Database Resources of the National Genomics Data Center, China National Center for Bioinformation in 2023

CNCB-NGDC Members and Partners*,†

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ABSTRACT

The National Genomics Data Center (NGDC), part of the China National Center for Bioinformation (CNCB). provides a family of database resources to support global academic and industrial communities. With the explosive accumulation of multi-omics data generated at an unprecedented rate. CNCB-NGDC constantly expands and updates core database resources by big data archive, integrative analysis and value-added curation. In the past year, efforts have been devoted to integrating multiple omics data, synthesizing the growing knowledge, developing new resources and upgrading a set of major resources. Particularly, several database resources are newly developed for infectious diseases and microbiology (MPoxVR, KGCoV, ProPan), cancer-trait association (ASCancer Atlas, TWAS Atlas, Brain Catalog, CCAS) as well as tropical plants (TCOD). Importantly, given the global health threat caused by monkeypox virus and SARS-CoV-2, CNCB-NGDC has newly constructed the monkeypox virus resource, along with frequent updates of SARS-CoV-2 genome sequences, variants as well as haplotypes. All the resources and services are publicly accessible at https://ngdc.cncb.ac.cn.

INTRODUCTION

The National Genomics Data Center (NGDC) is affiliated to Beijing Institute of Genomics (BIG), Chinese Academy of Sciences (CAS) & China National Center for Bioinformation (CNCB). Since its foundation in 2019, CNCB-NGDC has been constructed in collaborations with additional two CAS institutions, viz., Institute of Biophysics and Shanghai Institute of Nutrition and Health, as well as by joint efforts with partners (https://ngdc.cncb.ac.cn/ partners). Over the last decades, an increasing number of large-scale high-throughput sequencing projects have been conducted globally, advancing the understanding of the genetic basis of diseases, genetic epidemiology and public health (1-3) For example, UK Biobank collects a rich variety of genome-wide genotype data and enables populationbased cohort studies on genetic and epidemiological associations for a broad range of health-related traits (1). Such large-scale cohort studies have uncovered novel biomarkers and drug targets, which have greatly contributed to disease molecular diagnosis and precision medicine. Meanwhile, single-cell sequencing technologies have been rapidly developed and widely adopted to elucidate genomic (4), transcriptomic (5), epigenomic (6) and proteomic (7) heterogeneities in cellular populations and to disentangle complex mechanisms of diseases at single-cell resolution (8). As a result, immense amount of multi-omics data has been generated at an ever-increasing rate and scale. Therefore, synthesizing and sharing such massive quantities of data and knowledge is increasingly important for a wide range of research activities worldwide.

In the past year, CNCB-NGDC has made continuous efforts in developing new resources and updating relevant resources, accordingly providing open access to a family of resources for advancing life and health sciences globally (9–18) Particularly, in the context of monkeypox outbreak and COVID-19 pandemic, considerable efforts have been devoted to integrating, analyzing and updating the virus genome sequences, variants, and haplotypes (19-21). Importantly, several core database resources have been recommended by major publishers, greatly accelerating the efficient deposition and open sharing of biomedical data. Meanwhile, in addition to data sharing of SARS-CoV-2 genomes with NCBI, CNCB-NGDC is building close collaborations with INSDC (22) by mirroring the metadata and sequence data from NCBI SRA (23). Here, we provide a brief overview of new developments and recent updates in CNCB-NGDC and describe its core resources and services (Figure 1). All these resources and services are publicly available in the home page of CNCB-NGDC (https: //ngdc.cncb.ac.cn).

*To whom correspondence should be addressed. Yongbiao Xue Email: ybxue@big.ac.cn [†]Full list provided in the Appendix.

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Figure 1. Core database resources of CNCB-NGDC classified by database categories. These database resources are publicly available and searchable through the home page of CNCB-NGDC at https://ngdc.cncb.ac.cn. A full list of data resources is shown at https://ngdc.cncb.ac.cn/databases.

NEW DEVELOPMENTS

Health and disease

MPoxVR. The Monkeypox Virus Resource (MPoxVR; https://ngdc.cncb.ac.cn/gwh/poxvirus) is a one-stop portal that integrates monkeypox virus genome sequences, variants, publications and online tools (21). MPoxVR collects all public genome sequences and metadata for the *Poxviridae* family from GenBank (24), accompanying with daily update through in-house automatic pipelines. Of note, MPoxVR performs systematic analysis to obtain a dynamic landscape of genomic variations from a global perspective, providing all identified variants and detailed statistics for each virus isolate and attributing functional annotation and population frequency to each variant. It also equips with online tools for sequence alignment, genome annotation and variant annotation. In addition, it provides a full list of relevant publications, including published articles from PubMed as well as preprints from bioRxiv and medRxiv. Furthermore, MPoxVR offers data submission services to accept raw sequences and assembled genomes in cooperation with the Genome Sequence Archive (25) and Genome Warehouse (26) of CNCB-NGDC. Given the spread of recent outbreak caused by monkeypox virus, MPoxVR serves as a valuable resource for the global research community.

KGCoV. The Knowledge Graph of SARS-CoV-2 (KG-CoV; https://www.biosino.org/kgcov) (27) is an online database centered on virus genomic information and epidemiological data, which is helpful to identify relevant knowledge and devise epidemic prevention and control policies in collaboration with disease control personnel. To help analyze the spread and evolution of the virus, KG-CoV collates a wide range of data covering viral genomes, sequence variations, and locations in temporal and spatial distribution from GISAID. Thus, it collects 445 470 genomic records and 2 571 621 epidemiological records from Wikipedia and research papers. As a result, a total of 11 412 genome-case pairs are generated for the surveillance of virus transmission and reconstruction of infection paths. In conclusion, KGCoV conducts standardized processing on viral genomic and epidemiological data and produces a new genomic epidemiology knowledge graph to show the genomic mutation sites, epidemiological information and their connections in SARS-CoV-2.

