

## Drug Discovery and Medicinal Chemistry

### Short Course Outline

	TOPIC	Description
1	Overview, Orientation of students.	<ul style="list-style-type: none"> <li>◆ Course outline, delivery mode, staff introduction, scope of training, Pre-test.</li> </ul>
2	Drug Discovery Process	<ul style="list-style-type: none"> <li>◆ Selecting a disease, pre-clinical research, clinical trials &amp; approval</li> <li>◆ Drug costs &amp; failure, intellectual property, module review</li> </ul>
3	Drug Targets	<ul style="list-style-type: none"> <li>◆ Protein structure, enzymes &amp; inhibitors, receptors &amp; ligands, potency &amp; binding, efficacy, Module review</li> </ul>
4	Drug Metabolism and Pharmacokinetics	<ul style="list-style-type: none"> <li>◆ Therapeutic window &amp; ADME, exposure &amp; bioavailability,</li> <li>◆ Metabolic reactions, clearance &amp; distribution, controlling CL &amp; Vd, Module review.</li> </ul>
5	Lead Discovery and Optimisation	<ul style="list-style-type: none"> <li>◆ Finding hits, lead selection, structure-activity relationships,</li> <li>◆ ADME optimization, Toxicity, Module review</li> </ul>
6	Case Studies from Literature	<ul style="list-style-type: none"> <li>◆ Case study 1, Case study 2</li> </ul>

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7	Special topic 1:  Structure-guided Drug Design (SGDD)	<ul style="list-style-type: none"> <li>◆ Overview of Structure-guided drug design</li> <li>◆ Application of SGDD in hit identification, maturation and lead optimization.</li> <li>◆ SGDD Workflows and examples</li> <li>◆ SGDD Tools and Methods.</li> </ul>
8	Special Topic 2:  Computation and Artificial Intelligence in Drug Discovery	<ul style="list-style-type: none"> <li>◆ General Evolution of Computer Technology and Usage</li> <li>◆ Scientific Computing</li> <li>◆ Machine Learning and Artificial Intelligence in Drug Discovery</li> <li>◆ Example of ML/AI Enabled Drug Discovery</li> <li>◆ Role of Computing in Different Stages of the Drug Discovery Pipeline</li> <li>◆ Current Challenges</li> </ul>
10	Special Topic 3: Drug Repurposing	<ul style="list-style-type: none"> <li>◆ Overview of Drug Repurposing</li> <li>◆ Strategies and approaches to repurpose existing medicines for new indications.</li> <li>◆ Examples of Medicine Repurposing</li> </ul>
11	Special Topic 4: Herbal Medicine Integration into Modern Drug Discovery (Cross-taught	<ul style="list-style-type: none"> <li>◆ Definition of Class of Herbal Medicines</li> <li>◆ Analysis of Complex Natural Products.</li> <li>◆ Methodologies for formal evaluation of herbal medicines.</li> </ul>

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	with Herbal Medicines Module)	<ul style="list-style-type: none"> <li>◆ Examples of successful transformation of herbal medicines into conventional medicines.</li> </ul>
12	Special Topic 5: Non-small molecule therapies	<p><u>Peptide Therapies:</u></p> <ul style="list-style-type: none"> <li>◆ Overview</li> <li>◆ Advantages, Disadvantages and Challenges</li> <li>◆ Discovery, Development and Manufacturing</li> </ul> <p><u>Nucleic Acid Therapies:</u></p> <ul style="list-style-type: none"> <li>◆ Overview</li> <li>◆ RNA Therapies</li> <li>◆ DNA/Genetic Therapies</li> <li>◆ Challenges</li> </ul> <p><u>Cell Therapies:</u></p> <ul style="list-style-type: none"> <li>◆ Overview</li> <li>◆ Cell Engineering</li> <li>◆ Cell Product Manufacturing</li> <li>◆ Administration and Treatment Facilities.</li> </ul>
<u>13</u>	Field Trip	<ul style="list-style-type: none"> <li>◆ UVRI or Makerere</li> </ul>
14	Assessment of the modules	<ul style="list-style-type: none"> <li>◆ Knowledge Test</li> <li>◆ Project Presentation</li> </ul>