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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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Table S1. Optimization of reaction conditions for the oxidative bromination catalyzed by VO-2-L hydrogel.



Entry	Molar ratio				Temperature	Time	Isolated
	V-comlex: S	S: KBr	Br:H ₂ O ₂	HClO ₄	(°C)	(min)	yield (%)
				(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°	1:4	4	RT	30	15
13	-	1:4 ^d	1:4	4	RT	30	28

^aAll 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.

^bEt₄NBr used as bromide source.

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

^dControl reaction with HClO₄: 2-hydroxyacetophenone (1.0 mmol), KBr (4.0 mmol), H₂O₂ (16.0 mmol), HClO₄ (4.0 mmol) and H₂O (5 mL).



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



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



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



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



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



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





Fig S7. ¹H NMR of ligand



Fig S8. ¹H NMR of complex



Fig. S9. Experimental and simulated powder XRD patterns of VO₂-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 VO₂-L metallogel and its corresponding EDS spectrum