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

WORLDWIDE PDB
PROTEIN DATA BANK

Members:

RCSB PDB PROTEIN DATA BANK

PDBe Protein Data Bank in Europe

PDBj Protein Data Bank Japan

BMRB

PDBj BMRB

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

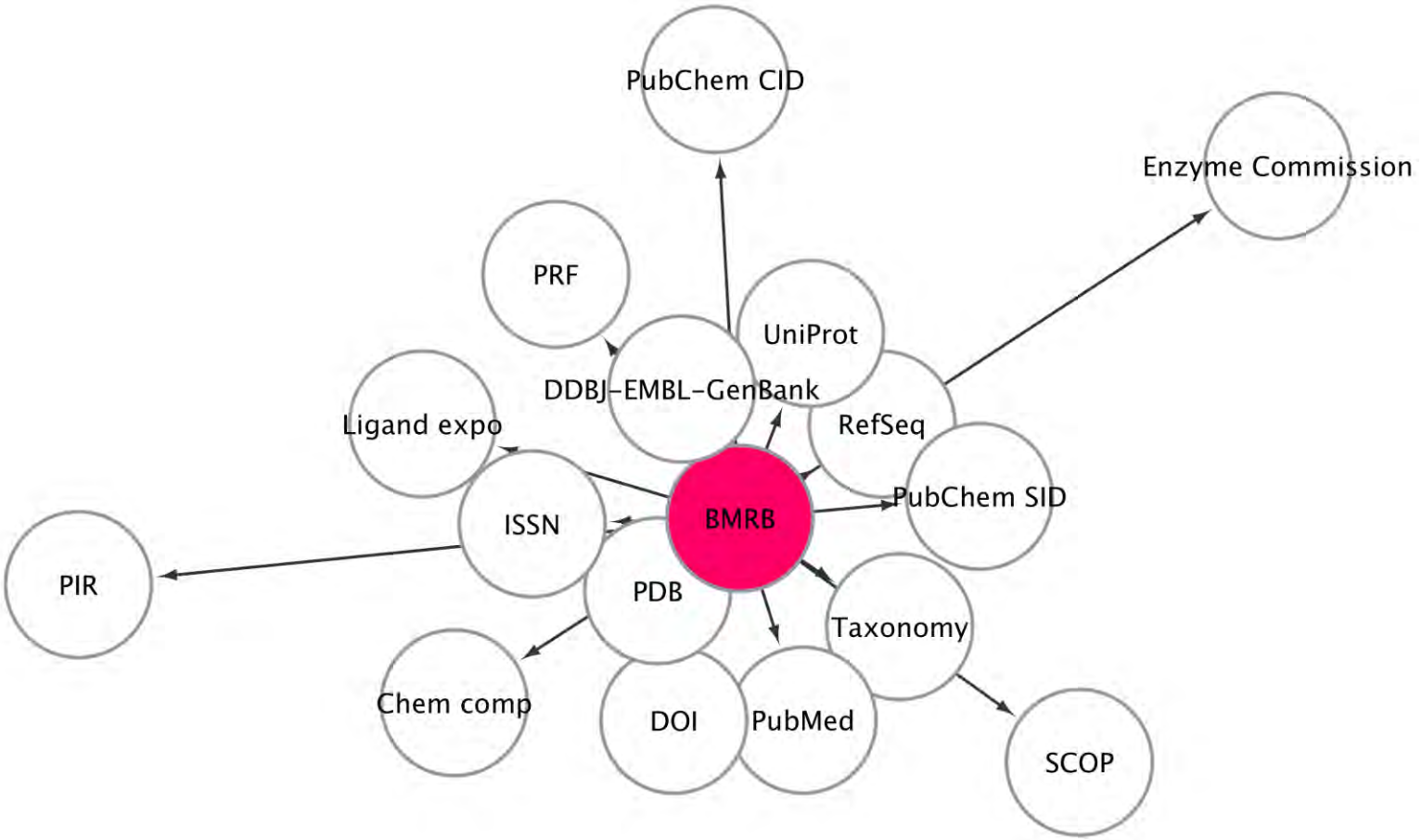
1. http://bmrb.pdbj.org/ftp/pub/bmrb/entry_lists/nmr-star3.1/
2. http://bmrb.pdbj.org/ftp/pub/bmrb/nmr_pdb_integrated_data/coordinates_restraints_chemshifts/bmrb_plus_pdb/
3. http://pacsy.nmrfam.wisc.edu/
4. http://bmrb.pdbj.org/ftp/pub/bmrb/validation_reports/LACS/
5. http://bmrbpub.protein.osaka-u.ac.jp/archive/pb/
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/bmr11300/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"
                 rdfs:label="info:refseq/NP_001008202"/>
   <rdfs:seeAlso rdf:resource="http://identifiers.org/refseq/NP_001008202"
                 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.seq_identity>100.00</BMRBo:entity_db_link.seq_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

PDBj-BMRB web services to enhance interoperability of NMR data

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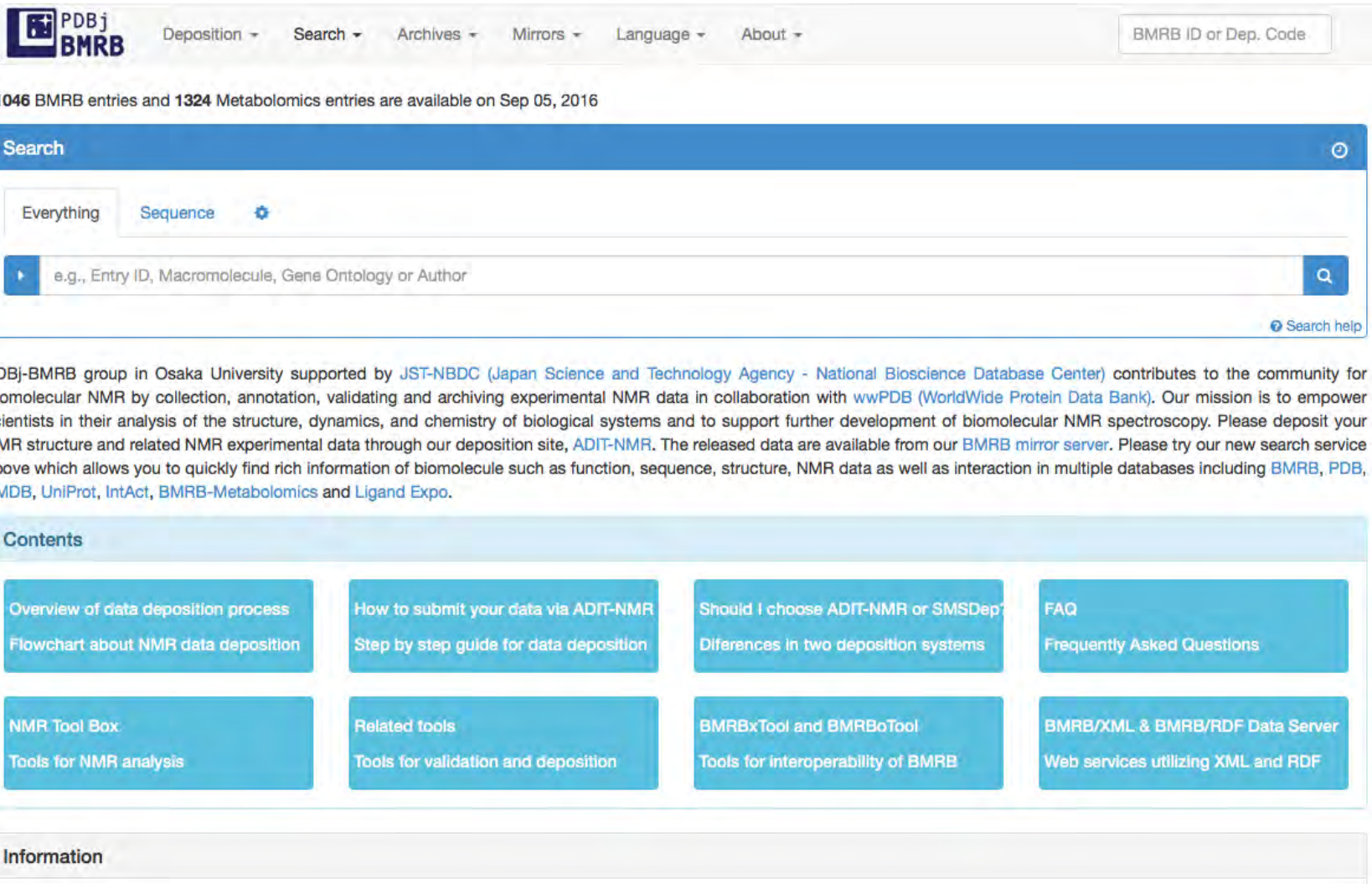
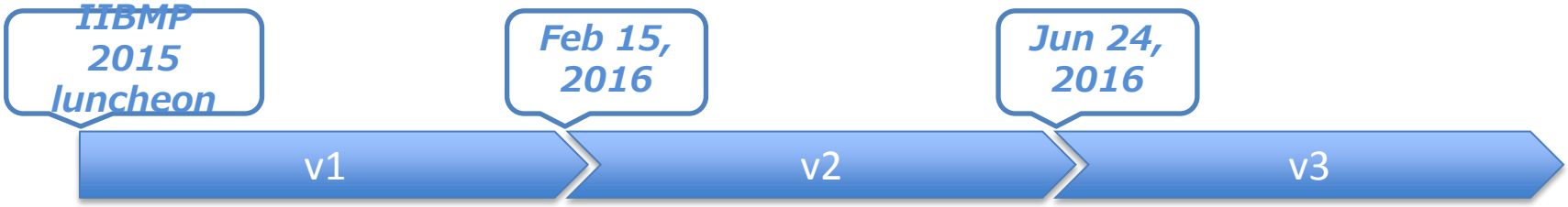
http://bmrbdep.pdbj.org



