Jonas Boström

List of Publications by Year in descending order

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ΙΩΝΛς ΒΩςτρöΜ

#	Article	IF	CITATIONS
1	On the Value of Using 3D Shape and Electrostatic Similarities in Deep Generative Methods. Journal of Chemical Information and Modeling, 2022, 62, 1388-1398.	2.5	11
2	Transformers for future medicinal chemists. Nature Machine Intelligence, 2021, 3, 102-103.	8.3	5
3	Reusability report: Learning the language of synthetic methods used in medicinal chemistry. Nature Machine Intelligence, 2021, 3, 572-575.	8.3	3
4	Can easy chemistry produce complex, diverse, and novel molecules?. Drug Discovery Today, 2020, 25, 2174-2181.	3.2	33
5	Design of a small molecule that stimulates vascular endothelial growth factor A enabled by screening RNA fold–small molecule interactions. Nature Chemistry, 2020, 12, 952-961.	6.6	51
6	Identification and analyses of inhibitors targeting apolipoprotein(a) kringle domains KIV-7, KIV-10, and KV provide insight into kringle domain function. Journal of Biological Chemistry, 2020, 295, 5136-5151.	1.6	6
7	Deep Convolutional Neural Networks for the Prediction of Molecular Properties: Challenges and Opportunities Connected to the Data. Journal of Integrative Bioinformatics, 2019, 16, .	1.0	9
8	Improving the Use of Deep Convolutional Neural Networks for the Prediction ofÂMolecular Properties. Advances in Intelligent Systems and Computing, 2019, , 71-79.	0.5	0
9	Deep Reinforcement Learning for Multiparameter Optimization in <i>de novo</i> Drug Design. Journal of Chemical Information and Modeling, 2019, 59, 3166-3176.	2.5	130
10	ReFlex3D: Refined Flexible Alignment of Molecules Using Shape and Electrostatics. Journal of Chemical Information and Modeling, 2018, 58, 747-760.	2.5	7
11	Expanding the medicinal chemistry synthetic toolbox. Nature Reviews Drug Discovery, 2018, 17, 709-727.	21.5	391
12	Where Do Recent Small Molecule Clinical Development Candidates Come From?. Journal of Medicinal Chemistry, 2018, 61, 9442-9468.	2.9	131
13	Discovery and Evaluation of Anti-Fibrinolytic Plasmin Inhibitors Derived from 5-(4-Piperidyl)isoxazol-3-ol (4-PIOL). Journal of Chemical Information and Modeling, 2017, 57, 1703-1714.	2.5	7
14	3D-Lab: a collaborative web-based platform for molecular modeling. Future Medicinal Chemistry, 2016, 8, 1739-1752.	1.1	20
15	Analysis of Past and Present Synthetic Methodologies on Medicinal Chemistry: Where Have All the New Reactions Gone?. Journal of Medicinal Chemistry, 2016, 59, 4443-4458.	2.9	1,187
16	Stuck in a rut with old chemistry. Drug Discovery Today, 2016, 21, 701-703.	3.2	11
17	Understanding Our Love Affair with <i>p</i> -Chlorophenyl: Present Day Implications from Historical Biases of Reagent Selection. Journal of Medicinal Chemistry, 2015, 58, 2390-2405.	2.9	54
18	Molecular Rift: Virtual Reality for Drug Designers. Journal of Chemical Information and Modeling, 2015, 55, 2475-2484.	2.5	88

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19	Lactam sulfonamides as potent inhibitors of the Kv1.5 potassium ion channel. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 1269-1273.	1.0	9
20	Using Matched Molecular Series as a Predictive Tool To Optimize Biological Activity. Journal of Medicinal Chemistry, 2014, 57, 2704-2713.	2.9	50
21	Discovery of the Fibrinolysis Inhibitor AZD6564, Acting via Interference of a Protein–Protein Interaction. ACS Medicinal Chemistry Letters, 2014, 5, 538-543.	1.3	31
22	Synthesis and evaluation of diphenylphosphinic amides and diphenylphosphine oxides as inhibitors of Kv1.5. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 706-710.	1.0	19
23	Potent Fibrinolysis Inhibitor Discovered by Shape and Electrostatic Complementarity to the Drug Tranexamic Acid. Journal of Medicinal Chemistry, 2013, 56, 3273-3280.	2.9	33
24	Synthesis, structure–property relationships and pharmacokinetic evaluation of ethyl 6-aminonicotinate sulfonylureas as antagonists of the P2Y12 receptor. European Journal of Medicinal Chemistry, 2013, 65, 360-375.	2.6	36
25	5-alkyl-1,3-oxazole derivatives of 6-amino-nicotinic acids as alkyl ester bioisosteres are antagonists of the P2Y ₁₂ receptor. Future Medicinal Chemistry, 2013, 5, 2037-2056.	1.1	13
26	Symmetric Kv1.5 Blockers Discovered by Focused Screening. ACS Medicinal Chemistry Letters, 2012, 3, 769-773.	1.3	6
27	Exploiting Structural Information in Patent Specifications for Key Compound Prediction. Journal of Chemical Information and Modeling, 2012, 52, 1480-1489.	2.5	17
28	Oxadiazoles in Medicinal Chemistry. Journal of Medicinal Chemistry, 2012, 55, 1817-1830.	2.9	458
29	Exploiting personalized information for reagent selection in drug design. Drug Discovery Today, 2011, 16, 181-187.	3.2	13
30	Follow-on drugs: How far should chemists look?. Drug Discovery Today, 2011, 16, 722-732.	3.2	28
31	A novel series of piperazinyl-pyridine ureas as antagonists of the purinergic P2Y12 receptor. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 2877-2881.	1.0	26
32	Novel thioamide derivatives as neutral CB1 receptor antagonists. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 479-482.	1.0	25
33	Scaffold hopping, synthesis and structure–activity relationships of 5,6-diaryl-pyrazine-2-amide derivatives: A novel series of CB1 receptor antagonists. Bioorganic and Medicinal Chemistry, 2007, 15, 4077-4084.	1.4	62
34	Do Structurally Similar Ligands Bind in a Similar Fashion?. Journal of Medicinal Chemistry, 2006, 49, 6716-6725.	2.9	171
35	MIMUMBA Revisited:  Torsion Angle Rules for Conformer Generation Derived from X-ray Structures. Journal of Chemical Information and Modeling, 2006, 46, 2305-2309.	2.5	32
36	Computational chemistry-driven decision making in lead generation. Drug Discovery Today, 2006, 11, 43-50.	3.2	70

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37	Assessing the performance of OMEGA with respect to retrieving bioactive conformations. Journal of Molecular Graphics and Modelling, 2003, 21, 449-462.	1.3	281
38	A 3D QSAR Study on a Set of Dopamine D4Receptor Antagonists. Journal of Chemical Information and Computer Sciences, 2003, 43, 1020-1027.	2.8	49
39	Reproducing the conformations of protein-bound ligands: a critical evaluation of several popular conformational searching tools. Journal of Computer-Aided Molecular Design, 2001, 15, 1137-1152.	1.3	164
40	A pharmacophore model for dopamine D4 receptor antagonists. Journal of Computer-Aided Molecular Design, 2000, 14, 769-786.	1.3	21
41	Conformational energy penalties of protein-bound ligands. Journal of Computer-Aided Molecular Design, 1998, 12, 383-383.	1.3	223