The BMRB archive of Protein, Nucleic Acid and Metabolite NMR Data

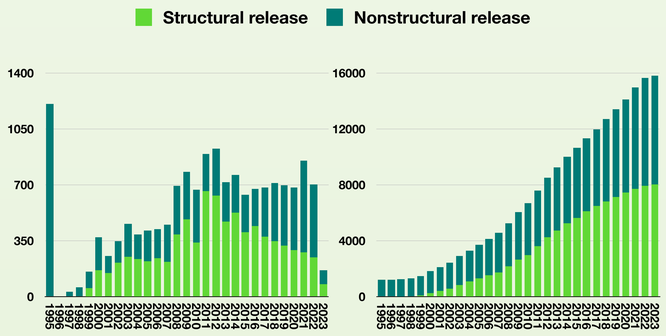
Kumaran Baskaran, Jonathan R. Wedell, Hongyang Yao, Dimitri Maziuk, Hamid R. Eghbalnia, Michael M. Gryk, and Jeffrey C. Hoch

Department of Molecular Biology and Biophysics, UConn Health,
263 Farmington Avenue, Farmington, CT 06030, USA

The Biological Magnetic Resonance Data Bank[1] (BMRB: https://bmrb.io) serves the biomolecular NMR community by supporting a curated archive of primary and derived data and metadata linked to scientific investigations under the "FAIR Principles" (Findable, Accessible, Interoperable, and Reusable)[2]. BMRB is a member and a core archive of the Worldwide Protein Data Bank (wwPDB: https://www.wwpdb.org), which collects the coordinate data along with assigned chemical shifts and restraints from NMR structural studies through the OneDep (https://deposit.wwpdb.org) deposition system. NMR data from other studies are collected by the BMRBdep (https://deposit.bmrb.io) deposition system. BMRB's goal is to empower scientists in their analysis of the structure, dynamics, and chemistry of biological systems and to support further developments in the field of biomolecular NMR spectroscopy.

BMRB growth statistics

The bar graph shows the growth of the BMRB archive. As of April 2023, BMRB holds 15793 entries with 8008 entries having corresponding coordinate data in the PDB archive and 7785 BMRB only entries.



Data access

Find data using the instant search or advance search

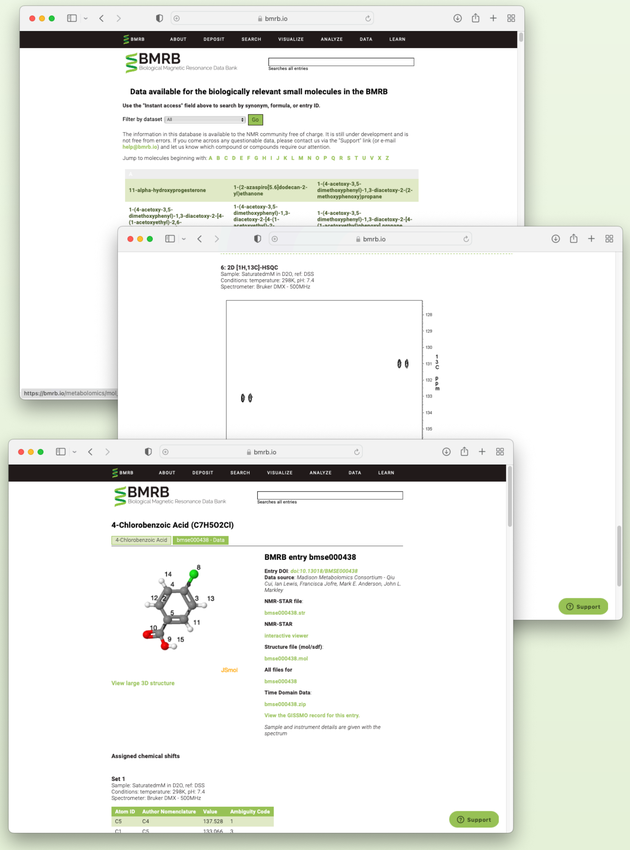
Access through web browser or BMRB API

Interoperate with the help of PyNMRSTAR

Reuse/reinterpret with new software tools

Small molecules library

BMRB maintains a library of carefully curated NMR spectroscopic data of over 1000 biologically important small molecules.

