## Marc van Dijk

List of Publications by Year in descending order

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MARC VAN DUK

#	Article	IF	CITATIONS
1	The HADDOCK web server for data-driven biomolecular docking. Nature Protocols, 2010, 5, 883-897.	12.0	1,167
2	3D-DART: a DNA structure modelling server. Nucleic Acids Research, 2009, 37, W235-W239.	14.5	330
3	WeNMR: Structural Biology on the Grid. Journal of Grid Computing, 2012, 10, 743-767.	3.9	170
4	Information-driven protein-DNA docking using HADDOCK: it is a matter of flexibility. Nucleic Acids Research, 2006, 34, 3317-3325.	14.5	169
5	Mass Spec Studio for Integrative Structural Biology. Structure, 2014, 22, 1538-1548.	3.3	86
6	A protein-DNA docking benchmark. Nucleic Acids Research, 2008, 36, e88-e88.	14.5	67
7	A Comparative Linear Interaction Energy and MM/PBSA Study on SIRT1–Ligand Binding Free Energy Calculation. Journal of Chemical Information and Modeling, 2019, 59, 4018-4033.	5.4	60
8	Pushing the limits of what is achievable in protein–DNA docking: benchmarking HADDOCK's performance. Nucleic Acids Research, 2010, 38, 5634-5647.	14.5	51
9	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	2.6	50
10	Strengths and weaknesses of dataâ€driven docking in critical assessment of prediction of interactions. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3242-3249.	2.6	36
11	Rapid prediction of multi-dimensional NMR data sets. Journal of Biomolecular NMR, 2012, 54, 377-387.	2.8	35
12	A Flexible, Grid-Enabled Web Portal for GROMACS Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3463-3472.	5.3	32
13	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.	3.3	28
14	Solvated protein–DNA docking using HADDOCK. Journal of Biomolecular NMR, 2013, 56, 51-63.	2.8	23
15	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.	5.4	20
16	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.	2.9	19
17	Inter-individual Variability in Activity of the Major Drug Metabolizing Enzymes in Liver Homogenates of 20 Individuals. Current Drug Metabolism, 2018, 19, 370-381.	1.2	16
18	Recent Developments in Linear Interaction Energy Based Binding Free Energy Calculations. Frontiers in Molecular Biosciences, 2020, 7, 114.	3.5	14

#	Article	IF	CITATIONS
19	eTOX ALLIES: an automated pipeLine for linear interaction energy-based simulations. Journal of Cheminformatics, 2017, 9, 58.	6.1	7
20	Drug toxicity profiling of a Saccharomyces cerevisiae deubiquitinase deletion panel shows that acetaminophen mimics tyrosine. Toxicology in Vitro, 2018, 47, 259-268.	2.4	5