Alexandre Varnek

List of Publications by Year in Descending Order

209 papers	6,608 citations	39 h-index	74 g-index
242 ext. papers	7,744 ext. citations	4.7 avg, IF	5.79 L-index

#	Paper	IF	Citations
209	Exploration of the chemical space of DNA-encoded libraries.. *Molecular Informatics*, **2022**,	3.8	1
208	Molecular Similarity Perception Based on Machine-Learning Models. *International Journal of Molecular Sciences*, **2022**, 23, 6114	6.3	
207	NP Navigator: A New Online Tool for the Exploration of the Natural Products Chemical Space. *Medical Sciences Forum*, **2021**, 7, 1		
206	Atom-to-atom Mapping: A Benchmarking Study of Popular Mapping Algorithms and Consensus Strategies. *Molecular Informatics*, **2021**, e2100138	3.8	2
205	Chemoinformatics-Driven Design of New Physical Solvents for Selective CO Absorption. *Environmental Science & Technology*, **2021**, 55, 15542-15553	10.3	1
204	SynthI: A New Open-Source Tool for Synthon-Based Library Design. *Journal of Chemical Information and Modeling*, **2021**,	6.1	3
203	CATMoS: Collaborative Acute Toxicity Modeling Suite. *Environmental Health Perspectives*, **2021**, 129, 47013	8.4	14
202	NP Navigator: A New Look at the Natural Product Chemical Space. *Molecular Informatics*, **2021**, 40, e2100068	3.8	9
201	Computer-Aided Design of New Physical Solvents for Hydrogen Sulfide Absorption. *Industrial & Engineering Chemistry Research*, **2021**, 60, 8588-8596	3.9	4
200	DMSO Solubility Assessment for Fragment-Based Screening. *Molecules*, **2021**, 26,	4.8	2
199	Visualization and Analysis of the REACH-chemical Space with Generative Topographic Mapping. *Molecular Informatics*, **2021**, 40, e2000232	3.8	1
198	Chemography: Searching for Hidden Treasures. *Journal of Chemical Information and Modeling*, **2021**, 61, 179-188	6.1	8
197	Combined Graph/Relational Database Management System for Calculated Chemical Reaction Pathway Data. *Journal of Chemical Information and Modeling*, **2021**, 61, 554-559	6.1	2
196	Modern Trends in Chemical Reactions Modeling **2021**, 190-197		
195	Cross-validation strategies in QSPR modelling of chemical reactions. *SAR and QSAR in Environmental Research*, **2021**, 32, 207-219	3.5	2
194	Discovery of novel chemical reactions by deep generative recurrent neural network. *Scientific Reports*, **2021**, 11, 3178	4.9	11
193	Reaction Data Curation I: Chemical Structures and Transformations Standardization. *Molecular Informatics*, **2021**, 40, e2100119	3.8	3

192	QSAR Modeling Based on Conformation Ensembles Using a Multi-Instance Learning Approach. *Journal of Chemical Information and Modeling*, **2021**, 61, 4913-4923	6.1	2
191	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
190	Endocrine disruption: the noise in available data adversely impacts the models' performance. *SAR and QSAR in Environmental Research*, **2021**, 32, 111-131	3.5	0
189	Machine learning modelling of chemical reaction characteristics: yesterday, today, tomorrow. *Mendeleev Communications*, **2021**, 31, 769-780	1.9	0
188	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	5.6	1
187	A Close-up Look at the Chemical Space of Commercially Available Building Blocks for Medicinal Chemistry.. *Journal of Chemical Information and Modeling*, **2021**,	6.1	5
186	A Chemographic Audit of anti-Coronavirus Structure-activity Information from Public Databases (ChEMBL). *Molecular Informatics*, **2020**, 39, e2000080	3.8	8
185	"Big Data" 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	6.1	
184	Publicly available QSPR models for environmental media persistence. *SAR and QSAR in Environmental Research*, **2020**, 31, 493-510	3.5	1
183	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. *Environmental Health Perspectives*, **2020**, 128, 27002	8.4	70
182	Application of the mol2vec Technology to Large-size Data Visualization and Analysis. *Molecular Informatics*, **2020**, 39, e1900170	3.8	5
181	Modelling of ready biodegradability based on combined public and industrial data sources. *SAR and QSAR in Environmental Research*, **2020**, 31, 171-186	3.5	8
180	Parallel Generative Topographic Mapping: An Efficient Approach for Big Data Handling. *Molecular Informatics*, **2020**, 39, e2000009	3.8	2
179	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
178	QSPR Modeling of Potentiometric Mg2+/Ca2+ Selectivity for PVC-plasticized Sensor Membranes. *Electroanalysis*, **2020**, 32, 792-798	3	4
177	Thermodynamic radii of lanthanide ions derived from metal□gand complexes stability constants. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2020**, 98, 69-78	1.7	2
176	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	6.1	1
175	Comprehensive Analysis of Applicability Domains of QSPR Models for Chemical Reactions. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	8

