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Editorial

DrugBank as a recognized bank of drugs having ATM card in database

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Abstract
The Drug Bank database is an unique bioinformatics and cheminformatics resource that combines detailed about drug (i.e. chemical, pharmacological and pharmaceutical) data with comprehensive drug target (i.e. sequence, structure and pathway) information. The database contains 7740 drug entries including 1584 FDA-approved small molecule drugs, 157 FDA-approved biotech (protein/peptide) drugs, 89 nutraceuticals and over 6000 experimental drugs. Additionally, 4282 non-redundant protein (i.e. drug target/ enzyme/ transporter/carrier) sequences are linked to these drug entries. Each DrugCard entry contains more than 200 data fields with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data. Chemical structures, small molecule drugs, biotech drugs, drug targets, drug transporters, drug target sequences, drug target SNPs, drug metabolites, drug descriptions, disease associations, dosage data, food and drug interactions, adverse drug reactions, pharmacology, mechanisms of action, drug metabolism, chemical synthesis, patent and pricing data, chemical properties, nomenclature, synonyms, chemical taxonomy, drug NMR spectra, drug GC-MS spectra, drug LC-MS spectra are mentioned in this database.

Keywords: Bioinformatics, Cheminformatics, *in-silico* database, Nutraceuticals, Drug target, Protein, Peptide, HMDB, T3DB, SMPDB, FooDB, Metabolomics, DrugCard, MetaboCard, ToxCard, KEGG, PubChem, MetaCyc, ChEBI, PDB, UniProt and GenBank.

INTRODUCTION

The **DrugBank** database is a comprehensive, high-quality, freely accessible, *in-silico* online database containing information on drugs and drug targets. As both a bioinformatics and a cheminformatics resource, DrugBank combines detailed drug (i.e. chemical, pharmacological and pharmaceutical) data with comprehensive drug target (i.e. sequence, structure and pathway) information. Because of its broad scope, comprehensive referencing and unusually detailed data descriptions, DrugBank is more akin to a drug encyclopedia than a drug database. As a result, links to DrugBank are maintained for nearly all drugs listed in Wikipedia. DrugBank is widely used by the drug industry, medicinal chemists, pharmacists, physicians, students and the general public. Its extensive drug and drug-target

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data has enabled the discovery and repurposing of a number of existing drugs to treat rare and newly identified illnesses. The latest release of the database (version 4.0) contains 7677 drug entries including 1558 FDA-approved small molecule drugs, 155 FDA-approved biotech (protein/peptide) drugs, 87 nutraceuticals and over 6000 experimental drugs. Additionally, 4270 non-redundant protein (i.e. drug target/ enzyme/ transporter/ carrier) sequences are linked to this drug entries.[1]

Figure-1: DrugBank[1,2]

(1. Law V, Knox C, Djoumbou Y, Jewison T, et al. DrugBank 4.0: shedding new light on drug metabolism. Nucleic Acids Res. 2014; 42(1): D 1091-1097.
2. Knox C, Law V, Jewison T, et al. DrugBank 3.0: a comprehensive resource for 'omics' research on drugs. Nucleic Acids Res. 2011; 39: D 1035-41.)

Each DrugCard entry contains more than 200 data fields with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data. Four additional databases, HMDB, T3DB, SMPDB and FooDB are also part of a general suite of metabolomics/cheminformatics databases. HMDB contains equivalent information on more than 40,000 human metabolites, T3DB contains information on 3100 common toxins and environmental pollutants and SMPDB contains pathway diagrams for nearly 700 human metabolic pathways and disease pathways, while FooDB contains equivalent information on ~ 28,000 food components and food additives.[2]

