In this example we will illustrate how knowledge-based predictions of toxicity can be used within a MPO environment to guide the selection and design of compounds with a good balance of properties and reduced risk of toxicity. We will explore a library of compounds with COX2 inhibition data, with the goal of identifying a high quality lead series, using StarDrop's Probabilistic Scoring to integrate experimental data, predicted ADME properties from the ADME QSAR module and predictions of toxicity risk from the Derek Nexus module.

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.
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To hear the narration, please increase your speaker volume.