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Combining Ion Mobility Mass Spectrometry and Molecular Dynamics - a look at the conformational behaviour during water droplet evaporation. LUKASZ MIGAS, ELEANOR DICKINSON, Univ of Manchester, REBECCA BEVERIDGE, Vienna Biocenter, RICHARD KRIWACKI, St. Jude Children's Research Hospital, GARY DAUGHDRILL, USF, PERDITA BARRAN, Univ of Manchester — Intrinsically Disordered Proteins (IDPs) lack stable secondary and tertiary structure yet fulfil a myriad of functions within their native environments. Determination of the conformational landscape of such heterogeneous ensemble is challenging and mass spectrometry (MS) and ion mobility mass spectrometry (IM-MS) offer unique benefits for structural biology, complementing existing techniques. IM-MS is able to determine the conformational spread of a given protein or protein-complex in vacuo in terms of a collision cross section. In order to best relate the gas phase conformational diversity to that present in solution it is essential to consider how desolvation alters the stable conformations and the increased importance of self-solvation in a solvent-free environment. Here we present the results of MD and IM-MS experiments from oncogenic IDPs, namely the C-terminus of the KID domain of p27 and the N-terminal transactivation domain of p53. For both proteins the experimental charge state distribution is used to prepare starting structures with different protonation states. Independent MD trajectories of each charge state are performed with explicit solvent which is then 'evaporated' as water molecules move further from the protein core simulating the desolvation process.

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