

Jiye Shi

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/7002825/jiye-shi-publications-by-year.pdf>

Version: 2024-04-19

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

196
papers

9,577
citations

50
h-index

92
g-index

215
ext. papers

11,418
ext. citations

8.6
avg, IF

6.24
L-index

#	Paper	IF	Citations
196	Benzyl-rich ligand engineering of the photostability of atomically precise gold nanoclusters.. <i>Chemical Communications</i> , 2022 ,	5.8	1
195	Recent Advances in Prescribing Chiral Plasmonics with DNA Frameworks. <i>ChemNanoMat</i> , 2022 , 8,	3.5	0
194	Water-Dispersible Gold Nanoclusters: Synthesis Strategies, Optical Properties, and Biological Applications. <i>Chemistry - A European Journal</i> , 2021 , e202103736	4.8	0
193	Nanomechanical Induction of Autophagy-Related Fluorescence in Single Cells with Atomic Force Microscopy. <i>Advanced Science</i> , 2021 , 8, e2102989	13.6	2
192	Public Baseline and shared response structures support the theory of antibody repertoire functional commonality. <i>PLoS Computational Biology</i> , 2021 , 17, e1008781	5	8
191	Membrane Interactions of β -Synuclein Revealed by Multiscale Molecular Dynamics Simulations, Markov State Models, and NMR. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 2929-2941	3.4	1
190	The Promise of AI for DILI Prediction. <i>Frontiers in Artificial Intelligence</i> , 2021 , 4, 638410	3	6
189	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	9.5	12
188	Modulating Target Protein Biology Through the Re-mapping of Conformational Distributions Using Small Molecules. <i>Frontiers in Chemistry</i> , 2021 , 9, 668186	5	1
187	Biocomputing Based on DNA Strand Displacement Reactions. <i>ChemPhysChem</i> , 2021 , 22, 1151-1166	3.2	7
186	Remote Photothermal Control of DNA Origami Assembly in Cellular Environments. <i>Nano Letters</i> , 2021 , 21, 5834-5841	11.5	3
185	Encoding Fluorescence Anisotropic Barcodes with DNA Frameworks. <i>Journal of the American Chemical Society</i> , 2021 , 143, 10735-10742	16.4	6
184	Probing Transient DNA Conformation Changes with an Intercalative Fluorescent Excimer. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 6624-6630	16.4	2
183	Programming folding cooperativity of the dimeric i-motif with DNA frameworks for sensing small pH variations. <i>Chemical Communications</i> , 2021 , 57, 3247-3250	5.8	5
182	Ab-Ligity: identifying sequence-dissimilar antibodies that bind to the same epitope. <i>MAbs</i> , 2021 , 13, 1873-1878	14.8	9
181	Probing Transient DNA Conformation Changes with an Intercalative Fluorescent Excimer. <i>Angewandte Chemie</i> , 2021 , 133, 6698-6704	3.6	
180	Cryogenic Electron Microscopy for Resolving DNA Nanostructures and Their Complexes. <i>Small Structures</i> , 2021 , 2, 2100053	8.7	1

