



Robotic Platforms for Qualitative and Quantitative Real-time Analysis

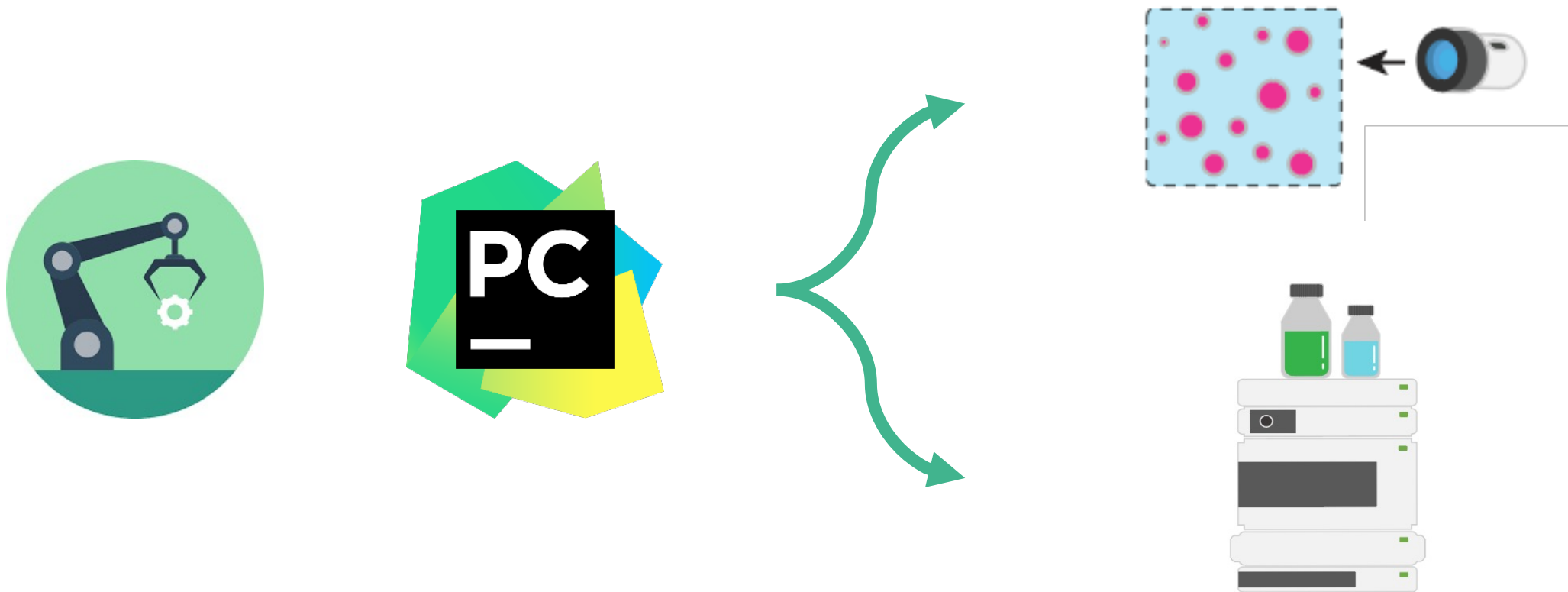
Fan (Luke) Yang

Supervisor: Dr. Jason Hein

April 30th, 2021



Outline



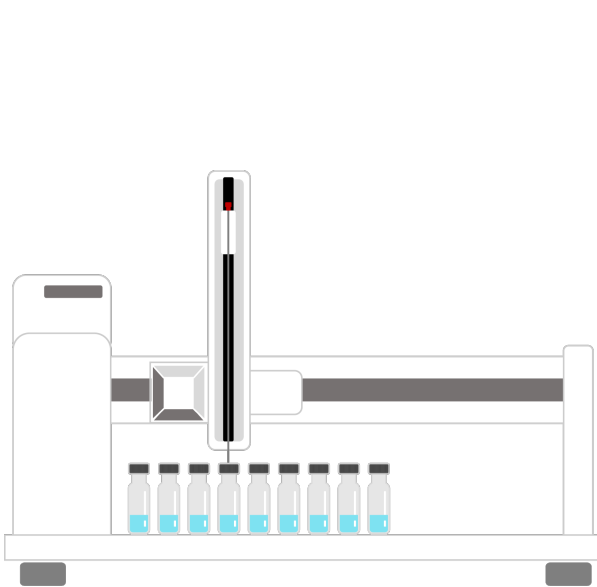
PC: PyCharm, a development software for Python programming

