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RESEARCH ARTICLE

COMPILATION AND COMPARISON OF VIROLOGICAL AND BIOCHEMICAL RESOURCES *Vishalavani Nidagundi, Kusum Paul and Shambhu M. G.

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ARTICLE INFO	ABSTRACT

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INTRODUCTION

Studying microbes are important for various purposes from evolution to the understanding of infectious diseases in humans, animals and plants [1], [2]. Microbial and biochemical data generated from diverse perspectives have been stored systematically in specific as well as general databases. To counter the data growth, scientists have created specific databases in specific areas. While this is supposed to help scientists to cope with the data explosion, the flood of such Bioinformatics resources has created a huge problem. Microbiological data is particularly interesting from the system biology point of view in the current post-genomic era. Similarly, there are several software designed for microbial and biochemical data analysis. Such databases and software are crucial for microbiologists as well as biochemists. Data analysis is the area which has been neglected by most of the people. With increasing number of software, tools and databases, researchers face a problem in selecting the resources that could suit their needs. Data analysis plays an important role in identifying the proper tool or resource for particular applications. In this context, a systematic comparative analysis of resources would be most helpful for the research community. The numbers of studies about comparative analysis are very less. There are large numbers of resources available like different databases, tools, and software. Data analysis act as a middleware, this can create a bridge between the available resources and end users. To help scientists in making scientific-database-selection there is an urgent need to compile all resources in single new database and provide additional guidance. Such a need is particularly high in the areas of microbiology and some aspects of biochemistry such as carbohydrates and lipids.

METHODS

Data Collection

The literature in Pub med database was searched to identify the available microbiological, biochemical (carbohydrate, lipid) resources. The Pub med query terms are used to retrieve the available

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To counter the data growth, scientists have created curated databases in specific areas. While this is supposed to help scientists to cope with the data explosion, the flood of such bioinformatics resources has created a huge problem. To help scientists in making scientific-database-selection there is an urgent need to compile all resources in one place and provide additional guidance. Such a need is particularly high in the areas of microbiology and some aspects of biochemistry such as carbohydrates and lipids. The current work involved, a) listing the bioinformatics resources relevant to microbiology, carbohydrates and lipids; b) cataloging them systematically and then c) comparing the databases from selected categories. A first time compilation of maximum number of databases has been achieved. A total of 173 microbiology databases have been listed and categorized into viral (28), fungal (23), bacterial (71), antimicrobial peptide databases (4), plant pathogen databases (3) and others (42).

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resources are as follows, a) Microbiology: ((Microbe OR microbes OR microbial) AND (Database OR databases)) b) HIV: ((HIV OR Human Immunodeficiency Virus) AND (Database OR databases)) c) Carbohydrate: ((Carbohydrate OR carbohydrates) AND (database OR databases)) d) Lipid: ((Lipid OR lipids) AND (database OR databases)). The Pub med query returned many numbers of articles. We screened many articles; however the majority of them was not providing the desired data. This could be due to the above keywords are quite frequently used in the research articles. Therefore, we limited our query term in the title field to retrieve articles and screened articles based on abstracts or full paper to shortlist potential articles having the required data.

Rank by Usage Frequency Calculation

The rank by usage frequency for each of the identified resources is calculated using the manual approach method. The resources are ranked based on their "usage frequency" (widely-used being 1st and less-used to be 100th rank).

Manual approach

This method identifies the average of the ranks calculated by each of the following estimation methods.

Method 1: Estimates the number of articles containing the resourcename along with the application-related terms.

Method 2: Estimating the citations of the resource-reporting article(s).

Method 3: Estimates the number of articles containing the URL(s) of the resource.

Google Scholar

A full text search engine was used to obtain the hits by using appropriate query terms in each of the methods.

Categorization of Microbiology Resources

Microbiology resources obtained from literature search are listed. This list of microbiology resources is categorized based on the important features, characteristics and their application area.

