The 2014 *Nucleic Acids Research* Database Issue and an updated NAR online Molecular Biology Database Collection

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**ABSTRACT**

The 2014 *Nucleic Acids Research* Database Issue includes descriptions of 58 new molecular biology databases and recent updates to 123 databases previously featured in *NAR* or other journals. For convenience, the issue is now divided into eight sections that reflect major subject categories. Among the highlights of this issue are six databases of the transcription factor binding sites in various organisms and updates on such popular databases as CAZy, Database of Genomic Variants (DGV), dbGaP, DrugBank, KEGG, miRBase, Pfam, Reactome, SEED, TCDB and UniProt. There is a strong block of structural databases, which includes, among others, the new RNA Bricks database, updates on PDBe, PDBsum, ArchDB, Gene3D, ModBase, Nucleic Acid Database and the recently revived iPfam database. An update on the NCBI’s MMDB describes VAST+, an improved tool for protein structure comparison. Two articles highlight the development of the Structural Classification of Proteins (SCOP) database: one describes SCOPe, which automates assignment of new structures to the existing SCOP hierarchy; the other one describes the first version of SCOP2, with its more flexible approach to classifying protein structures. This issue also includes a collection of articles on bacterial taxonomy and metagenomics, which includes updates on the List of Prokaryotic Names with Standing in Nomenclature (LPSN), Ribosomal Database Project (RDP), the SILVA/LTP project and several new metagenomics resources. The NAR online Molecular Biology Database Collection, [http://www.oxfordjournals.org/nar/database/c/](http://www.oxfordjournals.org/nar/database/c/), has been expanded to 1552 databases. The entire Database Issue is freely available online on the *Nucleic Acids Research* website (http://nar.oxfordjournals.org/).

**NEW AND UPDATED DATABASES**

The 21st annual Nucleic Acids Research Database Issue is the largest ever. It includes 185 articles that provide (i) descriptions of the database resources at the NCBI, European Bioinformatics Institute (EBI) and the US Department of Energy Joint Genome Institute (JGI); (ii) 58 new molecular biology databases (Table 1); (iii) updates on 100 databases previously featured in NAR; and (iv) updated descriptions of 23 databases that had been previously described in other journals (Table 2). For the past several years, the order of articles in the Database Issue reflected the categorization of the databases in the NAR online Molecular Biology Database Collection ([http://www.oxfordjournals.org/nar/database/c/](http://www.oxfordjournals.org/nar/database/c/)). Acting on the advice of many readers, we have now made the categories visible and divided the entire Database Issue into the following eight sections: (i) nucleic acid sequence and structure, transcriptional regulation; (ii) protein sequence and structure, motifs and domains, protein–protein interactions; (iii) metabolic and signalling pathways, enzymes, protein modification; (iv) viruses, bacteria, protozoa and fungi; (v) human genome, model organisms, comparative genomics; (vi) genomic variation, diseases and drugs; (vii) plant databases; and (viii) other molecular biology databases. Although each of these sections unifies several of the categories and/or subcategories of the NAR online Database Collection, we believe that they provide an easy-to-use guide to navigate this huge volume and help placing related databases next to each other.

The first section, in addition to the annual descriptions of GenBank, the European Nucleotide Archive and the DNA Data Bank of Japan, includes update papers on
Table 1. Descriptions of new online databases in the 2014 NAR Database issue

