# Automating chemical research: a step closer to a more experimental chemistry.

Research in chemistry is hard work. It requires diligence to carry and analyse hundreds of reactions. Research could be boosted if a chemist could define a chemistry of interest, and have a robotic platform to autonomously schedule carry out and analyse reactions. This will permit the chemist to run hundreds of reactions. The problem then becomes finding a method to analyse such vast data to come to new chemical conclusions. Borrowing machine learning tools, from our computer science friends, allows chemists to then fully automate inference too. This idea was applied to the area of imine organometallic supramolecular chemistry. Where the platform found X supramolecular structures in a search space of 720 reactions. Of which, one was taken for x-ray crystallography leading to the discovery of a novel supramolecular structure.

## Introduction

A big portion of chemistry is about experimentation. As the title suggests, the paper will focus on key ideas that allows a chemist to do so. Achieving a more experimental approach to chemistry is made possible with tools developed by the robotics and machine learning domains.

When applied to chemistry they come hand in hand: robots carry out the labour-intensive experiments, and machine learning carries out inference. The advantage of robotics comes from their work ethic, as shown by the workflow developed by Dr.Burger et al. where a robotic platform carried out 688 experiments in the span of 8 days1. The advantage of ML comes from their ability to analyse huge amounts of data and to come to conclusions often unintuitive to the chemist2.

If it is possible to define a chemistry, the robotic platform could run the experiments and analysis for the chemist. Chemistry then becomes more experimental – reagents just need to be typed in and the workflow does the rest.

The chemistry used as a proof of concept is supramolecular chemistry, imine-based metal organic complexes to be more specific. The simplicity, low temperatures, reversibility, and combinatorial accessibility of a reaction makes it easy to work with in a robotic platform. Additionally, due to supramolecular chemistry’s complexity, arising from its dynamic nature, it remains an unexplored field. A perfect opportunity to be exploited by machine learning (ML) systems, and a true challenge for reactivity prediction2,3. Lastly, the importance of supramolecular chemistry comes from its ability to form recognition and reaction networks4 Therefore utilizing this workflow to gaining a deeper understanding of supramolecular chemistry will help speed up discovery of such new materials.

Not only does the workflow developed in this paper add chemical understanding, it also helps tackle the main issue with current digital chemistry: bias and a lack of data2,5. The data of the reactions and their analysis can be found *section1* and bias is partially mitigated by the paper’s formal definition of chemistry. Unfortunately, in the workflow bias is not fully eliminated, and is further discussed in *section2*.

## Chemistry and workflow Description

‘Chemistry’ in this paper is defined by combinations, where each object in a class is combined with all other objects on a class basis (see figure x). When applied to chemistry, classes are groups of chemicals that exhibit similar reactivities, such as functional groups. This paper uses diamines, monoaldehydes and transition metals as classes (see figure x). On the other hand, objects are specific reagents. This paper uses 10 different diamines, 12 different monoaldehydes, and 5 different transition metals (of which silver was considered to have coordination numbers of 4 and 6) for a total of 720 combinations (see figure x). With the addition of reaction parameters (such as reagent concentrations, transfer volumes, reaction temperature, heating duration) combinations are turned to reactions (see figure x).

Defining chemistry in such a way comes with the following advantages:  
the addition of the ketene

#have a section describing the chemist time vs reaction time (i.e. robotic platform v human chemist time)

## References

Workflow setup and explanation:

Data analysis:

Conclusions:

Here is a problem. Here why its interesting. (this is the hook).

Structure: Title

Abstract:

* State the problem
* Say why its an interesting problem
* Say what your solution achieves
* Say what follows from your solutions

Introduction (here is why you’d want to read this paper):

* Say what the problem is
  + Give example don’t be to ambitious
* Say what your contributions are
  + Add some form of refuitability (i.e. what are the failures that you might have come across)
  + Add structure of the essay in an interesting way
  + Minimise related work (add only when it makes sense in that narrative)
  + Its got to be intuitive

The problem:

My idea:

The details:

Related work:

Conclusions and further work: