Timur I Madzhidov

List of Publications by Year
in descending order

59	1,107	471509 17	434195 31
papers	citations	h-index	g-index

63	63	63	1208
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.	2.5	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.	5.4	3
3	Theoretical insight into the catalytic effect of transition metal ions on the aquathermal degradation of heavy oil: A DFT study of cyclohexyl phenyl ether cleavage. Fuel, 2022, 311, 122595.	6.4	4
4	Theoretical insight into the catalytic effect of transition metal ions on the aquathermal degradation of heavy oil: A DFT study of cyclohexyl phenyl amine cleavage. Fuel, 2022, 312, 123002.	6.4	3
5	Editorial: Chemical Reactions Mining. Molecular Informatics, 2022, 41, .	2.5	0
6	Prediction of Optimal Conditions of Hydrogenation Reaction Using the Likelihood Ranking Approach. International Journal of Molecular Sciences, 2022, 23, 248.	4.1	4
7	A new algorithm to assess the risk of malignancy in premenopausal patients with pelvic mass. Opuholi Zenskoj Reproduktivnoj Sistemy, 2022, 18, 76-86.	0.4	0
8	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
9	Cross-validation strategies in QSPR modelling of chemical reactions. SAR and QSAR in Environmental Research, 2021, 32, 207-219.	2.2	12
10	Discovery of novel chemical reactions by deep generative recurrent neural network. Scientific Reports, 2021, 11, 3178.	3.3	40
11	Multi-Instance Learning Approach to Predictive Modeling of Catalysts Enantioselectivity. Synlett, 2021, 32, 1833-1836.	1.8	8
12	Reaction Data Curation I: Chemical Structures and Transformations Standardization. Molecular Informatics, 2021, 40, e2100119.	2.5	15
13	Multiple Conformer Descriptors for QSAR Modeling. Molecular Informatics, 2021, 40, e2060030.	2.5	7
14	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
15	Machine learning modelling of chemical reaction characteristics: yesterday, today, tomorrow. Mendeleev Communications, 2021, 31, 769-780.	1.6	9
16	Comprehensive Analysis of Applicability Domains of QSPR Models for Chemical Reactions. International Journal of Molecular Sciences, 2020, 21, 5542.	4.1	32
17	Theoretical Insights into the Catalytic Effect of Transition-Metal Ions on the Aquathermal Degradation of Sulfur-Containing Heavy Oil: A DFT Study of Cyclohexyl Phenyl Sulfide Cleavage. ACS Omega, 2020, 5, 19589-19597.	3.5	6
18	Probabilistic Approach for Virtual Screening Based on Multiple Pharmacophores. Molecules, 2020, 25, 385.	3.8	5

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19	Multi-instance Learning for Structure-Activity Modeling for Molecular Properties. Communications in Computer and Information Science, 2020, , 62-71.	0.5	0
20	Predictive Models for Kinetic Parameters of Cycloaddition Reactions. Molecular Informatics, 2019, 38, e1800077.	2.5	25
21	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
22	Sydnone-alkyne cycloaddition: Which factors are responsible for reaction rate ?. Journal of Molecular Structure, 2019, 1198, 126897.	3.6	7
23	â€œLpâ‹¯synthonâ€•interaction as a reason for the strong amplification of synthon-forming hydrogen bonds. CrystEngComm, 2019, 21, 1499-1511.	2.6	3
24	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
25	Virtual Screening Using Pharmacophore Models Retrieved from Molecular Dynamic Simulations. International Journal of Molecular Sciences, 2019, 20, 5834.	4.1	16
26	Bimolecular Nucleophilic Substitution Reactions: Predictive Models for Rate Constants and Molecular Reaction Pairs Analysis. Molecular Informatics, 2019, 38, e1800104.	2.5	23
27	Assessment of tautomer distribution using the condensed reaction graph approach. Journal of Computer-Aided Molecular Design, 2018, 32, 401-414.	2.9	20
28	Prediction of Aromatic Hydroxylation Sites for Human CYP1A2 Substrates Using Condensed Graph of Reactions. BioNanoScience, 2018, 8, 384-389.	3.5	3
29	Hydration of copper(II) amino acids complexes. Journal of Computational Chemistry, 2018, 39, 821-826.	3.3	9
30	Effect of core substituents on the intramolecular exchange interaction in N,Nâ€²â€dioxyâ€2,6â€diazaadamantane biradical: DFT studies. International Journal of Quantum Chemistry, 2018, 118, e25568.	2.0	0
31	Ligand-Based Pharmacophore Modeling Using Novel 3D Pharmacophore Signatures. Molecules, 2018, 23, 3094.	3.8	41
32	Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. Molecular Informatics, 2018, 37, e1800056.	2.5	7
33	Modern Trends of Organic Chemistry in Russian Universities. Russian Journal of Organic Chemistry, 2018, 54, 157-371.	0.8	68
34	Structureâ€“reactivity relationship in Dielsâ€“Alder reactions obtained using the condensed reaction graph approach. Journal of Structural Chemistry, 2017, 58, 650-656.	1.0	15
35	Structureâ€“reactivity modeling using mixture-based representation of chemical reactions. Journal of Computer-Aided Molecular Design, 2017, 31, 829-839.	2.9	23
36	Artificial intelligence in synthetic chemistry: achievements and prospects. Russian Chemical Reviews, 2017, 86, 1127-1156.	6.5	45

