# Yu-Shan Lin

List of Publications by Year
in descending order



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|---|---|---|---|
| 57 papers | 3,347 citations | 236925 25 h-index | 144013 57 g-index |
| 61 all docs | 61 docs citations | 61 times ranked | 4242 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | A Perfluoroaryl-Cysteine S<sub>N</sub>Ar Chemistry Approach to Unprotected Peptide Stapling. Journal of the American Chemical Society, 2013, 135, 5946-5949. | 13.7 | 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. | 5.3 | 347 |
| 3 | Collagen interactions: Drug design and delivery. Advanced Drug Delivery Reviews, 2016, 97, 69-84. | 13.7 | 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. | 7.1 | 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. | 7.1 | 151 |
| 6 | Water structure, dynamics, and vibrational spectroscopy in sodium bromide solutions. Journal of Chemical Physics, 2009, 131, 144511. | 3.0 | 135 |
| 7 | Vibrational Spectroscopy and Dynamics of Water Confined inside Reverse Micelles. Journal of Physical Chemistry B, 2009, 113, 15017-15028. | 2.6 | 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. | 2.6 | 129 |
| 9 | Diversity-Oriented Stapling Yields Intrinsically Cell-Penetrant Inducers of Autophagy. Journal of the American Chemical Society, 2017, 139, 7792-7802. | 13.7 | 121 |
| 10 | Gating Mechanism of the Influenza A M2 Channel Revealed by 1D and 2D IR Spectroscopies. Structure, 2009, 17, 247-254. | 3.3 | 116 |
| 11 | Robust three-body water simulation model. Journal of Chemical Physics, 2011, 134, 184501. | 3.0 | 115 |
| 12 | Investigating How Peptide Length and a Pathogenic Mutation Modify the Structural Ensemble of Amyloid Beta Monomer. Biophysical Journal, 2012, 102, 315-324. | 0.5 | 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. | 13.7 | 90 |
| 14 | Convergent diversity-oriented side-chain macrocyclization scan for unprotected polypeptides. Organic and Biomolecular Chemistry, 2014, 12, 566-573. | 2.8 | 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. | 3.0 | 63 |
| 16 | Solution Structures of Rat Amylin Peptide: Simulation, Theory, and Experiment. Biophysical Journal, 2010, 98, 443-451. | 0.5 | 51 |
| 17 | Toward structure prediction of cyclic peptides. Physical Chemistry Chemical Physics, 2015, 17, 4210-4219. | 2.8 | 50 |
| 18 | A Molecular Interpretation of 2D IR Protein Folding Experiments with Markov State Models. Biophysical Journal, 2014, 106, 1359-1370. | 0.5 | 48 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Effects of Familial Mutations on the Monomer Structure of AÎ²42. Biophysical Journal, 2012, 103, L47-L49. | 0.5 | 47 |
| 20 | Insights into How Cyclic Peptides Switch Conformations. Journal of Chemical Theory and Computation, 2016, 12, 2480-2488. | 5.3 | 47 |
| 21 | Elucidating Solution Structures of Cyclic Peptides Using Molecular Dynamics Simulations. Chemical Reviews, 2021, 121, 2292-2324. | 47.7 | 45 |
| 22 | Host proteostasis modulates influenza evolution. ELife, 2017, 6, . | 6.0 | 34 |
| 23 | A bicyclic peptide scaffold promotes phosphotyrosine mimicry and cellular uptake. Bioorganic and Medicinal Chemistry, 2014, 22, 6387-6391. | 3.0 | 30 |
| 24 | <scp>d</scp>-Amino Acid Scan of Two Small Proteins. Journal of the American Chemical Society, 2016, 138, 12099-12111. | 13.7 | 30 |
| 25 | Destabilized adaptive influenza variants critical for innate immune system escape are potentiated by host chaperones. PLoS Biology, 2018, 16, e3000008. | 5.6 | 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. | 1.9 | 26 |
| 27 | Collagen Gly missense mutations: Effect of residue identity on collagen structure and integrin binding. Journal of Structural Biology, 2018, 203, 255-262. | 2.8 | 26 |
| 28 | Enhanced ER proteostasis and temperature differentially impact the mutational tolerance of influenza hemagglutinin. ELife, 2018, 7, . | 6.0 | 25 |
