# Arieh Warshel

List of Publications by Year
in descending order



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|---|---|---|---|
| 158 papers | 21,502 citations | 16791 66 h-index | 10399 144 g-index |
| 159 all docs | 159 docs citations | 159 times ranked | 14851 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Effect of Environmental Factors on the Catalytic Activity of Intramembrane Serine Protease. Journal of the American Chemical Society, 2022, 144, 1251-1257. | 6.6 | 4 |
| 2 | Enhancing computational enzyme design by a maximum entropy strategy. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, . | 3.3 | 18 |
| 3 | Electrostatic influence on IL-1 transport through the GSDMD pore. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, . | 3.3 | 13 |
| 4 | Fast and Effective Prediction of the Absolute Binding Free Energies of Covalent Inhibitors of SARS-CoV-2 Main Protease and 20S Proteasome. Journal of the American Chemical Society, 2022, 144, 7568-7572. | 6.6 | 10 |
| 5 | A new class of Î±-ketoamide derivatives with potent anticancer and anti-SARS-CoV-2 activities. European Journal of Medicinal Chemistry, 2021, 215, 113267. | 2.6 | 13 |
| 6 | Simulating the directional translocation of a substrate by the AAA+ motor in the 26S proteasome. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, . | 3.3 | 7 |
| 7 | Exploring the Activation Process of the Î²2AR-G<sub>s</sub>Complex. Journal of the American Chemical Society, 2021, 143, 11044-11051. | 6.6 | 14 |
| 8 | Predicting Mutational Effects on Receptor Binding of the Spike Protein of SARS-CoV-2 Variants. Journal of the American Chemical Society, 2021, 143, 17646-17654. | 6.6 | 39 |
| 9 | Exploring alternative catalytic mechanisms of the Cas9 HNH domain. Proteins: Structure, Function and Bioinformatics, 2020, 88, 260-264. | 1.5 | 17 |
| 10 | A freeâ€energy landscape for the glucagonâ€like peptide 1 receptor GLP1R. Proteins: Structure, Function and Bioinformatics, 2020, 88, 127-134. | 1.5 | 11 |
| 11 | Exploring the activation pathway and G <sub>i</sub> -coupling specificity of the Î¼-opioid receptor. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26218-26225. | 3.3 | 15 |
| 12 | Exploring the Mechanism of Covalent Inhibition: Simulating the Binding Free Energy of Î±-Ketoamide Inhibitors of the Main Protease of SARS-CoV-2. Biochemistry, 2020, 59, 4601-4608. | 1.2 | 45 |
| 13 | Exploring the Catalytic Reaction of Cysteine Proteases. Journal of Physical Chemistry B, 2020, 124, 11349-11356. | 1.2 | 18 |
| 14 | The catalytic dwell in ATPases is not crucial for movement against applied torque. Nature Chemistry, 2020, 12, 1187-1192. | 6.6 | 11 |
| 15 | Exploring the Proteolysis Mechanism of the Proteasomes. Journal of Physical Chemistry B, 2020, 124, 5626-5635. | 1.2 | 12 |
| 16 | Critical Differences between the Binding Features of the Spike Proteins of SARS-CoV-2 and SARS-CoV. Journal of Physical Chemistry B, 2020, 124, 5907-5912. | 1.2 | 52 |
| 17 | Combinatorial Approach for Exploring Conformational Space and Activation Barriers in Computer-Aided Enzyme Design. ACS Catalysis, 2020, 10, 6002-6012. | 5.5 | 16 |
| 18 | Exploring the Effectiveness of Binding Free Energy Calculations. Journal of Physical Chemistry B, 2019, 123, 8910-8915. | 1.2 | 16 |

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| 19 | Revisiting the protomotive vectorial motion of F <sub>0</sub> -ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 19484-19489. | 3.3 | 36 |
| 20 | ZnT2 is an electroneutral proton-coupled vesicular antiporter displaying an apparent stoichiometry of two protons per zinc ion. PLoS Computational Biology, 2019, 15, e1006882. | 1.5 | 31 |
| 21 | Exploring the challenges of computational enzyme design by rebuilding the active site of a dehalogenase. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 389-394. | 3.3 | 28 |
| 22 | Exploring the Catalytic Mechanism of Cas9 Using Information Inferred from Endonuclease VII. ACS Catalysis, 2019, 9, 1329-1336. | 5.5 | 26 |
| 23 | EF-Tu and EF-G are activated by allosteric effects. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3386-3391. | 3.3 | 18 |
