Citation Report
List of articles citing

Electrophilicity Index

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398	DFT rationalization of metal-catalyst-controlled coupling of carbazole with diazo-naphthalen-2(1H)-one. **2022**, 529, 112574	
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396	Introducing a new model based on electronegativity equalization principle for the analysis of the natural bond orbital reactivity in the c-DFT background.	
395	AIEgens-NLOphores coumarin-triphenylamine chalcone derivatives: Synthesis, photophysical properties and DFT computational study. **2022**, 134009	0
394	Density Functional Theoretical Computational Studies on 3-Methyl 2-Vinyl Pyridinium Phosphate. **2022**, 2022, 1-14	
393	Hardness of Molecules and Bandgap of Solids from a Generalized Gradient Approximation Exchange Energy Functional.	
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391	Synthesis, In´ Vitro and in Cell Study of a New Spirooxindoles-Based N-Alkylated Maleimides Targeting HER2/3 Signaling Pathway. 1-25	
390	Unexpected kinetically controlled organoselenium-based isomaleimide: X-ray structure, hirshfeld surface analysis, 3D energy framework approach, and density functional theory calculation. 10,	0
389	Why Ortho- and Para-Hydroxy Metabolites Can Scavenge Free Radicals That the Parent Atorvastatin Cannot? Important Pharmacologic Insight from Quantum Chemistry.	0
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385	Bromochlorodifluoromethane interaction with pristine and doped BN nanosheets: A DFT study. **2022**, 10, 108367	1
384	The effects of biologically important divalent and trivalent metal cations on the cyclization step of dopamine autoxidation reaction: A quantum chemical study. **2022**, 15, 104153	1

383	Experimental, DFT and MD simulation studies of Mordant Black 11 dye adsorption onto polyaniline in aqueous solution. **2022**, 364, 120045	1
382	Nonlinear optical and quantum chemical studies of Palladium benzimidazole Schiff base complex. **2022**, 151, 107012	1
381	Effect of porogen agent on bio-based membranes filtration performances: Experimental and theoritical study. **2022**, 1269, 133863	
380	Regioselective synthesis of spirooxindole-pyrolidine via (GAP) chemistry process: Experimental and DFT study. **2022**, 1270, 133891	
379	A convenient one-pot synthesis, theoretical studies, and NMR-based conformational analysis of nitroarylidene dimalonates. **2022**, 1269, 133848	0
378	Theoretical vibrational spectroscopy (FT-IR), PED and DFT calculations of chromones and thiochromones. **2022**, 1270, 133972	3
377	Dianionic or tetraanionic ligand: Synthesis, Hirshfeld surface analysis, DFT, electrochemical and magnetic properties of mono- and dinuclear Cu(II) complexes derived from a deprotonated Schiff base. **2022**, 1269, 133857	
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375	TD-DFT and optical properties of 9,9-dioctyl-9Hfluorene-based oligomer in a thin film and design of DFB laser using ellipsometry studies.	0
374	Density Functional Theory Study of the Regioselectivity in Copolymerization of bis-Styrenic Molecules with Propylene Using Zirconocene Catalyst. **2022**, 12, 1039	1
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372	Theoretical insight and molecular recognition of oxatub[4]arene-based organic macrocycle as a supramolecular host for antipsychotic drug risperidone. **2022**, 366, 120195	0
371	An experimental and theoretical investigation of cationic azine dye adsorption on natural sepiolite in single and multi-component systems. **2022**, 187, 507-515	1
370	Design, synthesis and evaluate of imidazole, triazine and metastable oxazolone derivatives as chemosensor for detecting metals. **2022**, 26, 101537	0
