Project title: **Building meaningful atomic models of polysaccharides automatically**
Supervisor name(s): **Dr Jon Agirre, Dr Kevin Cowtan**
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**Project Description:**

**Context:** We have recently assessed the methodological support for building atomic models of carbohydrates using data from macromolecular crystallography (MX) and electron cryo-microscopy (cryoEM), and found it to be very incomplete [1]. As part of our analysis, we have found thousands of unlikely or indeed wrong carbohydrate structures in public macromolecular structure databases. One of the widely-accepted reasons for this is the lack of automated tools for creating and fitting atomic models of carbohydrates to the experimental data [2]. This is a problem now for MX, and it is likely to become a major problem for cryoEM as the technique becomes ever more popular.

**Project:** We have an evolving set of high-performance tools – e.g. Privateer [3] – which can be used as building blocks for creating a much bigger and capable computer program. While our software is built on efficient but harder to maintain languages (C++ with use of parallelism), the successful candidate will use the high-level, easy to learn Python programming language to combine pre-existing modular code in logical ways. The ultimate goal is to build a computer program that combines all our knowledge of carbohydrate chemistry and glycobiology to create meaningful atomic models of branched polysaccharides. The tool will be evaluated against all published protein-carbohydrate structures – the results are expected to enhance or even increase our glycobiological insight.

**Research group:** The successful candidate will join the world-renowned York Structural Biology Laboratory (YSBL, for more information please refer to [https://www.york.ac.uk/chemistry/research/ysbl](https://www.york.ac.uk/chemistry/research/ysbl)). Research in YSBL covers, among other topics, glycobiology and method development for both MX and cryoEM. The laboratory provides a highly collaborative environment for creative individuals to thrive.

**Dissemination:** The successful candidate is expected to present their work at UK and international conferences, and to demonstrate their software’s use to other research groups in the UK and abroad.

**Relevant publications:**

1. *Carbohydrate anomalies in the PDB.*

2. *Carbohydrate structure: the rocky road to automation.*

Training:

All research students follow our innovative Doctoral Training in Chemistry (iDTC): cohort-based training to support the development of scientific, transferable and employability skills. All research students take the core training package which provides both a grounding in the skills required for their research, and transferable skills to enhance employability opportunities following graduation. Core training is progressive and takes place at appropriate points throughout a student’s higher degree programme, with the majority of training taking place in Year 1. In conjunction with the Core training, students, in consultation with their supervisor(s), select training related to the area of their research.

Depending on the successful candidate’s qualifications, taking an ‘Introduction to Python programming’ course might be desirable. This runs regularly in the Department of Chemistry at the University of York, and familiarises the students with programmatic access to public databases, which is one of the features we expect to incorporate to our software.

The project will also provide externally-funded opportunities for teaching and training in specialised structural biology workshops in the UK and overseas through the Collaborative Computational Projects for macromolecular crystallography (CCP4) and electron cryo-microscopy (CCP-EM).

Equality and Diversity:

The Department of Chemistry holds an Athena SWAN Gold Award and is committed to supporting equality and diversity for all staff and students. The Department strives to provide a working environment which allows all staff and students to contribute fully, to flourish, and to excel. Chemistry at York was the first academic department in the UK to receive the Athena SWAN Gold award, first attained in 2007 and then renewed in October 2010 and in April 2015. This PhD project is available to study full-time or part-time (50%).

Funding:

This project has guaranteed funding, providing a suitable candidate can be found.

Value: Studentships are fully funded either by the EPSRC or a Department of Chemistry Teaching Studentship, and cover: (i) a tax-free annual stipend at the standard Research Council rate (£14,553 for 2017-18), (ii) tuition fees at the UK/EU rate.

Eligibility: EPSRC studentships are available to UK and EU students who meet the UK residency requirements. Students from EU countries who do not meet the residency requirements may still be eligible for a fees-only award. Chemistry Teaching Studentships are available to any student who is eligible to pay tuition fees at the home rate. Further information about eligibility for Research Council UK funding can be found at the following website: [http://www.bbsrc.ac.uk/documents/studentship-eligibility-pdf/](http://www.bbsrc.ac.uk/documents/studentship-eligibility-pdf/)

Candidate selection process:

- Applicants should submit an application for a PhD in Chemistry by **17:00 on Wednesday 28 February 2018**
- Supervisors will interview their preferred candidates either by email, telephone, web-chat or in person
- Supervisors may nominate up to two candidates to the assessment panel
- Nominated candidates will be invited to a panel interview at the University of York in mid March (date TBC)
- The Chemistry Graduate Awards Panel will award studentships following the panel interviews
- Candidates will be notified of the outcome of the panel’s decision by email

For more information contact chemgrad@york.ac.uk or see our web page: [http://www.york.ac.uk/chemistry/postgraduate/](http://www.york.ac.uk/chemistry/postgraduate/)