Electronic Supplementary Material (ESI) for CrystEngComm.

A *de novo* strategy for the development of a Zn^{II}–organic framework based luminescent "switch-on" assay for size-exclusive sensitization of the oxidised form of glutathione (GSSG) over the reduced form (GSH): insights into the sensing mechanism through DFT

Sourav Bej,[ab] Riyanka Das,[ab] Debojyoti Kundu,[ab] Tapan K. Pal[c] and Priyabrata Banerjee*[ab]

* E-mail: pr_banerjee@cmeri.res.in & priyabrata_banerjee@yahoo.co.in Webpage: www.cmeri.res.in & www.priyabratabanerjee.in Fax: +91-343-2546745; Tel: +91-343-6452220.

[a] Surface Engineering & Tribology Group, CSIR-Central Mechanical Engineering Research Institute, Mahatma Gandhi Avenue, Durgapur 713209, West Bengal, India.

[b] Academy of Scientific & Innovative Research (AcSIR),Ghaziabad – 201002, Uttar Pradesh, India

[c] Department of Chemistry, Pandit Deendayal Energy University, Gandhinagar- 382426, Gujarat, India

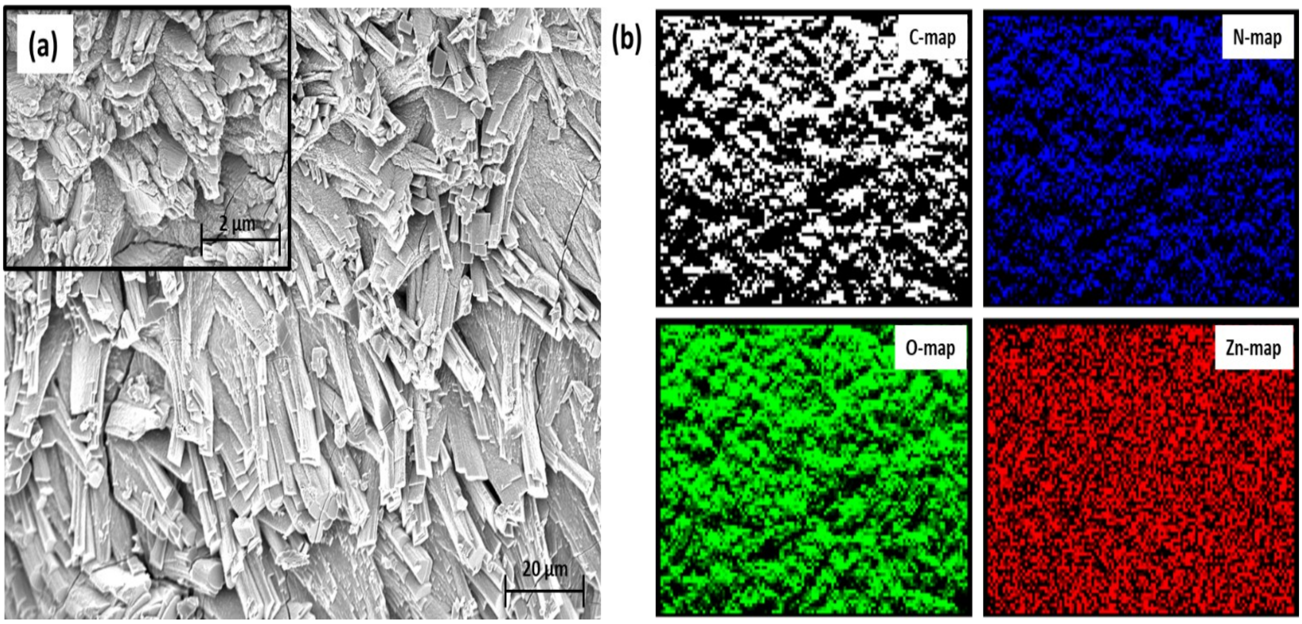

Fig. S1 (a) FE-SEM image of **Zn-CMERI**, **(b)** EDX mapping images of carbon, nitrogen, oxygen and Zn.

Thermogravimetric analysis (TGA) and framework rigidity of Zn-CMERI

TGA was carried out at a temperature range between 0-600 °C with a heating rate of 5 ^{0}C/min under nitrogenous environment. The MOF is quite stable upto ~350 °C and the thermal decomposition is presumably due to release of uncoordinated guest solvent molecules. Beyond 350 °C the framework started gradual decomposition.

