BMRBに登録されたNMRデータの検索 - SPARQLクエリを中心にして

How to retrieve NMR data archived at BMRB with SPARQL

IIBMP2016 (生命医薬情報学連合大会2016) Oct 1, 2016

PDBj&創薬等ランチョンセミナー

PDBj-BMRB Masashi Yokochi(横地政志)

PDBj-BMRB, satellite site of BMRB, serves deposition, annotation and distribution sites of experimental NMR data written in NMR-STAR format



Members:











PDBj-BMRB web services to enhance interoperability of NMR data



BMRB/XML, BMRB/RDF

representations of BMRB NMR-STAR data in XML and RDF formats



PDBj-BMRB integrated search service

search biological/biochemical DBs at once



PDBj-BMRB SPARQL server

a programmable API for federated search



BMRB SQL on your PC

periodically updated BMRB relational DB for intensive search

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BMRB/XML: The most comprehensive NMR-STAR data repository as a single format

We have converted canonical NMR-STAR data and diverse repositories such as atomic coordinate of NMR structures, LACS chemical shift validation, PACSY structural annotations, etc. into a single BMRB/XML format.

BMRB/XML

canonical NMR-STAR

- 1. Conventional NMR-STAR
- 2. BMRB+PDB NMR-STAR
- 3. PACSY structural annotation
- 4. LACS chemical shift validation report
- 5. Protein Blocks structural annotation
- 6. Completeness of assigned chemical shifts

URLs of each data repository

- 1. http://bmrb.pdbj.org/ftp/pub/bmrb/entry_lists/nmr-star3.1/
- 2. http://bmrb.pdbj.org/ftp/pub/bmrb/nmr_pdb_integrated_dat a/coordinates_restraints_chemshifts/bmrb_plus_pdb/
- 3. http://pacsy.nmrfam.wisc.edu/
- 4. http://bmrb.pdbj.org/ftp/pub/bmrb/validation_reports/LACS/
- 5. http://bmrbpub.protein.osaka-u.ac.jp/archive/pb/
- 6. http://bmrbpub.protein.osaka-u.ac.jp/archive/cs complete/



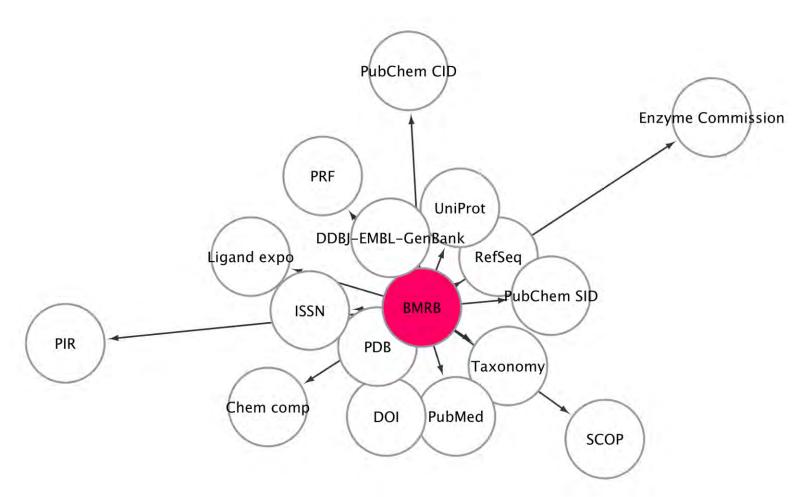
BMRB/RDF: In compliance with standards of 'Linked Data' and biological DB community

```
<BMRBo:entity db link rdf:about="http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmrl1300/entity db link/NP 001008202,REF,1,11300">
   <BMRBo:of datablock rdf:resource="http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr11300"/>
   <BMRBo:entity db link.accession code>NP 001008202</BMRBo:entity db link.accession code>
   <BMRBo:entity db link.database code>REF</BMRBo:entity db link.database code>
   <BMRBo:entity db link.entity id>1/BMRBo:entity db link.entity id>
   <BMRBo:entity db link.entry id>11300/BMRBo:entity db link.entry id>
   <rdfs:seeAlso rdf:resource="http://www.ncbi.nlm.nih.gov/protein/NP 001008202"</pre>
                 rdfs:label="info:refseq/NP 001008202"/>
   <rdfs:seeAlso rdf:resource="http://identifiers.org/refseq/NP 001008202"</pre>
                 rdfs:label="urn:miriam:refseq:NP 001008202"/>
   <BMRBo:entity db link.author supplied>no/BMRBo:entity db link.author supplied>
   <BMRBo:entity db link.entry mol name>cell division cycle 5-like protein [Xenopus (Silurana) tropicalis]/BMRBo:entity db link.entry mol name>
   <BMRBo:entity db link.ordinal>16</BMRBo:entity db link.ordinal>
   <BMRBo:entity db link.seq homology expectation val>8.17E-32/BMRBo:entity db link.seq homology expectation val>
   <BMRBo:entity db link.seg identity>100.00/BMRBo:entity db link.seg identity>
   <BMRBo:entity db link.seq positive>100.00/BMRBo:entity db link.seq positive>
   <BMRBo:entity db link.seq query to submitted percent>82.86/BMRBo:entity db link.seq query to submitted percent>
   <BMRBo:entity db link.seq subject length>804/BMRBo:entity db link.seq subject length>
</BMRBo:entity db link>
```

Two statements using **rdfs:seeAlso** appear, the former one represents **polite URL** pointing original resource of NCBI RefSeq database and the resource has a label written in the **formal URN**, the latter one is a statement semantically equivalent to the former one, but utilizes a **persistent URI** resolving system of Identifiers.org with the **MIRIAM URN** widely accepted by biological database community.



