

Lokanath Neratur

List of Publications by Year in descending order

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262
papers

1,926
citations

411340

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536525

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all docs

264
docs citations

264
times ranked

1843
citing authors

#	ARTICLE	IF	CITATIONS
1	Design, crystal structure determination, molecular dynamic simulation and MMGBSA calculations of novel p38-alpha MAPK inhibitors for combating Alzheimer's disease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 6114-6127.	2.0	6
2	4-acetamido-3-nitrobenzoic acid - structural, quantum chemical studies, ADMET and molecular docking studies of SARS-CoV2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 6656-6670.	2.0	5
3	Synthesis, crystal structure, anticancer and molecular docking studies of quinolinone-thiazolidinone hybrid molecules. Journal of the Iranian Chemical Society, 2022, 19, 793-808.	1.2	5
4	Design, synthesis, structural analysis and quantum chemical insight into the molecular structure of coumarin derivatives. Molecular Systems Design and Engineering, 2022, 7, 132-157.	1.7	20
5	Analysis of structural conformation and supramolecular self-assembly of novel oxalate-bridged tetranuclear Cu(II) complex by combined crystallographic and computational studies. Journal of Molecular Structure, 2022, 1250, 131658.	1.8	0
6	Structure-property relationship in thioxotriaza-spiro derivative: Crystal structure and molecular docking analysis against SARS-CoV-2 main protease. Journal of Molecular Structure, 2022, 1250, 131746.	1.8	8
7	Study of the crystal structure, H-bonding and noncovalent interactions of novel cocrystal by systematic computational search approach. Journal of Molecular Structure, 2022, 1251, 131936.	1.8	18
8	Synthesis, structural characterization and biological properties of cyclometalated iridium(III) complexes containing 2-methyl-3-((E)-[(quinolin-2-yl)methylidene]amino)quinazolin-4(3H)-one. Inorganica Chimica Acta, 2022, 531, 120735.	1.2	2
9	Synthesis, molecular structure, Hirshfeld surface, energy framework and DFT studies of 1,3,4-oxadiazole derivative. Journal of Molecular Structure, 2022, 1252, 132203.	1.8	17
10	Surface defect-engineered CeO ₂ by ultrasound treatment for superior photocatalytic H ₂ production and water treatment. Catalysis Science and Technology, 2022, 12, 2071-2083.	2.1	16
11	Synthesis and characterization of Zinc(II) complex with ONO donor type new phenylpropanehydrazide based ligand: Crystal structure, Hirshfeld surface analysis, DFT, energy frameworks and molecular docking. Journal of Molecular Structure, 2022, 1255, 132429.	1.8	5
12	Highly Efficient Degradation of Organic Compounds via Bi ₂ O ₃ Semiconductor Under Visible Illumination. IOP Conference Series: Materials Science and Engineering, 2022, 1221, 012040.	0.3	2
13	Enchant O...O interactions in hydrated 6-amino-2-methoxypyrimidin-4(3H)one resembles as water flow in the channel: Crystallographic and theoretical investigations. Journal of Molecular Structure, 2022, 1263, 133098.	1.8	2
14	Structural, Optical, Spectral, Thermal and Third-order NLO Behaviour of 4-Chlorobenzhydrazide Trichloro Acetate Single Crystal. Brazilian Journal of Physics, 2022, 52, 1.	0.7	0
15	Rational design of a 2D TiO ₂ MoO ₃ step-scheme heterostructure for boosted photocatalytic overall water splitting. New Journal of Chemistry, 2022, 46, 9629-9640.	1.4	21
16	Persistent prevalence of non-covalent interaction in pyrimidine containing sulfonamide derivative: A quantum computational analysis. Journal of Molecular Structure, 2022, 1266, 133378.	1.8	18
17	Structural-property relationship in halogen-bonded Schiff base derivative: Crystal structure, computational and SARS-CoV-2 docking studies. Journal of Molecular Structure, 2022, 1265, 133409.	1.8	6
18	existence of H-bond and halogen bond interactions assisted supramolecular architecture A quantum chemical investigation. Journal of Molecular Structure, 2022, 1267, 133476.	1.8	15

