

Jiye Shi

List of Publications by Year in descending order

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Version: 2024-02-01

201
papers

13,411
citations

23567

58
h-index

27406

106
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215
all docs

215
docs citations

215
times ranked

15183
citing authors

#	ARTICLE	IF	CITATIONS
1	Water-Dispersible Gold Nanoclusters: Synthesis Strategies, Optical Properties, and Biological Applications. <i>Chemistry - A European Journal</i> , 2022, 28, e202103736.	3.3	10
2	Benzyl-rich ligand engineering of the photostability of atomically precise gold nanoclusters. <i>Chemical Communications</i> , 2022, , .	4.1	1
3	Chemical Flocculation-Based Green Algae Materials for Photobiological Hydrogen Production. <i>ACS Applied Bio Materials</i> , 2022, 5, 897-903.	4.6	12
4	DNA origami nanocalipers for pH sensing at the nanoscale. <i>Chemical Communications</i> , 2022, 58, 3673-3676.	4.1	3
5	Frontispiece: Water-Dispersible Gold Nanoclusters: Synthesis Strategies, Optical Properties, and Biological Applications. <i>Chemistry - A European Journal</i> , 2022, 28, .	3.3	1
6	Single-Stranded DNA-Encoded Gold Nanoparticle Clusters as Programmable Enzyme Equivalents. <i>Journal of the American Chemical Society</i> , 2022, 144, 6311-6320.	13.7	37
7	Recent Advances in Prescribing Chiral Plasmonics with DNA Frameworks. <i>ChemNanoMat</i> , 2022, 8, .	2.8	2
8	Driving DNA Origami Assembly with a Terahertz Wave. <i>Nano Letters</i> , 2022, 22, 468-475.	9.1	23
9	Phase transferring luminescent gold nanoclusters via single-stranded DNA. <i>Science China Chemistry</i> , 2022, 65, 1212-1220.	8.2	10
10	Scaling Up Multi-bit DNA Full Adder Circuits with Minimal Strand Displacement Reactions. <i>Journal of the American Chemical Society</i> , 2022, 144, 9479-9488.	13.7	24
11	Probing Transient DNA Conformation Changes with an Intercalative Fluorescent Excimer. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6624-6630.	13.8	13
12	Programming folding cooperativity of the dimeric i-motif with DNA frameworks for sensing small pH variations. <i>Chemical Communications</i> , 2021, 57, 3247-3250.	4.1	9
13	Ab-Ligity: identifying sequence-dissimilar antibodies that bind to the same epitope. <i>MAbs</i> , 2021, 13, 1873478.	5.2	31
14	Probing Transient DNA Conformation Changes with an Intercalative Fluorescent Excimer. <i>Angewandte Chemie</i> , 2021, 133, 6698-6704.	2.0	0
15	Public Baseline and shared response structures support the theory of antibody repertoire functional commonality. <i>PLoS Computational Biology</i> , 2021, 17, e1008781.	3.2	26
16	Membrane Interactions of Î±-Synuclein Revealed by Multiscale Molecular Dynamics Simulations, Markov State Models, and NMR. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2929-2941.	2.6	17
17	The Promise of AI for DILI Prediction. <i>Frontiers in Artificial Intelligence</i> , 2021, 4, 638410.	3.4	31
18	Multichannel Immunosensor Platform for the Rapid Detection of SARS-CoV-2 and Influenza A(H1N1) Virus. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 22262-22270.	8.0	41