Laboratory Automation Increases Productivity

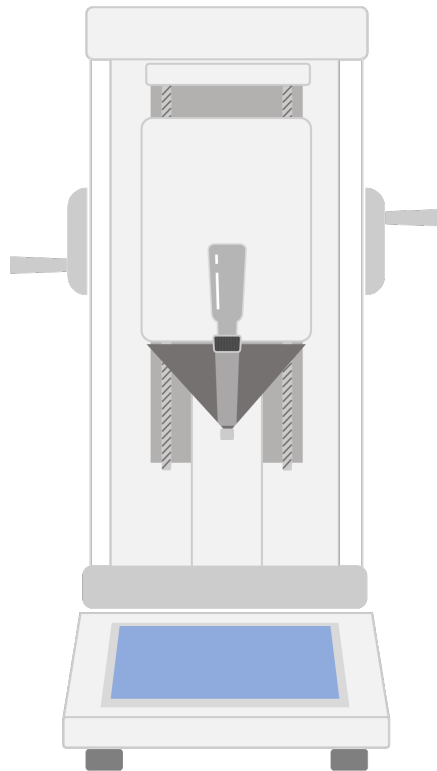


- Using robots...
 - Saves research time
 - Reduces human error

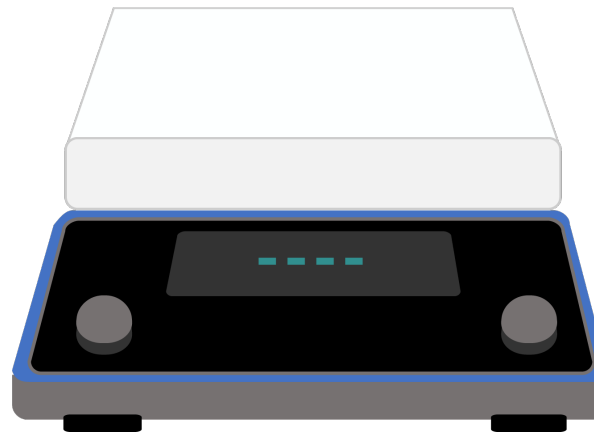
What Our System Can Do



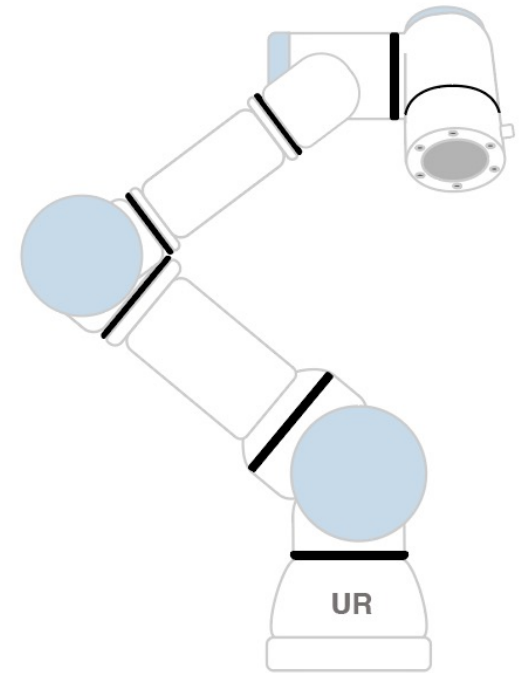
Liquid Handling



Solid Handling



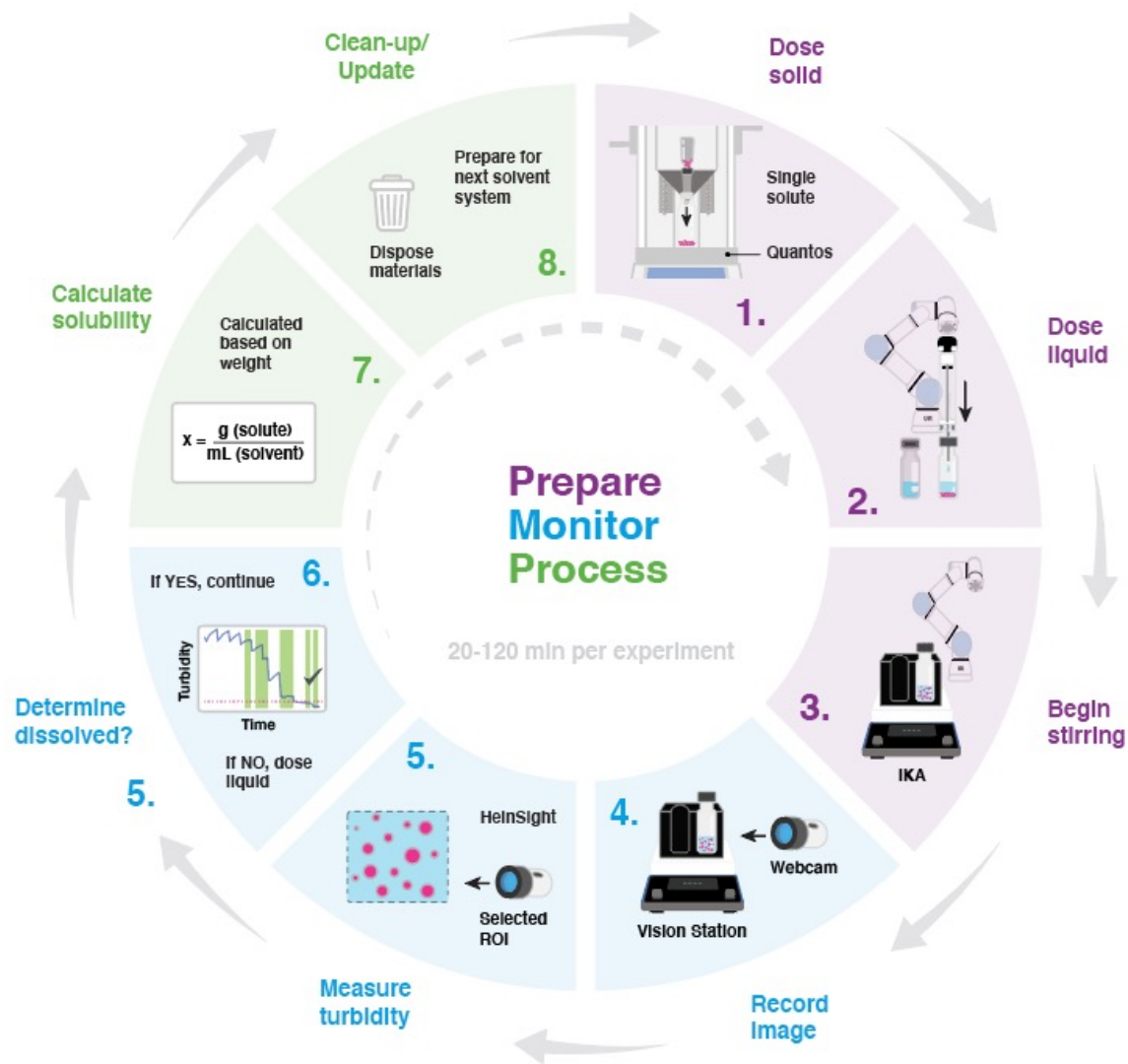
Heating and Stirring



Arm 4

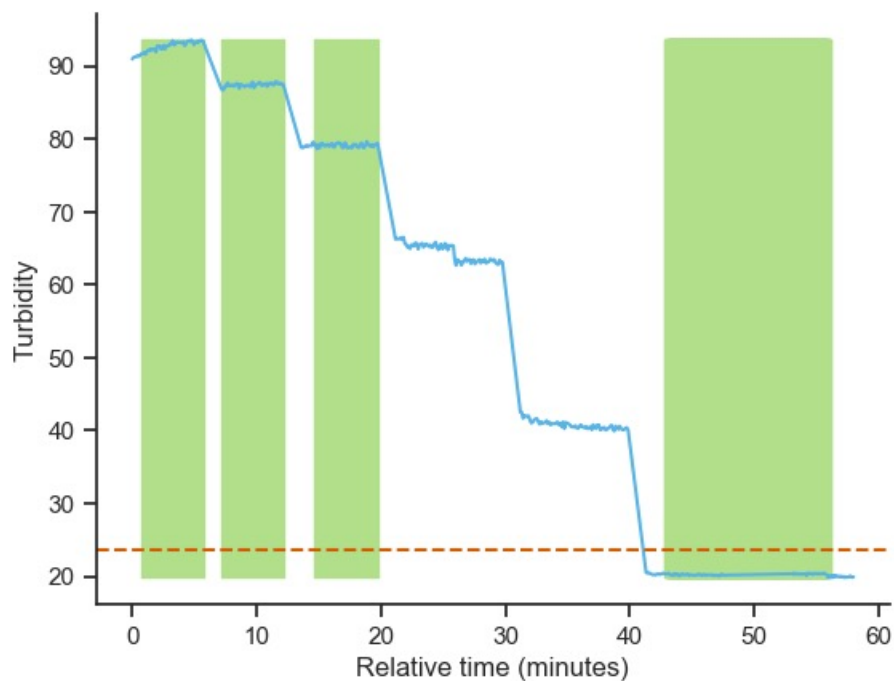
Qualitative Analysis - Solubility Tests

- Solute/solvent
- Important for the solvent system choices
- Titration-like procedure

