Olivier Sperandio

List of Publications by Year in Descending Order

54 papers	2,262 citations	23 h-index	47 g-index
59 ext. papers	2,538 ext. citations	6 avg, IF	4.71 L-index

#	Paper	IF	Citations
54	Characterization of the interaction domains between the phosphoprotein and the nucleoprotein of human Metapneumovirus. *Journal of Virology*, **2021**, JVI0090921	6.6	0
53	Phylogenetic analysis of Harmonin homology domains. *BMC Bioinformatics*, **2021**, 22, 190	3.6	0
52	The iPPI-DB initiative: A Community-centered database of Protein-Protein Interaction modulators. *Bioinformatics*, **2021**,	7.2	4
51	New machine learning and physics-based scoring functions for drug discovery. *Scientific Reports*, **2021**, 11, 3198	4.9	17
50	InDeep: 3D fully convolutional neural networks to assist in silico drug design on protein-protein interactions.. *Bioinformatics*, **2021**,	7.2	2
49	Fr-PPIChem: An Academic Compound Library Dedicated to Protein-Protein Interactions. *ACS Chemical Biology*, **2020**, 15, 1566-1574	4.9	13
48	Privileged Substructures to Modulate Protein-Protein Interactions. *Journal of Chemical Information and Modeling*, **2017**, 57, 2448-2462	6.1	5
47	iPPI-DB: an online database of modulators of protein-protein interactions. *Nucleic Acids Research*, **2016**, 44, D542-7	20.1	38
46	Stabilization of protein-protein interaction complexes through small molecules. *Drug Discovery Today*, **2016**, 21, 48-57	8.8	32
45	Imbalance in chemical space: How to facilitate the identification of protein-protein interaction inhibitors. *Scientific Reports*, **2016**, 6, 23815	4.9	22
44	In silico design of low molecular weight protein-protein interaction inhibitors: Overall concept and recent advances. *Progress in Biophysics and Molecular Biology*, **2015**, 119, 20-32	4.7	46
43	MTiOpenScreen: a web server for structure-based virtual screening. *Nucleic Acids Research*, **2015**, 43, W448-54	20.1	101
42	Sampling of conformational ensemble for virtual screening using molecular dynamics simulations and normal mode analysis. *Future Medicinal Chemistry*, **2015**, 7, 2317-31	4.1	18
41	An exploration of the 3D chemical space has highlighted a specific shape profile for the compounds intended to inhibit protein-protein interactions. *BMC Bioinformatics*, **2015**, 16, A5	3.6	2
40	In Silico Approaches Assisting the Rational Design of Low Molecular Weight Protein-Protein Interaction Modulators **2015**, 441-482		
39	FAF-Drugs3: a web server for compound property calculation and chemical library design. *Nucleic Acids Research*, **2015**, 43, W200-7	20.1	192
38	Which three-dimensional characteristics make efficient inhibitors of protein-protein interactions?. *Journal of Chemical Information and Modeling*, **2014**, 54, 3067-79	6.1	33

37	Identification of Small Inhibitory Molecules Targeting the Bfl-1 Anti-Apoptotic Protein That Alleviates Resistance to ABT-737. *Journal of Biomolecular Screening*, **2014**, 19, 1035-46		10
36	Ligand efficiency driven design of new inhibitors of Mycobacterium tuberculosis transcriptional repressor EthR using fragment growing, merging, and linking approaches. *Journal of Medicinal Chemistry*, **2014**, 57, 4876-88	8.3	50
35	Identification of novel small molecule inhibitors of activated protein C. *Thrombosis Research*, **2014**, 133, 1105-14	8.2	12
34	Rational design of small molecules targeting the C2 domain of coagulation factor VIII. *Blood*, **2014**, 123, 113-20	2.2	17
33	Drug-Like Protein-Protein Interaction Modulators: Challenges and Opportunities for Drug Discovery and Chemical Biology. *Molecular Informatics*, **2014**, 33, 414-437	3.8	84
32	Imidazole-derived 2-[N-carbamoylmethyl-alkylamino]acetic acids, substrate-dependent modulators of insulin-degrading enzyme in amyloid-hydrolysis. *European Journal of Medicinal Chemistry*, **2014**, 79, 184-93	6.8	22
31	Computational analysis of protein-protein interfaces involving an alpha helix: insights for terphenyl-like molecules binding. *BMC Pharmacology & Toxicology*, **2013**, 14, 31	2.6	7
30	Aggrecanase-2 inhibitors based on the acylthiosemicarbazide zinc-binding group. *European Journal of Medicinal Chemistry*, **2013**, 69, 244-61	6.8	10
29	A Leap into the Chemical Space of Protein Protein Interaction Inhibitors **2013**, 63-83		1
28	iPPI-DB: a manually curated and interactive database of small non-peptide inhibitors of protein-protein interactions. *Drug Discovery Today*, **2013**, 18, 958-68	8.8	79
27	One hundred thousand mouse clicks down the road: selected online resources supporting drug discovery collected over a decade. *Drug Discovery Today*, **2013**, 18, 1081-9	8.8	68
26	Thymoquinone as an anticancer agent: evidence from inhibition of cancer cells viability and invasion in vitro and tumor growth in vivo. *Fundamental and Clinical Pharmacology*, **2013**, 27, 557-69	3.1	89
25	Insights into an original pocket-ligand pair classification: a promising tool for ligand profile prediction. *PLoS ONE*, **2013**, 8, e63730	3.7	15
24	1,2,4-Oxadiazoles identified by virtual screening and their non-covalent inhibition of the human 20S proteasome. *Current Medicinal Chemistry*, **2013**, 20, 2351-62	4.3	23
23	A leap into the chemical space of protein-protein interaction inhibitors. *Current Pharmaceutical Design*, **2012**, 18, 4648-67	3.3	53
22	Target-Based Virtual Screening to Address Protein Protein Interfaces. *Methods and Principles in Medicinal Chemistry*, **2011**, 435-465	0.4	
21	The FAF-Drugs2 server: a multistep engine to prepare electronic chemical compound collections. *Bioinformatics*, **2011**, 27, 2018-20	7.2	70
20	In Silico ADME/Tox Predictions **2010**, 29-124		4

