

**SPRING 2021**  
**PHM809 (SECTION 001)/ CEM809 (SECTION 001) /BMB961 (SECTION 004): DRUG**  
**DISCOVERY AND MEDICINAL CHEMISTRY (2 CREDITS)**  
**TUE-THU 9:10 – 10:00 AM (SYNCHRONIZED ZOOM)**

**Instructor:** Drs. Kin Sing Stephen Lee, Edmund Ellsworth, Rick Neubig, Bin Chen, Erika Lisabeth, Alex Dickson, Bryan Copple, Jay Sisco, Andy Vick, Marc Bailie

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**Zoom link:** <https://msu.zoom.us/j/96064486636> Passcode: 809

**Course Description:**

Drug Discovery is a complicated and fascinating adventure, engaging multiple disciplines, strategic decision-making, and problem-solving skills. The selection of a finalist from a pool of drug candidates is often driven by a careful balance of efficacy, safety, and economic considerations. Expert practitioners have some knowledge in chemistry, biochemistry, molecular biology, pharmacology, informatics, toxicology, and physiology to make key decisions.

This course will provide the fundamentals for the drug discovery process including but not limited to basic chemical knowledge, drug design principles, high-throughput screening, computational modeling, drug metabolic pathways and pharmacokinetic/pharmacodynamic analysis. The goal of this course is to equip students with a basic knowledge of discovery pharmaceutical research and to prepare them ultimately to work as a team-member in a discovery program.

**Grading:**

The course grade will be based on the participation in team presentations, the preparation and presentation of the final group project and course attendance (**90% attendance is required** and the attendance will be recorded by iClicker):

<b>Group Presentations</b>	<b>50%</b>
<b>Group Written Report</b>	<b>40%</b>
<b>Attendance</b>	<b>10%</b>

**The group project will** include written reports and presentations. Each group will be assigned a drug discovery project. We will provide each project group a list of potential drug candidates with structural, potency, pharmacokinetic, etc. information. Based on the data provided, each team member should be engaged in the selection of the best candidate from a group of compounds for the next development phase. It is anticipated that each group meet together outside of class time for scholarly discussion for the preparation of their final project and during the semester.

**The written report** will be graded by the instructors while the presentations (Open to Public) will be graded by both students (40% of the grade of the presentation) and the attending faculty (60% of the grade of the presentation). The detailed breakdown of the grade for written report and the presentation is listed below:

<b>Written Report</b>		<b>Presentation</b>	
<b>Criteria</b>	<b>Contribution to the grade (%)</b>	<b>Criteria</b>	<b>Contribution to the grade (%)</b>
Organization	20	Organization	20
Significance	20	Significance	20
Lab Objective and Data Analysis	40	Lab Objective and/or Data Analysis	40
Rationale of the Decision	20	Rationale of the Decision	20

During the semester, each group is required to give **4 presentations (including the final presentation)**, each presentation account for 10% of the final grading except final presentation account for 20%).

Each group will submit **3 short reports (due on Friday before the short presentation, template will be provided)** for instructors' comments. The short report should contain individual answer on the questions in the template and a summary statement from the team after the discussion within the group. Please considered to incorporate our comments into your final report. Instructors and external guest lecturers will provide suggestions and feedbacks for the project during the presentations and teams are encouraged to contact instructors for questions and advices.

**The final report** is due on Apr 20<sup>th</sup>.

#### **Americans with Disabilities Act Accommodations:**

Michigan State University is committed to providing equal opportunity for participation in all programs, services, and activities. Requests for accommodations by persons with disabilities may be made by contacting the Resource Center for Persons with Disabilities by phone at 517-884-RCPD or through the web at [rcpd.msu.edu](http://rcpd.msu.edu). Once your eligibility for an accommodation has been determined, you will be issued a verified individual services accommodation ("VISA") form. Please present this form at the start of the semester and/or at least two weeks prior to the accommodation date. Requests received after this date will be honored whenever possible.

