



Why NMR Matters in Metabolomics

11am Monday 25th July
F10 room G37, UNSW

In principle, NMR is an ideal technique for metabolomics. It is non-destructive, non-biased, highly quantitative, requires no prior separation, permits the identification of novel compounds and needs no chemical derivatization. However, relative to other analytical techniques NMR is slow and relatively insensitive. Furthermore the identification and quantification of compounds in mixtures by NMR is manually intensive and often error-prone. Because of these limitations, NMR is being supplanted by mass spectrometry for many metabolomic applications. In this presentation I will highlight some recent developments in the field of NMR-based metabolomics and show how NMR can be used to match or even exceed the speed, sensitivity and metabolite coverage claimed by various mass spectrometry methods. In particular, I will describe our recent efforts to completely automate NMR-based metabolomics using a software program called Bayesil as well as NMR-based metabolomics kits that we are developing. I will also describe other activities being conducted both in our lab and elsewhere to: 1) enhance the sensitivity of NMR to nanomolar detection; 2) extend the capabilities of NMR to work with tiny samples; 3) provide new vistas for chemical and/or metabolite imaging; 4) measure both metabolites and proteins simultaneously and 5) facilitate novel compound identification and characterization. I will also show how NMR can – and should -- play a complementary role to mass spectrometry for metabolomics research, and that NMR still really matters in metabolomics.