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

**report\_chroms** shows all chromatograms of the campaign consisting of “training runs” (runs, the tool learns from), which are one internal standard run, two quantitative calibration runs of substrate and product each and one qualitative compound run for two aryl CN-sources. All subsequent runs are reaction runs on the wellplate, which are analyzed by the tool.

**report\_hplc\_input** shows all given user input. Note how the compound object is used to train the tool on qualitative + quantitative information (indices 2–5) and qualitative information (indices 1, 6, 7). Note moreover, how the internal standard is added to the campaign (index 1) and how the internal standard information is given in all subsequent runs.

**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.

**report\_quant\_db** shows all “quantitative components”, i.e., compound information which is used to quantify peaks (integral 🡪 concentration). Note, that we only find compounds, which had quantitative compound objects in the user input to be trained on.

**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**).