

Joel T Mague

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405
papers

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ext. papers

2,833
ext. citations

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avg, IF

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L-index

#	Paper	IF	Citations
405	Diastereoselective synthesis of polysubstituted tetrahydropyrans and thiacyclohexanes via indium trichloride mediated cyclizations. <i>Journal of Organic Chemistry</i> , 2001 , 66, 739-47	4.2	100
404	Rationalization of Noncovalent Interactions within Six New MII/8-Aminoquinoline Supramolecular Complexes (MII = Mn, Cu, and Cd): A Combined Experimental and Theoretical DFT Study. <i>Crystal Growth and Design</i> , 2015 , 15, 1351-1361	3.5	88
403	Tetranuclear Rhodium(I) Macrocycle Containing Cyclodiphosphazane [Rh ₂ (EtCl) ₂ (CO) ₂ {(tBuNP(OC ₆ H ₄ OMe-o)) ₂ -P] ₂ and Its Reversible Conversion into trans-[Rh(CO)Cl{(tBuNP(OC ₆ H ₄ OMe-o)) ₂ -P] ₂ . <i>Organometallics</i> , 2005 , 24, 3780-3783	3.8	66
402	Novel Carbocycle Enlargement in Aqueous Medium. <i>Journal of the American Chemical Society</i> , 1996 , 118, 4216-4217	16.4	62
401	On the importance of tetrel bonding interactions in lead(II) complexes with (iso)nicotinohydrazide based ligands and several anions. <i>Dalton Transactions</i> , 2016 , 45, 10708-16	4.3	60
400	Crystal engineering with coordination compounds of NiII, CoII, and CrIII bearing dipicolinic acid driven by the nature of the noncovalent interactions. <i>CrystEngComm</i> , 2014 , 16, 5352	3.3	44
399	Facile reductive elimination of ethane from strained dimethylpalladium(II) complexes. <i>Journal of the American Chemical Society</i> , 2001 , 123, 4081-2	16.4	43
398	Thioether-functionalized ferrocenyl-bis(phosphonite), Fe{(C ₅ H ₄)P(-OC ₁₀ H ₆ (micro-S)C ₁₀ H ₆ O-)} ₂ : synthesis, coordination behavior, and application in Suzuki-Miyaura cross-coupling reactions. <i>Inorganic Chemistry</i> , 2007 , 46, 10268-75	5.1	40
397	Synthetic and structural studies of the coordination behavior of 2-pyridylbis(diphenylphosphino)methane. <i>Inorganic Chemistry</i> , 2001 , 40, 1962-71	5.1	37
396	Synthesis and derivatization, structures and transition metal chemistry of a new large bite bis(phosphinite) derived from bis(2-hydroxy-1-naphthyl)methane. <i>Dalton Transactions RSC</i> , 2002 , 4617-4621		36
395	Crystal engineering with coordination compounds of 2,6-dicarboxy-4-hydroxypyridine and 9-aminoacridine fragments driven by different nature of the face-to-face π-stacking. <i>CrystEngComm</i> , 2014 , 16, 1359-1377	3.3	33
394	Novel Co(II) and Cu(II) coordination complexes constructed from pyrazole-acetamide: Effect of hydrogen bonding on the self assembly process and antioxidant activity. <i>Journal of Inorganic Biochemistry</i> , 2019 , 191, 21-28	4.2	30
393	On the importance of non covalent interactions in the structure of coordination Cu(II) and Co(II) complexes of pyrazine- and pyridine-dicarboxylic acid derivatives: experimental and theoretical views. <i>CrystEngComm</i> , 2014 , 16, 6149-6158	3.3	29
392	Hierarchical Assembly of Organic/Inorganic Building Molecules with π-Interactions. <i>Advanced Functional Materials</i> , 2008 , 18, 1526-1535	15.6	29
391	Synthesis, spectroscopic characterization, crystal structure, DFT, molecular docking and in vitro antibacterial potential of novel quinoline derivatives. <i>Journal of Molecular Structure</i> , 2020 , 1209, 127940 ³⁻⁴		28
390	Synthesis, structural and molecular characterization of 2,2-diphenyl-2H,3H,5H,6H,7H-imidazo[2,1-b][1,3]thiazin-3-one. <i>Journal of Molecular Structure</i> , 2019 , 1197, 369-376	3.4	28
389	Two Triazole-Based Phosphine Ligands Prepared via Temperature-Mediated Li/H Exchange: Cu(I) and Au(I) Complexes and Structural Studies. <i>Inorganic Chemistry</i> , 2016 , 55, 8514-26	5.1	27

388	Dodecaphenyltetracene. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 2831-2833	16.4	27
387	Curcumin and derivatives. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2004 , 60, o608-10		26
386	Importance of polarization assisted/resonance assisted hydrogen bonding interactions and unconventional interactions in crystal formations of five new complexes bearing chelidamic acid through a proton transfer mechanism. <i>RSC Advances</i> , 2015 , 5, 72923-72936	3.7	25
385	Structural scope of six new layered to pillar-layered hybrid inorganic-organic networks bearing [BW12O40]5- and lanthanoid-cluster; database study toward ligand role in assemblies. <i>CrystEngComm</i> , 2016 , 18, 6724-6737	3.3	25
384	Synthesis, crystal structure, DFT, molecular dynamics simulation and evaluation of the anticorrosion performance of a new pyrazolotriazole derivative. <i>Journal of Molecular Structure</i> , 2019 , 1176, 290-297	3.4	23
383	Hydrothermal synthesis, X-ray structure and DFT and magnetic studies of a (H2SiW12O40)(2-) based one-dimensional linear coordination polymer. <i>Dalton Transactions</i> , 2015 , 44, 8824-32	4.3	22
382	Synthesis of a novel phenytoin derivative: Crystal structure, Hirshfeld surface analysis and DFT calculations. <i>Journal of Molecular Structure</i> , 2020 , 1205, 127630	3.4	22
381	Diamondoid-Type Copper Coordination Polymers Containing Soft Cyclodiphosphazane Ligands. <i>Inorganic Chemistry</i> , 2015 , 54, 6063-5	5.1	21
380	Synthesis, transition metal chemistry and catalytic reactions of ferrocenylbis(phosphonite), [Fe{C5H4P(OC6H3(OMe-o)(C3H5-p))2}2]. <i>Dalton Transactions</i> , 2013 , 42, 11695-708	4.3	20
379	Cyclodiphosphazane cis-{(o-MeOC6H4O)P(EntBu)}2 as a Bridging Bidentate Ligand: Synthesis, Structures of Heterometallic Complexes, and Halogen Exchange Between RhIII and CuX (X = Br, I). <i>European Journal of Inorganic Chemistry</i> , 2007 , 2007, 4988-4997	2.3	20
378	Synthesis, crystal structure, spectroscopic characterization, Hirshfeld surface analysis, molecular docking studies and DFT calculations, and antioxidant activity of 2-oxo-1,2-dihydroquinoline-4-carboxylate derivatives. <i>Journal of Molecular Structure</i> , 2019 , 1188, 255-268	3.4	19
377	Tribenzodecacyclene and hexabenzodecacyclene. <i>Journal of Organic Chemistry</i> , 2015 , 80, 4824-7	4.2	19
376	Self-Assembled Cyclophane-Type Copper(I) Complexes of 2,4,6-Tris(diphenylphosphino)-1,3,5-triazine and Their Catalytic Application. <i>Inorganic Chemistry</i> , 2015 , 54, 10985-92	5.1	19
375	Synthesis and structure elucidation of novel salophen-based dioxo-uranium(VI) complexes: In-vitro and in-silico studies of their DNA/BSA-binding properties and anticancer activity. <i>European Journal of Medicinal Chemistry</i> , 2017 , 140, 172-186	6.8	19
374	Potential antidiabetic activity and molecular docking studies of novel synthesized 3,6-dimethyl-5-oxo-pyrido[3,4-f][1,2,4]triazepino[2,3-a]benzimidazole and 10-amino-2-methyl-4-oxo-pyrimido[1,2-a]benzimidazole derivatives. <i>Journal of Molecular Modeling</i> , 2018 , 24, 179	2	19
373	Sterically Demanding Phosphines with 2,6-Dibenzhydryl-4-methylphenyl Core: Synthesis of Ru, Pd, and Pt Complexes, and Structural and Catalytic Studies. <i>Inorganic Chemistry</i> , 2018 , 57, 7468-7480	5.1	18
372	Radicals organized by disk shaped aromatics [polymorphism and co-crystals that tune inter-electron exchange. <i>CrystEngComm</i> , 2012 , 14, 1515-1526	3.3	18
371	A hybrid terpyridine-based bis(diphenylphosphino)amine ligand, terpy-CHN(PPh): synthesis, coordination chemistry and photoluminescence studies. <i>Dalton Transactions</i> , 2016 , 45, 18434-18437	4.3	17

