Effects of Ion Mobility, LC Separation, and Mass Spectrometry on Quantitation of Water-Soluble B Vitamins in Market Product Vapor Devices

Dr. R. Owen Bussey, III

8/16/2022

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Presentation Contents

IMS/MS Method for Fast Analysis of B Vitamins in E-liquid Samples

Purpose

01

Goal 1

Create fast analytical method for B vitamins.

02

Goal 2

Maintain low interference by adding orthogonal separation technique to shorter liquid chromatography mass spectrometry method.

03

Goal 3

Apply technique to quantitate B vitamins with low interference in the e-liquid of market product vapor devices.

Study Design: B Vitamin Experiments Performed

Longer LC method

Calibration Curve 1 Creation
Mass spec quantitation **with** and **without ion mobility** to maxmize peak resolution and **minimize co-elution**.

Shorter LC Method

Calibration Curve 2 Creation
Mass spec quantitation **with and without ion mobility** to **force co-elution**.

Products Quantitation

Quantitate Market Poducts
Spike pure vitamins into e-liquid to show low interference.
Quantitate market vapor products that contain B vitamins.

Study Design: Equipment and LC Parameters

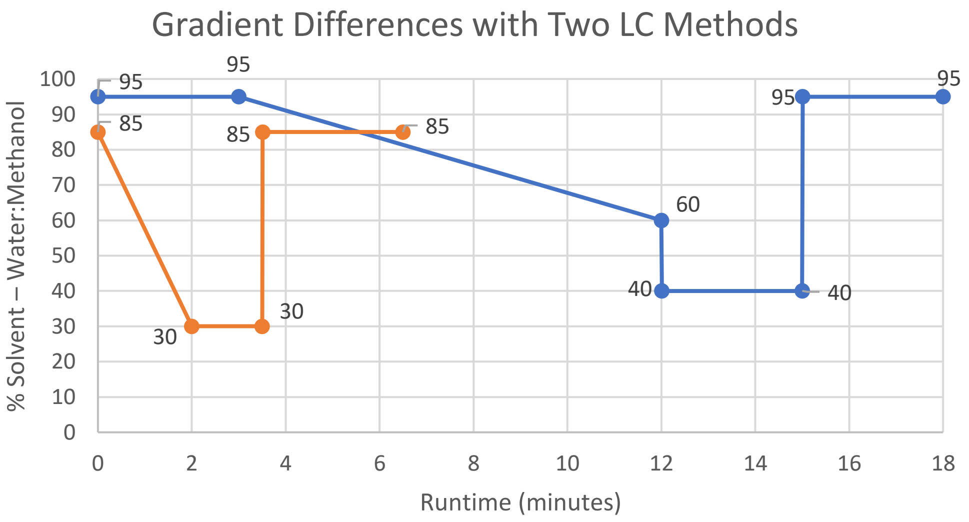
Waters Acquity I-Class LC

Vion IMS QToF

Column:
Acquity HSS T3 1.8 µm 2.1 x 150 mm

LC Solvents:

Solvent A: Methanol + 10 mM Ammonium Acetate + 0.1% Formic Acid
Solvent B: Water + 10 mM Ammonium Acetate + 0.1% Formic Acid



Study Design: MS and IMS Parameters

High Resolution Mass Spectrometer Settings

MS Parameter	Values
Ionization Type	Electrospray Ionization
Capillary Voltage	2.8 kV
Source Temperature	120 °C
Desolvation Temperature	300 °C
Cone Gas Flow	0 L/hour
Desolvation Gas Flow	800 L/hour
MS Scan Settings	HRMS and High-Definition MS Mode
MS Scan Masses	100-700 Da
Scan Time	0.5 seconds

Traveling Wave Ion Mobility

Collects “Full Scan” Ion Mobility

Word Association: Ion Mobility?

