Asuka A Orr

List of Publications by Citations

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	Self-assembly of phenylalanine oligopeptides: insights from experiments and simulations. *Biophysical Journal*, **2009**, 96, 5020-9	2.9	187
54	Structure-Dependent Modulation of Aryl Hydrocarbon Receptor-Mediated Activities by Flavonoids. *Toxicological Sciences*, **2018**, 164, 205-217	4.4	48
53	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, 855-69	5.7	47
52	Molecular recognition of CCR5 by an HIV-1 gp120 V3 loop. *PLoS ONE*, **2014**, 9, e95767	3.7	44
51	Molecular recognition of CXCR4 by a dual tropic HIV-1 gp120 V3 loop. *Biophysical Journal*, **2013**, 105, 1502-14	2.9	39
50	Elucidating a key component of cancer metastasis: CXCL12 (SDF-1) binding to CXCR4. *Journal of Chemical Information and Modeling*, **2014**, 54, 1174-88	6.1	37
49	Amyloid-like self-assembly of peptide sequences from the adenovirus fiber shaft: insights from molecular dynamics simulations. *Journal of Physical Chemistry B*, **2009**, 113, 15639-47	3.4	35
48	Elucidating a key anti-HIV-1 and cancer-associated axis: the structure of CCL5 (Rantes) in complex with CCR5. *Scientific Reports*, **2014**, 4, 5447	4.9	32
47	Species specificity of the complement inhibitor compstatin investigated by all-atom molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 2655-67	4.2	32
46	Molecular dynamics in drug design: new generations of compstatin analogs. *Chemical Biology and Drug Design*, **2012**, 79, 703-18	2.9	31
45	Self-Assembled Amyloid Peptides with Arg-Gly-Asp (RGD) Motifs As Scaffolds for Tissue Engineering. *ACS Biomaterials Science and Engineering*, **2017**, 3, 1404-1416	5.5	28
44	Enhanced Fluorescence for Bioassembly by Environment-Switching Doping of Metal Ions. *Advanced Functional Materials*, **2020**, 30, 1909614	15.6	24
43	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. *Toxicological Sciences*, **2017**, 155, 458-473	4.4	23
42	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	3.7	23
41	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, 3166-79	4.2	23
40	High-Efficiency Fluorescence through Bioinspired Supramolecular Self-Assembly. *ACS Nano*, **2020**, 14, 2798-2807	16.7	22
39	Princeton_TIGRESS: protein geometry refinement using simulations and support vector machines. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 794-814	4.2	21

38	Highly Accurate Structure-Based Prediction of HIV-1 Coreceptor Usage Suggests Intermolecular Interactions Driving Tropism. *PLoS ONE*, **2016**, 11, e0148974	3.7	21
37	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, 1765-74	3.4	20
36	Insights into the mechanism of C5aR inhibition by PMX53 via implicit solvent molecular dynamics simulations and docking. *BMC Biophysics*, **2014**, 7, 5	0	20
35	Uncovering the Binding and Specificity of Wrapins for Amyloid- and Synuclein. *Journal of Physical Chemistry B*, **2016**, 120, 12781-12794	3.4	19
34	Interactions between Curcumin Derivatives and Amyloid-Fibrils: Insights from Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2020**, 60, 289-305	6.1	18
33	Enhanced adsorption of per- and polyfluoroalkyl substances (PFAS) by edible, nutrient-amended montmorillonite clays. *Water Research*, **2021**, 188, 116534	12.5	18
32	Montmorillonites Can Tightly Bind Glyphosate and Paraquat Reducing Toxin Exposures and Toxicity. *ACS Omega*, **2019**, 4, 17702-17713	3.9	17
31	Insights into the structure, correlated motions, and electrostatic properties of two HIV-1 gp120 V3 loops. *PLoS ONE*, **2012**, 7, e49925	3.7	17
30	Isoflavones as Ah Receptor Agonists in Colon-Derived Cell Lines: Structure-Activity Relationships. *Chemical Research in Toxicology*, **2019**, 32, 2353-2364	4	16
29	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, 814-26	8.3	16
28	Exploring Protein-Protein and Protein-Ligand Interactions in the Immune System using Molecular Dynamics and Continuum Electrostatics. *Current Physical Chemistry*, **2012**, 2, 324-343	0.5	16
27	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	3.9	16
26	Combination of theoretical and experimental approaches for the design and study of fibril-forming peptides. *Methods in Molecular Biology*, **2014**, 1216, 53-70	1.4	15
25	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. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 1078-1098	4.2	12
24	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	4.6	12
23	Virtual Screening of Chemical Compounds for Discovery of Complement C3 Ligands. *ACS Omega*, **2018**, 3, 6427-6438	3.9	11
22	Designer Amyloid Cell-Penetrating Peptides for Potential Use as Gene Transfer Vehicles. *Biomolecules*, **2019**, 10,	5.9	10
21	Elucidating the multi-targeted anti-amyloid activity and enhanced islet amyloid polypeptide binding of -wrapins. *Computers and Chemical Engineering*, **2018**, 116, 322-332	4	10

