Alexandre Varnek

List of Publications by Year
in descending order

220	9,116	61984	49909
papers	citations	43 h-index	87 g-index

242	242	242	6902
all docs	docs citations	times ranked	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.	5.4	18
2	Atomâ€toâ€atom Mapping: A Benchmarking Study of Popular Mapping Algorithms and Consensus Strategies. Molecular Informatics, 2022, 41, e2100138.	2.5	17
3	CGRdb2.0: A Python Database Management System for Molecules, Reactions, and Chemical Data. Journal of Chemical Information and Modeling, 2022, 62, 2015-2020.	5.4	3
4	Exploration of the Chemical Space of DNAâ€encoded Libraries. Molecular Informatics, 2022, 41, .	2.5	9
5	HIV-1 drug resistance profiling using amino acid sequence space cartography. Bioinformatics, 2022, 38, 2307-2314.	4.1	5
6	Computational screening methodology identifies effective solvents for CO2 capture. Communications Chemistry, 2022, 5, .	4.5	17
7	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.	4.1	4
8	Editorial: Chemical Reactions Mining. Molecular Informatics, 2022, 41, .	2.5	0
9	Prediction of Optimal Conditions of Hydrogenation Reaction Using the Likelihood Ranking Approach. International Journal of Molecular Sciences, 2022, 23, 248.	4.1	4
10	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.	5.4	32
11	Toward in Silico Modeling of Dynamic Combinatorial Libraries. ACS Central Science, 2022, 8, 804-813.	11.3	3
12	Molecular Similarity Perception Based on Machine-Learning Models. International Journal of Molecular Sciences, 2022, 23, 6114.	4.1	0
13	Visualization and Analysis of the REACHâ€chemical Space with Generative Topographic Mapping. Molecular Informatics, 2021, 40, 2000232.	2.5	2
14	Chemography: Searching for Hidden Treasures. Journal of Chemical Information and Modeling, 2021, 61, 179-188.	5.4	14
15	Combined Graph/Relational Database Management System for Calculated Chemical Reaction Pathway Data. Journal of Chemical Information and Modeling, 2021, 61, 554-559.	5.4	6
16	Modern Trends in Chemical Reactions Modeling. , 2021, , 190-197.		0
17	Cross-validation strategies in QSPR modelling of chemical reactions. SAR and QSAR in Environmental Research, 2021, 32, 207-219.	2.2	12
18	Discovery of novel chemical reactions by deep generative recurrent neural network. Scientific Reports, 2021, 11, 3178.	3.3	40

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19	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
20	NP Navigator: A New Look at the Natural Product Chemical Space. Molecular Informatics, 2021, 40, e2100068.	2.5	16
21	Computer-Aided Design of New Physical Solvents for Hydrogen Sulfide Absorption. Industrial & Engineering Chemistry Research, 2021, 60, 8588-8596.	3.7	9
22	DMSO Solubility Assessment for Fragment-Based Screening. Molecules, 2021, 26, 3950.	3.8	2
23	Multi-Instance Learning Approach to Predictive Modeling of Catalysts Enantioselectivity. Synlett, 2021, 32, 1833-1836.	1.8	8
24	Reaction Data Curation I: Chemical Structures and Transformations Standardization. Molecular Informatics, 2021, 40, e2100119.	2.5	15
25	QSAR Modeling Based on Conformation Ensembles Using a Multi-Instance Learning Approach. Journal of Chemical Information and Modeling, 2021, 61, 4913-4923.	5.4	15
26	A critical overview of computational approaches employed for COVID-19 drug discovery. Chemical Society Reviews, 2021, 50, 9121-9151.	38.1	128
27	Endocrine disruption: the noise in available data adversely impacts the modelsâ€™ performance. SAR and QSAR in Environmental Research, 2021, 32, 111-131.	2.2	4
28	Chemoinformatics-Driven Design of New Physical Solvents for Selective CO₂ Absorption. Environmental Science & Technology, 2021, 55, 15542-15553.	10.0	16
29	NP Navigator: A New Online Tool for the Exploration of the Natural Products Chemical Space. Medical Sciences Forum, 2021, 7, .	0.5	0
30	Machine learning modelling of chemical reaction characteristics: yesterday, today, tomorrow. Mendeleev Communications, 2021, 31, 769-780.	1.6	9
31	Pre-Steady-State Kinetics of the SARS-CoV-2 Main Protease as a Powerful Tool for Antiviral Drug Discovery. Frontiers in Pharmacology, 2021, 12, 773198.	3.5	5
32	Diversifying chemical libraries with generative topographic mapping. Journal of Computer-Aided Molecular Design, 2020, 34, 805-815.	2.9	7
33	QSPR Modeling of Potentiometric Mg²⁺/Ca²⁺ Selectivity for PVCâ€plasticized Sensor Membranes. Electroanalysis, 2020, 32, 792-798.	2.9	9
34	Thermodynamic radii of lanthanide ions derived from metalâ€“ligand complexes stability constants. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2020, 98, 69-78.	1.6	4
35	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.	5.4	1
36	Comprehensive Analysis of Applicability Domains of QSPR Models for Chemical Reactions. International Journal of Molecular Sciences, 2020, 21, 5542.	4.1	32

