

# Accurate and Efficient Model Energies for Exploring Intermolecular Crystals

Journal of Physical Chemistry Letters

5, 4249-4255

DOI: [10.1021/jz502271c](https://doi.org/10.1021/jz502271c)

Citation Report

#	ARTICLE	IF	CITATIONS
1	Predicting Energetics of Supramolecular Systems Using the XDM Dispersion Model. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4033-4040.	2.3	39
2	How Reliable Are Intermolecular Interaction Energies Estimated from Topological Analysis of Experimental Electron Densities?. <i>Crystal Growth and Design</i> , 2015, 15, 5624-5628.	1.4	105
3	Organic alloys of room temperature liquids thiophenol and selenophenol. <i>Chemical Communications</i> , 2015, 51, 14255-14258.	2.2	46
4	S $\pi$ O chalcogen bonding in sulfa drugs: insights from multipole charge density and X-ray wavefunction of acetazolamide. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25411-25420.	1.3	74
5	Supramolecular Recognition and Energy Frameworks in Host-Guest Complexes of 18-Crown-6 and Sulfonamides. <i>Crystal Growth and Design</i> , 2015, 15, 5892-5900.	1.4	34
6	Energy frameworks: insights into interaction anisotropy and the mechanical properties of molecular crystals. <i>Chemical Communications</i> , 2015, 51, 3735-3738.	2.2	515
7	Molecular Electrostatic Potentials from Invariom Point Charges. <i>ChemPhysChem</i> , 2016, 17, 2238-2246.	1.0	5
8	Structural Collapse of the Hydroquinone-Formic Acid Clathrate: A Pressure-Medium-Dependent Phase Transition. <i>Chemistry - A European Journal</i> , 2016, 22, 4061-4069.	1.7	18
9	Isostructural polymorphs: qualitative insights from energy frameworks. <i>CrystEngComm</i> , 2016, 18, 8497-8505.	1.3	35
10	Effects of the crystal structure and thermodynamic stability on solubility of bioactive compounds: DFT study of isoniazid cocrystals. <i>Computational and Theoretical Chemistry</i> , 2016, 1092, 1-11.	1.1	19
11	Geometries, interaction energies and complexation free energies of 18-crown-6 with neutral molecules. <i>CrystEngComm</i> , 2016, 18, 8653-8663.	1.3	1
12	Quantifying Host-Guest Interaction Energies in Clathrates of Dianin's Compound. <i>Crystal Growth and Design</i> , 2016, 16, 6858-6866.	1.4	12
13	Energy frameworks and a topological analysis of the supramolecular features in in situ cryocrystallized liquids: tuning the weak interaction landscape via fluorination. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 31811-31820.	1.3	48
14	q-GRID: A New Method To Calculate Lattice and Interaction Energies for Molecular Crystals from Electron Densities. <i>Crystal Growth and Design</i> , 2016, 16, 662-671.	1.4	6
15	Quasi-isostructural polymorphism in molecular crystals: inputs from interaction hierarchy and energy frameworks. <i>Chemical Communications</i> , 2016, 52, 2141-2144.	2.2	44
16	The S66x8 benchmark for noncovalent interactions revisited: explicitly correlated ab initio methods and density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20905-20925.	1.3	182
17	Silver(i), gold(i) and palladium(ii) complexes of a NHC-pincer ligand with an aminotriazine core: a comparison with pyridyl analogues. <i>Dalton Transactions</i> , 2016, 45, 1484-1495.	1.6	15
18	Approaching an experimental electron density model of the biologically active trans-epoxysuccinyl amide group-Substituent effects vs. crystal packing. <i>Journal of Physical Organic Chemistry</i> , 2017, 30, e3683.	0.9	4

#	ARTICLE	IF	CITATIONS
19	Supramolecular Chemistry of BrettPhos and BrettPhos Oxide: Breakup of Isostructurality via Orderâ€“Disorder Phase Transitions. <i>Crystal Growth and Design</i> , 2017, 17, 1982-1990.	1.4	7
20	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasiâ€“isotropic Crystal Packing. <i>Angewandte Chemie</i> , 2017, 129, 8588-8592.	1.6	29
21	The Elusive Structural Origin of Plastic Bending in Dimethyl Sulfone Crystals with Quasiâ€“isotropic Crystal Packing. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 8468-8472.	7.2	104
22	Intermolecular Interaction Energies in Hydroquinone Clathrates at High Pressure. <i>Crystal Growth and Design</i> , 2017, 17, 3834-3846.	1.4	21
23	Intermolecular interactions in molecular crystals: whatâ€™s in a name?. <i>Faraday Discussions</i> , 2017, 203, 93-112.	1.6	121
24	New Chargeâ€“Transfer Complexes with 1,2,5â€“Thiadiazoles as Both Electron Acceptors and Donors Featuring an Unprecedented Addition Reaction. <i>Chemistry - A European Journal</i> , 2017, 23, 852-864.	1.7	25
25	Relationships among Crystal Structures, Mechanical Properties, and Tableting Performance Probed Using Four Salts of Diphenhydramine. <i>Crystal Growth and Design</i> , 2017, 17, 6030-6040.	1.4	56
26	Way to Highly Emissive Materials: Increase of Rigidity by Introduction of a Furan Moiety in Co-Oligomers. <i>Journal of Physical Chemistry C</i> , 2017, 121, 23359-23369.	1.5	32
27	Benchmark Databases of Intermolecular Interaction Energies: Design, Construction, and Significance. <i>Annual Reports in Computational Chemistry</i> , 2017, 13, 3-91.	0.9	8
28	Molecular Level Understanding of the Reversible Phase Transformation between Forms III and II of Dapsone. <i>Crystal Growth and Design</i> , 2017, 17, 5054-5060.	1.4	19
29	Liquid Nicotine Tamed in Solid Forms by Cocrystallization. <i>Crystal Growth and Design</i> , 2017, 17, 4958-4964.	1.4	35
30	Quantitative investigation of Câ€“Hâ€“â€“ and other intermolecular interactions in a series of crystalline N-(substituted phenyl)-2-naphthamide derivatives. <i>CrystEngComm</i> , 2017, 19, 5473-5491.	1.3	13
31	New insights about the hydrogen bonds formed between acetylene and hydrogen fluoride: Î€â€“H, Câ€“H and Fâ€“H. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 173, 160-169.	2.0	10
32	Structural characterization, gelation ability, and energy-framework analysis of two bis(long-chain) Tj ETQq1 1 0.784314 rgBT /Overl... 2017, 73, 791-796.	0.2	5
33	Exploring the rare Sâ€“H...S hydrogen bond using charge density analysis in isomers of mercaptobenzoic acid. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 626-633.	0.5	13
34	<i>CrystalExplorer</i> model energies and energy frameworks: extension to metal coordination compounds, organic salts, solvates and open-shell systems. <i>IUCrJ</i> , 2017, 4, 575-587.	1.0	848
35	New Insights into Solid Form Stability and Hydrate Formation: o-Phenanthroline HCl and Neocuproine HCl. <i>Molecules</i> , 2017, 22, 2238.	1.7	8
36	Interplay of point multipole moments and charge penetration for intermolecular electrostatic interaction energies from the University at Buffalo pseudoatom databank model of electron density. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2017, 73, 598-609.	0.5	9

