

Electronic Supplementary Information

***In situ* fabricated MOF-cellulose composite as an advanced ROS deactivator-convertor: fluoroswitchable bi-phasic tweezer for free chlorine detoxification and size-exclusive catalytic insertion of aqueous H₂O₂**

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1. Materials and methods

All the reagents employed were commercially available and used as provided without further purification. Metal nitrate and acetate salts, 2-Aminoterephthalic acid (2-ATA), hydrazine monohydrate, 4-cyano pyridine were purchased from Sigma–Aldrich and TCI chemicals, respectively. All the solvents such as HPLC grade N, N′-dimethylformamide (DMF), dichloromethane (CH₂Cl₂) were procured from Loba chemie Pvt. Ltd., India. All the ROS species were synthesized following the reported protocol.¹ Linker *dpta* was synthesized according to the reported literature procedure and characterized.² All spectroscopic, catalytic and crystallographic studies are provided in the following sections.

Caution!!! Being hazardous and corrosive in nature, all ROS species should be handled carefully.

2. Physical measurements

The infrared spectra (IR) of the samples were recorded using the KBr pellet method on a Perkin–Elmer GX FTIR spectrometer in the region of 400–4000 cm^{−1}. Powder X-ray diffraction

(PXRD) data were collected using a PANalytical Empyrean (PIXcel 3D detector) system equipped with Cu K α ($\lambda=1.54$ Å) radiation. Microanalyses of the compounds were conducted using elemental vario MICRO CUBE analyzer. Thermogravimetric analyses (TGA) (heating rate of 10 °C/min under N₂ atmosphere) were performed with a Mettler Toledo Star SW 8.10 system. Prior to sensing and catalysis measurement, as-synthesized compounds were immersed in dichloromethane for 2 days at room temperature to replace lattice guest molecules. The solvent-exchanged frameworks were then degassed overnight under vacuum at 120 °C to generate **14a**. UV-Vis spectra recorded using Shimadzu UV-3101 PC spectrometer and the luminescence experiments were performed at room temperature using a Fluorolog Horiba JobinYvon spectrophotometer. Inductively coupled plasma-optical emission spectrometry (ICP-OES) analysis was measured by Perkin Elmer, Optima 2000. The XPS analysis was carried out using a Thermo Scientific ESCALAB 250 Xi photoelectron spectrometer (XPS) using a monochromatic Al K α X-ray as an excitation source outfitted with an X-ray spot size of 650 $\times$ 650 μm^2 .

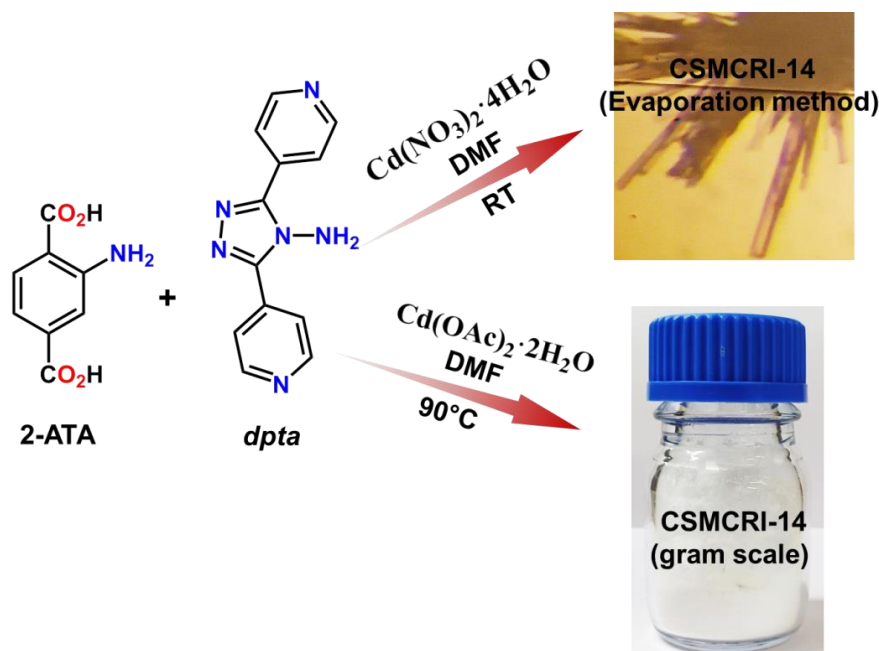
3. Single Crystal X-ray Crystallography

Single crystals with suitable dimensions were chosen under an optical microscope and mounted on a glass fibre for data collection. The crystal data for as synthesized crystal of **CSMCRI-14** were collected on a Bruker D8 Quest diffractometer, with CMOS detector in shutter less mode. The crystals were cooled to low temperature using an Oxford Cryostream liquid nitrogen cryostat. The instrument was equipped with a graphite monochromatized MoK α X-ray source ($\lambda = 0.71073$ Å), with Triumph™ X-ray source optics. Data collection and initial indexing and cell refinement were handled using APEX II software.³ Frame integration, including Lorentz-polarization corrections, and final cell parameter calculations were carried out using SAINT+ software.⁴ The data were corrected for absorption using the SADABS program.⁵ Decay of reflection intensity was monitored by analysis of redundant frames. The structure was solved using Direct methods and difference Fourier techniques. All non-hydrogen atoms were refined anisotropically. All H atoms were placed in calculated positions using idealized geometries (riding model) and assigned fixed isotropic displacement parameters. The SHELXL-2014 package within the OLEX2 crystallographic software⁶ was applied for structure refinement with several full-matrix least-squares/difference Fourier cycles.⁷ The disordered guest solvent molecules in the crystal lattice were treated with solvent mask option in OLEX2 software.⁶ The potential solvent accessible void space was calculated using the PLATON⁸ software. The crystal and refinement data for solvent free **CSMCRI-14** is listed in Table S1. Topological analysis

was performed by using TOPOS software.⁹ Structure of thereacting molecules in catalysis were drawn and optimized using Avogadro software.¹⁰

4. Computational Details

The Luminescence quenching of **14a** in presence of ROS and AA are defined via the aid of periodic DFT probe. Herein, a group of ROS (ClO^- , AA, H_2O_2 , $\text{OH}\cdot$) as well as AA are being the analytes and the Photo induced electron transfer (PET) during sensing is theoretically assigned with the help of HOMO-LUMO energy gap. The parental activated framework along with analytes is optimised using PBE functional¹¹ by Quickstep module of the CP2K package.¹² All the DFT calculations are performed by Unrestricted Kohn-sham (UKS) with spin multiplicity.¹³ A triple zeta (TZVP-MOLOPT)¹⁴ basis sets were considered for the elements such as carbon, oxygen, nitrogen, hydrogen, but cadmium followed by a double zeta (DZVP-MOLOPT)¹⁴ basis set, additionally van der walls corrections were applied by DFT-D3 method¹⁵ and optimized at the triclinic symmetry. These optimised structures were used to explore the quenching mechanism by photo excitation via HOMO-LUMO energy gap Fig. S29a. Additionally, it includes the DFT optimized intermediate in alkene epoxidation reaction catalysed by **14a** based on same as the mentioned concept.



Scheme S1. Synthetic scheme for **CSMCRI-14** as single crystals and in gram scale.

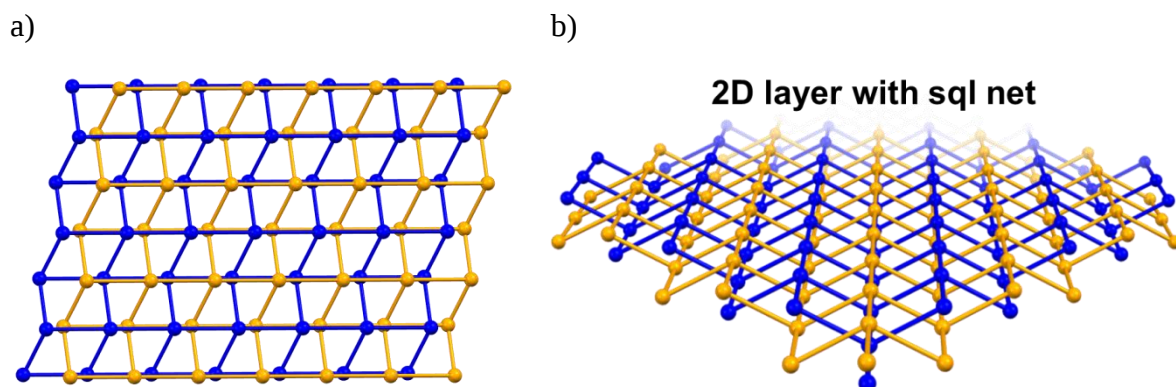


Fig. S2. a) Top and b) sideways topological representation of **CSMCRI-14** showing 2-fold interpenetrated sql-net) with Schlafli symbol $\{4^4 \cdot 6^2\}$.

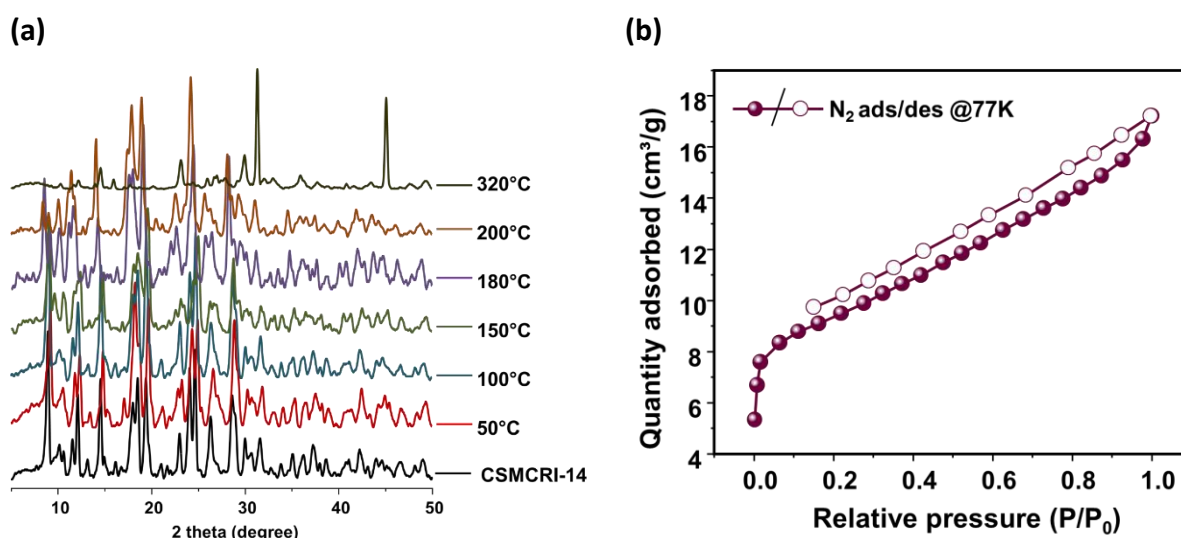


Fig. S3. a) Variable Temperature PXRD of the **CSMCRI-14**, and b) N_2 adsorption/desorption isotherms of activated **CSMCRI-14** at 77 K.

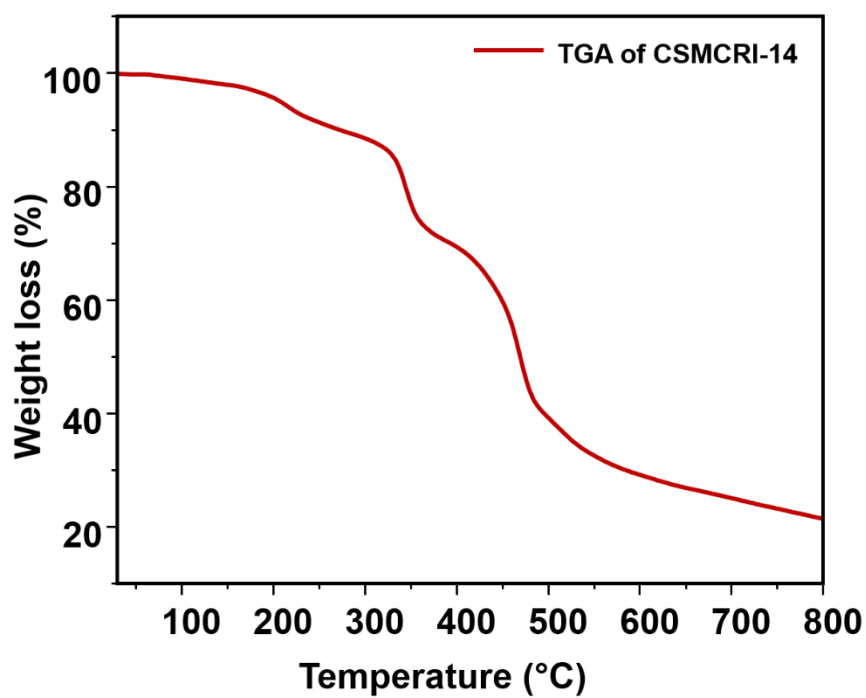
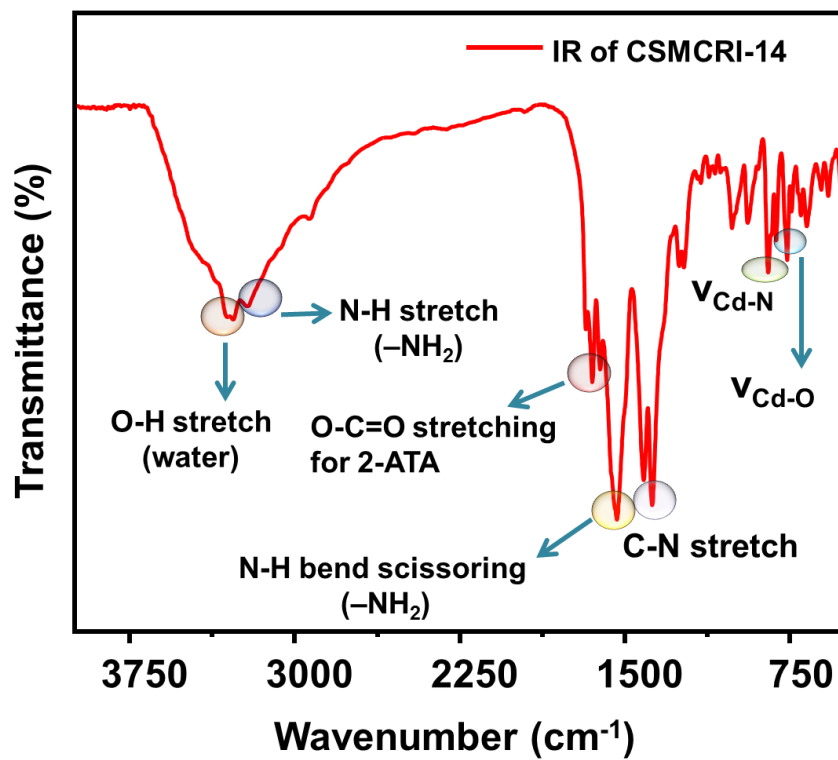


Fig. S4. Thermogravimetric analysis of as-synthesized CSMCRI-14.

a)



b)

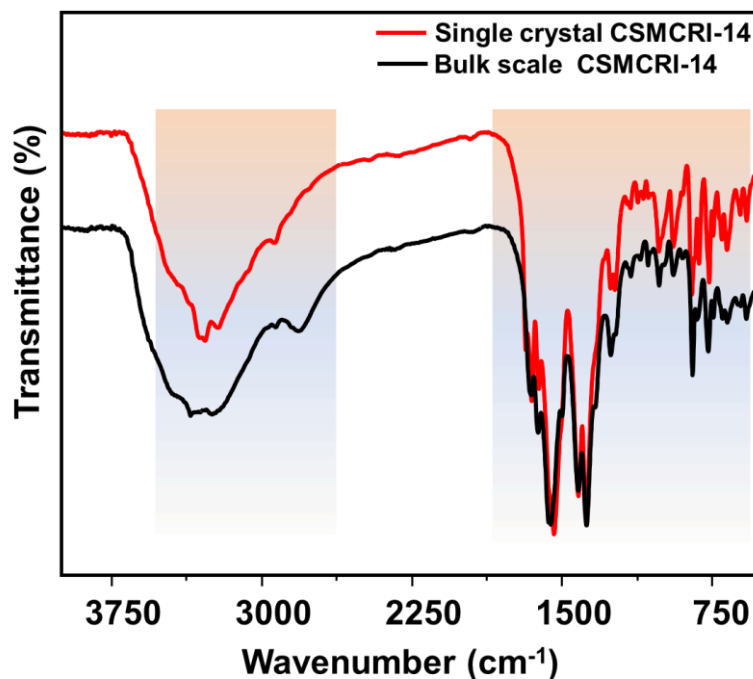
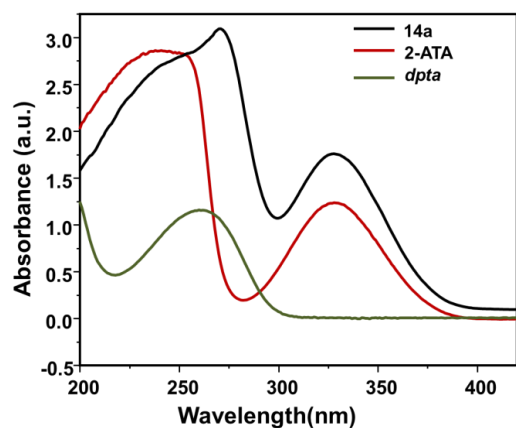
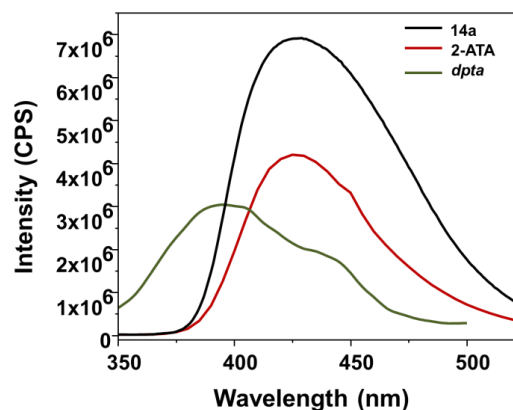


Fig. S5. FT-IR profile of a) as-synthesized and b) bulk scale powder **CSMCRI-14**.

a)



b)



c)



Fig. S6. (a) UV-Vis spectra of MOF constituents and activated **CSMCRI-14**. (b) Comparison of emission intensity of 2-ATA, *dpta*, and **14a** (all dispersed in water). (c) Digital photographs of **CSMCRI-14** and **14a** (before and after excitation).

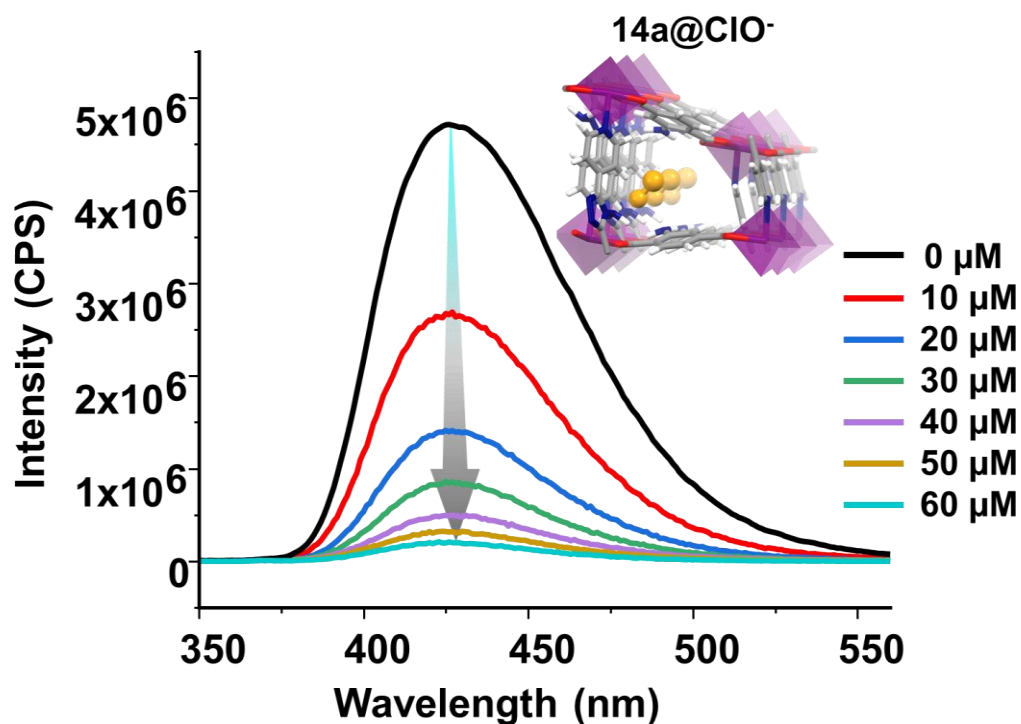


Fig. S7. Emission spectra of **14a** upon incremental addition of ClO^- solution (1 mM) in water. Inset represents DFT optimised view of **14a@ClO⁻**.

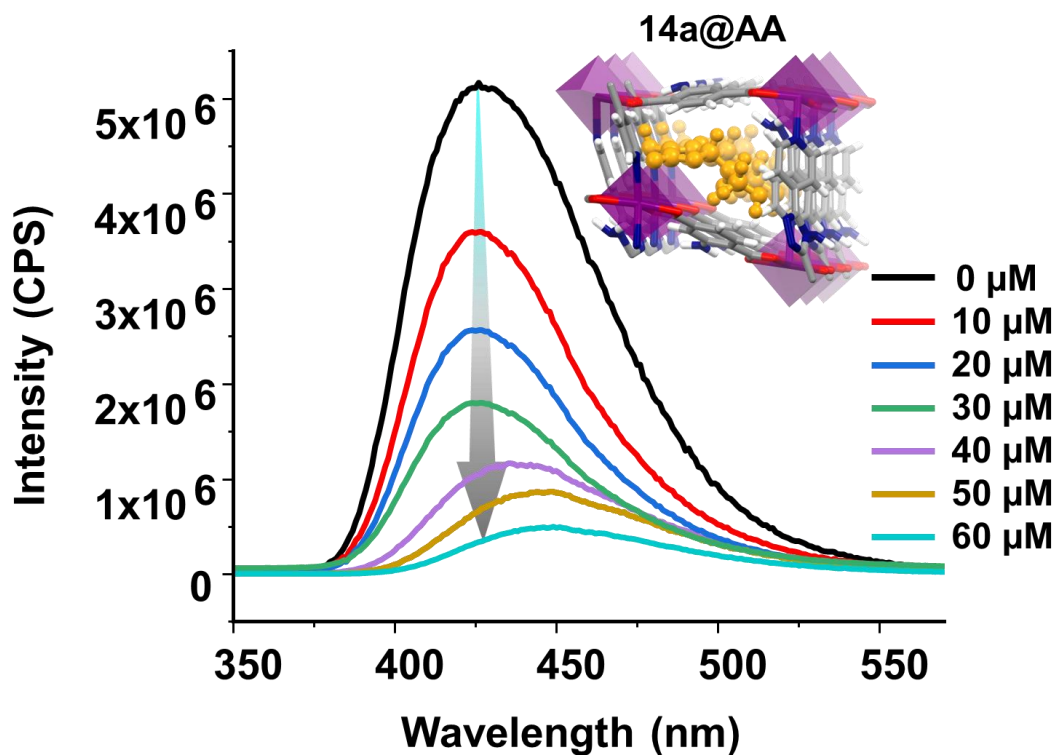


Fig. S8. Emission spectra of **14a** upon incremental addition of AA solution (1 mM) in water. Inset represents DFT optimised view of **14a@AA**.

