Mathy Mc Froeyen

List of Publications by Year
in descending order

139 papers	3,992 citations	117453 34 h-index	155451 55 g-index
153 all docs	153 docs citations	153 times ranked	5004 citing authors

#	Article	IF	Citations
1	Structural elucidation of SARS-CoV-2 vital proteins: Computational methods reveal potential drug candidates against main protease, Nsp12 polymerase and Nsp13 helicase. Journal of Pharmaceutical Analysis, 2020, 10, 320-328.	2.4	207
2	Mutations in the chikungunya virus non-structural proteins cause resistance to favipiravir (T-705), a broad-spectrum antiviral. Journal of Antimicrobial Chemotherapy, 2014, 69, 2770-2784.	1.3	187
3	Novel Inhibitors of Influenza Virus Fusion: Structure-Activity Relationship and Interaction with the Viral Hemagglutinin. Journal of Virology, 2010, 84, 4277-4288.	1.5	137
4	Cyclohexene Nucleic Acids (CeNA):Â Serum Stable Oligonucleotides that Activate RNase H and Increase Duplex Stability with Complementary RNA. Journal of the American Chemical Society, 2000, 122, 8595-8602.	6.6	129
5	Deoxythreosyl Phosphonate Nucleosides as Selective Anti-HIV Agents. Journal of the American Chemical Society, 2005, 127, 5056-5065.	6.6	114
6	Carbohydrate-binding Agents Cause Deletions of Highly Conserved Glycosylation Sites in HIV GP120. Journal of Biological Chemistry, 2005, 280, 41005-41014.	1.6	108
7	Molecular dynamics simulation of polarizable water by an extended Lagrangian method. Molecular Physics, 1992, 77, 239-255.	0.8	107
8	Pharmacoinformatics and molecular dynamics simulation studies reveal potential covalent and FDA-approved inhibitors of SARS-CoV-2 main protease 3CL^{pro}. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4936-4948.	2.0	103
9	Rational Design of 5â€˜-Thiourea-Substituted Î±-Thymidine Analogues as Thymidine Monophosphate Kinase Inhibitors Capable of Inhibiting Mycobacterial Growth. Journal of Medicinal Chemistry, 2007, 50, 5281-5292.	2.9	82
10	The Cyclohexene Ring System as a Furanose Mimic:â€‰ Synthesis and Antiviral Activity of Both Enantiomers of Cyclohexenylguanine. Journal of Medicinal Chemistry, 2000, 43, 736-745.	2.9	81
11	A Novel, Highly Selective Inhibitor of Pestivirus Replication That Targets the Viral RNA-Dependent RNA Polymerase. Journal of Virology, 2006, 80, 149-160.	1.5	78
12	A Derivate of the Antibiotic Doxorubicin Is a Selective Inhibitor of Dengue and Yellow Fever Virus Replication In Vitro. Antimicrobial Agents and Chemotherapy, 2010, 54, 5269-5280.	1.4	72
13	Discovery of human coronaviruses pan-papain-like protease inhibitors using computational approaches. Journal of Pharmaceutical Analysis, 2020, 10, 546-559.	2.4	67
14	Marked Depletion of Glycosylation Sites in HIV-1 gp120 under Selection Pressure by the Mannose-Specific Plant Lectins ofHippeastrumHybrid andGalanthus nivalis. Molecular Pharmacology, 2005, 67, 1556-1565.	1.0	62
15	Understanding the Mechanism of the Broad-Spectrum Antiviral Activity of Favipiravir (T-705): Key Role of the F1 Motif of the Viral Polymerase. Journal of Virology, 2017, 91, .	1.5	62
16	Investigation of the DNA-dependent cyclohexenyl nucleic acid polymerization and the cyclohexenyl nucleic acid-dependent DNA polymerization. Nucleic Acids Research, 2005, 33, 3828-3836.	6.5	60
17	The Capsid Binder Vapendavir and the Novel Protease Inhibitor SG85 Inhibit Enterovirus 71 Replication. Antimicrobial Agents and Chemotherapy, 2014, 58, 6990-6992.	1.4	60
18	Comparative Study of the Genetic Barriers and Pathways towards Resistance of Selective Inhibitors of Hepatitis C Virus Replication. Antimicrobial Agents and Chemotherapy, 2011, 55, 4103-4113.	1.4	54

