

Muhammad Khalid

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170
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32
h-index

44
g-index

180
ext. papers

4,353
ext. citations

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avg, IF

6.06
L-index

#	Paper	IF	Citations
170	First Theoretical Framework of TriphenylamineDicyanovinylene-Based Nonlinear Optical Dyes: Structural Modification of Linkers. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 4009-4018	3.8	111
169	Efficiency of electron transfer initiated chemiluminescence. <i>Photochemistry and Photobiology</i> , 2013 , 89, 1299-317	3.6	74
168	First theoretical probe for efficient enhancement of nonlinear optical properties of quinacridone based compounds through various modifications. <i>Chemical Physics Letters</i> , 2019 , 715, 222-230	2.5	72
167	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells.. <i>RSC Advances</i> , 2019 , 9, 26402-26418	3.7	68
166	Synthesis, crystal structures, spectroscopic and nonlinear optical properties of chalcone derivatives: A combined experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2017 , 1141, 142-156	3.4	62
165	Designing indenothiophene-based acceptor materials with efficient photovoltaic parameters for fullerene-free organic solar cells. <i>Journal of Molecular Modeling</i> , 2020 , 26, 137	2	62
164	Designing N-phenylaniline-triazol configured donor materials with promising optoelectronic properties for high-efficiency solar cells. <i>Computational and Theoretical Chemistry</i> , 2020 , 1186, 112908	2	62
163	Prediction of Second-Order Nonlinear Optical Properties of D _{3h} Compounds Containing Novel Fluorene Derivatives: A Promising Route to Giant Hyperpolarizabilities. <i>Journal of Cluster Science</i> , 2019 , 30, 415-430	3	61
162	Synthesis, crystal structure analysis, spectral IR, UV-Vis, NMR assessments, electronic and nonlinear optical properties of potent quinoline based derivatives: Interplay of experimental and DFT study. <i>Journal of Saudi Chemical Society</i> , 2019 , 23, 546-560	4.3	61
161	Quantum chemical designing of indolo[3,2,1-jk]carbazole-based dyes for highly efficient nonlinear optical properties. <i>Chemical Physics Letters</i> , 2019 , 719, 59-66	2.5	59
160	Enhancement in Photovoltaic Properties of N,N-diethylaniline based Donor Materials by Bridging Core Modifications for Efficient Solar Cells. <i>ChemistrySelect</i> , 2020 , 5, 5022-5034	1.8	58
159	Facile synthesis, single crystal analysis, and computational studies of sulfanilamide derivatives. <i>Journal of Molecular Structure</i> , 2017 , 1127, 766-776	3.4	58
158	Synthesis, structural, DFT studies, docking and antibacterial activity of a xanthene based hydrazone ligand. <i>Journal of Molecular Structure</i> , 2017 , 1143, 235-244	3.4	55
157	Synthetic, XRD, non-covalent interactions and solvent dependent nonlinear optical studies of Sulfadiazine-Ortho-Vanillin Schiff base: (E)-4-((2-hydroxy-3-methoxy- benzylidene) amino)-N-(pyrimidin-2-yl)benzene-sulfonamide. <i>Journal of Molecular Structure</i> , 2018 , 1161, 66-75	3.4	52
156	Molecular engineering of AD ₂ DA configured small molecular acceptors (SMAs) with promising photovoltaic properties for high-efficiency fullerene-free organic solar cells. <i>Optical and Quantum Electronics</i> , 2020 , 52, 1	2.4	52
155	Designing of benzothiazole based non-fullerene acceptor (NFA) molecules for highly efficient organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020 , 1181, 112833	2	51
154	First principles study of electronic and nonlinear optical properties of A-D-DA and D-A-D-DA configured compounds containing novel quinoline-carbazole derivatives.. <i>RSC Advances</i> , 2020 , 10, 22273-22283	3.7	48

