Xavier Daura

List of Publications by Year
in descending order

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127 papers	9,670 citations	76196 40 h-index	45213 90 g-index
138 all docs	138 docs citations	138 times ranked	10308 citing authors

#	Article	IF	Citations
1	Peptide Folding: When Simulation Meets Experiment. Angewandte Chemie - International Edition, 1999, 38, 236-240.	7.2	1,611
2	AGGRESCAN: a server for the prediction and evaluation of "hot spots" of aggregation in polypeptides. BMC Bioinformatics, 2007, 8, 65.	1.2	845
3	An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. Journal of Computational Chemistry, 2001, 22, 1205-1218.	1.5	814
4	Biomolecular Modeling: Goals, Problems, Perspectives. Angewandte Chemie - International Edition, 2006, 45, 4064-4092.	7.2	503
5	Reversible peptide folding in solution by molecular dynamics simulation 1 1Edited by R. Huber. Journal of Molecular Biology, 1998, 280, 925-932.	2.0	379
6	Parametrization of aliphatic CHn united atoms of GROMOS96 force field. , 1998, 19, 535-547.		370
7	Folding-unfolding thermodynamics of a ?-heptapeptide from equilibrium simulations. , 1999, 34, 269-280.		370
8	Derivation of an improved simple point charge model for liquid water: SPC/A and SPC/L. Journal of Chemical Physics, 2002, 116, 9811-9828.	1.2	203
9	Îhe Î²-Peptide Hairpin in Solution:Â Conformational Study of a Î²-Hexapeptide in Methanol by NMR Spectroscopy and MD Simulation. Journal of the American Chemical Society, 2001, 123, 2393-2404.	6.6	193
10	Can One Derive the Conformational Preference of a Î²-Peptide from Its CD Spectrum?. Journal of the American Chemical Society, 2002, 124, 12972-12978.	6.6	162
11	Assessing equilibration and convergence in biomolecular simulations. Proteins: Structure, Function and Bioinformatics, 2002, 48, 487-496.	1.5	128
12	Essential dynamics of reversible peptide folding: memory-free conformational dynamics governed by internal hydrogen bonds. Journal of Molecular Biology, 2001, 309, 299-313.	2.0	126
13	The Key to Solving the Protein-Folding Problem Lies in an Accurate Description of the Denatured State. Angewandte Chemie - International Edition, 2001, 40, 351-355.	7.2	124
14	Studying the Stability of a Helical Î²â€Heptapeptide by Molecular Dynamics Simulations. Chemistry - A European Journal, 1997, 3, 1410-1417.	1.7	120
15	PARS: a web server for the prediction of Protein Allosteric and Regulatory Sites. Bioinformatics, 2014, 30, 1314-1315.	1.8	117
16	Comparing geometric and kinetic cluster algorithms for molecular simulation data. Journal of Chemical Physics, 2010, 132, 074110.	1.2	110
17	The effect of motional averaging on the calculation of NMR-derived structural properties. , 1999, 36, 542-555.		103
18	Validation of Molecular Simulation: An Overview of Issues. Angewandte Chemie - International Edition, 2018, 57, 884-902.	7.2	101

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19	Structure and Conformation ofÎ²-Oligopeptide Derivatives with Simple Proteinogenic Side Chains: Circular Dichroism and Molecular Dynamics Investigations. Helvetica Chimica Acta, 2000, 83, 34-57.	1.0	100
20	Computation of Free Energy. Helvetica Chimica Acta, 2002, 85, 3113-3129.	1.0	99
21	Configurational entropy elucidates the role of salt-bridge networks in protein thermostability. Protein Science, 2007, 16, 1349-1359.	3.1	99
22	Entropy calculations on a reversibly folding peptide: Changes in solute free energy cannot explain folding behavior. Proteins: Structure, Function and Bioinformatics, 2001, 43, 45-56.	1.5	97
