Bioinspired catalysis and Bromoperoxidase like activity of Multistimuli-Responsive Supramolecular Metallogel: Supramolecular assembly triggered by pi-pi stacking and hydrogen bonding interactions

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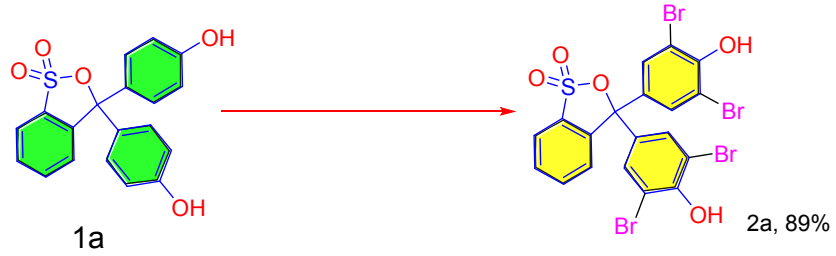
Supporting information

Table S1. Optimization of reaction conditions for the oxidative bromination catalyzed by VO-$_2$-L hydrogel.



Entry	Molar ratio				Temperature (°C)	Time (min)	Isolated yield (%)
	V-comlex: S	S: KBr	Br:H_2O_2	$HClO_4$ (mmol)			
1	1:10	1:2	1:1	2	RT	40	90
2	1:10	1:4	1:1	2	RT	30	89
3	1:10	1:4	1:2	2	RT	35	94
4	1:10	1:4	1:4	2	RT	25	97
5	1:20	1:4	1:4	2	RT	50	96
6	1:05	1:4	1:4	2	RT	20	92
7	1:10	1:4	1:4	2	40	30	93
8	1:10	1:4	1:4	2	55	30	95
9	1:10	1:4	1:4	2	70	30	98
10	1:10	1:4[b]	1:4	2	RT	60	94
11	1:10	1:4	1:4	4	RT	15	96
12	-	1:4[c]	1:4	4	RT	30	15
13	-	1:4[d]	1:4	4	RT	30	28

[a]All the reactions were carried out using 0.129 g catalyst (0.1 mmol), phenol red as substrate, KBr as bromide source and H_2O (5 mL) as solvent unless stated.

[b]Et_4NBr used as bromide source.

[c]Control reaction: 2-hydroxyacetophenone (1.0 mmol), KBr (4.0 mmol), H_2O_2 (16.0 mmol) and H_2O (5 mL).

[d]Control reaction with $HClO_4$: 2-hydroxyacetophenone (1.0 mmol), KBr (4.0 mmol), H_2O_2 (16.0 mmol), $HClO_4$ (4.0 mmol) and H_2O (5 mL).