ASCancer Atlas. ASCancer Atlas (https://ngdc.cncb.ac. cn/ascancer) is a comprehensive knowledgebase designed to provide a complete landscape of carcinogenic alternative splicing (AS) in human cancers (28). The current version of ASCancer Atlas houses about 2 million computationally putative splicing events identified from largescale cancer transcriptome datasets. Different from existing databases of AS in cancers, it has unique features as follows: (i) high-confidence collection of 2,006 experimentally validated cancer-associated splicing events; (ii) complete splicing regulatory network and (iii) a suite of multi-dimensional online splicing analysis tools. In summary, ASCancer Atlas provides a repository of oncogenic AS to help researchers study a full spectrum of splicing disorders in human cancers.

Brain catalog. Brain Catalog (https://ngdc.cncb.ac.cn/ braincatalog) presents a resource for a variety of disorders, diseases, and risk factors that are broadly related to the dysfunctions of the brain (29). Specifically, we collected more than 500 GWAS summary statistics datasets for psychiatric disorders, neurodevelopmental disorders, cognitive disorders, substance use disorders, behavioral habits, psychosocial and personality traits, and neurodegenerative diseases. Brain Catalog estimates the SNP-based heritability, the partitioning heritability based on functional annotations, and genetic correlations among traits. Augmented by a list of comprehensive annotation datasets including 58 QTL datasets spanning 6 types of QTLs, Brain Catalog hosts inferring results from multiple methods for the candidate causal variants, causal genes, and functional tissues and cell types for each trait. Finally, Brain Catalog presents inferred risk factors that are likely causal to each trait. In conclusion, Brain Catalog serves as a valuable resource to delineate the genetic components of brain-related traits.

CCAS. CCAS (https://ngdc.cncb.ac.cn/ccas) is a one-stop and comprehensive annotation system for individual cancer genome at multi-omics level (30). CCAS integrates 20 widely recognized resources in the field to support data annotation for 10 categories of cancers covering 395 sub-

types. Data from each resource are curated and standardized by using multiple ontology frameworks. The inputs of CCAS include abnormalities on single nucleotide variant/insertion or deletion, expression, copy number variation, and methylation level. Consensus outputs are arranged in a tabular form and visualized in figures. Expanded panels with additional information are used for conciseness, and most figures are interactive to show additional information. Moreover, CCAS offers multi-dimensional annotation information, including mutation signature pattern, gene set enrichment analysis, pathways, and clinical trial related information. In summary, CCAS is designed to help users intuitively understand the molecular mechanisms of tumors and discover key functional genes.

Genome and variation

HGD. The Homologous Gene Database (HGD; https: //ngdc.cncb.ac.cn/hgd) integrates multi-species and multiomics data and provides one-stop public data services for browsing, retrieval, comparison and downloading (31). By integrating several existing homologous resources that vary in terms of inferring method and homology relationship, HGD is able to efficiently eliminate the difficulties for researchers in choosing and mapping homology results from one species to another. Besides, by offering various gene function annotations, HGD makes it convenient to conduct comprehensive homologous functional studies on largescale genome sequences. Currently, HGD houses a total of 112 383 644 homologous pairs for 37 species, including 19 animals, 16 plants and 2 microorganisms. Specifically, 10 of the 37 species are model organisms. Meanwhile, HGD integrates various annotations including 16 909 homologs with traits, 276 670 homologs with variants, 398 573 homologs with expression profiles and 536 852 homologs with gene ontology annotations, which can help users gain a deeper understanding of homologous gene function.

ProPan. ProPan (https://ngdc.cncb.ac.cn/propan) is a public database for comprehensively profiling prokaryotic pan-genome dynamics (32). In the current version, it covers 51 882 high-quality strain genomes and provides a total of 1504 pangenomes, with 23 in archaea and 1481 bacteria. ProPan offers multi-dimensional insights into species, such as pan-genome dynamics characteristics, multiple gene functional annotation, functional protein association networks, pathway map association, resistance gene prediction for 126 substances (antimicrobial drug, biocide, and metal), and evaluation of 31 metabolic cycle processes (e.g. organic carbon oxidation, nitrite oxidation, and sulfur oxidation). Collectively, ProPan bears great utility for studying prokaryotic pan-genome dynamics, species classification and identification, pan-genome metabolism and further beyond.

Biodiversity

TCOD. The Tropical Crops Omics Database (TCOD; https://ngdc.cncb.ac.cn/tcod) is a comprehensive omics data resource for tropical crops. By integrating diverse data from five economic tropical crops, namely, cassava, rubber tree, sugarcane, mango and pineapple, TCOD houses

1253 samples with whole-genome raw sequencing data, 14 chromosome-level genome assemblies, 565 185 genes with functional annotations, 111 934 324 unique variants, 10 433 germplasm items and 23 279 publications. In addition, TCOD embeds BLAST for finding homologous genes across multiple species as well as a genome browser for visualizing the distribution of SNPs and indels on the genome. Taken together, TCOD functions as a multi-omics data platform for tropical crops and thereby provides data services for researchers to conduct selective breeding and trait improvement research.

Expression

TWAS Atlas. TWAS Atlas (https://ngdc.cncb.ac.cn/twas) is a curated knowledgebase of transcriptome-wide association studies (TWAS) (33). Based on manual curation of TWAS related publications and integration of external relevant datasets, the current implementation of TWAS Atlas contains a curated collection of 401 266 gene-trait associations, which are derived from a total of 200 publications and encompass 22 247 genes and 257 traits that are classified into diseases, phenotypic abnormalities, measurements and others. Most importantly, an interactive knowledge graph covering all catalogued gene-trait associations is constructed, which can be used to add remarkable SNPgene associations to achieve the integration and visualization of SNP-gene-trait associations. Collectively, TWAS Atlas provides comprehensive and visualized regulatory relationships, enabling researchers to better understand the genetic mechanisms of various phenotypes and complex diseases.