BMRB/RDF: Linked external information resources via RDF links



Shorter distances from BMRB indicate closer relationships with BMRB

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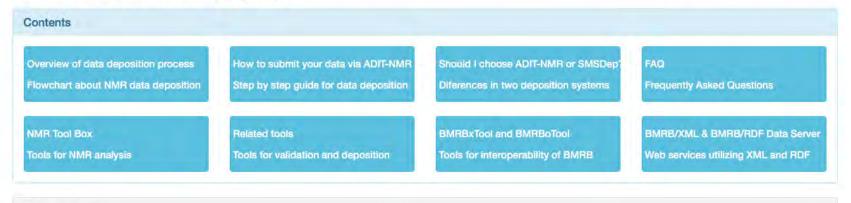
Information

PDBj-BMRB integrated search service: Search biological/biochemical DBs at once

http://bmrbdep.pdbj.org

PDBj BMRB Deposition - Search - Archives - Mirrors - Language - About -	BMRB ID or Dep. Code
1046 BMRB entries and 1324 Metabolomics entries are available on Sep 05, 2016	
Search	0
Everything Sequence •	
e.g., Entry ID, Macromolecule, Gene Ontology or Author	Q
	Search help

PDBj-BMRB group in Osaka University supported by JST-NBDC (Japan Science and Technology Agency - National Bioscience Database Center) contributes to the community for Biomolecular NMR by collection, annotation, validating and archiving experimental NMR data in collaboration with wwPDB (WorldWide Protein Data Bank). Our mission is to empower scientists in their analysis of the structure, dynamics, and chemistry of biological systems and to support further development of biomolecular NMR spectroscopy. Please deposit your NMR structure and related NMR experimental data through our deposition site, ADIT-NMR. The released data are available from our BMRB mirror server. Please try our new search service above which allows you to quickly find rich information of biomolecule such as function, sequence, structure, NMR data as well as interaction in multiple databases including BMRB, PDB, EMDB, UniProt, IntAct, BMRB-Metabolomics and Ligand Expo.





Timeline of PDBj-BMRB search service



- Keyword search
- Sequence search
- Auto suggest
- Search settings
- Search filter
- BMRB, PDB, Swiss-Prot, Ligand expo and BMRB-Metabolomics
- Mutual reference using PubMed, BLAST, IntAct and PubChem
- Entry list view
- Sort search results

- Lower latency (4~100 times faster)
- System stability
- EMDB integration

- Entry page with static URL
- Entry tracking by Dep. ID
- Query history
- Search help page
- Unified file exportation
- Chart displays
- Entries sharing articles
- Details of experiment
- Hit context with highlight
- Statistics on search results



Basic query composition

A query is broken up into single term, phrases (a group of terms surrounded by double quotes) and operators. Multiple terms and phrases separated by a white space are automatically conjugated by "AND" operator.

The query syntax allows you to use:

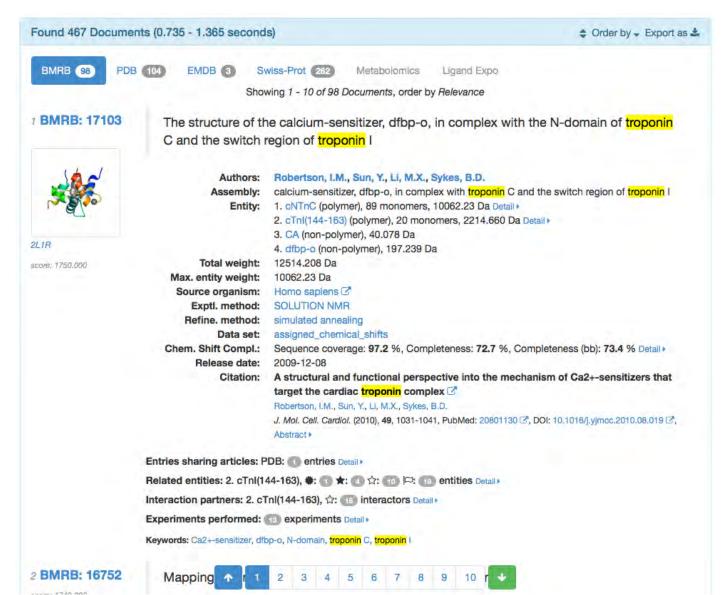
- phrases in the specified attribute (e.g. data_set.type:order_parameters)
- wild card (either ? or * character in term)
- regular expression surrounded by slashes
- fuzzy search based on Demerau-Levenshtein distance using a tilde character in term end, proximity search(e.g. "ph domain"~3, which searches for "ph" and "domain" within 3 words.)
- range search for decimal or date attributes (e.g. entry.original_release_date:[20010101 TO 20051231])
- a series of Boolean operators ("OR", "AND" and "NOT")
- grouping using parentheses to form sub queries that is useful if you want to control Boolean logic for a query.

