Francesca Grisoni

List of Publications by Citations

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	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. *Environmental Health Perspectives*, **2016**, 124, 1023-33	8.4	206
61	De Novo Design of Bioactive Small Molecules by Artificial Intelligence. *Molecular Informatics*, **2018**, 37, 1700153	3.8	155
60	Drug discovery with explainable artificial intelligence. *Nature Machine Intelligence*, **2020**, 2, 573-584	22.5	116
59	Multivariate comparison of classification performance measures. *Chemometrics and Intelligent Laboratory Systems*, **2018**, 174, 33-44	3.8	115
58	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. *Environmental Health Perspectives*, **2020**, 128, 27002	8.4	70
57	Beware of Unreliable Q! A Comparative Study of Regression Metrics for Predictivity Assessment of QSAR Models. *Journal of Chemical Information and Modeling*, **2016**, 56, 1905-1913	6.1	59
56	Generative molecular design in low data regimes. *Nature Machine Intelligence*, **2020**, 2, 171-180	22.5	44
55	Designing Anticancer Peptides by Constructive Machine Learning. *ChemMedChem*, **2018**, 13, 1300-1302	3.7	44
54	Tuning artificial intelligence on the de novo design of natural-product-inspired retinoid X receptor modulators. *Communications Chemistry*, **2018**, 1,	6.3	44
53	Chemical profiling and multivariate data fusion methods for the identification of the botanical origin of honey. *Food Chemistry*, **2018**, 266, 79-89	8.5	42
52	Bidirectional Molecule Generation with Recurrent Neural Networks. *Journal of Chemical Information and Modeling*, **2020**, 60, 1175-1183	6.1	39
51	In Silico Prediction of Cytochrome P450-Drug Interaction: QSARs for CYP3A4 and CYP2C9. *International Journal of Molecular Sciences*, **2016**, 17,	6.3	38
50	Scaffold hopping from natural products to synthetic mimetics by holistic molecular similarity. *Communications Chemistry*, **2018**, 1,	6.3	29
49	QSAR models for bioconcentration: is the increase in the complexity justified by more accurate predictions?. *Chemosphere*, **2015**, 127, 171-9	8.4	28
48	Computer-Assisted Discovery of Retinoid X Receptor Modulating Natural Products and Isofunctional Mimetics. *Journal of Medicinal Chemistry*, **2018**, 61, 5442-5447	8.3	28
47	Artificial intelligence in drug discovery: recent advances and future perspectives. *Expert Opinion on Drug Discovery*, **2021**, 16, 949-959	6.2	27
46	De novo design of anticancer peptides by ensemble artificial neural networks. *Journal of Molecular Modeling*, **2019**, 25, 112	2	25

45	Geographical identification of Chianti red wine based on ICP-MS element composition. *Food Chemistry*, **2020**, 315, 126248	8.5	22
44	Design of Natural-Product-Inspired Multitarget Ligands by Machine Learning. *ChemMedChem*, **2019**, 14, 1129-1134	3.7	21
43	Investigating the mechanisms of bioconcentration through QSAR classification trees. *Environment International*, **2016**, 88, 198-205	12.9	21
42	A QSTR-Based Expert System to Predict Sweetness of Molecules. *Frontiers in Chemistry*, **2017**, 5, 53	5	21
41	Machine Learning Consensus To Predict the Binding to the Androgen Receptor within the CoMPARA Project. *Journal of Chemical Information and Modeling*, **2019**, 59, 1839-1848	6.1	20
40	Expert QSAR system for predicting the bioconcentration factor under the REACH regulation. *Environmental Research*, **2016**, 148, 507-512	7.9	20
39	Integrated QSAR Models to Predict Acute Oral Systemic Toxicity. *Molecular Informatics*, **2019**, 38, e1800124	3.8	20
38	A new concept of higher-order similarity and the role of distance/similarity measures in local classification methods. *Chemometrics and Intelligent Laboratory Systems*, **2016**, 157, 50-57	3.8	18
37	On the Misleading Use of Q F 3 2 for QSAR Model Comparison. *Molecular Informatics*, **2019**, 38, e1800029	3.8	17
36	Scaffold-Hopping from Synthetic Drugs by Holistic Molecular Representation. *Scientific Reports*, **2018**, 8, 16469	4.9	17
35	Matrix-based Molecular Descriptors for Prospective Virtual Compound Screening. *Molecular Informatics*, **2017**, 36, 1600091	3.8	16
34	Impact of Molecular Descriptors on Computational Models. *Methods in Molecular Biology*, **2018**, 1825, 171-209	1.4	16
33	Reshaped Sequential Replacement algorithm: An efficient approach to variable selection. *Chemometrics and Intelligent Laboratory Systems*, **2014**, 133, 136-148	3.8	15
32	Geometric deep learning on molecular representations. *Nature Machine Intelligence*, **2021**, 3, 1023-1032	22.5	15
31	Combining generative artificial intelligence and on-chip synthesis for de novo drug design. *Science Advances*, **2021**, 7,	14.3	15
30	CATMoS: Collaborative Acute Toxicity Modeling Suite. *Environmental Health Perspectives*, **2021**, 129, 47013	8.4	14
29	Lipophilicity prediction of peptides and peptide derivatives by consensus machine learning. *MedChemComm*, **2018**, 9, 1538-1546	5	13
28	Scaffold hopping from synthetic RXR modulators by virtual screening and design. *MedChemComm*, **2018**, 9, 1289-1292	5	13

