OPRLM: A Web Tool and a Database for Positioning and Simulations of Proteins in Realistic Lipid Membranes ☆,☆☆

Sang-Jun Park [1], Kyle A. Schnitzer [2], Alexey Kovalenko [3], Stanislav Cherepanov [4], L. Ponoop Prasad Patro [5], Zigang Song [5], Irina D. Pogozheva [6], Andrei L. Lomize [6,*], and Wonpil Im [1,5,*]

*1 - **Department of Computer Science and Engineering,** Lehigh University, 111 Research Drive, Bethlehem, PA 18015, United States*

*2 - **Department of Electrical Engineering and Computer Science,** College of Engineering, University of Michigan, 1221 Beal Ave, Ann Arbor, MI 48109-2102, United States*

*3 - **Department of Computer Science,** College of Literature, Science, and the Arts, University of Michigan, 2260 Hayward Street, Ann Arbor, MI 48109-2121, United States*

*4 - **Biophysics Program,** University of Michigan, 930 N. University Avenue, Ann Arbor, MI 48109-1065, United States*

*5 - **Department of Biological Sciences,** Lehigh University, 111 Research Drive, Bethlehem, PA 18015, United States*

*6 - **Department of Medicinal Chemistry,** College of Pharmacy, University of Michigan, 428 Church St., Ann Arbor, MI 48109-1065, United States*

Correspondence to Andrei L. LomizeWonpil Im: Department of Biological Sciences, Lehigh University, 111 Research Drive, Bethlehem, PA 18015, United States (W. Im). *almz@umich.edu (A.L. Lomize), wonpil@lehigh.edu (W. Im)*

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Abstract

Molecular dynamics (MD) simulations in explicit lipid bilayers enable modeling of protein-lipid interactions essential for membrane protein functions and regulation. The newly developed computational web tool, OPRLM (**O**rientations of **P**roteins in **R**ealistic **L**ipid **M**embranes), automates the assembly of membrane protein structures with explicit lipids corresponding to 18 biological membrane types with symmetric or asymmetric lipid distributions, as well as 5 types of two-component lipid bilayers with varying cholesterol content. Built upon the CHARMM-GUI toolset and the PPM method, OPRLM simplifies the setup of complex simulation system involving integral and/or peripheral membrane proteins with explicit lipid mixtures and generates all necessary files for subsequent all-atom MD simulations. OPRLM has successfully generated protein-membrane systems for 286 tested protein structures in various biomembranes, including 138 structures containing ligands. The OPRLM database, an advanced successor of the OPM database, includes explicit protein-lipid systems for tested proteins in their native biomembranes. It provides coordinates of integral and peripheral membrane proteins from the Protein Data Bank embedded in planar or curved implicit lipid bilayers. Additionally, it includes the classification of proteins into types, superfamilies, and families, along with the information on intracellular localizations and membrane topology and visualization options. The OPRLM web tool and the database are publicly accessible at https://oprlm.org.

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☆☆ Link to resource: https://www.oprlm.org.

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Introduction

Biological membranes create protective barriers for living cells and their intracellular compartments. These membranes are composed of numerous lipid types[1–3] and are populated with diverse membrane proteins, including membrane-spanning transmembrane (TM) proteins, permanently embedded (from one side) monotopic proteins, and temporarily associated peripheral proteins. Lipid membranes form unique anisotropic environments for these proteins, where various lipids modulate membrane protein structure and function through specific or non-specific protein-lipid interactions.[4] Understanding the structure and dynamics of membrane proteins within their native membrane environment is essential for elucidating the molecular mechanisms underlying their folding, stability, function, and regulation.

Recent progress in structure determination techniques, such as X-ray crystallography, NMR spectroscopy, and cryo-electron microscopy (cryo-EM), have led to an almost exponential growth of the number of three-dimensional (3D) structures of membrane proteins and their complexes deposited in databases,[5] such as RCSB PDB,[6] EMDataBank,[7] and related resources. Despite this progress, the spatial positions of proteins within membranes are not immediately apparent from experimental 3D structures and require computational analysis.

