Ricardo D Enriz

List of Publications by Year
in descending order

138	3,141	159525	197736
papers	citations	30 h-index	49 g-index

139	139	139	3780
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Pseudorotaxane formation affected by stereo-electronic effects. A theoretical and experimental study. Physical Chemistry Chemical Physics, 2022, 24, 1654-1665.	1.3	0
2	Evaluating the conformational space of the active site of <scp>D₂</scp> dopamine receptor. Scope and limitations of the standard docking methods. Journal of Computational Chemistry, 2022, 43, 1298-1312.	1.5	2
3	Covalence and Ï€-electron delocalization influence on hydrogen bonds in proton transfer process of o-hydroxy aryl Schiff bases: A combined NMR and QTAIM analysis. Journal of Chemical Physics, 2021, 155, 054307.	1.2	2
4	Novel Sulfonamide-Based Carbamates as Selective Inhibitors of BChE. International Journal of Molecular Sciences, 2021, 22, 9447.	1.8	11
5	Structure, interface stability and hot-spots identification for RBD(SARS-CoV-2):hACE2 complex formation. Molecular Simulation, 2021, 47, 1443-1454.	0.9	3
6	Quinazolineâ€tethered hydrazone: A versatile scaffold toward dual antiâ€TB and EGFR inhibition activities in NSCLC. Archiv Der Pharmazie, 2021, 354, e2100281.	2.1	5
7	New short cationic antibacterial peptides. Synthesis, biological activity and mechanism of action. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183665.	1.4	13
8	Design, synthesis, biological evaluation and molecular modelling of substituted pyrrolo[2,1-a]isoquinolinone derivatives: discovery of potent inhibitors of AChE and BChE. New Journal of Chemistry, 2021, 45, 8321-8334.	1.4	3
9	Design of new quinolin-2-one-pyrimidine hybrids as sphingosine kinases inhibitors. Bioorganic Chemistry, 2020, 94, 103414.	2.0	19
10	Combined MD/QTAIM techniques to evaluate ligand-receptor interactions. Scope and limitations. European Journal of Medicinal Chemistry, 2020, 208, 112792.	2.6	19
11	Hydroxynaphthalenecarboxamides and substituted piperazinylpropandiols, two new series of BRAF inhibitors. A theoretical and experimental study. Bioorganic Chemistry, 2020, 103, 104145.	2.0	8
12	Conformational and electronic study of dopamine interacting with the <scp>D₂</scp> dopamine receptor. Journal of Computational Chemistry, 2020, 41, 1898-1911.	1.5	9
13	Second-generation 4,5,6,7-tetrahydrobenzo[d]thiazoles as novel DNA gyrase inhibitors. Future Medicinal Chemistry, 2020, 12, 277-297.	1.1	9
14	Synthesis, biological evaluation and molecular modeling studies of substitutedN-benzyl-2-phenylethanamines as cholinesterase inhibitors. New Journal of Chemistry, 2020, 44, 9466-9476.	1.4	8
15	Targeting defective sphingosine kinase 1 in Niemannâ€“Pick type C disease with an activator mitigates cholesterol accumulation. Journal of Biological Chemistry, 2020, 295, 9121-9133.	1.6	19
16	Searching new structural scaffolds for BRAF inhibitors. An integrative study using theoretical and experimental techniques. Bioorganic Chemistry, 2019, 91, 103125.	2.0	9
17	Polycerasoidol, a Natural Prenylated Benzopyran with a Dual PPARÎ±/PPARÎ³ Agonist Activity and Anti-inflammatory Effect. Journal of Natural Products, 2019, 82, 1802-1812.	1.5	16
18	The nitrone spin trap 5,5â€dimethylâ€1â€pyrroline Nâ€oxide binds to toll-like receptor-2-TIR-BB-loop domain and dampens downstream inflammatory signaling. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2019, 1865, 1152-1159.	1.8	9

