

Annotation validation guide

A. INTRODUCTION

The goal of this tool is the fine-tuning and validation of the annotations produced by the chemical literature annotation tool.

Validation Instructions (Click to expand)

[Download the detailed validation instructions here](#)

Validate the **Products** in the description

(14) For the reaction of N,-acylated indoles with dimethyldioxirane , see : (a) Zhang,,X. ; Foote , C. S. J. Am. Chem. SOC. 1993 , 115 , 8867. (b) Adam , W. ; Ahrweiler , M. ; Peters , K. ; **Schmiedeskamp** , B. J. Org. Chem. 1994 , 59 , 2733 and references therein. (15) Diketopiperazine 12 can be prepared directly , albeit only in 35 % yield , by heating tryptophan methyl ester (9) at 140 °C for 3 h , thus saving four steps in the synthetic sequence described above. (16) There are relatively few direct methods for the preparation of 2,3-disubstituted indoles. For some current methods , see : (a) Saulnier , M. G. ; Gribble , G. W. J. Org. Chem. 1982 , 47 , 2810. (b) Fukuyama , T. F. ; Chen , X. ; Peng , G. J. Am. Chem. SOC. 1994 , 126 , 3127 and references therein .

Undo Reset

Reactants
Products
Yield
Reaction
Catalyst
Solvent
Temperature
Time

Reactants

tryptophan methyl ester (9)

☐ There is no Reactants

Products

Schmiedeskamp

☐ There is no Products

Yield

35 %

☐ There is no Yield

Reaction

☒ There is no Reaction

Catalyst

☒ There is no Catalyst

Solvent

☒ There is no Solvent

Temperature

140 °C

☐ There is no Temperature

Time

3 h

☐ There is no Time

Validate annotation

☐ There is no reaction

B. VALIDATION PROCESS

1. The text paragraph to be validated will be shown in the text window on the left side of the screen.
 - The paragraph shown may include from none to multiple chemical reactions.
 - The validation tool will automatically go through each and every reaction annotated in the paragraph, one at a time.
 - The annotated entities are automatically highlighted in order to facilitate the validation.

Validate the **Products** in the description

(14) For the reaction of N,-acylated indoles with dimethyldioxirane , see : (a) Zhang,X. ; Foote , C. S. J. Am. Chem. SOC. 1993 , 115 , 8867. (b) Adam , W. ; Ahrweiler , M. ; Peters , K. : **Schmiedeskamp** , B. J. Org. Chem. 1994 , 59 , 2733 and references therein. (15) Diketopiperazine 12 can be prepared directly , albeit only in 35 % yield , by heating tryptophan methyl ester (9) at 140 'C for 3 h , thus saving four steps in the synthetic sequence described above. (16) There are relatively few direct methods for the preparation of 2,3-disubstituted indoles. For some current methods , see : (a) Saulnier , M. G. ; Gribble , G. W. J. Org. Chem. 1982 , 47 , 2810. (b) Fukuyama , T. F. ; Chen , X. ; Peng , G. J. Am. Chem. SOC. 1994 , 126 , 3127 and references therein .

FOR EACH PARAGRAPH REPEAT SETPS 2 – 6 BELOW:

2. If a change is required, select (highlight in green) in the window on the right the entity class to be modified.

Reactants
Products
Yield
Reaction
Catalyst
Solvent
Temperature
Time

3. Proceed as per one of the following three options depending on the required type of modification:
 1. If there should be no annotation at all, reset it by clicking the reset button and check the “There is no XXX” box next to the entity class:

 Reset

☒ There is no Catalyst

- If the entity class contains no annotation but one or more entities should be included, add them by selecting the relevant word(s) or span(s) in the paragraph.

Validate the **Products** in the description

(14) For the reaction of N,-acylated indoles with dimethyldioxirane , see : (a) Zhang,X. ; Foote , C. S. J. Am. Chem. SOC. 1993 , 115 , 8867. (b) Adam , W. ; Ahrweiler , M. ; Peters , K. ; Schmiedeskamp , B. J. Org. Chem. 1994 , 59 , 2733 and references therein. (15) **Diketopiperazine 12 can** be prepared directly , albeit only in 35 % yield , by heating tryptophan methyl ester (9) at 140 °C for 3 h , thus saving four steps in the synthetic sequence described above. (16) There are relatively few direct methods for the preparation of 2,3-disubstituted indoles. For some current methods , see : (a) Saulnier , M. G. ; Gribble , G. W. J. Org. Chem. 1982 , 47 , 2810. (b) Fukuyama , T. F. ; Chen , X. ; Peng , G. J. Am. Chem. SOC. 1994 , 126 , 3127 and references therein .

⏮ Undo
✖ Reset

Reactants
Products
Yield
Reaction
Catalyst
Solvent
Temperature
Time

Reactants

tryptophan methyl ester (9)

Products

Diketopiperazine 12 can

☐ There is no Reactants

☐ There is no Products

- If the entity class contains an incorrect annotation that should be substituted, reset the field and annotate the entity class as described above.
- In case that, after the review, no entity should be annotated, the **‘There is no reaction’** box must be checked in order to proceed to the next annotation.

Validate annotation

☒ **There is no reaction**

- Once the current reaction has been validated annotated click on **‘Validate annotation’** in order to review the next annotation.

Validate annotation

☐ **There is no reaction**

D. CORRECTIONS

The **‘Undo’** and **‘Reset’** buttons allow to make corrections during the validation process:

- Undo: Undoes the last action
- Reset: Clears the active entity field

⏮ Undo

✖ Reset