369	Structure, electronic and optical properties of chalcopyrite-type semiconducting materials XGaY2 (X′ =′ Cu, Ag, Au; Y′ =′ S, Se, Te) for solar cell applications: A DFT study. **2022**, 646, 414305	0
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364	Nitrobenzamido substitution on thiophene-3-carboxylate: Electrochemical investigation, antioxidant activity, molecular docking, DFT calculations. **2023**, 1271, 134030	0
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362	Design, synthesis, and in vitro anticancer activity of thiophene substituted pyridine derivatives. **2023**, 127-143	0
361	Investigation (IR, UV-visible, fluorescence, X-ray diffraction and thermogravimetric) studies of Mn(II), Fe(III) and Cr(III) complexes of thiosemicarbazone derived from 4- pyridyl thiosemicarbazide and monosodium 5-sulfonatosalicylaldehyde and evaluation of their biological applications. **2023**, 1271, 134139	0
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355	Experimental, NBO, NLO and docking analysis of a novel ligand derived from vanillin and N(4)-methyl-N(4)-phenylthiosemicarbazide and its transition metal complexes. **2022**, 4, 100453	0
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353	Unveiling the [3+2] cycloaddition between difluoromethyl diazomethane and 3-ylideneoxindole from the perspective of molecular electron density theory.	2
352	Mixed-ligand complexes of copper(ii) with thienoyltrifluoroacetonate and nitrogen containing ligands: synthesis, structures, antimicrobial activity, cytotoxicity, Hirshfeld surface analysis and DFT studies. **2022**, 12, 23513-23526	0
351	Electronic properties of amino acids and nucleobases: similarity classes and pairing principles from chemical reactivity indices. **2022**, 24, 22477-22486	2
350	Impact of Doping on the Optoelectronic, Electronic and Nonlinear Optical Properties and on the Reactivity of Photochromic Polymers Containing Styrylquinoline Fragments.	0
349	DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science.	9
348	Spectroscopic and quantum chemical investigations to explore the effect of intermolecular interactions in a diuretic drug: Hydrochlorothiazide. **2023**, 285, 121931	0

347	Supramolecular association of (1,4-phenylenedimethanaminium) bis(perchlorate) monohydrate: A combined experimental and theoretical study. **2023**, 1272, 134212	0
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342	Crystal structure determination, Hirshfeld surface, crystal void, intermolecular interaction energy analyses, as well as DFT and energy framework calculations of 2-(4-oxo-4,5-dihydro-1H-pyrazolo[3,4-d]pyrimidin-1-yl)acetic acid. **2022**, 78, 953-960	0
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340	Theoretical Study on the Diels–Alder Reaction of Fullerenes: Analysis of Isomerism, Aromaticity, and Solvation. **2022**, 3, 364-379	0
339	Kinetic and Computational Study of Degradation of Two Azo Dyes, Metanil Yellow and Orange II, by Iron Oxide Nanoparticles Synthesized Using Hylocereus undatus. **2022**, 7, 31667-31681	1
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333	An Experimental and Theoretical Study on Essential Oil of Aethionema sancakense: Characterization, Molecular Properties and RDG Analysis. **2022**, 27, 6129	5
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331	Experimental and Theoretical Assessments on Anticorrosion Performance of 2-(1H-benzimidazol-2-yl)-3-(4-hydroxyphenyl) Acrylonitrile for Copper in 1M HNO3. 17-45	0
330	Self-assembly of new cobalt complexes based on [Co (SCN)4], synthesis, empirical, antioxidant activity, and quantum theory investigations. **2022**, 12,	1

329	New insight into the substituent effects on the hydrolytic deamination of saturated and unsaturated cytosine.	0
328	Modelling of Aminothiophene-Carbonitrile Derivatives as Potential Drug Candidates for Hepatitis B and C.	6
