



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: <https://digitalcommons.iwu.edu/jwprc>

Kasper, Douglas and Bailey, Faculty Advisor, David N., "Conformations of a Cocaine Metabolite" (2000). *John Wesley Powell Student Research Conference*. 18.
<https://digitalcommons.iwu.edu/jwprc/2000/posters2/18>

This is protected by copyright and/or related rights. It has been brought to you by Digital Commons @ IWU with permission from the rights-holder(s). You are free to use this material in any way that is permitted by the copyright and related rights legislation that applies to your use. For other uses you need to obtain permission from the rights-holder(s) directly, unless additional rights are indicated by a Creative Commons license in the record and/ or on the work itself. This material has been accepted for inclusion by faculty at Illinois Wesleyan University. For more information, please contact 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.