

# Houssein Boulebd

## List of Publications by Year in descending order

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45  
papers

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430874  
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552781  
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docs citations

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532  
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#	ARTICLE	IF	CITATIONS
1	Structure-activity relationship of antioxidant prenylated (iso)flavonoid-type compounds: quantum chemistry and molecular docking studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 10373-10382.	3.5	15
2	Radical scavenging behavior of butylated hydroxytoluene against oxygenated free radicals in physiological environments: Insights from DFT calculations. <i>International Journal of Chemical Kinetics</i> , 2022, 54, 50-57.	1.6	20
3	New benzimidazolium N-heterocyclic carbene precursors and their related Pd-NHC complex PEPPSI-type: Synthesis, structures, DFT calculations, biological activity, docking study, and catalytic application in the direct arylation. <i>Journal of Molecular Structure</i> , 2022, 1248, 131504.	3.6	12
4	Synthesis and radical scavenging activity of new phenolic hydrazone/hydrazide derivatives: Experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2022, 1249, 131546.	3.6	25
5	Assessment of the free radical scavenging potential of cannabidiol under physiological conditions: Theoretical and experimental investigations. <i>Journal of Molecular Liquids</i> , 2022, 346, 118277.	4.9	17
6	Insights on the kinetics and mechanisms of the peroxy radical scavenging capacity of caftaric acid: the important role of the acid–base equilibrium. <i>New Journal of Chemistry</i> , 2022, 46, 7403-7409.	2.8	6
7	Preparation, DFT calculations, docking studies, antioxidant, and anticancer properties of new pyrazole and pyridine derivatives. <i>Journal of Biochemical and Molecular Toxicology</i> , 2022, 36, .	3.0	9
8	The radical scavenger capacity and mechanism of prenylated coumestan-type compounds: a DFT analysis. <i>Free Radical Research</i> , 2022, 56, 273-281.	3.3	5
9	Synthesis, biological evaluation, theoretical investigations, docking study and ADME parameters of some 1,4-bisphenylhydrazone derivatives as potent antioxidant agents and acetylcholinesterase inhibitors. <i>Molecular Diversity</i> , 2021, 25, 279-290.	3.9	21
10	The role of benzylic-allylic hydrogen atoms on the antiradical activity of prenylated natural chalcones: a thermodynamic and kinetic study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 1955-1964.	3.5	27
11	Synthesis, crystal structure, Hirshfeld surface analysis, biological evaluation, DFT calculations, and in silico ADME analysis of 4-arylidene pyrazolone derivatives as promising antibacterial agents. <i>Journal of Molecular Structure</i> , 2021, 1229, 129586.	3.6	11
12	Synthesis, in vitro and in silico studies of naphtho-1,3-oxazin-3(2H)-one derivatives as promising inhibitors of cholinesterase and $\alpha$ -glucosidase. <i>Journal of Molecular Structure</i> , 2021, 1225, 129103.	3.6	6
13	Insights into the mechanisms and kinetics of the hydroperoxyl radical scavenging activity of Artepillin C. <i>New Journal of Chemistry</i> , 2021, 45, 7774-7780.	2.8	12
14	Are thymol, rosefuran, terpinolene and umbelliferone good scavengers of peroxy radicals?. <i>Phytochemistry</i> , 2021, 184, 112670.	2.9	23
15	Free radical scavenging activity and mechanisms of amidoalkyl-2-naphthol derivative: a joint experimental and theoretical study. <i>Chemical Papers</i> , 2021, 75, 6651.	2.2	1
16	A detailed DFT-based study of the free radical scavenging activity and mechanism of daphnetin in physiological environments. <i>Phytochemistry</i> , 2021, 189, 112831.	2.9	25
17	Modeling the peroxy radical scavenging behavior of Carnosic acid: Mechanism, kinetics, and effects of physiological environments. <i>Phytochemistry</i> , 2021, 192, 112950.	2.9	21
18	Synthesis, structures, DFT calculations, and catalytic application in the direct arylation of five-membered heteroarenes with aryl bromides of novel palladium-N-heterocyclic carbene PEPPSI-type complexes. <i>New Journal of Chemistry</i> , 2021, 45, 17878-17892.	2.8	14

