Hamilton Napolitano

List of Publications by Year
in descending order

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99 papers	1,498 citations	430442 18 h-index	360668 35 g-index
100 all docs	100 docs citations	100 times ranked	2064 citing authors

#	Article	IF	Citations
1	Structural insights and antioxidant analysis of a tri-methoxy chalcone with potential as a diesel-biodiesel blend additive. Fuel Processing Technology, 2022, 227, 107122.	3.7	11
2	Cyclohexanone-Based Chalcones as Alternatives for Fuel Additives. ACS Omega, 2022, 7, 11871-11886.	1.6	6
3	Synthesis, Molecular Structure, Thermal and Spectroscopic Analysis of a Novel Bromochalcone Derivative with Larvicidal Activity. Crystals, 2022, 12, 440.	1.0	7
4	Remarkable Nonlinear Properties of a Novel Quinolidone Derivative: Joint Synthesis and Molecular Modeling. Molecules, 2022, 27, 2379.	1.7	3
5	A new quinolinone-chalcone hybrid with potential antibacterial and herbicidal properties using in silico approaches. Journal of Molecular Modeling, 2022, 28, .	0.8	5
6	Molecular modeling and nonlinear optical properties of new isostructural halogenated dihydroquinolinones. New Journal of Chemistry, 2022, 46, 14192-14204.	1.4	2
7	Comparative Conformational Study of a New Terpenoid-like Chalcone. Journal of Molecular Structure, 2021, 1228, 129743.	1.8	3
8	In silico-driven identification and structural analysis of nitrodihydroquinolinone pesticide candidates with antifungal activity. Journal of Molecular Structure, 2021, 1226, 129326.	1.8	6
9	Dihydroquinoline derivative as a potential anticancer agent: synthesis, crystal structure, and molecular modeling studies. Molecular Diversity, 2021, 25, 55-66.	2.1	6
10	A new isostructural halogenated chalcone with optical properties. Journal of Molecular Modeling, 2021, 27, 52.	0.8	3
11	Effect of ortho- and para-chlorine substitution on hydroxychlorochalcone. Journal of Molecular Modeling, 2021, 27, 65.	0.8	6
12	Structural insights into the biological activity of a thioxopyrimidine derivative. Journal of Molecular Modeling, 2021, 27, 73.	0.8	0
13	Insights on a new sulfonamide chalcone with potential antineoplastic application. Journal of Molecular Modeling, 2021, 27, 211.	0.8	3
14	Synthesis and Structural Studies of Two New Anthracene Derivatives. Crystals, 2021, 11, 934.	1.0	1
15	Aqueous solvation study of melatonin using ab initio molecular dynamics. Journal of Molecular Liquids, 2021, 343, 117451.	2.3	4
16	Second-order nonlinear optical properties of two chalcone derivatives: insights from sum-over-states. Physical Chemistry Chemical Physics, 2021, 23, 6128-6140.	1.3	16
17	Comparative Study of Chalcones and Their Potential as Additives for Biofuels. Energy & Fuels, 2021, 35, 552-560.	2.5	6
18	Molecular modelling and optical properties of a novel fluorinated chalcone. Arabian Journal of Chemistry, 2020, 13, 3362-3371.	2.3	12

