Shailesh Kumar Panday

List of Publications by Year
in descending order

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11 papers	149 citations	1684129 5 h-index	1281846 11 g-index
11 all docs	11 docs citations	11 times ranked	160 citing authors

#	Article	IF	Citations
1	Proteinâ€“Protein Binding Free Energy Predictions with the MM/PBSA Approach Complemented with the Gaussian-Based Method for Entropy Estimation. ACS Omega, 2022, 7, 11057-11067.	3.5	9
2	SAAFEC-SEQ: A Sequence-Based Method for Predicting the Effect of Single Point Mutations on Protein Thermodynamic Stability. International Journal of Molecular Sciences, 2021, 22, 606.	4.1	63
3	SAMPDI-3D: predicting the effects of protein and DNA mutations on proteinâ€“DNA interactions. Bioinformatics, 2021, 37, 3760-3765.	4.1	8
4	BION-2: Predicting Positions of Non-Specifically Bound Ions on Protein Surface by a Gaussian-Based Treatment of Electrostatics. International Journal of Molecular Sciences, 2021, 22, 272.	4.1	5
5	Application and Comprehensive Analysis of Neighbor Approximated Information Theoretic Configurational Entropy Methods to Proteinâ€“Ligand Binding Cases. Journal of Chemical Theory and Computation, 2020, 16, 7581-7600.	5.3	2
6	Capturing the Effects of Explicit Waters in Implicit Electrostatics Modeling: Qualitative Justification of Gaussian-Based Dielectric Models in DelPhi. Journal of Chemical Information and Modeling, 2020, 60, 2229-2246.	5.4	8
7	DelPhi Suite: New Developments and Review of Functionalities. Journal of Computational Chemistry, 2019, 40, 2502-2508.	3.3	38
8	Coupling Supervised Molecular Dynamics (SuMD) with Entropy Estimations To Shine Light on the Stability of Multiple Binding Sites. ACS Medicinal Chemistry Letters, 2019, 10, 444-449.	2.8	5
9	In Silico Structure-Based Prediction of Receptorâ€“Ligand Binding Affinity: Current Progress and Challenges. Challenges and Advances in Computational Chemistry and Physics, 2019, , 109-175.	0.6	3
10	Modeling electrostatics in molecular biology: A tutorial of DelPhi and associated resources [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	5
11	ProLego: tool for extracting and visualizing topological modules in protein structures. BMC Bioinformatics, 2018, 19, 167.	2.6	3