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Public Notice - International Selection Procedure

PhD Scientific Researcher Recruitment

FCiências.ID/2018/DL57/BiolSI/11

FCiências.ID - Associação para a Investigação e Desenvolvimento de Ciências, through its Chairman of the Board of Directors, hereby announces the opening of an international call for the recruitment of a scientific researcher with a PhD degree, within the scope of **Project** IN SILICO NANOBIO SOLUTIONS: COMPUTATIONAL DESIGN OF BIOACTIVE METAL COMPLEXES AND POLYOXOMETALATES FOR MEDICAL APPLICATIONS, PTDC/QUI-QFI/29236/2017, in the form of an employment contract with an uncertain term, according to the Portuguese Labour Code and Decree-Law No. 57/2016, of August 29th, as amended by Law No. 57/2017, of July 19th, and complementary legislation.

I - Admission Requirements

Portuguese nationals, foreign and stateless persons may submit applications to this selection procedure, provided they hold a doctoral degree¹ in Chemistry or Biochemistry or related areas and comply with the following requirements:

- The PhD should have been granted at least 3 years ago, preferably no earlier than 2006.
- Scientific and/or professional experience in the area of chemistry and/or biochemistry. Knowledge in computational chemistry and/or computational biochemistry will be evaluated very positively.
- Experience in the application of topological techniques such as QTAIM, ELF and/or NCI analyses and/or in the calculation of reaction mechanisms. Familiarity with a variety of quantum mechanics computational packages (Gaussian, ADF, etc.) and availability for scientific meetings every two weeks will be evaluated positively.

¹ Applicants with doctoral degrees obtained in foreign countries need, in accordance with Decree-Law No. 341/2007, of October 12th, as regulated by Government Order No. 227/2017, of July 25th, to be registered as holders of a doctoral degree, with all inherent entitlements. Applicants to whom, under the terms of Decree-Law No. 283/83, of June 21th, equivalence or recognition of the degree of Doctor has been granted are also valid. The presentation of the registration / recognition /equivalence certificate is mandatory for contract signature.

II. Applicable Law

- Decree-Law No. 57/2016, of August 29th, in the wording conferred on it by Law No. 57/2017, of July 19 (RJEC), taking also into account the provisions of Regulatory Decree No. 11-A/2017, of December 29;
- Portuguese Labour Code, as approved by Law No. 7/2009, of February 12, in its current version (CT);
- Administrative Procedure Code, as published in Decree-Law No. 4/2015, of January 7, in its current version (CPA).

III. Work Plan

The aim of the work plan is to explore modifications of $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)(\text{CO})_2\text{Br(phen)}]$, namely by changing the substituents of the ligands (CH_3 , OH , NH_2 , Ph , COOH , etc), in order to optimize the interaction of the complexes with DNA and/or G-quadruplexes. Other complexes of V, Co, Ni, Cu and Zn with the same phenanthroline ligands will be also studied. Gaussian or MOPAC software will be used to study the interactions and to rationalize the origin of substituent effects. The ADF software will be employed to complement the previous study with the energy decomposition analysis.

The project also includes the study of the phosphoester bond hydrolysis mechanism with the $[\text{Mo}_7\text{O}_{24}]^{6-}$ and DNA model substrates (NPP, BNPP and HPNP) for which experimental studies are available. Calculations (BP86/TZ2P with ADF) on several polyoxometallates (POMs) with different shape, charge, composition and other inherent properties of POMs will be carried out to understand how these modifications change the energy profiles and the mechanism of the catalytic phosphoester bond hydrolysis in DNA model substrates. Biofunctionalized POMs, carrying amino acids belonging to different groups and peptides, will also be addressed and their reactivity compared with that of $[\text{Mo}_7\text{O}_{24}]^{6-}$.

The objectives of the work plan are:

- 1) To give insight and provide rationalization of the interaction of transition metal complexes containing phenanthroline (phen) derivatives with DNA (regular and G-quadruplexes).
- 2) To understand how substitution in number and position in phen derivatives modulates the preference for groove binding or intercalation in DNA (regular and G-quadruplexes).
- 3) Design of optimal polyoxometalate-based artificial phosphoesterases by means of changes in inherent properties of POMs and biofunctionalization.

The work plan is mainly included in task 3 (Analysis of the modulation of the interaction between transition metal complexes containing phen derivatives and DNA (regular DNA and G-quadruplexes) by means of substitution in the phen ligand and changes in the metal), and task 5 (Optimization of the performance of POMs to act as phosphoesterases) of the project “IN SILICO NANOBIO SOLUTIONS: COMPUTATIONAL DESIGN OF BIOACTIVE METAL COMPLEXES AND POLYOXOMETALATES FOR MEDICAL APPLICATIONS” (Project PTDC/QUI-QFI/29236/2017).

IV. Composition of the Jury

In accordance to article 13 of the RJEC, the members of the jury are:

- President – Adrià Gil-Mestres
- 1st Evaluator - Maria José Calhorda
- 2nd Evaluator - Nuno A. G. Bandeira
- 1st Alternate Evaluator - Nuno Galamba
- 2nd Alternate Evaluator - Paulo J. Costa

V. Place of work

The work will be developed at the facilities of the Research Center: BioISI – Biosystems and Integrative Sciences Institute, in Campo Grande, Lisbon, Portugal.

VI. Contract Duration

The full-time employment contract with an uncertain term is expected to start on 01/02/2019, and will last until the Work Plan referred to in section III is completed. It will have an expected duration of 30 months, with a maximum duration of 30 months, including an initial trial period of 30 days.

