Abdelkader Chouaih

List of Publications by Year
in descending order

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41 papers	624 citations	623188 14 h-index	642321 23 g-index
41 all docs	41 docs citations	41 times ranked	421 citing authors

#	Article	IF	Citations
1	Theoretical and Experimental Electrostatic Potential around the m-Nitrophenol Molecule. Molecules, 2015, 20, 4042-4054.	1.7	111
2	On the molecular structure, vibrational spectra, HOMO-LUMO, molecular electrostatic potential, UVâ€“Vis, first order hyperpolarizability, and thermodynamic investigations of 3-(4-chlorophenyl)-1-(1yridine-3-yl) prop-2-en-1-one by quantum chemistry calculations. Journal of Molecular Structure, 2018, 1155, 484-495.	1.8	57
3	Synthesis, crystal structure, spectroscopic characterization and nonlinear optical properties of (Z)-N'-(2,4-dinitrobenzylidene)-2-(quinolin-8-yloxy) acetohydrazide. Journal of Molecular Structure, 2019, 1194, 112-123.	1.8	50
4	Synthesis, crystal structure, vibrational spectral investigation, intermolecular interactions, chemical reactivity, NLO properties and molecular docking analysis on (E)-N-(4-nitrobenzylidene)-3-chlorobenzenamine: A combined experimental and theoretical study. Journal of Molecular Structure, 2021, 1240, 130589.	1.8	37
5	Synthesis, PXRD structural determination, Hirshfeld surface analysis and DFT/TD-DFT investigation of 3N-ethyl-2Nâ€™-(2-ethylphenylimino) thiazolidin-4-one. Journal of Molecular Structure, 2019, 1189, 8-20.	1.8	28
6	Synthesis, crystal structure, Hirshfeld surface analysis, spectral characterization, reduced density gradient and nonlinear optical investigation on (E)-N'-(4-nitrobenzylidene)-2-(quinolin-8-yloxy) acetohydrazide monohydrate: A combined experimental and DFT approach. Journal of Molecular Structure, 2020, 1222, 128952.	1.8	25
7	DFT studies of disubstituted diphenyldithiophosphates of nickel(II): Structural and some spectral parameters. Journal of Molecular Structure, 2019, 1185, 212-218.	1.8	23
8	Spectroscopic (FT-IR,1H and 13C NMR) characterization and density functional theory calculations for (Z)-5-(4-nitrobenzyliden)-3-N(2-ethoxyphenyl)-2-thioxo-thiazolidin-4-one (ARNO). Journal of Molecular Structure, 2017, 1147, 569-581.	1.8	22
9	2-thioxo- 3N-(2-methoxyphenyl)Âå˜5 [4â€²-methyl -3â€²N -(2â€²-methoxyphenyl) thiazol-2â€²(3â€²H)-ylidene] thiazolidin-4-one: Synthesis, characterization, X-ray single crystal structure investigation and quantum chemical calculations. Journal of Molecular Structure, 2019, 1177, 186-192.	1.8	18
10	Crystal Structure, Hirshfeld Surface Analysis and Computational Studies of Thiazolidin-4-one derivative: (Z)-5-(4-Chlorobenzylidene)-3-(2-ethoxyphenyl)-2-thioxothiazolidin-4-one. Acta Chimica Slovenica, 2016, 63, 619-626.	0.2	17
11	Synthesis and Molecular Structure Investigation by DFT and X-Ray Diffraction of ARNO. Journal of Chemical Crystallography, 2011, 41, 1729-1736.	0.5	15
12	Synthesis and Structural Determination of Novel 5-Arylidene-3-N(2-alkyloxyaryl)-2-thioxothiazolidin-4-ones. Molecules, 2012, 17, 3501-3509.	1.7	15
13	Synthesis and evaluation of new isatin-aminorhodanine hybrids as PIM1 and CLK1 kinase inhibitors. Journal of Molecular Structure, 2019, 1192, 82-90.	1.8	15
14	Synthesis, X-Ray Structure Determination and Related Physical Properties of Thiazolidinone Derivative by DFT Quantum Chemical Method. Acta Chimica Slovenica, 2019, 66, 490-500.	0.2	15
15	Capability of X-ray diffraction to the determination of the macroscopic linear susceptibility in a crystalline environment: the case of 3-Methyl 4-Nitropyridine N-oxide (POM). Journal of Molecular Structure, 2005, 738, 33-38.	1.8	14
16	Molecular Structure, Experimental and Theoretical Vibrational Spectroscopy, (HOMO-LUMO, NBO) Investigation, (RDG, AIM) Analysis, (MEP, NLO) Study and Molecular Docking of Ethyl-2-{[4-Ethyl-5-(Quinolin-8-yloxyMethyl)-4H-1,2,4-Triazol-3-yl] Sulfanyl} Acetate. Polycyclic Aromatic Compounds, 2023, 43, 2152-2176.	1.4	14
17	Experimental spectral characterization, Hirshfeld surface analysis, DFT/TD-DFT calculations and docking studies of (2Z,5Z)-5-(4-nitrobenzylidene)-3-N(2-methoxyphenyl)-2-Nâ€™(2-methoxyphenylimino) thiazolidin-4-one. Heliyon, 2020, 6, e05754.	1.4	13
18	Solvent Effects on Molecular Structure, Vibrational Frequencies, and NLO Properties of N-(2,3-Dichlorophenyl)-2-Nitrobenzeneâ€“Sulfonamide: a Density Functional Theory Study. Brazilian Journal of Physics, 2016, 46, 371-383.	0.7	12

