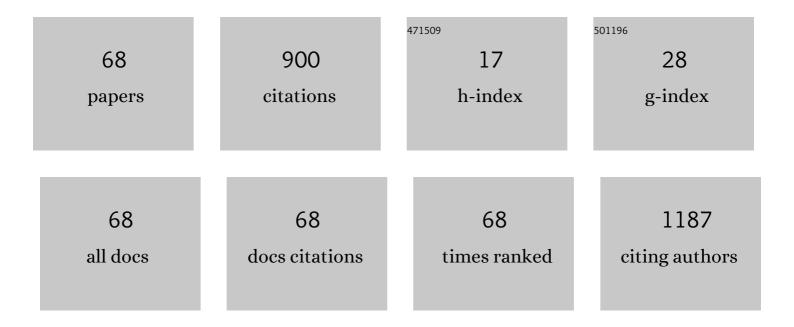
List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/1924284/publications.pdf Version: 2024-02-01



#	Article	IF	CITATIONS
1	Title is missing!. Journal of Solution Chemistry, 2000, 29, 1047-1060.	1.2	126
2	Stereodynamical Origin of Anti-Arrhenius Kinetics: Negative Activation Energy and Roaming for a Four-Atom Reaction. Journal of Physical Chemistry Letters, 2015, 6, 1553-1558.	4.6	63
3	Ruthenium Tetraammines as a Model of Nitric Oxide Donor Compounds. European Journal of Inorganic Chemistry, 2004, 2004, 1879-1885.	2.0	48
4	Theoretical investigation of the intramolecular hydrogen bond formation, non-linear optic properties, and electronic absorption spectra of the 8-hydroxiquinoline. Computational and Theoretical Chemistry, 2007, 816, 145-151.	1.5	46
5	Synthesis, characterization, and computational study of a new dimethoxy-chalcone. Journal of Molecular Modeling, 2014, 20, 2526.	1.8	42
6	On-line mass spectrometry investigation of the reduction of carbon dioxide in acidic media on polycrystalline Pt. Electrochemistry Communications, 2001, 3, 603-607.	4.7	40
7	Stereodirectional Origin of <i>anti</i> -Arrhenius Kinetics for a Tetraatomic Hydrogen Exchange Reaction: Born–Oppenheimer Molecular Dynamics for OH + HBr. Journal of Physical Chemistry A, 2016, 120, 5408-5417.	2.5	30
8	Biological and structure-activity evaluation of chalcone derivatives against bacteria and fungi. Journal of the Brazilian Chemical Society, 2013, 24, 133-144.	0.6	29
9	Methanol Solvation Effect on the Proton Rearrangement of Curcumin's Enol Forms: An <i>Ab Initio</i> Molecular Dynamics and Electronic Structure Viewpoint. Journal of Physical Chemistry C, 2016, 120, 19923-19931.	3.1	27
10	A structure–activity relationship study of HEPT-analog compounds with anti-HIV activity. Computational and Theoretical Chemistry, 2000, 530, 39-47.	1.5	26
11	Reactivity of Radicals Generated on Irradiation oftrans-[Ru(NH3)4(NO2)P(OEt)3](PF6). Journal of the American Chemical Society, 2004, 126, 2546-2555.	13.7	25
12	A quantum chemical and statistical study of flavonoid compounds with anti-HIV activity. Computational and Theoretical Chemistry, 1999, 491, 123-131.	1.5	24
13	A multiple linear regression and partial least squares study of flavonoid compounds with anti-HIV activity. Computational and Theoretical Chemistry, 2001, 541, 81-88.	1.5	24
14	A quantum chemical and statistical study of flavonoid compounds (flavones) with anti-HIV activity. European Journal of Medicinal Chemistry, 2003, 38, 929-938.	5.5	22
15	Contribution of Directional Dihydrogen Interactions in the Supramolecular Assembly of Single Crystals: Quantum Chemical and Structural Investigation of C ₁₇ H ₁₇ N ₃ O ₂ Azine. Crystal Growth and Design, 2017, 17. 5145-5153.	3.0	22
16	Antioxidant effects of polyphenolic compounds and structure-activity relationship predicted by multivariate regression tree. LWT - Food Science and Technology, 2021, 137, 110366.	5.2	20
17	A structure–activity relationship (SAR) study of synthetic neolignans and related compounds with biological activity against Escherichia coli. Computational and Theoretical Chemistry, 2002, 583, 105-116.	1.5	19
18	A study of neolignan compounds with biological activity against Paracoccidioides brasiliensis by using quantum chemical and chemometric methods. Journal of the Brazilian Chemical Society, 2003, 14, 809-814.	0.6	19

#	Article	IF	CITATIONS
19	A Structure-Activity Relationship (SAR) Study of Neolignan Compounds with Anti-schistosomiasis Activity. Journal of the Brazilian Chemical Society, 2002, 13, 300-307.	0.6	18
20	Study of the O–Ru–N bonding in trans-[Ru(NH3)4(SO4)L]+ complexes (L=imidazole, histidine and) Tj ETQq 2004, 357, 3147-3154.	0 0 0 rgBT 2.4	Overlock 10 16