| 24 | On the control of the proton current in the voltage-gated proton channel Hv1. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10321-10326. | 3.3 | 28 |
| 25 | Exploring the free-energy landscape of GPCR activation. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10327-10332. | 3.3 | 43 |
| 26 | Demonstrating aspects of multiscale modeling by studying the permeation pathway of the human ZnT2 zinc transporter. PLoS Computational Biology, 2018, 14, e1006503. | 1.5 | 13 |
| 27 | Simulating the dynamics of the mechanochemical cycle of myosin-V. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2259-2264. | 3.3 | 25 |
| 28 | Origin of the Non-Arrhenius Behavior of the Rates of Enzymatic Reactions. Journal of Physical Chemistry B, 2017, 121, 6520-6526. | 1.2 | 14 |
| 29 | Simulating the fidelity and the three Mg mechanism of pol Î· and clarifying the validity of transition state theory in enzyme catalysis. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1446-1453. | 1.5 | 27 |
| 30 | Exploring the Development of Ground-State Destabilization and Transition-State Stabilization in Two Directed Evolution Paths of Kemp Eliminases. ACS Catalysis, 2017, 7, 3301-3305. | 5.5 | 27 |
| 31 | Validating the Water Flooding Approach by Comparing It to Grand Canonical Monte Carlo Simulations. Journal of Physical Chemistry B, 2017, 121, 9358-9365. | 1.2 | 13 |
| 32 | Reexamining the origin of the directionality of myosin V. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 10426-10431. | 3.3 | 16 |
| 33 | Misunderstanding the preorganization concept can lead to confusions about the origin of enzyme catalysis. Proteins: Structure, Function and Bioinformatics, 2017, 85, 2157-2161. | 1.5 | 23 |
| 34 | The FOF1 ATP synthase: from atomistic three-dimensional structure to the rotary-chemical function. Photosynthesis Research, 2017, 134, 1-15. | 1.6 | 28 |
| 35 | Validating a Coarse-Grained Voltage Activation Model by Comparing Its Performance to the Results of Monte Carlo Simulations. Journal of Physical Chemistry B, 2017, 121, 11284-11291. | 1.2 | 12 |
| 36 | Exploring the Drug Resistance of HCV Protease. Journal of Physical Chemistry B, 2017, 121, 6831-6840. | 1.2 | 8 |

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| 37 | Perspective: Defining and quantifying the role of dynamics in enzyme catalysis. Journal of Chemical Physics, 2016, 144, 180901. | 1.2 | 163 |
| 38 | Refining the treatment of membrane proteins by coarseâ€grained models. Proteins: Structure, Function and Bioinformatics, 2016, 84, 92-117. | 1.5 | 37 |
| 39 | Enhancing Paradynamics for QM/MM Sampling of Enzymatic Reactions. Journal of Physical Chemistry B, 2016, 120, 2155-2164. | 1.2 | 22 |
| 40 | Simulating the Function of the MjNhaP1 Transporter. Journal of Physical Chemistry B, 2016, 120, 10951-10958. | 1.2 | 4 |
| 41 | The control of the discrimination between dNTP and rNTP in DNA and RNA polymerase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1616-1624. | 1.5 | 8 |
| 42 | Exploring the mechanism of DNA polymerases by analyzing the effect of mutations of active site acidic groups in Polymerase Î². Proteins: Structure, Function and Bioinformatics, 2016, 84, 1644-1657. | 1.5 | 18 |
| 43 | Exploring the Dependence of QM/MM Calculations of Enzyme Catalysis on the Size of the QM Region. Journal of Physical Chemistry B, 2016, 120, 9913-9921. | 1.2 | 94 |
| 44 | Cover Image, Volume 84, Issue 11. Proteins: Structure, Function and Bioinformatics, 2016, 84, C4. | 1.5 | 0 |
| 45 | The Physics and Physical Chemistry of Molecular Machines. ChemPhysChem, 2016, 17, 1719-1741. | 1.0 | 120 |
| 46 | Analyzing the electrogenicity of cytochrome c oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 7810-7815. | 3.3 | 6 |
| 47 | A Microscopic Capacitor Model of Voltage Coupling in Membrane Proteins: Gating Charge Fluctuations in Ci-VSD. Journal of Physical Chemistry B, 2016, 120, 418-432. | 1.2 | 6 |
| 48 | Torque, chemistry and efficiency in molecular motors: a study of the rotaryâ€“chemical coupling in F<sub>1</sub>-ATPase. Quarterly Reviews of Biophysics, 2015, 48, 395-403. | 2.4 | 24 |
