Ficha LA - versão 2.1

A - Caracterização do LA	**LA**	1. Nome/Designação do LA	Institute of Molecular Sciences
		2. Acrónimo do LA	IMS
		3. Referência FCT	LA/P/00056/2020
		4. Coordenador do LA	José Nuno Canongia Lopes; jnlopes@tecnico.ulisboa.pt
		5. Data da atribuição do estatuto de LA	NA
		6. Webpage	NA
		7. Classificação FCT	4,25
		8. Financiamento Complementar FCT Total	1200 k€
	Unidade de I&D Principal	1. Nome/Designação da Unidade de I&D	Centro de Química Estrutural
		2. Acrónimo	CQE
		3. Personalidade jurídica	IST-ID
		4. Coordenador	José Nuno Canongia Lopes; jnlopes@tecnico.ulisboa.pt
		5. Contactos gerais	https://cqe.tecnico.ulisboa.pt/
		6. Webpage	https://cqe.tecnico.ulisboa.pt/
		7. Classificação FCT	Excelente
		8. Financiamento Base FCT Total	3258 k€
		9. Financiamento Programático FCT Total	940 k€
	Unidade de Gestão Principal	1. Nome/Designação	IST-ID, Associação do Instituto Superior Técnico para a Investigação e Desenvolvimento
		2. Personalidade jurídica	IST-ID, Associação do Instituto Superior Técnico para a Investigação e Desenvolvimento, instituição privada sem fins lucrativos

B - Constituição da equipa de investigação do LA	N.º de investigadores integrados com PhD		270
	N.º de ETIs integrados		NA
	N.º de técnicos		4
	N.º de doutorandos		100
	N.º de outros colaboradores com PhD		50
	N.º de outros colaboradores sem PhD		120

C - Missão do LA	1. Mission Statement/Objetivos principais		The Institute of Molecular Sciences, IMS, is composed of three R&D units, CQE, CQC and CIQUP, that excel in the scientific area of chemical sciences. Unlike R&D models that are mainly focused on a single facet or application of the chemical sciences, the three R&D units of IMS are involved in a plethora of sub-areas ranging from single-molecule processes and catalysis to functional materials and soft matter, from specialty chemicals to heavy-duty commodities, from environmental concerns to health-related matters, from fundamental to applied research, from issues related to the awareness of the Chemical Sciences to their communication. The impact of this research and its socioeconomic value is well evidenced by the multiple patents applications over the last 5 years and creation of +10 spin-off companies. The multi-disciplinarity and inter-disciplinarity character of IMS enables the development of both blue-sky and applied research lines aimed to provide solutions of specific societal challenges that can be confronted using chemistry and molecular-based tools. Research is organized around five Thematic Lines (TLs): MATsoft (Materials, soft matter and nanoscience); MEDlife (Medicinal, biological and biophysical chemistry for health); H2Oenv (Technologies for water, environment and energy); SYNcat (Synthesis, catalysis and chemical processes); and CHEMfocus (Fundamentals and

D - Áreas Científicas	1. Área Científica 1		Materials, soft matter and nanosciences
	2. Área Científica 2		Medicinal, biological and biophysical chemistry for Health
	3. Área Científica 3		Technologies for water and environment
	4. Área Científica 4		Synthesis, catalysis and chemical processes
	5. Área científica 5		Fundamentals and Awareness