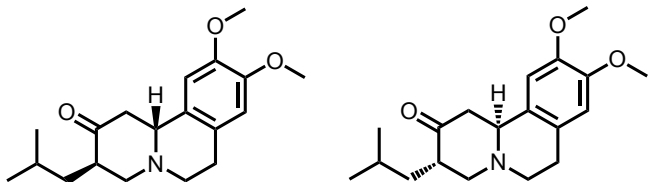


Turbidity Versus Time Results

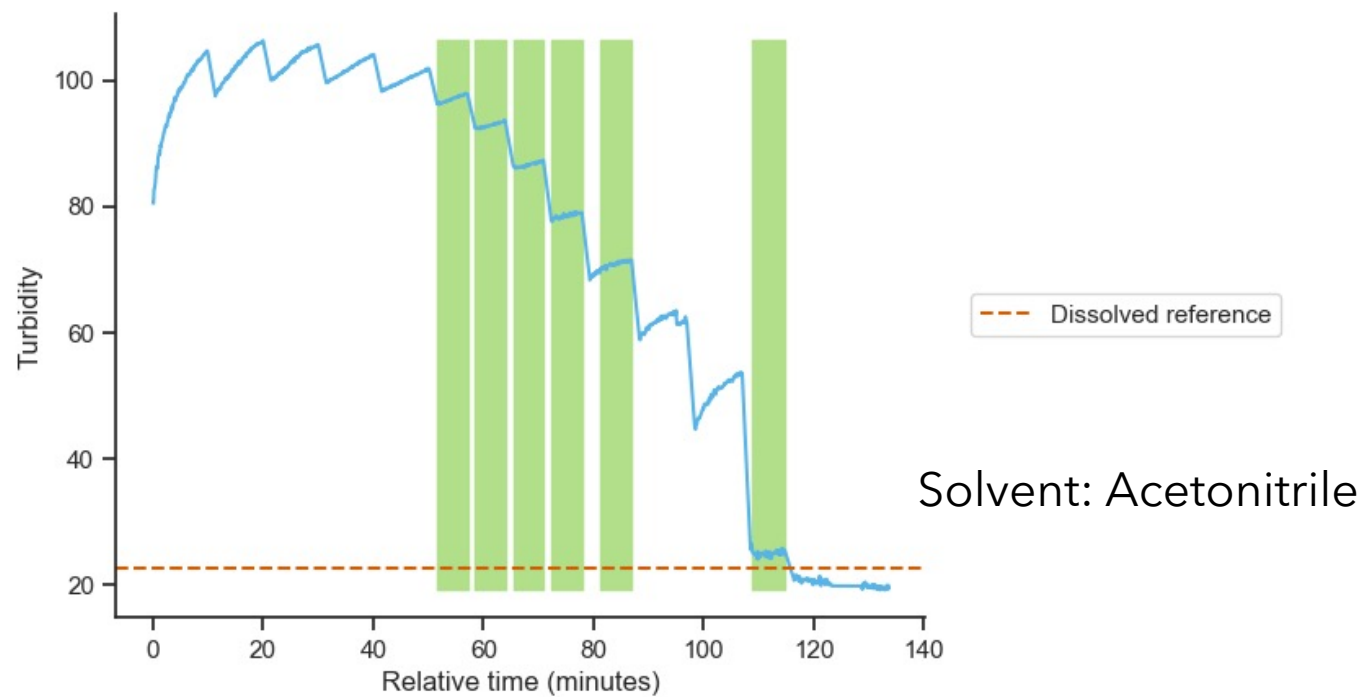
Turbidity over time



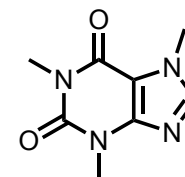
Tetrabenazine



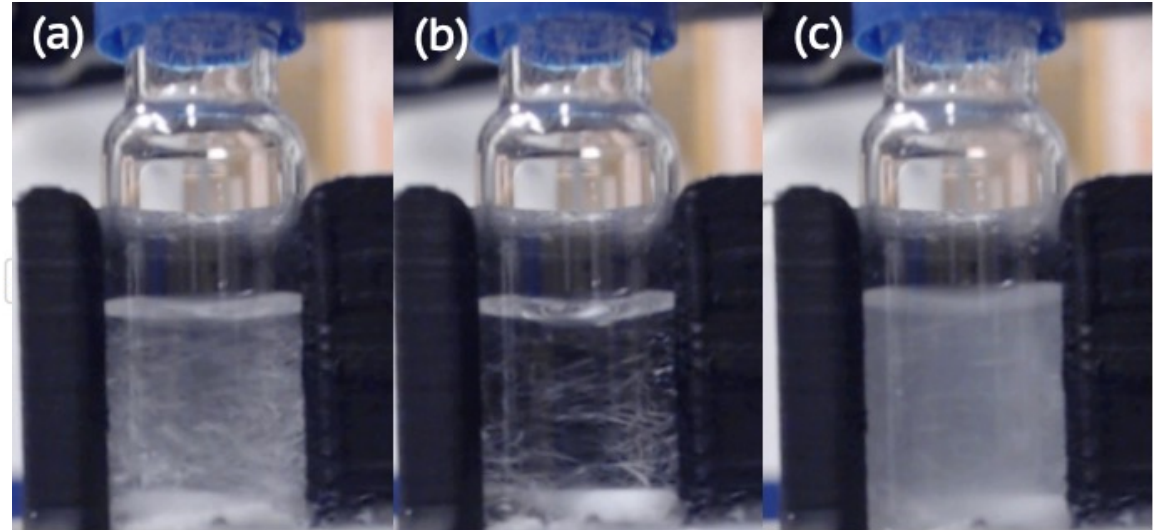
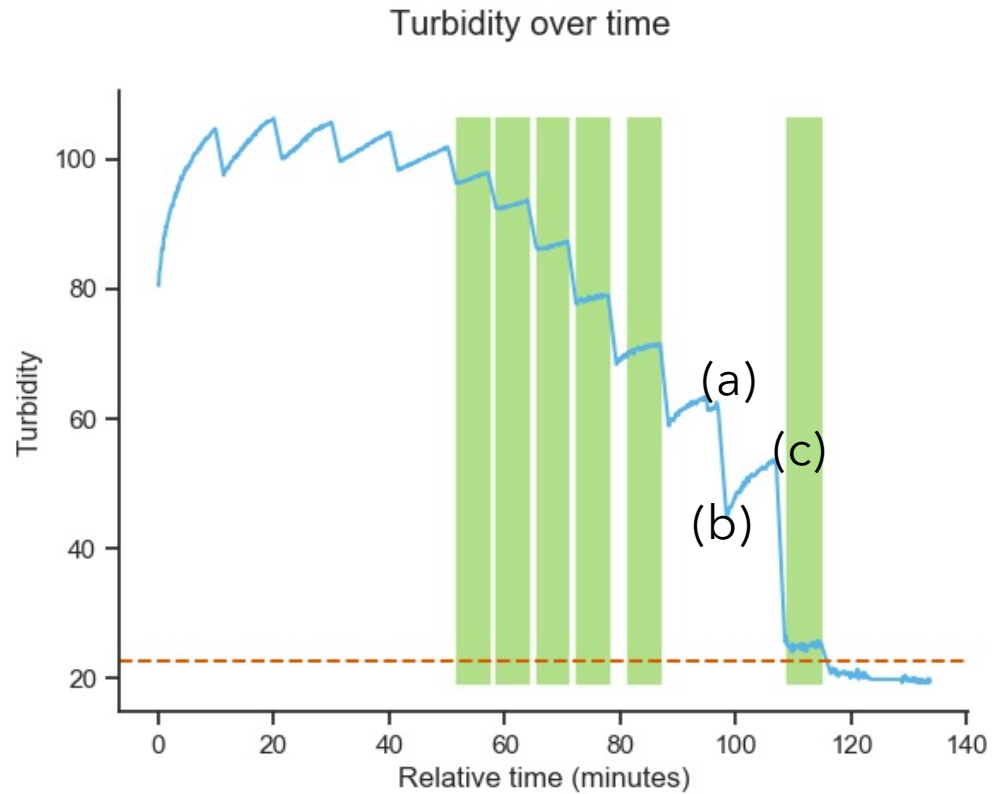
Turbidity over time



Caffeine



Further Look into the Caffeine's Turbidity Plot



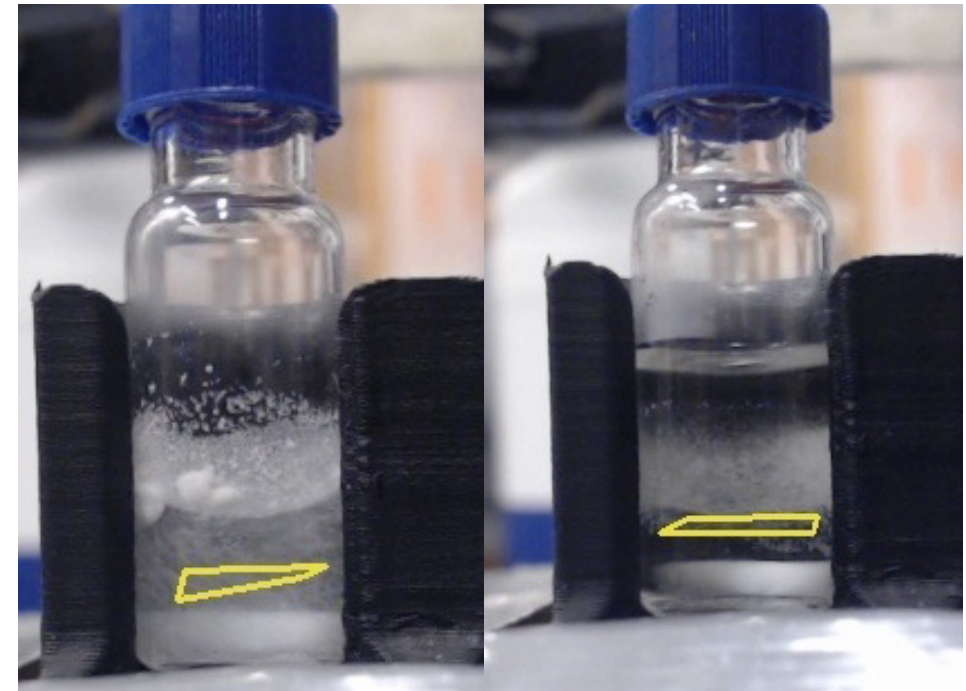
Robotic and Manual Data Comparison of Tetrabenazine Solubility

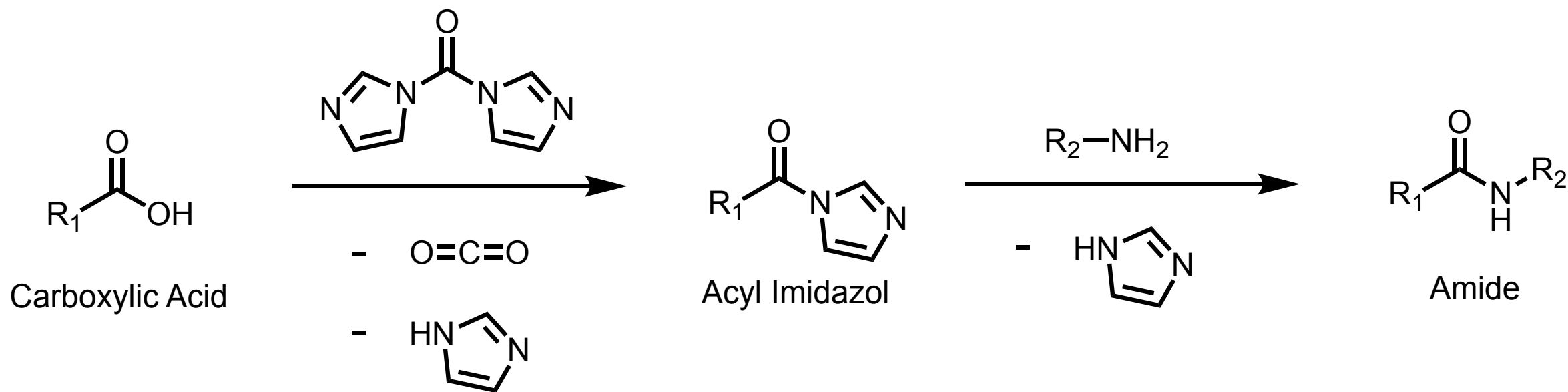
Solvent	Ethanol	Isopropanol	Ethyl Acetate	Methanol	Acetonitrile	Acetone
Robotic $\pm$ SE (mg/mL)	16.18 $\pm$ 0.79	9.72 $\pm$ 0.18	64.54 $\pm$ 1.75	24.51 $\pm$ 0.206	64.54 $\pm$ 1.75	87.97 $\pm$ 0.88
Manual (mg/mL)	17.08	9.74	65.29	24.63	65.29	88.34

SE: Standard Error

Limitations

- Only suitable for white/whitish chemicals
- Needs colorless dissolution
- Requires uniform particle size

