Evaluating the Use of ASAP-HMQC and Sensitivity-Edited HSQC Spectra Acquired with Non-Uniform Sampling for Rapid Screening of Organic Samples

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There has been increasing interest in using edited HSQC spectra in combination with $^1$H and $^{13}$C data sets for screening organic compounds. However, the time and/or sample concentration still inhibits this approach unless one has access to a cryoprobe. An alternative would be to use the ASAP-HMQC sequence of Freeman and Kupce, which allows for faster acquisition but does not provide spectral editing and gives slightly poorer $^{13}$C resolution. However, significant further improvements are possible with the availability of software for acquiring and processing non-uniformed sampled (NUS) 2D data.

We have investigated this possibility using an Agilent DD2-600 NMR spectrometer equipped with a OneNMR (room temperature) probe. Using 10mM (ca 2 mg) solutions of representative organic compounds, we find that, with the aid of NUS, it is feasible to obtain high quality 2D shift-correlated spectra in 1.5 minutes or less with ASAP-HMQC and as little as 3 minutes with the sensitivity-enhanced CRISIS2-gHSQC sequence. In each case, the time to acquire a spectrum is less than the ‘overhead’ time required for a sample changer to replace one sample with another, followed by locking, tuning and shimming. Thus, there would be limited advantage in further decreasing acquisition times, although a cryoprobe would allow one to further decrease the sample concentration requirements.