

Upasana Issar

List of Publications by Year in descending order

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189
citing authors

#	ARTICLE	IF	CITATIONS
1	Structures and Stabilities of Alkaline Earth Metal Oxide Nanoclusters: A DFT Study. Journal of Theoretical Chemistry, 2013, 2013, 1-14.	1.5	21
2	In Silico study of the active site of Helicobacter pylori urease and its inhibition by hydroxamic acids. Journal of Molecular Graphics and Modelling, 2018, 83, 64-73.	2.4	20
3	Docking Modes of BB-3497 into the PDF Active Site – A Comparison of the Pure MM and QM/MM Based Docking Strategies. Current Computer-Aided Drug Design, 2015, 10, 315-326.	1.2	11
4	Assessment of molecular binding of Hoechst 33258 analogues into DNA using docking and MM/GBSA approach. Journal of Computational Science, 2015, 10, 166-177.	2.9	11
5	Conformational properties of DNA minor groove binder Hoechst 33258 in gas phase and in aqueous solution. Computational and Theoretical Chemistry, 2017, 1113, 32-41.	2.5	9
6	Identification of novel urease inhibitors: pharmacophore modeling, virtual screening and molecular docking studies. Journal of Biomolecular Structure and Dynamics, 2019, 37, 4312-4326.	3.5	9
7	Combined pharmacophore-guided 3D-QSAR, molecular docking, and virtual screening on bis-benzimidazoles and ter-benzimidazoles as DNA topoisomerase I poisons. Structural Chemistry, 2019, 30, 1185-1201.	2.0	8