To The Systems Biology Institute

# CellDesigner Extension Tag Specification Document

Fourth Edition

September 28, 2009
Mitsui Knowledge Industry Co., Ltd.

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Revision Record

First Edition

Created on January 31, 2006

Second Edition

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| Revised Content | Revised Section |
|---|---|
| “DRUG” was added to the class of Species. | 7.3.1 Element celldesigner:class |
| CompartmentAliasType/namePoint was added. | 8.4.2. Element compartmentAliasType/namePoint |
| ListOfBindingRegionsType and bindingRegionType were added as BindingRegions of proteins. | 8.8.1.1, 8.8.1.2 |
| A complex type that represents state was added. | 8.8.2. Element celldesigner:proteinType/listOfStructuralStates |
| BackupSize and backupView were added to elements, and complexSpeciesAlias was added to attributes. | 8.5.1. Element celldesigner:listOfComplexSpeciesAliasesType/complexSpeciesAlias |
| Active was added to attributes. | 8.9.1.1. Element celldesigner:listOfRegionsType/region |
| State details were changed. | 10.3.6.2.1 Element celldesigner:listOfModificationsType/modification |
| A complex type for layers was added. | 8.13 |
| Type details were added. ModificationType was added to attributes. | 11.10.1 Element celldesigner:listOfModificationType/modification |
| “RectangleIndex” was added to attributes. | 11.1.3. ComplexType celldesigner:connectSchemeType |

Third Edition

Revised on August 6, 2008

| Revised Content | Revised Section |
|---|---|
| StructuralStateAngle,listOfSpeciesTag and their child element data were added to complexSpeciesAlias. | 8.5.1.1, 8.5.1.2.x |
| A spelling error in the phrase listOfBindingRegions was corrected. | 8.8.1 |
| The attributes of listOfBindingRegionsType/bindingRegion were rewritten. | 8.8.1.2 |
| Celldesigner:proteinType/listOfStructuralStates was deleted. | |
| The diagram of celldesigner:speciesIdentityType/state was revised. ListOfStructuralStates was added to child elements. | 10.3.6. |
| Element celldesigner: structuralState was added. | 10.3.6.3.1. |
| Line was deleted from the attributes of celldesigner:lineType. | 11.1.2 |
| ComplexType celldesigner:lineType2 was added. | 11.1.4 |
| Two types, TRANSCRIPTION and TRANSLATION were added to celldesigner:reactionType. | 11.2 |
| Examples were revised. | 11.5.1. Element celldesigner:listOfReactantLinksType/reactantLink<br>11.6.1. Element celldesigner:listOfProductLinksType/productLink |
| Description of celldesigner:reactionAnnotationType/editPoints was revised. | 11.9 |
| BOOLEAN_LOGIC_GATE_NOT and TRIGGER were added to the type of celldesigner:listOfModificationType/modification. | 11.10.1 |

Fourth Edition

Revised on September 28, 2008

| Revised Content | Revised Section |
|---|---|
| Extension was added to the parent elements. | 8. Model annotation, 9. Compartment annotation, 10. Species annotation, 11. reaction annotation |
| InfoType was added. | 7.2.12 ComplexType celldesigner:infoType |
| Info was added to the child elements of compartmentAlias. | 8.4.1. Element celldesigner:listOfCompartmentAliasesType/compartmentAlias |
| Info was added to the child elements of complexSpeciesAlias. | 8.5.1. Element celldesigner:listOfComplexSpeciesAliasesType/complexSpeciesAlias |
| Info was added to the child elements of speciesAlias. | 8.6.1. Element celldesigner:listOfSpeciesAliasesType/speciesAlias |

# Contents

## 1. Introduction

CellDesigner[1] is a software that allows a graphical description of networks consisting of information related to components such as biomolecules and metabolites that are frequently used in the field of molecular biology, particularly systems biology research. Typical examples of target networks are gene regulatory networks that describe transcription and regulatory relationships among genes; metabolic networks (metabolic pathways) that describe the relationships of the substrates, products and enzymes of metabolic reactions; and signal transduction networks that describe intercellular signal transduction derived from activation or inactivation of molecules, changes in post-translational modification, and complex association/dissociation.

There are considerable numbers of commercial and non-commercial software programs that describe such networks, and they employ many different notational systems. CellDesigner uses the notational system developed by Kitano[2]. The main features are its high descriptive ability of biological processes, and that as much as possible, it eliminates the ambiguity so often found in many conventional systems of notation. Of particular note is the possibility to describe in detail modification states and changes in the activities of biomolecules such as proteins and nucleic acids. CellDesigner's graphical user interface allows the description of a biological process by combining such graphical notations, and enables the creation of biological process models.

CellDesigner saves created models in the SBML (Systems Biology Markup Language) format[3]. The SBML format is a standard description language for systems biology models. Systems biology is a field of study that attempts to understand target biological units as a system; the components of such biological units, e.g. cells, cell colonies, tissues, individuals, populations and their environments, are listed, and simulation is carried out for the increase/decrease of volume and quantity of such components. SBML is designed to retain minimal common information when a variety of simulations are carried out in research. SBML's descriptive core is the data needed to simulate processes, e.g. components, mathematical relationships between volume and quantity, units of volume, and parameters. CellDesigner has additional functions to edit such data; it facilitates the creation of simulation models used in the field of systems biology, and by outputting in SBML, models can be directly run or conveniently given to other researchers.

CellDesigner is an excellent tool for the efficient creation and verification of SBML models. However, the description space of a graphical model described by CellDesigner extends beyond the scope of the description space of an SBML simulation model; therefore, to enable the saving of models, any data unique to CellDesigner needs to be kept to hand. Such data is classified as: **the molecular biological meaning of components** that represent a model (e.g. molecular species, modification state, reaction type); **data to distinguish elements** when representing a model, although they do not have molecular biological meaning (e.g. type and shape of a compartment); **graphical data for elements** (e.g. color, line width, space between lines); **layout data** (e.g. display position, size); and **meta data** for a model (e.g. size and version of a model). CellDesigner is compliant with the SBML format and uses these pieces of data by appropriately embedding them as extension tags in the SBML structure.

This document explains the extension tag specifications of CellDesigner in relation to SBML. The specifications cover CellDesigner Version 4.0 (released on July 15, 2007) and SBML Level 2 Version 1[4] for the SBML file format. To use this document, basic knowledge of the SBML format is required. If necessary, refer to the specification document of the SBML format[4]. For graphical models represented by CellDesigner, refer to Reference[2] and for block diagrams of proteins particularly, refer to Reference section[5].

## 2. Graphical Model

This chapter explains the key features of models described by CellDesigner.

### 2.1. Alias

This section gives a summary of CompartmentAlias and SpeciesAlias described by CellDesigner.

Firstly, related SBML elements are explained. For example, the following components are set as XML elements in SBML: a Compartment that represents a bounded space -- a biological unit -- such as nuclei, endoplasmic reticula or cells; and a Species that represents the molecular biological components of a Compartment such as proteins, metabolites or nucleic acids. Moreover, relations between Species are associated with Reactions. The user decides what kind of item is to be actually associated with Compartment, Species, or Reaction. In fact, in many cases the three-dimensional structure of organisms are not taken into account, and simulation is conducted after creating a model based on an abstract bounded space with biological meaning and the volume of its components. Therefore, Species are usually distinguished according to the differences of chemical species and the bounded space to which they belong, and then individual Species are set. Among these elements Reactions that represent biochemical processes, such as changes and transfers due to reactions, are set to create a graph structure.

Next, we examine how to describe such a structure on a plane as a graphical network. In an organism various kinds of elements exist and when the biochemical processes are described in detail, the following problems may occur.

1. Hub elements: An element that takes part in numerous processes can be called a hub; many elements fulfill this role. This feature can be called scale-free, and reflects the fact that any combination of elements that triggers a process is not just selected at random. When a graphical model is edited, flexibility in the edit operation (change or delete) is lost for those elements that bind very closely with other elements.
2. Combining models: To combine two graphs, e.g. two logical abstract models, is a simple operation. However, when graphical data is added to these graphs, the combination of displayed items needs to be considered.

To deal with these problems CellDesigner avoids the direct display of graph structures and incorporates CompartmentAlias and SpeciesAlias into the structure (Fig. 1). In this case an SBML model corresponds to a logical abstract model with a graph-like structure. For an element that is considered to be identical to a Compartment or Species in an SBML model, multiple CompartmentAliases or SpeciesAliases can be created in a graphical model of CellDesigner (the correspondence of each Compartment and Species is indicated by pink and blue lines in Fig. 1). This enables any elements that frequently appear in a model to be arranged in separate locations, and avoids such problems as the obstruction of edit operations, or links set between elements (represented by Reactions) converging into a hub and becoming unreadable. In addition, when graphical models are combined, the drawn item of one model is just simply pasted to the drawn item of the other model. At this time, SBML models -- abstract models -- also need to be combined.

As mentioned above, CompartmentAlias and SpeciesAlias play a key role in the representation of a graphical model (Sections 8.4, 8.4.2, 8.6). Compartments and Species that appear to be created by CellDesigner are actually all CompartmentAlias and SpeciesAlias. By creating and editing CompartmentAlias and SpeciesAlias in a graphical model, Compartments and Species in an SBML model are created and updated in the background. To decide whether to add generated CompartmentAlias and SpeciesAlias to an SBML model, it is necessary to verify their identity. The identity of a Compartment is

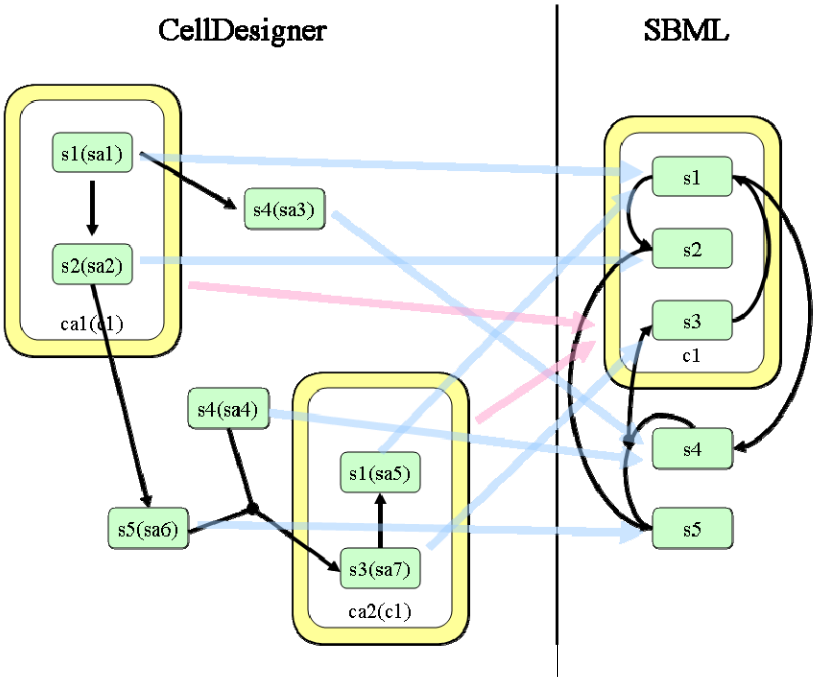


**Fig. 1 Correspondence of CompartmentAlias - Compartment and SpeciesAlias - Species, and Reactions**

## 2.2. Complex

This section describes a complex view and an object structure representing a complex.

Protein in an organism makes up many different complexes by binding with other proteins; for example, dimerization of EGF receptors during ligand binding (small scale); preinitiation complex (medium scale); and very large complex such as proteasome. As a method to conveniently create a variety of complexes in a graphical model, CellDesigner is equipped with ComplexSpeciesAlias that is a virtual container of complexes, and adopts a method to keep adding SpeciesAlias that are complex elements.

A complex created in this manner represents its elements in detail in the model; however, on the other hand, the complex will occupy a larger area in the model, and if more detailed models are created, it may be difficult to understand the overall picture of relationships among elements. In order to solve the inefficient use of display space and facilitate intuitive understanding of the overall picture, it is possible to display a generated complex in a compact way (Fig. 2). In Fig. 2, s3(sa3) and s3(sa6) are individual ComplexSpeciesAliases that refer to the same SpeciesAlias, and the figure gives a view just after the display is changed. A ComplexSpeciesAlias represents a complex, and in usual view, SpeciesAliases representing complex elements are shown inside, whereas in a compact or brief display the ComplexSpeciesAlias becomes a small bounding box (standard size) and does not display the elements inside. When the display is changed, view data before the change is retained inside the complex (ComplexSpeciesAlias) and complex elements (SpeciesAliases), in readiness for when the original view is changed again. Therefore, these elements need to retain data for the usual and brief views, and the present state (Sections 7.2.8, 7.2.9, 7.2.10).

SBML itself does not have a structure representing complexes; the graphical model shown on the left in Fig. 2 for example, corresponds to the SBML model with three Species and one Reaction shown at the upper right. To represent such a structure, CellDesigner internally retains Species corresponding to complex elements shown at the lower right in Fig. 2 (Section 8.3).

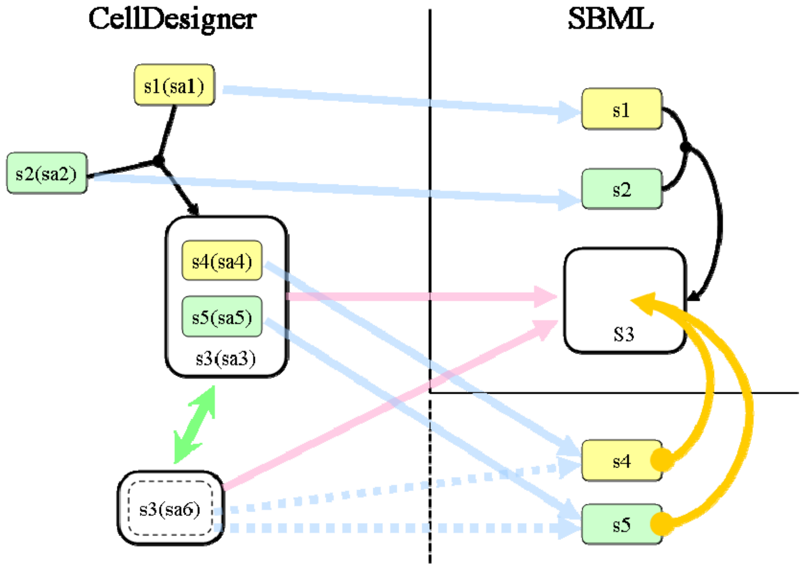


Fig. 2 Complex

### 2.3. Biomolecule

In vivo molecules such as proteins and nucleic acids are subject to modification, e.g. phosphorylation of amino-acid residues and methylation of bases, and thus change their activities in many ways resulting in their involvement in diverse biochemical processes. For partial nucleic acid sequences such as genes and RNAs, annotation relating to the gene expression process is given.

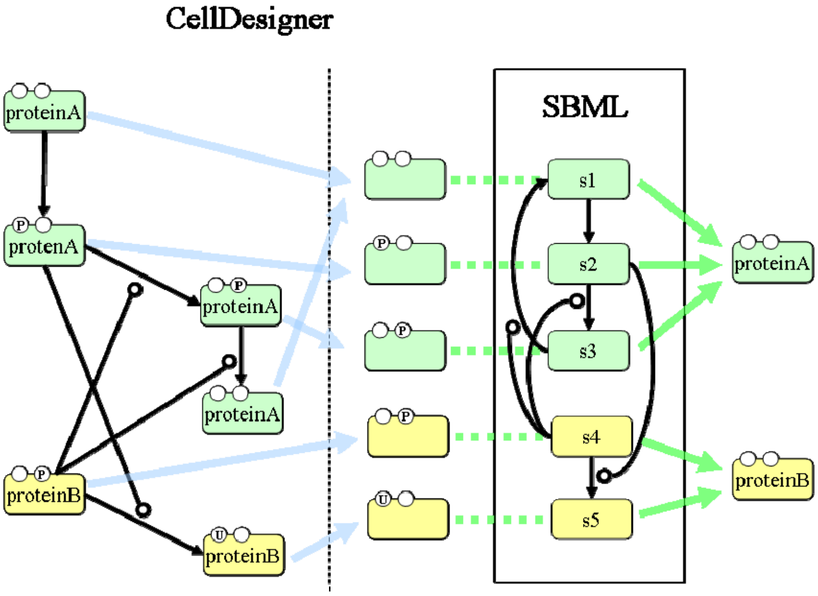


Fig. 3 Biomolecule (Protein)

In order to enable these kinds of description, CellDesigner provides data structures for proteins, genes, RNAs, and antisense RNAs (Sections 8.8, 8.10, 8.11, 8.12). For proteins and genes, "slots" can be physically provided for modification of amino-acid residues and bases. Depending on how a "slot" is modified, chemical species are distinguished and used in the identity verification of a Species (Fig. 3, Section 10.3.6).

### 2.4. Reaction

In the graphical model created by CellDesigner, biochemical processes and regulatory relationships among molecular biological elements are represented as links between (Complex)SpeciesAliases. In an SBML model this link corresponds to the Reaction between Species equivalent to (Complex)SpeciesAliases (Fig. 1). Moreover, when such regulation as enzymic activity or inhibition of biochemical processes and regulatory relationships are described in a graphical model, the regulation is represented by another link that connects a (Complex)SpeciesAlias (modifier) with the Reaction link (regulation target) (green link in Fig. 4). The next section describes the notational structure of these links in the graphical model.

Links in the graphical model are divided broadly into two categories: a link that is called the Base Reaction and can be directly set between (Complex)SpeciesAliases (black link in Fig. 4); and a link that connects a (Complex)SpeciesAlias with the Base Reaction. The latter is further divided into two categories: a Modification Link that represents regulation applied to the Base Reaction (green link in Fig. 4); and a link to describe additional reactants and products (light blue link in Fig. 4).

Reactants and products of the Base Reaction are called BaseReactant and BaseProduct (Sections 11.3, 11.4). The links to describe additional reactants/products are called ReactantLink/ProductLink (Sections 11.5, 11.6). In an SBML model there is no distinction made between the reactants/products derived from the Base Reaction and any additional reactants/products, and the relevant Species are listed as Reactant/Product. In addition, a Species corresponding to a (Complex)SpeciesAlias that is connected to a Modification Link (Modification, Section 11.10) is listed as a Modifier.

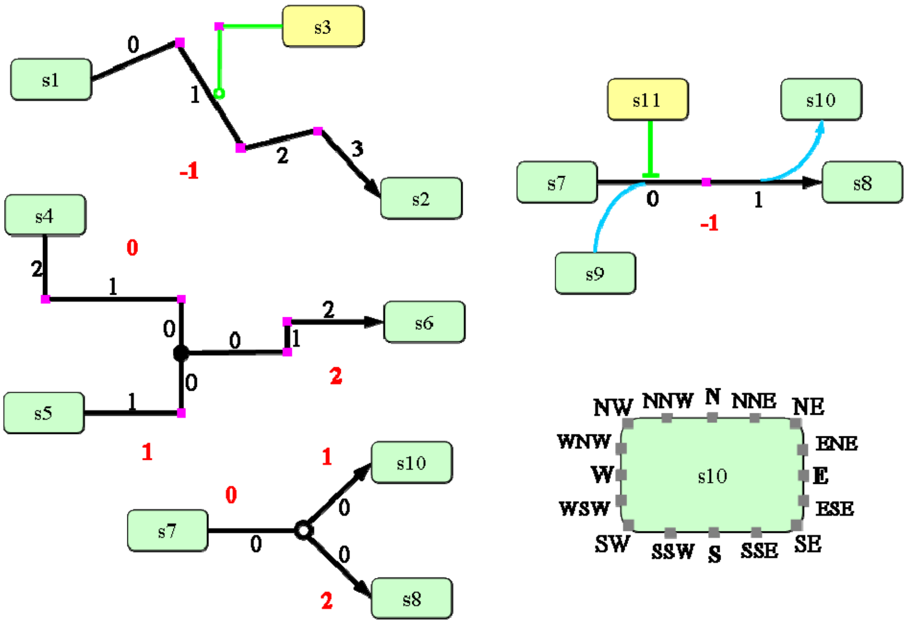


**Fig. 4 Information associated with Reactions**

An arbitrary number of edit points can be set for the Base Reactions and Modification Links, and links can be bent using these edit points. The base links are classified into non-branch type and branch type, and to identify them a “branch index” (-1 for a non-branch type, and 0, 1, 2 for a branch type) is set (red numerals in Fig. 4). To distinguish individual line segments from a set of line segments that form each branch, a "line segment index" (0, 1, 2...) is set from the starting point side for the non-branch type, and from the branch point side for the branch type.

On a Base Reaction link line, a process box that represents the type of reaction is displayed. On the process box perimeter point indexes (2, 3, 4, 5, 6, and 7) to add Modification Links are set (Fig. 4.2). Modification Links can only be connected with these index points. A ReactantLink can only be connected with Index 0 and a ProductLink only with Index 1 (specifications available from Ver.4.0).

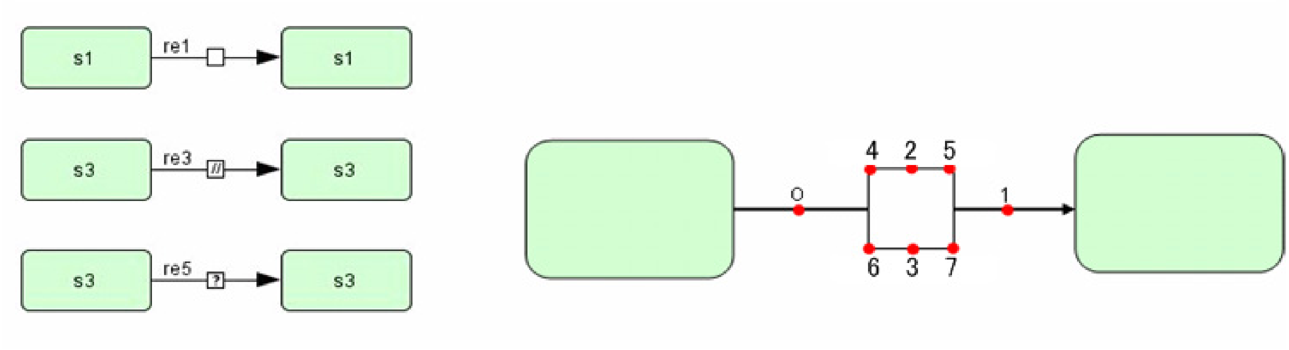


Fig. 4.2

When a Base Reaction, Modification Link or ReactantLink/ProductLink is connected on the (Complex)SpeciesAlias side, they are connected to any of the 16 points on the perimeter. A connection point is specified using abbreviations representing the 16 directions (lower right in Fig. 4).

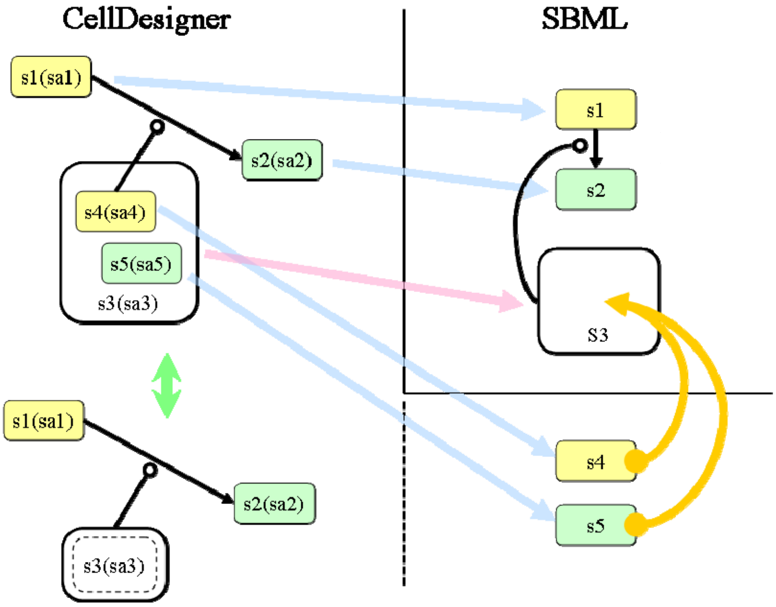


**Fig. 5 Reaction and complex**

When a link is set for a complex, the link can be drawn from either ComplexSpeciesAlias (a virtual container of complexes) or SpeciesAlias (a complex element) (Fig. 5 shows an example of links drawn from complex elements). In the corresponding SBML model, both cases are interpreted as a link from a complex Species.

### 2.5. Block Diagram

This section describes a block diagram associated with protein.

A block diagram is a diagram that focuses on a specific protein and represents an overall picture of the biochemical processes associated with the protein, including other enzymes that affect the modification of residues, partner molecules forming a complex, activities that change according to states and the effect on targets, or self-degradation (e.g. [5], Figure 1 (b)). It is also possible to provide internal logic to represent the different kinds of relationships between each process.

From a graphical model of a biochemical process, CellDesigner extracts the relationships with other biomolecules such as protein (e.g. influence on modification state of residues, complex formation, enzymic activity in the reaction with other molecules) and automatically creates a block diagram (red-circled sections in Fig. 6). The mutual relationships between these elements can be created and edited as internal logic. The created block diagram is also saved in an SBML file for each target protein (Section 8.13).

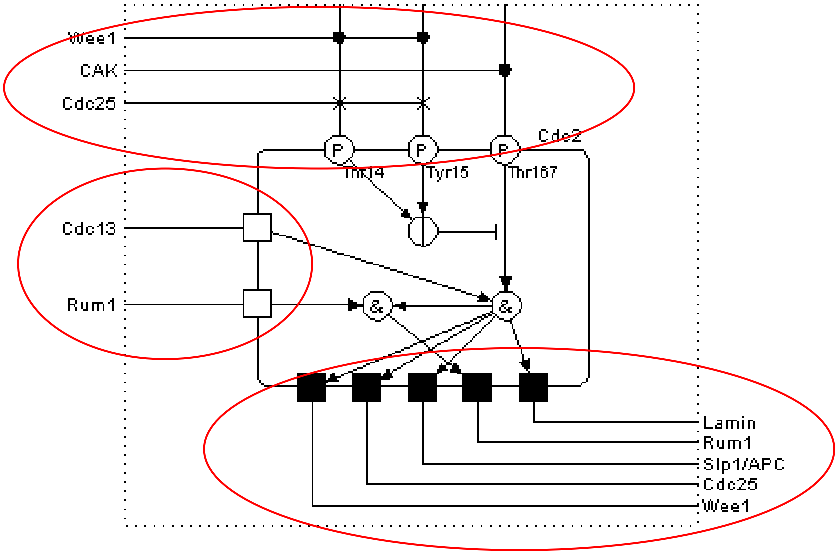


**Fig. 6 Block diagram (the red-circled sections indicate relationships with other biomolecules)**

## 3. Namespace and Schema

In relation to SBML, CellDesigner extension tags are defined as XML elements that belong to namespace,

http://www.sbml.org/2001/ns/celldesigner

and in an XML schema file,

sbmlCellDesignerExtension_v2_5.xsd.

| | |
|---|---|
| schema file: | **sbmlCellDesignerExtension_v2_5.xsd** |
| attribute form default: | **unqualified** |
| element form default: | **qualified** |
| targetNamespace: | **http://www.sbml.org/2001/ns/celldesigner** |

In the input/output SBML files of the actual CellDesigner application, CellDesigner extension tags are embedded under the annotation elements of SBase derived classes defined in SBML -- Model, Compartment, Species, Reaction, SpeciesReference, and ModifierSpeciesReference. To restrict the structure under annotation, each SBase derived class is redefined in a schema file,

CellDesigner.xsd.

| | |
|---|---|
| schema file: | **CellDesigner.xsd** |
| attribute form default: | **unqualified** |
| element form default: | **qualified** |
| targetNamespace: | **http://www.sbml.org/sbml/level2** |

## 4. Description Rules

This document aims to define extension tags for those tags defined in SBML; therefore, the same names or similar names can be found in their definitions. To distinguish them, for XML elements defined in SBML, `SBML.` is used in an abstract data model, and a prefix `sbml:` is used for actual description in an XML file. For XML elements defined in CellDesigner extension, `CellDesigner.` is used for an abstract data model, and a prefix `celldesigner:` is used for actual description in an XML file.

Namespace that represents XML schema is

`http://www.w3.org/2001/XMLSchema.`

For XML elements to describe XML schema, a prefix `xs:` is used.

The description format in this document conforms to the description format of XML schema, and the description within CellDesigner extension tag schema and SBML redefinition schema. Definitions of complex data type (complexType) are used as elements in the definitions of schema or others. The name of this complex data type is given as an option; however, “someElementNameType” is given to an element name “someElementName”. Therefore, when a complex data type is used as an XML element, the tag name is created by removing “Type” from the end of the name. However, for a complex type to redefine an annotation tag in SBML, to avoid name collision, the annotation of Model, for example, is named “modelAnnotationType”.

## 5. Notational System

### 5.1. Notational Format

Chapter 7 and the following chapters describe CellDesigner extension tag specifications in accordance with the definitions of the CellDesigner extension tags in XML schema. These specifications describe the built-in data types of XML schema, user definition of data types, and derivations. A summary and structure of XML schema, and specifications of the data types are given in Bibliography [6], [7], and [8].

Moreover, these specifications use diagrams to represent structural definitions of tags represented by XML schema. The next section explains the notational system of diagrams.

### 5.2. Structural Display Diagram

#### 5.2.1. Element Declaration

Declares a tag in XML representation.

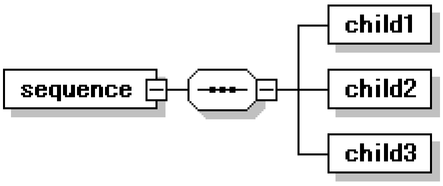
#### 5.2.2. Complex Type Definition

Defines a complex type that has child elements or attributes.

#### 5.2.3. Compositor

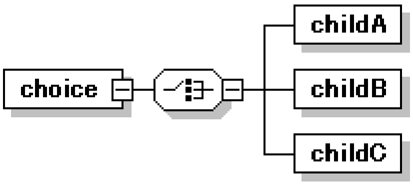
Stipulates behavior of element occurrence in the complex type definition. The following two are used.

#### 5.2.3.1. Sequence



Represents that child elements occur (in the order of definition).

#### 5.2.3.2. Choice



Represents that any one of the defined children occurs.

#### 5.2.4. Elements Including Characters

Represents that an element including characters exists between a start tag and end tag.

### 5.2.5. Optional Element

Represents an element used as an option.

### 5.2.6. Reference

Represents that an element defined globally (i.e. at the top level in schema) is referred to.

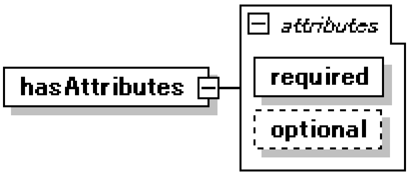
### 5.2.7. Multiple Elements

Represents inclusion of multiple elements. The numerals at the lower part represent a restriction in the number of element occurrences.

### 5.2.8. Existence of Lower Structure

Represents that attributes or child elements are defined (omitted in notation).

### 5.2.9. Display of Attributes



Represents that attributes are defined. A solid line box represents an essential attribute, and a dotted line box represents an optional attribute.

