CHEMNER ANNOTATION

Thank you for helping with this task!

Entity Types and Definitions

The entity ontology: Chemical Fine-grained Entity Ontology.pdf.
In the given ontology, the entity type is defined in a hierarchical structure across the first four columns of each row. The first column represents the most general or highest-level type, while the fourth column represents the most specific or lowest-level type. The last two columns in each row provide a detailed description of the corresponding type and its associated external link. Some rows may not have entries in the second to fourth columns, indicating that they are general types. When performing annotations, please aim to assign each entity to the most specific type available.

Please annotate chemical compound entities mentioned **either in natural language or chemical formulas**, such as *H2O* and *water*. Additionally, please annotate IUPAC names (e.g., *(4R,4aR,7S,7aR,12bS)-3-methyl-2,4,4a*), and IDs (e.g., MFCD00003299). Please also annotate other chemical entities defined in the ontology.
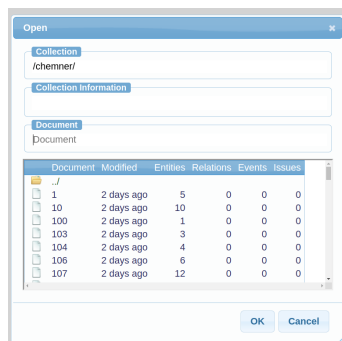
Annotation Guideline

STEP 1: Visit the annotation page for a document

The home URL to the annotation interface is
http:/XXXX:8001/index.xhtml#/chemne_test/
There will be two ways to annotate a document.

Firstly, visit the home URL above. A document selection window will show up. Select the document id to proceed to the document annotation page.
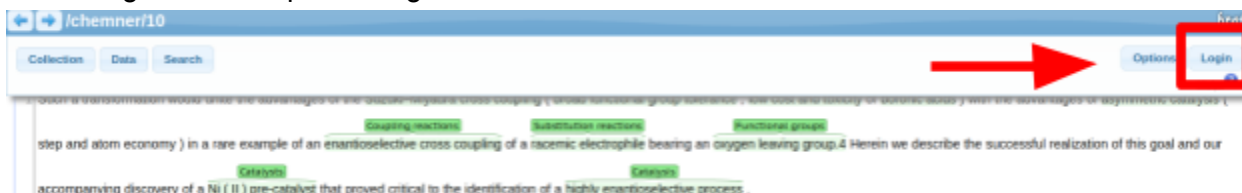
Secondly, directly access the annotation pages of documents:
http://XXX:8001/index.xhtml#/chemner_test/{document_id}

STEP2 Log In

Please log in with the private login credentials we sent.

STEP3 Annotate the Document

Your job is to annotate entity mentions in the document. Each entity mention is a consecutive text span. The annotation interface will provide entity types (see the above figure in Step 2 for an example). However, it's important to note that these annotations are not comprehensive or entirely accurate. Please ensure to check for possible mentions that are not included in the preset annotations, and consider providing more specific subtypes or different entity types for the preset annotations. Additionally, some text spans are labeled as the type **PHRASE**. For these spans, please assign the appropriate type from the ontology mentioned above, if applicable. If there is no suitable match is found, please remove the **PHRASE** annotation.

Please carefully read the annotation examples below. These examples cover four major annotation scenarios.

