Welcome to

Advanced Organic Chemistry!

Markus Kärkäs

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Division of Organic Chemistry
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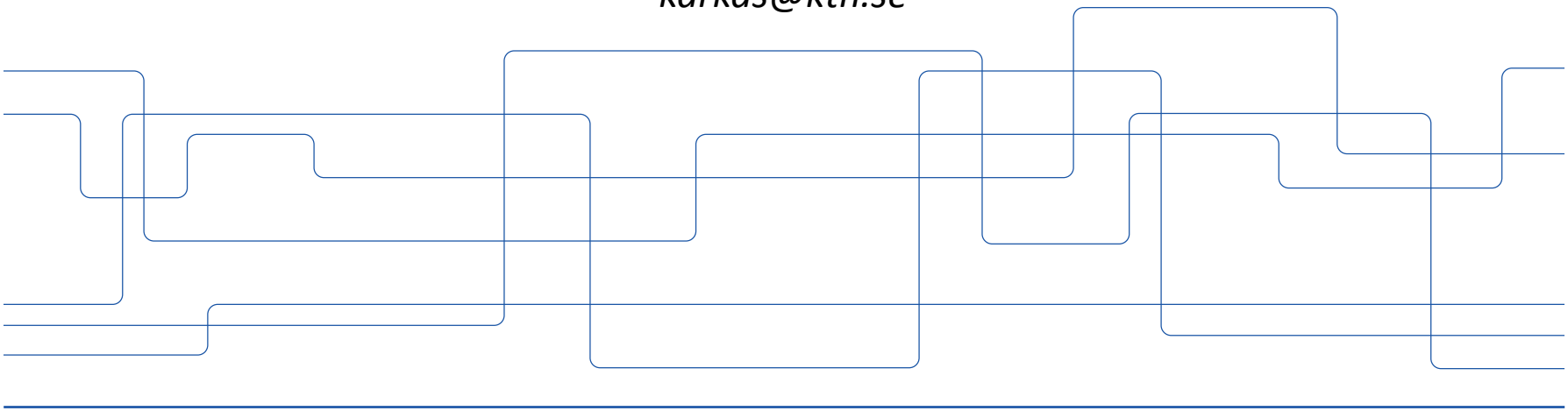
karkas@kth.se



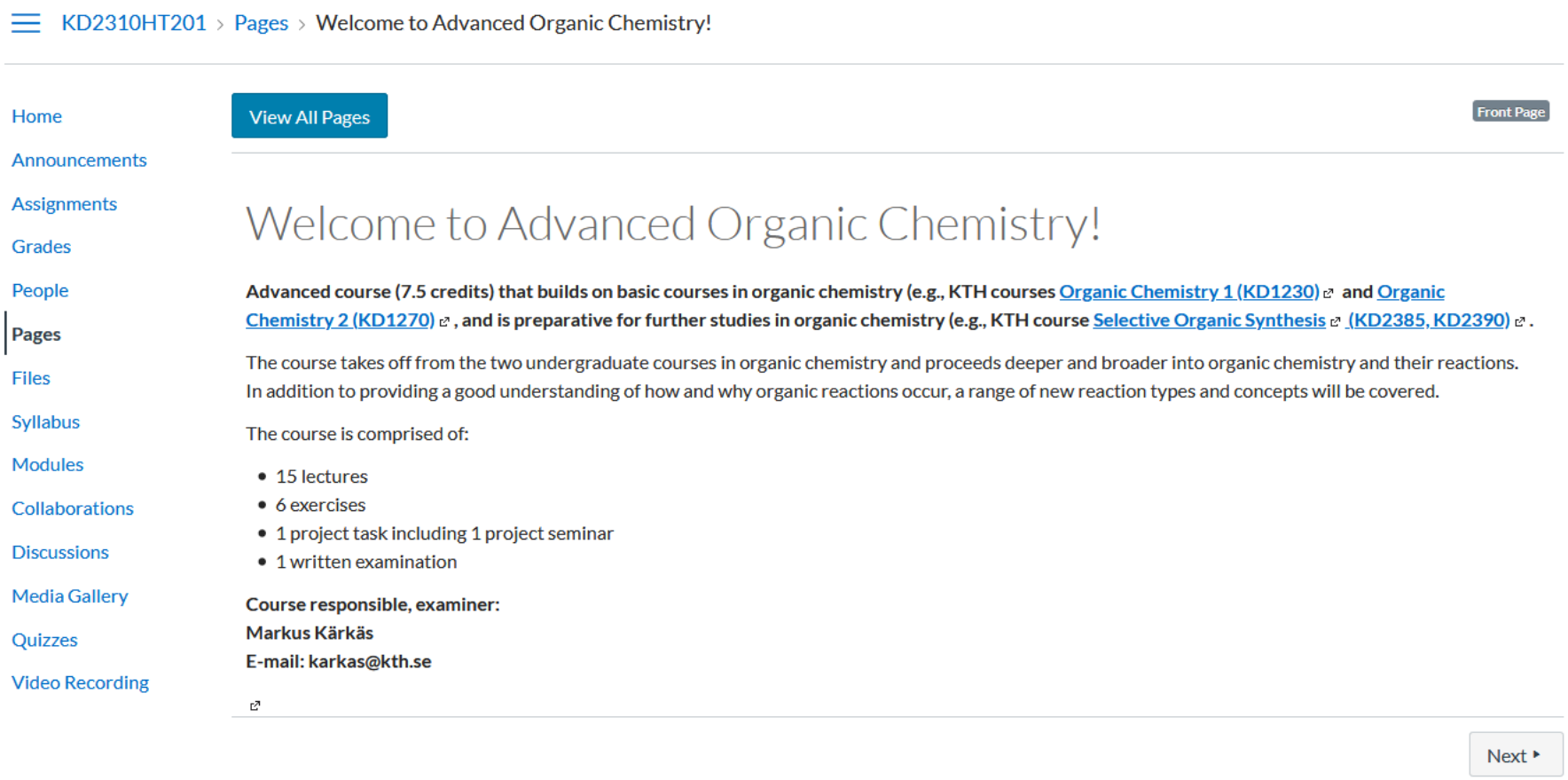
General course information

- All course information can be found in Canvas
- Including this information!

Canvas = web tool

Canvas

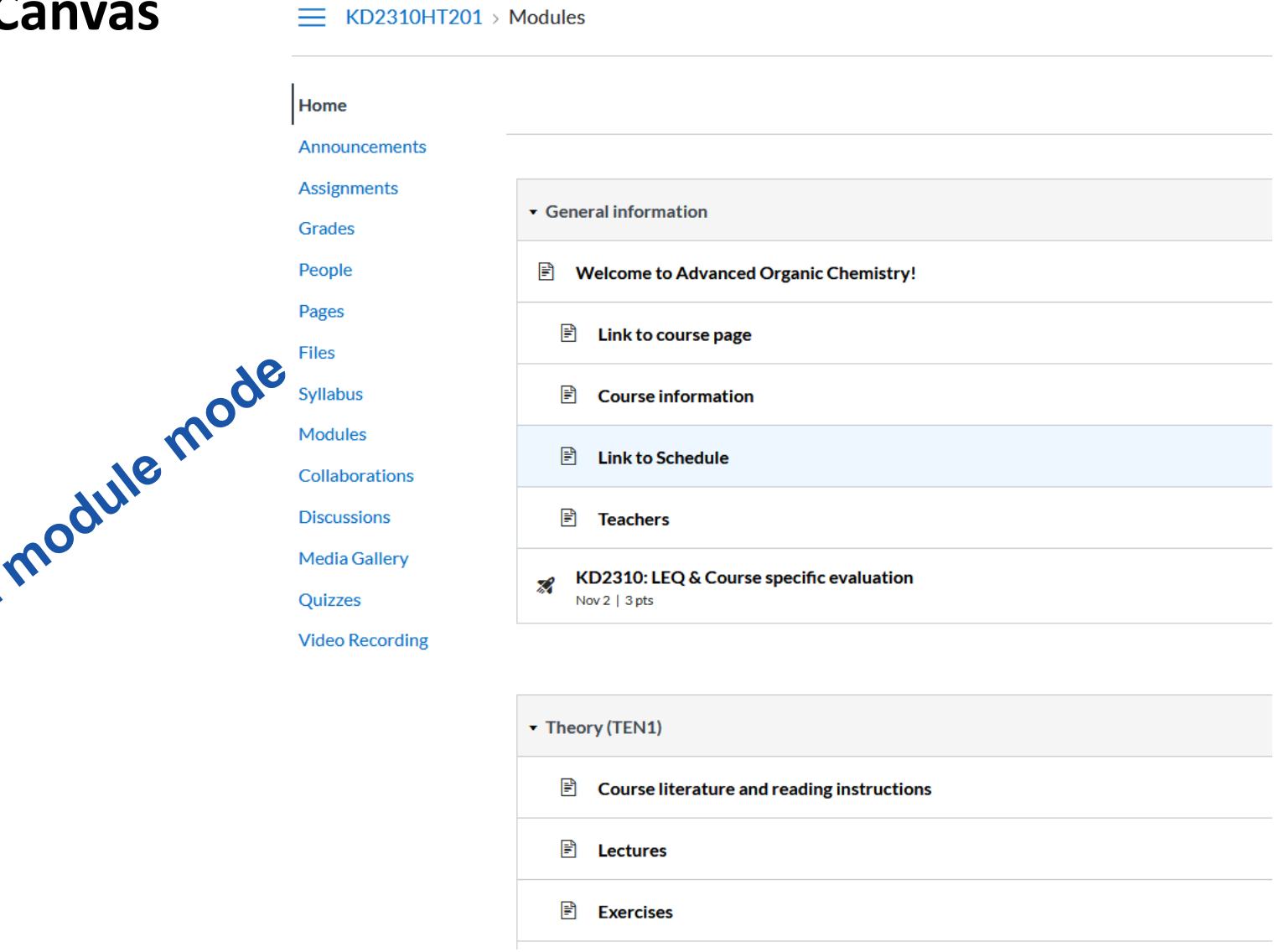
https://kth.instructure.com/login/canvas



