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

Megha. P Nambiar & Biju AR*

Department of Chemistry, Sir Syed College, Kannur, Taliparamba-670141, Kerala, India

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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