Yuriy A Abramov

List of Publications by Year
in descending order

26	1,153	471509 17	580821 25
papers	citations	h-index	g-index

34	34	34	1307
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Emerging Landscape of Computational Modeling in Pharmaceutical Development. Journal of Chemical Information and Modeling, 2022, 62, 1160-1171.	5.4	18
2	Selecting a stable solid form of remdesivir using microcrystal electron diffraction and crystal structure prediction. RSC Advances, 2021, 11, 17408-17412.	3.6	9
3	Virtual coformer screening by a combined machine learning and physics-based approach. CrystEngComm, 2021, 23, 6039-6044.	2.6	15
4	Current State-of-the-art In-house and Cloud-Based Applications of Virtual Polymorph Screening of Pharmaceutical Compounds: A Challenging Case ofAZD1305. Crystal Growth and Design, 2021, 21, 1972-1983.	3.0	17
5	Computational Insights into Kinetic Hindrance Affecting Crystallization of Stable Forms of Active Pharmaceutical Ingredients. Crystal Growth and Design, 2020, 20, 1512-1525.	3.0	20
6	Applications of Quantum Chemistry in Pharmaceutical Process Development: Current State and Opportunities. Organic Process Research and Development, 2020, 24, 1496-1507.	2.7	25
7	Virtual Coformer Screening by Crystal Structure Predictions: Crucial Role of Crystallinity in Pharmaceutical Cocrystallization. Journal of Physical Chemistry Letters, 2020, 11, 8832-8838.	4.6	40
8	Guiding Lead Optimization for Solubility Improvement with Physics-Based Modeling. Molecular Pharmaceutics, 2020, 17, 666-673.	4.6	17
9	Solid-Form Transition Temperature Prediction from a Virtual Polymorph Screening: A Reality Check. Crystal Growth and Design, 2019, 19, 7132-7137.	3.0	12
10	Rational Solvent Selection for Pharmaceutical Impurity Purge. Crystal Growth and Design, 2018, 18, 1208-1214.	3.0	14
11	Understanding the Risk of Agglomeration of Polar Pharmaceutical Crystals. Crystal Growth and Design, 2017, 17, 2873-2880.	3.0	10
12	Quantification of Tribocharging of Pharmaceutical Powders in V-Blenders: Experiments, Multiscale Modeling, and Simulations. Journal of Pharmaceutical Sciences, 2016, 105, 1467-1477.	3.3	22
13	An experimental and numerical modeling study of tribocharging in pharmaceutical granular mixtures. Powder Technology, 2016, 297, 211-219.	4.2	30
14	Virtual hydrate screening and coformer selection for improved relative humidity stability. CrystEngComm, 2015, 17, 5216-5224.	2.6	27
15	Low solubility in drug development: de-convoluting the relative importance of solvation and crystal packing. Journal of Pharmacy and Pharmacology, 2015, 67, 847-856.	2.4	48
16	Major Source of Error in QSPR Prediction of Intrinsic Thermodynamic Solubility of Drugs: Solid vs Nonsolid State Contributions?. Molecular Pharmaceutics, 2015, 12, 2126-2141.	4.6	33
17	A Computational Approach to Enzyme Design: Predicting Ï‰-Aminotransferase Catalytic Activity Using Docking and MM-GBSA Scoring. Journal of Chemical Information and Modeling, 2014, 54, 2334-2346.	5.4	78
18	Current Computational Approaches to Support Pharmaceutical Solid Form Selection. Organic Process Research and Development, 2013, 17, 472-485.	2.7	75

#	Article	IF	Citations
19	Integrating Intramolecular Hydrogen Bonding (IMHB) Considerations in Drug Discovery Using Î”logP As a Tool. Journal of Medicinal Chemistry, 2013, 56, 4870-4879.	6.4	79
20	Evaluation of Milling Method on the Surface Energetics of Molecular Crystals Using Inverse Gas Chromatography. Crystal Growth and Design, 2012, 12, 5271-5282.	3.0	22
21	Rational Coformer or Solvent Selection for Pharmaceutical Cocrystallization or Desolvation. Journal of Pharmaceutical Sciences, 2012, 101, 3687-3697.	3.3	150
22	QTAIM Application in Drug Development: Prediction of Relative Stability of Drug Polymorphs from Experimental Crystal Structures. Journal of Physical Chemistry A, 2011, 115, 12809-12817.	2.5	27
23	Development of machine learning models of Î²-cyclodextrin and sulfobutylether-Î²-cyclodextrin complexation free energies. International Journal of Pharmaceutics, 2011, 418, 207-216.	5.2	26
24	Development of a Targeted Polymorph Screening Approach for a Complex Polymorphic and Highly Solvating API. Journal of Pharmaceutical Sciences, 2010, 99, 3874-3886.	3.3	111
25	Solid-State Acidâ^'Base Interactions in Complexes of Heterocyclic Bases with Dicarboxylic Acids:â€‰ Crystallography, Hydrogen Bond Analysis, and 15N NMR Spectroscopy. Journal of the American Chemical Society, 2006, 128, 8199-8210.	13.7	181
26	Uncertainty Distribution of Crystal Structure Prediction. Crystal Growth and Design, 0, , .	3.0	5