

Mohamed El Hafi

List of Publications by Year in descending order

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papers

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149
citing authors

#	ARTICLE	IF	CITATIONS
1	Synthesis, crystal structure, DFT calculations, Hirshfeld surface analysis, energy frameworks, molecular dynamics and docking studies of novel isoxazolequinoxaline derivative (IZQ) as anti-cancer drug. Journal of Molecular Structure, 2021, 1232, 130004.	3.6	40
2	Synthesis, structural analysis and corrosion inhibition application of a new indazole derivative on mild steel surface in acidic media complemented with DFT and MD studies. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 617, 126373.	4.7	32
3	Synthesis, X-ray, spectroscopic characterization, DFT and antioxidant activity of 1,2,4-triazolo[1,5-a]pyrimidine derivatives. Journal of Molecular Structure, 2019, 1177, 131-142.	3.6	18
4	Solvent induced supramolecular polymorphism in Cu(II) coordination complex built from 1,2,4-triazolo[1,5-a]pyrimidine: Crystal structures and anti-oxidant activity. Journal of Inorganic Biochemistry, 2020, 208, 111092.	3.5	15
5	Palladium-catalyzed regioselective direct CH arylation of 1-pyrazolo[3,4-d]pyrimidines. Comptes Rendus Chimie, 2017, 20, 927-933.	0.5	10
6	Spectral, DFT/B3LYP and molecular docking analyses on ethyl 2-(5-methyl-1,2,4-triazolo[1,5-a]pyrimidin-7-yl)pent-4-enoate. Journal of Molecular Structure, 2020, 1206, 127680.	3.6	9
7	Synthesis of diverse isoxazolylamino-2-(aryl)acetamides using one-pot Multicomponent Reactions: X-ray, Hirshfeld analysis and DFT modeling. Journal of Molecular Structure, 2020, 1201, 127178.	3.6	5
8	Synthesis, Crystal structure, Hirshfeld surface analysis, Spectral characterizations and Quantum computational assessments of 1-hydroxy-3-methyl-1H-pyrido[2,1-b]quinazolin-11-one. Journal of Molecular Structure, 2021, , 131592.	3.6	5
9	Crystal structure and Hirshfeld surface analysis of 1-benzyl-3-(prop-2-yn-1-yl)-2,3-dihydro-1H-1,3-benzodiazol-2-one. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1842-1846.	0.5	3
10	Crystal structure and Hirshfeld surface analysis of 5-[(5-nitro-1H-indazol-1-yl)methyl]-3-phenyl-4,5-dihydroisoxazole. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 71-74.	0.5	3
11	One-step Synthesis of novel N1-substituted benzimidazole derivatives: Experimental and theoretical investigations. Journal of Heterocyclic Chemistry, 0, , .	2.6	3
12	A new synthetic route for the preparation of 2,2,5-trimethyl-7-oxo-4,7-dihydro-6,7-bipyrazolo[1,5-a]pyrimidine]tricarbonitrile, structural elucidation, Hirshfeld surface analysis, energy framework, density functional theory and molecular docking investigations. Journal of the Chinese Chemical Society, 2022, 69, 717-730.	1.4	3
13	Synthesis, structural elucidation, and antioxidant activity of new phenolic derivatives containing piperidine moiety: Experimental and theoretical investigations. Journal of Heterocyclic Chemistry, 2021, 58, 1268-1277.	2.6	2
14	Crystal structure and Hirshfeld surface analysis of N-(tert-butyl)-2-(phenylethynyl)imidazo[1,2-a]pyridin-3-amine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1564-1567.	0.5	2
15	Crystal structure and Hirshfeld surface analysis of 3-(4-methoxyphenyl)-1-methyl-4-phenyl-1H-pyrazolo[3,4-d]pyrimidine. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 638-641.	0.5	1
16	Crystal structure, Hirshfeld surface analysis and interaction energy calculation of 4-(furan-2-yl)-2-(6-methyl-2,4-dioxopyran-3-ylidene)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepine. Acta Crystallographica Section E: Crystallographic Communications, 2021, 77, 834-838.	0.5	0