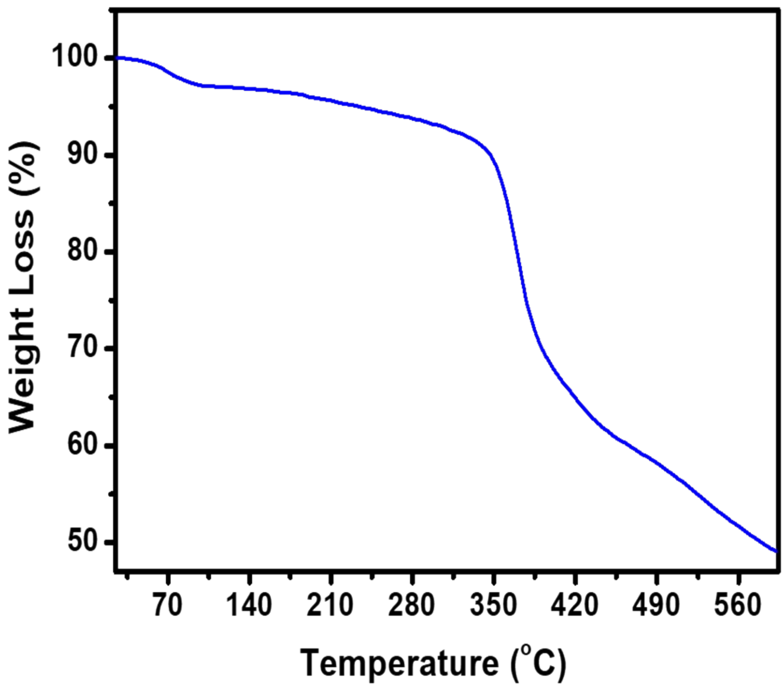

Fig. S2 TGA curve of **Zn-CMERI** in nitrogen gas medium with a heating rate of 5^{0}C/min.

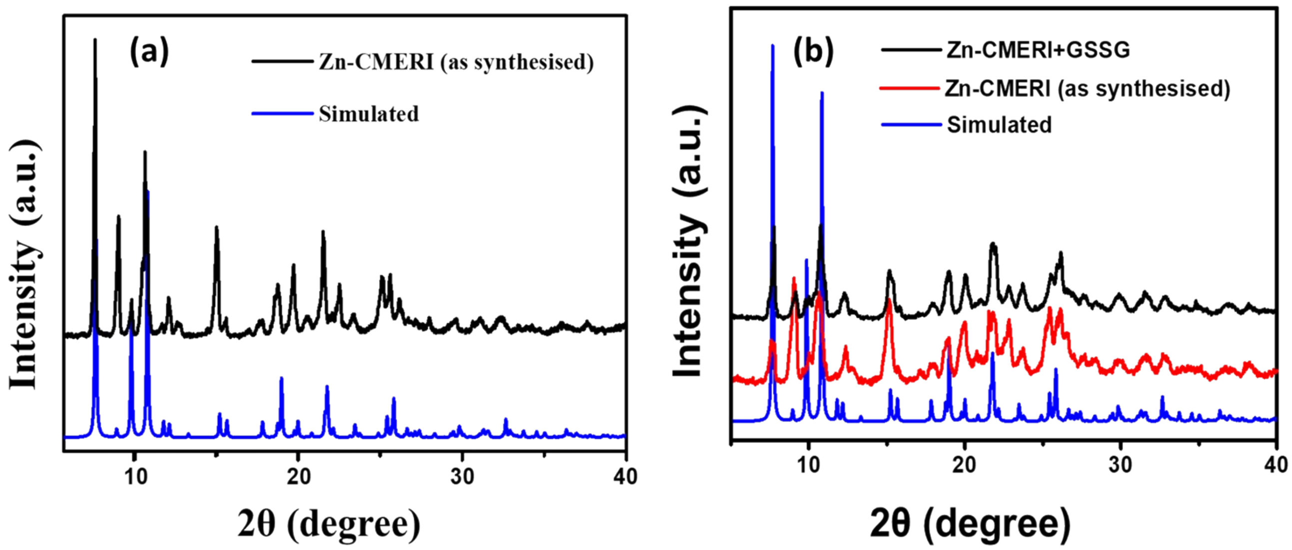

Fig. S3 (a) PXRD pattern of as-synthesised **Zn-CMERI** with its simulated spectra, **(b)** Different PXRD patterns of **Zn-CMERI** confirming its structural stability