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19	On the potential as nonlinear optical material of a new chalcone derivative and its crystal and topological analysis. Journal of Molecular Structure, 2020, 1201, 127131.	1.8	5
20	Growth and characterization of a new chlorine substituted chalcone: A third order nonlinear optical material. Journal of Molecular Structure, 2020, 1201, 127137.	1.8	10
21	Enhanced nonlinear optics properties of a bromine chalcone from a novel polymorph. Chemical Physics Letters, 2020, 738, 136852.	1.2	8
22	Halogen bonds on substituted dibromonitrobenzene derivatives. Journal of Molecular Modeling, 2020, 26, 319.	0.8	0
23	Synthesis, characterization, and computational study of a new heteroaryl chalcone. Journal of Molecular Modeling, 2020, 26, 243.	0.8	2
24	Structural comparison of five new halogenated dihydroquinoline-4(1H)-ones. Journal of Molecular Structure, 2020, 1219, 128559.	1.8	2
25	Synthesis and structural studies on (E)-3-(2,6-difluorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one: a promising nonlinear optical material. RSC Advances, 2020, 10, 22542-22555.	1.7	15
26	Theoretical study of solvent effects on the hyperpolarizabilities of two chalcone derivatives. Revista Colombiana De Quimica, 2020, 49, 33-39.	0.2	6
27	Benzenesulfonyl incorporated chalcones: Synthesis, structural and optical properties. Journal of Molecular Structure, 2020, 1208, 127845.	1.8	18
28	On the in silico and in vitro anticancer activity of sulfonamide chalcones: potential JNKK3 inhibitors. New Journal of Chemistry, 2020, 44, 3294-3309.	1.4	10
29	Machine learning prediction of the potential pesticide applicability of three dihydroquinoline derivatives: Syntheses, crystal structures and physical properties. Journal of Molecular Structure, 2020, 1206, 127732.	1.8	12
30	Synthesis, crystal structure and molecular modeling of a novel Chalcone-Quinolone Hybrid. Journal of Molecular Structure, 2020, 1217, 128355.	1.8	2
31	New Halogen Chalcone with Potential for Application in Biofuels. Energy & Fuels, 2020, 34, 5958-5968.	2.5	11
32	Microscopic Image Segmentation to Quantification of Leishmania Infection in Macrophages. Fronteiras, 2020, 9, 488-498.	0.0	2
33	Solvent-driven structural adaptation in a novel anticancer sulfonamide chalcone. Journal of Molecular Structure, 2019, 1175, 389-397.	1.8	14
34	Different reactivity to glutathione but similar tumor cell toxicity of chalcones and their quinolinone analogues. Medicinal Chemistry Research, 2019, 28, 1448-1460.	1.1	15
35	Sulphonamide chalcones: Conformationally diverse yet optically similar. Journal of Molecular Structure, 2019, 1198, 126896.	1.8	9
36	A comprehensive study on crystal structure of a novel sulfonamide-dihydroquinolinone through experimental and theoretical approaches. Journal of Molecular Modeling, 2019, 25, 205.	0.8	7

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37	Experimental and molecular modeling study of a novel arylsulfonamide chalcone. Journal of Molecular Modeling, 2019, 25, 208.	0.8	4
38	Hyperpolarizability studies and Hirshfeld surface analysis of two heterocyclic chalcones. Journal of Molecular Modeling, 2019, 25, 324.	0.8	4
39	Benzodioxol Group Driving Supramolecular Arrangement of Two Tri-Methoxy Chalcones onto Î²-Secretase 1 Enzyme Active Site. Journal of the Brazilian Chemical Society, 2019, , .	0.6	1
40	Flavonoids from Brazilian Cerrado: Biosynthesis, Chemical and Biological Profile. Molecules, 2019, 24, 2891.	1.7	10
41	A Comprehensive Topological Analysis on a New Bromine-Chalcone with Potential Nonlinear Optical Properties. Journal of Physical Chemistry A, 2019, 123, 8632-8643.	1.1	5
42	Structural studies on dihydropyrimidine derivatives as Mycobacterium tuberculosis coenzyme-A carboxylase inhibitors. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 657-669.	0.4	3
43	Synthesis, conformational analysis and molecular docking studies on three novel dihydropyrimidine derivatives. Journal of Molecular Structure, 2019, 1192, 274-287.	1.8	9
44	Chalcone as Potential Nonlinear Optical Material: A Combined Theoretical, Structural, and Spectroscopic Study. Journal of Physical Chemistry C, 2019, 123, 5931-5941.	1.5	40
45	Analysis of two novel 1â€“4 quinolinone structures with bromine and nitrobenzyl ligands. Journal of Molecular Modeling, 2019, 25, 55.	0.8	6
46	Chalcone as Potential Nonlinear Optical Material: A Combined Theoretical, Structural and Spectroscopic Study. Journal of Physical Chemistry A, 2019, , .	1.1	6
47	Molecular modeling of cytotoxic activity of a new terpenoid-like bischalcone. New Journal of Chemistry, 2019, 43, 18451-18460.	1.4	6
48	A Comprehensive Topological Analysis of a Novel Flavonoid Extracted from Brazilian Cerrado Plants. ChemistrySelect, 2019, 4, 14012-14020.	0.7	3
49	Using the Supermolecule Approach To Predict the Nonlinear Optics Potential of a Novel Asymmetric Azine. Journal of Physical Chemistry A, 2019, 123, 153-162.	1.1	20
50	Structural insights into a novel anticancer sulfonamide chalcone. New Journal of Chemistry, 2018, 42, 3426-3434.	1.4	26
51	Molecular structure of hybrid imino-chalcone in the solid state: X-ray diffraction, spectroscopy study and third-order nonlinear optical properties. Journal of Molecular Structure, 2018, 1157, 210-221.	1.8	19
52	A novel potential anticancer chalcone: Synthesis, crystal structure and cytotoxic assay. Journal of Molecular Structure, 2018, 1168, 309-315.	1.8	11
53	Synthesis, characterization, and computational study of the supramolecular arrangement of a novel cinnamic acid derivative. Journal of Molecular Modeling, 2017, 23, 35.	0.8	7
54	Substitution effect on a hydroxylated chalcone: Conformational, topological and theoretical studies. Journal of Molecular Structure, 2017, 1136, 69-79.	1.8	16

