RuleBuilder 1.0

Getting Started Guide

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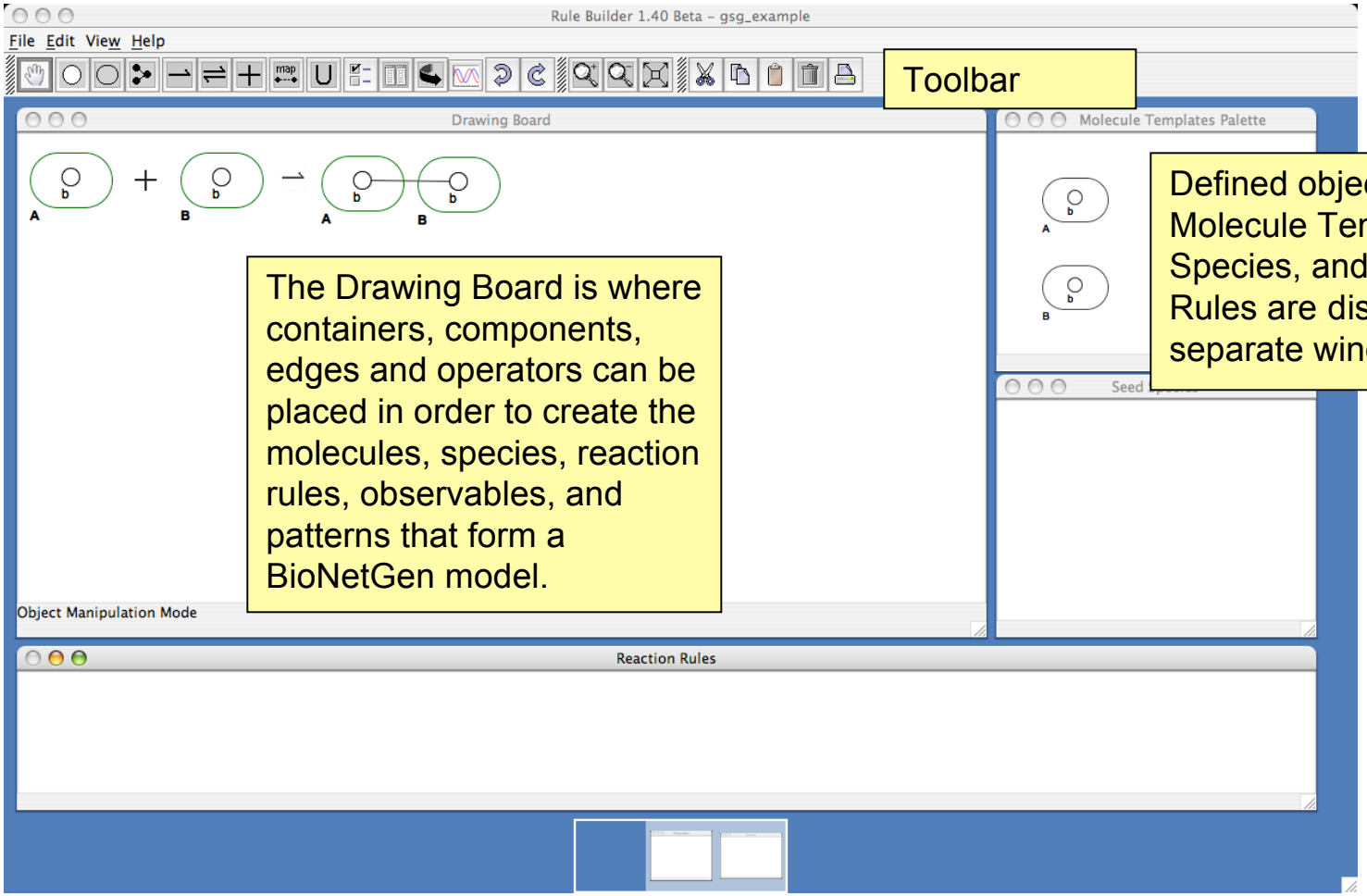
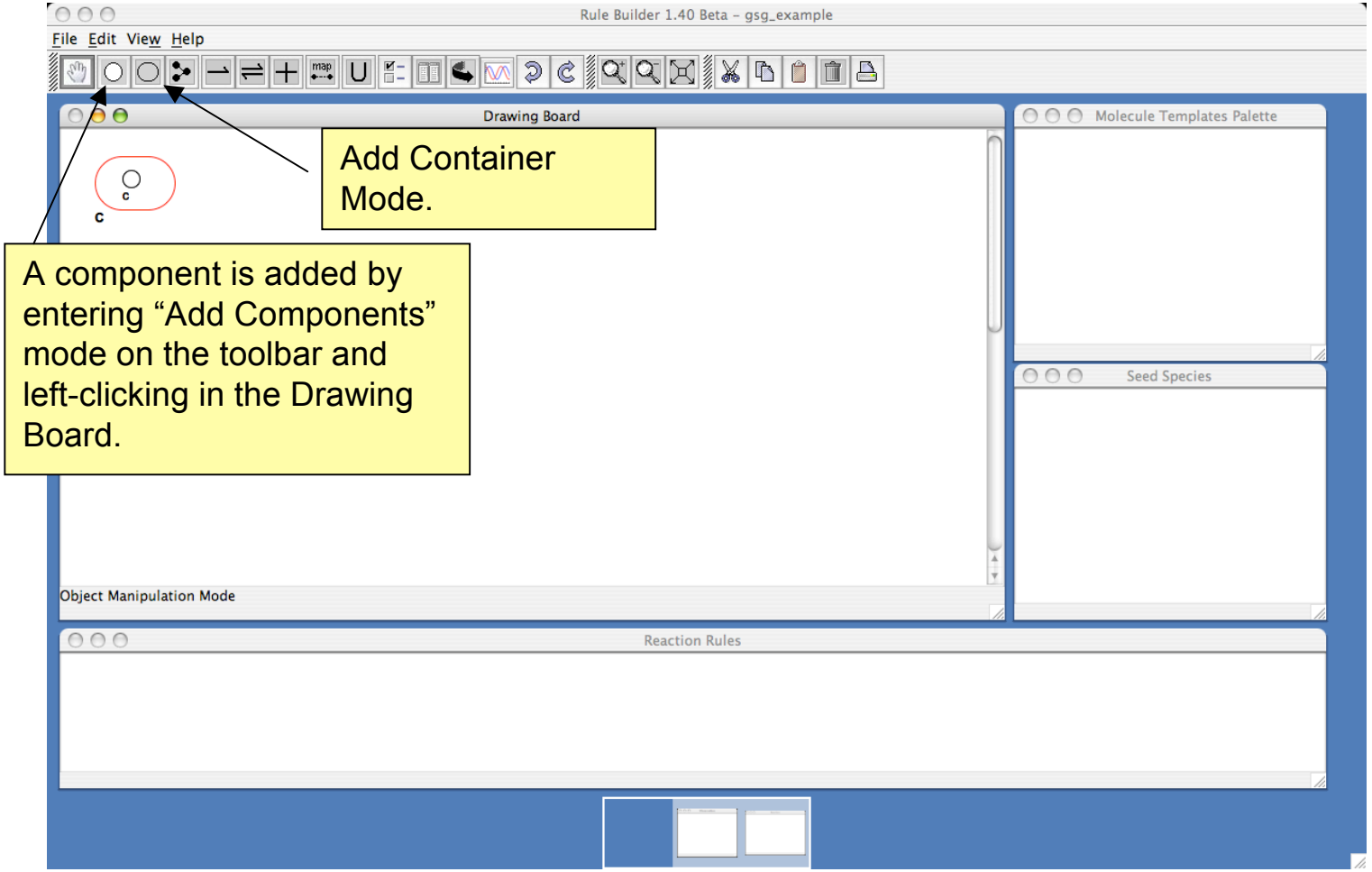
Introduction

RuleBuilder enables you to define, generate, and simulate graphical rule-based models of biochemical systems. Objects and rules created in RuleBuilder are passed to the BioNetGen program in the form of a BioNetGen Language (BNGL) file in order to generate and simulate the reaction network. RuleBuilder enables you to control both the network generation and simulation steps and to view the generated network and plot the simulation results. This guide takes you through all of the basic steps involved in using RuleBuilder.