#	ARTICLE	IF	CITATIONS
37	Linear MgCp* <sub>2</sub> vs Bent CaCp* <sub>2</sub> : London Dispersion, Ligand-Induced Charge Localizations, and Pseudo-Pregostic C-H...Ca Interactions. <i>Inorganic Chemistry</i> , 2018, 57, 4906-4920.	1.9	17
38	Accurate Lattice Energies for Molecular Crystals from Experimental Crystal Structures. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1614-1623.	2.3	164
39	Identifying Slip Planes in Organic Polymorphs by Combined Energy Framework Calculations and Topology Analysis. <i>Crystal Growth and Design</i> , 2018, 18, 1909-1916.	1.4	63
40	Concomitance, Reversibility, and Switching Ability of Centrosymmetric and Non-Centrosymmetric Crystal Forms: Polymorphism in an Organic Nonlinear Optical Material. <i>Crystal Growth and Design</i> , 2018, 18, 1126-1135.	1.4	18
41	Crystal packing analysis of 1-(3,4-dimethoxyphenyl)-3-(4-bromophenyl)prop-2-en-1-one exhibiting a putative halogen bond C-Br...O. <i>Journal of Molecular Structure</i> , 2018, 1156, 216-223.	1.8	17
42	Tetraiodoallene, I <sub>2</sub> C=C=CI <sub>2</sub> – the missing link between I <sub>2</sub> C=CI <sub>2</sub> and I <sub>2</sub> C=C=C=CI <sub>2</sub> – and the oxidation product, 2,2-diiodoacrylic acid, I <sub>2</sub> C=CH(CO <sub>2</sub> H). <i>Australian Journal of Chemistry</i> , 2018, 71, 70.	0.5	5
43	An exploration of O-H...O and C-H...N interactions in a long-chain-ester-substituted phenylphenol: methyl 10-[4-(4-hydroxyphenyl)phenoxy]decanoate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 594-599.	0.2	2
44	Observation of 3D isostructurality in halogen substituted N-benzoyl-N-phenylbenzamides. <i>Journal of Molecular Structure</i> , 2018, 1164, 280-288.	1.8	1
45	Computational and analytical approaches for investigating hydrates: the neat and hydrated solid-state forms of 3-(3-methylimidazolium-1-yl)propanoate. <i>CrystEngComm</i> , 2018, 20, 7826-7837.	1.3	6
46	Shape-selective crystallisation of fluxional carbon cages. <i>Chemical Science</i> , 2018, 9, 8631-8636.	3.7	22
47	Synthesis of chiral nopinane annelated 3-methyl-1-aryl-1H-pyrazolo[3,4-b]pyridines by condensation of pinocarovone oxime with 1-aryl-1H-pyrazol-5-amines. <i>Mendeleev Communications</i> , 2018, 28, 584-586.	0.6	12
48	Hydrogen dynamics in solid formic acid: insights from simulations with quantum colored-noise thermostats. <i>Journal of Physics: Conference Series</i> , 2018, 1055, 012003.	0.3	8
49	Exploring the Solubility of the Carbamazepine-Saccharin Cocrystal: A Charge Density Study. <i>Crystal Growth and Design</i> , 2021, 21, 4259-4275.	1.4	8
50	Diversity in Mechanical Response in Donor-Acceptor Coupled Cocrystal Stoichiomorphs Based on Pyrene and 1,8-Dinitroanthraquinone Systems. <i>Crystal Growth and Design</i> , 2018, 18, 6670-6680.	1.4	28
51	Non-Steroidal Biphenyl Gelators: Correlation of Xerogel Structure with Solid-State Structure and Circular Dichroism Spectroscopy. <i>Gels</i> , 2018, 4, 34.	2.1	1
52	Conformational trimorphism of bis(2,6-dimesitylphenyl)ditelluride. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 707-721.	0.4	1
53	Quantifying intermolecular interactions for isoindole derivatives: substituent effect vs. crystal packing. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 675-687.	0.4	7
54	Rationalizing Distinct Mechanical Properties of Three Polymorphs of a Drug Adduct by Nanoindentation and Energy Frameworks Analysis: Role of Slip Layer Topology and Weak Interactions. <i>Crystal Growth and Design</i> , 2018, 18, 3927-3937.	1.4	59

#	ARTICLE	IF	CITATIONS
55	3D energy frameworks of a potential nutraceutical. <i>Journal of Molecular Structure</i> , 2018, 1173, 300-306.	1.8	19
56	Crystal structure, Hirshfeld surface analysis and energy framework calculation of the first oxoanion salt containing 1,3-cyclohexanebis(methylammonium): [3-(azaniumylmethyl)cyclohexyl]methanaminium dinitrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 949-954.	0.2	10
57	Supramolecular Organization of Nonstoichiometric Drug Hydrates: Dapsone. <i>Frontiers in Chemistry</i> , 2018, 6, 31.	1.8	23
58	Intermolecular interactions in crystals of small unsubstituted cyclic ethers and substituted epoxides. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2018, 233, 641-648.	0.4	2
59	The Polymorphs of ROY: A Computational Study of Lattice Energies and Conformational Energy Differences. <i>Australian Journal of Chemistry</i> , 2018, 71, 279.	0.5	36
60	Unsubstituted Oxalix[ <i>n</i> ]arenes ( <i>n</i> =4 and 8): A Conformational Study in Solution and Solid State and Interaction Studies with Aromatic Guests. <i>ChemistrySelect</i> , 2018, 3, 9091-9095.	0.7	2
61	Towards the use of experimental electron densities to estimate reliable lattice energies. <i>CrystEngComm</i> , 2018, 20, 5340-5347.	1.3	13
62	On the kinetics of solvate formation through mechanochemistry. <i>CrystEngComm</i> , 2019, 21, 2097-2104.	1.3	14
64	Understanding the Tabletability Differences between Indomethacin Polymorphs Using Powder Brillouin Light Scattering. <i>Pharmaceutical Research</i> , 2019, 36, 150.	1.7	8
65	Experimental and computational approaches to produce and characterise isostructural solvates. <i>CrystEngComm</i> , 2019, 21, 5533-5545.	1.3	18
66	Charge Transfer Versus Arene-Perfluoroarene Interactions in Modulation of Optical and Conductivity Properties in Cocrystals of 2,7-Di- <i>tert</i> -butylpyrene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 18198-18206.	1.5	29
67	Effect of high pressure on the typical 2D hydrogen-bonded crystal azodicarbonamide. <i>Journal of Physics and Chemistry of Solids</i> , 2019, 135, 109096.	1.9	1
68	Experimental and computational approaches to rationalise multicomponent supramolecular assemblies: dapsone monosolvates. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 17288-17305.	1.3	13
69	Crystal structures and supramolecular architectures of ONO donor hydrazone and solvent exchangeable dioxidomolybdenum(VI) complexes derived from 3,5-diiodosalicylaldehyde-4-methoxybenzoylhydrazone: Hirshfeld surface analysis and interaction energy calculations. <i>Polyhedron</i> , 2019, 170, 749-761.	1.0	16
70	Structure Property Correlation of a Series of Halogenated Schiff Base Crystals and Understanding of the Molecular Basis Through Nanoindentation. <i>Crystal Growth and Design</i> , 2019, 19, 6698-6707.	1.4	19
71	Impact of Crystal Structure and Molecular Conformation on the Hydration Kinetics of Fluconazole. <i>Crystal Growth and Design</i> , 2019, 19, 7193-7205.	1.4	17
72	Fast and Accurate Quantum Crystallography: From Small to Large, from Light to Heavy. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6973-6982.	2.1	48
73	Experimental Insights into the Electronic Nature, Spectral Features, and Role of Entropy in Short CH <sub>3</sub> - $\dot{A}$ -CH <sub>3</sub> Hydrophobic Interactions. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7224-7229.	2.1	7

#	ARTICLE	IF	CITATIONS
74	Enhancing the solubility of natural compound xanthotoxin by modulating stability via cocrystallization engineering. <i>International Journal of Pharmaceutics</i> , 2019, 572, 118776.	2.6	12
75	Synthesis and structural study of 2-(haloalkyl)-3-methylchromones. <i>Monatshefte für Chemie</i> , 2019, 150, 1929-1940.	0.9	5
76	Mesogens with Aggregation-Induced Emission Formed by Hydrogen Bonding. , 2019, 1, 589-593.		19
77	Surface Induced Phenytoin Polymorph. 1. Full Structure Solution by Combining Grazing Incidence X-ray Diffraction and Crystal Structure Prediction. <i>Crystal Growth and Design</i> , 2019, 19, 6058-6066.	1.4	5
78	Remarkably Distinct Mechanical Flexibility in Three Structurally Similar Semiconducting Organic Crystals Studied by Nanoindentation and Molecular Dynamics. <i>Chemistry of Materials</i> , 2019, 31, 1391-1402.	3.2	84
79	Relationship between hydrate stability and accuracy of true density measured by helium pycnometry. <i>International Journal of Pharmaceutics</i> , 2019, 567, 118444.	2.6	17
80	X-ray crystal structure, Hirshfeld surface analysis and DFT study on symmetrical trans-1,2-diformyldiimide: An unusual One-pot condensation of formic acid and hydrazine hydrate mediated by metal(II) nitrate hexahydrates. <i>Chemical Data Collections</i> , 2019, 22, 100239.	1.1	4
81	Orientation-dependent conformational polymorphs in two similar pyridine/pyrazine phenolic esters. <i>CrystEngComm</i> , 2019, 21, 3721-3730.	1.3	8
82	Seeking the best model for non-covalent interactions within the crystal structure of meloxicam. <i>Computational and Theoretical Chemistry</i> , 2019, 1157, 47-53.	1.1	10
83	Structure-property relationships in aromatic thioethers featuring aggregation-induced emission: solid-state structures and theoretical analysis. <i>CrystEngComm</i> , 2019, 21, 3097-3105.	1.3	8
84	Computational Techniques for Predicting Mechanical Properties of Organic Crystals: A Systematic Evaluation. <i>Molecular Pharmaceutics</i> , 2019, 16, 1732-1741.	2.3	62
85	Structure-property Relationship in an Organic Semiconductor: Insights from Energy Frameworks, Charge Density Analysis, and Diode Devices. <i>Crystal Growth and Design</i> , 2019, 19, 3019-3029.	1.4	6
86	3D energy frameworks of dimethylbenzophenone tetramorphs. <i>Heliyon</i> , 2019, 5, e01209.	1.4	13
87	Measurement of Electric Fields Experienced by Urea Guest Molecules in the 18-Crown-6/Urea (1:5) Host-Guest Complex: An Experimental Reference Point for Electric-Field-Assisted Catalysis. <i>Journal of the American Chemical Society</i> , 2019, 141, 3965-3976.	6.6	35
88	First-Principles-Based Force Field for 2,6-Diamino-3,5-dinitropyrazine-1-oxide (LLM-105). <i>ACS Omega</i> , 2019, 4, 21054-21062.	1.6	4
89	Polymorphs of 2,4,6-tris(4-pyridyl)-1,3,5-triazine and their mechanical properties. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 987-993.	0.5	2
90	Crystallographic and Energetic Insights into Reduced Dissolution and Physical Stability of a Drug-Surfactant Salt: The Case of Norfloxacin Lauryl Sulfate. <i>Molecular Pharmaceutics</i> , 2019, 17, 579-587.	2.3	3
91	Symmetric Fluoroborate and its Boron Modification: Crystal and Electronic Structures. <i>Crystals</i> , 2019, 9, 662.	1.0	6

