

Youness El Bakri

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Electrochemical, DFT and MD simulation of newly synthesized triazolotriazepine derivatives as corrosion inhibitors for carbon steel in 1M HCl. Journal of Molecular Liquids, 2019, 274, 759-769.	4.9	49
2	Synthesis, NMR characterization, DFT and anti-corrosion on carbon steel in 1M HCl of two novel 1,5-benzodiazepines. Journal of Molecular Structure, 2019, 1182, 123-130.	3.6	30
3	Potential antidiabetic activity and molecular docking studies of novel synthesized 3,6-dimethyl-5-oxo-pyrido[3,4-f][1,2,4]triazepino[2,3-a]benzimidazole and 10-amino-2-methyl-4-oxo-pyrimido[1,2-a]benzimidazole derivatives. Journal of Molecular Modeling, 2018, 24, 179.	1.8	28
4	Synthesis, crystal structure, DFT, molecular dynamics simulation and evaluation of the anticorrosion performance of a new pyrazolotriazole derivative. Journal of Molecular Structure, 2019, 1176, 290-297.	3.6	27
5	Synthesis, biological activity and molecular modeling of a new series of condensed 1,2,4-triazoles. Bioorganic Chemistry, 2019, 92, 103193.	4.1	23
6	Synthesis, crystal structure, spectroscopic characterization, Hirshfeld surface analysis, and DFT calculations of 1,4-dimethyl-2-oxo-pyrimido[1,2-a]benzimidazole hydrate. Journal of Molecular Structure, 2018, 1152, 154-162.	3.6	16
7	In silico approach for potential antimicrobial agents through antiviral, molecular docking, molecular dynamics, pharmacokinetic and bioactivity predictions of galactopyranoside derivatives. Arab Journal of Basic and Applied Sciences, 2022, 29, 99-112.	2.1	15
8	1-Benzyl-3-methylquinoxalin-2(1H)-one. IUCrData, 2018, 3, .	0.3	13
9	Synthesis, crystal structure, Hirshfeld surface analysis, and DFT calculations of new 1-[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl]-6-methoxy-1H-benzimidazol-2(3H)-one. Chemical Data Collections, 2018, 17-18, 472-482.	2.3	10
10	Synthesis, anticancer evaluation in vitro, DFT, Hirshfeld surface analysis of some new 4-(1,3-benzothiazol-2-yl)-3-methyl-1-phenyl-4,5-dihydro-1H-pyrazol-5-one derivatives. Journal of Molecular Structure, 2019, 1198, 126910.	3.6	10
11	Synthesis, spectroscopic characterization, thermal, XRD crystal structure, the PLATON structural analysis, and theoretical studies of a new 1,2,4-triazolo-[1,5-a]pyrimidines derivatives. Journal of Molecular Structure, 2019, 1184, 12-24.	3.6	10
12	Synthesis, Crystal structure, Hirshfeld surface Analysis and computational approach of new 2-methylbenzimidazo[1,2-a]pyrimidin-4(1H)-one. Journal of Molecular Structure, 2021, 1239, 130497.	3.6	10
13	Synthesis and Identification of Novel Potential Molecules Against COVID-19 Main Protease Through Structure-Guided Virtual Screening Approach. Applied Biochemistry and Biotechnology, 2021, 193, 3602-3623.	2.9	9
14	Multidimensional insights involving electrochemical and in silico investigation into the corrosion inhibition of newly synthesized pyrazolotriazole derivatives on carbon steel in a HCl solution. RSC Advances, 2019, 9, 34761-34771.	3.6	8
15	Synthesis, crystal structure, and a molecular modeling approach to identify effective antiviral hydrazide derivative against the main protease of SARS-CoV-2. Journal of Molecular Structure, 2022, 1265, 133391.	3.6	6
16	Synthesis, spectroscopic characterizations, DFT, molecular docking and molecular dynamics simulations of a novel 2-methyl-3H-benzimidazo[1,2-b][1,2,4]triazepin-4(5H)-one. Journal of Molecular Structure, 2020, 1202, 127317.	3.6	5
17	Ethyl 2-(2-oxo-3-phenyl-1,2-dihydroquinoxalin-1-yl)acetate. IUCrData, 2018, 3, .	0.3	5
18	Novel 3-chloro-6-nitro-1H-indazole derivatives as promising antileishmanial candidates: synthesis, biological activity, and molecular modelling studies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 151-167.	5.2	4