174	Autoignition temperature: comprehensive data analysis and predictive models. *SAR and QSAR in Environmental Research*, **2020**, 31, 597-613	3.5	2
173	Consensus QSAR models estimating acute toxicity to aquatic organisms from different trophic levels: algae, and fish. *SAR and QSAR in Environmental Research*, **2020**, 31, 655-675	3.5	8
172	Diversifying chemical libraries with generative topographic mapping. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 805-815	4.2	5
171	Sydnone-alkyne cycloaddition: Which factors are responsible for reaction rate ?. *Journal of Molecular Structure*, **2019**, 1198, 126897	3.4	3
170	QSPR modeling of potentiometric sensitivity towards heavy metal ions for polymeric membrane sensors. *Sensors and Actuators B: Chemical*, **2019**, 301, 126941	8.5	7
169	Generative Topographic Mapping of the Docking Conformational Space. *Molecules*, **2019**, 24,	4.8	4
168	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	3.5	8
167	In silico Design, Virtual Screening and Synthesis of Novel Electrolytic Solvents. *Molecular Informatics*, **2019**, 38, e1900014	3.8	4
166	Serum-based differentiation between multiple sclerosis and amyotrophic lateral sclerosis by Random Forest classification of FTIR spectra. *Analyst, The*, **2019**, 144, 4647-4652	5	10
165	CGRtools: Python Library for Molecule, Reaction, and Condensed Graph of Reaction Processing. *Journal of Chemical Information and Modeling*, **2019**, 59, 2516-2521	6.1	17
164	Prediction of the Glass-Transition Temperatures of Linear Homo/Heteropolymers and Cross-Linked Epoxy Resins. *ACS Applied Polymer Materials*, **2019**, 1, 1430-1442	4.3	13
163	CovaDOTS: In Silico Chemistry-Driven Tool to Design Covalent Inhibitors Using a Linking Strategy. *Journal of Chemical Information and Modeling*, **2019**, 59, 1472-1485	6.1	11
162	Classification of Metal Binders by Naïve Bayes Classifier on the Base of Molecular Fragment Descriptors and Ensemble Modeling. *Molecular Informatics*, **2019**, 38, e1900002	3.8	4
161	Getting to Know the Neighbours with GTM: The Case of Antiviral Compounds. *Molecular Informatics* , **2019**, 38, e1800166	3.8	5
160	Multi-task generative topographic mapping in virtual screening. *Journal of Computer-Aided Molecular Design*, **2019**, 33, 331-343	4.2	12
159	Predictive Models for Kinetic Parameters of Cycloaddition Reactions. *Molecular Informatics*, **2019**, 38, e1800077	3.8	16
158	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	3.5	12
157	Conjugated Quantitative Structure-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	6.1	4