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19	Computational design of new tacrine analogs: an in silico prediction of their cholinesterase inhibitory, antioxidant, and hepatotoxic activities. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-15.	3.5	2
20	Is cannabidiolic acid an overlooked natural antioxidant? Insights from quantum chemistry calculations. <i>New Journal of Chemistry</i> , 2021, 46, 162-168.	2.8	12
21	Comparative study of the radical scavenging behavior of ascorbic acid, BHT, BHA and Trolox: Experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2020, 1201, 127210.	3.6	80
22	Substitution effects on the antiradical activity of hydralazine: a DFT analysis. <i>New Journal of Chemistry</i> , 2020, 44, 16577-16583.	2.8	12
23	Synthesis, Docking Study and Biological Activities Evaluation of 1- <i>N</i> -amidoalkyl-2-naphthol Derivatives as Dual Inhibitors of Cholinesterase and $\alpha$ -Glucosidase. <i>ChemistrySelect</i> , 2020, 5, 5515-5520.	1.5	12
24	Green one-pot multicomponent synthesis, biological evaluation and theoretical investigations of some novel 1'-acetamido ketone derivatives as potent cholinesterase inhibitors. <i>Tetrahedron</i> , 2020, 76, 131260.	1.9	6
25	Thermodynamic and kinetic studies of the antiradical activity of 5-hydroxymethylfurfural: computational insights. <i>New Journal of Chemistry</i> , 2020, 44, 9863-9869.	2.8	41
26	Design, synthesis, biological evaluation, molecular docking, DFT calculations and in silico ADME analysis of (benz)imidazole-hydrazone derivatives as promising antioxidant, antifungal, and anti-acetylcholinesterase agents. <i>Journal of Molecular Structure</i> , 2020, 1218, 128527.	3.6	38
27	New chalcone-type compounds and 2-pyrazoline derivatives: synthesis and caspase-dependent anticancer activity. <i>Future Medicinal Chemistry</i> , 2020, 12, 493-509.	2.3	32
28	Combined experimental and theoretical studies of the structure-antiradical activity relationship of heterocyclic hydrazone compounds. <i>Journal of Molecular Structure</i> , 2020, 1221, 128858.	3.6	12
29	Synthesis, biological evaluation and molecular docking studies of novel 2-alkylthiopyrimidino-tacrine derivatives as anticholinesterase agents and their DFT calculations. <i>Journal of Molecular Structure</i> , 2020, 1209, 127902.	3.6	14
30	Synthesis, crystal structure, biological evaluation, docking study, and DFT calculations of 1-amidoalkyl-2-naphthol derivative. <i>Journal of Molecular Structure</i> , 2020, 1212, 128179.	3.6	5
31	Theoretical insights into the antioxidant activity of moracin T. <i>Free Radical Research</i> , 2020, 54, 221-230.	3.3	40
32	Thermodynamic and Kinetic Studies of the Radical Scavenging Behavior of Hydralazine and Dihydralazine: Theoretical Insights. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4123-4131.	2.6	24
33	Co(II) complexes derived from (1-methyl-1H-imidazol-2-yl)methanol: Synthesis, characterization, spectroscopic study, DFT/TD-DFT calculations and biological evaluation. <i>Inorganica Chimica Acta</i> , 2019, 497, 119073.	2.4	6
34	Dinuclear Hg(II) complex of new benzimidazole-based Schiff base: one-pot synthesis, crystal structure, spectroscopy, and theoretical investigations. <i>Journal of Coordination Chemistry</i> , 2019, 72, 3156-3170.	2.2	6
35	DFT study of the antiradical properties of some aromatic compounds derived from antioxidant essential oils: C-H bond vs. O-H bond. <i>Free Radical Research</i> , 2019, 53, 1125-1134.	3.3	49
36	New Schiff bases derived from benzimidazole as efficient mercury-complexing agents in aqueous medium. <i>Journal of Molecular Structure</i> , 2019, 1196, 58-65.	3.6	23

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37	Cobalt(II) complexes based on (1-methyl-1 <i>H</i> -benzo[ <i>d</i> ]imidazol-2-yl) methanol derivative: synthesis, crystal structure, spectroscopy, DFT calculations, and antioxidant activity. Journal of Coordination Chemistry, 2018, 71, 311-328.	2.2	9
38	New highly fluorescent hybrids (benz)imidazol-2-aminonicotinonitrile and -2-aminoisophthalonitrile: synthesis, characterization, fluorescence study, and theoretical calculations. Monatshefte für Chemie, 2018, 149, 1125-1136.	1.8	1
39	Copper(II) and zinc(II) as metal-carboxylate coordination complexes based on (1-methyl-1 <i>H</i> -benzo[ <i>d</i> ]imidazol-2-yl) methanol derivative: Synthesis, crystal structure, spectroscopy, DFT calculations and antioxidant activity. Journal of Molecular Structure, 2018, 1160, 406-414.	3.6	26
40	A silver nanoparticles-catalyzed efficient three-component synthesis of polysubstituted 4 <i>H</i> -chromenylphosphonates and their antioxidant activity. Synthetic Communications, 2018, 48, 2366-2381.	2.1	12
41	New (benz)imidazolopyridino tacrines as nonhepatotoxic, cholinesterase inhibitors for Alzheimer disease. Future Medicinal Chemistry, 2017, 9, 723-729.	2.3	25
42	Imidazopyranotacrines as Non-Hepatotoxic, Selective Acetylcholinesterase Inhibitors, and Antioxidant Agents for Alzheimer's Disease Therapy. Molecules, 2016, 21, 400.	3.8	19
43	Synthesis and biological evaluation of heterocyclic privileged medicinal structures containing (benz)imidazole unit. Monatshefte für Chemie, 2016, 147, 2209-2220.	1.8	16
44	3-Anilino-5,5-dimethylcyclohex-2-enone. Acta Crystallographica Section E: Structure Reports Online, 2014, 70, o233-o234.	0.2	1
45	2-Halogeno-N-phenacylimidazolium salts and their reactions with active methylene species, arylamines and thiocyanate ions. Tetrahedron Letters, 2014, 55, 4701-4704.	1.4	5