Albert Jelke Kooistra

List of Publications by Year
in descending order

50 papers	2,743 citations	172207 29 h-index	197535 49 g-index
53 all docs	53 docs citations	53 times ranked	3253 citing authors

#	Article	IF	Citations
1	GPCRdb in 2021: integrating GPCR sequence, structure and function. Nucleic Acids Research, 2021, 49, D335-D343.	6.5	254
2	KLIFS: A Knowledge-Based Structural Database To Navigate Kinaseâ€“Ligand Interaction Space. Journal of Medicinal Chemistry, 2014, 57, 249-277.	2.9	243
3	Community assessment to advance computational prediction of cancer drug combinations in a pharmacogenomic screen. Nature Communications, 2019, 10, 2674.	5.8	240
4	Crystal Structure-Based Virtual Screening for Fragment-like Ligands of the Human Histamine H₁ Receptor. Journal of Medicinal Chemistry, 2011, 54, 8195-8206.	2.9	189
5	KLIFS: a structural kinase-ligand interaction database. Nucleic Acids Research, 2016, 44, D365-D371.	6.5	132
6	Differential GLP-1R Binding and Activation by Peptide and Non-peptide Agonists. Molecular Cell, 2020, 80, 485-500.e7.	4.5	111
7	GPCR activation mechanisms across classes and macro/microscales. Nature Structural and Molecular Biology, 2021, 28, 879-888.	3.6	98
8	The Landscape of Atypical and Eukaryotic Protein Kinases. Trends in Pharmacological Sciences, 2019, 40, 818-832.	4.0	87
9	Function-specific virtual screening for GPCR ligands using a combined scoring method. Scientific Reports, 2016, 6, 28288.	1.6	79
10	A structural chemogenomics analysis of aminergic <scp>GPCRs</scp>: lessons for histamine receptor ligand design. British Journal of Pharmacology, 2013, 170, 101-126.	2.7	74
11	KLIFS: an overhaul after the first 5 years of supporting kinase research. Nucleic Acids Research, 2021, 49, D562-D569.	6.5	74
12	Chemical Diversity in the G Protein-Coupled Receptor Superfamily. Trends in Pharmacological Sciences, 2018, 39, 494-512.	4.0	67
13	Virtual Fragment Screening: Discovery of Histamine H₃ Receptor Ligands Using Ligand-Based and Protein-Based Molecular Fingerprints. Journal of Chemical Information and Modeling, 2012, 52, 3308-3324.	2.5	64
14	Structure-Based Virtual Screening for Ligands of G Proteinâ€“Coupled Receptors: What Can Molecular Docking Do for You?. Pharmacological Reviews, 2021, 73, 1698-1736.	7.1	61
15	Structure of the class D GPCR Ste2 dimer coupled to two G proteins. Nature, 2021, 589, 148-153.	13.7	55
16	PDEStrIAn: A Phosphodiesterase Structure and Ligand Interaction Annotated Database As a Tool for Structure-Based Drug Design. Journal of Medicinal Chemistry, 2016, 59, 7029-7065.	2.9	54
17	Aminergic GPCRâ€“Ligand Interactions: A Chemical and Structural Map of Receptor Mutation Data. Journal of Medicinal Chemistry, 2019, 62, 3784-3839.	2.9	53
18	Discovery of Novel Trypanosoma brucei Phosphodiesterase B1 Inhibitors by Virtual Screening against the Unliganded TbrPDEB1 Crystal Structure. Journal of Medicinal Chemistry, 2013, 56, 2087-2096.	2.9	51

