

Fast atomic charge calculation for implementation into a polarizable force field and application to an ion channel protein

Witter, Raiker; Möllhoff, Margit; Koch, Frank-Thomas; **Sternberg, Ulrich** Journal of chemistry 2015 / p. 1-14 : ill

<https://doi.org/10.1155/2015/908204> [Journal metrics at Scopus](#) [Article at Scopus](#) [Article at WOS](#)

¹H line width dependence on MAS speed in solid state NMR - comparison of experiment and simulation

Sternberg, Ulrich; **Witter, Raiker**; Kuprov, Ilya; Lamley, Jonathan M.; **Oss, Andres**; Lewandowski, Jozef R.; **Samoson, Ago** Journal of magnetic resonance 2018 / p. 32-39 : ill <https://doi.org/10.1016/j.jmr.2018.04.003> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Molecular dynamics simulations on PGLa using NMR orientational constraints

Sternberg, Ulrich; Witter, Raiker Journal of biomolecular NMR 2015 / p. 265-274 : ill <https://doi.org/10.1007/s10858-015-9983-y>

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Simulation of oriented NMR spectra : combining molecular dynamics and chemical shift tensor calculations

Sternberg, Ulrich; **Witter, Raiker** Magnetic resonance in chemistry 2024 / p. 125-144 <https://doi.org/10.1002/mrc.5403> [Journal metrics at Scopus](#) [Article at Scopus](#)