



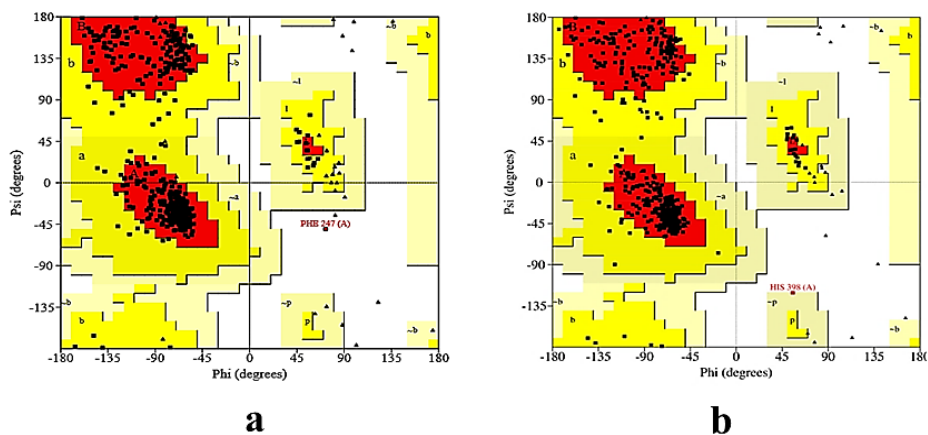
Designing of promising Tromethamine-Diflunisal-Pyrrole combinations based on COX binding, drug-properties and safety

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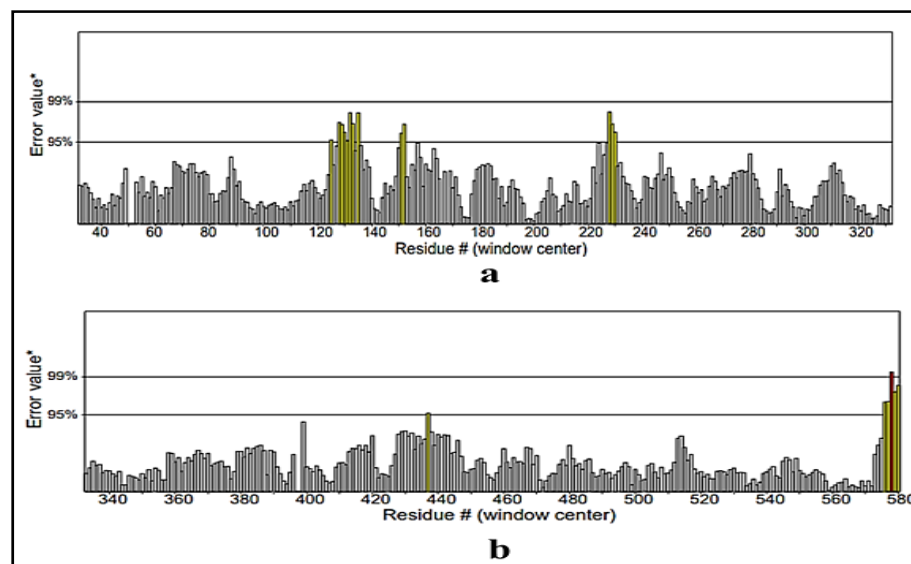
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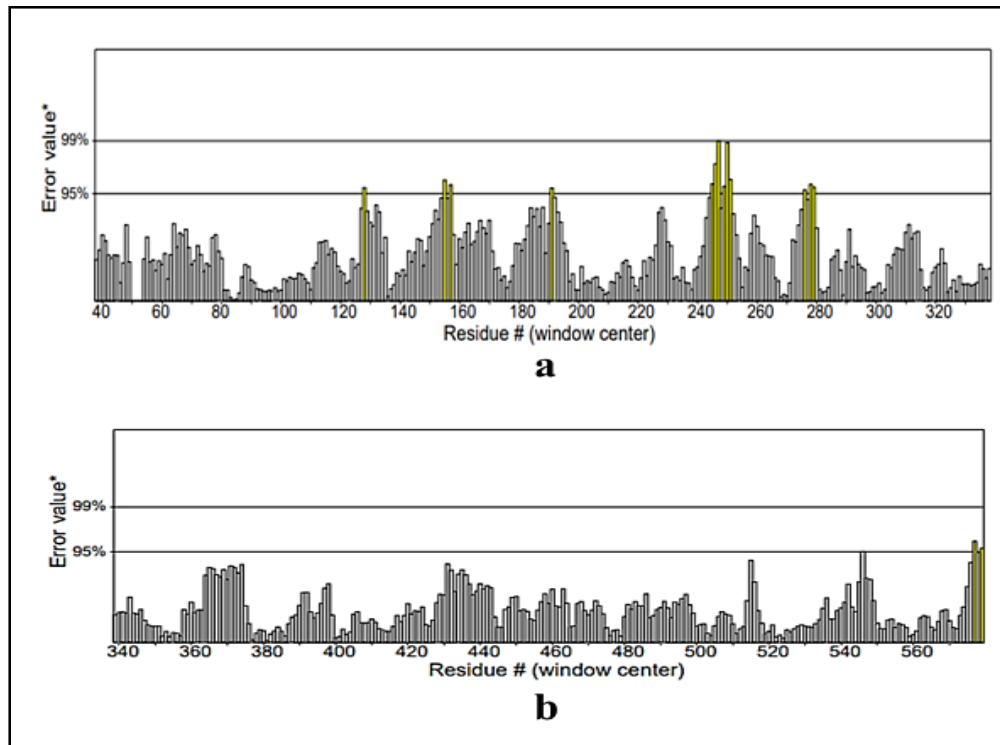
Supplementary Data



Suppl. Fig. 1—Ramachandran plots of refined COX-1 (PDB ID: 6Y3C) and COX-2 (PDB ID: 5IKR) models



Suppl. Fig. 2—Errat plot of residues of refined COX-1 (PDB ID: 6Y3C) enzyme model



Suppl. Fig. 3—Errat plot of residues of refined COX-2 (PDB ID: 5IKR) enzyme model