El Hassane Anouar

List of Publications by Year
in descending order

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119 papers	2,466 citations	249298 26 h-index	299063 42 g-index
119 all docs	119 docs citations	119 times ranked	2825 citing authors

#	Article	IF	Citations
1	Synthesis,inÂvitrobiological screening and docking study of benzo[d]oxazolebisSchiff base derivatives as a potent anti-Alzheimer agent. Journal of Biomolecular Structure and Dynamics, 2023, 41, 1649-1664.	2.0	9
2	Synthesis, Spectroscopic Characterization, DFT, Molecular Docking and Antidiabetic Activity of N-Isonicotinoyl Arylaldehyde Hydrazones. Polycyclic Aromatic Compounds, 2023, 43, 1469-1481.	1.4	1
3	Synthesis, Characterization, Antibacterial Evaluation, and Molecular Docking of New Quinazolinone-Based Derivatives. Polycyclic Aromatic Compounds, 2023, 43, 1879-1887.	1.4	3
4	Synthesis, characterization, biological evaluation and molecular docking of a new quinazolinone-based derivative as a potent dual inhibitor for VEGFR-2 and EGFR tyrosine kinases. Journal of Biomolecular Structure and Dynamics, 2022, 40, 6810-6816.	2.0	12
5	An effort to find new Î±-amylase inhibitors as potent antidiabetics compounds based on indole-based-thiadiazole analogs. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13103-13114.	2.0	4
6	New spiropyrrolothiazole derivatives bearing an oxazolone moiety as potential antidiabetic agent: Design, synthesis, crystal structure, Hirshfeld surface analysis, ADME and molecular docking studies. Journal of Molecular Structure, 2022, 1254, 132398.	1.8	8
7	A new synthetic route for the preparation of 2,2â€²,5â€²â€trimethylâ€7â€oxoâ€4,7â€dihydroâ€[6,7â€²â€bipyrazolo[1,5â€a]pyrimidine]â€3,3â€²â€dicarbonitrile, structural elucidation, Hirshfeld surface analysis, energy framework, density functional theory and molecular docking investigations. Journal of the Chinese Chemical Society, 2022, 69, 717-730.	0.8	3
8	Synthesis, characterization and bioactivity of novel 8-hydroxyquinoline derivatives: Experimental, molecular docking, DFT and POM analyses. Journal of Molecular Structure, 2022, 1258, 132688.	1.8	26
9	Palladium(II) complexes bearing N,O-bidentate Schiff base ligands: Experimental, in-silico, antibacterial, and catalytic properties. Journal of Molecular Structure, 2022, 1260, 132821.	1.8	8
10	Synthesis, structural confirmation, antibacterial properties and bio-informatics computational analyses of new pyrrole based on 8-hydroxyquinoline. Journal of Molecular Structure, 2022, 1259, 132683.	1.8	37
11	Synthesis, crystal structures, Î±-glucosidase and Î±-amylase inhibition, DFT and molecular docking investigations of two thiazolidine-2,4-dione derivatives. Journal of Molecular Structure, 2022, 1261, 132960.	1.8	7
12	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.	2.5	4
13	Synthesis, structural characterization, antioxidant and antidiabetic activities, DFT calculation, and molecular docking of novel substituted phenolic and heterocyclic compounds. Journal of Biomolecular Structure and Dynamics, 2022, , 1-13.	2.0	0
14	Molecular docking and anticancer evaluation of some newly synthesized 4-aryl-2-(2-oxopropoxy)-6-(cyclohexyl)nicotinonitrile and their furo[2,3-b]pyridine derivatives. Journal of Molecular Structure, 2022, 1263, 133148.	1.8	4
15	antimicrobial evaluation, DFT, chemical approach, in silico ADME and molecular docking studies. Journal of Molecular Structure, 2022, 1264, 133299.	1.8	5
16	Unexpected synthesis of novel 2-pyrone derivatives: crystal structures, Hirshfeld surface analysis and computational studies. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4859-4877.	2.0	7
17	Characteristics of multidentate schiff base ligand and its complexes using cyclic voltammetry, fluorescence, antimicrobial behavior and DFT-calculations. Journal of Molecular Structure, 2021, 1224, 129263.	1.8	14