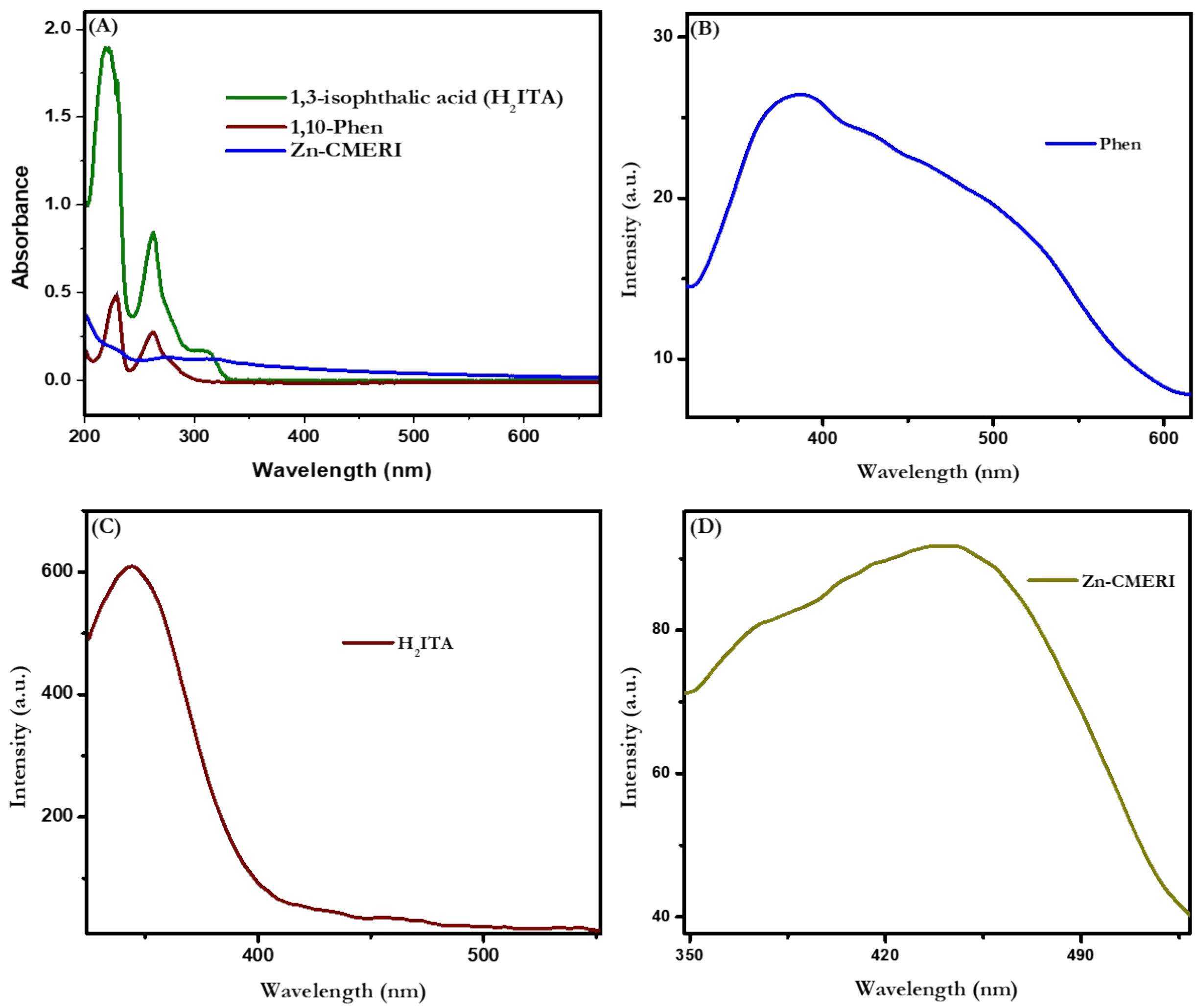

Fig. S4 (A) UV-vis spectra of **Zn-CMERI** and the co-ligands; fluorescence emission spectra of **(B)** Phen, **(C)** H_2ITA and **(D) Zn-CMERI**.

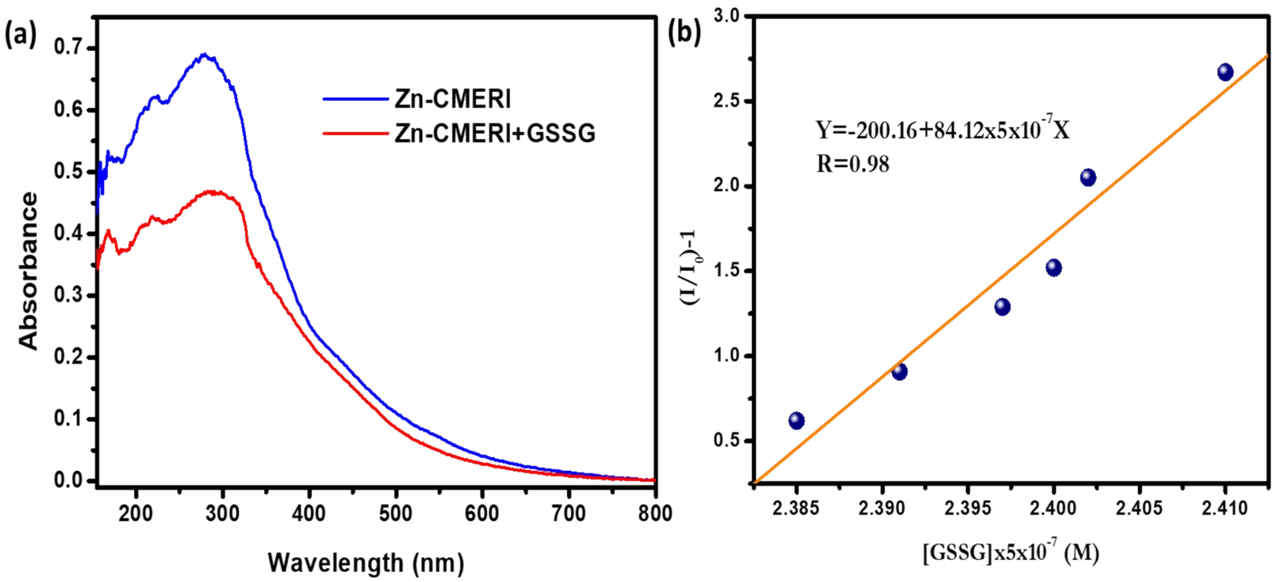

Fig. S5 (a) UV-vis DRS (Diffuse Reflection Spectroscopy) spectra of **Zn-CMERI** before and after interaction with GSSG, **(b)** Change of (I/I_0)-1 as the linear function of the concentration of GSSG for the calculation of LOD of **Zn-CMERI** towards GSSG.

