Ulrich Sternberg

List of Publications by Year
in descending order

24	636	567281 15	642732 23
papers	citations	h-index	g-index

24	24	24	509
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Statistical evaluation of simulated NMR data of flexible molecules. Physical Chemistry Chemical Physics, 2022, , .	2.8	0
2	The simulation of NMR data of flexible molecules: sagittamide A as an example for MD simulations with orientational constraints. Physical Chemistry Chemical Physics, 2020, 22, 17375-17384.	2.8	8
3	Fundamental and practical aspects of molecular dynamics using tensorial orientational constraints. Liquid Crystals, 2020, 47, 2043-2057.	2.2	7
4	Configuration determination by residual dipolar couplings: accessing the full conformational space by molecular dynamics with tensorial constraints. Chemical Science, 2019, 10, 8774-8791.	7.4	40
5	Investigation of backbone dynamics and local geometry of bio-molecules using calculated NMR chemical shifts and anisotropies. Journal of Biomolecular NMR, 2019, 73, 727-741.	2.8	4
6	Molecular Dynamics with Orientational Tensorial Constraints: A New Approach to Probe the Torsional Angle Distributions of Small Rotationally Flexible Molecules. Journal of Physical Chemistry B, 2019, 123, 8480-8491.	2.6	25
7	Conformational Investigations in Flexible Molecules Using Orientational NMR Constraints in Combination with 3J-Couplings and NOE Distances. Molecules, 2019, 24, 4417.	3.8	12
8	1H line width dependence on MAS speed in solid state NMR â€“ Comparison of experiment and simulation. Journal of Magnetic Resonance, 2018, 291, 32-39.	2.1	80
9	Molecular dynamics simulations on PGLa using NMR orientational constraints. Journal of Biomolecular NMR, 2015, 63, 265-274.	2.8	8
10	Fast Atomic Charge Calculation for Implementation into a Polarizable Force Field and Application to an Ion Channel Protein. Journal of Chemistry, 2015, 2015, 1-14.	1.9	6
11	Structural characterization of a peptoid with lysine-like side chains and biological activity using NMR and computational methods. Organic and Biomolecular Chemistry, 2013, 11, 640-647.	2.8	15
12	Rapid calculation of protein chemical shifts using bond polarization theory and its application to protein structure refinement. Physical Chemistry Chemical Physics, 2012, 14, 12263.	2.8	14
13	Irregular structure of the HIV fusion peptide in membranes demonstrated by solid-state NMR and MD simulations. European Biophysics Journal, 2011, 40, 529-543.	2.2	38
14	Calculation of fluorine chemical shift tensors for the interpretation of oriented 19F-NMR spectra of gramicidin A in membranes. Physical Chemistry Chemical Physics, 2009, 11, 7048.	2.8	30
15	All-atom molecular dynamics simulations using orientational constraints from anisotropic NMR samples. Journal of Biomolecular NMR, 2007, 38, 23-39.	2.8	27
16	13C Chemical Shift Constrained Crystal Structure Refinement of Cellulose Iα and Its Verification by NMR Anisotropy Experiments. Macromolecules, 2006, 39, 6125-6132.	4.8	74
17	3D Structure Elucidation Using NMR Chemical Shifts. Annual Reports on NMR Spectroscopy, 2004, , 53-104.	1.5	17
18	Chemical shift driven geometry optimization. Journal of Computational Chemistry, 2002, 23, 298-305.	3.3	26

#	Article	IF	Citations
19	Structure determination of a pseudotripeptide zinc complex with the COSMOS-NMR force field and DFT methods. Journal of Biomolecular NMR, 2002, 24, 277-289.	2.8	17
20	Molecular mechanics for zinc complexes with fluctuating atomic charges. Journal of Molecular Modeling, 2001, 7, 54-64.	1.8	31
21	Molecular mechanics with fluctuating atomic charges â€“ a new force field with a semi-empirical charge calculation. Journal of Molecular Modeling, 2001, 7, 90-102.	1.8	41
22	New Semi-empirical Approach for the Calculation of13C Chemical-Shift Tensors. Journal of Magnetic Resonance, 1997, 125, 8-19.	2.1	22
23	New approach to the semiempirical calculation of atomic charges for polypeptides and large molecular systems. Journal of Computational Chemistry, 1994, 15, 524-531.	3.3	39
24	Theory of the influence of the second co-ordination sphere on the chemical shift. Molecular Physics, 1988, 63, 249-267.	1.7	55