

Resource Summary Report

Generated by SPARC SAWG on Jul 28, 2026

TOPOFIT Database

RRID:SCR_006936

Type: Tool

Proper Citation

TOPOFIT Database (RRID:SCR_006936)

Resource Information

URL: http://topofit.ilyinlab.org/topofit/topofit_db.php

Proper Citation: TOPOFIT Database (RRID:SCR_006936)

Description: THIS RESOURCE IS NO LONGER IN SERVICE, documented on August 26, 2016. The T-DB contains millions of structural alignments between all proteins in the PDB as of July 2005 found by the TOPOFIT method. Structural neighbors to the query protein structure can be retrieved by the PDB code and chain id. Pairwise or multiple structural alignments can be visualized in 3D with the FRIEND software. In the TOPOFIT method, similarity of protein structures is analyzed using three-dimensional Delaunay triangulation patterns derived from backbone representation. It has been found that structurally related proteins have a common spatial invariant part, a set of tetrahedrons, mathematically described as a common spatial sub-graph volume of the three-dimensional contact graph derived from Delaunay tessellation (DT). Based on this property of protein structures we present a novel common volume superimposition (TOPOFIT) method to produce structural alignments of proteins. The superimposition of the DT patterns allows one to uniquely identify a common number of equivalent residues in the structural alignment, in other words, TOPOFIT identifies a feature point on the RMSD/Ne curve, a topomax point, until which two structures correspond to each other including backbone and inter-residue contacts, while the growing number of mismatches between the DT patterns occurs at larger RMSD (Ne) after topomax point. The topomax point is present in all alignments from different protein structural classes; therefore, the TOPOFIT method identifies common, invariant structural parts between proteins. The TOPOFIT method adds new opportunities for the comparative analysis of protein structures and for more detailed studies on understanding the molecular principles of tertiary structure organization and functionality. It helps to detect conformational changes, topological differences in variable parts, which are particularly important for studies of variations in active/binding sites and protein classification.

Synonyms: T-DB

Resource Type: database, data or information resource

Availability: THIS RESOURCE IS NO LONGER IN SERVICE

Resource Name: TOPOFIT Database

Resource ID: SCR_006936

Alternate IDs: nif-0000-03569

Old URLs: <http://mozart.bio.neu.edu/topofit/>

Record Creation Time: 20220129T080238+0000

Record Last Update: 20260725T191143+0000

Ratings and Alerts

No rating or validation information has been found for TOPOFIT Database.

No alerts have been found for TOPOFIT Database.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We have not found any literature mentions for this resource.