Da-Wei Li

List of Publications by Year
in descending order

62 papers	2,355 citations	201674 27 h-index	223800 46 g-index
65 all docs	65 docs citations	65 times ranked	2509 citing authors

#	Article	IF	Citations
1	Cadaverine Is a Switch in the Lysine Degradation Pathway in Pseudomonas aeruginosa Biofilm Identified by Untargeted Metabolomics. Frontiers in Cellular and Infection Microbiology, 2022, 12, 833269.	3.9	9
2	Fundamental and practical aspects of machine learning for the peak picking of biomolecular NMR spectra. Journal of Biomolecular NMR, 2022, 76, 49-57.	2.8	5
3	COLMARq: A Web Server for 2D NMR Peak Picking and Quantitative Comparative Analysis of Cohorts of Metabolomics Samples. Analytical Chemistry, 2022, 94, 8674-8682.	6.5	8
4	Systematic Differences between Current Molecular Dynamics Force Fields To Represent Local Properties of Intrinsically Disordered Proteins. Journal of Physical Chemistry B, 2021, 125, 798-804.	2.6	18
5	2D NMR-Based Metabolomics with HSQC/TOCSY NOAH Supersequences. Analytical Chemistry, 2021, 93, 6112-6119.	6.5	28
6	DEEP picker is a deep neural network for accurate deconvolution of complex two-dimensional NMR spectra. Nature Communications, 2021, 12, 5229.	12.8	55
7	Balanced Amino-Acid-Specific Molecular Dynamics Force Field for the Realistic Simulation of Both Folded and Disordered Proteins. Journal of Chemical Theory and Computation, 2020, 16, 1311-1318.	5.3	43
8	Quantitative Cooperative Binding Model for Intrinsically Disordered Proteins Interacting with Nanomaterials. Journal of the American Chemical Society, 2020, 142, 10730-10738.	13.7	22
9	COLMAR Lipids Web Server and Ultrahigh-Resolution Methods for Two-Dimensional Nuclear Magnetic Resonance- and Mass Spectrometry-Based Lipidomics. Journal of Proteome Research, 2020, 19, 1674-1683.	3.7	23
10	Accurate and Efficient Determination of Unknown Metabolites in Metabolomics by NMR-Based Molecular Motif Identification. Analytical Chemistry, 2019, 91, 15686-15693.	6.5	16
11	Extreme Nonuniform Sampling for Protein NMR Dynamics Studies in Minimal Time. Journal of the American Chemical Society, 2019, 141, 16829-16838.	13.7	12
12	Identification of Unknown Metabolomics Mixture Compounds by Combining NMR, MS, and Cheminformatics. Methods in Enzymology, 2019, 615, 407-422.	1.0	19
13	Quantitative Binding Behavior of Intrinsically Disordered Proteins to Nanoparticle Surfaces at Individual Residue Level. Chemistry - A European Journal, 2018, 24, 16997-17001.	3.3	21
14	Nonâ€Uniform and Absolute Minimal Sampling for Highâ€Throughput Multidimensional NMR Applications. Chemistry - A European Journal, 2018, 24, 11535-11544.	3.3	14
15	Improved Quantum Chemical NMR Chemical Shift Prediction of Metabolites in Aqueous Solution toward the Validation of Unknowns. Journal of Physical Chemistry A, 2017, 121, 3071-3078.	2.5	29
16	Statistical database analysis of the role of loop dynamics for proteinâ€“protein complex formation and allostery. Bioinformatics, 2017, 33, 1814-1819.	4.1	5
17	Absolute Minimal Sampling of Homonuclear 2D NMR TOCSY Spectra for Highâ€Throughput Applications of Complex Mixtures. Angewandte Chemie - International Edition, 2017, 56, 8149-8152.	13.8	16
18	Maximal clique method for the automated analysis of NMR TOCSY spectra of complex mixtures. Journal of Biomolecular NMR, 2017, 68, 195-202.	2.8	14

