Gilles Marcou

List of Publications by Year
in descending order

110 papers	3,725 citations	185998 28 h-index	143772 57 g-index
113 all docs	113 docs citations	113 times ranked	3366 citing authors

#	Article	IF	Citations
1	Synthl: A New Open-Source Tool for Synthon-Based Library Design. Journal of Chemical Information and Modeling, 2022, 62, 2151-2163.	2.5	18
2	Exploration of the Chemical Space of DNAâ€encoded Libraries. Molecular Informatics, 2022, 41, .	1.4	9
3	Comprehensive analysis of commercial fragment libraries. RSC Medicinal Chemistry, 2022, 13, 300-310.	1.7	11
4	Computational screening methodology identifies effective solvents for CO2 capture. Communications Chemistry, 2022, 5, .	2.0	17
5	Rapid Discrimination of Neuromyelitis Optica Spectrum Disorder and Multiple Sclerosis Using Machine Learning on Infrared Spectra of Sera. International Journal of Molecular Sciences, 2022, 23, 2791.	1.8	4
6	A Close-up Look at the Chemical Space of Commercially Available Building Blocks for Medicinal Chemistry. Journal of Chemical Information and Modeling, 2022, 62, 2171-2185.	2.5	32
7	Toward in Silico Modeling of Dynamic Combinatorial Libraries. ACS Central Science, 2022, 8, 804-813.	5.3	3
8	Molecular Similarity Perception Based on Machine-Learning Models. International Journal of Molecular Sciences, 2022, 23, 6114.	1.8	0
9	Visualization and Analysis of the REACHâ€chemical Space with Generative Topographic Mapping. Molecular Informatics, 2021, 40, 2000232.	1.4	2
10	Chemography: Searching for Hidden Treasures. Journal of Chemical Information and Modeling, 2021, 61, 179-188.	2.5	14
11	Discovery of novel chemical reactions by deep generative recurrent neural network. Scientific Reports, 2021, 11, 3178.	1.6	40
12	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	2.8	63
13	NP Navigator: A New Look at the Natural Product Chemical Space. Molecular Informatics, 2021, 40, e2100068.	1.4	16
14	Computer-Aided Design of New Physical Solvents for Hydrogen Sulfide Absorption. Industrial & Engineering Chemistry Research, 2021, 60, 8588-8596.	1.8	9
15	DMSO Solubility Assessment for Fragment-Based Screening. Molecules, 2021, 26, 3950.	1.7	2
16	Endocrine disruption: the noise in available data adversely impacts the modelsâ€™ performance. SAR and QSAR in Environmental Research, 2021, 32, 111-131.	1.0	4
17	Chemoinformatics-Driven Design of New Physical Solvents for Selective CO₂ Absorption. Environmental Science & Technology, 2021, 55, 15542-15553.	4.6	16
18	NP Navigator: A New Online Tool for the Exploration of the Natural Products Chemical Space. Medical Sciences Forum, 2021, 7, .	0.5	0

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19	Diversifying chemical libraries with generative topographic mapping. Journal of Computer-Aided Molecular Design, 2020, 34, 805-815.	1.3	7
20	Trustworthiness, the Key to Grid-Based Map-Driven Predictive Model Enhancement and Applicability Domain Control. Journal of Chemical Information and Modeling, 2020, 60, 6020-6032.	2.5	1
21	Autoignition temperature: comprehensive data analysis and predictive models. SAR and QSAR in Environmental Research, 2020, 31, 597-613.	1.0	4
22	Consensus QSAR models estimating acute toxicity to aquatic organisms from different trophic levels: algae, Daphnia and fish. SAR and QSAR in Environmental Research, 2020, 31, 655-675.	1.0	19
23	A Chemographic Audit of antiâ€Coronavirus Structureâ€activity Information from Public Databases (ChEMBL). Molecular Informatics, 2020, 39, e2000080.	1.4	16
24	â€œBig Dataâ€•Fast Chemoinformatics Model to Predict Generalized Born Radius and Solvent Accessibility as a Function of Geometry. Journal of Chemical Information and Modeling, 2020, 60, 2951-2965.	2.5	1
25	Publicly available QSPR models for environmental media persistence. SAR and QSAR in Environmental Research, 2020, 31, 493-510.	1.0	3
26	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
27	Application of the mol2vec Technology to Largeâ€size Data Visualization and Analysis. Molecular Informatics, 2020, 39, e1900170.	1.4	8
28	Modelling of ready biodegradability based on combined public and industrial data sources. SAR and QSAR in Environmental Research, 2020, 31, 171-186.	1.0	14
29	Parallel Generative Topographic Mapping: An Efficient Approach for Big Data Handling. Molecular Informatics, 2020, 39, 2000009.	1.4	6
30	Predictive Models for Kinetic Parameters of Cycloaddition Reactions. Molecular Informatics, 2019, 38, e1800077.	1.4	25
31	Consensus models to predict oral rat acute toxicity and validation on a dataset coming from the industrial context. SAR and QSAR in Environmental Research, 2019, 30, 879-897.	1.0	22
32	Generative Topographic Mapping of the Docking Conformational Space. Molecules, 2019, 24, 2269.	1.7	4
33	QSPR models for bioconcentration factor (BCF): are they able to predict data of industrial interest?. SAR and QSAR in Environmental Research, 2019, 30, 507-524.	1.0	18
34	In silico Design, Virtual Screening and Synthesis of Novel Electrolytic Solvents. Molecular Informatics, 2019, 38, 1900014.	1.4	5
35	Serum-based differentiation between multiple sclerosis and amyotrophic lateral sclerosis by Random Forest classification of FTIR spectra. Analyst, The, 2019, 144, 4647-4652.	1.7	20
36	Prediction of the Glass-Transition Temperatures of Linear Homo/Heteropolymers and Cross-Linked Epoxy Resins. ACS Applied Polymer Materials, 2019, 1, 1430-1442.	2.0	25