179	Reconstructing Soma-Soma Synapse-like Vesicular Exocytosis with DNA Origami. <i>ACS Central Science</i> , 2021 , 7, 1400-1407	16.8	6
178	The Chemical Synthesis of Knob Domain Antibody Fragments. <i>ACS Chemical Biology</i> , 2021 , 16, 1757-1769	4.9	4
177	Programming cell communications with pH-responsive DNA nanodevices. <i>Chemical Communications</i> , 2021 , 57, 4536-4539	5.8	4
176	The prospects of quantum computing in computational molecular biology. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021 , 11, e1481	7.9	28
175	Driving DNA Origami Assembly with a Terahertz Wave.. <i>Nano Letters</i> , 2021 ,	11.5	5
174	Programming Switchable Transcription of Topologically Constrained DNA. <i>Journal of the American Chemical Society</i> , 2020 , 142, 10739-10746	16.4	20
173	Encapsulation and release of living tumor cells using hydrogels with the hybridization chain reaction. <i>Nature Protocols</i> , 2020 , 15, 2163-2185	18.8	25
172	TCRBuilder: multi-state T-cell receptor structure prediction. <i>Bioinformatics</i> , 2020 , 36, 3580-3581	7.2	4
171	DNA Origami-Enabled Engineering of Ligand-Drug Conjugates for Targeted Drug Delivery. <i>Small</i> , 2020 , 16, e1904857	11	25
170	A DNA tetrahedral structure-mediated ultrasensitive fluorescent microarray platform for nucleic acid test. <i>Sensors and Actuators B: Chemical</i> , 2020 , 321, 128538	8.5	13
169	Programming bulk enzyme heterojunctions for biosensor development with tetrahedral DNA framework. <i>Nature Communications</i> , 2020 , 11, 838	17.4	44
168	Exploring Conformational Change of Adenylate Kinase by Replica Exchange Molecular Dynamic Simulation. <i>Biophysical Journal</i> , 2020 , 118, 1009-1018	2.9	11
167	Implementing digital computing with DNA-based switching circuits. <i>Nature Communications</i> , 2020 , 11, 121	17.4	50
166	Blood exposure to graphene oxide may cause anaphylactic death in non-human primates. <i>Nano Today</i> , 2020 , 35, 100922	17.9	16
165	Programmable Live-Cell CRISPR Imaging with Toehold-Switch-Mediated Strand Displacement. <i>Angewandte Chemie</i> , 2020 , 132, 20793-20799	3.6	5
164	Programmable Live-Cell CRISPR Imaging with Toehold-Switch-Mediated Strand Displacement. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 20612-20618	16.4	19
163	Computational study of the substituent effect of halogenated fused-ring heteroaromatics on halogen bonding. <i>Journal of Molecular Modeling</i> , 2020 , 26, 270	2	2
162	DNA Framework-Supported Electrochemical Analysis of DNA Methylation for Prostate Cancers. <i>Nano Letters</i> , 2020 , 20, 7028-7035	11.5	9

161	Thera-SAbDab: the Therapeutic Structural Antibody Database. <i>Nucleic Acids Research</i> , 2020 , 48, D383-D388	3.1	34
160	Halogen bonding in differently charged complexes: basic profile, essential interaction terms and intrinsic Ehole. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 15106-15119	3.6	25
159	An Intelligent DNA Nanorobot with Enhanced Protein Lysosomal Degradation of HER2. <i>Nano Letters</i> , 2019 , 19, 4505-4517	11.5	91
158	Improving the accuracy of predicting protein-ligand binding-free energy with semiempirical quantum chemistry charge. <i>Future Medicinal Chemistry</i> , 2019 , 11, 303-321	4.1	9
157	Underestimated Noncovalent Interactions in Protein Data Bank. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 3389-3399	6.1	10
156	Fractal Nanoplasmonic Labels for Supermultiplex Imaging in Single Cells. <i>Journal of the American Chemical Society</i> , 2019 , 141, 11938-11946	16.4	23
155	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	6.1	19
154	B-cell epitopes: Discontinuity and conformational analysis. <i>Molecular Immunology</i> , 2019 , 114, 643-650	4.3	9
153	Programming chain-growth copolymerization of DNA hairpin tiles for in-vitro hierarchical supramolecular organization. <i>Nature Communications</i> , 2019 , 10, 1006	17.4	18
152	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	11.5	109
151	DNA origami cryptography for secure communication. <i>Nature Communications</i> , 2019 , 10, 5469	17.4	36
150	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	3.9	7
149	Programming biosensing sensitivity by controlling the dimension of nanostructured electrode. <i>Analytical and Bioanalytical Chemistry</i> , 2019 , 411, 4085-4092	4.4	3
148	Solving mazes with single-molecule DNA navigators. <i>Nature Materials</i> , 2019 , 18, 273-279	27	121
147	Poly-adenine-mediated spherical nucleic acids for strand displacement-based DNA/RNA detection. <i>Biosensors and Bioelectronics</i> , 2019 , 127, 85-91	11.8	23
146	Molecular Threading-Dependent Mass Transport in Paper Origami for Single-Step Electrochemical DNA Sensors. <i>Nano Letters</i> , 2019 , 19, 369-374	11.5	26
145	Systematic Study in Mammalian Cells Showing No Adverse Response to Tetrahedral DNA Nanostructure. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 15442-15448	9.5	31
144	Computational Exploration of Conformational Transitions in Protein Drug Targets. <i>Methods in Molecular Biology</i> , 2018 , 1762, 339-365	1.4	1