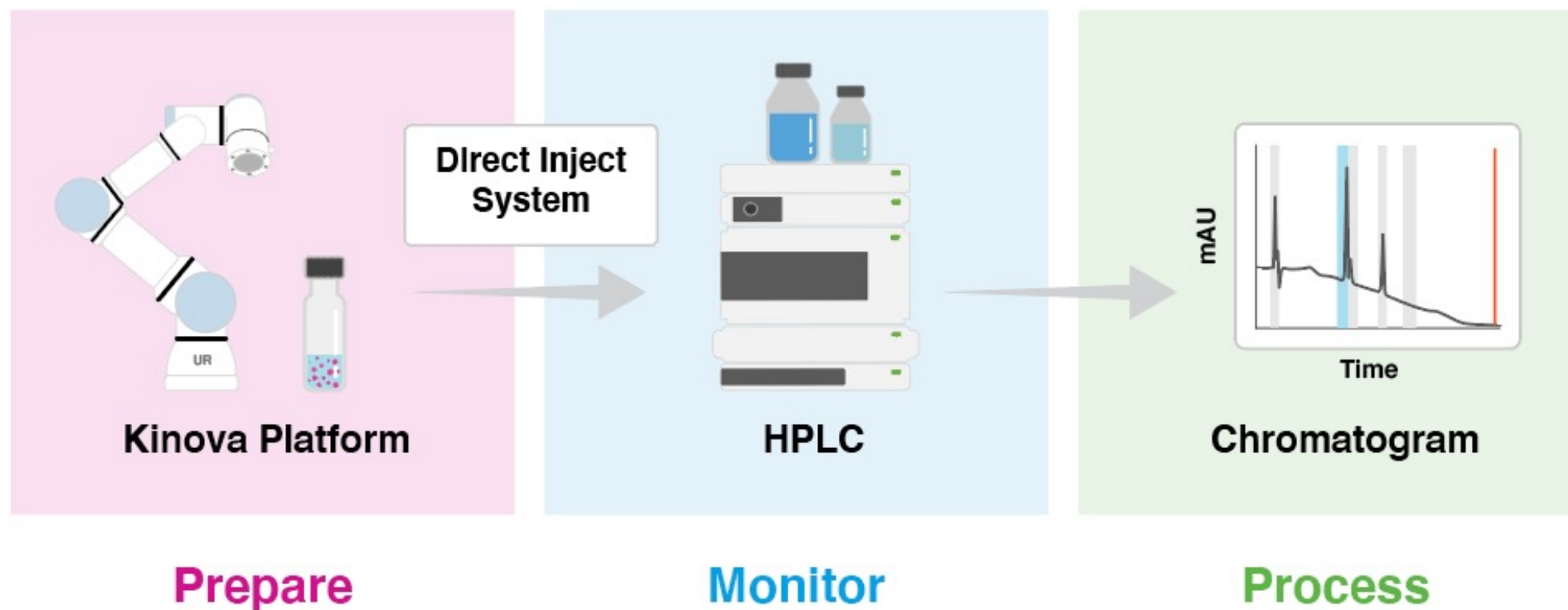




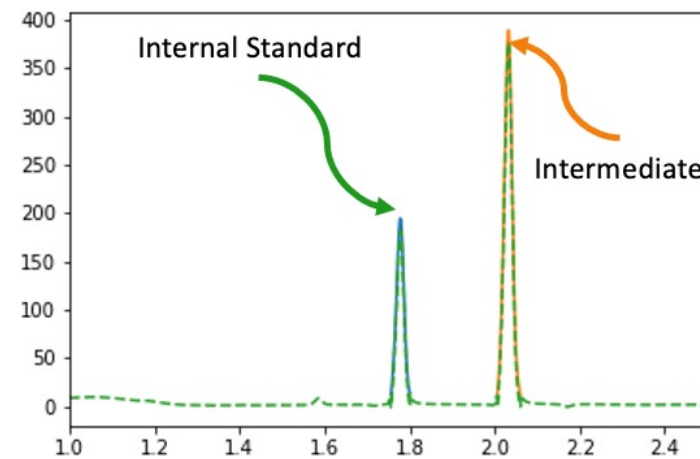
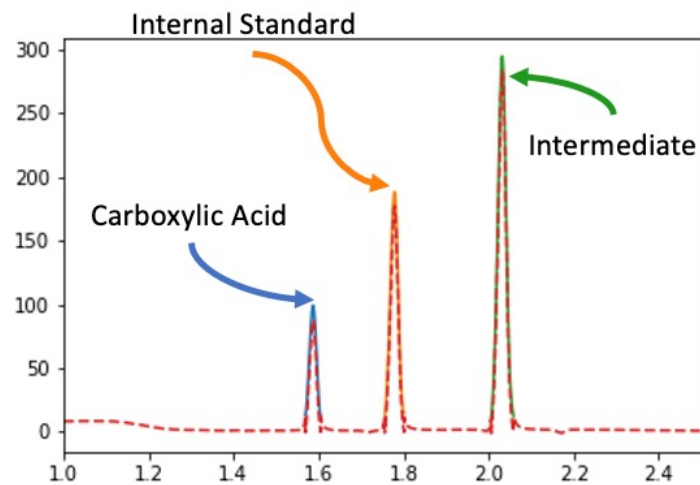
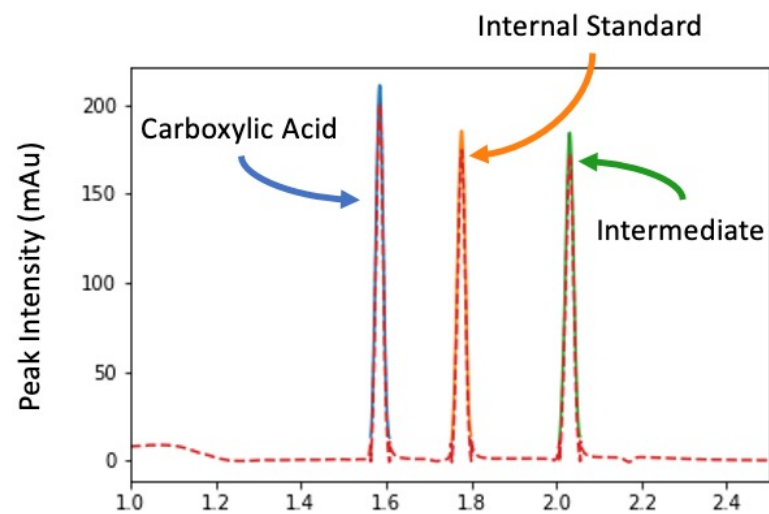
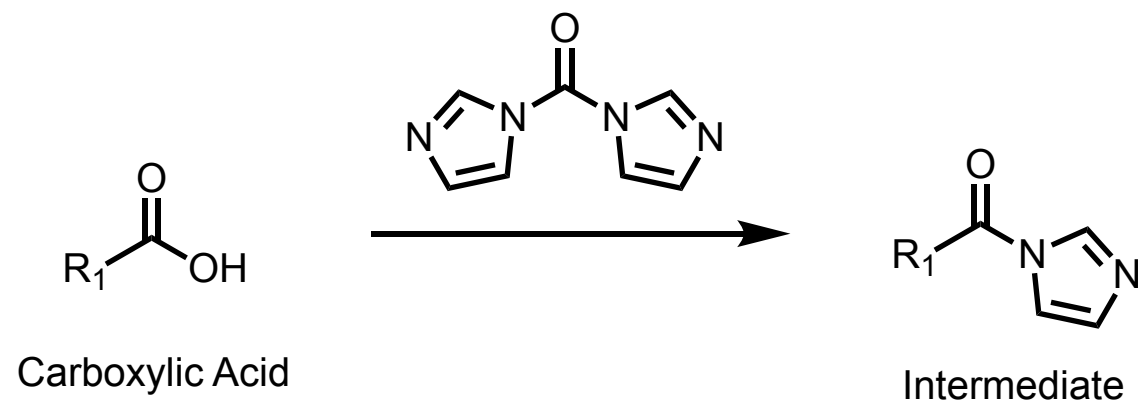
Quantitative Analysis - Amide Bond Formation

- Important synthesis in industrial and pharmaceutical sectors¹
- Involves two reaction steps

