



Department of Chemistry
NMR Facilities
Director: Dr. Carlos A. Steren

NMR NEWS

July 2009

* To check on the [instrumental status](#) and [reservation system](#), and find tutorials, links and more, visit our website www.chem.utk.edu/nmr

*** New student operator in the NMR Facilities.**

The NMR Committee has selected Mr. Jonathan Horton to replace Mr. Julio Gutierrez as student operator in the NMR Facilities. Jonathan is starting his third year as a graduate student in our Chemistry Department. He works in Dr. Bin Zhao's research group. Jon, among other responsibilities, will be in charge of training and helping users with the Bruker AC250 and Varian 300 instruments. Jon will start in this position on August 1st.

On the other hand, Mr. Josh Abbott, who has been the student operator in charge of the Bruker AC250, Bruker 400 and Solid State Varian 400, will remain in charge of the two 400 MHz spectrometers.

* **Varian Mercury 300 MHz Autosampler**

The autosampler on the Varian 300 has been repaired. The undergraduate Organic Lab (CHEM 369) is taking full advantage of it. Thanks to the coordination with Dr. L. Smith and help from Mr. Costyl Njiojob, every student is getting a ^1H and a ^{13}C NMR spectra on his/her sample. Next semester we will also acquire 2D-COSY on their samples.

* **NMR in Forensics.**

*2009 UTK
Forensic Chemistry Camp*



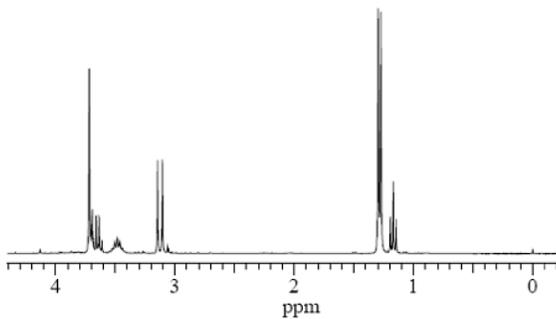
Kids assisting the 2009 UTK Forensic Camp had the opportunity to solve a poisoning case using NMR.

In more specific chemistry terms, identification of glyphosate in cases of poisoning using nuclear magnetic resonance spectroscopy of biological fluids.

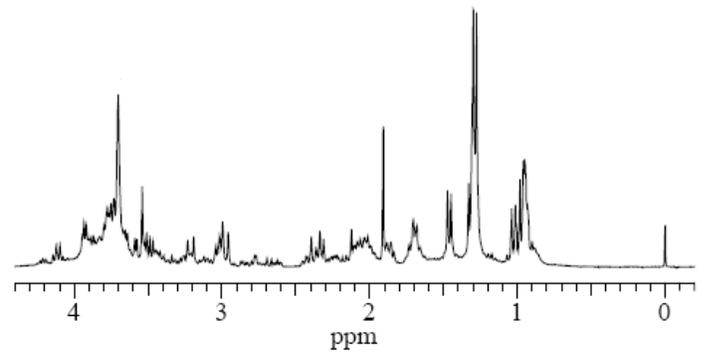
Glyphosate (N-phosphonomethylglycine; CAS registry number: 1071-83-6) is a broad-spectrum, relatively nonselective and post-emergence herbicide. It is used worldwide in the form of an aqueous solution of isopropylamine (I.P.) salt under trade names such as Roundup, Rodeo, Glyfonox and Glycel.

A 40-year-old man, treated for depression, ingested about 20 ml of Roundup. ^1H NMR measurements of biological fluid samples were performed on a 300 NMR spectrometer (extracted from Forensic Science International 143 (2004) 141–145)

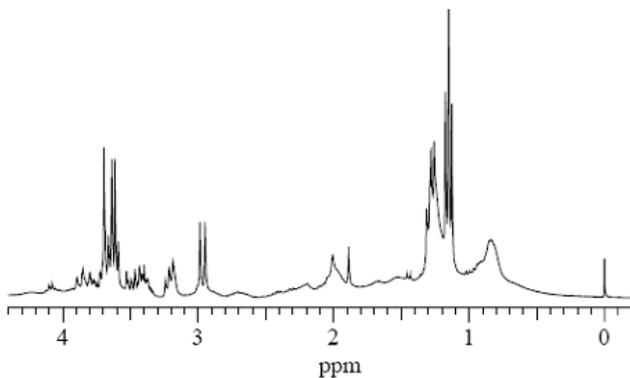
A



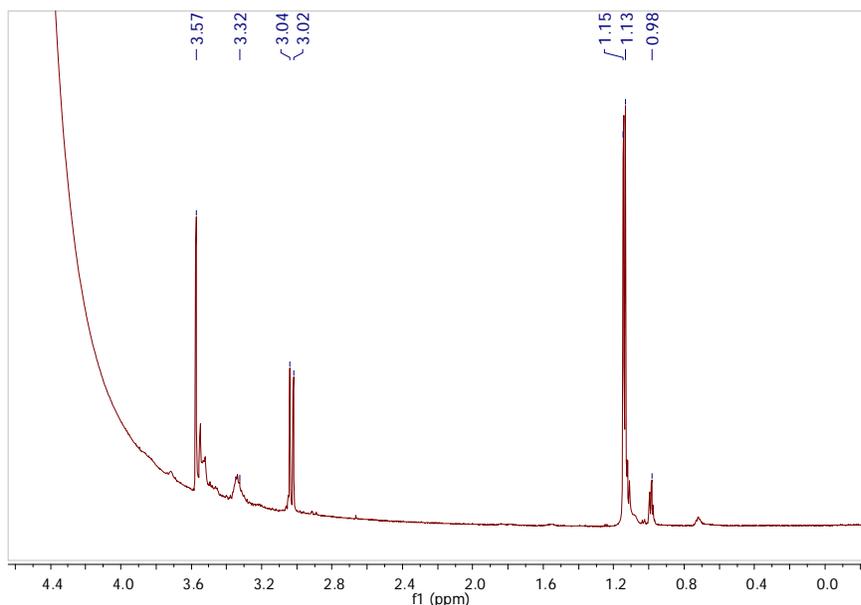
B



C



- A: ^1H spectrum of Urine
- B: ^1H spectrum Gastric fluid
- C: ^1H spectrum Serum



The figure above shows a partial ^1H spectrum of Roundup taken on our Varian 600 MHz instrument. During the Camp, the kids watched how the same spectrum was acquired on the Varian 300 MHz using the autosampler.

The ^1H NMR lines of Roundup can be identified in the ^1H spectra of the biological fluid samples of the patient (A, B and C).

Acknowledgment: Dr. Al Hazari for allowing NMR to participate in the Forensic Chemistry Camp.