Xingqing Xiao

List of Publications by Year in descending order

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29	472	687363 13	752698 20
papers	citations	h-index	g-index

30	30	30	456
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advancing Peptide-Based Biorecognition Elements for Biosensors Using in-Silico Evolution. ACS Sensors, 2018, 3, 1024-1031.	7.8	50
2	Potent aromatase inhibitors and molecular mechanism of inhibitory action. European Journal of Medicinal Chemistry, 2018, 143, 426-437.	5.5	49
3	Insights into the solvation and dynamic behaviors of a lithium salt in organic- and ionic liquid-based electrolytes. Physical Chemistry Chemical Physics, 2019, 21, 19216-19225.	2.8	29
4	Amino Acid Signature Enables Proteins to Recognize Modified tRNA. Biochemistry, 2014, 53, 1125-1133.	2.5	28
5	Morphology Transition of Block Copolymers under Curved Confinement. Macromolecular Theory and Simulations, 2007, 16, 732-741.	1.4	25
6	The design of a peptide sequence to inhibit HIV replication: a search algorithm combining Monte Carlo and self-consistent mean field techniques. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1523-1536.	3.5	25
7	Capture of pure toxic gases through porous materials from molecular simulations. Molecular Physics, 2018, 116, 2095-2107.	1.7	24
8	Novel peptide ligands for antibody purification provide superior clearance of host cell protein impurities. Journal of Chromatography A, 2020, 1625, 461237.	3.7	21
9	Monte Carlo Simulation of ABA Triblock Copolymer Melts Confined in a Cylindrical Nanotube. Macromolecular Theory and Simulations, 2007, 16, 166-177.	1.4	20
10	De novo design of peptides that coassemble into Î² sheetâ€“based nanofibrils. Science Advances, 2021, 7, eabf7668.	10.3	20
11	Designing Peptide Sequences in Flexible Chain Conformations to Bind RNA: A Search Algorithm Combining Monte Carlo, Self-Consistent Mean Field and Concerted Rotation Techniques. Journal of Chemical Theory and Computation, 2015, 11, 740-752.	5.3	18
12	Introducing folding stability into the score function for computational design of RNAâ€binding peptides boosts the probability of success. Proteins: Structure, Function and Bioinformatics, 2016, 84, 700-711.	2.6	17
13	Adding energy minimization strategy to peptideâ€design algorithm enables better search for RNAâ€binding peptides: Redesigned Î» N peptide binds boxB RNA. Journal of Computational Chemistry, 2016, 37, 2423-2435.	3.3	16
14	Molecular recognition mechanism of peptide chain bound to the tRNALys3anticodon loopin silico. Journal of Biomolecular Structure and Dynamics, 2015, 33, 14-27.	3.5	13
15	Simulation study of the ability of a computationallyâ€designed peptide to recognize target tRNA Lys3 and other decoy tRNAs. Protein Science, 2016, 25, 2243-2255.	7.6	13
16	De novo discovery of peptide-based affinity ligands for the fab fragment of human immunoglobulin G. Journal of Chromatography A, 2022, 1669, 462941.	3.7	13
17	Extended Concerted Rotation Technique Enhances the Sampling Efficiency of the Computational Peptide-Design Algorithm. Journal of Chemical Theory and Computation, 2017, 13, 5709-5720.	5.3	12
18	All-silica zeolites screening for capture of toxic gases from molecular simulation. Chinese Journal of Chemical Engineering, 2019, 27, 174-181.	3.5	12

#	Article	IF	Citations
19	In Silico Discovery and Validation of Neuropeptide-Y-Binding Peptides for Sensors. Journal of Physical Chemistry B, 2020, 124, 61-68.	2.6	11
20	Computational study of transition states for reaction path of energetic material TKX-50. Journal of Energetic Materials, 2019, 37, 240-250.	2.0	10
21	Engineering Î²-Sheet Peptide Coassemblies for Biomaterial Applications. Journal of Physical Chemistry B, 2021, 125, 13599-13609.	2.6	10
22	In Silico Identification and Experimental Validation of Peptide-Based Inhibitors Targeting Clostridium difficile Toxin A. ACS Chemical Biology, 2022, 17, 118-128.	3.4	9
23	Microphase Separation of a Diblock Copolymer Dispersed in Nanorod Arrays Grafted on a Plate: A Monte Carlo Study. Macromolecular Theory and Simulations, 2011, 20, 124-132.	1.4	8
24	Computational insights into the destabilization of Î±-helical conformations formed by leucine zipper peptides in response to temperature. Physical Chemistry Chemical Physics, 2016, 18, 25465-25473.	2.8	8
25	Probe the Binding Mode of Aristololactamâ€Î²â€Dâ€glucoside to Phenylalanine Transfer RNA in Silico. ChemistrySelect, 2016, 1, 5430-5439.	1.5	4
26	24 Interference of PNA binding to the non-template strand with transcription supports the general model for transcription blockage by R-loop formation. Journal of Biomolecular Structure and Dynamics, 2015, 33, 14-14.	3.5	3
27	Modulation of phase transition of thermosensitive liposomes with leucine zipper-structured lipopeptides. Physical Chemistry Chemical Physics, 2018, 20, 15916-15925.	2.8	3
28	Effect of curvature on properties of diblock copolymers confined between two coaxial cylinders: 1. Layer thickness of a curved monolayer. Chemical Physics Letters, 2015, 633, 58-64.	2.6	1
29	Effect of curvature on properties of diblock copolymers confined between two coaxial cylinders: 2. Domain adjustment in a curved bilayer. Chemical Physics Letters, 2015, 639, 326-334.	2.6	0