| 49 | Dissecting the role of the Î³-subunit in the rotaryâ€“chemical coupling and torque generation of F <sub>1</sub> -ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2746-2751. | 3.3 | 51 |
| 50 | The entropic contributions in vitamin B <sub>12</sub> enzymes still reflect the electrostatic paradigm. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 4328-4333. | 3.3 | 26 |
| 51 | BrÃ¸nsted slopes based on single-molecule imaging data help to unveil the chemically coupled rotation in F1-ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14121-14122. | 3.3 | 8 |
| 52 | Simulating the function of sodium/proton antiporters. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12378-12383. | 3.3 | 23 |
| 53 | Equilibrium fluctuation relations for voltage coupling in membrane proteins. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2985-2997. | 1.4 | 6 |
| 54 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215. | 0.8 | 2,561 |

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| 55 | Multiskalenmodellierung biologischer Funktionen: Von Enzymen zu molekularen Maschinen (Nobelâ€Aufsatz). Angewandte Chemie, 2014, 126, 10182-10194. | 1.6 | 15 |
| 56 | Computer aided enzyme design and catalytic concepts. Current Opinion in Chemical Biology, 2014, 21, 56-62. | 2.8 | 78 |
| 57 | Multiscale Modeling of Biological Functions: From Enzymes to Molecular Machines (Nobel Lecture). Angewandte Chemie - International Edition, 2014, 53, 10020-10031. | 7.2 | 201 |
| 58 | Modeling gating charge and voltage changes in response to charge separation in membrane proteins. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11353-11358. | 3.3 | 13 |
| 59 | An effective Coarseâ€grained model for biological simulations: Recent refinements and validations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1168-1185. | 1.5 | 45 |
| 60 | Realistic simulations of the coupling between the protomotive force and the mechanical rotation of the F0-ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 14876-14881. | 3.3 | 54 |
| 61 | Prechemistry barriers and checkpoints do not contribute to fidelity and catalysis as long as they are not rate limiting. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 29 |
| 62 | Paradynamics: An Effective and Reliable Model for Ab Initio QM/MM Free-Energy Calculations and Related Tasks. Journal of Physical Chemistry B, 2011, 115, 7950-7962. | 1.2 | 101 |
| 63 | Coarse-Grained (Multiscale) Simulations in Studies of Biophysical and Chemical Systems. Annual Review of Physical Chemistry, 2011, 62, 41-64. | 4.8 | 176 |
| 64 | The empirical valence bond model: theory and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 30-45. | 6.2 | 141 |
| 65 | Simulating electrostatic energies in proteins: Perspectives and some recent studies of pK<sub>a</sub>s, redox, and other crucial functional properties. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3469-3484. | 1.5 | 44 |
| 66 | Prechemistry versus preorganization in DNA replication fidelity. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2900-2919. | 1.5 | 37 |
| 67 | Electrostatic origin of the mechanochemical rotary mechanism and the catalytic dwell of F1-ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 20550-20555. | 3.3 | 93 |
| 68 | At the dawn of the 21st century: Is dynamics the missing link for understanding enzyme catalysis?. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1339-1375. | 1.5 | 399 |
| 69 | Absolute binding free energy calculations: On the accuracy of computational scoring of proteinâ€“ligand interactions. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1705-1723. | 1.5 | 180 |
| 70 | Ketosteroid isomerase provides further support for the idea that enzymes work by electrostatic preorganization. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 4075-4080. | 3.3 | 81 |
| 71 | Reply to Karplus: Conformational dynamics have no role in the chemical step. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, E72-E72. | 3.3 | 23 |