143	Valency-Controlled Framework Nucleic Acid Signal Amplifiers. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 7131-7135	16.4	70
142	Valency-Controlled Framework Nucleic Acid Signal Amplifiers. <i>Angewandte Chemie</i> , 2018 , 130, 7249-7253	3.6	5
141	MoS Nanoprobe for MicroRNA Quantification Based on Duplex-Specific Nuclease Signal Amplification. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 7852-7858	9.5	58
140	Nanoscale delivery systems for cancer immunotherapy. <i>Materials Horizons</i> , 2018 , 5, 344-362	14.4	43
139	Antibody side chain conformations are position-dependent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018 , 86, 383-392	4.2	12
138	Inhibition of Epithelial-Mesenchymal Transition and Tissue Regeneration by Waterborne Titanium Dioxide Nanoparticles. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 3449-3458	9.5	14
137	Targeted Imaging of Brain Tumors with a Framework Nucleic Acid Probe. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 3414-3420	9.5	50
136	MoS ₂ @Au@Pt nano hybrids as a sensing platform for electrochemical nonenzymatic glucose detection. <i>New Journal of Chemistry</i> , 2018 , 42, 6750-6755	3.6	28
135	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	3.6	14
134	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	16.4	48
133	Structurally Mapping Antibody Repertoires. <i>Frontiers in Immunology</i> , 2018 , 9, 1698	8.4	25
132	Inhibiting Methicillin-Resistant Staphylococcus aureus by Tetrahedral DNA Nanostructure-Enabled Antisense Peptide Nucleic Acid Delivery. <i>Nano Letters</i> , 2018 , 18, 5652-5659	11.5	82
131	Guiding protein delivery into live cells using DNA-programmed membrane fusion. <i>Chemical Science</i> , 2018 , 9, 5967-5975	9.4	39
130	Deciphering active biocompatibility of iron oxide nanoparticles from their intrinsic antagonism. <i>Nano Research</i> , 2018 , 11, 2746-2755	10	30
129	DNA origami nanostructures can exhibit preferential renal uptake and alleviate acute kidney injury. <i>Nature Biomedical Engineering</i> , 2018 , 2, 865-877	19	184
128	Hydrogen Sulfide-Activatable Second Near-Infrared Fluorescent Nanoassemblies for Targeted Photothermal Cancer Therapy. <i>Nano Letters</i> , 2018 , 18, 6411-6416	11.5	115
127	Graphene oxide-silver nanocomposites modulate biofilm formation and extracellular polymeric substance (EPS) production. <i>Nanoscale</i> , 2018 , 10, 19603-19611	7.7	30
126	Nanodiamond autophagy inhibitor allosterically improves the arsenical-based therapy of solid tumors. <i>Nature Communications</i> , 2018 , 9, 4347	17.4	52