Table S1: Comparative literature survey of **Zn-CMERI** with recently reported chemosensors for GSSG/GSH

Sl. No.	Chemosensor	Type of analyte	Type of Chemosensor	Method of detection	pH range	LOD	Response time	Biological Applications	Application in molecular circuitry	Ref
1	PSMOF	GSH	MOF	Colorimetry	4	~0.68 µM		Detection from the HeLa and LO2 cells	NA	1
2	Cu-MOF(II)	GSH	MOF	Colorimetry	7	0.97 µM		Detection from serum samples	NA	2
3	Eu(DTBA)	GSH	MOF	Fluorimetry		0.35 µM	~180 s	HEP 1-6 and Hacat cells in the CCK-8 assay	NA	3
4	ZIF-67	GSH	Nanosheets of a metal organic framework (MOF)	Colorimetry	5.5	0.07 µM		Detection from human serum samples	NA	4
5	Ni/Fe MOF nanosheet	GSH	Nanosheets of a metal organic framework (MOF)	Colorimetry	3	10 nM		NA	NA	5

6	GSSH-2TPE		Peptide	Fluorimetry	NA	1.5 nM	~60 s	Detection from HeLa cells	NA	6
7	Eu^{3+}/Cu^{2+}@UiO-67-bpydc	GSH	MOF	Fluorimetry	7.0	54.3 nM	~150 s	Detection from human serum samples	NA	7
8	UiO-66-NH_2 MOF	GSH	MOF	Fluorimetry	7.3	0.57 µM	NA	Detection from human serum samples	NA	8
9	CIA	GSSG	Small molecule	Fluorimetry	7.5	0.226 mM	NA	NA	NA	9
10	UiO-68-An/Ma	GSH	MOF	Fluorimetry	NA	50 µM	NA	NA	NA	10
11	Zn-CMERI	GSSG	MOF	Fluorimetry	6-8	34 nM (20.8 ppb)	~12 sec	Detection from urine and serum samples	Yes	**Present work**

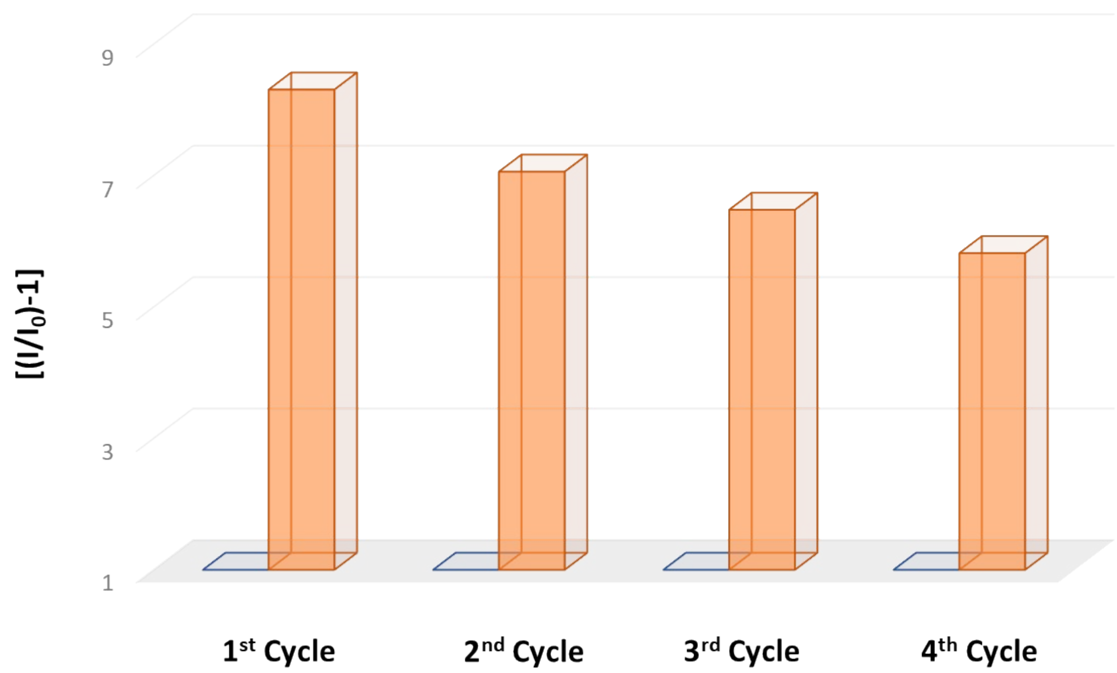

Fig. S6 Recyclable nature of **Zn-CMERI** towards GSSG upto 3 cycles without any hassle.

