

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

1 Research Fellowship (BI) for 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 “INSILNANOBIO SOL - 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 interactions of metal complexes with DNA.
3. **Additional optional skills and qualifications:** Experience in the following computational techniques: Linear-Scaling Density Functional Theory like SIESTA, use of semi-empirical methods with MOPAC, QM/MM calculations with Gaussian, use of tools on the energy decomposition analysis with ADF, experience in QTAIM calculations and use of docking software.
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:** Non-covalent interactions produced by means of weak interactions of ligands, isolated or included in metal complexes, with DNA is one crucial process in the study of alternative chemotherapies against cancer and in the studies of innovative processes against bacterial antibiotic resistance. In the case of the duplex DNA we have information in the bibliography about some kinetic equilibrium where a competence between the groove binding and intercalation is found and such equilibrium may be modulated by means of substitutions in the ligands and changes in the metal centre of the metal complex and therefore its nature. On the other hand, in the case of the G-quadruplex structures we have also different points of interactions (end-stacking, intercalation, groove biniding, interaction with loops, etc.), which may also be modulated by means of substitutions in the ligands and changes in the metal centre. Once the interaction of the [Mo(phen)(C3H5)Br(CO)2(phen)] metal complex with the duplex DNA and G-quadruplexes was studied, we want to analyse how the substitution in phen, in the other ligands or the change in the metal centre modulates this kind of interactions with regular duplex DNA and G-quadruplexes. Thus, the work plan and research in this fellowship aims at the comprehension and rationalization about how substitutions in different number and position in phenanthroline with functional groups like -CH3, -NH2, -OH, =O, -Ph, -Cl, -COOH and substitutions of the other ligands and changes in the metal centres modulate the interaction of the metal complexes that we are going to study with the DNA not only with regular duplex DNA but also with G-quadruplexes and therefore the selectivity for one or the other DNA structure in the interaction is obtained. In order to achieve this objective, the candidate will have to develop the following tasks:
 1. Docking calculations for the different situations that will be studied in which the [Mo(phen)(C3H5)Br(CO)2(phen)] metal complex will interact with regular duplex DNA and in the form of G-quadruplexes once we make the different substitutions in phen and in the other ligands.
 2. Optimizations at semi-empirical level or at LS-DFT level for the most representative results of the docking studies.
 3. EDA's of the most representative optimized systems.

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4. QTAIM and NCI calculations for the same systems in which the EDA's were carried out in order to know the nature of the weak interactions.

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 16th December: <https://dre.pt/application/file/a/127230968>, or at the FCT website: <https://www.fct.pt/apoios/bolsas/regulamento.phtml.pt>), and FCiências.ID Fellowship Regulation, as approved on 12th 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 Ángel Sánchez González.

8. **Fellowship duration:** This position is initially opened for 3 months due to start in March 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 € 1104,64 ,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*. The fellowship will be paid monthly by bank transfer

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: Doutor Ángel Sánchez González e Doutor Paulo Nuno Martinho; Alternate member: Doutor Nuno Bandeira.

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 31/01/22 to 14/02/2022 .

14. **Application:** Applications should be sent via e-mail to 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) 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>.