

# Xingqing Xiao

## List of Publications by Year in descending order

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29  
papers

472  
citations

687363

13  
h-index

752698

20  
g-index

30  
all docs

30  
docs citations

30  
times ranked

456  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	<i>In Silico</i> Identification and Experimental Validation of Peptide-Based Inhibitors Targeting <i>Clostridium difficile</i> Toxin A. ACS Chemical Biology, 2022, 17, 118-128.	3.4	9
3	De novo design of peptides that coassemble into $\beta^2$ sheet-based nanofibrils. Science Advances, 2021, 7, eabf7668.	10.3	20
4	Engineering $\beta^2$ -Sheet Peptide Coassemblies for Biomaterial Applications. Journal of Physical Chemistry B, 2021, 125, 13599-13609.	2.6	10
5	In Silico Discovery and Validation of Neuropeptide-Y-Binding Peptides for Sensors. Journal of Physical Chemistry B, 2020, 124, 61-68.	2.6	11
6	Novel peptide ligands for antibody purification provide superior clearance of host cell protein impurities. Journal of Chromatography A, 2020, 1625, 461237.	3.7	21
7	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
8	Computational study of transition states for reaction path of energetic material TKX-50. Journal of Energetic Materials, 2019, 37, 240-250.	2.0	10
9	All-silica zeolites screening for capture of toxic gases from molecular simulation. Chinese Journal of Chemical Engineering, 2019, 27, 174-181.	3.5	12
10	Capture of pure toxic gases through porous materials from molecular simulations. Molecular Physics, 2018, 116, 2095-2107.	1.7	24
11	Potent aromatase inhibitors and molecular mechanism of inhibitory action. European Journal of Medicinal Chemistry, 2018, 143, 426-437.	5.5	49
12	Advancing Peptide-Based Biorecognition Elements for Biosensors Using <i>in-Silico</i> Evolution. ACS Sensors, 2018, 3, 1024-1031.	7.8	50
13	Modulation of phase transition of thermosensitive liposomes with leucine zipper-structured lipopeptides. Physical Chemistry Chemical Physics, 2018, 20, 15916-15925.	2.8	3
14	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
15	Introducing folding stability into the score function for computational design of RNA-binding peptides boosts the probability of success. Proteins: Structure, Function and Bioinformatics, 2016, 84, 700-711.	2.6	17
16	Adding energy minimization strategy to peptide design algorithm enables better search for RNA-binding peptides: Redesigned $\beta$ N peptide binds $\alpha$ RNA. Journal of Computational Chemistry, 2016, 37, 2423-2435.	3.3	16
17	Computational insights into the destabilization of $\beta$ -helical conformations formed by leucine zipper peptides in response to temperature. Physical Chemistry Chemical Physics, 2016, 18, 25465-25473.	2.8	8
18	Simulation study of the ability of a computationally designed peptide to recognize target tRNA Lys3 and other decoy tRNAs. Protein Science, 2016, 25, 2243-2255.	7.6	13

#	ARTICLE	IF	CITATIONS
19	Probe the Binding Mode of Aristololactam- $\beta$ -D-glucoside to Phenylalanine Transfer RNA <i>in Silico</i> . ChemistrySelect, 2016, 1, 5430-5439.	1.5	4
20	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
21	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
22	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
23	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
24	Molecular recognition mechanism of peptide chain bound to the tRNA <sup>Lys</sup> 3anticodon loop in silico. Journal of Biomolecular Structure and Dynamics, 2015, 33, 14-27.	3.5	13
25	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
26	Amino Acid Signature Enables Proteins to Recognize Modified tRNA. Biochemistry, 2014, 53, 1125-1133.	2.5	28
27	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
28	Monte Carlo Simulation of ABA Triblock Copolymer Melts Confined in a Cylindrical Nanotube. Macromolecular Theory and Simulations, 2007, 16, 166-177.	1.4	20
29	Morphology Transition of Block Copolymers under Curved Confinement. Macromolecular Theory and Simulations, 2007, 16, 732-741.	1.4	25