Stanislav Geidl

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	NEEMP: software for validation, accurate calculation and fast parameterization of EEM charges. Journal of Cheminformatics, 2016, 8, 57.	6.1	5
2	Detection and Extraction of Fragments. SpringerBriefs in Biochemistry and Molecular Biology, 2016, , 43-57.	0.3	0
3	Characterization via Charges. SpringerBriefs in Biochemistry and Molecular Biology, 2016, , 73-80.	0.3	0
4	How Does the Methodology of 3D Structure Preparation Influence the Quality of p <i>K</i> _a Prediction?. Journal of Chemical Information and Modeling, 2015, 55, 1088-1097.	5.4	10
5	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
6	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
7	High-quality and universal empirical atomic charges for chemoinformatics applications. Journal of Cheminformatics, 2015, 7, 59.	6.1	32
8	MotiveValidator: interactive web-based validation of ligand and residue structure in biomolecular complexes. Nucleic Acids Research, 2014, 42, W227-W233.	14.5	11
9	Predicting pK a values from EEM atomic charges. Journal of Cheminformatics, 2013, 5, 18.	6.1	15
10	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
11	SiteBinder: An Improved Approach for Comparing Multiple Protein Structural Motifs. Journal of Chemical Information and Modeling, 2012, 52, 343-359.	5.4	10
12	QSPR designer – employ your own descriptors in the automated QSAR modeling process. Journal of Cheminformatics, 2012, 4, .	6.1	2
13	How the methodology of 3D structure preparation influences the quality of QSPR models?. Journal of Cheminformatics, 2012, 4, .	6.1	0
14	Predicting p <i>K</i> _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