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19	Antiviral Activity of Broad-Spectrum and Enterovirus-Specific Inhibitors against Clinical Isolates of Enterovirus D68. Antimicrobial Agents and Chemotherapy, 2015, 59, 7782-7785.	1.4	54
20	3â€˜-C-Branched-Chain-Substituted Nucleosides and Nucleotides as Potent Inhibitors of Mycobacterium tuberculosis Thymidine Monophosphate Kinase. Journal of Medicinal Chemistry, 2003, 46, 3811-3821.	2.9	53
21	Reverse transcriptase incorporation of 1,5-anhydrohexitol nucleotides. Nucleic Acids Research, 2001, 29, 3154-3163.	6.5	52
22	Polymerase-catalyzed synthesis of DNA from phosphoramidate conjugates of deoxynucleotides and amino acids. Nucleic Acids Research, 2007, 35, 5060-5072.	6.5	51
23	Difference in conformational diversity between nucleic acids with a six-membered 'sugar' unit and natural 'furanose' nucleic acids. Nucleic Acids Research, 2003, 31, 2975-2989.	6.5	48
24	Discovery of Bicyclic Thymidine Analogues as Selective and High-Affinity Inhibitors of Mycobacterium tuberculosis Thymidine Monophosphate Kinase. Journal of Medicinal Chemistry, 2004, 47, 6187-6194.	2.9	48
25	Helical Structure of Xylose-DNA. Journal of the American Chemical Society, 2010, 132, 587-595.	6.6	47
26	Structural Characterization and Biological Evaluation of Small Interfering RNAs Containing Cyclohexenyl Nucleosides. Journal of the American Chemical Society, 2007, 129, 9340-9348.	6.6	46
27	Binary Genetic Cassettes for Selecting XNAâ€Templated DNA Synthesis In Vivo. Angewandte Chemie - International Edition, 2013, 52, 8139-8143.	7.2	45
28	Synthesis and Structureâ€“Activity Relationships of 3,5-Disubstituted-pyrrolo[2,3-b]pyridines as Inhibitors of Adaptor-Associated Kinase 1 with Antiviral Activity. Journal of Medicinal Chemistry, 2019, 62, 5810-5831.	2.9	44
29	The Imidazopyrrolopyridine Analogue AG110 Is a Novel, Highly Selective Inhibitor of Pestiviruses That Targets the Viral RNA-Dependent RNA Polymerase at a Hot Spot for Inhibition of Viral Replication. Journal of Virology, 2007, 81, 11046-11053.	1.5	43
30	DNA Polymerase Mutations in Drug-Resistant Herpes Simplex Virus Mutants Determine In Vivo Neurovirulence and Drug-Enzyme Interactions. Antiviral Therapy, 2007, 12, 719-732.	0.6	42
31	Baseâ‹¯Base Interactions in the Minor Groove of Double-Stranded DNA. Journal of Organic Chemistry, 2006, 71, 5423-5431.	1.7	40
32	Exploring the conformational changes of the ATP binding site of gyrase B from Escherichia coli complexed with different established inhibitors by using molecular dynamics simulation. Journal of Molecular Graphics and Modelling, 2011, 29, 726-739.	1.3	40
33	Circular trimers of gelatinase B/matrix metalloproteinase-9 constitute a distinct population of functional enzyme molecules differentially regulated by tissue inhibitor of metalloproteinases-1. Biochemical Journal, 2015, 465, 259-270.	1.7	39
34	Synthesis and Biological Evaluation of Bicyclic Nucleosides as Inhibitors ofM.â€…tuberculosis Thymidylate Kinase. ChemMedChem, 2006, 1, 1081-1090.	1.6	35
35	Discovery of 7-N-Piperazinylthiazolo[5,4-d]pyrimidine Analogues as a Novel Class of Immunosuppressive Agents with in Vivo Biological Activity. Journal of Medicinal Chemistry, 2011, 54, 655-668.	2.9	35
36	Perspectives towards antiviral drug discovery against Ebola virus. Journal of Medical Virology, 2019, 91, 2029-2048.	2.5	35

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37	In Vitro Antidiabetic, Anti-Obesity and Antioxidant Analysis of Ocimum basilicum Aerial Biomass and in Silico Molecular Docking Simulations with Alpha-Amylase and Lipase Enzymes. Biology, 2019, 8, 92.	1.3	32
