

Charlotte M Deane

List of Publications by Year in descending order

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Version: 2024-02-01

189
papers

9,609
citations

57631

44
h-index

58464

82
g-index

290
all docs

290
docs citations

290
times ranked

10289
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|---|-----|-----------|
| 1 | Learning from Docked Ligands: Ligand-Based Features Rescue Structure-Based Scoring Functions When Trained on Docked Poses. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 5329-5341. | 2.5 | 10 |
| 2 | The Therapeutic Antibody Profiler for Computational Developability Assessment. <i>Methods in Molecular Biology</i> , 2022, 2313, 115-125. | 0.4 | 7 |
| 3 | DLAB: deep learning methods for structure-based virtual screening of antibodies. <i>Bioinformatics</i> , 2022, 38, 377-383. | 1.8 | 48 |
| 4 | SABDab in the age of biotherapeutics: updates including SABDab-nano, the nanobody structure tracker. <i>Nucleic Acids Research</i> , 2022, 50, D1368-D1372. | 6.5 | 49 |
| 5 | Observed Antibody Space: A diverse database of cleaned, annotated, and translated unpaired and paired antibody sequences. <i>Protein Science</i> , 2022, 31, 141-146. | 3.1 | 98 |
| 6 | ABlooper: fast accurate antibody CDR loop structure prediction with accuracy estimation. <i>Bioinformatics</i> , 2022, 38, 1877-1880. | 1.8 | 78 |
| 7 | Current structure predictors are not learning the physics of protein folding. <i>Bioinformatics</i> , 2022, 38, 1881-1887. | 1.8 | 50 |
| 8 | Current advances in biopharmaceutical informatics: guidelines, impact and challenges in the computational developability assessment of antibody therapeutics. <i>MAbs</i> , 2022, 14, 2020082. | 2.6 | 35 |
| 9 | AI in 3D compound design. <i>Current Opinion in Structural Biology</i> , 2022, 73, 102326. | 2.6 | 8 |
| 10 | Challenges and Opportunities for Bayesian Statistics in Proteomics. <i>Journal of Proteome Research</i> , 2022, 21, 849-864. | 1.8 | 5 |
| 11 | Ranking of communities in multiplex spatiotemporal models of brain dynamics. <i>Applied Network Science</i> , 2022, 7, 15. | 0.8 | 0 |
| 12 | Membranome 3.0: Database of single-pass membrane proteins with <i>AlphaFold</i> models. <i>Protein Science</i> , 2022, 31, e4318. | 3.1 | 20 |
| 13 | Incorporating Target-Specific Pharmacophoric Information into Deep Generative Models for Fragment Elaboration. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2280-2292. | 2.5 | 10 |
| 14 | Advances in computational structure-based antibody design. <i>Current Opinion in Structural Biology</i> , 2022, 74, 102379. | 2.6 | 32 |
| 15 | Extracting Information from Gene Coexpression Networks of <i>Rhizobium leguminosarum</i> . <i>Journal of Computational Biology</i> , 2022, , . | 0.8 | 1 |
| 16 | Generating weighted and thresholded gene coexpression networks using signed distance correlation. <i>Network Science</i> , 2022, 10, 131-145. | 0.8 | 1 |
| 17 | AbLang: an antibody language model for completing antibody sequences. <i>Bioinformatics Advances</i> , 2022, 2, . | 0.9 | 48 |
| 18 | Empirical Bayes functional models for hydrogen deuterium exchange mass spectrometry. <i>Communications Biology</i> , 2022, 5, . | 2.0 | 1 |

