Membranome: an active web site

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Motivation

Membrane proteins play key role in cell biology e.g. as ion channels, drug receptors, and solute transporters. It has been estimated that ∼25% of genes code for membrane proteins, and that ca. 50% of potential new drug targets are membrane proteins. Despite the central importance of membrane proteins, the number of high resolution structures (from X-ray diffraction and more recently from NMR) remains small but the literature about experimental data available is huge. Literature gives a large amount of disjointed information about this essential group of proteins that needs to be organized to give a direct access to the researcher. In order to ease the browse of experimental data we are preparing the "membranome" site. Membranome site will select, store and efficiently organize literature data about: - classification; - genomic and protein sequences; - expression, purification, crystallization and structure determination; - structure and function; - transmembrane regions predictions (if the structure is not available); - interactions between membrane proteins and the rest of cell components: ions, lipids, sugars, ligands, substrates, solvent, a variety of molecules and other proteins; - mutants, mutation technique, altered functionality and pathological consequences of mutations; - publication references.

Methods

Membranome site is suited with an http server (Apache 2), a web application server (Zope 8.0), a dbms (PostgreSQL 7.4). The host operating system is Gentoo Linux. Most scripts and several tools are being written in Python. The heuristics of the agent and an ancillary application server (acting as client for nested dynamic remote queries and as a second level server for the membranome site) are currently being implemented in haskell.

Results

The membranome site consists of a database, a web interface and a set of software agents. The site is built around software agents, which: o gather data interactively from a network of collaborators; o gather data automatically from existing public protein databases (especially dealing with membrane proteins and protein interactions); o gather data automatically from the literature; o filter information from any of these sources; o convert data according to an internal, source independent, structure; o build dynamical interfaces for the collaborators and the public-domain access. The software agents are currently under development. In a first stage the database, the web interface and the agents to gather data from existing databases are developed. At a later phase, an empirical search engine will be implemented, in order to automatically extract relevant information from online literature data-banks. In both stages, results will be evaluated through human expertise.

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