#	ARTICLE	IF	CITATIONS
92	Nonclassical Synthons: Supramolecular Recognition by Sâ€¦â€¦â€¦O Chalcogen Bonding in Molecular Complexes of Riluzole. <i>Chemistry - A European Journal</i> , 2019, 25, 3591-3597.	1.7	28
93	The conformation of chloramphenicol in the ordered and disordered phases. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 211, 383-392.	2.0	2
94	Synthesis, Elucidation, Hirshfeld surface analysis, and DFT calculations of 4-chloro-N-[2-(2-1H-indol-3-yl-acetylamino)-phenyl]-benzamide. <i>Journal of Molecular Structure</i> , 2019, 1178, 384-393.	1.8	25
95	Exploring the Relationship between Intermolecular Interactions and Solid-State Photophysical Properties of Organic Co-Crystals. <i>Journal of Physical Chemistry C</i> , 2019, 123, 9311-9322.	1.5	31
96	A Practical Guide to the Design of Molecular Crystals. <i>Crystal Growth and Design</i> , 2019, 19, 1426-1453.	1.4	222
97	Role of Side Chains in the Solid State Assembly of Cyclic Peptoids. <i>Crystal Growth and Design</i> , 2019, 19, 125-133.	1.4	13
98	3D energy framework of a benzophenone acidic dimer. <i>Chemical Data Collections</i> , 2019, 19, 100168.	1.1	4
99	Assessing the impact on aqueous solubility of berberine chloride via co-crystallization with different stoichiometric ratios of pyromellitic dianhydride. <i>Journal of Molecular Structure</i> , 2020, 1200, 127086.	1.8	13
100	Design-based synthesis, molecular docking analysis of an anti-inflammatory drug, and geometrical optimization and interaction energy studies of an indole acetamide derivative. <i>Journal of Molecular Structure</i> , 2020, 1202, 127244.	1.8	27
101	Hexaiododiplatinate( <i>ii</i> ) as a useful supramolecular synthon for halogen bond involving crystal engineering. <i>Dalton Transactions</i> , 2020, 49, 356-367.	1.6	49
102	Photo-switching and -cyclisation of hydrogen bonded liquid crystals based on resveratrol. <i>Chemical Communications</i> , 2020, 56, 1105-1108.	2.2	12
103	Structural and Noncovalent Interactions Study of 2-Pyridone Based Flexible Unsymmetrical Dimer. <i>Crystal Research and Technology</i> , 2020, 55, 1900136.	0.6	9
104	Boron-Nitrogen Double Tweezers Comprising Arylboronic Esters and Diamines: Self-Assembly in Solution and Adaptability as Hosts for Aromatic Guests in the Solid State. <i>ChemPlusChem</i> , 2020, 85, 548-560.	1.3	10
105	Mononuclear and binuclear dioxidomolybdenum(VI) complexes of ONO appended aroylhydrazone: Crystal structures, interaction energy calculation and cytotoxicity. <i>Journal of Molecular Structure</i> , 2020, 1204, 127467.	1.8	9
106	Applications of charge-density analysis to the rational design of molecular materials: A mini review on how to engineer optical or magnetic crystals. <i>Journal of Molecular Structure</i> , 2020, 1203, 127431.	1.8	4
107	Quantitative investigation on the intermolecular interactions present in 8-(4-ethoxyphenyl)-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione with insight from interaction energies, energy framework, electrostatic potential map and fingerprint analysis. <i>Journal of Chemical Sciences</i> , 2020, 132, 1.	0.7	5
108	COMPARISON OF DIFFERENT COMPUTATIONAL APPROACHES FOR UNVEILING THE HIGH-PRESSURE BEHAVIOR OF ORGANIC CRYSTALS AT A MOLECULAR LEVEL. CASE STUDY OF TOLAZAMIDE POLYMORPHS. <i>Journal of Structural Chemistry</i> , 2020, 61, 1356-1366.	0.3	8
109	Development of piroxicam mini-tablets enabled by spherical cocrystallization. <i>International Journal of Pharmaceutics</i> , 2020, 590, 119953.	2.6	22

#	ARTICLE	IF	CITATIONS
110	Nanoindentation of Molecular Crystals: Lessons Learned from Aspirin. <i>Crystal Growth and Design</i> , 2020, 20, 5956-5966.	1.4	31
111	Chiral mesophases of hydrogen-bonded liquid crystals. <i>Molecular Systems Design and Engineering</i> , 2020, 5, 1299-1306.	1.7	10
112	Accurate Modelling of Group Electrostatic Potential and Distributed Polarizability in Dipeptides. <i>ChemPhysChem</i> , 2020, 21, 2155-2165.	1.0	8
113	Novel Quasi-Emulsion Solvent Diffusion-Based Spherical Cocrystallization Strategy for Simultaneously Improving the Manufacturability and Dissolution of Indomethacin. <i>Crystal Growth and Design</i> , 2020, 20, 6752-6762.	1.4	23
114	The Impact of the Next-Nearest Neighbor Dispersion Interactions on Spin Crossover Transition Enthalpy Evidenced by Experimental and Computational Analyses of Neutral $\pi$ -Extended Heteroleptic Fe(III) Complexes. <i>Inorganic Chemistry</i> , 2020, 59, 12295-12303.	1.9	6
115	2-Mercaptoimidazolium halides: structural diversity, stability and spontaneous racemisation. <i>CrystEngComm</i> , 2020, 22, 6034-6046.	1.3	2
116	4 <i>H</i> -[1,2,3]Triazolo[4,5- <i>c</i> ][1,2,5]oxadiazole 5-oxide and Its Salts: Promising Multipurpose Energetic Materials. <i>ACS Applied Energy Materials</i> , 2020, 3, 9401-9407.	2.5	22
117	Tuning of Molecular Electrostatic Potential Enables Efficient Charge Transport in Crystalline Azaacenes: A Computational Study. <i>International Journal of Molecular Sciences</i> , 2020, 21, 5654.	1.8	6
118	Design, Synthesis, In Silico Analysis, and Structural Study of 4,6-Dimethyl-2-(3-( <i>p</i> -tolylloxy)propoxy)nicotinonitrile Fleximer. <i>Crystal Research and Technology</i> , 2020, 55, 2000100.	0.6	7
119	Sila-Ibuprofen. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 12614-12622.	2.9	14
120	Cyclic hexapeptoids with N-alkyl side chains: solid-state assembly and thermal behaviour. <i>CrystEngComm</i> , 2020, 22, 6371-6384.	1.3	6
121	The Advent of Quantum Crystallography: Form and Structure Factors from Quantum Mechanics for Advanced Structure Refinement and Wavefunction Fitting. <i>Structure and Bonding</i> , 2020, , 65-144.	1.0	17
122	Experimental charge density of ferrocenyl derivative of $\beta$ -lactam. <i>Journal of Molecular Structure</i> , 2020, 1217, 128274.	1.8	3
123	Engineering Crystals Using $sp^3$ Centred Tetrel Bonding Interactions. <i>Chemistry - A European Journal</i> , 2020, 26, 10126-10132.	1.7	28
124	Solid-State Landscape of 4,4'-Azobis(3,5-dimethyl-1 <i>H</i> -pyrazole) with the Isolation of Conformer-Dependent Polymorphs. <i>Crystal Growth and Design</i> , 2020, 20, 2721-2733.	1.4	4
125	Exploring Ambipolar Semiconductor Nature of Binary and Ternary Charge-Transfer Cocrystals of Triphenylene, Pyrene, and TCNQ. <i>Journal of Physical Chemistry C</i> , 2020, 124, 6544-6553.	1.5	23
126	Effect of the substituent position on the electrochemical, optical and structural properties of donor-acceptor type acridone derivatives. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8522-8534.	1.3	10
127	Melting point-solubility-structure correlations in chiral and racemic model cocrystals. <i>CrystEngComm</i> , 2020, 22, 2766-2771.	1.3	11