#	Article	IF	Citations
19	Accurate Identification of Unknown and Known Metabolic Mixture Components by Combining 3D NMR with Fourier Transform Ion Cyclotron Resonance Tandem Mass Spectrometry. Journal of Proteome Research, 2017, 16, 3774-3786.	3.7	26
20	Absolute Minimal Sampling of Homonuclear 2D NMR TOCSY Spectra for Highâ€Throughput Applications of Complex Mixtures. Angewandte Chemie, 2017, 129, 8261-8264.	2.0	8
21	Model for the allosteric regulation of the <scp>N</scp>a⁺/<scp>C</scp>a²⁺ exchanger <scp>NCX</scp>. Proteins: Structure, Function and Bioinformatics, 2016, 84, 580-590.	2.6	11
22	Comprehensive Metabolite Identification Strategy Using Multiple Two-Dimensional NMR Spectra of a Complex Mixture Implemented in the COLMARm Web Server. Analytical Chemistry, 2016, 88, 12411-12418.	6.5	95
23	Emerging new strategies for successful metabolite identification in metabolomics. Bioanalysis, 2016, 8, 557-573.	1.5	79
24	Decoding the Mobility and Time Scales of Protein Loops. Journal of Chemical Theory and Computation, 2015, 11, 1308-1314.	5.3	39
25	PPM_One: a static protein structure based chemical shift predictor. Journal of Biomolecular NMR, 2015, 62, 403-409.	2.8	40
26	Reliable resonance assignments of selected residues of proteins with known structure based on empirical NMR chemical shift prediction. Journal of Magnetic Resonance, 2015, 254, 93-97.	2.1	1
27	Unified and Isomer-Specific NMR Metabolomics Database for the Accurate Analysis of ¹³Câ€“¹H HSQC Spectra. ACS Chemical Biology, 2015, 10, 452-459.	3.4	96
28	Protocol To Make Protein NMR Structures Amenable to Stable Long Time Scale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 1781-1787.	5.3	8
29	Customized Metabolomics Database for the Analysis of NMR ¹Hâ€“¹H TOCSY and ¹³Câ€“¹H HSQC-TOCSY Spectra of Complex Mixtures. Analytical Chemistry, 2014, 86, 5494-5501.	6.5	96
30	NMR Order Parameter Determination from Long Molecular Dynamics Trajectories for Objective Comparison with Experiment. Journal of Chemical Theory and Computation, 2014, 10, 2599-2607.	5.3	54
31	PPM: a side-chain and backbone chemical shift predictor for the assessment of protein conformational ensembles. Journal of Biomolecular NMR, 2012, 54, 257-265.	2.8	75
32	Probing Side-Chain Dynamics in Proteins by the Measurement of Nine Deuterium Relaxation Rates Per Methyl Group. Journal of Physical Chemistry B, 2012, 116, 606-620.	2.6	30
33	Competitive Binding between Dynamic p53 Transactivation Subdomains to Human MDM2 Protein. Journal of Biological Chemistry, 2012, 287, 30376-30384.	3.4	25
34	Dynamic and Thermodynamic Signatures of Native and Non-Native Protein States with Application to the Improvement of Protein Structures. Journal of Chemical Theory and Computation, 2012, 8, 2531-2539.	5.3	7
35	Dynamics of Lysine Side-Chain Amino Groups in a Protein Studied by Heteronuclear ¹Hâ€™¹⁵N NMR Spectroscopy. Journal of the American Chemical Society, 2011, 133, 909-919.	13.7	71
36	Signature of Mobile Hydrogen Bonding of Lysine Side Chains from Long-Range ¹⁵Nâ€“¹³C Scalar J-Couplings and Computation. Journal of the American Chemical Society, 2011, 133, 9192-9195.	13.7	40