23	Calculation of NMR-relaxation parameters for flexible molecules from molecular dynamics simulations. Journal of Biomolecular NMR, 2001, 20, 297-310.	1.6	89
24	In Vivo Architectonic Stability of Fully de Novo Designed Protein-Only Nanoparticles. ACS Nano, 2014, 8, 4166-4176.	7.3	89
25	Validation of the GROMOS force-field parameter set 45A3 against nuclear magnetic resonance data of hen egg lysozyme. Journal of Biomolecular NMR, 2004, 30, 407-422.	1.6	87
26	Understanding the Molecular Determinants Driving the Immunological Specificity of the Protective Pilus 2a Backbone Protein of Group B Streptococcus. PLoS Computational Biology, 2013, 9, e1003115.	1.5	82
27	The phylogenetic landscape and nosocomial spread of the multidrug-resistant opportunist Stenotrophomonas maltophilia. Nature Communications, 2020, 11, 2044.	5.8	76
28	PrionW: a server to identify proteins containing glutamine/asparagine rich prion-like domains and their amyloid cores. Nucleic Acids Research, 2015, 43, W331-W337.	6.5	74
29	Molecular Dynamics Simulations of a Reversibly Folding Î²-Heptapeptide in Methanol: Influence of the Treatment of Long-Range Electrostatic Interactions. Journal of Physical Chemistry B, 2009, 113, 3112-3128.	1.2	72
30	Exploiting protein flexibility to predict the location of allosteric sites. BMC Bioinformatics, 2012, 13, 273.	1.2	72
31	Bottomâ€Up Instructive Quality Control in the Biofabrication of Smart Protein Materials. Advanced Materials, 2015, 27, 7816-7822.	11.1	61
32	Peptides of Aminoxy Acids:â€‰ A Molecular Dynamics Simulation Study of Conformational Equilibria under Various Conditions. Journal of the American Chemical Society, 2000, 122, 7461-7466.	6.6	60
33	Protein nanodisk assembling and intracellular trafficking powered by an arginine-rich (R9) peptide. Nanomedicine, 2010, 5, 259-268.	1.7	59
34	Peptide Folding: When Simulation Meets Experiment. , 1999, 38, 236.		57
35	Two Different rpf Clusters Distributed among a Population of Stenotrophomonas maltophilia Clinical Strains Display Differential Diffusible Signal Factor Production and Virulence Regulation. Journal of Bacteriology, 2014, 196, 2431-2442.	1.0	55
36	HLA and microtubule-associated protein tau H1 haplotype associations in anti-IgLON5 disease. Neurology: Neuroimmunology and NeuroInflammation, 2019, 6, .	3.1	55

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37	Circular dichroism spectra of Î²-peptides: sensitivity to molecular structure and effects of motional averaging. European Biophysics Journal, 2003, 32, 661-670.	1.2	53
38	Effect of Oxidative Damage on the Stability and Dimerization of Superoxide Dismutase 1. Biophysical Journal, 2016, 110, 1499-1509.	0.2	53
39	Free Energies of Transfer of Trp Analogs from Chloroform to Water:Â Comparison of Theory and Experiment and the Importance of Adequate Treatment of Electrostatic and Internal Interactions. Journal of the American Chemical Society, 1996, 118, 6285-6294.	6.6	52
40	The Role of Hydration in Protein Stability: Comparison of the Cold and Heat Unfolded States of Yfh1. Journal of Molecular Biology, 2012, 417, 413-424.	2.0	52
41	Exploiting the Burkholderia pseudomallei Acute Phase Antigen BPSL2765 for Structure-Based Epitope Discovery/Design in Structural Vaccinology. Chemistry and Biology, 2013, 20, 1147-1156.	6.2	50
42	A Structure-Based Strategy for Epitope Discovery in Burkholderia pseudomallei OppA Antigen. Structure, 2013, 21, 167-175.	1.6	49
43	Thyroglobulin Peptides Associate In Vivo to HLA-DR in Autoimmune Thyroid Glands. Journal of Immunology, 2008, 181, 795-807.	0.4	48
