

# Yang Shen

## List of Publications by Year in descending order

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Version: 2024-02-01

54  
papers

6,761  
citations

236925

25  
h-index

168389

53  
g-index

58  
all docs

58  
docs citations

58  
times ranked

8036  
citing authors

| #  | ARTICLE   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | TALOS+: a hybrid method for predicting protein backbone torsion angles from NMR chemical shifts. <i>Journal of Biomolecular NMR</i> , 2009, 44, 213-223.  | 2.8  | 2,305     |
| 2  | Protein backbone and sidechain torsion angles predicted from NMR chemical shifts using artificial neural networks. <i>Journal of Biomolecular NMR</i> , 2013, 56, 227-241.                                      | 2.8  | 939       |
| 3  | Consistent blind protein structure generation from NMR chemical shift data. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 4685-4690.                      | 7.1  | 776       |
| 4  | SPARTA+: a modest improvement in empirical NMR chemical shift prediction by means of an artificial neural network. <i>Journal of Biomolecular NMR</i> , 2010, 48, 13-22.  | 2.8  | 468       |
| 5  | Protein backbone chemical shifts predicted from searching a database for torsion angle and sequence homology. <i>Journal of Biomolecular NMR</i> , 2007, 38, 289-302.   | 2.8  | 287       |
| 6  | De novo protein structure generation from incomplete chemical shift assignments. <i>Journal of Biomolecular NMR</i> , 2009, 43, 63-78.  | 2.8  | 234       |
| 7  | Protein Structural Information Derived from NMR Chemical Shift with the Neural Network Program TALOS-N. <i>Methods in Molecular Biology</i> , 2015, 1260, 17-32.  | 0.9  | 196       |
| 8  | Monomeric $\alpha^1$ and $\alpha^2$ Peptides in Solution Adopt Very Similar Ramachandran Map Distributions That Closely Resemble Random Coil. <i>Biochemistry</i> , 2016, 55, 762-775.                          | 2.5  | 168       |
| 9  | Simultaneous prediction of protein folding and docking at high resolution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 18978-18983.                     | 7.1  | 145       |
| 10 | Prediction of Xaa-Pro peptide bond conformation from sequence and chemical shifts. <i>Journal of Biomolecular NMR</i> , 2010, 46, 199-204.  | 2.8  | 124       |
| 11 | NMR data collection and analysis protocol for high-throughput protein structure determination. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 10487-10492. | 7.1  | 108       |
| 12 | Identification of helix capping and $\beta^2$ -turn motifs from NMR chemical shifts. <i>Journal of Biomolecular NMR</i> , 2012, 52, 211-232.  | 2.8  | 81        |
| 13 | A maximum entropy approach to the study of residue-specific backbone angle distributions in $\beta$ -synuclein, an intrinsically disordered protein. <i>Protein Science</i> , 2014, 23, 1275-1290.              | 7.6  | 73        |
| 14 | De novo structure generation using chemical shifts for proteins with high sequence identity but different folds. <i>Protein Science</i> , 2010, 19, 349-356.  | 7.6  | 59        |
| 15 | G-Matrix Fourier Transform NOESY-Based Protocol for High-Quality Protein Structure Determination. <i>Journal of the American Chemical Society</i> , 2005, 127, 9085-9099.                                       | 13.7 | 54        |
| 16 | Homology modeling of larger proteins guided by chemical shifts. <i>Nature Methods</i> , 2015, 12, 747-750.  | 19.0 | 51        |
| 17 | Total Synthesis of Aplydactone by a Conformationally Controlled C <sup>α</sup> H Functionalization. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8187-8190.                                     | 13.8 | 46        |
| 18 | Protecting-Group-Free Total Synthesis of (±)-Jiadifenolide: Development of a [4 + 1] Annulation toward Multisubstituted Tetrahydrofurans. <i>Organic Letters</i> , 2015, 17, 5480-5483.                         | 4.6  | 44        |

