Knoevenagel reports information (for information to the reaction, see tutorial slides):

**Please not that we are aware of the issues with PARAFAC for the decomposition of impure peaks in this campaign. We are already actively working to resolve this issue.**

**report\_chroms** shows all chromatograms of the campaign consisting of “training runs” (runs, the tool learns from), which are four quantitative calibration runs for each aldehyde (indices 1–16). All subsequent runs are reaction runs, which are recorded in the following order:

* Indices 17 + i \* 5 with i = 0, 1, 2, 3, 4, 5: Benzaldehyde reaction
* Indices 18 + i \* 5 with i = 0, 1, 2, 3, 4, 5: 4-Chlorobenzaldehyde reaction
* Indices 19 + i \* 5 with i = 0, 1, 2, 3, 4, 5: 4-Methoxybenzaldehyde reaction
* Indices 20 + i \* 5 with i = 0, 1, 2, 3, 4, 5: 4-Dimethylaminobenzaldehyde reaction
* Indices 21 + i \* 5 with i = 0, 1, 2, 3, 4, 5: All four benzaldehydes in one reaction (mix)

**report\_hplc\_input** shows all given user input. Note how the compound object is used to train the tool on qualitative + quantitative information (indices 1–16).

**report\_peak\_db** shows all peaks found in all chromatograms over the campaign.

**report\_quali\_comp\_db** shows all “qualitative components”, i.e., compound information which is used to assign peaks to compound names. Note, that we find all compounds we trained the tool on plus all “unknown” compounds. “Impurity” compounds are minor inpurities found in pure compound runs.

**report\_quant\_db** shows all “quantitative components”, i.e., compound information which is used to quantify peaks (integral 🡪 concentration).

**report\_runs** tracks the integrals and, if available, the concentrations of all “qualitative components” over all chromatograms of the campaign.

**report\_parafac** shows all information to the PARAFAC decomposition of impure peaks (**not yet in final version**).