38	Computational alanine scanning and free energy decomposition for E. coli type I signal peptidase with lipopeptide inhibitor complex. Journal of Molecular Graphics and Modelling, 2008, 26, 813-823.	1.3	31
39	Identification of novel human USP2 inhibitor and its putative role in treatment of COVID-19 by inhibiting SARS-CoV-2 papain-like (PLpro) protease. Computational Biology and Chemistry, 2020, 89, 107376.	1.1	31
40	Quantification of Berberine in Berberis vulgaris L. Root Extract and Its Curative and Prophylactic Role in Cisplatin-Induced In Vivo Toxicity and In Vitro Cytotoxicity. Antioxidants, 2019, 8, 185.	2.2	29
41	Synthesis and Stability of Oligonucleotides Containing Acyclic Achiral Nucleoside Analogues with Two Base Moieties. Organic Letters, 2004, 6, 51-54.	2.4	28
42	Synthesis and inhibitory activity of thymidine analogues targeting Mycobacterium tuberculosis thymidine monophosphate kinase. Bioorganic and Medicinal Chemistry, 2011, 19, 7603-7611.	1.4	28
43	Discovery of an Acyclic Nucleoside Phosphonate that Inhibits Mycobacterium tuberculosis ThyX Based on the Binding Mode of a 5â€Alkynyl Substrate Analogue. ChemMedChem, 2013, 8, 1373-1383.	1.6	28
44	A novel benzonitrile analogue inhibits rhinovirus replication. Journal of Antimicrobial Chemotherapy, 2014, 69, 2723-2732.	1.3	27
45	Aminopurine and aminoquinazoline scaffolds for development of potential dengue virus inhibitors. European Journal of Medicinal Chemistry, 2017, 126, 101-109.	2.6	27
46	A pyrazolotriazolopyrimidinamine inhibitor of bovine viral diarrhea virus replication that targets the viral RNA-dependent RNA polymerase. Antiviral Research, 2009, 82, 141-147.	1.9	26
47	Role of the viral hemagglutinin in the anti-influenza virus activity of newly synthesized polycyclic amine compounds. Antiviral Research, 2013, 99, 281-291.	1.9	26
48	In silico structural elucidation of RNA-dependent RNA polymerase towards the identification of potential Crimean-Congo Hemorrhagic Fever Virus inhibitors. Scientific Reports, 2019, 9, 6809.	1.6	26
49	Inhibition of Oncogenic Kinases: An In Vitro Validated Computational Approach Identified Potential Multi-Target Anticancer Compounds. Biomolecules, 2019, 9, 124.	1.8	26
50	Comparison of the Complexation between Methylprednisolone and Different Cyclodextrins in Solution by 1H-NMR and Molecular Modeling Studies. Journal of Pharmaceutical Sciences, 2010, 99, 3863-3873.	1.6	25
51	Invading Escherichia coli Genetics with a Xenobiotic Nucleic Acid Carrying an Acyclic Phosphonate Backbone (ZNA). Journal of the American Chemical Society, 2019, 141, 10844-10851.	6.6	25
52	GA(M)E-QSAR: A Novel, Fully Automatic Genetic-Algorithm-(Meta)-Ensembles Approach for Binary Classification in Ligand-Based Drug Design. Journal of Chemical Information and Modeling, 2012, 52, 2366-2386.	2.5	23
53	Rational design of an XNA ligase through docking of unbound nucleic acids to toroidal proteins. Nucleic Acids Research, 2019, 47, 7130-7142.	6.5	23
54	Highly potent and selective inhibition of bovine viral diarrhea virus replication by Î³-carboline derivatives. Antiviral Research, 2010, 88, 263-268.	1.9	22

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55	Discovery of HIV entry inhibitors via a hybrid CXCR4 and CCR5 receptor pharmacophoreâ€based virtual screening approach. European Journal of Pharmaceutical Sciences, 2020, 155, 105537.	1.9	22
56	CYCLOHEXENE NUCLEIC ACIDS (CeNA) FORM STABLE DUPLEXES WITH RNA AND INDUCE RNASE H ACTIVITY. Nucleosides, Nucleotides and Nucleic Acids, 2001, 20, 785-788.	0.4	21
