Jiye Shi

List of Publications by Year in descending order

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201 papers	13,411 citations	23567 58 h-index	27406 106 g-index
215 all docs	215 docs citations	215 times ranked	15183 citing authors

#	Article	IF	Citations
1	FUGUE: sequence-structure homology recognition using environment-specific substitution tables and structure-dependent gap penalties11Edited by B. Honig. Journal of Molecular Biology, 2001, 310, 243-257.	4.2	1,185
2	Hybridization Chain Reaction Amplification of MicroRNA Detection with a Tetrahedral DNA Nanostructure-Based Electrochemical Biosensor. Analytical Chemistry, 2014, 86, 2124-2130.	6.5	460
3	Singleâ€Particle Tracking and Modulation of Cell Entry Pathways of a Tetrahedral DNA Nanostructure in Live Cells. Angewandte Chemie - International Edition, 2014, 53, 7745-7750.	13.8	430
4	Smart Drug Delivery Nanocarriers with Selfâ€Assembled DNA Nanostructures. Advanced Materials, 2013, 25, 4386-4396.	21.0	378
5	SAbDab: the structural antibody database. Nucleic Acids Research, 2014, 42, D1140-D1146.	14.5	374
6	Programmable Engineering of a Biosensing Interface with Tetrahedral DNA Nanostructures for Ultrasensitive DNA Detection. Angewandte Chemie - International Edition, 2015, 54, 2151-2155.	13.8	350
7	An Exonuclease IIIâ€Powered, Onâ€Particle Stochastic DNA Walker. Angewandte Chemie - International Edition, 2017, 56, 1855-1858.	13.8	325
8	Electrochemical detection of nucleic acids, proteins, small molecules and cells using a DNA-nanostructure-based universal biosensing platform. Nature Protocols, 2016, 11, 1244-1263.	12.0	320
9	DNA origami nanostructures can exhibit preferential renal uptake and alleviate acute kidney injury. Nature Biomedical Engineering, 2018, 2, 865-877.	22.5	297
10	An Exonuclease IIIâ€Powered, Onâ€Particle Stochastic DNA Walker. Angewandte Chemie, 2017, 129, 1881-1884.	2.0	252
11	Five computational developability guidelines for therapeutic antibody profiling. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4025-4030.	7.1	221
12	ABodyBuilder: Automated antibody structure prediction with dataâ€“driven accuracy estimation. MAbs, 2016, 8, 1259-1268.	5.2	208
13	Graphene Oxideâ€Based Antibacterial Cotton Fabrics. Advanced Healthcare Materials, 2013, 2, 1259-1266.	7.6	207
14	Multicolor Goldâ€“Silver Nano-Mushrooms as Ready-to-Use SERS Probes for Ultrasensitive and Multiplex DNA/miRNA Detection. Analytical Chemistry, 2017, 89, 2531-2538.	6.5	205
15	DNA Hydrogel with Aptamer-Toehold-Based Recognition, Cloaking, and Decloaking of Circulating Tumor Cells for Live Cell Analysis. Nano Letters, 2017, 17, 5193-5198.	9.1	204
16	Solving mazes with single-molecule DNA navigators. Nature Materials, 2019, 18, 273-279.	27.5	190
17	Nanoscale optical probes for cellular imaging. Chemical Society Reviews, 2014, 43, 2650.	38.1	179
18	Yolkâ€“shell nanostructured Fe₃O₄@C magnetic nanoparticles with enhanced peroxidase-like activity for label-free colorimetric detection of H₂O₂and glucose. Nanoscale, 2017, 9, 4508-4515.	5.6	175

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19	Hydrogen Sulfide-Activatable Second Near-Infrared Fluorescent Nanoassemblies for Targeted Photothermal Cancer Therapy. Nano Letters, 2018, 18, 6411-6416.	9.1	164
20	Real-time visualization of clustering and intracellular transport of gold nanoparticles by correlative imaging. Nature Communications, 2017, 8, 15646.	12.8	163
