

Resource Summary Report

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NCBI Structure

RRID:SCR_004218

Type: Tool

Proper Citation

NCBI Structure (RRID:SCR_004218)

Resource Information

URL: <http://www.ncbi.nlm.nih.gov/structure>

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Description: Database of three-dimensional structures of macromolecules that allows the user to retrieve structures for specific molecule types as well as structures for genes and proteins of interest. Three main databases comprise Structure-The Molecular Modeling Database; Conserved Domains and Protein Classification; and the BioSystems Database. Structure also links to the PubChem databases to connect biological activity data to the macromolecular structures. Users can locate structural templates for proteins and interactively view structures and sequence data to closely examine sequence-structure relationships. * Macromolecular structures: The three-dimensional structures of biomolecules provide a wealth of information on their biological function and evolutionary relationships. The Molecular Modeling Database (MMDB), as part of the Entrez system, facilitates access to structure data by connecting them with associated literature, protein and nucleic acid sequences, chemicals, biomolecular interactions, and more. It is possible, for example, to find 3D structures for homologs of a protein of interest by following the Related Structure link in an Entrez Protein sequence record. * Conserved domains and protein classification: Conserved domains are functional units within a protein that act as building blocks in molecular evolution and recombine in various arrangements to make proteins with different functions. The Conserved Domain Database (CDD) brings together several collections of multiple sequence alignments representing conserved domains, in addition to NCBI-curated domains that use 3D-structure information explicitly to define domain boundaries and provide insights into sequence/structure/function relationships. * Small molecules and their biological activity: The PubChem project provides information on the biological activities of small molecules and is a component of NIH's Molecular Libraries Roadmap Initiative. PubChem includes three databases: PCSubstance, PCBioAssay, and PCCompound. The PubChem data are linked to other data types (illustrated example) in the Entrez system, making it possible, for example, to retrieve information about a compound and then Link to its biological activity data, retrieve 3D protein structures bound to the compound and interactively view their active sites, and find biosystems that include the compound as a component. * Biological Systems: A

biosystem, or biological system, is a group of molecules that interact directly or indirectly, where the grouping is relevant to the characterization of living matter. The NCBI BioSystems Database provides centralized access to biological pathways from several source databases and connects the biosystem records with associated literature, molecular, and chemical data throughout the Entrez system. BioSystem records list and categorize components (illustrated example), such as the genes, proteins, and small molecules involved in a biological system. The companion FLink icon FLink tool, in turn, allows you to input a list of proteins, genes, or small molecules and retrieve a ranked list of biosystems.

Abbreviations: NCBI Structure

Resource Type: data or information resource, database

Keywords: macromolecule, conserved domain, protein classification, protein, small molecule, biological activity, molecule, biosystem, biological system, structure, gene, alignment, biomolecule, interaction, function, evolution, 3d spatial image, visualization, gold standard

Availability: Free, Public, Acknowledgement requested

Resource Name: NCBI Structure

Resource ID: SCR_004218

Alternate IDs: nlx_23947, r3d100010927

Alternate URLs: <http://www.ncbi.nlm.nih.gov/sites/entrez?db=structure>,
<https://doi.org/10.17616/R3PP7J>

Record Creation Time: 20220129T080223+0000

Record Last Update: 20260905T133123+0000

Ratings and Alerts

No rating or validation information has been found for NCBI Structure.

No alerts have been found for NCBI Structure.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 26 mentions in open access literature.

Listed below are recent publications. The full list is available at [Kravitz](#) .

Xu M, et al. (2024) Genome-wide analysis of the MYB gene family in pumpkin. *PeerJ*, 12, e17304.

Zhang J, et al. (2022) Potential antagonistic relationship of *fgf9* and *rspo1* genes in WNT4 pathway to regulate the sex differentiation in Chinese giant salamander (*Andrias davidianus*). *Frontiers in molecular biosciences*, 9, 974348.

Qi Q, et al. (2021) Cloning, expression and functional analysis of the desert hedgehog (*dhh*) gene in Chinese tongue sole (*Cynoglossus semilaevis*). *Gene expression patterns : GEP*, 39, 119163.

Fu X, et al. (2021) Identification and functional analysis of the perforin-1 like gene in disease resistance in half smooth tongue sole (*Cynoglossus semilaevis*). *Developmental and comparative immunology*, 122, 104135.

Gao BJ, et al. (2020) Subtilisin-like Pr1 proteases marking the evolution of pathogenicity in a wide-spectrum insect-pathogenic fungus. *Virulence*, 11(1), 365.

Nilsson J, et al. (2019) Human Leukocyte Antigen-Based Risk Stratification in Heart Transplant Recipients-Implications for Targeted Surveillance. *Journal of the American Heart Association*, 8(15), e011124.

Visentin J, et al. (2019) Measuring anti-HLA antibody active concentration and affinity by surface plasmon resonance: Comparison with the luminex single antigen flow beads and T-cell flow cytometry crossmatch results. *Molecular immunology*, 108, 34.

Goh GK, et al. (2019) Zika and Flavivirus Shell Disorder: Virulence and Fetal Morbidity. *Biomolecules*, 9(11).

Arenas AF, et al. (2019) Time-Frequency Approach Applied to Finding Interaction Regions in Pathogenic Proteins. *Bioinformatics and biology insights*, 13, 1177932219850172.

Moreno Amador ML, et al. (2019) A new microbial gluten-degrading prolyl endopeptidase: Potential application in celiac disease to reduce gluten immunogenic peptides. *PloS one*, 14(6), e0218346.

Meng L, et al. (2018) Molecular characterization and expression analysis of *strbp* in Chinese tongue sole (*Cynoglossus semilaevis*). *Theriogenology*, 118, 225.

Kourghi M, et al. (2018) Identification of Loop D Domain Amino Acids in the Human Aquaporin-1 Channel Involved in Activation of the Ionic Conductance and Inhibition by AqB011. *Frontiers in chemistry*, 6, 142.

Bergendahl LT, et al. (2017) Functional determinants of protein assembly into homomeric complexes. *Scientific reports*, 7(1), 4932.

Rasheed MA, et al. (2017) Comparative Genomics of *Mycoplasma bovis* Strains Reveals That Decreased Virulence with Increasing Passages Might Correlate with Potential Virulence-Related Factors. *Frontiers in cellular and infection microbiology*, 7, 177.

Galperin MY, et al. (2017) The 24th annual Nucleic Acids Research database issue: a look back and upcoming changes. *Nucleic acids research*, 45(D1), D1.

Guo H, et al. (2017) Molecular cloning and expression analysis of the aqp1aa gene in half-smooth tongue sole (*Cynoglossus semilaevis*). PloS one, 12(4), e0175033.

Wang Z, et al. (2016) Molecular Characterization and Functional Analysis of a Novel Calcium-Dependent Protein Kinase 4 from *Eimeria tenella*. PloS one, 11(12), e0168132.

Kennedy H, et al. (2016) Sudden Cardiac Death Due to Deficiency of the Mitochondrial Inorganic Pyrophosphatase PPA2. American journal of human genetics, 99(3), 674.

Martín-Gómez L, et al. (2014) Molecular characterisation of TNF, AIF, dermatopontin and VAMP genes of the flat oyster *Ostrea edulis* and analysis of their modulation by diseases. Gene, 533(1), 208.

Goh GK, et al. (2013) Prediction of Intrinsic Disorder in MERS-CoV/HCoV-EMC Supports a High Oral-Fecal Transmission. PLoS currents, 5.