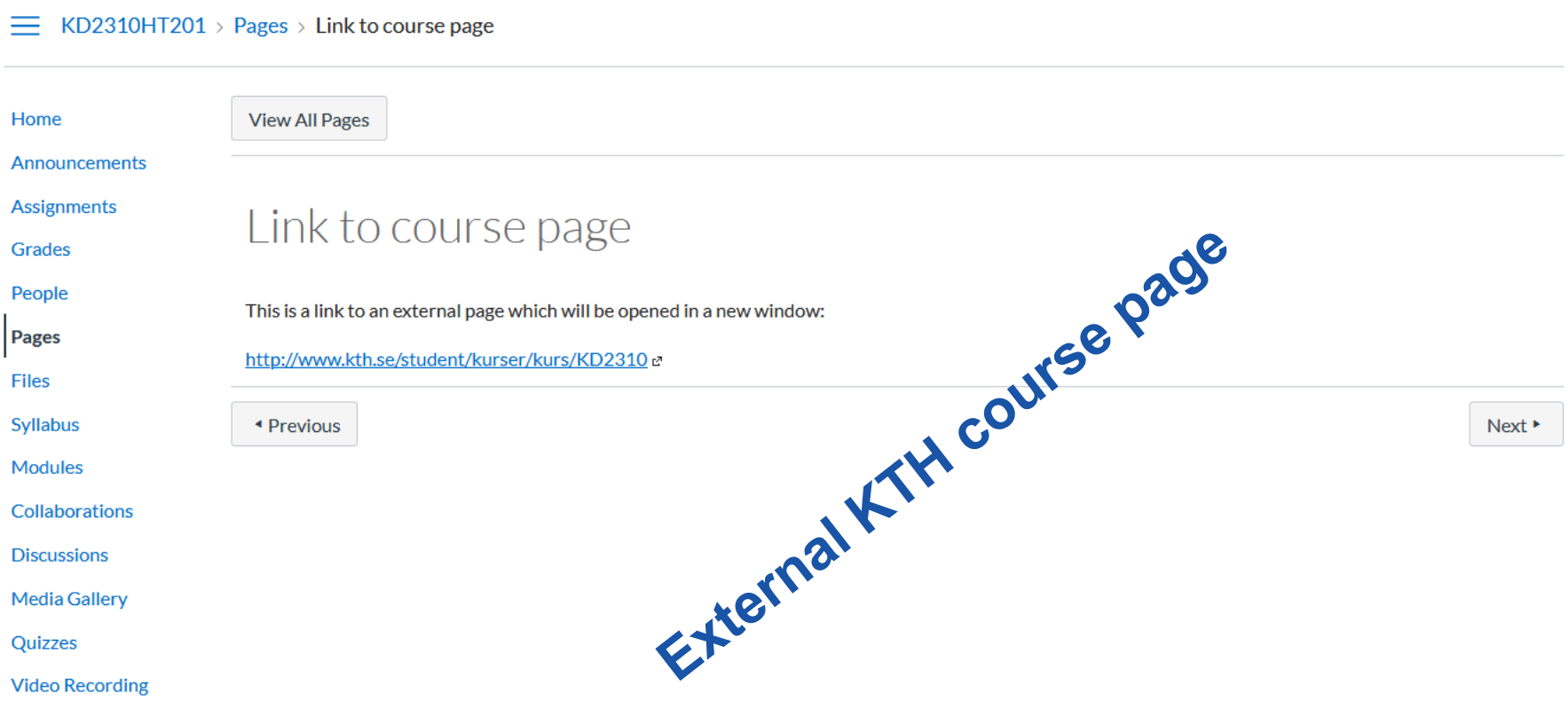
Contact course administration for access!

Canvas

Overview in module mode



Canvas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This is a link to an external page which will be opened in a new window:
http://www.kth.se/student/kurser/kurs/KD2310
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KTH / STUDENT AT KTH / COURSE AND PROGRAMME DIRECTORY / CBH/Chemistry

KD2310 Advanced Organic Chemistry 7.5 credits

Organisk kemi, fortsättningskurs

About course Administrate →

Course information

Course development and history

Advanced Organic Chemistry (KD2310, 7.5 credits) builds on basic courses in organic chemistry (e.g., KTH courses Organic Chemistry 1 (KD1230) and Organic Chemistry 2 (KD1270), and is preparative for further studies in organic chemistry (e.g., KTH course Selective Organic Synthesis (KD2385, KD2390).

The course uses Canvas as a Learning Management System and in order to access Canvas you have to register for the course. If you study the course for the first time, register on the web.

If you have read the course earlier and want to re-register on the course, please contact the course expedition and they will assist you. Teachers can NOT register students or give access to Canvas.

Markus Kärkäs (Course responsible, examiner)
Email: karkas@kth.se

Course information

* Retrieved from Course syllabus (Autumn 2019 -)

Content and learning outcomes

Course contents *

Short course description:

Show course information based on the chosen semester and course offering:

Autumn 2020

Autumn 2020 Start date 24/08/2020 programme students

Offering and execution

Intended learning outcomes

After completing the course the student should be able to:

- Describe, explain, and compare the reactivity in organic chemistry and synthesis with for example reaction mechanisms and concepts in physical organic chemistry
- Analyze and evaluate processes in organic chemistry from a green and sustainable perspective

Course content

Detailed course description:

- Delineate mechanisms for reactions in organic chemistry
- Application of organic reactions in multi-step synthesis
- Principles regarding reaction energetics and reaction kinetics
- Application of molecular orbital theory on reactivity and stereochemistry
- Principles for the rationalization of regio- or enantioselective reaction outcomes
- Basic metal-organic chemistry
- Silicon, phosphorus, and sulfur in organic chemistry
- The process of drug discovery in the pharmaceutical industry
- Application of knowledge in organic chemistry on pharmaceutical and medicinal chemistry
- Principles concerning green- and sustainable chemistry

Course content

- **Theory (TEN2) 6 credits**
  - Lectures
  - Exercises

  Written exam ⟵ ***Determines the final grade!***

Grade:	A	B	C	D	E	F_x	F
Points:	90–100	80–89	70–79	60–69	50–59	45–49	0–44

Complementary exam

- **Project (PRO1) 1.5 credits**
  - Green/sustainable organic chemistry

  Zoom-seminar

Theory (TEN2) 6 credits

- **15 Lectures (Videos!)**
  - 14 on general course material
  - 1 on “synthetic chemistry in the pharmaceutical industry”

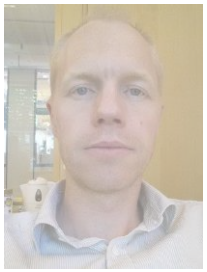
- **6 Exercises**
  - ”learning-by-doing” **IMPORTANT!**
  - up to **15 bonus credits** from voluntary hand-in problems (added to final exam!)

Theory (TEN2) 6 credits

Markus

Peter

Helena



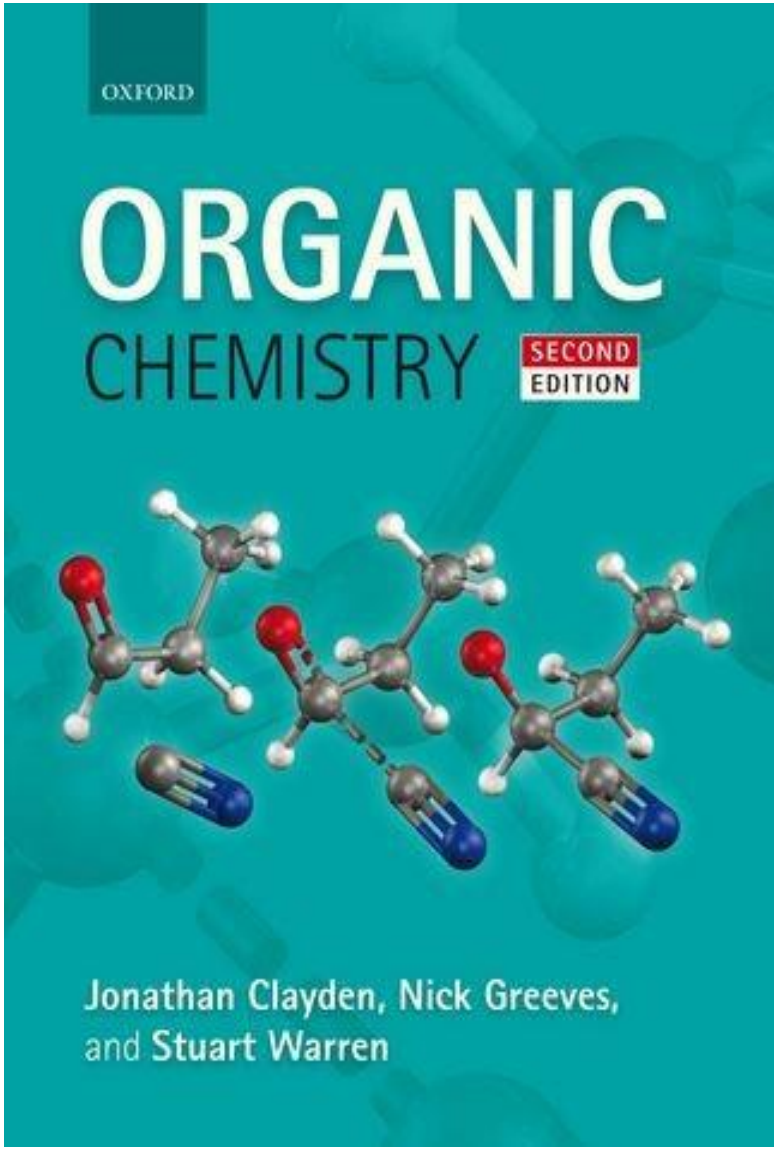
Anders

Daniel

Course coordination	Lectures	Exercises
Course responsible	Peter Dinér	Markus Kärkäs
Markus Kärkäs	Markus Kärkäs	Helena Lundberg
Examiner	Helena Lundberg	
Markus Kärkäs	**External**	
	Anders Bøgevig (Chemnotia) Daniel Pettersen (AstraZeneca)	