Several computational methods have been developed to determine positioning of proteins in implicit membranes, including PPM,[8–10] Memembed,[11] Ez-3D,[12–14] and TMDET.[15,16] Our PPM[8–10] method optimizes protein positions in membranes by minimizing their transfer energy from water to the non-polar membrane environment. The latest version, PPM 3.0,[10] offers a significant advantage over other methods by calculating orientations of TM and peripheral proteins not only in planar membranes but also in curved and multiple membranes. The results of PPM 3.0 calculations for membrane proteins with known 3D structures are regularly deposited into the well-recognized OPM database.[9,17]

However, the key limitation of the current PPM method is the membrane approximation by an implicit lipid model. This model combines the polarity profiles of a 1,2-dioleoyl-*sn*-glycero-3-phosphatidylcholine (DOPC) bilayer with a variable bilayer thickness and a penalty for a hydrophobic mismatch. Such a simplistic membrane representation does not capture the complex lipid composition of natural biomembranes[1–3] or specific protein-lipid interactions, which can only be observed in explicit protein-membrane systems. To address this limitation, we have developed the OPRLM web tool for an automated construction of multicomponent membrane systems composed of membrane proteins and explicit lipids from various biomembranes. The tool also generates all necessary files for molecular dynamics (MD) simulations. The OPRLM web tool, publicly accessible from the OPRLM database at https://oprlm.org, allows researchers to better understand membrane protein interactions in realistic membrane environments.

OPRLM Web Tool

A new OPRLM web tool has been developed based on the widely used CHARMM-GUI pipeline[18] and the PPM 2.0 method.[10] This tool simplifies the setup of protein-membrane systems for all-atom MD simulations using pre-defined 18 biomembranes[19] and 5 types of two-component lipid bilayers with variable cholesterol content. OPRLM allows users to pack explicit lipids around any experimental or modeled protein structure. The tool is directly linked to the OPRLM database, which includes membrane protein structures from the RCSB PDB[6] database with pre-oriented position in their primary location membrane.

OPRLM web interface

The OPRLM web server offers a simple, streamlined web interface for users to download the atomic coordinate files of existing protein entries from the RCSB PDB and OPRLM databases or upload custom files from their computers for modeling protein with explicit lipids suitable for MD simulations (Figure 1). Users can select either the asymmetric unit or the biological assembly for each PDB protein entry. The biological assembly is created based on the transformation matrix in the PDB file header. The NGL viewer[20] provides a visual depiction of the atomic coordinates, while protein chains, N- or O-linked glycans, and hetero-ligands are listed in a table. For all selected hetero chains from RCSB PDB or OPRLM entries, the server systematically retrieves associated SDF files from the RCSB PDB database for each ligand and handles non-standard amino acid residue and post-translational modification that are supported by CHARMM-GUI.[21–25] A custom PDB file must be supplemented with each ligand's proper SDF file. Users can specify the membrane type, protein topology in a membrane ("in" or "out" position of the first protein chain N-terminus relative to the membrane sides), subunits to be included in modeling, system size in the XY membrane plane, water layer thickness above and below the membrane or protein, ion types and concentrations, requirement for CHARMM minimization, and input option for MD simulations. In other words, the multiple building steps of CHARMM-GUI Membrane Builder[26,27] are simplified in one page (and its consequent advantages and limitations are elaborated below).