Comparison of Resources

After categorization, some of the categories are selected for comparative analysis. From microbiology database, virus and fungal databases are selected. Similarly, carbohydrate databases, lipid databases, are selected from biochemical databases. The selected categories are compared based on important parameters such as number of species covered in a database, disease caused by the species, genome etc. Under virus category it has been noticed that, there is an urgent need for the creation of new databases in certain areas [3]. One of the areas is HIV. Comparative analysis of HIV databases is made based on certain parameters like, type of HIV explained in databases, genes and proteins available in databases etc [4],[5].

RESULTS AND DISCUSSIONS

A total of 173 microbiology databases is listed as shown in Table 1. The listed microbiology databases provide details about databases, short description, URL and rank by usage frequency of each database. The 6 categories are made from the listed microbiology resources based on their important features and application area as shown in Table 2.

Bacterial (71 databases)
 Virus (28 databases)
 Fungal (23 databases)
 Antimicrobial peptide databases (4 databases)
 Plant pathogen databases (3 databases)
 Other databases (42 databases)

Microbiology databases are compared based on important parameters. Virus databases, fungal databases were selected out of six categories. The virus databases were compared with the help of some of the important parameters such as number of virus species covered, host information, disease caused by species etc... shown in Table 3. This list will provide knowledge about virus databases and their application area. This comparative analysis of databases will guide the user to select the relevant resources for their studies. The notorious retrovirus - HIV has been dreaded for several years. A few databases created to help researchers to facilitate easy access to related data [6], [7]. But a comparative analysis showed that existing databases have shortcomings [8]. After recognizing a specific need in the area of HIV, compiled a total of 17 HIV relevant databases. Out of 17 databases 7 databases are HIV specific Table 4 and 10 are general virus databases. Also provides a comparative analysis of 17

Table 1. List of microbiology databases

	Cor	npilation of N	Aicrobiology Resources	
				Rank by Usage
<u>N(▼</u>	DATABASES/RESOURSES	Short Description 💌	UNL	Frequency
1	AgBase-AgricultureBase database		http://www.agbase.msstate.edu/	100
2	AgDB-Ashbya Genome Database	It is a comprehensive onli	http://agd.unibas.ch/	100
3	AgdbNet-antigen sequence database	It is an antigen sequence	http://pubmlst.org/software/database/agdbnet/	100
4	AHMII-Agent to Help Microbial Information Integration	Act as search engine for t	http://www.wdcm.org/AHMII/ahmii.html.	100
5	AHOD- Australian HIV Observational Database		http://www.acronymfinder.com/Australian-HIV- Observational-Database-%28AHOD%29.html	100
6	AMIGene-Annotation of MIcrobial Genes	Provides raw DNA sequence information for bacterial species.	http://www.genoscope.cns.fr/agc/tools/amigene/index.html	100
7	ANTIMIC-Antimicrobial peptides		http://research.i2r.a-star.edu.sg/Templar/DB/ANTIMIC/	100
8	APD2-antimicrobial peptide database		http://aps.unmc.edu/AP/main.php	100
9	BacMap-Bacterial Genomes BacterialLectinDb-Bacterial Lectin	Database provides the m	http://wishart.biology.ualberta.ca/BacMap/	100
10	Database		http://www.research-bioinformatics.in	100
11	regulator database		www.bactregulators.org	100
12	monophosphate kinase	Provides details about ho	http://www.ces.clemson.edu/compbio/banmoki	100

The table provides details about microbiology databases, short description and URL and rank by usage frequency.

Table 2. Categorization of microbiology databases

Toolname 🖵	Bacterial	Virus	Fungal 🝷	Antimicrobial Peptides databases 💌	Fungi,	Plant pathogen Databas∵	URL 🖵	Important features	Citations
AgBase - Ag	Bacterial	Virus					http://www.	AgBase provides information about	McCarthy FM
AgDB - Ashb AgdbNet - ar		Databa	Fungal					It is a comprehensive It is an antigen	Gattiker A, R Dietrich FS, V
AHMII-Agent AMIGene-Ar	Bacterial		Fungal				<u>.wdcm.org/</u> AHMII/ahm		Miyazaki S. AHMII:
AHOD- Aust		Maria					http://www.	Provides HIV inform	D
ANTIMIC - A Database of		virus					nup.//www.	1. Provides details about approximately	Petoumenos
Antimicrobi				Antimicrobial	Peptides dat	tabases	http://resea		Brahmachary
antimicrobi al peptide				Antimicrobial	Peptides dat	tabases	<u>unmc.edu/</u> AP/main.ph		X, Wang Z. APD2: the
Bacterial Genomes	Bacterial						art.biology.	provides the	Stothard P, Va

The above table provides six different categories of microbiology databases along with their URL, important features and Citations.

