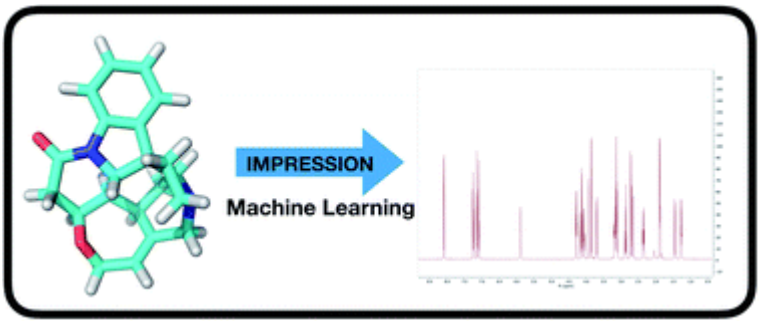
Digital Chemistry – Machine learning, computation and chemical properties

About the project or challenge area: The project will develop new directions for our machine learning tool – IMPRESSION (see ref. below) – which predicts chemical/physical/spectroscopic/biological properties directly from 3D molecular structures. The first generation of IMPRESSION was used to predict NMR parameters with accuracies that approached quantum mechanical methods (such as Density Functional Theory – DFT), but hundreds of thousands of times faster. However, IMPRESSION Generation 1 was limited to prediction for molecules containing H, C, N and O only, used resource-heavy machine learning tools and could only predict NMR parameters. Recent results in our group suggest that IMPRESSION can applied to many other types of predictions, including ligand-binding efficiency (used in early-stage pharmaceutical development), solubility, acidity – pretty much any property that can be predicted by quantum mechanical methods. We have also developed a neural-network based approach which as the potential to deal with 1000-fold more classes of molecules, allowing us to move beyond H, C, N, O and into the entire range of relevant chemical space in the periodic table.



So we want you to explore this new world – building new generations of our IMPRESSION machine, building new datasets on which we can train it, and setting it new challenges to address.

Why choose this opportunity? The focus of your project will be on predicting chemical properties and behaviours using *machine learning and computational chemistry* which will provide an excellent platform to learn how computation and machine learning are applied to *modern chemical research problems*. Your work in this area can make a real impact on cutting edge scientific problems and global challenges, such as molecular design for drug development. You will develop expertise in *computational chemistry*, *coding* and *machine learning*, whilst becoming more familiar with the fundamentals of molecular structure and dynamics. Furthermore, this project will require your collaboration across research groups, including *synthetic chemists* and *spectroscopists*, and working our *industrial collaborators*, thus improving your teamwork and networking skills. You will be developing a range of additional transferable skills, including presentation, scientific writing, and project and time management. Finally, you will be interacting with students from all over the world learning from their culture and skills, adding to your professional and personal development.

Full training will be provided for all aspects of this project. You will be embedded in the Supervisor's research group, who will provide support. In addition, you will be assigned a mentor for the duration of your project, who will provide extra support and help you to identify any additional training needs or opportunities.

About you: You will have skills and knowledge to understand the physical or chemical concepts behind molecular structure and chemical computation and an enthusiasm (but necessarily experience of!) coding and machine learning. You will enjoy working in teams and have good time management. These skills are desirable but not essential – what you don't have, we will teach you.

Bench fees: A bench fee of £5,500 is required.

How to apply: Applications are accepted throughout the year and you should complete the online application form for Chemistry (MSc by Research).

Supervisor: Your supervisor for this project will be Craig Butts, Professor of Structural and Mechanistic Chemistry in the School of Chemistry. You can contact him at Craig.Butts@bristol.ac.uk

Find out more about your prospective research program: This article demonstrates our machine learning tools applied to property prediction (in this case NMR):

IMPRESSION – Prediction of NMR parameters for 3D Chemical Structures https://doi.org/10.1039/C9SC03854J