

Resource Summary Report

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PyRosetta

RRID:SCR_018541

Type: Tool

Proper Citation

PyRosetta (RRID:SCR_018541)

Resource Information

URL: <http://www.pyrosetta.org/>

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Description: Interactive Python based interface to Rosetta molecular modeling suite. Stand alone Python based implementation of Rosetta molecular modeling package that allows users to write custom structure prediction and design algorithms using major Rosetta sampling and scoring functions.

Synonyms: Python Rosetta

Resource Type: software resource, software application, standalone software

Defining Citation: [PMID:20061306](#)

Keywords: Molecular modeling, custom structure prediction, design algorithm, energy function, scoring function, bio.tools

Funding: NIGMS R01 GM73151;
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NSF 0846324

Availability: Free, Freely available

Resource Name: PyRosetta

Resource ID: SCR_018541

Alternate IDs: biotools:pyrosetta

Alternate URLs: <https://bio.tools/pyrosetta>

Record Creation Time: 20220129T080340+0000

Record Last Update: 20260731T043024+0000

Ratings and Alerts

No rating or validation information has been found for PyRosetta.

No alerts have been found for PyRosetta.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 20 mentions in open access literature.

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

Vanguru S, et al. (2025) To pack or not to pack: revisiting protein side-chain packing in the post-AlphaFold era. bioRxiv : the preprint server for biology.

Vanguru S, et al. (2025) To pack or not to pack: revisiting protein side-chain packing in the post-AlphaFold era. Briefings in bioinformatics, 26(3).

Riveros Maidana RLB, et al. (2025) Benchmarking Machine Learning Models for HIV-1 Protease Inhibitor Resistance Prediction: Impact of Data Set Construction and Feature Representation. Journal of chemical information and modeling, 65(19), 10037.

Roel-Touris J, et al. (2024) The structural landscape of the immunoglobulin fold by large-scale de novo design. Protein science : a publication of the Protein Society, 33(4), e4936.

Richards LS, et al. (2023) Cryo-EM Structure of a Human LECT2 Amyloid Fibril Reveals a Network of Polar Ladders at its Core. bioRxiv : the preprint server for biology.

Custodio JM, et al. (2023) Structural and physical features that distinguish tumor-controlling from inactive cancer neoepitopes. Proceedings of the National Academy of Sciences of the United States of America, 120(51), e2312057120.

Bhardwaj G, et al. (2022) Accurate de novo design of membrane-traversing macrocycles. Cell, 185(19), 3520.

Hickerson BT, et al. (2022) Host receptor-targeted therapeutic approach to counter pathogenic New World mammarenavirus infections. Nature communications, 13(1), 558.

Koehler Leman J, et al. (2021) Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature communications, 12(1), 6947.

Milighetti M, et al. (2021) Predicting T Cell Receptor Antigen Specificity From Structural Features Derived From Homology Models of Receptor-Peptide-Major Histocompatibility Complexes. Frontiers in physiology, 12, 730908.

Maguire JB, et al. (2021) XENet: Using a new graph convolution to accelerate the timeline for protein design on quantum computers. PLoS computational biology, 17(9), e1009037.

Julian AT, et al. (2021) 3DFI: a pipeline to infer protein function using structural homology. *Bioinformatics advances*, 1(1).

Pan X, et al. (2021) De novo protein fold families expand the designable ligand binding site space. *PLoS computational biology*, 17(11), e1009620.

Zheng Y, et al. (2020) Histone Deacetylase HDA9 and WRKY53 Transcription Factor Are Mutual Antagonists in Regulation of Plant Stress Response. *Molecular plant*, 13(4), 598.

Yang J, et al. (2020) Predicting the viability of beta-lactamase: How folding and binding free energies correlate with beta-lactamase fitness. *PloS one*, 15(5), e0233509.

Chowdhury R, et al. (2020) Computational biophysical characterization of the SARS-CoV-2 spike protein binding with the ACE2 receptor and implications for infectivity. *Computational and structural biotechnology journal*, 18, 2573.

Chowdhury R, et al. (2020) IPRO+/-: Computational Protein Design Tool Allowing for Insertions and Deletions. *Structure (London, England : 1993)*, 28(12), 1344.

Kurczynska M, et al. (2018) Automated method to differentiate between native and mirror protein models obtained from contact maps. *PloS one*, 13(5), e0196993.

Newman HA, et al. (2017) A high throughput mutagenic analysis of yeast sumo structure and function. *PLoS genetics*, 13(2), e1006612.

Gavenonis J, et al. (2014) Comprehensive analysis of loops at protein-protein interfaces for macrocycle design. *Nature chemical biology*, 10(9), 716.