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19	Modulating Target Protein Biology Through the Re-mapping of Conformational Distributions Using Small Molecules. <i>Frontiers in Chemistry</i> , 2021, 9, 668186.	3.6	4
20	Biocomputing Based on DNA Strand Displacement Reactions. <i>ChemPhysChem</i> , 2021, 22, 1151-1166.	2.1	23
21	Remote Photothermal Control of DNA Origami Assembly in Cellular Environments. <i>Nano Letters</i> , 2021, 21, 5834-5841.	9.1	18
22	Encoding Fluorescence Anisotropic Barcodes with DNA Frameworks. <i>Journal of the American Chemical Society</i> , 2021, 143, 10735-10742.	13.7	31
23	Cryogenic Electron Microscopy for Resolving DNA Nanostructures and Their Complexes. <i>Small Structures</i> , 2021, 2, 2100053.	12.0	4
24	Reconstructing Soma-like Soma Synapse-like Vesicular Exocytosis with DNA Origami. <i>ACS Central Science</i> , 2021, 7, 1400-1407.	11.3	14
25	The Chemical Synthesis of Knob Domain Antibody Fragments. <i>ACS Chemical Biology</i> , 2021, 16, 1757-1769.	3.4	10
26	Programming cell communications with pH-responsive DNA nanodevices. <i>Chemical Communications</i> , 2021, 57, 4536-4539.	4.1	6
27	The prospects of quantum computing in computational molecular biology. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1481.	14.6	108
28	Nanomechanical Induction of Autophagy-Related Fluorescence in Single Cells with Atomic Force Microscopy. <i>Advanced Science</i> , 2021, 8, e2102989.	11.2	10
29	Thera-SAbDab: the Therapeutic Structural Antibody Database. <i>Nucleic Acids Research</i> , 2020, 48, D383-D388.	14.5	88
30	Exploring Conformational Change of Adenylate Kinase by Replica Exchange Molecular Dynamic Simulation. <i>Biophysical Journal</i> , 2020, 118, 1009-1018.	0.5	21
31	Implementing digital computing with DNA-based switching circuits. <i>Nature Communications</i> , 2020, 11, 121.	12.8	114
32	Blood exposure to graphene oxide may cause anaphylactic death in non-human primates. <i>Nano Today</i> , 2020, 35, 100922.	11.9	29
33	Programmable Live-Cell CRISPR Imaging with Toehold-Switch-Mediated Strand Displacement. <i>Angewandte Chemie</i> , 2020, 132, 20793-20799.	2.0	9
34	Programmable Live-Cell CRISPR Imaging with Toehold-Switch-Mediated Strand Displacement. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 20612-20618.	13.8	48
35	Computational study of the substituent effect of halogenated fused-ring heteroaromatics on halogen bonding. <i>Journal of Molecular Modeling</i> , 2020, 26, 270.	1.8	5
36	DNA Framework-Supported Electrochemical Analysis of DNA Methylation for Prostate Cancers. <i>Nano Letters</i> , 2020, 20, 7028-7035.	9.1	31

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37	Programming Switchable Transcription of Topologically Constrained DNA. <i>Journal of the American Chemical Society</i> , 2020, 142, 10739-10746.	13.7	41
38	Encapsulation and release of living tumor cells using hydrogels with the hybridization chain reaction. <i>Nature Protocols</i> , 2020, 15, 2163-2185.	12.0	54
39	TCRBuilder: multi-state T-cell receptor structure prediction. <i>Bioinformatics</i> , 2020, 36, 3580-3581.	4.1	10
40	DNA Origami-Enabled Engineering of Ligand-Drug Conjugates for Targeted Drug Delivery. <i>Small</i> , 2020, 16, e1904857.	10.0	58
41	A DNA tetrahedral structure-mediated ultrasensitive fluorescent microarray platform for nucleic acid test. <i>Sensors and Actuators B: Chemical</i> , 2020, 321, 128538.	7.8	26
42	Programming bulk enzyme heterojunctions for biosensor development with tetrahedral DNA framework. <i>Nature Communications</i> , 2020, 11, 838.	12.8	84
43	Underestimated Noncovalent Interactions in Protein Data Bank. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3389-3399.	5.4	25
44	Fractal Nanoplasmonic Labels for Supermultiplex Imaging in Single Cells. <i>Journal of the American Chemical Society</i> , 2019, 141, 11938-11946.	13.7	37
45	D3Pockets: A Method and Web Server for Systematic Analysis of Protein Pocket Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3353-3358.	5.4	54
46	B-cell epitopes: Discontinuity and conformational analysis. <i>Molecular Immunology</i> , 2019, 114, 643-650.	2.2	28
47	Halogen bonding in differently charged complexes: basic profile, essential interaction terms and intrinsic π -hole. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15106-15119.	2.8	37
48	An Intelligent DNA Nanorobot with <i>in Vitro</i> Enhanced Protein Lysosomal Degradation of HER2. <i>Nano Letters</i> , 2019, 19, 4505-4517.	9.1	153
49	Improving the accuracy of predicting protein-ligand binding-free energy with semiempirical quantum chemistry charge. <i>Future Medicinal Chemistry</i> , 2019, 11, 303-321.	2.3	13
50	Programming chain-growth copolymerization of DNA hairpin tiles for in-vitro hierarchical supramolecular organization. <i>Nature Communications</i> , 2019, 10, 1006.	12.8	26
51	Five computational developability guidelines for therapeutic antibody profiling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 4025-4030.	7.1	221
52	DNA origami cryptography for secure communication. <i>Nature Communications</i> , 2019, 10, 5469.	12.8	84
53	Conformation of the Macrocyclic Drug Lorlatinib in Polar and Nonpolar Environments: A MD Simulation and NMR Study. <i>ACS Omega</i> , 2019, 4, 22245-22250.	3.5	13
54	Programming biosensing sensitivity by controlling the dimension of nanostructured electrode. <i>Analytical and Bioanalytical Chemistry</i> , 2019, 411, 4085-4092.	3.7	4

