

Muhammad Khalid

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/3305168/muhammad-khalid-publications-by-year.pdf>

Version: 2024-04-28

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

170
papers

2,935
citations

32
h-index

44
g-index

180
ext. papers

4,353
ext. citations

3.4
avg, IF

6.06
L-index

#	Paper	IF	Citations
170	Donor moieties with D- π A framing modulated electronic and nonlinear optical properties for non-fullerene-based chromophores.. <i>RSC Advances</i> , 2022 , 12, 4209-4223	3.7	3
169	Influence of acceptor tethering on the performance of nonlinear optical properties for pyrene-based materials with A- π - π D architecture. <i>Arabian Journal of Chemistry</i> , 2022 , 15, 103673	5.9	5
168	Iron (III) complex exhibiting efficient catechol oxidase activity: Experimental, kinetic and theoretical approach. <i>Journal of Molecular Structure</i> , 2022 , 1252, 131685	3.4	2
167	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
166	A facile synthesis and structural elucidation for furfural based chromophores: Prediction of linear and nonlinear optical properties. <i>Journal of Molecular Structure</i> , 2022 , 1249, 131543	3.4	1
165	Nickel -doped iron oxide nanoparticle-conjugated porphyrin interface (porphyrin/FeO@Ni) for the non-enzymatic detection of dopamine from lacrimal fluid.. <i>Dalton Transactions</i> , 2022 ,	4.3	3
164	Quantum chemical designing of novel fullerene-free acceptor molecules for organic solar cell applications.. <i>Journal of Molecular Modeling</i> , 2022 , 28, 67	2	4
163	Influence of Peripheral Modification of Electron Acceptors in Nonfullerene (O-IDTBR1)-Based Derivatives on Nonlinear Optical Response: DFT/TDDFT Study.. <i>ACS Omega</i> , 2022 , 7, 11631-11642	3.9	0
162	Ab Initio Study of Two-Dimensional Cross-Shaped Non-Fullerene Acceptors for Efficient Organic Solar Cells.. <i>ACS Omega</i> , 2022 , 7, 10638-10648	3.9	0
161	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
160	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
159	First example of vinylbenzene based small photovoltaic molecules: Towards the development of efficient D- π A configured optoelectronic materials for bulk heterojunction solar cells. <i>Physica B: Condensed Matter</i> , 2022 , 633, 413769	2.8	5
158	A combined experimental and theoretical study of alkyl 2-(3-benzoyl-4-hydroxy-1,1-dioxido-2H-benzo[e][1,2]thiazin-2-yl)acetates: Synthesis, X-ray crystallography and DFT. <i>Journal of Molecular Structure</i> , 2022 , 1258, 132671	3.4	0
157	Efficient designing of half-moon-shaped chalcogen heterocycles as non-fullerene acceptors for organic solar cells.. <i>Journal of Molecular Modeling</i> , 2022 , 28, 125	2	2
156	Functionalized thiazolidone-decorated lanthanum-doped copper oxide: novel heterocyclic sea sponge morphology for the efficient detection of dopamine. <i>RSC Advances</i> , 2022 , 12, 14439-14449	3.7	1
155	Enriching NLO efficacy designing non-fullerene molecules with the modification of acceptor moieties into ICIF2F: an emerging theoretical approach.. <i>RSC Advances</i> , 2022 , 12, 13412-13427	3.7	4
154	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