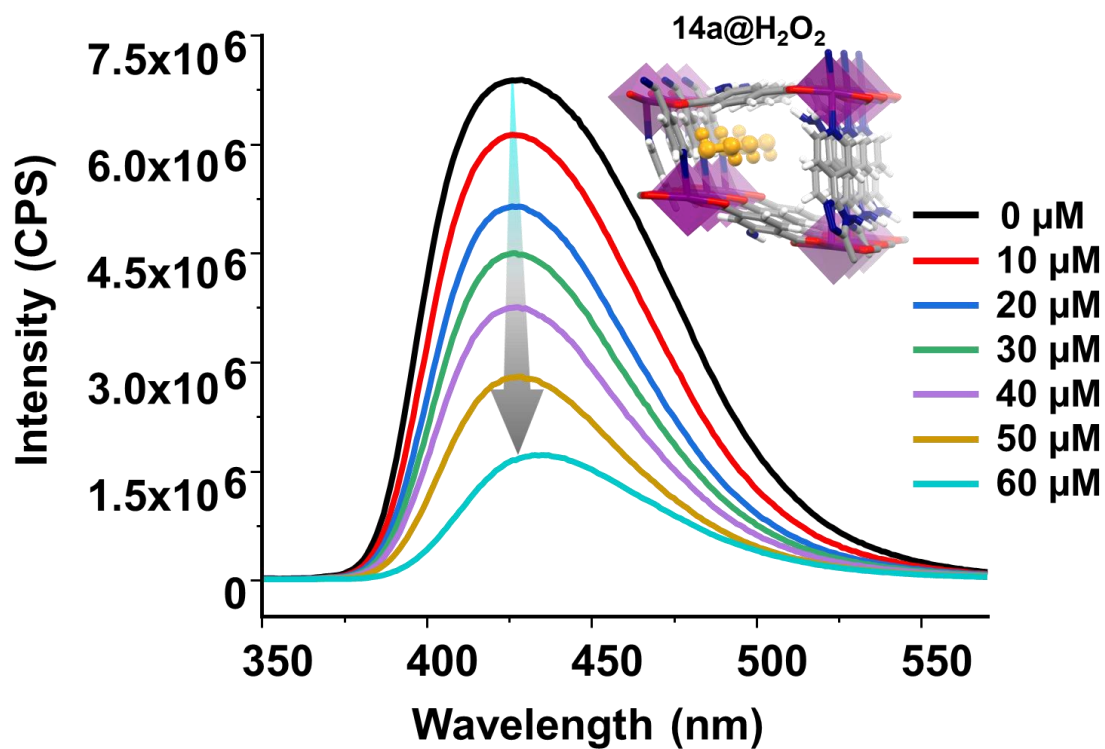


Fig. S9. Emission spectra of **14a** upon incremental addition of H_2O_2 solution (1 mM) in water. Inset represents DFT optimised view of **14a**@ H_2O_2 .

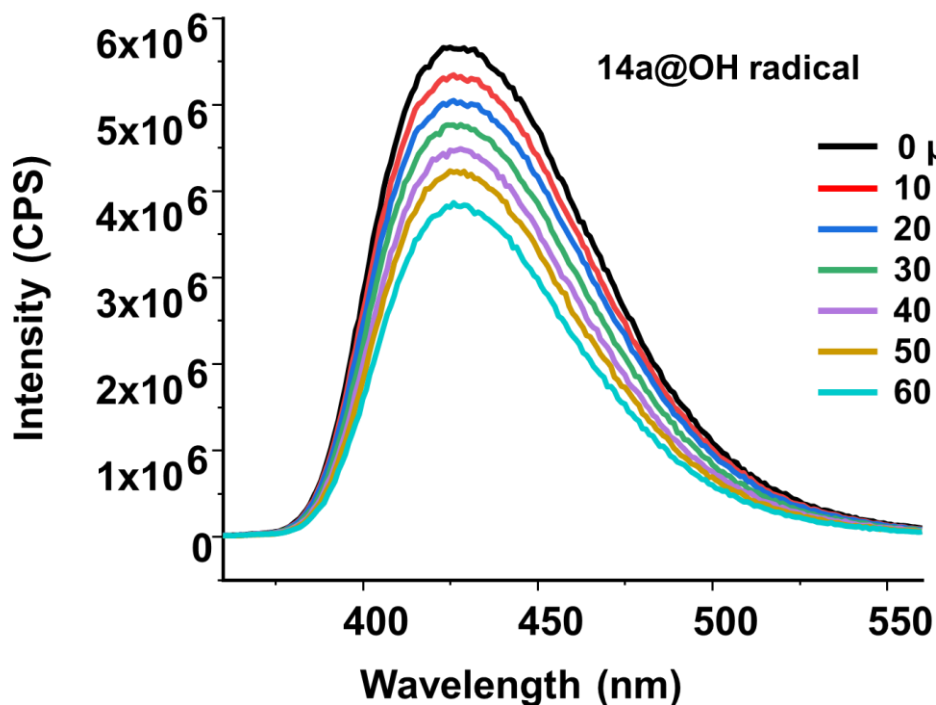


Fig. S10. Emission spectra of **14a** upon incremental addition of hydroxyl radical ($\text{OH}^\bullet$) (1 mM) in water.

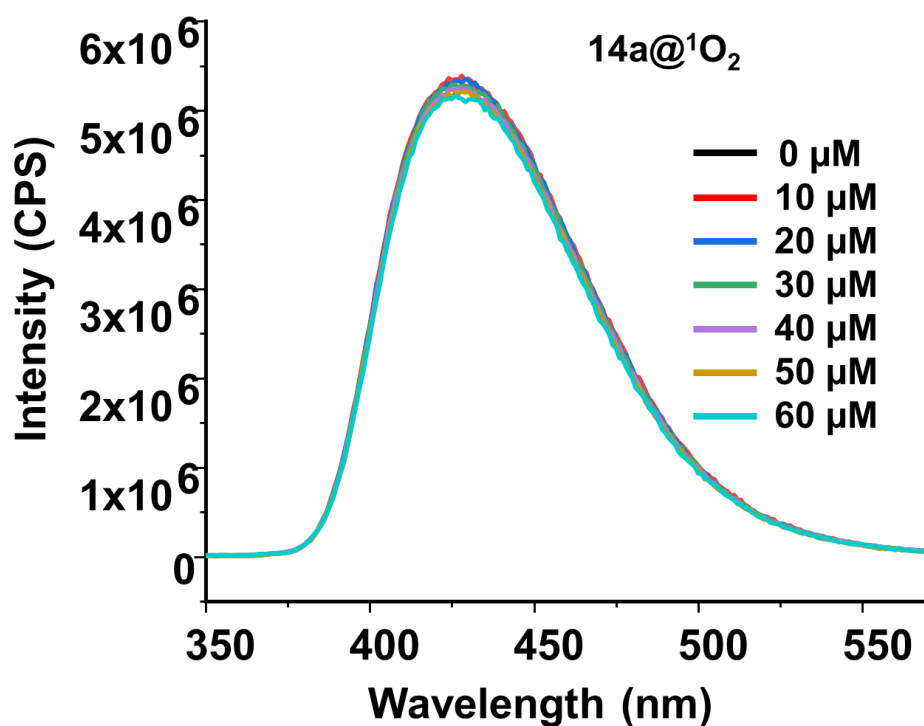


Fig. S11. Emission spectra of **14a** upon incremental addition of singlet oxygen ($^1\text{O}_2$) solution (1 mM) in water.

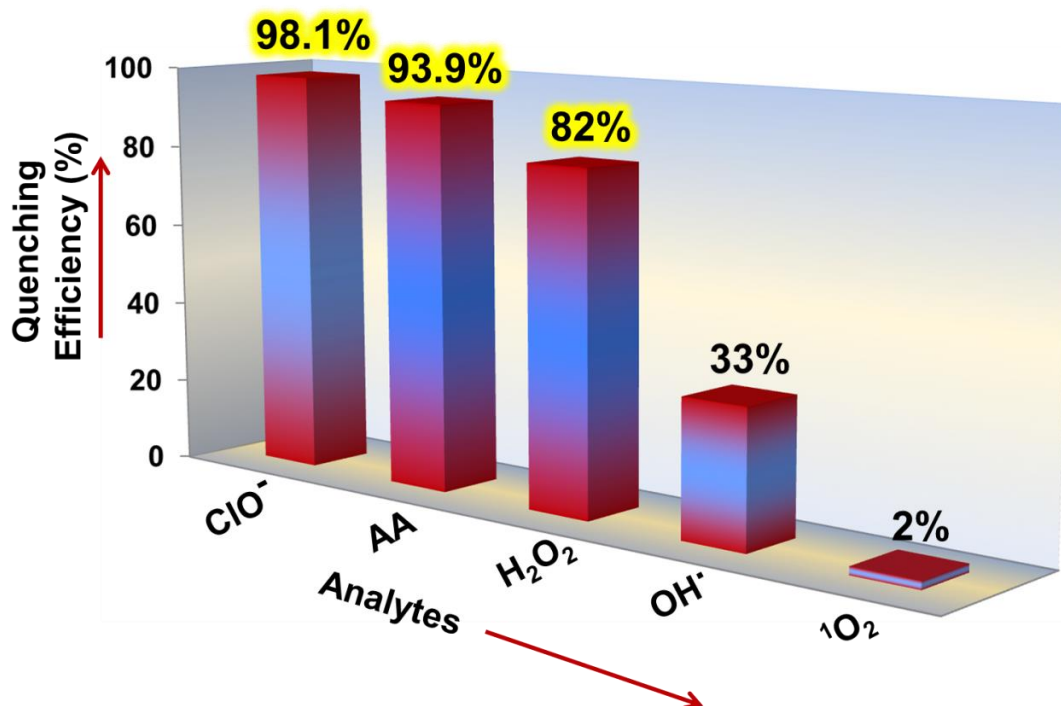
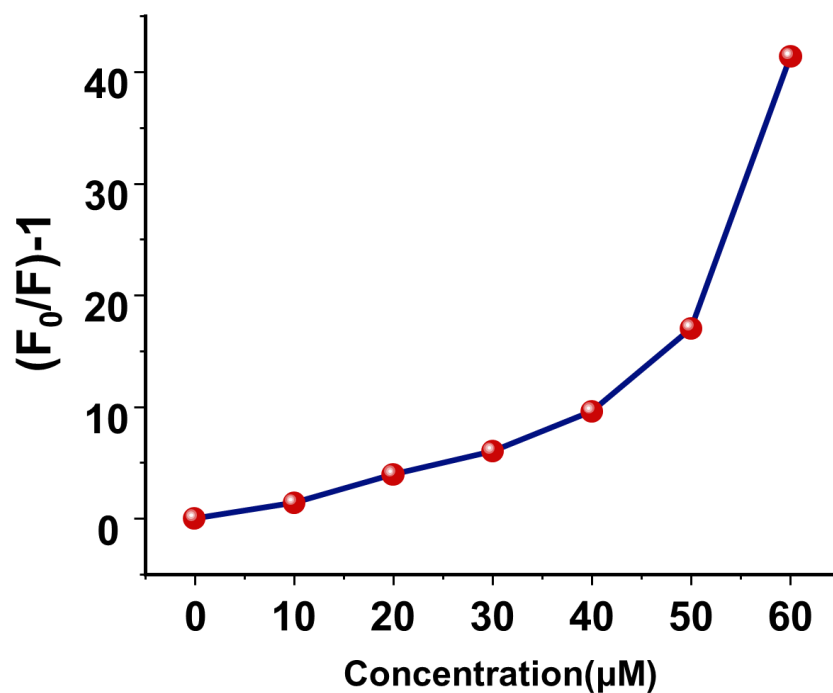


Fig. S12. Fluorescence quenching efficiency of aqueous suspensions of **14a** (1 mg/ 2 mL) for different reactive oxygen species (ROS) and AA.

a)



b)

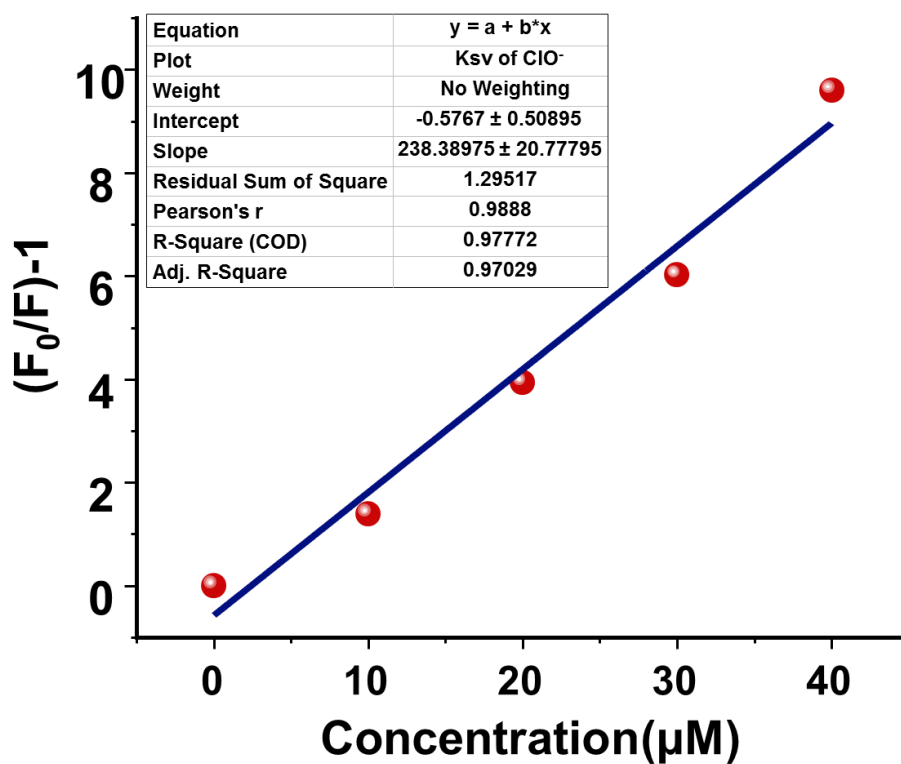
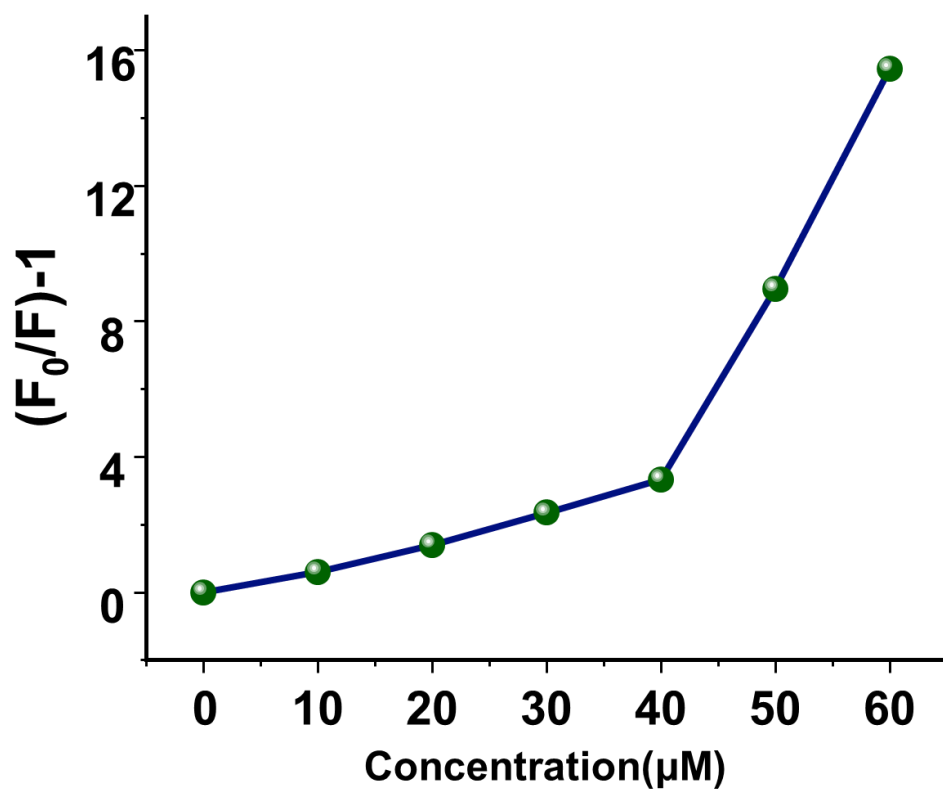


Fig. S13. a) The curvature of the S–V plot for ClO[−] (0–60 μM). (b) S–V plot for ClO[−] in aqueous suspensions of **14a**. The relative fluorescence intensity [(F₀/F)-1] is linear with ClO[−] concentration in the range of 0–40 μM.

a)



b)

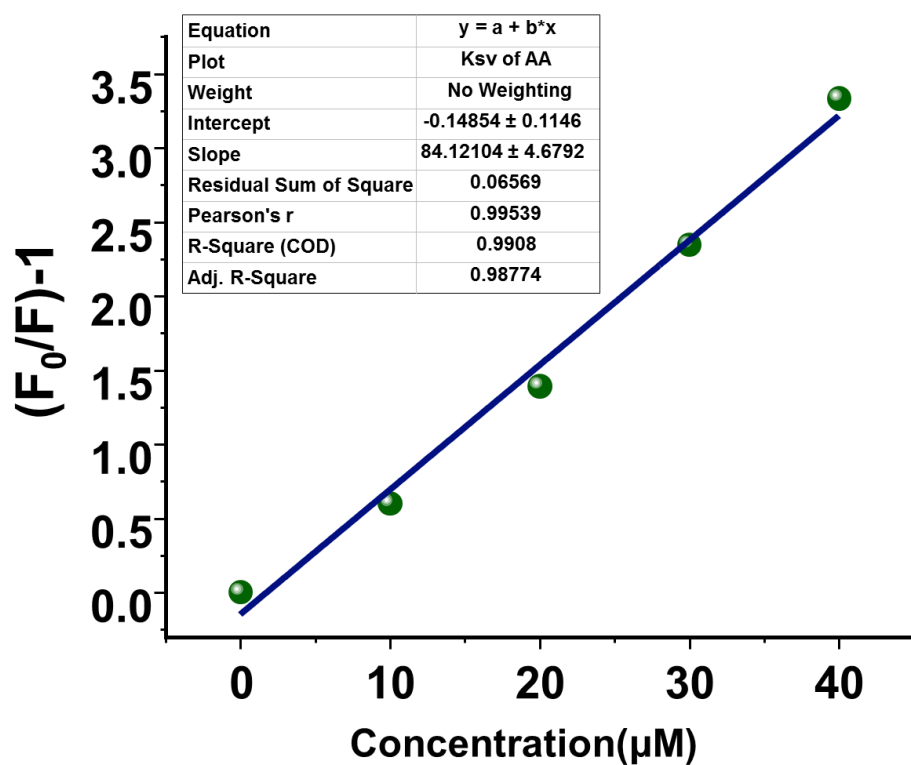
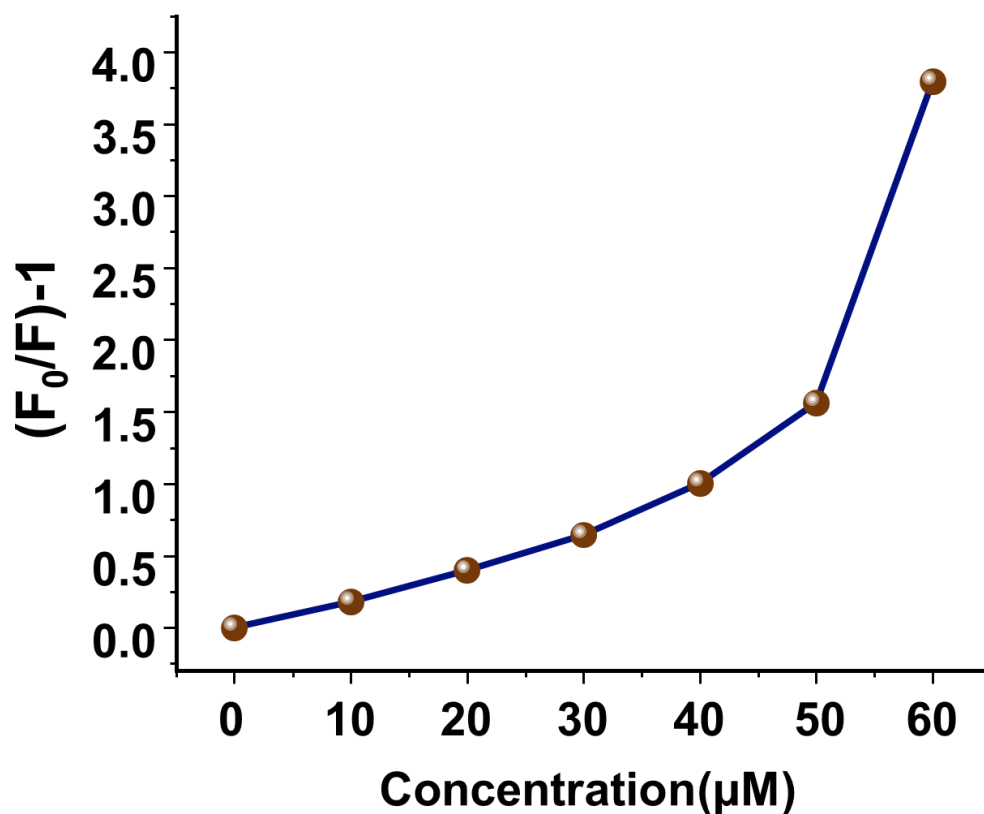


Fig. S14. a) The curvature of the S–V plot for AA (0–60 μM). (b) S–V plot for AA in aqueous suspensions of 14a. The relative fluorescence intensity $[(F_0/F)-1]$ is linear with AA concentration in the range of 0–40 μM.

a)



b)

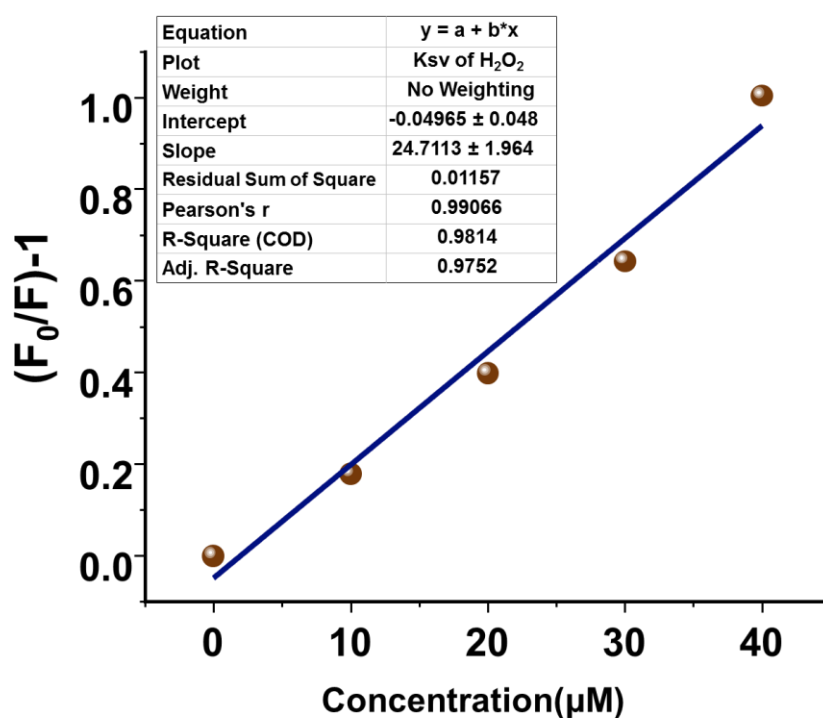


Fig. S15. a) The curvature of the S–V plot for H₂O₂ (0–60 μM). (b) S–V plot for H₂O₂ in aqueous suspensions of **14a**. The relative fluorescence intensity [(F₀/F)-1] is linear with H₂O₂ concentration in the range of 0–40 μM.

