

TECHNICAL NOTE

Mark J. Bennett,¹ B.S. and Robert R. Steiner,² M.S.

Detection of Gamma-Hydroxybutyric Acid in Various Drink Matrices via AccuTOF-DART*

ABSTRACT: A new screening method for detecting *gamma*-hydroxybutyric acid (GHB) in drink matrices, using the IonSense, Inc. (Saugus, MA) direct analysis in real time (DART) ion source coupled to a JEOL exact mass time-of-flight mass spectrometer (AccuTOF), was validated and compared with the current screening methodology. The DART ion source allows for analysis of samples under ambient conditions with little to no sample preparation. Fifty drink specimens were spiked at levels of 1, 2, 3, and 4 mg/mL GHB, and analyzed on the AccuTOF-DART. Positive detection of GHB occurred for each of the samples at each concentration level, giving 100% accuracy for the samples tested. Twenty-five of the 50 drink specimens were spiked at 1 mg/mL GHB and tested using a color test known as the GHB Color Test #3. Only two of these 25 specimens tested positive for the presence of GHB, giving only 8% accuracy. Implementation of this new methodology as a screening tool for GHB analysis will quickly eliminate negative specimens allowing the examiner to focus analysis time on those that screened positive.

KEYWORDS: forensic science, controlled substances, screening, *gamma*-hydroxybutyric acid, *gamma*-hydroxybutyrate, direct analysis in real time, mass spectrometry, time of flight

Gamma-hydroxybutyric acid (GHB) is a naturally occurring compound in the human body and a minor metabolite and precursor to the inhibitory neurotransmitter, *gamma*-aminobutyric acid (GABA). GHB is considered a strong central nervous system depressant, and has long been studied for its ability to induce short-term comas, as well as a potential use in surgical anesthesia. GHB easily and rapidly dissolves in most liquid matrices and, in the proper dosage, can induce sleep, cause memory loss, lower inhibitions, and cause mild euphoria. These characteristics have led to GHB being increasingly seen in sexual assault cases and commonly referred to as a “date rape drug.” In the forensic setting, GHB is most commonly encountered dissolved in various drinks, with the most frequently encountered drink being alcohol-based (i.e. beer, wine, liquor) (1). Other drinks commonly encountered include non-alcoholic beverages often seen in social settings such as juices, sodas, and bottled water. Drinks served commercially are typically offered in amounts of 8, 12, and 20 ounces. The reported dose of GHB needed for sleep induction ranges from 1 to 5 g depending on the body type of the exposed subject. This places the dosage range of GHB commonly encountered in drink matrices at 1.7–21.1 mg/mL, based on the amount of drink matrix. GHB is a Schedule I controlled substance, except when found as a treatment for narcolepsy in the form of a drug preparation called Xyrem[®] (Schedule III) (1).

Color tests are typically employed for screening of drink matrices for the presence of GHB. Positive results for a color test are only indicative of a particular chemical functionality being present; however, combinations of different color tests may be employed to help in narrowing down the possible identity of the unknown sample to a specific drug or a class of drugs (2). The primary color test

used in screening for GHB at the Virginia Department of Forensic Science is the GHB Color Test #3 (3). This test was first reported by Smith et al. (4) and has a reported sensitivity of 3 mg/mL.

Direct Analysis in Real Time (DART), developed by IonSense, Inc. (Saugus, MA), is a new mass spectrometry ion source that allows for real-time data collection under ambient conditions. The DART performs positive- and/or negative-ion, noncontact detection of gases, liquids, and materials on surfaces. Quick and simple analyses with little to no sample preparation, no carryover issues, and the capability to analyze polar and nonpolar compounds are all hallmarks of this new technology (5). DART employs a gas, such as helium or nitrogen, to produce metastable species that in turn ionize water (positive mode) or oxygen (negative mode) molecules. These ions then ionize sample molecules on the surface of the sample probe which is held in the DART gas stream. While positive ion detection is the more commonly employed method, analysis of GHB is best accomplished using negative ion detection. The mechanism of negative ion detection using the DART was previously described by Cody et al. (6).

The DART ion source is coupled with an accurate mass time-of-flight (TOF) mass spectrometer, called the AccuTOF (JEOL USA, Inc., Peabody, MA). TOF mass analyzers provide the advantage of rapid data acquisition rates, simplicity of design, a very wide observed mass range and exact mass measurements, which can give rise to accurate elemental composition information (7).

