K54 A Nuclear Magnetic Resonance (NMR) Based Study of Urine Samples Containing Drug of Abuse: Scope and Limitations of the Technique

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After attending this presentation, attendees will learn about the use of NMR spectroscopy in drug of abuse detection.

This presentation will impact the forensic science community by exploring a new spectroscopic technique for the analysis of forensic samples.

Testing for substances of abuse in urine has great forensic relevance. The need for testing arises in many different situations: identifying drugs of abuse, supporting or denying a person's statement that they have or have not taken drugs, or determining what drug may have caused an overdose. In the following presentation, the advantages and limitations of using nuclear magnetic resonance (NMR) spectroscopy for the identification of substances of abuse in urine is explored. Opioids were chosen for analysis as federal drug testing in urine mandates a higher cutoff level than other substances of abuse. NMR spectroscopy is the method chosen for the analysis on the basis of many advantages: it allows positive identifications of chemically different species (very similar substrates can be usually identified); very little sample preparation or operator training is needed; and, spectra could be gathered in very short times.

Codeine, morphine, and oxycodone were used in this study. Initially, these compounds were dissolved in an artificial urine solution of ten components formulated to model the NMR spectrum of real urine and NMR spectra were recorded. Later, real urine and forensic samples from deceased patients were used in the investigation.

From preliminary data, NMR spectroscopy has proven to be a novel, feasible, and useful technique for the study of opioids in urine samples. The three opioids, which present very similar structures, could be distinguished from one another in both water and artificial urine. Moreover, all three drugs could be identified at a concentration of 2000 ng/ml, equal to the federal cutoff limit given by the United States Department of Health and Human Services. This was easily done with a simple analysis of chemical shift differences. These characteristic peaks were observed at low concentrations suitable for drug testing. These peaks, arising from two protons on the phenyl group of phenanthrene opioids, were found between 6 and 7 ppm. For morphine, the difference in frequency was near 41 Hz while for codeine is near 71 Hz. For oxycodone, the difference in frequency is near 43 Hz. The ease of use NMR instrumentation, speed of analysis, as well as the small sample amount needed and the fact that is a non-destructive technique render NMR spectroscopy an advantage over current forensic methods used to analyze substance of abuse in urine.

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