153	Designing spirobifullerene core based three-dimensional cross shape acceptor materials with promising photovoltaic properties for high-efficiency organic solar cells. <i>International Journal of Quantum Chemistry</i> , 2020 , 120, e26377	2.1	48
152	In Silico Modeling of New "Y-Series"-Based Near-Infrared Sensitive Non-Fullerene Acceptors for Efficient Organic Solar Cells. <i>ACS Omega</i> , 2020 , 5, 24125-24137	3.9	48
151	First theoretical framework of Z-shaped acceptor materials with fused-chrysene core for high performance organic solar cells. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021 , 245, 118938	4.4	44
150	A combined experimental and computational study of 3-bromo-5-(2,5-difluorophenyl) pyridine and 3,5-bis(naphthalen-1-yl)pyridine: Insight into the synthesis, spectroscopic, single crystal XRD, electronic, nonlinear optical and biological properties. <i>Journal of Molecular Structure</i> , 2018 , 1160, 129-141	3.4	43
149	Synthesis and XRD, FT-IR vibrational, UV-Vis, and nonlinear optical exploration of novel tetra substituted imidazole derivatives: A synergistic experimental-computational analysis. <i>Journal of Physics and Chemistry of Solids</i> , 2018 , 115, 265-276	3.9	43
148	Efficient designing of triphenylamine-based hole transport materials with outstanding photovoltaic characteristics for organic solar cells. <i>Journal of Materials Science</i> , 2021 , 56, 5113-5131	4.3	40
147	Synthesis, crystal structure analysis, spectral characterization and nonlinear optical exploration of potent thiosemicarbazones based compounds: A DFT refine experimental study. <i>Inorganica Chimica Acta</i> , 2019 , 486, 162-171	2.7	38
146	Synthesis, single crystal analysis and DFT based computational studies of 2,4-diamino-5-(4-chlorophenyl)-6-ethylpyrimidin-1-ium 3,4,5-trihydroxybenzoate -methanol (DETM). <i>Journal of Molecular Structure</i> , 2019 , 1180, 119-126	3.4	36
145	Molecular designing of high-performance 3D star-shaped electron acceptors containing a truxene core for nonfullerene organic solar cells. <i>Journal of Physical Organic Chemistry</i> , 2021 , 34,	2.1	35
144	Structural parameters, electronic, linear and nonlinear optical exploration of thiopyrimidine derivatives: A comparison between DFT/TDDFT and experimental study. <i>Journal of Molecular Structure</i> , 2020 , 1201, 127183	3.4	34
143	Synthesis, spectroscopic, SC-XRD characterizations and DFT based studies of ethyl-2-(substituted-(2-benzylidenehydrazinyl))thiazole-4-carboxylate derivatives. <i>Journal of Molecular Structure</i> , 2019 , 1187, 164-171	3.4	33
142	Efficient Synthesis, SC-XRD, and Theoretical Studies of -Benzenesulfonylated Pyrimidines: Role of Noncovalent Interaction Influence in Their Supramolecular Network. <i>ACS Omega</i> , 2020 , 5, 15115-15128	3.9	33
141	Facile preparation, characterization, SC-XRD and DFT/DTDFT study of diversely functionalized unsymmetrical bis-aryl- β -unsaturated ketone derivatives. <i>Journal of Molecular Structure</i> , 2020 , 1206, 127755	3.4	33
140	Benchmark study of the linear and nonlinear optical polarizabilities in proto-type NLO molecule of para-nitroaniline. <i>Journal of Theoretical and Computational Chemistry</i> , 2019 , 18, 1950030	1.8	32
139	DFT and single crystal analysis of the pyrimethamine-based novel co-crystal salt: 2,4-diamino-5-(4-chloro-phenyl)-6-ethylpyrimidin-1-ium:4-hydroxybenzoate:methanol:hydrate (1:1:1:1) (DEHMH). <i>Journal of Molecular Structure</i> , 2020 , 1199, 127041	3.4	32
138	RuO ₂ nanorods decorated CNTs grown carbon cloth as a free standing electrode for supercapacitor and lithium ion batteries. <i>Electrochimica Acta</i> , 2019 , 326, 135009	6.7	31
137	Synthesis, X-ray crystallographic, spectroscopic and computational studies of aminothiazole derivatives. <i>Journal of Molecular Structure</i> , 2017 , 1131, 136-148	3.4	31
136	Theoretical and Conceptual Framework to Design Efficient Dye-Sensitized Solar Cells (DSSCs): Molecular Engineering by DFT Method. <i>Journal of Cluster Science</i> , 2021 , 32, 243-253	3	30