21	Substitution effect on a hydroxylated chalcone: Conformational, topological and theoretical studies. Journal of Molecular Structure, 2017, 1136, 69-79.	3.6	16
22	Synthesis, structure, electronic and vibrational spectra of 9-(Diethylamino)-benzo(a)phenoxazin-7-ium-5-N-methacrylamide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 3103-3111.	3.9	15
23	A quantum chemical and photophysical study of acridine-9-N-methacrylamide. Computational and Theoretical Chemistry, 2004, 674, 213-225.	1.5	15
24	Synthesis and structural studies on (<i>E</i>)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one: a promising nonlinear optical material. RSC Advances, 2020, 10, 22542-22555.	3.6	15
25	Structure characterization of molecular complexes for non-linear optical materials I. X-ray analysis and AM1 calculations of 1 : 1 complexes of 8-hydroxiquinoline (1) and isonicotinamide (2) with 2,4,6-trinitrophenol. Zeitschrift Fur Kristallographie - Crystalline Materials, 2003, 218, 575-580.	0.8	12
26	Theoretical investigation of nitric oxide interaction with aluminum phthalocyanine. Journal of Molecular Graphics and Modelling, 2011, 29, 777-783.	2.4	9
27	Synthesis, Antimicrobial Activity and Structure-Activity Relationship of Some 5-Arylidene-thiazolidine-2,4-dione Derivatives. Journal of the Brazilian Chemical Society, 0, , .	0.6	8
28	A quantum chemical and chemometrical study of indolo[2,1- <i>b</i>]quinazoline and their analogues with cytotoxic activity against breast cancer cells. SAR and QSAR in Environmental Research, 2009, 20, 537-549.	2.2	7
29	Theoretical investigation of the interaction of glycerol with aluminum and magnesium phthalocyanines. Journal of Molecular Graphics and Modelling, 2010, 29, 206-213.	2.4	7
30	Synthesis, characterization, and computational study of the supramolecular arrangement of a novel cinnamic acid derivative. Journal of Molecular Modeling, 2017, 23, 35.	1.8	7
31	Explicit Aqueous Solvation Treatment of Epinephrine from Car–Parrinello Molecular Dynamics: Effect of Hydrogen Bonding on the Electronic Absorption Spectrum. Journal of Physical Chemistry B, 2018, 122, 8439-8450.	2.6	7
32	Molecular orbital calculations, experimental and theoretical UV spectra of granulatimides and didemnimides, biologically active polycyclic heteroaromatic alkaloids from the ascidian Didemnum granulatum. Journal of Molecular Structure, 2001, 559, 67-77.	3.6	6
33	X-ray diffraction and theoretical investigation of the Gedunin crystal structure. Journal of Molecular Structure, 2012, 1008, 83-87.	3.6	6
34	Conformation analysis of a novel fluorinated chalcone. Journal of Molecular Modeling, 2017, 23, 97.	1.8	6
35	Molecular modeling of cytotoxic activity of a new terpenoid-like bischalcone. New Journal of Chemistry, 2019, 43, 18451-18460.	2.8	6
36	Ab Initio Molecular Dynamics Simulations of Aqueous Glucosamine Solutions: Solvation Structure and Mechanism of Proton Transfer from Water to Amino Group. Journal of Physical Chemistry B, 2020, 124, 6986-6997.	2.6	6

#	Article	IF	CITATIONS
37	Effect of ortho- and para-chlorine substitution on hydroxychlorochalcone. Journal of Molecular Modeling, 2021, 27, 65.	1.8	6
38	Cyclohexanone-Based Chalcones as Alternatives for Fuel Additives. ACS Omega, 2022, 7, 11871-11886.	3.5	6
39	Structure-activity relationship study of rutaecarpine analogous active against central nervous system cancer. Journal of the Brazilian Chemical Society, 2012, 23, 2183-2190.	0.6	5
40	Effect of the Methanol Molecule on the Stabilization of C ₁₈ H ₁₈ O ₄ Crystal: Combined Theoretical and Structural Investigation. Journal of Physical Chemistry A, 2014, 118, 10048-10056.	2.5	5
41	A novel dihydrocoumarin under experimental and theoretical characterization. Journal of Molecular Modeling, 2017, 23, 315.	1.8	5
42	Conformational variability in a new terpenoid-like bischalcone: Structure and theoretical studies. Journal of Structural Chemistry, 2013, 54, 1112-1121.	1.0	4