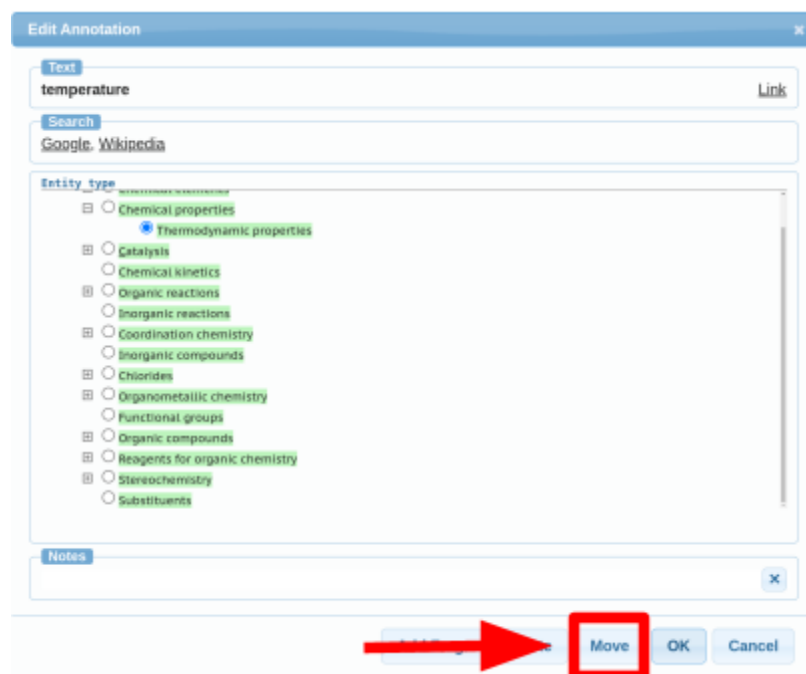### Correct the entity mention span if it is wrong

The preset annotation may consist of partial mentions or include extra tokens as part of the mentions.
Example:
- In this sentence, *high temperature* should be the (*Thermodynamic properties*) entity.

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- To fix the annotations:
    1. Double-click on the *Thermodynamic properties* label. An edit annotation menu will pop up.

2. Click the **Move** button from the menu
3. Re-select *high temperature* as the new entity mention.

4. The label will be updated automatically.

Correct the entity type if the entity mention span is correct but the entity type is wrong

The provided annotation may contain incorrect entity types assigned to certain entity mentions.

Example:
- In this sentence. the phrase *high temperature* should be labeled as *Thermodynamic properties*, rather than *Chemical properties*

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- To fix the annotations:
   1. Double-click the *Chemical properties* label. An edit annotation menu will pop up.

2. Choose the correct entity type from the list (Thermodynamic properties).

3. Click **OK**. The label will be promptly updated.

Label an entity with the appropriate entity type if there was no entity type assigned to it

An entity might not be annotated.
Example:
- In this sentence, the phrase *Suzuki-Miyaura reaction* is not annotated.

  les

-   and amount of base required for the Suzuki-Miyaura reaction ,

- To fix the annotations:

  1. Use your mouse to highlight *Suzuki-Miyaura reaction* on the annotation tool. An annotation menu will pop up.

     les

       and amount of base required for the Suzuki-Miyaura reaction ,

  2. Select the correct label for *Suzuki-Miyaura reaction*

     New Annotation   ×

     Text
     Suzuki-Miyaura reaction

     Search
     Google, Wikipedia

     Entity type
     - ⊞ ○ Chemical elements
     - ⊞ ○ Chemical properties
     - ⊞ ○ Catalysis
     - ○ Chemical kinetics
     - ⊟ ○ Organic reactions
       - ○ Carbon-carbon bond forming reactions
       - ● Coupling reactions
       - ○ Addition reactions
       - ○ Elimination reactions
       - ○ Substitution reactions
       - ○ Polymerization reactions
       - ○ Name reactions
       - ○ Organic redox reactions
       - ○ Ring forming reactions
     - ○ Inorganic reactions

