Annick Dejaegere

List of Publications by Year
in descending order

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45	1,983	304743	243625
papers	citations	22 h-index	44 g-index

46	46	46	2656
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Frontier Bonds in QM/MM Methods: A Comparison of Different Approaches. Journal of Physical Chemistry A, 2000, 104, 1720-1735.	2.5	367
2	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	3.3	285
3	Theoretical Evaluation of pKain Phosphoranes:Â Implications for Phosphate Ester Hydrolysis. Journal of the American Chemical Society, 2002, 124, 5010-5018.	13.7	120
4	Protein/Ligand Binding Free Energies Calculated with Quantum Mechanics/Molecular Mechanics. Journal of Physical Chemistry B, 2005, 109, 10474-10483.	2.6	97
5	Protein-protein recognition and interaction hot spots in an antigen-antibody complex: Free energy decomposition identifies â€œefficient amino acidsâ€• Proteins: Structure, Function and Bioinformatics, 2007, 67, 418-434.	2.6	92
6	Nucleophilic Attack on Phosphate Diesters:Â A Density Functional Study of Inâ^'Line Reactivity in Dianionic, Monoanionic, and Neutral Systems. Journal of Physical Chemistry B, 2006, 110, 11525-11539.	2.6	71
7	Dual Specificity of the Interfacial Inhibitor Brefeldin A for Arf Proteins and Sec7 Domains. Journal of Biological Chemistry, 2006, 281, 11805-11814.	3.4	71
8	Hydrolysis rate difference between cyclic and acyclic phosphate esters: solvation versus strain. Journal of the American Chemical Society, 1993, 115, 5316-5317.	13.7	70
9	Phosphate ester hydrolysis: calculation of gas-phase reaction paths and solvation effects. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1763.	1.7	69
10	The â€œPhantom Effectâ€•of the Rexinoid LG100754: Structural and Functional Insights. PLoS ONE, 2010, 5, e15119.	2.5	64
11	Solvent Effects on the Reaction Coordinate of the Hydrolysis of Phosphates and Sulfates:Â Application of Hammond and Anti-Hammond Postulates to Understand Hydrolysis in Solution. Journal of the American Chemical Society, 2001, 123, 11755-11763.	13.7	53
12	Structural Insights into the Molecular Mechanism of Vitamin D Receptor Activation by Lithocholic Acid Involving a New Mode of Ligand Recognition. Journal of Medicinal Chemistry, 2014, 57, 4710-4719.	6.4	46
13	Theoretical studies on the hydrolysis of phosphate diesters in the gas phase, solution, and RNase A. International Journal of Quantum Chemistry, 2002, 86, 10-26.	2.0	41
14	On the Affinity Regulation of the Metal-Ion-Dependent Adhesion Sites in Integrins. Journal of the American Chemical Society, 2006, 128, 3554-3563.	13.7	39
15	The Asymmetric Binding of PGC-1Î± to the ERRÎ± and ERRÎ³ Nuclear Receptor Homodimers Involves a Similar Recognition Mechanism. PLoS ONE, 2013, 8, e67810.	2.5	34
16	Structural Basis for the Accommodation of Bis- and Tris-Aromatic Derivatives in Vitamin D Nuclear Receptor. Journal of Medicinal Chemistry, 2012, 55, 8440-8449.	6.4	30
17	Differential Modes of Peptide Binding onto Replicative Sliding Clamps from Various Bacterial Origins. Journal of Medicinal Chemistry, 2014, 57, 7565-7576.	6.4	29
18	Structure Activity Relationship by NMR and by Computer:Â A Comparative Study. Journal of the American Chemical Society, 2002, 124, 11073-11084.	13.7	27