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19	Quinoline analogs of 2-aminoindane as potential central dopaminergic agents. Medicinal Chemistry Research, 2019, 28, 1168-1181.	1.1	1
20	Synthesis and biological evaluation of sphingosine kinase 2 inhibitors with antiâ€inflammatory activity. Archiv Der Pharmazie, 2019, 352, e1800298.	2.1	6
21	New substituted aminopyrimidine derivatives as BACE1 inhibitors: in silico design, synthesis and biological assays. Journal of Biomolecular Structure and Dynamics, 2019, 37, 229-246.	2.0	7
22	Cholinesterase-inhibitory effect and in silico analysis of alkaloids from bulbs of Hieronymiella species. Phytomedicine, 2018, 39, 66-74.	2.3	27
23	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. Tetrahedron, 2018, 74, 7047-7057.	1.0	4
24	Antinociceptive effect of neo-clerodane diterpenes obtained from Baccharis flabellata. FÃ¬toterapÃ¬Ã¢, 2018, 130, 94-99.	1.1	6
25	Small Cationic Peptides: Influence of Charge on Their Antimicrobial Activity. ACS Omega, 2018, 3, 5390-5398.	1.6	51
26	Theoretical models to predict the inhibitory effect of ligands of sphingosine kinase 1 using QTAIM calculations and hydrogen bond dynamic propensity analysis. Journal of Computer-Aided Molecular Design, 2018, 32, 781-791.	1.3	9
27	The Antimicrobial Activity of Annona emarginata (Schltdl.) H. Rainer and Most Active Isolated Compounds against Clinically Important Bacteria. Molecules, 2018, 23, 1187.	1.7	16
28	Synthesis, anti-parasitic activity and QSAR study of a new library of polysubstituted tetrahydronaphtho[1,2-b]azepines. Medicinal Chemistry Research, 2018, 27, 2239-2264.	1.1	8
29	Searching for improved mimetic peptides inhibitors preventing conformational transition of amyloid-Î²42 monomer. Bioorganic Chemistry, 2018, 81, 211-221.	2.0	7
30	New small-size peptides modulators of the exosite of BACE1 obtained from a structure-based design. Journal of Biomolecular Structure and Dynamics, 2017, 35, 413-426.	2.0	17
31	Molecular design and synthesis of novel peptides from amphibians skin acting as inhibitors of cholinesterase enzymes. Journal of Peptide Science, 2017, 23, 236-244.	0.8	12
32	The electronic density obtained from a QTAIM analysis used as molecular descriptor. A study performed in a new series of DHFR inhibitors. Journal of Molecular Structure, 2017, 1134, 464-474.	1.8	16
33	Tetrahydroisoquinolines functionalized with carbamates as selective ligands of D2 dopamine receptor. Journal of Molecular Modeling, 2017, 23, 273.	0.8	9
34	An integrative study to identify novel scaffolds for sphingosine kinase 1 inhibitors. European Journal of Medicinal Chemistry, 2017, 139, 461-481.	2.6	33
35	Dihydrofolate reductase inhibitors: a quantitative structureâ€“activity relationship study using 2D-QSAR and 3D-QSAR methods. Medicinal Chemistry Research, 2017, 26, 247-261.	1.1	8
36	Synthesis, Analysis, Cholinesterase-Inhibiting Activity and Molecular Modelling Studies of 3-(Dialkylamino)-2-hydroxypropyl 4-[(Alkoxy-carbonyl)amino]benzoates and Their Quaternary Ammonium Salts. Molecules, 2017, 22, 2048.	1.7	9

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37	The Long and Winding Road to Convert an Antimicrobial Compound into an Antimicrobial Drug: An Overview from a Medicinal Chemistry Point of View. Current Organic Chemistry, 2017, 21, .	0.9	3
38	Halogen bonding in biological context: a computational study of D2 dopamine receptor. Journal of Physical Organic Chemistry, 2016, 29, 645-655.	0.9	21
39	Small Peptides Derived from Penetratin as Antibacterial Agents. Archiv Der Pharmazie, 2016, 349, 242-251.	2.1	8
