"Supporting Information"

Design and synthesis of hydrophobic mixed organogel with complementary hydrogen-bond donor-acceptor sites: removal of heavy metal ions Hg^{+2}, Cd^{+2} and Pb^{+2} from aqueous solution

Reena Kyarikwal,[a] Ritika Munjal,[a] Probal Nag,[b] Sivaranjana Reddy Vennapusa[b] and Suman Mukhopadhyay[a]*

[a]Department of Chemistry, School of basic science, Indian Institute of Technology Indore, Khandwa Road, Simrol, Indore, 453552, India

[b]School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, Thiruvananthapuram 695551, India

*Email: suman@iiti.ac.in

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Table S11. Cartesian coordinates of **GE**.
Table S12. Cartesian coordinates of **G8**.
Table S13. Cartesian coordinates of **2GE-2G8** (**G8GE**).

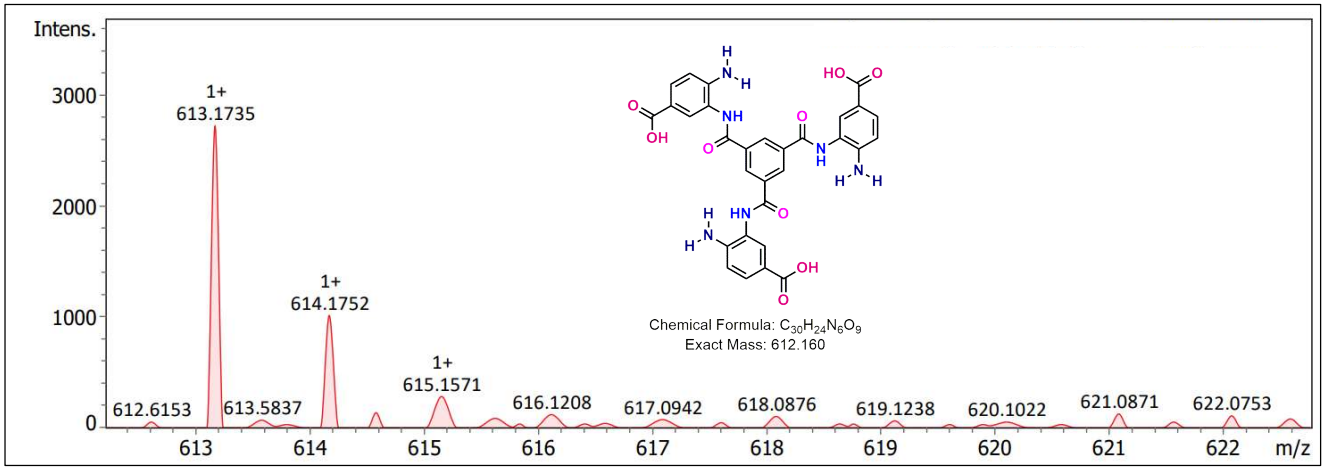


Fig. S1: ESI-MS data of gelator component **GE**.

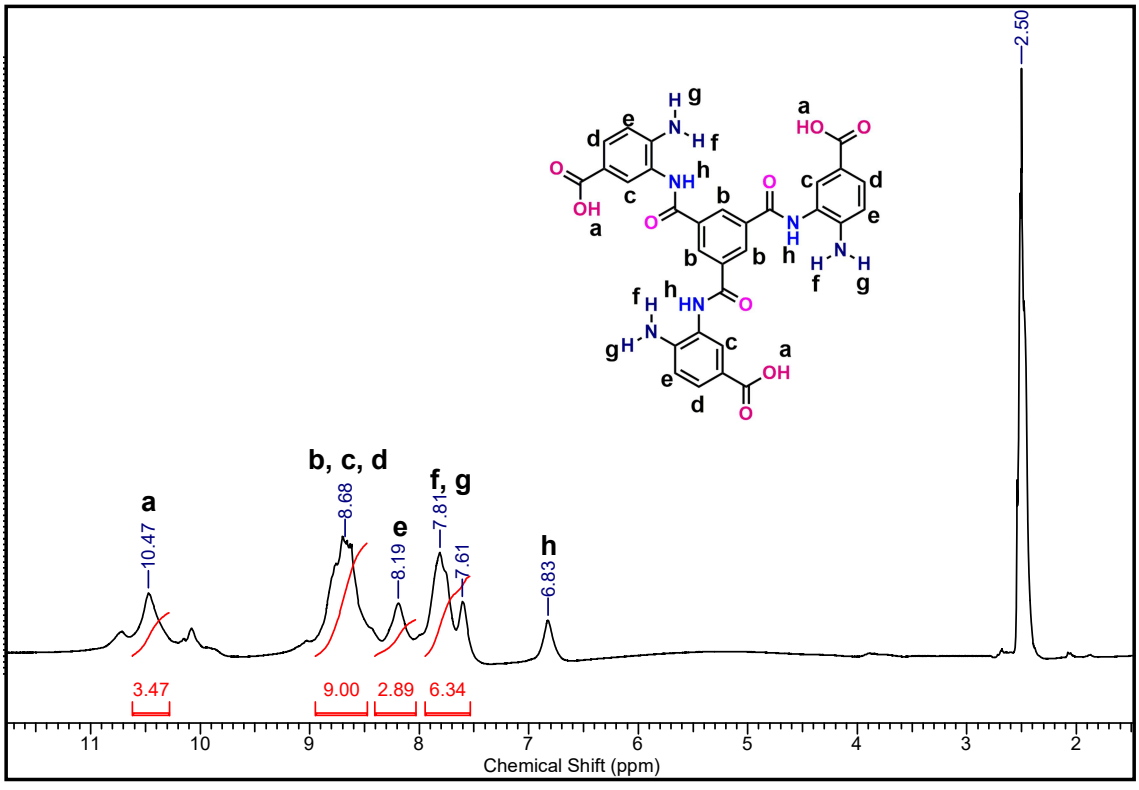


Fig. S2: ^{1}H NMR data of gelator component **GE**.

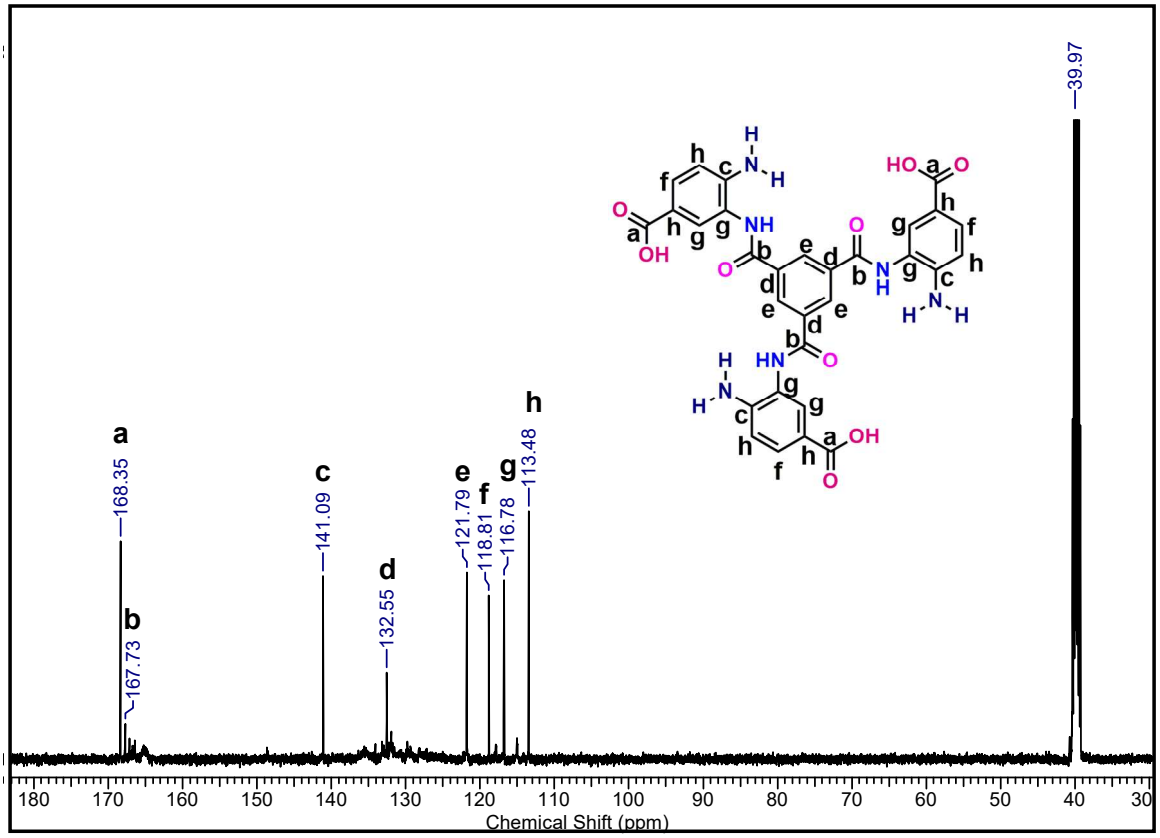


Fig. S3: ^{13}C NMR data of gelator component **GE**.

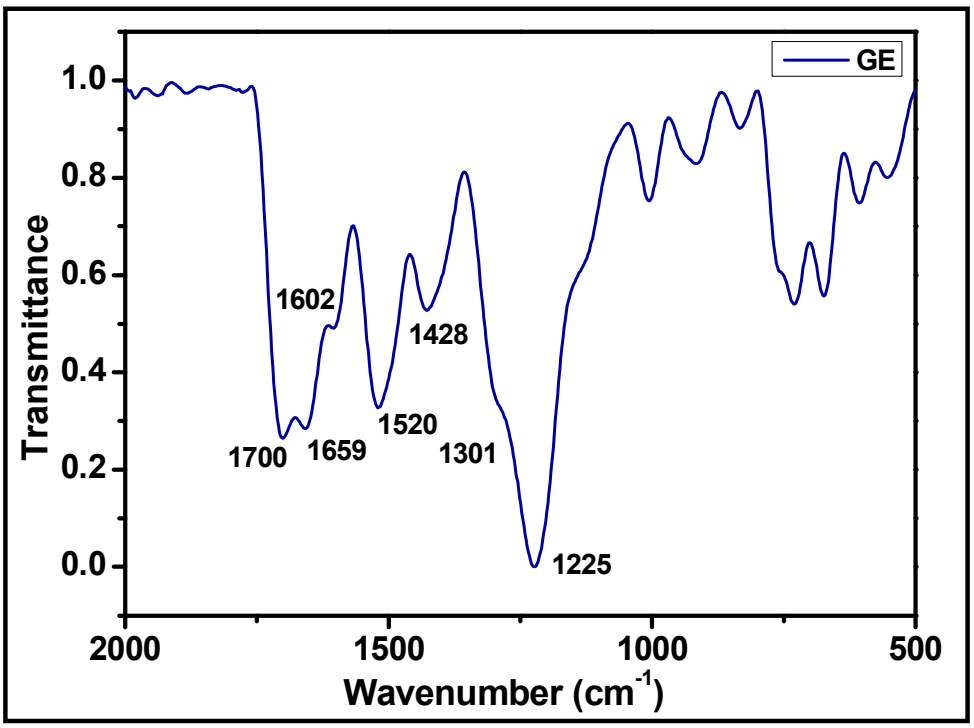


Fig. S4: FTIR data of gelator enhancer molecule **GE**.

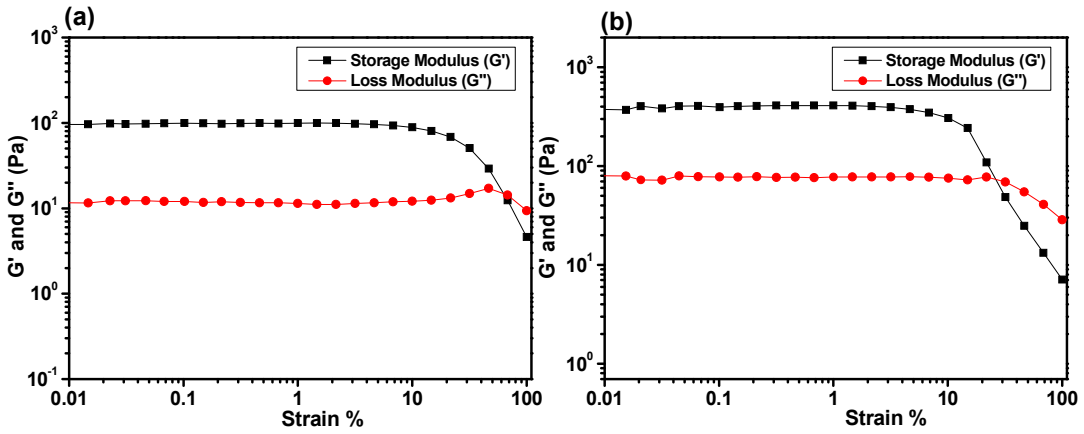


Fig. S5: Angular sweep experiment of organogel **G8GE** with (a) 0.01: 0.01 mmol (b) 0.02: 0.02 mmol in 1:1 ratio of 2 mL DMSO: H_2O mixture.

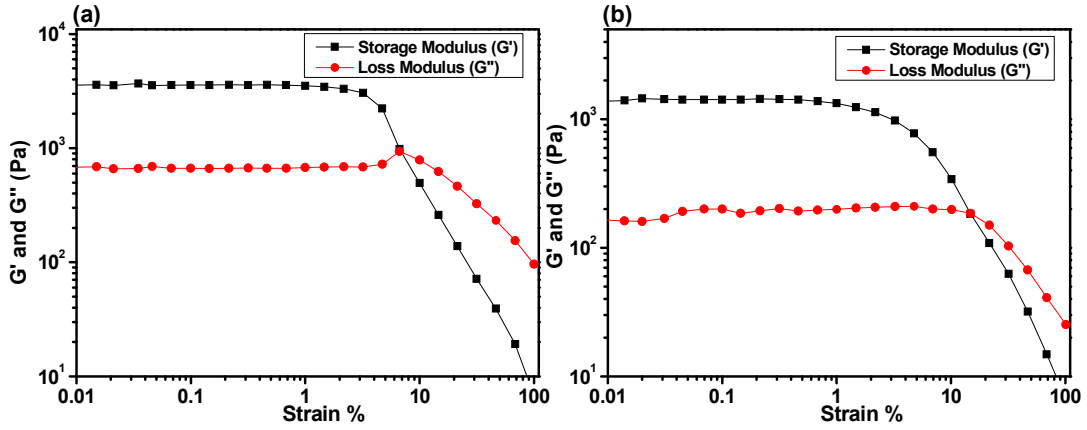


Fig. S6: Angular sweep experiment of organogel **G8GE** with (a) 0.03: 0.03 mmol (b) 0.04: 0.04 mmol in 1:1 ratio of 2 mL DMSO: H_2O mixture.

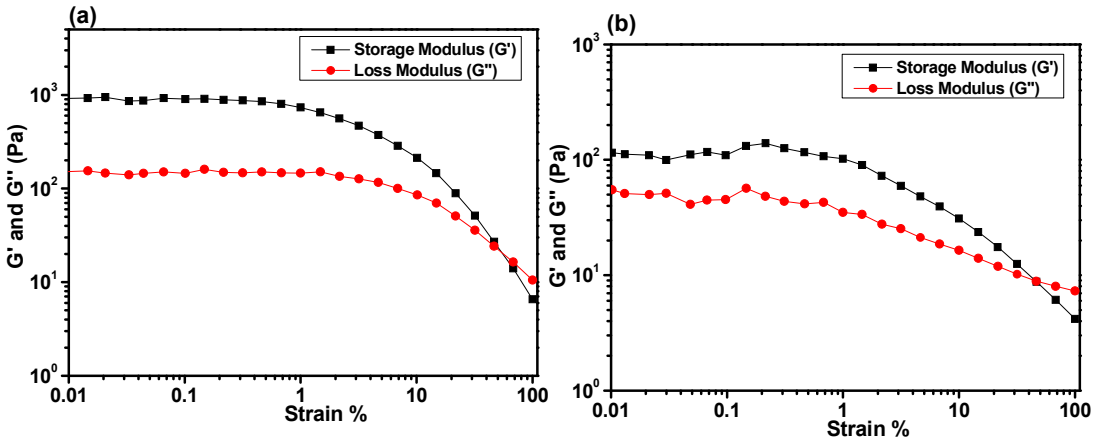


Fig. S7: Angular sweep experiment of organogel **G8GE** with (a) 0.07: 0.07 mmol (b) 0.1: 0.1 mmol in 1:1 ratio of 2 mL DMSO: H_2O mixture.

Table S1: Concentration dependent rheological study of organogel **G8GE**.

S. No.	mmol of G8	mmol of GE	Ratio of G8 and GE	Observation in 1 mL DMSO: 1 mL H_2O	Value of G'	Value of crossover point	Non- deformation range
1	0.01	0.01	1:1	Gel	95 Pa	68 strain %	0.01- 4.85 strain %
2	0.02	0.02	1:1	Gel	392 Pa	26 strain %	0.01- 2.16 strain %
3	**0.03**	**0.03**	**1:1**	**Strong Gel**	**3517 Pa**	**6 strain %**	**0.01- 1.01 strain %**
4	0.04	0.04	1:1	Strong Gel	1456 Pa	14 strain %	0.01- 0.47 strain %
5	0.07	0.07	1:1	Gel	922 Pa	47 strain %	0.01- 0.22 strain %
6	0.1	0.1	1:1	Gel	144 Pa	46 strain %	0.01- 0.15 strain %
7	0.03	0.02	3:2	Strong Gel	1593 Pa	25 strain %	0.01- 2.16 strain %

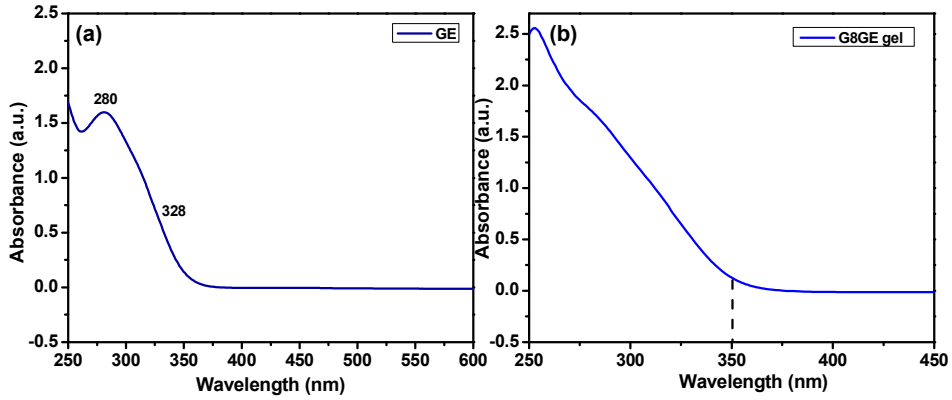


Fig. S8: UV-Vis spectrum of (a) **GE** and (c) **G8GE**.

