



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

## **NMR NEWS**

**December 2011**

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

\* **The Facilities Website** [www.chem.utk.edu/nmr](http://www.chem.utk.edu/nmr) has been updated.

### **\* Diffusion-Ordered Spectroscopy (DOSY)**

The NMR Facilities has purchased the DOSY package and installed it in the Varian 500. The package includes several 2D and 3D diffusion experiments.

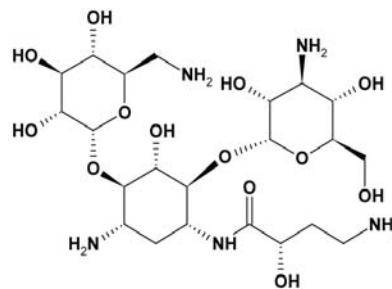
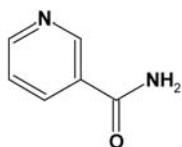
“NMR diffusion experiments provide a way to separate the different compounds in a mixture based on the differing translation diffusion coefficients (and therefore differences in the size and shape of the molecule, as well as physical properties of the surrounding environment such as viscosity, temperature, etc) of each chemical species in solution.”

“In a certain way, it can be regarded as a special chromatographic method for physical component separation, but unlike those techniques, it does not require any particular sample

preparation or chromatographic method optimization and maintains the innate chemical environment of the sample during analysis.”

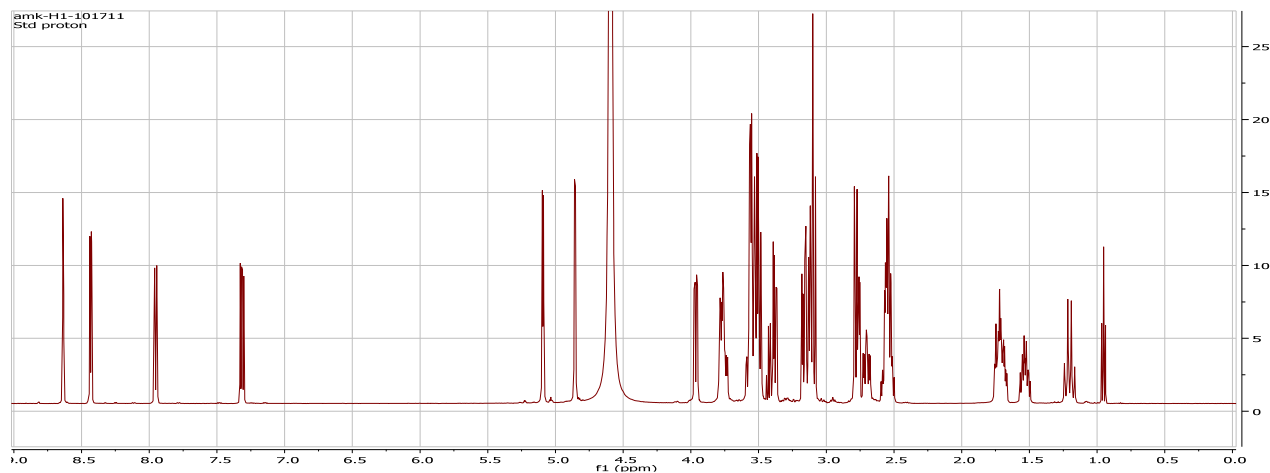
Example: A mixture of Nicotinic acid amide and Amikacin in D<sub>2</sub>O;

