

README

Data folder:

Contains files data and holdout_test.

Data includes all previous data + 24 OH-PCBs (LC and FIA).

Holdout_test includes 12 OH-PCBs (LC and FIA) which model has never been introduced too.

Scripts:

- load_and_predict: Load model from Model-folder and predict IE-values. Saves result in Result-folder.
- train_eval_model: Script for training a new model. Separating test and train so that no compound appears in both. Saves completed model in Model-folder. Saves result of predictions in Result-folder.
- descriptor_calculator: Only calculates descriptors. Saves result in Result-folder.