Academic Year	AY20/21	**Semester**	1
Course Coordinator	Mihaiela Corina Stuparu, Xuewei Liu, Yanli Zhao		
Course Code	CM3031		
Course Title	Organic Reaction Mechanism and Synthesis		
Pre-requisites	CM2031 or by permission		
No of AUs	3 AUs		
Contact Hours	Lectures: 39, Tutorials: 3		

Course Aims

This core chemistry course aims to develop your understanding of fundamentals of organic chemistry concepts that are essential for future advance chemistry courses and any practicing chemists. This course is also great preparation for a PhD and a career in chemistry research.

On completing this course, you have extended your understanding of organic reaction mechanisms beyond the first- and second-year contents to more advanced chemistry. You will understand issues of selectivity and specificity, especially in terms of regio-, stereo-, and chemo-selectivity and specificity. You will be able to propose syntheses of molecules of higher complexity.

Intended Learning Outcomes (ILO)

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

1. explain basic concept of chirality.
2. describe and rationalise 1,3-allylic strain reactions.
3. describe and rationalise the conformation and addition reactions based on carbonyl molecules.
4. describe and rationalise stereoselective aldol reactions.
5. describe and rationalise reactions on monocyclic and bicyclic rings over cyclic stereocontrol.
6. define the various types of pericyclic reaction; define such terms as conrotatory", "suprafacial", etc; explain and apply the Woodward-Hoffmann Rules.
7. state that the outcomes of pericyclic reactions may be understood in terms of frontier orbital interactions.
8. predict and rationalise the outcomes of Diels-Alder cycloadditions, including stereospecificity, regioselectivity, and stereoselectivity.
9. predict and rationalise the outcomes of other cycloaddition reactions, including 1,3- dipolar and [2+2] cycloadditions, cheletropic reactions, and the ene reaction.
10. predict and rationalise the outcomes of electrocyclic reactions.
11. predict and rationalise the outcomes of [1,n]-, [2,3]- and [3,3]-sigmatropic rearrangements.
12. state the synthetic importance of cycloaddition and rearrangement reactions.
13. design and propose synthetic pathway to new molecules.

Course Content

1. 1,3-Allylic strain: lowest-energy conformation; cis/trans substituents; Houk model
2. Conformation and addition reactions of carbonyls: Felkin-Anh model; effect of electronegative atoms; chelation control
3. Stereoselective aldol reaction: stereoselective aldol reactions; control of enolate geometry; Zimmerman-Traxler model
4. Cyclic stereocontrol: reactions on monocyclic rings; reactions on bicyclic rings
5. Introduction: Isomerism; Selectivity; Selectivity
6. Diels-Alder Cycloaddition: The basic reaction and its disconnection; Substituted dienes and dienophiles and their effect on reaction rates; Regioselectivity; Stereoselectivity and Stereoselectivity (exo/endo) governed by secondary orbital interactions and chirality of starting materials.

7. Other Cycloadditions: 1,3-Dipolar cycloadditions; [2+2] cycloadditions; Cheletropic reactions; More than 6e cycloadditions; Photochemical cycloadditions
8. Woodward- Hoffmann Rules as applied to cycloadditions; Frontier Molecular Orbital Theory applied to cycloadditions
9. Electrocyclic Reactions: Occurrence with 2, 3, 4, etc. electron pairs; Direction of equilibrium; Con- and dis-rotatory reaction; Woodward-Hoffmann Rules as applied to electrocyclic reactions.
10. Simgatropic Rearrangements: Prototropic and sigmatropic rearrangements; [1,3], [1,5], [1,7] hydrogen shifts; Cope, Claisen and related rearrangements; Orbital involvement; Chair-shaped transition states; Stereochemical control; Woodward-Hoffmann Rules as applied to electrocyclic simgatropic rearrangements.

Formative feedback

Formative feedback: Lecturers and TAs will be closely working with you to monitor your learning progress. They will provide you with timely feedback to improve your understanding and design. Furthermore, you can feel free to express your ideas and discuss them with lecturers and TAs as course progresses. You will have opportunities to practise the key learning aspects during lectures and tutorials.

After each item of CA, you will be given written and/or verbal feedback on your work. An examiner report will be provided to you after the final exam, as a way to allow you to reflect on the areas for improvement and allow you to achieve intended learning outcomes 1-13.

Assessment (includes both continuous and summative assessment)

This is a graded course. There is a checklist of ALL the components of the assessments.

Component	Course LO Tested	Related Programme LO or Graduate Attributes	Weighting	Team/ Individual	Assessment rubrics
Midterm Test 1	1 – 5	Communication, Competence, Creativity	15%	Individual	See Appendix 1
Homework / Quiz	1 – 13	Communication, Competence, Creativity	10%	Individual	See Appendix 1
Midterm Test 2	6 – 13	Competence, Creativity Communication	15%	Individual	See Appendix 1
Final Examination	1 – 13	Competence, Competence, Creativity	60%	Individual	See Appendix 1
Total			100%		

Learning and Teaching approach

Approach	How does this approach support students in achieving the learning outcomes?
Lectures	Face to face lectures will be conducted for ILO 1 – 13. This is to

(39 hours)	allow you to interact directly with the instructor. Students could also immediately clarify their doubts/questions during the lectures. You will be spending time to learn detailed organic chemistry principles, structures and reactions. This will enable you to possess the ability for designing new organic chemistry experiments and addressing scientific problems in organic chemistry.
Tutorials (3 hours)	TAs will provide materials containing concepts taught in classes and cover related applications derived from corresponding lectures. You will be assigned to a small group for interactive discussions toward some representative questions, which will help you develop your own critical thinking capability and problem solving skills.
Homework	You will work independently, apply the knowledge you learn to solve scientific problems, develop self-discipline to take initiative and responsibility for completing a task.