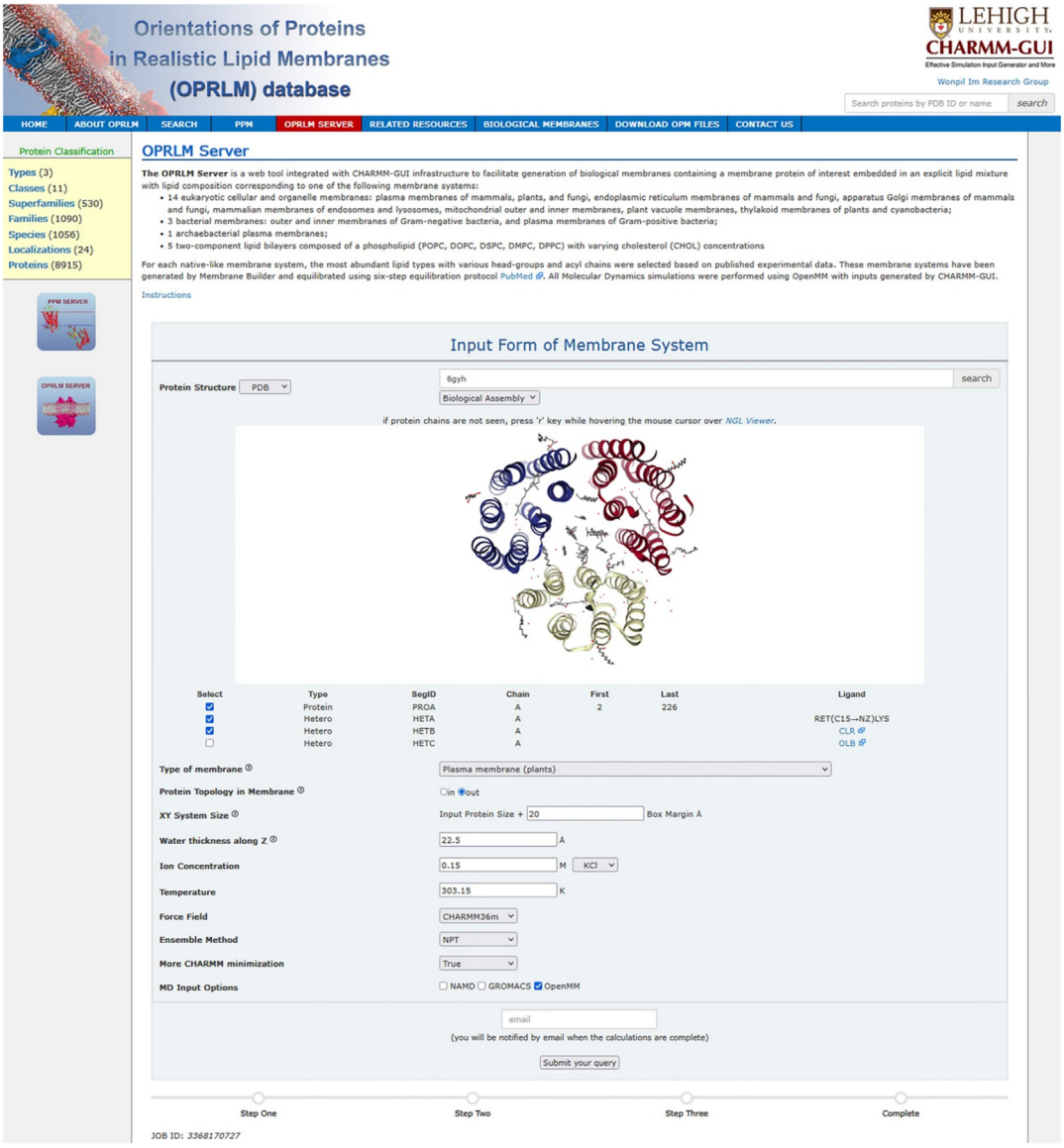

Figure 1. The web interface of the OPRLM web server integrated in the OPRLM database (https://oprlm.org/oprlm_server).

OPRLM supports 18 types of biomembranes: 14 eukaryotic cellular and organelle membranes, (such as mammalian, plant, and fungal plasma membranes, mammalian and fungal endoplasmic reticulum and apparatus Golgi membranes, mammalian endosomal and lysosomal membranes, mitochondrial outer and inner membranes, plant vacuole membranes, thylakoid membranes of plants and cyanobacteria), Gram-negative bacteria (*E. coli*) outer and inner membranes, and Gram-positive bacteria and archaebacteria cell membranes.[19] OPRLM also offers custom two-component membrane system composed of a phospholipid, such as DOPC, 1-palmitoyl-2-oleoyl-*sn*-glycero-3-phosphatidylcholine (POPC), 1,2-distearoyl-*sn*-glycero-3-phosphatidylcholine (DSPC), 1,2-dimyristoyl-*sn*-glycero-3-phosphatidylcholine (DMPC), or 1,2-dipalmitoyl-*sn*-glycero-3-phosphatidylcholine (DPPC), with varying cholesterol (CHOL) concentrations (Figure 1).

The system size in the XY membrane plane is mainly depends on the protein size and the user-defined box margin, with a default margin of 20 Å corresponding to 2–3 lipid layers. The water thickness setting determines the system size along the Z-axis, specifying the thickness of the bulk water layer from the protein or membrane boundaries. For ion modeling, users can set the concentration of selected ions (KCl, NaCl, $CaCl_2$, and $MgCl_2$). Note that only the CHARMM36 force field (FF) is supported in OPRLM with NPT (constant particle number, pressure, and temperature) production ensemble. An optional

CHARMM minimization runs 400 minimization steps to remove major steric hindrances before equilibration process. OPRLM generates input files for MD programs, such as NAMD, GROMACS, and OpenMM. Users can monitor the progress of OPRLM computations from the web interface after submitting the input form. Upon completion of calculations, users will receive email notifications with a link to downloadable files. The user-friendly interface makes the OPRLM web tool handy for non-experts and experimentalists.

OPRLM server workflow

The workflow of OPRLM for protein-membrane construction integrates a series of CHARMM-GUI pipeline components, as shown in Figure 2. This backend process includes the CHARMM-GUI *PDB Reader and Manipulator*,[21] *Membrane Builder*,[26,27] *Ligand Reader and Modeler*,[28] and *FF-Converter and Input Generator*.[29] The module enables users to model protein chains, nucleic acids, carbohydrates, and ligands using the CHARMM FF. All protein residues and organic molecules supported by the CHARMM FF are documented on the CHARMM-GUI archive (https://www.charmm-gui.org/docs/archive/csml). For ligands not supported by the CHARMM FF, the CHARMM General Force Field (CGenFF) program[30] is used to generate necessary topologies and parameters. OPRLM also utilizes the default settings of CHARMM-GUI *PDB Reader and Manipulator* to select terminal groups for each protein chain and to form disulfide bonds and other post-translational modifications.