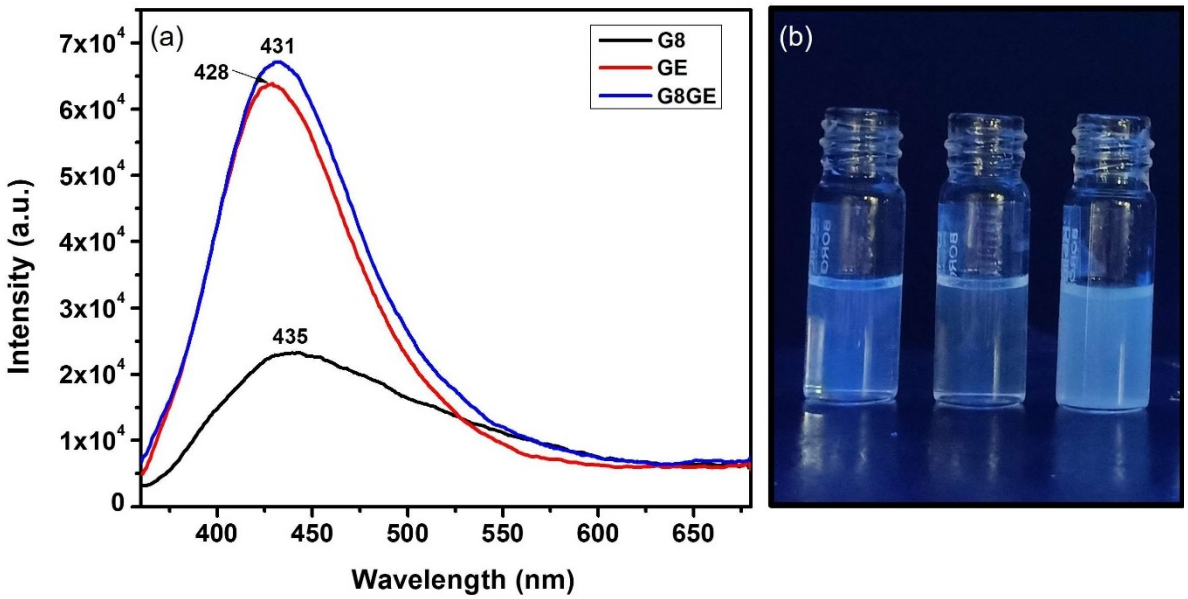


Fig. S9: Fluorescence spectrum of (a) **G8**, **GE**, **G8GE** (b) 1 mM solution of **G8**, **GE** and **G8GE** under UV chamber.

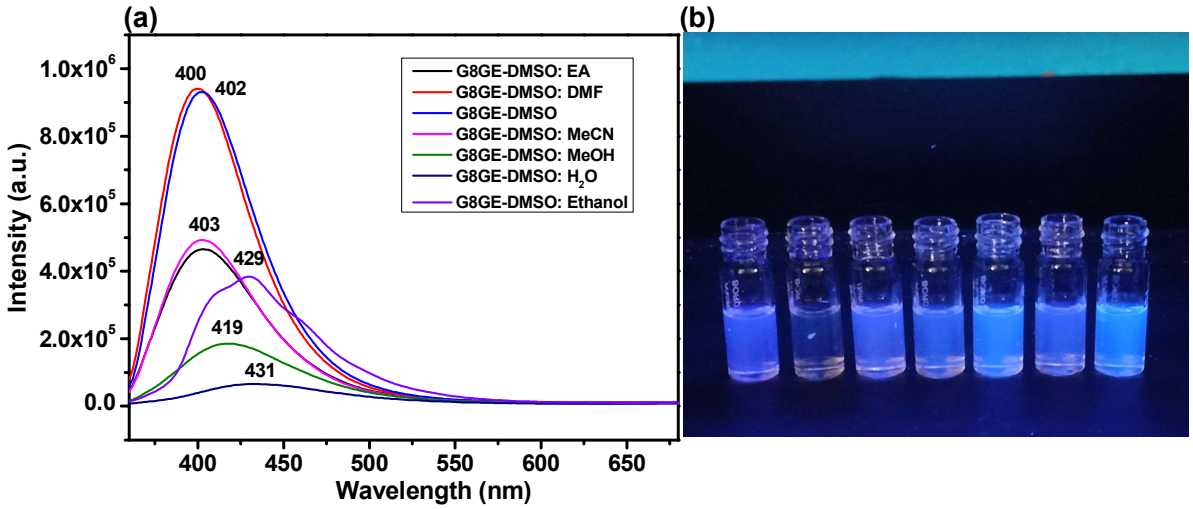


Fig. S10: (a) Fluorescence study of **G8GE** gelator component with different polar protic and polar aprotic solvents (b) 0.3 mM solution of **G8GE** component in different solvents under UV chamber.

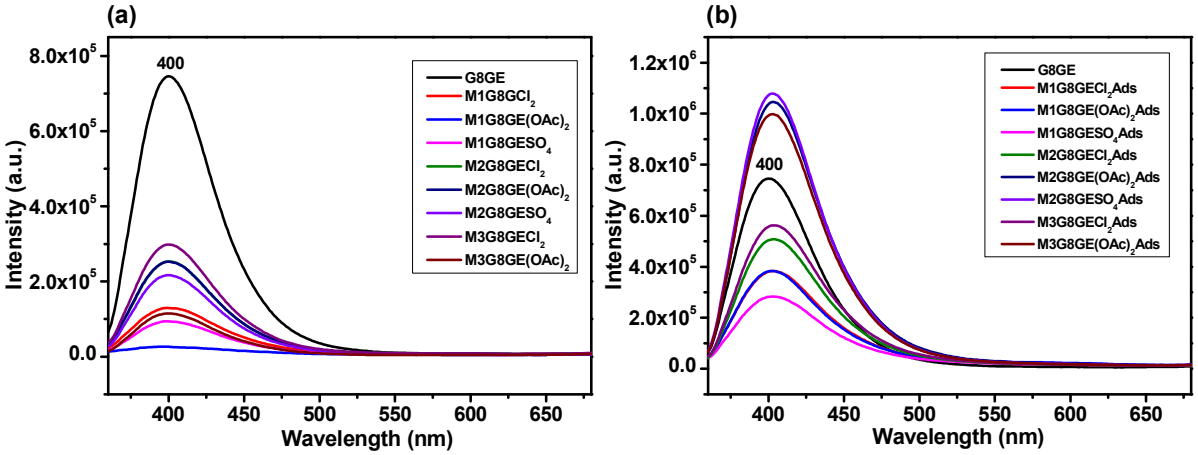


Fig. S11: Fluorescence study of **G8GE** organogel and metallogels formed by (a) mixing method and (b) adsorption method.

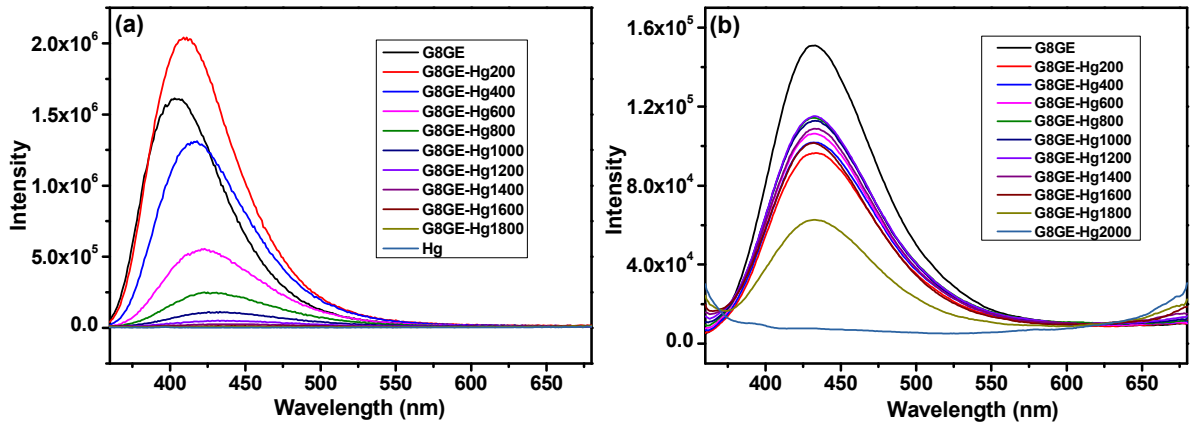


Fig. S12: Fluorescence study of (a) 1 mM solution of **G8GE** (in DMSO) and $HgCl_2$ (in H_2O) and (b) 1 mM solution of **G8GE** (in DMSO: H_2O) and $HgCl_2$ (in DMSO: H_2O).

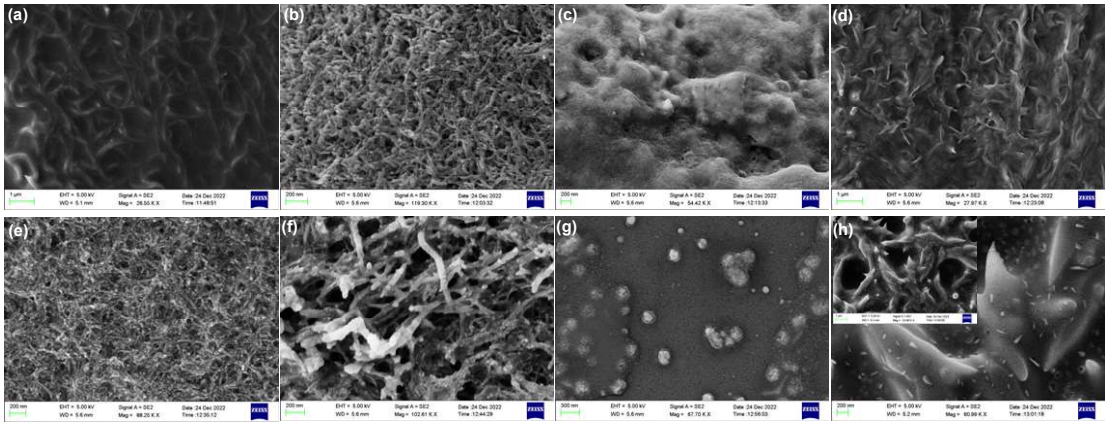


Fig. S13: FE-SEM images of (a) **M1G8GECl_2Ads** (b) **M1G8GE$(OAc)_2$Ads** (c) **M1G8GESO_4Ads** (d) **M2G8GECl_2Ads** (e) **M2G8GE$(OAc)_2$Ads** (f) **M2G8GESO_4Ads** (g) **M3G8GECl_2Ads and** (h) **M3G8GE$(OAc)_2$Ads** formed by adsorption method.

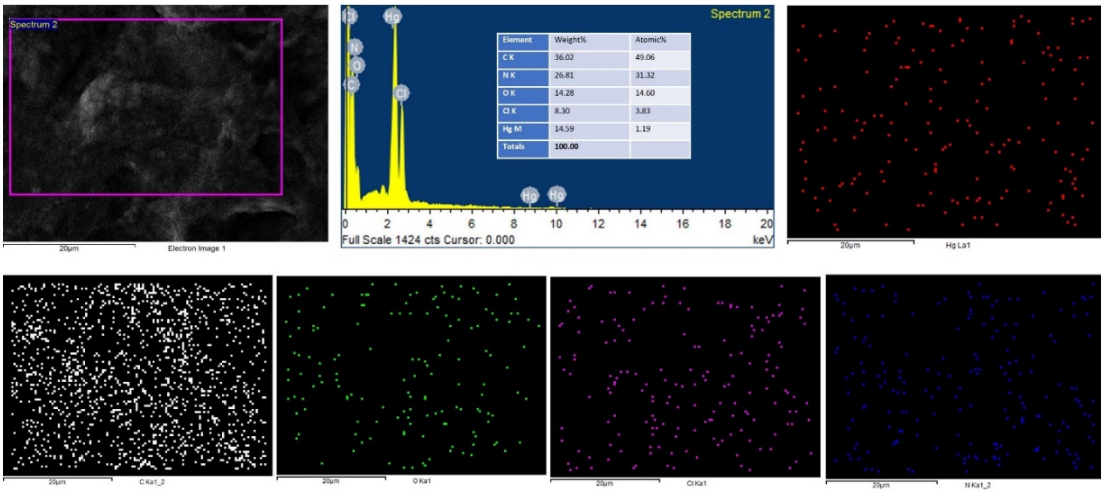


Fig. S14: EDX and Mapping analysis of **M1G8GECl_2** showing the presence of C, N, O, Hg and Cl inside gel matrix.

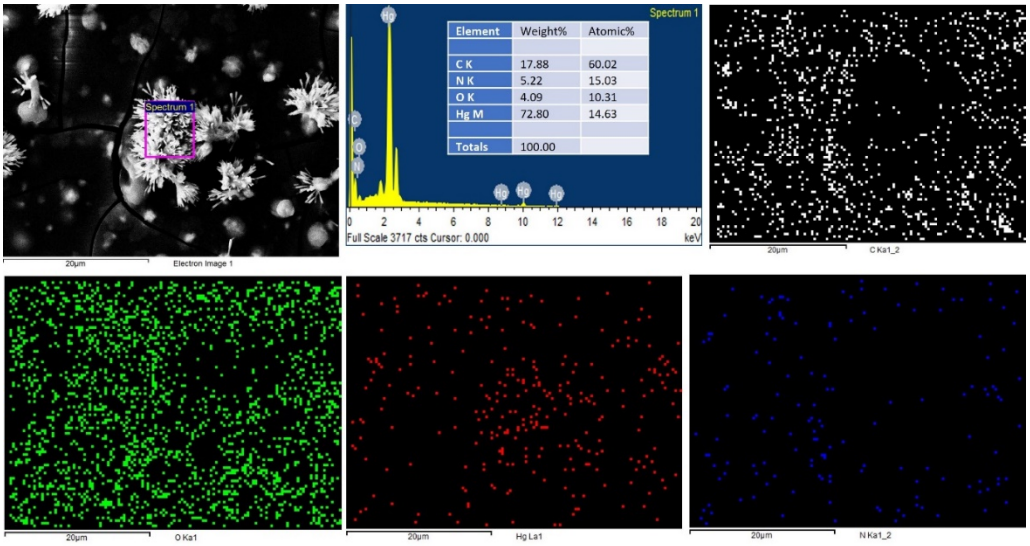


Fig. S15: EDX and Mapping analysis of **M1G8GE$(OAc)_2$** showing the presence of C, N, O and Hg inside gel matrix.

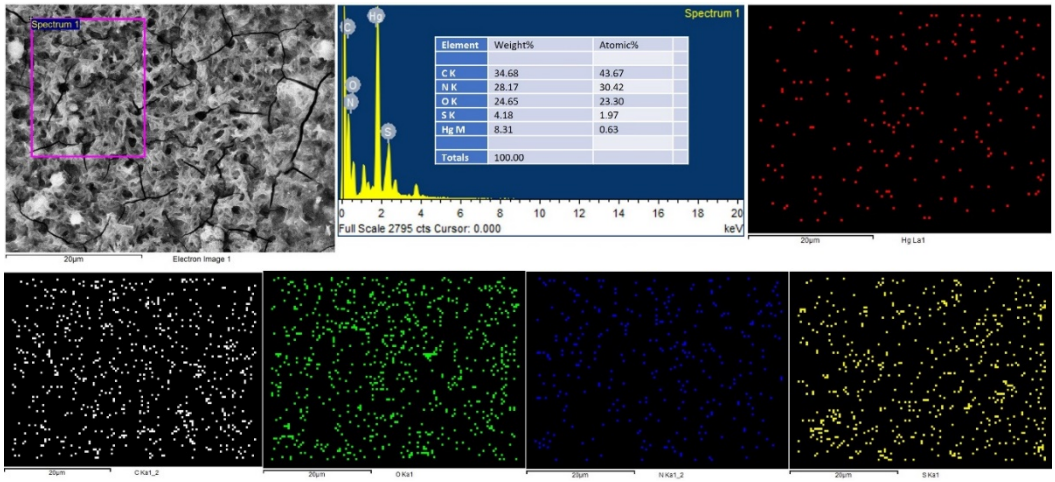


Fig. S16: EDX and Mapping analysis of **M1G8GESO$_4$** showing the presence of C, N, O, Hg and S inside gel matrix.

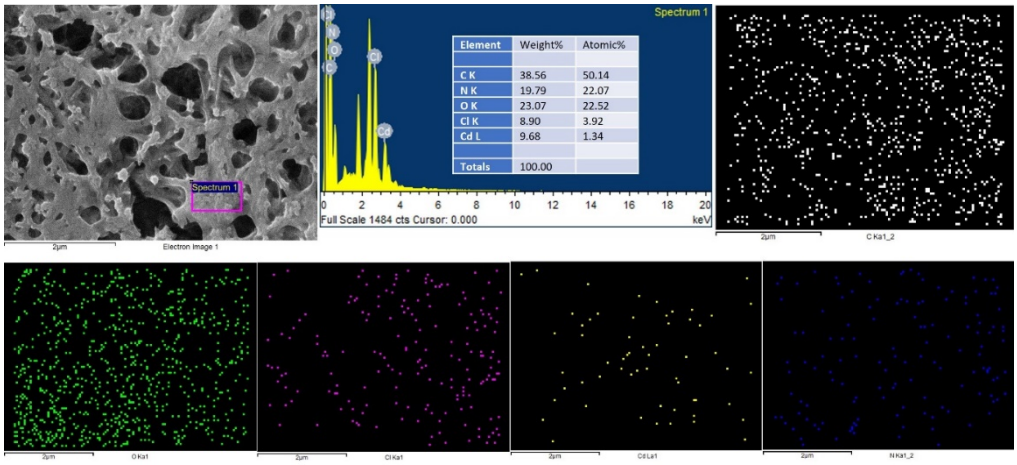


Fig. S17: EDX and Mapping analysis of **M2G8GECl$_2$** showing the presence of C, N, O, Cd and Cl inside gel matrix.

