Combining Robotics and Artificial Intelligence for Search & Discovery in Chemical Space

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What constitutes a new discovery in chemistry and how does a synthetic chemist set out to make a discovery? Whilst it is possible to design experiments to explore and extend the properties of a given chemical system, the discovery of new reactions, phenomenon, and properties representing entirely new knowledge is a harder problem. If the experimental outcomes are not predictable using the current rules of science, then I suggest they are unexpected and so not merely new but also novel. However, this classification requires an expert and access to all current chemical knowledge to avoid the lack of information being considered as unpredictable. In this talk I will describe how searching chemical space using automation and algorithmic approaches improves the probability of discovery where the former enables performing routine tasks in the chemical laboratory faster and more consistently and the latter utilizes algorithmic searching as well as databases of current chemical knowledge. However, this talk is not about fast automation, but more deeply about how we can find new knowledge beyond the bias of the observer, see Fig. 1.

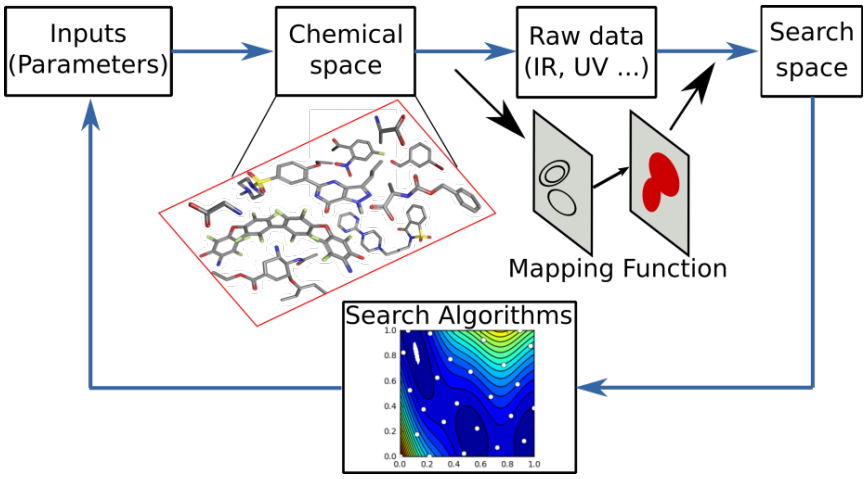

Figure 1 – A framework for searching chemical space. The schematic shows how the input parameters constrain chemical space to a limited section which in turn defines a search space using a mapping function. Feedback from measurements can then be used by the algorithm to assess the outcome of the reaction for use in the search algorithm.

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