Benchmarking spectral simulation protocols for amide I.

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A benchmark of amide I spectral simulation protocols is presented. Results allow choosing the optimal frequency mapping and coupling model for the tested force fields. We further find that due to the sensitivity of two-dimensional spectroscopy there is room for improving the protocols.

In the current work a benchmark of amide I spectral simulation protocols is presented. This provides insights to the best force fields, frequency mappings and coupling models for this type of modelling. The amide I mode is widely used in IR spectroscopy of proteins due to the high sensitivity to hydrogen bonding and secondary structure [1,2]. FTIR and 2DIR of this band, thus, report important information regarding the local environment. Here, we benchmark spectral simulation protocols using all atom as well as united atom force fields. These were combined with different electrostatic mappings/coupling models [3,5]. The results were validated against spectral experimental data of three well-studied proteins. We found that the OPLS-AA/Jansen/TDC combination predicts the best FTIR, while the best agreement for 2DIR is given by the OPLS-AA/Skinner/TCC combination. Our findings give room for new ideas to improve the existing models [6,7].

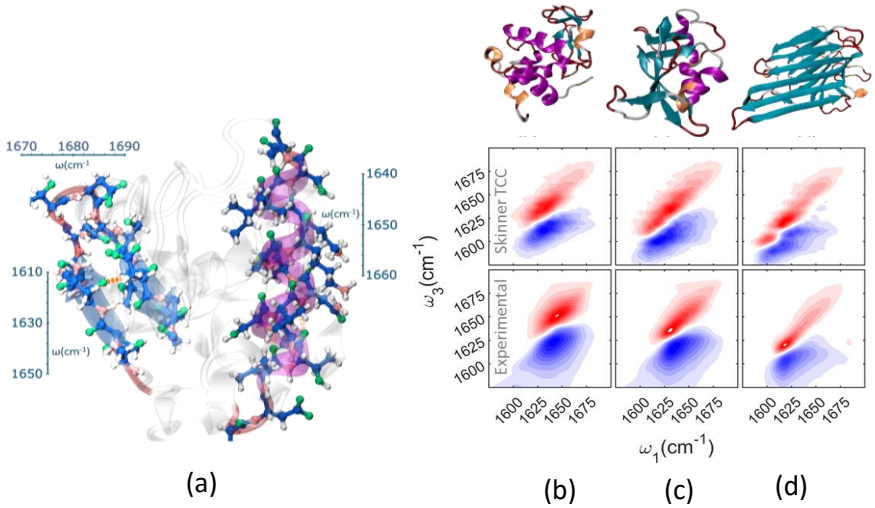

Figure 1: (a) Relationship between secondary structure and amide I vibrational frequency in the infrared spectrum, where the protein structure is represented in new cartoon. Two dimensional infrared spectra of the proteins: (b) Lysozyme,(c) Ribonuclease A,(d) Concanavalin A, simulated with the OPLS-AA force field. The countour lines are equidistant, and separed by 10% of the maximum value.

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