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37	Classification of Metal Binders by NaÃ¯ve Bayes Classifier on the Base of Molecular Fragment Descriptors and Ensemble Modeling. Molecular Informatics, 2019, 38, e1900002.	1.4	8
38	Multi-task generative topographic mapping in virtual screening. Journal of Computer-Aided Molecular Design, 2019, 33, 331-343.	1.3	17
39	De Novo Molecular Design by Combining Deep Autoencoder Recurrent Neural Networks with Generative Topographic Mapping. Journal of Chemical Information and Modeling, 2019, 59, 1182-1196.	2.5	93
40	Generative topographic mapping in drug design. Drug Discovery Today: Technologies, 2019, 32-33, 99-107.	4.0	19
41	Virtual Screening with Generative Topographic Maps: How Many Maps Are Required?. Journal of Chemical Information and Modeling, 2019, 59, 564-572.	2.5	20
42	Prediction of Aromatic Hydroxylation Sites for Human CYP1A2 Substrates Using Condensed Graph of Reactions. BioNanoScience, 2018, 8, 384-389.	1.5	3
43	Monitoring of the Conformational Space of Dipeptides by Generative Topographic Mapping. Molecular Informatics, 2018, 37, 1700115.	1.4	3
44	Transductive Ridge Regression in Structureâ€activity Modeling. Molecular Informatics, 2018, 37, 1700112.	1.4	3
45	Mapping of the Available Chemical Space versus the Chemical Universe of Leadâ€Like Compounds. ChemMedChem, 2018, 13, 540-554.	1.6	33
46	Rescoring of docking poses under Occamâ€™s Razor: are there simpler solutions?. Journal of Computer-Aided Molecular Design, 2018, 32, 877-888.	1.3	15
47	Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. Molecular Informatics, 2018, 37, e1800056.	1.4	7
48	AntiMalarial Mode of Action (AMMA) Database: Data Selection, Verification and Chemical Space Analysis. Molecular Informatics, 2018, 37, e1800021.	1.4	4
49	Generative Topographic Mapping of Conformational Space. Molecular Informatics, 2017, 36, 1700036.	1.4	10
50	Virtual screening, synthesis and biological evaluation of DNA intercalating antiviral agents. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3915-3919.	1.0	15
51	QSAR modeling and chemical space analysis of antimalarial compounds. Journal of Computer-Aided Molecular Design, 2017, 31, 441-451.	1.3	13
52	Neighboring Structure Visualization on a Gridâ€based Layout. Molecular Informatics, 2017, 36, 1700047.	1.4	0
53	Generative Topographic Mapping Approach to Chemical Space Analysis. Challenges and Advances in Computational Chemistry and Physics, 2017, , 167-199.	0.6	4
54	In Silico Mining for Antimalarial Structure-Activity Knowledge and Discovery of Novel Antimalarial Curcuminoids. Molecules, 2016, 21, 853.	1.7	16

