



## Illinois Wesleyan University Digital Commons @ IWU

John Wesley Powell Student Research  
Conference

2000, 11th Annual JWP Conference

Apr 15th, 2:00 PM - 3:00 PM

# Conformations of a Cocaine Metabolite

Douglas Kasper

*Illinois Wesleyan University*

David N. Bailey, Faculty Advisor

*Illinois Wesleyan University*

Follow this and additional works at: <http://digitalcommons.iwu.edu/jwprc>

Douglas Kasper and David N. Bailey, Faculty Advisor, "Conformations of a Cocaine Metabolite" (April 15, 2000). *John Wesley Powell Student Research Conference*. Paper 18.

<http://digitalcommons.iwu.edu/jwprc/2000/posters2/18>

This Event is brought to you for free and open access by The Ames Library, the Andrew W. Mellon Center for Curricular and Faculty Development, the Office of the Provost and the Office of the President. It has been accepted for inclusion in Digital Commons @ IWU by the faculty at Illinois Wesleyan University. For more information, please contact [digitalcommons@iwu.edu](mailto:digitalcommons@iwu.edu).

©Copyright is owned by the author of this document.

Poster Presentation 24

CONFORMATIONS OF A COCAINE METABOLITE

Douglas Kasper and David N. Bailey\*

Department of Chemistry, Illinois Wesleyan University

Benzoyllecognine, the principle metabolite of cocaine, is the target molecule of choice for detecting illicit use of cocaine. Benzoyllecognine 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 Benzoyllecognine: 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 Benzoyllecognine 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 Benzoyllecognine will then be analyzed by High Pressure Liquid Chromatography (HPLC) to determine its concentration.