Nanyang Technological University
Division of Chemistry and Biological Chemistry

Academic Year	2022/23	**Semester**	2
Course Coordinator	Liu Xuewei		
Course Code	CM5082[1]		
Course Title	Drug Design and Synthesis		
Pre-requisites	(CM1051 and CM2031 and CM9081) or (CM2031 and CM9081/CM5081 and CY1101) or (CM1002 and CM2031 and CM9081/CM5081) or by permission		
No of AUs	3		
Contact Hours	Lecture: 39 hours (3 hours per week)		
Proposal Date	21 October 2021		

Course Aims

This course aims to equip you with the theoretical and practical knowledge on the new trends in drug design and synthesis. You will be introduced with the chemistry behind the design the synthesis of some drug molecules. This course will also introduce the drug, discovery and development process and its basic principles, medicinal chemistry, fundamental molecular basis of drug action, drug target discovery and "drugability", structure-activity relationships, new design and high throughput screening methods to discover new drugs and classes of drugs. The course will improve your communication skills by requiring you to deliver technical presentations to a broad audience.

Intended Learning Outcomes (ILO)

By the end of this course, you (as a student) would be able to:

Drug design and drug discovery technologies

1. Apply structural activity relationships to explain the biological activities
2. Collect and extract knowledge on the common methods used in design, synthesis and testing of drugs
3. Extract concepts in drug discovery and development to align them into existing examples
4. Identify the key timelines of an utility patent
5. Relate the importance of key timelines of an utility patent to the drug discovery cycle

Medicinal chemistry concepts

6. Use small molecules and orally active drugs to illustrate lead generation and optimization
7. Identify some representative drugs as chemical entities
8. Apply knowledge in chemical functional groups and their properties to correlate the biological activities

Organic chemistry in process chemistry

9. Identify key synthetic strategies in process chemistry and manufacturing
10. Apply formulation methods for some drug entities

Course Content

[1] Previously listed as CM9082

Drug design and drug discovery technologies

1. Introduction to drug discovery process
2. Introduction to drug development process
3. Serendipity in drug discovery
4. Introduction to patents in pharmaceutical industry
5. Introduction to protein kinases and enzymes as drug targets

Medicinal chemistry concepts

6. Introduction to Lead optimization
7. Introduction to targets and lead finding

Organic chemistry in process chemistry

8. Introduction to organic chemistry in process development
9. Introduction to formulation in drug manufacturing

Assessment (includes both continuous and summative assessment)

Component	Course LO Tested	Related Programme LO or Graduate Attributes	Weighting	Team/Individual	Assessment Rubrics
Mid-term 1	1-5	competence and creativity	20	individual	see appendix 1
Mid-term 2	5-10		20	individual	
Assignment	all		20	individual	
Final exam	all		40	individual	
Total			100%		

Formative feedback

You will be given feedback in three ways:
1. By response to postings on the course discussion board and face to face consultations
2. Through the marking of CA1 and CA2.
3. General feedback will be provided to the students following the final exam.

Learning and Teaching approach

Approach	How does this approach support students in achieving the learning outcomes?
Lectures	Present the key ideas and important steps used to solve different types of problems. graphics display and a mixture of modern and old school humour. In addition, you will be encouraged to ask questions or have discussions after the lecture.
Video	Youtube videos and animations are prepared for technology enhance learning. These videos will be presented between slides presentation. This will facilitate the understanding of certain concepts. Besides reading references, this would offer students alternative learning materials for better comprehension.

Reading and References

1. An Introduction to Medicinal Chemistry
   Sixth Edition, G.L. Patrick, Oxford University Press, 2017. ISBN 978-0198749691.
2. The Organic Chemistry of Drug Design and Drug Action, Richard B. Silverman, Elsevier, January 2016. ISBN 978-0123959034.
3. Foye's Principles of Medicinal Chemistry, 5th edition; David A. Williams, William O. Foye, Thomas L. Lemke; Sixth Edition, Lippincott Williams & Wilkins: Philadelphia, 2012. ISBN 978-1609133450.
4. Molecules and Medicine, by EJ Corey, B Czako, L Kurti, Wiley, 2007. ISBN 978-0470227497.
5. Medicinal Chemistry – Principles and Practice, Edited by F. D. King, Royal Society of Chemistry (UK), 2014. ISBN 978-1849736251.

Course Policies and Student Responsibilities

(1) General

You are expected to complete all assigned pre-class readings and activities, attend all classes punctually and take all scheduled assignments and tests by due dates. You are expected to participate in all lecture discussions and activities.