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19	Synthesis, molecular and solid state structure of 5-(5-nitro furan-2-ylmethylen), 3- N -(2-methoxy) Tj ETQq1 1 0.784314 rgBT /Overlock 1 Journal of Molecular Structure, 2017, 1143, 259-264.	1.8	12
20	Conformational, spectroscopic and nonlinear optical investigations on 1-(4-chlorophenyl)-3-(4-chlorophenyl)-2-propen-1-one: a DFT study. Indian Journal of Physics, 2017, 91, 501-511.	0.9	10
21	Synthesis, structural determination, molecular docking and biological activity of 1-(4-fluorobenzyl)-5-bromolindolin-2,3-dione. Journal of Molecular Structure, 2022, 1265, 133342.	1.8	10
22	Molecular structure investigation of Z-3N(2-ethoxyphenyl)-2-Nâ€²(2-ethoxyphenyl)-imino-thiazolidin-4-one by ab initio, DFT and X-ray diffraction methods. Journal of Structural Chemistry, 2015, 56, 1373-1378.	0.3	9
23	Synthesis, structural, spectroscopic, intermolecular interactions, kinetic stability, charge transfer method with DNA bases and electronic properties of (E)-3-(2-ethoxyphenyl)-5-(3-(2-methoxyphenyl)-4methylthiazol-2(3H)-ylidene)-2-thioxothiazolidin-4-one: Computational and experimental approach. Journal of Molecular Structure, 2022, 1262, 133002.	1.8	9
24	Determination of electrostatic parameters of a coumarin derivative compound C₁₇H₁₃NO₃by x-ray and density functional theory. Chinese Physics B, 2015, 24, 106103.	0.7	8
25	Synthesis, characterization, single crystal X-ray and DFT analysis of disubstituted phosphorodithioates. Journal of Molecular Structure, 2018, 1157, 708-715.	1.8	8
26	Molecular Structure, FT-IR, NMR (13C/1H), UV-Vis Spectroscopy and DFT Calculations on (2Z,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 467 thiazolidin-4-one. South African Journal of Chemistry, 2019, 72, 176-188.	0.3	8
27	Crystal and molecular structure of (2Z,5Z)-3-(2-methoxyphenyl)-2-[(2-methoxyphenyl)imino]-5-(4-nitrobenzylidene)thiazolidin-4-one. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 511-514.	0.2	6
28	Crystal structure and Hirshfeld surface analysis of ethyl 2-{[4-ethyl-5-(quinolin-8-yloxymethyl)-4H-1,2,4-triazol-3-yl]sulfanyl}acetate. Acta Crystallographica Section E: Crystallographic Communications, 2017, 73, 173-176.	0.2	6
29	Electron Charge Density Distribution from X-ray Diffraction Study of the M-Nitrophenol Compound in the Monoclinic Form. International Journal of Molecular Sciences, 2007, 8, 103-115.	1.8	5
30	Electron Charge Density Distribution from X-Ray Diffraction Study of the 4-Methoxybenzenecarbothioamide Compound. Journal of Crystallography, 2013, 2013, 1-7.	0.0	5
31	Quantum chemical investigation of spectroscopic, electronic and NLO properties of (1E,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 121-131.	0.1	5
32	Synthesis, structural determination, Hirshfeld surface analysis, 3D energy frameworks, electronic and (static, dynamic) NLO properties of o-Nitroacetanilide (o-NAA): A combined experimental and quantum chemical study. Inorganic Chemistry Communication, 2021, 133, 108884.	1.8	5
33	Crystal structure of (2Z,5Z)-3-(4-methoxyphenyl)-2-[(4-methoxyphenyl)imino]-5-[(E)-3-(2-nitrophenyl)allylidene]-1,3-thiazolidin-4-one. Acta Crystallographica Section E: Crystallographic Communications, 2016, 72, 155-157.	0.2	4
34	FTIR, NMR and UVâ€“Visible Spectral Investigations, Theoretical Calculations, Topological Analysis, Chemical Stablity, and Molecular Docking Study on Novel Bioactive Compound: The 5-(5-Nitro) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 14 Thiazolidin-4-One. Polycyclic Aromatic Compounds, 2023, 43, 4685-4706.	1.4	4
35	Structural and electron charge density studies of a nonlinear optical compound 4,4 di-methyl amino cyano biphenyl. Chinese Physics B, 2014, 23, 016103.	0.7	3
36	Triflic Acid Functionalized Carbon@Silica Composite: Synthesis and Applications in Organic Synthesis; DFT Studies of Indeno[1,2â€b]indole. ChemistrySelect, 2020, 5, 2201-2213.	0.7	2

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37	Molecular and crystal structure, Hirshfeld analysis and DFT investigation of 5-(furan-2-ylmethylidene)thiazolo[3,4-a]benzimidazole-2-thione. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1832-1836.	0.2	2
38	Evolution structurale en fonction de la tempÃ©rature du composÃ© LiNbO3. European Journal of Control, 2006, 31, 431-438.	1.6	1
39	Synthesis, X-Ray Structure Determination and Related Physical Properties of Thiazolidinone Derivative by DFT Quantum Chemical Method. Acta Chimica Slovenica, 2019, 66, 490-500.	0.2	1
40	A Comparative X-ray Diffraction Study and Ab Initio Calculation on RU60358, a New Pyrethroid. International Journal of Molecular Sciences, 2006, 7, 255-265.	1.8	0
41	Mol-ecular and crystal structure, Hirshfeld analysis and DFT investigation of 5-(furan-2-yl-methyl-idene)thia-zolo[3,4-]benzimidazole-2-thione. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1832-1836.	0.2	0