- 135 Designing of benzodithiophene acridine based Donor materials with favorable photovoltaic parameters for efficient organic solar cell. *Computational and Theoretical Chemistry*, **2021**, 1200, 113238² 29
- 134 Structural parameter-modulated nonlinear optical amplitude of acceptor-Donor-configured pyrene derivatives: a DFT approach. *RSC Advances*, **2021**, 11, 14237-14250 3.7 28
- 133 Experimental and computational investigations of new indole derivatives: A combined spectroscopic, SC-XRD, DFT/TD-DFT and QTAIM analysis. *Journal of Molecular Structure*, **2020**, 1207, 127803 27
- 132 Synthesis and structural analysis of novel indole derivatives by XRD, spectroscopic and DFT studies. *Journal of Molecular Structure*, **2020**, 1203, 127438 3.4 27
- 131 Synthesis, XRD, spectral (IR, UV-Vis, NMR) characterization and quantum chemical exploration of benzoimidazole-based hydrazones: A synergistic experimental-computational analysis. *Applied Organometallic Chemistry*, **2019**, 33, e5182 3.1 25
- 130 Novel W-Shaped Oxygen Heterocycle-Fused Fluorene-Based Non-Fullerene Acceptors: First Theoretical Framework for Designing Environment-Friendly Organic Solar Cells. *Energy & Fuels*, **2021**, 35, 12436-12450 4.1 24
- 129 Electron Donor and Acceptor Influence on the Nonlinear Optical Response of Diacetylene-Functionalized Organic Materials (DFOMs): Density Functional Theory Calculations. *Molecules*, **2019**, 24, 4.8 22
- 128 Synthesis, crystal structure, spectral and DFT studies of potent isatin derived metal complexes. *Journal of Molecular Structure*, **2018**, 1166, 110-120 3.4 22
- 127 Facile synthesis, crystal growth, characterization and computational study of new pyridine-based halogenated hydrazones: Unveiling the stabilization behavior in terms of noncovalent interactions. *Applied Organometallic Chemistry*, **2020**, 34, e5399 3.1 21
- 126 Designing Star-Shaped Subphthalocyanine-Based Acceptor Materials with Promising Photovoltaic Parameters for Non-fullerene Solar Cells. *ACS Omega*, **2020**, 5, 23039-23052 3.9 21
- 125 Synthesis of Diaminopyrimidine Sulfonate Derivatives and Exploration of Their Structural and Quantum Chemical Insights via SC-XRD and the DFT Approach. *ACS Omega*, **2021**, 6, 7047-7057 3.9 21
- 124 Molecular structure of 1,4-bis(substituted-carbonyl)benzene: A combined experimental and theoretical approach. *Journal of Molecular Structure*, **2020**, 1205, 127633 3.4 19
- 123 Synthesis, characterization, and biological screening of metal complexes of novel sulfonamide derivatives: Experimental and theoretical analysis of sulfonamide crystal. *Applied Organometallic Chemistry*, **2020**, 34, e5623 3.1 18
- 122 Designing benzothiadiazole based non-fullerene acceptors with high open circuit voltage and higher LUMO level to increase the efficiency of organic solar cells. *Optik*, **2021**, 228, 166138 2.5 18
- 121 Structural, optical and photovoltaic properties of unfused Non-Fullerene acceptors for efficient solution processable organic solar cell (Estimated PCE greater than 2.4%): A DFT approach. *Journal of Molecular Liquids*, **2021**, 341, 117428 6 18
- 120 Efficient Synthesis by Mono-Carboxy Methylation of 4,4'-Biphenol, X-ray Diffraction, Spectroscopic Characterization and Computational Study of the Crystal Packing of Ethyl 2-((4'-hydroxy-[1,1'-biphenyl]-4-yl)oxy)acetate. *ChemistrySelect*, **2019**, 4, 9274-9284 1.8 17
- 119 Facile Ultrasound-Based Synthesis, SC-XRD, DFT Exploration of the Substituted Acyl-Hydrazones: An Experimental and Theoretical Slant towards Supramolecular Chemistry. *ChemistrySelect*, **2020**, 5, 14844-14856 1.8 17
- 118 Molecular salts of terephthalic acids with 2-aminopyridine and 2-aminothiazole derivatives as potential antioxidant agents; Base-Acid-Base type architectures. *Journal of Molecular Structure*, **2020**, 1200, 127126 3.4 17