| Database name                  | URL                                           | Brief description                                                                 |
|--------------------------------|-----------------------------------------------|-----------------------------------------------------------------------------------|
| 1000 Genomes Selection Browser| http://hsb.upf.edu                           | Signatures of selection in the human genomes                                      |
| AgeFactDB                      | http://agefactdb.jenage.de                    | Aging Factors, phenotypes and lifespan data                                       |
| AVpdb                          | http://crdd.osdd.net/servers/avpdb            | A database of experimentally validated AntiViral Peptides                        |
| BacDive                        | http://bacdive.dsmz.de                        | Bacterial Diversity metadata                                                      |
| BacMet                         | http://bacmet.biomedicine.gu.se              | Antibacterial bioicide and Metal resistance Genes                                 |
| BloodChIP                      | http://149.171.101.136/python/BloodChIP       | Transcription factor binding profiles in human haematopoietic stem/progenitor cells|
| bNAber                         | http://bnaibs.org                             | A database of broadly Neutralizing HIV-1 Antibodies                               |
| CellFinder                     | http://www.cellfinder.org                     | Gene and protein expression, phenotype and images mapped to the cell types        |
| ClinVar                        | http://www.ncbi.nlm.nih.gov/clinvar           | Collection of verified bacterial Taxonomic Factor binding sites                   |
| CollecTF                       | http://collect.umbc.edu                      | Chromatin Regulators and histone modifications in human and mouse                 |
| CR Cistrome                    | http://compbio.tongji.edu.cn/cr               | A database of recent Positive Selection across Human Populations                  |
| dbPShP                         | http://jjwanglab.org/dbpshp                   | Phenotype-specific Regulatory Programs derived from TF binding data               |
| DPRP                           | http://syslab.nchu.edu.tw/DPRP               | Cancer driver genes/mutations deduced from cancer exome-seq results              |
| DriverDB                       | https://ngs.ym.edu.tw/drivedb/               | An automated pipeline for the analysis and archiving of metagenomic data          |
| EBI metagenomics               | https://www.ebi.ac.uk/metagenomics/           | Eukaryotic protein Kinase and Phosphatase Database                                |
| EPKD                           | http://ekpd.biocuckoo.us                      | Protein-coding exons from complete vertebrate genomes                            |
| ExoLocator                     | http://exolocator.eopsf.org                   | Unified plant-specific gene ontology                                              |
| GoMapMan                       | http://www.gomapman.org                       | Genome-Wide Information on Protein Synthesis in vivo using ribosome profiling     |
| GWIPS-viz                      | http://gwips.ucc.ie                          | Haemolytic and non-haemolytic peptides                                            |
| Hemolytik                      | http://crdd.osdd.net/raghava/hemolytik       | Host-Pathogen Interactions of Pseudomonas aeruginosa and Coxiella spp.           |
| HoPaC-DB                       | http://mips.helmholtz-muenchen.de/HoPaC/      | DNA shape                                                                        |
| HrAP                           | http://bioinfo.protres.ru/hrap               | DNA shape                                                                        |
| InvFEST                        | http://invfstedb.uab.cat                      |Polymeric inversions in the human genome                                           |
| IUPHAR/BPS guide to pharmacology| http://www.guideopharmacology.org             | Properties of established and potential drug targets: GPCRs, ion channels, nuclear Silence of protein domains                                      |
| LenVarDB                       | http://caps.ncbs.res.in/lenvardb             | Localization and Quantitation Atlas of the yeast proteome                          |
| LoQAIE                         | http://www.weizmann.ac.il/molgen/loqate      | Genomic and clinical data on complex heritable disorders                           |
| Lynx                           | http://lynx.ciu.uchicago.edu                 | Embryonic development of the mouse, chicken, zebrafish and human                   |
| Manteia                        | http://manteia.ibmc.fr                        | Manually Curated Database of Rice Proteins                                        |
| MCDRiceProt                    | http://www.genomeindia.org/biocuration        | Reference clade-specific microbial genes for Metagenomic studies                  |
| MetaRef                        | http://metaref.org                            | Mitochondrial DNA Breakpoints in human, mouse and rat                              |
| MitoBreak                      | http://mitobreak.portugene.com               | Membrane Proteins: Packing Densities, packing defects and internal water molecules |
| MP:PD                          | http://proteinf ormatics.charite.de/mppd      | Moonlighting proteins database                                                    |
| MultiTaskDB                    | http://wallace.uab.es/multitask              | Microbial Volatile Organic Compounds                                              |
| mVOC                           | http://bioinformatics.charite.de/mvoc        | Disease-related non-synonymous mutations                                           |
| NECTAR                         | http://cardiodb.org/nectar                    | A database of gene transcription regulatory networks                              |
| Network Portal                 | http://networkportal.systemsbiology.net      | Network Extracted Ontology database                                               |
| NcXO                           | http://nexontology.org/                      | A catalog of published Genome-Wide Association Studies, maintained at the NHGRI and EBI |
| NHGRI GWAS Catalog             | http://www.ebi.ac.uk/gpvt/gwas               | DNA-binding specificities of transcription factors in Drosophila                  |
| OnTheFly                       | http://bhapp.c2b2.columbia.edu/OnTheFly      | Protein Ensemble Database: ensembles of intrinsically disordered and unfolded proteins |
| pEB-D                          | http://pedb.vib.be                           | Plant Miniature Inverted-repeat Transposable Elements (MITEs)                     |
| P-MITE                         | http://pmite.hzau.edu.cn/django/mite          | Fairwise comparisons Of Genomes and universal Orthologous genes                  |
| POGO-DB                        | http://pogo.ece.drexel.edu                   | Escherichia coli K-12 Knowledgebase Portal                                       |
| PortEco                        | http://porteco.org                           | A Rigorously Annotated Database of A-to-I RNA editing                             |
| RADAR                          | http://rnaedit.com                           | Repeats in protein structures                                                     |
| RepeatsDB                      | http://repeatsdb.bio.unipd.it                | Manually curated annotations for rhiobial genomes                                  |
| RhizoBase                      | http://genome.microbed.jp/rhizobase          | Wiki-based open-content platform for community curation of rice genes              |
| RicWiki                        | http://ricwiki.big.ac.cn                     | RNA structural modules and their interactions                                      |
| RNA Bricks                     | http://iimcb.genesilico.pl/rbricks            | Annotated SNPs within regulatory DNA elements                                      |
| rSNPBase                       | http://rsnp.psych.ac.cn                      | Structural Antibody Database                                                      |
| SAbDab                         | http://opig.stats.oa.ac.uk/webapps/sabdab    | Small Molecule inhibitors of RNA                                                  |
| SMMRNA                         | http://www.smmrna.org                        | Regulatory pathways during the sporulation cycle of Bacillus subtilis             |
| SporeWeb                       | http://sporeweb.molgenrug.nl                 | Compounds that stimulate or relieve pain                                           |
| SuperPain                      | http://bioinformatics.charite.de/superpain   | DNA shape features of Transcription Factor Binding Sites                          |
| TFBSShape                      | http://roslab.cnb.usc.edu/TFBSshape          | Alternative Translation Initiation Sites                                          |
| TISdb                          | http://tisdb.human.cornell.edu               | Biotransformation of drugs and food ingredients by human enzymes                 |
| Transformer                    | http://bioinformatics.charite.de/transformer | Upstream ORFs and their effect of translation of downstream CDSs                  |
| uORFdb                         | http://cdnh.mdc-berlin.de/tools/uorfdb       | Links from human disease to natural variation data in Caenorhabditis elegans     |
Table 2. Updated descriptions of online databases not previously featured in the NAR Database issue

