

# Youness El Bakri

## List of Publications by Year in descending order

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36  
papers

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citations

933447

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h-index

888059

17  
g-index

36  
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docs citations

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times ranked

258  
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#	ARTICLE	IF	CITATIONS
1	Molecular docking study and molecular dynamics simulation of ethyl 3,5-diphenyl-1-pyrroline-2-carboxylate and (Z)-ethyl-(3-oxo-1,3-diphenylpropyl-1-enylamino)acetate. Journal of Biochemical and Molecular Toxicology, 2022, , e23013.		
2	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
3	Synthesis, crystal structure investigation and computational approach to discover potential hydrazone derivatives as a potent inhibitor of cyclooxygenase-2 enzyme. Journal of Biochemical and Molecular Toxicology, 2022, , e23082.	3.0	3
4	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
5	Synthesis, crystal structure, and a molecular modeling approach to identify effective antiviral hydrazone derivative against the main protease of SARS-CoV-2. Journal of Molecular Structure, 2022, 1265, 133391.	3.6	6
6	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. Journal of Molecular Structure, 2021, 1234, 130146.	3.6	3
7	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
8	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
9	Synthesis, Crystal Structure, DFT Calculations and Hirshfeld Surface Analysis of 5-Bromo-1-decyl-2,3-dihydro-1H-indolin-2-one. Journal of Chemical Crystallography, 2020, 50, 330-337.	1.1	1
10	A newly synthesized 6-methyl-7H,8H,9H-[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. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3578-3586.	3.5	2
11	Synthesis, spectroscopic characterizations, DFT, molecular docking and molecular dynamics simulations of a novel 2-methyl-3H-benzimidazolo[1,2-b][1,2,4]triazepin-4(5H)-one. Journal of Molecular Structure, 2020, 1202, 127317.	3.6	5
12	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
13	Synthesis, biological activity and molecular modeling of a new series of condensed 1,2,4-triazoles. Bioorganic Chemistry, 2019, 92, 103193.	4.1	23
14	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
15	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
16	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
17	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
18	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

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19	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
20	Crystal structure, DFT study and Hirshfeld surface analysis of 1-nonyl-2,3-dihydro-1 <i>H</i> -indole-2,3-dione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1140-1144.	0.5	2
21	Crystal structure, computational study and Hirshfeld surface analysis of ethyl (2 <i>S</i> ,3 <i>R</i> )-3-(3-amino-1 <i>H</i> -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
22	Synthesis, crystal structure, spectroscopic characterization, Hirshfeld surface analysis, and DFT calculations of 1,4-dimethyl-2-oxo-pyrimido[1,2- <i>a</i> ]benzimidazole hydrate. <i>Journal of Molecular Structure</i> , 2018, 1152, 154-162.	3.6	16
23	Synthesis, crystal structure, Hirshfeld surface analysis, and DFT calculations of new 1-[(1-benzyl-1 <i>H</i> -1,2,3-triazol-4-yl)methyl]-6-methoxy-1 <i>H</i> -benzimidazol-2(3 <i>H</i> )-one. <i>Chemical Data Collections</i> , 2018, 17-18, 472-482.	2.3	10
24	Potential antidiabetic activity and molecular docking studies of novel synthesized 3,6-dimethyl-5-oxo-pyrido[3,4- <i>f</i> ][1,2,4]triazepino[2,3- <i>a</i> ]benzimidazole and 10-amino-2-methyl-4-oxo-pyrimido[1,2- <i>a</i> ]benzimidazole derivatives. <i>Journal of Molecular Modeling</i> , 2018, 24, 179.	1.8	28
25	Crystal structure, DFT calculations and Hirshfeld surface analysis of 3-(4-methylphenyl)-6-nitro-1 <i>H</i> -indazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1857-1861.	0.5	2
26	1-Benzyl-3-methylquinoxalin-2(1 <i>H</i> )-one. <i>IUCrData</i> , 2018, 3, .	0.3	13
27	(3 <i>R</i> ,4 <i>Z</i> )-1,3-Diethyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1 <i>H</i> -1,5-benzodiazepin-2-one. <i>IUCrData</i> , 2018, 3, .	0.3	1
28	Ethyl 2-(3-oxo-1,2,3,4-tetrahydroquinoxalin-2-yl)acetate. <i>IUCrData</i> , 2018, 3, .	0.3	2
29	Ethyl 2-[(2 <i>E</i> )-4-decyl-3-oxo-1,2,3,4-tetrahydroquinoxalin-2-ylidene]acetate. <i>IUCrData</i> , 2018, 3, .	0.3	2
30	3-Bromo-6-nitro-1-(prop-2-en-1-yl)-1 <i>H</i> -indazole. <i>IUCrData</i> , 2018, 3, .	0.3	0
31	2-Benzyl-6-nitro-2 <i>H</i> -indazole. <i>IUCrData</i> , 2018, 3, .	0.3	0
32	A monoclinic modification of (4 <i>Z</i> )-1-benzyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1 <i>H</i> -1,5-benzodiazepin-2-one. <i>IUCrData</i> , 2018, 3, .	0.3	1
33	Ethyl 2-(2-oxo-3-phenyl-1,2-dihydroquinoxalin-1-yl)acetate. <i>IUCrData</i> , 2018, 3, .	0.3	5
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-4 <i>H</i> -1,4-benzothiazine-2-carboxylate monohydrate. <i>IUCrData</i> , 2018, 3, .	0.3	0
36	Insight into the Crystal Structures and Potential of Two Newly Synthesized Naproxen-Based Hydrazide Derivatives as Potent COX-2 Inhibitors. <i>Applied Biochemistry and Biotechnology</i> , 0, , .	2.9	1