## 6. General Composition

Fig. 1 shows the whole structure of SBML and extension points of CellDesigner extension tags in relation to the SBML structure. CellDesigner stores extension tags as child elements of `Sbase.annotations` that are created in order to store data unique to applications under SBML specifications. More specifically, extension is applied to the following:

- `Model.annotation`
- `Compartment.annotation`
- `Species.annotation`
- `Reaction.annotation`
- `SpeciesReference.annotation`
- `ModifierSpeciesReference.annotation`

Most of the extension tags in CellDesigner exist under `Model.annotation`.

Chapter 7 describes XML elements that are widely used in the extension tag specifications.

Chapter 8 and the following chapters describe the specifications of extension tags at each extension point mentioned above in accordance with the SBML structure.

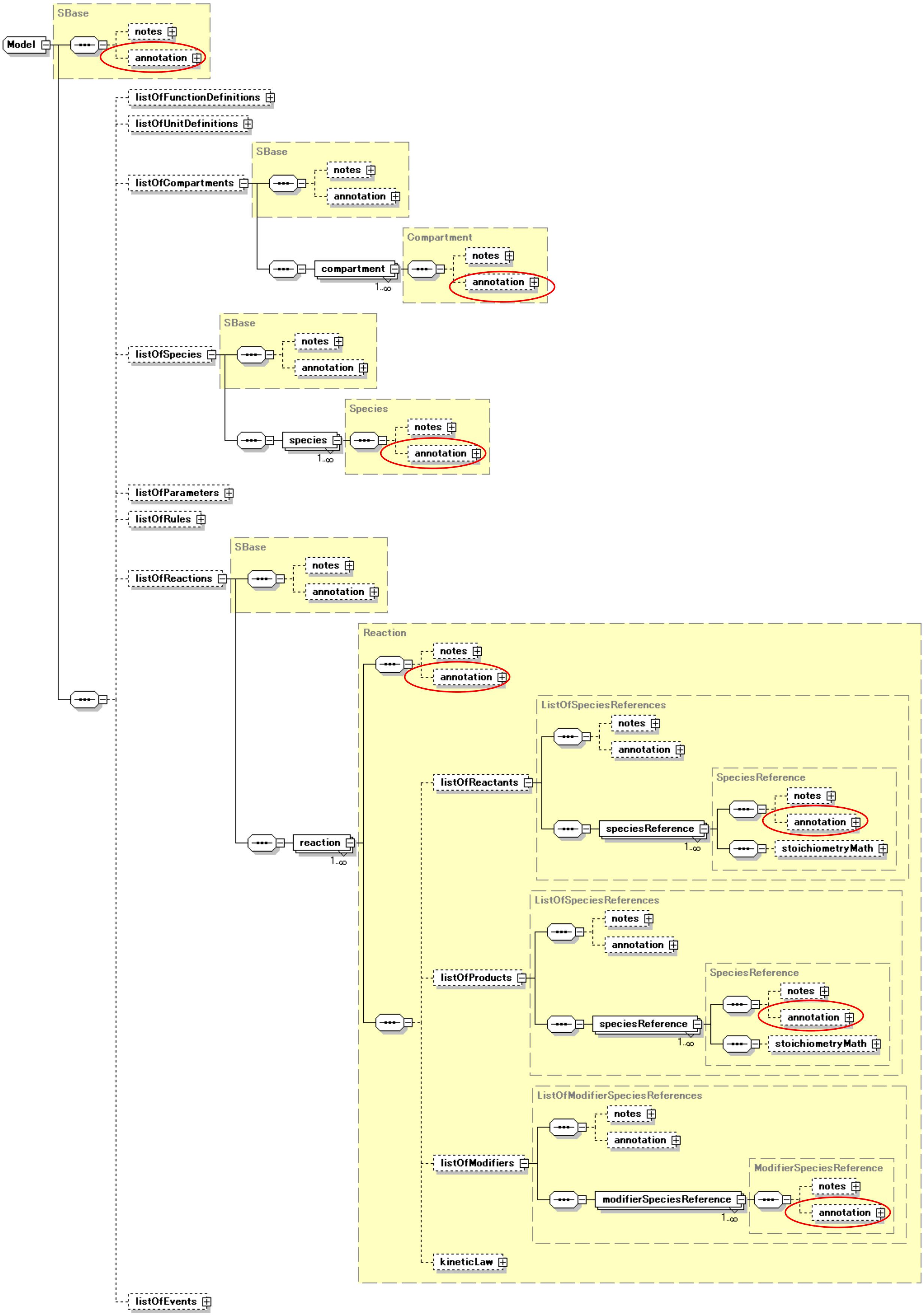


**Fig. 7 SBML structure (Model and under) and CellDesigner extension points (circled in red)**

# 7. Common Elements

## 7.1. Simple Type Definition

### 7.1.1. SimpleType celldesigner:SId

This is a data type to be used when identification is needed in a substantial data structure of CellDesigner extension tags. Restriction of the pattern is subject to specifications of CellDesigner application; however there is still a need to refer to SId in SBML definitions and therefore, equal definitions are provided.

<table>
<tr><td>namespace</td><td colspan="2">http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td colspan="2">restriction of **xs:string**</td></tr>
<tr><td>used by</td><td>elements</td><td>celldesigner:alias celldesigner:antisensernaReference<br>celldesigner:complexSpecies celldesigner:geneReference<br>celldesigner:proteinReference celldesigner:rnaReference</td></tr>
<tr><td></td><td>complexTypes</td><td>celldesigner:AntisenseRNAType celldesigner:baseProductType<br>celldesigner:baseReactantType<br>celldesigner:bindingSiteInBlockDiagramType<br>celldesigner:blockDiagramType<br>celldesigner:compartmentAliasType<br>celldesigner:compartmentAliasType<br>celldesigner:complexSpeciesAliasType<br>celldesigner:complexSpeciesAliasType<br>celldesigner:effectTargetInBlockDiagramType<br>celldesigner:geneType celldesigner:groupType<br>celldesigner:linkTargetType celldesigner:modificationResidueType<br>celldesigner:productLinkType celldesigner:proteinType<br>celldesigner:reactantLinkType celldesigner:regionType<br>celldesigner:residueInBlockDiagramType celldesigner:RNAType<br>celldesigner:speciesAliasType celldesigner:speciesAliasType<br>celldesigner:speciesAliasType</td></tr>
<tr><td></td><td>attributes</td><td>celldesigner:speciesType/@compartment<br>celldesigner:speciesType/@id<br>celldesigner:productLinkType/@product<br>celldesigner:reactantLinkType/@reactant<br>celldesigner:catalyzedType/@reaction<br>celldesigner:effectSiteInBlockDiagramType/@reaction<br>celldesigner:listOfModificationsType/modification/@residue<br>celldesigner:speciesType/@spatialSizeUnits<br>celldesigner:complexSpeciesAliasType/@species<br>celldesigner:speciesAliasType/@species<br>celldesigner:effectSiteInBlockDiagramType/@species<br>celldesigner:baseReactantType/@species<br>celldesigner:baseProductType/@species<br>celldesigner:linkTargetType/@species<br>celldesigner:speciesType/@substanceUnits</td></tr>
<tr><td>facets</td><td>pattern</td><td>(_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*</td></tr>
</table>

### 7.1.2. SimpleType celldesigner:SIdSet

This is a data type introduced for convenience to restrict a character pattern. This is a string in which SIds are connected with a comma ",".

<table>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>restriction of <b>xs:string</b></td></tr>
<tr><td>used by</td><td>complexTypes <b>celldesigner:modificationType</b><br><b>celldesigner:modificationType</b></td></tr>
<tr><td>facets</td><td>pattern (_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*(,(_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*)*</td></tr>
</table>

### 7.1.3. SimpleType celldesigner:point2D

This is a data type; two strings that represent numerical values corresponding to two-dimensional coordinates are connected with a comma ",". This is introduced to restrict data content.

<table>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>restriction of <b>xs:string</b></td></tr>
<tr><td>used by</td><td>simpleType <b>celldesigner:point2DList</b></td></tr>
<tr><td>facets</td><td>pattern (\+|-)?[0-9]+(\.[0-9]*)?((e|E)(\+|-)?[0-9]+)?,(\+|-)?[0-9]+(\.[0-9]*)?((e|E)(\+|-)?[0-9]+)?</td></tr>
</table>

### 7.1.4. SimpleType celldesigner:point2Dlist

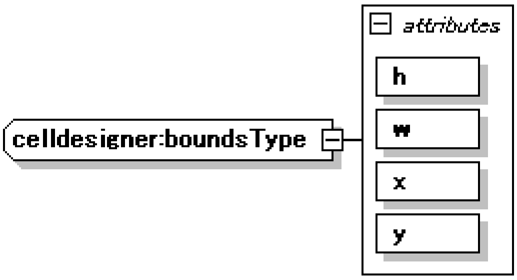
This is a data type and simple type point2Ds are connected with a comma ",". This is introduced to restrict data content.

| | |
|---|---|
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | list of **celldesigner:point2D** |
| properties | final list |
| used by | complexTypes **celldesigner:editPointsType**<br>**celldesigner:modificationType** |

## 7.2. Complex Type Definition

### 7.2.1. ComplexType celldesigner:boundsType

This is an XML element that represents a bounding box for an element represented by a box in a graphical model.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>used by</td><td>elements <b>celldesigner:compartmentAliasType/bounds</b><br><b>celldesigner:complexSpeciesAliasType/bounds</b><br><b>celldesigner:speciesAliasType/bounds</b></td></tr>
</table>

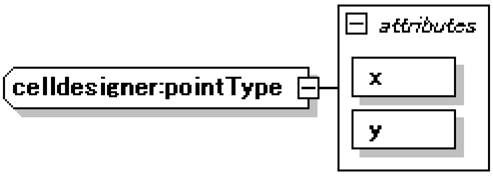
| | | | | | |
|---|---|---|---|---|---|
| attributes | Name | Type | Use | Default | Fixed |
| | h | **derived by: xs:decimal** | required | | |
| | w | **derived by: xs:decimal** | required | | |
| | x | **derived by: xs:decimal** | required | | |
| | y | **derived by: xs:decimal** | required | | |

Example

```
<celldesigner:bounds h="240.0" w="720.0" x="140.0" y="80.0" />
```

### 7.2.2. ComplexType celldesigner:pointType

This is an XML element that represents the position of an element represented by a point in a graphical model.

| | | | | | |
|---|---|---|---|---|---|
| diagram |  | | | | |
| namespace | http://www.sbml.org/2001/ns/celldesigner | | | | |
| used by | element | **celldesigner:compartmentAliasType/point** | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | x | **derived by: xs:decimal** | required | | |
| | y | **derived by: xs:decimal** | required | | |

Example

```
<celldesigner:point x="160.0" y="500.0" />
```

### 7.2.3. ComplexType celldesigner:innerPositionType

When a displayed item is located inside another element, this XML element specifies the relative position to the upper element.

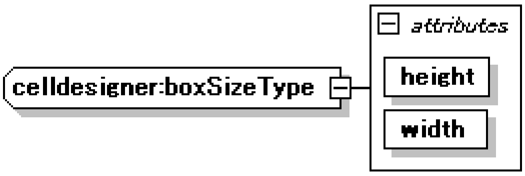
| | | | | | |
|---|---|---|---|---|---|
| diagram |  | | | | |
| namespace | http://www.sbml.org/2001/ns/celldesigner | | | | |
| used by | elements | **celldesigner:usualViewType/innerPosition**<br>**celldesigner:briefViewType/innerPosition** | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | x | **derived by: xs:decimal** | required | | |
| | y | **derived by: xs:decimal** | required | | |

Example

```
<celldesigner:innerPosition x="-159.75" y="970.28125" />
```

### 7.2.4. ComplexType celldesigner:boxSizeType

When a displayed item is represented by a box, this XML element specifies the width and height of the box.

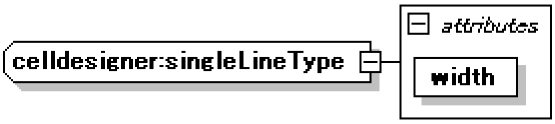
<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>used by</td><td><table><tr><td>elements</td><td><b>celldesigner:usualViewType/boxSize celldesigner:briefViewType/boxSize</b></td></tr></table></td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr>
<tr><td>height</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>width</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
</table></td></tr>
</table>

Example

```
<celldesigner:boxSize height="89.0" width="163.0" />
```

### 7.2.5. ComplexType celldesigner:singleLineType

This is an XML element that indicates a displayed item as a single line, and the line width is specified by the attribute value.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>used by</td><td><table><tr><td>elements</td><td><b>celldesigner:usualViewType/singleLine<br>celldesigner:briefViewType/singleLine</b></td></tr></table></td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr>
<tr><td>width</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
</table></td></tr>
</table>

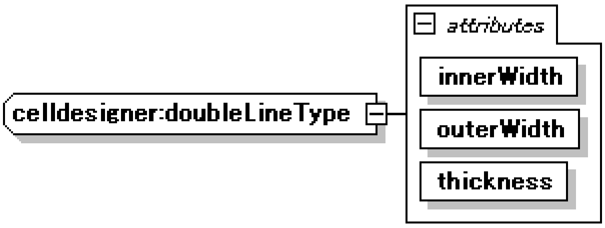
Example

```
<celldesigner:singleLine width="2.0" />
```

### 7.2.6. ComplexType celldesigner:doubleLineType

This is an XML element that indicates an item is displayed as two lines, and the width of the inside and outside line is specified by innerWidth and outerWidth, and the distance between the two lines is specified by the thickness value.

Tomoko Tanabe

<table>
<tr><td>diagram</td><td> </td></tr>
</table>

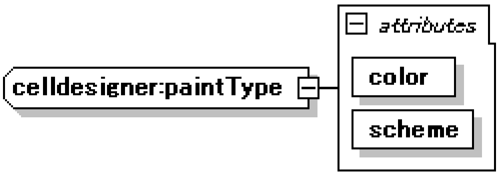
| | | | | | |
|---|---|---|---|---|---|
| namespace | http://www.sbml.org/2001/ns/celldesigner | | | | |
| used by | element | **celldesigner:compartmentAliasType/doubleLine** | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | innerWidth | **derived by: xs:decimal** | required | | |
| | outerWidth | **derived by: xs:decimal** | required | | |
| | thickness | **derived by: xs:decimal** | required | | |

Example

```
<celldesigner:doubleLine innerWidth="1.0" outerWidth="2.0" thickness="12.0" />
```

### 7.2.7. ComplexType celldesigner:paintType

This is an XML element to paint a displayed item and specify its color. The attribute for color is an 8-digit hexadecimal number that specifies αRGB, and for scheme is either “Color” (painted with a specified color) or “Gradation” (gradation with a specified color and white).

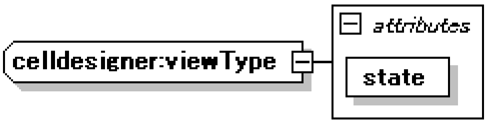
| | | | | | |
|---|---|---|---|---|---|
| diagram |  | | | | |
| namespace | http://www.sbml.org/2001/ns/celldesigner | | | | |
| used by | elements | **celldesigner:usualViewType/paint celldesigner:briefViewType/paint celldesigner:compartmentAliasType/paint** | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | color | **derived by: xs:string** | required | | |
| | scheme | **derived by: xs:string** | optional | | |

Example

```
<celldesigner:paint color="ff7f0000" scheme="Color" />
```

### 7.2.8. ComplexType celldesigner:viewType

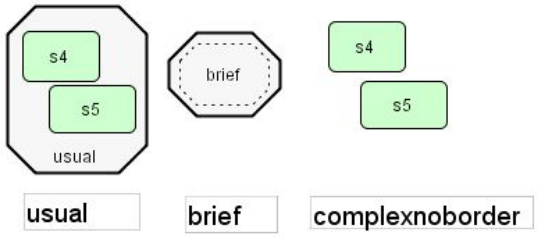
This is an XML element to specify the viewing state: usual or brief. The attribute state is any string of “usual”, “brief”, “complexnoborder”, “complexparentbrief”, or “none”. For the display of each state in celldesigner, refer to Fig. 7.2.8. Complexnoborder is used only for the viewType of complexSpeciesAlias. From Ver. 4.0, a complex can include other complexes; when the state of a parent complex (a complex includes complexes inside) is “brief”, the state of a child (an included complex) is “complexparentbrief”.

| | | | | | |
|---|---|---|---|---|---|
| diagram |  | | | | |
| namespace | http://www.sbml.org/2001/ns/celldesigner | | | | |
| used by | elements | **celldesigner:complexSpeciesAliasType/view<br>celldesigner:speciesAliasType/view** | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | state | **derived by: xs:string** | required | | |

Example

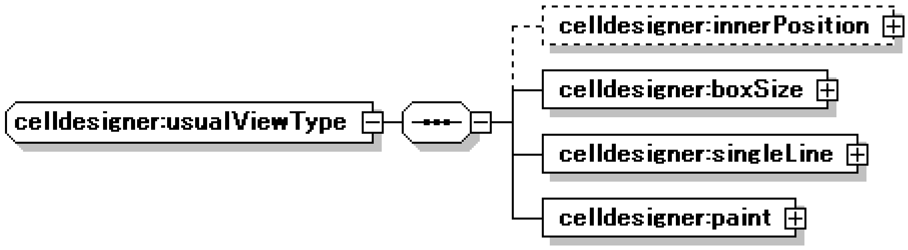
```
<celldesigner:view state="usual" />
```

Fig. 7.2.8 Display of usual, brief, and complexnoborder



### 7.2.9. ComplexType celldesigner:usualViewType

This is an XML element that retains the usual view data of a displayed item.

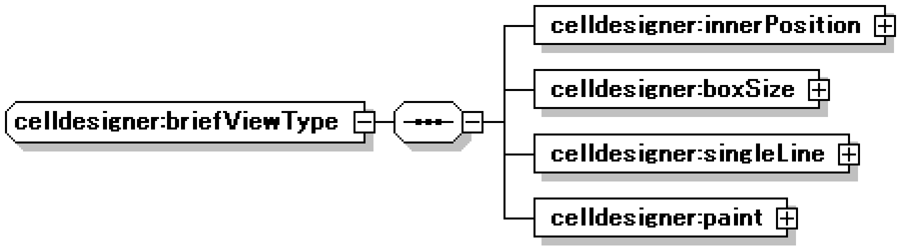
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| children | **celldesigner:innerPosition celldesigner:boxSize celldesigner:singleLine celldesigner:paint** |
| used by | elements **celldesigner:complexSpeciesAliasType/usualView**<br>**celldesigner:speciesAliasType/usualView** |

Example

```
<celldesigner:usualView>
  <celldesigner:innerPosition x="-135.0" y="-1.0" />
  <celldesigner:boxSize height="88.0" width="110.0" />
  <celldesigner:singleLine width="2.0" />
  <celldesigner:paint color="ffffffff" scheme="Color" />
</celldesigner:usualView>
```

### 7.2.10. ComplexType celldesigner:briefViewType

This is an XML element that retains brief view data of a displayed item.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| children | **celldesigner:innerPosition celldesigner:boxSize celldesigner:singleLine celldesigner:paint** |

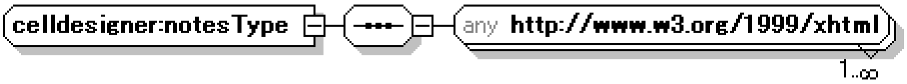
| | | |
|---|---|---|
| used by | elements | **celldesigner:complexSpeciesAliasType/briefView**<br>**celldesigner:speciesAliasType/briefView** |

Example

```
<celldesigner:briefView>
  <celldesigner:innerPosition x="0.0" y="0.0" />
  <celldesigner:boxSize height="60.0" width="80.0" />
  <celldesigner:singleLine width="2.0" />
  <celldesigner:paint color="ffffffff" scheme="Color" />
</celldesigner:briefView>
```

### 7.2.11. ComplexType celldesigner:notesType

This is an XML element that represents CellDesigner.Notes equivalent to SBML.Notes. This element is redefined because SBML.Notes cannot be reused.

| | | |
|---|---|---|
| diagram | |  |
| namespace | | http://www.sbml.org/2001/ns/celldesigner |
| used by | elements | **celldesigner:speciesType/notes celldesigner:proteinType/notes celldesigner:geneType/notes celldesigner:RNAType/notes celldesigner:AntisenseRNAType/notes** |

Example

```
<celldesigner:notes>
  <html xmlns="http://www.w3.org/1999/xhtml">
    <!-- Notes by CellDesigner -->
    <body>This is protein notes.</body>
  </html>
</celldesigner:notes>
```

### 7.2.12. ComplexType celldesigner:infoType

This is an element to store data for unit of information. For state, “open” or “close” is set. The value of prefix or label is a value defined by “unit of information” in SBGN (for details, refer to the SBGN specification document).

| | | |
|---|---|---|
| diagram | |  |
| namespace | | http://www.sbml.org/2001/ns/celldesigner |
| used by | elements | **compartmentAliasType/info complexSpeciesAliasType/info speciesAliasType/info** |

attributes

| Name | Type | Use | Default | Fixed | annotation |
|---|---|---|---|---|---|
| state | xs:string | optional | | | |
| prefix | xs:string | optional | | | |
| label | xs:string | optional | | | |
| angle | xs:decimal | required | | | |

source

```
<xs:complexType name="infoType">
  <xs:attribute name="state" type="xs:string" use="optional"/>
  <xs:attribute name="prefix" type="xs:string" use="optional"/>
  <xs:attribute name="label" type="xs:string" use="optional"/>
  <xs:attribute name="angle" type="xs:decimal" use="required"/>
</xs:complexType>
```

## 7.3. Element Declaration

### 7.3.1. Element celldesigner:class

This is an XML element to identify a class of a Species or Compartment as an element of a graphical model.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | restriction of **xs:string** |
| properties | content simple |
| used by | complexTypes **celldesigner:compartmentAliasType celldesigner:speciesIdentityType** |
| facets | enumeration PROTEIN<br>enumeration GENE<br>enumeration RNA<br>enumeration ANTISENSE_RNA<br>enumeration PHENOTYPE<br>enumeration ION<br>enumeration SIMPLE_MOLECULE<br>Enumeration DRUG<br>enumeration UNKNOWN<br>enumeration COMPLEX<br>enumeration SQUARE<br>enumeration OVAL<br>enumeration SQUARE_CLOSEUP_NORTHWEST<br>enumeration SQUARE_CLOSEUP_NORTHEAST<br>enumeration SQUARE_CLOSEUP_SOUTHWEST<br>enumeration SQUARE_CLOSEUP_SOUTHEAST<br>enumeration SQUARE_CLOSEUP_NORTH<br>enumeration SQUARE_CLOSEUP_EAST<br>enumeration SQUARE_CLOSEUP_WEST<br>enumeration SQUARE_CLOSEUP_SOUTH<br>enumeration DEGRADED |

Example

```
<celldesigner:class>SIMPLE_MOLECULE</celldesigner:class>
```

### 7.3.2. Element celldesigner:name

This is an XML element to represent the name of an element in a graphic model.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | restriction of **xs:string** |
| properties | content simple |
| used by | complexTypes **celldesigner:compartmentAnnotationType**<br>**celldesigner:reactionAnnotationType**<br>**celldesigner:speciesIdentityType** |

Example

```
<celldesigner:name>MAPK</celldesigner:name>
```

### 7.3.3. Element celldesigner:activity

This is an XML element that indicates the activity state of a biomolecule: active or inactive.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | restriction of **xs:string** |
| properties | content simple |
| used by | complexTypes **celldesigner:complexSpeciesAliasType**<br>**celldesigner:speciesAliasType** |
| facets | enumeration active<br>enumeration inactive |

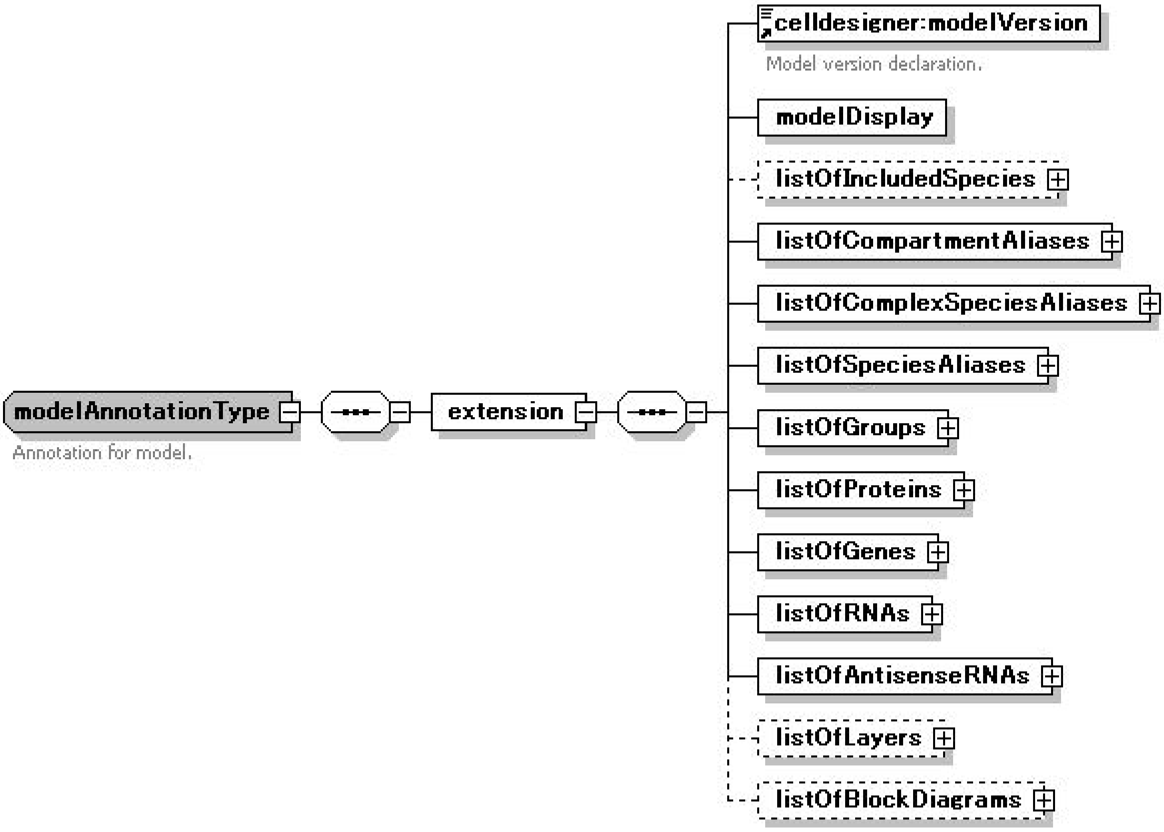
Example

```
<celldesigner:activity>inactive</celldesigner:activity>
```

## 8. Extension of Model.Annotation

Most of the graphical model data is stored under Model.Annotation.

### Element Model/annotation

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| children | celldesigner:modelVersion celldesigner:modelDisplay celldesigner:listOfIncludedSpecies celldesigner:listOfCompartmentAliases celldesigner:listOfComplexSpeciesAliases celldesigner:listOfSpeciesAliases celldesigner:listOfGroups celldesigner:listOfProteins celldesigner:listOfGenes celldesigner:listOfRNAs celldesigner:listOfAntisenseRNAs celldesigner:listOfLayers celldesigner:listOfBlockDiagrams |
| annotation | documentation<br>Annotation for model. |

### 8.1. Element modelVersion

This is an XML element to describe the internal identification number of a graphical model represented by CellDesigner. For CellDesigner3.0, 2.5 is set for the fixed value.

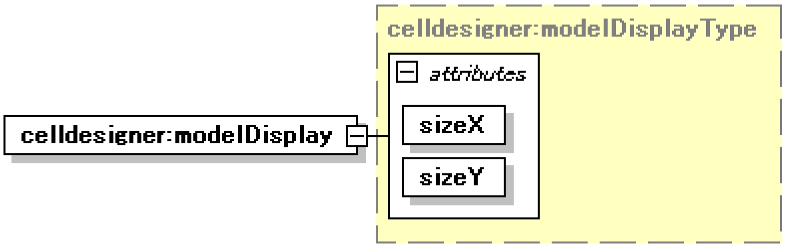
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | restriction of **xs:decimal** |
| properties | content simple<br>fixed 2.5 |
| used by | complexType **celldesigner:modelAnnotationType** |
| facets | minInclusive 0.0 |

Example

```
<celldesigner:modelVersion>2.5</celldesigner:modelVersion>
```

### 8.2. Element celldesigner:modelAnnotationType/modelDisplay

This is an XML element to describe the canvas size for the display of graphical objects in CellDesigner.

