Supporting Information

Schiff base complexes conjugate of bovine serum albumins as artificial metalloenzymes for eco-friendly enantioselective sulfoxidation

Table S1 Selected bond lengths (Å) and angles (º) for complex CrL

Symmetry code: (A) −x+1, −y+1, −z.					
Cr1—O4	1.983 (3)	Cr1—O5	1.994 (4)	Cr1—O6	1.915 (3)
Cr1—O6A	1.915 (3)	Cr1—N1	1.991 (3)	Cr1—N1A	1.991 (3)
O4—Cr1—O5	179.57 (15)	O4—Cr1—N1A	89.69 (10)	O4—Cr1—N1	89.69 (10)
O6A—Cr1—O4	91.38 (10)	O6—Cr1—O4	91.38 (10)	O6—Cr1—O5	88.34 (12)
O6A—Cr1—O5	88.34 (12)	O6A—Cr1—O6	96.06 (17)	O6—Cr1—N1A	172.87 (11)
O6A—Cr1—N1A	90.96 (11)	O6A—Cr1—N1	172.87 (11)	O6—Cr1—N1	90.96 (11)
N1—Cr1—O5	90.63 (12)	N1A—Cr1—O5	90.63 (12)	N1—Cr1—N1A	81.99 (15)

Table S2 Enantioselective oxidation of various prochiral sulfides using BSA-**ML**[a]

	Yield (%) Chemoselectivity (%) *ee* (%) TOF (h^{-1}) Configuration[f]				
Substrate	BSA-CoL[b]	BSA-MnL[c]	BSA-VL[d]	BSA-FeL[d]	BSA-CrL[e]
1	93, 98, 40, 465, R	80, 100, 32, 400, R	75, 100, 34, 375, R	75, 98, 27, 375, R	68, 89, 24, 340, R
2	24, 100, 51, 120, R	6, 100, 2, 30, S	93, 100, 62, 465, R	94, 100, 3, 470, S	15, 100, 5, 75, R
3	48, 100, 67, 240, R	58, 94, 4, 290, R	100, 100, 24, **500**, R	98, 99, 4, 490, S	44, 100, 6, 220, R
4	77, 98, 80, 385, R	26, 98, 4, 130, R	95, 99, 68, 475, R	87, 95, 94, 435, S	16, 100, 8, 80, R
5	56, 99, 7, 280, R	97, 98, 6, 485, R	100, 100, 32, **500**, R	98, 100, 5, 490, S	100, 100, 3, **500**, R
6	81, 85, 66, 405, R	98, 100, 6, 490, R	86, 100, 16, 430, R	92, 100, 7, 460, R	98, 100, 2, 490, R
7	95, 95, 3, 475, R	99, 99, 8, 495, S	99, 99, 14, 495, R	100, 100, 3, **500**, R	99, 99, 4, 495, R

8	90, 90, 5, 450, R	89, 100, 9, 445, R	99, 100, 96, 495, R	82, 100, 8, 410, S	80, 100, 8, 400, R
9	45, 90, 18, 225, R	29, 92, 20, 145, S	84, 91, 5, 420, S	98, 100, 19, 490, R	15, 100, 16, 75, S
10	52, 78, 55, 260, R	94, 95, 1, 376, R	97, 99, 3, 485, R	22, 27, 5, 110, S	87, 88, 5, 435, R
11	40, 100, —,200, —	94, 99, 4, 470, R	84, 99, 3, 420, R	98, 100, 490, —	86, 90, 9, 430, R
12	89, 96, 16, 445, R	94, 99, 3, 470, S	98, 100, 22, 490, S	93, 98, 24, 465, S	90, 92, 2, 450, S
13	38, 83, 7, 190, R	31, 100, 15, 155, S	71, 98, —, 355, —	79, 98, 3, 395, R	10, 100, 5, 50, R

[a] Reactions were performed in PB (2 ml) at room temperature for 20 h. [b] pH = 6; The ratios of H_2O_2: substrate (0.068 mM): BSA-CoL were 150:100:1. [c] pH = 5.1; The ratios of H_2O_2: substrate (0.135 mM): BSA-MnL were 150:100:1. [d] pH = 8; The ratios of H_2O_2: substrate (0.203 mM): BSA-**ML** were 100:100:1.[e] pH = 6; The ratios of H_2O_2: substrate (0.135 mM): BSA-CrL were 200:100:1. [f] Assigned by HPLC elution order with known literature data.

