
OPMxplore

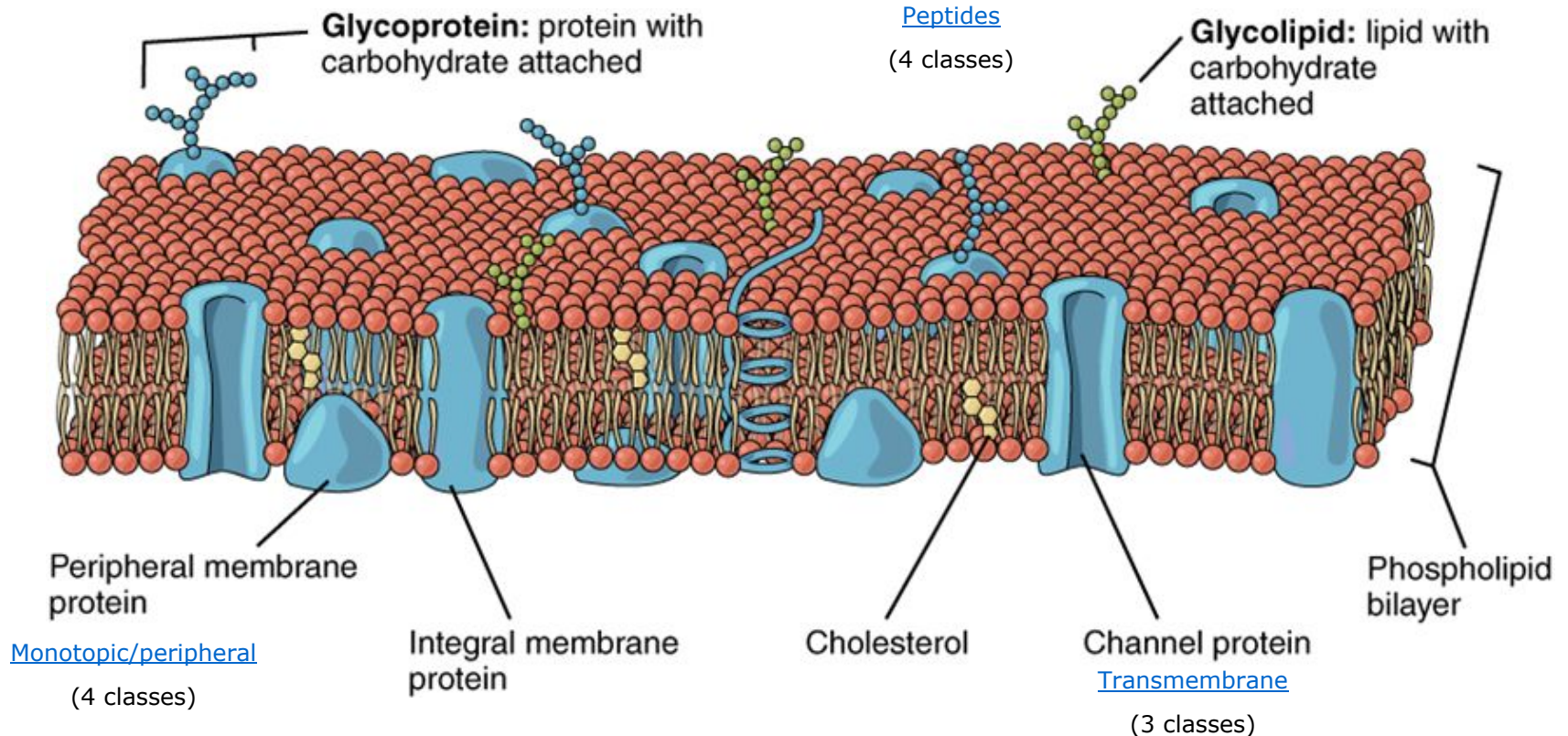
— Sinduja, David and Felcy —

Agenda

- Background
- Mission statement
- Data
- Users and Use Cases
- Project Structure
- Design
- Demo
- Lessons learned and future work