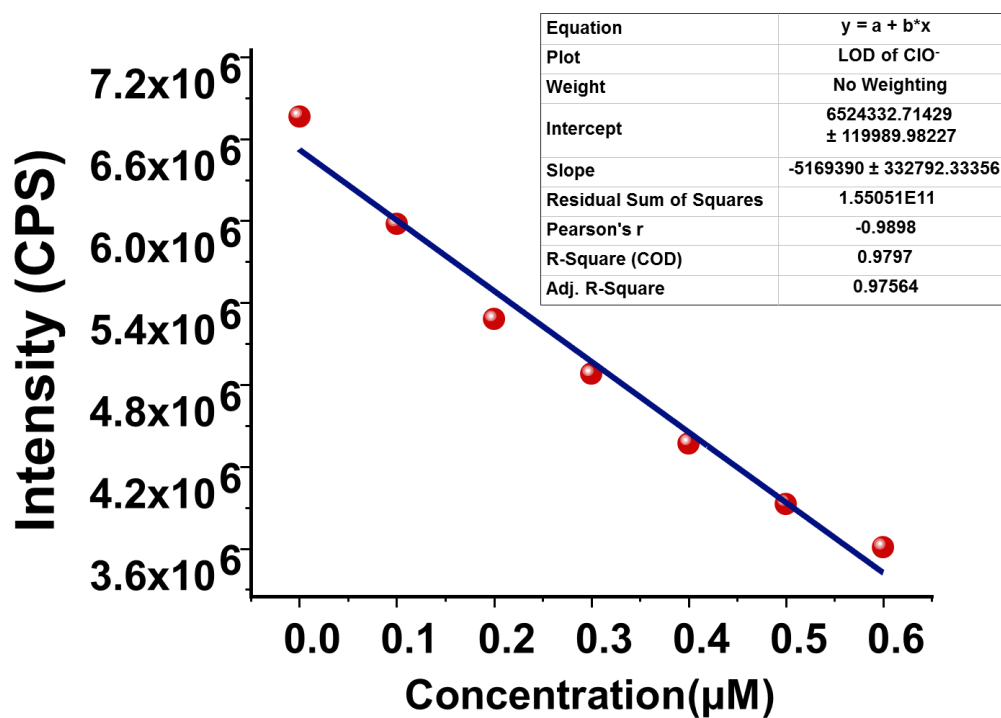


Fig. S16. Linear region of fluorescence intensity of **14a** upon addition of ClO^- (0 – 120 μL , 10 μM stock solution).

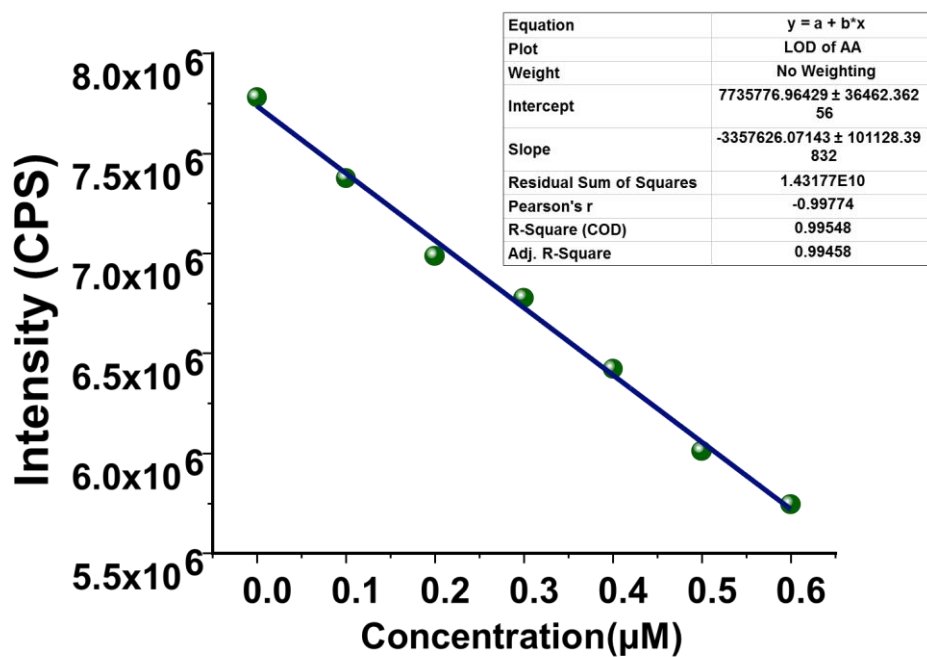


Fig. S17. Linear region of fluorescence intensity of **14a** upon addition of AA (0 – 120 μL , 10 μM stock solution).

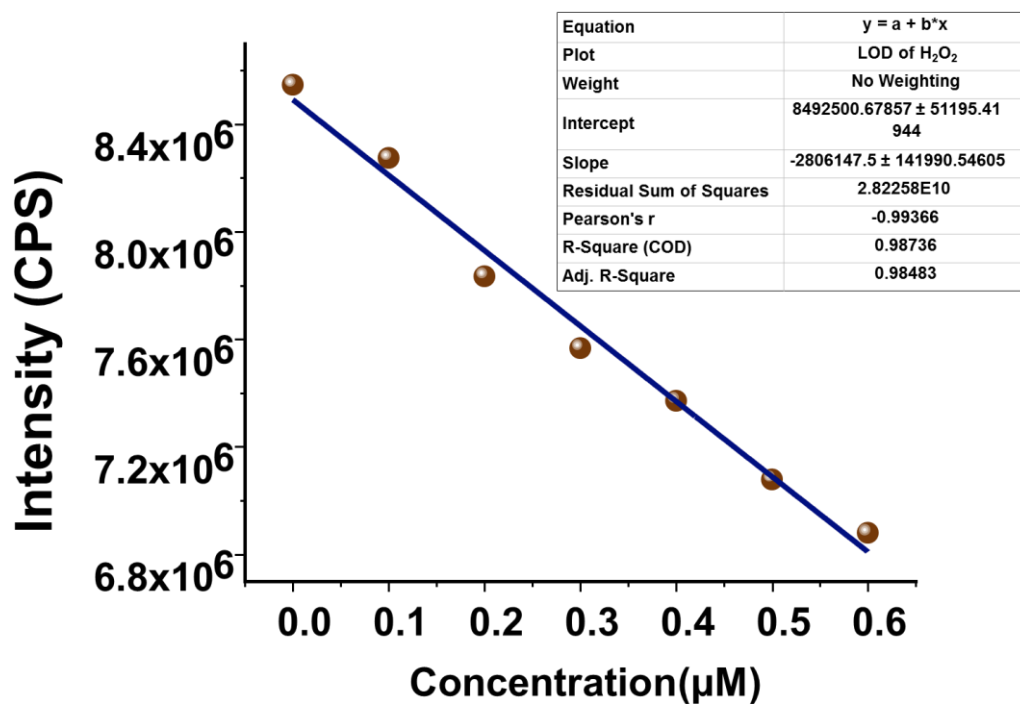


Fig. S18. Linear region of fluorescence intensity of **14a** upon addition of H_2O_2 (0 – 120 μ L, 10 μ M stock solution).

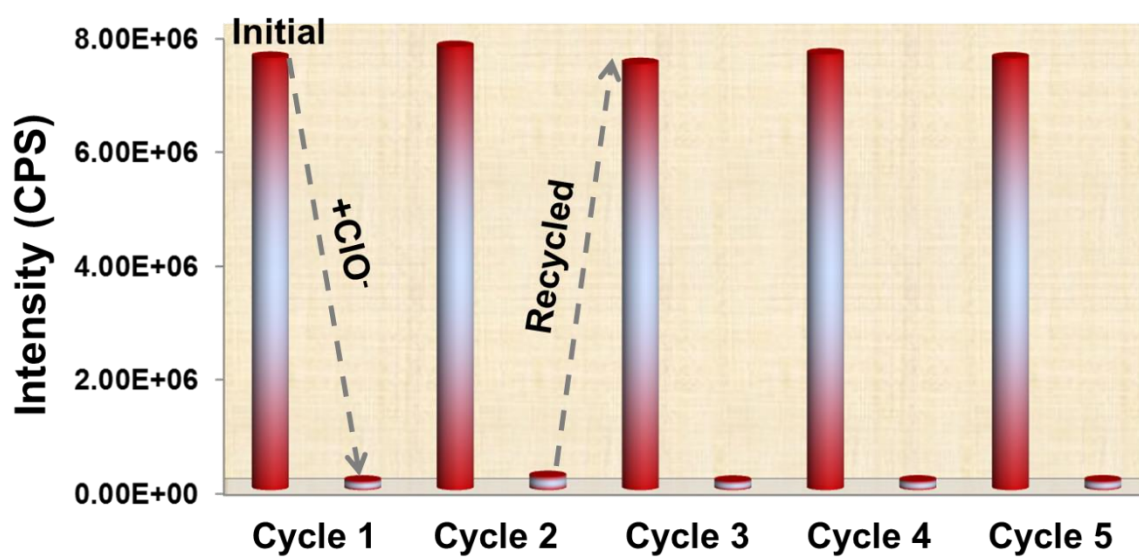


Fig. S19. Recyclable nature of quenching efficiency of **14a** towards 1 mM ClO^- solution for 5 cycles.

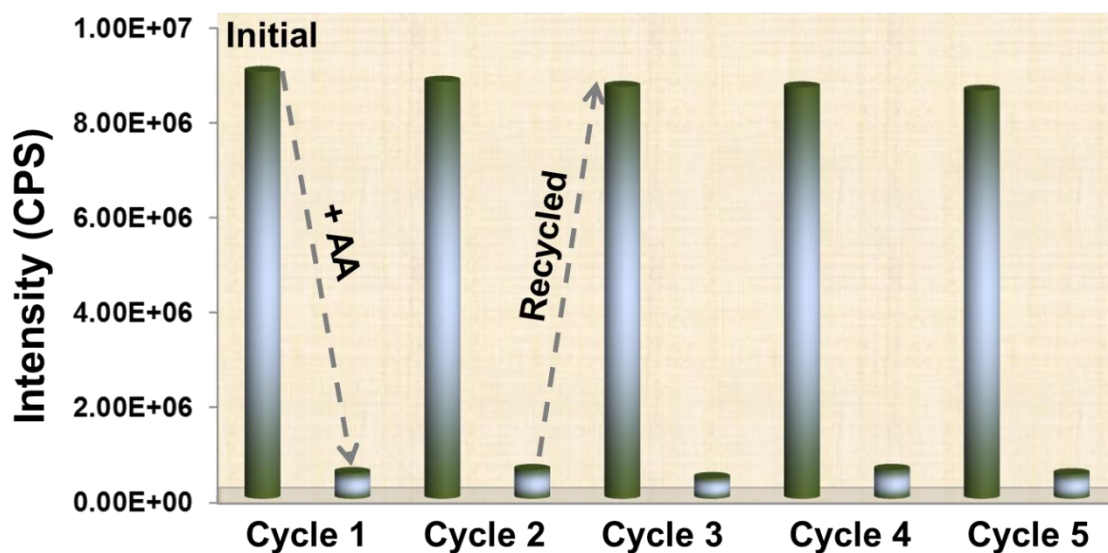


Fig. S20. Recyclable nature of quenching efficiency of **14a** towards 1 mM AA solution for 5 cycles.

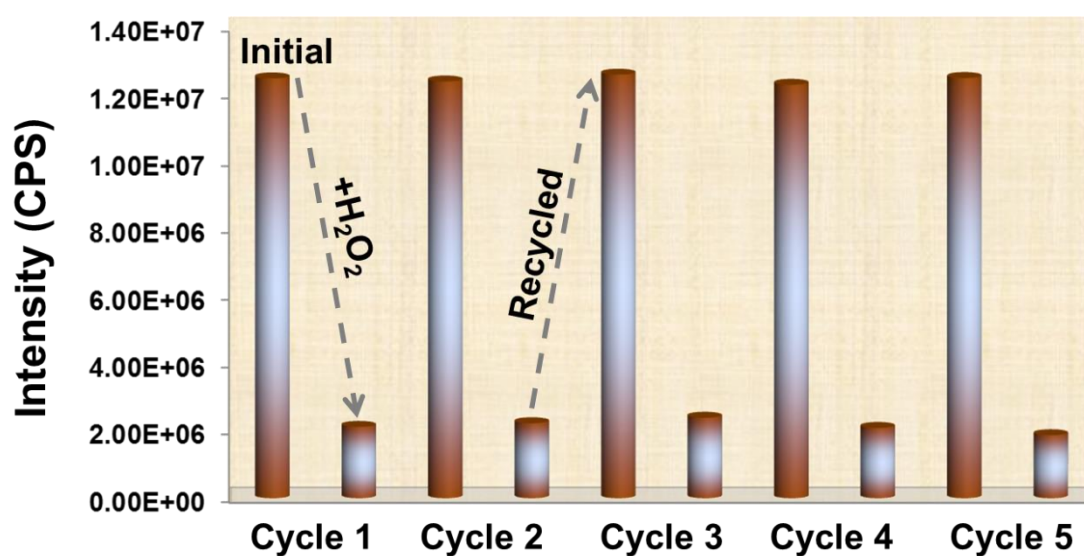


Fig. S21. Recyclable nature of quenching efficiency of **14a** towards 1 mM H₂O₂ solution for 5 cycles.

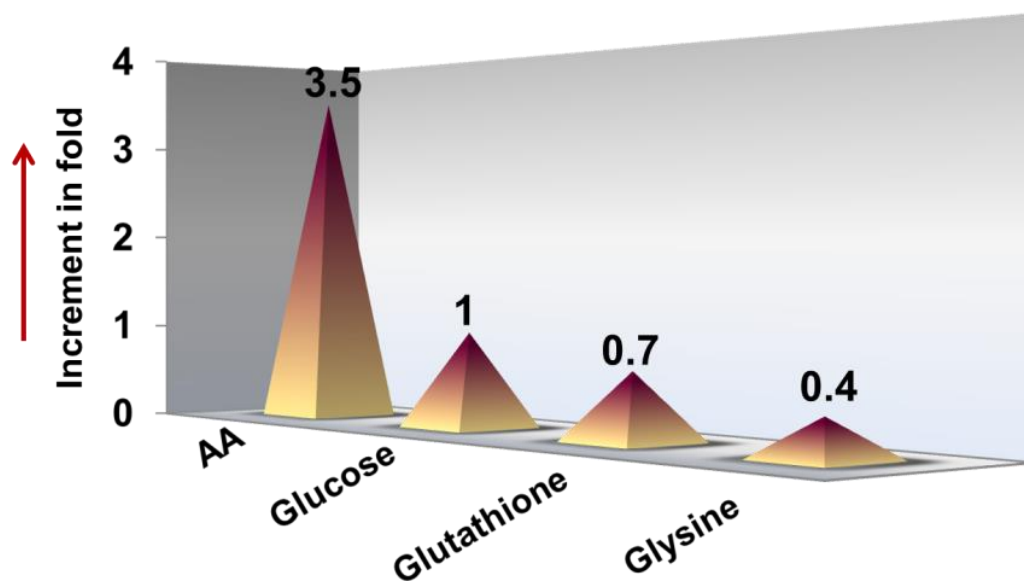


Fig. S22. Emission intensity increment (in fold) in **14a**@ClO⁻ for various reductants.

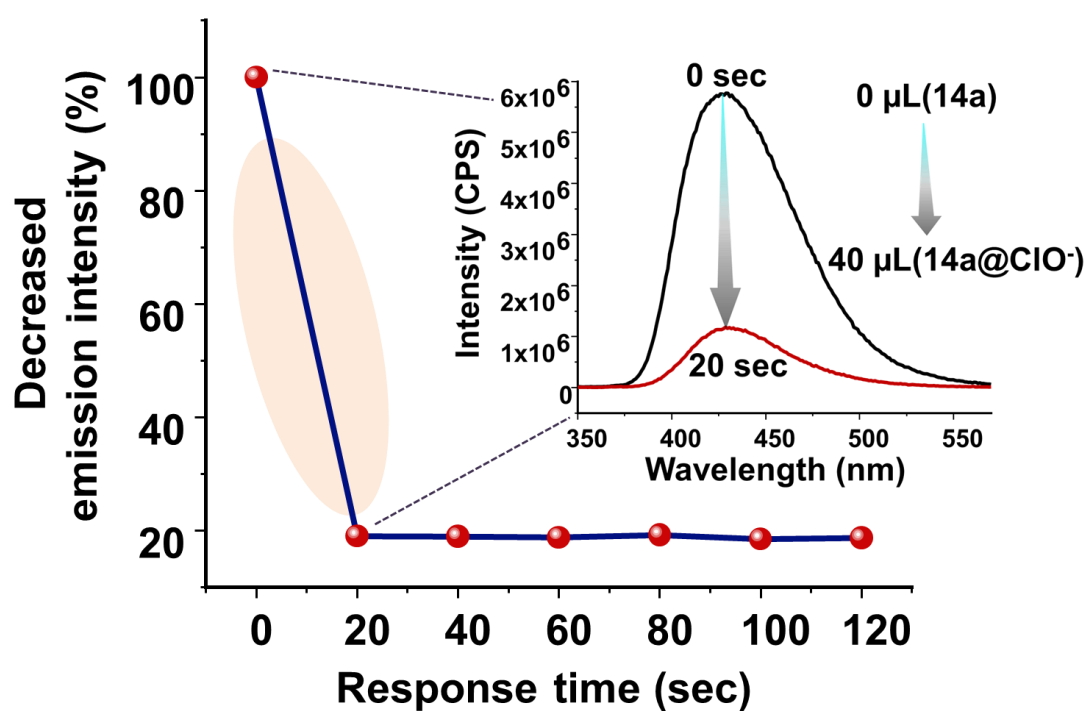


Fig. S23. Plot of decrease in emission intensity percentage at different time intervals for ClO⁻ (inset shows fluorescence spectra of **14a** before (0 sec) and after (20 sec) addition of 40 μL ClO⁻).

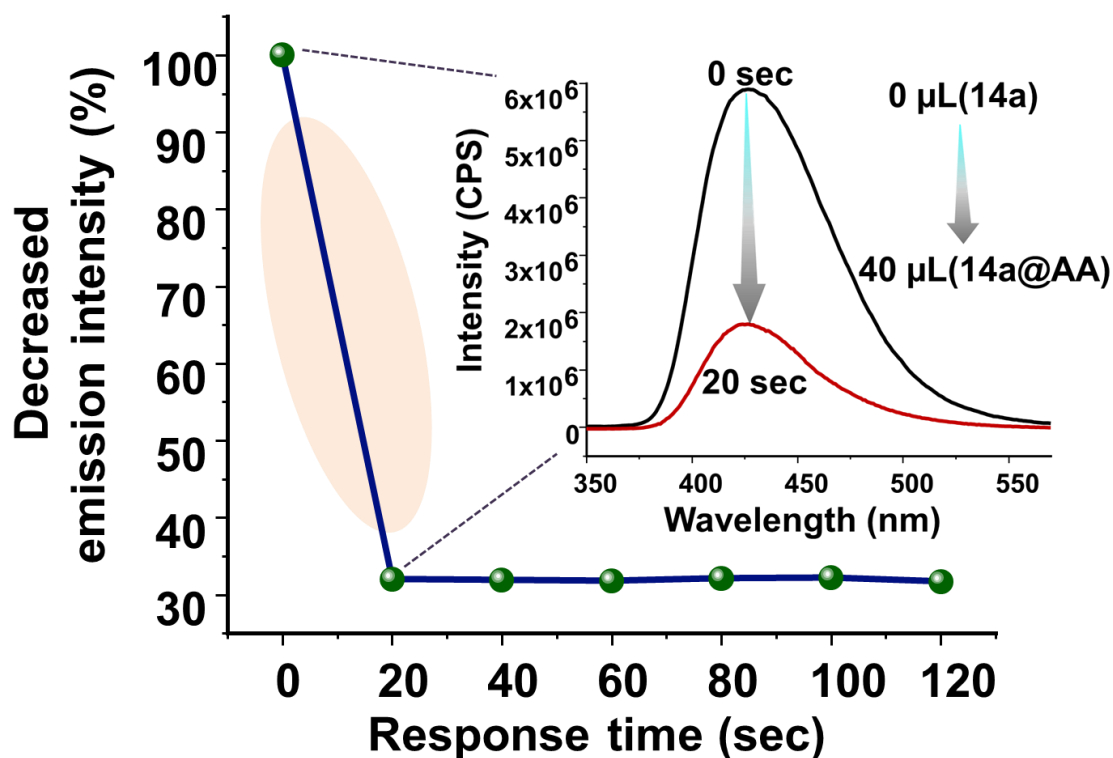


Fig. S24. Plot of decrease in emission intensity percentage at different time intervals for AA (inset shows fluorescence spectra of **14a** before (0 sec) and after (20 sec) addition of 40 μL AA).

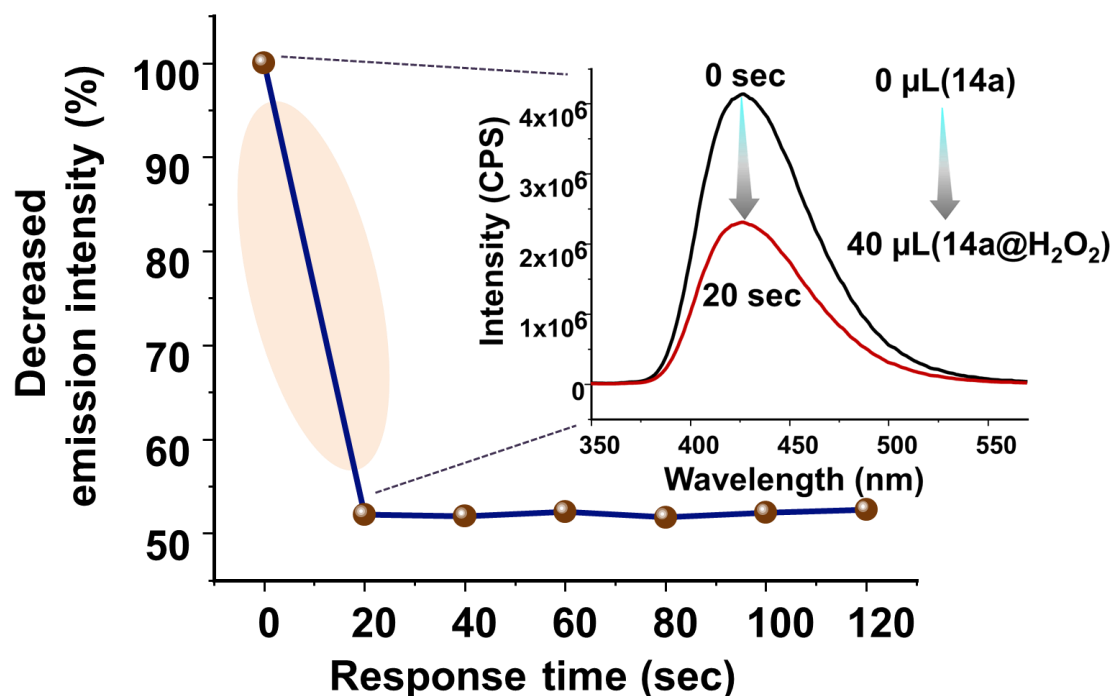


Fig. S25. Plot of decrease in emission intensity percentage at different time intervals for H_2O_2 (inset shows fluorescence spectra of **14a** before (0 sec) and after (20 sec) addition of 40 μL H_2O_2).

