Christian Bartels

List of Publications by Year in descending order

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430874 552781 10,271 29 18 26 citations h-index g-index papers 31 31 31 13165 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077
2	The program XEASY for computer-supported NMR spectral analysis of biological macromolecules. Journal of Biomolecular NMR, 1995, 6, 1-10.	2.8	1,570
3	Multidimensional adaptive umbrella sampling: Applications to main chain and side chain peptide conformations. Journal of Computational Chemistry, 1997, 18, 1450-1462.	3.3	289
4	Solution conformations and thermodynamics of structured peptides: molecular dynamics simulation with an implicit solvation model. Journal of Molecular Biology, 1998, 284, 835-848.	4.2	228
5	Probability Distributions for Complex Systems:  Adaptive Umbrella Sampling of the Potential Energy. Journal of Physical Chemistry B, 1998, 102, 865-880.	2.6	178
6	QSAR â° How Good Is It in Practice? Comparison of Descriptor Sets on an Unbiased Cross Section of Corporate Data Sets. Journal of Chemical Information and Modeling, 2006, 46, 1924-1936.	5.4	135
7	GARANT-a general algorithm for resonance assignment of multidimensional nuclear magnetic resonance spectra. Journal of Computational Chemistry, 1997, 18, 139-149.	3.3	129
8	Automated sequence-specific NMR assignment of homologous proteins using the program GARANT. Journal of Biomolecular NMR, 1996, 7, 207-13.	2.8	117
9	Fast algorithm for peptide sequencing by mass spectroscopy. Biological Mass Spectrometry, 1990, 19, 363-368.	0.5	112
10	Analyzing biased Monte Carlo and molecular dynamics simulations. Chemical Physics Letters, 2000, 331, 446-454.	2.6	83
11	Effective atom volumes for implicit solvent models: comparison between Voronoi volumes and minimum fluctuation volumes. Journal of Computational Chemistry, 2001, 22, 1857-1879.	3.3	61
12	Correlations between FEV1 and patient-reported outcomes: A pooled analysis of 23 clinical trials in patients with chronic obstructive pulmonary disease. Pulmonary Pharmacology and Therapeutics, 2018, 49, 11-19.	2.6	41
13	Determination of equilibrium properties of biomolecular systems using multidimensional adaptive umbrella sampling. Journal of Chemical Physics, 1999, 111, 8048-8067.	3.0	40
14	Determination of the pharmacokinetics of glycopyrronium in the lung using a population pharmacokinetic modelling approach. British Journal of Clinical Pharmacology, 2013, 76, 868-879.	2.4	40
15	A Novel Reduced-Dimensionality Triple-Resonance Experiment for Efficient Polypeptide Backbone Assignment, 3D HN N. Journal of Magnetic Resonance Series B, 1995, 108, 197-203.	1.6	37
16	Solution conformations of structured peptides: continuum electrostatics versus distance-dependent dielectric functions. Theoretical Chemistry Accounts, 1999, 101, 194-204.	1.4	30
17	Characterization of flexible molecules in solution: the RGDW peptide 1 1Edited by B. Honig. Journal of Molecular Biology, 1998, 284, 1641-1660.	4.2	23
18	A randomized, double-blind study to compare the efficacy and safety of two doses of mometasone furoate delivered via Breezhaler \hat{A}^{\otimes} or Twisthaler \hat{A}^{\otimes} in patients with asthma. Pulmonary Pharmacology and Therapeutics, 2020, 62, 101919.	2.6	14

#	Article	IF	CITATIONS
19	Adaptive umbrella sampling of the potential energy: modified updating procedure of the umbrella potential and application to peptide folding. Theoretical Chemistry Accounts, 1999, 101, 62-66.	1.4	13
20	Absolute free energies of binding of peptide analogs to the HIV-1 protease from molecular dynamics simulations. Journal of Computational Chemistry, 2005, 26, 1294-1305.	3.3	8
21	A spectral correlation function for efficient sequential NMR assignments of uniformly 15N-labeled proteins. Journal of Biomolecular NMR, 1994, 4, 775-785.	2.8	7
22	Estimandsâ€"What they are and why they are important for pharmacometricians. CPT: Pharmacometrics and Systems Pharmacology, 2021, 10, 279-282.	2.5	6
23	Dose bridging data for mometasone furoate in once-daily fixed-dose inhaled combinations of mometasone furoate/indacaterol and mometasone furoate/ indacaterol/glycopyrronium in patients with asthma. Pulmonary Pharmacology and Therapeutics, 2021, 70, 102068.	2.6	6
24	Population pharmacokinetics of IND/GLY (indacaterol/glycopyrronium) in COPD patients. International Journal of Clinical Pharmacology and Therapeutics, 2016, 54, 405-414.	0.6	5
25	Population Pharmacokinetic Analysis of Indacaterol/Glycopyrronium/Mometasone Furoate After Administration of Combination Therapies Using the Breezhaler® Device in Patients with Asthma. European Journal of Drug Metabolism and Pharmacokinetics, 2021, 46, 487-504.	1.6	2
26	Relationship between change in trough FEV1and COPD patient outcomes: Pooled analysis of 23 clinical trials in patients with COPD. , 2015, , .		2
27	Relationship Between Change in Trough FEV 1 and COPD Patient Outcomes: Exploring the Pharmacological Class Effect of Bronchodilators. Chest, 2015, 148, 719A.	0.8	O
28	Confidence intervals with maximal average power. Communications in Statistics - Theory and Methods, 2020, , 1-17.	1.0	0
29	Inverse probability of censoring weighting for visual predictive checks of timeâ€toâ€event models with timeâ€varying covariates. Pharmaceutical Statistics, 2021, 20, 1051-1060.	1.3	O