Reductive amination –Validation kit

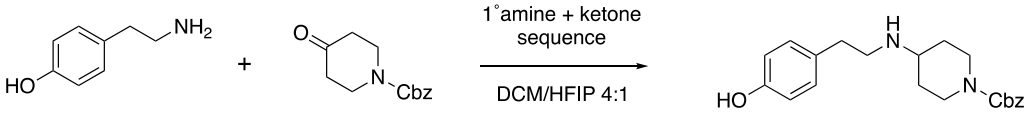
The initialization kit serves to provide benchmark data, that the instrument is set up correctly and the performance is optimal. The kit contains all reagents and substrate for a defined reaction, where yield, purity and analytical data is available.

The kit contains:

- 1 reductive amination cartridge (includes Si-$CNBH_3$ and SCX-2)
- Tyramine (99%, Fluka): 0.5 mmol, 68.6 mg
- 1-Z-4-Piperidone (99%, Sigma-Aldrich): 0.55 mmol, 122.5 mg

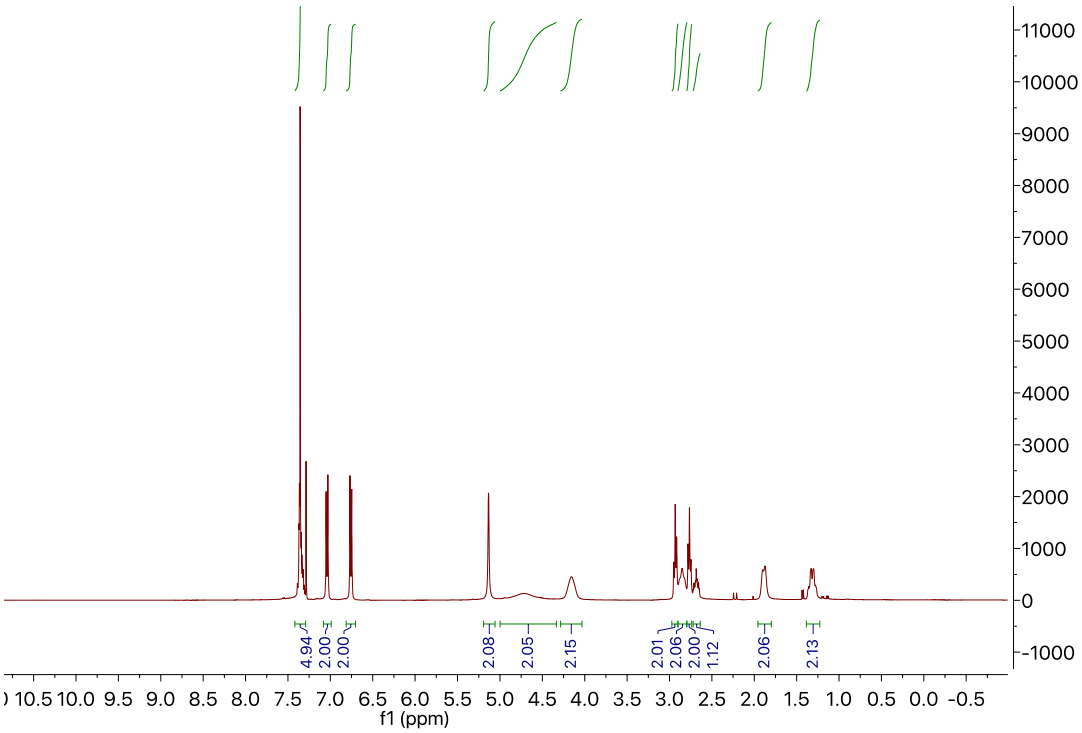
Reaction Setup Instructions:

Place the two starting materials (Tyramine and 1-Z-4-Piperidone) in the reaction vial and dissolve them into the reaction solvent (4 ml CH_2Cl_2 + 1 ml HFIP). Add a stir bar of suitable size into the vial. Load the sequence on the machine by scanning the microchip present on the capsule and select the variant “primary amine and ketone”. Insert the reaction vial and the reagent cartridge into their compartment, then start the sequence. After the sequence is complete (about 4 hours) concentrate the solvent in the vial to collect the product.

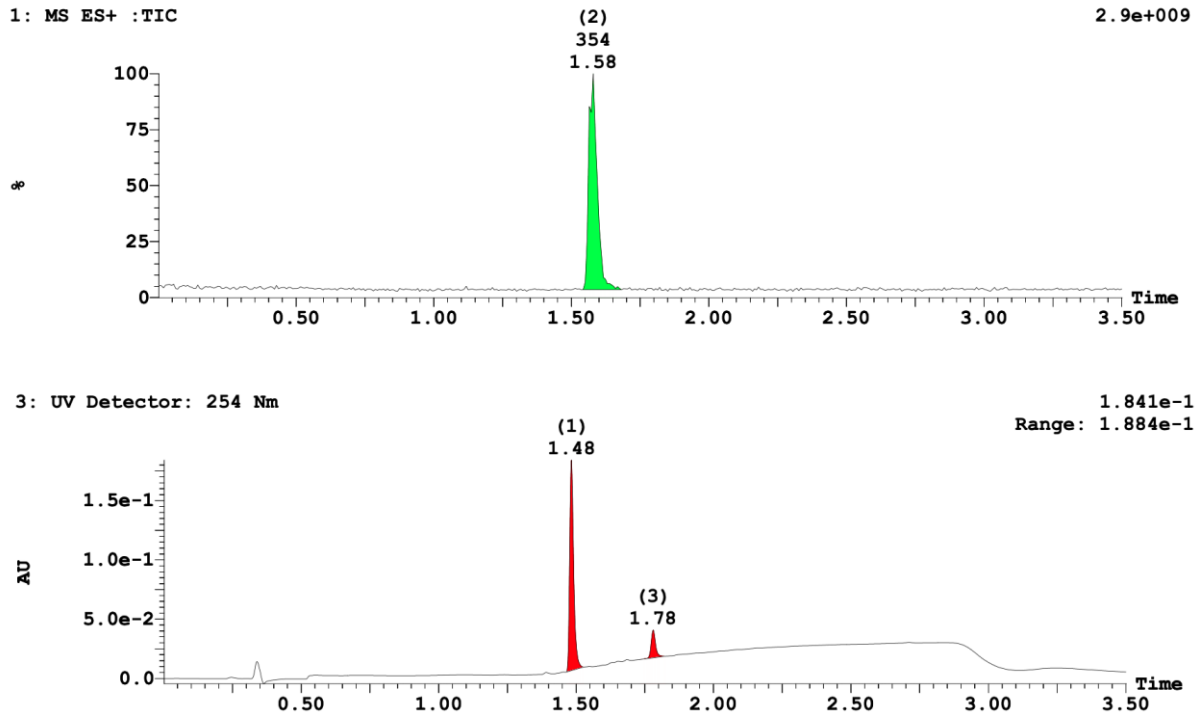


expected yield: 75-80%
expected purity: >95%

HNMR spectrum of the product (solvent $CDCl_3$):



LCMS data of the product:
Gradient: H_2O to MeCN, 5-95% in 3.5 min on C18 column



The peak at 1.48 min was identified as the product and matches with the expected mass. The second peak at 1.78 is a known contamination of the LCMS-instrument and can be ignored.