UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2018/19
Subject (*)	Stereoselective Synthesis		Code	610509113
Study programme	Mestrado Universitario en Investigación Química e Química Industrial (Plan 2017)			
Descriptors				
Cycle	Period	Year	Type	Credits
Official Master's Degree	Yearly	First	Optional	3
Language	Spanish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
Coordinador	Perez Sestelo, Jose	E-mail	jose.perez.sestelo@udc.es	
Lecturers	Perez Sestelo, Jose Sarandeses Da Costa, Luis Alberto	E-mail	jose.perez.sestelo@udc.es luis.sarandeses@udc.es	
Web	www.usc.es/gl/centros/quimica/curso/master.html			
General description	The subject covers the study of the generation of (new) stereocenters starting from substrates that contain stereocenters or proestereogenic units (C=C or C=X bonds). Therefore, incorporates fundamental concepts for the training in synthesis, such as the analysis of the Stereochemistry in chemical reactions, the conformational analysis of organic compounds and the reactivity models, including the diastereoselectivity induced by the substrate, the chiral auxiliary or a chiral-non racemic additive (catalyst, ligand).			

Study programme competences	
Code	Study programme competences
A1	Define concepts, principles, theories and specialized facts of different areas of chemistry.
A2	Suggest alternatives for solving complex chemical problems related to the different areas of chemistry.
A3	Innovate in the methods of synthesis and chemical analysis related to the different areas of chemistry
A8	Analyze and use the data obtained independently in complex laboratory experiments and relating them with the chemical, physical or biological appropriate techniques, including the use of primary literature sources
B1	Possess knowledge and understanding to provide a basis or opportunity for originality in developing and / or applying ideas, often within a research context
B2	Students should apply their knowledge and ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.
B4	Students should be able to communicate their conclusions, and the knowledge and the reasons that support them to specialists and non-specialists in a clear and unambiguous manner
B5	Students must possess learning skills to allow them to continue studying in a way that will have to be largely self-directed or autonomous.
B7	Identify information from scientific literature by using appropriate channels and integrate such information to raise and contextualize a research topic
B10	Use of scientific terminology in English to explain the experimental results in the context of the chemical profession

Learning outcomes			
Learning outcomes	Study programme competences		
? Use of the terms and definitions of chemical reactivity, and the proper description of stereoselective reactions	AC1	BC1 BC10	
? Use of the terms and definitions of chemical reactivity, and the proper description of stereoselective reactions	AC1	BC10	
? Capacity to visualise molecular structures using models generated by quantum mechanical computations	AC8	BC2	
? Ability to use and communicate, both in written and oral forms, the basic concepts of dynamic stereochemistry in Organic Chemistry		BC4	
Understand the relationship between the tridimensional structure of the organic compounds and their reactivity	AC3	BC5 BC7	

? Be familiar with the tridimensional representation of molecules, building the capacity to estimate their possible conformations.	AC1 AC8	BC1 BC7	
Understand the structural properties and the reactivity of the prostereogenic centers in those processes that generate new stereogenic elements.	AC3 AC8	BC1	
? Capacity to visualise molecular structures using models generated by quantum mechanical computations.	AC8	BC4	
? Rationally explain the outcome of a chemical reaction in terms of the Stereochemistry.	AC2 AC8	BC10	
? Understand the relationship between the tridimensional structure of the organic compounds and their reactivity		BC1 BC5	
? Understand the stereoelectronic effects and their role in chemical reactivity	AC8	BC1	
? Understand the value of the analysis of transition structures in chemical reactions, and be able to visualise those generated by quantum mechanical computations	AC8		
? Understand how the chirality of enantiopure compounds can be transmited to other chiral non-racemic products through chemical transformations	AC8	BC2	
? Quantity the relative ration of diastereoisomers and enantiomers using phisical and chemical methods.	AC3	BC1 BC7	
? Predict the outcome of a chemical reaction that generates novel stereocenters	AC8	BC1	
? Acquire and utilize the existing literature on synthetic processes in which stereocenters are generated.	AC8	BC5	
? Understand the structural properties and the reactivity of the prostereogenic centers in those processes that generate new stereogenic elements.	AC8	BC1 BC7	
? Rationally explain the outcome of a chemical reaction in terms of the Stereochemistry		BC1 BC7	
? To know the main classes of reactions that generate stereocenters, and understand their mechanisms.	AC3 AC8		

Contents	
Topic	**Sub-topic**
Chapter 1. Stereochemistry in chemical reactions. Conformational control of stereoselectivity	Chirality. Stereogenic units. Topicity. Diastereoselectivity and enantioselectivity. The ?chiral pool?: chiral auxiliaries and chiral ligands. Kinetic resolution. Conformational control of the diastereoselectivity. Stereoelectronic effects. The Curtin-Hammett principle.
Chapter 2. Additions to C=C trigonal centers	Additions to C=C bonds. Diastereoselective epoxidations of acyclic and cyclic olefins. Enantioselective epoxidations (Sharpless, Jacobsen, Shi). Synthetic applications of epoxyalcohols. Diastereoselective dihydroxylations of acyclic and cyclic olefins. Sharpless enantioselective dihydroxylation (SAD). Sharpless enantioselective aminohydroxylation (SAA). Diastereoselective olefin hydrogenation. Enantioselective hydrogenation
Chapter 3. Additions to C=O trigonal centers.	Addition to C=X bonds. Sterecontrol in nucleophilic additions to carbonyl groups in acyclic and cyclic compounds. 1,2 and 1,3-Asymmetric induction models. Enantioselective additions to ketones. Nucleophilic additions to imines and sulfinamides.
Chapter 4. Conjugate additions to C=C-C=X systems	Conjugate additions to C=C-C=O systems. Diastereoselective conjugate additions. Catalytic asymmetric conjugate additions. Reduction of conjugated systems. Asymmetric epoxidation of enones.
Chapter 5. Additions to C=C-X systems	Additions to C=C-OM bonds. Regio- y stereoselective synthesis of enolates. Diastereoselective reactions of chiral enolates: alkylation, halogenation, amination and hydroxilation. Diastereoselective reactions of chiral azaenolates