#	ARTICLE	IF	CITATIONS
128	syn and anti polymorphs of 2,6-dimethoxy benzoic acid and its molecular and ionic cocrystals: Structural analysis and energetic perspective. <i>Journal of Molecular Structure</i> , 2020, 1221, 128721.	1.8	7
129	Molecular Origin of the Distinct Tabletability of Loratadine and Desloratadine: Role of the Bonding Area " Bonding Strength Interplay. <i>Pharmaceutical Research</i> , 2020, 37, 133.	1.7	7
130	Improving solubility and intrinsic dissolution rate of ofloxacin API through salt formation via mechanochemical synthesis with diphenic acid. <i>Journal of Molecular Structure</i> , 2020, 1221, 128806.	1.8	19
131	Synthesis, crystal structure and electron density analysis of a sulfanyl 2-pyridone analogue: Tautomeric preference and conformation locking by S...O chalcogen bonding. <i>Journal of Molecular Structure</i> , 2020, 1222, 128798.	1.8	3
132	Synthesis, physicochemical, and thermal characterization of coordination compounds of Cu(II) with a pyrazole-type ligand. <i>Journal of Thermal Analysis and Calorimetry</i> , 2020, 142, 451-460.	2.0	5
133	Metal-like Ductility in Organic Plastic Crystals: Role of Molecular Shape and Dihydrogen Bonding Interactions in Aminoboranes. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 10971-10980.	7.2	65
134	Metal-like Ductility in Organic Plastic Crystals: Role of Molecular Shape and Dihydrogen Bonding Interactions in Aminoboranes. <i>Angewandte Chemie</i> , 2020, 132, 11064-11073.	1.6	24
135	Structural chemistry and anti-inflammatory activity of flexible/restricted phenyl dimers. <i>Journal of the Iranian Chemical Society</i> , 2020, 17, 1289-1303.	1.2	7
136	Structural elucidation, theoretical insights and thermal properties of three novel multicomponent molecular forms of gallic acid with hydroxypyridines. <i>Journal of Molecular Structure</i> , 2020, 1207, 127828.	1.8	18
137	Supramolecular frameworks formed via hydrogen bonding and non-covalent interactions and interaction energy calculations of solvent coordinated cis-dioxomolybdenum(VI) complexes derived from ONO donor aroylhydrazone: Cytotoxicity studies. <i>Inorganica Chimica Acta</i> , 2020, 505, 119472.	1.2	4
138	Supramolecular organisation of sulphate salt hydrates exemplified with brucine sulphate. <i>CrystEngComm</i> , 2020, 22, 7204-7216.	1.3	4
139	Polymorph induced diversity of photomechanical motions of molecular crystals. <i>CrystEngComm</i> , 2020, 22, 3279-3286.	1.3	17
140	Alkyl-Alkyl Interactions in the Periphery of Supramolecular Entities: From the Evaluation of Weak Forces to Applications. <i>ChemPlusChem</i> , 2020, 85, 715-724.	1.3	14
141	Photophysical and crystallographic study of three integrated pyrazolo[1,5-a]pyrimidine-triphenylamine systems. <i>Dyes and Pigments</i> , 2021, 184, 108730.	2.0	26
142	Investigation of intermolecular interactions in fluoro/trifluoromethyl derivatives of benzoylferrocene. <i>Journal of Molecular Structure</i> , 2021, 1224, 129045.	1.8	1
143	Synthesis of 1-aryl-3-methylsulfanyl-5-amino-1,2,4-triazoles and their analysis by spectroscopy, X-ray crystallography and theoretical calculations. <i>Journal of Molecular Structure</i> , 2021, 1226, 129317.	1.8	14
144	Analysis of supramolecular self-assembly of two chromene derivatives: Synthesis, crystal structure, Hirshfeld surface, quantum computational and molecular docking studies. <i>Journal of Molecular Structure</i> , 2021, 1225, 129104.	1.8	9
145	Design, synthesis, in silico analysis with PPAR $\beta$ receptor and study of non-covalent interactions in unsymmetrical heterocyclic/phenyl fleximer. <i>Journal of the Chinese Chemical Society</i> , 2021, 68, 150-158.	0.8	6

#	ARTICLE	IF	CITATIONS
146	DFT and IsoStar Analyses to Assess the Utility of $\pi$ - and $\pi$ -Hole Interactions for Crystal Engineering. <i>ChemPhysChem</i> , 2021, 22, 141-153.	1.0	9
147	Spectral studies and crystal structures of molybdenum(VI) complexes containing pyridine or picoline as auxiliary ligands: interaction energy calculations and free radical scavenging studies. <i>Transition Metal Chemistry</i> , 2021, 46, 241-253.	0.7	1
148	<i>CrystalGrower</i> : a generic computer program for Monte Carlo modelling of crystal growth. <i>Chemical Science</i> , 2021, 12, 1126-1146.	3.7	18
149	Experimental and computational evidence for a stabilising Cl(lone-pair) $\cdots$ (chelate-ring) interaction. <i>CrystEngComm</i> , 2021, 23, 119-130.	1.3	4
150	Sublimation thermodynamics of pyrazinoic, dipicolinic and quinolinic acids: Experiment and theoretical prediction. <i>Journal of Chemical Thermodynamics</i> , 2021, 155, 106369.	1.0	6
151	Accurate crystal structures and chemical properties from NoSpherA2. <i>Chemical Science</i> , 2021, 12, 1675-1692.	3.7	147
152	Reversible order-disorder phase transition and interaction topology in 4-carboxyanilinium nitrate. <i>Journal of Molecular Structure</i> , 2021, 1227, 129542.	1.8	5
153	Interplay of weak noncovalent interactions in alkoxybenzylidene derivatives of benzohydrazide and acetohydrazide: a combined experimental and theoretical investigation and lipoxigenase inhibition (LOX) studies. <i>CrystEngComm</i> , 2021, 23, 955-971.	1.3	9
154	Synthesis and X-ray crystallographic analysis of free base and hexafluorophosphate salts of 3,4-dihydroisoquinolines from the Bischler-Napieralski reaction. <i>New Journal of Chemistry</i> , 2021, 45, 1565-1572.	1.4	2
155	Predicting molecular isomerism of symmetrical and unsymmetrical <i>N,N</i> -diphenyl formamidines in the solid-state: crystal structure, Hirshfeld surface analysis, pairwise interaction energy, and $\int^{\infty} H <sub>fusion</sub>$ and $\int^{\infty} S <sub>fusion</sub>$ correlations. <i>CrystEngComm</i> , 2021, 23, 4459-4474.	1.3	3
156	Solid-State Conformational Flexibility at Work: Energetic Landscape of a Single Crystal-to-Single Crystal Transformation in a Cyclic Hexapeptoid. <i>Crystal Growth and Design</i> , 2021, 21, 897-907.	1.4	13
157	Sweet Sulfamethazine Acesulfamate Crystals with Improved Compaction Property. <i>Crystal Growth and Design</i> , 2021, 21, 1077-1085.	1.4	5
158	Dissecting the packing forces in mixed perfluorocarbon/aromatic co-crystals. <i>CrystEngComm</i> , 0, , .	1.3	2
159	Self-organization of 1,6-dialkyl-3a,6a-diphenylglycolurils in the crystalline state. <i>CrystEngComm</i> , 2021, 23, 4312-4319.	1.3	4
160	Naturally occurring polyphenols as building blocks for supramolecular liquid crystals – substitution pattern dominates mesomorphism. <i>Molecular Systems Design and Engineering</i> , 2021, 6, 390-397.	1.7	5
161	Modulation of the powder properties of lamotrigine by crystal forms. <i>International Journal of Pharmaceutics</i> , 2021, 595, 120274.	2.6	16
162	Crystal Structures of New Ivermectin Pseudopolymorphs. <i>Crystals</i> , 2021, 11, 172.	1.0	6
163	Multidentate, V-shaped Pyridine Building Blocks as Tectons for Crystal Engineering. <i>Chemistry - A European Journal</i> , 2021, 27, 4660-4669.	1.7	2