44	Exploiting Antigenic Diversity for Vaccine Design. Journal of Biological Chemistry, 2010, 285, 30126-30138.	1.6	44
45	Folding study of an Aib-rich peptide in DMSO by molecular dynamics simulations. Chemical Biology and Drug Design, 2001, 57, 107-118.	1.2	42
46	From crystal structure to inÂsilico epitope discovery in the BurkholderiaÂpseudomallei flagellar hookâ€associated protein FlgK. FEBS Journal, 2015, 282, 1319-1333.	2.2	42
47	Unfolded state of peptides. Advances in Protein Chemistry, 2002, 62, 341-360.	4.4	40
48	Sequence- and Structure-Based Immunoreactive Epitope Discovery for Burkholderia pseudomallei Flagellin. PLoS Neglected Tropical Diseases, 2015, 9, e0003917.	1.3	40
49	Quorum Sensing Signaling and Quenching in the Multidrug-Resistant Pathogen Stenotrophomonas maltophilia. Frontiers in Cellular and Infection Microbiology, 2018, 8, 122.	1.8	39
50	Validation of molecular simulation by comparison with experiment: Rotational reorientation of tryptophan in water. Journal of Chemical Physics, 1999, 110, 3049-3055.	1.2	38
51	Stenotrophomonas maltophilia responds to exogenous AHL signals through the LuxR solo SmoR (Smlt1839). Frontiers in Cellular and Infection Microbiology, 2015, 5, 41.	1.8	38
52	On the sensitivity of MD trajectories to changes in water-protein interaction parameters: The potato carboxypeptidase inhibitor in water as a test case for the GROMOS force field. , 1996, 25, 89-103.		37
53	Decoding the genetic and functional diversity of the DSF quorum-sensing system in Stenotrophomonas maltophilia. Frontiers in Microbiology, 2015, 6, 761.	1.5	37
54	Peptide folding simulations: no solvent required?. Computer Physics Communications, 1999, 123, 97-102.	3.0	35

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55	The rheumatoid arthritisâ€“associated allele HLAâ€“DR10 (DRB1*1001) shares part of its repertoire with HLAâ€“DR1 (DRB1*0101) and HLAâ€“DR4 (DRB*0401). Arthritis and Rheumatism, 2008, 58, 1630-1639.	6.7	34
56	Assessing the structural conservation of protein pockets to study functional and allosteric sites: implications for drug discovery. BMC Structural Biology, 2010, 10, 9.	2.3	34
57	Abundance of the Quorum-Sensing Factor Ax21 in Four Strains of Stenotrophomonas maltophilia Correlates with Mortality Rate in a New Zebrafish Model of Infection. PLoS ONE, 2013, 8, e67207.	1.1	33
58	Heterogeneous Colistin-Resistance Phenotypes Coexisting in Stenotrophomonas maltophilia Isolates Influence Colistin Susceptibility Testing. Frontiers in Microbiology, 2018, 9, 2871.	1.5	29
59	A strategy for analysis of (molecular) equilibrium simulations: Configuration space density estimation, clustering, and visualization. Journal of Chemical Physics, 2001, 114, 2079-2089.	1.2	28
60	Procarboxypeptidase A from the insect pestHelicoverpa armigeraand its derived enzyme. FEBS Journal, 2003, 270, 3026-3035.	0.2	27
61	Sheltering DNA in self-organizing, protein-only nano-shells as artificial viruses for gene delivery. Nanomedicine: Nanotechnology, Biology, and Medicine, 2014, 10, 535-541.	1.7	27
62	Î²-Hairpin folding and stability: molecular dynamics simulations of designed peptides in aqueous solution. Journal of Peptide Science, 2004, 10, 546-565.	0.8	26
63	Enhanced Conformational Sampling in Molecular Dynamics Simulations of Solvated Peptides: Fragment-Based Local Elevation Umbrella Sampling. Journal of Chemical Theory and Computation, 2010, 6, 2598-2621.	2.3	25
64	Molecular dynamics simulation study of the effect of glycerol dialkyl glycerol tetraether hydroxylation on membrane thermostability. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 966-974.	1.4	25