Features	Dr.VIS-Viral Integration sites database	euHCVdb- European Hepatitis C Virus database	FLAN -FLu Annotation database	FluGenome- Genotyping Influenza A viruses with full genome	HBVRegDB- Hepatitis B Virus Regulatory Sequence Database
Status	Working	Working	Working	Working	Working
Developed by	Not available	et RMN Structurales	NIAID and NCBI	Not available	Not available
Important features	human disease-related	hepatitis C virus (HCV) protein	virus or influenza B virus	on lineages and genotypes	elements in hepatitis B
No. of viral species covere	type 6, human	Hepatitis C virus	Influenza virus A and B	Influenza A virus	Orthohepadnavirus, (OHV)
Host	Homo sapiens	Human	Human, Mouse	species	Human
Disease caused by species	Available	Available	H1N1(subtypes)	H1N1 and H9N2 (subtypes)	Not available
Human disease information	cervical carcinoma,	cirrhosis and hepatocellular	H1N1(subtypes)	Available	Hepatitis and carcinoma
miRNA	Not available	Not available	Not available	Not available	Not available
siRNA	Not available	Not available	Not available	Not available	Not available
Taxonomy	Not available	Not available	Available	Available	Available
Viral-cellular sequence info	Available	Not available	Not available	Not available	Not available
Viral-host junction sequence	Available	Not available	Not available	Not available	Not available
Lineages information	Not available	Not available	Not available	Lineages information	Available
Gene	Available	Available (HCV)	Available	Available	Available
Genome	Not available	Available (HCV)	Available	Virus genome information	virus genome sequence info
Genome sequence	Available	Available (HCV)	Available	Available	Available

Table 3. Comparison of virus databases based on application area

The table shows a comparison of virus databases. In the table top most horizontal line represents a database name and left most vertical lines represents features, are used for comparison of virus databases.

Table 4. List of HIV specific databases

Databases	URL	Important Features	Citations	PMID	Year of publication	Limitations
AHOD - Australian HIV Observational Database	http://www.acronymfinder. com/Australian-HIV- Observational-Database- %28AIIOD%29.html	Provides information on cancer cases, which were diagnosed after HIV infection.	Leuwen MT, Vajdic CM, Woolley I, Chuah J, Templeton DJ, Grulich AE, Law MG; HIV Med. 2013	22934689	2013	Acts as a search engine for HIV related studies and provides links.
HIVKT & PrDB	http://sierra2.stanford.edu/ sierra/servlet/JSierra	Provides list of sequences useful for the development of viral resistance against anti-retroviral drugs and also focuses on the analysis of those sequences.	Kulken C, Korber B, Shafer RW, HIV sequence databases. AIDS Rev. 2003 Jan-Mar,5(1) 52-61. Review. PubMed PMID: 12875108; PubMed Central PMC/D: PMC2613779	12875108	2003	submitted protease and RT sequences and returns inferred levels of resistance to 19 commonly used protease and RT inhibitors.
HIVsirDB	http://crdd.osdd.net/raghav a/hivsir/	siRNAs, which are responsible for silencing HIV genes. 2. Provides 26 HIV Strains and 28 cell types.	, Four N, Sharma A, Raghava GP, Kumar M. HIVsirDB: a database of HIV	22022467	2011	Only provides details about HIV inhibiting siRNA/shRNA .
HIVBrainSeqDB	http://www.HIVBrainSeqDB	HIV envelope sequences, which are directly sequenced from the brain and other tissues from the same patients.	ME, O'Connor N, Gabuzda D. HIVBrainSeqDB: a database of	21156070	2010	Contains only brain sequences.
HIVPSMDB	http://www.bioinformatics. ucla.edu/HIV/	datasets such as, 1.Stanford- Ireated dataset, which consists of 1797 subtype B samples with known drug treatments.	Wang Q, Lee C. The HIV positive selection mutation database. Nucleic	17108357	2007	Only provides detailed selection pressure maps of HIV protease and reverse transcriptase.
TAHOD - Treat Asia HIV Observational Database	http://www.amfar.org/arou nd the world/treat asia/re search and treatment/treat asia hiv aids observation	Provides the details of HIV dIsease in treated and untreated patients throughout Asia and the Pacific.	Petoumenos K, Hui E, Kumarasamy N, Kerr SJ, Choi JY, Chen YM, Merati T, Zhang	21143940	2010	TREAT Asia (Therapeutics Research, Education, and AIDS Training in Asia) is a
HIP Database	http://crdd.osdd.net/server s/hipdb	 Hirdb contains 981 peptides and are checked for anti HIV activity. 2. This database is useful for people working on peptide based therapy against HIV. 3. Statistics provides information about targets, cell lines, peptide 	Qureshi A, Thakur N, Kumar M. HIPdb: a database of experimentally validated HIV inhibiting peptides. PLoS One.	23359817	2013	This database is useful for people working on peptide based therapy against HIV and also in identifying the best inhibitory peptides for further research.