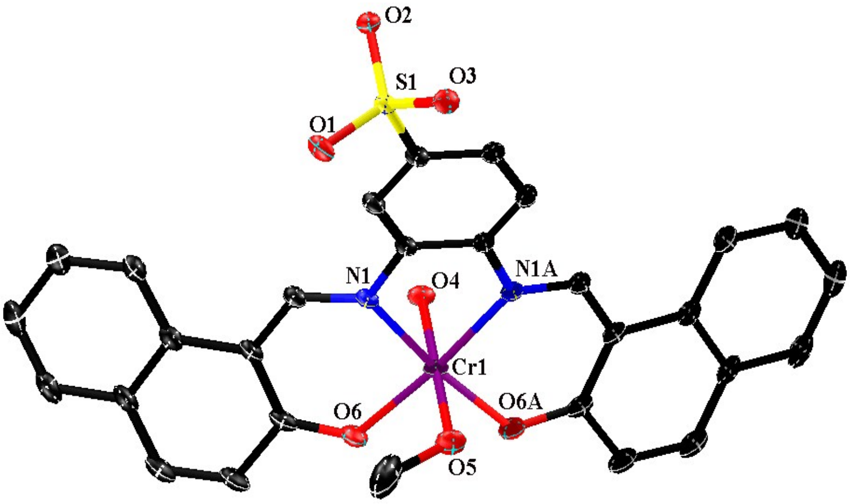

Fig. S1 The local coordination environments of complex CrL.

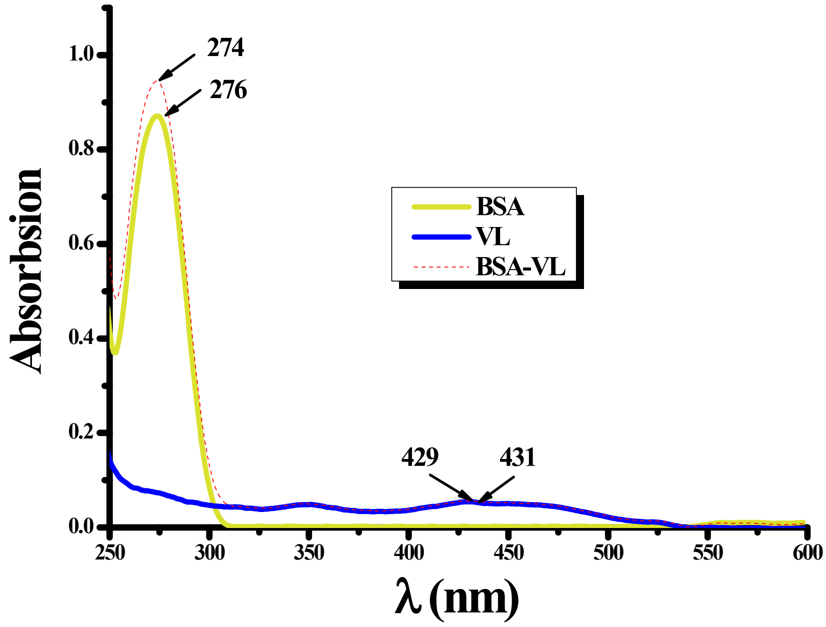

Fig. S2 UV-visible spectra of 20 μM BSA (yellow solid line), 20 μM VL complex (blue solid line) and 20 μM BSA-VL hybrid (red dashed line) in 50 mM PBS buffer pH 7.45.

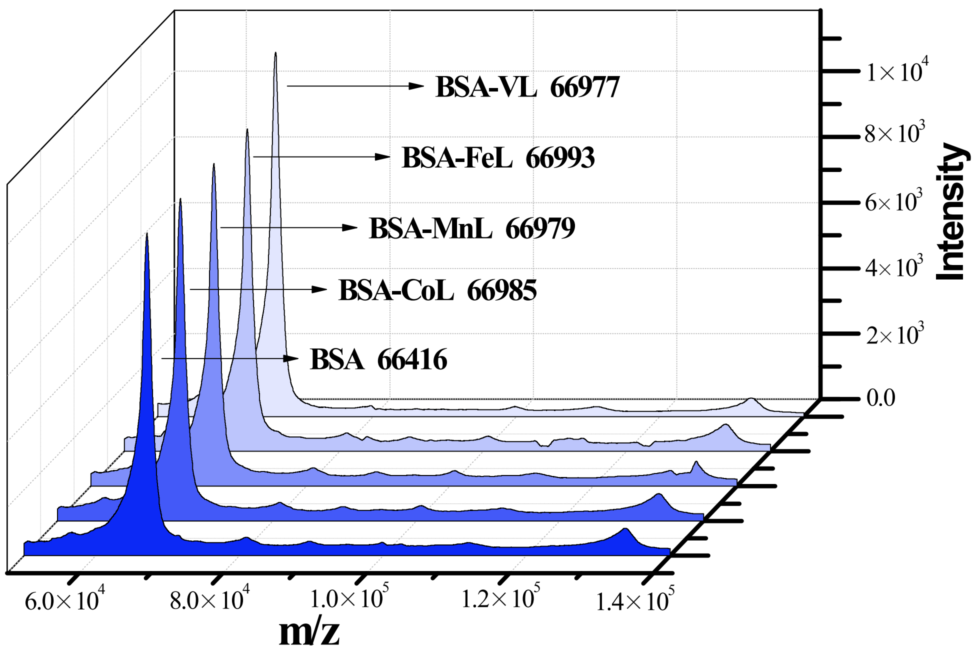

Fig. S3 ESI-TOF MS spectrum of BSA and BSA-**ML** (M= Co, Mn, Fe, V).