21	An Intelligent DNA Nanorobot with in Vitro Enhanced Protein Lysosomal Degradation of HER2. Nano Letters, 2019, 19, 4505-4517.	9.1	153
22	Multiple-Armed Tetrahedral DNA Nanostructures for Tumor-Targeting, Dual-Modality in Vivo Imaging. ACS Applied Materials & Interfaces, 2016, 8, 4378-4384.	8.0	142
23	Label-Free Electrochemical Sensing Platform for MicroRNA-21 Detection Using Thionine and Gold Nanoparticles Co-Functionalized MoS₂ Nanosheet. ACS Applied Materials & Interfaces, 2017, 9, 35597-35603.	8.0	141
24	Improving B-cell epitope prediction and its application to global antibody-antigen docking. Bioinformatics, 2014, 30, 2288-2294.	4.1	137
25	Evolutionary trace analysis of TGF-Î² and related growth factors: implications for site-directed mutagenesis. Protein Engineering, Design and Selection, 2000, 13, 839-847.	2.1	130
26	Biodistribution and pulmonary toxicity of intratracheally instilled graphene oxide in mice. NPG Asia Materials, 2013, 5, e44-e44.	7.9	125
27	DNA-Directed Assembly of Gold Nanohalo for Quantitative Plasmonic Imaging of Single-Particle Catalysis. Journal of the American Chemical Society, 2015, 137, 4292-4295.	13.7	125
28	Inhibiting Methicillin-Resistant Staphylococcus aureus by Tetrahedral DNA Nanostructure-Enabled Antisense Peptide Nucleic Acid Delivery. Nano Letters, 2018, 18, 5652-5659.	9.1	117
29	Implementing digital computing with DNA-based switching circuits. Nature Communications, 2020, 11, 121.	12.8	114
30	Scaffolded biosensors with designed DNA nanostructures. NPG Asia Materials, 2013, 5, e51-e51.	7.9	111
31	The prospects of quantum computing in computational molecular biology. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1481.	14.6	108
32	ABangle: characterising the VH-VL orientation in antibodies. Protein Engineering, Design and Selection, 2013, 26, 611-620.	2.1	105
33	MEDELLER: homology-based coordinate generation for membrane proteins. Bioinformatics, 2010, 26, 2833-2840.	4.1	103
34	Programming Cell Adhesion for On-Chip Sequential Boolean Logic Functions. Journal of the American Chemical Society, 2017, 139, 10176-10179.	13.7	103
35	Oneâ€Shot Immunomodulatory Nanodiamond Agents for Cancer Immunotherapy. Advanced Materials, 2016, 28, 2699-2708.	21.0	102
36	A Bubbleâ€Mediated Intelligent Microscale Electrochemical Device for Singleâ€Step Quantitative Bioassays. Advanced Materials, 2014, 26, 4671-4676.	21.0	99

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37	Goldâ€Nanoparticleâ€Mediated Jigsawâ€Puzzleâ€like Assembly of Supersized Plasmonic DNA Origami. Angewandte Chemie - International Edition, 2015, 54, 2966-2969.	13.8	94
38	Catalysisâ€Driven Selfâ€Thermophoresis of Janus Plasmonic Nanomotors. Angewandte Chemie - International Edition, 2017, 56, 515-518.	13.8	93
39	Selfâ€Assembly of Polyâ€Adenineâ€Tailed CpG Oligonucleotideâ€Gold Nanoparticle Nanoconjugates with Immunostimulatory Activity. Small, 2014, 10, 368-375.	10.0	92
40	The H3 loop of antibodies shows unique structural characteristics. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1311-1318.	2.6	89
41	Thera-SAbDab: the Therapeutic Structural Antibody Database. Nucleic Acids Research, 2020, 48, D383-D388.	14.5	88
42	The role of the TolC family in protein transport and multidrug efflux.. FEBS Journal, 2001, 268, 5011-5026.	0.2	85