- 125 Serum protein corona-responsive autophagy tuning in cells. *Nanoscale*, **2018**, 10, 18055-18063 7.7 19
- 124 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 6.11
- 123 Determining Protein Folding Pathway and Associated Energetics through Partitioned Integrated-Tempering-Sampling Simulation. *Journal of Chemical Theory and Computation*, **2017**, 13, 1229-1243 6.15
- 122 Computational design of an epitope-specific Keap1 binding antibody using hotspot residues grafting and CDR loop swapping. *Scientific Reports*, **2017**, 7, 41306 4.9 15
- 121 An Exonuclease III-Powered, On-Particle Stochastic DNA Walker. *Angewandte Chemie - International Edition*, **2017**, 56, 1855-1858 16.4 248
- 120 Multicolor Gold-Silver Nano-Mushrooms as Ready-to-Use SERS Probes for Ultrasensitive and Multiplex DNA/miRNA Detection. *Analytical Chemistry*, **2017**, 89, 2531-2538 7.8 161
- 119 Yolk-shell nanostructured FeO@C magnetic nanoparticles with enhanced peroxidase-like activity for label-free colorimetric detection of HO and glucose. *Nanoscale*, **2017**, 9, 4508-4515 7.7 136
- 118 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 4.9 10
- 117 The Inhibition Effect of Graphene Oxide Nanosheets on the Development of Streptococcus mutans Biofilms. *Particle and Particle Systems Characterization*, **2017**, 34, 1700001 3.1 18
- 116 Graphene Nanoprobes for Real-Time Monitoring of Isothermal Nucleic Acid Amplification. *ACS Applied Materials & Interfaces*, **2017**, 9, 15245-15253 9.5 20
- 115 DNA-Origami-Based Assembly of Anisotropic Plasmonic Gold Nanostructures. *Small*, **2017**, 13, 1603991 11 30
- 114 Design, Synthesis, and Structure-Activity Relationships of Bavachinin Analogues as Peroxisome Proliferator-Activated Receptor α Agonists. *ChemMedChem*, **2017**, 12, 183-193 3.7 12
- 113 Cavity-Type DNA Origami-Based Plasmonic Nanostructures for Raman Enhancement. *ACS Applied Materials & Interfaces*, **2017**, 9, 21942-21948 9.5 13
- 112 Real-Time Imaging of Endocytosis and Intracellular Trafficking of Semiconducting Polymer Dots. *ACS Applied Materials & Interfaces*, **2017**, 9, 21200-21208 9.5 27
- 111 Preservation of DNA Nanostructure Carriers: Effects of Freeze-Thawing and Ionic Strength during Lyophilization and Storage. *ACS Applied Materials & Interfaces*, **2017**, 9, 18434-18439 9.5 13
- 110 Real-time visualization of clustering and intracellular transport of gold nanoparticles by correlative imaging. *Nature Communications*, **2017**, 8, 15646 17.4 116
- 109 An Exonuclease III-Powered, On-Particle Stochastic DNA Walker. *Angewandte Chemie*, **2017**, 129, 1881-1884 9.31
- 108 The H3 loop of antibodies shows unique structural characteristics. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 1311-1318 4.2 52

107	Catalysis-Driven Self-Thermophoresis of Janus Plasmonic Nanomotors. <i>Angewandte Chemie</i> , 2017 , 129, 530-533	3.6	17
106	Catalysis-Driven Self-Thermophoresis of Janus Plasmonic Nanomotors. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 515-518	16.4	70
105	Energetics and structural characterization of the "DFG-flip" conformational transition of B-RAF kinase: a SITS molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 1257-1267	3.6	13
104	Label-Free Electrochemical Sensing Platform for MicroRNA-21 Detection Using Thionine and Gold Nanoparticles Co-Functionalized MoS Nanosheet. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 35597-35603 ¹⁰⁴	9.5	23
103	PCR-Free Colorimetric DNA Hybridization Detection Using a 3D DNA Nanostructured Reporter Probe. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 38281-38287	9.5	23
102	Sphinx: merging knowledge-based and ab initio approaches to improve protein loop prediction. <i>Bioinformatics</i> , 2017 , 33, 1346-1353	7.2	25
101	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	9.5	14
100	DNA-Encoded Raman-Active Anisotropic Nanoparticles for microRNA Detection. <i>Analytical Chemistry</i> , 2017 , 89, 9850-9856	7.8	67
99	Structural insights into HIV-1 protease flap opening processes and key intermediates. <i>RSC Advances</i> , 2017 , 7, 45121-45128	3.7	12
98	Real-Time Continuous Identification of Greenhouse Plant Pathogens Based on Recyclable Microfluidic Bioassay System. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 31568-31575	9.5	18
97	Programming Cell Adhesion for On-Chip Sequential Boolean Logic Functions. <i>Journal of the American Chemical Society</i> , 2017 , 139, 10176-10179	16.4	85
96	Humidity-Responsive Single-Nanoparticle-Layer Plasmonic Films. <i>Advanced Materials</i> , 2017 , 29, 160679624	24	21
95	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	11.5	144
94	Recognizing single phospholipid vesicle collisions on carbon fiber nanoelectrode. <i>Science China Chemistry</i> , 2017 , 60, 1474-1480	7.9	14
93	Underestimated Halogen Bonds Forming with Protein Backbone in Protein Data Bank. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 1529-1534	6.1	17
92	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	10.3	12
91	Dynamic Modulation of DNA Hybridization Using Allosteric DNA Tetrahedral Nanostructures. <i>Analytical Chemistry</i> , 2016 , 88, 8043-9	7.8	37
90	Electrochemical detection of PCR amplicons of Escherichia coli genome based on DNA nanostructural probes and polyHRP enzyme. <i>Analyst, The</i> , 2016 , 141, 5304-10	5	21