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37	Autoignition temperature: comprehensive data analysis and predictive models. SAR and QSAR in Environmental Research, 2020, 31, 597-613.	2.2	4
38	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.	2.2	19
39	A Chemographic Audit of antiâ€Coronavirus Structureâ€activity Information from Public Databases (ChEMBL). Molecular Informatics, 2020, 39, e2000080.	2.5	16
40	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.	5.4	1
41	Publicly available QSPR models for environmental media persistence. SAR and QSAR in Environmental Research, 2020, 31, 493-510.	2.2	3
42	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
43	Application of the mol2vec Technology to Largeâ€size Data Visualization and Analysis. Molecular Informatics, 2020, 39, e1900170.	2.5	8
44	Modelling of ready biodegradability based on combined public and industrial data sources. SAR and QSAR in Environmental Research, 2020, 31, 171-186.	2.2	14
45	Parallel Generative Topographic Mapping: An Efficient Approach for Big Data Handling. Molecular Informatics, 2020, 39, 2000009.	2.5	6
46	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
47	Predictive Models for Kinetic Parameters of Cycloaddition Reactions. Molecular Informatics, 2019, 38, e1800077.	2.5	25
48	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.	2.2	22
49	Conjugated Quantitative Structureâ€“Property Relationship Models: Application to Simultaneous Prediction of Tautomeric Equilibrium Constants and Acidity of Molecules. Journal of Chemical Information and Modeling, 2019, 59, 4569-4576.	5.4	5
50	An Investigation into the Stephensâ€“Castro Synthesis of Dehydrotriaryl[12]annulenes: Factors Influencing the Cyclotrimerization. European Journal of Organic Chemistry, 2019, 2019, 6783-6795.	2.4	1
51	Sydnone-alkyne cycloaddition: Which factors are responsible for reaction rate ?. Journal of Molecular Structure, 2019, 1198, 126897.	3.6	7
52	QSPR modeling of potentiometric sensitivity towards heavy metal ions for polymeric membrane sensors. Sensors and Actuators B: Chemical, 2019, 301, 126941.	7.8	11
53	Generative Topographic Mapping of the Docking Conformational Space. Molecules, 2019, 24, 2269.	3.8	4
54	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.	2.2	18

