

Jeffrey J Gray

List of Publications by Year in descending order

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157
papers

13,755
citations

36203

51
h-index

26548

107
g-index

191
all docs

191
docs citations

191
times ranked

15495
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 1 | Rosetta3. <i>Methods in Enzymology</i> , 2011, 487, 545-574. | 0.4 | 1,620 |
| 2 | The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3031-3048. | 2.3 | 1,032 |
| 3 | Protein-Protein Docking with Simultaneous Optimization of Rigid-body Displacement and Side-chain Conformations. <i>Journal of Molecular Biology</i> , 2003, 331, 281-299. | 2.0 | 1,017 |
| 4 | The interaction of proteins with solid surfaces. <i>Current Opinion in Structural Biology</i> , 2004, 14, 110-115. | 2.6 | 740 |
| 5 | PyRosetta: a script-based interface for implementing molecular modeling algorithms using Rosetta. <i>Bioinformatics</i> , 2010, 26, 689-691. | 1.8 | 601 |
| 6 | Macromolecular modeling and design in Rosetta: recent methods and frameworks. <i>Nature Methods</i> , 2020, 17, 665-680. | 9.0 | 513 |
| 7 | The RosettaDock server for local protein-protein docking. <i>Nucleic Acids Research</i> , 2008, 36, W233-W238. | 6.5 | 508 |
| 8 | Serverification of Molecular Modeling Applications: The Rosetta Online Server That Includes Everyone (ROSIE). <i>PLoS ONE</i> , 2013, 8, e63906. | 1.1 | 348 |
| 9 | A Comprehensive, High-Resolution Map of a Gene's Fitness Landscape. <i>Molecular Biology and Evolution</i> , 2014, 31, 1581-1592. | 3.5 | 291 |
| 10 | Benchmarking and Analysis of Protein Docking Performance in Rosetta v3.2. <i>PLoS ONE</i> , 2011, 6, e22477. | 1.1 | 272 |
| 11 | Modeling and docking of antibody structures with Rosetta. <i>Nature Protocols</i> , 2017, 12, 401-416. | 5.5 | 236 |
| 12 | Toward high-resolution homology modeling of antibody F _v regions and application to antibody-antigen docking. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 74, 497-514. | 1.5 | 198 |
| 13 | Scientific Benchmarks for Guiding Macromolecular Energy Function Improvement. <i>Methods in Enzymology</i> , 2013, 523, 109-143. | 0.4 | 195 |
| 14 | Large-scale sequence and structural comparisons of human naive and antigen-experienced antibody repertoires. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E2636-45. | 3.3 | 179 |
| 15 | High-resolution protein-protein docking. <i>Current Opinion in Structural Biology</i> , 2006, 16, 183-193. | 2.6 | 176 |
| 16 | Targeting the CoREST complex with dual histone deacetylase and demethylase inhibitors. <i>Nature Communications</i> , 2018, 9, 53. | 5.8 | 175 |
| 17 | RosettaAntibody: antibody variable region homology modeling server. <i>Nucleic Acids Research</i> , 2009, 37, W474-W479. | 6.5 | 157 |
| 18 | Conformer Selection and Induced Fit in Flexible Backbone Protein-Protein Docking Using Computational and NMR Ensembles. <i>Journal of Molecular Biology</i> , 2008, 381, 1068-1087. | 2.0 | 152 |