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55	Solving mazes with single-molecule DNA navigators. <i>Nature Materials</i> , 2019, 18, 273-279.	27.5	190
56	Poly-adenine-mediated spherical nucleic acids for strand displacement-based DNA/RNA detection. <i>Biosensors and Bioelectronics</i> , 2019, 127, 85-91.	10.1	33
57	Molecular Threading-Dependent Mass Transport in Paper Origami for Single-Step Electrochemical DNA Sensors. <i>Nano Letters</i> , 2019, 19, 369-374.	9.1	37
58	Systematic Study in Mammalian Cells Showing No Adverse Response to Tetrahedral DNA Nanostructure. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 15442-15448.	8.0	43
59	Computational Exploration of Conformational Transitions in Protein Drug Targets. <i>Methods in Molecular Biology</i> , 2018, 1762, 339-365.	0.9	1
60	Valency-Controlled Framework Nucleic Acid Signal Amplifiers. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 7131-7135.	13.8	85
61	Valency-Controlled Framework Nucleic Acid Signal Amplifiers. <i>Angewandte Chemie</i> , 2018, 130, 7249-7253.	2.0	9
62	MoS ₂ Nanoprobe for MicroRNA Quantification Based on Duplex-Specific Nuclease Signal Amplification. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 7852-7858.	8.0	81
63	Nanoscale delivery systems for cancer immunotherapy. <i>Materials Horizons</i> , 2018, 5, 344-362.	12.2	57
64	Antibody side chain conformations are position-dependent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 383-392.	2.6	21
65	Inhibition of Epithelial-Mesenchymal Transition and Tissue Regeneration by Waterborne Titanium Dioxide Nanoparticles. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 3449-3458.	8.0	22
66	Targeted Imaging of Brain Tumors with a Framework Nucleic Acid Probe. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 3414-3420.	8.0	77
67	MoS ₂ -Au@Pt nanohybrids as a sensing platform for electrochemical nonenzymatic glucose detection. <i>New Journal of Chemistry</i> , 2018, 42, 6750-6755.	2.8	40
68	In-Situ Spatial Complementation of Aptamer-Mediated Recognition Enables Live-Cell Imaging of Native RNA Transcripts in Real Time. <i>Angewandte Chemie</i> , 2018, 130, 984-988.	2.0	21
69	In-Situ Spatial Complementation of Aptamer-Mediated Recognition Enables Live-Cell Imaging of Native RNA Transcripts in Real Time. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 972-976.	13.8	71
70	Deciphering active biocompatibility of iron oxide nanoparticles from their intrinsic antagonism. <i>Nano Research</i> , 2018, 11, 2746-2755.	10.4	42
71	DNA origami nanostructures can exhibit preferential renal uptake and alleviate acute kidney injury. <i>Nature Biomedical Engineering</i> , 2018, 2, 865-877.	22.5	297
72	Hydrogen Sulfide-Activatable Second Near-Infrared Fluorescent Nanoassemblies for Targeted Photothermal Cancer Therapy. <i>Nano Letters</i> , 2018, 18, 6411-6416.	9.1	164