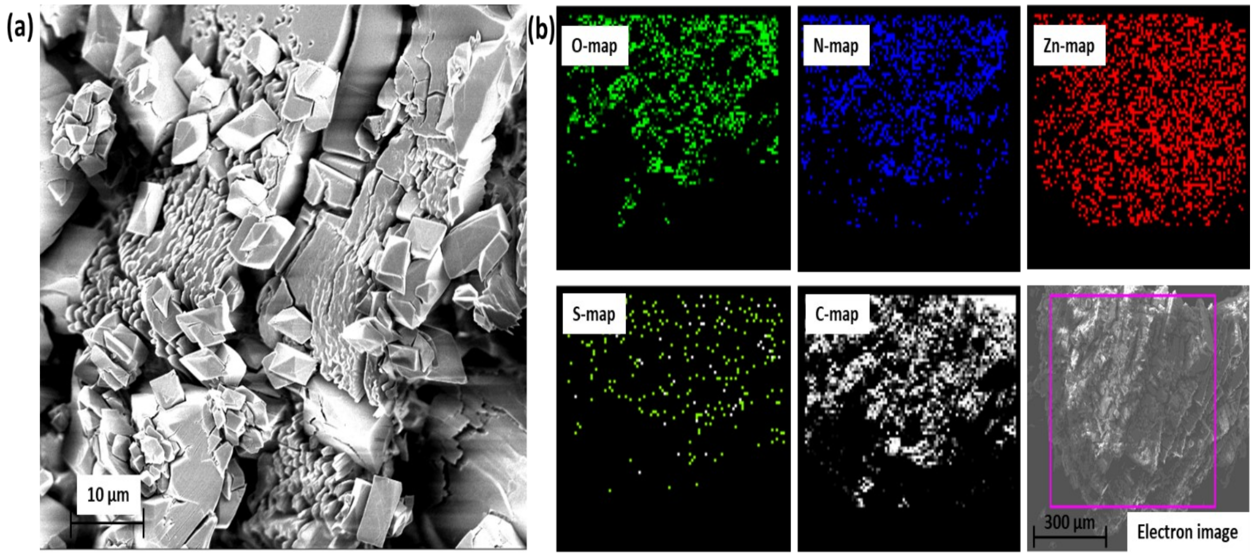

Fig. S7 (a) FE-SEM image of unaffected needle shaped morphology of **Zn-CMERI** after interaction with GSSG, **(b)** EDX mapping image of **Zn-CMERI**@GSSG confirming presence of respective elements.

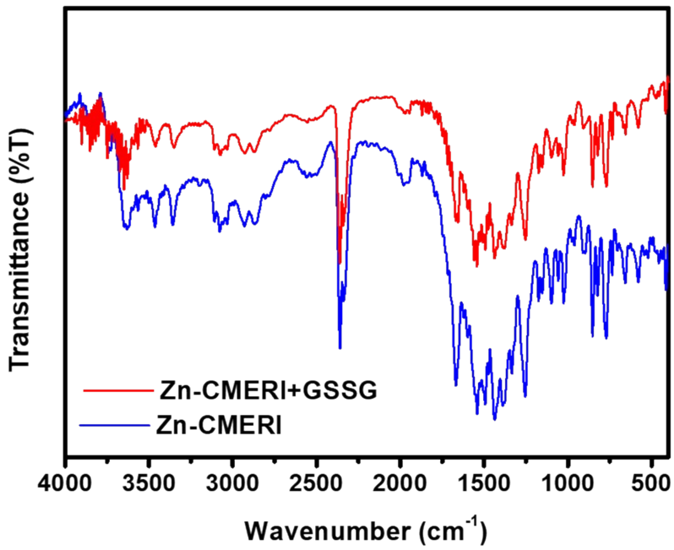

Fig. S8 FTIR spectra of **Zn-CMERI** before and after interaction with GSSG.

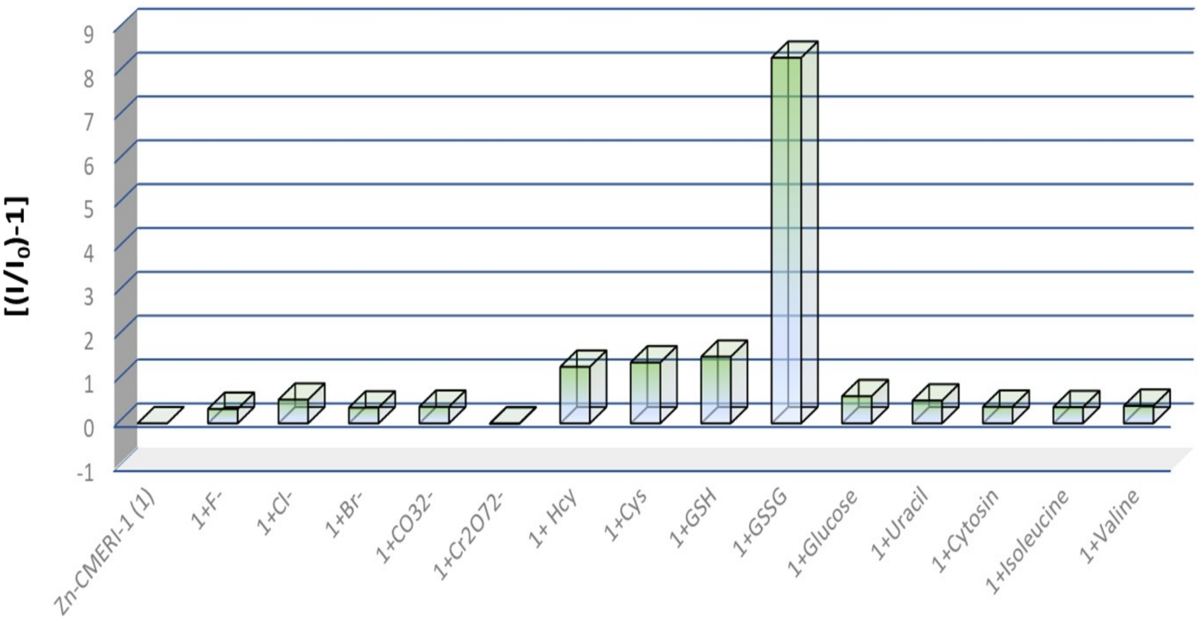

Fig. S9 Selectivity studies of **Zn-CMERI** towards different biologically relevant interferents in similar sensing environment.