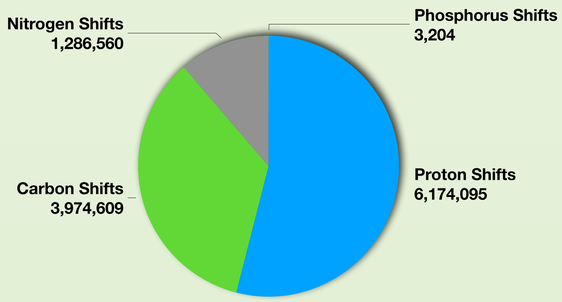


NMR-STAR data model

NMR-STAR[3] is the official data format of BMRB and the deposition and archival format of NMR spectroscopic data at the wwPDB. It is a Self-defining Text Archive and Retrieval (STAR) format with controlled vocabularies(tags) defined by the NMR-STAR dictionary. The NMR-STAR data model supports many kinds of NMR data, metadata and derived data.

BMRB data content (chemical shifts)

As of April 2023, BMRB holds over 11 million chemical shifts from 14463 protein, 565 DNA and 535 RNA entries. In addition to the chemical shift data, other NMR data are also available at the BMRB



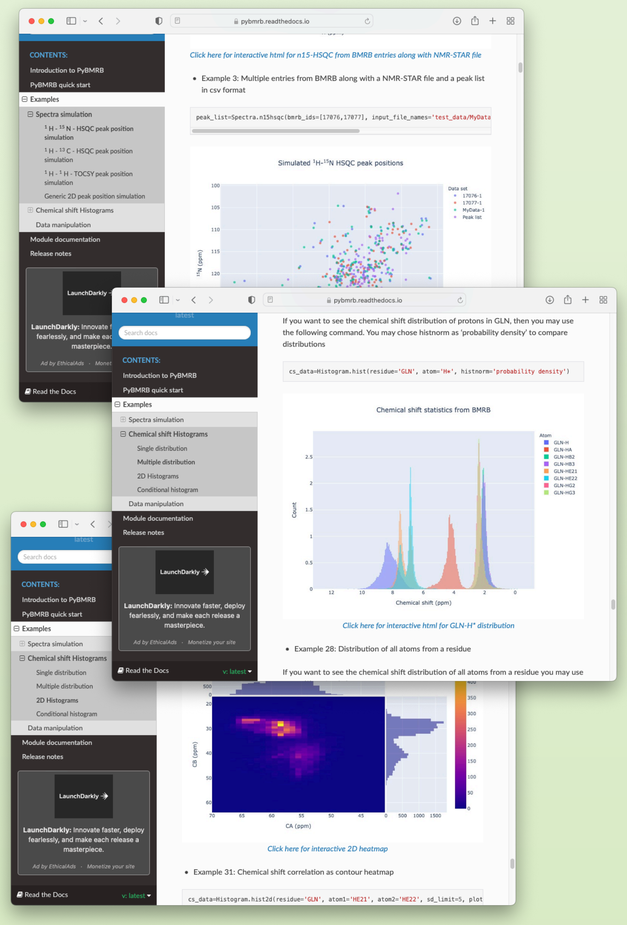
BMRB Software resouce

BMRB GitHub: https://github.com/bmrb-io

- BMRB - API : provides machine to machine access to BMRB data base
- PyNMRSTAR : Python NMR-STAR parser
- PyBMRB: BMRB data visualization tool in Python
- RBMRB: BMRB data visualization tool in R

