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Dynamics of IDP Histatin 5 probed by QENS and compared with simulation

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Intrinsically disordered proteins (IDPs) adopt a wide variety of conformations in solution, without a distinct equilibrium structure. Here, we investigate the dynamics of IDPs, using the antimicrobial saliva protein Histatin 5 as model. A suitable technique for this purpose is quasi-elastic neutron scattering (QENS), which through the incoherent scattering probes the self-diffusion of particles on biologically relevant length- and timescales. Here, focus is on the center-of-mass diffusion, considering dynamics with respect to temperature and self-crowding effects. The diffusion obtained is a convolution of translational and rotational diffusion, but implicit relations between these are known. Therefore, atomistic molecular dynamics simulations previously performed are analyzed to compare with the experimentally achieved results, providing further insight into the dynamical properties of IDPs and how these are affected by self-crowding and temperature.

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