

Doree F Sitkoff

List of Publications by Year in descending order

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32
papers

5,279
citations

394286

19
h-index

395590

33
g-index

33
all docs

33
docs citations

33
times ranked

5243
citing authors

#	ARTICLE	IF	CITATIONS
1	Accurate Calculation of Hydration Free Energies Using Macroscopic Solvent Models. <i>The Journal of Physical Chemistry</i> , 1994, 98, 1978-1988.	2.9	1,971
2	Accurate First Principles Calculation of Molecular Charge Distributions and Solvation Energies from Ab Initio Quantum Mechanics and Continuum Dielectric Theory. <i>Journal of the American Chemical Society</i> , 1994, 116, 11875-11882.	6.6	1,026
3	New Model for Calculation of Solvation Free Energies: A Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. <i>The Journal of Physical Chemistry</i> , 1996, 100, 11775-11788.	2.9	936
4	Theories of chemical shift anisotropies in proteins and nucleic acids. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 1998, 32, 165-190.	3.9	164
5	Free Energy of Amide Hydrogen Bond Formation in Vacuum, in Water, and in Liquid Alkane Solution. <i>Journal of Physical Chemistry B</i> , 1997, 101, 450-457.	1.2	143
6	A comparative study of available software for high-accuracy homology modeling: From sequence alignments to structural models. <i>Protein Science</i> , 2006, 15, 808-824.	3.1	134
7	Calculation of Alkane to Water Solvation Free Energies Using Continuum Solvent Models. <i>The Journal of Physical Chemistry</i> , 1996, 100, 2744-2752.	2.9	110
8	Correlating solvation free energies and surface tensions of hydrocarbon solutes. <i>Biophysical Chemistry</i> , 1994, 51, 397-409.	1.5	109
9	Pharmacologic Profile of the Adnectin BMS-962476, a Small Protein Biologic Alternative to PCSK9 Antibodies for Low-Density Lipoprotein Lowering. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2014, 350, 412-424.	1.3	107
10	Synthesis of Novel Potent Dipeptidyl Peptidase IV Inhibitors with Enhanced Chemical Stability: A Interplay between the N-Terminal Amino Acid Alkyl Side Chain and the Cyclopropyl Group of β -Aminoacyl-L-cis-4,5-methanoprolinonitrile-Based Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 2587-2598.	2.9	102
11	Density Functional Calculations of Proton Chemical Shifts in Model Peptides. <i>Journal of the American Chemical Society</i> , 1997, 119, 12262-12273.	6.6	85
12	Tryptamine and homotryptamine-based sulfonamides as potent and selective inhibitors of 15-lipoxygenase. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 1435-1440.	1.0	49
13	Analysis and optimization of structure-based virtual screening protocols. <i>Journal of Molecular Graphics and Modelling</i> , 2003, 22, 31-40.	1.3	36
14	(3 <i>R</i> ,5 <i>S</i> ,7 <i>E</i>)-7-(4-(4-Fluorophenyl)-6-isopropyl-2-(methyl(1-methyl-1 <i>H</i> -1,2,4-triazol-5-yl)amino)pyrimidin-5-yl)-3,5-dihydroxy-3-methylglutaryl Coenzyme-A Reductase Inhibitor with Reduced Myotoxicity Potential. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 2722-2733.	2.9	36
15	Design, Structure-Activity Relationships, X-ray Crystal Structure, and Energetic Contributions of a Critical P1 Pharmacophore: 3-Chloroindole-7-yl-Based Factor Xa Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 7541-7551.	2.9	33
16	The Surprising Importance of Peptide Bond Contacts in Drug-Protein Interactions. <i>Chemistry - A European Journal</i> , 2017, 23, 7887-7890.	1.7	28
17	Discovery of Pyrrolidine-Containing GPR40 Agonists: Stereochemistry Effects a Change in Binding Mode. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 1417-1431.	2.9	25
18	Diphenylpyridylethanamine (DPPE) Derivatives as Cholesteryl Ester Transfer Protein (CETP) Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 6162-6175.	2.9	24

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19	Diproyl nitriles as potent dipeptidyl peptidase IV inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 3992-3995.	1.0	22
20	Aroylguanidine-based factor Xa inhibitors: The discovery of BMS-344577. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 6882-6889.	1.0	20
21	Ketene aminal-based lactam derivatives as a novel class of orally active FXa inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 5453-5458.	1.0	18
22	Cyanoguanidine-based lactam derivatives as a novel class of orally bioavailable factor Xa inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 4034-4041.	1.0	17
23	Theoretical calculations of the permeability of monensin ⁺ cation complexes in model bio-membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2000, 1466, 221-233.	1.4	15
24	Arylsulfonamidopiperidone derivatives as a novel class of factor Xa inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 7516-7521.	1.0	14
25	Amino(methyl) pyrrolidines as novel scaffolds for factor Xa inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2007, 17, 5952-5958.	1.0	11
26	Reductions in log P Improved Protein Binding and Clearance Predictions Enabling the Prospective Design of Cannabinoid Receptor (CB1) Antagonists with Desired Pharmacokinetic Properties. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 9586-9600.	2.9	10
27	Cannabinoid CB1 receptor ligand binding and function examined through mutagenesis studies of F200 and S383. <i>European Journal of Pharmacology</i> , 2011, 651, 9-17.	1.7	8
28	Initial Structure-Activity Relationships for a Caprolactam-based Series of Neutral Factor Xa Inhibitors: Lead Identification. <i>Letters in Drug Design and Discovery</i> , 2005, 2, 625-630.	0.4	7
29	The influence of a solvent environment on direct non-covalent interactions between two molecules: A symmetry-adapted perturbation theory study of polarization tuning of π - π interactions by water. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	6
30	Discovery of BMS-986339, a Pharmacologically Differentiated Farnesoid X Receptor Agonist for the Treatment of Nonalcoholic Steatohepatitis. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 8948-8960.	2.9	6
31	Optimized damping parameters for empirical dispersion corrections to symmetry-adapted perturbation theory. <i>Journal of Chemical Physics</i> , 2021, 154, 234107.	1.2	3
32	Discovery of BMS-986318, a Potent Nonbile Acid FXR Agonist for the Treatment of Nonalcoholic Steatohepatitis. <i>ACS Medicinal Chemistry Letters</i> , 2021, 12, 1413-1420.	1.3	3