NMRbox: National Center for Biomolecular NMR Data Processing and Analysis

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NMRbox is a new software platform for biomolecular NMR. Computation is crucial for applications of NMR that provide insights into biomolecular structure, dynamics, interactions, and stability, and have translational applications including diagnostics and drug discovery. Spectrum analysis, parametric data reduction, computer-aided assignment, spectral databases, and structure computation and validation are just some of the methods dependent on software, and have all been vital for extending the size and complexity of biomolecular systems amenable to NMR. The amount and variety of NMR software is exploding, making it more difficult to discover new software, and to support a full complement of software on a diverse set of computer platforms, or maintain legacy packages that are no longer actively developed. Communication between software packages also becomes more challenging. Removing barriers to interoperability is essential for NMR software to be fully utilized. The broad aim of NMRbox is to simplify and integrate dissemination, maintenance, support, and application of a range of widely used NMR data processing and analysis software packages. By facilitating the use and persistence of advanced software for biomolecular NMR, the resource will advance the application of biomolecular NMR for challenging applications in biomedicine, including structural biology, drug discovery, and metabolomics. A unifying theme is that the center will foster reproducible research in bio-NMR.

NMRbox staff will be on hand to provide live demonstrations and conduct signups for this free service, which includes downloadable pre-configured virtual machines (VMs) and hosted VMs running on a Center-supported compute cloud.

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