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73	Graphene oxide-silver nanocomposites modulate biofilm formation and extracellular polymeric substance (EPS) production. <i>Nanoscale</i> , 2018, 10, 19603-19611.	5.6	41
74	Nanodiamond autophagy inhibitor allosterically improves the arsenical-based therapy of solid tumors. <i>Nature Communications</i> , 2018, 9, 4347.	12.8	77
75	Serum protein corona-responsive autophagy tuning in cells. <i>Nanoscale</i> , 2018, 10, 18055-18063.	5.6	30
76	Poly-adenine-mediated fluorescent spherical nucleic acid probes for live-cell imaging of endogenous tumor-related mRNA. <i>Nanomedicine: Nanotechnology, Biology, and Medicine</i> , 2018, 14, 1797-1807.	3.3	18
77	A PIP2 Binding Site on a Human TRP Channel: Simulation Studies of PKD2. <i>Biophysical Journal</i> , 2018, 114, 397a.	0.5	2
78	Structurally Mapping Antibody Repertoires. <i>Frontiers in Immunology</i> , 2018, 9, 1698.	4.8	36
79	Efficient Sampling for the Prediction of Long and Multidomain Protein Structures. <i>Biophysical Journal</i> , 2018, 114, 574a.	0.5	0
80	Inhibiting Methicillin-Resistant <i>Staphylococcus aureus</i> by Tetrahedral DNA Nanostructure-Enabled Antisense Peptide Nucleic Acid Delivery. <i>Nano Letters</i> , 2018, 18, 5652-5659.	9.1	117
81	Guiding protein delivery into live cells using DNA-programmed membrane fusion. <i>Chemical Science</i> , 2018, 9, 5967-5975.	7.4	66
82	Determining Protein Folding Pathway and Associated Energetics through Partitioned Integrated-Tempering-Sampling Simulation. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1229-1243.	5.3	20
83	Computational design of an epitope-specific Keap1 binding antibody using hotspot residues grafting and CDR loop swapping. <i>Scientific Reports</i> , 2017, 7, 41306.	3.3	27
84	An Exonuclease III-Powered, On-Particle Stochastic DNA Walker. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 1855-1858.	13.8	325
85	Multicolor Gold-Silver Nano-Mushrooms as Ready-to-Use SERS Probes for Ultrasensitive and Multiplex DNA/miRNA Detection. <i>Analytical Chemistry</i> , 2017, 89, 2531-2538.	6.5	205
86	Yolk-shell nanostructured Fe ₃ O ₄ @C magnetic nanoparticles with enhanced peroxidase-like activity for label-free colorimetric detection of H ₂ O ₂ and glucose. <i>Nanoscale</i> , 2017, 9, 4508-4515.	5.6	175
87	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. <i>Scientific Reports</i> , 2017, 7, 41287.	3.3	12
88	The Inhibition Effect of Graphene Oxide Nanosheets on the Development of <i>Streptococcus mutans</i> Biofilms. <i>Particle and Particle Systems Characterization</i> , 2017, 34, 1700001.	2.3	27
89	Graphene Nanoprobes for Real-Time Monitoring of Isothermal Nucleic Acid Amplification. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 15245-15253.	8.0	23
90	DNA-Origami-Based Assembly of Anisotropic Plasmonic Gold Nanostructures. <i>Small</i> , 2017, 13, 1603991.	10.0	35

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91	Design, Synthesis, and Structure-Activity Relationships of Bavachinin Analogues as Peroxisome Proliferator-Activated Receptor- β Agonists. <i>ChemMedChem</i> , 2017, 12, 183-193.	3.2	20
92	Cavity-Type DNA Origami-Based Plasmonic Nanostructures for Raman Enhancement. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 21942-21948.	8.0	15
93	Real-Time Imaging of Endocytosis and Intracellular Trafficking of Semiconducting Polymer Dots. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 21200-21208.	8.0	36
94	Preservation of DNA Nanostructure Carriers: Effects of Freeze-Thawing and Ionic Strength during Lyophilization and Storage. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 18434-18439.	8.0	27
95	Real-time visualization of clustering and intracellular transport of gold nanoparticles by correlative imaging. <i>Nature Communications</i> , 2017, 8, 15646.	12.8	163
96	Investigating Cotranslational Folding in Membrane Proteins using Fragment-Based Structure Prediction. <i>Biophysical Journal</i> , 2017, 112, 61a.	0.5	1
97	An Exonuclease III-Powered, On-Particle Stochastic DNA Walker. <i>Angewandte Chemie</i> , 2017, 129, 1881-1884.	2.0	252
98	The H3 loop of antibodies shows unique structural characteristics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1311-1318.	2.6	89
99	Catalysis-Driven Self-Thermophoresis of Janus Plasmonic Nanomotors. <i>Angewandte Chemie</i> , 2017, 129, 530-533.	2.0	23
100	Catalysis-Driven Self-Thermophoresis of Janus Plasmonic Nanomotors. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 515-518.	13.8	93
101	Energetics and structural characterization of the α -DFG-flip-conformational transition of B-RAF kinase: a SITS molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1257-1267.	2.8	17
102	Label-Free Electrochemical Sensing Platform for MicroRNA-21 Detection Using Thionine and Gold Nanoparticles Co-Functionalized MoS ₂ Nanosheet. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 35597-35603.	8.0	141
103	PCR-Free Colorimetric DNA Hybridization Detection Using a 3D DNA Nanostructured Reporter Probe. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 38281-38287.	8.0	28
104	Multifunctional Yolk-Shell Nanostructure as a Superquencher for Fluorescent Analysis of Potassium Ion Using Guanine-Rich Oligonucleotides. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 30406-30413.	8.0	16
105	DNA-Encoded Raman-Active Anisotropic Nanoparticles for microRNA Detection. <i>Analytical Chemistry</i> , 2017, 89, 9850-9856.	6.5	85
106	Structural insights into HIV-1 protease flap opening processes and key intermediates. <i>RSC Advances</i> , 2017, 7, 45121-45128.	3.6	16
107	Real-Time Continuous Identification of Greenhouse Plant Pathogens Based on Recyclable Microfluidic Bioassay System. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 31568-31575.	8.0	28
108	Programming Cell Adhesion for On-Chip Sequential Boolean Logic Functions. <i>Journal of the American Chemical Society</i> , 2017, 139, 10176-10179.	13.7	103