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19	Synthesis, characterisation, biological and theoretical studies of novel pyridine derivatives. <i>Molecular Physics</i> , 2022, 120, .	0.8	3
20	N,N'-bis(2-bromobenzylidene)-2,2'-diaminodiphenyldisulfide (BBDD): Insights of crystal structure, DFT, QTAIM, PASS, ADMET and molecular docking studies. <i>Journal of Molecular Structure</i> , 2022, 1268, 133657.	1.8	5
21	Synthesis, structure, quantum computational and biological studies of novel thiophene derivatives. <i>Journal of Molecular Structure</i> , 2021, 1229, 129587.	1.8	5
22	Synthesis, spectral characterization, crystal structure and theoretical investigation of (E)-3-(4-bromothiophen-2-yl)-1-(5-bromothiophen-2-yl)prop-2-en-1-one. <i>Chemical Data Collections</i> , 2021, 31, 100587.	1.1	19
23	Hydroxyacetone derived N4-methyl substituted thiosemicarbazone: Syntheses, crystal structures and spectroscopic characterization of later first-row transition metal complexes. <i>Journal of Molecular Structure</i> , 2021, 1224, 129055.	1.8	4
24	Thermal, optical, etching, structural studies and theoretical calculations of [1-(2,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 547 Td (5-Dichloro Molecular Structure, 2021, 1224, 129077.	1.8	11
25	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
26	Synthesis, characterization, crystal structure, Hirshfeld surface analysis, antioxidant properties and DFT calculations of a novel pyrazole derivative: Ethyl 1-(2,4-dimethylphenyl)-3-methyl-5-phenyl-1H-pyrazole-4-carboxylate. <i>Journal of Molecular Structure</i> , 2021, 1226, 129350.	1.8	19
27	Molecular structure, Hirshfeld surface and density functional theoretical analysis of a NLO active chalcone derivative single crystal. A quantum chemical approach. <i>Journal of Molecular Structure</i> , 2021, 1228, 129739.	1.8	35
28	Environmentally benign synthesis of substituted pyrazoles as potent antioxidant agents, characterization and docking studies. <i>Journal of the Iranian Chemical Society</i> , 2021, 18, 479-493.	1.2	2
29	Post-synthetic modification of supramolecular assemblies of β^2 -diketonato Cu(II) complexes: comparing and contrasting the molecular topology by crystal structure and quantum computational studies. <i>CrystEngComm</i> , 2021, 23, 4344-4369.	1.3	14
30	Synthesis, Crystal Structure, Hirshfeld, DFT, Quorum Sensing Inhibition and Molecular Docking Studies of N'-{(E)-[3-(3,5-Difluorophenyl)1H-pyrazol-4-yl]methylidene}-4-methoxybenzohydrazide. <i>Asian Journal of Chemistry</i> , 2021, 33, 1796-1804.	0.1	3
31	Magnetic recyclable β -Fe ₂ O ₃ /Co ₃ O ₄ nanocomposite with a dual Z-scheme charge transfer pathway for quick photo-Fenton degradation of organic pollutants. <i>Catalysis Science and Technology</i> , 2021, 11, 3084-3097.	2.1	32
32	Square Planar <i>trans</i> -[N ₂ O ₂] Cu(II) Complex: Synthesis, Crystal Structure, Hirshfeld Surface, DFT, Antimicrobial and Docking Studies. <i>ChemistrySelect</i> , 2021, 6, 6240-6255.	0.7	21
33	Cis and trans isomers of 1-(5-bromothiophen-2-yl)-3-(10-chloroanthracen-9-yl)prop-2-en-1-one: Synthesis and characterization. <i>Journal of Molecular Structure</i> , 2021, 1236, 130228.	1.8	8
34	Construction of Bi ₂ S ₃ /TiO ₂ /MoS ₂ S-scheme Heterostructure with a Switchable Charge Migration Pathway for Selective CO ₂ Reduction. <i>Solar Rrl</i> , 2021, 5, 2100501.	3.1	27
35	Enhanced photo-Fenton activity over a sunlight-driven ignition synthesized β -Fe ₂ O ₃ -Fe ₃ O ₄ /CeO ₂ heterojunction catalyst enriched with oxygen vacancies. <i>Journal of Molecular Liquids</i> , 2021, 335, 116186.	2.3	31
36	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