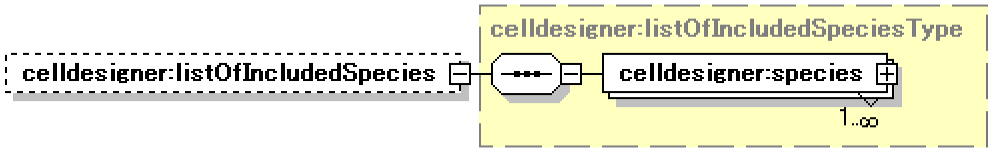
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:modelDisplayType</b></td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>attributes</td><td><table><tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr><tr><td>sizeX</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr><tr><td>sizeY</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr></table></td></tr>
</table>

Example

```
<celldesigner:modelDisplay sizeX="2400" sizeY="2400" />
```

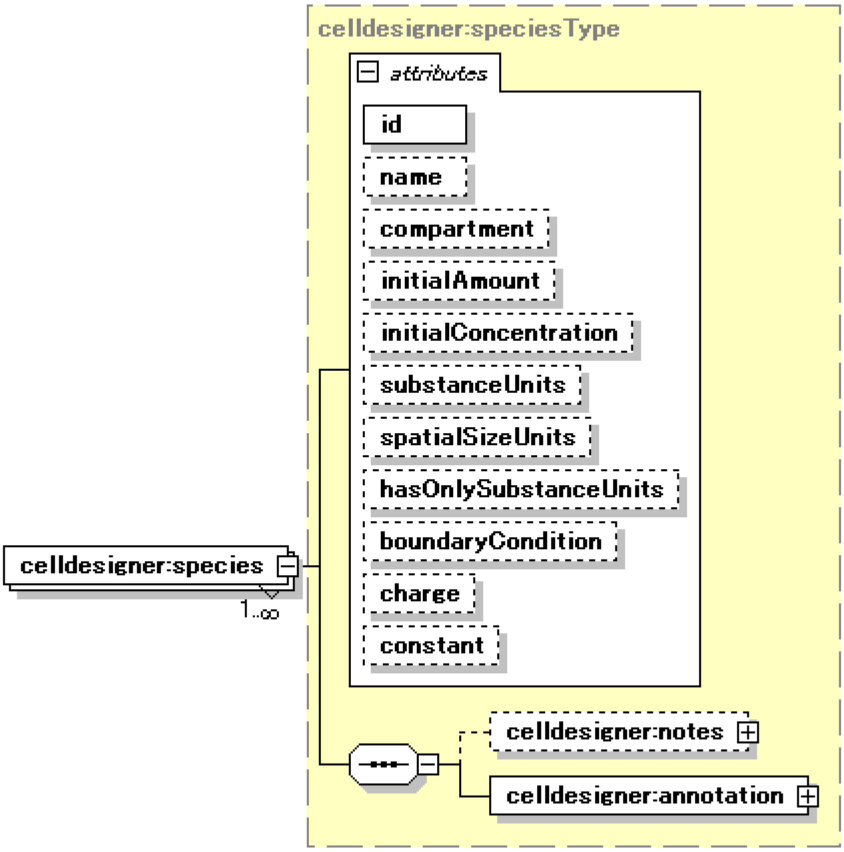
### 8.3. Element celldesigner:modelAnnotationType/listOfIncludedSpecies

This is an XML element to store a list of complex internal elements (CellDesigner.Species) described in CellDesigner.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:listOfIncludedSpeciesType</b></td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>minOcc</td><td>0</td></tr><tr><td>maxOcc</td><td>1</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td><b>celldesigner:species</b></td></tr>
</table>

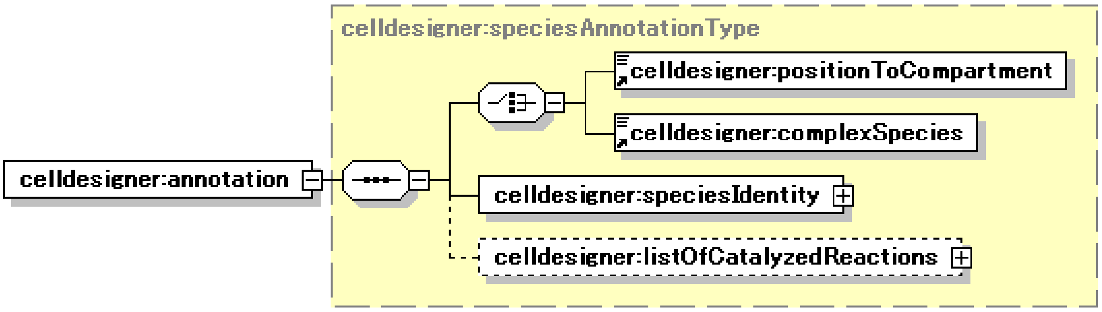
### 8.3.1. Element celldesigner:listOfIncludedSpeciesType/species

This is an XML element to represent a complex internal element described in CellDesigner. The definition is equal to SBML.Species; SBML.Species cannot be carried over because of the schema structure. CellDesigner.notes and CellDesigner.annotation were newly defined and created because SBML.notes and SBML.annotation are closed specifications.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:speciesType</b></td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>1</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>children</td><td><b>celldesigner:notes celldesigner:annotation</b></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>id</td><td><b>celldesigner:SId</b></td><td>required</td><td></td><td></td></tr>
<tr><td>name</td><td><b>xs:string</b></td><td>optional</td><td></td><td></td></tr>
<tr><td>compartment</td><td><b>celldesigner:SId</b></td><td></td><td></td><td></td></tr>
<tr><td>initialAmount</td><td><b>xs:double</b></td><td>optional</td><td></td><td></td></tr>
<tr><td>initialConcentration</td><td><b>xs:double</b></td><td>optional</td><td></td><td></td></tr>
<tr><td>substanceUnits</td><td><b>celldesigner:SId</b></td><td>optional</td><td></td><td></td></tr>
<tr><td>spatialSizeUnits</td><td><b>celldesigner:SId</b></td><td>optional</td><td></td><td></td></tr>
<tr><td>hasOnlySubstanceUnits</td><td><b>xs:boolean</b></td><td>optional</td><td>false</td><td></td></tr>
<tr><td>boundaryCondition</td><td><b>xs:boolean</b></td><td>optional</td><td>false</td><td></td></tr>
<tr><td>charge</td><td><b>xs:integer</b></td><td>optional</td><td></td><td></td></tr>
<tr><td>constant</td><td><b>xs:boolean</b></td><td>optional</td><td>false</td><td></td></tr>
</table></td></tr>
</table>

### 8.3.1.1. Element celldesigner:speciesType/annotation

This is an XML element to describe annotation for a CellDesigner.Species that represents a complex internal element. The element stores data needed to distinguish a CellDesigner.Species (a complex internal element in this case) in the CellDesigner application (details are described in Chapter 10).

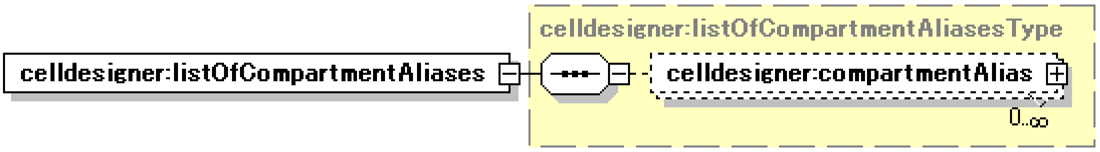
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:speciesAnnotationType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:positionToCompartment celldesigner:complexSpecies celldesigner:speciesIdentity celldesigner:listOfCatalyzedReactions** |

Example

```
<celldesigner:listOfIncludedSpecies>
    <celldesigner:species id="s111" initialAmount="0.0" name="Cdc2">
        <celldesigner:annotation>
            <celldesigner:complexSpecies>s109</celldesigner:complexSpecies>
            <celldesigner:speciesIdentity>
                <celldesigner:class>PROTEIN</celldesigner:class>
                <celldesigner:proteinReference>pr32</celldesigner:proteinReference>
                <celldesigner:state>
                <celldesigner:listOfModifications>
                    <celldesigner:modification residue="rs1" state="phosphorylated" />
                    <celldesigner:modification residue="rs2" state="phosphorylated" />
                </celldesigner:listOfModifications>
            </celldesigner:state>
            </celldesigner:speciesIdentity>
        </celldesigner:annotation>
    </celldesigner:species>
    .
    .
    .
<celldesigner:listOfIncludedSpecies>
```

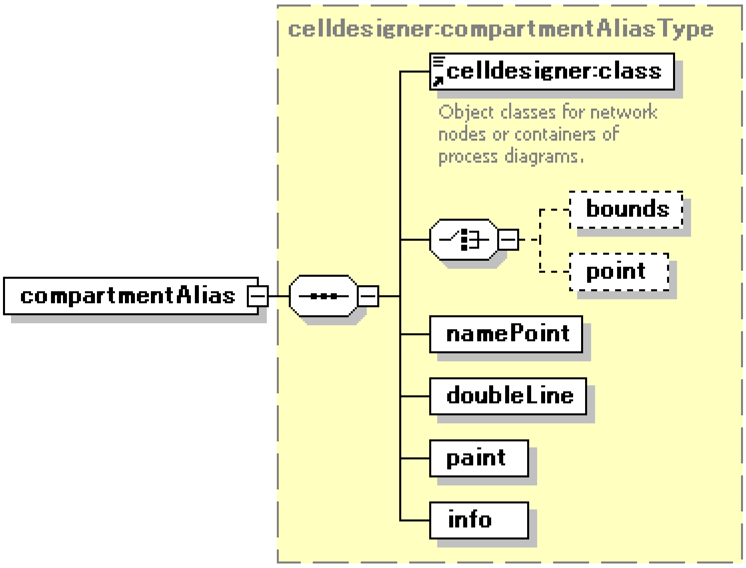
### 8.4. Element celldesigner:modelAnnotationType/listOfCompartmentAliases

This is an XML element to store a list of CellDesigner.CompartmentAliases.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfCompartmentAliasesType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:compartmentAlias** |

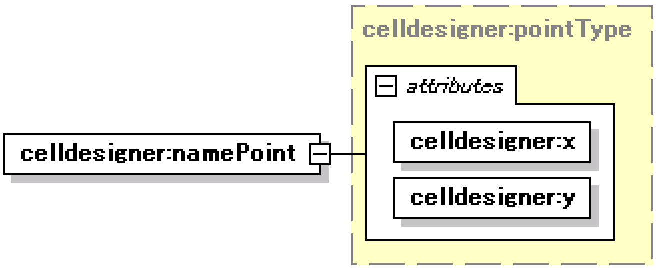
### 8.4.1. Element celldesigner:listOfCompartmentAliasesType/compartmentAlias

This is an XML element to represent a CompartmentAlias (refer to 2. Graphical Model). For the attribute compartment, the id of the referred SBML.Compartment is described. The attribute id is a string to identify a CompartmentAlias (ca123 is a standard type). A child element “namePoint” is an element to describe coordinates data of the compartment name. Other elements are described in 7. Common Elements.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>celldesigner:compartmentAliasType</td></tr>
<tr><td>properties</td><td>isRef 0<br>minOcc 0<br>maxOcc unbounded<br>content complex</td></tr>
<tr><td>children</td><td><b>celldesigner:class celldesigner:bounds celldesigner:point celldesigner:namePoint celldesigner:doubleLine celldesigner:paint</b></td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td><td>annotation</td></tr>
<tr><td>celldesigner:compartment</td><td><b>derived by: celldesigner:SId</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>celldesigner:id</td><td><b>derived by: celldesigner:SId</b></td><td>required</td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

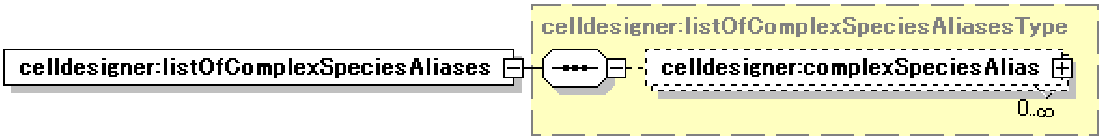
### 8.4.2. Element compartmentAliasType/namePoint

This is an element to describe position data of a compartment name. The attributes “x” and “y” retain x-coordinate and y-coordinate.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:pointType** |
| properties | isRef 0<br>content complex |
| attributes | Name / Type / Use / Default / Fixed / annotation<br>celldesigner:x / **derived by: xs:decimal** / required<br>celldesigner:y / **derived by: xs:decimal** / required |

### 8.5. Element celldesigner:modelAnnotationType/listOfComplexSpeciesAliases

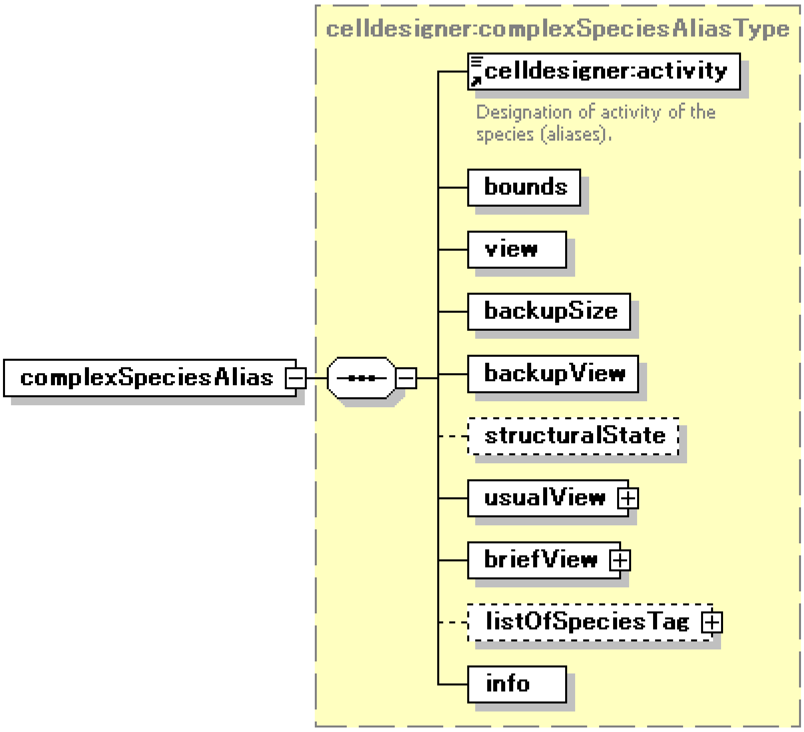
This is an XML element that stores a list of CellDesigner.ComplexSpeciesAliases, each of which corresponds to a complex Species.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfComplexSpeciesAliasesType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:complexSpeciesAlias** |

### 8.5.1. Element celldesigner:listOfComplexSpeciesAliasesType/complexSpeciesAlias

This is an XML element representing a CellDesigner.ComplexSpeciesAlias that corresponds to a complex Species. For the attribute “compartmentAlias”, the id of a CellDesigner.CompartmentAlias in which this complexSpeciesAlias is located is described. The attribute “id” is an identification string to distinguish a complexSpeciesAlias (csa123 is a standard type). For the attribute “species” the id of an SBML.Species that is the source of this complexSpeciesAlias is described. “complexSpeciesAlias” is an attribute that is used when a complex includes other complexes, and the id of the parent complex (a complex that includes the relevant complex inside) is described.

The lower elements apart from “backupSize” and “backupView” are described in 7. Common Elements.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | extension of **celldesigner:complexSpeciesAliasType** |
| children | **celldesigner:activity bounds view backupSize backupView usualView briefView celldesigner:structuralState celldesigner:listOfSpeciesTag** |

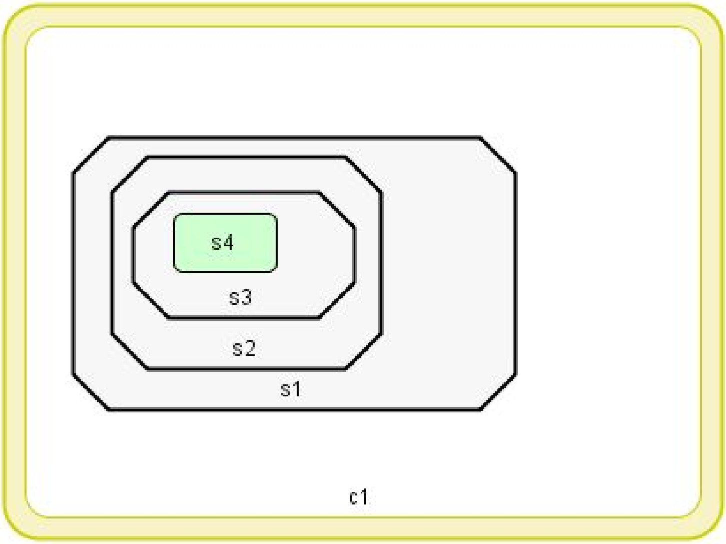
attributes

| Name | Type | Use | Default | Fixed | annotation |
|---|---|---|---|---|---|
| compartmentAlias | celldesigner:SId | optional | | | |
| id | celldesigner:SId | required | | | |
| species | celldesigner:SId | required | | | |
| complexSpeciesAlias | celldesigner:SId | optional | | | |

source

```
<xs:element name="complexSpeciesAlias" minOccurs="0" maxOccurs="unbounded">
  <xs:complexType>
    <xs:complexContent>
      <xs:extension base="celldesigner:complexSpeciesAliasType">
        <xs:attribute name="complexSpeciesAlias" type="celldesigner:SId" use="optional"/>
      </xs:extension>
    </xs:complexContent>
  </xs:complexType>
</xs:element>
```

Example 1. Notation of a complex with multiple complexes inside.



```
<celldesigner:listOfComplexSpeciesAliases>
                <celldesigner:complexSpeciesAlias id="csa1" species="s1" compartmentAlias="ca1">
                    <celldesigner:activity>inactive</celldesigner:activity>
                    <celldesigner:bounds x="83.0" y="106.0" w="250.0" h="154.0"/>
                    <celldesigner:view state="usual"/>
                    <celldesigner:backupSize w="0.0" h="0.0"/>
                    <celldesigner:backupView state="none"/>
                    <celldesigner:usualView>
                        <celldesigner:innerPosition x="39.0" y="75.0"/>
                        <celldesigner:boxSize width="250.0" height="154.0"/>
                        <celldesigner:singleLine width="2.0"/>
                        <celldesigner:paint color="fff7f7f7" scheme="Color"/>
                    </celldesigner:usualView>
                    <celldesigner:briefView>
                        <celldesigner:innerPosition x="0.0" y="0.0"/>
                        <celldesigner:boxSize width="80.0" height="60.0"/>
                        <celldesigner:singleLine width="2.0"/>
                        <celldesigner:paint color="fff7f7f7" scheme="Color"/>
                    </celldesigner:briefView>
                       <celldesigner:info state="empty" angle="-1.5707963267948966"/>
                </celldesigner:complexSpeciesAlias>
                <celldesigner:complexSpeciesAlias id="csa2" species="s2" complexSpeciesAlias="csa1">
                    <celldesigner:activity>inactive</celldesigner:activity>
                    <celldesigner:bounds x="105.0" y="117.0" w="152.0" h="120.0"/>
                    <celldesigner:view state="usual"/>
                    <celldesigner:backupSize w="0.0" h="0.0"/>
                    <celldesigner:backupView state="none"/>
                    <celldesigner:usualView>
                        <celldesigner:innerPosition x="22.0" y="11.0"/>
                        <celldesigner:boxSize width="152.0" height="120.0"/>
                        <celldesigner:singleLine width="2.0"/>
                        <celldesigner:paint color="fff7f7f7" scheme="Color"/>
                    </celldesigner:usualView>
                    <celldesigner:briefView>
                        <celldesigner:innerPosition x="0.0" y="0.0"/>
                        <celldesigner:boxSize width="80.0" height="60.0"/>
                        <celldesigner:singleLine width="2.0"/>
                        <celldesigner:paint color="fff7f7f7" scheme="Color"/>
                    </celldesigner:briefView>
                       <celldesigner:info state="empty" angle="-1.5707963267948966"/>
                </celldesigner:complexSpeciesAlias>
                <celldesigner:complexSpeciesAlias id="csa3" species="s3" complexSpeciesAlias="csa2">
                    <celldesigner:activity>inactive</celldesigner:activity>
                    <celldesigner:bounds x="117.0" y="137.0" w="125.0" h="71.0"/>
```

```
        <celldesigner:view state="usual"/>
        <celldesigner:backupSize w="0.0" h="0.0"/>
        <celldesigner:backupView state="none"/>
        <celldesigner:usualView>
          <celldesigner:innerPosition x="12.0" y="20.0"/>
          <celldesigner:boxSize width="125.0" height="71.0"/>
          <celldesigner:singleLine width="2.0"/>
          <celldesigner:paint color="fff7f7f7" scheme="Color"/>
        </celldesigner:usualView>
        <celldesigner:briefView>
          <celldesigner:innerPosition x="0.0" y="0.0"/>
          <celldesigner:boxSize width="80.0" height="60.0"/>
          <celldesigner:singleLine width="2.0"/>
          <celldesigner:paint color="fff7f7f7" scheme="Color"/>
        </celldesigner:briefView>
        <celldesigner:info state="empty" angle="-1.5707963267948966"/>
      </celldesigner:complexSpeciesAlias>
    </celldesigner:listOfComplexSpeciesAliases>
```

ComplexSpeciesAliases “csa3” and “csa2” have ”csa2” and “csa1” respectively, each of which is the ID of the parent complex (a complex that includes the relevant complex), for the attribute “complexSpeciesAlias”. In addition, complexSpeciesAlias has ca1 that is the ID of the compartment (speciesID=c1) for the attribute compartmentAlias.

BackupSize and backupView

From ver. 4.0, a complex can have other complexes inside. Along with this specification, brief was changed as follows:

Before the change

State of a complex: brief

After the change

**When there is no complex with the relevant complex inside: the state of the relevant complex is brief.**

**When there is a complex with the relevant complex inside (parent complex): the state of the parent complex is brief.**

For example, as shown in Fig. 8.5.1.2, when complexes s2 and s1 are both brief, the size described in the briefView of s2 is the same size as s1; therefore, when s1 is brief, the state and size of s2 must be retained (Note). To retain the values, from ver.4.0, backupView and backupSize are available. The complexSpeciesAlias of s2 in the state on the right side in Fig. 8.5.1.2 is as follows:

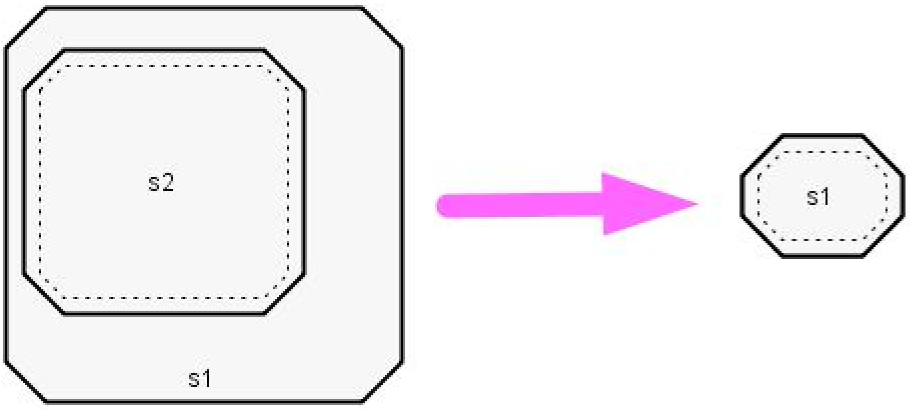


Fig. 8.5.1.2

```
<celldesigner:complexSpeciesAlias id="csa2" species="s2" complexSpeciesAlias="csa1">
                  <celldesigner:activity>inactive</celldesigner:activity>
                  <celldesigner:bounds x="93.0" y="163.0" w="80.0" h="60.0"/>
          ①       <celldesigner:view state="complexparentbrief"/>
                  <celldesigner:backupSize w="140.0" h="132.0"/>
                  <celldesigner:backupView state="brief"/>
                  <celldesigner:usualView>
                      <celldesigner:innerPosition x="0.0" y="0.0"/>
                      <celldesigner:boxSize width="72.0" height="65.0"/>
                      <celldesigner:singleLine width="2.0"/>
                      <celldesigner:paint color="fff7f7f7" scheme="Color"/>
                  </celldesigner:usualView>
          ②       <celldesigner:briefView>
                      <celldesigner:innerPosition x="9.0" y="21.5"/>
                      <celldesigner:boxSize width="140.0" height="132.0"/>
                      <celldesigner:singleLine width="2.0"/>
                      <celldesigner:paint color="fff7f7f7" scheme="Color"/>
                  </celldesigner:briefView>
                     <celldesigner:info state="empty" angle="-1.5707963267948966"/>
            </celldesigner:complexSpeciesAlias>
```

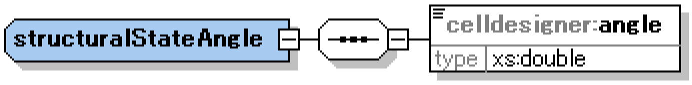
① In backupView and backupSize, the brief state and the size of s2 are both retained.

② In “briefView”, the brief state of the parent complex is retained. However, in the element “innerPostion” the relative coordinates of s2 in relation to s1 are retained.

(Note) As in the past, it is better that the “briefView” of a complex retains the size in its brief state. However, in implementation up to ver.3.5.x the following specifications were applied: when the state of a complex is changed to brief, the size of species (e.g. protein, gene, or RNA) inside the complex is also changed to the same size of the complex and drawn, and each “briefView” retains the size of the complex. Therefore, these specifications are applied to the complexes inside a complex so as to minimize the number of sections to be changed.

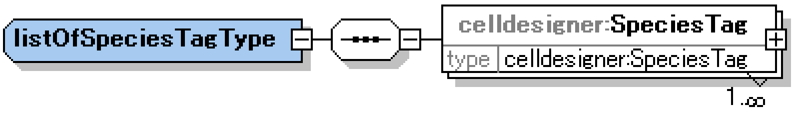
### 8.5.1.1. Element celldesigner: structuralStateAngle

This is an XML element that represents the angle of the State of a Complex.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner: structuralStateAngle** |
| properties | minOcc 0<br>maxOcc 1<br>content simple |
| children | |
| attributes | Name Type Use Default Fixed annotation<br>angle **xs:double** required |

### 8.5.1.2. Element celldesigner: listOfSpeciesTag

This is an XML element that represents a list of Tag data given to a Species.

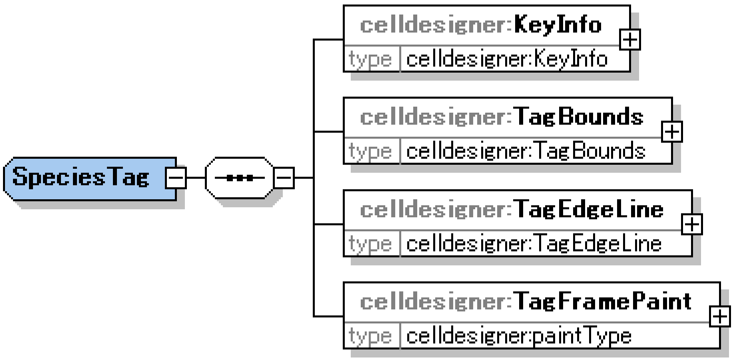
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:** listOfSpeciesTagType |
| properties | minOcc 0<br>maxOcc unbounded<br>content complex |
| children | SpeciesTag |

Example

```
<celldesigner:listOfSpeciesTag>
  <celldesigner:SpeciesTag>
    <celldesigner:KeyInfo name="s2_tag" direct="LEFT"/>
    <celldesigner:TagBounds x="520.0" y="197.5" w="50.0" h="25.0"/>
    <celldesigner:TagEdgeLine width="1.0"/>
    <celldesigner:TagFramePaint color="ff00ff96" scheme="Color"/>
  </celldesigner:SpeciesTag>
  <celldesigner:SpeciesTag>
    <celldesigner:KeyInfo name="s2_tag" direct="DOWN"/>
    <celldesigner:TagBounds x="407.5" y="50.0" w="25.0" h="50.0"/>
    <celldesigner:TagEdgeLine width="1.0"/>
    <celldesigner:TagFramePaint color="ff00ff96" scheme="Color"/>
  </celldesigner:SpeciesTag>
  <celldesigner:SpeciesTag>
    <celldesigner:KeyInfo name="s2_tag" direct="RIGHT"/>
    <celldesigner:TagBounds x="270.0" y="197.5" w="50.0" h="25.0"/>
    <celldesigner:TagEdgeLine width="1.0"/>
    <celldesigner:TagFramePaint color="ff00ff96" scheme="Color"/>
  </celldesigner:SpeciesTag>
  <celldesigner:SpeciesTag>
    <celldesigner:KeyInfo name="s2_tag" direct="UP"/>
    <celldesigner:TagBounds x="407.5" y="320.0" w="25.0" h="50.0"/>
    <celldesigner:TagEdgeLine width="1.0"/>
    <celldesigner:TagFramePaint color="ff00ff96" scheme="Color"/>
  </celldesigner:SpeciesTag>
</celldesigner:listOfSpeciesTag>
```

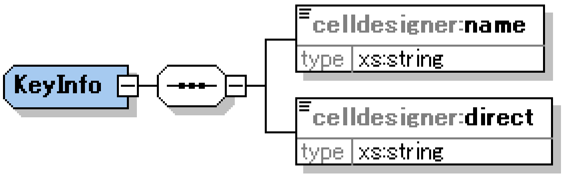
### 8.5.1.2.1. Element celldesigner: SpeciesTag

This is an XML element that represents Tag data given to a Species.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:** SpeciesTag |
| properties | complex |
| children | celldesigner:KeyInfo celldesigner: TagBounds celldesigner: TagEdgeLine celldesigner: TagFramePaint |

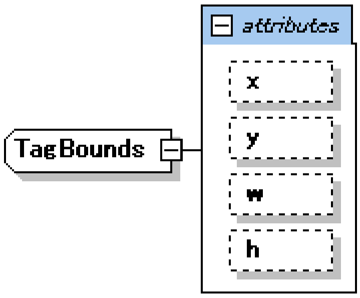
### 8.5.1.2.2. Element celldesigner: KeyInfo

The name of a Tag and the direction of an arrow are described.

<table>
<tr><td>diagram</td><td colspan="6"> </td></tr>
<tr><td>namespace</td><td colspan="6">http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td colspan="6"><b>celldesigner:</b> KeyInfo</td></tr>
<tr><td>properties</td><td colspan="6">complex</td></tr>
<tr><td>children</td><td colspan="6"></td></tr>
<tr><td rowspan="3">attributes</td><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td><td>annotation</td></tr>
<tr><td>Name</td><td><b>xs:string</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>direct</td><td><b>xs: string</b></td><td>required</td><td></td><td></td><td></td></tr>
</table>

### 8.5.1.2.3. Element celldesigner: TagBounds

Frame data of a Tag is described.

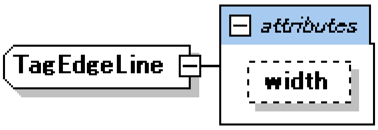
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |

| | |
|---|---|
| type | **celldesigner:** TagBounds |
| properties | complex |
| children | |

| attributes | Name | Type | Use | Default | Fixed | annotation |
|---|---|---|---|---|---|---|
| | x | **xs:double** | required | | | |
| | y | **xs: double** | required | | | |
| | w | **xs: double** | required | | | |
| | h | **xs: double** | required | | | |

### 8.5.1.2.4. Element celldesigner: TagEdgeLine

Frame width data of a Tag is described.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:** TagEdgeLine |
| properties | complex |
| children | |

| attributes | Name | Type | Use | Default | Fixed | annotation |
|---|---|---|---|---|---|---|
| | width | **xs:double** | required | | | |

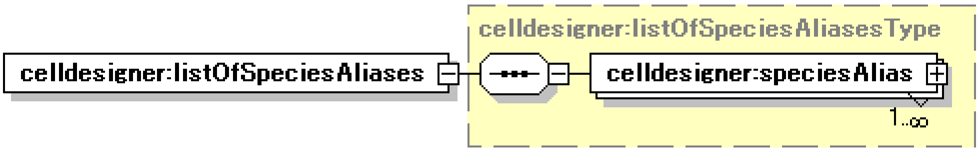
### 8.5.1.2.5. Element celldesigner: TagFramePaint

Data for painting and the color of a displayed item is described.

| | |
|---|---|
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:** paintType |
| properties | complex |

### 8.6. Element celldesigner:modelAnnotationType/listOfSpeciesAliases

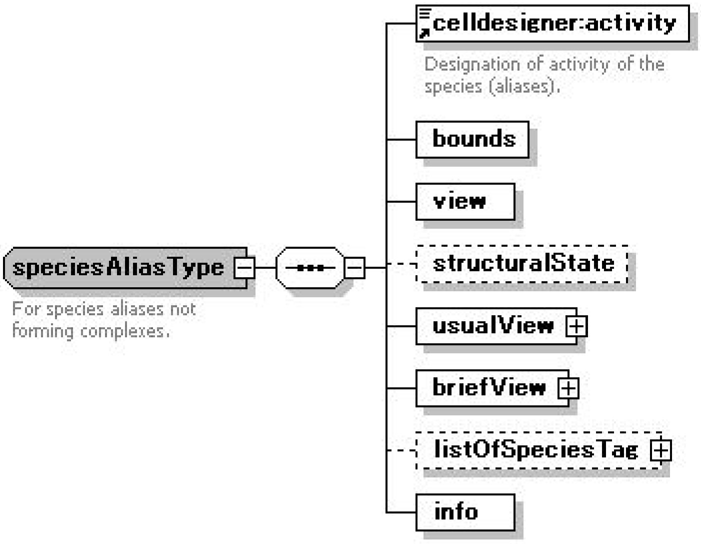
This is an XML element that stores a list of CellDesigner.SpeciesAliases, each of which corresponds to a Species that is not a complex.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfSpeciesAliasesType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:speciesAlias** |

### 8.6.1. Element celldesigner:listOfSpeciesAliasesType/speciesAlias

This is an XML element representing a CellDesigner.SpeciesAlias that corresponds to a Species that is not a complex. When this Species is not a complex element, for the attribute “compartmentAlias” the id of the CellDesigner.CompartmentAlias in which this speciesAlias is located is described. When this Species is a complex element, for the attribute “complexSpeciesAlias” the id of the CellDesigner.ComplexSpeciesAlias in which this speciesAlias is located is described. Only one of “compartmentAlias” or “complexSpeciesAlias” is used. If there is no description for both attributes, this means this speciesAlias belongs to a “default” compartment (canvas for editing).