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|----|---|-----|-----------|
| 19 | CoV-AbDab: the coronavirus antibody database. <i>Bioinformatics</i> , 2021, 37, 734-735. | 1.8 | 273 |
| 20 | COGENT: evaluating the consistency of gene co-expression networks. <i>Bioinformatics</i> , 2021, 37, 1928-1929. | 1.8 | 6 |
| 21 | Ribosome occupancy profiles are conserved between structurally and evolutionarily related yeast domains. <i>Bioinformatics</i> , 2021, 37, 1853-1859. | 1.8 | 4 |
| 22 | Ab-Ligity: identifying sequence-dissimilar antibodies that bind to the same epitope. <i>MAbs</i> , 2021, 13, 1873478. | 2.6 | 31 |
| 23 | A computational method for immune repertoire mining that identifies novel binders from different clonotypes, demonstrated by identifying anti-pertussis toxoid antibodies. <i>MAbs</i> , 2021, 13, 1869406. | 2.6 | 31 |
| 24 | Robust gene coexpression networks using signed distance correlation. <i>Bioinformatics</i> , 2021, 37, 1982-1989. | 1.8 | 10 |
| 25 | The allosteric modulation of complement C5 by knob domain peptides. <i>ELife</i> , 2021, 10, . | 2.8 | 21 |
| 26 | Generating property-matched decoy molecules using deep learning. <i>Bioinformatics</i> , 2021, 37, 2134-2141. | 1.8 | 30 |
| 27 | Public Baseline and shared response structures support the theory of antibody repertoire functional commonality. <i>PLoS Computational Biology</i> , 2021, 17, e1008781. | 1.5 | 26 |
| 28 | Hypergraphs for predicting essential genes using multiprotein complex data. <i>Journal of Complex Networks</i> , 2021, 9, . | 1.1 | 16 |
| 29 | Humanization of antibodies using a machine learning approach on large-scale repertoire data. <i>Bioinformatics</i> , 2021, 37, 4041-4047. | 1.8 | 49 |
| 30 | Co-evolutionary distance predictions contain flexibility information. <i>Bioinformatics</i> , 2021, , . | 1.8 | 9 |
| 31 | The prospects of quantum computing in computational molecular biology. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1481. | 6.2 | 108 |
| 32 | Deep generative design with 3D pharmacophoric constraints. <i>Chemical Science</i> , 2021, 12, 14577-14589. | 3.7 | 36 |
| 33 | Different B cell subpopulations show distinct patterns in their IgH repertoire metrics. <i>ELife</i> , 2021, 10, . | 2.8 | 22 |
| 34 | Current strategies for detecting functional convergence across B-cell receptor repertoires. <i>MAbs</i> , 2021, 13, 1996732. | 2.6 | 18 |
| 35 | Epitope profiling using computational structural modelling demonstrated on coronavirus-binding antibodies. <i>PLoS Computational Biology</i> , 2021, 17, e1009675. | 1.5 | 33 |
| 36 | Learning from the ligand: using ligand-based features to improve binding affinity prediction. <i>Bioinformatics</i> , 2020, 36, 758-764. | 1.8 | 60 |

