**Setup:**

1. The required chemicals in 4mL vials are transferred from the back of the SMOLE part to the transfer MTP plate, and then the plate is transferred to the Mbraun platform. At the same time, the MTP plate with 16 capped MTP vials is transferred from the chemical storage to the evacuation chamber. After 3 times of evacuation, the MTP plate is transferred to the Mbraun platform.
2. The empty vials and the chemical vials are unscrewed.
3. The solid chemicals in 4mL vials are transferred to the tilt-shake rack
4. Solid dispensing (GDU-Pfd, GDU-SWILE)
5. Solvent dispensing
6. Liquid+stock solution dispensing (GDU-V, 4NH)
7. The reaction vials and the chemical vials are screwed back.
8. The reaction vials are transferred to 440nm photoreactor, shaking at 400rpm, water cooling at room temperature, for 8h.
9. In the meantime, all the chemicals in 4mL vials are transferred back to the SMOLE part.
10. After 8h, the reaction vials are putting back to the MTP plate
11. The MTP plate is transferred to workup station (SWING-XL).

**Work up:**

1. The GC vial MTP plate is transferred from chemical storage to the work-up station.
2. The 4NH adds 0.5 mL of the internal standard stock solution dodecane (0.2 M) to all of the reaction vials (1.5X dilution).
3. 0.5 mL of the reaction mixture from each reaction is filtered through the SPE filtration rack, then 1.5 mL of EtOAc is filtered through the filter cartridge. 10 mL of air is pushed into the filter cartridge using 4NH. (4X dilution) After all 16 reaction mixtures are filtered, 0.3 mL of the filtrate is transferred to a GC vial, using the 4NH.
4. The 4NH filled the GC vial with EtOAc (1.2 mL) (5X dilution, 30X dilution in total).
5. The GC-MTP plate is transferred to the shaking rack.
6. The rack is shaken for 2 minutes.
7. The GC auto-sampler rack is transferred with the multigripper to the transfer station. At the same time, the reaction vials MTP plate is transferred to chemical storage for storage.
8. The GC auto-sampler rack is then moved with the robot to the Triplus auto-sampler.
9. All samples are injected into the GC. After the analysis is completed, the GC-MTP plate is transferred to chemical storage.
10. Resulting GCs are analyzed and resulting peak data is linked to sample data in ArkSuite.
11. A csv of sample data along with results is output for use with SyCoFinder or other 3rd party software to be used for the next optimization iteration.
12. The second iteration is started in simulation using a json file.