The Human Metabolome Database (HMDB) is a freely available electronic database containing detailed information about small molecule metabolites found in the human body. It is intended to be used for applications in metabolomics, clinical chemistry, biomarker discovery and general education. The database is designed to contain or link three kinds of data: 1) chemical data, 2) clinical data, and 3) molecular biology/biochemistry data. The database contains 41,808 metabolite entries including both water-soluble and lipid soluble metabolites as well as metabolites that would be regarded as either abundant (> 1 uM) or relatively rare (< 1 nM). Additionally, 5,688 protein sequences are linked to these metabolite entries. Each MetaboCard entry contains more than 110 data fields with 2/3 of the information being devoted to chemical/clinical data and the other 1/3 devoted to enzymatic or biochemical data. Many data fields are hyperlinked to other databases (KEGG, PubChem, MetaCyc, ChEBI, PDB, UniProt and GenBank) and a variety of structure and pathway viewing applets.[3]

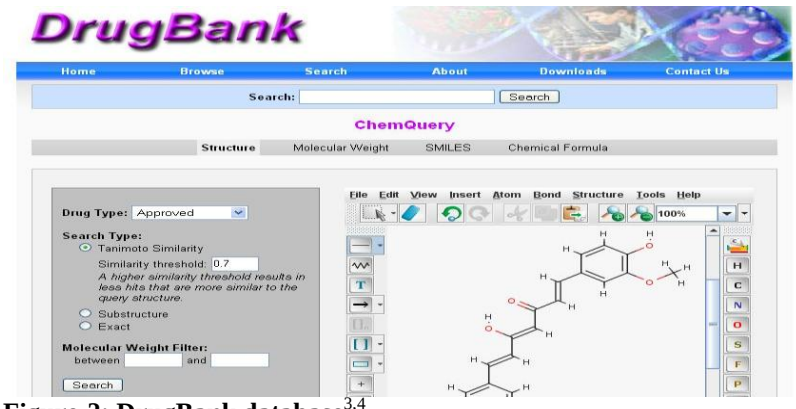


Figure-2: DrugBank database[3,4]

(3. Wishart DS, Knox C, Guo AC, et al. DrugBank: a knowledgebase for drugs, drug actions and drug targets. Nucleic Acids Res. 2008; 36: D 901-906.
4. Wishart DS, Knox C, Guo AC, et al. DrugBank: a comprehensive resource for in silico drug discovery and exploration. Nucleic Acids Res. 2006; 34: D 668-672.)

KEGG (Kyoto Encyclopedia of Genes and Genomes) is a collection of databases dealing with genomes, biological pathways, diseases, drugs, and chemical substances. KEGG is utilized for bioinformatics research and education,

including data analysis in genomics, metagenomics, metabolomics and other omics studies, modeling and simulation in systems biology, and translational research in drug development.

PubChem is a database of chemical molecules and their activities against biological assays. The system is maintained by the National Center for Biotechnology Information (NCBI), a component of the National Library of Medicine, which is part of the United States National Institutes of Health(NIH). PubChem can be accessed for free through a web user interface. Millions of compound structures and descriptive datasets can be freely downloaded via FTP. PubChem contains substance descriptions and small molecules with fewer than 1000 atoms and 1000 bonds. More than 80 database vendors contribute to the growing PubChem database. The **MetaCyc** database contains extensive information on metabolic pathways and enzymes from many organisms. MetaCyc data cover all domains of life and have been curated from more than 41,000 publications. MetaCyc applications include use as a reference data set for computationally predicting the metabolic pathways of organisms from their sequenced genomes; it has been used to perform pathway predictions for thousands of organisms, including those in the BioCyc Database Collection. MetaCyc is also used in metabolic engineering and metabolomics research. MetaCyc contains extensive data on individual enzymes, describing their subunit structure, cofactors, activators and inhibitors, substrate specificity, and, in some cases, kinetic constants. MetaCyc data on reactions includes predicted atom mappings that describe the correspondence between atoms in the reactant compounds and the product compounds. It also provides enzyme mini-reviews and literature references. MetaCyc data on metabolites includes chemical structures, predicted Gibbs free energies of formation, and links to external databases.

