Doree F Sitkoff

List of Publications by Year
in descending order

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Version: 2024-02-01

32	5,279	394286	395590
papers	citations	19 h-index	33 g-index

33	33	33	5243
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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, .	1.2	6
2	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.	2.9	6
3	Optimized damping parameters for empirical dispersion corrections to symmetry-adapted perturbation theory. Journal of Chemical Physics, 2021, 154, 234107.	1.2	3
4	Discovery of BMS-986318, a Potent Nonbile Acid FXR Agonist for the Treatment of Nonalcoholic Steatohepatitis. ACS Medicinal Chemistry Letters, 2021, 12, 1413-1420.	1.3	3
5	Discovery of Pyrrolidine-Containing GPR40 Agonists: Stereochemistry Effects a Change in Binding Mode. Journal of Medicinal Chemistry, 2017, 60, 1417-1431.	2.9	25
6	The Surprising Importance of Peptide Bond Contacts in Drugâ€“Protein Interactions. Chemistry - A European Journal, 2017, 23, 7887-7890.	1.7	28
7	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.	1.3	107
8	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.	2.9	10
9	Diphenylpyridylethanamine (DPPE) Derivatives as Cholesteryl Ester Transfer Protein (CETP) Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 6162-6175.	2.9	24
10	Cannabinoid CB1 receptor ligand binding and function examined through mutagenesis studies of F200 and S383. European Journal of Pharmacology, 2011, 651, 9-17.	1.7	8
11	Arylsulfonamidopiperidone derivatives as a novel class of factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 7516-7521.	1.0	14
12	Aroylguanidine-based factor Xa inhibitors: The discovery of BMS-344577. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6882-6889.	1.0	20
13	Cyanoguanidine-based lactam derivatives as a novel class of orally bioavailable factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 4034-4041.	1.0	17
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.	2.9	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.	2.9	33
16	Amino(methyl) pyrrolidines as novel scaffolds for factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 5952-5958.	1.0	11
17	A comparative study of available software for high-accuracy homology modeling: From sequence alignments to structural models. Protein Science, 2006, 15, 808-824.	3.1	134
18	Tryptamine and homotryptamine-based sulfonamides as potent and selective inhibitors of 15-lipoxygenase. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 1435-1440.	1.0	49

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19	Diprolyl nitriles as potent dipeptidyl peptidase IV inhibitors. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3992-3995.	1.0	22
20	Ketene aminal-based lactam derivatives as a novel class of orally active FXa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5453-5458.	1.0	18
21	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.	0.4	7
22	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.	2.9	102
23	Analysis and optimization of structure-based virtual screening protocols. Journal of Molecular Graphics and Modelling, 2003, 22, 31-40.	1.3	36
24	Theoretical calculations of the permeability of monensinâ€“cation complexes in model bio-membranes. Biochimica Et Biophysica Acta - Biomembranes, 2000, 1466, 221-233.	1.4	15
25	Theories of chemical shift anisotropies in proteins and nucleic acids. Progress in Nuclear Magnetic Resonance Spectroscopy, 1998, 32, 165-190.	3.9	164
26	Density Functional Calculations of Proton Chemical Shifts in Model Peptides. Journal of the American Chemical Society, 1997, 119, 12262-12273.	6.6	85
27	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.	1.2	143
28	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
29	Calculation of Alkane to Water Solvation Free Energies Using Continuum Solvent Models. The Journal of Physical Chemistry, 1996, 100, 2744-2752.	2.9	110
30	Correlating solvation free energies and surface tensions of hydrocarbon solutes. Biophysical Chemistry, 1994, 51, 397-409.	1.5	109
31	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.	6.6	1,026
32	Accurate Calculation of Hydration Free Energies Using Macroscopic Solvent Models. The Journal of Physical Chemistry, 1994, 98, 1978-1988.	2.9	1,971