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55	In silico Design, Virtual Screening and Synthesis of Novel Electrolytic Solvents. Molecular Informatics, 2019, 38, 1900014.	2.5	5
56	Serum-based differentiation between multiple sclerosis and amyotrophic lateral sclerosis by Random Forest classification of FTIR spectra. Analyst, The, 2019, 144, 4647-4652.	3.5	20
57	CGRtools: Python Library for Molecule, Reaction, and Condensed Graph of Reaction Processing. Journal of Chemical Information and Modeling, 2019, 59, 2516-2521.	5.4	34
58	Prediction of the Glass-Transition Temperatures of Linear Homo/Heteropolymers and Cross-Linked Epoxy Resins. ACS Applied Polymer Materials, 2019, 1, 1430-1442.	4.4	25
59	CovaDOTS: In Silico Chemistry-Driven Tool to Design Covalent Inhibitors Using a Linking Strategy. Journal of Chemical Information and Modeling, 2019, 59, 1472-1485.	5.4	13
60	Classification of Metal Binders by NaÃ¯ve Bayes Classifier on the Base of Molecular Fragment Descriptors and Ensemble Modeling. Molecular Informatics, 2019, 38, e1900002.	2.5	8
61	Getting to Know the Neighbours with GTM: The Case of Antiviral Compounds. Molecular Informatics, 2019, 38, 1800166.	2.5	7
62	Multi-task generative topographic mapping in virtual screening. Journal of Computer-Aided Molecular Design, 2019, 33, 331-343.	2.9	17
63	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.	5.4	93
64	Generative topographic mapping in drug design. Drug Discovery Today: Technologies, 2019, 32-33, 99-107.	4.0	19
65	Virtual Screening with Generative Topographic Maps: How Many Maps Are Required?. Journal of Chemical Information and Modeling, 2019, 59, 564-572.	5.4	20
66	Bimolecular Nucleophilic Substitution Reactions: Predictive Models for Rate Constants and Molecular Reaction Pairs Analysis. Molecular Informatics, 2019, 38, e1800104.	2.5	23
67	Pros and cons of virtual screening based on public â€œBig Dataâ€ In silico mining for new bromodomain inhibitors. European Journal of Medicinal Chemistry, 2019, 165, 258-272.	5.5	12
68	Evolution of commercially available compounds for HTS. Drug Discovery Today, 2019, 24, 390-402.	6.4	53
69	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Kimito Funatsu â€“ Driving Force of Japanese-French Collaboration in Chemoinformatics. Journal of Computer Aided Chemistry, 2019, 20, 47-49.	0.3	0
70	Assessment of tautomer distribution using the condensed reaction graph approach. Journal of Computer-Aided Molecular Design, 2018, 32, 401-414.	2.9	20
71	Prediction of Aromatic Hydroxylation Sites for Human CYP1A2 Substrates Using Condensed Graph of Reactions. BioNanoScience, 2018, 8, 384-389.	3.5	3
72	Monitoring of the Conformational Space of Dipeptides by Generative Topographic Mapping. Molecular Informatics, 2018, 37, 1700115.	2.5	3

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73	Transductive Ridge Regression in Structureâ€activity Modeling. Molecular Informatics, 2018, 37, 1700112.	2.5	3
74	Mapping of the Available Chemical Space versus the Chemical Universe of Leadâ€Like Compounds. ChemMedChem, 2018, 13, 540-554.	3.2	33
75	6th Strasbourg Summer School in Chemoinformatics. Molecular Informatics, 2018, 37, 1880931.	2.5	0
76	Rescoring of docking poses under Occamâ€™s Razor: are there simpler solutions?. Journal of Computer-Aided Molecular Design, 2018, 32, 877-888.	2.9	15
77	Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. Molecular Informatics, 2018, 37, e1800056.	2.5	7
78	AntiMalarial Mode of Action (AMMA) Database: Data Selection, Verification and Chemical Space Analysis. Molecular Informatics, 2018, 37, e1800021.	2.5	4
79	Integrated Strategy for Lead Optimization Based on Fragment Growing: The Diversity-Oriented-Target-Focused-Synthesis Approach. Journal of Medicinal Chemistry, 2018, 61, 5719-5732.	6.4	51
80	Generative Topographic Mapping of Conformational Space. Molecular Informatics, 2017, 36, 1700036.	2.5	10
81	Privileged Structural Motif Detection and Analysis Using Generative Topographic Maps. Journal of Chemical Information and Modeling, 2017, 57, 1218-1232.	5.4	9
82	Virtual screening, synthesis and biological evaluation of DNA intercalating antiviral agents. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3915-3919.	2.2	15
83	QSAR modeling and chemical space analysis of antimalarial compounds. Journal of Computer-Aided Molecular Design, 2017, 31, 441-451.	2.9	13
84	From birdâ€™s eye views to molecular communities: two-layered visualization of structureâ€“activity relationships in large compound data sets. Journal of Computer-Aided Molecular Design, 2017, 31, 961-977.	2.9	5
85	A Direct Oneâ€Pot Synthesis of Asymmetric Dehydrobenzopyrido[12]annulenes and Their Physicochemical Properties. European Journal of Organic Chemistry, 2017, 2017, 4625-4632.	2.4	1
86	Neighboring Structure Visualization on a Gridâ€based Layout. Molecular Informatics, 2017, 36, 1700047.	2.5	0
87	Structureâ€“reactivity modeling using mixture-based representation of chemical reactions. Journal of Computer-Aided Molecular Design, 2017, 31, 829-839.	2.9	23
88	Artificial intelligence in synthetic chemistry: achievements and prospects. Russian Chemical Reviews, 2017, 86, 1127-1156.	6.5	45
89	Chemoinformatics in France. Molecular Informatics, 2017, 36, 1781031.	2.5	0
90	Predictive cartography of metal binders using generative topographic mapping. Journal of Computer-Aided Molecular Design, 2017, 31, 701-714.	2.9	6