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|----|---|-----|-----------|
| 37 | The evolution of contact prediction: evidence that contact selection in statistical contact prediction is changing. <i>Bioinformatics</i> , 2020, 36, 1750-1756. | 1.8 | 5 |
| 38 | Thera-SAbDab: the Therapeutic Structural Antibody Database. <i>Nucleic Acids Research</i> , 2020, 48, D383-D388. | 6.5 | 88 |
| 39 | Data Set Augmentation Allows Deep Learning-Based Virtual Screening to Better Generalize to Unseen Target Classes and Highlight Important Binding Interactions. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3722-3730. | 2.5 | 36 |
| 40 | Maturation of the Human Immunoglobulin Heavy Chain Repertoire With Age. <i>Frontiers in Immunology</i> , 2020, 11, 1734. | 2.2 | 46 |
| 41 | Functional module detection through integration of single-cell RNA sequencing data with protein-protein interaction networks. <i>BMC Genomics</i> , 2020, 21, 756. | 1.2 | 13 |
| 42 | How repertoire data are changing antibody science. <i>Journal of Biological Chemistry</i> , 2020, 295, 9823-9837. | 1.6 | 43 |
| 43 | TCRBuilder: multi-state T-cell receptor structure prediction. <i>Bioinformatics</i> , 2020, 36, 3580-3581. | 1.8 | 10 |
| 44 | Deep Generative Models for 3D Linker Design. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1983-1995. | 2.5 | 126 |
| 45 | Structural diversity of B-cell receptor repertoires along the B-cell differentiation axis in humans and mice. <i>PLoS Computational Biology</i> , 2020, 16, e1007636. | 1.5 | 27 |
| 46 | Deep Sequencing of B Cell Receptor Repertoires From COVID-19 Patients Reveals Strong Convergent Immune Signatures. <i>Frontiers in Immunology</i> , 2020, 11, 605170. | 2.2 | 101 |
| 47 | Title is missing!. , 2020, 16, e1007636. | | 0 |
| 48 | Title is missing!. , 2020, 16, e1007636. | | 0 |
| 49 | Title is missing!. , 2020, 16, e1007636. | | 0 |
| 50 | Title is missing!. , 2020, 16, e1007636. | | 0 |
| 51 | Assessment of model fit via network comparison methods based on subgraph counts. <i>Journal of Complex Networks</i> , 2019, 7, 226-253. | 1.1 | 3 |
| 52 | Comparative Analysis of the CDR Loops of Antigen Receptors. <i>Frontiers in Immunology</i> , 2019, 10, 2454. | 2.2 | 40 |
| 53 | RFQAmode: Random Forest Quality Assessment to identify a predicted protein structure in the correct fold. <i>PLoS ONE</i> , 2019, 14, e0218149. | 1.1 | 3 |
| 54 | Measuring rank robustness in scored protein interaction networks. <i>BMC Bioinformatics</i> , 2019, 20, 446. | 1.2 | 30 |

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| 55 | Looking for therapeutic antibodies in next-generation sequencing repositories. <i>MAbs</i> , 2019, 11, 1197-1205. | 2.6 | 29 |
| 56 | Modeling conformational flexibility of kinases in inactive states. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 943-951. | 1.5 | 11 |
| 57 | Ligity: A Non-Superpositional, Knowledge-Based Approach to Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2600-2616. | 2.5 | 9 |
| 58 | HLA-DM Stabilizes the Empty MHCII Binding Groove: A Model Using Customized Natural Move Monte Carlo. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2894-2899. | 2.5 | 1 |
| 59 | Antibody-antigen complex modelling in the era of immunoglobulin repertoire sequencing. <i>Molecular Systems Design and Engineering</i> , 2019, 4, 679-688. | 1.7 | 20 |
| 60 | 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. | 3.3 | 221 |
| 61 | MHC binding affects the dynamics of different T-cell receptors in different ways. <i>PLoS Computational Biology</i> , 2019, 15, e1007338. | 1.5 | 13 |
| 62 | Increasing the accuracy of protein loop structure prediction with evolutionary constraints. <i>Bioinformatics</i> , 2019, 35, 2585-2592. | 1.8 | 8 |
| 63 | SCALOP: sequence-based antibody canonical loop structure annotation. <i>Bioinformatics</i> , 2019, 35, 1774-1776. | 1.8 | 29 |
| 64 | High-Throughput Antibody Structure Modeling and Design Using ABodyBuilder. <i>Methods in Molecular Biology</i> , 2019, 1851, 367-380. | 0.4 | 3 |
| 65 | A Statistical Model for Helices with Applications. <i>Biometrics</i> , 2018, 74, 845-854. | 0.8 | 2 |
| 66 | Identifying networks with common organizational principles. <i>Journal of Complex Networks</i> , 2018, 6, 887-913. | 1.1 | 20 |
| 67 | Combining co-evolution and secondary structure prediction to improve fragment library generation. <i>Bioinformatics</i> , 2018, 34, 2219-2227. | 1.8 | 7 |
| 68 | pyHVis3D: visualising molecular simulation deduced H-bond networks in 3D: application to T-cell receptor interactions. <i>Bioinformatics</i> , 2018, 34, 1941-1943. | 1.8 | 6 |
| 69 | Predicting loop conformational ensembles. <i>Bioinformatics</i> , 2018, 34, 949-956. | 1.8 | 20 |
| 70 | Antibody side chain conformations are position-dependent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 383-392. | 1.5 | 21 |
| 71 | <i>In silico</i> structural modeling of multiple epigenetic marks on DNA. <i>Bioinformatics</i> , 2018, 34, 41-48. | 1.8 | 4 |
| 72 | STCRDab: the structural T-cell receptor database. <i>Nucleic Acids Research</i> , 2018, 46, D406-D412. | 6.5 | 69 |

