Bogdan I Iorga

List of Publications by Year in descending order

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121 papers	3,027 citations	201385 27 h-index	214527 47 g-index
140 all docs	140 docs citations	140 times ranked	3943 citing authors

#	Article	IF	Citations
1	Optimization of the rapid carbapenem inactivation method for use with AmpC hyperproducersâ€"authorsâ€™ response. Journal of Antimicrobial Chemotherapy, 2022, 77, 1210-1211.	1.3	0
2	Class C Î²-Lactamases: Molecular Characteristics. Clinical Microbiology Reviews, 2022, 35, e0015021.	5.7	15
3	Carbapenemase -producing Pseudomonas aeruginosa isolates from Turkey: first report of P. aeruginosa high-risk clones with VIM-5â€" and IMP-7â€"type carbapenemases in a tertiary hospital. Diagnostic Microbiology and Infectious Disease, 2021, 99, 115174.	0.8	14
4	From Synthetic Simplified Marine Metabolite Analogues to New Selective Allosteric Inhibitor of Aurora B Kinase. Journal of Medicinal Chemistry, 2021, 64, 1197-1219.	2.9	8
5	Baseâ€Mediated Generation of Ketenimines from Ynamides: [3+2] Annulation with Azaallyl Anions. Advanced Synthesis and Catalysis, 2021, 363, 2903-2908.	2.1	6
6	Biochemical characterization of OXA-244, an emerging OXA-48 variant with reduced Î²-lactam hydrolytic activity. Journal of Antimicrobial Chemotherapy, 2021, 76, 2024-2028.	1.3	6
7	Optimization of the rapid carbapenem inactivation method for use with AmpC hyperproducers. Journal of Antimicrobial Chemotherapy, 2021, 76, 2294-2301.	1.3	9
8	Precise force-field-based calculations of octanol-water partition coefficients for the SAMPL7 molecules. Journal of Computer-Aided Molecular Design, 2021, 35, 853-870.	1.3	5
9	Azetidinimines as a novel series of non-covalent broad-spectrum inhibitors of Î²-lactamases with submicromolar activities against carbapenemases KPC-2 (class A), NDM-1 (class B) and OXA-48 (class D). European Journal of Medicinal Chemistry, 2021, 219, 113418.	2.6	14
10	Disorder is a critical component of lipoprotein sorting in Gram-negative bacteria. Nature Chemical Biology, 2021, 17, 1093-1100.	3.9	13
11	Detection and Characterization of VIM-52, a New Variant of VIM-1 from a Klebsiella pneumoniae Clinical Isolate. Antimicrobial Agents and Chemotherapy, 2021, 65, e0266020.	1.4	2
12	KPC-39-Mediated Resistance to Ceftazidime-Avibactam in a Klebsiella pneumoniae ST307 Clinical Isolate. Antimicrobial Agents and Chemotherapy, 2021, 65, e0116021.	1.4	14
13	Evaluation of borinic acids as new, fast hydrogen peroxideâ€"responsive triggers. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	14
14	Different phenotypic expression of KPC Î²-lactamase variants and challenges in their detection. Journal of Antimicrobial Chemotherapy, 2020, 75, 769-771.	1.3	16
15	LMB-1 producing Citrobacter freundii from Argentina, a novel player in the field of MBLs. International Journal of Antimicrobial Agents, 2020, 55, 105857.	1.1	14
16	Biochemical and Structural Characterization of OXA-405, an OXA-48 Variant with Extended-Spectrum Î²-Lactamase Activity. Microorganisms, 2020, 8, 24.	1.6	12
17	Pyridinium derivatives of 3-aminobenzenesulfonamide are nanomolar-potent inhibitors of tumor-expressed carbonic anhydrase isozymes CA IX and CA XII. Bioorganic Chemistry, 2020, 103, 104204.	2.0	24
18	NMR Characterization of the Influence of Zinc(II) Ions on the Structural and Dynamic Behavior of the New Delhi Metallo-Î²-Lactamase-1 and on the Binding with Flavonols as Inhibitors. ACS Omega, 2020, 5, 10466-10480.	1.6	19

