

Supplementary Materials

Table S1. Organic acids & furans standards: amounts used in grams (gr) and concentrations in (mg/ml) of each individual standard.

Formic Acid (FA)	m FA (gr)	m H₂O (gr)	C FA (mg/ml)
Dilution 1	2.7472	44.5413	58.7095
Dilution 2	4.0003	44.0137	84.5861
Dilution 3	5.0056	43.0422	106.1742
Acetic Acid (Ac.Ac.)	m Ac.Ac. (gr)	m H₂O (gr)	C Ac.Ac. (mg/ml)
Dilution 1	2.5243	44.5782	53.7261
Dilution 2	4.0202	44.0559	83.9495
Dilution 3	5.0053	42.0235	106.9622
Citric Acid (Cit.)	m Cit. (gr)	m H₂O (gr)	C Cit. (mg/ml)
Dilution 1	2.3720	44.1124	53.7717
Dilution 2	3.5152	44.0480	79.8038
Dilution 3	4.7198	44.5039	106.0536
Levulinic Acid (LA)	m LA (gr)	m H₂O (gr)	C LA (mg/ml)
Dilution 1	2.3766	44.1031	53.8873
Dilution 2	3.5262	44.0462	80.0568
Dilution 3	4.7091	44.5782	105.6368
Hydroxymethylfurfural (HMF)	m HMF (gr)	m H₂O (gr)	C HMF (mg/ml)
Dilution 1	0.0034	14.5460	0.2337
Dilution 2	0.0080	14.3089	0.5591
Dilution 3	0.0142	14.5085	0.9787
Gamma Valerolactone (GVL)	m GVL (gr)	m H₂O (gr)	C GVL (mg/ml)
Dilution 1	2.5098	44.0277	54.0695
Dilution 2	4.0190	44.1294	83.8042
Dilution 3	5.2267	44.0672	106.5694
Furfural (Fur.)	m Fur. (gr)	m H₂O (gr)	C Fur. (mg/ml)
Dilution 1	0.9557	44.0497	21.2976
Dilution 2	1.6235	44.0706	35.7047
Dilution 3	2.4931	44.0130	54.0073
Diformylfuran (DFF)	m DFF (gr)	m H₂O (gr)	C DFF (mg/ml)
Dilution 1	0.0050	14.0270	0.3564
Dilution 2	0.0080	14.1720	0.5644
Dilution 3	0.0130	14.3750	0.9043

Table S2. Mix standard solutions of V=15 ml: amounts used in grams (gr) and concentrations (mg/ml) of each individual standard.

Mix Standard Solutions	Components	Masses (gr)	C (mg/ml)
STD1	FA	0.3048	1.1799
	Cit.	0.3074	1.1019
	LA	1.0146	3.6449
	HMF	1.5017	0.0991
STD2	FA	0.6111	2.3658
	Cit.	0.6159	2.2078
	LA	1.0323	3.7085

STD3	HMF	3.0123	0.1987
	FA	0.8603	3.3305
	Cit.	0.8671	3.1083
	LA	1.0380	3.7290
	HMF	4.6098	0.3042
STD4	FA	0.1457	0.5640
	Ac.Ac.	0.1507	0.5381
	LA	1.0187	3.6596
	HMF	0.8572	0.0565
STD5	FA	0.8679	3.3599
	Ac.Ac.	0.8580	3.0639
	LA	1.0095	3.6266
	HMF	2.5014	0.1651
STD6	FA	1.7125	6.6297
	Ac.Ac.	1.7042	6.0857
	LA	1.0117	3.6345
	HMF	3.5120	0.2317

Table S3. Recipe of commercial products samples with internal standard (LA) of V=15ml.

	m B.VIN (gr)	m LA (gr)	Vmix (ml)	C LA (mg/ml)	C B.VIN (mg/ml)
B.VIN	0.325	1.0201	15	3.6647	0.0216
	m ACV (gr)	m LA (gr)	Vmix (ml)	C LA (mg/ml)	C ACV (mg/ml)
ACV	0.3226	1.0199	15	3.6639	0.0215
	m Pom (gr)	m LA (gr)	Vmix (ml)	C LA (mg/ml)	C Pom (mg/ml)
POM	0.3315	1.0154	15	3.6478	0.0221

Table S4. Linear calibration of individual standards: 3-pts concentrations run at 0.5ml/min mobile phase.