Table 5. List of HIV genes

Gene	Gene ID	Gene Length	Gene Symbol	Gene Description	Locus Tag	Gene Type	Genomic Context
Gag-Pol	155348	1435 aa	gag-pol	Gag-Pol	HIV1gp1	protein coding	NC 001802.
Pr55(Gag)	155030	500 aa	gag	Pr55(Gag)	HIV1gp2	protein coding	NC_001802.1
Vif	155459	192 aa	vif	p23	HIV1gp3	protein coding	NC_001802.1
Vpr	155807	96 aa	vpr	p15	HIV1gp4	protein coding	NC_001802.1
Tat	155871	86 aa	tat	p14	HIV1gp5	protein coding	NC_001802.1
Rev	155908	116 aa	rev	p19	HIV1gp6	protein coding	NC_001802.1
Vpu	155945	82 aa	vpu	p16	HIV1gp7	protein coding	NC_001802.1
Env	155971	856 aa	env	gp160; envelope glycoprotein	HIV1gp8	protein coding	NC_001802.1
Nef	156110	206 aa	nef	p27	HIV1gp9	protein coding	NC_001802.1

Protiens	length	Accession	GI	Region name	Superfamily	Source	Taxonomy	Conserved Domain
							Primate lentivirus	
<u>Nef</u>	206 aa	NP_057857.2	28872818	F-protein	<u>cl02874</u>	pfam00469	group	Negative factor, (F-I
							Primate lentivirus	
Vpu	82 aa	NP_057855.1	9629366	Vpu	cl02898	pfam00558	group	Vpu protein
							Primate lentivirus	
<u>Vif</u>	192 aa	NP_057851.1	9629361	Vif	<u>cl02899</u>	pfam00559	group	Retroviral Vif (Viral
							Primate lentivirus	
Rev	116 aa	NP_057854.1	9629359	REV	cl02864	pfam00424	group	REV protein (anti-rej
							Primate lentivirus	
Gag-Pol	1435 aa	NP_057849.4	28872819	Gag_p17	cl02892	pfam00540	group	gag gene protein p17
							Primate lentivirus	
Vpr	96 aa	NP_057852.2	28872817	VPR	<u>cl02887</u>	pfam00522	group	VPR/VPX protein
							Primate lentivirus	
Env	856 aa	NP_057856.1	9629363	GP120	cl02884	pfam00516	group	Envelope glycoprotei
							Primate lentivirus	
Pr55(Gag)	500 aa	NP_057850.1	9629360		<u>cl02892</u>	<u>pfam00540</u>	group	gag gene protein p17
Tat	86 aa	NP_057853.1	9629358	Tat	cl08273	pfam00539	Lentivirus	Transactivating regul