Chapter 6. Reactions between trigonal centers	Reactions between trigonal centers: generation of two or more stereocenters. Aldol reaction: control of the diastereoselectivity. The Zimmerman-Traxler model. Organocatalyzed aldol reactions. Aldol Mukaiyama reaction of latent enolates. Double diastereoselection: chiral centers on the components of the aldol reaction. Addition of allyl organometals to carbonyl groups. Allylic boranes. Allylic stannanes and silanes: catalysis by chiral Lewis acids and bases. Addition of allyl organometals to imines. Diastereoselectivity in Diels-Alder cycloadditions

Planning				
Methodologies / tests	Competencies	Ordinary class hours	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A1 B1 B10	12	24	36
Seminar	A8 B1	5	20	25
ICT practicals	A2 A3 A8 B2 B4 B5 B7	2	4	6
Objective test	A1 A8 B1 B2 B10	3	3	6
Personalized attention		2	0	2
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	Description
Guest lecture / keynote speech	It will be held 12 sessions of lectures in one group where the theoretical contents of the course will be presented with illustrative examples. It will consist mainly of PowerPoint presentations. Copies of these presentations will be made available to the students in advance of the course via the virtual campus. This will allow the students to study ahead the contents of the course and will facilitate the monitoring of explanations. Attendance to these lectures is mandatory
Seminar	4 sessions in small group seminars where students will present the work proposed by the professor followed by a discussion section. Students will have access to the proposed exercises and papers in advance via the virtual campus of the course. Attendance to these classes is mandatory
ICT practicals	3 sessions in small group seminars where students will have the opportunity to visualize the transition structures generated by computational methods that correspond to the main reaction of the course. Attendance to these classes is mandatory.
Objective test	A written exam will be performed with the purpose to measure the knowledge adquired during the course

Personalized attention	
Methodologies	Description
Guest lecture / keynote speech Seminar ICT practicals Objective test	Tutoring scheduled by the professor and coordinated by the Centre. It will be 2 hours per student and will involve the supervision of proposed work, clarifying doubts, etc. Attendance to these classes is mandatory.

Assessment			
Methodologies	Competencies	Description	**Qualification**
Guest lecture / keynote speech	A1 B1 B10	Attendance and participation	5
Seminar	A8 B1	Continuous assessment (N1) will be 35% of the qualification and will consist of two components: interactive class in small groups (seminars) and interactive class in very small groups (tutorials). Seminars and tutorials include the following: resolution of exercises and practical cases (15%), realization of homework and reports (10%), oral presentations [(papers, reviews and practical cases), 10%].	35

Objective test	A1 A8 B1 B2 B10	The final exam (N2) will cover all the contents of the course.	60

Assessment comments
The student's score will result of applying the following formula: Final score = 0.4 x N1 + 0.6 x N2 N1 and N2 are the marks corresponding to the continuous assessment (0-10 scale) and the final exam (0-10 scale), respectively. The repeaters will have the same system of class attendance than those who study the course for first time.

Sources of information	
Basic	- Corey, E. J.; Kürti, L. (2010). Enantioselective Chemical Synthesis. Methods, Logic and Practice. Direct Book Publishing: LLC - Mulzer, J.; , Jacobsen, E. N.; Pfaltz, A.; Yamamoto, Y. (1999). Basic Principles of Asymmetric Synthesis, In Comprehensive Asymmetric Catalysis. Springer, Heidelberg - Koskinen, A. M. P (2012). Asymmetric Synthesis of Natural Products. Wiley, New York
Complementary	- Procter, G. (1996). Asymmetric Synthesis. Oxford University Press, Oxford - Corey, E. J.; Kürti, L. (2010). Enantioselective Chemical Synthesis.Methods, Logic and Practice. Direct Book Publishing: LLC - Atkinson, R. S. (1995). Stereoselective Synthesis. Chichester, UK:John Wiley & Sons - Ager, D. J.; East, M. B. (1996). Asymmetric Synthetic Methodology. CRC Press, Boca Raton, FL

Recommendations
Subjects that it is recommended to have taken before
/ /
Subjects that are recommended to be taken simultaneously
/
Subjects that continue the syllabus
Other comments
The students should review the theoretical concepts introduced in each chapter using the reference manual and the material provided by the professor. Those students, which have significant difficulties when working the proposed activities, should contact with the professor during the tutorials, in order to analyze the problem and to receive the necessary support. The professor will analyze with those students who do not successfully pass the evaluation, and so wish, their difficulties in learning the course content. Additional material (questions, exercises, tests, etc..) to strengthen the learning of the course might be also provided.