What entries can be retrieved using the query below?

"ph domain" 3 AND data_set.type:order_parameters



Search results





Unified file exportation of derived data

BMRB Mirror server:

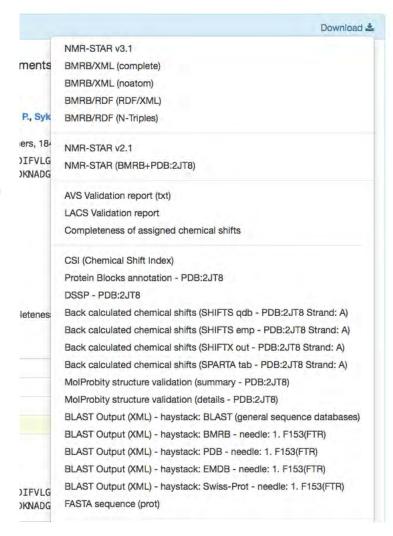
- NMR-STAR
- PDB+BMRB*
- AVS validation report
- LACS validation report
- CSI
- CS-Rosetta structures
- DSSP*
- Watson Click basepairs (Wattos)*
- Backcalculated CS (SHIFTS, SHIFTX, SPARTA)*
- MolProbity validation*
- BLAST Output (general)
- Timedomain

BMRB/XML & BMRB/RDF Data server:

- BMRB/XML
- BMRB/RDF
- CS completeness
- Protein Blocks (NMR structure)
- Protein Blocks (related X-ray structure)*
- BLAST Output (DB specific)
- FASTA

PDBj-BMRB entry page:

Download menu button







Statistics on search results

Statistics on search results are shown as charts summarizing the following points:

- Released entries
- Total molecular weights
- Available data sets (BMRB)
- Completeness of assigned chemical shifts
- Highest resolution (PDB, EMDB)
- R-value (PDB)
- Applied experimental methods
- Applied refinement methods
- Cited journal names
- Most frequent keywords
- Most frequent entry author names

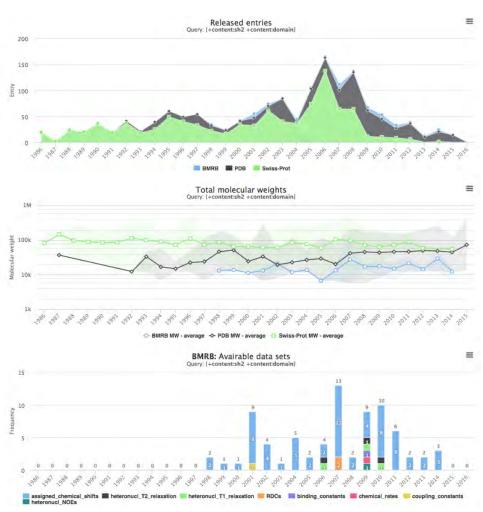




Chart displays: Assigned chemical shifts

Chem. Shift Compl.:

Sequence coverage: 97.5 %, Completeness: 75.9 %, Completeness (bb): 81.7 % Detail -

Polymer type: polypeptide(L)

Dow		

	Total	¹ H	¹³ C	15N
All	75.9 % (1398 of 1842)	76.8 % (737 of 960)	71.7 % (509 of 710)	88.4 % (152 of 172)
Backbone	81.7 % (771 of 944)	95.6 % (304 of 318)	67.5 % (316 of 468)	95.6 % (151 of 158)
Sidechain	73.8 % (772 of 1046)	67.6 % (434 of 642)	86.4 % (337 of 390)	7.1 % (1 of 14)
Aromatic	24.0 % (25 of 104)	25.0 % (13 of 52)	23.1 % (12 of 52)	
Methyl	100.0 % (148 of 148)	100.0 % (74 of 74)	100.0 % (74 of 74)	

1. F153(FTR)

MDDIYKAAVE QLTEEQKNEF KAAFDIFVLG AEDGSISTKE LGKVMRMLGQ NPTPEELQEM IDEVDEDGSG TVDFDEFLVM MVRSMKDDSK GKSEEELSDL FRMFDKNADG YIDLDELKIM LQATGETITE DDIEELMKDG DKNNDGRIDY DEXLEFMKGV E

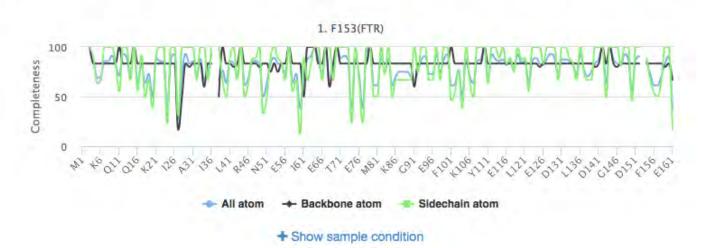




Chart displays: Heteronuclear T₁, T₂, NOE and S²

Exptl. method:

Data set: heteronucl_NOEs, heteronucl_T1_relaxation, heteronucl_T2_relaxation

Heteronucl. T1: 1680 T1 values in 30 lists

NMR

Coherence: Sz, Field strength (1H): 500 MHz, 600 MHz, 800 MHz, Temperature: 278 (±0.1) K, 283 (±0.1) K, 283 (±0.1) K, 293 (±0.1) K, 293 (±0.1) K, 298 (±0.1)