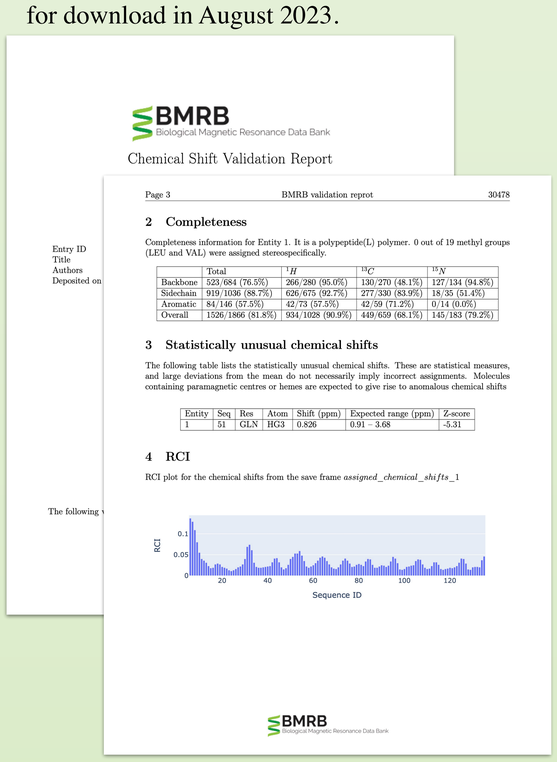
BMRB data visualization

Chemical shift histograms and simulated HSQCs can be generated using PyBMRB or RBMRB.



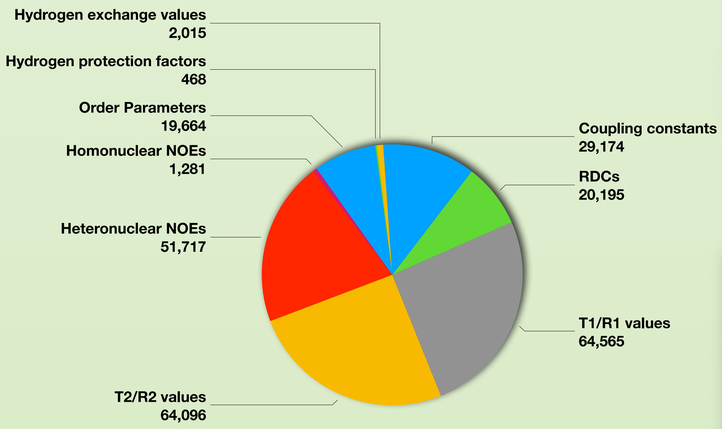
BMRB validation report

BMRB is working on generating validation reports in PDF and XML formats which include completeness of resonance assignment, chemical shift outliers, RCI plots and other useful information. It will be available for download in August 2023.



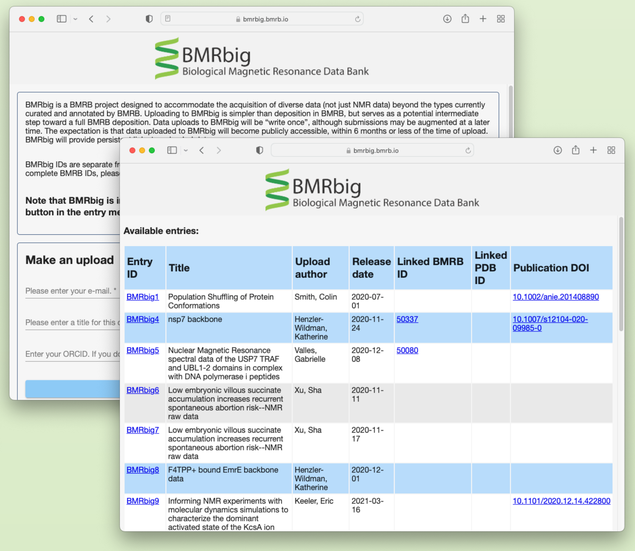
PDF version of the poster

BMRB data content (other NMR data)



BMRBig

BMRbig is a BMRB project designed to accommodate the acquisition of diverse data (not just NMR data) beyond the types currently curated and annotated by BMRB. Uploading to BMRbig is simpler than deposition in BMRB, but serves as a potential intermediate step toward a full BMRB deposition. Data uploads to BMRbig will be "write once", although submissions may be augmented at a later time



1. *Hoch, J. C.; et al. Nucleic Acids Research 2023, 51.*
2. *Ulrich, E. L.; et al. J. Biomol. NMR 2019, 73 (1-2), 5.*
3. *Wilkinson, M. D.; et al. Scientific data 2016, 3, 160018.*

BMRB is supported by NIH through grant R01GM109046