Reaction Inspection Method - HPLC

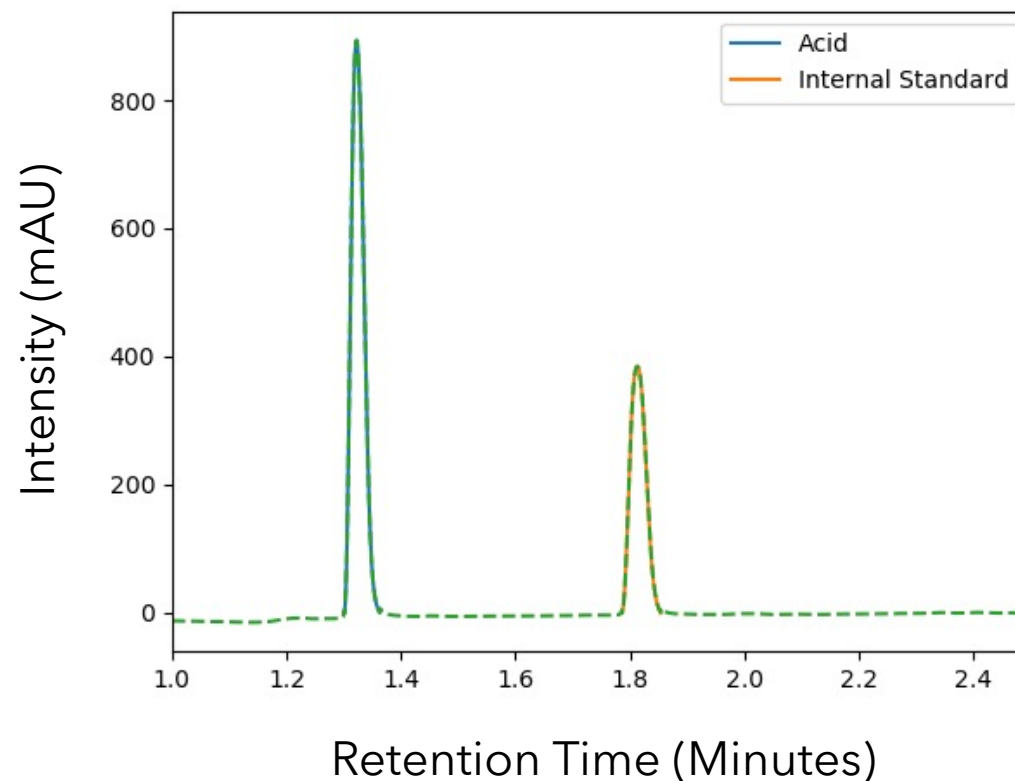
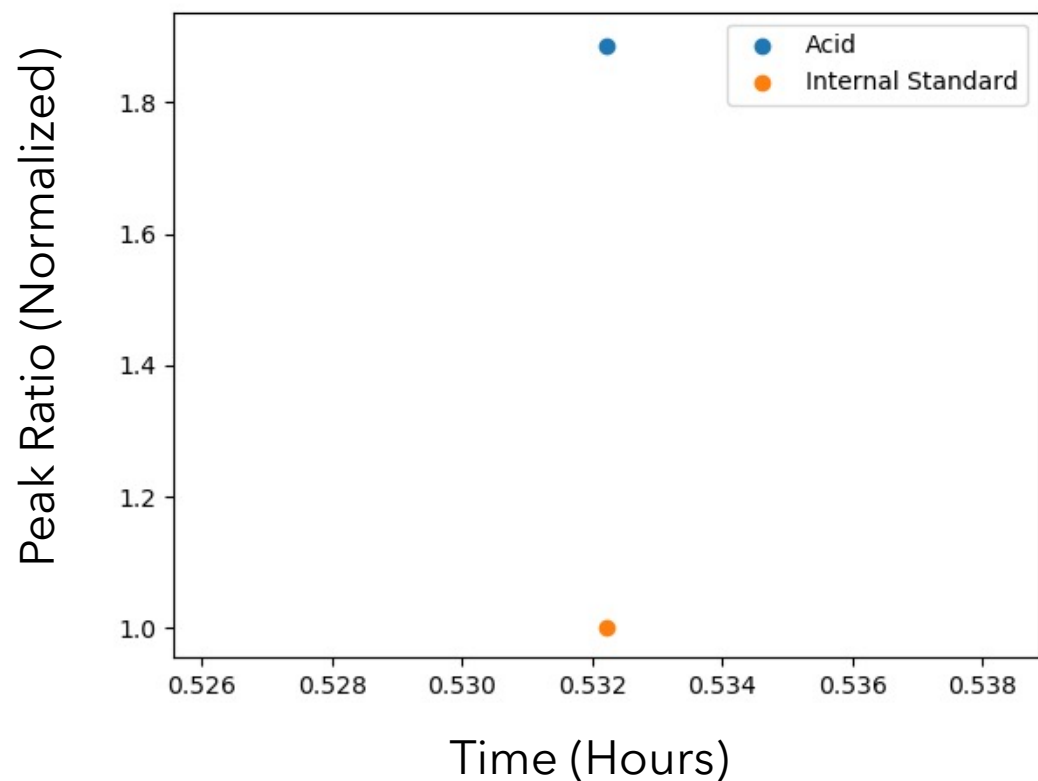


Acid Peak Tracking

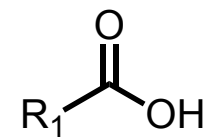


Retention Time (min)

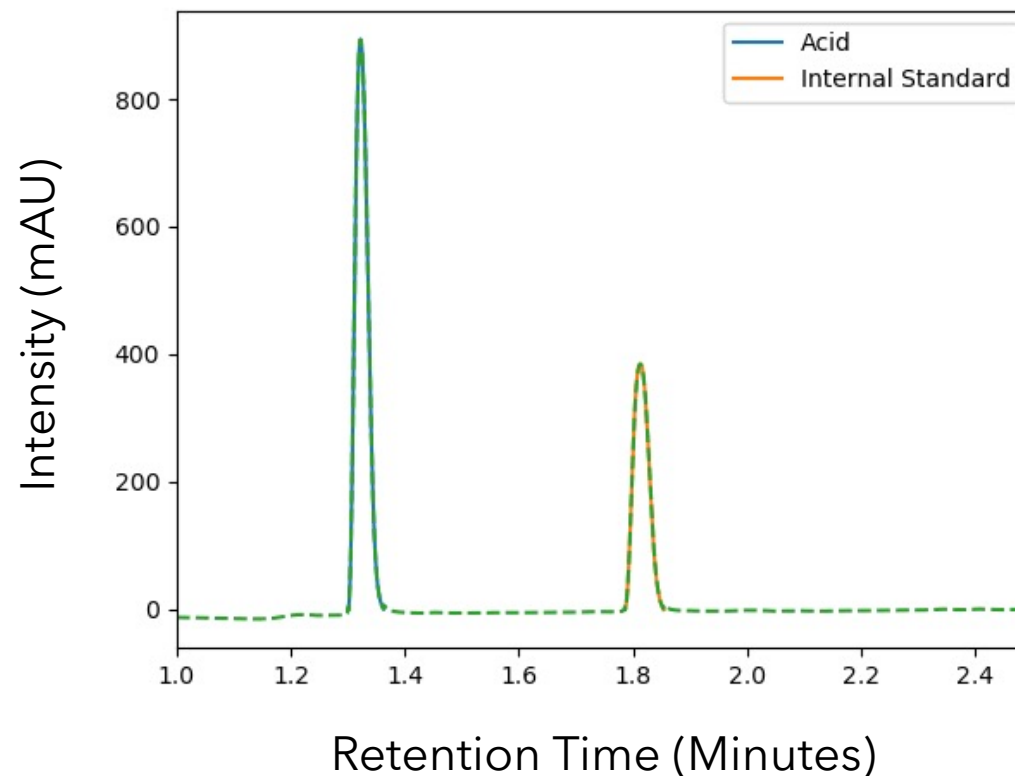
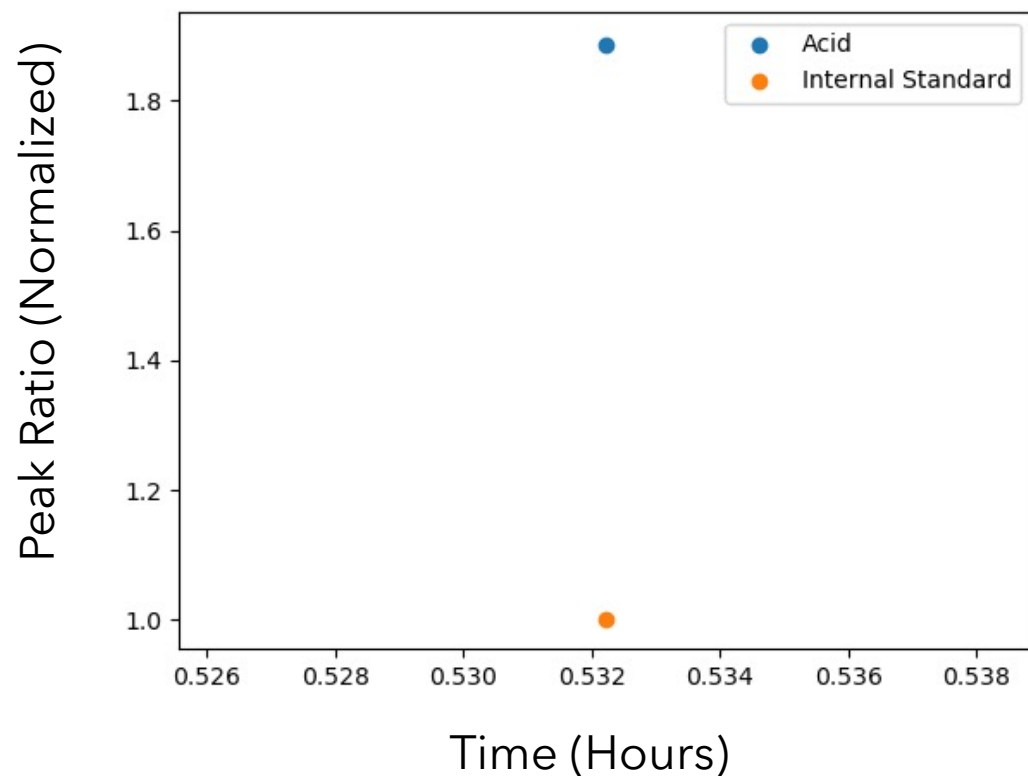
Reaction Progress and Data Output



