



Reference: REQUIMTE 2021-38

Main research field: Chemistry

Sub research field: Computational Chemistry

1. The Board of Directors of REQUIMTE – Rede de Química e Tecnologia – Associação, has decided to open an international call for position of PhD holder Researcher, under a work contract for a non-fixed term. This announcement is intended to 1 (one) research position (**Reference REQUIMTE 2021-38**) on the project PTDC/QUI-QFI/31689/2017 entitled: " RDB-TS: A reaction database for transition state information from quantum chemical calculations", supported by national funds by FCT / MCTES and co-supported by Fundo Europeu de Desenvolvimento Regional (FEDER) throughout COMPETE 2020 – Programa Operacional Competitividade (NORTE-01-0145-FEDER-31689), to pursue scientific research activities in the area of chemistry, scientific sub-area computational chemistry, in order to work in the determination, optimization, characterization and organization of transition states from chemical reactions into the RDB-TS database.

2. **Applicable Legislation** Decree-Law no. 57/2016 of August 29th, amended by Law 57/2017 and Regulatory Decree No. 11- A / 2017 which approved the doctorate hiring regime destined to stimulate scientific and technological employment for all knowledge areas (RJEC); Portuguese Labour Code, approved by Law 7/2009 of February 12, in its actual form.

3. Pursuant to article 13 of RJEC, the tender selection panel is to be formed by: Dr. Nuno Manuel Ferreira de Sousa de Azevedo Cerqueira (Researcher at UCIBIO/REQUIMTE, chair of the jury by delegation of the Director of REQUIMTE), Dr. Sérgio Filipe Sousa (Researcher at UCIBIO/REQUIMTE) and Professor Dr. Pedro Jorge Araújo Alves da Silva (Professor Associado, Universidade Fernando Pessoa and Researcher at UCIBIO/REQUIMTE).

4. The workplace shall be at the Faculdade de Medicina da Universidade do Porto.

5. The gross monthly salary entitle is stipulated in clause 1 a) of article 15 of the Regulatory Decree No. 57/2016, of August 29th, amended by the law nº 57/2017 of July 29th, corresponding to level 33 of the Consolidated Table of Allowances, as approved by Government Order No. 1553-C/2008, of December 31st, being 2.134,73 Euros.

6. Application can be submitted by any national, foreign and stateless candidate(s) holding a doctorate degree in Chemistry, Biochemistry, or related areas and a scientific and professional curriculum whose profile is suited for the activity described below.

In case the doctorate degree was awarded by a foreign higher education institution, it must comply with the provisions of Decree-Law no. 341/2007 of October 12th, and all formalities established therein must be complied with at the signature of work contract.

7. The tender admission requirements are those defined in the previous point 6, and specific requirements to have: (1) proven experience in the determination of transition state structures; (2) proven experience in computational enzymatic catalysis; (3) Proven experience in the use of the

softwares Gaussian, ORCA and VMD; (4) Proven experience in the computational study of catalytic triads and in the determination of concerted transition states.

8. Pursuant to article 5 of RJEC, the selection is to be made based on the evaluation of the scientific and curricular career of the candidate.

9. Scientific and curricular career evaluation focuses on relevance, quality and up-to-datedness:

a) of scientific, technological, cultural or artistic production, considered most relevant by the candidate;

b) of research activities, fundamental or applied science, considered of higher impact by the candidate;

c) of knowledge extension and dissemination activities, namely under the scope of the promotion of culture and scientific practices, deemed most relevant by the candidate.

10. Evaluation criteria are the following:

The evaluation of the CV of the candidates, in particular the scientific merit and research experience will take into consideration the elements presented falling within the scope of the specific areas of the tender (see Point 1) and will be performed according to the following criteria:

10.1 Integrated assessment of the curriculum trajectory of the candidate, based on an overview of their scientific merits, namely:

I. overall scientific coherence of the CV – 10%

II. diversity and quality of scientific indicators, including relevant published peer-reviewed articles in the specific areas of announce (see point 1) – 25 %

III. participation in research projects related to the present topic – 5 %

10.2 Relevant experience, proved by the CV, in:

I. Computational Study of Reaction Mechanisms by QM and QM/MM - 15%

II. Determination of Transition State Structures by Computational Methods - 15%

III. Use of softwares Gaussian, ORCA and VMD – 15%

IV. Computational treatment of catalytic triads and determinations of concerted transition states – 15%

11. In the case of admitted candidates whose evaluation does not differ more than 10% from that obtained by the best positioned candidate, the jury will interview these candidates. This will be aimed at obtaining clarifications and explanations about the curricular elements and additional information as well as to evaluate the attitude profile and motivation of the candidate.

The final score of each jury member is obtained by the following assessment: 90% scientific and curricular career evaluation and 10% interview.

12. Candidate final classification system shall be given based on a scale 0 to 100.

13. The panel shall deliberate by means of roll-call vote justified under adopted and disclosed selection criteria, with no abstentions allowed.

14. Minutes of panel meetings shall be executed and include a summary of all occurrences of said meeting, as well as of all votes casted by the members and respective reasoning, and shall be provided to candidates whenever required.

15. After selection criteria application, the panel shall prepare a sorted list of approved candidates and respective classification.

16. Panel's final decision shall be validated by the leader of the institution, who is also in charge of deciding about the hiring.

17. Application formalization:

17.1 The applications are formalized at the electronic address <https://www.requimte.com/> with following documents in a digital form, in PDF format:

- i) Curriculum vitae;
- ii) Motivational Letter;
- iii) Qualifications Certificate;
- iv) other relevant documentation.

17.2. The application period is from **30/09/2021 to 14/10/2021**.

18. All candidates who formalize their applications in an improper way or fail to prove the requirements imposed by this tender are excluded from admission. In case of doubt, the panel is entitled to request any candidate to present further documentation supporting their statements.

19. False statements provided by the candidates shall be punished by law.

20. Both admitted and excluded candidate list and final classification list shall be published in the website of the Institute and the selected candidate shall be notified by email.

21. Preliminary Hearing and Final Decision Deadline: After publication, all candidates have 10 working days to respond. Panel's final decisions are pronounced within a period of 90 working days, from response period deadline.

22. This tender is exclusively destined to fill this specify position and can be terminated at any time until approval of final candidate list, expiring with the respective occupation of said position.

23. Non-discrimination and equal access policy: ICETA actively promotes a non-discrimination and equal access policy, wherefore no candidate can be privileged, benefited, impaired or deprived of any rights whatsoever, or be exempt of any duties based on their ancestry, age, sex, sexual preference, marital status, family and economic conditions, instruction, origin or social conditions, genetic heritage, reduced work capacity, disability, chronic illness, nationality, ethnic origin or race, origin territory, language, religion, political or ideological convictions and union membership.

24. The panel has approved this announcement in meeting held on 28/09/2021.

25. According to Decree-Law no. 29/2001 of 3 February, disabled candidates shall be preferred in a situation of equal classification, and said preference supersedes any legal preferences. Candidates must declare, on their honour, their respective disability degree, type of disability and communication/expression means to be used during selection period on their application form, under the regulations above.