

PhD Programme in CHEMICAL SCIENCE AND TECHNOLOGY in collaboration with the University of Sassari	
DISCIPLINARY SCIENTIFIC AREAS	02 - PHYSICAL SCIENCES; 03 - CHEMICAL SCIENCES; 09 - INDUSTRIAL AND INFORMATION ENGINEERING
COORDINATOR	PROF. CARLA CANNAS
HEAD DEPARTMENT	DEPARTMENT OF CHEMICAL AND GEOLOGICAL SCIENCES
DURATION	3 YEARS
LEARNING OUTCOMES AND RESEARCH TOPICS	<p>The activity of the PhD in Chemical Sciences and Technologies mainly includes 18 key research topics that constitute the cultural basis of PhDs. Within them, the training of the PhD provides a specific and personalized program with the aim of orienting the pre-existing basic preparation of the PhD student towards the acquisition of specialized skills, beside the general methodological aspects of the research approach.</p> <p>The main issues proposed for the research activities are the following:</p> <ol style="list-style-type: none"> 1. Nanostructured materials. Synthesis, functionalization and chemical-physical characterization of new nanostructured, inorganic and hybrid materials for applications in heterogeneous catalysis, energy, environment, sensors, cultural heritage, and biomedicine. Development of eco-friendly synthesis strategies and from industrial and mining waste. 2. Complex biological systems. Experimental and theoretical studies and metabolomic investigations. 3. Modeling and computational chemistry. Development of simulation techniques, computational studies of complex systems of chemical interest. Applied quantum electrodynamics and development of the theory of dispersion forces. 4. Thermodynamic characterization of liquid mixtures. Experimental and theoretical studies of the thermodynamic properties of mixing of binary or ternary liquid mixtures containing ionic liquids. 5. Industrial catalytic processes. Process chemical technologies. Study of catalytic processes (preparation, stability, regeneration). 6. Bio-nanointerphases. Study of the interactions between biomacromolecules and 'hard' and 'soft' nanostructures. Experimental and theoretical-computational studies on the specific effects of electrolytes on biomolecules and/or nanostructures. 7. Development of analytical methodologies for the characterization of metallic, polymeric, nanomaterials and functionalized surfaces for applications in the field of renewable energy, the environment, sensors, health and cultural heritage. 8. Application of conventional and supercritical carbon dioxide extraction technologies on vegetable and agro-food matrices, and chemical and biological characterization of the extracts. 9. Design and development of new synthesis methodologies for obtaining complex organic molecules and their applications in the biomedical and technological fields. Design of new catalytic and environmentally friendly processes with low environmental impact and valorisation of agricultural and industrial waste. 10. Synthesis, characterization, properties and reactivity of new inorganic or organometallic compounds. Structural, spectroscopic, computational characterization and catalytic, biological and pharmacological properties of compounds of applicative interest.

11. Molecular materials. Development of coordination polymer complexes and polymers, 2D and 3D Metal Organic Frameworks, for applications in electronics, spintronics, energy and as molecular fluorescence and redox sensors for metal ions and inorganic anions and organic molecules. Supramolecular architectures based on weak interactions for the development of new intelligent materials. Reactivity studies, molecular spectroscopies, solution equilibria and calculation methodologies.
12. Analytical methodologies and applications. Synthesis and spectroscopic and electrochemical characterization of organic, inorganic and organometallic based materials for applications in sensors, photosensitive devices, electrocatalysis. Setting up, validation and application of instrumental analysis methods to real matrices. Analytical typification of agri-food productions. Food safety. Studies on bioaccumulation of toxic elements in biotic matrices. Environmental analysis and monitoring, bioanalysis.
13. Design, synthesis and characterization of new metal ligands and complexes with biological properties (antitumor, antioxidants) and of interest in the environmental field (sensors for toxic metals). Calculations of molecular mechanics, molecular docking and chemometric approach for the determination of structure-activity relationships.
14. Design, synthesis and biological evaluation of small molecules. Synthesis, characterization and biological evaluation of new chemical structures with potential pharmacological activity.
15. Chemistry and pharmaceutical technologies. Design and development of nanosystems for site-specific delivery of bioactive molecules and for diagnostics/theranostics. Design and testing of innovative platforms for the delivery of drugs through different routes of administration.
16. Pharmaceutical and toxicological chemical analysis. Validation of analytical methodologies for the determination of drugs, designer drugs and metabolites in biological matrices.
17. Cultural heritage. Archaeometric studies on ceramics, pigments, obsidian and metal-based finds. Application of diagnostic techniques for in-situ analysis. Synthesis, characterization and application of inorganic consolidants for the conservation and restoration of stone cultural heritage. Innovative strategies for conservation through the kinetic control of mineralogical and inhibitory processes.
18. Polymeric materials. Synthesis and characterization of new polymeric materials and polymeric devices for applications in energy, environment and biomedicine. Innovative processing techniques.