40	Alkaloids from Hippeastrum argentinum and Their Cholinesterase-Inhibitory Activities: An in Vitro and in Silico Study. Journal of Natural Products, 2016, 79, 1241-1248.	1.5	32
41	Dopaminergic isoquinolines with hexahydrocyclopenta[ij]-isoquinolines as D 2 -like selective ligands. European Journal of Medicinal Chemistry, 2016, 122, 27-42.	2.6	17
42	A QM/MM study of the molecular recognition site of bapineuzumab toward the amyloid-Î² peptide isoforms. Molecular Simulation, 2016, 42, 196-207.	0.9	12
43	Theoretical and Experimental Study of Inclusion Complexes of Î²-Cyclodextrins with Chalcone and 2â€²,4â€²-Dihydroxychalcone. Journal of Physical Chemistry B, 2016, 120, 3000-3011.	1.2	46
44	Conformational transition of AÎ² 42 inhibited by a mimetic peptide. A molecular modeling study using QM/MM calculations and QTAIM analysis. Computational and Theoretical Chemistry, 2016, 1080, 56-65.	1.1	23
45	Pentameric models as alternative molecular targets for the design of new antiaggregant agents. Current Protein and Peptide Science, 2016, 17, 156-168.	0.7	12
46	Mass spectrometry and theoretical calculations about the loss of methyl radical from methoxilated coumarins. Journal of Molecular Structure, 2015, 1093, 49-58.	1.8	7
47	New mimetic peptides inhibitors of ÎŴ aggregation. Molecular guidance for rational drug design. European Journal of Medicinal Chemistry, 2015, 95, 136-152.	2.6	19
48	A New Series of Antibacterial Nitrosopyrimidines: Synthesis and Structureâ€“Activity Relationship. Archiv Der Pharmazie, 2015, 348, 68-80.	2.1	7
49	3â€Chlorotyramine Acting as Ligand of the D₂ Dopamine Receptor. Molecular Modeling, Synthesis and D₂ Receptor Affinity. Molecular Informatics, 2015, 34, 28-43.	1.4	10
50	Non-covalent interactions in receptor-ligand complexes. A study based on the electron charge density. Journal of Physical Organic Chemistry, 2014, 27, 128-134.	0.9	29
51	Easy synthesis of new series of pteridine analogs: di- and tetra-hydropyrimido[4,5-d]pyrimidines via 5-pyrimidinecarbaldehydes. Arkivoc, 2014, 2014, 42-63.	0.3	2
52	Molecular Modeling Study of Dihydrofolate Reductase Inhibitors. Molecular Dynamics Simulations, Quantum Mechanical Calculations, and Experimental Corroboration. Journal of Chemical Information and Modeling, 2013, 53, 2018-2032.	2.5	56
53	2,3,9- and 2,3,11-Trisubstituted tetrahydroprotoberberines as D2 dopaminergic ligands. European Journal of Medicinal Chemistry, 2013, 68, 150-166.	2.6	37
54	Penetratin and Derivatives Acting as Antibacterial Agents. Chemical Biology and Drug Design, 2013, 82, 167-177.	1.5	13

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55	Structural Requirements for the Antifungal Activities of Natural Drimane Sesquiterpenes and Analogues, Supported by Conformational and Electronic Studies. Molecules, 2013, 18, 2029-2051.	1.7	26
56	Structureâ€“activity relationship study of nitrosopyrimidines acting as antifungal agents. Bioorganic and Medicinal Chemistry, 2012, 20, 6109-6122.	1.4	10
57	Amyloid-Î² fibril disruption by C60â€”molecular guidance for rational drug design. Physical Chemistry Chemical Physics, 2012, 14, 8599.	1.3	56
58	Synthesis and cytotoxic activity of 4-N-carboxybutyl-5-fluorocytosyl-Arg-Gln-Trp-Arg-Arg-Trp-Trp-Gln-Arg-NH2. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 4233-4237.	1.0	2
59	Catalytic and Molecular Properties of Rabbit Liver Carboxylesterase Acting on 1,8-Cineole Derivatives. Natural Product Communications, 2012, 7, 1934578X1200700.	0.2	0
