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Electronic Supplementary Information

The vital role of ditopic N-N bridging ligands with different lengths in the formation of new binuclear dioxomolybdenum(VI) complexes: Synthesis, crystal structures, supramolecular framework and protein binding studies

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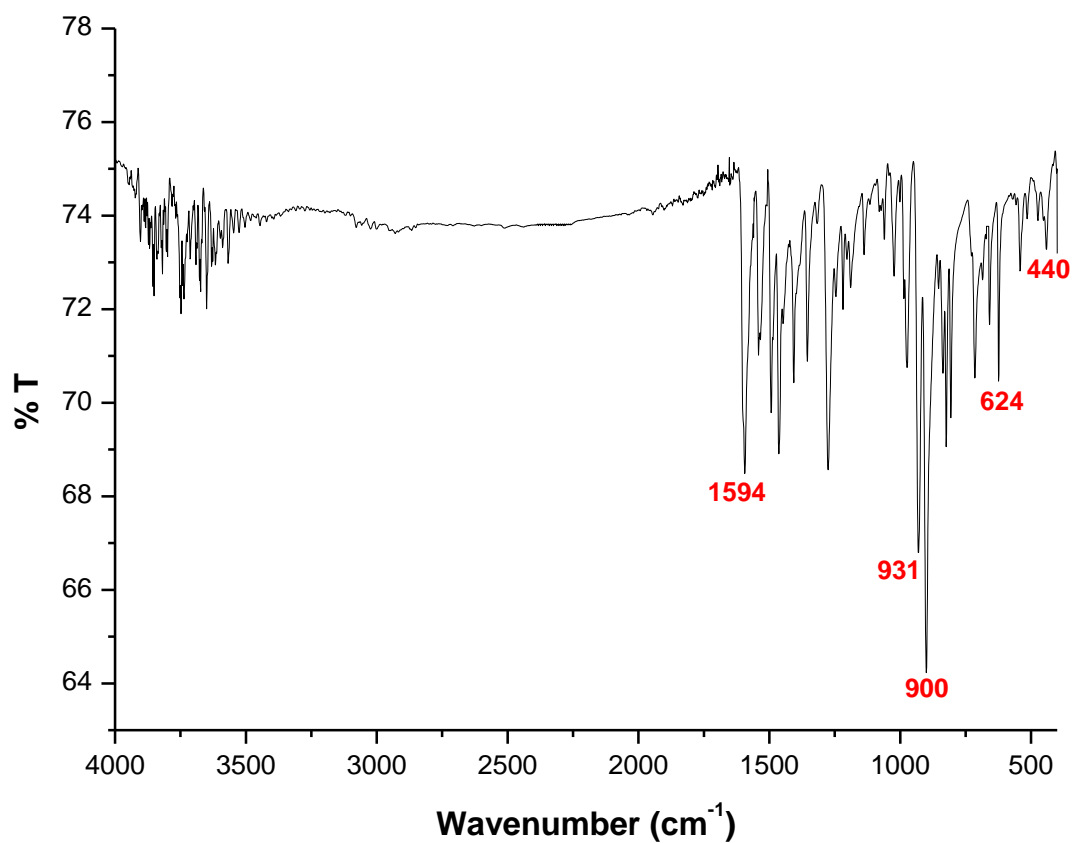
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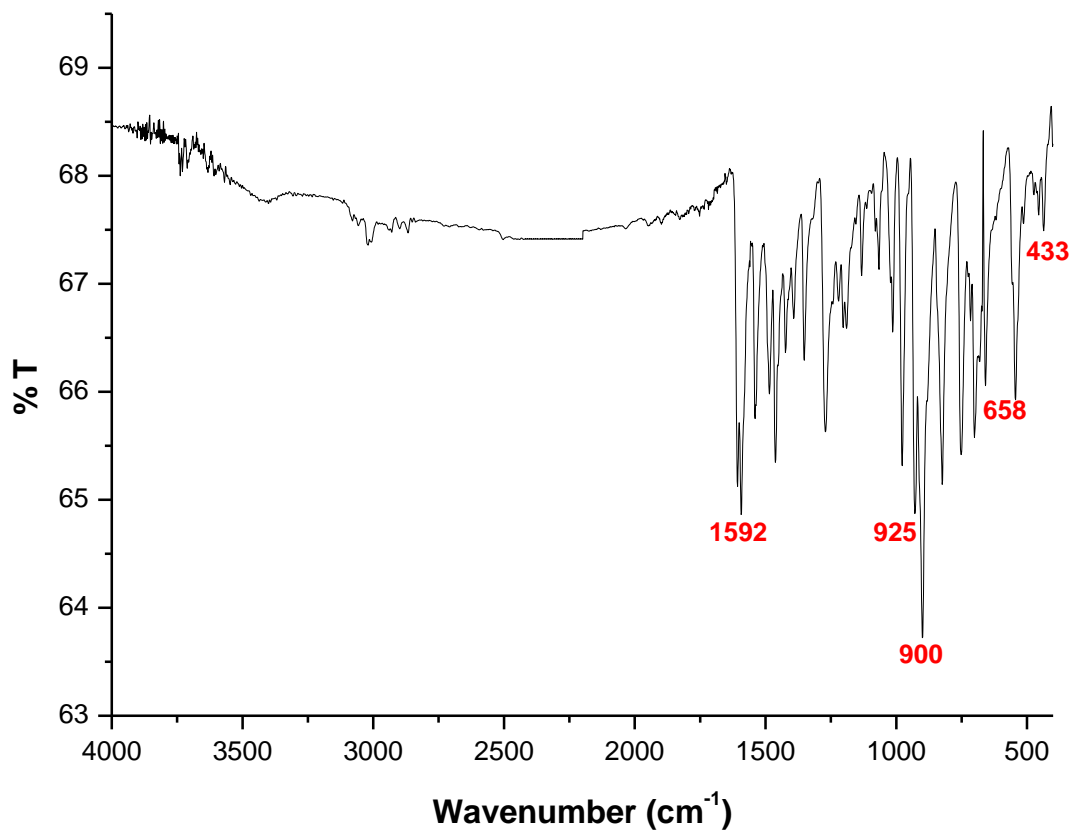
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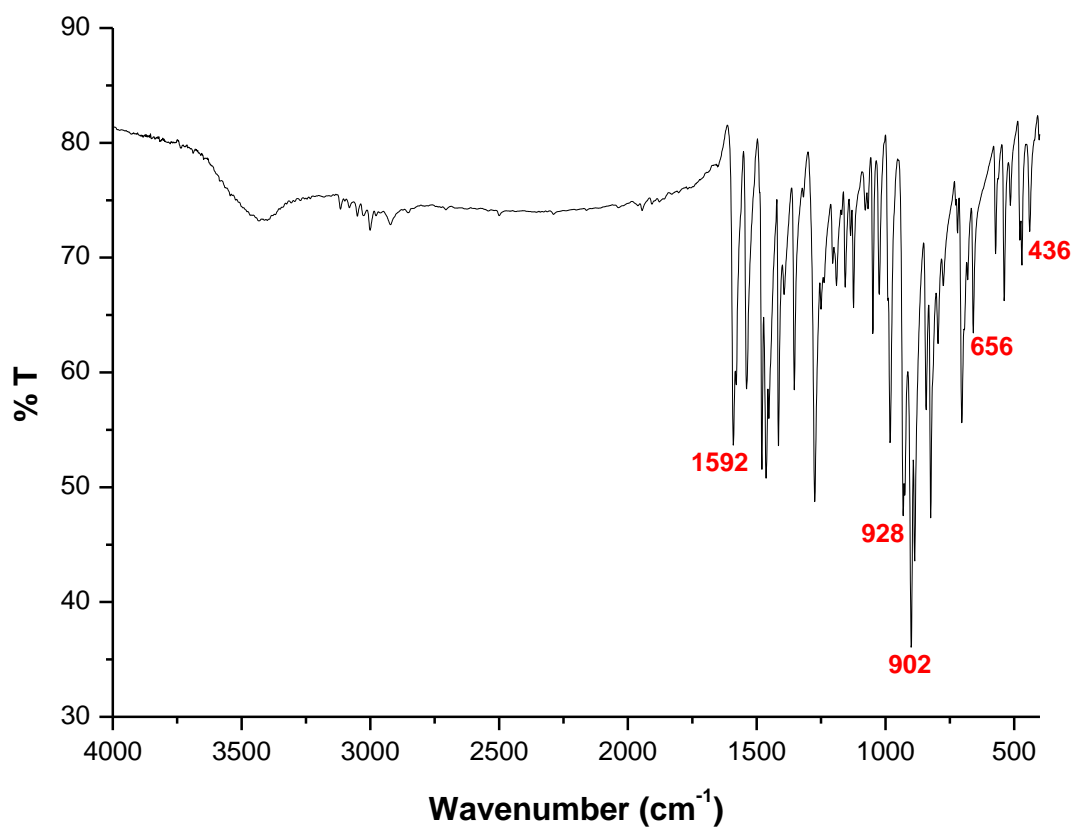
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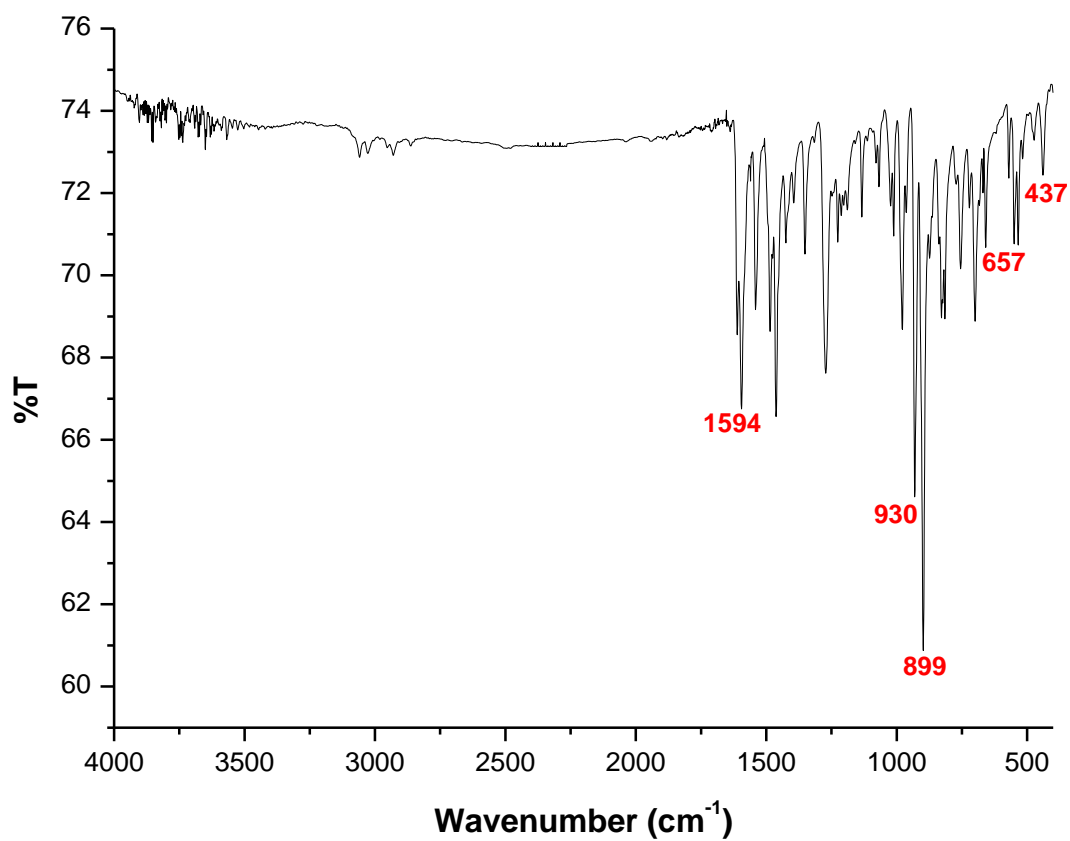
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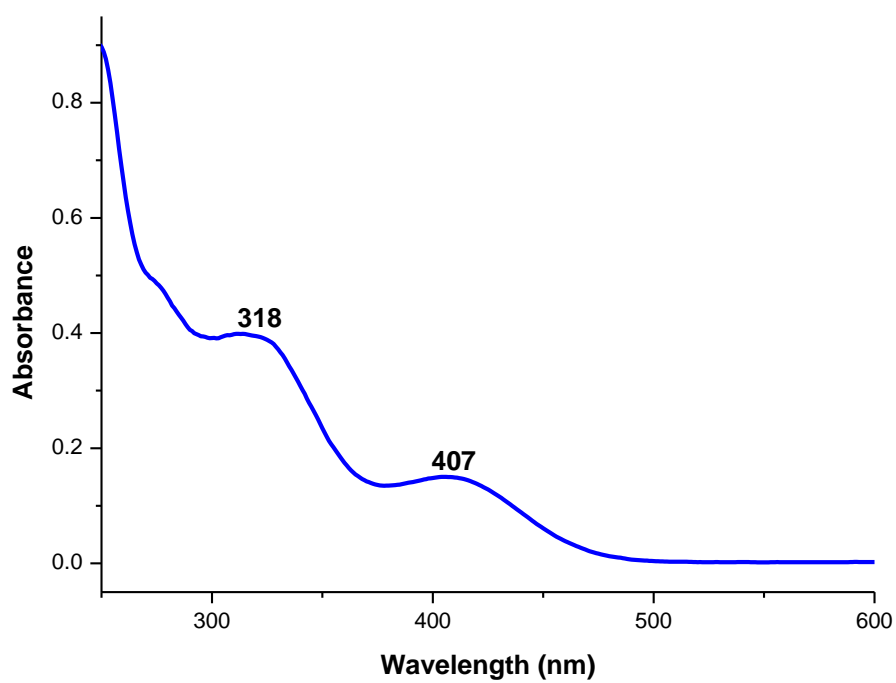


