

Ricardo D Enriz

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4716111/publications.pdf>

Version: 2024-02-01

138
papers

3,141
citations

159585

30
h-index

197818

49
g-index

139
all docs

139
docs citations

139
times ranked

3780
citing authors

#	ARTICLE	IF	CITATIONS
1	In vitro antifungal evaluation and structure-activity relationships of a new series of chalcone derivatives and synthetic analogues, with inhibitory properties against polymers of the fungal cell wall. <i>Bioorganic and Medicinal Chemistry</i> , 2001, 9, 1999-2013.	3.0	275
2	Synthesis and antifungal activity of (Z)-5-arylidenerhodanines. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 484-494.	3.0	175
3	In vitro antifungal activity of new series of homoallylamines and related compounds with inhibitory properties of the synthesis of fungal cell wall polymers. <i>Bioorganic and Medicinal Chemistry</i> , 2003, 11, 1531-1550.	3.0	108
4	Antimicrobial activity of aqueous extracts and of berberine isolated from <i>Berberis heterophylla</i> . <i>FÁ-toterapĀ-Āç</i> , 2003, 74, 702-705.	2.2	105
5	Inhibitors of the fungal cell wall. Synthesis of 4-aryl-4-N-arylamine-1-butenes and related compounds with inhibitory activities on $\beta(1\rightarrow3)$ glucan and chitin synthases. <i>Bioorganic and Medicinal Chemistry</i> , 2000, 8, 691-698.	3.0	94
6	In Vitro Evaluation of Antifungal Properties of 8-O- β -Neolignans. <i>Journal of Natural Products</i> , 1997, 60, 659-662.	3.0	84
7	<i>In Silico</i> Study of Full-Length Amyloid β^{1-42} Tri- and Penta-Oligomers in Solution. <i>Journal of Physical Chemistry B</i> , 2009, 113, 11710-11719.	2.6	81
8	Structure-activity relationship in the gastric cytoprotective effect of several sesquiterpene lactones. <i>Journal of Medicinal Chemistry</i> , 1992, 35, 2452-2458.	6.4	80
9	Structure-Activity Relationship of Cinnamic Acid Derivatives. <i>Journal of Agricultural and Food Chemistry</i> , 2007, 55, 10635-10640.	5.2	76
10	In Vitro Evaluation of Antifungal Properties of Phenylpropanoids and Related Compounds Acting Against Dermatophytes. <i>Journal of Natural Products</i> , 1999, 62, 1353-1357.	3.0	61
11	Amyloid- β fibril disruption by C60 molecular guidance for rational drug design. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8599.	2.8	56
12	Molecular Modeling Study of Dihydrofolate Reductase Inhibitors. Molecular Dynamics Simulations, Quantum Mechanical Calculations, and Experimental Corroboration. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2018-2032.	5.4	56
13	Syntheses and Antitumor Targeting G1 Phase of the Cell Cycle of Benzoyldihydroisoquinolines and Related 1-Substituted Isoquinolines. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 5058-5068.	6.4	54
14	Small Cationic Peptides: Influence of Charge on Their Antimicrobial Activity. <i>ACS Omega</i> , 2018, 3, 5390-5398.	3.5	51
15	Structure-Activity Relationship of Clerodane Diterpenoids. Comparative Study with Withanolides and Azadirachtin. <i>Journal of Agricultural and Food Chemistry</i> , 2000, 48, 1384-1392.	5.2	49
16	Peptide models XXIV: An ab initio study on N-formyl-L-prolinamide with trans peptide bond. The existence or non-existence of β and μ L conformations. <i>Computational and Theoretical Chemistry</i> , 1999, 465, 79-91.	1.5	48
17	New small-size peptides possessing antifungal activity. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 158-167.	3.0	48
18	Searching the Biologically Relevant Conformation of Dopamine: A Computational Approach. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 99-112.	5.4	48