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|----|---|-----|-----------|
| 19 | Phosphorylation-dependent inhibition of mineralization by osteopontin ASARM peptides is regulated by PHEX cleavage. <i>Journal of Bone and Mineral Research</i> , 2010, 25, 695-705. | 3.1 | 151 |
| 20 | Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 323-348. | 1.5 | 148 |
| 21 | An Integrated Framework Advancing Membrane Protein Modeling and Design. <i>PLoS Computational Biology</i> , 2015, 11, e1004398. | 1.5 | 145 |
| 22 | SnugDock: Paratope Structural Optimization during Antibody-Antigen Docking Compensates for Errors in Antibody Homology Models. <i>PLoS Computational Biology</i> , 2010, 6, e1000644. | 1.5 | 139 |
| 23 | Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. <i>Journal of Molecular Biology</i> , 2011, 414, 289-302. | 2.0 | 131 |
| 24 | Chiral acidic amino acids induce chiral hierarchical structure in calcium carbonate. <i>Nature Communications</i> , 2017, 8, 15066. | 5.8 | 129 |
| 25 | Structure-Based Design of Supercharged, Highly Thermoresistant Antibodies. <i>Chemistry and Biology</i> , 2012, 19, 449-455. | 6.2 | 127 |
| 26 | Efficient flexible backbone protein-protein docking for challenging targets. <i>Bioinformatics</i> , 2018, 34, 3461-3469. | 1.8 | 121 |
| 27 | Deep Learning in Protein Structural Modeling and Design. <i>Patterns</i> , 2020, 1, 100142. | 3.1 | 119 |
| 28 | Functional Loss of Semaphorin 3C and/or Semaphorin 3D and Their Epistatic Interaction with Ret Are Critical to Hirschsprung Disease Liability. <i>American Journal of Human Genetics</i> , 2015, 96, 581-596. | 2.6 | 118 |
| 29 | Structure Prediction of Protein-Solid Surface Interactions Reveals a Molecular Recognition Motif of Statherin for Hydroxyapatite. <i>Journal of the American Chemical Society</i> , 2007, 129, 13713-13722. | 6.6 | 114 |
| 30 | Enzyme Replacement Therapy Prevents Dental Defects in a Model of Hypophosphatasia. <i>Journal of Dental Research</i> , 2011, 90, 470-476. | 2.5 | 106 |
| 31 | Antibody structure prediction using interpretable deep learning. <i>Patterns</i> , 2022, 3, 100406. | 3.1 | 106 |
| 32 | Local motions in a benchmark of allosteric proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 67, 385-399. | 1.5 | 103 |
| 33 | Protein-protein docking predictions for the CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 52, 118-122. | 1.5 | 102 |
| 34 | Allosteric Communication Occurs via Networks of Tertiary and Quaternary Motions in Proteins. <i>PLoS Computational Biology</i> , 2009, 5, e1000293. | 1.5 | 98 |
| 35 | Blind prediction performance of RosettaAntibody 3.0: Grafting, relaxation, kinematic loop modeling, and full CDR optimization. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1611-1623. | 1.5 | 91 |
| 36 | Contact rearrangements form coupled networks from local motions in allosteric proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 455-466. | 1.5 | 89 |