57	3-Phosphono-l-alanine as pyrophosphate mimic for DNA synthesis using HIV-1 reverse transcriptase. Organic and Biomolecular Chemistry, 2011, 9, 111-119.	1.5	21
58	Solution Structure and Conformational Dynamics of Deoxyxylonucleic Acids (dXNA): An Orthogonal Nucleic Acid Candidate. Chemistry - A European Journal, 2012, 18, 869-879.	1.7	21
59	1,2,4-Triazole Derivatives Inhibiting the Human Immunodeficiency Virus Type 1 (HIV-1) in vitro. Helvetica Chimica Acta, 2002, 85, 1883.	1.0	20
60	Iminodiacetic-phosphoramidates as metabolic prototypes for diversifying nucleic acid polymerization in vivo. Nucleic Acids Research, 2010, 38, 2541-2550.	6.5	20
61	A Synthetic Substrate of DNA Polymerase Deviating from the Bases, Sugar, and Leaving Group of Canonical Deoxynucleoside Triphosphates. Chemistry and Biology, 2013, 20, 416-423.	6.2	20
62	Substituted 2,6-bis(benzimidazol-2-yl)pyridines: A novel chemical class of pestivirus inhibitors that targets a hot spot for inhibition of pestivirus replication in the RNA-dependent RNA polymerase. Antiviral Research, 2014, 106, 71-79.	1.9	20
63	New naphthalene derivative for cost-effective AChE inhibitors for Alzheimerâ€™s treatment: In silico identification, in vitro and in vivo validation. Computational Biology and Chemistry, 2020, 89, 107378.	1.1	20
64	Î±-Homo-DNA and RNA Form a Parallel Oriented Non-A, Non-B-Type Double Helical Structure. Chemistry - A European Journal, 2001, 7, 5183-5194.	1.7	19
65	Correct Bond Order Assignment in a Molecular Framework Using Integer Linear Programming with Application to Molecules Where Only Non-Hydrogen Atom Coordinates Are Available. Journal of Chemical Information and Modeling, 2005, 45, 1267-1274.	2.5	19
66	Polymeraseâ€Catalysed Incorporation of Glucose Nucleotides into a DNA Duplex. Chemistry - A European Journal, 2009, 15, 5463-5470.	1.7	19
67	Insight into ligand selectivity in HCV NS5B polymerase: molecular dynamics simulations, free energy decomposition and docking. Journal of Molecular Modeling, 2010, 16, 49-59.	0.8	19
68	Identification of a novel resistance mutation for benzimidazole inhibitors of the HCV RNA-dependent RNA polymerase. Antiviral Research, 2012, 93, 30-38.	1.9	19
69	Family-wide analysis of aminoacyl-sulfamoyl-3-deazaadenosine analogues as inhibitors of aminoacyl-tRNA synthetases. European Journal of Medicinal Chemistry, 2018, 148, 384-396.	2.6	19
70	Deleterious Variants in WNT10A, EDAR, and EDA Causing Isolated and Syndromic Tooth Agenesis: A Structural Perspective from Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2019, 20, 5282.	1.8	19
71	Base substituted 5â€²-O-(N-isoleucyl)sulfamoyl nucleoside analogues as potential antibacterial agents. Bioorganic and Medicinal Chemistry, 2014, 22, 2875-2886.	1.4	18
72	Conformational and Chiral Selection of Oligonucleotides. Chemistry and Biodiversity, 2007, 4, 803-817.	1.0	17

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73	Molecular dynamics and docking simulations as a proof of high flexibility in E. coli FabH and its relevance for accurate inhibitor modeling. Journal of Computer-Aided Molecular Design, 2011, 25, 371-393.	1.3	17
74	A Putative Prophylactic Solution for COVID-19: Development of Novel Multiepitope Vaccine Candidate against SARS-COV-2 by Comprehensive Immunoinformatic and Molecular Modelling Approach. Biology, 2020, 9, 296.	1.3	17
75	Development of a Functionalizable External Î²-Turn Mimic Based on a cis-Fused 1,7-Naphthyridine Scaffold. European Journal of Organic Chemistry, 2003, 2003, 1868-1878.	1.2	16
76	Isolation of Antidiabetic Withanolides from Withania coagulans Dunal and Their In Vitro and In Silico Validation. Biology, 2020, 9, 197.	1.3	16