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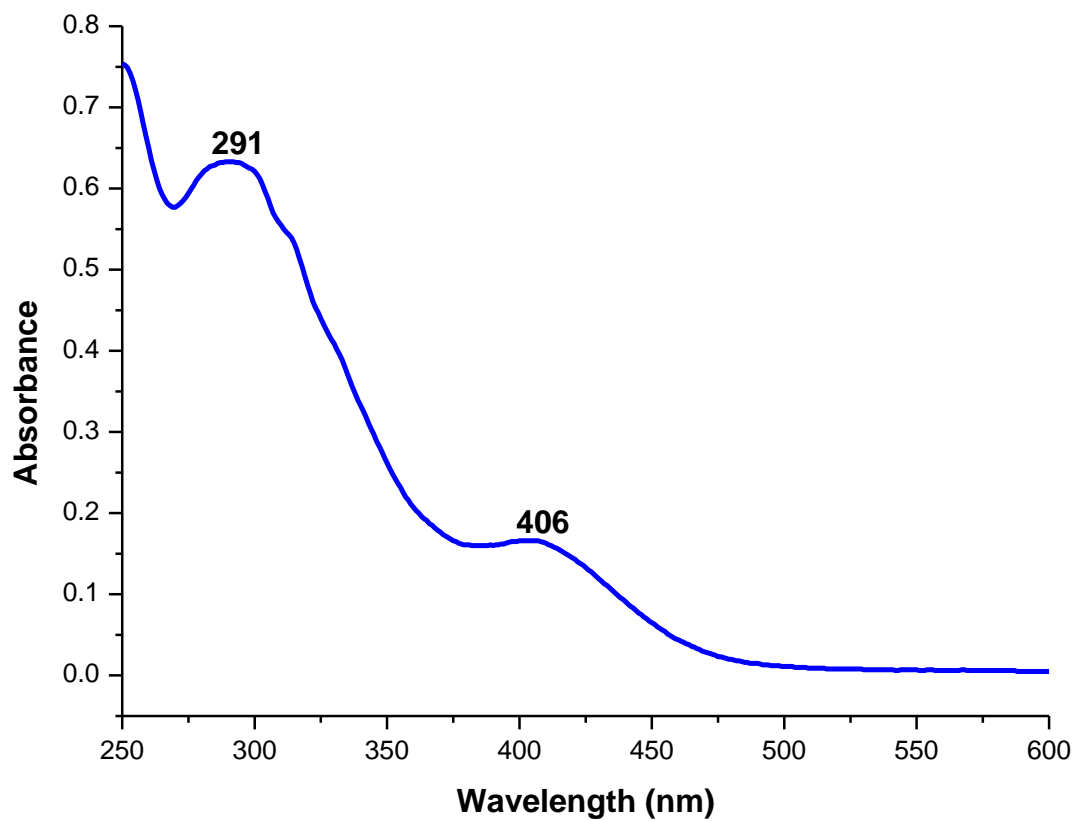


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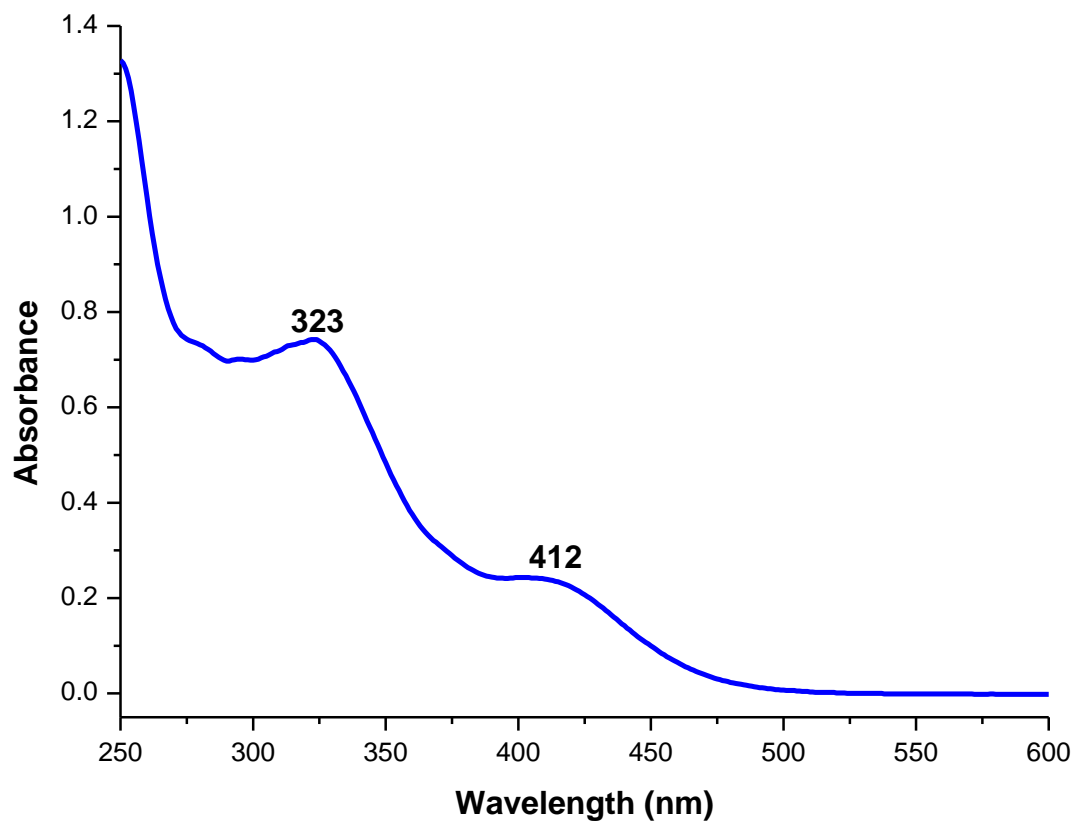
Fig. S1: IR spectra of (a) complex 1, (b) complex 2, (c) complex 3 and (d) complex 4 in KBr pellets.