| Database name         | URL                               | Brief description                                                                 |
|-----------------------|-----------------------------------|----------------------------------------------------------------------------------|
| COLOMBOS              | http://colombos.net               | Collections of Microarrays for Bacterial Organisms                               |
| Consensus CDS         | http://www.ncbi.nlm.nih.gov/projects/CCDS | A collaborative effort to identify a core set of human protein coding regions |
| CottonGen             | http://www.cottongen.org          | Cotton Genomics, genetics and breeding                                             |
| Database of Genomic Variants dbGaP | http://www.ncbi.nlm.nih.gov/gap            | Curated catalog of human genomic structural variation                             |
| DECIPHER              | http://decipher.sanger.ac.uk      | Database of Genotypes and Phenotypes                                              |
| GEISHA                | http://geisha.arizona.edu         | Database of Chromosomal Imbalance and Phenotype in Humans Using Ensembl Resources |
| GeneProf              | http://www.geneprof.org           | *Gaub’s Expression In Situ Hybridization Analysis*                                 |
| GGBN                  | http://www.ggbn.org/dataportal    | Human and mouse gene expression data from RNA-seq and ChIP-seq                    |
| HMDD                  | http://cmbi.bjmu.edu.cn/hmdd      | The Global Genome Biodiversity Network portal                                     |
| Human Phenotype Ontology | http://www.human-phenotype-ontology.org | Human MicroRNA and Disease Associations Database                                    |
| IMPC                  | http://www.mousephenotype.org     | Standardized vocabulary of phenotypic abnormalities in human disease             |
| iPfam                 | http://www.ipfam.org              | International Mouse Phenotyping Consortium portal                                 |
| KBDOCK                | http://kbdock.loria.fr            | Protein family interactions mapped to Pfam domains                                 |
| Locus Reference Genomic | http://www.lrg-sequence.org       | Knowledge-Based Docking: protein domain interfaces                                |
| LPSN                  | http://www.bacterio.net           | Each LRG is a stable genomic DNA sequence for a region of the human genome        |
| NDB                   | http://ndbserver.rutgers.edu      | List of Prokaryotic names with Standing in Nomenclature                           |
| Plasma Proteome Database | http://www.plasmaproteomedatabase.org | Nucleic Acid Database, nucleic acids-containing structures                        |
| Progenetix            | http://www.progenetix.org         | Quantitative information on proteins in human plasma and serum                   |
| SEED                  | http://pubseed.theseed.org or http://www.theseed.org | Copy number abnormalities in human cancer                                         |
| SFLD                  | http://sfdl.rubi.ua.edu            | Genome annotations based on curated functional systems                            |
| SoyKB                 | http://soykb.org                   | Structure-Function Linkage Database: sequence conservation in enzyme superfamilies |
| Virus variation       | http://www.ncbi.nlm.nih.gov/genomes/VirusVariation | Soybean Knowledge Base                                                             |
| YeastNet              | http://www.inetbio.org/yeastnet   | Variation data on influenza, dengue and West Nile viruses                         |
|
| Bricks                |                                    | Functional gene networks for *Saccharomyces cerevisiae*                           |

