Ultrahigh-Resolution NMR at Full Sensitivity

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Abstract

We present CUPID (Computer-assisted Undiminished-sensitivity Protocol for Ideal Decoupling), a technique which uses parametric estimation to produce pure shift spectra from easy-to-acquire J-Resolved datasets without loss of sensitivity, and with absorption-mode lineshapes. We illustrate that it is effective even in scenarios where state-of-the-art pure shift experimental techniques are too insensitive, and where undesired solvent/impurity peaks overlap with signals of interest. The method also enables the assignment of multiplet structures based on a simple criterion involving the relationship between a particular resonance's direct- and indirect-dimension frequencies. The functionality required to use CUPID is provided by NMR Estimation in Python (NMR-EsPy), an open source package with a simple-to-use API and supporting graphical interface.