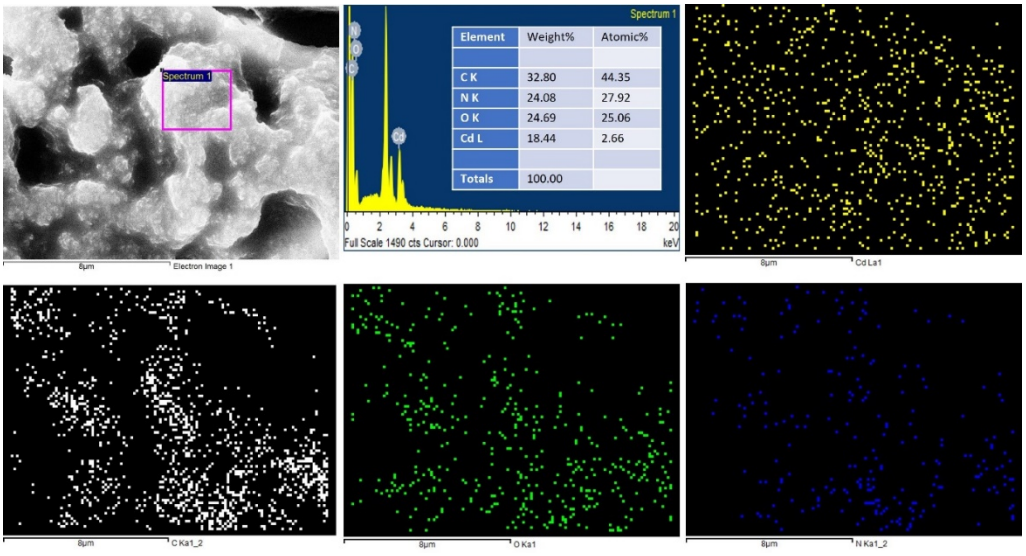


Fig. S18: EDX and Mapping analysis of **M2G8GE(OAc)$_2$** showing the presence of C, N, O and Cd inside gel matrix.

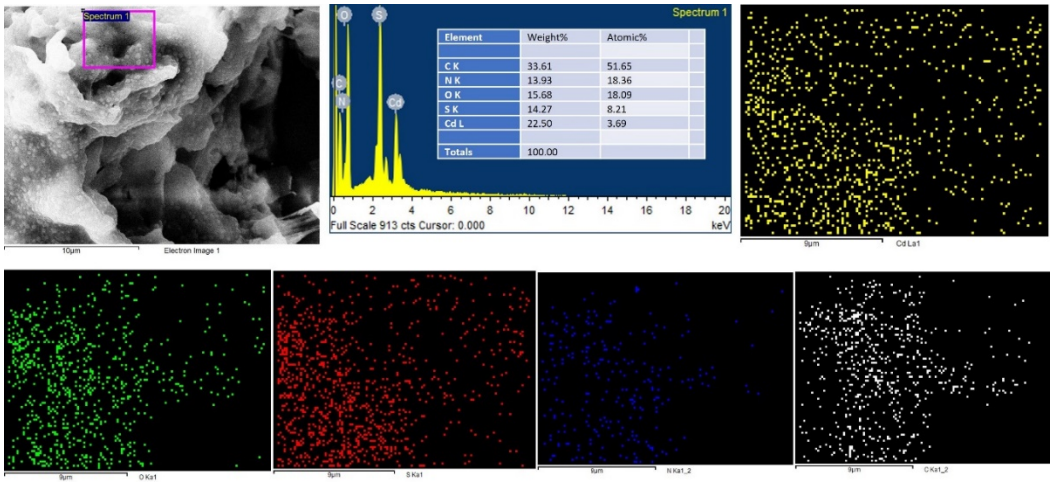


Fig. S19: EDX and Mapping analysis of **M2G8GESO$_4$** showing the presence of C, N, O, Cd and S inside gel matrix.

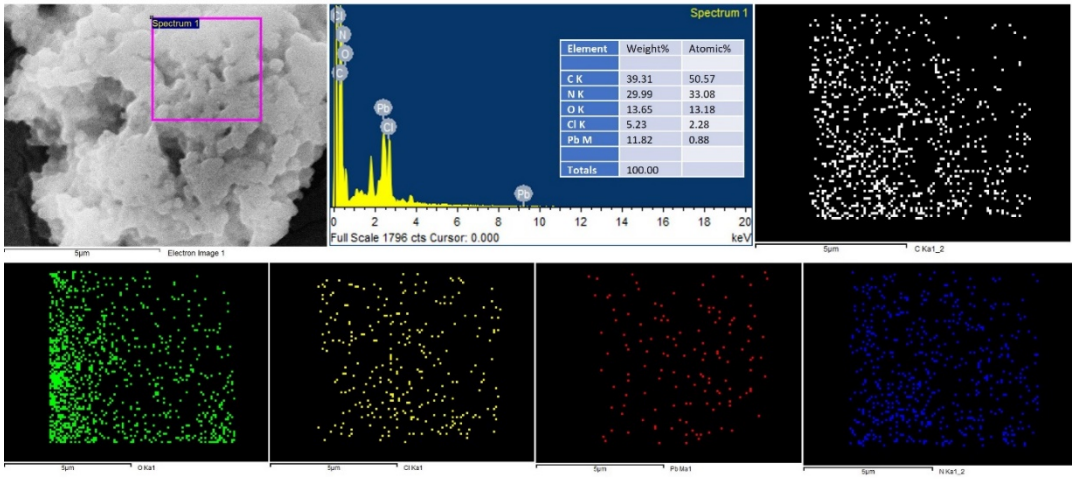


Fig. S20: EDX and Mapping analysis of **M3G8GECl$_2$** showing the presence of C, N, O, Pb and Cl inside gel matrix.

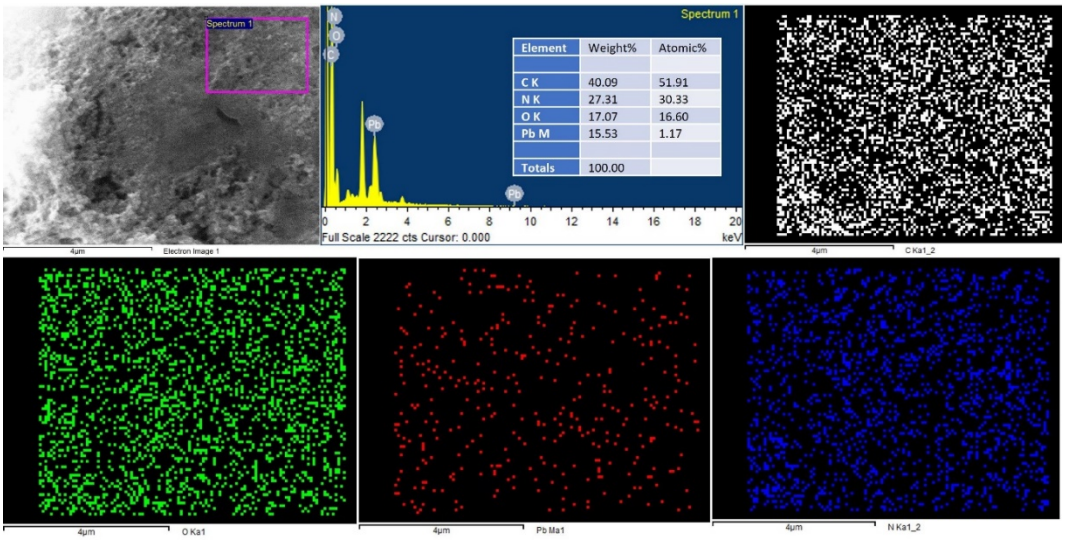


Fig. S21: EDX and Mapping analysis of **M3G8GE(OAc)$_2$** showing the presence of C, N, O and Pb inside gel matrix.

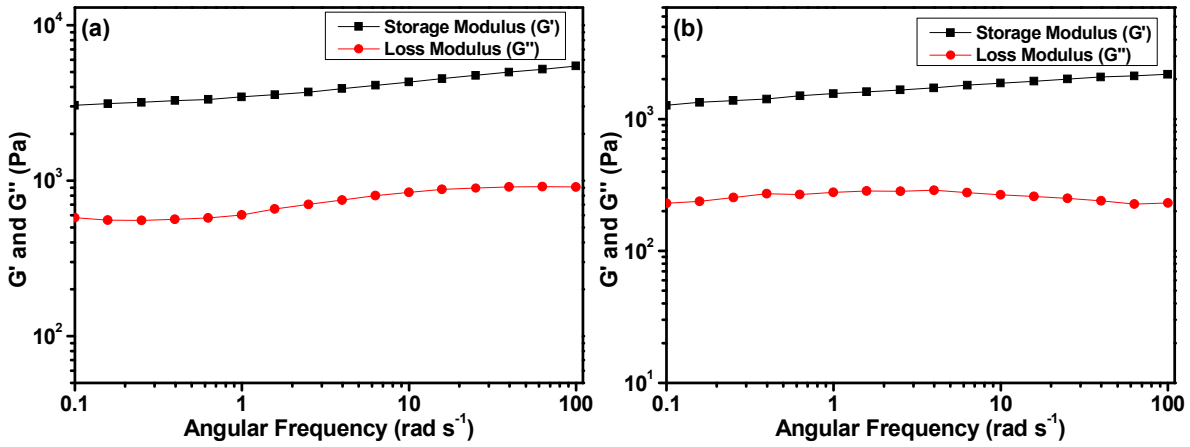


Fig. S22: (a) Frequency sweep experiment of organogel **G8GE** at 1:1 molar ratio (0.03: 0.03 mmol) (b) Frequency sweep experiment of organogel **G8GE** at 3: 2 molar ratio (0.03: 0.02 mmol).

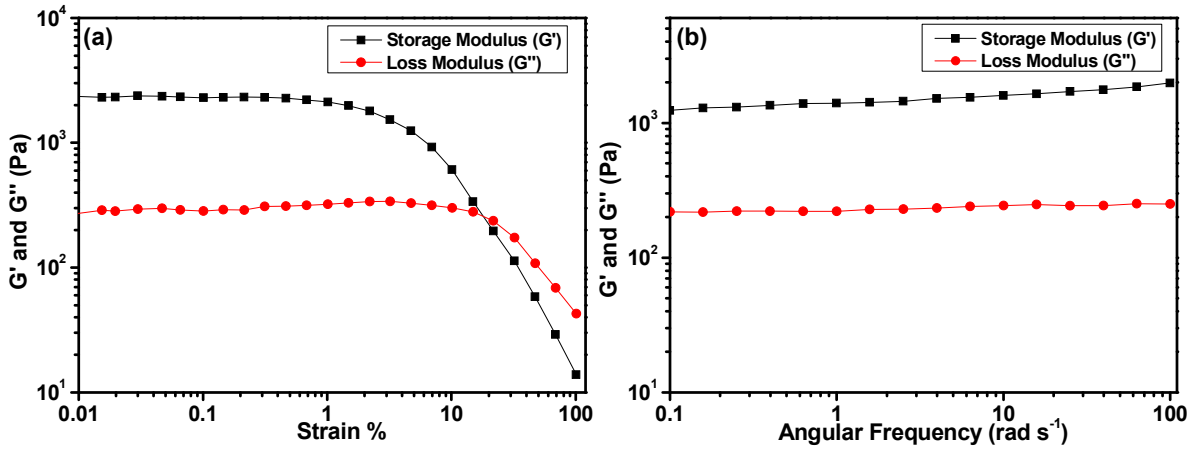


Fig. S23: (a) Angular sweep experiment of metallogel **M1G8GECl$_2$** (b) Frequency sweep experiment of metallogel **M1G8GECl$_2$**.

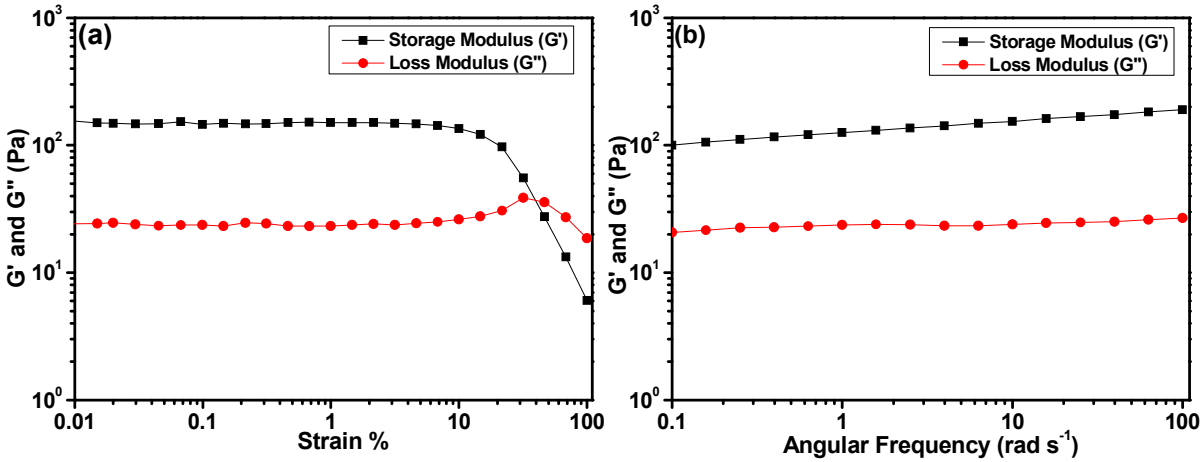


Fig. S24: (a) Angular sweep experiment of metallogel **M1G8GE(OAc)$_2$** (b) Frequency sweep experiment of metallogel **M1G8GE(OAc)$_2$**.

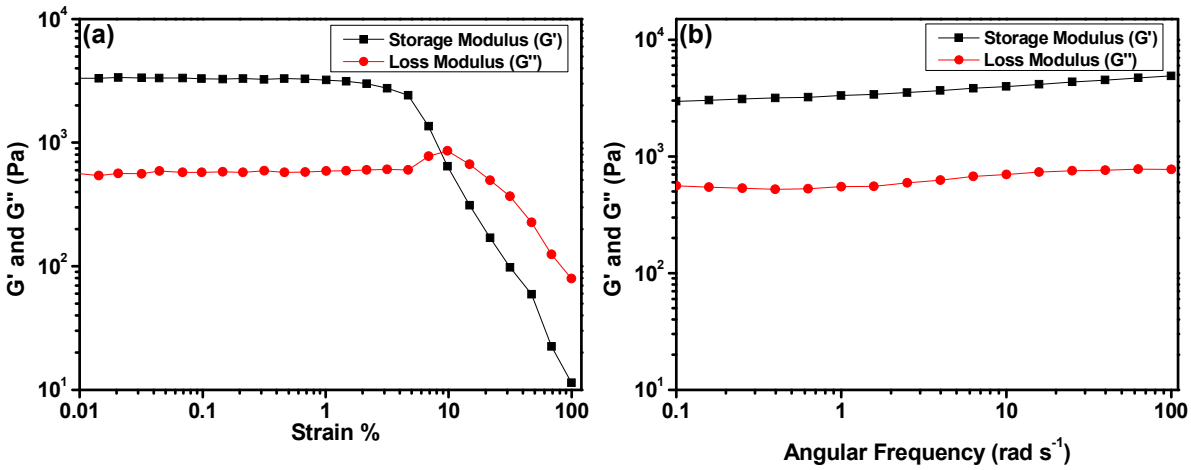


Fig. S25: (a) Angular sweep experiment of metallogel **M1G8GESO$_4$** (b) Frequency sweep experiment of metallogel **M1G8GESO$_4$**.

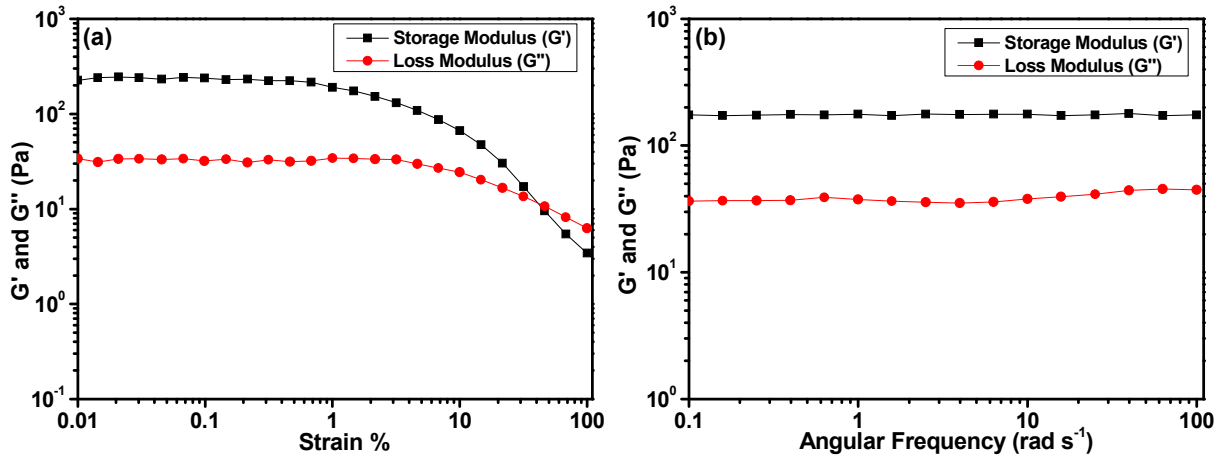


Fig. S26: (a) Angular sweep experiment of metallogel **M2G8GECl$_2$** (b) Frequency sweep experiment of metallogel **M2G8GECl$_2$**.

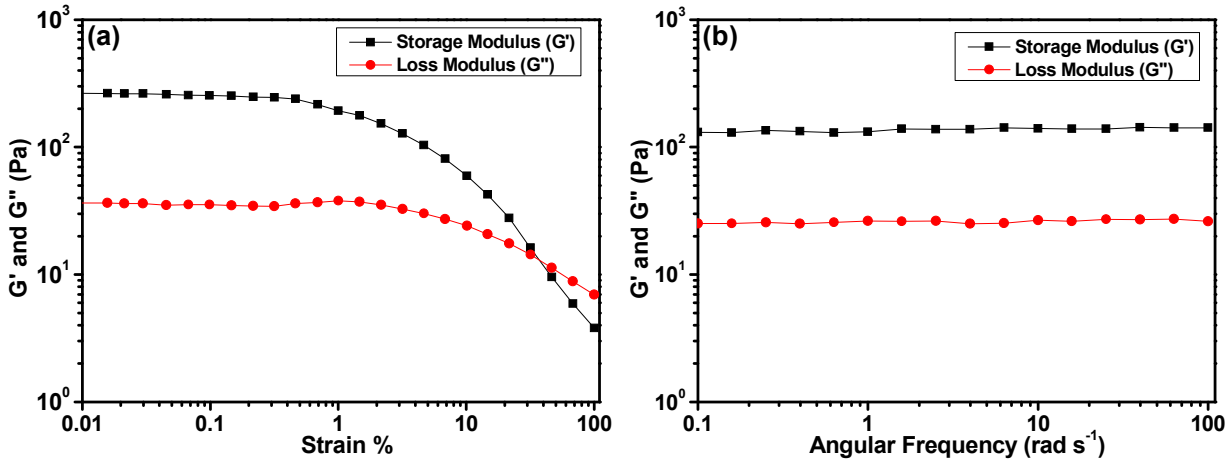


Fig. S27: (a) Angular sweep experiment of metallogel **M3G8GECl$_2$** (b) Frequency sweep experiment of metallogel **M3G8GECl$_2$**.

