J Willem M Nissink

List of Publications by Year
in descending order

51 papers	3,956 citations	257357 24 h-index	175177 52 g-index
53 all docs	53 docs citations	53 times ranked	6277 citing authors

#	Article	IF	Citations
1	Highly Stable Siâ^'C Linked Functionalized Monolayers on the Silicon (100) Surface. Langmuir, 1998, 14, 1759-1768.	1.6	495
2	Seven Year Itch: Pan-Assay Interference Compounds (PAINS) in 2017â€"Utility and Limitations. ACS Chemical Biology, 2018, 13, 36-44.	1.6	444
3	A new test set for validating predictions of protein-ligand interaction. Proteins: Structure, Function and Bioinformatics, 2002, 49, 457-471.	1.5	416
4	Modeling Water Molecules in Proteinâ^'Ligand Docking Using GOLD. Journal of Medicinal Chemistry, 2005, 48, 6504-6515.	2.9	354
5	PAINS in the Assay: Chemical Mechanisms of Assay Interference and Promiscuous Enzymatic Inhibition Observed during a Sulfhydryl-Scavenging HTS. Journal of Medicinal Chemistry, 2015, 58, 2091-2113.	2.9	284
6	Comparing protein-ligand docking programs is difficult. Proteins: Structure, Function and Bioinformatics, 2005, 60, 325-332.	1.5	275
7	Discovery and Characterization of AZD6738, a Potent Inhibitor of Ataxia Telangiectasia Mutated and Rad3 Related (ATR) Kinase with Application as an Anticancer Agent. Journal of Medicinal Chemistry, 2018, 61, 9889-9907.	2.9	204
8	Discovery of 4-{4-[(3R)-3-Methylmorpholin-4-yl]-6-[1-(methylsulfonyl)cyclopropyl]pyrimidin-2-yl}-1H-indole (AZ20): A Potent and Selective Inhibitor of ATR Protein Kinase with Monotherapy in Vivo Antitumor Activity. Journal of Medicinal Chemistry, 2013, 56, 2125-2138.	2.9	190
9	Potent and Selective Inhibitors of MTH1 Probe Its Role in Cancer Cell Survival. Journal of Medicinal Chemistry, 2016, 59, 2346-2361.	2.9	121
10	Simple Size-Independent Measure of Ligand Efficiency. Journal of Chemical Information and Modeling, 2009, 49, 1617-1622.	2.5	94
11	Promiscuous 2-Aminothiazoles (PrATs): A Frequent Hitting Scaffold. Journal of Medicinal Chemistry, 2015, 58, 1205-1214.	2.9	75
12	(Thio)urea Resorcinarene Cavitands. Complexation and Membrane Transport of Halide Anions. Journal of Organic Chemistry, 1998, 63, 4174-4180.	1.7	74
13	Drugging ATR: progress in the development of specific inhibitors for the treatment of cancer. Future Medicinal Chemistry, 2015, 7, 873-891.	1.1	68
14	Mimicry by asx- and ST-turns of the four main types of Î²-turn in proteins. Protein Science, 2008, 13, 3051-3055.	3.1	64
15	Discovery of AZD9833, a Potent and Orally Bioavailable Selective Estrogen Receptor Degrader and Antagonist. Journal of Medicinal Chemistry, 2020, 63, 14530-14559.	2.9	59
16	Cellularly active N-hydroxyurea FEN1 inhibitors block substrate entry to the active site. Nature Chemical Biology, 2016, 12, 815-821.	3.9	57
17	Proteinâ€šÃ„Ã¬Ligand Docking Virtual Screening with GOLD. Drug Discovery Series, 2005, , 379-415.	0.1	52
18	Quantification of frequent-hitter behavior based on historical high-throughput screening data. Future Medicinal Chemistry, 2014, 6, 1113-1126.	1.1	47

