Didier Rognan

List of Publications by Year
in descending order

71 papers	6,913 citations	76031 42 h-index	104191 69 g-index
75 all docs	75 docs citations	75 times ranked	7674 citing authors

#	Article	IF	Citations
1	High-Throughput Screening for Extracellular Inhibitors of the FLT3 Receptor Tyrosine Kinase Reveals Chemically Diverse and Druggable Negative Allosteric Modulators. ACS Chemical Biology, 2022, 17, 709-722.	1.6	2
2	On the Frustration to Predict Binding Affinities from Proteinâ€“Ligand Structures with Deep Neural Networks. Journal of Medicinal Chemistry, 2022, 65, 7946-7958.	2.9	68
3	Targeting undruggable carbohydrate recognition sites through focused fragment library design. Communications Chemistry, 2022, 5, .	2.0	9
4	Nonâ€Carbohydrate Glycomimetics as Inhibitors of Calcium(II)â€Binding Lectins. Angewandte Chemie, 2021, 133, 8185-8195.	1.6	3
5	Nonâ€Carbohydrate Glycomimetics as Inhibitors of Calcium(II)â€Binding Lectins. Angewandte Chemie - International Edition, 2021, 60, 8104-8114.	7.2	17
6	Modeling Protein-Ligand Interactions: Are We Ready for Deep Learning?. , 2021, , 163-173.		0
7	True Accuracy of Fast Scoring Functions to Predict High-Throughput Screening Data from Docking Poses: The Simpler the Better. Journal of Chemical Information and Modeling, 2021, 61, 2788-2797.	2.5	30
8	Unexpected similarity between HIV-1 reverse transcriptase and tumor necrosis factor binding sites revealed by computer vision. Journal of Cheminformatics, 2021, 13, 90.	2.8	2
9	Targeting the Central Pocket of the Pseudomonas aeruginosa Lectin LecA. ChemBioChem, 2021, , .	1.3	12
10	Anticancer activity of ruthenium and osmium cyclometalated compounds: identification of ABCB1 and EGFR as resistance mechanisms. Inorganic Chemistry Frontiers, 2020, 7, 678-688.	3.0	34
11	A Computer Vision Approach to Align and Compare Protein Cavities: Application to Fragment-Based Drug Design. Journal of Medicinal Chemistry, 2020, 63, 7127-7142.	2.9	14
12	Benchmarking Data Sets from PubChem BioAssay Data: Current Scenario and Room for Improvement. International Journal of Molecular Sciences, 2020, 21, 4380.	1.8	8
13	LIT-PCBA: An Unbiased Data Set for Machine Learning and Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4263-4273.	2.5	92
14	Unsupervised Classification of G-Protein Coupled Receptors and Their Conformational States Using IChem Intramolecular Interaction Patterns. Journal of Chemical Information and Modeling, 2019, 59, 3611-3618.	2.5	0
15	Local Interaction Density (LID), a Fast and Efficient Tool to Prioritize Docking Poses. Molecules, 2019, 24, 2610.	1.7	4
16	Exhaustive Repertoire of Druggable Cavities at Proteinâ€“Protein Interfaces of Known Three-Dimensional Structure. Journal of Medicinal Chemistry, 2019, 62, 9732-9742.	2.9	17
17	Ureidopeptide GLP-1 analogues with prolonged activity in vivo via signal bias and altered receptor trafficking. Chemical Science, 2019, 10, 9872-9879.	3.7	31
18	All in One: Cavity Detection, Druggability Estimate, Cavity-Based Pharmacophore Perception, and Virtual Screening. Journal of Chemical Information and Modeling, 2019, 59, 573-585.	2.5	25