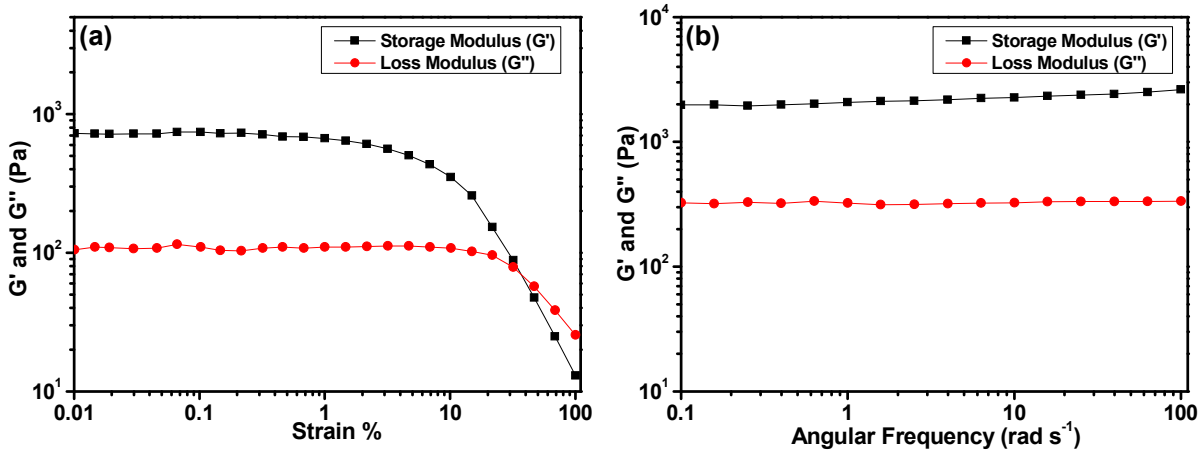


Fig. S28: (a) Angular sweep experiment of metallogel **M3G8GESO$_4$** (b) Frequency sweep experiment of metallogel **M3G8GESO$_4$**.

Table S2: Storage modulus and loss modulus of metallogels formed by mixing method.

Metallogel	Storage Modulus (G')	Loss Modulus (G'')
M1G8GECl$_2$	1976 Pa	247 Pa
M1G8GE(OAc)$_2$	189 Pa	27 Pa
M1G8GESO$_4$	4838 Pa	792 Pa
M2G8GECl$_2$	176 Pa	44 Pa
M2G8GE(OAc)$_2$	Gelatinous Solution	Gelatinous Solution
M2G8GESO$_4$	Gelatinous Solution	Gelatinous Solution
M3G8GECl$_2$	140 Pa	26 Pa
M3G8GE(OAc)$_2$	2646 Pa	338 Pa

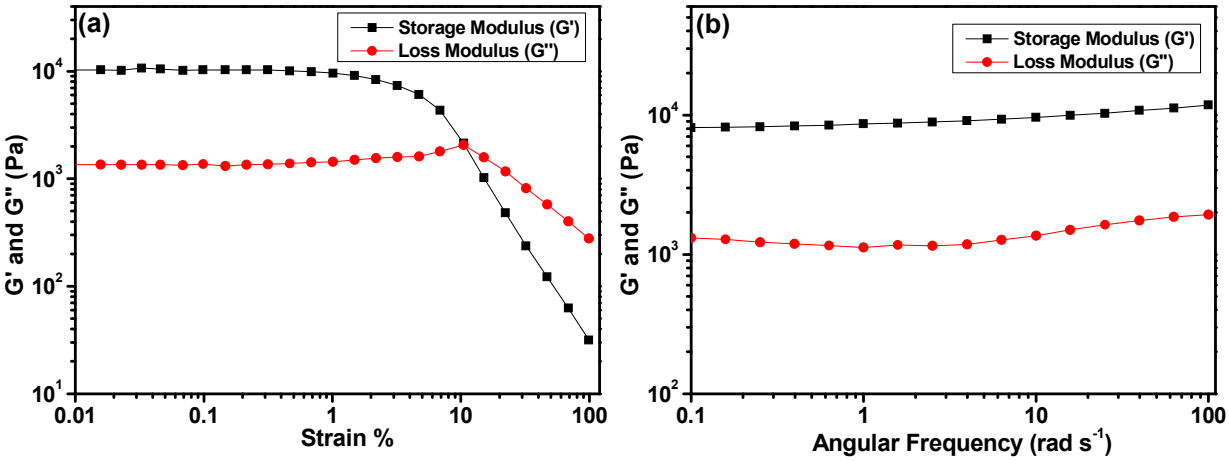


Fig. S29: (a) Angular sweep experiment of metallogel **M1G8GECl$_2$Ads** (b) Frequency sweep experiment of metallogel **M1G8GECl$_2$Ads**.

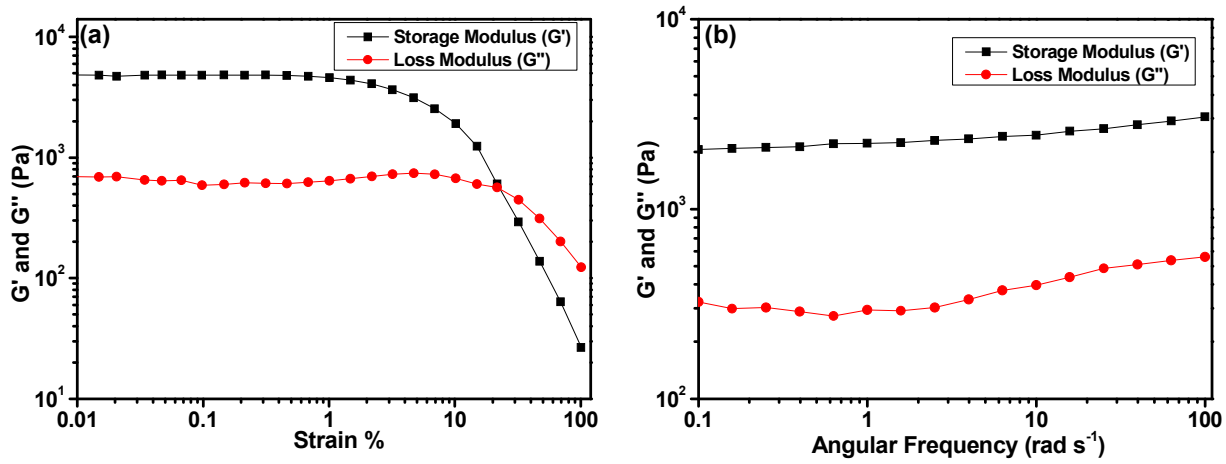


Fig. S30: (a) Angular sweep experiment of metallogel **M1G8GE(OAc)$_2$Ads** (b) Frequency sweep experiment of metallogel **M1G8GE(OAc)$_2$Ads.**

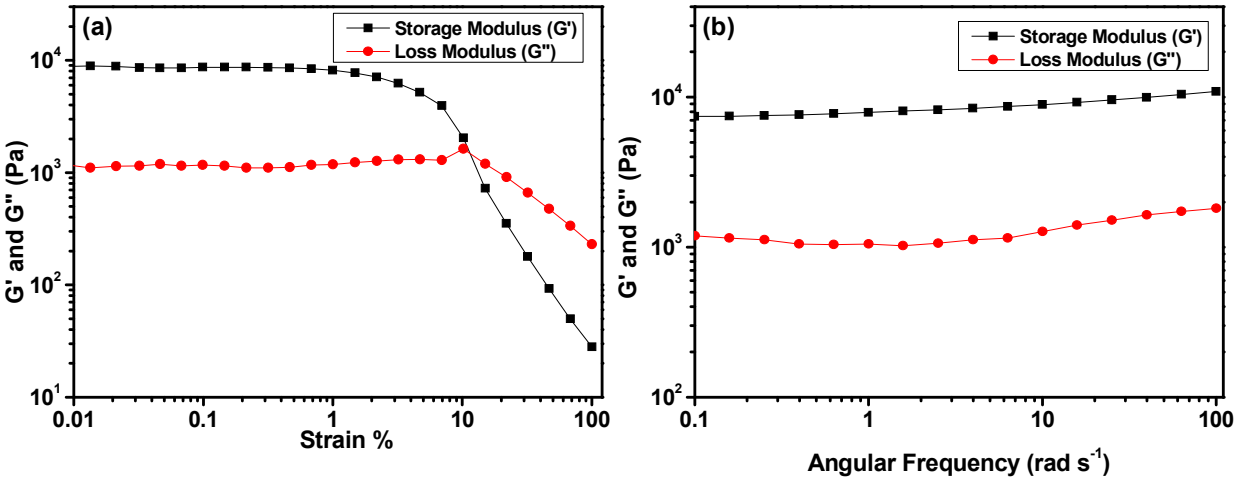


Fig. S31: (a) Angular sweep experiment of metallogel **M1G8GESO$_4$Ads** (b) Frequency sweep experiment of metallogel **M1G8GESO$_4$Ads**.

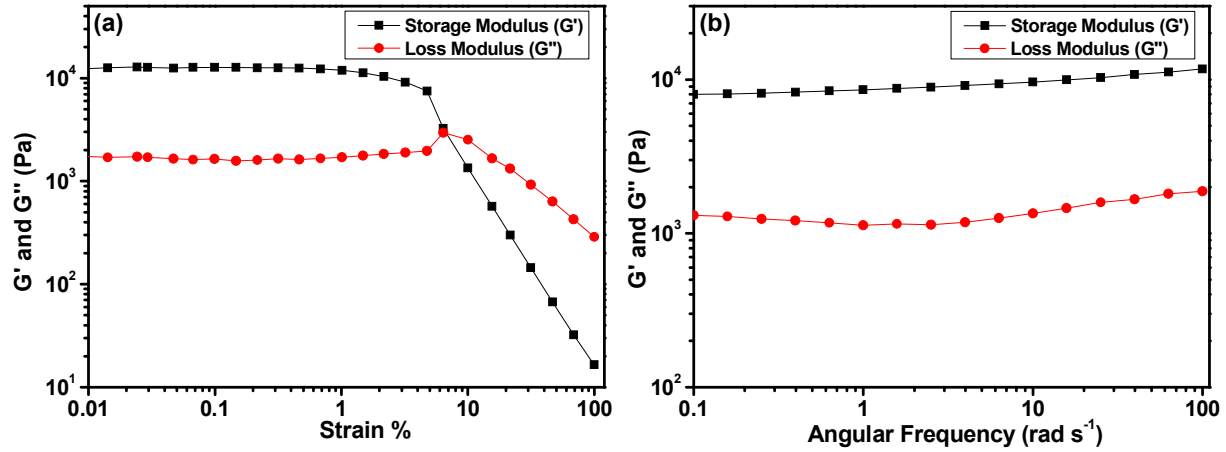


Fig. S32: (a) Angular sweep experiment of metallogel **M2G8GECl$_2$Ads** (b) Frequency sweep experiment of metallogel **M2G8GECl$_2$Ads**.

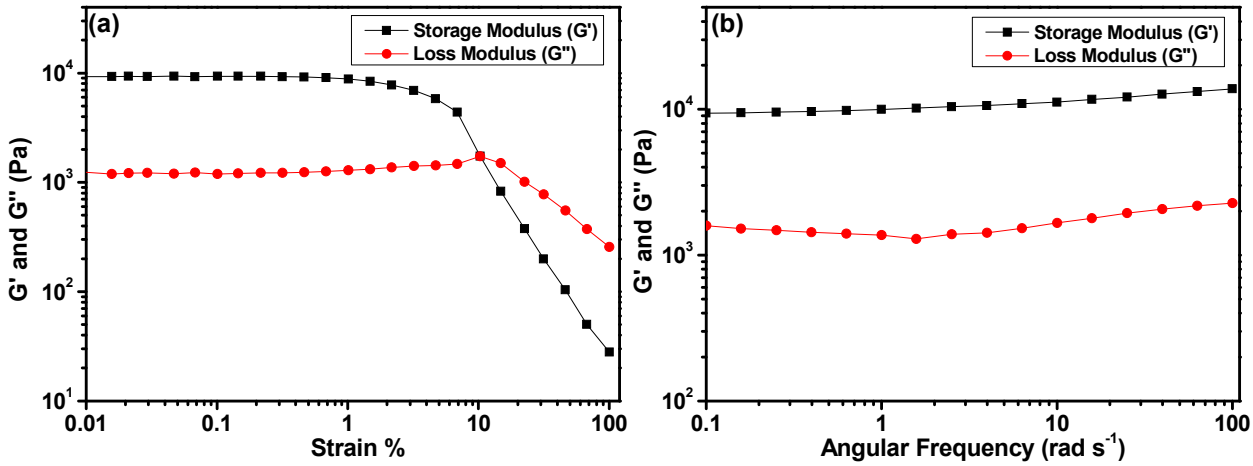


Fig. S33: (a) Angular sweep experiment of metallogel **M2G8GE(OAc)$_2$Ads** (b) Frequency sweep experiment of metallogel **M2G8GE(OAc)$_2$Ads.**

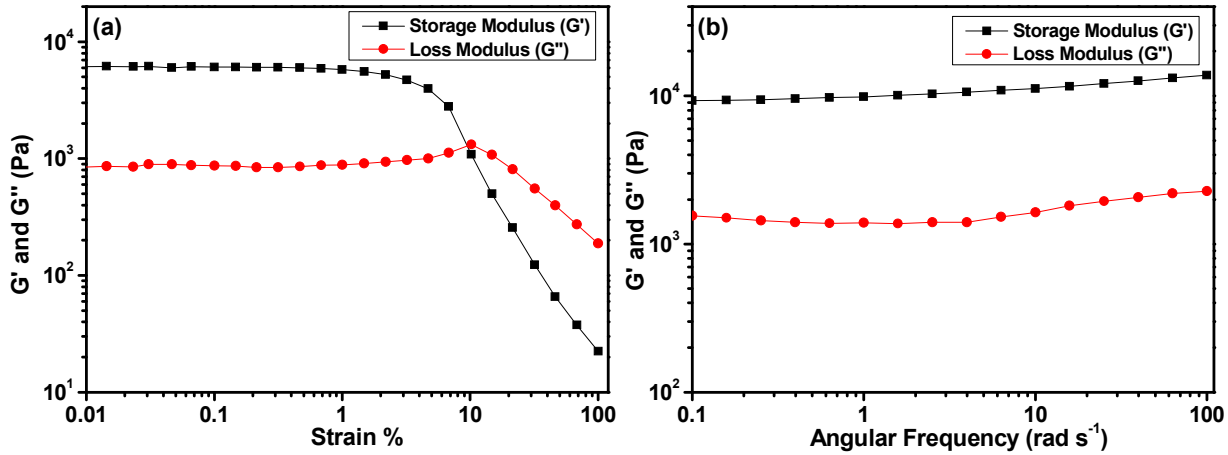


Fig. S34: (a) Angular sweep experiment of metallogel **M2G8GESO$_4$Ads** (b) Frequency sweep experiment of metallogel **M2G8GESO$_4$Ads.**

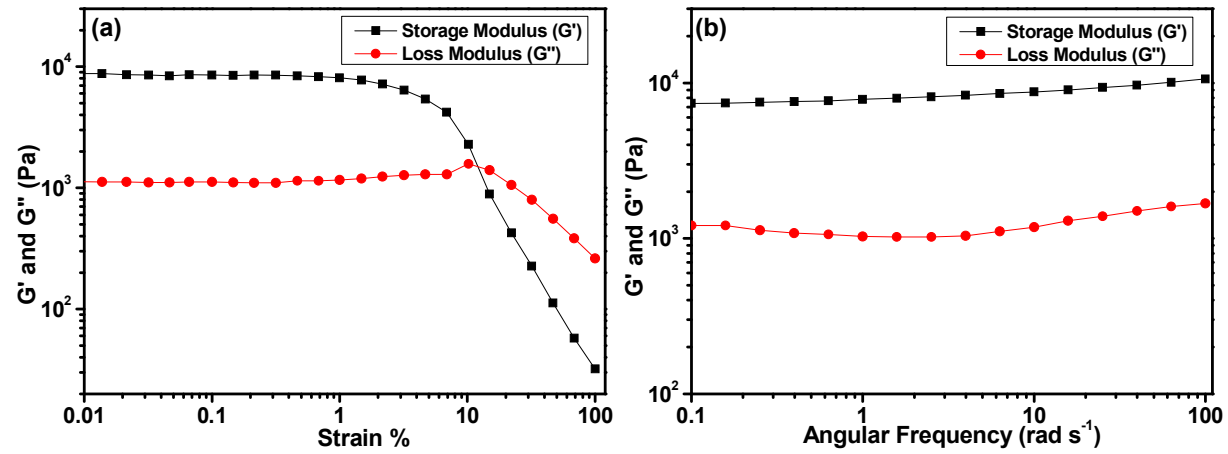


Fig. S35: (a) Angular sweep experiment of metallogel **M3G8GECl$_2$Ads** (b) Frequency sweep experiment of metallogel **M3G8GECl$_2$Ads.**

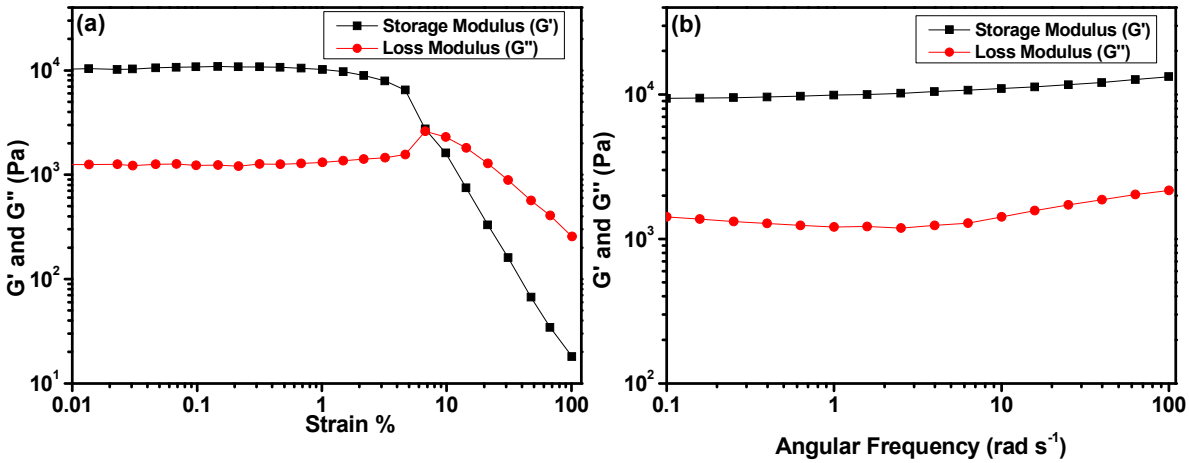


Fig. S36: (a) Angular sweep experiment of metallogel **M3G8GE(OAc)$_2$Ads** (b) Frequency sweep experiment of metallogel **M3G8GE(OAc)$_2$Ads.**

Table S3: Storage modulus and loss modulus of metallogels formed by adsorption method.

