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Research Position at Acellera, Barcelona
DEVELOPING AND APPLYING SIMULATIONS METHODS FOR DRUG DISCOVERY

Acellera is seeking an exceptional medicinal chemist / computational biologist / biophysicist, with a strong background in development of scientific software, to join our Barcelona-based team. This is a unique opportunity to participate in the design and development of new tools for computational chemistry of interest for pharmaceutical companies based on the in-silico software platform, HTMD (http://www.htmd.org).

The work will include developing new methods for simulation based drug discovery in partnerships with top pharmaceutical industries worldwide, applying simulation-based methods to specific problems, participating in research papers with our scientific and industrial partners, and giving support, and producing tutorial materials and work-flow protocols for HTMD.

Applications are invited from individuals with a technical and scientific background with excellent programming skills in a scientific research context. The ideal candidate should have a strong hands-on, proactive spirit with a passion for working in a start-up environment, autonomy and an ability to go beyond the state-of-the-art.

Essential:
- PhD in medicinal chemistry, chemistry, computational biology or biophysics
- Proven track record of developing scientific software
- Very good knowledge of Python
- Very good knowledge of molecular simulations
- Fluent in English and with excellent communication skills
- EU citizen or suitable work visa, able to travel to the USA
- Residing in, or willing to relocate to, Barcelona

Desirable:
- Experience with computational chemistry packages (e.g. Maestro and Maestro API)
- A good publication record
- Some experience with Amazon Web Services
- Familiarity with the pharmaceutical industry

Contract & Remuneration
The position is full-time. We are committed to fostering a rewarding and flexible work environment, and offer competitive salary in the context of Barcelona area. Salary is negotiable depending on the expertise.

Applying: To apply, please send your CV and cover letter to jobs@acellera.com
Any other enquires should also be directed to that email.
Indicative timetable: position to be filled by early 2017.
Location: Barcelona at the Barcelona biomedical research park (http://www.prbb.org)

About Acellera

Since 2006, Acellera has innovated in the field of molecular dynamics simulations for graphical processing units (GPUs). Our mission is to accelerate the transition to computerized drug discovery by developing in silico simulation assay technologies that deliver solutions for estimating common physical chemistry properties as binding affinities, kinetics, poses and pathways with experimental accuracy. Acellera is currently active in production of molecular dynamics software specially optimized to run on GPUs (ACEMD) and Amazon cloud (AceCloud). Acellera offers its expertise in molecular simulations to improve the effectiveness of the drug discovery processes. We have had contracts with several of the top 20 pharmas and participate in two EU research and drug discovery projects.

Selected references

• S. Doerr, M.J. Harvey, F. Noé, G. De Fabritiis. HTMD: High-Throughput Molecular Dynamics for Molecular Discovery. J Chem Theory Comput 12 (4), 1845-1852. (2016)
• M. J. Harvey and G. De Fabritiis. High-throughput molecular dynamics: The powerful new tool for drug discovery, Drug Discovery Today, 17, 1059–1062 (2012).
• I. Buch, T. Giorgino and G. De Fabritiis. Complete reconstruction of an enzyme-inhibitor binding process by molecular dynamics simulations, PNAS 108, 10184-10189 (2011).
• M. J. Harvey and G. De Fabritiis. An implementation of the smooth particle-mesh Ewald (PME) method on GPU hardware, J. Chem. Theory Comput. 5, 2371–2377 (2009).
• M. Harvey, G. Giupponi and G. De Fabritiis. ACEMD: Accelerated molecular dynamics simulations in the microseconds timescale, J. Chem. Theory and Comput. 5, 1632 (2009)