NOAH Supersequences for Small Molecule Structure Elucidation

Ēriks Kupče[1] and Tim D. W. Claridge[2]

[1]Bruker UK Limited, Banner Lane, Coventry, CV4 9GH, UK
[2]Department of Chemistry, University of Oxford, Chemistry Research Laboratory, Mansfield Road, Oxford, OX1 3TA, UK

e-mail: eriks.kupce@bruker.com; tim.claridge@chem.ox.ac.uk;

Section: liquids

Abstract We provide a suite of NOAH pulse sequences, parameter sets and processing scripts (au-programs) for structure elucidation of small organic molecules at the natural isotopic abundance. The core 2D NMR techniques routinely employed in small molecule NMR spectroscopy, such as HSQC, HMQC, HMBC, COSY, NOESY, TOCSY, and similar, are combined into NMR supersequences (NOAH – NMR by Ordered Acquisition using ^{1}H-detection) that can be recorded in a single measurement involving a single recovery delay. In this way the data collection time is dramatically reduced and sample throughput increased for basic NMR applications, such as structure elucidation and verification in synthetic, medicinal, and natural product chemistry. The technique is based on an assumption that the sensitivity (as determined by the sample concentration and the available NMR probes) is sufficient to record the experiments with one or two scans per increment.

Keywords: NOAH, supersequences, structure elucidation, fast techniques.

Contents: pulse programs, parameter sets, au-programs, and README file.

Reference: Ē. Kupče and T. D. W. Claridge, Angew. Chem. Int. Ed. Eng., vol. 56, pp. 11779-11783 (2017).

Compatibility: Avance III, TS3, prosol, WaveMaker (wvm).

Submission Date: 3rd November 2017.