Myungshim Kang

List of Publications by Year
in descending order

28	821	623734	526287
papers	citations	14 h-index	27 g-index

30	30	30	1031
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Recent Applications of Kirkwoodâ€“Buff Theory to Biological Systems. Cell Biochemistry and Biophysics, 2008, 50, 1-22.	1.8	199
2	N-(3-Acyloxy-2-benzylpropyl)-Nâ€˜-[4-(methylsulfonylamino)benzyl]thiourea Analogues:Â Novel Potent and High Affinity Antagonists and Partial Antagonists of the Vanilloid Receptor. Journal of Medicinal Chemistry, 2003, 46, 3116-3126.	6.4	110
3	A Kirkwood-Buff derived force field for amides. Journal of Computational Chemistry, 2006, 27, 1477-1485.	3.3	69
4	Preferential interaction parameters in biological systems by Kirkwoodâ€“Buff theory and computer simulation. Fluid Phase Equilibria, 2007, 256, 14-19.	2.5	53
5	Ï€â€“Ï€ Stacking Mediated Chirality in Functional Supramolecular Filaments. Macromolecules, 2016, 49, 994-1001.	4.8	41
6	Molecular simulations of peptide amphiphiles. Organic and Biomolecular Chemistry, 2017, 15, 7993-8005.	2.8	38
7	Gating and Intermolecular Interactions in Ligand-Protein Association: Coarse-Grained Modeling of HIV-1 Protease. Journal of Chemical Theory and Computation, 2011, 7, 3438-3446.	5.3	36
8	Molecular Simulation of the Concentration-Dependent Interaction of Hydrophobic Drugs with Model Cellular Membranes. Journal of Physical Chemistry B, 2014, 118, 11965-11972.	2.6	33
9	Molecular Mechanism for the Role of the H2A and H2B Histone Tails in Nucleosome Repositioning. Journal of Physical Chemistry B, 2018, 122, 11827-11840.	2.6	22
10	MspA Porinâ^'Gold Nanoparticle Assemblies: Enhanced Binding through a Controlled Cysteine Mutation. Nano Letters, 2008, 8, 1229-1236.	9.1	21
11	Kirkwoodâ€“Buff theory of four and higher component mixtures. Journal of Chemical Physics, 2008, 128, 244511.	3.0	21
12	Switches of hydrogen bonds during ligandâ€“protein association processes determine binding kinetics. Journal of Molecular Recognition, 2014, 27, 537-548.	2.1	21
13	The paradox of conformational constraint in the design of Cbl(TKB)-binding peptides. Scientific Reports, 2013, 3, 1639.	3.3	17
14	Coarse-grained molecular dynamics studies of the structure and stability of peptide-based drug amphiphile filaments. Soft Matter, 2017, 13, 7721-7730.	2.7	16
15	Analysis of structureâ€“activity relationships with the N-(3-acyloxy-2-benzylpropyl)-Nâ€²-[4-(methylsulfonylamino)benzyl]thiourea template for vanilloid receptor 1 antagonism. Bioorganic and Medicinal Chemistry, 2004, 12, 3411-3420.	3.0	14
16	Kirkwoodâ€“Buff-Derived Force Field for Peptides and Proteins: Philosophy and Development of KBFF20. Journal of Chemical Theory and Computation, 2021, 17, 2964-2990.	5.3	14
17	Direct Observation of Gold Nanoparticle Assemblies with the Porin MspA on Mica. ACS Nano, 2009, 3, 462-466.	14.6	11
18	Effect of Nucleotide State on the Protofilament Conformation of Tubulin Octamers. Journal of Physical Chemistry B, 2018, 122, 6164-6178.	2.6	10

#	Article	IF	Citations
19	Structureâ€“activity relationships of simplified resiniferatoxin analogues with potent VR1 agonism elucidates an active conformation of RTX for VR1 binding. Bioorganic and Medicinal Chemistry, 2004, 12, 1055-1069.	3.0	9
20	Rational Coarse-Grained Molecular Dynamics Simulations of Supramolecular Anticancer Nanotubes. Journal of Physical Chemistry B, 2019, 123, 10582-10593.	2.6	9
21	Molecular Dynamics Simulations of Supramolecular Anticancer Nanotubes. Journal of Chemical Information and Modeling, 2018, 58, 1164-1168.	5.4	8
22	Mechanistic Insights into Phosphopeptideâ€“BRCT Domain Association: Preorganization, Flexibility, and Phosphate Recognition. Journal of Physical Chemistry B, 2012, 116, 10247-10258.	2.6	6
23	Isomeric control of the mechanical properties of supramolecular filament hydrogels. Biomaterials Science, 2018, 6, 216-224.	5.4	6
24	Comment on â€œCan existing models quantitatively describe the mixing behavior of acetone with waterâ€• [J. Chem. Phys. 130, 124516 (2009)]. Journal of Chemical Physics, 2009, 131, 157101.	3.0	5
25	Interaction of Camptothecin with Model Cellular Membranes. Journal of Chemical Theory and Computation, 2020, 16, 3373-3384.	5.3	5
26	The interaction of supramolecular anticancer drug amphiphiles with phospholipid membranes. Nanoscale Advances, 2021, 3, 370-382.	4.6	3
27	A Pairwise Preferential Interaction Model for Understanding Peptide Aggregation. International Journal of Thermophysics, 2010, 31, 793-804.	2.1	2
28	Molecular Modeling of Paclitaxel Interacting with Membranes. Biophysical Journal, 2014, 106, 801a.	0.5	0