Chemical Entities of Biological Interest, also known as **ChEBI**, is a database and ontology of molecular entities focused on 'small' chemical compounds, that is part of the Open Biomedical Ontologies effort. The term "molecular entity" refers to any "constitutionally or isotopically distinct atom, molecule, ion, ion pair, radical, radical ion, complex, conformer, etc., identifiable as a separately distinguishable entity". The molecular entities in question are either product of nature or synthetic products which have potential bioactivity. Molecules directly encoded by the genome, such as nucleic acids, proteins and peptides derived from proteins by proteolytic cleavage, are not as a rule included in ChEBI. ChEBI uses nomenclature, symbolism and terminology endorsed by the International Union of Pure and Applied Chemistry (IUPAC) and Nomenclature Committee of the International Union of Biochemistry and Molecular Biology (NC-IUBMB).

The **Protein Data Bank** (**PDB**) is a repository for the three-dimensional structural data of large biological molecules, such as proteins and nucleic acids. The data, typically obtained by X-ray crystallography or NMR spectroscopy and submitted by biologists and biochemists from around the world, are freely accessible on the Internet via the websites of its member organizations (PDBe, PDBj and RCSB). The PDB is overseen by an organization called the Worldwide Protein Data Bank.

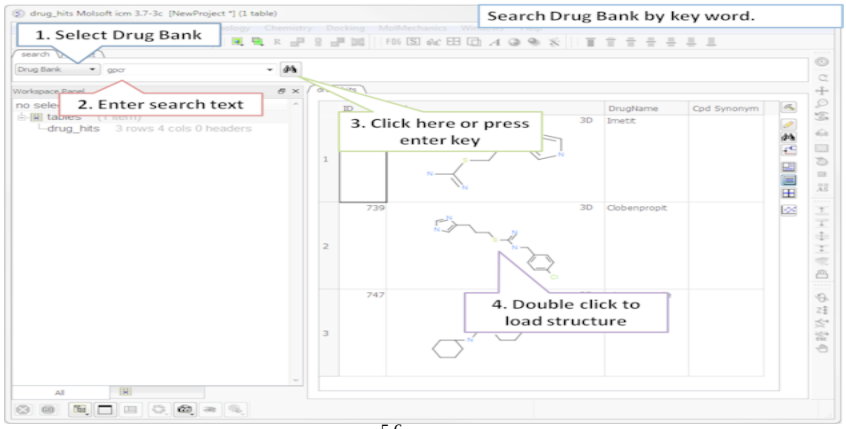


Figure-3: Browsing in DrugBank[5,6]

(5. Wishart DS, Tzur D, Knox C, et al. HMDB: the Human Metabolome Database. Nucleic Acids Research. 2007; 35: D 521–526.
6. Law V, Knox C, Djoumbou Y, et al. DrugBank 4.0: shedding new light on drug metabolism. Nucleic Acids Research. 2014; 42: D 1091-1097.)

The PDB is a key resource in areas of structural biology, such as structural genomics. Most major scientific journals, and some funding agencies, now require scientists to submit their structure data to the PDB. If the contents of the PDB are thought of as primary data, then there are hundreds of derived (i.e., secondary) databases that categorize the data differently. For example, both SCOP and CATH categorize structures according to type of structure and assumed evolutionary relations; GO categorize structures based on genes.

UniProt is a comprehensive, high-quality and freely accessible database of protein sequence and functional information, many entries being derived from genome sequencing projects. It contains a large amount of information about the biological function of proteins derived from the research literature.

The **GenBank** sequence database is an open access, annotated collection of all publicly available nucleotide sequences and their protein translations. This database is produced and maintained by the National Center for Biotechnology Information (NCBI) as part of the International Nucleotide Sequence Database Collaboration (INSDC). The National Center for Biotechnology Information is a part of the National Institutes of Health in the United States. GenBank and its collaborators receive sequences produced in laboratories throughout the world from more than 100,000 distinct organisms. In the more than 30 years since its establishment, GenBank has become the most important and most influential database for research in almost all biological fields, whose data are accessed and cited by millions of researchers around the world. GenBank continues to grow at an exponential rate, doubling every 18 months. Release 194, produced in February 2013 and contained over 150 billion nucleotide bases in more than 162 million sequences. GenBank is built by direct submissions from individual laboratories, as well as from bulk submissions from large-scale sequencing centers.[4]

Figure-4: *in-silico* Database of DrugBank[7]

(7. Lim E, Pon A, Djoumbou Y, Knox C, et al. T3DB: a comprehensively annotated database of common toxins and their targets. Nucleic Acids Research. 2010; 38: D 781-786.)