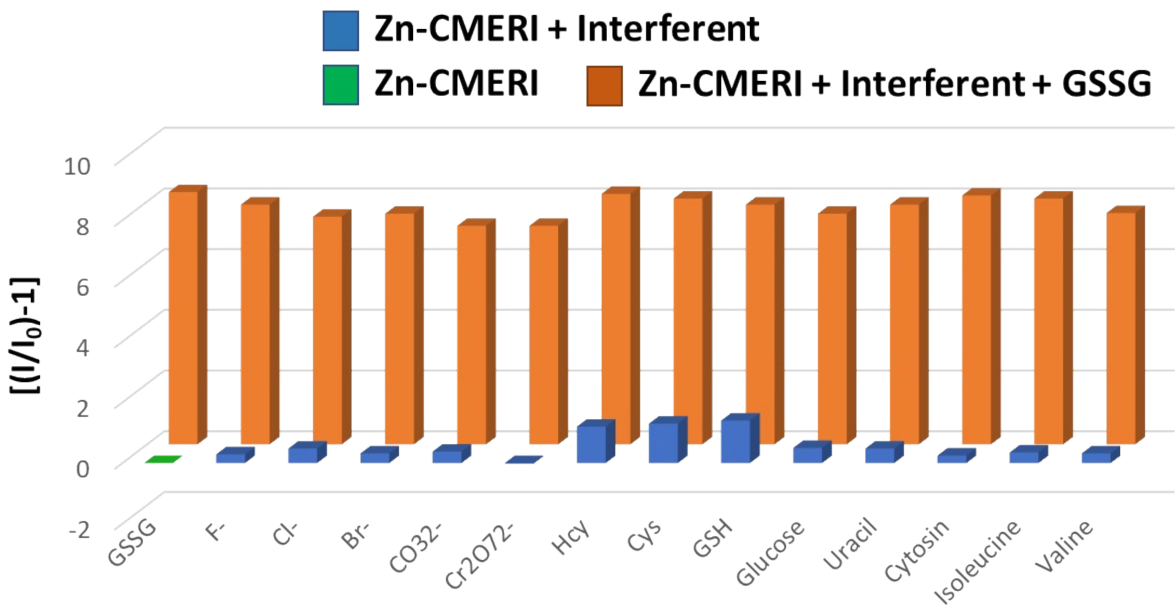

Fig. S10 Relative fluorescence intensity of **Zn-CMERI** towards GSSG in presence of different biologically relevant interferents in similar sensing environment.

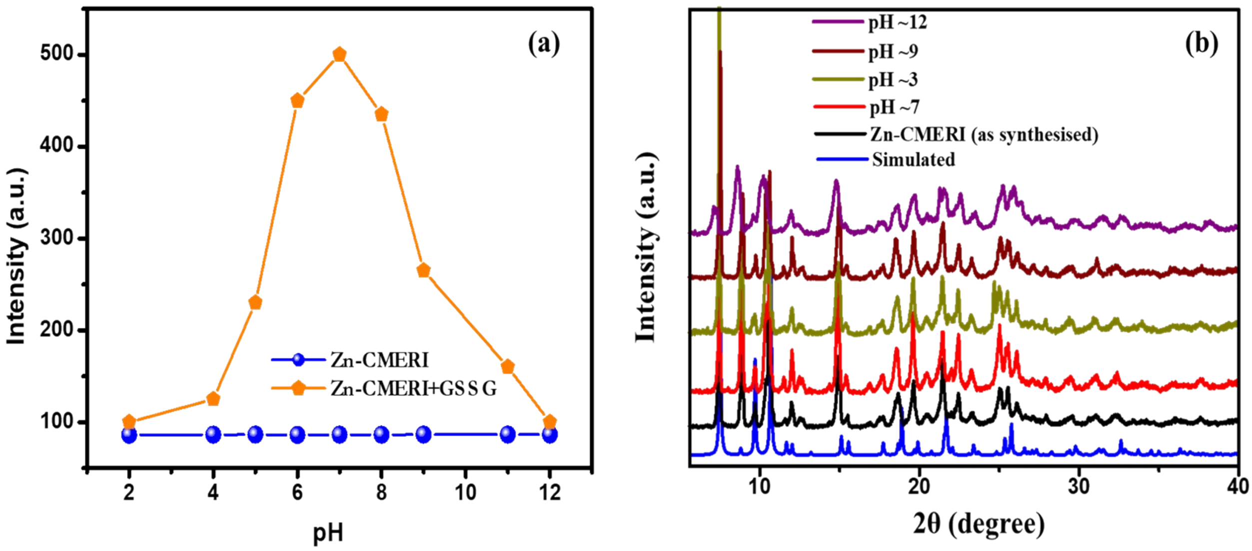

Fig. S11 (a) Effect of fluorescence emission intensity of **Zn-CMERI** at 415 nm at different pH (λ_{ex}=290 nm), **(b)** PXRD spectra of **Zn-CMERI** at different pH.

