

Michal Vieth

List of Publications by Year in descending order

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Version: 2024-02-01

41
papers

4,058
citations

218677

26
h-index

265206

42
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42
all docs

42
docs citations

42
times ranked

5175
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|---|-----|-----------|
| 1 | Detailed analysis of grid-based molecular docking: A case study of CDOCKER?A CHARMM-based MD docking algorithm. <i>Journal of Computational Chemistry</i> , 2003, 24, 1549-1562. | 3.3 | 1,299 |
| 2 | Lessons in Molecular Recognition: The Effects of Ligand and Protein Flexibility on Molecular Docking Accuracy. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 45-55. | 6.4 | 358 |
| 3 | Characteristic Physical Properties and Structural Fragments of Marketed Oral Drugs. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 224-232. | 6.4 | 350 |
| 4 | Synthesis and Activity of New Aryl- and Heteroaryl-Substituted Pyrazole Inhibitors of the Transforming Growth Factor- β Type I Receptor Kinase Domain. <i>Journal of Medicinal Chemistry</i> , 2003, 46, 3953-3956. | 6.4 | 225 |
| 5 | Kinomics structural biology and chemogenomics of kinase inhibitors and targets. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2004, 1697, 243-257. | 2.3 | 168 |
| 6 | Kinomics: characterizing the therapeutically validated kinase space. <i>Drug Discovery Today</i> , 2005, 10, 839-846. | 6.4 | 164 |
| 7 | Assessing energy functions for flexible docking. <i>Journal of Computational Chemistry</i> , 1998, 19, 1612-1622. | 3.3 | 144 |
| 8 | Assessing search strategies for flexible docking. <i>Journal of Computational Chemistry</i> , 1998, 19, 1623-1631. | 3.3 | 112 |
| 9 | Lessons in Molecular Recognition. 2. Assessing and Improving Cross-Docking Accuracy. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 2293-2302. | 5.4 | 112 |
| 10 | Dependence of Molecular Properties on Proteomic Family for Marketed Oral Drugs. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 3451-3453. | 6.4 | 95 |
| 11 | Do active site conformations of small ligands correspond to low free-energy solution structures?. <i>Journal of Computer-Aided Molecular Design</i> , 1998, 12, 563-572. | 2.9 | 94 |
| 12 | DoMCoSAR: A Novel Approach for Establishing the Docking Mode That Is Consistent with the Structure-Activity Relationship. Application to HIV-1 Protease Inhibitors and VEGF Receptor Tyrosine Kinase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2000, 43, 3020-3032. | 6.4 | 77 |
| 13 | Drugs in other drugs: a new look at drugs as fragments. <i>Drug Discovery Today</i> , 2007, 12, 71-79. | 6.4 | 73 |
| 14 | Chemical Fragments as Foundations for Understanding Target Space and Activity Prediction. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 2689-2700. | 6.4 | 70 |
| 15 | Structural insights into probe-dependent positive allostereism of the GLP-1 receptor. <i>Nature Chemical Biology</i> , 2020, 16, 1105-1110. | 8.0 | 58 |
| 16 | Design of Potent and Selective 2-Aminobenzimidazole-Based p38 MAP Kinase Inhibitors with Excellent in Vivo Efficacy. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 2270-2273. | 6.4 | 49 |
| 17 | SDOCKER: A Method Utilizing Existing X-ray Structures To Improve Docking Accuracy. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 3142-3148. | 6.4 | 47 |
| 18 | Predicting the Conformational Variability of Abl Tyrosine Kinase using Molecular Dynamics Simulations and Markov State Models. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2721-2732. | 5.3 | 47 |

