

# MOE Forum 2020

Drug Modalities

Developability

Workflow FMO

AI SBDD

Medicinal Chemist

Antibody PROTAC

HLA / Antigenic Peptide

**Webinar with Zoom  
Japanese–English Simultaneous  
Interpretation Available**



Date: Thursday, September 3<sup>rd</sup> – Friday, September 4<sup>th</sup>, 2020

Registration Fee: Free

Audience: Researchers in Drug Discovery and Life Science Field

## The Latest Development and Application of MOE, an Optimal Molecular Operating Environment for Drug Discovery and Life Science

In the MOE Forum, MOE developers introduce the latest basic research in the computational chemistry field.

Lecturers active at the forefront of drug discovery and life science research present their latest knowledge obtained with MOE.

This year, it will be held online with ZOOM on Thursday, September 3<sup>rd</sup> and Friday through September 4<sup>th</sup>. Details will be provided on our [web page](#). Please feel free to join us.

### MOE Updates

**MOEsaic: Guiding Multi-Parameter Optimization in Ligand-Based Design**  
Fred Parsons, Chemical Computing Group ULC

**Developability Assessment and Property Prediction by pH-Dependent Conformational Sampling**  
David Thompson, Chemical Computing Group ULC

**MOE 2020 Release Overview**  
Matthias Keil, Chemical Computing Group ULC

### MOE & PSILO Technical Information

**Development of Tools to Build Model and Predict Antigenic Peptide for HLA**

**In Silico Modeling Tools for PROTAC-Mediated Ternary Complexes**

**Introduction to MOE Antibody Design Application**

**Introduction to PSILO**

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### Online events by Zoom

In-house, on-campus, home, etc.  
You can join anywhere you like.

**Simultaneous Japanese–English interpretation is available**

You can listen to the lecture in the language of your choice.

### Invited Lectures

**Research on pocket prediction using 3D-CNN**

Takeshi Baba, Toray Industries, Inc.

**Semi-automation of in silico analysis using MOE and KNIME**

Akitoshi Okada, Japan Tobacco Inc.

**Quantum Structural Life Science by Combining FMO and Structural Biology**  
Kaori Fukuzawa, Hoshi University

**Considering what's the literacy to extract useful information for drug discovery from amino acid sequence = In order to use MOE more effectively=**

Hiroki Shirai, Astellas Pharma Inc.

**My experience with structure-based ligand design (SBDD)**

Qian Liu, Sichuan Kelun Pharmaceutical Co., Ltd.

### Virtual Booth

**Demonstration of the New Versions of MOE & PSILO**

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\* The content of the lecture and the speaker are subject to change without prior notice.

For more information: [https://www.molsis.co.jp/seminar/moe\\_forum2020\\_en/](https://www.molsis.co.jp/seminar/moe_forum2020_en/)  
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