Pieter F W Stouten

List of Publications by Year in descending order

48 papers	2,118 citations	304602 22 h-index	233338 45 g-index
50 all docs	50 docs citations	50 times ranked	2490 citing authors

#	Article	IF	Citations
1	Multitask machine learning models for predicting lipophilicity (logP) in the SAMPL7 challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 901-909.	1.3	13
2	Identification of GLPG/ABBV-2737, a Novel Class of Corrector, Which Exerts Functional Synergy With Other CFTR Modulators. Frontiers in Pharmacology, 2019, 10, 514.	1.6	29
3	Shedding Light on Important Waters for Drug Design: Simulations versus Grid-Based Methods. Journal of Chemical Information and Modeling, 2018, 58, 692-699.	2.5	41
4	Discovery of N-(3-Carbamoyl-5,5,7,7-tetramethyl-5,7-dihydro-4H-thieno[2,3-c]pyran-2-yl)-lH-pyrazole-5-carboxamide (GLPG1837), a Novel Potentiator Which Can Open Class III Mutant Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) Channels to a High Extent. Journal of Medicinal Chemistry, 2018, 61, 1425-1435.	2.9	52
5	Identification and Characterization of Novel CFTR Potentiators. Frontiers in Pharmacology, 2018, 9, 1221.	1.6	32
6	Reinvestigation of the Branimycin Stereochemistry at Position 17-C. Organic Letters, 2016, 18, 780-783.	2.4	11
7	Strategies for Small Molecule Library Design. Current Pharmaceutical Design, 2014, 20, 3314-3322.	0.9	13
8	Identification of phosphorylase kinase as a novel therapeutic target through high-throughput screening for anti-angiogenesis compounds in zebrafish. Oncogene, 2012, 31, 4333-4342.	2.6	43
9	The Design and Application of Target-Focused Compound Libraries. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 521-531.	0.6	98
10	Novel, Customizable Scoring Functions, Parameterized Using N-PLS, for Structure-Based Drug Discovery. Journal of Chemical Information and Modeling, 2007, 47, 85-91.	2.5	25
11	Inhibition of proteinâ€“protein interactions: The discovery of druglike Î²â€catenin inhibitors by combining virtual and biophysical screening. Proteins: Structure, Function and Bioinformatics, 2006, 64, 60-67.	1.5	177
12	Quantitative determination of the topological propensities of amyloidogenic peptides. Biophysical Chemistry, 2006, 120, 55-61.	1.5	9
13	Linear and Nonlinear Methods in Modeling the Aqueous Solubility of Organic Compounds.. ChemInform, 2005, 36, no.	0.1	0
14	Understanding and modulating cyclin-dependent kinase inhibitor specificity: molecular modeling and biochemical evaluation of pyrazolopyrimidinones as CDK2/cyclin A and CDK4/cyclin D1 inhibitors. Journal of Computer-Aided Molecular Design, 2005, 19, 111-122.	1.3	13
15	Virtual screening to enrich a compound collection with CDK2 inhibitors using docking, scoring, and composite scoring models. Proteins: Structure, Function and Bioinformatics, 2005, 60, 629-643.	1.5	19
16	Linear and Nonlinear Methods in Modeling the Aqueous Solubility of Organic Compounds. Journal of Chemical Information and Modeling, 2005, 45, 170-176.	2.5	41
17	Assessment of Docking Poses: Interactions-Based Accuracy Classification (IBAC) versus Crystal Structure Deviations.. ChemInform, 2004, 35, no.	0.1	0
18	Novel Scoring Functions Comprising QXP, SASA, and Protein Side-Chain Entropy Terms.. ChemInform, 2004, 35, no.	0.1	0