327	Radical scavenging capacity, antibacterial activity, and quantum chemical aspects of the spectrophotometrically investigated iridium (III) complex with benzopyran derivative. 13,	0
326	Corrosion Inhibition Properties of Phenyl Phthalimide Derivatives against Carbon Steel in the Acidic Medium: DFT, MP2, and Monte Carlo Simulation Studies. **2022**, 7, 33054-33066	2
325	Electrophilicity of Hoveyda-Grubbs Olefin Metathesis Catalysts as the Driving Force that Controls Initiation Rates.	0
324	Computational study of the effects of static electric field on the interaction of 5-Fluorouracil anti-cancer drug with pristine and Sc- and Ti-doped B12P12 nanocage as drug delivery.	1
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321	Catalytic performance of pyridinium dihydrogen phosphate ionic liquid for butyl acetate production: theoretical insights and reaction kinetic studies.	0
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318	Solvent Effects in the Regioselective N-Functionalization of Tautomerizable Heterocycles Catalyzed by Methyl Trifluoromethanesulfonate: A Density Functional Theory Study with Implicit Solvent Model. **2022**, 10, 172	0
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315	Coupling of pseudoradical centers in the synthesis of oxazine fused-spiroindoline: a two-stage one-step double cyclization. **2022**, 134,	0
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309	Solvent effect, quantification and correlation analysis of the nucleophilicities of cyclic secondary amines.	0
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307	On the Periodicity of the Information Theory and Conceptual DFT-Based Reactivity Descriptors. **2022**, 126, 6801-6813	0
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301	Investigating the third-order NLO properties of 4-[(Z)-(6-nitro-1,3-benzothiazol-2-yl)diazinyl]naphthalen-1-ol for nonlinear applications using the Z-scan technique and quantum chemical computations.. **2022**, 134288	0
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299	Unravelling the Effect of Donor-□Acceptor Architecture in Designing 1,3-Indanedione Based Sensitizers for DSSC Applications. **2022**, 114328	0
298	Fluorination of 2,5-diphenyl-1,3,4-oxadiazole enhances the electron transport properties for OLED devices: a DFT analysis. 1-13	0
297	Electrochemistry, DFT Calculations, and Antioxidant Capability of Cobalt Cefazolin Complex. 1083-1090	0
296	Bonding nature, nucleophilic reactivity and Electron excitation of NLO active 2,6 Dichloroindophenol Sodium Salt (Polar and Non Polar Solvents) with Topology analysis- Bacterial pathogens study. **2022**, 120533	0
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294	DFT study of regio- and stereo-selective 13DC reaction between diazopropane and substituted chalcone derivatives: Molecular docking of novel pyrazole derivatives as Anti-Alzheimer□ Agents.	0

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284	A theoretical study on aza-Michael additions. **2022**, 141,	1
283	Silylium ion migration dominated hydroamidation of siloxy-alkynes. **2022**, 5,	0
282	[3 + 2] Cycloadditions in Asymmetric Synthesis of Spirooxindole Hybrids Linked to Triazole and Ferrocene Units: X-ray Crystal Structure and MEDT Study of the Reaction Mechanism. **2022**, 14, 2071	0
281	A safe alternative synthesis of primary carbamates from alcohols; in vitro and in silico assessments as an alternative acetylcholinesterase inhibitors. 1-10	0
280	The First Examples of [3+2] Cycloadditions with the Participation of (E)-3,3,3-tribromo-1-nitroprop-1-ene. **2022**, 15, 7584	1
279	Superstrong Chemical Bonding of Noble Gases with Oxidoboron (BO+) and Sulfidoboron (BS+). **2022**, 126, 7888-7900	0