#	ARTICLE	IF	CITATIONS
164	Synthesis, structural characterization, and DFT studies of anti-cancer drug N-(2-Aminophenyl)-2-(4-bromophenoxy)acetamide. <i>Heliyon</i> , 2021, 7, e06464.	1.4	8
165	Bandgap Tuning in Molecular Alloy Crystals Formed by Weak Chalcogen Interactions. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3059-3065.	2.1	12
166	Weak yet Decisive: Molecular Halogen Bond and Competing Weak Interactions of Iodobenzene and Quinuclidine. <i>Journal of the American Chemical Society</i> , 2021, 143, 4133-4137.	6.6	25
167	Influence of the haloaryl moiety over the molecular packing in N-phenacylbenzimidazoles crystallizing in the same space group. <i>Journal of Molecular Structure</i> , 2021, 1230, 129869.	1.8	5
168	Crystallographic investigation, Hirshfeld surface analysis, NLO characterization and experimental spectral (UV and NMR) studies with DFT probe on(R)-9-(2-hydroxy propyl)adenine. <i>Heliyon</i> , 2021, 7, e06593.	1.4	4
169	<i>CrystalExplorer</i>: a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals. <i>Journal of Applied Crystallography</i> , 2021, 54, 1006-1011.	1.9	1,744
170	Crystal structure, Hirshfeld surface analysis and interaction energy calculation of 1-decyl-2,3-dihydro-1<i>H</i>-benzimidazol-2-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 559-563.	0.2	2
171	Drugâ€“Drug Cocrystallization Simultaneously Improves Pharmaceutical Properties of Genistein and Ligustrazine. <i>Crystal Growth and Design</i> , 2021, 21, 3461-3468.	1.4	15
172	Polymorphism of coumarin thione-triazole - 4-methyl-7-[(4-phenyl-5-thioxo-4,5-dihydro-1H-1,2,4-triazol-3-yl)methoxy]-2H-chromen-2-one. <i>Journal of Molecular Structure</i> , 2021, 1231, 129957.	1.8	3
173	Qualitative and Quantitative Study of Intermolecular Interactions in Imidazo[2,1- <i>b</i> ] [1,3,4] Thiadiazoles. <i>ChemistrySelect</i> , 2021, 6, 4265-4272.	0.7	3
174	Functional substituted Cu(II) Schiff base complexes, syntheses, X-ray and theoretical characterizations, and investigations of their polyphenol oxidase- and peroxidase-like activities. <i>Journal of Molecular Structure</i> , 2021, 1232, 129975.	1.8	5
175	Synthesis, crystal structure, DFT calculations, Hirshfeld surface analysis, energy frameworks, molecular dynamics and docking studies of novel isoxazolequinoxaline derivative (IZQ) as anti-cancer drug. <i>Journal of Molecular Structure</i> , 2021, 1232, 130004.	1.8	40
176	Crystal structure, Hirshfeld surface analysis, interaction energy, and DFT studies of cholesteryl heptanoate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 686-691.	0.2	0
177	Structural investigations into a new polymorph of F<sub>4</sub>TCNQ: towards enhanced semiconductor properties. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021, 77, 426-434.	0.2	2
178	Combining Molecular Dynamic Information and an Aspherical-Atom Data Bank in the Evaluation of the Electrostatic Interaction Energy in Multimeric Protein-Ligand Complex: A Case Study for HIV-1 Protease. <i>Molecules</i> , 2021, 26, 3872.	1.7	6
179	Crystallography, Molecular Modeling, and COX-2 Inhibition Studies on Indolizine Derivatives. <i>Molecules</i> , 2021, 26, 3550.	1.7	10
180	Insights into Intermolecular Interactions of Spironolactone Solvates. <i>Crystal Growth and Design</i> , 2021, 21, 3677-3688.	1.4	14
181	Synthesis, structural characterisation and theoretical studies of a novel pyridazine derivative: Investigations of anti-inflammatory activity and inhibition of $\alpha$ -glucosidase. <i>Journal of Molecular Structure</i> , 2021, 1234, 130177.	1.8	11

#	ARTICLE	IF	CITATIONS
182	Crystal structure, Hirshfeld surface analysis and interaction energy calculation of 4-(furan-2-yl)-2-(6-methyl-2,4-dioxopyran-3-ylidene)-2,3,4,5-tetrahydro-1 <i>H</i> -1,5-benzodiazepine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021, 77, 834-838.	0.2	0
183	Experimental and in silico studies of dichloro-tetrakis(1 <i>H</i> -pyrazole)-cobalt(II): Structural description, photoluminescent behavior and molecular docking. <i>Journal of Molecular Structure</i> , 2021, 1235, 130266.	1.8	5
184	Estudio estructural y supramolecular del Ácido 2-E-((4-hidroxifenil) diazenil) benzoico. <i>Revista Colombiana De Quimica</i> , 2021, 50, 40-48.	0.2	0
185	Interplay of Halogen and Hydrogen Bonding through Co <sup>2+</sup> Crystallization in Pharmacologically Active Dihydropyrimidines: Insights from Crystal Structure and Energy Framework. <i>ChemPlusChem</i> , 2021, 86, 1167-1176.	1.3	10
186	Easy preparation of novel 3,3-dimethyl-3,4-dihydro-2 <i>H</i> -1,2,4-benzothiadiazine 1,1-dioxide: Molecular structure, Hirshfeld surface, NCI analyses and molecular docking on AMPA receptors. <i>Journal of Molecular Structure</i> , 2021, 1238, 130435.	1.8	9
187	Synthesis, structure analysis, DFT calculations, Hirshfeld surface studies, and energy frameworks of 6-Chloro-3-[(4-chloro-3-methylphenoxy)methyl][1,2,4]triazolo[4,3- <i>b</i> ]pyridazine. <i>Journal of Molecular Structure</i> , 2021, 1237, 130282.	1.8	9
188	Study of the structure-bioactivity of fleximers: synthesis, crystal structure, Hirshfeld surface analysis, and anti-inflammatory assays. <i>Journal of Molecular Structure</i> , 2021, 1239, 130513.	1.8	8
189	Synthesis, conformation and Hirshfeld surface analysis of benzoxazole methyl ester as a versatile building block for heterocycles. <i>Heliyon</i> , 2021, 7, e08042.	1.4	4
190	Structural Insights and Docking Analysis of Adamantane-Linked 1,2,4-Triazole Derivatives as Potential 11 $\beta$ -HSD1 Inhibitors. <i>Molecules</i> , 2021, 26, 5335.	1.7	4
191	Synthesis, crystal structure elucidation, Hirshfeld surface analysis, 3D energy frameworks and DFT studies of 2-(4-fluorophenoxy) acetic acid. <i>European Journal of Chemistry</i> , 2021, 12, 304-313.	0.3	1
192	Synthesis, structural determination, Hirshfeld surface analysis, 3D energy frameworks, electronic and (static, dynamic) NLO properties of <i>o</i> -Nitroacetanilide ( <i>o</i> -NAA): A combined experimental and quantum chemical study. <i>Inorganic Chemistry Communication</i> , 2021, 133, 108884.	1.8	5
193	Crystal structures and photoluminescence properties of chromium(III) complexes with 2-thenyltrifluoroacetone ligand. <i>Journal of Molecular Structure</i> , 2021, 1245, 131023.	1.8	1
194	Hirshfeld surface analysis, enrichment ratio, energy frameworks and third-order nonlinear optical studies of a hydrazone derivative for optical limiting applications. <i>Journal of Molecular Structure</i> , 2021, 1245, 131019.	1.8	3
195	Isomeric nitro substituted symmetrical benzamides: Crystal Structures, Hirshfeld surface analysis, 3D energy frameworks, DNA binding and cell line studies. <i>Journal of Molecular Structure</i> , 2022, 1247, 131396.	1.8	4
196	Non-covalent interactions involving remote substituents influence the topologies of supramolecular chains featuring hydroxyl-O $\cdots$ H $\cdots$ O(hydroxyl) hydrogen bonding in crystals of (HOCH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> NC(=S)N(H)(C <sub>6</sub> H <sub>4</sub> Y-4) for Y = H, Me, Cl and NO <sub>2</sub> . <i>CrystEngComm</i> , 2021, 23, 1723-1743.	1.3	6
197	The trimorphism of 3-hydroxybenzoic acid: an experimental and computational study. <i>CrystEngComm</i> , 2021, 23, 2513-2519.	1.3	3
198	Conformational aspects of polymorphs and phases of 2-propyl-1 <i>H</i> -benzimidazole. <i>IUCr</i> , 2018, 5, 706-715.	1.0	7
199	Insight from electron density and energy framework analysis on the structural features of F <sub>x</sub> -TCNQ (x = 0, 2, 4) family of molecules. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2019, 75, 71-78.	0.5	7