The HMDB database supports extensive text, sequence, chemical structure and relational query searches. Four additional databases, DrugBank, T3DB, SMPDB and FooDB are also part of the HMDB suite of databases. DrugBank contains equivalent information on ~1600 drug and drug metabolites, T3DB contains information on 3100 common toxins and environmental pollutants, and SMPDB contains pathway diagrams for 440 human metabolic and disease pathways, while FooDB contains equivalent information on ~ 28,000 food components and food additives.[5]

The Toxin and Toxin-Target Database (T3DB) is a comprehensive, high-quality, freely accessible, online database of common toxic substances and their protein/DNA or organ targets. The database currently houses 3,053 toxic compounds or poisons described by 32,276 synonyms. This list includes common pollutants, pesticides, drugs, and food toxins. These toxic substances are linked to 1,670 corresponding protein/DNA target records. In total there are 37,084 toxic substance-toxin target associations. Each toxic compound record (ToxCard) in T3DB contains nearly 60 data fields and holds information such as chemical properties and descriptors, mechanisms of action, toxicity or lethal dose values, molecular and cellular interactions, and medical (symptom and treatment) information. This information has been extracted from over 5,454 sources, which include other databases, government documents, books, and scientific literature. The primary focus of the T3DB is on providing mechanisms of toxicity and identifying target proteins for common toxic substances. While a number of other toxic compound databases do exist, their emphasis is on covering large numbers of chemical compounds that are almost never seen outside a chemical laboratory. T3DB attempts to capture data on only those toxic substances that are abundant or in widespread use and have been detected or measured in humans. T3DB is fully searchable and supports extensive text, sequence, chemical structure, and relational query searches. It is both modelled after and closely linked to the Human Metabolome Database (HMDB) and DrugBank. Potential applications of T3DB include metabolomics and environmental exposure studies, toxic compound metabolism prediction, toxin/drug interaction prediction, and general toxic substance awareness. All data in T3DB is non-proprietary or is derived from a non-proprietary source. It is freely accessible and available to anyone. In addition, nearly every data item is fully traceable and explicitly referenced to the original source. T3DB data is available through a public web interface and downloads.[6]