Individual Standards	Equation	R ²
Formic Acid (FA)	y = 204.93x + 73.732	1.0000
Acetic Acid (Ac.Ac.)	y = 123.26x - 153.48	1.0000
Citric Acid (Cit.)	y = 203.31x + 2989.6	0.9993
Levulinic Acid (LA)	y = 62.721x + 103.13	1.0000
Hydroxymethylfurfural (HMF)	y = 28021x - 577.24	0.9998
Gamma Valerolactone (GVL)	y = 75.847x - 451.04	0.9999
Furfural (Fur.)	y = 2358.3x + 473.06	0.9998
Diformylfuran (DFF)	y = 26035x + 1295.7	0.9979

Table S5. Linear calibration of standards in mix solutions: 3-pts concentrations run at 0.3ml/min mobile phase.

Standard Solutions in mixes STD1, STD2, & STD3	Equation	R ²
Formic Acid (FA)	y = 234.53x - 3.1603	0.9995
Citric Acid (Cit.)	y = 690.72x + 54.291	0.9998
Hydroxymethylfurfural (HMF)	y = 3783.3x - 15.679	1.0000
Standard Solutions in mixes STD4, STD5, & STD6	Equation	R ²

Formic Acid (FA)	$y = 313.03x - 8.4127$	1.0000
Acetic Acid (Ac.Ac.)	$y = 235.13x - 2.6383$	1.0000
Hydroxymethylfurfural (HMF)	$y = 3669.2x + 6.5032$	1.0000

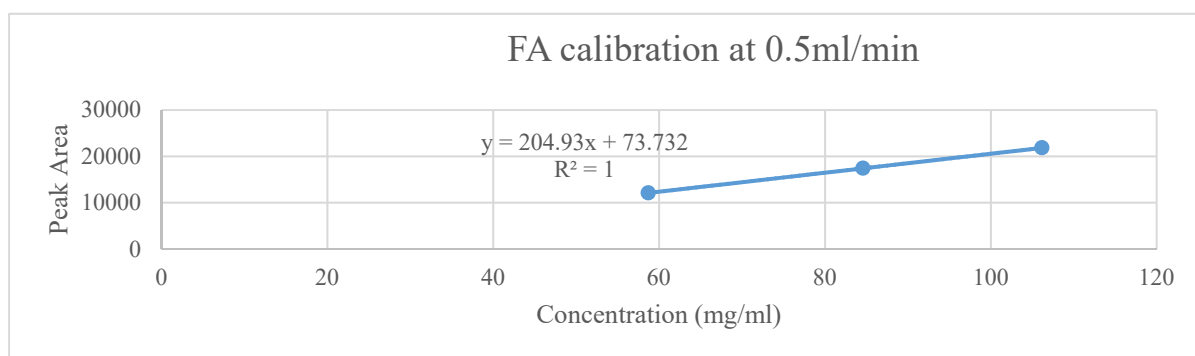


Figure S1. Formic acid (FA) standard calibration curve at mobile phase flow rate 0.5 ml/min.

