A175 Spectral Analysis of the Interconversion of Gamma-Hydroxybutyrate (GHB) and Gamma-Butyrolactone (GBL) Using Near Infrared Spectroscopy

Kristen J. Johnson, BS, and Thomas A. Brettell, PhD, Cedar Crest College, 100 College Drive, Allentown, PA 10104*

After attending this presentation, attendees will have a better understanding of the use of Near Infrared Spectroscopy (NIRS) to study the chemistry and equilibrium between the cyclization of gamma-hydroxybutyrate (GHB) to gamma-butyrolactone (GBL).

This presentation will impact the forensic science community by serving to provide a critical understanding of the rate of interconversion of GHB to GBL, and vice versa, at different matrix conditions of GHB in evidential samples.

GHB is a central nervous system depressant classified as a sedative- hypnotic and abused for it's euphoric, sedative, and anabolic effects. GHB and its many derivatives can be studied using the spectroscopic technique of NIRS because it is a quick non-destructive technique that allows for the measurement of organic compounds with vibrational overtones between 700nm and 2500nm. GHB is classified as a federal Schedule I illicit substance, but can also be obtained in prescription form. GHB commonly cycilizes into a lactone, GBL, and the equilibrium depends upon the matrix conditions. The equilibrium ratio between GHB and GBL can vary with the pH of the medium and the temperature of the matrix. The equilibrium reactions can be measured accurately using NIRS in the transmittance mode. Due to the solutions being clear and colorless, the transmittance mode is most appropriate for this equilibrium study. The unique changes in the carbon groups can be used as the main

parameter of comparison in shape, size, and intensity of each spectrum with the intention of understanding the rate of interconversion at different specific conditions. All samples were diluted in deionized water, measured in the same cuvette (2mm) using NIRS, while varying the pH with a phosphate buffer. Thirty-two scans for each run were taken and the interconversion was measured as it occurred at a given time interval. To standardize the spectral data, all spectra were analyzed using the multivariable mathematical software provided with the instrument. Using a specific time interval, the conversion rate can be seen at the various pH levels using the spectra generated by the NIR software. The fanning of the spectra over the time interval clearly demonstrates the conversion of the alcohol to the lactone or the lactone to the alcohol depending on the pH tested. The fanning demonstrates a reaction rate which can be measured using a regression plot.

The results in this study agree with that as measured by Ciolino et al.[1] When GHB is exposed to a basic solution with a pH = 12, the solution is stable. If GBL is added to this basic medium instead, a rapid conversion takes place with 100% completion to form GHB. The basic medium de-cycilizes the GBL and forms GHB due to the introduction of more free OH^- molecules in the medium. The reaction also goes to completion very rapidly due to the amount of free OH^- groups present at this pH. The reaction time for 100% GHB at pH=12 is approximately 15 minutes. Once the pH begins to lower toward the acidic region, the reaction rate of GBL to GHB drops off significantly and the reaction no longer goes to 100% GHB. The pH has a drastic effect on the reaction rate as well as the equilibrium concentrations of the two drugs. At an acidic pH, the GBL is stable, but upon addition of GHB to a solution with a pH of two, the reaction rate of conversion to GBL is very fast and the relative concentration of GBL to GHB is much greater. At a pH of seven, the reaction is very stable, amounting to a longer period to equilibrate and relatively equal concentrations of GHB and GBL in an aqueous solution.

Reference:

1. Ciolino L.A., Mesmer M.Z., Satzger R.D., Machal A.C., McCauley H.A., Mohrhaus A.S. The chemical interconversion of GHB and GBL: forensic issues and implications. J Forensic Sci 2001 46(6):1315–1323.

Forensic Science, GHB, Near Infrared Spectroscopy

 ** Presenting Author*