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19	Structure-Based Design of Short Peptide Ligands Binding onto the E. coli Processivity Ring. Journal of Medicinal Chemistry, 2011, 54, 4627-4637.	6.4	26
20	Comparative Normal Mode Analysis of LFA-1 Integrin I-domains. Journal of Molecular Biology, 2007, 374, 231-249.	4.2	25
21	Molecular Basis for Bcl-2 Homology 3 Domain Recognition in the Bcl-2 Protein Family. Journal of Biological Chemistry, 2009, 284, 17499-17511.	3.4	25
22	Force field parameters for the simulation of modified histone tails. Journal of Computational Chemistry, 2010, 31, 2434-2451.	3.3	24
23	Phosphorylation of the Retinoic Acid Receptor Alpha Induces a Mechanical Allosteric Regulation and Changes in Internal Dynamics. PLoS Computational Biology, 2013, 9, e1003012.	3.2	24
24	Histone H3 Tails Containing Dimethylated Lysine and Adjacent Phosphorylated Serine Modifications Adopt a Specific Conformation during Mitosis and Meiosis. Molecular and Cellular Biology, 2008, 28, 1739-1754.	2.3	23
25	Evolution of Nuclear Retinoic Acid Receptor Alpha (RARÂ) Phosphorylation Sites. Serine Gain Provides Fine-Tuned Regulation. Molecular Biology and Evolution, 2011, 28, 2125-2137.	8.9	23
26	Design, Synthesis, and Functional Evaluation of Leukocyte Function Associated Antigen-1 Antagonists in Early and Late Stages of Cancer Development. Journal of Medicinal Chemistry, 2013, 56, 735-747.	6.4	21
27	Functional relationship between matrix metalloproteinaseâ€11 and matrix metalloproteinaseâ€14. Cancer Medicine, 2014, 3, 1197-1210.	2.8	21
28	Mechanism of Alkaline Hydrolysis of Cyclic and Acyclic Sulfates:â€‰ An ab Initio Study with Solvation Correction. Journal of the American Chemical Society, 1999, 121, 5548-5558.	13.7	19
29	Alternative dimerization interfaces in the glucocorticoid receptor-Î± ligand binding domain. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1810-1825.	2.4	18
30	Dynamics of Î²3 integrin Iâ€like and hybrid domains: Insight from simulations on the mechanism of transition between open and closed forms. Proteins: Structure, Function and Bioinformatics, 2009, 76, 977-994.	2.6	17
31	Dynamic correlation networks in human peroxisome proliferator-activated receptor-Î³ nuclear receptor protein. European Biophysics Journal, 2010, 39, 1503-1512.	2.2	15
32	Quantitative sampling of conformational heterogeneity of a DNA hairpin using molecular dynamics simulations and ultrafast fluorescence spectroscopy. Nucleic Acids Research, 2016, 44, 3408-3419.	14.5	14
33	Challenges in pKa Predictions for Proteins: The case of Asp213 in Human Proteinase 3. Journal of Physical Chemistry A, 2009, 113, 11783-11792.	2.5	12
34	Protein Structural Statistics with PSS. Journal of Chemical Information and Modeling, 2013, 53, 2471-2482.	5.4	11
35	Agonistic and potentiating effects of perfluoroalkyl substances (PFAS) on the Atlantic cod (Gadus) Tj ETQq1 1 0.784314 rgBT /Overlo 107203.	10.0	11
36	PSSweb: protein structural statistics web server. Nucleic Acids Research, 2016, 44, W401-W405.	14.5	8

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37	Self-Associating Peptides for Modular Bifunctional Conjugation of Tetramer Macromolecules in Living Cells. Bioconjugate Chemistry, 2019, 30, 1734-1744.	3.6	7
38	Molecular dynamics for computational proteomics of methylated histone H3. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1026-1040.	2.4	6
39	Allosteric Regulation in the Ligand Binding Domain of Retinoic Acid Receptorî³. PLoS ONE, 2017, 12, e0171043.	2.5	6
40	Interaction of a Model Peptide on Gram Negative and Gram Positive Bacterial Sliding Clamps. ACS Infectious Diseases, 2019, 5, 1022-1034.	3.8	6
41	Insights into mineralocorticoid receptor homodimerization from a combined molecular modeling and bioinformatics study. Proteins: Structure, Function and Bioinformatics, 2021, 89, 952-965.	2.6	6
42	Magnetic Effects of Disulfide Bridges:Â A Density Functional and Semiempirical Study. Journal of Physical Chemistry B, 2005, 109, 3627-3638.	2.6	5
43	Tex19 and Sectm1 concordant molecular phylogenies support co-evolution of both eutherian-specific genes. BMC Evolutionary Biology, 2015, 15, 222.	3.2	2
44	Unrolr: Structural analysis of protein conformations using stochastic proximity embedding. Journal of Computational Chemistry, 2018, 39, 2551-2557.	3.3	2
45	Metal Ion Dependent Adhesion Sites in Integrins:â€‰A Combined DFT and QMC Study on Mn2+. Journal of Physical Chemistry B, 2007, 111, 9099-9103.	2.6	1