Dalton Transactions

Electronic Supplementary Information (ESI)

Syntheses, crystal structures, DFT calculations, protein interaction and anticancer activities of water soluble dipicolinic acid - imidazole based oxidovanadium(IV) complexes

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Table S2 Results of molecular docking: Adjacent residues and hydrogen bonding interactions

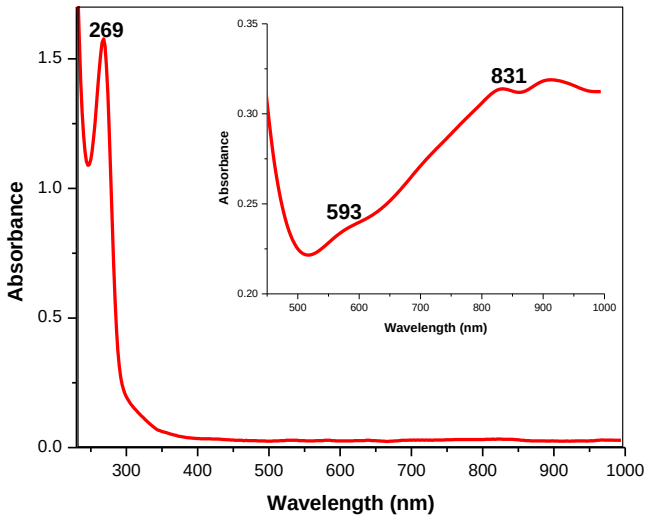


Fig. S1 Electronic spectra of complex **1** in water at room temperature. Inset: Peaks in the visible region obtained at higher complex concentration.

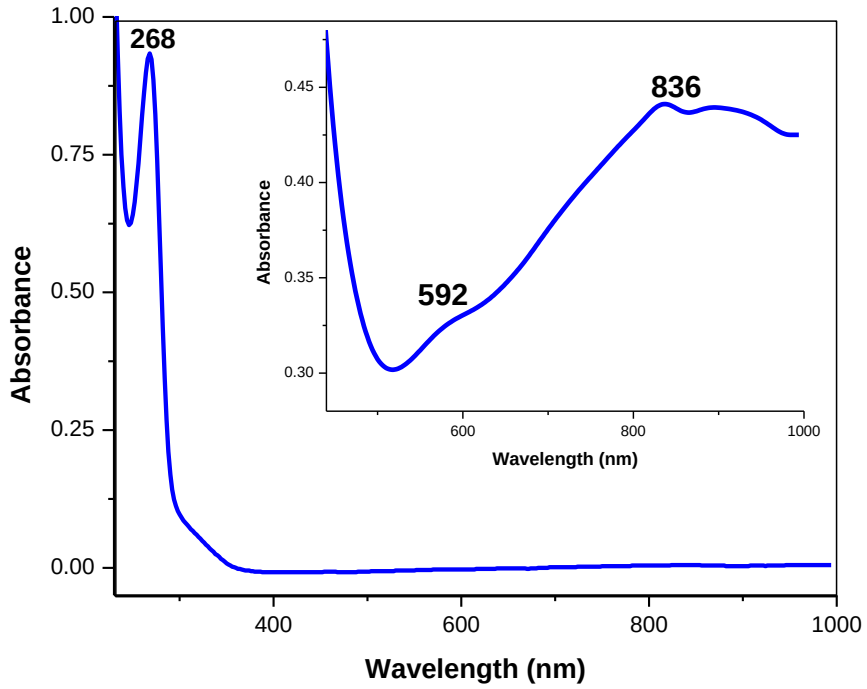


Fig. S2 Electronic spectra of complex **2** in water at room temperature. Inset: Peaks in the visible region obtained at higher complex concentration.

