



## Activity details in response to the international MOU with Simulation Plus Inc., Lancaster, US (AY 2023-24)

Date: 04/03/2024

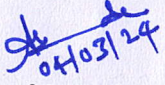
In response to the international MOU and software license agreement established in between faculty of Oriental college of Pharmacy and Simulation Plus Inc., Lancaster, US, a part of research-oriented lectures were conducted for M. Pharm (Pharmaceutics) Sem II students during the academic year 2023-24. These lectures were part of the subject "Computer-Aided Drug Development." The sessions focused on Unit IV, specifically covering computer-aided biopharmaceutical characterization and gastrointestinal absorption simulation using the cloud-access software GastroPlus.

The lectures provided a comprehensive introduction to GastroPlus, explaining its theoretical background and practical applications. Students learned about the fundamentals of computer-aided biopharmaceutical characterization. The gastrointestinal absorption simulation segment emphasized modelling techniques and the construction of predictive models for drug behaviour in the human body.

Through hands-on sessions with GastroPlus, students gained practical experience in simulating gastrointestinal absorption, enabling them to visualize and predict the biopharmaceutical properties of various drug compounds. These simulations helped illustrate the impact of physiological variables on drug absorption and overall bioavailability.

The initiative aimed to enhance the students' understanding of advanced drug development tools and methodologies, preparing them for future research and professional endeavours in pharmaceuticals. The collaboration with Simulation Plus Inc. provided access to state-of-the-art software, bridging the gap between theoretical knowledge and practical application.

### Activity Conducted by:

  
Dr. Amol Borade  
Assistant Professor  
Oriental college of Pharmacy, Sanpada,  
Navi Mumbai.



  
Principal

Dr. (Mrs.) Sudha Rathod  
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Plot No. 3, 4 & 5, Sector-2,  
Sanpada, Navi Mumbai.

### Enclosures:

1. Syllabus copy of subject Computer Aided Drug Development, M. Pharm. Sem II (Pharmaceutics branch)
2. Attendance sheet of students attended the lectures.



Enclosure 2: Syllabus copy of subject covered by using Gastroplus Simulation

## COMPUTER AIDED DRUG DEVELOPMENT

(MPH 203T)

### Scope

This course is designed to impart knowledge and skills necessary for computer Applications in pharmaceutical research and development who want to understand the application of computers across the entire drug research and development process. Basic theoretical discussions of the principles of more integrated and coherent use of computerized information (informatics) in the drug development process are provided to help the students to clarify the concepts.

### Objectives

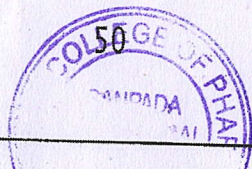
Upon completion of this course it is expected that students will be able to understand,

- History of Computers in Pharmaceutical Research and Development
- Computational Modeling of Drug Disposition
- Computers in Preclinical Development
- Optimization Techniques in Pharmaceutical Formulation
- Computers in Market Analysis
- Computers in Clinical Development
- Artificial Intelligence (AI) and Robotics
- Computational fluid dynamics(CFD)

### THEORY

60 Hrs

1. a. Computers in Pharmaceutical Research and Development: A General Overview: History of Computers in Pharmaceutical Research and Development. **Statistical modeling in Pharmaceutical research and development: Descriptive versus Mechanistic Modeling,** Statistical Parameters, Estimation, Confidence Regions, Nonlinearity at the Optimum, Sensitivity Analysis, Optimal Design, Population Modeling  
PHS (b. Quality-by-Design In Pharmaceutical Development: Introduction, ICH Q8 guideline, Regulatory and industry views on QbD, Scientifically based QbD - examples of application.)
2. Computational Modeling Of Drug Disposition: Introduction ,Modeling Techniques: Drug Absorption, Solubility, Intestinal Permeation, Drug Distribution ,Drug Excretion, Active Transport; P-gp, BCRP, Nucleoside Transporters, hPEPT1, ASBT, OCT, OATP, BBB-Choline Transporter. 12 Hrs



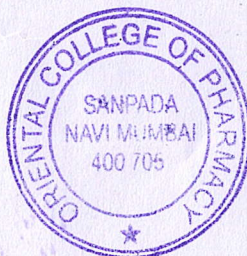
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- 3 (Computer-aided formulation development:: Concept of optimization, Optimization parameters, Factorial design, Optimization technology & Screening design. Computers in Pharmaceutical Formulation: Development of pharmaceutical emulsions, microemulsion) drug carriers Legal Protection of Innovative Uses of Computers in R&D; The Ethics of Computing in Pharmaceutical Research, Computers in Market analysis 12 Hrs
- 4 a. Computer-aided biopharmaceutical characterization: 12 Hrs  
 Gastrointestinal absorption simulation. Introduction, Theoretical background, Model construction, Parameter sensitivity analysis, Virtual trial, Fed vs. fasted state, In vitro dissolution and in vitro-in vivo correlation, Biowaiver considerations  
 b. Computer Simulations in Pharmacokinetics and Pharmacodynamics: Introduction, Computer Simulation: Whole Organism, Isolated Tissues, Organs, Cell, Proteins and Genes.  
 c. Computers in Clinical Development: Clinical Data Collection and Management, Regulation of Computer Systems
- 5 Artificial Intelligence (AI), Robotics and Computational fluid dynamics: General overview, Pharmaceutical Automation, Pharmaceutical applications, Advantages and Disadvantages. Current Challenges and Future Directions. 12 Hrs