Metallogel	Storage Modulus (G')	Loss Modulus (G")
M1G8GECl$_2$Ads	11730 Pa	1943 Pa
M1G8GE(OAc)$_2$Ads	3055 Pa	559 Pa
M1G8GESO$_4$Ads	10872 Pa	1803 Pa
M2G8GECl$_2$Ads	11830 Pa	1855 Pa
M2G8GE(OAc)$_2$Ads	13815 Pa	2291 Pa
M2G8GESO$_4$Ads	13635 Pa	2266 Pa
M3G8GECl$_2$Ads	10747 Pa	1688 Pa
M3G8GE(OAc)$_2$Ads	13119 Pa	2179 Pa

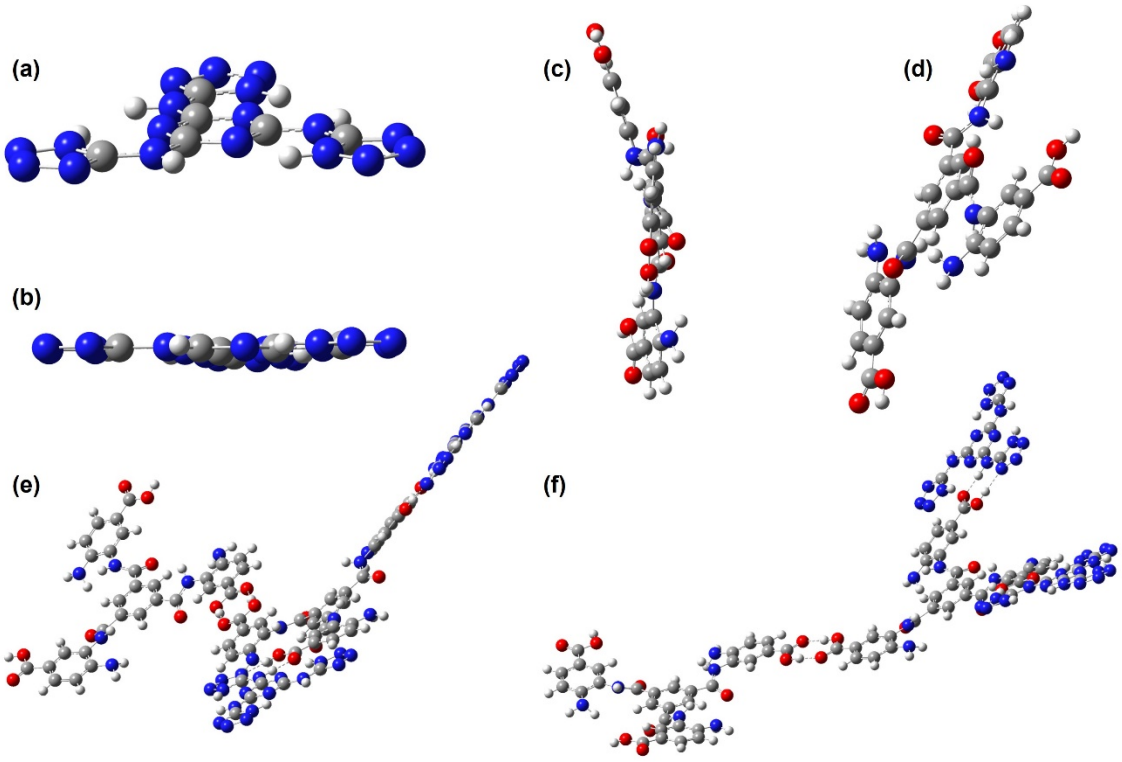


Fig. S37: DFT structure showing (a, b) Planarity of **G8** (c, d) Tilted structure of **GE** and (e, f) Less tilted structure of **G8GE** as compared to **GE** after interaction with **G8**.

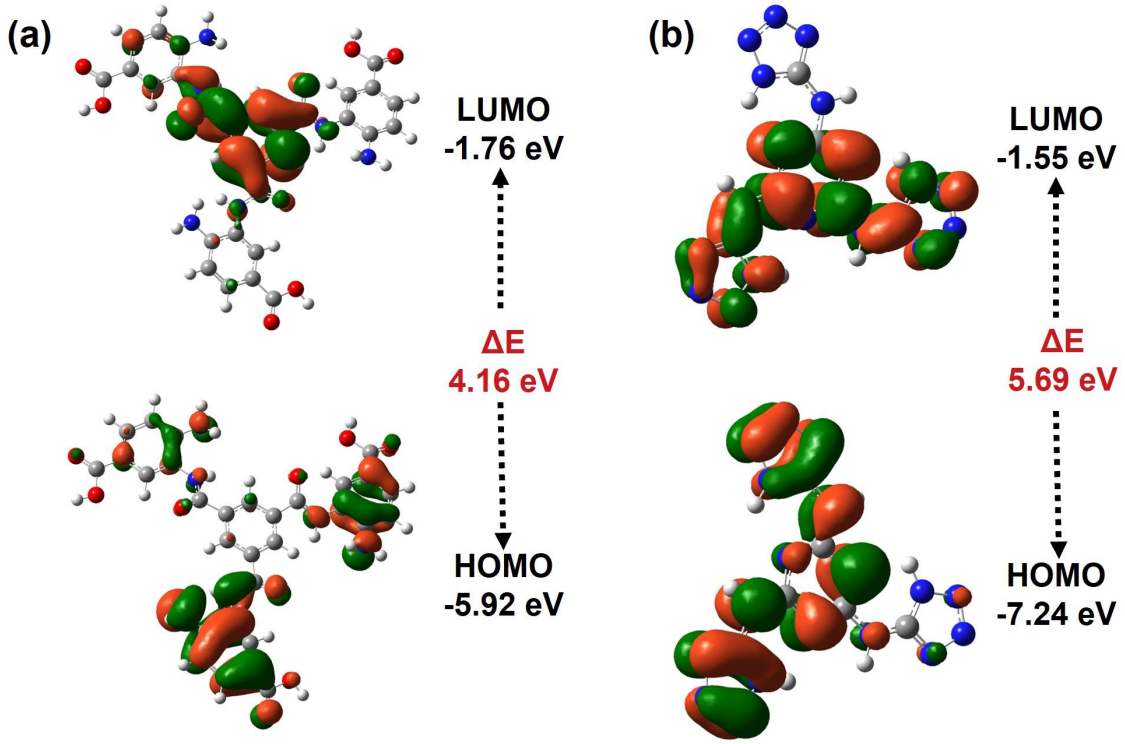
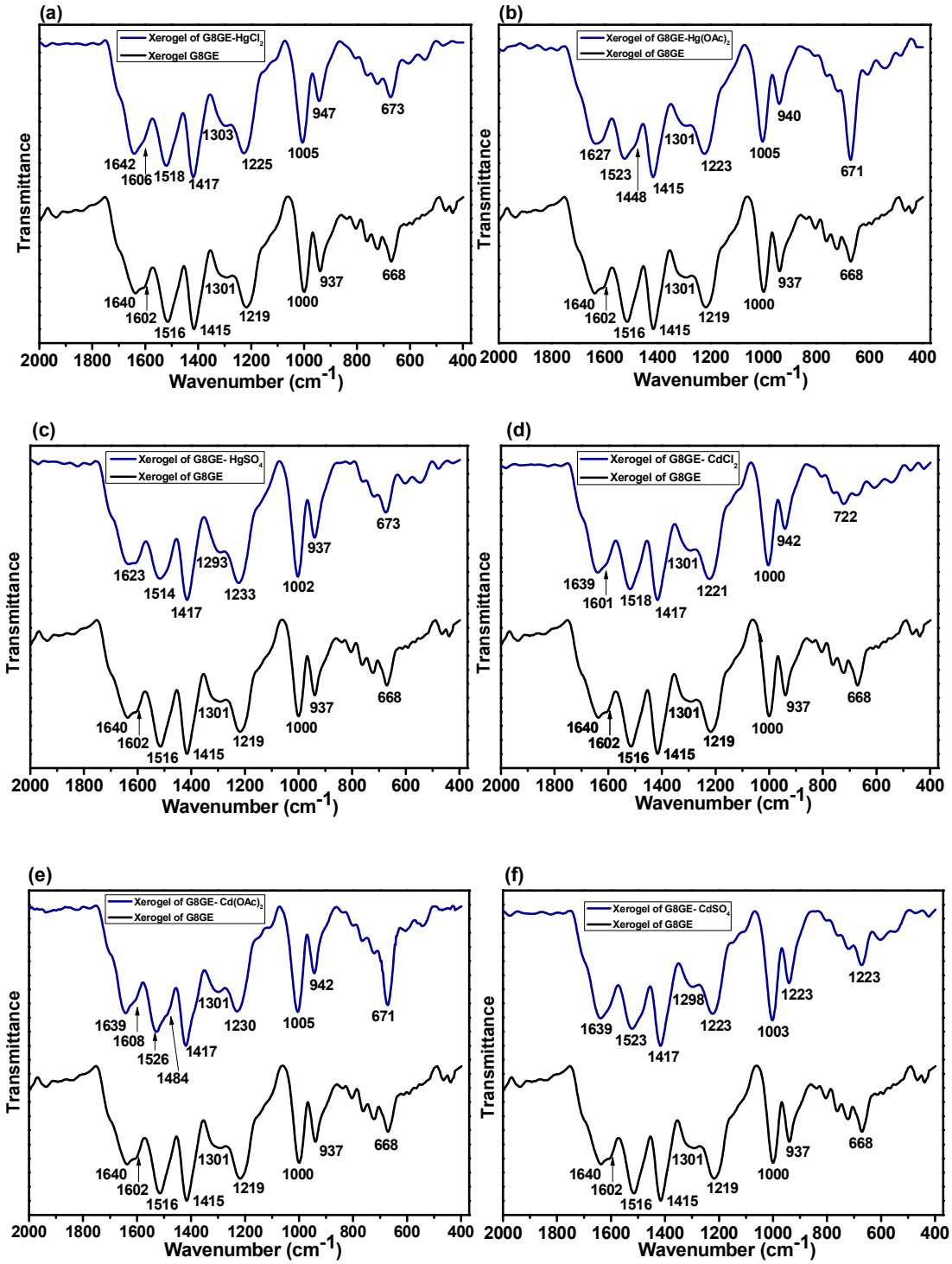


Fig. S38: HOMO-LUMO energy orbitals of (a) **G8** and (b) **GE**.


(a)
Xerogel of G8GE-HgCl2
Xerogel G8GE
1642
1606
1518
1417
1303
1225
1005
947
673
1640
1602
1516
1415
1301
1219
1000
937
668
Transmittance
Wavenumber (cm-1)
(b)
Xerogel of G8GE-Hg(OAc)2
Xerogel of G8GE
1627
1523
1448
1415
1301
1223
1005
940
671
1640
1602
1516
1415
1301
1219
1000
937
668
Transmittance
Wavenumber (cm-1)
(c)
Xerogel of G8GE- HgSO4
Xerogel of G8GE
1623
1514
1417
1293
1233
1002
937
673
1640
1602
1516
1415
1301
1219
1000
937
668
Transmittance
Wavenumber (cm-1)
(d)
Xerogel of G8GE- CdCl2
Xerogel of G8GE
1639
1601
1518
1417
1301
1221
1000
942
722
1640
1602
1516
1415
1301
1219
1000
937
668
Transmittance
Wavenumber (cm-1)
(e)
Xerogel of G8GE- Cd(OAc)2
Xerogel of G8GE
1639
1608
1526
1484
1417
1301
1230
1005
942
671
1640
1602
1516
1415
1301
1219
1000
937
668
Transmittance
Wavenumber (cm-1)
(f)
Xerogel of G8GE- CdSO4
Xerogel of G8GE
1639
1523
1417
1298
1223
1003
1223
1640
1602
1516
1415
1301
1219
1000
937
668
Transmittance
Wavenumber (cm-1)

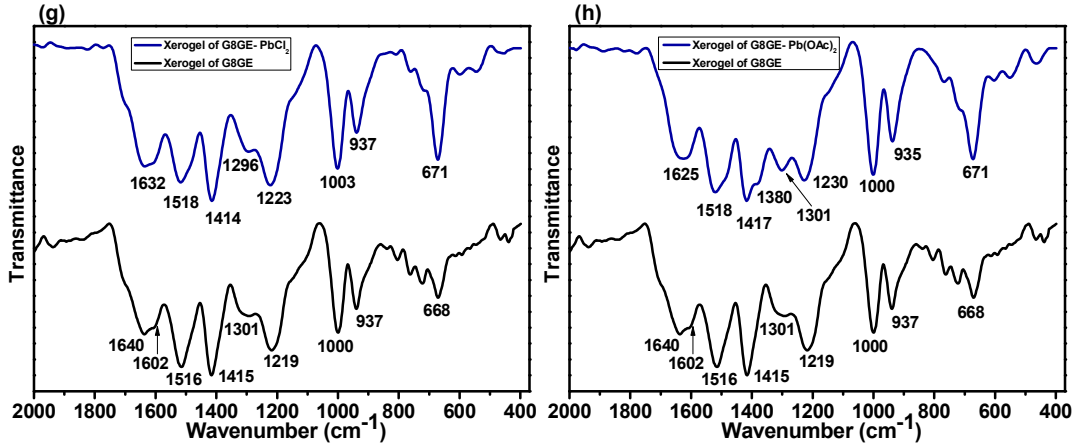


Fig. 39: FTIR data analysis of (a) **M1G8GECl$_2$** (b) **M1G8GE(OAc)$_2$** (c) **M1G8GESO$_4$** (d) **M2G8GECl$_2$** (e) precipitate of **M2G8GE(OAc)$_2$** (f) precipitate of **M2G8GESO$_4$** (g) **M3G8GECl$_2$** (h) **M3G8GE(OAc)$_2$.**

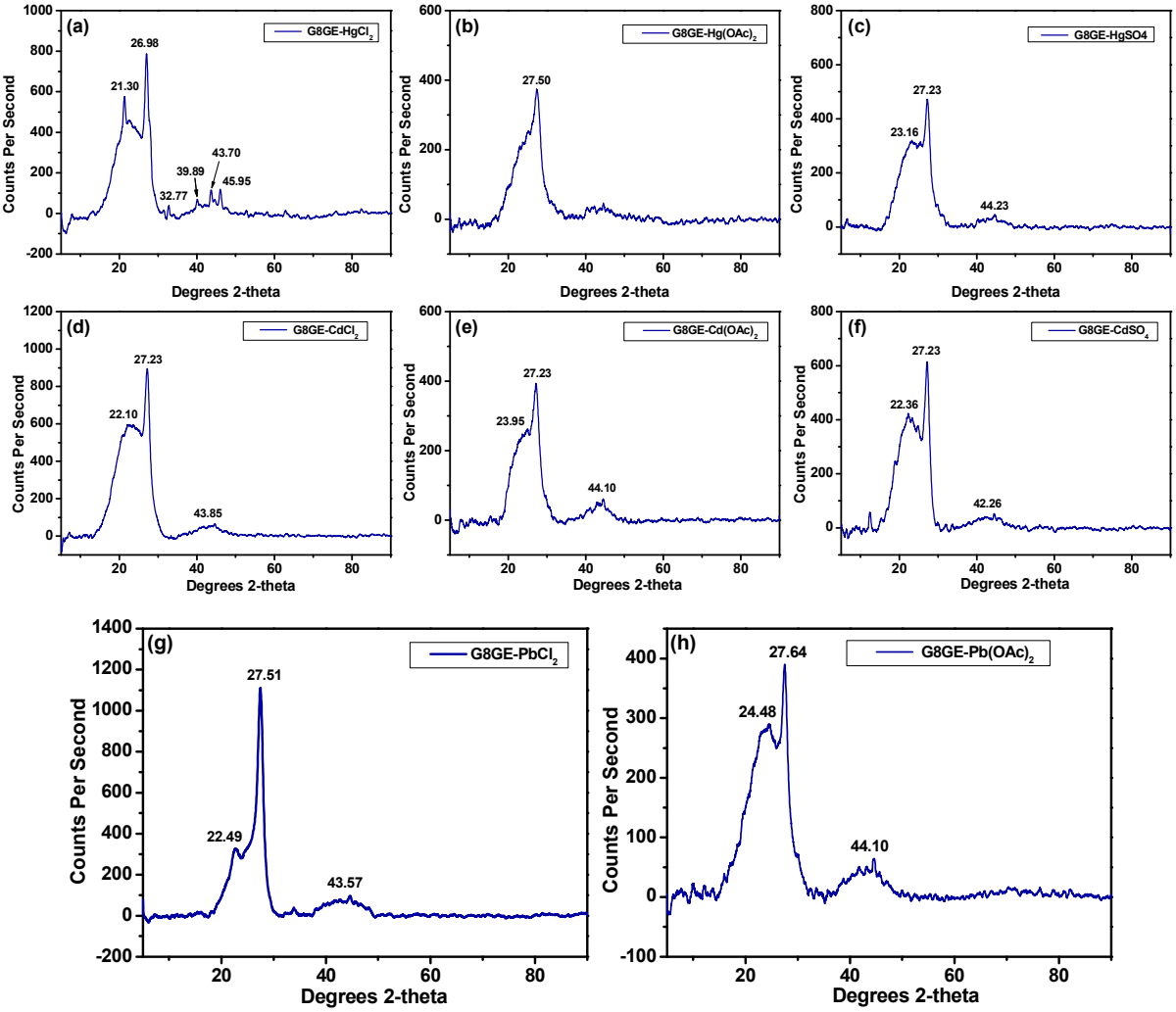


Fig. S40: PXRD data of metallogels (a) **M1G8GECl$_2$** (b) **M1G8GE(OAc)$_2$** (c) **M1G8GESO$_4$** (d) **M2G8GECl$_2$** (e) precipitate of **M2G8GE(OAc)$_2$** (f) precipitate of **M2G8GESO$_4$** (g) **M3G8GECl$_2$** (h) **M3G8GE(OAc)$_2$.**

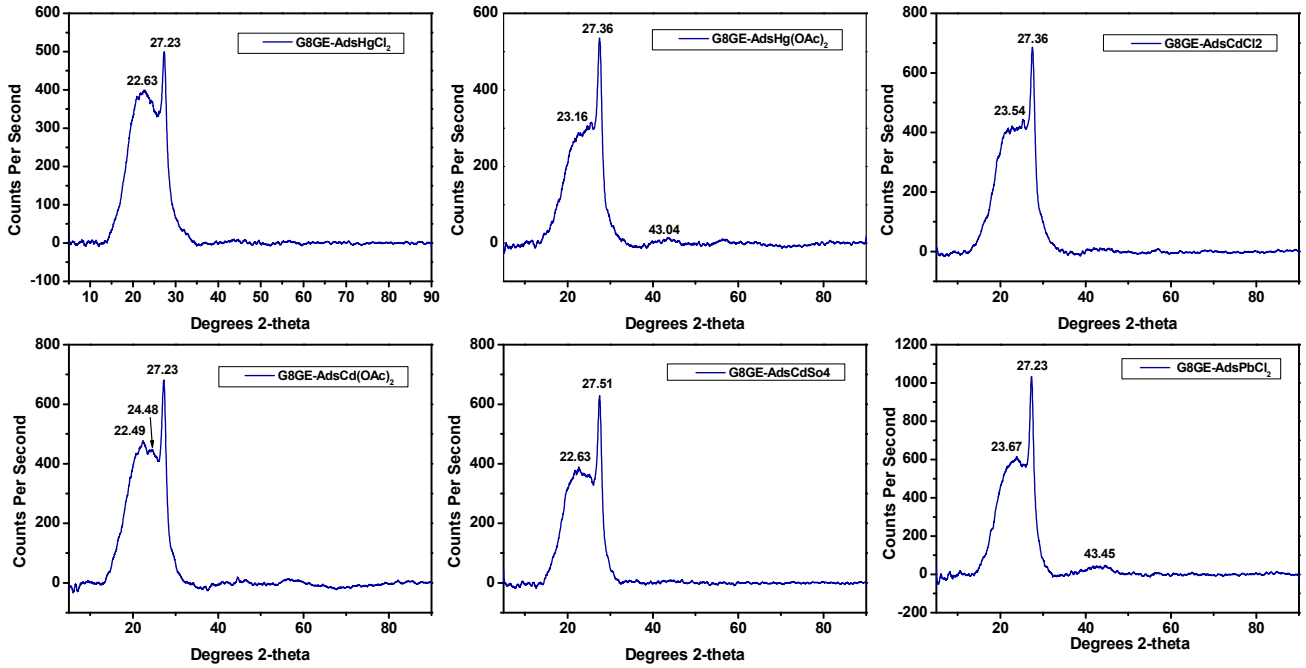


Fig. S41: PXRD data of metallogels (a) **M1G8GECl_2Ads** (b) **M1G8GE$(OAc)_2$ Ads** (c) **M2G8GECl_2 Ads** (d) **M2G8GE$(OAc)_2$ Ads** (e) **M2G8GESO_4 Ads** (f) **M3G8GECl_2 Ads.**

Table S4: Optimization of heavy metal removal reaction by xerogel of organogel **G8GE**, analysed by ICP-AES.