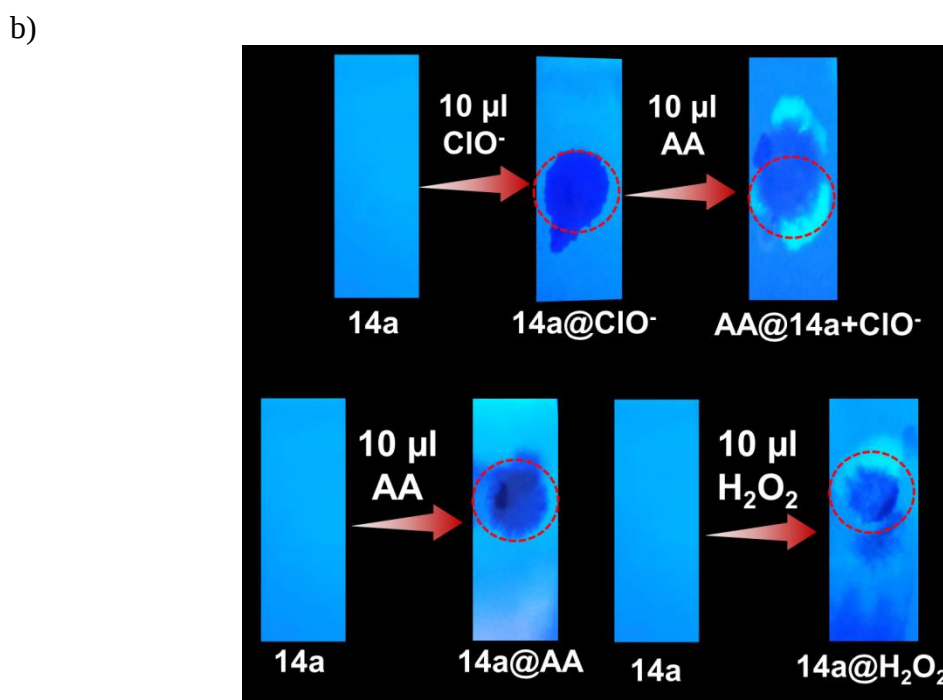
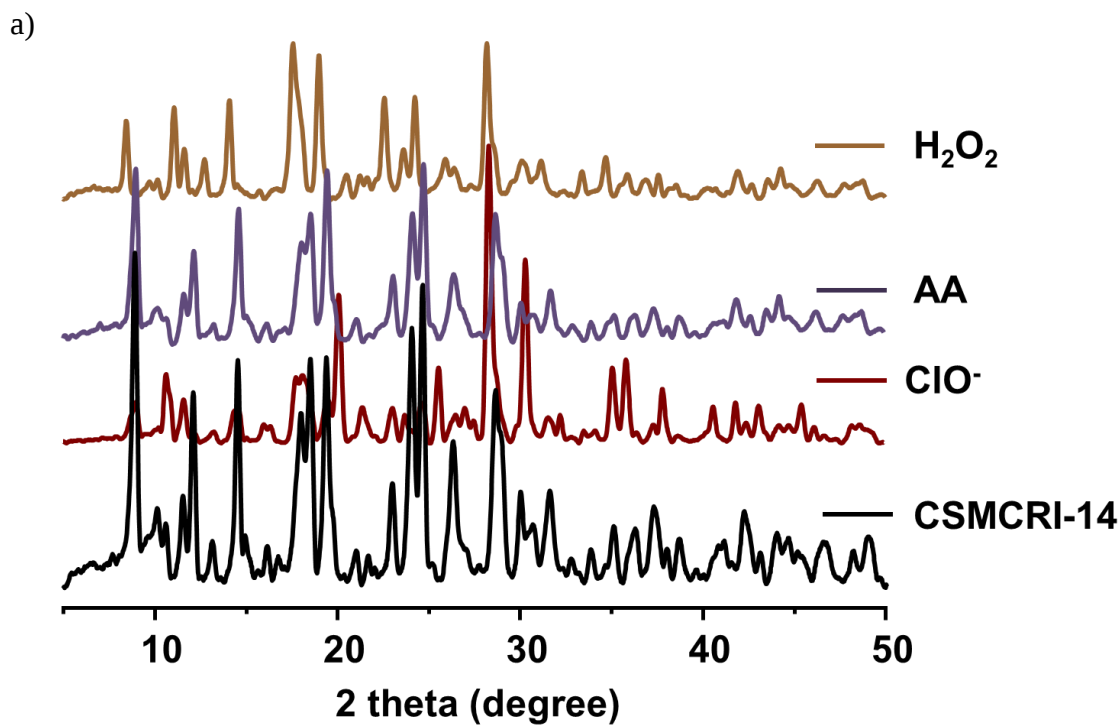


Fig. S26. a) PXRD patterns of CSMCRI-14 obtained after five sensing-recovery cycles for all studied analytes, b) Photographs of the paper strip coated with **14a** dispersion, showing fluorescence “on-off-on” switching in alternative presence of ClO^- and AA (Top) and quenching (Down) by individual analyte AA and H_2O_2 .

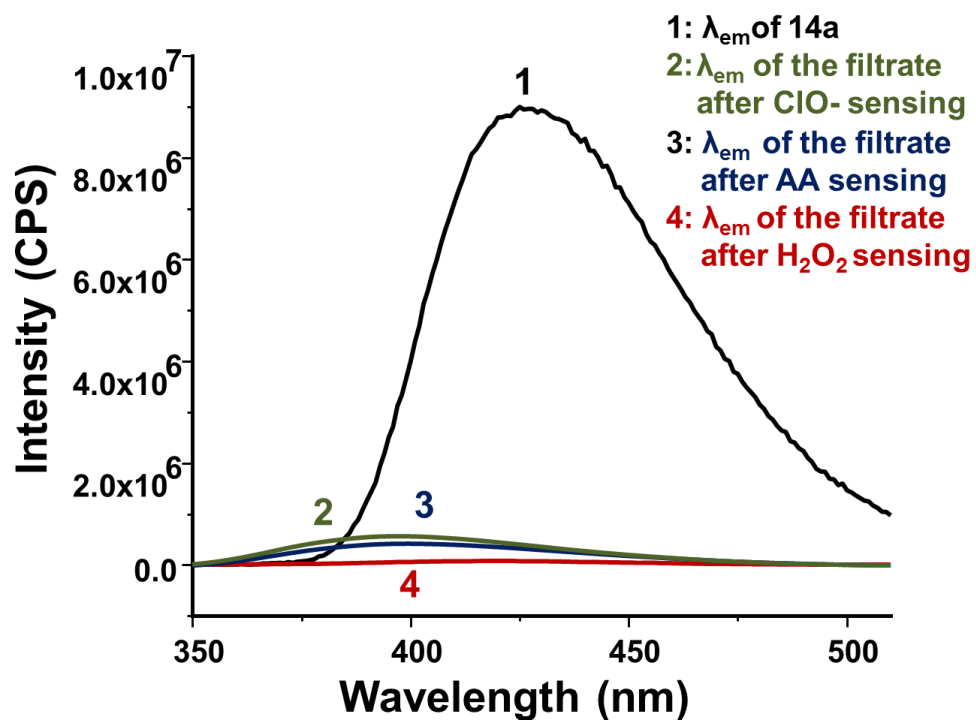
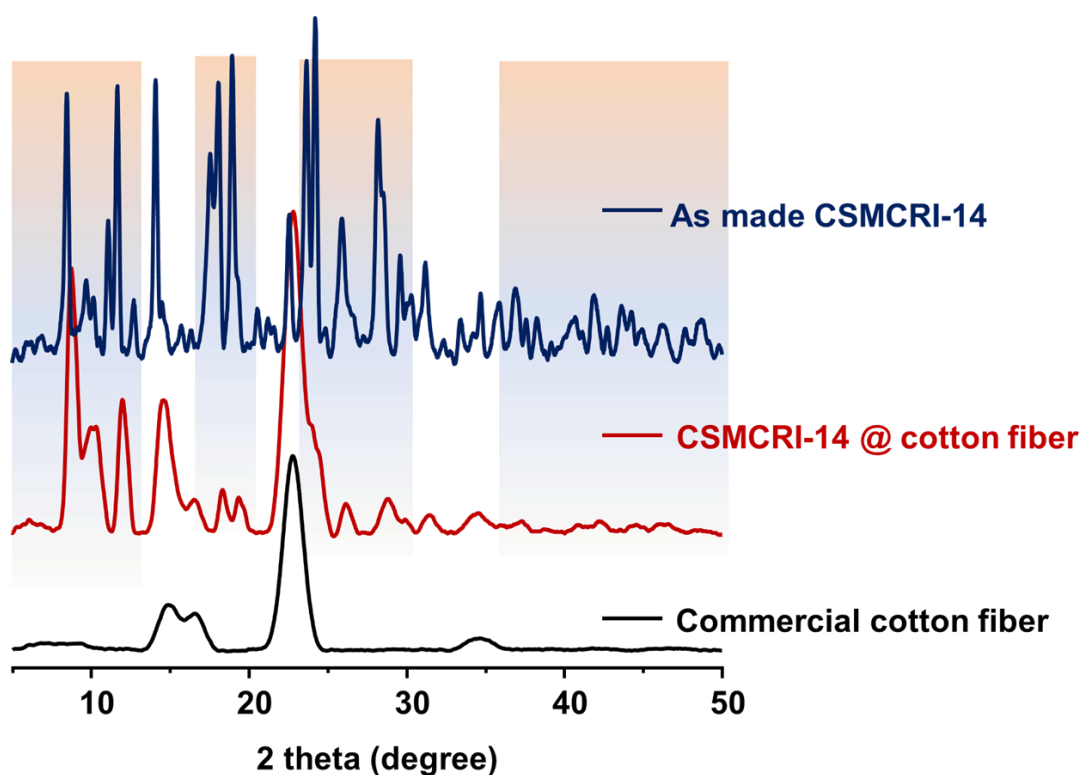


Fig. S27. Emission spectra of the filtrate after 5 sensing-recovery cycle, corroborating no leaching and heterogeneous nature of the fluoroprobe.

a)



b)

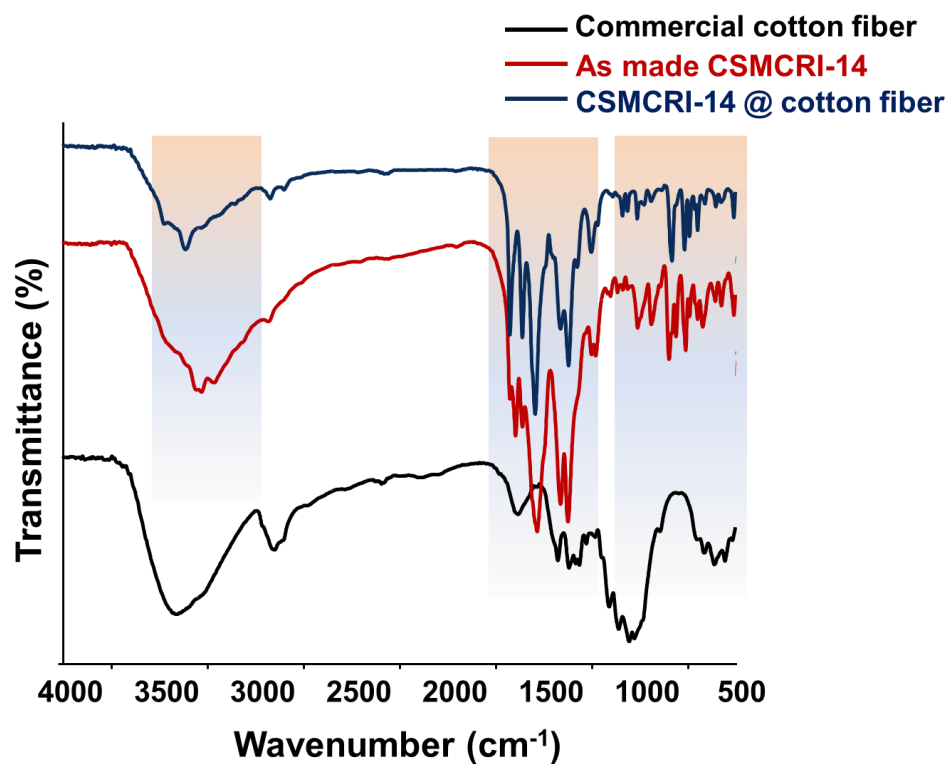
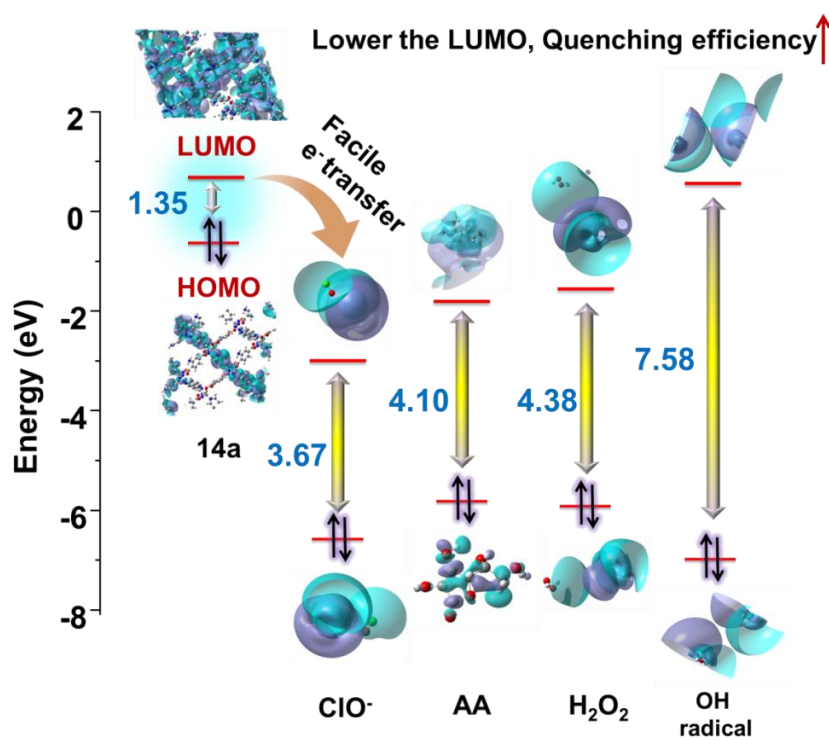
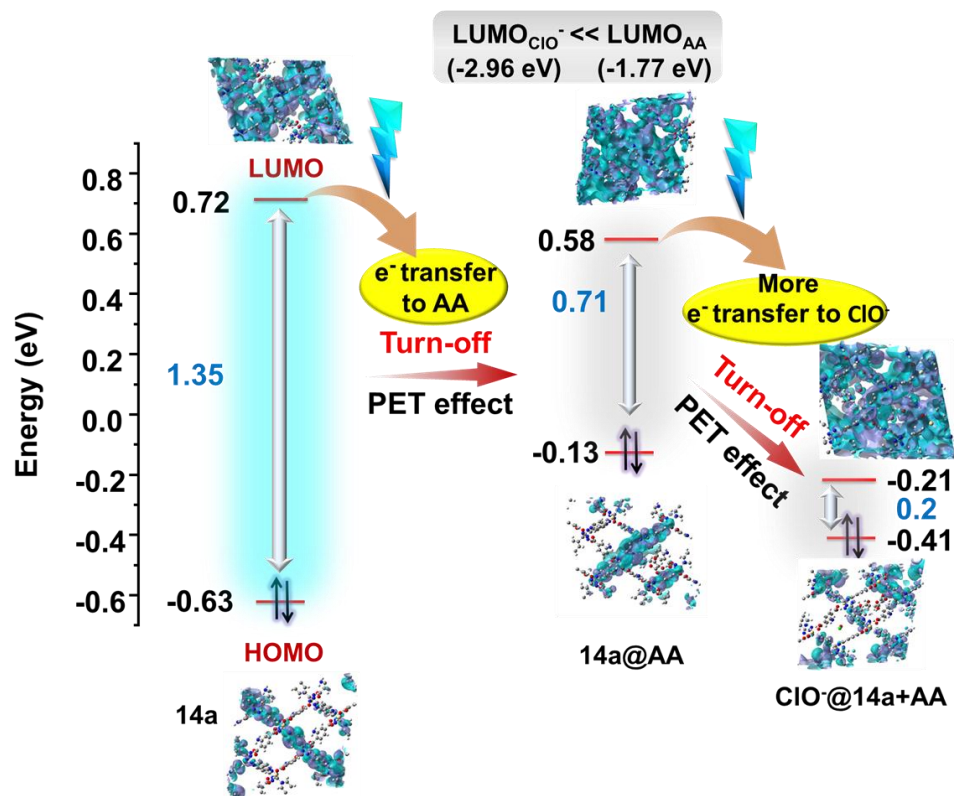


Fig. S28. a) PXRD pattern and b) FT-IR spectra of commercial cotton fiber (CF), CSMCRI-14 and CSMCRI-14@CF.

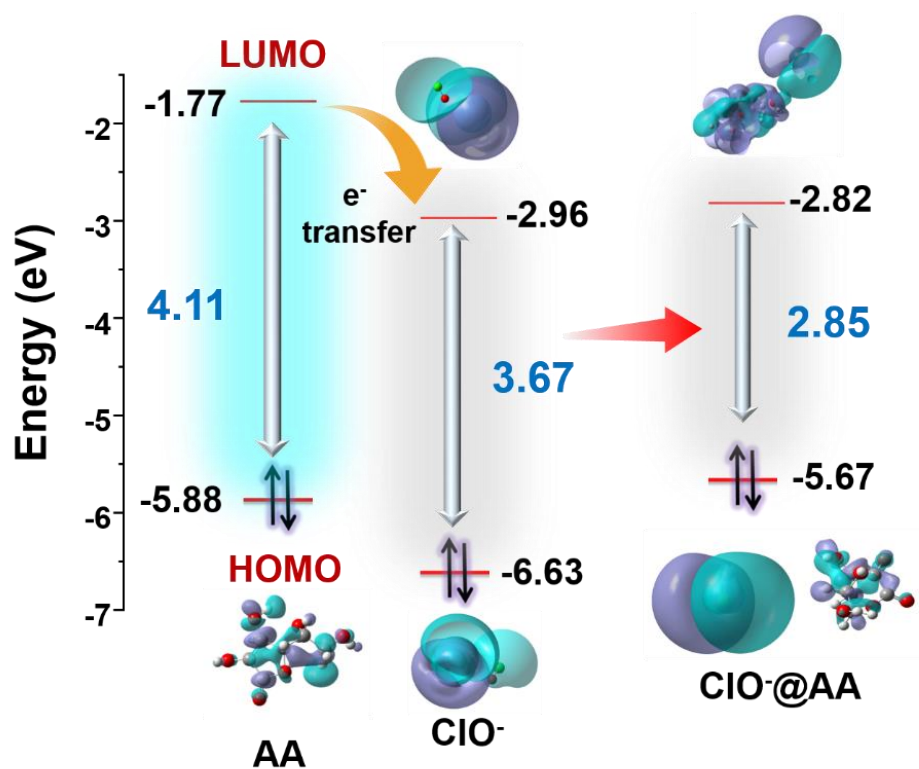
a)



b)



c)



d)

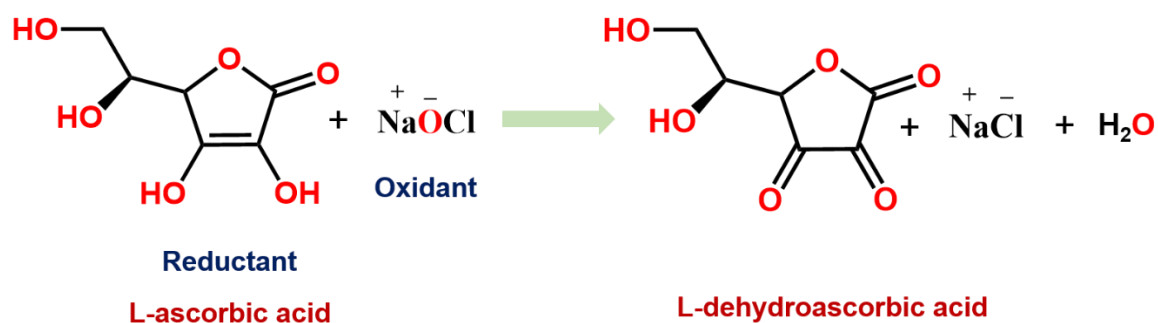


Fig. S29. a) HOMO–LUMO energies for **14a**, studied ROS and AA. b) Demonstration of electronic aspects behind the consecutive fluorescence quenching of **14a** in concurrent presence of AA and ClO[−]. c) HOMO-LUMO energy levels of AA, ClO[−] and ClO[−]@AA along with redistribution of the HOMO-LUMO energy gaps for ClO[−] in the presence of the AA. d) Oxidation-reduction reaction between L-ascorbic acid and sodium hypochlorite (NaClO).

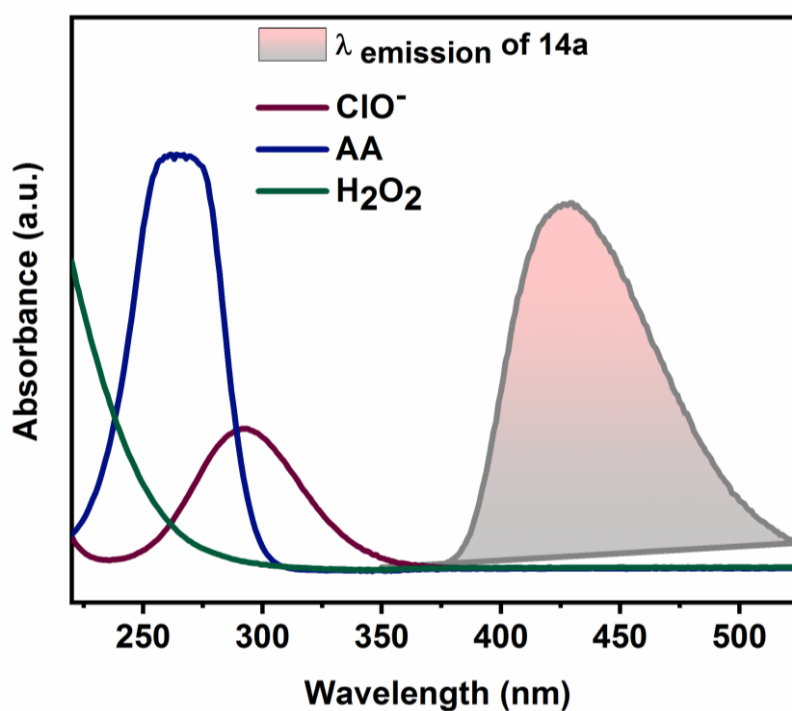


Fig. S30. Spectral overlap between the absorption spectra of the ROS and AA and emission spectrum of **14a**.

