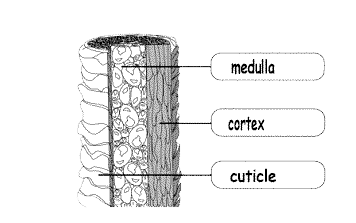
**Determining Time of Death Based on Drug Docking Hair Samples in Overdose Cases**

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When drugs enter the body, it is a biological response that the body wants to break them down. During this process or breakdown, metabolites of the drug consumed are produced, and can linger around in the hair while the effects of the drug are being felt. Even after those effects end, those metabolites of the drug stay, and these metabolites can later be found as traces in drug testing. The typical method of drug analysis is performed using Gas Chromatography / Mass Spectrometry (GC/MS) [1]. Hair drug testing searches for drugs that are within the hair shaft. Placement of drugs in the shaft guarantees the victim had the drug in their system rather than it being deposited by some exposure method. Getting a hair sample requires a small lock of the person’s hair, generally about 100 strands. The hair is washed to prevent getting results of potential surface exposure, and then run through the GC/MS in order to detect any possible metabolites. Hair has three main sections, the cuticle, the cortex, the medulla (Figure 1). The medulla is the innermost core of the hair that not all people present, depending mainly on hair color and thickness, so any traces of drugs of abuse that are looked for, will be found in the middle layer, cortex [2]. The cuticle is the outer layer of the hair shaft that acts as a protectant to the cortex.



*Figure 1 – Anatomy of a hair strand*

Detection times of drugs found in hair samples is mainly dependent on the dose of the drug, but also if the person was a chronic or acute user, how the drug was administered, and the concentration of the drug. Overall, detection time is longest in hair, lasting anywhere between 7 to 100 days, which is a much larger window for detection than other drug testing methods [2]. While the detection of the drug and its dose have a big window, the concentration of the drug in a post-mortem case can be overlooked. Many times, the concentration of a drug will increase after death. For many drugs concentrations may increase by as much as 10-fold [3]. This is mainly because no blood is circulating in the body, leaving no cells or responses to help break down the drug and wear off [4]. In turn, the environment allows for the drug to manifest on its own and the concentration begins to increase. In order to gain an accurate perspective on what the actual concentration of the drug was at the time of death, drug docking software can be used to visualize how the molecules react in the body after death.

By using drug docking software to mimic the drug that was detected in the victim’s hair sample, it is possible to simulate how the drug will react in the body post-mortem. You can set the software to match conditions in the body as they change from when the drug was introduced to the system, through death, and once the blood stops circulating how the drug changes in the system. Being able to visualize this reaction in the body can give a time frame on how long it takes before the drugs concentration will increase, and how long the victim has been passed since the drug was introduced. Piecing these together can lead back to time of death, which is a key in any overdose case.

The procedure would start by creating a drug commonly abused in a drug docking software and placing it under body conditions to note how the drug reacts. This would match what the drug in the hair sample would be right before death. Next altering the conditions to match what happens in the body once it shuts down and recording how the drug changes and what increases in the concentration. This will match how the drug and its concentration will look once analyzed in a GC/MS spectrum. Watching how the drug changes in the software and increase over a specific time, should be comparable to if another spectrum was taken of the same hair sample a certain time mark later depending on how long the simulation on the computer was run. The spectrum after a certain amount of time has gone by should show an increased spike in the concentration from the initial spectrum taken when the hair was first taken.

**Intellectual Merit**

The final result will show how drug docking can accurately simulate the post-mortem reaction of a drug and how the concentration increases in the body. This result will allow researchers to find time of death of the victim.

**Broader Impacts**

If this experiment is successful it will give the opportunity to be used in the Forensic Science field as an indicator in discovering time of death. Using this method in a case can aid in investigations where life and death comes into play. Helping to speed up the time it could take to solve an overdose crime can help investigators close a case quicker.

**References**

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