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

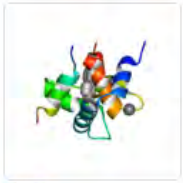
Found 467 Documents (0.735 - 1.365 seconds)

Order by Export as

BMRB 98 | PDB 104 | EMDB 3 | Swiss-Prot 262 | Metabolomics | Ligand Expo

Showing *1 - 10 of 98 Documents*, order by *Relevance*

1 **BMRB: 17103**



2L1R

score: 1750.000

The structure of the calcium-sensitizer, dfbp-o, in complex with the N-domain of troponin C and the switch region of troponin I

Authors: Robertson, I.M., Sun, Y., Li, M.X., Sykes, B.D.
Assembly: calcium-sensitizer, dfbp-o, in complex with troponin C and the switch region of troponin I
Entity: 1. cNTnC (polymer), 89 monomers, 10062.23 Da Detail
2. cTnI(144-163) (polymer), 20 monomers, 2214.660 Da Detail
3. CA (non-polymer), 40.078 Da
4. dfbp-o (non-polymer), 197.239 Da
Total weight: 12514.208 Da
Max. entity weight: 10062.23 Da
Source organism: Homo sapiens
Exptl. method: SOLUTION NMR
Refine. method: simulated annealing
Data set: assigned_chemical_shifts
Chem. Shift Compl.: Sequence coverage: **97.2** %, Completeness: **72.7** %, Completeness (bb): **73.4** % Detail
Release date: 2009-12-08
Citation: **A structural and functional perspective into the mechanism of Ca2+-sensitizers that target the cardiac troponin complex**
Robertson, I.M., Sun, Y., Li, M.X., Sykes, B.D.
J. Mol. Cell. Cardiol. (2010), **49**, 1031-1041, PubMed: 20801130, DOI: 10.1016/j.yjmcc.2010.08.019, Abstract

Entries sharing articles: PDB: 1 **entries** Detail

Related entities: 2. cTnI(144-163), ✹: 1 ★: 4 ☆: 10 ⚐: 18 **entities** Detail

Interaction partners: 2. cTnI(144-163), ☆: 16 **interactors** Detail

Experiments performed: 13 **experiments** Detail

Keywords: Ca2+-sensitizer, dfbp-o, N-domain, troponin C, troponin I

2 **BMRB: 16752**

Mapping 1 2 3 4 5 6 7 8 9 10

Unified file exportation of derived data

BMRB Mirror server:

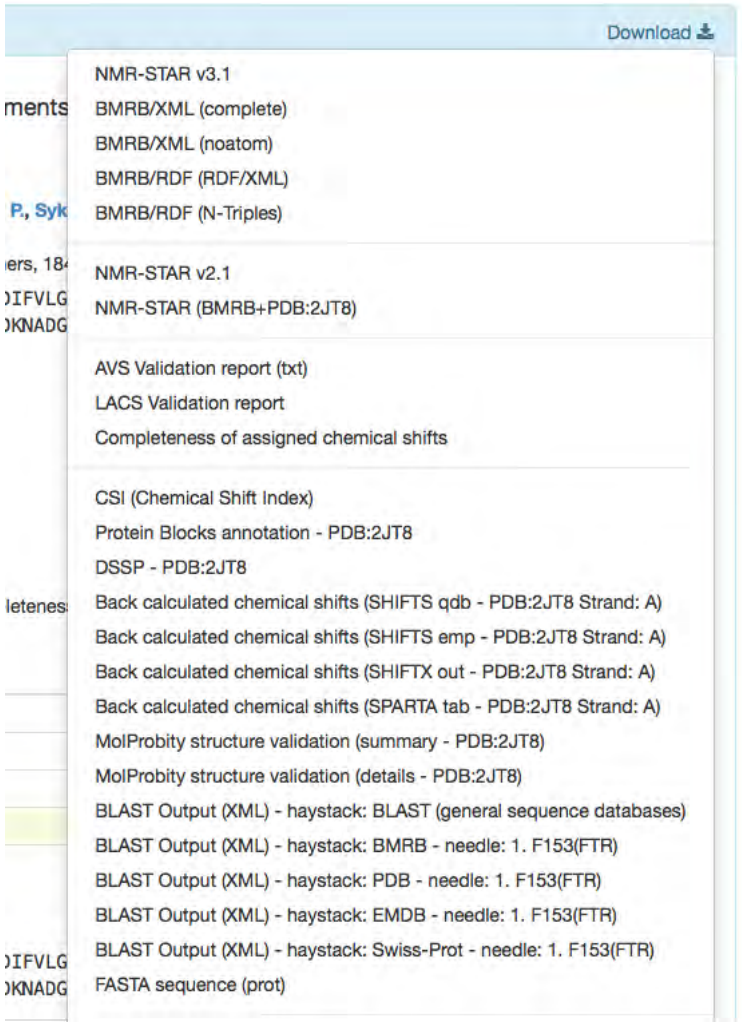
- NMR-STAR
- PDB+BMRB*
- AVS validation report
- LACS validation report
- CSI
- CS-Rosetta structures
- DSSP*
- Watson Click basepairs (Wattos)*
- Backcalculated CS (SHIFTS, SHIFTX, SPARTA)*
- MolProbity validation*
- BLAST Output (general)
- Timedomain