F - Linhas Temáticas	1. Linha Temática 1		
		1. Designação da LT	MATsoft – Materials, soft matter and nanosciences
		2. Coordenador da LT	
		3. Contactos do Coordenador	
		4. Descrição da LT	The TL Materials, Soft Matter and Nanosciences (MATsoft) gathers complementary and multidisciplinary expertise from dynamic research groups in the three research units of IMS, that work in different areas of materials chemistry, nanosciences, materials science and engineering, strongly underpinned in powerful research infrastructures and instrumental platforms. MATsoft researchers address a wide range of themes, not only from a fundamental curiosity-driven approach, deeply rooted in molecular sciences, but also targeting applications, transfer of knowledge, intellectual property and response to direct societal challenges. These valences will be strongly valorised thanks to the IMS ecosystem and scientific synergies among the different research groups, allowing to reach highly competitive critical mass and top international indicators. One important added value of this cross fertilization through IMS is a unique interdisciplinary vision supported by advanced research in physical chemistry, computational chemistry, materials science and myconanotechnology embedded with Artificial Intelligence techniques.
	2. Linha Temática 2	1. Designação da LT	MEDlife – Medicinal, biological and biophysical chemistry for Health
		2. Coordenador da LT	
		3. Contactos do Coordenador	
		4. Descrição da LT	MEDlife researchers tackle a wide variety of topics in HEALTH, firmly grounded upon a range of multidisciplinary skills that encompass physical and computational approaches, synthetic and analytical chemistry, structural analysis, biological chemistry, biochemistry, biophysics, chemical toxicology, and pharmacology. Acting in all stages of drug discovery from therapeutic concepts to clinical translation, MEDlife researchers identify and validate therapeutic targets, explore biological pathways, validate early disease biomarkers, study ADME-Tox properties, improve the activity and/or bioavailability of active pharmaceutical ingredients, optimize lead compounds, design and synthesize drug candidates, and support clinical trials. MEDlife researchers advance knowledge and share breakthroughs in high-impact scientific publications in all fields mentioned above. However, in an area known for the long and expensive path from therapeutic concepts to approved medicines, MEDlife members also value intellectual property (IP) protection as a means to translate practical solutions to health problems
	3. Linha Temática 3	1. Designação da LT	H2Oenv – Technologies for water and environment
		2. Coordenador da LT	
		3. Contactos do Coordenador	
		4. Descrição da LT	H2Oenv brings an integrated multidisciplinary approach to tackle the technological challenges of the waterenvironment-energy nexus. Researchers with a strong background on chemistry, materials science, and engineering will create synergistic efforts to develop innovative solutions and deliver cutting edge technologies to address the European Green Deal Challenge, and to make Europe the first climate neutral continent by 2050. In particular this TL aims at i) carrying out forefront research, through strong national and international cooperation, ii) conducting advanced training on those subjects, and iii) play a major role in technology transfer as part of its achievements. H2Oenv research is structured according to three strategic axes:
	3. Linha Temática 4	1. Designação da LT	SYNcat -
		2. Coordenador da LT	
		3. Contactos do Coordenador	
		4. Descrição da LT	The main goal of SYNcat is the development of sustainable and economically efficient synthetic and catalytic processes/strategies towards value-added products for all economy sectors, in a constant effort to mitigate pollution, as well as to save energy. Thus, this TL aims to provide a dialogue platform with industry, attracting funding and answering to important challenges of the Portuguese and EU industries. This strategy will foster the creation of knowledge and will attract highly skilled human resources that can complement and leverage the expertise of IMS researchers.
	3. Linha Temática 5	1. Designação da LT	CHEMfocus – Fundamentals and awareness
		2. Coordenador da LT	
		3. Contactos do Coordenador	
		4. Descrição da LT	The Thematic Line CHEMfocus addresses the fundamental issue of how to develop, transform and update those molecular-based tools (the essence of Chemistry). It provides a scientific foundation to the other four thematic lines and it will also channel part of its research towards the awareness of Chemistry in the present-day society. Thus, CHEMfocus encompasses two axes of action: a) it considers innovative, ground-breaking science, where new theories, models, experimental setups and techniques or more broad research strategies will be tested and developed, without targeting necessarily a short-term specific practical application, but rather a more fundamental issue or problem. This is what generally is designated by fundamental science, in opposition to what is commonly known as applied science, which is mostly focused on the finding of solutions for a particular societal or technological problem. The outputs will be new molecular-based tools, often cited in the context of the other four TLs. Moreover, and since it will deal with the most fundamental aspects of the Chemical Sciences (interactions, reactivity and structure at a molecular level and how they can be interpreted, modelled or probed experimentally) it can provide important answers and insights related to the question "what is Chemistry?". Such outputs can be used in the second axis of CHEMfocus where b) existing and new lines of research will be directed towards the promotion of the awareness in Chemistry. These lines of research will stress the importance of IMS (an Associate Laboratory focused in the Chemical Sciences) as an active player towards the urgent persecution of a more sustainable world, and will be able to develop guidelines and scientific documents capable of influencing the strategic options, at the national and international levels, of the policy-makers of our society.