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19	Role of Arginine 214 in the Substrate Specificity of OXA-48. Antimicrobial Agents and Chemotherapy, 2020, 64, .	1.4	17
20	How the assembly and protection of the bacterial cell envelope depend on cysteine residues. Journal of Biological Chemistry, 2020, 295, 11984-11994.	1.6	29
21	Structural insight into the formation of lipoprotein-Î²-barrel complexes. Nature Chemical Biology, 2020, 16, 1019-1025.	3.9	34
22	Discovery of simplified benzazole fragments derived from the marine benzosceptrin B as necroptosis inhibitors involving the receptor interacting protein Kinase-1. European Journal of Medicinal Chemistry, 2020, 201, 112337.	2.6	9
23	Substrate Specificity of OXA-48 after Î²5â^'Î²6 Loop Replacement. ACS Infectious Diseases, 2020, 6, 1032-1043.	1.8	10
24	Mutational analysis of the Qi-site proton pathway in yeast cytochrome bc1 complex. Biochemical and Biophysical Research Communications, 2020, 523, 615-619.	1.0	2
25	Prediction of octanol-water partition coefficients for the SAMPL6-$$log P$$ molecules using molecular dynamics simulations with OPLS-AA, AMBER and CHARMM force fields. Journal of Computer-Aided Molecular Design, 2020, 34, 543-560.	1.3	30
26	Defining the function of OmpA in the Rcs stress response. ELife, 2020, 9, .	2.8	23
27	Performance evaluation of molecular docking and free energy calculations protocols using the D3R Grand Challenge 4 dataset. Journal of Computer-Aided Molecular Design, 2019, 33, 1031-1043.	1.3	12
28	Synthetic Pinnatoxins A and G Reversibly Block Mouse Skeletal Neuromuscular Transmission In Vivo and In Vitro. Marine Drugs, 2019, 17, 306.	2.2	10
29	Unravelling ceftazidime/avibactam resistance of KPC-28, a KPC-2 variant lacking carbapenemase activity. Journal of Antimicrobial Chemotherapy, 2019, 74, 2239-2246.	1.3	48
30	Genetic, Biochemical, and Structural Characterization of CMY-136 Î²-Lactamase, a Peculiar CMY-2 Variant. ACS Infectious Diseases, 2019, 5, 528-538.	1.8	5
31	Deleting a Chromatin Remodeling Gene Increases the Diversity of Secondary Metabolites Produced by Colletotrichum higginsianum. Journal of Natural Products, 2019, 82, 813-822.	1.5	17
32	Blinded evaluation of cathepsin S inhibitors from the D3RGC3 dataset using molecular docking and free energy calculations. Journal of Computer-Aided Molecular Design, 2019, 33, 93-103.	1.3	9
33	Mitochondrial complex III Q_iâ€site inhibitor resistance mutations found in laboratory selected mutants and field isolates. Pest Management Science, 2019, 75, 2107-2114.	1.7	23
34	The antimalarial compound <scp>ELQ</scp>â€400 is an unusual inhibitor of the bc₁ complex, targeting both Q_o and Q_i sites. FEBS Letters, 2018, 592, 1346-1356.	1.3	30
35	Blinded evaluation of farnesoid X receptor (FXR) ligands binding using molecular docking and free energy calculations. Journal of Computer-Aided Molecular Design, 2018, 32, 273-286.	1.3	11
36	mTOR Inhibition via Displacement of Phosphatidic Acid Induces Enhanced Cytotoxicity Specifically in Cancer Cells. Cancer Research, 2018, 78, 5384-5397.	0.4	14

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37	Prorocentrolide-A from Cultured Prorocentrum lima Dinoflagellates Collected in Japan Blocks Sub-Types of Nicotinic Acetylcholine Receptors. Toxins, 2018, 10, 97.	1.5	18
38	Genetic and Biochemical Characterization of OXA-535, a Distantly Related OXA-48-Like Î²-Lactamase. Antimicrobial Agents and Chemotherapy, 2018, 62, .	1.4	10
