

Timur I Madzhidov

List of Publications by Year in descending order

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58
papers

1,107
citations

471061

17
h-index

433756

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. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 675-679.	1.3	319
2	Modern Trends of Organic Chemistry in Russian Universities. <i>Russian Journal of Organic Chemistry</i> , 2018, 54, 157-371.	0.3	68
3	Artificial intelligence in synthetic chemistry: achievements and prospects. <i>Russian Chemical Reviews</i> , 2017, 86, 1127-1156.	2.5	45
4	Ligand-Based Pharmacophore Modeling Using Novel 3D Pharmacophore Signatures. <i>Molecules</i> , 2018, 23, 3094.	1.7	41
5	Discovery of novel chemical reactions by deep generative recurrent neural network. <i>Scientific Reports</i> , 2021, 11, 3178.	1.6	40
6	Automatized Assessment of Protective Group Reactivity: A Step Toward Big Reaction Data Analysis. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2140-2148.	2.5	37
7	CGRtools: Python Library for Molecule, Reaction, and Condensed Graph of Reaction Processing. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2516-2521.	2.5	34
8	Comprehensive Analysis of Applicability Domains of QSPR Models for Chemical Reactions. <i>International Journal of Molecular Sciences</i> , 2020, 21, 5542.	1.8	32
9	Structure-reactivity relationships in terms of the condensed graphs of reactions. <i>Russian Journal of Organic Chemistry</i> , 2014, 50, 459-463.	0.3	29
10	Structure-reactivity relationship in bimolecular elimination reactions based on the condensed graph of a reaction. <i>Journal of Structural Chemistry</i> , 2015, 56, 1227-1234.	0.3	25
11	Predictive Models for Kinetic Parameters of Cycloaddition Reactions. <i>Molecular Informatics</i> , 2019, 38, e1800077.	1.4	25
12	The nature of hydrogen bonds with divalent selenium compounds. <i>Computational and Theoretical Chemistry</i> , 2010, 959, 1-7.	1.5	23
13	Structure-reactivity modeling using mixture-based representation of chemical reactions. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 829-839.	1.3	23
14	Bimolecular Nucleophilic Substitution Reactions: Predictive Models for Rate Constants and Molecular Reaction Pairs Analysis. <i>Molecular Informatics</i> , 2019, 38, e1800104.	1.4	23
15	Assessment of tautomer distribution using the condensed reaction graph approach. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 401-414.	1.3	20
16	The Nature of the Interaction of Organoselenium Molecules with Diiodine. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10069-10077.	1.1	19
17	Theoretical and experimental study on cyclic 6-methyl-2,3,4-tris(hydroxymethyl)pyridin-5-ol acetonides. <i>Russian Journal of Organic Chemistry</i> , 2010, 46, 561-567.	0.3	17
18	Atom-to-atom Mapping: A Benchmarking Study of Popular Mapping Algorithms and Consensus Strategies. <i>Molecular Informatics</i> , 2022, 41, e2100138.	1.4	17

