Mohammed Bouachrine

List of Publications by Year
in descending order

182 papers	3,111 citations	185998 28 h-index	253896 43 g-index
182 all docs	182 docs citations	182 times ranked	2437 citing authors

#	Article	IF	Citations
1	Gravimetric, electrochemical and quantum chemical studies of some pyridazine derivatives as corrosion inhibitors for mild steel in 1ÂM HCl solution. Journal of the Taiwan Institute of Chemical Engineers, 2016, 58, 552-564.	2.7	130
2	A theoretical study on the inhibition efficiencies of some quinoxalines as corrosion inhibitors of copper in nitric acid. Journal of Saudi Chemical Society, 2014, 18, 450-455.	2.4	111
3	Inhibitive properties, adsorption and theoretical study of 3,7-dimethyl-1-(prop-2-yn-1-yl)quinoxalin-2(1H)-one as efficient corrosion inhibitor for carbon steel in hydrochloric acid solution. Journal of Molecular Liquids, 2016, 222, 239-252.	2.3	110
4	DFT and TD-DFT calculation of new thienopyrazine-based small molecules for organic solar cells. Chemistry Central Journal, 2016, 10, 67.	2.6	97
5	Dielectric Properties, AC Conductivity, and Electric Modulus Analysis of Bulk Ethylcarbazole-Terphenyl. Advances in Materials Science and Engineering, 2020, 2020, 1-8.	1.0	83
6	Theoretical investigation of new thiazolothiazole-based D-Ï€-A organic dyes for efficient dye-sensitized solar cell. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 124, 646-654.	2.0	79
7	Weight Loss, Electrochemical, Quantum Chemical Calculation, and Molecular Dynamics Simulation Studies on 2-(Benzylthio)-1,4,5-triphenyl-1H-imidazole as an Inhibitor for Carbon Steel Corrosion in Hydrochloric Acid. Industrial & Engineering Chemistry Research, 2013, 52, 14315-14327.	1.8	71
8	Density functional theory (B3LYP/6-31G*) study of oligothiophenes in their aromatic and polaronic states. Computational and Theoretical Chemistry, 2005, 726, 271-276.	1.5	61
9	Theoretical design of thiazolothiazole-based organic dyes with different electron donors for dye-sensitized solar cells. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 232-238.	2.0	61
10	Ground state geometries, UV/vis absorption spectra and charge transfer properties of triphenylamine-thiophenes based dyes for DSSCs: A TD-DFT benchmark study. Computational and Theoretical Chemistry, 2018, 1125, 39-48.	1.1	56
11	A Combined Experimental and Theoretical Study on the Corrosion Inhibition and Adsorption Behaviour of Quinoxaline Derivative During Carbon Steel Corrosion in Hydrochloric Acid. Portugaliae Electrochimica Acta, 2012, 30, 405-417.	0.4	56
12	Identification of a novel dual-target scaffold for 3CLpro and RdRp proteins of SARS-CoV-2 using 3D-similarity search, molecular docking, molecular dynamics and ADMET evaluation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4522-4535.	2.0	49
13	Inhibition of copper corrosion by bipyrazole compound in aerated 3% NaCl. Journal of Saudi Chemical Society, 2012, 16, 413-418.	2.4	48
14	Quantum Chemical Studies on the Inhibiting Effect of Bipyrazoles on Steel Corrosion in HCl. E-Journal of Chemistry, 2010, 7, 419-424.	0.4	44
15	DFT/TD-DFT characterization of conjugational electronic structures and spectral properties of materials based on thieno[3,2-b][1]benzothiophene for organic photovoltaic and solar cell applications. Journal of Saudi Chemical Society, 2017, 21, 563-574.	2.4	44
16	QSAR study of unsymmetrical aromatic disulfides as potent avian SARS-CoV main protease inhibitors using quantum chemical descriptors and statistical methods. Chemometrics and Intelligent Laboratory Systems, 2021, 210, 104266.	1.8	40
17	Discovery of Potent SARS-CoV-2 Inhibitors from Approved Antiviral Drugs via Docking and Virtual Screening. Combinatorial Chemistry and High Throughput Screening, 2021, 24, 441-454.	0.6	39
18	Effects of electron acceptor groups on triphenylamine-based dyes for dye-sensitized solar cells: Theoretical investigation. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 398, 112572.	2.0	39