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55	Conformation analysis of a novel fluorinated chalcone. Journal of Molecular Modeling, 2017, 23, 97.	0.8	6
56	Theoretical investigations of nonlinear optical properties of two crystalline acetamides structures including polarization effects of their environment. Chemical Physics Letters, 2017, 681, 110-123.	1.2	24
57	Synthesis, structural characterization and computational study of a novel amino chalcone: a potential nonlinear optical material. New Journal of Chemistry, 2017, 41, 1744-1754.	1.4	61
58	A novel dihydrocoumarin under experimental and theoretical characterization. Journal of Molecular Modeling, 2017, 23, 315.	0.8	5
59	The solid state structure and environmental polarization effect of a novel asymmetric azine. New Journal of Chemistry, 2017, 41, 11361-11371.	1.4	22
60	Contribution of Directional Dihydrogen Interactions in the Supramolecular Assembly of Single Crystals: Quantum Chemical and Structural Investigation of C₁₇H₁₇N₃O₂ Azine. Crystal Growth and Design, 2017, 17, 5145-5153.	1.4	22
61	Solid state characterization and theoretical study of non-linear optical properties of a Fluoro-N-Acylhydrazide derivative. PLoS ONE, 2017, 12, e0175859.	1.1	26
62	Structural and Theoretical Investigation of Anhydrous 3,4,5-Triacetoxybenzoic Acid. PLoS ONE, 2016, 11, e0158029.	1.1	3
63	Theoretical study on the third-order nonlinear optical properties and structural characterization of 3-Acetyl-6-Bromocoumarin. Chemical Physics Letters, 2016, 653, 122-130.	1.2	49
64	Polarization effects on the third-order nonlinear optical properties of two polymorphs of enamine derivative. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	20
65	Synthesis, characterization, and third-order nonlinear optical properties of a new neolignane analogue. RSC Advances, 2016, 6, 79215-79227.	1.7	31
66	InovaÃ§Ã£o e Biotecnologia na Biodiversidade do Cerrado. Fronteiras, 2016, 5, 162.	0.0	1
67	How genomics is contributing to the fight against artemisinin-resistant malaria parasites. Acta Tropica, 2015, 148, 1-7.	0.9	21
68	DFT investigation on hydrogen bonding in cyclohexane-1,2,3,4,5-pentol crystal structure. Journal of Structural Chemistry, 2014, 55, 1596-1606.	0.3	3
69	Synthesis, characterization, and computational study of a new dimethoxy-chalcone. Journal of Molecular Modeling, 2014, 20, 2526.	0.8	42
70	Effect of the Methanol Molecule on the Stabilization of C₁₈H₁₈O₄ Crystal: Combined Theoretical and Structural Investigation. Journal of Physical Chemistry A, 2014, 118, 10048-10056.	1.1	5
71	Conformational variability in a new terpenoid-like bischalcone: Structure and theoretical studies. Journal of Structural Chemistry, 2013, 54, 1112-1121.	0.3	4
72	An additional methylene group driving the conformation and assembly of two arylsulfonamidepara-alkoxychalcone hybrids. Acta Crystallographica Section C: Crystal Structure Communications, 2013, 69, 267-272.	0.4	4