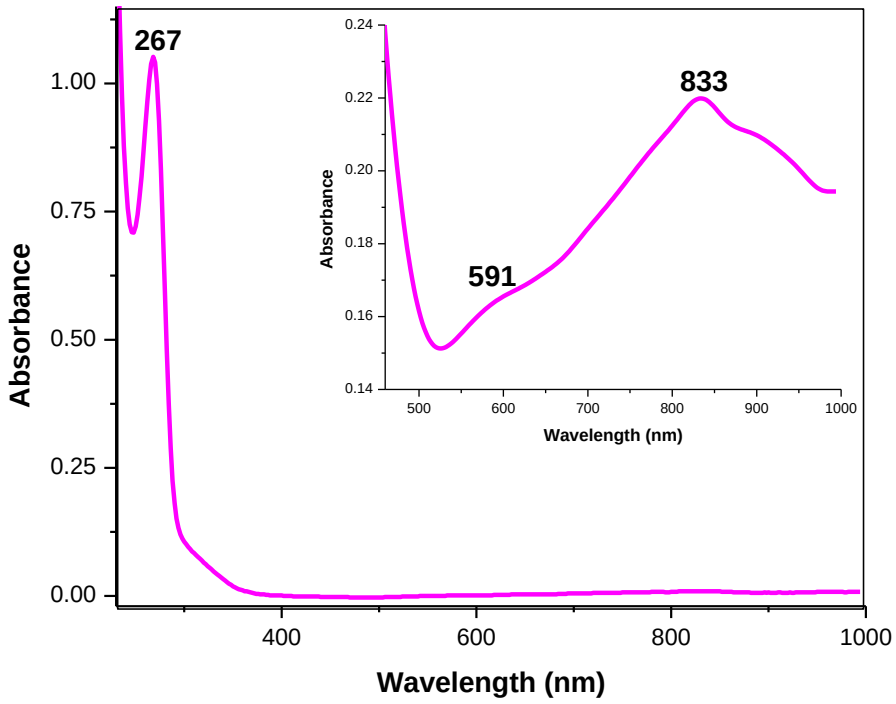


Fig. S3 Electronic spectra of complex **3** in water at room temperature. Inset: Peaks in the visible region obtained at higher complex concentration.

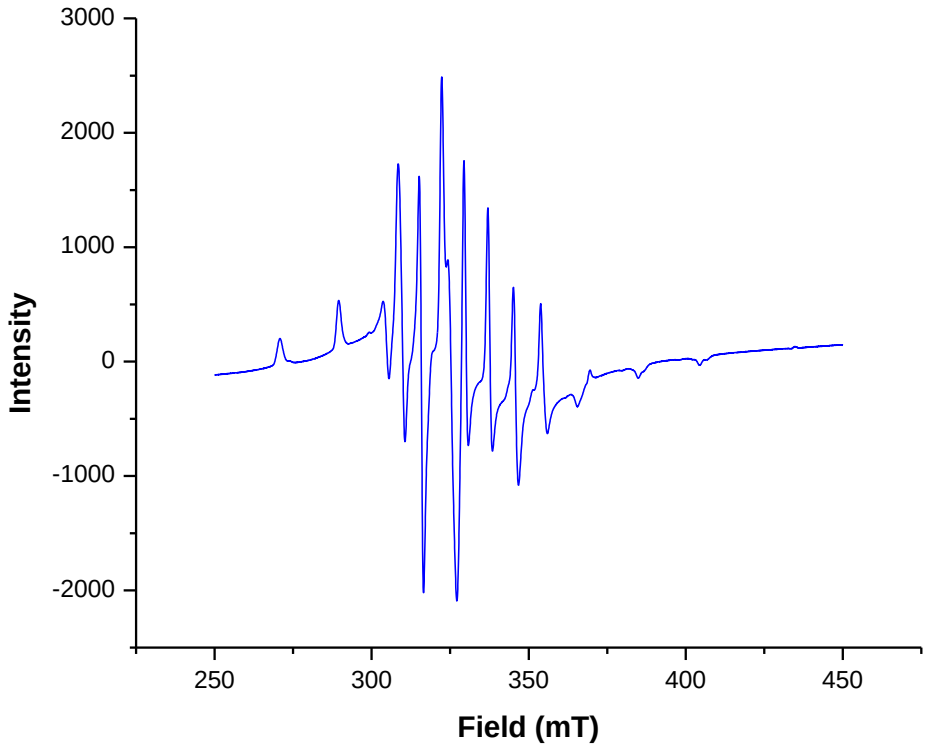


Fig. S4 EPR Spectrum of complex **2** at liquid nitrogen temperature.