The attribute “id” is an identification string to distinguish a speciesAlias (sa123 is a standard type). For the attribute “species”, if the Species is not a complex element, the id of the SBML.Species that is the source of this speciesAlias is described; if the Species is a complex element, the id of the CellDesigner.Species is described. Other lower elements are described in 7. Common Elements.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:speciesAliasType</b></td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>1</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>children</td><td><b>celldesigner:activity celldesigner:bounds celldesigner:view celldesigner:usualView celldesigner:briefView celldesigner:structuralState celldesigner:listOfSpeciesTag</b></td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr>
<tr><td>id</td><td><b>derived by: celldesigner:SId</b></td><td>required</td><td></td><td></td></tr>
<tr><td>species</td><td><b>celldesigner:SId</b></td><td>required</td><td></td><td></td></tr>
<tr><td>compartmentAlias</td><td><b>derived by: celldesigner:SId</b></td><td>optional</td><td></td><td></td></tr>
<tr><td>complexSpeciesAlias</td><td><b>derived by: celldesigner:SId</b></td><td>optional</td><td></td><td></td></tr>
</table></td></tr>
</table>

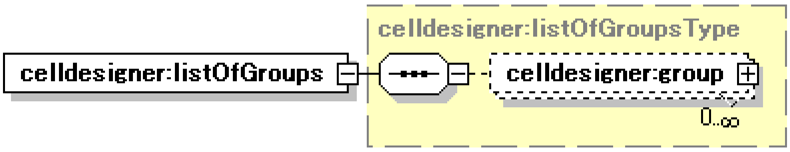
Example

```
<celldesigner:listOfSpeciesAliases>
  <celldesigner:speciesAlias id="a1" species="s1">
    <celldesigner:activity>inactive</celldesigner:activity>
    <celldesigner:bounds h="30.0" w="80.0" x="40.0" y="25.0" />
    <celldesigner:view state="usual" />
    <celldesigner:usualView>
      <celldesigner:innerPosition x="0.0" y="0.0" />
      <celldesigner:boxSize height="30.0" width="80.0" />
      <celldesigner:singleLine width="1.0" />
```

```
      <celldesigner:paint color="ff7f0000" scheme="Gradation" />
    </celldesigner:usualView>
    <celldesigner:briefView>
      <celldesigner:innerPosition x="0.0" y="0.0" />
      <celldesigner:boxSize height="60.0" width="80.0" />
      <celldesigner:singleLine width="1.0" />
      <celldesigner:paint color="3fff0000" scheme="Color" />
    </celldesigner:briefView>
    <celldesigner:info state="empty" angle="-1.5707963267948966"/>
  </celldesigner:speciesAlias>
  .
  .
  .
<celldesigner:listOfSpeciesAliases>
```

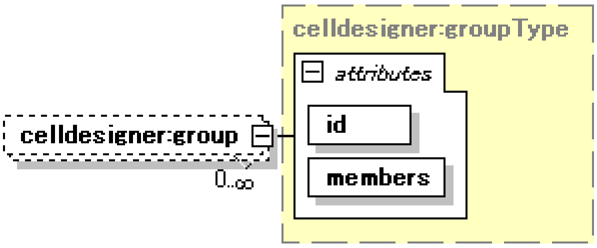
### 8.7. Element celldesigner:modelAnnotationType/listOfGroups

This is an XML element that stores a list of (Complex)SpeciesAliases groups created in a graphic model; a group is regarded as a unit for editing.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>**celldesigner:listOfGroupsType**</td></tr>
<tr><td>properties</td><td>isRef 0<br>content complex</td></tr>
<tr><td>children</td><td>**celldesigner:group**</td></tr>
</table>

### 8.7.1. Element celldesigner:listOfGroupsType/group

This is an XML element that represents a group of (Complex)SpeciesAliases created in a graphic model; a group is regarded as a unit for editing.

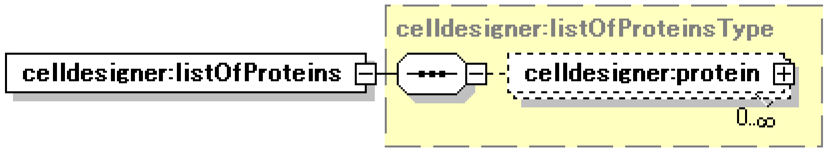
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>**celldesigner:groupType**</td></tr>
<tr><td>properties</td><td>isRef 0<br>minOcc 0<br>maxOcc unbounded<br>content complex</td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr>
<tr><td>id</td><td>**derived by: celldesigner:SId**</td><td>required</td><td></td><td></td></tr>
<tr><td>members</td><td>**derived by: xs:string**</td><td>required</td><td></td><td></td></tr>
</table></td></tr>
</table>

Example

```
<celldesigner:listOfGroups>
  <celldesigner:group id="g1" members="sa536,sa533,sa534,sa537,sa535,sa198" />
  <celldesigner:group id="g2" members="a70,a62,a71,a57,a56,a63,a51,a50" />
</celldesigner:listOfGroups>
```

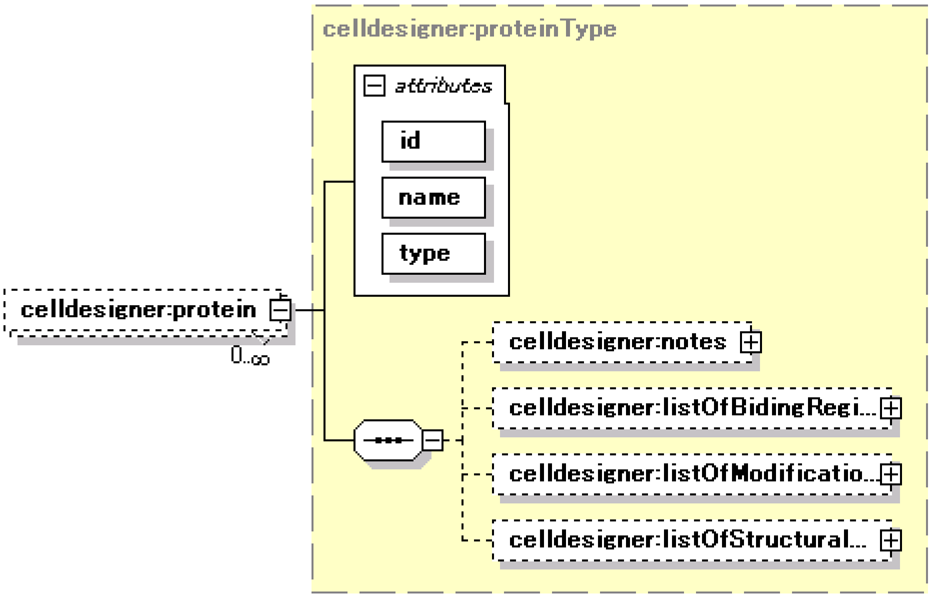
## 8.8. Element celldesigner:modelAnnotationType/listOfProteins

This is an XML element that stores a list of CellDesigner.Proteins.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfProteinsType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:protein** |

### 8.8.1. Element celldesigner:listOfProteinsType/protein

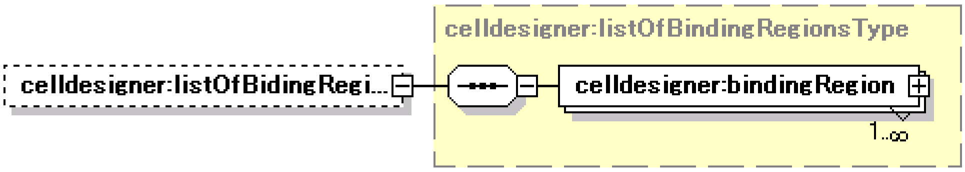
This is an XML element representing a CellDesigner.Protein that means a protein. The attribute id is a string to uniquely identify a Protein (pr123 is a standard type). The attribute name is the name of the Protein and used for identifying the uniqueness of the Protein. The attribute type is any string of “GENERIC”, “ION_CHANNEL”, “RECEPTOR”, or “TRUNCATED”. The lower element CellDesigner.Notes is described in 7.2.11, and other lower elements are described in the following sections.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:proteinType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc unbounded<br>content complex |
| children | **celldesigner:notes celldesigner:listOfBindingRegions celldesigner:listOfModificationResidues celldesigner:listOfStructuralStates** |

| attributes | Name | Type | Use | Default | Fixed | annotation |
|---|---|---|---|---|---|---|
| | id | **derived by: celldesigner:SId** | required | | | |
| | name | **derived by: xs:string** | required | | | |
| | type | **derived by: xs:string** | required | | | |

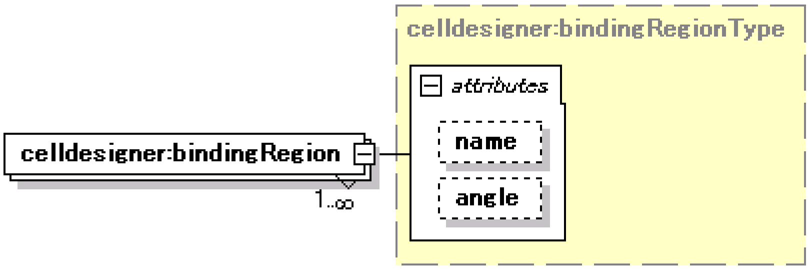
### 8.8.1.1. Element celldesigner:proteinType/listOfBindingRegions

This is an XML element that stores a list of celldesigner:bindingRegions, each of which binds to other proteins, GENEs, or RNAs on the Protein.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfBindingRegionsType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:bindingRegion** |

### 8.8.1.2. Element celldesigner:listOfBindingRegionsType/bindingRegion

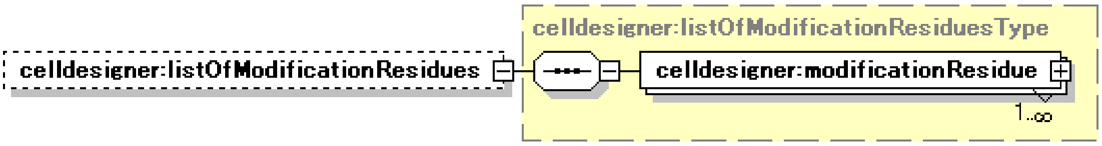
This is an XML element that stores data of a region that binds to other proteins, GENEs, or RNAs on the protein. The attribute name stores the string of a label attached to the region. The attribute angle is a numerical value [0, 2π] that specifies the display position of the binding region in the displayed protein.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:bindingRegionType** |
| properties | isRef 0<br>minOcc 1<br>maxOcc unbounded<br>content complex |

| attributes | Name | Type | Use | Default | Fixed | annotation |
|---|---|---|---|---|---|---|
| | angle | **xs: decimal** | optional | | | |
| | Id | **xs:string** | optional | | | |
| | Name | **xs: string** | optional | | | |
| | size | **xs:decimal** | optional | | | |

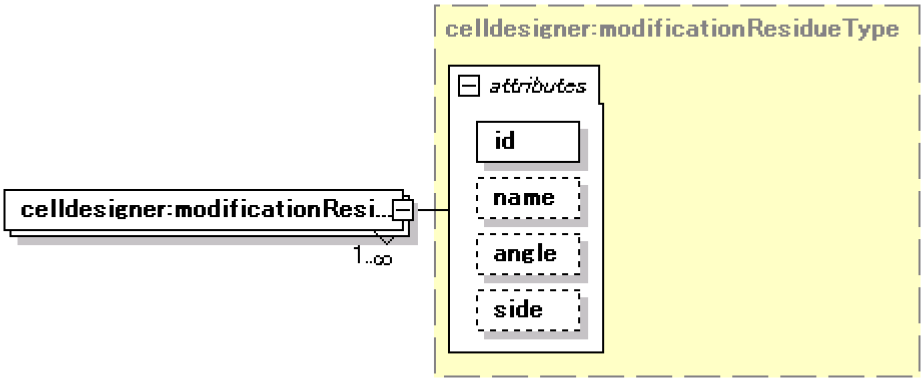
### 8.8.1.3. Element celldesigner:proteinType/listOfModificationResidues

This is an XML element that stores a list of CellDesigner.ModificationResidues, each of which is a residue subject to protein modification.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfModificationResiduesType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:modificationResidue** |

### 8.8.1.3.1. Element celldesigner:listOfModificationResiduesType/modificationResidue

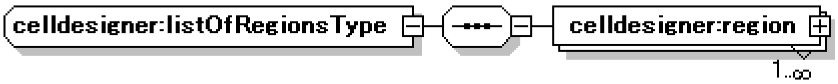
This is an XML element representing a CellDesigner.ModificationResidue that is a residue subject to protein modification. The attribute id is an identification string uniquely determined within one protein (rs12 is a standard type). The attribute name stores a label attached to the residue (e.g. a string “Ser178”). The attribute angle is a numerical value [0, 2π] that specifies the display position of the residue in the displayed protein.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:modificationResidueType</b></td></tr>
<tr><td>properties</td><td>isRef 0<br>minOcc 1<br>maxOcc unbounded<br>content complex</td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th><th>annotation</th></tr>
<tr><td>id</td><td><b>derived by: celldesigner:SId</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>name</td><td><b>derived by: xs:string</b></td><td>optional</td><td></td><td></td><td></td></tr>
<tr><td>angle</td><td><b>derived by: xs:decimal</b></td><td>optional</td><td></td><td></td><td></td></tr>
<tr><td>side</td><td></td><td></td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

## 8.9. Common Elements for Genes, RNAs, and Antisense RNAs

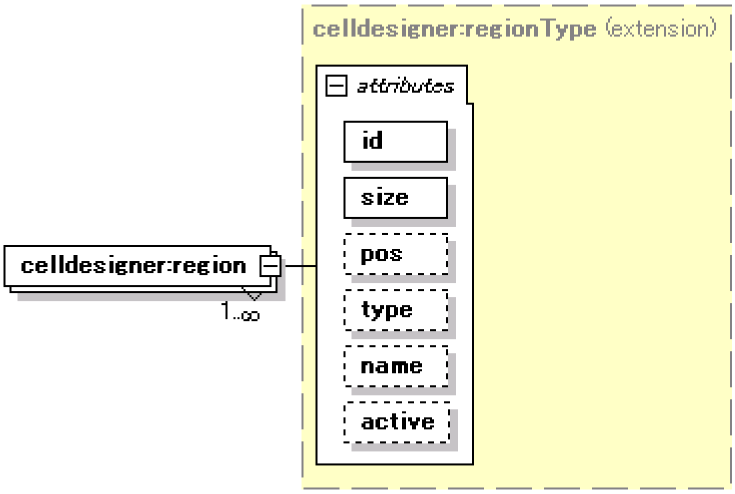
### 8.9.1. ComplexType celldesigner:listOfRegionsType

This is an XML element that stores a list of CellDesigner.Regions, each of which represents a specific region in a nucleotide sequence.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| children | **celldesigner:region** |
| used by | elements **celldesigner:geneType/listOfRegions**<br>**celldesigner:RNAType/listOfRegions**<br>**celldesigner:AntisenseRNAType/listOfRegions** |

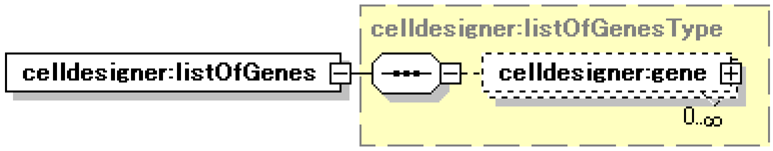
### 8.9.1.1. Element celldesigner:listOfRegionsType/region

This is an XML element representing a CellDesigner.Region that represents a specific region in a nucleotide sequence. The attribute id is an identification string uniquely determined within one nucleic acid (tr12 is a standard type). The attribute size is the relative size [0,1] of a box representing the region in relation to the displayed nucleic acid, and in the same manner, the attribute pos is a relative position [0,1]. For the attribute type any of the following is set: “proteinBindingDomain”, “Modification Site”, “transcriptionStartingSiteL”, “transcriptionStartingSiteR”, “CodingRegion”, “RegulatoryRegion”, or ”empty”. If no type is set, the region is regarded as a modification site. The attribute name stores a label attached to the region (e.g. a string “TATA box”). The attribute “active” represents the state of “transcriptionStartingSiteL” and “transcriptionStartingSiteR”, and for other types, “false” is set.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>extension of celldesigner:regionType</td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>1</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td><td>annotation</td></tr>
<tr><td>id</td><td><b>derived by: celldesigner:SId</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>size</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>pos</td><td><b>derived by: xs:decimal</b></td><td>optional</td><td></td><td></td><td></td></tr>
<tr><td>type</td><td><b>derived by: xs:string</b></td><td></td><td></td><td></td><td></td></tr>
<tr><td>name</td><td><b>derived by: xs:string</b></td><td></td><td></td><td></td><td></td></tr>
<tr><td>active</td><td><b>xs:boolean</b></td><td>optional</td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

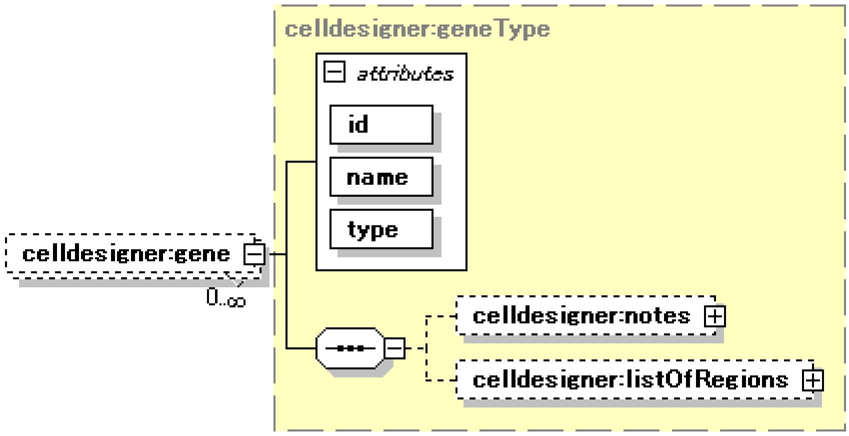
### 8.10. Element celldesigner:modelAnnotationType/listOfGenes

This is an XML element that stores a list of CellDesigner.Genes.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:listOfGenesType</b></td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td><b>celldesigner:gene</b></td></tr>
</table>

### 8.10.1. Element celldesigner:listOfGenesType/gene

This is an XML element representing a CellDesigner.Gene that means a gene. The attribute id is a string to uniquely identify a Gene (gn123 is a standard type). The attribute name is the name of the Gene and used for identifying the uniqueness of the Gene. For the attribute type only “GENE” can be set. The lower element CellDesigner.Notes are described in 7.2.11, and CellDesigner.ListOfRegions are described in 8.9.1.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:geneType</b></td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>minOcc</td><td>0</td></tr><tr><td>maxOcc</td><td>unbounded</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td><b>celldesigner:notes celldesigner:listOfRegions</b></td></tr>
<tr><td>attributes</td><td><table><tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr><tr><td>id</td><td><b>derived by: celldesigner:SId</b></td><td>required</td><td></td><td></td></tr><tr><td>name</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td></tr><tr><td>type</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td></tr></table></td></tr>
</table>

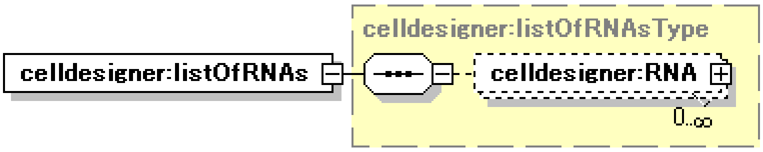
Example

```
<celldesigner:listOfGenes>
  <celldesigner:gene id="gn1" name="s5" type="GENE" />
  <celldesigner:gene id="gn2" name="histon1" type="GENE">
    <celldesigner:listOfRegions>
```

```
      <celldesigner:region id="tr1" size="0.0" />
    </celldesigner:listOfRegions>
  </celldesigner:gene>
  <celldesigner:gene id="gn4" name="Cre1" type="GENE">
    <celldesigner:listOfRegions>
      <celldesigner:region id="tr1" pos="0.12" size="0.36" type="codingRegion" />
    </celldesigner:listOfRegions>
  </celldesigner:gene>
  .
  .
  .
<celldesigner:listOfGenes>
```

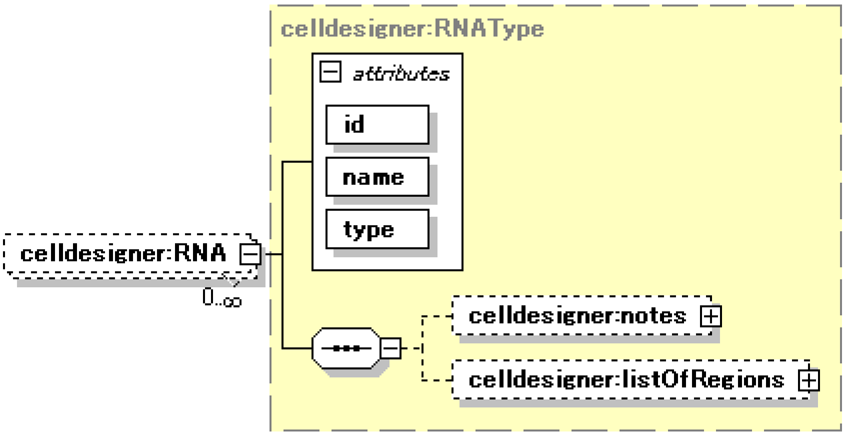
### 8.11. Element celldesigner:modelAnnotationType/listOfRNAs

This is an XML element that stores a list of CellDesigner.RNAs.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfRNAsType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:RNA** |

### 8.11.1. Element celldesigner:listOfRNAsType/RNA

This is an XML element representing a CellDesigner.RNA that means an RNA. The attribute id is a string to uniquely identify an RNA (rn123 is a standard type). The attribute name is the name of an RNA and used for identifying the uniqueness of a Gene. For the attribute “type”, only “RNA” can be set. The lower element CellDesigner.Notes are described in 7.2.11, and CellDesigner.ListOfRegions are described in 8.9.1.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:RNAType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc unbounded<br>content complex |

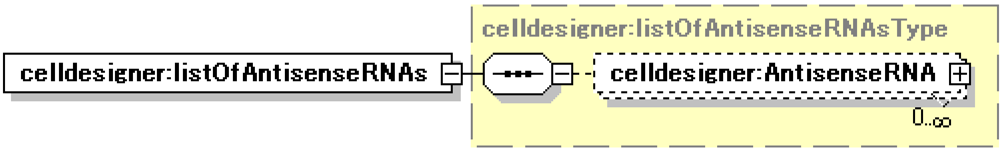
| | | | | | |
|---|---|---|---|---|---|
| children | **celldesigner:notes celldesigner:listOfRegions** | | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | id | **derived by: celldesigner:SId** | required | | |
| | name | **derived by: xs:string** | required | | |
| | type | **derived by: xs:string** | required | | |

Example

```
<celldesigner:listOfRNAs>
  <celldesigner:RNA id="rn1" name="s6" type="RNA" />
  <celldesigner:RNA id="rn2" name="RNA" type="RNA" />
  <celldesigner:RNA id="rn3" name="exon" type="RNA">
    <celldesigner:notes>
      <html xmlns="http://www.w3.org/1999/xhtml">
        <!-- Notes by CellDesigner -->
        <body>This is RNA notes.</body>
      </html>
    </celldesigner:notes>
    <celldesigner:listOfRegions>
      <celldesigner:region id="tr1" size="0.3" type="exon" />
    </celldesigner:listOfRegions>
  </celldesigner:RNA>
  <celldesigner:RNA id="rn4" name="proteinBindingDomain" type="RNA">
    <celldesigner:listOfRegions>
      <celldesigner:region id="tr1" pos="0.20999999999999996" size="0.48"
        type="proteinBindingDomain" />
    </celldesigner:listOfRegions>
  </celldesigner:RNA>
  .
  .
  .
</celldesigner:listOfRNAs>
```

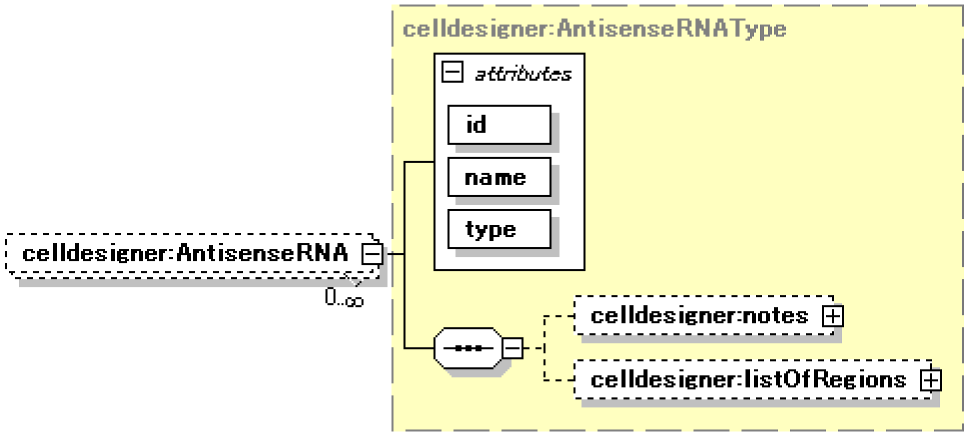
### 8.12. Element celldesigner:modelAnnotationType/listOfAntisenseRNAs

This is an XML element that stores a list of CellDesigner.AntisenseRNAs.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfAntisenseRNAsType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:AntisenseRNA** |

### 8.12.1. Element celldesigner:listOfAntisenseRNAsType/AntisenseRNA

This is an XML element representing a CellDesigner.AntisenseRNA that means an antisenseRNA. The attribute id is a string to uniquely identify an AntisenseRNA (arn123 is a standard type). The attribute name is the name of the AntisenseRNA and used for identifying the uniqueness of the AntisenseRNA. For the

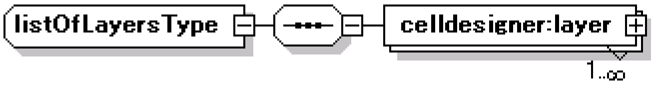
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>**celldesigner:AntisenseRNAType**</td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>0</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>children</td><td>**celldesigner:notes celldesigner:listOfRegions**</td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr>
<tr><td>id</td><td>**derived by: celldesigner:SId**</td><td>required</td><td></td><td></td></tr>
<tr><td>name</td><td>**derived by: xs:string**</td><td>required</td><td></td><td></td></tr>
<tr><td>type</td><td>**derived by: xs:string**</td><td>required</td><td></td><td></td></tr>
</table></td></tr>
</table>

Example

```
<celldesigner:listOfAntisenseRNAs>
  <celldesigner:AntisenseRNA id="arn2" name="asRNA" type="ANTISENSE_RNA" />
  <celldesigner:AntisenseRNA id="arn3" name="s451" type="ANTISENSE_RNA" />
  <celldesigner:AntisenseRNA id="arn4" name="s452" type="ANTISENSE_RNA">
    <celldesigner:listOfRegions>
      <celldesigner:region id="tr1" name="sta" pos="0.29999999999999993"
        size="0.3" type="exon" />
    </celldesigner:listOfRegions>
  </celldesigner:AntisenseRNA>
  <celldesigner:AntisenseRNA id="arn1" name="s7" type="ANTISENSE_RNA">
    <celldesigner:listOfRegions>
      <celldesigner:region id="tr1" name="CreBinding" pos="0.32999999999999996"
        size="0.52" type="proteinBindingDomain" />
    </celldesigner:listOfRegions>
  </celldesigner:AntisenseRNA>
</celldesigner:listOfAntisenseRNAs>
```

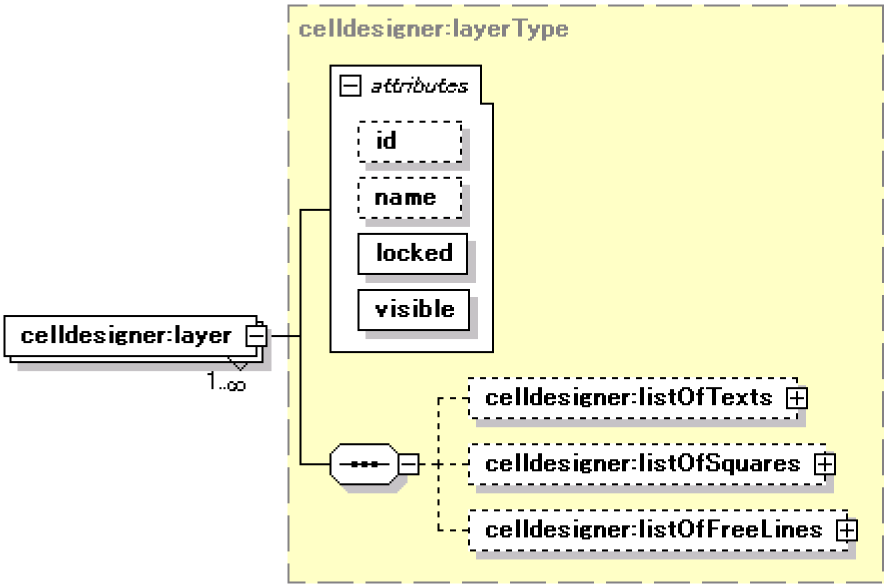
### 8.13. Element celldeisgner:modelAnnotationType/listOflayers

This is a complex type that manages a list of celldesigner:layers.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| children | **celldesigner:layer** |
| used by | element **modelAnnotationType/listOfLayers** |

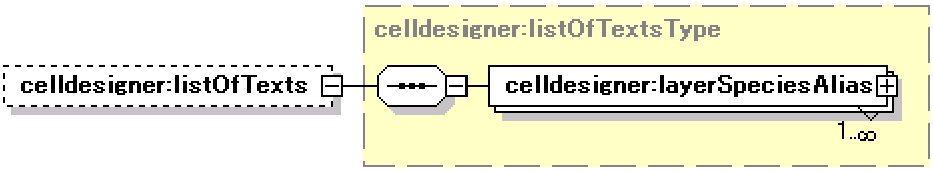
### 8.13.1. Element listOfLayersType/layer

This is an XML element that represents a layer. The attributes "id" and "name" retains the ID and name; the attribute "locked" indicates the layer cannot be edited; and the attribute "visible" retains the visible/invisible state of components in the layer.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:layerType</b></td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>minOcc</td><td>1</td></tr><tr><td>maxOcc</td><td>unbounded</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td><b>celldesigner:listOfTexts celldesigner:listOfSquares celldesigner:listOfFreeLines</b></td></tr>
<tr><td>attributes</td><td><table><tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th><th>annotation</th></tr><tr><td>id</td><td></td><td></td><td></td><td></td><td></td></tr><tr><td>name</td><td></td><td></td><td></td><td></td><td></td></tr><tr><td>locked</td><td><b>xs:boolean</b></td><td>required</td><td></td><td></td><td></td></tr><tr><td>visible</td><td><b>xs:boolean</b></td><td>required</td><td></td><td></td><td></td></tr></table></td></tr>
</table>

