

Yurii S Moroz

List of Publications by Year in descending order

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72

papers

3,623

citations

257101

24

h-index

143772

57

g-index

81

all docs

81

docs citations

81

times ranked

3990

citing authors

#	ARTICLE	IF	CITATIONS
1	One-pot parallel synthesis of 1,3,5-trisubstituted 1,2,4-triazoles. <i>Molecular Diversity</i> , 2022, 26, 993-1004.	2.1	4
2	Synthon-based ligand discovery in virtual libraries of over 11 billion compounds. <i>Nature</i> , 2022, 601, 452-459.	13.7	153
3	A Close-up Look at the Chemical Space of Commercially Available Building Blocks for Medicinal Chemistry. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 2171-2185.	2.5	32
4	Drug building blocks and libraries at risk in Ukraine. <i>Science</i> , 2022, 376, 929-929.	6.0	1
5	The Ukrainian Factor in Early-Stage Drug Discovery in the Context of Russian Invasion: The Case of Enamine Ltd. <i>ACS Medicinal Chemistry Letters</i> , 2022, 13, 992-996.	1.3	1
6	Synthesis of Spirocyclic 1,2,4- and 1,3,5- Sultams by One-Pot Reductive Cyclization of Cyanoalkylsulfonyl Fluorides. <i>European Journal of Organic Chemistry</i> , 2021, 2021, 6530-6540.	1.2	7
7	A multi-pronged approach targeting SARS-CoV-2 proteins using ultra-large virtual screening. <i>IScience</i> , 2021, 24, 102021.	1.9	66
8	Synthesis of 1-substituted 2-(1H-1,2,4-triazol-3-yl)acetates and 5-amino-2,4-dihydro-3H-pyrazol-3-ones via the Pinner strategy. <i>Tetrahedron Letters</i> , 2021, 69, 152956.	0.7	6
9	Structures of the 5-HT ₂ receptor enable docking for bioactive ligand discovery. <i>Nature</i> , 2021, 600, 759-764.	13.7	113
10	The iterative application of a large chemical space in the drug discovery process. <i>Journal of Organic and Pharmaceutical Chemistry</i> , 2021, 19, 3-11.	0.0	2
11	SAVI, in silico generation of billions of easily synthesizable compounds through expert-system type rules. <i>Scientific Data</i> , 2020, 7, 384.	2.4	34
12	ZINC20 – A Free Ultralarge-Scale Chemical Database for Ligand Discovery. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 6065-6073.	2.5	321
13	Generating Multibillion Chemical Space of Readily Accessible Screening Compounds. <i>IScience</i> , 2020, 23, 101681.	1.9	90
14	Virtual discovery of melatonin receptor ligands to modulate circadian rhythms. <i>Nature</i> , 2020, 579, 609-614.	13.7	184
15	An open-source drug discovery platform enables ultra-large virtual screens. <i>Nature</i> , 2020, 580, 663-668.	13.7	345
16	Synthesis of 5-(Fluoroalkyl)isoxazole Building Blocks by Regioselective Reactions of Functionalized Halogenoximes. <i>Journal of Organic Chemistry</i> , 2019, 84, 15877-15899.	1.7	26
17	Regioselective Synthesis of Functionalized 3- or 5-Fluoroalkyl Isoxazoles and Pyrazoles from Fluoroalkyl Ynones and Binucleophiles. <i>Journal of Organic Chemistry</i> , 2019, 84, 15212-15225.	1.7	22
18	SAR by Space: Enriching Hit Sets from the Chemical Space. <i>Molecules</i> , 2019, 24, 3096.	1.7	24