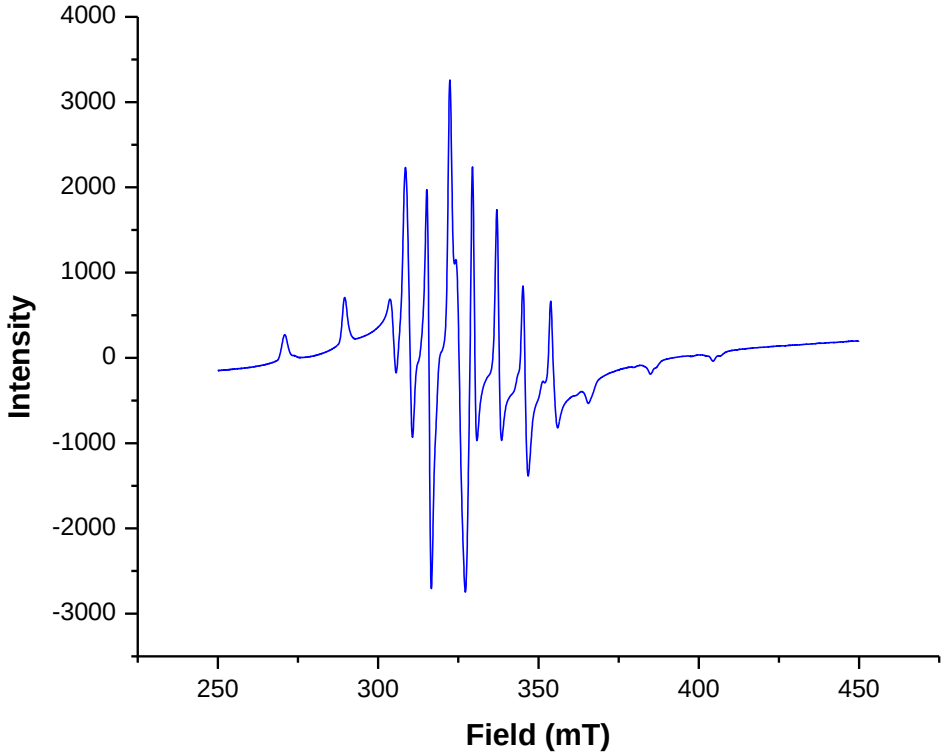


Fig. S5 EPR Spectrum of complex **3** at liquid nitrogen temperature

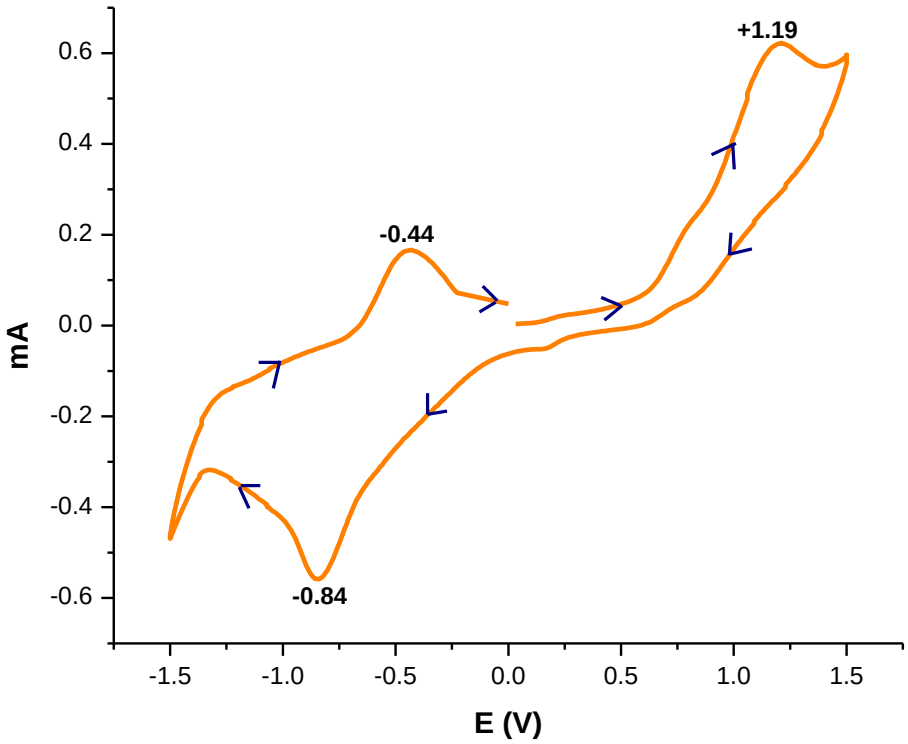


Fig. S6 Cyclic voltammogram of complex **2** in DMF at 298K