The PhD programme aims to train highly qualified young scientists in the field of chemistry, offering to young Italian and foreign graduates the opportunity to independently develop an original and innovative research project in the most advanced fields of chemical sciences and technologies. To this end, PhD students are trained, within the different research topics, through a constant experimental and / or theoretical research activity and an appropriate educational path.

The PhD student will acquire the knowledge, the scientific method and will develop a careful critical spirit to carry out high-level research activities in multiple interdisciplinary fields of interest in Chemistry both nationally and internationally. The centrality of Chemical Sciences is widely recognized and has a transversal character to different scientific disciplines (physics, biology, engineering, geology, pharmacy, archeology) for which it finds applications in a wide variety of fields ranging from materials science to biomedicine, from energy to agriculture, from electronics to biology, from the conservation of cultural heritage to the environment protection. This training path will allow

	<p>the PhD to acquire a deep basic as well as specialized knowledge that will allow him to actively contribute to the progress of chemical sciences both in the industrial field and in the academic one, in a context of global international competition. To achieve this goal, the PhD student is offered the opportunity to come into contact with national and foreign researchers and research institutions and to carry out a period of research activity abroad, in highly qualified foreign research institutions and to get in touch with the world of industry. In addition, the Doctoral Course provides a great variety of advanced courses and seminars for PhD students and it promotes the participation to national and international schools, workshops and conferences.</p>
<p>ELIGIBILITY AND OTHER REQUIREMENTS FOR CANDIDATES (ART. 2 - NOTICE OF COMPETITION)</p>	<p>LM-6 Biologia LM-8 Biotecnologie industriali LM-9 Biotecnologie mediche, veterinarie e farmaceutiche LM-11 Scienze per la conservazione dei beni culturali LM-13 Farmacia e farmacia industriale LM-17 Fisica LM-22 Ingegneria chimica LM-35 Ingegneria per l'ambiente e il territorio LM-53 Scienza e ingegneria dei materiali LM-54 Scienze chimiche LM-71 Scienze e tecnologie della chimica industriale LM-75 Scienze e tecnologie per l'ambiente e il territorio LM Sc. Mat. Scienze dei materiali LM-53. Ingegneria dei materiali 61/S (specialistiche in scienza e ingegneria dei materiali) 62/S (specialistiche in scienze chimiche) 81/S (specialistiche in scienze e tecnologie della chimica industriale) 82/S (specialistiche in scienze e tecnologie per l'ambiente e il territorio)</p> <p>Foreign candidates: Similar qualification awarded abroad and declared equivalent by the PhD Academic Board, for the only purpose of admission to the PhD programme.</p>
<p>ADMISSION TESTS</p>	<p>ASSESSMENT OF QUALIFICATIONS AND CURRICULUM VITAE, AND INTERVIEW The interview will be aimed at verifying the candidate's ability to orient himself/herself on the main fields of study related to the Doctorate and to verify his/her knowledge in chemical sciences and technologies, skills of analysis, elaboration and communication, and can take place, at the request of the candidate, also in English. During the interview, the candidate will discuss his/her 3-year research project. The project (preferably written in English) must be uploaded along with the documents listed in art. 3 of the PhD notice of competition (<i>Annex A "Titoli valutabili e Curriculum Vitae"; Annex B "Dichiarazione sostitutiva di certificazioni del/i titolo/i di accesso con esami e voti"; two-sided coloured scanned copy of a valid ID, with a clear photo</i>), within the deadline (file name: progetto_di_ricerca_surname_name). Candidates who are unable, for justified reasons, to take the interview at the established location, may be given the opportunity to conduct it by teleconference, on the same date and time established for face-to-face interviews, according to the instructions of the notice of competition.</p>
<p>ADMISSION TESTS FOR FOREIGN CANDIDATES APPLYING FOR RESERVED POSITIONS SUPPORTED BY A SCHOLARSHIP</p>	<p>ASSESSMENT OF QUALIFICATIONS AND CV, VIDEO CONFERENCE INTERVIEW The interview will focus mainly on the experiences gained by the candidate in the topics specific to the Doctorate and on the topics that he/she would propose as a possible object of the activity to be developed during the three-year PhD programme. During the interview, the candidate will discuss a three-year research project, which must be submitted in addition to the documents required in art. 3 of the</p>