Literature

Clayden, Greeves & Warren
Organic Chemistry
Oxford University Press, 2012
ISBN: 978-0-19-927029-3



Content

1. What is organic chemistry?
2. Organic structures
3. Determining organic structures
4. Structure of molecules
5. Organic reactions
6. Nucleophilic addition to the carbonyl group
7. Delocalization and conjugation
8. Acidity, basicity, and pK_a
9. Using organometallic reagents to make C-C bonds
10. Nucleophilic substitution at the carbonyl group
11. Nucleophilic substitution at C=O with loss of carbonyl oxygen
12. Equilibria, rates and mechanisms
13. ^1H NMR: Proton nuclear magnetic resonance
14. Stereochemistry
15. Nucleophilic substitution at saturated carbon
16. Conformational analysis
17. Elimination reactions
18. Review of spectroscopic methods
19. Electrophilic addition to alkenes
20. Formation and reactions of enols and enolates
21. Electrophilic aromatic substitution
22. Conjugate addition and nucleophilic aromatic substitution
23. Chemoselectivity and protecting groups
24. Regioselectivity
25. Alkylation of enolates
26. Reactions of enolates with carbonyl compounds: the aldol and Claisen reactions
27. Sulfur, silicon and phosphorus in organic chemistry
28. Retrosynthetic analysis
29. Aromatic heterocycles 1: structures and reactions
30. Aromatic heterocycles 2: synthesis
31. Saturated heterocycles and stereoelectronics
32. Stereoselectivity in cyclic molecules
33. Diastereoselectivity
34. Pericyclic reactions 1: cycloadditions
35. Pericyclic reactions 2: sigmatropic and electrocyclic reactions
36. Participation, rearrangement and fragmentation
37. Radical reactions
38. Synthesis and reactions of carbenes
39. Determining reaction mechanisms
40. Organometallic chemistry
41. Asymmetric synthesis
42. Organic chemistry of life
43. Organic chemistry today

Content

1. **What is organic chemistry?**
2. **Organic structures**
3. **Determining organic structures**
4. **Structure of molecules**
5. **Organic reactions**
6. **Nucleophilic addition to the carbonyl group**
7. **Delocalization and conjugation**
8. **Acidity, basicity, and pK_a**
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Previous knowledge

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This course (AOC)

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Complementary course (SOS)

