# Flemming Steen JÃ¸rgensen

List of Publications by Year
in descending order



| 82 | 2,569 | 185998 28 | 214527 47 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 83 | 83 | 83 | 3170 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Synthesis and Structureâ€“Activity Relationships of Novel Non-Steroidal CYP17A1 Inhibitors as Potential Prostate Cancer Agents. Biomolecules, 2022, 12, 165. | 1.8 | 8 |
| 2 | 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 |
| 3 | PTR2/POT/NPF transporters: what makes them tick?. Advances in Protein Chemistry and Structural Biology, 2021, 123, 219-240. | 1.0 | 9 |
| 4 | Biased cytochrome P450-mediated metabolism via small-molecule ligands binding P450 oxidoreductase. Nature Communications, 2021, 12, 2260. | 5.8 | 34 |
| 5 | 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 |
| 6 | 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 |
| 7 | SMARTCyp 3.0: enhanced cytochrome P450 site-of-metabolism prediction server. Bioinformatics, 2019, 35, 3174-3175. | 1.8 | 53 |
| 8 | Structural analysis of Cytochrome P450 BM3 mutant M11 in complex with dithiothreitol. PLoS ONE, 2019, 14, e0217292. | 1.1 | 5 |
| 9 | Fast Methods for Prediction of Aldehyde Oxidase-Mediated Site-of-Metabolism. Computational and Structural Biotechnology Journal, 2019, 17, 345-351. | 1.9 | 16 |
| 10 | 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 |
| 11 | 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 |
| 12 | The anti-epileptic drug lamotrigine inhibits the CYP17A1 lyase reaction in vitroâ€. Biology of Reproduction, 2018, 99, 888-897. | 1.2 | 3 |
| 13 | 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 |
| 14 | Structure-based optimisation of non-steroidal cytochrome P450 17A1 inhibitors. Chemical Communications, 2017, 53, 3118-3121. | 2.2 | 9 |
| 15 | 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 |
| 16 | Mechanism of Cytochrome P450 17A1-Catalyzed Hydroxylase and Lyase Reactions. Journal of Chemical Information and Modeling, 2017, 57, 1123-1133. | 2.5 | 24 |
| 17 | Aldehyde Oxidase: Reaction Mechanism and Prediction of Site of Metabolism. ACS Omega, 2017, 2, 4237-4244. | 1.6 | 33 |
| 18 | Promising Tools in Prostate Cancer Research: Selective Non-Steroidal Cytochrome P450 17A1 Inhibitors. Scientific Reports, 2016, 6, 29468. | 1.6 | 43 |

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|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Salt Bridge Swapping in the EXXERFXYY Motif of Proton-coupled Oligopeptide Transporters. Journal of Biological Chemistry, 2015, 290, 29931-29940. | 1.6 | 40 |
| 22 | 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 |
| 23 | Prediction of cytochrome P450 mediated metabolism. Advanced Drug Delivery Reviews, 2015, 86, 61-71. | 6.6 | 78 |
| 24 | Use of density functional theory in drug metabolism studies. Expert Opinion on Drug Metabolism and Toxicology, 2014, 10, 215-227. | 1.5 | 25 |
| 25 | 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 |
| 26 | Synthesis and Antiangiogenic Activity of N-Alkylated Levamisole Derivatives. PLoS ONE, 2012, 7, e45405. | 1.1 | 8 |
| 27 | A Steered Molecular Dynamics Study of Binding and Translocation Processes in the GABA Transporter. PLoS ONE, 2012, 7, e39360. | 1.1 | 26 |
| 28 | 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 |
| 29 | 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 |
| 30 | Identification of CYP1A2 ligands by structure-based and ligand-based virtual screening. MedChemComm, 2011, 2, 853. | 3.5 | 8 |
| 31 | 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 |
| 32 | Homology Modelling of the GABA Transporter and Analysis of Tiagabine Binding. ChemMedChem, 2010, 5, 986-1000. | 1.6 | 50 |
| 33 | 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 |
| 34 | 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 |
| 35 | Classification of Cytochrome P450 1A2 Inhibitors and Noninhibitors by Machine Learning Techniques. Drug Metabolism and Disposition, 2009, 37, 658-664. | 1.7 | 91 |
| 36 | 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 |