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37	Synthesis, crystal structure characterization, Hirshfeld surface analysis, and Quantum chemical computations of Ethyl 5-(thiophene-2-carbonyl)thiazole-4-carboxylate. <i>Journal of Molecular Structure</i> , 2021, 1242, 130747.	1.8	7
38	4,4,4-trifluoro-1-phenylbutane-1,3-dione metal [Cu(II) and Ni(II)] complexes as an superlative antibacterial agent against MRSA: Synthesis, structural quantum-chemical and molecular docking studies. <i>Journal of Molecular Structure</i> , 2021, 1243, 130774.	1.8	11
39	Synthesis, Crystal Structure, Biological Evaluation, DFT Calculations and Third Order Nonlinear Optical Studies of Pyrazolines. <i>Journal of Molecular Structure</i> , 2021, 1243, 130780.	1.8	5
40	Towards the Synthesis of Imidazopyridine Derivatives: Characterization, Single Crystal XRD, Hirshfeld Analysis, and Biological Evaluation. <i>ChemistrySelect</i> , 2021, 6, 843-851.	0.7	4
41	Fluorophore Tagged Mixed Ligand Copper(II) Complexes: Synthesis, Structural Characterization, Protein Binding, DNA Cleavage and Anticancer Activity. <i>ChemistrySelect</i> , 2021, 6, 12666-12676.	0.7	2
42	Synthesis, characterization and hydrogen bonding attributes of halogen bonded O-hydroxy Schiff bases: Crystal structure, Hirshfeld surface analysis and DFT studies. <i>Journal of Molecular Structure</i> , 2020, 1202, 127238.	1.8	17
43	Synthesis, characterization, crystal structure, Hirshfeld surface analysis and DFT calculations of two novel pyrrole derivatives. <i>Journal of Molecular Structure</i> , 2020, 1199, 127033.	1.8	5
44	4,4,4-Trifluoro-1-(thiophen-2-yl)butane-1,3-dione nickel(II) complex: Synthesis, structure, quantum chemical and DNA binding studies. <i>Journal of Molecular Structure</i> , 2020, 1202, 127277.	1.8	8
45	Structural and optical characterization of novel nitro substituted D-π-A-π type chalcone single crystal showing second-order and third-order nonlinear optical properties. <i>Physica B: Condensed Matter</i> , 2020, 580, 411830.	1.3	11
46	Understanding the Formation of Novel Hydrated Gallic Acid-Creatinine Molecular Salt: Crystal Structure, Hirshfeld Surface and DFT Studies. <i>Journal of Chemical Crystallography</i> , 2020, 50, 410-421.	0.5	5
47	Design and synthesis of coumarin-triazole hybrids: biocompatible anti-diabetic agents, in silico molecular docking and ADME screening. <i>Heliyon</i> , 2020, 6, e05290.	1.4	19
48	Solvent induced mononuclear and dinuclear mixed ligand Cu(II) complex: structural diversity, supramolecular packing polymorphism and molecular docking studies. <i>New Journal of Chemistry</i> , 2020, 44, 18048-18068.	1.4	17
49	Synthesis, Characterization, Crystallographic Studies of 5-Acetyl-8-hydroxyquinoline and Their Chalcone Derivatives. <i>Asian Journal of Chemistry</i> , 2020, 32, 1609-1613.	0.1	0
50	Synthesis, structural characterization and biological properties of cyclometalated iridium(III) complexes containing [1,2,5]-thiadiazolo-[3,4-f]-[1,10]-phenanthroline. <i>New Journal of Chemistry</i> , 2020, 44, 17442-17452.	1.4	2
51	A solid state analysis of metformin picrate salt. <i>Chemical Data Collections</i> , 2020, 30, 100577.	1.1	2
52	Solid state and Computational studies of Ambroxol hydrochloride drug. <i>Chemical Data Collections</i> , 2020, 27, 100377.	1.1	3
53	Fluorine substituted thiomethyl pyrimidine derivatives as efficient inhibitors for mild steel corrosion in hydrochloric acid solution: Thermodynamic, electrochemical and DFT studies. <i>Journal of Molecular Liquids</i> , 2020, 311, 113311.	2.3	14
54	N-(4-bromobenzylidene)-2,3-dihydrobenzo[b][1,4]dioxin-6-amine: Synthesis, crystal structure, docking and in-vitro inhibition of PLA2. <i>Journal of Molecular Structure</i> , 2020, 1218, 128441.	1.8	6