#	ARTICLE	IF	CITATIONS
19	Theoretical and Experimental Study of Inclusion Complexes of β -Cyclodextrins with Chalcone and 2,4-Dihydroxychalcone. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3000-3011.	2.6	46
20	Structure-activity relationship study of homoallylamines and related derivatives acting as antifungal agents. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 1851-1862.	3.0	44
21	Peptide and protein folding. <i>Computational and Theoretical Chemistry</i> , 2001, 537, 319-361.	1.5	43
22	Tetrahydroisoquinolines as dopaminergic ligands: 1-Butyl-7-chloro-6-hydroxy-tetrahydroisoquinoline, a new compound with antidepressant-like activity in mice. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 4968-4980.	3.0	39
23	2,3,9- and 2,3,11-Trisubstituted tetrahydroprotoberberines as D2 dopaminergic ligands. <i>European Journal of Medicinal Chemistry</i> , 2013, 68, 150-166.	5.5	37
24	Penetratin and derivatives acting as antifungal agents. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 212-228.	5.5	35
25	Characteristics of Ramachandran maps of L-alanine diamides as computed by various molecular mechanics, semiempirical and ab initio MO methods.. <i>Computational and Theoretical Chemistry</i> , 1998, 455, 275-301.	1.5	34
26	Structure-Cytoprotective Activity Relationship of Simple Molecules Containing an α,β -Unsaturated Carbonyl System. <i>Journal of Medicinal Chemistry</i> , 1997, 40, 1827-1834.	6.4	33
27	An integrative study to identify novel scaffolds for sphingosine kinase 1 inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2017, 139, 461-481.	5.5	33
28	Antifungal and cytotoxic activities of some N-substituted aniline derivatives bearing a hetaryl fragment. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 794-809.	3.0	32
29	Antioxidant and cytotoxic activities of canadine: Biological effects and structural aspects. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 3641-3651.	3.0	32
30	Alkaloids from <i>Hippeastrum argentinum</i> and Their Cholinesterase-Inhibitory Activities: An in Vitro and in Silico Study. <i>Journal of Natural Products</i> , 2016, 79, 1241-1248.	3.0	32
31	An exploratory ab initio study of the full conformational space of N-acetyl-L-cysteine-N-methylamide. <i>Computational and Theoretical Chemistry</i> , 2001, 540, 271-283.	1.5	30
32	Non-covalent interactions in receptor-ligand complexes. A study based on the electron charge density. <i>Journal of Physical Organic Chemistry</i> , 2014, 27, 128-134.	1.9	29
33	Antifungal Activity of Extracts and Prenylated Coumarins Isolated from <i>Baccharis darwinii</i> Hook & Arn. (Asteraceae). <i>Molecules</i> , 2010, 15, 4898-4907.	3.8	28
34	Cholinesterase-inhibitory effect and in silico analysis of alkaloids from bulbs of <i>Hieronymiella</i> species. <i>Phytomedicine</i> , 2018, 39, 66-74.	5.3	27
35	Structural Requirements for the Antifungal Activities of Natural Drimane Sesquiterpenes and Analogues, Supported by Conformational and Electronic Studies. <i>Molecules</i> , 2013, 18, 2029-2051.	3.8	26
36	Tetrahydroisoquinolines acting as dopaminergic ligands. A molecular modeling study using MD simulations and QM calculations. <i>Journal of Molecular Modeling</i> , 2012, 18, 419-431.	1.8	25

