B181 The Detection and Differentiation of Controlled Substances by Gas Chromatography-Vacuum Ultraviolet (GC-VUV) and Chemometrics

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Learning Overview: The goal of this presentation is to bring an understanding of gas chromatography-vacuum ultraviolet spectrophotometry (GC-VUV) as applied to traditional controlled substances.

Impact on the Forensic Science Community: This presentation will impact the forensic science community by highlighting the capabilities of gas chromatography-vacuum ultraviolet (GC-VUV) spectrophotometry to detect and differentiate controlled substances.

The region of the electromagnetic spectrum known as "vacuum ultraviolet" extends below 200nm where the electronic transitions of sigma bonds lie. A new Vacuum Ultraviolet (VUV) spectrophotometer has been made available for coupling to gas chromatographs allowing spectra to be obtained from 125-430nm. All gas phase compounds except the smallest molecule, H_2, absorb above 125 nm.[1] Thus, the VUV detector should be able to detect any molecule analyzable by gas chromatography. Though virtually any molecule can be detected, the question arises of how differentiable the spectra are. To answer this question, several controlled substances were analyzed.

Phenethylamines are a common drug class including pseudoephedrine and illicit drugs such as methamphetamine. Several of the phenethylamines are difficult to analyze by electron impact mass spectrometry due to the fragmentation giving the same mass to charge ratio fragments at similar ratios. While phenethylamines are generally differentiable by retention time, an extra layer of specificity is preferred. Eight structurally similar phenethylamines were found to be differentiable using their VUV spectra. A calibration curve and limit of detection study was performed for two phenethylamines that indicated a limit of detection around 1 ng on-column and upper limit of linearity around 1 µg on-column using gas chromatography–vacuum ultraviolet spectrophotometry (GC-VUV). The spectral data obtained were analyzed by the multivariate statistical techniques Principal Component Analysis and Discriminant Analysis. The results indicate the ability to differentiate each of the phenethylamines based upon their repeatable VUV spectra.

The most exciting results from the phenethylamines are the ability to differentiate the VUV spectra of the diastereomers ephedrine and pseudoephedrine. While the two compounds give very similar spectra, chemometric analyses indicate the ability to correctly associate the spectra with the corresponding molecule. It should be noted that the spectra are similar enough that the 95% confidence interval around the discriminant analysis results overlap slightly. The control software for the VUV detector was also able to distinguish the two with some degree of reliability based on the produced "Match coefficient." The ability of VUV to distinguish diastereomers also lends itself to the diastereomers of cocaine.

GC-VUV of other drugs such as heroin, γ-butyrolactone, and 3,4-Methyl enedioxy methamphetamine (MDMA) provides results of similar promise for forensic chemistry. Several de-identified seized drugs "street" samples were analyzed to show "real world" performance. It should be noted that VUV has difficulties differentiating small alkanes and should be considered as complimentary to GC/MS rather than a replacement. Overall, GC-VUV continues to show promise for future use in forensic drug analyses as a technique complimentary to GC/MS.

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Reference(s):

1. Schug KA, Sawicki I, Carlton DD, Jr., Fan H, McNair HM, Nimmo JP, et al. Vacuum ultraviolet detector for gas chromatography. *Anal Chem*. 2014 Aug 19;86(16):8329-35.

Vacuum Ultraviolet Detection, Phenethylamines, GC-VUV