43	DNA-Encoded Raman-Active Anisotropic Nanoparticles for microRNA Detection. Analytical Chemistry, 2017, 89, 9850-9856.	6.5	85
44	Valencyâ€Controlled Framework Nucleic Acid Signal Amplifiers. Angewandte Chemie - International Edition, 2018, 57, 7131-7135.	13.8	85
45	DNA origami cryptography for secure communication. Nature Communications, 2019, 10, 5469.	12.8	84
46	Programming bulk enzyme heterojunctions for biosensor development with tetrahedral DNA framework. Nature Communications, 2020, 11, 838.	12.8	84
47	MoS₂ Nanoprobe for MicroRNA Quantification Based on Duplex-Specific Nuclease Signal Amplification. ACS Applied Materials & Interfaces, 2018, 10, 7852-7858.	8.0	81
48	Antibody i-Patch prediction of the antibody binding site improves rigid local antibody-antigen docking. Protein Engineering, Design and Selection, 2013, 26, 621-629.	2.1	80
49	A Surfaceâ€Confined Protonâ€Driven DNA Pump Using a Dynamic 3D DNA Scaffold. Advanced Materials, 2016, 28, 6860-6865.	21.0	79
50	Characterization of the Interaction of Sclerostin with the Low Density Lipoprotein Receptor-related Protein (LRP) Family of Wnt Co-receptors. Journal of Biological Chemistry, 2012, 287, 26464-26477.	3.4	77
51	Targeted Imaging of Brain Tumors with a Framework Nucleic Acid Probe. ACS Applied Materials & Interfaces, 2018, 10, 3414-3420.	8.0	77
52	Nanodiamond autophagy inhibitor allosterically improves the arsenical-based therapy of solid tumors. Nature Communications, 2018, 9, 4347.	12.8	77
53	Analysis and Modeling of the Variable Region of Camelid Single-Domain Antibodies. Journal of Immunology, 2011, 186, 6357-6367.	0.8	75
54	Transfer of Twoâ€Dimensional Oligonucleotide Patterns onto Stereocontrolled Plasmonic Nanostructures through DNAâ€Origamiâ€Based Nanoimprinting Lithography. Angewandte Chemie - International Edition, 2016, 55, 8036-8040.	13.8	74

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55	Inâ€…Situ Spatial Complementation of Aptamerâ€Mediated Recognition Enables Liveâ€Cell Imaging of Native RNA Transcripts in Real Time. Angewandte Chemie - International Edition, 2018, 57, 972-976.	13.8	71
56	Guiding protein delivery into live cells using DNA-programmed membrane fusion. Chemical Science, 2018, 9, 5967-5975.	7.4	66
57	Size-Dependent Programming of the Dynamic Range of Graphene Oxideâ€“DNA Interaction-Based Ion Sensors. Analytical Chemistry, 2014, 86, 4047-4051.	6.5	63
58	Helix kinks are equally prevalent in soluble and membrane proteins. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1960-1970.	2.6	61
59	Pattern Recognition Analysis of Proteins Using DNAâ€Decorated Catalytic Gold Nanoparticles. Small, 2013, 9, 2844-2849.	10.0	59
60	Exploring Transition Pathway and Free-Energy Profile of Large-Scale Protein Conformational Change by Combining Normal Mode Analysis and Umbrella Sampling Molecular Dynamics. Journal of Physical Chemistry B, 2014, 118, 134-143.	2.6	58
61	DNA Origamiâ€Enabled Engineering of Ligandâ€“Drug Conjugates for Targeted Drug Delivery. Small, 2020, 16, e1904857.	10.0	58
62	Nanoscale delivery systems for cancer immunotherapy. Materials Horizons, 2018, 5, 344-362.	12.2	57
63	Activity modulation and allosteric control of a scaffolded DNAzyme using a dynamic DNA nanostructure. Chemical Science, 2016, 7, 1200-1204.	7.4	56
64	Dynamic Modulation of DNA Hybridization Using Allosteric DNA Tetrahedral Nanostructures. Analytical Chemistry, 2016, 88, 8043-8049.	6.5	54