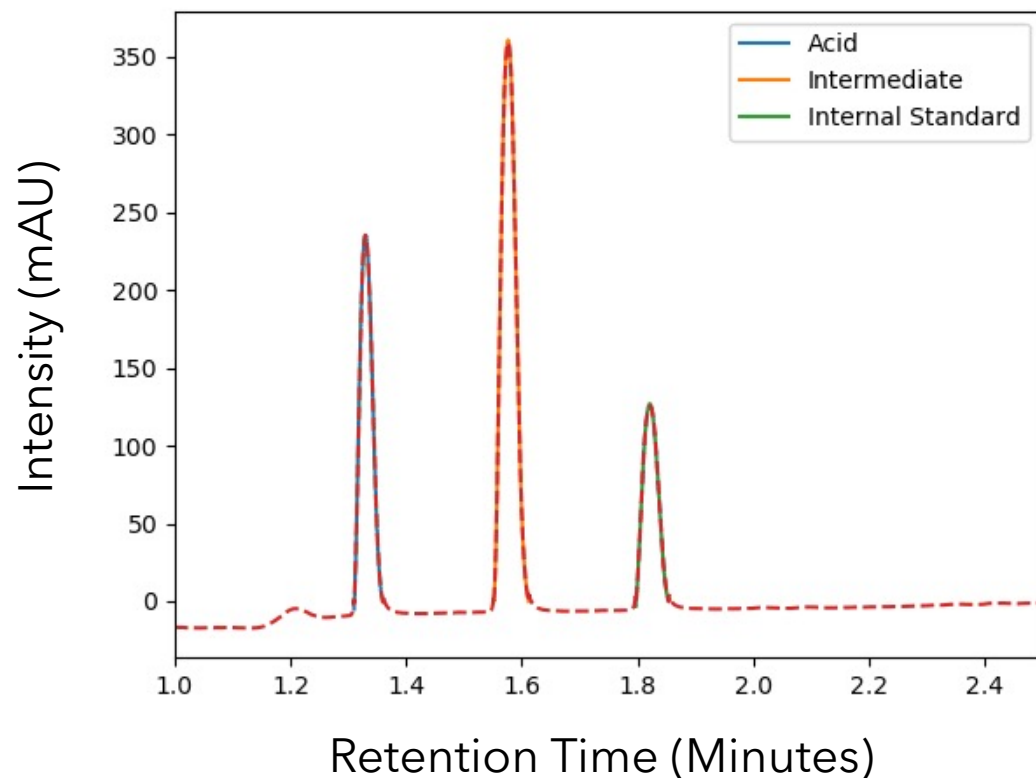
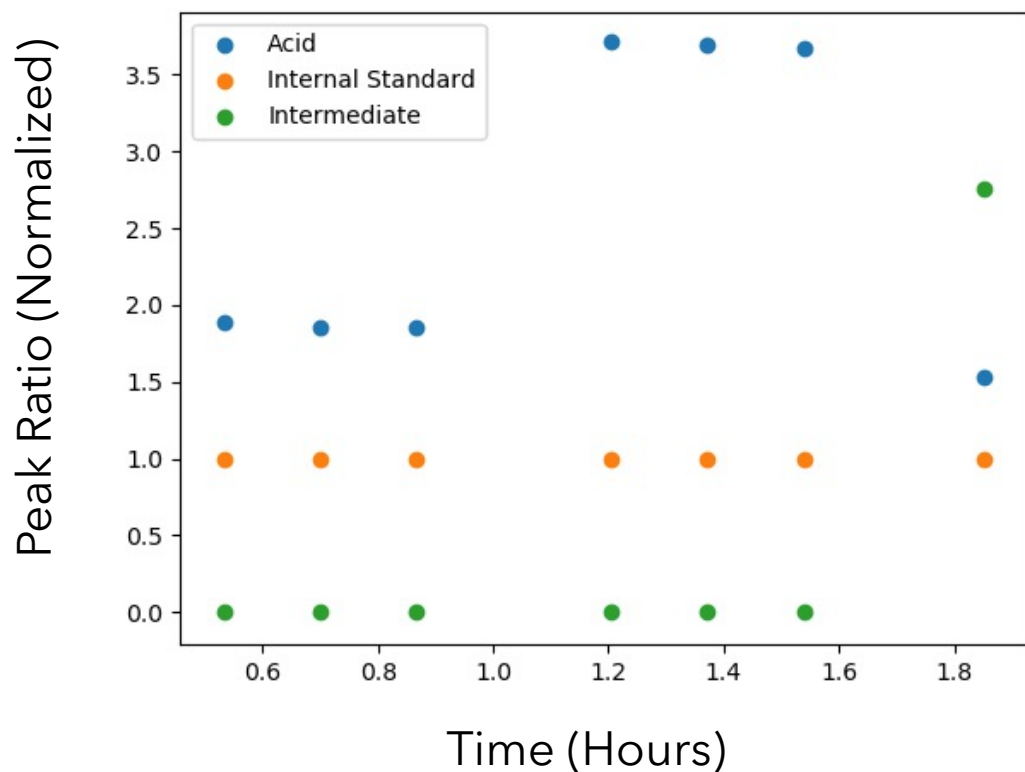
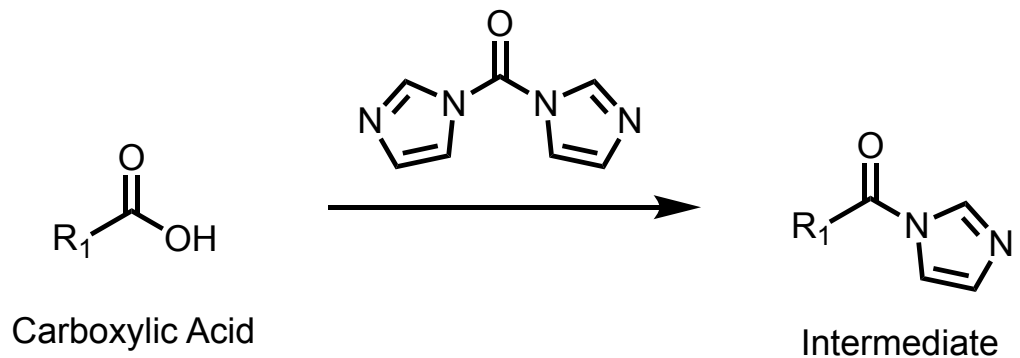
1: Acid Addition