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19	Virtual Screening Using Pharmacophore Models Retrieved from Molecular Dynamic Simulations. <i>International Journal of Molecular Sciences</i> , 2019, 20, 5834.	1.8	16
20	Development of σ -structure-property models in nucleophilic substitution reactions involving azides. <i>Journal of Structural Chemistry</i> , 2014, 55, 1026-1032.	0.3	15
21	Structure-reactivity relationship in Diels-Alder reactions obtained using the condensed reaction graph approach. <i>Journal of Structural Chemistry</i> , 2017, 58, 650-656.	0.3	15
22	Reaction Data Curation I: Chemical Structures and Transformations Standardization. <i>Molecular Informatics</i> , 2021, 40, e2100119.	1.4	15
23	QSAR Modeling Based on Conformation Ensembles Using a Multi-Instance Learning Approach. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4913-4923.	2.5	15
24	Using semantic analysis of texts for the identification of drugs with similar therapeutic effects. <i>Russian Chemical Bulletin</i> , 2017, 66, 2180-2189.	0.4	13
25	Predictive Models for Halogen-bond Basicity of Binding Sites of Polyfunctional Molecules. <i>Molecular Informatics</i> , 2016, 35, 70-80.	1.4	12
26	Cross-validation strategies in QSPR modelling of chemical reactions. <i>SAR and QSAR in Environmental Research</i> , 2021, 32, 207-219.	1.0	12
27	S=O \cdots S=O Interactions as a Driving Force for Low-Temperature Conformational Rearrangement of Stable H-Bonding {S(O)-CH ₂ -CH ₂ -OH} ₂ Synthon in two Modifications of Diastereomeric Pinanyl Sulfoxides Co-Crystal. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2015, 190, 2222-2231.	0.8	9
28	Predictive Models for the Free Energy of Hydrogen Bonded Complexes with Single and Cooperative Hydrogen Bonds. <i>Molecular Informatics</i> , 2016, 35, 629-638.	1.4	9
29	Hydration of copper(II) amino acids complexes. <i>Journal of Computational Chemistry</i> , 2018, 39, 821-826.	1.5	9
30	Machine learning modelling of chemical reaction characteristics: yesterday, today, tomorrow. <i>Mendeleev Communications</i> , 2021, 31, 769-780.	0.6	9
31	Multi-Instance Learning Approach to Predictive Modeling of Catalysts Enantioselectivity. <i>Synlett</i> , 2021, 32, 1833-1836.	1.0	8
32	σ -Additive-cooperativity of hydrogen bonds in complexes of catechol with proton acceptors in the gas phase: FTIR spectroscopy and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 75-82.	2.0	7
33	The Nature of the Interaction of Dimethylselenide with IIIA Group Element Compounds. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4011-4024.	1.1	7
34	Visualization and Analysis of Complex Reaction Data: The Case of Tautomeric Equilibria. <i>Molecular Informatics</i> , 2018, 37, e1800056.	1.4	7
35	Sydnone-alkyne cycloaddition: Which factors are responsible for reaction rate ?. <i>Journal of Molecular Structure</i> , 2019, 1198, 126897.	1.8	7
36	Multiple Conformer Descriptors for QSAR Modeling. <i>Molecular Informatics</i> , 2021, 40, e2060030.	1.4	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. <i>Russian Journal of General Chemistry</i> , 2009, 79, 1919-1928.	0.3	6
38	Experimental and theoretical study on 6-substituted pyridoxine derivatives. Synthesis of cyclic 2,4,5,6-tetrakis-(hydroxymethyl)pyridin-3-ol acetonides. <i>Russian Journal of Organic Chemistry</i> , 2011, 47, 100-108.	0.3	6
39	Generative Topographic Mapping Approach to Modeling and Chemical Space Visualization of Human Intestinal Transporters. <i>BioNanoScience</i> , 2016, 6, 464-472.	1.5	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. <i>ACS Omega</i> , 2020, 5, 19589-19597.	1.6	6
41	Combined Graph/Relational Database Management System for Calculated Chemical Reaction Pathway Data. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 554-559.	2.5	6
42	Conjugated Quantitative Structure-Property Relationship Models: Application to Simultaneous Prediction of Tautomeric Equilibrium Constants and Acidity of Molecules. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4569-4576.	2.5	5
43	Probabilistic Approach for Virtual Screening Based on Multiple Pharmacophores. <i>Molecules</i> , 2020, 25, 385.	1.7	5
44	Electrochemically driven molecular rotors based on ferrocene-1,1'-diyl-bisphosphinic acids. <i>Russian Journal of Electrochemistry</i> , 2015, 51, 645-664.	0.3	4
45	Quantum chemical calculation of exchange interactions in supramolecularly arranged $\langle i \rangle N \langle /i \rangle$, $\langle i \rangle N \langle /i \rangle$ $\hat{\alpha}^2$ -dioxy-2,6-diazaadamantane organic biradical. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 1064-1070.	1.0	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. <i>Fuel</i> , 2022, 311, 122595.	3.4	4
47	Prediction of Optimal Conditions of Hydrogenation Reaction Using the Likelihood Ranking Approach. <i>International Journal of Molecular Sciences</i> , 2022, 23, 248.	1.8	4
48	Prediction of Aromatic Hydroxylation Sites for Human CYP1A2 Substrates Using Condensed Graph of Reactions. <i>BioNanoScience</i> , 2018, 8, 384-389.	1.5	3
49	$\hat{\alpha}$ -synthon interaction as a reason for the strong amplification of synthon-forming hydrogen bonds. <i>CrystEngComm</i> , 2019, 21, 1499-1511.	1.3	3
50	CGRdb2.0: A Python Database Management System for Molecules, Reactions, and Chemical Data. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2015-2020.	2.5	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. <i>Fuel</i> , 2022, 312, 123002.	3.4	3
52	Dimethyl selenide complexes with compounds of Group IIIA elements: electron density redistribution and interaction energy partitioning. <i>Russian Chemical Bulletin</i> , 2014, 63, 43-53.	0.4	1
53	STRUCTURE-REACTIVITY RELATIONSHIP IN DIELS-ALDER REACTIONS OBTAINED USING THE CONDENSED REACTION GRAPH APPROACH. <i>Journal of Structural Chemistry</i> , 2017, , .	0.0	1
54	Exchange interaction mechanisms in 1,3,5,7-tetramethyl-2,6-diazaadamantane N,N $\hat{\alpha}$ -dioxyl biradical. <i>Russian Chemical Bulletin</i> , 2017, 66, 2028-2034.	0.4	0

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55	Effect of core substituents on the intramolecular exchange interaction in <i>N,N</i> -dioxo-2,6-diazaadamantane biradical: DFT studies. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25568.	1.0	0
56	Multi-instance Learning for Structure-Activity Modeling for Molecular Properties. <i>Communications in Computer and Information Science</i> , 2020, , 62-71.	0.4	0
57	Editorial: Chemical Reactions Mining. <i>Molecular Informatics</i> , 2022, 41, .	1.4	0
58	A new algorithm to assess the risk of malignancy in premenopausal patients with pelvic mass. <i>Opuholi Zenskoj Reproktivnoj Sistemy</i> , 2022, 18, 76-86.	0.1	0