89	One-Shot Immunomodulatory Nanodiamond Agents for Cancer Immunotherapy. <i>Advanced Materials</i> , 2016 , 28, 2699-708	24	85
88	Electrochemical detection of nucleic acids, proteins, small molecules and cells using a DNA-nanostructure-based universal biosensing platform. <i>Nature Protocols</i> , 2016 , 11, 1244-63	18.8	234
87	Thermodynamics calculation of protein-ligand interactions by QM/MM polarizable charge parameters. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016 , 34, 163-76	3.6	24
86	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, 380-3	6.2	24
85	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, 610-20	3.4	40
84	Multiple-Armed Tetrahedral DNA Nanostructures for Tumor-Targeting, Dual-Modality in Vivo Imaging. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 4378-84	9.5	110
83	Facile Synthesis of Substituted 4-Alkoxy-2-oxazolines and Exploration of the Reaction Mechanism. <i>Synthesis</i> , 2016 , 48, 1331-1343	2.9	4
82	Length-independent structural similarities enrich the antibody CDR canonical class model. <i>MAbs</i> , 2016 , 8, 751-60	6.6	30
81	DNA orientation-specific adhesion and patterning of living mammalian cells on self-assembled DNA monolayers. <i>Chemical Science</i> , 2016 , 7, 2722-2727	9.4	26
80	Activity modulation and allosteric control of a scaffolded DNAzyme using a dynamic DNA nanostructure. <i>Chemical Science</i> , 2016 , 7, 1200-1204	9.4	49
79	Volunteer Computing on Mobile Devices 2016 , 2171-2198		
78	Examining the Conservation of Kinks in Alpha Helices. <i>PLoS ONE</i> , 2016 , 11, e0157553	3.7	17
77	Transfer of Two-Dimensional Oligonucleotide Patterns onto Stereocontrolled Plasmonic Nanostructures through DNA-Origami-Based Nanoimprinting Lithography. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 8036-40	16.4	60
76	ABodyBuilder: Automated antibody structure prediction with data-driven accuracy estimation. <i>MAbs</i> , 2016 , 8, 1259-1268	6.6	104
75	A Surface-Confined Proton-Driven DNA Pump Using a Dynamic 3D DNA Scaffold. <i>Advanced Materials</i> , 2016 , 28, 6860-5	24	70
74	How Do Distance and Solvent Affect Halogen Bonding Involving Negatively Charged Donors?. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8784-93	3.4	18
73	Gold-Nanoparticle-Mediated Jigsaw-Puzzle-like Assembly of Supersized Plasmonic DNA Origami. <i>Angewandte Chemie</i> , 2015 , 127, 3009-3012	3.6	15
72	Cotranscriptionally folded RNA nanostructures pave the way to intracellular nanofabrication. <i>ChemBioChem</i> , 2015 , 16, 39-41	3.8	4

71	Separation and peroxisome proliferator-activated receptor- β agonist activity evaluation of synthetic racemic bavachinin enantiomers. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015 , 25, 2579-83 ^{2.9}	16
70	Alchembed: A Computational Method for Incorporating Multiple Proteins into Complex Lipid Geometries. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 2743-2754	6.4 37
69	DNA-directed assembly of gold nanohalo for quantitative plasmonic imaging of single-particle catalysis. <i>Journal of the American Chemical Society</i> , 2015 , 137, 4292-5	16.4 111
68	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 ^{3.9}	3
67	Nanoplasmonic imaging of latent fingerprints with explosive RDX residues. <i>Analytical Chemistry</i> , 2015 , 87, 9403-7	7.8 40
66	Recent progress in natural products as DPP-4 inhibitors. <i>Future Medicinal Chemistry</i> , 2015 , 7, 1079-89	4.1 39
65	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, 11988-97	3.4 21
64	Constructing Higher-Order DNA Nanoarchitectures with Highly Purified DNA Nanocages. <i>ACS Applied Materials & Interfaces</i> , 2015 , 7, 13174-9	9.5 29
63	Force fields and scoring functions for carbohydrate simulation. <i>Carbohydrate Research</i> , 2015 , 401, 73-81 ^{2.9}	41
62	Reversible Regulation of Catalytic Activity of Gold Nanoparticles with DNA Nanomachines. <i>Scientific Reports</i> , 2015 , 5, 14402	4.9 15
61	Programmable Engineering of a Biosensing Interface with Tetrahedral DNA Nanostructures for Ultrasensitive DNA Detection. <i>Angewandte Chemie</i> , 2015 , 127, 2179-2183	3.6 39
60	Exploring the interaction of SV2A with racetams using homology modelling, molecular dynamics and site-directed mutagenesis. <i>PLoS ONE</i> , 2015 , 10, e0116589	3.7 14
59	Building a better fragment library for de novo protein structure prediction. <i>PLoS ONE</i> , 2015 , 10, e0123998 ^{3.7}	16
58	The Cloudlet Accelerator: Bringing Mobile-Cloud Face Recognition into Real-Time 2015 ,	18
57	Programmable engineering of a biosensing interface with tetrahedral DNA nanostructures for ultrasensitive DNA detection. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 2151-5	16.4 264
56	Unraveling the role of hydrogen peroxide in β -synuclein aggregation using an ultrasensitive nanoplasmonic probe. <i>Analytical Chemistry</i> , 2015 , 87, 1968-73	7.8 31
55	Gold-nanoparticle-mediated jigsaw-puzzle-like assembly of supersized plasmonic DNA origami. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 2966-9	16.4 88
54	Accelerating Mobile-Cloud Computing 2015 , 1933-1955	2

