Resource Summary Report

Generated by RRID on May 17, 2025

Structure modeling of 907 G protein coupled receptors in the human genome

RRID:SCR_008351
Type: Tool

Proper Citation

Structure modeling of 907 G protein coupled receptors in the human genome (RRID:SCR_008351)

Resource Information

URL: http://cssb.biology.gatech.edu/skolnick/files/gpcr/gpcr.html

Proper Citation: Structure modeling of 907 G protein coupled receptors in the human genome (RRID:SCR_008351)

Description: THIS RESOURCE IS NO LONGER IN SERVICE, documented on August 19,2019.Database of tertiary structural modeling results of threading assembly refinement (TASSER) method for all 907 G protein-coupled receptors (GPCRs) in human genome. All sequences were collected from GPCR database http://www.gpcr.org/7tm/ and http://www.expasy.org/cgi-bin/lists?7tmrlist.txt. Unlike traditional homology modeling approaches, TASSER modeling does not require solved homologous template structures; moreover, it often refines the structures closer to native. G protein-coupled receptors (GPCRs), encoded by about 5% of human genes, comprise the largest family of integral membrane proteins and act as cell surface receptors responsible for the transduction of endogenous signal into a cellular response. Although tertiary structural information is crucial for function annotation and drug design, there are few experimentally determined GPCR structures. To address this issue, we employ the recently developed threading assembly refinement (TASSER) method to generate structure predictions for all 907 putative GPCRs in the human genome. Unlike traditional homology modeling approaches, TASSER modeling does not require solved homologous template structures; moreover, it often refines the structures closer to native. These features are essential for the comprehensive modeling of all human GPCRs when close homologous templates are absent. Based on a benchmarked confidence score, approximately 820 predicted models should have the correct folds. The majority of GPCR models share the characteristic seven-transmembrane helix topology, but 45 ORFs are predicted to have different structures. This is due to GPCR fragments that are predominantly from extracellular or intracellular domains as well as database annotation

errors. Our preliminary validation includes the automated modeling of bovine rhodopsin, the only solved GPCR in the Protein Data Bank. With homologous templates excluded, the final model built by TASSER has a global C(alpha) root-mean-squared deviation from native of 4.6 angstroms, with a root-mean-squared deviation in the transmembrane helix region of 2.1 angstroms. Models of several representative GPCRs are compared with mutagenesis and affinity labeling data, and consistent agreement is demonstrated. Structure clustering of the predicted models shows that GPCRs with similar structures tend to belong to a similar functional class even when their sequences are diverse. These results demonstrate the usefulness and robustness of the in silico models for GPCR functional analysis. Sponsors: GPCR is funded by the University at Buffalo, Buffalo, New York.

Synonyms: GPCR

Resource Type: database, data or information resource

Keywords: endogenous, extracellular, family, functional, gene, cellular, couple, genome, gpcr, g protein, helix, homology, human, membrane, model, modeling, orf, protein, receptor, response, signal, structural, structural model, structure, template, tertiary, topology, transduction, transmembrane

Funding:

Availability: THIS RESOURCE IS NO LONGER IN SERVICE

Resource Name: Structure modeling of 907 G protein coupled receptors in the human genome

Resource ID: SCR_008351

Alternate IDs: nif-0000-25215

Record Creation Time: 20220129T080247+0000

Record Last Update: 20250517T055856+0000

Ratings and Alerts

No rating or validation information has been found for Structure modeling of 907 G protein coupled receptors in the human genome.

No alerts have been found for Structure modeling of 907 G protein coupled receptors in the human genome.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 3 mentions in open access literature.

Listed below are recent publications. The full list is available at RRID.

Veselkov K, et al. (2018) BASIS: High-performance bioinformatics platform for processing of large-scale mass spectrometry imaging data in chemically augmented histology. Scientific reports, 8(1), 4053.

Shiau JY, et al. (2017) Phytoagent Deoxyelephantopin and Its Derivative Inhibit Triple Negative Breast Cancer Cell Activity through ROS-Mediated Exosomal Activity and Protein Functions. Frontiers in pharmacology, 8, 398.

Dou D, et al. (2013) Novel selective and irreversible mosquito acetylcholinesterase inhibitors for controlling malaria and other mosquito-borne diseases. Scientific reports, 3, 1068.