## PhD Studentship in Data Mining in Chemical Space

Contact: Dr Michael Schmuker (m.schmuker@herts.ac.uk)

Our group translates processes from the brain into algorithms for efficient computing. One of the specialties of our group is data mining in chemical space, where we study how the brain processes olfactory signals to efficiently encode chemical information. We thus aim to learn from the sense of smell how to achieve a powerful understanding of chemical space, with potential applications in fragrance and aroma chemistry, and potential wider impact in drug discovery.

A PhD studentship is available in Data mining in chemical space, with Principal Investigator Dr Michael Schmuker. Potential topics include but are not limited to:

- Supervised and unsupervised pattern recognition in chemical space
- Model structure-activity relationships for odorant receptors using machine learning
- Scent prediction for small molecules using Artificial Intelligence

We pursue multiple collaborative projects with neuroscientists and perfumers to gain insight into how the brain extracts information from the chemical world. This guarantees a stimulating environment for a project that aims not only at generating theoretical insight but also validating the findings with experimental scientists and pursuing applications in the real world.

We are looking for highly motivated candidates who are keen to explore the interface between the chemical world and the brain. Previous exposure to pattern recognition methods, supervised and unsupervised learning, or molecular modelling is a plus.

Successful candidates are eligible for a research studentship award from the University (approximately GBP 14,777 per annum bursary plus the payment of the standard UK student fees). Applicants from outside the UK or EU are eligible but will have to pay half of the overseas fees out of their bursary.

Please contact Principal Investigator Dr. Michael Schmuker prior to application to scope out a project proposal that is tailored to your background, via email: <a href="mailto:m.schmuker@herts.ac.uk">m.schmuker@herts.ac.uk</a>.

Application forms can be downloaded from <a href="https://www.herts.ac.uk/study/schools-of-study/computer-science/our-research/the-phd-programme-in-computer-science">https://www.herts.ac.uk/study/schools-of-study/computer-science/our-research/the-phd-programme-in-computer-science</a>.

Completed forms should be returned to

Mrs Emma Thorogood Research Student Administrator University of Hertfordshire College Lane Hatfield, Herts AL10 9AB

tel: +44 (0)1707 286083

doctoralcollegeadmissions@herts.ac.uk

Applications should also include two references and transcripts of previous academic degrees. We accept applications for self-funded places throughout the year.

The next short-listing process for studentship applications will begin on 25 June 2018.