156	An Investigation into the Stephens□Castro Synthesis of Dehydrotriaryl[12]annulenes: Factors Influencing the Cyclotrimerization. *European Journal of Organic Chemistry*, **2019**, 2019, 6783-6795	3.2	1
155	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Kimito Funatsu □Driving Force of Japanese-French Collaboration in Chemoinformatics. *Journal of Computer Aided Chemistry*, **2019**, 20, 47-49	0.2	
154	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	6.1	56
153	Generative topographic mapping in drug design. *Drug Discovery Today: Technologies*, **2019**, 32-33, 99-107	7.1	8
152	Virtual Screening with Generative Topographic Maps: How Many Maps Are Required?. *Journal of Chemical Information and Modeling*, **2019**, 59, 564-572	6.1	13
151	Bimolecular Nucleophilic Substitution Reactions: Predictive Models for Rate Constants and Molecular Reaction Pairs Analysis. *Molecular Informatics*, **2019**, 38, e1800104	3.8	13
150	Pros and cons of virtual screening based on public "Big Data": In silico mining for new bromodomain inhibitors. *European Journal of Medicinal Chemistry*, **2019**, 165, 258-272	6.8	10
149	Evolution of commercially available compounds for HTS. *Drug Discovery Today*, **2019**, 24, 390-402	8.8	27
148	Assessment of tautomer distribution using the condensed reaction graph approach. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 401-414	4.2	16
147	Prediction of Aromatic Hydroxylation Sites for Human CYP1A2 Substrates Using Condensed Graph of Reactions. *BioNanoScience*, **2018**, 8, 384-389	3.4	3
146	Monitoring of the Conformational Space of Dipeptides by Generative Topographic Mapping. *Molecular Informatics*, **2018**, 37, 1700115	3.8	3
145	Transductive Ridge Regression in Structure-activity Modeling. *Molecular Informatics*, **2018**, 37, 1700112	3.8	2
144	Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. *Molecular Informatics*, **2018**, 37, e1800056	3.8	6
143	AntiMalarial Mode of Action (AMMA) Database: Data Selection, Verification and Chemical Space Analysis. *Molecular Informatics*, **2018**, 37, e1800021	3.8	3
142	Integrated Strategy for Lead Optimization Based on Fragment Growing: The Diversity-Oriented-Target-Focused-Synthesis Approach. *Journal of Medicinal Chemistry*, **2018**, 61, 5719-5732	8.3	35
141	Mapping of the Available Chemical Space versus the Chemical Universe of Lead-Like Compounds. *ChemMedChem*, **2018**, 13, 540-554	3.7	28
140	Rescoring of docking poses under Occam's Razor: are there simpler solutions?. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 877-888	4.2	14
139	Generative Topographic Mapping of Conformational Space. *Molecular Informatics*, **2017**, 36, 1700036	3.8	9

138	Privileged Structural Motif Detection and Analysis Using Generative Topographic Maps. *Journal of Chemical Information and Modeling*, **2017**, 57, 1218-1232	6.1	6
137	Cross-Validation and the Variable Selection Bias **2017**, 163-173		0
136	3D Pharmacophore Modeling Techniques in Computer-Aided Molecular Design Using LigandScout **2017**, 279-309		8
135	Data Visualization and Analysis Using Kohonen Self-Organizing Maps **2017**, 119-126		1
134	QSPR Models on Fragment Descriptors **2017**, 135-162		3
133	Virtual screening, synthesis and biological evaluation of DNA intercalating antiviral agents. *Bioorganic and Medicinal Chemistry Letters*, **2017**, 27, 3915-3919	2.9	5
132	QSAR modeling and chemical space analysis of antimalarial compounds. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 441-451	4.2	11
131	From bird's eye views to molecular communities: two-layered visualization of structure-activity relationships in large compound data sets. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 961-977	4.2	4
130	A Direct One-Pot Synthesis of Asymmetric Dehydrobenzopyrido[12]annulenes and Their Physicochemical Properties. *European Journal of Organic Chemistry*, **2017**, 2017, 4625-4632	3.2	1
129	Neighboring Structure Visualization on a Grid-based Layout. *Molecular Informatics*, **2017**, 36, 1700047	3.8	
128	Structure-reactivity modeling using mixture-based representation of chemical reactions. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 829-839	4.2	20
127	Artificial intelligence in synthetic chemistry: achievements and prospects. *Russian Chemical Reviews* , **2017**, 86, 1127-1156	6.8	37
126	Predictive cartography of metal binders using generative topographic mapping. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 701-714	4.2	4
125	Generative Topographic Mapping Approach to Chemical Space Analysis. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 167-199	0.7	4
124	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, 1631-40	6.1	18
123	Predictive Models for the Free Energy of Hydrogen Bonded Complexes with Single and Cooperative Hydrogen Bonds. *Molecular Informatics*, **2016**, 35, 629-638	3.8	9
122	Chemical Space Mapping and Structure-Activity Analysis of the ChEMBL Antiviral Compound Set. *Journal of Chemical Information and Modeling*, **2016**, 56, 1438-54	6.1	26
121	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, 1455-69	6.1	27