370	Tris(4-methylpiperazin-1-yl)phosphane, P(NC ₄ H ₈ NMe) ₃ : Synthesis, Structural Studies, Group 10 and 11 Metal Complexes and Catalytic Investigations. <i>European Journal of Inorganic Chemistry</i> , 2008 , 2008, 596-604	2.3	17
369	Synthesis, Thermal Behavior, and Structure of Hexaaquanickel(II) Chloro(hydrogenethylenediaminetetraacetato)ferrate(III): A Molecular Precursor for Stoichiometric Nickel Ferrite. <i>Chemistry of Materials</i> , 1996 , 8, 650-655	9.6	17
368	Mono-, Bi-, Tri- and Tetranuclear Palladium(II), Copper(I), and Gold(I) Complexes of Morpholine- and N-Methylpiperazine-Functionalized Cyclodiphosph(III)azans, cis-[(tBuN) ₂ P(NC ₄ H ₈ X) ₂] (X = O, NMe). <i>European Journal of Inorganic Chemistry</i> , 2010 , 2010, 4201-4210	2.3	16
367	Two new copper and nickel complexes of pyridine-2,6-dicarboxylic acid N-oxide and their proton transferred salts: Solid state and DFT insights. <i>Inorganica Chimica Acta</i> , 2015 , 438, 135-145	2.7	15
366	An Exceptionally Close, Non-Bonded Hydrogen-Hydrogen Contact with Strong Through-Space Spin-Spin Coupling. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 2244-2247	16.4	15
365	The Hairpin Furans: Easily Prepared Hybrids of Helicenes and Twisted Acenes. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 13957-60	16.4	15
364	Coordination of bis(azol-1-yl)methane-based bisphosphines towards Ru, Rh, Pd and Pt: synthesis, structural and catalytic studies. <i>Dalton Transactions</i> , 2016 , 46, 227-241	4.3	14
363	A newly synthesized nitrogen-rich derivative of bicyclic quinoxaline—Structural and conceptual DFT reactivity study. <i>Journal of Physical Organic Chemistry</i> , 2020 , 33, e4055	2.1	14
362	Co(III) and Fe(III) complexes of Schiff bases derived from 2,4-dihydroxybenzaldehyde S-allyl-isothiosemicarbazonehydrobromide. <i>Journal of Coordination Chemistry</i> , 2013 , 66, 3915-3925	1.6	14
361	Mononuclear, Tetranuclear and 1D Polymeric Copper(I) Complexes of Large Bite Bisphosphines Containing Nitrogen and Oxygen Donor Atoms. <i>European Journal of Inorganic Chemistry</i> , 2015 , 2015, 3949-3958	2.3	14
360	Synthesis and Spectroscopic and Thermal Decomposition Studies of Alkali Metal Salts of 2-Oximidopropionate. <i>Inorganic Chemistry</i> , 1997 , 36, 2656-2661	5.1	14
359	2-pyridylbis(diphenylphosphino)methane chemistry. Synthesis and structures of [Cu(μ ₂ -(Ph ₂ P) ₂ HC ₅ H ₄ N)(THF)] ₂ (BF ₄) ₂ and [Ni(Ph ₂ PCH ₂ C ₅ H ₄ N) ₂]-[NiCl ₄] ₂ ·0.85CH ₂ Cl ₂ and [Ni(Ph ₂ PCH ₂ C ₅ H ₄ N) ₂]-[NiCl ₄] ₂ ·0.85CH ₂ Cl ₂ . <i>Journal of Chemical Crystallography</i> , 1997 , 27, 603-608	0.5	14
358	Synthesis, X-ray characterization and DFT study of a novel Fe(III)–pyridine-2,6-dicarboxylic acid N-oxide complex with unusual coordination mode. <i>Inorganica Chimica Acta</i> , 2016 , 449, 44-51	2.7	14
357	Surface-grafted lanthanoid complexes of the tungstosilicate polyanion [SiWO]: a synthetic, structural and computational investigation. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018 , 74, 1300-1309	0.8	14
356	Dodecaphenyltetracene. <i>Angewandte Chemie</i> , 2019 , 131, 2857-2859	3.6	13
355	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	3.4	13
354	Synthesis and antibacterial activity of new 1,2,3-triazolymethyl-2H-1,4-benzothiazin-3(4H)-one derivatives. <i>Chemistry Central Journal</i> , 2018 , 12, 123		13
353	HSA-interaction studies of uranyl complexes of alkyl substituted isothiosemicarbazone. <i>Journal of Molecular Structure</i> , 2019 , 1193, 53-61	3.4	12