     Notes
       ×

     OK   Cancel

  3. Click **OK**. The label will be promptly updated.

  s
                                                    Coupling reactions
       and amount of base required for the Suzuki-Miyaura reaction ,
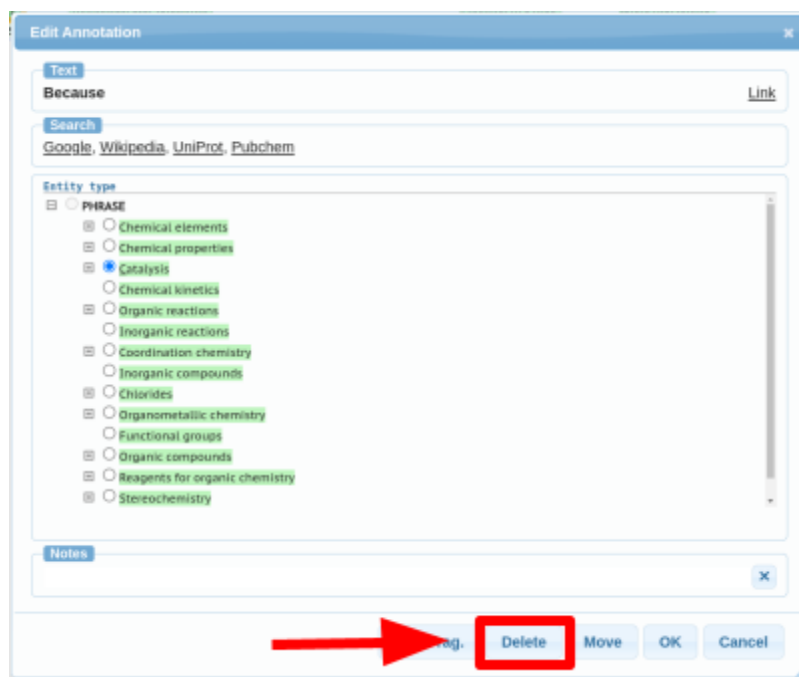
Remove the entity type if both the entity type and its mention span are incorrect

Entity types may mistakenly be assigned to non-entity phrases.
Example:

- In this sentence, the word *Because* is mistakenly annotated as *Catalysis,* and there is no appropriate label for this term

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- To fix the annotations:
    1. Double-click on the *Because* label. An edit annotation menu will pop-up.

    2. Click the **Delete** button. The annotation will be removed.

Tips

1. A common error found in the preset annotations is mislabeling *catalysts* as "*chemical_reactions/catalysis*".
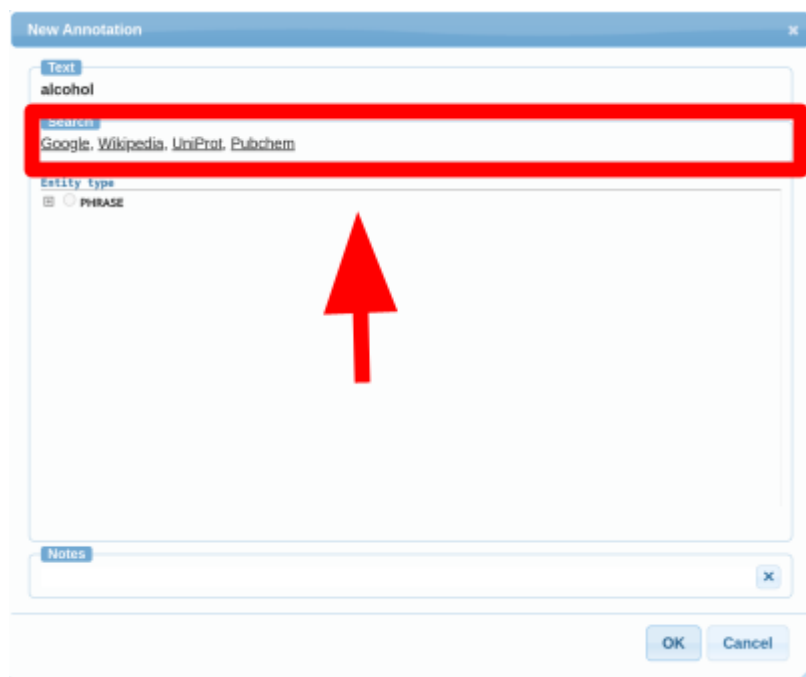   For example:

2. Another common error is mislabelling *organic acid* as "Inorganic_compound/metal_halides/oxoacids"

broad functional group tolerance , low cost and toxicity of boronic acids)

3. If you are not sure about a chemical, you can click the search button inside the pop-up menu

Thank you so much for your help and contribution to our project. We really appreciate the efforts of everyone involved. If you have any questions or if anything is unclear, please don't hesitate to reach out to us.