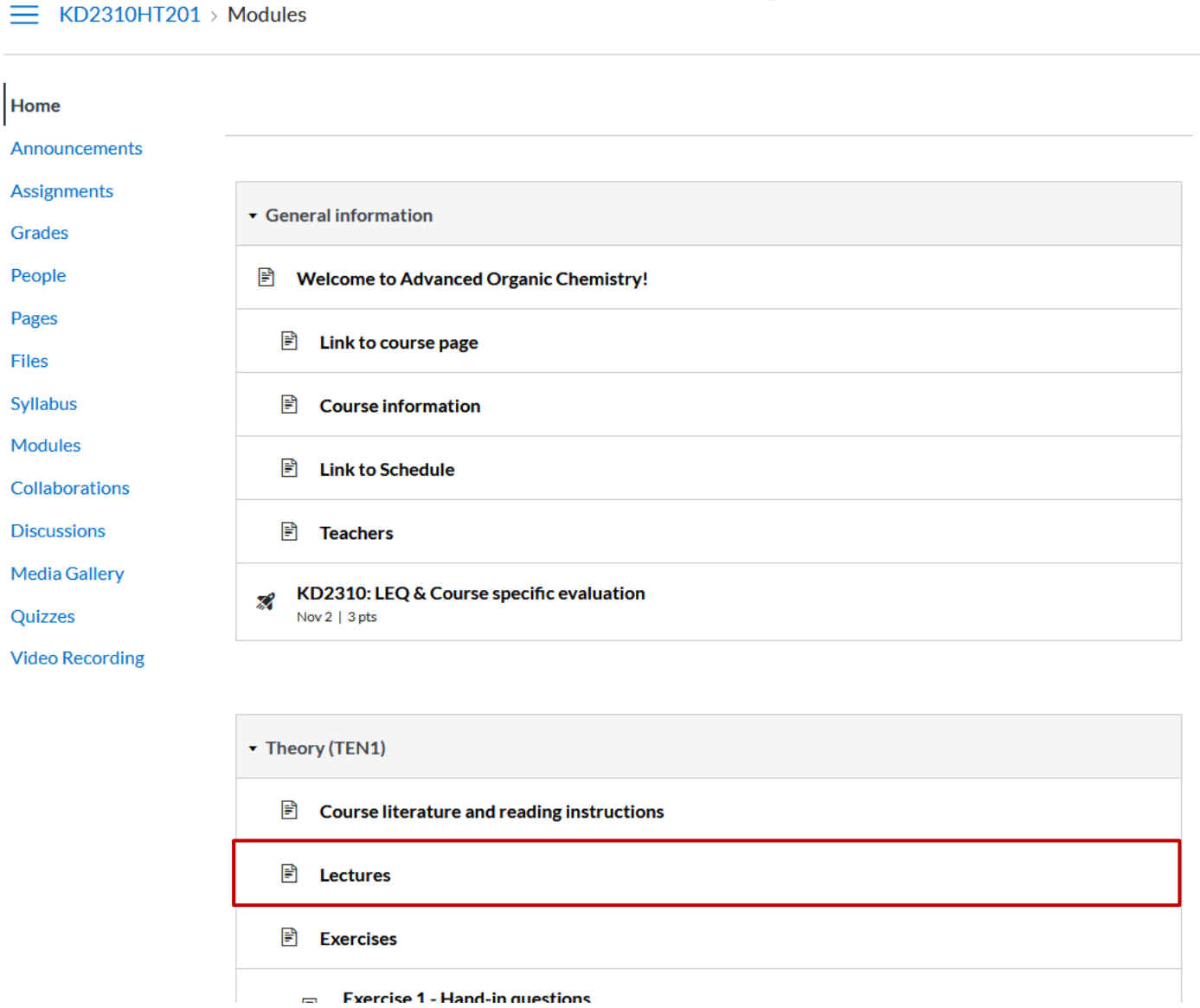
Lectures

- **No lectures at campus!**
- **Videos will be uploaded to Canvas!**

Peter

Markus

Helena

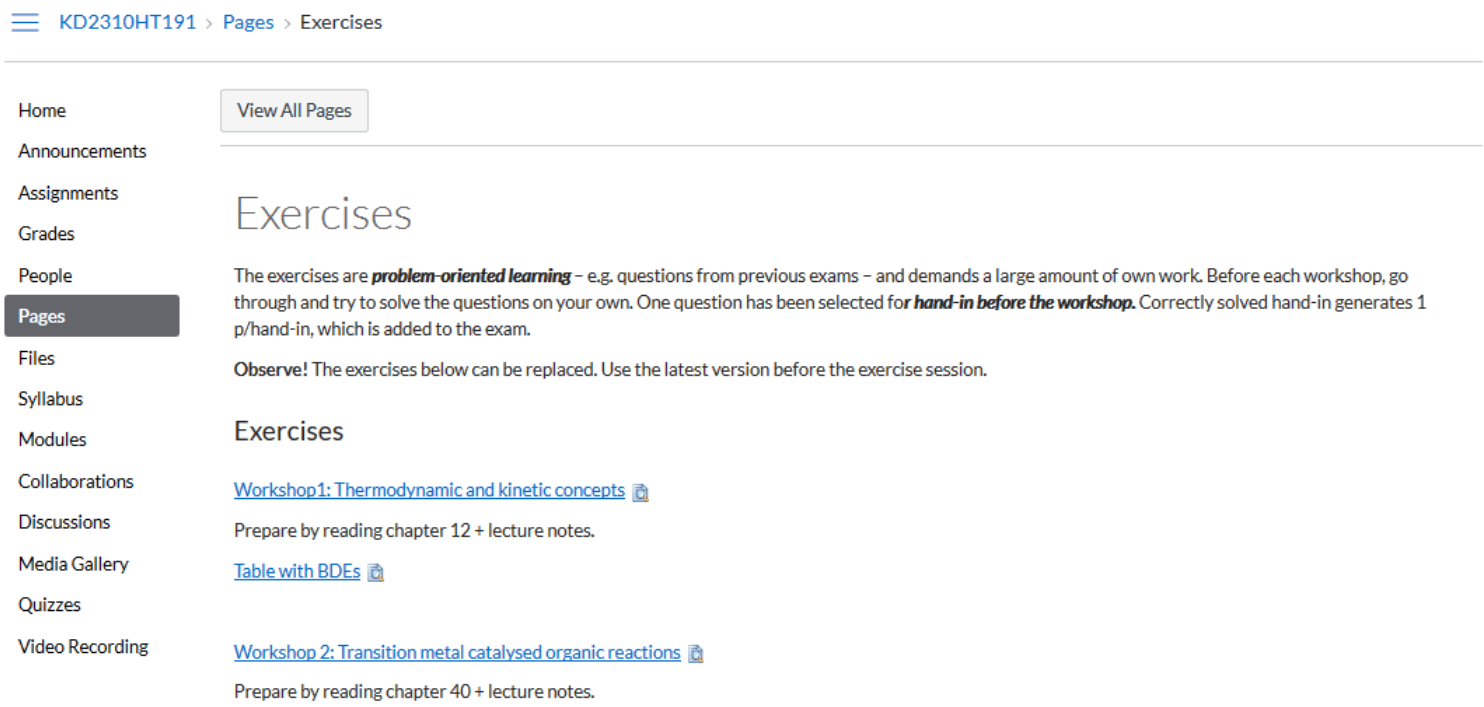


Exercises

- **Two exercise groups!**

Markus

Helena



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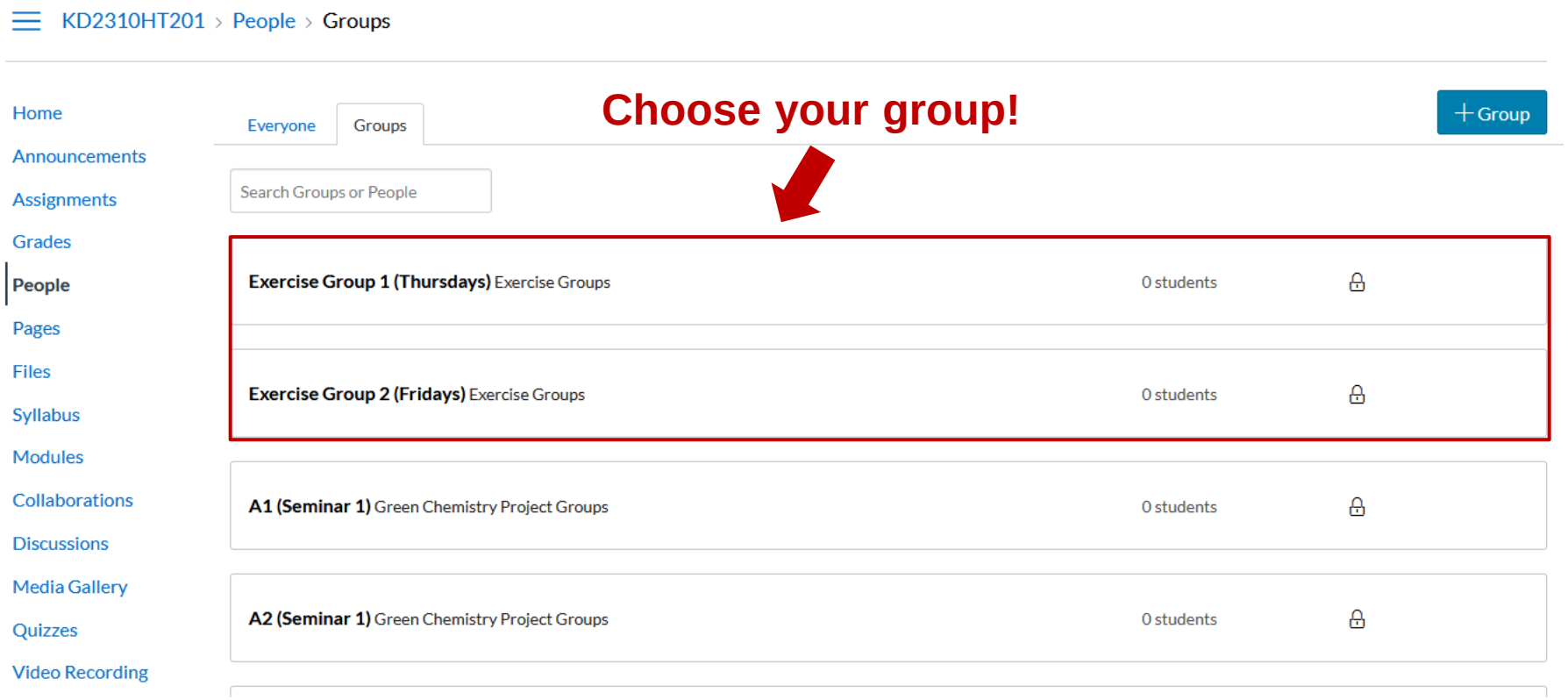
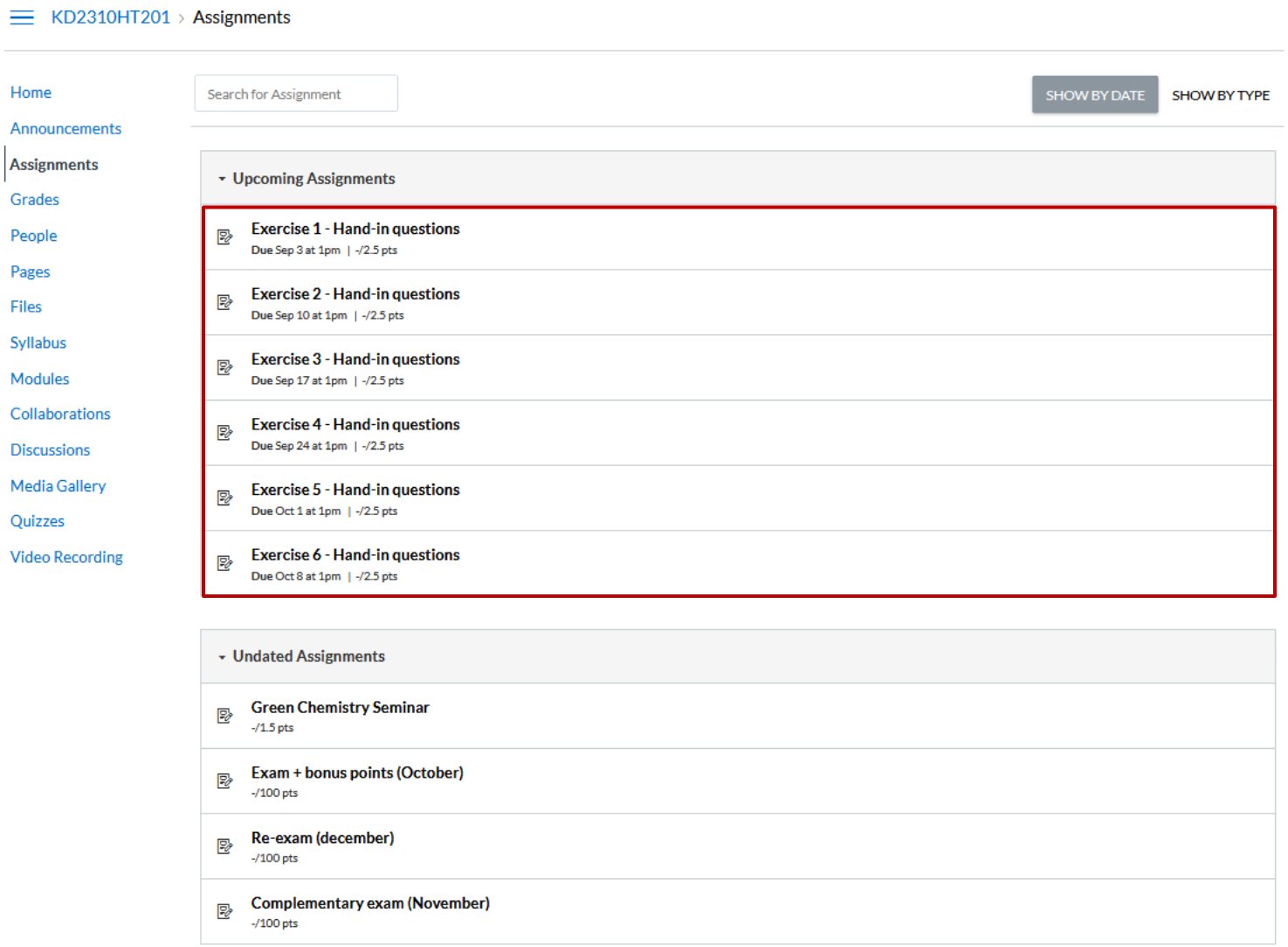
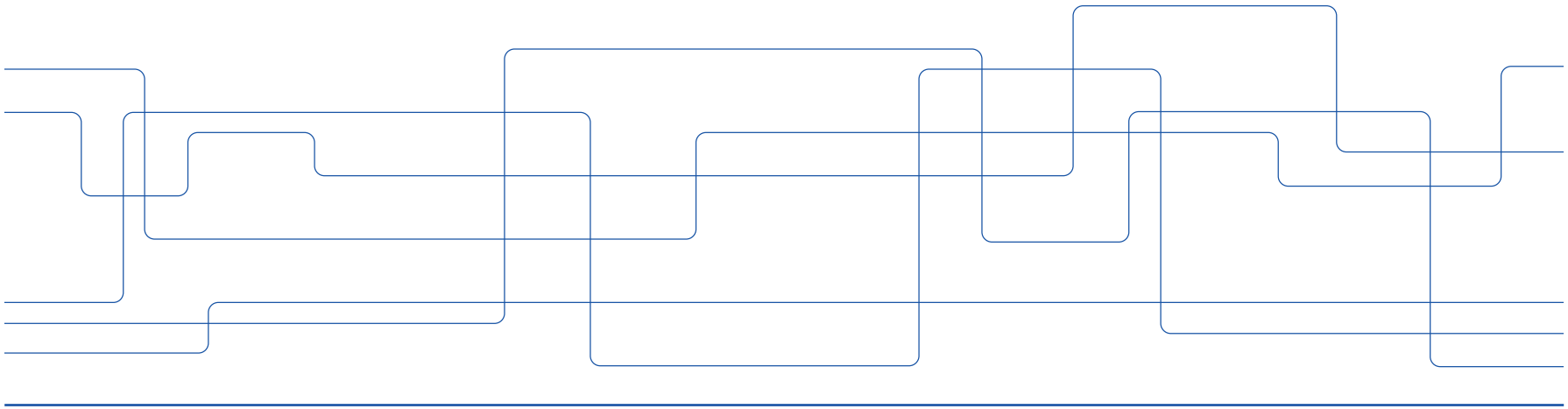


