ChromSoc Summer Studentship Experience Report 2021

I'm Scott, a graduate M.Chem Chemistry student from Sheffield Hallam University. I have always been very analytically minded which posed me to always ask 'why?' as a kid. This has led me down the path of science and in particular chemistry as a way to understand what goes on around us and provide an explanation to processes we see every day.

Near the end of my research project Rachel Schwartz-Narbonne approached me with a series of summer projects that were on offer the university. These projects had initially been offered to second and third year students but after a lack of applicants for some projects, the Masters students were also included. After spending a year working with bacteriohopanepolyols (BHPs) and lipid extraction techniques, the summer project Rachel presented me with worked well as a way to extend the work I had been doing. As I already had the core knowledge on the bacterial process and structures we would be looking at, Rachel saw me as a good fit for the project.

The work aimed to build on preliminary studies by Allcock *et al.* over the previous summer, where the group established the potential of a computational chromatography approach to model Gas Chromatography (GC) retention time of BHPs by demonstrating a linear correlation between computationally predicted BHP polarizability and GC retention time. Our work would focus on building on the knowledge gained by using additional BHPs, different chromatographic conditions and more advanced computational methods. This is with the end goal of identifying an unknown BHT-isomer that can serve as a specific biomarker for annamox bacteria. This project allowed me to gain further lab skills, particularly in the areas of gas chromatography, of which I have only used at undergraduate level. The use of computational chemistry allowed me to try something new and learn how computational studies can be used to calculate a wide range of electronic and thermodynamic properties that can be of interest to a chemist. I found the process of research work to be eye opening as it provided a less structured, more curiosity driven way to learn and gain practical skills. It also provided me with the challenge of having to problem solve in real time and work around other researchers in the lab to ensure everyone got

access to the equipment they required. Research work is definitely something I plan to return to in the future.

The results for the project were included in a presentation at the British Mass Spectrometry Society's annual conference (BMSS41). I also presented, but focused on data from subjects in my M.Chem year. I found the process of report to presentation to be more difficult than expected, as there was a lot of interesting data produced that I would not be able to cover within the 5-minute flash poster talk. Overcoming this required considering the audience I would be presenting to, and what areas of my project would be most relevant. As it was a BMSS meeting, I focused mainly on the mass spectrometry development work I completed for the analysis of mycolic acids. In regard to my conference experience as a whole, I was pleasantly surprised by the relaxed atmosphere and the efforts by all attendees to make the early career researchers like me feel welcome. I found the talk itself to be an enjoyable experience and I felt a real sense of achievement being able to present work that I had put so much time and effort into.

I now work in the pharmaceutical industry in a quality control role where chromatography techniques such as GC and HPLC are used daily to confirm the contents of drug tablets and any relevant impurities. This is in the effort to provide safe and affordable drugs to millions of people across the country. The addition of a multidisciplinary project involving GC and computational chromatography has been of particular interest within job interviews, as it's an unusual combination of subject areas. The experience gave me the chance to talk in detail about how the two disciplines can be connected and provided an opportunity to talk about something I had a deep understanding of.

I would like to thank everyone at ChromSoc for this opportunity, it has been an enriching and eye-opening experience that I cannot recommend enough. I would encourage any students who are looking to enhance their laboratory, presentation, and scientific writing skills to apply.

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