117	DFT and single-crystal investigation of the pyrimethamine-based novel co-crystal salt: 2,4-diamino-5-(4-chlorophenyl)-6-ethylpyrimidin-1-ium-4-methylbenzoate hydrate (1:1:1) (DEMH). <i>Journal of Molecular Structure</i> , 2021 , 1228, 129445	3.4	17
116	Synthesis, spectroscopic, single crystal diffraction and potential nonlinear optical properties of novel pyrazoline derivatives: Interplay of experimental and computational analyses. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018 , 202, 146-158	4.4	16
115	Solvent viscosity influence on the chemiexcitation efficiency of inter and intramolecular chemiluminescence systems. <i>Photochemical and Photobiological Sciences</i> , 2015 , 14, 1296-305	4.2	15
114	Surface assembly of Fe ₃ O ₄ nanodiscs embedded in reduced graphene oxide as a high-performance negative electrode for supercapacitors. <i>Ceramics International</i> , 2020 , 46, 19499-19505	5.1	15
113	Synthesis, crystal structure, spectroscopic, electronic and nonlinear optical properties of potent thiazole based derivatives: Joint experimental and computational insight. <i>Journal of Molecular Structure</i> , 2020 , 1202, 127354	3.4	15
112	Exploring the impact of central core modifications among several push-pull configurations to enhance nonlinear optical response. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 100, 107665	2.8	15
111	Probing 2-acetylbenzofuran hydrazones and their metal complexes as α -glucosidase inhibitors. <i>Bioorganic Chemistry</i> , 2020 , 102, 104082	5.1	15
110	Persistent prevalence of supramolecular architectures of novel ultrasonically synthesized hydrazones due to hydrogen bonding [XH \cdots O; X=N]: Experimental and density functional theory analyses. <i>Journal of Physics and Chemistry of Solids</i> , 2021 , 148, 109679	3.9	15
109	O-4-Acetylamino-benzenesulfonylated pyrimidine derivatives: synthesis, SC-XRD, DFT analysis and electronic behaviour investigation. <i>Journal of Molecular Structure</i> , 2021 , 1224, 129308	3.4	15
108	NLO potential exploration for D π A heterocyclic organic compounds by incorporation of various linkers and acceptor units. <i>Arabian Journal of Chemistry</i> , 2021 , 14, 103295	5.9	15
107	Exploration of Noncovalent Interactions, Chemical Reactivity, and Nonlinear Optical Properties of Piperidone Derivatives: A Concise Theoretical Approach. <i>ACS Omega</i> , 2020 , 5, 13236-13249	3.9	14
106	Synthesis, spectral characterization and computed optical analysis of potent triazole based compounds. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018 , 190, 197-207	4.4	14
105	Stabilization of Supramolecular Assembly of N-Substituted Benzylidene Acetohydrazone Analogs by Non-Covalent Interactions: A Concise Experimental and Theoretical Approach. <i>ChemistrySelect</i> , 2020 , 5, 10618-10631	1.8	14
104	Exploring the optoelectronic and third-order nonlinear optical susceptibility of cross-shaped molecules: insights from molecule to material level. <i>Journal of Molecular Modeling</i> , 2021 , 27, 12	2	14
103	Tuning the optoelectronic properties of scaffolds by using variable central core unit and their photovoltaic applications. <i>Chemical Physics Letters</i> , 2021 , 782, 139018	2.5	14
102	An efficient synthesis, structural (SC-XRD) and spectroscopic (FTIR, ¹ HNMR, MS spectroscopic) characterization of novel benzofuran-based hydrazones: An experimental and theoretical studies. <i>Journal of Molecular Structure</i> , 2020 , 1216, 128318	3.4	13
101	A facile microwave assisted synthesis and structure elucidation of (3R)-3-alkyl-4,1-benzoxazepine-2,5-diones by crystallographic, spectroscopic and DFT studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 230, 117995	4.4	13
100	Exploration of CH \cdots F & CF \cdots H mediated supramolecular arrangements into fluorinated terphenyls and theoretical prediction of their third-order nonlinear optical response.. <i>RSC Advances</i> , 2021 , 11, 7766-7778	3.7	13

