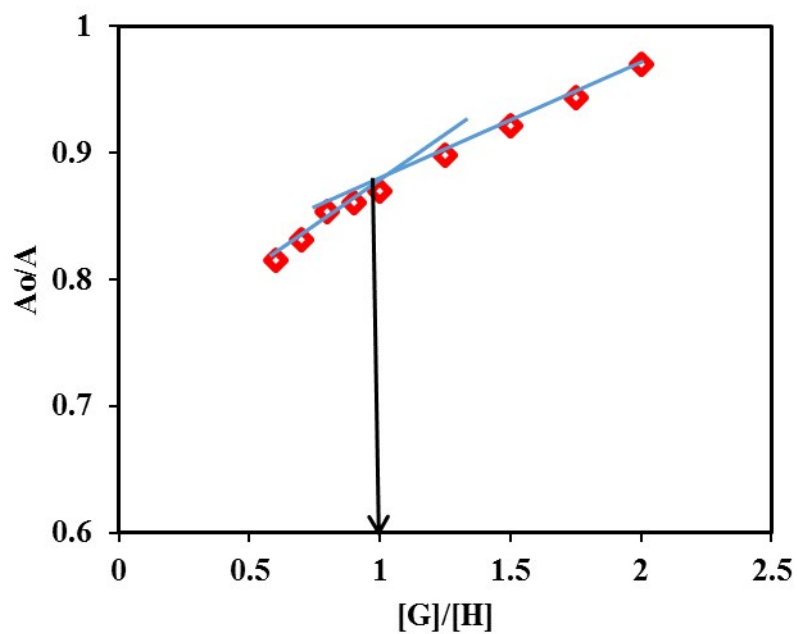


Fig S5.3. Mole ratio plot for Receptor 2. Hg(II)

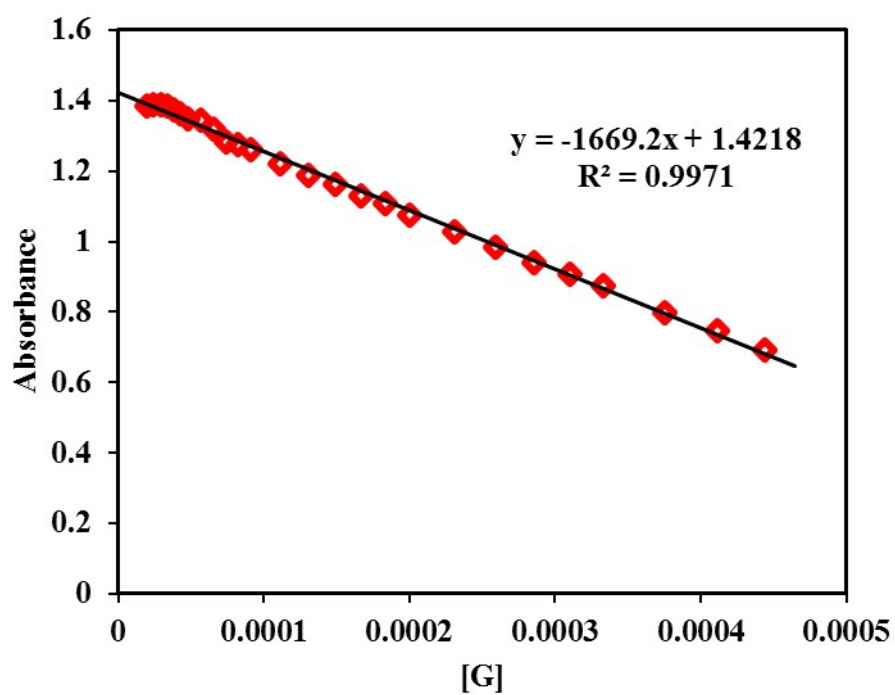


Fig S5.4. Normalized plot for Receptor 2. Hg(II)