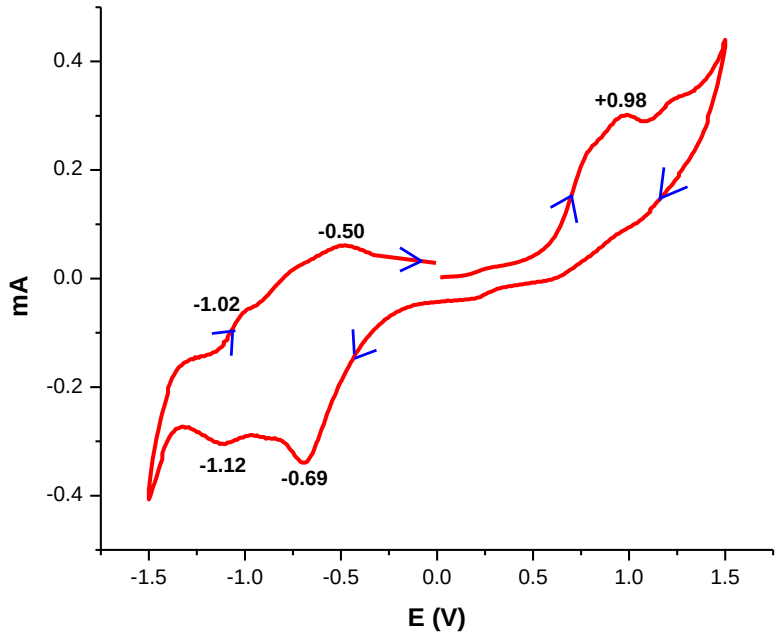


Fig. S7 Cyclic voltammogram of complex **3** in DMF at 298K

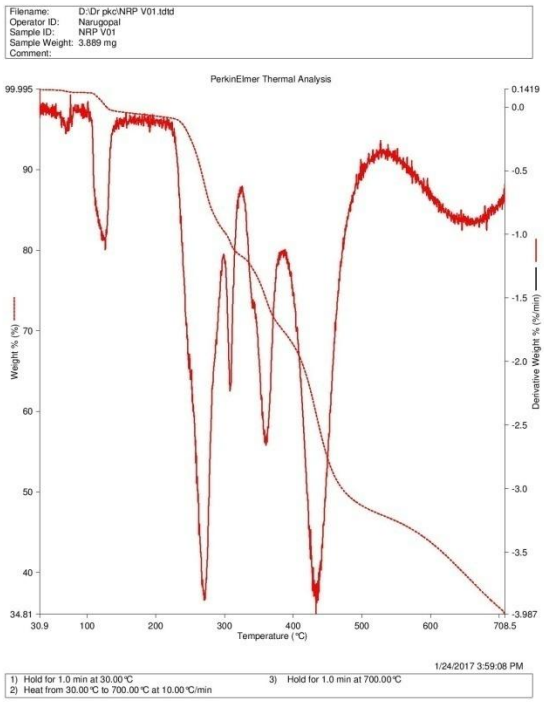


Fig. S8 TG-DT curve of complex **1** under N_2 atmosphere.