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109	Humidity-Responsive Single-Nanoparticle-Layer Plasmonic Films. <i>Advanced Materials</i> , 2017, 29, 1606796.	21.0	25
110	DNA Hydrogel with Aptamer-Toehold-Based Recognition, Cloaking, and Decloaking of Circulating Tumor Cells for Live Cell Analysis. <i>Nano Letters</i> , 2017, 17, 5193-5198.	9.1	204
111	Recognizing single phospholipid vesicle collisions on carbon fiber nanoelectrode. <i>Science China Chemistry</i> , 2017, 60, 1474-1480.	8.2	17
112	Underestimated Halogen Bonds Forming with Protein Backbone in Protein Data Bank. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1529-1534.	5.4	19
113	Sphinx: merging knowledge-based and <i>ab initio</i> approaches to improve protein loop prediction. <i>Bioinformatics</i> , 2017, 33, 1346-1353.	4.1	49
114	Titanium Dioxide Nanoparticles Trigger Non-Canonical Receptor Endocytosis to Inhibit Wnt Signaling. <i>Journal of Biomedical Nanotechnology</i> , 2017, 13, 1522-1532.	1.1	4
115	Examining the Conservation of Kinks in Alpha Helices. <i>PLoS ONE</i> , 2016, 11, e0157553.	2.5	20
116	Transfer of Two-Dimensional Oligonucleotide Patterns onto Stereocontrolled Plasmonic Nanostructures through DNA-Origami-Based Nanoimprinting Lithography. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8036-8040.	13.8	74
117	ABodyBuilder: Automated antibody structure prediction with data-driven accuracy estimation. <i>MAbs</i> , 2016, 8, 1259-1268.	5.2	208
118	A Surface-Confined Proton-Driven DNA Pump Using a Dynamic 3D DNA Scaffold. <i>Advanced Materials</i> , 2016, 28, 6860-6865.	21.0	79
119	How Do Distance and Solvent Affect Halogen Bonding Involving Negatively Charged Donors?. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8784-8793.	2.6	19
120	Deciphering buried air phases on natural and bioinspired superhydrophobic surfaces using synchrotron radiation-based X-ray phase-contrast imaging. <i>NPG Asia Materials</i> , 2016, 8, e306-e306.	7.9	13
121	Dynamic Modulation of DNA Hybridization Using Allosteric DNA Tetrahedral Nanostructures. <i>Analytical Chemistry</i> , 2016, 88, 8043-8049.	6.5	54
122	Electrochemical detection of PCR amplicons of <i>Escherichia coli</i> genome based on DNA nanostructural probes and polyHRP enzyme. <i>Analyst</i> , The, 2016, 141, 5304-5310.	3.5	25
123	One-Shot Immunomodulatory Nanodiamond Agents for Cancer Immunotherapy. <i>Advanced Materials</i> , 2016, 28, 2699-2708.	21.0	102
124	Electrochemical detection of nucleic acids, proteins, small molecules and cells using a DNA-nanostructure-based universal biosensing platform. <i>Nature Protocols</i> , 2016, 11, 1244-1263.	12.0	320
125	Thermodynamics calculation of protein-ligand interactions by QM/MM polarizable charge parameters. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 163-176.	3.5	26
126	Access to Different Isomeric Dibenzoxazepinones through Copper-Catalyzed C-H Etherification and C-N Bond Construction with Controllable Smiles Rearrangement. <i>Organic Letters</i> , 2016, 18, 380-383.	4.6	29

