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# Determination of pK Values for the Ionic Pairing of Benzoylecognine

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Poster Presentation 40

**DETERMINATION OF pK VALUES FOR THE IONIC PAIRING OF  
BENZOYLECOGNINE**

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Benzoyllecognine is the most abundant metabolite of cocaine in the human body. In forensic science, analysis of benzoyllecognine in urine, using gas chromatography/mass spectroscopy, is used to identify cocaine abuse. GC/MS requires derivatization of benzoyllecognine samples, which is costly. Liquid chromatography is a cheaper and faster way of quantifying, since derivatization is not needed. However, the benzoyllecognine ion has both a positive and a negative charge, with a net charge of zero. This makes benzoyllecognine extremely water soluble and difficult to extract from urine into a non-polar solvent. This research concentrates on finding the best environment to isolate benzoyllecognine as a charged molecule. By experimentally obtaining the pK<sub>a</sub> values for benzoyllecognine, the ideal pH can be obtained for isolating benzoyllecognine in a negatively charged form. This information can be used to complex benzoyllecognine with a bulky positive counter ion. The ion-pair can then be extracted into an organic solvent for quantification by liquid chromatography.