#	ARTICLE	IF	CITATIONS
37	Exploration of the Full Conformational Space of N-Acetyl-L-glutamine-N-methylamide. An ab Initio and Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5079-5091.	2.5	23
38	Structural and Thermodynamic Characteristics of the Exosite Binding Pocket on the Human BACE1: A Molecular Modeling Approach. <i>Journal of Physical Chemistry A</i> , 2010, 114, 10261-10269.	2.5	23
39	Conformational transition of A β 42 inhibited by a mimetic peptide. A molecular modeling study using QM/MM calculations and QTAIM analysis. <i>Computational and Theoretical Chemistry</i> , 2016, 1080, 56-65.	2.5	23
40	A search for C-H \cdots O type hydrogen bonds in Lamivudine (3TC). An exploratory conformational and electronic analysis. <i>Computational and Theoretical Chemistry</i> , 2001, 543, 185-193.	1.5	22
41	Synthesis and conformational analysis of His-Phe-Arg-Trp-NH ₂ and analogues with antifungal properties. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 7604-7614.	3.0	22
42	Structure-activity relationship of dopaminergic halogenated 1-benzyl-tetrahydroisoquinoline derivatives. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 4616-4621.	5.5	22
43	Halogen bonding in biological context: a computational study of D2 dopamine receptor. <i>Journal of Physical Organic Chemistry</i> , 2016, 29, 645-655.	1.9	21
44	New antitumoral acetogenin -Guanacone type- derivatives: Isolation and bioactivity. Molecular dynamics simulation of diacetyl-guanacone. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 4369-4381.	3.0	19
45	New mimetic peptides inhibitors of A β aggregation. Molecular guidance for rational drug design. <i>European Journal of Medicinal Chemistry</i> , 2015, 95, 136-152.	5.5	19
46	Design of new quinolin-2-one-pyrimidine hybrids as sphingosine kinases inhibitors. <i>Bioorganic Chemistry</i> , 2020, 94, 103414.	4.1	19
47	Combined MD/QTAIM techniques to evaluate ligand-receptor interactions. Scope and limitations. <i>European Journal of Medicinal Chemistry</i> , 2020, 208, 112792.	5.5	19
48	Targeting defective sphingosine kinase 1 in Niemann-Pick type C disease with an activator mitigates cholesterol accumulation. <i>Journal of Biological Chemistry</i> , 2020, 295, 9121-9133.	3.4	19
49	Gastric cytoprotective activity of ilicic aldehyde: Structure-activity relationships. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 3547-3550.	2.2	18
50	Comprehensive conformational analysis of N-acetyl-L-tryptophane-N-methylamide. An ab initio and DFT study. <i>Computational and Theoretical Chemistry</i> , 2005, 724, 173-184.	1.5	17
51	Penetratin analogues acting as antifungal agents. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 370-377.	5.5	17
52	Dopaminergic isoquinolines with hexahydrocyclopenta[ij]-isoquinolines as D ₂ -like selective ligands. <i>European Journal of Medicinal Chemistry</i> , 2016, 122, 27-42.	5.5	17
53	New small-size peptides modulators of the exosite of BACE1 obtained from a structure-based design. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 413-426.	3.5	17
54	Ab Initio and DFT Study of the Conformational Energy Hypersurface of Cyclic Gly-Gly-Gly. <i>Journal of Physical Chemistry A</i> , 2009, 113, 10818-10825.	2.5	16