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|----|---|------|-----------|
| 19 | Remarkable Rigidity of the Single $\alpha$ -Helical Domain of Myosin-VI As Revealed by NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2019, 141, 9004-9017.  | 13.7 | 42        |
| 20 | MERA: a webserver for evaluating backbone torsion angle distributions in dynamic and disordered proteins from NMR data. <i>Journal of Biomolecular NMR</i> , 2015, 63, 85-95.   | 2.8  | 40        |
| 21 | Concordance of X-ray and AlphaFold2 Models of SARS-CoV-2 Main Protease with Residual Dipolar Couplings Measured in Solution. <i>Journal of the American Chemical Society</i> , 2021, 143, 19306-19310.  | 13.7 | 40        |
| 22 | Improved chemical shift based fragment selection for CS-Rosetta using Rosetta3 fragment picker. <i>Journal of Biomolecular NMR</i> , 2013, 57, 117-127.   | 2.8  | 38        |
| 23 | Building native protein conformation from NMR backbone chemical shifts using Monte Carlo fragment assembly. <i>Protein Science</i> , 2007, 16, 1515-1521.   | 7.6  | 33        |
| 24 | Conformational Design Principles in Total Synthesis. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 14198-14210.  | 13.8 | 30        |
| 25 | Advances in NMR Spectroscopy of Weakly Aligned Biomolecular Systems. <i>Chemical Reviews</i> , 2022, 122, 9307-9330.  | 47.7 | 27        |
| 26 | Gating Mechanism of Aquaporin Z in Synthetic Bilayers and Native Membranes Revealed by Solid-State NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2018, 140, 7885-7895.  | 13.7 | 26        |
| 27 | Site-Specific Photochemical Desaturation Enables Divergent Syntheses of <i>Illicium</i> Sesquiterpenes. <i>Journal of the American Chemical Society</i> , 2021, 143, 3256-3263.   | 13.7 | 26        |
| 28 | Improving 3D structure prediction from chemical shift data. <i>Journal of Biomolecular NMR</i> , 2013, 57, 27-35.   | 2.8  | 25        |
| 29 | J-GFT NMR for Precise Measurement of Mutually Correlated Nuclear Spin-Spin Couplings. <i>Journal of the American Chemical Society</i> , 2007, 129, 680-692.   | 13.7 | 24        |
| 30 | Solution Conformation and Dynamics of the HIV-1 Integrase Core Domain. <i>Journal of Biological Chemistry</i> , 2010, 285, 18072-18084.   | 3.4  | 24        |
| 31 | Prediction of nearest neighbor effects on backbone torsion angles and NMR scalar coupling constants in disordered proteins. <i>Protein Science</i> , 2018, 27, 146-158.   | 7.6  | 24        |
| 32 | Merging $^1\text{H}$ Vinylation with Switchable $^6\text{Li}$ -Electrocyclizations for Divergent Heterocycle Synthesis. <i>Journal of the American Chemical Society</i> , 2020, 142, 15585-15594.   | 13.7 | 21        |
| 33 | A lowly populated, transient $\beta$ -sheet structure in monomeric A $\beta$ 1-42 identified by multinuclear NMR of chemical denaturation. <i>Biophysical Chemistry</i> , 2021, 270, 106531.  | 2.8  | 21        |
| 34 | NMR structure of the 18 kDa protein CC1736 from <i>Caulobacter crescentus</i> identifies a member of the $\alpha$ -START domain superfamily and suggests residues mediating substrate specificity. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 58, 747-750. | 2.6  | 18        |
| 35 | Hybrid measurement of respiratory aerosol reveals a dominant coarse fraction resulting from speech that remains airborne for minutes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .                                     | 7.1  | 17        |
| 36 | Probing transient excited states of the bacterial cell division regulator MinE by relaxation dispersion NMR spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 25446-25455.                                      | 7.1  | 16        |