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



* represents derived data accessible by PDB ID

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

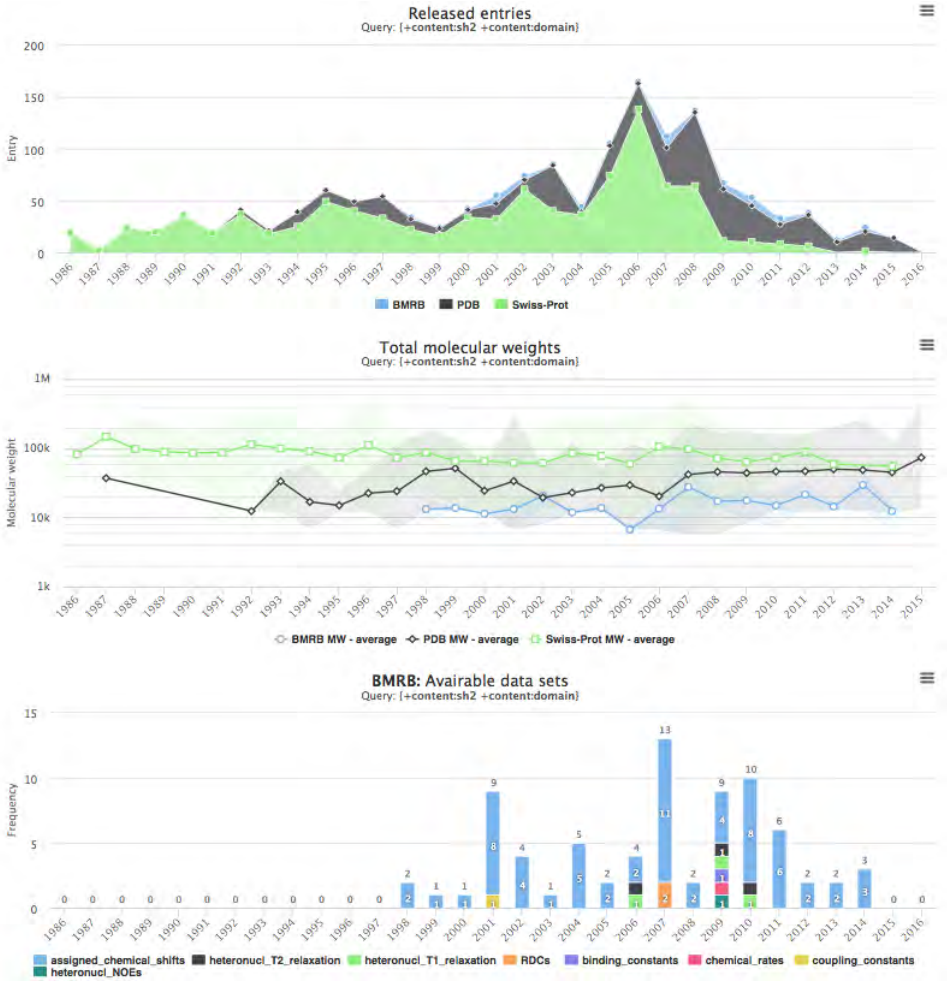


Chart displays:
Assigned chemical shifts

Chem. Shift Compl.: Sequence coverage: **97.5** %, Completeness: **75.9** %, Completeness (bb): **81.7** % Detail

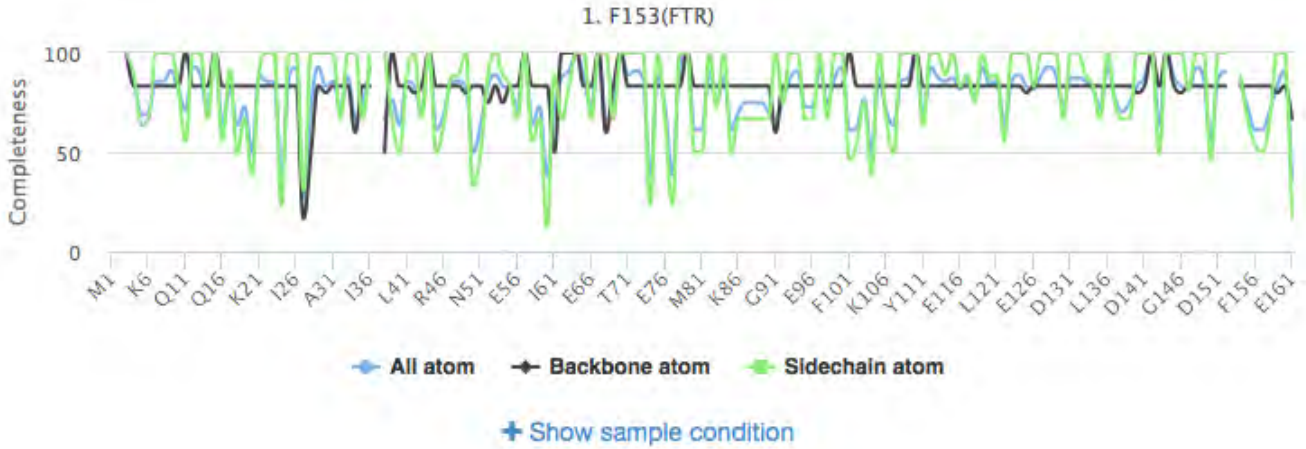
Polymer type: **polypeptide(L)**

Download

	Total	^{1}H	^{13}C	^{15}N
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



+ Show sample condition

Chart displays: Heteronuclear T_1, T_2, NOE and S^2

Exptl. method: NMR

Data set: heteronucl_NOEs, heteronucl_T1_relaxation, heteronucl_T2_relaxation

Heteronucl. T_1: 1680 T_1 values in 30 lists

Coherence: Sz, **Field strength (^{1}H):** 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

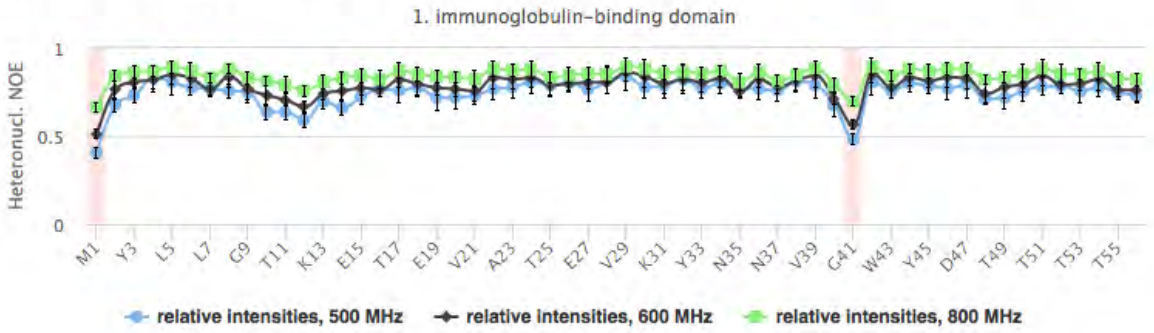
Heteronucl. T_2: 1680 T_2 values in 30 lists

Coherence: S(+,-), **Field strength (^{1}H):** 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

