# 3D REAGENT LIBRARIES AND THE AUTOMATED SYNTHESIS LAB

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**Abstract**: Eli Lilly has developed the Automated Synthesis Lab (ASL) [1]- an automation platform which allows reaction schemes to be devised and executed remotely from a user's PC anywhere in the world. In parallel to this the Proximal Lilly Collection[2] has been developed to categorize available reagents internally and externally into classes which are appropriate to the most common reaction types, and enumerate and make searchable these virtual libraries, which are then synthesizable in one or two steps on the ASL. [3]

We present work to convert these reagent libraries into 3D representations (Cresset, MOE) and exemplify their use in sidechain replacement and fragment elaboration. The conversion into 3D enables their use to be informed by ligand and protein structural information, and we will describe prospective examples where novel isosteres were found as well as a validation experiment where the performance of the computational method is assessed.

We will also describe how the ASL is accessible to external collaborators via the Open Innovation in Drug Discovery platform.

## References

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