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19	Theoretical approach to the corrosion inhibition efficiency of some quinoxaline derivatives of steel in acid media using the DFT method. Research on Chemical Intermediates, 2013, 39, 1125-1133.	1.3	38
20	The optoelectronic properties of organic materials based on triphenylamine that are relevant to organic solar photovoltaic cells. New Journal of Chemistry, 2017, 41, 13336-13346.	1.4	38
21	Designing Donor-Acceptor thienopyrazine derivatives for more efficient organic photovoltaic solar cell: A DFT study. Physica B: Condensed Matter, 2019, 560, 111-125.	1.3	38
22	In silico detection of potential inhibitors from vitamins and their derivatives compounds against SARS-CoV-2 main protease by using molecular docking, molecular dynamic simulation and ADMET profiling. Journal of Molecular Structure, 2022, 1258, 132652.	1.8	36
23	DFT theoretical investigations of Ï€-conjugated molecules based on thienopyrazine and different acceptor moieties for organic photovoltaic cells. Journal of Saudi Chemical Society, 2016, 20, S415-S425.	2.4	35
24	Synthesis and ionochromic properties of chelating conjugated polymers. Journal of Materials Chemistry, 2000, 10, 263-268.	6.7	33
25	Camphor, Artemisinin and Sumac Phytochemicals as inhibitors against COVID-19: Computational approach. Computers in Biology and Medicine, 2021, 136, 104758.	3.9	33
26	The bridged effect on the geometric, optoelectronic and charge transfer properties of the triphenylamineâ€“bithiophene-based dyes: a DFT study. Research on Chemical Intermediates, 2018, 44, 2009-2023.	1.3	32
27	Quantitative structureâ€“activity relationship studies of dibenzo[a,d]cycloalkenimine derivatives for non-competitive antagonists ofN-methyl-<scp>d</scp>-aspartate based on density functional theory with electronic and topological descriptors. Journal of Taibah University for Science, 2015, 9, 143-154.	1.1	31
28	Density functional theory study of conformational and opto-electronic properties of oligo-para-phenylenes. Computational and Theoretical Chemistry, 2005, 725, 39-44.	1.5	29
29	Synthesis and characterization of novel graft copolymers of Poly(N-vinylcarbazole) and Poly(3-methylthiophene) for optoelectronic applications. Synthetic Metals, 2010, 160, 2306-2314.	2.1	29
30	QSAR study of anti-Human African Trypanosomiasis activity for 2-phenylimidazopyridines derivatives using DFT and Lipinski's descriptors. Heliyon, 2019, 5, e01304.	1.4	29
31	Biological activities of triazine derivatives. Combining DFT and QSAR results. Arabian Journal of Chemistry, 2017, 10, S946-S955.	2.3	28
32	2D-QSAR and docking study of a series of coumarin derivatives as inhibitors of CDK (anticancer) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 2	1.4	28
33	Theoretical design and characterization of D-A1-A based organic dyes for efficient DSSC by altering promising acceptor (A1) moiety. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 407, 113048.	2.0	28
34	Quantitative structureâ€“activity relationships analysis, homology modeling, docking and molecular dynamics studies of triterpenoid saponins as Kirsten rat sarcoma inhibitors. Journal of Biomolecular Structure and Dynamics, 2021, 39, 152-170.	2.0	27
35	In silico design of novel PIN1 inhibitors by combined of 3D-QSAR, molecular docking, molecular dynamic simulation and ADMET studies. Journal of Molecular Structure, 2022, 1253, 132291.	1.8	27
36	Bridging effect on structural and optoelectronic properties of oligothiophene. Computational and Theoretical Chemistry, 2008, 851, 254-262.	1.5	26

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37	QSAR study of N-substituted oseltamivir derivatives as potent avian influenza virus H5N1 inhibitors using quantum chemical descriptors and statistical methods. New Journal of Chemistry, 2020, 44, 1747-1760.	1.4	26
38	New organic materials based on Dâ€“Ï€â€“A structure for application in dye-sensitized solar cells. Research on Chemical Intermediates, 2018, 44, 6071-6085.	1.3	25