18	Corrosion inhibition potential of 2-[(5-methylpyrazol-3-yl)methyl]benzimidazole against carbon steel corrosion in 1ÂM HCl solution: Combining experimental and theoretical studies. Journal of Molecular Liquids, 2021, 321, 114750.	2.3	75

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19	Efficient novel eutectic-mixture-mediated synthesis of benzoxazole-linked pyrrolidin-2-one heterocycles. Journal of Molecular Liquids, 2021, 323, 115011.	2.3	13
20	Synthesis, antibacterial evaluation, crystal structure and molecular interactions analysis of new 6-Bromo-2â€'chloroâ€'3-butylquinazolin-4(3H)-one. Journal of Molecular Structure, 2021, 1225, 129166.	1.8	12
21	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.	1.4	2
22	New substituted pyrazolones and dipyrazolotriazines as promising tyrosyl-tRNA synthetase and peroxiredoxin-5 inhibitors: Design, synthesis, molecular docking and structure-activity relationship (SAR) analysis. Bioorganic Chemistry, 2021, 109, 104704.	2.0	17
23	An unprecedented diterpene with three new neoclerodanes from Teucrium sandrasicum O. Schwarz. Journal of Molecular Structure, 2021, 1231, 129919.	1.8	5
24	Synthesis, characterization, biological evaluation, and kinetic study of indole base sulfonamide derivatives as acetylcholinesterase inhibitors in search of potent anti-Alzheimer agent. Journal of King Saud University - Science, 2021, 33, 101401.	1.6	19
25	Adsorption and corrosion inhibition accomplishment for thiosemicarbazone derivatives for mild steel in 1.0ÂM HCl medium: Electrochemical, XPS and DFT studies. Journal of Molecular Liquids, 2021, 329, 115553.	2.3	30
26	Synthesis, structure elucidation, Hirshfeld surface analysis, DFT, molecular docking and Monte Carlo simulation of new quinoline-4-carboxylate derivatives. Journal of Molecular Structure, 2021, 1234, 130195.	1.8	3
27	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.	1.8	3
28	Adsorption, electrochemistry, DFT and inhibitive effect of imines derived from tribulin on corrosion of mild steel in 1ÂM HCl. Journal of Molecular Structure, 2021, 1235, 130206.	1.8	10
29	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.	1.4	9
30	Growth, single crystal investigation, hirshfeld surface analysis, DFT studies, molecular docking, physico-chemical characterization and, in vitro, antioxidant activity of a novel hybrid complex. Journal of Solid State Chemistry, 2021, 301, 122319.	1.4	5
31	Exploring indole-based-thiadiazole derivatives as potent acetylcholinesterase and butyrylcholinesterase enzyme inhibitors. International Journal of Biological Macromolecules, 2021, 188, 1025-1036.	3.6	20
32	New 1,2,3-triazole containing benzimidazolone derivatives: Syntheses, crystal structures, spectroscopic characterizations, Hirshfeld surface analyses, DFT calculations, anti-corrosion property anticipation, and antibacterial activities. Journal of Molecular Structure, 2021, 1242, 130719.	1.8	6
33	Synthesis of indole derivatives as diabetics II inhibitors and enzymatic kinetics study of Î±-glucosidase and Î±-amylase along with their in-silico study. International Journal of Biological Macromolecules, 2021, 190, 301-318.	3.6	23
34	Synthesis, bioinformatics and biological evaluation of novel pyridine based on 8-hydroxyquinoline derivatives as antibacterial agents: DFT, molecular docking and ADME/T studies. Journal of Molecular Structure, 2021, 1244, 130934.	1.8	25
35	Synthesis, crystal structure, DFT, Î±-glucosidase and Î±-amylase inhibition and molecular docking studies of (E)-N'-(4-chlorobenzylidene)-5-phenyl-1H-pyrazole-3-carbohydrazide. Journal of Molecular Structure, 2021, 1245, 131067.	1.8	35