65	Human Leukocyte Antigen (HLA)-DRB1*15:01 and HLA-DRB5*01:01 Present Complementary Peptide Repertoires. Frontiers in Immunology, 2017, 8, 984.	2.2	25
66	A novel approach for designing simple point charge models for liquid water with three interaction sites. Journal of Computational Chemistry, 2003, 24, 1087-1096.	1.5	24
67	Deriving Structural Information from Experimentally Measured Data on Biomolecules. Angewandte Chemie - International Edition, 2016, 55, 15990-16010.	7.2	24
68	-Peptides with Different Secondary-Structure Preferences: How Different Are Their Conformational Spaces?. Helvetica Chimica Acta, 2002, 85, 3872-3882.	1.0	23
69	On the Influence of Charged Side Chains on the Foldingâ€“Unfolding Equilibrium of Î²-Peptides: A Molecular Dynamics Simulation Study. Chemistry - A European Journal, 2005, 11, 7276-7293.	1.7	23
70	EsiB, a Novel Pathogenic Escherichia coli Secretory Immunoglobulin A-Binding Protein Impairing Neutrophil Activation. MBio, 2013, 4, .	1.8	22
71	Genetic Variants of the DSF Quorum Sensing System in Stenotrophomonas maltophilia Influence Virulence and Resistance Phenotypes Among Genotypically Diverse Clinical Isolates. Frontiers in Microbiology, 2020, 11, 1160.	1.5	22
72	Stability of SIV gp32 Fusionâ€Peptide Singleâ€Layer Protofibrils as Monitored by Molecularâ€Dynamics Simulations. Angewandte Chemie - International Edition, 2005, 44, 1065-1067.	7.2	21

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73	Molecular Dynamics Simulation of Peptide Folding. Theoretical Chemistry Accounts, 2006, 116, 297-306.	0.5	20
74	The Key to Solving the Protein-Folding Problem Lies in an Accurate Description of the Denatured State Financial support from the Schweizerischer Nationalfonds (Project no. 21-50929.97) is gratefully acknowledged.. Angewandte Chemie - International Edition, 2001, 40, 351-355.	7.2	20
75	Molecular dynamics simulations of peptides containing an unnatural amino acid: Dimerization, folding, and protein binding. Proteins: Structure, Function and Bioinformatics, 2003, 54, 116-127.	1.5	17
76	Molecular-Dynamics Simulations of C- and N-Terminal Peptide Derivatives of GCN4-p1 in Aqueous Solution. Chemistry and Biodiversity, 2005, 2, 1086-1104.	1.0	17
77	Crystal structure of c5321: a protective antigen present in uropathogenic Escherichia coli strains displaying an SLR fold. BMC Structural Biology, 2013, 13, 19.	2.3	17
78	Proteomic analysis of outer membrane proteins and vesicles of a clinical isolate and a collection strain of Stenotrophomonas maltophilia. Journal of Proteomics, 2016, 142, 122-129.	1.2	17
79	Estimating the Temperature Dependence of Peptide Folding Entropies and Free Enthalpies from Total Energies in Molecular Dynamics Simulations. Chemistry - A European Journal, 2008, 14, 5039-5046.	1.7	16
80	Structural and Biochemical Characterization of NarE, an Iron-containing ADP-ribosyltransferase from Neisseria meningitidis. Journal of Biological Chemistry, 2011, 286, 14842-14851.	1.6	16
81	RGD-based cell ligands for cell-targeted drug delivery act as potent trophic factors. Nanomedicine: Nanotechnology, Biology, and Medicine, 2012, 8, 1263-1266.	1.7	16
82	Methods to Develop an in silico Clinical Trial: Computational Head-to-Head Comparison of Lisdexamfetamine and Methylphenidate. Frontiers in Psychiatry, 2021, 12, 741170.	1.3	16
83	Conformational and functional variants of CD44-targeted protein nanoparticles bio-produced in bacteria. Biofabrication, 2016, 8, 025001.	3.7	15