**Policy Regarding Academic Dishonesty:** Academic dishonesty of any kind will not be tolerated in this course. Please see the following website for information regarding Michigan State University's policy regarding academic dishonesty:

<https://www.msu.edu/~ombud/academic-integrity/index.html>

**TENTATIVE SCHEDULE (THE SCHEDULE MAY SUBJECT CHANGES DUE TO UNFORSEEN EVENTS SUCH AS: WEATHER CONDITION, ETC)**

<b>Date</b>	<b>Topic</b>
<b>Introduction</b>	
Jan 12 <sup>th</sup> - Jan 14 <sup>th</sup>	1. Different Aspects of Drug Discovery ( <b>Dr. Ellsworth</b> ) 2. From Hit-to-Drug Candidate ( <b>Dr. Ellsworth</b> )
Jan 19 <sup>th</sup> - Jan 21 <sup>th</sup>	3. Lab Objectives, Product Profile, Guidance for Lead Selection. ( <b>Dr. Ellsworth</b> ) 4. Druggable Target and Target Identification ( <b>Dr. Neubig</b> )
Jan 26 <sup>nd</sup> – Jan 28 <sup>th</sup>	5. Druggable Target and Target Identification ( <b>Dr. Neubig</b> ) 6. Bioinformatics in Drug discovery ( <b>Dr. Chen</b> )
<b>Identification of the Lead Compounds</b>	
Feb 2 <sup>nd</sup> - Feb 4 <sup>th</sup>	7. <b>Group presentations (Disease Target, current treatment limitations, your target and advantages, product profile)</b> 8. Sources of Chemical Matter – principle of medicinal chemistry ( <b>Dr. Lee</b> )
Feb 9 <sup>th</sup> – Feb 11 <sup>th</sup>	9. Pitfalls of Chasing Drug-Target Binding Affinity ( <b>Dr. Lee</b> ) 10. Important Parameters for Lead Optimization ( <b>Dr. Lee</b> )
Feb 16 <sup>th</sup> – Feb 18 <sup>th</sup>	11. Concepts of Multiparameter Optimization (Use of Data Warrior) ( <b>Dr. Ellsworth</b> ) 12. High-Throughput Screening (*include screening strategy, <b>Dr. Lisabeth</b> )
Feb 23 <sup>rd</sup> - Feb 25 <sup>th</sup>	13. <b>Group presentation: Define lab objective and screening Strategy.</b> 14. <b>Breakout Room discussion: Identifying leading candidates for PK/ in vivo experiment or drug modifications</b>
Mar 4 <sup>th</sup>	15. Drug Metabolic Pathway and Prediction ( <b>Dr. Copple</b> )
Mar 9 <sup>th</sup> – Mar 11 <sup>th</sup>	16. Drug-Drug Interaction + Computational tools for drug discovery (PAINs compound and metabolism prediction) ( <b>Drs. Ellsworth and Lee</b> ) 17. Crystal Structure and Computational Model Guided Drug Design ( <b>Dr. Dickson</b> )
<b>In vivo Aspects in Drug Discovery</b>	
Mar 16 <sup>th</sup> – Mar 18 <sup>th</sup>	18. Pharmacokinetic/ Toxicokinetic And Pharmacodynamic

Date	Topic
	<p>(Dr. Vick)</p> <p>19. Pharmacokinetic/ Toxicokinetic And Pharmacodynamic (Dr. Vick)</p>
Mar 23 <sup>rd</sup> – Mar 25 <sup>th</sup>	<p>20. Computational tools for drug discovery (Simcyps workshop) (Dr. Lee/ M.Pharm. Maghami)</p> <p>21. Different Aspects of Chemical Structure in Drug Design (Dr. Ellsworth and Dr. Lee)</p>
Mar 30 <sup>th</sup> – Apr 1 <sup>st</sup>	<p>22. Different Aspects of Chemical Structure in Drug Design (Dr. Ellsworth and Dr. Lee)</p> <p>23. Group presentation: Identification of Lead and Backup Candidate for Efficacy Model Testing and the Potential Limitation of the Candidates</p>
Apr 6 <sup>th</sup> – Apr 8 <sup>th</sup>	<p>24. Group presentation: Identification of Lead and Backup Candidate for Efficacy Model Testing and the Potential Limitation of the Candidates</p> <p>25. Major topic: Bioinformatics Assessment on Safety and Other Consideration before Moving to Pre-IND/IND Application (Dr. Chen)</p>
Apr 13 <sup>th</sup> – Apr 15 <sup>th</sup>	<p>26. Drug Formulation (Dr. Sisco)</p> <p>27. in vivo Model and Biomarkers (Dr. Bailie)</p>
Apr 20 <sup>th</sup>	28. In vivo Toxicology Study (Dr. Bailie)
Apr 27 <sup>th</sup> – Apr 29 <sup>th</sup> (Final Week)	<p>29. Final Group presentation</p> <p>30. Final Group presentation</p>