153	The theoretical investigation of the opto-electronic properties of designed molecules having 2-(2-Methylene-3-oxo-indane-1-ylidene)malononitrile as end-capped acceptors. <i>Zeitschrift Fur Physikalische Chemie</i> , 2021 , 235, 785-804	3.1	
152	Exploration of Photophysical and Nonlinear Properties of Salicylaldehyde-Based Functionalized Materials: A Facile Synthetic and DFT Approach.. <i>ACS Omega</i> , 2021 , 6, 33914-33922	3.9	3
151	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
150	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
149	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
148	2-Nitro- and 4-fluorocinnamaldehyde based receptors as naked-eye chemosensors to potential molecular keypad lock. <i>Scientific Reports</i> , 2021 , 11, 20847	4.9	1
147	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
146	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
145	Synthesis of Diaminopyrimidine Sulfonate Derivatives and Exploration of Their Structural and Quantum Chemical Insights via SC-XRD and the DFT Approach. <i>ACS Omega</i> , 2021 , 6, 7047-7057	3.9	21
144	A comprehensive study of structural, non-covalent interactions and electronic insights into N-aryl substituted thiosemicarbazones via SC-XRD and first-principles DFT approach. <i>Journal of Molecular Structure</i> , 2021 , 1230, 129852	3.4	3
143	In-vitro and in-silico antioxidant, α -glucosidase inhibitory potentials of abutilins C and D, new flavonoid glycosides from <i>Abutilon pakistanicum</i> . <i>Arabian Journal of Chemistry</i> , 2021 , 14, 103021	5.9	2
142	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
141	Synthesis, antioxidant, antimicrobial and antiviral docking studies of ethyl 2-(2-(arylidene)hydrazinyl)thiazole-4-carboxylates. <i>Zeitschrift Fur Naturforschung - Section C Journal of Biosciences</i> , 2021 , 76, 467-480	1.7	4
140	Smart Parking Systems: Reviewing the Literature, Architecture and Ways Forward. <i>Smart Cities</i> , 2021 , 4, 623-642	3.3	6
139	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
138	Key Electronic, Linear and Nonlinear Optical Properties of Designed Disubstituted Quinoline with Carbazole Compounds. <i>Molecules</i> , 2021 , 26,	4.8	6
137	Designing of benzodithiophene acridine based Donor materials with favorable photovoltaic parameters for efficient organic solar cell. <i>Computational and Theoretical Chemistry</i> , 2021 , 1200, 113238 ²		29
136	High-throughput calculations and experimental insights towards the development of potent thiazoline based functional materials. <i>Materials Today Communications</i> , 2021 , 27, 102485	2.5	0

135	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
134	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
133	Persistent prevalence of supramolecular architectures of novel ultrasonically synthesized hydrazones due to hydrogen bonding [XH ⁺ O; X=N]: Experimental and density functional theory analyses. <i>Journal of Physics and Chemistry of Solids</i> , 2021 , 148, 109679	3.9	15
132	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
131	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
130	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
129	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
128	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
127	Designing benzothiadiazole based non-fullerene acceptors with high open circuit voltage and higher LUMO level to increase the efficiency of organic solar cells. <i>Optik</i> , 2021 , 228, 166138	2.5	18
126	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
125	Nifedipine degradation by an electro-oxidation process using titanium-based RuO ₂ /TiO ₂ /TiO ₂ mixed metal oxide electrode. <i>Chemical Papers</i> , 2021 , 75, 681-690	1.9	3
124	Exploration of CH ₂ F & CF ₂ 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
123	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
122	Structural parameter-modulated nonlinear optical amplitude of acceptor-donor-configured pyrene derivatives: a DFT approach. <i>RSC Advances</i> , 2021 , 11, 14237-14250	3.7	28
121	Novel W-Shaped Oxygen Heterocycle-Fused Fluorene-Based Non-Fullerene Acceptors: First Theoretical Framework for Designing Environment-Friendly Organic Solar Cells. <i>Energy & Fuels</i> , 2021 , 35, 12436-12450	4.1	24
120	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
119	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
118	Phenolic and flavonoid contents in <i>Malva sylvestris</i> 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