120	Generative Topographic Mapping Approach to Chemical Space Analysis. *ACS Symposium Series*, **2016**, 211-241	0.4	10
119	Automatized Assessment of Protective Group Reactivity: A Step Toward Big Reaction Data Analysis. *Journal of Chemical Information and Modeling*, **2016**, 56, 2140-2148	6.1	30
118	Redox Polypharmacology as an Emerging Strategy to Combat Malarial Parasites. *ChemMedChem*, **2016**, 11, 1339-51	3.7	21
117	Predictive Models for Halogen-bond Basicity of Binding Sites of Polyfunctional Molecules. *Molecular Informatics*, **2016**, 35, 70-80	3.8	10
116	Kernel Target Alignment Parameter: A New Modelability Measure for Regression Tasks. *Journal of Chemical Information and Modeling*, **2016**, 56, 6-11	6.1	11
115	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. *Environmental Health Perspectives*, **2016**, 124, 1023-33	8.4	206
114	In Silico Mining for Antimalarial Structure-Activity Knowledge and Discovery of Novel Antimalarial Curcuminoids. *Molecules*, **2016**, 21,	4.8	14
113	Generative Topographic Mapping Approach to Modeling and Chemical Space Visualization of Human Intestinal Transporters. *BioNanoScience*, **2016**, 6, 464-472	3.4	6
112	Visualization of a Multidimensional Descriptor Space. *ACS Symposium Series*, **2016**, 243-267	0.4	4
111	Prediction of Optimal Salinities for Surfactant Formulations Using a Quantitative Structure□Property Relationships Approach. *Energy & Fuels*, **2015**, 29, 4281-4288	4.1	10
110	Stargate GTM: Bridging Descriptor and Activity Spaces. *Journal of Chemical Information and Modeling*, **2015**, 55, 2403-10	6.1	26
109	Design, Virtual Screening, and Synthesis of Antagonists of □b□3 as Antiplatelet Agents. *Journal of Medicinal Chemistry*, **2015**, 58, 7681-94	8.3	18
108	Chemical data visualization and analysis with incremental generative topographic mapping: big data challenge. *Journal of Chemical Information and Modeling*, **2015**, 55, 84-94	6.1	56
107	Continuous indicator fields: a novel universal type of molecular fields. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 233-47	4.2	3
106	S4MPLE--Sampler for Multiple Protein-Ligand Entities: Methodology and Rigid-Site Docking Benchmarking. *Molecules*, **2015**, 20, 8997-9028	4.8	21
105	Structure□reactivity relationship in bimolecular elimination reactions based on the condensed graph of a reaction. *Journal of Structural Chemistry*, **2015**, 56, 1227-1234	0.9	19
104	Mappability of drug-like space: towards a polypharmacologically competent map of drug-relevant compounds. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 1087-108	4.2	41
103	Electrochemical properties of substituted 2-methyl-1,4-naphthoquinones: redox behavior predictions. *Chemistry - A European Journal*, **2015**, 21, 3415-24	4.8	24

102	Expert system for predicting reaction conditions: the Michael reaction case. *Journal of Chemical Information and Modeling*, **2015**, 55, 239-50	6.1	40
101	GTM-Based QSAR Models and Their Applicability Domains. *Molecular Informatics*, **2015**, 34, 348-56	3.8	48
100	Prediction of drug induced liver injury using molecular and biological descriptors. *Combinatorial Chemistry and High Throughput Screening*, **2015**, 18, 315-22	1.3	20
99	Computational chemogenomics: is it more than inductive transfer?. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 597-618	4.2	26
98	QSPR ensemble modelling of the 1:1 and 1:2 complexation of Co□+, Ni□+, and Cu□+ with organic ligands: relationships between stability constants. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 549-64	4.2	15
97	QSAR modeling: where have you been? Where are you going to?. *Journal of Medicinal Chemistry*, **2014**, 57, 4977-5010	8.3	996
96	Individual Hydrogen-Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. *Molecular Informatics*, **2014**, 33, 477-87	3.8	16
95	Design of a general-purpose European compound screening library for EU-OPENSCREEN. *ChemMedChem*, **2014**, 9, 2309-26	3.7	21
94	Quantitative structure-property relationship modeling: a valuable support in high-throughput screening quality control. *Analytical Chemistry*, **2014**, 86, 2510-20	7.8	14
93	Structure-reactivity relationships in terms of the condensed graphs of reactions. *Russian Journal of Organic Chemistry*, **2014**, 50, 459-463	0.7	24
92	Simple Ligand-Receptor Interaction Descriptor (SILIRID) for alignment-free binding site comparison. *Computational and Structural Biotechnology Journal*, **2014**, 10, 33-7	6.8	15
91	Development of □tructure-property□models in nucleophilic substitution reactions involving azides. *Journal of Structural Chemistry*, **2014**, 55, 1026-1032	0.9	14
90	An Evolutionary Optimizer of libsvm Models. *Challenges*, **2014**, 5, 450-472	3.4	40
89	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 □b□□ *Bioorganic and Medicinal Chemistry*, **2013**, 21, 4646-61	3.4	6
88	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, 3318-25	6.1	53
87	Estimation of the size of drug-like chemical space based on GDB-17 data. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 675-9	4.2	184
86	Synthesis of a strained acetylenic macrocycle incorporating a para-oligo[2]cruciform bridge bent over nanoscopic dimensions: structural, electronic, spectroscopic, and ion-sensing properties. *Chemistry - A European Journal*, **2013**, 19, 12336-49	4.8	7
85	Transductive Support Vector Machines: Promising Approach to Model Small and Unbalanced Datasets. *Molecular Informatics*, **2013**, 32, 261-6	3.8	16

