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Determining the pK_a of Benzoylecognine

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Poster Presentation 53

DETERMINING THE pK_a OF BENZOYLECOGNINE

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The most abundant cocaine metabolite found in the human body is benzoylecognine. To recognize cocaine abuse, gas chromatography/mass spectroscopy is currently used to analyze urine for benzoylecognine. However, GC/MS requires benzoylecognine to be derivitized before analysis, which is expensive. Derivitization is not needed when analyzing by liquid chromatography and therefore is cheaper. Benzoylecognine however is a zwitterion and possesses both a positive charge and a negative charge. This makes benzoylecognine highly soluble in water, making it difficult to extract into a non-polar solvent. Much of this research focuses on the determination of the pK_a of benzoylecognine in order to isolate it as a singly charged molecule. One of the pK_as is determined to be 2.47. Once benzoylecognine is in its positively charged form, it can be complexed with a large negative counter ion. This ion pair can then be extracted into an organic solvent analyzed using liquid chromatography.