Flemming Steen JÃ¸rgensen

List of Publications by Year
in descending order

82 papers	2,569 citations	186209 28 h-index	214721 47 g-index
83 all docs	83 docs citations	83 times ranked	3170 citing authors

#	Article	IF	Citations
1	A New Concept for Multidimensional Selection of Ligand Conformations (MultiSelect) and Multidimensional Scoring (MultiScore) of Proteinâ˜Ligand Binding Affinities. Journal of Medicinal Chemistry, 2001, 44, 2333-2343.	2.9	110
2	GABAA Receptor Agonists, Partial Agonists, and Antagonists. Design and Therapeutic Prospects. Journal of Medicinal Chemistry, 1994, 37, 2489-2505.	2.9	99
3	Evaluation and Comparison of 3D-QSAR CoMSIA Models for CDK1, CDK5, and GSK-3 Inhibition by Paullones. Journal of Medicinal Chemistry, 2004, 47, 22-36.	2.9	98
4	Prediction methods and databases within chemoinformatics: emphasis on drugs and drug candidates. Bioinformatics, 2005, 21, 2145-2160.	1.8	98
5	hERG Classification Model Based on a Combination of Support Vector Machine Method and GRIND Descriptors. Molecular Pharmaceutics, 2008, 5, 117-127.	2.3	91
6	Classification of Cytochrome P450 1A2 Inhibitors and Noninhibitors by Machine Learning Techniques. Drug Metabolism and Disposition, 2009, 37, 658-664.	1.7	91
7	Mutational Mapping and Modeling of the Binding Site for (S)-Citalopram in the Human Serotonin Transporter. Journal of Biological Chemistry, 2010, 285, 2051-2063.	1.6	91
8	Structural Differences of Matrix Metalloproteinases with Potential Implications for Inhibitor Selectivity Examined by the GRID/CPCA Approach. Journal of Medicinal Chemistry, 2002, 45, 2675-2684.	2.9	90
9	Prediction of pH-Dependent Aqueous Solubility of Druglike Molecules. Journal of Chemical Information and Modeling, 2006, 46, 2601-2609.	2.5	84
10	Virtual Screening and Prediction of Site of Metabolism for Cytochrome P450 1A2 Ligands. Journal of Chemical Information and Modeling, 2009, 49, 43-52.	2.5	78
11	Prediction of cytochrome P450 mediated metabolism. Advanced Drug Delivery Reviews, 2015, 86, 61-71.	6.6	78
12	Identification of a gene on chromosome 12q22 uniquely overexpressed in chronic lymphocytic leukemia. Blood, 2006, 107, 2904-2911.	0.6	55
13	SMARTCyp 3.0: enhanced cytochrome P450 site-of-metabolism prediction server. Bioinformatics, 2019, 35, 3174-3175.	1.8	53
14	Towards an understanding of drug resistance in malaria: Three-dimensional structure of Plasmodium falciparum dihydrofolate reductase by homology building. Bioorganic and Medicinal Chemistry, 1999, 7, 1003-1011.	1.4	52
15	Solvent Diversity in Polymorph Screening. Journal of Pharmaceutical Sciences, 2008, 97, 2145-2159.	1.6	51
16	New leads of metallo-Î²-lactamase inhibitors from structure-based pharmacophore design. Bioorganic and Medicinal Chemistry, 2006, 14, 2627-2635.	1.4	50
17	Homology Modelling of the GABA Transporter and Analysis of Tiagabine Binding. ChemMedChem, 2010, 5, 986-1000.	1.6	50
18	Cyclynes. Part 5. Pericyclynes: "exploded cycloalkanes" with unusual orbital interactions and conformational properties. MM2 and STO-3G calculations, x-ray crystal structures, photoelectron spectra, and electron transmission spectra. Journal of the American Chemical Society, 1985, 107, 6556-6562.	6.6	49

