

Albert Jelke Kooistra

List of Publications by Year in descending order

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Version: 2024-02-01

50
papers

2,743
citations

172457

29
h-index

197818

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. <i>Nucleic Acids Research</i> , 2021, 49, D335-D343.	14.5	254
2	KLIFS: A Knowledge-Based Structural Database To Navigate Kinase–Ligand Interaction Space. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 249-277.	6.4	243
3	Community assessment to advance computational prediction of cancer drug combinations in a pharmacogenomic screen. <i>Nature Communications</i> , 2019, 10, 2674.	12.8	240
4	Crystal Structure-Based Virtual Screening for Fragment-like Ligands of the Human Histamine H ₁ Receptor. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 8195-8206.	6.4	189
5	KLIFS: a structural kinase-ligand interaction database. <i>Nucleic Acids Research</i> , 2016, 44, D365-D371.	14.5	132
6	Differential GLP-1R Binding and Activation by Peptide and Non-peptide Agonists. <i>Molecular Cell</i> , 2020, 80, 485-500.e7.	9.7	111
7	GPCR activation mechanisms across classes and macro/microscales. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 879-888.	8.2	98
8	The Landscape of Atypical and Eukaryotic Protein Kinases. <i>Trends in Pharmacological Sciences</i> , 2019, 40, 818-832.	8.7	87
9	Function-specific virtual screening for GPCR ligands using a combined scoring method. <i>Scientific Reports</i> , 2016, 6, 28288.	3.3	79
10	A structural chemogenomics analysis of aminergic GPCRs: lessons for histamine receptor ligand design. <i>British Journal of Pharmacology</i> , 2013, 170, 101-126.	5.4	74
11	KLIFS: an overhaul after the first 5 years of supporting kinase research. <i>Nucleic Acids Research</i> , 2021, 49, D562-D569.	14.5	74
12	Chemical Diversity in the G Protein-Coupled Receptor Superfamily. <i>Trends in Pharmacological Sciences</i> , 2018, 39, 494-512.	8.7	67
13	Virtual Fragment Screening: Discovery of Histamine H ₃ Receptor Ligands Using Ligand-Based and Protein-Based Molecular Fingerprints. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 3308-3324.	5.4	64
14	Structure-Based Virtual Screening for Ligands of G Protein–Coupled Receptors: What Can Molecular Docking Do for You?. <i>Pharmacological Reviews</i> , 2021, 73, 1698-1736.	16.0	61
15	Structure of the class D GPCR Ste2 dimer coupled to two G proteins. <i>Nature</i> , 2021, 589, 148-153.	27.8	55
16	PDEStrIA: A Phosphodiesterase Structure and Ligand Interaction Annotated Database As a Tool for Structure-Based Drug Design. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 7029-7065.	6.4	54
17	Aminergic GPCR–Ligand Interactions: A Chemical and Structural Map of Receptor Mutation Data. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 3784-3839.	6.4	53
18	Discovery of Novel <i>Trypanosoma brucei</i> Phosphodiesterase B1 Inhibitors by Virtual Screening against the Unliganded TbrPDEB1 Crystal Structure. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 2087-2096.	6.4	51

