# Johan Ãqvist

List of Publications by Year
in descending order



| 184 | 12,882 | 26630 | 26613 |
|---|---|---|---|
| papers | citations | 56 h-index | 107 g-index |

| 188 | 188 | 188 | 9959 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
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| 1 | Computer Simulations Reveal an Entirely Entropic Activation Barrier for the Chemical Step in a Designer Enzyme. ACS Catalysis, 2022, 12, 1452-1460. | 11.2 | 10 |
| 2 | The Activation Parameters of a Cold-Adapted Short Chain Dehydrogenase Are Insensitive to Enzyme Oligomerization. Biochemistry, 2022, 61, 514-522. | 2.5 | 6 |
| 3 | Structure and Mechanism of a Cold-Adapted Bacterial Lipase. Biochemistry, 2022, 61, 933-942. | 2.5 | 8 |
| 4 | Free Energy Calculations for Proteinâ€“Ligand Binding Prediction. Methods in Molecular Biology, 2021, 2266, 203-226. | 0.9 | 11 |
| 5 | Structure and mechanism of a phage-encoded SAM lyase revises catalytic function of enzyme family. ELife, 2021, 10, . | 6.0 | 15 |
| 6 | Structural Basis of Inhibition of Human Insulin-Regulated Aminopeptidase (IRAP) by Benzopyran-Based Inhibitors. Frontiers in Molecular Biosciences, 2021, 8, 625274. | 3.5 | 3 |
| 7 | Transition States for Psychrophilic and Mesophilic (R)-3-Hydroxybutyrate Dehydrogenase-Catalyzed Hydride Transfer at Sub-zero Temperatures. Biochemistry, 2021, 60, 2186-2194. | 2.5 | 1 |
| 8 | 3,4-Dihydropyrimidin-2(1H)-ones as Antagonists of the Human A<sub>2B</sub> Adenosine Receptor: Optimization, Structureâ€“Activity Relationship Studies, and Enantiospecific Recognition. Journal of Medicinal Chemistry, 2021, 64, 458-480. | 6.4 | 19 |
| 9 | Deciphering conformational selectivity in the A2A adenosine G protein-coupled receptor by free energy simulations. PLoS Computational Biology, 2021, 17, e1009152. | 3.2 | 5 |
| 10 | Macrocyclic peptidomimetics as inhibitors of insulin-regulated aminopeptidase (IRAP). RSC Medicinal Chemistry, 2020, 11, 234-244. | 3.9 | 9 |
| 11 | Hidden Conformational States and Strange Temperature Optima in Enzyme Catalysis. Biochemistry, 2020, 59, 3844-3855. | 2.5 | 16 |
| 12 | Dissecting the Mechanism of (R)-3-Hydroxybutyrate Dehydrogenase by Kinetic Isotope Effects, Protein Crystallography, and Computational Chemistry. ACS Catalysis, 2020, 10, 15019-15032. | 11.2 | 8 |
| 13 | Computer simulations explain the anomalous temperature optimum in a cold-adapted enzyme. Nature Communications, 2020, 11, 2644. | 12.8 | 35 |
| 14 | Xâ€Ray Crystallography and Free Energy Calculations Reveal the Binding Mechanism of A<sub>2A</sub> Adenosine Receptor Antagonists. Angewandte Chemie - International Edition, 2020, 59, 16536-16543. | 13.8 | 23 |
| 15 | Synthesis, Evaluation and Proposed Binding Pose of Substituted Spiroâ€Oxindole Dihydroquinazolinones as IRAP Inhibitors. ChemistryOpen, 2020, 9, 325-337. | 1.9 | 7 |
| 16 | Xâ€Ray Crystallography and Free Energy Calculations Reveal the Binding Mechanism of A<sub>2A</sub> Adenosine Receptor Antagonists. Angewandte Chemie, 2020, 132, 16679-16686. | 2.0 | 1 |
| 17 | Evolution of Angiotensin Peptides and Peptidomimetics as Angiotensin II Receptor Type 2 (AT2) Receptor Agonists. Biomolecules, 2020, 10, 649. | 4.0 | 12 |
| 18 | Inhibition of translation termination by small molecules targeting ribosomal release factors. Scientific Reports, 2019, 9, 15424. | 3.3 | 6 |

