Iteration Number:	
Experiment Name:	**Description:**

1 Computational Requirements for Bayesian Optimization

- ☐ Generate samples using Sobol sampling
- ☐ Generate the layout for **Opentrons II robot** transfer, generate a tick box list for the manual mixes, and the automated csv file for the **Triple Quadrupole mass spectrometer**

  This will generate 5 files: A master table with the run information, a Opentrons II robot script, an QqQ csv table for mass spec run, a diagram with the microplate and the corresponding condition, and a table with the microplate layout and the colors.
- ☐ Generate tables for the microtubes mixes

Pause!

- ☐ Dataset prepared and preprocessed for the optimization task
- ☐ Give new recommendations using the acquisition function

  This will give files:
- ☐ Come back to the second step in a new sheet, all the boxes should be ticked

2 Opentrons II Robot Preparation

- ☐ Test the programmed protocol with water and dummy plates

On the preparation day!

- ☐ Check the stock solutions that are needed for the experiment. Prepare fresh ones when required. Keep it fridged. Filter-sterilise when it's possible, specially with concentrated solutions.
- ☐ Prepare the necessary mixes and keep in the fridge
- ☐ Calibration of the robot (very important)
- ☐ Loading of necessary labware (pipette tips, plates, etc.)
- ☐ Programming the experimental protocol (it's given before)
- ☐ Loading of samples and reagents
- ☐ Run the programmed protocol

After samples are collected

- ☐ Run the programmed protocol to make the QC pool

3 Plate Reader Preparation

- ☐ Prepare agar plate with the bacteria (one day before)
- ☐ Prepare complete media for pre-cultures
- ☐ Prepare precultures (5ml complete media)
- ☐ Calibration of the plate reader **(Currently not done by user)**
- ☐ Setting up the main script with the correct parameters (wavelength, time, temperature, etc.)
- ☐ Book the slot for the plater reader in the building system

On the day of the experiment!

- ☐ Setting up the software with the preheating programme (15 minutes before)
- ☐ Preparing and loading the sample plate (Come from **Opentrons II robot**
- ☐ Verifying the functioning and cleanliness of the reading chamber **(Currently not done by user)**
- ☐ Running the plate

On between!

- ☐ Prepare ice before taking off the plates
- ☐ Weight and label every tube that will be used

After 24 / 36 / 48 hrs

- ☐ Take off the plate from the reader
- ☐ Put the plate on ice, mix the wells with the tip, and move 500 ul to the tubes (that are on ice **Keep the plates for biofilm assay**)
- ☐ Quenching with cold methanol/water, the ratio should be
- ☐ Centrifuge the tubes in a cold centrifuge
- ☐ Take 400ul of the tubes into new ones cold, remove the rest of supernatant, keep everything on ice **Weight the pellet quickly**
- ☐ Move the tubes to the -80 freezer

4 Triple Quadrupole Mass Spectrometer Preparation

- ☐ Calibration of the mass spectrometer**(Currently not done by user)**
- ☐ Cleaning and verifying the ion source and detector **Has to be done once a while**
- ☐ Open csv for the sequence list, create new sequence from this file
- ☐ Check that there's enough mobile phase solvent for the run and miliQ water for the seal wash
- ☐ Check the status of the mass spec by looking at the parameters, and if they are in range
- ☐ Run a few blanks, plus system suitability sample, plus a few blanks
- ☐ Preparing and loading the samples from the experiment
- ☐ Perform the run