RECENT UPDATES

Raw data and metadata

BioProject and BioSample. BioProject (https://ngdc.cncb. ac.cn/bioproject) and BioSample (https://ngdc.cncb.ac.cn/ biosample) are two public repositories of biological research projects and samples, respectively. They collect descriptive metadata on biological projects and samples investigated in experiments and provide centralized accesses to all public projects and samples as well as cross links to their related data resources. Till September 2022, there are a total of 7906 biological projects and 783 267 biological samples submitted by 4312 users from 1027 organizations (Figure 2A), clearly showing a rapid increase by comparison with 4514 projects and 482 577 samples in August 2021. In addition, this year, BioProject and BioSample have mirrored the data of INSDC (International Nucleotide Sequence Database Collaboration) by downloading and integrating all metadata of 596 052 projects and 27 977 897 samples from NCBI.

GSA, GSA-Human and OMIX. The Genome Sequence Archive (GSA; https://ngdc.cncb.ac.cn/gsa) (25,34) is a public data repository for raw sequence reads, which accepts worldwide data submissions, performs data curation and quality control for all submitted data, and provides free open data for sharing services for sharing all publicly available data. GSA for Human (GSA-Human; https:

//ngdc.cncb.ac.cn/gsa-human) (25) is a data archive specialized for human genetic related omics data with controlledaccess and security services. As of September 2022, GSA and GSA-Human have together collected 654 635 experiments and 773 032 runs and archived a total of 16.3 PB data, showing a rapid increase of data volume by comparison with the previous release last September (~ 10 PB) (Figure 2B and 2C). Similar to BioProject and BioSample, GSA has also mirrored the INSDC's data by collecting and integrating the relevant metadata and raw data from NCBI SRA, covering 20 488 321 experiments, 21 963 869 runs and 962 TB of sequence files. The Open Archive for Miscellaneous Data database (OMIX; https://ngdc.cncb.ac.cn/omix), as a member of the GSA family, accepts miscellaneous data with different types as well as supplementary information and materials with various formats. OMIX has archived 952 submissions with 20.30 TB, demonstrating its dramatic growth in contrast to 269 submissions and 13.3 TB last September.

Database commons. Database Commons (https://ngdc. cncb.ac.cn/databasecommons) is a global catalog of biological databases. It provides easy access and retrieval to a full collection of worldwide biological databases, assesses the database impact by factoring both citation and age, and delivers a series of useful statistics and trends to investigate their status and impact on biomedical research. Since its inception in 2015, it has been expanded frequently to incorporate more databases and enriched gradually with a series of user-friendly functionalities. Currently, with the efforts of more than 50 curators, it catalogues a total of 5825 databases, involving 8929 publications and 1976 institutions throughout the world. Notably, Database Commons has been recommended by Cell Press and Bioinformatics Advances to provide registry services for biological data repositories. In addition, Database Commons, in collaboration with Nucleic Acids Research (NAR), provides registration services for databases published in the NAR Database Issue.

Genome and variation

Genome warehouse. The Genome Warehouse (GWH; https://ngdc.cncb.ac.cn/gwh) is a public resource for archiving assembled genome sequences and their detailed metadata (26). Compared to 20 606 assemblies last August, GWH hosts a total of 24 781 assemblies for 1792 species as of September 2022 (Figure 2D). Among them, 12 887 assemblies are publicly released and reported in 206 journal articles, by comparison with 9886 assemblies and 97 articles in August 2021. All released sequences have passed strict quality control, and are searchable and freely accessible in GWH. Of interest, 25 protist genome assemblies mainly from the Protist 10 000 Genomes Project (P10K) (35) are deposited in the current release of GWH. Particularly, GWH has received and released telomereto-telomere gap-free assemblies for organisms such as Arabidopsis thaliana (36). In support of MPoxVR (21), GWH has integrated NCBI genome and protein sequences of all viruses in the *Poxviridae* family (https://ngdc. cncb.ac.cn/gwh/browse/virus/poxviridae), with the aim to



Figure 2. Statistics of data submissions to CNCB-NGDC. (A) Data statistics of BioProject and BioSample. (B) Data statistics of Experiments and Runs in GSA. (C) Timeline of data growth in GSA. (D) Statistics of genome assemblies in GWH. All statistics are frequently updated and publicly available at https://ngdc.cncb.ac.cn/bioproject, https://ngdc.cncb.ac.cn/biosample, https://ngdc.cncb.ac.cn/gsa and https://ngdc.cncb.ac.cn/gwh.

enable researchers to conduct comparative analysis on poxviruses.

GVM and GWAS atlas. The Genome Variation Map (GVM; https://ngdc.cncb.ac.cn/gvm) (37,38) and GWAS Atlas (https://ngdc.cncb.ac.cn/gwas) (39,40) are two public variation-related resources. GVM is a public repository of genome variations, including single nucleotide polymorphisms (SNP) and small insertions and deletions (indel), features data collection for a wide range of species and accepts data submissions from all over the world. GWAS Atlas (39,40) is a curated resource of genome-wide variant-trait associations in plants and animals. Till August 2022, GVM has received 244 data submissions involving 165 243 samples from 37 species and contained a total of ~ 1055 million variants, encompassing 330 projects and 65 862 samples and covering 18 animals, 26 plants and 3 viruses. GWAS Atlas integrates 233 599 associations across ten cultivated plants and five domesticated animals that were manually curated from 3072 studies in 771 publications. As a result, a total of 36 874 genes and 1395 traits are annotated based on a set of ontologies. To prioritize the most important loci for functional follow-up studies, a total of 4492 unique lead SNPs for 407 traits and 361 unique experiment-validated causal variants for 131 traits are newly provided. To facilitate comparative analysis across species, GWAS Atlas unifies trait vocabularies and defines new ontology terms for 1056 traits, resulting in a total of 1172 Plant Phenotype/Trait Ontology (PPTO) and 431 Animal Phenotype/Trait Ontology (APTO) terms. Together, GVM provides high-density reference variations and GWAS Atlas integrates high-quality curated GWAS associations for plants and animals, which serve as valuable resources for genomic variation research of important traits.