84	Sulfonamide-based diffusible signal factor analogs interfere with quorum sensing in Stenotrophomonas maltophilia and Burkholderia cepacia. Future Medicinal Chemistry, 2019, 11, 1565-1582.	1.1	15
85	The Pseudomonas aeruginosa substrate-binding protein Ttg2D functions as a general glycerophospholipid transporter across the periplasm. Communications Biology, 2021, 4, 448.	2.0	15
86	Nanoparticulate architecture of protein-based artificial viruses is supported by proteinâ€“DNA interactions. Nanomedicine, 2011, 6, 1047-1061.	1.7	14
87	Advances in the Computational Identification of Allosteric Sites and Pathways in Proteins. Advances in Experimental Medicine and Biology, 2019, 1163, 141-169.	0.8	14
88	Reply. Angewandte Chemie - International Edition, 2001, 40, 4616-4618.	7.2	13
89	Interaction of camel Lactoferrin derived peptides with DNA: a molecular dynamics study. BMC Genomics, 2020, 21, 60.	1.2	13
90	An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase. , 2001, 22, 1205.		13

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91	Structure-Based Design of a B Cell Antigen from B. pseudomallei. ACS Chemical Biology, 2015, 10, 803-812.	1.6	12
92	The fusogenic peptide HA2 impairs selectivity of CXCR4-targeted protein nanoparticles. Chemical Communications, 2017, 53, 4565-4568.	2.2	12
93	On the Effect of the Various Assumptions and Approximations used in Molecular Simulations on the Properties of Bioâ€Molecular Systems: Overview and Perspective on Issues. ChemPhysChem, 2021, 22, 264-282.	1.0	12
94	Factor Xa: simulation studies with an eye to inhibitor design. Journal of Computer-Aided Molecular Design, 2000, 14, 507-529.	1.3	11
95	BPSL1626: Reverse and Structural Vaccinology Reveal a Novel Candidate for Vaccine Design Against Burkholderia pseudomallei. Antibodies, 2018, 7, 26.	1.2	11
96	Aggregation-prone peptides modulate activity of bovine interferon gamma released from naturally occurring protein nanoparticles. New Biotechnology, 2020, 57, 11-19.	2.4	11
97	A generalized Langevin dynamics approach to model solvent dynamics effects on proteins via a solvent-accessible surface. The carboxypeptidase A inhibitor protein as a model. Theoretical Chemistry Accounts, 2000, 105, 101-109.	0.5	10
98	Oligonucleotide Analogues with a Nucleobase-Including Backbone, Part 7, Molecular Dynamics Simulation of a DNA Duplex Containing a 2â€²-Deoxyadenosine 8-(Hydroxymethyl)-Derived Nucleotide. Helvetica Chimica Acta, 2001, 84, 2132-2145.	1.0	10
99	Free energy calculations offer insights into the influence of receptor flexibility on ligandâ€“receptor binding affinities. Journal of Computer-Aided Molecular Design, 2011, 25, 709-716.	1.3	10
100	antibacTR: dynamic antibacterial-drug-target ranking integrating comparative genomics, structural analysis and experimental annotation. BMC Genomics, 2014, 15, 36.	1.2	10
101	A Comparative Analysis of the Peptide Repertoires of HLAâ€“DR Molecules Differentially Associated With Rheumatoid Arthritis. Arthritis and Rheumatology, 2016, 68, 2412-2421.	2.9	10
102	A Molecular Dynamics Simulation of the Binding Modes of d-Glutamate and d-Glutamine to Glutamate Racemase. Journal of Chemical Theory and Computation, 2005, 1, 737-749.	2.3	9
103	On the Relative Merits of Equilibrium and Nonâ€Equilibrium Simulations for the Estimation of Freeâ€Energy Differences. ChemPhysChem, 2010, 11, 3734-3743.	1.0	9
104	Disulfide Bond Formation and Activation of Escherichia coli Î²-Galactosidase under Oxidizing Conditions. Applied and Environmental Microbiology, 2012, 78, 2376-2385.	1.4	9
105	Structure and atomic fluctuation patterns of potato carboxypeptidase a inhibitor protein. European Biophysics Journal, 1995, 24, 1-11.	1.2	7