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19	Human peptide transporters: therapeutic applications. Expert Opinion on Therapeutic Patents, 2002, 12, 1329-1350.	2.4	48
20	Primary structure and conformational analysis of peptide methionine-tyrosine, a peptide related to neuropeptide Y and peptide YY isolated from lamprey intestine. FEBS Journal, 1991, 199, 293-298.	0.2	47
21	G Protein- and Agonist-Bound Serotonin 5-HT2A Receptor Model Activated by Steered Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2011, 51, 315-325.	2.5	47
22	In Silico Predictions of hERG Channel Blockers in Drug Discovery: From Ligand-Based and Target-Based Approaches to Systems Chemical Biology. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 375-387.	0.6	44
23	Promising Tools in Prostate Cancer Research: Selective Non-Steroidal Cytochrome P450 17A1 Inhibitors. Scientific Reports, 2016, 6, 29468.	1.6	43
24	Salt Bridge Swapping in the EXXERFXYY Motif of Proton-coupled Oligopeptide Transporters. Journal of Biological Chemistry, 2015, 290, 29931-29940.	1.6	40
25	Assessing the relative importance of the biophysical properties of amino acid substitutions associated with human genetic disease. Human Mutation, 2002, 20, 98-109.	1.1	39
26	Biased cytochrome P450-mediated metabolism via small-molecule ligands binding P450 oxidoreductase. Nature Communications, 2021, 12, 2260.	5.8	34
27	Computational Prediction of Binding Affinity for CYP1A2-Ligand Complexes Using Empirical Free Energy Calculations. Drug Metabolism and Disposition, 2010, 38, 1347-1354.	1.7	33
28	Aldehyde Oxidase: Reaction Mechanism and Prediction of Site of Metabolism. ACS Omega, 2017, 2, 4237-4244.	1.6	33
29	Dissecting the Cytochrome P450 1A2â€•and 3A4â€Mediated Metabolism of Aflatoxin B1 in Ligand and Protein Contributions. Chemistry - A European Journal, 2017, 23, 2884-2893.	1.7	31
30	Disulfide conformational analysis. Tetrahedron, 1979, 35, 1399-1407.	1.0	29
31	Docking and scoring of metallo-Î²-lactamases inhibitors. Journal of Computer-Aided Molecular Design, 2004, 18, 287-302.	1.3	29
32	Insights into regioselective metabolism of mefenamic acid by cytochrome <scp>P</scp>450 <scp>BM</scp>3 mutants through crystallography, docking, molecular dynamics, and free energy calculations. Proteins: Structure, Function and Bioinformatics, 2016, 84, 383-396.	1.5	29
33	The electronic structure of .beta.-thioxoketones. A photoelectron spectroscopic study of the enol-enethiol tautomerism of thioacetylacetone and related compounds. Journal of the American Chemical Society, 1981, 103, 1350-1353.	6.6	26
34	Substrate-enzyme interactions and catalytic mechanism in phospholipase C: A molecular modeling study using the GRID program. Proteins: Structure, Function and Bioinformatics, 1992, 12, 331-338.	1.5	26
35	A Steered Molecular Dynamics Study of Binding and Translocation Processes in the GABA Transporter. PLoS ONE, 2012, 7, e39360.	1.1	26
36	QSAR Models for the Human H+/Peptide Symporter, hPEPT1:â€‰ Affinity Prediction Using Alignment-Independent Descriptors. Journal of Chemical Information and Modeling, 2008, 48, 233-241.	2.5	25