#	ARTICLE	IF	CITATIONS
200	Interplay between packing, dimer interaction energy and morphology in a series of tricyclic imide crystals. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2020, 76, 157-165.	0.5	2
201	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of 3-[(2 <i>Z</i> )-2-[(2,4-dichlorophenyl)methylidene]-3-oxo-3,4-dihydro-2 <i>H</i> -1,4-benzothiazin-4-yl]propanenitrile. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 721-727.	0.2	12
202	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of 5,5-diphenyl-1,3-bis(prop-2-yn-1-yl)imidazolidine-2,4-dione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 951-956.	0.2	2
203	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of 2-chloroethyl 2-oxo-1-(prop-2-yn-1-yl)-1,2-dihydroquinoline-4-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1411-1417.	0.2	2
204	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of 1-(1,3-benzothiazol-2-yl)-3-(2-hydroxyethyl)imidazolidin-2-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 370-376.	0.2	1
205	Crystal structure, Hirshfeld surface analysis, interaction energy and DFT studies of 4-[(4-allyl-2-methoxyphenoxy)methyl]-1-(4-methoxyphenyl)-1 <i>H</i> -1,2,3-triazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 962-966.	0.2	6
206	Crystal structure, Hirshfeld surfaces, topology, energy frameworks and dielectric studies of 1-(2-chlorophenyl)-3,3-bis(methylthio)prop-2-en-1-one. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2020, 235, 85-93.	0.4	6
207	Theoretical and experimental solid state studies of Ethyl 1-benzyl-2-(thiophen-3-yl)-1 <i>H</i> -benzo[d]imidazole-5-carboxylate. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2020, 235, 569-579.	0.4	2
208	A combined structural and computational investigation of aminobenzyl-naphthol compounds derived from the Betti reaction using valine methyl ester. <i>New Journal of Chemistry</i> , 2021, 45, 20735-20742.	1.4	5
209	Maximizing completeness in single-crystal high-pressure diffraction experiments: phase transitions in 2Å <sup>3</sup> AP. <i>IUCr</i> , 2021, 8, 1006-1017.	1.0	4
210	Charge-assisted hydrogen bonding in three diaminobenzene salts. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 1725-1731.	0.2	2
211	A 1:2 co-crystal of 2,2- <sup>2</sup> -thiodibenzoic acid and triphenylphosphane oxide: crystal structure, Hirshfeld surface analysis and computational study. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1764-1771.	0.2	9
212	Intermolecular interactions in a phenol-substituted benzimidazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 272-276.	0.2	0
213	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of 4-[(prop-2-en-1-yloxy)methyl]-3,6-bis(pyridin-2-yl)pyridazine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1321-1326.	0.2	1
214	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of methyl 4-[3,6-bis(pyridin-2-yl)pyridazin-4-yl]benzoate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1672-1678.	0.2	0
215	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of (2 <i>Z</i> )-4-benzyl-2-(2,4-dichlorobenzylidene)-2 <i>H</i> -1,4-benzothiazin-3(4 <i>H</i> )-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1650-1656.	0.2	3
216	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of 1-methyl-3-(prop-2-yn-1-yl)-2,3-dihydro-1 <i>H</i> -1,3-benzodiazol-2-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 1940-1946.	0.2	0
217	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of 2-(2,3-dihydro-1 <i>H</i> -perimidin-2-yl)-6-methoxyphenol. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020, 76, 605-610.	0.2	0

#	ARTICLE	IF	CITATIONS
218	Crystal structure, Hirshfeld surface analysis and interaction energy, DFT and antibacterial activity studies of ( <i>Z</i> )-4-hexyl-2-(4-methylbenzylidene)-2 <i>H</i> -benzo[ <i>b</i> ][1,4]thiazin-3(4 <i>H</i> )-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 889-895.	0.2	0
219	Regiospecific substitution of the $\hat{1}^2$ -vinylic sp <sup>2</sup> carbon of cyclohexenones bearing the $\hat{1}\pm$ -chloro- and $\hat{1}^2$ -tosylate-groups: Single crystal XRD/Hirshfeld surface/in-silico studies of three representative compounds. European Journal of Chemistry, 2020, 11, 261-275.	0.3	1
220	Crystal structure and Hirshfeld surface analysis of dl-methionine polymorphs ( $\hat{1}\pm$ and $\hat{1}^2$ ). Journal of Molecular Structure, 2022, 1250, 131721.	1.8	9
221	Crystal structure, Hirshfeld surface analysis, interaction energy and DFT studies of (2 <i>Z</i> )-2-(2,4-dichlorobenzylidene)-4-nonyl-3,4-dihydro-2 <i>H</i> -1,4-benzothiazin-3-one. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 281-287.	0.2	1
222	Interactions in flavanone and chalcone derivatives: Hirshfeld surface analysis, energy frameworks and global reactivity descriptors. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 212-224.	0.2	2
223	Crystal structure, Hirshfeld surface analysis and interaction energy and DFT studies of ( <i>S</i> )-10-propargylpyrrolo[2,1- <i>c</i> ][1,4]benzodiazepine-5,11-dione. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 467-472.	0.2	2
224	Crystal structure, Hirshfeld surface analysis and interaction energy, DFT and antibacterial activity studies of ethyl 2-[(2 <i>Z</i> )-2-(2-chlorobenzylidene)-3-oxo-3,4-dihydro-2 <i>H</i> -1,4-benzothiazin-4-yl]acetate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 629-636.	0.2	1
225	Expanding the Solid Form Landscape of Bipyridines. Crystal Growth and Design, 2021, 21, 7201-7217.	1.4	5
226	Pseudopolymorphism Driven by Stoichiometry and Hydrated/Anhydrous Reagents: The Riveting Case of Methyl Gallate- <i>scp</i> -Proline. Crystal Growth and Design, 2021, 21, 6776-6785.	1.4	4
227	Four Directional Twinning Deformation of an Anisotropic Molecular Single Crystal Based on Three Different Modes of Mechanical Twinning. Crystal Growth and Design, 2022, 22, 174-179.	1.4	3
228	1-Hydroxynaphthalene-4-trifluoromethylphenyl chalcone and 3- $\hat{c}$ 'hydroxy-4-trifluoromethylphenyl flavone: A combined experimental, structural, in vitro AChE, BChE and in silico studies. Journal of Molecular Structure, 2022, 1253, 132253.	1.8	1
229	COMPUTATIONAL INVESTIGATIONS, HIRSHFELD SURFACE ANALYSIS, INTERACTION ENERGY CALCULATIONS, AND ENERGY FRAMEWORK CRYSTAL STRUCTURE OF METHYL 2-AMINO-5-HYDROXYBENZOATE. Journal of Structural Chemistry, 2021, 62, 1745-1758.	0.3	1
230	Synthesis, elucidation, DFT computations, Hirshfeld surface analysis and docking study of 6-chloro-3-[(4-fluoro-phenoxy)methyl][1, 2, 4]triazolo[4,3- <i>b</i> ]pyridazine against fungi pathogen. Molecular Crystals and Liquid Crystals, 2022, 738, 76-90.	0.4	1
231	Bendable and Twistable Crystals of Flufenamic Acid Form III with Bending Mechanofluorochromism Behavior. Crystal Growth and Design, 2022, 22, 1312-1318.	1.4	17
232	Shedding Light on the Synthesis, Crystal Structure, Characterization, and Computational Study of Optoelectronic Properties and Bioactivity of Imine derivatives. ACS Omega, 2022, 7, 5217-5230.	1.6	18
233	Inclusion of CO <sub>2</sub> , NH <sub>3</sub> , SO <sub>2</sub> , Cl <sub>2</sub> and H <sub>2</sub> S in porous N <sub>4</sub> O <sub>4</sub> -donor macrocyclic Schiff base. Microporous and Mesoporous Materials, 2022, 332, 111708.	2.2	3
234	Crystal structure, Hirshfeld, computational biomolecular investigations, and MTT assay studies of amino pyrimidine derivative as EGFR kinase domain inhibitor. Journal of Molecular Structure, 2022, 1254, 132416.	1.8	9
235	Crystal structures of <i>N</i> -[4-(trifluoromethyl)phenyl]benzamide and <i>N</i> -(4-methoxyphenyl)benzamide at 173 K: a study of the energetics of conformational changes due to crystal packing. Acta Crystallographica Section E: Crystallographic Communications, 2022, 78, 297-305.	0.2	1

