



GastroPlus®



ADMET Predictor®

Application-Based Virtual Workshop: Drug Discovery "Drug Design ... Meet PBPK"

October 3rd - November 4th, 2022

Workshop Overview

In silico approaches can drive drug discovery by speeding up the process, improving compound quality, and reducing *in vitro/in vivo* testing. This Next-Gen Discovery Workshop will show you how to combine machine learning and PBPK modeling seamlessly to support lead optimization and candidate selection tasks in innovative ways! This workshop is geared towards computational/medicinal chemists and DMPK scientists.

Pre-requisite: Completion of a GastroPlus® Introductory Workshop within the past 3 years – OR – confirmation that participant is proficient in the following:

- Database and support file structure
- Understanding and implementing inputs for physicochemical and pharmacokinetic parameters
- Running basic GastroPlus simulations
- Understanding and implementing physiology options for human and animal simulations (ACAT™ and PBPK)
- General concepts with respect to:
 - o Processes that govern absorption
 - o Processes that govern distribution and elimination of compounds (including metabolism and/or transporter effects)

Note: This workshop will run over 5 weeks. During these 5 weeks attendees can expect a total time commitment of 15 to 20 hours engaging in on-demand content, live virtual sessions, hands-on applications, and implementation of concepts in a "real world" group exercise. Background on the general capabilities of ADMET Predictor can be found via online tutorial videos: <https://www.youtube.com/playlist?list=PLQuCii74Pfd2vZ2SugsWbWHSnWPdK7yo>

Learning Objectives

At workshop completion, you should be able to:

- Rank order compounds correctly based on PK and/or dose
- Communicate results cross-functionally to help move compounds from discovery into the pre-clinical/clinical stages



Register online! simulations-plus.com/register-training-workshop

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Course Instruction

This workshop will be taught by Neil Miller (Vice President, Simulation Sciences), Becky Graves (Associate Director, Simulation Sciences), and Michael Lawless (Sr. Principal Applications Scientist).



Agenda

Week 1 (October 3rd – 7th): On-demand Lectures

Lectures will be available on-demand and accessible to view for the entire length of the workshop.

- Introduction to the Drug Discovery Process – Neil Miller
- Lead Candidate Selection: ADMET Predictor (including AI-Driven Drug Design [AIDD], DELTA Model) – Michael Lawless
- Linking HTPK to GastroPlus: A Bridge to Early Development – Becky Graves

Week 2 (October 10th – 14th): Live Session with Instructor

Participants will attend a 2-hour live session that will include an in-depth discussion with a hands-on exercise using AIDD, Q&A, and introduction to the group project.

Date/Time to be communicated to participants once all preferences are received.

Weeks 3 & 4 (October 17th – October 28th): Group Project

Participants will meet for a 2-hour live session with their group members to discuss the project. Key discussion points will be provided by instructors prior to the session.

Date/Time to be communicated to participants once all preferences are received.

Week 5 (October 31st – November 4th): Live Session with Instructor

Participants will meet for a 3-hour live session to discuss the project with instructors and the larger group.

Date/Time to be communicated to participants once all preferences are received.

Note: All attendees will be required to attend the live sessions and participate in the discussion in order to receive a Certificate of Completion. Certificate of Completion provided to participants approximately 2 weeks after the end of the workshop.



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Virtual Platform

Participants will virtually attend using their PCs with enabling of cameras and microphones *optional but encouraged*.

Technical Requirements

PCs equipped with internet access and Google Chrome with Flash 9+ plugins are required to participate.

Registration Details

Week 2: Live Session with Instructor Date Options (rank order 1-3):

Tuesday, October 11th
Wednesday, October 12th
Thursday, October 13th

Times for all dates are 07:00-09:00PT / 10:00-12:00ET / 16:00-18:00CET

Weeks 3 & 4: Group Project Date Options (choose one):

Monday, October 17th - 09:00-11:00PT / 12:00-14:00ET / 18:00-20:00CET
Thursday, October 20th - 00:00-02:00PT / 03:00-05:00ET / 9:00-11:00CET
Tuesday, October 25th - 09:00-11:00PT / 12:00-14:00ET / 18:00-20:00CET
Wednesday, October 26th - 06:00-08:00PT / 09:00-11:00ET / 15:00-17:00CET

Week 5: Live Session with Instructor Date Options (rank order 1-3):

Tuesday, November 1st
Wednesday, November 2nd
Thursday, November 3rd

Times for all dates are 07:00-09:00PT / 10:00-12:00ET / 16:00-18:00CET



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Virtual Workshop:

Application-Based Discovery Workshop

October 3rd – November 4th, 2022 – Register by September 14th, 2022

Title: Professor Dr. Mr. Mrs. Miss Ms. Industry
Academia

First name:

Last name: Company:

Job Title: Department:

Address:

Telephone: Email:

Purchase Order No. (if applicable):

Industry: \$2,500 USD
Academia: \$1,250 USD (2 academic slots available).
Coupon codes will be accepted.

*You must register with a valid .edu email address

Method of payment (Please check one)

- Payment by check (you will be invoiced upon receipt of your completed registration form)
- Payment online (you will be redirected to the payment portal when registering online at simulations-plus.com/register-training-workshop)

Terms and Conditions

Registration: The course is limited to 20 participants (no exceptions). An email confirming registration will be issued within 2 business days upon receipt of registration.

Cancellations: Cancellations with a refund minus 4% credit card fees may be made two weeks before course date. No refunds will be given for cancellations received after this date. Substitutions may be made at any time.

Payment Terms: Following completion and return of the registration form, the total fee must be paid within 30 days of receipt of invoice. All fees must be paid in full prior to the start of the workshop.