65	D3Pockets: A Method and Web Server for Systematic Analysis of Protein Pocket Dynamics. Journal of Chemical Information and Modeling, 2019, 59, 3353-3358.	5.4	54
66	Encapsulation and release of living tumor cells using hydrogels with the hybridization chain reaction. Nature Protocols, 2020, 15, 2163-2185.	12.0	54
67	HOMSTRAD: adding sequence information to structure-based alignments of homologous protein families. Bioinformatics, 2001, 17, 748-749.	4.1	49
68	Encapsulation of curcumin within poly(amidoamine) dendrimers for delivery to cancer cells. Journal of Materials Science: Materials in Medicine, 2013, 24, 2137-2144.	3.6	49
69	Nanoplasmonic Imaging of Latent Fingerprints with Explosive RDX Residues. Analytical Chemistry, 2015, 87, 9403-9407.	6.5	49
70	Force fields and scoring functions for carbohydrate simulation. Carbohydrate Research, 2015, 401, 73-81.	2.3	49
71	Length-independent structural similarities enrich the antibody CDR canonical class model. MAbs, 2016, 8, 751-760.	5.2	49
72	Sphinx: merging knowledge-based and ab initio approaches to improve protein loop prediction. Bioinformatics, 2017, 33, 1346-1353.	4.1	49

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73	Recent progress in natural products as DPP-4 inhibitors. Future Medicinal Chemistry, 2015, 7, 1079-1089.	2.3	48
74	Programmable Liveâ€Cell CRISPR Imaging with Toeholdâ€Switchâ€Mediated Strand Displacement. Angewandte Chemie - International Edition, 2020, 59, 20612-20618.	13.8	48
75	Stability and Characteristics of the Halogen Bonding Interaction in an Anionâ€“Anion Complex: A Computational Chemistry Study. Journal of Physical Chemistry B, 2016, 120, 610-620.	2.6	44
76	Systematic Study in Mammalian Cells Showing No Adverse Response to Tetrahedral DNA Nanostructure. ACS Applied Materials & Interfaces, 2018, 10, 15442-15448.	8.0	43
77	Alchembed: A Computational Method for Incorporating Multiple Proteins into Complex Lipid Geometries. Journal of Chemical Theory and Computation, 2015, 11, 2743-2754.	5.3	42
78	Deciphering active biocompatibility of iron oxide nanoparticles from their intrinsic antagonism. Nano Research, 2018, 11, 2746-2755.	10.4	42
79	Graphene oxideâ€“silver nanocomposites modulate biofilm formation and extracellular polymeric substance (EPS) production. Nanoscale, 2018, 10, 19603-19611.	5.6	41
80	Programming Switchable Transcription of Topologically Constrained DNA. Journal of the American Chemical Society, 2020, 142, 10739-10746.	13.7	41
81	Multichannel Immunosensor Platform for the Rapid Detection of SARS-CoV-2 and Influenza A(H1N1) Virus. ACS Applied Materials & Interfaces, 2021, 13, 22262-22270.	8.0	41
82	High Resolution NMR-based Model for the Structure of a scFv-IL-1Î² Complex. Journal of Biological Chemistry, 2009, 284, 31928-31935.	3.4	40
83	Enhanced sampling molecular dynamics simulation captures experimentally suggested intermediate and unfolded states in the folding pathway of Trp-cage miniprotein. Journal of Chemical Physics, 2012, 137, 125103.	3.0	40
84	MoS₂â€“Au@Pt nanohybrids as a sensing platform for electrochemical nonenzymatic glucose detection. New Journal of Chemistry, 2018, 42, 6750-6755.	2.8	40
85	Memoir: template-based structure prediction for membrane proteins. Nucleic Acids Research, 2013, 41, W379-W383.	14.5	38