#	ARTICLE	IF	CITATIONS
236	Unique sandwich structure of the pyrazinamide–methylmalonic acid cocrystal: ternary phase diagrams, characterization and property evaluation. <i>CrystEngComm</i> , 2022, 24, 2650-2659.	1.3	2
237	Dielectric response of 1,1-difluorosumanene caused by an in-plane motion. <i>Materials Chemistry Frontiers</i> , 2022, 6, 1752-1758.	3.2	10
238	BN-Substitution in Dithienylpyrenes Prevents Excimer Formation in Solution and in the Solid State. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4563-4576.	1.5	5
239	Quantum, Hirshfeld surface, crystal voids, energy framework and molecular docking analysis of two halogen-containing benzimidazole-2-thione structures. <i>Molecular Crystals and Liquid Crystals</i> , 0, , 1-15.	0.4	2
240	Understanding Poor Milling Behavior of Voriconazole from Crystal Structure and Intermolecular Interactions. <i>Molecular Pharmaceutics</i> , 2022, 19, 985-997.	2.3	6
241	π-Hole bonding in a new co-crystal hydrate of gallic acid and pyrazine: static and dynamic charge density analysis. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2022, 78, 231-246.	0.5	4
242	Crystal structure, Hirshfeld surface analysis, interaction energy and DFT calculations and energy frameworks of methyl 6-chloro-1-methyl-2-oxo-1,2-dihydroquinoline-4-carboxylate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 425-432.	0.2	2
243	Investigation of crystal structures, energetics and isostructurality in halogen-substituted phosphoramidates. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2022, 78, 179-194.	0.5	1
244	Mechanisms of Crystal Plasticization by Lattice Water. <i>Pharmaceutical Research</i> , 2022, 39, 3113-3122.	1.7	3
245	Diverse Mechanical Properties of 1,3-Bis(4-nitrophenyl) thiourea–DMSO Dimorphic Solvates. <i>Crystal Growth and Design</i> , 2022, 22, 2058-2065.	1.4	9
246	Tunable Solid–State Thermochromism: Alkyl Chain Length–Dependent Conformational Isomerization of Bianthrone. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	2
247	Azide–Alkyne Interactions: A Crucial Attractive Force for Their Preorganization for Topochemical Cycloaddition Reaction. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	11
248	Crystal structure, Hirshfeld surface, and DFT studies of 4-((pyrrolidin-1-ylsulfonyl)methyl)aniline. <i>European Journal of Chemistry</i> , 2021, 12, 419-431.	0.3	1
249	Energetic Co-Crystal of a Primary Metal-Free Explosive with BTF. Ideal Pair for Co-Crystallization. <i>Molecules</i> , 2021, 26, 7452.	1.7	10
250	Structural, Computational and 3D Interaction Energy Calculations of the Compound 2-chloro-3-(1-naphthyl)-5,5-dimethyl-2-cyclohexenone. <i>Crystallography Reports</i> , 2022, 67, 201-208.	0.1	7
252	Thorough investigation on the high-temperature polymorphism of dipentyl-perylenediimide: thermal expansion vs. polymorphic transition. <i>Journal of Materials Chemistry C</i> , 2022, 10, 8089-8100.	2.7	6
253	Synthesis, X-ray, characterization and HSA and energy framework analysis of novel pyridine-hydrazone based ligand and its Co(II) complex biological activity prediction and experimental antibacterial properties. <i>Molecular Crystals and Liquid Crystals</i> , 0, , 1-20.	0.4	2
254	Multiple Mechanical Behaviors in One Crystal of 2,4-Dichlorophenoxyacetic Acid Form II: Thermomechanical Effect and Elastic Deformation. <i>Crystal Growth and Design</i> , 2022, 22, 3680-3687.	1.4	4

#	ARTICLE	IF	CITATIONS
255	Cocrystal design of vanillin with amide drugs: Crystal structure determination, solubility enhancement, DFT calculation. <i>Chemical Engineering Research and Design</i> , 2022, 183, 170-180.	2.7	7
256	Synthesis, Crystal Structure, Hirshfeld Surface Analysis and Interaction Energy and Energy Framework Studies of Novel Hydrazone Derivative Containing Barbituric Acid Moiety. <i>Journal of Chemical Crystallography</i> , 2023, 53, 81-92.	0.5	2
257	A comparison of three crystalline forms of miconazole: solvent-free, ethanol monosolvate and hemihydrate. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 343-350.	0.2	2
258	Optimized Structure, in Silico interaction and Molecular Docking Analysis of Two Benzimidazole-2-Thione Derivatives. <i>Material Science Research India</i> , 2022, 19, 01-16.	0.9	0
259	Experimental and theoretical investigation of hydrogen bonded supramolecular assemblies through water molecules in a copper(II)-EGTA complex. <i>Journal of Molecular Structure</i> , 2022, , 133400.	1.8	7
260	Theoretical Prediction of Structures and Properties of 2,4,6-Trinitro-1,3,5-Triazine (TNTA) Green Energetic Materials from DFT and ReaxFF Molecular Modeling. <i>Materials</i> , 2022, 15, 3873.	1.3	3
261	Classical Intermolecular Hydrogen Bonding Motifs of Heterocyclic <i>rac</i>-2-Amino-3-carbonitrile Derivatives: Linking Hirshfeld Surface Analysis, CT-DNA Binding Affinity, and Molecular Docking. <i>Crystal Growth and Design</i> , 2022, 22, 5814-5834.	1.4	5
262	Solid-state landscape and biopharmaceutical implications of novel metformin-based salts. <i>New Journal of Chemistry</i> , 0, , .	1.4	4
263	Crystal Engineering of Ionic Cocrystals Sustained by the Phenolâ€“Phenolate Supramolecular Heterosynthon. <i>Crystal Growth and Design</i> , 2022, 22, 4582-4591.	1.4	8
264	Synchrotron Xâ€ray Electron Density Analysis of Chemical Bonding in the Graphitic Carbon Nitride Precursor Melamine. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	5
265	Synthesis, characterization and self assembly of dinuclear zinc Schiff base complexes: A combined experimental and theoretical study. <i>Polyhedron</i> , 2022, 225, 116044.	1.0	5
266	N-Fluoroalkylpyrazolyl-substituted Nitronyl Nitroxides. <i>Journal of Molecular Structure</i> , 2022, 1269, 133739.	1.8	5
267	Structural, vibrational and thermal study of Bis(4-Carboxyanilinium) sulphate a new organo-sulphate adduct of 4-amino benzoic acid. <i>Journal of Molecular Structure</i> , 2022, 1267, 133631.	1.8	2
268	X-ray structure analysis of the cholesterol 25- and 20-hydroperoxides, the elusive primary sidechain autoxidation products of cholesterol. <i>Steroids</i> , 2022, 187, 109092.	0.8	1
269	Fast photoactuation of elastic crystals based on 3-(naphthalen-1-yl)-2-phenylacrylonitriles triggered by subtle photoisomerization. <i>Journal of Materials Chemistry C</i> , 2022, 10, 14273-14281.	2.7	16
270	Exploring Highly Functionalized Tetrahydropyridine as a Dual Inhibitor of Monoamine Oxidase A and B: Synthesis, Structural Analysis, Single Crystal XRD, Supramolecular Assembly Exploration by Hirshfeld Surface Analysis, and Computational Studies. <i>ACS Omega</i> , 2022, 7, 29452-29464.	1.6	12
271	On the influence of pnictogen bonding on acidity. <i>Polyhedron</i> , 2022, 227, 116145.	1.0	2
272	Unravelling the semiconductor properties of mixed stack donor acceptor cocrystals of pyrene derivatives and TCNQ: effect of crystal packing <i>versus</i> super-exchange mechanism. <i>CrystEngComm</i> , 2022, 24, 6579-6586.	1.3	1