We report here the validation of a new and reliable screening method for GHB analysis in various commonly encountered drink matrices using the AccuTOF-DART. This method was compared with the currently accepted screening method, GHB Color Test #3, to offer potential benefits.

Methods

Materials and Equipment

The GHB standard was obtained from Sigma (St. Louis, MO), *gamma*-butyrolactone (GBL), 1,3 butanediol (1,3-BD), and

¹Department of Forensic Science, Virginia Commonwealth University, Richmond, VA 23284.

²Virginia Department of Forensic Science, Richmond, VA 23219.

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1,4-butanediol (1,4-BD) from Aldrich (Milwaukee, WI), malic acid from Eastman Organic Chemicals (Rochester, NY), and the methanol was HPLC grade from Fisher Scientific (Fairlawn, NJ). The GHB Color Test #3 reagent consisted of bromocresol green (JT Baker Chemical Company, Phillipsburg, NJ), methyl orange (Coleman and Bell Company, Norwood, OH), dextrose (JT Baker Chemical Company), aniline hydrochloride (Sigma-Aldrich, St. Louis, MO), sodium hydroxide (EM Science, Gibbstown, NJ) and HPLC grade ethanol (Fisher Scientific). Test tubes used for color testing were borosilicate FisherBrand 10 × 75 mm. Melting point tubes used for DART testing were borosilicate glass, 0.8 × 90 mm obtained from Kimble Glass, Inc (Vineland, NJ). Polyethylene Glycol (PEG) 600 for AccuTOF calibration was obtained from Chem. Service, West Chester, PA.

Stock solutions were prepared in methanol with GHB at concentrations of 1.0 mg/mL and 100 mg/mL, GBL at 2.0 mg/mL, 1,3-BD at 3.0 mg/mL, and 1,4-BD at 2.0 mg/mL. The GHB Color Test #3 reagent was prepared by mixing bromocresol green solution (0.03 g bromocresol green in 100 mL 4:1 methanol:water, adjusted to pH 7.0 with 0.1 N sodium hydroxide) and methyl orange solution (0.01 g methyl orange in 100 mL methanol, adjusted to pH 7 with 0.1 N sodium hydroxide) in a 1:1 ratio. The combined reagent was then mixed in a 3:1 ratio with a modified Schwebbes reagent (solution A: 2 g dextrose in 20 mL water; solution B: 2.4 g aniline hydrochloride in 20 mL ethanol. Solutions A and B were mixed and diluted to a total volume of 80 mL with methanol) (4).

Fifty different drink specimens were typed into six drink groups; soda, beer, wine, liquor, juice, and "other" (e.g. well water). Each respective drink specimen was stored in 2 ounce Qorpak™ glass bottles (Bridgeville, PA). pH readings were taken of all drink specimens using EM-Reagents® Color pHast pH paper (EM Science). Table 1 shows a summary of all drinks received and measured pH values. One milliliter aliquots of each drink specimen were transferred to respective autosampler vials for testing. All drink specimens were stored in the refrigerator when not in use.

Experiments were carried out using the DART ion source coupled to a JEOL AccuTOF™ mass spectrometer (JMS-100LC) operated in negative-ion mode. This system was controlled by JEOL's "Mass Center" software. All measurements were taken with the ion guide peak voltage set at 650 V, the reflectron voltage at -950 V, orifice 1 voltage at -20 V, orifice 2 voltage at -10 V, ring lens voltage at -17 V, and an orifice 1 temperature of 80°C. The mass range was 65–300 Daltons (Da). The DART ion source was used for all specimens with a helium gas flow rate of 4.0 L/min, gas heater temperature of 300°C, discharge electrode needle set at 4000 V, electrode 1 at -150 V, and electrode 2 at -350 V. These DART parameters represent the optimum response for GHB in negative ion mode. Internal mass calibration was achieved using PEG600 run within each data file. Instrument calibration was performed daily by sampling malic acid. Calibration was deemed acceptable if the measured mass of the deprotonated molecule of malic acid was within 3 millimass units (mmu) of the calculated ([M-H] - of 133.0137) mass. Each individual specimen in a respective run was sampled two times. Sampling was done using the closed end of cleaned glass melting point tubes. Area count values for both the blank and spiked specimens were obtained using the "Peak Integration" software in MSTools (ChemSW, Inc., Fairfield, CA).