(±0.1) K, 303 (±0.1) K, 308 (±0.1) K, 313 (±0.1) K, 318 (±0.1) K, 323 (±0.1) K, pH: 5.25 (±0.1) Detail

Heteronucl. T2: 1680 T2 values in 30 lists

Coherence: S(+,-), Field strength (1H): 500 MHz, 600 MHz, 800 MHz, Temperature: 278 (±0.1) K, 283 (±0.1) K, 283 (±0.1) K, 293 (±0.1) K,

298 (±0.1) K, 303 (±0.1) K, 308 (±0.1) K, 313 (±0.1) K, 318 (±0.1) K, 323 (±0.1) K, pH: 5.25 (±0.1) Detail >

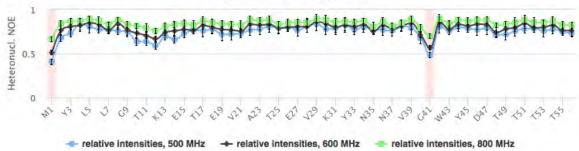
Heteronucl. NOE: 1680 NOE values in 30 lists

Value type: relative intensities, Field strength (1H): 500 MHz, 600 MHz, 800 MHz, Temperature: 278 (±0.1) K, 283 (±0.1) K, 288 (±0.1) K, 293

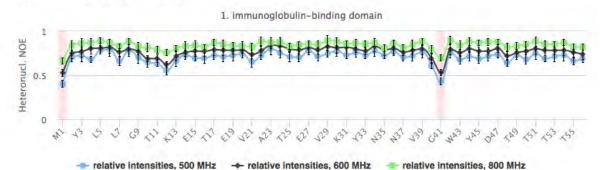
(±0.1) K, 298 (±0.1) K, 303 (±0.1) K, 308 (±0.1) K, 313 (±0.1) K, 318 (±0.1) K, 323 (±0.1) K, pH: 5.25 (±0.1) Detail

Temperature: 278 (±0.1) K, pH: 5.25 (±0.1)





Temperature: 283 (±0.1) K, pH: 5.25 (±0.1)



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PDBj-BMRB SPARQL server: Graphical interface for querying RDF data

http://bmrbpub.protein.osaka-u.ac.jp/search/rdf

Default Data Cat Nam	o (Graph IDI)		About Namespace Prefixes Inference rules
Default Data Set Nam http://bmrbpub.protein.os			
nttp://orniopoo.protein.oo	aka-u,ac.jp/rui/oiiii		
Query Text			
			11
		to retrieve remote RDF data, see <u>details</u> .)	12
Results Format:	HTML	<u> </u>	re ignored)
Results Format: Execution timeout:	HTML 0	milliseconds (values less than 1000 a	re ignored)
Results Format: Execution timeout: Options:	HTML 0 Strict checking of	milliseconds (values less than 1000 at f void variables	re ignored)
Results Format: Execution timeout: Options:	HTML 0 Strict checking of	milliseconds (values less than 1000 a	re ignored)



PDBj-BMRB SPARQL server: A programmable API for federated search

6 Graph URIs

- http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr (for BMRB entries)
- http://bmrbpub.protein.osaka-u.ac.jp/rdf/bms (for Metabolomics entries)
- http://rdf.wwpdb.org/pdb (for PDB entries)

Prefixes

- rdf: http://www.w3.org/1999/02/22-rdf-syntax-ns#
- rdfs: <http://www.w3.org/2000/01/rdf-schema#>
- owl: http://www.w3.org/2002/07/owl#
- BMRBo: http://bmrbpub.protein.osaka-u.ac.jp/schema/mmcif_nmr-star.owl#
- PDBo: http://rdf.wwpdb.org/schema/pdbx-v40.owl#

Reference Ontorogies

- BMRB/OWL: BMRB/RDF ontology
- PDBx OWL: PDB/RDF ontology
- 1 How to run SPARQL query via curl command. Please include FROM clause in a query to select Graph URI.

```
% curl -F "query=QUERY" -F "format=FORMAT" http://bmrbpub.protein.osaka-u.ac.jp/search/rdf
```

```
% curl -F "query=@QFILE" -F "format=FORMAT" http://bmrbpub.protein.osaka-u.ac.jp/search/rdf
```

, where QUERY and QFILE stand for actual query strings and query file name, respectively. FORMAT represents MIME type selected from either text/html, application/vnd.ms-excel, application/results-xml, application/results-json, text/plane, application/rdf+xml, text/csv or text/tabseparated-values.