39	Synthesis and characterization of thienyleneâ€“phenylene copolymers with oligo(ethylene oxide) side chains. Journal of Materials Chemistry, 2004, 14, 3043-3050.	6.7	24
40	Inhibition of corrosion of copper in nitric acid solution by four amino acids. Research on Chemical Intermediates, 2014, 40, 991-1002.	1.3	24
41	DFT Study of Polythiophene Energy Band Gap and Substitution Effects. Journal of Chemistry, 2015, 2015, 1-12.	0.9	24
42	The inhibitory activity of aldose reductase of flavonoid compounds: Combining DFT and QSAR calculations. Journal of Taibah University for Science, 2016, 10, 534-542.	1.1	24
43	Combined 3D-QSAR and molecular docking study on 7,8-dialkyl-1,3-diaminopyrrolo-[3,2-f] Quinazoline series compounds to understand the binding mechanism of DHFR inhibitors. Journal of Molecular Structure, 2017, 1139, 319-327.	1.8	24
44	Structureâ€“property relationships of soluble poly(2,5-dibutoxyethoxy-1,4-phenylene-alt-2,5-thienylene) (PBuPT) for organic-optoelectronic devices. Journal of Molecular Structure, 2013, 1036, 7-18.	1.8	23
45	Furanone derivatives as new inhibitors of CDC7 kinase: development of structure activity relationship model using 3D QSAR, molecular docking, and in silico ADMET. Structural Chemistry, 2018, 29, 1031-1043.	1.0	23
46	Molecular Design of D-Ï€-A-A Organic Dyes Based on Triphenylamine Derivatives with Various Auxiliary Acceptors for High Performance DSSCs. Journal of Electronic Materials, 2019, 48, 4452-4462.	1.0	23
47	Theoretical investigation on Ï€-spacer effect of the Dâ€“Ï€â€“A organic dyes for dye-sensitized solar cell applications: a DFT and TD-BHandH study. Journal of Molecular Modeling, 2019, 25, 92.	0.8	23
48	Computational design of new organic (Dâ€“Ï€â€“A) dyes based on benzothiadiazole for photovoltaic applications, especially dye-sensitized solar cells. Research on Chemical Intermediates, 2020, 46, 3247-3262.	1.3	23
49	Spectroscopic investigations of copolymers incorporating various thiophene and phenylene monomers. Synthetic Metals, 2006, 156, 318-326.	2.1	22
50	Investigation of Antileishmanial Activities of Acridines Derivatives against Promastigotes and Amastigotes Form of Parasites Using Quantitative Structure Activity Relationship Analysis. Advances in Physical Chemistry, 2016, 2016, 1-16.	2.0	22
51	QSAR analysis of the toxicity of phenols and thiophenols using MLR and ANN. Journal of Taibah University for Science, 2017, 11, 1-10.	1.1	22
52	The optoelectronic properties of new dyes based onÂthienopyrazine. Comptes Rendus Chimie, 2017, 20, 461-466.	0.2	22
53	3D-QSAR modeling and molecular docking studies on a series of 2,5 disubstituted 1,3,4-oxadiazoles. Journal of Molecular Structure, 2017, 1145, 278-284.	1.8	22
54	Role of silicon in polymer synthesis: activation of the oxidative coupling of thiophene by trimethylsilyl substituents; a route to high molecular weight poly(3-alkyl)thiophene. Journal of Materials Chemistry, 1995, 5, 797-799.	6.7	21

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55	Theoretical study of structural and electronic properties of oligo(thiophene-phenylene)s in comparison with oligothiophenes and oligophenylenes. Chinese Chemical Letters, 2008, 19, 123-126.	4.8	21
56	QSPR studies of 9-aniliioacridine derivatives for their DNA drug binding properties based on density functional theory using statistical methods: Model, validation and influencing factors. Journal of Taibah University for Science, 2016, 10, 868-876.	1.1	21
57	Theoretical study of the effects of modifying the structures of organic dyes based on N,N-alkylamine on their efficiencies as DSSC sensitizers. Journal of Molecular Modeling, 2019, 25, 9.	0.8	20
58	Experimental and theoretical study for corrosion inhibition of mild steel 1ÂM HCl solution by some new diaminopropanenitrile compounds. Research on Chemical Intermediates, 2012, 38, 1669-1690.	1.3	18