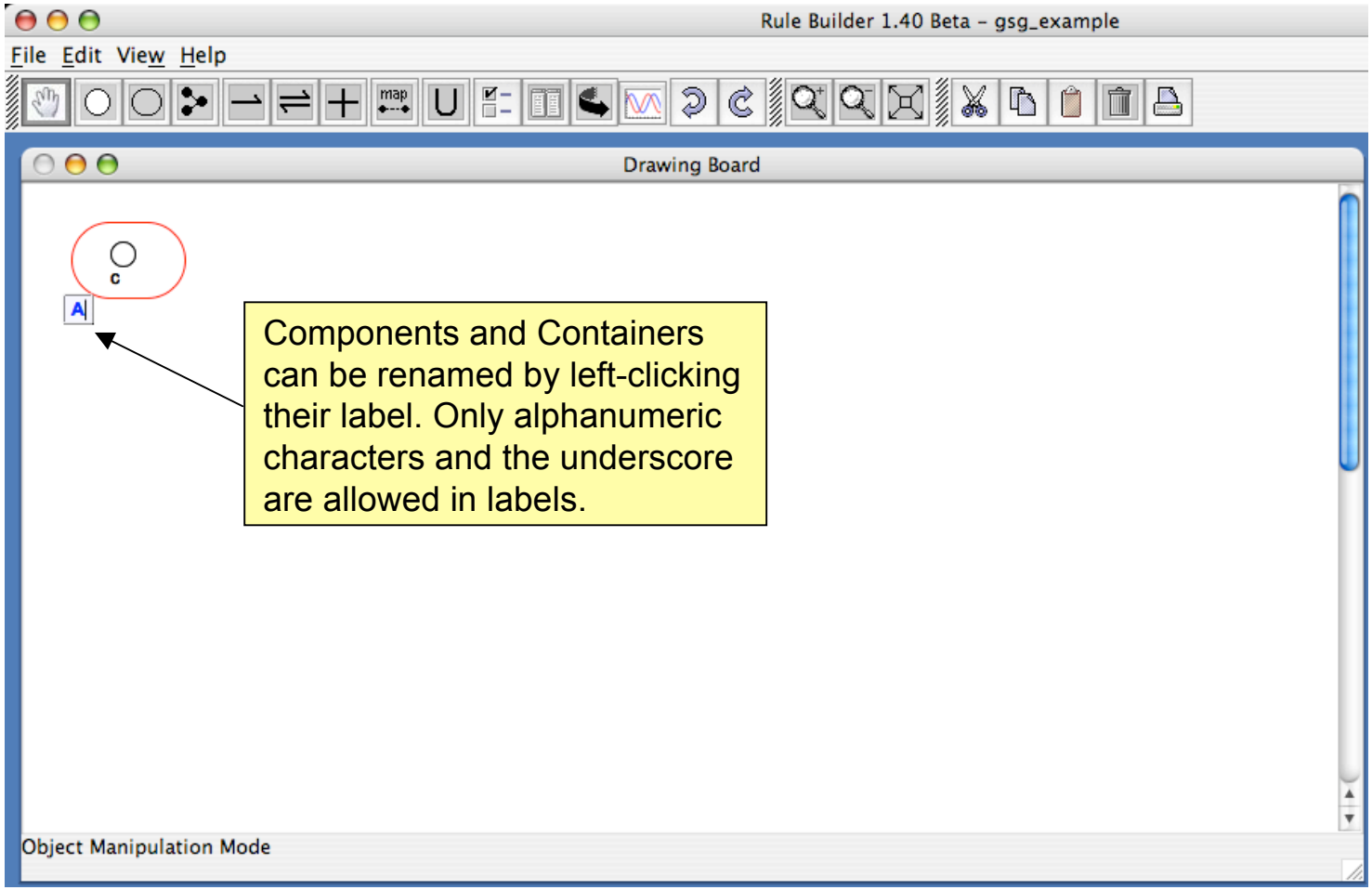
RuleBuilder Layout



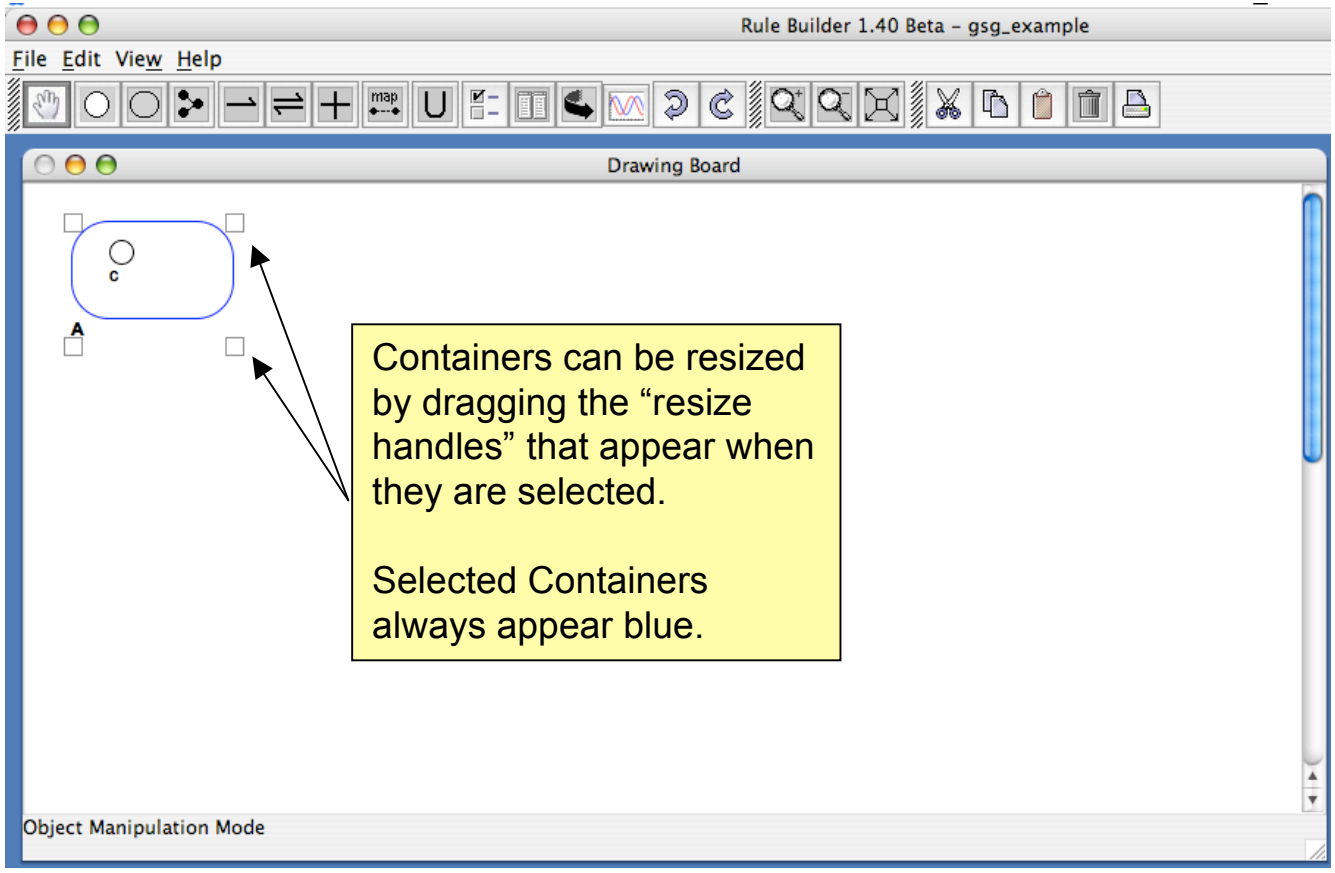
Adding Containers and Components



Renaming Components and Containers

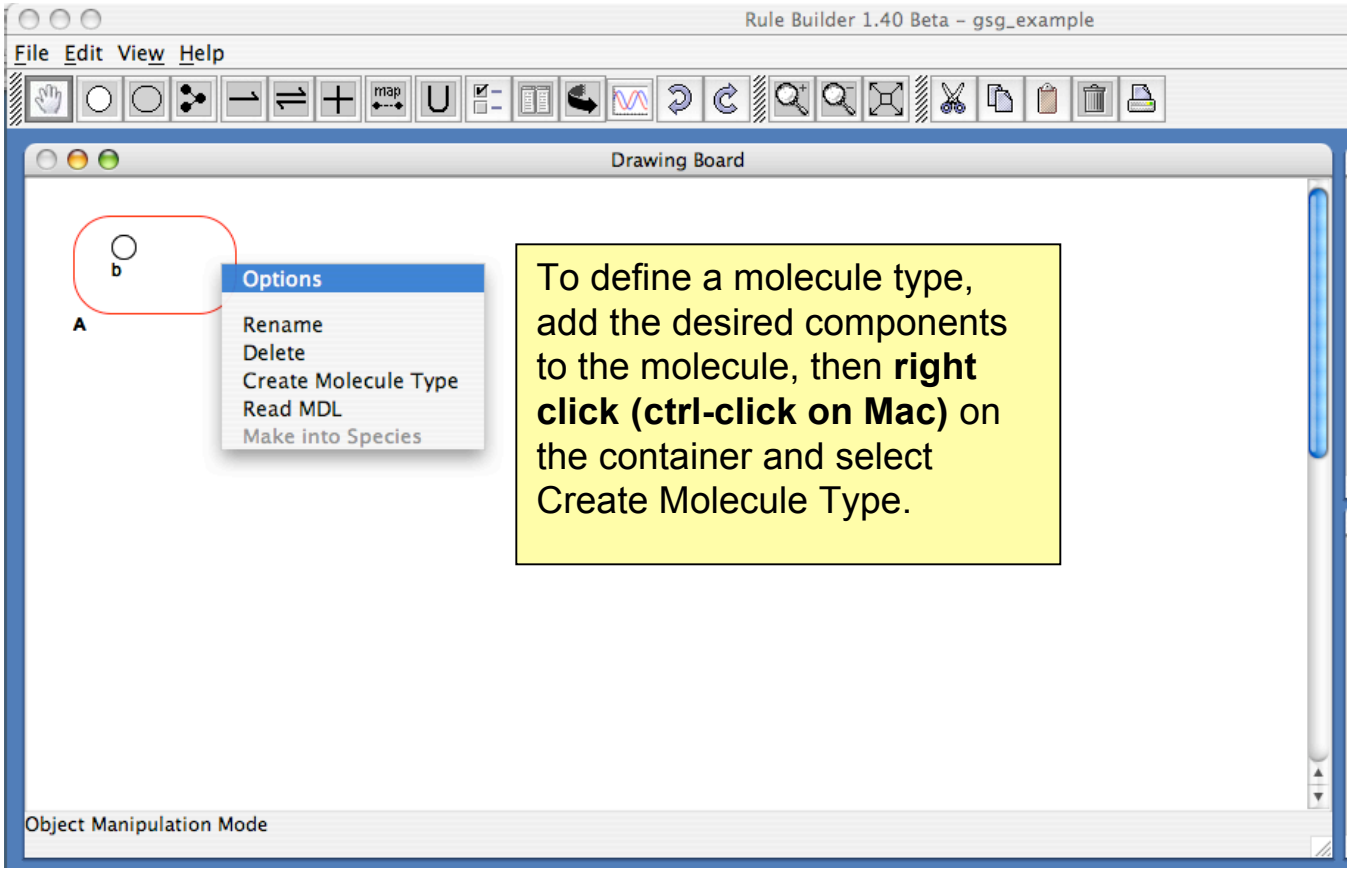


Resizing Containers



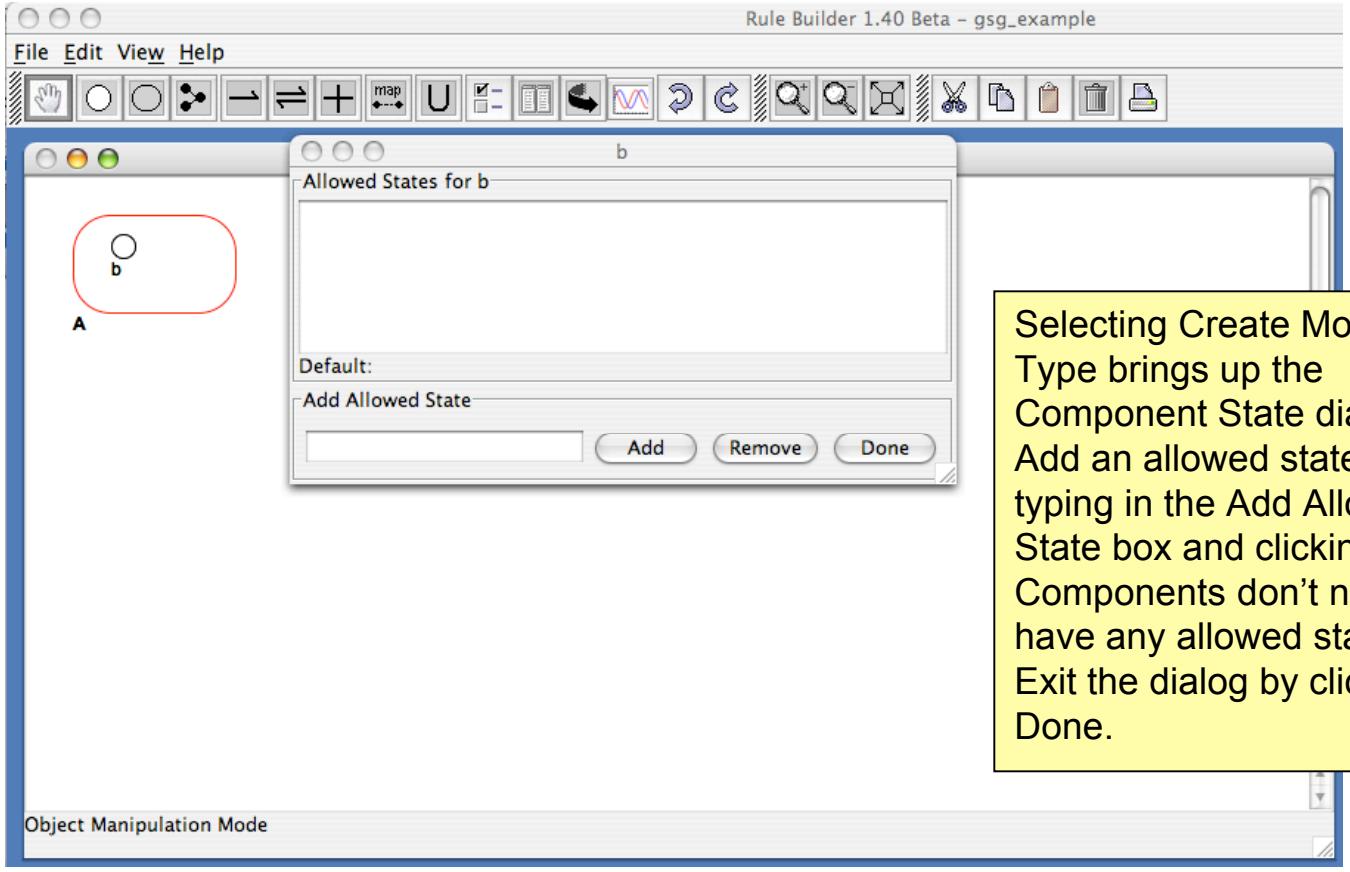
Creating Molecule Types

Molecules used in a model have to be defined and registered as a “Molecule Type” before they can be used in reaction rules and species.



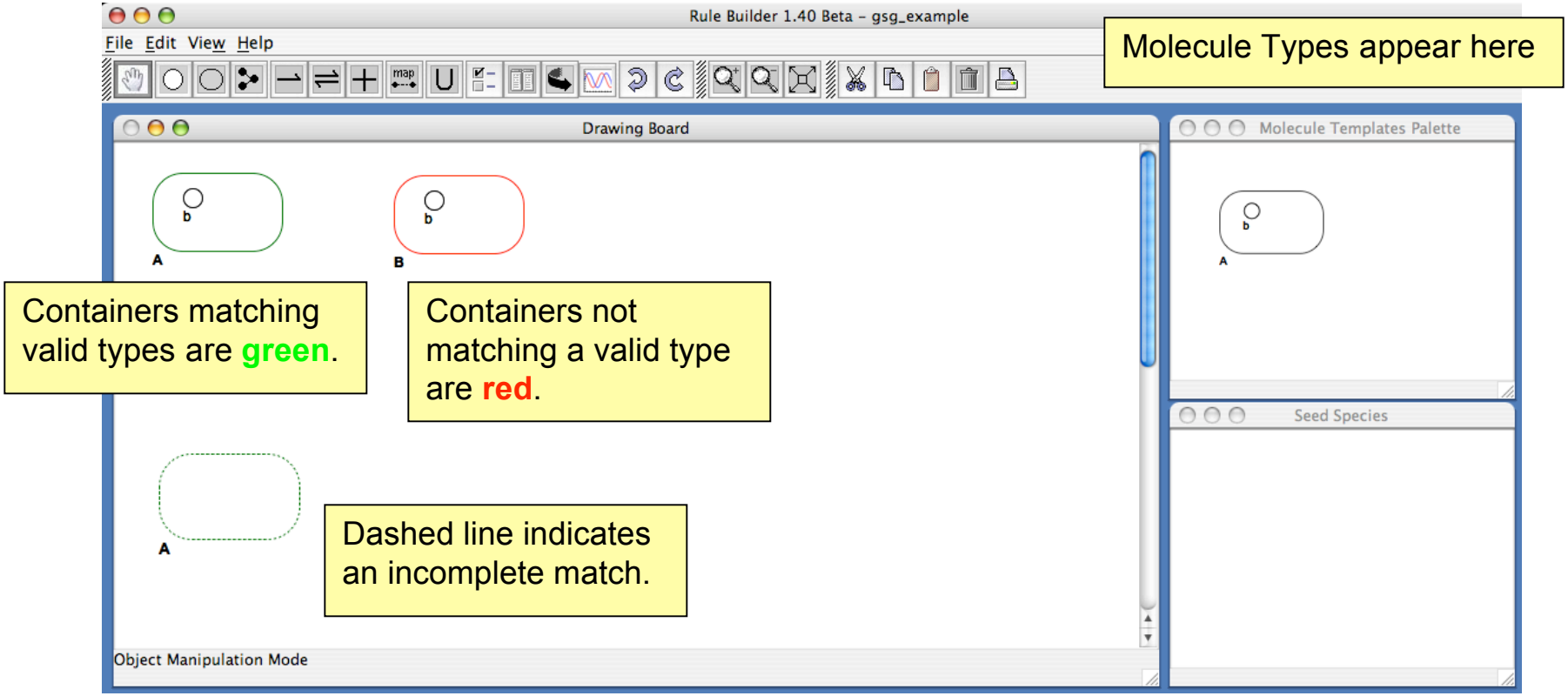
Setting Allowed Component States

Components may take on different states to indicate conformation or covalent modification, such as phosphorylation.

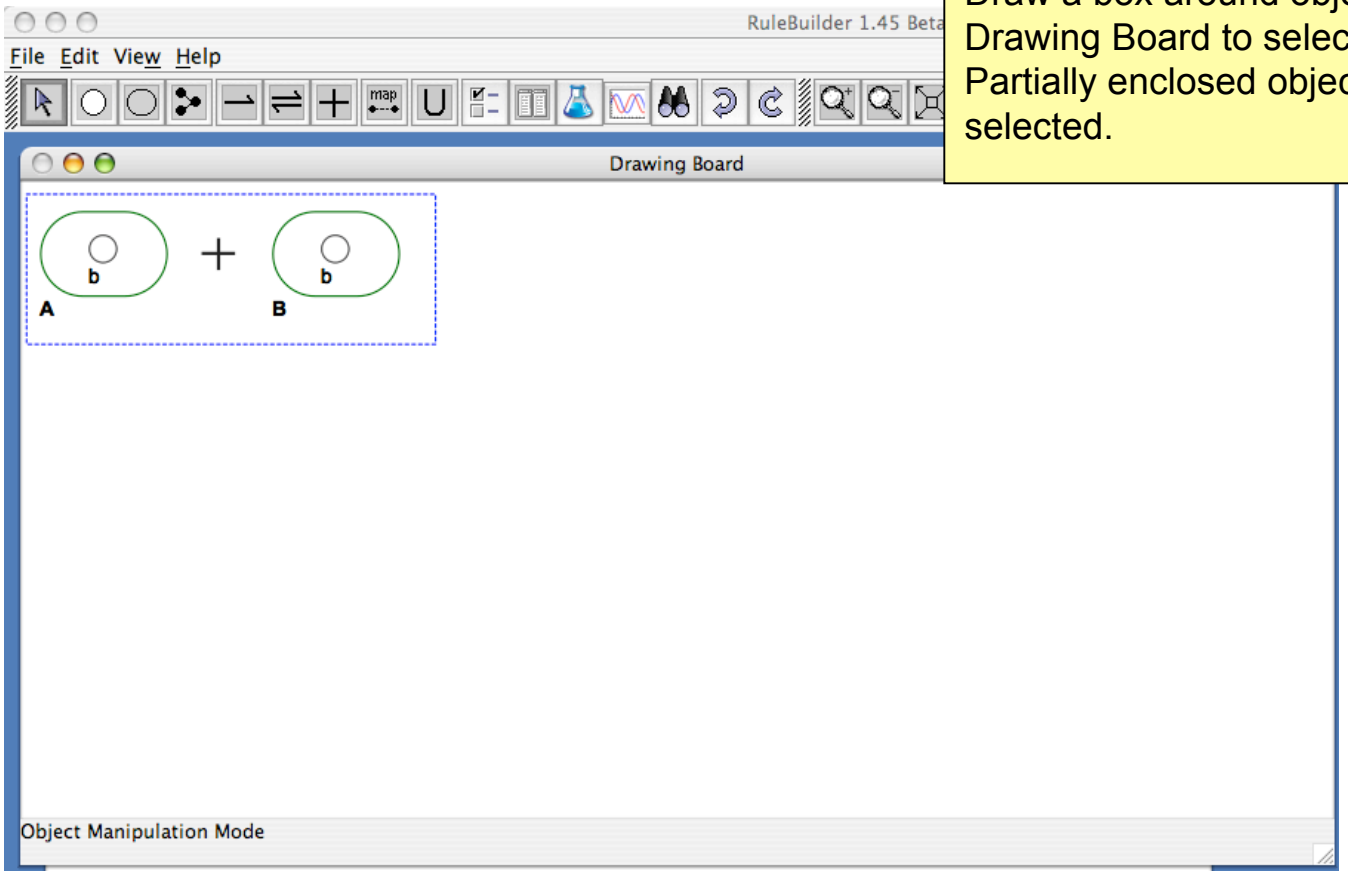


Selecting Create Molecule Type brings up the Component State dialog. Add an allowed state by typing in the Add Allowed State box and clicking Add. Components don't need to have any allowed states. Exit the dialog by clicking Done.