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55	Generative Topographic Mapping Approach to Modeling and Chemical Space Visualization of Human Intestinal Transporters. BioNanoScience, 2016, 6, 464-472.	1.5	6
56	Prediction of Activity Cliffs Using Condensed Graphs of Reaction Representations, Descriptor Recombination, Support Vector Machine Classification, and Support Vector Regression. Journal of Chemical Information and Modeling, 2016, 56, 1631-1640.	2.5	28
57	Predictive Models for the Free Energy of Hydrogen Bonded Complexes with Single and Cooperative Hydrogen Bonds. Molecular Informatics, 2016, 35, 629-638.	1.4	9
58	Chemical Space Mapping and Structureâ€“Activity Analysis of the ChEMBL Antiviral Compound Set. Journal of Chemical Information and Modeling, 2016, 56, 1438-1454.	2.5	31
59	Generative Topographic Mapping Approach to Chemical Space Analysis. ACS Symposium Series, 2016, , 211-241.	0.5	15
60	Redox Polypharmacology as an Emerging Strategy to Combat Malarial Parasites. ChemMedChem, 2016, 11, 1339-1351.	1.6	28
61	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	1.4	12
62	Kernel Target Alignment Parameter: A New Modelability Measure for Regression Tasks. Journal of Chemical Information and Modeling, 2016, 56, 6-11.	2.5	14
63	S4MPLEâ€”Sampler for Multiple Protein-Ligand Entities: Methodology and Rigid-Site Docking Benchmarking. Molecules, 2015, 20, 8997-9028.	1.7	25
64	Mappability of drug-like space: towards a polypharmacologically competent map of drug-relevant compounds. Journal of Computer-Aided Molecular Design, 2015, 29, 1087-1108.	1.3	52
65	Electrochemical Properties of Substituted 2â€Methylâ€1,4â€Naphthoquinones: Redox Behavior Predictions. Chemistry - A European Journal, 2015, 21, 3415-3424.	1.7	35
66	Expert System for Predicting Reaction Conditions: The Michael Reaction Case. Journal of Chemical Information and Modeling, 2015, 55, 239-250.	2.5	65
67	GTMâ€Based QSAR Models and Their Applicability Domains. Molecular Informatics, 2015, 34, 348-356.	1.4	52
68	Stargate GTM: Bridging Descriptor and Activity Spaces. Journal of Chemical Information and Modeling, 2015, 55, 2403-2410.	2.5	28
69	Chemical Data Visualization and Analysis with Incremental Generative Topographic Mapping: Big Data Challenge. Journal of Chemical Information and Modeling, 2015, 55, 84-94.	2.5	67
70	Prediction of Drug Induced Liver Injury Using Molecular and Biological Descriptors. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 315-322.	0.6	23
71	An Evolutionary Optimizer of libsvm Models. Challenges, 2014, 5, 450-472.	0.9	52
72	The use of three-dimensional similarity in assessing the risk of cross-reactivity between carbamazepine and psychotropic drugs. European Journal of Clinical Pharmacology, 2014, 70, 495-498.	0.8	1

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73	Computational chemogenomics: Is it more than inductive transfer?. Journal of Computer-Aided Molecular Design, 2014, 28, 597-618.	1.3	26
74	Individual Hydrogenâ€Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487.	1.4	19
75	Design of a Generalâ€Purpose European Compound Screening Library for EUâ€OPENSCREEN. ChemMedChem, 2014, 9, 2309-2326.	1.6	29
76	Quantitative Structureâ€“Property Relationship Modeling: A Valuable Support in High-Throughput Screening Quality Control. Analytical Chemistry, 2014, 86, 2510-2520.	3.2	18
77	Simple Ligandâ€“Receptor Interaction Descriptor (SILIRID) for alignment-free binding site comparison. Computational and Structural Biotechnology Journal, 2014, 10, 33-37.	1.9	25
78	Generative Topographic Mapping-Based Classification Models and Their Applicability Domain: Application to the Biopharmaceutics Drug Disposition Classification System (BDDCS). Journal of Chemical Information and Modeling, 2013, 53, 3318-3325.	2.5	55
79	Publicly available models to predict normal boiling point of organic compounds. Thermochimica Acta, 2013, 553, 60-67.	1.2	7
80	Predicting Ligand Binding Modes from Neural Networks Trained on Proteinâ€“Ligand Interaction Fingerprints. Journal of Chemical Information and Modeling, 2013, 53, 763-772.	2.5	47
81	Do Not Hesitate to Use Tverskyâ€”and Other Hints for Successful Active Analogue Searches with Feature Count Descriptors. Journal of Chemical Information and Modeling, 2013, 53, 1543-1562.	2.5	19
82	Models for Identification of Erroneous Atom-to-Atom Mapping of Reactions Performed by Automated Algorithms. Journal of Chemical Information and Modeling, 2012, 52, 3116-3122.	2.5	20
83	Using self-organizing maps to accelerate similarity search. Bioorganic and Medicinal Chemistry, 2012, 20, 5396-5409.	1.4	17
84	Mining Chemical Reactions Using Neighborhood Behavior and Condensed Graphs of Reactions Approaches. Journal of Chemical Information and Modeling, 2012, 52, 2325-2338.	2.5	24
85	Complexation of Mn²⁺, Fe²⁺, Y³⁺, La³⁺, Pb²⁺, and UO₂²⁺ with Organic Ligands: QSPR Ensemble Modeling of Stability Constants. Industrial & Engineering Chemistry Research, 2012, 51, 13482-13489.	1.8	16
86	Interpretability of SAR/QSAR Models of any Complexity by Atomic Contributions. Molecular Informatics, 2012, 31, 639-642.	1.4	32
87	Generative Topographic Mapping (GTM): Universal Tool for Data Visualization, Structureâ€Activity Modeling and Dataset Comparison. Molecular Informatics, 2012, 31, 301-312.	1.4	107
88	QSPR Approach to Predict Nonadditive Properties of Mixtures. Application to Bubble Point Temperatures of Binary Mixtures of Liquids. Molecular Informatics, 2012, 31, 491-502.	1.4	59
89	Stability constants of complexes of Zn2+, Cd2+, and Hg2+ with organic ligands: QSPR consensus modeling and design of new metal binders. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2012, 72, 309-321.	1.6	19
90	In Silico Design of New Ionic Liquids Based on Quantitative Structureâ˜Property Relationship Models of Ionic Liquid Viscosity. Journal of Physical Chemistry B, 2011, 115, 93-98.	1.2	48