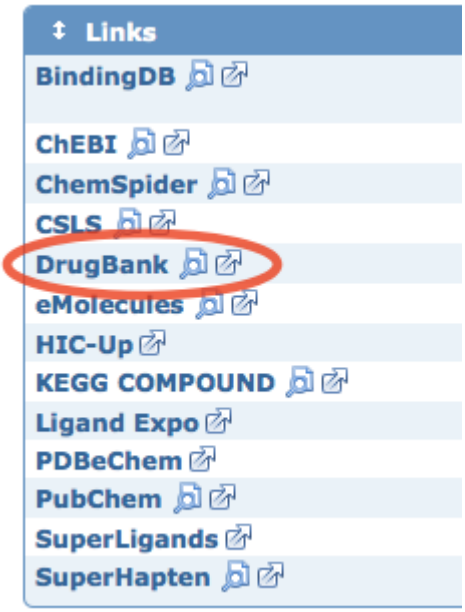
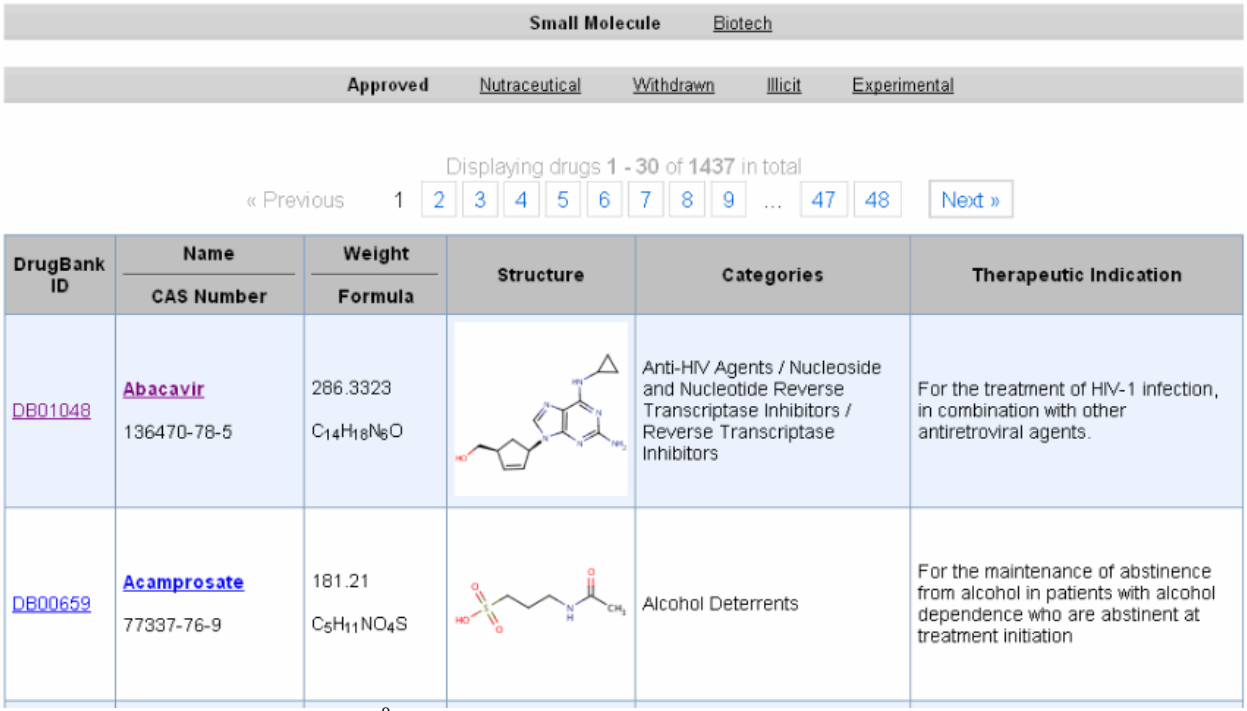


Figure-5: Drug Ligand binding database of DrugBank[8]
(8. Frolkis A, Knox C, Lim E, et al. SMPDB: The Small Molecule Pathway Database. Nucleic Acids Research. 2010; 38: D 480-487.)

The Small Molecule Pathway Database (SMPDB) is a comprehensive, high-quality, freely accessible, online database containing more than 600 small molecule (i.e. metabolic) pathways found in humans. SMPDB is designed specifically to support pathway elucidation and pathway discovery in metabolomics, transcriptomics, proteomics and systems biology. It is able to do so, in part, by providing colorful, detailed, fully searchable, hyperlinked diagrams of five types of