five microRNA databases: miRBase, miRNEST, mirTarBase, PolymiRTS and starBASE, and on the NONCODE database of various types of non-coding RNA. There are also several databases of transcription factor (TF) binding sites (TFBSs), including updates on JASPAR and YEASTRACT and new databases of TFBS in *Escherichia coli*, *Drosophila* and human haematopoietic stem cells (1–5). An interesting work, chosen by the reviewers and NAR editors as a ‘Breakthrough paper’, describes TFBSshape (6), a database of DNA structural features (minor groove width, roll, propeller twist and helix twist) of TFBSs for various TFs, which have been collected from the JASPAR (1) and UniProbe (7) databases. The TFBSshape website, http://rohslab.cmbusc.edu/TFBSshape/, allows the users to submit their own aligned TFBS sequences, which could be used, for example, to compare the DNA binding specificities of closely related TFs (6).

The protein database section includes annual updates on UniProt and KEGG, as well as updates of such popular databases as Pfam, eggNOG, ELM, FireDB, SEED, SIMAP and Transporter protein Classification Database (TCDB). Two new databases, HRaP and RepeatsDB, collect information on protein repeats, the former at the sequence level (runs of the same amino acid residue) and the latter at the structural level (8,9).

As in previous years, this Database Issue features an impressive selection of structural databases. Two of them deal with nucleic acid structure: an update on the well-known Nucleic Acids Database (NDB) and RNA Bricks, a new database of RNA 3D motifs and their contacts (10,11). The block of protein structure databases includes, among others, updates on Protein Data Bank in Europe (PDBe), PDBsum, ArchDB, Gen3D, ModBase, SCOP and the recently revived Pfam database. Diverse improvements at PDBe include comprehensive visualization and analysis of the rapidly growing collection of electron microscopy-derived structures, whereas PDBsum now offers facilities to browse domain architectures and new connections to ligand and SNP data (12).

For the past 18 years, the NCBI’s Molecular Modeling Database (MMDB) displayed the lists of structural neighbours of a given protein, calculated using the Vector Alignment Search Tool (VAST) (13). The MMDB update paper describes VAST+, a recent extension of that tool, which allows calculation of structural similarity at the level of ‘biological assemblies’ (hetero- or homooligomeric protein complexes). Accordingly, for macro-molecular complexes, MMDB now displays precalculated lists of similar protein complexes ranked by the extent of similarity (14). Several databases, including iPfam, 3did and UniHI, reflect current interest in the structural basis of protein interaction networks and take on the challenge of presenting complex protein–protein and protein–ligand interaction data in clear and useful ways (15–17). The aptly named Negatome database (18) provides a useful
benchmark, documenting protein pairs that definitely do not interact, and could be used as negative control for the constantly growing protein ‘interactome’. A pair of papers published back-to-back highlight two different directions in the development of the Structural Classification of Proteins (SCOP) database: one of them describes SCOPe, an extension of SCOP that focuses on regularly and automatically assigning new structures to the existing SCOP hierarchy, whereas the other one describes the birth of SCOP2, with its more flexible graph-based approach to classifying protein structures and documenting the subtleties of their relationships (19,20).