(2) Absenteeism

If you miss a lecture, you are expected to make up for the lost learning activities. If you miss the mid-term exam with approval, you will either be offered a make up exam or grading based upon the final.

All project assignments must be submitted on time. Failure to do so will affect your score.

Academic Integrity

Good academic work depends on honesty and ethical behavior. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values.

As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Course Instructors

Instructor	Office Location	Phone	Email
LIU Xuewei	SPMS-CBC-05-02	6316 8901	xuewei@ntu.edu.sg

Planned Weekly Schedule

Week	Topic	Course ILO	Readings/ Activities
1	Course introduction and introduction to drug discovery and development	1	Lecture

2	Drug discovery targets and lead finding	2	Lecture
3	Lead optimization 1	3	Lecture
4	Lead optimization 2 and 3	4	Lecture
5	Protein kinases and enzymes as drug targets	3, 4	Lecture
6	Patents and case study	4, 5	Lecture
7	Mid-term 1 and discussion	1-5	Lecture
8	Drug development and serendipity in drug discovery	6	Lecture
9	Privileged structures and process development 1	7	Lecture
10	Process development 2 and rationales	8	Lecture
11	Formulation	9	Lecture
12	Assignment and Presentation	1-10	Lecture
13	Mid-term 2 and discussion	5-10	Lecture

Appendix 1: Assessment Criteria for all components

Mid-terms 1 and 2 (MCQ and short answer questions)

Standards		
Fail standard (0-9 marks)	**Pass standard (10-14 marks)**	**High standard (15-20 marks)**
Answers to the questions are mostly incorrect.	Answers to the questions are mostly correct.	Answers to the questions are almost always correct.

Final exam (MCQ and short answer questions)

Standards		
Fail standard (0-49 marks)	**Pass standard (50-74 marks)**	**High standard (75-100 marks)**
Answers demonstrate the ability to repeat factual knowledge but not to apply it outside of the lecture context. Answers do not have a strong logical underpinning or maybe attempts to answer both ways at the same time.	Answers to the standard level question are correct and show the ability to apply concepts from the course, but a high level of critical thinking is absent. Answers are reasonably logical, but with gaps.	Answers to all questions show a high and consistent level of critical analysis of the information presented and creative solutions to the problems. Answers are highly logical and demonstrate strong reasoning. Answers are concise and to the point.

Assignment – Presentation

Performance Level	**Criteria**
Excellent	Demonstrates complete achievement of the learning outcomes 1-10. Able to connect to the topics covered and how it can be used to solve the problem. Able to organize the slides to present the assigned topic and answer the comments/questions after the oral presentation.

Good	Demonstrates complete achievement of the learning outcomes 1-10. Able to connect to the topics covered and how it can be used to solve the problem at hand.
Satisfactory	Demonstrates partial achievement of the learning outcomes 1-10. Able to apply the technique or methodology taught in class only in direct way. Able to present the assigned topic but may not be precise or concise enough.
Unsatisfactory	Demonstrates minimal achievement of the learning outcomes 1-10. Not able to apply the knowledge to the problems or not able to present the assigned topic well.
Poor	Do not possess sufficient understanding of problem and lack solution for it. Not able to complete presentation.

CBC Programme Learning Outcome

The Division of Chemistry and Biological Chemistry (CBC) offers an undergraduate degree major in Chemistry that satisfies the American Chemical Society (ACS) curricular guidelines and equips students with knowledge relevant to the industry. Graduates of the Division of Chemistry and Biological Chemistry should have the following key attributes:

1. Competence

Graduates should be well-versed in the foundational and advanced concepts of chemical science, be able to evaluate chemistry-related information critically and independently, and be able to use complex reasoning to solve emergent chemical problems.

2. Creativity

Graduates should be able to synthesize and integrate multiple ideas across the curriculum, and propose innovative solutions to emergent chemistry-related problems based on their training in chemistry.

3. Communication

Graduates should be able to demonstrate clarity of thought, independent thinking, and sound scientific analysis and reasoning through written and oral reports to audiences with varying technical backgrounds. They should also be able to effectively engage other professional chemists in collaborative endeavours.

4. Character

Graduates should be able to act in responsible ways and uphold the high ethical standards that the society expects of professional chemists.

5. Civic-mindedness

Graduates should be aware of the impact of chemistry on society, and how chemistry can be applied to benefit mankind. They should also be aware of and uphold the best chemical safety practices.