| # | ARTICLE | IF | CITATIONS |
|----|---|-----|-----------|
| 37 | Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 1980-1987. | 1.5 | 87 |
| 38 | Computational modeling of membrane proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 1-24. | 1.5 | 86 |
| 39 | Nanostructure, osteopontin, and mechanical properties of calcitic avian eggshell. <i>Science Advances</i> , 2018, 4, eaar3219. | 4.7 | 86 |
| 40 | The Origin of CDR H3 Structural Diversity. <i>Structure</i> , 2015, 23, 302-311. | 1.6 | 78 |
| 41 | Analysis and Modeling of the Variable Region of Camelid Single-Domain Antibodies. <i>Journal of Immunology</i> , 2011, 186, 6357-6367. | 0.4 | 75 |
| 42 | Prediction of protein assemblies, the next frontier: The <sc>CASP14</sc> CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 1800-1823. | 1.5 | 73 |
| 43 | Alternative Computational Protocols for Supercharging Protein Surfaces for Reversible Unfolding and Retention of Stability. <i>PLoS ONE</i> , 2013, 8, e64363. | 1.1 | 73 |
| 44 | Shape complementarity and hydrogen bond preferences in protein-protein interfaces: implications for antibody modeling and protein-protein docking. <i>Bioinformatics</i> , 2016, 32, 2451-2456. | 1.8 | 70 |
| 45 | An expanded benchmark for antibody-antigen docking and affinity prediction reveals insights into antibody recognition determinants. <i>Structure</i> , 2021, 29, 606-621.e5. | 1.6 | 65 |
| 46 | Rapid Calculation of Protein pKa Values Using Rosetta. <i>Biophysical Journal</i> , 2012, 103, 587-595. | 0.2 | 61 |
| 47 | Plasma Cells Are the Most Abundant Gluten Peptide MHC-expressing Cells in Inflamed Intestinal Tissues From Patients With Celiac Disease. <i>Gastroenterology</i> , 2019, 156, 1428-1439.e10. | 0.6 | 61 |
| 48 | Modulation of Calcium Oxalate Dihydrate Growth by Selective Crystal-face Binding of Phosphorylated Osteopontin and Polyaspartate Peptide Showing Occlusion by Sectoral (Compositional) Zoning. <i>Journal of Biological Chemistry</i> , 2009, 284, 23491-23501. | 1.6 | 60 |
| 49 | Structural Diversity in the Type IV Pili of Multidrug-resistant <i>Acinetobacter</i> . <i>Journal of Biological Chemistry</i> , 2016, 291, 22924-22935. | 1.6 | 60 |
| 50 | Adding Diverse Noncanonical Backbones to Rosetta: Enabling Peptidomimetic Design. <i>PLoS ONE</i> , 2013, 8, e67051. | 1.1 | 59 |
| 51 | Protein Structure Prediction and Design in a Biologically Realistic Implicit Membrane. <i>Biophysical Journal</i> , 2020, 118, 2042-2055. | 0.2 | 59 |
| 52 | Real-Time PyMOL Visualization for Rosetta and PyRosetta. <i>PLoS ONE</i> , 2011, 6, e21931. | 1.1 | 55 |
| 53 | Solution- and Adsorbed-State Structural Ensembles Predicted for the Statherin-Hydroxyapatite System. <i>Biophysical Journal</i> , 2009, 96, 3082-3091. | 0.2 | 54 |
| 54 | Acidic C-terminal domains autoregulate the RNA chaperone Hfq. <i>ELife</i> , 2017, 6, . | 2.8 | 53 |

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|----|---|-----|-----------|
| 55 | CAPRI rounds 3-5 reveal promising successes and future challenges for RosettaDock. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 60, 181-186. | 1.5 | 52 |
| 56 | Structural Model of the mAb 806-EGFR Complex Using Computational Docking followed by Computational and Experimental Mutagenesis. <i>Structure</i> , 2006, 14, 401-414. | 1.6 | 52 |
| 57 | Improved prediction of antibody V _L –V _H orientation. <i>Protein Engineering, Design and Selection</i> , 2016, 29, 409-418. | 1.0 | 52 |
| 58 | De Novo Design of Peptide–Calcite Biom mineralization Systems. <i>Journal of the American Chemical Society</i> , 2010, 132, 12252-12262. | 6.6 | 51 |
| 59 | Enzymatic Excision of Uracil Residues in Nucleosomes Depends on the Local DNA Structure and Dynamics. <i>Biochemistry</i> , 2012, 51, 6028-6038. | 1.2 | 50 |
| 60 | Blind prediction of interfacial water positions in CAPRI. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 620-632. | 1.5 | 50 |
| 61 | Geometric potentials from deep learning improve prediction of CDR H3 loop structures. <i>Bioinformatics</i> , 2020, 36, i268-i275. | 1.8 | 48 |
| 62 | Web-accessible molecular modeling with Rosetta: The Rosetta Online Server that Includes Everyone (ROSIE). <i>Protein Science</i> , 2018, 27, 259-268. | 3.1 | 47 |
| 63 | A generalized approach to sampling backbone conformations with RosettaDock for CAPRI rounds 13–19. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 3115-3123. | 1.5 | 46 |
| 64 | Pushing the Backbone in Protein-Protein Docking. <i>Structure</i> , 2016, 24, 1821-1829. | 1.6 | 46 |
| 65 | Accurate Structure Prediction of CDR H3 Loops Enabled by a Novel Structure-Based C-Terminal Constraint. <i>Journal of Immunology</i> , 2017, 198, 505-515. | 0.4 | 43 |
| 66 | Partial High-Resolution Structure of Phosphorylated and Non-phosphorylated Leucine-Rich Amelogenin Protein Adsorbed to Hydroxyapatite. <i>Journal of Physical Chemistry C</i> , 2011, 115, 13775-13785. | 1.5 | 42 |
| 67 | Adsorption of colloidal particles by Brownian dynamics simulation: Kinetics and surface structures. <i>Journal of Chemical Physics</i> , 2001, 114, 1366-1381. | 1.2 | 41 |
| 68 | Residue-centric modeling and design of saccharide and glycoconjugate structures. <i>Journal of Computational Chemistry</i> , 2017, 38, 276-287. | 1.5 | 41 |
| 69 | Chiral switching in biomineral suprastructures induced by homochiral α -amino acid. <i>Science Advances</i> , 2018, 4, eaas9819. | 4.7 | 41 |
| 70 | Advances to tackle backbone flexibility in protein docking. <i>Current Opinion in Structural Biology</i> , 2021, 67, 178-186. | 2.6 | 41 |
| 71 | Repertoire Analysis of Antibody CDR-H3 Loops Suggests Affinity Maturation Does Not Typically Result in Rigidification. <i>Frontiers in Immunology</i> , 2018, 9, 413. | 2.2 | 39 |
| 72 | Incorporating biochemical information and backbone flexibility in RosettaDock for CAPRI rounds 6–12. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 793-800. | 1.5 | 37 |