117	Palladium-catalyzed synthesis of 5-(arylated) pyrimidines, their characterization, electronic communication, and non-linear optical evaluations. <i>Journal of Molecular Structure</i> , 2021 , 1237, 130408	3-4	4
116	Tris-isopropyl-sily-ethynyl anthracene based small molecules for organic solar cells with efficient photovoltaic parameters. <i>Computational and Theoretical Chemistry</i> , 2021 , 1202, 113305	2	3
115	Exploration of Nonlinear Optical Properties of Triphenylamine-Dicyanovinylene Coexisting Donor-Acceptor Architecture by the Modification of Conjugated Linker. <i>Frontiers in Materials</i> , 2021 , 8,	4	3
114	NLO potential exploration for heterocyclic organic compounds by incorporation of various linkers and acceptor units. <i>Arabian Journal of Chemistry</i> , 2021 , 14, 103295	5-9	15
113	Efficient tuning of small acceptor chromophores with A1-A2-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
112	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
111	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
110	Facile Synthesis of Diversely Functionalized Peptoids, Spectroscopic Characterization, and DFT-Based Nonlinear Optical Exploration. <i>ACS Omega</i> , 2021 , 6, 26016-26025	3-9	1
109	Chemically Modified Quinoidal Oligothiophenes for Enhanced Linear and Third-Order Nonlinear Optical Properties. <i>ACS Omega</i> , 2021 , 6, 24602-24613	3-9	8
108	Synthesis, biological activity and docking calculations of bis-naphthoquinone derivatives from Lawsone. <i>Bioorganic Chemistry</i> , 2021 , 114, 105069	5-1	11
107	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
106	Theoretical investigation of nonlinear optical behavior for rod and T-Shaped phenothiazine based D-A organic compounds and their derivatives. <i>Journal of Saudi Chemical Society</i> , 2021 , 25, 101339	4-3	6
105	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
104	2-amino-6-methylpyridine based salt converted to carbon electrode material for supercapacitive application. <i>Journal of Molecular Structure</i> , 2021 , 1244, 130895	3-4	
103	Experimental and computational study of naphthalimide derivatives: Synthesis, optical, nonlinear optical and antiviral properties. <i>Optik</i> , 2021 , 246, 167748	2-5	3
102	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
101	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
100	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. <i>Journal of Molecular Liquids</i> , 2021 , 341, 117428	6	18

99	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
98	Alkyl 2-(2-(arylidene)alkylhydrazinyl)thiazole-4-carboxylates: Synthesis, acetyl cholinesterase inhibition and docking studies. <i>Journal of Molecular Structure</i> , 2021 , 1245, 131063	3.4	1
97	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
96	Facile Ultrasound-Based Synthesis, SC-XRD, DFT Exploration of the Substituted Acyl-Hydrazones: An Experimental and Theoretical Slant towards Supramolecular Chemistry. <i>ChemistrySelect</i> , 2020 , 5, 14844-14856	1.8	17
95	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
94	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
93	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
92	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
91	Chemical Composition and Bioactivities of Essential Oil from Leaves of <i>Syzygium cumini</i> (L.) Skeels Native to Punjab, Pakistan. <i>Chemistry and Biodiversity</i> , 2020 , 17, e1900733	2.5	2
90	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
89	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
88	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
87	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
86	First principles study of electronic and nonlinear optical properties of A-D-EA and D-A-D-EA configured compounds containing novel quinoline-carbazole derivatives.. <i>RSC Advances</i> , 2020 , 10, 22273-22283	3.7	48
85	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
84	Synthesis, characterization, and biological screening of metal complexes of novel sulfonamide derivatives: Experimental and theoretical analysis of sulfonamide crystal. <i>Applied Organometallic Chemistry</i> , 2020 , 34, e5623	3.1	18
83	Crystal and Quantum Chemical Exploration of the Potent Monocarbonyl Curcuminoids to Unveil Their Structural and Intriguing Electronic Properties. <i>ChemistrySelect</i> , 2020 , 5, 3735-3745	1.8	4
82	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