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37	Exchange interaction mechanisms in 1,3,5,7-tetramethyl-2,6-diazaadamantane N,Nâ€™-dioxyl biradical. Russian Chemical Bulletin, 2017, 66, 2028-2034.	1.5	0
38	Using semantic analysis of texts for the identification of drugs with similar therapeutic effects. Russian Chemical Bulletin, 2017, 66, 2180-2189.	1.5	13
39	STRUCTURE-REACTIVITY RELATIONSHIP IN DIELS-ALDER REACTIONS OBTAINED USING THE CONDENSED REACTION GRAPH APPROACH. Journal of Structural Chemistry, 2017, , .	0.0	1
40	Quantum chemical calculation of exchange interactions in supramolecularly arrangedN,Nâ€²-dioxy-2,6-diazaadamantane organic biradical. International Journal of Quantum Chemistry, 2016, 116, 1064-1070.	2.0	4
41	Generative Topographic Mapping Approach to Modeling and Chemical Space Visualization of Human Intestinal Transporters. BioNanoScience, 2016, 6, 464-472.	3.5	6
42	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
43	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
44	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	2.5	12
45	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
46	S=oâ€¦s=o Interactions as a Driving Force for Low-Temperature Conformational Rearrangement of Stable H-Bonding {S(O)-Ch2-Ch2-OHÂ·Â·Â·}2 Synthon in two Modifications of Diastereomeric Pinanyl Sulfoxides Co-Crystal. Phosphorus, Sulfur and Silicon and the Related Elements, 2015, 190, 2222-2231.	1.6	9
47	Electrochemically driven molecular rotors based on ferrocene-1,1'-diyl-bisphosphinic acids. Russian Journal of Electrochemistry, 2015, 51, 645-664.	0.9	4
48	STRUCTURE-REACTIVITY RELATIONSHIP IN BIMOLECULAR ELIMINATION REACTIONS BASED ON THE CONDENSED GRAPH OF A REACTION. Journal of Structural Chemistry, 2015, 56, .	0.0	0
49	Development of â€œstructure-propertyâ€•models in nucleophilic substitution reactions involving azides. Journal of Structural Chemistry, 2014, 55, 1026-1032.	1.0	15
50	Dimethyl selenide complexes with compounds of Group IIIA elements: electron density redistribution and interaction energy partitioning. Russian Chemical Bulletin, 2014, 63, 43-53.	1.5	1
51	Structure-reactivity relationships in terms of the condensed graphs of reactions. Russian Journal of Organic Chemistry, 2014, 50, 459-463.	0.8	29
52	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
53	The Nature of the Interaction of Dimethylselenide with IIIA Group Element Compounds. Journal of Physical Chemistry A, 2013, 117, 4011-4024.	2.5	7
54	â€œAdditiveâ€•cooperativity of hydrogen bonds in complexes of catechol with proton acceptors in the gas phase: FTIR spectroscopy and quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 75-82.	3.9	7

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55	The Nature of the Interaction of Organoselenium Molecules with Diiodine. Journal of Physical Chemistry A, 2011, 115, 10069-10077.	2.5	19
56	Experimental and theoretical study on 6-substituted pyridoxine derivatives. Synthesis of cyclic 2,4,5,6-tetrakis-(hydroxymethyl)pyridin-3-ol acetonides. Russian Journal of Organic Chemistry, 2011, 47, 100-108.	0.8	6
57	Theoretical and experimental study on cyclic 6-methyl-2,3,4-tris(hydroxymethyl)pyridin-5-ol acetonides. Russian Journal of Organic Chemistry, 2010, 46, 561-567.	0.8	17
58	The nature of hydrogen bonds with divalent selenium compounds. Computational and Theoretical Chemistry, 2010, 959, 1-7.	1.5	23
59	Quantum-chemical investigation of structure and reactivity of pyrazol-5-ones and their thio- and seleno-analogs: X. Solvent effect on the chemical shifts of nuclei in the molecules of 3-methylpyrazol-5-ones and 1-phenyl-3-methylchalcogenepyrazol-5-ones and characteristics of tautomeric equilibrium in these compounds. Russian Journal of General Chemistry, 2009, 79, 1919-1928.	0.8	6