Herman W T Van Vlijmen

List of Publications by Year
in descending order

65 papers	3,902 citations	126907 33 h-index	123424 61 g-index
66 all docs	66 docs citations	66 times ranked	5808 citing authors

#	Article	IF	Citations
1	Divide and Conquer. Pocket-Opening Mixed-Solvent Simulations in the Perspective of Docking Virtual Screening Applications for Drug Discovery. Journal of Chemical Information and Modeling, 2022, 62, 533-543.	5.4	3
2	The Impact of Experimental and Calculated Error on the Performance of Affinity Predictions. Journal of Chemical Information and Modeling, 2022, 62, 703-717.	5.4	4
3	The performance of ensemble-based free energy protocols in computing binding affinities to ROS1 kinase. Scientific Reports, 2022, 12, .	3.3	2
4	Identification of novel inhibitors of rat Mrp3. European Journal of Pharmaceutical Sciences, 2021, 162, 105813.	4.0	1
5	Mechanism of covalent binding of ibrutinib to Bruton's tyrosine kinase revealed by QM/MM calculations. Chemical Science, 2021, 12, 5511-5516.	7.4	22
6	DrugEx v2: de novo design of drug molecules by Pareto-based multi-objective reinforcement learning in polypharmacology. Journal of Cheminformatics, 2021, 13, 85.	6.1	30
7	The Need of Industry to Go FAIR. Data Intelligence, 2020, 2, 276-284.	1.5	20
8	Large scale relative protein ligand binding affinities using non-equilibrium alchemy. Chemical Science, 2020, 11, 1140-1152.	7.4	147
9	Accuracy and Precision of Alchemical Relative Free Energy Predictions with and without Replicaâ€Exchange. Advanced Theory and Simulations, 2020, 3, 1900195.	2.8	30
10	Annotation of Allosteric Compounds to Enhance Bioactivity Modeling for Class A GPCRs. Journal of Chemical Information and Modeling, 2020, 60, 4664-4672.	5.4	2
11	FEP+ calculations predict a stereochemical SAR switch for first-in-class indoline NIK inhibitors for multiple myeloma. Future Drug Discovery, 2020, 2, .	2.1	2
12	Assessment of the Fragment Docking Program SEED. Journal of Chemical Information and Modeling, 2020, 60, 4881-4893.	5.4	9
13	Successive Statistical and Structure-Based Modeling to Identify Chemically Novel Kinase Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 4283-4295.	5.4	4
14	Quantitative prediction of selectivity between the A1 and A2A adenosine receptors. Journal of Cheminformatics, 2020, 12, 33.	6.1	10
15	Accurate Prediction of GPCR Ligand Binding Affinity with Free Energy Perturbation. Journal of Chemical Information and Modeling, 2020, 60, 5563-5579.	5.4	45
16	Application of the ESMACS Binding Free Energy Protocol to a Multiâ€Binding Site Lactate Dehydogenase A Ligand Dataset. Advanced Theory and Simulations, 2020, 3, 1900194.	2.8	9
17	Limitations of Ligand-Only Approaches for Predicting the Reactivity of Covalent Inhibitors. Journal of Chemical Information and Modeling, 2019, 59, 4220-4227.	5.4	15
18	An exploration strategy improves the diversity of de novo ligands using deep reinforcement learning: a case for the adenosine A2A receptor. Journal of Cheminformatics, 2019, 11, 35.	6.1	58

