Epithelial Modelling Platform: A Tool for Investigating Hypotheses through Discovery and Assembly of Computational Models of Epithelial Transport

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Background

Scientists often leverage computational models of biological systems to investigate hypotheses which are difficult or prohibitively expensive to achieve experimentally. Such investigations are best achieved by utilizing suitable computational models, reusing existing validated models where possible and creating novel models consistently as needed. This requires tools which enable the discovery and exploration of existing models matched with assistance in constructing and testing new models. Enabling biomedical engineers to use such a tool by allowing them to describe their requirements in a manner familiar to them greatly improves the utility of the tool. This tool is not quite ready for pure biologists or clinicians to use.

We have developed a web-based tool, the Epithelial Modelling Platform, for discovery of relevant models and assemble them into a novel model customized for investigating their hypotheses. While our tool specifically focuses on epithelial transport, by utilizing relevant community standards and publicly accessible knowledge repositories, it is extensible to other areas of application. The platform abstracts underlying mathematics of the computational models and provides a visual environment which mimics biophysical phenomena of an epithelial cell.

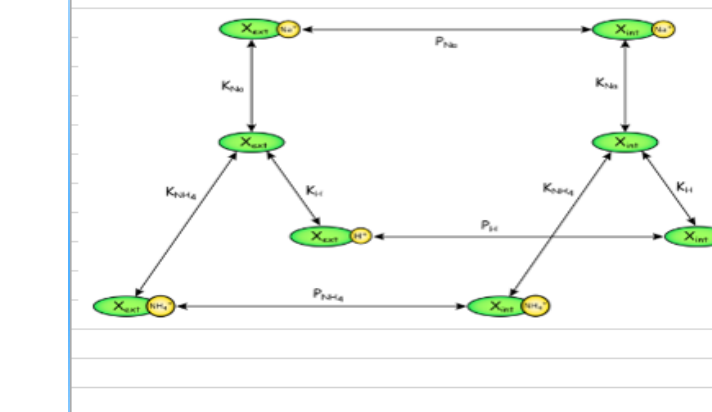Presented below is an overview of our knowledge management platform being developed and utilized in this work.
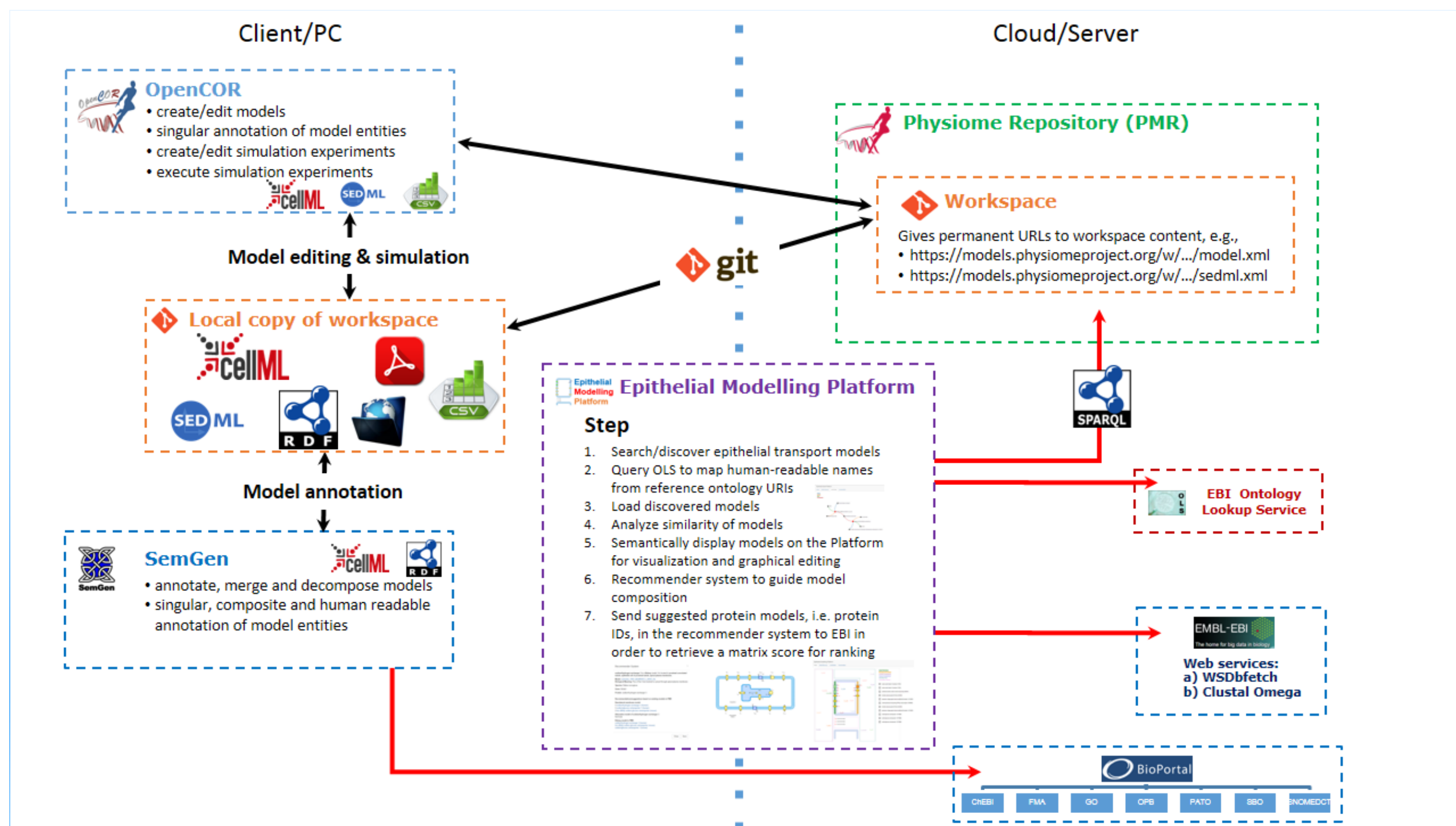
### This poster at
figshare

