

Automatic Generation of New Compound Ideas

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Wednesday, 16 October 2013 20:50 - Last Updated Thursday, 11 January 2018 16:02

The objective in this tutorial is to evolve the chemistry around three lead compounds which have good ADME properties but which have insufficient inhibition of the target, the Serotonin transporter. Using Nova and Probabilistic Scoring we look at how we can generate new ideas for compounds to improve the potency while maintaining the balance of other properties.

To try this example yourself, please visit the [Tutorials](#) section of the Community. If you don't have access to StarDrop or the optional modules and would like to arrange a free trial license, please email us at

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