86	Constructing Higher-Order DNA Nanoarchitectures with Highly Purified DNA Nanocages. ACS Applied Materials & Interfaces, 2015, 7, 13174-13179.	8.0	37
87	Fractal Nanoplasmonic Labels for Supermultiplex Imaging in Single Cells. Journal of the American Chemical Society, 2019, 141, 11938-11946.	13.7	37
88	Halogen bonding in differently charged complexes: basic profile, essential interaction terms and intrinsic Ïƒ-hole. Physical Chemistry Chemical Physics, 2019, 21, 15106-15119.	2.8	37
89	Molecular Threading-Dependent Mass Transport in Paper Origami for Single-Step Electrochemical DNA Sensors. Nano Letters, 2019, 19, 369-374.	9.1	37
90	Single-Stranded DNA-Encoded Gold Nanoparticle Clusters as Programmable Enzyme Equivalents. Journal of the American Chemical Society, 2022, 144, 6311-6320.	13.7	37

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91	Real-Time Imaging of Endocytosis and Intracellular Trafficking of Semiconducting Polymer Dots. ACS Applied Materials & Interfaces, 2017, 9, 21200-21208.	8.0	36
92	Structurally Mapping Antibody Repertoires. Frontiers in Immunology, 2018, 9, 1698.	4.8	36
93	Mobile computing - A green computing resource. , 2013, , .		35
94	Unraveling the Role of Hydrogen Peroxide in Î±-Synuclein Aggregation Using an Ultrasensitive Nanoplasmonic Probe. Analytical Chemistry, 2015, 87, 1968-1973.	6.5	35
95	DNAâ€Origamiâ€Based Assembly of Anisotropic Plasmonic Gold Nanostructures. Small, 2017, 13, 1603991.	10.0	35
96	Poly-adenine-mediated spherical nucleic acids for strand displacement-based DNA/RNA detection. Biosensors and Bioelectronics, 2019, 127, 85-91.	10.1	33
97	DNA orientation-specific adhesion and patterning of living mammalian cells on self-assembled DNA monolayers. Chemical Science, 2016, 7, 2722-2727.	7.4	31
98	DNA Framework-Supported Electrochemical Analysis of DNA Methylation for Prostate Cancers. Nano Letters, 2020, 20, 7028-7035.	9.1	31
99	Ab-Ligity: identifying sequence-dissimilar antibodies that bind to the same epitope. MAbs, 2021, 13, 1873478.	5.2	31
100	The Promise of AI for DILI Prediction. Frontiers in Artificial Intelligence, 2021, 4, 638410.	3.4	31
101	Encoding Fluorescence Anisotropic Barcodes with DNA Frameworks. Journal of the American Chemical Society, 2021, 143, 10735-10742.	13.7	31
102	Serum protein corona-responsive autophagy tuning in cells. Nanoscale, 2018, 10, 18055-18063.	5.6	30
103	iMembrane: homology-based membrane-insertion of proteins. Bioinformatics, 2009, 25, 1086-1088.	4.1	29
104	Examining Variable Domain Orientations in Antigen Receptors Gives Insight into TCR-Like Antibody Design. PLoS Computational Biology, 2014, 10, e1003852.	3.2	29
105	Access to Different Isomeric Dibenzoxazepinones through Copper-Catalyzed Câ€“H Etherification and Câ€“N Bond Construction with Controllable Smiles Rearrangement. Organic Letters, 2016, 18, 380-383.	4.6	29
106	Blood exposure to graphene oxide may cause anaphylactic death in non-human primates. Nano Today, 2020, 35, 100922.	11.9	29
107	PCR-Free Colorimetric DNA Hybridization Detection Using a 3D DNA Nanostructured Reporter Probe. ACS Applied Materials & Interfaces, 2017, 9, 38281-38287.	8.0	28
108	Real-Time Continuous Identification of Greenhouse Plant Pathogens Based on Recyclable Microfluidic Bioassay System. ACS Applied Materials & Interfaces, 2017, 9, 31568-31575.	8.0	28