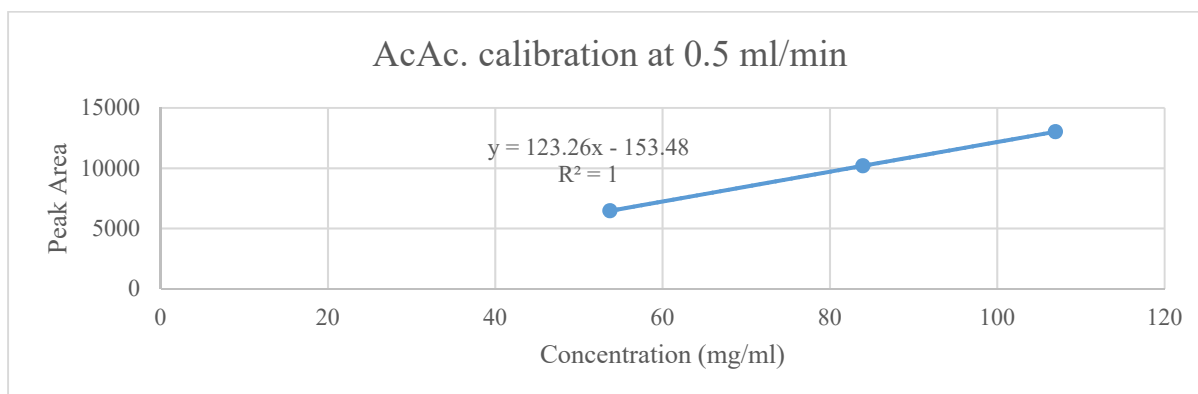


Figure S2. Acetic acid (AcAc) standard calibration curve at mobile phase flow rate 0.5 ml/min.

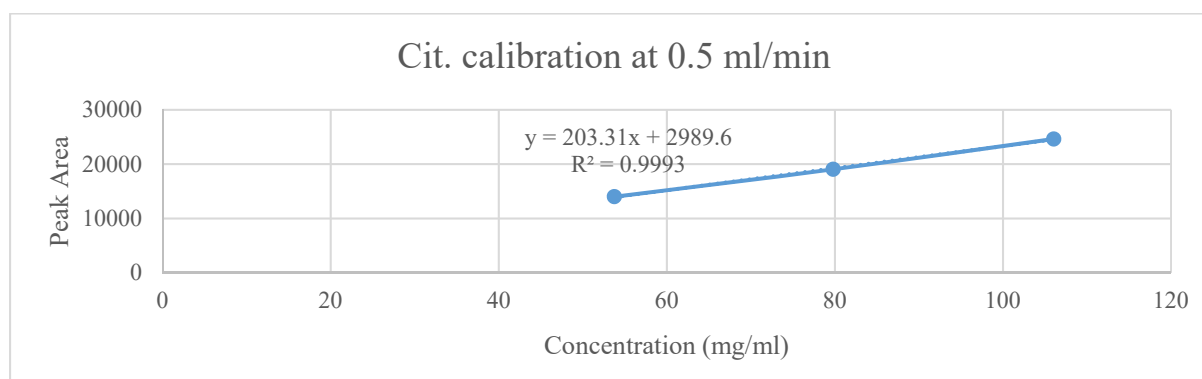


Figure S3. Citric acid (Cit) standard calibration curve at mobile phase flow rate 0.5 ml/min.

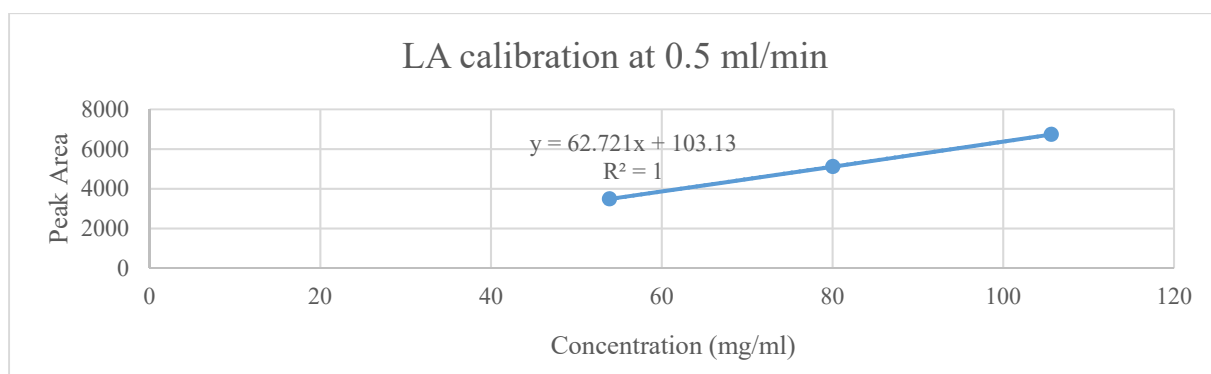


Figure S4. Levulinic acid (LA) standard calibration curve at mobile phase flow rate 0.5 ml/min.