small molecule pathways: 1) general human metabolic pathways; 2) human metabolic disease pathways; 3) human metabolite signaling pathways; 4) drug-action pathways and 5) drug metabolism pathways. SMPDB pathways may be navigated, viewed and zoomed interactively using a Google Maps-like interface. All SMPDB pathways include information on the relevant organs, sub cellular compartments, protein cofactors, protein locations, metabolite locations, chemical structures and protein quaternary structures. Each small molecule in SMPDB is hyperlinked to detailed descriptions contained in the HMDB or DrugBank and each protein or enzyme complex is hyperlinked to UniProt. Additionally, all SMPDB pathways are accompanied with detailed descriptions and references, providing an overview of the pathway, condition or processes depicted in each diagram. Users can browse the SMPDB or search its contents by text searching, sequence searching, or chemical structure searching. More powerful queries are also possible including searching with lists of gene or protein names, drug names, metabolite names, GenBank IDs, Swiss-Prot IDs, Agilent or Affymetrix microarray IDs. These queries will produce lists of matching pathways and highlight the matching molecules on each of the pathway diagrams. Gene, metabolite and protein concentration data can also be visualized through SMPDB's mapping interface. SMPDB is part of a suite of metabolomics databases that also includes Human Metabolome Database, DrugBank, and the Toxin and Toxin-Target Database (T3DB). While DrugBank includes information on 7000 drugs and >4200 non-redundant drug targets, enzymes, transporters, and carriers, HMDB houses over 40,000 small molecule metabolites found in the human body. The suite is complemented by T3DB with its over 3100 common toxic substances and over 1300 corresponding toxin targets. The first version of SMPDB was released on January 1, 2010. This release contained more than 350 image-mapped pathways for small molecule pathways. The viewer interface was limited to scroll-bar image navigation with 3-step (small, medium, large) zooming. The pathways in this first version were limited to 1) human metabolic pathways; 2) human metabolic disease pathways; and 3) human metabolite signaling pathways. The second version of SMPDB was released in 2014. This version contained more than 620 small molecule pathways. The viewer interface was enhanced to include a Google-Map-like interface with click-n-drag image navigation and unlimited, interactive zooming. The pathways in this second version were expand to include: 1) general human metabolic pathways; 2) human metabolic disease pathways; 3) human metabolite signaling pathways; 4) drug action pathways and 5) drug metabolism pathways.[7]



Small Molecule Biotech

Approved Nutraceutical Withdrawn Illicit Experimental

Displaying drugs 1 - 30 of 1437 in total

« Previous 1 2 3 4 5 6 7 8 9 ... 47 48 Next »

DrugBank ID	Name / CAS Number	Weight / Formula	Structure	Categories	Therapeutic Indication
DB01048	Abacavir 136470-78-5	286.3323 $C_{14}H_{18}N_6O$		Anti-HIV Agents / Nucleoside and Nucleotide Reverse Transcriptase Inhibitors / Reverse Transcriptase Inhibitors	For the treatment of HIV-1 infection, in combination with other antiretroviral agents.
DB00659	Acamprosate 77337-76-9	181.21 $C_5H_{11}NO_4S$		Alcohol Deterrents	For the maintenance of abstinence from alcohol in patients with alcohol dependence who are abstinent at treatment initiation

Figure-6: DrugBank search result[9]

(9. Scalbert A, Andres-Lacueva C, Arita M, et al. Databases on Food Phytochemicals and Their Health-Promoting Effects. J. Agric. Food Chem. 2011; 59(9): 4331-4348.)

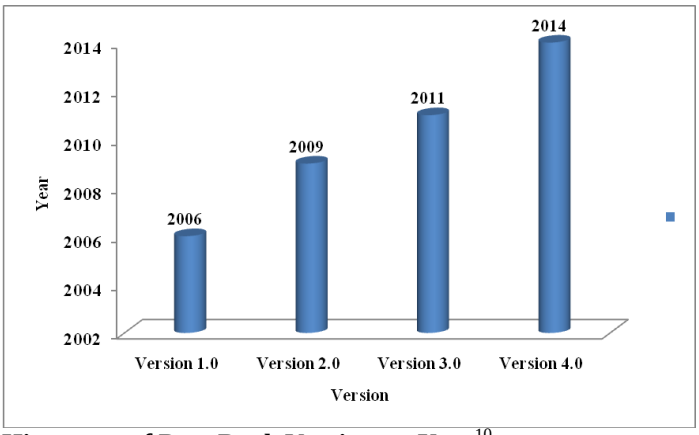
FooDB (The Food Database) is a freely available, open-access database containing chemical (micronutrient and macronutrient) composition data on common, unprocessed foods. It also contains extensive data on flavour/aroma constituents, food additives as well as positive/negative health effects associated with food constituents. The database currently contains information on more than 28,000 chemicals found in >1000 raw or unprocessed food products. The data in FooDB was collected from many sources including textbooks, scientific journals, on-line food composition or nutrient databases, flavour and aroma databases and various on-line metabolomic databases. This literature-derived information has been combined with experimentally-derived data measured on 1000's of compounds from more than 40 very common food products through the Alberta Food Metabolome Project which is led by Dr. David Wishart of the University of Alberta. Users are able to browse through the FooDB data by food source, name, descriptors or function. Chemical structures and molecular weights for compounds in FooDB may be searched via a specialized chemical structure search utility. Users are able to view the content of FooDB using two different "Viewing" options: FoodView, which lists foods by their chemical compounds or ChemView, which lists chemicals by their food sources. Knowledge about the precise chemical composition of foods can be used to guide public health policies, assist food companies with improved food labeling, help dieticians prepare better dietary plans, support nutraceutical companies with their submissions of health claims and guide consumer choices with regard to food purchases. [8]