Table 6. List of HIV proteins

Table 7. Comparison of fungal databases based on application area

Features	CADRE-Central Aspergillus Data Repository Database	Candida DB- Candida Database	CFGP- Comparative Fungal Genomics Platform Database	CGD - Candida Genome Database	FC P450 database- Fungal Cytochrome P450 Database	FFGED- Filamentous Fungal Gene Expression Database	FGDB-Fusarium Graminearum Genome Database
Status	Working	Not working as o	Working	Working	Working	Working	Working
No. of fungal species/strains	Many species cove	Many species co	80 species	8 strains covere	66 species	Available	Fusarium graminearu
Cluster information	Not available	Protein cluster in	Not available	Not available	Available	Not available	Not available
Genome	Available	Available	Available	Available	Available	Not available	Available
Gene	Available (Gene exo	Available	Available	Available	Available	Available	Available
Chromosome information	Available	Available	Available	Available	Available	Not available	Available
Contigs information	Available	Available	Available	Available	Available	Not available	Available
Sequence	Available	Available	Available	Available	Available (Genome	Not available	Available
Protein	Available	Available	Available	Available	Available	Not available	Available (Molecular we
Protein sequence	Available	Available	Available	Available	Available	Not available	Available
Protein length	Available	Available	Available	Not available	Not available	Not available	Available
Domain information	Not available	Available (Functi	Available	Available	Available	Not available	Available
Conserved domains	Not available	Not available	Not available	Not available	Not available	Not available	Available
Structure	Not available	Available (Struct	Not available	Not available	Not available	Not available	Not available
Important features	Provides details abo	Provides detailed	Provides compara	Provides function	Cytochrome P450	Provides fungal ge	FGDB provides informati

Table 8. List of carbohydrate databases

Resource	URL	Important features / utilities	Citations	Year of publication
dbCAN-Carbohydra	http://csbl.bmb.uga.ed	Provides signature domai	Yin Y. Mao X. Yang J. Ch	2012
~ ~ ~		Provides detailed carboh		2011
GlycomeDB	N. INCOM	Provides the structural in		2010
PROCARB	http://www.procarb.or	Provides information abo	Malik A, Firoz A, Jha V,	2010
MatrixDB	http://matrixdb.ibcp.fr	Provides information abo	Chautard E, Ballut L, Th	2009
3DSDSCAR-Three	http://www.3dsdscar.o	Provides information abo	Veluraja K, Selvin JF, V	2010
GLYCOSCIENCES	http://www.glycoscien	Provides details about gly	Lütteke T, Bohne-Lang	2006
Mucin Database	http://www.medkem.g	Provides details about m	Lang T, Hansson GC, Sar	2007
3D Lectine Database	http://lectin3d.cermav.	Provides information abo	Not available	Not available
GLYCO3D	http://glyco3d.cermav.	Provides the integration (Not available	Not available
O-GlycBase	http://www.cbs.dtu.dk	Provides details about gly	Gupta R, Birch H, Rapa	1999
BPGD	http://sydney.edu.au/s	Database describes about	Not available	Not available
EuroCarbDB	http://www.ebi.ac.uk/	Database with structures	von der Lieth CW, Freir	2010
KEGG GLYCAN	http://www.genome.jp	Database provides the inf	Hashimoto K, Goto S, K	2006
CFG Functional Glyc	http://www.functional	Provides access to prim	Not available	Not available
CAZy	http://www.cazy.org	Provides details about the	Cantarel BL, Coutinho P	2008
GBP-Glycan Binding	http://www.functional	Provides the information	Not available	Not available