Lower Limit of Detection

GHB solutions were prepared in test tubes using the 1 mg/mL stock solution of GHB. A series of dilutions in methanol was made to obtain concentrations of 0.5, 0.25, 0.12, 0.06, 0.03, and

TABLE 1—Drink specimen and pH reading summary.

Name of Drink	Type of Drink	pH
Seagram's Ginger Ale	Soda	2
Kroger Cranberry Raspberry Juice	Juice	2
Private Selection Apple Juice	Juice	3
Tropicana Original Orange Juice	Juice	3
Tropicana Fruit Punch	Juice	2
Minute Maid Lemonade	Juice	2
Gatorade-Lemon Lime	Juice	3
Gatorade-Fruit Punch	Juice	3
Minute Maid Apple Juice	Juice	3
Campbell's Tomato Juice	Juice	4
Gatorade-Orange (Powder in Tap Water)	Juice	3
Aromasde Toris with Sengria	Red wine	3
Elijah Craig Bourbon Whiskey 12	Liquor	4
Gordon's Vodka Deluxe	Liquor	4
Barefoot Sauvignon Blanc	White wine	3
Captain Morgan Parrot Bay Pineapple Colada	Liquor	2
Ocean Spray Cranberry Juice (no sugar)	Juice	2
Stewart's Ginger Beer	Soda	3
Nature's Place Organic Vanilla Soy Milk	Other	7
Green Springs Winery Chardonnay	White wine	3
Peels Blueberry Pomegranate Malt	Beer	3
Yuengling Lager Beer	Beer	4
Vampyre Vodka	Liquor	N/A*
Smirnoff Raspberry	Beer	3
Berry Gatorade Rain	Juice	3
Smirnoff Vodka (Triple Distilled)	Liquor	5
Aristocrat Rum	Liquor	5
Well water (Dinwiddie County)	Other	6
Franklin County's Finest (Grape)	Liquor	3
Propel water (with calcium)	Other	3
Diet Coke	Soda	3
Coca-Cola Classic	Soda	2
Sprite	Soda	3
A&W Root Beer	Soda	5
Tilt Alcohol Malt Beverage/Energy Drink	Other	3
Cocaine Energy Drink	Other	3
Contadino Pinot Grigio (2006)	White wine	3
Mano A Mano Tempranillo	Red wine	N/A*
Sam's Choice Diet Sam's Cola	Soda	3
Jim Beam Kentucky Straight Bourbon Whiskey	Liquor	4
Southern Comfort Liqueur	Liquor	5
Vendage 2003 California Shira	Red wine	5
Hiram Walker Dry Gin	Liquor	4
DeKuyper Peachtree Schnapps	Liquor	4
Old Mr. Boston Peppermint Schnapps	Liquor	4
Hiram Walker Blended Whiskey	Liquor	4
Hiram Walker Blackberry Flavored Brandy	Liquor	5
Goldschlager	Liquor	5
Keswick Vineyards 2005 Rose	White wine	3
Red Bull Energy Drink	Other	3

*Nature of sample did not allow for pH testing

0.015 mg/mL. Sampling was done by dipping a glass melting point tube into each respective solution and holding it in the gas stream of the DART. The serial dilutions were run on the AccuTOF-DART, with averaged, centroided, background subtracted spectra produced. An acceptance criterion was established such that the difference between the measured mass and the calculated mass was required to be within the instrument manufacturer's specification of ±5 mmu. The lower limit of detection was established at the concentration just above where this criterion was no longer met.

Selectivity

The prepared GBL, 1,3-BD, and 1,4-BD stock solutions were run on the AccuTOF-DART to determine whether these compounds would interfere with GHB analysis. pH readings were taken

for each respective drink specimen. Each blank drink specimen was run four times on the AccuTOF-DART to determine if any endogenous levels of GHB were present, and to look for interfering ions at the specific mass of the GHB anion. Blank levels were determined by constructing a mass chromatogram over a mass range ± 5 mmu from the calculated exact mass of the GHB anion at 103.0395 Da, integrating these mass chromatograms and determining the amount of area counts present. Data from these runs were organized by corresponding drink type, and an average area count value was tabulated for each respective group. The average area count of the four runs for each group was then multiplied by 3 to establish a blank administrative cutoff value for each drink group. A blank administrative cutoff value was calculated for each individual drink within the "other" group.