60	Cinnamic Acid Derivatives Acting against Aspergillus Fungi.Taq Polymerase I a Potential Molecular Target. Natural Product Communications, 2012, 7, 1934578X1200701.	0.2	0
61	Multistep conformational interconversion mechanism of cyclododecane. A simple and fast analysis using potential energy curves. International Journal of Quantum Chemistry, 2012, 112, 2382-2391.	1.0	2
62	Theoretical study of the conformational energy hypersurface of cyclotrisarcosyl. Open Chemistry, 2012, 10, 248-255.	1.0	6
63	Searching the â€œBiologically Relevantâ€Conformation of Dopamine: A Computational Approach. Journal of Chemical Information and Modeling, 2012, 52, 99-112.	2.5	48
64	Tetrahydroisoquinolines acting as dopaminergic ligands. A molecular modeling study using MD simulations and QM calculations. Journal of Molecular Modeling, 2012, 18, 419-431.	0.8	25
65	Cinnamic acid derivatives acting against Aspergillus fungi. Taq polymerase I a potential molecular target. Natural Product Communications, 2012, 7, 1639-44.	0.2	3
66	New Small-Size Antifungal Peptides: Design, Synthesis and Antifungal Activity. Letters in Drug Design and Discovery, 2011, 8, 562-567.	0.4	8
67	Theoretical and experimental study of the interactions of annonaceous acetogenins with artificial lipid bilayers. Journal of Molecular Structure, 2011, 1003, 87-91.	1.8	9
68	Penetratin analogues acting as antifungal agents. European Journal of Medicinal Chemistry, 2011, 46, 370-377.	2.6	17
69	Synthesis and antifungal activity of N-aryl-N-benzylamines and of their homoallyl analogues. Arkivoc, 2011, 2011, 149-161.	0.3	9
70	Structure of isolated tyrosyl-glycyl-glycine tripeptide. A comparative conformational study with peptides containing an aromatic ring. Open Chemistry, 2010, 8, 566-575.	1.0	1
71	Advances in correlation between experimental and DFT/GIAO computed 13C NMR chemical shifts: A theoretical study on pentacyclic terpenoids (fernenes). Computational and Theoretical Chemistry, 2010, 953, 83-90.	1.5	13
72	New small-size peptides possessing antifungal activity. Bioorganic and Medicinal Chemistry, 2010, 18, 158-167.	1.4	48

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73	New antifungal peptides. Synthesis, bioassays and initial structure prediction by CD spectroscopy. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4808-4811.	1.0	11
74	Structural and Thermodynamic Characteristics of the Exosite Binding Pocket on the Human BACE1: A Molecular Modeling Approach. Journal of Physical Chemistry A, 2010, 114, 10261-10269.	1.1	23
75	Antifungal Activity of Extracts and Prenylated Coumarins Isolated from Baccharis darwinii Hook & Arn. (Asteraceae). Molecules, 2010, 15, 4898-4907.	1.7	28
76	Conformational and electronic study of cis-peptides (non-proline residues) occurring in natural proteins. Journal of Molecular Structure, 2009, 934, 103-111.	1.8	4
77	Penetratin and derivatives acting as antifungal agents. European Journal of Medicinal Chemistry, 2009, 44, 212-228.	2.6	35
78	Structureâ€“activity relationship of dopaminergic halogenated 1-benzyl-tetrahydroisoquinoline derivatives. European Journal of Medicinal Chemistry, 2009, 44, 4616-4621.	2.6	22
79	Tetrahydroisoquinolines as dopaminergic ligands: 1-Butyl-7-chloro-6-hydroxy-tetrahydroisoquinoline, a new compound with antidepressant-like activity in mice. Bioorganic and Medicinal Chemistry, 2009, 17, 4968-4980.	1.4	39
80	In Silico Study of Full-Length Amyloid Î² 1â^'42 Tri- and Penta-Oligomers in Solution. Journal of Physical Chemistry B, 2009, 113, 11710-11719.	1.2	81