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19	One-Pot Parallel Synthesis of 5-(Dialkylamino)tetrazoles. ACS Combinatorial Science, 2019, 21, 635-642.	3.8	6
20	Kemp Eliminases of the AlleyCat Family Possess High Substrate Promiscuity. ChemCatChem, 2019, 11, 1377-1377.	1.8	0
21	Ultra-large library docking for discovering new chemotypes. Nature, 2019, 566, 224-229.	13.7	595
22	Kemp Eliminases of the AlleyCat Family Possess High Substrate Promiscuity. ChemCatChem, 2019, 11, 1425-1430.	1.8	3
23	Pros and cons of virtual screening based on public "Big Data": In silico mining for new bromodomain inhibitors. European Journal of Medicinal Chemistry, 2019, 165, 258-272.	2.6	12
24	Evolution of commercially available compounds for HTS. Drug Discovery Today, 2019, 24, 390-402.	3.2	53
25	Saturated Heterocyclic Aminosulfonyl Fluorides: New Scaffolds for Protecting "Group-Free Synthesis of Sulfonamides. Chemistry - A European Journal, 2018, 24, 8343-8349.	1.7	19
26	An Old Story in the Parallel Synthesis World: An Approach to Hydantoin Libraries. ACS Combinatorial Science, 2018, 20, 35-43.	3.8	16
27	Copper-Containing Catalytic Amyloids Promote Phosphoester Hydrolysis and Tandem Reactions. ACS Catalysis, 2018, 8, 59-62.	5.5	81
28	(Chlorosulfonyl)benzenesulfonyl Fluorides "Versatile Building Blocks for Combinatorial Chemistry: Design, Synthesis and Evaluation of a Covalent Inhibitor Library. ACS Combinatorial Science, 2018, 20, 672-680.	3.8	12
29	Straightforward hit identification approach in fragment-based discovery of bromodomain-containing protein 4 (BRD4) inhibitors. Bioorganic and Medicinal Chemistry, 2018, 26, 3399-3405.	1.4	16
30	The correction of the metabolic parameters of msg-induced obesity in rats by 2-[4-(benzyloxy) phenoxy] acetic acid. Journal of Nutrition & Intermediary Metabolism, 2018, 13, 1-9.	1.7	3
31	Facile One-Pot Parallel Synthesis of 3-Amino-1,2,4-triazoles. ACS Combinatorial Science, 2018, 20, 461-466.	3.8	13
32	Wpływ Z56822977 na biosyntezę serotonininy w mózgu szczurów z otępieniem... wywołaną przez podawanie glutaminianu sodu. Endokrynologia Polska, 2018, 69, 536-544.	0.3	0
33	Expanding Synthesizable Space of Disubstituted 1,2,4-Oxadiazoles. ACS Combinatorial Science, 2016, 18, 616-624.	3.8	25
34	2,2,2-Trifluoroethyl Oxalates in the One-Pot Parallel Synthesis of Hindered Aliphatic Oxamides. European Journal of Organic Chemistry, 2016, 2016, 2120-2130.	1.2	5
35	Î²-(1-Azulenyl)-L-alanine "a functional probe for determination of pK _a of histidine residues. Chemical Communications, 2015, 51, 5347-5350.	2.2	28
36	New Tricks for Old Proteins: Single Mutations in a Nonenzymatic Protein Give Rise to Various Enzymatic Activities. Journal of the American Chemical Society, 2015, 137, 14905-14911.	6.6	68

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37	Design of an allosterically regulated retroaldolase. <i>Protein Science</i> , 2015, 24, 561-570.	3.1	17
38	Functional characterization of a melittin analog containing a non-natural tryptophan analog. <i>Biopolymers</i> , 2015, 104, 384-394.	1.2	24
39	One-Pot Parallel Synthesis of Alkyl Sulfides, Sulfoxides, and Sulfones. <i>ACS Combinatorial Science</i> , 2015, 17, 348-354.	3.8	22
40	2,2,2-Trifluoroethyl Chlorooxoacetate—Universal Reagent for One-Pot Parallel Synthesis of N1-Aryl-N2-alkyl-Substituted Oxamides. <i>ACS Combinatorial Science</i> , 2015, 17, 615-622.	3.8	8
41	Facile one-pot synthesis of 4-substituted semicarbazides. <i>RSC Advances</i> , 2015, 5, 1063-1069.	1.7	9
42	2D IR spectroscopy reveals the role of water in the binding of channel-blocking drugs to the influenza M2 channel. <i>Journal of Chemical Physics</i> , 2014, 140, 235105.	1.2	23
43	One-Pot Parallel Synthesis Approach to Secondary Amines Based on the Reductive Amination of Ketones. <i>Synthesis</i> , 2014, 46, 1765-1772.	1.2	7
44	Short peptides self-assemble to produce catalytic amyloids. <i>Nature Chemistry</i> , 2014, 6, 303-309.	6.6	510
45	Sulfonyl Fluorides as Alternative to Sulfonyl Chlorides in Parallel Synthesis of Aliphatic Sulfonamides. <i>ACS Combinatorial Science</i> , 2014, 16, 192-197.	3.8	58
46	H ₂ O ₂ activation with biomimetic non-haem iron complexes and AcOH: connecting the g = 2.7 EPR signal with a visible chromophore. <i>Chemical Communications</i> , 2014, 50, 645-648.	2.2	51
47	Enzyme-Catalyzed Kinetic Resolution of 2,2,2-Trifluoro-1-(heteroaryl)ethanols: Experimental and Docking Studies. <i>European Journal of Organic Chemistry</i> , 2014, 2014, 7692-7698.	1.2	8
48	A One-Pot Parallel Reductive Amination of Aldehydes with Heteroaromatic Amines. <i>ACS Combinatorial Science</i> , 2014, 16, 375-380.	3.8	16
49	Bis(2,2,2-trifluoroethyl) Carbonate as a Condensing Agent in One-Pot Parallel Synthesis of Unsymmetrical Aliphatic Ureas. <i>ACS Combinatorial Science</i> , 2014, 16, 303-308.	3.8	20
50	Painting proteins blue: Î ² -(1-azulenyl)-l-alanine as a probe for studying protein-protein interactions. <i>Chemical Communications</i> , 2013, 49, 490-492.	2.2	47
51	Reprogramming EF-hands for design of catalytically amplified lanthanide sensors. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 411-418.	1.1	12
52	A Single Mutation in a Regulatory Protein Produces Evolvable Allosterically Regulated Catalyst of Nonnatural Reaction. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 6246-6249.	7.2	30
53	Novel pyrazolate-based copper(II) [2D—2] grid complexes: Synthesis, structure and properties. <i>Inorganica Chimica Acta</i> , 2012, 392, 322-330.	1.2	14
54	Isolated Toll-like Receptor Transmembrane Domains Are Capable of Oligomerization. <i>PLoS ONE</i> , 2012, 7, e48875.	1.1	66