59	New organic dyes based on phenylenevinylene for solar cells: DFT and TD-DFT investigation. Karbala International Journal of Modern Science, 2017, 3, 75-82.	0.5	18
60	Identification of Novel SARS-CoV-2 Inhibitors: A Structure-Based Virtual Screening Approach. Journal of Chemistry, 2021, 2021, 1-7.	0.9	18
61	A thienylene-phenylene copolymer with di(ethylene oxide) side chains and its use in light emitting diodes. Synthetic Metals, 2002, 126, 241-244.	2.1	17
62	Theoretical Investigations on the Electronic and Optical Properties of Bridged Oligothiophenes. Journal of Physical Chemistry A, 2012, 116, 9730-9738.	1.1	17
63	Inhibiting effects of benzamide derivatives on the corrosion of mild steel in hydrochloric acid solution. Research on Chemical Intermediates, 2013, 39, 2417-2433.	1.3	17
64	In Silico Exploration of Aryl Halides Analogues as CheckpointKinase 1 Inhibitors by Using 3D QSAR, Molecular Docking Study,and ADMET Screening. Advanced Pharmaceutical Bulletin, 2019, 9, 84-92.	0.6	17
65	The photophysical properties and electronic structures of bis[1]benzothieno[6,7-d:6â€²,7â€²-dâ€²]benzo[1,2-b:4,5-bâ€²]dithiophene (BBTBDT) derivatives as hole-transporting materials for organic light-emitting diodes (OLEDs). New Journal of Chemistry, 2019, 43, 15899-15909.	1.4	17
66	3D-QSAR Study of the Chalcone Derivatives as Anticancer Agents. Journal of Chemistry, 2020, 2020, 1-12.	0.9	17
67	Molecular docking analysis of N-substituted oseltamivir derivatives with the SARS-Cov-2 main protease. Bioinformation, 2020, 16, 404-410.	0.2	17
68	Computational investigation of pyrrolidin derivatives as novel GPX4/MDM2â€“p53 inhibitors using 2D/3D-QSAR, ADME/toxicity, molecular docking, molecular dynamics simulations, and MM-GBSA free energy. Structural Chemistry, 2022, 33, 1019-1039.	1.0	17
69	DFT calculations of the local spin densities and oligomerization mechanism of thiopheneâ€“phenylene (TP) co-oligomers and derivatives. Computational and Theoretical Chemistry, 2007, 814, 25-32.	1.5	16
70	Prediction of potential inhibitors of SARS-CoV-2 using 3D-QSAR, molecular docking modeling and ADMET properties. Heliyon, 2021, 7, e06603.	1.4	16
71	Theoretical study using DFT calculations on inhibitory action of four pyridazines on corrosion of copper in nitric acid. Research on Chemical Intermediates, 2012, 38, 2327-2334.	1.3	15
72	3D QSAR studies, molecular docking and ADMET evaluation, using thiazolidine derivatives as template to obtain new inhibitors of PIM1 kinase. Computational Biology and Chemistry, 2018, 74, 201-211.	1.1	15

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73	In silico investigation of phytoconstituents from Cameroonian medicinal plants towards COVID-19 treatment. Structural Chemistry, 2022, 33, 1799-1813.	1.0	15
74	Synthesis, characterization and theoretical study of new organic copolymer based on PVK and PEDOT. Journal of Non-Crystalline Solids, 2010, 356, 467-473.	1.5	14
75	Quantitative structureâ€“activity relationship of antitumor and neurotoxic Î²-carbolines alkaloids: nine harmine derivatives. Research on Chemical Intermediates, 2013, 39, 2219-2236.	1.3	14
76	Investigation of indirubin derivatives: a combination of 3D-QSAR, molecular docking, and ADMET towards the design of new DRAK2 inhibitors. Structural Chemistry, 2018, 29, 1609-1622.	1.0	14
77	Non-fullerene acceptor IDIC based on indacinodithiophene used as an electron donor for organic solar cells: A computational study. Journal of Molecular Liquids, 2022, 348, 118289.	2.3	14
78	Density functional theory [B3LYP/6â€311G(d,p)] study of a new copolymer based on carbazole and (3,4â€ethylenedioxythiophene) in their aromatic and polaronic states. Journal of Applied Polymer Science, 2011, 122, 3351-3360.	1.3	13
79	Inhibition of copper corrosion in acid solution by N-1-naphthylethylenediamine dihydrochloride monomethanolate: experimental and theoretical study: part-1. Research on Chemical Intermediates, 2012, 38, 1079-1089.	1.3	13
