

Resource Summary Report

Generated by [FDI Lab - SciCrunch.org](#) on Apr 30, 2025

MODELLER

RRID:SCR_008395

Type: Tool

Proper Citation

MODELLER (RRID:SCR_008395)

Resource Information

URL: <http://salilab.org/modeller/modeller.html>

Proper Citation: MODELLER (RRID:SCR_008395)

Description: Software tool as Program for Comparative Protein Structure Modelling by Satisfaction of Spatial Restraints. Used for homology or comparative modeling of protein three dimensional structures. User provides alignment of sequence to be modeled with known related structures and MODELLER automatically calculates model containing all non hydrogen atoms.

Resource Type: simulation software, software resource, topical portal, software application, portal, data or information resource

Keywords: comparative, protein, structure, modelling, satisfaction, spatial, restrain, homology, 3D, alignment, sequence, hydrogen, atom, cluster

Funding: Sandler Family Supporting Foundation ;
NIGMS R01 GM54762;
NIGMS P01 GM71790;
NIH P01 A135707;
NIGMS U54 GM62529;
IBM ;
Intel

Availability: Restricted

Resource Name: MODELLER

Resource ID: SCR_008395

Alternate IDs: nif-0000-30054

License URLs: https://salilab.org/modeller/download_installation.html

Record Creation Time: 20220129T080247+0000

Record Last Update: 20250430T055613+0000

Ratings and Alerts

No rating or validation information has been found for MODELLER.

No alerts have been found for MODELLER.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 5463 mentions in open access literature.

Listed below are recent publications. The full list is available at [FDI Lab - SciCrunch.org](#).

Basrai A, et al. (2025) Computational analyses of drug resistance mutations in katG and emb complexes in Mycobacterium tuberculosis. Proteins, 93(1), 359.

Alrouji M, et al. (2025) Virtual screening and molecular dynamics simulations identify repurposed drugs as potent inhibitors of Histone deacetylase 1: Implication in cancer therapeutics. PloS one, 20(1), e0316343.

Wang R, et al. (2025) Development of a recombinant Ang1 variant with enhanced Tie2 binding and its application to attenuate sepsis in mice. Science advances, 11(3), eads1796.

Zheng B, et al. (2025) Discovery of a heparan sulfate binding domain in monkeypox virus H3 as an anti-poxviral drug target combining AI and MD simulations. eLife, 13.

Escalera-Balsera A, et al. (2025) A rare haplotype of the GJD3 gene segregating in familial Meniere's disease interferes with connexin assembly. Genome medicine, 17(1), 4.

Lloyd AR, et al. (2025) In silico drug repurposing at the cytoplasmic surface of human aquaporin 1. PloS one, 20(1), e0314151.

Machado LA, et al. (2025) Engineering Protein Dynamics through Mutational Energy Landscape Traps. Journal of chemical information and modeling, 65(2), 517.

Tae HS, et al. (2025) Molecular determinants of the selectivity and potency of α -conotoxin Vc1.1 for human nicotinic acetylcholine receptors. *The Journal of biological chemistry*, 301(1), 108017.

Bheemireddy S, et al. (2025) Computational analysis of the effect of a binding protein (RbpA) on the dynamics of *Mycobacterium tuberculosis* RNA polymerase assembly. *PloS one*, 20(1), e0317187.

Xie S, et al. (2025) Molecular basis of the CYFIP2 and NCKAP1 autism-linked variants in the WAVE regulatory complex. *Protein science : a publication of the Protein Society*, 34(1), e5238.

Yu T, et al. (2025) Enhanced dynamic coupling in a nuclear receptor underlies ligand activity. *The Journal of biological chemistry*, 301(2), 108081.

Younus I, et al. (2025) A Structural Bioinformatics-Guided Study of Adenosine Triphosphate-Binding Cassette (ABC) Transporters and Their Substrates. *Membranes*, 15(1).

Bhattacharya S, et al. (2025) Conformational dynamics and multi-modal interaction of Paxillin with the Focal Adhesion Targeting Domain. *bioRxiv : the preprint server for biology*.

Hussain SFJ, et al. (2025) Molecular analysis of HPV16 and HPV18 oncogenes in oral squamous cell carcinoma: Structural, transcriptomic and in vitro insights. *Oncology letters*, 29(3), 115.

Uddin ME, et al. (2025) Identification and Characterization of a Protease Producing *Bacillus cereus* Strain From Tannery Waste for Efficient Dehairing of Goat Skin. *BioMed research international*, 2025, 7639181.

Singh S, et al. (2025) Molecular mechanisms underlying allosteric behavior of *Escherichia coli* DgoR, a GntR/FadR family transcriptional regulator. *Nucleic acids research*, 53(1).

Tani K, et al. (2025) A Native LH1-RC-HiPIP Supercomplex from an Extremophilic Phototroph. *Communications biology*, 8(1), 42.

Ali-Ahmad A, et al. (2025) Non-nucleosomal (CENP-A/H4)₂ - DNA complexes as a possible platform for centromere organization. *bioRxiv : the preprint server for biology*.

Chen H, et al. (2025) Impact of sodium alginate hydrogel containing bacteriophage peptides that specifically bind to the EtCab protein on the inhibition of *Eimeria tenella* infection. *Veterinary research*, 56(1), 18.

Shin Y, et al. (2025) *Mycobacterium tuberculosis* CrgA Forms a Dimeric Structure with Its Transmembrane Domain Sandwiched between Cytoplasmic and Periplasmic α -Sheets, Enabling Multiple Interactions with Other Divisome Proteins. *bioRxiv : the preprint server for biology*.