Title: In silico time-resolved infrared spectroscopy of biomolecules in solution

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Infrared (IR) absorption spectra of amide modes (particularly of the amide I mode, mostly corresponding to the peptide-group C=O stretching) have long provided a tool for determining the secondary structure of peptides and proteins. Our group recently developed a computational approach to calculate amide I IR spectra of peptides and proteins based on the joint use of extended molecular dynamics (MD) simulations and a mixed quantum/classical theoretical methodology: the Perturbed Matrix Method (PMM) [1,2]. As the method makes use of classical MD to provide phase space sampling, statistically relevant sampling of the system configurations can be achieved, which is required for an accurate calculation of the spectra of complex systems. The use of the MD-PMM procedure has allowed the theoretical investigation of the amide I spectra of both helical [3,4] and β [1,4-6] peptides as well as amyloids [7] and peptides unfolded states [1,4,6]. Comparison between calculated spectra with experimental IR temperature-dependent and isotope-labelled spectra provided a mean for the interpretation of the experimental spectra at the molecular level. More recently, we focused on modelling the time-dependence of the amide I IR signal, to be compared with experimental time-resolved IR spectra, commonly used to monitor folding kinetics [6]. The possibility of quantitatively modelling time resolved spectra can provide a detailed interpretation of the time evolution of the spectroscopic signal, permitting a full characterization of the kinetics of complex chemical-biochemical processes.

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