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|----|--|-----|-----------|
| 73 | Structure-based cross-docking analysis of antibody-antigen interactions. <i>Scientific Reports</i> , 2017, 7, 8145. | 1.6 | 37 |
| 74 | Toward a Structure Determination Method for Biomineral-Associated Protein Using Combined Solid-State NMR and Computational Structure Prediction. <i>Structure</i> , 2010, 18, 1678-1687. | 1.6 | 36 |
| 75 | Identification of Structural Mechanisms of HIV-1 Protease Specificity Using Computational Peptide Docking: Implications for Drug Resistance. <i>Structure</i> , 2009, 17, 1636-1648. | 1.6 | 34 |
| 76 | Modeling the structure of mAb 14B7 bound to the anthrax protective antigen. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 218-230. | 1.5 | 32 |
| 77 | Expanding the toolkit for membrane protein modeling in Rosetta. <i>Bioinformatics</i> , 2017, 33, 754-756. | 1.8 | 32 |
| 78 | Applying Linear Interaction Energy Method for Rational Design of Noncompetitive Allosteric Inhibitors of the Sarco- and Endoplasmic Reticulum Calcium-ATPase. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 3005-3014. | 2.9 | 31 |
| 79 | Targeted DNA Methylation Using an Artificially Bisected M.HhaI Fused to Zinc Fingers. <i>PLoS ONE</i> , 2012, 7, e44852. | 1.1 | 30 |
| 80 | Microstructure Formation and Kinetics in the Random Sequential Adsorption of Polydisperse Tethered Nanoparticles Modeled as Hard Disks. <i>Langmuir</i> , 2001, 17, 2317-2328. | 1.6 | 28 |
| 81 | Neutron Reflectometry Studies of the Adsorbed Structure of the Amelogenin, LRAP. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3098-3109. | 1.2 | 28 |
| 82 | Rheology and dynamics of sheared arrays of colloidal particles. <i>Journal of Rheology</i> , 1998, 42, 1121-1151. | 1.3 | 27 |
| 83 | Better together: Elements of successful scientific software development in a distributed collaborative community. <i>PLoS Computational Biology</i> , 2020, 16, e1007507. | 1.5 | 27 |
| 84 | Using the RosettaSurface Algorithm to Predict Protein Structure at Mineral Surfaces. <i>Methods in Enzymology</i> , 2013, 532, 343-366. | 0.4 | 25 |
| 85 | Nonequilibrium Phase Behavior during the Random Sequential Adsorption of Tethered Hard Disks. <i>Physical Review Letters</i> , 2000, 85, 4430-4433. | 2.9 | 23 |
| 86 | Structurally distinct toxicity inhibitors bind at common loci on β -amyloid fibril. <i>Protein Science</i> , 2010, 19, 2291-2304. | 3.1 | 23 |
| 87 | Extending RosettaDock with water, sugar, and pH for prediction of complex structures and affinities for CAPRI rounds 20-27. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013, 81, 2201-2209. | 1.5 | 22 |
| 88 | Interfacial Mineral-Peptide Properties of a Mineral Binding Peptide from Osteonectin and Bone-like Apatite. <i>Chemistry of Materials</i> , 2015, 27, 5562-5569. | 3.2 | 21 |
| 89 | The structure of the colorectal cancer-associated enzyme GalNAc-T12 reveals how nonconserved residues dictate its function. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 20404-20410. | 3.3 | 21 |
| 90 | Structure-based non-canonical amino acid design to covalently crosslink an antibody-antigen complex. <i>Journal of Structural Biology</i> , 2014, 185, 215-222. | 1.3 | 20 |