43	Aqueous solvation study of melatonin using ab initio molecular dynamics. Journal of Molecular Liquids, 2021, 343, 117451.	4.9	4
44	An Update on the Synthesis and Pharmacological Properties of Pyrazoles Obtained from Chalcone. Current Organic Chemistry, 2022, 26, 81-90.	1.6	4
45	Crystal, Molecular, and Electronic Structure of 1-Acetyl-indoline and Derivatives. Structural Chemistry, 1998, 9, 365-373.	2.0	3
46	Structural and Theoretical Investigation of Anhydrous 3,4,5-Triacetoxybenzoic Acid. PLoS ONE, 2016, 11, e0158029.	2.5	3
47	Structural studies on dihydropyrimidine derivatives as Mycobacterium tuberculosis coenzyme-A carboxylase inhibitors. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 657-669.	0.8	3
48	A Comprehensive Topological Analysis of a Novel Flavonoid Extracted from Brazilian Cerrado Plants. ChemistrySelect, 2019, 4, 14012-14020.	1.5	3
49	A new isostructural halogenated chalcone with optical properties. Journal of Molecular Modeling, 2021, 27, 52.	1.8	3
50	Structure–activity relationship of tacrine and its analogues in relation to inhibitory activity against Alzheimer's disease. Journal of Molecular Modeling, 2019, 25, 116.	1.8	2
51	Synthesis, characterization, and computational study of a new heteroaryl chalcone. Journal of Molecular Modeling, 2020, 26, 243.	1.8	2
52	Aproximações da Mecânica Quântica no Estudo de Propriedades Moleculares. Revista Processos QuÃmicos, 2009, 3, 9-16.	0.0	2
53	Molecular modeling and nonlinear optical properties of new isostructural halogenated dihydroquinolinones. New Journal of Chemistry, 2022, 46, 14192-14204.	2.8	2
54	Theoretical investigation on ruthenium tetraazaporphyrin as potential nitric oxide carrier in biological systems. Journal of Molecular Modeling, 2013, 19, 1727-1737.	1.8	1

#	Article	IF	CITATIONS
55	Synthesis and Structural Studies of Two New Anthracene Derivatives. Crystals, 2021, 11, 934.	2.2	1
56	Estudo QuÃmico Quântico da Adsorção dos Gases O2 e H2 sobre a Ftalocianina de AlumÃnio. Revista Processos QuÃmicos, 2008, 2, 23-30.	0.0	1
57	Análise da difração dos Raios X. Revista Processos QuÃmicos, 2007, 1, 35-45.	0.0	1
58	Halogen bonds on substituted dibromonitrobenzene derivatives. Journal of Molecular Modeling, 2020, 26, 319.	1.8	0
59	Structural insights of a potential inhibition against leishmania major. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c290-c290.	0.3	Ο
60	Estudo teórico quÃmico-quântico das propriedades geométricas e fÃsico-quÃmicas das Ftalocianinas de Co, Cr, Cu, Mn, Ni, Fe, Sc, Ti, VO. Revista Processos QuAmicos, 2007, 1, 21-34.	0.0	0
61	Análise Quantitativa do Solvente em Cristais. Revista Processos QuÃmicos, 2007, 1, 42-50.	0.0	0
62	Estudo QuÃmico Quântico da Atividade da Indolo [2,1b] Quinazolina e seus Derivados Análogos Contra o Câncer de Mama. Revista Processos QuÃmicos, 2008, 2, 51-61.	0.0	0
63	Dinâmica Molecular de Car-Parrinello. Revista Processos QuÃmicos, 2009, 3, 59-72.	0.0	0
64	Estudo Teórico da Relação Estrutura Atividade da Indolo [2,1b] Quinazolina e seus Derivados Análogos Contra o Câncer de Ovário. Revista Processos QuÃmicos, 2009, 3, 24-30.	0.0	0
65	A Quantum Chemical and Chemometrical Study of Styrylbenzylsulfones and their Analogues with Citotoxic Activity against Prostate Cancer Cells. Revista Virtual De Quimica, 2016, 8, 506-514.	0.4	0
66	Estudo Teórico dos Parâmetros Estruturais da CafeÃna no Vácuo Usando Dinâmica Molecular de Car-Parrinello. Revista Processos QuÃmicos, 2017, 11, 17-24.	0.0	0
67	Theoretical Studies on the Glucosamine: A Systematic Review. Revista Virtual De Quimica, 2019, 11, 1835-1852.	0.4	Ο
68	Uma Revisão Sistemática sobre Interações de Halogênio em Derivados de Nitrobenzeno SubstituÃdos. Revista Processos QuÃmicos, 2019, 13, 23-30.	0.0	0