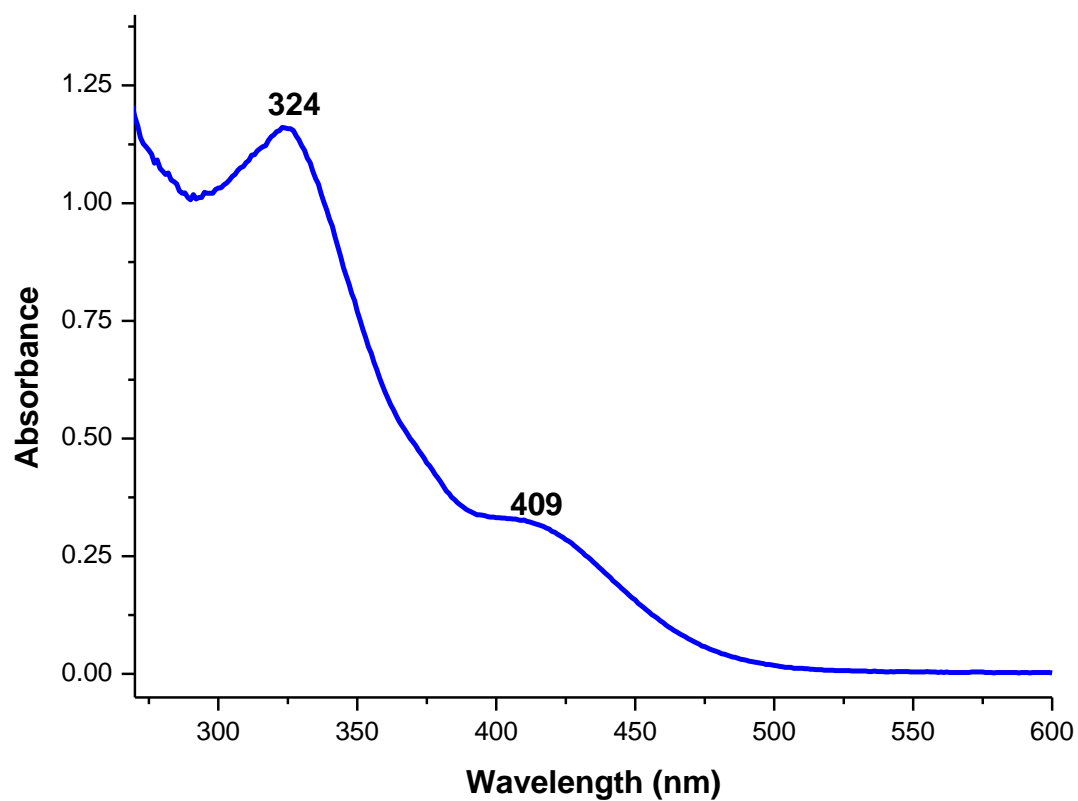
(a)



(b)



(c)



(d)

Fig. S2: UV-Vis spectra of (a) complex 1, (b) complex 2, (c) complex 3 and (d) complex 4 in CH_2Cl_2 at 298 K.

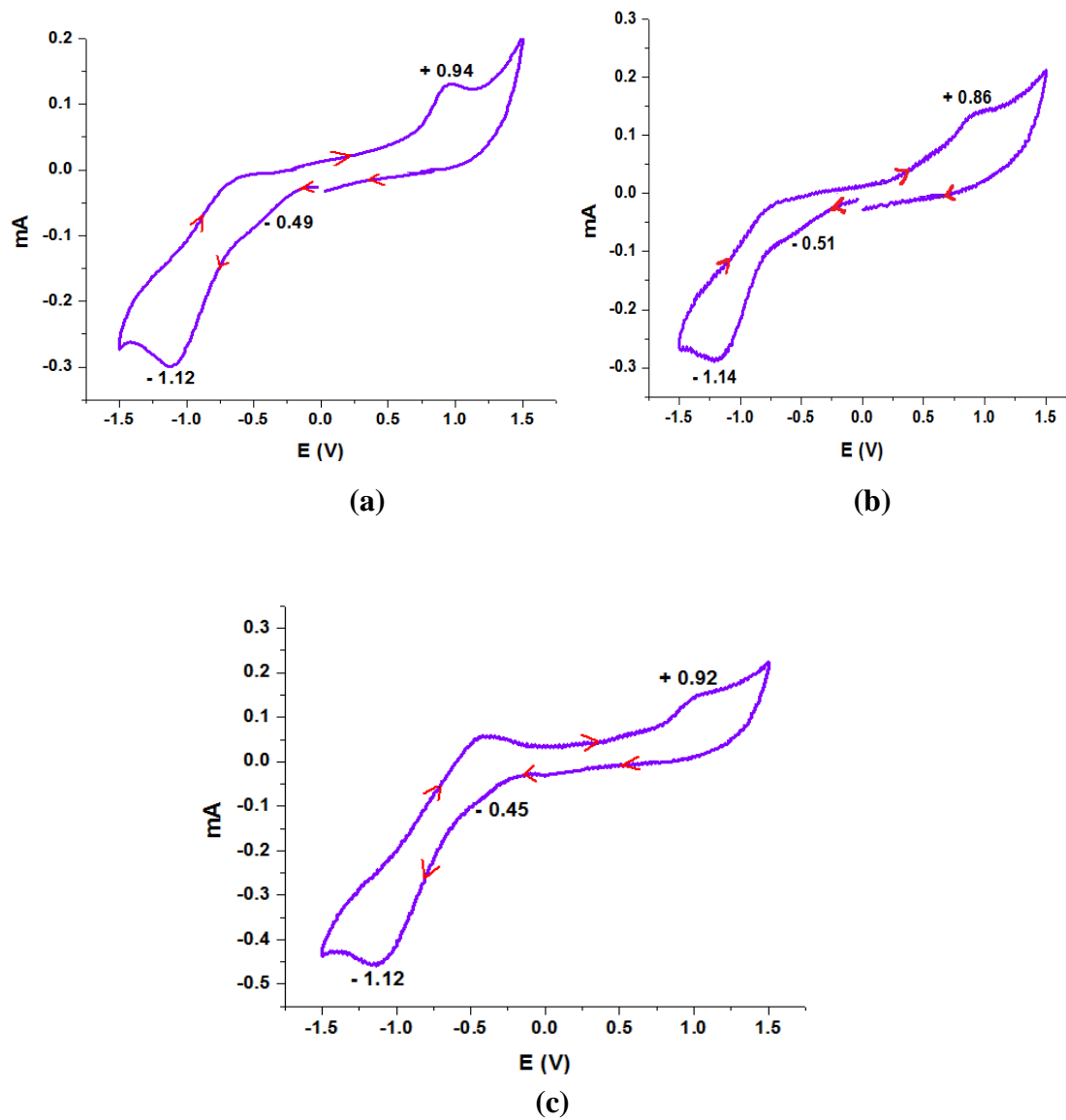
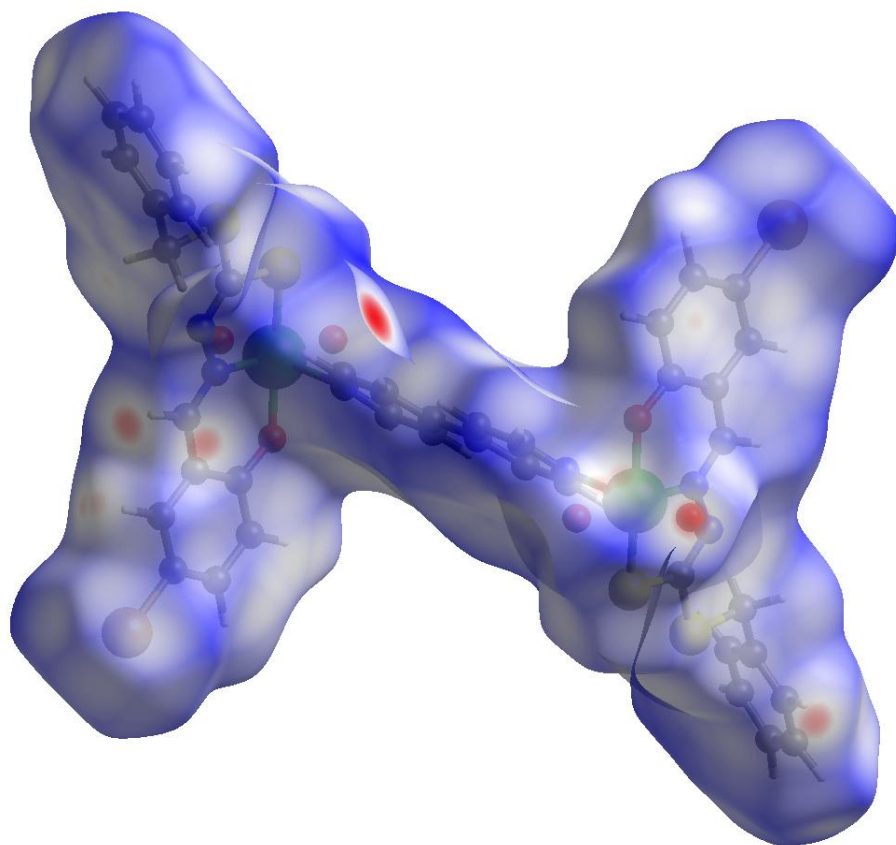
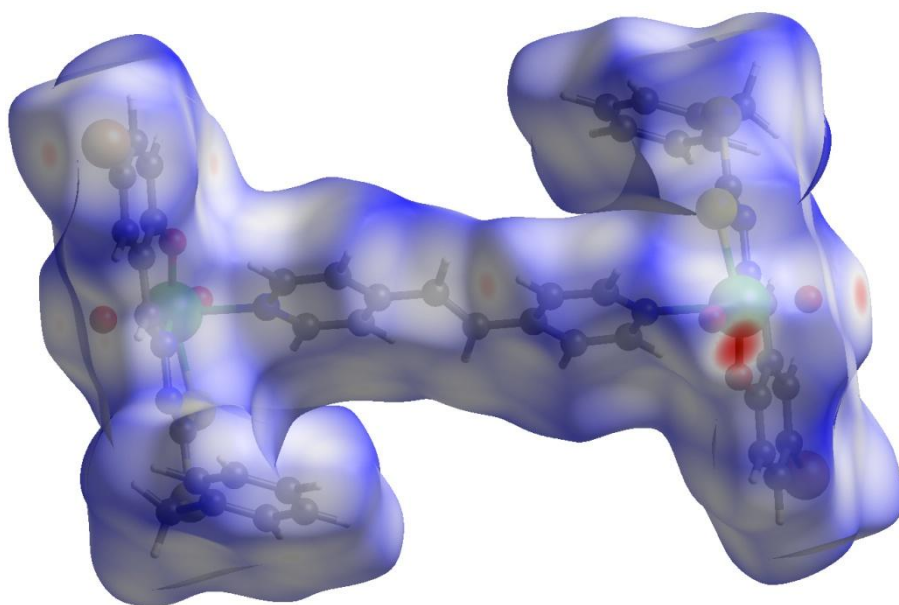