### 8.13.2. Element layerType/listOfTexts

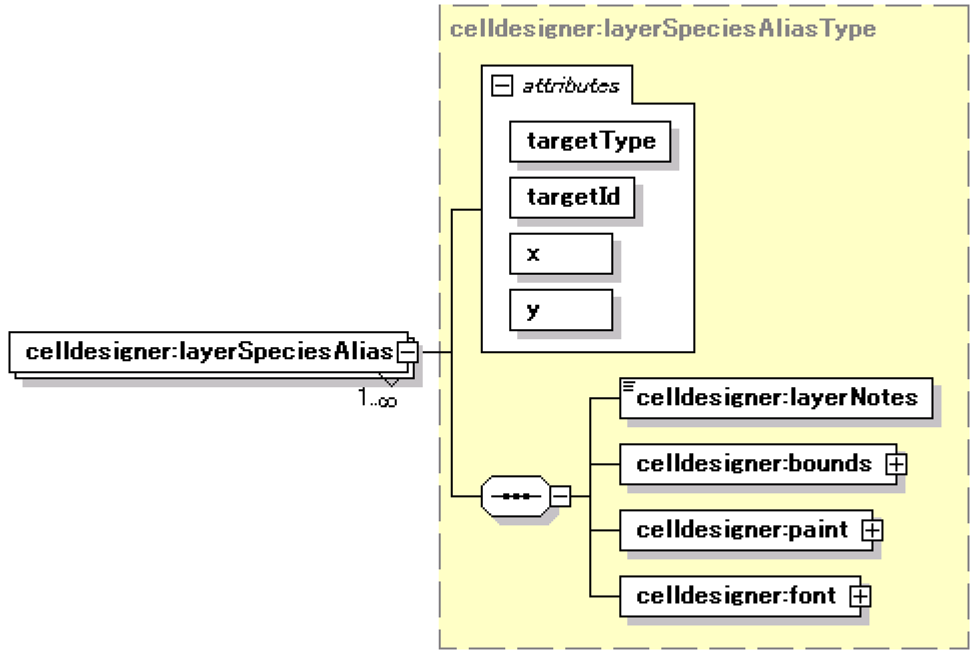
This is an element that represents a list of celldesigner:layerSpeciesAliases.

| | |
|---|---|
| diagram |  |

|  |  |
|---|---|
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfTextsType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:layerSpeciesAlias** |

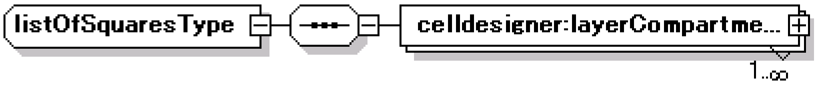
### 8.13.3. Element listOfTextsType/layerSpeciesAlias

This is an element that represents text notes added to a layer. The attribute “targetType” retains the type of a component to which notes are added, and “targetID” retains the ID of the component. If there is no component as directed by the notes, null is set for both targetType and targetID. “x” and “y” represent the coordinates of the arrow tip as directed by the notes. The child element “layerNotes” represents a string for the notes. For other elements, refer to Chapter 7. Common Elements.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:layerSpeciesAliasType</b></td></tr>
<tr><td>properties</td><td>isRef 0<br>minOcc 1<br>maxOcc unbounded<br>content complex</td></tr>
<tr><td>children</td><td><b>celldesigner:layerNotes celldesigner:bounds celldesigner:paint celldesigner:font</b></td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td><td>annotation</td></tr>
<tr><td>targetType</td><td><b>xs:string</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>targetId</td><td><b>xs:string</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>x</td><td><b>xs:decimal</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>y</td><td><b>xs:decimal</b></td><td>required</td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

### 8.13.4. Element layerType/listOfSquares

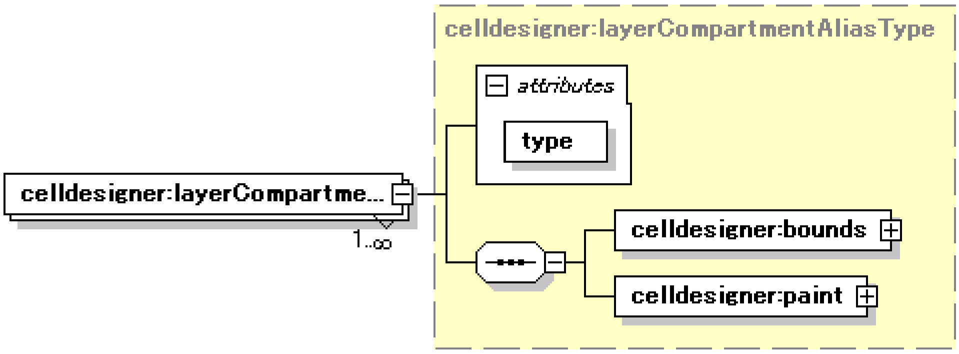
This is an XML element that represents a list of celldesigner:layerCompartmentAliases.

|  |  |
|---|---|
| diagram |  |

| | |
|---|---|
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| children | **celldesigner:layerCompartmentAlias** |

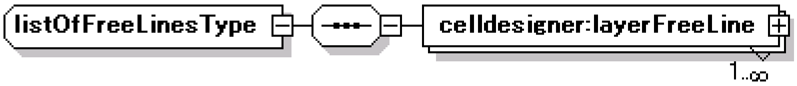
### 8.13.5. Element listOfSquaresType/layerCompartmentAlias

This is an element that represents a shape (square or oval) drawn in a layer. The attribute “type” represents the type of the shape, and “Oval” or “Square” is set. For the child elements “bound” and “paint”, refer to Chapter 7. Common Elements.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:layerCompartmentAliasType** |
| properties | isRef 0<br>minOcc 1<br>maxOcc unbounded<br>content complex |
| children | **celldesigner:bounds celldesigner:paint** |
| attributes | Name Type Use Default Fixed annotation<br>type **derived by: xs:string** required |

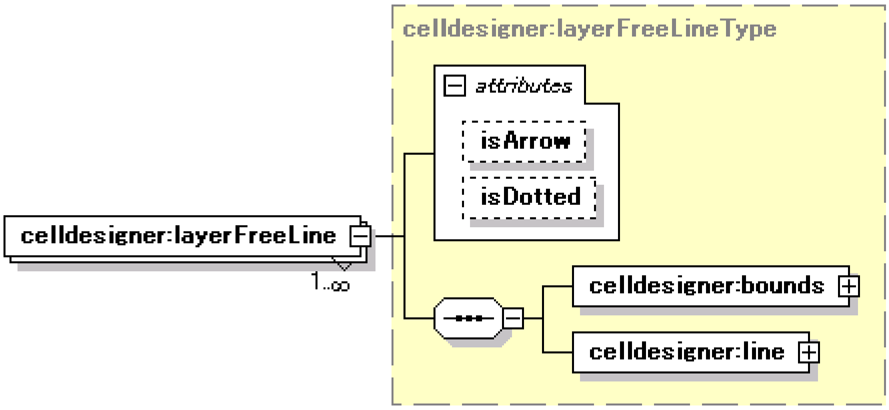
### 8.13.6. Element layerType/listOfFreeLines

This is an XML element that represents a list of celldesigner:layerFreeLines.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| children | **celldesigner:layerFreeLine** |

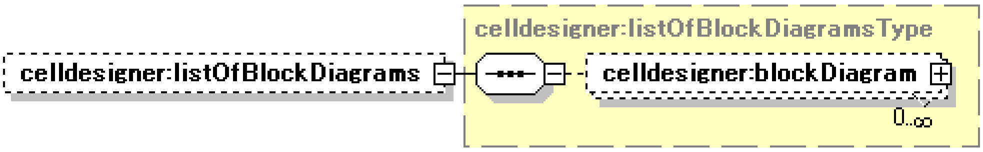
### 8.13.7. Element listOfFreeLinesType/layerFreeLine

This is an element that represents lines and arrows drawn in a layer. When the attribute “isArrow” is true, this refers to an arrow, and when “isDotted” is true, this refers to a dotted line. For the child elements “bounds” and “line”, refer to Chapter 7. Common Elements.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:layerFreeLineType** |
| properties | isRef 0<br>minOcc 1<br>maxOcc unbounded<br>content complex |
| children | **celldesigner:bounds celldesigner:line** |
| attributes | Name Type Use Default Fixed annotation<br>isArrow **xs:boolean**<br>isDotted **xs:boolean** |

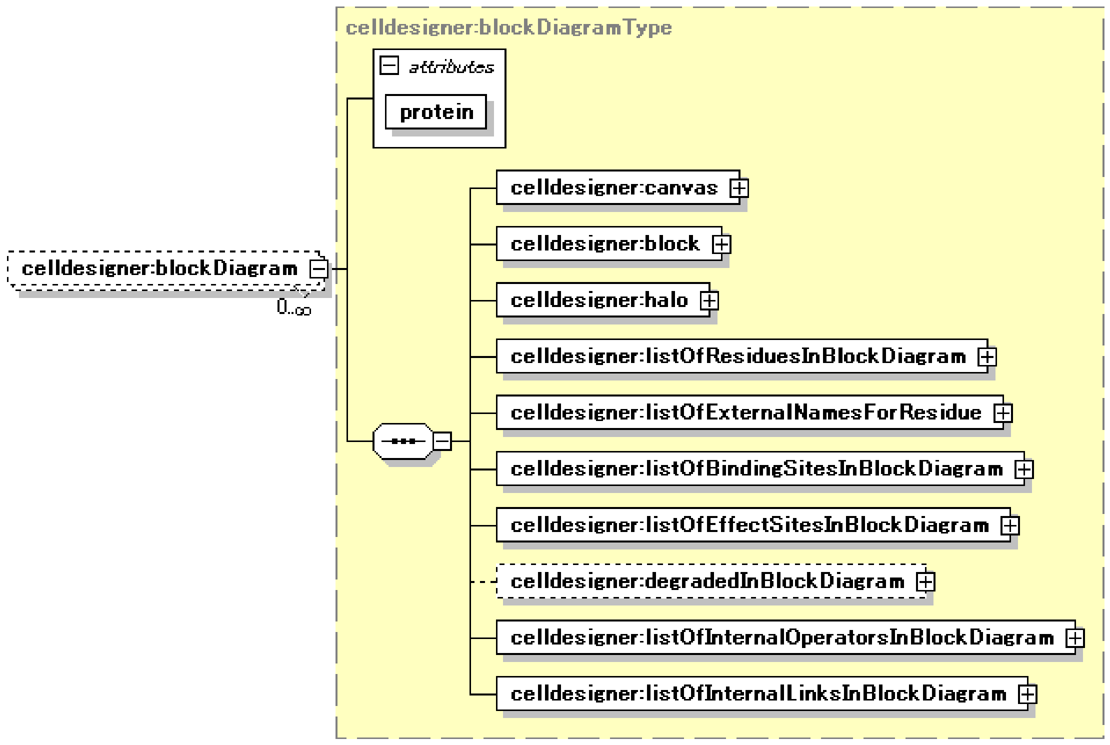
### 8.14. Element celldesigner:modelAnnotationType/listOfBlockDiagrams

This is an XML element to store a list of CellDesigner.BlockDiagrams.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfBlockDiagramsType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:blockDiagram** |

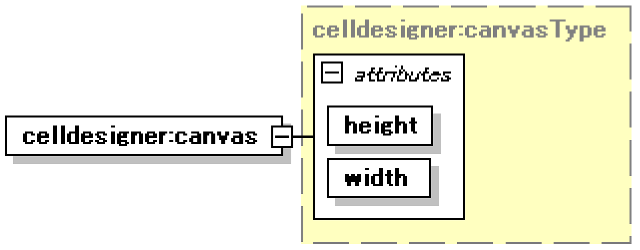
### 8.14.1. Element celldesigner:listOfBlockDiagramsType/blockDiagram

This is an XML element representing a CellDesigner.BlockDiagram that retains data concerning a block diagram with a focus on a specific protein (refer to Section 2.5). For the attribute protein the id of the target Protein is set. The lower XML elements are explained in the next sections.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:blockDiagramType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc unbounded<br>content complex |
| children | **celldesigner:canvas celldesigner:block celldesigner:halo celldesigner:listOfResiduesInBlockDiagram celldesigner:listOfExternalNamesForResidue celldesigner:listOfBindingSitesInBlockDiagram celldesigner:listOfEffectSitesInBlockDiagram celldesigner:degradedInBlockDiagram celldesigner:listOfInternalOperatorsInBlockDiagram celldesigner:listOfInternalLinksInBlockDiagram** |
| attributes | Name: protein<br>Type: **derived by: celldesigner:SId**<br>Use: required<br>Default:<br>Fixed: |

### 8.14.1.1. Element celldesigner:blockDiagramType/canvas

This is an XML element to specify the size of a window canvas for the display of the block diagram. For the attributes width and height, the width and height of the canvas are set.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:canvasType** |

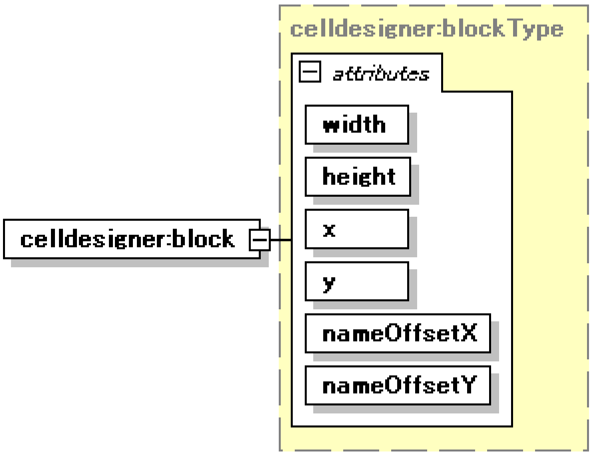
| | | | | | |
|---|---|---|---|---|---|
| properties | isRef 0<br>content complex | | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | height | **derived by: xs:short** | required | | |
| | width | **derived by: xs:short** | required | | |

Example

```
<celldesigner:canvas height="308" width="474" />
```

### 8.14.1.2. Element celldesigner:blockDiagramType/block

This is an XML element to describe a block in the block diagram, i.e. display area data of the target Protein. In an actual diagram, the area is displayed as a rounded box with a solid line. The attributes width and height give the width and height of the box; x and y describe the position within the window canvas; and nameOffsetX and nameOffsetY describe the offset values between the center of the protein name label and the upper right of the block.

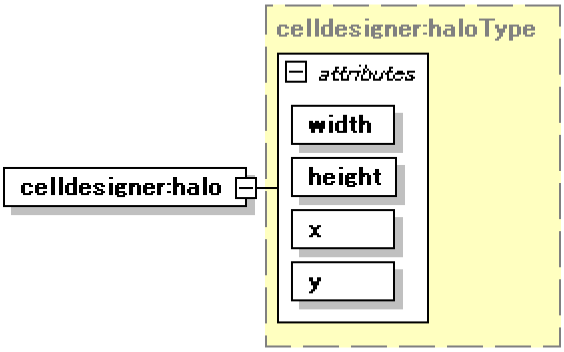
| | | | | | |
|---|---|---|---|---|---|
| diagram |  | | | | |
| namespace | http://www.sbml.org/2001/ns/celldesigner | | | | |
| type | **celldesigner:blockType** | | | | |
| properties | isRef 0<br>content complex | | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | width | **derived by: xs:short** | required | | |
| | height | **derived by: xs:short** | required | | |
| | x | **derived by: xs:short** | required | | |
| | y | **derived by: xs:short** | required | | |
| | nameOffsetX | **derived by: xs:decimal** | required | | |
| | nameOffsetY | **derived by: xs:decimal** | required | | |

Example

```
<celldesigner:block height="90" nameOffsetX="-8.0" nameOffsetY="-8.0" width="210"
  x="100" y="50" />
```

### 8.14.1.3. Element celldesigner:blockDiagramType/halo

This is an XML element that retains data for the block diagram extension or halo to describe other proteins, etc., which are associated with the target Protein. The attributes width and height give the width and height of the halo, and x and y describe the position within the canvas.

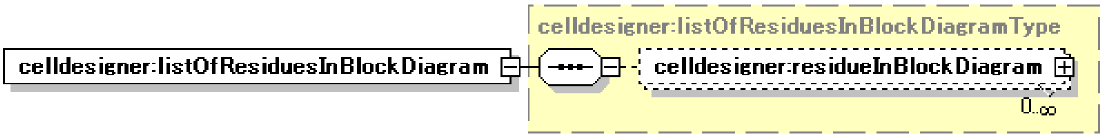
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:haloType</b></td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>width</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr>
<tr><td>height</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr>
<tr><td>x</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr>
<tr><td>y</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr>
</table></td></tr>
</table>

Example

```
<celldesigner:halo height="150" width="270" x="70" y="20" />
```

### 8.14.1.4. Element celldesigner:blockDiagramType/listOfResiduesInBlockDiagram

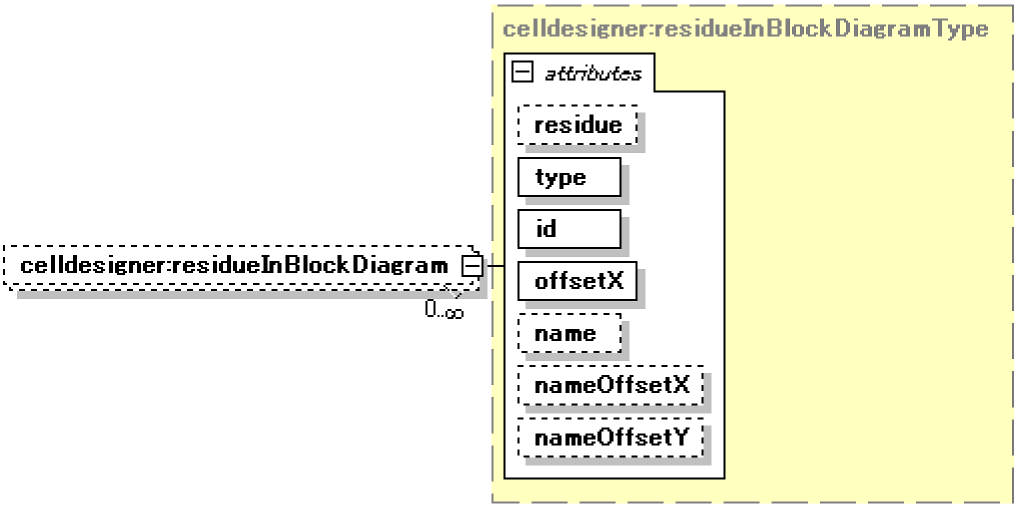
This is an XML element to store a list of ResiduesInBlockDiagram, each of which describes a residue arranged at the top side of the block diagram.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:listOfResiduesInBlockDiagramType</b></td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td><b>celldesigner:residueInBlockDiagram</b></td></tr>
</table>

### 8.14.1.4.1. Element celldesigner:listOfResiduesInBlockDiagramType/residueInBlockDiagram

This is an XML element representing a ResidueInBlockDiagram that describes a residue arranged at the top side of the block diagram. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| residue | The SId of a corresponding residue in a process diagram. |
| type | Type of residue. |
| id | A unique identifier in the list. An integer of 0 or more is used. |
| offsetX | The offset position is determined by assuming the center of the top side of the block is 0. |
| name | Residue name. This is omitted if a residue name is not displayed in the block diagram. |
| nameOffsetX<br>nameOffsetY | When a residue name is displayed, the offsets are located between the center of the name and the center of the residue. |

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:residueInBlockDiagramType</b></td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>0</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>residue</td><td><b>derived by: celldesigner:SId</b></td><td>optional</td><td></td><td></td></tr>
<tr><td>type</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td></tr>
<tr><td>id</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr>
<tr><td>offsetX</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>name</td><td><b>derived by: xs:string</b></td><td></td><td></td><td></td></tr>
<tr><td>nameOffsetX</td><td><b>derived by: xs:decimal</b></td><td></td><td></td><td></td></tr>
<tr><td>nameOffsetY</td><td><b>derived by: xs:decimal</b></td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

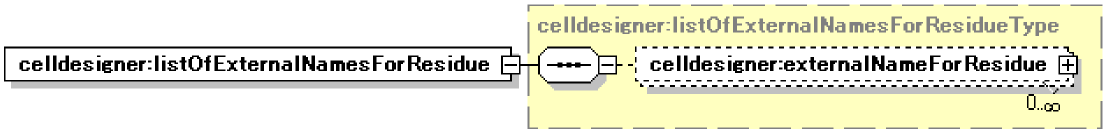
Example

```
<celldesigner:listOfResiduesInBlockDiagram>
  <celldesigner:residueInBlockDiagram id="0" name="Ser225" nameOffsetX="17.0"
    nameOffsetY="12.0" offsetX="-75.0" residue="rs1" type="acetylated" />
  <celldesigner:residueInBlockDiagram id="1" name="Ser225" nameOffsetX="17.0"
```

```
    nameOffsetY="12.0" offsetX="-45.0" residue="rs1" type="dontcare" />
  <celldesigner:residueInBlockDiagram id="2" name="Ser225" nameOffsetX="17.0"
    nameOffsetY="12.0" offsetX="-15.0" residue="rs1" type="methylated" />
  <celldesigner:residueInBlockDiagram id="3" name="Ser225" nameOffsetX="17.0"
    nameOffsetY="12.0" offsetX="15.0" residue="rs1" type="phosphorylated" />
  <celldesigner:residueInBlockDiagram id="4" name="Ser225" nameOffsetX="17.0"
    nameOffsetY="12.0" offsetX="45.0" residue="rs1" type="ubiquitinated" />
  <celldesigner:residueInBlockDiagram id="5" name="Ser225" nameOffsetX="17.0"
    nameOffsetY="12.0" offsetX="75.0" residue="rs1" type="unknown" />
</celldesigner:listOfResiduesInBlockDiagram>
```

### 8.14.1.5. Element celldesigner:blockDiagramType/listOfExternalNamesForResidue

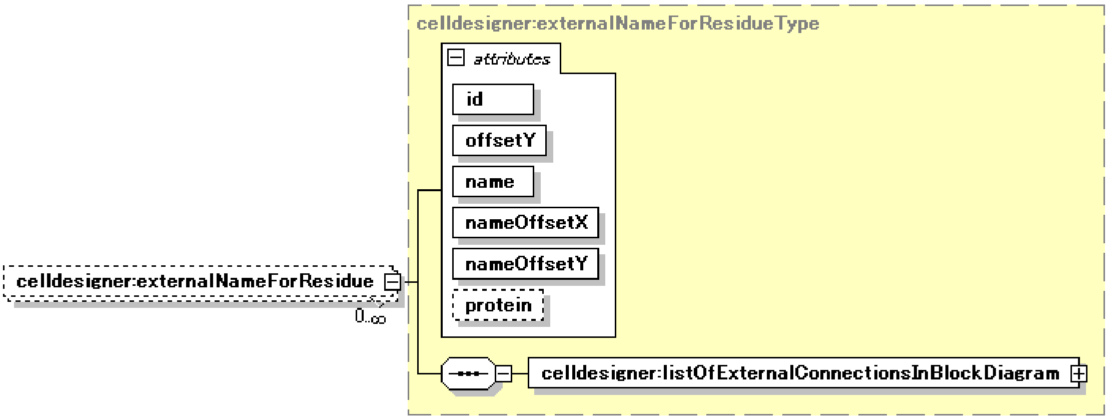
This is an XML element that stores a list of ExternalNamesResidue to describe modifiers that affect modification states of protein residues.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfExternalNamesForResidueType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:externalNameForResidue** |

#### 8.14.1.5.1. Element celldesigner:listOfExternalNamesForResidueType/externalNameForResidue

This is an XML element that represents an ExternalNameResidue to describe a modifier that affects the modification states of protein residues. The meaning of each attribute is as follows:

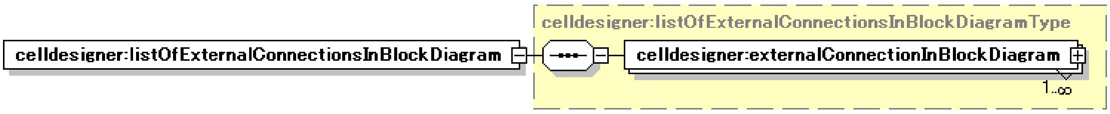
| Attribute name | Content |
|---|---|
| id | A unique identifier in the list. An integer of 0 or more is used. |
| offsetY | The offset position is determined by assuming the central point between the block halo left side and the block left side is 0. |
| name | Name. |
| nameOffsetX<br>nameOffsetY | When a name is displayed, the offsets are located between the center of the name and the link line left end. |
| protein | Optional. When automatically generated from a process diagram, a string in which the id of the Protein is connected with a slash "/" is described. |

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |

<table>
<tr><td>type</td><td><b>celldesigner:externalNameForResidueType</b></td></tr>
<tr><td>properties</td><td>isRef 0<br>minOcc 0<br>maxOcc unbounded<br>content complex</td></tr>
<tr><td>children</td><td><b>celldesigner:listOfExternalConnectionsInBlockDiagram</b></td></tr>
<tr><td>attributes</td><td>
<table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>id</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr>
<tr><td>offsetY</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>name</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td></tr>
<tr><td>nameOffsetX</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>nameOffsetY</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>protein</td><td><b>derived by: xs:string</b></td><td>optional</td><td></td><td></td></tr>
</table>
</td></tr>
</table>

### 8.14.1.5.1.1. Element celldesigner:externalNameForResidueType/listOfExternalConnectionsInBlockDiagram

This is an XML element that stores a list of ExternalConnectionsInBlockDiagram, each of which describes a connection line to a residue affected by an external modifier.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfExternalConnectionsInBlockDiagramType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:externalConnectionInBlockDiagram** |

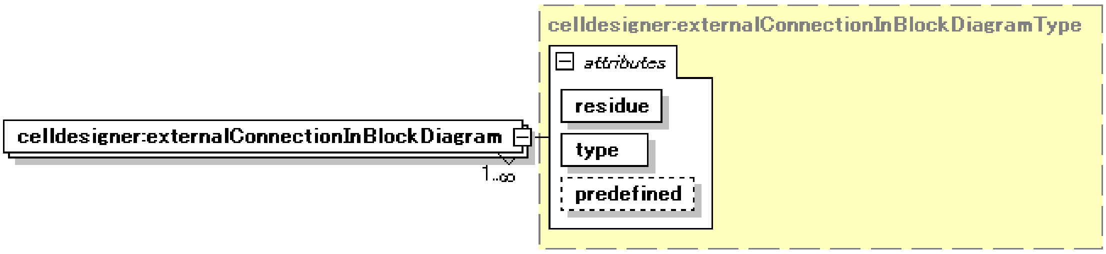
### 8.14.1.5.1.1.1. Element celldesigner:listOfExternalConnectionsInBlockDiagramType/externalConnectionInBlockDiagram

This is an XML element representing an ExternalConnectionInBlockDiagram that describes a connection line to a residue affected by an external modifier. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| residue | The id of corresponding ResiduesInBlockDiagram. |
| type | Type of link line (activation/activationMaybe1[1]/inhibition). |
| predefined | Optional. When automatically generated from a process diagram, “true” is set. |

---

[1] Activation (whether modification is triggered or not) is not determined. In a diagram the line drawn to the upper part from the residue is linked by a gray small circle.

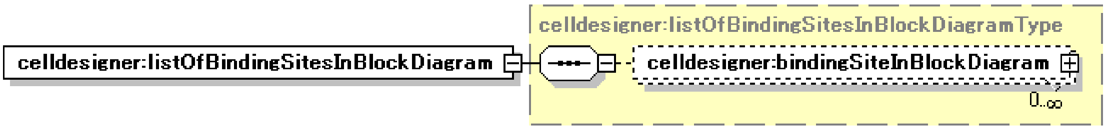
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:externalConnectionInBlockDiagramType</b></td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>1</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>residue</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr>
<tr><td>type</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td></tr>
<tr><td>predefined</td><td><b>derived by: xs:boolean</b></td><td>optional</td><td></td><td></td></tr>
</table></td></tr>
</table>

Example

```xml
<celldesigner:listOfExternalNamesForResidue>
  <celldesigner:externalNameForResidue id="0" name="PP2B" nameOffsetX="-17.0"
    nameOffsetY="0.0" offsetY="-7.0" protein="p101">
    <celldesigner:listOfExternalConnectionsInBlockDiagram>
      <celldesigner:externalConnectionInBlockDiagram predefined="true" residue="1"
        type="inhibition" />
      <celldesigner:externalConnectionInBlockDiagram predefined="true" residue="0"
        type="inhibition" />
    </celldesigner:listOfExternalConnectionsInBlockDiagram>
  </celldesigner:externalNameForResidue>
  <celldesigner:externalNameForResidue id="1" name="nuc.ERK1/2" nameOffsetX="-32.0"
    nameOffsetY="0.0" offsetY="9.0" protein="p91">
    <celldesigner:listOfExternalConnectionsInBlockDiagram>
      <celldesigner:externalConnectionInBlockDiagram predefined="true" residue="1"
        type="activation" />
      <celldesigner:externalConnectionInBlockDiagram predefined="true" residue="0"
        type="activation" />
    </celldesigner:listOfExternalConnectionsInBlockDiagram>
  </celldesigner:externalNameForResidue>
</celldesigner:listOfExternalNamesForResidue>
```

### 8.14.1.6. Element celldesigner:blockDiagramType/listOfBindingSitesInBlockDiagram

This is an XML element that stores a list of BindingSitesInBlockDiagram, each of which describes a binding site with another molecule, and is displayed on the left side of the block diagram.