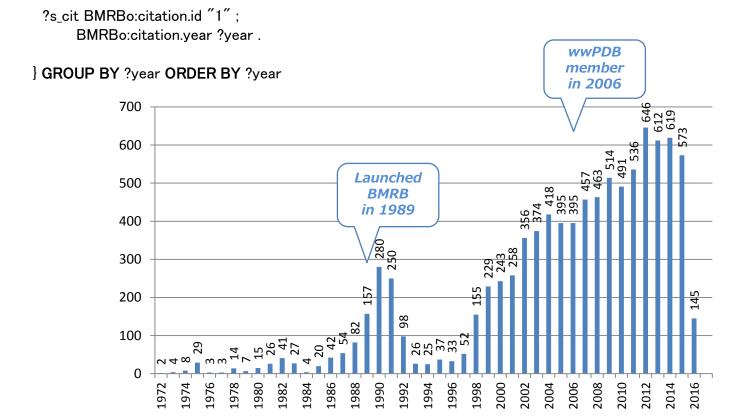


Basic SPARQL query composition

Count the number of primary publications cited by BMRB entries per year:

PREFIX BMRBo: http://bmrbpub.protein.osaka-u.ac.jp/schema/mmcif_nmr-star.owl#

SELECT ?year (COUNT(?year) AS ?count)
FROM http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr
WHERE {



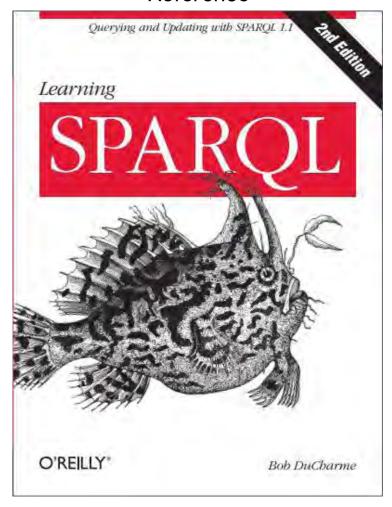


Federated SPARQL query using 'SERVICE' clause

... While typical SPARQL query or subquery retrieves data from somewhere local or remote and applies a query to it, the **SERVICE** keyword lets you say "send this query off to the specified SPARQL endpoint service, which will run the query, and then retrieve the result." It's a great keyword to know, ...

Learning SPARQL by Bob DuCharme

Reference











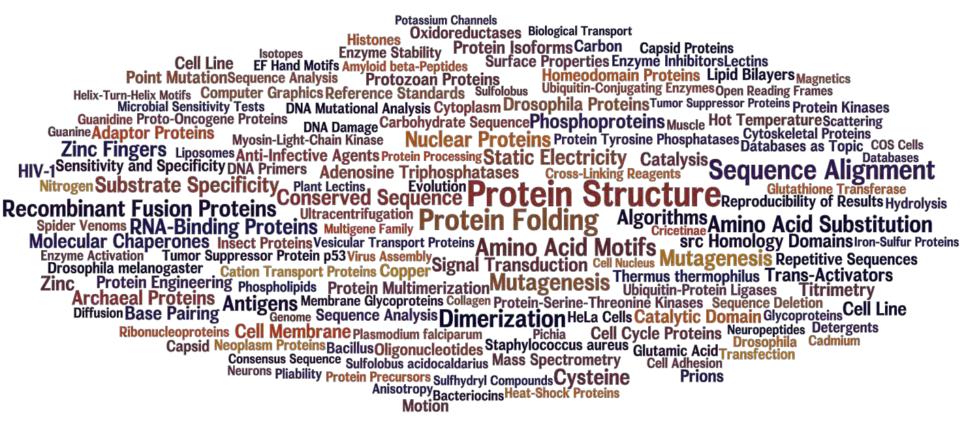
Retrieve a list of MeSH (Medical Subject Headings) words in publications of a period of time:

```
PREFIX BMRBo: <a href="http://bmrbpub.protein.osaka-u.ac.jp/schema/mmcif">http://bmrbpub.protein.osaka-u.ac.jp/schema/mmcif</a> nmr-star.owl#>
PREFIX pubmed v: <a href="http://bio2rdf.org/pubmed">http://bio2rdf.org/pubmed</a> vocabulary:>
SELECT ?word (COUNT(?word) AS ?count)
FROM <a href="http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr">http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr</a> FROM <a href="http://bio2rdf.org/pubmed">http://bio2rdf.org/pubmed</a>
WHERE {
   SELECT DISTINCT ?pubmed_id ?word
   WHERE {
     ?s_citation BMRBo:citation.pubmed_id ?pubmed_id ; BMRBo:citation.year ?year .
     FILTER (bound(?pubmed id) && xsd:integer(?year) >= 2001 && xsd:integer(?year) <= 2010)
     BIND (IRI(CONCAT("http://bio2rdf.org/pubmed:", ?pubmed id)) AS ?s pubmed)
     SERVICE <a href="http://cu.pubmed.bio2rdf.org/sparql">http://cu.pubmed.bio2rdf.org/sparql</a> {
      ?s pubmed_v:mesh_heading ?s_meshhd .
      ?s meshhd pubmed v:mesh descriptor name ?mesh descriptor .
     FILTER NOT EXISTS { ?s_meshhd pubmed_v:mesh_qualifier_name ?mesh_qualifier .
     BIND ((IF (CONTAINS(?mesh descriptor, ","), STRBEFORE(?mesh descriptor, ","), ?mesh descriptor)) AS ?word)
     FILTER (?word NOT IN ("Magnetic Resonance Spectroscopy", "Nuclear Magnetic Resonance"))
     FILTER (?word NOT IN ("X-Ray Diffraction", "X-rays", "Crystallography", "Crystallization"))
} ORDER BY DESC(?count)
```

