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	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
2	13C Chemical Shift Constrained Crystal Structure Refinement of Cellulose Iβ and Its Verification by NMR Anisotropy Experiments. Macromolecules, 2006, 39, 6125-6132.	4.8	74
3	Theory of the influence of the second co-ordination sphere on the chemical shift. Molecular Physics, 1988, 63, 249-267.	1.7	55
4	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
5	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
6	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
7	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
8	Molecular mechanics for zinc complexes with fluctuating atomic charges. Journal of Molecular Modeling, 2001, 7, 54-64.	1.8	31
9	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
10	All-atom molecular dynamics simulations using orientational constraints from anisotropic NMR samples. Journal of Biomolecular NMR, 2007, 38, 23-39.	2.8	27
11	Chemical shift driven geometry optimization. Journal of Computational Chemistry, 2002, 23, 298-305.	3.3	26
12	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
13	New Semi-empirical Approach for the Calculation of13C Chemical-Shift Tensors. Journal of Magnetic Resonance, 1997, 125, 8-19.	2.1	22
14	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
15	3D Structure Elucidation Using NMR Chemical Shifts. Annual Reports on NMR Spectroscopy, 2004, , 53-104.	1.5	17
16	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
17	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
18	Conformational Investigations in Flexible Molecules Using Orientational NMR Constraints in Combination with 3J-Couplings and NOE Distances. Molecules, 2019, 24, 4417.	3.8	12

#	Article	IF	Citations
19	Molecular dynamics simulations on PGLa using NMR orientational constraints. Journal of Biomolecular NMR, 2015, 63, 265-274.	2.8	8
20	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
21	Fundamental and practical aspects of molecular dynamics using tensorial orientational constraints. Liquid Crystals, 2020, 47, 2043-2057.	2.2	7
22	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
23	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
24	Statistical evaluation of simulated NMR data of flexible molecules. Physical Chemistry Chemical Physics, 2022, , .	2.8	0