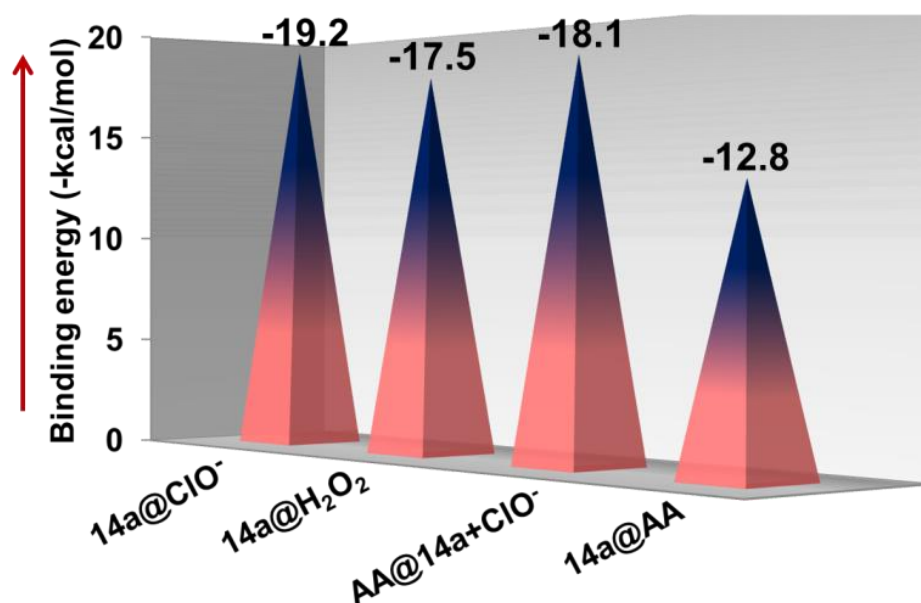


Fig. S31. Binding energy values of **14a** in presence of studied ROS, AA and AA@**14a**+ClO⁻.

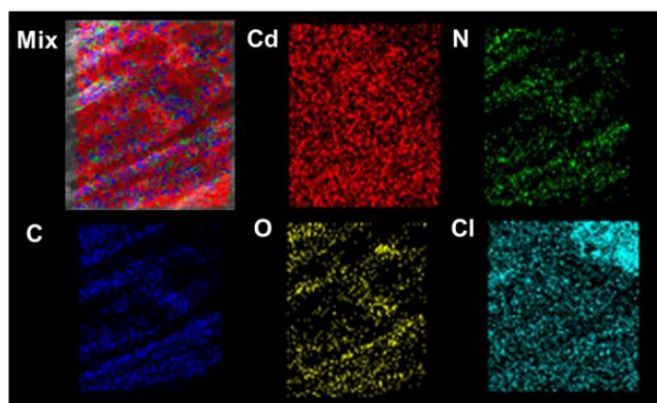
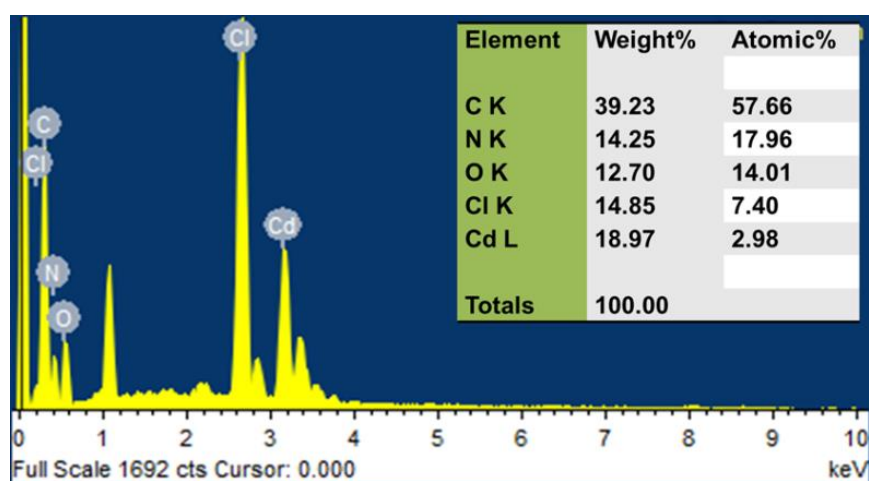


Fig. S32. EDX-elemental mapping of **14a**@ClO⁻ showing presences of all expected elements.

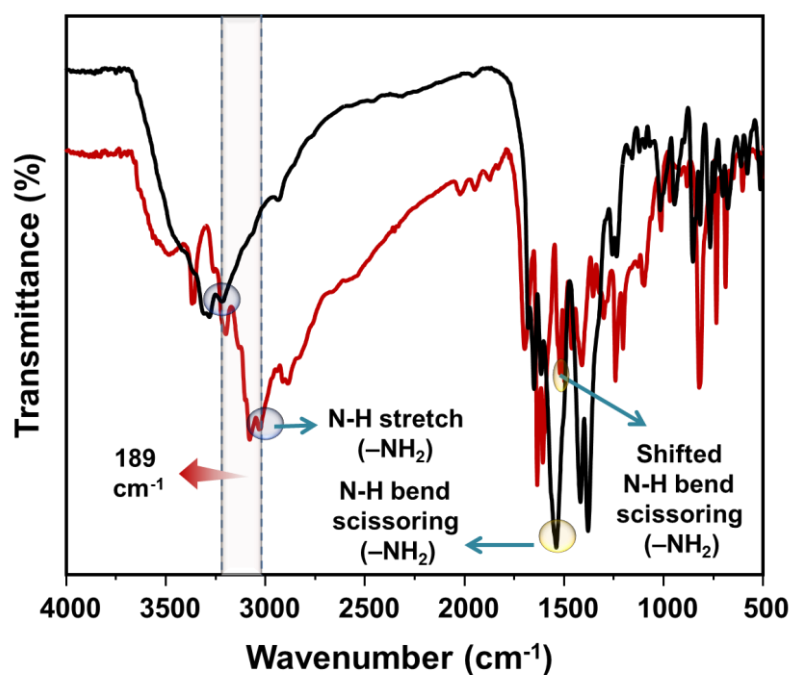


Fig. S33. FT-IR spectra of as made **CSMCRI-14** (Black) and **14a@ClO⁻** (red).

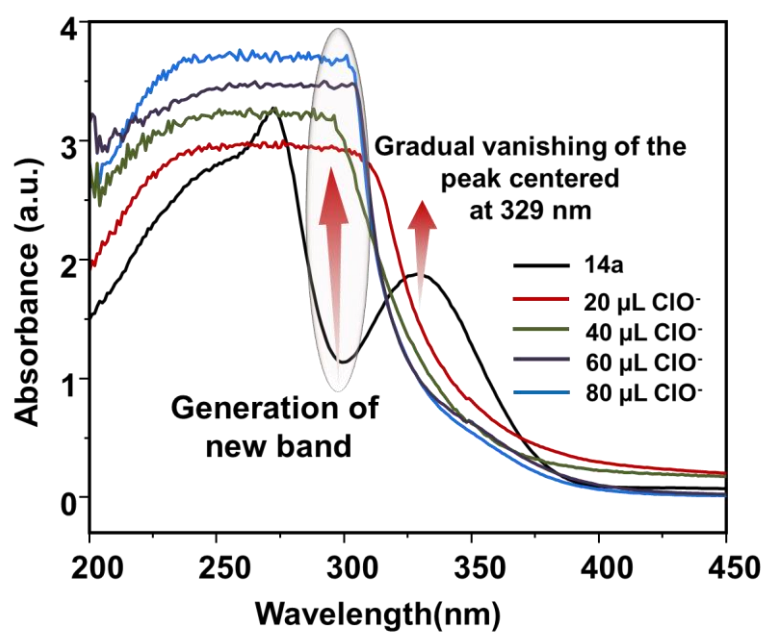


Fig. S34. UV-Vis spectra of **14a** (Black) and upon gradual addition ClO^- to the dispersion of **14a**.

Line#:1 R.Time:9.310(Scan#:663)
 MassPeaks:323
 RawMode:Averaged 9.305-9.315(662-664) BasePeak:55(8353394)
 BG Mode:Calc. from Peak Group 1 - Event 1

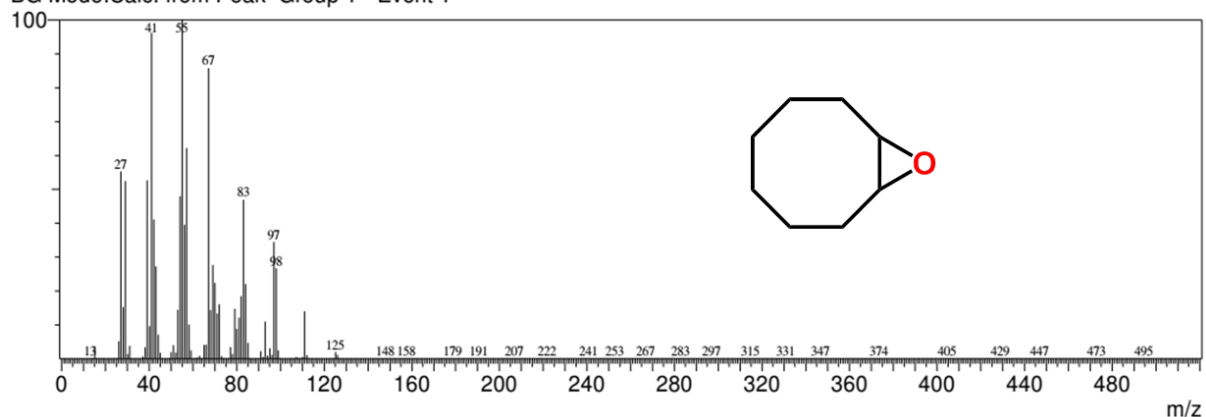


Fig. S35. GC-MS spectra of product 1b.

Line#:2 R.Time:7.720(Scan#:925)
 MassPeaks:289
 RawMode:Averaged 7.715-7.725(924-926) BasePeak:41(1675147)
 BG Mode:Calc. from Peak Group 1 - Event 1

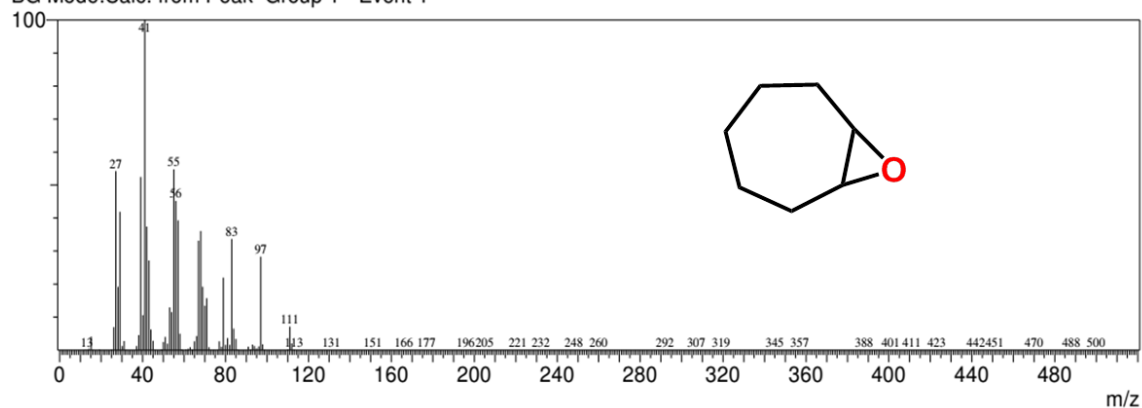


Fig. S35. GC-MS spectra of product 2b.

Line#:3 R.Time:9.380(Scan#:1257)
 MassPeaks:310
 RawMode:Averaged 9.375-9.385(1256-1258) BasePeak:67(3652605)
 BG Mode:Calc. from Peak Group 1 - Event 1

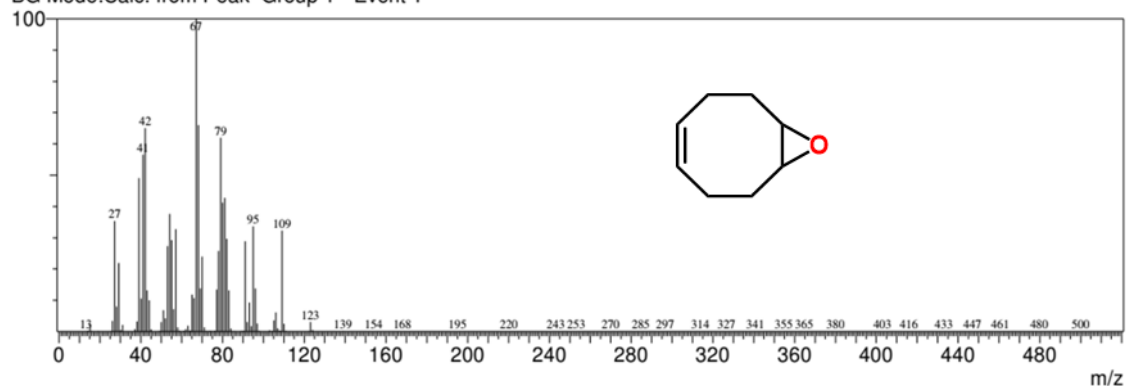


Fig. S36. GC-MS spectra of product 3b.

Line#:6 R.Time:14.995(Scan#:2380)
 MassPeaks:324
 RawMode:Averaged 14.990-15.000(2379-2381) BasePeak:167(3834399)
 BG Mode:Calc. from Peak Group 1 - Event 1

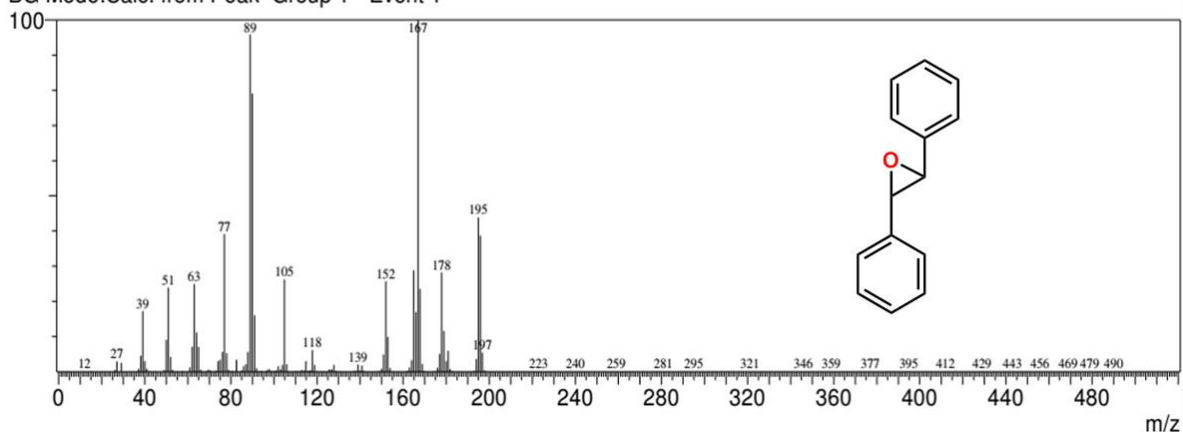


Fig. S37. GC-MS spectra of product 4b.

Line#:3 R.Time:12.070(Scan#:1795)
 MassPeaks:295
 RawMode:Averaged 12.065-12.075(1794-1796) BasePeak:59(224694)
 BG Mode:Calc. from Peak Group 1 - Event 1

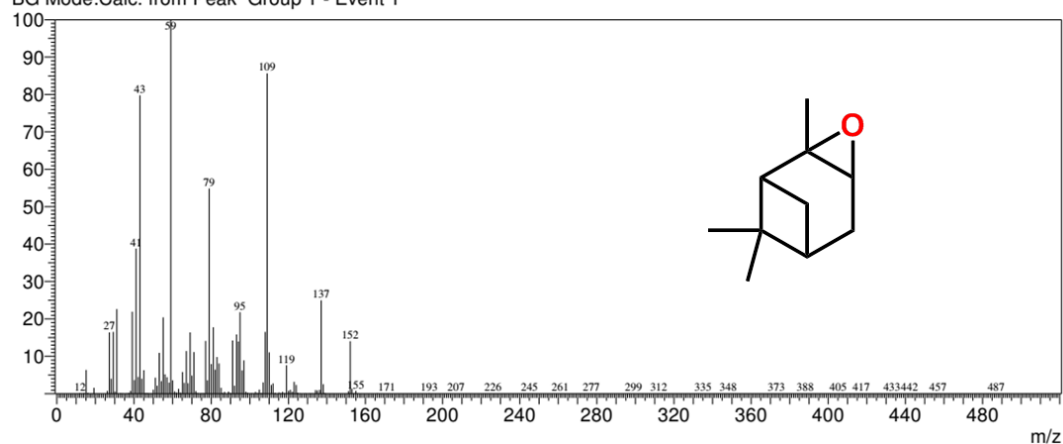


Fig. S38. GC-MS spectra of product 5b.

Line#:3 R.Time:4.955(Scan#:192)
 MassPeaks:302
 RawMode:Averaged 4.950-4.960(191-193) BasePeak:71(445075)
 BG Mode:Calc. from Peak Group 1 - Event 1

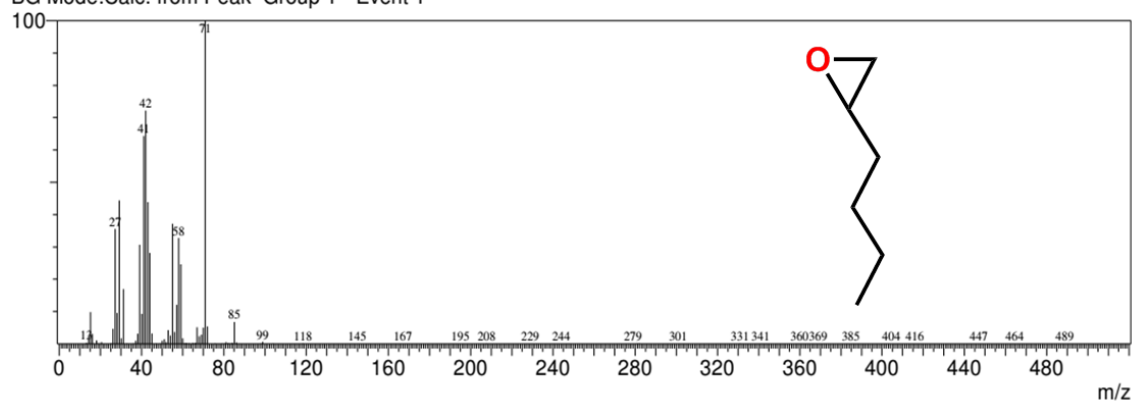


Fig. S39. GC-MS spectra of product 6b.

Line#:5 R.Time:6.200(Scan#:1221)
 MassPeaks:310
 RawMode:Averaged 6.195-6.205(1220-1222) BasePeak:45(1811853)
 BG Mode:Calc. from Peak Group 1 - Event 1

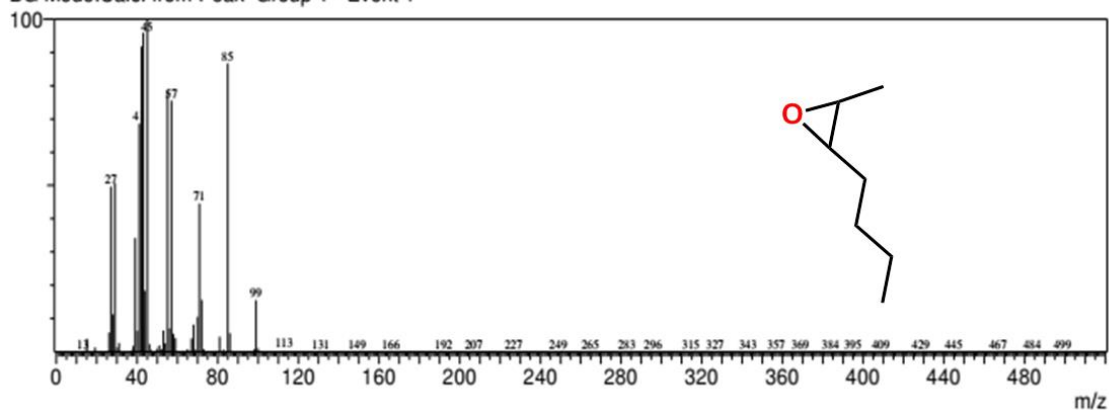


Fig. S40. GC-MS spectra of product 7b.

Line#:7 R.Time:11.415(Scan#:2264)
 MassPeaks:310
 RawMode:Averaged 11.410-11.420(2263-2265) BasePeak:71(3027171)
 BG Mode:Calc. from Peak Group 1 - Event 1

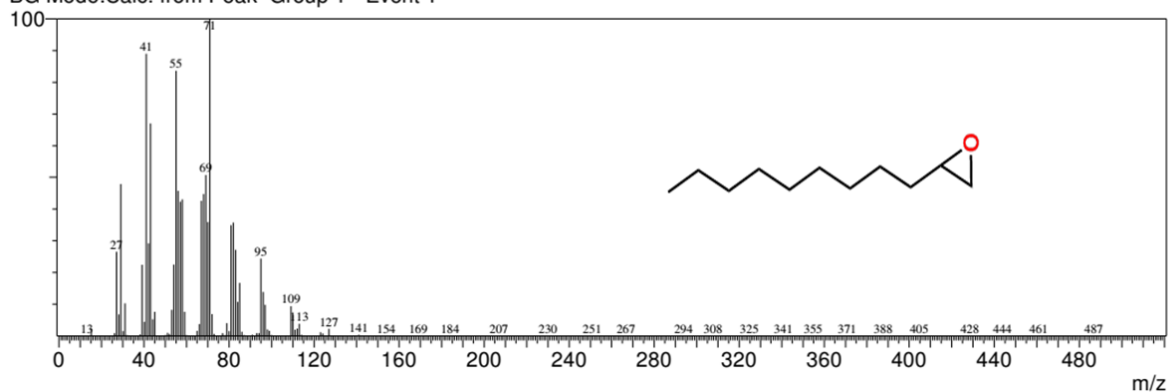


Fig. S41. GC-MS spectra of product 8b.

Line#:3 R.Time:13.455(Scan#:2072)
 MassPeaks:299
 RawMode:Averaged 13.450-13.460(2071-2073) BasePeak:41(158690)
 BG Mode:Calc. from Peak Group 1 - Event 1

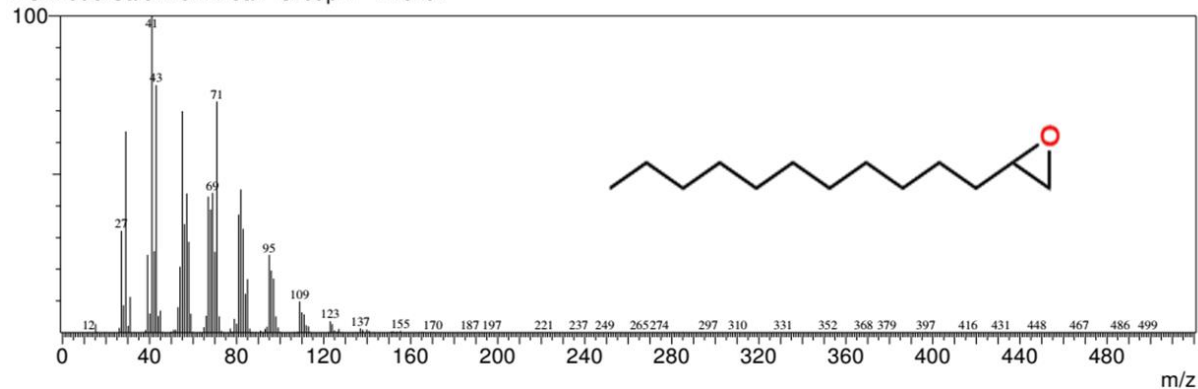


Fig. S42. GC-MS spectra of product 9b.