80	Theoretical investigation of electroluminescent alkoxy substituted 4,4â€²-bis(2-phenylethenyl)biphenyls as guest in blue OLEDs. Solar Energy Materials and Solar Cells, 2006, 90, 1393-1402.	3.0	12
81	Computer aided drug design based on 3D-QSAR and molecular docking studies of 5-(1H-indol-5-yl)-1,3,4-thiadiazol-2-amine derivatives as PIM2 inhibitors: a proposal to chemists. In Silico Pharmacology, 2018, 6, 5.	1.8	12
82	Development of novel monoamine oxidase B (MAO-B) inhibitors by combined application of docking-based alignment, 3D-QSAR, ADMET prediction, molecular dynamics simulation, and MM_GBSA binding free energy. Journal of Biomolecular Structure and Dynamics, 2023, 41, 4667-4680.	2.0	12
83	Synthesis and characterization of co-polymers involving various thiophene and phenylene monomers. Synthetic Metals, 2004, 145, 237-243.	2.1	11
84	Exchange with temperature of the electronâ€vibrational mode interaction between thienyleneâ€“phenylene copolymer rings. Journal of Polymer Science, Part B: Polymer Physics, 2010, 48, 964-971.	2.4	11
85	Molecular design of Dâ€“Aâ€“D conjugated molecules based on fluorene for organic solar cells. Optical and Quantum Electronics, 2019, 51, 1.	1.5	11
86	Antibacterial study of 3-(2-amino-6-phenylpyrimidin-4-yl)-N-cyclopropyl-1-methyl-1H-indole-2-carboxamide derivatives: CoMFA, CoMSIA analyses, molecular docking and ADMET properties prediction. Journal of Molecular Structure, 2019, 1177, 275-285.	1.8	11
87	Prediction of electropolymerization mechanisms of two substituted phenylene: Poly-3-methoxy-toluenes (P3mt1 and P3mt2). Journal of Applied Polymer Science, 2006, 100, 57-64.	1.3	10
88	Quantum chemical investigations study of the effect of electron donor units on the structural, electronic and optoelectronic properties of diarylthienopyrazine analogs. Computational and Theoretical Chemistry, 2014, 1036, 22-30.	1.1	10
89	3D-QSAR models to predict anti-cancer activity on a series of protein P38 MAP kinase inhibitors. Journal of Taibah University for Science, 2017, 11, 392-407.	1.1	10
90	Synthesis, characterization, DFT and TD-DFT studies of novel carbazole-based copolymer used in high efficient dye-sensitized solar cells. Polymer Testing, 2018, 66, 78-86.	2.3	10

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91	Structural and photophysical studies of triphenylamine-based nonlinear optical dyes: effects of Ï€-linker moieties on the D-Ï€-A structure. Comptes Rendus Chimie, 2019, 22, 373-385.	0.2	10
92	DFT-based reactivity and combined QSAR, molecular docking of 1,2,4,5-Tetrazine derivatives as inhibitors of Pim-1 kinase. Heliyon, 2019, 5, e02451.	1.4	10
93	Assessment of effective imidazole derivatives against SARS-CoV-2 main protease through computational approach. Life Sciences, 2020, 262, 118469.	2.0	10
94	Theoretical study of organic sensitizers based on 2, 6-diphenyl-4H-pyranylidene/1, 3, 4-oxadiazole for dye-sensitized solar cells. Journal of Molecular Modeling, 2020, 26, 346.	0.8	10
95	Integrated 3D-QSAR, molecular docking, and molecular dynamics simulation studies on 1,2,3-triazole based derivatives for designing new acetylcholinesterase inhibitors. Turkish Journal of Chemistry, 2021, 45, 647-660.	0.5	10
96	QSAR study and rustic ligand-based virtual screening in a search for aminooxadiazole derivatives as PIM1 inhibitors. Chemistry Central Journal, 2018, 12, 32.	2.6	9
97	New organic molecular based on Bis-Dipolar Diphenylamino-EndcappedOligo Aryl Fluorene Application for organic solar cells. Materials Today: Proceedings, 2019, 13, 1178-1187.	0.9	9
98	Opto-electronic properties and molecular design of new materials based on pyrrole studied by DFT. Research on Chemical Intermediates, 2012, 38, 1375-1388.	1.3	8
99	The effect of 2-aminoquinoline-6-carboxylic acid on the corrosion behavior of mild steel in hydrochloric acid. Journal of the Iranian Chemical Society, 2012, 9, 635-641.	1.2	8
100	New materials based on thiazolothiazole and thiophene candidates for optoelectronic device applications: theoretical investigations. Research on Chemical Intermediates, 2013, 39, 2679-2695.	1.3	8
