

Mohamed El Hafi

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	A new synthetic route for the preparation of 2,2â€²,5â€²â€¢trimethylâ€¢oxoâ€¢4,7â€¢dihydroâ€¢[6,7â€¢1 <i>a</i>]pyrimidine]â€¢3,3â€¢dicarbonitrile, structural elucidation, Hirshfeld surface analysis, energy framework, density functional theory and molecular docking investigations. <i>Journal of the Chinese Chemical Society</i> , 2022, 69, 717-730.	1.4	3
2	Synthesis, structural elucidation, and antioxidant activity of new phenolic derivatives containing piperidine moiety: Experimental and theoretical investigations. <i>Journal of Heterocyclic Chemistry</i> , 2021, 58, 1268-1277.	2.6	2
3	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. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021, 617, 126373.	4.7	32
4	Synthesis, crystal structure, DFT calculations, Hirshfeld surface analysis, energy frameworks, molecular dynamics and docking studies of novel isoxazolequinoxaline derivative (IZQ) as anti-cancer drug. <i>Journal of Molecular Structure</i> , 2021, 1232, 130004.	3.6	40
5	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-1 <i>H</i> -1,5-benzodiazepine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 834-838.	0.5	0
6	Synthesis, Crystal structure, Hirshfeld surface analysis, Spectral characterizations and Quantum computational assessments of 1-hydroxy-3-methyl-11 <i>H</i> -pyrido[2,1-b] quinazolin-11-one. <i>Journal of Molecular Structure</i> , 2021, , 131592.	3.6	5
7	Synthesis of diverse isoxazolylamino-2-(aryl)acetamides using one-pot Multicomponent Reactions: X-ray, Hirshfeld analysis and DFT modeling. <i>Journal of Molecular Structure</i> , 2020, 1201, 127178.	3.6	5
8	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. <i>Journal of Molecular Structure</i> , 2020, 1206, 127680.	3.6	9
9	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. <i>Journal of Inorganic Biochemistry</i> , 2020, 208, 111092.	3.5	15
10	Synthesis, X-ray, spectroscopic characterization, DFT and antioxidant activity of 1,2,4-triazolo[1,5-a]pyrimidine derivatives. <i>Journal of Molecular Structure</i> , 2019, 1177, 131-142.	3.6	18
11	Crystal structure and Hirshfeld surface analysis of <math>\text{N}(\text{H})-\text{tert-butyl}-2-(\text{phenylethynyl})\text{imidazo}[1,2-\text{i}]\text{a}\text{mino}\text{pyridin-3-amine}. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1564-1567.	0.5	2
12	Crystal structure and Hirshfeld surface analysis of 5-[5-nitro-1 <i>H</i> -indazol-1-yl)methyl]-3-phenyl-4,5-dihydroisoxazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 71-74.	0.5	3
13	Crystal structure and Hirshfeld surface analysis of 3-(4-methoxyphenyl)-1-methyl-4-phenyl-1 <i>H</i> -pyrazolo[3,4-d]pyrimidine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 638-641.	0.5	1
14	Crystal structure and Hirshfeld surface analysis of 1-benzyl-3-(prop-2-yn-1-yl)-2,3-dihydro-1 <i>H</i> -1,3-benzodiazol-2-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1842-1846.	0.5	3
15	Palladium-catalyzed regioselective direct CH arylation of pyrazolo[3,4-d]pyrimidines. <i>Comptes Rendus Chimie</i> , 2017, 20, 927-933.	0.5	10
16	One-step Synthesis of novel N1 substituted benzimidazole derivatives: Experimental and theoretical investigations. <i>Journal of Heterocyclic Chemistry</i> , 0, , .	2.6	3