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277	Computational Insights on Periodicity in Bonding and Lewis Acidity and Basicity of the p-Block Trispyrazolylborate Complexes.	0
276	A Molecular Electron Density Theory Study of the [3+2] Cycloaddition Reaction of an Azomethine Ylide with an Electrophilic Ethylene Linked to Triazole and Ferrocene Units. **2022**, 27, 6532	1

275	Synthesis of eugenol derivative by the ring opening of epoxide eugenol and its analysis through chemical reactivity: a DFT approach. 1-9	0
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273	Bromine Substitution Effect on Structure, Reactivity, and Linear and Third-Order Nonlinear Optical Properties of 2,3-Dimethoxybenzaldehyde. **2022**, 126, 7852-7863	0
272	Computational investigations on acceptor substituent influence of metal-free efficient chromophores for optoelectronic properties. **2022**, 28,	1
271	5,5,5-Trichloropent-3-en-one as a Precursor of 1,3-Bi-centered Electrophile in Reactions with Arenes in Brønsted Superacid CF3SO3H. Synthesis of 3-Methyl-1-trichloromethylindenes. **2022**, 27, 6675	0
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269	CHEMISORPTION OF C2H2 ON C20 BOWL: A COMPUTATIONAL INVESTIGATION. **2022**, 63, 1600-1609	0
268	Molecular structure and biological activities of 4-thiazolidinone derivatives: a combined theoretical and experimental study. 1-10	0
267	New Theoretical Insights about Anticorrosive Effects and Adsorption Mechanism of Some α-Amino Acids on Al Surface: DFT, MEP, FMO, NBO, QSAR, Fukui Functions and Monte Carlo Simulation.	0
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264	In silico designing of Si- and Ge-doped imidazolium: a new heterocyclic aromatic superacid. **2022**, 141,	0
263	Synthesis, characterization and computational studies for (2? S *,3 R *,3? S *,8a? R *)-2?,3?-bis(ethoxycarbonyl)-2-oxo-2?,3?-dihydro-8a?H-spiro[indoline-3,1?-indolizine]-6?-carboxylic acid and some derivatives.	1
262	Hydrogen storage in SiC, GeC, and SnC nanocones functionalized with nickel, Density Functional Theory□Study.	0
261	Electronic Spectra (Experimental and Simulated), and DFT Investigation of NLO, FMO, NBO, and MESP Characteristics of Some Biphenylcarboxaldehydes. 1-14	0
260	Theoretical Studies, Spectroscopic Investigation, Molecular Docking, Molecular Dynamics and MMGBSA Calculations with 2-Hydrazinoquinoline. **2022**, 134482	0
259	Glutathione as green corrosion inhibitor for 6061Al-SiC(p) composite in HCl medium: electrochemical and theoretical investigation.	1
258	Theoretical and photophysical investigation of biologically active fluorophore: 2-amino-6-chlorofluoren-9-one. **2022**, 99, 100767	0

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255	Modeling of pristine, Ir- and Au-decorated C60 fullerenes as sensors for detection of hydroxyurea and nitrosourea drugs. **2022**, 10, 108802	4
254	Structural insights into conformational stability and binding of thiazolo-[2,3-b] quinazolinone derivatives with EGFR-TKD and in-vitro study. **2022**, 29, 103478	0
253	Synthesis of new halogenated compounds based on 8-hydroxyquinoline derivatives for the inhibition of acid corrosion: Theoretical and experimental investigations. **2022**, 33, 104654	1
252	Experimental and theoretical studies of hexylmeythylimidazolium tetrafluoroborate ionic liquid as cathodic corrosion inhibitor for mild steel. **2022**, 146, 110110	0
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250	Diaminoalkanes functionalized graphene oxide as corrosion inhibitors against carbon steel corrosion in simulated oil/gas well acidizing environment. **2023**, 630, 591-610	1
249	Synthesis and spectral studies of Ni(II) complexes involving functionalized dithiocarbamates and triphenylphosphine: X-ray crystal structure, thermal stability, Hirshfeld surface analysis, DFT and biological evaluation. **2023**, 545, 121271	0
