# Introduction

# Technical specification

This section formally defines the spreadsheet-based annotation format for logical models. It describes thetabular structure, element attributes for qualitative species and transitions, recommended format for annotations, and intended mappings between spreadsheet entries and the SBML-qual elements.

## 2.1 Data Organization

The spreadsheet consists of several tables (sheets), where each **row** represents a distinct model entity (**species**, **transition**, or **interaction**). And each **column** corresponds to a defined attribute or annotation of that entity. In addition, a **model** sheet is used to provide other information about the model as a whole.

At minimum, three core tables are required to define a logical model, with the last one being optional:

* **Model** sheet: Defines the model and its metadata.
* **Species** sheet: Defines QualitativeSpecies (nodes), their attributes and annotations.
* **Transitions** sheet: Defines transitions (logical rules), their attributes and annotations.
* (Optional) **Interactions** sheet: Provides annotations of the interactions (each edge) between two species.

Each sheet contains one or two data fields (columns) that are required to define a model. In addition,optional columns for annotation can be used to store external references and provenance data. For example, species can be linked with their biological entity ID from UniProt or NCBI gene; transitions and interactions can be supported by evidence from literature, etc.

Additional sheets and columns may be included if needed, but they will not be considered as part of the standard nor be kept in the converted SBML-qual model. In the template, two additional sheets are provided:

* **README** sheet: Provides basic instructions for using the template.
* **Appendix** sheet: Describe the options for certain columns (see 2.2).

## 2.2 Definitions of the tables

This section provides definitions of the fields in each table. Order of the tables can be changed, as long as the tab names and headers remain the same.

Typically there is only one entry per cell, if multiple entries are provided, they should be comma-separated. For identifiers used in the spreadsheet, we recommend using compact identifiers that follow the [prefix]:[accession] pattern registered at identifiers.org when possible. Additional URLs are supported for other resources.

### 2.2.1 Model sheet

The model sheet contains general information about the model, only **Model\_ID** is required, other fields are optional annotation of model provenance and metadata.

Table 1 provides the definition and an example entry of each field in the model sheet. In the Mapping column, blue represents the corresponding SBML attributes of model elements; green represents the [qualifier](#_x3pmcgi6qdzs) used for annotations of the model object.

Table 1: Definition of the fields in the **Model** sheet.

|  |  |  |  |
| --- | --- | --- | --- |
| **Field** | **Mapping** | **Definition** | **Example** |
| **Model\_source** | bqmodel:is | URL or accession of the model or the spreadsheet itself. | https://www.ebi.ac.uk/biomodels/MODEL2307180001 |
| **Model\_ID** | model.id | Identifier for the model; must be a valid SBML *SId* (ASCII, no spaces). | ToyExample\_boolean |
| **Name** | model.name | Descriptive label of the model, can be any text. | Example Boolean model of NF-κB signaling pathway |
| **Publication** | bqmodel:isDescribedBy | Primary publication(s) supporting the encoded model; compact IDs stored with qualifier. | DOI:10.1093/bib/bbac212 |
| **Origin\_publication** | bqmodel:isDerivedFrom | Paper(s) describing the biological system from which the present model was derived. | pubmed:38272919 |
| **Origin\_model** | bqmodel:isDerivedFrom | Accession(s) of parent model in [compact identifier](#_qo707ctcmg6x). | biomodels.db:MODEL2307180001 |
| **Taxon** | bqbiol:hasTaxon | NCBI taxonomy compact ID of the species (animal) described by the model. | taxonomy:9606 |
| **Biological\_process** | bqbiol:isVersionOf | Biological process(es) described in the model. | GO:0007249 |
| **Created** | dcterms:created | ISO-8601 timestamp when this model is created. | 2025-04-04T17:08:28Z |
| **Modified** | dcterms:modified | Last edit timestamp when the model is modified. | 2025-07-29T16:56:00Z |
| **Creator[1, 2, …]** | dcterms:creator | Information about the creator of the model: [family name, given name, "organization", email]; if more than one creator, add new rows with header “**Creator2**”, “**Creator3**”, … | Li, Luna, "Center for Reproducible Biomedical Modeling", lixy@uw.edu |
| **Contributor[1, 2, …]** | dcterms:contributor | Additional person or organization that have contributed to the model; encoded like **Creator**. |
| **Version** | model.notes | Other versions of the model can be listed here using the file name. | ToyExample\_multivalue.xlsx |
| **Notes[1, 2, …]** | model.notes | Free-text as *notes* in the SBML model. | “This is an example note.” |
| **Comments** |  | Informal comments NOT exported to SBML. |  |

### 2.2.2 Species sheet

The species sheet lists every *QualitativeSpecies* (node) that appears in the logical model, usually this refers to genes or gene products in biological processes.

Only **Species\_ID** is required for a valid SBML-qual model; all other columns provide optional attributes or annotations.