352	Solvent induced supramolecular polymorphism in Cu(II) coordination complex built from 1,2,4-triazolo[1,5-a]pyrimidine: Crystal structures and anti-oxidant activity. <i>Journal of Inorganic Biochemistry</i> , 2020 , 208, 111092	4.2	12
351	Synthesis of a tert-butyl substituted bis(silirane) and comparison with its methyl and phenyl analogs. <i>Journal of Organometallic Chemistry</i> , 2011 , 696, 1957-1963	2.3	12
350	Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of 3-((2,2-((2,4-dichlorophenyl)methylidene)-3-oxo-3,4-dihydro-2-1,4-benzothiazin-4-yl)propyl)propane-nitrile. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019 , 75, 721-727	0.7	12
349	1-Benzyl-3-methylquinoxalin-2(1H)-one. <i>IUCrData</i> , 2018 , 3,	0.7	12
348	Novel antioxidant quinoxaline derivative: Synthesis, crystal structure, theoretical studies, antidiabetic activity and molecular docking study. <i>Journal of Molecular Structure</i> , 2021 , 1239, 130484	3.4	12
347	Synthesis, biological activity and molecular modeling of a new series of condensed 1,2,4-triazoles. <i>Bioorganic Chemistry</i> , 2019 , 92, 103193	5.1	11
346	An inorganic-organic hybrid material based on a Keggin-type polyoxometalate@Dysprosium as an effective and green catalyst in the synthesis of 2-amino-4H-chromenes via multicomponent reactions. <i>Applied Organometallic Chemistry</i> , 2020 , 34, e5793	3.1	11
345	A Novel Method for the Synthesis of Furo-imidazo[3.3.3]propellanes from Thiocarbonohydrazides. <i>Synlett</i> , 2016 , 27, 412-416	2.2	11
344	A luminescent heteroleptic five-coordinate cadmium(II) complex containing a bridging dithiolate ligand. <i>Journal of Chemical Crystallography</i> , 2001 , 31, 295-300	0.5	11
343	Synthesis, single crystal X-ray characterization, and solution studies of Zn(II)-, Cu(II)-, Ag(I)- and Ni(II)-pyridine-2,6-dipicolinate N-oxide complexes with different topologies and coordination modes. <i>Inorganica Chimica Acta</i> , 2017 , 458, 84-96	2.7	10
342	Redox-Active Metallodithiolene Groups Separated by Insulating Tetraphosphinobenzene Spacers. <i>Inorganic Chemistry</i> , 2018 , 57, 4023-4038	5.1	10
341	A Straightforward Approach for the Synthesis of Novel Derivatives of Benzo[b]pyrazolo[5',1':2,3]pyrimido[4,5-e][1,4]thiazine. <i>Journal of Heterocyclic Chemistry</i> , 2016 , 53, 1231-1235	1.9	10
340	Facile and convenient synthesis of 2,4-disubstituted and 2,3,4-trisubstituted 1,3-thiazoles. <i>Journal of Sulfur Chemistry</i> , 2016 , 37, 162-175	2.3	10
339	Ethyl 2-(2,5-dioxo-4,4-diphenylimidazolidin-1-yl)acetate. <i>IUCrData</i> , 2017 , 2,	0.7	10
338	1,1'-Bis(dipyrrolylphosphino)ferrocene: Synthesis, coordination chemistry and structural studies. <i>Journal of Organometallic Chemistry</i> , 2016 , 824, 15-24	2.3	10
337	Synthesis, crystal structure, Hirshfeld surface analysis, and DFT calculations of new 1-[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl]-6-methoxy-1H-benzimidazol-2(3H)-one. <i>Chemical Data Collections</i> , 2018 , 17-18, 472-482	2.1	10
336	Structure and characterization of charge transfer complexes of benzo[1,2-b:3,4-b':5,6-b'']trithiophene [C3h-BTT]. <i>CrystEngComm</i> , 2017 , 19, 6355-6364	3.3	9
335	An inorganic-organic hybrid supramolecular framework based on the [MoO] cluster and cobalt complex of aspartic acid: X-ray structure and DFT study. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2019 , 75, 469-477	0.8	9

334	Synthesis, crystal structure, spectroscopic characterization, Hirshfeld surface analysis, and DFT calculations of 1,4-dimethyl-2-oxo-pyrimido[1,2-a]benzimidazole hydrate. <i>Journal of Molecular Structure</i> , 2018 , 1152, 154-162	3.4	9
333	Synthesis and Structures of [LCu(I)(SSi(i)Pr ₃)] (L = triphos, carbene) and Related Compounds. <i>Inorganic Chemistry</i> , 2016 , 55, 9173-7	5.1	9
332	Expanding the Scope of Ligand Substitution from [M(SCPh)] (M = Ni, Pd, Pt) To Afford New Heteroleptic Dithiolene Complexes. <i>Inorganic Chemistry</i> , 2017 , 56, 10257-10267	5.1	9
331	Chemistry of diaminomaleonitrile: synthesis and structure of two unexpected products from its condensation with 2,5-hexanedione. <i>Journal of Chemical Crystallography</i> , 2000 , 30, 311-320	0.5	9
330	Docking of disordered independent molecules of novel crystal structure of (N-(4-methoxyphenyl)-2-(3-methyl-2-oxo-3,4-dihydroquinoxalin-1(2H)-yl)acetamide as anti-COVID-19 and anti-Alzheimer's disease. Crystal structure, HSA/DFT/XRD. <i>Journal of Molecular Structure</i> , 2022 , 1247, 131420	3.4	9
329	Supramolecular network of a framework material supported by the anion-π linkage of Keggin-type heteropolyoxotungstates: experimental and theoretical insights. <i>Dalton Transactions</i> , 2021 , 50, 1895-1900	4.3	9
328	Synthesis, spectroscopic characterization, thermal, XRD crystal structure, the PLATON structural analysis, and theoretical studies of a new 1,2,4-triazolo-[1,5-a]pyrimidines derivatives. <i>Journal of Molecular Structure</i> , 2019 , 1184, 12-24	3.4	8
327	The first mixed-ligand coordination compound involving 8-aminoquinoline and pyridine-2,6-dicarboxylate: synthesis, X-ray crystal structure, and DFT studies. <i>Journal of Coordination Chemistry</i> , 2015 , 68, 3599-3610	1.6	8
326	A co-crystal of 2-(1-pyrenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl with octafluoronaphthalene. <i>CrystEngComm</i> , 2013 , 15, 831-835	3.3	8
325	The influence of weak hydrogen bonds on the properties of 3-cyano-N-methylpyridinium chloride and iodide. <i>Journal of Chemical Crystallography</i> , 2003 , 33, 391-402	0.5	8
324	Structural characterization and excited-state properties of luminescent Tris-(β ³ -methyl-5-trifluoromethylpyrazolato)trigold(I). <i>Journal of Chemical Crystallography</i> , 2005 , 35, 5-12	0.5	8
323	Crystal structure and Hirshfeld surface analysis of -{2-[(-)-(4-methyl-benzyl-idene)amino]-phen-yl}-2-(5-methyl-1-pyrazol-3-yl)acetamide hemihydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019 , 75, 154-158	0.7	8
322	3-Ethyl-5,5-diphenylimidazolidine-2,4-dione. <i>IUCrData</i> , 2017 , 2,	0.7	8
321	Two polyoxometalate-based hybrids constructed from trinuclear lanthanoid clusters with single-molecule magnet behavior. <i>Polyhedron</i> , 2021 , 194, 114903	2.7	8
320	Ni(II), Co(II), and Cu(II) complexes incorporating 2-pyrazinecarboxylic acid: Synthesis, characterization, electrochemical evaluation, and catalytic activity for the synthesis of 2H-indazolo[2,1-b]phthalazine-triones. <i>Chinese Journal of Catalysis</i> , 2015 , 36, 1101-1108	11.3	7
319	Crystal structure of 2-(2,3-di-methyl-anilino)-NN'[(1E)-2-hydroxy-benzyl-idene]benzohydrazide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, 0957-8	0.7	7
318	Synthesis, anticancer evaluation in vitro, DFT, Hirshfeld surface analysis of some new 4-(1,3-benzothiazol-2-yl)-3-methyl-1-phenyl-4,5-dihydro-1H-pyrazol-5-one derivatives. <i>Journal of Molecular Structure</i> , 2019 , 1198, 126910	3.4	7
317	Square planar nickel(II) complexes derived from 5-bromo-2-hydroxybenzaldehyde S-ethylisothiosemicarbazone: Preparation, characterization and structural studies. <i>Polyhedron</i> , 2014 , 80, 243-249	2.7	7