The section on enzymes and metabolism includes updates on three metabolic pathway databases, MetaCyc, Reactome and the Small Molecule Pathway Database (21–23). This issue also features updates of two excellent databases of the active sites in various enzyme superfamilies, the Catalytic Site Atlas and the Structure-Function Linkage Database (SFLD) (24,25). There are also updates of the Carbohydrate-Active enzymes database (CAZY) and the protease database MEROPS, as well as new databases: EKPD, a database of eukaryotic protein kinases and protein phosphatases, and MultiTaskDB, a database of ‘moonlighting’ enzymes (26–29).

The increased interest in microbial genomics, fuelled in part by the Human Microbiome Project, led to several important developments in database construction. Many databases now emphasize improved genome annotation for a variety of microbes, including human pathogens (IMG, PATRIC, SEED), and for selected free-living microorganisms (CyanoBase, PortEco, Rhizobase, SubtiWiki). A number of databases, such as JGI’S IMG/M (30) and the newly created EBI metagenomics resource (31), strive to capture microbial diversity in natural environments. The rapid growth of completely or partially sequenced microbial genomes makes particularly important their proper classification, which increasingly relies on such resources as the Ribosomal Database Project (RDP), the SILVA/LTP project, BacDive at the DSMZ-German Collection of Microorganisms and Cell Cultures and the List of Prokaryotic Names with Standing in Nomenclature (LPSN) (32–35). The new MetaRef database collects from reference microbial genomes clade-specific genes that could be useful for taxonomic assignments of metagenomic reads (36).

One of the major highlights of this issue is the block of articles on the improved annotation of human genome and detailed analysis of genome variation and its potential clinical significance. These articles include, among others, updates on the Consensus CDS project, a collaborative effort to identify a core set of human protein-coding regions, and on the dbGaP, a database of genotyping results and related clinically relevant phenotypes (37,38). dbGaP contains openly available study data but requires pre-authorization for access to personal health information, such as individual-level data including phenotypic data tables and genotypes (see http://www.ncbi.nlm.nih.gov/gap for details). This issue also includes descriptions of several related databases: Locus Reference Genomic, a set of reference sequences for reporting of clinically relevant sequence variants; the NCBI’s ClinVar, a database documenting these clinically relevant sequence variants; the NHGRI GWAS Catalog, a curated resource of SNP-trait associations; Sanger Institute’s DECIPHER, a database of pathogenic single nucleotide variants, indels and copy-number variants; and the Database of Genomic Variants (DGV) at the Toronto’s Centre for Applied Genomics (39–43). There are also several more specialized databases (canSAR, DriverDB, FINDBase, HbVar, Lynx, NECTAR, Progenetix) that cover genetic defects leading to various human diseases, including cancer. In addition, three separate databases, Selectome, dbPSPHP and 1000 Genomes Selection Browser, report the sites of likely positive selection in human genomes.

Model organism databases featured in this issue include regular updates from Saccharomyces Genome Database (SGD), WormBase, FlyBase, Mouse Genome Database (MGD), Mouse Gene Expression Database, Mouse Phenome Database and Vertebrate Genome Annotation (VEGA) database, as well as a description of the International Mouse Phenotyping Consortium (IMPC) web portal.

NAR ONLINE MOLECULAR BIOLOGY DATABASE COLLECTION

The NAR online Molecular Biology Database Collection (freely available at http://www.oxfordjournals.org/nar/database/) has been updated by including the databases introduced in the 2014 NAR Database Issue. This list has been expanded by including such databases as CREDO, DoSA, DBATE, RedoxDB and TMBB-DB, whose descriptions had been published in our sister journals Bioinformatics and Database (Oxford) and are freely available online, as well as selected databases published elsewhere. The entire collection has been carefully curated by checking all non-responsive database websites; coordinators of such databases have been asked to confirm their commitment to maintaining their resources. Based on the received responses (or a lack thereof), URLs of 193 databases have been corrected and 24 obsolete databases have been removed from the list. As a result of these changes, the online collection now includes 1552 databases that are sorted into 14 categories and 41 subcategories.

Suggestions for inclusion in the collection of additional databases are welcome. They should include extended databases summaries in plain text, generally formatted according to the http://www.oxfordjournals.org/nar/database/summary/1 template, including references to the published database descriptions freely available online, and should be addressed to XMFS at xose.m.fernandez@gmail.com.

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