99	Facile Synthesis, Spectral (IR, Mass, UV-Vis, NMR), Linear and Nonlinear Investigation of the Novel Phosphonate Compounds: A Combined Experimental and Simulation Study. <i>ChemistrySelect</i> , 2020 , 5, 2994-3006	1.8	12
98	Efficient synthesis, characterization, and in vitro bactericidal studies of unsymmetrically substituted triazole-derived Schiff base ligand and its transition metal complexes. <i>Monatshefte Für Chemie</i> , 2020 , 151, 549-557	1.4	12
97	Peroxyoxalate chemiluminescence efficiency in polar medium is moderately enhanced by solvent viscosity. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016 , 321, 143-150	4.7	12
96	Tuning of a A-A-D-A-A-Type Small Molecule with Benzodithiophene as a Central Core with Efficient Photovoltaic Properties for Organic Solar Cells. <i>ACS Omega</i> , 2021 , 6, 28923-28935	3.9	12
95	Efficiency of intermolecular chemiluminescence systems lacks significant solvent cavity effect in binary toluene/diphenylmethane mixtures. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2015 , 312, 81-87	4.7	11
94	Green Synthesis, SC-XRD, Non-Covalent Interactive Potential and Electronic Communication via DFT Exploration of Pyridine-Based Hydrazone. <i>Crystals</i> , 2020 , 10, 778	2.3	11
93	Non-covalent interactions abetted supramolecular arrangements of N-Substituted benzylidene acetohydrazide to direct its solid-state network. <i>Journal of Molecular Structure</i> , 2021 , 1230, 129827	3.4	11
92	Efficient tuning of small acceptor chromophores with A1- π A2- π A1 configuration for high efficacy of organic solar cells via end group manipulation. <i>Journal of Saudi Chemical Society</i> , 2021 , 25, 101305	4.3	11
91	Synthesis, biological activity and docking calculations of bis-naphthoquinone derivatives from Lawsone. <i>Bioorganic Chemistry</i> , 2021 , 114, 105069	5.1	11
90	A facile and concise route to (hydroxybenzoyl)pyrido[2,3-]pyrimidine heterocycle derivatives: synthesis, and structural, spectral and computational exploration.. <i>RSC Advances</i> , 2019 , 9, 34567-34580	3.7	10
89	Structural modulation of π -conjugated linkers in D- π A dyes based on triphenylamine dicyanovinylene framework to explore the NLO properties. <i>Royal Society Open Science</i> , 2021 , 8, 210570	3.3	10
88	A combined experimental and computational study of 2,2M(diazene-1,2-diylbis(4,1-phenylene))bis(6-(butylamino)-1H-benzo[de]isoquinoline-1,3(2H)-dione): Synthesis, optical and nonlinear optical properties. <i>Optik</i> , 2019 , 192, 162952	2.5	9
87	Rational design of naphthalimide based small molecules non-fullerene acceptors for organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020 , 1187, 112916	2	9
86	Exploration of efficient electron acceptors for organic solar cells: rational design of indacenodithiophene based non-fullerene compounds. <i>Scientific Reports</i> , 2021 , 11, 19931	4.9	9
85	Tuning the optoelectronic properties of ZOPTAN core-based derivatives by varying acceptors to increase efficiency of organic solar cell. <i>Journal of Molecular Modeling</i> , 2021 , 27, 316	2	9
84	Exploration of Chromone-Based Thiosemicarbazone Derivatives: SC-XRD/DFT, Spectral (IR, UV-Vis) Characterization, and Quantum Chemical Analysis. <i>ACS Omega</i> , 2020 , 5, 30176-30188	3.9	9
83	Synthetic, spectroscopic, SC-XRD and nonlinear optical analysis of potent hydrazide derivatives: A comparative experimental and DFT/TD-DFT exploration. <i>Journal of Molecular Structure</i> , 2020 , 1200, 127140	3.4	9
82	Cyclization of chalcones into N-propionyl pyrazolines for their single crystal X-ray, computational and antibacterial studies. <i>Journal of Molecular Structure</i> , 2020 , 1201, 127186	3.4	9