#	Article	IF	Citations
19	Application of ESMACS binding free energy protocols to diverse datasets: Bromodomain-containing protein 4. Scientific Reports, 2019, 9, 6017.	3.3	18
20	Identification of novel small molecule inhibitors for solute carrier SGLT1 using proteochemometric modeling. Journal of Cheminformatics, 2019, 11, 15.	6.1	17
21	Advances and Challenges in Computational Target Prediction. Journal of Chemical Information and Modeling, 2019, 59, 1728-1742.	5.4	76
22	Predicting Activity Cliffs with Free-Energy Perturbation. Journal of Chemical Theory and Computation, 2019, 15, 1884-1895.	5.3	37
23	Large-Scale Validation of Mixed-Solvent Simulations to Assess Hotspots at Proteinâ€“Protein Interaction Interfaces. Journal of Chemical Information and Modeling, 2018, 58, 784-793.	5.4	29
24	Predicting Binding Free Energies of PDE2 Inhibitors. The Difficulties of Protein Conformation. Scientific Reports, 2018, 8, 4883.	3.3	43
25	Chemical space screening around Phe3 in opioid peptides: Modulating Âµ versus Î´ agonism by Suzuki-Miyaura cross-couplings. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 2320-2323.	2.2	4
26	Molecular Modeling of Drugâ€“Transporter Interactionsâ€”An International Transporter Consortium Perspective. Clinical Pharmacology and Therapeutics, 2018, 104, 818-835.	4.7	43
27	Acylguanidine Beta Secretase 1 Inhibitors: A Combined Experimental and Free Energy Perturbation Study. Journal of Chemical Theory and Computation, 2017, 13, 1439-1453.	5.3	67
28	Beyond the hype: deep neural networks outperform established methods using a ChEMBL bioactivity benchmark set. Journal of Cheminformatics, 2017, 9, 45.	6.1	219
29	Identification of Allosteric Modulators of Metabotropic Glutamate 7 Receptor Using Proteochemometric Modeling. Journal of Chemical Information and Modeling, 2017, 57, 2976-2985.	5.4	18
30	The Suzukiâ€“Miyaura Cross-Coupling as a Versatile Tool for Peptide Diversification and Cyclization. Catalysts, 2017, 7, 74.	3.5	58
31	The ELF Honest Data Broker: informatics enabling publicâ€“private collaboration in a precompetitive arena. Drug Discovery Today, 2016, 21, 97-102.	6.4	21
32	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. ACS Omega, 2016, 1, 293-304.	3.5	108
33	Interacting with GPCRs: Using Interaction Fingerprints for Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 2053-2060.	5.4	12
34	In search of novel ligands using a structure-based approach: a case study on the adenosine A2A receptor. Journal of Computer-Aided Molecular Design, 2016, 30, 863-874.	2.9	20
35	Extending kinome coverage by analysis of kinase inhibitor broad profiling data. Drug Discovery Today, 2015, 20, 652-658.	6.4	46
36	Selecting an Optimal Number of Binding Site Waters To Improve Virtual Screening Enrichments Against the Adenosine A_{2A} Receptor. Journal of Chemical Information and Modeling, 2014, 54, 1737-1746.	5.4	49