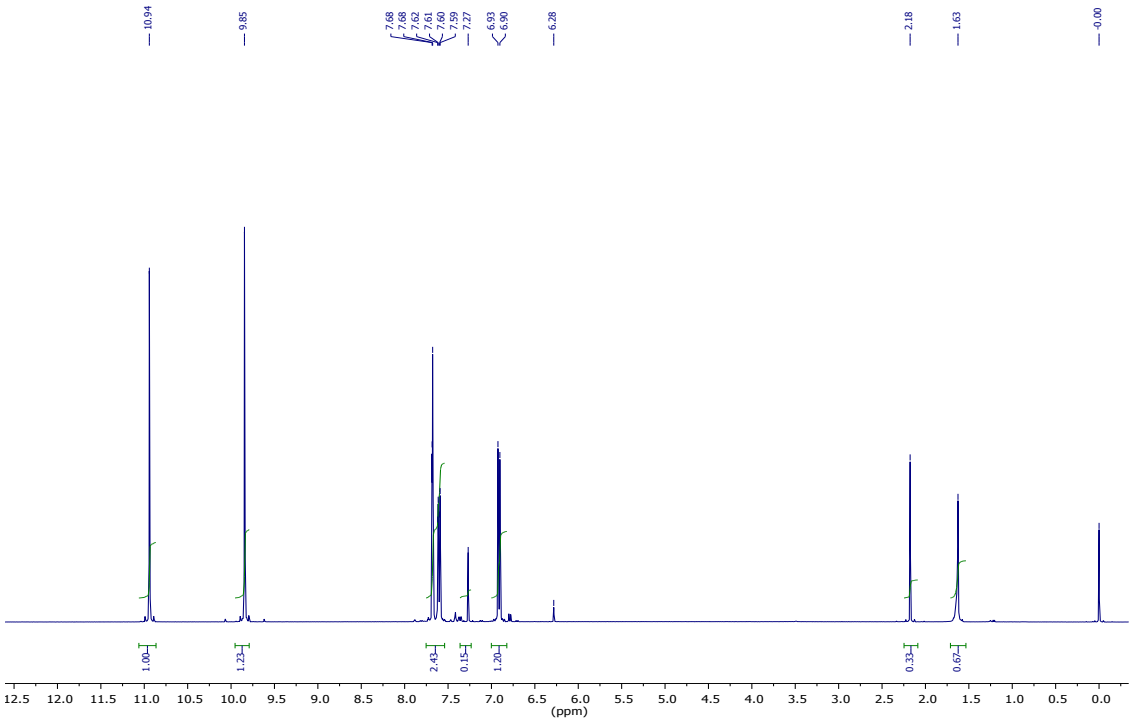


Fig S1. ^{1}H NMR of 5-bromo-2-hydroxybenzaldehyde

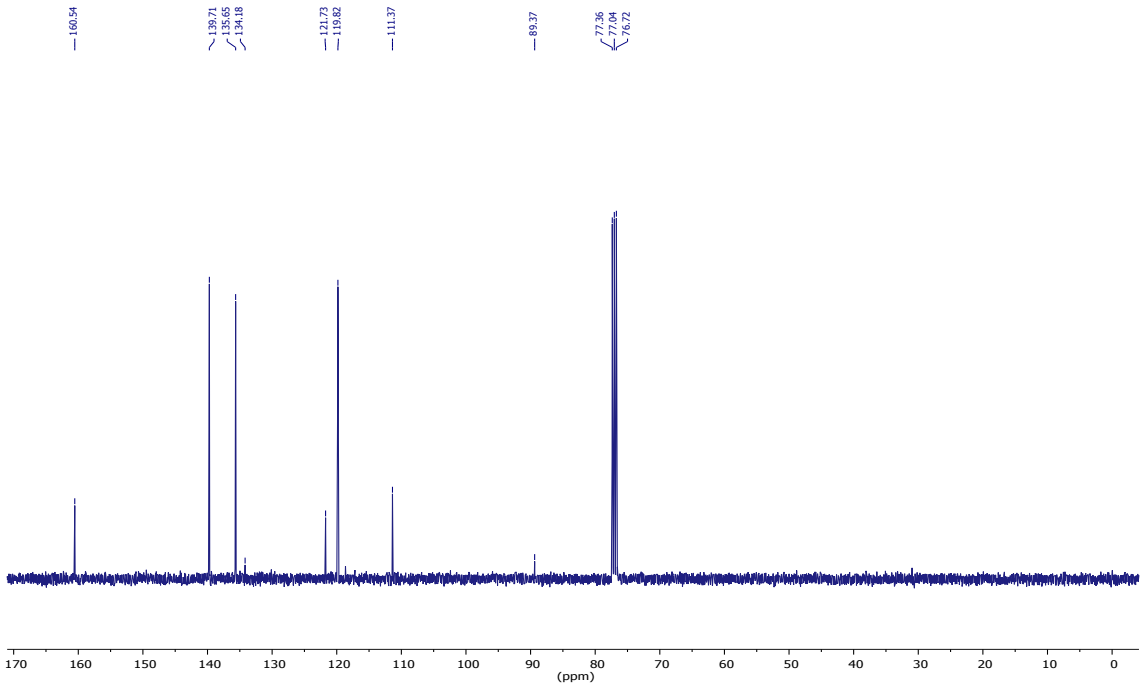


Fig S2. ^{13}C NMR of 5-bromo-2-hydroxybenzaldehyde