77	Effect of Berberis vulgaris L. root extract on ifosfamide-induced in vivo toxicity and in vitro cytotoxicity. Scientific Reports, 2021, 11, 1708.	1.6	16
78	Improved algorithm for the discrete Fourier transform. Review of Scientific Instruments, 1985, 56, 2325-2327.	0.6	15
79	A novel highâ€vacuum and variableâ€temperature stoppedâ€flow device for highâ€purity polymerization kinetics. Makromolekulare Chemie Macromolecular Symposia, 1991, 47, 271-275.	0.6	15
80	Enantiomeric Selection Properties of Î²â€homoDNA: Enhanced Pairing for Heterochiral Complexes. Angewandte Chemie - International Edition, 2013, 52, 6662-6665.	7.2	14
81	5â€²-(N-aminoacyl)-sulfonamido-5â€²-deoxyadenosine: Attempts for a stable alternative for aminoacyl-sulfamoyl adenosines as aaRS inhibitors. European Journal of Medicinal Chemistry, 2015, 93, 227-236.	2.6	14
82	New class of early-stage enterovirus inhibitors with a novel mechanism of action. Antiviral Research, 2017, 147, 67-74.	1.9	14
83	Structure-activity relationship study of the pyridine moiety of isothiazolo[4,3-b]pyridines as antiviral agents targeting cyclin G-associated kinase. Bioorganic and Medicinal Chemistry, 2020, 28, 115188.	1.4	14
84	Translational Properties of mHNA, a Messenger RNA Containing Anhydrohexitol Nucleotidesâ€. Biochemistry, 2001, 40, 11777-11784.	1.2	13
85	Combining molecular docking and QSAR studies for modelling the antigyrase activity of cyclothialidine derivatives. European Journal of Medicinal Chemistry, 2011, 46, 2736-2747.	2.6	13
86	1â€²,5â€²-Anhydro-<scp>l</scp>-ribo-hexitol Adenine Nucleic Acids (Î±-<scp>l</scp>-HNA-A): Synthesis and Chiral Selection Properties in the Mirror Image World. Journal of Organic Chemistry, 2015, 80, 5014-5022.	1.7	13
87	Discovery of novel Hepatitis C virus inhibitor targeting multiple allosteric sites of NS5B polymerase. Infection, Genetics and Evolution, 2020, 84, 104371.	1.0	13
88	Comparative structural dynamics of Tyrosyl-tRNA synthetase complexed with different substrates explored by molecular dynamics. European Biophysics Journal, 2008, 38, 25-35.	1.2	12
89	Mutagenesis of DsbAss is Crucial for the Signal Recognition Particle Mechanism in Escherichia coli: Insights from Molecular Dynamics Simulations. Biomolecules, 2019, 9, 133.	1.8	12
90	In vitro evaluation of arylsubstituted imidazoles derivatives as antiprotozoal agents and docking studies on sterol 14Î±-demethylase (CYP51) from Trypanosoma cruzi, Leishmania infantum, and Trypanosoma brucei. Parasitology Research, 2019, 118, 1533-1548.	0.6	12

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91	New isolate from <scp>Salvinia molesta</scp> with antioxidant and urease inhibitory activity. Drug Development Research, 2021, 82, 1169-1181.	1.4	12
92	Oxygen vacancy generation in rareâ€earthâ€doped SrTiO₃. Physica Status Solidi (B): Basic Research, 2016, 253, 2197-2203.	0.7	11
93	A novel pathogenic missense variant in CNNM4 underlying Jalili syndrome: Insights from molecular dynamics simulations. Molecular Genetics & Genomic Medicine, 2019, 7, e902.	0.6	11
94	Experimental and theoretical study of electrostatic effects on the isoelectric pH and the pKa of the catalytic residue His-102 of the recombinant ribonuclease fromBacillus amyloliquefaciens (barnase). , 1996, 24, 370-378.		10
95	(D)- AND (L)-CYCLOHEXENYL-G, A NEW CLASS OF ANTIVIRAL AGENTS: SYNTHESIS, CONFORMATIONAL ANALYSIS, MOLECULAR MODELING, AND BIOLOGICAL ACTIVITY. Nucleosides, Nucleotides and Nucleic Acids, 2001, 20, 727-730.	0.4	10
96	Poly(2-acrylamido-2-methyl-1-propanamide) (PAMPA): A Neutral, Water-Soluble Synthetic Polymer with Double-Stranded Helix Conformation. Helvetica Chimica Acta, 2001, 84, 2398-2408.	1.0	10
