Yu-Shan Lin

List of Publications by Year
in descending order

57 papers	3,347 citations	270111 25 h-index	162838 57 g-index
61 all docs	61 docs citations	61 times ranked	4845 citing authors

#	Article	IF	Citations
1	A Perfluoroaryl-Cysteine S_NAr Chemistry Approach to Unprotected Peptide Stapling. Journal of the American Chemical Society, 2013, 135, 5946-5949.	6.6	389
2	Are Protein Force Fields Getting Better? A Systematic Benchmark on 524 Diverse NMR Measurements. Journal of Chemical Theory and Computation, 2012, 8, 1409-1414.	2.3	347
3	Collagen interactions: Drug design and delivery. Advanced Drug Delivery Reviews, 2016, 97, 69-84.	6.6	195
4	Water inertial reorientation: Hydrogen bond strength and the angular potential. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 5295-5300.	3.3	181
5	Simple few-state models reveal hidden complexity in protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17807-17813.	3.3	151
6	Water structure, dynamics, and vibrational spectroscopy in sodium bromide solutions. Journal of Chemical Physics, 2009, 131, 144511.	1.2	135
7	Vibrational Spectroscopy and Dynamics of Water Confined inside Reverse Micelles. Journal of Physical Chemistry B, 2009, 113, 15017-15028.	1.2	134
8	Empirical Amide I Vibrational Frequency Map: Application to 2D-IR Line Shapes for Isotope-Edited Membrane Peptide Bundles. Journal of Physical Chemistry B, 2009, 113, 592-602.	1.2	129
9	Diversity-Oriented Stapling Yields Intrinsically Cell-Penetrant Inducers of Autophagy. Journal of the American Chemical Society, 2017, 139, 7792-7802.	6.6	121
10	Gating Mechanism of the Influenza A M2 Channel Revealed by 1D and 2D IR Spectroscopies. Structure, 2009, 17, 247-254.	1.6	116
11	Robust three-body water simulation model. Journal of Chemical Physics, 2011, 134, 184501.	1.2	115
12	Investigating How Peptide Length and a Pathogenic Mutation Modify the Structural Ensemble of Amyloid Beta Monomer. Biophysical Journal, 2012, 102, 315-324.	0.2	114
13	2D IR Line Shapes Probe Ovispirin Peptide Conformation and Depth in Lipid Bilayers. Journal of the American Chemical Society, 2010, 132, 2832-2838.	6.6	90
14	Convergent diversity-oriented side-chain macrocyclization scan for unprotected polypeptides. Organic and Biomolecular Chemistry, 2014, 12, 566-573.	1.5	73
15	On the calculation of rotational anisotropy decay, as measured by ultrafast polarization-resolved vibrational pump-probe experiments. Journal of Chemical Physics, 2010, 132, 174505.	1.2	63
16	Solution Structures of Rat Amylin Peptide: Simulation, Theory, and Experiment. Biophysical Journal, 2010, 98, 443-451.	0.2	51
17	Toward structure prediction of cyclic peptides. Physical Chemistry Chemical Physics, 2015, 17, 4210-4219.	1.3	50
18	A Molecular Interpretation of 2D IR Protein Folding Experiments with Markov State Models. Biophysical Journal, 2014, 106, 1359-1370.	0.2	48

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19	Effects of Familial Mutations on the Monomer Structure of AÎ²42. Biophysical Journal, 2012, 103, L47-L49.	0.2	47
20	Insights into How Cyclic Peptides Switch Conformations. Journal of Chemical Theory and Computation, 2016, 12, 2480-2488.	2.3	47
21	Elucidating Solution Structures of Cyclic Peptides Using Molecular Dynamics Simulations. Chemical Reviews, 2021, 121, 2292-2324.	23.0	45
22	Host proteostasis modulates influenza evolution. ELife, 2017, 6, .	2.8	34
23	A bicyclic peptide scaffold promotes phosphotyrosine mimicry and cellular uptake. Bioorganic and Medicinal Chemistry, 2014, 22, 6387-6391.	1.4	30
24	<scp>d</scp>-Amino Acid Scan of Two Small Proteins. Journal of the American Chemical Society, 2016, 138, 12099-12111.	6.6	30
25	Destabilized adaptive influenza variants critical for innate immune system escape are potentiated by host chaperones. PLoS Biology, 2018, 16, e3000008.	2.6	28
26	Design and synthesis of intramolecular hydrogen bonding systems. Their application in metal cation sensing based on excited-state proton transfer reaction. Tetrahedron, 2004, 60, 11861-11868.	1.0	26
27	Collagen Gly missense mutations: Effect of residue identity on collagen structure and integrin binding. Journal of Structural Biology, 2018, 203, 255-262.	1.3	26
28	Enhanced ER proteostasis and temperature differentially impact the mutational tolerance of influenza hemagglutinin. ELife, 2018, 7, .	2.8	25
29	Computational methods to design cyclic peptides. Current Opinion in Chemical Biology, 2016, 34, 95-102.	2.8	24
30	Structure prediction of cyclic peptides by molecular dynamics + machine learning. Chemical Science, 2021, 12, 14927-14936.	3.7	24
31	Competitive intramolecular hydrogen bonding formation and excited-state proton transfer reaction in 1-[(diethylamino)-methyl]-2-hydroxy-3-naphthaldehyde. Chemical Physics Letters, 2004, 384, 203-209.	1.2	23
32	Light-responsive bicyclic peptides. Organic and Biomolecular Chemistry, 2018, 16, 7588-7594.	1.5	23
33	Structural basis for the antiarrhythmic blockade of a potassium channel with a small molecule. FASEB Journal, 2018, 32, 1778-1793.	0.2	22
34	Mapping the Effect of Gly Mutations in Collagen on Î±2Î²1 Integrin Binding. Journal of Biological Chemistry, 2016, 291, 19196-19207.	1.6	21
35	Correlated rotational switching in two-dimensional self-assembled molecular rotor arrays. Nature Communications, 2017, 8, 16057.	5.8	21
36	Mapping the sequenceâ€“structure relationships of simple cyclic hexapeptides. Physical Chemistry Chemical Physics, 2017, 19, 3315-3324.	1.3	20