Identifying Valid and Invalid Molecules

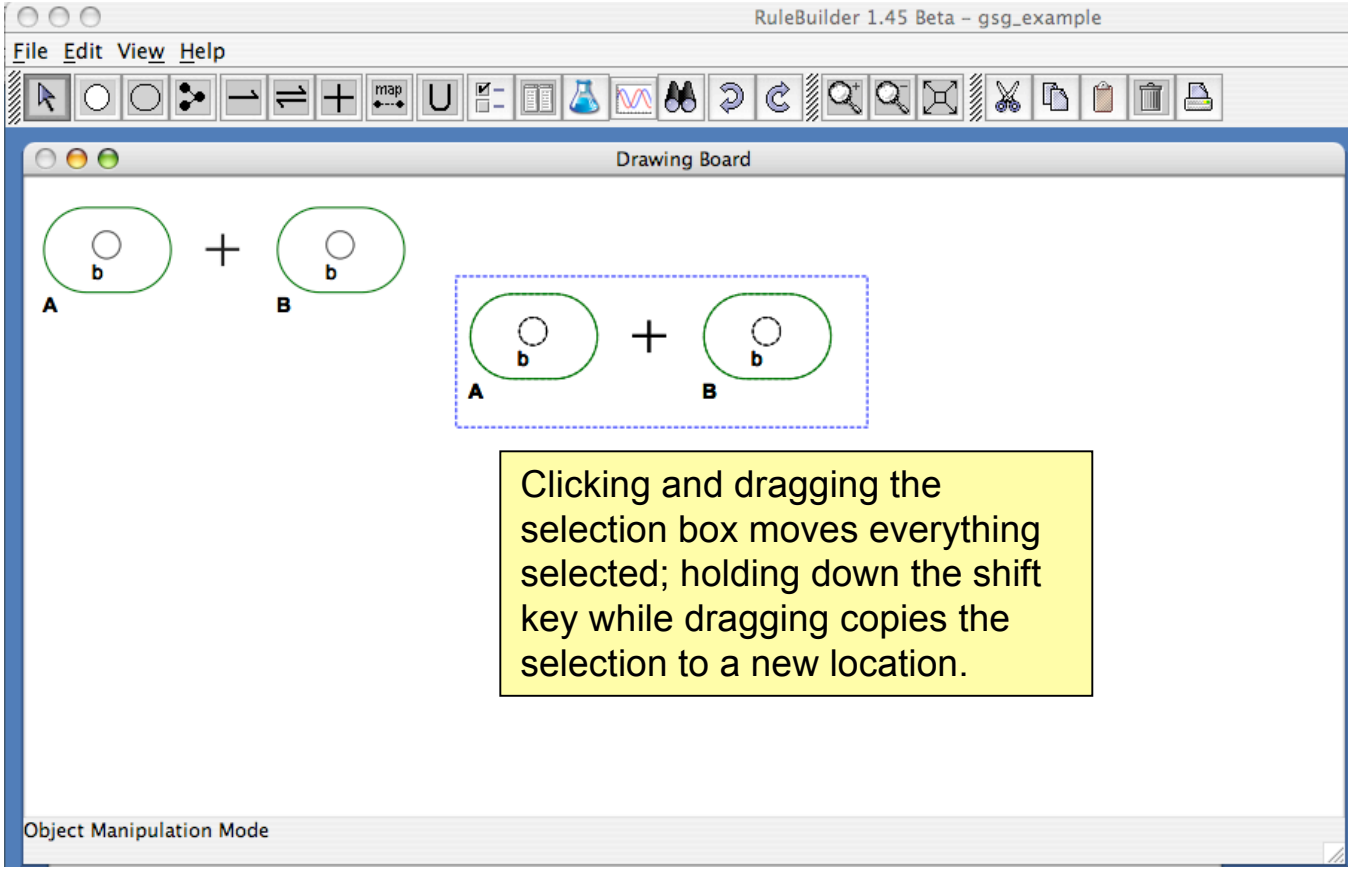


Copying Objects with the Selection Box



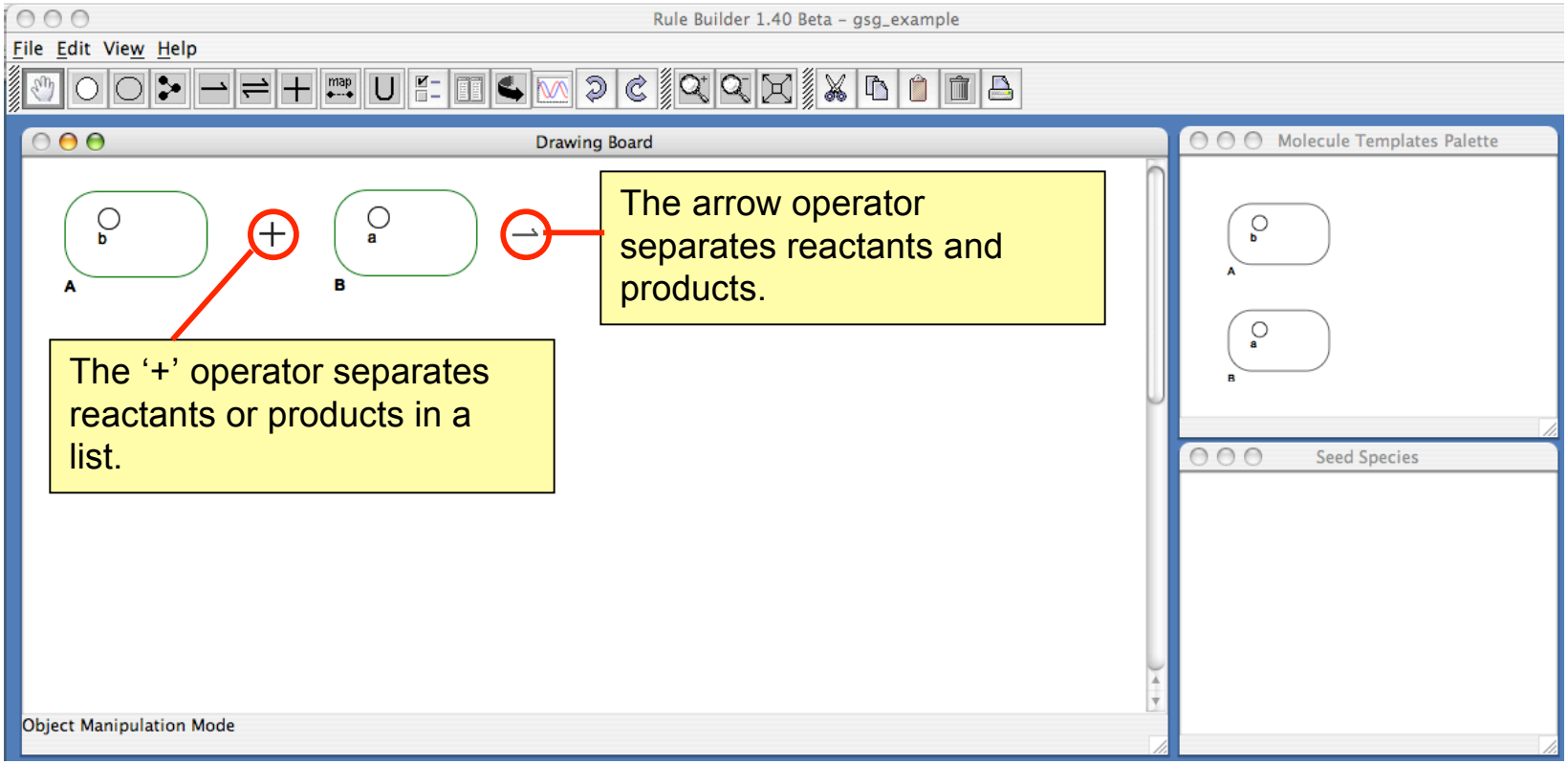
Draw a box around objects on the Drawing Board to select them. Partially enclosed objects are not selected.

Copying Objects with the Selection Box



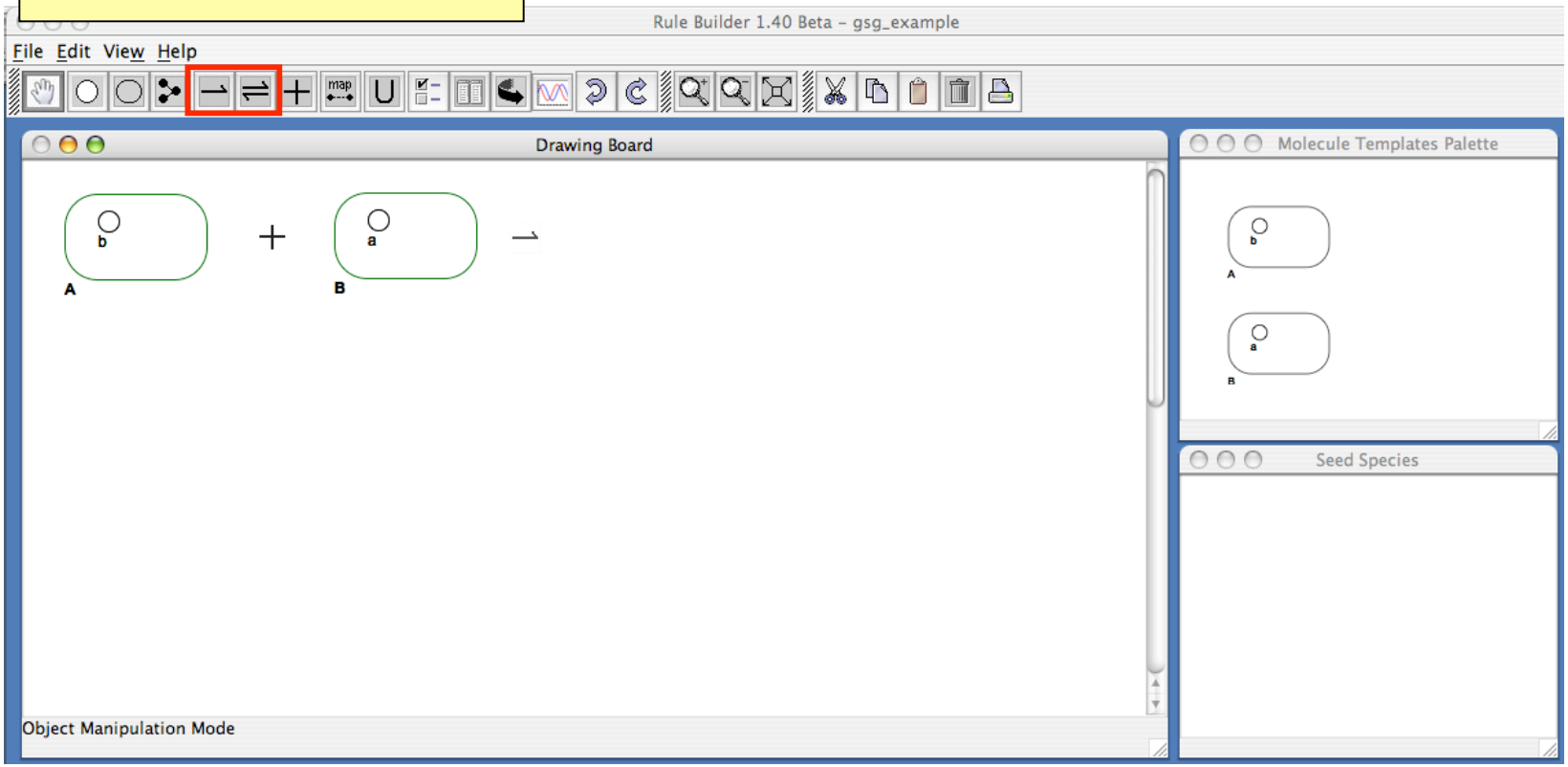
Creating a Reaction Rule

Reaction rules are created by arranging containers and operators to construct a formula for the reaction.

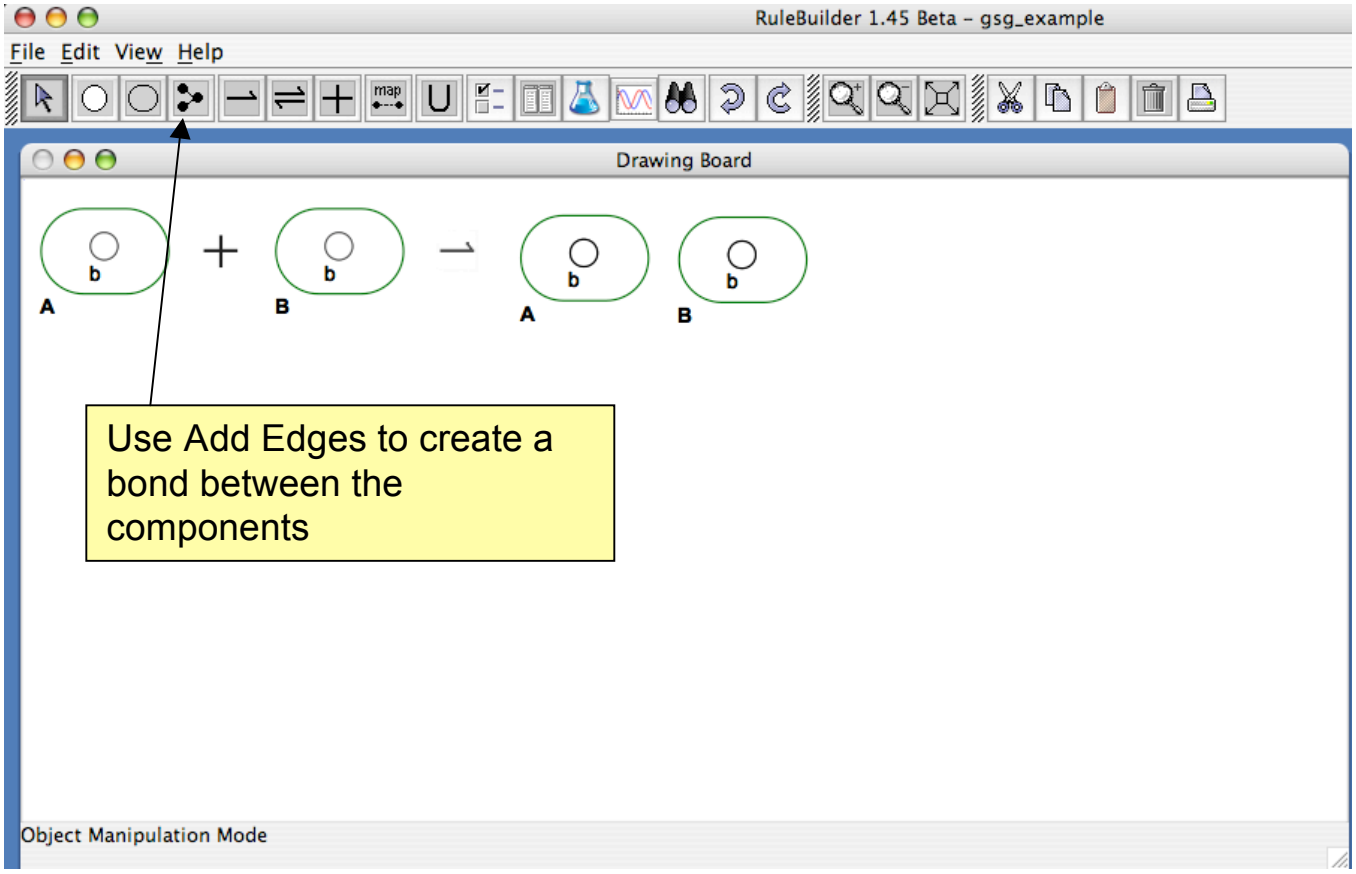


Creating a Reaction Rule

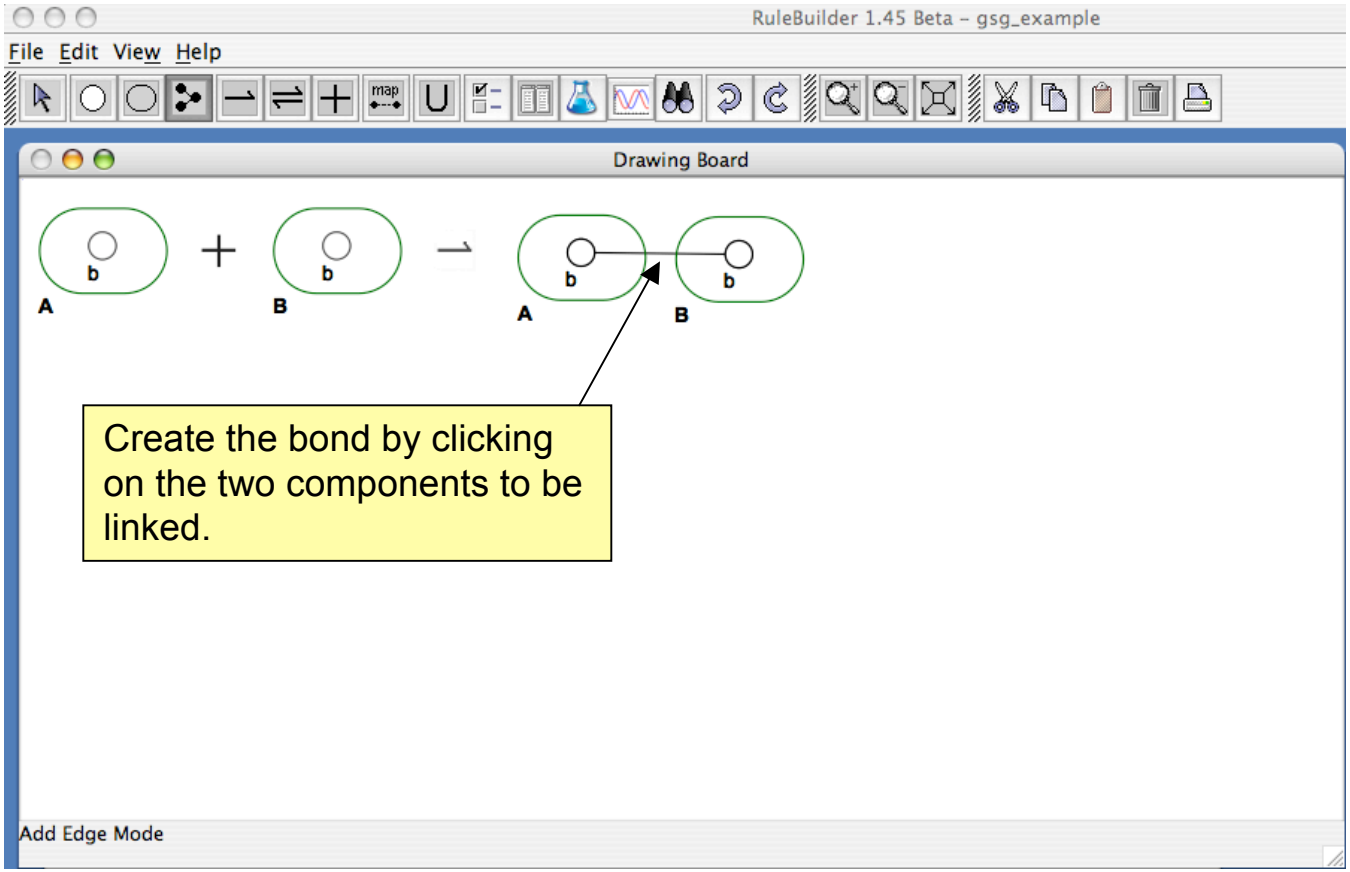
The type of arrow determines whether a reaction is reversible or irreversible.



