

UK 850 MHz Solid-State NMR Facility Travel Fund Report

Jonathan Bradley, PhD Student, University of Warwick

From 1 – 5 August 2010 I attended the Solid-State NMR Symposium of the Rocky Mountain Conference on Analytical Chemistry, held in Snowmass, Colorado, USA. Financial support for this trip was provided by the UK 850 MHz Solid-State NMR Facility Travel Fund.

I presented a talk on the second day of the conference on “ ^1H double-quantum build-up curves from double-quantum filtered ^1H – ^{13}C correlation spectra of Indomethacin- γ ”. This work concerns the extraction of ^1H double-quantum data, used to obtain relative H – H distance information, from complex pharmaceutical systems. The majority of the experimental work I presented in this talk was acquired using the 850 MHz facility, which was necessary to achieve the required spectral resolution, and to acquire data in a reasonable timeframe. In addition to the talk, I presented a poster on the same topic.

The talk and poster led to several interesting conversations regarding my work with other conference attendees. Topics that were discussed included details of the experimental procedure, suggestions for methods to further improve the resolution of the spectra, and comparisons with other experimental techniques. Additionally several people were interested in the methods used to perform simulations, which I presented alongside the experimental results, and I was able to discuss ways to perform simulations more efficiently.

Other presentations at the conference were of great interest. In particular, a number of talks on dipolar decoupling and recoupling methods, fast MAS, and computational techniques were of particular relevance to my research. A talk on “Characterisation of Pharmaceuticals Using Solid-State NMR spectroscopy” concerned many areas of relevance to my work, and in particular, provided significant insight into understanding data I had recently acquired.