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19	Influence of Molecular Flexibility and Polar Surface Area Metrics on Oral Bioavailability in the Rat. Journal of Medicinal Chemistry, 2004, 47, 6104-6107.	2.9	167
20	Novel Scoring Functions Comprising QXP, SASA, and Protein Side-Chain Entropy Terms. Journal of Chemical Information and Computer Sciences, 2004, 44, 882-893.	2.8	34
21	Assessment of Docking Poses:â€‰ Interactions-Based Accuracy Classification (IBAC) versus Crystal Structure Deviations. Journal of Chemical Information and Computer Sciences, 2004, 44, 871-881.	2.8	116
22	Synthesis and Biological Evaluation of 1-Aryl-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-4-one Inhibitors of Cyclin-Dependent Kinases. Journal of Medicinal Chemistry, 2004, 47, 5894-5911.	2.9	93
23	Does a diol cyclic urea inhibitor of HIV-1 protease bind tighter than its corresponding alcohol form? A study by free energy perturbation and continuum electrostatics calculations. Journal of Computer-Aided Molecular Design, 2001, 15, 145-156.	1.3	12
24	Synthesis and activity studies of conformationally restricted Î±-ketoamide factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 1253-1256.	1.0	14
25	The de novo design and synthesis of cyclic urea inhibitors of factor Xa: optimization of the S4 ligand. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 301-304.	1.0	15
26	Design, Synthesis, and Biological Evaluation of Potent and Selective Amidino Bicyclic Factor Xa Inhibitors. Journal of Medicinal Chemistry, 2000, 43, 4398-4415.	2.9	46
27	Preparation of pyrrolidine and isoxazolidine benzamidines as potent inhibitors of coagulation factor Xa. Bioorganic and Medicinal Chemistry Letters, 1999, 9, 1195-1200.	1.0	12
28	The de novo design and synthesis of cyclic urea inhibitors of factor Xa: Initial sar studies. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 2705-2710.	1.0	22
29	Rational Design and Synthesis of Novel, Potent Bis-phenylamidine Carboxylate Factor Xa Inhibitors. Journal of Medicinal Chemistry, 1998, 41, 53-62.	2.9	49
30	Bisbenzamidine isoxazoline derivatives as factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 1997, 7, 2813-2818.	1.0	31
31	The synthesis of lysine Î±-ketoamide thrombin inhibitord via an epoxy amide ring opening. Tetrahedron Letters, 1997, 38, 5741-5744.	0.7	8
32	A comparison of structural and dynamic properties of different simulation methods applied to SH3. Biophysical Journal, 1996, 70, 684-692.	0.2	48
33	Type IIâ€˜ to Type I Î²-Turn Swap Changes Specificity for Integrins. Journal of the American Chemical Society, 1996, 118, 293-294.	6.6	118
34	(N-acyl-N-alkyl)glycyl borolysine analogs: A new class of potent thrombin inhibitors. Bioorganic and Medicinal Chemistry Letters, 1996, 6, 2913-2918.	1.0	15
35	A molecular mechanics/grid method for evaluation of ligand-receptor interactions. Journal of Computational Chemistry, 1995, 16, 454-464.	1.5	175
36	How does the switch II region of G-domains work?. FEBS Letters, 1993, 320, 1-6.	1.3	75

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37	An Effective Solvation Term Based on Atomic Occupancies for Use in Protein Simulations. Molecular Simulation, 1993, 10, 97-120.	0.9	271
38	Interchain cysteine bridges control entry of progesterone to the central cavity of the uteroglobin dimer. Protein Engineering, Design and Selection, 1992, 5, 351-359.	1.0	17
39	New triple-helical model for the shaft of the adenovirus fibre. Journal of Molecular Biology, 1992, 226, 1073-1084.	2.0	83
40	Structure-function relationship for the highly toxic crotoxin from Crotalus durissus terrificus. European Biophysics Journal, 1992, 21, 199-205.	1.2	6
41	Hydrogen bonds in concreto and in computro: the sequel. Journal of Molecular Structure, 1991, 243, 61-87.	1.8	8
42	Crystal and molecular structure of sodium picrate monohydrate. Journal of Crystallographic and Spectroscopic Research, 1991, 21, 553-557.	0.3	3
43	Computation Confirms Contraction: A Molecular Dynamics Study of Liquid Methanol, Water and a Methanol-Water Mixture. Molecular Simulation, 1990, 5, 175-179.	0.9	16
44	Molecular Dynamics Simulations of some Small Organic Molecules. Molecular Simulation, 1989, 4, 193-207.	0.9	5
45	Conformational aspects of Î±-hydroxy carboxylic acids, the heralds of stereochemistry. Computational and Theoretical Chemistry, 1989, 200, 169-187.	1.5	13
46	Hydrogen bonds in concreto and in computro. Journal of Molecular Structure, 1988, 177, 467-475.	1.8	17
47	Conformational aspects of malic acid: A multidisciplinary approach. Journal of Molecular Structure, 1988, 189, 65-80.	1.8	8
48	Coordination chemistry of alkali and alkaline earth cationsâ€"synthesis and X-ray structural analysis of sodium(picrate)-(1,10-phenanthroline)2. Polyhedron, 1987, 6, 1833-1837.	1.0	5