316	Crystal structure and Hirshfeld surface analysis of (4)-1-butyl-4-(2-oxo-propyl-idene)-2,3,4,5-tetra-hydro-1-1,5-benzodiazepin-2-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018 , 74, 1669-1673	0.7	7
315	Crystal structure and Hirshfeld surface analysis of a new benzodiazepine derivative: 4-di-chloro-methyl-2,3-di-hydro-1-1,5-benzodiazepin-2-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019 , 75, 33-37	0.7	7
314	2-{3-[2-(2-Chlorophenyl)ethyl]-2-oxo-1,2-dihydroquinoxalin-1-yl}acetohydrazide. <i>IUCrData</i> , 2017 , 2,	0.7	7
313	Ethyl 2-[(3-methylquinoxalin-2-yl)sulfanyl]acetate. <i>IUCrData</i> , 2017 , 2,	0.7	7
312	Buffer and Salt Effects in Aqueous Host-Guest Systems: Screening, Competitive Binding, or Both?. <i>Journal of the American Chemical Society</i> , 2021 , 143, 18605-18616	16.4	7
311	Synthesis and HSA-interaction of a new mixed ligand Cu-isothiosemicarbazonato complex with adenine nucleobase. <i>Polyhedron</i> , 2020 , 179, 114357	2.7	7
310	Synthesis, structural characterisation and theoretical studies of a novel pyridazine derivative: Investigations of anti-inflammatory activity and inhibition of α -glucosidase. <i>Journal of Molecular Structure</i> , 2021 , 1234, 130177	3.4	7
309	Photocatalytic H-Evolution by Homogeneous Molybdenum Sulfide Clusters Supported by Dithiocarbamate Ligands. <i>Inorganic Chemistry</i> , 2019 , 58, 16458-16474	5.1	7
308	Synthesis of New Pyrimido[4,5-e][1,2,4]triazolo[3,4-b][1,3,4]thiadiazine Derivatives via S/N Smiles Rearrangement. <i>Journal of Heterocyclic Chemistry</i> , 2017 , 54, 235-241	1.9	6
307	Effect of solvents in mixed-ligand supramolecular self-assembly architectures. <i>Polyhedron</i> , 2017 , 134, 41-49	2.7	6
306	Synthesis, characterization and bioactivity studies of new dithiocarbamate complexes. <i>New Journal of Chemistry</i> , 2020 , 44, 8878-8889	3.6	6
305	Palladium-catalyzed regioselective direct C-H arylation of pyrazolo[3,4-d]pyrimidines. <i>Comptes Rendus Chimie</i> , 2017 , 20, 927-933	2.7	6
304	2-Cyano-1-methyl-pyridinium nitrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1653		6
303	Aryl acetylene inhibitors for cytochrome P450-based monooxygenase isozymes. <i>Journal of Chemical Crystallography</i> , 1997 , 27, 183-189	0.5	6
302	2-Cyano-1-methyl-pyridinium iodide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o1281		6
301	3-[2-(5-Oxo-4,4-diphenyl-2-sulfanylideneimidazolidin-1-yl)ethyl]-1,3-oxazolidin-2-one. <i>IUCrData</i> , 2017 , 2,	0.7	6
300	A possible potential COVID-19 drug candidate: Diethyl 2-(2-(2-(3-methyl-2-oxoquinoxalin-1(2H)-yl)acetyl)hydrazono)malonate: Docking of disordered independent molecules of a novel crystal structure, HSA/DFT/XRD and cytotoxicity.. <i>Arabian Journal of Chemistry</i> , 2022 , 15, 103595	5.9	6
299	Syntheses, single crystal X-ray structure, Hirshfeld surface analyses, DFT computations and Monte Carlo simulations of New Eugenol derivatives bearing 1,2,3-triazole moiety. <i>Journal of Molecular Structure</i> , 2021 , 1234, 130189	3.4	6