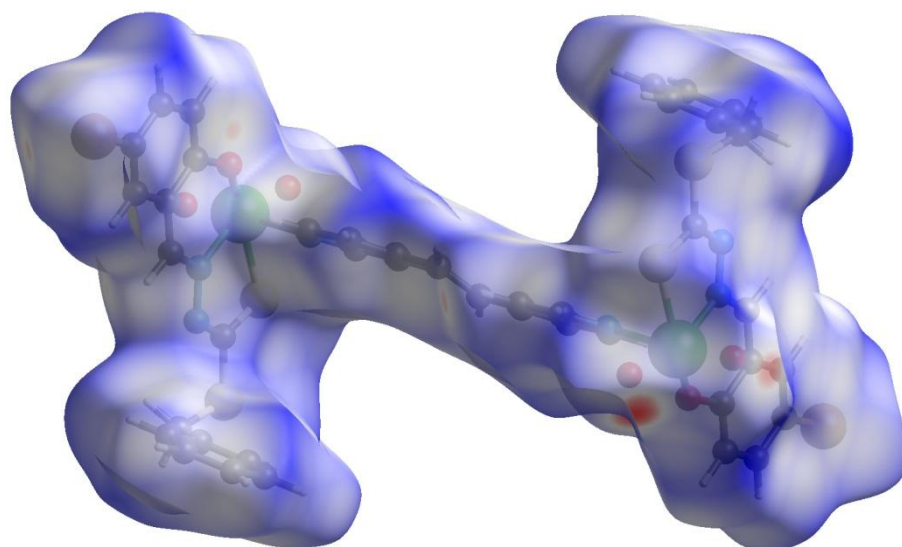
Fig. S3: Cyclic voltammograms of (a) complex 2, (b) complex 3 and (c) complex 4 in DMF at 298K.



(a)

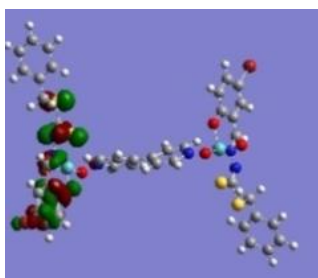


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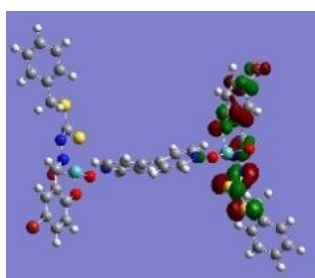


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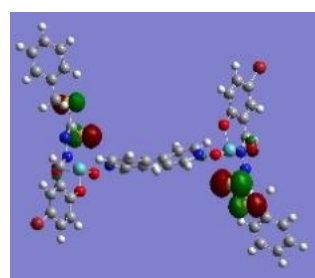
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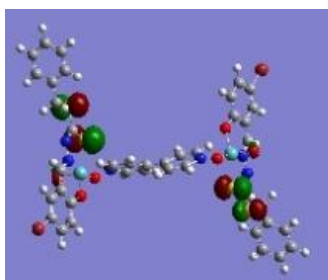
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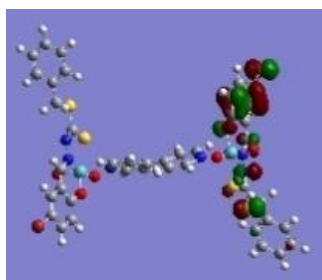
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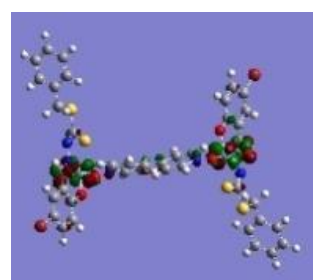
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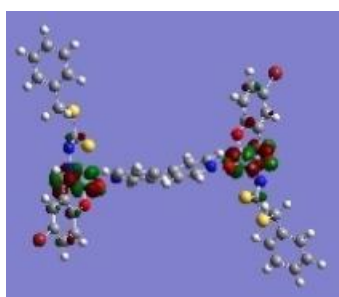
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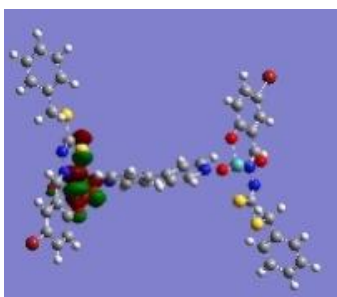
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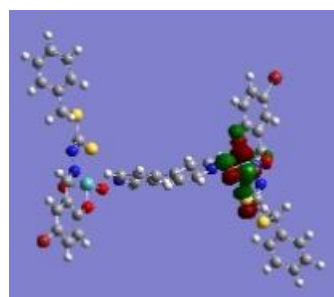
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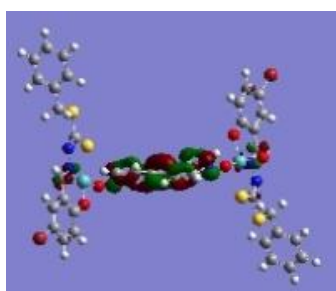
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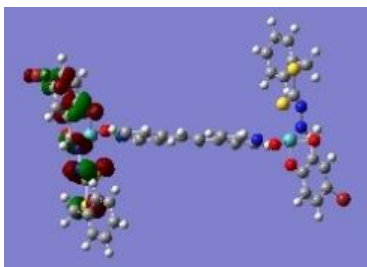


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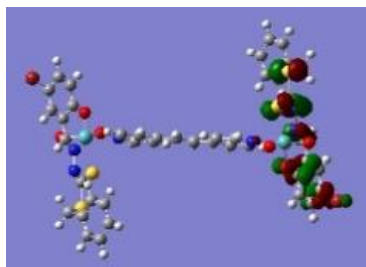


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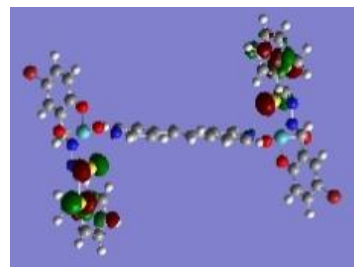
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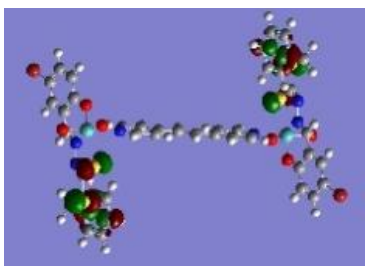
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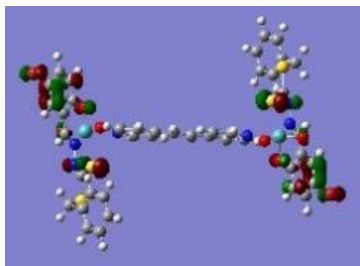
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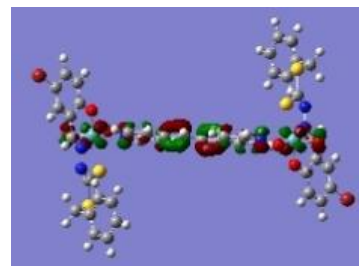
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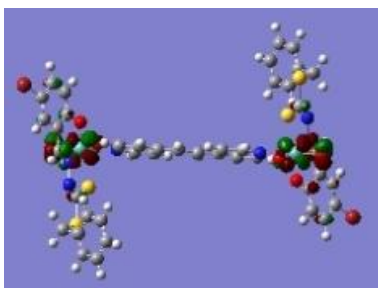
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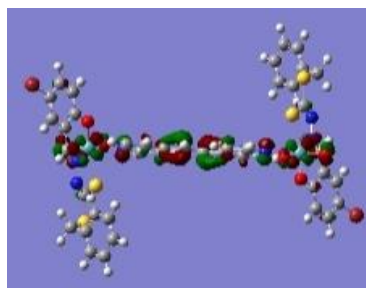
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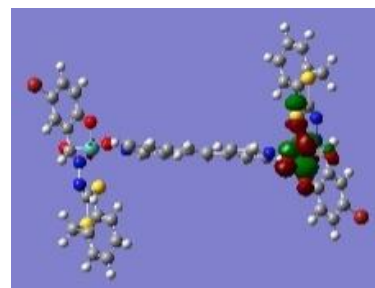
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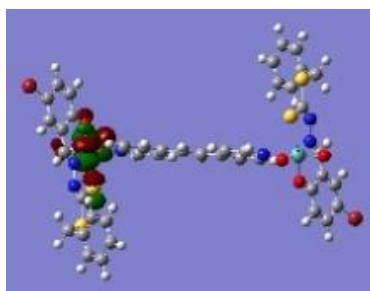
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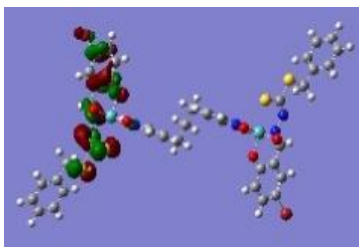


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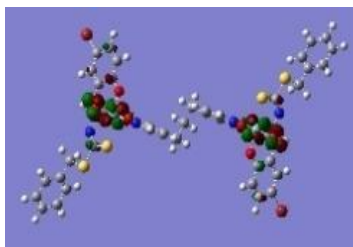