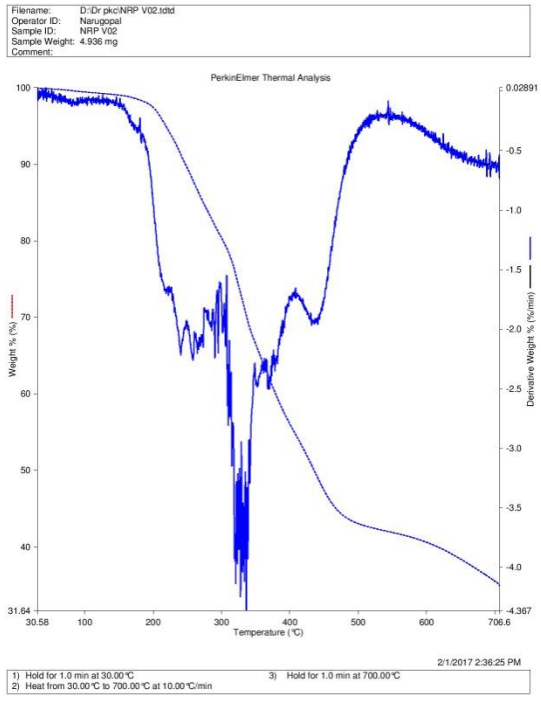


Fig. S9 TG-DT curve of complex **2** under N_2 atmosphere.

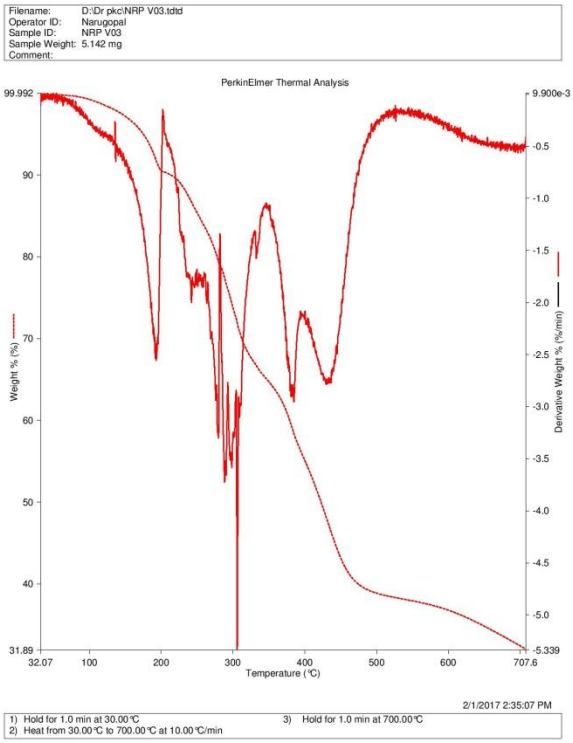
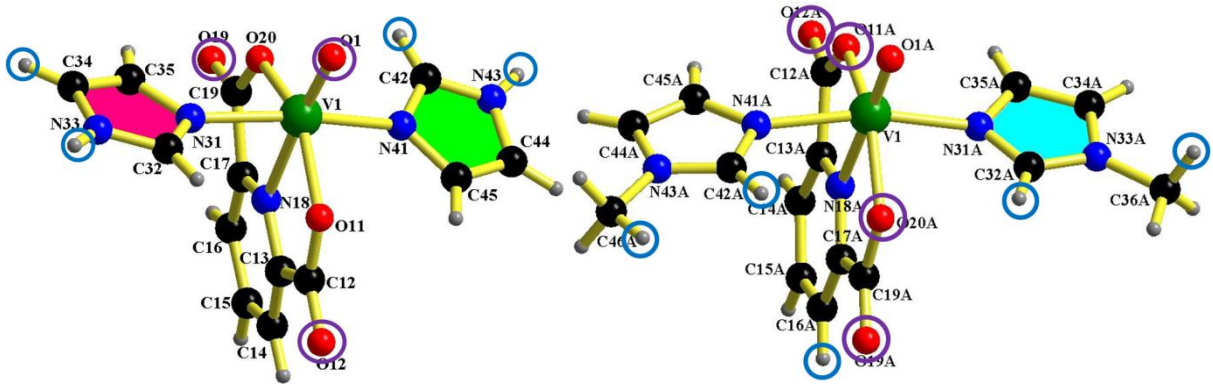


Fig. S10 TG-DT curve of complex **3** under N_2 atmosphere.



