

Asuka A Orr

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

55
papers

1,077
citations

20
h-index

30
g-index

60
ext. papers

1,352
ext. citations

5.1
avg. IF

4.51
L-index

#	Paper	IF	Citations
55	Computational and Experimental Protocols to Study Cyclo-dihistidine Self- and Co-assembly: Minimalistic Bio-assemblies with Enhanced Fluorescence and Drug Encapsulation Properties.. <i>Methods in Molecular Biology</i> , 2022 , 2405, 179-203	1.4	1
54	Computational design of a ßwrapin α N-terminal domain with canonical and non-canonical amino acid modifications mimicking curcumin α proposed inhibitory function.. <i>Biophysical Chemistry</i> , 2022 , 286, 106805	3.5	0
53	Montmorillonite clay-based sorbents decrease the bioavailability of per- and polyfluoroalkyl substances (PFAS) from soil and their translocation to plants. <i>Environmental Research</i> , 2021 , 205, 112433	7.9	3
52	Protection of Oxygen-Sensitive Enzymes by Peptide Hydrogel. <i>ACS Nano</i> , 2021 , 15, 6530-6539	16.7	9
51	Combining Experimental Isotherms, Minimalistic Simulations, and a Model to Understand and Predict Chemical Adsorption onto Montmorillonite Clays. <i>ACS Omega</i> , 2021 , 6, 14090-14103	3.9	2
50	Self-Assembled Peptide Nano-Superstructure towards Enzyme Mimicking Hydrolysis. <i>Angewandte Chemie</i> , 2021 , 133, 17301-17307	3.6	1
49	Self-Assembled Peptide Nano-Superstructure towards Enzyme Mimicking Hydrolysis. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 17164-17170	16.4	9
48	Hydroxylated Chalcones as Aryl Hydrocarbon Receptor Agonists: Structure-Activity Effects. <i>Toxicological Sciences</i> , 2021 , 180, 148-159	4.4	0
47	Enhanced adsorption of per- and polyfluoroalkyl substances (PFAS) by edible, nutrient-amended montmorillonite clays. <i>Water Research</i> , 2021 , 188, 116534	12.5	18
46	EDTA-mimicking amino acid-metal ion coordination for multifunctional packings. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 20385-20394	13	1
45	High-Efficiency Fluorescence through Bioinspired Supramolecular Self-Assembly. <i>ACS Nano</i> , 2020 , 14, 2798-2807	16.7	22
44	Enhanced Fluorescence for Bioassembly by Environment-Switching Doping of Metal Ions. <i>Advanced Functional Materials</i> , 2020 , 30, 1909614	15.6	24
43	Computational evolution of an RNA-binding protein towards enhanced oxidized-RNA binding. <i>Computational and Structural Biotechnology Journal</i> , 2020 , 18, 137-152	6.8	2
42	Amyloid Peptide Scaffolds Coordinate with Alzheimer's Disease Drugs. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 487-503	3.4	4
41	Molecular Mechanism for Attractant Signaling to DHMA by E. coli Tsr. <i>Biophysical Journal</i> , 2020 , 118, 492-504	2.9	6
40	Interactions between Curcumin Derivatives and Amyloid- β Fibrils: Insights from Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 289-305	6.1	18
39	Insights into the interactions of bisphenol and phthalate compounds with unamended and carnitine-amended montmorillonite clays. <i>Computers and Chemical Engineering</i> , 2020 , 143, 107063-107063	4.3	7