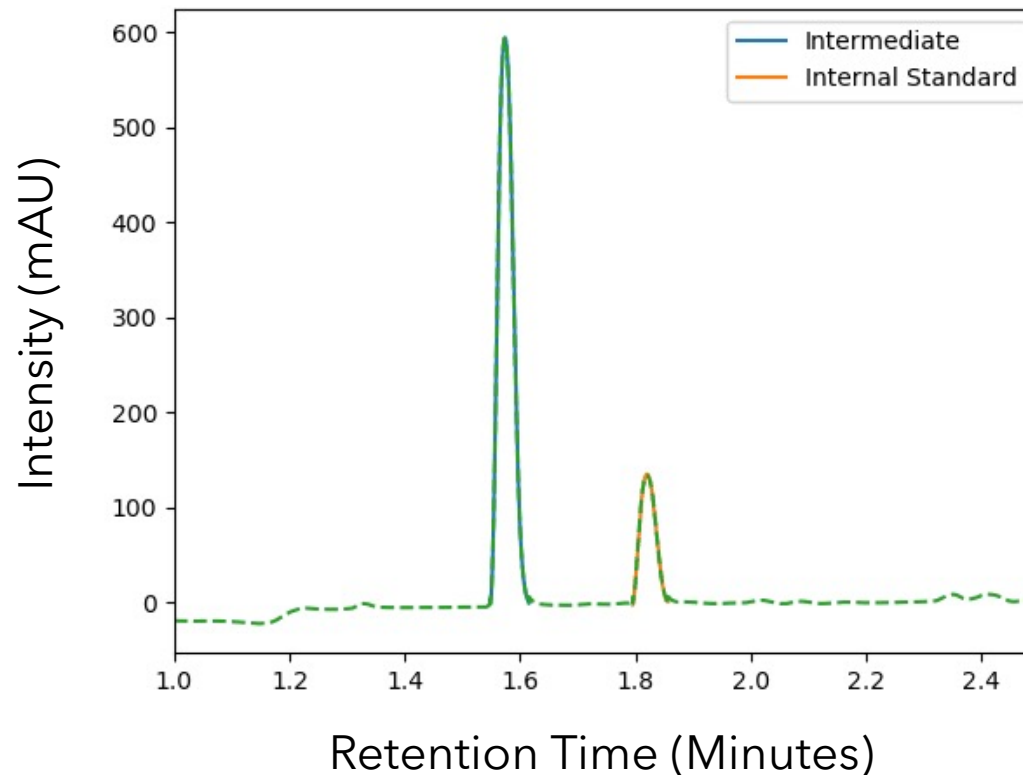
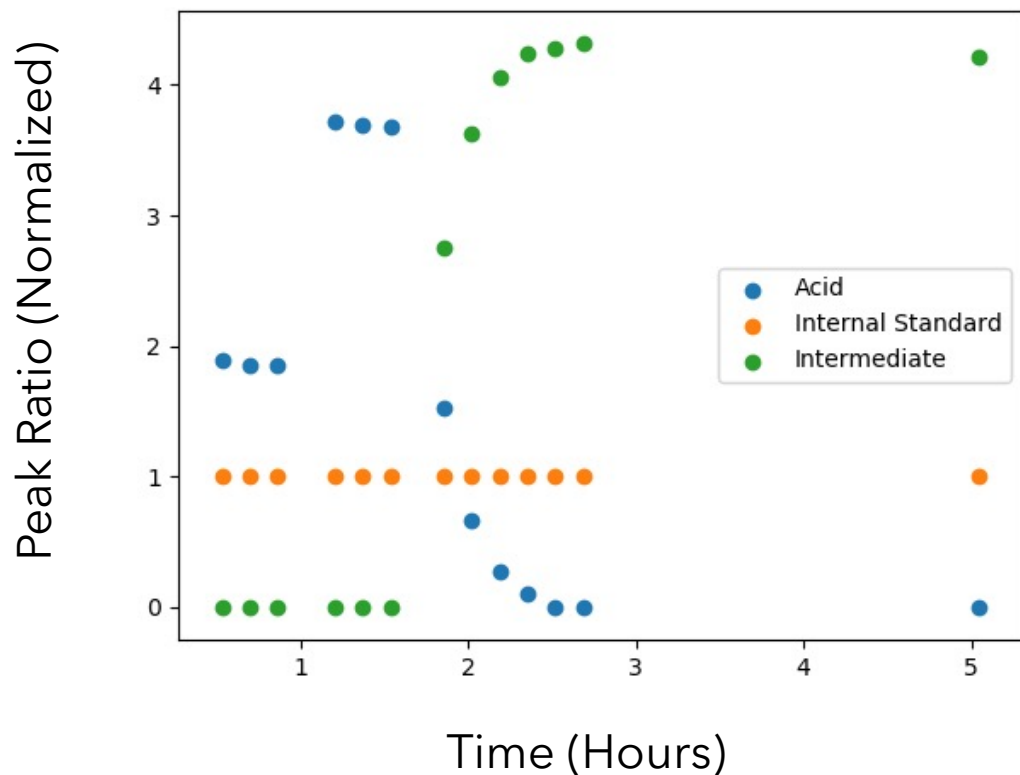
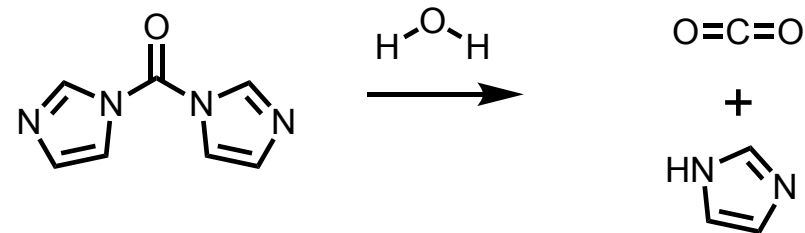
Carboxylic Acid



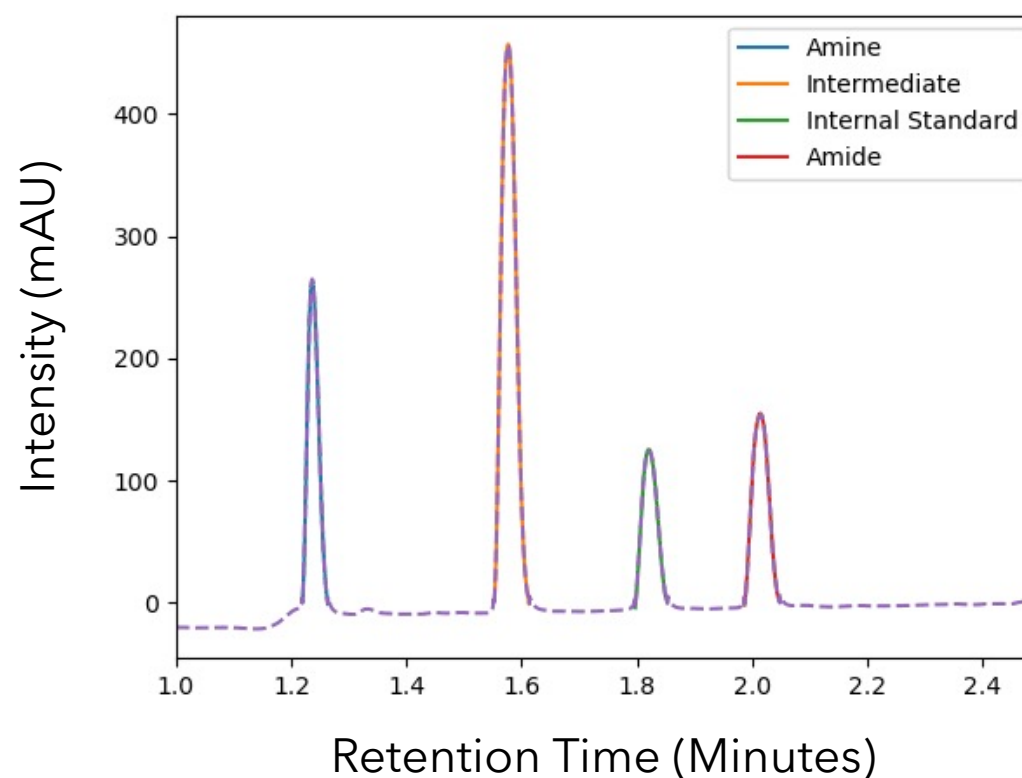
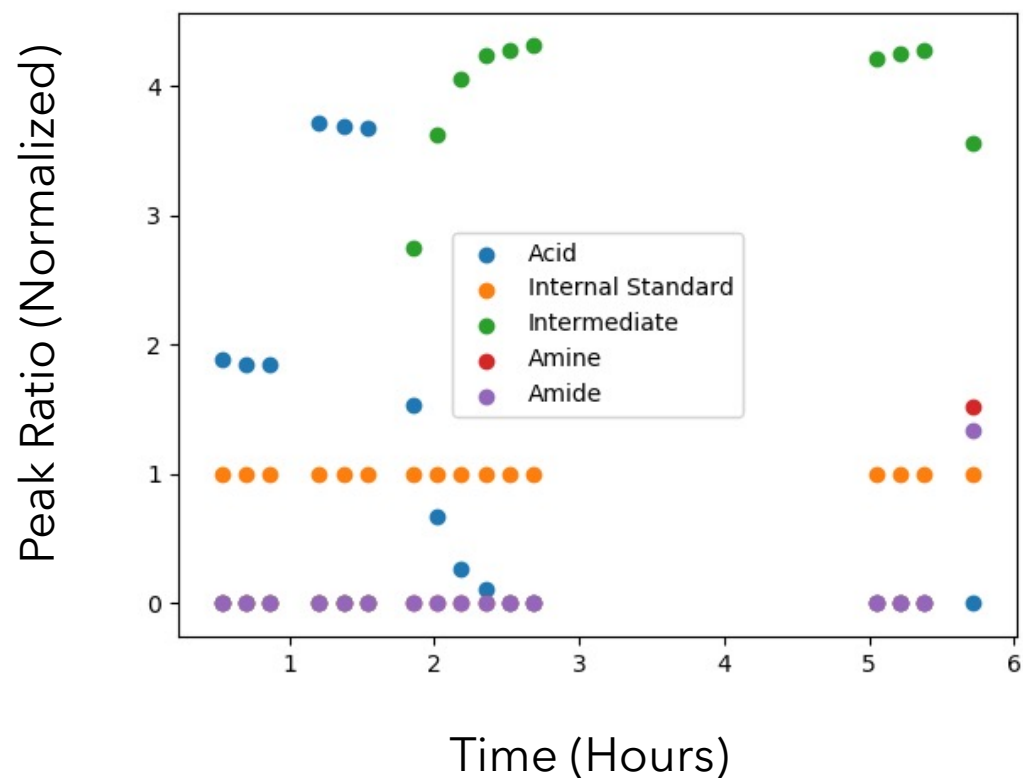
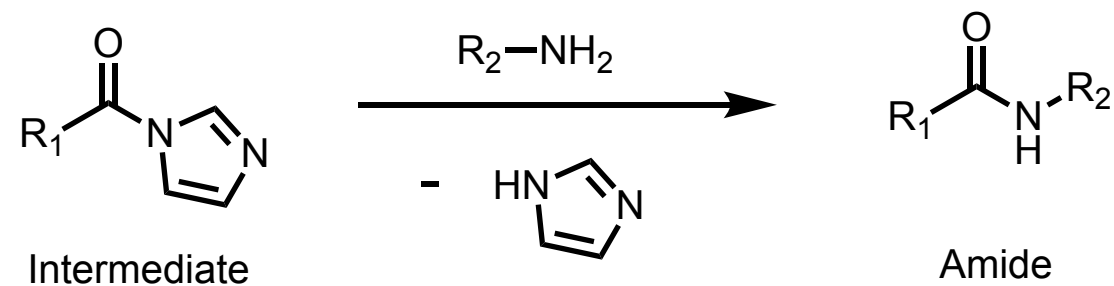
2. CDI Addition