	<p>notice of competition (<i>certificate attesting the award of a 2nd level foreign degree needed to access a PhD programme, including exams and marks, with a translation in Italian or English; certificate attesting the award of a 1st level foreign degree, including and marks, with a translation in Italian or English; signed Curriculum Vitae preferably in EU format, in English or Italian; additional qualifications, certifications, publications (up to 5) and work experiences, detailed in English or in Italian; two-sided coloured scanned copy of a valid passport, with a clear photo</i>), within the deadline (file name: research project_surname_name).</p> <p>During the interview, the candidate's language skills in English will be assessed. His/Her exposition skills, clarity in describing the objectives and methods of the project, as well as the accuracy of his/her scientific language will also be evaluated.</p> <p>Reference letters must be written in English, using the form available on the webpage https://unica.it/dottoraticerca (How to apply for PhD selection: Guidelines and forms- Annex D), by a university professor or an expert in the research fields of the PhD programme, on letterhead of their institution, dated and signed. Evaluators will send their letters directly to the email address phdcall_referenceletter@unica.it (object: surname and name of the candidate being evaluated and name of the PhD programme for which he/she is applying).</p>
POSITIONS	14
SCHOLARSHIPS	12: 1 funded by UniCa; 3 funded by Ministerial Decree no. 118/2023: 1 NRRP Research, 1 Public Administration, 1 Cultural Heritage; 4 funded by Ministerial Decree no. 117/2023; 4 funded by the affiliated institution: 4 funded by the University of Sassari with funds from Ministerial Decree no. 118/2023: 2 NRRP Research, 1 Public Administration, 1 Cultural Heritage
POSITIONS WITHOUT SCHOLARSHIP	2
CONTACT PERSON	PROF. CARLA CANNAS EMAIL: ccannas@unica.it - TEL. +39 0706754380
WEBSITE	https://people.unica.it/dottoratoinchimica https://www.uniss.it/node/8694

SCHOLARSHIPS FUNDED BY MINISTERIAL DECREE NO. 118/2023

SCHOLARSHIP 1

TYPOLOGY	NRRP Research
RESEARCH PROJECT	Complex biological systems and related experimental and theoretical studies
PRINCIPAL INVESTIGATOR	Prof. Carla Cannas
DESCRIPTION OF DOCTORAL TRAINING	The doctoral programme will be characterized by an appropriate training path, through the attendance of advanced and transversal specialist courses, scientific schools and national and international congresses, and by a constant experimental and/or theoretical research activity developed within the institutions and industries involved. The PhD student will carry out periods of research activity in highly qualified foreign/Italian institutions and/or industries to promote the transfer of technology from basic to applied research. Through this path, the doctoral student will develop the skills, the scientific method and a careful critical spirit in order to carry out high-level research activities in multiple interdisciplinary fields of interest in Chemistry both at national and international level.
COMPANY/RESEARCH INSTITUTION/PUBLIC ADMINISTRATION	The company/research institution where the activity will be carried out and the relative contact person will be defined after the conclusion of the selection proceedings.