20	Computational Design of Functional Amyloid Materials with Cesium Binding, Deposition, and Capture Properties. *Journal of Physical Chemistry B*, **2018**, 122, 7555-7568	3.4	10
19	Protection of Oxygen-Sensitive Enzymes by Peptide Hydrogel. *ACS Nano*, **2021**, 15, 6530-6539	16.7	9
18	Self-Assembled Peptide Nano-Superstructure towards Enzyme Mimicking Hydrolysis. *Angewandte Chemie - International Edition*, **2021**, 60, 17164-17170	16.4	9
17	Ecotoxic effects of paclitaxel-loaded nanotherapeutics on freshwater algae, Raphidocelis subcapitata and Chlamydomonas reinhardtii. *Environmental Science: Nano*, **2017**, 4, 1077-1085	7.1	7
16	Insights into the interactions of bisphenol and phthalate compounds with unamended and carnitine-amended montmorillonite clays. *Computers and Chemical Engineering*, **2020**, 143, 107063-107063	4	7
15	Activation of COUP-TFI by a Novel Diindolylmethane Derivative. *Cells*, **2019**, 8,	7.9	6
14	Molecular Mechanism for Attractant Signaling to DHMA by E.□coli Tsr. *Biophysical Journal*, **2020**, 118, 492-504	2.9	6
13	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	4.6	5
12	Molecular Modeling of Chemoreceptor:Ligand Interactions. *Methods in Molecular Biology*, **2018**, 1729, 353-372	1.4	4
11	Amyloid Peptide Scaffolds Coordinate with Alzheimer's Disease Drugs. *Journal of Physical Chemistry B*, **2020**, 124, 487-503	3.4	4
10	Montmorillonite clay-based sorbents decrease the bioavailability of per- and polyfluoroalkyl substances (PFAS) from soil and their translocation to plants. *Environmental Research*, **2021**, 205, 112433	7.9	3
9	Computational evolution of an RNA-binding protein towards enhanced oxidized-RNA binding. *Computational and Structural Biotechnology Journal*, **2020**, 18, 137-152	6.8	2
8	Combining Experimental Isotherms, Minimalistic Simulations, and a Model to Understand and Predict Chemical Adsorption onto Montmorillonite Clays. *ACS Omega*, **2021**, 6, 14090-14103	3.9	2
7	Self-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	0.8	1
6	Self-Assembled Peptide Nano-Superstructure towards Enzyme Mimicking Hydrolysis. *Angewandte Chemie*, **2021**, 133, 17301-17307	3.6	1
5	EDTA-mimicking amino acid□metal ion coordination for multifunctional packings. *Journal of Materials Chemistry A*, **2021**, 9, 20385-20394	13	1
4	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	1.4	1
3	Hydroxylated Chalcones as Aryl Hydrocarbon Receptor Agonists: Structure-Activity Effects. *Toxicological Sciences*, **2021**, 180, 148-159	4.4	0

List of Publications

2	Computational design of a β-wrapin's N-terminal domain with canonical and non-canonical amino acid modifications mimicking curcumin's proposed inhibitory function.. *Biophysical Chemistry*, **2022**, 286, 106805	3.5	0
1	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		