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91	Generative Topographic Mapping Approach to Chemical Space Analysis. Challenges and Advances in Computational Chemistry and Physics, 2017, , 167-199.	0.6	4
92	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	6.0	264
93	In Silico Mining for Antimalarial Structure-Activity Knowledge and Discovery of Novel Antimalarial Curcuminoids. Molecules, 2016, 21, 853.	3.8	16
94	5th Strasbourg Summer School in Chemoinformatics. Molecular Informatics, 2016, 35, 540-540.	2.5	0
95	Generative Topographic Mapping Approach to Modeling and Chemical Space Visualization of Human Intestinal Transporters. BioNanoScience, 2016, 6, 464-472.	3.5	6
96	Visualization of a Multidimensional Descriptor Space. ACS Symposium Series, 2016, , 243-267.	0.5	8
97	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.	5.4	28
98	Predictive Models for the Free Energy of Hydrogen Bonded Complexes with Single and Cooperative Hydrogen Bonds. Molecular Informatics, 2016, 35, 629-638.	2.5	9
99	Chemical Space Mapping and Structureâ€“Activity Analysis of the ChEMBL Antiviral Compound Set. Journal of Chemical Information and Modeling, 2016, 56, 1438-1454.	5.4	31
100	Structural and Physico-Chemical Interpretation (SPCI) of QSAR Models and Its Comparison with Matched Molecular Pair Analysis. Journal of Chemical Information and Modeling, 2016, 56, 1455-1469.	5.4	35
101	Generative Topographic Mapping Approach to Chemical Space Analysis. ACS Symposium Series, 2016, , 211-241.	0.5	15
102	Automatized Assessment of Protective Group Reactivity: A Step Toward Big Reaction Data Analysis. Journal of Chemical Information and Modeling, 2016, 56, 2140-2148.	5.4	37
103	Redox Polypharmacology as an Emerging Strategy to Combat Malarial Parasites. ChemMedChem, 2016, 11, 1339-1351.	3.2	28
104	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	2.5	12
105	Kernel Target Alignment Parameter: A New Modelability Measure for Regression Tasks. Journal of Chemical Information and Modeling, 2016, 56, 6-11.	5.4	14
106	S4MPLEâ€”Sampler for Multiple Protein-Ligand Entities: Methodology and Rigid-Site Docking Benchmarking. Molecules, 2015, 20, 8997-9028.	3.8	25
107	Structureâ€“reactivity relationship in bimolecular elimination reactions based on the condensed graph of a reaction. Journal of Structural Chemistry, 2015, 56, 1227-1234.	1.0	25
108	Mappability of drug-like space: towards a polypharmacologically competent map of drug-relevant compounds. Journal of Computer-Aided Molecular Design, 2015, 29, 1087-1108.	2.9	52