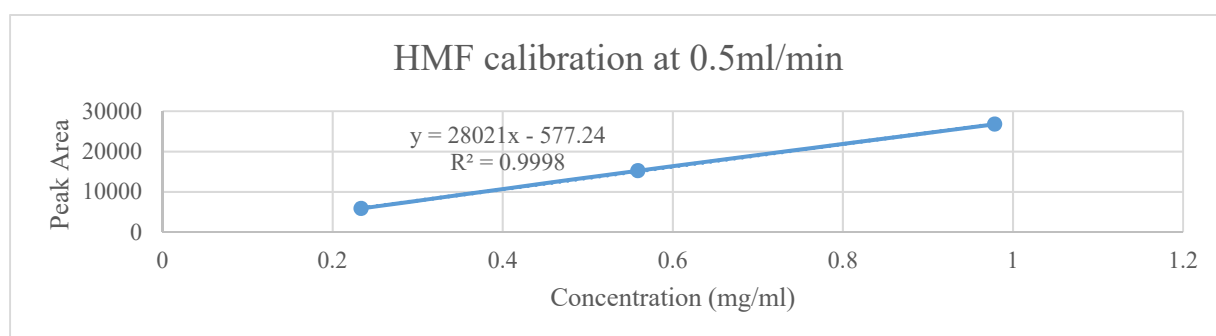


Figure S5. Hydroxymethylfurfural (HMF) standard calibration curve at mobile phase flow rate 0.5 ml/min.

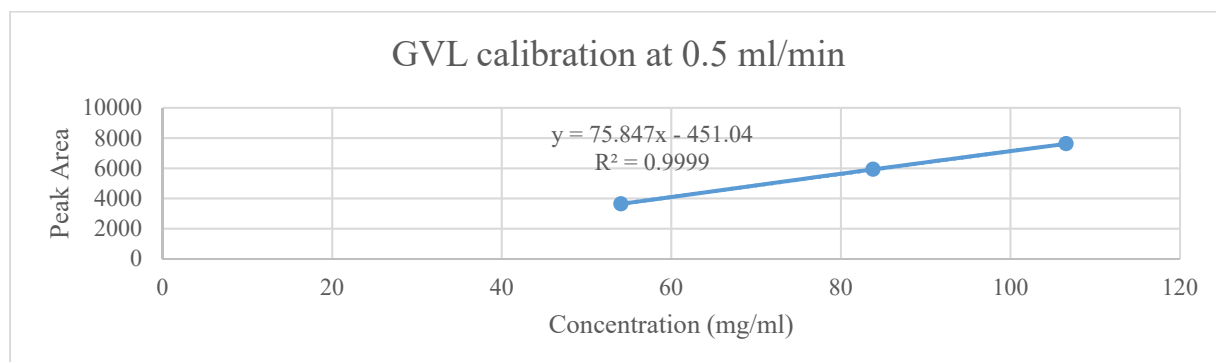


Figure S6. Gamma valerolactone (GVL) standard calibration curve at mobile phase flow rate 0.5 ml/min.