To determine the orientation of the input protein in a membrane, we use PPM 2.0, except for the input coordinate file obtained directly from the OPRLM database. After orientation, the dimensions of the XY plane are calculated based on the size of the protein structure with an added user-specified margin to ensure sufficient space between the protein and the simulation box boundaries. Using the protein areas calculated in the previous step and the cross-sectional areas per lipid molecules, the numbers of molecules for each lipid type are determined to construct a system with the specific size in the XY plane. A specific lipid ratio composition table of 18 biomembranes (https://www.charmm-gui.org/docs/archive/biomembrane) is used to achieve the appropriate lipid composition for the user-specified biomembrane type.

To generate a protein-membrane system, pseudo-atoms that mimic lipid head groups are

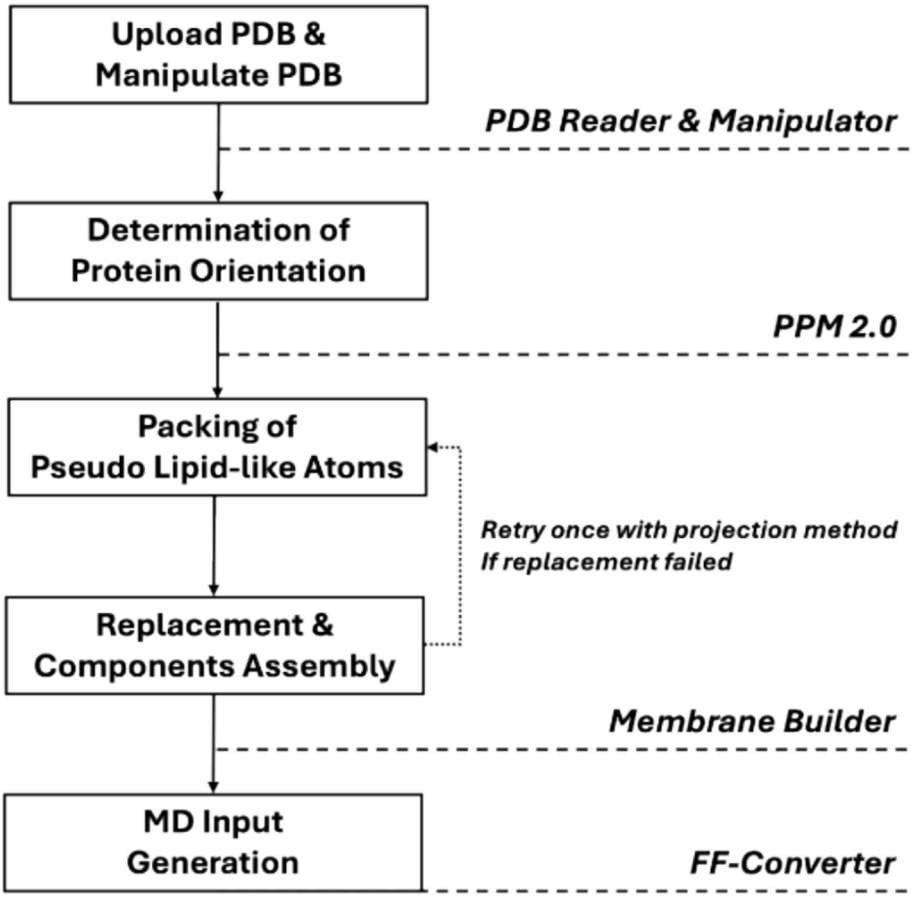

Figure 2. OPRLM workflow of protein-membrane system construction.

first placed on the membrane surface (typically ±12 Å along the *Z*-axis) to define lipid head group positions packed around a protein. The pseudo-atoms are subsequently replaced by the corresponding all-atom lipid structures from the lipid conformation library. If the replacement step failed due to bad contacts between protein and lipids (Figure S1), the current workflow reiterates the placement of the pseudo-atoms by applying a "projection method" to avoid the bad contact between the protein and surrounding lipids. This method makes the projection of protein atoms onto the XY plane at the membrane surface to consider a protein shape above or below the membrane surface (Figure S1). Upon successful replacement, interactions between lipid tails and sterol ring structures, aromatic side chains, carbohydrate groups, and protein surfaces are reevaluated, with necessary adjustments made to avoid clashes or ring penetration. Other components such as ions and water are then integrated into the membrane system once the replacement is successful. Finally, the topology and input files required for equilibration and production MD simulations are generated.