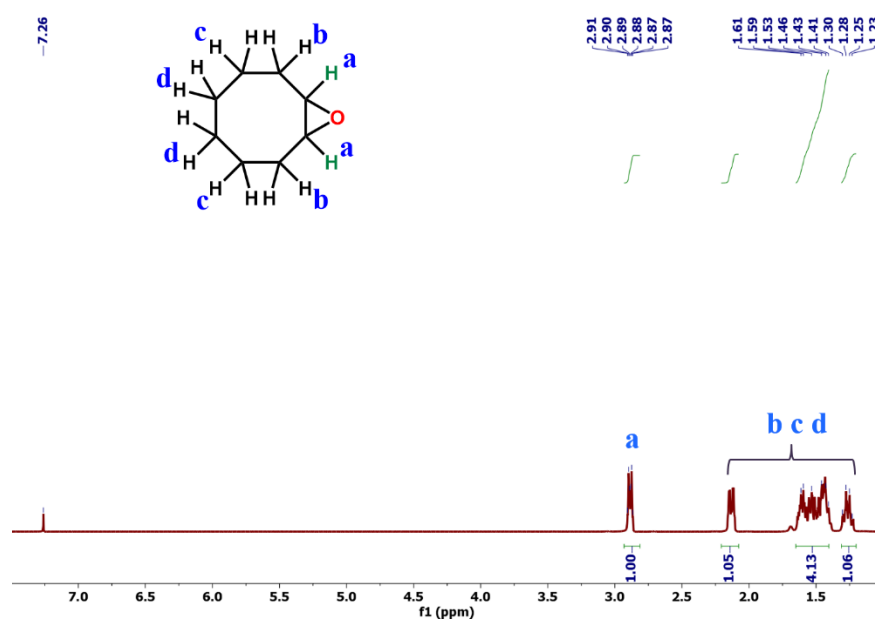


Fig. S43. ¹H-NMR spectrum of 1b in CDCl₃.

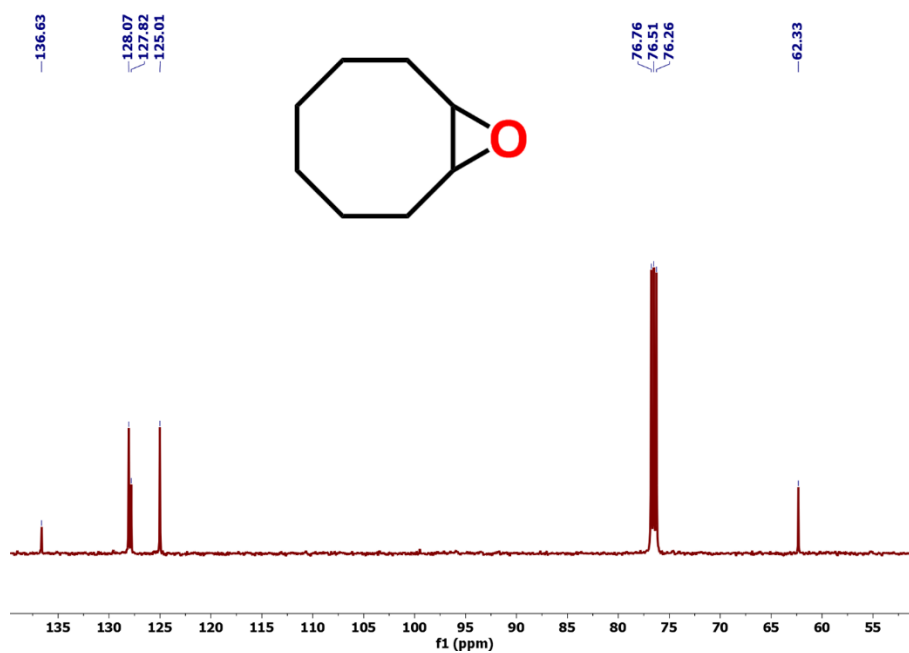


Fig. S44. ¹³C-NMR spectrum of 1b in CDCl₃.

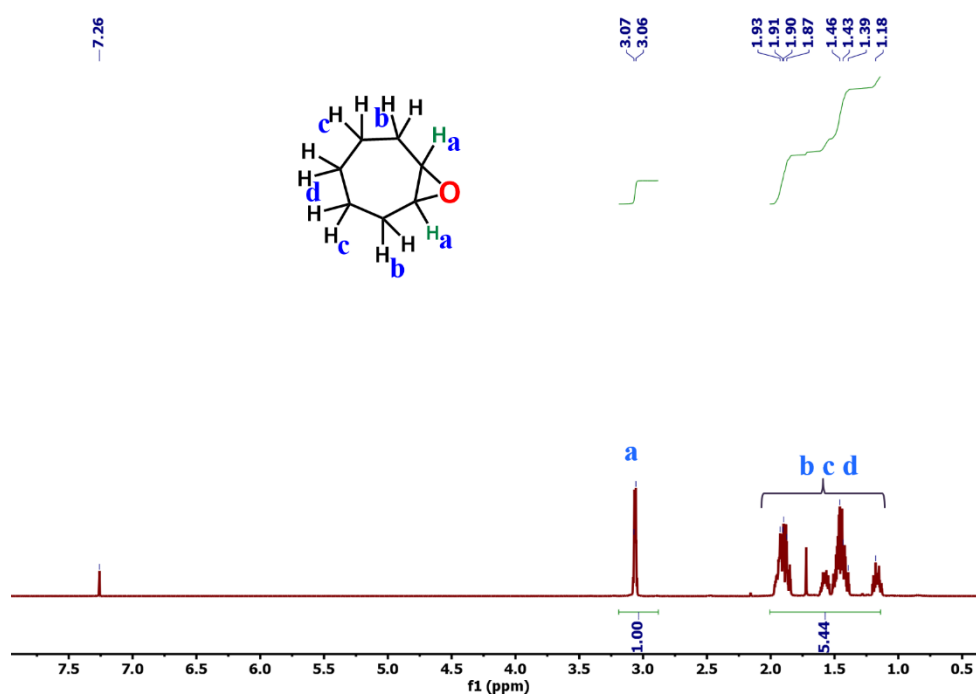


Fig. S45. ¹H-NMR spectrum of 2b in CDCl₃.

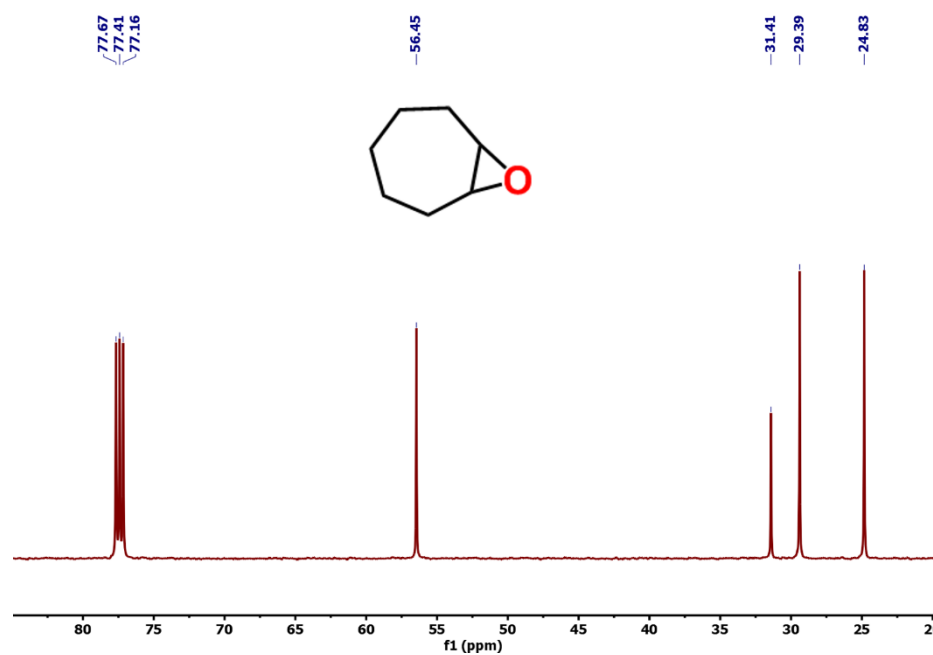


Fig. S46. ¹³C-NMR spectrum of 2b in CDCl₃.

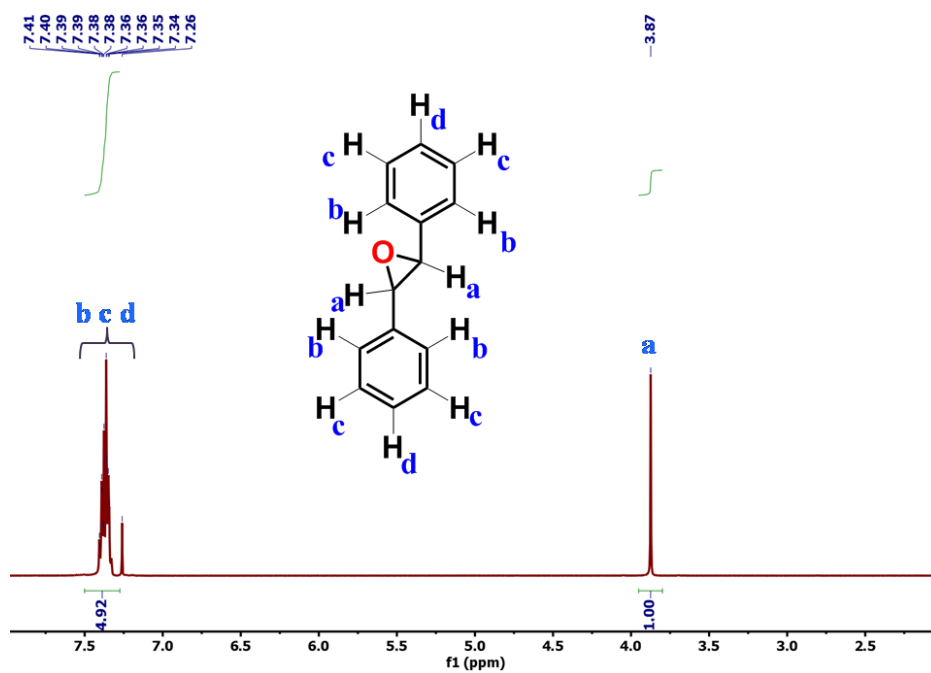


Fig. S47. ¹H-NMR spectrum of 4b in CDCl₃.

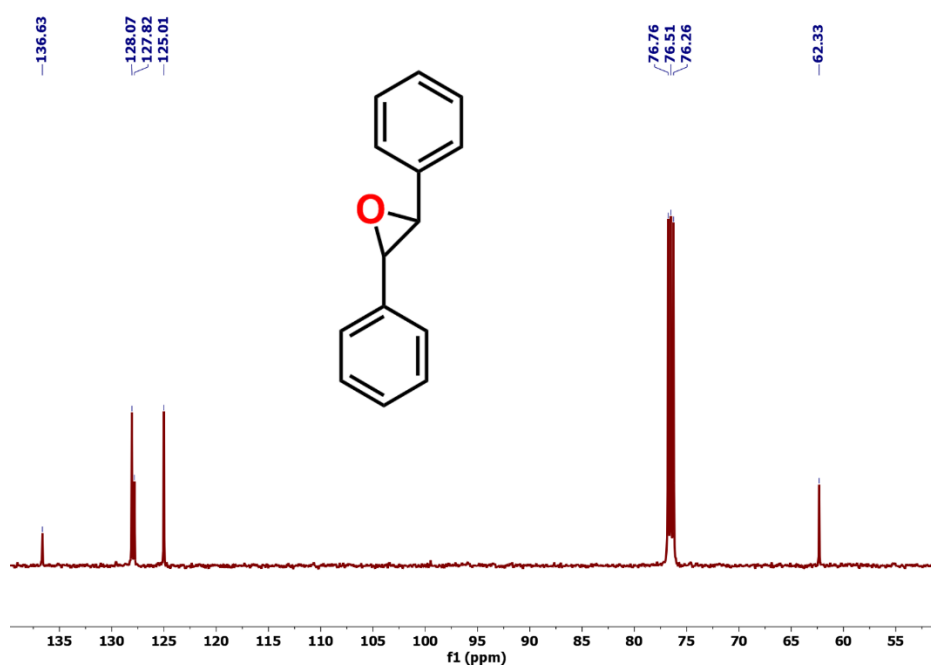


Fig. S48. ¹³C-NMR spectrum of 4b in CDCl₃.

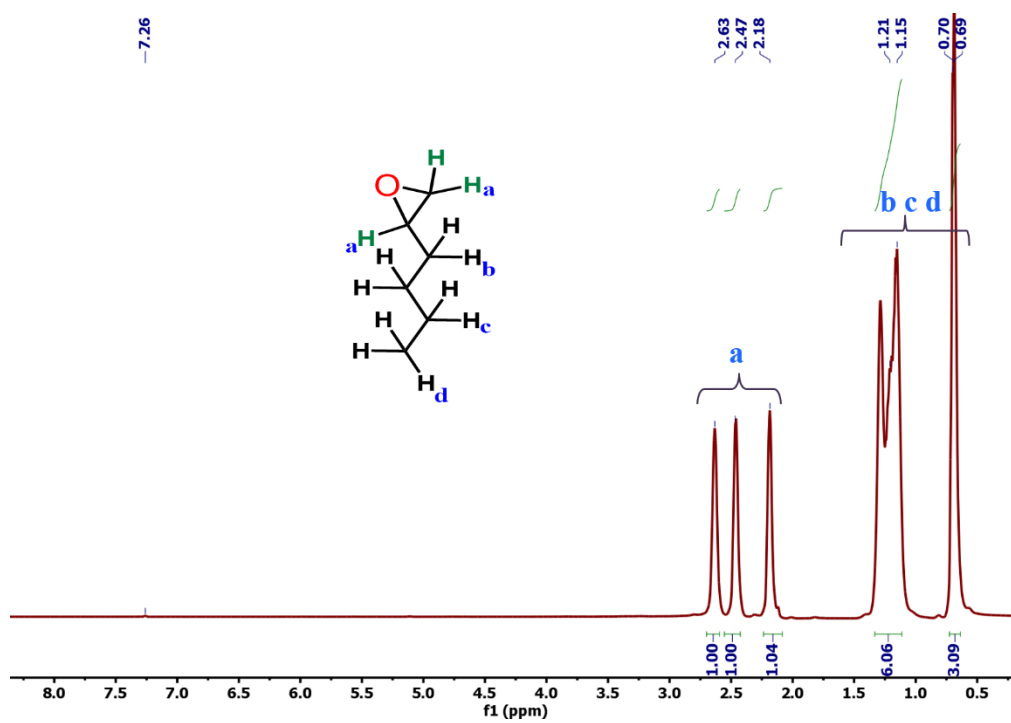


Fig. S49. ¹H-NMR spectrum of 6b in CDCl₃.

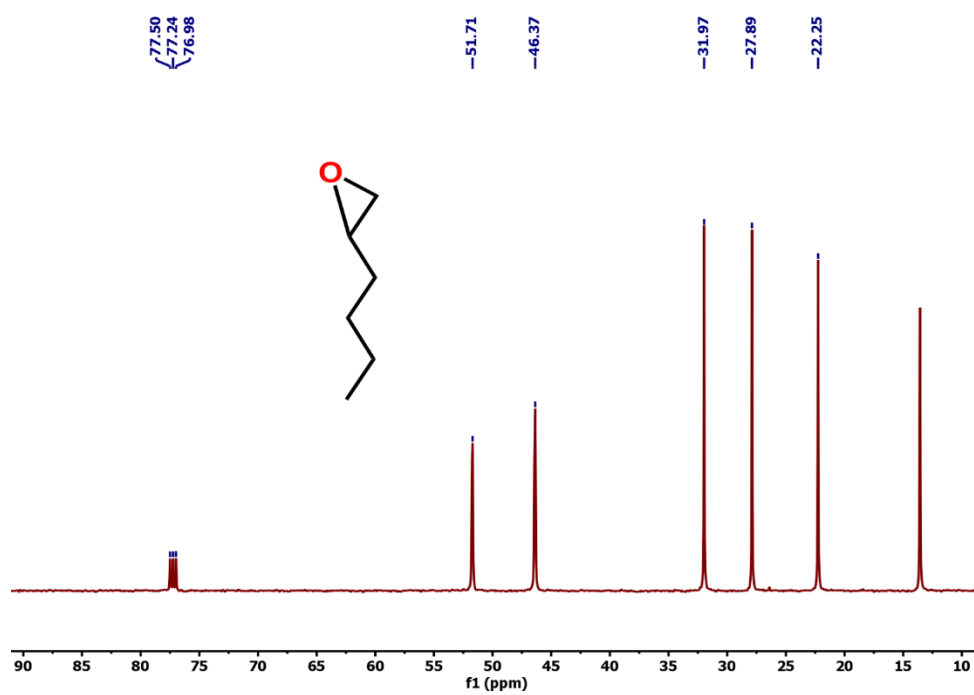


Fig. S50. ¹³C-NMR spectrum of 6b in CDCl₃.

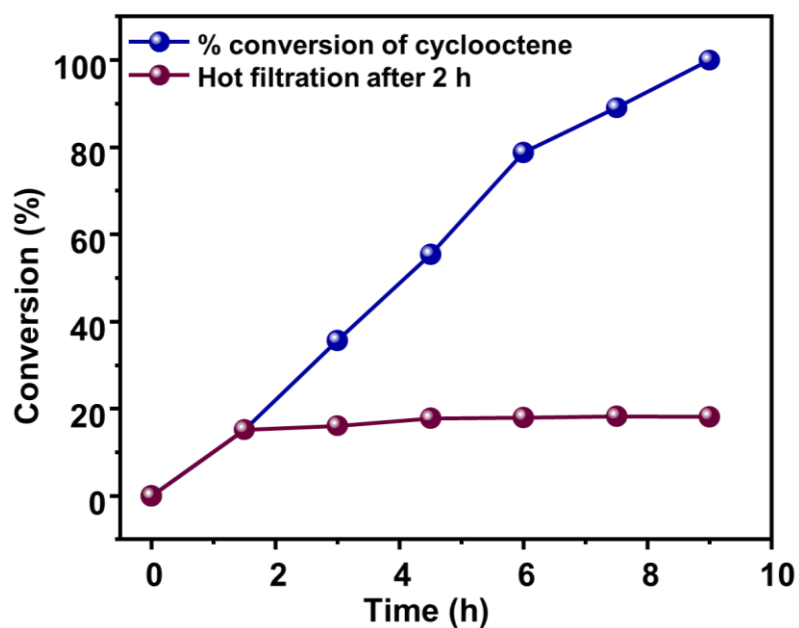


Fig. S51. Hot filtration test for cyclooctene epoxidation reaction.

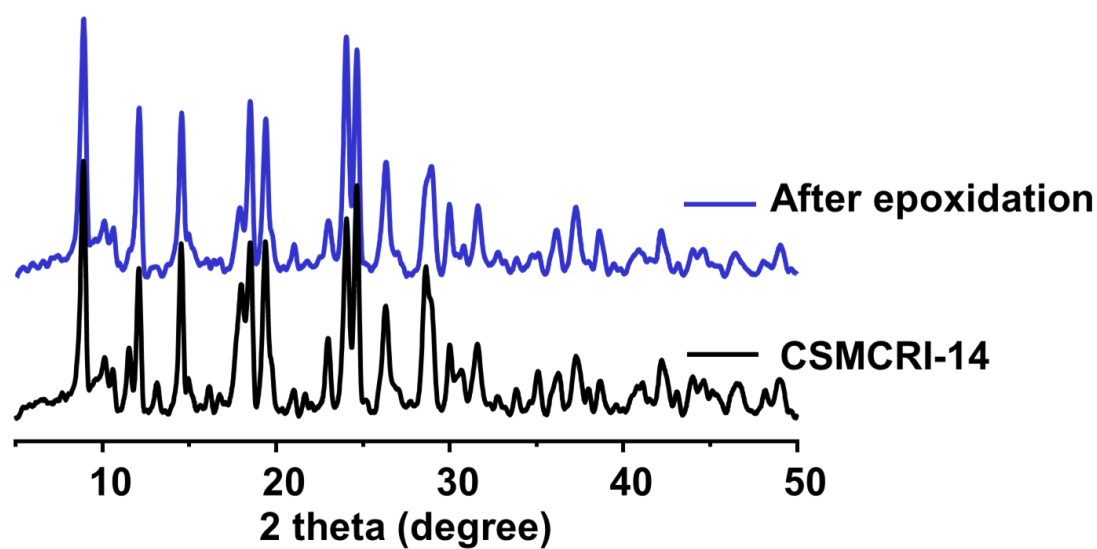


Fig. S52. PXRD patterns of as made CSMCRI-14 and recovered catalyst after five catalytic cycles, corroborating retention of structural integrity during catalytic reactions.

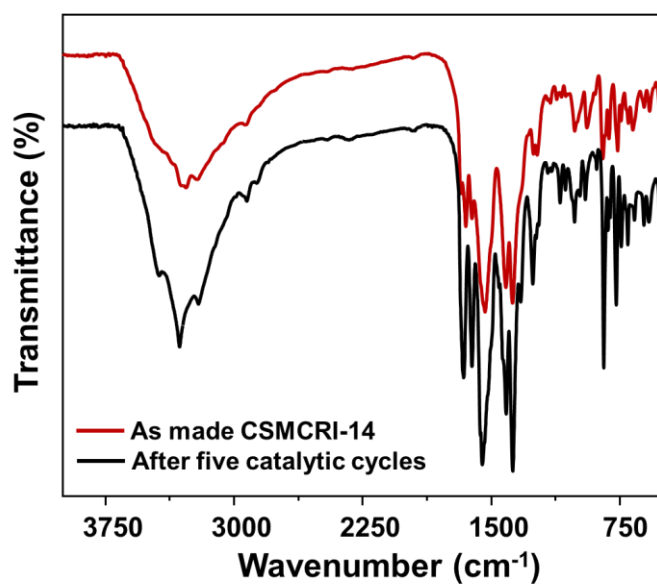


Fig. S53. FT-IR spectra of as made **CSMCRI-14** and recovered catalyst after five catalytic cycles, corroborating retention of structural integrity during catalytic reactions.

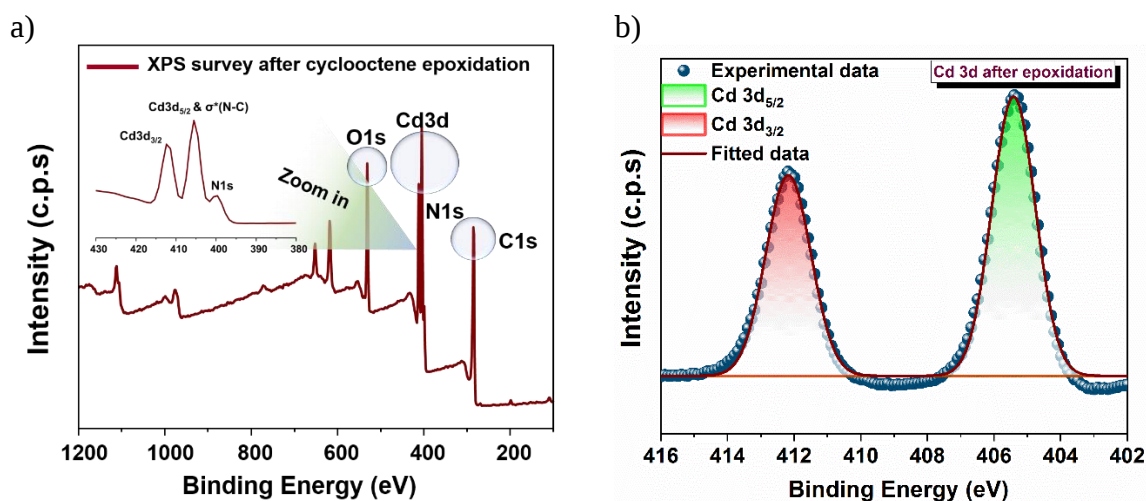


Fig. S54. (a) XPS survey spectrum and (b) deconvoluted Cd 3d XPS spectrum after cyclooctene epoxidation reaction, showing substantial stability of the MOF and no leaching of Cd(II) during catalytic runs.