248	A density functional theory study of H3+ and Li3+ clusters: Similar structures with different bonding, aromaticity, and reactivity properties. **2023**, 237-245	0
247	Conceptual density functional theory and all metal aromaticity. **2023**, 87-98	0
246	Combined experimental, computational studies (synthesis, crystal structural, DFT calculations, spectral analysis) and biological evaluation of the new homonuclear complex Di-´ μ-benzoato-bis [benzoatodipyridine-cobalt (II)]. **2023**, 1273, 134331	0
245	Investigation of embelin synthetic hybrids as potential COVID-19 and COX inhibitors: Synthesis, spectral analysis, DFT calculations and molecular docking studies. **2023**, 1273, 134356	2
244	Hydrogen trapping potential of a few novel molecular clusters and ions. **2023**, 297-312	0
243	Ultra High Reversible Hydrogen Storage Capacity of Li4B2 Cluster: A Quantum Chemical Study.	0
242	Effects of edge hydrogenation and applied electric field on the structure and electrical properties of zigzag silicene nanoribbons by SCC-DFTB calculations. **2023**, 649, 414445	0
241	Theoretical study of the adsorption mechanism of ioversol contrast agent on the single-walled carbon nanotube surface. **2023**, 1274, 134504	0
240	Spectroscopic, reactivity analysis and docking studies of 3-(adamantan-1-yl)-4-(4-fluorophenyl)-1-[(4-phenylpiperazin-1-yl)methyl]-4,5-dihdyro-1H-1,2,4-triazole-5-thione: DFT and MD simulations. **2023**, 1274, 134418	0

239	Quantum Chemical Benchmark Study on Valdecoxib, a Potent and Selective Inhibitor of COX-2, and its Hydroxylated Derivative. **2022**, 43, 221-231	0
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237	A Molecular Electron Density Theory Study of the Polar Diels-Alder Reaction of Naphtoquinone:Cr(CO)3 Complex with Cyclic Dienes. 1-17	0
236	Conversion of lignin oil and hemicellulose derivative into high-density jet fuel. **2022**,	1
235	Chemical reactivity, molecular electrostatic potential and in-silico analysis on benzimidazole fungicide benomyl. **2022**, 8, e11417	0
234	Unveiling the zwitterionic and stepwise mechanism for the domino reactions of amidine with 1,2,4,5- and 1,2,3,5-tetrazines.	0
233	Quantitative Structure□Toxicity Relationship in Bioactive Molecules from a Conceptual DFT Perspective. **2022**, 15, 1383	0
232	On the possibility of using the Ti@Si16 superatom as a novel drug delivery carrier for different drugs: A DFT study. **2022**, 108378	0
231	Choline amino acid ionic liquids as green corrosion inhibitors of mild steel in acidic medium. **2022**, 130541	2
230	An account of noncovalent interactions in homoleptic palladium(II) and platinum(II) complexes within the DFT framework: A correlation between geometries, energy components of symmetry-adapted perturbation theory and NCI descriptors. **2022**, 8, e11408	0
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228	Radical scavenging capacity, UV activity, and molecular docking studies of 2?, 5?, 3, 4-Tetrahydroxychalcone: An insight into the photoprotection. **2022**, 100126	0
227	Structural, electronic, spectroscopic and molecular docking analysis of novel hetero oxetane ring compound. **2022**, 1217, 113919	1
226	Quantum Chemical Investigation on Hydrolysis of Orally Active Organometallic Ruthenium(II) and Osmium(II) Anticancer Drugs and Their Interaction with Histidine.	0
225	Impact of doping on the optoelectronic, electronic and nonlinear optical properties and on the reactivity of photochromic polymers containing styrylquinoline fragments: Hartree-Fock and DFT study. **2022**, 8, e11491	1
224	Effects of chelate ligands containing NN, PN, and PP on the performance of half-sandwich ruthenium metal complexes as sensitizers in dye sensitized solar cells (DSSCs): quantum chemical investigation. **2022**, 116190	0