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37	Use of density functional theory in drug metabolism studies. Expert Opinion on Drug Metabolism and Toxicology, 2014, 10, 215-227.	1.5	25
38	A Quantitative Structureâ€“Activity Relationship for Translocation of Tripeptides via the Human Proton-Coupled Peptide Transporter, hPEPT1 (SLC15A1). AAPS Journal, 2010, 12, 385-396.	2.2	24
39	Mechanism of Cytochrome P450 17A1-Catalyzed Hydroxylase and Lyase Reactions. Journal of Chemical Information and Modeling, 2017, 57, 1123-1133.	2.5	24
40	Search for a trans-disulfide: structural analysis of di-tert-adamantyl disulfide by photoelectron spectroscopy, derivation of .sigma.I(t-Ad), and molecular mechanics calculations for related bulky disulfides. Journal of Organic Chemistry, 1980, 45, 1015-1020.	1.7	23
41	Molecular Mechanics Calculations of Proteins. Comparison of Different Energy Minimization Strategies. Journal of Biomolecular Structure and Dynamics, 1997, 15, 473-488.	2.0	22
42	Structural Differences of Matrix Metalloproteinases. Homology Modeling and Energy Minimization of Enzyme-Substrate Complexes. Journal of Biomolecular Structure and Dynamics, 2000, 17, 933-946.	2.0	22
43	.beta.-Thioxo ketones. 8. X-ray photoelectron-spectroscopic study of the enol-enethiol tautomerism of thioacetylacetone and related .beta.-thioxo ketones. Journal of the American Chemical Society, 1982, 104, 5922-5926.	6.6	20
44	Relationship between structure, conformational flexibility, and biological activity of agonists and antagonists at the N-methyl-D-aspartic acid subtype of excitatory amino acid receptors. Journal of Medicinal Chemistry, 1990, 33, 374-380.	2.9	20
45	Crystal and molecular structure of di-tert-adamantyl disulfide. Extension of the correlation between the sulfur-sulfur dihedral angle and the sulfur lone-pair energy gap. Journal of Organic Chemistry, 1980, 45, 5343-5347.	1.7	18
46	Substrate binding and catalytic mechanism in phospholipase C fromBacillus Cereus: A molecular mechanics and molecular dynamics study. , 1997, 42, 319-336.		18
47	Isolation of a Library of Aromadendranes fromLandolphiadulcisand Its Characterization Using the VolSurf Approach. Journal of Natural Products, 2004, 67, 799-805.	1.5	18
48	Development of a QSAR Model for Binding of Tripeptides and Tripeptidomimetics to the Human Intestinal Di-/Tripeptide Transporter hPEPT1. Pharmaceutical Research, 2006, 23, 483-492.	1.7	18
49	Correlations between core photoionization energies (EB1s) and gas-phase basicity. A general method for determining sites of protonation and intramolecular ion reorganization energies. Journal of the American Chemical Society, 1982, 104, 5019-5025.	6.6	17
50	An Optimized Screen Reduces the Number of GA Transporters and Provides Insights Into Nitrate Transporter 1/Peptide Transporter Family Substrate Determinants. Frontiers in Plant Science, 2019, 10, 1106.	1.7	17
51	Determination of protein conformation by isotopically labelled cross-linking and dedicated software: Application to the chaperone, calreticulin. International Journal of Mass Spectrometry, 2007, 268, 217-226.	0.7	16
52	Fast Methods for Prediction of Aldehyde Oxidase-Mediated Site-of-Metabolism. Computational and Structural Biotechnology Journal, 2019, 17, 345-351.	1.9	16
53	The low binding affinity of D-serine at the ionotropic glutamate receptor GluD2 can be attributed to the hinge region. Scientific Reports, 2017, 7, 46145.	1.6	15
54	Crystal structure of merosinigrin, an (ap,ap)-monothioacetal; structural properties of the thioglycosidic linkage. Carbohydrate Research, 1983, 123, 1-11.	1.1	14