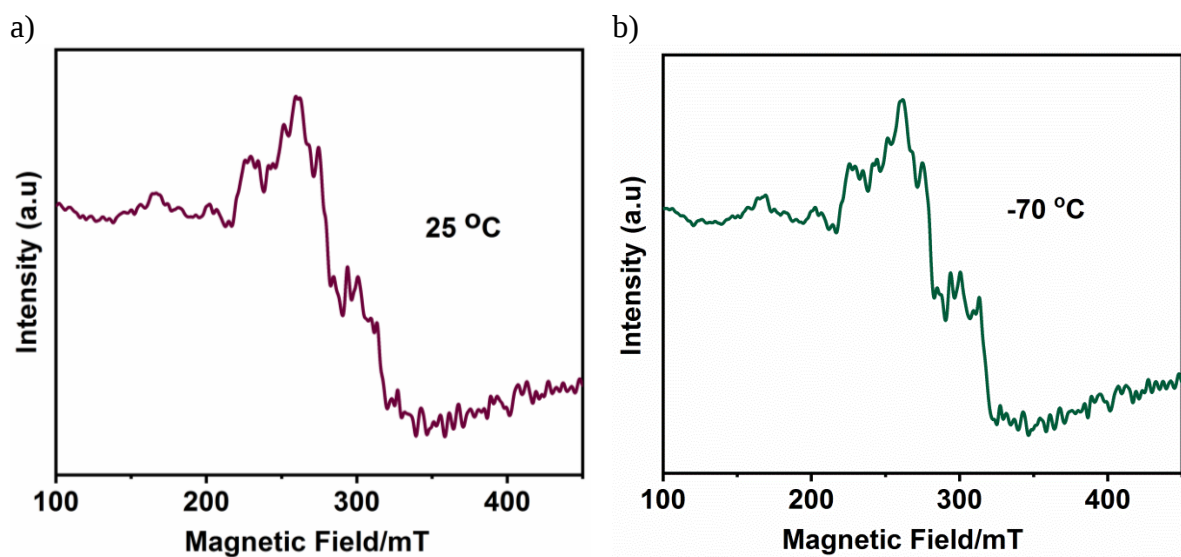


Fig. S55. a) Room temperature and b) low temperature EPR spectra of **14a** showing absence of hyperfine splitting.

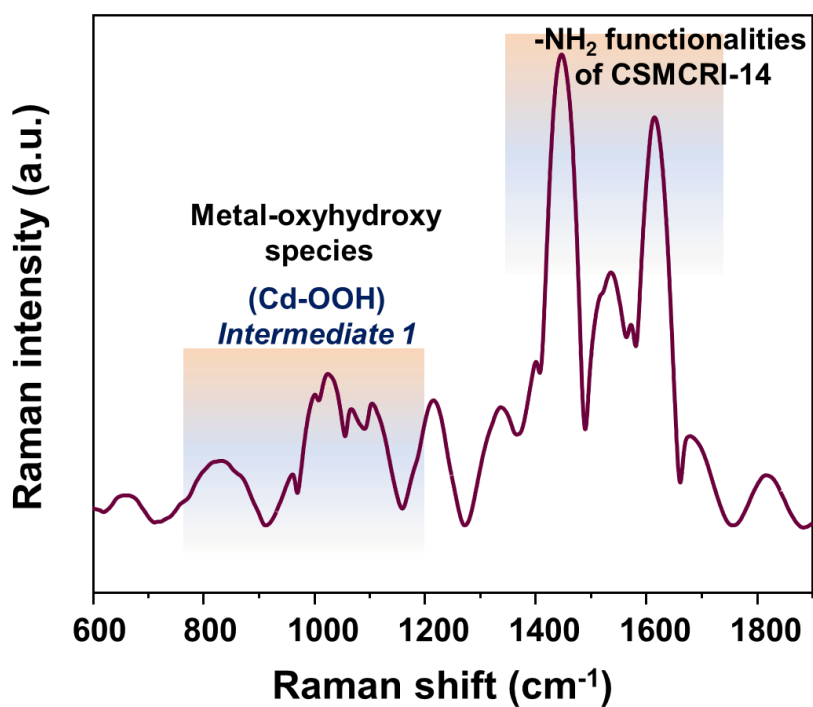


Fig. S56. SERS spectra of activated **CSMCRI-14** in presence of H_2O_2 .

Table S1. Crystal data and refinement parameters for **CSMCRI-14**

Identification code	CSMCRI-14
Empirical formula	C ₂₀ H ₁₆ N ₈ O ₅ Cd
Formula weight	562.83
Temperature/K	103.15
Crystal system	triclinic
Space group	P-1
a/Å	10.762(3)
b/Å	11.619(3)
c/Å	13.482(4)
$\alpha/^\circ$	72.923(8)
$\beta/^\circ$	78.124(9)
$\gamma/^\circ$	67.674(8)
Volume/Å ³	1482.2(7)
Z	2
$\rho_{\text{calc}}/\text{g cm}^{-3}$	1.2610
μ/mm^{-1}	0.775
F(000)	562.6
Crystal size/mm ³	0.16 × 0.14 × 0.12
Radiation	Mo K α (λ = 0.71073)
2 Θ range for data collection/ $^\circ$	4.76 to 54.52
Index ranges	-13 ≤ h ≤ 12, -14 ≤ k ≤ 14, -17 ≤ l ≤ 17
Reflections collected	12729
Independent reflections	6449 [R _{int} = 0.0710, R _{sigma} = 0.0996]
Data/restraints/parameters	6449/0/317
Goodness-of-fit on F ²	0.996
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0547, wR ₂ = 0.1399
Final R indexes [all data]	R ₁ = 0.0653, wR ₂ = 0.1466
Largest diff. peak/hole / e Å ⁻³	0.96/-1.26

Alert level A for **CSMCRI-14**

PLAT213_ALERT_2_A Atom C3 has ADP max/min Ratio 5.1 prolat

PLAT353_ALERT_3_A Long N-H (N0.87,N1.01A) N00 - H00D . 1.24 Ang.

Explanation: These two alerts have been generated probably due to the presences of disorder in the structure.

Determination of Formula & Solvent Composition of CSMCRI-14 from PLATON Squeeze and Thermogravimetric Analysis Data:

From the TGA plot of as-synthesized **CSMCRI-14**, the observed mass loss is 21.3 %

The framework is neutral. In the asymmetric unit one of each 2-ATA, *dpta*, H₂O molecule are coordinated with single Cd (II) metal centre.

So, formula of the asymmetric unit excluding the guest solvents is $[\text{Cd}(2\text{-ATA})(\text{dpta})(\text{H}_2\text{O})]$

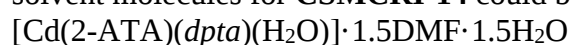
From OLEX2, void electron count comes out to be 78

Now, according to the above formula, mass of the asymmetric unit is 560.81

Table S2. Number of electrons and molecular masses of guest solvent molecules associated with **CSMCRI-14** for determination of solvent composition and molecular formula

	Dimethyl formamide (DMF)	Water
No. of electrons	40	10
mass	73	18

Considering the above mentioned number of electrons, the best possible combination of solvent molecules for **CSMCRI-14** could be:



The total number of electrons contributed by lattice solvent molecules will be $[(40 \times 1.5) + (10 \times 1.5)] = 75$, which is in good agreement with the OLEX result and thus validates the above formula.

The aforementioned combination was further cross-checked from TGA analysis.

Mass loss due to guest solvents is $[(73 \times 1.5) + (18 \times 1.5)] = 136.5$

Therefore, total mass of **CSMCRI-14** including the guests is $(560.81 + 136.5) = 697.31$

So, mass loss due to coordinated water molecule = $(18/697.31) \times 100\% = 2.58\%$

Mass loss due to lattice water molecules = $[(18 \times 1.5)/697.31] \times 100\% = 3.87\%$

Mass loss due to lattice DMF molecules = $[(73 \times 1.5)/697.31] \times 100\% = 15.7\%$

Therefore, total mass loss for coordinated and guest solvents = $(2.58 + 3.87 + 15.7)\% = 22.15\%$, which is in good agreement with that of the TGA result.

Table S3. Calculation of standard deviation of fluorescence intensity and limit of detection for **14a** towards ClO^-

Blank Readings (14a)	Fluorescence Intensity(CPS)
Reading 1	5400396
Reading 2	5488954
Reading 3	5300569
Reading 4	5287956
Reading 5	5355789
<i>Standard Deviation (σ)</i>	81814.47
<i>Slope from Graph (K)</i>	5169390 μM^{-1}
<i>Detection limit ($3\sigma/K$)</i>	47.4 nM
<i>Limit of Detection (LOD)</i>	26.7 ppb

Table S4. Calculation of standard deviation of fluorescence intensity and limit of detection for **14a** towards AA

Blank Readings (14a)	Fluorescence Intensity(CPS)
Reading 1	5400396
Reading 2	5488954
Reading 3	5300569
Reading 4	5287956
Reading 5	5355789
<i>Standard Deviation (σ)</i>	81814.47
<i>Slope from Graph (K)</i>	3357626 μM^{-1}
<i>Detection limit ($3\sigma/K$)</i>	73.1 nM
<i>Limit of Detection (LOD)</i>	41.1 ppb

Table S5. Calculation of standard deviation of fluorescence intensity and limit of detection for **14a** towards H_2O_2

Blank Readings (14a)	Fluorescence Intensity(CPS)
Reading 1	5400396
Reading 2	5488954
Reading 3	5300569
Reading 4	5287956
Reading 5	5355789
<i>Standard Deviation (σ)</i>	81814.47
<i>Slope from Graph (K)</i>	2806147 μM^{-1}
<i>Detection limit ($3\sigma/K$)</i>	87.4 nM
<i>Limit of Detection (LOD)</i>	49.2 ppb

Table S6. A comparison of quenching constant, their LOD values, of various luminescent MOFs used for detection of ClO⁻

Sl.no.	Materials	Limit of detection (μM)	Medium used	Reference
1.	In1-NH ₂	0.64	water	<i>Dalton Trans.</i> , 2021, 50 , 7554-7562
2.	Eu/BPyDC@M OF-253-NH ₂	0.094	Tris-HCl	<i>Inorg. Chem.</i> , 2019, 58 , 13360-13369
3.	Zr-UiO-66-DMTCM))1	1.22	Water	<i>New J. Chem.</i> , 2021, 45 , 14211-14217
4.	UiO-68-ol	0.7	PBS buffer	<i>Inorg. Chem.</i> , 2017, 56 , 13241-13248
5.	Eu-BDC-NH ₂ /DPA	0.037	-	<i>Anal. Chem.</i> 2021, 93 , 3559-3566
6.	UiO-68-PT	0.28	water	<i>Inorg. Chem.</i> , 2019, 58 , 9890-9896
7.	UiO-Eu-L1	0.016	pure water	<i>Chem. Eng. J.</i> , 2018, 351 , 364-370
8.	PDA@ERGO/G C	0.044	Water	<i>Sensors and Actuators B: Chemical</i> , 2017, 240 , 818-828
9.	Poly(luminol) reagent film	0.5	Water	<i>Sensors and Actuators B: Chemical</i> , 2014, 192 , 92-98
10.	CSMCRI-14	0.047 μM/26.7 ppb	Water	Present work

Table S7. A comparison of quenching constant, their LOD values, of various luminescent MOFs used for detection of AA

Sl.no.	Material	Analytical method	Limit of detection (μM)	Reference
1.	$\text{Hf}_6\text{O}_4(\text{OH})_4(\text{C}_{15}\text{H}_8\text{O}_4\text{S}_2)_6$	FS	2.9	<i>Chem. - Asian J.</i> 2019, 14 , 2822–2830
2.	ZIF-8	ECS	740	<i>J. Mater. Chem. B</i> , 2013 , 1 , 2742-2749
3.	$[\{(\text{H}_3\text{O})[\text{Eu}(\text{SBDB})(\text{H}_2\text{O})_2]\}_n]$	FS	5.0	<i>CrystEngComm</i> , 2018, 20 , 6989-6994
4.	ZJU-136- $\text{Ce}_{1-x}\text{Eu}_x$ ($x = 0.24, 0.36$)	FS	12.6	<i>J. Mater. Chem. C</i> , 2018, 6 , 2054–2059.
5.	$[\text{Tb}(\text{Cm}(\text{dcp})(\text{H}_2\text{O})_3)_2(\text{NO}_3)_2 \cdot 5\text{H}_2\text{O}]$	FS	5.9	<i>Dalton Trans.</i> , 2019, 48 , 8911-8919
6.	ZJU-137	FS	0.034	<i>Eur. J. Inorg. Chem.</i> , 2018, 173 —177
7.	ZJU-136-Ce	FS	0.007	<i>Chem. Commun.</i> 2017, 53 , 11221-11224
8.	MOF-5/3D-KSC	ECS	0.24	<i>Anal. Methods</i> , 2016, 8 , 2290-2296
9.	GO@HKUST-1	CL	0.35	<i>RSC Adv.</i> , 2016, 6 , 25047-25055
10.	CSMCRI-14	FS	.073 μM / 41.1 ppb	Present work

ECS: Electrochemical sensors; CL: Chemiluminescence; FS: Fluorescent sensors.

Table S8. A comparison of quenching constant, their LOD values, of various luminescent MOFs used for detection of H₂O₂

Sl.no.	Material	Analytical method	Limit of detection (μM)	Reference
1.	FePt-Au HNPs	FS	12.33	<i>Sens. Actuators, B</i> , 2018, 259 , 775-783
2.	PBA-In1	FS	0.42	<i>Dalton Trans.</i> , 2021, 50 , 7554-7562
3.	Au NPs-NH ₂ /Cu-MOF/GCE	FS	1.20	<i>J. Electro anal. Chem.</i> , 2020, 856, 113592
4.	CoFe-PBA/Co-ZIF/NF	FS	0.00108	<i>ACS Appl. Mater. Interfaces</i> , 2020, 12 , 35365–35374
5.	Pt@UiO-66/GC	FS	3.06	<i>J. Am. Chem. Soc.</i> 2010, 132 , 1490–1491
6.	AP-Ni-MOF	electrochemistry	0.9	<i>Sens. Actuators, B</i> , 2018, 254 , 1148–1156
7.	Co/DOBDC	electrochemistry	0.5	<i>Sens. Actuators, B</i> , 2015, 221 , 224–229
8.	Cu-MOF	electrochemistry	1.0	<i>Talanta</i> , 2015, 144 , 1176–1181
9.	Co-MOF	electrochemistry	3.76	<i>Sens. Actuators, B</i> , 2015, 215 , 489–496
10.	CSMCRI-14	FS	0.087 μM/49.2 ppb	Present work

FS: Fluorescent sensors.

Table S9. A comparison of reaction condition, conversion and selectivity of materials used for alkene epoxidation

Sl.No.	Catalyst	Reaction Condition	Conversion (Selectivity%)	References
1	Fe(III) and Mn(III) porphyrins supported carbon (NT)	Catalyst : substrate : isobutyraldehyde was 1:45:135 and O ₂ (balloon), 1 mL CH ₃ CN, temperature: 40–45°C in water bath	98 (100)	<i>Appl. Organomet. Chem.</i> , 2019, 33 , e4789
2	Zn-Mo-ICP	Catalyst (50 mg), olefin (4 mmol), TBHP (7.2 mmol), chloroform (5 ml) Time: 22 h.	87 (99)	<i>Appl Organometal Chem.</i> , 2019, 33 , e5052
3	MNP@PMA-SB-Mo nanocatalyst	0.004 g catalyst: 1 mmol alkene: 1 mmol TBHP. The reactions were run under reflux in 1 ml dichloroethane, Time: 1 h.	98 (100)	<i>Appl Organometal Chem.</i> , 2019, 34 , e5410
4	2D Cu-MOF	1 mmol of olefin, 3 mmol of isobutyraldehyde and 5 mL of CH ₃ CN were mixed with 10 mol% catalyst in a	92(99)	<i>Chem.–Eur. J.</i> , 2020, 26 , 4333-4340

		25 mL three-necked round-bottomed flask along with a condensation tube. The mixture was stirred with air bubbling at 80°C for 24 h.		
5	Co(II)-complex supported on graphene oxide	Alkene (10 mmol), catalyst (50 mg, 0.2 mol%), 60 °C, CH ₃ CN (10 mL), O ₂ (~1 atm. bubbling 15 mL/min), Time: 1 h.	99(99)	<i>Journal of Organometallic Chemistry</i> , 896 , 2019, 59-69
6	Mn-MOF	Cyclohexene (0.2 mmol), CPF-5 (5 mg, 0.004 mmol based on Mn ₅ SBU), TBHP (0.25 equiv.), mesitylene (3 µL), CH ₃ CN (1 mL), O ₂ (1 bar), 24 h. 1.2 equiv. of TBHP. Temperature: 60 °C.	62(76)	<i>Green Chem.</i> , 2019, 21 , 3629-3636
7	Fe ₃ O ₄ @SiO ₂ -[MnL(OAc)]	Catalyst: (0.0017 mmol), molar ratio of cat : imidazole : cyclooctene : H ₂ O ₂ is 1 : 100 : 150 : 750, EtOH (1 mL), room temperature, potential: 60 V, and time: 90 min	97 (100)	<i>RSC Adv.</i> , 2020, 10 , 17026-17036
8	MoO ₂ L ₁ -GO	Alkene (5 mmol), TBHP (10 mmol), catalyst (20 mg), 1,2-DCE (5 mL), Time 1 h.	98 (100)	<i>Journal of Coordination Chemistry</i> , 2019, 72 , 3401-3416
9	CoPMA@UiO-bpy	catalyst (10 mg), cyclooctene (1 mmol), H ₂ O ₂ (2 mmol), CH ₃ CN (1 ml), temperature (70 °C). Time: 6 h.	91 (99)	<i>ACS Sustainable Chem. Eng.</i> , 2019, 7 , 3624–3631
10	SBA-15-NH ₃	Catalyst (9 ×10 mmol), alkene (0.2 mmol), TBHP (0.4 mmol) in water Time: 1.5 h.	>99 (98)	<i>ChemistrySelect</i> , 2019, 4 , 5911 – 5917
11	CSMCRI-14	Alkene (1 mmol), catalyst amount (1.8 mol %), acetonitrile (2 mL), temperature (70 °C), time (9 h).	100	Present work

Cartesian coordinates of optimized structures

1. 14a

Cd	6.582367861	6.334551668	9.632682647
O	5.380257800	4.599331467	8.203644217
O	7.615492880	4.757427096	8.267202598
O	7.360209099	7.874420665	11.189094123
O	8.966111186	6.595474832	10.292100847
N	6.277642411	7.683009949	7.725931227
N	5.012116922	8.848280325	2.942137945
N	5.206266391	9.393382518	1.709669184
N	7.052866615	9.698082741	2.886268078
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H	8.421481657	8.638188128	5.311737896
N	6.039754826	4.919172084	11.425131496
C	6.535748254	4.161326413	7.908405287
C	8.575272672	7.473157458	11.139375067
C	9.547484316	8.001805998	12.144776387
C	7.414335109	8.011092946	7.080608636
H	8.339077486	7.898876792	7.649814940
C	6.128224151	9.012102349	3.657938579
C	6.696664371	2.868148369	7.172614517
C	6.431737040	9.921741026	1.678915129
C	6.240506360	8.575348315	5.050072143
N	8.406297320	10.002642758	3.122049168
C	6.932044451	10.697592278	0.543321641
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C	7.944978694	2.524458529	6.658765512
H	8.760948925	3.244535412	6.730524974
C	5.050280333	8.249047427	5.735118722
H	4.084659872	8.344717900	5.240491001
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H	8.320824684	13.026959047	12.229093755
C	7.286058564	6.259998874	0.946968615
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C	5.115942119	7.803166739	7.047035459
H	4.210311258	7.520804316	7.584206289
C	5.619683886	1.971300465	7.075995527
C	5.103091745	3.955272199	11.303140411
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H	7.423563504	5.829781529	12.680409515
C	3.577613598	1.030270004	0.648910564
H	4.129636398	1.159953183	1.575376476
H	8.518983541	10.351794451	4.075681162
H	8.919645202	9.111653010	3.046701732
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O	9.171561175	7.231783901	2.790417939
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C	10.630899616	5.980465618	6.099554276
H	9.702820397	6.259583747	5.598263176
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C	11.446716122	11.014776476	5.930919540
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H	10.590509550	8.096560603	0.473099882
C	14.465969665	12.849950872	12.476920183
H	13.913876115	12.724315655	11.549429136
H	9.566583462	3.518004162	8.997098840
H	9.153610220	4.706564526	10.067339960
H	14.560387233	12.203353026	5.767154196
H	13.922816346	10.661444607	5.225113974
H	4.655213201	2.247379260	7.495532097
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C	12.313207361	13.161548982	6.658765512
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H	11.792095686	16.467086942	12.680409515
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H	8.497953340	11.797258596	1.575376476
H	12.887244992	20.989037054	4.075424878
H	13.287942800	19.749173383	3.046701732
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C	14.999304833	16.617985991	6.099554276
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C	16.318940353	15.438577166	9.440726086
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C	15.724599640	19.506370949	0.535120560
H	14.958934111	18.733866016	0.473099882
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H	18.282248547	23.361683879	11.549685420
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H	18.928900071	22.840873400	5.767154196
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O	11.787311775	9.782569685	23.351554092
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O	16.286811571	21.032176899	15.862429090
N	17.412678425	18.001870834	13.092513854
N	18.970237899	19.923680623	18.402714047
N	20.254317421	18.825550393	23.188557599
N	20.039984530	18.325885562	24.441529064
N	18.222445341	17.954314768	23.244683750
C	17.820923762	19.345250366	20.441195337
H	16.867032275	19.306098824	20.961195154
N	19.194426065	22.795218627	14.755283104
C	18.745805813	23.520543672	18.294562286
C	16.689840175	20.116028499	15.062567372
C	15.762213925	19.544936440	14.062035443
C	17.838280129	19.781901808	19.120564952
H	16.911362930	20.058599586	18.614660744
C	19.153591049	18.618204585	22.465324735
C	18.627566572	24.821658852	18.993448190
C	18.822250536	17.776352108	24.469207714
C	19.037428982	19.014361960	21.061914684
N	16.876595519	17.634663060	22.989425092
C	18.313519706	17.016939655	25.612233431
C	16.161889123	18.544209567	13.119679936
C	17.380275607	25.191207900	19.530362737
H	16.572951412	24.463139650	19.474236586

C	20.217971564	19.114981936	20.297163846
H	21.185962285	18.841516349	20.719775821
C	20.494894315	24.589023099	13.821897529
H	16.927517008	14.675592079	13.953883683
C	18.026863674	21.323308246	25.207305038
H	18.293290086	20.568327728	24.471257984
C	20.136389010	19.580516072	18.990885352
H	21.037073426	19.693029888	18.386055601
C	19.719521746	25.732444445	19.072383598
N	20.945812419	25.448728884	18.519066889
C	20.138267079	23.752551107	14.872404797
H	20.636961184	23.817028398	15.836288143
C	18.549724391	22.683675551	13.573045966
H	17.789773798	21.905830164	13.505899612
C	21.658075314	26.693785721	25.513051603
H	21.106044068	26.565392303	24.586585691
H	16.777377763	17.312842129	22.024516611
H	16.351495453	18.517900197	23.073486176
H	21.732247420	26.027710373	18.790471426
H	21.110449503	24.465223911	18.298662827
H	11.842248213	16.061884335	20.559342166
H	15.360739049	23.267718179	26.066368312