Table 2 provides the definition and an example entry of each field in the species sheet. SBML-qual attributes (blue in the Mapping column) are written exactly as they appear in the specification with capitalization; annotation [qualifiers](#_x3pmcgi6qdzs) (green) should follow the BioModels Qualifiers vocabulary.

Table 2: Definition of the fields in the **Species** sheet.

|  |  |  |  |
| --- | --- | --- | --- |
| **Field** | **Mapping** | **Definition** | **Example** |
| **Species\_ID** | QualitativeSpecies.id | Identifier for the species; must be a valid SBML *SId* (ASCII, no spaces). | NFKB1 |
| **Name** | QualitativeSpecies.name | Descriptive label of the species. | NFκB protein p50 subunit |
| **Relation[1, 2, …]** | bqbiol qualifiers | [Qualifier](#_x3pmcgi6qdzs) for identifier[1, 2, …], respectively; defaults to 'is' | is |
| **Identifier[1, 2, …]** |  | [Compact identifiers](#_qo707ctcmg6x) for Relation[1, 2, …], respectively. | uniprot:P19838 |
| **Compartment** | QualitativeSpecies.compartment | The compartment in which the species is located. | cytosol |
| **Type** |  | Describe the role of the species in a network; Choose from: Input, Internal, output. | Internal |
| **Constant** | QualitativeSpecies.constant | Whether the level of the species is fixed or can be varied; Choose from: True, False. | False |
| **InitialLevel** | QualitativeSpecies.initialLevel | Initial value of the species; non-negative integer; cannot exceed MaxLevel if both are set. | 0 |
| **MaxLevel** | QualitativeSpecies.maxLevel | Maximum value of the species; non-negative integer; default ‘1’ for Boolean models. | 1 |
| **Notes[1, 2, …]** | QualitativeSpecies.notes | Free-text as *notes* for the species. | “p50 subunit of the NF-κB complex” |
| **Comments** |  | Informal comments NOT exported to SBML. |  |

### 2.2.3 Interactions sheet

The Interactions sheet records evidence and provenance for pairwise influences between species.

It is an **optional** sheet and purely for annotating pair-wise relations between nodes, rather than the transitions as a whole. In addition, softwares may use it to decorate graphical views or to auto-generate default Transition inputs/outputs.

Table 3: Definition of the fields in the **Interactions** sheet.

|  |  |  |  |
| --- | --- | --- | --- |
| **Field** | **Mapping** | **Definition** | **Example** |
| **Target** | Transition.Output.id (QualitativeSpecies.id) | Identifier for the regulated species; the output that participates in a transition. Must be an existing Species\_ID. | A |
| **Source** | Transition.Input.id (QualitativeSpecies.id) | Identifier for the regulator species; the input that is affected by a transition. Must be an existing Species\_ID. | D |
| **Sign** | Transition.Input.sign | Whether the contribution of this input is positive, negative, both (dual) or unknown. | positive |
| **Relation[1, 2, …]** | bqbiol qualifiers | [Qualifier](#_x3pmcgi6qdzs) for identifier[1, 2, …], respectively; defaults to 'isDescribedBy' | isDescribedBy |
| **Identifier[1, 2, …]** |  | [Compact identifiers](#_qo707ctcmg6x) for Relation[1, 2, …], respectively. | pubmed:20300203, ECO:0007392 |
| **Notes[1, 2, …]** | Transition.Input.notes | Free-text as *notes* for the interaction. | “IKK complex activates RELA by phosphorylating IκBα.The activation of RELA by IKK has been supported by immunohistochemistry evidence” |
| **Comments** |  | Informal comments NOT exported to SBML. |

### 2.2.4 Transitions sheet

The transitions sheet provides core regulatory information of the model. Each row in the Transitions sheet defines the logical rule (*Transition*) that governs one output species.

Only **Target** and **Rule** are required. Transition\_ID and Name are optional and will be assigned a default value in the SBML model.

Table 4: Definition of the fields in the **Transitions** sheet.

|  |  |  |  |
| --- | --- | --- | --- |
| **Field** | **Mapping** | **Definition** | **Example** |
| **Transitions\_ID** | Transition.id | Identifier for the transition; Optional, if provided, must be a valid SBML *SId* (ASCII, no spaces). | tr\_A |
| **Name** | Transition.name | Descriptive label of the transition. | RELA activation |
| **Target** | Transition.Output.id (QualitativeSpecies.id) | Identifier for the regulated species; the output that participates in a transition. Must be an existing Species\_ID. | A |
| **Level** | Transition.functionTerm.resultLevel | Effect of the transition on the corresponding target species; non-negative integer; default ‘1’ for Boolean models. | 1 |
| **Rule** | Transition.functionTerm.math | Logical rules of the transition; expressions using Boolean operators AND (&), or (|), and NOT (!). See Table 5. | A | (D & !C) |
| **Relation[1, 2, …]** | bqbiol qualifiers | [Qualifier](#_x3pmcgi6qdzs) for identifier[1, 2, …], respectively; defaults to 'isDescribedBy' | isDescribedBy |
| **Identifier[1, 2, …]** |  | [Compact identifiers](#_qo707ctcmg6x) for Relation[1, 2, …], respectively. | pubmed:20300203, ECO:0007392 |
| **Notes[1, 2, …]** | Transition.notes | Free-text as *notes* for the interaction. | “IKK complex activates RELA by phosphorylating IκBα.The activation of RELA by IKK has been supported by immunohistochemistry evidence” |
| **Comments** |  | Informal comments NOT exported to SBML. |

