

Wipf Group CBIS Guidelines

The following information is required for every CBIS page entry:

- A reaction scheme, showing all used reactants in front or above the arrow and reaction conditions such as solvent, temperature and time under the arrow.
- A complete reactant table, including names of starting material and used amounts in g and mmol.
- A complete product row entry, containing product name, amount in g, mmol as well as yield in %.
- Specify the solvent in the solvent row with the amount in mL.
- Start and stop times of the experiment.
- The procedure should contain the names of all used reactants as well as the amount in g, mmol, with the same number of significant figures, usually three (0.123). A detailed description of performed steps (work-up, purification, etc.) and significant observations according to the ACS style is absolutely required. Every procedure has to end with the result of the reaction, for example: “to obtain ABC.0123.04 (60.2 mg, 0.0522 mmol, 99%) as a colorless solid.”
- For all unknown/new compounds, the following analytical data are required and need to be listed or attached to the CBIS page of the representative procedure:
 - ¹H NMR
 - ¹³C NMR
 - TLC
 - High resolution mass (LCMS with LC/UVD/ELSD trace and correct mass if HRMS is not possible)
 - IR
 - Melting point if solid
 - Optical rotation if enantiomerically enriched
- For all known compounds the following analytical data are required:
 - ¹H NMR (as an attachment to every CBIS page)
 - TLC (as an attachment to every CBIS page)
 - Reference to the source of complete analytical data, for example in a previous publication or an earlier CBIS page.

Please note that the number of pending pages is limited to 40. If you reach this limit, you will need to add all missing data, upload spectra, etc., and approve the page(s) in order to be able to continue your research. It is important that your approved pages are complete, which means you have to attach all appropriate analytical data.