36	Nano-synthesis, spectroscopic characterization, quantum chemical calculations, thermal properties and antimicrobial activity of (E)-Nâ€²-(2-hydroxybenzylidene)morpholine-4-carbothiohydrazide ligand and its metal complexes. Inorganica Chimica Acta, 2020, 500, 119221.	1.2	4

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37	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.	2.0	2
38	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.	1.8	5
39	Synthesis of Benzimidazoleâ€“Based Analogs as Anti Alzheimerâ€™s Disease Compounds and Their Molecular Docking Studies. Molecules, 2020, 25, 4828.	1.7	23
40	Experimental and theoretical studies of azomethines derived from benzylamine as corrosion inhibitors of mild steel in 1ÂM HCl. Journal of Molecular Structure, 2020, 1222, 128899.	1.8	26
41	Design, synthesis ADMET and molecular docking of new imidazo[4,5-b]pyridine-5-thione derivatives as potential tyrosyl-tRNA synthetase inhibitors. Bioorganic Chemistry, 2020, 102, 104105.	2.0	31
42	Syntheses, crystal structures, spectroscopic characterizations, DFT calculations, hirshfeld surface analyses and monte carlo simulations of novel long-chain alkyl-substituted 1,4-benzothiazine derivatives. Journal of Molecular Structure, 2020, 1221, 128886.	1.8	2
43	Structure Elucidation of the spiro-Polyketide Svalbardine B from the Arctic Fungal Endophyte Poaceicola sp. E1PB with Support from Extensive ESI-MSn Interpretation. Journal of Natural Products, 2020, 83, 3493-3501.	1.5	8
44	Spectroscopic Characterization, Hirshfeld Surface, DFT, and TD-DFT of tert-Butyl Phenethylcarbamate and 1,1-Dimethyl-3-Phenethylurea. Journal of Applied Spectroscopy, 2020, 87, 736-744.	0.3	1
45	HR-LCMS-Based Metabolite Profiling, Antioxidant, and Anticancer Properties of Teucrium polium L. Methanolic Extract: Computational and In Vitro Study. Antioxidants, 2020, 9, 1089.	2.2	36
46	Synthesis of diindolylmethane (DIM) bearing thiadiazole derivatives as a potent urease inhibitor. Scientific Reports, 2020, 10, 7969.	1.6	13
47	Novel fused pyridine derivatives containing pyrimidine moiety as prospective tyrosyl-tRNA synthetase inhibitors: Design, synthesis, pharmacokinetics and molecular docking studies. Journal of Molecular Structure, 2020, 1219, 128651.	1.8	38
48	Inhibition potential of phenyl linked benzimidazole-triazolothiadiazole modular hybrids against Î²-glucuronidase and their interactions thereof. International Journal of Biological Macromolecules, 2020, 161, 355-363.	3.6	9
49	DFT study and radical scavenging activity of 2-phenoxypyridotriazolo pyrimidines by DPPH, ABTS, FRAP and reducing power capacity. Chemical Papers, 2020, 74, 2893-2899.	1.0	17
50	Exploring efficacy of indole-based dual inhibitors for Î±-glucosidase and Î±-amylase enzymes: In silico, biochemical and kinetic studies. International Journal of Biological Macromolecules, 2020, 154, 217-232.	3.6	26
51	Synthesis of indole based acetohydrazide analogs: Their in vitro and in silico thymidine phosphorylase studies. Bioorganic Chemistry, 2020, 98, 103745.	2.0	11
52	An Improved Synthesis of Key Intermediate to the Formation of Selected Indolin-2-Ones Derivatives Incorporating Ultrasound and Deep Eutectic Solvent (DES) Blend of Techniques, for Some Biological Activities and Molecular Docking Studies. Molecules, 2020, 25, 1118.	1.7	5
53	Synthesis, crystal structure, photophysical properties, DFT studies and Hirshfeld surface analysis of a phosphorescent 1,2,4-triazole-based iridium(III) complex. Polyhedron, 2020, 188, 114690.	1.0	2
54	Cytotoxicity, alpha-glucosidase inhibition and molecular docking studies of hydroxamic acid chromium(III) complexes. Journal of Biological Inorganic Chemistry, 2020, 25, 239-252.	1.1	8

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55	Synthesis of symmetrical bis-Schiff base-disulfide hybrids as highly effective anti-leishmanial agents. Bioorganic Chemistry, 2020, 99, 103819.	2.0	6
