ChEBI Guidelines

URL
https://www.ebi.ac.uk/chebi/

Description
Chemical Entities of Biological Interest (ChEBI) is a freely available dictionary of molecular entities focused on 'small' chemical compounds. Small chemical compounds are usually drugs that help regulate biological processes.

A Warning On Nomenclature
As stated in other guideline sheets, some authors may use a word to describe a chemical compound that is not included in the ChEBI database. If you find that you are having a difficult time finding anything on a particular compound, consult Wikipedia or PubMed for alternate terms.

Guidelines
If your BioModel includes instances of pharmaceutical intervention, then this database will be of use to you. This guide will be using 'caffeine' as an example.

The homepage contains a search bar at the center of the page, with two filters. The first filter says "Search for *** only", and the second says "All in ChEBI". You will be checking the circle that says "All in ChEBI". The "***" indicate that the small molecule was curated by the ChEBI team, but we don't want to limit our search to only this category.

In the search bar, type in 'caffeine' (without the quotes). You will be taken to the search results page for your query.

These results contain pure caffeine along with its metabolites. You're interested in the "caffeine" hyperlink. When you click on this link, you will be taken to the record for caffeine. The record contains six tabs: Main, ChEBI Ontology, Automatic Xrefs, Reactions, Pathways, Models.

Main

This tab contains basic information, such as: definition, molecular weight, ChEBI ID (which is what you will be using to tag the BioModel), and a Wikipedia entry about the small molecule. Also includes a "Roles and Classification" section and a "ChEBI Ontology" section which shows its biochemical role in certain pathways and organisms.

The ‘synonym’ section contains all of the databases this small molecule is listed in. Notice how most of these entries use different terms in the place of our ‘caffeine’ example. This is where you could find additional terms to add to the BioModel, such as KEGG C07481.

ChEBI Ontology

This section is split into two groups. The first lists the related structures of caffeine: The Functional Parent Of (Child) terms and the Structural Derivative Of (Parent) terms. If you needed to annotate your BioModel further, you could use the qualifiers bqbiol: hasPart and bqbiol: isVersionOf and include these terms.

The second section is a visual display of this small molecule’s place in the biochemical hierarchy. All of the parent and child relations of caffeine are shown here, and the types of relations are indicated by the shape to the left of the term.

Automatic Xrefs

This section contains a complete list of associations and cross-references in other databases. It may be useful to look at this section for an annotation for a pathway or reaction associated with this small molecule.

For example, if the ODE in your paper described the N-atom dealkylation of caffeine, then you would use the Reactome record R-HSA-76426 to annotate the ‘Math’ and ‘Physical Entities’ tabs of your BioModel record.

Reactions

This page lists the various molecular species that are involved with the listed reactions of caffeine. May be helpful when annotating the ‘Math’ and ‘Physical Entities’ tabs of the BioModel.

Pathways

Shows a diagram of a list of associated pathways that caffeine utilizes in biological systems. These pathways could be used in the BioModel under the “Math” tab.

Models

This tab lists curated models that contain this term. It could be useful to look at these models (if any are listed) to see how others curated their model.

For more help

The ChEBI Help Page

https://www.ebi.ac.uk/chebi/userManualForward.do;jsessionid=7682AA1381C4CFDFECCD753AD5285CEE?printerFriendlyView=true#Searching%20the%20ChEBI%20database

The ChEBI Tutorial Page

https://www.ebi.ac.uk/chebi/tutorialForward.do