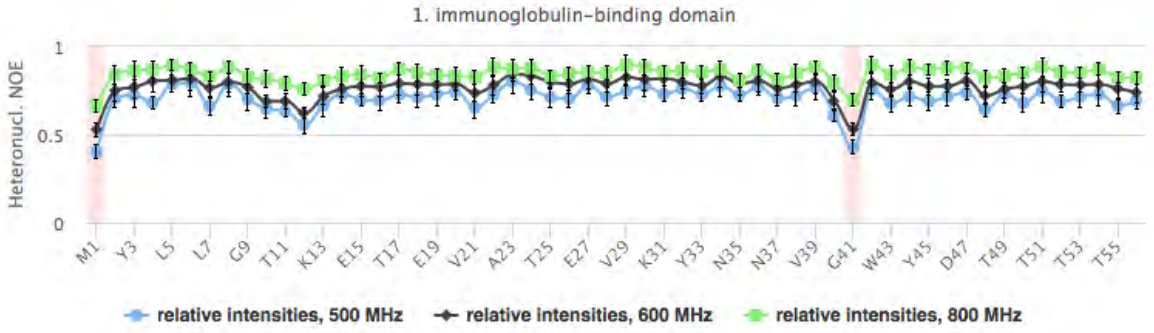
Heteronucl. NOE: 1680 NOE values in 30 lists

Value type: relative intensities, **Field strength (^{1}H)**: 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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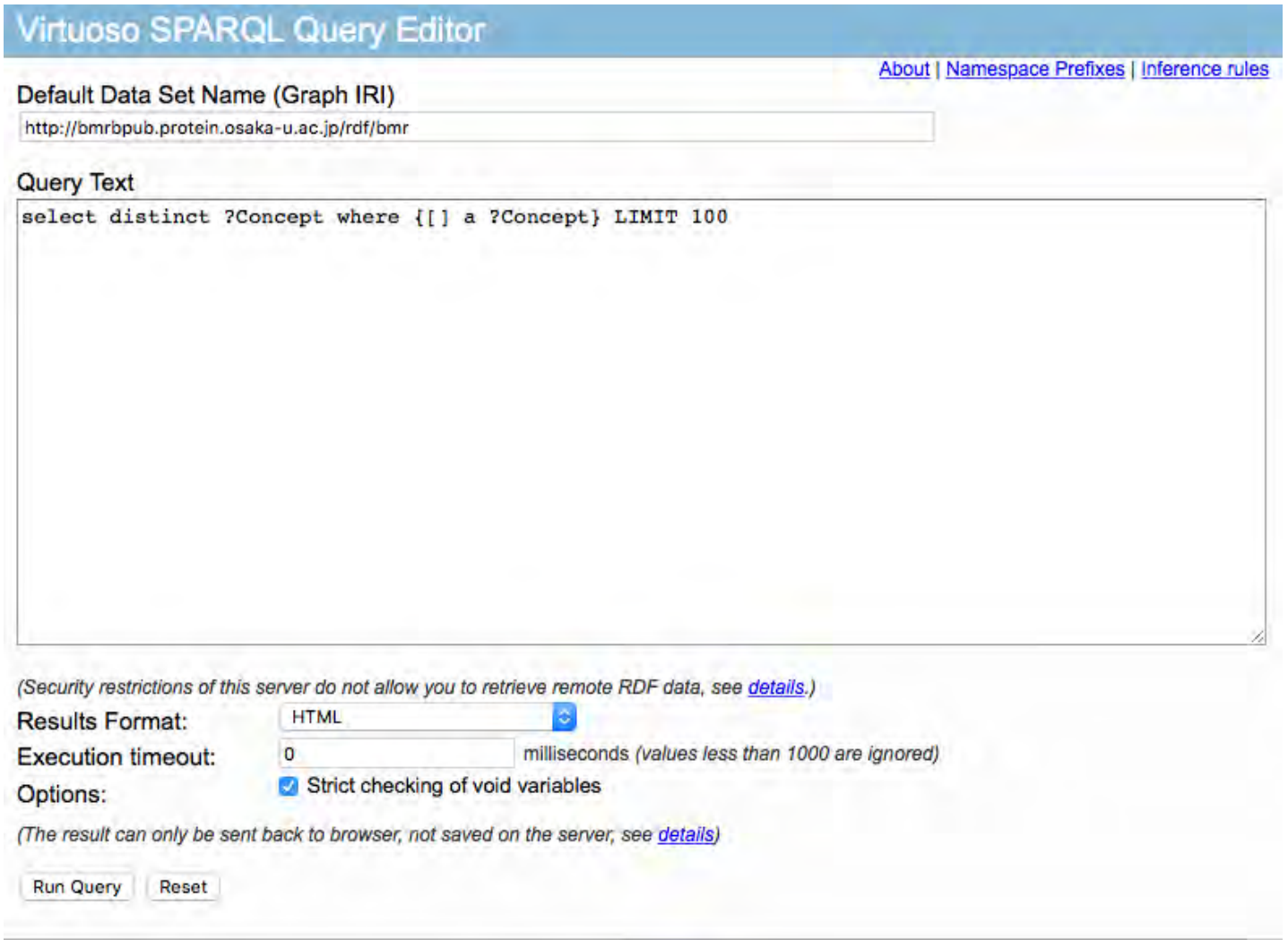
PDBj-BMRB SPARQL server: Graphical interface for querying RDF data

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



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

ℹ 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)

ℹ 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#>

ℹ Reference Ontorogies

- BMRB/OWL: BMRB/RDF ontology
- PDBx OWL: PDB/RDF ontology

ℹ 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
```

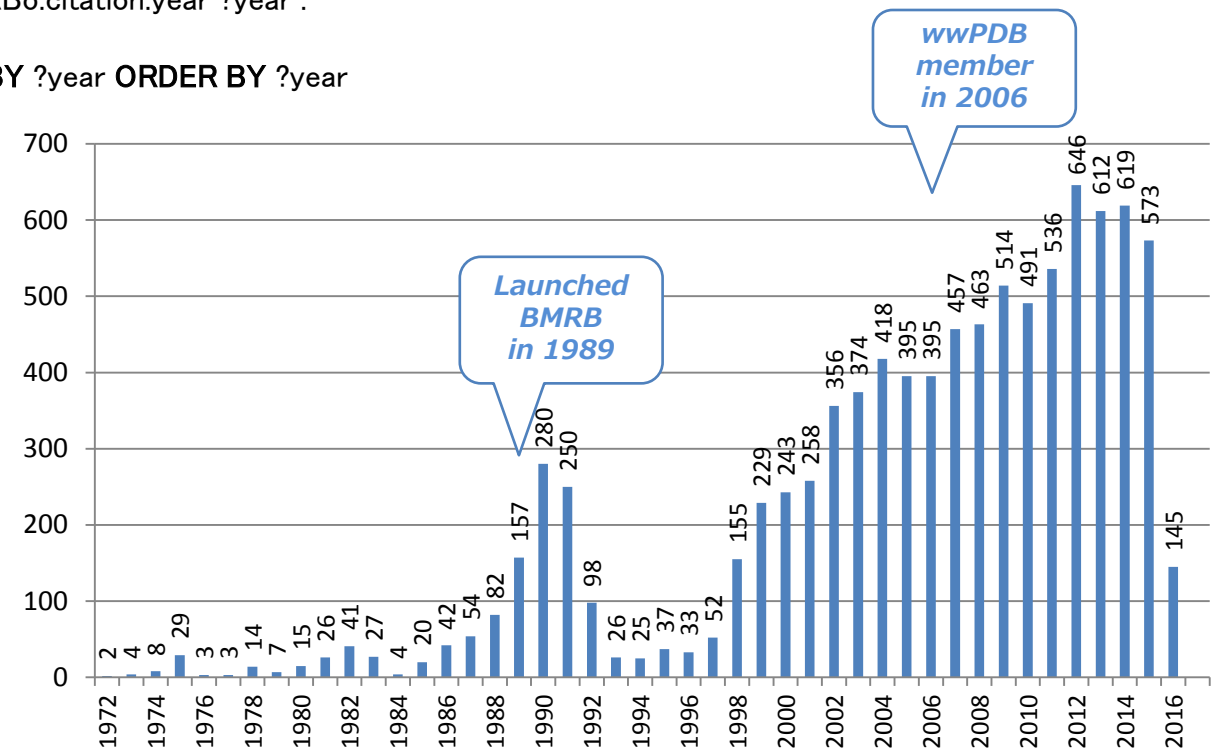
```
% curl -F "query=@QFILE" -F "format=FORMAT" http://bmrbpub.protein.osaka-u.ac.jp/search/rdf
```

, 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/tab-separated-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 {

  ?s_cit BMRBo:citation.id "1" ;
         BMRBo:citation.year ?year .

} GROUP BY ?year ORDER BY ?year
```