81	Ab Initio and DFT Study of the Conformational Energy Hypersurface of Cyclic Gly-Gly-Gly. Journal of Physical Chemistry A, 2009, 113, 10818-10825.	1.1	16
82	Ring inversion in 1,4,7 cyclononatriene and analogues:Ab initio and DFT calculations and topological analysis. Journal of Computational Chemistry, 2008, 29, 280-290.	1.5	4
83	Antifungal and cytotoxic activities of some N-substituted aniline derivatives bearing a hetaryl fragment. Bioorganic and Medicinal Chemistry, 2008, 16, 794-809.	1.4	32
84	Synthesis, dopaminergic profile, and molecular dynamics calculations of N-aralkyl substituted 2-aminoindans. Bioorganic and Medicinal Chemistry, 2008, 16, 3233-3244.	1.4	10
85	Antioxidant and cytotoxic activities of canadine: Biological effects and structural aspects. Bioorganic and Medicinal Chemistry, 2008, 16, 3641-3651.	1.4	32
86	Structureâ€“antifungal activity relationship of His-Phe-Arg-Trp-Gly-Lys-Pro-Val-NH2 and analogues. Bioorganic and Medicinal Chemistry, 2008, 16, 4347-4358.	1.4	9
87	A Comprehensive Conformational Analysis of Bullacin B, a Potent Inhibitor of Complex I. Molecular Dynamics Simulations and Ab Initio Calculations. Journal of Physical Chemistry A, 2008, 112, 7426-7438.	1.1	11
88	Synthesis and Antibacterial Activity of Highly Oxygenated 1,8-Cineole Derivatives. Natural Product Communications, 2008, 3, 1934578X0800300.	0.2	4
89	Structureâ^'Antifungal Activity Relationship of Cinnamic Acid Derivatives. Journal of Agricultural and Food Chemistry, 2007, 55, 10635-10640.	2.4	76
90	Conformational Preferences of N-Acetyl-<scp>l</scp>-leucine-Nâ€˜-methylamide. Gas-Phase and Solution Calculations on the Model Dipeptide. Journal of Physical Chemistry A, 2007, 111, 10682-10691.	1.1	14

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91	Synthesis and antifungal activity of (Z)-5-arylidenerhodanines. Bioorganic and Medicinal Chemistry, 2007, 15, 484-494.	1.4	175
92	New antitumoral acetogenin â€˜Guanacone typeâ€™ derivatives: Isolation and bioactivity. Molecular dynamics simulation of diacetyl-guanacone. Bioorganic and Medicinal Chemistry, 2007, 15, 4369-4381.	1.4	19
93	Conformational and electronic study ofN-acetyl-L-isoleucine-N-methylamide using DFT and IPCM calculations. International Journal of Quantum Chemistry, 2006, 106, 1580-1595.	1.0	5
94	Synthesis and conformational analysis of His-Phe-Arg-Trp-NH2 and analogues with antifungal properties. Bioorganic and Medicinal Chemistry, 2006, 14, 7604-7614.	1.4	22
95	Structureâ€“activity relationship study of homoallylamines and related derivatives acting as antifungal agents. Bioorganic and Medicinal Chemistry, 2006, 14, 1851-1862.	1.4	44
96	Dynamics of flexible cycloalkanes.Ab initio and DFT study of the conformational energy hypersurface of cyclononane. Journal of Computational Chemistry, 2006, 27, 188-202.	1.5	10
97	Comprehensive conformational analysis of N-acetyl-l-tryptophane-N-methylamide. An ab initio and DFT study. Computational and Theoretical Chemistry, 2005, 724, 173-184.	1.5	17
98	Ab initio conformational study of vinylogues. 2-Butene, stilbene and their conjugated polyenes. Computational and Theoretical Chemistry, 2005, 731, 107-114.	1.5	7
99	Conformational study of â€˜Cis and transâ€™ N-formyl-N-methyl-l-glycine-Nâ€²-amide and N-acetyl-N-methyl-l-glycine-Nâ€²-methylamide. An ab-initio and DFT study. Computational and Theoretical Chemistry, 2005, 731, 177-185.	1.5	7
