Ramil I Nugmanov

List of Publications by Year
in descending order

35	608	566801 15	610482 24
papers	citations	h-index	g-index

36	36	36	475
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Atomâ€toâ€atom Mapping: A Benchmarking Study of Popular Mapping Algorithms and Consensus Strategies. Molecular Informatics, 2022, 41, e2100138.	1.4	17
2	CGRdb2.0: A Python Database Management System for Molecules, Reactions, and Chemical Data. Journal of Chemical Information and Modeling, 2022, 62, 2015-2020.	2.5	3
3	Prediction of Optimal Conditions of Hydrogenation Reaction Using the Likelihood Ranking Approach. International Journal of Molecular Sciences, 2022, 23, 248.	1.8	4
4	Bidirectional Graphormer for Reactivity Understanding: Neural Network Trained to Reaction Atom-to-Atom Mapping Task. Journal of Chemical Information and Modeling, 2022, 62, 3307-3315.	2.5	2
5	Combined Graph/Relational Database Management System for Calculated Chemical Reaction Pathway Data. Journal of Chemical Information and Modeling, 2021, 61, 554-559.	2.5	6
6	Cross-validation strategies in QSPR modelling of chemical reactions. SAR and QSAR in Environmental Research, 2021, 32, 207-219.	1.0	12
7	Discovery of novel chemical reactions by deep generative recurrent neural network. Scientific Reports, 2021, 11, 3178.	1.6	40
8	Switching Ion Binding Selectivity of Thiacalix[4]arene Monocrowns at Liquidâ€“Liquid and 2D-Confined Interfaces. International Journal of Molecular Sciences, 2021, 22, 3535.	1.8	4
9	Reaction Data Curation I: Chemical Structures and Transformations Standardization. Molecular Informatics, 2021, 40, e2100119.	1.4	15
10	QSAR Modeling Based on Conformation Ensembles Using a Multi-Instance Learning Approach. Journal of Chemical Information and Modeling, 2021, 61, 4913-4923.	2.5	15
11	Azocalix[4]arene-Rhodamine Supramolecular Hypoxia-Sensitive Systems: A Search for the Best Calixarene Hosts and Rhodamine Guests. Molecules, 2021, 26, 5451.	1.7	10
12	Functional supramolecular systems: design and applications. Russian Chemical Reviews, 2021, 90, 895-1107.	2.5	93
13	Machine learning modelling of chemical reaction characteristics: yesterday, today, tomorrow. Mendeleev Communications, 2021, 31, 769-780.	0.6	9
14	Alkyl-malonate-substituted thiacalix[4]arenes as ligands for bottom-up design of paramagnetic Gd(III)-containing colloids with low cytotoxicity. Arabian Journal of Chemistry, 2020, 13, 453-463.	2.3	3
15	Comprehensive Analysis of Applicability Domains of QSPR Models for Chemical Reactions. International Journal of Molecular Sciences, 2020, 21, 5542.	1.8	32
16	Predictive Models for Kinetic Parameters of Cycloaddition Reactions. Molecular Informatics, 2019, 38, e1800077.	1.4	25
17	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.	2.5	5
18	CGRtools: Python Library for Molecule, Reaction, and Condensed Graph of Reaction Processing. Journal of Chemical Information and Modeling, 2019, 59, 2516-2521.	2.5	34

#	Article	IF	Citations
19	Bimolecular Nucleophilic Substitution Reactions: Predictive Models for Rate Constants and Molecular Reaction Pairs Analysis. Molecular Informatics, 2019, 38, e1800104.	1.4	23
20	Assessment of tautomer distribution using the condensed reaction graph approach. Journal of Computer-Aided Molecular Design, 2018, 32, 401-414.	1.3	20
21	Synthesis of new p-tert-butylcalix[4]arene-based polyammonium triazolyl amphiphiles and their binding with nucleoside phosphates. Beilstein Journal of Organic Chemistry, 2018, 14, 1980-1993.	1.3	16
22	Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. Molecular Informatics, 2018, 37, e1800056.	1.4	7
23	Detection of sulfate surface-active substances via fluorescent response using new amphiphilic thiacalix[4]arenes bearing cationic headgroups with Eosin Y dye. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2017, 515, 41-49.	2.3	13
24	Structureâ€“reactivity relationship in Dielsâ€“Alder reactions obtained using the condensed reaction graph approach. Journal of Structural Chemistry, 2017, 58, 650-656.	0.3	15
25	Structureâ€“reactivity modeling using mixture-based representation of chemical reactions. Journal of Computer-Aided Molecular Design, 2017, 31, 829-839.	1.3	23
26	Unusual Reactivity of Aliphatic and Aromatic Amines with Bromoalkyl Derivatives of Thiacalix[4]arene in 1,3-Alternate Stereoisomeric Form. Macroheterocycles, 2017, 10, 215-220.	0.9	4
27	Automatized Assessment of Protective Group Reactivity: A Step Toward Big Reaction Data Analysis. Journal of Chemical Information and Modeling, 2016, 56, 2140-2148.	2.5	37
28	Effect of copper(I) on the conformation of the thiacalixarene platform in azide-alkyne cycloaddition. Russian Chemical Bulletin, 2015, 64, 2114-2124.	0.4	3
29	â€˜Click chemistryâ€™ in the synthesis of new amphiphilic 1,3-alternate thiacalixarenes. Mendeleev Communications, 2015, 25, 177-179.	0.6	26
30	Structureâ€“reactivity relationship in bimolecular elimination reactions based on the condensed graph of a reaction. Journal of Structural Chemistry, 2015, 56, 1227-1234.	0.3	25
31	Synthesis and structure of lower rim-substituted alkynyl derivatives of thiacalix[4]arene. Russian Journal of Organic Chemistry, 2015, 51, 1334-1342.	0.3	9
32	Development of â€œstructure-propertyâ€•models in nucleophilic substitution reactions involving azides. Journal of Structural Chemistry, 2014, 55, 1026-1032.	0.3	15
33	Structure-reactivity relationships in terms of the condensed graphs of reactions. Russian Journal of Organic Chemistry, 2014, 50, 459-463.	0.3	29
34	Bifunctional Derivatives of (Thia)calix[4]-arenes with Terminal Double and Triple Bonds: Synthesis and Azide-Alkyne Click Reactions. Macroheterocycles, 2014, 7, 10-17.	0.9	4
35	Microwave-assisted Alkylation of p-tert-butylcalix[4]arene Lower Rim: The Effect of Alkyl Halides. Mendeleev Communications, 2013, 23, 113-115.	0.6	10