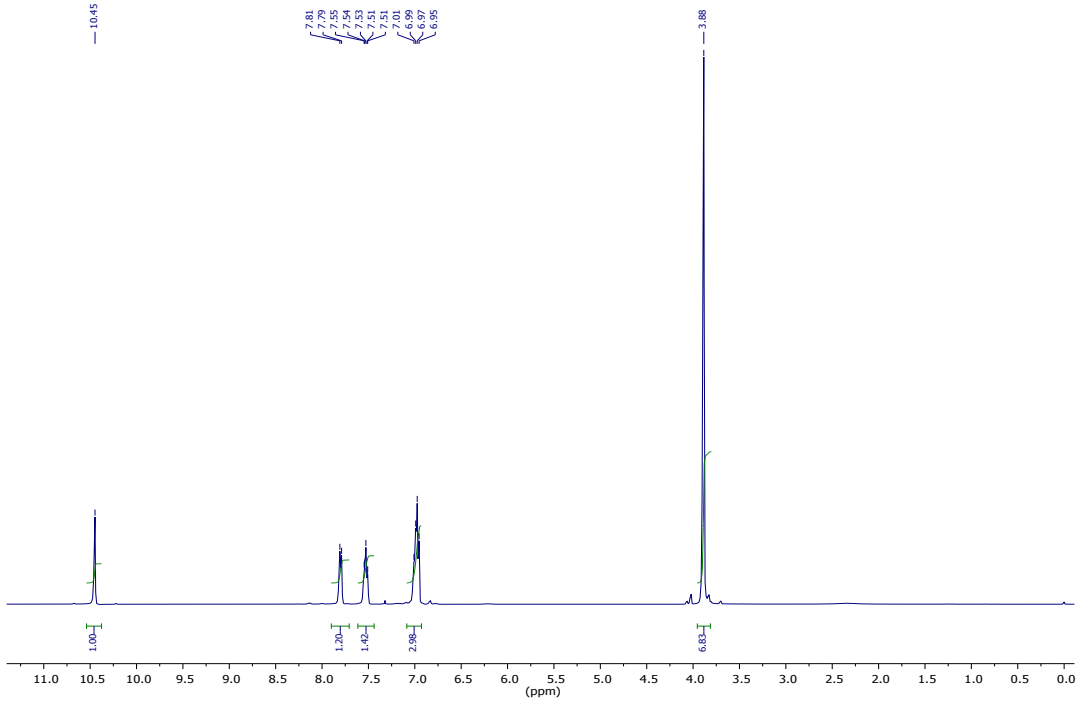


Fig S3. ^{1}H NMR of 2-bromo-1-(2-hydroxyphenyl) ethan-1-one

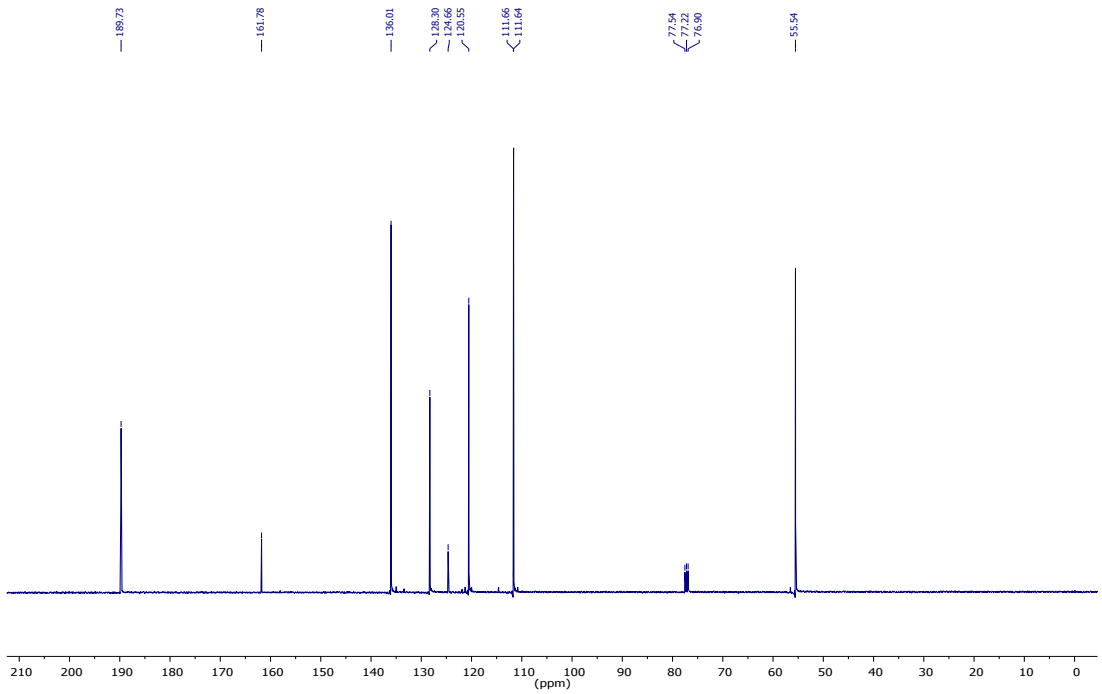