#	ARTICLE	IF	CITATIONS
273	Profoundly improved photostability of dimetronidazole by cocrystallization. <i>CrystEngComm</i> , 2022, 24, 6165-6171.	1.3	4
274	Conformational preferences in a series of $\beta$ -hydroxy ketone derivatives: interplay of conformational energies and lattice cohesive energies. <i>CrystEngComm</i> , 2022, 24, 7306-7314.	1.3	1
275	Unravelling supramolecular features and opto-electronic properties of a binary charge transfer cocrystal of a blue fluorescent di-carbazole and TFT. <i>CrystEngComm</i> , 2022, 24, 6669-6676.	1.3	1
276	Structural systematics in isomorphous binary co-crystal solvates comprising 2,2-dithiodibenzoic acid, 4-halobenzoic acid and dimethylformamide (1:1), for halide = chloride, bromide and iodide. <i>CrystEngComm</i> , 2022, 24, 5907-5921.	1.3	1
277	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-1 <i>H</i> -pyrazolo[3,4- <i>d</i> ]pyrimidin-1-yl)acetic acid. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022, 78, 953-960.	0.2	5
278	A structural and computational comparison of close contacts and related intermolecular energies of interaction in the structures of 1,3-diiodo-5-nitrobenzene, 1,3-dibromo-5-nitrobenzene, and 1,3-dichloro-5-nitrobenzene. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 552-558.	0.2	0
279	ANALYSIS OF THE CRYSTAL STRUCTURE AND ENERGY FRAMEWORKS OF 5-ACETIL-1,3-DIMETHYL BARBITURIC ACID. <i>Muğla Journal of Science and Technology</i> , 0, , .	0.1	0
280	Antispasmodic activity of novel 2,4-dichloroanilinium perchlorate hybrid material: X-ray crystallography, DFT studies and molecular docking approach. <i>Journal of Molecular Structure</i> , 2023, 1274, 134440.	1.8	5
281	Synthesis, Structural, and Intriguing Electronic Properties of Symmetrical Bis-Aryl- $\beta,\beta$ -Unsaturated Ketone Derivatives. <i>ACS Omega</i> , 2022, 7, 39294-39309.	1.6	22
282	Weak Noncovalent Interactions in Three Closely Related Adamantane-Linked 1,2,4-Triazole N-Mannich Bases: Insights from Energy Frameworks, Hirshfeld Surface Analysis, In Silico $11^2$ -HSD1 Molecular Docking and ADMET Prediction. <i>Molecules</i> , 2022, 27, 7403.	1.7	0
283	Green synthesis, X-ray crystallography, DFT and Hirshfeld analysis of C-2 symmetric 1,3-bis(4-ethylphenyl)triaz-1-ene. <i>Journal of Molecular Structure</i> , 2023, 1274, 134523.	1.8	0
284	Synthesis, crystal structure, Hirshfeld surface analysis, DNA binding, optical and nonlinear optical properties of Schiff bases derived from o-aminophenol. <i>Journal of Molecular Structure</i> , 2023, 1274, 134427.	1.8	18
285	Multivariate Analysis of a Highly Effective Drug Combination Tablet Containing the Antiepileptic Drug Gabapentin to Enhance Pharmaceutical Properties with a Multicomponent Crystal Strategy. <i>Crystal Growth and Design</i> , 2022, 22, 7234-7247.	1.4	3
286	Synthesis, Characterization, Crystal Structure and Computational Study of Third-Order NLO Properties of Schiff bases. <i>ChemistrySelect</i> , 2022, 7, .	0.7	7
287	The discovery of new cocrystals of 5-fluorocytosine using amine-carboxylate supramolecular synthon. <i>Journal of Drug Delivery Science and Technology</i> , 2022, 78, 103934.	1.4	2
288	Zwitterionic versus neutral molecules of fluoroquinolones: crystal structure of danofloxacin dihydrate. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2022, 78, 722-729.	0.2	1
289	Three for the Price of One: Concomitant $\text{N}$ , $\text{O}$ , and $\text{H}$ Halogen Bonds in the Same Crystal Structure. <i>Molecules</i> , 2022, 27, 7550.	1.7	3
290	DFT Investigation, Hirshfeld Analysis and Molecular Docking of Cu(II) Complex of O-Vanillin Based Ligand. <i>ChemistrySelect</i> , 2022, 7, .	0.7	1

#	ARTICLE	IF	CITATIONS
291	Assessment of solid-liquid equilibrium behavior and thermodynamic analysis of natural plant extracts artemisinin (Form I) in twelve mono-solvents. <i>Journal of Molecular Liquids</i> , 2023, 369, 120975.	2.3	0
292	Polymorphism in carboxamide compounds with high- $Z$ crystal structures. <i>CrystEngComm</i> , 0, , .	1.3	4
293	New charge-transfer complexes of 1,2,5-chalcogenadiazoles with tetrathiafulvalenes. <i>CrystEngComm</i> , 2023, 25, 391-402.	1.3	3
294	Hydrogen-Bonded Chain of Rings Motif in N-(4-Methoxyphenyl)piperazin-1-ium Salts with Benzoate Anions: Supramolecular Assemblies and Their Energy Frameworks. <i>Crystals</i> , 2022, 12, 1807.	1.0	2
295	The investigation of modification in structural flexibility and coordination modes in a solvent free $\beta$ -diketone Cu(II) complex by crystal structure and DFT studies. <i>Polyhedron</i> , 2023, , 116293.	1.0	0
296	Structure, Optical and Magnetic Properties of Two Isomeric 2-Bromomethylpyridine Cu(II) Complexes [Cu(C <sub>6</sub> H <sub>9</sub> NBr) <sub>2</sub> (NO <sub>3</sub> ) <sub>2</sub> ] with Very Different Binding Motives. <i>Molecules</i> , 2023, 28, 731.	1.7	0
297	Charge Transport in Organic Semiconducting Crystals Exhibiting TADF: Insight from Quantum Chemical Calculations. <i>Crystals</i> , 2023, 13, 55.	1.0	1
298	Acid catalyzed one-pot approach towards the synthesis of curcuminoid systems: unsymmetrical diarylidene cycloalkanones, exploration of their single crystals, optical and nonlinear optical properties. <i>RSC Advances</i> , 2023, 13, 4476-4494.	1.7	19
299	Aryl Boronic Acids in Columnar Stacked Co-crystalline Materials: Key Factors Governing the Assembly with Quinones. <i>ChemPhysChem</i> , 0, , .	1.0	0
300	Assessing Solvate Prediction Approaches: A Case of Spironolactone. <i>Crystal Growth and Design</i> , 2023, 23, 832-841.	1.4	4
301	Synthesis, single crystal structure determinations, Hirshfeld surface analysis, crystal voids, interaction energies, and density functional theory studies of functionalized 1,3-thiazoles. <i>Journal of Molecular Structure</i> , 2023, 1281, 135108.	1.8	3
302	Arsenic-Involving Intermolecular Interactions in Crystal Structures: The Dualistic Behavior of As(III) as Electron-Pair Donor and Acceptor. <i>Crystal Growth and Design</i> , 2023, 23, 1033-1048.	1.4	0
303	Searching for Suitable Kojic Acid Coformers: From Cocrystals and Salt to Eutectics. <i>Crystal Growth and Design</i> , 2023, 23, 1874-1887.	1.4	1
304	Elastic and bright assembly-induced luminescent crystals of platinum( $\text{II}$ ) complexes with near-unity emission quantum yield. <i>Dalton Transactions</i> , 0, , .	1.6	0
305	Stability and Mechanical Properties of Darunavir Isostructural Solvates: An Experimental and Computational Study. <i>Crystal Growth and Design</i> , 2023, 23, 2905-2915.	1.4	4
306	SYNTHESIS, CRYSTAL STRUCTURE, SUPRAMOLECULAR ASSEMBLY EXPLORATION BY HIRSHFELD SURFACE ANALYSIS AND COMPUTATIONAL STUDY OF 6-BROMO-2-OXO-2H-CHROMENE-3-CARBONITRILE (BOCC). <i>Journal of Structural Chemistry</i> , 2023, 64, 302-313.	0.3	12
307	Experimental and Computational Study on the Effects of High Pressure on the Crystal Structure of Boron Nitrilotriacetate. <i>Crystal Growth and Design</i> , 2023, 23, 2745-2754.	1.4	1
308	Polymorphism of Butyl Ester of Oleanolic Acid—The Dominance of Dispersive Interactions over Electrostatic. <i>International Journal of Molecular Sciences</i> , 2023, 24, 6572.	1.8	0

#	ARTICLE	IF	CITATIONS
309	Competing and directing interactions in new phosphoramidate/thiophosphoramidate structures: energy considerations and evidence for CH $\cdots$ HC contacts and aliphatic $\cdots$ aromatic stacking. CrystEngComm, 0, , .	1.3	0
310	Synthesis, Crystal Structure, Supramolecular Assembly Inspection by Hirshfeld Surface Analysis and Computational Exploration of 4-Phenyl-6-(p-Tolyl)Pyrimidin-2 (1H)-One (PPTP). Journal of Structural Chemistry, 2023, 64, 437-449.	0.3	15
311	An investigation into the Br $\cdots$ sted acidity of the perfluorinated alkoxy silanes $\{(F_{3})_{3}CO\}_{3}SiH$ and $\{(F_{6})_{5}C_{5}\}_{3}CO\}_{2}Si(Cl)H$ . Dalton Transactions, 2023, 52, 5918-5925.	1.6	2
312	Preparation and Characterization of N-benzyl-2-methyl-4-nitroaniline (BNA) Single Crystals by Physical Vapour Transport (PVT) Technique. Journal of Molecular Structure, 2023, , 135593.	1.8	0
313	Mechanical properties and peculiarities of molecular crystals. Chemical Society Reviews, 2023, 52, 3098-3169.	18.7	48
314	Synthesis, X-ray, DFT, Hirshfeld surface analysis, molecular docking, urease inhibition, antioxidant, cytotoxicity, DNA protection, and DNA binding properties of 5-(tert-butyl)-N-(2,4-dichlorophenyl)-1H-1,2,4-triazol-3-amine. Structural Chemistry, 2024, 35, 7-23.	1.0	1
315	Synthesis, spectroscopic, crystallographic, quantum and molecular docking investigations of cis-4,5-diphenylimidazolidine-2-thione. Journal of Molecular Structure, 2023, 1286, 135633.	1.8	16