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127	Stability and Characteristics of the Halogen Bonding Interaction in an Anion-Anion Complex: A Computational Chemistry Study. <i>Journal of Physical Chemistry B</i> , 2016, 120, 610-620.	2.6	44
128	Multiple-Armed Tetrahedral DNA Nanostructures for Tumor-Targeting, Dual-Modality in Vivo Imaging. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 4378-4384.	8.0	142
129	Facile Synthesis of Substituted 4-Alkoxy-2-oxazolines and Exploration of the Reaction Mechanism. <i>Synthesis</i> , 2016, 48, 1331-1343.	2.3	5
130	Length-independent structural similarities enrich the antibody CDR canonical class model. <i>MAbs</i> , 2016, 8, 751-760.	5.2	49
131	DNA orientation-specific adhesion and patterning of living mammalian cells on self-assembled DNA monolayers. <i>Chemical Science</i> , 2016, 7, 2722-2727.	7.4	31
132	Activity modulation and allosteric control of a scaffolded DNAzyme using a dynamic DNA nanostructure. <i>Chemical Science</i> , 2016, 7, 1200-1204.	7.4	56
133	Volunteer Computing on Mobile Devices. , 2016, , 2171-2198.		0
134	Reversible Regulation of Catalytic Activity of Gold Nanoparticles with DNA Nanomachines. <i>Scientific Reports</i> , 2015, 5, 14402.	3.3	22
135	Exploring the Interaction of SV2A with Racetams Using Homology Modelling, Molecular Dynamics and Site-Directed Mutagenesis. <i>PLoS ONE</i> , 2015, 10, e0116589.	2.5	18
136	Building a Better Fragment Library for De Novo Protein Structure Prediction. <i>PLoS ONE</i> , 2015, 10, e0123998.	2.5	25
137	The Cloudlet Accelerator: Bringing Mobile-Cloud Face Recognition into Real-Time. , 2015, , .		23
138	Programmable Engineering of a Biosensing Interface with Tetrahedral DNA Nanostructures for Ultrasensitive DNA Detection. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 2151-2155.	13.8	350
139	Unraveling the Role of Hydrogen Peroxide in β -Synuclein Aggregation Using an Ultrasensitive Nanoplasmonic Probe. <i>Analytical Chemistry</i> , 2015, 87, 1968-1973.	6.5	35
140	Gold-Nanoparticle-Mediated Jigsaw-Puzzle-Like Assembly of Supersized Plasmonic DNA Origami. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 2966-2969.	13.8	94
141	Gold-Nanoparticle-Mediated Jigsaw-Puzzle-Like Assembly of Supersized Plasmonic DNA Origami. <i>Angewandte Chemie</i> , 2015, 127, 3009-3012.	2.0	17
142	Cotranscriptionally Folded RNA Nanostructures Pave the Way to Intracellular Nanofabrication. <i>ChemBioChem</i> , 2015, 16, 39-41.	2.6	4
143	Separation and peroxisome proliferator-activated receptor- β agonist activity evaluation of synthetic racemic bavachinin enantiomers. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 2579-2583.	2.2	17
144	Alchembed: A Computational Method for Incorporating Multiple Proteins into Complex Lipid Geometries. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2743-2754.	5.3	42

