# 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 | A Toolkit for the Analysis of Free-Energy Perturbation Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2606-2616. | 2.3 | 153 |
| 2 | 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 |
| 3 | 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 |
| 4 | Conformational transitions of the serotonin 5-HT3 receptor. Nature, 2018, 563, 275-279. | 13.7 | 128 |
| 5 | Modeling Membranes under a Transmembrane Potential. Journal of Physical Chemistry B, 2008, 112, 5547-5550. | 1.2 | 94 |
| 6 | 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 |
| 7 | Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. Molecules, 2018, 23, 228. | 1.7 | 85 |
| 8 | Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141. | 5.5 | 56 |
| 9 | On the Electroporation Thresholds of Lipid Bilayers: Molecular Dynamics Simulation Investigations. Journal of Membrane Biology, 2013, 246, 843-850. | 1.0 | 54 |
| 10 | The substrate specificity of the human ADP/ATP carrier AAC1. Molecular Membrane Biology, 2013, 30, 160-168. | 2.0 | 50 |
| 11 | Energetics of Ion Transport in a Peptide Nanotube. Journal of Physical Chemistry B, 2007, 111, 10633-10635. | 1.2 | 49 |
| 12 | Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913. | 2.3 | 41 |
| 13 | 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 |
| 14 | Mechanism of the allosteric activation of the ClpP protease machinery by substrates and active-site inhibitors. Science Advances, 2019, 5, eaaw3818. | 4.7 | 41 |
| 15 | Distributed polarizabilities derived from induction energies: A finite perturbation approach. Journal of Chemical Physics, 2000, 112, 2709-2717. | 1.2 | 40 |
| 16 | Conformational transitions and ligand-binding to a muscle-type nicotinic acetylcholine receptor. Neuron, 2022, 110, 1358-1370.e5. | 3.8 | 39 |
| 17 | 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 |
| 18 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | Water Conduction through a Peptide Nanotube. Journal of Physical Chemistry C, 2013, 117, 26797-26803. | 1.5 | 30 |
| 22 | 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 |
| 23 | Polarization effects in molecular interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 844-854. | 6.2 | 28 |
| 24 | 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 |
| 25 | 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 |
| 26 | Charge Transfer and Chemo-Mechanical Coupling in Respiratory Complex I. Journal of the American Chemical Society, 2020, 142, 9220-9230. | 6.6 | 22 |
| 27 | 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 |
| 28 | The Binding of Palonosetron and Other Antiemetic Drugs to the Serotonin 5-HT3 Receptor. Structure, 2020, 28, 1131-1140.e4. | 1.6 | 20 |
| 29 | 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 |
| 30 | Structural and energetic study of cationâ€“Ï€â€“cation interactions in proteins. Physical Chemistry Chemical Physics, 2017, 19, 9849-9861. | 1.3 | 19 |
| 31 | 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 |
| 32 | Mitochondrial ADP/ATP Carrier in Dodecylphosphocholine Binds Cardiolipins with Non-native Affinity. Biophysical Journal, 2017, 113, 2311-2315. | 0.2 | 18 |
| 33 | Deciphering the photosensitization mechanisms of hypericin towards biological membranes. Physical Chemistry Chemical Physics, 2017, 19, 23187-23193. | 1.3 | 18 |
| 34 | Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. Nucleic Acids Research, 2017, 45, 3654-3662. | 6.5 | 17 |
| 35 | The three Endonuclease III variants of Deinococcus radiodurans possess distinct and complementary DNA repair activities. DNA Repair, 2019, 78, 45-59. | 1.3 | 17 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Targeting G-quadruplexes with Organic Dyes: Chelerythrineâ€“DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. Antioxidants, 2019, 8, 472. | 2.2 | 15 |
| 38 | Modeling induction phenomena in amino acid cationâ€“ $$pi $$ Ï€ interactions. Theoretical Chemistry Accounts, 2018, 137, 1. | 0.5 | 14 |
| 39 | Re-evaluating the p7 viroporin structure. Nature, 2018, 562, E8-E18. | 13.7 | 14 |
| 40 | Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. Journal of Physical Chemistry Letters, 2019, 10, 7133-7140. | 2.1 | 14 |
| 41 | Impaired Transport of Nucleotides in a Mitochondrial Carrier Explains Severe Human Genetic Diseases. ACS Chemical Biology, 2012, 7, 1164-1169. | 1.6 | 13 |
| 42 | Hepatitis C virus sequence divergence preserves p7 viroporin structural and dynamic features. Scientific Reports, 2019, 9, 8383. | 1.6 | 13 |
| 43 | Changes in Microenvironment Modulate the B- to A-DNA Transition. Journal of Chemical Information and Modeling, 2019, 59, 2324-2330. | 2.5 | 11 |
| 44 | Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. Physical Chemistry Chemical Physics, 2016, 18, 33180-33186. | 1.3 | 10 |
| 45 | 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 |
| 46 | 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 |
| 47 | 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 |
| 48 | Binding properties of the quaternary assembly protein SPAG1. Biochemical Journal, 2019, 476, 1679-1694. | 1.7 | 9 |
| 49 | Dynamics and interactions of AAC3 in DPC are not functionally relevant. Nature Structural and Molecular Biology, 2018, 25, 745-747. | 3.6 | 8 |
| 50 | 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 |
| 51 | 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 |
| 52 | 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 |
| 53 | An ab initio strategy for handling induction phenomena in metal ion complexes. Molecular Physics, 2008, 106, 1685-1696. | 0.8 | 3 |
| 54 | Chemomechanical Coupling of Mitochondrial Complex I. Biophysical Journal, 2019, 116, 155a. | 0.2 | 0 |

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|---|---|---|---|
| 55 | Molecular simulation: a virtual microscope in the toolbox of integrated structural biology. , 2016, , 413-436. | | 0 |