223	Sustainable corrosion inhibitor for steel embedded in concrete by Guar Gum: Electrochemical and theoretical analyses. **2022**, 12, 100328	0
222	Theoretical Study of Cyano-Promoted Intramolecular Aza-Diels□Alder Reaction.	0

221	In-silico and in-detail experimental interaction studies of new antitumor Zn(II) complex with CT-DNA and serum albumin. 1-18	0
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125	Molecular engineering on D-□A organic dyes with flavone-based different acceptors for highly efficient dye-sensitized solar cells using experimental and computational study. **2023**, 29,	1
124	Spectroscopic, crystal structure and DFT-assisted studies of some nickel(II) chelates of a heterocyclic-based NNO donor aroylhydrazone: in vitro DNA binding and docking studies.	0
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93	Molecular modeling and solubility of olopatadine hydrochloride polymorphs. **2023**, 1224, 114110	0
92	Corrosion inhibition of Schiff base and their metal complexes with [Mn (II), Co (II) and Zn (II)]: Experimental and quantum chemical studies. **2023**, 378, 121637	0
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90	Reduction potential of benzophenones, hydroxyphenones and bis(2-hydroxyphenone)copper molecules. **2023**, 443, 141931	0
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85	Synthesis, X-Ray Structure Analysis, Computational Investigations, and In´ Vitro Biological Evaluation of New Thiazole-Based Heterocycles as Possible Antimicrobial Agents. 1-14	0
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73	Theoretical Study on the Origin of Abnormal Regioselectivity in Ring-Opening Reaction of Hexafluoropropylene Oxide. **2023**, 28, 1669	0
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69	1,3,4-Oxadiazole derivatives as potential antifungal agents: Synthesis, characterization, Ct-DNA binding, molecular docking, and TD-DFT studies.	0
68	New Xanthene Diones Compounds as a Corrosion Inhibitor of Mild Steel in Acid Medium: Electrochemical, Surface Characterization and Theoretical Insights.	0
67	Role of electron-withdrawing groups on nonlinear optical response of conjugated anthracenyl fused rings chalcone: Experimental and DFT study. **2023**, 655, 414744	0
66	A comprehensive DFT study on organosilicon-derived fungicide flusilazole and its germanium analogue: A computational approach to Si/Ge bioisosterism. **2023**, 100, 100939	0
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63	Photocatalytic degradation and pollutant-oriented structure-activity analysis of carbamazepine, ibuprofen and acetaminophen over faceted TiO2. **2023**, 11, 109553	0
62	Nucleophilicity Parameters for Nitroalkyl Anions in Methanol and Structure-Reactivity Analysis. **2023**, 8,	0
61	Generating Fischer-Type Rh-Carbenes with Rh-Carbynoids. **2023**, 145, 4975-4981	0
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59	Synthesis of a Novel Hydrazone of Thieno[2,3-d]pyrimidine Clubbed with Ninhydrin: X-ray Crystal Structure and Computational Investigations. **2023**, 13, 384	0
58	Comparative Study of Molecular Docking, Structural, Electronic, and Fukui Function Studies on Favipiravir and its Newly Designed Derivatives (Potential Inhibitors) for COVID-19 Protease. **2023**, 407,	0
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54	Inhibition of corrosion of an aluminum alloy by Rosemary and Eucalyptus extracted oils in 1M hydrochloric acid medium: Experimental and theoretical study.	0
53	Theoretical descriptions of novel silicon analogs of cyclo[18]carbon.	0
52	Mono-/multiadsorption of chlorobenzene compounds on biochar: influence of the properties of the chlorobenzene molecules and biochar. **2023**, 23, 2120-2135	0
