This whitepaper describing Nova's technology has not yet been published.

## Abstract

Using *in silico* predictive models and multi-parameter optimisation techniques allows large numbers of compounds to be quickly assessed with respect to a profile of properties required for a successful compound in a drug discovery project. With these predictive methods, it becomes possible to consider a large number of ideas for potential compounds that can be easily created and entered into a computer by an individual. In this article we describe a method that automatically generates chemically relevant compound ideas from an initial molecule, based on medicinal chemistry 'transformation rules' taken from examples in the literature. These are then prioritised using *in silico* models and a probabilistic scoring algorithm to identify the compound ideas most likely to satisfy a user-defined profile of required properties. Embedded in an intuitive, visual user interface, this approach provides a powerful means to explore potential chemistry to identify high quality leads or to improve properties in lead optimisation. We demonstrate that the set of 206 transformations employed is generally applicable, produces a wide range of new compounds and is representative of the types of modifications previously made to move from lead-like to drug-like compounds. Furthermore, we show that more than 94% of the compounds generated by transformation of typical drug-like molecules are acceptable to experienced medicinal chemists. Finally, we illustrate an application of our approach to the lead that ultimately led to the discovery of Duloxetine, a marketed serotonin reuptake inhibitor. Our analysis results in the identification of a diverse range of high scoring compounds, including Duloxetine itself.

You can download a preprint here.