

Francesca Grisoni

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

62

papers

1,577

citations

21

h-index

38

g-index

73

ext. papers

2,184

ext. citations

5.7

avg, IF

5.55

L-index

#	Paper	IF	Citations
62	De Novo Molecular Design with Chemical Language Models. <i>Methods in Molecular Biology</i> , 2022 , 2390, 207-232	1.4	1
61	Perplexity-Based Molecule Ranking and Bias Estimation of Chemical Language Models.. <i>Journal of Chemical Information and Modeling</i> , 2022 ,	6.1	4
60	Identification of novel off targets of baricitinib and tofacitinib by machine learning with a focus on thrombosis and viral infection.. <i>Scientific Reports</i> , 2022 , 12, 7843	4.9	1
59	Geometric deep learning on molecular representations. <i>Nature Machine Intelligence</i> , 2021 , 3, 1023-1032	22.5	15
58	Artificial intelligence in drug discovery: recent advances and future perspectives. <i>Expert Opinion on Drug Discovery</i> , 2021 , 16, 949-959	6.2	27
57	CATMoS: Collaborative Acute Toxicity Modeling Suite. <i>Environmental Health Perspectives</i> , 2021 , 129, 47013	8.4	14
56	Combining generative artificial intelligence and on-chip synthesis for de novo drug design. <i>Science Advances</i> , 2021 , 7,	14.3	15
55	Beam Search for Automated Design and Scoring of Novel ROR Ligands with Machine Intelligence*. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 19477-19482	16.4	7
54	Molecular Scaffold Hopping via Holistic Molecular Representation. <i>Methods in Molecular Biology</i> , 2021 , 2266, 11-35	1.4	3
53	Beam-Search zum automatisierten Entwurf und Scoring neuer ROR-Liganden mithilfe maschineller Intelligenz**. <i>Angewandte Chemie</i> , 2021 , 133, 19626-19632	3.6	
52	Generative molecular design in low data regimes. <i>Nature Machine Intelligence</i> , 2020 , 2, 171-180	22.5	44
51	Verification of Chromatographic Profile of Primary Essential Oil of L. Combined with Chemometric Analysis. <i>Molecules</i> , 2020 , 25,	4.8	5
50	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. <i>Environmental Health Perspectives</i> , 2020 , 128, 27002	8.4	70
49	Consensus versus Individual QSARs in Classification: Comparison on a Large-Scale Case Study. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 1215-1223	6.1	9
48	Geographical identification of Chianti red wine based on ICP-MS element composition. <i>Food Chemistry</i> , 2020 , 315, 126248	8.5	22
47	NURA: A curated dataset of nuclear receptor modulators. <i>Toxicology and Applied Pharmacology</i> , 2020 , 407, 115244	4.6	6
46	Bidirectional Molecule Generation with Recurrent Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 1175-1183	6.1	39

45	Chemometrics for QSAR Modeling 2020 , 599-634		5
44	Drug discovery with explainable artificial intelligence. <i>Nature Machine Intelligence</i> , 2020 , 2, 573-584	22.5	116
43	Predicting molecular activity on nuclear receptors by multitask neural networks. <i>Journal of Chemometrics</i> , 2020 , e3325	1.6	8
42	Machine Learning Consensus To Predict the Binding to the Androgen Receptor within the CoMPARA Project. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 1839-1848	6.1	20
41	Design of Natural-Product-Inspired Multitarget Ligands by Machine Learning. <i>ChemMedChem</i> , 2019 , 14, 1129-1134	3.7	21
40	De novo design of anticancer peptides by ensemble artificial neural networks. <i>Journal of Molecular Modeling</i> , 2019 , 25, 112	2	25
39	On the Misleading Use of Q F 3 2 for QSAR Model Comparison. <i>Molecular Informatics</i> , 2019 , 38, e1800029	3.8	17
38	Structural alerts for the identification of bioaccumulative compounds. <i>Integrated Environmental Assessment and Management</i> , 2019 , 15, 19-28	2.5	9
37	Deep Ranking Analysis by Power Eigenvectors (DRAPE): A wizard for ranking and multi-criteria decision making. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2019 , 191, 129-137	3.8	5
36	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Molecular Design With Long Short-Term Memory Networks. <i>Journal of Computer Aided Chemistry</i> , 2019 , 20, 35-42	0.2	
35	Predictive models in ecotoxicology: Bridging the gap between scientific progress and regulatory applicability-Remarks and research needs. <i>Integrated Environmental Assessment and Management</i> , 2019 , 15, 345-351	2.5	3
34	Molecular Design with Generative Long Short-term Memory. <i>Chimia</i> , 2019 , 73, 1006-1011	1.3	12
33	Integrated QSAR Models to Predict Acute Oral Systemic Toxicity. <i>Molecular Informatics</i> , 2019 , 38, e1800124	3.8	20
32	Acceptable-by-design QSARs to predict the dietary biomagnification of organic chemicals in fish. <i>Integrated Environmental Assessment and Management</i> , 2019 , 15, 51-63	2.5	6
31	Discovery of Novel Molecular Frameworks of Farnesoid X Receptor Modulators by Ensemble Machine Learning. <i>ChemistryOpen</i> , 2019 , 8, 3	2.3	0
30	Discovery of Novel Molecular Frameworks of Farnesoid X Receptor Modulators by Ensemble Machine Learning. <i>ChemistryOpen</i> , 2019 , 8, 7-14	2.3	1
29	Designing Anticancer Peptides by Constructive Machine Learning. <i>ChemMedChem</i> , 2018 , 13, 1300-1302	3.7	44
28	Predictive Models in Ecotoxicology: Bridging the Gap Between Scientific Progress and Regulatory Applicability. <i>Integrated Environmental Assessment and Management</i> , 2018 , 14, 601-603	2.5	2