84	Recovery of uranium (VI) from concentrated phosphoric acid by mixtures of new bis(1,3-dialkyloxypropan-2-yl) phosphoric acids and tri-n-octylphosphine oxide. *Hydrometallurgy*, **2013**, 140, 28-33	4	26
83	Publicly available models to predict normal boiling point of organic compounds. *Thermochimica Acta*, **2013**, 553, 60-67	2.9	4
82	Predicting ligand binding modes from neural networks trained on protein-ligand interaction fingerprints. *Journal of Chemical Information and Modeling*, **2013**, 53, 763-72	6.1	39
81	Do not hesitate to use Tversky-and other hints for successful active analogue searches with feature count descriptors. *Journal of Chemical Information and Modeling*, **2013**, 53, 1543-62	6.1	18
80	QSPR ensemble modelling of alkaline-earth metal complexation. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2013**, 76, 159-171		16
79	Models for identification of erroneous atom-to-atom mapping of reactions performed by automated algorithms. *Journal of Chemical Information and Modeling*, **2012**, 52, 3116-22	6.1	17
78	Using self-organizing maps to accelerate similarity search. *Bioorganic and Medicinal Chemistry*, **2012** , 20, 5396-409	3.4	13
77	Mining chemical reactions using neighborhood behavior and condensed graphs of reactions approaches. *Journal of Chemical Information and Modeling*, **2012**, 52, 2325-38	6.1	19
76	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	3.9	13
75	Interpretability of SAR/QSAR Models of any Complexity by Atomic Contributions. *Molecular Informatics*, **2012**, 31, 639-42	3.8	27
74	Electronic, spectroscopic, and ion-sensing properties of a dehydro[m]pyrido[14]- and [15]annulene isomer library. *Journal of Organic Chemistry*, **2012**, 77, 126-42	4.2	12
73	Generative Topographic Mapping (GTM): Universal Tool for Data Visualization, Structure-Activity Modeling and Dataset Comparison. *Molecular Informatics*, **2012**, 31, 301-12	3.8	88
72	QSPR Approach to Predict Nonadditive Properties of Mixtures. Application to Bubble Point Temperatures of Binary Mixtures of Liquids. *Molecular Informatics*, **2012**, 31, 491-502	3.8	50
71	Machine learning methods for property prediction in chemoinformatics: Quo Vadis?. *Journal of Chemical Information and Modeling*, **2012**, 52, 1413-37	6.1	146
70	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		14
69	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	2.2	16
68	In silico design of new ionic liquids based on quantitative structure-property relationship models of ionic liquid viscosity. *Journal of Physical Chemistry B*, **2011**, 115, 93-8	3.4	43
67	Quantitative Structure−Property Relationship (QSPR) Modeling of Normal Boiling Point Temperature and Composition of Binary Azeotropes. *Industrial & Engineering Chemistry Research*, **2011**, 50, 14162-14167	3.9	25