Verification of Known Samples

Ten microliter aliquots of the 100 mg/mL stock solution of GHB were added to 1.0 mL of each individual drink sample (from the blank runs) with a 10 μ L Hamilton syringe to obtain a concentration of 1 mg/mL in each respective drink sample. These were then run on the AccuTOF-DART. This process was repeated to obtain sample concentrations of 2, 3, and 4 mg/mL, respectively. These concentration levels were chosen for this study because they mimic the low end of the concentration range needed to induce clinical effects. The assumption was made that detection at these levels would extend to detection at the upper levels seen in illicit

use. Data was organized by drink type and compared with the established administrative cutoffs from the blank specimens to determine if GHB could be considered present.

GHB Color Test #3

GHB Color Test #3 was performed on 25 of the 50 specimens (all six drink types included) using the protocol established by Smith et al. (4). Each drink specimen within the "other" group was included in this sampling. One-half milliliter aliquots of each sample were placed in a test tube and spiked with 5 μ L of the 100 mg/mL GHB stock solution to give a concentration of 1 mg/mL in each drink. A positive result for the presence of GHB was indicated by an immediate green color. Negative results showed either orange-red, in white or colorless drinks, or a solution slightly darker in color than the original drink solution. One-half milliliter of tap water served as the negative control for this test (4).

Results and Discussion

Lower Limit of Detection

The acceptance criterion of ± 5 mmu failed at 0.03 mg/mL, while the criterion was met at 0.06 mg/mL. A solution with a concentration between these two values was made at 0.05 mg/mL, sampled 10 separate times, and found to meet the acceptance criterion in all runs. The lower limit of detection was set at 0.05 mg/mL.