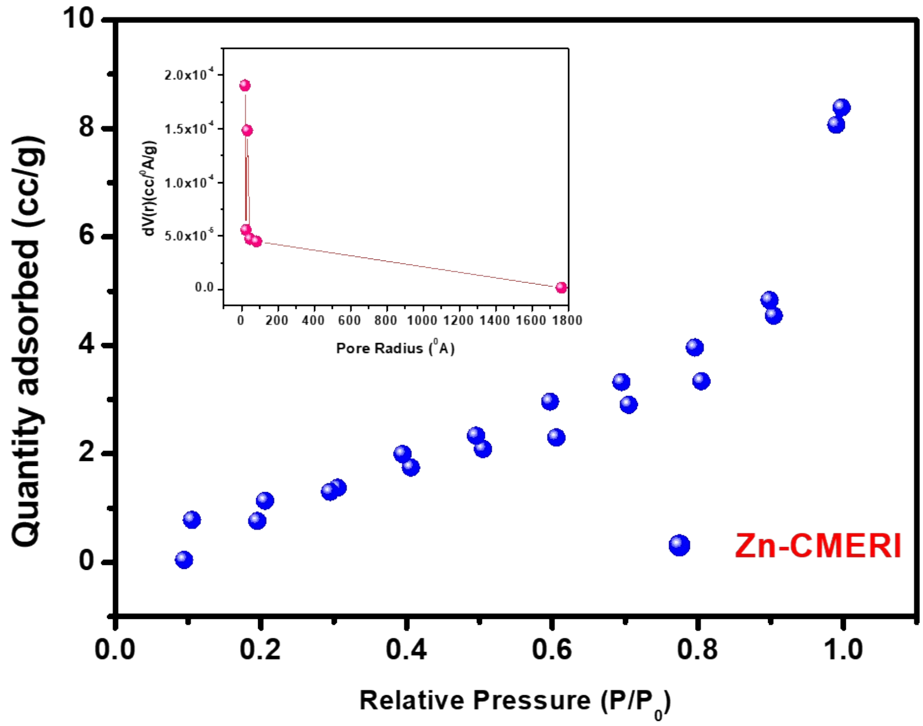

Fig. S12 N_2 sorption analysis of **Zn-CMERI** at 77K; inset: pore size distribution of **Zn-CMERI** as derived from BJH method.