56	Anti-corrosion performance of 8-hydroxyquinoline derivatives for mild steel in acidic medium: Gravimetric, electrochemical, DFT and molecular dynamics simulation investigations. Journal of Molecular Liquids, 2020, 308, 113042.	2.3	113
57	Synthesis, antibacterial evaluation, Raman, Crystal Structure and Hirshfeld Surface analysis of a new 3-(4-fluorophenyl)-6-methyl-2-(propylthio)quinazolin-4(3H)-one. Journal of Molecular Structure, 2020, 1215, 128265.	1.8	13
58	Synthesis, characterization, quantum chemical calculations and anticancer activity of a Schiff base NNOO chelate ligand and Pd(II) complex. PLoS ONE, 2020, 15, e0231147.	1.1	16
59	Synthesis, Characterization and Corrosion Inhibition of decyl-2-[(5-methylisoxazol-2-yl)methyl]benzimidazole: Experimental and DFT Approaches. Portugaliae Electrochimica Acta, 2020, 38, 281-297.	0.4	4
60	Structural cytotoxicity relationship of 2-phenoxy(thiomethyl)pyridotriazolopyrimidines: Quantum chemical calculations and statistical analysis. Open Chemistry, 2020, 18, 740-751.	1.0	0
61	Electrophilic Aromatic Synthesis of Radioiodinated Aripiprazole: Experimental and DFT Investigations. Current Organic Synthesis, 2020, 17, 295-303.	0.7	1
62	Evaluation of Cytotoxic and Tyrosinase Inhibitory Activities of 2-phenoxy(thiomethyl) pyridotriazolopyrimidines: In Vitro and Molecular Docking Studies. Anti-Cancer Agents in Medicinal Chemistry, 2020, 20, 1714-1721.	0.9	2
63	Triazoloquinazolines as a new class of potent Î±-glucosidase inhibitors: in vitro evaluation and docking study. PLoS ONE, 2019, 14, e0220379.	1.1	29
64	Synthesis of new heterocyclic systems oxazino derivatives of 8-Hydroxyquinoline: Drug design and POM analyses of substituent effects on their potential antibacterial properties. Chemical Data Collections, 2019, 24, 100306.	1.1	22
65	Absolute Configuration of Alkaloids from Uncaria longiflora through Experimental and Computational Approaches. Journal of Natural Products, 2019, 82, 2933-2940.	1.5	3
66	Synthesis, biological activity and molecular modeling of a new series of condensed 1,2,4-triazoles. Bioorganic Chemistry, 2019, 92, 103193.	2.0	23
67	XPS and DFT investigations of corrosion inhibition of substituted benzylidene Schiff bases on mild steel in hydrochloric acid. Applied Surface Science, 2019, 476, 861-877.	3.1	162
68	Synthesis, X-Ray, spectroscopic characterization (FT-IR, NMR, UVâ€“Vis) and quantum chemical calculations of some substituted benzoylthiourea derivatives. Journal of Molecular Structure, 2019, 1194, 48-56.	1.8	18
69	Synthesis, biological activity and molecular docking of new tricyclic series as Î±-glucosidase inhibitors. BMC Chemistry, 2019, 13, 52.	1.6	22
70	Synthesis, crystal structure, spectroscopic characterization, hirshfeld surface analysis, DFT calculations and antibacterial activity of ethyl 2-(4-vinylbenzyl)-2-(5-methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)-3-(4-vinylphenyl)propanoate. Journal of Molecular Structure, 2019, 1191, 66-75.	1.8	12
71	Anti-HAV evaluation and molecular docking of newly synthesized 3-benzyl(phenethyl)benzo[g]quinazolines. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 1614-1619.	1.0	10
72	Synthesis, Molecular Docking and Î²-Glucuronidase Inhibitory Potential of Indole Base Oxadiazole Derivatives. Molecules, 2019, 24, 963.	1.7	17

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73	Synthesis of Thymidine Phosphorylase Inhibitor Based on Quinoxaline Derivatives and Their Molecular Docking Study. Molecules, 2019, 24, 1002.	1.7	9
74	Indole bearing thiadiazole analogs: synthesis, Î²-glucuronidase inhibition and molecular docking study. BMC Chemistry, 2019, 13, 14.	1.6	10
