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Conformations of a Cocaine Metabolite

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Poster Presentation 24

CONFORMATIONS OF A COCAINE METABOLITE

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Benzoylecognine, the principle metabolite of cocaine, is the target molecule of choice for detecting illicit use of cocaine. Benzoylecognine is not organic solvent soluble because the molecule is a charged species, therefore cannot be easily extracted from aqueous urine. There are three different species of Benoylecognine: a positively charged (protonated) species, a negatively charged (deprotonated) species, and the zwitterion ion (containing both positive and negative charges) species.

The shape of each species has been determined using the Computer Animated Chemistry program (C.A.Che) and the most stable conformation found. The next step is to attempt to design another molecule with opposite charges and an inverse shape that will 'dock' with BE to form an uncharged ion pair. Upon docking the two molecules, the charge of Benzoylecognine will be hidden in the interior of the newly-formed ion pair. This ion pair has an overall charge of zero and should, therefore, mimic a non-polar molecule. The ion–pair should also be organic solvent-soluble. This allows extraction of the ion pair from urine using an organic solvent. The Benzoylecognine will then be analyzed by High Pressure Liquid Chromatography (HPLC) to determine its concentration.