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|----|--|-----|-----------|
| 19 | Prediction of Quaternary Structure of Coiled Coils. Application to Mutants of the GCN4 Leucine Zipper. <i>Journal of Molecular Biology</i> , 1995, 251, 448-467. | 4.2 | 45 |
| 20 | Molecular Basis for Necitumumab Inhibition of EGFR Variants Associated with Acquired Cetuximab Resistance. <i>Molecular Cancer Therapeutics</i> , 2018, 17, 521-531. | 4.1 | 45 |
| 21 | Kinase Inhibitor Data Modeling and de Novo Inhibitor Design with Fragment Approaches. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 6456-6466. | 6.4 | 41 |
| 22 | Predicting leucine zipper structures from sequence. <i>Protein Engineering, Design and Selection</i> , 1996, 9, 657-662. | 2.1 | 35 |
| 23 | A High-Throughput Screen against Pantothenate Synthetase (PanC) Identifies 3-Biphenyl-4-Cyanopyrrole-2-Carboxylic Acids as a New Class of Inhibitor with Activity against <i>Mycobacterium tuberculosis</i> . <i>PLoS ONE</i> , 2013, 8, e72786. | 2.5 | 35 |
| 24 | Aminoimidazo[1,2-a]pyridines as a new structural class of cyclin-dependent kinase inhibitors. Part 1: Design, synthesis, and biological evaluation. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 6095-6099. | 2.2 | 34 |
| 25 | Structural determinants of dual incretin receptor agonism by tirzepatide. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, e2116506119. | 7.1 | 31 |
| 26 | Molecular properties that influence oral drug-like behavior. <i>Current Opinion in Drug Discovery & Development</i> , 2004, 7, 470-7. | 1.9 | 29 |
| 27 | What general conclusions can we draw from kinase profiling data sets?. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 1425-1433. | 2.3 | 28 |
| 28 | Oxadiazoles Have Butyrate-Specific Conditional Activity against <i>Mycobacterium tuberculosis</i> . <i>Antimicrobial Agents and Chemotherapy</i> , 2016, 60, 3608-3616. | 3.2 | 26 |
| 29 | Structure-guided expansion of kinase fragment libraries driven by support vector machine models. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2010, 1804, 642-652. | 2.3 | 23 |
| 30 | Geometric Accuracy of Three-Dimensional Molecular Overlays. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 1996-2002. | 5.4 | 17 |
| 31 | Novel route to the synthesis of 4-quinolyl isothiocyanates. <i>Tetrahedron Letters</i> , 2006, 47, 2161-2164. | 1.4 | 17 |
| 32 | Crystal structure of human RIOK2 bound to a specific inhibitor. <i>Open Biology</i> , 2019, 9, 190037. | 3.6 | 15 |
| 33 | Identification of tyrosine kinase inhibitors that halt <i>Plasmodium falciparum</i> parasitemia. <i>PLoS ONE</i> , 2020, 15, e0242372. | 2.5 | 13 |
| 34 | Identification of Î²-Lactams Active against <i>Mycobacterium tuberculosis</i> by a Consortium of Pharmaceutical Companies and Academic Institutions. <i>ACS Infectious Diseases</i> , 2022, 8, 557-573. | 3.8 | 13 |
| 35 | A simple technique to estimate partition functions and equilibrium constants from Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 1995, 102, 6189-6193. | 3.0 | 12 |
| 36 | Knowledge-Based Strategy to Improve Ligand Pose Prediction Accuracy for Lead Optimization. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1460-1468. | 5.4 | 12 |

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|----|---|-----|-----------|
| 37 | Selectivity Data: Assessment, Predictions, Concordance, and Implications. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 6991-7002. | 6.4 | 11 |
| 38 | Are induced fit protein conformational changes caused by ligand binding predictable? A molecular dynamics investigation. <i>Journal of Computational Chemistry</i> , 2017, 38, 1229-1237. | 3.3 | 10 |
| 39 | Reconstruction of 3D structures of MET antibodies from electron microscopy 2D class averages. <i>PLoS ONE</i> , 2017, 12, e0175758. | 2.5 | 10 |
| 40 | The discovery of a new structural class of cyclin-dependent kinase inhibitors, aminoimidazo[1,2-a]pyridines. <i>Molecular Cancer Therapeutics</i> , 2004, 3, 1-9. | 4.1 | 8 |
| 41 | Perspective on computational and structural aspects of kinase discovery from IPK2014. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2015, 1854, 1595-1604. | 2.3 | 4 |