100	Gastric cytoprotective activity of ilicic aldehyde: Structureâ€“activity relationships. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3547-3550.	1.0	18
101	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. Arzneimittelforschung, 2005, 55, 123-132.	0.5	12
102	Conformational study of internally retrograde and quasi-retrograde molecules Â— An ab initio and DFT study. Canadian Journal of Chemistry, 2005, 83, 122-137.	0.6	4
103	In vitroâ€“in vivo antifungal evaluation and structureâ€“activity relationships of 3H-1,2-dithiole-3-thione derivatives. Il Farmaco, 2004, 59, 245-254.	0.9	13
104	In vitroâ€”in vivo Antifungal Evaluation and Structureâ€”Activity Relationships of 3H-1,2-Dithiole-3-thione Derivatives.. ChemInform, 2004, 35, no.	0.1	0
105	Antimicrobial activity of aqueous extracts and of berberine isolated from Berberis heterophylla. FÃ¬toterapÃ¬Â¢, 2003, 74, 702-705.	1.1	105
106	Conformational study of N-alkyl-benzyltetrahydroisoquinolines alkaloid. Computational and Theoretical Chemistry, 2003, 666-667, 109-116.	1.5	5
107	Molecular recognition and binding mechanism of N-alkyl-benzyltetrahydroisoquinolines to the D1 dopamine receptor. A computational approach. Computational and Theoretical Chemistry, 2003, 666-667, 455-467.	1.5	10
108	Conformational and electronic study of homoallylamines with inhibitory properties against polymers of fungal cell wall. Computational and Theoretical Chemistry, 2003, 666-667, 587-598.	1.5	2

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109	An ab initio conformational study on captopril. Computational and Theoretical Chemistry, 2003, 666-667, 599-608.	1.5	7
110	Exploratory conformational analysis of N-acetyl-L-Tryptophan-N-methylamide. An ab initio study. Computational and Theoretical Chemistry, 2003, 631, 277-290.	1.5	9
111	Comprehensive conformational analysis of N-acetyl-l-isoleucine-N-methylamide: an ab initio study. Computational and Theoretical Chemistry, 2003, 634, 201-213.	1.5	9
112	Conformational and electronic study ofN-phenylalkyl-3,4-dichloromaleimides: Ab initio and DFT study. International Journal of Quantum Chemistry, 2003, 93, 32-46.	1.0	6
113	In vitro antifungal activity of new series of homoallylamines and related compounds with inhibitory properties of the synthesis of fungal cell wall polymers. Bioorganic and Medicinal Chemistry, 2003, 11, 1531-1550.	1.4	108
114	Exploration of the Full Conformational Space ofN-Acetyl-l-glutamine-N-methylamide. An ab Initio and Density Functional Theory Study. Journal of Physical Chemistry A, 2003, 107, 5079-5091.	1.1	23
115	Synthesis, in vitro/in vivo Antifungal Evaluation and Structure-Activity Relationship Study of 3(2H)-Pyridazinones. Arzneimittelforschung, 2003, 53, 738-743.	0.5	0
116	Syntheses and Antitumor Targeting G1 Phase of the Cell Cycle of Benzoyldihydroisoquinolines and Related 1-Substituted Isoquinolines. Journal of Medicinal Chemistry, 2002, 45, 5058-5068.	2.9	54
117	In vitro antifungal evaluation and structureâ€“activity relationships of a new series of chalcone derivatives and synthetic analogues, with inhibitory properties against polymers of the fungal cell wall. Bioorganic and Medicinal Chemistry, 2001, 9, 1999-2013.	1.4	275
118	Partially relaxed ring closure conditions for geometrical algorithm to search the conformational space for minimum energy conformations. Computational and Theoretical Chemistry, 2001, 536, 173-188.	1.5	14
119	Peptide and protein folding. Computational and Theoretical Chemistry, 2001, 537, 319-361.	1.5	43