NO. OF MONTHS TO BE SPENT IN THE COMPANY/RESEARCH INSTITUTION/PUBLIC ADMINISTRATION	6-12
FOREIGN INSTITUTION	The foreign institution where the activity will be carried out and the relative contact person will be defined after the conclusion of the selection proceedings.
NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6
SCHOLARSHIP 2	
TYPOLOGY	Public Administration
RESEARCH PROJECT	Innovative organic and hybrid materials for energy efficiency, construction industry, and improvement of air quality in public buildings
PRINCIPAL INVESTIGATOR	Prof. Carla Cannas
DESCRIPTION OF DOCTORAL TRAINING	The doctoral programme will be characterized by an appropriate training path, through the attendance of advanced and transversal specialist courses, scientific schools and national and international congresses, and by a constant experimental and/or theoretical research activity developed within the institutions and industries involved. The PhD student will carry out periods of research activity in highly qualified foreign/Italian institutions and/or industries to promote the transfer of technology from basic to applied research. Through this path, the doctoral student will develop the skills, the scientific method and a careful critical spirit in order to carry out high-level research activities in multiple interdisciplinary fields of interest in Chemistry both at national and international level.
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FOREIGN INSTITUTION	The foreign institution where the activity will be carried out and the relative contact person will be defined after the conclusion of the selection proceedings.
NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6
SCHOLARSHIP 3	
TYPOLOGY	Cultural Heritage
RESEARCH PROJECT	Design of innovative materials and application and development of analytical and chemical-physical techniques for the study and valorization of cultural heritage
PRINCIPAL INVESTIGATOR	Prof. Carla Cannas
DESCRIPTION OF DOCTORAL TRAINING	The doctoral programme will be characterized by an appropriate training path, through the attendance of advanced and transversal specialist courses, scientific schools and national and international congresses, and by a constant experimental and/or theoretical research activity developed within the institutions and industries involved. The PhD student will carry out periods of research activity in highly qualified foreign/Italian institutions and/or industries to promote the transfer of technology from basic to applied research. Through this path, the doctoral student will develop the skills, the scientific method and a careful critical spirit in order to carry out high-level research activities in multiple interdisciplinary fields of interest in Chemistry both at national and international level.
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NO. OF MONTHS TO BE SPENT	6-12

IN THE COMPANY/RESEARCH INSTITUTION/PUBLIC ADMINISTRATION	
FOREIGN INSTITUTION	The foreign institution where the activity will be carried out and the relative contact person will be defined after the conclusion of the selection proceedings.
NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6
SCHOLARSHIPS FUNDED BY MINISTERIAL DECREE NO. 117/2023	
SCHOLARSHIP 1	
TYPOLOGY	Innovative doctorates responding to the innovation needs of companies and promoting the recruitment of researchers by companies (M4C2 - Inv. 3.3)
RESEARCH PROJECT	Production of fertilizers from agricultural and industrial waste
PRINCIPAL INVESTIGATORS	Prof. Tiziana Pivetta
DESCRIPTION OF DOCTORAL TRAINING	The doctoral student will carry out the curricular training courses provided by the PhD programme in Chemical Sciences and Technologies, choosing among the various courses, on basis of relevance to the topics of his/her own research project. He/She will have to participate in schools, conferences or workshops to present the results of his/her research.
COMPANY/RESEARCH INSTITUTION	Comase srl Santa Vittoria d'Alba (CN), Italia Contact person: dott.ssa Paola Casti
NO. OF MONTHS TO BE SPENT IN THE COMPANY/RESEARCH INSTITUTION	10
FOREIGN INSTITUTION	SALVUM INVESTMENT Bucarest, Romania Contact person: Dr. Emilio Brunetti
NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6
SCHOLARSHIP 2	
TYPOLOGY	Innovative doctorates responding to the innovation needs of companies and promoting the recruitment of researchers by companies (M4C2 - Inv. 3.3)
RESEARCH PROJECT	Mechanochemistry in Cosmetics: Beauty turns Green
PRINCIPAL INVESTIGATORS	Prof. Andrea Porcheddu
DESCRIPTION OF DOCTORAL TRAINING	During the three-year period, the PhD student will gain theoretical and practical skills in synthesizing molecules of cosmetic relevance by mechanochemical activation. The student will attend several national and international schools to improve his knowledge of the main green techniques of organic synthesis. During the period abroad, he/she will work on organic synthesis using extruders. During the six months in the company, all synthetic and regulatory issues related to the industrial production of biochemicals will be explored.
COMPANY/RESEARCH INSTITUTION	CRB Benelux BV Legal head office: Oxfordlaan 70 - 6229 Maastricht, The Netherlands Contact person: Pietro Agostino Rando
NO. OF MONTHS TO BE SPENT IN THE COMPANY/RESEARCH INSTITUTION	6
FOREIGN INSTITUTION	Aachen University, Institute of Organic Chemistry, RWTH Legal head office: Landoltweg 1 - 52074 Aachen, Germany Contact person: Prof. Dr. Carsten Bolm
NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6
SCHOLARSHIP 3	
TYPOLOGY	Innovative doctorates responding to the innovation needs of companies and promoting the recruitment of researchers by companies (M4C2 - Inv. 3.3)

