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	Functional supramolecular systems: design and applications. Russian Chemical Reviews, 2021, 90, 895-1107.	2.5	93
2	Discovery of novel chemical reactions by deep generative recurrent neural network. Scientific Reports, 2021, 11, 3178.	1.6	40
3	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
4	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
5	Comprehensive Analysis of Applicability Domains of QSPR Models for Chemical Reactions. International Journal of Molecular Sciences, 2020, 21, 5542.	1.8	32
6	Structure-reactivity relationships in terms of the condensed graphs of reactions. Russian Journal of Organic Chemistry, 2014, 50, 459-463.	0.3	29
7	â€˜Click chemistryâ€™ in the synthesis of new amphiphilic 1,3-alternate thiacalixarenes. Mendeleev Communications, 2015, 25, 177-179.	0.6	26
8	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
9	Predictive Models for Kinetic Parameters of Cycloaddition Reactions. Molecular Informatics, 2019, 38, e1800077.	1.4	25
10	Structureâ€“reactivity modeling using mixture-based representation of chemical reactions. Journal of Computer-Aided Molecular Design, 2017, 31, 829-839.	1.3	23
11	Bimolecular Nucleophilic Substitution Reactions: Predictive Models for Rate Constants and Molecular Reaction Pairs Analysis. Molecular Informatics, 2019, 38, e1800104.	1.4	23
12	Assessment of tautomer distribution using the condensed reaction graph approach. Journal of Computer-Aided Molecular Design, 2018, 32, 401-414.	1.3	20
13	Atomâ€toâ€atom Mapping: A Benchmarking Study of Popular Mapping Algorithms and Consensus Strategies. Molecular Informatics, 2022, 41, e2100138.	1.4	17
14	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
15	Development of â€œstructure-propertyâ€•models in nucleophilic substitution reactions involving azides. Journal of Structural Chemistry, 2014, 55, 1026-1032.	0.3	15
16	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
17	Reaction Data Curation I: Chemical Structures and Transformations Standardization. Molecular Informatics, 2021, 40, e2100119.	1.4	15
18	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

#	Article	IF	Citations
19	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
20	Cross-validation strategies in QSPR modelling of chemical reactions. SAR and QSAR in Environmental Research, 2021, 32, 207-219.	1.0	12
21	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
22	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
23	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
24	Machine learning modelling of chemical reaction characteristics: yesterday, today, tomorrow. Mendeleev Communications, 2021, 31, 769-780.	0.6	9
25	Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. Molecular Informatics, 2018, 37, e1800056.	1.4	7
26	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
27	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
28	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
29	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
30	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
31	Prediction of Optimal Conditions of Hydrogenation Reaction Using the Likelihood Ranking Approach. International Journal of Molecular Sciences, 2022, 23, 248.	1.8	4
32	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
33	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
34	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
35	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