Fig S4. ^{13}C NMR of 2-bromo-1-(2-hydroxyphenyl) ethan-1-one

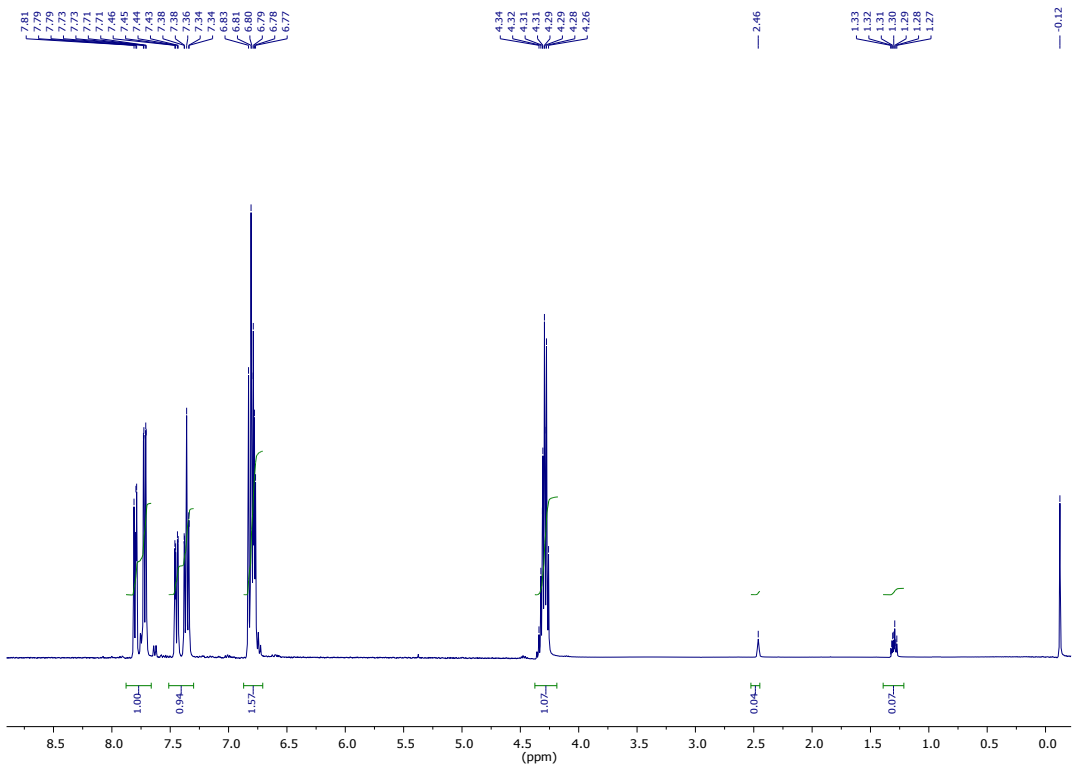


Fig S5. ^{1}H NMR of ethyl 5-bromo-2-hydroxybenzoate

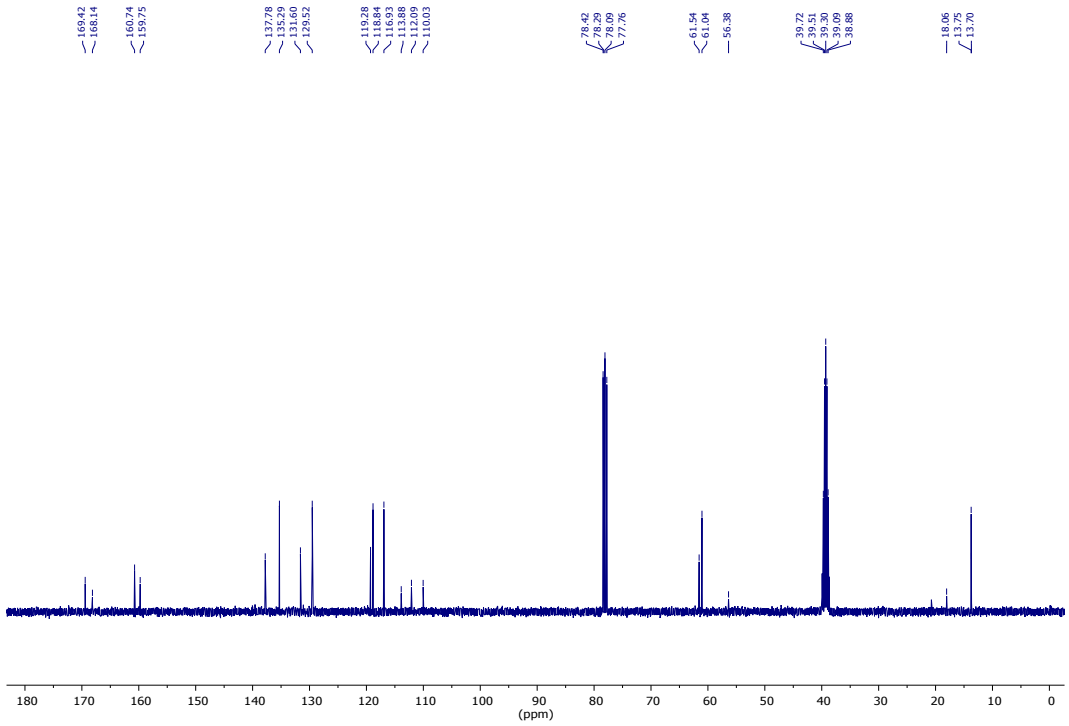


