FranÃ§ois Dehez

List of Publications by Year
in descending order

55	1,874	279487	288905
papers	citations	23 h-index	40 g-index

58	58	58	2999
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Conformational transitions and ligand-binding to a muscle-type nicotinic acetylcholine receptor. Neuron, 2022, 110, 1358-1370.e5.	3.8	39
2	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	5.5	56
3	Computational Assessment of Proteinâ€“Protein Binding Specificity within a Family of Synaptic Surface Receptors. Journal of Physical Chemistry B, 2022, 126, 7510-7527.	1.2	6
4	Structure, substrate binding and symmetry of the mitochondrial ADP/ATP carrier in its matrix-open state. Biophysical Journal, 2021, 120, 5187-5195.	0.2	5
5	The Binding of Palonosetron and Other Antiemetic Drugs to the Serotonin 5-HT3 Receptor. Structure, 2020, 28, 1131-1140.e4.	1.6	20
6	Charge Transfer and Chemo-Mechanical Coupling in Respiratory Complex I. Journal of the American Chemical Society, 2020, 142, 9220-9230.	6.6	22
7	Chemomechanical Coupling of Mitochondrial Complex I. Biophysical Journal, 2019, 116, 155a.	0.2	0
8	Targeting G-quadruplexes with Organic Dyes: Chelerythrineâ€“DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. Antioxidants, 2019, 8, 472.	2.2	15
9	Molecular Bases of DNA Packaging in Bacteria Revealed by All-Atom Molecular Dynamics Simulations: The Case of Histone-Like Proteins inBorrelia burgdorferi. Journal of Physical Chemistry Letters, 2019, 10, 7200-7207.	2.1	19
10	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. Journal of Physical Chemistry Letters, 2019, 10, 7133-7140.	2.1	14
11	Mechanism of the allosteric activation of the ClpP protease machinery by substrates and active-site inhibitors. Science Advances, 2019, 5, eaaw3818.	4.7	41
12	Hepatitis C virus sequence divergence preserves p7 viroporin structural and dynamic features. Scientific Reports, 2019, 9, 8383.	1.6	13
13	Binding properties of the quaternary assembly protein SPAG1. Biochemical Journal, 2019, 476, 1679-1694.	1.7	9
14	The three Endonuclease III variants of Deinococcus radiodurans possess distinct and complementary DNA repair activities. DNA Repair, 2019, 78, 45-59.	1.3	17
15	Enthalpyâ€“Entropy Interplay in Ï€-Stacking Interaction of Benzene Dimer in Water. Journal of Chemical Theory and Computation, 2019, 15, 1538-1545.	2.3	16
16	Changes in Microenvironment Modulate the B- to A-DNA Transition. Journal of Chemical Information and Modeling, 2019, 59, 2324-2330.	2.5	11
17	Effects of hydration on the protonation state of a lysine analog crossing a phospholipid bilayer â€“ insights from molecular dynamics and free-energy calculations. Physical Chemistry Chemical Physics, 2018, 20, 9101-9107.	1.3	9
18	Perturbations of Native Membrane Protein Structure in Alkyl Phosphocholine Detergents: A Critical Assessment of NMR and Biophysical Studies. Chemical Reviews, 2018, 118, 3559-3607.	23.0	132