Category	**1.0**	**2.0**	**3.0**	**4.0**
No. of data fields per DrugCard	88	108	148	208
No. of search types	8	12	16	18
No. of illustrated drug-action pathways	0	0	168	232
No. of drugs with metabolizing enzyme data	0	0	762	1,037
No. of drug metabolites with structures	0	0	0	1,239
No. of drug-metabolism reactions	0	0	0	1,308
No. of illustrated drug metabolism pathways	0	0	0	53
No. of drugs with drug transporter data	0	0	516	623
No. of drugs with taxonomic classification information	0	0	0	6,713
No. of SNP-associated drug effects	0	0	113	20
No. of drugs with patent/pricing/manufacturer data	0	0	1,208	1,450
'No. of food–drug interactions	0	714	1,039	1,180
No. of drug–drug interactions	0	13,242	13,795	14,150
No. of ADMET parameters (Caco-2, LogS)	0	276	890	6,667
No. of QSAR parameters per drug	5	6	14	23
No. of drugs with drug-target binding constant data	0	0	0	791
No. of drugs with NMR spectra	0	0	0	306
No. of drugs with MS spectra	0	0	0	384
No. of drugs with chemical synthesis information	0	38	38	1,285
No. of FDA-approved small molecule drugs	841	1,344	1,424	1,558
No. of biotech drugs	113	123	132	155
No. of nutraceutical drugs	61	69	82	87
No. of withdrawn drugs	0	57	68	78
No. of illicit drugs	0	188	189	190
No. of experimental drugs	2,894	3,116	5,210	6,009
Total No. of experimental and FDA small molecule drugs	3,796	4,774	6,684	7,561
Total No. of experimental and FDA drugs (all types)	3,909	4,897	6,816	7,713
No. of all drug targets (unique)	2,133	3,037	4,326	4,115
No. of approved-drug enzymes/carriers (unique)	0	0	164	245
No. of all drug enzymes/carriers (unique)	0	0	169	253
No. of external database links	12	18	31	3

Table-1: Comparison between the DrugBank with Version 1.0, 2.0, 3.0 and 4.0. [10]

(10. Wishart DS, Guo AC, Eisner R, et al. HMDB: a knowledgebase for the human metabolome. Nucleic Acids Research. 2009; 37: D 603-610.)

Version 1.0 of DrugBank was released in **2006**. This early release contained relatively modest information about 841 FDA-approved small molecule drugs and 113 biotech drugs. It also included information on 2133 drug targets. **Version 2.0** of DrugBank was released in **2009**. This greatly expanded and improved version of the database included 1344 approved small molecule drugs and 123 biotech drugs as well as 3037 unique drug targets. This also included, for the first time, withdrawn drugs and illicit drugs, extensive food-drug and drug-drug interactions as well as ADMET (absorption, distribution, metabolism, excretion and toxicity) parameters. **Version 3.0** was released in **2011**. This version contained 1424 approved small molecule drugs and 132 biotech drugs as well as >4000 unique drug targets. Version 3.0 also included drug transporter data, drug pathway data, drug pricing, patent and manufacturing data as well as data on >5000 experimental drugs. **Version 4.0** was released in **2014**. This version included 1558 FDA-approved small molecule drugs, 155 biotech drugs and 4200 unique drug targets. Version 4.0 also incorporated extensive information on drug metabolites (structures and reactions), drug taxonomy, drug spectra, drug binding constants and drug synthesis information. Table-1 provides a more complete statistical summary of the history of Drug Bank's development.[9]



Histogram of DrugBank Version vs. Year[10]

(10. Wishart DS, Guo AC, Eisner R, et al. HMDB: a knowledgebase for the human metabolome. Nucleic Acids Research. 2009; 37: D 603-610.)