Health and disease

RCoV19. The 2019 Novel Coronavirus Resource (RCoV19; https://ngdc.cncb.ac.cn/ncov) (41,42) provides a series of functional modules on SARS-CoV-2 genome sequences, genomic mutations, variant monitoring, online data analysis toolkits and literatures. As of September 2022, a total of 13 345 020 SARS-CoV-2 sequences and meta data are integrated, and 188 100 genomic mutations are identified based on those complete and high-quality genome sequences. To meet the need for near real-time mutation surveillance and early-warning of high-risk variants, RCoV19 offers the genomic prevalence of lineages globally and nationally, and allows mutation prevalence comparison across lineages. It also provides potential high-risk variants predicted weekly by a machine

learning model based on several important haplotype network features, and estimates the percentage of high-risk lineages among all sequences since its emergence. More importantly, RCoV19 provides curated knowledge of host susceptibility to SARS-CoV-2 and mutation effects on transmission and pathogenicity, which are of great usefulness for origin tracing and transmission preventing.

Expression

Gene expression nebulas. Gene Expression Nebulas (GEN; https://ngdc.cncb.ac.cn/gen) is a data portal integrating transcriptomic profiles at both bulk and single-cell levels in various conditions across multiple species (43). In the current release, 146 gene expression profiling datasets related to SARS-CoV-2 infection (101 bulk and 45 scRNA-seq) derived from 140 original high-throughput sequencing projects are systematically incorporated. In comparison to the previous release (August 2021), total number of incorporated datasets increases from 323 to 469, covering 54 448 samples and 18 966 983 cells of 34 species, involving 21 animals, 10 plants, 2 protists and 1 fungus. In addition to the enrichment of data volume, GEN has also been significantly upgraded by providing an easy-to-use one-stop offline RNA-seq data analysis pipeline, named GENToolkit, which aims to facilitate the standardization of expression profiling analysis of both bulk RNA-seq and scRNA-seq data across various technical and biological conditions.

Internal control genes. The database of Internal Control Genes (ICG; https://ngdc.cncb.ac.cn/icg) is a wellestablished knowledgebase of experiment-validated internal control genes and their respective applicable scenarios for RT-qPCR normalization across a wide variety of species (44). In the current version, ICG houses a total of 2514 high-quality verified internal control genes from 509 species (188 animals, 264 plants, 28 fungi and 29 bacteria), associating with 2725 corresponding applicable scenarios. Particularly, a new module 'Health & Disease portal' is set up to facilitate the application of RT-qPCR in precision medicine research, which currently supports 27 cancer types, 15 diseases and 17 human molecular biological models. In addition to mRNAs, effective normalization strategies for diverse types of non-coding RNAs are also integrated. Moreover, to improve the flexibility and functionality, ICG is implemented based on MySQL/Java, greatly facilitating structured management, access, utilization and knowledge enrichment.

Epigenomics

EWAS open platform. The EWAS Open Platform (https: //ngdc.cncb.ac.cn/ewas) (45) is a one-stop resource for epigenome-wide association studies (EWAS). It is made up of three parts: EWAS Data Hub (46) for data collection and standardized normalization, EWAS Atlas (47) for knowledge extraction and curation, and EWAS Toolkit for downstream analysis and visualization. The current version of EWAS Open Platform is updated by adding 17 820 samples and 25 526 associations. Among them, all DNA methylation array data was normalized with batch effect removal using GMQN (48), a reference-based method for correcting batch effects as well as probe bias in the Human Methylation BeadChip. At present, EWAS Open Platform houses 133 672 DNA methylation array data, including 1099 tissues/cell types and 612 diseases, as well as 642 544 high-quality EWAS associations manually curated from 1586 studies in 991 publications, covering 717 traits and 3497 cohorts. In addition, taking advantage of the high-quality knowledge and data, EWAS Open Platform provides a number of reference DNA methylation profiles and offers online services for enrichment, annotation, and network visualization.

MethBank. The Methylation Bank (MethBank; https: //ngdc.cncb.ac.cn/methbank) (49-51) is a comprehensive database of whole-genome DNA methylation across a variety of species. In the current release of MethBank, significant improvements and updates have been made in data volume, downstream data mining for differential methylation and web interfaces. Specifically, the updated MethBank features: (i) an increase in single-base resolution methylomes, from 855 last August to 1449 across 23 species and 236 tissues/cell lines in different biological scenarios including development, cancer and physiology; (ii) computational identification of differentially methylated regions related to 887 different biological groups and characterization of enriched biological pathways to expand the methylation traits/biomarkers resource; (iii) a new knowledge module that consists of a curation network for 266 associations of biological contexts and featured differentially methylated genes; (iv) an increasing amount of microarray data with up to 111 tissue/cell type specific samples and (v) significant improvements in visualization together with the completely redesigned web interfaces.

Noncoding RNA

LncBook (https://ngdc.cncb.ac.cn/lncbook) is a comprehensive database of human long non-coding RNAs (lncR-NAs) as well as their annotations (52,53). The updated release of LncBook integrates more lncRNA genes, characterizes their molecular signatures in more biological contexts, and incorporates more annotations by including new omics features. First, it incorporates 119 722 new transcripts and 9632 new genes, updates gene structure of 21 305 lncRNAs, and provides 323 950 high-quality lncRNA transcripts and 95 243 genes. Second, it enriches the expression and methylation annotations with more biological contexts, highlights disease/trait-associated variants, and predicts lncRNA-miRNA binding sites. Third, it integrates new omics features of lncRNA genes including sequence conservation across 40 vertebrates, small protein expression, and interaction with proteins. LncRNAWiki (https://ngdc.cncb. ac.cn/lncrnawiki), a knowledgebase of human lncRNAs, incorporates comprehensive annotations of functional lncR-NAs based on a standardized curation model and provides user-friendly web interfaces to facilitate data curation, retrieval and visualization (54,55). This year, based on manual curation of 535 publications, we have expanded LncR-NAWiki by adding 97 experiment-validated human lncR-NAs, updating 191 existing lncRNAs and integrating 4761 newly-curated associations.