| 29 | Computational methods to design cyclic peptides. Current Opinion in Chemical Biology, 2016, 34, 95-102. | 6.1 | 24 |
| 30 | Structure prediction of cyclic peptides by molecular dynamics + machine learning. Chemical Science, 2021, 12, 14927-14936. | 7.4 | 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. | 2.6 | 23 |
| 32 | Light-responsive bicyclic peptides. Organic and Biomolecular Chemistry, 2018, 16, 7588-7594. | 2.8 | 23 |
| 33 | Structural basis for the antiarrhythmic blockade of a potassium channel with a small molecule. FASEB Journal, 2018, 32, 1778-1793. | 0.5 | 22 |
| 34 | Mapping the Effect of Gly Mutations in Collagen on Î±2Î²1 Integrin Binding. Journal of Biological Chemistry, 2016, 291, 19196-19207. | 3.4 | 21 |
| 35 | Correlated rotational switching in two-dimensional self-assembled molecular rotor arrays. Nature Communications, 2017, 8, 16057. | 12.8 | 21 |
| 36 | Mapping the sequenceâ€“structure relationships of simple cyclic hexapeptides. Physical Chemistry Chemical Physics, 2017, 19, 3315-3324. | 2.8 | 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. | 2.6 | 20 |
| 38 | Genetically-encoded discovery of proteolytically stable bicyclic inhibitors for morphogen NODAL. Chemical Science, 2021, 12, 9694-9703. | 7.4 | 20 |
| 39 | Consequences of Glycine Mutations in the Fibronectin-binding Sequence of Collagen. Journal of Biological Chemistry, 2016, 291, 27073-27086. | 3.4 | 19 |
| 40 | Toward accurately modeling N-methylated cyclic peptides. Physical Chemistry Chemical Physics, 2017, 19, 5377-5388. | 2.8 | 19 |
| 41 | Understanding and designing headâ€toâ€tail cyclic peptides. Biopolymers, 2018, 109, e23113. | 2.4 | 17 |
| 42 | Using synthetic peptides and recombinant collagen to understand DDRâ€“collagen interactions. Biochimica Et Biophysica Acta - Molecular Cell Research, 2019, 1866, 118458. | 4.1 | 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. | 2.6 | 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. | 2.8 | 14 |
| 45 | Enzymatic Phosphorylation of Ser in a Type I Collagen Peptide. Biophysical Journal, 2018, 115, 2327-2335. | 0.5 | 13 |
| 46 | Consequences of Depsipeptide Substitution on the ClpP Activation Activity of Antibacterial Acyldepsipeptides. ACS Medicinal Chemistry Letters, 2017, 8, 1171-1176. | 2.8 | 11 |
| 47 | The Antimalarial Chloroquine Reduces the Burden of Persistent Atrial Fibrillation. Frontiers in Pharmacology, 2019, 10, 1392. | 3.5 | 11 |
| 48 | Î²-Branched Amino Acids Stabilize Specific Conformations of Cyclic Hexapeptides. Biophysical Journal, 2019, 116, 433-444. | 0.5 | 11 |
| 49 | Stapled Î²-Hairpins Featuring 4-Mercaptoproline. Journal of the American Chemical Society, 2021, 143, 15039-15044. | 13.7 | 11 |
| 50 | Heterochiral Knottin Protein: Folding and Solution Structure. Biochemistry, 2017, 56, 5720-5725. | 2.5 | 10 |
| 51 | Cyclic peptides: backbone rigidification and capability of mimicking motifs at proteinâ€“protein interfaces. Physical Chemistry Chemical Physics, 2021, 23, 607-616. | 2.8 | 10 |
| 52 | Controlling Molecular Switching via Chemical Functionality: Ethyl vs Methoxy Rotors. Journal of Physical Chemistry C, 2019, 123, 23738-23746. | 3.1 | 9 |
| 53 | CATBOSS: Cluster Analysis of Trajectories Based on Segment Splitting. Journal of Chemical Information and Modeling, 2021, 61, 5066-5081. | 5.4 | 9 |
| 54 | N-Amination Converts Amyloidogenic Tau Peptides into Soluble Antagonists of Cellular Seeding. ACS Chemical Neuroscience, 2021, 12, 3928-3938. | 3.5 | 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. | 5.6 | 7 |
| 56 | Predictions for Î±-Helical Glycopeptide Design from Structural Bioinformatics Analysis. Journal of Chemical Information and Modeling, 2017, 57, 2598-2611. | 5.4 | 2 |
| 57 | Visualizing and Understanding Ordered Surface Phases during the Ullmann Coupling Reaction. Journal of Physical Chemistry C, 2021, 125, 7675-7685. | 3.1 | 2 |