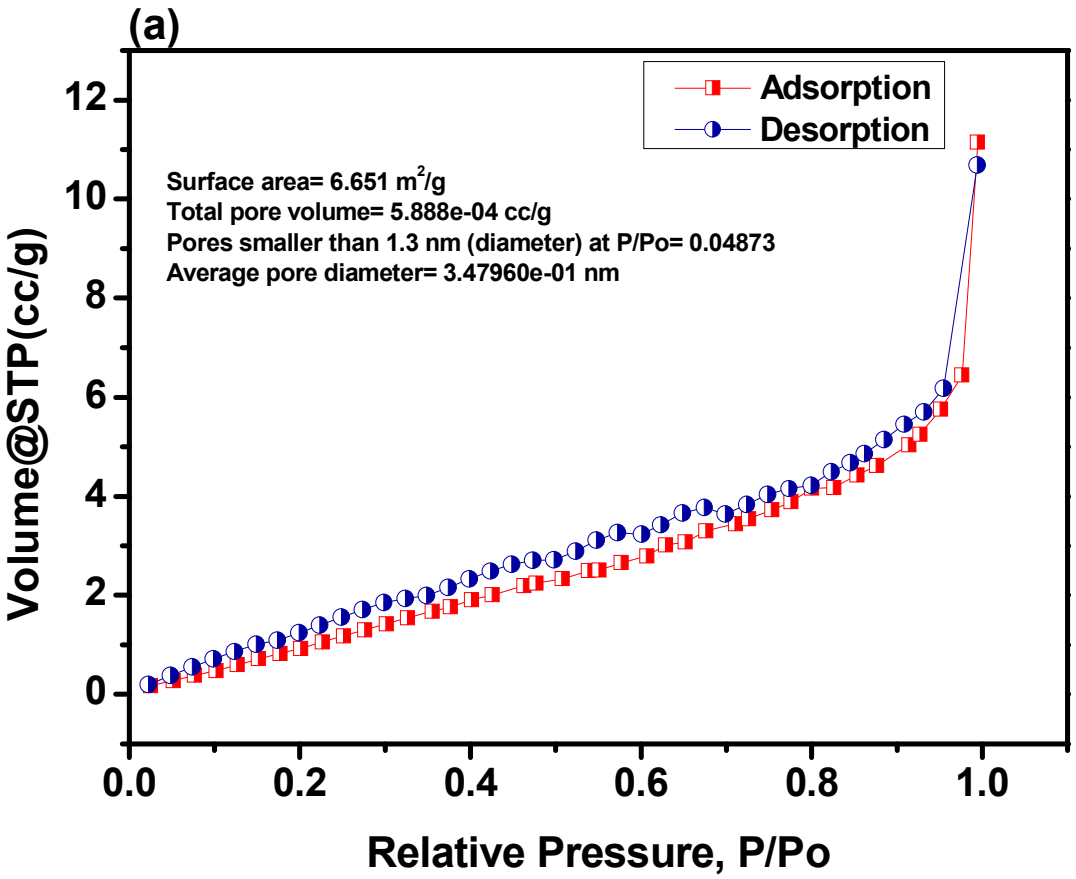
S.No.	Volume of solvent (H_2O) used	Metal salt and concentration used	Amount of xerogel used	Time for removal operation (hour)	Removal %
1	20 mL water	$Hg(OAc)_2$, 1 mM	10 mg	3	57.45
2				6	60.48
3			20 mg	3	72.52
4				6	80.12
5			40 mg	3	90.56
6				6	99.24

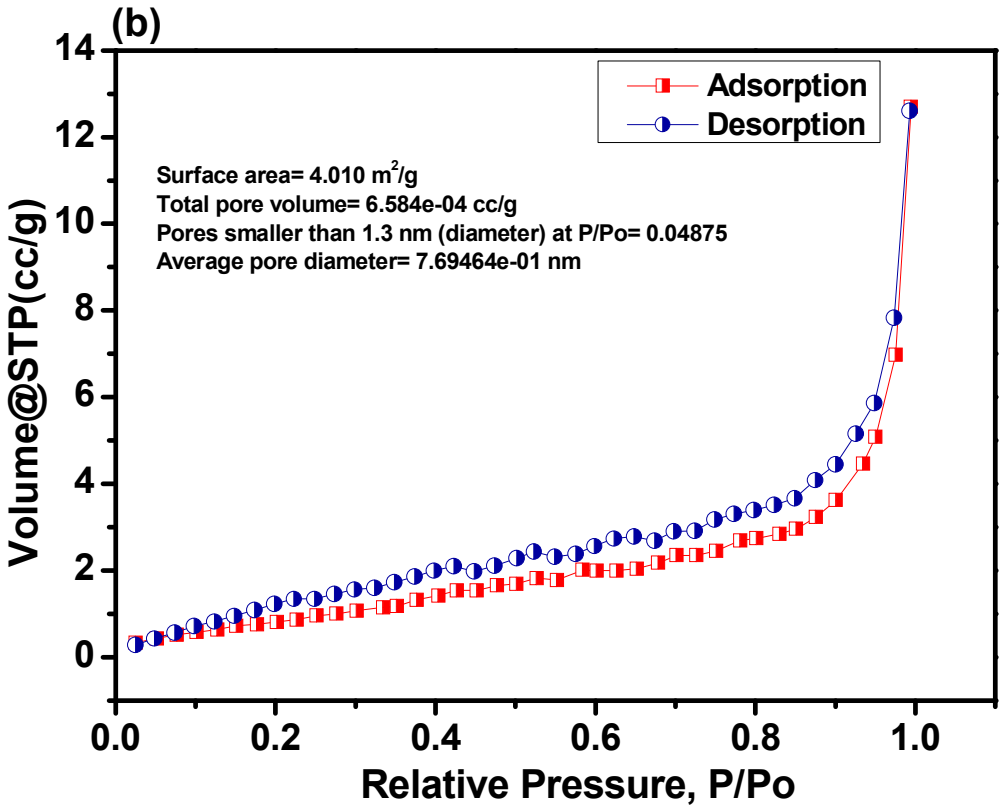
Table S5: ICP-AES analysis of study of adsorption property of organogel **G8GE.**

Heavy metal salt	Concentration in ppm before treatment in 20 mL water	Concentration in ppm after treatment by xerogel G8GE (ppm)	Adsorption capacity (q) in (mg/g)	% of heavy metal separation from water
$HgCl_2$	271 ppm (1 mM)	118.517	76.24	56.27 %
$Hg(CH_3COO)_2$	318 ppm (1 mM)	2.42	157.79	99. 24 %
$HgSO_4$	296 ppm (1 mM)	0.289	147.81	99.90 %
$CdCl_2$	201 ppm (1 mM)	96.818	52.09	51.83 %
$Cd(CH_3COO)_2$	266 ppm (1 mM)	3.501	131.25	98.68 %
$CdSO_4$	769 ppm (1 mM)	119.437	284.93	84.47%
$PbCl_2$	278 ppm (1 mM)	112.033	83	59.70 %
$Pb(CH_3COO)_2$	443 ppm (1 mM)	0.432	221.02	99.90 %

Table S6: Adsorption capacity of various gel-based adsorbent.

S. No.	Adsorbent	Adsorbate	Adsorption capacity (q)	References
1	Bi-component supramolecular gel (RQ)	Hg^{2+}	59 mg/g	Ref. 1
2	Alginate cryogel of sweet lime-derived activated carbon (SLACC)	Cr^{6+}, Cd^{2+}, Pb^{2+}, Hg^{2+} and As^{3+}	3.71, 4.22, 20.04, 4.37 and 7.31 mg/g	Ref. 2
3	Xerogel of BTG organogel	Cu^{2+} and Hg^{2+}	99.02 % and 99.46 % (1×10^{-5} M metal salt by 1 mg of xerogel)	Ref. 3
4	G-L organogel	Pb^{2+} and Hg^{2+}	85.63 % and 99.95 % (For Pb^{2+} it is from 301.5 mg/L to 43.34 mg/L and for Hg^{2+}, it is from 24.12 to 0.011 mg/L) with xerogel 1 wt. %in 2mL	Ref. 4
5	Xerogel of G8GE organogel	Chloride, acetate and sulphate salt of Hg^{2+} and Cd^{2+} , Chloride and acetate of Pb^{2+}	76.24, 157.79, 147.81, 52.09, 131.25, 284.93, 83 and 221.02 respectively.	This work


(a)
Adsorption
Desorption
Surface area= 6.651 m²/g
Total pore volume= 5.888e-04 cc/g
Pores smaller than 1.3 nm (diameter) at P/Po= 0.04873
Average pore diameter= 3.47960e-01 nm
Volume@STP(cc/g)
Relative Pressure, P/Po
0
2
4
6
8
10
12
0.0
0.2
0.4
0.6
0.8
1.0


(b)
Adsorption
Desorption
Surface area= 4.010 m²/g
Total pore volume= 6.584e-04 cc/g
Pores smaller than 1.3 nm (diameter) at P/Po= 0.04875
Average pore diameter= 7.69464e-01 nm
Volume@STP(cc/g)
Relative Pressure, P/Po
0
2
4
6
8
10
12
14
0.0
0.2
0.4
0.6
0.8
1.0

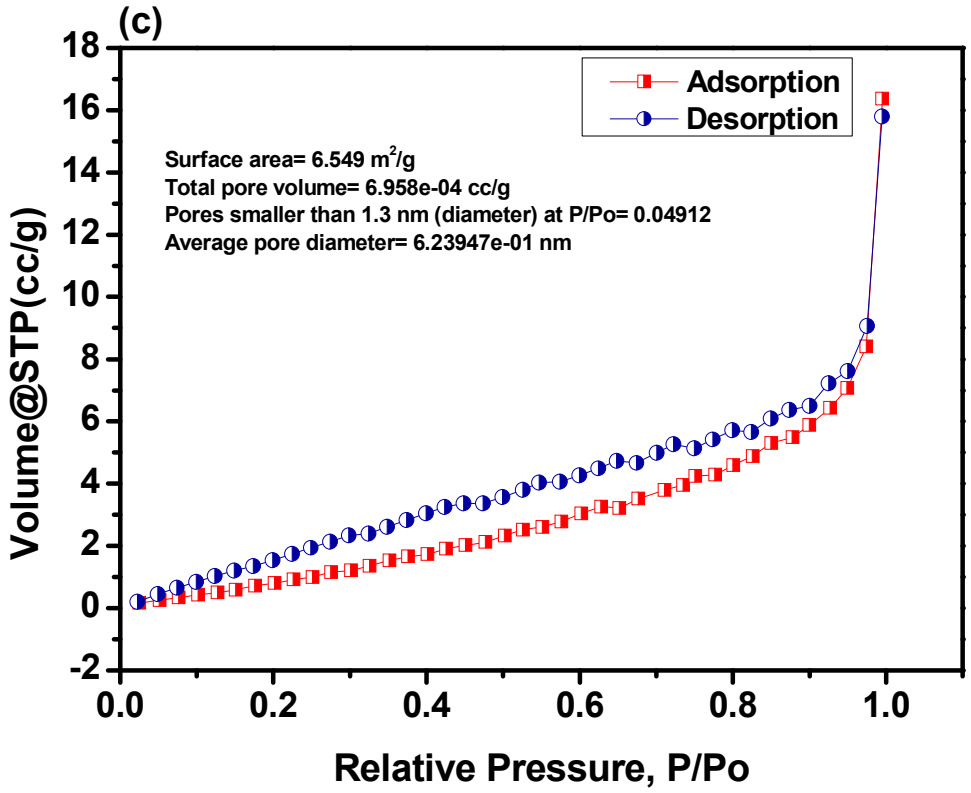


Fig. S42: BET analysis data of (a) Xerogel **G8GE** before $Hg(OAc)_2$ adsorption (b) After $Hg(OAc)_2$ adsorption and (c) after $Hg(OAc)_2$ removal from xerogel **G8GE** or recovery of xerogel **G8GE**.

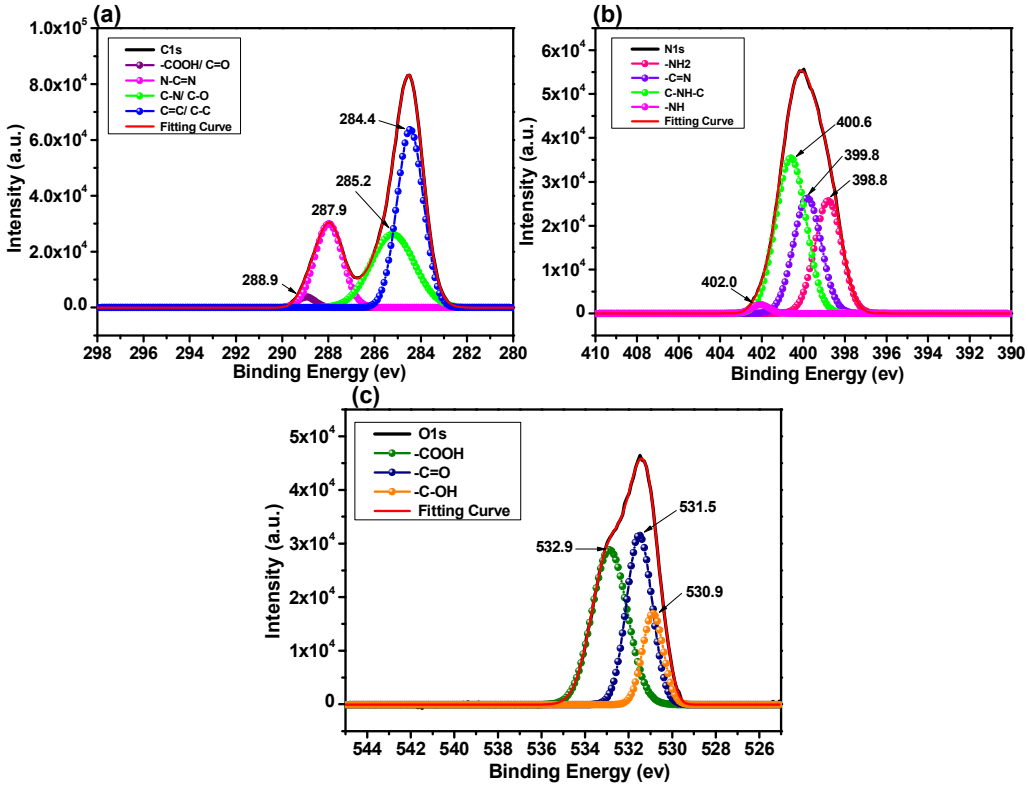


Fig. S43: XPS analysis of xerogel **G8GE** showing (a) C1s spectrum (b) N1s spectrum and (c) O1s spectrum.

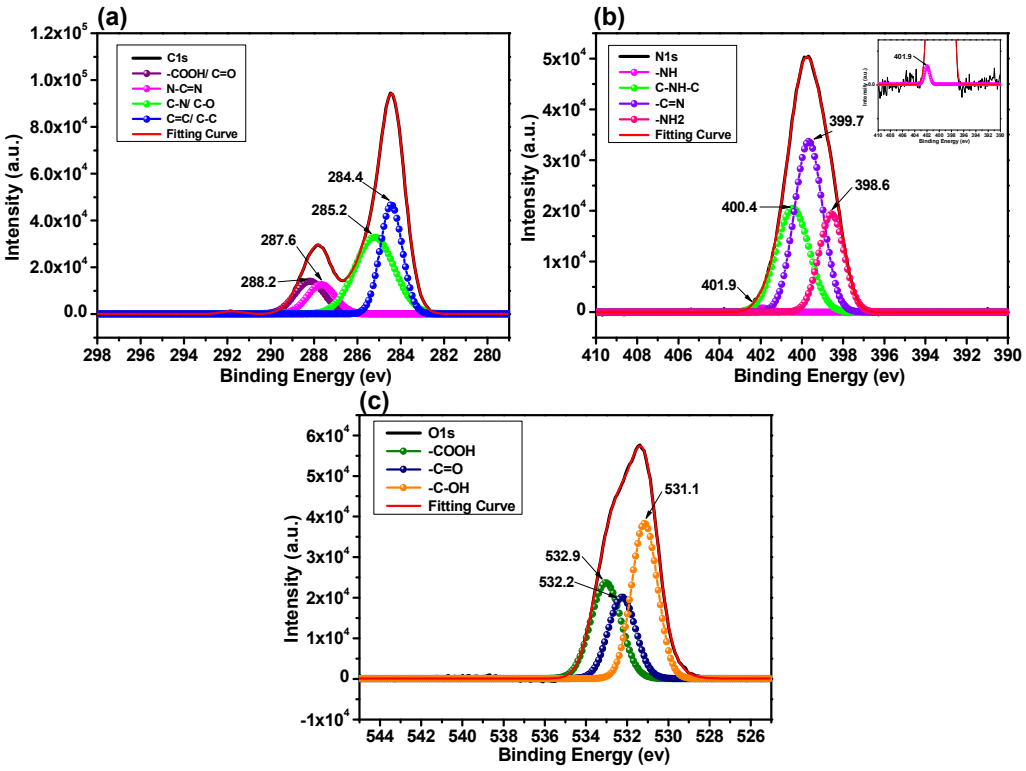


Fig. S44: XPS analysis of xerogel **mtG8GE** showing (a) C1s spectrum (b) N1s spectrum and (c) O1s spectrum.

