Tejender S Thakur

List of Publications by Year
in descending order

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44 papers	3,048 citations	257450 24 h-index	254184 43 g-index
46 all docs	46 docs citations	46 times ranked	3567 citing authors

#	Article	IF	Citations
1	Computational Screening of Multicomponent Solid Forms of 2-Aryl-Propionate Class of NSAID, Zaltoprofen, and Their Experimental Validation. Crystal Growth and Design, 2021, 21, 449-461.	3.0	13
2	Understanding the guest binding in the cucurbit[7]uril inclusion complexes of CDK4/6 inhibitors, palbociclib, and ribociclib from a combined experimental and computational study. Journal of Molecular Structure, 2021, 1241, 130637.	3.6	2
3	Photoinstability in Active Pharmaceutical Ingredients: Crystal Engineering as a Mitigating Measure. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2021, 49, 100455.	11.6	7
4	Crystalline Multicomponent Solids: An Alternative for Addressing the Hygroscopicity Issue in Pharmaceutical Materials. Crystal Growth and Design, 2020, 20, 6245-6265.	3.0	45
5	Comment on â€œPolymorphism of levofloxacin: structure, properties and phase transformationâ€•by N. Wei, L. Jia, Z. Shang, J. Gong, S. Wu, J. Wang and W. Tang, CrystEngComm, 2019, 21, 6196â€“6207. CrystEngComm, 2020, 22, 1885-1888.	2.6	2
6	Cationâ‹¯cation hydrogen bonds in synephrine salts: a typical interaction in an unusual environment. Physical Chemistry Chemical Physics, 2019, 21, 20647-20660.	2.8	13
7	Structural Landscape-Guided Exploration of a New Polymorph of 4-Nitrobenzoic Acid. Crystal Growth and Design, 2019, 19, 952-958.	3.0	3
8	Rational Coformer Selection and the Development of New Crystalline Multicomponent Forms of Resveratrol with Enhanced Water Solubility. Crystal Growth and Design, 2018, 18, 1581-1592.	3.0	22
9	Preparation of Pyrazinamide Eutectics versus Cocrystals Based on Supramolecular Synthon Variations. Crystal Growth and Design, 2018, 18, 6640-6651.	3.0	24
10	S-Enantiomer of the Antitubercular Compound S006-830 Complements Activity of Frontline TB Drugs and Targets Biogenesis of Mycobacterium tuberculosis Cell Envelope. ACS Omega, 2017, 2, 8453-8465.	3.5	12
11	Crystal Polymorphism in Pharmaceutical Science. , 2017, , 283-309.		9
12	Synthesis of Octabromoperylene Dianhydride and Diimides: Evidence of Halogen Bonding and Semiconducting Properties. Organic Letters, 2016, 18, 472-475.	4.6	39
13	Experimental and computational crystal structure landscape study of nigerloxin: a fungal metabolite from Aspergillus niger. CrystEngComm, 2016, 18, 1740-1751.	2.6	4
14	Studying the Role of Câ•OÂ·Â·Â·Câ•O, Câ•OÂ·Â·Â·Nâ€“O, and Nâ€“OÂ·Â·Â·Nâ€“O Dipoleâ€“Dipole Interactions in the Crystal Packing of 4-Nitrobenzoic Acid and 3,3â€²-Dinitrobenzophenone Polymorphs: An Experimental Charge Density Study. Crystal Growth and Design, 2015, 15, 3280-3292.	3.0	13
15	Intermolecular atomâ€“atom bonds in crystals â€“ a chemical perspective. IUCrJ, 2015, 2, 159-160.	2.2	63
16	Crystal Structure and Prediction. Annual Review of Physical Chemistry, 2015, 66, 21-42.	10.8	65
17	New crystalline salt forms of levofloxacin: conformational analysis and attempts towards the crystal structure prediction of the anhydrous form. CrystEngComm, 2014, 16, 4215.	2.6	37
18	Versatile coordination environment and interplay of metal assisted secondary interactions in the organization of supramolecular motifs in new Hg(II)/PhHg(II) dithiolates. Polyhedron, 2014, 69, 225-233.	2.2	19