#	Article	IF	Citations
37	Iterative Optimization of Molecular Mechanics Force Fields from NMR Data of Full-Length Proteins. Journal of Chemical Theory and Computation, 2011, 7, 1773-1782.	5.3	78
38	Observation of Two Families of Folding Pathways of BBL. Biophysical Journal, 2011, 100, 2457-2465.	0.5	9
39	Toward a Predictive Understanding of Slow Methyl Group Dynamics in Proteins. Biophysical Journal, 2011, 101, 910-915.	0.5	37
40	NMRâ€Based Protein Potentials. Angewandte Chemie - International Edition, 2010, 49, 6778-6780.	13.8	173
41	Entropy Localization in Proteins. Journal of Physical Chemistry B, 2010, 114, 16036-16044.	2.6	49
42	Variation in Quadrupole Couplings of Î± Deuterons in Ubiquitin Suggests the Presence of C^{Î±}â^'H^{Î±}Â·Â·Â·Oâ•€ Hydrogen Bonds. Journal of the American Chemical Society, 2010, 132, 7709-7719.	13.7	26
43	Certification of Molecular Dynamics Trajectories with NMR Chemical Shifts. Journal of Physical Chemistry Letters, 2010, 1, 246-248.	4.6	79
44	In silicoRelationship between Configurational Entropy and Soft Degrees of Freedom in Proteins and Peptides. Physical Review Letters, 2009, 102, 118108.	7.8	43
45	Protein Conformational Flexibility from Structureâ€Free Analysis of NMR Dipolar Couplings: Quantitative and Absolute Determination of Backbone Motion in Ubiquitin. Angewandte Chemie - International Edition, 2009, 48, 4154-4157.	13.8	87
46	Deuterium Spin Probes of Backbone Order in Proteins: 2H NMR Relaxation Study of Deuterated Carbon Î± Sites. Journal of the American Chemical Society, 2009, 131, 15853-15865.	13.7	41
47	A Dictionary for Protein Side-Chain Entropies from NMR Order Parameters. Journal of the American Chemical Society, 2009, 131, 7226-7227.	13.7	67
48	Short-Range Coherence of Internal Protein Dynamics Revealed by High-Precision in Silico Study. Journal of the American Chemical Society, 2009, 131, 14610-14611.	13.7	61
49	All-Atom Contact Model for Understanding Protein Dynamics from Crystallographic B-Factors. Biophysical Journal, 2009, 96, 3074-3081.	0.5	36
50	Predicting the Folding Pathway of Engrailed Homeodomain with a Probabilistic Roadmap Enhanced Reaction-Path Algorithm. Biophysical Journal, 2008, 94, 1622-1629.	0.5	11
51	Formation and Growth of Oligomers: A Monte Carlo Study of an Amyloid Tau Fragment. PLoS Computational Biology, 2008, 4, e1000238.	3.2	104
52	Structural and Pathway Complexity of Î²-Strand Reorganization within Aggregates of Human Transthyretin(105â^'115) Peptide. Journal of Physical Chemistry B, 2007, 111, 5425-5433.	2.6	21
53	Temperature-Dependent Probabilistic Roadmap Algorithm for Calculating Variationally Optimized Conformational Transition Pathways. Journal of Chemical Theory and Computation, 2007, 3, 17-25.	5.3	14
54	Evaluation of Configurational Entropy Methods from Peptide Foldingâ^'Unfolding Simulation. Journal of Physical Chemistry B, 2007, 111, 13807-13813.	2.6	25

#	Article	IF	Citations
55	A lateral growth mode leading to successive rotation of crystallographic orientation. Surface and Interface Analysis, 2006, 38, 1024-1027.	1.8	0
56	Examination of membrane fusion by dissipative particle dynamics simulation and comparison with continuum elastic models. Journal of Chemical Physics, 2005, 122, 174909.	3.0	37
57	Consecutive Rotation of Crystallographic Orientation in Lateral Growth. Physical Review Letters, 2005, 94, 125505.	7.8	14
58	Bond-Angle-Potential-Dependent Dissipative Particle Dynamics Simulation and Lipid Inverted Phase. Journal of Physical Chemistry B, 2004, 108, 11206-11213.	2.6	27
59	Optical and thermal properties of nonlinear optical crystal LaCa4O(BO3)3. Chemical Physics Letters, 2003, 372, 788-793.	2.6	26
60	Spontaneous Correlation of Crystallographic Orientations in Crystallite Aggregation:Â Physical Origin and Its Influence on Pattern Formation. Journal of Physical Chemistry B, 2003, 107, 96-101.	2.6	10
61	Nucleation-limited aggregation of crystallites in fractal growth. Journal of Crystal Growth, 2000, 208, 687-695.	1.5	16
62	Evaluation of Solvent Accessibility to the [Fe4S4] Binding Pocket in Native and Tyr19 Mutant High Potential Iron Proteins by1Hâ^'15N HMQC and19F NMR Experimentsâ€. Inorganic Chemistry, 1996, 35, 1121-1125.	4.0	19