PhD in Machine Learning for NMR Prediction in Pharmaceutical Development

We have a PhD project available from Sept/Oct 2020, co-funded by Genentech (San Francisco, USA), in the application of machine learning tools to the prediction of Nuclear Magnetic Resonance (NMR) spectroscopy data, which is used to understand the 3-dimensional structure of molecules in the development of new pharmaceutical products.

The project will develop the next generations of our machine learning (ML) system, IMPRESSION (https://pubs.rsc.org/en/content/articlelanding/2020/sc/c9sc03854j#IdivAbstract), which is the world’s first ML tool for predicting 3D solution-state NMR parameters with quantum chemical accuracy. We will work with implementing neural network architectures, improving the underpinning quantum chemical datasets, extending to multi-conformer predictions and expanding the range of NMR parameters predicted the ML system.

Candidates with backgrounds in chemistry, physics, computer science are all invited to apply. Experience in coding, quantum chemical calculations or NMR is helpful, but not critical (we can’t imagine anyone will have them all!) as you’ll be able to learn everything you need to know on-the-fly. Most importantly we want someone with a problem-solving mindset, who loves a challenge and working on a cutting-edge scientific problem with some of the leading academic and industrial scientists in the world!

For further details please contact Prof Craig Butts (Craig.Butts@bristol.ac.uk)

Please apply here: http://www.bristol.ac.uk/study/postgraduate/apply/