Total query execution time: about 10 minutes

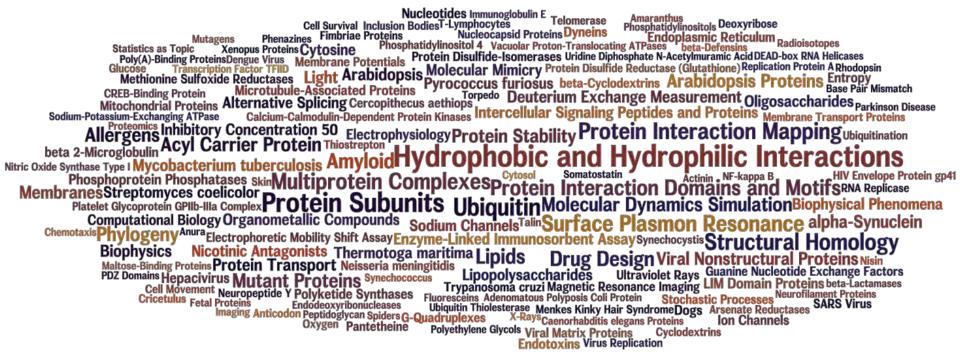


Newly appeared MeSH words in abstracts of publications cited by BMRB entries in the 1990s





Newly appeared MeSH words in abstracts of publications cited by BMRB entries in the 2000s





Compering BMRB and PDB by the MeSH words in the same period

PDB: 2000s

BMRB: 1990s BMRB: 2000s

Potassium Channels
Oxidoreductases Biological Transport
Cell Line
Er Hand Motifs Amyloid beta-Peptides
Protein Isoforms Carbon
Cell Line
Fried Motifs Amyloid beta-Peptides
Protein Surface
Proteins
Helix-Turn-Helix Motifs Computer Graphics Reference Standards
Microbial Sensitivity Tests
Microbial Sensitivity Tests
Microbial Sensitivity Tests
Mosification
Guanidine Prote-Oncogene Proteins
Guanidine Prote-Oncogene Proteins
Mosification
Guanidine Prote-Oncogene Proteins
Myosin-Light-Chain Kinases
Nuclear Proteins Protein Turns-Helix Muscle Hot Temperature Scattering
Guanine Adaptor Proteins
Myosin-Light-Chain Kinase
Nuclear Proteins Protein Turns-House Phosphatases Cytoskeletal Proteins
Countier Froteins Protein Proteins Protein Turns-House Phosphatases Stoph Databases
HIV-1 Sensitivity and Specificity DNA Primers Adenosine Triphosphatases
Recombinant Fusion Proteins
Spider Venoms RNA-Binding Proteins Multigene Family
Molecular Chapperones Insect Proteins Venecular Transport Protein Folding
Molecular Chapperones Insect Proteins Venecular Transport Proteins Amino Acid Molecular Chapperones Insect Proteins Proteins Multigene Family
Drosophila melanogaster Caton Transport Proteins Copper Signal Transduction
Protein Engineering Phospholipids Protein Multimerization Mutagenesis
Mitigenes Membrane Glycoproteins Soldgeser Protein-Serine-Threomine Kinases Sequence Deteron Cell Line
Genome Sequence Analysis

Rebonucleoproteins Cell Membrane Proteins Sequence Consensus Sequence Molecular Union Consensus Sequence Molecular Staphylococcus aureus
Consensus Sequence Multimerization Mass Spectrometry
Neurons Plability Proteins Protein Proteins Staphylococcus aureus
Consensus Sequence Calofouris Mass Spectrometry
Neurons Plability Protein Protein Proteins Staphylococcus aureus
Colle Proteins Mutagenesis
Mitigenesis Multimerization Mass Spectrometry
Neurons Plability Protein Proteins Suppressor Supplydy Compounds Cycle Proteins Neuropetides Detergents
Mitigenesis Multimerization Mass Spectrometry
Neurons Plability Protein Proteins

Nucleotides immonodoulin E Telomerase

Matagens Plenarine, Findriae Proteins

Micrographic Proteins Dyneins

Statistics as Topic Xenopus Proteins Dyneins

Micrographic Proteins Dyneins

Phyly Al-Binding Proteins Degue Virus

Methionina Strotiens Degue Degue Vi

PDB: 1990s

Glutamine Neoplasms Nucleotides Arabidopsis

Primidines Poptide Library

Trans-Activators

Databases Protozoan Proteins

Sulfornamides Libid Blayers

Primidines Poptide Library

Trans-Activators

DNA Primers Microfilament Proteins Anti-HIV Agents

Nucleotides Administration Molecular Mimicry

Reproducibility of Results

Arabidopsis Proteins Proteins Methiorine Viral Nonstructural Proteins Mass Spectrometry Glutathione

Transcriptase Protein Subunits Alloy and Aryl Transferases Cytoplasm Crypelectron Microscopy Nuclear Proteins

Polymerases Chain Reaction Antineoplastic Agents Molecular Chaperones

DNA-Directed RNA Polymerases Hydro-Lyases Tumor Suppressor Protein P53

Oxygenase Catalytic Domain Thermotoga maritima Protein Structure Proteins Green Microscopy Nuclear Proteins

Strict Homology Domains Mycobacterium tuberculosis Potassium

Protein Interaction Mapping Methanecoccus Hydrophobic and Hydrophilic Interactions DNA Replication Pose Response Relationship

Conserved Sequence Protein Tyrosine Phosphatases Light Sequence Alignment Proteins

