# Olivier Sperandio

## List of Publications by Citations



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|---|---|---|---|
| 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 | Druggable pockets and binding site centric chemical space: a paradigm shift in drug discovery. *Drug Discovery Today*, **2010**, 15, 656-67 | 8.8 | 214 |
| 53 | FAF-Drugs3: a web server for compound property calculation and chemical library design. *Nucleic Acids Research*, **2015**, 43, W200-7 | 20.1 | 192 |
| 52 | FAF-Drugs2: free ADME/tox filtering tool to assist drug discovery and chemical biology projects. *BMC Bioinformatics*, **2008**, 9, 396 | 3.6 | 192 |
| 51 | Rationalizing the chemical space of protein-protein interaction inhibitors. *Drug Discovery Today*, **2010**, 15, 220-9 | 8.8 | 158 |
| 50 | MTiOpenScreen: a web server for structure-based virtual screening. *Nucleic Acids Research*, **2015**, 43, W448-54 | 20.1 | 101 |
| 49 | Designing focused chemical libraries enriched in protein-protein interaction inhibitors using machine-learning methods. *PLoS Computational Biology*, **2010**, 6, e1000695 | 5 | 94 |
| 48 | Free resources to assist structure-based virtual ligand screening experiments. *Current Protein and Peptide Science*, **2007**, 8, 381-411 | 2.8 | 91 |
| 47 | 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 |
| 46 | Drug-Like Protein-Protein Interaction Modulators: Challenges and Opportunities for Drug Discovery and Chemical Biology. *Molecular Informatics*, **2014**, 33, 414-437 | 3.8 | 84 |
| 45 | 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 |
| 44 | The FAF-Drugs2 server: a multistep engine to prepare electronic chemical compound collections. *Bioinformatics*, **2011**, 27, 2018-20 | 7.2 | 70 |
| 43 | 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 |
| 42 | 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 |
| 41 | A leap into the chemical space of protein-protein interaction inhibitors. *Current Pharmaceutical Design*, **2012**, 18, 4648-67 | 3.3 | 53 |
| 40 | 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 |
| 39 | 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 |
| 38 | 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 |

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| 37 | 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 |
| 36 | Receptor-based computational screening of compound databases: the main docking-scoring engines. *Current Protein and Peptide Science*, **2006**, 7, 369-93 | 2.8 | 40 |
| 35 | iPPI-DB: an online database of modulators of protein-protein interactions. *Nucleic Acids Research*, **2016**, 44, D542-7 | 20.1 | 38 |
| 34 | Which three-dimensional characteristics make efficient inhibitors of protein-protein interactions?. *Journal of Chemical Information and Modeling*, **2014**, 54, 3067-79 | 6.1 | 33 |
| 33 | Stabilization of protein-protein interaction complexes through small molecules. *Drug Discovery Today*, **2016**, 21, 48-57 | 8.8 | 32 |
| 32 | 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 |
| 31 | 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 |
| 30 | 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 |
| 29 | Imidazole-derived 2-[N-carbamoylmethyl-alkylamino]acetic acids, substrate-dependent modulators of insulin-degrading enzyme in amyloid-β hydrolysis. *European Journal of Medicinal Chemistry*, **2014**, 79, 184-93 | 6.8 | 22 |
| 28 | Imbalance in chemical space: How to facilitate the identification of protein-protein interaction inhibitors. *Scientific Reports*, **2016**, 6, 23815 | 4.9 | 22 |
| 27 | Combining Ligand- and Structure-Based Methods in Drug Design Projects. *Current Computer-Aided Drug Design*, **2008**, 4, 250-258 | 1.4 | 21 |
| 26 | wwLigCSRre: a 3D ligand-based server for hit identification and optimization. *Nucleic Acids Research* , **2009**, 37, W504-9 | 20.1 | 19 |
| 25 | 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 |
| 24 | 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 |
| 23 | Rational design of small molecules targeting the C2 domain of coagulation factor VIII. *Blood*, **2014**, 123, 113-20 | 2.2 | 17 |
| 22 | Ligand scaffold hopping combining 3D maximal substructure search and molecular similarity. *BMC Bioinformatics*, **2009**, 10, 245 | 3.6 | 17 |
| 21 | New machine learning and physics-based scoring functions for drug discovery. *Scientific Reports*, **2021**, 11, 3198 | 4.9 | 17 |
| 20 | Insights into an original pocket-ligand pair classification: a promising tool for ligand profile prediction. *PLoS ONE*, **2013**, 8, e63730 | 3.7 | 15 |

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| 19 | 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 |
| 18 | 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 |
| 17 | Fr-PPIChem: An Academic Compound Library Dedicated to Protein-Protein Interactions. *ACS Chemical Biology*, **2020**, 15, 1566-1574 | 4.9 | 13 |
| 16 | Identification of novel small molecule inhibitors of activated protein C. *Thrombosis Research*, **2014**, 133, 1105-14 | 8.2 | 12 |
| 15 | 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 |
| 14 | 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 |
| 13 | Aggrecanase-2 inhibitors based on the acylthiosemicarbazide zinc-binding group. *European Journal of Medicinal Chemistry*, **2013**, 69, 244-61 | 6.8 | 10 |
| 12 | 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 |
| 11 | Privileged Substructures to Modulate Protein-Protein Interactions. *Journal of Chemical Information and Modeling*, **2017**, 57, 2448-2462 | 6.1 | 5 |
| 10 | In Silico ADME/Tox Predictions **2010**, 29-124 | | 4 |
| 9 | The iPPI-DB initiative: A Community-centered database of Protein-Protein Interaction modulators. *Bioinformatics*, **2021**, | 7.2 | 4 |
| 8 | 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 |
| 7 | InDeep: 3D fully convolutional neural networks to assist in silico drug design on protein-protein interactions.. *Bioinformatics*, **2021**, | 7.2 | 2 |
| 6 | A Leap into the Chemical Space of Protein–Protein Interaction Inhibitors **2013**, 63-83 | | 1 |
| 5 | InDeep : 3D fully convolutional neural networks to assist in silico drug design on protein-protein interactions | | 1 |
| 4 | Characterization of the interaction domains between the phosphoprotein and the nucleoprotein of human Metapneumovirus. *Journal of Virology*, **2021**, JVI0090921 | 6.6 | 0 |
| 3 | Phylogenetic analysis of Harmonin homology domains. *BMC Bioinformatics*, **2021**, 22, 190 | 3.6 | 0 |
| 2 | In Silico Approaches Assisting the Rational Design of Low Molecular Weight Protein–Protein Interaction Modulators **2015**, 441-482 | | |

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| 1 | Target-Based Virtual Screening to Address Protein–Protein Interfaces. *Methods and Principles in Medicinal Chemistry*, **2011**, 435-465 | 0.4 |