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55	Cu^{2+} -Catalyzed transformation of <i>o</i> -aminobenzamide to <i>o</i> -ureidobenzonitrile using isothiocyanates. <i>Organic and Biomolecular Chemistry</i> , 2020, 18, 2678-2684.	1.5	9
56	XRD/DFT/HSA-interactions in Cu(II)Cl/phen/ β -diketonato complex: Physicochemical, solvatochromism, thermal and DNA-binding analysis. <i>Journal of Molecular Structure</i> , 2020, 1210, 128000.	1.8	21
57	Synthesis of novel Cubane $[\text{Ni}_4(\text{O}^\ominus\text{O})_4(\text{OCH}_3)_4(\text{OOH})_4]$ cluster: XRD/HSA-interactions, spectral, DNA-binding, docking and subsequent thermolysis to NiO nanocrystals. <i>Journal of Molecular Liquids</i> , 2020, 315, 113756.	2.3	15
58	Protection of mild steel corrosion by three new quinazoline derivatives: experimental and DFT studies. <i>Surfaces and Interfaces</i> , 2020, 18, 100446.	1.5	12
59	Synthesis, Characterization and Anticancer Studies of Rh(I), Rh(III), Pd(II) and Pt(II) Complexes Bearing A Dithiooxamide Ligand. <i>ChemistrySelect</i> , 2020, 5, 810-817.	0.7	3
60	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
61	A third-order nonlinear optical single crystal of 3,4-dimethoxy-substituted chalcone derivative with high laser damage threshold value: a potential material for optical power limiting. <i>Journal of Materials Science: Materials in Electronics</i> , 2020, 31, 9133-9150.	1.1	31
62	Synthesis of novel spirobibenzopyrans as potent anticancer leads inducing apoptosis in HeLa cells. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 127199.	1.0	6
63	A long-chain based bromo and methyl substituted chalcone derivatives; experimental and theoretical approach on nonlinear optical single crystals. <i>Materials Research Express</i> , 2020, 7, 055101.	0.8	15
64	Synthesis, characterization, crystal structure and theoretical simulation of novel ethyl 2-(7-hydroxy-4-methyl-2-oxo-2H-chromen-3-yl)acetate. <i>Chemical Data Collections</i> , 2020, 28, 100425.	1.1	4
65	Synthesis, characterization, structural exploration and quantum chemical calculations of (E)-8-(1-((4-aminobenzyl)imino)ethyl)-7-hydroxy-4-methyl-coumarin. <i>Oriental Journal of Chemistry</i> , 2020, 37, 484-492.	0.1	0
66	Synthesis, Structural Characterization and Hirshfeld Surface Analysis of Mixed Ligand Copper(II) Complex. <i>Chemical Data Collections</i> , 2020, 28, 100374.	1.1	1
67	Crystal Structure, Hirshfeld Surface and Frontier Molecular Orbital Analyses of N-[2-(trifluoromethyl)phenyl]succinamic Acid. <i>Asian Journal of Chemistry</i> , 2020, 32, 3179-3185.	0.1	0
68	Design, Synthesis, and Biological Evaluation of (E)-N ¹ -((1-Chloro-3,4-Dihydronaphthalen-2-yl)Methylene)Benzohydrazide Derivatives as Anti-prostate Cancer Agents. <i>Frontiers in Chemistry</i> , 2019, 7, 474.	1.8	17
69	Synthesis, characterization crystal and molecular structure studies of 5-(3-Methylbenzoyl)-4-methyl-1,3,4,5-tetrahydro-2H-1,5-benzodiazepin-2-one: Hirshfeld surface analysis and DFT calculations. <i>Chemical Data Collections</i> , 2019, 24, 100292.	1.1	2
70	Synthesis, crystal structure and molecular docking studies of novel 2-(4-benzoylpiperazin-1-yl)quinoline-3-carbaldehyde. <i>Chemical Data Collections</i> , 2019, 24, 100282.	1.1	2
71	Cocrystals of Gallic Acid with Urea and Propionamide: Supramolecular Structures, Hirshfeld Surface Analysis, and DFT Studies. <i>Crystal Research and Technology</i> , 2019, 54, 1900016.	0.6	13
72	One-dimensional copper(II) coordination polymers based on 1,3-bis(pyridin-4-yl)propane and diimine ligands. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019, 75, 496-503.	0.2	1