#	ARTICLE	IF	CITATIONS
55	The electronic density obtained from a QTAIM analysis used as molecular descriptor. A study performed in a new series of DHFR inhibitors. <i>Journal of Molecular Structure</i> , 2017, 1134, 464-474.	3.6	16
56	The Antimicrobial Activity of <i>Annona emarginata</i> (Schltdl.) H. Rainer and Most Active Isolated Compounds against Clinically Important Bacteria. <i>Molecules</i> , 2018, 23, 1187.	3.8	16
57	Polycerasoidol, a Natural Prenylated Benzopyran with a Dual PPAR α /PPAR γ Agonist Activity and Anti-inflammatory Effect. <i>Journal of Natural Products</i> , 2019, 82, 1802-1812.	3.0	16
58	An analytic ring closure condition for geometrical algorithm to search the conformational space. <i>Computational and Theoretical Chemistry</i> , 2000, 507, 89-95.	1.5	14
59	Partially relaxed ring closure conditions for geometrical algorithm to search the conformational space for minimum energy conformations. <i>Computational and Theoretical Chemistry</i> , 2001, 536, 173-188.	1.5	14
60	An exploratory study of side-chain π -backbone interaction in selected conformations of N-acetyl-L-glutamate-N-methylamide. An ab initio study. <i>Computational and Theoretical Chemistry</i> , 2001, 543, 203-222.	1.5	14
61	Conformational Preferences of N-Acetyl-L-leucine-N-methylamide. Gas-Phase and Solution Calculations on the Model Dipeptide. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10682-10691.	2.5	14
62	In vitro π -in vivo antifungal evaluation and structure π -activity relationships of 3H-1,2-dithiole-3-thione derivatives. <i>Il Farmaco</i> , 2004, 59, 245-254.	0.9	13
63	Advances in correlation between experimental and DFT/GIAO computed ¹³ C NMR chemical shifts: A theoretical study on pentacyclic terpenoids (ferrenes). <i>Computational and Theoretical Chemistry</i> , 2010, 953, 83-90.	1.5	13
64	Penetratin and Derivatives Acting as Antibacterial Agents. <i>Chemical Biology and Drug Design</i> , 2013, 82, 167-177.	3.2	13
65	New short cationic antibacterial peptides. Synthesis, biological activity and mechanism of action. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2021, 1863, 183665.	2.6	13
66	A potentiometric and spectrophotometric study on acid π -base equilibria in ethanol-aqueous solution of acetazolamide and related compounds. <i>Talanta</i> , 1999, 49, 859-868.	5.5	12
67	In vitro Antifungal Properties, Structure-activity Relationships and Studies on the Mode of Action of N-Phenyl, N-Aryl, N-Phenylalkyl Maleimides and Related Compounds. <i>Arzneimittelforschung</i> , 2005, 55, 123-132.	0.4	12
68	A QM/MM study of the molecular recognition site of bapineuzumab toward the amyloid- β peptide isoforms. <i>Molecular Simulation</i> , 2016, 42, 196-207.	2.0	12
69	Molecular design and synthesis of novel peptides from amphibians skin acting as inhibitors of cholinesterase enzymes. <i>Journal of Peptide Science</i> , 2017, 23, 236-244.	1.4	12
70	Pentameric models as alternative molecular targets for the design of new antiaggregant agents. <i>Current Protein and Peptide Science</i> , 2016, 17, 156-168.	1.4	12
71	A Comprehensive Conformational Analysis of Bullacin B, a Potent Inhibitor of Complex I. Molecular Dynamics Simulations and Ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7426-7438.	2.5	11
72	New antifungal peptides. Synthesis, bioassays and initial structure prediction by CD spectroscopy. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 4808-4811.	2.2	11

#	ARTICLE	IF	CITATIONS
73	Novel Sulfonamide-Based Carbamates as Selective Inhibitors of BChE. <i>International Journal of Molecular Sciences</i> , 2021, 22, 9447.	4.1	11
74	A theoretical study on the conformations of azadirachtin. <i>Computational and Theoretical Chemistry</i> , 1996, 363, 167-178.	1.5	10
75	A matrix representation for the geometrical algorithm to search the conformational space (GASCOS) for flexible linear molecules. <i>Computational and Theoretical Chemistry</i> , 2001, 571, 91-98.	1.5	10
76	Molecular recognition and binding mechanism of N-alkyl-benzyltetrahydroisoquinolines to the D1 dopamine receptor. A computational approach. <i>Computational and Theoretical Chemistry</i> , 2003, 666-667, 455-467.	1.5	10
77	Dynamics of flexible cycloalkanes. Ab initio and DFT study of the conformational energy hypersurface of cyclononane. <i>Journal of Computational Chemistry</i> , 2006, 27, 188-202.	3.3	10
78	Synthesis, dopaminergic profile, and molecular dynamics calculations of N-aralkyl substituted 2-aminoindans. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 3233-3244.	3.0	10
79	Structure-activity relationship study of nitrosopyrimidines acting as antifungal agents. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 6109-6122.	3.0	10
80	3- α -Chlorotyramine Acting as Ligand of the D ₂ Dopamine Receptor. <i>Molecular Modeling, Synthesis and D₂ Receptor Affinity</i> . <i>Molecular Informatics</i> , 2015, 34, 28-43.	2.5	10
81	Exploratory conformational analysis of N-acetyl-L-Tryptophan-N-methylamide. An ab initio study. <i>Computational and Theoretical Chemistry</i> , 2003, 631, 277-290.	1.5	9
82	Comprehensive conformational analysis of N-acetyl-L-isoleucine-N-methylamide: an ab initio study. <i>Computational and Theoretical Chemistry</i> , 2003, 634, 201-213.	1.5	9
83	Structure-antifungal activity relationship of His-Phe-Arg-Trp-Gly-Lys-Pro-Val-NH ₂ and analogues. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 4347-4358.	3.0	9
84	Theoretical and experimental study of the interactions of annonaceous acetogenins with artificial lipid bilayers. <i>Journal of Molecular Structure</i> , 2011, 1003, 87-91.	3.6	9
85	Tetrahydroisoquinolines functionalized with carbamates as selective ligands of D ₂ dopamine receptor. <i>Journal of Molecular Modeling</i> , 2017, 23, 273.	1.8	9
86	Synthesis, Analysis, Cholinesterase-Inhibiting Activity and Molecular Modelling Studies of 3-(Dialkylamino)-2-hydroxypropyl 4-[(Alkoxy-carbonyl)amino]benzoates and Their Quaternary Ammonium Salts. <i>Molecules</i> , 2017, 22, 2048.	3.8	9
87	Theoretical models to predict the inhibitory effect of ligands of sphingosine kinase 1 using QTAIM calculations and hydrogen bond dynamic propensity analysis. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 781-791.	2.9	9
88	Searching new structural scaffolds for BRAF inhibitors. An integrative study using theoretical and experimental techniques. <i>Bioorganic Chemistry</i> , 2019, 91, 103125.	4.1	9
89	The nitron spin trap 5,5-dimethyl-1-pyrroline N-oxide binds to toll-like receptor-2-TIR-BB-loop domain and dampens downstream inflammatory signaling. <i>Biochimica Et Biophysica Acta - Molecular Basis of Disease</i> , 2019, 1865, 1152-1159.	3.8	9
90	Conformational and electronic study of dopamine interacting with the D ₂ dopamine receptor. <i>Journal of Computational Chemistry</i> , 2020, 41, 1898-1911.	3.3	9