- 298 An Unexpected Diastereoselective Synthesis of Novel Substituted Pyridines via One-Pot, Four-Component Reaction. *Synlett*, **2016**, 27, 1669-1673 2.2 6
- 297 Syntheses of N-substituted benzimidazolone derivatives: DFT calculations, Hirshfeld surface analysis, molecular docking studies and antibacterial activities. *Journal of Molecular Structure*, **2020**, 1200, 127174 3.4 6
- 296 Synthesis, Characterization and Fluorescence Properties of Zn(II) and Cu(II) Complexes: DNA Binding Study of Zn(II) Complex. *Journal of Fluorescence*, **2016**, 26, 333-44 2.4 5
- 295 New 5-bromo-2-hydroxybenzaldehyde S-ethylisothiosemicarbazone and its mixed-ligand Cu(II) complex with imidazole: synthesis, characterization and DFT calculation. *Open Chemistry*, **2013**, 11, 1844-1851 1.6 5
- 294 The Hairpin Furans: Easily Prepared Hybrids of Helicenes and Twisted Acenes. *Angewandte Chemie*, **2015**, 127, 14163-14166 3.6 5
- 293 Crystal structure of 1-(2-amino-phen-yl)-3-phenyl-urea. *Acta Crystallographica Section E: Crystallographic Communications*, **2015**, 71, o88-9 0.7 5
- 292 4-Cyano-1-methyl-pyridinium iodide. *Acta Crystallographica Section E: Structure Reports Online*, **2012**, 68, o2514 5
- 291 Structural characterization and photophysical properties of a luminescent trinuclear zinc(II) complex exhibiting multiple coordination geometries. *Journal of Chemical Crystallography*, **2005**, 35, 327-338 0.5 5
- 290 Lower rim modification of calix[4]arenes to incorporate a single group functionality. Single crystal X-ray structures of 5-(3-bromopropyl)-25,26,27,28-tetrahydroxycalix[4]arene and 25,27-diallyloxy-26,28-dibenzoyloxycalix[4]arene. *Supramolecular Chemistry*, **1993**, 2, 53-60 1.8 5
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- 288 3-Methyl-5,5-diphenylimidazolidine-2,4-dione. *IUCrData*, **2017**, 2, 0.7 5
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215	2-Methoxy-4,6-diphenyl-nicotino-nitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o228		2
214	2-Cycloheptyl-ylidene-N-phenylhydrazine-carbothioamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o359		2
213	Methyl (2Z)-2-[(2Z)-3-[(cyclopentyl-ylidene)amino]-4-oxo-2-phenylimino-1,3-thiazolidin-5-yl-ylidene]acetate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o366-7		2
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208	Methyl (2Z)-((2Z)-2-((2E)-[1-(4-methyl-phen-yl)ethyl-idene]hydrazinyl-idene)-4-oxo-3-phenyl-1,3-thia-zolidin-5-yl-idene)ethano-ate <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o1401-2		
207	Dimethyl (2Z)-2-[4-((1Z)-1-(2-[(2Z,5Z)-5-(2-meth-oxy-2-oxo-ethyl-idene)-4-oxo-3-phenyl-1,3-thia-zolidin-2-yl-idene]hydra-zin-1-yl-idene)]-1,2,3-triazol-1-yl]acetate <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o1844-5		
206	Crystal structure of ethyl 3-amino-6-methyl-2-[(4-methyl-phen-yl)carbamo-yl]-4-[(E)-2-phenyl-ethen-yl]thieno[2,3-b]pyridine-5-carboxyl-ate monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016 , 72, 297-9		
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203	Crystal structure and Hirshfeld surface analysis of 3,4-dihydro-2-(2,4-dioxo-6-methylpyran-3-ylidene)-4-(4-pyridin-4-yl)-1,5-benzodiazepine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019 , 75, 94-98	0.7	2
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198	1-Ethyl-5-nitro-1H-indazole. <i>IUCrData</i> , 2016 , 1,	0.7	2
197	4-Benzyl-2-(4-chlorobenzylidene)-3,4-dihydro-2H-1,4-benzothiazin-3(4H)-one. <i>IUCrData</i> , 2016 , 1,	0.7	2
196	Dichlorido{2-[(5-methyl-1H-pyrazol-3-yl-N2)methyl]-1H-1,3-benzimidazole-N3}zinc. <i>IUCrData</i> , 2017 , 2,	0.7	2
195	trans-Bis(N-{2-[2-(3-methyl-1H-pyrazol-5-yl-N2)acetamido-D]phenyl}benzamide)bis(perchlorato-D)copper(II). <i>IUCrData</i> , 2017 , 2,	0.7	2
194	1-[[3-(Thiophen-2-yl)-4,5-dihydro-1,2-oxazol-5-yl]methyl]-2,3-dihydro-1H-indole-2,3-dione. <i>IUCrData</i> , 2017 , 2,	0.7	2
193	7-Acetyl-8-(4-chlorophenyl)-3-ethylsulfonyl-6-hydroxy-1,6-dimethyl-5,6,7,8-tetrahydroisoquinoline-4-carbonitrile. <i>IUCrData</i> , 2017 , 2,	0.7	2
192	3-Chloro-2-ethyl-6-nitro-2H-indazole. <i>IUCrData</i> , 2017 , 2,	0.7	2
191	(E)-N-[(Anthracen-9-yl)methylidene]hydroxylamine. <i>IUCrData</i> , 2017 , 2,	0.7	2

190	Methyl 2-[[[(6S*,7R*,8S*)-7-acetyl-8-(4-chlorophenyl)-4-cyano-6-hydroxy-1,6-dimethyl-5,6,7,8-tetrahydroisoquinolin-3-yl]sulfanyl]methyl]quinolin-8-ol. <i>IUCrData</i> , 2017 , 2,		
189	3-Benzyl-5,5-diphenylimidazolidine-2,4-dione. <i>IUCrData</i> , 2018 , 3,	0.7	2
188	3-Hexyl-5,5-diphenylimidazolidine-2,4-dione. <i>IUCrData</i> , 2018 , 3,	0.7	2
187	(Z)-1-(1,3-Diphenyl-1H-pyrazol-4-yl)-N-phenylmethanimineN-oxide. <i>IUCrData</i> , 2018 , 3,	0.7	2
186	Ethyl 2-(3-oxo-1,2,3,4-tetrahydroquinoxalin-2-yl)acetate. <i>IUCrData</i> , 2018 , 3,	0.7	2
185	Ethyl 2-[(2E)-4-decyl-3-oxo-1,2,3,4-tetrahydroquinoxalin-2-ylidene]acetate. <i>IUCrData</i> , 2018 , 3,	0.7	2
184	5-[[2-Hydroxyethyl]sulfanyl]methyl]quinolin-8-ol. <i>IUCrData</i> , 2019 , 4,	0.7	2
183	Synthesis and crystal structure of 3-octyl-5,5-diphenylimidazolidine-2,4-dione, C ₂₃ H ₂₈ N ₂ O ₂ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2020 , 235, 1425-1427	0.2	2
182	Crystal structure, Hirshfeld surface analysis and DFT studies of 6-bromo-3-(12-bromo-dodecyl)-2-(4-nitro-phen-yl)-4-imidazo[4,5-]pyridine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020 , 76, 677-682	0.7	2
181	Coordination complexes of zinc and manganese based on pyridine-2,5-dicarboxylic acid -oxide: DFT studies and antiproliferative activities consideration.. <i>RSC Advances</i> , 2021 , 11, 37403-37412	3.7	2
180	1-Bromo-2,4,6-tricyclo-hexyl-benzene. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2007 , 64, o335		2
179	Crystal structure and Hirshfeld surface analysis of 5-[(5-nitro-1-indazol-1-yl)meth-yl]-3-phenyl-4,5-di-hydro-isoxazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019 , 75, 71-74	0.7	2
178	Crystal structure of 2-cyano-1-methyl-pyridinium tetra-fluoro-borate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, o697-8	0.7	2
177	(4Z)-4-(2-Oxopropylidene)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one. <i>IUCrData</i> , 2017 , 2,	0.7	2
176	Dimroth rearrangement-based synthesis of novel derivatives of [1,3]selenazolo[5,4-e][1,2,4]triazolo[1,5-c]pyrimidine as a new class of selenium-containing heterocyclic architecture. <i>Molecular Diversity</i> , 2021 , 1	3.1	2
175	Synthesis, Characterization, and Crystal Structure of Some New Tetrahydroisoquinolines and Related Tetrahydrothieno[2,3-]isoquinolines. <i>ACS Omega</i> , 2021 , 6, 8332-8339	3.9	2
174	Crystal structure, Hirshfeld surface analysis and DFT study of -(2-amino-5-methyl-phen-yl)-2-(5-methyl-1-pyrazol-3-yl)acetamide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021 , 77, 638-642	0.7	2
173	Synthesis, X-ray, spectroscopic characterization, Hirshfeld surface analysis, DFT calculation and molecular docking investigations of a novel 7-phenyl-2,3,4,5-tetrahydro-1H-1,4- diazepin-5-one derivative. <i>Journal of Molecular Structure</i> , 2021 , 1234, 130146	3.4	2