101	Predictive modelling of the LD50 activities of coumarin derivatives using neural statistical approaches: Electronic descriptor-based DFT. Journal of Taibah University for Science, 2016, 10, 451-461.	1.1	8
102	QSPR study of the retention/release property of odorant molecules in pectin gels using statistical methods. Journal of Taibah University for Science, 2017, 11, 1030-1046.	1.1	8
103	Study of novel triazolo-benzodiazepine analogues as antidepressants targeting by molecular docking and ADMET properties prediction. Heliyon, 2019, 5, e02446.	1.4	8
104	DFT and TD-DFT calculations on thieno[2,3-b]indole-based compounds for application in organic bulk heterojunction (BHJ) solar cells. Research on Chemical Intermediates, 2019, 45, 1327-1340.	1.3	8
105	3D-QSAR modeling and molecular docking studies on a series of 2, 4, 5-trisubstituted imidazole derivatives as CK2 inhibitors. Journal of Biomolecular Structure and Dynamics, 2023, 41, 234-248.	2.0	8
106	QSAR Study of Anthra[1,9-cd]pyrazol-6(2H)-one Derivatives as Potential Anticancer Agents Using Statistical Methods. Advances in Chemistry, 2018, 2018, 1-16.	1.1	7
107	New dehydroabietic acid (DHA) derivatives with anticancer activity against HepG2 cancer cell lines as a potential drug targeting EGFR kinase domain. CoMFA study and virtual ligand-based screening. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2993-3003.	2.0	7
108	Molecular docking of potential cytotoxic alkylating carmustine derivatives 2-chloroethylnitrososulfamides analogues of 2-chloroethylnitrosoureas. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4256-4269.	2.0	7

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109	3D-QSAR modeling, molecular docking and ADMET properties of benzothiazole derivatives as Î±-glucosidase inhibitors. Materials Today: Proceedings, 2021, 45, 7643-7652.	0.9	7
110	Molecular Modeling Studies of C-Glycosylfavone Derivatives as GSK-3Î² Inhibitors Based on QSAR and Docking Analysis. Journal of Solution Chemistry, 2021, 50, 808-822.	0.6	7
111	Identification of novel acetylcholinesterase inhibitors through 3D-QSAR, molecular docking, and molecular dynamics simulation targeting Alzheimerâ€™s disease. Journal of Molecular Modeling, 2021, 27, 302.	0.8	7
112	A study of polymers obtained by oxidative coupling of furan monomers. Synthetic Metals, 2011, 161, 2220-2225.	2.1	6
113	Tetrathiafulvalene-based azine ligands for anion and metal cation coordination. Beilstein Journal of Organic Chemistry, 2015, 11, 1379-1391.	1.3	6
114	Optoelectronic properties of four azobenzene-based iminopyridine ligands for photovoltaic application. Journal of Taibah University for Science, 2017, 11, 930-938.	1.1	6
115	Chemical composition andin vitroantibacterial activity ofArtemisia ifranensisJ. Didier essential oil Growing Wild in Middle Moroccan Atlas. Journal of Essential Oil Research, 2018, 30, 142-151.	1.3	6
116	Molecular Docking and 3D-QSAR Studies on 7-azaindole Derivatives as Inhibitors of Trk A: A Strategic Design in Novel Anticancer Agents. Letters in Drug Design and Discovery, 2018, 15, 1211-1223.	0.4	6
117	Design of Novel Benzimidazole Derivatives as Potential Î±-amylase Inhibitors by 3D-QSAR Modeling and Molecular Docking Studies. Journal of the Turkish Chemical Society, Section A: Chemistry, 2020, 7, 471-480.	0.4	6
118	Rational design of novel potential EGFR inhibitors by 3D-QSAR, molecular docking, molecular dynamics simulation, and pharmacokinetics studies. Chemical Data Collections, 2022, 39, 100851.	1.1	6
119	A study of drug candidates derived from pleconaril for inhibiting coxsackievirus B3 (Cvb3) by ADMET, molecular docking, molecular dynamics and retrosynthesis. New Journal of Chemistry, 2022, 46, 10154-10161.	1.4	6
120	Homology modeling, virtual screening, molecular docking, molecular dynamic (MD) simulation, and ADMET approaches for identification of natural anti-Parkinson agents targeting MAO-B protein. Neuroscience Letters, 2022, 786, 136803.	1.0	6
