

MICROME SOPs		
Title: <b>Compound curation in ChEBI environment</b>		Pages: 4
SOP01	Revision level: 1	Effective date: 08/25/2011
Author(s): AM/EB/DV/FLF		

## 1-Overview

In the context of Microme project, ChEBI (<http://www.ebi.ac.uk/chebi/>) is used as the reference resource for chemical compounds and Rhea (<http://www.ebi.ac.uk/rhea/>) as the reference resource for chemical reactions. Rhea is also based on ChEBI. Prior to the creation of a new reaction, the Microme curator has to check that all the chemical entities needed are available in ChEBI. The 2D structure of the compound should be the major form at pH 7.3 (the pH used in Rhea for all reactions). If a compound is missing, it is submitted by the Microme curators using the ChEBI submission tool.

### 1.1-Scope

This SOP describes the submission of a chemical compound using the ChEBI submission tool. In particular, the check to ensure that the submitted compound corresponds to the major form at pH 7.3.

### 1.2-Related documents

**ChEBI Submission Tool User Manual:** <https://www.ebi.ac.uk/chebi/submissions/help>

**ChEBI annotation manual:** <http://www.ebi.ac.uk/chebi/userManualForward.do>

**MarvinSketch user guide:** <http://www.chemaxon.com/marvin/help/sketch/sketch-index.html>

SOP02 – Reaction curation in Rhea environment

SOP03 – De-novo pathway creation in Microme environment

### 1.3-Revision history

Author	Date	Change
EB	07/27/2011	Creation of the document
AM	08/23/2011	Revision
DV	08/24/2011	Revision
FLF	08/25/2011	Revision

## 2-Requirements

To register as a new user for ChEBI submission, Microme curators has to enter their details at <https://www.ebi.ac.uk/chebi/submissions/register>. The registration is performed in two steps. First, the email address is validated. Then, the account is validated by the ChEBI team before it is activated. This process may take a few days. A new user is notified by email that he/she may proceed with submissions.

## 3-Procedure

The ChEBI Submission tool (<https://www.ebi.ac.uk/chebi/submissions>) allows the submission of compounds, chemical entities, and chemical classes to the ChEBI database. ChEBI annotators will then review the submission: if it is deemed appropriate they will approve the entry and it will be made publicly visible at the next ChEBI release (ChEBI database is updated once a month).

### 3.1 Login to the submission tool

Once you are registered, enter your name and password.

### 3.2 Creating a submission

To create a new submission, click the link 'Create new submission' which is near the bottom of the page.

A newly created submission will have the status 'Initialised'. A submission which has been edited but not submitted will have the status 'Edited'. A submission which has been submitted with a future release date will have status 'Pending'.

### 3.3 Editing a submission

To edit a submission, click on the 'Edit submission' link next to the submission details in the submission table. On the ensuing page, entitled 'Edit ChEBI Submission', clicking on the tabs in turn will guide you through the submission process.

Submission Step 1:

#### ChEBI name

The ChEBI Name will be the primary name of the ChEBI entry being submitted. It is highly desirable that such names be kept short - abbreviations (similar to ATP, NAD, etc.) are acceptable. Unless it is an abbreviation, a ChEBI Name should start with a lower-case letter, not a capital (unless this is a special character relating to stereochemistry or denoting an element).

Additionally to the name, either a structure or a definition must be added. Definition: They are especially relevant to classes of compounds. See the ChEBI Submission Tool User Manual for guidance. No sources of definitions need to be cited.

#### Capturing a structure

To capture a structure, click on the 'Edit Structure' tab. The MarvinSketch applet will be displayed, which should be used to capture the structure as required. Submitters are recommended to consult the MarvinSketch User's Guide (a structure can be drawn or imported).

The Microme curator will have to check that the displayed structure is the major form at the pH used in Rhea for all reactions, i.e. pH 7.3. From the top menu, clicking on **Tools->Protonation->Major Microspecies at pH 7.3** will compute the major structure and will allow comparison with the drawn structure. In case of differences, the user may save the structure at pH 7.3 then loads it into the canvas before clicking the 'Update structure' button.

#### Submission Step 2: Capturing cross-references

Clicking on the link 'Add cross-reference' will open up two boxes, in the left-hand one the cross-reference may be added, with the source of the reference being selected from the drop-down menu of the right-hand box.

#### Submission Step 3: Capturing synonyms

Clicking on the link 'Add synonym' opens boxes in which the name, type and language may be specified. A synonym taken from an external source should not normally be altered when being entered into ChEBI. Further guidance on the capture of synonyms, including IUPAC Names, is given in the ChEBI Annotation Manual (section 4.6).

#### Submission Step 4: Classifying a submission

a) to classify the entity in the Simple Classification View, select one of the available classification parents from the radio options provided. The classification relationship will be automatically added.

b) to classify the entity in the Advanced View, select 'Advanced' from the drop-down selection box. Select the Relationship type from the drop-down selection box. Enter the name/ID of the related term then select the proposed term then click on the 'Select' button. Clicking the 'Add relationship' button then saves the relationship.

#### Preview: Final Submission

This page summarizes any outstanding errors with the submission. The submitter will be notified at this point and submission will be impossible until all errors have been fixed.

If there are no errors, leave the required submission date blank (i.e. submission with immediate effect), and click 'Submit'.

An acknowledgement will be displayed which will include the assigned ChEBI identifier.

ChEBI annotators will then review the submission; if it is deemed appropriate they will approve the entry and it will be made publicly visible in the next ChEBI release. However if it is inappropriate the entry will be deleted and will not be publicly visible as a normal entry but rather as a deleted entry in the following release.

### 3.4 Listing submissions

Click the link 'Historical submission' to list all your submissions and their status. A submission which has been submitted will have the ChEBI status SUBMITTED. A submission which has been approved by the ChEBI curation team will have the status CHECKED. A submission which has been deleted by ChEBI curation team will have the status DELETED.

### 3.5 Use in Rhea

Once a new compound has been submitted and has received an identifier (ChEBI ID), this can be used in Rhea to create a new reaction.

## **4-Data management**

### **4.1-Quality control**

The ChEBI resource has its own internal quality control procedure. Microme submissions are approved by the ChEBI curation team.