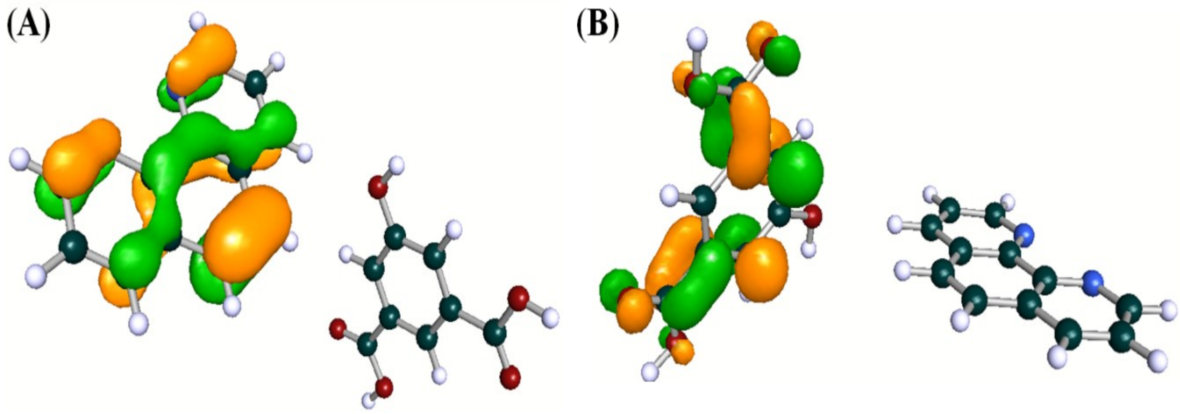

Fig. S13 (A) HOMO and **(B)** LUMO of the co-ligands assembly in **Zn-CMERI**

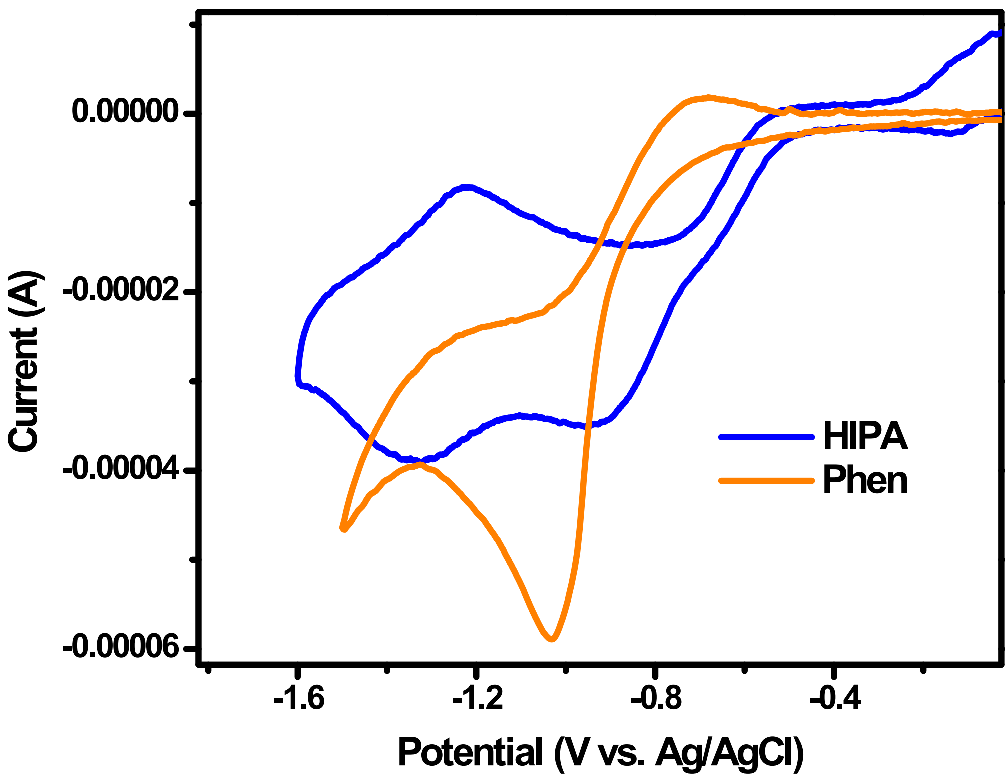

Fig. S14 Cyclic voltammogram of Phen and HIPA in acetonitrile using tetrabutylammonium hexafluorophosphate as supporting electrolyte, scan rate= 0.05 V/s.

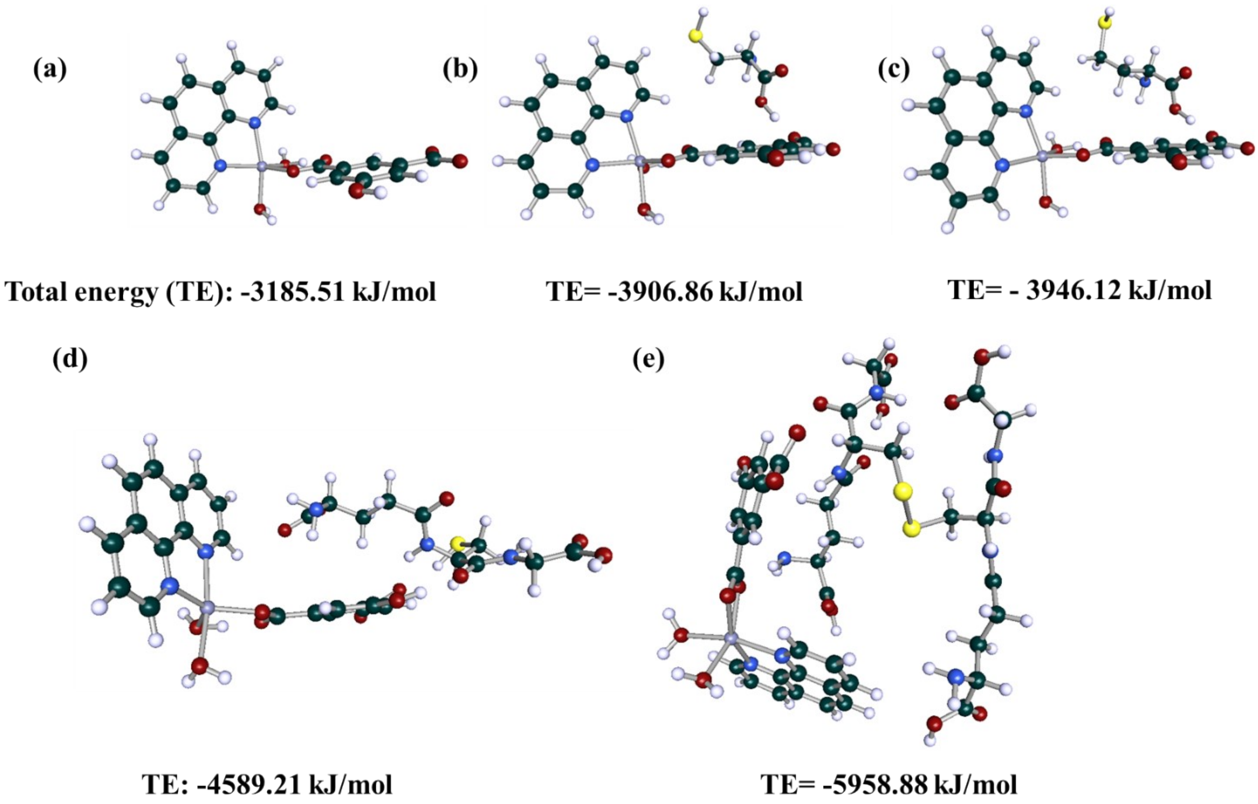

Fig. S15 Total energy values of **(a) Zn-CMERI** MOF fragment and **Zn-CMERI** MOF fragment with **(b)** Cys, **(c)** Hcy, **(d)** GSH and **(e)** GSSG respectively.

Table S2 Truth table presenting output at the emission wavelength of 415 nm for the chemosensor, **Zn-CMERI** in presence of the targeted analyte, GSSG

IN 1 (Zn-CMERI)	IN2 (GSSG)	OUT1 (415 nm)
0	0	0
0	1	0
1	0	0
1	1	1

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