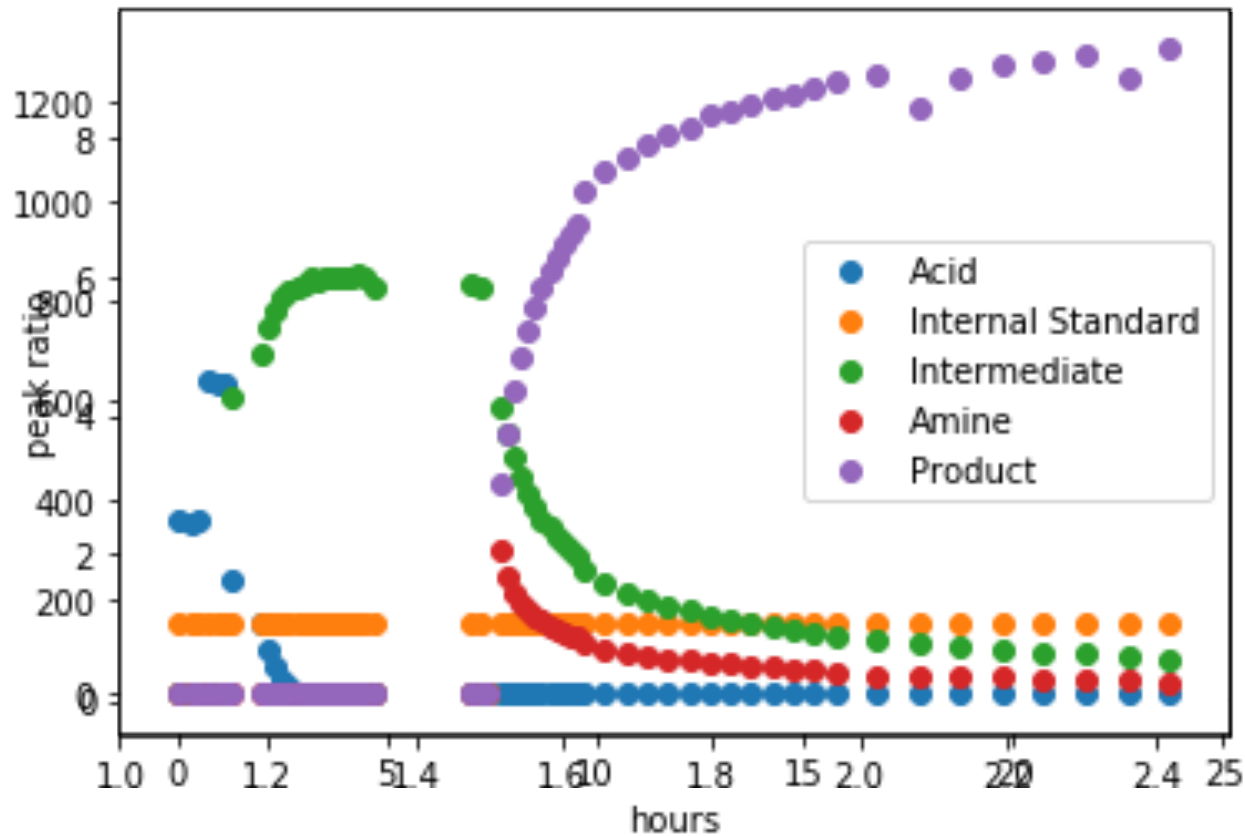
3. CDI Quenching



4. Amine Addition

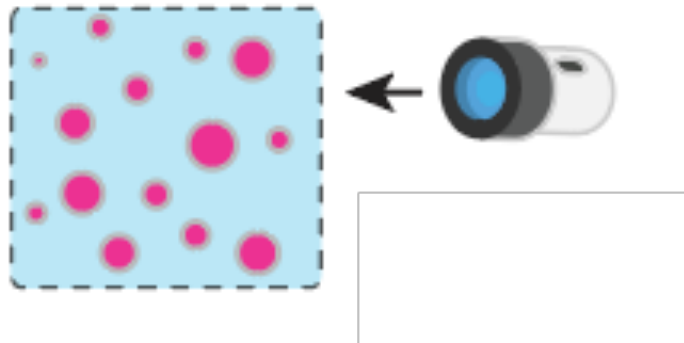


Limitations

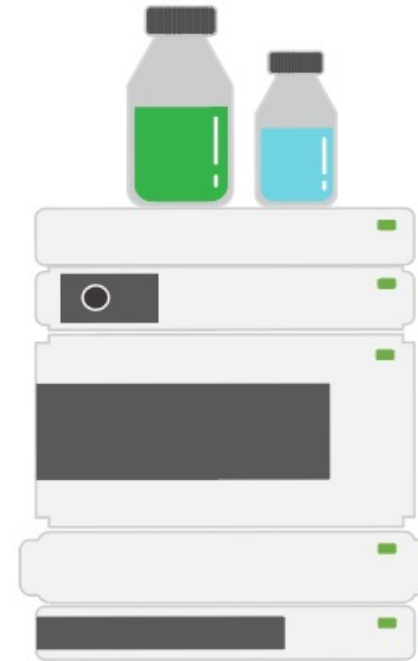


- Long computational time
- Requires clear peak separation
- Only applies in this specific experimental procedures

Conclusion

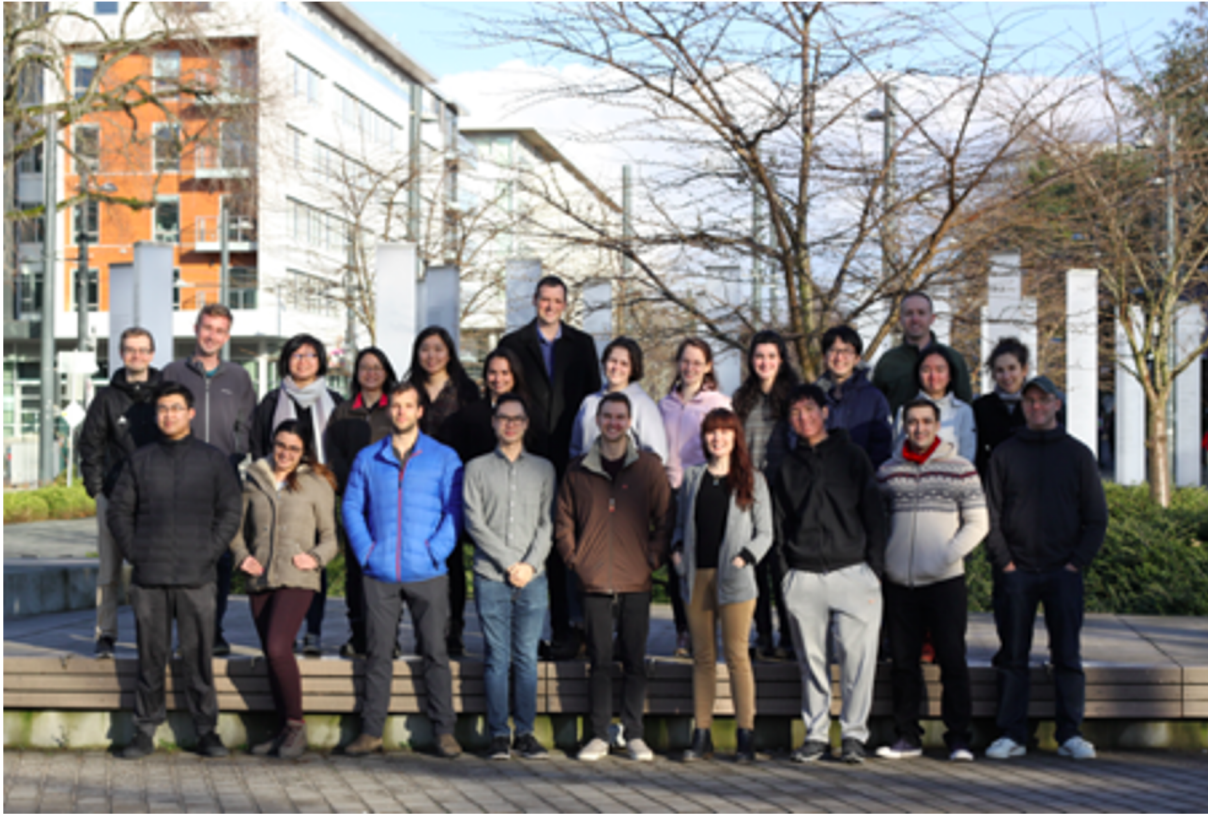


Qualitative Analysis
Solubility Tests via Computer Vision



Quantitative Analysis
Amide Bond Formation via HPLC

Acknowledgement



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