81	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
80	Spectroscopic and DFT/TDDFT insights of the novel phosphonate imine compounds. <i>Journal of Molecular Structure</i> , 2020 , 1207, 127838	3-4	8
79	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
78	Facile preparation, characterization, SC-XRD and DFT/DTDFT study of diversely functionalized unsymmetrical bis-aryl- π -unsaturated ketone derivatives. <i>Journal of Molecular Structure</i> , 2020 , 1206, 127755	3-4	33
77	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
76	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
75	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
74	N-Trifluoroacetylated pyrazolines: Synthesis, characterization and antimicrobial studies. <i>Bioorganic Chemistry</i> , 2020 , 99, 103842	5-1	8
73	Highly efficient one pot palladium-catalyzed synthesis of 3,5-bis (arylated) pyridines: Comparative experimental and DFT studies. <i>Journal of Molecular Structure</i> , 2020 , 1213, 128131	3-4	0
72	Experimental and computational investigations of new indole derivatives: A combined spectroscopic, SC-XRD, DFT/TD-DFT and QTAIM analysis. <i>Journal of Molecular Structure</i> , 2020 , 1207, 127803	3-4	27
71	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
70	Molecular structure of 1,4-bis(substituted-carbonyl)benzene: A combined experimental and theoretical approach. <i>Journal of Molecular Structure</i> , 2020 , 1205, 127633	3-4	19
69	An untargeted C isotopic evaluation approach for the discrimination of fermented food matrices at natural abundance: Application to vinegar. <i>Talanta</i> , 2020 , 210, 120679	6.2	3
68	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
67	Facile synthesis, crystal growth, characterization and computational study of new pyridine-based halogenated hydrazones: Unveiling the stabilization behavior in terms of noncovalent interactions. <i>Applied Organometallic Chemistry</i> , 2020 , 34, e5399	3-1	21
66	Synthesis and structural analysis of novel indole derivatives by XRD, spectroscopic and DFT studies. <i>Journal of Molecular Structure</i> , 2020 , 1203, 127438	3-4	27
65	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
64	Probing 2-acetylbenzofuran hydrazones and their metal complexes as β -glucosidase inhibitors. <i>Bioorganic Chemistry</i> , 2020 , 102, 104082	5-1	15

63	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
62	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
61	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
60	Molecular engineering of ADODA 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
59	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
58	Palladium-catalyzed synthesis of pyrimidine substituted diaryl ethers through Suzuki Miyaura coupling reactions: Experimental and DFT studies. <i>Optik</i> , 2020 , 219, 165285	2.5	4
57	Synthesis, Structure Study, First-Principles Investigations and Luminescence Properties of Europium and Terbium Complexes. <i>Journal of Fluorescence</i> , 2020 , 30, 1345-1355	2.4	1
56	A Spellbinding Interplay Between Biological Barcoding and Nanotechnology. <i>Frontiers in Bioengineering and Biotechnology</i> , 2020 , 8, 883	5.8	4
55	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
54	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
53	Designing Star-Shaped Subphthalocyanine-Based Acceptor Materials with Promising Photovoltaic Parameters for Non-fullerene Solar Cells. <i>ACS Omega</i> , 2020 , 5, 23039-23052	3.9	21
52	Stabilization of Supramolecular Assembly of N-Substituted Benzylidene Acetohydrazide Analogs by Non-Covalent Interactions: A Concise Experimental and Theoretical Approach. <i>ChemistrySelect</i> , 2020 , 5, 10618-10631	1.8	14
51	Molecular salts of terephthalic acids with 2-aminopyridine and 2-aminothiazole derivatives as potential antioxidant agents; Base-Acid-Base type architectures. <i>Journal of Molecular Structure</i> , 2020 , 1200, 127126	3.4	17
50	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
49	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
48	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
47	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
46	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. <i>ChemistrySelect</i> , 2019 , 4, 9274-9284	1.8	17