Upload your answers to Canvas



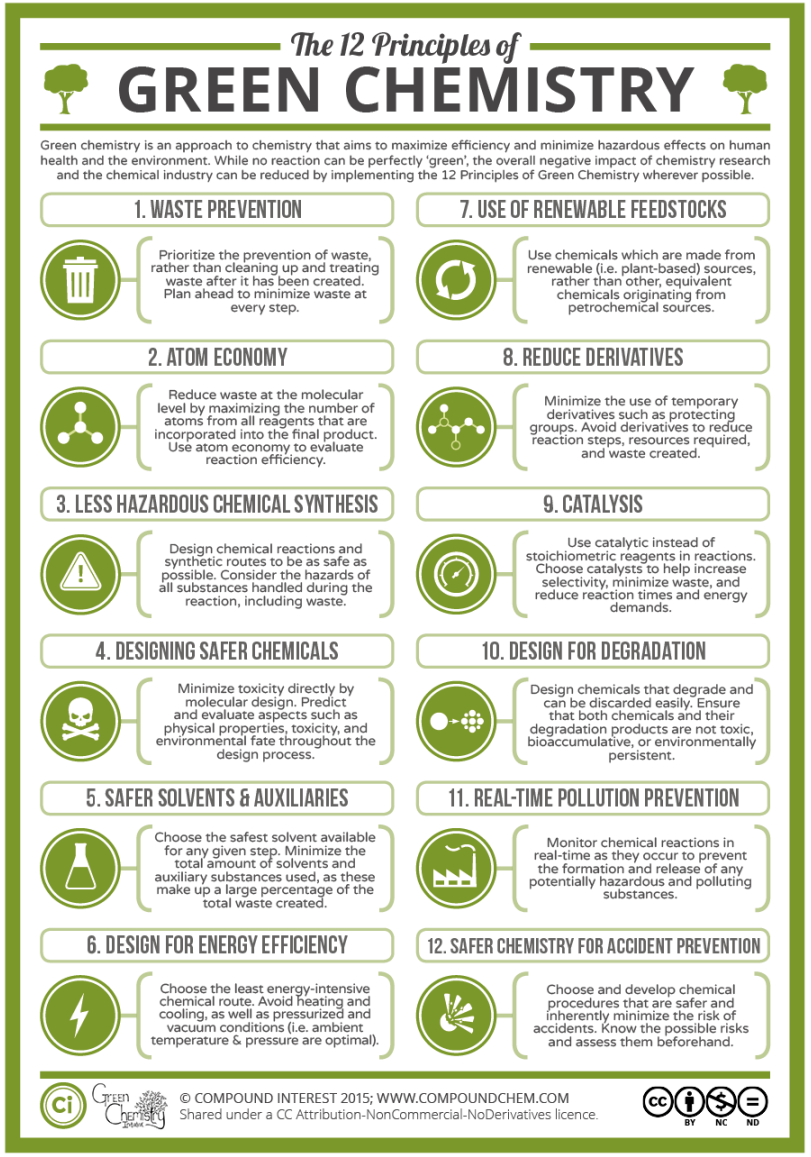
Introduction to Green Chemistry Project

KD2310 Advanced Organic Chemistry



Green chemistry project, 1.5 credits

- Practice in **how to analyse** different organic chemistry processes from a sustainability perspective
- Based on a **set of principles and tools** to aid in the design and analysis of different routes



Project (PRO1) 1.5 credits

- Groups of ~4 students
- Choose 1 of the 4 projects/molecules
- Green organic chemistry problems
- Introductory lecture by Anders Bøgevig/Markus + own studies
- Presentation at one of the seminars – end of course

Project task

- To use the green chemistry principles/tools to analyze the synthesis of a specific pharmaceutical drug (active pharmaceutical ingredient, API)

1) **Sildenafil** (Groups A1 and B1)
2) **Ibuprofen** (Groups A2 and B2)
3) **Pregabalin** (Groups A3 and B3)
4) **Lipoxygenase inhibitor PF-04191834** (Groups A4 and B4)

- To present this analysis at a common seminar at the end of the course

Project (PRO1) 1.5 credits – Canvas

Discussions

Media Gallery

Quizzes

Video Recording

- Teachers
- KD2310: LEQ & Course specific evaluation
  Nov 2 | 3 pts

Theory (TEN1)

- Course literature and reading instructions
- Lectures
- Exercises
  - Exercise 1 - Hand-in questions
    Sep 3 | 2.5 pts
  - Exercise 2 - Hand-in questions
    Sep 10 | 2.5 pts
  - Exercise 3 - Hand-in questions
    Sep 17 | 2.5 pts
  - Exercise 4 - Hand-in questions
    Sep 24 | 2.5 pts
  - Exercise 5 - Hand-in questions
    Oct 1 | 2.5 pts
  - Exercise 6 - Hand-in questions
    Oct 8 | 2.5 pts
- Exam

Green Chemistry Projekt (PRO1)

- Green Chemistry Project

Link to project

Project (PRO1) 1.5 credits

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Green Chemistry Project

Aim of Green Chemistry Project:

- Practice in how to design new, efficient, and environmentally benign organic chemistry processes.
- Based on a set of principles and tools to aid in the design and analysis of different routes.

An overview of these principles, tools, and guidelines will be presented partly by Anders Bøgevig in Lecture 5.

Task:

- To use the green chemistry principles/tools to analyze the synthesis of a specific pharmaceutical drug (active pharmaceutical ingredient, API)

Background review: R. A. Sheldon, Chem. Soc. Rev., 2012,41, 1437-1451. (+ supporting information).

Green chemistry review

1. Sildenafil (Groups A1 and B1)

Synthesis of sildenafil

Project assignment

Literature 1: xlink.rsc.org/?doi=10.1039/b312329d

Literature 2: pubs.acs.org/doi/abs/10.1021/op9900683

Literature

2. Ibuprofen (Groups A2 and B2)

Synthesis of ibuprofen

Route 1: https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.200903055

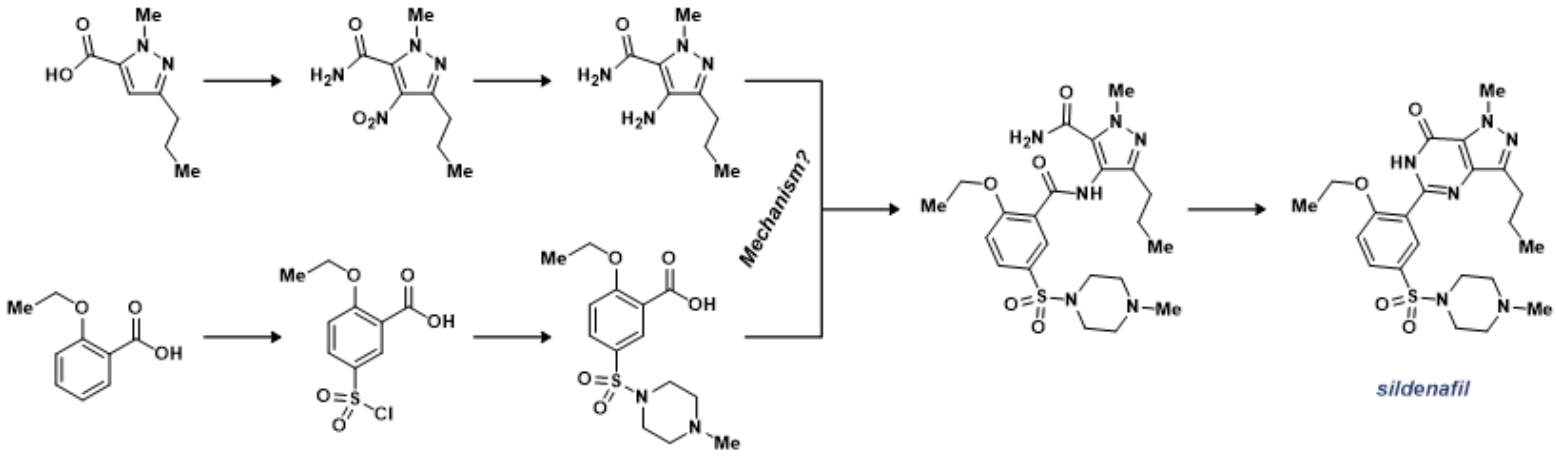
Route 2: US4981995.pdf, EP0284310B1.pdf

Literature extra: pubs.acs.org/doi/abs/10.1021/ed100892p

Resolution: WO9619431.pdf

Project assignment – Example

Synthesis of sildenafil (Viagra™)



1) Calculate atom economy (AE), reaction mass efficiency (RME) and E factor (if possible) for the different steps and the overall process
2) Discuss the synthesis using the 12 principles of green chemistry
   - Any particular hazardous reactions?
   - Any potential for improvements
3) Draw and discuss the mechanism for the indicated step

Data is available in Dale *et al*. *Organic Process Research & Development* **2000**, *4*, 17–22