51	New Diacetic Acids Containing Quinazolin-4(3 H)-one: Synthesis, Characterization, Anticholinergic Properties, DFT Analysis and Molecular Docking Studies. **2023**, 8,	0
50	Anthrone-Based Carbocyclic Azo Dyes: Synthesis, Dyeing, UV Protection, Anti-microbial Activity and Computational Study. **2023**, 24, 1285-1296	0
49	A dispersion-corrected DFT calculations on encapsulation of Favipiravir drug used as antiviral against COVID-19 into carbon-, boron-, and aluminum-nitride nanotubes for optimal drug delivery systems combined with molecular docking simulations.	0
48	Kinetic and computational study of the oxidative degradation of an amebicide by acid bromate in perchlorate solutions and the effect of Ruthenium (III) catalyst in micro molar concentration: a mechanistic approach.	0
47	Crystal structure, Hirshfeld surface analysis and DFT study of (5E,5?E,6Z,6?Z)-6,6?-[ethane-1,2-diylbis(azanylylidene)]bis{5-[2-(4-fluorophenyl)hydrazono]-3,3-dimethylcyclohexanone} 2.5-hydrate. **2023**, 79, 297-301	
46	Facile Synthesis, Crystal Structure, Hirshfeld Surface Analysis, DFT Calculation and in´ vitro Antifungal Evaluation of 4-Arylidene-1H-pyrazol-5(4H)-ones. 1-15	0
45	Determination of the molecular structure and spectroscopic properties of capsaicin. **2023**, 208, 110879	0
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40	Aromatic Clusters and Hydrogen Storage. **2023**, 16, 2833	0
39	A DFT study of structural-stability, Mulliken charges, MEP, FMO, and NLO properties of trans alkenyl substituted chalcones conformers: theoretical study.	0
38	Amazon raw clay as a precursor of a clay-based adsorbent: experimental study and DFT analysis for the adsorption of Basic Yellow 2 dye.	0
37	Insights into the crystal structure and computational studies of newly synthesized thiazolopyrimidine derivatives against adenosine receptor (Thermostabilised HUMAN A2a). **2023**, 1284, 135372	0
36	Molecular Assembly of Rhodanine with Torus-Shaped Cyclodextrins and Their Innovative Applications by Physicochemical Contrivance Simultaneously Optimized by Computational Study. **2023**, 8,	0
35	Synthetic, Structural and Supramolecular Features of a New Dithiocyanato-κN, κS-Copper(II) Complex: Insights Through Computational Studies.	0
34	Insights into the Three-Component Coupling Reactions of Aldehydes, Alkynes, and Amines Catalyzed by N-heterocyclic Carbene Silver: A DFT Study. **2023**, 13, 646	0
33	New azo-azomethine derivatives: Synthesis, characterization, computational, solvatochromic UV-Vis absorption and antibacterial studies. **2023**, 1284, 135451	0
32	Identification of Novel Tau-Tubulin Kinase 2 Inhibitors Using Computational Approaches. **2023**, 8, 13026-13037	0
31	Quantum computational investigation into structural, spectroscopic, topological and electronic properties of L-histidinium-L-tartrate hemihydrate: Nonlinear optical organic single crystal. **2023**, 9, e14879	0
30	Local reactivity descriptors of the important atoms in chelotropic reactions provide insight into their global variants along the reaction path.	0
29	Computational investigation of dimethoate and β-cyclodextrin inclusion complex: molecular structures, intermolecular interactions, and electronic analysis.	0
28	Efficient green synthesis of a potential novel nosylation reagent and its DFT study. 1-5	0
27	Identifying novel therapeutic inhibitors to target FMS-like tyrosine kinase-3 (FLT3) against acute myeloid leukemia: a molecular docking, molecular dynamics, and DFT study. 1-19	0
26	Free radical scavenging activity of gallic acid toward various reactive oxygen, nitrogen, and sulfur species: a DFT approach. 1-10	0
25	Synthesis, characterization, and quantum chemistry local chemical reactivity description of new phosphorylated derivatives of piperazine. 1-11	0
24	Novel asymmetrical azines appending 1,3,4-thiadiazole sulfonamide: synthesis, molecular structure analyses, in silico ADME, and cytotoxic effect. **2023**, 13, 10353-10366	0