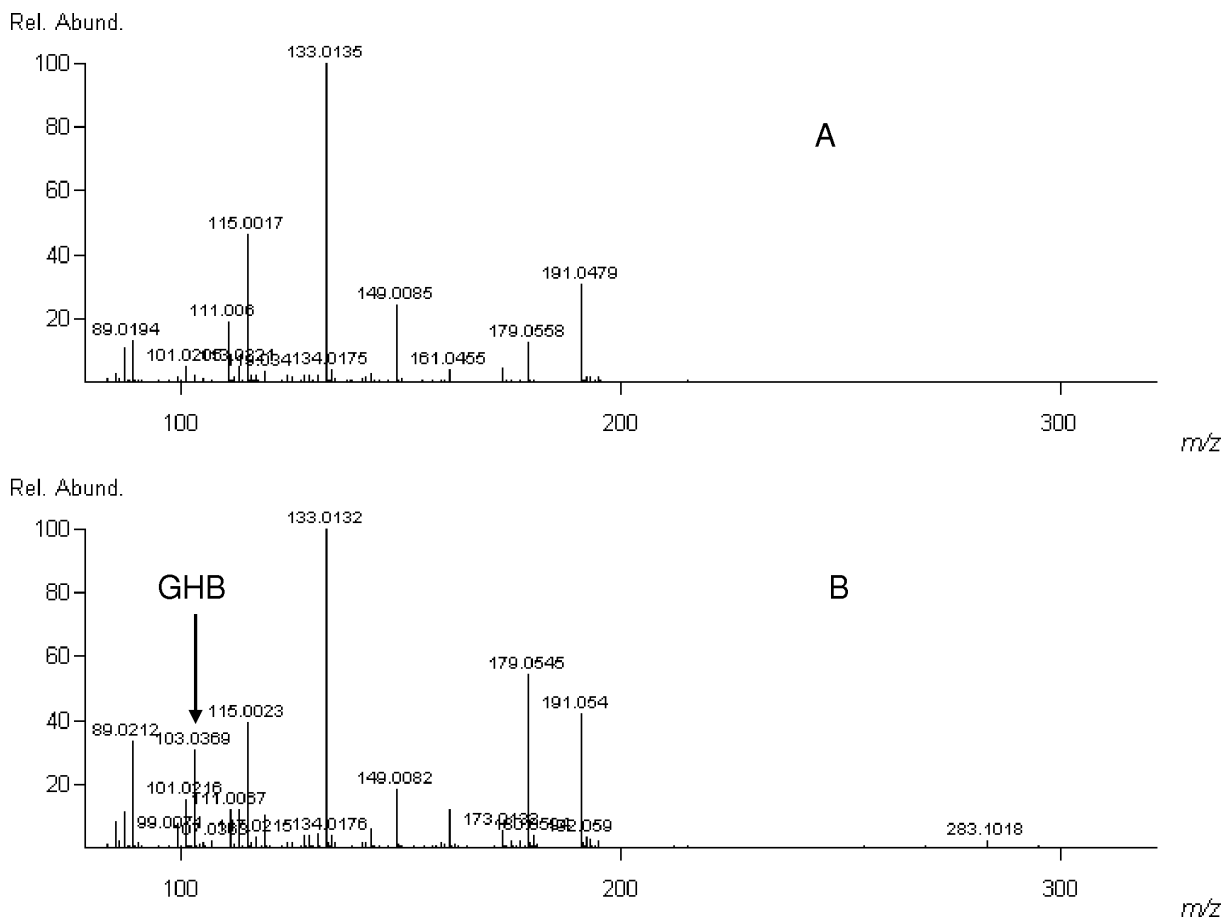


FIG. 1—AccuTOF-DART mass spectra of (A) blank Ocean Spray Cranberry Juice and (B) 2 mg/mL spike of same with GHB.

TABLE 2—Average blank area counts for each drink type.

Drink Type	Blank Average (Area Counts)	Established Administrative Cutoff
Soda	1502	4506
Juice	2277	6831
Liquor	2595	7785
Beer	2154	6462
White wine	5136	15,408
Red wine	5488	16,464
Organic Vanilla Soy Milk	618	1854
Well water	0	0
Propel water with calcium	0	0
TILT Alcohol Malt Beverage/Energy Drink	1961	5883
Cocaine Energy Drink	1130	3390
Red Bull Energy Drink	2909	8727

Selectivity and Verification of Known Samples

The GBL, 1,3-BD, and 1,4-BD samples were observed to not give any mass signal in negative-ion mode. As these compounds would therefore not interfere with GHB analysis, no further testing was done with these compounds.

Table 1 shows the results of pH readings taken for all 50 specimens. pH readings taken for 46 of the 50 specimens showed moderate to relatively strong acidic readings (i.e., pH 2–5). These pH readings were important to account for any GHB to GBL inter-conversion. Previous studies, conducted by Ciolino et al. (8) and Chappell (9), determined the primary factors involved in the inter-conversion of these two components to be pH, time, and storage temperature. The pH readings for all specimens ranged from 2 to 7 with the majority of the values falling in the 3–5 range. GHB is considered to be stable for several days at strongly acidic to neutral

TABLE 3—Average area counts for all specimens at 1 mg/mL GHB spiked.

Name of Drink	Type of Drink	Administrative Cutoff Value (Area Counts)	Specimen 1 mg/mL Average (Area Counts)
Seagram's Ginger Ale	Soda	4506	75,841
Kroger Cranberry Raspberry Juice	Juice	6831	127,550
Private Selection Apple Juice	Juice	6831	28,440
Tropicana Original Orange Juice	Juice	6831	185,001
Tropicana Fruit Punch	Juice	6831	95,204
Minute Maid Lemonade	Juice	6831	165,538
Gatorade—Lemon Lime	Juice	6831	107,522
Gatorade—Fruit Punch	Juice	6831	288,826
Minute Maid Apple Juice	Juice	6831	53,304
Campbell's Tomato Juice	Juice	6831	179,960
Gatorade—Orange (powder in tap water)	Juice	6831	97,019
Aromasde Toris with Sangria	Red wine	16,464	195,854
Elijah Craig Bourbon Whiskey 12	Liquor	7785	746,805
Gordon's Vodka Deluxe	Liquor	7785	411,876
Barefoot Sauvignon Blanc	White wine	15,408	87,506
Captain Morgan Parrot Bay Pineapple Colada	Liquor	7785	408,869
Ocean Spray Cranberry Juice (no sugar)	Juice	6831	57,173
Stewart's Ginger Beer	Soda	4506	228,583
Nature's Place Organic Vanilla Soy Milk	Other	1854	823,590
Green Springs Winery Chardonnay	White wine	15,408	91,894
Peels Blueberry Pomegranate Malt	Beer	6462	182,858
Yuengling Lager Beer	Beer	6462	350,128
Vampyre Vodka	Liquor	7785	322,696
Smirnoff Raspberry	Beer	6462	183,561
Berry Gatorade Rain	Juice	6831	98,827
Smirnoff Vodka (Triple Distilled)	Liquor	7785	31,898
Aristocrat Rum	Liquor	7785	42,414
Well water (Dinwiddie County)	Other	0	24,095
Franklin County's Finest (Grape)	Liquor	7785	109,672
Propel water (with calcium)	Other	0	35,764
Diet Coke	Soda	4506	218,847
Coca-Cola Classic	Soda	4506	63,536
Sprite	Soda	4506	154,867
A&W Root Beer	Soda	4506	47,659
Tilt Alcohol Malt Beverage/Energy Drink	Other	5883	147,651
Cocaine Energy Drink	Other	3390	60,028
Contadino Pinot Grigio (2006)	White wine	15,408	43,010
Mano A Mano Tempranillo	Red wine	16,464	98,267
Sam's Choice Diet Sam's Cola	Soda	4506	436,988
Jim Beam Kentucky Straight Bourbon Whiskey	Liquor	7785	447,326
Southern Comfort Liqueur	Liquor	7785	158,610
Vendage 2003 California Shira	Red wine	16,464	100,392
Hiram Walker Dry Gin	Liquor	7785	361,117
DeKuyper Peachtree Schnapps	Liquor	7785	333,916
Old Mr. Boston Peppermint Schnapps	Liquor	7785	267,760
Hiram Walker Blended Whiskey	Liquor	7785	525,500
Hiram Walker Blackberry Flavored Brandy	Liquor	7785	433,894
Goldschlager	Liquor	7785	467,984
Keswick Vineyards 2005 Rose	White wine	15,408	144,529
Red Bull Energy Drink	Other	5727	423,147