Antineoplastic Agents Immunoglobulin Variable Region Uria Bacterial Outer Membrane Proteins

Dimerization Amino Acid Motifs Thiazoles DNA-Directed DNA Primers

Ribosomes Hydrolases

Genome

Genome

Transferase Naminopeptidases Allosteric Site

Transferase Naminopeptidases Allosteric Site

Transferase Archaea Proteins Sequence Analysis Oxidored Conserved Sequence Oxidored Sequence Proteins

Ribosomes Hydrolases

Genome

Transferase Archaea Proteins Sequence Analysis Oxidored Repetitive Sequence Septoment Proteins Sequence DNA Damage Adaptor Proteins

Ribosomes Hydrolases

Genome

Transferase Archaea Proteins Sequence Analysis Open Reading Frames

Genome

Transferase Archaea Proteins Sequence Analysis Open Reading Frames

Genome

Transferase Archaea Proteins Sequence Analysis Open Reading Frames

Aminopeptidases Allosteric Site

Malaria Indezoles
RNA Editing













Retrieve phenotypes annotated with the information for SNPs from the human genome in BMRB entities:

```
PREFIX BMRBo: <a href="http://bmrbpub.protein.osaka-u.ac.jp/schema/mmcif">http://bmrbpub.protein.osaka-u.ac.jp/schema/mmcif</a> nmr-star.owl#>
PREFIX rdfs: <a href="http://www.w3.org/2000/01/rdf-schema#">http://www.w3.org/2000/01/rdf-schema#</a>>
PREFIX omim v: <a href="http://bio2rdf.org/omim">http://bio2rdf.org/omim vocabulary:></a>
SELECT DISTINCT ?entity_id ?uniprot_id ?label ?omim_id ?dbsnp_id ?mutation ?phenotype
FROM <a href="http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr">http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr</a> FROM <a href="http://purl.uniprot.org/uniprot">http://purl.uniprot.org/uniprot</a>
FROM <a href="http://bio2rdf.org/omim">http://bio2rdf.org/omim</a>
WHERE {
 ?s up BMRBo:entity_db_link.entry_id "4280"; BMRBo:entity_db_link.entity_id ?entity_id;
       BMRBo:entity_db_link.database_code "SP"; BMRBo:entity_db_link.accession_code ?uniprot_id;
       rdfs:seeAlso ?s uniprot.
  ?s uniprot rdfs:label ?info .
  FILTER (STRSTARTS(?info, "info:uniprot"))
  SERVICE <a href="http://sparql.uniprot.org/sparql">http://sparql.uniprot.org/sparql</a> {
   ?s uniprot rdfs:label ?label ; rdfs:seeAlso ?o purl .
  FILTER (STRSTARTS(STR(?o_purl), "http://purl.uniprot.org/mim/"))
  BIND (STRAFTER(STR(?o_purl), "http://purl.uniprot.org/mim/") AS ?omim_id)
  BIND (IRI(CONCAT("http://bio2rdf.org/omim:", ?omim id)) AS ?s omim)
  SERVICE <a href="http://omim.bio2rdf.org/sparql">http://omim.bio2rdf.org/sparql</a> {
   ?s_omim omim_v:variant ?s_allele .
   ?s_allele omim_v:dbsnp ?s_dbsnp ; omim_v:mutation ?mutation ; rdfs:label ?phenotype .
   BIND (STRAFTER(STR(?s dbsnp), "http://bio2rdf.org/dbsnp:") AS ?dbsnp id)
```



Federated search beyond DB boundaries: BMRB, UniProt and OMIM

4597 phenotype annotated SNPs in all BMRB entities



574 residues having backbone chemical shifts



74 residues having structural information



Classification by structural parameters archived at BMRB

- Degeneration of protein fold or its function by stop codon: 12
- Mutation of inherently hydrophilic amino acids (Arg, Lys and Pro) in a hydrophobic environment: **11**
- Mutation of Arg, Lys and Pro in mostly buried residues (rSASA<10%): 15
- Substitution of residues on the protein surface (rSASA>50%) with different charge: 14
- Substitution of residues on the protein surface to bulky aromatic residue:
- The other cases having little relation with the structural parameters above: 20

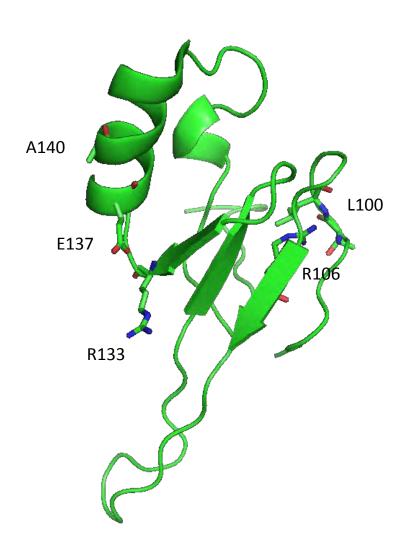


Federated search beyond DB boundaries: BMRB, UniProt and OMIM

Results performed by the SPARQL query for BMRB entry 4280, showing BMRB ID, mutation, OMIM ID, dbSNP ID, secondary structure, and SASA.

