

Byungchan Kim

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/11024748/publications.pdf>

Version: 2024-02-01

11
papers

2,885
citations

840776

11
h-index

1281871

11
g-index

11
all docs

11
docs citations

11
times ranked

3246
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|--|------|-----------|
| 1 | Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 42-54. | 5.3 | 103 |
| 2 | Accurate and Reliable Prediction of Relative Ligand Binding Potency in Prospective Drug Discovery by Way of a Modern Free-Energy Calculation Protocol and Force Field. <i>Journal of the American Chemical Society</i> , 2015, 137, 2695-2703. | 13.7 | 931 |
| 3 | Docking and Free Energy Perturbation Studies of Ligand Binding in the Kappa Opioid Receptor. <i>Journal of Physical Chemistry B</i> , 2015, 119, 824-835. | 2.6 | 26 |
| 4 | Modeling Local Structural Rearrangements Using FEP/REST: Application to Relative Binding Affinity Predictions of CDK2 Inhibitors. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1282-1293. | 5.3 | 179 |
| 5 | Thermodynamic analysis of water molecules at the surface of proteins and applications to binding site prediction and characterization. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 871-883. | 2.6 | 118 |
| 6 | Motifs for molecular recognition exploiting hydrophobic enclosure in protein-ligand binding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 808-813. | 7.1 | 633 |
| 7 | Serial Replica Exchange. <i>Journal of Physical Chemistry B</i> , 2007, 111, 1416-1423. | 2.6 | 35 |
| 8 | Replica Exchange with Solute Tempering: Efficiency in Large Scale Systems. <i>Journal of Physical Chemistry B</i> , 2007, 111, 5405-5410. | 2.6 | 103 |
| 9 | Replica exchange with solute tempering: A method for sampling biological systems in explicit water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 13749-13754. | 7.1 | 634 |
| 10 | Structure and Dynamics of the Solvation of Bovine Pancreatic Trypsin Inhibitor in Explicit Water: A Comparative Study of the Effects of Solvent and Protein Polarizability. <i>Journal of Physical Chemistry B</i> , 2005, 109, 16529-16538. | 2.6 | 55 |
| 11 | Efficient Simulation Method for Polarizable Protein Force Fields: Application to the Simulation of BPTI in Liquid Water. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 169-180. | 5.3 | 68 |