A lingua franca for robot chemists

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It is 2020 and synthetic chemistry is still laborious, time-consuming, and at times difficult to reproduce. Successful synthesis needs precision in execution and special care in communication, requirements that are hard to enforce when synthetic procedures are recorded and communicated in prose. Meanwhile, we and others have been building robot chemists that promise to relieve our manual burden, but each robot only understands its own esoteric language, meaning only the designers know how to talk to them. It is also not clear how to make a chemical program written for one robot work on another machine, or whether it would even work correctly once "translated". Because of this gap, advances in chemical robotics have yet to fulfil their potential and synthesis is far from truly automated.

This talk is about our work[1] to build a bridge between chemists, robots, and chemical synthesis, so that chemists can automate their syntheses (without having to learn programming) and run them on any robot. To this end, we had to create an abstraction of synthesis: we had to imagine the execution of a procedure but without the details specific to a human performing the steps (see Figure 1). We then created a language that could capture these abstract actions with enough detail to make them executable but not so much that it would tie the execution to any particular hardware system. At the same time, we created a translator that could convert literature procedures to our new language. By doing this, we steered the design of our language to cover the common scenarios encountered in practical synthesis. Finally, we created a visual environment that lets chemist express and manipulate synthetic actions using English sentences; describe their robot using a graph; and compile their procedure to hardware instructions that will run their synthesis on the robot. We experimentally validated our approach by converting the literature synthesis of 12 molecules into chemical code, which we successfully executed on our robot to give the product.

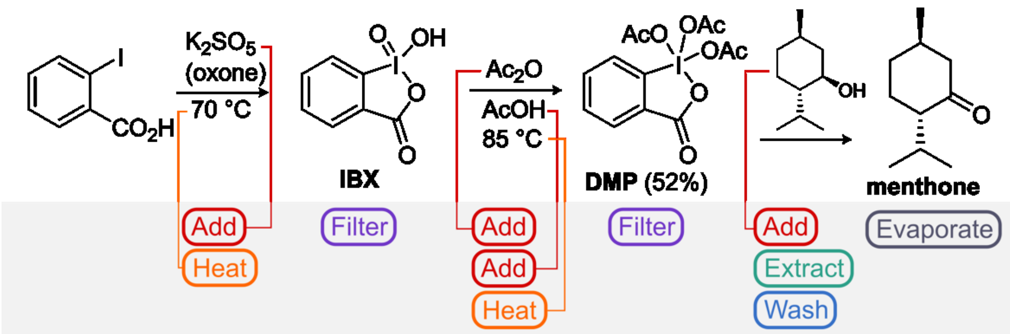

Figure 1. Schematic representation of actions involved in the literature synthesis of the Dess-Martin periodinane (DMP) and its use as an oxidizer to convert menthol to menthone. This synthesis, along with 11 others, was used for experimental validation of our system.

References:

[1] S. Hessam M. Mehr, Matthew Craven, Artem I. Leonov, Graham Keenan, and Leroy Cronin *Science* **2020** *in press*