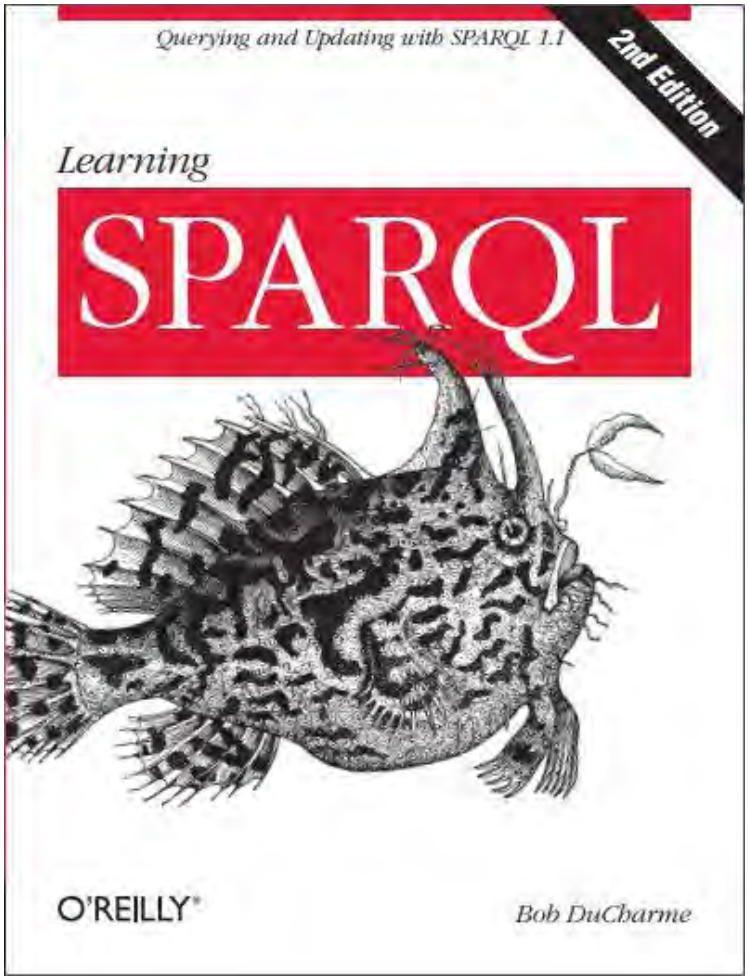


Federated SPARQL query using ‘SERVICE’ clause

… 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

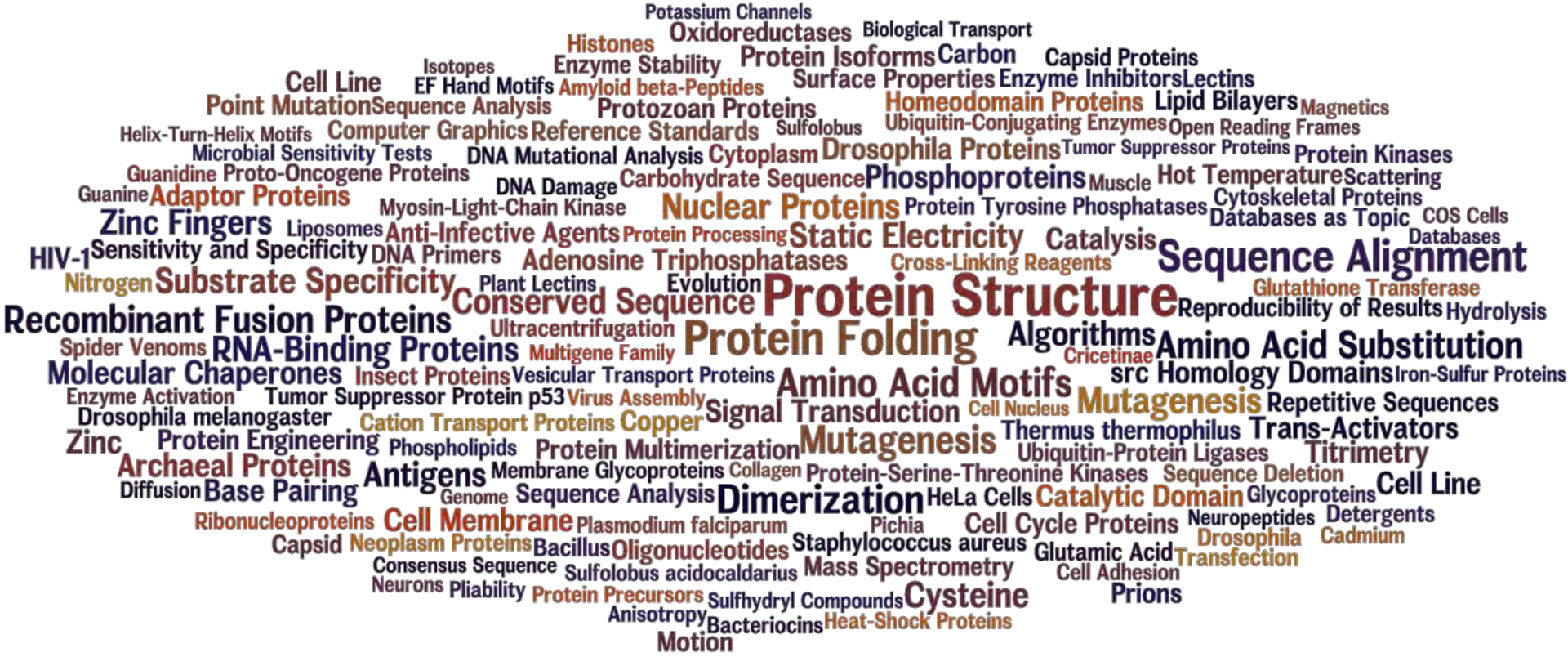


Retrieve a list of MeSH (Medical Subject Headings) words in publications of a period of time:

```
PREFIX BMRBo: <http://bmrbpub.protein.osaka-u.ac.jp/schema/mmcif_nmr-star.owl#>
PREFIX pubmed_v: <http://bio2rdf.org/pubmed_vocabulary:>

SELECT ?word (COUNT(?word) AS ?count)
FROM <http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr> FROM <http://bio2rdf.org/pubmed>
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 <http://cu.pubmed.bio2rdf.org/sparql> {
        ?s_pubmed 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)
```