The representation of logical rules use a conventional expression as in many popular logical modeling tools (e.g., GINsim, BoolNet), where the regulatory effect can be described as Boolean operations of regulators. Table 5 gives a list of allowed symbols to be used in this expression.

Table 5: Symbols that can be used in **Transitions** - **Rule** field.

|  |  |  |
| --- | --- | --- |
| **Symbol** | **Definition** | **Example** |
| & | Boolean “AND” operator | A & B |
| | | Boolean “OR” operator | A | C |
| ! | Boolean “NOT” operator | !A |
| () | Parentheses to prioritize regulation | A | (D & !C) |
| : | Used only in multi-valued models to represent the threshold level of an input; can be omitted for value of 1. | A & B:2 |
| `space` | Spaces will be ignored in parsing the expression |  |

### 2.2.5 Other sheets

* **README** – instructions on using the template. Content is ignored by converters but for user guidance only.
* **Appendix** – controlled vocabularies and allowed option lists referenced by Type, Constant, Relation, Sign.

Both sheets are informational only and may be removed from the spreadsheet.

# Concepts used

### Compact identifier

A Compact Identifier is a unique string consisting of a Prefix (assigned by curator), a colon (‘:’), and an Accession (e.g. local identifier string). The Prefix is composed of an optional Provider Code, and an assigned Namespace, separated by a slash (‘/’).

They will be put as identifiers.org URLs in the SBML model using the following form:

https://identifiers.org/[provider\_code/]namespace:accession

**Examples**: uniprot:P19838, [pubmed:22140103](https://identifiers.org/pubmed:22140103), [ec-code:1.1.1.1](https://identifiers.org/ec-code:1.1.1.1), [taxonomy:9606](https://identifiers.org/taxonomy:9606)

**Reference**: <https://docs.identifiers.org/pages/identification_scheme.html>

### Qualifiers (bqmodel/bqbiol)

Qualifiers are used to describe the relation between a model component and the resource used to annotate it.

One can view the annotation of a model component as a statement in the form of a 'triple'. The resource used in the annotation is the 'object', while the qualifier is the 'predicate'. In the cases of the model qualifiers, the 'subject' of the relation is the modelling concept represented by the model component referenced by the annotation. The modelling concept may be the model itself, a mathematical construct, or a hypothesis that is proposed, changing the way we previously understood the model, etc. In the cases of the biology qualifiers, the 'subject' of the relation is the biological or biochemical object represented by the enclosing model element.

There are two kinds of qualifiers used for different purposes: 1) model qualifiers, and 2) biology qualifiers. Below is the list of qualifiers that may be used in a model:

**Model qualifiers**: is, isDerivedFrom, isDescribedBy, isInstanceOf, hasInstance

**Biology qualifiers**: is, hasVersion, isVersionOf, isDescribedBy, hasPart, isPartOf, hasProperty, isPropertyOf, encodes, isEncodedBy, isHomologTo, occursIn, hasTaxon, hasSource, hasSink, hasMediator, hasMultiplier, hasPhysicalEntity

**Reference**: <https://identifiers.org/combine.specifications:qualifiers-1.1>

# Examples

[ToyExample.xlsx](https://docs.google.com/spreadsheets/d/1_xY0VboBhejg8tWnGNyAFpEA_ZU762B0/edit?usp=sharing&ouid=105819375684543832411&rtpof=true&sd=true): A toy model in Boolean formalism.

[ToyExample\_multivalue.xlsx](https://docs.google.com/spreadsheets/d/1gcRtkNhJDny3R5ZtimwIIu-s5okNmp35/edit?usp=sharing&ouid=105819375684543832411&rtpof=true&sd=true): A multi-valued version of the toy model.

[Faure2006\_MammalianCellCycle.xlsx](https://docs.google.com/spreadsheets/d/1B9SUcuY_ioQVlY9y351yIHnW45oZ8J1t/edit?usp=sharing&ouid=105819375684543832411&rtpof=true&sd=true): The Fauré 2006 model, widely used in tools such as GINsim, Cell Collective, MaBoSS, BoolNet, etc.

[Faure2006\_MammalianCellCycle.sbml](https://drive.google.com/file/d/1JtgSUQxFxfJAjJ9wfg0xhgroMajAz-US/view?usp=sharing): Equivalent SBML file of the Fauré 2006 model.