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	An Effective Solvation Term Based on Atomic Occupancies for Use in Protein Simulations. Molecular Simulation, 1993, 10, 97-120.	0.9	271
2	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
3	A molecular mechanics/grid method for evaluation of ligand-receptor interactions. Journal of Computational Chemistry, 1995, 16, 454-464.	1.5	175
4	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
5	Type Iâ€˜ to Type I Î²-Turn Swap Changes Specificity for Integrins. Journal of the American Chemical Society, 1996, 118, 293-294.	6.6	118
6	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
7	The Design and Application of Target-Focused Compound Libraries. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 521-531.	0.6	98
8	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
9	New triple-helical model for the shaft of the adenovirus fibre. Journal of Molecular Biology, 1992, 226, 1073-1084.	2.0	83
10	How does the switch II region of G-domains work?. FEBS Letters, 1993, 320, 1-6.	1.3	75
11	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
12	Rational Design and Synthesis of Novel, Potent Bis-phenylamidine Carboxylate Factor Xa Inhibitors. Journal of Medicinal Chemistry, 1998, 41, 53-62.	2.9	49
13	A comparison of structural and dynamic properties of different simulation methods applied to SH3. Biophysical Journal, 1996, 70, 684-692.	0.2	48
14	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
15	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
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	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
18	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

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19	Identification and Characterization of Novel CFTR Potentiators. Frontiers in Pharmacology, 2018, 9, 1221.	1.6	32
20	Bisbenzamidine isoxazoline derivatives as factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 1997, 7, 2813-2818.	1.0	31
21	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
22	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
23	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
24	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
25	Hydrogen bonds in concreto and in computro. Journal of Molecular Structure, 1988, 177, 467-475.	1.8	17
26	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
27	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
28	(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
29	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
30	Synthesis and activity studies of conformationally restricted Î±-ketoamide factor Xa inhibitors. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 1253-1256.	1.0	14
31	Conformational aspects of Î±-hydroxy carboxylic acids, the heralds of stereochemistry. Computational and Theoretical Chemistry, 1989, 200, 169-187.	1.5	13
32	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
33	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
34	Strategies for Small Molecule Library Design. Current Pharmaceutical Design, 2014, 20, 3314-3322.	0.9	13
35	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
36	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

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37	Reinvestigation of the Branimycin Stereochemistry at Position 17-C. Organic Letters, 2016, 18, 780-783.	2.4	11
38	Quantitative determination of the topological propensities of amyloidogenic peptides. Biophysical Chemistry, 2006, 120, 55-61.	1.5	9
39	Conformational aspects of malic acid: A multidisciplinary approach. Journal of Molecular Structure, 1988, 189, 65-80.	1.8	8
40	Hydrogen bonds in concreto and in computro: the sequel. Journal of Molecular Structure, 1991, 243, 61-87.	1.8	8
41	The synthesis of lysine Î±-ketoamide thrombin inhibitord via an epoxy amide ring opening. Tetrahedron Letters, 1997, 38, 5741-5744.	0.7	8
42	Structure-function relationship for the highly toxic crotoxin from Crotalus durissus terrificus. European Biophysics Journal, 1992, 21, 199-205.	1.2	6
43	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
44	Molecular Dynamics Simulations of some Small Organic Molecules. Molecular Simulation, 1989, 4, 193-207.	0.9	5
45	Crystal and molecular structure of sodium picrate monohydrate. Journal of Crystallographic and Spectroscopic Research, 1991, 21, 553-557.	0.3	3
46	Assessment of Docking Poses: Interactions-Based Accuracy Classification (IBAC) versus Crystal Structure Deviations.. ChemInform, 2004, 35, no.	0.1	0
47	Novel Scoring Functions Comprising QXP, SASA, and Protein Side-Chain Entropy Terms.. ChemInform, 2004, 35, no.	0.1	0
48	Linear and Nonlinear Methods in Modeling the Aqueous Solubility of Organic Compounds.. ChemInform, 2005, 36, no.	0.1	0