Second Dimension Separation

Electric Field

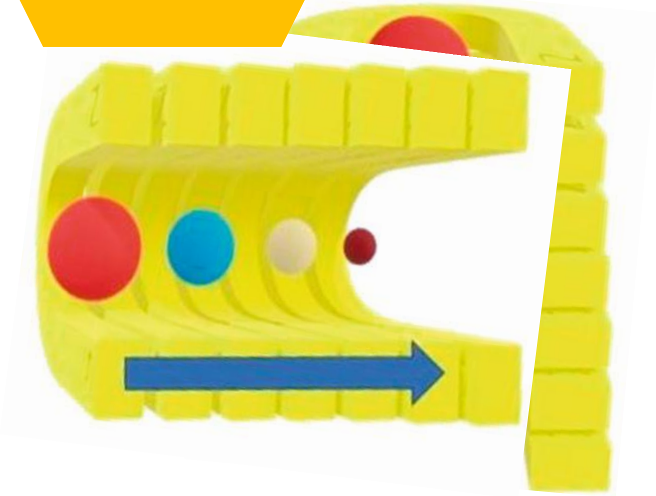
Paper Drop Demo

Orthogonal Separation

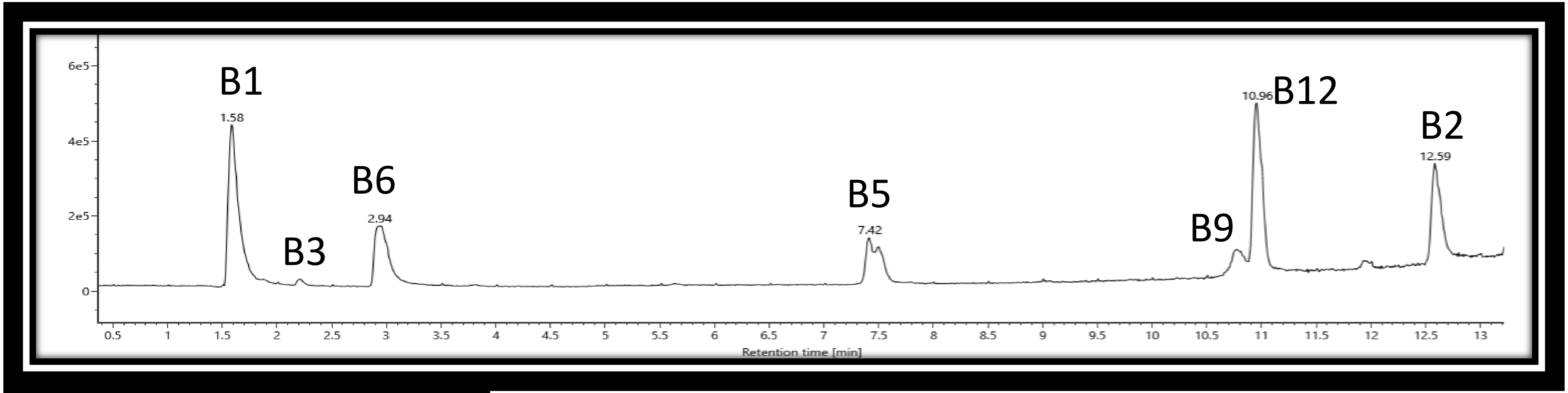
Cross Sectional Area

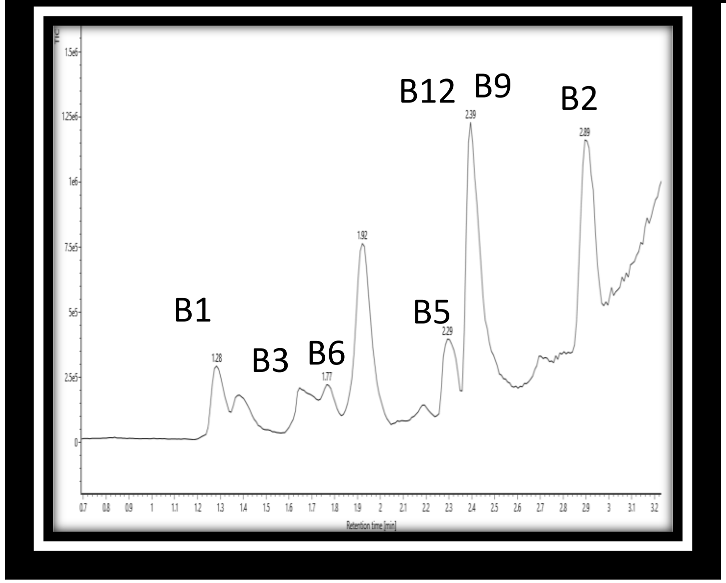
Gas Phase Separation

Drift Time



LC Chromatograms



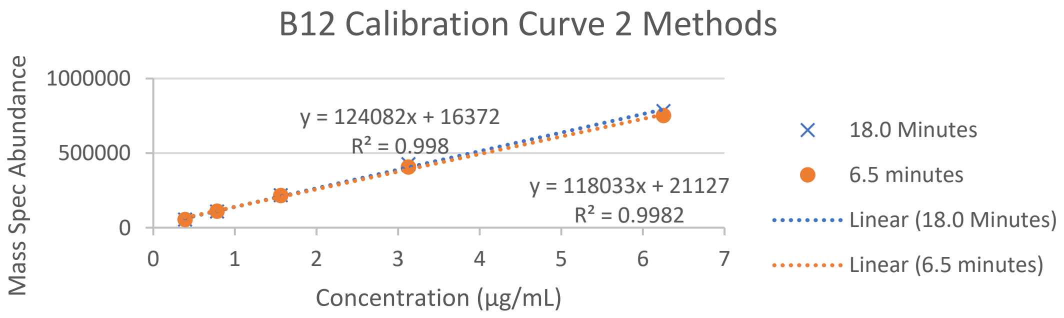


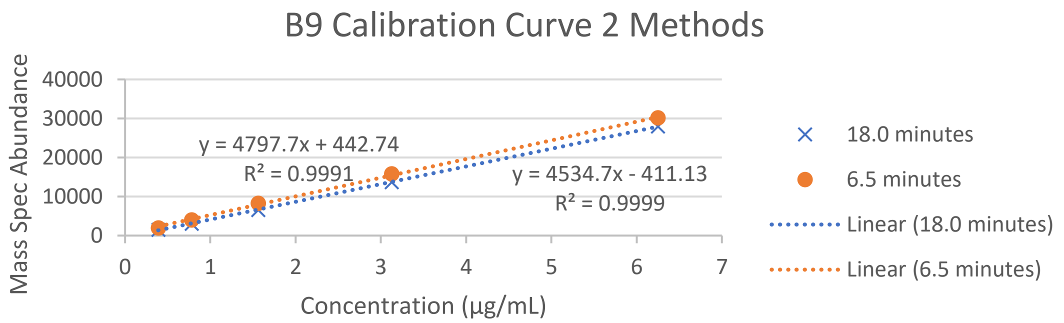
B Vitamin Descriptive Data

Chemical Name	Common Name	Main Ion (m/Z)	Drift (ms)	CCS (Å)
Cyanocobalamine	Vitamin B12	678.2930	6.37	187.10
Pyridoxine HCl	Vitamin B6	134.0602	3.83	133.88
Pantothenic acid hemicalcium salt	Vitamin B5	202.1076	4.50	145.54
Thiamine HCl	Vitamin B1	265.1124	5.19	161.25
Riboflavin	Vitamin B2	377.1457	6.31	185.20
Nicotinic Acid	Vitamin B3	124.0398	3.38	124.97
Folic Acid	Vitamin B9	295.0944	6.75	196.71

Calibration Curve Data with Ion Mobility

Vitamin	Slope at 18.0 min	Slope at 6.5 min	Slope Percent Difference	Quantitation Range (µg/mL)	Trendline	R^2
B5	2746	2669	2.8 %	0.78-3.13	Linear	0.9993-0.9999
B12	125010	119217	4.6 %	0.20-6.25	Linear	0.9980-0.9982
B9	4534	4797	5.5 %	0.39-6.25	Linear	0.9991-0.9999
B2	61902	66221	6.5 %	0.098-12.50	Linear	0.9927-0.9998
B6	26334	28643	8.1 %	0.20-0.78	Linear	0.9723-0.9973
B3	409	429	4.7 %	3.13-12.50	Linear	0.9606-0.9932
B1	2692	902	66%	3.13-12.50	Linear	0.9892-0.999