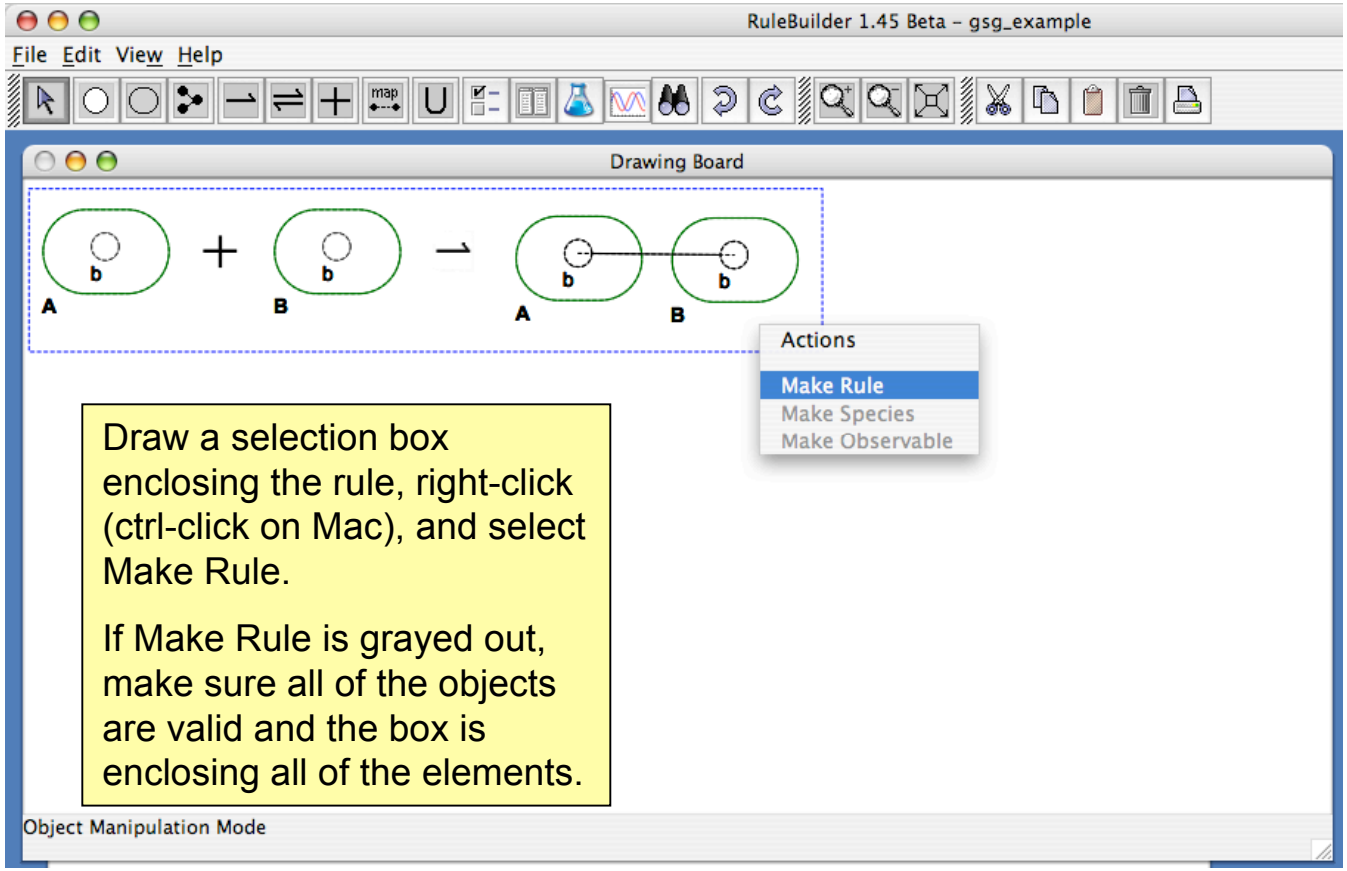
Defining Products



Defining Products



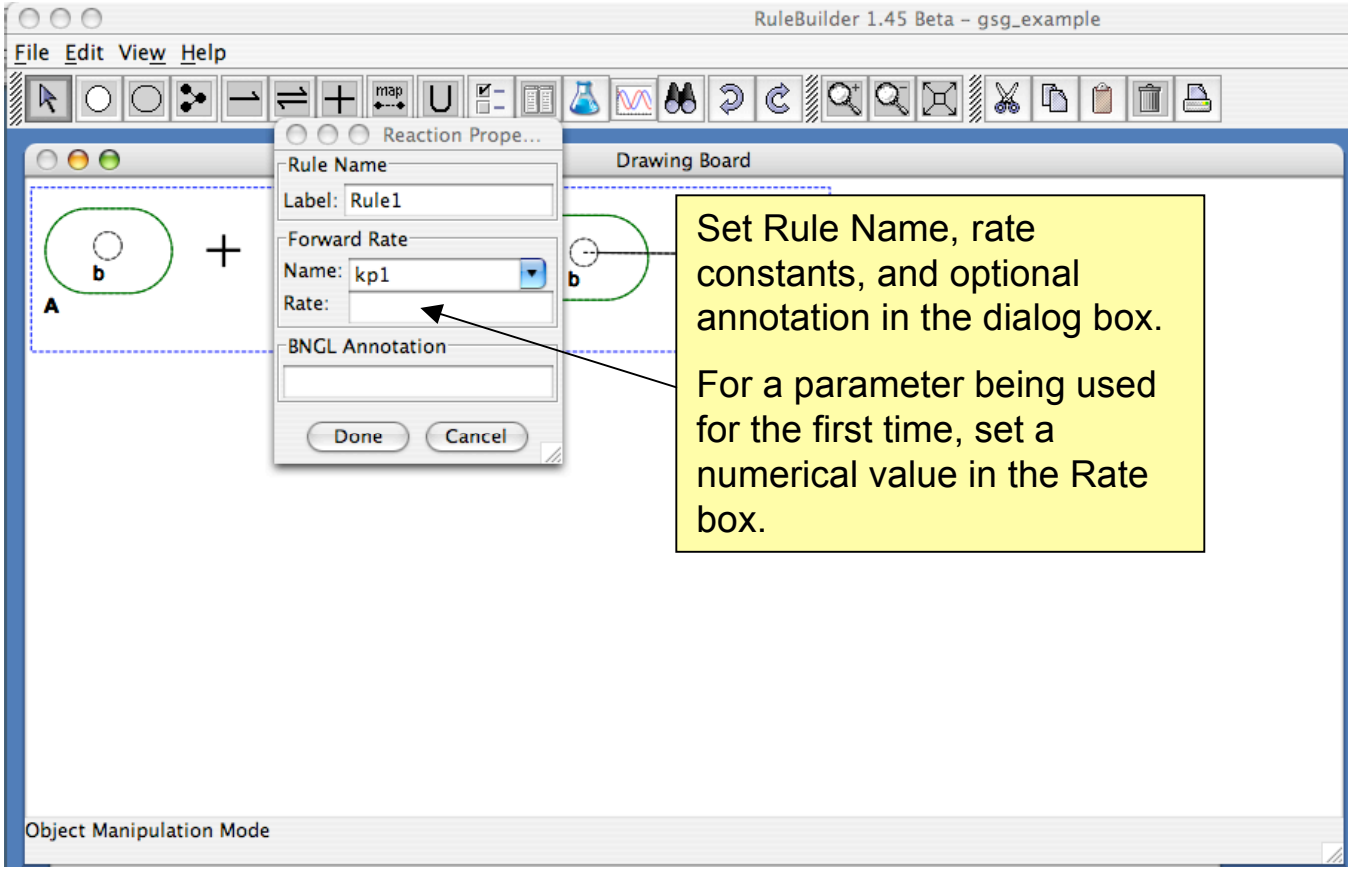
Creating the Rule



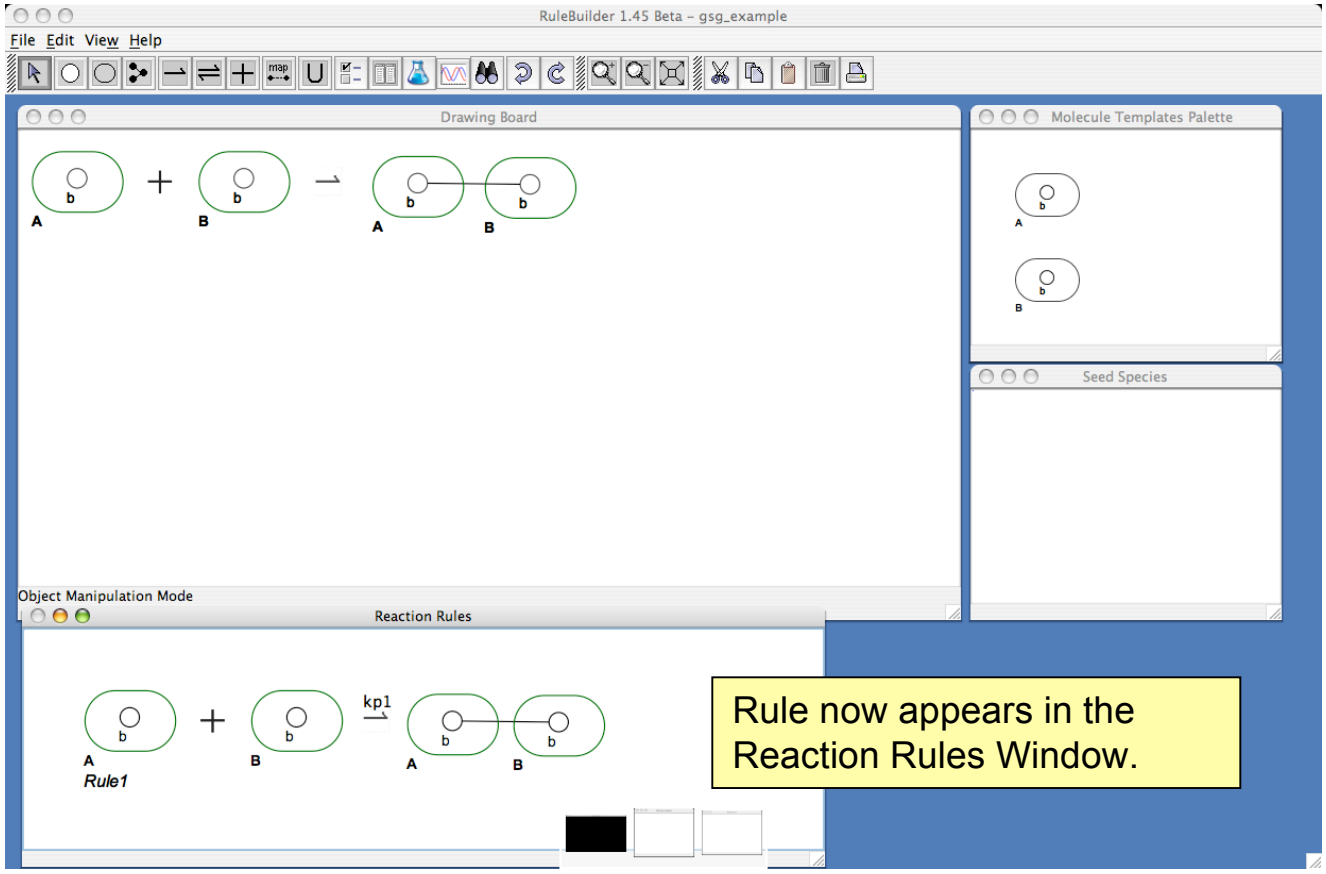
Draw a selection box enclosing the rule, right-click (ctrl-click on Mac), and select Make Rule.

If Make Rule is grayed out, make sure all of the objects are valid and the box is enclosing all of the elements.