Testing and Application of the OPRLM Web Tool to Membrane Proteins

The dataset used for testing the OPRLM web tool includes 286 membrane protein entries from RCSB PDB representing different protein families residing in various biomembranes (Table S1). Most structures in the dataset were resolved using X-ray crystallography. The biologically relevant assembly and oligomeric form of each individual protein or a complex was usually generated automatically by applying the symmetry transformation provided in the corresponding PDB file. However, in a number of cases, the proper functional assembly was generated manually by taking the asymmetric unit and selecting certain chains or using structures from the OPRLM database (Table S2). We used the default values of a 20 Å box margin for the XY dimensions, a 22.5 Å water thickness for the Z dimension, and a KCl concentration of 0.15 M. We found that various errors may arise due to complex lipid composition or ligand reading. Therefore, three series of tests were conducted using an automated script.

Test 1: Ligand-free proteins in two-component lipid bilayers

The applicability of the OPRLM web server was initially evaluated using simple lipid bilayers consisting of 80% POPC and 20% CHOL. Among the 286 RCSB PDB entries tested, 20 have glycosylated residues, 179 structures include one or more ligands, while 107 structures contain no ligands. In this test, all structures were modeled without ligands and glycans. Overall, all 286 protein structures were successfully modeled in the simple two-component lipid bilayers.

Test 2: Ligand-free proteins in 18 types of biomembranes

The performance of OPRLM for multicomponent biological membranes was evaluated using 18 native-like membranes and the same set of 286 protein entries as for Test 1 (see Table S1 for their native membrane type of each protein). In Test 2, 238 protein-lipid systems were successfully modeled using the original lipid packing method (without protein projection). Some errors occasionally occurred during the replacement step because some pseudo-atom spheres were too closely packed near proteins, making it impossible to replace them by all-atom lipid structures due to too many protein-lipid clashes. Therefore, the 46 protein-membrane systems among the remaining 47 protein entries were successfully constructed using the projection method after the original packing method failed (Figure S1). Both methods failed only for the large TM pore formed by gasdermin A3 (PDB ID: 6cb8) in a Gram-negative bacterial outer membrane, although it was successfully inserted into a simple two-component bilayer.

Test 3: Proteins with ligands in biomembranes

The performance of the OPRLM web tool for modeling proteins with ligands was tested for 179 PDB entries containing at least one ligand (excluding detergents and solvents). In this set, the automatic parametrization of ligands failed for 41 PDB entries, accounting for 23% of complexes in this set. These errors generally fall into two categories. The first type is related to a failure of the CGenFF program to parameterize certain molecules (Table S3). CGenFF automatically assigns atom types, bond parameters (bond lengths, angles, and dihedrals), and charges based on its chemical structure and sets up the FF parameters by analogy with previously parameterized molecules. However, CGenFF may fail to parameterize ligand containing rare atoms, such as rubidium (RB), cadmium (CD), or tungstate (VI) (WO4) ions, as well as compounds with coordinated metals such as derivatives of porphyrins, chlorins, bacteriochlorins, and corrins (e.g., HEA, HEC, CLA, BLC, CNC), or Fe-S clusters (e.g., FES, F3S, SF4). The second type of errors occurs when the coordinates of heterochains in the PDB file do not match the topology and parameter files generated by the CGenFF program (Table S4). This discrepancy arises because the CGenFF input is based on ideal SDF files downloaded from RCSB, while the actual Cartesian coordinates of the heterochains

are taken from the PDB file. Mismatches may also occur if the PDB file has missing atoms in the heterochains.

For 179 protein entries containing ligands, the protein-membrane systems were generated for the corresponding native membranes. Among them, there were 10 proteins structures with N- or O-glycosylated residues. Only for three protein entries (PDB IDsL 4k1c, 6lkd, and 6sek, see Table S1), incorporation of ligands prevented the modeling of protein-lipid systems in biomembranes. Therefore, these proteins were modeled in POPC/CHOL (8:2) bilayers.

Advantages and Limitations of the OPRLM web tool

The OPRLM web tool is an efficient and user-friendly platform for constructing explicit protein-lipid systems using 18 predefined types of biomembranes.[19] It builds molecular systems utilizing several well-established and validated programs and tools: CHARMM GUI *PDB Reader and Manipulator*,[21] *Membrane Builder*,[31] *Ligand Reader and Modeler*,[28] *FF-Converter*[32], *and Input Generator*,[29] CGenFF,[30] and PPM.[10] OPRLM effectively arranges explicit lipids around membrane proteins using the original lipid packing method. Occasional clashes between proteins and lipids are resolved using the protein projection method.