53	Helix kinks are equally prevalent in soluble and membrane proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 1960-70	4.2	52
52	Nanoscale optical probes for cellular imaging. <i>Chemical Society Reviews</i> , 2014 , 43, 2650-61	58.5	166
51	Multi-algorithm and multi-model based drug target prediction and web server. <i>Acta Pharmacologica Sinica</i> , 2014 , 35, 419-31	8	5
50	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, 14223-33	3.4	8
49	SABDab: the structural antibody database. <i>Nucleic Acids Research</i> , 2014 , 42, D1140-6	20.1	193
48	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, 134-43	3.4	49
47	Mapping central α -helix linker mediated conformational transition pathway of calmodulin via simple computational approach. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 9677-85	3.4	13
46	Hybridization chain reaction amplification of microRNA detection with a tetrahedral DNA nanostructure-based electrochemical biosensor. <i>Analytical Chemistry</i> , 2014 , 86, 2124-30	7.8	392
45	Size-dependent programming of the dynamic range of graphene oxide-DNA interaction-based ion sensors. <i>Analytical Chemistry</i> , 2014 , 86, 4047-51	7.8	59
44	Crowdsourcing yields a new standard for kinks in protein helices. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 2585-93	6.1	6
43	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, 204-10	6.8	10
42	Fragment-based modeling of membrane protein loops: successes, failures, and prospects for the future. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 175-86	4.2	7
41	Examining variable domain orientations in antigen receptors gives insight into TCR-like antibody design. <i>PLoS Computational Biology</i> , 2014 , 10, e1003852	5	20
40	Improving B-cell epitope prediction and its application to global antibody-antigen docking. <i>Bioinformatics</i> , 2014 , 30, 2288-94	7.2	86
39	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, 7745-50	16.4	326
38	Single-Particle Tracking and Modulation of Cell Entry Pathways of a Tetrahedral DNA Nanostructure in Live Cells. <i>Angewandte Chemie</i> , 2014 , 126, 7879-7884	3.6	31
37	A bubble-mediated intelligent microscale electrochemical device for single-step quantitative bioassays. <i>Advanced Materials</i> , 2014 , 26, 4671-6	24	87
36	Titelbild: Single-Particle Tracking and Modulation of Cell Entry Pathways of a Tetrahedral DNA Nanostructure in Live Cells (Angew. Chem. 30/2014). <i>Angewandte Chemie</i> , 2014 , 126, 7809-7809	3.6	1