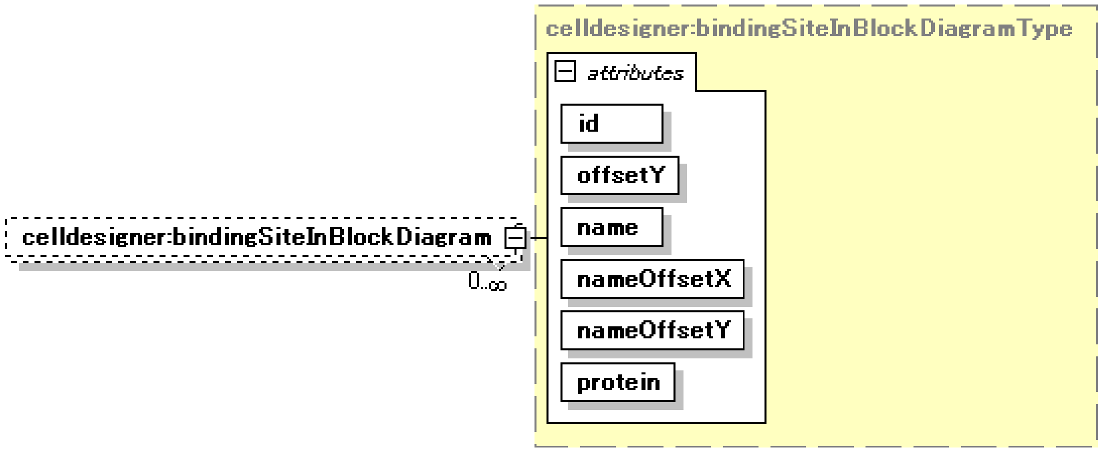
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:listOfBindingSitesInBlockDiagramType</b></td></tr>
</table>

| | |
|---|---|
| properties | isRef 0<br>content complex |
| children | **celldesigner:bindingSiteInBlockDiagram** |

### 8.14.1.6.1. Element celldesigner:listOfBindingSitesInBlockDiagramType/bindingSiteInBlockDiagram

This is an XML element representing a BindingSiteInBlockDiagram that describes a binding site with another molecule, and is displayed on the left side of the block diagram. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| id | A unique identifier in the list. An integer of 0 or more is used. |
| offsetY | The offset position is determined by assuming the center of the left side of the block is 0. |
| name | The name of a Species that is a binding partner. |
| nameOffsetX<br>nameOffsetY | When the name of the binding partner is displayed, the offsets are located between the center of the name and the link line endpoint. |
| protein | The id of a Species that is a binding partner. |

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:bindingSiteInBlockDiagramType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc unbounded<br>content complex |

| attributes | Name | Type | Use | Default | Fixed |
|---|---|---|---|---|---|
| | id | **derived by: xs:short** | required | | |
| | offsetY | **derived by: xs:decimal** | required | | |
| | name | **derived by: xs:string** | required | | |
| | nameOffsetX | **derived by: xs:decimal** | required | | |
| | nameOffsetY | **derived by: xs:decimal** | required | | |
| | protein | **derived by: celldesigner:SId** | required | | |

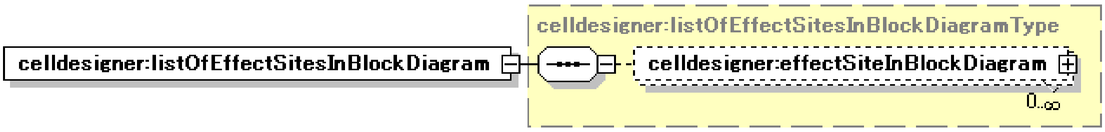
Example

```
<celldesigner:listOfBindingSitesInBlockDiagram>
  <celldesigner:bindingSiteInBlockDiagram id="0" name="Slp1" nameOffsetX="-14.0"
    nameOffsetY="0.0" offsetY="-30.0" protein="pr34" />
```

```
   <celldesigner:bindingSiteInBlockDiagram id="1" name="A" nameOffsetX="-7.0"
     nameOffsetY="0.0" offsetY="0.0" protein="pr42" />
   <celldesigner:bindingSiteInBlockDiagram id="2" name="B" nameOffsetX="-7.0"
     nameOffsetY="0.0" offsetY="30.0" protein="pr43" />
</celldesigner:listOfBindingSitesInBlockDiagram>
```

### 8.14.1.7. Element celldesigner:blockDiagramType/listOfEffectSitesInBlockDiagram

This is an XML element that stores a list of EffectSitesInBlockDiagram, each of which describes such effects as enzymic activity with an external molecule, and is displayed on the bottom side of the block diagram.

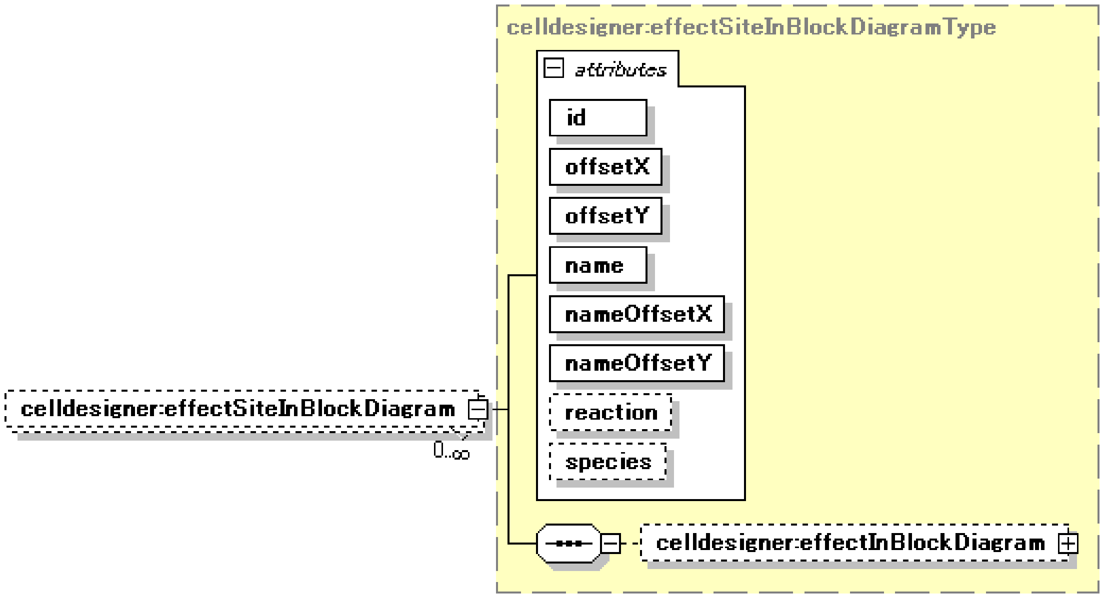
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfEffectSitesInBlockDiagramType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:effectSiteInBlockDiagram** |

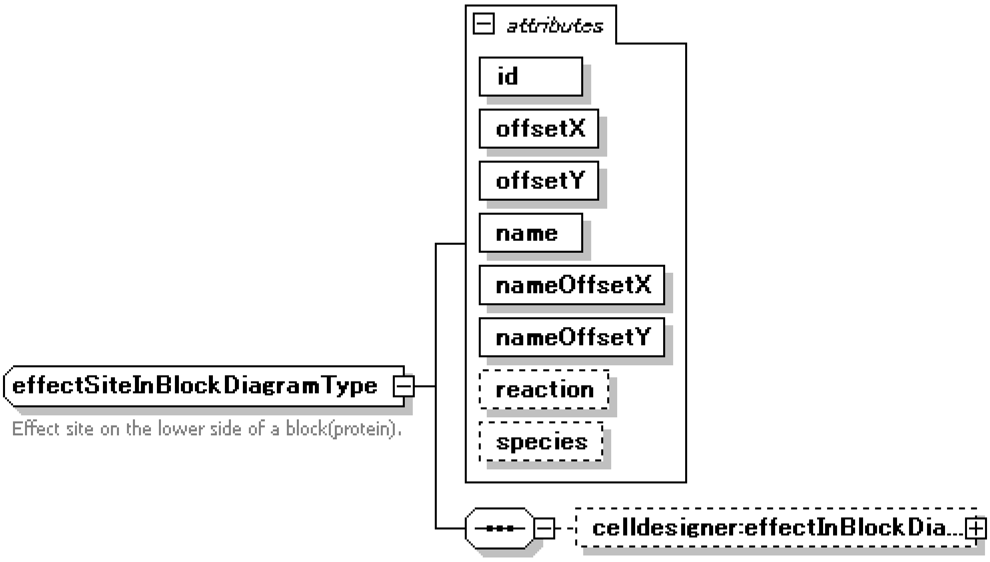
### 8.14.1.7.1. Element celldesigner:listOfEffectSitesInBlockDiagramType/effectSiteInBlockDiagram

This is an XML element representing a EffectSiteInBlockDiagram to describe such effects as enzymic activity with an external molecule, and is displayed on the bottom side of the block diagram. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| id | A unique identifier in the list. An integer of 0 or more is used. |
| offsetX | When a black box is positioned, the offset position is determined by assuming the center of the bottom side of the block is 0. |
| offsetY | When a point for bending is determined, the offset position is determined by assuming the midpoint between the block bottom side and the block halo bottom side is 0. |
| name | The name of a Species that is affected. |
| nameOffsetX<br>nameOffsetY | Regarding the name label of the affected target, the offsets are located between the center of the label and the link line endpoint. |
| species | The SId of a Species that is affected. |
| reaction | The id of a Reaction that is the actual process of the effect. |

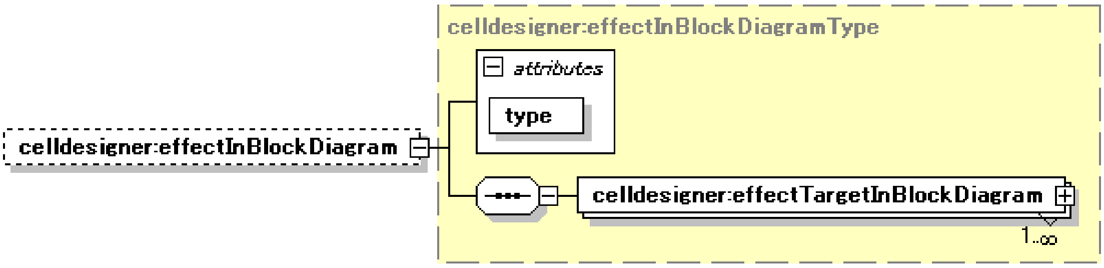
EffectInBlockDiagram is described later.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:effectSiteInBlockDiagramType</b></td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>0</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>children</td><td><b>celldesigner:effectInBlockDiagram</b></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>id</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr>
<tr><td>offsetX</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>offsetY</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>name</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td></tr>
<tr><td>nameOffsetX</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>nameOffsetY</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>reaction</td><td><b>celldesigner:SId</b></td><td></td><td></td><td></td></tr>
<tr><td>species</td><td><b>celldesigner:SId</b></td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>children</td><td><b>celldesigner:effectInBlockDiagram</b></td></tr>
<tr><td>used by</td><td>element <b>listOfEffectSitesInBlockDiagramType/effectSiteInBlockDiagram</b></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th><th>annotation</th></tr>
<tr><td>id</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>offsetX</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>offsetY</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>name</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>nameOffsetX</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>nameOffsetY</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>reaction</td><td><b>derived by: sbml:SId</b></td><td></td><td></td><td></td><td></td></tr>
<tr><td>species</td><td><b>derived by: sbml:SId</b></td><td></td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

### 8.14.1.7.1.1. Element celldesigner:effectSiteInBlockDiagramType/effectInBlockDiagram

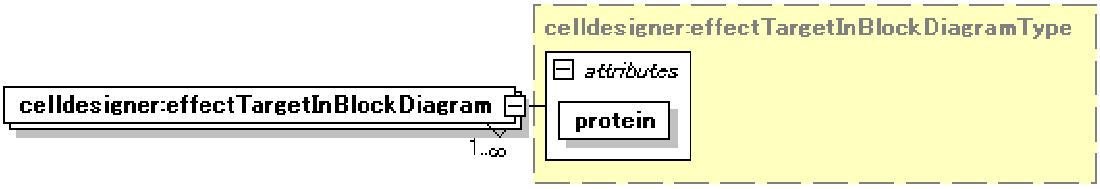
This is an XML element to describe an effect given to an external molecule. For the attribute type either "CATALYSIS" or "INHIBITION" is specified as a type of activity. EffectTargetInBlockDiagram is described in the next section.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:effectInBlockDiagramType</b></td></tr>
</table>

| | |
|---|---|
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:effectTargetInBlockDiagram** |
| attributes | Name Type Use Default Fixed<br>type **derived by: xs:string** required |

### 8.14.1.7.1.1.1. Element celldesigner:effectInBlockDiagramType/effectTargetInBlockDiagram

This is an XML element to describe a Protein that is an effect target. For the attribute protein, the id of the target Protein is described.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:effectTargetInBlockDiagramType** |
| properties | isRef 0<br>minOcc 1<br>maxOcc unbounded<br>content complex |
| attributes | Name Type Use Default Fixed<br>protein **derived by: celldesigner:SId** required |

Example

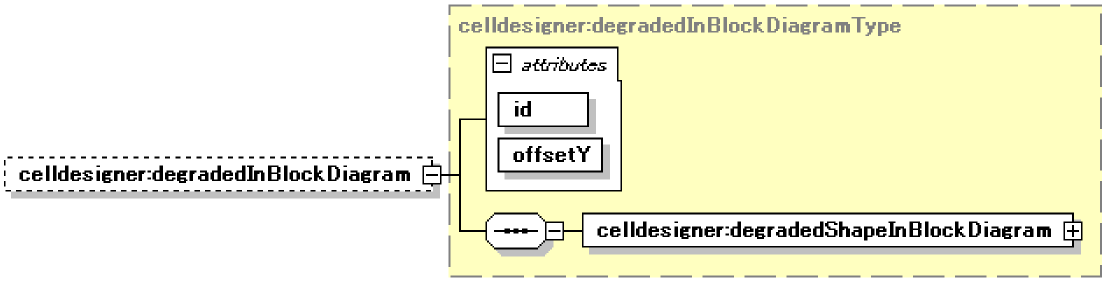
```
<celldesigner:listOfEffectSitesInBlockDiagram>
  <celldesigner:effectSiteInBlockDiagram id="1" name="B/A/Slp1/APC|B/Slp1/APC"
    nameOffsetX="66.0" nameOffsetY="0.0" offsetX="30.0" offsetY="-16.0"
    reaction="re31" species="s115">
    <celldesigner:effectInBlockDiagram type="CATALYSIS">
      <celldesigner:effectTargetInBlockDiagram protein="pr43" />
      <celldesigner:effectTargetInBlockDiagram protein="pr34" />
      <celldesigner:effectTargetInBlockDiagram protein="p11" />
    </celldesigner:effectInBlockDiagram>
  </celldesigner:effectSiteInBlockDiagram>
  <celldesigner:effectSiteInBlockDiagram id="2" name="Rum1" nameOffsetX="18.0"
    nameOffsetY="0.0" offsetX="60.0" offsetY="-32.0" reaction="re32" species="s115">
    <celldesigner:effectInBlockDiagram type="CATALYSIS">
      <celldesigner:effectTargetInBlockDiagram protein="p13" />
    </celldesigner:effectInBlockDiagram>
  </celldesigner:effectSiteInBlockDiagram>
</celldesigner:listOfEffectSitesInBlockDiagram>
```

### 8.14.1.8. Element celldesigner:blockDiagramType/degradedInBlockDiagram

This is an XML element representing a DegragedInBlockDiagram that describes self-degradation and is displayed on the right side of the block diagram. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| id | A unique identifier in the list. An integer of 0 or more is used. |
| offsetY | The offset position is determined by assuming the center of the right side of the block is 0. |

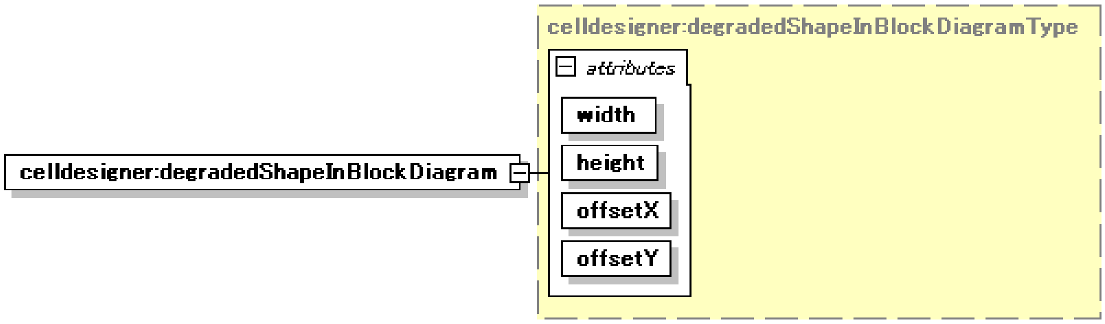
The lower element DegradedShapeInBlockDiagram is described in the next section.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>**celldesigner:degradedInBlockDiagramType**</td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>minOcc</td><td>0</td></tr><tr><td>maxOcc</td><td>1</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td>**celldesigner:degradedShapeInBlockDiagram**</td></tr>
<tr><td>attributes</td><td><table><tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr><tr><td>id</td><td>**derived by: xs:short**</td><td>required</td><td></td><td></td></tr><tr><td>offsetY</td><td>**derived by: xs:decimal**</td><td>required</td><td></td><td></td></tr></table></td></tr>
</table>

### 8.14.1.8.1. Element celldesigner:degradedInBlockDiagramType/degradedShapeInBlockDiagram

This is an XML element to describe a symbol that means degradation. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| width | The width and height for a circle with oblique line. |
| height | |
| offsetX | The offset position is determined by assuming the right endpoint of the link line to the above shape is (0,0). |
| offsetY | |

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>**celldesigner:degradedShapeInBlockDiagramType**</td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>attributes</td><td><table><tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr><tr><td>width</td><td>**derived by: xs:short**</td><td>required</td><td></td><td></td></tr><tr><td>height</td><td>**derived by: xs:short**</td><td>required</td><td></td><td></td></tr><tr><td>offsetX</td><td>**derived by: xs:decimal**</td><td>required</td><td></td><td></td></tr></table></td></tr>
</table>

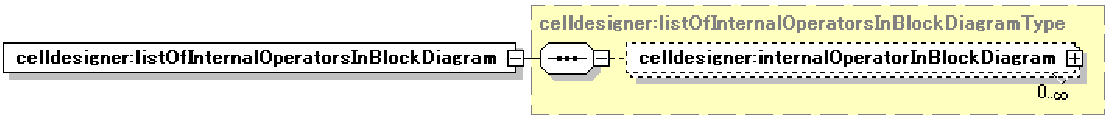
| | | | |
|---|---|---|---|
| | offsetY | **derived by: xs:decimal** | required |

Example

```
<celldesigner:degradedInBlockDiagram id="0" offsetY="0.0">
  <celldesigner:degradedShapeInBlockDiagram height="22" offsetX="11.0" offsetY="0.0"
    width="22" />
</celldesigner:degradedInBlockDiagram>
```

### 8.14.1.9. Element celldesigner:blockDiagramType/listOfInternalOperatorsInBlockDiagram

This is an XML element that stores a list of InternalOperatorsInBlockDiagram, each of which is needed to describe the internal logic of the protein described by the block diagram.

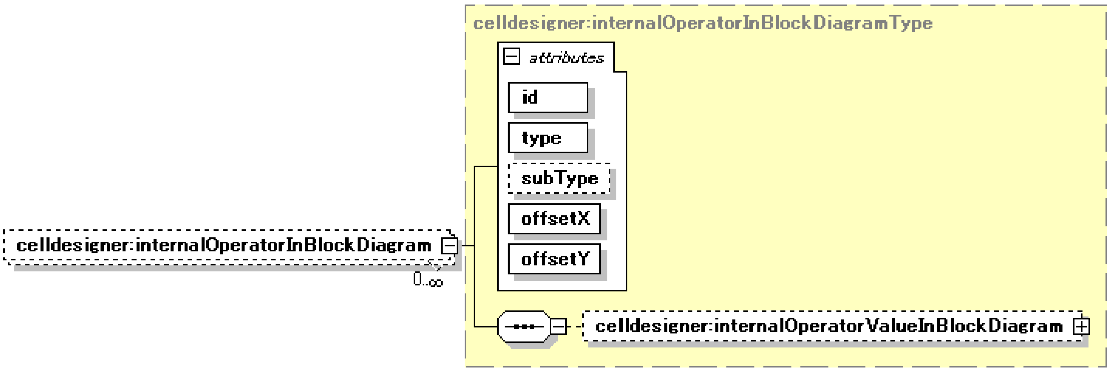
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfInternalOperatorsInBlockDiagramType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:internalOperatorInBlockDiagram** |

#### 8.14.1.9.1. Element celldesigner:listOfInternalOperatorsInBlockDiagramType/internalOperatorInBlockDiagram

This is an XML element to describe an InternalOperatorInBlockDiagram, an operator needed to describe the internal logic of the protein described by the block diagram. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| id | A unique identifier in the list. An integer of 0 or more is used. |
| type | Type (and/or/add/multiply/threshold/autoActivate/assign). |
| subType | Optional. When the type is “threshold”, the subtype is (ge/gt/le/lt). |
| offsetX<br>offsetY | When an operator is displayed, the offsets are located from the center of the block. |

The lower element InternalOperatorValueInBlockDiagram is explained in the next section.

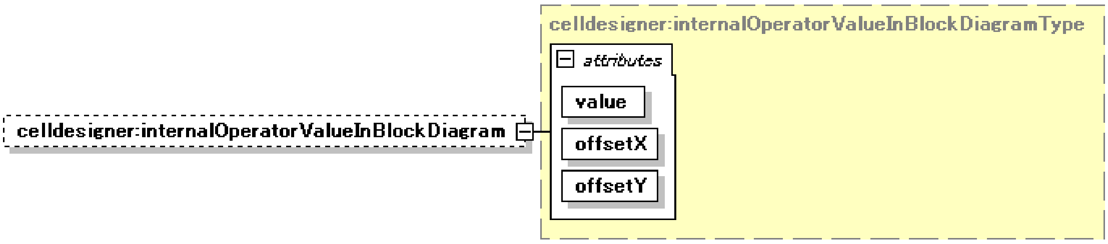
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:internalOperatorInBlockDiagramType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc unbounded<br>content complex |

| | | | | | |
|---|---|---|---|---|---|
| children | **celldesigner:internalOperatorValueInBlockDiagram** | | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | id | **derived by: xs:short** | required | | |
| | type | **derived by: xs:string** | required | | |
| | subType | **derived by: xs:string** | optional | | |
| | offsetX | **derived by: xs:decimal** | required | | |
| | offsetY | **derived by: xs:decimal** | required | | |

### 8.14.1.9.1.1. Element celldesigner:internalOperatorInBlockDiagramType/internalOperatorValueInBlockDiagram

This is an XML element representing an InternalOperatorValueInBlockDiagram that describes a value accompanying an InternalOperatorInBlockDiagram, an operator needed to describe the internal logic. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| value | A value represented by a real number. |
| offsetX<br>offsetY | When the value is displayed, the offsets are located from the center of the operator. |

| | | | | | |
|---|---|---|---|---|---|
| diagram |  | | | | |
| namespace | http://www.sbml.org/2001/ns/celldesigner | | | | |
| type | **celldesigner:internalOperatorValueInBlockDiagramType** | | | | |
| properties | isRef | 0 | | | |
| | minOcc | 0 | | | |
| | maxOcc | 1 | | | |
| | content | complex | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | value | **derived by: xs:decimal** | required | | |
| | offsetX | **derived by: xs:decimal** | required | | |
| | offsetY | **derived by: xs:decimal** | required | | |

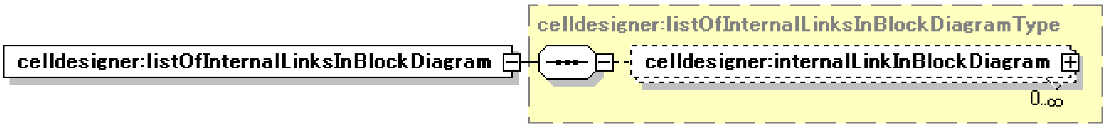
Example

```
<celldesigner:listOfInternalOperatorsInBlockDiagram>
  <celldesigner:internalOperatorInBlockDiagram id="0" offsetX="35.0" offsetY="-36.0"
    type="and" />
  <celldesigner:internalOperatorInBlockDiagram id="1" offsetX="46.0" offsetY="6.0"
    type="add" />
  <celldesigner:internalOperatorInBlockDiagram id="2" offsetX="-42.0" offsetY="-20.0"
    subType="ge" type="threshold">
    <celldesigner:internalOperatorValueInBlockDiagram offsetX="16.0" offsetY="12.0"
      value="1.0" />
  </celldesigner:internalOperatorInBlockDiagram>
```

```
  <celldesigner:internalOperatorInBlockDiagram id="3" offsetX="49.0" offsetY="40.0"
    type="autoActivate" />
  <celldesigner:internalOperatorInBlockDiagram id="4" offsetX="-20.0" offsetY="29.0"
    type="assign">
    <celldesigner:internalOperatorValueInBlockDiagram offsetX="7.0" offsetY="8.0"
      value="1.0" />
  </celldesigner:internalOperatorInBlockDiagram>
</celldesigner:listOfInternalOperatorsInBlockDiagram>
```

### 8.14.1.10. Element celldesigner:blockDiagramType/listOfInternalLinksInBlockDiagram

This is an XML element that stores a list of InternalLinksInBlockDiagram, each of which describes a link to describe the internal logic of the protein described by the block diagram.

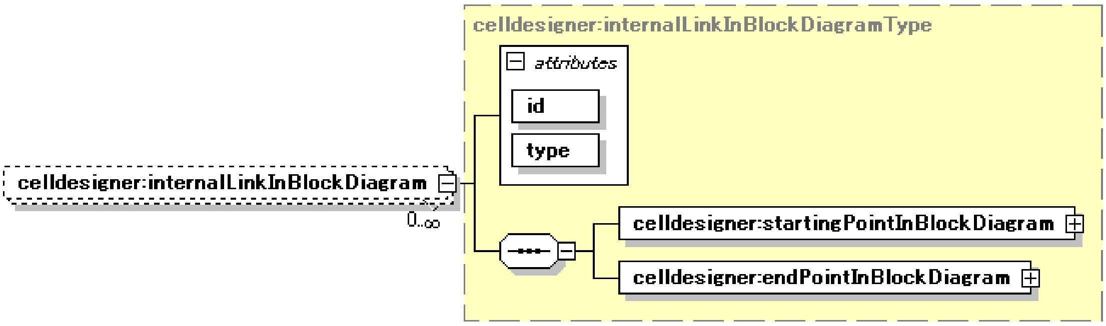
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfInternalLinksInBlockDiagramType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:internalLinkInBlockDiagram** |

### 8.14.1.10.1. Element celldesigner:listOfInternalLinksInBlockDiagramType/internalLinkInBlockDiagram

This is an XML element representing an InternalLinkInBlockDiagram to describe a link that describes the internal logic of the protein described by the block diagram. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| id | A unique identifier in the list. An integer of 0 or more is used. |
| type | Link type.<br>activation/absoluteActivation/inhibition/absoluteInhibition |

The lower elements StartingPointInBlockDiagram and EndPointInBlockDiagram are explained in the next sections.

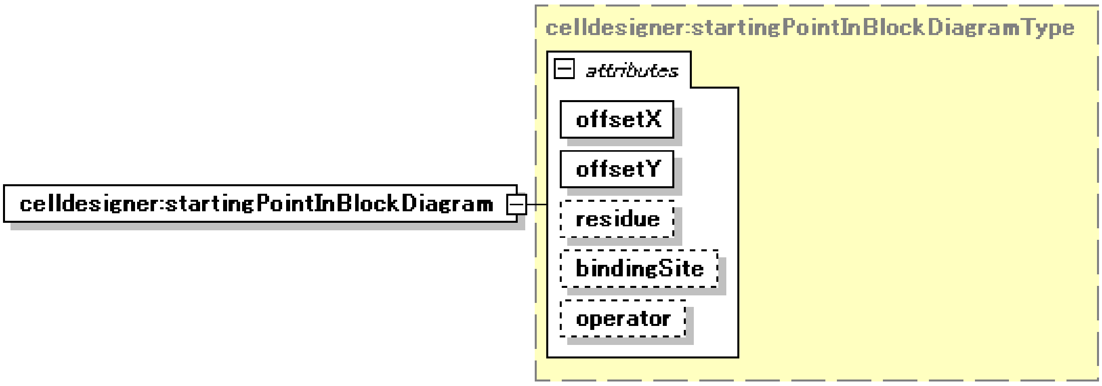
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:internalLinkInBlockDiagramType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc unbounded<br>content complex |

|  |  |  |  |  |  |
|---|---|---|---|---|---|
| children | **celldesigner:startingPointInBlockDiagram celldesigner:endPointInBlockDiagram** |  |  |  |  |
| attributes | Name | Type | Use | Default | Fixed |
|  | id | **derived by: xs:short** | required |  |  |
|  | type | **derived by: xs:string** | required |  |  |

### 8.14.1.10.1.1. Element celldesigner:internalLinkInBlockDiagramType/startingPointInBlockDiagram

This is an XML element representing a StartingPointInBlockDiagram to describe a starting point of a link that describes the internal logic of the protein described by the block diagram. The meaning of each attribute is as follows:

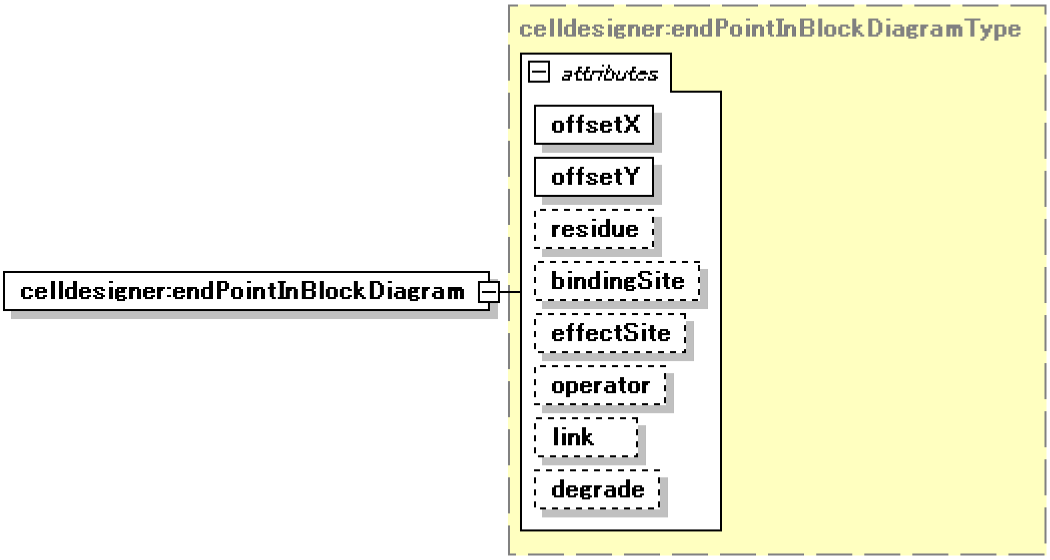
| Attribute name | Content |
|---|---|
| offsetX<br>offsetY | The offsets are located between the link starting point and the center of the target shape. |
| An attribute representing the link destination (any of residue, bindingSite, or operator) | id. The id of the element representing the link starting point. |

|  |  |  |  |  |  |
|---|---|---|---|---|---|
| diagram |  |  |  |  |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |  |  |  |  |
| type | **celldesigner:startingPointInBlockDiagramType** |  |  |  |  |
| properties | isRef 0<br>content complex |  |  |  |  |
| attributes | Name | Type | Use | Default | Fixed |
|  | offsetX | **derived by: xs:decimal** | required |  |  |
|  | offsetY | **derived by: xs:decimal** | required |  |  |
|  | residue | **derived by: xs:short** |  |  |  |
|  | bindingSite | **derived by: xs:short** |  |  |  |
|  | operator | **derived by: xs:short** |  |  |  |

### 8.14.1.10.1.2. Element celldesigner:internalLinkInBlockDiagramType/endPointInBlockDiagram

This is an XML element representing an EndPointInBlockDiagram to describe an end point of a link that describes the internal logic of the protein described by the block diagram. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| offsetX<br>offsetY | The offsets are located between the link end point and the center of the target shape. |
| An attribute representing the link destination (any of residue, bindingSite, effectSite, operator, link, or degrade) | id. The id of the element representing the link end point. |

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:endPointInBlockDiagramType** |
| properties | isRef 0<br>content complex |

attributes

| Name | Type | Use | Default | Fixed |
|---|---|---|---|---|
| offsetX | **derived by: xs:list** | required | | |
| offsetY | **derived by: xs:decimal** | required | | |
| residue | **derived by: xs:short** | | | |
| bindingSite | **derived by: xs:short** | | | |
| effectSite | **derived by: xs:short** | | | |
| operator | **derived by: xs:short** | | | |
| link | **derived by: xs:short** | | | |
| degrade | **derived by: xs:short** | | | |

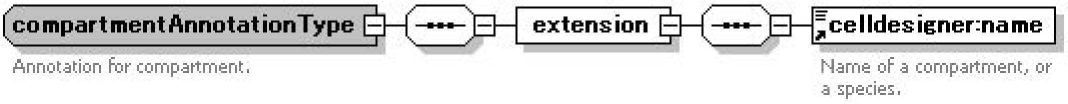
Example

```
<celldesigner:listOfInternalLinksInBlockDiagram>
  <celldesigner:internalLinkInBlockDiagram id="0" type="inhibition">
    <celldesigner:startingPointInBlockDiagram bindingSite="0" offsetX="0.0" offsetY="0.0" />
    <celldesigner:endPointInBlockDiagram effectSite="1" offsetX="0.0" offsetY="0.0" />
  </celldesigner:internalLinkInBlockDiagram>
  <celldesigner:internalLinkInBlockDiagram id="1" type="absoluteInhibition">
    <celldesigner:startingPointInBlockDiagram bindingSite="1" offsetX="0.0" offsetY="0.0" />
    <celldesigner:endPointInBlockDiagram effectSite="0" offsetX="0.0" offsetY="0.0" />
  </celldesigner:internalLinkInBlockDiagram>
  <celldesigner:internalLinkInBlockDiagram id="2" type="activation">
    <celldesigner:startingPointInBlockDiagram offsetX="0.0" offsetY="0.0" residue="0" />
    <celldesigner:endPointInBlockDiagram effectSite="2" offsetX="0.0" offsetY="0.0" />
  </celldesigner:internalLinkInBlockDiagram>
  <celldesigner:internalLinkInBlockDiagram id="3" type="absoluteActivation">
    <celldesigner:startingPointInBlockDiagram bindingSite="2" offsetX="0.0" offsetY="0.0" />
    <celldesigner:endPointInBlockDiagram effectSite="3" offsetX="0.0" offsetY="0.0" />
  </celldesigner:internalLinkInBlockDiagram>
</celldesigner:listOfInternalLinksInBlockDiagram>
```

## 9. Extension of Compartment.Annotation

Data used for identity verification of a Compartment is stored as the lower elements of Annotation.