See also: Dunn *et al*. *Green Chemistry* **2004**, *6*, 43–48

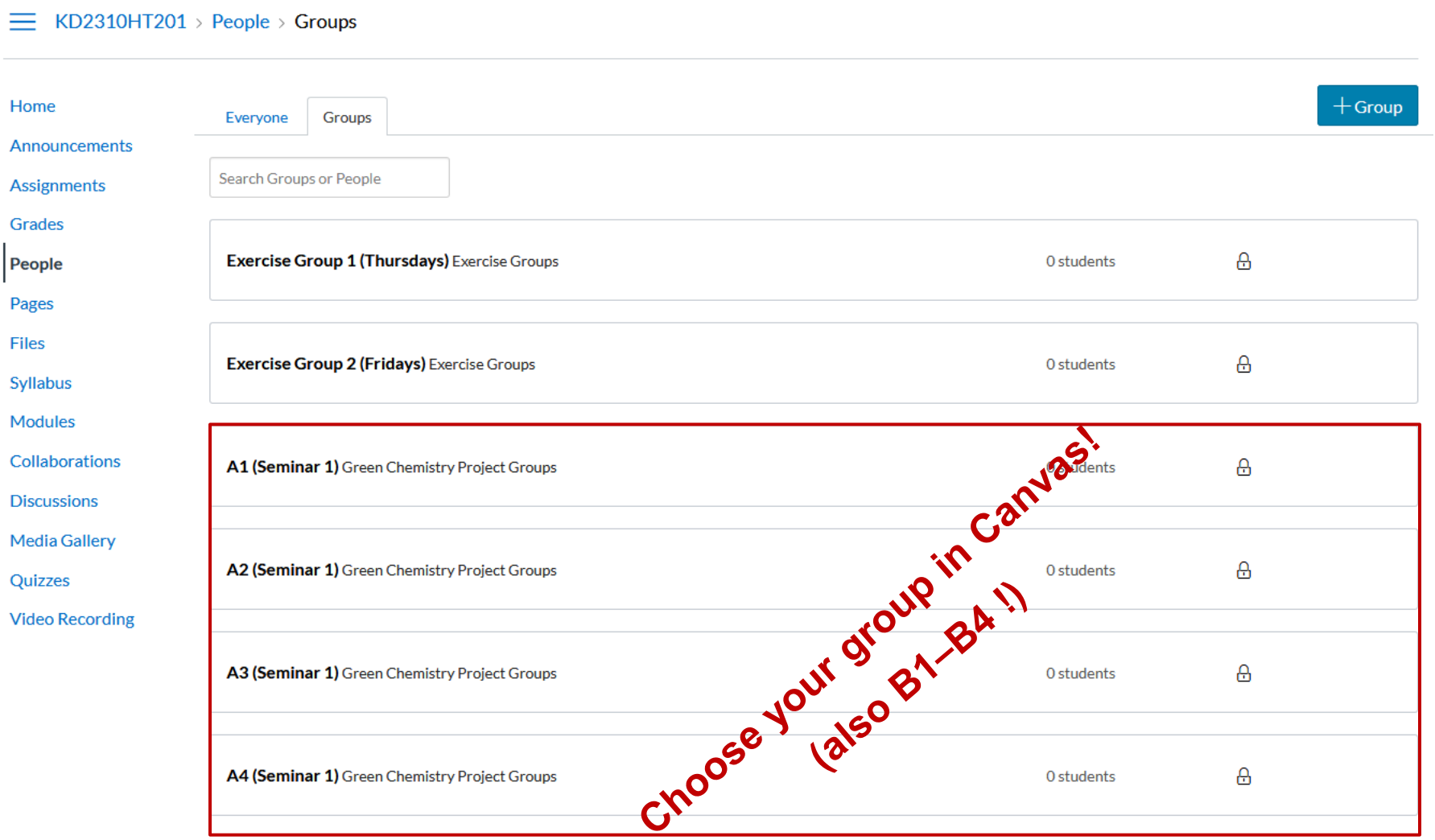
Project (PRO1) 1.5 credits – Groups & presentations

- Groups
  - Ca 4 participants per group (8 groups)
  - Join group yourself in Canvas
  - Access to messaging through Canvas if needed
  - Specific Canvas folders for common access of documents if needed
- Presentations
  - 2 presentation seminars (2 hours each) at the end of the course
  - 4 groups per seminar

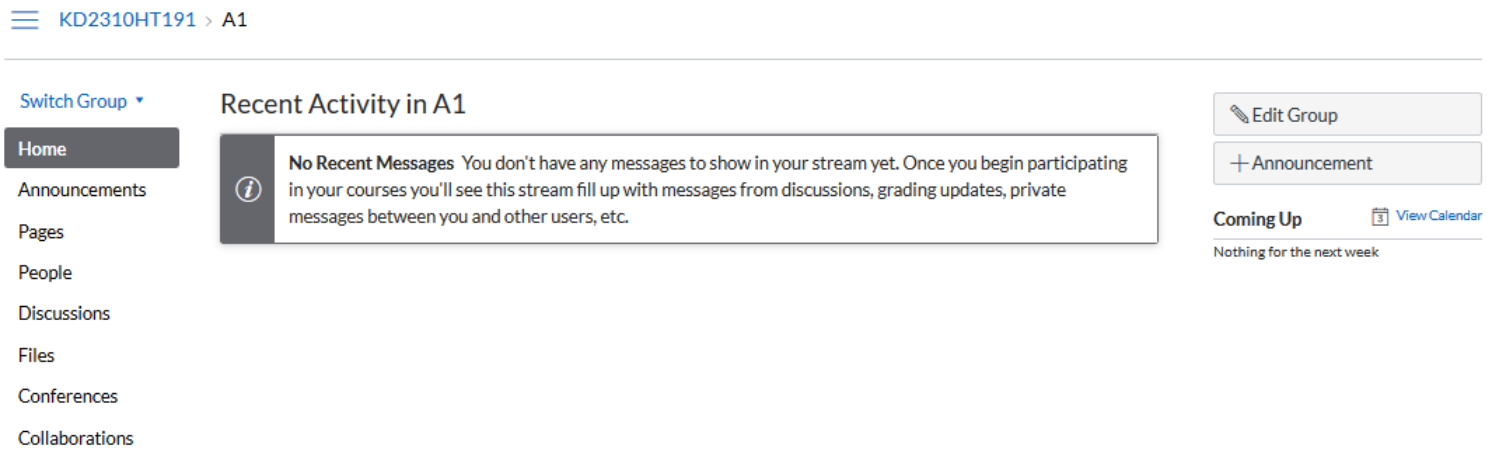
    A-groups: Wednesday, October 9, 2019, 10:00–12.00 (sharp)

    B-groups: Thursday, October 10, 2019, 13:00–15:00 (sharp)
  - Ca 20 minutes per presentation including questions/comments
  - **All group members need to upload the presentation to Canvas (at least) the day before the seminar**

Project (PRO1) 1.5 credits – Joining a group



Project (PRO1) 1.5 credits – Communication & collaboration



You have to initiate and plan the collaboration within the group!

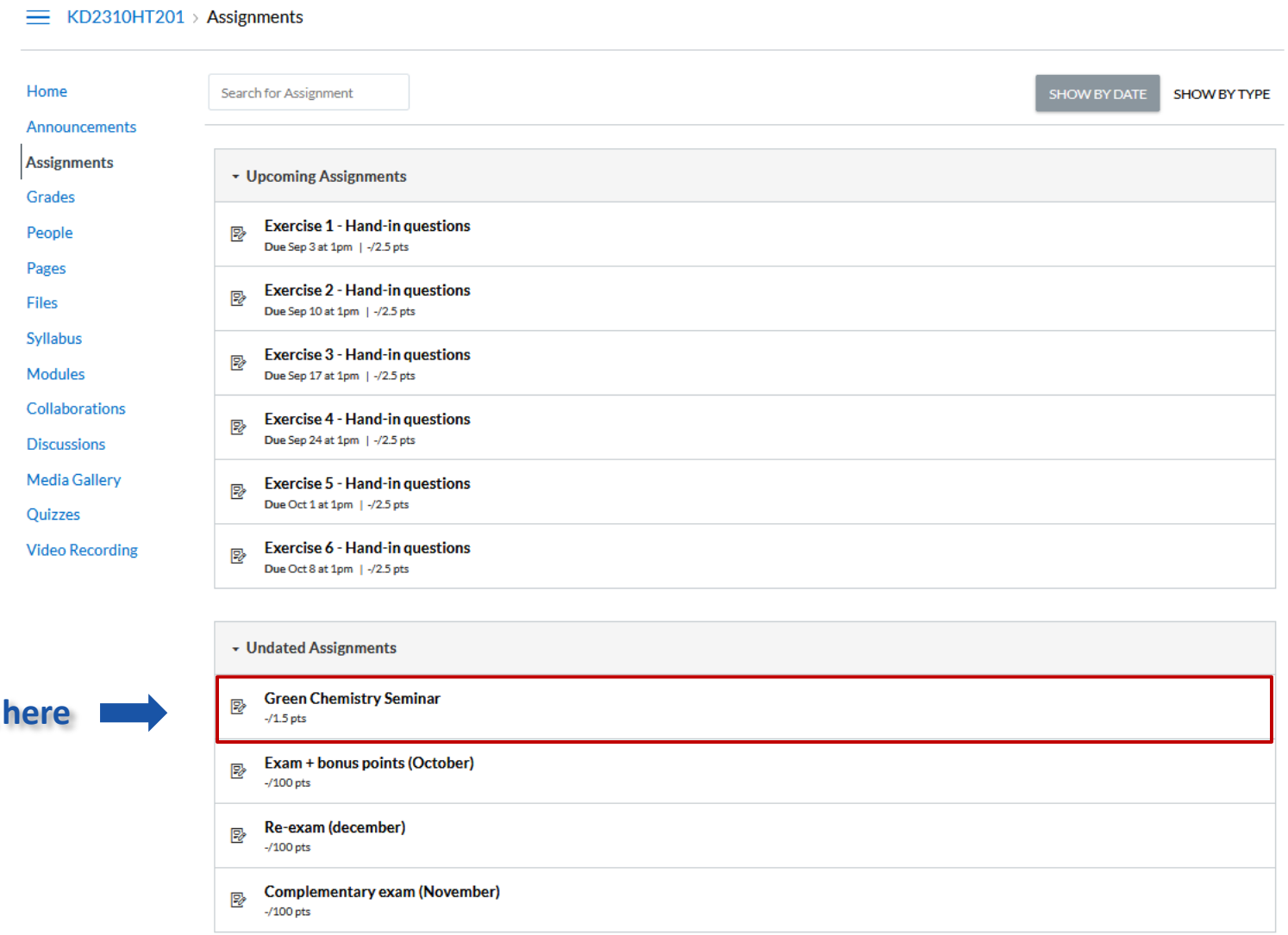
Project (PRO1) 1.5 credits – Groups & presentations

