CHANGES IN CELLDESIGNER™ 1.1

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0 Attention

If you have been a user of CellDesigner 1.0, DO NOT OPEN 1.0 files with CellDesigner 1.1 and DO NOT UNINSTALL CellDesigner 1.0 before finishing reading throughout this document. Carelessly opening and saving the 1.0 files with the version 1.1 application may corrupt your data.

1 New Features in CellDesigner 1.1

1.1 SBML Level 1 Version 2 Compliant

CellDesigner 1.1 supports input/output of SBML Level 1 Version 2 files.

1.2 Species Identification on Compartments

The way of **Species** identification on the edit canvas is changed. Criteria of **Species** identification, in addition to ones of CellDesigner 1.0, include **Compartment**s that **Species** belong to and positions to their membranes where the **Species** are placed. You can treat the same biochemical **Species** in different positions as different **Species** by just placing them.

There are four distinguishable positions to membrane of a **Compartment**:

Position	Description	Usage
inside	inside, not touching to the membrane	For **Species** freely diffusing inside of the **Compartment**.
innerSurface	inside, touching to the membrane	For **Species** adsorbed on inner surface of the **Compartment**.
transmemebrane	appearing in both sides of the membrane	For **Species** spanning the membrane of the **Compartment**.
outerSurface	outside, touching to the membrane	For **Species** adsorbed on outer surface of the **Compartment**.

2 Read in CellDesigner 1.0 File

Because of change in **Species** identification, it is necessary to change format of CellDesigner 1.0 files.

CellDesigner 1.1 can automatically convert 1.0 files for the current version, but some original data may be lost in conversion process. This is caused by the fact that new **Species** and/or **Compartment**s should be created if several numbers of the same **Species** and/or the same **Compartment**s exist in 1.0 model and if they are different in 1.1 model.

(Important)
If you want to read in CellDesigner 1.0 files, make backup of the files first. Next read all the following subsections [2.1 to 2.4] to know what to be changed in automatic conversion and how to avoid it.

2.1 Read-in Steps

When you open a CellDesigner 1.0 file by CellDesigner1.1, you see the following dialog.

<The file seems to be created by lower version of CellDesigner. Do you convert it for the current version?   **Yes/No**>

Select "**No**," and reading in the file is canceled. Select "**Yes**," and the file is automatically converted and one of the following dialogs comes up.

[A]
<The conversion has finished successfully. **OK**>

[B]
<The conversion has finished successfully. But species in <listOfSpecies> and compartments in <listOfCompartments> were remade, so that their id numbers were renewed and their SBML field values were initialized. Please input the values and

check consistency in the model. (See documents attached.)   **OK**>

The former [A] indicates nothing wrong happened in conversion, while the latter [B] indicates list of **Species** and/or **Compartment**s were remade and prompts users to input the data again and check consistency.

Click **OK**, and converted model (no change in the canvas) are displayed. If the message [B] was appeared, you should check and edit SBML field data described the next subsection [2.2].

2.2 <u>What may be changed or inconsistent, when Species and Compartments are remade?</u>

The following is list of SBML fields changed in the case that list of **Species** and/or **Compartment**s were remade in automatic conversion process.

Species	
id	Changed by CellDesigner1.1
initialAmount	Initialized to "0"
units	Initialized to ""
boundaryCondition	Initialized to "false"
charge	Initialized to "0"
constant	Initialize to "false"

Compartment	
id	Changed by CellDesigner1.1
volume	Initialized to "1.0"
units	Initialized to ""
constant	Initialized to "true"

AlgabraicRule	
formula	Unchanged. ids of **Species** and **Compartment**s are also unchanged, to lead to inconsistency.

SpeciesConcentrationRule	
formula	Unchanged. ids of **Species** and **Compartment**s are also unchanged, to lead to inconsistency.
species	ids for **Species** unchanged, to lead to inconsistency.

ComparmentVolumeRule	
formula	Unchanged. ids of **Species** and **Compartment**s are also unchanged, to lead to inconsistency.
compartment	ids for **Compartment**s unchanged, to lead to inconsistency.

ParameterRule	
formula	Unchanged. ids of **Species** and **Compartment**s are also unchanged, to lead to inconsistency.

KineticLaw of Reaction	
formula	Unchanged. ids of **Species** and **Compartment**s are also unchanged, to lead to inconsistency.

2.3 What kinds of models are safe in automatic conversion?

CellDesigner 1.1 does not remake lists of **Species** and **Compartment**s for the models:

(a) Without any **Compartment**s except the default **Compartment** (edit canvas itself).

(b) With several **Compartment**s, except the default, which do not contain and do not touch any **Species**.

(c) With several **Compartment**s, only one of them includes all the **Species** "inside"(1.1 terminology) completely.

The automatic conversion also keeps consistency of original 1.0 files. So, these models are safe in conversion process.

In the other conditions, CellDesigner 1.1 may remake the lists. Even if the lists are not remade, consistency of the original 1.0 files is not guaranteed.

2.4 Instruction for Read-in 1.0 Files

When you intend to read in a 1.0 file, the following instructions are helpful.

[i] If nothing about SBML fields described in 2-2 has been edited in the 1.0 file, the result of the automatic conversion keeps consistency of the original file in any case.

[ii] If the SBML fields described in 2-2 have been edited and the edited parts are few enough to edit again, do automatic conversion and edit the parts.

[iii] If the SBML fields described in 2-2 have been edited and the edited parts are too many to edit again, first check the safe conditions (a)--(c) in 2-3.

    [iii-1] If a model in the file satisfies one of the conditions, do automatic conversion.

    [iii-2] If the model is not satisfies either of the conditions, edit the file with CellDesigner 1.0 to satisfy one of the conditions, and then read in the edited file by CellDesigner 1.1. (Removing all **Compartment**s but the default could always do this, since **Species** are global to a model created with CellDesigner 1.0.)

3 Known Bugs

(a) On Windows platforms, when a function of an SBW application or an SBW application is called from the SBW menu, sometimes the linkage to SBW is not sufficient to fail in unspecific conditions.

If the problem is due to insufficient linkage, a possible workaround is to start the SBW Broker before calling from the SBW menu. The SBW Broker can be started by selecting the "Broker start" menu from the Windows start menu -> Programs -> Systems Biology Workbench -> Utilities.

4 Fixed Bugs

(a) Fix the bugs on Sec. 8.2 in CellDesigner1.0 STARTUP GUIDE.

(b) When a type other than PROTEIN is selected in class pulldown in a dialog to appear by double-clicking **Species**, and when its name field is empty, clicking Apply button makes a **Species** with no name.

Fixed.

(c) When scrolling a large document in a small window, labels concerned with residues out from the top and/or the left of the window are disappeared.

Fixed.

(d) When there are some ModificationLinks attached, by using "add reactant" and/or "add product" buttons, to a BaseLink, and then its type is changed in a dialog to appear by double-clicking its Reaction arrow, the ModificationLinks do not move so as to keep their links to the BaseLink.

Fixed.

(e) When a BaseLink are folded by using editing points of Reactions, and then its type is changed in a dialog to appear by double-clicking its Reaction arrow, UNDO does not recover the arrow before folded.

Fixed.

(f) When height or width of a **Species** or a **Compartment** is zero by reducing its size with dragging its handle point, the Species or the **Compartment** jumps to top-left positions of the edit canvas.

Fixed.