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73	Solvent induced 4,4,4-trifluoro-1-(2-naphthyl)-1,3-butanedione Cu(II) complexes: Synthesis, structure, DFT calculation and biocidal activity. <i>Polyhedron</i> , 2019, 168, 127-137.	1.0	9
74	Crystal interactions, computational, spectral and thermal analysis of (E)-N'-(thiophen-2-ylmethylene)isonicotinohydrazide as O-N-S-tridentate schiff base ligand. <i>Journal of Molecular Structure</i> , 2019, 1185, 290-299.	1.8	3
75	Synthesis, crystal structure and 3D energy frameworks of ethyl 2-[5-nitro-2-oxopyridine-1(2H)-yl] acetate: Hirshfeld surface analysis and DFT calculations. <i>Chemical Data Collections</i> , 2019, 20, 100195.	1.1	18
76	SiCl ₄ mediated one-pot synthesis of novel spirobibenzopyrans as potent anticancer agents. <i>New Journal of Chemistry</i> , 2019, 43, 4669-4673.	1.4	5
77	Pyridine solvated dioxouranium complex with salen ligand: Synthesis, characterization and luminescence properties. <i>Journal of Saudi Chemical Society</i> , 2019, 23, 636-641.	2.4	5
78	Design, synthesis and biological evaluation of 2-(phenoxymethyl)-5-phenyl-1,3,4-oxadiazole derivatives as anti-breast cancer agents. <i>European Journal of Medicinal Chemistry</i> , 2019, 168, 1-10.	2.6	45
79	Synthesis, Optical and Thermal Properties of 1-(4-Methoxyphenyl)-2-((5-(1-(Naphthalene-1-Yloxy)Ethyl)-[1,3,4]-Oxadiazol-2-Yl)Sulfanyl)Ethanoic Acid - A Novel Heterocyclic Compound. <i>Materials Science Forum</i> , 2019, 962, 10-16.	0.3	0
80	Design, structural, H ¹ H ¹³ C supramolecular interactions and computational investigations of Cd(N ⁺ ON ³)X ₂ complexes based on an asymmetrical 1,2-diamine ligand: physicochemical and thermal analysis. <i>Journal of Coordination Chemistry</i> , 2019, 72, 3285-3297.	0.8	4
81	X-ray crystal structure, Hirshfeld surface analysis, DFT and electronic properties of (E)-4-chloro-N ² -(2,4-dihydroxybenzylidene) benzohydrazide. <i>Chemical Data Collections</i> , 2019, 19, 100174.	1.9	4
82	Impact of Barium cationic mixing on Cadmium and Strontium oxalate crystals. <i>Materials Research Express</i> , 2019, 6, 035506.	0.8	1
83	Excited state hydrogen atom transfer in micro-solvated dicoumarol: A TDDFT/EFP1 study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 208, 325-330.	2.0	1
84	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
85	3D energy framework of a benzophenone acidic dimer. <i>Chemical Data Collections</i> , 2019, 19, 100168.	1.1	4
86	<i>N</i> -[2-(Trifluoromethyl)phenyl]maleamic acid: crystal structure and Hirshfeld surface analysis. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019, 75, 766-769.	0.2	1
87	Synthesis of cocrystals/salts of flucytosine: Structure and stability. <i>New Journal of Chemistry</i> , 2018, 42, 5433-5446.	1.4	20
88	Synthesis, spectral characterization and X-ray crystal structure studies of 3-(benzo[d][1,3]dioxol-5-yl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazole-1-carboxamide: Hirshfeld surface, DFT and thermal analysis. <i>Journal of Molecular Structure</i> , 2018, 1161, 285-298.	1.8	55
89	Synthesis, spectral and X-ray crystal structure of 3-(3-methoxyphenyl)-5-(3-methylthiophen-2-yl)-4,5-dihydro-1H-pyrazole-1-carboxamide: Hirshfeld surface, DFT calculations and thermo-optical studies. <i>Chemical Data Collections</i> , 2018, 13-14, 40-59.	1.1	15
90	Synthesis, crystal structure and excellent photoluminescence properties of copper (II) and cobalt (II) complexes with Bis(1[(4-butylphenyl)imino]methyl naphthalen-2-ol) Schiff base. <i>Journal of Science: Advanced Materials and Devices</i> , 2018, 3, 51-58.	1.5	9