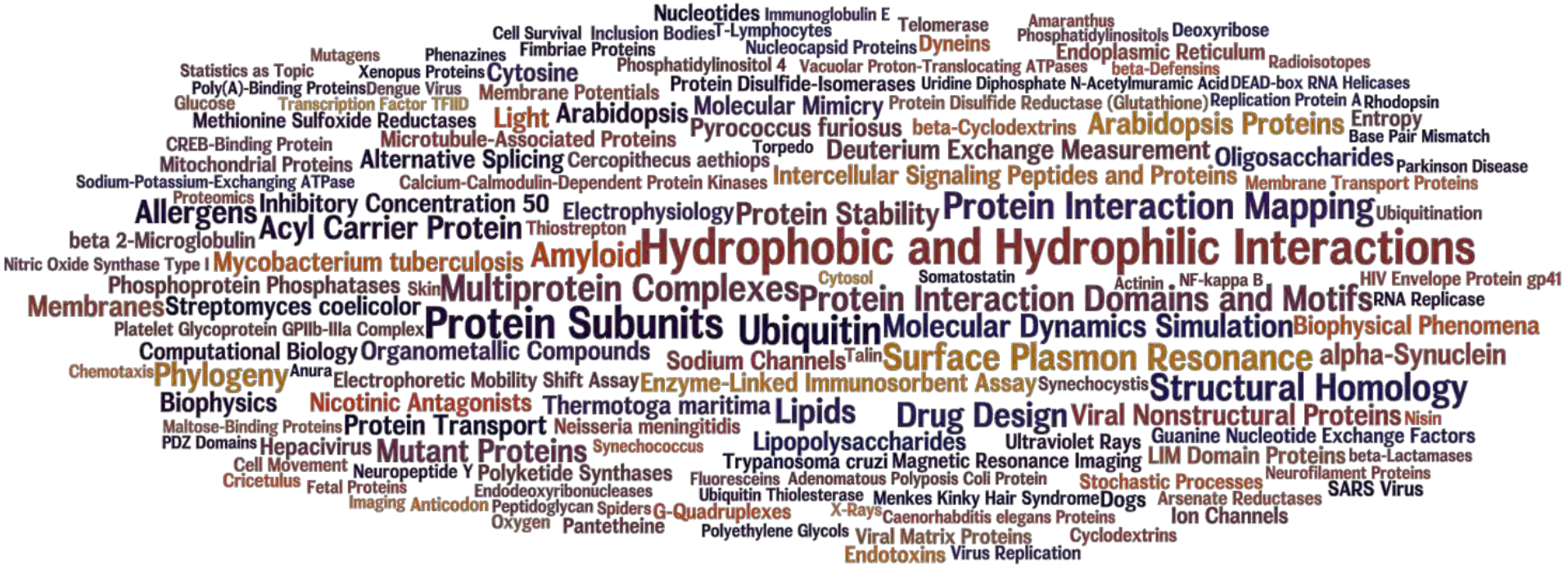
Total query execution time: about 10 minutes

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



where relative font sizes corresponded to quotation frequencies of the words to date

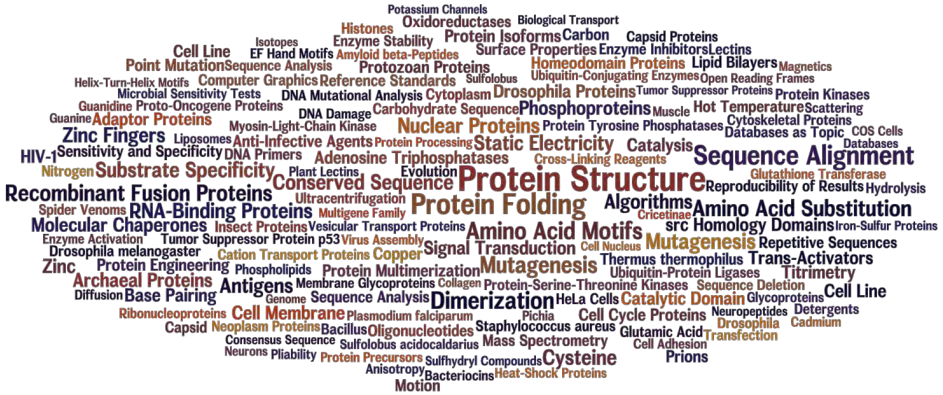
Newly appeared MeSH words in abstracts of publications cited by BMRB entries in the 2000s



where relative font sizes corresponded to quotation frequencies of the words to date

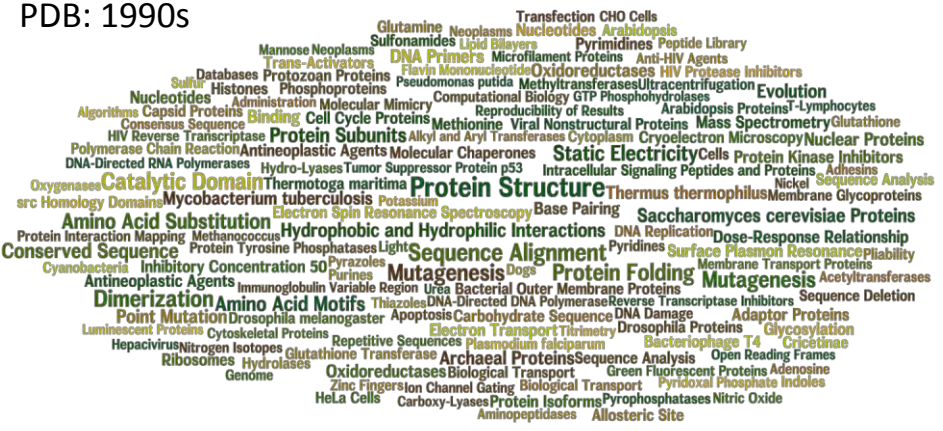
Compering BMRB and PDB by the MeSH words in the same period

BMRB: 1990s



BMRB: 2000s

PDB: 1990s



PDB: 2000s

where relative font sizes corresponded to quotation frequencies of the words to date

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

```
PREFIX BMRBo: <http://bmrbpub.protein.osaka-u.ac.jp/schema/mmcif_nmr-star.owl#>
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX omim_v: <http://bio2rdf.org/omim_vocabulary:>

SELECT DISTINCT ?entity_id ?uniprot_id ?label ?omim_id ?dbsnp_id ?mutation ?phenotype
FROM <http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr> FROM <http://purl.uniprot.org/uniprot>
FROM <http://bio2rdf.org/omim>
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 <http://sparql.uniprot.org/sparql> {
    ?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 <http://omim.bio2rdf.org/sparql> {
    ?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)
  }
}
```