Single-cell omics

Cell taxonomy. Cell Taxonomy (https://ngdc.cncb.ac.cn/ celltaxonomy) is a comprehensive and curated repository of cell types and associated cell markers encompassing a wide range of species, tissues and conditions (56). Combined with literature curation and data integration, up to September 2022, Cell Taxonomy houses 3143 cell types and 26 613 associated cell markers in 257 conditions and 387 tissues across 34 species based on 4299 publications and scRNA-seq profiles of ~3.5 million cells. It presents a significant increase in comparison to the last version in September 2021 (containing 2650 cell types and 25 087 cell markers in 157 conditions, 296 tissues, 21 species supported by 3402 publications and 1.9 million scRNA-seq profiles). Collectively, Cell Taxonomy represents a fundamentally useful reference to systematically and accurately characterize cell types and thus lays an important foundation for deeply understanding and exploring cellular biology in diverse species.

CONCLUDING REMARKS

With the explosive growth of multi-omics data, CNCB-NGDC keeps putting efforts to provide a suite of newly developed and updated database resources, with the aim to accept data submissions and provide value-added annotations and curated knowledge for the global research community. Ongoing efforts include, but not limited to, automation of data submission, curation, integration and analysis procedures, infrastructure upgrades for big data storage and transmission, and development of new tools and pipelines in aid of big data analysis. As one of major global centers, CNCB-NGDC will continue to expand and provide a family of data resources and services to support knowledge discovery for a wide range of research activities in life and health sciences.

DATA AVAILABILITY

All resources and services are publicly available in the home page of CNCB-NGDC (https://ngdc.cncb.ac.cn).

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APPENDIX

Corresponding author: Yongbiao Xue^{1,2,3,*}

Co-corresponding authors: Yiming Bao^{1,2,3,*}, Zhang Zhang^{1,2,3,*}, Wenming Zhao^{1,2,3,*}, Jingfa Xiao^{1,2,3,*}, Shunmin He^{3,4,*}, Guoqing Zhang^{3,5,*}, Yixue Li^{3,5,*}, Guoping Zhao^{3,5,6,7,*}, Runsheng Chen^{4,8,*}

CNCB-NGDC MEMBERS (Arranged by project role and then by contribution except for Team Leader (TL), as indicated)

MPoxVR: Yingke Ma^{1,2,#}, Meili Chen^{1,2,#}, Cuiping Li^{1,2,#}, Shuai Jiang^{1,2}, Dong Zou^{1,2}, Zheng Gong^{1,2}, Xuetong Zhao^{1,2,3}, Yanqing Wang^{1,2}, Junwei Zhu^{1,2}, Zhang Zhang^{1,2,3}, Wenming Zhao^{1,2,3}, Yongbiao Xue^{1,2,3}, Yiming Bao^{1,2,3,*} (TL), Shuhui Song^{1,2,3,#} (TL)

KGCoV: Guoqing Zhang^{5,#}, Yunchao Ling⁵, Yiwei Wang⁵, Jiaxin Yang⁵, Xinhao Zhuang⁵

Jiaxin Yang', Xinhao Zhuang' **HGD:** Guangya Duan^{1,2,3,#}, Gangao Wu^{1,2,3,#}, Xiaon-ing Chen^{1,2,3}, Dongmei Tian^{1,2}, Zhaohua Li^{1,2,3}, Yan-ling Sun^{1,2}, Zhenglin Du^{1,2}, Lili Hao^{1,2}, Shuhui Song^{1,2,3}, Yuan Gao^{1,2,3}, Jingfa Xiao^{1,2,3}, Zhang Zhang^{1,2,3}, Yiming Bao^{1,2,3}, Bixia Tang^{1,2,#}, Wenming Zhao^{1,2,3,#}, Zaichao Zhang⁹, Qiheng Qian^{1,2,3}, Zhewen Zhang^{1,2,#}, Jingfa Xiao^{1,2,3,*}

TCOD: Hailong Kang^{1,2,3,#}, Tianhao Huang^{1,2,3,#}, Xiaon-**ICOD:** Hallong Kang^{1,2,3,#}, Hanhao Huang^{1,2,3,#}, Xiaon-ing Chen^{1,2,3,#}, Zhiqiang Xia¹⁰, Xincheng Zhou¹¹, Jin-quan Chao¹², Bixia Tang^{1,2}, Zhonghuang Wang^{1,2,3}, Jun-wei Zhu^{1,2}, Zhenglin Du^{1,2}, Sisi Zhang^{1,2}, Jingfa Xiao^{1,2,3}, Weimin Tian¹², Wenquan Wang^{10,#}, Wenming Zhao^{1,2,3,*} **ASCancer Atlas:** Song Wu^{1,2,3,#}, Yue Huang^{2,3,13,#}, Mochen Zhang^{1,2,3}, Zheng Gong^{1,2,3}, Guoliang Wang^{1,2,3}, Xin-chang Zheng^{1,2}, Wenting Zong^{1,2,3}, Wei Zhao^{1,2,3}, Peiqi Xing^{2,13}, Puigo Li^{1,2,3,#} (TL), Zhaogi Liu^{2,3,13,#} (TL), Xim

Xing^{2,13}, Rujiao Li^{1,2,3,#} (TL), Zhaoqi Liu^{2,3,13,#} (TL), Yiming Bao^{1,2,3,*} (TL)

TWAS Atlas: Mingming Lu^{1,2,3,#}, Yadong Zhang^{1,2,#}, Fengchun Yang^{14,#}, Jialin Mai ^{1,2,3,#}, Qianwen Gao^{1,2,3,15}, Xiaowei Xu¹⁴, Hongyu Kang¹⁴, Li Hou¹⁴, Yunfei Shang^{1,2,3}, Qiheng Qain^{1,2,3}, Jie Liu¹⁶, Meiye Jiang^{1,2,3}, Hao Zhang^{1,2,3}, Congfan Bu^{1,2}, Jinyue Wang¹⁷, Zhewen Zhang^{1,2}, Zaichao Zhang⁹, Jingyao Zeng^{1,2,#}, Jiao Li^{14,#}, Jingfa Xiao^{1,2,3,}