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109	B-cell epitopes: Discontinuity and conformational analysis. Molecular Immunology, 2019, 114, 643-650.	2.2	28
110	Computational design of an epitope-specific Keap1 binding antibody using hotspot residues grafting and CDR loop swapping. Scientific Reports, 2017, 7, 41306.	3.3	27
111	The Inhibition Effect of Graphene Oxide Nanosheets on the Development ofStreptococcus mutansBiofilms. Particle and Particle Systems Characterization, 2017, 34, 1700001.	2.3	27
112	Preservation of DNA Nanostructure Carriers: Effects of Freezeâ€“Thawing and Ionic Strength during Lyophilization and Storage. ACS Applied Materials & Interfaces, 2017, 9, 18434-18439.	8.0	27
113	Thermodynamics calculation of proteinâ€“ligand interactions by QM/MM polarizable charge parameters. Journal of Biomolecular Structure and Dynamics, 2016, 34, 163-176.	3.5	26
114	Programming chain-growth copolymerization of DNA hairpin tiles for in-vitro hierarchical supramolecular organization. Nature Communications, 2019, 10, 1006.	12.8	26
115	A DNA tetrahedral structure-mediated ultrasensitive fluorescent microarray platform for nucleic acid test. Sensors and Actuators B: Chemical, 2020, 321, 128538.	7.8	26
116	Public Baseline and shared response structures support the theory of antibody repertoire functional commonality. PLoS Computational Biology, 2021, 17, e1008781.	3.2	26
117	Building a Better Fragment Library for De Novo Protein Structure Prediction. PLoS ONE, 2015, 10, e0123998.	2.5	25
118	Electrochemical detection of PCR amplicons of Escherichia coli genome based on DNA nanostructural probes and polyHRP enzyme. Analyst, The, 2016, 141, 5304-5310.	3.5	25
119	Humidityâ€Responsive Singleâ€Nanoparticleâ€Layer Plasmonic Films. Advanced Materials, 2017, 29, 1606796.	21.0	25
120	Underestimated Noncovalent Interactions in Protein Data Bank. Journal of Chemical Information and Modeling, 2019, 59, 3389-3399.	5.4	25
121	Like-Charge Guanidinium Pairing between Ligand and Receptor: An Unusual Interaction for Drug Discovery and Design?. Journal of Physical Chemistry B, 2015, 119, 11988-11997.	2.6	24
122	Scaling Up Multi-bit DNA Full Adder Circuits with Minimal Strand Displacement Reactions. Journal of the American Chemical Society, 2022, 144, 9479-9488.	13.7	24
123	The Cloudlet Accelerator: Bringing Mobile-Cloud Face Recognition into Real-Time. , 2015, , .		23
124	Graphene Nanoprobes for Real-Time Monitoring of Isothermal Nucleic Acid Amplification. ACS Applied Materials & Interfaces, 2017, 9, 15245-15253.	8.0	23
125	Catalysisâ€Driven Selfâ€Thermophoresis of Janus Plasmonic Nanomotors. Angewandte Chemie, 2017, 129, 530-533.	2.0	23
126	Biocomputing Based on DNA Strand Displacement Reactions. ChemPhysChem, 2021, 22, 1151-1166.	2.1	23

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127	Driving DNA Origami Assembly with a Terahertz Wave. Nano Letters, 2022, 22, 468-475.	9.1	23
128	Combining modelling and mutagenesis studies of synaptic vesicle protein 2A to identify a series of residues involved in racetam binding. Biochemical Society Transactions, 2011, 39, 1341-1347.	3.4	22
129	Reversible Regulation of Catalytic Activity of Gold Nanoparticles with DNA Nanomachines. Scientific Reports, 2015, 5, 14402.	3.3	22
130	Inhibition of Epithelialâ€“Mesenchymal Transition and Tissue Regeneration by Waterborne Titanium Dioxide Nanoparticles. ACS Applied Materials & Interfaces, 2018, 10, 3449-3458.	8.0	22