Model Annotation

The figure below presents some of the information with which we have enriched a cohort of kidney models meta-data in the form of semantic annotations available in the Physiome Model Repository (PMR). In particular, we extracted each of the mathematical variables from the models and associated them with a biologically meaningful knowledge.

Model Discovery

Utilizing these biological annotations, we are able to frame queries to PMR using biologically relevant terms. Our prototype web interface presents the search results obtained from querying the PMR services with the biological context; including models of similar biology and a recommender system.

https://github.com/dewancse/model-discovery-tool
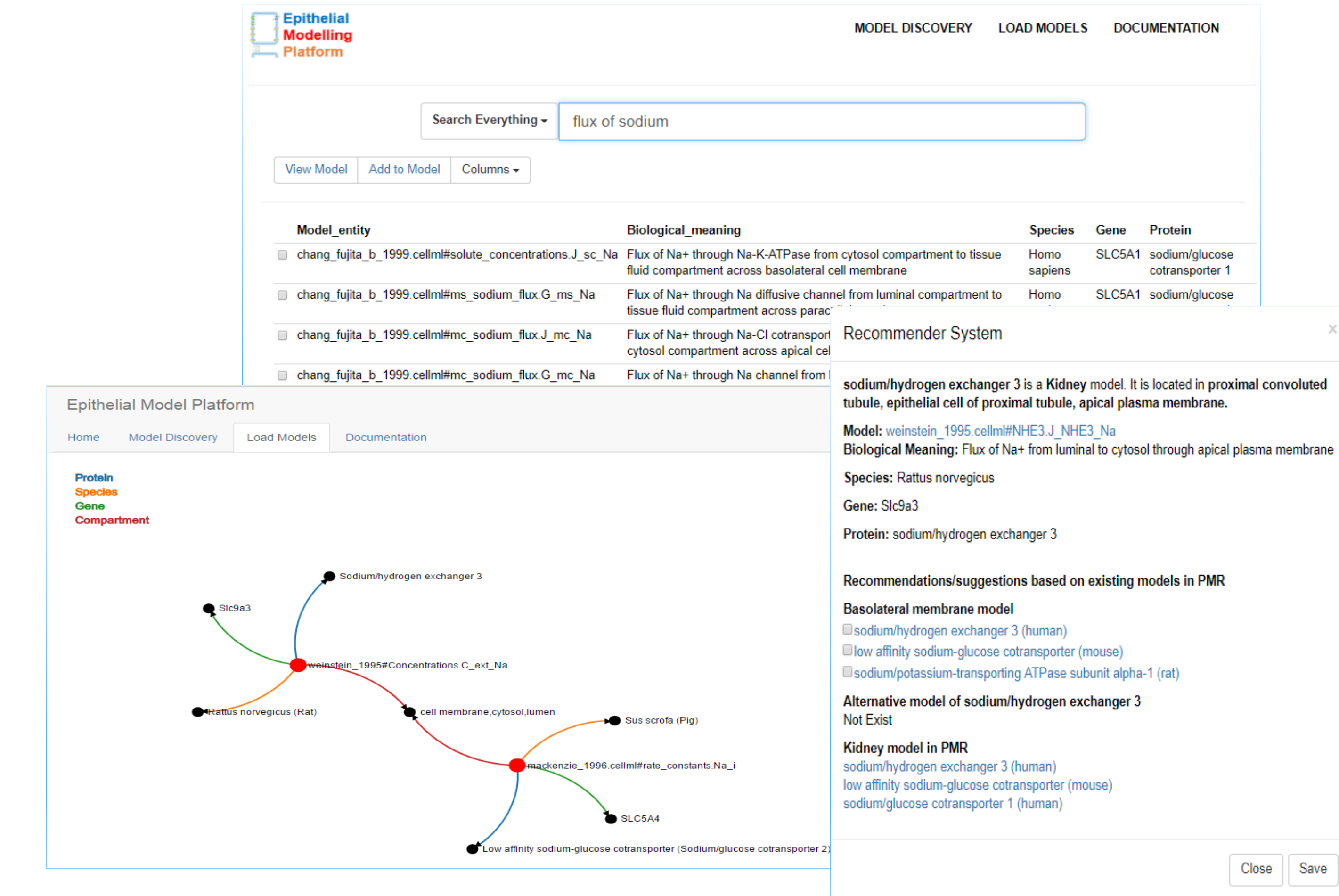
Modeling Platform

Presented on the top-right column is the web-based epithelial modelling platform to discover, explore and assemble models where users would be able to create and verify new epithelial models. This platform allows users to drag and drop models between apical and basolateral membranes. Solutes, e.g. sodium, potassium, will be floating in specific compartments. Modelers and clinicians can use this platform to build models to help investigate specific research questions and hypotheses.