Resource	URL	Important features / utilities	Citations	Year of publication
CYBERLIPID CENTER	http://www.cyberlipid.org	Provides description of diff	Not available	Not available
Lipid Bank	http://lipidbank.jp	Provides information about	Yasugi E, Seyama Y.	2007
LIPIDAT	http://www.lipidat.tcd.ie	Provides information about th	Caffrey M, Hogan J.	1992
THE LIPID LIBRARY	http://lipidlibrary.aocs.org	Provides information about	Not available	Not available
Lipid Bilayer Membranes for	http://www.umass.edu/m	Provides lipid bilayer mem	Not available	Not available
Lipids Online	http://www.lipidsonline.c	An online resource, which I	Not available	Not available
LMPD-LIPID MAPS Prote	http://www.lipidmaps.org	Provides information about	Cotter D, Maer A, G	2006
LMSD-LIPID MAPS Struct	http://www.lipidmaps.org	Provides information about	Sud M, Fahy E, Cott	2007
LOX-DB-LipOXygenases D	http://www.glycosciences	Provides information about	Lütteke T, Krieg P, F	2003
Lipidomics Gateway	http://www.lipidmaps.org	Provides detailed informat	Not available	Not available
LIPIDAG	http://www.lipidag.tcd.ie	Provides lipid miscibility and	Not available	Not available

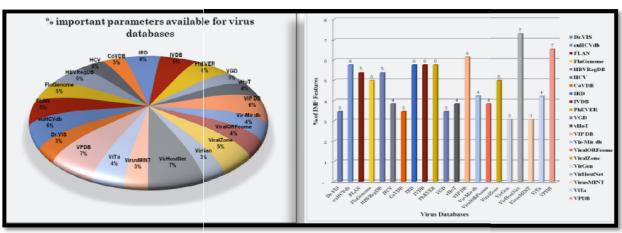
Table 9. List of lipid databases

Table 10. Comparison of carbohydrate databases based on application area

Features	dbCAN-Carbohydrate- active enzymes	BCSDB-Bacterial carbohydrate structure database	GlycomeDB	PROCARB	MatrixDB
Status	Working	Working	Working	Working	Working
Source	Available	Available	Available	Available (Source na	Available
Species	Many species covered	Bacterial species cover	Many species cover	Many species covere	Available
Taxonomy	Available	Available	Available (Taxonom	Not available	Available
Families	Available	Not available	Not available	Not available	Not available
Sub-families	Available	Not available	Not available	Not available	Not available
Genome	Available	Available	Available	Not available	Not available
Gene	Available	Available	Not available	Available (Gene nam	Available
Protein properties (Available	Available (protein deta	Available (Protein d	Available (Protein na	Available (Protein)
Domain	Available	Not available	Not available	Not available	Available
Conserved domain d	Available	Not available	Not available	Not available	Not available
Sequence	Available (Sequence so	Not available	Available (Carbohyd	Available (Amino aci	Available (Sequence ar
Signature domain	Available	Not available	Not available	Not available	Not available
Structural information	Not available	Available (Chemical st	Available (Structura	Available (3D structu	Available (2D, 3D Struct
Methods used	Hidden Markov Models	Many methods used	Not available	Not available	Available
Carbohydrate inform	Available	Available	Available	Available (Name, Fo	Available
Important features	Provides signature dom	Provides detailed carb	Provides the structu	Provides information	Provides information a

Table 11. Comparison of lipid databases based on application area

Features	CYBERLIPID CENTER	Lipid Bank	LIPIDAT	THE LIPID LIBRARY	Lipid Bilayer Membranes for RasMol
Status	Working	Working	Not working	Working	Working
Source	Available	Available	Not available	Available	Not available
Lipid information	Available (Simple lip	Available (Fatty acid	Available	Available	Available
Oxidation informati	Available	Not available	Not available	Not available	Not available
Techniques used	Available (Many tech	Not available	Not available	Available	Not available
Information on the	Available	Available	Not available	Available	Not available
Molecular structure	Available	Available (ChemDra	Not available	Available	Available
Spectral information	Not available	Available (Mass, UV,	Available	Not available	Not available
Physical and chemic	Not available	Available (Melting p	Not available	Available	Available (Some pr
Species information	Not available	Not available	Not available	Not available	Not available
Gene information	Not available	Not available	Not available	Not available	Not available
Protein information	Not available	Not available	Not available	Not available	Not available
Pathways information	Not available	Not available	Not available	Not available	Not available
Important features	Provides description	Provides information	Provides informati	Provides informati	Provides lipid bilay