39	SAMPL6: calculation of macroscopic pKa values from ab initio quantum mechanical free energies. Journal of Computer-Aided Molecular Design, 2018, 32, 1203-1216.	1.3	21
40	Genetic and Biochemical Characterization of OXA-519, a Novel OXA-48-Like Î²-Lactamase. Antimicrobial Agents and Chemotherapy, 2018, 62, .	1.4	20
41	Characterization of BRP _{MBL} , the Bleomycin Resistance Protein Associated with the Carbapenemase NDM. Antimicrobial Agents and Chemotherapy, 2017, 61, .	1.4	22
42	Stereoselective Synthesis of 1,2â€transâ€Diamines Using the Threeâ€Component Boronoâ€Mannich Condensation â€“ Reaction Scope and Mechanistic Insights. European Journal of Organic Chemistry, 2017, 2017, 1940-1951.	1.2	9
43	Selective trihydroxylated azepane inhibitors of NagZ, a glycosidase involved in Pseudomonas aeruginosa resistance to Î²-lactam antibiotics. Organic and Biomolecular Chemistry, 2017, 15, 4609-4619.	1.5	12
44	Cyclic imine toxins from dinoflagellates: a growing family of potent antagonists of the nicotinic acetylcholine receptors. Journal of Neurochemistry, 2017, 142, 41-51.	2.1	59
45	Beta-lactamase database (BLDB) â€“ structure and function. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 917-919.	2.5	405
46	In Silico Self-Assembly of Nanoparticles with Applications in Drug Delivery. ACS Symposium Series, 2017, , 95-113.	0.5	0
47	(+)- and (â^')-Ecarlottones, Uncommon Chalconoids from Fissistigma latifolium with Pro-Apoptotic Activity. Journal of Natural Products, 2017, 80, 3179-3185.	1.5	13
48	Ligandbook: an online repository for small and drug-like molecule force field parameters. Bioinformatics, 2017, 33, 1747-1749.	1.8	17
49	Structural and Functional Aspects of Class A Carbapenemases. Current Drug Targets, 2016, 17, 1006-1028.	1.0	115
50	The Dinoflagellate Toxin 20-Methyl Spirolide-G Potently Blocks Skeletal Muscle and Neuronal Nicotinic Acetylcholine Receptors. Toxins, 2016, 8, 249.	1.5	16
51	Spirolides and Cyclic Imines: Toxicological Profile. , 2016, , 193-217.		2
52	Selectivity of Spiroimine Phycotoxins Toward Nicotinic Acetylcholine Receptors. Biophysical Journal, 2016, 110, 603a.	0.2	0
53	Molecular docking performance evaluated on the D3R Grand Challenge 2015 drug-like ligand datasets. Journal of Computer-Aided Molecular Design, 2016, 30, 829-839.	1.3	14
54	Prediction of cyclohexane-water distribution coefficients for the SAMPL5 data set using molecular dynamics simulations with the OPLS-AA force field. Journal of Computer-Aided Molecular Design, 2016, 30, 1045-1058.	1.3	19

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55	Euphorbia dendroides Latex as a Source of Jatrophane Esters: Isolation, Structural Analysis, Conformational Study, and Anti-CHIKV Activity. Journal of Natural Products, 2016, 79, 2873-2882.	1.5	52
56	Blind Pose Prediction, Scoring, and Affinity Ranking of the CSAR 2014 Dataset. Journal of Chemical Information and Modeling, 2016, 56, 996-1003.	2.5	13
57	Saccharomyces cerevisiae-Based Mutational Analysis of the bc ₁ Complex Q _o Site Residue 279 To Study the Trade-Off between Atovaquone Resistance and Function. Antimicrobial Agents and Chemotherapy, 2015, 59, 4053-4058.	1.4	12
58	The unexpected increase of clotrimazole apparent solubility using randomly methylated Î²â€cyclodextrin. Journal of Molecular Recognition, 2015, 28, 96-102.	1.1	13
59	Advanced Structural Determination of Diterpene Esters Using Molecular Modeling and NMR Spectroscopy. Journal of Natural Products, 2015, 78, 2423-2431.	1.5	24