131	Antibody side chain conformations are positionâ€dependent. Proteins: Structure, Function and Bioinformatics, 2018, 86, 383-392.	2.6	21
132	Inâ€…Situ Spatial Complementation of Aptamerâ€Mediated Recognition Enables Liveâ€Cell Imaging of Native RNA Transcripts in Real Time. Angewandte Chemie, 2018, 130, 984-988.	2.0	21
133	Exploring Conformational Change of Adenylate Kinase by Replica Exchange Molecular Dynamic Simulation. Biophysical Journal, 2020, 118, 1009-1018.	0.5	21
134	Environment specific substitution tables improve membrane protein alignment. Bioinformatics, 2011, 27, i15-i23.	4.1	20
135	Conjugation of Dexamethasone to C60 for the Design of an Anti-Inflammatory Nanomedicine with Reduced Cellular Apoptosis. ACS Applied Materials & Interfaces, 2013, 5, 5291-5297.	8.0	20
136	Examining the Conservation of Kinks in Alpha Helices. PLoS ONE, 2016, 11, e0157553.	2.5	20
137	Determining Protein Folding Pathway and Associated Energetics through Partitioned Integrated-Tempering-Sampling Simulation. Journal of Chemical Theory and Computation, 2017, 13, 1229-1243.	5.3	20
138	Design, Synthesis, and Structureâ€“Activity Relationships of Bavachinin Analogues as Peroxisome Proliferatorâ€Activated Receptorâ€…Î³ Agonists. ChemMedChem, 2017, 12, 183-193.	3.2	20
139	How Do Distance and Solvent Affect Halogen Bonding Involving Negatively Charged Donors?. Journal of Physical Chemistry B, 2016, 120, 8784-8793.	2.6	19
140	Underestimated Halogen Bonds Forming with Protein Backbone in Protein Data Bank. Journal of Chemical Information and Modeling, 2017, 57, 1529-1534.	5.4	19
141	Exploring the Interaction of SV2A with Racetams Using Homology Modelling, Molecular Dynamics and Site-Directed Mutagenesis. PLoS ONE, 2015, 10, e0116589.	2.5	18
142	Poly-adenine-mediated fluorescent spherical nucleic acid probes for live-cell imaging of endogenous tumor-related mRNA. Nanomedicine: Nanotechnology, Biology, and Medicine, 2018, 14, 1797-1807.	3.3	18
143	Remote Photothermal Control of DNA Origami Assembly in Cellular Environments. Nano Letters, 2021, 21, 5834-5841.	9.1	18
144	Goldâ€Nanoparticleâ€Mediated Jigsawâ€Puzzleâ€like Assembly of Supersized Plasmonic DNA Origami. Angewandte Chemie, 2015, 127, 3009-3012.	2.0	17

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145	Separation and peroxisome proliferator-activated receptor-Î³ agonist activity evaluation of synthetic racemic bavachinin enantiomers. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2579-2583.	2.2	17
146	Energetics and structural characterization of the â€œDFG-flipâ€•conformational transition of B-RAF kinase: a SITS molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 1257-1267.	2.8	17
147	Recognizing single phospholipid vesicle collisions on carbon fiber nanoelectrode. Science China Chemistry, 2017, 60, 1474-1480.	8.2	17
148	Membrane Interactions of Î±-Synuclein Revealed by Multiscale Molecular Dynamics Simulations, Markov State Models, and NMR. Journal of Physical Chemistry B, 2021, 125, 2929-2941.	2.6	17
149	Mapping Central Î±-Helix Linker Mediated Conformational Transition Pathway of Calmodulin via Simple Computational Approach. Journal of Physical Chemistry B, 2014, 118, 9677-9685.	2.6	16