#	ARTICLE	IF	CITATIONS
91	Second-generation 4,5,6,7-tetrahydrobenzo[<i>c</i>]thiazoles as novel DNA gyrase inhibitors. <i>Future Medicinal Chemistry</i> , 2020, 12, 277-297.	2.3	9
92	Synthesis and antifungal activity of N-aryl-N-benzylamines and of their homoallyl analogues. <i>Arkivoc</i> , 2011, 2011, 149-161.	0.5	9
93	SYNTHESIS AND PRELIMINARY CYTOTOXIC AND ANTIFUNGAL EVALUATION OF SOME 6-N,N-DIALKYL 2-ARYL-4(3H)-QUINAZOLINONE DERIVATIVES. <i>Heterocyclic Communications</i> , 2001, 7, .	1.2	8
94	New Small-Size Antifungal Peptides: Design, Synthesis and Antifungal Activity. <i>Letters in Drug Design and Discovery</i> , 2011, 8, 562-567.	0.7	8
95	Small Peptides Derived from Penetratin as Antibacterial Agents. <i>Archiv Der Pharmazie</i> , 2016, 349, 242-251.	4.1	8
96	Dihydrofolate reductase inhibitors: a quantitative structure-activity relationship study using 2D-QSAR and 3D-QSAR methods. <i>Medicinal Chemistry Research</i> , 2017, 26, 247-261.	2.4	8
97	Synthesis, anti-parasitic activity and QSAR study of a new library of polysubstituted tetrahydronaphtho[1,2-b]azepines. <i>Medicinal Chemistry Research</i> , 2018, 27, 2239-2264.	2.4	8
98	Hydroxynaphthalenecarboxamides and substituted piperazinypropandiols, two new series of BRAF inhibitors. A theoretical and experimental study. <i>Bioorganic Chemistry</i> , 2020, 103, 104145.	4.1	8
99	Synthesis, biological evaluation and molecular modeling studies of substituted N-benzyl-2-phenylethanamines as cholinesterase inhibitors. <i>New Journal of Chemistry</i> , 2020, 44, 9466-9476.	2.8	8
100	Theoretical study on the conformations of 3-tigloyl-azadirachtol and azadirachtin derivatives. <i>Computational and Theoretical Chemistry</i> , 1997, 391, 27-38.	1.5	7
101	An ab initio conformational study on captopril. <i>Computational and Theoretical Chemistry</i> , 2003, 666-667, 599-608.	1.5	7
102	Ab initio conformational study of vinyllogues. 2-Butene, stilbene and their conjugated polyenes. <i>Computational and Theoretical Chemistry</i> , 2005, 731, 107-114.	1.5	7
103	Conformational study of <i>cis</i> and <i>trans</i> N-formyl-N-methyl-L-glycine-N ² -amide and N-acetyl-N-methyl-L-glycine-N ² -methylamide. An ab-initio and DFT study. <i>Computational and Theoretical Chemistry</i> , 2005, 731, 177-185.	1.5	7
104	Mass spectrometry and theoretical calculations about the loss of methyl radical from methoxilated coumarins. <i>Journal of Molecular Structure</i> , 2015, 1093, 49-58.	3.6	7
105	A New Series of Antibacterial Nitrosopyrimidines: Synthesis and Structure-Activity Relationship. <i>Archiv Der Pharmazie</i> , 2015, 348, 68-80.	4.1	7
106	Searching for improved mimetic peptides inhibitors preventing conformational transition of amyloid- β 42 monomer. <i>Bioorganic Chemistry</i> , 2018, 81, 211-221.	4.1	7
107	New substituted aminopyrimidine derivatives as BACE1 inhibitors: in silico design, synthesis and biological assays. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 229-246.	3.5	7
108	Conformational and electronic study of N-phenylalkyl-3,4-dichloromaleimides: Ab initio and DFT study. <i>International Journal of Quantum Chemistry</i> , 2003, 93, 32-46.	2.0	6