- Groups
  - Ca 4 participants per group (8 groups)
  - Join group yourself in Canvas
  - Access to messaging through Canvas if needed
  - Specific Canvas folders for common access of documents if needed
- Presentations
  - 2 presentation Zoom-seminars (2 hours each) at the end of the course
  - 4 groups per Zoom-seminar

    A-groups: Wednesday, October 7, 2020, 10:00–12.00 (sharp)

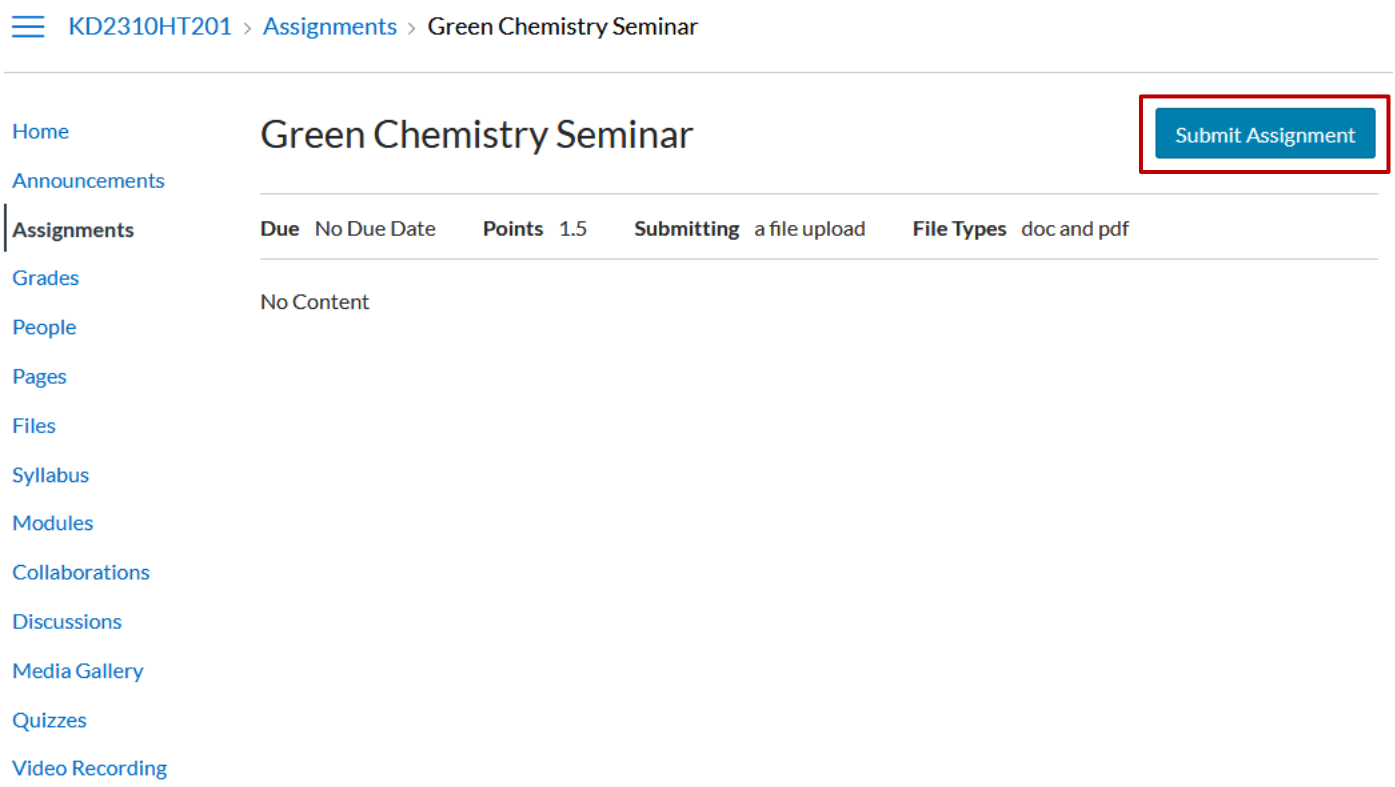
    B-groups: Friday, October 9, 2019, 10:00–12:00 (sharp)
  - Ca 20 minutes per presentation
  - **Everyone need to upload their group´s presentation to Canvas before the first seminar**

Upload your group´s presentation to Canvas



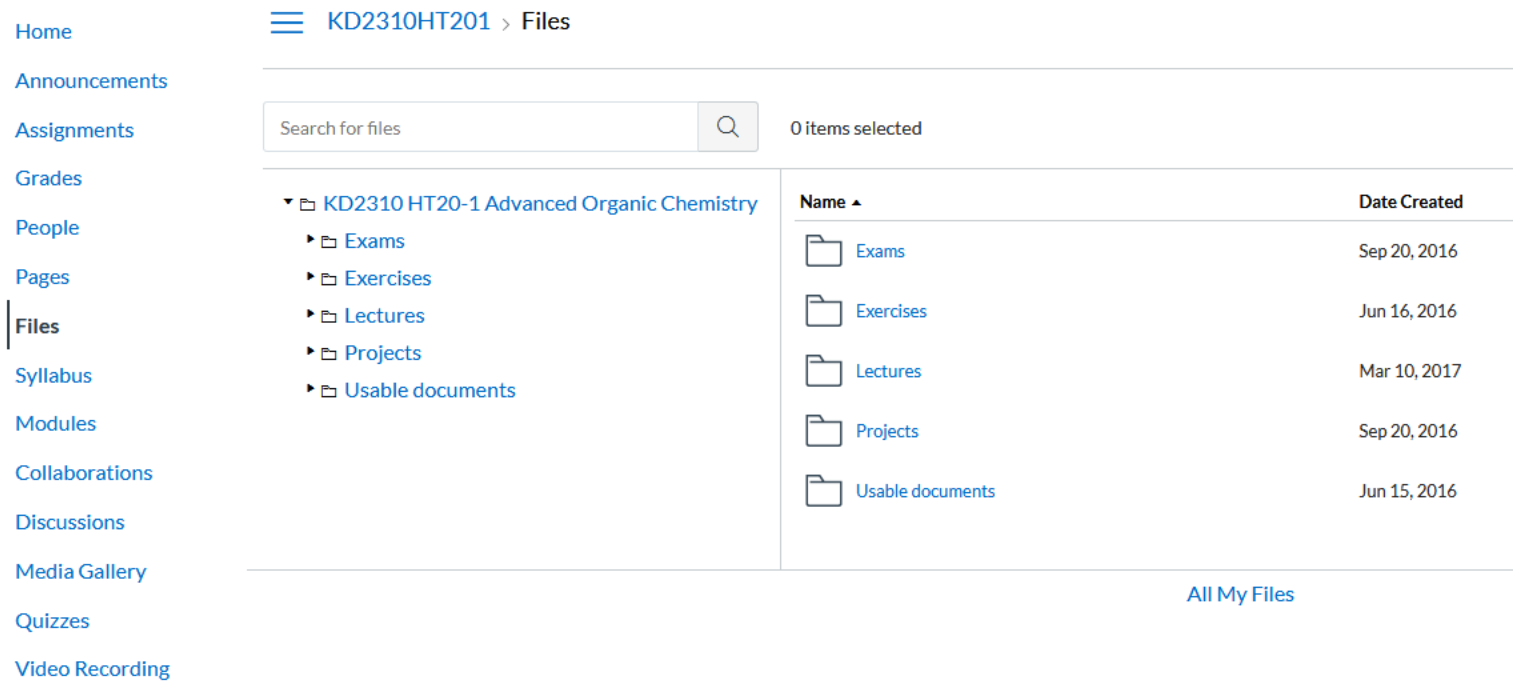
Click here

Upload your group´s presentation to Canvas



Click here to upload your presentation

Canvas: Files



Schedule week 35

w35	Monday 24/8	Tuesday 25/8	Wednesday 26/8	Thursday 27/8	Friday 28/8	Saturday 29/8	Sunday 30/8
8	08:00 Lecture KD2310 Helklass KD2310 D2 Peter Dinér TMMMM1 TMVTM1				08:00 Lecture KD2310 Helklass KD2310 Digital Peter Dinér TMMMM1 TMVTM1		
9							
10	10:00 		10:00 Lecture KD2310 Helklass KD2310 Digital Peter Dinér TMMMM1 TMVTM1		10:00 		
11							
12			12:00 				
13							
14							
15							
16							
17							

Schedule week 36

w36	Monday 31/8	Tuesday 1/9	Wednesday 2/9	Thursday 3/9	Friday 4/9	Saturday 5/9	Sunday 6/9
8	08:00 Lecture KD2310 Helklass KD2310 Digital Peter Dinér TMMMM1 TMVTM1						
9				**Exercise 1**			
10	10:00 		10:00 Lecture KD2310 Helklass KD2310 Digital Peter Dinér TMMMM1 TMVTM1		10:00 Exercise KD2310 grupp B KD2310 Q15 Markus Kärkäs TMMMM1 TMVTM1		
11							
12			12:00 		 		
13				Exercise KD2310 grupp A KD2310 D41 Markus Kärkäs TMMMM1 TMVTM1			
14							
15							
16							
17							

