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Isolation of a Cocaine Derivative and Its Quantification in Urine

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Poster Presentation P5

ISOLATION OF A COCAINE DERIVATIVE AND ITS QUANTIFICATION IN URINE

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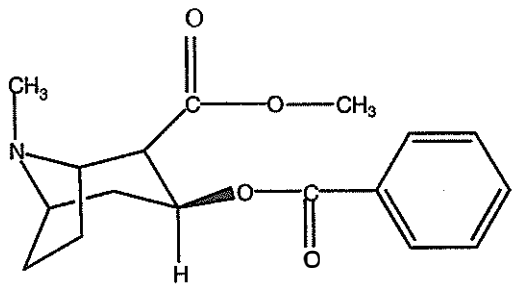
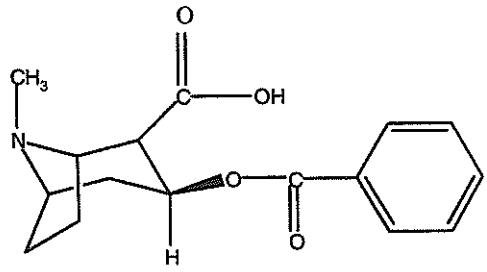


Cocaine



Benzoylecognine

Benzoylecognine (BE) is the most abundant metabolite of cocaine found in the human body. Analysis of BE in urine by gas chromatography/mass spectrometry is the method currently used to detect cocaine abuse. This current method is costly and time consuming, so finding an easier and more cost-effective approach is the goal of this research.

Due to BE being a zwitterion, it is highly soluble in water and very difficult to extract from urine. Once the pKa values of BE are determined, either the cation or anion form of BE can be formed from the zwitterion by adjusting the pH appropriately. When BE is in a cationic or anionic state, it can be ion-paired with an appropriate counter-ion to form a neutral ion pair. This ion pair can then be extracted into a non-polar solvent, concentrated, and quantitatively determined by UV-Vis spectroscopy.
The following portions of this project have been completed: BE was synthesized, characterized, and purity tests were performed. Preliminary UV-Vis spectra of BE were measured to determine absorption bands of BE in various solvents. Based on these preliminary UV-Vis spectra, dichloromethane was determined to be the best organic extracting agent. Next, pK_a values were experimentally determined, with a pK_{a1} of 2.15 +/- .01 and a pK_{a2} of 11.41 +/- .01. The pH of the BE zwitterion solution was adjusted according to these values, and ion pairings and extractions were performed using various ions. Many ion pairs failed to give clear results. There has been some initial success with the ion pair formed between BE and Dragendorf's reagant. This ion pair is currently being tested and data gathered in order to generate a clear calibration curve.