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| 91 | <i>Caulobacter crescentus</i> Hfq structure reveals a conserved mechanism of RNA annealing regulation. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10978-10987. | 3.3 | 20 |
| 92 | The structural basis of PTEN regulation by multi-site phosphorylation. Nature Structural and Molecular Biology, 2021, 28, 858-868. | 3.6 | 20 |
| 93 | Analysis of Protein Kinase Autophosphorylation Using Expressed Protein Ligation and Computational Modeling. Journal of the American Chemical Society, 2008, 130, 5667-5669. | 6.6 | 19 |
| 94 | Structure Prediction of Domain Insertion Proteins from Structures of Individual Domains. Structure, 2008, 16, 513-527. | 1.6 | 18 |
| 95 | Modeling oblong proteins and water-mediated interfaces with RosettaDock in CAPRI rounds 28-35. Proteins: Structure, Function and Bioinformatics, 2017, 85, 479-486. | 1.5 | 18 |
| 96 | Robustification of RosettaAntibody and Rosetta SnugDock. PLoS ONE, 2021, 16, e0234282. | 1.1 | 18 |
| 97 | Protein-Protein Docking with Dynamic Residue Protonation States. PLoS Computational Biology, 2014, 10, e1004018. | 1.5 | 17 |
| 98 | Modulation of calcium oxalate dihydrate growth by phosphorylated osteopontin peptides. Journal of Structural Biology, 2018, 204, 131-144. | 1.3 | 17 |
| 99 | How Do We Do This at a Distance? A Descriptive Study of Remote Undergraduate Research Programs during COVID-19. CBE Life Sciences Education, 2022, 21, ar1. | 1.1 | 17 |
| 100 | Origin of anomalous multibody interactions. Nature, 1999, 402, 750-750. | 13.7 | 16 |
| 101 | Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947. | 5.8 | 16 |
| 102 | Novel sampling strategies and a coarse-grained score function for docking homomers, flexible heteromers, and oligosaccharides using Rosetta in CAPRI rounds 37-45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 973-985. | 1.5 | 15 |
| 103 | Protein docking and steered molecular dynamics suggest alternative phospholamban-binding sites on the SERCA calcium transporter. Journal of Biological Chemistry, 2020, 295, 11262-11274. | 1.6 | 15 |
| 104 | A high-affinity human TCR-like antibody detects celiac disease gluten peptide-MHC complexes and inhibits T cell activation. Science Immunology, 2021, 6, . | 5.6 | 15 |
| 105 | Development of a Broadly Accessible, Computationally Guided Biochemistry Course-Based Undergraduate Research Experience. Journal of Chemical Education, 2021, 98, 400-409. | 1.1 | 15 |
| 106 | A high throughput mutagenic analysis of yeast sumo structure and function. PLoS Genetics, 2017, 13, e1006612. | 1.5 | 15 |
| 107 | Glycoengineering of Esterase Activity through Metabolic Flux-Based Modulation of Sialic Acid. ChemBioChem, 2017, 18, 1204-1215. | 1.3 | 14 |
| 108 | Effect of trisodium citrate treatment on hybridoma cell viability. Biotechnology Letters, 1991, 5, 295-298. | 0.5 | 13 |