Make Rule Dialog

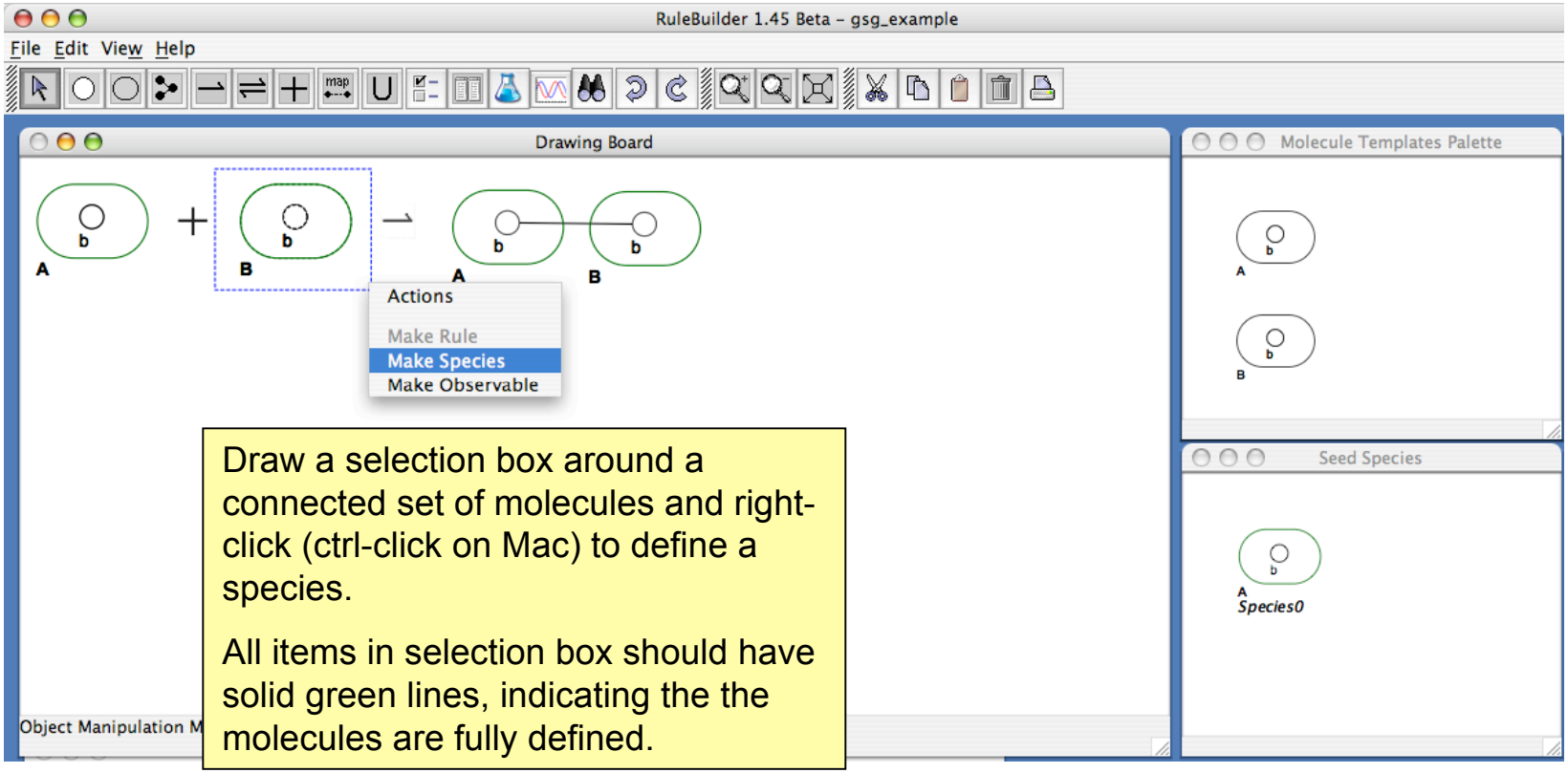


Reaction Rules Window



Defining Seed Species

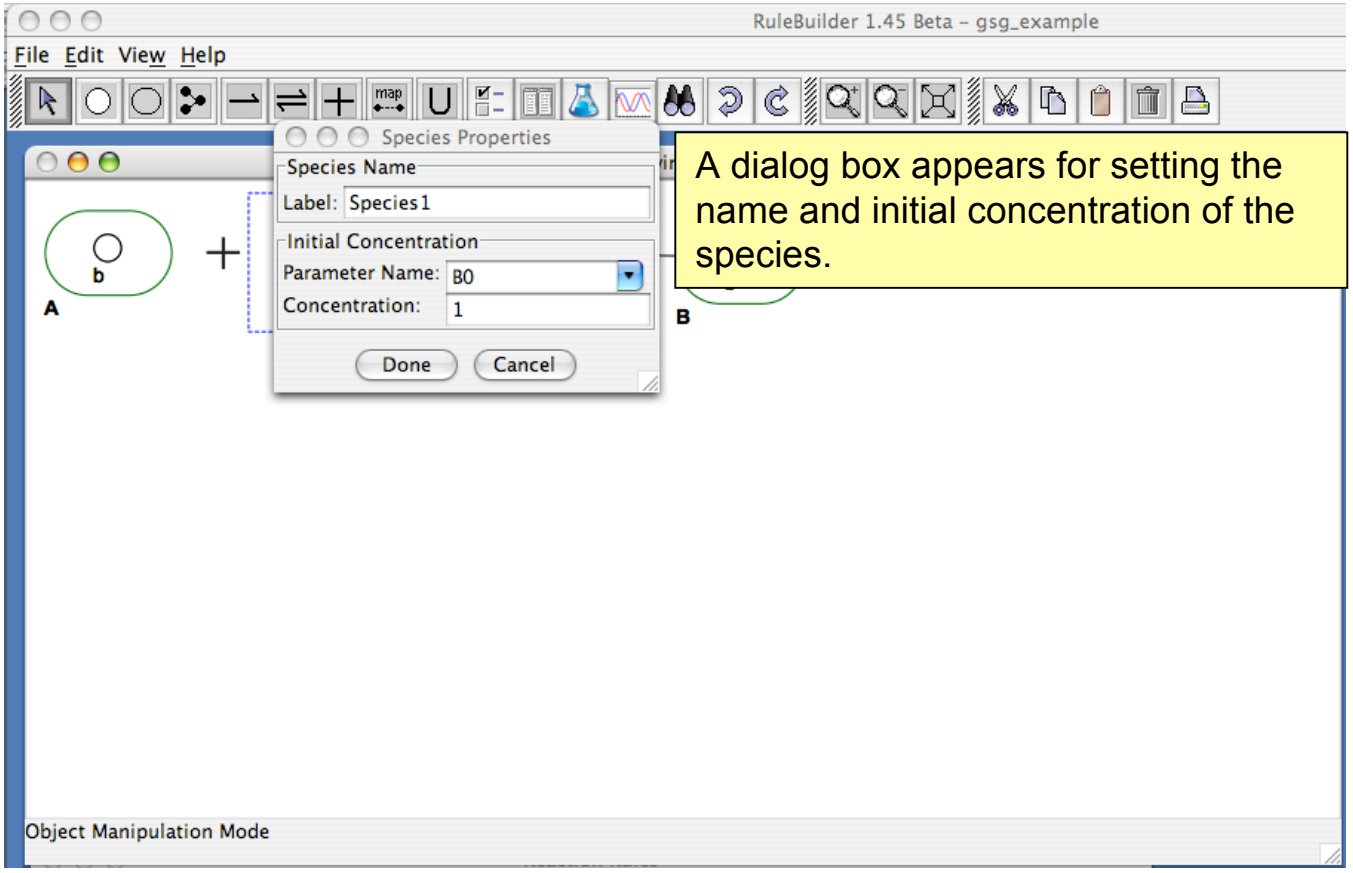
The network is defined by applying the reaction rules to a set of seed species.



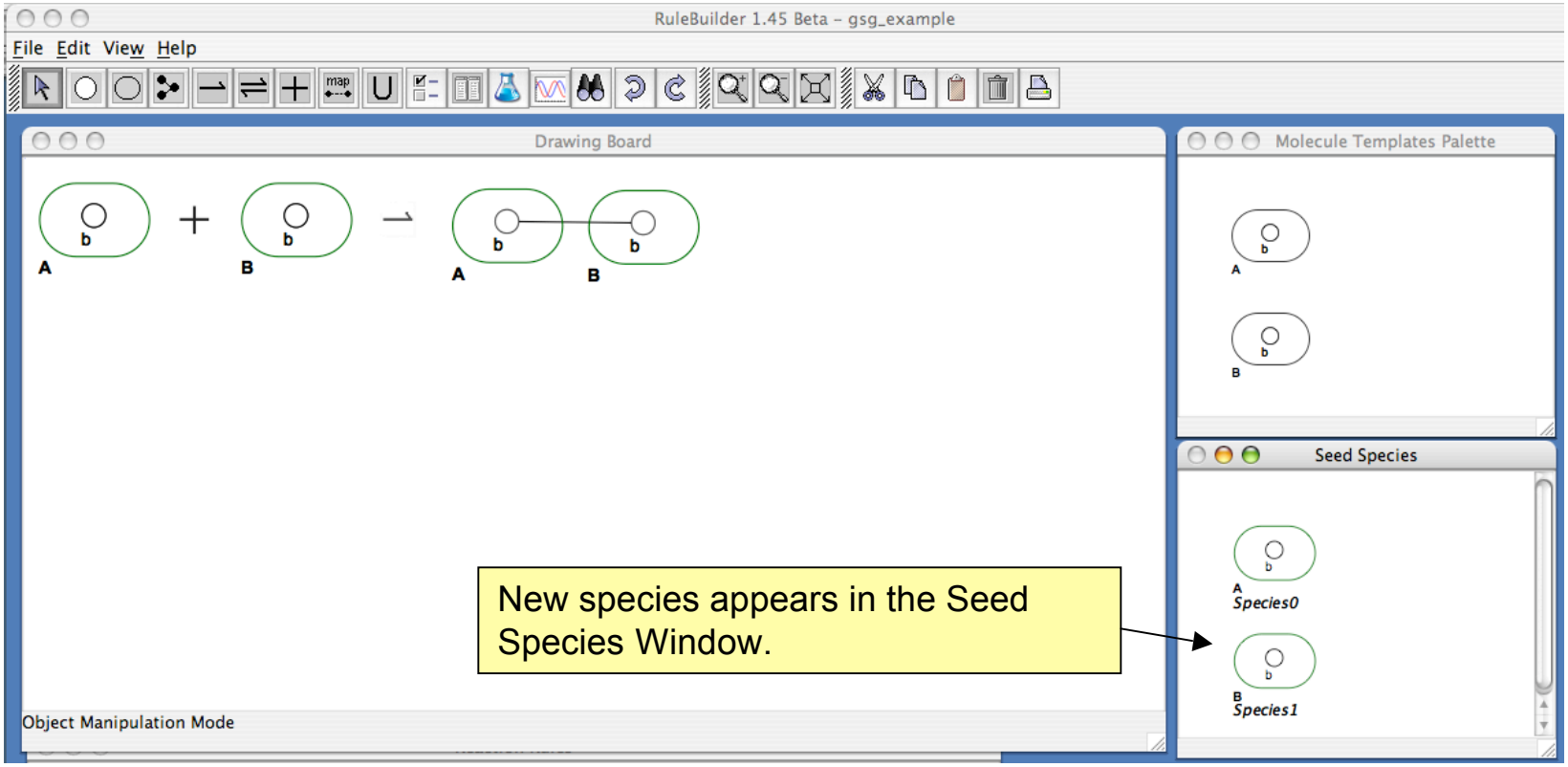
Draw a selection box around a connected set of molecules and right-click (ctrl-click on Mac) to define a species.

All items in selection box should have solid green lines, indicating the the molecules are fully defined.

Species Dialog Box

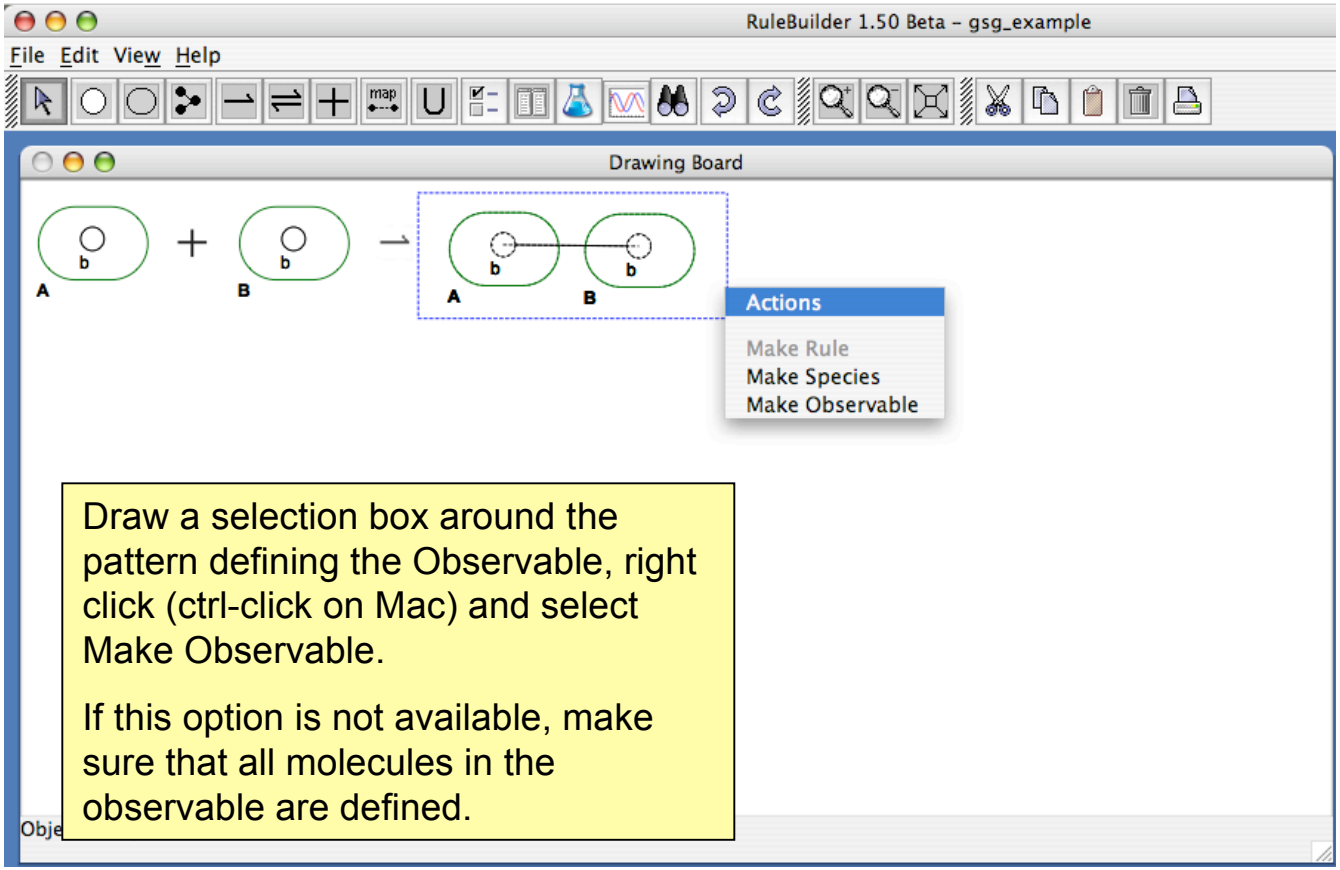


Seed Species Window

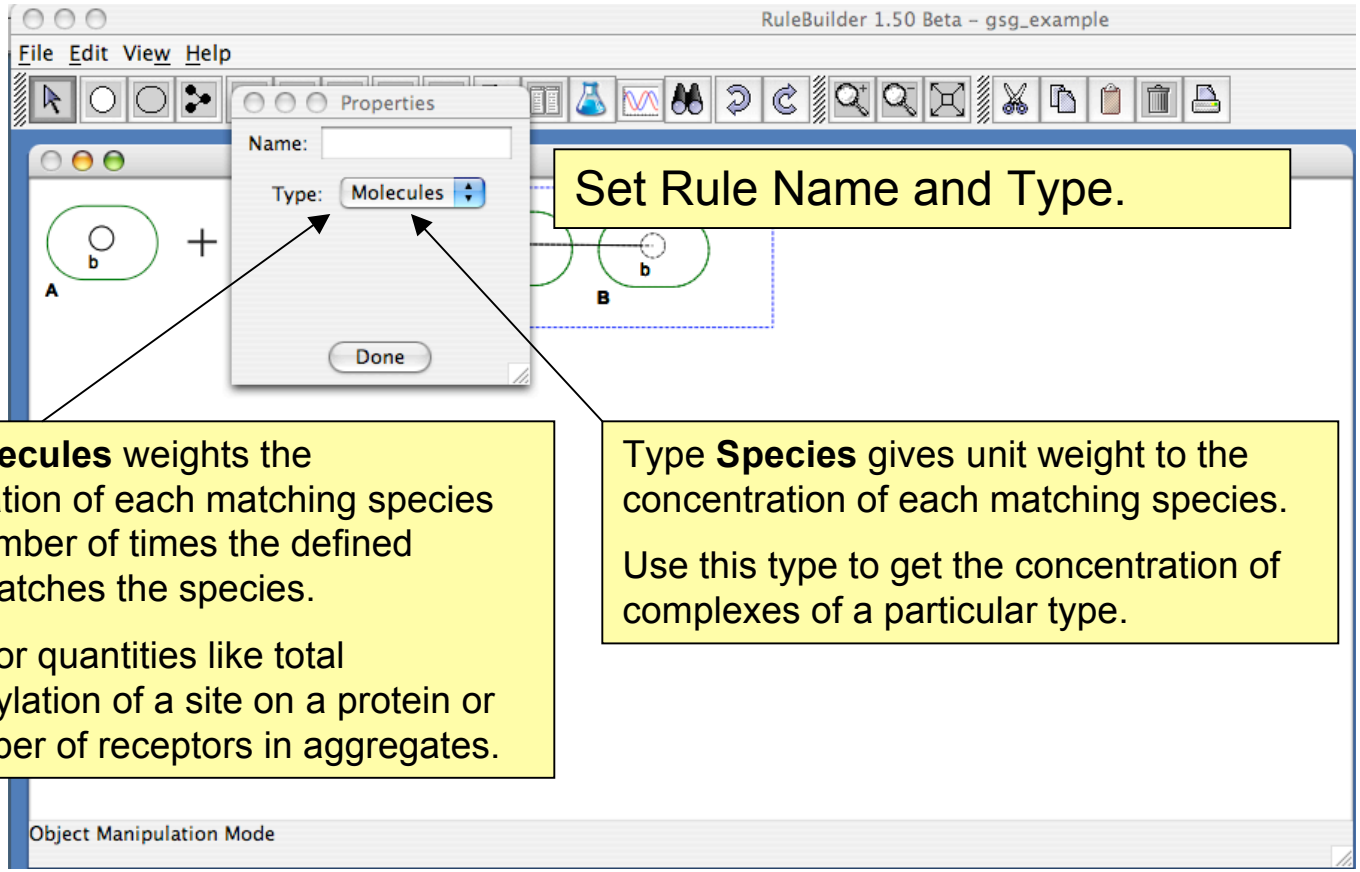


Defining Observables

Observables are concentration sums over species with particular properties and correspond to model outputs, such as total phosphorylation of a protein.