#	ARTICLE	IF	CITATIONS
109	Theoretical study of the conformational energy hypersurface of cyclotrisarcosyl. <i>Open Chemistry</i> , 2012, 10, 248-255.	1.9	6
110	Antinociceptive effect of neo-clerodane diterpenes obtained from <i>Baccharis flabellata</i> . <i>Farmacologia</i> , 2018, 130, 94-99.	2.2	6
111	Synthesis and biological evaluation of sphingosine kinase 2 inhibitors with anti-inflammatory activity. <i>Archiv Der Pharmazie</i> , 2019, 352, e1800298.	4.1	6
112	Conformational study of N-alkyl-benzyltetrahydroisoquinolines alkaloid. <i>Computational and Theoretical Chemistry</i> , 2003, 666-667, 109-116.	1.5	5
113	Conformational and electronic study of N-acetyl-L-isoleucine-N-methylamide using DFT and IPCM calculations. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1580-1595.	2.0	5
114	Quinazoline ethered hydrazone: A versatile scaffold toward dual anti-TB and EGFR inhibition activities in NSCLC. <i>Archiv Der Pharmazie</i> , 2021, 354, e2100281.	4.1	5
115	Cytoprotective Activity of Minor Constituents of <i>Artemisia Douglasiana</i> . <i>Natural Product Research</i> , 1995, 6, 269-280.	0.4	4
116	Conformational study of internally retrograde and quasi-retrograde molecules – An ab initio and DFT study. <i>Canadian Journal of Chemistry</i> , 2005, 83, 122-137.	1.1	4
117	Ring inversion in 1,4,7 cyclononatriene and analogues: Ab initio and DFT calculations and topological analysis. <i>Journal of Computational Chemistry</i> , 2008, 29, 280-290.	3.3	4
118	Synthesis and Antibacterial Activity of Highly Oxygenated 1,8-Cineole Derivatives. <i>Natural Product Communications</i> , 2008, 3, 1934578X0800300.	0.5	4
119	Conformational and electronic study of cis-peptides (non-proline residues) occurring in natural proteins. <i>Journal of Molecular Structure</i> , 2009, 934, 103-111.	3.6	4
120	Indole-substituted 2,4-diamino-5,8-dihydropyrido[2,3-d]pyrimidines from one-pot process and evaluation of their ability to bind dopamine receptors. <i>Tetrahedron</i> , 2018, 74, 7047-7057.	1.9	4
121	Structure, interface stability and hot-spots identification for RBD(SARS-CoV-2):hACE2 complex formation. <i>Molecular Simulation</i> , 2021, 47, 1443-1454.	2.0	3
122	Design, synthesis, biological evaluation and molecular modelling of substituted pyrrolo[2,1-a]isoquinolinone derivatives: discovery of potent inhibitors of AChE and BChE. <i>New Journal of Chemistry</i> , 2021, 45, 8321-8334.	2.8	3
123	The Long and Winding Road to Convert an Antimicrobial Compound into an Antimicrobial Drug: An Overview from a Medicinal Chemistry Point of View. <i>Current Organic Chemistry</i> , 2017, 21, .	1.6	3
124	Cinnamic acid derivatives acting against <i>Aspergillus</i> fungi. Taq polymerase I a potential molecular target. <i>Natural Product Communications</i> , 2012, 7, 1639-44.	0.5	3
125	Conformational and electronic study of homoallylamines with inhibitory properties against polymers of fungal cell wall. <i>Computational and Theoretical Chemistry</i> , 2003, 666-667, 587-598.	1.5	2
126	Synthesis and cytotoxic activity of 4-N-carboxybutyl-5-fluorocytosyl-Arg-Gln-Trp-Arg-Arg-Trp-Trp-Gln-Arg-NH ₂ . <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 4233-4237.	2.2	2

