Centro de Química de Évora (CQE) and the Laboratory for Chemio-Physio Development and Characterization (*O Laboratório de Desenvolvimento e Caracterização Físico-Química*-LADECA), University of Évora, PORTUGAL.

Post-Doctoral Grant in Molecular Modeling and Drug Design

14 Nov. 2013

A Post-Doctoral grant is available for a highly motivated individual with a proven track record in molecular modeling/structure based drug screening/ligand-protein docking to work as a key team member of the project: INMOLFARM - Molecular Innovation and Drug Discovery ALENT-07-0224-FEDER-001743).This project is co-financed by FEDER through the "INALENTEJO Program".

The selected candidate will have the opportunity to work with an interdisciplinary multinational team, that will look at an innovative synthetic route to key potential pharmaceutical compounds. This project will be undertaken at the Centro de Química de Évora and the Laboratory for Chemio-Physio Development and Characterization (LADECA, part of the Alentejo Science and Technology Park - PCTA) at the University of Évora.

Scientific Area: Molecular modeling/ligand-protein docking/structure based drug screening/in silico drug design

Academic Requirements: A PhD degree in Chemistry/pharmacy/Biochemistry in the area of molecular modeling studies of enzyme target inhibition by lead compounds, ideally experience with the targets involved in neurodegenerative diseases such Alzheimer's, Parkinson's and depression. It is essential that the candidate have experience with ligand-protein docking methodologies and structure based drug screening. His/Her academic background (from first or second cycles) should include subjects of relevance to the theme of this project (for example, medicinal chemistry, organic chemistry etc).

Specific Entry Requirements: The candidate should have significant (documented) experience in molecular modeling and structure based drug screening, particularly, regarding the preparation of targets for and application of known docking (ideally protein-ligand docking) methods to access the potential inhibitory properties of the drugs under study. The candidate should have experience with GOLD, AutoDoc and AutoGrow suites. Ideally the candidate should have experience with neurodegenerative disease targets like for example, N-methyl-D-aspartate (NMDA) receptor, monoamine oxidase B (MAOB), catechol-O-methyl transferase (COMT), acetylcholine esterase and indoleamine 2,3-Dioxygenase etc. He/she should have a strong publication record in this field. The candidate should be a highly motivated, organized individual, with the

ability to be able to work autonomously but at the same time being a good team-player and with a track-record in accomplishing deadlines. The candidate should have good english language skills.

Work Plan: The aim of this project is to develop a cutting edge innovative catalytic process into a state of the art process for the discovery and eventual production of key neurodegenerative disease and anti-infectious disease lead compounds. This experienced scientist will be expected to apply molecular modeling and structure based drug screening techniques and in silico methods, which will entail docking simulations (i.e. ligand-protein docking) in the target active site (which may include homology models), the compounds will be ranked in order to predict the potential inhibitory properties of our lead compound libraries. The targets that have been identified are: N-methyl-D-aspartate (NMDA) receptor, monoamine oxidase B (MAOB), acetylcholine esterase and indoleamine 2,3-dioxygenase etc. The GOLD, AutoDoc and AutoGrow suites will be used for this purpose. The most promising lead compounds will then be structurally modified in order to optimize their inhibitory potential. They will be synthesized and biologically screened. This group member will be expected to liaise with both the medicinal chemistry and the biological assay teams in order to optimize the design of our neurodegenerative and anti-infectious disease leads.

This post-doc project will be conducted under the direct supervision of Prof. Anthony Burke (CQE-UE, and LADECA-UE) in collaboration with Prof. João Paulo Ramalho (CQE-UE).

Legislation and applicable regulations: This scholarship will be carried on the basis of a signed contract between the University of Évora and the scholarship recipient, under the terms of the Research Scholarship Regulations of the University of Évora, (Regulamento de Bolsas de Investigação da Universidade de Évora) (Ordem de Serviço nº1/2011), the Scientific Research Grant Holder Statute (Estatuto do Bolseiro de Investigação Científica) (Decree-Law nº40/2004 of the 18 of August) and according to the Regulations and legislation for advanced training and qualifications for human resources of the Fundação para a Ciência e a Tecnólagia (FCT).

Work location: This project will be carried out in the department of chemistry at the University of Évora, Portugal, under the direct supervision of Prof. Anthony Burke in collaboration with Prof. João Paulo Ramalho.

Grant Duration: 12 months with the expected starting date of January 2014.

Stipend value: 1495€ per month (tax free). according to the Regulation of advanced training and qualification of human resources for 2012 of the Portuguese Foundation for Science and Technology (http://www.fct.pt/apoios/bolsas/regulamento.phtml). This stipend will be paid monthly by check or bank transfer.

Selection Method: The evaluation criteria are: i) Academic/Scientific record (a. CV , 50%; ii. previous experience in the context of this Post-doctoral project, 35%; iii, letter of motivation, 15%. shortlisted candidates - those with the highest classifications, and who are deemed to have the most suitable profiles that match the requirements for this position - may be called for interview.

Selection Committee:
Prof. Anthony Burke (President of the Jury); Prof. Paulo Mendes (1º Member); Prof. João Paulo Ramalho (2º Member); and Prof.ª Maria do Rosário Martins (Reserve member) all from Dept of Chemistry/CQE, University of Evora.

Advertisement/Notification of the results: The final result of the assessment will be made public through a ranking list which will be exhibited in a visible public place in the Chemistry Department/CQE of the University of Évora, the candidates being notified by email.

Call opening and closing dates: The call will be opened from the 15th of November to the 29th of November 2013 and the results are expected to be published on the 06st of December 2013.

Applications will be formalized, mandatorily, by sending a letter of motivation, which will be accompanied by the following relevant documents: a very detailed Curriculum Vitae (which includes, candidates address, telephone number and email address and the same contacts for the named referees), a motivation letter, two letters of recommendation (most recent possible), photocopy or scanned copy of identity card/passport and degree certificates, university grade cards/transcripts and any other documents that are considered relevant for the selection process.

These documents must be sent or emailed (before the closing date) to:

Prof. Anthony Burke,
Chemistry Department and Centro de Química de Évora,
Universidade de Évora,
Rua Romão Ramalho, 59
7000 Évora,
PORTUGAL.
e-mail: ajb@uevora.pt
For any queries please contact Prof. Anthony Burke (telefone: +351 266 745310; e-mail: ajb@uevora.pt)

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