ACS Local Section
North Jersey

# Unequivocal Identification of Two-bond Heteronuclear Correlations by i-HMBC to Facilitate the Elucidation of Complex Natural Product Structures at Nanomole Scale


**Speaker:** **Xiao Wang**
Associate Principal Scientist
Merck


**Date:** **March 23rd, 2023**

**Time:** 12:00 pm ET via Microsoft Teams

## Abstract

HMBC is an essential NMR experiment for determining multiple bond heteronuclear correlations in small to medium-sized organic molecules, including natural products, yet its major limitation is the inability to differentiate two-bond from longer-range correlations. There have been several attempts to address this issue, but all reported approaches suffer various drawbacks, such as restricted utility and poor sensitivity. Here we present a sensitive and universal methodology to identify two-bond HMBC correlations using isotope shifts, referred to as i-HMBC (isotope shift detection HMBC). Experimental utility was demonstrated at the sub-milligram / nanomole scale with only a few hours of acquisition time required for structure elucidation of several complex proton-deficient natural products, which could not be fully elucidated by conventional 2D NMR experiments. Because i-HMBC overcomes the key limitation of HMBC without significant reduction in sensitivity or performance, i-HMBC can be used as a complement to HMBC when unambiguous identifications of two-bond correlations are needed.


## Connection Information

This will be a virtual meeting hosted via Microsoft Teams. A direct link to the meeting is located HERE.

Further information can be found on the NMR Topical Group website.

Please reach out to Tom Osborn Popp (thomas.osbornpopp@rutgers.edu) or Christine Jorge (christine.jorge@bms.com) with any questions.

*Presented by the NMR Topical Group – North Jersey ACS*