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|----|---|------|-----------|
| 37 | Fully automated high-quality NMR structure determination of small 2H-enriched proteins. <i>Journal of Structural and Functional Genomics</i> , 2010, 11, 223-232.   | 1.2  | 12        |
| 38 | Conformational Bias by a Removable Silyl Group: Construction of Bicyclo[ <i>n</i> .3.1]alkenes by Ring Closing Metathesis. <i>Chemistry - A European Journal</i> , 2018, 24, 2334-2338.                       | 3.3  | 10        |
| 39 | Stabilizing <i>p</i> -Dithiobenzyl Urethane Linkers without Rate-Limiting Self-Immolation for Traceless Drug Release. <i>ChemMedChem</i> , 2019, 14, 1196-1203.   | 3.2  | 9         |
| 40 | Residual Dipolar Couplings for Resolving Cysteine Bridges in Disulfide-Rich Peptides. <i>Frontiers in Chemistry</i> , 2019, 7, 889.   | 3.6  | 9         |
| 41 | Hydrophobic Gate of Mechanosensitive Channel of Large Conductance in Lipid Bilayers Revealed by Solid-State NMR Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2477-2490.                  | 2.6  | 9         |
| 42 | De novo design and directed folding of disulfide-bridged peptide heterodimers. <i>Nature Communications</i> , 2022, 13, 1539.   | 12.8 | 9         |
| 43 | ARTSY-J: Convenient and precise measurement of $^3\text{J}_{\text{HNH}}$ couplings in medium-size proteins from TROSY-HSQC spectra. <i>Journal of Magnetic Resonance</i> , 2016, 268, 73-81.                  | 2.1  | 8         |
| 44 | Total Synthesis of Aplydactone by a Conformationally Controlled $^{\text{C}}\text{H}$ Functionalization. <i>Angewandte Chemie</i> , 2017, 129, 8299-8302.   | 2.0  | 8         |
| 45 | Structure of membrane diacylglycerol kinase in lipid bilayers. <i>Communications Biology</i> , 2021, 4, 282.  | 4.4  | 7         |
| 46 | Two-Stage Syntheses of Clonastatins A and B. <i>Journal of the American Chemical Society</i> , 2022, 144, 8938-8944.  | 13.7 | 7         |
| 47 | Structure of the Protein BPTI Derived with NOESY in Supercooled Water: Validation and Refinement of Solution Structures. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 324-326.                | 13.8 | 5         |
| 48 | Letter to the Editor: Resonance assignments for the 18 kDa protein CC1736 from <i>Caulobacter crescentus</i> . <i>Journal of Biomolecular NMR</i> , 2004, 29, 549-550.  | 2.8  | 3         |
| 49 | NMR structure of protein $\gamma\text{q}b\text{G}$ from <i>Bacillus subtilis</i> reveals a novel $\alpha$ -helical protein fold. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 288-291. | 2.6  | 3         |
| 50 | Simultaneous Determination of Vitamin B Complex Using Wavelet Neural Network. <i>Chinese Journal of Chemistry</i> , 2001, 19, 836-841.  | 4.9  | 2         |
| 51 | Modulating the Stiffness of the Myosin VI Single $\alpha$ -Helical Domain. <i>Biophysical Journal</i> , 2020, 118, 1119-1128.   | 0.5  | 2         |
| 52 | Conformational Design Principles in Total Synthesis. <i>Angewandte Chemie</i> , 2020, 132, 14302-14314.   | 2.0  | 2         |
| 53 | NMR structure of protein PA2021 from <i>Pseudomonas aeruginosa</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 65, 767-770.   | 2.6  | 1         |
| 54 | Innenteilbild: Total Synthesis of Aplydactone by a Conformationally Controlled $^{\text{C}}\text{H}$ Functionalization (Angew. Chem. 28/2017). <i>Angewandte Chemie</i> , 2017, 129, 8130-8130.               | 2.0  | 0         |