

# Stanislav Geidl

## List of Publications by Year in descending order

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14  
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1040056

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16  
times ranked

411  
citing authors

#	ARTICLE	IF	CITATIONS
1	Predicting $pK_a$ Values of Substituted Phenols from Atomic Charges: Comparison of Different Quantum Mechanical Methods and Charge Distribution Schemes. Journal of Chemical Information and Modeling, 2011, 51, 1795-1806.	5.4	50
2	AtomicChargeCalculator: interactive web-based calculation of atomic charges in large biomolecular complexes and drug-like molecules. Journal of Cheminformatics, 2015, 7, 50.	6.1	50
3	High-quality and universal empirical atomic charges for cheminformatics applications. Journal of Cheminformatics, 2015, 7, 59.	6.1	32
4	ValidatorDB: database of up-to-date validation results for ligands and non-standard residues from the Protein Data Bank. Nucleic Acids Research, 2015, 43, D369-D375.	14.5	22
5	Rapid Calculation of Accurate Atomic Charges for Proteins via the Electronegativity Equalization Method. Journal of Chemical Information and Modeling, 2013, 53, 2548-2558.	5.4	20
6	Predicting $pK_a$ values from EEM atomic charges. Journal of Cheminformatics, 2013, 5, 18.	6.1	15
7	MotiveValidator: interactive web-based validation of ligand and residue structure in biomolecular complexes. Nucleic Acids Research, 2014, 42, W227-W233.	14.5	11
8	SiteBinder: An Improved Approach for Comparing Multiple Protein Structural Motifs. Journal of Chemical Information and Modeling, 2012, 52, 343-359.	5.4	10
9	How Does the Methodology of 3D Structure Preparation Influence the Quality of $pK_a$ Prediction?. Journal of Chemical Information and Modeling, 2015, 55, 1088-1097.	5.4	10
10	NEEMP: software for validation, accurate calculation and fast parameterization of EEM charges. Journal of Cheminformatics, 2016, 8, 57.	6.1	5
11	QSPR designer “employ your own descriptors in the automated QSAR modeling process. Journal of Cheminformatics, 2012, 4, .	6.1	2
12	How the methodology of 3D structure preparation influences the quality of QSPR models?. Journal of Cheminformatics, 2012, 4, .	6.1	0
13	Detection and Extraction of Fragments. SpringerBriefs in Biochemistry and Molecular Biology, 2016, , 43-57.	0.3	0
14	Characterization via Charges. SpringerBriefs in Biochemistry and Molecular Biology, 2016, , 73-80.	0.3	0