172	Single-molecule magnets within polyoxometalate-based frameworks. <i>Dalton Transactions</i> , 2021 , 50, 15047-15056	4.5	2
171	Unusual Rearrangement-Remercuration Reactions of Allylic Silanols. <i>Organic Chemistry Frontiers</i> , 2021 , 8, 5361-5368	5.2	2
170	Synthesis, Crystal structure, Hirshfeld surface analysis, Spectral characterizations and Quantum computational assessments of 1-hydroxy-3-methyl-11H-pyrido[2,1-b]quinazolin-11-one. <i>Journal of Molecular Structure</i> , 2021 , 131592	3.4	2
169	Convenient one-pot access to novel densely functionalized pyrano[2,3-d][1,3,4]thiadiazolo[3,2-a]pyrimidines via three component reaction. <i>Research on Chemical Intermediates</i> , 2017 , 43, 4683-4696	2.8	1
168	Synthesis, resolution and crystal structures of two enanti-omeric rhodamine derivatives. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017 , 73, 327-333	0.7	1
167	Crystal structure of poly[di-aqua-{5-[(1Z)-2-(4-chloro-phen-yl)-1-cyano-ethenyl]-1,2,3,4-tetra-zol-1-ido-N (1)}sodium]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, m102-3	0.7	1
166	Crystal structure of methyl 2-hydroxy-5-[(4-oxo-4,5-dihydro-1,3-thiazol-2-yl)amino]benzoate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, o282-3	0.7	1
165	The 2-(4-Phenyl-1H-1,2,3-triazol-1-yl)ethanol-Based Phosphinite Ligand Ph2POCH2CH2[1,2,3-N3C(Ph)C(H)] [Synthesis, Transition-Metal Complexes, and Structural Studies. <i>European Journal of Inorganic Chemistry</i> , 2018 , 2018, 1694-1694	2.3	1
164	A Simple, Serendipitous Synthesis of Heterohexahelicenes. <i>European Journal of Organic Chemistry</i> , 2019 , 2019, 6534-6538	3.2	1
163	Silylated gallium and indium chalcogenide ring systems as potential precursors to ME (E=O, S) materials. <i>Open Chemistry</i> , 2013 , 11, 1225-1238	1.6	1
162	Crystal structure of unsymmetrical di-imine palladium(II) complex -[ArN=C(Me)-(Et)C=NAr]PdCl [Ar = 2,6-(iPr)CH]. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017 , 73, 1148-1150	0.7	1
161	Crystal structure of ethyl 2-[2-[(1Z)-1-hydroxy-3-(4-nitro-phen-yl)-3-oxoprop-1-en-1-yl]phen-oxy]acetate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, o917-8	0.7	1
160	Crystal structure of [(E)-{2-[3-(2-[(1E)-[(carbamo-thioyl-amino)-imino]-meth-yl]phen-oxy)prop-oxy]phen-yl)methyl-idene)amino]-thio-urea with an unknown solvate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, o530-1	0.7	1
159	Crystal structure of (E)-4-[[2-(2,4-di-nitro-phen-yl)hydrazin-1-yl-idene]meth-yl]-3-methyl-1-phenyl-5-(1H-pyrrol-1-yl)-1H-pyrazole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o1246-7	1	1
158	3-[2-(4-Fluoro-phen-yl)-2-oxoeth-yl]-5,5-di-phenyl-imidazolidine-2,4-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o226-7	1	1
157	4-Phenyl-1,2,4-tri-aza-spiro-[4.4]non-1-ene-3-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o433-4	1	1
156	N-(12-Amino-9,10-di-hydro-9,10-ethano-anthracen-11-yl)-4-methyl-benzene-sulfonamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o248-9	1	1
155	3-Amino-5,5-di-phenyl-imidazolidine-2,4-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o262-3	1	1

154	4-[(1,3-Dioxoisindolin-2-yl)methyl]benzene-sulfonamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o291-2		1
153	Methyl 2-((2Z,5Z)-4-oxo-3-phenyl-2-[2-[(1E)-1,2,3,4-tetra-hydro-naphthalen-1-yl-idene]hydrazin-1-yl-idene]-1,3-thia-zolidin-5-yl)ethane. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o436-7		
152	4-Phenyl-1,2,4-tri-aza-spiro-[4.6]undec-1-ene-3-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o640		1
151	(Z)-1-[(2E)-3,4-Diphenyl-2,3-di-hydro-1,3-thia-zol-2-yl-idene]-2-[1-(4-hydroxy-phen-yl)ethyl-idene]hydrazinium bromide including an unknown solvate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o647-8		1
150	(2E)-4-(4-Bromo-phen-yl)-2-[2-[(1E)-cyclo-pentyl-idene]hydrazin-1-yl-idene]-3-phenyl-2,3-di-hydro-1,3-thia-zole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o669		1
149	Ethyl 2-[[[4-amino-5-cyano-6-(methyl-sulfan-yl)pyridin-2-yl]carbamo-yl]meth-yl]sulfan-yl]acetate monohydrate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o745-6		1
148	Crystal structure of 2-[(E)-2-(2-chloro-benzyl-idene)hydrazin-1-yl]-4-phenyl-1,3-thia-zole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o907-8		1
147	Crystal structure of 2-[12-methyl-14-phenyl-10,13,14,16-tetra-aza-tetra-cyclo[7.7.0.0(2,7).0(11,15)]hexa-deca-1(16),2,4,6,9,11(15),12-hepta-2,5,8-triene]. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o1244-5		
146	2,2N[(1,3,4-Thia-diazole-2,5-di-yl)bis-(sulfanedi-yl)]diaceto-nitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o1855		1
145	NN[(E)-Benzyl-idene]-2-(6-meth-oxy-naphthalen-2-yl)propano-hydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o1614		1
144	Synthesis and crystal structure of N 12-(7-chloro-4-quinoliny)-N 1,N 1-diethyl-1,1,12-diaminododecane (AQ-40). <i>Journal of Chemical Crystallography</i> , 1998 , 28, 925-929	0.5	1
143	Synthesis and X-ray crystal structure of an organometallic phosphonate [B-1,2-C6H4(OCH3)(P(O)(OCH2CH3)2)]Cr(CO)3. <i>Journal of Chemical Crystallography</i> , 2003 , 33, 497-501	0.5	1
142	Crystal structures of three sterically congested disilanes. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017 , 73, 448-452	0.7	1
141	Crystal structure and Hirshfeld surface analysis of 1-[(1-butyl-1-1,2,3-triazol-4-yl)methyl]-3-methyl-quinoxalin-2(1)-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2018 , 74, 1815-1820	0.7	1
140	Crystal structure, Hirshfeld surface analysis and DFT studies of 1-benzyl-3-[(1-benzyl-1-1,2,3-triazol-5-yl)methyl]-2,3-di-hydro-1-1,3-benzo-diazol-2-one monohydrate. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020 , 76, 95-101	0.7	1
139	Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of 1-(1,3-benzo-thia-zol-2-yl)-3-(2-hydroxy-ethyl)imidazolidin-2-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020 , 76, 370-376	0.7	1
138	A redetermination of the crystal structure of the mannitol complex NH[MoO(CHO)]HO: hydrogen-bonding scheme and Hirshfeld surface analysis. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020 , 76, 518-522	0.7	1
137	1-Ethyl-4-phenyl-1,5-benzodiazepine-2-thione. <i>IUCrData</i> , 2017 , 2,	0.7	1