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145	DNA-Directed Assembly of Gold Nanohalo for Quantitative Plasmonic Imaging of Single-Particle Catalysis. <i>Journal of the American Chemical Society</i> , 2015, 137, 4292-4295.	13.7	125
146	Increasing the sampling efficiency of protein conformational transition using velocity-scaling optimized hybrid explicit/implicit solvent REMD simulation. <i>Journal of Chemical Physics</i> , 2015, 142, 125105.	3.0	4
147	Nanoplasmonic Imaging of Latent Fingerprints with Explosive RDX Residues. <i>Analytical Chemistry</i> , 2015, 87, 9403-9407.	6.5	49
148	Recent progress in natural products as DPP-4 inhibitors. <i>Future Medicinal Chemistry</i> , 2015, 7, 1079-1089.	2.3	48
149	Like-Charge Guanidinium Pairing between Ligand and Receptor: An Unusual Interaction for Drug Discovery and Design?. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11988-11997.	2.6	24
150	Constructing Higher-Order DNA Nanoarchitectures with Highly Purified DNA Nanocages. <i>ACS Applied Materials & Interfaces</i> , 2015, 7, 13174-13179.	8.0	37
151	Force fields and scoring functions for carbohydrate simulation. <i>Carbohydrate Research</i> , 2015, 401, 73-81.	2.3	49
152	Accelerating Mobile-Cloud Computing. , 2015, , 1933-1955.		2
153	Examining Variable Domain Orientations in Antigen Receptors Gives Insight into TCR-Like Antibody Design. <i>PLoS Computational Biology</i> , 2014, 10, e1003852.	3.2	29
154	Improving B-cell epitope prediction and its application to global antibody-antigen docking. <i>Bioinformatics</i> , 2014, 30, 2288-2294.	4.1	137
155	Single-Particle Tracking and Modulation of Cell Entry Pathways of a Tetrahedral DNA Nanostructure in Live Cells. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 7745-7750.	13.8	430
156	A Bubble-Mediated Intelligent Microscale Electrochemical Device for Single-Step Quantitative Bioassays. <i>Advanced Materials</i> , 2014, 26, 4671-4676.	21.0	99
157	Titelbild: Single-Particle Tracking and Modulation of Cell Entry Pathways of a Tetrahedral DNA Nanostructure in Live Cells (<i>Angew. Chem.</i> 30/2014). <i>Angewandte Chemie</i> , 2014, 126, 7809-7809.	2.0	1
158	Self-Assembly of Poly-Adenine-Tailed CpG Oligonucleotide-Gold Nanoparticle Nanoconjugates with Immunostimulatory Activity. <i>Small</i> , 2014, 10, 368-375.	10.0	92
159	Helix kinks are equally prevalent in soluble and membrane proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1960-1970.	2.6	61
160	Nanoscale optical probes for cellular imaging. <i>Chemical Society Reviews</i> , 2014, 43, 2650.	38.1	179
161	Multi-algorithm and multi-model based drug target prediction and web server. <i>Acta Pharmacologica Sinica</i> , 2014, 35, 419-431.	6.1	7
162	Unstable, Metastable, or Stable Halogen Bonding Interaction Involving Negatively Charged Donors? A Statistical and Computational Chemistry Study. <i>Journal of Physical Chemistry B</i> , 2014, 118, 14223-14233.	2.6	9

#	ARTICLE	IF	CITATIONS
163	SAbDab: the structural antibody database. <i>Nucleic Acids Research</i> , 2014, 42, D1140-D1146.	14.5	374
164	Exploring Transition Pathway and Free-Energy Profile of Large-Scale Protein Conformational Change by Combining Normal Mode Analysis and Umbrella Sampling Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2014, 118, 134-143.	2.6	58
165	Mapping Central α -Helix Linker Mediated Conformational Transition Pathway of Calmodulin via Simple Computational Approach. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9677-9685.	2.6	16
166	Hybridization Chain Reaction Amplification of MicroRNA Detection with a Tetrahedral DNA Nanostructure-Based Electrochemical Biosensor. <i>Analytical Chemistry</i> , 2014, 86, 2124-2130.	6.5	460
167	Size-Dependent Programming of the Dynamic Range of Graphene Oxide-DNA Interaction-Based Ion Sensors. <i>Analytical Chemistry</i> , 2014, 86, 4047-4051.	6.5	63
168	Crowdsourcing Yields a New Standard for Kinks in Protein Helices. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2585-2593.	5.4	7
169	Discovery of N-substituted 3-arylisquinolone derivatives as antitumor agents originating from O-substituted 3-arylisquinolines via [2,3] or [3,3] rearrangement. <i>European Journal of Medicinal Chemistry</i> , 2014, 77, 204-210.	5.5	11
170	Fragment-based modeling of membrane protein loops: Successes, failures, and prospects for the future. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 175-186.	2.6	15
171	Encapsulation of curcumin within poly(amidoamine) dendrimers for delivery to cancer cells. <i>Journal of Materials Science: Materials in Medicine</i> , 2013, 24, 2137-2144.	3.6	49
172	Biodistribution and pulmonary toxicity of intratracheally instilled graphene oxide in mice. <i>NPG Asia Materials</i> , 2013, 5, e44-e44.	7.9	125
173	Mobile computing - A green computing resource. , 2013, , .		35
174	Antibody i-Patch prediction of the antibody binding site improves rigid local antibody-antigen docking. <i>Protein Engineering, Design and Selection</i> , 2013, 26, 621-629.	2.1	80
175	Molecular dynamics simulation indicating cold denaturation of β -hairpins. <i>Journal of Chemical Physics</i> , 2013, 138, 085102.	3.0	10
176	The universality of β -hairpin misfolding indicated by molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2013, 139, 165103.	3.0	9
177	Graphene Oxide-Based Antibacterial Cotton Fabrics. <i>Advanced Healthcare Materials</i> , 2013, 2, 1259-1266.	7.6	207
178	Pattern Recognition Analysis of Proteins Using DNA-Decorated Catalytic Gold Nanoparticles. <i>Small</i> , 2013, 9, 2844-2849.	10.0	59
179	Smart Drug Delivery Nanocarriers with Self-Assembled DNA Nanostructures. <i>Advanced Materials</i> , 2013, 25, 4386-4396.	21.0	378
180	Scaffolded biosensors with designed DNA nanostructures. <i>NPG Asia Materials</i> , 2013, 5, e51-e51.	7.9	111

