MSc Thesis in Computational Chemistry

Computationally-driven purification processes for small molecules

We are looking for a motivated and talented **MSc Student** to join our laboratory of **Computer-Aided Molecular Design** at the **Medical University of Graz (Austria)**. The successful MSc candidate will work in the context of the COMET project *Digital and Green (Twin) Transition of Pharmaceutical Product and Process Development* **Twin4Pharma** (https://www.rcpe.at/en/twin4pharma) lead by the Research Center Pharmaceutical Engineering (RCPE). The main goal of Twin4Pharma is to deliver novel **computational methods** to speed up sustainable process development, and to reduce failures and the experimental burden.

What iis this position about?

This MSc thesis is planned for **6-months** and is entirely computational (do not worry: you may not enter the wet-lab). Your tasks will focus on the computation and prediction of **molecular properties** of **relevant pharmaceutical molecules** (i.e. solubility, stability) as well as in their interactions with other molecules of interest, to help in the pharmaceutical production and purification processes. A variety of methods will be use, from classical to quantum mechanics, including artificial intelligence algorithms.

Why should you apply to this position?

- Interdisciplinary team, with players from both Academia and Industry
- Hands on a plethora of computational methods for computing molecular properties
- We offer economical support upon completion of the MSc Thesis
- We are nice people and Graz is beautiful

How to apply for?

If you are interested on the position, you can send (1) your CV and (2) a letter of motivation as PDF files to pedro.murcia@medunigraz.at.

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