## Era Singam

## List of Publications by Year in descending order

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623188 610482 31 575 14 24 h-index citations g-index papers 32 32 32 1022 all docs docs citations times ranked citing authors

#	Article	IF	CITATIONS
1	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
2	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
3	Predicting the binding of small molecules to nuclear receptors using machine learning. Briefings in Bioinformatics, 2022, 23, .	3.2	7
4	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
5	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
6	Structure-based discovery of the endocrine disrupting effects of hydraulic fracturing chemicals as novel androgen receptor antagonists. Chemosphere, 2020, 257, 127178.	4.2	6
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	Thermodynamics of Adsorption on Graphenic Surfaces from Aqueous Solution. Journal of Chemical Theory and Computation, 2019, 15, 1302-1316.	2.3	41
9	Interactions between Triterpenes and a P-I Type Snake Venom Metalloproteinase: Molecular Simulations and Experiments. Toxins, 2018, 10, 397.	1.5	5
10	Experimental and Computational Characterization of the Interaction between Gold Nanoparticles and Polyamidoamine Dendrimers. Langmuir, 2018, 34, 10063-10072.	1.6	11
11	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
12	Variable Dynamics of IgG4 Monoclonal Antibody Controlled by Single Point Mutations. Biophysical Journal, 2017, 112, 355a.	0.2	0
13	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
14	JED: a Java Essential Dynamics Program for comparative analysis of protein trajectories. BMC Bioinformatics, 2017, 18, 271.	1.2	11
15	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
16	Interaction of collagen like peptides with gold nanosurfaces: a molecular dynamics investigation. Physical Chemistry Chemical Physics, 2015, 17, 5172-5186.	1.3	26
17	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
18	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

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19	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
20	AntiAngioPred: A Server for Prediction of Anti-Angiogenic Peptides. PLoS ONE, 2015, 10, e0136990.	1.1	51
21	Molecular dynamics simulation study on the interaction of collagenâ€ike peptides with gelatinaseâ€A (MMPâ€2). Biopolymers, 2014, 101, 779-794.	1.2	12
22	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
23	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
24	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
25	Structure-based virtual screening of novel, high-affinity BRD4 inhibitors. Molecular BioSystems, 2014, 10, 2384.	2.9	33
26	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
27	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
28	Molecular dynamic simulation studies on the effect of one residue chain staggering on the structure and stability of heterotrimeric collagenâ€ike peptides with interruption. Biopolymers, 2012, 97, 847-863.	1.2	10
29	Effect of Curvature on the $\hat{l}\pm$ -Helix Breaking Tendency of Carbon Based Nanomaterials. Journal of Physical Chemistry C, 2011, 115, 8886-8892.	1.5	57
30	Adsorption of collagen onto single walled carbon nanotubes: a molecular dynamics investigation. Physical Chemistry Chemical Physics, 2011, 13, 13046.	1.3	21
31	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