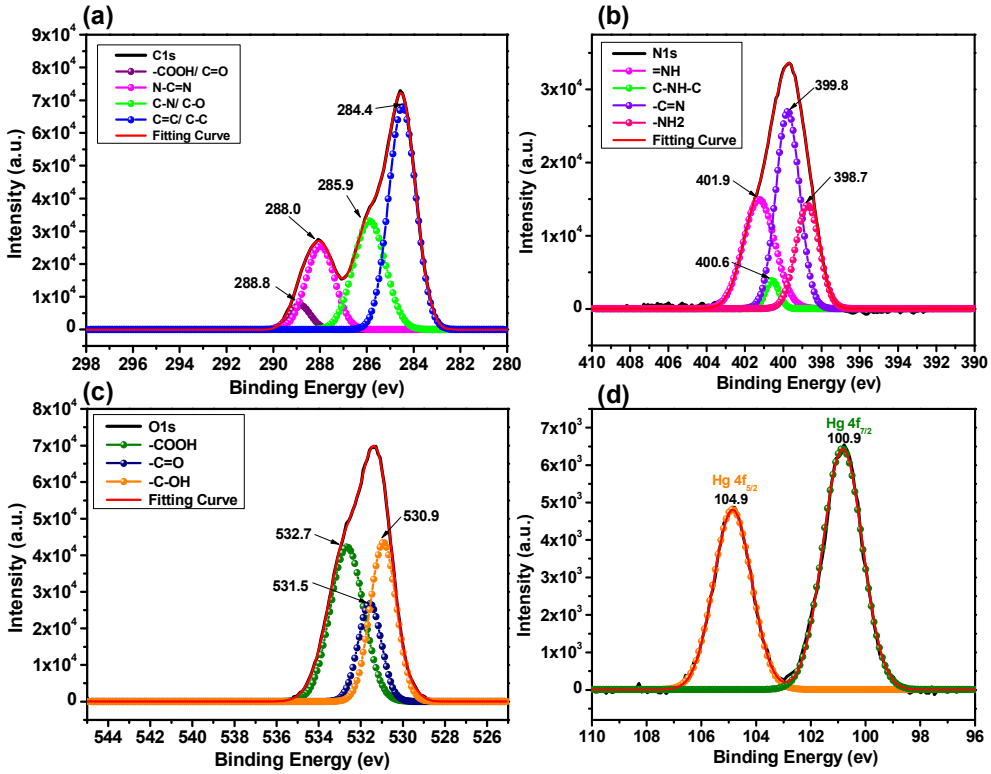


Fig. S45: XPS analysis of xerogel **mrG8GE** showing (a) C1s spectrum (b) N1s spectrum and (c) O1s spectrum and (d) Hg 4f spectrum.

Table S7: XPS peaks position of various groups for **G8GE**, **mtG8GE** and recovered **mrG8GE**.

Groups or Element present	Xerogel G8GE Binding Energy (eV)	mtG8GE Binding Energy (eV)	mrG8GE Binding Energy (eV)
-COOH/ C=O	288.9	288.2	288.8
N-C=N	287.9	287.6	288.0
C-N/ C-O	285.2	285.2	285.9
C=C/ C-C	284.4	284.4	284.4
-NH	402.0	401.9	401.9
C-NH-C	400.6	400.4	400.6
-C=N	399.8	399.7	399.8
-NH2	398.8	398.6	398.7
-COOH	532.9	532.9	532.7
C=O	531.5	532.2	531.5
C-OH	530.9	531.1	530.9
Hg^{2+} (Hg $4f_{7/2}$)	-	100.9	100.9
Hg^{2+} (Hg $4f_{5/2}$)	-	104.9	104.9

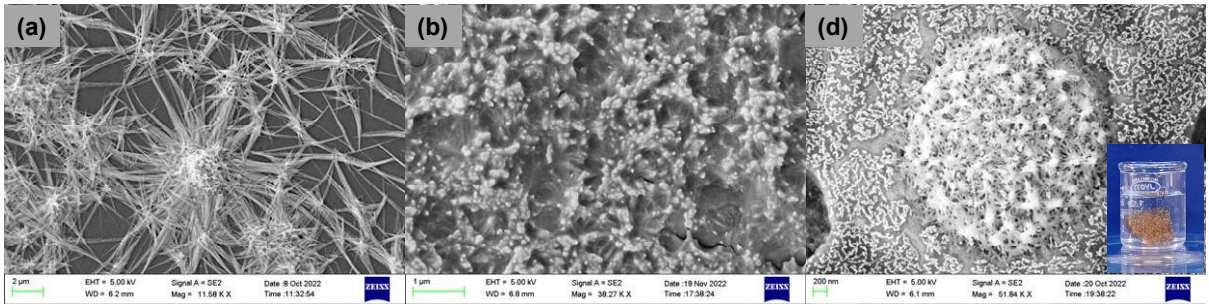


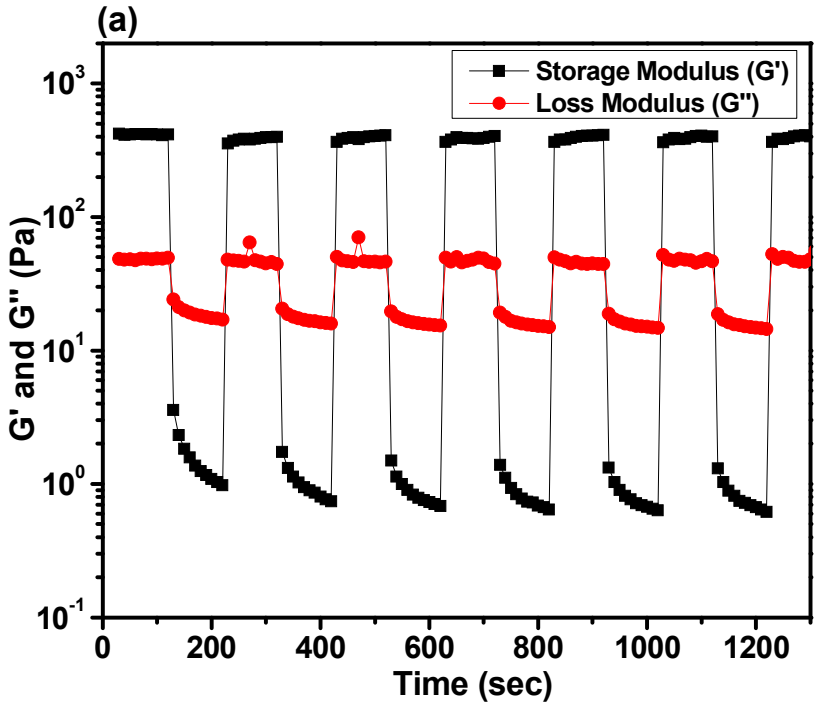
Fig. S46: FE-SEM images of (a) **M1G8GECl$_2$** gel by mixing (b) **M1G8GECl$_2$Ads** by adsorption (c) **M1G8GECl$_2$Ads** when **G8GE** inserted inside the aqueous solution of $HgCl_2$.

Table S8: Recyclability of xerogel **G8GE** for heavy metal separation.

Concentration of $Hg(CH_3COO)_2$ in ppm before treatment (20 mL water)	Concentration in ppm after treatment by xerogel G8GE (ppm)	Removal % from water
318 ppm (1 mM)	2.514	99.21
318 ppm (1 mM)	5.092	98.39
318 ppm (1 mM)	5.271	98.34
318 ppm (1 mM)	6.003	98.11
318 ppm (1 mM)	8.311	97.39

Table S9: Water remediation at different pH by xerogel **G8GE**.

Concentration of $Hg(CH_3COO)_2$ in ppm before treatment (20 mL water)	pH of contaminated water system	Concentration in ppm after treatment by xerogel G8GE (ppm)	Removal % from water
318 ppm (1 mM)	3	87.876	72.36
318 ppm (1 mM)	5.4	2.405	99.24
318 ppm (1 mM)	7	7.338	97.69
318 ppm (1 mM)	10	5.514	98.26



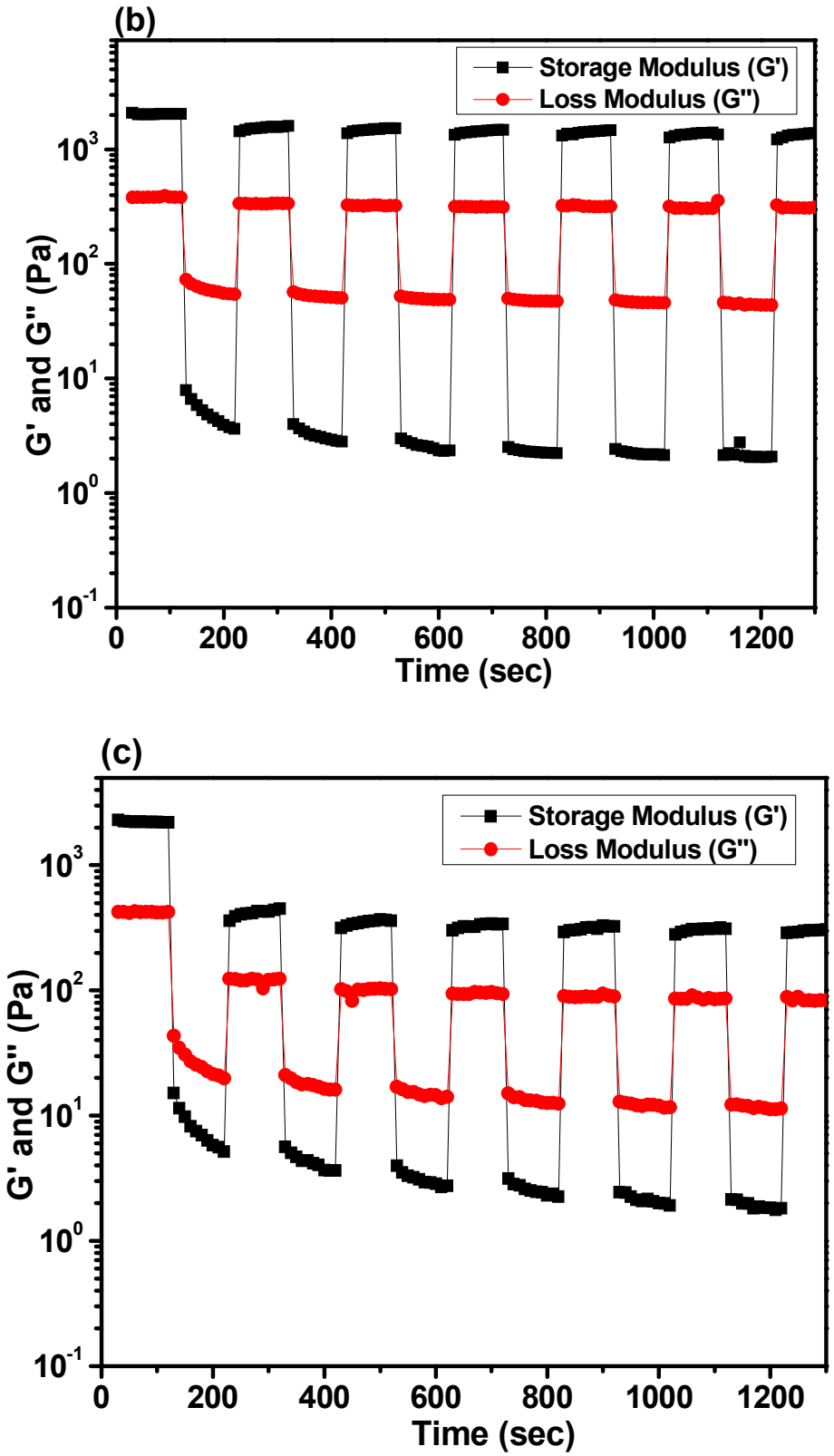


Fig. S47: Time oscillation sweep experiment of organogel **G8GE** at (a) 0.02: 0.02 mmol (b) 0.03: 0.03 mmol and (c) 0.04: 0.04 mmol.

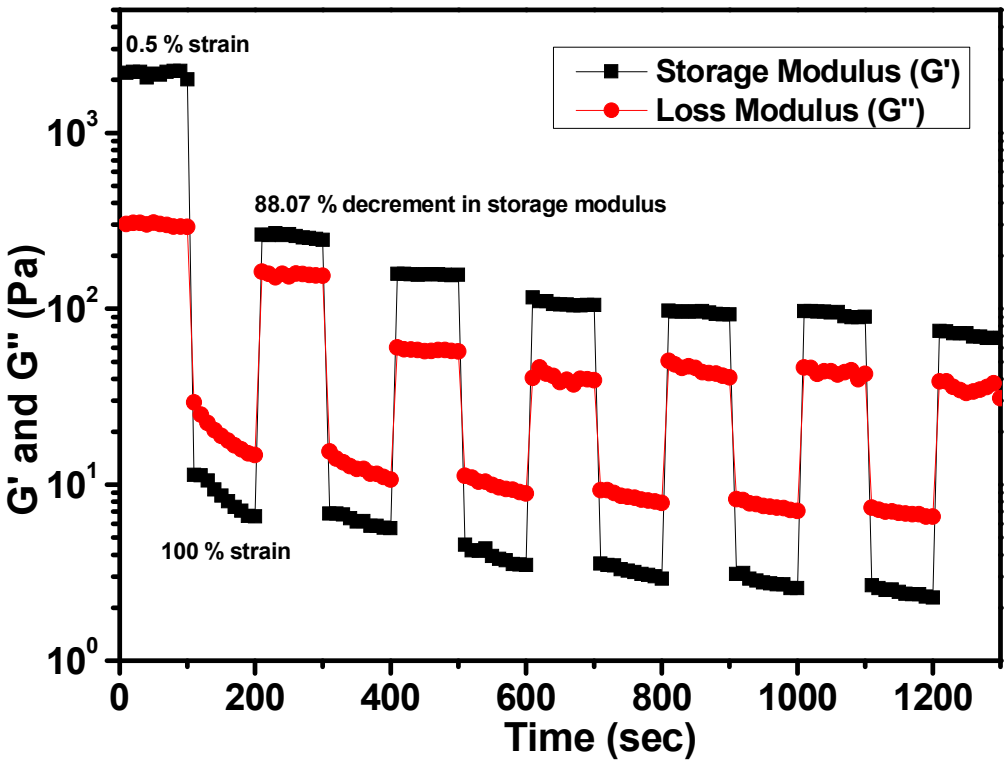


Fig. S48: Time oscillation sweep experiment of metallogel **M3G8GECl$_2$.**

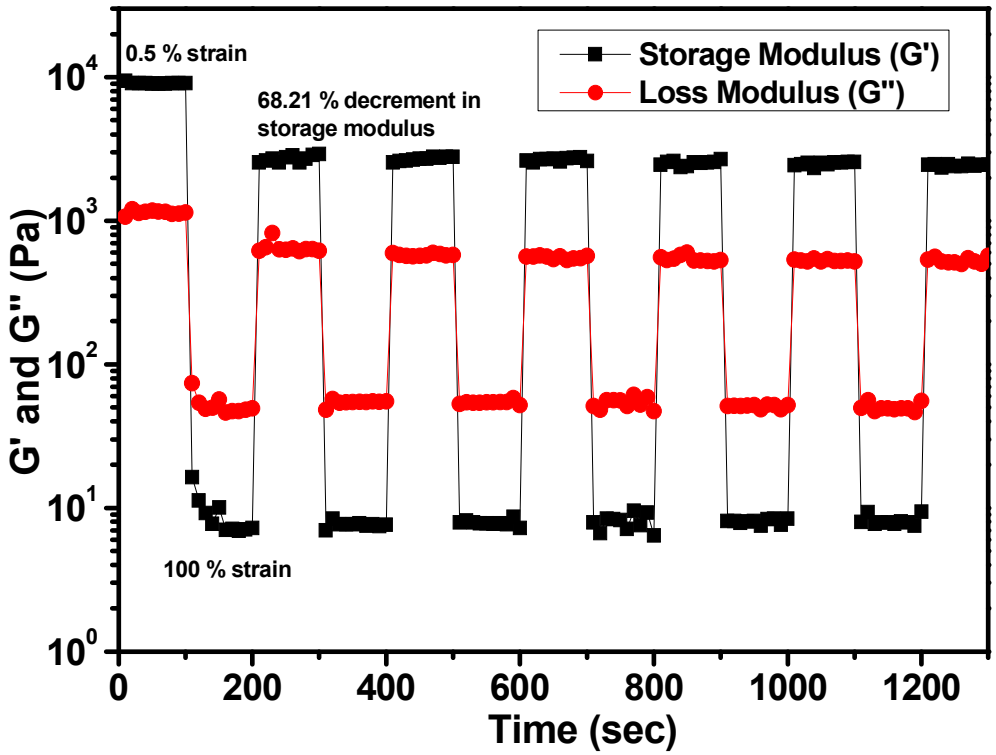


Fig. S49: Time oscillation sweep experiment of metallogel **M2G8GECl$_2$Ads.**

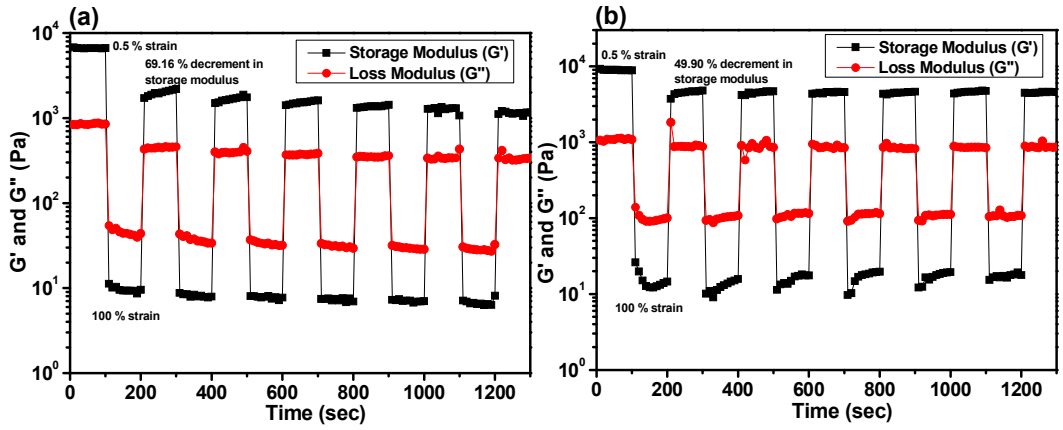


Fig. S50: Time oscillation sweep experiment of metallogel (a) **M2G8GE(OAc)$_2$Ads** and **(b) M2G8GESO$_4$Ads.**

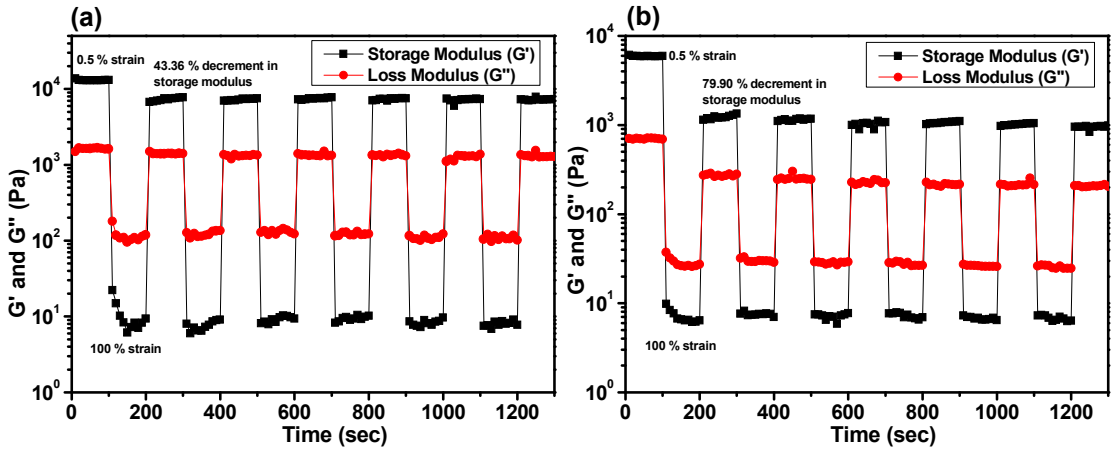


Fig. S51: Time oscillation sweep experiment of metallogel (a) **M3G8GECl$_2$Ads** and **(b) M3G8GE(OAc)$_2$Ads.**

Table S10. Intermolecular H-bond binding energies of individual sites along with the associated bond lengths of structure **G8GE**.