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| 19 | QresFEP: An Automated Protocol for Free Energy Calculations of Protein Mutations in Q. Journal of Chemical Theory and Computation, 2019, 15, 5461-5473. | 5.3 | 33 |
| 20 | Principles of tRNA<sup>Ala</sup> Selection by Alanylâ€“tRNA Synthetase Based on the Critical G3Â·U70 Base Pair. ACS Omega, 2019, 4, 15539-15548. | 3.5 | 7 |
| 21 | A Series of Analogues to the AT<sub>2</sub>R Prototype Antagonist C38 Allow Fine Tuning of the Previously Reported Antagonist Binding Mode. ChemistryOpen, 2019, 8, 114-125. | 1.9 | 8 |
| 22 | QligFEP: an automated workflow for small molecule free energy calculations in Q. Journal of Cheminformatics, 2019, 11, 26. | 6.1 | 51 |
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| 24 | Towards Rational Computational Engineering of Psychrophilic Enzymes. Scientific Reports, 2019, 9, 19147. | 3.3 | 20 |
| 25 | Structural Basis of Inhibition of Human Insulin-Regulated Aminopeptidase (IRAP) by Aryl Sulfonamides. ACS Omega, 2018, 3, 4509-4521. | 3.5 | 14 |
| 26 | Complementary charge-based interaction between the ribosomal-stalk protein L7/12 and IF2 is the key to rapid subunit association. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 4649-4654. | 7.1 | 21 |
| 27 | Elucidation of the Binding Mode of the Carboxyterminal Region of Peptide YY to the Human Y<sub>2</sub>Receptor. Molecular Pharmacology, 2018, 93, 323-334. | 2.3 | 28 |
| 28 | Molecular Mechanisms in the Selectivity of Nonsteroidal Anti-Inflammatory Drugs. Biochemistry, 2018, 57, 1236-1248. | 2.5 | 19 |
| 29 | Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. SoftwareX, 2018, 7, 388-395. | 2.6 | 47 |
| 30 | Catalytic Adaptation of Psychrophilic Elastase. Biochemistry, 2018, 57, 2984-2993. | 2.5 | 18 |
| 31 | Characterization of Ligand Binding to GPCRs Through Computational Methods. Methods in Molecular Biology, 2018, 1705, 23-44. | 0.9 | 6 |
| 32 | Mechanistic alternatives for peptide bond formation on the ribosome. Nucleic Acids Research, 2018, 46, 5345-5354. | 14.5 | 12 |
| 33 | Entropy and Enzyme Catalysis. Accounts of Chemical Research, 2017, 50, 199-207. | 15.6 | 96 |
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| 37 | Thermodynamics of the Purine Nucleoside Phosphorylase Reaction Revealed by Computer Simulations. Biochemistry, 2017, 56, 306-312. | 2.5 | 4 |
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| 39 | Cold Adaptation of Triosephosphate Isomerase. Biochemistry, 2017, 56, 4169-4176. | 2.5 | 24 |
| 40 | Effect of Nitrogen Atom Substitution in A<sub>3</sub> Adenosine Receptor Binding: N-(4,6-Diarylpyridin-2-yl)acetamides as Potent and Selective Antagonists. Journal of Medicinal Chemistry, 2017, 60, 7502-7511. | 6.4 | 14 |
| 41 | Origin of the omnipotence of eukaryotic release factor 1. Nature Communications, 2017, 8, 1425. | 12.8 | 15 |
| 42 | Structure-Based Design of Potent and Selective Ligands at the Four Adenosine Receptors. Molecules, 2017, 22, 1945. | 3.8 | 30 |
| 43 | Enzyme surface rigidity tunes the temperature dependence of catalytic rates. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 7822-7827. | 7.1 | 74 |
| 44 | Computer Simulations Reveal Substrate Specificity of Glycosidic Bond Cleavage in Native and Mutant Human Purine Nucleoside Phosphorylase. Biochemistry, 2016, 55, 2153-2162. | 2.5 | 11 |
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| 46 | Aryl Sulfonamide Inhibitors of Insulin-Regulated Aminopeptidase Enhance Spine Density in Primary Hippocampal Neuron Cultures. ACS Chemical Neuroscience, 2016, 7, 1383-1392. | 3.5 | 27 |
| 47 | The Competing Mechanisms of Phosphate Monoester Dianion Hydrolysis. Journal of the American Chemical Society, 2016, 138, 10664-10673. | 13.7 | 46 |
| 48 | Peptide Release on the Ribosome Involves Substrate-Assisted Base Catalysis. ACS Catalysis, 2016, 6, 8432-8439. | 11.2 | 15 |
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| 64 | Protein Surface Softness Is the Origin of Enzyme Cold-Adaptation of Trypsin. PLoS Computational Biology, 2014, 10, e1003813. | 3.2 | 63 |
| 65 | Computational Prediction of Alanine Scanning and Ligand Binding Energetics in G-Protein Coupled Receptors. PLoS Computational Biology, 2014, 10, e1003585. | 3.2 | 58 |
| 66 | Why base tautomerization does not cause errors in mRNA decoding on the ribosome. Nucleic Acids Research, 2014, 42, 12876-12884. | 14.5 | 27 |
| 67 | Permeation Redux: Thermodynamics and Kinetics of Ion Movement through Potassium Channels. Biophysical Journal, 2014, 106, 1859-1863. | 0.5 | 30 |
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