RESEARCH PROJECT	Enabling technologies lay the ground for more sustainable production processes
PRINCIPAL INVESTIGATORS	Prof. Andrea Porcheddu
DESCRIPTION OF DOCTORAL TRAINING	Over the course of three years, the Ph.D. student will acquire theoretical and practical skills in synthesizing molecules of pharmaceutical interest using the latest and most advanced technologies (enabling technologies) available in academia and industry. The student will attend various national and international schools to improve their knowledge of the leading green techniques of organic synthesis. During the period abroad, at Prof. C. Oliver Kappe's laboratory, University of Graz, Institute of Chemistry Heinrichstrasse 28, 8010 Graz, Austria, he/she will work on organic synthesis using continuous flow devices. During the in-company training period, the student will gain access to several cutting edge flow devices do not present in the laboratories of the University of Cagliari. In addition, the training provided within the company will address synthetic and regulatory concerns regarding manufacturing active ingredients in an industrial setting.
COMPANY/RESEARCH INSTITUTION	Chiesi Farmaceutici S.p.A. Legal head office: Largo F. Belloli, 11 - 43122 Parma Contact person: Dr. Edoardo Mariani
NO. OF MONTHS TO BE SPENT IN THE COMPANY/RESEARCH INSTITUTION	9
FOREIGN INSTITUTION	University of Graz, Institute of Chemistry Legal head office: Heinrichstrasse 28, Graz - Austria Contact person: Prof. C. Oliver Kappe
NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6
SCHOLARSHIP 4	
TYPOLOGY	Innovative doctorates responding to the innovation needs of companies and promoting the recruitment of researchers by companies (M4C2 - Inv. 3.3)
RESEARCH PROJECT	Mechanochemistry and Enabling Technologies: a Revolutionary and Environmentally-friendly Approach to Active Pharmaceutical Ingredients
PRINCIPAL INVESTIGATORS	Prof. Andrea Porcheddu
DESCRIPTION OF DOCTORAL TRAINING	During the three-year period, the doctoral student will gain theoretical and practical skills in synthesizing molecules of pharmaceutical relevance by mechanochemical activation. The student will attend several national and international schools to improve his knowledge of the main green techniques of organic synthesis. During the period abroad, he/she will work on organic synthesis using extruders. During the six months in the company, all synthetic and regulatory issues related to the industrial production of active ingredients will be explored.
COMPANY/RESEARCH INSTITUTION	Angelini Pharma S.p.A. Legal head office: Viale Amelia, 70 - 00181 Roma Contact person: Dr. Giuliano Caracciolo Torchiarolo
NO. OF MONTHS TO BE SPENT IN THE COMPANY/RESEARCH INSTITUTION	8
FOREIGN INSTITUTION	Ruhr-Universität Bochum, Lehrstuhl für Anorganische Chemie Legal head office: Universitätsstraße 150, NCDF 04/399 - 44801 Bochum, Germany Contact person: Prof. Lars Borhardt
NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6