BMRB	Mutation	OMIM	dbSNP	2nd	SASA%
4280	L100V	300005	rs28935168	Coil	22.5
4280	R106W	300005	rs28934907	Strand	8.0
4280	R133C	300005	rs28934904	Coil	49.4
4280	E137G	300005	rs61748392	Helix	41.7
4280	A140V	300005	rs28934908	Helix	42.0

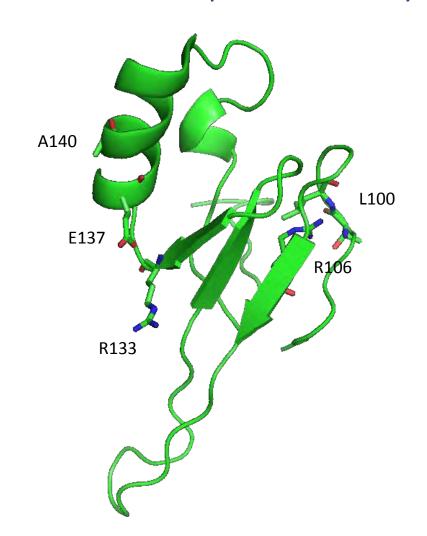
Ribbon models of NMR structure (PDB: 1QK9) of MECP2. The side-chains for the mutation (E137 and A140) exposed to solvent. R133 is critical residue for CpG DNA recognition. L100 and R106 are located in hydrophobic environment. All residues are responsible for X-linked mental retardation (Rett syndrome).

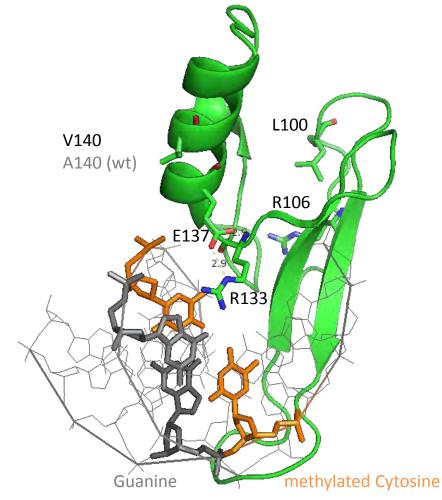


Solution structure of MeCP2 methyl CpG binding domain



Rett syndrome related residues of MeCP2 in complex with methylated DNA (CpG motif)





Solution structure of MeCP2 MBD, PDB: 1QK9

J. Mol. Biol. (1999) 291:1055

MeCP2 MBD (A140V) in complex with CpG DNA, PDB: 5BT2

Scientific report (2016) **6**:31210



Search

Home.

Examples

PDBj-BMRB SPARQL server: Other 30 SPARQL query examples

http://bmrbpub.protein.osaka-u.ac.jp

BMRB/XML & BMRB/RDF Data Server:

Resources

Download

common open representations of BMRB NMR-STAR data in XML and RDF formats

NEWS

Virtuoso SPARQL Query Editor

Default Data Set Name (Graph IRI)

http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr

Query Text

1. Select all category holders of datablock class of BMRB entry 15400:

SELECT *
FROM FROM FROM red">red"red">red"red">red"red"<a href="mailto:re

Query examples

Category holders

- Select all category holders of datablock class
 of BMRB entry 15400: Show
- Select all category holders of datablock class of Metabolomics entry bmse000400: Show

Entry statistics

 Count entries per submission year and experimental method (subtype): Show

Assembly descriptions

 Select all assembly names, asym IDs, entity IDs, polymer types, formula weights and functions in a assembly: Show

PDBj-BMRB web services to enhance interoperability of NMR data



BMRB/XML, BMRB/RDF

representations of BMRB NMR-STAR data in XML and RDF formats



PDBj-BMRB integrated search service

search biological/biochemical DBs at once



PDBj-BMRB SPARQL server

a programmable API for federated search



BMRB SQL on your PC

periodically updated BMRB relational DB for intensive search



BMRB SQL on your PC: periodically updated BMRB relational DB for intensive search

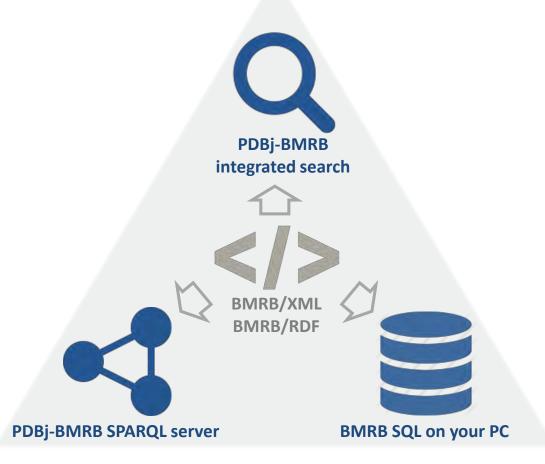
BMRB PostgreSQL 9.5 dump file (noatom):

```
% rsync -av --delete rsync://bmrbpub.protein.osaka-u.ac.jp/bmrb-pg-dump .
% pg_restore -c -d $DB_NAME -U $USER bmrb_clone.sql
```

- Easy to install
- Updated every week
- Data remediation equivalent to BMRB/XML
- Reducing latency as much as you want

A selection of PDBj-BMRB web services for researchers

Easy-to-use



Linked data

Low latency

Collaborators



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