27	Mapping of Activity through Dichotomic Scores (MADS): A new chemoinformatic approach to detect activity-rich structural regions. <i>Journal of Chemometrics</i> , 2018 , 32, e2994	1.6	0
26	De Novo Design of Bioactive Small Molecules by Artificial Intelligence. <i>Molecular Informatics</i> , 2018 , 37, 1700153	3.8	155
25	Molecular Descriptors for Structure-Activity Applications: A Hands-On Approach. <i>Methods in Molecular Biology</i> , 2018 , 1800, 3-53	1.4	10
24	Lipophilicity prediction of peptides and peptide derivatives by consensus machine learning. <i>MedChemComm</i> , 2018 , 9, 1538-1546	5	13
23	Scaffold hopping from natural products to synthetic mimetics by holistic molecular similarity. <i>Communications Chemistry</i> , 2018 , 1,	6.3	29
22	Scaffold hopping from synthetic RXR modulators by virtual screening and design. <i>MedChemComm</i> , 2018 , 9, 1289-1292	5	13
21	Computer-Assisted Discovery of Retinoid X Receptor Modulating Natural Products and Isofunctional Mimetics. <i>Journal of Medicinal Chemistry</i> , 2018 , 61, 5442-5447	8.3	28
20	Multivariate comparison of classification performance measures. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2018 , 174, 33-44	3.8	115
19	Scaffold-Hopping from Synthetic Drugs by Holistic Molecular Representation. <i>Scientific Reports</i> , 2018 , 8, 16469	4.9	17
18	Tuning artificial intelligence on the de novo design of natural-product-inspired retinoid X receptor modulators. <i>Communications Chemistry</i> , 2018 , 1,	6.3	44
17	Impact of Molecular Descriptors on Computational Models. <i>Methods in Molecular Biology</i> , 2018 , 1825, 171-209	1.4	16
16	Detecting the bioaccumulation patterns of chemicals through data-driven approaches. <i>Chemosphere</i> , 2018 , 208, 273-284	8.4	10
15	Chemical profiling and multivariate data fusion methods for the identification of the botanical origin of honey. <i>Food Chemistry</i> , 2018 , 266, 79-89	8.5	42
14	Matrix-based Molecular Descriptors for Prospective Virtual Compound Screening. <i>Molecular Informatics</i> , 2017 , 36, 1600091	3.8	16
13	A QSTR-Based Expert System to Predict Sweetness of Molecules. <i>Frontiers in Chemistry</i> , 2017 , 5, 53	5	21
12	Beware of Unreliable Q! A Comparative Study of Regression Metrics for Predictivity Assessment of QSAR Models. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 1905-1913	6.1	59
11	A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2016 , 157, 50-57	3.8	18
10	Investigating the mechanisms of bioconcentration through QSAR classification trees. <i>Environment International</i> , 2016 , 88, 198-205	12.9	21

9	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. <i>Environmental Health Perspectives</i> , 2016 , 124, 1023-33	8.4	206
8	In Silico Prediction of Cytochrome P450-Drug Interaction: QSARs for CYP3A4 and CYP2C9. <i>International Journal of Molecular Sciences</i> , 2016 , 17,	6.3	38
7	Expert QSAR system for predicting the bioconcentration factor under the REACH regulation. <i>Environmental Research</i> , 2016 , 148, 507-512	7.9	20
6	QSAR models for bioconcentration: is the increase in the complexity justified by more accurate predictions?. <i>Chemosphere</i> , 2015 , 127, 171-9	8.4	28
5	Weighted power/weakness ratio for multi-criteria decision making. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015 , 146, 329-336	3.8	12
4	How to weight Hasse matrices and reduce incomparabilities. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2015 , 147, 95-104	3.8	11
3	Reshaped Sequential Replacement algorithm: An efficient approach to variable selection. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2014 , 133, 136-148	3.8	15
2	Reshaped Sequential Replacement for variable selection in QSPR: comparison with other reference methods. <i>Journal of Chemometrics</i> , 2014 , 28, 249-259	1.6	12
1	Combining Generative Artificial Intelligence and On-Chip Synthesis for De Novo Drug Design		2