97	Characterization and molecular modeling of the inclusion complexes of 2-(2-nitrovinyl) furan (G-0) with cyclodextrines. International Journal of Pharmaceutics, 2012, 439, 275-285.	2.6	10
98	Hepatitis C virus polymeraseâ€“polymerase contact interface: Significance for virus replication and antiviral design. Antiviral Research, 2014, 108, 14-24.	1.9	10
99	Achiral, acyclic nucleic acids: synthesis and biophysical studies of a possible prebiotic polymer. Organic and Biomolecular Chemistry, 2015, 13, 9249-9260.	1.5	10
100	Structural properties and mechanical stability of lithium-ion based materials. A theoretical study. Computational Materials Science, 2017, 136, 271-279.	1.4	10
101	Galactosylsphingamides: new Î±-GalCer analogues to probe the Fâ€™-pocket of CD1d. Scientific Reports, 2017, 7, 4276.	1.6	10
102	Cyclin G-associated kinase (GAK) affinity and antiviral activity studies of a series of 3-C-substituted isothiazolo[4,3-b]pyridines. European Journal of Medicinal Chemistry, 2019, 163, 256-265.	2.6	10
103	Discovery of 3-phenyl- and 3-N-piperidinyl-isothiazolo[4,3-b]pyridines as highly potent inhibitors of cyclin G-associated kinase. European Journal of Medicinal Chemistry, 2021, 213, 113158.	2.6	10
104	Comparative analysis of the molecular mechanism of resistance to vapendavir across a panel of picornavirus species. Antiviral Research, 2021, 195, 105177.	1.9	10
105	Elaboration of a proprietary thymidylate kinase inhibitor motif towards anti-tuberculosis agents. Bioorganic and Medicinal Chemistry, 2016, 24, 5172-5182.	1.4	9
106	Molecular Dynamics of Double Stranded Xylo-Nucleic Acid. Journal of Chemical Theory and Computation, 2017, 13, 5028-5038.	2.3	9
107	Chimeric XNA: An Unconventional Design for Orthogonal Informational Systems. Chemistry - A European Journal, 2018, 24, 12811-12819.	1.7	9
108	Toxicity Evaluation of the Naphthalen-2-yl 3,5-Dinitrobenzoate: A Drug Candidate for Alzheimer Disease. Frontiers in Pharmacology, 2021, 12, 607026.	1.6	9

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109	N-Alkylated Aminoacyl sulfamoyladenosines as Potential Inhibitors of Aminoacylation Reactions and Microcin C Analogues Containing D-Amino Acids. PLoS ONE, 2013, 8, e79234.	1.1	9
110	Hydrolysis of aspartic acid phosphoramidate nucleotides: a comparative quantum chemical study. Physical Chemistry Chemical Physics, 2009, 11, 7274.	1.3	8
111	Toward the computer-aided discovery of FabH inhibitors. Do predictive QSAR models ensure high quality virtual screening performance?. Molecular Diversity, 2014, 18, 637-654.	2.1	8
112	3-(imidazo[1,2- a :5,4- b â€²]dipyridin-2-yl)aniline inhibits pestivirus replication by targeting a hot spot drug binding pocket in the RNA-dependent RNA polymerase. Antiviral Research, 2016, 129, 99-103.	1.9	8
113	1-(Piperidin-3-yl)thymine amides as inhibitors of M. tuberculosis thymidylate kinase. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 1730-1739.	2.5	8
114	Quinolinecarboxamides Inhibit the Replication of the Bovine Viral Diarrhea Virus by Targeting a Hot Spot for the Inhibition of Pestivirus Replication in the RNA-Dependent RNA Polymerase. Molecules, 2020, 25, 1283.	1.7	8
115	Asymmetric Synthesis of New Î²â€Lactam Lipopeptides as Bacterial Signal Peptidase I Inhibitors. European Journal of Organic Chemistry, 2011, 2011, 3437-3449.	1.2	7
116	Efficient and Accurate Potential Energy Surfaces of Puckering in Sugar-Modified Nucleosides. Journal of Chemical Theory and Computation, 2021, 17, 3814-3823.	2.3	7