Make Observables Dialog



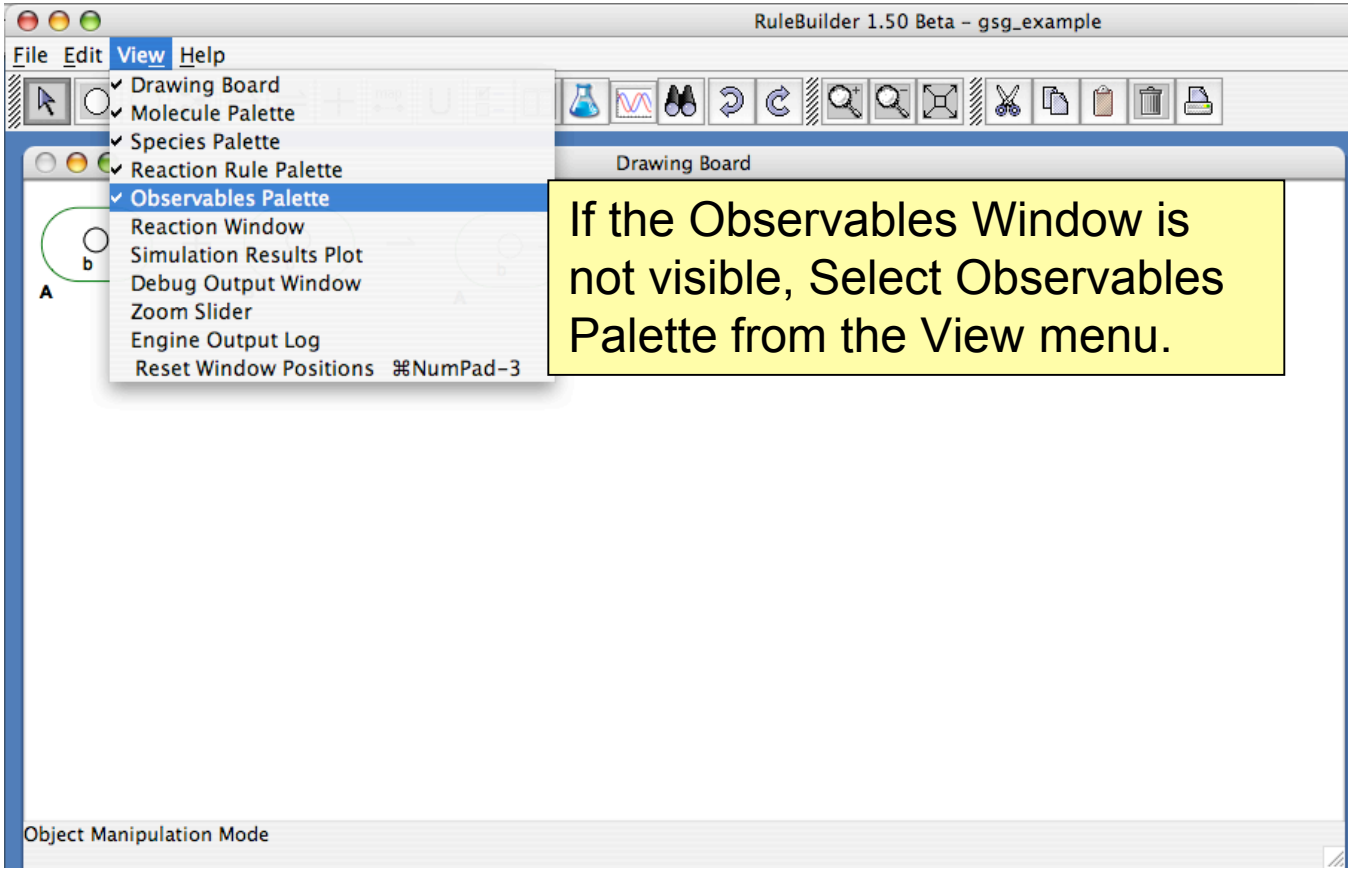
Type **Molecules** weights the concentration of each matching species by the number of times the defined pattern matches the species.

Use this for quantities like total phosphorylation of a site on a protein or total number of receptors in aggregates.

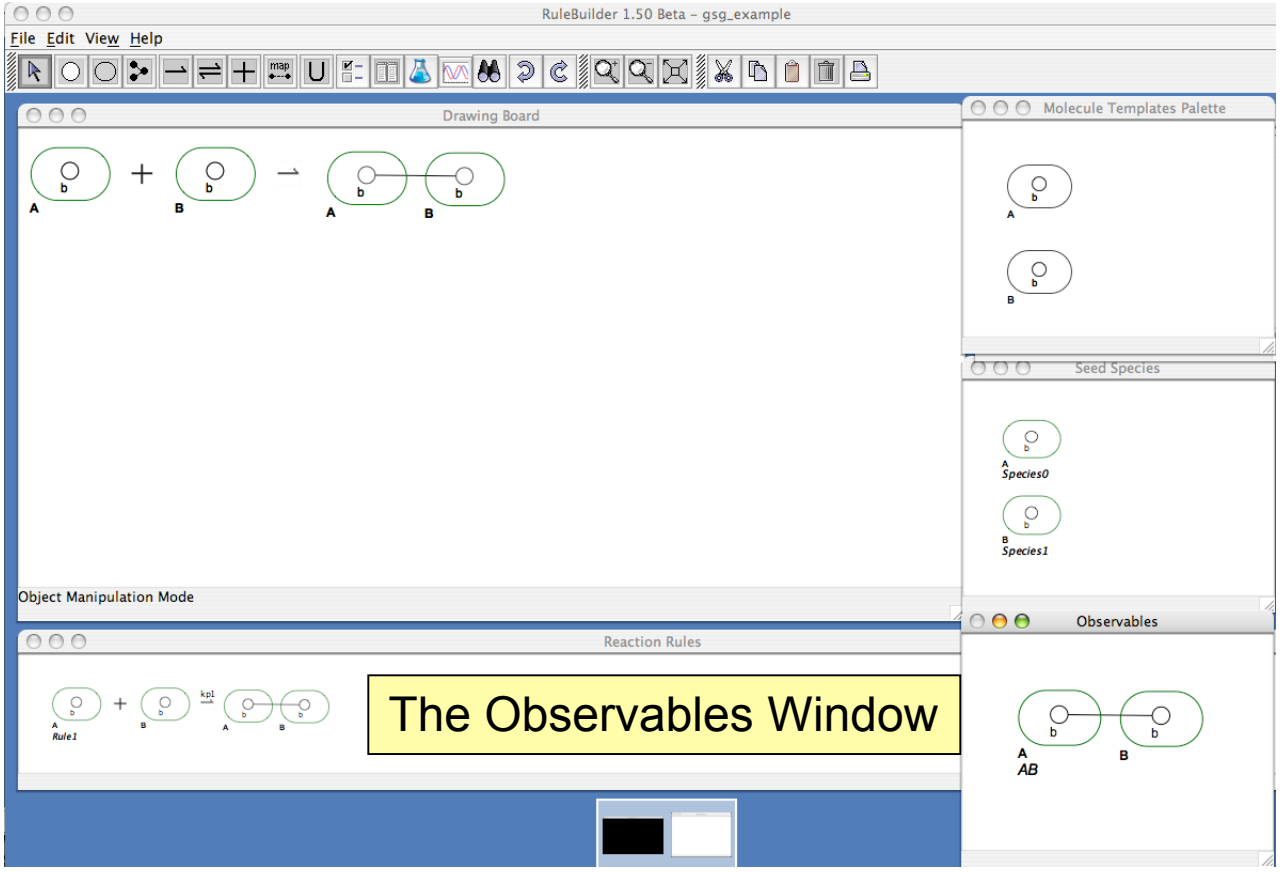
Type **Species** gives unit weight to the concentration of each matching species.

Use this type to get the concentration of complexes of a particular type.

Observables Window

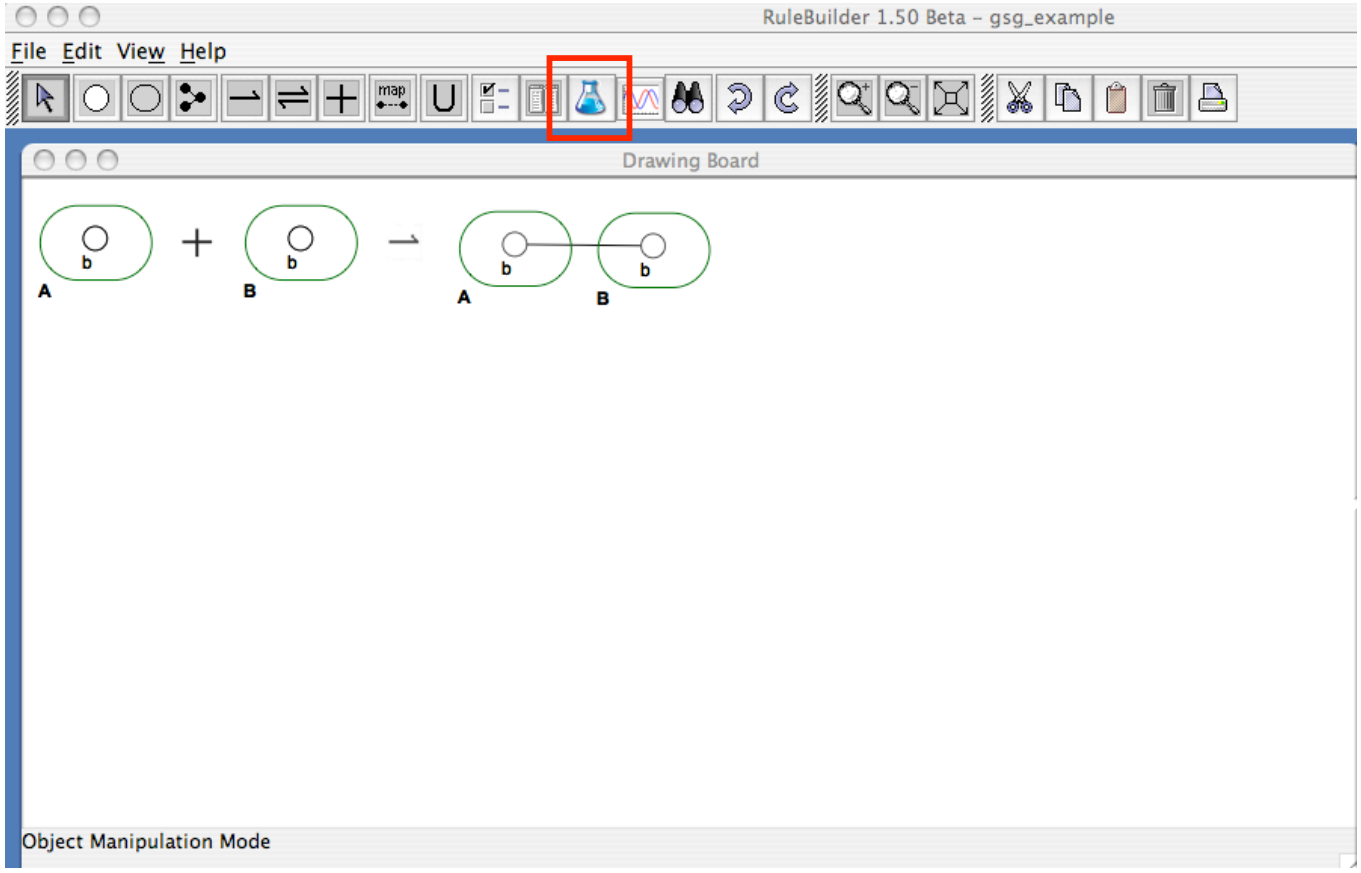


Observables Window

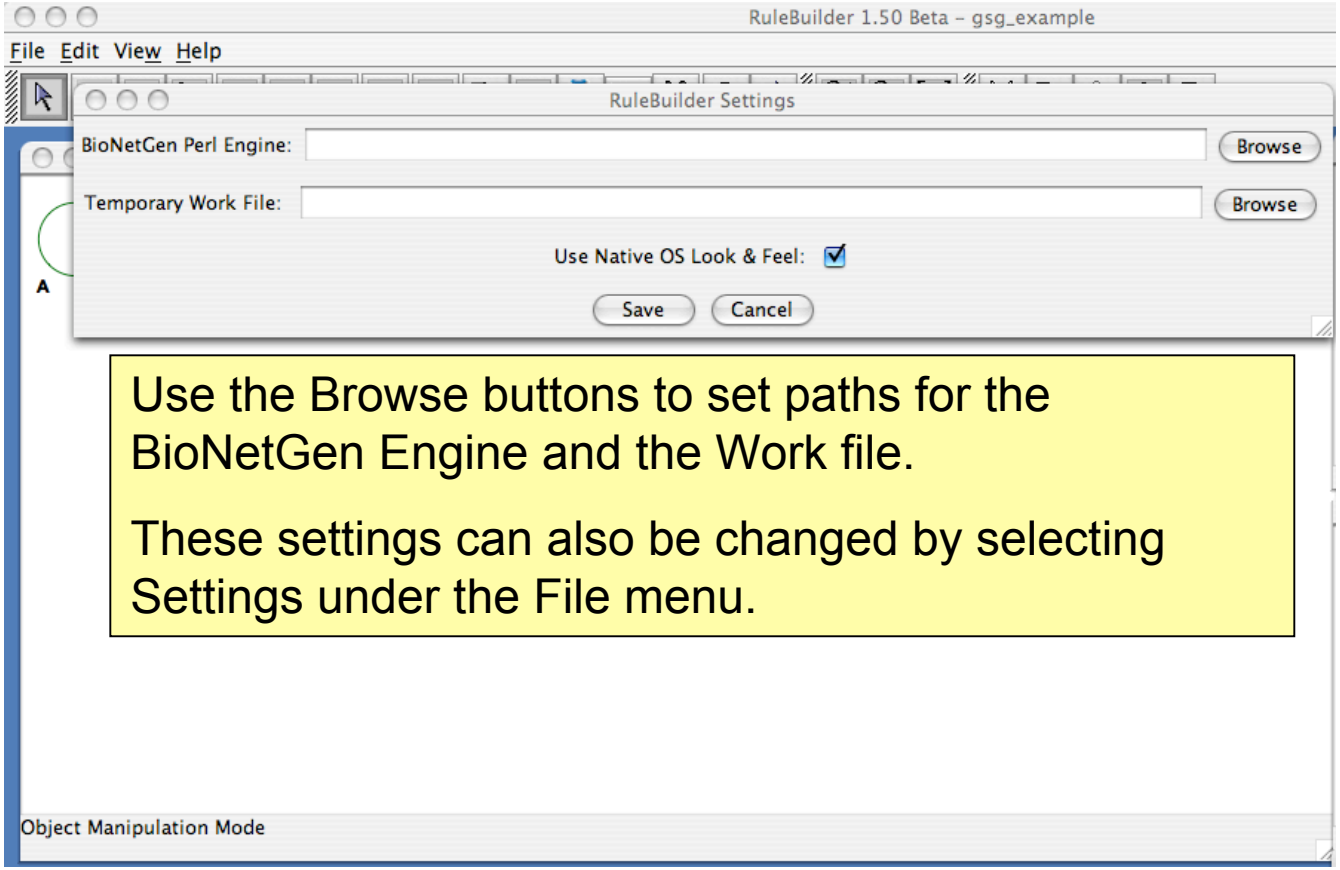


Running the Model

Once Reaction Rules, Seed Species, and Observables (optional) have been defined, the model can be simulated by pressing Run BioNetGen button.