23	Computational evaluation on molecular stability and binding affinity of methyldopa against Lysine-specific demethylase 4D Enzyme through quantum chemical computations and molecular docking analysis. **2023**, 135518	0
22	Computational study and quantum chemical investigation on bambuterol hydrochloride compound drug: ADFT approach.	0
21	Design new organic material based on triphenylamine (TPA) with D-A-D structure used as an electron donor for organic solar cells: A DFT approach. **2023**, 108470	0
20	Design, Synthesis, and Density Functional Theory Studies of Indole Hydrazones as Colorimetric Naked Eye Sensors for F Ions. **2023**, 8, 14131-14143	0
19	Two new Schiff bases of (E)-2,4-di-tert-butyl-6-((4-fluorophenylimino)methyl)phenol (I) and (E)-2,4-di-tert-butyl-6-((3-iodo-4-methylphenylimino)methyl)phenol (II): structural, spectroscopic and quantum chemical calculations. 1-18	0
18	Study of N -methyl-5-nitroindazolylacrylonitriles as a Function of Quantum Parameters Employing Density Function Theory Methods: Comparative Theoretical Study and Nonlinear Optical Properties. **2023**, 8,	0
17	Theoretical investigation of some transition metal sulfides nanomaterials: CDFT approach. **2023**, 142,	0
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15	Synthesis, Crystal structure, Hirshfeld surface interactions, anti-corrosion analysis, DFT calculations, Docking studies and evaluation of the antioxidant activity of a new zwitterion Schiff base. **2023**, 1286, 135569	0
14	Benzethonium chloride as a tungsten corrosion inhibitor in neutral and alkaline media for the post-chemical mechanical planarization application. **2023**,	0
13	Electronic effects of the substituted dopants on stability and reactivity of difuranosilapyridine-4-ylidenes: DFT approach.	0
12	Newly designed triazatruxene-based dye-sensitized solar cells containing different benzothiazine linkers: Geometric, optoelectronic, charge transfer properties, and cyanoacrylic acid versus benzoic acid. **2023**, 1224, 114127	0
11	Optoelectronic properties fine-tuning through chalcogenide-based bridge for dye molecules featuring hydantoin anchoring group: first-principle calculations.	0
10	Crystal Structure, Hirshfeld Surface Analysis, and Computational Study of Quinolin-8-yl 4-Chlorobenzoate: Insights from Spectroscopic, Thermal, and Antitumor Properties. **2023**, 13, 694	0
9	Spectroscopic (FT-IR, FT-Raman, UV-vis and NMR) Investigation, Molecular Structure, Docking and Chemical Reactivity Elucidation of Antifungal Drug Tioconazole. 1-25	0
8	Investigation of the solvent effect, regioselectivity, and the mechanism of the cycloaddition reaction between 2-chlorobenzimidazole and benzonitrile oxide.	0
7	Molecular Structure, Hydrogen Bonding Interactions and Docking Simulations of Nicotinamide (Monomeric and Trimeric Models) by Using Spectroscopy and Theoretical Approach. 1-19	0
6	Density functional theory-based molecular modeling. **2023**, 95-113	0

5	A molecular electron density theory study of mechanism and selectivity of the intramolecular [3+2] cycloaddition reaction of a nitrone–vinylphosphonate adduct.	0
4	[3′ +′ 2] Cycloaddition reaction of disubstituted-3-benzylidene succinimide with C, N-disubstituted nitrile imines for synthesizing spiro-heterocycles: A computational study. **2023**, 1225, 114138	0
3	Adsorption mechanism of AsH3 pollutant on metal-functionalized coronene C24H12-X (X′ =′ Mg, Al, K) quantum dots. **2023**, 6, 100224	0
2	Direct sunlight photodegradation of congo red in aqueous solution by TiO2/rGO binary system: Experimental and DFT study. **2023**, 16, 104992	0
1	Synthesis, physico-chemical characterization and theoretical exploration of some 2,4,5-triaryl imidazole derivatives.	0