45	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
44	A combined experimental and computational study of 2,2Mdiazene-1,2-diybis(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
43	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
42	Electron Donor and Acceptor Influence on the Nonlinear Optical Response of Diacetylene-Functionalized Organic Materials (DFOMs): Density Functional Theory Calculations. <i>Molecules</i> , 2019 , 24,	4.8	22
41	Synthesis, spectroscopic, SC-XRD characterizations and DFT based studies of ethyl2-(substituted-(2-benzylidenehydrazinyl))thiazole-4-carboxylate derivatives. <i>Journal of Molecular Structure</i> , 2019 , 1187, 164-171	3.4	33
40	Effects of bismuth on structural and dielectric properties of cobalt-cadmium spinel ferrites fabricated via micro-emulsion route. <i>Chinese Physics B</i> , 2019 , 28, 088701	1.2	2
39	Designing triazatruxene-based donor materials with promising photovoltaic parameters for organic solar cells.. <i>RSC Advances</i> , 2019 , 9, 26402-26418	3.7	68
38	Synthesis, XRD, spectral (IR, UVVis, NMR) characterization and quantum chemical exploration of benzoimidazole-based hydrazones: A synergistic experimental-computational analysis. <i>Applied Organometallic Chemistry</i> , 2019 , 33, e5182	3.1	25
37	A dual approach to study the synthesis, crystal structure, thermal, optical and nonlinear optical properties of copper (II) malonate complex {(C ₇ H ₈ O ₂ N) ₂ [Cu(C ₃ H ₂ O ₄) ₂ (H ₂ O) ₂]}. <i>Inorganic Chemistry Communication</i> , 2019 , 107, 107450	3.1	1
36	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
35	Phytochemicals: Key to Effective Anticancer Drugs. <i>Mini-Reviews in Organic Chemistry</i> , 2019 , 16, 141-158	1.7	4
34	EGlucosidase Inhibition and Docking Studies of 5-Deoxyflavonols and Dihydroflavonols Isolated from <i>Abutilon pakistanicum</i> . <i>Current Organic Chemistry</i> , 2019 , 23, 1857-1866	1.7	0
33	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
32	A computational approach to study the optoelectronic properties of F-BODIPY derivatives at the bulk level for photovoltaic applications. <i>Materials Research Express</i> , 2019 , 6, 125110	1.7	0
31	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
30	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
29	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
28	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

27	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
26	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
25	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
24	Synthesis, crystal structure, spectral and DFT studies of potent isatin derived metal complexes. <i>Journal of Molecular Structure</i> , 2018 , 1166, 110-120	3-4	22
23	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
22	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
21	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
20	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
19	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
18	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
17	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
16	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
15	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
14	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
13	Facile synthesis, single crystal analysis, and computational studies of sulfanilamide derivatives. <i>Journal of Molecular Structure</i> , 2017 , 1127, 766-776	3-4	58
12	Synthesis, X-ray crystallographic, spectroscopic and computational studies of aminothiazole derivatives. <i>Journal of Molecular Structure</i> , 2017 , 1131, 136-148	3-4	31
11	Biological evaluation of potent antioxidant, lipoxigenase inhibitor and antibacterial: A comparative study. <i>Journal of Saudi Chemical Society</i> , 2016 , 20, 45-48	4-3	6
10	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

9	Chemiexcitation 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
8	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
7	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
6	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
5	Pakistamide C, a new sphingolipid from <i>Abutilon pakistanicum</i> . <i>Revista Brasileira De Farmacognosia</i> , 2014 , 24, 277-281	2	6
4	Efficiency of electron transfer initiated chemiluminescence. <i>Photochemistry and Photobiology</i> , 2013 , 89, 1299-317	3.6	74
3	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
2	Thermodynamic and solubilization properties of a polynuclear copper complex in ionic surfactants media. <i>Journal of Dispersion Science and Technology</i> , 1-9	1.5	3
1	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