

AUGMENTED DESIGN USING REACTION VECTORS

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Abstract:

Given that the organic chemist's transform compendium increases year by year how can we couple those advances in synthetic chemistry with the desire for novelty and excellence in small molecule drug design? Molecular design tools will often use a subset of reactions or a cut down set of medchem transforms which rarely take advantage of the full breadth of synthetic transformations and reagents available. With access to a full suite of synthetic chemistry options how can we answer the question –What should I make next? This talk will describe how we can use Chemistry ELNs and reaction databases for *in-situ* fragment growth and compound design using the reaction vector approach. It will highlight some of the options and issues associated with multi-objective optimisation and scoring of designs from fragments and will introduce the use of reaction pathways and reaction networks that aim to overcome such issues. Alongside several examples the opensource application framework will be discussed.