75	An Improved Synthesis of Key Intermediate to the Formation of Selected Indolin-2-ones Derivatives Incorporating Ultrasound and Deep Eutectic Solvent (DES) Blend of Techniques, for Some Biological Activities and Molecular Docking Studies. Proceedings (mdpi), 2019, 41, 8.	0.2	0
76	Multidimensional insights involving electrochemical andin silicoinvestigation into the corrosion inhibition of newly synthesized pyrazolotriazole derivatives on carbon steel in a HCl solution. RSC Advances, 2019, 9, 34761-34771.	1.7	8
77	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.	1.8	27
78	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.	1.8	18
79	Electrochemical, DFT and MD simulation of newly synthesized triazolotriazepine derivatives as corrosion inhibitors for carbon steel in 1â€M HCl. Journal of Molecular Liquids, 2019, 274, 759-769.	2.3	49
80	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.	1.8	30
81	Crystal structure, DFT study and Hirshfeld surface analysis of ethyl 6-chloro-2-ethoxyquinoline-4-carboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 912-916.	0.2	7
82	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.	1.8	16
83	Synthesis, characterization, crystal structures and DFT studies of some new 1,2,4-triazole and triazolidin derivatives. Journal of Molecular Structure, 2018, 1151, 315-326.	1.8	4
84	Laevifins Aâ€“G, clerodane diterpenoids from the Bark of Croton oblongus Burm.f.. Phytochemistry, 2018, 156, 193-200.	1.4	7
85	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.	0.8	28
86	Quantum Chemical Calculations and Statistical Analysis: Structural Cytotoxicity Relationships of some Synthesized 2-thiophen-naphtho(benzo)oxazinone Derivatives. Cell Biochemistry and Biophysics, 2018, 76, 377-389.	0.9	1
87	Synthesis, spectroscopic characterization, DFT and antibacterial studies of newly synthesized cobalt(II, III), nickel(II) and copper(II) complexes with salicylaldehyde N(4)-antipyrinylthiosemicarbazone. Inorganica Chimica Acta, 2018, 483, 116-128.	1.2	16
88	3-Benzyl(phenethyl)-2-thioxobenzo[g]quinazolines as a new class of potent Î±-glucosidase inhibitors: synthesis and molecular docking study. Future Medicinal Chemistry, 2018, 10, 1889-1905.	1.1	26
89	Organic Synthesis of Iodinated Atorvastatin via Nucleophilic Substitution Reaction: Experimental and DFT Studies. Current Organic Chemistry, 2018, 22, 2017-2022.	0.9	3
90	Screening and evaluation of antioxidant activity of some 1,2,4-triazolo[1,5-a]quinazoline derivatives. Future Medicinal Chemistry, 2018, 10, 379-390.	1.1	30

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91	Synthesis and molecular modelling studies of phenyl linked oxadiazole-phenylhydrazone hybrids as potent antileishmanial agents. European Journal of Medicinal Chemistry, 2017, 126, 1021-1033.	2.6	34
92	3,4-Dimethoxybenzohydrazide derivatives as antiulcer: Molecular modeling and density functional studies. Bioorganic Chemistry, 2017, 75, 235-241.	2.0	7
93	Molecular modeling, enzyme activity, anti-inflammatory and antiarthritic activities of newly synthesized quinazoline derivatives. Future Medicinal Chemistry, 2017, 9, 1995-2009.	1.1	12
94	A novel l-leucine modified Sol-Gel-Carbon electrode for simultaneous electrochemical detection of homovanillic acid, dopamine and uric acid in neuroblastoma diagnosis. Materials Science and Engineering C, 2017, 71, 870-878.	3.8	19
95	DFT analysis and bioactivity of 2-((E)-(4-methoxybenzylimino)methyl)phenol and its Ni(II) and Pd(II) complexes. Arabian Journal of Chemistry, 2017, 10, 769-780.	2.3	12
96	Molecular Docking and Anticonvulsant Activity of Newly Synthesized Quinazoline Derivatives. Molecules, 2017, 22, 1094.	1.7	52
97	Identification of bisindolylmethaneâ€“hydrazone hybrids as novel inhibitors of Î²-glucuronidase, DFT, and in silico SAR intimations. RSC Advances, 2016, 6, 3276-3289.	1.7	29