All data in DrugBank is non-proprietary or is derived from a non-proprietary source. It is freely accessible and available to anyone. In addition, nearly every data item is fully traceable and explicitly referenced to the original source. DrugBank data is available through a public web interface and downloads.

Users may query DrugBank in a number of ways: Simple text queries of the entire textual component of the database are supported. Clicking on the Browse button generates a tabular synopsis of DrugBank's content. This view allows users to casually scroll through the database or re-sort its contents. Clicking on a given DrugCard button brings up the full data content for the corresponding drug. A complete explanation of all the DrugCard fields and sources is given there. The Pharma Browse button allows users to browse through drugs as grouped by their indication. This is particularly useful for pharmacists and physicians, but also for pharmaceutical researchers looking for potential drug leads.[10] The ChemQuery button allows users to draw (using ChemAxon applets) or write (as a SMILES string) a chemical compound and to search DrugBank for chemicals similar or identical to the query compound. The TextQuery button supports a more sophisticated text search (partial word matches, case sensitive, misspellings, etc.) of the text portion of DrugBank. The Seq Search button allows users to conduct BLAST (protein) sequence searches of the 18,000 sequences contained in DrugBank. Both single and multiple sequence (i.e. whole proteome) BLAST queries are supported. The Data Extractor button opens an easy-to-use relational query search tool that allows users to select or search over various combinations of subfields. The Data Extractor is the most sophisticated search tool for DrugBank.[11] Users may download selected text components and sequence data from DrugBank and track the latest news about DrugBank through regular news feeds through its website as well as through Twitter and Face book.

Conclusion

The DrugBank database is a unique bioinformatics and cheminformatics resource that combines

detailed drug (i.e. chemical, pharmacological and pharmaceutical) data with comprehensive drug target (i.e. sequence, structure, and pathway) information. The database contains 7740 drug entries including 1584 FDA-approved small molecule drugs, 157 FDA-approved biotech (protein/peptide) drugs, 89 nutraceuticals and over 6000 experimental drugs. Each DrugCard entry contains more than 200 data fields with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data.

Figure-7: Drugs in Medicine form[11]
(11. Jewison T, Su Y, Disfany FM. et al. Small Molecule Pathway Database. Nucleic Acids Research. 2014; 42: D 478-484.)

Operational approach of DrugBank

Users may query DrugBank in any number of ways. The simple text query (above) supports general text queries of the entire textual component of the database. Clicking on the Browse button (on the DrugBank navigation panel above) generates a tabular synopsis of Drug Bank's content. This browse view allows users to casually scroll through the database or re-sort its contents. Clicking on a given DrugCard button brings up the full data content for the corresponding drug. A complete explanation of all the DrugCard fields and sources is given here. The Pharma Browse button allows users to browse through drugs as grouped by their indication. This is particularly useful for pharmacists and physicians, but also for pharmaceutical researchers looking for potential drug leads. The ChemQuery button allows users to draw (using Marvin Sketch applet or a ChemSketch applet) or write (SMILES string) a chemical compound and to search DrugBank for chemicals similar or identical to the query compound. The SeqSearch button allows users to conduct BLASTP (protein) sequence searches of the 18,000 sequences contained in DrugBank. Both single and multiple sequence (i.e. whole proteome) BLAST queries are supported. The Advanced Search button opens an easy-to-use relational query search tool that allows users to select or search over various combinations of subfields. The Data Extractor is the most sophisticated search tool for DrugBank. Users may download selected text components and sequence data from DrugBank and track the latest DrugBank statistics by clicking on the Download button.

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