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	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
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	In silico investigation of phytoconstituents from Cameroonian medicinal plants towards COVID-19 treatment. Structural Chemistry, 2022, 33, 1799-1813.	1.0	15
11	Designing new donors organic compounds with IDIC core for photovoltaic application. Optik, 2022, 262, 169174.	1.4	2
12	Modeling study, 3D-QSAR and molecular docking of 9H-purine derivatives as EGFR inhibitors. Materials Today: Proceedings, 2022, 62, 6312-6323.	0.9	2
13	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
14	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
15	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
16	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
17	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
18	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

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19	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
20	Design of new 3, 5-disubstituted indole as hematological anticancer agents using 3D-QSAR, molecular docking and drug-likeness studies. Materials Today: Proceedings, 2021, 45, 7608-7614.	0.9	3
21	QSAR Study of Î±-Glucosidase Inhibitors for Benzimidazole Bearing Bis-Schiff Bases Using CoMFA, CoMSIA, and Molecular Docking. International Journal of Quantitative Structure-Property Relationships, 2021, 6, 9-24.	1.1	3
22	Frequency and Temperature Effects on Dielectric Properties of PEDOT-VC Copolymer. E3S Web of Conferences, 2021, 229, 01054.	0.2	0
23	Identification of Novel SARS-CoV-2 Inhibitors: A Structure-Based Virtual Screening Approach. Journal of Chemistry, 2021, 2021, 1-7.	0.9	18
24	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
25	Prediction of potential inhibitors of SARS-CoV-2 using 3D-QSAR, molecular docking modeling and ADMET properties. Heliyon, 2021, 7, e06603.	1.4	16
26	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
27	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
28	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
29	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
30	Optical Properties of (C2H5C6H4NH2)2ZnBr2 Complex: Experimental and Quantum Chemical Studies. Russian Journal of Physical Chemistry A, 2021, 95, 1864-1870.	0.1	0
31	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
32	Camphor, Artemisinin and Sumac Phytochemicals as inhibitors against COVID-19: Computational approach. Computers in Biology and Medicine, 2021, 136, 104758.	3.9	33
33	Catastrophic Collision Between Obesity and COVID-19 Have Evoked the Computational Chemistry for Research in Silico Design of New CaMKKII Inhibitors Against Obesity by Using 3D-QSAR, Molecular Docking, and ADMET. Orbital, 2021, 13, .	0.1	0
34	Combined Conceptual-DFT, Quantitative MEP Analysis, and Molecular Docking Study of Benzodiazepine Analogs. Orbital, 2021, 13, .	0.1	2
35	3D-QSAR and molecular docking studies of 4-methyl quinazoline derivatives as PI3KÎ± inhibitors. Journal of the Indian Chemical Society, 2021, 98, 100183.	1.3	3
36	Organic dyes based on selenophene for efficient dye-sensitized solar cell. Journal of Molecular Modeling, 2021, 27, 333.	0.8	3

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37	Assessment of asthma treatment against SARS CoV-2 by using a computer approach. E3S Web of Conferences, 2021, 319, 01024.	0.2	1
38	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
39	Study of dipolar 1.3 cycloaddition reaction by DFT method, as well as study of antibacterial activity of two isomers 1.4 and 1.5 on two therapeutic targets E. coli and Helicobacter pylori, by molecular docking. Turkish Computational and Theoretical Chemistry, 2021, 5, 46-55.	0.5	2
40	DFT/TDDFT studies of the structural, electronic, NBO and non-linear optical proper-ties of triphenylamine functionalized tetrathiafulvalene. Turkish Computational and Theoretical Chemistry, 2021, 5, 24-34.	0.5	2
41	2-Oxoquinoline Arylaminothiazole Derivatives in Identifying Novel Potential Anticancer Agents by Applying 3D-QSAR, Docking, and Molecular Dynamics Simulation Studies. Journal of the Mexican Chemical Society, 2021, 66, .	0.2	3
42	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
43	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
44	2D- and 3D-QSAR and Molecular Docking of 2-Hydroxyisoquinoline-1,3-Diones as Inhibitors of HIV Reverse Transcriptase. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 32-52.	1.1	0
45	Assessment of effective imidazole derivatives against SARS-CoV-2 main protease through computational approach. Life Sciences, 2020, 262, 118469.	2.0	10
46	Photophysical properties of electroluminescent molecules based on thiophene and oxadiazole. Computational investigations. Results in Chemistry, 2020, 2, 100068.	0.9	3
47	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
48	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 3	1.4	28
49	3D-QSAR Study of the Chalcone Derivatives as Anticancer Agents. Journal of Chemistry, 2020, 2020, 1-12.	0.9	17
50	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
51	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
52	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
53	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
54	Optimization and Simulation of the photovoltaic properties of modified Donor-Acceptor Conjugated Oligomers for Organic Solar Cells. , 2020, , .		1

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55	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
56	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
57	Molecular docking analysis of N-substituted oseltamivir derivatives with the SARS-Cov-2 main protease. Bioinformation, 2020, 16, 404-410.	0.2	17
58	Molecular docking investigation of cytotoxic phenanthrene derivatives. Comptes Rendus Chimie, 2020, 23, 329-342.	0.2	0
59	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
60	Ã‰tude structurale des systÃ¨mes dissymÃ©triques de structure D-Ï€-A Ã base de thiÃ©nopyrazine destinÃ©s aux cellules solaires organiques de type Â« bulk heterojunction Â» (BHJ). Canadian Journal of Chemistry, 2019, 97, 745-755.	0.6	1
61	QSPR Study of the Retention/Release Property of Odorant Molecules in Water, Dairy and Pectin gels. Materials Today: Proceedings, 2019, 13, 621-629.	0.9	3
62	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
63	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
64	Study of novel triazolo-benzodiazepine analogues as antidepressants targeting by molecular docking and ADMET properties prediction. Heliyon, 2019, 5, e02446.	1.4	8
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	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
67	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
68	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
69	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
70	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
71	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
72	Machine learning algorithms used in Quantitative structure-activity relationships studies as new approaches in drug discovery. , 2019, , .		2