#	ARTICLE	IF	CITATIONS
181	Conjugation of Dexamethasone to C60 for the Design of an Anti-Inflammatory Nanomedicine with Reduced Cellular Apoptosis. <i>ACS Applied Materials & Interfaces</i> , 2013, 5, 5291-5297.	8.0	20
182	Real Time in Vitro Regulation of DNA Methylation Using a 5-Fluorouracil Conjugated DNA-Based Stimuli-Responsive Platform. <i>ACS Applied Materials & Interfaces</i> , 2013, 5, 2604-2609.	8.0	7
183	ABangle: characterising the VH-VL orientation in antibodies. <i>Protein Engineering, Design and Selection</i> , 2013, 26, 611-620.	2.1	105
184	Memoir: template-based structure prediction for membrane proteins. <i>Nucleic Acids Research</i> , 2013, 41, W379-W383.	14.5	38
185	Characterization of the Interaction of Sclerostin with the Low Density Lipoprotein Receptor-related Protein (LRP) Family of Wnt Co-receptors. <i>Journal of Biological Chemistry</i> , 2012, 287, 26464-26477.	3.4	77
186	Enhanced sampling molecular dynamics simulation captures experimentally suggested intermediate and unfolded states in the folding pathway of Trp-cage miniprotein. <i>Journal of Chemical Physics</i> , 2012, 137, 125103.	3.0	40
187	Combining modelling and mutagenesis studies of synaptic vesicle protein 2A to identify a series of residues involved in racetam binding. <i>Biochemical Society Transactions</i> , 2011, 39, 1341-1347.	3.4	22
188	Analysis and Modeling of the Variable Region of Camelid Single-Domain Antibodies. <i>Journal of Immunology</i> , 2011, 186, 6357-6367.	0.8	75
189	Environment specific substitution tables improve membrane protein alignment. <i>Bioinformatics</i> , 2011, 27, i15-i23.	4.1	20
190	MEDELLER: homology-based coordinate generation for membrane proteins. <i>Bioinformatics</i> , 2010, 26, 2833-2840.	4.1	103
191	iMembrane: homology-based membrane-insertion of proteins. <i>Bioinformatics</i> , 2009, 25, 1086-1088.	4.1	29
192	High Resolution NMR-based Model for the Structure of a scFv-IL-1 β Complex. <i>Journal of Biological Chemistry</i> , 2009, 284, 31928-31935.	3.4	40
193	DDBASE2.0: updated domain database with improved identification of structural domains. <i>Bioinformatics</i> , 2003, 19, 1760-1764.	4.1	11
194	FUGUE: sequence-structure homology recognition using environment-specific substitution tables and structure-dependent gap penalties. Edited by B. Honig. <i>Journal of Molecular Biology</i> , 2001, 310, 243-257.	4.2	1,185
195	The role of the TolC family in protein transport and multidrug efflux. <i>FEBS Journal</i> , 2001, 268, 5011-5026.	0.2	85
196	HOMSTRAD: adding sequence information to structure-based alignments of homologous protein families. <i>Bioinformatics</i> , 2001, 17, 748-749.	4.1	49
197	Evolutionary trace analysis of TGF- β and related growth factors: implications for site-directed mutagenesis. <i>Protein Engineering, Design and Selection</i> , 2000, 13, 839-847.	2.1	130
198	Accelerating Mobile-Cloud Computing. <i>Advances in Systems Analysis, Software Engineering, and High Performance Computing Book Series</i> , 0, , 175-197.	0.5	14

#	ARTICLE	IF	CITATIONS
199	Investigating the potential for a limited quantum speedup on protein lattice problems. <i>New Journal of Physics</i> , 0, , .	2.9	6
200	Volunteer Computing on Mobile Devices. <i>Advances in Wireless Technologies and Telecommunication Book Series</i> , 0, , 153-181.	0.4	11
201	Directing Multivalent Aptamerâ€Receptor Binding on the Cell Surface with Programmable Atomâ€Like Nanoparticles. <i>Angewandte Chemie</i> , 0, , .	2.0	2