SCHOLARSHIPS FUNDED BY THE AFFILIATED INSTITUTION UNDER MINISTERIAL DECREE NO. 118/2023	
SCHOLARSHIP 1 - University of Sassari	
TYPOLOGY	NRRP Research
RESEARCH PROJECT	Experimental and/or theoretical studies of complex inorganic/organic systems for environment/energy/biomedicine or construction industry
PRINCIPAL INVESTIGATORS	Prof. Carla Cannas
DESCRIPTION OF DOCTORAL TRAINING	The doctoral programme will be characterized by an appropriate training path, through the attendance of advanced and transversal specialist courses, scientific schools and national and international congresses, and by a constant experimental and/or theoretical research activity developed within the institutions and industries involved. The PhD student will carry out periods of research activity in highly qualified foreign/Italian institutions and/or industries to promote the transfer of technology from basic to applied research. Through this path, the doctoral student will develop the skills, the scientific method and a careful critical spirit in order to carry out high-level research activities in multiple interdisciplinary fields of interest in Chemistry both at national and international level.
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NO. OF MONTHS TO BE SPENT IN THE COMPANY/RESEARCH INSTITUTION	6-12
FOREIGN INSTITUTION	The foreign institution where the activity will be carried out and the relative contact person will be defined after the conclusion of the selection proceedings.
NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6
SCHOLARSHIP 2 - University of Sassari	
TYPOLOGY	NRRP Research
RESEARCH PROJECT	Design, synthesis, and biological evaluation of novel molecular scaffolds for pharmaceutical
PRINCIPAL INVESTIGATORS	Prof. Carla Cannas
DESCRIPTION OF DOCTORAL TRAINING	The doctoral path will be characterized by an appropriate training path, through the attendance of advanced and transversal specialist courses, scientific schools and national and international conferences, and by a constant activity of experimental and/or theoretical research developed within the institutions and companies involved. The PhD student will carry out periods of research activity in highly qualified foreign institutions and/or industrial realities to favour the transfer of technology from basic to applied research. Through this path, the PhD student will develop the skills, the scientific method and a careful critical spirit in order to carry out high-level research activities in multiple interdisciplinary fields of interest in Chemistry both at national and international level.
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NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6

SCHOLARSHIP 3 - University of Sassari	
TYPOLOGY	Public Administration
RESEARCH PROJECT	Design, synthesis and public regulation of new drugs of strategic interest for pathologies with a high national impact
PRINCIPAL INVESTIGATORS	Prof. Carla Cannas
DESCRIPTION OF DOCTORAL TRAINING	The doctoral path will be characterized by an appropriate training path, through the attendance of advanced and transversal specialist courses, scientific schools and national and international conferences, and by a constant activity of experimental and/or theoretical research developed within the institutions and companies involved. The PhD student will carry out periods of research activity in highly qualified foreign institutions and/or industrial realities to favour the transfer of technology from basic to applied research. Through this path, the PhD student will develop the skills, the scientific method and a careful critical spirit in order to carry out high-level research activities in multiple interdisciplinary fields of interest in Chemistry both at national and international level.
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FOREIGN INSTITUTION	The foreign institution where the activity will be carried out and the relative contact person will be defined after the conclusion of the selection proceedings.
NO. OF MONTHS TO BE SPENT IN THE FOREIGN INSTITUTION	6
SCHOLARSHIP 4 - University of Sassari	
TYPOLOGY	Cultural Heritage
RESEARCH PROJECT	Innovative diagnostic techniques for the study of materials and the valorization of cultural heritage
PRINCIPAL INVESTIGATORS	Prof. Carla Cannas
DESCRIPTION OF DOCTORAL TRAINING	The doctoral path will be characterized by an appropriate training path, through the attendance of advanced and transversal specialist courses, scientific schools and national and international conferences, and by a constant activity of experimental and/or theoretical research developed within the institutions and companies involved. The PhD student will carry out periods of research activity in highly qualified foreign institutions and/or industrial realities to favour the transfer of technology from basic to applied research. Through this path, the PhD student will develop the skills, the scientific method and a careful critical spirit in order to carry out high-level research activities in multiple interdisciplinary fields of interest in Chemistry both at national and international level.
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