27	Weighted power□weakness ratio for multi-criteria decision making. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 146, 329-336	3.8	12
26	Reshaped Sequential Replacement for variable selection in QSPR: comparison with other reference methods. *Journal of Chemometrics*, **2014**, 28, 249-259	1.6	12
25	Molecular Design with Generative Long Short-term Memory. *Chimia*, **2019**, 73, 1006-1011	1.3	12
24	How to weight Hasse matrices and reduce incomparabilities. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 147, 95-104	3.8	11
23	Molecular Descriptors for Structure-Activity Applications: A Hands-On Approach. *Methods in Molecular Biology*, **2018**, 1800, 3-53	1.4	10
22	Detecting the bioaccumulation patterns of chemicals through data-driven approaches. *Chemosphere*, **2018**, 208, 273-284	8.4	10
21	Consensus versus Individual QSARs in Classification: Comparison on a Large-Scale Case Study. *Journal of Chemical Information and Modeling*, **2020**, 60, 1215-1223	6.1	9
20	Structural alerts for the identification of bioaccumulative compounds. *Integrated Environmental Assessment and Management*, **2019**, 15, 19-28	2.5	9
19	Predicting molecular activity on nuclear receptors by multitask neural networks. *Journal of Chemometrics*, **2020**, e3325	1.6	8
18	Beam Search for Automated Design and Scoring of Novel ROR Ligands with Machine Intelligence*. *Angewandte Chemie - International Edition*, **2021**, 60, 19477-19482	16.4	7
17	NURA: A curated dataset of nuclear receptor modulators. *Toxicology and Applied Pharmacology*, **2020**, 407, 115244	4.6	6
16	Acceptable-by-design QSARs to predict the dietary biomagnification of organic chemicals in fish. *Integrated Environmental Assessment and Management*, **2019**, 15, 51-63	2.5	6
15	Verification of Chromatographic Profile of Primary Essential Oil of L. Combined with Chemometric Analysis. *Molecules*, **2020**, 25,	4.8	5
14	Deep Ranking Analysis by Power Eigenvectors (DRAPE): A wizard for ranking and multi-criteria decision making. *Chemometrics and Intelligent Laboratory Systems*, **2019**, 191, 129-137	3.8	5
13	Chemometrics for QSAR Modeling **2020**, 599-634		5
12	Perplexity-Based Molecule Ranking and Bias Estimation of Chemical Language Models.. *Journal of Chemical Information and Modeling*, **2022**,	6.1	4
11	Predictive models in ecotoxicology: Bridging the gap between scientific progress and regulatory applicability-Remarks and research needs. *Integrated Environmental Assessment and Management*, **2019**, 15, 345-351	2.5	3
10	Molecular Scaffold Hopping via Holistic Molecular Representation. *Methods in Molecular Biology*, **2021**, 2266, 11-35	1.4	3

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9	Predictive Models in Ecotoxicology: Bridging the Gap Between Scientific Progress and Regulatory Applicability. *Integrated Environmental Assessment and Management*, **2018**, 14, 601-603	2.5	2
8	Combining Generative Artificial Intelligence and On-Chip Synthesis for De Novo Drug Design		2
7	De Novo Molecular Design with Chemical Language Models. *Methods in Molecular Biology*, **2022**, 2390, 207-232	1.4	1
6	Discovery of Novel Molecular Frameworks of Farnesoid X Receptor Modulators by Ensemble Machine Learning. *ChemistryOpen*, **2019**, 8, 7-14	2.3	1
5	Identification of novel off targets of baricitinib and tofacitinib by machine learning with a focus on thrombosis and viral infection.. *Scientific Reports*, **2022**, 12, 7843	4.9	1
4	Mapping of Activity through Dichotomic Scores (MADS): A new chemoinformatic approach to detect activity-rich structural regions. *Journal of Chemometrics*, **2018**, 32, e2994	1.6	0
3	Discovery of Novel Molecular Frameworks of Farnesoid X Receptor Modulators by Ensemble Machine Learning. *ChemistryOpen*, **2019**, 8, 3	2.3	0
2	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Molecular Design With Long Short-Term Memory Networks. *Journal of Computer Aided Chemistry*, **2019**, 20, 35-42	0.2	
1	Beam-Search zum automatisierten Entwurf und Scoring neuer ROR-Liganden mithilfe maschineller Intelligenz**. *Angewandte Chemie*, **2021**, 133, 19626-19632	3.6	