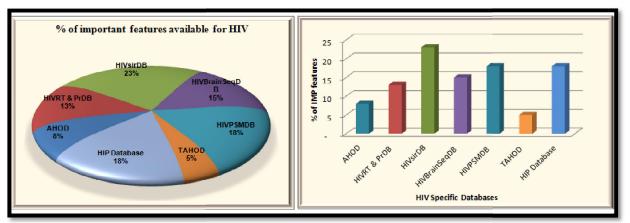
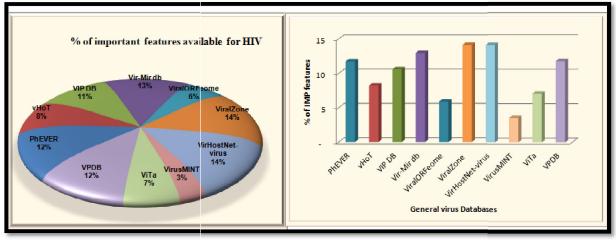
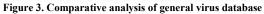


Figure 2. Comparative analysis of HIV specific database





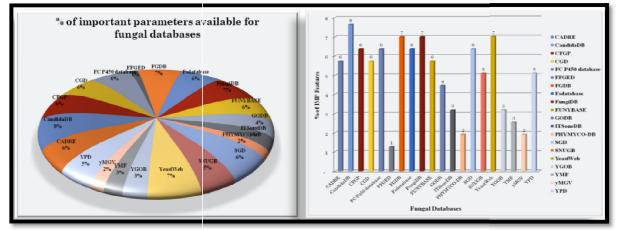


Figure 4. Comparative analysis of fungal databases

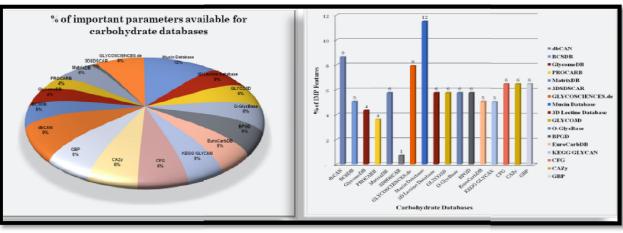


Figure 5. Comparative analysis of carbohydrate databases

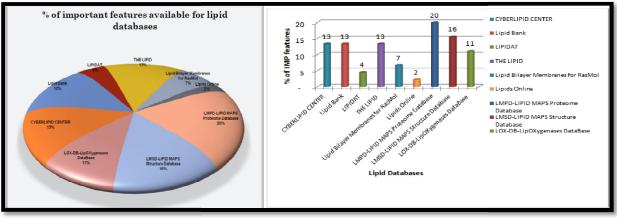


Figure 6. Comparative analysis lipid of databases

databases. In additional the list of HIV genes and proteins are also provided Table 5, Table 6. Fungal databases were compared using some of the important parameters such as number of fungal species/strains covered, cluster information, chromosome etc... Table 7. This gives knowledge about fungal databases and their application area. From the comparative study user can evaluate that some of the resources cover all most all the information and some of them are not.

Compilation and Comparison of Biochemical Resources

A total of 17 carbohydrate and 11 lipid databases are listed Table- 8, Table-9. The list provides a list of databases along with the URL, important features, citations and year of publications. Comparisons of carbohydrate and lipid databases are made based on their important parameters. This will be helpful for study of carbohydrate and lipid databases and their application area Table-10, Table-11.

Conclusions

The present study has achieved compilation of 173 microbiology databases and also listed biochemical molecule databases such as, carbohysdrate databases (17), lipid (11) databases. Microbiology databases were further categorized as viral (28) databases, fungal (23) databases, bacterial (71) databases, antimicrobial peptide databases (4), plant pathogen databases (3) and other (42) databases. Certain categories are selected for comparison such as virus, fungal categories from microbiology databases. After performing comparative analysis we came to know that there is no such database which provides knowledge on virus, fungal, carbohydrate, lipid databases. The present database provides information about HIV genes, proteins, existing HIV database details and comparison of other databases. This database will be helpful for people who are all working on HIV and also easy access to HIV related data.

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