Fig S6. ^{13}C NMR of ethyl 5-bromo-2-hydroxybenzoate

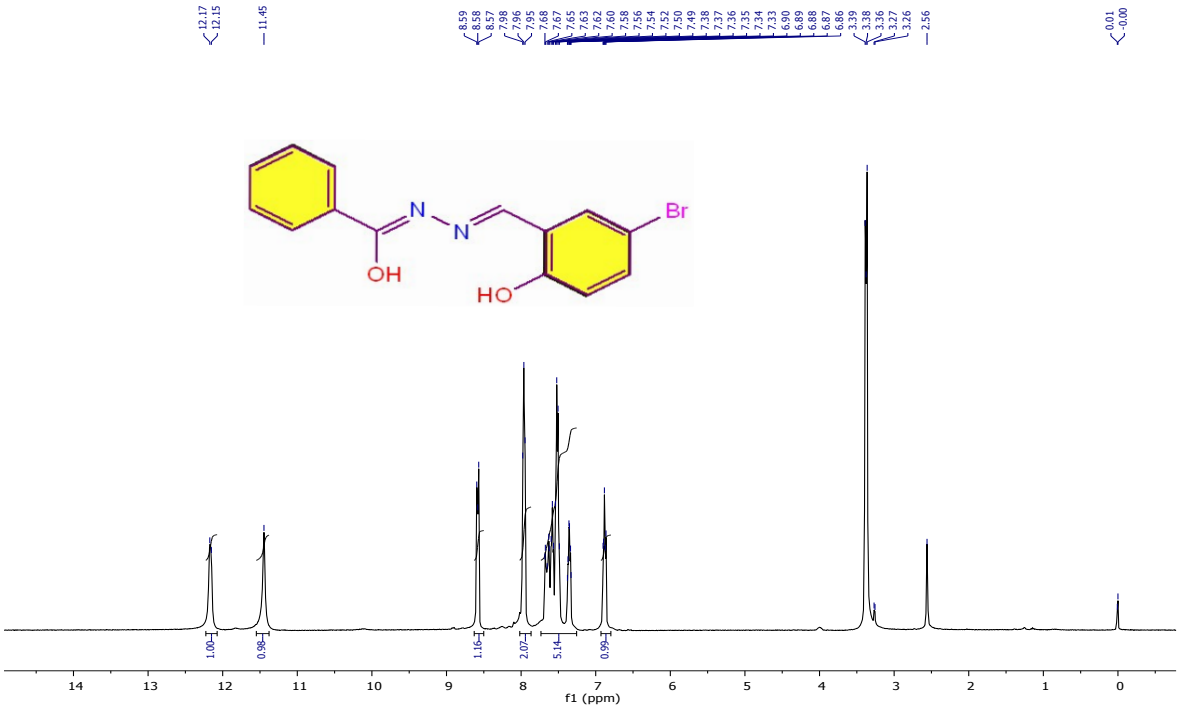


Fig S7. ^{1}H NMR of ligand

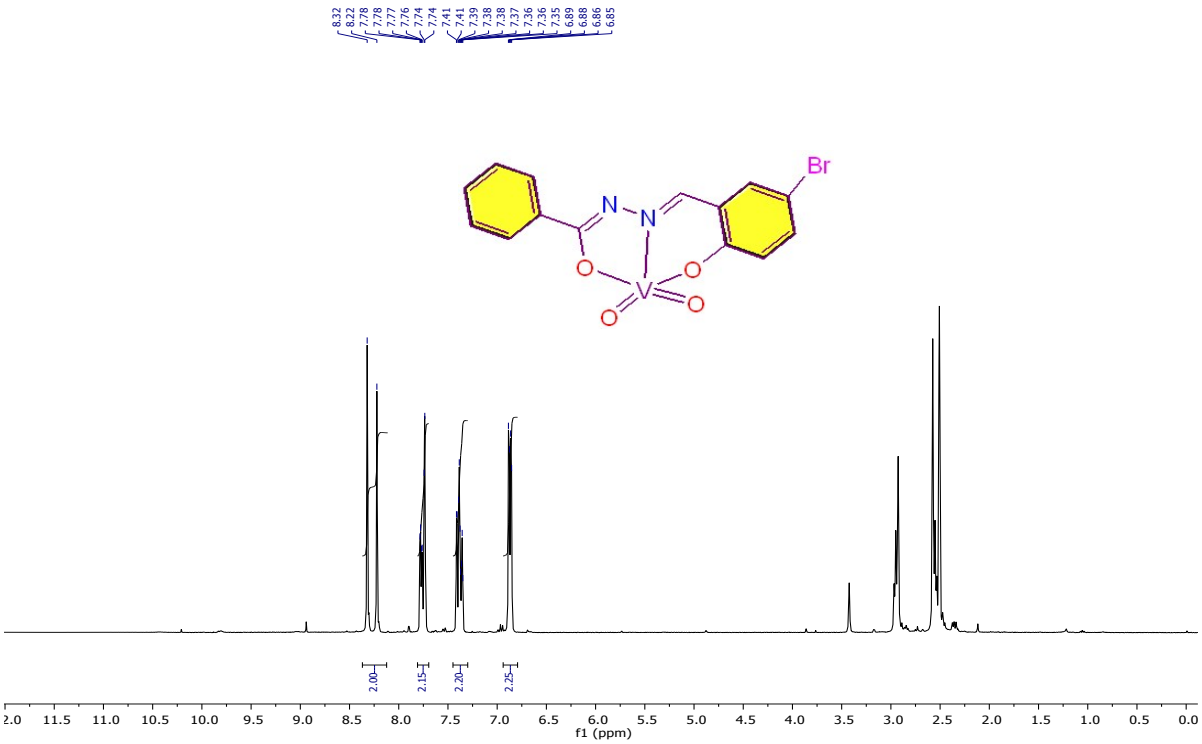


