Timur I Madzhidov

List of Publications by Year
in descending order

59 papers	1,107 citations	471509 17 h-index	434195 31 g-index
63 all docs	63 docs citations	63 times ranked	1208 citing authors

#	Article	IF	Citations
1	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
2	Modern Trends of Organic Chemistry in Russian Universities. Russian Journal of Organic Chemistry, 2018, 54, 157-371.	0.8	68
3	Artificial intelligence in synthetic chemistry: achievements and prospects. Russian Chemical Reviews, 2017, 86, 1127-1156.	6.5	45
4	Ligand-Based Pharmacophore Modeling Using Novel 3D Pharmacophore Signatures. Molecules, 2018, 23, 3094.	3.8	41
5	Discovery of novel chemical reactions by deep generative recurrent neural network. Scientific Reports, 2021, 11, 3178.	3.3	40
6	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
7	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
8	Comprehensive Analysis of Applicability Domains of QSPR Models for Chemical Reactions. International Journal of Molecular Sciences, 2020, 21, 5542.	4.1	32
9	Structure-reactivity relationships in terms of the condensed graphs of reactions. Russian Journal of Organic Chemistry, 2014, 50, 459-463.	0.8	29
10	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
11	Predictive Models for Kinetic Parameters of Cycloaddition Reactions. Molecular Informatics, 2019, 38, e1800077.	2.5	25
12	The nature of hydrogen bonds with divalent selenium compounds. Computational and Theoretical Chemistry, 2010, 959, 1-7.	1.5	23
13	Structureâ€“reactivity modeling using mixture-based representation of chemical reactions. Journal of Computer-Aided Molecular Design, 2017, 31, 829-839.	2.9	23
14	Bimolecular Nucleophilic Substitution Reactions: Predictive Models for Rate Constants and Molecular Reaction Pairs Analysis. Molecular Informatics, 2019, 38, e1800104.	2.5	23
15	Assessment of tautomer distribution using the condensed reaction graph approach. Journal of Computer-Aided Molecular Design, 2018, 32, 401-414.	2.9	20
16	The Nature of the Interaction of Organoselenium Molecules with Diiodine. Journal of Physical Chemistry A, 2011, 115, 10069-10077.	2.5	19
17	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
18	Atomâ€toâ€atom Mapping: A Benchmarking Study of Popular Mapping Algorithms and Consensus Strategies. Molecular Informatics, 2022, 41, e2100138.	2.5	17

#	ARTICLE	IF	CITATIONS
19	Virtual Screening Using Pharmacophore Models Retrieved from Molecular Dynamic Simulations. International Journal of Molecular Sciences, 2019, 20, 5834.	4.1	16
20	Development of â€œstructure-propertyâ€•models in nucleophilic substitution reactions involving azides. Journal of Structural Chemistry, 2014, 55, 1026-1032.	1.0	15
21	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
22	Reaction Data Curation I: Chemical Structures and Transformations Standardization. Molecular Informatics, 2021, 40, e2100119.	2.5	15
23	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
24	Using semantic analysis of texts for the identification of drugs with similar therapeutic effects. Russian Chemical Bulletin, 2017, 66, 2180-2189.	1.5	13
25	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	2.5	12
26	Cross-validation strategies in QSPR modelling of chemical reactions. SAR and QSAR in Environmental Research, 2021, 32, 207-219.	2.2	12
27	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
28	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
29	Hydration of copper(II) amino acids complexes. Journal of Computational Chemistry, 2018, 39, 821-826.	3.3	9
30	Machine learning modelling of chemical reaction characteristics: yesterday, today, tomorrow. Mendeleev Communications, 2021, 31, 769-780.	1.6	9
31	Multi-Instance Learning Approach to Predictive Modeling of Catalysts Enantioselectivity. Synlett, 2021, 32, 1833-1836.	1.8	8
32	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
33	The Nature of the Interaction of Dimethylselenide with IIIA Group Element Compounds. Journal of Physical Chemistry A, 2013, 117, 4011-4024.	2.5	7
34	Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. Molecular Informatics, 2018, 37, e1800056.	2.5	7
35	Sydnone-alkyne cycloaddition: Which factors are responsible for reaction rate ?. Journal of Molecular Structure, 2019, 1198, 126897.	3.6	7
36	Multiple Conformer Descriptors for QSAR Modeling. Molecular Informatics, 2021, 40, e2060030.	2.5	7

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37	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
38	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
39	Generative Topographic Mapping Approach to Modeling and Chemical Space Visualization of Human Intestinal Transporters. BioNanoScience, 2016, 6, 464-472.	3.5	6
40	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
41	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
42	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
43	Probabilistic Approach for Virtual Screening Based on Multiple Pharmacophores. Molecules, 2020, 25, 385.	3.8	5
44	Electrochemically driven molecular rotors based on ferrocene-1,1'-diyl-bisphosphinic acids. Russian Journal of Electrochemistry, 2015, 51, 645-664.	0.9	4
45	Quantum chemical calculation of exchange interactions in supramolecularly arranged<i>N</i>,<i>N</i>â€²-dioxy-2,6-diazaadamantane organic biradical. International Journal of Quantum Chemistry, 2016, 116, 1064-1070.	2.0	4
46	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
47	Prediction of Optimal Conditions of Hydrogenation Reaction Using the Likelihood Ranking Approach. International Journal of Molecular Sciences, 2022, 23, 248.	4.1	4
48	Prediction of Aromatic Hydroxylation Sites for Human CYP1A2 Substrates Using Condensed Graph of Reactions. BioNanoScience, 2018, 8, 384-389.	3.5	3
49	â€œLpâ‹¯synthonâ€•interaction as a reason for the strong amplification of synthon-forming hydrogen bonds. CrystEngComm, 2019, 21, 1499-1511.	2.6	3
50	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
51	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
52	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
53	STRUCTURE-REACTIVITY RELATIONSHIP IN DIELS-ALDER REACTIONS OBTAINED USING THE CONDENSED REACTION GRAPH APPROACH. Journal of Structural Chemistry, 2017, , .	0.0	1
54	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

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55	Effect of core substituents on the intramolecular exchange interaction in <i>N</i>,<i>N</i>â€²â€•dioxyâ€•2,6â€•diazaadamantane biradical: DFT studies. International Journal of Quantum Chemistry, 2018, 118, e25568.	2.0	0
56	STRUCTURE-REACTIVITY RELATIONSHIP IN BIMOLECULAR ELIMINATION REACTIONS BASED ON THE CONDENSED GRAPH OF A REACTION. Journal of Structural Chemistry, 2015, 56, .	0.0	0
57	Multi-instance Learning for Structure-Activity Modeling for Molecular Properties. Communications in Computer and Information Science, 2020, , 62-71.	0.5	0
58	Editorial: Chemical Reactions Mining. Molecular Informatics, 2022, 41, .	2.5	0
59	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