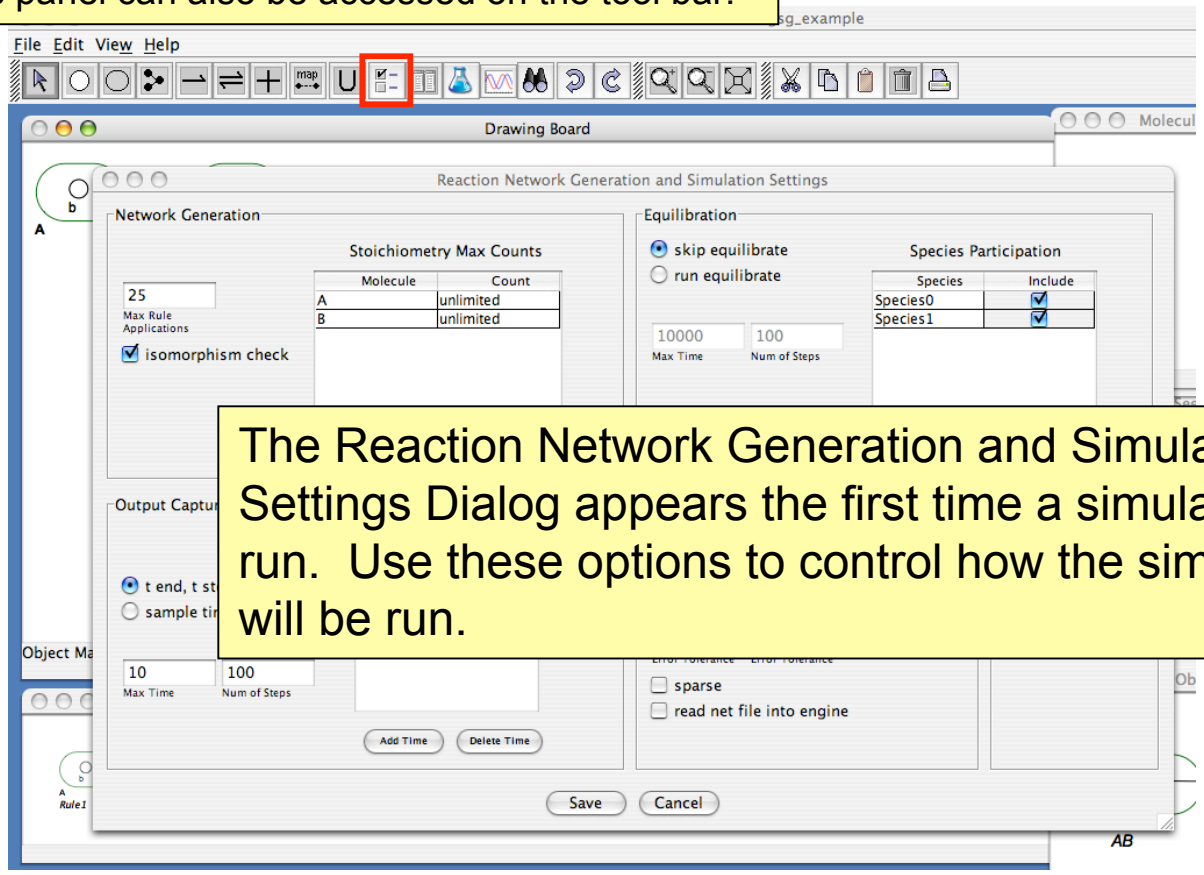


BioNetGen Engine Settings



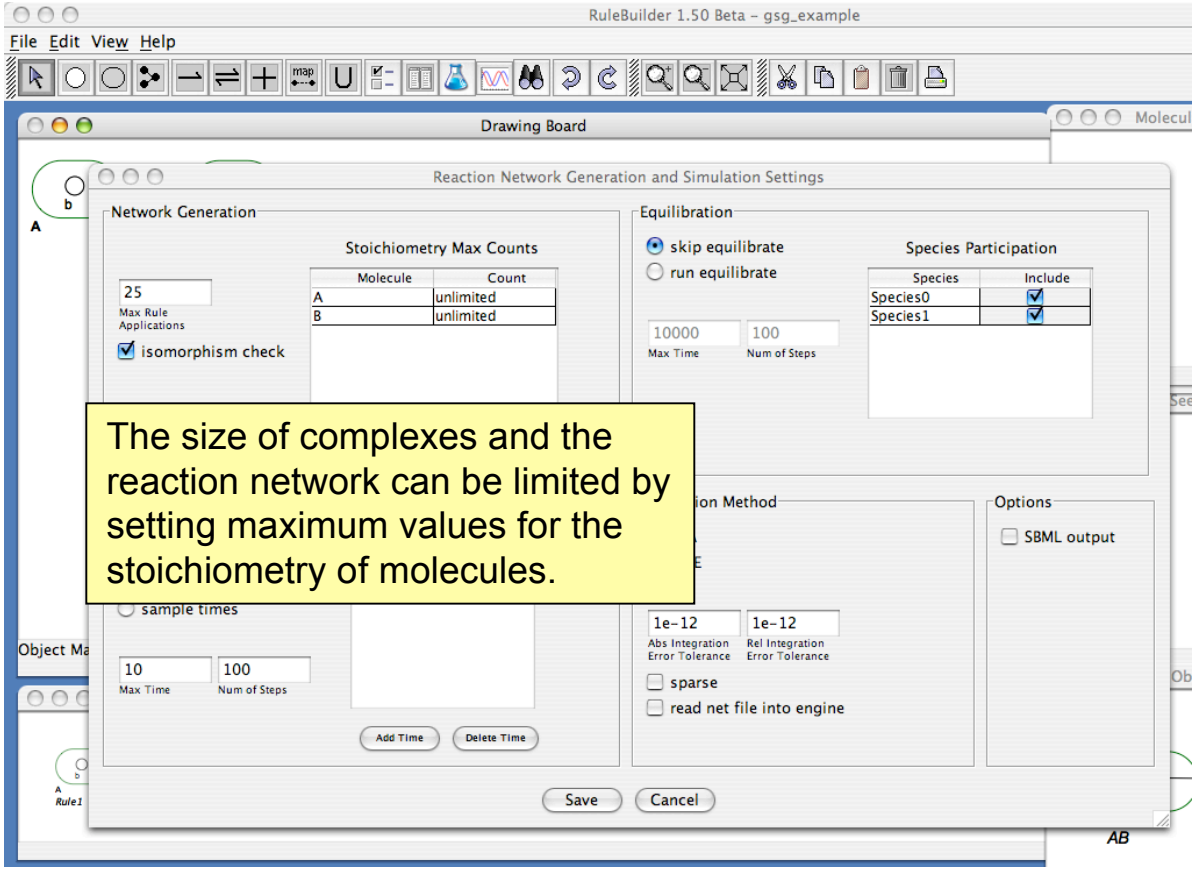
The SimConfig Panel

This panel can also be accessed on the tool bar.

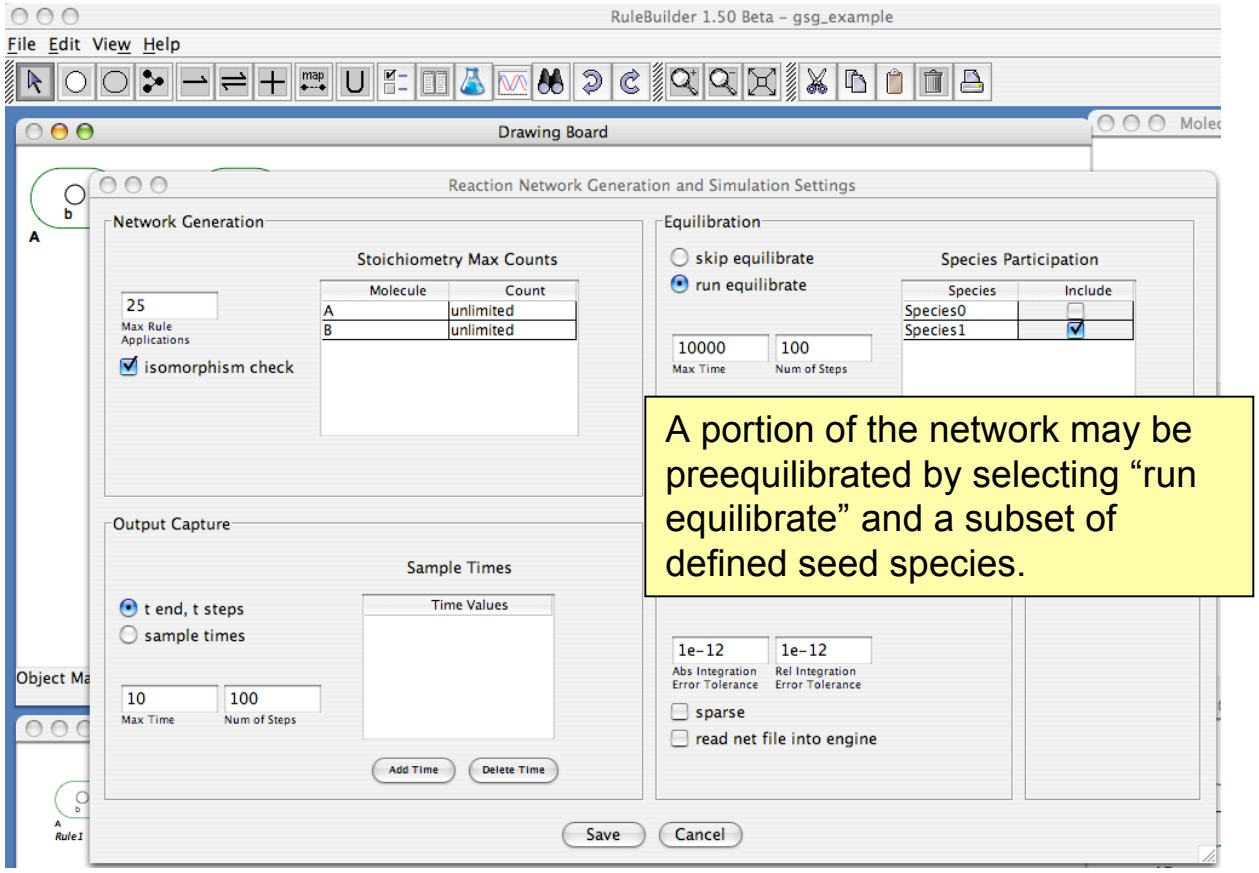


The Reaction Network Generation and Simulation Settings Dialog appears the first time a simulation is run. Use these options to control how the simulation will be run.

