Using the CcpNmr software for assignment, screening, metabolomics, dynamics and structure

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In my presentation I will show the latest progress and versatility of the CcpNmr software suite for covering all aspects NMR data analysis. I will show an example of using AnalysisAssign for spectral assignment using chemical shift distribution information.

Using AnalysisStructure and starting from a single source of NEF-formatted input data, different computational engines result in variable results. I will address the question of structural variability; i.e. how to assess similarity in structure and conformation and how to quantify it.

AnalysisDynamics features a sophisticated and expandable framework for NMR dynamics analysis, aiming to optimise complex workflows and incorporate advanced modelling techniques, including simultaneous multi-model fittings. The software automates key routines, facilitating the seamless execution of multi-step analyses across diverse NMR datasets, including CEST, CPMG relaxation dispersion, and ZZ-exchange. A newly implemented framework for the Lipari-Szabo formalism leverages speed-optimised minimisers and parallel processing. It includes multi-spectral density parameter minimisations, automated model selection, and tensor shape analysis. I will present the results of the analysis of 72 remediated BMRB ^{15}N-relaxation datasets.