Era Singam

List of Publications by Year in descending order

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EDA SINCAM

#	Article	IF	CITATIONS
1	Effect of Curvature on the α-Helix Breaking Tendency of Carbon Based Nanomaterials. Journal of Physical Chemistry C, 2011, 115, 8886-8892.	1.5	57
2	AntiAngioPred: A Server for Prediction of Anti-Angiogenic Peptides. PLoS ONE, 2015, 10, e0136990.	1.1	51
3	Investigation on interaction of tannic acid with type I collagen and its effect on thermal, enzymatic, and conformational stability for tissue engineering applications. Biopolymers, 2014, 101, 471-483.	1.2	47
4	Discovery of potent inhibitor for matrix metalloproteinase-9 by pharmacophore based modeling and dynamics simulation studies. Journal of Molecular Graphics and Modelling, 2014, 49, 25-37.	1.3	45
5	Thermodynamics of Adsorption on Graphenic Surfaces from Aqueous Solution. Journal of Chemical Theory and Computation, 2019, 15, 1302-1316.	2.3	41
6	Inhibition of insulin amyloid fibril formation by ferulic acid, a natural compound found in many vegetables and fruits. RSC Advances, 2014, 4, 62326-62336.	1.7	35
7	Structural Dynamics of Agonist and Antagonist Binding to the Androgen Receptor. Journal of Physical Chemistry B, 2019, 123, 7657-7666.	1.2	34
8	Structure-based virtual screening of novel, high-affinity BRD4 inhibitors. Molecular BioSystems, 2014, 10, 2384.	2.9	33
9	Interaction of collagen like peptides with gold nanosurfaces: a molecular dynamics investigation. Physical Chemistry Chemical Physics, 2015, 17, 5172-5186.	1.3	26
10	Adsorption of collagen onto single walled carbon nanotubes: a molecular dynamics investigation. Physical Chemistry Chemical Physics, 2011, 13, 13046.	1.3	21
11	Structure-based virtual screening of perfluoroalkyl and polyfluoroalkyl substances (PFASs) as endocrine disruptors of androgen receptor activity using molecular docking and machine learning. Environmental Research, 2020, 190, 109920.	3.7	21
12	Decomposing Dynamical Couplings in Mutated scFv Antibody Fragments into Stabilizing and Destabilizing Effects. Journal of the American Chemical Society, 2017, 139, 17508-17517.	6.6	18
13	Enhancement of Internal Motions of Lysozyme through Interaction with Gold Nanoclusters and its Optical Imaging. Journal of Physical Chemistry C, 2015, 119, 653-664.	1.5	15
14	Investigation of nuclease, proteolytic and antiproliferative effects of copper(II) complexes of thiophenylmethanamine derivatives. European Journal of Medicinal Chemistry, 2013, 70, 280-293.	2.6	14
15	Molecular dynamics simulation study on the interaction of collagenâ€like peptides with gelatinaseâ€A (MMPâ€2). Biopolymers, 2014, 101, 779-794.	1.2	12
16	Influence of the size and charge of gold nanoclusters on complexation with siRNA: a molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2015, 17, 30307-30317.	1.3	12
17	JED: a Java Essential Dynamics Program for comparative analysis of protein trajectories. BMC Bioinformatics, 2017, 18, 271.	1.2	11
18	Experimental and Computational Characterization of the Interaction between Gold Nanoparticles and Polyamidoamine Dendrimers. Langmuir, 2018, 34, 10063-10072.	1.6	11

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19	In Vitro characterization of the endocrine disrupting effects of per- and poly-fluoroalkyl substances (PFASs) on the human androgen receptor. Journal of Hazardous Materials, 2022, 429, 128243.	6.5	11
20	Molecular dynamic simulation studies on the effect of one residue chain staggering on the structure and stability of heterotrimeric collagenâ€like peptides with interruption. Biopolymers, 2012, 97, 847-863.	1.2	10
21	Design and synthesis of sugar-triazole based uracil appended sugar-imine derivatives – an application in DNA binding studies. New Journal of Chemistry, 2015, 39, 4575-4582.	1.4	9
22	3Dâ€QSAR and Docking Studies on the HEPT Derivatives of HIVâ€1 Reverse Transcriptase. Chemical Biology and Drug Design, 2011, 78, 418-426.	1.5	7
23	Predicting the binding of small molecules to nuclear receptors using machine learning. Briefings in Bioinformatics, 2022, 23, .	3.2	7
24	Structure-based discovery of the endocrine disrupting effects of hydraulic fracturing chemicals as novel androgen receptor antagonists. Chemosphere, 2020, 257, 127178.	4.2	6
25	Beta-1,3 Oligoglucans Specifically Bind to Immune Receptor CD28 and May Enhance T Cell Activation. International Journal of Molecular Sciences, 2021, 22, 3124.	1.8	6
26	Interactions between Triterpenes and a P-I Type Snake Venom Metalloproteinase: Molecular Simulations and Experiments. Toxins, 2018, 10, 397.	1.5	5
27	3D-QSAR studies on the biological activity of juvenile hormone mimetic compounds for Culex pipiens Larvae. Medicinal Chemistry Research, 2013, 22, 5948-5960.	1.1	3
28	Identification of an Electrostatic Ruler Motif for Sequence-Specific Binding of Collagenase to Collagen Journal of Physical Chemistry B, 2016, 120, 8580-8589.	1.2	3
29	Molecular clustering and percolation characteristics near the glass transition in aqueous trehalose and choline dihydrogen phosphate solutions. Physical Chemistry Chemical Physics, 2018, 20, 20899-20909.	1.3	1
30	Local immune checkpoint blockade therapy by an adenovirus encoding a novel PD-L1 inhibitory peptide inhibits the growth of colon carcinoma in immunocompetent mice. Translational Oncology, 2022, 16, 101337.	1.7	1
31	Variable Dynamics of IgG4 Monoclonal Antibody Controlled by Single Point Mutations. Biophysical Journal, 2017, 112, 355a.	0.2	0