81	Spectroscopic and DFT/TDDFT insights of the novel phosphonate imine compounds. <i>Journal of Molecular Structure</i> , 2020 , 1207, 127838	3.4	8
80	A potent synthesis and supramolecular synthon hierarchy percipience of (E)-N [?] -(Naphthalen-1-yl-methylene)-benzenesulfonylhydrazide and 1-Napthaldehyde: A combined experimental and DFT studies. <i>Journal of Molecular Structure</i> , 2020 , 1221, 128797	3.4	8
79	N-Trifluoroacetylated pyrazolines: Synthesis, characterization and antimicrobial studies. <i>Bioorganic Chemistry</i> , 2020 , 99, 103842	5.1	8
78	Chemexcitation Efficiency of Intermolecular Electron-transfer Catalyzed Peroxide Decomposition Shows Low Sensitivity to Solvent-cavity Effects. <i>Photochemistry and Photobiology</i> , 2016 , 92, 537-45	3.6	8
77	Impact of linker modifications on the photovoltaic performance of rainbow-shaped acceptor molecules for high performance organic solar cell applications. <i>Physica B: Condensed Matter</i> , 2022 , 625, 413465	2.8	8
76	An Efficient Synthesis, Spectroscopic Characterization, and Optical Nonlinearity Response of Novel Salicylaldehyde Thiosemicarbazone Derivatives. <i>ACS Omega</i> , 2021 , 6, 16058-16065	3.9	8
75	Determination of Paraquat Dichloride from Water Samples Using Differential Pulse Cathodic Stripping Voltammetry. <i>Russian Journal of Electrochemistry</i> , 2018 , 54, 1155-1163	1.2	8
74	Facile synthesis, DNA binding, Urease inhibition, anti-oxidant, molecular docking and DFT studies of 3-(3-Bromo-phenyl)-1-(2-trifluoromethyl-phenyl)-propenone and 3-(3-Bromo-5-chloro-phenyl)-1-(2-trifluoromethyl-phenyl)-propenone. <i>Journal of Molecular Liquids</i> , 2021 , 336, 116302	6	8
73	Phenolic and flavonoid contents in Malva sylvestris and exploration of active drugs as antioxidant and anti-COVID19 by quantum chemical and molecular docking studies. <i>Journal of Saudi Chemical Society</i> , 2021 , 25, 101277	4.3	8
72	Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. <i>ACS Omega</i> , 2021 , 6, 24602-24613	3.9	8
71	Synthesis and solid state self-assembly of a 1,4-diazepine derivative: Water cluster as molecular glue and conformational isomerism. <i>Journal of Molecular Structure</i> , 2020 , 1207, 127811	3.4	7
70	Structural, SC-XRD and spectroscopic investigation of schiff base derivatives: A joint experimental and DFT investigation. <i>Journal of Molecular Structure</i> , 2018 , 1167, 57-68	3.4	7
69	Synthesis, crystal structure, Hirshfeld surface analysis and theoretical investigation of polynuclear coordination polymers of cobalt and manganese complexes with nitrobenzene and pyrazine. <i>Journal of Molecular Structure</i> , 2021 , 1250, 131851	3.4	7
68	An Experimental and Computational Exploration on the Electronic, Spectroscopic, and Reactivity Properties of Novel Halo-Functionalized Hydrazones. <i>ACS Omega</i> , 2020 , 5, 18907-18918	3.9	7
67	Green synthesis of Ag@CdO nanocomposite and their application towards brilliant green dye degradation from wastewater. <i>Journal of Nanostructure in Chemistry</i> , 1	7.6	7
66	Exploration of structural, electronic and third order nonlinear optical properties of crystalline chalcone systems: Monoarylidene and unsymmetrical diarylidene cycloalkanones. <i>Journal of Molecular Structure</i> , 2021 , 1241, 130685	3.4	7
65	Copper oxide integrated perylene diimide self-assembled graphitic pencil for robust non-enzymatic dopamine detection.. <i>RSC Advances</i> , 2021 , 11, 25084-25095	3.7	7
64	Biological evaluation of potent antioxidant, lipoxxygenase inhibitor and antibacterial: A comparative study. <i>Journal of Saudi Chemical Society</i> , 2016 , 20, 45-48	4.3	6