Fig S8. ^{1}H NMR of complex

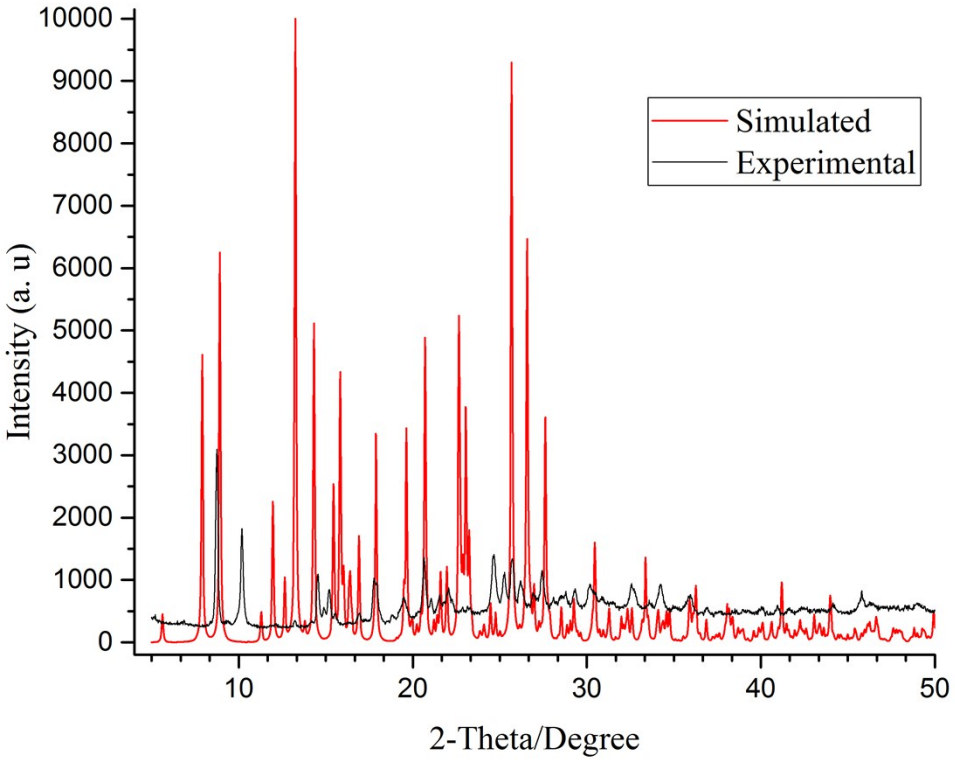


Fig. S9. Experimental and simulated powder XRD patterns of VO_2-L metallogel