### Element Compartment/annotation

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/sbml/level2 |
| type | **celldesigner:compartmentAnnotationType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:name** |

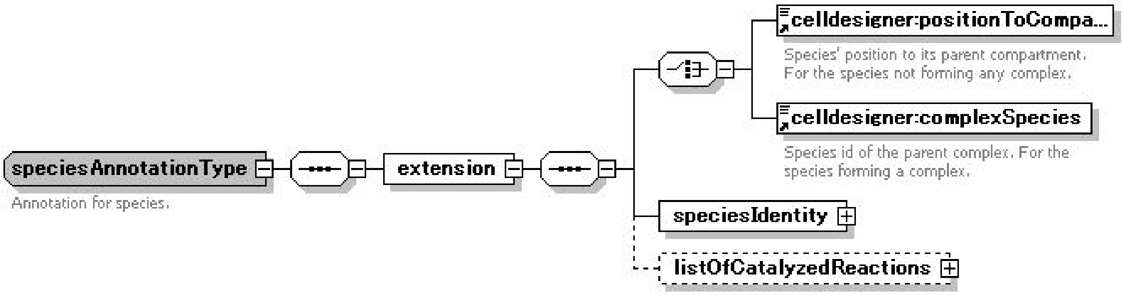
### 9.1. Element name

This is an XML element used for storing the name of a Compartment. The definition is described in 7.3.2. Although the attribute name of an SBML.Compartment is optional, in CellDesigner it is essential, and therefore, it is retained by creating a tag in the Compartment.Annotation. This value is used for verifying the identity of the Compartment.

## 10. Extension of Species.Annotation

Data used for identity verification of a Species is stored in the lower elements of Annotation.

### Element Species/annotation

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/sbml/level2 |
| type | **celldesigner:speciesAnnotationType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:positionToCompartment celldesigner:complexSpecies celldesigner:speciesIdentity celldesigner:listOfCatalyzedReactions** |

### 10.1. Element celldesigner:positionToCompartment

This element describes the relative position to a membrane of the Compartment to which the Species belongs. A string representing any of “outerSurface”, “transmembrane”, “innerSurface”, “inside” or “insideOfMembrane” is set.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | restriction of **xs:string** |
| properties | content simple |
| used by | complexType **celldesigner:speciesAnnotationType** |
| facets | enumeration outerSurface<br>enumeration transmembrane<br>enumeration innerSurface<br>enumeration inside<br>enumeration insideOfMembrane |

Example

```
<celldesigner:positionToCompartment>outerSurface</celldesigner:positionToCompartment>
```

### 10.2. Element celldesigner:complexSpecies

This is an XML element to store the SId of an SBML.Species that is a complex of the parent element. The SId must be for a Species listed in the SBML.listOfSpecies.

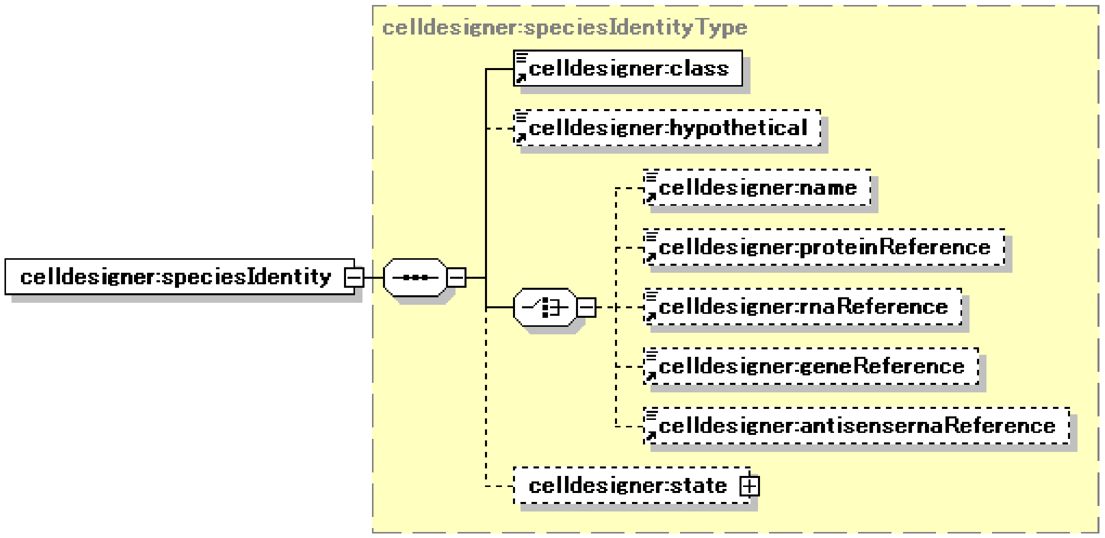
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:SId** |
| properties | content simple |
| used by | complexType **celldesigner:speciesAnnotationType** |
| facets | pattern (_\|[a-z]\|[A-Z])(_\|[a-z]\|[A-Z]\|[0-9])* |

Example

```
<celldesigner:complexSpecies>s109</celldesigner:complexSpecies>
```

### 10.3. Element celldesigner:speciesAnnotationType/speciesIdentity

This is an XML element that stores data to mainly distinguish the chemical species of the Species. The lower element Class represents the category of molecules (refer to Section 7.3.1) and Hypothetical is an element to represent that the relevant Species is hypothetical. From among the following lower elements one is selected as an element: Name, ProteinReference, GeneReference, RnaReference, and AntisensernaReference. State is an element to stipulate the modification state of the chemical species.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:speciesIdentityType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:class celldesigner:hypothetical celldesigner:name celldesigner:proteinReference celldesigner:rnaReference celldesigner:geneReference celldesigner:antisensernaReference celldesigner:state** |

### 10.3.1. Element celldesigner:hypothetical

This is an XML element representing Hypothetical that indicates the Species is hypothetical. In case of False, this element can be omitted.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | restriction of **xs:boolean** |
| properties | content simple |
| used by | complexType **celldesigner:speciesIdentityType** |

Example

```
<celldesigner:hypothetical>true</celldesigner:hypothetical>
```

### 10.3.2. Element celldesigner:proteinReference

This is an XML element to describe the id of a Protein that is referred to.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | restriction of **celldesigner:SId** |
| properties | content simple |
| used by | complexType **celldesigner:speciesIdentityType** |
| facets | pattern (_\|[a-z]\|[A-Z])(_\|[a-z]\|[A-Z]\|[0-9])* |

Example

```
<celldesigner:proteinReference>pr2</celldesigner:proteinReference>
```

### 10.3.3. Element celldesigner:geneReference

This is an XML element to describe the id of a Gene that is referred to.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>restriction of <b>celldesigner:SId</b></td></tr>
<tr><td>properties</td><td>content simple</td></tr>
<tr><td>used by</td><td>complexType <b>celldesigner:speciesIdentityType</b></td></tr>
<tr><td>facets</td><td>pattern (_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*</td></tr>
</table>

Example

```
<celldesigner:geneReference>gn1</celldesigner:geneReference>
```

### 10.3.4. Element celldesigner:rnaReference

This is an XML element to describe the id of an RNA that is referred to.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>restriction of <b>celldesigner:SId</b></td></tr>
<tr><td>properties</td><td>content simple</td></tr>
<tr><td>used by</td><td>complexType <b>celldesigner:speciesIdentityType</b></td></tr>
<tr><td>facets</td><td>pattern (_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*</td></tr>
</table>

Example

```
<celldesigner:rnaReference>rn1</celldesigner:rnaReference>
```

### 10.3.5. Element celldesigner:antisensernaReference

This is an XML element to describe the id of an AntisenseRNA that is referred to.

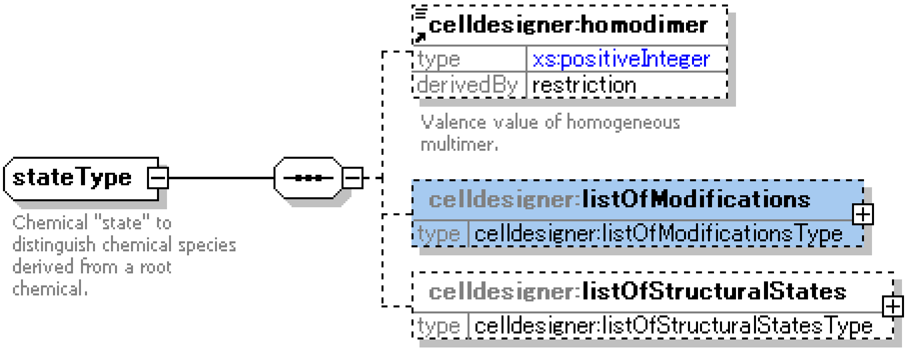
<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>restriction of <b>celldesigner:SId</b></td></tr>
<tr><td>properties</td><td>content simple</td></tr>
<tr><td>used by</td><td>complexType <b>celldesigner:speciesIdentityType</b></td></tr>
<tr><td>facets</td><td>pattern (_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*</td></tr>
</table>

Example

```
<celldesigner:antisensernaReference>arn2</celldesigner:antisensernaReference>
```

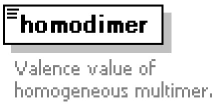
### 10.3.6. Element celldesigner:speciesIdentityType/state

This is an XML element representing a State that stipulates the modification state of the species. The lower elements are described in the following sections.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:stateType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:homodimer celldesigner:listOfModifications** listOfStructuralStates |

### 10.3.6.1. Element homodimer

This is an XML element representing a Homodimer that indicates a homogenous species forms a multimer. The valence of the multimer is described. When the valence is 1, this element can be omitted.

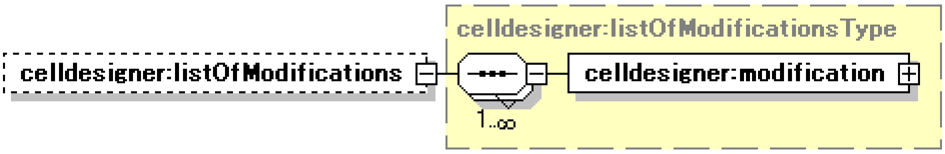
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | restriction of **xs:positiveInteger** |
| properties | content simple |
| used by | complexType **stateType** |

Example

```
<celldesigner:homodimer>2</celldesigner:homodimer>
```

### 10.3.6.2. Element celldesigner:stateType/listOfModifications

This is an XML element to store a list of Modifications, each of which represents the modification state of a chemical species.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfModificationsType** |

|  |  |
|---|---|
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:modification** |

### 10.3.6.2.1. Element celldesigner:listOfModificationsType/modification

This is an XML element to store a list of Modifications, each of which represents the modification state of a chemical species. For the attribute residue, the id of a Protein residue or the id of a Gene region is described. For the attribute state, the modification sate is described with any of “phosphorylated”, “acetylated”, “ubiquitinated”, “methylated”, “hydroxylated”, “don't care”, “unknown”, “glycosylated”, “myristoylated”, “palmytoylated”, “prenylated”, “protonated”, or “sulfated”.

“Histone1” and “histone2” used up to Ver. 3.x were removed from ver. 4.0.

|  |  |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| properties | isRef 0<br>content complex |

attributes:

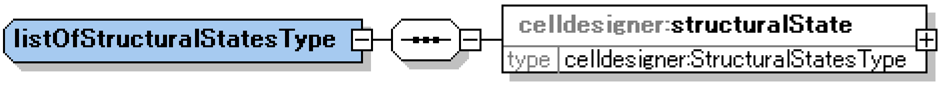
| Name | Type | Use | Default | Fixed |
|---|---|---|---|---|
| residue | **celldesigner:SId** | required |  |  |
| state | **derived by: xs:string** | required |  |  |

Example

```
<celldesigner:listOfModifications>
  <celldesigner:modification residue="rs1" state="phosphorylated" />
  <celldesigner:modification residue="rs2" state="phosphorylated" />
  <celldesigner:modification residue="rs3" state="ubiquitinated" />
  <celldesigner:modification residue="rs4" state="ubiquitinated" />
  </celldesigner:listOfModifications>
</celldesigner:state>
```

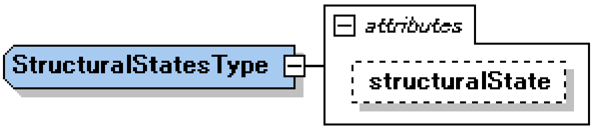
### 10.3.6.3. Element celldesigner:proteinType/listOfStructuralStates

This is an XML element representing a list of celldesigner:structuralStates, each of which is the state of a protein. The child element “structuralState” retains a string of “open”, “close”, or an arbitrary string input by a user.

|  |  |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfStructuralStatesType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:** structuralState (**celldesigner:** structuralStateType) |

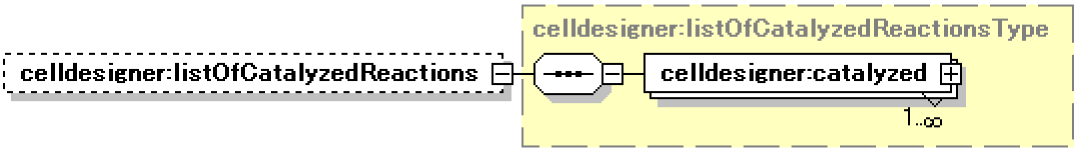
### 10.3.6.3.1. Element celldesigner: StructuralStatesType

**StructuralState** retains a string of “open”, “close”, or an arbitrary string input by a user.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:StructuralStatesType** |
| properties | content complex |
| used by | complexType **celldesigner: listOfStructuralStatesType** |
| attributes | Name: structuralState<br>Type: **xs:string**<br>Use: required<br>Default:<br>Fixed: |

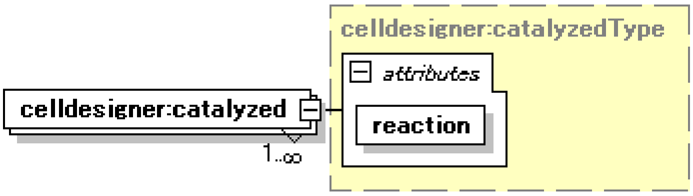
### 10.4. Element celldesigner:speciesAnnotationType/listOfCatalyzedReactions

This is an XML element to store a list of CellDesigner.Catalyzed that means a target on which the Species acts as a regulator, e.g. enzymic activity.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfCatalyzedReactionsType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:catalyzed** |

### 10.4.1. Element celldesigner:listOfCatalyzedReactionsType/catalyzed

This is an XML element representing a CellDesigner.Catalyzed that means a target on which the Species acts as a regulator e.g. enzymic activity.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:catalyzedType** |
| properties | isRef 0<br>minOcc 1<br>maxOcc unbounded<br>content complex |
| attributes | Name: reaction<br>Type: **celldesigner:SId**<br>Use: required<br>Default:<br>Fixed: |

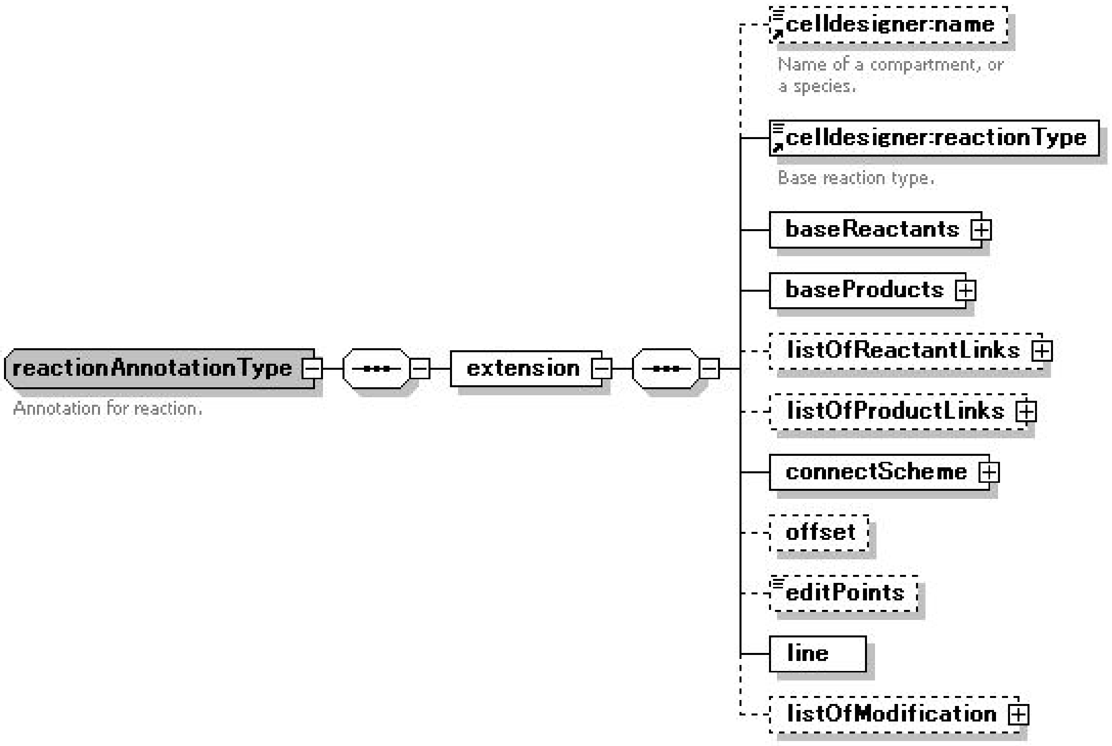
Example

```
<celldesigner:listOfCatalyzedReactions>
    <celldesigner:catalyzed reaction="re18" />
    <celldesigner:catalyzed reaction="re19" />
    <celldesigner:catalyzed reaction="re137" />
    <celldesigner:catalyzed reaction="re138" />
</celldesigner:listOfCatalyzedReactions>
```

## 11. Extension of Reaction.Annotation

Data is stored that stipulates Reaction types and connection conditions in a graphical model.

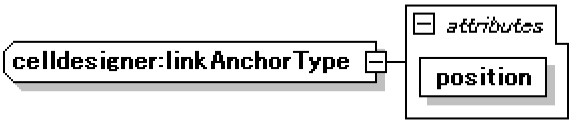
### Element Reaction/annotation

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/sbml/level2 |
| type | **celldesigner:reactionAnnotationType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:name celldesigner:reactionType celldesigner:baseReactants celldesigner:baseProducts celldesigner:listOfReactantLinks celldesigner:listOfProductLinks celldesigner:connectScheme celldesigner:offset celldesigner:editPoints celldesigner:line celldesigner:listOfModification** |

### 11.1. Common Elements in Reaction.Annotation

#### 11.1.1. ComplexType celldesigner:linkAnchorType

This is an XML element that indicates the position of the connection destination element (e.g. SpeciesAlias) to which the connection point of a Reaction or the like is connected. For the attribute position, any of the following abbreviations is described: “N”, “NNE”, “NE”, “ENE”, “E”, “ESE”, “SE”, “SSE”, “S”, “SSW”, “SW”, “WSW”, “W”, “WNW”, “NW”, or “NNW”.

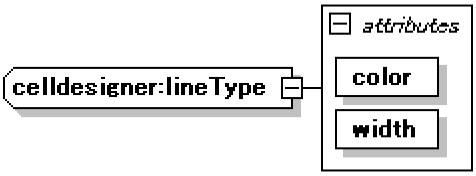
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>used by</td><td><table><tr><td>elements</td><td>**celldesigner:baseReactantType/linkAnchor**<br>**celldesigner:baseProductType/linkAnchor**<br>**celldesigner:reactantLinkType/linkAnchor**<br>**celldesigner:productLinkType/linkAnchor**<br>**celldesigner:linkTargetType/linkAnchor**</td></tr></table></td></tr>
<tr><td>attributes</td><td><table><tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr><tr><td>position</td><td>**derived by: xs:string**</td><td>required</td><td></td><td></td></tr></table></td></tr>
</table>

Example

```
<celldesigner:linkAnchor position="S" />
```

### 11.1.2. ComplexType celldesigner:lineType

This is an XML representation of a Line that retains data for the color and line width of a Reaction link. For the attribute color, a hexadecimal string representing αRGB is described and for width, the line width is described.

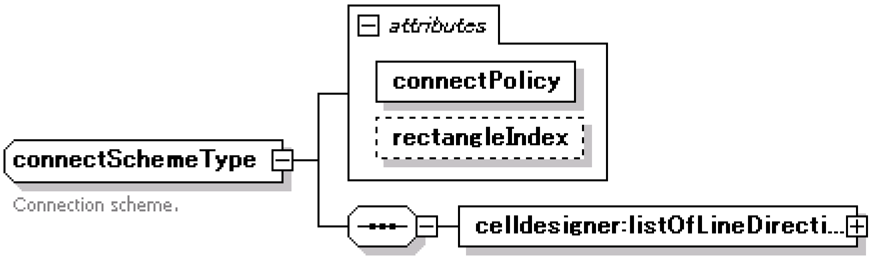
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>used by</td><td><table><tr><td>elements</td><td>**celldesigner:modificationType/line**<br>**celldesigner:reactionAnnotationType/line**</td></tr></table></td></tr>
<tr><td>attributes</td><td><table><tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr><tr><td>color</td><td>**derived by: xs:string**</td><td>required</td><td></td><td></td></tr><tr><td>width</td><td>**derived by: xs:decimal**</td><td>required</td><td></td><td></td></tr></table></td></tr>
</table>

Example

```
<celldesigner:line color="ff000000" width="1.0" />
```

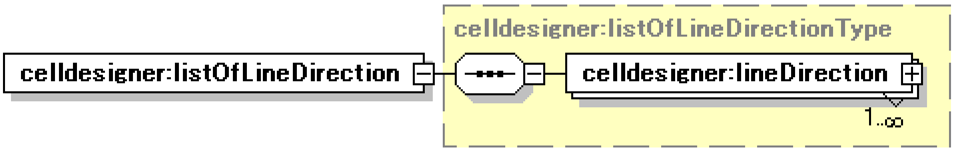
### 11.1.3. ComplexType celldesigner:connectSchemeType

This is an XML element representing a ConnectScheme that describes a connection format of a Reaction link in a graphical model. For the attribute connectPolicy, either “direct” (free angle line segments are connected) or “square” (horizontal and vertical line segments are connected) is described. For the attribute rectangleIndex, an index of a line segment on which a process box is located is described. The lower elements are explained in the following sections.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>children</td><td>**celldesigner:listOfLineDirection**</td></tr>
<tr><td>used by</td><td><table><tr><td>elements</td><td>**modificationType/connectScheme**<br>**reactionAnnotationType/connectScheme**</td></tr></table></td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td><td>annotation</td></tr>
<tr><td>connectPolicy</td><td>**derived by: xs:string**</td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>rectangleIndex</td><td></td><td>optional</td><td></td><td></td><td></td></tr>
</table></td></tr>
<tr><td>annotation</td><td>documentation<br>Connection scheme.</td></tr>
</table>

### 11.1.3.1. Element celldesigner:connectSchemeType/listOfLineDirection

This is an XML element that stores a list of LineDirections, each of which describes the direction of a line segment that forms a Reaction link.

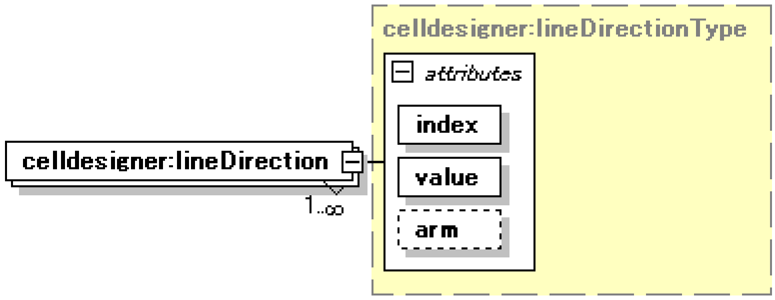
<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>**celldesigner:listOfLineDirectionType**</td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td>**celldesigner:lineDirection**</td></tr>
</table>

### 11.1.3.2. Element celldesigner:listOfLineDirectionType/lineDirection

This is an XML element representing a LineDirection that describes the direction of a line segment that forms a Reaction link. For the attribute index, a line segment index of the link is specified. A line segment index is used to identify an element line segment in a link consisting of multiple line segments. When a Base Reaction is a non-branch type, a number 0, 1, 2… is given from the starting point side, and for a branch type, the number is given from the center of the branches.

The attribute value represents the direction of a line segment; for a horizontal or vertical direction, “horizontal” or “vertical” is specified; for other directions, “unknown” is specified.

The attribute arm is used for a branch type Reaction, and a branch number is specified. For a non-branch type Base Reaction, -1 is given as a branch number, and for a branch type, a branch number 0, 1, 2 is given from the branch on the starting side.

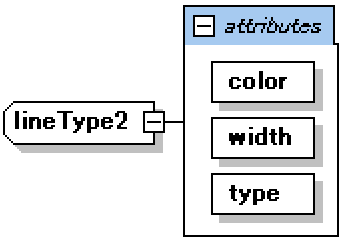
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:lineDirectionType</b></td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>1</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>index</td><td><b>derived by: xs:short</b></td><td>required</td><td></td><td></td></tr>
<tr><td>value</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td></tr>
<tr><td>arm</td><td><b>derived by: xs:short</b></td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

Example

```
<celldesigner:connectScheme connectPolicy="direct">
  <celldesigner:listOfLineDirection>
    <celldesigner:lineDirection index="0" value="unknown" />
    <celldesigner:lineDirection index="1" value="unknown" />
    <celldesigner:lineDirection index="2" value="unknown" />
  </celldesigner:listOfLineDirection>
</celldesigner:connectScheme>
```

### 11.1.4. ComplexType celldesigner:lineType2

This is an XML representation of a Line that retains data for the color and line width of a Reaction link. For the attribute color a hexadecimal string representing αRGB is described; for width a line width is described; and for type Curve or Straight is specified.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>used by</td><td><table>
<tr><td>elements</td><td><b>celldesigner:reactantLinkType/line celldesigner:productLinkType/line</b></td></tr>
</table></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>color</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td></tr>
<tr><td>width</td><td><b>derived by: xs:decimal</b></td><td>required</td><td></td><td></td></tr>
<tr><td>type</td><td><b>derived by: xs:string</b></td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

Example

```
<celldesigner:line width="1.0" color="ff000000" type="Straight"/>
```

### 11.2. Element celldesigner:reactionType

This is an XML element that stipulates a basic Reaction type in a graphical model.

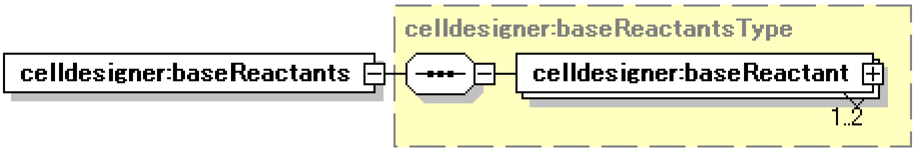
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | restriction of **xs:string** |
| properties | content simple |
| used by | complexType **celldesigner:reactionAnnotationType** |
| facets | enumeration STATE_TRANSITION<br>enumeration KNOWN_TRANSITION_OMITTED<br>enumeration UNKNOWN_TRANSITION<br>enumeration CATALYSIS<br>enumeration UNKNOWN_CATALYSIS<br>enumeration INHIBITION<br>enumeration UNKNOWN_INHIBITION<br>enumeration TRANSPORT<br>enumeration HETERODIMER_ASSOCIATION<br>enumeration DISSOCIATION<br>enumeration TRUNCATION<br>enumeration TRANSCRIPTIONAL_ACTIVATION<br>enumeration TRANSCRIPTIONAL_INHIBITION<br>enumeration TRANSLATIONAL_ACTIVATION<br>enumeration TRANSLATIONAL_INHIBITION<br>enumeration TRANSCRIPTION<br>enumeration TRANSLATION |

Example

```
<celldesigner:reactionType>TRANSCRIPTIONAL_INHIBITION</celldesigner:reactionType>
```

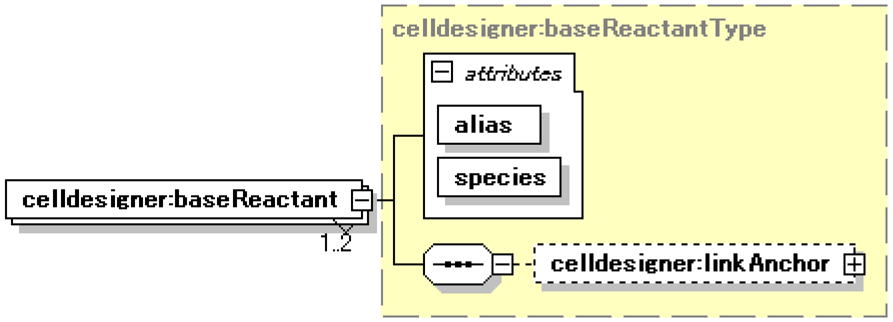
### 11.3. Element celldesigner:reactionAnnotationType/baseReactants

This is an XML element that stores a list of BaseReactants, each of which is a reactant of a Base Reaction.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:baseReactantsType** |
| properties | isRef 0<br>content complex |
| children | **celldesigner:baseReactant** |

#### 11.3.1. Element celldesigner:baseReactantsType/baseReactant

This is an XML element representing a BaseReactant that is a reactant of a Base Reaction. For the attribute alias, the id of a (Complex)SpeciesAlias that is the BaseReactant is described. For the attribute species, a Species that the (Complex)SpeciesAlias refers to is described. The lower element LinkAnchor is explained in 11.1.1.