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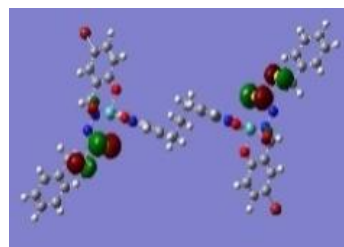
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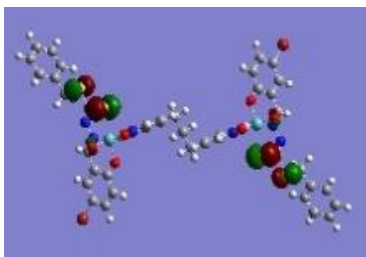
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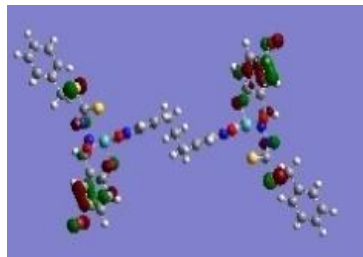
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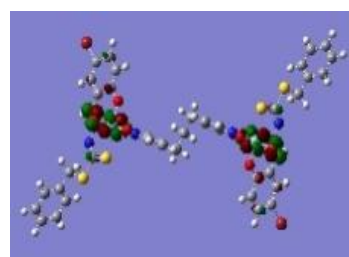
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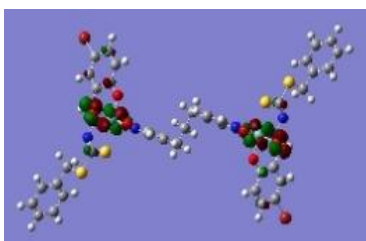
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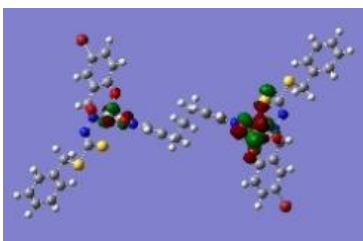
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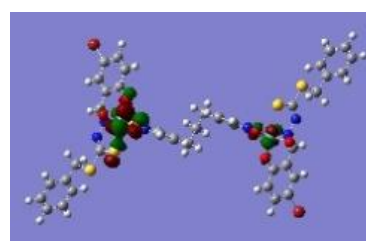
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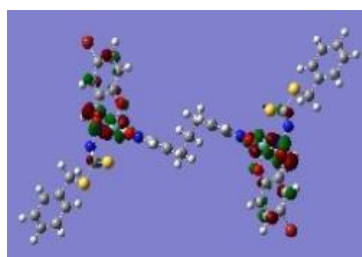
LUMO+1



LUMO+2



LUMO+3



LUMO+4

(c)

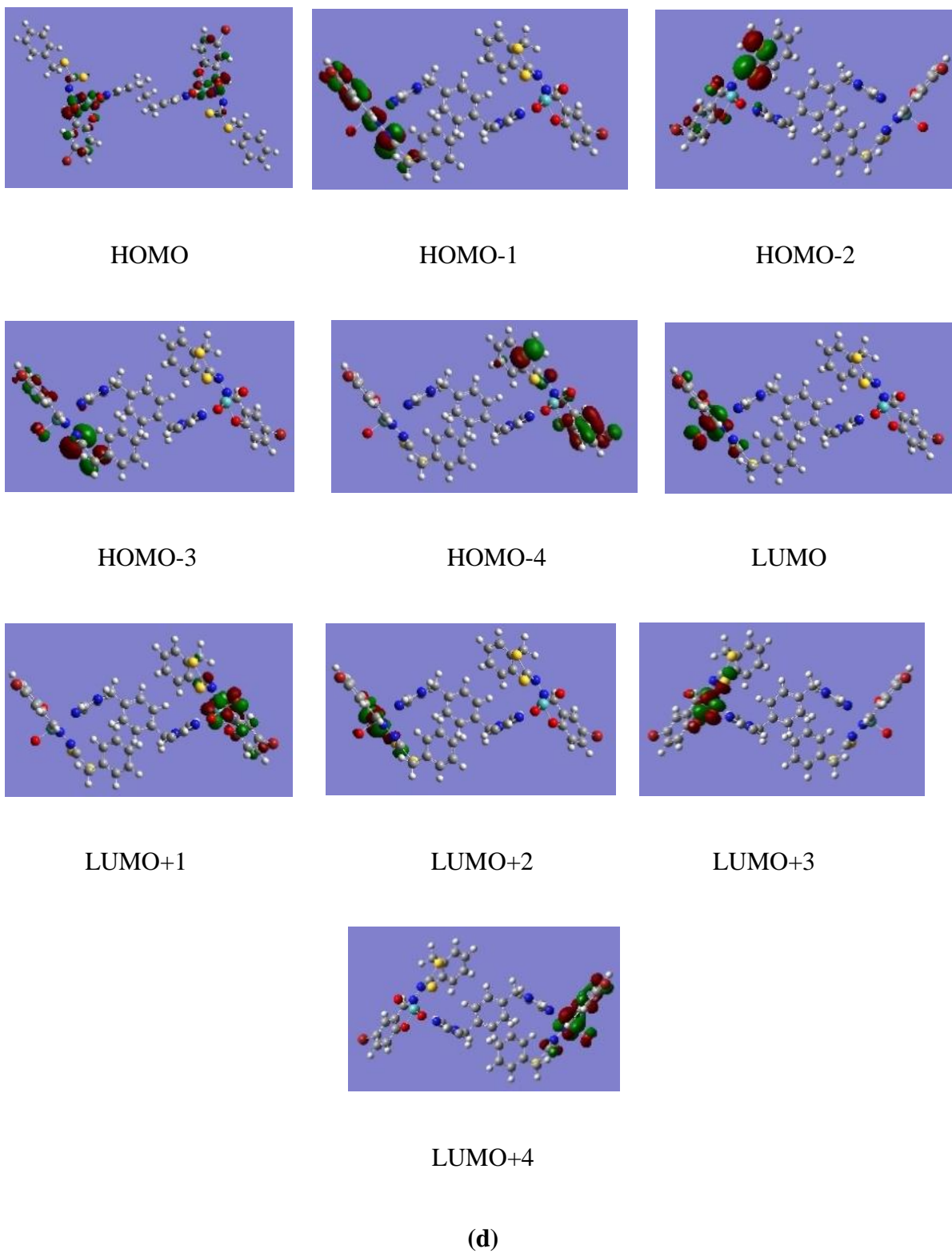
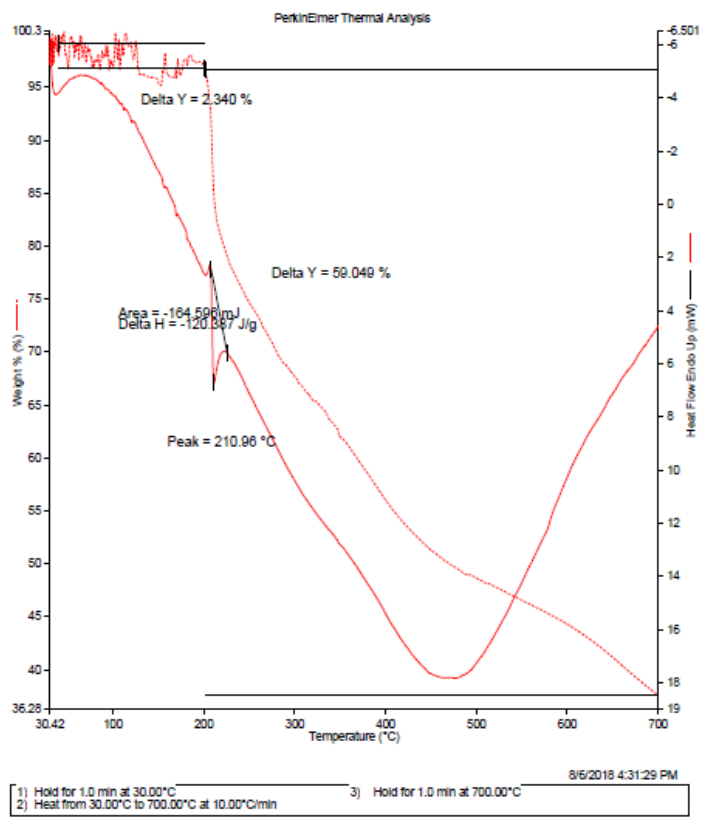


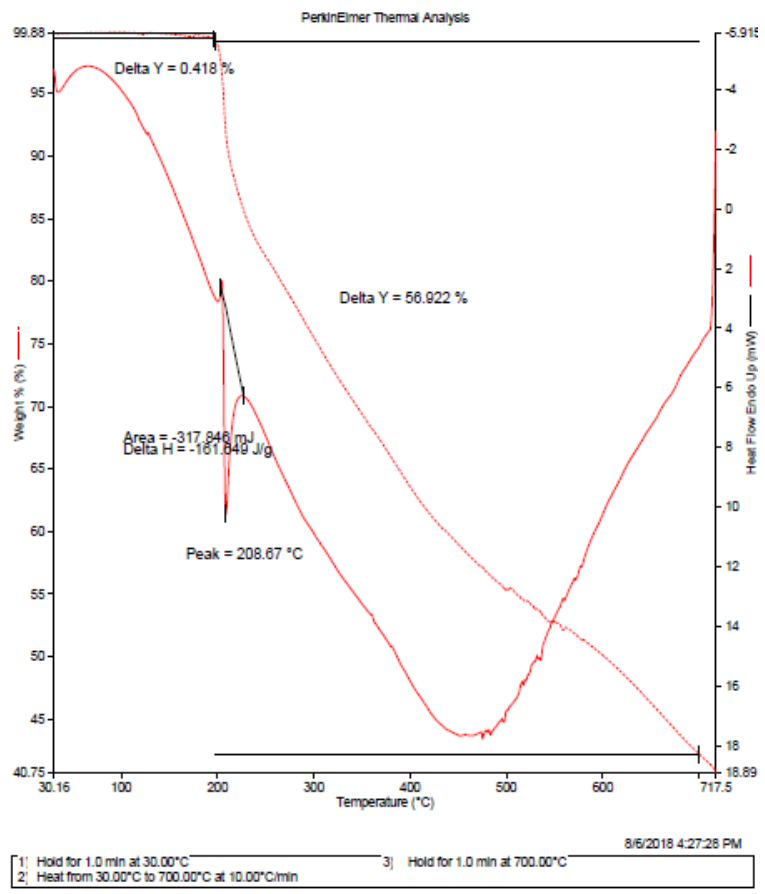
Fig. S5: Frontier orbitals of (a) complex 1, (b) complex 2, (c) complex 3 and (d) complex 4.