120	1,2-Dipolar addition model for the cytoprotective activity of selected Î±,Î²-unsaturated compounds with C˜...O functionality: an ab initio study. Computational and Theoretical Chemistry, 2001, 538, 225-233.	1.5	1
121	A search for Câ€“Hâ‹¯O type hydrogen bonds in Lamivudine (3TC). An exploratory conformational and electronic analysis. Computational and Theoretical Chemistry, 2001, 543, 185-193.	1.5	22
122	An exploratory ab initio study of the full conformational space of N -acetyl- l -cysteine- N -methylamide. Computational and Theoretical Chemistry, 2001, 540, 271-283.	1.5	30
123	An exploratory study of side-chainâ€“backbone interaction in selected conformations of N -acetyl- l -glutamate- N -methylamide. An ab initio study. Computational and Theoretical Chemistry, 2001, 543, 203-222.	1.5	14
124	A matrix representation for the geometrical algorithm to search the conformational space (GASCOS) for flexible linear molecules. Computational and Theoretical Chemistry, 2001, 571, 91-98.	1.5	10
125	SYNTHESIS AND PRELIMINARY CYTOTOXIC AND ANTIFUNGAL EVALUATION OF SOME 6-N,N-DIALKYL 2-ARYL-4(3H)-QUINAZOLINONE DERIVATIVES. Heterocyclic Communications, 2001, 7, .	0.6	8
126	Inhibitors of the fungal cell wall. Synthesis of 4-aryl-4- N -arylamine-1-butenes and related compounds with inhibitory activities on Î²(1â€“3) glucan and chitin synthases. Bioorganic and Medicinal Chemistry, 2000, 8, 691-698.	1.4	94

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127	An analytic ring closure condition for geometrical algorithm to search the conformational space. Computational and Theoretical Chemistry, 2000, 507, 89-95.	1.5	14
128	Structureâ^'Antifeedant Activity Relationship of Clerodane Diterpenoids. Comparative Study with Withanolides and Azadirachtin. Journal of Agricultural and Food Chemistry, 2000, 48, 1384-1392.	2.4	49
129	Peptide models XXIV: An ab initio study on N-formyl-L-prolinamide with trans peptide bond. The existence or non-existence of Î±L and ÏµL conformations. Computational and Theoretical Chemistry, 1999, 465, 79-91.	1.5	48
130	A potentiometric and spectrophotometric study on acidâ€"base equilibria in ethanol-aqueous solution of acetazolamide and related compounds. Talanta, 1999, 49, 859-868.	2.9	12
131	In Vitro Evaluation of Antifungal Properties of Phenylpropanoids and Related Compounds Acting Against Dermatophytes. Journal of Natural Products, 1999, 62, 1353-1357.	1.5	61
132	Characteristics of Ramachandran maps of L-alanine diamides as computed by various molecular mechanics, semiempirical and ab initio MO methods.. Computational and Theoretical Chemistry, 1998, 455, 275-301.	1.5	34
133	In Vitro Evaluation of Antifungal Properties of 8.O.4â€˜-Neolignans. Journal of Natural Products, 1997, 60, 659-662.	1.5	84
134	Structureâ^'Cytoprotective Activity Relationship of Simple Molecules Containing an Î±,Î²-Unsaturated Carbonyl System. Journal of Medicinal Chemistry, 1997, 40, 1827-1834.	2.9	33
135	Theoretical study on the conformations of 3-tigloyl-azadirachtol and azadirachtin derivatives. Computational and Theoretical Chemistry, 1997, 391, 27-38.	1.5	7
136	A theoretical study on the conformations of azadirachtin. Computational and Theoretical Chemistry, 1996, 363, 167-178.	1.5	10
137	Cytoprotective Activity of Minor Constituents ofArtemisia Douglasiana. Natural Product Research, 1995, 6, 269-280.	0.4	4
138	Structure-activity relationship in the gastric cytoprotective effect of several sesquiterpene lactones. Journal of Medicinal Chemistry, 1992, 35, 2452-2458.	2.9	80