Anders Bøgevig

Green and safe synthesis, medchem, industrial processes

Schedule week 37

w37	Monday 7/9	Tuesday 8/9	Wednesday 9/9	Thursday 10/9	Friday 11/9	Saturday 12/9	Sunday 13/9
8	08:00 Lecture KD2310 Helklass KD2310 Digital Peter Dinér TMMMM1 TMVTM1				08:00 Lecture KD2310 Helklass KD2310 Digital Markus Kärkäs TMMMM1 TMVTM1		
9							
10	10:00 		10:00 Lecture KD2310 Helklass KD2310 Digital Markus Kärkäs TMMMM1 TMVTM1		10:00 		
11							
12			12:00 	**Exercise 2**			
13				Exercise KD2310 grupp A KD2310 Q26 Markus Kärkäs TMMMM1 TMVTM1	Exercise KD2310 grupp B KD2310 Q2 Markus Kärkäs TMMMM1 TMVTM1		
14							
15				15:00 	15:00 		
16							
17							

Schedule week 38

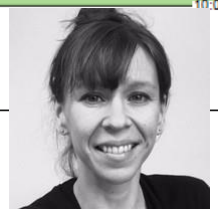
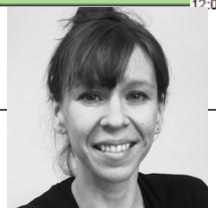
w38	Monday 14/9	Tuesday 15/9	Wednesday 16/9	Thursday 17/9	Friday 18/9	Saturday 19/9	Sunday 20/9
8	08:00 Lecture KD2310 Helklass KD2310 Digital Markus Kärkäs TMMMM1 TMVTM1						
9							
10			10:00 Lecture KD2310 Helklass KD2310 Digital Markus Kärkäs TMMMM1 TMVTM1		10:00 Exercise KD2310 grupp B KD2310 Q15 Markus Kärkäs TMMMM1 TMVTM1		
11							
12					 		
13				12:00 Exercise KD2310 grupp A KD2310 Q15 Markus Kärkäs TMMMM1 TMVTM1			
14							
15							
16							
17							

Exercise 3

Schedule week 39

w39	Monday 21/9	Tuesday 22/9	Wednesday 23/9	Thursday 24/9	Friday 25/9	Saturday 26/9	Sunday 27/9
8	08:00 Lecture KD2310 Helklass KD2310 Digital Markus Kärkäs TMMMM1 TMVTM1				08:00 Lecture KD2310 Helklass KD2310 Digital Helena Lundberg TMMMM1 TMVTM1		
9							
10	10:00 		10:00 Lecture KD2310 Helklass KD2310 Digital Markus Kärkäs TMMMM1 TMVTM1		10:00 		
11							
12			12:00 	**Exercise 4**			
13				Exercise KD2310 grupp A KD2310 D34 Markus Kärkäs TMMMM1 TMVTM1	Exercise KD2310 grupp B KD2310 Q22 Markus Kärkäs TMMMM1 TMVTM1		
14							
15							
16							
17							

Schedule week 40

w40	Monday 28/9	Tuesday 29/9	Wednesday 30/9	Thursday 1/10	Friday 2/10	Saturday 3/10	Sunday 4/10
8	08:00 Lecture KD2310 Helklass KD2310 Digital Helena Lundberg TMMMM1 TMVTM1						
9							
10	10:00 		10:00 Lecture KD2310 Helklass KD2310 Digital Helena Lundberg TMMMM1 TMVTM1				
11							
12			12:00 				
13				Exercise KD2310 grupp A KD2310 Q22 Markus Kärkäs TMMMM1 TMVTM1	Exercise KD2310 grupp B KD2310 V2 Markus Kärkäs TMMMM1 TMVTM1		
14							
15							
16							
17							

Exercise 5

Schedule week 41

w41	Monday 5/10	Tuesday 6/10	Wednesday 7/10	Thursday 8/10	Friday 9/10	Saturday 10/10	Sunday 11/10
8	08:00 Lecture KD23 lass KD23 Digital Helena Lu TMMMM1 TMVTM 10:00						
9			Group A		Group B		
10			Seminar KD2310 grupp A KD2310 Digital Markus Kärkäs TMMMM1 TMVTM1		Seminar KD2310 grupp B KD2310 Digital Markus Kärkäs TMMMM1 TMVTM1		
11							
12				Exercise 6			
13		Project seminars		Exercise KD2310 grupp A KD2310 Q36 Markus Kärkäs TMMMM1 TMVTM1	Exercise KD2310 grupp B KD2310 Q22 Markus Kärkäs TMMMM1 TMVTM1		
14							
15							
16							
17							

Schedule week 42

w42	Monday 12/10	Tuesday 13/10	Wednesday 14/10	Thursday 15/10	Friday 16/10	Saturday 17/10	Sunday 18/10
8							
9							
10							
11							
12							
13							
14							
15							
16							
17							

EXAM STUDY!

Schedule week 43

w43	Monday 19/10	Tuesday 20/10	Wednesday 21/10	Thursday 22/10	Friday 23/10	Saturday 24/10	Sunday 25/10
8							
9							
10							
11							
12							
13			EXAM				
14			Written Exam KD2310 Helklass KD2310 U41 U51 Markus Kärkäs TMMMM1 TMVTM1				
15							
16							
17							

Schedule week 45

w45	Monday 2/11	Tuesday 3/11	Wednesday 4/11	Thursday 5/11	Friday 6/11	Saturday 7/11	Sunday 8/11
8							
9							
10							
11							
12		12:00 Virtual KTH Global 2020	12:00 Virtual KTH Global 2020	12:00 Virtual KTH Global 2020			
13							
14		14:00	14:00	14:00			
15							
16							
17							

Complementary Exam

For exam results: 45–49 p (grade F_x)

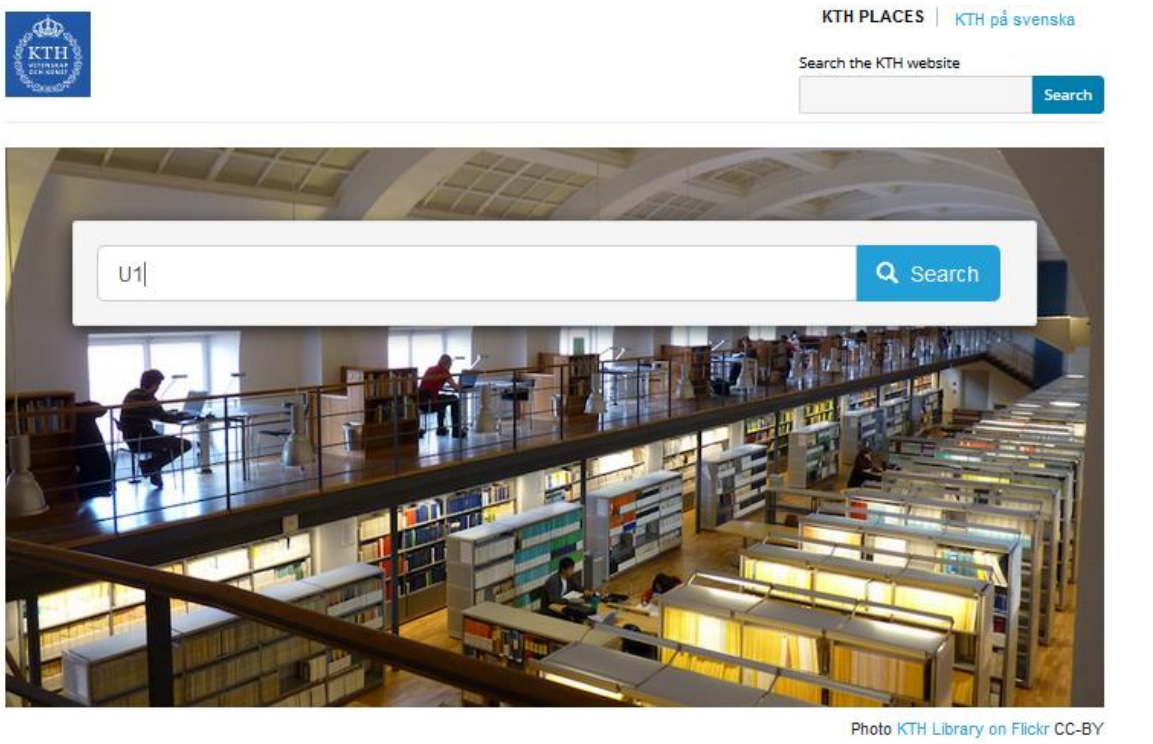
Re-exam (December 16, 2020)

w51	Monday 14/12	Tuesday 15/12	Wednesday 16/12	Thursday 17/12	Friday 18/12	Saturday 19/12	Sunday 20/12
8							
9							
10							
11							
12							
13							
14			14:00 Re-exam KD2310 K51 Markus Kärkäs TMMMM1 TMVTM1 20:00				
15							
16							
17							

RE-EXAM

Most difficult part of the course…

https://www.kth.se/places



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U1

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Address: Brinellvägen 28A

Floor: 6

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☐ Places 1

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Help us be better at search, share your ideas.

Some advice from previous students

"…ask as many questions as you can! The teachers are very approachable, and care about your learning, so take the opportunity when it's there!"

"Work hard before and during the workshops!"

"Prepare before the workshops"

"Work together to figure out mechanisms and solve problems continuously throughout the course. The workshop problems that are given are a good representation of what you will need to know on the exam, so use them! The book is also very helpful. Even though it is a big chunk of text associated with this course, the more you can prepare for lectures by reading ahead, the better!"

"Study consistently and do not hesitate to ask questions!"

Some advice from previous students

"Start going through the theory/different reactions as soon as you learn them in class! It will help you a lot!"

"Be prepared that there is a lot of mechanisms and very much information that you need to remember. Try to plan ahead and do not have too much on your plate while taking the course!"

"Work continuously during the period!"

"Keep up with the course content as much as possible! It is a lot better to understand the mechanisms and at least some of the exercises for each section of the course before the exam period than trying to learn everything at the end!"

…and don’t forget to have fun!