121	Absorption and photoluminescence of a new thienyleneâ€“phenylene copolymer. Journal of Non-Crystalline Solids, 2006, 352, 3685-3688.	1.5	5
122	Structureâ€“olfactive threshold relationships for pyrazine derivatives. Journal of Molecular Modeling, 2006, 12, 985-989.	0.8	5
123	New low band-gap conjugated organic materials based on fluorene, thiophene and phenylene for photovoltaic applications: Theoretical study. Materials Today: Proceedings, 2016, 3, 2578-2586.	0.9	5
124	3D-QSAR and Molecular Docking Studies of p-Aminobenzoic Acid Derivatives to Explore the Features Requirements of Alzheimer Inhibitors. Orbital, 2020, 12, .	0.1	5
125	New Organic Materials Based on Thiophene for Photovoltaic Device: Theoretical investigation. Turkish Computational and Theoretical Chemistry, 2018, 2, 36-48.	0.5	5
126	Molecular docking, molecular dynamics simulation, and ADMET analysis of levamisole derivatives against the SARS-CoV-2 main protease (M^{Pro}). BioImpacts, 2021, 12, 107-113.	0.7	5

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127	REACTIVITY OF SILYL MONOMERS FOR THE OXIDATIVE POLYMERIZATION OF PHENYLENE UNITS. Phosphorus, Sulfur and Silicon and the Related Elements, 1999, 152, 265-278.	0.8	4
128	New materials based on carbazole for optoelectronic device applications: Theoretical investigation. Chinese Chemical Letters, 2008, 19, 488-492.	4.8	4
129	Correlation structureâ€“properties of poly(3-methyl-thiophene) (P3MTh) synthesized using TiCl4 as an oxidant. Synthetic Metals, 2012, 162, 1724-1730.	2.1	4
130	DFT study of opto-electronic properties of benzothiazole derivatives for use in solar cells. Journal of Theoretical and Computational Chemistry, 2016, 15, 1650023.	1.8	4
131	Study of interactions between odorant molecules and the hOR1G1 olfactory receptor by molecular modeling. Egyptian Journal of Ear, Nose, Throat and Allied Sciences, 2017, 18, 257-265.	0.0	4
132	Structural basis of pyrazolopyrimidine derivatives as CAMKIIÎ´ kinase inhibitors: insights from 3D QSAR, docking studies and in silico ADMET evaluation. Chemical Papers, 2018, 72, 2833-2847.	1.0	4
133	Elaboration of low-band-gap Ï€-conjugated systems based on thieno[3,4-b]pyrazines. Pure and Applied Chemistry, 2020, 92, 335-353.	0.9	4
134	Characterization and simulation study of organic solar cells based on donorâ€“acceptor (Dâ€“Ï€â€“A) molecular materials. RSC Advances, 2020, 10, 18816-18823.	1.7	4
135	In Silico Drug Design: Development of New Pyrimidine-based Benzothiazole Derivatives, Selective for CDK2. Letters in Drug Design and Discovery, 2021, 18, 961-975.	0.4	4
136	QSPR Study of the Retention/release Property of Odorant Molecules in Water Using Statistical Methods. Orbital, 2017, 9, .	0.1	4
137	Low Band Gap of Novel Compounds Having Triphenylamine and Oligothiophenes Based Donor-acceptor Organic Dyes for Photovoltaic Applications: A DFT-B3LYP Calculation. International Journal of Advanced Research in Computer Science and Software Engineering, 2017, 7, 96-107.	0.1	4
138	2-Aminopyridine Cadmium (II) meso-chlorophenylporphyrin coordination compound. Photophysical properties, X-ray molecular structure, antimicrobial activity, and molecular docking analysis. Journal of Chemical Sciences, 2022, 134, 1.	0.7	4
139	Characterization and structureâ€“property relationship of chemical oxidative polymerization of poly(paraâ€hydroquinone). Journal of Applied Polymer Science, 2010, 118, 711-720.	1.3	3
140	Quantitative Structureâ€“Activity Relationship Studies of Anticancer Activity for Isatin (1H-indole-2,3-dione) Derivatives Based on Density Functional Theory. International Journal of Quantitative Structure-Property Relationships, 2017, 2, 90-115.	1.1	3
141	Theoretical Study of Copper Acetonitrile Effects on Parr Functions Indices and Regioselectivity Using Density Functional Theory (DFT). Russian Journal of Physical Chemistry A, 2018, 92, 2464-2471.	0.1	3
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