

# Forensic Research & Technology

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## Isotopic quantitative NMR as a tool for authentication and traceability of drugs

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Isotopic quantitative NMR (iqNMR) has been successfully applied to  $^2\text{H}$  since the 80's (SNIF-NMR). Recently, EBSI team has been able to extend it to  $^{13}\text{C}$ . It is now possible to measure with a precision as low as 1‰, the  $^{13}\text{C}/^{12}\text{C}$  ratio on each carbon ( $\delta^{13}\text{C}_i$ ), giving a lot more information than the global  $^{13}\text{C}/^{12}\text{C}$  ratio on the whole molecule ( $\delta^{13}\text{C}_g$ ) obtained from isotope ratio measurement by mass spectrometry (irm-MS). Indeed, only knowing the mean  $\delta^{13}\text{C}_g$  could be misleading. If the measured value is null, is it because there is no fractionation or because there is counteractive normal and inverse isotopic effects on different positions? Quantitative  $^{13}\text{C}$  NMR has already been successfully applied to a range of molecules including glucose, vanillin, paracetamol and aspirin and used to show the position-dependent isotopic fractionation occurring during reactions or purifications. We developed new applications of this powerful technique. In environmental studies,  $^{13}\text{C}$  iqNMR can be used to study the fate of pollutants. As an example, oxidation of a fuel additive, Methyl tert-butyl ether has been done. MTBE was oxidized by potassium permanganate and the eventuality of a position-specific fractionation has been investigated. In the actual debate around the origin of Tramadol, natural or anthropogenic, mean values cannot give a clear answer and  $^{13}\text{C}$  iqNMR can help to establish a possible biosynthetic pathway. The isotopic fingerprint could provide a unique tool for the authentication of drugs, depending of their synthesis, manufacturer or the origin of reactants.

### Biography

Pierrick Nun has completed his PhD in 2009 from Montpellier University, France, where he worked on the application of alternative methodologies as mechanochemistry in organic solvent-free synthesis. After Post-doctoral positions at St. Andrews University, Scotland, on gold catalysis and University of Caen, France, on phosphine-boranes reactivity, he was appointed as an Assistant Professor in Nantes in 2012. He is currently working on applications of iqNMR in environmental and pharmaceutical sciences and has published 27 papers and book chapters in peer-reviewed journals.

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