

Turning failure into success: New perspectives for unsupervised NMR studies of proteins

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In the first part of the presentation, the J-UNIO protocol for structure determination of small globular proteins by solution NMR will be introduced. The J-UNIO protocol requires only a minimal set of NMR spectra and allows efficient interactive validation of intermediate and final results. Application of the J-UNIO protocol to more than 40 *de novo* protein structures with sizes up to 180 residues shows that the procedure is highly robust and efficient, and well road-tested.

In the second part, new concepts for homology modeling–driven NMR structure determination of complex biological systems will be described. We will show how database knowledge can be effectively incorporated into backbone, side-chain and NOE assignment in order to enable structural and dynamical studies of large biological systems. Applications of homology-driven NMR structure determination to proton-detected solid-state NMR studies will conclude the presentation.