Doree F Sitkoff

List of Publications by Year
in descending order

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32 papers	5,279 citations	394421 19 h-index	395702 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. The Journal of Physical Chemistry, 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. Journal of the American Chemical Society, 1994, 116, 11875-11882.	13.7	1,026
3	New Model for Calculation of Solvation Free Energies:Â Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. The Journal of Physical Chemistry, 1996, 100, 11775-11788.	2.9	936
4	Theories of chemical shift anisotropies in proteins and nucleic acids. Progress in Nuclear Magnetic Resonance Spectroscopy, 1998, 32, 165-190.	7.5	164
5	Free Energy of Amide Hydrogen Bond Formation in Vacuum, in Water, and in Liquid Alkane Solution. Journal of Physical Chemistry B, 1997, 101, 450-457.	2.6	143
6	A comparative study of available software for high-accuracy homology modeling: From sequence alignments to structural models. Protein Science, 2006, 15, 808-824.	7.6	134
7	Calculation of Alkane to Water Solvation Free Energies Using Continuum Solvent Models. The Journal of Physical Chemistry, 1996, 100, 2744-2752.	2.9	110
8	Correlating solvation free energies and surface tensions of hydrocarbon solutes. Biophysical Chemistry, 1994, 51, 397-409.	2.8	109
9	Pharmacologic Profile of the Adnectin BMS-962476, a Small Protein Biologic Alternative to PCSK9 Antibodies for Low-Density Lipoprotein Lowering. Journal of Pharmacology and Experimental Therapeutics, 2014, 350, 412-424.	2.5	107
10	Synthesis of Novel Potent Dipeptidyl Peptidase IV Inhibitors with Enhanced Chemical Stability:Â Interplay between the N-Terminal Amino Acid Alkyl Side Chain and the Cyclopropyl Group of Î±-Aminoacyl-l-cis-4,5-methanoprolinenitrile-Based Inhibitors. Journal of Medicinal Chemistry, 2004, 47, 2587-2598.	6.4	102
11	Density Functional Calculations of Proton Chemical Shifts in Model Peptides. Journal of the American Chemical Society, 1997, 119, 12262-12273.	13.7	85
12	Tryptamine and homotryptamine-based sulfonamides as potent and selective inhibitors of 15-lipoxygenase. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 1435-1440.	2.2	49
13	Analysis and optimization of structure-based virtual screening protocols. Journal of Molecular Graphics and Modelling, 2003, 22, 31-40.	2.4	36
14	(3R,5S,E)-7-(4-(4-Fluorophenyl)-6-isopropyl-2-(methyl(1-methyl-1H-1,2,4-triazol-5-yl)amino)pyrimidin-5-yl)-3,5-dihyd Acid (BMS-644950): A Rationally Designed Orally Efficacious 3-Hydroxy-3-methylglutaryl Coenzyme-A Reductase Inhibitor with Reduced Myotoxicity Potential. Journal of Medicinal Chemistry, 2008, 51, 2722-2733.	6.4	36
15	Design, Structureâ"Activity Relationships, X-ray Crystal Structure, and Energetic Contributions of a Critical P1 Pharmacophore: 3-Chloroindole-7-yl-Based Factor Xa Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 7541-7551.	6.4	33
16	The Surprising Importance of Peptide Bond Contacts in Drugâ€"Protein Interactions. Chemistry - A European Journal, 2017, 23, 7887-7890.	3.3	28
17	Discovery of Pyrrolidine-Containing GPR40 Agonists: Stereochemistry Effects a Change in Binding Mode. Journal of Medicinal Chemistry, 2017, 60, 1417-1431.	6.4	25
18	Diphenylpyridylethanamine (DPPE) Derivatives as Cholesteryl Ester Transfer Protein (CETP) Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 6162-6175.	6.4	24

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19	Diprolyl nitriles as potent dipeptidyl peptidase IV inhibitors. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3992-3995.	2.2	22
20	Aroylguanidine-based factor Xa inhibitors: The discovery of BMS-344577. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6882-6889.	2.2	20
21	Ketene aminal-based lactam derivatives as a novel class of orally active FXa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5453-5458.	2.2	18
22	Cyanoguanidine-based lactam derivatives as a novel class of orally bioavailable factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 4034-4041.	2.2	17
23	Theoretical calculations of the permeability of monensinâ€“cation complexes in model bio-membranes. Biochimica Et Biophysica Acta - Biomembranes, 2000, 1466, 221-233.	2.6	15
24	Arylsulfonamidopiperidone derivatives as a novel class of factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 7516-7521.	2.2	14
25	Amino(methyl) pyrrolidines as novel scaffolds for factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 5952-5958.	2.2	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. Journal of Medicinal Chemistry, 2013, 56, 9586-9600.	6.4	10
27	Cannabinoid CB1 receptor ligand binding and function examined through mutagenesis studies of F200 and S383. European Journal of Pharmacology, 2011, 651, 9-17.	3.5	8
28	Initial Structure-Activity Relationships for a Caprolactam-based Series of Neutral Factor Xa Inhibitors: Lead Identification. Letters in Drug Design and Discovery, 2005, 2, 625-630.	0.7	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 Ï€â€“Ï€ interactions by water. Journal of Chemical Physics, 2022, 156, .	3.0	6
30	Discovery of BMS-986339, a Pharmacologically Differentiated Farnesoid X Receptor Agonist for the Treatment of Nonalcoholic Steatohepatitis. Journal of Medicinal Chemistry, 2022, 65, 8948-8960.	6.4	6
31	Optimized damping parameters for empirical dispersion corrections to symmetry-adapted perturbation theory. Journal of Chemical Physics, 2021, 154, 234107.	3.0	3
32	Discovery of BMS-986318, a Potent Nonbile Acid FXR Agonist for the Treatment of Nonalcoholic Steatohepatitis. ACS Medicinal Chemistry Letters, 2021, 12, 1413-1420.	2.8	3