#### REFERENCES

1. Computer Applications in Pharmaceutical Research and Development, Sean Ekins, 2006, John Wiley & Sons.
2. Computer-Aided Applications in Pharmaceutical Technology, 1<sup>st</sup> Edition, Jelena Djuris, Woodhead Publishing
3. Encyclopedia of Pharmaceutical Technology, Vol 13, James Swarbrick, James. G.Boylan, Marcel Dekker Inc, New York, 1996.

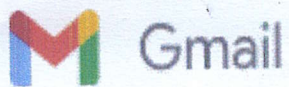


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Amol Borade &lt;amol.borade@ocp.edu.in&gt;

## Simulations Plus University+ Account

2 messages

Wed, Aug 2, 2023 at 1:38 AM

SLP Academic <slpacademic@simulations-plus.com>  
To: "amol.borade@ocp.edu.in" <amol.borade@ocp.edu.in>  
Cc: Jennifer Dilts <jennifer.dilts@simulations-plus.com>

Hi Amol,

Your account has been set up to access Simulations Plus software from our virtual cloud infrastructure until **8/1/2024**.

This access grants use of GastroPlus, ADMET Predictor, PKPlus, DDDPlus, & MembranePlus.

If you are using a Windows PC, you may download our cloud access installer from the following location:

<https://simplus-downloads.com/MB/CloudAccess.zip>

USER: **CloudAccess**

PASS: **SLP\_Access1!**

If you are using a Mac, you will need the Microsoft Remote Desktop application: [Microsoft Remote Desktop on the Mac App Store \(apple.com\)](https://www.apple.com/app-store/microsoft-remote-desktop/)

On a Mac you will need to enter this computer name when creating the connection: [cloud2.slp-access.com](https://cloud2.slp-access.com)

Under Gateway name, set the Gateway name as: [cloud2.slp-access.com](https://cloud2.slp-access.com)

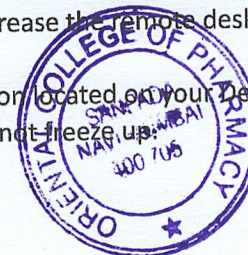
After you install the package, you may connect to the server with the following credentials:

User: **User00237**

Password: **ChangeMe\_PLZ!**

We recommend that you change your password (instructions attached). Instructions on how to exit "Demo mode" to get full functionality of GastroPlus, DDDPlus, and MembranePlus are also attached, as well as instructions on how to increase the remote desktop's resolution.

Please practice proper disconnecting procedures by double-clicking on the Log Off icon located on your Desktop rather than clicking on the X at the top of your session. This will ensure a fresh session every time so the programs you use do not freeze up.



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If the FlexNET License Finder appears, choose "License Server System", click "Next", then input 1.0.1 in the next window, and click "Next" then "Finish".

To ensure the privacy of your files, we strongly encourage users not to store their data on our servers. To move files from the remote desktop to your computer, simply cut them from where they are saved in the remote desktop (Ctrl+X) and paste them onto your computer (Ctrl+V).

Please let me know if you have any issues.

Thank you,

**Jennifer Dilts**

*Operations Specialist*

[jennifer.dilts@simulations-plus.com](mailto:jennifer.dilts@simulations-plus.com)

Simulations Plus, Inc. (NASDAQ: SLP)




42505 10th Street West, Lancaster, CA 93534

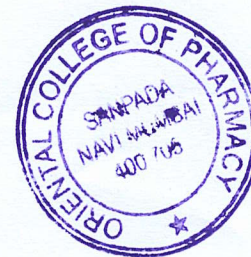
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**3 attachments**

-  **CHANGING YOUR PASSWORD ON THE SIMULATIONS PLUS CLOUD.PDF**  
145K
-  **How do I get out of Demo mode.pdf**  
78K
-  **How to Increase Virtual Computer Resolution.pdf**  
389K



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**Amol Borade** <amol.borade@ocp.edu.in>  
To: SLP Academic <slpacademic@simulations-plus.com>

Wed, Aug 2, 2023 at 10:31 PM