Background

Membrane Proteins



Protein Data Bank

RCSB PDB

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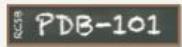


135787 Biological
Macromolecular Structures
Enabling Breakthroughs in
Research and Education

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EMDataBank
Verified Data Resource for 3D EM



NUCLEIC ACID
DATABASE



Worldwide
Protein Data Bank
Foundation



Welcome

A Structural View of Biology

This resource is powered by the Protein Data Bank
archive-information about the 3D shapes of proteins,

December Molecule of the Month

Orientation of Membrane Proteins (OPM)

← → ↻ opm.phar.umich.edu

orientations of (OPM) database
proteins in membranes

UNIVERSITY OF MICHIGAN | COLLEGE OF PHARMACY | LOMIZE GROUP

PDB ID or protein name Search OPM

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Protein Classification

- Types (3 types)
- Classes (11 classes)
- Superfamilies (474 superfamilies)
- Families (884 families)
- Species (745 species)
- Localization (24 types)
- All proteins in OPM (3622 proteins)

Orientations of Proteins in Membranes (OPM) database

OPM provides spatial arrangements of membrane proteins with respect to the hydrocarbon core of the lipid bilayer.

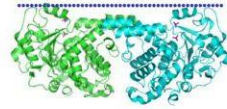
OPM includes all unique experimental structures of transmembrane proteins and some peripheral proteins and membrane-active peptides (Features).

Each protein is positioned in a lipid bilayer of adjustable thickness by minimizing its transfer energy from water to the membrane (Methods).

OPM provides structural classification and sorting according to different criteria (Classification).

Our calculations are in agreement with experimental studies of 24 transmembrane and 39 peripheral peptides and proteins (Comparison with Experiments).

For more information on single-spanning transmembrane proteins please see our [Membranome database](#)



4y71 » Myotubularin-related protein 8,

All proteins in OPM (3622 proteins)

Family	Protein Name	PDB ID	Species	Localization	Num. Subunits	Num. TM Sec. Structs.	Hydrophobic Thickness or Depth (Å)	Tilt Angle (°)	$\Delta G_{\text{transfer}}$ (kcal/mol)
1.1.01.01.	Archaeorhodopsin-2, trimeric	2ei4	<i>Halobacterium sp.</i>	Archaeobac.	3	21	30.5 ± 1.2	0 ± 1	-143.9
1.1.01.01.	Archaeorhodopsin-1	1uaz	<i>Halobacterium sp.</i>	Archaeobac.	1	7	31.8 ± 1.3	9 ± 2	-65.3
1.1.01.01.	Bacteriorhodopsin	5azd	<i>Thermus thermophilus</i>	Bact. Gram-neg inner	4	28	30.0 ± 0.5	3 ± 1	-121.3

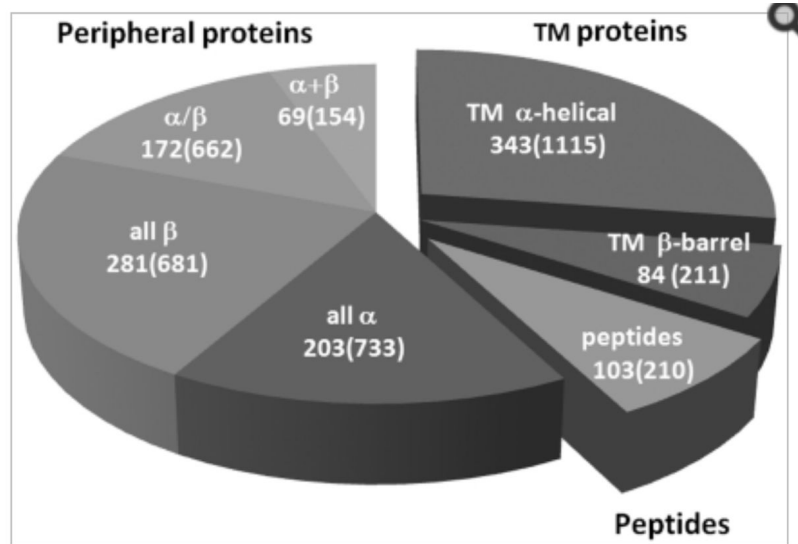
Mission Statement

Develop tools to:

- **Query the PDB/OPM database**
- **Identify relationships between different categories of membrane proteins**
- **Interactively visualize the results**

DATA

1. RCSB-PDB (135,787 experimentally determined protein structures)
2. OPM dataset (3622 membrane proteins)



Current distribution of different OPM entry types (as of 20 July 2011).

User and Use Cases

- Educational setting:
 - Interactive graph to intuitively explore properties of proteins of interest.
 - Research setting:
 - Researchers with basic python/jupyter notebook knowledge can ***query*** OPM database for computationally and experimentally derived measures and ***view*** statistical plots.
- User Interface : **Jupyter notebook** and visualizations on **Plotly Dash**.

Design

Components Design

1. **Convert database into str searchable format**
 - a. **Python: Sqlite3, pandasql, pypdb**
 - b. **Functions: load_data(), sql_query()**
 - c. **Specs: programmatic access to data and custom query**

2. **Interactive graphs based on database query**
 - a. **Python: Plotly, seaborn, ipywidgets**
 - b. **Functions: query_hash(), make_plot_*type*()**
 - c. **Specs: guided statistical plots and interactive discovery**

Components

1. Searching and displaying desired proteins:

- This will let the user search for desired list of membrane protein(s), usually with a generic name such as "channels" from PDB and match with the list of membrane proteins on OPM. The user will get a data frame with details such as PDBIDs, names of proteins, location of the membrane protein, membrane depth, tilt and transfer energy from water to the membrane.

2. Displaying data visualization:

- This will let the user view the basic statistical features of the desired group of proteins obtained in component 1.

3. Displaying 3D protein Visualization:

- This will let the user visualize 3D structure of a selected membrane protein from the list obtained in component 1.

4. User Interface:

- Building Plotly Dash to allow the user visualize the results from components 2 and 3.

Project Structure

GitHub Repository

UWSEDS-aut17 / OPMxplore

<> Code 1 Issues 3 Pull requests 0

uwseds-group-OPMxplore created by GitHub Clas

membrane-proteins pdb pdb-database Manage topic

80 commits 1 branch

Branch: master New pull request

fpDNA Delete github.py

OPMxplore	Migrated all of the files b
dev	all
doc	Delete github.py
examples	all
external_scripts	static plots, dynamic plots
.gitignore	Updated .gitignore to ger
LICENSE	Initial commit
README.md	Update README.md
requirements.txt	Added pdb-search.py, a n
setup.py	Migrated all of the files b

Python package folder

Branch: master OPMxplore / OPMxplore /

dstarkebaum Migrated all of the files based on the

..

data	Migrated all of the files t
tests	Migrated all of the files t
OPMxplore.py	Migrated all of the files t
__init__.py	Migrated all of the files t
version.py	Migrated all of the files t

Doc folder

Branch: master OPMxplore / doc /

fpDNA Delete github.py

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Component_design.md	ad
Functional_specification.md	mc
OPMpresentation.pdf	Ba
data.md	Mc

Required packages:

Standard tools:

numpy
scipy
matplotlib
pandas
sqlite3

Specialized analysis:

pypdb
biopython
biopandas

Visualization:

nglview
plotly
seaborn
ipywidgets
jupyter-notebook

Demo

Video of the demo: <https://youtu.be/8AhEcPVn3ac>

Lessons learned and Future Work

Lessons:

- ★ Cyclic Development Process
- ★ Data Munging
- ★ Git Branches

Road Map:

- ★ Stand Alone app for intuitively converging on proteins of interest
- ★ Integrate more computational tools to add to the database
 - Pore profile for channel like proteins

Thanks!