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109	Electrochemical Properties of Substituted 2â€Methylâ€1,4â€Naphthoquinones: Redox Behavior Predictions. Chemistry - A European Journal, 2015, 21, 3415-3424.	3.3	35
110	Expert System for Predicting Reaction Conditions: The Michael Reaction Case. Journal of Chemical Information and Modeling, 2015, 55, 239-250.	5.4	65
111	GTMâ€Based QSAR Models and Their Applicability Domains. Molecular Informatics, 2015, 34, 348-356.	2.5	52
112	Prediction of Optimal Salinities for Surfactant Formulations Using a Quantitative Structureâ€“Property Relationships Approach. Energy & Fuels, 2015, 29, 4281-4288.	5.1	10
113	Stargate GTM: Bridging Descriptor and Activity Spaces. Journal of Chemical Information and Modeling, 2015, 55, 2403-2410.	5.4	28
114	Design, Virtual Screening, and Synthesis of Antagonists of Îł_{IIb}Î²₃ as Antiplatelet Agents. Journal of Medicinal Chemistry, 2015, 58, 7681-7694.	6.4	22
115	Chemical Data Visualization and Analysis with Incremental Generative Topographic Mapping: Big Data Challenge. Journal of Chemical Information and Modeling, 2015, 55, 84-94.	5.4	67
116	Continuous indicator fields: a novel universal type of molecular fields. Journal of Computer-Aided Molecular Design, 2015, 29, 233-247.	2.9	3
117	Prediction of Drug Induced Liver Injury Using Molecular and Biological Descriptors. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 315-322.	1.1	23
118	A Summer School for Structuring the Chemoinformatics Community. Molecular Informatics, 2014, 33, 390-390.	2.5	0
119	Development of â€œstructure-propertyâ€•models in nucleophilic substitution reactions involving azides. Journal of Structural Chemistry, 2014, 55, 1026-1032.	1.0	15
120	An Evolutionary Optimizer of libsvm Models. Challenges, 2014, 5, 450-472.	1.7	52
121	Computational chemogenomics: Is it more than inductive transfer?. Journal of Computer-Aided Molecular Design, 2014, 28, 597-618.	2.9	26
122	QSPR ensemble modelling of the 1:1 and 1:2 complexation of Co2+, Ni2+, and Cu2+ with organic ligands: relationships between stability constants. Journal of Computer-Aided Molecular Design, 2014, 28, 549-564.	2.9	19
123	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	6.4	1,401
124	Individual Hydrogenâ€Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487.	2.5	19
125	Design of a Generalâ€Purpose European Compound Screening Library for EUâ€OPENSCREEN. ChemMedChem, 2014, 9, 2309-2326.	3.2	29
126	Quantitative Structureâ€“Property Relationship Modeling: A Valuable Support in High-Throughput Screening Quality Control. Analytical Chemistry, 2014, 86, 2510-2520.	6.5	18

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127	Structure-reactivity relationships in terms of the condensed graphs of reactions. Russian Journal of Organic Chemistry, 2014, 50, 459-463.	0.8	29
128	Simple Ligandâ€“Receptor Interaction Descriptor (SILIRID) for alignment-free binding site comparison. Computational and Structural Biotechnology Journal, 2014, 10, 33-37.	4.1	25
129	Synthesis, biological evaluation, X-ray molecular structure and molecular docking studies of RGD mimetics containing 6-amino-2,3-dihydroisoindolin-1-one fragment as ligands of integrin Î±IIbÎ²3. Bioorganic and Medicinal Chemistry, 2013, 21, 4646-4661.	3.0	7
130	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.	5.4	55
131	Estimation of the size of drug-like chemical space based on GDB-17 data. Journal of Computer-Aided Molecular Design, 2013, 27, 675-679.	2.9	319
132	Synthesis of a Strained Acetylenic Macrocycle Incorporating a paraâ€Oligo[2]cruciform Bridge Bent over Nanoscopic Dimensions: Structural, Electronic, Spectroscopic, and Ionâ€Sensing Properties. Chemistry - A European Journal, 2013, 19, 12336-12349.	3.3	8
133	Transductive Support Vector Machines: Promising Approach to Model Small and Unbalanced Datasets. Molecular Informatics, 2013, 32, 261-266.	2.5	26
134	Recovery of uranium (VI) from concentrated phosphoric acid by mixtures of new bis(1,3-) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 467 Td (28-33.	4.3	28
135	Publicly available models to predict normal boiling point of organic compounds. Thermochimica Acta, 2013, 553, 60-67.	2.7	7
136	Predicting Ligand Binding Modes from Neural Networks Trained on Proteinâ€“Ligand Interaction Fingerprints. Journal of Chemical Information and Modeling, 2013, 53, 763-772.	5.4	47
137	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.	5.4	19
138	QSPR ensemble modelling of alkaline-earth metal complexation. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2013, 76, 159-171.	1.6	21
139	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.	5.4	20
140	Using self-organizing maps to accelerate similarity search. Bioorganic and Medicinal Chemistry, 2012, 20, 5396-5409.	3.0	17
141	Mining Chemical Reactions Using Neighborhood Behavior and Condensed Graphs of Reactions Approaches. Journal of Chemical Information and Modeling, 2012, 52, 2325-2338.	5.4	24
142	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.	3.7	16
143	Interpretability of SAR/QSAR Models of any Complexity by Atomic Contributions. Molecular Informatics, 2012, 31, 639-642.	2.5	32
144	Electronic, Spectroscopic, and Ion-Sensing Properties of a Dehydro[m]pyrido[14]- and [15]annulene Isomer Library. Journal of Organic Chemistry, 2012, 77, 126-142.	3.2	14

