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
Email address protected by JavaScript.
Please enable JavaScript to view email address.

To hear the narration, please increase your speaker volume.