19	Tensin2 reduces intracellular phosphatidylinositol 3,4,5-trisphosphate levels at the plasma membrane. *Biochemical and Biophysical Research Communications*, **2010**, 399, 396-401	3.4	12
18	Designing focused chemical libraries enriched in protein-protein interaction inhibitors using machine-learning methods. *PLoS Computational Biology*, **2010**, 6, e1000695	5	94
17	How to choose relevant multiple receptor conformations for virtual screening: a test case of Cdk2 and normal mode analysis. *European Biophysics Journal*, **2010**, 39, 1365-72	1.9	65
16	In silico studies of blood coagulation proteins: from mosaic proteases to nonenzymatic cofactor inhibitors. *Current Opinion in Structural Biology*, **2010**, 20, 168-79	8.1	14
15	Rationalizing the chemical space of protein-protein interaction inhibitors. *Drug Discovery Today*, **2010**, 15, 220-9	8.8	158
14	Druggable pockets and binding site centric chemical space: a paradigm shift in drug discovery. *Drug Discovery Today*, **2010**, 15, 656-67	8.8	214
13	New non-hydroxamic ADAMTS-5 inhibitors based on the 1,2,4-triazole-3-thiol scaffold. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 6213-6	2.9	19
12	wwLigCSRre: a 3D ligand-based server for hit identification and optimization. *Nucleic Acids Research* , **2009**, 37, W504-9	20.1	19
11	Ligand scaffold hopping combining 3D maximal substructure search and molecular similarity. *BMC Bioinformatics*, **2009**, 10, 245	3.6	17
10	MED-3DMC: a new tool to generate 3D conformation ensembles of small molecules with a Monte Carlo sampling of the conformational space. *European Journal of Medicinal Chemistry*, **2009**, 44, 1405-9	6.8	23
9	FAF-Drugs2: free ADME/tox filtering tool to assist drug discovery and chemical biology projects. *BMC Bioinformatics*, **2008**, 9, 396	3.6	192
8	In silico-in vitro screening of protein-protein interactions: towards the next generation of therapeutics. *Current Pharmaceutical Biotechnology*, **2008**, 9, 103-22	2.6	47
7	Combining Ligand- and Structure-Based Methods in Drug Design Projects. *Current Computer-Aided Drug Design*, **2008**, 4, 250-258	1.4	21
6	Screening Outside the Catalytic Site: Inhibition of Macromolecular Inter-actions Through Structure-Based Virtual Ligand Screening Experiments. *The Open Biochemistry Journal*, **2008**, 2, 29-37	0.9	14
5	MED-SuMoLig: a new ligand-based screening tool for efficient scaffold hopping. *Journal of Chemical Information and Modeling*, **2007**, 47, 1097-110	6.1	31
4	Free resources to assist structure-based virtual ligand screening experiments. *Current Protein and Peptide Science*, **2007**, 8, 381-411	2.8	91
3	Design of protein membrane interaction inhibitors by virtual ligand screening, proof of concept with the C2 domain of factor V. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 12697-702	11.5	41
2	Receptor-based computational screening of compound databases: the main docking-scoring engines. *Current Protein and Peptide Science*, **2006**, 7, 369-93	2.8	40

List of Publications

1 InDeep : 3D fully convolutional neural networks to assist in silico drug design on protein-protein interactions 1