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Determination of a Simpler Method to Detect Benzoyllecgonine in Urine

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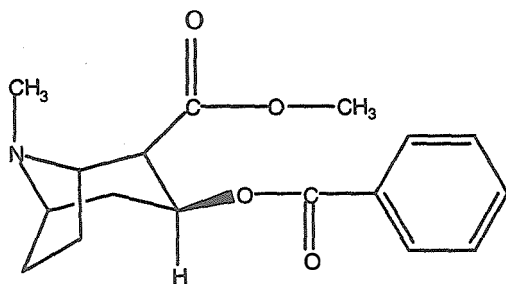
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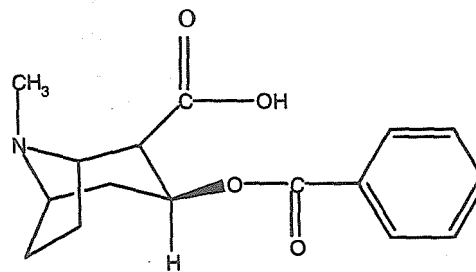
DETERMINATION OF A SIMPLER METHOD TO DETECT
BENZOYLECGONINE IN URINE

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Benzoylecgonine (BE) is the most abundant metabolite of cocaine found in the



Cocaine



Benzoylecgonine

human body. Analysis of BE in urine by gas chromatography/mass spectrometry is currently the method used to detect cocaine abuse. The current method is costly and time consuming, so an easier and more cost effective approach is being sought after. Because BE is a zwitterion, it is highly soluble in water and very difficult to extract from urine. To isolate BE in an environment where it is a charged molecule, the pK_a values were obtained experimentally, with a pK_{a1} of 2.15 ± 0.01 and a pK_{a2} of 11.41 ± 0.01 . Preliminary UltraViolet-Visible (UV-Vis) spectra were obtained to determine absorption bands of BE in various solvents. Based off of these spectra, dichloromethane was determined to be the best organic extracting agent. BE was synthesized, characterized, and purity tests were performed.

Future work includes further purification of BE, ion pairings, and finally extractions. Using the pK_a values, BE can be paired with another ion to form an ion pair at an appropriate pH. By extraction the ion pair into an organic solvent, it will be possible to detect small quantities of BE by UV-Visible spectroscopy.