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55	Zinc(II) Complexes with Asymmetric 3,5-Substituted 1 <i>H</i> -Pyrazoles. <i>European Journal of Inorganic Chemistry</i> , 2012, 2012, 1639-1649.	1.0	7
56	Regular High-Nuclearity Species from Square Building Blocks: A Triangular 3 Å— [2 Å— 2] Ni ₁₂ Complex Generated by the Self-assembly of Three [2 Å— 2] Ni ₄ Molecular Grids. <i>Inorganic Chemistry</i> , 2012, 51, 7445-7447.	1.9	56
57	Synthesis of cobalt(III) complexes with new oxime-containing Schiff base ligands and metal–ligand coordination in solution. <i>Polyhedron</i> , 2012, 33, 410-416.	1.0	18
58	Facile synthesis of Cu(II) complexes of mono- and bicondensed N donor Schiff base 1 <i>H</i> -pyrazolate ligands: Crystal structures, spectroscopic and magnetic properties. <i>Polyhedron</i> , 2012, 37, 77-84.	1.0	12
59	Bis(½-2,2,4,6-trimethylbenzonitrile)bis[(N-isopropyl-3,5-dimethylanilido)molybdenum(III)](Mo–Mo). <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, m1643-m1644.	0.2	0
60	N–(2-Hydroxybenzylidene)-2-(hydroxyimino)propanohydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o3282-o3283.	0.2	2
61	Tris{2-[(2,6-dimethylphenyl)amino]ethyl}amine. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o3421-o3421.	0.2	2
62	catena-Poly[[[aquacopper(II)]bis(¼-bis(3,5-dimethyl-1 <i>H</i> -pyrazol-4-yl) selenide)] bis(tetrafluoroborate) bis(triphenylphosphine oxide) monohydrate]. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, m527-m527.	0.2	2
63	One-Pot Synthesis of a New Magnetically Coupled Heterometallic Cu ₂ Mn ₂ [2 Å— 2] Molecular Grid. <i>Inorganic Chemistry</i> , 2010, 49, 4750-4752.	1.9	47
64	Bis{2-hydroxyimino-N–[1-(2-pyridyl)ethylidene]propanohydrazidato}zinc(II) dihydrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, m242-m243.	0.2	1
65	catena-Poly[[[aquacopper(II)]-bis(¼-bis(3,5-dimethyl-1 <i>H</i> -pyrazol-4-yl) selenide-2N2:N2)] dichloride monohydrate]. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, m363-m363.	0.2	3
66	New copper(II) 1D polymer containing dimethyl(phenylsulfonyl)amidophosphate: Synthesis, crystal structure and magnetic properties. <i>Polyhedron</i> , 2009, 28, 1331-1335.	1.0	22
67	2-Hydroxyimino-N–[1-(2-pyridyl)ethylidene]propanohydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2009, 65, o2242-o2242.	0.2	4
68	(2 <i>E</i>)-2-Hydroxyimino-N–[1-(2-pyridyl)ethylidene]propanohydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2009, 65, o2413-o2413.	0.2	8
69	A square-planar Ni ^{II} complex with an asymmetric coordination of a novel polynucleative 2,6-diacetylpyridine bis{[2-(hydroxyimino)propanoyl]hydrazone} ligand. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2008, 64, m137-m139.	0.4	4
70	Synthesis and Structure of [2 Å— 2] Molecular Grid Copper(II) and Nickel(II) Complexes with a New Polydentate Oxime-Containing Schiff Base Ligand. <i>Inorganic Chemistry</i> , 2008, 47, 5656-5665.	1.9	70
71	Dichlorido{2-hydroxyimino-N–[1-(2-pyridyl)ethylidene]propanohydrazide-½ ³ N ₃ , N ₃ , Q}zinc(II) hemihydrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2008, 64, m353-m354.	0.2	9
72	Bis(ethylenediaminium) bis[oxalohydroxamato(3–)]nickelate(II) dihydrate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, m498-m500.	0.4	3