

## Guided Multi-Parameter Optimisation of 2D and 3D SAR

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Wednesday, 22 June 2016 08:56 - Last Updated Monday, 18 June 2018 20:42

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This example uses a combination of 2D and 3D methods to understand and optimise a virtual library of Heat Shock Protein 90 (HSP90) inhibitors. The library, created by a de novo design process, is based around an amide substitution on a beta resorcylic acid core. The objective in this example is to use the SeeSAR™ module to develop an understanding of the 3D structure-activity relationships (SAR) and then use multi-parameter optimisation to further develop the absorption, distribution, metabolism and excretion (ADME) and physicochemical properties of a potent inhibitor without losing efficacy.

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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