98	Antioxidant activity of mildbone and mildbenone secondary metabolites of Erythrina mildbraedii Harms: A theoretical approach. Computational and Theoretical Chemistry, 2016, 1077, 106-112.	1.1	10
99	Synthesis, X-ray, NMR, FT-IR, UV/vis, DFT and TD-DFT studies of N-(4-chlorobutanoyl)-Nâ€²-(2-, 3- and) Tj ETQq1 1 0.784314 rgBT /Ove Spectroscopy, 2015, 144, 115-124.	2.0	22
100	Spectrofluorometric and Molecular Docking Studies on the Binding of Curcumenol and Curcumenone to Human Serum Albumin. International Journal of Molecular Sciences, 2015, 16, 5180-5193.	1.8	26
101	A Quantum Chemical and Statistical Study of Cytotoxic Activity of Compounds Isolated from Curcuma zedoaria. International Journal of Molecular Sciences, 2015, 16, 9450-9468.	1.8	11
102	Evaluation of 2-indolcarbohydrazones as potent Î±-glucosidase inhibitors, in silico studies and DFT based stereochemical predictions. Bioorganic Chemistry, 2015, 63, 24-35.	2.0	37
103	Î±-Glucosidase activity of oleanolic acid and its oxidative metabolites: DFT and Docking studies. Mini-Reviews in Medicinal Chemistry, 2015, 15, 1148-1158.	1.1	7
104	Synthesis of novel derivatives of 4-methylbenzimidazole and evaluation of their biological activities. European Journal of Medicinal Chemistry, 2014, 84, 731-738.	2.6	69
105	UV/Visible spectra of a series of natural and synthesised anthraquinones: experimental and quantum chemical approaches. SpringerPlus, 2014, 3, 233.	1.2	28
106	Antioxidant activity, NMR, X-ray, ECD and UV/vis spectra of (+)-terrein: Experimental and theoretical approaches. Journal of Molecular Structure, 2014, 1060, 102-110.	1.8	20
107	A Quantum Chemical and Statistical Study of Phenolic Schiff Bases with Antioxidant Activity against DPPH Free Radical. Antioxidants, 2014, 3, 309-322.	2.2	22
108	Synthesis, Crystal Structure, DFT Studies and Evaluation of the Antioxidant Activity of 3,4-Dimethoxybenzenamine Schiff Bases. Molecules, 2014, 19, 8414-8433.	1.7	38

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109	Antioxidant Activity of Hispidin Oligomers from Medicinal Fungi: A DFT Study. Molecules, 2014, 19, 3489-3507.	1.7	40
110	Structure and Absolute Configuration of 20Î²-Hydroxyprednisolone, a Biotransformed Product of Predinisolone by the Marine Endophytic Fungus Penicilium lapidosum. Molecules, 2014, 19, 13775-13787.	1.7	10
111	Time-dependent density functional theory study of UV/vis spectra of natural styrylpyrones. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 675-682.	2.0	8
112	Antioxidant properties of phenolic Schiff bases: structureâ€“activity relationship and mechanism of action. Journal of Computer-Aided Molecular Design, 2013, 27, 951-964.	1.3	70
113	UV/Visible spectra of natural polyphenols: A time-dependent density functional theory study. Food Chemistry, 2012, 131, 79-89.	4.2	181
114	Hâ€atom acceptor capacity of free radicals used in antioxidant measurements. International Journal of Quantum Chemistry, 2011, 111, 1131-1142.	1.0	20
115	DFT study of the reaction of quercetin with and radicals. Computational and Theoretical Chemistry, 2009, 904, 35-42.	1.5	51
116	New aspects of the antioxidant properties of phenolic acids: a combined theoretical and experimental approach. Physical Chemistry Chemical Physics, 2009, 11, 7659.	1.3	60
117	Free Radical Scavenging Properties of Guaiacol Oligomers: A Combined Experimental and Quantum Study of the Guaiacyl-Moiety Role. Journal of Physical Chemistry A, 2009, 113, 13881-13891.	1.1	76
118	Evaluation of the inhibition effect of novel cyclohepta[b]pyridine derivatives for copper corrosion and theoretical calculations. Journal of Physical Organic Chemistry, 0, , e4297.	0.9	2
119	Synthesis of Oxadiazole-Based-Thiourea, Evaluation of Their Î²-Glucuronidase Inhibitory Potential, and Molecular Docking Study. Polycyclic Aromatic Compounds, 0, , 1-16.	1.4	0