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