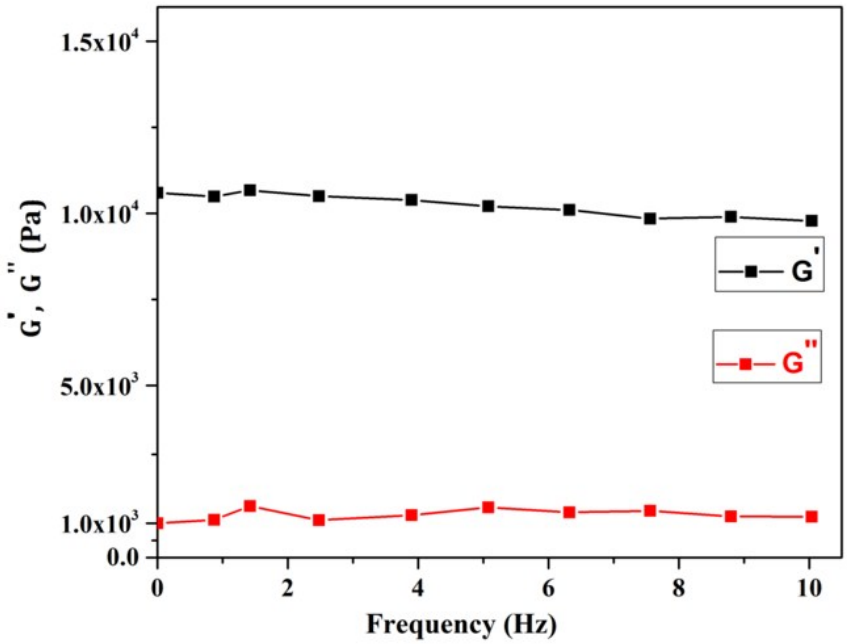


Fig S10a. Variation of storage modulus (G′) and loss modulus (G″) with frequency

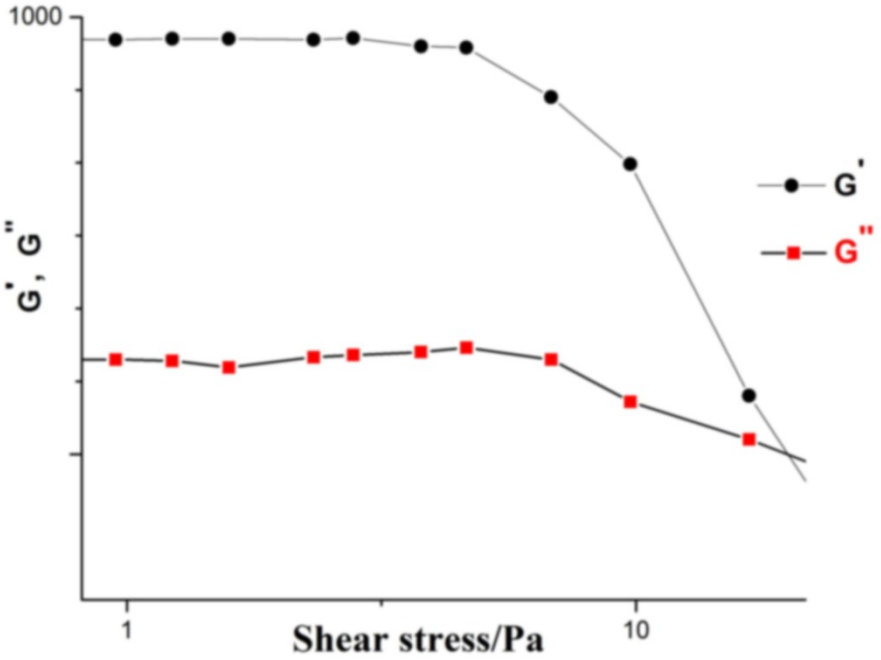