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19	Synthesis, X-ray, spectroscopic characterization, Hirshfeld surface analysis, DFT calculation and molecular docking investigations of a novel 7-phenyl-2,3,4,5-tetrahydro-1H-1,4-diazepin-5-one derivative. <i>Journal of Molecular Structure</i> , 2021, 1234, 130146.	3.6	3
20	Synthesis, crystal structure, DFT calculations and Hirshfeld surface analysis of 2-(1-decyl-2-oxoindolin-3-ylidene)propanedinitrile. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 21-25.	0.5	3
21	Synthesis, crystal structure investigation and computational approach to discover potential hydrazone derivatives as a potent inhibitor of cyclooxygenase-2 enzyme. <i>Journal of Biochemical and Molecular Toxicology</i> , 2022, , e23082.	3.0	3
22	A newly synthesized 6-methyl-7,8,9-[1,2,4]triazolo[4,3-b][1,2,4]triazepin-8-one for potential inhibitor of adenosine A1 receptor: a combined experimental and computational studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 3578-3586.	3.5	2
23	Crystal structure, DFT calculations and Hirshfeld surface analysis of 3-(4-methylphenyl)-6-nitro-1H-indazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1857-1861.	0.5	2
24	Ethyl 2-(3-oxo-1,2,3,4-tetrahydroquinoxalin-2-yl)acetate. <i>IUCrData</i> , 2018, 3, .	0.3	2
25	Ethyl 2-[(2E)-4-decyl-3-oxo-1,2,3,4-tetrahydroquinoxalin-2-ylidene]acetate. <i>IUCrData</i> , 2018, 3, .	0.3	2
26	Crystal structure, DFT study and Hirshfeld surface analysis of 1-nonyl-2,3-dihydro-1H-indole-2,3-dione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1140-1144.	0.5	2
27	Synthesis, Crystal Structure, DFT Calculations and Hirshfeld Surface Analysis of 5-Bromo-1-decyl-2,3-dihydro-1H-indolin-2-one. <i>Journal of Chemical Crystallography</i> , 2020, 50, 330-337.	1.1	1
28	(3R,4Z)-1,3-Diethyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one. <i>IUCrData</i> , 2018, 3, .	0.3	1
29	A monoclinic modification of (4Z)-1-benzyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one. <i>IUCrData</i> , 2018, 3, .	0.3	1
30	Crystal structure, computational study and Hirshfeld surface analysis of ethyl (2S,3R)-3-(3-amino-1H-1,2,4-triazol-1-yl)-2-hydroxy-3-phenylpropanoate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1919-1924.	0.5	1
31	Insight into the Crystal Structures and Potential of Two Newly Synthesized Naproxen-Based Hydrazone Derivatives as Potent COX-2 Inhibitors. <i>Applied Biochemistry and Biotechnology</i> , 0, , .	2.9	1
32	3-Bromo-6-nitro-1-(prop-2-en-1-yl)-1H-indazole. <i>IUCrData</i> , 2018, 3, .	0.3	0
33	2-Benzyl-6-nitro-2H-indazole. <i>IUCrData</i> , 2018, 3, .	0.3	0
34	1-[(Oxiran-2-yl)methyl]-3-phenyl-1,2-dihydroquinoxalin-2-one. <i>IUCrData</i> , 2018, 3, .	0.3	0
35	Ethyl 3-methyl-1-oxo-4H-1,4-benzothiazine-2-carboxylate monohydrate. <i>IUCrData</i> , 2018, 3, .	0.3	0
36	Molecular docking study and molecular dynamics simulation of ethyl 3,5-diphenyl-1H-pyrrole-2-carboxylate and (Z)-ethyl 2-(3-oxo-1,3-diphenylpropyl)enylamino)acetate. <i>Journal of Biochemical and Molecular Toxicology</i> , 2022, , e23013.	0.3	0