

Benefits of NMRbox for Users

The NMRbox platform delivered by the Center for Biomolecular NMR Data Processing and Analysis simplifies development, support, collection of usage metrics, and provides persistence:



Zero-Configuration

NMRbox comes with a wide variety of commonly used NMR software installed and configured.

Access

Users may access NMRbox as a Platform-as-a-Service (PaaS), hosted on our servers, via a free VNC client, or download NMRbox for local execution. The PaaS platform allows users to open and close VNC connections to their dedicated NMRbox session.

Training

The NMRbox.org website and VM will contain software user manuals, tutorials, and rich multimedia resources to assist novice users.

Community

The NMRbox user community will be engaged through workshops, tutorials, forums, and email lists.

Computational Resources

A dedicated cloud provides powerful, free parallel computing via shared-memory, distributed, and GPU-accelerated models. The PaaS platform removes the entire computational burden from the user.

Discovery

A searchable software registry describes each installed package, including primary citations, a table of versions included in each NMRbox release, and links to BMRB entries citing the software.

Persistence

Software captured by NMRbox will be made available through the Center's archive. Software that is no longer actively developed remains accessible, long after OSes, programming languages, or hardware become obsolete.

Reproducibility

A version-controlled archive of NMRbox releases ensures that the exact computational environment used in a study can be recapitulated. The NMRbox version number may be cited in publications and used to allow readers to access the primary data and computational resources employed in the study.

Availability

Redundant high-bandwidth network connections and geodispersed hierarchical file storage offer high performance and secure access to programs and data.

Support

The Center works with developers to migrate packages into NMRbox, including development of unit tests to validate the correct operation of each software package.

Think inside the box.