The OPRLM server has several advantages. First, it allows for the quick and easy generation of complex membrane systems with native-like lipid compositions and distributions between leaflets (Figure S3). The 18 membrane systems encompass a variety of uncommon membrane-specific lipids, such as various sphingolipids from mammalian membranes, essential glycerol-based glycolipids from plant and bacterial thylakoid membranes (*e.g.*, monogalactosyldiacylglycerol, digalactosyldiacylglycerol, and sulfoquinovosyl-dia cylglycerol), ergosterol from yeast and diverse phytosterols from plant membranes *(e.g.*, stigmasterol, campesterol, and sitosterol), unique lipopolysaccharides from the outer membranes of Gram-negative bacteria (*e.g.*, lipid A of *E. coli*), lipids with branched side chains and cyclic moieties from bacterial membranes, and diether lipids with phytanyl side chains from archaebacterial membranes. The OPRLM web tool successfully generated native-like membrane systems for all tested proteins without errors. However, while it is convenient for users to operate with predefined membrane compositions, the server is currently limited to these predefined 18 native-like membranes and five types of lipids for building two-component lipid-cholesterol membranes. For generating protein-membrane systems with customized lipid composition, users can directly use the CHARMM-GUI platform,[18] which requires a more significant effort and expertise.

Second, OPRLM web tool operates not only with membrane protein entries from RCSB PDB or OPRLM databases but also with user-generated structures of individual membrane proteins or their complexes. Third, OPRLM is a unique tool that allows generating protein models with ligands. It accommodates ligands such as glycans and ions through parameterization by the CGenFF program. However, during testing, OPRLM successfully modeled only 77% of proteins with ligands; in other cases, ligand parameterization by CGenFF failed. Users are also advised to check the penalty scores in the provided ligand topology file to ensure the validity of ligand parameterizations. Finally, the OPRLM web tool employs the CHARMM-GUI *FF-Converter and Input Generator*[29] to provide input files for MD simulations compatible with major molecular simulation programs, including NAMD, OpenMM, and GROMACS.

As mentioned above, the OPRLM web tool employs a second packing method of pseudo spheres with protein projection, when some pseudo spheres in the first packing trial are too closely packed near protein to be replaced by all-atom lipid structures due to too many protein-lipid bad contacts. The protein projection generally works well for a cylindrical protein shape with similar protein area in the TM region and above and below the membrane. However, when the protein area above or below the membrane is much larger than the TM region, the projected protein ends up occupying a large membrane area into which pseudo lipid atoms could not pack. In this case, too many pseudo lipid atoms packed too tightly in the reaming lipid accessible area, causing the replacement failure due to too many lipid-lipid bad contacts. We strongly recommend users to check “step3_packing.pdb” to visualize any issues during the packing and use the CHARMM-GUI platform with more protein orientation options that may solve the issues.

The OPRLM Database

The OPRLM (**O**rientations of **P**roteins in **R**ealistic **L**ipid **M**embranes) is the successor to the OPM database.[9] This new database represents a significant advancement by providing access to atomic-level protein models with explicit lipids that mimic native-like membranes (Figure 1). Similar to OPM, the OPRLM database includes experimental structures of TM, peripheral membrane proteins, and membrane-interacting peptides from the RCSB PDB[6]. These proteins are oriented with respect to flat or curved lipid bilayers by PPM 3.0.[10] OPRLM provides structural classification of proteins into families and superfamilies, protein topology, preferred intracellular localization, and calculated parameters of spatial positioning within membranes.

OPRLM offers several features for the comparative analysis of membrane-associated proteins, including options for browsing, sorting, searching, and visualization. Users can display images for all proteins within a specific family, superfamily, or membrane type simultaneously. The advanced search function supports precise queries using keywords, PDB IDs, UniProt entry names, membrane types, species, taxons, families, superfamilies, number of helices, subunits, TM secondary structures, membrane thickness, and transfer energies to membranes.

For interactive visualization, the database provides four web-based 3D viewers: iCn3D,[33] LiteMol,[34] GLmol,[35] and JMol.[36] The database also includes links to related web resources, such as RCSB PDB,[6] PDBsum,[37] MSD (PDBe),[38] TCDB,[39] UniProt,[40] and EncoMPASS.[41] It also presents a web interface for the PPM,[10] the TMPfold,[42] and the OPRLM web tools. The OPRLM database currently (as of November 2024) contains 16,873 protein entries (including 10,312 TM proteins, 5,247 peripheral proteins, and 1,314 peptides) from 24 membrane types across 1,056 organisms. The coordinate files for 286 explicit protein-membrane systems of tested proteins, mainly in corresponding biomembranes, have been included in the OPRLM database (Figure 3).