Brain Catalog: Siyu Pan^{2,3,13,#}, Hongen Kang^{2,3,13,#}, Xinxuan Liu^{2,13,18,#}, Shiqi Lin^{2,3,13}, Na Yuan^{2,13}, Zhang Zhang^{1,2,3}, Yiming Bao^{1,2,3}, Peilin Jia^{2,13,#}

Zhang^{1,2,3}, Yiming Bao^{1,2,3}, Peilin Jia^{2,13,#} CCAS: Xinchang Zheng^{1,2,#}, Wenting Zong^{1,2,3,#}, Zhaohua Li^{1,2,3,#}, Yanling Sun^{1,2,#}, Yingke Ma^{1,2}, Zhuang Xiong^{1,2,3}, Song Wu^{1,2,3}, Fei Yang^{1,2,3}, Wei Zhao^{1,2,3}, Congfan Bu^{1,2}, Zhenglin Du^{1,2}, Jingfa Xiao^{1,2,3,*}, Yiming Bao^{1,2,3,*} **BioProject & BioSample & GSA & BIG Submission:** Xu Chen^{1,2,#}, Tingting Chen^{1,2,#}, Sisi Zhang^{1,2,#}, Yanling Sun^{1,2,#}, Caixia Yu^{1,2}, Bixia Tang^{1,2}, Junwei Zhu^{1,2}, Lili Dong^{1,2}, Shuang Zhai^{1,2}, Yubin Sun^{1,2}, Qiancheng Chen^{1,2}, Xiaoyu Yang^{1,2} Xin Zhang^{1,2} Zhengqi Sang^{1,2} Vongcong Xiaoyu Yang^{1,2}, Xin Zhang^{1,2}, Zhengqi Sang^{1,2}, Yonggang Wang^{1,2}, Yilin Zhao^{1,2}, Huanxin Chen^{1,2}, Li Lan^{1,2}, Yan-qing Wang^{1,2,#} (TL), Wenming Zhao^{1,2,3,*} (TL)

OMIX: Anke Wang^{1,2,#}, Caixia Yu^{1,2,#}, Yanqing Wang^{1,2}, Sisi Zhang^{1,2,#} (TL)

GWH: Yingke Ma^{1,2,#}, Yaokai Jia^{1,2,#}, Xuetong Zhao^{1,2}, Meili Chen^{1,2,#} (TL)

GVM: Cuiping Li^{1,2,#}, Dongmei Tian^{1,2,#}, Bixia Tang^{1,2,#}, Yitong Pan^{1,2,3}, Lili Dong^{1,2}, Xiaonan Liu^{1,2,3}, Shuhui Song^{1,2,3,#} (TL)

GWAS Atlas: Xiaonan Liu^{1,2,3,#}, Dongmei Tian^{1,2,#}, Cuiping Li^{1,2,#}, Bixia Tang^{1,2}, Zhonghuang Wang^{1,2,3}, Rongqin Zhang^{1,2,3}, Yitong Pan^{1,2,3}, Yi Wang^{1,2,3}, Dong Zou^{1,2}, Shuhui Song^{1,2,3,#} (TL)

RCoV19: Cuiping Li^{1,2,#}, Dong Zou^{1,2,#}, Lina Ma^{1,2,3,#}, Zheng Gong^{1,2,3,#}, Junwei Zhu^{1,2}, Xufei Teng^{1,2,3}, Lun Li^{1,2}, Na Li^{1,2}, Ying Cui^{1,2,3}, Guangya Duan^{1,2,3}, Mochen Zhang^{1,2,3}, Tong Jin^{1,2,3}, Hailong Kang^{1,2,3}, Zhonghuang Wang^{1,2,3}, Gangao Wu^{1,2,3}, Tianhao Huang^{1,2,3}, Wei Zhao^{1,2,3}, Enhui Jin^{1,2,3}, Tao Zhang^{1,2,3}, Zhang Zhang^{1,2,3}, Wenming Zhao^{1,2,3}, Yongbiao Xue^{1,2,3}, Yiming Bao^{1,2,3,*} (TL), Shuhui Song^{1,2,3,#} (TL)

GEN: Tianyi Xu^{1,2,#}, Dong Zou^{1,2,#}, Ming Chen^{1,2,3,#}, Guangyi Niu^{1,2,3,#}, Rong Pan^{1,2,3}, Tongtong Zhu^{1,2,3}, Yuan Chu^{1,2,3}, Lili Hao^{1,2,#} (TL)

ICG: Jian Sang^{1,2,3,#}, Rong Pan^{1,2,3,#}, Dong Zou^{1,2,#}, Yuanpu Zhang¹⁹, Zhennan Wang²⁰, Ming Chen^{1,2,3}, Yuan-sheng Zhang^{1,2,3}, Tianyi Xu^{1,2}, Qiliang Yao²¹, Tongtong Zhu^{1,2,3}, Guangyi Niu^{1,2,3}, Lili Hao^{1,2,#} (TL)

EWAS Open Platform: Zhuang Xiong^{1,2,3,#}, Fei Yang^{1,2,3,#}. Guoliang Wang^{1,2,3,#}, Rujiao $Li^{1,2,3,#}$ (TL)

Guoliang Wang^{1,2,3,#}, Rujiao Li^{1,2,3,#}, Mochen Zhang^{1,2,3,#}, Dong Zou^{1,2,#}, Wei Zhao^{1,2,3,#}, Guoliang Wang^{1,2,3}, Fei Yang^{1,2}, Song Wu^{1,2,3}, Xinran Zhang^{1,2,3}, Xutong Guo^{1,2,3}, Yingke Ma^{1,2}, Zhuang Xiong^{1,2,3}, Rujiao Li^{1,2,3,#} (TL) **LncBook:** Zhao Li^{1,2,3,#}, Lin Liu^{1,2,#}, Changrui Feng^{1,2,3,#},