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19	Molecular Determinants of Ligand Binding Modes in the Histamine H ₄ Receptor: Linking Ligand-Based Three-Dimensional Quantitative Structure-Activity Relationship (3D-QSAR) Models to <i>In Silico</i> Guided Receptor Mutagenesis Studies. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 8136-8147.	6.4	50
20	Synthesis and Characterization of a Bidirectional Photoswitchable Antagonist Toolbox for Real-Time GPCR Photopharmacology. <i>Journal of the American Chemical Society</i> , 2018, 140, 4232-4243.	13.7	50
21	Structure-Based Prediction of G-Protein-Coupled Receptor Ligand Function: A β^2 -Adrenoceptor Case Study. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1045-1061.	5.4	49
22	The G protein database, GproteinDb. <i>Nucleic Acids Research</i> , 2022, 50, D518-D525.	14.5	49
23	Development of novel fluorescent histamine H ₁ -receptor antagonists to study ligand-binding kinetics in living cells. <i>Scientific Reports</i> , 2018, 8, 1572.	3.3	48
24	From Heptahelical Bundle to Hits from the Haystack. <i>Methods in Enzymology</i> , 2013, 522, 279-336.	1.0	47
25	Molecular interaction fingerprint approaches for GPCR drug discovery. <i>Current Opinion in Pharmacology</i> , 2016, 30, 59-68.	3.5	43
26	Crowdsourced mapping of unexplored target space of kinase inhibitors. <i>Nature Communications</i> , 2021, 12, 3307.	12.8	41
27	Structure-based virtual screening for fragment-like ligands of the G protein-coupled histamine H ₄ receptor. <i>MedChemComm</i> , 2015, 6, 1003-1017.	3.4	33
28	Small and colorful stones make beautiful mosaics: fragment-based chemogenomics. <i>Drug Discovery Today</i> , 2013, 18, 323-330.	6.4	30
29	From Three-Dimensional GPCR Structure to Rational Ligand Discovery. <i>Advances in Experimental Medicine and Biology</i> , 2014, 796, 129-157.	1.6	30
30	Mapping histamine H ₄ receptor ligand binding modes. <i>MedChemComm</i> , 2013, 4, 193-204.	3.4	27
31	Identification of Ligand Binding Hot Spots of the Histamine H ₁ Receptor following Structure-Based Fragment Optimization. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 9047-9061.	6.4	26
32	Analyzing Multitarget Activity Landscapes Using Protein-Ligand Interaction Fingerprints: Interaction Cliffs. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 251-262.	5.4	23
33	3D-e-Chem-VM: Structural Cheminformatics Research Infrastructure in a Freely Available Virtual Machine. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 115-121.	5.4	21
34	The Viral G Protein-Coupled Receptor ORF74 Hijacks β^2 -Arrestins for Endocytic Trafficking in Response to Human Chemokines. <i>PLoS ONE</i> , 2015, 10, e0124486.	2.5	17
35	Combinatorial Consensus Scoring for Ligand-Based Virtual Fragment Screening: A Comparative Case Study for Serotonin 5-HT _{3A} , Histamine H ₁ , and Histamine H ₄ Receptors. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1030-1044.	5.4	17
36	3D-e-Chem: Structural Cheminformatics Workflows for Computer-Aided Drug Discovery. <i>ChemMedChem</i> , 2018, 13, 614-626.	3.2	17

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37	An online GPCR structure analysis platform. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 875-878.	8.2	16
38	Route to Prolonged Residence Time at the Histamine H ₁ Receptor: Growing from Desloratadine to Rupatadine. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 6630-6644.	6.4	15
39	Identification of novel β_7 nicotinic receptor ligands by in silico screening against the crystal structure of a chimeric β_7 receptor ligand binding domain. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 5992-6002.	3.0	11
40	Alkynamide phthalazinones as a new class of TbrPDEB1 inhibitors (Part 2). <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 4013-4029.	3.0	11
41	Kinase-Centric Computational Drug Development. <i>Annual Reports in Medicinal Chemistry</i> , 2017, , 197-236.	0.9	9
42	Structural insights into serotonin receptor ligands polypharmacology. <i>European Journal of Medicinal Chemistry</i> , 2018, 151, 797-814.	5.5	7
43	Electron Density Fingerprints (EDprints): Virtual Screening Using Assembled Information of Electron Density. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1772-1780.	5.4	6
44	The Receptor Concept in 3D: From Hypothesis and Metaphor to GPCRâ€™Ligand Structures. <i>Neurochemical Research</i> , 2014, 39, 1850-1861.	3.3	6
45	A Structural Framework for GPCR Chemogenomics: Whatâ€™s In a Residue Number?. <i>Methods in Molecular Biology</i> , 2018, 1705, 73-113.	0.9	6
46	Covalent Inhibition of the Histamine H3 Receptor. <i>Molecules</i> , 2019, 24, 4541.	3.8	5
47	Utilizing drug-target-event relationships to unveil safety patterns in pharmacovigilance. <i>Expert Opinion on Drug Safety</i> , 2020, 19, 961-968.	2.4	5
48	Discovery of Diaryl Ether Substituted Tetrahydrophthalazinones as TbrPDEB1 Inhibitors Following Structure-Based Virtual Screening. <i>Frontiers in Chemistry</i> , 2020, 8, 608030.	3.6	5
49	KiSSim: Predicting Off-Targets from Structural Similarities in the Kinome. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2600-2616.	5.4	3
50	Structural Chemogenomics Databases to Navigate Proteinâ€™Ligand Interaction Space. , 2017, , 444-471.		1