Total query execution time: about 125 minutes

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

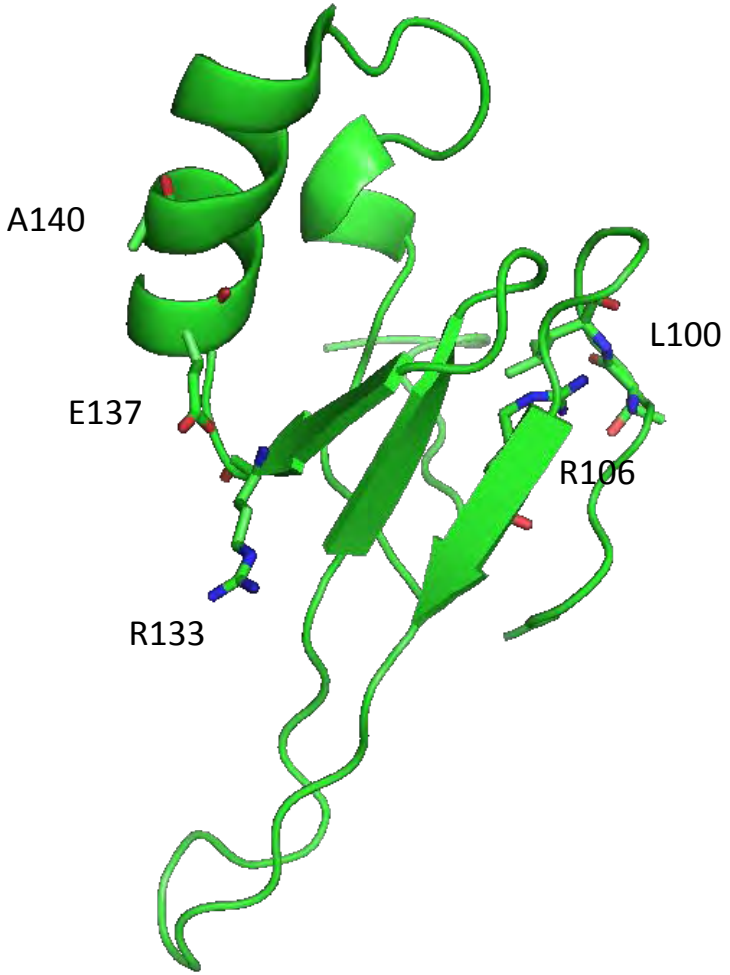
- Degeneration of protein fold or its function by stop codon: **12**
- Mutation of inherently hydrophilic amino acids (Arg, Lys and Pro) in a hydrophobic environment: **11**
- Mutation of Arg, Lys and Pro in mostly buried residues (rSASA<10%): **15**
- Substitution of residues on the protein surface (rSASA>50%) with different charge: **14**
- Substitution of residues on the protein surface to bulky aromatic residue: **4**
- 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.

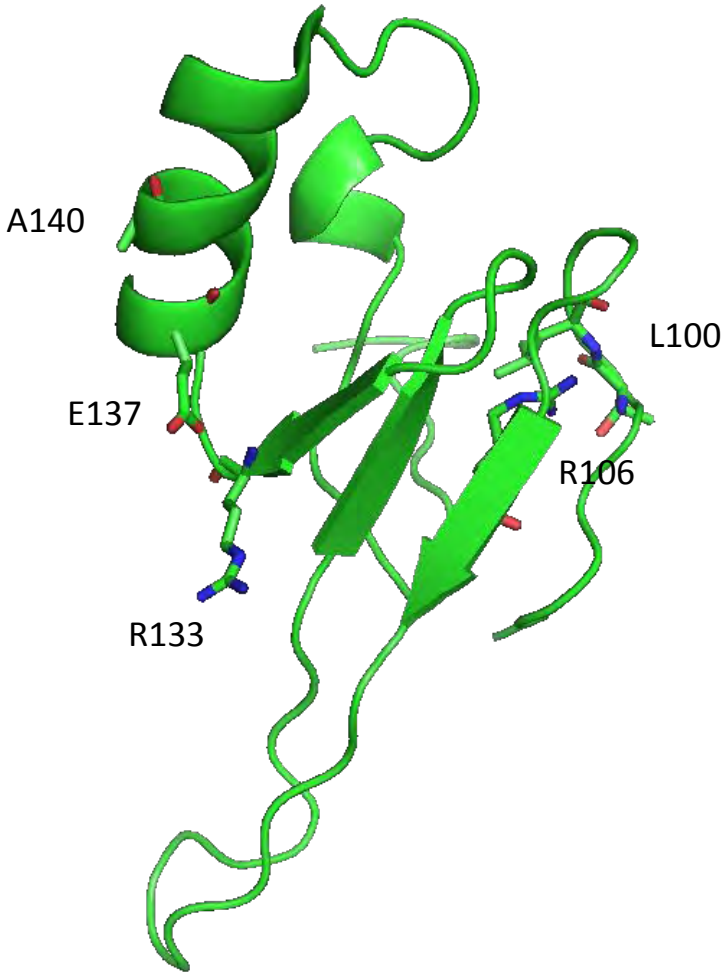
BMRB	Mutation	OMIM	dbSNP	2nd	SASA%
4280	L100V	300005	rs28935168	Coil	22.5
4280	R106W	300005	rs28934907	Strand	8.0
4280	R133C	300005	rs28934904	Coil	49.4
4280	E137G	300005	rs61748392	Helix	41.7
4280	A140V	300005	rs28934908	Helix	42.0

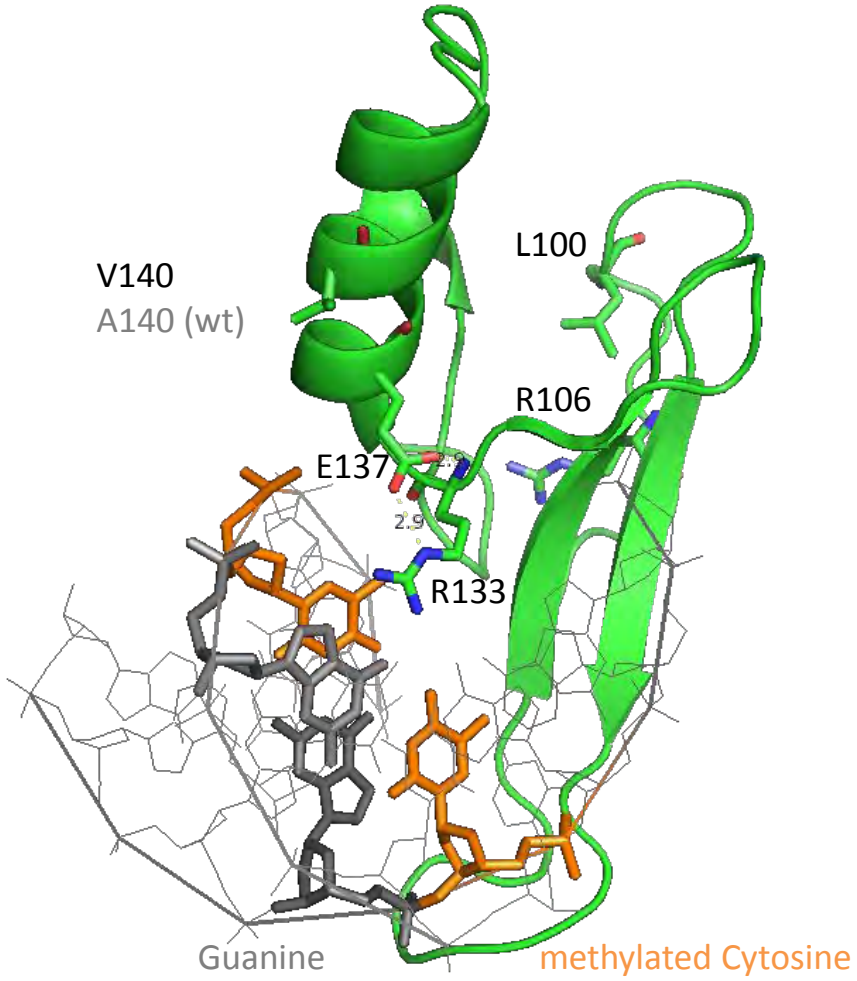
Ribbon models of NMR structure (PDB: 1QK9) of MECP2. The side-chains for the mutation (E137 and A140) exposed to solvent. R133 is critical residue for CpG DNA recognition. L100 and R106 are located in hydrophobic environment. All residues are responsible for X-linked mental retardation (Rett syndrome).



