Nicolas Panel

List of Publications by Year in descending order

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NICOLAS PANEL

#	Article	IF	CITATIONS
1	Ligand design by targeting a binding site water. Chemical Science, 2021, 12, 960-968.	7.4	34
2	Computational Design of PDZ-Peptide Binding. Methods in Molecular Biology, 2021, 2256, 237-255.	0.9	3
3	Structureâ€Guided Design of Gâ€Proteinâ€Coupled Receptor Polypharmacology. Angewandte Chemie, 2021, 133, 18170-18178.	2.0	Ο
4	Structureâ€Guided Design of Gâ€Proteinâ€Coupled Receptor Polypharmacology. Angewandte Chemie - International Edition, 2021, 60, 18022-18030.	13.8	12
5	Positive allosteric mechanisms of adenosine A1 receptor-mediated analgesia. Nature, 2021, 597, 571-576.	27.8	84
6	Physics-Based Computational Protein Design: An Update. Journal of Physical Chemistry A, 2020, 124, 10637-10648.	2.5	16
7	A physics-based energy function allows the computational redesign of a PDZ domain. Scientific Reports, 2020, 10, 11150.	3.3	7
8	Adaptive landscape flattening in amino acid sequence space for the computational design of protein:peptide binding. Journal of Chemical Physics, 2018, 149, 072302.	3.0	22
9	Accurate PDZ/Peptide Binding Specificity with Additive and Polarizable Free Energy Simulations. Biophysical Journal, 2018, 114, 1091-1102.	0.5	30
10	Computational Design of the Tiam1 PDZ Domain and Its Ligand Binding. Journal of Chemical Theory and Computation, 2017, 13, 2271-2289.	5.3	12
11	A Simple PB/LIE Free Energy Function Accurately Predicts the Peptide Binding Specificity of the Tiam1 PDZ Domain. Frontiers in Molecular Biosciences, 2017, 4, 65.	3.5	10
12	Insight on Mutation-Induced Resistance from Molecular Dynamics Simulations of the Native and Mutated CSF-1R and KIT. PLoS ONE, 2016, 11, e0160165.	2.5	8
13	Protein side chain conformation predictions with an <scp>MMGBSA</scp> energy function. Proteins: Structure, Function and Bioinformatics, 2016, 84, 803-819.	2.6	21
14	Differential Effects of CSF-1R D802V and KIT D816V Homologous Mutations on Receptor Tertiary Structure and Allosteric Communication. PLoS ONE, 2014, 9, e97519.	2.5	11
15	Hotspot Mutations in KIT Receptor Differentially Modulate Its Allosterically Coupled Conformational Dynamics: Impact on Activation and Drug Sensitivity. PLoS Computational Biology, 2014, 10, e1003749.	3.2	27
16	Characterization of S628N. JAMA Dermatology, 2014, 150, 1345.	4.1	6