Bridging the gap between the latest technology advancements and pharmaceutical research

The Rational Solid Form Design and Development Summit hopes to facilitate conversations between trailblazing researchers and industry players in the field of rational drug design and development and bridge the gap between newly available technologies and pharmaceutical research. The summit also offers insights on data strategy, IT security, and patent strategies relevant to implementing new technologies into existing R&D workflows to help pharmaceutical key decision-makers prepare for the future R&D and mitigate new challenges.

Conference Highlights

1. Focus on in silico technologies ready to be implemented into existing process and pipeline

2. High profile speakers presenting on state-of-the-art developments in the fields of molecular simulation, AI drug development, solid-state development, and computer-aided drug design

3. New insights and case studies on adopting cutting-edge technologies and their implications for the future of R&D

4. IP and data strategies to prepare pharmaceutical companies for the future of cloud computing and AI applications
Workshop Overview

Given the complexity of the pharmaceutical solid-state landscape and challenges facing the pharmaceutical industry, an accelerated drug design process could greatly benefit from the guidance and insights provided by computational methods. During the RSFD workshop, the attendees will learn about the state-of-the-art computational solid form screening and designing solutions developed by XtalPi that are cloud-based and AI-powered. With a mixture of discussions, lectures, and activities, the workshop offers real-life case studies to illustrate how such technologies can support the crucial steps related to solid state design of pharmaceuticals. This includes virtual polymorph screening and stable solid form selection, virtual design of solid form changes for drug properties improvement, and in silico screening of molecules for poor solubility improvement during lead optimization. Computational support is complemented by XtalPi’s internal experimental solid form screening capabilities.

Summit-at-a-glance

**October 20th, Sunday**
Pre-summit Workshop

**October 21th, Monday**
Stephen Kennedy Smith
Welcome address

**Session 1**
In silico solid state
Chair: Greg Beran
Ahmad Sheikhi
Director, Solid State, AbbVie
Solid-State Chemistry from Lead Optimization to Product Launch with Evolving Paradigms and Modalities

Bruno Hancock
Global Head of Materials Science, Pfizer
Predicting the Crystallization Propensity of Active Pharmaceutical Ingredients

Shawn Yin
Research Fellow, BMS
The API Form in Pharmaceutical Drug Product – Risks and Mitigation Strategies

Alfred Lee
Principal Scientist, Merck
Molecular Modeling Applications in Crystallization

Michael Lovette
Senior Scientist, Amgen
Solubility in the Age of a Data Lake

**October 22th, Tuesday**

**Session 2**
Advancing CSP
Chair: TBD
Michael Shirts
Associate Professor, UC Boulder
Entropy and Conformational Heterogeneity in Molecular Solids

Alexandre Tkatchenko
Professor, University of Luxembourg
Reliable and Practical Computational Prediction of Molecular Crystal Polymorphs

Michael Bellucci
Director of Solid Form Design, XtalPi
Intelligent Cloud-Based Algorithms for Pharmaceutical Sciences

Greg Beran
Professor of Chemistry, UC Riverside
Restoring the Balance: Accurate Treatment of Intra- and Intermolecular Interactions in Conformational Polymorphs

Noa Marom
Assistant Professor, Carnegie Mellon University
Property-Based Genetic Algorithm Optimization of Molecular Crystals for High Carrier Mobility

**Session 3**
CSP industrial applications
Chair: Yuriy Abramov
Geoff Wood
Senior Principal Scientist, Pfizer
Going Beyond Lattice Energy Approximations in Solid Form Selection

Sten Nilson
Associate Principal Scientist, AstraZeneca
A Smorgasbord of Predictive and Analysis Tools for Crystal Structure

Susan Reutzel-Edens
Senior Research Advisor, Lily
Inconvenient Truths about Solid Form Landscapes

Jane Li
Vice President of Material Science, Pharmanova
A Case Study of Successful Polymorph Prediction of a Salt Form

Moderator, Alexandre Tkatchenko
CSP Panel Discussion

Dongyue Xin
Senior Scientist, Boehringer Ingelheim
A Machine Learning Approach for Pharmaceutical Solvent Prediction

Lipeng Lai
Co-Founder, XtalPi
Discover the Ultimate Solution in the Dark Space: How Can AI Help Us

Alex Tropsha
Professor and Associate Dean, UNC Chapel Hill
Prediction of Physical Properties and Safety of Chemicals and Materials: Methods and Applications

Oles Isayev
Assistant Professor, Carnegie Mellon University
Restoring the Balance: Accurate Treatment of Intra- and Intermolecular Interactions in Conformational Polymorphs

Eyal Barash
Pharmaceutical Patent Attorney, Barash Law LLC
Using AI in Solid-Form Patent Strategies – Challenges and Opportunities

Yuriy Abramov
Concluding Remarks

**Session 4**
AI and Machine Learning
Chair: TBD

2019
Rational Solid Form Design Summit