1 **2**

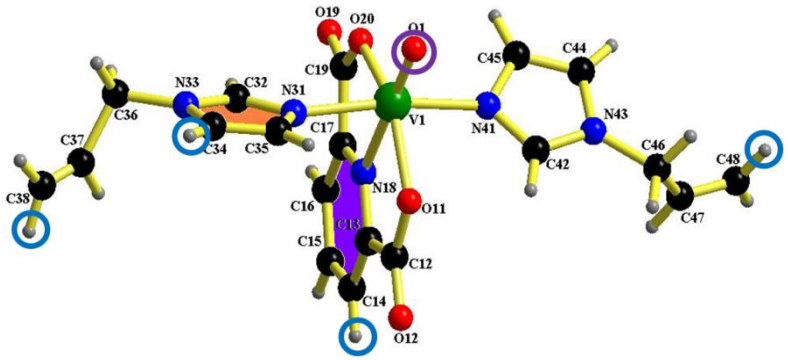


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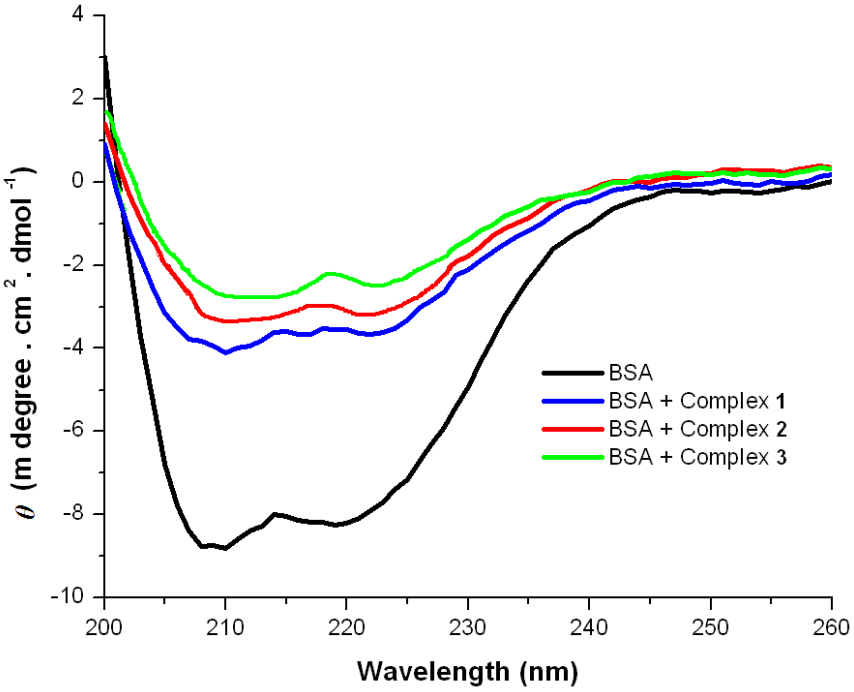
Fig. S11 Diagrams showing the atoms taking part in H-bonding and the aromatic rings involved in π···π stacking interaction