60	Interplay between the hinge region of iron sulphur protein and the Qo site in the bc1 complex â€" Analysis of Plasmodium-like mutations in the yeast enzyme. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 1487-1494.	0.5	5
61	Regio-, Diastereo-, and Enantioselective Nitroso-Dielsâ€"Alder Reaction of 1,3-Diene-1-carbamates Catalyzed by Chiral Phosphoric Acids. Journal of the American Chemical Society, 2015, 137, 11950-11953.	6.6	79
62	The Neurotoxic Effect of 13,19-Didesmethyl and 13-Desmethyl Spirolide C Phycotoxins Is Mainly Mediated by Nicotinic Rather Than Muscarinic Acetylcholine Receptors. Toxicological Sciences, 2015, 147, 156-167.	1.4	28
63	Spirolides and Cyclic Imines: Toxicological Profile. , 2015, , 1-19.		3
64	Prediction of hydration free energies for the SAMPL4 diverse set of compounds using molecular dynamics simulations with the OPLS-AA force field. Journal of Computer-Aided Molecular Design, 2014, 28, 265-276.	1.3	37
65	Virtual screening of the SAMPL4 blinded HIV integrase inhibitors dataset. Journal of Computer-Aided Molecular Design, 2014, 28, 455-462.	1.3	13
66	Bicyclic and tetracyclic diterpenes from a Trichoderma symbiont of Taxus baccata. Phytochemistry, 2014, 97, 55-61.	1.4	54
67	From meiogynin A to the synthesis of dual inhibitors of Bcl-xL and Mcl-1 anti-apoptotic proteins. Chemical Communications, 2014, 50, 8593.	2.2	27
68	Pro-apoptotic meiogynin A derivatives that target Bcl-xL and Mcl-1. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 5086-5088.	1.0	9
69	From Enantiopure Hydroxyaldehydes to Complex Heterocyclic Scaffolds: Development of Domino Petasis/Dielsâ€"Alder and Crossâ€Metathesis/Michael Addition Reactions. Chemistry - A European Journal, 2014, 20, 12133-12143.	1.7	22
70	0310 Assay development and high-throughput screening to identify PDE2A activators to treat heart failure. Archives of Cardiovascular Diseases Supplements, 2014, 6, 43.	0.0	0
71	Investigation of the complexation of albendazole with cyclodextrins for the design of new antiparasitic formulations. Carbohydrate Research, 2014, 398, 50-55.	1.1	29
72	Acridone Alkaloids from Glycosmis chlorosperma as DYRK1A Inhibitors. Journal of Natural Products, 2014, 77, 1117-1122.	1.5	51

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73	Poly(Î³-benzyl-l-glutamate)-PEG-alendronate multivalent nanoparticles for bone targeting. International Journal of Pharmaceutics, 2014, 460, 73-82.	2.6	37
74	Calcium Channels for Exocytosis and Endocytosis: Pharmacological Modulation. , 2014, , 1091-1138.		3
75	Cyclic Imine Toxins: Chemistry, Origin, Metabolism, Pharmacology, Toxicology, and Detection. , 2014, , 951-990.		15
76	Molecular Mechanisms of Maitotoxin Action. , 2014, , 77-101.		1
77	Physical and virtual screening methods for marine toxins and drug discovery targeting nicotinic acetylcholine receptors. Expert Opinion on Drug Discovery, 2013, 8, 1203-1223.	2.5	13
78	Carbonic anhydrase binding site parameterization in OPLS-AA force field. Bioorganic and Medicinal Chemistry, 2013, 21, 1427-1430.	1.4	7
79	Isolation and Characterization of Unusual Hydrazides from Streptomyces sp. Impact of the Cultivation Support and Extraction Procedure. Journal of Natural Products, 2013, 76, 142-149.	1.5	29
80	Fast Synthesis of Complex Enantiopure Heterocyclic Scaffolds by a Tandem Sequence of Simple Transformations on Î±â€Hydroxyaldehydes. Chemistry - A European Journal, 2013, 19, 9127-9131.	1.7	25