150	Multifunctional Yolkâ€“Shell Nanostructure as a Superquencher for Fluorescent Analysis of Potassium Ion Using Guanine-Rich Oligonucleotides. ACS Applied Materials & Interfaces, 2017, 9, 30406-30413.	8.0	16
151	Structural insights into HIV-1 protease flap opening processes and key intermediates. RSC Advances, 2017, 7, 45121-45128.	3.6	16
152	Fragment-based modeling of membrane protein loops: Successes, failures, and prospects for the future. Proteins: Structure, Function and Bioinformatics, 2014, 82, 175-186.	2.6	15
153	Cavity-Type DNA Origami-Based Plasmonic Nanostructures for Raman Enhancement. ACS Applied Materials & Interfaces, 2017, 9, 21942-21948.	8.0	15
154	Accelerating Mobile-Cloud Computing. Advances in Systems Analysis, Software Engineering, and High Performance Computing Book Series, 0, , 175-197.	0.5	14
155	Reconstructing Somaâ€“Soma Synapse-like Vesicular Exocytosis with DNA Origami. ACS Central Science, 2021, 7, 1400-1407.	11.3	14
156	Deciphering buried air phases on natural and bioinspired superhydrophobic surfaces using synchrotron radiation-based X-ray phase-contrast imaging. NPG Asia Materials, 2016, 8, e306-e306.	7.9	13
157	Improving the accuracy of predicting proteinâ€“ligand binding-free energy with semiempirical quantum chemistry charge. Future Medicinal Chemistry, 2019, 11, 303-321.	2.3	13
158	Conformation of the Macrocyclic Drug Lorlatinib in Polar and Nonpolar Environments: A MD Simulation and NMR Study. ACS Omega, 2019, 4, 22245-22250.	3.5	13
159	Probing Transient DNA Conformation Changes with an Intercalative Fluorescent Excimer. Angewandte Chemie - International Edition, 2021, 60, 6624-6630.	13.8	13
160	Regioselectivity and Mechanism of Synthesizing N-Substituted 2-Pyridones and 2-Substituted Pyridines via Metal-Free C-O and C-N Bond-Cleaving of Oxazoline[3,2-a]pyridiniums. Scientific Reports, 2017, 7, 41287.	3.3	12
161	Chemical Flocculation-Based Green Algae Materials for Photobiological Hydrogen Production. ACS Applied Bio Materials, 2022, 5, 897-903.	4.6	12
162	DDBASE2.0: updated domain database with improved identification of structural domains. Bioinformatics, 2003, 19, 1760-1764.	4.1	11

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163	Discovery of N-substituted 3-arylisoquinolone derivatives as antitumor agents originating from O-substituted 3-arylisoquinolines via [2,3] or [3,3] rearrangement. European Journal of Medicinal Chemistry, 2014, 77, 204-210.	5.5	11
164	Volunteer Computing on Mobile Devices. Advances in Wireless Technologies and Telecommunication Book Series, 0, , 153-181.	0.4	11
165	Molecular dynamics simulation indicating cold denaturation of Î²-hairpins. Journal of Chemical Physics, 2013, 138, 085102.	3.0	10
166	TCRBuilder: multi-state T-cell receptor structure prediction. Bioinformatics, 2020, 36, 3580-3581.	4.1	10
167	The Chemical Synthesis of Knob Domain Antibody Fragments. ACS Chemical Biology, 2021, 16, 1757-1769.	3.4	10
168	Nanomechanical Induction of Autophagyâ€Related Fluorescence in Single Cells with Atomic Force Microscopy. Advanced Science, 2021, 8, e2102989.	11.2	10
169	Waterâ€Dispersible Gold Nanoclusters: Synthesis Strategies, Optical Properties, and Biological Applications. Chemistry - A European Journal, 2022, 28, e202103736.	3.3	10
170	Phase transferring luminescent gold nanoclusters via single-stranded DNA. Science China Chemistry, 2022, 65, 1212-1220.	8.2	10
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