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| 37 | 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 |
| 38 | Solvent Diversity in Polymorph Screening. Journal of Pharmaceutical Sciences, 2008, 97, 2145-2159. | 1.6 | 51 |
| 39 | hERG Classification Model Based on a Combination of Support Vector Machine Method and GRIND Descriptors. Molecular Pharmaceutics, 2008, 5, 117-127. | 2.3 | 91 |
| 40 | 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 |
| 41 | Computational prediction of solubilizersâ€™ effect on partitioning. International Journal of Pharmaceutics, 2007, 329, 46-52. | 2.6 | 4 |
| 42 | 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 |
| 43 | Identification of a gene on chromosome 12q22 uniquely overexpressed in chronic lymphocytic leukemia. Blood, 2006, 107, 2904-2911. | 0.6 | 55 |
| 44 | New leads of metallo-Î²-lactamase inhibitors from structure-based pharmacophore design. Bioorganic and Medicinal Chemistry, 2006, 14, 2627-2635. | 1.4 | 50 |
| 45 | Prediction of pH-Dependent Aqueous Solubility of Druglike Molecules. Journal of Chemical Information and Modeling, 2006, 46, 2601-2609. | 2.5 | 84 |
| 46 | 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 |
| 47 | 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 |
| 48 | 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 |
| 49 | Prediction methods and databases within chemoinformatics: emphasis on drugs and drug candidates. Bioinformatics, 2005, 21, 2145-2160. | 1.8 | 98 |
| 50 | Docking and scoring of metallo-Î²-lactamases inhibitors. Journal of Computer-Aided Molecular Design, 2004, 18, 287-302. | 1.3 | 29 |
| 51 | Isolation of a Library of Aromadendranes fromLandolphiadulcisand Its Characterization Using the VolSurf Approach. Journal of Natural Products, 2004, 67, 799-805. | 1.5 | 18 |
| 52 | 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 |
| 53 | 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 |
| 54 | Human peptide transporters: therapeutic applications. Expert Opinion on Therapeutic Patents, 2002, 12, 1329-1350. | 2.4 | 48 |

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| 55 | 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 |
| 56 | 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 |
| 57 | 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 |
| 58 | 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 |
| 59 | Conformational Analysis and Pharmacophore Identification of Potential Drugs for Osteoporosis. , 2000, , 373-374. | | 0 |
| 60 | 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 |
| 61 | Molecular Mechanics Calculations of Proteins. Comparison of Different Energy Minimization Strategies. Journal of Biomolecular Structure and Dynamics, 1997, 15, 473-488. | 2.0 | 22 |
| 62 | Conformational analysis of six- and twelve-membered ring compounds by molecular dynamics. , 1997, 11, 385-394. | | 14 |
| 63 | Substrate binding and catalytic mechanism in phospholipase C fromBacillus Cereus: A molecular mechanics and molecular dynamics study. , 1997, 42, 319-336. | | 18 |
| 64 | Crystallization and preliminary X-ray analysis of a PNA-DNA complex. FEBS Letters, 1995, 363, 115-117. | 1.3 | 8 |
| 65 | GABAA Receptor Agonists, Partial Agonists, and Antagonists. Design and Therapeutic Prospects. Journal of Medicinal Chemistry, 1994, 37, 2489-2505. | 2.9 | 99 |
| 66 | 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 |
| 67 | 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 |
| 68 | 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 |
| 69 | Cyclic Acetals. Structural Analysis of 1,3-Dioxepine and Related Compounds. Helvetica Chimica Acta, 1985, 68, 2148-2157. | 1.0 | 4 |
| 70 | 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 |
| 71 | Crystal and molecular structure of anti-sesquinorbornene. Journal of Organic Chemistry, 1985, 50, 4395-4397. | 1.7 | 12 |
| 72 | cis-disulfides protelectron spectrum of a 6,7-dithiabicyclo[3.2.1]octane. Tetrahedron Letters, 1983, 24, 319-322. | 0.7 | 8 |

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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 | Crystal structure of merosinigrin, an (ap,ap)-monothioacetal; structural properties of the thioglycosidic linkage. Carbohydrate Research, 1983, 123, 1-11. | 1.1 | 14 |
| 75 | .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 |
| 76 | 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 |
| 77 | Anti,anti acetals. Tetrahedron Letters, 1982, 23, 5221-5224. | 0.7 | 13 |
| 78 | 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 |
| 79 | Polyethers. Tetrahedron, 1981, 37, 3671-3679. | 1.0 | 10 |
| 80 | 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 |
| 81 | 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 |
| 82 | Disulfide conformational analysis. Tetrahedron, 1979, 35, 1399-1407. | 1.0 | 29 |