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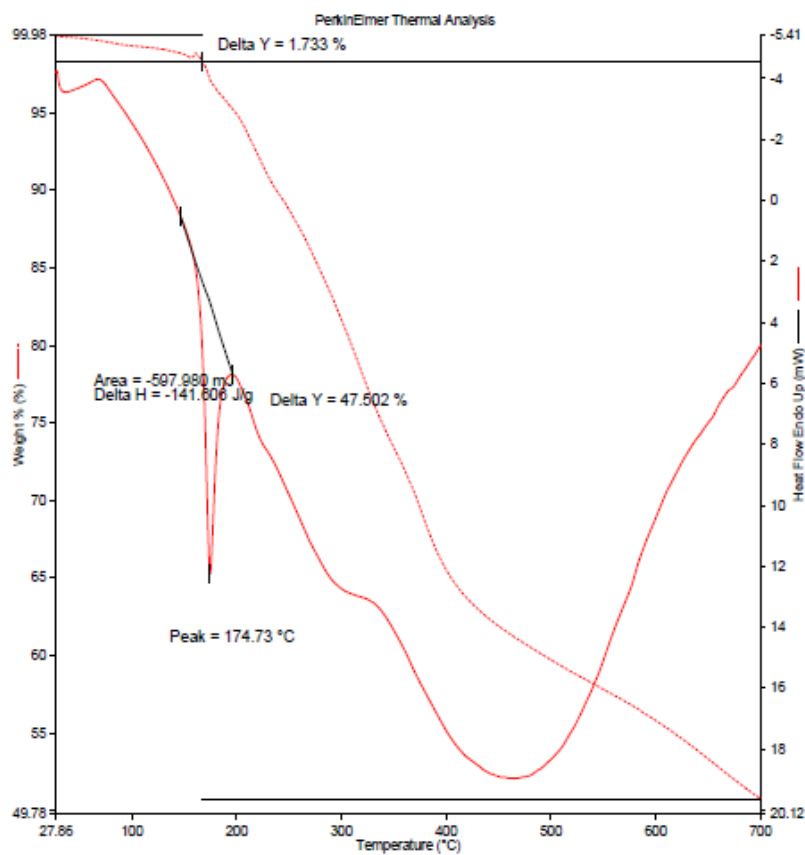
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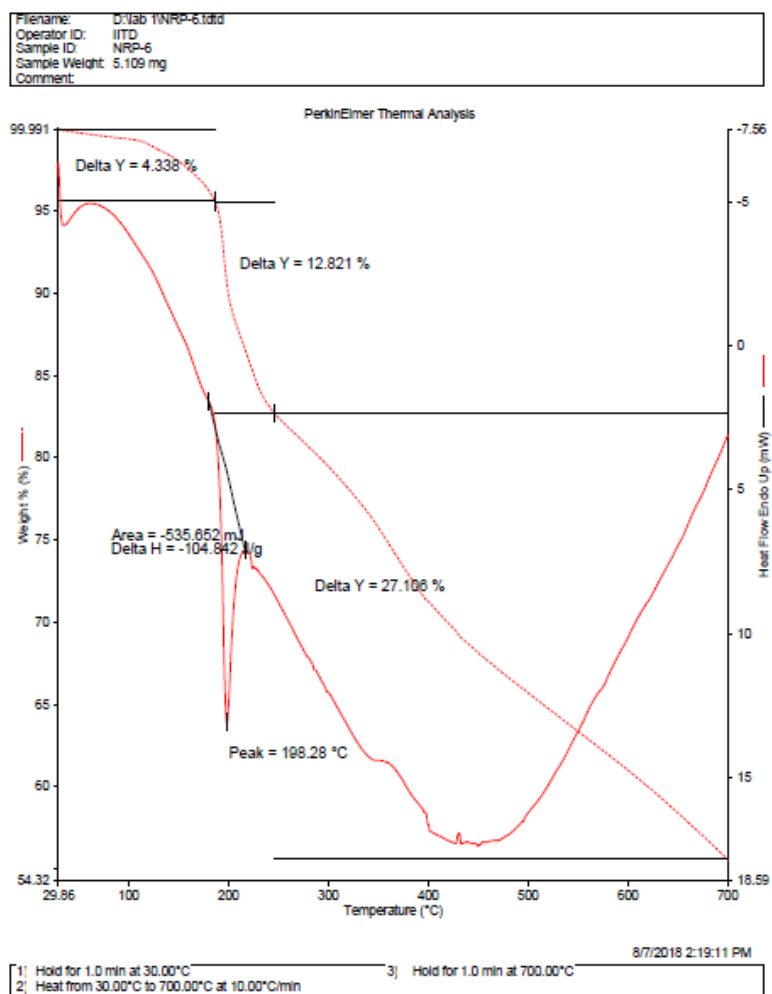
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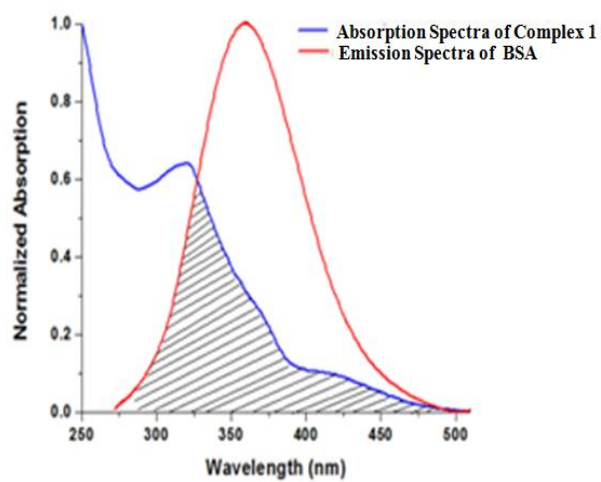
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(c)

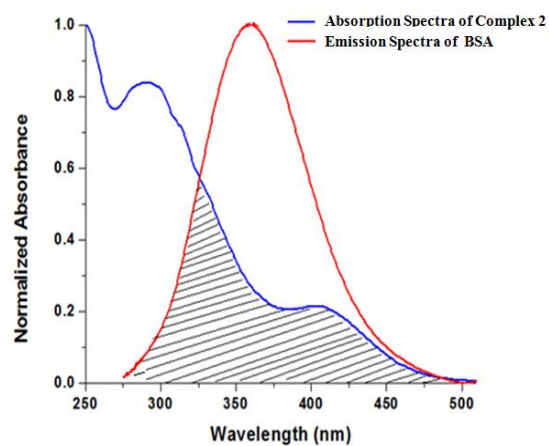


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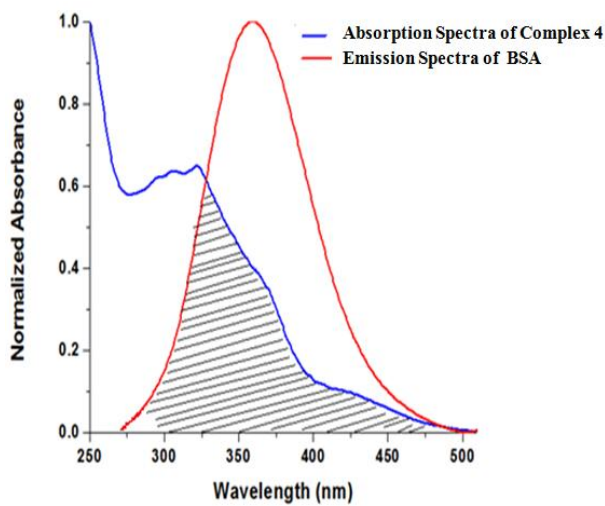
Fig. S6: TG-DTA curves for (a) complex 1, (b) complex 2, (c) complex 3 and (d) complex 4.



(a)

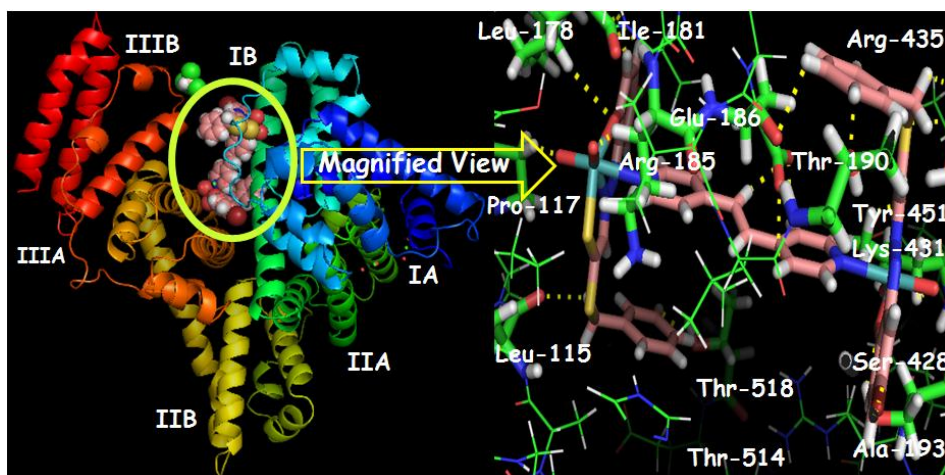


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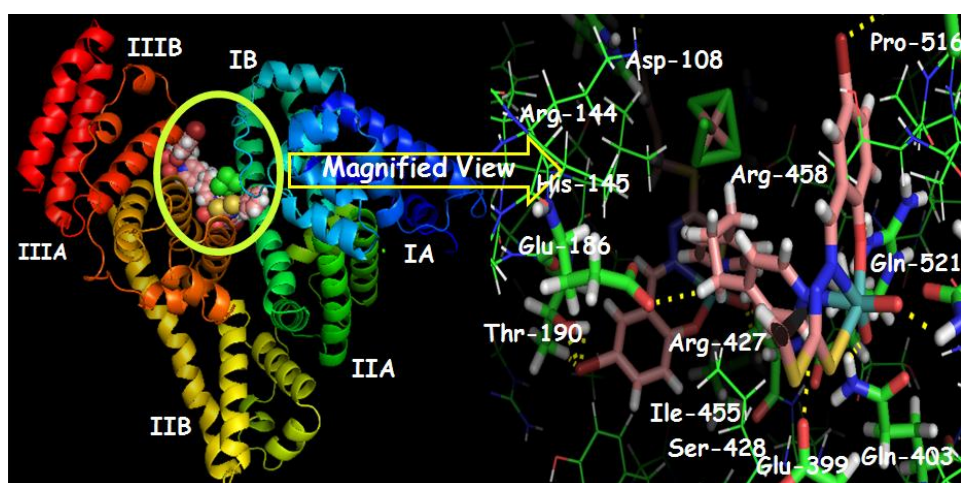


