RESEARCH & PUBLICATIONS

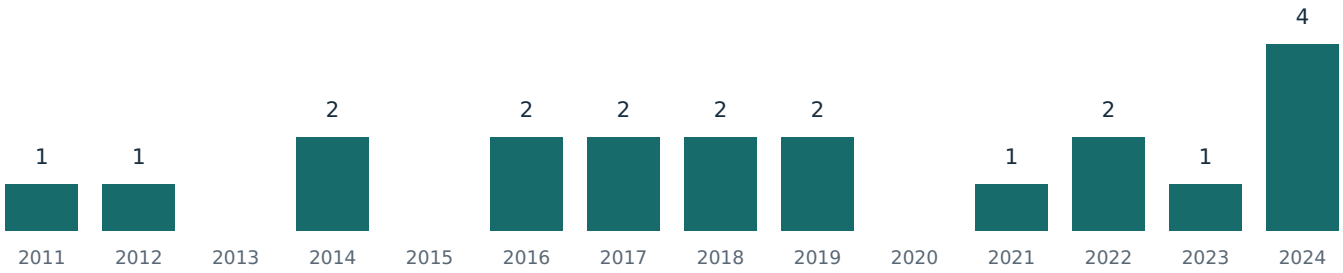
Antoine Daina

A publication record at a glance

20	25,458	16
ARTICLES	CITATIONS	h-INDEX

PUBLICATION ACTIVITY

Articles by publication year



MOST CITED IN THIS LIST

SwissADME: A Free Web Tool to Evaluate Pharmacokinetics, Drug-Likeness and Medicinal Chemistry Friendliness of Small Molecules — 16,667

2017 Scientific Reports

SwissTargetPrediction: Updated Data and New Features for Efficient Prediction of Protein Targets of Small Molecules — 4,347

2019 Nucleic Acids Research

SwissTargetPrediction: A Web Server for Target Prediction of Bioactive Small Molecules. — 1,646

2014 Nucleic Acids Research

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Ordered by publication year, newest first

2024

01 **Open Access Databases and Datasets for Computer-Aided Drug Design. A Short List Used in the Molecular Modelling Group of the SIB**

0 citations

Methods and Principles in Medicinal Chemistry

https://exaly.com/article/170769689

02 **Bioisosteric Replacement for Drug Discovery Supported by the SwissBioisostere Database**

3 citations

Methods and Principles in Medicinal Chemistry

https://exaly.com/article/170791519

03 **SwissDock 2024: Major Enhancements for Small-Molecule Docking With Attracting Cavities and AutoDock Vina.**

556 citations

Nucleic Acids Research · 52, W324-W332

https://exaly.com/article/185021913

04 **Testing the Predictive Power of Reverse Screening to Infer Drug Targets, With the Help of Machine Learning**

120 citations

Communications Chemistry · 7, 1-8

https://exaly.com/article/185307216

2023

05 **SwissParam 2023: A Modern Web-Based Tool for Efficient Small Molecule Parametrization**

330 citations

Journal of Chemical Information and Modeling · 63, 6469-6475

https://exaly.com/article/170754040

2022

06 **SwissBioisostere 2021: Updated Structural, Bioactivity and Physicochemical Data Delivered by a Reshaped Web Interface**

51 citations

Nucleic Acids Research · 50, D1382-D1390

https://exaly.com/article/120396235

07 **The SwissSimilarity 2021 Web Tool: Novel Chemical Libraries and Additional Methods for an Enhanced Ligand-Based Virtual Screening Experience**

134 citations

International Journal of Molecular Sciences · 23, 811

https://exaly.com/article/125267125

2021

08 **Computer-Aided Drug Design for Cancer Therapy**

3 citations

Journal unavailable

https://exaly.com/article/77878027

Ordered by publication year, newest first

2019

09 **Application of the SwissDrugDesign Online Resources in Virtual Screening**
108 citations
International Journal of Molecular Sciences · 20, 4612
https://exaly.com/article/72803347

10 **SwissTargetPrediction: Updated Data and New Features for Efficient Prediction of Protein Targets of Small Molecules**
4,347 citations
Nucleic Acids Research · 47, W357-W364
https://exaly.com/article/73132169

2018

11 **Rational Design, Synthesis, and Pharmacological Characterization of Novel Ghrelin Receptor Inverse Agonists as Potential Treatment Against Obesity-Related Metabolic Diseases**
17 citations
Journal of Medicinal Chemistry · 61, 11039-11060
https://exaly.com/article/70662162

12 **Educational Tools to Introduce Computer-Aided Drug Design to Students and to the Public at Large**
3 citations
Chimia · 72, 55
https://exaly.com/article/71727651

2017

13 **Drug Design Workshop: A Web-Based Educational Tool to Introduce Computer-Aided Drug Design to the General Public**
55 citations
Journal of Chemical Education · 94, 335-344
https://exaly.com/article/66084447

14 **SwissADME: A Free Web Tool to Evaluate Pharmacokinetics, Drug-Likeness and Medicinal Chemistry Friendliness of Small Molecules**
16,667 citations
Scientific Reports · 7, 1-13
https://exaly.com/article/66132810

2016

15 **SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening**
337 citations
Journal of Chemical Information and Modeling · 56, 1399-404
https://exaly.com/article/63467227

16 **Attracting Cavities for Docking. Replacing the Rough Energy Landscape of the Protein by a Smooth Attracting Landscape**
69 citations
Journal of Computational Chemistry · 37, 437-447
https://exaly.com/article/63895387

Ordered by publication year, newest first

2014

17 **SwissTargetPrediction: A Web Server for Target Prediction of Bioactive Small Molecules.**

1,646 citations

Nucleic Acids Research · 42, W32-8

https://exaly.com/article/57732633

18 **iLOGP: A Simple, Robust, and Efficient Description of n-Octanol/Water Partition Coefficient for Drug Design Using the GB/SA Approach**

936 citations

Journal of Chemical Information and Modeling · 54, 3284-301

https://exaly.com/article/58237677

2012

19 **Glycosaminoglycans Are Interactants of Langerin: Comparison With gp120 Highlights an Unexpected Calcium-Independent Binding Mode**

51 citations

PLoS ONE · 7, e50722

https://exaly.com/article/54060144

2011

20 **A Practical Introduction to Molecular Dynamics Simulations: Applications to Homology Modeling**

25 citations

Methods in Molecular Biology · 857, 137-173

https://exaly.com/article/50339612

End of list · 20 articles. Citation counts use Exaly’s peer-reviewed cohort.