66	RGD mimetics containing phthalimidine fragment as novel ligands of fibrinogen receptor. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 5971-4	2.9	5
65	Local neighborhood behavior in a combinatorial library context. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 237-52	4.2	9
64	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, 533-54	4.2	311
63	Chemoinformatics as a Theoretical Chemistry Discipline. *Molecular Informatics*, **2011**, 30, 20-32	3.8	64
62	A REPRESENTATION TO APPLY USUAL DATA MINING TECHNIQUES TO CHEMICAL REACTIONS ILLUSTRATION ON THE RATE CONSTANT OF SN2 REACTIONS IN WATER. *International Journal on Artificial Intelligence Tools*, **2011**, 20, 253-270	0.9	27
61	Fragment descriptors in structure-property modeling and virtual screening. *Methods in Molecular Biology*, **2011**, 672, 213-43	1.4	6
60	Applicability domains for classification problems: Benchmarking of distance to models for Ames mutagenicity set. *Journal of Chemical Information and Modeling*, **2010**, 50, 2094-111	6.1	169
59	The One-Class Classification Approach to Data Description and to Models Applicability Domain. *Molecular Informatics*, **2010**, 29, 581-7	3.8	44
58	ISIDA Property-Labelled Fragment Descriptors. *Molecular Informatics*, **2010**, 29, 855-68	3.8	92
57	A Representation to Apply Usual Data Mining Techniques to Chemical Reactions. *Lecture Notes in Computer Science*, **2010**, 318-326	0.9	2
56	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, 133-44	6.1	55
55	Predicting the predictability: a unified approach to the applicability domain problem of QSAR models. *Journal of Chemical Information and Modeling*, **2009**, 49, 1762-76	6.1	132
54	Quantitative Structure-Property Relationships in Solvent Extraction and Complexation of Metals. *Ion Exchange and Solvent Extraction*, **2009**, 319-358		11
53	Combinatorial QSAR modeling of chemical toxicants tested against Tetrahymena pyriformis. *Journal of Chemical Information and Modeling*, **2008**, 48, 766-84	6.1	222
52	Computer-aided design of new metal binders. *Radiochimica Acta*, **2008**, 96, 505-511	1.9	12
51	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, 1733-46	6.1	296
50	Building a chemical space based on fragment descriptors. *Combinatorial Chemistry and High Throughput Screening*, **2008**, 11, 661-8	1.3	13
49	ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. *Current Computer-Aided Drug Design*, **2008**, 4, 191-198	1.4	152

48	Stochastic versus stepwise strategies for quantitative structure-activity relationship generation--how much effort may the mining for successful QSAR models take?. *Journal of Chemical Information and Modeling*, **2007**, 47, 927-39	6.1	30
47	Successful In Silico Design of New Efficient Uranyl Binders. *Solvent Extraction and Ion Exchange*, **2007**, 25, 433-462	2.5	22
46	Synthesis and structure of heterometallic compounds of [RuNO(NO2)4OH]2- with triphenyl phosphine oxide complexes of Co(II), Ni (II), and Zn(II). *Journal of Molecular Structure*, **2007**, 837, 63-71	3.4	19
45	QSPR Modeling of the AmIII/EuIII Separation Factor: How Far Can we Predict ?. *Solvent Extraction and Ion Exchange*, **2007**, 25, 1-26	2.5	20
44	Exhaustive QSPR studies of a large diverse set of ionic liquids: how accurately can we predict melting points?. *Journal of Chemical Information and Modeling*, **2007**, 47, 1111-22	6.1	115
43	Skin permeation rate as a function of chemical structure. *Journal of Medicinal Chemistry*, **2006**, 49, 3305-14	5.3	46
42	Benchmarking of linear and nonlinear approaches for quantitative structure-property relationship studies of metal complexation with ionophores. *Journal of Chemical Information and Modeling*, **2006**, 46, 808-19	6.1	59
41	Correlation of blood-brain penetration using structural descriptors. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 4888-917	3.4	71
40	Structure-property modelling of complex formation of strontium with organic ligands in water. *Journal of Structural Chemistry*, **2006**, 47, 298-311	0.9	15
39	QSAR modeling of blood:air and tissue:air partition coefficients using theoretical descriptors. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 6450-63	3.4	30
38	Substructural fragments: an universal language to encode reactions, molecular and supramolecular structures. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 693-703	4.2	127
37	"In silico" design of potential anti-HIV actives using fragment descriptors. *Combinatorial Chemistry and High Throughput Screening*, **2005**, 8, 403-16	1.3	17
36	Upper Rim Thioether Derivatives of Calix[4,6]Arenes: Extraction of Fission Pd(II) and Ag(I). *Solvent Extraction and Ion Exchange*, **2005**, 23, 781-801	2.5	26
35	New Wide Rim Phosphomethylated Calix[4]arenes in Extraction of Americium and Europium. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, **2004**, 49, 47-56		40
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