pH values. It is not until pH values of 2 or lower that an equilibrium will be established in a 2:1 ratio of GBL to GHB, respectively; however, this process occurs over roughly 9 days (8). Interconversion can be delayed if the GHB or GBL containing solutions are stored at refrigeration temperatures when not in use. Several specimens showed a pH value that would lead to slow interconversion. Certain measures were taken to prevent any interconversion that could take place in these samples. The stock standard of GHB used for spiking all specimens was stored in a refrigerator when not in use, and all sampling was done immediately following the spiking of actual specimens.

The AccuTOF-DART mass spectra of a blank specimen of Ocean Spray Cranberry Juice and the same specimen spiked with 2 mg/mL of GHB are shown in Figs. 1A and 1B. The peak at 103.0369 Da seen in Fig. 1B is within 3 mmu of the calculated mass of the GHB anion (103.0395 Da).

Table 2 shows the averaged values of four replicate runs of signal detected on the AccuTOF-DART at the calculated mass of the GHB anion, and the corresponding calculated administrative cutoff value for each drink type and each drink in the "other" category for all blank specimens. Forty three of the 50 specimens showed very low levels of signal (area counts) at the calculated mass of the GHB anion. These signal levels could be attributed to instrument noise or interference from peaks associated with compounds in the drink matrices. By setting the blank administrative cutoffs at three times the blank signal levels, it could be established that signal levels higher than these values could be directly attributed to the addition of GHB to the drink matrices. The wine drink type showed blank signals significantly higher than all other drink types. This is consistent with the previous findings of Elliott and Burgess (10), which showed that GHB is a naturally occurring component in some wines.

Average area count values for each specimen at 1 mg/mL were chosen to demonstrate the lowest value for GHB in the spiked

specimens relative to the administrative cutoff value established from the blank specimen runs for each drink type. Table 3 shows the average area count value of GHB detected in all specimens at 1 mg/mL. Area count values of GHB in the spiked specimens far exceeded the established blank administrative cutoff for their corresponding drink type. All drink specimens showed a difference >24,095 area counts. There is considerable variability in area counts in the spiked specimens. This variability is thought to arise from the various ionization potentials of other components present in each different drink matrix. Each separate drink contains different constituents in its makeup allowing for different degrees of ionization observed for each specimen. An additional factor that could contribute to this variability is viscosity of the specimen. Specimens exhibiting very viscous characteristics allow for more sample to adhere to the melting point tube during sampling, while specimens showing a less viscous nature would have a tendency to quickly run off the tube. Some specimens tested, such as the Vampyre Vodka, were noticeably thicker in viscosity than the other samples and these samples did show higher area counts of GHB in all spiked specimens.

Human variability does exist in the sampling technique used. The "wandering" technique used in analysis can affect the final area count readings of GHB. "Wandering" refers to the overall technique or motion used by the analyst when drawing the melting point tube through the gas stream of the sampling area of the DART source. The amount of sample detected is directly related to the time the sample tube is held in the gas stream and the amount of liquid adhered to the tube, as described above. With a small amount of practice, better accuracy and consistency can be achieved with this technique. Two "wandings" for each specimen were done in order to obtain consistent and reproducible data.