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55	Conformational analysis of six- and twelve-membered ring compounds by molecular dynamics. , 1997, 11, 385-394.		14
56	Anti,anti acetals. Tetrahedron Letters, 1982, 23, 5221-5224.	0.7	13
57	Enantioselective endocrine disrupting effects of omeprazole studied in the H295R cell assay and by molecular modeling. Toxicology in Vitro, 2016, 34, 71-80.	1.1	13
58	Both Reactivity and Accessibility Are Important in Cytochrome P450 Metabolism: A Combined DFT and MD Study of Fenamic Acids in BM3 Mutants. Journal of Chemical Information and Modeling, 2019, 59, 743-753.	2.5	13
59	Crystal and molecular structure of anti-sesquinorbornene. Journal of Organic Chemistry, 1985, 50, 4395-4397.	1.7	12
60	HETEROTROPIC MODULATION OF SULFOTRANSFERASE 2A1 ACTIVITY BY CELECOXIB: PRODUCT RATIO SWITCHING OF ETHYNYLESTRADIOL SULFATION. Drug Metabolism and Disposition, 2004, 32, 1260-1264.	1.7	12
61	Polyethers. Tetrahedron, 1981, 37, 3671-3679.	1.0	10
62	Conformational restrictions in ligand binding to the human intestinal di-/tripeptide transporter: implications for design of hPEPT1 targeted prodrugs. Bioorganic and Medicinal Chemistry, 2005, 13, 1977-1988.	1.4	10
63	Structure-based optimisation of non-steroidal cytochrome P450 17A1 inhibitors. Chemical Communications, 2017, 53, 3118-3121.	2.2	9
64	PTR2/POT/NPF transporters: what makes them tick?. Advances in Protein Chemistry and Structural Biology, 2021, 123, 219-240.	1.0	9
65	cis-disulfides protelectron spectrum of a 6,7-dithiabicyclo[3.2.1]octane. Tetrahedron Letters, 1983, 24, 319-322.	0.7	8
66	Crystallization and preliminary X-ray analysis of a PNA-DNA complex. FEBS Letters, 1995, 363, 115-117.	1.3	8
67	Discovery of Ligands for the Human Intestinal Diâ€/Tripeptide Transporter (hPEPT1) Using a QSARâ€Assisted Virtual Screening Strategy. ChemMedChem, 2009, 4, 1439-1445.	1.6	8
68	Identification of CYP1A2 ligands by structure-based and ligand-based virtual screening. MedChemComm, 2011, 2, 853.	3.5	8
69	Synthesis and Antiangiogenic Activity of N-Alkylated Levamisole Derivatives. PLoS ONE, 2012, 7, e45405.	1.1	8
70	Density Functional Theory Study on the Formation of Reactive Benzoquinone Imines by Hydrogen Abstraction. Journal of Chemical Information and Modeling, 2015, 55, 660-666.	2.5	8
71	Synthesis and Structureâ€“Activity Relationships of Novel Non-Steroidal CYP17A1 Inhibitors as Potential Prostate Cancer Agents. Biomolecules, 2022, 12, 165.	1.8	8
72	In vitro evaluation of N-methyl amide tripeptidomimetics as substrates for the human intestinal di-/tri-peptide transporter hPEPT1. European Journal of Pharmaceutical Sciences, 2006, 28, 325-335.	1.9	7

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73	On the presence of extremely short Hâ€¦H non-bonded distances, and orbital interactions through eight Ïƒ bonds or through two methylene groups in tetramethanonaphthacenes.. Tetrahedron Letters, 1983, 24, 5415-5418.	0.7	6
74	Discovery of Novel Non-Steroidal Cytochrome P450 17A1 Inhibitors as Potential Prostate Cancer Agents. International Journal of Molecular Sciences, 2020, 21, 4868.	1.8	6
75	A Robust Force Field Based Method for Calculating Conformational Energies of Charged Drug-Like Molecules. Journal of Chemical Information and Modeling, 2012, 52, 409-419.	2.5	5
76	Structural analysis of Cytochrome P450 BM3 mutant M11 in complex with dithiothreitol. PLoS ONE, 2019, 14, e0217292.	1.1	5
77	Cyclic Acetals. Structural Analysis of 1,3-Dioxepine and Related Compounds. Helvetica Chimica Acta, 1985, 68, 2148-2157.	1.0	4
78	Computational prediction of solubilizersâ€™ effect on partitioning. International Journal of Pharmaceutics, 2007, 329, 46-52.	2.6	4
79	The anti-epileptic drug lamotrigine inhibits the CYP17A1 lyase reaction in vitroâ€. Biology of Reproduction, 2018, 99, 888-897.	1.2	3
80	Molecular Dynamics Simulations Reveal the Proton:Peptide Coupling Mechanism in the Bacterial Proton-Coupled Oligopeptide Transporter YbgH. ACS Omega, 2019, 4, 2040-2046.	1.6	3
81	Is the unique benzodiazepine structure interacting with CYP enzymes to affect steroid synthesis in vitro?. Journal of Steroid Biochemistry and Molecular Biology, 2021, 205, 105765.	1.2	0
82	Conformational Analysis and Pharmacophore Identification of Potential Drugs for Osteoporosis. , 2000, , 373-374.		0