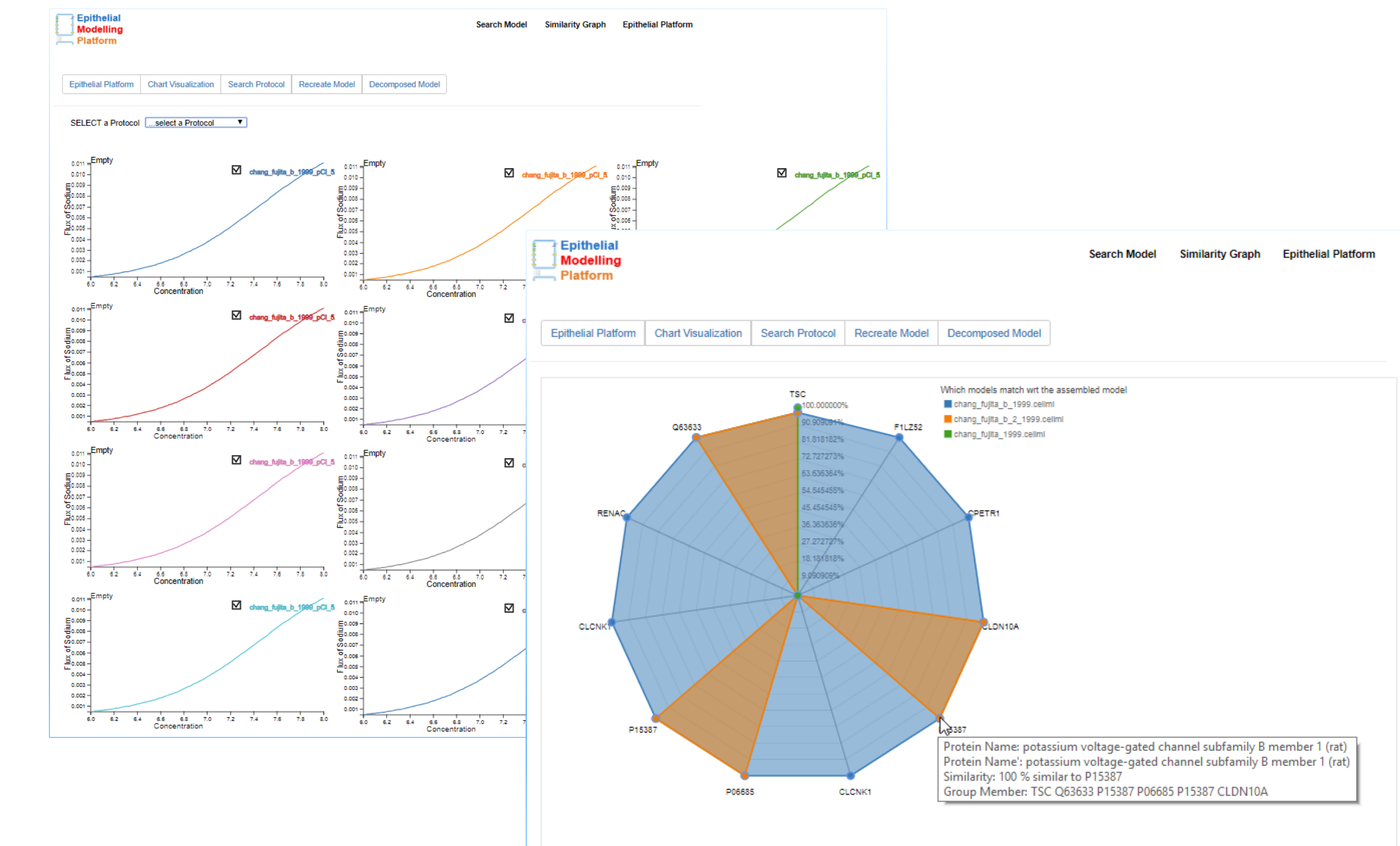https://github.com/dewancse/epithelial-modelling-platform
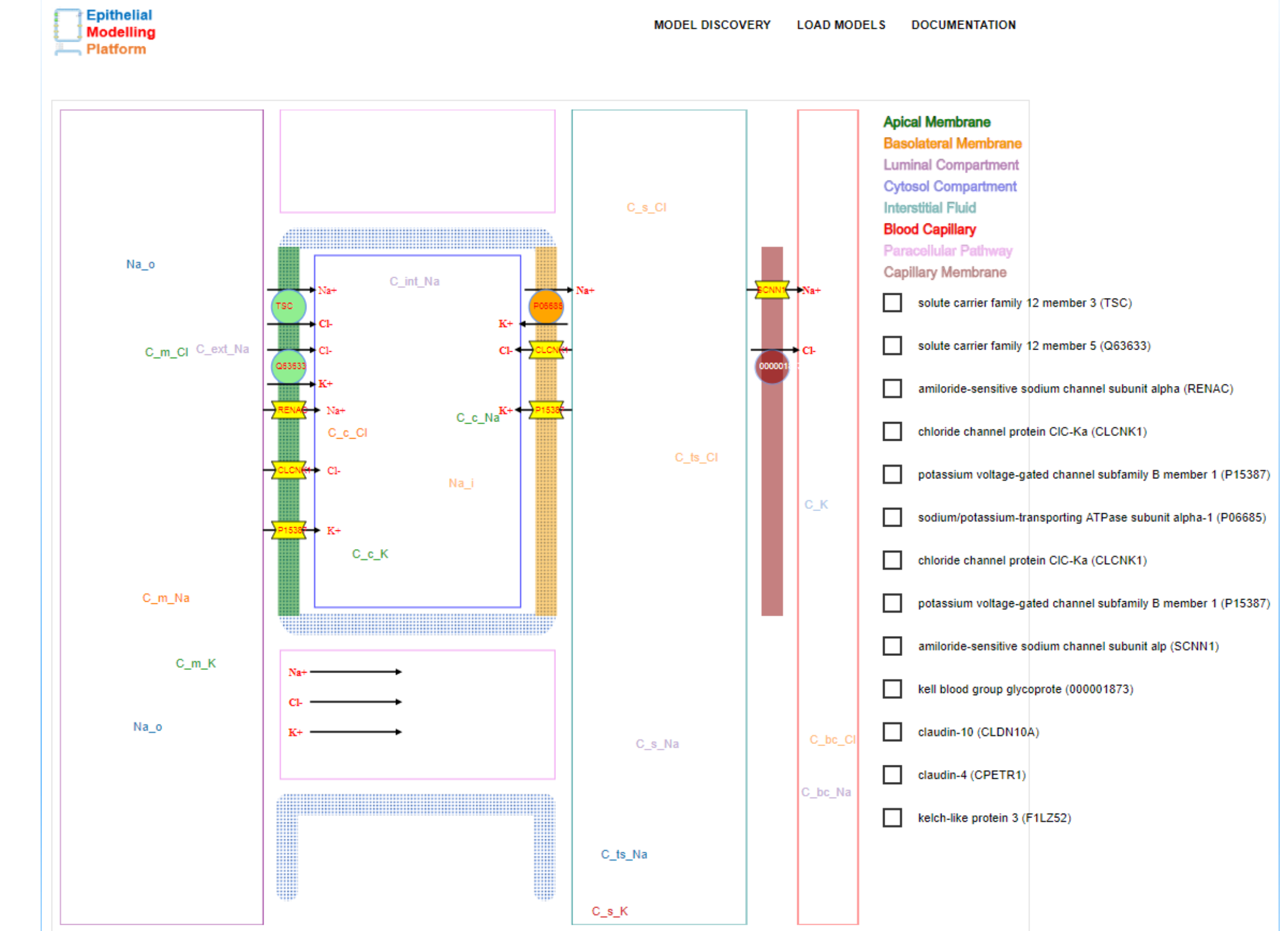
Model Composition

Once a user is satisfied with the model built and graphically edited using our platform, they will then be able to generate a novel model meeting their requirements. Utilizing the modularity and reuse capabilities of CellML, we are able to create a new CellML model by directly reusing and customizing the existing models discovered by the user.

Model Verification

For testing purpose, we have begun implementing a verification system which allows users to discover simulation experiments which match the features of the novel models users create. By executing these simulation experiments with the novel models and comparing to previous model predictions and/or experimental or clinical observations we are able to provide the user with some measure of verification that their model matches, or doesn't match, existing knowledge captured in the various repositories utilized.