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List of Publications by Year
in descending order

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59 papers	1,583 citations	279778 23 h-index	330122 37 g-index
60 all docs	60 docs citations	60 times ranked	1869 citing authors

#	Article	IF	Citations
1	Self-Assembly of Phenylalanine Oligopeptides: Insights from Experiments and Simulations. Biophysical Journal, 2009, 96, 5020-5029.	0.5	212
2	Structure-Dependent Modulation of Aryl Hydrocarbon Receptor-Mediated Activities by Flavonoids. Toxicological Sciences, 2018, 164, 205-217.	3.1	82
3	Selfâ€Assembled Peptide Nanoâ€Superstructure towards Enzyme Mimicking Hydrolysis. Angewandte Chemie - International Edition, 2021, 60, 17164-17170.	13.8	69
4	Enhanced adsorption of per- and polyfluoroalkyl substances (PFAS) by edible, nutrient-amended montmorillonite clays. Water Research, 2021, 188, 116534.	11.3	62
5	Forcefield_NCAA: Ab Initio Charge Parameters to Aid in the Discovery and Design of Therapeutic Proteins and Peptides with Unnatural Amino Acids and Their Application to Complement Inhibitors of the Compstatin Family. ACS Synthetic Biology, 2014, 3, 855-869.	3.8	59
6	Molecular Recognition of CCR5 by an HIV-1 gp120 V3 Loop. PLoS ONE, 2014, 9, e95767.	2.5	56
7	Molecular Recognition of CXCR4 by a Dual Tropic HIV-1 gp120 V3 Loop. Biophysical Journal, 2013, 105, 1502-1514.	0.5	52
8	Elucidating a Key Component of Cancer Metastasis: CXCL12 (SDF-1Î±) Binding to CXCR4. Journal of Chemical Information and Modeling, 2014, 54, 1174-1188.	5.4	49
9	High-Efficiency Fluorescence through Bioinspired Supramolecular Self-Assembly. ACS Nano, 2020, 14, 2798-2807.	14.6	49
10	Interactions between Curcumin Derivatives and Amyloid-Î² Fibrils: Insights from Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2020, 60, 289-305.	5.4	44
11	Amyloid-Like Self-Assembly of Peptide Sequences from the Adenovirus Fiber Shaft: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 15639-15647.	2.6	42
12	Editorâ€™s Highlight: Microbial-Derived 1,4-Dihydroxy-2-naphthoic Acid and Related Compounds as Aryl Hydrocarbon Receptor Agonists/Antagonists: Structureâ€“Activity Relationships and Receptor Modeling. Toxicological Sciences, 2017, 155, 458-473.	3.1	40
13	Elucidating a Key Anti-HIV-1 and Cancer-Associated Axis: The Structure of CCL5 (Rantes) in Complex with CCR5. Scientific Reports, 2014, 4, 5447.	3.3	38
14	Self-Assembled Amyloid Peptides with Arg-Gly-Asp (RGD) Motifs As Scaffolds for Tissue Engineering. ACS Biomaterials Science and Engineering, 2017, 3, 1404-1416.	5.2	38
15	Species specificity of the complement inhibitor compstatin investigated by allâ€atom molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2655-2667.	2.6	34
16	Molecular Dynamics in Drug Design: New Generations of Compstatin Analogs. Chemical Biology and Drug Design, 2012, 79, 703-718.	3.2	34
17	Montmorillonites Can Tightly Bind Glyphosate and Paraquat Reducing Toxin Exposures and Toxicity. ACS Omega, 2019, 4, 17702-17713.	3.5	33
18	Enhanced Fluorescence for Bioassembly by Environmentâ€Switching Doping of Metal Ions. Advanced Functional Materials, 2020, 30, 1909614.	14.9	33