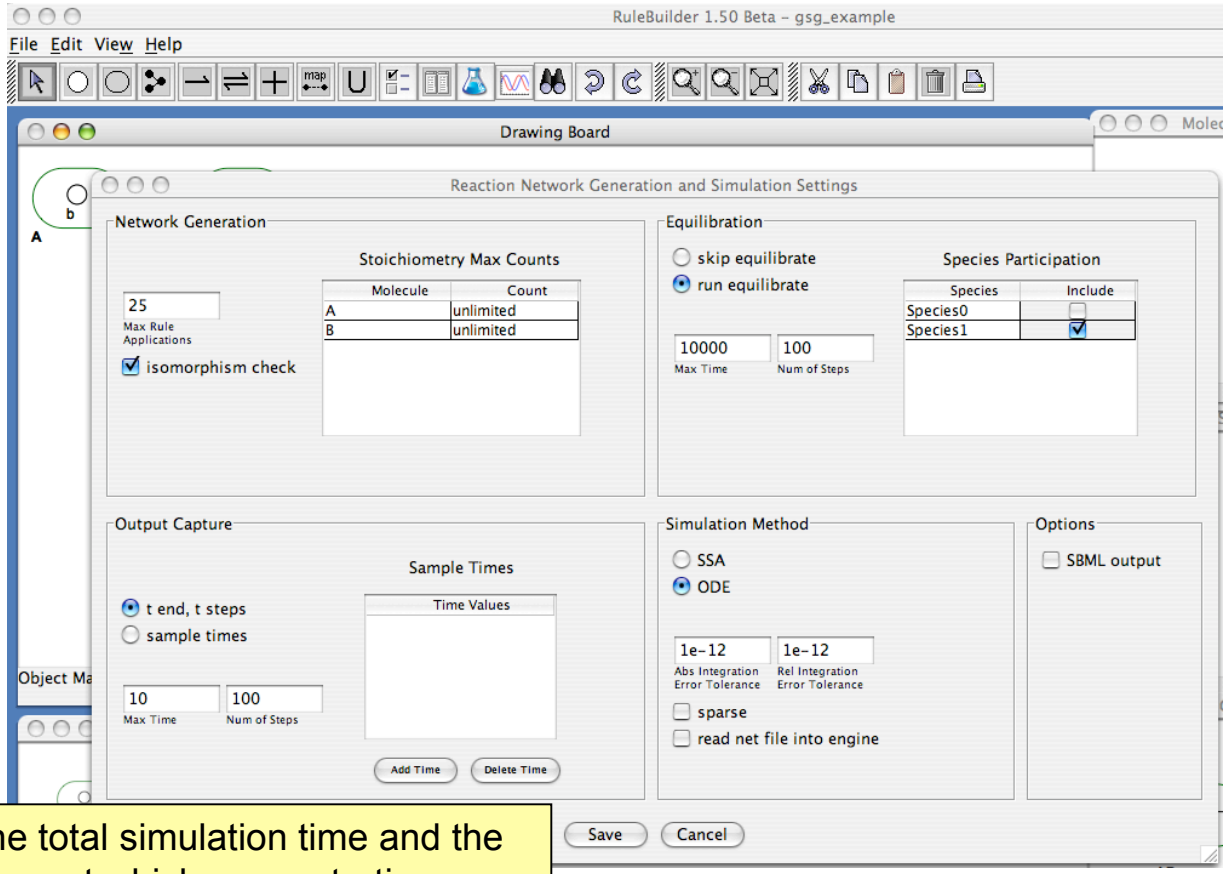
The SimConfig Panel



The SimConfig Panel

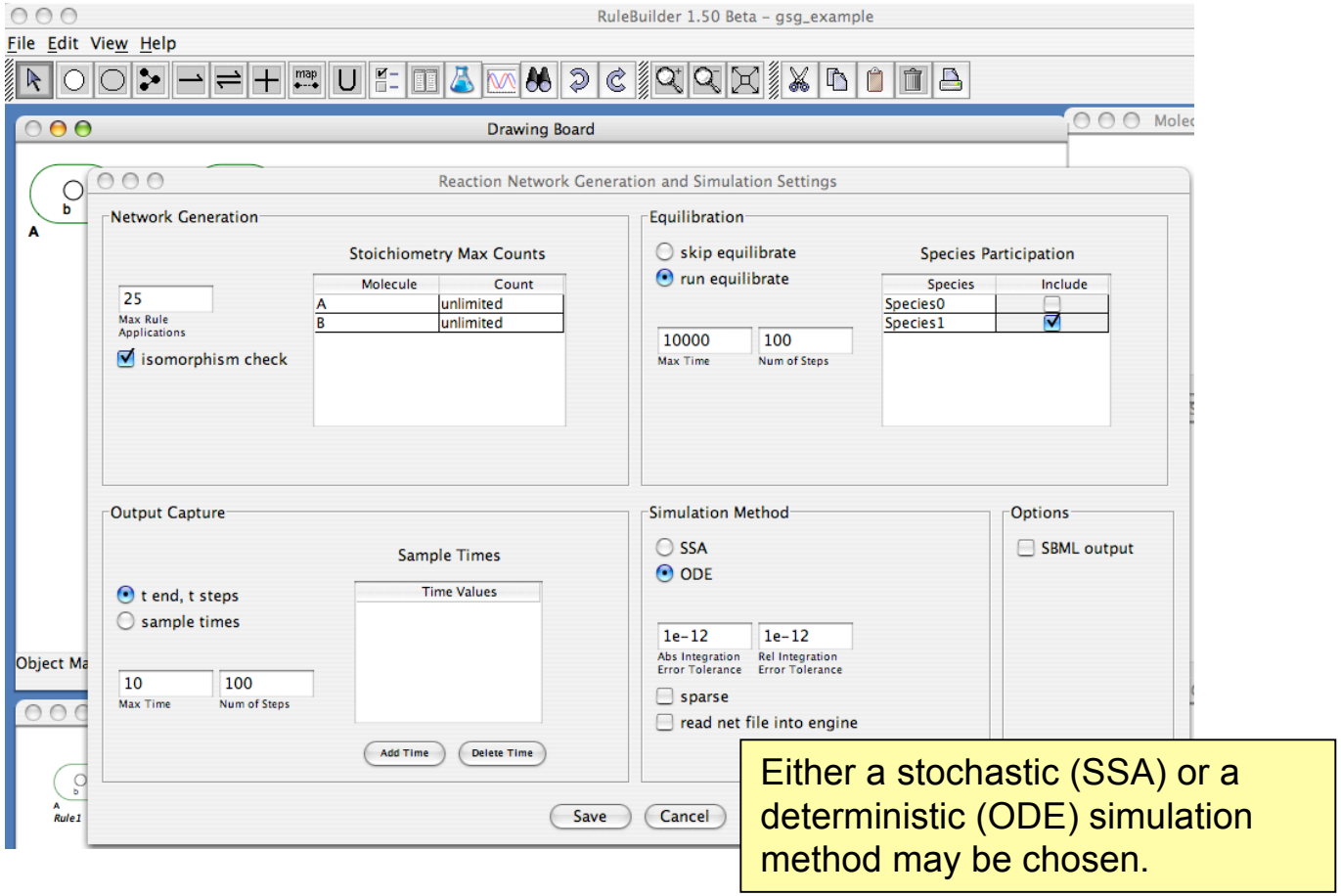


The SimConfig Panel

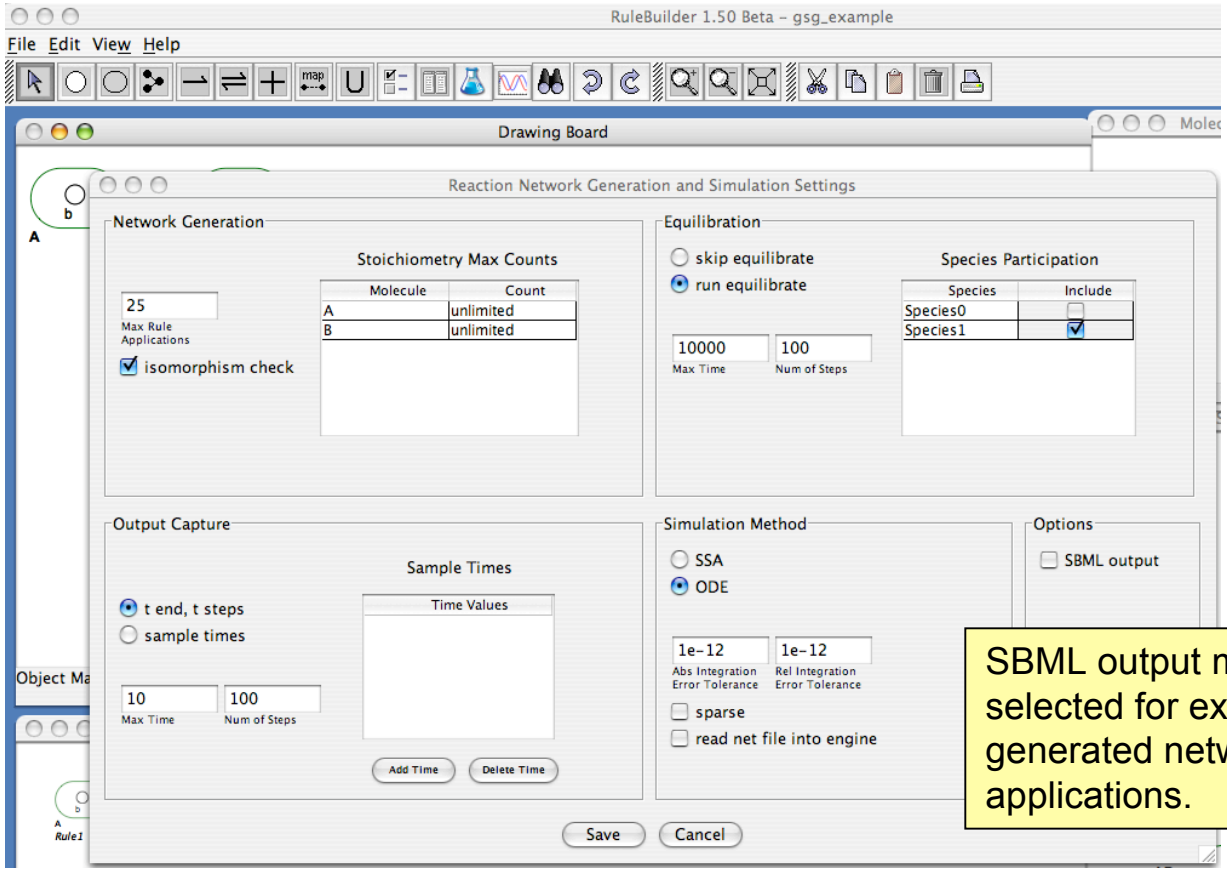


The total simulation time and the times at which concentrations are sampled are set here.

The SimConfig Panel



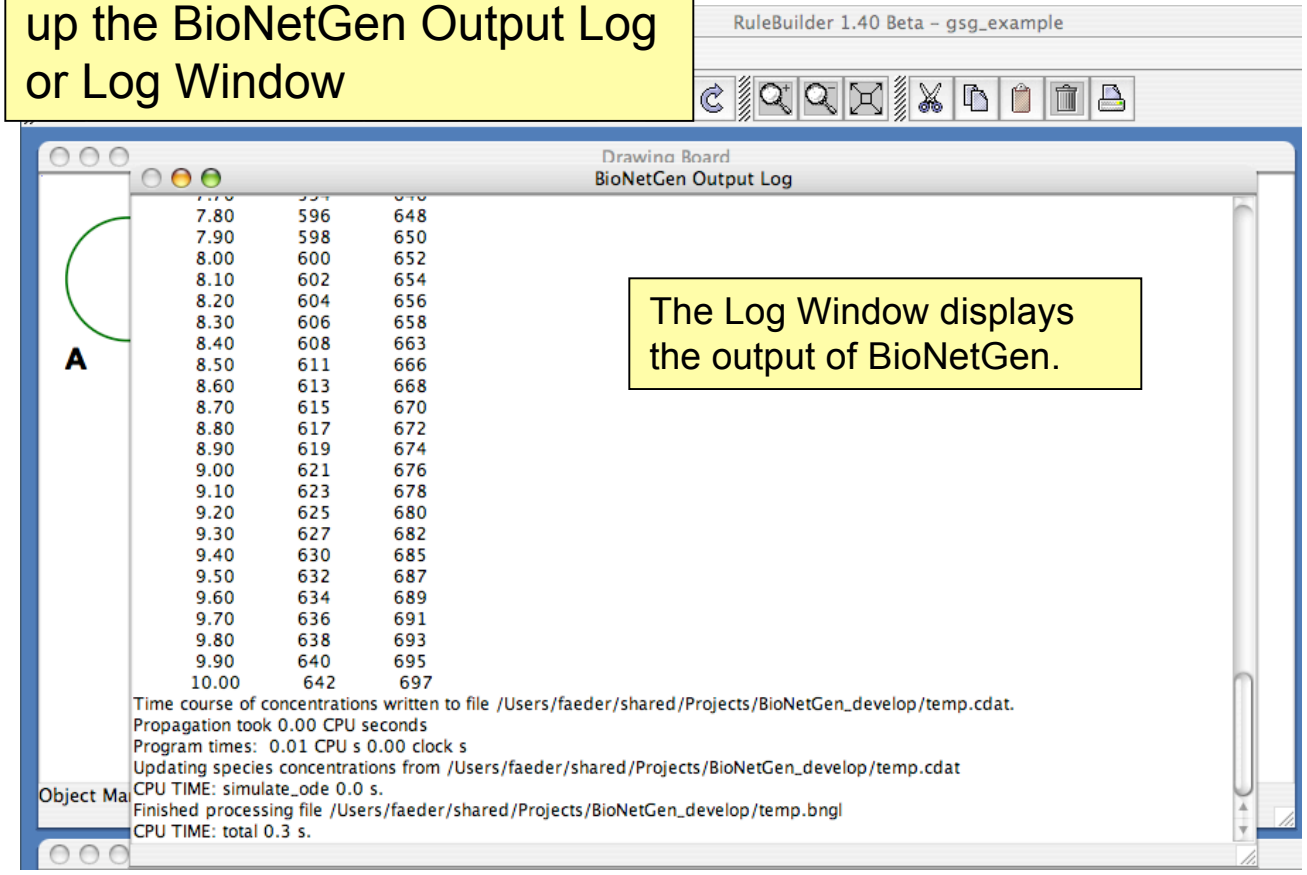
The SimConfig Panel



SBML output may be selected for export of the generated network to other applications.

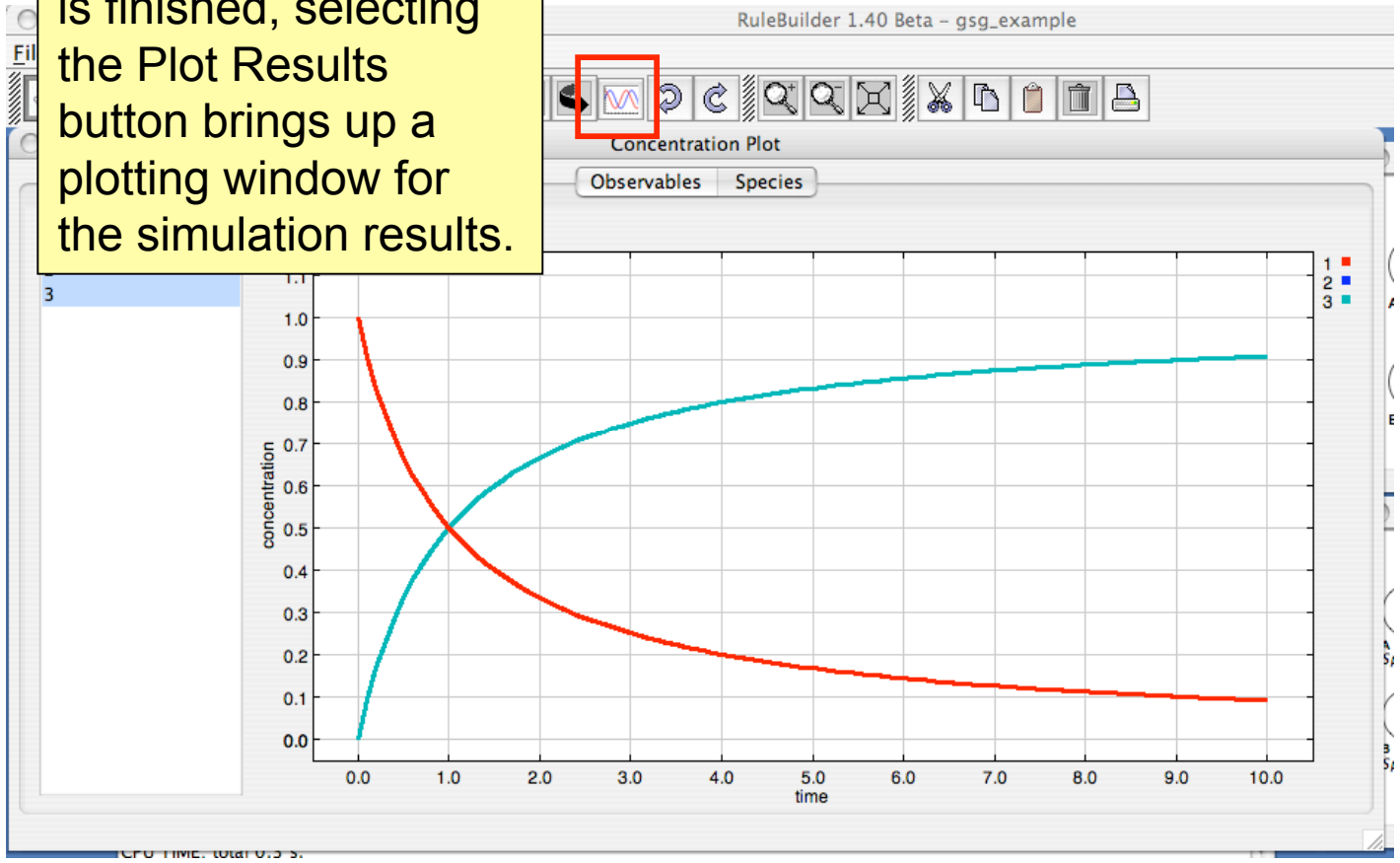
The Log Window

Running the simulation brings up the BioNetGen Output Log or Log Window

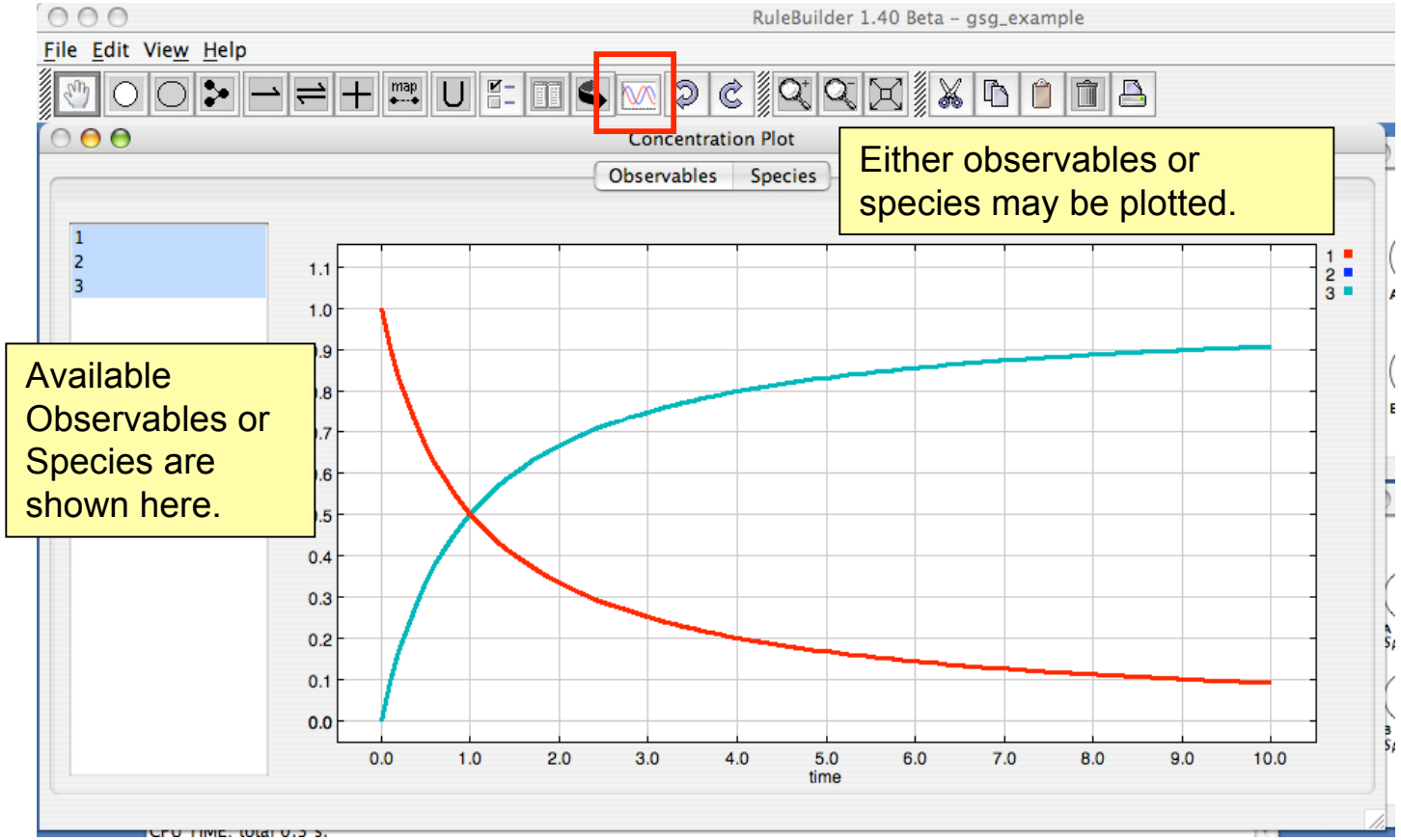


Plotting the Results

Once the simulation is finished, selecting the Plot Results button brings up a plotting window for the simulation results.



Plotting the Results



Plotting the Results