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

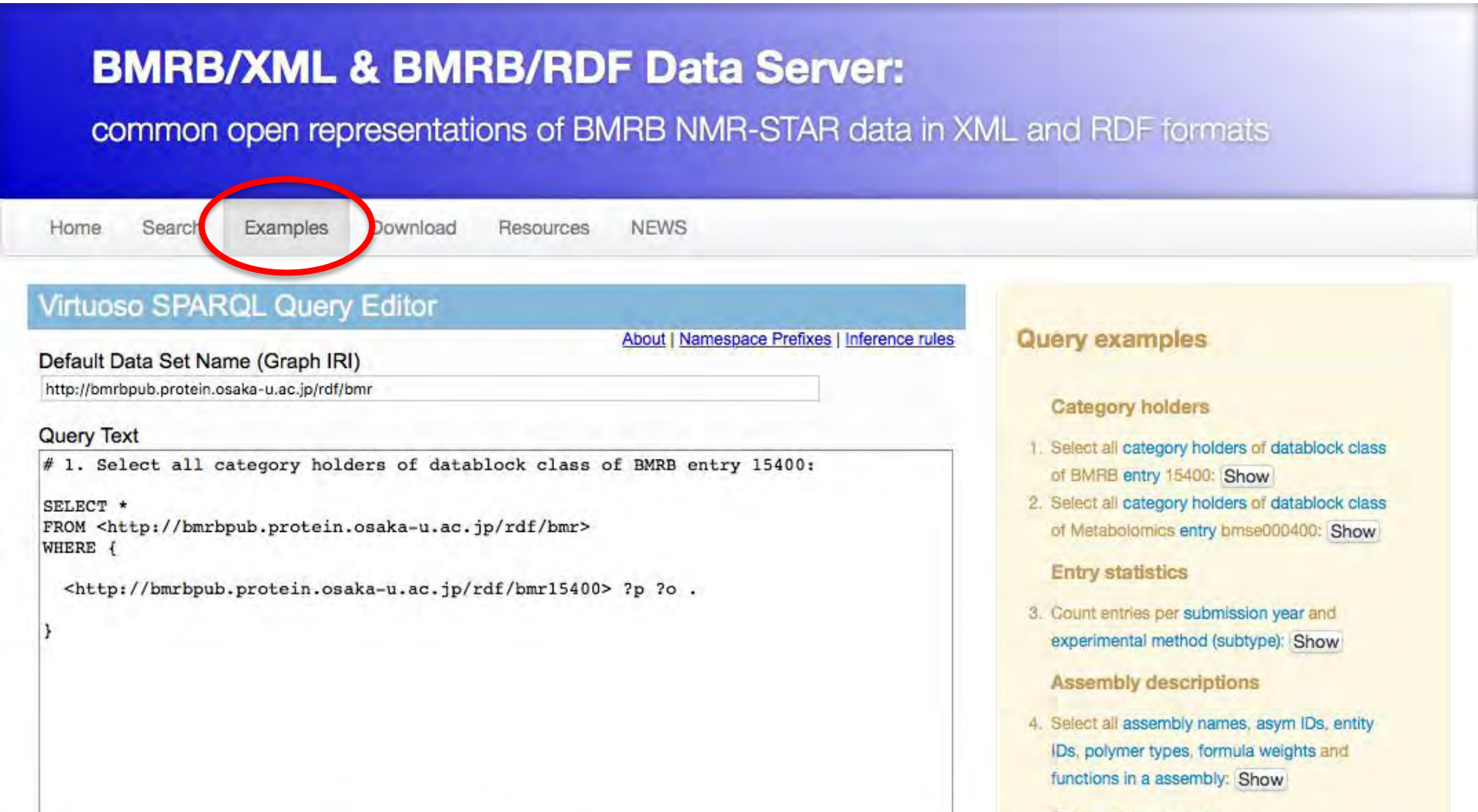
J. Mol. Biol. (1999) **291**:1055

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

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

PDBj-BMRB SPARQL server:
Other 30 SPARQL query examples

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



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

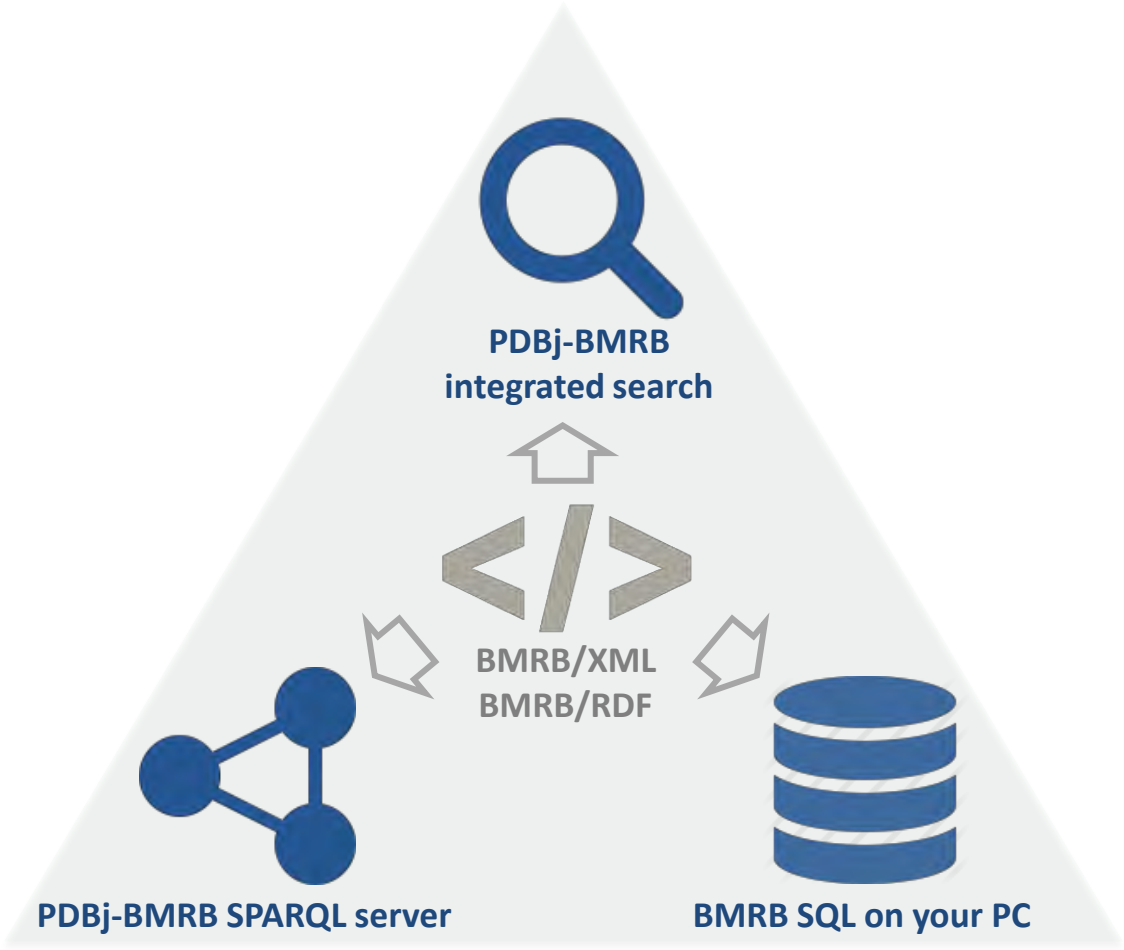
BMRB PostgreSQL 9.5 dump file (noatom):

```
% 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

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