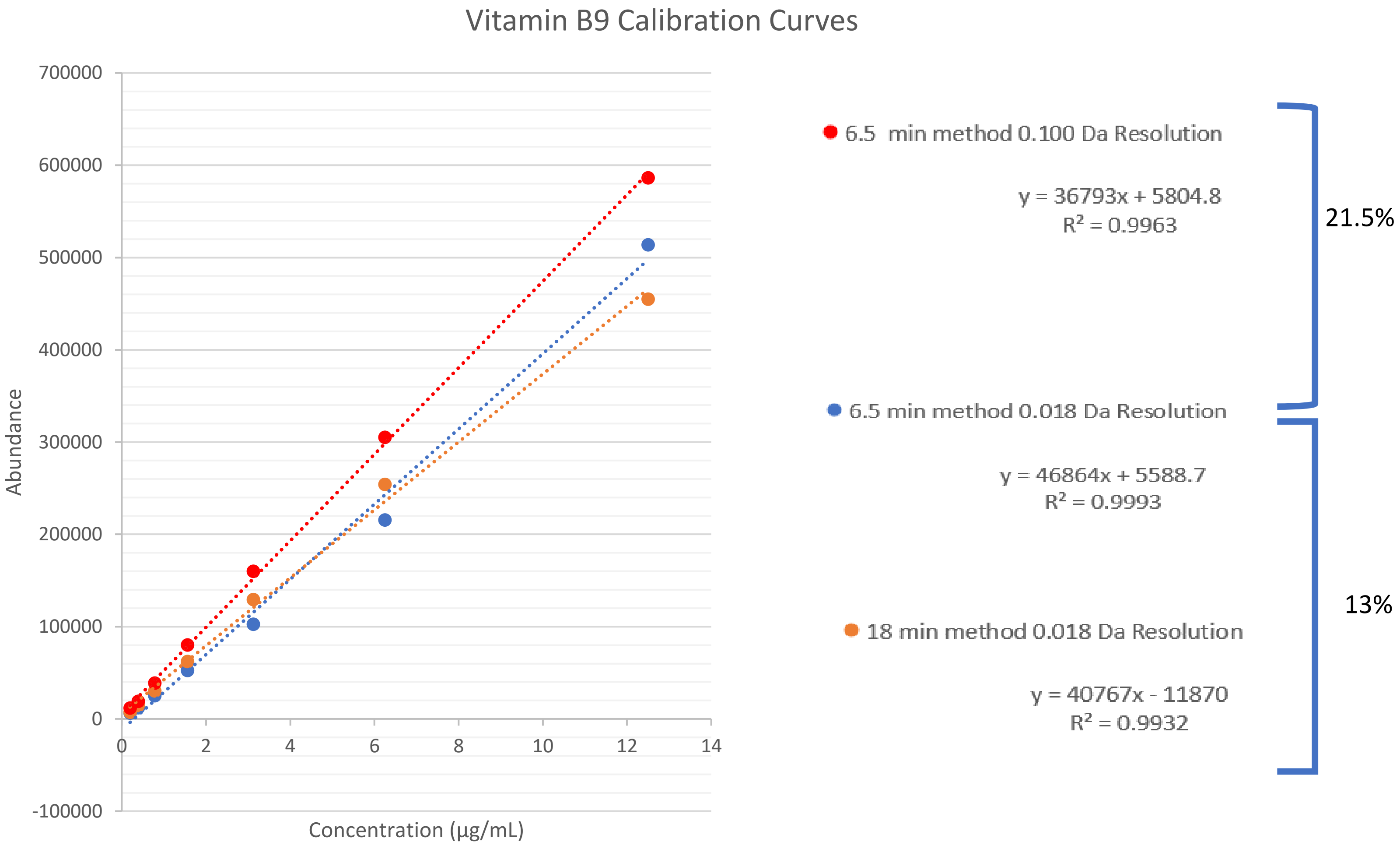


More Descriptive Data for Short Method:

Vitamin	%RSD intraday for Standards	LOQ (ppm)	LOD (ppm)
B12	0.38-2.53	0.39	0.13
B9	0.78-2.28	0.39	0.13
B5	1.36-1.66	0.78	0.26
B6	0.19-3.89	0.20	0.07
B3	3.89-13.57	3.13	1.04
B1	0.98-1.78	3.13	1.04
B2	1.98-5.51	0.098	0.03

Data without IMS and HRMS Contribution.

- Ran standards without IMS and % RSD between long and short method slopes was larger than experiments with IMS.
- Filtered at high and low mass resolution and % RSD increased.
- Will test on low resolution MS single quad mass spectrometer to confirm.



E-liquids with B vitamins

E-liquid with B-vitamins	B Vitamin	Label Claims (µg/cartridge)	µg/g	Calculated Minimum Mass per Cartridge (µg)	Calculated Maximum Mass per Cartridge (µg)
Product 1	B12	No Number Available	3.1	5.5	7.0
Product 2	B12	40	3.0	5.4	6.9
	B2	9000	3.0	5.4	6.9
	B6	9000	6.4	11.5	14.6
Product 3	B12	4000	255.9	2300.4	2898.5

Calculated Minimum Mass based on density of water at 0.999 mg/mL and listed volume of e-liquid per cartridge

Calculated Maximum Mass based on density of glycerin at 1.26 mg/mL and listed volume of e-liquid per cartridge.

*All products have Best By date in 2020. Product was sourced in 2019 for this study. New product difficult to source.

Peak Area Precision: Long and Short Methods WITH and WITHOUT Ion Mobility

Two commercial B vitamin e-liquids with low B vitamin levels were spiked.

Ion mobility helped to **eliminate** potential **interferences** and allowed for **better precision** between the long and short methods compared to the experiments without ion mobility.

Spiked B12 Peak Area Comparison WITH Ion Mobility			
	Long Method	Short Method	%RSD
Product 1	1278422	1315117	2.8
Product 2	843511	861614	2.1

Spiked B12 Peak Area Comparison WITHOUT Ion Mobility			
	Long Method	Short Method	%RSD
Product 1	4001426	4511561	11.3
Product 2	3333704	3691021	9.5

Summary:

- Developed faster analytical method for most B vitamins.
- Ion mobility produced better precision between long and short methods by eliminating potential interferences
- High-resolution mass spectrometry potentially contributed to better precision between methods.
- Quantitated B vitamins in market B vitamins vapor products using short LC method with ion mobility.

Questions