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| 73 | Phosphate ester analogues as probes for understanding enzyme catalysed phosphoryl transfer. Faraday Discussions, 2010, 145, 281-299. | 1.6 | 21 |
| 74 | The EVB as a quantitative tool for formulating simulations and analyzing biological and chemical reactions. Faraday Discussions, 2010, 145, 71-106. | 1.6 | 96 |
| 75 | Enzyme millisecond conformational dynamics do not catalyze the chemical step. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 17359-17364. | 3.3 | 195 |
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| 78 | Electrostatic Contributions to Binding of Transition State Analogues Can Be Very Different from the Corresponding Contributions to Catalysis:Â Phenolates Binding to the Oxyanion Hole of Ketosteroid Isomeraseâ€. Biochemistry, 2007, 46, 1466-1476. | 1.2 | 71 |
| 79 | Chapter 15. Challenges and Progresses in Calculations of Binding Free Energies â€“ What Does it Take to Quantify Electrostatic Contributions to Proteinâ€“Ligand Interactions?. RSC Biomolecular Sciences, 2007, , 268-290. | 0.4 | 7 |
| 80 | Electrostatic Basis for Enzyme Catalysis. Chemical Reviews, 2006, 106, 3210-3235. | 23.0 | 1,117 |
| 81 | Modeling electrostatic effects in proteins. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2006, 1764, 1647-1676. | 1.1 | 472 |
| 82 | On the Mechanism of Hydrolysis of Phosphate Monoesters Dianions in Solutions and Proteins. Journal of the American Chemical Society, 2006, 128, 15310-15323. | 6.6 | 191 |
| 83 | Computer simulations of protein functions: Searching for the molecular origin of the replication fidelity of DNA polymerases. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6819-6824. | 3.3 | 103 |
| 84 | Inverting the selectivity of aquaporin 6: Gating versus direct electrostatic interaction. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 1813-1814. | 3.3 | 10 |
| 85 | The low barrier hydrogen bond (LBHB) proposal revisited: The case of the Asp Â·Â·Â· His pair in serine proteases. Proteins: Structure, Function and Bioinformatics, 2004, 55, 711-723. | 1.5 | 155 |
| 86 | Computer Simulation of the Chemical Catalysis of DNA Polymerases:â€‰ Discriminating between Alternative Nucleotide Insertion Mechanisms for T7 DNA Polymerase. Journal of the American Chemical Society, 2003, 125, 8163-8177. | 6.6 | 145 |
| 87 | Computer simulation studies of the fidelity of DNA polymerases. Biopolymers, 2003, 68, 286-299. | 1.2 | 39 |
| 88 | Computer Simulations of Enzyme Catalysis: Methods, Progress, and Insights. Annual Review of Biophysics and Biomolecular Structure, 2003, 32, 425-443. | 18.3 | 467 |
| 89 | Comment on â€œEffect of Active Site Mutation Phe93 â†' Trp in the Horse Liver Alcohol Dehydrogenase Enzyme on Catalysis:Â A Molecular Dynamics Studyâ€. Journal of Physical Chemistry B, 2003, 107, 12370-12371. | 1.2 | 15 |
| 90 | Converting conformational changes to electrostatic energy in molecular motors: The energetics of ATP synthase. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 14834-14839. | 3.3 | 75 |

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| 91 | Ab Initio QM/MM Simulation with Proper Sampling:â€‰â€œFirst Principleâ€•Calculations of the Free Energy of the Autodissociation of Water in Aqueous Solution. Journal of Physical Chemistry B, 2002, 106, 13333-13343. | 1.2 | 150 |
| 92 | Molecular Dynamics Simulations of Biological Reactions. Accounts of Chemical Research, 2002, 35, 385-395. | 7.6 | 186 |
| 93 | Dynamics of biochemical and biophysical reactions: insight from computer simulations. Quarterly Reviews of Biophysics, 2001, 34, 563-679. | 2.4 | 257 |
| 94 | Energetics and Dynamics of Enzymatic Reactions. Journal of Physical Chemistry B, 2001, 105, 7887-7907. | 1.2 | 326 |
| 95 | Ab Initio Evaluation of the Free Energy Surfaces for the General Base/Acid Catalyzed Thiolysis of Formamide and the Hydrolysis of Methyl Thiolformate:Â A Reference Solution Reaction for Studies of Cysteine Proteases. Journal of Physical Chemistry B, 2001, 105, 4471-4484. | 1.2 | 66 |