Binding Site	H-bond length (Å)	$\rho(r_{BCP})$ (a.u.)	HBE (kcal/mol)
O-H...O	1.66	0.0497	-10.33
O-H...O	1.66	0.0497	-10.34
O-H...N	1.86	0.0367	-7.44
O-H...N	1.86	0.0368	-7.46
N-H...O	1.70	0.0466	-9.65
N-H...O	1.70	0.0466	-9.66

Table S11. Cartesian coordinates of **GE**.

69
Energy = -2163.413966 Hartree

C	-1.19846001	0.73221939	0.55276116
C	0.02869176	1.39738300	0.56213802
C	1.23003830	0.67766094	0.55260126
C	1.19265187	-0.71858676	0.56012894
C	-0.03149061	-1.39932539	0.55113776
C	-1.22115608	-0.66837765	0.55842979
H	0.09482226	2.47894230	0.61111845
H	2.09676942	-1.31610398	0.60662826
H	-2.19116349	-1.15159696	0.60271265
C	-2.53040615	1.43298728	0.59024847
C	2.50319919	1.48026541	0.58766266
C	0.02672127	-2.90351111	0.58828944
H	-1.69591308	3.06402567	-0.32700222
H	3.48836622	-0.05008641	-0.35052830
H	-1.79486736	-2.99561167	-0.34384610
O	-3.53239696	0.86264417	1.02043008
O	2.51412792	2.62875394	1.02920696
O	1.01880192	-3.48687147	1.02417157
C	-3.67362612	3.56646183	0.01825512
C	-4.94035382	3.08690831	-0.29865477
C	-3.46068302	4.95505480	0.21597418
C	-6.02112368	3.97076342	-0.43468672
H	-5.08282387	2.02479357	-0.43534854
C	-4.54838969	5.83238796	0.04587756
C	-5.80695046	5.34856871	-0.27196254
H	-4.39162436	6.89825656	0.18773794
H	-6.64446209	6.02871452	-0.38427905
C	4.92117952	1.39886617	0.00186529
C	5.14931034	2.74147218	-0.28165803
C	6.01048431	0.50387486	0.16070418
C	6.45866579	3.22388696	-0.42477201
H	4.30655347	3.40904848	-0.38841409
C	7.31677893	0.99635421	-0.01750844
C	7.53749157	2.33375664	-0.30392747
H	8.15565912	0.31476730	0.09308936
H	8.54788170	2.71038291	-0.42269269
C	-1.25132415	-4.95943801	0.01454531
C	-2.56626639	-5.46187043	0.19459111
C	-0.20215316	-5.82343438	-0.28090611
C	-2.78691305	-6.84189881	0.02567421
C	-0.43242739	-7.20047990	-0.41412560
H	0.79330722	-5.42166667	-0.40347363
C	-1.73781901	-7.69659024	-0.27157829
H	-3.79237242	-7.23349374	0.15244468
H	-1.91225248	-8.76140573	-0.38295918
N	-2.54061117	2.71611234	0.11108099

N	3.61582580	0.85010705	0.09618788
N	-1.07672698	-3.55354985	0.10268612
N	-2.18885498	5.42512489	0.50559506
H	-2.14854878	6.39616001	0.79387656
H	-1.63683265	4.83785119	1.12171081
N	-3.60892083	-4.58824108	0.46447757
H	-4.47681386	-5.03391113	0.74009931
H	-3.38189235	-3.81753399	1.08386301
N	5.76930442	-0.83685005	0.42136554
H	6.58858045	-1.37483920	0.67989169
H	4.99724589	-1.02457113	1.05250428
C	-7.38188170	3.50139610	-0.76107190
O	-8.35423701	4.22567990	-0.91309939
O	-7.47136060	2.15255980	-0.87750096
H	-8.40105968	1.95039289	-1.09269482
C	6.74356996	4.64290164	-0.71580212
O	7.85962324	5.11389602	-0.87680826
O	5.62698998	5.40969911	-0.79477948
H	5.92315514	6.31814743	-0.99063721
C	0.65532893	-8.15091367	-0.71756123
O	0.51133837	-9.35519420	-0.86687932
O	1.87198729	-7.55939426	-0.82097735
H	2.51305501	-8.26623023	-1.02367954

Table S12. Cartesian coordinates of **G8**.

30
Energy = -1217.738870 Hartree

C	-1.21535050	-0.45363285	0.00000422
C	1.00077919	-0.82616842	-0.00000089
C	0.21537843	1.27937668	-0.00001944
N	1.29445634	0.47734839	-0.00001501
N	-1.06028443	0.88191256	-0.00000903
N	-0.23333181	-1.35970545	0.00000765
H	1.45750405	2.89693034	-0.00004038
H	-3.23673369	-0.18562011	0.00000489
H	1.78025422	-2.71064685	0.00001968
C	-0.43229902	3.64706277	-0.00002452
N	-1.77192724	3.53584929	-0.00000207
H	-2.32050158	2.68258413	0.00001786
C	-2.94288617	-2.19764829	0.00002517
N	-2.17720375	-3.30241305	0.00003900
H	-1.16400359	-3.35118725	0.00004321
C	3.37514475	-1.44933687	-0.00000462
N	3.94865196	-0.23366423	-0.00002590
H	3.48364934	0.66788400	-0.00004194
N	2.02973759	-1.72823997	0.00000503
N	-2.51111901	-0.89334606	0.00001080
N	0.48204458	2.62151062	-0.00002832

N	-0.11085780	4.93340497	-0.00003809
N	-1.29798669	5.59703553	-0.00002258
N	-2.30170728	4.78205726	-0.00000139
N	-4.21779186	-2.56193236	0.00003046
N	-4.19944401	-3.92190063	0.00004837
N	-2.99192505	-4.38404027	0.00004962
N	4.32844276	-2.37094191	0.00000747
N	5.49678629	-1.67469416	-0.00000696
N	5.29277809	-0.39793515	-0.00003232

Table S13. Cartesian coordinates of **2GE**-**2G8** (**G8GE**).

198
Energy = -6762.402264 Hartree

C	15.66640983	-2.02490993	0.20242577
C	14.38171527	-1.62059262	0.57047069
C	14.04557966	-0.26134741	0.61166582
C	15.01742918	0.69309369	0.30485513
C	16.31078690	0.30201333	-0.06474111
C	16.63121680	-1.05649365	-0.10275531
H	13.62051544	-2.33424720	0.86678293
H	14.81894157	1.75699772	0.37400013
H	17.63292493	-1.40335896	-0.33243728
C	16.10881778	-3.46320766	0.16576719
C	12.64347236	0.07776183	1.04279347
C	17.29812290	1.40274929	-0.34774425
H	14.19271342	-4.03186566	-0.27486556
H	12.73685965	1.82089448	-0.02929387
H	18.32547195	0.15395330	-1.60418552
O	17.29342354	-3.76390595	0.30980829
O	11.98449629	-0.70941573	1.72148305
O	17.14363463	2.52708770	0.12814428
C	15.26987022	-5.78946935	-0.13441296
C	16.40388325	-6.38636499	-0.67592073
C	14.18415911	-6.58633843	0.31336846
C	16.48234934	-7.78181884	-0.79577680
H	17.22420261	-5.76320586	-1.00085918
C	14.26547498	-7.98233061	0.15694574
C	15.39596655	-8.57073983	-0.38691647
H	13.43427045	-8.59811888	0.48935252
H	15.45911210	-9.64888138	-0.48830186
C	10.87094099	1.81565790	0.85879390
C	9.73969052	1.01079357	0.93556339
C	10.75546641	3.22609706	0.96966265
C	8.47083820	1.58347742	1.10999219
H	9.84618242	-0.06162325	0.86152945
C	9.47248321	3.78724137	1.11090924
C	8.34856847	2.98026344	1.18087450
H	9.37615724	4.86669115	1.18710182

H	7.36525554	3.41985018	1.30806782
C	19.38399420	1.93145602	-1.59698326
C	20.66535701	1.35605545	-1.79806223
C	19.16799421	3.27906585	-1.86624056
C	21.69332271	2.16855083	-2.31220073
C	20.21118836	4.08301678	-2.34857646
H	18.18758201	3.70019532	-1.69707769
C	21.47096216	3.50924575	-2.58118495
H	22.67503996	1.73316674	-2.47675245
H	22.27279455	4.13345791	-2.96078055
N	15.11525939	-4.38214841	-0.04568519
N	12.16720585	1.29052658	0.61937315
N	18.34539415	1.06624611	-1.16407217
N	13.04842482	-5.97908812	0.83007917
H	12.38876501	-6.61342760	1.26575768
H	13.21639299	-5.17022027	1.41914773
N	20.86461134	0.00602048	-1.55063636
H	21.83373735	-0.29056294	-1.56311396
H	20.38045925	-0.36517308	-0.74010218
N	11.88804855	4.02008940	0.87305146
H	11.74742896	4.99493078	1.11230383
H	12.71829294	3.65016837	1.32377569
C	17.67124647	-8.45400465	-1.35624424
O	17.78610783	-9.66103854	-1.50771536
O	18.66172403	-7.59363187	-1.70208382
H	19.39042132	-8.13418596	-2.06027687
C	7.25968393	0.74888320	1.20680791
O	6.12584283	1.23716855	1.32216546
O	7.48104555	-0.55978715	1.16212171
H	6.61124072	-1.05750675	1.23985874
C	20.02502893	5.51856791	-2.63755278
O	20.88840591	6.26036260	-3.08190606
O	18.77392274	5.96453394	-2.36030827
H	18.75748919	6.91307490	-2.58719549
C	-5.04765182	-1.07179686	1.92715093
C	-5.38135077	0.28398872	1.91298225
C	-4.38558316	1.26634518	1.99129977
C	-3.04933087	0.87862368	2.10976507
C	-2.69919476	-0.47745330	2.11981104
C	-3.70220024	-1.44502694	2.03886847
H	-6.41068344	0.62332780	1.87353185
H	-2.24964718	1.60147512	2.22878957
H	-3.48028756	-2.50496113	2.09535248
C	-6.05683574	-2.18838956	1.87859199
C	-4.84790061	2.69937057	1.98814770
C	-1.23777565	-0.80325695	2.27415870
H	-7.39916188	-0.95370591	0.93746015
H	-3.03309927	3.29532761	1.23842149
H	-1.52736687	-2.54103471	1.23384363
O	-5.77253372	-3.31418238	2.28563520

O	-5.99972640	2.99219594	2.30618874
O	-0.46712700	-0.00975267	2.81341094
C	-8.36470864	-2.77418674	1.18507509
C	-8.17340238	-4.07631460	0.74155508
C	-9.67196160	-2.29071833	1.45251835
C	-9.26859418	-4.93202606	0.54550278
H	-7.16837758	-4.42709335	0.55412107
C	-10.76450100	-3.14977622	1.21809093
C	-10.56790636	-4.44688065	0.77685153
H	-11.77027973	-2.78656089	1.41035551
H	-11.42278813	-5.09572492	0.62182224
C	-4.15143282	5.02578545	1.48076880
C	-5.32950034	5.53107787	0.94640033
C	-3.11266721	5.90268011	1.88827846
C	-5.50981114	6.91488670	0.79612078
H	-6.11074493	4.84539881	0.65014854
C	-3.29545025	7.28819029	1.70407307
C	-4.47187842	7.78624811	1.17136707
H	-2.50324511	7.96793090	2.00535436
H	-4.59640581	8.85713506	1.05448521
C	0.47122062	-2.54130124	1.75680210
C	0.60153788	-3.95419217	1.80870548
C	1.60033075	-1.73646140	1.65000195
C	1.88780675	-4.51569125	1.70501107
C	2.87843423	-2.31096132	1.57965586
H	1.48510521	-0.66285371	1.62306788
C	3.00832304	-3.70862000	1.59307651
H	1.99351644	-5.59664960	1.73537268
H	3.99730396	-4.14944473	1.53104254
N	-7.28110619	-1.87022535	1.35198143
N	-3.91827074	3.62881085	1.60073011
N	-0.84576999	-2.01443241	1.76741473
N	-9.85653730	-0.98888996	1.87536625
H	-10.78109902	-0.77025220	2.22699891
H	-9.12742467	-0.60685684	2.46708673
N	-0.53133920	-4.74991286	1.89217826
H	-0.35016547	-5.73094113	2.07102993
H	-1.26744678	-4.40080491	2.49671340
N	-1.93357646	5.39294441	2.39457337
H	-1.32117931	6.06533940	2.84059990
H	-2.01264487	4.53685378	2.93163215
C	-9.08498804	-6.31880610	0.09111935
O	-10.03674909	-7.09015581	-0.10463392
O	-7.81395921	-6.67299782	-0.09087078
H	-7.71168666	-7.61728832	-0.39913592
C	-6.75224592	7.46833334	0.23615319
O	-6.92809718	8.68545149	0.07248899
O	-7.66676115	6.55310001	-0.08030036
H	-8.49872992	6.94847792	-0.46599446
C	4.08908200	-1.47625909	1.47600757

O	5.22431200	-1.96468225	1.37569289
O	3.86580973	-0.16739668	1.49903395
H	4.73619630	0.33020679	1.42719151
C	-10.09450635	13.13389251	-1.53464278
C	-8.03447388	13.01566563	-0.64546821
C	-9.20267208	11.13791890	-1.04539470
N	-8.06679529	11.68820111	-0.59011279
N	-10.25771827	11.79669388	-1.53280148
N	-9.01781983	13.80780873	-1.10811824
H	-8.34865488	9.34594666	-0.57721138
H	-11.95574318	13.31399719	-2.34410127
H	-6.85655263	14.64075891	-0.22717519
C	-10.19176363	8.91684556	-1.33022264
N	-11.39579528	9.18093872	-1.85921638
H	-11.79122282	10.08693891	-2.08727707
C	-11.25031779	15.21270791	-2.14230339
N	-10.32255323	16.11891194	-1.78818021
H	-9.40985392	15.93831290	-1.38300662
C	-5.79160284	12.99071857	0.32309428
N	-5.60169462	11.66518841	0.47709705
H	-6.22836849	10.89513100	0.24769472
N	-6.89874044	13.62897195	-0.19067773
N	-11.15390201	13.84752909	-2.02817700
N	-9.20685613	9.77896415	-0.97118817
N	-10.07798322	7.59905266	-1.19250112
N	-11.24454833	7.07502997	-1.65225653
N	-12.04530304	8.00175766	-2.05491534
N	-12.30468091	15.85079952	-2.63225554
N	-11.98543484	17.17118180	-2.56316924
N	-10.80721074	17.35315104	-2.06267156
N	-4.71118139	13.62724869	0.75681124
N	-3.86282452	12.65247721	1.17724757
N	-4.37689050	11.47654773	1.01808683
C	-12.18175796	-12.16617263	-1.52525789
C	-13.17447733	-10.25603046	-0.88157965
C	-10.93628633	-10.36471775	-1.05408000
N	-12.01352510	-9.62049605	-0.76076236
N	-10.94318432	-11.64296609	-1.44214942
N	-13.33458038	-11.53580928	-1.26262912
H	-9.84777392	-8.69711138	-0.61459537
H	-11.34758908	-13.93096277	-2.11020448
H	-15.20010217	-10.01273810	-0.67632253
C	-8.49983204	-10.13464699	-1.12836619
N	-8.08674892	-11.35010215	-1.51717596
H	-8.65514911	-12.16330878	-1.72908593
C	-13.35820349	-14.24581948	-2.08912460
N	-14.63293746	-13.86309690	-1.89959164
H	-14.96313655	-12.95044930	-1.60315430
C	-14.34447733	-8.22882349	-0.18105780
N	-13.30351175	-7.39426789	0.01045255

H	-12.30714227	-7.57139473	-0.10858550
N	-14.30609695	-9.54319510	-0.59106661
N	-12.23340783	-13.47620965	-1.92054972
N	-9.76400145	-9.68625113	-0.92059797
N	-7.42821350	-9.36542753	-0.95918916
N	-6.35796304	-10.14855710	-1.25599769
N	-6.72847210	-11.33694553	-1.59162710
N	-13.34653847	-15.51455030	-2.47524600
N	-14.65424398	-15.88701848	-2.51322684
N	-15.43833771	-14.91673564	-2.17335749
N	-15.46695297	-7.57690881	0.09401176
N	-15.07807834	-6.32655452	0.45716177
N	-13.79188356	-6.19944340	0.41331586

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