Fig S10b. Variation of storage modulus (G′) and loss modulus (G″) with shear stress

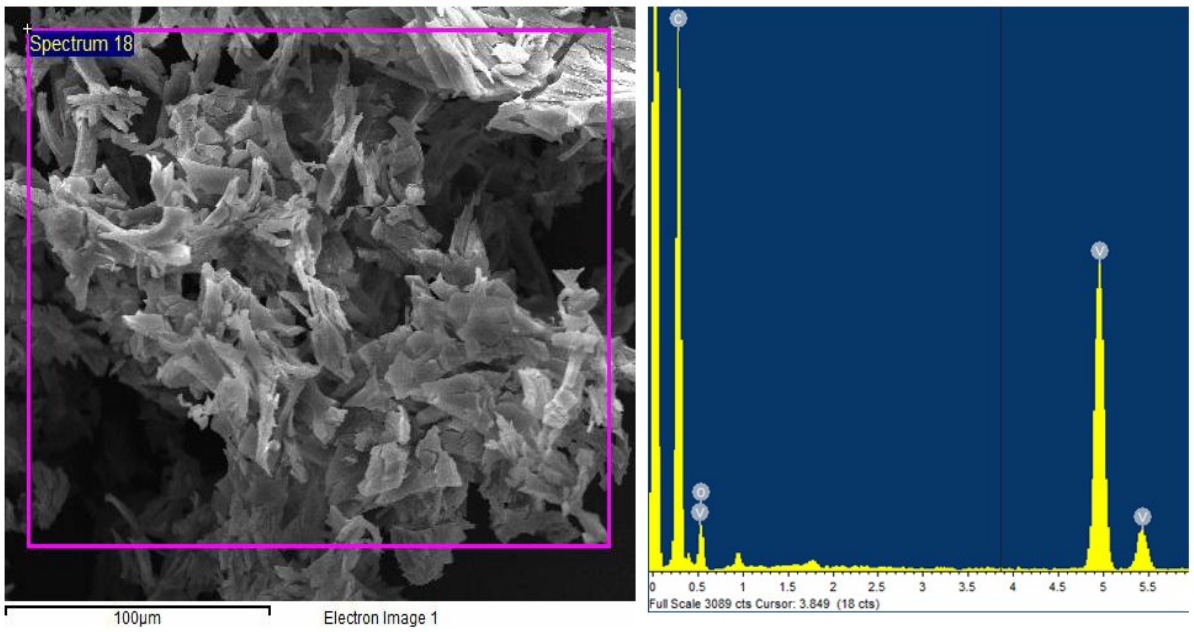


Fig S11. SEM image of VO_2-L metallogel and its corresponding EDS spectrum