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|-----|--|-----|-----------|
| 109 | Mechanism of Polyubiquitin Chain Recognition by the Human Ubiquitin Conjugating Enzyme Ube2g2. <i>Journal of Biological Chemistry</i> , 2011, 286, 3981-3991. | 1.6 | 13 |
| 110 | Flexible Backbone Assembly and Refinement of Symmetrical Homomeric Complexes. <i>Structure</i> , 2019, 27, 1041-1051.e8. | 1.6 | 13 |
| 111 | Truncation of the caspase-related subunit (Gpi8p) of <i>Saccharomyces cerevisiae</i> GPI transamidase: Dimerization revealed. <i>Archives of Biochemistry and Biophysics</i> , 2007, 462, 83-93. | 1.4 | 12 |
| 112 | Molecular Determinants for Protein Stabilization by Insertional Fusion to a Thermophilic Host Protein. <i>ChemBioChem</i> , 2015, 16, 2392-2402. | 1.3 | 12 |
| 113 | A cyber-linked undergraduate research experience in computational biomolecular structure prediction and design. <i>PLoS Computational Biology</i> , 2017, 13, e1005837. | 1.5 | 12 |
| 114 | A Benchmarking Study of Peptide-Biomaterial Interactions. <i>Crystal Growth and Design</i> , 2018, 18, 607-616. | 1.4 | 12 |
| 115 | A humanized yeast system to analyze cleavage of prelamin A by ZMPSTE24. <i>Methods</i> , 2019, 157, 47-55. | 1.9 | 12 |
| 116 | Computer-aided engineering of thermostabilized antibody fragments. <i>AIChE Journal</i> , 2020, 66, e16864. | 1.8 | 12 |
| 117 | Development and Evaluation of GlycanDock: A Protein-Glycoligand Docking Refinement Algorithm in Rosetta. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6807-6820. | 1.2 | 12 |
| 118 | Adsorption of Charge-Disperse Mixtures of Colloidal Particles. <i>Langmuir</i> , 2001, 17, 7935-7947. | 1.6 | 11 |
| 119 | Non-H3 CDR template selection in antibody modeling through machine learning. <i>PeerJ</i> , 2019, 7, e6179. | 0.9 | 10 |
| 120 | Shotgun scanning glycomutagenesis: A simple and efficient strategy for constructing and characterizing neoglycoproteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, . | 3.3 | 9 |
| 121 | Prediction of Calcite Morphology from Computational and Experimental Studies of Mutations of a De Novo-Designed Peptide. <i>Langmuir</i> , 2011, 27, 11520-11527. | 1.6 | 8 |
| 122 | Computed structures of point deletion mutants and their enzymatic activities. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 2844-2860. | 1.5 | 8 |
| 123 | PyRosetta Jupyter Notebooks Teach Biomolecular Structure Prediction and Design. <i>The Biophysicist</i> , 2021, 2, 108-122. | 0.1 | 8 |
| 124 | Computational Predictions of the Mutant Behavior of AraC. <i>Journal of Molecular Biology</i> , 2010, 398, 462-470. | 2.0 | 7 |
| 125 | Colicin-Mediated Transport of DNA through the Iron Transporter FepA. <i>MBio</i> , 2021, 12, e0178721. | 1.8 | 7 |
| 126 | Comparison of NMR and crystal structures of membrane proteins and computational refinement to improve model quality. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 57-74. | 1.5 | 6 |