Nicotinic acid amide

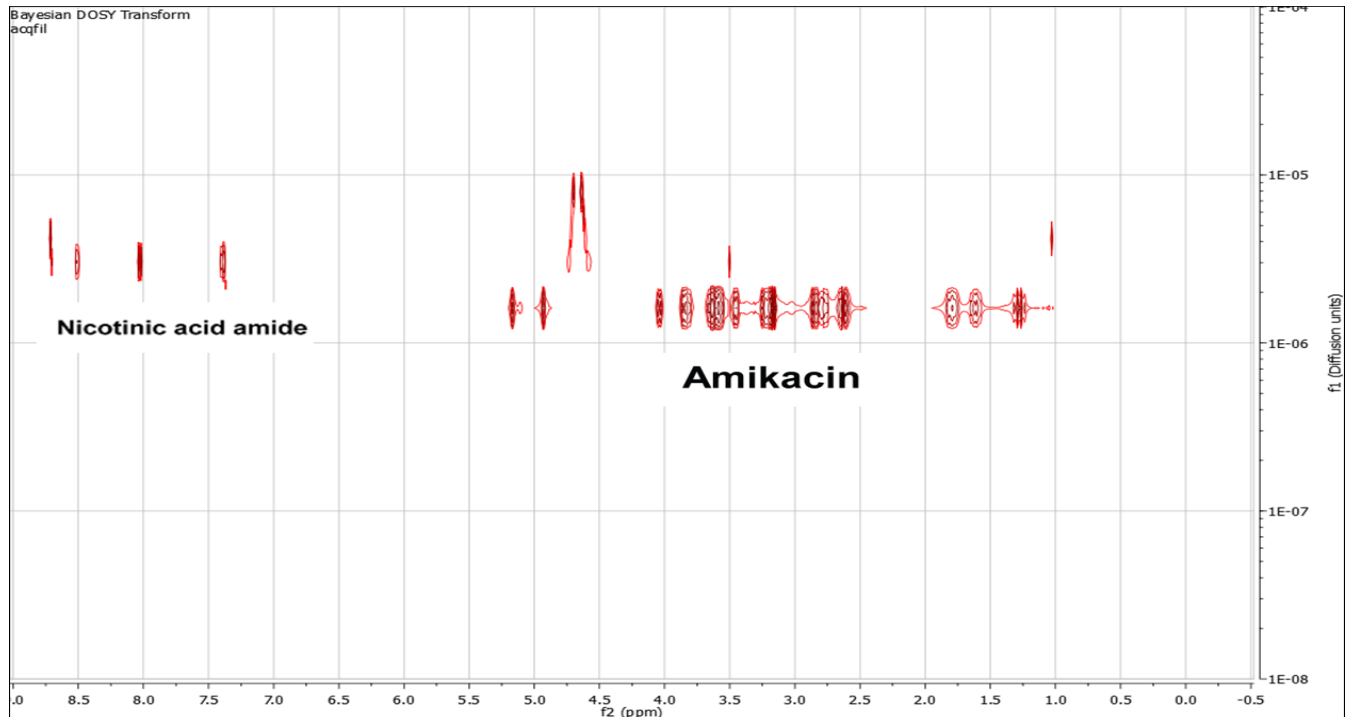


Amikacin

**<sup>1</sup>H spectrum of the mixture:**

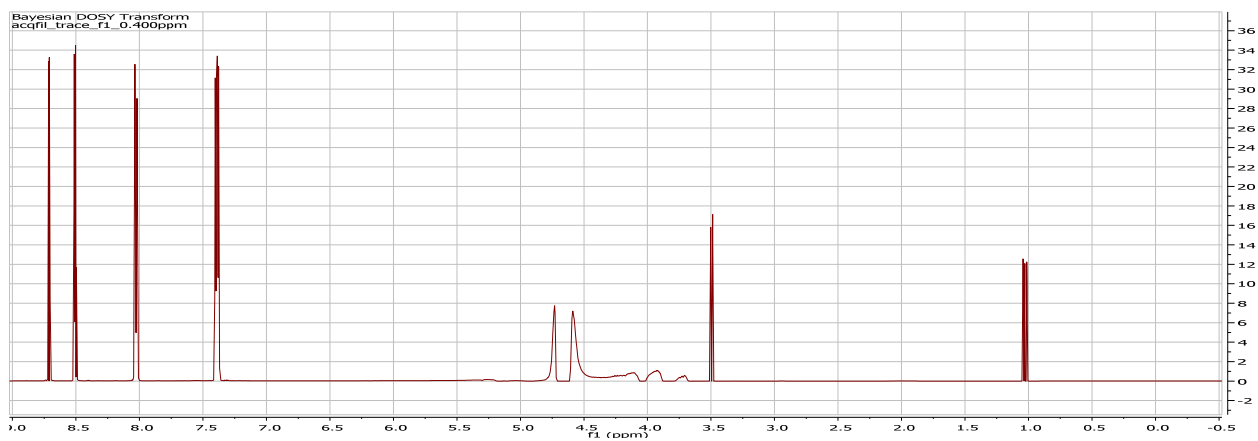


## 2D-DOSY experiment.

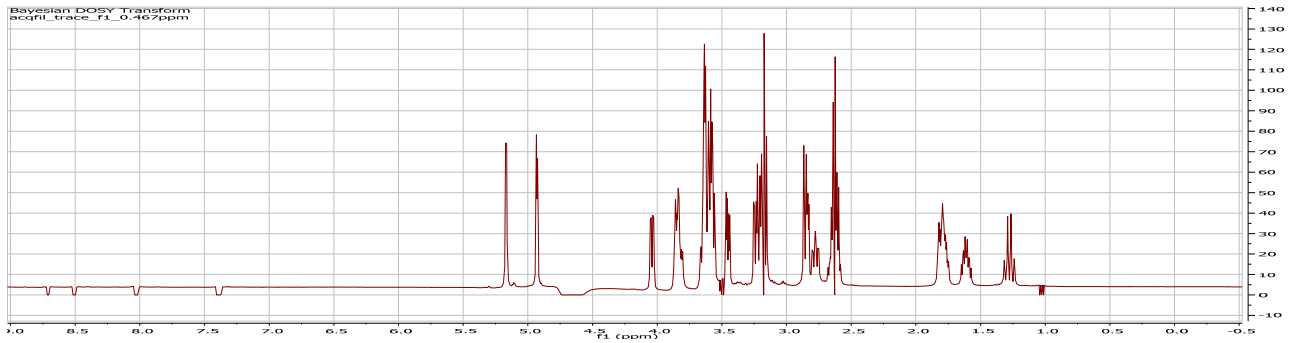


The <sup>1</sup>H spectra of each component of the mixture, can be extracted from the 2D-DOSY experiment.

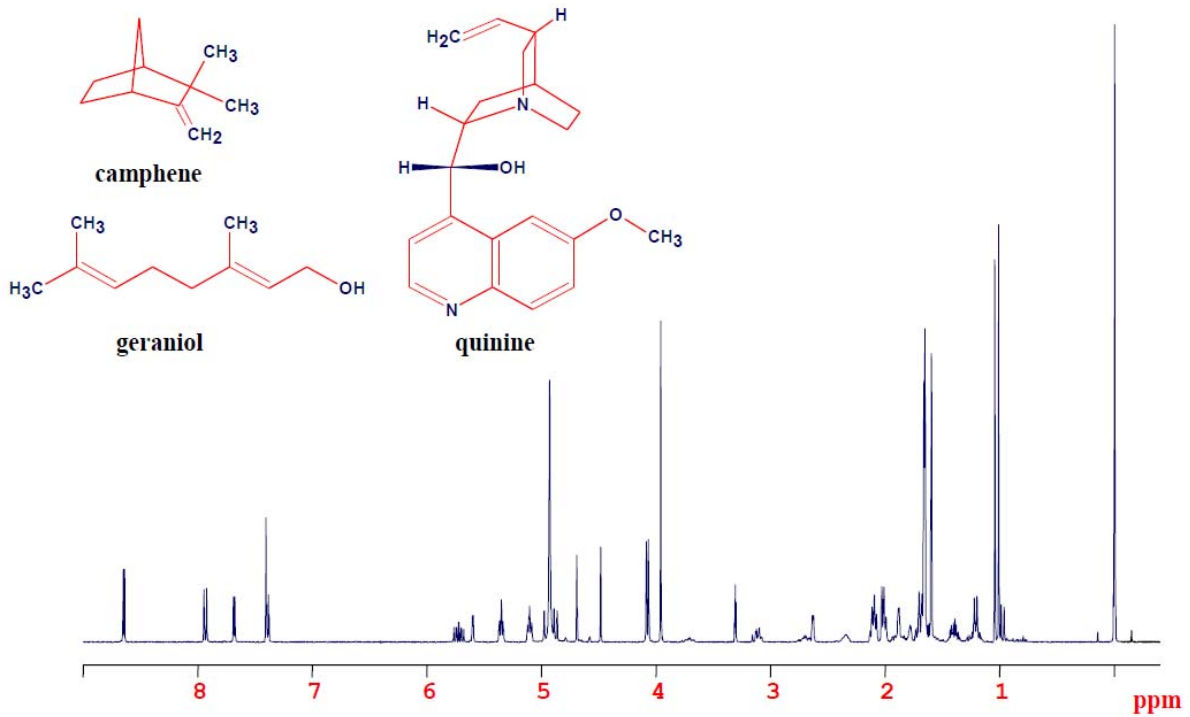
**Nicotinic acid amide:**



# Amikacin:



## Structures and <sup>1</sup>H spectrum of the QGC mixture (in CD<sub>3</sub>OD)



A standard 2D homonuclear and heteronuclear NMR experiment can be combined with a diffusion experiment into a 3D experiment as the DOSYHMQC shown in the figure below.

### DOSY 3.1 - What to do with overlapping peaks?