38	Activation of COUP-TFI by a Novel Diindolylmethane Derivative. <i>Cells</i> , 2019 , 8,	7.9	6
37	Designer Amyloid Cell-Penetrating Peptides for Potential Use as Gene Transfer Vehicles. <i>Biomolecules</i> , 2019 , 10,	5.9	10
36	Self-Assembling Amyloid Sequences as Scaffolds for Material Design: A Case Study of Building Blocks Inspired From the Adenovirus Fiber Protein. <i>Macromolecular Symposia</i> , 2019 , 386, 1900005	0.8	1
35	Isoflavones as Ah Receptor Agonists in Colon-Derived Cell Lines: Structure-Activity Relationships. <i>Chemical Research in Toxicology</i> , 2019 , 32, 2353-2364	4	16
34	Montmorillonites Can Tightly Bind Glyphosate and Paraquat Reducing Toxin Exposures and Toxicity. <i>ACS Omega</i> , 2019 , 4, 17702-17713	3.9	17
33	Molecular Modeling of Chemoreceptor:Ligand Interactions. <i>Methods in Molecular Biology</i> , 2018 , 1729, 353-372	1.4	4
32	A high-throughput and rapid computational method for screening of RNA post-transcriptional modifications that can be recognized by target proteins. <i>Methods</i> , 2018 , 143, 34-47	4.6	5
31	Structure-Dependent Modulation of Aryl Hydrocarbon Receptor-Mediated Activities by Flavonoids. <i>Toxicological Sciences</i> , 2018 , 164, 205-217	4.4	48
30	Elucidating the multi-targeted anti-amyloid activity and enhanced islet amyloid polypeptide binding of -wrapins. <i>Computers and Chemical Engineering</i> , 2018 , 116, 322-332	4	10
29	Virtual Screening of Chemical Compounds for Discovery of Complement C3 Ligands. <i>ACS Omega</i> , 2018 , 3, 6427-6438	3.9	11
28	Computational Design of Functional Amyloid Materials with Cesium Binding, Deposition, and Capture Properties. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 7555-7568	3.4	10
27	O2-02-04: BETA-WRAPIN PROTEINS SEQUESTERING AMYLOID PROTEINS INVOLVED IN ALZHEIMER'S DISEASE: UNDERSTANDING THEIR FUNCTION AND DESIGNING NOVEL, IMPROVED BETA-WRAPINS AS POTENTIAL THERAPEUTICS 2018 , 14, P611-P612		
26	Princeton_TIGRESS 2.0: High refinement consistency and net gains through support vector machines and molecular dynamics in double-blind predictions during the CASP11 experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017 , 85, 1078-1098	4.2	12
25	Ecotoxic effects of paclitaxel-loaded nanotherapeutics on freshwater algae, <i>Raphidocelis subcapitata</i> and <i>Chlamydomonas reinhardtii</i> . <i>Environmental Science: Nano</i> , 2017 , 4, 1077-1085	7.1	7
24	Computational design of amyloid self-assembling peptides bearing aromatic residues and the cell adhesive motif Arg-Gly-Asp. <i>Molecular Systems Design and Engineering</i> , 2017 , 2, 321-335	4.6	12
23	Self-Assembled Amyloid Peptides with Arg-Gly-Asp (RGD) Motifs As Scaffolds for Tissue Engineering. <i>ACS Biomaterials Science and Engineering</i> , 2017 , 3, 1404-1416	5.5	28
22	Editor's Highlight: Microbial-Derived 1,4-Dihydroxy-2-naphthoic Acid and Related Compounds as Aryl Hydrocarbon Receptor Agonists/Antagonists: Structure-Activity Relationships and Receptor Modeling. <i>Toxicological Sciences</i> , 2017 , 155, 458-473	4.4	23
21	Highly Accurate Structure-Based Prediction of HIV-1 Coreceptor Usage Suggests Intermolecular Interactions Driving Tropism. <i>PLoS ONE</i> , 2016 , 11, e0148974	3.7	21

20	Uncovering the Binding and Specificity of BWrapins for Amyloid- β and β Synuclein. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 12781-12794	3.4	19
19	New compstatin peptides containing N-terminal extensions and non-natural amino acids exhibit potent complement inhibition and improved solubility characteristics. <i>Journal of Medicinal Chemistry</i> , 2015 , 58, 814-26	8.3	16
18	Elucidating a key anti-HIV-1 and cancer-associated axis: the structure of CCL5 (Rantes) in complex with CCR5. <i>Scientific Reports</i> , 2014 , 4, 5447	4.9	32
17	Princeton_TIGRESS: protein geometry refinement using simulations and support vector machines. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 794-814	4.2	21
16	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. <i>ACS Synthetic Biology</i> , 2014 , 3, 855-69	5.7	47
15	Elucidating a key component of cancer metastasis: CXCL12 (SDF-1 β) binding to CXCR4. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 1174-88	6.1	37
14	Self-assembly of an aspartate-rich sequence from the adenovirus fiber shaft: insights from molecular dynamics simulations and experiments. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 1765-74	3.4	20
13	Insights into the mechanism of C5aR inhibition by PMX53 via implicit solvent molecular dynamics simulations and docking. <i>BMC Biophysics</i> , 2014 , 7, 5	0	20
12	Molecular recognition of CCR5 by an HIV-1 gp120 V3 loop. <i>PLoS ONE</i> , 2014 , 9, e95767	3.7	44
11	Combination of theoretical and experimental approaches for the design and study of fibril-forming peptides. <i>Methods in Molecular Biology</i> , 2014 , 1216, 53-70	1.4	15
10	Molecular recognition of CXCR4 by a dual tropic HIV-1 gp120 V3 loop. <i>Biophysical Journal</i> , 2013 , 105, 1502-14	2.9	39
9	Novel compstatin family peptides inhibit complement activation by drusen-like deposits in human retinal pigmented epithelial cell cultures. <i>Experimental Eye Research</i> , 2013 , 116, 96-108	3.7	23
8	Molecular dynamics in drug design: new generations of compstatin analogs. <i>Chemical Biology and Drug Design</i> , 2012 , 79, 703-18	2.9	31
7	Exploring Protein-Protein and Protein-Ligand Interactions in the Immune System using Molecular Dynamics and Continuum Electrostatics. <i>Current Physical Chemistry</i> , 2012 , 2, 324-343	0.5	16
6	Insights into the structure, correlated motions, and electrostatic properties of two HIV-1 gp120 V3 loops. <i>PLoS ONE</i> , 2012 , 7, e49925	3.7	17
5	Amyloid-like self-assembly of a dodecapeptide sequence from the adenovirus fiber shaft: Perspectives from molecular dynamics simulations. <i>Journal of Non-Crystalline Solids</i> , 2011 , 357, 717-722	3.9	16
4	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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 3166-79	4.2	23
3	Species specificity of the complement inhibitor compstatin investigated by all-atom molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 2655-67	4.2	32

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| 2 | Amyloid-like self-assembly of peptide sequences from the adenovirus fiber shaft: insights from molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 15639-47 | 3.4 | 35 |
| 1 | Self-assembly of phenylalanine oligopeptides: insights from experiments and simulations. <i>Biophysical Journal</i> , 2009 , 96, 5020-9 | 2.9 | 187 |