81	Plasma distribution of tetraphenylporphyrin derivatives relevant for Photodynamic Therapy: Importance and limits of hydrophobicity. European Journal of Pharmaceutics and Biopharmaceutics, 2013, 83, 244-252.	2.0	19
82	Stability of Cyclic Imine Toxins: Interconversion of Pinnatoxin Amino Ketone and Pinnatoxin A in Aqueous Media. Journal of Organic Chemistry, 2012, 77, 10435-10440.	1.7	27
83	Cyanomethylene-bis(phosphonate) as ditopical ligand: stepwise formation of a 2-D heterometallic Fe(iii)â€“Ag(i) coordination network. CrystEngComm, 2012, 14, 3096.	1.3	7
84	Conformational Study of Glycal-Type Neuraminidase Inhibitors. Journal of Carbohydrate Chemistry, 2012, 31, 114-129.	0.4	1
85	Synthesis, Biological Evaluation, and Molecular Modeling of Natural and Unnatural Flavonoidal Alkaloids, Inhibitors of Kinases. Journal of Medicinal Chemistry, 2012, 55, 2811-2819.	2.9	36
86	Ionontropic Glutamate Receptors: Insight into the Mechanism of Desensitization and Deactivation using Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 114a.	0.2	0
87	Evaluation of docking performance in a blinded virtual screening of fragment-like trypsin inhibitors. Journal of Computer-Aided Molecular Design, 2012, 26, 595-601.	1.3	16
88	Prediction of hydration free energies for aliphatic and aromatic chloro derivatives using molecular dynamics simulations with the OPLS-AA force field. Journal of Computer-Aided Molecular Design, 2012, 26, 635-645.	1.3	23
89	Pharmacomodulation of Meiogynin A, a dimeric sesquiterpenoid inhibiting BCL-XL and BAK interaction. Planta Medica, 2012, 78, .	0.7	0
90	Rigid Analogues of Antimitotic Indolobenzazepinones: New Insights into Tubulin Binding via Molecular Modeling. ACS Medicinal Chemistry Letters, 2011, 2, 565-570.	1.3	18

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91	Spiroimine Toxins in Complex with Nicotinic Acetylcholine Receptors: Structure and Dynamics. Biophysical Journal, 2011, 100, 347a.	0.2	0
92	Benzofurans from Styrax agrestis As Acetylcholinesterase Inhibitors: Structureâ€“Activity Relationships and Molecular Modeling Studies. Journal of Natural Products, 2011, 74, 2081-2088.	1.5	30
93	Total Synthesis of Pinnatoxins A and G and Revision of the Mode of Action of Pinnatoxin A. Journal of the American Chemical Society, 2011, 133, 10499-10511.	6.6	122
94	Bivalent sequential binding of docetaxel to methyl-Î²-cyclodextrin. International Journal of Pharmaceutics, 2011, 416, 171-180.	2.6	44
95	New potent human acetylcholinesterase inhibitors in the tetracyclic triterpene series with inhibitory potency on amyloid Î² aggregation. European Journal of Medicinal Chemistry, 2011, 46, 2193-2205.	2.6	36
96	NADH oxidase activity of Bacillus subtilis nitroreductase NfrA1: Insight into its biological role. FEBS Letters, 2010, 584, 3916-3922.	1.3	22
97	Design, synthesis and In Vitro evaluation on glucosamine-6P synthase of aromatic analogs of 2-Aminohexitols-6P. Journal of the Brazilian Chemical Society, 2010, 21, 680-685.	0.6	6
98	Computational Approaches to Ionotropic Glutamate Receptors. RSC Biomolecular Sciences, 2010, , 203-224.	0.4	0
99	Diastereoselective Total Synthesis of (Â±)â€Codeine. Chemistry - A European Journal, 2008, 14, 6606-6608.	1.7	45
100	A New Access to Dihydrotropones through Ring Expansion of Spirocyclohexadienones:Â Synthesis and Mechanismâ€. Journal of Organic Chemistry, 2007, 72, 6421-6426.	1.7	12