#	Article	IF	Citations
37	Significantly Improved HIV Inhibitor Efficacy Prediction Employing Proteochemometric Models Generated From Antivirogram Data. PLoS Computational Biology, 2013, 9, e1002899.	3.2	42
38	Cheminformatics. Communications of the ACM, 2012, 55, 65-75.	4.5	21
39	Identifying Novel Adenosine Receptor Ligands by Simultaneous Proteochemometric Modeling of Rat and Human Bioactivity Data. Journal of Medicinal Chemistry, 2012, 55, 7010-7020.	6.4	45
40	Proteochemometric modeling as a tool to design selective compounds and for extrapolating to novel targets. MedChemComm, 2011, 2, 16-30.	3.4	138
41	Structure-Based Site of Metabolism Prediction for Cytochrome P450 2D6. Journal of Medicinal Chemistry, 2011, 54, 6098-6105.	6.4	44
42	Chemogenomics Approaches for Receptor Deorphanization and Extensions of the Chemogenomics Concept to Phenotypic Space. Current Topics in Medicinal Chemistry, 2011, 11, 1964-1977.	2.1	18
43	Which Compound to Select in Lead Optimization? Prospectively Validated Proteochemometric Models Guide Preclinical Development. PLoS ONE, 2011, 6, e27518.	2.5	47
44	Mining protein dynamics from sets of crystal structures using â€œconsensus structuresâ€: Protein Science, 2010, 19, 742-752.	7.6	14
45	Binding of a potent small-molecule inhibitor of six-helix bundle formation requires interactions with both heptad-repeats of the RSV fusion protein. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 308-313.	7.1	81
46	Advantages of predicted phenotypes and statistical learning models in inferring virological response to antiretroviral therapy from HIV genotype. Antiviral Therapy, 2009, 14, 273-283.	1.0	10
47	A knowledgeâ€based forcefield for proteinâ€“protein interface design. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1540-1550.	2.6	13
48	Structureâ€“activity relationship of ortho- and meta-phenol based LFA-1 ICAM inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 5245-5248.	2.2	8
49	Recent Advances in Chemoinformatics. Journal of Chemical Information and Modeling, 2007, 47, 1279-1293.	5.4	57
50	Trends in Antibody Sequence Changes during the Somatic Hypermutation Process. Journal of Immunology, 2006, 177, 333-340.	0.8	102
51	Affinity enhancement of an in vivo matured therapeutic antibody using structure-based computational design. Protein Science, 2006, 15, 949-960.	7.6	160
52	Structure activity relationships of monocyte chemoattractant proteins in complex with a blocking antibody. Protein Engineering, Design and Selection, 2006, 19, 317-324.	2.1	27
53	Normal Mode Calculations of Icosahedral Viruses with Full Dihedral Flexibility by Use of Molecular Symmetry. Journal of Molecular Biology, 2005, 350, 528-542.	4.2	66
54	Mutations of the Anti-Mul̀lerian Hormone Gene in Patients with Persistent Mul̀lerian Duct Syndrome: Biosynthesis, Secretion, and Processing of the Abnormal Proteins and Analysis Using a Three-Dimensional Model. Molecular Endocrinology, 2004, 18, 708-721.	3.7	81

#	Article	IF	Citations
55	Novel Bicyclic Piperazine Derivatives of Triazolotriazine and Triazolopyrimidines as Highly Potent and Selective Adenosine A2A Receptor Antagonists. Journal of Medicinal Chemistry, 2004, 47, 6218-6229.	6.4	62
56	A classification of disulfide patterns and its relationship to protein structure and function. Protein Science, 2004, 13, 2045-2058.	7.6	31
57	A Novel Database of Disulfide Patterns and its Application to the Discovery of Distantly Related Homologs. Journal of Molecular Biology, 2004, 335, 1083-1092.	4.2	56
58	The CRIPTO/FRL-1/CRYPTIC (CFC) domain of human Cripto. FEBS Journal, 2003, 270, 3610-3618.	0.2	17
59	Identification of a New Murine Tumor Necrosis Factor Receptor Locus That Contains Two Novel Murine Receptors for Tumor Necrosis Factor-related Apoptosis-inducing Ligand (TRAIL). Journal of Biological Chemistry, 2003, 278, 5444-5454.	3.4	116
60	Identification of Potent and Novel Î±4Î²1 Antagonists Using in Silico Screening. Journal of Medicinal Chemistry, 2002, 45, 2988-2993.	6.4	67
61	Normal mode analysis of large systems with icosahedral symmetry: Application to (Dialanine)60 in full and reduced basis set implementations. Journal of Chemical Physics, 2001, 115, 691-698.	3.0	32
62	Analysis of Calculated Normal Modes of a Set of Native and Partially Unfolded Proteins. Journal of Physical Chemistry B, 1999, 103, 3009-3021.	2.6	48
63	The role of polar interactions in the molecular recognition of CD40L with its receptor CD40. Protein Science, 1998, 7, 1124-1135.	7.6	67
64	Evaluation of comparative protein modeling by MODELLER. Proteins: Structure, Function and Bioinformatics, 1995, 23, 318-326.	2.6	1,035
65	A model for the antagonist binding site on the adenosine A1 receptor, based on steric, electrostatic, and hydrophobic properties. Journal of Medicinal Chemistry, 1990, 33, 1708-1713.	6.4	52