## Jason W Labonte

List of Publications by Year in descending order

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| #  | Article  | IF   | CITATIONS |
|----|--|------|-----------|
| 1  | The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. Journal of Chemical Theory and Computation, 2017, 13, 3031-3048.  | 5.3  | 1,032     |
| 2  | Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.   | 19.0 | 513       |
| 3  | A Comprehensive, High-Resolution Map of a Gene's Fitness Landscape. Molecular Biology and Evolution, 2014, 31, 1581-1592.  | 8.9  | 291       |
| 4  | Adding Diverse Noncanonical Backbones to Rosetta: Enabling Peptidomimetic Design. PLoS ONE, 2013, 8, e67051.   | 2.5  | 59        |
| 5  | Active Site Comparisons and Catalytic Mechanisms of the Hot Dog Superfamily. Chemical Reviews, 2013, 113, 2182-2204.   | 47.7 | 43        |
| 6  | Residueâ€centric modeling and design of saccharide and glycoconjugate structures. Journal of<br>Computational Chemistry, 2017, 38, 276-287.  | 3.3  | 41        |
| 7  | Computationally designed peptide macrocycle inhibitors of New Delhi metallo-β-lactamase 1.<br>Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .  | 7.1  | 41        |
| 8  | Better together: Elements of successful scientific software development in a distributed collaborative community. PLoS Computational Biology, 2020, 16, e1007507.  | 3.2  | 27        |
| 9  | Extending RosettaDock with water, sugar, and pH for prediction of complex structures and affinities for CAPRI rounds 20–27. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2201-2209.   | 2.6  | 22        |
| 10 | Computational design of mixed chirality peptide macrocycles with internal symmetry. Protein Science, 2020, 29, 2433-2445.  | 7.6  | 16        |
| 11 | Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.   | 12.8 | 16        |
| 12 | Novel sampling strategies and a coarseâ€grained score function for docking homomers, flexible<br>heteromers, and oligosaccharides using Rosetta in CAPRI rounds 37–45. Proteins: Structure, Function<br>and Bioinformatics, 2020, 88, 973-985. | 2.6  | 15        |
| 13 | Molecular Determinants for Protein Stabilization by Insertional Fusion to a Thermophilic Host<br>Protein. ChemBioChem, 2015, 16, 2392-2402.  | 2.6  | 12        |
| 14 | Development and Evaluation of GlycanDock: A Protein–Glycoligand Docking Refinement Algorithm in<br>Rosetta. Journal of Physical Chemistry B, 2021, 125, 6807-6820.   | 2.6  | 12        |
| 15 | Shotgun scanning glycomutagenesis: A simple and efficient strategy for constructing and characterizing neoglycoproteins. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .                         | 7.1  | 9         |
| 16 | PyRosetta Jupyter Notebooks Teach Biomolecular Structure Prediction and Design. The Biophysicist, 2021, 2, 108-122.  | 0.3  | 8         |
| 17 | Engineering the synthetic potential of β-lactam synthetase and the importance of catalytic loop dynamics. MedChemComm, 2012, 3, 960.   | 3.4  | 6         |
| 18 | Structural Basis for Peptide Substrate Specificities of Glycosyltransferase GalNAc-T2. ACS Catalysis, 2021, 11, 2977-2991.   | 11.2 | 4         |