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19	Structures of the Human Poly (ADP-Ribose) Glycohydrolase Catalytic Domain Confirm Catalytic Mechanism and Explain Inhibition by ADP-HPD Derivatives. PLoS ONE, 2012, 7, e50889.	1.1	46
20	Discovery of novel imidazo[1,2-a]pyridines as inhibitors of the insulin-like growth factor-1 receptor tyrosine kinase. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 4698-4701.	1.0	44
21	Superposition of molecules: Electron density fitting by application of fourier transforms. Journal of Computational Chemistry, 1997, 18, 638-645.	1.5	37
22	Nuisance compounds in cellular assays. Cell Chemical Biology, 2021, 28, 356-370.	2.5	37
23	Increasing the delivery of next generation therapeutics from high throughput screening libraries. Current Opinion in Chemical Biology, 2015, 26, 104-110.	2.8	33
24	Recurring main-chain anion-binding motifs in short polypeptides: nests. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1935-1942.	2.5	31
25	Myc phosphorylation in its basic helixâ€“loopâ€“helix region destabilizes transient Î±-helical structures, disrupting Max and DNA binding. Journal of Biological Chemistry, 2018, 293, 9301-9310.	1.6	28
26	MTH1 Substrate Recognitionâ€”An Example of Specific Promiscuity. PLoS ONE, 2016, 11, e0151154.	1.1	24
27	Simple knowledge-based descriptors to predict protein-ligand interactions. methodology and validation. Journal of Computer-Aided Molecular Design, 2000, 14, 787-803.	1.3	22
28	Identification of Compounds That Interfere with Highâ€Throughput Screening Assay Technologies. ChemMedChem, 2019, 14, 1795-1802.	1.6	21
29	Discovery of a Thiadiazoleâ€“Pyridazine-Based Allosteric Glutaminase 1 Inhibitor Series That Demonstrates Oral Bioavailability and Activity in Tumor Xenograft Models. Journal of Medicinal Chemistry, 2019, 62, 6540-6560.	2.9	21
30	Development of a High-Throughput Fluorescence Polarization DNA Cleavage Assay for the Identification of FEN1 Inhibitors. Journal of Biomolecular Screening, 2013, 18, 567-575.	2.6	19
31	A Generic Platform for Cellular Screening Against Ubiquitin Ligases. Scientific Reports, 2016, 6, 18940.	1.6	18
32	Combined use of physicochemical data and small-molecule crystallographic contact propensities to predict interactions in protein binding sites. Organic and Biomolecular Chemistry, 2004, 2, 3238.	1.5	17
33	Mapping Hidden Residual Structure within the Myc bHLH-LZ Domain Using Chemical Denaturant Titration. Structure, 2019, 27, 1537-1546.e4.	1.6	17
34	Post-HTS case report and structural alert: Promiscuous 4-aroyl-1,5-disubstituted-3-hydroxy-2 H -pyrrol-2-one actives verified by ALARM NMR. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4740-4752.	1.0	15
35	An infrared study of hostâ€“guest association in solution by substituted resorcinarene cavitands. Part I. Structural aspects of halide complexation by a tetraurea cavitand. Journal of the Chemical Society Perkin Transactions II, 1998, , 2541-2546.	0.9	14
36	Analyzing compound and project progress through multi-objective-based compound quality assessment. Future Medicinal Chemistry, 2013, 5, 753-767.	1.1	14

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37	Optimization of an Imidazo[1,2-a]pyridine Series to Afford Highly Selective Type I1/2 Dual Mer/Axl Kinase Inhibitors with In Vivo Efficacy. Journal of Medicinal Chemistry, 2021, 64, 13524-13539.	2.9	13
38	An infrared study of hostâ€“guest association in solution by substituted resorcinarene cavitands. Part II.1 Comparison of halide complexation by tetrathiourea cavitands and a simple thiourea. Journal of the Chemical Society Perkin Transactions II, 1998, , 2623-2630.	0.9	12
39	Utility of Resazurin, Horseradish Peroxidase, and NMR Assays to Identify Redox-Related False-Positive Behavior in High-Throughput Screens. Assay and Drug Development Technologies, 2018, 16, 171-191.	0.6	11
40	Generating Selective Leads for Mer Kinase Inhibitorsâ€"Example of a Comprehensive Lead-Generation Strategy. Journal of Medicinal Chemistry, 2021, 64, 3165-3184.	2.9	11
41	Stratified High-Throughput Screening Sets Enable Flexible Screening Strategies from a Single Plated Collection. Journal of Biomolecular Screening, 2014, 19, 369-378.	2.6	10
42	A-loop interactions in Mer tyrosine kinase give rise to inhibitors with two-step mechanism and long residence time of binding. Biochemical Journal, 2020, 477, 4443-4452.	1.7	10
43	Building Bridges in a Series of Estrogen Receptor Degraders: An Application of Metathesis in Medicinal Chemistry. ACS Medicinal Chemistry Letters, 2019, 10, 1492-1497.	1.3	9
44	Adsorption and Ordering of Resorcinare Layers on Planar and Colloidal Gold and the Influence of Surface Modification: A SERS and IRRAS Study. Applied Spectroscopy, 1999, 53, 528-539.	1.2	8
45	Determination of the association constant of strongly bonded hostâ€“guest systems by multivariate regression of infrared spectroscopic data. Journal of the Chemical Society Perkin Transactions II, 1998, , 1671-1676.	0.9	7
46	Infrared Reflection-Absorption Study of Ordering and Hydrogen Bonding within Chiral and Nonchiral Self-Assembled Monolayers on Gold. Applied Spectroscopy, 1999, 53, 33-39.	1.2	6
47	Beyond the Scope of Free-Wilson Analysis. 2: Can Distance Encoded R-Group Fingerprints Provide Interpretable Nonlinear Models?. Journal of Chemical Information and Modeling, 2014, 54, 1117-1128.	2.5	6
48	Abstract 1823: AZ20, a novel potent and selective inhibitor of ATR kinase with in vivo antitumour activity. Cancer Research, 2012, 72, 1823-1823.	0.4	6
49	Targeting a Novel KRAS Binding Site: Application of One-Component Stapling of Small (5â€“6-mer) Peptides. Journal of Medicinal Chemistry, 2021, 64, 17287-17303.	2.9	6
50	Reversible binding of resorcin[4]arene cavitands onto a self-assembled monolayer. Journal of Molecular Structure, 1999, 479, 65-73.	1.8	5
51	Generation of Quantum Configurational Ensembles Using Approximate Potentials. Journal of Chemical Theory and Computation, 2021, 17, 7021-7042.	2.3	2