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73	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
74	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
75	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
76	The dielectric and electrical proprieties of Ethylcarbazole family based copolymer. Mediterranean Journal of Chemistry, 2019, 8, 191-197.	0.3	1
77	2D-QSPR Study of Olfactive Thresholds for Pyrazine Derivatives Using DFT and Statistical Methods. Emerging Science Journal, 2019, 3, 179-186.	1.4	2
78	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
79	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
80	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
81	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
82	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
83	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
84	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
85	Modulation on Dye/TiO2Bending Energy and Charge Transfer to High Performance Triphenylamine Based Sensitizers in Solar Cells: A DFT Study. , 2018, , .		0
86	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
87	3D QSAR Modeling and Molecular Docking Studies on a Series of Triazole Analogues as Antibacterial Agents. Journal of Structural Chemistry, 2018, 59, 1544-1554.	0.3	1
88	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
89	QSAR Study of (5-Nitroheteroaryl-1,3,4-Thiadiazole-2-yl) Piperazinyl Derivatives to Predict New Similar Compounds as Antileishmanial Agents. Advances in Physical Chemistry, 2018, 2018, 1-10.	2.0	3
90	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

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91	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
92	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
93	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
94	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
95	New Organic Materials Based on Thiophene for Photovoltaic Device: Theoretical investigation. Turkish Computational and Theoretical Chemistry, 2018, 2, 36-48.	0.5	5
96	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
97	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
98	The optoelectronic properties of new dyes based onÂthienopyrazine. Comptes Rendus Chimie, 2017, 20, 461-466.	0.2	22
99	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
100	Optoelectronic properties of four azobenzene-based iminopyridine ligands for photovoltaic application. Journal of Taibah University for Science, 2017, 11, 930-938.	1.1	6
101	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
102	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
103	QSAR studies on PIM1 and PIM2 inhibitors using statistical methods: a rustic strategy to screen for 5-(1H-indol-5-yl)-1,3,4-thiadiazol analogues and predict their PIM inhibitory activity. Chemistry Central Journal, 2017, 11, 41.	2.6	2
104	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
105	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
106	Small compounds based on 2,7-silafluorene and 4,7-di (2â€²-thienyl) for heterojunction organic solar cells: DFT study. Journal of the Iranian Chemical Society, 2017, 14, 2167-2176.	1.2	2
107	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
108	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

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109	Biological activities of triazine derivatives. Combining DFT and QSAR results. Arabian Journal of Chemistry, 2017, 10, S946-S955.	2.3	28
110	Organic Compounds Based on (E)-N-Aryl-2-ethene-sulfonamide as Microtubule Targeted Agents in Prostate Cancer: QSAR Study. Advances in Physical Chemistry, 2017, 2017, 1-14.	2.0	2
111	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
112	TUNING THE ELECTRONIC, PHOTOPHYSICAL AND CHARGE TRANSFER PROPERTIES OF SMALL D-A MOLECULES BASED ON THIENOPYRAZINE-TERTHIENYLS BY CHANGING THE DONOR FRAGMENT: A DFT STUDY. Journal of the Chilean Chemical Society, 2017, 62, 3637-3646.	0.5	2
113	DFT Study of Electronic and Optical Properties of Small Oligothiophenes Based on Terthiophene End-capped by Several Donor Groups. Orbital, 2017, 9, .	0.1	2
114	QSPR Study of the Retention/release Property of Odorant Molecules in Water Using Statistical Methods. Orbital, 2017, 9, .	0.1	4
115	Effect of the Alkyl Chain Length Incorporated into Donor Part on the Optoelectronic Properties of the Carbazole Based Dyes: Theoretical Study. Orbital, 2017, 9, .	0.1	1
116	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
117	Theoretical Study of 1,3-Dipolar Cycloadditions Regioselectivity of Benzyl Azide with Glycosyl-O Acetylene Using Density Functional Theory (DFT). Orbital, 2017, 9, .	0.1	0
118	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
119	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
120	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
121	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
122	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
123	DFT and TD-DFT calculation of new thienopyrazine-based small molecules for organic solar cells. Chemistry Central Journal, 2016, 10, 67.	2.6	97
124	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
125	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
126	Study of low band gap DSSCs based on bridging bithiophene and biphenyl: theoretical investigation. Journal of the Iranian Chemical Society, 2016, 13, 37-44.	1.2	2

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127	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
128	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
129	Tetrathiafulvalene-based azine ligands for anion and metal cation coordination. Beilstein Journal of Organic Chemistry, 2015, 11, 1379-1391.	1.3	6
130	DFT Study of Polythiophene Energy Band Gap and Substitution Effects. Journal of Chemistry, 2015, 2015, 1-12.	0.9	24
131	Combined experimental and theoretical study of structural and optoelectronic properties of Polyfuran with its oligomers. , 2015, , .		0
132	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
133	QSAR Studies of Toxicity Towards Monocytes with (1,3-benzothiazol-2-yl) amino-9-(10H)-acridinone Derivatives Using Electronic Descriptors. Orbital, 2015, 7, .	0.1	1
134	Spectroscopic analysis of polyfuran and theoretical investigation of electronic properties of oligofurans: Destined for the solar cell applications. , 2014, , .		2
135	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
136	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
137	Inhibition of corrosion of copper in nitric acid solution by four amino acids. Research on Chemical Intermediates, 2014, 40, 991-1002.	1.3	24
138	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
139	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
140	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
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