136	3-Phenylisoxazolin-5-one: a redetermination. <i>IUCrData</i> , 2017 , 2,	0.7	1
135	3-Hydroxy-3-(2-oxo-2,3-dihydro-1H-indol-3-yl)-2,3-dihydro-1H-indol-2-one. <i>IUCrData</i> , 2017 , 2,	0.7	1
134	1-[(1-[(1S,2R,6R,8R,9S)-4,4,11,11-Tetramethyl-3,5,7,10,12-pentaoxatricyclo[7.3.0.02,6]dodecan-8-yl)methyl]-1H-1,2,3-triazol-5-yl)methyl]pyrimidin-2(1H)-one. <i>IUCrData</i> , 2017 , 2,	0.7	1
133	Ethyl 2-allyl-2-(5-methyl-1,2,4-triazolo[1,5-a]pyrimidin-7-yl)pent-4-enoate. <i>IUCrData</i> , 2017 , 2,	0.7	1
132	2-[(Prop-2-yn-1-yl)amino]anilinium chloride. <i>IUCrData</i> , 2017 , 2,	0.7	1
131	Bis(2-formylphenyl) benzene-1,2-dicarboxylate. <i>IUCrData</i> , 2018 , 3,	0.7	1
130	(Pyridin-2-yl)methyl 6-bromo-2-oxo-1-[(pyridin-2-yl)methyl]-1,2-dihydroquinoline-4-carboxylate. <i>IUCrData</i> , 2018 , 3,	0.7	1
129	(3R,4Z)-1,3-Diethyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one. <i>IUCrData</i> , 2018 , 3,	0.7	1
128	2-Methyl-4-(pyridin-2-yl)-3H-1,5-benzodiazepine. <i>IUCrData</i> , 2018 , 3,	0.7	1
127	Ethyl 2-[2-(4-oxo-4-chromen-2-yl)phenoxy]acetate. <i>IUCrData</i> , 2018 , 3,	0.7	1
126	Crystal structure, Hirshfeld surface analysis, inter-action energy and DFT studies of (2)-2-(2,4-di-chloro-benzyl-idene)-4-nonyl-3,4-di-hydro-2-1,4-benzo-thia-zin-3-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020 , 76, 281-287	0.7	1
125	Crystal structure, Hirshfeld surface analysis and DFT study of 6-bromo-3-(5-bromo-hex-yl)-2-[4-(di-methyl-amino)-phen-yl]-3-imidazo[4,5-]pyridine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020 , 76, 1234-1238	0.7	1
124	N,N-Dimethyl-1H-pyrazolo[3,4-d]pyrimidin-4-amine monohydrate. <i>IUCrData</i> , 2018 , 3,	0.7	1
123	A monoclinic modification of (4Z)-1-benzyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one. <i>IUCrData</i> , 2018 , 3,	0.7	1
122	Crystal structure, DFT study and Hirshfeld surface analysis of 1-nonyl-2,3-di-hydro-1-indole-2,3-dione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019 , 75, 1140-1144	0.7	1
121	Crystal structure, Hirshfeld surface analysis and inter-action energy and DFT studies of 4-[(prop-2-en-1-yl-oxy)meth-yl]-3,6-bis-(pyridin-2-yl)pyridazine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019 , 75, 1321-1326	0.7	1
120	Synthesis, structural, characterization and Hirshfeld analysis of a bisselenide and a zinc complex of a new hemilabile ferrocenylbisphosphane, [Fe{CHP(CHCHNMe-o)}]. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2021 , 77, 725-733	0.8	1
119	Crystal structure of (4-meth-oxy-phen-yl)[(4-meth-oxy-phen-yl)phospho-nato]dioxidophosphate(1-)-2-amino-6-benzyl-3-eth-oxy-carbon-yl-4,5,6,7-tetra-hydro-thieno[2,3-c]pyridin-6-ium. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, o997-8	0.7	1

118	Crystal structure of 3-benzyl-1-[(1,2,3,4-tetra-hydro-naphthalen-1-yl-idene)amino]-thio-urea. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, o974-5	0.7	1
117	5-Nitro-1-(prop-2-yn-1-yl)-1H-indazole. <i>IUCrData</i> , 2016 , 1,	0.7	1
116	2-(2-Amino-5-methyl-1,2,4-triazolo[1,5-a]pyrimidin-7-yl)acetohydrazide monohydrate. <i>IUCrData</i> , 2016 , 1,	0.7	1
115	1-(5-Nitro-1H-indazol-1-yl)ethanone. <i>IUCrData</i> , 2016 , 1,	0.7	1
114	Cyclohexane-1,4-diammonium dithiocyanate. <i>IUCrData</i> , 2016 , 1,	0.7	1
113	2-[(2Z)-2-Benzylidene-3-oxo-3,4-dihydro-2H-1,4-benzothiazin-4-yl]acetic acid. <i>IUCrData</i> , 2016 , 1,	0.7	1
112	(E)-N ² -Benzylidene-2-phenylquinoline-4-carbohydrazide. <i>IUCrData</i> , 2016 , 1,	0.7	1
111	3-[2-(9H-Carbazol-9-yl)ethyl]-4-phenyl-1H-1,2,4-triazole-5(4H)-thione dimethyl sulfoxide monosolvate. <i>IUCrData</i> , 2016 , 1,	0.7	1
110	(4Z)-1-Dodecyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one. <i>IUCrData</i> , 2016 , 1,	0.7	1
109	(2Z)-2-Benzylidene-4-[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl]-3,4-dihydro-2H-1,4-benzothiazin-3-one. <i>IUCrData</i> , 2016 , 1,	0.7	1
108	(E)-4-Methoxy-3,5-dimethyl-2-[(3-nitrophenyl)ethenyl]pyridine. <i>IUCrData</i> , 2016 , 1,	0.7	1
107	N-{2-[2-(5-Methyl-1H-pyrazol-3-yl)acetamido]phenyl}benzamide monohydrate. <i>IUCrData</i> , 2017 , 2,	0.7	1
106	4-Methyl-3,4-dihydro-2H-1,4-benzothiazin-3-one. <i>IUCrData</i> , 2017 , 2,	0.7	1
105	3-Chloro-6-nitro-1-[(1-octyl-1H-1,2,3-triazol-4-yl)methyl]-1H-indazole. <i>IUCrData</i> , 2017 , 2,	0.7	1
104	Ethyl 2-(6-nitro-1H-indazol-1-yl)acetate. <i>IUCrData</i> , 2017 , 2,	0.7	1
103	(4Z)-4-(2-Oxopropylidene)-1,3-bis(prop-2-en-1-yl)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one. <i>IUCrData</i> , 2017 , 2,	0.7	1
102	(2Z)-2-Benzylidene-4-octadecyl-3,4-dihydro-2H-1,4-benzothiazin-3-one. <i>IUCrData</i> , 2017 , 2,	0.7	1
101	(2Z)-2-(4-Chlorobenzylidene)-4-[2-(2-oxooxazoliden-3-yl)ethyl]-3,4-dihydro-2H-1,4-benzothiazin-3-one. <i>IUCrData</i> , 2017 , 2,	0.7	1