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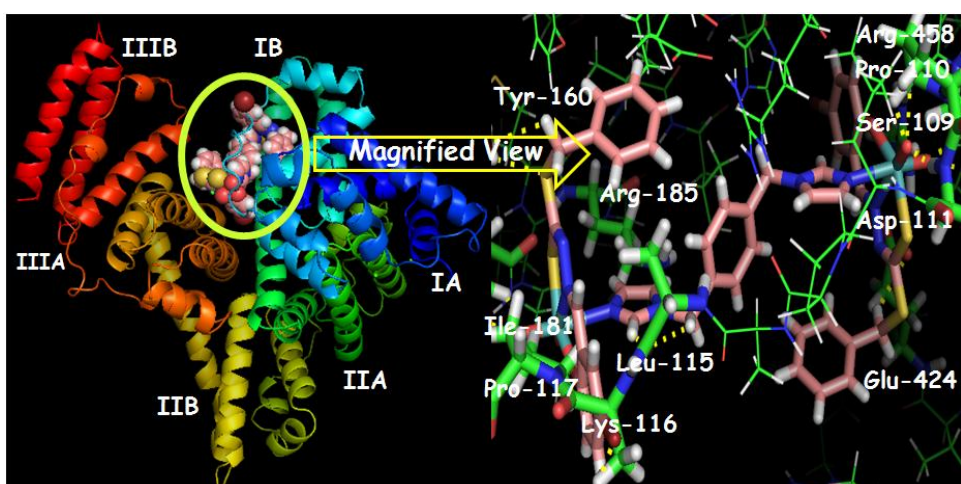
Fig. S7: Overlap of emission spectra of BSA and absorption spectra of (a) complex 1, (b) complex 2 and (c) complex 4.



(a)



(b)



(c)

Fig. S8: Molecular docking images of (a) complex 2 (b) complex 3 and (c) complex 4 with BSA, residues surrounding the binding sites is highlighted.