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91	Direct Aerobic Strategy for Synthesis of Imines via Alcohols and Amines Promoted by Ruthenium(II) (η^6 -p-cymene) Complexes. <i>ChemistrySelect</i> , 2018, 3, 1561-1568.	0.7	13
92	Molecular structure, Hirshfeld surface analysis, theoretical investigations and nonlinear optical properties of a novel crystalline chalcone derivative: (E)-1-(5-bromothiophen-2-yl)-3-(p-tolyl)prop-2-en-1-one. <i>Journal of Molecular Structure</i> , 2018, 1161, 9-17.	1.8	13
93	Growth, Characterization and Conductivity of Chromium Mixed Cadmium Oxalate Crystals. <i>Crystal Research and Technology</i> , 2018, 53, 1700261.	0.6	1
94	Crystal packing analysis of 1-(3,4-dimethoxyphenyl)-3-(4-bromophenyl)prop-2-en-1-one exhibiting a putative halogen bond C-Br \cdots O. <i>Journal of Molecular Structure</i> , 2018, 1156, 216-223.	1.8	17
95	Regular square planer bis-(4,4,4-trifluoro-1-(thiophen-2-yl)butane-1,3-dione)/copper(II) complex: Trans/cis-DFT isomerization, crystal structure, thermal, solvatochromism, hirshfeld surface and DNA-binding analysis. <i>Journal of Molecular Structure</i> , 2018, 1157, 69-77.	1.8	23
96	Synthesis, spectral studies, crystal structure and molecular docking of ethyl 6-[(4-methyl-2-oxo-2H-chromen-7-yl)oxy]hexanoate. <i>Chemical Data Collections</i> , 2018, 13-14, 17-27.	1.1	0
97	Synthesis, characterization, crystal structure and quantum chemical investigations of three novel coumarin-benzenesulfonohydrazide derivatives. <i>Journal of Molecular Structure</i> , 2018, 1158, 26-38.	1.8	19
98	Synthesis, structural exploration, spectral and combinatorial analysis of racemic-3-isobutyl-5-phenyl-5-(pyridin-4-yl)imida-zolidine-2,4-dione: Comparison between experimental and DFT calculations. <i>Journal of Molecular Structure</i> , 2018, 1167, 215-226.	1.8	31
99	Structural elucidation and Hirshfeld surface analysis of a novel pyrazole derivative: 3-(Benzo[d][1,3]dioxol-5-yl)-1-(3-chlorophenyl)-5-(2,4-dichlorophenyl)-4,5-dihydro-1H-pyrazole. <i>Chemical Data Collections</i> , 2018, 15-16, 89-96.	1.1	5
100	Synthesis of rhodamine based organic nanorods for efficient chemosensor probe for Al (III) ions and its biological applications. <i>Sensors and Actuators B: Chemical</i> , 2018, 254, 795-804.	4.0	65
101	Synthesis, spectra and X-ray crystallography of dipyridin-2-ylmethanone oxime and its CuX ₂ (oxime) ₂ complexes: Thermal, Hirshfeld surface and DFT analysis. <i>Journal of Molecular Structure</i> , 2018, 1154, 619-625.	1.8	14
102	Enzymatic Production of Non-Natural Nucleoside-5'-Monophosphates by a Thermostable Uracil Phosphoribosyltransferase. <i>ChemCatChem</i> , 2018, 10, 439-448.	1.8	12
103	p-halo N4-phenyl substituted thiosemicarbazones: Crystal structure, supramolecular architecture, characterization and bio-assay of their Co(III) and Ni(II) complexes. <i>Journal of Molecular Structure</i> , 2018, 1156, 115-126.	1.8	18
104	Synthesis, characterization and single crystal structures of chiral Schiff base and its tetranuclear palladium complex with Pd O Pd bridging and Pd Pd bonds. <i>Journal of Molecular Structure</i> , 2018, 1156, 301-307.	1.8	6
105	Crystal structures of 2-aminopyridine citric acid salts: C ₅ H ₇ N ₂ O ₇ and 3C ₅ H ₇ N ₂ O ₇ · C ₆ H ₅ O ₇ . <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018, 74, 1111-1116.	0.2	4
106	Phosphorescent cyclometalated iridium(III) complexes: synthesis, photophysics, DNA interaction, cellular internalization, and cytotoxic activity. <i>New Journal of Chemistry</i> , 2018, 42, 16846-16854.	1.4	11
107	Synthesis, structural, thermal and Hirshfeld surface analysis of novel [1,2,4]triazolo[3,4-b][1,3,4]thiadiazine carrying 1,4-benzothiazine-3-one moiety. <i>AIP Conference Proceedings</i> , 2018, , .	0.3	0
108	Synthesis, crystal structure and Hirshfeld surfaces of 1-(3,4-dimethoxyphenyl)-3-(3-hydroxyphenyl)prop-2-en-1-one. <i>Chemical Data Collections</i> , 2018, 15-16, 153-160.	1.1	7