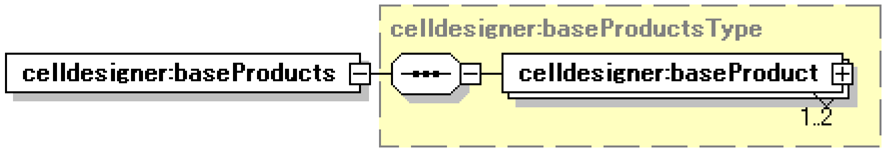
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:baseReactantType</b></td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>minOcc</td><td>1</td></tr><tr><td>maxOcc</td><td>2</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td><b>celldesigner:linkAnchor</b></td></tr>
<tr><td>attributes</td><td><table><tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr><tr><td>alias</td><td><b>derived by: celldesigner:SId</b></td><td>required</td><td></td><td></td></tr><tr><td>species</td><td><b>celldesigner:SId</b></td><td>required</td><td></td><td></td></tr></table></td></tr>
</table>

Example

```
<celldesigner:baseReactants>
  <celldesigner:baseReactant alias="sa305" species="s233">
    <celldesigner:linkAnchor position="E" />
  </celldesigner:baseReactant>
  <celldesigner:baseReactant alias="sa306" species="s234">
    <celldesigner:linkAnchor position="E" />
  </celldesigner:baseReactant>
</celldesigner:baseReactants>
```

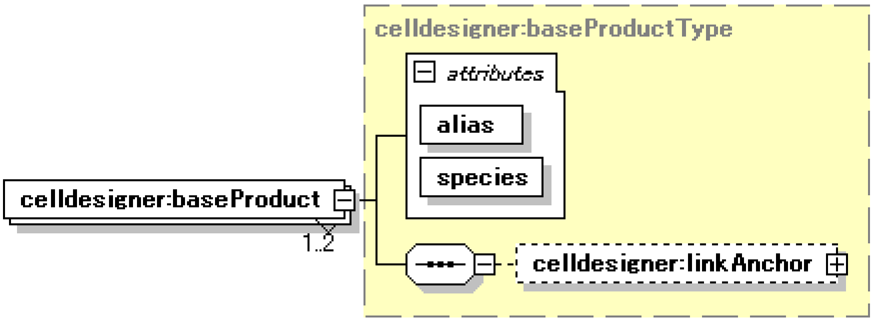
### 11.4. Element celldesigner:reactionAnnotationType/baseProducts

This is an XML element that stores a list of BaseProducts, each of which is a product of a Base Reaction.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:baseProductsType</b></td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td><b>celldesigner:baseProduct</b></td></tr>
</table>

### 11.4.1. Element celldesigner:baseProductsType/baseProduct

This is an XML element representing a BaseProduct that is a product of a Base Reaction. For the attribute alias, the id of a (Complex)SpeciesAlias that is the BaseProduct is described. For the attribute species, a Species that the (Complex)SpeciesAlias refers to is described. The lower element LinkAnchor is explained in 11.1.1.

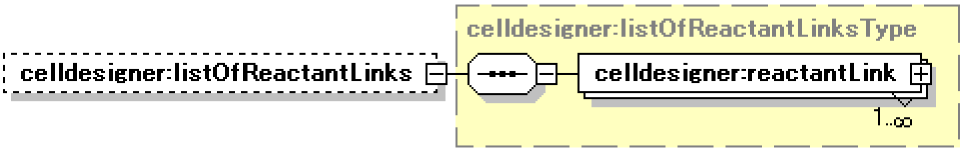
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>**celldesigner:baseProductType**</td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>minOcc</td><td>1</td></tr><tr><td>maxOcc</td><td>2</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td>**celldesigner:linkAnchor**</td></tr>
<tr><td>attributes</td><td><table><tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td></tr><tr><td>alias</td><td>**derived by: celldesigner:SId**</td><td>required</td><td></td><td></td></tr><tr><td>species</td><td>**celldesigner:SId**</td><td>required</td><td></td><td></td></tr></table></td></tr>
</table>

Example

```
<celldesigner:baseProducts>
  <celldesigner:baseProduct alias="csa22" species="s235">
    <celldesigner:linkAnchor position="W" />
  </celldesigner:baseProduct>
</celldesigner:baseProducts>
```

### 11.5. Element celldesigner:reactionAnnotationType/listOfReactantLinks

This is an XML element to store a list of ReactantLinks, each of which describes an additional reactant to a Base Reaction.

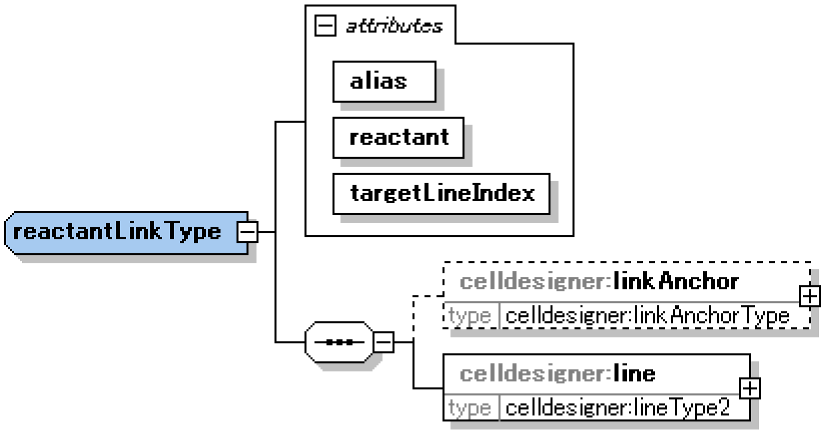
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>**celldesigner:listOfReactantLinksType**</td></tr>
<tr><td>properties</td><td><table><tr><td>isRef</td><td>0</td></tr><tr><td>minOcc</td><td>0</td></tr><tr><td>maxOcc</td><td>1</td></tr><tr><td>content</td><td>complex</td></tr></table></td></tr>
<tr><td>children</td><td>**celldesigner:reactantLink**</td></tr>
</table>

### 11.5.1. Element celldesigner:listOfReactantLinksType/reactantLink

This is an XML element representing a ReactantLink that describes an additional reactant to a Base Reaction. For the attribute alias, the id of a (Complex)SpeciesAlias that represents the additional reactant is described; for the attribute reactant, the id of a Species that represents the additional reactant is described. The attribute targetLineIndex is represented by a string in which a branch number of the Base Reaction link and a line segment index are connected with a comma “,”. From Ver. 4.0, positions to which reactants can be added are located together in one place; therefore, for targetLineIndex only “-1,0” can be used.

Reference) Regarding branch numbers used up to Ver.3.x, for a non-branch type Base Reaction, -1 is given as a branch number, and for a branch type, a branch number 0, 1, 2 is given from the branch on the starting side. A line segment index is used to identify an element line segment in a link consisting of multiple line segments. When a Base Reaction is a non-branch type, a number 0, 1, 2… is given from the starting point side, and for a branch type, the number is given from the center of the branches.

The lower elements LinkAnchor and Line are explained in 11.1.

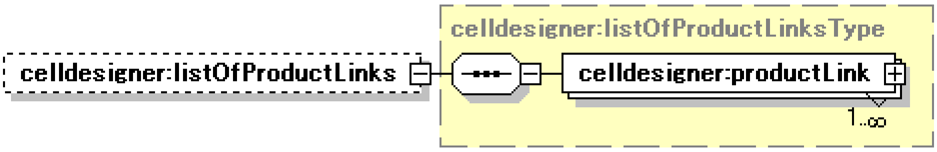
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:reactantLinkType</b></td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>1</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>children</td><td><b>celldesigner:linkAnchor celldesigner:line</b></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>alias</td><td><b>derived by: celldesigner:SId</b></td><td>required</td><td></td><td></td></tr>
<tr><td>reactant</td><td><b>celldesigner:SId</b></td><td>required</td><td></td><td></td></tr>
<tr><td>targetLineIndex</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td></tr>
</table></td></tr>
</table>

Example

```
<celldesigner:listOfReactantLinks>
  <celldesigner:reactantLink alias="sa5" reactant="s5" targetLineIndex="-1,2">
    <celldesigner:linkAnchor position="NW" />
    <celldesigner:line color="ff000000" width="1.0" />
    <celldesigner:line width="1.0" color="ff000000" type="Straight"/>
  </celldesigner:reactantLink>
</celldesigner:listOfReactantLinks>
```

### 11.6. Element celldesigner:reactionAnnotationType/listOfProductLinks

This is an XML element to store a list of ProductLinks, each of which describes an additional product to a Base Reaction.

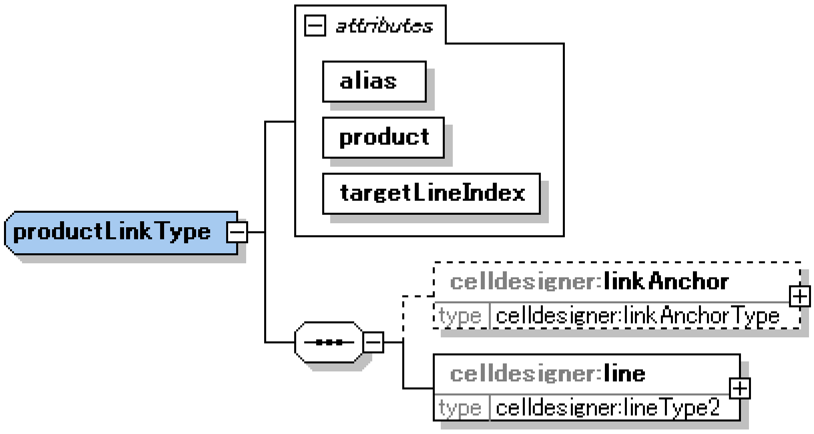
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfProductLinksType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:productLink** |

### 11.6.1. Element celldesigner:listOfProductLinksType/productLink

This is an XML element representing a ProductLink that describes an additional product to a Base Reaction. For the attribute alias, the id of a (Complex)SpeciesAlias that represents the additional product is described; for the attribute product, the id of a Species that represents the additional product is described. The attribute targetLineIndex is represented by a string in which a branch number of the Base Reaction link and a line segment index are connected with a comma “,”. From Ver. 4.0, points to which products can be connected are located together in one place; therefore, only “-1.1” can be used.

Reference) Regarding branch numbers used up to Ver.3.x, for a non-branch type Base Reaction, -1 is given as a branch number, and for a branch type, a branch number 0, 1, 2 is given from the branch on the starting side. A line segment index is used to identify an element line segment in a link consisting of multiple line segments. When a Base Reaction is a non-branch type, a number 0, 1, 2… is given from the starting point side, and for a branch type, the number is given from the center of the branches.

The lower elements LinkAnchor and Line are explained in 11.1.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:productLinkType** |
| properties | isRef 0<br>minOcc 1<br>maxOcc unbounded<br>content complex |
| children | **celldesigner:linkAnchor celldesigner:line** |
| attributes | Name Type Use Default Fixed<br>alias **derived by: celldesigner:SId** required |

| | | | |
|---|---|---|---|
| | product | **celldesigner:SId** | required |
| | targetLineIndex | **derived by: xs:string** | required |

Example

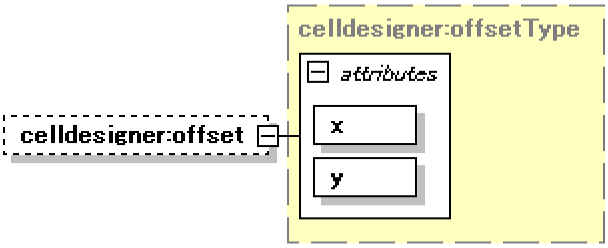
```
<celldesigner:listOfProductLinks>
  <celldesigner:productLink alias="sa5" product="s5" targetLineIndex="-1,1">
    <celldesigner:linkAnchor position="N" />
    <celldesigner:line color="ff000000" width="1.0" />
    <celldesigner:line width="1.0" color="ff000000" type="Curve"/>
  </celldesigner:productLink>
</celldesigner:listOfProductLinks>
```

### 11.7. Element celldesigner:reactionAnnotationType/connectScheme

This is an XML element representing a ConnectScheme that describes a connection format of a Reaction link in a graphical model. Details are given in 11.1.3

### 11.8. Element celldesigner:reactionAnnotationType/offset

This is an XML element representing a CellDesigner.OffsetReaction that indicates the distance which a Reaction link has moved as a whole in relation to a (Complex)SpeciesAlias -- connection destination -- and the center of the line segments consisting of a Base Reaction link. The distance is set in the attributes x and y.

| | | | | | |
|---|---|---|---|---|---|
| diagram |  | | | | |
| namespace | http://www.sbml.org/2001/ns/celldesigner | | | | |
| type | **celldesigner:offsetType** | | | | |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex | | | | |
| attributes | Name | Type | Use | Default | Fixed |
| | x | **derived by: xs:decimal** | required | | |
| | y | **derived by: xs:decimal** | required | | |

Example

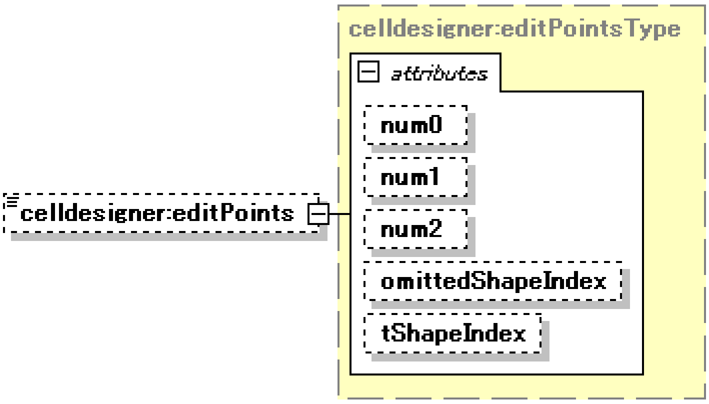
```
<celldesigner:offset x="14.0" y="-5.0" />
```

### 11.9. Element celldesigner:reactionAnnotationType/editPoints

When a Reaction link is made up of multiple line segments, this XML element represents Edit Points that describe its edit or connection points. For the attributes num0, num1, and num2, when the Reaction is a branch type, the number of edit points in each of the branch numbers 0, 1, and 2 is described. For a non-branch type Base Reaction, -1 is given as a branch number, and for a branch type, a branch number 0, 1, 2 is given from the branch on the starting side.

For the attributes tShapeIndex, the position of the ProcessNode of a three-forked ReactionLink is retained; and for the attribute omittedShapeIndex, in the case of ReactionLinks other than the former, if there is a ProcessNode, it is retained in this variable. When a Reaction type is “KNOWN_TRANSITION_OMITTED” or “TRUNCATION”, a line segment index to which an identification symbol is attached is specified in these attributes. A line segment index is used to identify an element line segment in a link consisting of multiple line segments. When a Base Reaction is a non-branch type, a number 0, 1, 2… is given from the starting point side, and for a branch type, the number is given from the center of the branches. A string described in a tag is a string in which coordinates x and y of an edit point stipulated by CellDesigner.Point2DList (7.1.4) are arranged.

The coordinates of an edit point are determined and retained by calculating local coordinates from line segments that connect the central points of (Complex)SpeciesAliases that are the starting point and end point of a Reaction.

<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:editPointsType</b></td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>0</td></tr>
<tr><td>maxOcc</td><td>1</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>attributes</td><td><table>
<tr><th>Name</th><th>Type</th><th>Use</th><th>Default</th><th>Fixed</th></tr>
<tr><td>num0</td><td><b>derived by: xs:short</b></td><td></td><td></td><td></td></tr>
<tr><td>num1</td><td><b>derived by: xs:short</b></td><td></td><td></td><td></td></tr>
<tr><td>num2</td><td><b>derived by: xs:short</b></td><td></td><td></td><td></td></tr>
<tr><td>omittedShapeIndex</td><td><b>derived by: xs:short</b></td><td></td><td></td><td></td></tr>
<tr><td>tShapeIndex</td><td><b>derived by: xs:short</b></td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

Example 1

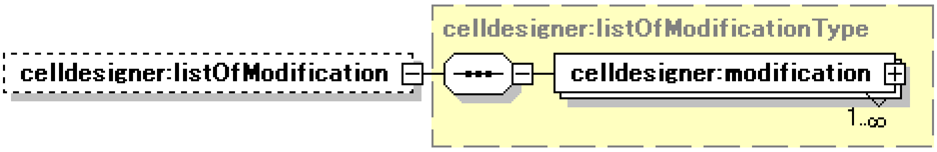
```
<celldesigner:editPoints omittedShapeIndex="0">0.12438587874696405,2.98381163386
09666E-4 0.6666666666666663,8.881784197001252E-16</celldesigner:editPoints>
```

Example 2

```
<celldesigner:editPoints num0="2" num1="2" num2="2">0.33246269555174024,-0.0065
46505318191009 0.664925391103476,-0.013093010636378466 0.2650906262742
7227,-0.07769315518193398 0.5301812525484877,-0.15538631036386352 0.3333
333333333357,-7.105427357601002E-15 0.6666666666666643,-1.4210854715202
004E-14 0.2431161049218673,0.5877571605694545</celldesigner:editPoints>
```

### 11.10. Element celldesigner:reactionAnnotationType/listOfModification

This is an XML element to store a list of Modifications, each of which describes enzymic activity or inhibition that gives reaction speed changes to a Base Reaction.

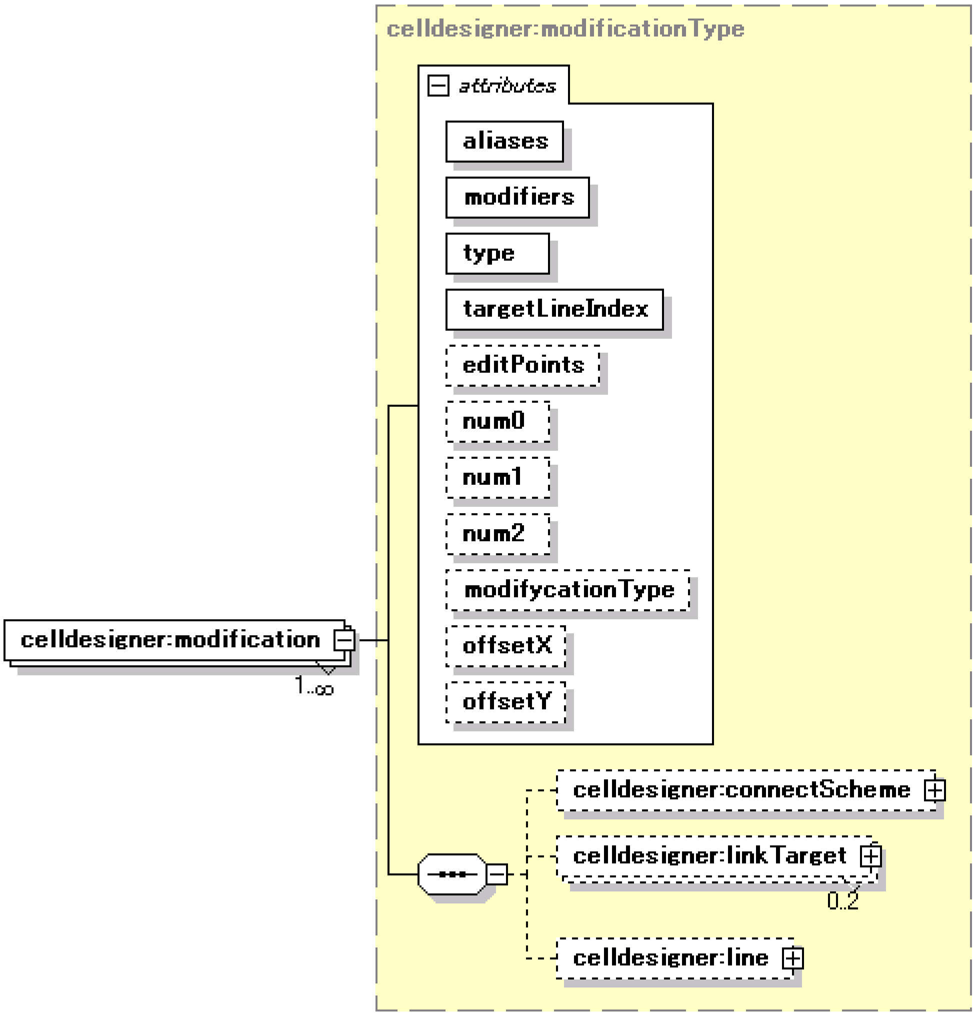
| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:listOfModificationType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:modification** |

### 11.10.1. Element celldesigner:listOfModificationType/modification

This is an XML element representing a Modification to describe enzymic activity or inhibition that gives reaction speed changes to a Base Reaction. The meaning of each attribute is as follows:

| Attribute name | Content |
|---|---|
| aliases | The id of the (Complex)SpeciesAlias of a Species that affects a Reaction; if there are multiple Species, a list connected with a comma “,” is described. |
| modifiers | The id of a Species that affects a Reaction; if there are multiple Species, a list connected with a comma “,” is described. |
| type | Type of a Modification Link. Any of the following is specified: “CATALYSIS”, “UNKNOWN_CATALYSIS”, “INHIBITION”, “UNKNOWN_INHIBITION”, “TRANSPORT”, “HETERODIMER_ASSOCIATION”, “TRANSCRIPTIONAL_ACTIVATION”, “TRANSCRIPTIONAL_INHIBITION”, “TRANSLATIONAL_ACTIVATION”, “TRANSLATIONAL_INHIBITION”, “PHYSICAL_STIMULATION”, “MODULATION”, “TRIGGER”, “BOOLEAN_LOGIC_GATE_AND”, “BOOLEAN_LOGIC_GATE_OR”, “BOOLEAN_LOGIC_GATE_NOT”, “BOOLEAN_LOGIC_GATE_UNKNOWN”. |
| targetLineIndex | Regarding the point at which a Modification is connected to a Reaction, a string in which a branch number and line segment index is connected with a comma “,” on the Reaction is described.<br>For the branch number, -1 is given, and for the line segment index, a number from between 2 and 7 is given according to the position on a process box. |
| num0, num1, num2 | In case of a branch type Modification Link, the number of edit points in each branch number 0, 1, or 2 is described. There is no branch type Modification; therefore, currently they are not used. |
| editPoints | A string in which edit points (x, y) in a Modification Link are arranged. However, when a Modification type is “BOOLEAN_*”, for the last coordinates in the string, the absolute coordinates of Logic Gate (HeaderPoint) is described. |
| modificationType | This is used when the type of a Modification Link is BOOLEAN_LOGIC_GATE_AND”, “BOOLEAN_LOGIC_GATE_OR”, or “BOOLEAN_LOGIC_GATE_UNKNOWN”. Any of the following is specified: “CATALYSIS”, “UNKNOWN_CATALYSIS”, “INHIBITION”, “UNKNOWN_INHIBITION”, “TRANSPORT”, “HETERODIMER_ASSOCIATION”, “TRANSCRIPTIONAL_ACTIVATION”, “TRANSCRIPTIONAL_INHIBITION”, “TRANSLATIONAL_ACTIVATION”, “TRANSLATIONAL_INHIBITION“, ”PHYSICAL_STIMULATION”, “MODULATION”. |
| offsetX<br>offsetY | Offset values for calculating internal coordinates. |

The lower elements Line and ConnectScheme are explained in 11.1. LinkTarget is explained in the next section.

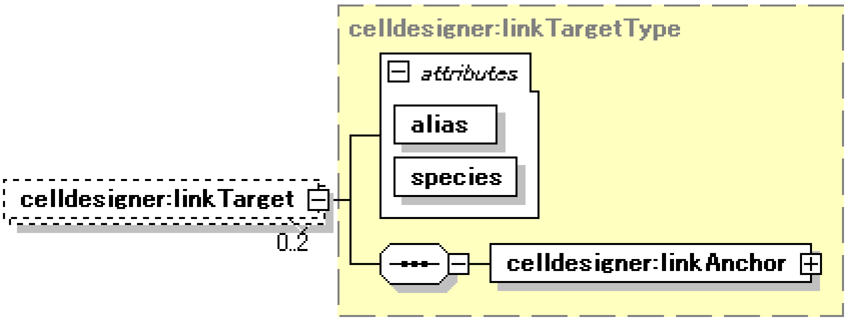
<table>
<tr><td>diagram</td><td>
</td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td><b>celldesigner:modificationType</b></td></tr>
<tr><td>properties</td><td><table>
<tr><td>isRef</td><td>0</td></tr>
<tr><td>minOcc</td><td>1</td></tr>
<tr><td>maxOcc</td><td>unbounded</td></tr>
<tr><td>content</td><td>complex</td></tr>
</table></td></tr>
<tr><td>children</td><td><b>celldesigner:connectScheme celldesigner:linkTarget celldesigner:line</b></td></tr>
<tr><td>attributes</td><td><table>
<tr><td>Name</td><td>Type</td><td>Use</td><td>Default</td><td>Fixed</td><td>annotation</td></tr>
<tr><td>aliases</td><td><b>derived by: celldesigner:SIdSet</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>modifiers</td><td><b>derived by: celldesigner:SIdSet</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>type</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>targetLineIndex</td><td><b>derived by: xs:string</b></td><td>required</td><td></td><td></td><td></td></tr>
<tr><td>editPoints</td><td><b>derived by: celldesigner:point2DList</b></td><td></td><td></td><td></td><td></td></tr>
<tr><td>num0</td><td><b>derived by: xs:nonNegativeInteger</b></td><td></td><td></td><td></td><td></td></tr>
<tr><td>num1</td><td><b>derived by: xs:nonNegativeInteger</b></td><td></td><td></td><td></td><td></td></tr>
<tr><td>num2</td><td><b>derived by: xs:nonNegativeInteger</b></td><td></td><td></td><td></td><td></td></tr>
<tr><td>modificationType</td><td><b>derived by: xs:string</b></td><td></td><td></td><td></td><td></td></tr>
<tr><td>offsetX</td><td><b>derived by: xs:decimal</b></td><td></td><td></td><td></td><td></td></tr>
<tr><td>offsetY</td><td><b>derived by: xs:decimal</b></td><td></td><td></td><td></td><td></td></tr>
</table></td></tr>
</table>

#### 11.10.1.1. Element celldesigner:modificationType/linkTarget

This is an XML element to describe a modifier that triggers enzymic activity or inhibition that gives reaction speed changes to a Base Reaction.

For the attribute alias, the id of a (Complex)SpeciesAlias, a modifier that affects reaction speed changes is described, and for species, the id of the Species is described.

The lower elements LinkAnchor and Line are explained in 11.1.

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/2001/ns/celldesigner |
| type | **celldesigner:linkTargetType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 2<br>content complex |
| children | **celldesigner:linkAnchor** |
| attributes | Name / Type / Use / Default / Fixed<br>alias / **derived by: celldesigner:SId** / required<br>species / **celldesigner:SId** / required |

Example

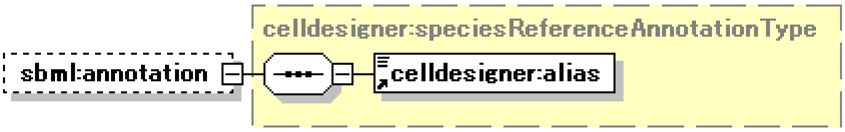
```
<celldesigner:listOfModification>
  <celldesigner:modification aliases="sa4"
      editPoints="0.7452364101614855,-0.10812008399079165"
      modifiers="s4" offsetX="35.0" offsetY="-23.0" targetLineIndex="1,0"
      type="CATALYSIS">
    <celldesigner:connectScheme connectPolicy="direct">
      <celldesigner:listOfLineDirection>
        <celldesigner:lineDirection index="0" value="unknown" />
        <celldesigner:lineDirection index="1" value="unknown" />
      </celldesigner:listOfLineDirection>
    </celldesigner:connectScheme>
    <celldesigner:linkTarget alias="sa4" species="s4">
      <celldesigner:linkAnchor position="W" />
    </celldesigner:linkTarget>
    <celldesigner:line color="ff000000" width="1.0" />
  </celldesigner:modification>
  <celldesigner:modification aliases="sa5" modifiers="s5" targetLineIndex="2,0"
    type="CATALYSIS">
    <celldesigner:connectScheme connectPolicy="direct">
      <celldesigner:listOfLineDirection>
        <celldesigner:lineDirection index="0" value="unknown" />
      </celldesigner:listOfLineDirection>
    </celldesigner:connectScheme>
    <celldesigner:linkTarget alias="sa5" species="s5">
      <celldesigner:linkAnchor position="E" />
```

```
    </celldesigner:linkTarget>
    <celldesigner:line color="ff000000" width="1.0" />
  </celldesigner:modification>
</celldesigner:listOfModification>
```

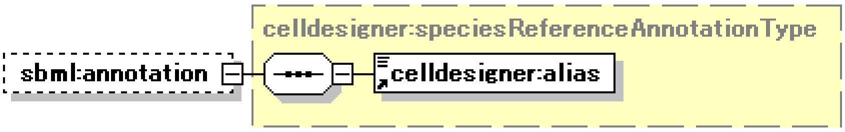
## 12. Extension of SpeciesReference.Annotation, and ModifierSpeciesReference.Annotation

To stipulate the storage format of connection destination data of a Reaction, annotation is redefined.

### Element SpeciesReference/annotation

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/sbml/level2 |
| type | **celldesigner:speciesReferenceAnnotationType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:alias** |

### Element ModifierSpeciesReference/annotation

| | |
|---|---|
| diagram |  |
| namespace | http://www.sbml.org/sbml/level2 |
| type | **celldesigner:speciesReferenceAnnotationType** |
| properties | isRef 0<br>minOcc 0<br>maxOcc 1<br>content complex |
| children | **celldesigner:alias** |

### 12.1. Element celldesigner:alias

This is an XML element to specify a (Complex)SpeciesAlias to which a Reaction is connected.

<table>
<tr><td>diagram</td><td> </td></tr>
<tr><td>namespace</td><td>http://www.sbml.org/2001/ns/celldesigner</td></tr>
<tr><td>type</td><td>restriction of **celldesigner:SId**</td></tr>
<tr><td>properties</td><td>content simple</td></tr>
<tr><td>used by</td><td>complexType **celldesigner:speciesReferenceAnnotationType**</td></tr>
<tr><td>facets</td><td>pattern (_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*</td></tr>
</table>

Example

```
<celldesigner:alias>sa464</celldesigner:alias>
```

## 13. Reference

[1] Funahashi, A., et al. (2003). "CellDesigner: a process diagram editor for gene-regulatory and biochemical networks." Biosilico 1, 159-162.

[2] Kitano, H., et al. (2005). "Using process diagrams for the graphical representation of biological networks." Nat Biotechnol. 2005 Aug; 23(8):961-6.

[3] Hucka, M., et al. (2003). "The systems biology markup language (SBML): a medium for representation and exchange of biochemical network models." Bioinformatics. 2003 Mar 1; 19(4):524-31.

[4] Finney, A. and Hucka, M. (2003). "Systems Biology Markup Language (SBML) Level 2: Structures and Facilities for Model Definitions." http://www.sbml.org/specifications/sbml-level-2/version-1/html/sbml-level-2.html.

[5] Kitano, H., (2003). "A graphical notation for biochemical networks." Biosilico 1, 169-176.

[6] "XML Schema Part 0: Primer Second Edition." http://www.w3.org/TR/xmlschema-0/.

[7] "XML Schema Part 1: Structures Second Edition." http://www.w3.org/TR/xmlschema-1/.

[8] "XML Schema Part 2: Datatypes Second Edition." http://www.w3.org/TR/xmlschema-2/.