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19	Inhibition of neuronal FLT3 receptor tyrosine kinase alleviates peripheral neuropathic pain in mice. Nature Communications, 2018, 9, 1042.	5.8	47
20	IChem: A Versatile Toolkit for Detecting, Comparing, and Predicting Proteinâ€“Ligand Interactions. ChemMedChem, 2018, 13, 507-510.	1.6	61
21	Ranking docking poses by graph matching of proteinâ€“ligand interactions: lessons learned from the D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 75-87.	1.3	12
22	Structure-Based Detection of Orthosteric and Allosteric Pockets at Proteinâ€“Protein Interfaces. Methods in Molecular Biology, 2018, 1825, 281-294.	0.4	0
23	The impact of in silico screening in the discovery of novel and safer drug candidates. , 2017, 175, 47-66.		85
24	Docking pose selection by interaction pattern graph similarity: application to the D3R grand challenge 2015. Journal of Computer-Aided Molecular Design, 2016, 30, 669-683.	1.3	15
25	sc-PDB: a 3D-database of ligandable binding sitesâ€”10 years on. Nucleic Acids Research, 2015, 43, D399-D404.	6.5	182
26	IChemPIC: A Random Forest Classifier of Biological and Crystallographic Proteinâ€“Protein Interfaces. Journal of Chemical Information and Modeling, 2015, 55, 2005-2014.	2.5	26
27	Novel aminotetrazole derivatives as selective STAT3 non-peptide inhibitors. European Journal of Medicinal Chemistry, 2015, 103, 163-174.	2.6	32
28	sc-PDB-Frag: A Database of Proteinâ€“Ligand Interaction Patterns for Bioisosteric Replacements. Journal of Chemical Information and Modeling, 2014, 54, 1908-1918.	2.5	20
29	Design of a Generalâ€Purpose European Compound Screening Library for EUâ€OPENSCREEN. ChemMedChem, 2014, 9, 2309-2326.	1.6	29
30	Beware of Machine Learning-Based Scoring Functionsâ€”On the Danger of Developing Black Boxes. Journal of Chemical Information and Modeling, 2014, 54, 2807-2815.	2.5	110
31	Computational Profiling of Bioactive Compounds Using a Target-Dependent Composite Workflow. Journal of Chemical Information and Modeling, 2013, 53, 2322-2333.	2.5	29
32	Proteome-scale docking: myth and reality. Drug Discovery Today: Technologies, 2013, 10, e403-e409.	4.0	20
33	Encoding Proteinâ€“Ligand Interaction Patterns in Fingerprints and Graphs. Journal of Chemical Information and Modeling, 2013, 53, 623-637.	2.5	139
34	Predicting Ligand Binding Modes from Neural Networks Trained on Proteinâ€“Ligand Interaction Fingerprints. Journal of Chemical Information and Modeling, 2013, 53, 763-772.	2.5	47
35	Comparison and Druggability Prediction of Proteinâ€“Ligand Binding Sites from Pharmacophore-Annotated Cavity Shapes. Journal of Chemical Information and Modeling, 2012, 52, 2287-2299.	2.5	118
36	Proteinâ€“Ligand-Based Pharmacophores: Generation and Utility Assessment in Computational Ligand Profiling. Journal of Chemical Information and Modeling, 2012, 52, 943-955.	2.5	116

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37	Fragment-Based Approaches and Computer-Aided Drug Discovery. Topics in Current Chemistry, 2011, 317, 201-222.	4.0	31
38	Identification of a lowâ€“molecular weight TrkB antagonist with anxiolytic and antidepressant activity in mice. Journal of Clinical Investigation, 2011, 121, 1846-1857.	3.9	319
39	Identification of Nonpeptide Oxytocin Receptor Ligands by Receptorâ€Ligand Fingerprint Similarity Search. Molecular Informatics, 2011, 30, 521-526.	1.4	14
40	Structureâ€Based Discovery of Allosteric Modulators of Two Related Classâ€…B Gâ€Proteinâ€Coupled Receptors. ChemMedChem, 2011, 6, 2159-2169.	1.6	62
41	Structureâ€Based Approaches to Target Fishing and Ligand Profiling. Molecular Informatics, 2010, 29, 176-187.	1.4	132
42	Estrogen Receptor Alpha as a Key Target of Red Wine Polyphenols Action on the Endothelium. PLoS ONE, 2010, 5, e8554.	1.1	102
43	Binding of Protein Kinase Inhibitors to Synapsin I Inferred from Pair-Wise Binding Site Similarity Measurements. PLoS ONE, 2010, 5, e12214.	1.1	60
44	Alignment-Free Ultra-High-Throughput Comparison of Druggable Proteinâ^'Ligand Binding Sites. Journal of Chemical Information and Modeling, 2010, 50, 123-135.	2.5	118
45	Customizing G Protein-Coupled Receptor Models for Structure-Based Virtual Screening. Current Pharmaceutical Design, 2009, 15, 4026-4048.	0.9	67
46	Development and Validation of a Novel Proteinâ^'Ligand Fingerprint To Mine Chemogenomic Space: Application to G Protein-Coupled Receptors and Their Ligands. Journal of Chemical Information and Modeling, 2009, 49, 1049-1062.	2.5	89
47	Molecular modeling of the second extracellular loop of Gâ€protein coupled receptors and its implication on structureâ€based virtual screening. Proteins: Structure, Function and Bioinformatics, 2008, 71, 599-620.	1.5	95
48	A simple and fuzzy method to align and compare druggable ligandâ€binding sites. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1755-1778.	1.5	96
49	Hot-Spots-Guided Receptor-Based Pharmacophores (HS-Pharm): A Knowledge-Based Approach to Identify Ligand-Anchoring Atoms in Protein Cavities and Prioritize Structure-Based Pharmacophores. Journal of Chemical Information and Modeling, 2008, 48, 1396-1410.	2.5	91
50	Ranking Targets in Structure-Based Virtual Screening of Three-Dimensional Protein Libraries: Methods and Problems. Journal of Chemical Information and Modeling, 2008, 48, 1014-1025.	2.5	61
51	Selective Structure-Based Virtual Screening for Full and Partial Agonists of the Î²2 Adrenergic Receptor. Journal of Medicinal Chemistry, 2008, 51, 4978-4985.	2.9	136
52	How to Measure the Similarity Between Protein Ligand-Binding Sites?. Current Computer-Aided Drug Design, 2008, 4, 209-220.	0.8	64
53	Identification of Nonpeptide CCR5 Receptor Agonists by Structure-based Virtual Screening. Journal of Medicinal Chemistry, 2007, 50, 1294-1303.	2.9	117
54	Optimizing Fragment and Scaffold Docking by Use of Molecular Interaction Fingerprints. Journal of Chemical Information and Modeling, 2007, 47, 195-207.	2.5	357