2. 14a@ClO⁻

Cd1	6.934356879	6.824397029	10.358453960	XXXX 1	xx	Cd	0.000
O2	5.656687473	4.954046573	8.821725725	XXXX 1	xx	O	0.000
O3	7.947947548	5.124545172	8.890042207	XXXX 1	xx	O	0.000
O4	7.774106986	8.483978182	12.031815161	XXXX 1	xx	O	0.000
O5	9.383260419	7.105263225	11.067531935	XXXX 1	xx	O	0.000
N6	6.642216415	8.280155264	8.307912486	XXXX 1	xx	N	0.000
N7	5.346421824	9.540863240	3.163759868	XXXX 1	xx	N	0.000
N8	5.550377794	10.129602051	1.838524805	XXXX 1	xx	N	0.000
N9	7.453585283	10.457471361	3.103819353	XXXX 1	xx	N	0.000
C10	7.846646870	9.103195798	6.191933767	XXXX 1	xx	C	0.000
H11	8.843844040	9.312245485	5.711886146	XXXX 1	xx	H	0.000
N12	6.357208759	5.296490851	12.285711668	XXXX 1	xx	N	0.000
C13	6.827530900	4.482012194	8.504224217	XXXX 1	xx	C	0.000
C14	9.008087633	8.051321611	11.978418370	XXXX 1	xx	C	0.000
C15	10.020616765	8.620692059	13.059441640	XXXX 1	xx	C	0.000
C16	7.809183599	8.634615391	7.614015951	XXXX 1	xx	C	0.000
H17	8.756095810	8.513161781	8.226246805	XXXX 1	xx	H	0.000
C18	6.496298174	9.716972004	3.933563605	XXXX 1	xx	C	0.000
C19	6.958612924	3.087657089	7.712957064	XXXX 1	xx	C	0.000
C20	6.816159289	10.699518666	1.805282685	XXXX 1	xx	C	0.000
C21	6.609121684	9.244705734	5.430505997	XXXX 1	xx	C	0.000
N22	8.846710063	10.785619964	3.357192361	XXXX 1	xx	N	0.000
C23	7.339384200	11.537433467	0.584223714	XXXX 1	xx	C	0.000
C24	9.640867583	9.672111735	14.067698694	XXXX 1	xx	C	0.000
C25	8.225311622	2.717457366	7.160404977	XXXX 1	xx	C	0.000

H26	9.077014069	3.494024062	7.237620924	XXXX 1	xx	H	0.000
C27	5.387672190	8.892173245	6.167067614	XXXX 1	xx	C	0.000
H28	4.398932797	8.995888904	5.635193696	XXXX 1	xx	H	0.000
C29	4.999037117	3.357112605	13.286116253	XXXX 1	xx	C	0.000
H30	8.879960429	14.040503079	13.150268534	XXXX 1	xx	H	0.000
C31	7.603090855	6.750864285	1.018203515	XXXX 1	xx	C	0.000
H32	7.347832534	7.570655417	1.803450442	XXXX 1	xx	H	0.000
C33	5.452363009	8.410410290	7.577894593	XXXX 1	xx	C	0.000
H34	4.522202848	8.105411406	8.155574582	XXXX 1	xx	H	0.000
C35	5.835609715	2.120466988	7.609042721	XXXX 1	xx	C	0.000
C36	5.376124326	4.257004712	12.154575431	XXXX 1	xx	C	0.000
H37	4.871161508	4.185254737	11.110720516	XXXX 1	xx	H	0.000
C38	7.019261510	5.426050119	13.559643932	XXXX 1	xx	C	0.000
H39	7.801037839	6.277633870	13.635551135	XXXX 1	xx	H	0.000
C40	3.688008981	1.110614183	0.697822769	XXXX 1	xx	C	0.000
H41	4.261078949	1.249817251	1.694039370	XXXX 1	xx	H	0.000
H42	8.975496976	11.161574913	4.382724847	XXXX 1	xx	H	0.000
H43	9.351481577	9.824785794	3.276311928	XXXX 1	xx	H	0.000
H44	10.697580931	3.567951354	-0.525591943	XXXX 1	xx	H	0.000
H45	11.222104381	4.791685200	0.852254665	XXXX 1	xx	H	0.000
Cd46	11.940917197	8.127828738	3.766567759	XXXX 1	xx	Cd	0.000
O47	13.232947862	9.964274260	5.245187722	XXXX 1	xx	O	0.000
O48	10.949410935	9.811339988	5.304604740	XXXX 1	xx	O	0.000
O49	11.166335321	6.339166391	2.170684255	XXXX 1	xx	O	0.000
O50	9.565157491	7.797505298	3.000690256	XXXX 1	xx	O	0.000
N51	10.538388038	4.456174484	0.084544919	XXXX 1	xx	N	0.000
N52	12.204268368	6.595436391	5.782820118	XXXX 1	xx	N	0.000
N53	13.530086243	5.384845008	10.927496233	XXXX 1	xx	N	0.000
N54	13.310018700	4.834776077	12.271315474	XXXX 1	xx	N	0.000
N55	11.429751072	4.450271003	10.989530741	XXXX 1	xx	N	0.000
C56	11.030983081	5.971668692	7.979155772	XXXX 1	xx	C	0.000
H57	10.058750841	5.930120948	8.541392572	XXXX 1	xx	H	0.000
N58	12.496418172	9.686093860	1.844283282	XXXX 1	xx	N	0.000
C59	12.077301913	10.472710987	5.621321000	XXXX 1	xx	C	0.000
C60	9.923439922	6.790291335	2.144771106	XXXX 1	xx	C	0.000
C61	8.932622678	6.186301326	1.081023269	XXXX 1	xx	C	0.000
C62	11.048821163	6.445263615	6.559167580	XXXX 1	xx	C	0.000
H63	10.102667974	6.746662420	6.019964690	XXXX 1	xx	H	0.000
C64	12.391580178	5.170840599	10.151934019	XXXX 1	xx	C	0.000
C65	11.997080361	11.875354850	6.377775539	XXXX 1	xx	C	0.000
C66	12.050137440	4.245092295	12.302201853	XXXX 1	xx	C	0.000
C67	12.271753169	5.609806546	8.644783417	XXXX 1	xx	C	0.000
N68	10.041695064	4.112849214	10.718620551	XXXX 1	xx	N	0.000
C69	11.520549696	3.416387179	13.527972306	XXXX 1	xx	C	0.000
C70	9.288910914	5.078471330	0.087162409	XXXX 1	xx	C	0.000
C71	10.729783750	12.274229716	6.949697051	XXXX 1	xx	C	0.000
H72	9.884869299	11.491671003	6.875098593	XXXX 1	xx	H	0.000
C73	13.476353288	5.722525154	7.820012395	XXXX 1	xx	C	0.000
H74	14.463836975	5.427547184	8.272314625	XXXX 1	xx	H	0.000
C75	13.867411952	11.612807842	0.831838244	XXXX 1	xx	C	0.000
H76	9.994067559	0.919698919	0.970565202	XXXX 1	xx	H	0.000

C77	11.330349447	8.066604691	13.080905056	XXXX 1	xx	C	0.000
H78	11.599972781	7.273018007	12.274979960	XXXX 1	xx	H	0.000
C79	13.393429467	6.225664111	6.415205643	XXXX 1	xx	C	0.000
H80	14.312628957	6.348027935	5.763188945	XXXX 1	xx	H	0.000
C81	13.137714888	12.853897007	6.480642887	XXXX 1	xx	C	0.000
N82	14.385298340	12.548153718	5.894325182	XXXX 1	xx	N	0.000
C83	13.488505219	10.714830714	1.964426062	XXXX 1	xx	C	0.000
H84	14.004741993	10.785021402	3.000952005	XXXX 1	xx	H	0.000
C85	11.824821962	9.565097693	0.575324248	XXXX 1	xx	C	0.000
H86	11.023338207	8.731933312	0.508840009	XXXX 1	xx	H	0.000
C87	15.165497289	13.849469684	13.416728991	XXXX 1	xx	C	0.000
H88	14.592453403	13.714684093	12.419203645	XXXX 1	xx	H	0.000
H89	9.920453573	3.787194435	9.675027385	XXXX 1	xx	H	0.000
H90	9.530962836	5.068252814	10.825675882	XXXX 1	xx	H	0.000
H91	15.209168668	13.157227025	6.201618479	XXXX 1	xx	H	0.000
H92	14.518622113	11.494578815	5.618703510	XXXX 1	xx	H	0.000
H93	4.857432052	2.417984582	8.060297955	XXXX 1	xx	H	0.000
H94	8.610222816	10.094496088	14.047282274	XXXX 1	xx	H	0.000
Cd95	11.645724064	18.297065413	10.358453960	XXXX 1	xx	Cd	0.000
O96	10.368163748	16.426714956	8.821725725	XXXX 1	xx	O	0.000
O97	12.659412023	16.597450468	8.890042207	XXXX 1	xx	O	0.000
O98	12.485571462	19.956883478	12.031815161	XXXX 1	xx	O	0.000
O99	14.094627605	18.577931608	11.067531935	XXXX 1	xx	O	0.000
N100	11.353680891	19.753060560	8.307912486	XXXX 1	xx	N	0.000
N101	10.057789010	21.013531624	3.163759868	XXXX 1	xx	N	0.000
N102	10.261842270	21.602507346	1.838524805	XXXX 1	xx	N	0.000
N103	12.164952469	21.930139745	3.103819353	XXXX 1	xx	N	0.000
C104	12.557957382	20.575800032	6.191672018	XXXX 1	xx	C	0.000
H105	13.555417606	20.785150780	5.711886146	XXXX 1	xx	H	0.000
N106	11.068685034	16.769159235	12.285711668	XXXX 1	xx	N	0.000
C107	11.538966560	15.954507816	8.504485966	XXXX 1	xx	C	0.000
C108	13.719357529	19.523753084	11.978418370	XXXX 1	xx	C	0.000
C109	14.731886661	20.093123531	13.059441640	XXXX 1	xx	C	0.000
C110	12.520659875	20.107283775	7.614015951	XXXX 1	xx	C	0.000
H111	13.467669376	19.986067076	8.226246805	XXXX 1	xx	H	0.000
C112	11.207665359	21.189640388	3.933563605	XXXX 1	xx	C	0.000
C113	11.670077400	14.560562384	7.712957064	XXXX 1	xx	C	0.000
C114	11.527623765	22.172423961	1.805282685	XXXX 1	xx	C	0.000
C115	11.320586160	20.717611029	5.430505997	XXXX 1	xx	C	0.000
N116	13.558065448	22.258525259	3.357192361	XXXX 1	xx	N	0.000
C117	12.050848676	23.010338762	0.584223714	XXXX 1	xx	C	0.000
C118	14.352332058	21.145017030	14.067698694	XXXX 1	xx	C	0.000
C119	12.936678808	14.190125750	7.160404977	XXXX 1	xx	C	0.000
H120	13.788433671	14.966628296	7.237359175	XXXX 1	xx	H	0.000
C121	10.099245756	20.365078540	6.167067614	XXXX 1	xx	C	0.000
H122	9.110299982	20.468557288	5.635193696	XXXX 1	xx	H	0.000
C123	9.710404303	14.829780989	13.286116253	XXXX 1	xx	C	0.000
H124	13.591327615	25.513171463	13.150268534	XXXX 1	xx	H	0.000
C125	12.314458041	18.223532669	1.018203515	XXXX 1	xx	C	0.000
H126	12.059199720	19.043323801	1.803450442	XXXX 1	xx	H	0.000
C127	10.163827485	19.883315585	7.577894593	XXXX 1	xx	C	0.000

H128	9.233776414	19.578316701	8.155574582	XXXX 1	xx	H	0.000
C129	10.546965100	13.593372283	7.609042721	XXXX 1	xx	C	0.000
C130	10.087697891	15.729910007	12.154575431	XXXX 1	xx	C	0.000
H131	9.582735073	15.658160032	11.110720516	XXXX 1	xx	H	0.000
C132	11.730737786	16.898718503	13.559643932	XXXX 1	xx	C	0.000
H133	12.512720495	17.750539165	13.635551135	XXXX 1	xx	H	0.000
C134	8.399473457	12.583519479	0.697822769	XXXX 1	xx	C	0.000
H135	8.972543425	12.722722546	1.694039370	XXXX 1	xx	H	0.000
H136	13.686807488	22.634179147	4.382463098	XXXX 1	xx	H	0.000
H137	14.062934253	21.297928000	3.276311928	XXXX 1	xx	H	0.000
H138	15.408948117	15.040619738	-0.525591943	XXXX 1	xx	H	0.000
H139	15.933471567	16.264353584	0.852254665	XXXX 1	xx	H	0.000
Cd140	16.652163493	19.600734033	3.766567759	XXXX 1	xx	Cd	0.000
O141	17.944371721	21.437006794	5.245449471	XXXX 1	xx	O	0.000
O142	15.660960901	21.284719106	5.304604740	XXXX 1	xx	O	0.000
O143	15.877702507	17.811834775	2.170684255	XXXX 1	xx	O	0.000
O144	14.276621967	19.270410594	3.000690256	XXXX 1	xx	O	0.000
N145	15.249852514	15.929079779	0.084544919	XXXX 1	xx	N	0.000
N146	16.915732844	18.068341687	5.782820118	XXXX 1	xx	N	0.000
N147	18.241562519	16.857513392	10.927496233	XXXX 1	xx	N	0.000
N148	18.021592266	16.307681373	12.271315474	XXXX 1	xx	N	0.000
N149	16.141227347	15.922939387	10.989530741	XXXX 1	xx	N	0.000
C150	15.742544847	17.444810899	7.979155772	XXXX 1	xx	C	0.000
H151	14.770118027	17.402789332	8.541392572	XXXX 1	xx	H	0.000
N152	17.207882648	21.158999155	1.844283282	XXXX 1	xx	N	0.000
C153	16.788863679	21.945853193	5.621321000	XXXX 1	xx	C	0.000
C154	14.634807107	18.262959718	2.144771106	XXXX 1	xx	C	0.000
C155	13.644196243	17.659206621	1.081023269	XXXX 1	xx	C	0.000
C156	15.760382929	17.918405821	6.559167580	XXXX 1	xx	C	0.000
H157	14.814132450	18.219567716	6.019964690	XXXX 1	xx	H	0.000
C158	17.103044653	16.643745894	10.151934019	XXXX 1	xx	C	0.000
C159	16.708613311	23.348087384	6.378037288	XXXX 1	xx	C	0.000
C160	16.761654332	15.717933440	12.301940104	XXXX 1	xx	C	0.000
C161	16.983229444	17.082474930	8.644783417	XXXX 1	xx	C	0.000
N162	14.753005576	15.585453448	10.718358802	XXXX 1	xx	N	0.000
C163	16.231916882	14.889055562	13.527972306	XXXX 1	xx	C	0.000
C164	14.000375390	16.551376626	0.087162409	XXXX 1	xx	C	0.000
C165	15.441316700	23.746962250	6.949958800	XXXX 1	xx	C	0.000
H166	14.596649245	22.964813209	6.875098593	XXXX 1	xx	H	0.000
C167	18.187720473	17.195193538	7.820012395	XXXX 1	xx	C	0.000
H168	19.175353867	16.900388330	8.272052876	XXXX 1	xx	H	0.000
C169	18.578681848	23.085239315	0.831838244	XXXX 1	xx	C	0.000
H170	14.705641125	12.392604214	0.970565202	XXXX 1	xx	H	0.000
C171	16.041813923	19.539509986	13.080905056	XXXX 1	xx	C	0.000
H172	16.311437257	18.745923303	12.274979960	XXXX 1	xx	H	0.000
C173	18.104882143	17.698806317	6.415205643	XXXX 1	xx	C	0.000
H174	19.023927669	17.820869080	5.762927196	XXXX 1	xx	H	0.000
C175	17.849247837	24.326629541	6.480904636	XXXX 1	xx	C	0.000
N176	19.096774616	24.020822102	5.894325182	XXXX 1	xx	N	0.000
C177	18.199969695	22.187736010	1.964426062	XXXX 1	xx	C	0.000
H178	18.716194669	22.258163609	3.000952005	XXXX 1	xx	H	0.000

C179	16.536189147	21.037766077	0.575324248	XXXX 1	xx	C	0.000
H180	15.734911773	20.204838607	0.508840009	XXXX 1	xx	H	0.000
C181	19.876767184	25.321901156	13.416728991	XXXX 1	xx	C	0.000
H182	19.303779973	25.187179716	12.419465394	XXXX 1	xx	H	0.000
H183	14.632015339	15.260336642	9.675027385	XXXX 1	xx	H	0.000
H184	14.242427312	16.541158109	10.825675882	XXXX 1	xx	H	0.000
H185	19.920742234	24.630132320	6.201618479	XXXX 1	xx	H	0.000
H186	19.230155063	22.967311349	5.618965259	XXXX 1	xx	H	0.000
H187	9.568690148	13.890652966	8.060297955	XXXX 1	xx	H	0.000
H188	13.321590002	21.567164472	14.047282274	XXXX 1	xx	H	0.000
Cd189	9.985413497	10.253044002	24.371447118	XXXX 1	xx	Cd	0.000
O190	8.684686325	8.384476438	22.812993717	XXXX 1	xx	O	0.000
O191	10.978076348	8.558420097	22.881833698	XXXX 1	xx	O	0.000
O192	10.825119636	11.971276938	26.017324677	XXXX 1	xx	O	0.000
O193	12.417053130	10.532521725	25.110626225	XXXX 1	xx	O	0.000
N194	9.675537474	11.700692622	22.327449368	XXXX 1	xx	N	0.000
N195	8.371501652	12.994222014	17.196384199	XXXX 1	xx	N	0.000
N196	8.575826650	13.589762019	15.873766625	XXXX 1	xx	N	0.000
N197	10.485246375	13.892721346	17.134087943	XXXX 1	xx	N	0.000
C198	10.878412417	12.526704392	20.211994147	XXXX 1	xx	C	0.000
H199	11.874743437	12.734767056	19.729852534	XXXX 1	xx	H	0.000
N200	9.393359651	8.725088927	26.289805360	XXXX 1	xx	N	0.000
C201	9.855689394	7.910333982	22.506223918	XXXX 1	xx	C	0.000
C202	12.049061578	11.511349492	25.990888030	XXXX 1	xx	C	0.000
C203	13.065439186	12.085399101	27.068770312	XXXX 1	xx	C	0.000
C204	10.841675839	12.054831999	21.632244089	XXXX 1	xx	C	0.000
H205	11.789364834	11.931270960	22.242642700	XXXX 1	xx	H	0.000
C206	9.525098917	13.155454909	17.962523451	XXXX 1	xx	C	0.000
C207	9.984666937	6.506363306	21.732755695	XXXX 1	xx	C	0.000
C208	9.845975676	14.147660305	15.840786254	XXXX 1	xx	C	0.000
C209	9.639544300	12.672794397	19.454754360	XXXX 1	xx	C	0.000
N210	11.882375413	14.206581598	17.380393729	XXXX 1	xx	N	0.000
C211	10.372444484	14.985032049	14.622344773	XXXX 1	xx	C	0.000
C212	12.705334714	13.158921414	28.061845925	XXXX 1	xx	C	0.000
C213	11.247665036	6.136953720	21.171827640	XXXX 1	xx	C	0.000
H214	12.096690835	6.918619418	21.239882374	XXXX 1	xx	H	0.000
C215	8.418972179	12.317764495	20.190792480	XXXX 1	xx	C	0.000
H216	7.430222916	12.423094072	19.659703808	XXXX 1	xx	H	0.000
C217	8.036211803	6.783879541	27.290471694	XXXX 1	xx	C	0.000
H218	11.918405892	17.465981931	27.152268235	XXXX 1	xx	H	0.000
C219	10.605285228	10.139945119	15.068888525	XXXX 1	xx	C	0.000
H220	10.346085267	10.948541703	15.863558415	XXXX 1	xx	H	0.000
C221	8.484709813	11.830449052	21.599263718	XXXX 1	xx	C	0.000
H222	7.555590857	11.521639898	22.175896711	XXXX 1	xx	H	0.000
C223	8.863202340	5.534354927	21.649781270	XXXX 1	xx	C	0.000
C224	8.411601336	7.686204911	26.159192622	XXXX 1	xx	C	0.000
H225	7.904608355	7.616004703	25.115861205	XXXX 1	xx	H	0.000
C226	10.058757256	8.851356209	27.561905382	XXXX 1	xx	C	0.000
H227	10.845013241	9.699327225	27.634671597	XXXX 1	xx	H	0.000
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O238	12.522261686	11.198421530	17.057133744	XXXX 1	xx	O	0.000
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C248	12.909459610	10.211266276	16.197026610	XXXX 1	xx	C	0.000
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C267	16.446400856	9.630610431	20.421393327	XXXX 1	xx	C	0.000
H268	17.367187577	9.752411509	19.770947123	XXXX 1	xx	H	0.000
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H276	17.629019955	17.159860230	26.438740527	XXXX 1	xx	H	0.000
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C307	15.959129512	17.609859015	21.171827640	XXXX 1	xx	C	0.000
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C309	13.130339365	23.790432879	20.190792480	XXXX 1	xx	C	0.000
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C311	12.747676279	18.256784836	27.290471694	XXXX 1	xx	C	0.000
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C313	15.316652413	21.612613502	15.068888525	XXXX 1	xx	C	0.000
H314	15.057549743	22.421446999	15.863558415	XXXX 1	xx	H	0.000
C315	13.196174289	23.303354347	21.599263718	XXXX 1	xx	C	0.000
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H321	15.556489517	21.171995609	27.634671597	XXXX 1	xx	H	0.000
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Cd328	19.670441958	23.020767711	17.790816123	XXXX 1	xx	Cd	0.000
O329	20.979063875	24.819964066	19.361048227	XXXX 1	xx	O	0.000
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O331	18.872072686	21.255918416	16.223463257	XXXX 1	xx	O	0.000

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H371	17.686464150	18.655199301	23.683570810	XXXX 1	xx	H	0.000
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O	20.983595429	24.834386725	19.366493146
O	18.697914997	24.735544050	19.300777453
O	18.875746608	21.268290304	16.228110648
O	17.238292288	22.684791611	17.061993042
N	18.304277021	19.416824259	14.082794374
N	19.972524093	21.486157463	19.794561502
N	21.288197459	20.296742617	24.942378025
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C	17.624791171	21.696593309	16.201667282
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C	18.815294336	21.332582628	20.566655436
H	17.870462940	21.631594052	20.022340994
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C	19.738317381	26.771752133	20.429725925
C	19.806354175	19.163310781	26.319789414
C	20.035447192	20.502263382	22.654634114
N	17.804038105	19.011734988	24.728212939
C	19.274895748	18.342589967	27.549275041
C	17.037220826	20.001919945	14.111855895
C	18.473920945	27.170048226	21.007290936
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H	17.736071064	15.826156093	15.009359457
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H	22.081503649	21.237312270	19.776496232
C	20.876945971	27.754630523	20.514815965
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H	21.752781147	25.690356430	17.033978783
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H	18.782463050	23.629673009	14.527357107
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H	17.689559031	18.665160184	23.690376265
H	17.287730923	19.964840718	24.818539290
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H	22.266168985	26.387587412	19.682504464
H	12.603615109	17.316380710	22.114246905
H	16.401061904	25.088391412	28.037822779
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Cl	14.449991960	15.931249583	17.556562537
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C	12.127791707	19.011506271	18.305354891
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O	13.178555128	20.028065990	16.487831633
O	14.663475024	21.062707421	18.664565768

C	15.968074663	19.118840697	17.839846917
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H	16.089450742	19.522812394	16.820337328
H	15.881609951	18.023320909	17.749782382
O	17.103160319	19.461072008	18.664565768
H	15.080468955	21.484900568	17.893519096
H	17.890169355	19.361667553	18.103233318
H	12.740203962	18.069775127	19.902953122
H	9.402164036	20.081337293	16.975070293

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