Abdulilah Ece

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Synthesis, molecular modeling, and biological evaluation of 4â€[5â€arylâ€3â€(thiophenâ€2â€yl)â€4,5â€dihydroâ€1 <i>H</i> â€pyrazolâ€1â€yl] benzenesulfonamides toward acetylcholinesterase, carbonic anhydrase I and <scp>II</scp> enzymes. Chemical Biology and Drug Design, 2018, 91, 854-866.	3.2	116
2	Design, synthesis, characterization, in vitro and in silico evaluation of novel imidazo[2,1-b][1,3,4]thiadiazoles as highly potent acetylcholinesterase and non-classical carbonic anhydrase inhibitors. Bioorganic Chemistry, 2021, 113, 105009.	4.1	78
3	Towards more effective acetylcholinesterase inhibitors: a comprehensive modelling study based on human acetylcholinesterase protein–drug complex. Journal of Biomolecular Structure and Dynamics, 2020, 38, 565-572.	3.5	43
4	Design, synthesis and molecular modelling studies of some pyrazole derivatives as carbonic anhydrase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 289-297.	5.2	38
5	Synthesis, biological evaluation and in silico modelling studies of 1,3,5-trisubstituted pyrazoles carrying benzenesulfonamide as potential anticancer agents and selective cancer-associated hCA IX isoenzyme inhibitors. Bioorganic Chemistry, 2019, 92, 103222.	4.1	34
6	Synthesis, characterization, preliminary SAR and molecular docking study of some novel substituted imidazo[2,1-b][1,3,4]thiadiazole derivatives as antifungal agents. Medicinal Chemistry Research, 2017, 26, 615-630.	2.4	33
7	Design, Synthesis, SAR and Molecular Modeling Studies of Novel Imidazo[2,1â€ <i>b</i>][1,3,4]Thiadiazole Derivatives as Highly Potent Antimicrobial Agents. Molecular Informatics, 2018, 37, 1700083.	2.5	32
8	New bis- and tetrakis-1,2,3-triazole derivatives: Synthesis, DNA cleavage, molecular docking, antimicrobial, antioxidant activity and acid dissociation constants. Bioorganic and Medicinal Chemistry Letters, 2022, 55, 128453.	2.2	32
9	Comprehensive study on potent and selective carbonic anhydrase inhibitors: Synthesis, bioactivities and molecular modelling studies of 4-(3-(2-arylidenehydrazine-1-carbonyl)-5-(thiophen-2-yl)-1H-pyrazole-1-yl) benzenesulfonamides. European Journal of Medicinal Chemistry, 2021, 217, 113351	5.5	30
10	The discovery of potential cyclin A/CDK2 inhibitors: a combination of 3D QSAR pharmacophore modeling, virtual screening, and molecular docking studies. Medicinal Chemistry Research, 2013, 22, 5832-5843.	2.4	26
11	A computational insight into acetylcholinesterase inhibitory activity of a new lichen depsidone. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 528-532.	5.2	23
12	Novel imidazo[2,1â€ <i>b</i>]thiazoleâ€based anticancer agents as potential focal adhesion kinase inhibitors: Synthesis, in silico and in vitro evaluation. Chemical Biology and Drug Design, 2021, 98, 270-282.	3.2	21
13	Epichlorohydrin and tripolyphosphate-crosslinked chitosan–kaolin composite for Auramine O dye removal from aqueous solutions: Experimental study and DFT calculations. International Journal of Biological Macromolecules, 2022, 199, 318-330.	7.5	21
14	A cooperative computational and experimental investigation on electrochemical behavior of metoprolol and its voltammetric determination. Canadian Journal of Chemistry, 2013, 91, 951-959.	1.1	18
15	An integrated approach towards the development of novel antifungal agents containing thiadiazole: synthesis and a combined similarity search, homology modelling, molecular dynamics and molecular docking study. Chemistry Central Journal, 2018, 12, 121.	2.6	18
16	Exploring QSAR on 4-Cyclohexylmethoxypyrimidines as Antitumor Agents for Their Inhibitory Activity of CDK2. Letters in Drug Design and Discovery, 2010, 7, 625-631.	0.7	17
17	Bioactive indanes: insight into the bioactivity of indane dimers related to the lead anti-inflammatory molecule PH46A. Journal of Pharmacy and Pharmacology, 2020, 72, 927-937.	2.4	17
18	Quinazolinone-based benzenesulfonamides with low toxicity and high affinity as monoamine oxidase-A inhibitors: Synthesis, biological evaluation and induced-fit docking studies. Bioorganic Chemistry, 2022, 124, 105822.	4.1	17

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19	Experimental and Theoretical Study on the Electrochemical Behavior of Zofenopril and its Voltammetric Determination. Current Pharmaceutical Analysis, 2012, 8, 339-348.	0.6	14
20	Experimental and theoretical studies on tautomeric structures of a newly synthesized 2,2′(hydrazine-1,2-diylidenebis(propan-1-yl-1-ylidene))diphenol. Chemical Physics Letters, 2018, 693, 132-145.	2.6	14
21	Application of carbon arcâ€generated Mo―and Wâ€based catalyst systems to the ROMP of norbornene. Applied Organometallic Chemistry, 2009, 23, 359-364.	3.5	13
22	Novel urea-thiourea hybrids bearing 1,4-naphthoquinone moiety: Anti-inflammatory activity on mammalian macrophages by regulating intracellular PI3K pathway, and molecular docking study. Journal of Molecular Structure, 2022, 1264, 133284.	3.6	12
23	E-pharmacophore based virtual screening for identification of dual specific PDE5A and PDE3A inhibitors as potential leads against cardiovascular diseases. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2302-2317.	3.5	11
24	Exploring the structural basis of conformational heterogeneity and autoinhibition of human cGMP-specific protein kinase lα through computational modelling and molecular dynamics simulations. Computational and Structural Biotechnology Journal, 2020, 18, 1625-1638.	4.1	10
25	Synthesis, Biological Evaluation, Molecular Docking, and Acid Dissociation Constant of New Bisâ€1,2,3â€triazole Compounds. ChemistrySelect, 2021, 6, 6994-7001.	1.5	10
26	Synthesis, structural characterization, and antiproliferative/cytotoxic effects of a novel modified poly(maleic anhydride-co-vinyl acetate)/doxorubicin conjugate. Polymer Bulletin, 2017, 74, 2159-2184.	3.3	9
27	The first example of tungsten-based carbene generation from WCl6 and atomic carbon and its use in olefin metathesis. Tetrahedron Letters, 2006, 47, 5167-5170.	1.4	7
28	Redox Pathways of Aliskiren Based on Experimental and Computational Approach and Its Voltammetric Determination. Journal of the Brazilian Chemical Society, 2013, , .	0.6	6
29	In Vitro Antibacterial and Antifungal Activity and Computational Evaluation of Novel Indole Derivatives Containing 4-Substituted Piperazine Moieties. Letters in Drug Design and Discovery, 2018, 15, 1079-1086.	0.7	6
30	Reaction of Atomic Carbon with Isomeric Cresols (Supplementary Material). Letters in Organic Chemistry, 2009, 6, 650-653.	0.5	1
31	E-Pharmacophore Mapping Combined with Virtual Screening and Molecular Docking to Identify Potent and Selective Inhibitors of P90 Ribosomal S6 Kinase (RSK). Turkish Journal of Pharmaceutical Sciences, 0, , .	1.4	1
32	Synthesis, Structure Elucidation and Biological Activities of Some Novel 4(3H)-Quinazolinones as Anti-Biofilm Agents. Letters in Drug Design and Discovery, 2019, 16, 313-321.	0.7	1