106	Bestimmung von Strukturinformation aus experimentellen Messdaten fÃ¼r BiomolekÃ¼le. Angewandte Chemie, 2016, 128, 16222-16244.	1.6	7
107	A Bowmanâ€“Birk protease inhibitor purified, cloned, sequenced and characterized from the seeds of Maclura pomifera (Raf.) Schneid. Planta, 2017, 245, 343-353.	1.6	7
108	CuBlock: a cross-platform normalization method for gene-expression microarrays. Bioinformatics, 2021, 37, 2365-2373.	1.8	7

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109	Prediction of Antigenic B and T Cell Epitopes via Energy Decomposition Analysis: Description of the Web-Based Prediction Tool BEPPE. Methods in Molecular Biology, 2015, 1348, 13-22.	0.4	6
110	Antigen Discovery in Bacterial Panproteomes. Methods in Molecular Biology, 2021, 2183, 43-62.	0.4	6
111	Why is a protective antigen protective?. Hum Vaccin, 2009, 5, 872-875.	2.4	5
112	Calcium binding to the purple membrane: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2009, 74, 669-681.	1.5	5
113	Draft Genome Sequence of Stenotrophomonas maltophilia Strain UV74 Reveals Extensive Variability within Its Genomic Group. Genome Announcements, 2015, 3, .	0.8	5
114	CNN-PepPred: an open-source tool to create convolutional NN models for the discovery of patterns in peptide setsâ€"application to peptideâ€"MHC class II binding prediction. Bioinformatics, 2021, 37, 4567-4568.	1.8	5
115	Antibacterial Activity of T22, a Specific Peptidic Ligand of the Tumoral Marker CXCR4. Pharmaceutics, 2021, 13, 1922.	2.0	5
116	Stability of SIV gp32 Fusionâ€Peptide Singleâ€Layer Protofibrils as Monitored by Molecularâ€Dynamics Simulations. Angewandte Chemie, 2005, 117, 1089-1091.	1.6	4
117	Draft Genome Sequence of Stenotrophomonas maltophilia Strain M30, Isolated from a Chronic Pressure Ulcer in an Elderly Patient. Genome Announcements, 2014, 2, .	0.8	4
118	Redefining the PF06864 Pfam Family Based on Burkholderia pseudomallei PilO2Bp S-SAD Crystal Structure. PLoS ONE, 2014, 9, e94981.	1.1	4
119	On the Entropic and Hydrophobic Properties Involved in the Inhibitory Mechanism of Carboxypeptidase A by its Natural Inhibitor from Potato. Journal of Molecular Modeling, 1995, 1, 54-67.	0.8	3
120	Modelling of the Complex between a 15-Residue Peptide from mSos2 and the N-Terminal SH3 Domain of Grb2 by Molecular-Dynamics Simulation. Chemistry and Biodiversity, 2004, 1, 505-519.	1.0	3
121	Engineering the E. coli Î²-galactosidase for the screening of antiviral protease inhibitors. Biochemical and Biophysical Research Communications, 2005, 329, 453-456.	1.0	3
122	Validierung von molekularen Simulationen: eine Ãœbersicht verschiedener Aspekte. Angewandte Chemie, 2018, 130, 894-915.	1.6	3
123	The Key to Solving the Protein-Folding Problem Lies in an Accurate Description of the Denatured State. Angewandte Chemie - International Edition, 2001, 40, 351-355.	7.2	3
124	Î±â€Cyclodextrin Hostâ€"Guest Binding: A Computational Study of the Different Driving Forces. Helvetica Chimica Acta, 2010, 93, 2318-2325.	1.0	2
125	Polypeptide folding on a conformationalâ€space network: Dependence of network topology on the structural discretization procedure. Journal of Computational Chemistry, 2010, 31, 1889-1903.	1.5	2
126	Entropy calculations on a reversibly folding peptide: Changes in solute free energy cannot explain folding behavior. , 2001, 43, 45.		1

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127	Aspects of Modeling Biomolecular Structure on the Basis of Spectroscopic or Diffraction Data. Biological Magnetic Resonance, 2002, , 3-35.	0.4	0