

## CALL FOR AWARDING RESEARCH FELLOWSHIPS WITHIN PROJECT GRANTS AND R&D INSTITUTIONS

### 1 Research Fellowship (BI) for a PhD Student

1 Research Fellowship(s) (BI) is(are) open at the **FCiências.ID – Associação para a Investigação e Desenvolvimento de Ciências**, for the project/R&D institution “NANOBIOSOLUÇÕES IN SILICO: Conceção Computacional de Complexos Metálicos Y Polioxometalatos Bioativos para Aplicações Médicas / Instituto de Biosistemas e Ciências Integrativas (BioISI), PTDC/QUI-QFI/29236/2017, funded by the Fundação para a Ciência e a Tecnologia, I.P./MCTES through national funds (PIDDAC) under the programme Programme All Scientific Domains, under the following conditions:

1. **Scientific Area:** Chemistry
2. **Requirements for admission:** Master in Chemistry with experience in Computational Chemistry and Molecular Modelling applied to the promotion and catalysis of the phosphoester bond by means of polyoxometalates and Mo-oxo species.
3. **Additional optional skills and qualifications:** Experience in DFT calculations.
4. **Contracting requirements:** Presentation of the academic qualifications and/or diplomas. Enrolment in Interuniversity doctoral programme on Theoretical Chemistry and Molecular Modelling
5. **Work plan:** The phosphoester bond hydrolysis is a very important reaction in chemistry and biochemistry and even though this reaction is known since many years ago, its catalysis is still a challenge in chemistry and an interesting topic of research. Such reaction is involved in several processes related to reduction of damaging species from pesticides in the environment, energy production, genetics, several processes where nucleotides are involved, etc. In standard conditions, this reaction is thermodynamically favourable. However, the important kinetic barrier, mainly because of Coulombic repulsion of phosphate anions with nucleophiles, makes that this reaction extremely slow and we need catalysts to produce it in reasonable times. We find in the nature the so-called phosphoesterases, which are enzymes that makes possible this reaction in reasonable times. Keeping the idea to assimilate nature in artificial processes, one of the challenges is the use of artificial phosphoesterases for the catalysis of the hydrolysis of the phosphoester bond. Such process may be applied to hydrolyze DNA chains and therefore, use such process as alternative chemotherapies for cancer disease or to fight against bacterial antibiotic resistance. One choice on the use of artificial phosphoesterases are the polyoxometalates. However, the problem with the use of polyoxometalates is that they may decompose easily in the organism. In order to avoid this decomposition different ideas arose from the literature, one of them being the functionalisation of polyoxometalates with amino acids and peptides. Thus, the aim of our work will be to study how the functionalisation of polyoxometalates with amino acids and peptides may affect in the catalysis of the hydrolysis of the phosphoester bond. In order to achieve this objective, the candidate will have to develop the following tasks:
  1. DFT calculations on the mechanism for the catalysis of the phosphoester bond by using different substrates and polyoxometalates.
  2. DFT calculations on the mechanisms for the catalysis of the phosphoester bond by using some model substrate for the phosphoester bond and different polyoxometalates functionalised with amino acids and peptides to compare with the results in which no biofunctionalisation was considered.

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6. **Legislation framework:** Research Fellowship Holder Statute, in accordance with Law 40/2004, of 18 August, in its current version and the FCT Regulation for Research Studentships and Fellowships, in its current version (Reg. 950/2019 published in DR on 16<sup>th</sup> December: <https://dre.pt/application/file/a/127230968>, or at the FCT website: <https://www.fct.pt/apoios/bolsas/regulamento.phtml>), and FCIências.ID Fellowship Regulation, as approved on 12<sup>th</sup> May 2020 (available at [Regulamento de Bolsas de Investigação Científica da FCIências.ID](#)).
7. **Place of work:** The work will be developed at the BioISI / Faculdade de Ciências da Universidade de Lisboa under the scientific supervision of Professor Adrià Gil Mestres e Doutor Nuno A. G. Bandeira.
8. **Fellowship duration:** This position is initially opened for 3 months due to start in April 2022. The fellowship contract may be potentially renewed for until the end of the project, in accordance with the provisions of Regulation of Research Fellowships from the Foundation for Science and Technology, I.P.
9. **Monthly allowance:** The fellowship amounts to € 1144,64 ,according to [table values](#) of the fellowships awarded directly by the FCT, IP. The fellowship holder will have a personal accident insurance and can ensure the right to social security through adherence to the voluntary social insurance scheme, if not covered by any other social protection scheme, pursuant to *Código dos Regimes Contributivos do Sistema Previdencial de Segurança Social*.
10. **Evaluation and selection process:** Candidates will be assessed by the quality of their CV 70% and motivation letter (30%).
11. **Selection Committee:** President of the jury: Doctor Adrià Gil Mestres; Chairs: Doctor Ángel Sánchez González and Doctor Nuno Bandeira; Alternate member: Doctor Paulo Nuno Martinho.
12. **Publication/notification of results:** All the candidates will be notified by e-mail, sent by the call holder, with the selection meeting minutes enclosed.
13. **Deadlines:** This call for applications is open from 16/02/22 to 01/03/2022 .
14. **Application:** Applications should be sent via e-mail to [agmestres@fc.ul.pt](mailto:agmestres@fc.ul.pt), by attaching the following documents:
  - a. Curriculum vitae - **CV may be provided in PDF or through the [CIÊNCIAVITAE](#) system**;
  - b. Certificate of completion of previous degree;
  - c. and other documents considered relevant.
15. **Time limits for the appeal procedure:** In case of negative decision, the candidates have 10 business days, after the date of announcement of the results of the candidates evaluation, to pronounce their disagreement in accordance with the *Código do Procedimento Administrativo*. Appeals against the final decision may be submitted to the Administration Board of FCIências.ID ([fciencias.id@fciencias-id.pt](mailto:fciencias.id@fciencias-id.pt)) within 15 business days after the notification date

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**Note 1:** The documents that prove the entitlement of the academic qualifications and diplomas, or the proof of registration in the academic degree or diploma requested on the call, can be dismissed during the application period and replaced by a declaration on their honour from the applicant. Their delivery is mandatory for the fellowship contractualization.

**Note 2:** Please note that - higher education degrees and diplomas awarded by foreign higher education institutions - need to be recognized by a Portuguese higher education institution, pursuant to the [Decree-Law nr. 66/2018](#) (August 16) and the [Ministerial Order nr. 33/2019](#) (January 25). The presentation of the recognition certificate is mandatory for contract signature. More information can be obtained at: <https://www.dges.gov.pt/en/pagina/degree-and-diploma-recognition>.