Yuxin Qin^{1,2,3}, Jingfa Xiao^{1,2,3}, Lina Ma^{1,2,3,#} (TL)

LucRNAWiki: Wei Jing^{1,2,3,#}, Sicheng Luo^{1,2,22,#}, Zhao Li^{1,2,3}, Lina Ma^{1,2,3,#} (TL)

Cell Taxonomy: Shuai Jiang^{1,2,#}, Qiheng Qian^{1,2,3,#}, Tongtong Zhu^{1,2,3,#}, Wenting Zong^{1,2,3}, Yunfei Shang^{1,2,3}, Tong Jin^{1,2,3}, Yuansheng Zhang^{1,2,3}, Ming Chen^{1,2,3}, Zis-han Wu^{1,2,3}, Yuan Chu^{1,2,3}, Rongqin Zhang^{1,2,3}, Sicheng Luo^{1,2,3}, Wei Jing^{1,2,3}, Dong Zou^{1,2}, Yiming Bao^{1,2,3}, Jingfa Xiao^{1,2,3,*} (TL), Zhang Zhang^{1,2,3,*} (TL)

Database Commons: Dong Zou^{1,2,#}, Lin Liu^{1,2,#}, Yuxin Qin^{1,2,3}, Sicheng Luo^{1,2,22}, Wei Jing^{1,2,3}, Qianpeng Li^{1,2,3}, Pei Liu⁴⁰, Yongqing Sun⁴⁰, Lina Ma^{1,2,3,#} (TL)

Writing Group: Shuai Jiang^{1,2}, Zhuojing Fan^{1,2}, Wen-ming Zhao^{1,2,3,*}, Jingfa Xiao^{1,2,3,*}, Yiming Bao^{1,2,3,*}, Zhang Zhang^{1,2,3,*}

CNCB-NGDC PARTNERS (Listed in alphabetical order by database names)

AnimalTFDB: Wen-Kang Shen²³, An-Yuan Guo²³

Animal I FDB: wen-Kang Shen 7, All-Tuan Guo BBCancer: Zhixiang Zuo²⁴, Jian Ren²⁴ CancerSEA: Xinxin Zhang²⁵, Yun Xiao²⁵, Xia Li²⁵ CellMarker: Xinxin Zhang²⁵, Yun Xiao²⁵, Xia Li²⁵ CGDB: Dan Liu²³, Chi Zhang²³, Yu Xue²³

CGGA: Zheng Zhao²⁶, Tao Jiang²⁶

circAtlas: Wanying Wu²⁷, Fangqing Zhao²⁷

CirFunBase: Xianwen Meng²⁸, Ming Chen²⁸

CPLM: Yujie Gou²³, Miaomiao Chen²³, Yu Xue²³

dbPSP & THANATOS: Di Peng²³, Yu Xue²³ **DEG & DoriC:** Hao Luo^{29,30,31}, Feng Gao^{29,30,31}

DrLLPS: Wanshan Ning²³, Yu Xue²³

eLMSG: Wan Liu⁵, Yunchao Ling⁵, Ruifang Cao⁵, Guoqing Zhang⁵

EPSD & WERAM: Yuxiang Wei²³, Yu Xue²³

EVAtlas: Chun-Jie Liu²³, An-Yuan Guo²³ **EVmiRNA:** Gui-Yan Xie²³, An-Yuan Guo²³ **GenTree:** Hao Yuan^{3,20}, Tianhan Su^{3,20}, Yong E. Zhang^{3,20,32}

GTDB: Chenfen Zhou⁵, Pengyu Wang⁵, Guoqing Zhang⁵

HCL: Yincong Zhou²⁸, Ming Chen²⁸, Guoji Guo³³

hTFtarget: Qiong Zhang²³, An-Yuan Guo²³

iEKPD: Shanshan Fu²³, Xiaodan Tan²³, Yu Xue²³

iPCD: Dachao Tang²³, Yu Xue²³ **iUUCD:** Weizhi Zhang²³, Yu Xue²³ **LeukemiaDB:** Mei Luo²³, An-Yuan Guo²³

InCAR: Yubin Xie²⁴, Jian Ren²⁴

IncRNASNP2: Ya-Ru Miao²³, An-Yuan Guo²³

MCA: Yincong Zhou²⁸, Ming Chen²⁸, Guoji Guo³³

MiCroKiTS: Xinhe Huang²³, Zihao Feng²³, Yu Xue²³ miRNASNP: Chun-Jie Liu²³, An-Yuan Guo²³

msRepDB: Xingyu Liao^{34,35}, Xin Gao³⁴, Jianxin Wang³⁵

PEA: Guiyan Xie²³, An-Yuan Guo²³

PceRBase: Chunhui Yuan²⁸, Ming Chen²⁸

PlantRegMap: Dechang Yang³⁶, Feng Tian³⁶, Ge Gao³⁶

Prantkegiviap: Dechang Fanger, Feng Fianer, Ge C PncStres: Wenyi Wu²⁸, Ming Chen²⁸ PTMD: Cheng Han²³, Yu Xue²³, Qinghua Cui^{37,38} RhesusBase: Chunfu Xiao³⁹, Chuan-Yun Li³⁹ RMVar: XiaoTong Luo²⁴, Jian Ren²⁴

SEECancer: Xinxin Zhang²⁵, Yun Xiao²⁵, Xia Li²⁵

SEGreg: Qing Tang²³, An-Yuan Guo²³

ZCURVE_CoVdb: Hao Luo^{29,30,31}, Feng Gao^{29,30,31}

*To whom correspondence should be addressed: Yongbiao Xue (ybxue@big.ac.cn).

Correspondence may also be addressed to Yim-Bao (baoym@big.ac.cn), Zhang Zhang ing (zhangzhang@big.ac.cn), Wenming Zhao (zhaowm@big.ac.cn), Jingfa Xiao (xiaojingfa@big.ac.cn), Shunmin He (heshunmin@ibp.ac.cn), Guoqing Zhang (gqzhang@picb.ac.cn), Yixue Li (yxli@sibs.ac.cn), Guoping Zhao (gpzhao@sibs.ac.cn) and Runsheng Chen (crs@ibp.ac.cn).

