# Biological Magnetic Resonance Data Bank

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#### ABSTRACT

The Biological Magnetic Resonance Data Bank (BMRB, https://bmrb.io) is the international open data repository for biomolecular nuclear magnetic resonance (NMR) data. Comprised of both empirical and derived data, BMRB has applications in the study of biomacromolecular structure and dynamics, biomolecular interactions, drug discovery, intrinsically disordered proteins, natural products, biomarkers, and metabolomics. Advances including GHz-class NMR instruments, national and trans-national NMR cyberinfrastructure, hybrid structural biology methods and machine learning are driving increases in the amount, type, and applications of NMR data in the biosciences. BMRB is a Core Archive and member of the World-wide Protein Data Bank (wwPDB).

#### INTRODUCTION

NMR is one of the most versatile analytic methods for analyzing matter, using atomic nuclei as embedded reporters. Applications of NMR to biomolecular science include structure, dynamics, and interactions of biomacromolecules in the solid and liquid solution state, the identity and composition of complex mixtures of small molecule metabolites, and the structure of natural products. BMRB is the open, international online repository for all types of biomolecular NMR data.

BMRB was founded by John Markley and Eldon Ulrich at the University of Wisconsin in 1988. Initial depositions were made by curators manually entering chemical shifts and assignments extracted from publications. With the development of the Adit-NMR deposition system, the primary means of accessions became depositor-driven. In 2006, BMRB joined the World-wide Protein Data Bank (wwPDB) (1) as a member and Core Archive. BMRB facilitates accession and validation of NMR-based biomacromolecular structures deposited to PDB via the OneDep system. BMRBj operating from Osaka University processes depositions in addition to serving as a mirror site. Another mirror site operates from CERM (https://bmrb.cerm. unifi.it/), at the University of Florence, IT. In 2020, BMRB moved to UConn Health in Farmington, CT.

BMRB depositions are linked to corresponding entries in PDB, the European Nucleotide Archive (2) (EMBL-EBI), the National Center for Biotechnology Information (3) (NCBI) and UniProt (4).

In addition to collaborations with wwPDB member organizations RCSB (5), PDBe (6), PDBj, (7) and EMDB (8), BMRB has close collaborations with the National Center for Biomolecular NMR Data Processing and Analysis (9) (NMR box.org), the Center for High-Throughput Computing and the University of Wisconsin-Madison, the Collaborative Computing Project for NMR (10) (CCPN), Rutgers University, and the University of Frankfurt.

BMRBj (7), formerly known as PDBj-BMRB at Osaka, Japan, is a satellite BMRB repository that accepts NMR experimental data via three deposition servers, (i) OneDep depositions containing NMR experimental data from Asian countries and regions, (ii) BMRBdep deposition server at Osaka and (iii) SMSDep deposition server, which accepts NMR derived structures of biologically interesting small molecules that are ineligible for OneDep deposition due to the limit on molecular size. 10% of BMRB entries have been processed at Osaka site since 2002 (7). The BMRB and BM-RBj sites share annotation tools and communicate closely on issues, assuring uniformity of annotation quality using either site.

#### MATERIALS AND METHODS

#### Accessions

Data housed at the BMRB are deposited, archived, and disseminated in the NMR-STAR file format (11). NMR-STAR is a variant of the STAR file format (12-14) intro-

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# **Magnetic Resonances In Biological Research**

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# Magnetic Resonances In Biological Research:

Magnetic Resonances in Biological Research Cafiero Franconi,1971-01-01 **Magnetic Resonances in Biological** Research, Edited by Cafiero Franconi International Conference on Magnetic Resonances in Biological Research, 3D, Santa Margherita, Cagliari, Italy, 1969, Cafiero Franconi (Ed), 1971 Biological Magnetic Resonance Lawrence J. Berliner, Jacques Reuben, 2012-12-06 We are pleased to present Volume 9 of our highly successful series which now celebrates 12 years of providing the magnetic resonance community with topical authoritative chapters on new aspects of biological magnetic resonance As always we try to present a diversity of topic coverage in each volume ranging from applications of in vivo magnetic resonance to more fundamental aspects of electron spin resonance and nuclear magnetic resonance Philip Yeagle presents an eagerly awaited chapter on 31p NMR studies of membranes and membrane protein interactions Alan Marshall has con tributed two chapters to the volume one with Jiejun Wu describes magnetic resonance studies of 5S RNA as probes of its structure and conformation the secon **Biological Magnetic Resonance** Lawrence Berliner, 2012-12-06 Judging from the articles published in Biochemistry magnetic resonance techniques NMR and ESR are now among the most popular methods in biochemical research The series Biological Magnetic Resonance the fifth volume of which we are proudly presenting is intended to provide authori tative coverage of topics of current interest Previous volumes have covered a number of aspects in a thorough and pedagogical fashion rarely found in other publications in this field Continuing to fulfill the mission of the series this volume presents a chapter by Baxter Mackenzie and Scott on the applications of carbon 13 NMR spectroscopy in investigations of methabolic pathways in vivo Blom berg and Ruterjans give a comprehensive summary of the use of nitrogen 15 NMR in studies of systems of biological interest Phosphorus 3I NMR investigations of enzyme systems are described by Rao Tsai and Bruzik outline the principles of and summarize the state of the art advances in the 18 use of oxygen isotopes e 70 and 0 in phosphorus 3I and oxygen 17 NMR studies of biophosphates Lipid protein interactions as reflected in ESR and NMR data are discussed by Devaux We wish to thank the authors for their cooperation in maintaining the and continued high standards of the series **Magnetic Resonance in Biological Systems** A. Ehrenberg, B. G. Malmström, T. Vänngård, 2013-09-24 Magnetic Resonance in Biological Systems Volume 9 is a collection of manuscripts presented at the Second International Conference on Magnetic Resonance in Biological Systems held in Wenner Gren Center Stockholm Sweden on June 1966 The conference is sponsored by International Union of Biochemistry Swedish Medical Research Council Swedish Natural Science Research Council Wenner Gren Center Foundation for Scientific Research This book contains 51 chapters and begins with reviews of NMR investigations of biological macromolecules including proteins amino acids and glycylglycine copper II Considerable chapters are devoted to numerous biological studies using the electronic paramagnetic resonance EPR thus introducing the branch of science called submolecular biology This book also explores other applications of NMR and EPR with special emphasis on blood component analysis and protein metal

complexes The final chapters survey the principles and applications of M ssbauer spectroscopy This book will prove useful to analytical chemists and biologists Biological Magnetic Resonance Lawrence Berliner, 2012-12-06 We have now reached our sixth volume in a series which has somewhat unintentionally become an annual event While we still intend to produce a volume only if a suitable number of excellent chapters in the forefront of biological magnetic resonance are available our philosophy is to present a pedagogical yet critical description and review of selected topics in mag netic resonance of current interest to the community of biomedical scien tists This volume fulfills our goals well As always we open the volume with a chapter which directly addresses an in vivo biological problem Phil Bolton's presentation of new techniques in measuring 31 P NMR in cells Lenkinski s chapter on the theory and applications of lanthanides in protein studies covers the details highlights and pitfalls of analysis of these complexes in biochemical NMR Reed and Markham summarize the interpreta tion of EPR spectra of manganese in terms of structure and function of proteins and enzymes Dalton and colleagues describe the applications to biological problems of the relatively new capability of time domain ESR Finally we are pleased to offer a departure from mainstream magnetic resonance with the comprehensive and stimulating chapter by Gus Maki on the theory instrumentation and applications of optically detected magnetic resonance **National Library of Medicine Current Catalog** National Library of Medicine (U.S.),1971 NMR Nuclear magnetic resonance. in biological research Kurt Wüthrich, 1976 **Research Grants Index** National Institutes of Health (U.S.). Division of Research Grants, 1967 Spectroscopic Properties of Inorganic and Organometallic Compounds E A V Ebsworth, 2007-10-31 Spectroscopic Properties of Inorganic and Organometallic Compounds provides a unique source of information on an important area of chemistry Divided into sections mainly according to the particular spectroscopic technique used coverage in each volume includes NMR with reference to stereochemistry dynamic systems paramagnetic complexes solid state NMR and Groups 13 18 nuclear guadrupole resonance spectroscopy vibrational spectroscopy of main group and transition element compounds and coordinated ligands and electron diffraction Reflecting the growing volume of published work in this field researchers will find this Specialist Periodical Report an invaluable source of information on current methods and applications Specialist Periodical Reports provide systematic and detailed review coverage in major areas of chemical research Compiled by teams of leading experts in their specialist fields this series is designed to help the chemistry community keep current with the latest developments in their field Each volume in the series is published either annually or biennially and is a superb reference point for researchers www rsc org spr

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web oh if you could see me now oh if you could see me now oh if you could see me now if you could see me now would you recognize me would you pat me on the back or would you criticise me would you follow every line on my tear stained face put your hand on a heart that s was cold as the day you were taken away

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