

**Fast atomic charge calculation for implementation into a polarizable force field and application to an ion channel protein**  
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**<sup>1</sup>H line width dependence on MAS speed in solid state NMR - comparison of experiment and simulation**  
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**Molecular dynamics simulations on PGLa using NMR orientational constraints**  
**Sternberg, Ulrich; Witter, Raiker** Journal of biomolecular NMR 2015 / p. 265-274 : ill <http://dx.doi.org/10.1007/s10858-015-9983-y>

**Simulation of oriented NMR spectra : combining molecular dynamics and chemical shift tensor calculations**  
Sternberg, Ulrich; **Witter, Raiker** Magnetic resonance in chemistry 2023 <https://doi.org/10.1002/mrc.5403>