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73	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
74	(2E)-3-(4-Methylphenyl)-1-(pyridin-3-yl)prop-2-en-1-one. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2585-o2585.	0.2	0
75	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
76	X-ray diffraction and theoretical investigation of the Gedunin crystal structure. Journal of Molecular Structure, 2012, 1008, 83-87.	1.8	6
77	(E)-1-(4-Methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2126-o2126.	0.2	6
78	Theoretical investigation of the interaction of glycerol with aluminum and magnesium phthalocyanines. Journal of Molecular Graphics and Modelling, 2010, 29, 206-213.	1.3	7
79	Determination of the molecular weight of proteins in solution from a single small-angle X-ray scattering measurement on a relative scale. Journal of Applied Crystallography, 2010, 43, 101-109.	1.9	389
80	Sugarcane Phosphoribosyl Pyrophosphate Synthetase: Molecular Characterization of a Phosphate-independent PRS. Plant Molecular Biology Reporter, 2008, 26, 301-315.	1.0	7
81	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
82	Synthesis, crystal structure and magnetic properties of a new dinuclear copper(II) amino acid complex [Cu2(l-arg)2(Î¼-HPO4-O)(Î¼-HPO4-O,Oâ€²)(Î¼-OH)]â˜Â·(H3O)+Â·(H2O)6. Polyhedron, 2007, 26, 5001-5008.	1.0	13
83	Estudo teÃ³rico quÃmico-quÂ¢ntico das propriedades geomÃ©tricas e fÃsico-quÃmicas das Ftalocianinas de Co, Cr, Cu, Mn, Ni, Fe, Sc, Ti, VO. Revista Processos QuÃmicos, 2007, 1, 21-34.	0.0	0
84	AnÃ¡lise da difraÃ§Ã£o dos Raios X. Revista Processos QuÃmicos, 2007, 1, 35-45.	0.0	1
85	Structural studies of 4-aminoantipyrine derivatives. Journal of Molecular Structure, 2005, 752, 32-39.	1.8	70
86	The first synthesis of pyridinium N-benzoylguanidines by bismuth- and mercury-promoted guanylation of N-iminopyridinium ylide with thioureas. Tetrahedron, 2005, 61, 10536-10540.	1.0	27
87	1-(4-Methoxyphenyl)-2-(6-methyl-2-nitro-3-pyridyloxy)propan-1-one. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o247-o249.	0.2	0
88	The polyfunctionalized enaminone ethyl [(Z)-2-(2,2-dimethyl-4,6-dioxo-1,3-dioxan-5-ylidenemethyl)-1-methyl-3-oxo-but-1-enylamino]acetate. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, o2479-o2481.	0.2	0
89	1-(4-Methoxyphenyl)-2-(2-nitrophenoxy)propan-1-one. Acta Crystallographica Section E: Structure Reports Online, 2004, 60, o2498-o2500.	0.2	0
90	Redetermination of skimmianine: a new inhibitor against the Leishmania APRT enzyme. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o1503-o1505.	0.2	9

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91	Redetermination and comparative structural study of isopimpinellin: a new inhibitor against the Leishmania APRT enzyme. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o1506-o1508.	0.2	7
92	3-(5,7-Dimethoxy-2,2-dimethyl-2H-benzo[b]pyran-6-yl)propionic acid: a potential inhibitor against Leishmania. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o1575-o1577.	0.2	0
93	Reaction of acyclic enaminones with methoxymethylene meldrum's acid: synthetic and structural implications. Journal of the Brazilian Chemical Society, 2003, 14, 107-112.	0.6	11
94	Study of N -benzoyl-activation in the HgCl 2 -promoted guanylation reaction of thioureas. Synthesis and structural analysis of N -benzoyl-guanidines. Tetrahedron, 2001, 57, 1671-1675.	1.0	55
95	Hirshfeld Surfaces and Nonlinear Optics on Two Conformers of a Heterocyclic Chalcone. Journal of the Brazilian Chemical Society, 0, , .	0.6	8
96	The Influence of Methoxy and Ethoxy Groups on Supramolecular Arrangement of Two Methoxy-chalcones. Journal of the Brazilian Chemical Society, 0, , .	0.6	6
97	Synthesis, Characterization and Conformational Analysis of Two Novel 4(1H)â€‘Quinolinones. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
98	A New Synthetic Route and Comprehensive Topological Study of a Benzimidazole Derivative. Journal of the Brazilian Chemical Society, 0, , .	0.6	0
99	Synthesis and Molecular Modeling Study of Two Bromo-Dimethoxybenzaldehydes. Journal of the Brazilian Chemical Society, 0, , .	0.6	2