# Herman W T Van Vlijmen

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Evaluation of comparative protein modeling by MODELLER. Proteins: Structure, Function and Bioinformatics, 1995, 23, 318-326. | 2.6 | 1,035 |
| 2 | Beyond the hype: deep neural networks outperform established methods using a ChEMBL bioactivity benchmark set. Journal of Cheminformatics, 2017, 9, 45. | 6.1 | 219 |
| 3 | Affinity enhancement of an in vivo matured therapeutic antibody using structure-based computational design. Protein Science, 2006, 15, 949-960. | 7.6 | 160 |
| 4 | Large scale relative protein ligand binding affinities using non-equilibrium alchemy. Chemical Science, 2020, 11, 1140-1152. | 7.4 | 147 |
| 5 | Proteochemometric modeling as a tool to design selective compounds and for extrapolating to novel targets. MedChemComm, 2011, 2, 16-30. | 3.4 | 138 |
| 6 | 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 |
| 7 | Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. ACS Omega, 2016, 1, 293-304. | 3.5 | 108 |
| 8 | Trends in Antibody Sequence Changes during the Somatic Hypermutation Process. Journal of Immunology, 2006, 177, 333-340. | 0.8 | 102 |
| 9 | Mutations of the Anti-MuÌllerian Hormone Gene in Patients with Persistent MuÌllerian 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 |
| 10 | 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 |
| 11 | Advances and Challenges in Computational Target Prediction. Journal of Chemical Information and Modeling, 2019, 59, 1728-1742. | 5.4 | 76 |
| 12 | The role of polar interactions in the molecular recognition of CD40L with its receptor CD40. Protein Science, 1998, 7, 1124-1135. | 7.6 | 67 |
| 13 | Identification of Potent and Novel Î±4Î²1 Antagonists Using in Silico Screening. Journal of Medicinal Chemistry, 2002, 45, 2988-2993. | 6.4 | 67 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | The Suzukiâ€“Miyaura Cross-Coupling as a Versatile Tool for Peptide Diversification and Cyclization. Catalysts, 2017, 7, 74. | 3.5 | 58 |
| 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 |

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|---|---|---|---|
| 19 | Recent Advances in Chemoinformatics. Journal of Chemical Information and Modeling, 2007, 47, 1279-1293. | 5.4 | 57 |
| 20 | 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 |
| 21 | 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 |
| 22 | Selecting an Optimal Number of Binding Site Waters To Improve Virtual Screening Enrichments Against the Adenosine A<sub>2A</sub> Receptor. Journal of Chemical Information and Modeling, 2014, 54, 1737-1746. | 5.4 | 49 |
| 23 | 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 |
| 24 | Which Compound to Select in Lead Optimization? Prospectively Validated Proteochemometric Models Guide Preclinical Development. PLoS ONE, 2011, 6, e27518. | 2.5 | 47 |
| 25 | Extending kinome coverage by analysis of kinase inhibitor broad profiling data. Drug Discovery Today, 2015, 20, 652-658. | 6.4 | 46 |
| 26 | 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 |
| 27 | Accurate Prediction of GPCR Ligand Binding Affinity with Free Energy Perturbation. Journal of Chemical Information and Modeling, 2020, 60, 5563-5579. | 5.4 | 45 |
| 28 | Structure-Based Site of Metabolism Prediction for Cytochrome P450 2D6. Journal of Medicinal Chemistry, 2011, 54, 6098-6105. | 6.4 | 44 |
| 29 | Predicting Binding Free Energies of PDE2 Inhibitors. The Difficulties of Protein Conformation. Scientific Reports, 2018, 8, 4883. | 3.3 | 43 |
| 30 | Molecular Modeling of Drugâ€“Transporter Interactionsâ€”An International Transporter Consortium Perspective. Clinical Pharmacology and Therapeutics, 2018, 104, 818-835. | 4.7 | 43 |
| 31 | Significantly Improved HIV Inhibitor Efficacy Prediction Employing Proteochemometric Models Generated From Antivirogram Data. PLoS Computational Biology, 2013, 9, e1002899. | 3.2 | 42 |
| 32 | Predicting Activity Cliffs with Free-Energy Perturbation. Journal of Chemical Theory and Computation, 2019, 15, 1884-1895. | 5.3 | 37 |
| 33 | 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 |
| 34 | A classification of disulfide patterns and its relationship to protein structure and function. Protein Science, 2004, 13, 2045-2058. | 7.6 | 31 |
| 35 | Accuracy and Precision of Alchemical Relative Free Energy Predictions with and without Replicaâ€Exchange. Advanced Theory and Simulations, 2020, 3, 1900195. | 2.8 | 30 |
| 36 | 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 |

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|---|---|---|---|
| 37 | 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 |
| 38 | 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 |
| 39 | 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 |
| 40 | Cheminformatics. Communications of the ACM, 2012, 55, 65-75. | 4.5 | 21 |
| 41 | The ELF Honest Data Broker: informatics enabling publicâ€“private collaboration in a precompetitive arena. Drug Discovery Today, 2016, 21, 97-102. | 6.4 | 21 |
| 42 | 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 |
| 43 | The Need of Industry to Go FAIR. Data Intelligence, 2020, 2, 276-284. | 1.5 | 20 |
| 44 | 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 |
| 45 | 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 |
| 46 | Application of ESMACS binding free energy protocols to diverse datasets: Bromodomain-containing protein 4. Scientific Reports, 2019, 9, 6017. | 3.3 | 18 |
| 47 | The CRIPTO/FRL-1/CRYPTIC (CFC) domain of human Cripto. FEBS Journal, 2003, 270, 3610-3618. | 0.2 | 17 |
| 48 | Identification of novel small molecule inhibitors for solute carrier SGLT1 using proteochemometric modeling. Journal of Cheminformatics, 2019, 11, 15. | 6.1 | 17 |
| 49 | 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 |
| 50 | Mining protein dynamics from sets of crystal structures using â€œconsensus structuresâ€: Protein Science, 2010, 19, 742-752. | 7.6 | 14 |
| 51 | A knowledgeâ€based forcefield for proteinâ€“protein interface design. Proteins: Structure, Function and Bioinformatics, 2008, 70, 1540-1550. | 2.6 | 13 |
| 52 | Interacting with GPCRs: Using Interaction Fingerprints for Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 2053-2060. | 5.4 | 12 |
| 53 | Quantitative prediction of selectivity between the A1 and A2A adenosine receptors. Journal of Cheminformatics, 2020, 12, 33. | 6.1 | 10 |
| 54 | 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 |

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| 55 | Assessment of the Fragment Docking Program SEED. Journal of Chemical Information and Modeling, 2020, 60, 4881-4893. | 5.4 | 9 |
| 56 | 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 |
| 57 | 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 |
| 58 | 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 |
| 59 | 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 |
| 60 | 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 |
| 61 | 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 |
| 62 | 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 |
| 63 | 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 |
| 64 | The performance of ensemble-based free energy protocols in computing binding affinities to ROS1 kinase. Scientific Reports, 2022, 12, . | 3.3 | 2 |
| 65 | Identification of novel inhibitors of rat Mrp3. European Journal of Pharmaceutical Sciences, 2021, 162, 105813. | 4.0 | 1 |