Reading and References

Organic Chemistry, Clayden, Greeves, Warren; Oxford University press ISBN: 9780199270293

Course Policies and Student Responsibilities

(1) General
You are expected to complete all online activities in good time.

(2) Absenteeism
If you miss a lecture, you are expected to make up for the lost learning activities. If you are sick and unable to attend your class, you have to:

1. send an email to the instructor regarding the absence
2. submit the original Medical Certificate‖ to the school. (‖ the medical certificate mentioned above should be issued in Singapore by a medical practitioner registered with the Singapore Medical Association.)

If you miss the mid-term exam with approval, you will be graded based upon the final.

Academic Integrity

Good academic work depends on honesty and ethical behaviour. 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 Instructor

Instructor	Office Location	Phone	Email
Mihaiela Stuparu	SPMS-CBC-05-01	6592 7765	mstuparu@ntu.edu.sg
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Planned Weekly Schedule

Week	Topic	Course LO	Readings/ Activities
1	Introduction, 1,3-Allylic strain	1, 2	Lecture, Responseware, Assignment
2	1,3-Allylic strain, Conformation and addition reactions of carbonyls	2, 3	Lecture, Responseware, Assignment
3	Tutorials	1-3	Lecture, Responseware, Assignment
4	Stereoselective aldol reactions	4	Lecture, Responseware, Assignment
5	Cyclic stereocontrol	5	Lecture, Responseware, Assignment
6	Tutorials	4, 5	Lecture, Responseware, Assignment
7	Midterm 1	1-5	Assignment
8	Cycloaddition Reactions	6, 7	Lecture, Responseware, Assignment
9	Woodward- Hoffmann Rules	8, 9	Lecture, Responseware, Assignment
10	Electrocyclic Reactions	10, 11	Lecture, Responseware, Assignment
11	Tutorials	6-11	Lecture, Responseware, Assignment
12	Simgatropic Rearrangements	12, 13	Lecture, Responseware, Assignment
13	Midterm 2	6 – 13	Assignment

The above schedule is for illustrative purposes and is subject to the exigencies of the calendar. Midterm 2 may be arranged in week 12 depending on the teaching progress.

Appendix 1:

Rubric for Homework Assignment

For the assignments, you will be expected to show your competency to understand the principle of pericyclic reactions. You are expected to apply the knowledge you learn to solve scientific problems. Marks will be scaled to 10% of the course. It is designed as an avenue for you to work independently, and apply the knowledge you learn to solve scientific problems.

0-3 marks	4-7 marks	8-10 marks
Shows little to no understanding of the theoretical and practical principles covered in the lectures. Not able to complete the assignments on time or achieve average marks	Shows moderate to good understanding of the theoretical and practical principles covered in the lectures Complete assignments with average marks	Shows a comprehensive or near comprehensive understanding of the theoretical and practical principles covered in the Complete assignment punctually is correct on majority of the questions.

Rubric for Midterm and Final Examination

For the questions in the exam, you will be expected to show your competency to understand organic chemistry principles, stereochemistry, synthesis, and reactivity, having critical thinking and practical skills to solve scientific problems. Marks will be scaled to 10% of the course total.

0-3 marks	4-7 marks	8-10 marks
Shows little to no understanding of the theoretical and practical principles covered in the lectures. Make no effort and often responds poorly to questions.	Shows moderate to good understanding of the theoretical and practical principles covered in the lectures. Understands and can address some of the questions.	Shows a comprehensive or near comprehensive understanding of the theoretical and practical principles covered in the lectures. Understands and can well address all the questions.

Grading Criteria for the Course

The following guideline describes the criteria expected of the different levels of performance in this course.

Standards	Criteria
A+ (Exceptional) A (Excellent)	Actively participate and answer Responseware and LAMS questions correctly in and out of class. Complete assignment punctually and correctly. Able to apply the knowledge learned very well with referenced to the learning outcomes (LO) 1 to 13 in order to answer the questions in written exams.
A- (Very good) B+ (Good)	Actively participate in Responseware and LAMS questions in and out of class. Complete assignment punctually and be correct on majority of the questions. Able to apply the knowledge learned with referenced to the LO 1 to 13 to answer most of the questions in written exams.
B (Average) B- (Satisfactory) C+ (Marginally satisfactory)	Participate in Responseware and LAMS questions in and out of class. Complete homework with average marks. Partially able to apply the knowledge learned with referenced to the LO 1 to 13 to answer some of the questions in written exams.

C (Bordering unsatisfactory) C- (Unsatisfactory)	Seldom participate in Responseware and LAMS questions in and out of class. Not able to complete homework on time or achieve average marks. Not able to apply the knowledge learned with referenced to the LO 1 to 13 to answer some of the questions in written exams.
D, F (Deeply unsatisfactory)	Does not participate in Responseware and LAMS questions in and out of class. Not able to complete homework. Not able to apply the knowledge learned with referenced to the LO 1 to 13 to answer most of the questions in written exams.

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.