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19	Montmorillonite clay-based sorbents decrease the bioavailability of per- and polyfluoroalkyl substances (PFAS) from soil and their translocation to plants. Environmental Research, 2022, 205, 112433.	7.5	27
20	Protection of Oxygen-Sensitive Enzymes by Peptide Hydrogel. ACS Nano, 2021, 15, 6530-6539.	14.6	26
21	Novel compstatin family peptides inhibit complement activation by drusen-like deposits in human retinal pigmented epithelial cell cultures. Experimental Eye Research, 2013, 116, 96-108.	2.6	25
22	Isoflavones as Ah Receptor Agonists in Colon-Derived Cell Lines: Structureâ€“Activity Relationships. Chemical Research in Toxicology, 2019, 32, 2353-2364.	3.3	25
23	Design of a modified mouse protein with ligand binding properties of its human analog by molecular dynamics simulations: The case of C3 inhibition by compstatin. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3166-3179.	2.6	24
24	Exploring Protein-Protein and Protein-Ligand Interactions in the Immune System using Molecular Dynamics and Continuum Electrostatics. Current Physical Chemistry, 2012, 2, 324-343.	0.2	24
25	Highly Accurate Structure-Based Prediction of HIV-1 Coreceptor Usage Suggests Intermolecular Interactions Driving Tropism. PLoS ONE, 2016, 11, e0148974.	2.5	23
26	Self-Assembly of an Aspartate-Rich Sequence from the Adenovirus Fiber Shaft: Insights from Molecular Dynamics Simulations and Experiments. Journal of Physical Chemistry B, 2014, 118, 1765-1774.	2.6	22
27	Uncovering the Binding and Specificity of Î²-Wrapins for Amyloid-Î² and Î±-Synuclein. Journal of Physical Chemistry B, 2016, 120, 12781-12794.	2.6	22
28	Insights into the mechanism of C5aR inhibition by PMX53 via implicit solvent molecular dynamics simulations and docking. BMC Biophysics, 2014, 7, 5.	4.4	21
29	Princeton_TIGRESS: Protein geometry refinement using simulations and support vector machines. Proteins: Structure, Function and Bioinformatics, 2014, 82, 794-814.	2.6	21
30	Insights into the Structure, Correlated Motions, and Electrostatic Properties of Two HIV-1 gp120 V3 Loops. PLoS ONE, 2012, 7, e49925.	2.5	20
31	A novel amyloid designable scaffold and potential inhibitor inspired by <scp>GAIIG</scp> of amyloid beta and the <scp>HIV</scp>â€1 V3 loop. FEBS Letters, 2018, 592, 1777-1788.	2.8	18
32	Designer Amyloid Cell-Penetrating Peptides for Potential Use as Gene Transfer Vehicles. Biomolecules, 2020, 10, 7.	4.0	18
33	Combination of Theoretical and Experimental Approaches for the Design and Study of Fibril-Forming Peptides. Methods in Molecular Biology, 2014, 1216, 53-70.	0.9	18
34	Amyloid-like self-assembly of a dodecapeptide sequence from the adenovirus fiber shaft: Perspectives from molecular dynamics simulations. Journal of Non-Crystalline Solids, 2011, 357, 717-722.	3.1	17
35	New Compstatin Peptides Containing N-Terminal Extensions and Non-Natural Amino Acids Exhibit Potent Complement Inhibition and Improved Solubility Characteristics. Journal of Medicinal Chemistry, 2015, 58, 814-826.	6.4	17
36	Virtual Screening of Chemical Compounds for Discovery of Complement C3 Ligands. ACS Omega, 2018, 3, 6427-6438.	3.5	15

