Thomas Fox

List of Publications by Year in descending order

48 papers	15,821 citations	172207 29 h-index	223531 46 g-index
50 all docs	50 docs citations	50 times ranked	14819 citing authors

#	Article	IF	Citations
1	A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules. Journal of the American Chemical Society, 1995, 117, 5179-5197.	6.6	12,116
2	Molecular Dynamics Simulations on Solvated Biomolecular Systems: The Particle Mesh Ewald Method Leads to Stable Trajectories of DNA, RNA, and Proteins. Journal of the American Chemical Society, 1995, 117, 4193-4194.	6.6	780
3	Application of the RESP Methodology in the Parametrization of Organic Solvents. Journal of Physical Chemistry B, 1998, 102, 8070-8079.	1.2	483
4	Energy decomposition analysis approaches and their evaluation on prototypical proteinâ€“drug interaction patterns. Chemical Society Reviews, 2015, 44, 3177-3211.	18.7	284
5	GRID/CPCA:Â A New Computational Tool To Design Selective Ligands. Journal of Medicinal Chemistry, 2000, 43, 3033-3044.	2.9	191
6	The development/application of a â€˜minimalistâ€™ organic/biochemical molecular mechanic force field using a combination of ab initio calculations and experimental data. , 1997, , 83-96.		176
7	Heteroaromatic Ï€-Stacking Energy Landscapes. Journal of Chemical Information and Modeling, 2014, 54, 1371-1379.	2.5	144
8	Accuracy Assessment and Automation of Free Energy Calculations for Drug Design. Journal of Chemical Information and Modeling, 2014, 54, 108-120.	2.5	111
9	A molecular level picture of the stabilization of A-DNA in mixed ethanol-water solutions. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 9626-9630.	3.3	104
10	Use of Locally Enhanced Sampling in Free Energy Calculations:â€‰ Testing and Application to the Î± â†’ Î² Anomerization of Glucose. Journal of the American Chemical Society, 1998, 120, 5771-5782.	6.6	88
11	The application of different solvation and electrostatic models in molecular dynamics simulations of ubiquitin: How well is the xâ€ray structure â€œmaintainedâ€?. , 1996, 25, 315-334.		81
12	Machine Learning Techniques for In Silico Modeling of Drug Metabolism. Current Topics in Medicinal Chemistry, 2006, 6, 1579-1591.	1.0	79
13	A challenging system: Free energy prediction for factor Xa. Journal of Computational Chemistry, 2011, 32, 1743-1752.	1.5	75
14	Dispersion dominated halogenâ€“Ï€ interactions: energies and locations of minima. Physical Chemistry Chemical Physics, 2010, 12, 14941.	1.3	73
15	The calculation of solvatochromic shifts: the n-Ï€* transition of acetone. Chemical Physics Letters, 1992, 191, 33-37.	1.2	65
16	Calculation of Ionization Potentials and Câˆ’H Bond Dissociation Energies of Toluene Derivatives. The Journal of Physical Chemistry, 1996, 100, 2950-2956.	2.9	60
17	Stabilizing of a Globular Protein by a Highly Complex Water Network: A Molecular Dynamics Simulation Study on Factor Xa. Journal of Physical Chemistry B, 2010, 114, 7405-7412.	1.2	59
18	Peptidic Macrocycles - Conformational Sampling and Thermodynamic Characterization. Journal of Chemical Information and Modeling, 2018, 58, 982-992.	2.5	55