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|----|--|-----|-----------|
| 73 | Filtering Next-Generation Sequencing of the Ig Gene Repertoire Data Using Antibody Structural Information. <i>Journal of Immunology</i> , 2018, 201, 3694-3704. | 0.4 | 11 |
| 74 | Protein Family-Specific Models Using Deep Neural Networks and Transfer Learning Improve Virtual Screening and Highlight the Need for More Data. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2319-2330. | 2.5 | 106 |
| 75 | Avoiding False Positive Conclusions in Molecular Simulation: The Importance of Replicas. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6127-6138. | 2.3 | 187 |
| 76 | Observed Antibody Space: A Resource for Data Mining Next-Generation Sequencing of Antibody Repertoires. <i>Journal of Immunology</i> , 2018, 201, 2502-2509. | 0.4 | 165 |
| 77 | Sequential search leads to faster, more efficient fragment-based <i>de novo</i> protein structure prediction. <i>Bioinformatics</i> , 2018, 34, 1132-1140. | 1.8 | 12 |
| 78 | Structurally Mapping Antibody Repertoires. <i>Frontiers in Immunology</i> , 2018, 9, 1698. | 2.2 | 36 |
| 79 | Efficient Sampling for the Prediction of Long and Multidomain Protein Structures. <i>Biophysical Journal</i> , 2018, 114, 574a. | 0.2 | 0 |
| 80 | Comparing co-evolution methods and their application to template-free protein structure prediction. <i>Bioinformatics</i> , 2017, 33, 373-381. | 1.8 | 28 |
| 81 | Antibody H3 Structure Prediction. <i>Computational and Structural Biotechnology Journal</i> , 2017, 15, 222-231. | 1.9 | 47 |
| 82 | Association between a common immunoglobulin heavy chain allele and rheumatic heart disease risk in Oceania. <i>Nature Communications</i> , 2017, 8, 14946. | 5.8 | 114 |
| 83 | A multi-crystal method for extracting obscured crystallographic states from conventionally uninterpretable electron density. <i>Nature Communications</i> , 2017, 8, 15123. | 5.8 | 186 |
| 84 | Computational Tools for Aiding Rational Antibody Design. <i>Methods in Molecular Biology</i> , 2017, 1529, 399-416. | 0.4 | 22 |
| 85 | Variable Regions of Antibodies and T-Cell Receptors May Not Be Sufficient in Molecular Simulations Investigating Binding. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3097-3105. | 2.3 | 21 |
| 86 | Investigating Cotranslational Folding in Membrane Proteins using Fragment-Based Structure Prediction. <i>Biophysical Journal</i> , 2017, 112, 61a. | 0.2 | 1 |
| 87 | The H3 loop of antibodies shows unique structural characteristics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1311-1318. | 1.5 | 89 |
| 88 | Partial-occupancy binders identified by the Pan-Dataset Density Analysis method offer new chemical opportunities and reveal cryptic binding sites. <i>Structural Dynamics</i> , 2017, 4, 032104. | 0.9 | 25 |
| 89 | Cross-linking mass spectrometry identifies new interfaces of Augmin required to localise the $\hat{1}^3$ -Tubulin Ring Complex to the mitotic spindle. <i>Biology Open</i> , 2017, 6, 654-663. | 0.6 | 25 |
| 90 | Co-evolution techniques are reshaping the way we do structural bioinformatics. <i>F1000Research</i> , 2017, 6, 1224. | 0.8 | 22 |