117	The discovery of Zika virus NS2B-NS3 inhibitors with antiviral activity via an integrated virtual screening approach. European Journal of Pharmaceutical Sciences, 2022, 175, 106220.	1.9	7
118	Six-membered Carbocyclic Nucleosides. Advances in Antiviral Drug Design, 2003, , 119-145.	0.7	6
119	Structural properties and mechanical stability of monoclinic lithium disilicate. Physica Status Solidi (B): Basic Research, 2017, 254, 1700108.	0.7	6
120	Methylated Nucleobases: Synthesis and Evaluation for Base Pairing Inâ€...Vitro and Inâ€...Vivo. Chemistry - A European Journal, 2018, 24, 12695-12707.	1.7	6
121	Enhanced Thermostability and Enzymatic Activity of cel6A Variants from Thermobifida fusca by Empirical Domain Engineering. Biology, 2020, 9, 214.	1.3	6
122	Chemical Etiology of Nucleic Acids: Aminopropyl Nucleic Acids (APNAs). Chemistry and Biodiversity, 2007, 4, 740-761.	1.0	5
123	Bioassay Directed Isolation, Biological Evaluation and in Silico Studies of New Isolates from Pteris cretica L.. Antioxidants, 2019, 8, 231.	2.2	5
124	Cleavage of DNA without loss of genetic information by incorporation of a disaccharide nucleoside. Nucleic Acids Research, 2003, 31, 6758-6769.	6.5	4
125	Structural basis for the role of LYS220 as proton donor for nucleotidyl transfer in HIV-1 reverse transcriptase. Biophysical Chemistry, 2011, 157, 1-6.	1.5	4
126	Regioselective 2â€²-O-debenzoylation of 2',3'-di-O-benzoyl threose nucleosides. Tetrahedron Letters, 2013, 54, 6084-6086.	0.7	4

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127	Thermodynamic computational approach to capture molecular recognition in the binding of different inhibitors to the DNA gyrase B subunit from Escherichia coli. Journal of Molecular Modeling, 2013, 19, 3187-3200.	0.8	3
128	Hybridisation Potential of 1',3'-Di-O-methylaltropyranoside Nucleic Acids. Molecules, 2015, 20, 4020-4041.	1.7	2
129	Molecular simulation of cyclohexanyl nucleic acid (CNA) duplexes with CNA, DNA and RNA and CNA triloop and tetraloop hairpin structures. Bioorganic and Medicinal Chemistry, 2016, 24, 1778-1785.	1.4	2
130	Synthesis, Enzyme Assays and Molecular Docking Studies of Fluorina ted Bioisosteres of Santacruzamate A as Potential HDAC Tracers. Letters in Drug Design and Discovery, 2017, 14, .	0.4	2
131	Thymidine (monophosphate) analogues as Mycobacterium tuberculosis thymidylate kinase inhibitors. , 2002, , .		2
132	Bacterial FabH: Towards the Discovery of New Broad-Spectrum Antibiotics. , 2014, , 131-158.		1
133	NMR study on the interaction of the conserved CREX â€˜stemâ€“loopâ€™ in the Hepatitis E virus genome with a naphthyridine-based ligand. Organic and Biomolecular Chemistry, 2015, 13, 9665-9672.	1.5	1
134	Conformational Analysis, Solvent-Accessible Surface and Geometric Extent of Inhibitors and Substrates. Collection of Czechoslovak Chemical Communications, 2006, 71, 842-858.	1.0	1
135	Reply to â€˜â€˜Comments on â€˜Improved algorithm for the discrete Fourier transformâ€™â€‰â€™â€™ [Rev. Sci. Instrum. 58, 714 (1987)]. Review of Scientific Instruments, 1987, 58, 715-715.	0.6	0
136	<title>Energy transfer and specific fluorescence quenching effects in barnase, studied via multifrequency phase-fluorometry of tryptophan mutants</title>. , 1992, 1640, 729.		0
137	Interactions of the Dimeric Triad of HIV-1 Aspartyl Protease with Inhibitors. Drug Design and Discovery, 2003, 18, 53-64.	0.3	0
138	Frontispiece: Chimeric XNA: An Unconventional Design for Orthogonal Informational Systems. Chemistry - A European Journal, 2018, 24, .	1.7	0
139	Interactions of the Dimeric Triad of HIV-1 Aspartyl Protease with Inhibitors. Drug Design and Discovery, 2003, 18, 53-64.	0.3	0