| 96 | What are the dielectric ?constants? of proteins and how to validate electrostatic models?. Proteins: Structure, Function and Bioinformatics, 2001, 44, 400-417. | 1.5 | 865 |
| 97 | Effective way of modeling chemical catalysis: Empirical valence bond picture of role of solvent and catalyst in alkylation reactions. Journal of Computational Chemistry, 2000, 21, 607-625. | 1.5 | 17 |
| 98 | Examining methods for calculations of binding free energies: LRA, LIE, PDLD-LRA, and PDLD/S-LRA calculations of ligands binding to an HIV protease. Proteins: Structure, Function and Bioinformatics, 2000, 39, 393-407. | 1.5 | 202 |
| 99 | Ab initio/LD studies of chemical reactions in solution: Reference free-energy surfaces for acylation reactions occurring in serine and cysteine proteases. International Journal of Quantum Chemistry, 2000, 77, 44-53. | 1.0 | 9 |
| 100 | Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548. | 1.5 | 617 |
| 101 | Constraining the electron densities in DFT method as an effective way forab initio studies of metal-catalyzed reactions. Journal of Computational Chemistry, 2000, 21, 1554-1561. | 1.5 | 44 |
| 102 | Perspective on "The energetics of enzymatic reactions". Theoretical Chemistry Accounts, 2000, 103, 337-339. | 0.5 | 6 |
| 103 | Calculations of Activation Entropies of Chemical Reactions in Solution. Journal of Physical Chemistry B, 2000, 104, 4578-4584. | 1.2 | 166 |
| 104 | How Does GAP Catalyze the GTPase Reaction of Ras?:â€‰ A Computer Simulation Study. Biochemistry, 2000, 39, 9641-9651. | 1.2 | 153 |
| 105 | Remarkable Rate Enhancement of Orotidine 5â€˜-Monophosphate Decarboxylase Is Due to Transition-State Stabilization Rather Than to Ground-State Destabilization. Biochemistry, 2000, 39, 14728-14738. | 1.2 | 135 |
| 106 | Ab Initio Evaluation of the Potential Surface for General Base- Catalyzed Methanolysis of Formamide:Â A Reference Solution Reaction for Studies of Serine Proteases. Journal of the American Chemical Society, 2000, 122, 5354-5366. | 6.6 | 115 |
| 107 | Examining methods for calculations of binding free energies: LRA, LIE, PDLD-LRA, and PDLD/S-LRA calculations of ligands binding to an HIV protease. , 2000, 39, 393. | | 4 |
| 108 | Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532. | | 2 |

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| 109 | Simulating proton translocations in proteins: Probing proton transfer pathways in theRhodobacter sphaeroides reaction center. Proteins: Structure, Function and Bioinformatics, 1999, 36, 484-500. | 1.5 | 81 |
| 110 | Calculations of Hydration Entropies of Hydrophobic, Polar, and Ionic Solutes in the Framework of the Langevin Dipoles Solvation Model. Journal of Physical Chemistry B, 1999, 103, 10282-10288. | 1.2 | 131 |
| 111 | Microscopic Based Density Matrix Treatments of Electron-Transfer Reactions in Condensed Phases. Journal of Physical Chemistry A, 1999, 103, 11378-11386. | 1.1 | 8 |
| 112 | Quantum Catalysis: The Modeling of Catalytic Transition States. ACS Symposium Series, 1999, , 2-17. | 0.5 | 7 |
| 113 | Energetics and Dynamics of Transition States of Reactions in Enzymes and Solutions. ACS Symposium Series, 1999, , 489-499. | 0.5 | 10 |
| 114 | Simulating proton translocations in proteins: Probing proton transfer pathways in the Rhodobacter sphaeroides reaction center. , 1999, 36, 484. | | 1 |
| 115 | Oscillations of the energy gap for the initial electron-transfer step in bacterial reaction centers. Photosynthesis Research, 1998, 55, 147-152. | 1.6 | 20 |
| 116 | Electrostatic contributions to proteinâ€“protein binding affinities: Application to Rap/Raf interaction. , 1998, 30, 407-423. | | 77 |
| 117 | Phosphate Ester Hydrolysis in Aqueous Solution:â€‰ Associative versus Dissociative Mechanisms. Journal of Physical Chemistry B, 1998, 102, 719-734. | 1.2 | 234 |
| 118 | Quantum Mechanical-Molecular Mechanical Approaches for Studying Chemical Reactions in Proteins and Solution. ACS Symposium Series, 1998, , 16-34. | 0.5 | 22 |
| 119 | Effect of Solvent Discreteness on Solvation. Journal of Physical Chemistry B, 1998, 102, 5348-5357. | 1.2 | 28 |