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91	Quantitative Structureâ€“Property Relationship (QSPR) Modeling of Normal Boiling Point Temperature and Composition of Binary Azeotropes. Industrial & Engineering Chemistry Research, 2011, 50, 14162-14167.	1.8	25
92	Local neighborhood behavior in a combinatorial library context. Journal of Computer-Aided Molecular Design, 2011, 25, 237-252.	1.3	9
93	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	1.3	453
94	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Cheminformatics, 2011, 3, .	2.8	4
95	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111.	2.5	202
96	ISIDA Propertyâ€Labelled Fragment Descriptors. Molecular Informatics, 2010, 29, 855-868.	1.4	111
97	A unified approach to the applicability domain problem of QSAR models. Journal of Cheminformatics, 2010, 2, .	2.8	5
98	Data integration and knowledge transfer: application to the tissue: air partition coefficients. Chemistry Central Journal, 2009, 3, .	2.6	0
99	Inductive Transfer of Knowledge: Application of Multi-Task Learning and Feature Net Approaches to Model Tissue-Air Partition Coefficients. Journal of Chemical Information and Modeling, 2009, 49, 133-144.	2.5	71
100	Predicting the Predictability: A Unified Approach to the Applicability Domain Problem of QSAR Models. Journal of Chemical Information and Modeling, 2009, 49, 1762-1776.	2.5	145
101	Hot-Spots-Guided Receptor-Based Pharmacophores (HS-Pharm): A Knowledge-Based Approach to Identify Ligand-Anchoring Atoms in Protein Cavities and Prioritize Structure-Based Pharmacophores. Journal of Chemical Information and Modeling, 2008, 48, 1396-1410.	2.5	91
102	Computer-aided design of new metal binders. Radiochimica Acta, 2008, 96, 505-511.	0.5	13
103	ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. Current Computer-Aided Drug Design, 2008, 4, 191-198.	0.8	173
104	Optimizing Fragment and Scaffold Docking by Use of Molecular Interaction Fingerprints. Journal of Chemical Information and Modeling, 2007, 47, 195-207.	2.5	357
105	First round of a focused library of cholera toxin inhibitors. Carbohydrate Research, 2007, 342, 1651-1660.	1.1	18
106	Synthesis and Conformational Analysis of Galactose-Derived Bicyclic Scaffolds. European Journal of Organic Chemistry, 2006, 2006, 2925-2933.	1.2	15
107	Synthesis, Conformational Studies and Mannosidase Stability of a Mimic of 1,2-Mannobioside. European Journal of Organic Chemistry, 2004, 2004, 5119-5225.	1.2	29
108	Exploring the natural conformational changes of the C-terminal domain of calmodulin. Physical Review E, 2002, 66, 031908.	0.8	5

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109	Coupling overall rotations with modal dynamics. Theoretical Chemistry Accounts, 2001, 106, 62-68.	0.5	1
110	The effect of ambient pressure and impactor geometry on low speed penetration of unconsolidated materials. Advances in Space Research, 1999, 23, 1229-1234.	1.2	7