

Database of Models for Ligand-Receptor Binding in Electronic Exchange Formats

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ABSTRACT

Cells need to respond to their environment. Cellular responses to environmental changes are often mediated by cell surface receptors, which generate signals when they interact with ligands. Models for many types of ligand-receptor interactions have been formulated [1]. These models are essential for understanding receptor-mediated cellular responses to environmental changes, as ligand-receptor binding is the first step in receptor signaling. To aid researchers studying receptor signaling, we are developing a database of models for ligand-receptor binding [2]. Models are encoded in electronic exchange, XML (Extensible Markup Language)-based formats, such as SBML and MathML. Models in these formats can be downloaded and used in application software, such as Jarnac, Maple or Mathematica, to perform calculations. The database provides access to such models in different XML-based formats, which enables one to perform calculations with these models using different application programs that are compliant with the XML formats provided. The database facilitates the development of models for receptor signaling which incorporate ligand-receptor binding, and the exchange of such models. The database is searchable. It includes a full description for each model, encodings in different formats, sample calculations, and downloadable XML and FORTRAN codes to use with different applications.

The database provides tools for

- ① search for a model by keywords or references
- ① view model description
- ① view graphical model description
- ① view references
- ① view mathematical description (governing differential equations and steady state equations)

- ① view sample computations and plots
- ① download different XML encodings of the model
- ① download FORTRAN code for computations

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REFERENCES

[1] <http://www.t10.lanl.gov/?http://cellsignaling.lanl.gov>

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The screenshot shows a web browser window displaying the 'Database' page for 'Model ID: 1: Monovalent Ligand/Monovalent Receptor Binding'. The page features a navigation menu on the left with links for 'Welcome', 'Home', 'Team', 'Models', 'Tools', 'Contact us', and 'Developers part'. The main content area includes a chemical reaction diagram showing a ligand (L) binding to a receptor (R) to form a complex (B). Below the diagram are three buttons: 'Download SBML code', 'Download MathML code', and 'View Model expression'. A 'Full Description' section follows, citing 'Douglas A. Lauffenburger and Jennifer J. Linderman (1993) Receptors: Models for Binding, Trafficking, and Signaling, Ch. 4, Oxford University Press (ISBN: 0195106666)'. The description states: 'This model is the simplest model for Ligand-Receptor binding on a cell surface: Monovalent Ligand binds to a Monovalent Receptor. We consider ligand and receptor each with one site, no diffusion effects. The dynamics of Ligand-Receptor Binding is given by the set of reactions L+R -> B with forward rate constant k_f B -> L+R with reverse rate constant k_r. The following variables are used in the model Variable Definitions L number of free ligands'.