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145	Generative Topographic Mapping (GTM): Universal Tool for Data Visualization, Structureâ€Activity Modeling and Dataset Comparison. Molecular Informatics, 2012, 31, 301-312.	2.5	107
146	QSPR Approach to Predict Nonadditive Properties of Mixtures. Application to Bubble Point Temperatures of Binary Mixtures of Liquids. Molecular Informatics, 2012, 31, 491-502.	2.5	59
147	Machine Learning Methods for Property Prediction in Chemoinformatics: Quo Vadis?. Journal of Chemical Information and Modeling, 2012, 52, 1413-1437.	5.4	191
148	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
149	New Approach for Accurate QSPR Modeling of Metal Complexation: Application to Stability Constants of Complexes of Lanthanide Ions Ln3+, Ag+, Zn2+, Cd2+ and Hg2+ with Organic Ligands in Water. Macroheterocycles, 2012, 5, 404-410.	0.5	21
150	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.	2.6	48
151	Quantitative Structureâ€“Property Relationship (QSPR) Modeling of Normal Boiling Point Temperature and Composition of Binary Azeotropes. Industrial & Engineering Chemistry Research, 2011, 50, 14162-14167.	3.7	25
152	RGD mimetics containing phthalimidine fragment as novel ligands of fibrinogen receptor. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5971-5974.	2.2	5
153	Local neighborhood behavior in a combinatorial library context. Journal of Computer-Aided Molecular Design, 2011, 25, 237-252.	2.9	9
154	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.	2.9	453
155	Chemoinformatics as a Theoretical Chemistry Discipline. Molecular Informatics, 2011, 30, 20-32.	2.5	78
156	A REPRESENTATION TO APPLY USUAL DATA MINING TECHNIQUES TO CHEMICAL REACTIONS â€" ILLUSTRATION ON THE RATE CONSTANT OF S_{N}2 REACTIONS IN WATER. International Journal on Artificial Intelligence Tools, 2011, 20, 253-270.	1.0	39
157	Fragment Descriptors in Structureâ€“Property Modeling and Virtual Screening. Methods in Molecular Biology, 2010, 672, 213-243.	0.9	7
158	Applicability Domains for Classification Problems: Benchmarking of Distance to Models for Ames Mutagenicity Set. Journal of Chemical Information and Modeling, 2010, 50, 2094-2111.	5.4	202
159	The Oneâ€Class Classification Approach to Data Description and to Models Applicability Domain. Molecular Informatics, 2010, 29, 581-587.	2.5	49
160	ISIDA Propertyâ€Labelled Fragment Descriptors. Molecular Informatics, 2010, 29, 855-868.	2.5	111
161	A Representation to Apply Usual Data Mining Techniques to Chemical Reactions. Lecture Notes in Computer Science, 2010, , 318-326.	1.3	2
162	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.	5.4	71

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163	Predicting the Predictability: A Unified Approach to the Applicability Domain Problem of QSAR Models. Journal of Chemical Information and Modeling, 2009, 49, 1762-1776.	5.4	145
164	Quantitative Structure-Property Relationships in Solvent Extraction and Complexation of Metals. Ion Exchange and Solvent Extraction, 2009, , 319-358.	0.3	12
165	Combinatorial QSAR Modeling of Chemical Toxicants Tested against Tetrahymena pyriformis. Journal of Chemical Information and Modeling, 2008, 48, 766-784.	5.4	258
166	Computer-aided design of new metal binders. Radiochimica Acta, 2008, 96, 505-511.	1.2	13
167	Critical Assessment of QSAR Models of Environmental Toxicity against Tetrahymena pyriformis: Focusing on Applicability Domain and Overfitting by Variable Selection. Journal of Chemical Information and Modeling, 2008, 48, 1733-1746.	5.4	350
168	Building a Chemical Space Based on Fragment Descriptors. Combinatorial Chemistry and High Throughput Screening, 2008, 11, 661-668.	1.1	17
169	ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. Current Computer-Aided Drug Design, 2008, 4, 191-198.	1.2	173
170	QSPR Modeling of the AmIII/EuIIISeparation Factor: How Far Can we Predict ?. Solvent Extraction and Ion Exchange, 2007, 25, 1-26.	2.0	21
171	Exhaustive QSPR Studies of a Large Diverse Set of Ionic Liquids:â€‰ How Accurately Can We Predict Melting Points?. Journal of Chemical Information and Modeling, 2007, 47, 1111-1122.	5.4	129
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