35	Self-assembly of poly-adenine-tailed CpG oligonucleotide-gold nanoparticle nanoconjugates with immunostimulatory activity. <i>Small</i> , 2014 , 10, 368-75	11	79
34	Encapsulation of curcumin within poly(amidoamine) dendrimers for delivery to cancer cells. <i>Journal of Materials Science: Materials in Medicine</i> , 2013 , 24, 2137-44	4.5	37
33	Biodistribution and pulmonary toxicity of intratracheally instilled graphene oxide in mice. <i>NPG Asia Materials</i> , 2013 , 5, e44-e44	10.3	102
32	Mobile computing - A green computing resource 2013 ,		31
31	Antibody i-Patch prediction of the antibody binding site improves rigid local antibody-antigen docking. <i>Protein Engineering, Design and Selection</i> , 2013 , 26, 621-9	1.9	55
30	Molecular dynamics simulation indicating cold denaturation of Ehairpins. <i>Journal of Chemical Physics</i> , 2013 , 138, 085102	3.9	10
29	The universality of Ehairpin misfolding indicated by molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2013 , 139, 165103	3.9	7
28	Graphene oxide-based antibacterial cotton fabrics. <i>Advanced Healthcare Materials</i> , 2013 , 2, 1259-66	10.1	173
27	Pattern recognition analysis of proteins using DNA-decorated catalytic gold nanoparticles. <i>Small</i> , 2013 , 9, 2844-9	11	52
26	Smart drug delivery nanocarriers with self-assembled DNA nanostructures. <i>Advanced Materials</i> , 2013 , 25, 4386-96	24	313
25	Scaffolded biosensors with designed DNA nanostructures. <i>NPG Asia Materials</i> , 2013 , 5, e51-e51	10.3	94
24	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, 5291-7	9.5	18
23	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, 2604-9	9.5	5
22	ABangle: characterising the VH-VL orientation in antibodies. <i>Protein Engineering, Design and Selection</i> , 2013 , 26, 611-20	1.9	69
21	Memoir: template-based structure prediction for membrane proteins. <i>Nucleic Acids Research</i> , 2013 , 41, W379-83	20.1	32
20	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	3.9	36
19	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, 26464-77	5.4	62
18	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, 1341-7	5.1	19

17	Analysis and modeling of the variable region of camelid single-domain antibodies. <i>Journal of Immunology</i> , 2011 , 186, 6357-67	5.3	57
16	Environment specific substitution tables improve membrane protein alignment. <i>Bioinformatics</i> , 2011 , 27, i15-23	7.2	19
15	MEDELLER: homology-based coordinate generation for membrane proteins. <i>Bioinformatics</i> , 2010 , 26, 2833-40	7.2	91
14	iMembrane: homology-based membrane-insertion of proteins. <i>Bioinformatics</i> , 2009 , 25, 1086-8	7.2	28
13	High resolution NMR-based model for the structure of a scFv-IL-1beta complex: potential for NMR as a key tool in therapeutic antibody design and development. <i>Journal of Biological Chemistry</i> , 2009 , 284, 31928-35	5.4	37
12	DDBASE2.0: updated domain database with improved identification of structural domains. <i>Bioinformatics</i> , 2003 , 19, 1760-4	7.2	8
11	The role of the TolC family in protein transport and multidrug efflux. From stereochemical certainty to mechanistic hypothesis. <i>FEBS Journal</i> , 2001 , 268, 5011-26		71
10	HOMSTRAD: adding sequence information to structure-based alignments of homologous protein families. <i>Bioinformatics</i> , 2001 , 17, 748-9	7.2	47
9	FUGUE: sequence-structure homology recognition using environment-specific substitution tables and structure-dependent gap penalties. <i>Journal of Molecular Biology</i> , 2001 , 310, 243-57	6.5	1102
8	Evolutionary trace analysis of TGF-beta and related growth factors: implications for site-directed mutagenesis. <i>Protein Engineering, Design and Selection</i> , 2000 , 13, 839-47	1.9	122
7	Accelerating Mobile-Cloud Computing. <i>Advances in Systems Analysis, Software Engineering, and High Performance Computing Book Series</i> , 175-197	0.4	9
6	Evidence of Antibody Repertoire Functional Convergence through Public Baseline and Shared Response Structures		4
5	Volunteer Computing on Mobile Devices. <i>Advances in Wireless Technologies and Telecommunication Book Series</i> , 153-181	0.2	7
4	A Multi-Crystal Method for Extracting Obscured Signal from Crystallographic Electron Density		5
3	Ab-Ligity: Identifying sequence-dissimilar antibodies that bind to the same epitope		3
2	Investigating the potential for a limited quantum speedup on protein lattice problems. <i>New Journal of Physics</i> ,	2.9	2
1	Phase transferring luminescent gold nanoclusters via single-stranded DNA. <i>Science China Chemistry</i> , 1	7.9	0