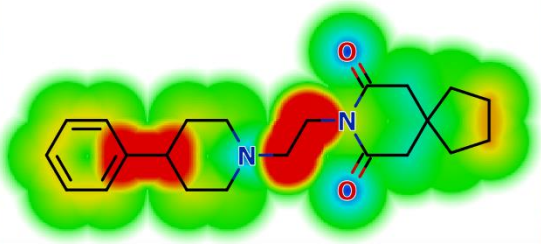
Optibrium and BITEKCHEMS present an interactive workshop:

Innovative Lead Optimization and Candidate Selection by *in Silico* Synthesis and ADMET Prediction



Agenda

Day 1

10:00 Opening of workshop and welcome

Introduction

10:05 The Importance of ADMET in Drug Discovery: Experimental and Predictive Methods

11:00 Introduction to Multi-Parameter Optimization – Prioritizing Compounds with a Balance of Properties

12:00 Lunch

Hands-On Workshop

13:00 Introduction to StarDrop – Getting started

14:45 Applying Probabilistic Scoring for Multi-Parameter Optimization

15:30 Coffee break

15:45 Exploring Chemical Space to Balance Quality and Diversity

16:30 Interactive Design and the Glowing Molecule™

17:00 Close of Day 1

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Day 2

9:00 Introduction to novel *in silico* lead optimization strategy

Hands-On Workshop

9:30 Building a QSAR model of target activity

10:15 Coffee Break

10:30 Introduction to P450 Metabolism

Hands-On Workshop

11:00 Predicting Metabolism by Cytochrome P450 to Guide Optimization of Metabolic Stability

11:30 Automatic Generation of Compound Ideas to Guide Optimization

12:00 Lunch

Hands-On Workshop

13:00 Applying Matched Series Analysis to Improve Target Activity

13:45 Applying Medicinal Chemistry Transformation Rules to Guide Optimization

14:30 Prioritizing compounds by a combination of potency (IC_{50}), *in vitro* CL prediction, and ADME properties by building predictive models

15:30 Thanks and close of workshop