63	Synthesis, crystal structure, DFT calculations, molecular docking study and Hirshfeld surface analysis of alkoxido-bridged dinuclear iron(III) complex. <i>Research on Chemical Intermediates</i> , 2020 , 46, 4155-4171	2.8	6
62	Pakistanamide C, a new sphingolipid from <i>Abutilon pakistanicum</i> . <i>Revista Brasileira De Farmacognosia</i> , 2014 , 24, 277-281	2	6
61	Novel Star-Shaped Benzotriindole-Based Nonfullerene Donor Materials: Toward the Development of Promising Photovoltaic Compounds for High-Performance Organic Solar Cells. <i>Energy Technology</i> , 2100751	3.5	6
60	Exploration of promising optical and electronic properties of (non-polymer) small donor molecules for organic solar cells. <i>Scientific Reports</i> , 2021 , 11, 21540	4.9	6
59	Molecular engineering of indenoindene-3-ethylrodanine acceptors with A2-A1-D-A1-A2 architecture for promising fullerene-free organic solar cells. <i>Scientific Reports</i> , 2021 , 11, 20320	4.9	6
58	2-Amino-3-methylpyridinium, 2-amino-4-methylbenzothiazolium and 2-amino-5-chloropyridinium salts. Experimental and theoretical findings. <i>Journal of Molecular Structure</i> , 2020 , 1222, 128914	3.4	6
57	Smart Parking Systems: Reviewing the Literature, Architecture and Ways Forward. <i>Smart Cities</i> , 2021 , 4, 623-642	3.3	6
56	Energy storage performance of binder-free ruthenium-oxide nano-needles based free-standing electrode in neutral pH electrolytes. <i>Electrochimica Acta</i> , 2021 , 378, 138139	6.7	6
55	Key Electronic, Linear and Nonlinear Optical Properties of Designed Disubstituted Quinoline with Carbazole Compounds. <i>Molecules</i> , 2021 , 26,	4.8	6
54	Effect of ZnO Nanoparticles Coating Layers on Top of ZnO Nanowires for Morphological, Optical, and Photovoltaic Properties of Dye-Sensitized Solar Cells. <i>Micromachines</i> , 2019 , 10,	3.3	6
53	Exploration of second and third order nonlinear optical properties for theoretical framework of organic DDA type compounds. <i>Optical and Quantum Electronics</i> , 2021 , 53, 1	2.4	6
52	Theoretical investigation of nonlinear optical behavior for rod and T-Shaped phenothiazine based D-BA organic compounds and their derivatives. <i>Journal of Saudi Chemical Society</i> , 2021 , 25, 101339	4.3	6
51	Synthesis, single-crystal exploration, and theoretical insights of arylsulfonylated 2-amino-6-methylpyrimidin derivatives. <i>Journal of Molecular Structure</i> , 2021 , 1243, 130789	3.4	6
50	Synthesis, characterization and DFT calculated properties of electron-rich hydrazinylthiazoles: Experimental and computational synergy. <i>Journal of Molecular Structure</i> , 2021 , 1245, 131043	3.4	6
49	Exploration of the Intriguing Photovoltaic Behavior for Fused Indacenodithiophene-Based A-D-A Conjugated Systems: A DFT Model Study.. <i>ACS Omega</i> , 2022 , 7, 11606-11617	3.9	6
48	Synthesis of Crystalline Fluoro-Functionalized Imines, Single Crystal Investigation, Hirshfeld Surface Analysis, and Theoretical Exploration.. <i>ACS Omega</i> , 2022 , 7, 9867-9878	3.9	6
47	Influence of acceptor tethering on the performance of nonlinear optical properties for pyrene-based materials with A-ED-ED architecture. <i>Arabian Journal of Chemistry</i> , 2022 , 15, 103673	5.9	5
46	Cationic dye adsorption and separation at discrete molecular level: first example of an iron cluster with rapid and selective adsorption of methylene blue from aqueous system. <i>New Journal of Chemistry</i> , 2021 , 45, 1415-1422	3.6	5

45	Electro-optical and charge transport properties of chalcone derivatives using a dual approach from molecule to material level simulations. <i>Computational and Theoretical Chemistry</i> , 2021 , 1203, 113349	2	5
44	β-Hydroxy Carbonyl compounds via aldol reaction: Single crystal investigation and quantum chemical exploration for the unveiling of supramolecular behavior. <i>Journal of Molecular Structure</i> , 2021 , 1241, 130650	3.4	5
43	First example of vinylbenzene based small photovoltaic molecules: Towards the development of efficient D-πA configured optoelectronic materials for bulk heterojunction solar cells. <i>Physica B: Condensed Matter</i> , 2022 , 633, 413769	2.8	5
42	Structural, optoelectronic and thermoelectric properties of FeSb ₂ under pressure: Bulk and monolayer. <i>Physica B: Condensed Matter</i> , 2019 , 570, 100-109	2.8	4
41	Synthesis, characterization and antibacterial investigation of divalent metal complexes of NO-donor ligand: {5-chloro-2-[(4-chlorobenzylidene)-amino]phenyl}(phenyl)methanone. <i>Journal of Saudi Chemical Society</i> , 2015 , 19, 322-326	4.3	4
40	The potential role of dietary plant ingredients against mammary cancer: a comprehensive review. <i>Critical Reviews in Food Science and Nutrition</i> , 2020 , 1-26	11.5	4
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