| 120 | On the Reactivity of Phosphate Monoester Dianions in Aqueous Solution:Â BrÃ¸nsted Linear Free-Energy Relationships Do Not Have an Unique Mechanistic Interpretation. Journal of the American Chemical Society, 1998, 120, 11524-11525. | 6.6 | 62 |
| 121 | Origin of the Catalytic Power of Acetylcholinesterase:Â Computer Simulation Studies. Journal of the American Chemical Society, 1998, 120, 183-194. | 6.6 | 116 |
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| 123 | The surface constraint all atom model provides size independent results in calculations of hydration free energies. Journal of Chemical Physics, 1998, 109, 7940-7944. | 1.2 | 60 |
| 124 | Continuum and Dipole-Lattice Models of Solvation. Journal of Physical Chemistry B, 1997, 101, 11254-11264. | 1.2 | 54 |
| 125 | A Fundamental Assumption about OH-Attack in Phosphate Ester Hydrolysis Is Not Fully Justified. Journal of the American Chemical Society, 1997, 119, 5473-5474. | 6.6 | 107 |
| 126 | Langevin Dipoles Model for ab Initio Calculations of Chemical Processes in Solution:â€‰ Parametrization and Application to Hydration Free Energies of Neutral and Ionic Solutes and Conformational Analysis in Aqueous Solution. Journal of Physical Chemistry B, 1997, 101, 5583-5595. | 1.2 | 275 |

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| 127 | Consistent Calculations of pKa's of Ionizable Residues in Proteins:â€‰ Semi-microscopic and Microscopic Approaches. Journal of Physical Chemistry B, 1997, 101, 4458-4472. | 1.2 | 357 |
| 128 | A stringent test of the cavity concept in continuum dielectrics. Journal of Chemical Physics, 1997, 107, 7975-7978. | 1.2 | 37 |
| 129 | How Important Are Quantum Mechanical Nuclear Motions in Enzyme Catalysis?. Journal of the American Chemical Society, 1996, 118, 11745-11751. | 6.6 | 185 |
| 130 | Calculations of the electrostatic free energy contributions to the binding free energy of sulfonamides to carbonic anhydrase. Structural Chemistry, 1996, 7, 131-138. | 1.0 | 21 |
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| 132 | Orientation of the OH Dipole of Tyrosine (M)210 and Its Effect on Electrostatic Energies in Photosynthetic Bacterial Reaction Centers. The Journal of Physical Chemistry, 1996, 100, 16761-16770. | 2.9 | 90 |
| 133 | Substrate-assisted catalysis as a mechanism for GTP hydrolysis of p21ras and other GTP-binding proteins. Nature Structural Biology, 1995, 2, 36-44. | 9.7 | 259 |
| 134 | Microscopic and semimicroscopic calculations of electrostatic energies in proteins by the POLARIS and ENZYMIX programs. Journal of Computational Chemistry, 1993, 14, 161-185. | 1.5 | 445 |
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| 138 | Microscopic simulations of macroscopic dielectric constants of solvated proteins. Journal of Chemical Physics, 1991, 95, 4366-4377. | 1.2 | 252 |
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| 148 | The extended Ewald method: A general treatment of longâ€range electrostatic interactions in microscopic simulations. Journal of Chemical Physics, 1988, 89, 3751-3759. | 1.2 | 45 |
| 149 | Theoretical correlation of structure and energetics in the catalytic reaction of trypsin. Journal of the American Chemical Society, 1986, 108, 6569-6579. | 6.6 | 169 |
| 150 | Simulation of the dynamics of electron transfer reactions in polar solvents: Semiclassical trajectories and dispersed polaron approaches. Journal of Chemical Physics, 1986, 84, 4938-4957. | 1.2 | 219 |
| 151 | Quantized semiclassical trajectory approach for evaluation of vibronic transitions in anharmonic molecules. Journal of Chemical Physics, 1985, 82, 1756-1771. | 1.2 | 18 |
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| 156 | Calculations of chemical processes in solutions. The Journal of Physical Chemistry, 1979, 83, 1640-1652. | 2.9 | 328 |
| 157 | Calculations of resonance Raman spectra of conjugated molecules. Journal of Chemical Physics, 1977, 66, 5477-5488. | 1.2 | 219 |
| 158 | Computer Simulations of Proton Transfer in Proteins and Solutions. , 0, , 1171-1205. | | 0 |