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37	Princeton_<scp>TIGRESS</scp> 2.0: High refinement consistency and net gains through support vector machines and molecular dynamics in doubleâ€blind predictions during the <scp>CASP</scp>11 experiment. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1078-1098.	2.6	14
38	Computational design of amyloid self-assembling peptides bearing aromatic residues and the cell adhesive motif Arg-Gly-Asp. Molecular Systems Design and Engineering, 2017, 2, 321-335.	3.4	14
39	Elucidating the multi-targeted anti-amyloid activity and enhanced islet amyloid polypeptide binding of Î²-wrapins. Computers and Chemical Engineering, 2018, 116, 322-332.	3.8	13
40	Development and characterization of chlorophyll-amended montmorillonite clays for the adsorption and detoxification of benzene. Water Research, 2022, 221, 118788.	11.3	13
41	Computational Design of Functional Amyloid Materials with Cesium Binding, Deposition, and Capture Properties. Journal of Physical Chemistry B, 2018, 122, 7555-7568.	2.6	12
42	Molecular Mechanism for Attractant Signaling to DHMA by E.Âcoli Tsr. Biophysical Journal, 2020, 118, 492-504.	0.5	12
43	Insights into the interactions of bisphenol and phthalate compounds with unamended and carnitine-amended montmorillonite clays. Computers and Chemical Engineering, 2020, 143, 107063.	3.8	12
44	Selfâ€Assembled Peptide Nanoâ€Superstructure towards Enzyme Mimicking Hydrolysis. Angewandte Chemie, 2021, 133, 17301-17307.	2.0	12
45	Activation of COUP-TFI by a Novel Diindolylmethane Derivative. Cells, 2019, 8, 220.	4.1	10
46	Modification of a Single Atom Affects the Physical Properties of Double Fluorinated Fmoc-Phe Derivatives. International Journal of Molecular Sciences, 2021, 22, 9634.	4.1	9
47	A high-throughput and rapid computational method for screening of RNA post-transcriptional modifications that can be recognized by target proteins. Methods, 2018, 143, 34-47.	3.8	8
48	Computational evolution of an RNA-binding protein towards enhanced oxidized-RNA binding. Computational and Structural Biotechnology Journal, 2020, 18, 137-152.	4.1	8
49	Ecotoxic effects of paclitaxel-loaded nanotherapeutics on freshwater algae, Raphidocelis subcapitata and Chlamydomonas reinhardtii. Environmental Science: Nano, 2017, 4, 1077-1085.	4.3	7
50	Combining Experimental Isotherms, Minimalistic Simulations, and a Model to Understand and Predict Chemical Adsorption onto Montmorillonite Clays. ACS Omega, 2021, 6, 14090-14103.	3.5	7
51	Amyloid Peptide Scaffolds Coordinate with Alzheimerâ€™s Disease Drugs. Journal of Physical Chemistry B, 2020, 124, 487-503.	2.6	5
52	Molecular Modeling of Chemoreceptor:Ligand Interactions. Methods in Molecular Biology, 2018, 1729, 353-372.	0.9	4
53	EDTA-mimicking amino acidâ€“metal ion coordination for multifunctional packings. Journal of Materials Chemistry A, 2021, 9, 20385-20394.	10.3	4
54	Computational and Experimental Protocols to Study Cyclo-dihistidine Self- and Co-assembly: Minimalistic Bio-assemblies with Enhanced Fluorescence and Drug Encapsulation Properties. Methods in Molecular Biology, 2022, 2405, 179-203.	0.9	3

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55	Selfâ€Assembling Amyloid Sequences as Scaffolds for Material Design: A Case Study of Building Blocks Inspired From the Adenovirus Fiber Protein. Macromolecular Symposia, 2019, 386, 1900005.	0.7	2
56	Hydroxylated Chalcones as Aryl Hydrocarbon Receptor Agonists: Structure-Activity Effects. Toxicological Sciences, 2021, 180, 148-159.	3.1	2
57	Exploring Protein-Protein and Protein-Ligand Interactions in the Immune System using Molecular Dynamics and Continuum Electrostatics. Current Physical Chemistry, 2012, 2, 324-343.	0.2	2
58	Computational design of a Î²-wrapin's N-terminal domain with canonical and non-canonical amino acid modifications mimicking curcumin's proposed inhibitory function. Biophysical Chemistry, 2022, 286, 106805.	2.8	1
59	O2â€02â€04: BETAâ€WRAPIN PROTEINS SEQUESTERING AMYLOID PROTEINS INVOLVED IN ALZHEIMER'S DISEASE: UNDERSTANDING THEIR FUNCTION AND DESIGNING NOVEL, IMPROVED BETAâ€WRAPINS AS POTENTIAL THERAPEUTICS. Alzheimer's and Dementia, 2018, 14, P611.	0.8	0