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|-----|--|-----|-----------|
| 91 | How B-Cell Receptor Repertoire Sequencing Can Be Enriched with Structural Antibody Data. <i>Frontiers in Immunology</i> , 2017, 8, 1753. | 2.2 | 48 |
| 92 | Sphinx: merging knowledge-based and <i>ab initio</i> approaches to improve protein loop prediction. <i>Bioinformatics</i> , 2017, 33, 1346-1353. | 1.8 | 49 |
| 93 | <i>WONKA</i> and <i>OOMMPPAA</i> : analysis of protein-ligand interaction data to direct structure-based drug design. <i>Acta Crystallographica Section D: Structural Biology</i> , 2017, 73, 279-285. | 1.1 | 5 |
| 94 | Ten simple rules for surviving an interdisciplinary PhD. <i>PLoS Computational Biology</i> , 2017, 13, e1005512. | 1.5 | 7 |
| 95 | ANARCI: antigen receptor numbering and receptor classification. <i>Bioinformatics</i> , 2016, 32, 298-300. | 1.8 | 237 |
| 96 | Exploring peptide/MHC detachment processes using hierarchical natural move Monte Carlo. <i>Bioinformatics</i> , 2016, 32, 181-186. | 1.8 | 21 |
| 97 | Examining the Conservation of Kinks in Alpha Helices. <i>PLoS ONE</i> , 2016, 11, e0157553. | 1.1 | 20 |
| 98 | ABodyBuilder: Automated antibody structure prediction with data-driven accuracy estimation. <i>MAbs</i> , 2016, 8, 1259-1268. | 2.6 | 208 |
| 99 | Modeling Functional Motions of Biological Systems by Customized Natural Moves. <i>Biophysical Journal</i> , 2016, 111, 710-721. | 0.2 | 7 |
| 100 | Tertiary Element Interaction in HIV-1 TAR. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1746-1754. | 2.5 | 8 |
| 101 | Comparison of large networks with sub-sampling strategies. <i>Scientific Reports</i> , 2016, 6, 28955. | 1.6 | 9 |
| 102 | The contribution of major histocompatibility complex contacts to the affinity and kinetics of T cell receptor binding. <i>Scientific Reports</i> , 2016, 6, 35326. | 1.6 | 18 |
| 103 | SAbPred: a structure-based antibody prediction server. <i>Nucleic Acids Research</i> , 2016, 44, W474-W478. | 6.5 | 155 |
| 104 | Progress and challenges in predicting protein interfaces. <i>Briefings in Bioinformatics</i> , 2016, 17, 117-131. | 3.2 | 115 |
| 105 | T-Cell Receptor Binding Affects the Dynamics of the Peptide/MHC-I Complex. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 46-53. | 2.5 | 21 |
| 106 | Length-independent structural similarities enrich the antibody CDR canonical class model. <i>MAbs</i> , 2016, 8, 751-760. | 2.6 | 49 |
| 107 | Prediction of VH-VL domain orientation for antibody variable domain modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 681-695. | 1.5 | 47 |
| 108 | Building a Better Fragment Library for De Novo Protein Structure Prediction. <i>PLoS ONE</i> , 2015, 10, e0123998. | 1.1 | 25 |

