Multi-Parameter Optimisation of 3D SAR

Written by Edmund Champness Wednesday, 16 October 2013 21:02 - Last Updated Thursday, 11 January 2018 16:04

In this example we will explore the multi-parameter optimisation of a series of CDK2 inhibitors, combining a 3D insight into the structure-activity-relationship (SAR) gained from StarDrop's torch3D™ module and predictions of ADME and physicochemical properties, using StarDrop's unique Probabilistic Scoring approach.

To try this example yourself, please visit the <u>Tutorials</u> 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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