[#] The authors wish it to be known that, in their opinion, these authors should be regarded as Joint First Authors.

¹ National Genomics Data Center & CAS Key Laboratory of Genome Sciences and Information, Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing 100101, China

China National Center for Bioinformation, Beijing 100101, China

³ University of Chinese Academy of Sciences, Beijing 100049, China

⁴ National Genomics Data Center & Key Laboratory of RNA Biology, Center for Big Data Research in Health, Institute of Biophysics, Chinese Academy of Sciences, Beijing 100101, China

⁵ National Genomics Data Center & Bio-Med Big Data Center, Key Laboratory of Computational Biology, Shanghai Institute of Nutrition and Health, University of Chinese Academy of Sciences, Chinese Academy of Sciences, 320 Yueyang Road, Xuhui, Shanghai 200031, China

⁶ CAS-Key Laboratory of Synthetic Biology, CAS Center for Excellence in Molecular Plant Sciences, Institute of Plant Physiology and Ecology, Chinese Academy of Sciences, 300 Fenglin Road, Xuhui, Shanghai 200032, China Center for Quantitative Synthetic Biology, Institute of

Synthetic Biology, Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, Shenzhen, China

Guangdong Geneway Decoding Bio-Tech Co. Ltd, Foshan, 528316, China

Department of Biology, The University of Western Ontario, London, Ontario N6A 5B7, Canada

¹⁰ College of Tropical Crops, Hainan University, Haikou 570228, China

¹¹ Institute of Tropical Biosciences and Biotechnology, Chinese Academy of Tropical Agricultural Sciences, Haikou 571101, China

¹² Rubber Research Institute, Chinese Academy of Tropical Agricultural Sciences, Haikou 571101, China

¹³ CAS Key Laboratory of Genomic and Precision Medicine, Beijing Institute of Genomics, Chinese Academy of Sciences, Beijing 100101, China

¹⁴ Institute of Medical Information, Chinese Academy of Medical Sciences/Peking Union Medical College, Beijing 100020, China

¹⁵ Current address: Beijing Novogene Bioinformatics Technology Co. Ltd, Beijing 100000, China

¹⁶ North China University of Science and Technology Affiliated Hospital, Tangshan 063000, China

¹⁷ Institute of Biophysics, Chinese Academy of Sciences, Beijing 100101, China

¹⁸ School of Future Technology, University of Chinese Academy of Sciences, Beijing 100049, China

¹⁹ College of Computer Science Technology, Inner Mongolia Normal University, Hohhot 010010, China

²⁰ Key Laboratory of Zoological Systematics and Evolution and State Key Laboratory of Integrated Management of Pest Insects and Rodents, Institute of Zoology, Chinese Academy of Sciences, Beijing 100101, China

²¹ Department of Civil and Environmental Engineering, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, China

²² Sino-Danish College, University of Chinese Academy of Sciences, Beijing 100049, China

²³ MOE Key Laboratory of Molecular Biophysics, Hubei Bioinformatics and Molecular Imaging Key Laboratory, Center for Artificial Intelligence Biology, College of Life Science and Technology, Huazhong University of Science and Technology, Wuhan 430074, Hubei, China

²⁴ State Key Laboratory of Oncology in South China, Cancer Center, Collaborative Innovation Center for Cancer Medicine, School of Life Sciences, Sun Yat-sen University, Guangzhou 510060, China

²⁵ College of Bioinformatics Science and Technology, Harbin Medical University, Harbin, Heilongjiang 150081, China

²⁶ Beijing Neurosurgical Institute, Capital Medical University, Beijing 100070, China

²⁷ Beijing Institutes of Life Science, Chinese Academy of Sciences, Beijing 100101, China ²⁸ Department of Bioinformatics, College of Life Sciences; The First Affiliated Hospital, School of Medicine, Zhejiang University, Hangzhou 310058, China

²⁹ Department of Physics, School of Science, Tianjin University, Tianjin 300072, China

³⁰ Frontiers Science Center for Synthetic Biology and Key Laboratory of Systems Bioengineering (Ministry of Education), Tianjin University, Tianjin 300072, China

³¹ SynBio Research Platform, Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Tianjin 300072, China

³² CAS Center for Excellence in Animal Evolution and Genetics, Chinese Academy of Sciences, Kunming, Yunnan 650223, China

 ³³ Center for Stem Cell and Regenerative Medicine, Zhejiang University School of Medicine, Hangzhou, China
³⁴ Computational Bioscience Research Center (CBRC),

³⁴ Computational Bioscience Research Center (CBRC), Computer, Electrical and Mathematical Sciences and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal 23955, Saudi Arabia

³⁵ Hunan Provincial Key Lab on Bioinformatics, School of Computer Science and Engineering, Central South University, Changsha 410083, China

³⁶ State Key Laboratory of Protein and Plant Gene Research, School of Life Sciences, Biomedical Pioneering Innovative Center (BIOPIC) & Beijing Advanced Innovation Center for Genomics (ICG), Center for Bioinformatics (CBI), Peking University, Beijing 100871, China

³⁷ Department of Biomedical Informatics, School of Basic Medical Sciences, MOE Key Lab of Cardiovascular Sciences, Center for Noncoding RNA Medicine, Peking University, Beijing 100190, China

³⁸ Center of Bioinformatics, Key Laboratory for NeuroInformation of Ministry of Education, School of Life Science and Technology, University of Electronic Science and Technology of China, Chengdu, Sichuan 610054, China

³⁹ Beijing Key Laboratory of Cardiometabolic Molecular Medicine, Institute of Molecular Medicine, College of Future Technology, Peking University, Beijing, China

⁴⁰ Huazhong University of Science and Technology, Wuhan, Hubei 430074, China

Present address: Jian Sang, Division of Cancer Epidemiology and Genetics, National Cancer Institute, National Institutes of Health, Bethesda, MD 20892, USA.