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|-----|---|-----|-----------|
| 109 | Structural Bridges through Fold Space. <i>PLoS Computational Biology</i> , 2015, 11, e1004466. | 1.5 | 16 |
| 110 | Rapid, Precise, and Reproducible Prediction of Peptide-MHC Binding Affinities from Molecular Dynamics That Correlate Well with Experiment. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3346-3356. | 2.3 | 122 |
| 111 | Misato Controls Mitotic Microtubule Generation by Stabilizing the TCP-1 Tubulin Chaperone Complex. <i>Current Biology</i> , 2015, 25, 1777-1783. | 1.8 | 25 |
| 112 | Current status and future challenges in T-cell receptor/peptide/MHC molecular dynamics simulations. <i>Briefings in Bioinformatics</i> , 2015, 16, 1035-1044. | 3.2 | 45 |
| 113 | Ten Simple Rules for a Successful Cross-Disciplinary Collaboration. <i>PLoS Computational Biology</i> , 2015, 11, e1004214. | 1.5 | 46 |
| 114 | Type II Inhibitors Targeting CDK2. <i>ACS Chemical Biology</i> , 2015, 10, 2116-2125. | 1.6 | 75 |
| 115 | Identifying and quantifying radiation damage at the atomic level. <i>Journal of Synchrotron Radiation</i> , 2015, 22, 201-212. | 1.0 | 51 |
| 116 | The <i>Caenorhabditis elegans</i> protein SAS-5 forms large oligomeric assemblies critical for centriole formation. <i>ELife</i> , 2015, 4, e07410. | 2.8 | 37 |
| 117 | Examining Variable Domain Orientations in Antigen Receptors Gives Insight into TCR-Like Antibody Design. <i>PLoS Computational Biology</i> , 2014, 10, e1003852. | 1.5 | 29 |
| 118 | Large Scale Characterization of the LC13 TCR and HLA-B8 Structural Landscape in Reaction to 172 Altered Peptide Ligands: A Molecular Dynamics Simulation Study. <i>PLoS Computational Biology</i> , 2014, 10, e1003748. | 1.5 | 32 |
| 119 | Ten Simple Rules for Effective Computational Research. <i>PLoS Computational Biology</i> , 2014, 10, e1003506. | 1.5 | 47 |
| 120 | Improving B-cell epitope prediction and its application to global antibody-antigen docking. <i>Bioinformatics</i> , 2014, 30, 2288-2294. | 1.8 | 137 |
| 121 | Alignment-free protein interaction network comparison. <i>Bioinformatics</i> , 2014, 30, i430-i437. | 1.8 | 48 |
| 122 | Helix kinks are equally prevalent in soluble and membrane proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1960-1970. | 1.5 | 61 |
| 123 | Protein Modeling and Structural Prediction. , 2014, , 171-182. | | 1 |
| 124 | SABDab: the structural antibody database. <i>Nucleic Acids Research</i> , 2014, 42, D1140-D1146. | 6.5 | 374 |
| 125 | OOMPPAA: A Tool To Aid Directed Synthesis by the Combined Analysis of Activity and Structural Data. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2636-2646. | 2.5 | 9 |
| 126 | Crowdsourcing Yields a New Standard for Kinks in Protein Helices. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2585-2593. | 2.5 | 7 |

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| 127 | Gro2mat: A package to efficiently read gromacs output in MATLAB. <i>Journal of Computational Chemistry</i> , 2014, 35, 1528-1531. | 1.5 | 18 |
| 128 | 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. | 1.5 | 15 |
| 129 | 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. | 1.0 | 80 |
| 130 | MP-T: improving membrane protein alignment for structure prediction. <i>Bioinformatics</i> , 2013, 29, 54-61. | 1.8 | 30 |
| 131 | Interactions of Two Amphipathic Cell-Penetrating Peptides with Complex Model Membranes: Insights from Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2013, 104, 600a. | 0.2 | 0 |
| 132 | Exploring Fold Space Preferences of New-born and Ancient Protein Superfamilies. <i>PLoS Computational Biology</i> , 2013, 9, e1003325. | 1.5 | 31 |
| 133 | Memoir: template-based structure prediction for membrane proteins. <i>Nucleic Acids Research</i> , 2013, 41, W379-W383. | 6.5 | 38 |
| 134 | Local Network Patterns in Protein-Protein Interfaces. <i>PLoS ONE</i> , 2013, 8, e57031. | 1.1 | 5 |
| 135 | How long is a piece of loop?. <i>PeerJ</i> , 2013, 1, e1. | 0.9 | 17 |
| 136 | What Evidence Is There for the Homology of Protein-Protein Interactions?. <i>PLoS Computational Biology</i> , 2012, 8, e1002645. | 1.5 | 41 |
| 137 | A maternally inherited autosomal point mutation in human phospholipase C zeta (PLC ζ) leads to male infertility. <i>Human Reproduction</i> , 2012, 27, 222-231. | 0.4 | 117 |
| 138 | Freely Available Conformer Generation Methods: How Good Are They?. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1146-1158. | 2.5 | 178 |
| 139 | The Importance of Age and High Degree, in Protein-Protein Interaction Networks. <i>Journal of Computational Biology</i> , 2012, 19, 785-795. | 0.8 | 11 |
| 140 | Mutual information and variants for protein domain-domain contact prediction. <i>BMC Research Notes</i> , 2012, 5, 472. | 0.6 | 5 |
| 141 | Producing High-Accuracy Lattice Models from Protein Atomic Coordinates Including Side Chains. <i>Advances in Bioinformatics</i> , 2012, 2012, 1-6. | 5.7 | 22 |
| 142 | Predicting Inter-Species Cross-Talk in Two-Component Signalling Systems. <i>PLoS ONE</i> , 2012, 7, e37737. | 1.1 | 2 |
| 143 | Predicting antibody complementarity determining region structures without classification. <i>Molecular BioSystems</i> , 2011, 7, 3327. | 2.9 | 39 |
| 144 | The imprint of codons on protein structure. <i>Biotechnology Journal</i> , 2011, 6, 641-649. | 1.8 | 17 |