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37	Designing Well-Structured Cyclic Pentapeptides Based on Sequenceâ€“Structure Relationships. Journal of Physical Chemistry B, 2018, 122, 3908-3919.	1.2	20
38	Genetically-encoded discovery of proteolytically stable bicyclic inhibitors for morphogen NODAL. Chemical Science, 2021, 12, 9694-9703.	3.7	20
39	Consequences of Glycine Mutations in the Fibronectin-binding Sequence of Collagen. Journal of Biological Chemistry, 2016, 291, 27073-27086.	1.6	19
40	Toward accurately modeling N-methylated cyclic peptides. Physical Chemistry Chemical Physics, 2017, 19, 5377-5388.	1.3	19
41	Understanding and designing headâ€toâ€tail cyclic peptides. Biopolymers, 2018, 109, e23113.	1.2	17
42	Using synthetic peptides and recombinant collagen to understand DDRâ€“collagen interactions. Biochimica Et Biophysica Acta - Molecular Cell Research, 2019, 1866, 118458.	1.9	16
43	Vibrational Energy Relaxation of the Bend Fundamental of Dilute Water in Liquid Chloroform and d-Chloroform. Journal of Physical Chemistry B, 2008, 112, 390-398.	1.2	14
44	Effects of flexibility of the Î±2 chain of type I collagen on collagenase cleavage. Journal of Structural Biology, 2018, 203, 247-254.	1.3	14
45	Enzymatic Phosphorylation of Ser in a Type I Collagen Peptide. Biophysical Journal, 2018, 115, 2327-2335.	0.2	13
46	Consequences of Depsipeptide Substitution on the ClpP Activation Activity of Antibacterial Acyldepsipeptides. ACS Medicinal Chemistry Letters, 2017, 8, 1171-1176.	1.3	11
47	The Antimalarial Chloroquine Reduces the Burden of Persistent Atrial Fibrillation. Frontiers in Pharmacology, 2019, 10, 1392.	1.6	11
48	Î²-Branched Amino Acids Stabilize Specific Conformations of Cyclic Hexapeptides. Biophysical Journal, 2019, 116, 433-444.	0.2	11
49	Stapled Î²-Hairpins Featuring 4-Mercaptoproline. Journal of the American Chemical Society, 2021, 143, 15039-15044.	6.6	11
50	Heterochiral Knottin Protein: Folding and Solution Structure. Biochemistry, 2017, 56, 5720-5725.	1.2	10
51	Cyclic peptides: backbone rigidification and capability of mimicking motifs at proteinâ€“protein interfaces. Physical Chemistry Chemical Physics, 2021, 23, 607-616.	1.3	10
52	Controlling Molecular Switching via Chemical Functionality: Ethyl vs Methoxy Rotors. Journal of Physical Chemistry C, 2019, 123, 23738-23746.	1.5	9
53	CATBOSS: Cluster Analysis of Trajectories Based on Segment Splitting. Journal of Chemical Information and Modeling, 2021, 61, 5066-5081.	2.5	9
54	N-Amination Converts Amyloidogenic Tau Peptides into Soluble Antagonists of Cellular Seeding. ACS Chemical Neuroscience, 2021, 12, 3928-3938.	1.7	7

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55	The endoplasmic reticulum proteostasis network profoundly shapes the protein sequence space accessible to HIV envelope. PLoS Biology, 2022, 20, e3001569.	2.6	7
56	Predictions for Î±-Helical Glycopeptide Design from Structural Bioinformatics Analysis. Journal of Chemical Information and Modeling, 2017, 57, 2598-2611.	2.5	2
57	Visualizing and Understanding Ordered Surface Phases during the Ullmann Coupling Reaction. Journal of Physical Chemistry C, 2021, 125, 7675-7685.	1.5	2