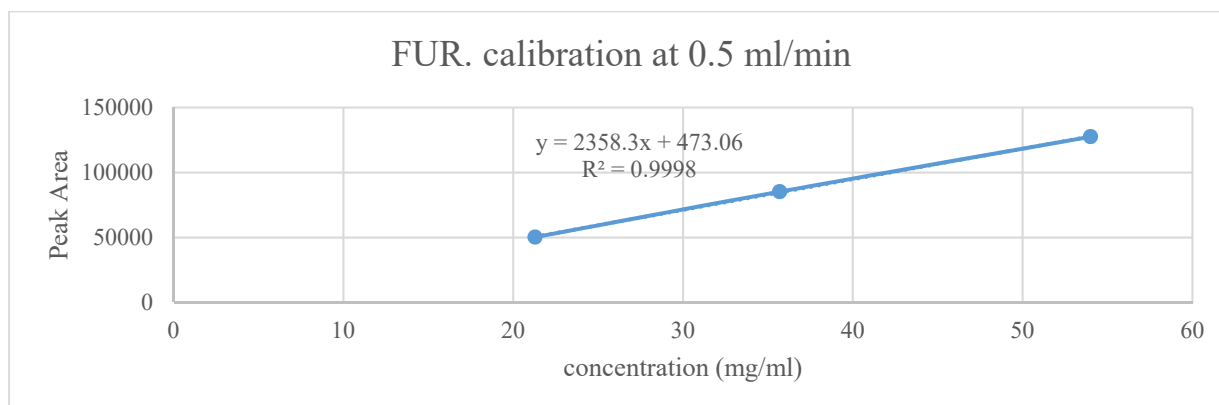


Figure S7. Furfural (FUR) standard calibration curve at mobile phase flow rate 0.5 ml/min.

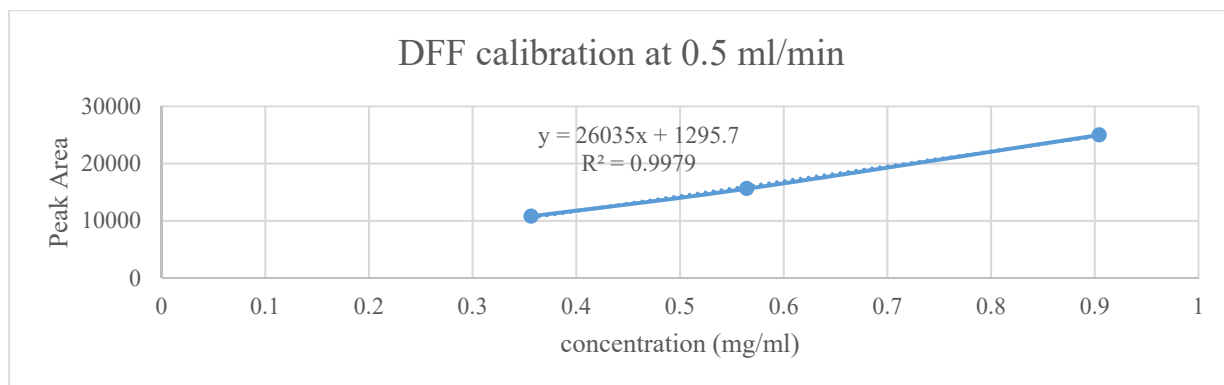


Figure S8. Diformylfuran (DFF) standard calibration curve at mobile phase flow rate 0.5ml/min.