Use of an autosampler device would reduce the number of variables involved in the introduction of samples into the DART gas stream. Delivery of the analyte to the gas stream would be more

TABLE 4—GHB Color Test #3 results.

Sample Type	Sample ID	Result	Immediate Color Change Observed
Soda	Seagram's Ginger Ale	NSR*	Clear → Light red
	Diet Coke	NSR	Brown → Brown
	Coca-Cola Classic	NSR	Brown → Brown
Liquor	Captain Morgan Parrot Bay Pineapple Colada	NSR	Light yellow → Light orange
	Vampyre Vodka	NSR	Red → Red
	Franklin County's Finest (Grape)	NSR	Clear → Light red
	Hiram Walker Blackberry Flavored Brandy	NSR	Brown → Brown
	Goldschlager	NSR	Clear → Light red
Juice	Kroger Cranberry Raspberry Juice	NSR	Red → Red
	Private Selection Apple Juice	NSR	Golden yellow → Light orange
	Tropicana Original Orange Juice (no pulp)	NSR	Orange → Red-orange
	Tropicana Fruit Punch	NSR	Red → Red
	Minute Maid Lemonade	NSR	Yellow → Light orange
	Gatorade-Fruit Punch	NSR	Red → Red
Beer	Peels Blueberry Pomegranate Malt	NSR	Purple → Light purple
	Yuengling Lager Beer	NSR	Golden yellow → Light orange
White wine	Contadino Pinot Grigio (2006)	NSR	Light yellow → Light orange
Red wine	Mano A Mano Tempranillo	NSR	Dark red → Dark red
	Vendage 2003 California Shira	NSR	Dark red → Dark red
Other	Nature's Place Organic Vanilla Soy Milk	Positive	Opaque white → Lime green
	Well water (Dinwiddie County)	Positive	Clear → Light green
	Propel water (with calcium)	NSR	Clear → Light red
	Tilt Alcohol Malt Beverage/Energy Drink	NSR	Golden yellow → Light orange
	Cocaine Energy Drink	NSR	Dark red → Dark red
	Red Bull Energy Drink	NSR	Yellow → Light orange
Controls	Positive	Positive	Clear → Dark green
	Negative	NSR	Clear → Light red

*No significant reaction.

precise and reproducible. While such devices currently exist, one was not available for this experiment.

GHB Color Test #3

A positive control consisting of a 10 mg/mL solution of GHB, and a negative control (tap water) were tested and gave expected results. These controls indicated the test reagent to be in working order. Table 4 shows the results obtained for the GHB Color Test #3 on the 25 drink specimens. When spiked with 1.0 mg/mL GHB, only two of the specimens, organic vanilla soy milk and well water, showed the desired green color change indicative of a positive result. All other specimens showed no significant reaction with a final solution color that was only different in appearance due to addition of the red-colored test reagent. At this concentration, screening for GHB using the AccuTOF-DART proved to be 100% effective at detecting GHB relative to GHB Color Test #3, which only showed detection of GHB in two of the 25 specimens (8%), for the drink matrices tested.

Identification of GHB on the AccuTOF-DART is not ideal. One issue is that the DART ion source utilizes no chromatographic input. The data obtained is a "mixture" mass spectrum of all the components that were ionized from the melting point tube. Other than the deprotonated molecule, no peaks are present that lead to a unique identification of GHB. Any fragmentation that occurs gives rise to relatively ubiquitous fragments that could originate from many species and not just GHB. This issue leads to a lack of useful data to exclusively identify GHB.

For screening purposes only, the data obtained shows the AccuTOF-DART to reliably detect the presence of GHB in drinks spiked at various levels relative to their corresponding blanks. In comparison with GHB Color Test #3, screening using AccuTOF-DART was more sensitive and reliable. While the AccuTOF-DART screening of drink matrices is no less time-consuming than the current screening methodology, its main advantage lies in the lowering of the detection limits for GHB in the wide range of drink matrices tested. This leads, overall, to a more efficient forensic analysis of this type of evidence submission.

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Additional information and reprint requests:

Robert R. Steiner, M.S.
Virginia Department of Forensic Science
700 N. 5th Street
Richmond, VA 23219
E-mail: robert.steiner@dfs.virginia.gov