VII. Monthly Allowance

The gross monthly salary entitle is stipulated in clause 1 of article 5 of the Regulatory Decree No. 11-A/2017, of December 29th, corresponding to level 28 of the Consolidated Table of Allowances, as approved by Government Order No. 1553-C/2008, of December 31st, to be 1,870.88 €, plus holiday and Christmas allowances, as well as food allowance, in value and conditions for workers with a legal relationship of employment under the Labour Code.

VIII. Evaluation of applications

1. Failure to comply with the Admission Requirements implies the non-admission of candidates in absolute merit.

2. According to article 5 of the RJEC, the selection of the candidates approved in absolute merit will rely essentially on the evaluation of their scientific and curricular achievements in the last five years, taking into consideration the quality and relevance of the scientific production, and the professional activity indicated as more relevant by the candidate, for the project.
3. The final classification of candidates is given on a scale of 0 to 100%.
4. Evaluation of the relative merit of candidates will rely on the following criteria: The candidate should have a demonstrable track record of his experience in scientific publications. A selection interview may be required from the applicants.
 - a) Scientific publications in the area – computational, physical, organic and inorganic chemistry 70 %;
 - b) Participation in relevant scientific projects in the area – computational, physical, organic and inorganic chemistry 15 %;
 - c) Pedagogical and outreach activities, in particular in the context of promoting scientific practices, organization of courses, seminars and conferences, in the area - 5 %;
 - d) Interview, if deemed necessary by the jury 10 %.
5. The jury may decide to interview the three best ranked [in criteria a) to c) of paragraph 4)] candidates, for clarification of curricular elements and additional information.
6. The jury will deliberate by means of a roll-call vote based on the evaluation criteria.
7. Minutes of the jury meetings are drawn up, summarizing all relevant elements considered by jury members, as well as their individual votes and justifications.
8. After completion of the evaluation process, the jury will draw up a ranking of successful candidates with their classifications.
9. Hiring will be decided by the Chairman of the Board of Directors of FCIências.ID, based on the final jury recommendation.
10. The evaluation results will be published on the website of the FCIências.ID ("Concursos" tab). The candidates will be individually notified of the evaluation results by e-mail sent to the address indicated in the "Personal Data" section of the submitted form.
11. With the notification referred to in paragraph 10, the hearing phase of interested parties referred to in Article 121 *et seq.* of the CPA will begin, and last for ten working days.
12. The possible pronouncement of the candidate in a prior hearing must be addressed to the President of the jury and submitted in writing to fciencias.id@fciencias-id.pt. The President of the jury will convene a jury's meeting to produce the final decision, within thirty working days.
13. Within five working days of the final jury decision, the Board of Directors Chairman of FCIências.ID will approve it and the candidates will be notified.
14. The communication between FCIências.ID and the candidates will be electronic and will comply with the following rules:
 - a) At the time of electronic submission of any document - namely in the case of paragraph no 11 - the candidates must generate proof of "sent message".
 - b) FCIências.ID will send an email message acknowledging documents received to the email address used by the candidates, within two working days.

- c) In case of absence of a confirmation receipt by FCIências.ID – showing the possibility of technical problems that should neither be the responsibility of the candidate nor FCIências.ID - the candidates should contact FCIências.ID, with the proof referred to in point (a), to ensure delivery and proper receipt of the documents concerned.

IX. Compliance with public policies

1. FCIências.ID actively promotes a policy of non-discrimination and equal access, so that no candidate can be privileged, benefited, disadvantaged or deprived of any right or exempt from any duty due to, inter alia, ancestry, age, sex, sexual orientation, marital status, family status, economic situation, education, social origin or condition, genetic heritage, reduced working capacity, disability, chronic illness, nationality, ethnic origin or race, territory of origin, language, religion, political or ideological beliefs and trade union membership.
2. Under the terms of D.L. No. 29/2001, of February 3, a disabled candidate has a preference in equal classification, which prevails over any other legal preference. Candidates must declare their respective degree of disability, the type of disability and the means of communication / expression to be used in the selection process, under the terms of the above-mentioned diploma.

X. Submission of Applications

1. The present call will be open from 11/12/2018 to 24/12/2018.
2. The application and all the required documents may be submitted in Portuguese or English.
3. Applications will be submitted online, through the electronic platform of FCIências.ID (<http://concursos.fcencias-id.pt>).
4. On the electronic platform, applicants will complete a *mandatory* section on Personal Data [name, address, date of birth, contact email, nationality and scientific identifiers] and upload files with the documents listed below:
 - i. Detailed curriculum vitae - *mandatory*;
 - ii. A motivation letter clearly demonstrating that the candidate has an adequate profile for the position and fully complies with the Admission Requirements - *mandatory*;
 - iii. Up to five publications relevant for the objectives of the Work Plan - *mandatory*;
 - iv. Digital copies of documents proving formal academic degrees (PhD) and/or other scientific and professional qualifications - original documents must be provided in case of actual recruitment- *mandatory*;
 - v. Other documents that candidates consider relevant for the assessment of their scientific merit, or to declare the personal situation in the cases covered in section IX-2 of this Notice - *optional*.
5. By decision of the Chairman of the Board of Directors of FCIências.ID, candidates who do not submit the documents identified in paragraph 4 will not be admitted to the call. In case of doubts, the Chairman may also invite candidates to substantiate specific data or statements with official supporting documents, before accepting the candidates' submission.

This Public Note was approved by the jury on 09/12/2018.