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|-----|---|-----|-----------|
| 127 | Toward the computational design of protein crystals with improved resolution. <i>Acta Crystallographica Section D: Structural Biology</i> , 2019, 75, 1015-1027. | 1.1 | 6 |
| 128 | An Expanded Benchmark for Antibody-Antigen Docking and Affinity Prediction Reveals Insights into Antibody Recognition Determinants. <i>SSRN Electronic Journal</i> , 0, , . | 0.4 | 6 |
| 129 | Accurate positioning of functional residues with robotics-inspired computational protein design. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2115480119. | 3.3 | 6 |
| 130 | Diverse Scientific Benchmarks for Implicit Membrane Energy Functions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5248-5261. | 2.3 | 5 |
| 131 | Induced fit with replica exchange improves protein complex structure prediction. <i>PLoS Computational Biology</i> , 2022, 18, e1010124. | 1.5 | 5 |
| 132 | Simultaneous prediction of antibody backbone and side-chain conformations with deep learning. <i>PLoS ONE</i> , 2022, 17, e0258173. | 1.1 | 5 |
| 133 | Solid-State NMR Studies of Biomineralization Peptides and Proteins. <i>ACS Symposium Series</i> , 2012, , 77-96. | 0.5 | 4 |
| 134 | Rosetta-MPDock: A Novel Computational Tool for Protein-Protein Docking within the Membrane Bilayer. <i>Biophysical Journal</i> , 2015, 108, 250a. | 0.2 | 4 |
| 135 | A Parametric Rosetta Energy Function Analysis with LK Peptides on SAM Surfaces. <i>Langmuir</i> , 2018, 34, 5279-5289. | 1.6 | 4 |
| 136 | Structural Basis for Peptide Substrate Specificities of Glycosyltransferase GalNAc-T2. <i>ACS Catalysis</i> , 2021, 11, 2977-2991. | 5.5 | 4 |
| 137 | Correction to "The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design". <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4594-4594. | 2.3 | 4 |
| 138 | Membrane Protein Engineering with Rosetta. <i>Methods in Molecular Biology</i> , 2021, 2315, 43-57. | 0.4 | 3 |
| 139 | Understanding the interactions between bone mineral crystals and their binding peptides derived from filamentous phage. <i>Materials Today Advances</i> , 2022, 15, 100263. | 2.5 | 3 |
| 140 | Efficient Flexible-Backbone Docking of Challenging Protein Complexes. <i>Biophysical Journal</i> , 2018, 114, 344a. | 0.2 | 2 |
| 141 | Big Data from Sparse Data: Diverse Scientific Benchmarks Reveal Optimization Imperatives for Implicit Membrane Energy Functions. <i>Biophysical Journal</i> , 2020, 118, 361a. | 0.2 | 1 |
| 142 | The Interaction of Proteins with Solid Surfaces. <i>ChemInform</i> , 2004, 35, no. | 0.1 | 0 |
| 143 | Fd Bacteriophage Coat Protein Structure Prediction and Design for the Assembly of Hydroxyapatite Nanorods and Bone Tissue Regeneration. <i>Biophysical Journal</i> , 2011, 100, 158a. | 0.2 | 0 |
| 144 | Towards Fast and Accurate Calculation of Protein pKa Values Exploiting Various Degrees of Conformational Flexibility. <i>Biophysical Journal</i> , 2012, 102, 169a-170a. | 0.2 | 0 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 145 | A Systematic Computational Method to Predict and Enhance Antibody-Antigen Binding in the Absence of Antibody Crystal Structures. <i>Biophysical Journal</i> , 2012, 102, 621a. | 0.2 | 0 |
| 146 | Docking and Design of Oligosaccharides, Glycoproteins, and Glycolipids. <i>Biophysical Journal</i> , 2015, 108, 470a. | 0.2 | 0 |
| 147 | Characterization of Peptides Designed to Control Crystal Nucleation and Growth. <i>Biophysical Journal</i> , 2015, 108, 633a. | 0.2 | 0 |
| 148 | The Origin of CDR H3 Structural Diversity. <i>Biophysical Journal</i> , 2015, 108, 510a. | 0.2 | 0 |
| 149 | A Deep-Dive into the Rosetta Energy Function for Biological Macromolecules. <i>Biophysical Journal</i> , 2017, 112, 194a. | 0.2 | 0 |
| 150 | Evolution of CDR H3 Flexibility at an Immunomic Scale. <i>Biophysical Journal</i> , 2018, 114, 189a-190a. | 0.2 | 0 |
| 151 | Fast Implicit Potentials for Accurate Prediction and Design of Membrane Protein Structures. <i>Biophysical Journal</i> , 2018, 114, 345a. | 0.2 | 0 |
| 152 | Computational Design of High-Resolution Protein Crystals. <i>Biophysical Journal</i> , 2018, 114, 575a. | 0.2 | 0 |
| 153 | Cover Image, Volume 86, Issue 1. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, C4. | 1.5 | 0 |
| 154 | Engineering immunity with quantitative tools. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 677-678. | 1.7 | 0 |
| 155 | Toward Accurate Prediction and Design of Kinked Alpha Helices in Membrane Proteins. <i>Biophysical Journal</i> , 2019, 116, 58a. | 0.2 | 0 |
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