#	ARTICLE	IF	CITATIONS
127	Multistep conformational interconversion mechanism of cyclododecane. A simple and fast analysis using potential energy curves. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 2382-2391.	2.0	2
128	Easy synthesis of new series of pteridine analogs: di- and tetra-hydropyrimido[4,5-d]pyrimidines via 5-pyrimidinecarbaldehydes. <i>Arkivoc</i> , 2014, 2014, 42-63.	0.5	2
129	Covalence and π -electron delocalization influence on hydrogen bonds in proton transfer process of <i>o</i> -hydroxy aryl Schiff bases: A combined NMR and QTAIM analysis. <i>Journal of Chemical Physics</i> , 2021, 155, 054307.	3.0	2
130	Evaluating the conformational space of the active site of D_2 dopamine receptor. Scope and limitations of the standard docking methods. <i>Journal of Computational Chemistry</i> , 2022, 43, 1298-1312.	3.3	2
131	1,2-Dipolar addition model for the cytoprotective activity of selected $\hat{1},\hat{2}$ -unsaturated compounds with $C\bar{r}\dots O$ functionality: an ab initio study. <i>Computational and Theoretical Chemistry</i> , 2001, 538, 225-233.	1.5	1
132	Structure of isolated tyrosyl-glycyl-glycine tripeptide. A comparative conformational study with peptides containing an aromatic ring. <i>Open Chemistry</i> , 2010, 8, 566-575.	1.9	1
133	Quinoline analogs of 2-aminoindane as potential central dopaminergic agents. <i>Medicinal Chemistry Research</i> , 2019, 28, 1168-1181.	2.4	1
134	Synthesis, in vitro/in vivo Antifungal Evaluation and Structure-Activity Relationship Study of 3(2H)-Pyridazinones. <i>Arzneimittelforschung</i> , 2003, 53, 738-743.	0.4	0
135	In vitro/in vivo Antifungal Evaluation and Structure-Activity Relationships of 3H-1,2-Dithiole-3-thione Derivatives. <i>ChemInform</i> , 2004, 35, no.	0.0	0
136	Catalytic and Molecular Properties of Rabbit Liver Carboxylesterase Acting on 1,8-Cineole Derivatives. <i>Natural Product Communications</i> , 2012, 7, 1934578X1200700.	0.5	0
137	Cinnamic Acid Derivatives Acting against <i>Aspergillus</i> Fungi. <i>Taq</i> Polymerase I a Potential Molecular Target. <i>Natural Product Communications</i> , 2012, 7, 1934578X1200701.	0.5	0
138	Pseudorotaxane formation affected by stereo-electronic effects. A theoretical and experimental study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1654-1665.	2.8	0