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19	How Detergent Impacts Membrane Proteins: Atomic-Level Views of Mitochondrial Carriers in Dodecylphosphocholine. Journal of Physical Chemistry Letters, 2018, 9, 933-938.	2.1	41
20	Modeling induction phenomena in amino acid cationâ€“ $$pi $$ Ï€ interactions. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	14
21	Re-evaluating the p7 viroporin structure. Nature, 2018, 562, E8-E18.	13.7	14
22	Conformational transitions of the serotonin 5-HT3 receptor. Nature, 2018, 563, 275-279.	13.7	128
23	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. Molecules, 2018, 23, 228.	1.7	85
24	Dynamics and interactions of AAC3 in DPC are not functionally relevant. Nature Structural and Molecular Biology, 2018, 25, 745-747.	3.6	8
25	Conformational changes of DNA induced by a trans-azobenzene derivative via non-covalent interactions. Physical Chemistry Chemical Physics, 2018, 20, 22645-22651.	1.3	5
26	Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. Nucleic Acids Research, 2017, 45, 3654-3662.	6.5	17
27	Structural and energetic study of cationâ€“Ï€â€“cation interactions in proteins. Physical Chemistry Chemical Physics, 2017, 19, 9849-9861.	1.3	19
28	Mitochondrial ADP/ATP Carrier in Dodecylphosphocholine Binds Cardiolipins with Non-native Affinity. Biophysical Journal, 2017, 113, 2311-2315.	0.2	18
29	Deciphering the photosensitization mechanisms of hypericin towards biological membranes. Physical Chemistry Chemical Physics, 2017, 19, 23187-23193.	1.3	18
30	Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. Physical Chemistry Chemical Physics, 2016, 18, 33180-33186.	1.3	10
31	Repair Rate of Clustered Abasic DNA Lesions by Human Endonuclease: Molecular Bases of Sequence Specificity. Journal of Physical Chemistry Letters, 2016, 7, 3760-3765.	2.1	30
32	Correlation of bistranded clustered abasic DNA lesion processing with structural and dynamic DNA helix distortion. Nucleic Acids Research, 2016, 44, 8588-8599.	6.5	37
33	Assessing the physiological relevance of alternate architectures of the p7 protein of hepatitis C virus in different environments. Bioorganic and Medicinal Chemistry, 2016, 24, 4920-4927.	1.4	9
34	Molecular simulation: a virtual microscope in the toolbox of integrated structural biology. , 2016, , 413-436.		0
35	Evidence of Conducting Hydrophobic Nanopores Across Membranes in Response to an Electric Field. Journal of Physical Chemistry C, 2014, 118, 6752-6757.	1.5	38
36	On the Electroporation Thresholds of Lipid Bilayers: Molecular Dynamics Simulation Investigations. Journal of Membrane Biology, 2013, 246, 843-850.	1.0	54

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37	How Do Membrane Transporters Sense pH? The Case of the Mitochondrial ADPâ€“ATP Carrier. Journal of Physical Chemistry Letters, 2013, 4, 3787-3791.	2.1	9
38	Dangerous Liaisons between Detergents and Membrane Proteins. The Case of Mitochondrial Uncoupling Protein 2. Journal of the American Chemical Society, 2013, 135, 15174-15182.	6.6	86
39	The substrate specificity of the human ADP/ATP carrier AAC1. Molecular Membrane Biology, 2013, 30, 160-168.	2.0	50
40	Effects of Phospholipid Composition on the Transfer of a Small Cationic Peptide Across a Model Biological Membrane. Journal of Chemical Theory and Computation, 2013, 9, 5675-5684.	2.3	25
41	Water Conduction through a Peptide Nanotube. Journal of Physical Chemistry C, 2013, 117, 26797-26803.	1.5	30
42	An â€˜openâ€™ structure of the RecOR complex supports ssDNA binding within the core of the complex. Nucleic Acids Research, 2013, 41, 7972-7986.	6.5	19
43	A Toolkit for the Analysis of Free-Energy Perturbation Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2606-2616.	2.3	153
44	Impaired Transport of Nucleotides in a Mitochondrial Carrier Explains Severe Human Genetic Diseases. ACS Chemical Biology, 2012, 7, 1164-1169.	1.6	13
45	Polarization effects in molecular interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 844-854.	6.2	28
46	Polarizable Intermolecular Potentials for Water and Benzene Interacting with Halide and Metal Ions. Journal of Chemical Theory and Computation, 2009, 5, 3022-3031.	2.3	34
47	High-Chloride Concentrations Abolish the Binding of Adenine Nucleotides in the Mitochondrial ADP/ATP Carrier Family. Biophysical Journal, 2009, 97, L25-L27.	0.2	20
48	Binding of ADP in the Mitochondrial ADP/ATP Carrier Is Driven by an Electrostatic Funnel. Journal of the American Chemical Society, 2008, 130, 12725-12733.	6.6	130
49	Modeling Membranes under a Transmembrane Potential. Journal of Physical Chemistry B, 2008, 112, 5547-5550.	1.2	94
50	An ab initio strategy for handling induction phenomena in metal ion complexes. Molecular Physics, 2008, 106, 1685-1696.	0.8	3
51	Energetics of Ion Transport in a Peptide Nanotube. Journal of Physical Chemistry B, 2007, 111, 10633-10635.	1.2	49
52	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913.	2.3	41
53	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. Journal of Chemical Theory and Computation, 2007, 3, 1914-1926.	2.3	34
54	Alternative Approaches for the Calculation of Induction Energies:Â Characterization, Effectiveness, and Pitfalls. Journal of Physical Chemistry A, 2001, 105, 11505-11514.	1.1	23

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55	Distributed polarizabilities derived from induction energies: A finite perturbation approach. Journal of Chemical Physics, 2000, 112, 2709-2717.	1.2	40