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19	A support vector machine approach to classify human cytochrome P450 3A4 inhibitors. Journal of Computer-Aided Molecular Design, 2005, 19, 189-201.	1.3	54
20	Electrostatic embedding in large-scale first principles quantum mechanical calculations on biomolecules. Journal of Chemical Physics, 2011, 135, 224107.	1.2	52
21	Protein and metal cluster structure of the wheat metallothionein domain Î³-Ec-1: the second part of the puzzle. Journal of Biological Inorganic Chemistry, 2011, 16, 683-694.	1.1	46
22	Computational approaches to predict drug metabolism. Expert Opinion on Drug Metabolism and Toxicology, 2009, 5, 15-27.	1.5	44
23	Assessing the accuracy of octanolâ€“water partition coefficient predictions in the SAMPL6 Part II logÂP Challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 335-370.	1.3	44
24	Multivariate modeling of cytochrome P450 3A4 inhibition. European Journal of Pharmaceutical Sciences, 2005, 24, 451-463.	1.9	43
25	Free Energies of Binding from Large-Scale First-Principles Quantum Mechanical Calculations: Application to Ligand Hydration Energies. Journal of Physical Chemistry B, 2013, 117, 9478-9485.	1.2	41
26	Prediction of Human Cytochrome P450 Inhibition Using Support Vector Machines. QSAR and Combinatorial Science, 2005, 24, 491-502.	1.5	37
27	Ligand Binding in the Catalytic Antibody 17E8. A Free Energy Perturbation Calculation Study. Journal of the American Chemical Society, 1997, 119, 11571-11577.	6.6	36
28	Electrostatic solvent effects on the electronic structure of ground and excited states of molecules: Applications of a cavity model based upon a finite element method. Journal of Computational Chemistry, 1993, 14, 253-262.	1.5	34
29	Largeâ€scale DFT calculations in implicit solventâ€”A case study on the T4 lysozyme L99A/M102Q protein. International Journal of Quantum Chemistry, 2013, 113, 771-785.	1.0	34
30	Density functional theory calculations on entire proteins for free energies of binding: Application to a model polar binding site. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3335-3346.	1.5	34
31	A â€œStepping Stoneâ€•Approach for Obtaining Quantum Free Energies of Hydration. Journal of Physical Chemistry B, 2015, 119, 7030-7040.	1.2	34
32	Onion design and its application to a pharmaceutical QSAR problem. Journal of Chemometrics, 2004, 18, 188-202.	0.7	30
33	Bias-Correction of Regression Models: A Case Study on hERG Inhibition. Journal of Chemical Information and Modeling, 2009, 49, 1486-1496.	2.5	29
34	Modeling of the geometry of densely packed chemisorbed overlayers: small organic molecules on Ni(110) and Pd(110). Surface Science, 1991, 256, 159-170.	0.8	21
35	Energy Decomposition Analysis Based on Absolutely Localized Molecular Orbitals for Large-Scale Density Functional Theory Calculations in Drug Design. Journal of Chemical Theory and Computation, 2016, 12, 3135-3148.	2.3	20
36	Proteinâ€“ligand free energies of binding from full-protein DFT calculations: convergence and choice of exchangeâ€“correlation functional. Physical Chemistry Chemical Physics, 2021, 23, 9381-9393.	1.3	20

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37	First Principles-Based Calculations of Free Energy of Binding: Application to Ligand Binding in a Self-Assembling Superstructure. Journal of Chemical Theory and Computation, 2011, 7, 1102-1108.	2.3	19
38	Intuitive Density Functional Theory-Based Energy Decomposition Analysis for Proteinâ€“Ligand Interactions. Journal of Chemical Theory and Computation, 2017, 13, 1837-1850.	2.3	19
39	Calculation of Electronic Spectra of Hydrated Ln(III) Ions within the INDO/S-CI Approach. The Journal of Physical Chemistry, 1995, 99, 600-605.	2.9	17
40	Application of Free Energy Perturbation Calculations to the â€œTennis Ballâ€•Dimer:â€‰ Why Is CF4 Not Encapsulated by This Host?. The Journal of Physical Chemistry, 1996, 100, 10779-10783.	2.9	17
41	Computer based screening of compound databases: 1. Preselection of benzamidine-based thrombin inhibitors. , 2000, 14, 411-425.		15
42	Economical and Accurate Protocol for Calculating Hydrogen-Bond-Acceptor Strengths. Journal of Chemical Information and Modeling, 2013, 53, 3262-3272.	2.5	14
43	On the cavity model for solvent shifts of excited states â€” a critical appraisal. Computational and Theoretical Chemistry, 1992, 276, 279-297.	1.5	13
44	A GRID-Derived Water Network Stabilizes Molecular Dynamics Computer Simulations of a Protease. Journal of Chemical Information and Modeling, 2011, 51, 2860-2867.	2.5	13
45	Design of rigid donor-acceptor systems with a low-lying charge-transfer state: an INDO model study of barrelene-based compounds. The Journal of Physical Chemistry, 1993, 97, 11420-11426.	2.9	8
46	On the electronic structure of barrelene-based rigid organic donor-acceptor systems. AnINDO model study including solvent effects. International Journal of Quantum Chemistry, 1992, 44, 551-561.	1.0	2
47	Chapter 5 Linear Quantitative Structureâ€“Activity Relationships for the Interaction of Small Molecules with Human Cytochrome P450 Isoenzymes. Annual Reports in Computational Chemistry, 2007, , 63-81.	0.9	2
48	On the electronic structure of barrelene-based rigid organic donor-acceptor systems. A comparison of INDO/S-CI calculations with absorption and fluorescence emission spectra. Chemical Physics, 1993, 175, 357-367.	0.9	1