Table S1: Fingerprint plots of complex 1

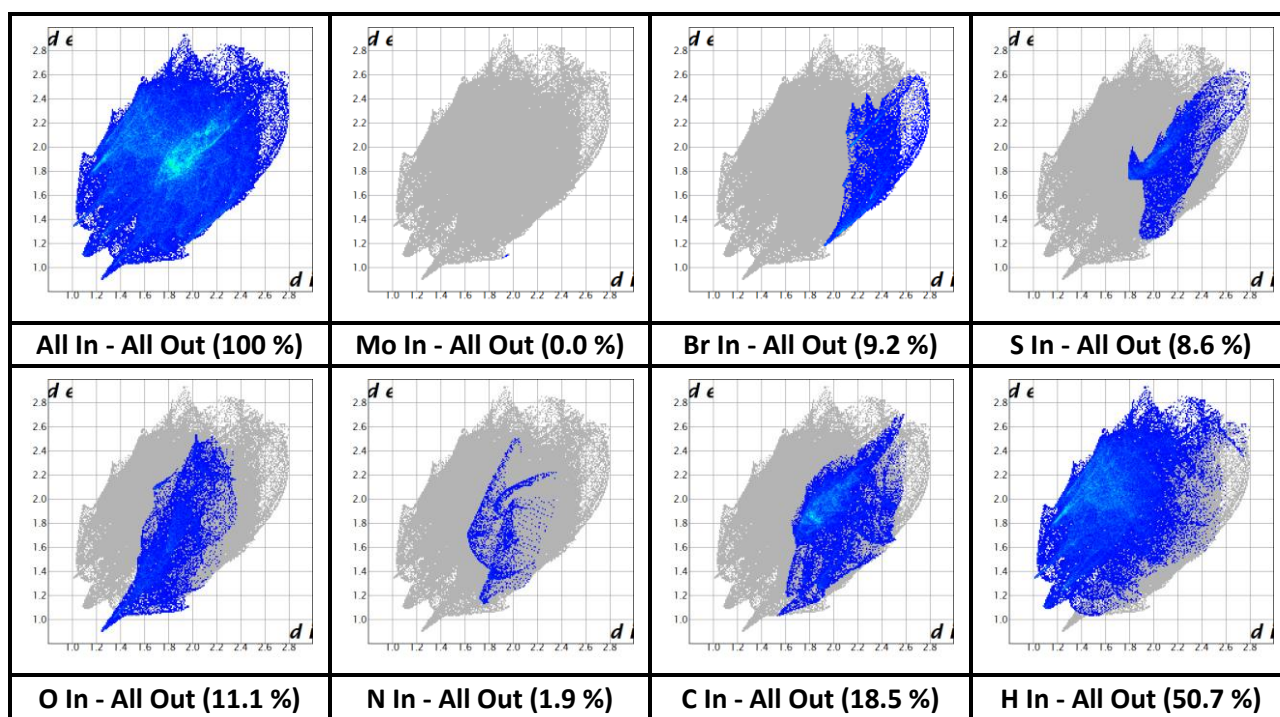


Table S2: Fingerprint plots of complex 2

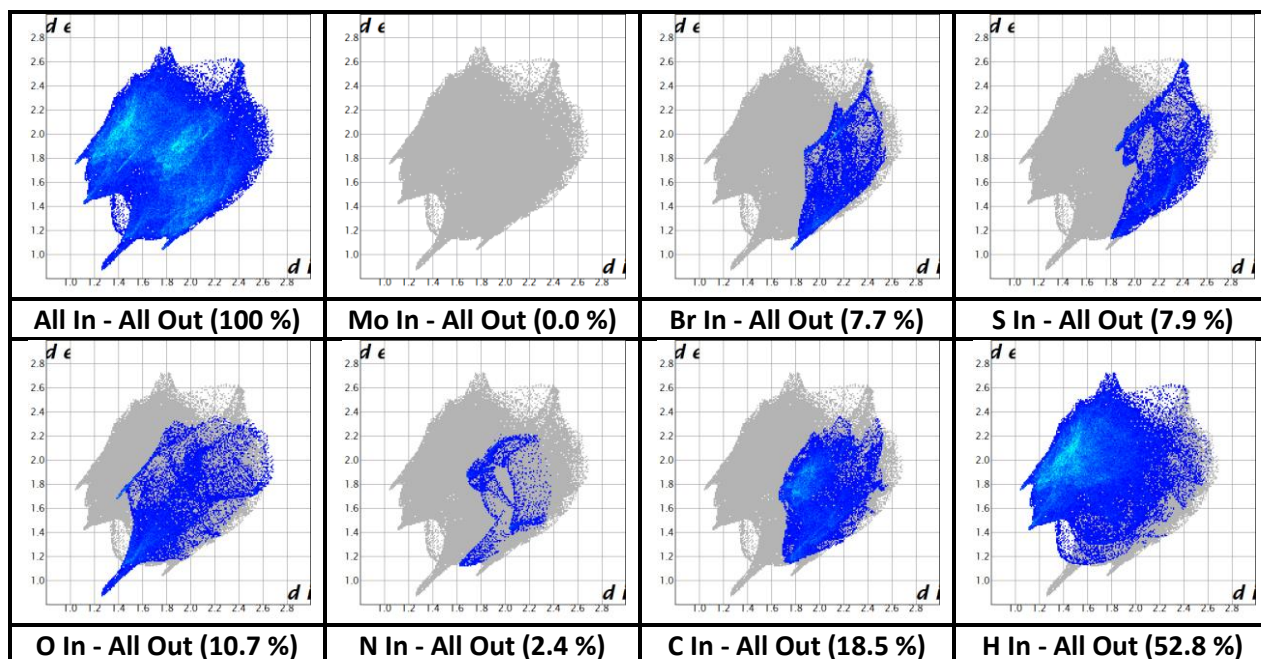


Table S3: Fingerprint plots of complex 3

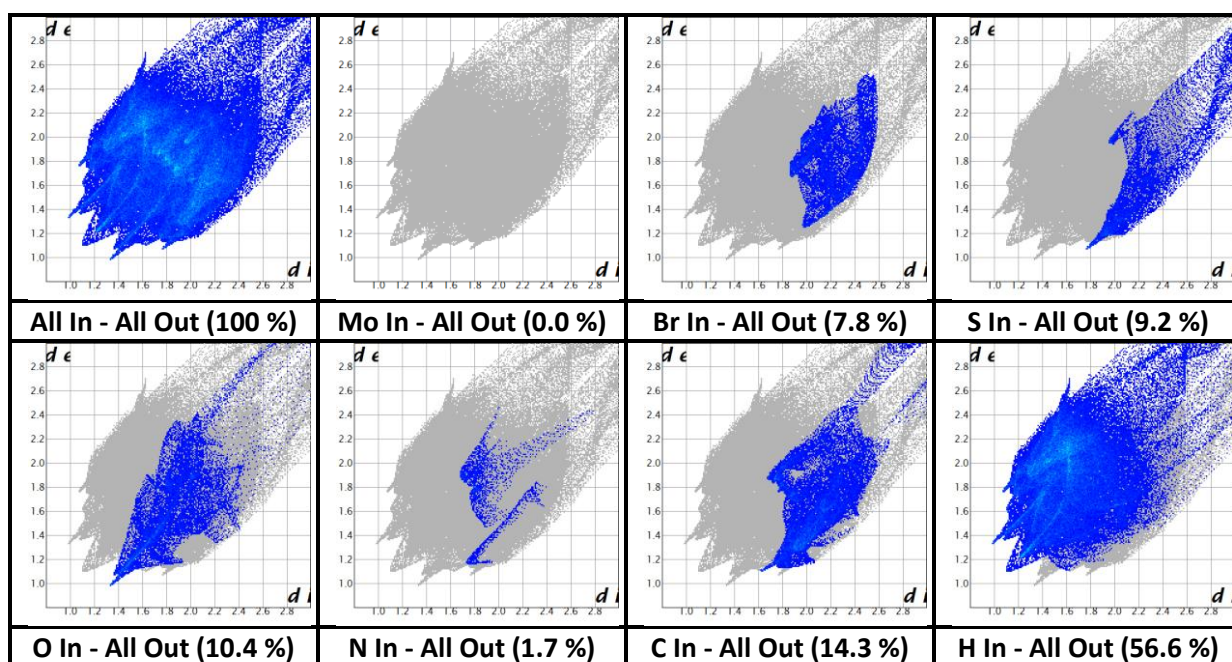


Table S4: Fingerprint plots of complex 4

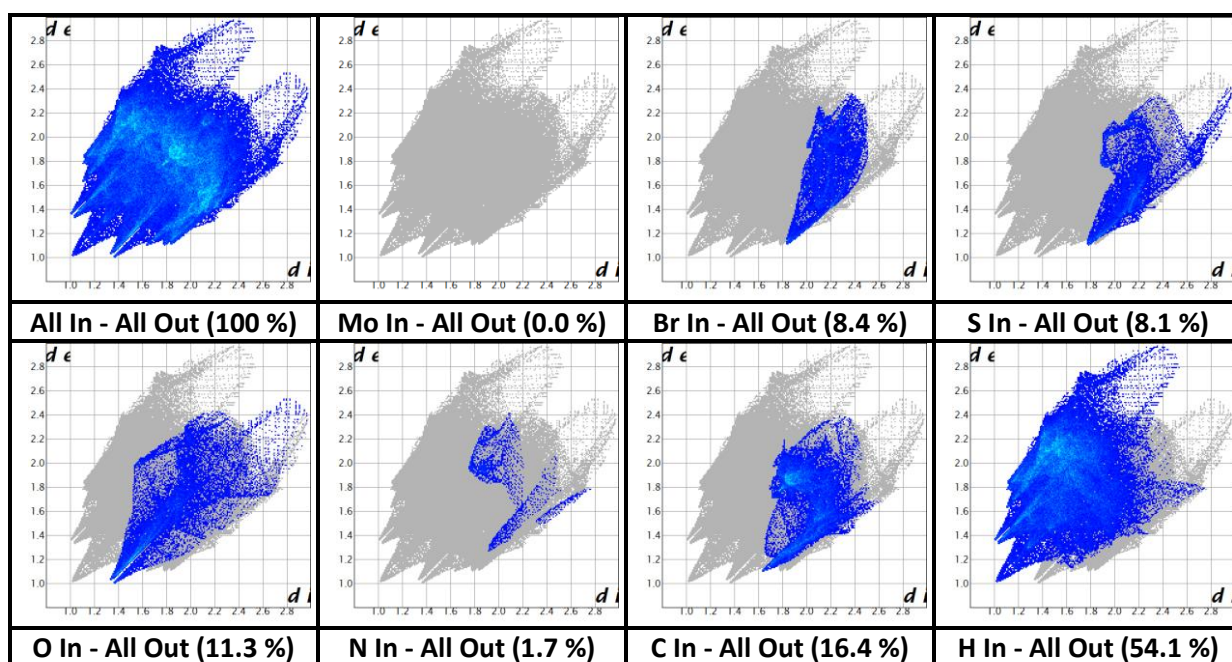


Table S5: Hirshfeld surface volume and surface area of complexes **1-4**

Complex	Surface Volume (\AA^3)	Surface Area (\AA^2)
1	1068.89	892.34
2	1078.04	909.29
3	1252.64	974.82
4	1169.43	896.26

Table S6: Förster Resonance Energy Transfer (FRET) parameters for the ligand and the complexes **1-4** with BSA

Compound	J ($\text{M}^{-1} \text{cm}^3$)	R_0 (nm)	r (nm)	E
H₂L	2.09×10^{-14}	2.87	2.90	0.68
1	1.77×10^{-14}	2.80	2.93	0.63
2	3.41×10^{-14}	2.13	2.25	0.59
3	3.25×10^{-14}	3.10	3.40	0.53
4	2.55×10^{-14}	2.98	3.31	0.54

Table S7: Results of molecular docking: Adjacent residues and hydrogen bonding interactions

Complex	Hydrogen bonding interactions	Adjacent amino acids
BSA...Complex 1	(Leu-115)-C-H...O-Mo = 2.5 \AA (Arg-185)-N-H...O-Mo = 1.7 \AA (Thr-518)-O-H...Br = 1.7 \AA (Arg-458)-N-H...O-Mo = 1.8 \AA (Arg-458)-C-H...O-Mo = 1.0 \AA (Asp-108)-O...H-C = 2.2 \AA (Tyr-147)-N-H...Br = 1.8 \AA (His-145)-C-H...Br = 2.2 \AA (Arg-458)-N-H...O-Mo = 2.5 \AA (Ser-192)-O...H-C = 2.3 \AA (Arg-144)-N-H...S = 1.9 \AA	Leu-112, Leu-115, Tyr-147, Lys-114, Arg-144, Arg-185, Arg-458, Ser-192, His-145, Thr-518, Asp-108

	<p>(Arg-144)-N-H...Cl-(solvent)= 2.7 Å (Leu-112)-N-H...Cl-(solvent)= 0.9 Å (Lys-114)-N...H-C-CH₂-S = 0.8 Å (Lys-114)-C-H...N-N = 0.8 Å (Arg-185)-N-H...O-Mo = 2.8 Å</p>	
BSA...Complex 2	<p>(Pro-117)-C-H...O-Mo = 1.7 Å (Arg-185)-C-H...O-Mo = 2.1 Å (Thr-518)-O...H-C = 2.4 Å (Ser-428)-O...H-C = 1.8 Å (Thr-514)-O...H-C-(solvent) = 2.9 Å (Thr-514)-C-H...Cl-(solvent)= 2.1 Å (Glu-186)-O...H-C-(bpe) = 2.2 Å (Glu-186)-O...H-C-(bpe) = 2.2 Å (Glu-186)-O...H-C-(bpe) = 3.0 Å (Lys-431)-C-H...O-Mo = 2.5 Å (Lys-431)-C-H...O-Mo = 2.0 Å (Ala-193)-C-H...Br = 1.1 Å (Ala-193)-C-H...Br = 2.3 Å (Ile-181)-C-H...O-Mo = 2.9 Å (Ser-428)-O-H...O-Mo = 2.2 Å (Leu-178)-O...H-C = 2.3 Å (Leu-178)-O...H-C = 2.9 Å (Tyr-451)-O...H-C-S = 2.4 Å (Arg-435)-C-H...S = 2.4 Å (Lys-431)-C-H...S-Mo = 1.6 Å (Leu-115)-O...H-C-S = 2.8 Å (Glu-186)-O...H-C = 2.5 Å (Thr-190)-O...H-C = 1.9 Å</p>	<p>Ala-193, Leu-115, Leu-178, Ile-181, Tyr-451, Glu-186, Arg-185, Arg-435, Pro-117, Thr-190, Thr-518, Lys-431, Ser-428</p>
BSA...Complex 3	<p>(Glu-186)-O...H-C-(tmp) = 2.7 Å (Gln-403)-N-H...O-Mo = 2.8 Å (Gln-521)-N-H...O-Mo = 2.0 Å</p>	<p>Glu-186, Glu-399, Gln-430, Gln-521, Arg-144, Arg-427, Arg-458, Pro-516, Thr-190,</p>

	<p>(Arg-427)-N-H...O-Mo = 2.9 Å (Arg-427)-N-H...O-Mo = 1.9 Å (Pro-156)-C-H...Br = 3.1 Å (Glu-399)-O...H-C-(tmp) = 2.8 Å (Thr-190)-O-H...Br = 1.6 Å (Thr-190)-C-H...Br = 2.0 Å (Arg-144)-O...H-C = 2.5 Å (His-145)-N...H-C = 2.4 Å (Asp-108)-O...H-C = 2.9 Å (Arg-458)-C-H...S = 1.9 Å (Ile-455)-C-H...O-Mo = 2.7 Å (Ser-428)-C-H...O-Mo = 1.6 Å (Ile-455)-C-H...O-Mo = 1.8 Å (Ser-428)-O...H-C-(tmp) = 1.0 Å (Thr-190)-O...Br-C = 1.8 Å</p>	<p>His-145, Asp-108, Ser-428, Ile-455</p>
<p>BSA...Complex 4</p>	<p>(Ser-109)-C-H...O-Mo = 1.9 Å (Arg-458)-N-H...O-Mo = 1.9 Å (Asp-111)-N-H...O-Mo = 2.1 Å (Pro-110)-C-H...O-Mo = 2.7 Å (Glu-424)-O...H-C=O = 2.9 Å (Pro-110)-C-H...O-Mo = 1.6 Å (Leu-115)-O...H-C-(bix) = 2.2 Å (Leu-115)-O...H-C-(bix) = 2.8 Å (Lys-116)-C-H...Br = 1.5 Å (Lys-116)-C-H...Br = 0.9 Å (Arg-185)-N...H-C-(bix) = 0.7 Å (Ile-181)-C-H...O-Mo = 1.8 Å (Pro-117)-C-H...O-Mo = 1.2 Å (Tyr-160)-C-H...S = 2.3 Å (Tyr-160)-O...H-C-S = 2.6 Å (Glu-424)-O...H-C-S = 2.8 Å</p>	<p>Leu-115, Ile-181, Tyr-160, Ser-109, Arg-185, Arg-458, Asp-111, Pro-110, Pro-117, Glu-424, Lys-116</p>

	(Ile-181)-C-H...O-Mo = 2.4 Å (Pro-117)-C-H...O-Mo = 2.2 Å	
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