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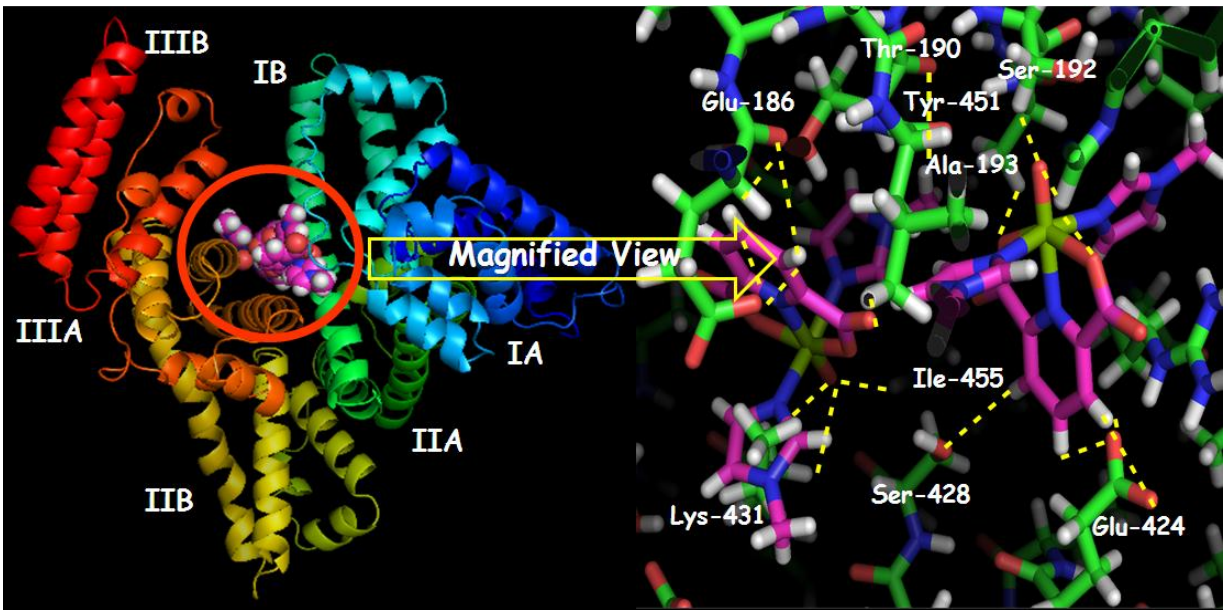

Fig. S13 Molecular docking image of complex **2** with BSA, residues surrounding the binding sites are highlighted.

