# The Detection of Date Rape Drug Residues Using Ray X Diffraction

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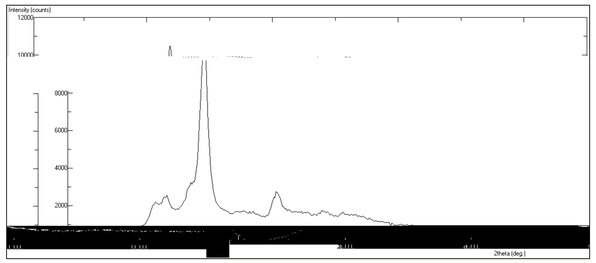


Figure 1: Spectrum of Denim Fabric. The sample was analyzed with a scan range of 2.000 – 90.00deg at a scan speed of 5.000 deg/min.

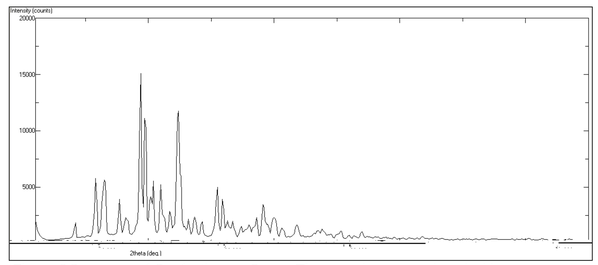


Figure 2: Spectrum of Confectionary Sugar. The sample was analyzed with a scan range of 2.000 – 90.00deg at a scan speed of 10.000 deg/min.

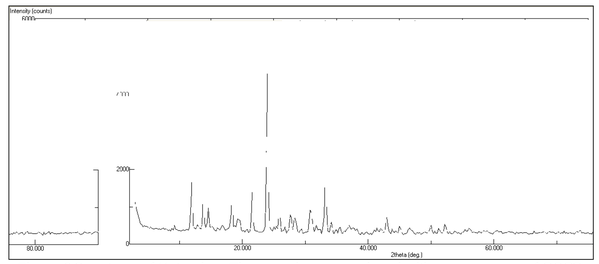


Figure 3: Spectrum of Ketamine. The sample was analyzed with a scan range of 2.000 – 90.00deg at a scan speed of 10.000 deg/min.

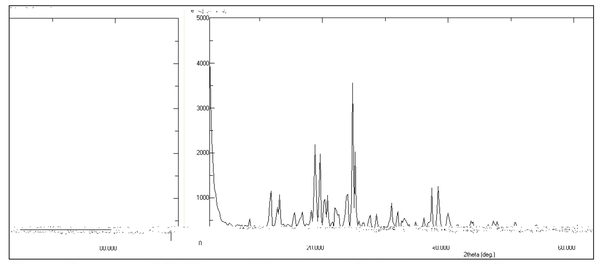


Figure 4: Spectrum of 10% Mixture of Ketamine and Confectionary sugar. The sample was analyzed with a scan range of 2.000 – 90.00deg at a scan speed of 5.000 deg/min.

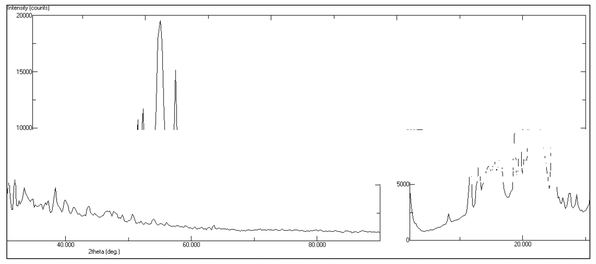


Figure 5: Spectrum of Denim Fabric with 10% Ketamine and Confectionary Sugar Paste. The sample was analyzed with a scan range of 2.000 – 90.00deg at a scan speed of 10.000 deg/min.

## Methods

The instrument used for this project was the Rigaku MiniFlex II Desktop X-ray Diffractometer. The software utilized for analyzing the obtained spectra was MDI Jade 9. Before every sample was run, a standard silicone test was performed to ensure the instrument was working properly.

Four fabric types: denim, white cotton, polyester, and grey cotton (90%) and polyester (10%), were cut to cover the 2 x 2 cm well on a zero background sample holder and mounted using cellophane tape. Individual spectra of the fabric samples were obtained and peak tables printed using Jade.

Puredate rape drug samples were loaded into the zero background holder with a small circular well about 2 mm in diameter using toothpicks. Spectra were obtained and analyzed using Jade.

Two mixtures of confectionary sugar and drug (Ketamine and Chloral Hydrate) were prepared to be 10% drug mixtures. After spectra of the two mixtures were obtained, peak tables were found using Jade. These peak tables were then compared to the pure drug and confectionary sugar peak tables found earlier, in order to assign the mixture peaks as being from the drug or sugar.

Pastes of the 10% drug mixtures were created using a single drop of water. The Ketamine paste was used in further testing by smearing it on the four fabric samples. These were then mounted on the zero background holder and tested with the X-ray diffractometer. Peak tables were then created using Jade and compared to find the peaks indicative of Ketamine.

Finally, a mixture of 5 mL ethanol and 0.0028 g Ketamine was prepared in a small falcon tube. A few drops of the mixture was pipetted onto a flat zero background holder. This was left out to evaporate and leave a residue behind. This was tested using XRD and peak tables were obtained and again compared to find the peaks resulting from the Ketamine.

Figure 6: Spectra and Peak Table analysis of the Ethanol and Ketamine Mixture using the MDI Jade 9 Software. This demonstrates how the software was utilized to further analyze all the samples. The peak positions, indicated above the peaks, were found by setting a background, which is the pink line. The software used threshold, intensity cutoff, and range to accurately pick and assign peak values.

## Results

The resulting spectra demonstrate the individualized diffraction patterns, ranging from simple to very complex, of the various samples analyzed using X-ray Diffraction. Samples were analyzed at angles within the range of 2° to 90° with both the sample holder and detector moving up to 45° each. The scan speed was varied between 10.000deg/min and 2.000deg/min. The use of XRD for the purposes of this project was validated by the results explained best in Figure 7. The chart clearly indicates Ketamine peaks can be detected amongst all the other components within the sam Figure 5 demonstrates how complex XRD spectra can be. Visual comparison with t spectra from Figures 1-

Figure 7: Chart of Peak Values from the Spectra shown in Figures 1-6. The peak values highlighted in yellow correspond to the peaks that were concluded to be the detected peaks of ketamine amongst the various other components of the samples.

## Acknowledgements