Incorporating new PDB entries into the OPRLM database involves several steps: assigning protein families, determining membrane topology and intracellular localization, identifying biological species, orienting proteins within lipid bilayers, and constructing explicit membrane-protein systems. To streamline this process, we have developed Python scripts that gather this information from the RCSB PDB and the UniProt databases. These scripts match newly released PDB structures with existing OPRLM entries using common UniProt and InterPro IDs, as well as sequence and structural alignments. By matching the new PDB entries with structures in OPRLM, we facilitate the classification of proteins into types, superfamily, and families, along with the assignment of membrane topology and localization. Additional scripts help position the new protein structures within membranes using PPM 3.0, generate corresponding figures and database tables, and create explicit lipid-protein systems for specified entries.

Comparison of the OPRLM Database With Other Resources

PDBTM[43] and MemProtMD[44] are two well-recognized databases that provide calculated spatial arrangements of proteins within lipid bilayers. However, these databases are focused principally on TM proteins. In contrast, OPRLM, like its parent OPM database, includes TM, monotopic and peripheral membrane proteins and peptides. While PDBTM presents the orientations of TM proteins only within a flat lipid bilayer, MemProtMD shows the local membrane deformations in planar membranes with TM proteins. Both OPM and OPRLM, however, offer spatial positions for integral and peripheral membrane proteins within flat, curved, or multiple membranes.

OPRLM and MemProtMD share the similar motivation: developing a reliable computational approach to explicitly model the membrane environment and collect 3D structures of membrane protein oriented within lipid bilayers in a database. The OPRLM database surpasses the capabilities of MemProtMD by offering more comprehensive data sets of membrane proteins and their complexes within various biomembranes. Each protein entry in OPRLM has a link to an integrated web tool for constructing explicit protein-membrane systems suitable for MD simulations. Additionally, 286 protein entries have been precomputed in explicit, native-like biomembranes and included to the OPRLM database; 138 of these entries also contain ligands, ions, and cofactors identified in experimental structures (Table S1, Figure 3). It is anticipated that the number of automatically generated explicit protein-membrane systems in the OPRLM database will grow over time.

Currently (as of July 2024), the MemProtDB database contains a significantly larger collection of precomputed TM proteins embedded in explicit lipid bilayers, totaling 7,792 TM proteins assembled with a DPPC bilayer by the MemProtMD pipeline.[45] However, the database has notable limitations, as it excludes protein ligands and cofactors, employs only one type of lipid, and omits large protein complexes (such as photosystems I and II), peripheral proteins, and membrane-associated peptides. Unlike MemProtDB, the OPRLM database does not have these limitations. Furthermore, the MemProtDB pipeline is not publicly available and does not allow calculation of custom proteins in user-defined membrane environments, unlike the OPRLM web tool.

Both OPRLM and MemProtDB databases provide atomic coordinates for membrane-protein systems and the necessary files for setting up all-atom MD simulations. However, MemProtMD exclusively uses the GROMACS simulation program, whereas OPRLM generates files compatible with various simulation programs, including NAMD, GROMACS, and OpenMM.

Implementation

The OPRLM utilizes a modified version of the OPM database leveraging the Ruby on Rails server-side web application framework and the PostgreSQL database management system for its backend, which is hosted at Lehigh University. The frontend application was developed using

