Geoffrey P F Wood

List of Publications by Year
in descending order

30 papers	872 citations	623574 14 h-index	477173 29 g-index
30 all docs	30 docs citations	30 times ranked	1067 citing authors

#	Article	IF	Citations
1	Kinetic Modeling of API Oxidation: (2) Imipramine Stress Testing. Molecular Pharmaceutics, 2022, 19, 1526-1539.	2.3	6
2	Investigating the Role of Solvent in the Formation of Vacancies on Ibuprofen Crystal Facets. Crystal Growth and Design, 2022, 22, 3034-3041.	1.4	0
3	Identifying Conformational Isomers of Organic Molecules in Solution via Unsupervised Clustering. Journal of Chemical Information and Modeling, 2021, 61, 2263-2273.	2.5	3
4	Kinetic Modeling of API Oxidation: (1) The AIBN/H₂O/CH₃OH Radical â€œSoupâ€• Molecular Pharmaceutics, 2021, 18, 3037-3049.	2.3	12
5	Five Degrees of Separation: Characterization and Temperature Stability Profiles for the Polymorphs of PD-0118057 (Molecule XXIII). Crystal Growth and Design, 2021, 21, 4435-4444.	1.4	4
6	Prediction of the Relative Free Energies of Drug Polymorphs above Zero Kelvin. Crystal Growth and Design, 2020, 20, 5211-5224.	1.4	26
7	Understanding Polymorph Selection of Sulfamerazine in Solution. Crystal Growth and Design, 2019, 19, 6925-6934.	1.4	8
8	Solvent Dynamics and Thermodynamics at the Crystalâ€“Solution Interface of Ibuprofen. Crystal Growth and Design, 2019, 19, 6534-6541.	1.4	5
9	Assessment of machine learning approaches for predicting the crystallization propensity of active pharmaceutical ingredients. CrystEngComm, 2019, 21, 1215-1223.	1.3	28
10	Harnessing Cloud Architecture for Crystal Structure Prediction Calculations. Crystal Growth and Design, 2018, 18, 6891-6900.	1.4	41
11	Dynamics and Thermodynamics of Ibuprofen Conformational Isomerism at the Crystal/Solution Interface. Journal of Chemical Theory and Computation, 2018, 14, 6484-6494.	2.3	13
12	Solvation of the Glycyl Radical. Journal of Physical Chemistry A, 2018, 122, 7212-7217.	1.1	3
13	Modelling nucleation from solution with the string method in the osmotic ensemble. Molecular Physics, 2018, 116, 2998-3007.	0.8	16
14	Drugâ€“Excipient Interactions in the Solid State: The Role of Different Stress Factors. Molecular Pharmaceutics, 2017, 14, 4560-4571.	2.3	15
15	Mechanistic Insights into Radical-Mediated Oxidation of Tryptophan from ab Initio Quantum Chemistry Calculations and QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2016, 120, 2926-2939.	1.1	6
16	Molecular Investigation of the Mechanism of Non-Enzymatic Hydrolysis of Proteins and the Predictive Algorithm for Susceptibility. Biochemistry, 2016, 55, 3315-3328.	1.2	6
17	Hydrogen Bond Hierarchy: Persistent PhenolÂ·Â·Â·Chloride Hydrogen Bonds in the Presence of Carboxylic Acid Moieties. Crystal Growth and Design, 2015, 15, 4341-4354.	1.4	49
18	Quantitative Solution Measurement for the Selection of Complexing Agents to Enable Purification by Impurity Complexation. Crystal Growth and Design, 2014, 14, 3649-3657.	1.4	13

#	Article	IF	Citations
19	Reactions of Benzene and 3-Methylpyrrole with the â€¢OH and â€¢OOH Radicals: An Assessment of Contemporary Density Functional Theory Methods. Journal of Physical Chemistry A, 2014, 118, 2667-2682.	1.1	7
20	Templated Nucleation of Acetaminophen on Spherical Excipient Agglomerates. Langmuir, 2013, 29, 3292-3300.	1.6	30
21	Secondary Structure Assignment of Amyloid-Î² Peptide Using Chemical Shifts. Journal of Chemical Theory and Computation, 2011, 7, 1552-1563.	2.3	14
22	Hydrogen Abstraction by Chlorine Atom from Small Organic Molecules Containing Amino Acid Functionalities: An Assessment of Theoretical Procedures. Journal of Physical Chemistry A, 2009, 113, 11817-11832.	1.1	18
23	Nature of Glycine and Its Î±-Carbon Radical in Aqueous Solution: A Theoretical Investigation. Journal of Chemical Theory and Computation, 2008, 4, 1788-1794.	2.3	24
24	Bond Dissociation Energies and Radical Stabilization Energies:â€‰ An Assessment of Contemporary Theoretical Procedures. Journal of Physical Chemistry A, 2007, 111, 13638-13644.	1.1	101
25	Effect of Side Chains on Competing Pathways for Î²-Scission Reactions of Peptide-Backbone Alkoxyl Radicals. Journal of Physical Chemistry A, 2006, 110, 10316-10323.	1.1	19
26	A restricted-open-shell complete-basis-set model chemistry. Journal of Chemical Physics, 2006, 125, 094106.	1.2	208
27	Bond Dissociation Energies and Radical Stabilization Energies Associated with Model Peptide-Backbone Radicals. Journal of Physical Chemistry A, 2005, 109, 6318-6325.	1.1	72
28	Modeling Î²-Scission Reactions of Peptide Backbone Alkoxy Radicals:Â Backbone Câ^'C Bond Fission. Journal of Chemical Theory and Computation, 2005, 1, 889-899.	2.3	6
29	Performance of the RB3-LYP, RMP2, and UCCSD(T) Procedures in Calculating Radical Stabilization Energies for â€¢NHX Radicals. Journal of Physical Chemistry A, 2003, 107, 7985-7990.	1.1	37
30	Methyl Radical Addition to CS Double Bonds:â€‰ Kinetic versus Thermodynamic Preferences. Journal of Physical Chemistry A, 2002, 106, 12124-12138.	1.1	82