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109	Synthesis, crystal structure, NLO and Hirshfeld surface analysis of 1,2,3-triazolyl chalcone single crystal. AIP Conference Proceedings, 2018, , .	0.3	0
110	3D energy frameworks of a potential nutraceutical. Journal of Molecular Structure, 2018, 1173, 300-306.	1.8	19
111	Design, synthesis and spectroscopic and crystallographic characterisation of novel functionalized pyrazole derivatives: biological evaluation for their cytotoxic, angiogenic and antioxidant activities. Research on Chemical Intermediates, 2018, 44, 5635-5652.	1.3	12
112	Ultrasound-assisted synthesis of two novel [CuBr(diamine)2·H ₂ O]Br complexes: Solvatochromism, crystal structure, physicochemical, Hirshfeld surface thermal, DNA/binding, antitumor and antibacterial activities. Ultrasonics Sonochemistry, 2018, 48, 1-10.	3.8	29
113	Synthesis, spectral characterization, crystal and molecular structure studies of 5-(5-bromo-2-thienyl)-1-(phenyl)-3-phenyl-2-pyrazoline. Chemical Data Collections, 2018, 17-18, 132-137.	1.1	1
114	Synthesis, single crystal, structure and Hirshfeld surface analysis of (E)-4-toluic- α -(2,4-dihydroxy-benzylidene) benzohydrazide. Chemical Data Collections, 2018, 17-18, 169-177.	1.1	7
115	Amberlyst-15 catalyzed synthesis of novel thiophene-pyrazoline derivatives: spectral and crystallographic characterization and anti-inflammatory and antimicrobial evaluation. Research on Chemical Intermediates, 2018, 44, 6453-6468.	1.3	11
116	Three novel coumarin-benzenesulfonylhydrazide hybrids: Synthesis, characterization, crystal structure, Hirshfeld surface, DFT and NBO studies. Journal of Molecular Structure, 2018, 1171, 564-577.	1.8	26
117	Design and Amberlyst-15 mediated synthesis of novel thienyl-pyrazole carboxamides that potently inhibit Phospholipase A2 by binding to an allosteric site on the enzyme. Bioorganic Chemistry, 2018, 80, 444-452.	2.0	14
118	Synthesis, molecular structure and Hirshfeld surface analysis of (4-methoxyphenyl)[2-(methylsulfanyl)thiophen-3-yl]methanone. Acta Crystallographica Section E: Crystallographic Communications, 2018, 74, 1800-1803.	0.2	0
119	Design, synthesis and biological evaluation of 2-(4-phenylthiazol-2-yl) isoindoline-1,3-dione derivatives as anti-prostate cancer agents. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 1199-1204.	1.0	25
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121	Crystal structure and Hirshfeld surface analysis of (E)-Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 262 Td (-)-2-(1-(2-phenylhydrazono	1.1	1
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