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19	Crystalline Supramolecular Nanofibers Based on Dehydrobenzoannulene Derivatives. Chemistry - A European Journal, 2013, 19, 15366-15377.	3.3	28
20	Structural Transformation between Supramolecular Nanofibers with Drastic Change of Conductivity by Heat and Ultrasound. Chemistry - an Asian Journal, 2013, 8, 1372-1376.	3.3	13
21	Crystal Engineering in the Desiraju Research Group in Bangalore. Crystal Growth and Design, 2012, 12, 4688-4691.	3.0	2
22	Polymorphs, Salts, and Cocrystals: Whatâ€™s in a Name?. Crystal Growth and Design, 2012, 12, 2147-2152.	3.0	767
23	Triclabendazole: An Intriguing Case of Coâ€existence of Conformational and Tautomeric Polymorphism. Chemistry - an Asian Journal, 2012, 7, 330-342.	3.3	34
24	Correction for Polymorphs, Salts and Cocrystals: Whatâ€™s in a Name?. Crystal Growth and Design, 2012, 12, 4290-4291.	3.0	17
25	Extending the Supramolecular Synthon Based Fragment Approach (SBFA) for Transferability of Multipole Charge Density Parameters to Monofluorobenzoic Acids and their Cocrystals with Isonicotinamide: Importance of Câ€“HÂ·Â·Â·O, Câ€“HÂ·Â·Â·F, and FÂ·Â·Â·F Intermolecular Regions. Journal of Physical Chemistry A, 2011, 115, 12852-12863.	2.5	57
26	Nature and strength of Câ€“Hâ‹¯O interactions involving formyl hydrogen atoms: computational and experimental studies of small aldehydes. Physical Chemistry Chemical Physics, 2011, 13, 14076.	2.8	83
27	Transferability of Multipole Charge Density Parameters for Supramolecular Synthons: A New Tool for Quantitative Crystal Engineering. Crystal Growth and Design, 2011, 11, 616-623.	3.0	65
28	Polymorphs, Pseudopolymorphs, and Co-Crystals of Orcinol: Exploring the Structural Landscape with High Throughput Crystallography. Crystal Growth and Design, 2011, 11, 2637-2653.	3.0	92
29	Weak Câ€”H...O hydrogen bonds in anisaldehyde, salicylaldehyde and cinnamaldehyde. Acta Crystallographica Section C: Crystal Structure Communications, 2011, 67, o387-o390.	0.4	20
30	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
31	Quinoxaline:Zâ€² = 1 form. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o2789-o2789.	0.2	4
32	New Solid State Forms of the Anti-HIV Drug Efavirenz. Conformational Flexibility and High Zâ€² Issues. Crystal Growth and Design, 2010, 10, 3191-3202.	3.0	71
33	Third Polymorph of Phenylacetylene. Crystal Growth and Design, 2010, 10, 4246-4249.	3.0	44
34	Câ€“Hâ‹¯Fâ€“C hydrogen bonding in 1,2,3,5-tetrafluorobenzene and other fluoroaromatic compounds and the crystal structure of alloxan revisited. CrystEngComm, 2010, 12, 2079.	2.6	95
35	Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
36	Structure-Based Design of DevR Inhibitor Active against Nonreplicating Mycobacterium tuberculosis. Journal of Medicinal Chemistry, 2009, 52, 6324-6334.	6.4	74

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37	Co-Crystals of the Anti-HIV Drugs Lamivudine and Zidovudine. Crystal Growth and Design, 2009, 9, 951-957.	3.0	148
38	1,2,3-Trifluorobenzene. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2670-o2670.	0.2	6
39	1,3-Difluorobenzene. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2668-o2669.	0.2	5
40	Crystal Structure Prediction of a Co-Crystal Using a Supramolecular Synthon Approach: 2-Methylbenzoic Acidâˆ'2-Amino-4-methylpyrimidine. Crystal Growth and Design, 2008, 8, 4031-4044.	3.0	75
41	Theoretical investigation of Câ€"Hâ‹¯M interactions in organometallic complexes: A natural bond orbital (NBO) study. Computational and Theoretical Chemistry, 2007, 810, 143-154.	1.5	82
42	Misassigned Câ€"Hâ‹¯Cu agostic interaction in a copper(ii) ephedrine derivative is actually a weak, multicentred hydrogen bond. Chemical Communications, 2006, , 552-554.	4.1	99
43	Five varieties of hydrogen bond in 1-formyl-3-thiosemicarbazide: an electron density study. Acta Crystallographica Section B: Structural Science, 2006, 62, 118-127.	1.8	27
44	Proton transfer and N(+)â€"Hâ‹¯S(â^')hydrogen bonds in the crystal structure of 4-aminothiophenol. Chemical Communications, 2004, , 2526-2527.	4.1	19