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55	Assessing the Scaffold Diversity of Screening Libraries. Journal of Chemical Information and Modeling, 2006, 46, 512-524.	2.5	122
56	sc-PDB:Â an Annotated Database of Druggable Binding Sites from the Protein Data Bank. Journal of Chemical Information and Modeling, 2006, 46, 717-727.	2.5	179
57	InSilico-Guided Target Identification of a Scaffold-Focused Library:Â 1,3,5-Triazepan-2,6-diones as Novel Phospholipase A2 Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 6768-6778.	2.9	64
58	A chemogenomic analysis of the transmembrane binding cavity of human G-protein-coupled receptors. Proteins: Structure, Function and Bioinformatics, 2005, 62, 509-538.	1.5	206
59	Delineating a Ca2+ Binding Pocket within the Venus Flytrap Module of the Human Calcium-sensing Receptor. Journal of Biological Chemistry, 2005, 280, 37917-37923.	1.6	126
60	N,Nâ€˜-Linked Oligoureas as Foldamers: Chain Length Requirements for Helix Formation in Protic Solvent Investigated by Circular Dichroism, NMR Spectroscopy, and Molecular Dynamics. Journal of the American Chemical Society, 2005, 127, 2156-2164.	6.6	156
61	Design of Small-Sized Libraries by Combinatorial Assembly of Linkers and Functional Groups to a Given Scaffold: Application to the Structure-Based Optimization of a Phosphodiesterase 4 Inhibitor. Journal of Medicinal Chemistry, 2005, 48, 3816-3822.	2.9	58
62	Positive and Negative Allosteric Modulators of the Ca2+-sensing Receptor Interact within Overlapping but Not Identical Binding Sites in the Transmembrane Domain. Journal of Biological Chemistry, 2004, 279, 18990-18997.	1.6	191
63	Comparative evaluation of eight docking tools for docking and virtual screening accuracy. Proteins: Structure, Function and Bioinformatics, 2004, 57, 225-242.	1.5	496
64	Recovering the true targets of specific ligands by virtual screening of the protein data bank. Proteins: Structure, Function and Bioinformatics, 2004, 54, 671-680.	1.5	103
65	High-Throughput Modeling of Human G-Protein Coupled Receptors:â€‰ Amino Acid Sequence Alignment, Three-Dimensional Model Building, and Receptor Library Screening. Journal of Chemical Information and Computer Sciences, 2004, 44, 1162-1176.	2.8	86
66	Modeling and Mutagenesis of the Binding Site of Calhex 231, a Novel Negative Allosteric Modulator of the Extracellular Ca2+-sensing Receptor. Journal of Biological Chemistry, 2003, 278, 49487-49494.	1.6	115
67	Probing the Cysteine-34 Position of Endogenous Serum Albumin with Thiol-Binding Doxorubicin Derivatives. Improved Efficacy of an Acid-Sensitive Doxorubicin Derivative with Specific Albumin-Binding Properties Compared to That of the Parent Compound. Journal of Medicinal Chemistry, 2002, 45, 5523-5533.	2.9	251
68	ConsDock: A new program for the consensus analysis of protein-ligand interactions. Proteins: Structure, Function and Bioinformatics, 2002, 47, 521-533.	1.5	125
69	Protein-based virtual screening of chemical databases. II. Are homology models of g-protein coupled receptors suitable targets?. Proteins: Structure, Function and Bioinformatics, 2002, 50, 5-25.	1.5	263
70	Protein-Based Virtual Screening of Chemical Databases. 1. Evaluation of Different Docking/Scoring Combinations. Journal of Medicinal Chemistry, 2000, 43, 4759-4767.	2.9	724
71	Predicting Binding Affinities of Protein Ligands from Three-Dimensional Models:Â Application to Peptide Binding to Class I Major Histocompatibility Proteins. Journal of Medicinal Chemistry, 1999, 42, 4650-4658.	2.9	176