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| 145 | Signatures of coâ€translational folding. <i>Biotechnology Journal</i> , 2011, 6, 742-751. | 1.8 | 15 |
| 146 | Environment specific substitution tables improve membrane protein alignment. <i>Bioinformatics</i> , 2011, 27, i15-i23. | 1.8 | 20 |
| 147 | Directionality in protein fold prediction. <i>BMC Bioinformatics</i> , 2010, 11, 172. | 1.2 | 17 |
| 148 | The function of communities in protein interaction networks at multiple scales. <i>BMC Systems Biology</i> , 2010, 4, 100. | 3.0 | 79 |
| 149 | Deciphering chemotaxis pathways using cross species comparisons. <i>BMC Systems Biology</i> , 2010, 4, 3. | 3.0 | 66 |
| 150 | Protein structure prediction begins well but ends badly. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1282-1290. | 1.5 | 15 |
| 151 | FREAD revisited: Accurate loop structure prediction using a database search algorithm. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1431-1440. | 1.5 | 154 |
| 152 | iâ€Patch: Interprotein contact prediction using local network information. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2781-2797. | 1.5 | 26 |
| 153 | How threshold behaviour affects the use of subgraphs for network comparison. <i>Bioinformatics</i> , 2010, 26, i611-i617. | 1.8 | 26 |
| 154 | Exploring the potential of template-based modelling. <i>Bioinformatics</i> , 2010, 26, 1849-1856. | 1.8 | 11 |
| 155 | Revisiting Date and Party Hubs: Novel Approaches to Role Assignment in Protein Interaction Networks. <i>PLoS Computational Biology</i> , 2010, 6, e1000817. | 1.5 | 128 |
| 156 | MEDELLER: homology-based coordinate generation for membrane proteins. <i>Bioinformatics</i> , 2010, 26, 2833-2840. | 1.8 | 103 |
| 157 | Synonymous codon usage influences the local protein structure observed. <i>Nucleic Acids Research</i> , 2010, 38, 6719-6728. | 6.5 | 148 |
| 158 | Predicting proteinâ€protein interactions in the context of protein evolution. <i>Molecular BioSystems</i> , 2010, 6, 55-64. | 2.9 | 42 |
| 159 | Evolutionary analysis reveals low coverage as the major challenge for protein interaction network alignment. <i>Molecular BioSystems</i> , 2010, 6, 2296. | 2.9 | 11 |
| 160 | iMembrane: homology-based membrane-insertion of proteins. <i>Bioinformatics</i> , 2009, 25, 1086-1088. | 1.8 | 29 |
| 161 | Reduced amounts and abnormal forms of phospholipase C zeta (PLC ζ) in spermatozoa from infertile men. <i>Human Reproduction</i> , 2009, 24, 2417-2428. | 0.4 | 257 |
| 162 | Proteomic Analysis of Microtubule-associated Proteins during Macrophage Activation. <i>Molecular and Cellular Proteomics</i> , 2009, 8, 2500-2514. | 2.5 | 41 |

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| 163 | Functionally guided alignment of protein interaction networks for module detection. <i>Bioinformatics</i> , 2009, 25, 3166-3173. | 1.8 | 31 |
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