

Floriane Montanari

List of Publications by Year in descending order

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Version: 2024-02-01

22
papers

1,095
citations

567281

15
h-index

677142

22
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docs citations

23
times ranked

1466
citing authors

#	ARTICLE	IF	CITATIONS
1	A Fast and Interpretable Deep Learning Approach for Accurate Electrostatics-Driven pK _a Predictions in Proteins. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 5068-5078.	5.3	11
2	Img2Mol – accurate SMILES recognition from molecular graphical depictions. <i>Chemical Science</i> , 2021, 12, 14174-14181.	7.4	32
3	Bayer’s in silico ADMET platform: a journey of machine learning over the past two decades. <i>Drug Discovery Today</i> , 2020, 25, 1702-1709.	6.4	92
4	Modeling Physico-Chemical ADMET Endpoints with Multitask Graph Convolutional Networks. <i>Molecules</i> , 2020, 25, 44.	3.8	67
5	Efficient multi-objective molecular optimization in a continuous latent space. <i>Chemical Science</i> , 2019, 10, 8016-8024.	7.4	143
6	Learning continuous and data-driven molecular descriptors by translating equivalent chemical representations. <i>Chemical Science</i> , 2019, 10, 1692-1701.	7.4	293
7	Vienna LiverTox Workspace – A Set of Machine Learning Models for Prediction of Interactions Profiles of Small Molecules With Transporters Relevant for Regulatory Agencies. <i>Frontiers in Chemistry</i> , 2019, 7, 899.	3.6	16
8	Virtual-screening workflow tutorials and prospective results from the Teach-Discover-Treat competition 2014 against malaria. <i>F1000Research</i> , 2018, 6, 1136.	1.6	6
9	Predicting drug-induced liver injury: The importance of data curation. <i>Toxicology</i> , 2017, 389, 139-145.	4.2	78
10	How Open Data Shapes In Silico Transporter Modeling. <i>Molecules</i> , 2017, 22, 422.	3.8	2
11	Virtual Screening of DrugBank Reveals Two Drugs as New BCRP Inhibitors. <i>SLAS Discovery</i> , 2017, 22, 86-93.	2.7	22
12	Virtual-screening workflow tutorials and prospective results from the Teach-Discover-Treat competition 2014 against malaria. <i>F1000Research</i> , 2017, 6, 1136.	1.6	7
13	Subtle Structural Differences Trigger Inhibitory Activity of Propafenone Analogues at the Two Polyspecific ABC Transporters: P-glycoprotein (P-gp) and Breast Cancer Resistance Protein (BCRP). <i>ChemMedChem</i> , 2016, 11, 1380-1394.	3.2	14
14	11th German Conference on Chemoinformatics (GCC 2015). <i>Journal of Cheminformatics</i> , 2016, 8, 18.	6.1	1
15	Selectivity profiling of BCRP versus P-gp inhibition: from automated collection of polypharmacology data to multi-label learning. <i>Journal of Cheminformatics</i> , 2016, 8, 7.	6.1	26
16	Flagging Drugs That Inhibit the Bile Salt Export Pump. <i>Molecular Pharmaceutics</i> , 2016, 13, 163-171.	4.6	24
17	Integrative Modeling Strategies for Predicting Drug Toxicities at the eTOX Project. <i>Molecular Informatics</i> , 2015, 34, 477-484.	2.5	17
18	The ABC of Phytohormone Translocation. <i>Planta Medica</i> , 2015, 81, 474-487.	1.3	18

#	ARTICLE	IF	CITATIONS
19	Prediction of drug-ABC-transporter interaction Recent advances and future challenges. <i>Advanced Drug Delivery Reviews</i> , 2015, 86, 17-26.	13.7	169
20	Exploiting open data: a new era in pharmacoinformatics. <i>Future Medicinal Chemistry</i> , 2014, 6, 503-514.	2.3	18
21	BCRP Inhibition: from Data Collection to Ligand-Based Modeling. <i>Molecular Informatics</i> , 2014, 33, 322-331.	2.5	27
22	Differences in the Number of Intrinsically Disordered Regions between Yeast Duplicated Proteins, and Their Relationship with Functional Divergence. <i>PLoS ONE</i> , 2011, 6, e24989.	2.5	12