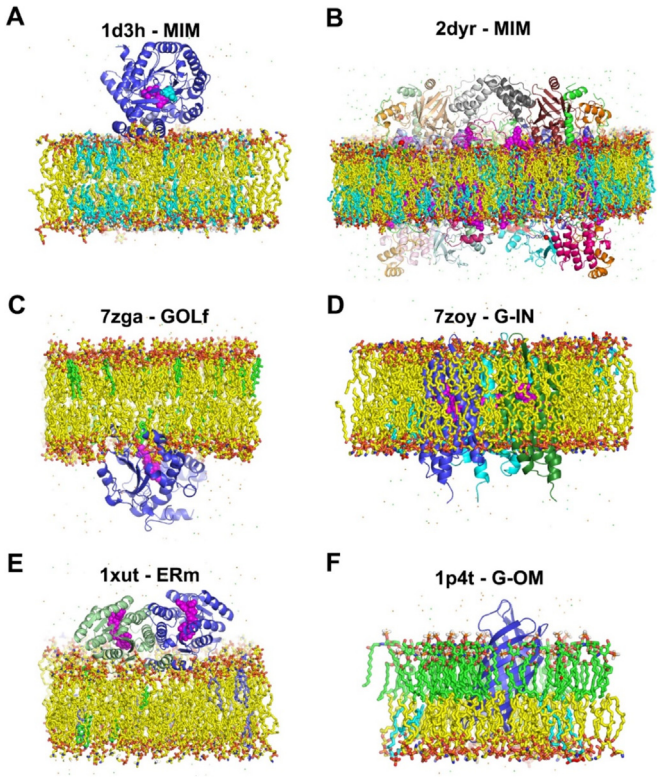

Figure 3. Examples of OPRLM-generated protein-membrane systems for monotopic/peripheral (**A, C, E**) and TM (**B, D, F**) proteins with ligands. Protein subunits are shown by cartoon colored differently for different subunits, ligands are shown by spheres, lipids are shown by sticks with color indicated for lipid tails. (**A**) Human dihydroorotate dehydrogenase (PDB ID: 1d3h) in a mitochondrial inner membrane (MIM) with 3 ligands: FMN (purple), A26 (light blue), and ORO (cyan). Phospholipids (PLs) are colored yellow, and cardiolipins (CLs) are colored cyan. **(B)** Bovine mitochondrial cytochrome *c* oxidase composed of dimer of 10-mers (PDB ID: 2dyr) in MIM; 4 ligands (CHD, CDL, PGV, TGL) are colored purple, 4 ions (CU, ZN, MG, NA) are colored red, PLs are colored yellow, and CLs are colored cyan. (**C**) Yeast phosphatidylinositol transfer protein Sec14p (PDB ID: 7zga) with ergoline (IUF, colored purple) in a fungal Golgi membrane (GOLf); PLs are colored yellow, and sterols (CHL1) are colored green. (**D**) Halorhodopsin trimer from *Synechocystis* sp. (PDB ID: 7zoy) in a Gram-negative bacteria inner membrane (G-IN). The covalently bound ligand (RET) is colored purple, PL are colored yellow, and CL are colored cyan. (**E**) Human corticosteroid 11-beta-dehydrogenase dimer (PDB ID: 1xu7) in a mammalian endoplasmic reticulum membrane (ERm); PL are colored yellow, sterols (CHL1) are colored green, sphingomyelins (SMs) are colored blue. (**F**) Outer membrane protein NspA from *Neisseria meningitidis* (PDB ID: 1p4t) in a Gram-negative bacterial outer membrane (G-OM). Lipid A (ECLI) is colored green, PLs are colored yellow, and CLs are colored cyan.

ReactJS. Certain database assets, such as static protein images and protein coordinate files, are stored on the Google Cloud platform. The application can also be built and run locally, using the source code from GitLab for both backend[47] and frontend.[48] There is also a dependency on the Membranome database,[46] which is also on GitLab: backend[49] and frontend.[50] The OPRLM web server can execute up to eight jobs in parallel. The time required for building the protein-membrane system by the OPRLM web tool ranges from 10 to 60 min.

Usage statistics

N/A (n.b., it has not been open to the public yet).

Authors contributions

Sang-Jun Park: Development of the OPRLM web server, paper writing.

Kyle A. Schnitzer: Development of the OPRLM website.

Alexey Kovalenko: Development and automated update of OPRLM database.

Stanislav Cherepanov: Web server testing, automated update of the OPRLM database.

L. Ponoop Prasad Patro: Web server testing, automated update of the OPRLM database.

Zigang Song: Web server testing, automated update of the OPRLM database.

Irina D. Pogozheva: Funding acquisition, paper writing.

Andrei L. Lomize: Funding acquisition, supervision, web server testing, project administration, paper writing, corresponding.
Wonpil Im: Funding acquisition, supervision, project administration, paper writing, corresponding author.

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Resource Maintenance

This resource will be maintained and updated during more than 3 years by the lab of Dr. Im (Lehigh University).

CRediT authorship contribution statement

Sang-Jun Park: Data curation, Methodology, Software, Visualization, Writing – original draft, Writing – review & editing. **Kyle A. Schnitzer:** Data curation, Methodology, Software. **Alexey Kovalenko:** Data curation, Methodology, Software. **Stanislav Cherepanov:** Data curation, Software, Validation. **L. Ponoop Prasad Patro:** Data curation, Software, Validation. **Zigang Song:** Data curation, Software. **Irina D. Pogozheva:** Funding acquisition, Validation, Writing – original draft, Writing – review & editing. **Andrei L. Lomize:** Data curation, Funding acquisition, Methodology, Project administration, Supervision, Writing – original draft, Writing – review & editing. **Wonpil Im:** Funding acquisition, Project administration, Supervision, Writing – review & editing.

DATA AVAILABILITY

All data are shared in the website

DECLARATION OF COMPETING INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary material

Supplementary material to this article can be found online at https://doi.org/10.1016/j.jmb.2025.168966.

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