101	Acetylcholine nicotinic receptors: finding the putative binding site of allosteric modulators using the â€œblind dockingâ€•approach. Journal of Molecular Modeling, 2006, 12, 366-372.	0.8	78
102	One or More C:C Bond(s) Formed by Condensation of P, As, Sb, Bi, Si, Ge, B, or Metal Functions. ChemInform, 2005, 36, no.	0.1	0
103	One or More CC Bond(s) Formed by Condensation: Condensation of P, As, Sb, Bi, Si, Ge, B, or Metal Functions. , 2005, , 723-759.		1
104	Ethyl Propiolate: A Simple and Convenient Peptide Coupling Reagent. Synlett, 2004, 2004, 1826-1828.	1.0	0
105	Controlled monohalogenation of phosphonates. Journal of Organometallic Chemistry, 2001, 624, 203-207.	0.8	10
106	Controlled Reactivity of Phosphonates by Temporary Silicon Connection. Synlett, 2001, 2001, 0447-0457.	1.0	10
107	Dialkyl 1-Alkynylphosphonates: a Range of Promising Reagents. European Journal of Organic Chemistry, 2000, 2000, 3103-3115.	1.2	64
108	Phosphonateâ€“phosphonochloridate conversion. Comptes Rendus De L'Academie Des Sciences - Series IIc: Chemistry, 2000, 3, 821-829.	0.1	7

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109	The Usefulness of Phosphorus Compounds in Alkyne Synthesis. Synthesis, 2000, 2000, 185-213.	1.2	74
110	Controlled Monohalogenation of Phosphonates, Part II: Preparation of Pure Diethyl Î±-Monohalogenated Alkylphosphonates. Synthesis, 2000, 2000, 576-580.	1.2	22
111	Protease Inhibitors. Part 2. Weakly Basic Thrombin Inhibitors Incorporating Sulfonyl-Aminoguanidine Moieties as S1 Anchoring Groups: Synthesis and Structure-Activity Correlations. Journal of Enzyme Inhibition and Medicinal Chemistry, 2000, 15, 235-264.	0.5	5
112	Carbonic Anhydrase Activators: Synthesis of High Affinity Isozymes I, II and IV Activators, Derivatives of 4-(4-Tosylureido-Amino Acyl)Ethyl-1H-Imidazole (Histamine Derivatives). Journal of Enzyme Inhibition and Medicinal Chemistry, 2000, 15, 139-161.	0.5	30
113	Carbanionic displacement reactions at phosphorus. Part III. Cyanomethylphosphonate vs. cyanomethylenediphosphonate. Synthesis and solid-state structures. Journal of the Chemical Society, Perkin Transactions 1, 2000, , 3311-3316.	1.3	19
114	The Syntheses and Properties of 1,2-Epoxyalkylphosphonates. Synthesis, 1999, 1999, 207-224.	1.2	30
115	Controlled monohalogenation of phosphonates: A new route to pure Î±-monohalogenated diethyl benzylphosphonates. Tetrahedron, 1999, 55, 2671-2686.	1.0	48
116	Synthesis of phosphonates by nucleophilic substitution at phosphorus: The SNP(V) reaction. Tetrahedron, 1999, 55, 13109-13150.	1.0	71
117	Phosphorylated aldehydes: Preparations and synthetic uses. Tetrahedron, 1998, 54, 14637-14677.	1.0	48
118	An efficient synthesis of tetraethyl fluoromethylenediphosphonate and derivatives from diethyl dibromofluoromethylphosphonate. Tetrahedron Letters, 1998, 39, 4477-4480.	0.7	22
119	A highly selective synthesis of Î±-monofluoro- and Î±-monochloro- benzylphosphonates using electrophilic halogenation of benzylphosphonates carbanions. Tetrahedron Letters, 1998, 39, 3693-3696.	0.7	25
120	Carbonic anhydrase inhibitors â€" Part 53. Synthesis of substituted-pyridinium derivatives of aromatic sulfonamides: The first non-polymeric membrane-impermeable inhibitors with selectivity for isozyme IV. European Journal of Medicinal Chemistry, 1998, 33, 577-594.	2.6	74
121	Chiral Phosphoric Acidâ€"Catalyzed Enantioselective Formal [4+2] Cycloaddition between Dienecarbamates and 2â€"Benzothioazolimines. Advanced Synthesis and Catalysis, 0, , .	2.1	10