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19	Molecular Determinants of Ligand Binding Modes in the Histamine H4Receptor: Linking Ligand-Based Three-Dimensional Quantitative Structureâ€“Activity Relationship (3D-QSAR) Models to in Silico Guided Receptor Mutagenesis Studies. Journal of Medicinal Chemistry, 2011, 54, 8136-8147.	2.9	50
20	Synthesis and Characterization of a Bidirectional Photoswitchable Antagonist Toolbox for Real-Time GPCR Photopharmacology. Journal of the American Chemical Society, 2018, 140, 4232-4243.	6.6	50
21	Structure-Based Prediction of G-Protein-Coupled Receptor Ligand Function: A Î²-Adrenoceptor Case Study. Journal of Chemical Information and Modeling, 2015, 55, 1045-1061.	2.5	49
22	The G protein database, GproteinDb. Nucleic Acids Research, 2022, 50, D518-D525.	6.5	49
23	Development of novel fluorescent histamine H1-receptor antagonists to study ligand-binding kinetics in living cells. Scientific Reports, 2018, 8, 1572.	1.6	48
24	From Heptahelical Bundle to Hits from the Haystack. Methods in Enzymology, 2013, 522, 279-336.	0.4	47
25	Molecular interaction fingerprint approaches for GPCR drug discovery. Current Opinion in Pharmacology, 2016, 30, 59-68.	1.7	43
26	Crowdsourced mapping of unexplored target space of kinase inhibitors. Nature Communications, 2021, 12, 3307.	5.8	41
27	Structure-based virtual screening for fragment-like ligands of the G protein-coupled histamine H₄receptor. MedChemComm, 2015, 6, 1003-1017.	3.5	33
28	Small and colorful stones make beautiful mosaics: fragment-based chemogenomics. Drug Discovery Today, 2013, 18, 323-330.	3.2	30
29	From Three-Dimensional GPCR Structure to Rational Ligand Discovery. Advances in Experimental Medicine and Biology, 2014, 796, 129-157.	0.8	30
30	Mapping histamine H4 receptorâ€“ligand binding modes. MedChemComm, 2013, 4, 193-204.	3.5	27
31	Identification of Ligand Binding Hot Spots of the Histamine H₁ Receptor following Structure-Based Fragment Optimization. Journal of Medicinal Chemistry, 2016, 59, 9047-9061.	2.9	26
32	Analyzing Multitarget Activity Landscapes Using Proteinâ€“Ligand Interaction Fingerprints: Interaction Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 251-262.	2.5	23
33	3D-e-Chem-VM: Structural Cheminformatics Research Infrastructure in a Freely Available Virtual Machine. Journal of Chemical Information and Modeling, 2017, 57, 115-121.	2.5	21
34	The Viral G Protein-Coupled Receptor ORF74 Hijacks Î²-Arrestins for Endocytic Trafficking in Response to Human Chemokines. PLoS ONE, 2015, 10, e0124486.	1.1	17
35	Combinatorial Consensus Scoring for Ligand-Based Virtual Fragment Screening: A Comparative Case Study for Serotonin 5-HT₃A, Histamine H₁, and Histamine H₄Receptors. Journal of Chemical Information and Modeling, 2015, 55, 1030-1044.	2.5	17
36	3Dâ€eâ€Chem: Structural Cheminformatics Workflows for Computerâ€Aided Drug Discovery. ChemMedChem, 2018, 13, 614-626.	1.6	17

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37	An online GPCR structure analysis platform. Nature Structural and Molecular Biology, 2021, 28, 875-878.	3.6	16
38	Route to Prolonged Residence Time at the Histamine H₁ Receptor: Growing from Desloratadine to Rupatadine. Journal of Medicinal Chemistry, 2019, 62, 6630-6644.	2.9	15
39	Identification of novel Î±7 nicotinic receptor ligands by in silico screening against the crystal structure of a chimeric Î±7 receptor ligand binding domain. Bioorganic and Medicinal Chemistry, 2012, 20, 5992-6002.	1.4	11
40	Alkynamide phthalazinones as a new class of TbrPDEB1 inhibitors (Part 2). Bioorganic and Medicinal Chemistry, 2019, 27, 4013-4029.	1.4	11
41	Kinase-Centric Computational Drug Development. Annual Reports in Medicinal Chemistry, 2017, , 197-236.	0.5	9
42	Structural insights into serotonin receptor ligands polypharmacology. European Journal of Medicinal Chemistry, 2018, 151, 797-814.	2.6	7
43	Electron Density Fingerprints (EDprints): Virtual Screening Using Assembled Information of Electron Density. Journal of Chemical Information and Modeling, 2010, 50, 1772-1780.	2.5	6
44	The Receptor Concept in 3D: From Hypothesis and Metaphor to GPCRâ€“Ligand Structures. Neurochemical Research, 2014, 39, 1850-1861.	1.6	6
45	A Structural Framework for GPCR Chemogenomics: Whatâ€™s In a Residue Number?. Methods in Molecular Biology, 2018, 1705, 73-113.	0.4	6
46	Covalent Inhibition of the Histamine H3 Receptor. Molecules, 2019, 24, 4541.	1.7	5
47	Utilizing drug-target-event relationships to unveil safety patterns in pharmacovigilance. Expert Opinion on Drug Safety, 2020, 19, 961-968.	1.0	5
48	Discovery of Diaryl Ether Substituted Tetrahydrophthalazinones as TbrPDEB1 Inhibitors Following Structure-Based Virtual Screening. Frontiers in Chemistry, 2020, 8, 608030.	1.8	5
49	KiSSim: Predicting Off-Targets from Structural Similarities in the Kinome. Journal of Chemical Information and Modeling, 2022, 62, 2600-2616.	2.5	3
50	Structural Chemogenomics Databases to Navigate Proteinâ€“Ligand Interaction Space. , 2017, , 444-471.		1