



Human blood serum spiked with N-nitrosodimethyl amine (NDMA)

Ashish Guleria, PhD, 2017

Biomolecular NMR and Disease Metabotyping | Centre of Biomedical Research (CBMR)

Field strength: 800 MHz

Why is this your favorite spectrum?

In a recent serum metabolomics study seeking metabolic discrimination between systemic sclerosis (SSc) patients and normal controls (NCs), we identified a metabolite entity of highest discriminatory significance resonating at chemical shift of 3.125 ppm w.r.t. lactate signal (methyl doublet peak referenced at chemical shift 1.3102 ppm). When we used the profiler module of CHENOMX (v8.1, containing 800 MHz data library of various endogenous metabolites), the singlet peak pattern nicely matched with that of simulated pattern of library compound known as *N*-nitrosodimethyl amine (NDMA). The identified NDMA resonances were further confirmed through NMR spiking experiments using NDMA pure compound. As such NDMA is highly toxic and is also a carcinogenic in nature. *In vivo* synthesis or accumulation of NDMA has also been demonstrated in several human pathologies.

Study reference: <http://acrabstracts.org/abstract/nuclear-magnetic-resonance-based-metabolomics-study-identifies-highly-discriminatory-metabolites-in-87-systemic-sclerosis-patients/>

Comments: The spectral signatures of NDMA established in our lab will form the basis for future metabolomics studies related to evaluating the elevated serum level of NDMA in patients with systemic sclerosis (SSc) and its metabolic reprogramming after clinical treatment.