Marc van Dijk

List of Publications by Year
in descending order

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20 papers	2,389 citations	516561 16 h-index	752573 20 g-index
22 all docs	22 docs citations	22 times ranked	4549 citing authors

#	Article	IF	Citations
1	Recent Developments in Linear Interaction Energy Based Binding Free Energy Calculations. Frontiers in Molecular Biosciences, 2020, 7, 114.	1.6	14
2	A Comparative Linear Interaction Energy and MM/PBSA Study on SIRT1â€“Ligand Binding Free Energy Calculation. Journal of Chemical Information and Modeling, 2019, 59, 4018-4033.	2.5	60
3	Drug toxicity profiling of a Saccharomyces cerevisiae deubiquitinase deletion panel shows that acetaminophen mimics tyrosine. Toxicology in Vitro, 2018, 47, 259-268.	1.1	5
4	Binding free energy predictions of farnesoid X receptor (FXR) agonists using a linear interaction energy (LIE) approach with reliability estimation: application to the D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 239-249.	1.3	19
5	Inter-individual Variability in Activity of the Major Drug Metabolizing Enzymes in Liver Homogenates of 20 Individuals. Current Drug Metabolism, 2018, 19, 370-381.	0.7	16
6	Comprehensive and Automated Linear Interaction Energy Based Binding-Affinity Prediction for Multifarious Cytochrome P450 Aromatase Inhibitors. Journal of Chemical Information and Modeling, 2017, 57, 2294-2308.	2.5	20
7	eTOX ALLIES: an automated pipeLine for linear interaction energy-based simulations. Journal of Cheminformatics, 2017, 9, 58.	2.8	7
8	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	1.5	50
9	Mass Spec Studio for Integrative Structural Biology. Structure, 2014, 22, 1538-1548.	1.6	86
10	Solvated proteinâ€“DNA docking using HADDOCK. Journal of Biomolecular NMR, 2013, 56, 51-63.	1.6	23
11	WeNMR: Structural Biology on the Grid. Journal of Grid Computing, 2012, 10, 743-767.	2.5	170
12	Rapid prediction of multi-dimensional NMR data sets. Journal of Biomolecular NMR, 2012, 54, 377-387.	1.6	35
13	A Flexible, Grid-Enabled Web Portal for GROMACS Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3463-3472.	2.3	32
14	The Structure of the XPF-ssDNA Complex Underscores the Distinct Roles of the XPF and ERCC1 Helix-Hairpin-Helix Domains in ss/ds DNA Recognition. Structure, 2012, 20, 667-675.	1.6	28
15	Strengths and weaknesses of dataâ€driven docking in critical assessment of prediction of interactions. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3242-3249.	1.5	36
16	The HADDOCK web server for data-driven biomolecular docking. Nature Protocols, 2010, 5, 883-897.	5.5	1,167
17	Pushing the limits of what is achievable in proteinâ€“DNA docking: benchmarking HADDOCKâ€™s performance. Nucleic Acids Research, 2010, 38, 5634-5647.	6.5	51
18	3D-DART: a DNA structure modelling server. Nucleic Acids Research, 2009, 37, W235-W239.	6.5	330

#	Article	IF	Citations
19	A protein-DNA docking benchmark. Nucleic Acids Research, 2008, 36, e88-e88.	6.5	67
20	Information-driven protein-DNA docking using HADDOCK: it is a matter of flexibility. Nucleic Acids Research, 2006, 34, 3317-3325.	6.5	169