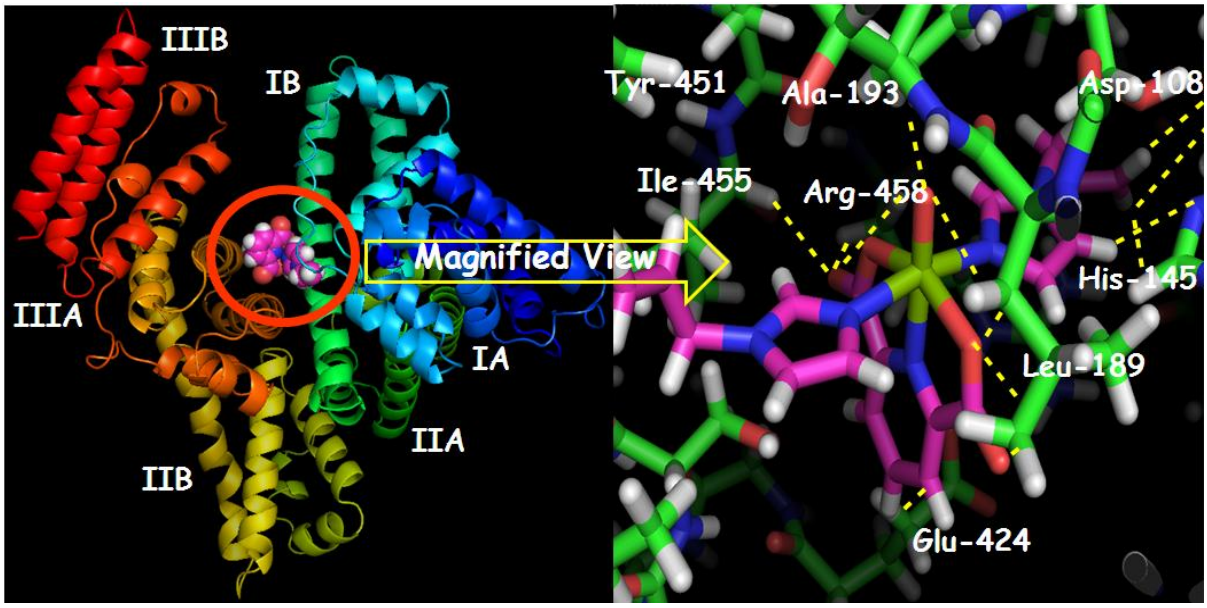

Fig. S14 Molecular docking image of complex **3** with BSA, residues surrounding the binding sites are highlighted.

Table S1

CD secondary structure estimation of BSA in the absence and presence of complexes **1-3** using CDNN Software

Components conformation	**Free BSA (1×10^{-5} M)**	**BSA + Complex 1 (2×10^{-5} M)**	**BSA + Complex 2 (2×10^{-5} M)**	**BSA + Complex 3 (2×10^{-5} M)**
α-Helix (%)	85.0	38.5	31.7	24.7
β-sheet (Antiparallel) (%)	1.3	7.3	9.0	11.6
β-sheet (Parallel) (%)	1.5	7.3	9.2	11.5
β-Turn (%)	9.3	16.1	17.2	18.6
Random Coil (%)	7.0	27.9	33.5	40.0

Table S2

Results of molecular docking: Adjacent residues and hydrogen bonding interactions

Complex	Hydrogen bonding interactions	Adjacent amino acids
BSA···Complex **1**	(Tyr-160)Ph-O-H···O=V = 2.2 Å (Tyr-160)Ph-H···O=V = 2.9 Å (Tyr-137)Ph-H···O-V=O 2.4 Å (Tyr-137)Ph-H···O=C-O-V = 2.4 Å (Ile-141)-CH_2-H···O=C-O-V = 1.3 Å (Lys-136)HO-C=O···H-(Imz)-V = 2.9 Å	Tyr-160, Tyr-137, Lys-136, Glu-140, Leu-115, Lys-116, Pro-117, Glu-182, Leu-122
BSA···Complex **2**	(Ile-455)-CH_2-H···O=V = 2.7 Å (Lys-431)-CH-H···O=V = 2.7, 2.9 Å (Arg-458)-C-H···O=C-O-V = 2.8 Å (Leu-189)-C-C-H···O=C-O-V = 2.8 Å (Glu-186)-CH_2-C-O···H-(Py) = 2.7, 2 Å (Glu-186)-C-C-O···H-(Py) = 3, 2.5 Å (Ser-192)-C-H···O=V = 1.7 Å (His-145)-Imz-H···O=V = 2.8 Å (Ala-193)-C-CH_2-H···O-V=O = 2.9 Å (Glu-424)-H_2C-C-O···H-(Py) = 1.7, 1.5, 2.4 Å (Thr-190)-NH_2-C-C-O···H-CH_2-(1-methimz) = 3Å	Ile-455, Lys-431, Arg-458, Glu-186, Leu-189, Ser-192, His-145, Thr-190, Glu-424, Ala-193, Tyr-451
BSA···Complex **3**	(Ala-193)-CH_2-H···O=V = 2.2 Å (Leu-189)-CH_2-H···O=V = 3.0 Å (Leu-189)-C-H···O-V=O = 2.2, 2.9 Å (Leu-189)-C-H···O=C-O-V = 1.8 Å (Glu-424)-C-O···H-(Py) = 2.9 Å (Arg-458)-CH-H···O=C-O-V = 2.7, 2.9 Å (Ile-455)-CH_2-H···O=C-O-V = 2.6 Å (His-145)-Imz-N···H-(1-allylimz) = 2.8 Å (Asp-108)-C-O···H-CH=CH-CH_2-N-(1-allylimz) = 3, 2.6, 2.9 Å	Ala-193, Leu-189, Glu-424, Arg-458, Ile-455, His-145, Asp-108