100	1-(3-Bromo-6-nitro-1H-indazol-1-yl)ethan-1-one. <i>IUCrData</i> , 2017 , 2,	0.7	1
99	1-Chloro-3-(6-nitro-1H-indazol-1-yl)propan-2-ol. <i>IUCrData</i> , 2017 , 2,	0.7	1
98	1-(6-Nitro-1H-indazol-1-yl)ethanone. <i>IUCrData</i> , 2017 , 2,	0.7	1
97	Insights into the crystal structure of two newly synthesized quinoxalines derivatives as potent inhibitor for -Jun -terminal kinases. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-18	3.6	1
96	Crystal structure and Hirshfeld surface analysis of 2-[[7-acetyl-8-(4-chloro-phen-yl)-4-cyano-6-hy-droxy-1,6-dimethyl-5,6,7,8-tetra-hydro-isoquinolin-3-yl]sulfa-nyl]-1(4-chloro-phen-yl)ethan-1-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021 , 77, 527-531	3.7	1
95	Crystal structure and Hirshfeld surface analysis of 2-[[7-acetyl-4-cyano-6-hy-droxy-8-(4-meth-oxy-phen-yl)-1,6-dimethyl-5,6,7,8-tetra-hydro-iso-quo-lin-3-yl]sulfa-nyl]-1(4-chloro-phen-yl)ethan-1-one. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2021 , 77, 663-667	3.7	1
94	Synthesis, Crystal Structure, DFT Calculations and Hirshfeld Surface Analysis of 5-Bromo-1-decyl-2,3-dihydro-1H- indolin-2-one. <i>Journal of Chemical Crystallography</i> , 2020 , 50, 330-337	0.5	1
93	A newly synthesized 6-methyl-7,8,9-[1,2,4]triazolo[4,3-][1,2,4]triazepin-8-one for potential inhibitor of adenosine A1 receptor: a combined experimental and computational studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 38, 3578-3586	3.6	1
92	An efficient diastereoselective synthesis of novel fused 5H-furo[2,3-d]thiazolo[3,2-a]pyrimidin-5-ones via one-pot three-component reaction. <i>Molecular Diversity</i> , 2021 , 1	3.1	1
91	Synthesis and characterization of Mo(0) and W(0) complexes of bis(azol-1-yl)methane based bisphosphines. <i>Journal of Coordination Chemistry</i> , 1-10	1.6	1
90	A Dimroth rearrangement approach for the synthesis of selenopheno[2,3-e][1,2,4]triazolo[1,5-c]pyrimidines with cytotoxic activity on breast cancer cells. <i>Molecular Diversity</i> , 2021 , 1	3.1	1
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88	Biological insights of a chiral hybrid-based Ectamolybdate and proline. <i>Journal of Molecular Structure</i> , 2022 , 1247, 131401	3.4	1
87	Coordination complexes constructed from pyrazole-acetamide and pyrazole-quinoxaline: effect of hydrogen bonding on the self-assembly process and antibacterial activity.. <i>RSC Advances</i> , 2022 , 12, 5324-5339	3.7	1
86	New styrylquinoxaline: synthesis, structural, biological evaluation, ADMET prediction and molecular docking investigations.. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022 , 1-17	3.6	1
85	Greener pastures in evaluating antidiabetic drug for a quinoxaline Derivative: Synthesis, Characterization, Molecular Docking, in vitro and HSA/DFT/XRD studies. <i>Arabian Journal of Chemistry</i> , 2022 , 15, 103851	5.9	1
84	Synthesis, crystal structure investigation and computational approach to discover potential hydrazide derivatives as a potent inhibitor of cyclooxygenase-2 enzyme.. <i>Journal of Biochemical and Molecular Toxicology</i> , 2022 , e23082	3.4	1
83	Synthesis, Crystal structure, and a molecular modeling approach to identify effective antiviral hydrazide derivative against the main protease of SARS-CoV-2. <i>Journal of Molecular Structure</i> , 2022 , 133391	3.4	1

82	Crystal structure of 4-amino-3-(3-methyl-5-phenyl-1H-pyrazol-1-yl)-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, o417	0.7	o
81	Crystal structure of 5-(4,5-di-hydro-1H-imidazol-2-yl)-3-methyl-1-phenyl-1H-pyrazolo-[3,4-b]pyrazin-6-amine. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o1212-3		o
80	Macrocyclic cyclodiphosphazane ($[(\mu\text{-}(\text{BuN}))_2(\text{O})\text{-m}(\text{C}_6\text{H}_4)_4\text{CHNCH}_2]_2$): synthesis of chalcogen derivatives and gold(I) complex. <i>Journal of Chemical Sciences</i> , 2017 , 129, 1531-1537	1.8	o
79	NN(E)-2-Chloro-benzyl-idene]-2-(6-meth-oxy-naphthalen-2-yl)propano-hydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o631-2		o
78	Synthesis and crystal structure of 2-azido-N-(4-nitrophenyl)acetamide, C ₈ H ₇ N ₅ O ₃ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2020 , 235, 1429-1430	0.2	o
77	Crystal structure and Hirshfeld surface analysis of 3-(4-meth-oxy-phen-yl)-1-methyl-4-phenyl-1-pyrazolo-[3,4]-pyrimidine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019 , 75, 638-641	0.7	o
76	Highly Regio- and Diastereoselective Tethered Aza-Wacker Cyclizations of Alkenyl Phosphoramidates. <i>Journal of Organic Chemistry</i> , 2021 , 86, 14732-14758	4.2	o
75	2-(5-Meth-oxy-2-methyl-1H-indol-3-yl)-NN(1E,2E)-3-phenyl-prop-2-en-1-yl-idene]acetohydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o1493		o
74	NN(E)-4-Meth-oxy-benzyl-idene]-2-(5-meth-oxy-2-methyl-1H-indol-3-yl)acetohydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o1660-1		o
73	Synthesis, structure elucidation, Hirshfeld surface analysis, DFT, molecular docking and Monte Carlo simulation of new quinoline-4-carboxylate derivatives. <i>Journal of Molecular Structure</i> , 2021 , 1234, 130195	3.4	o
72	Nitrophenyl-Group-Containing Heterocycles. I. Synthesis, Characterization, Crystal Structure, Anticancer Activity, and Antioxidant Properties of Some New 5,6,7,8-Tetrahydroisoquinolines Bearing 3(4)-Nitrophenyl Group.. <i>ACS Omega</i> , 2022 , 7, 8767-8776	3.9	o
71	Crystal structure, Hirshfeld surface analysis, inter-action energy and DFT calculations and energy frameworks of methyl 6-chloro-1-methyl-2-oxo-1,2-di-hydro-quinoline-4-carboxyl-ate.. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2022 , 78, 425-432	0.7	o
70	Novel 3-chloro-6-nitro-1-indazole derivatives as promising antileishmanial candidates: synthesis, biological activity, and molecular modelling studies.. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022 , 37, 151-167	5.6	o
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