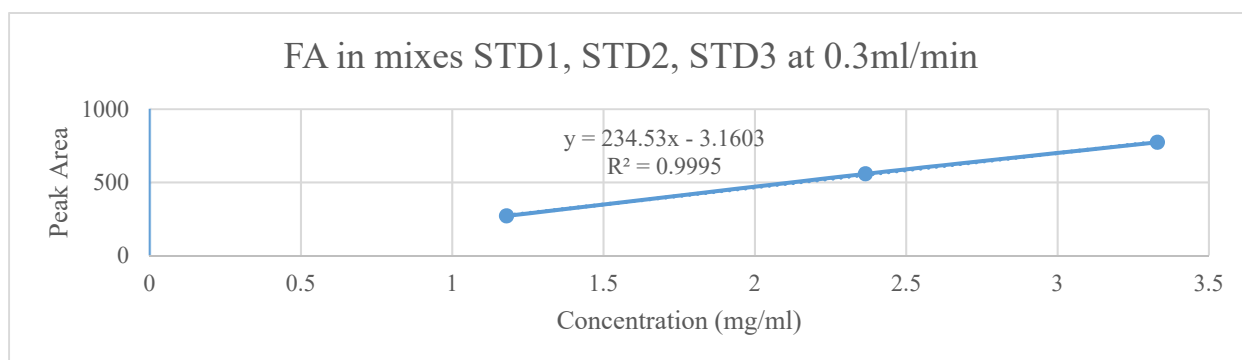


Figure S9. Formic acid (FA) in mix standard solutions STD1, STD2, & STD3 calibration curve at mobile phase flow rate 0.3 ml/min.

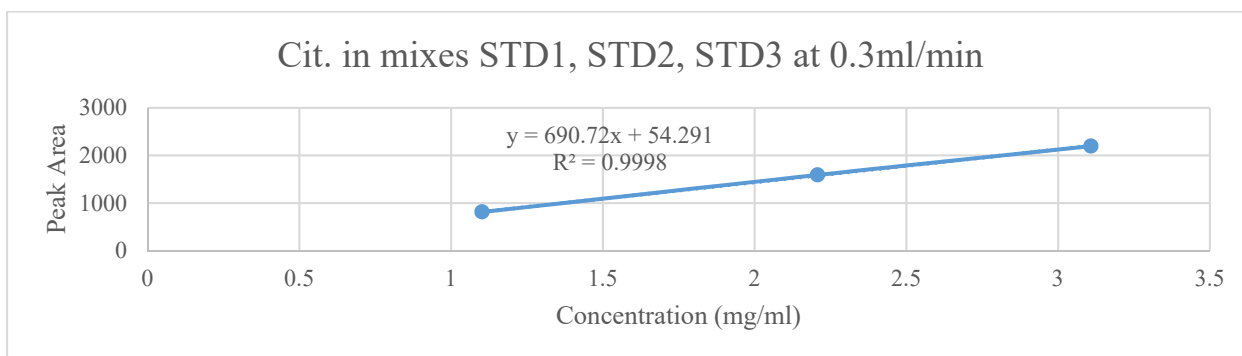


Figure S10. Citric (Cit) acid in mix standard solutions STD1, STD2, & STD3 calibration curve at mobile phase flow rate 0.3 ml/min.

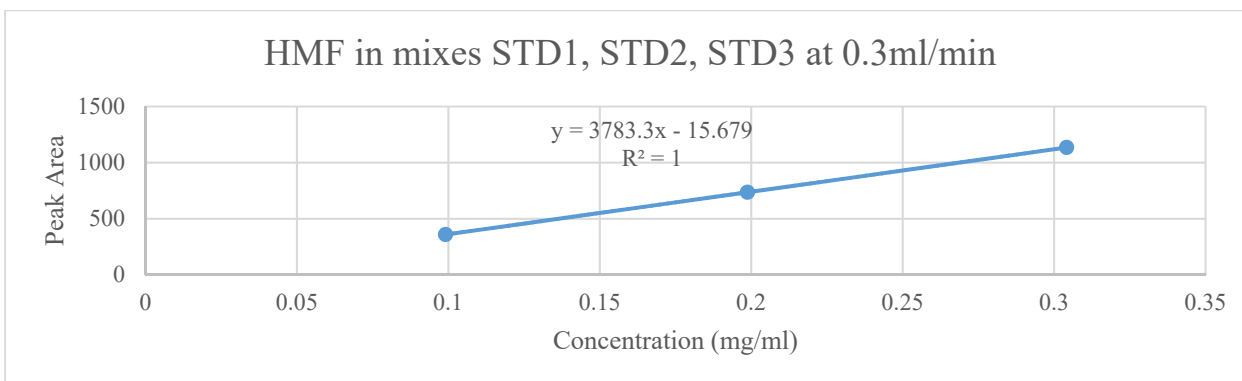


Figure S11. HMF in mix standard solutions STD1, STD2, & STD3 calibration curve at mobile phase flow rate 0.3 ml/min.

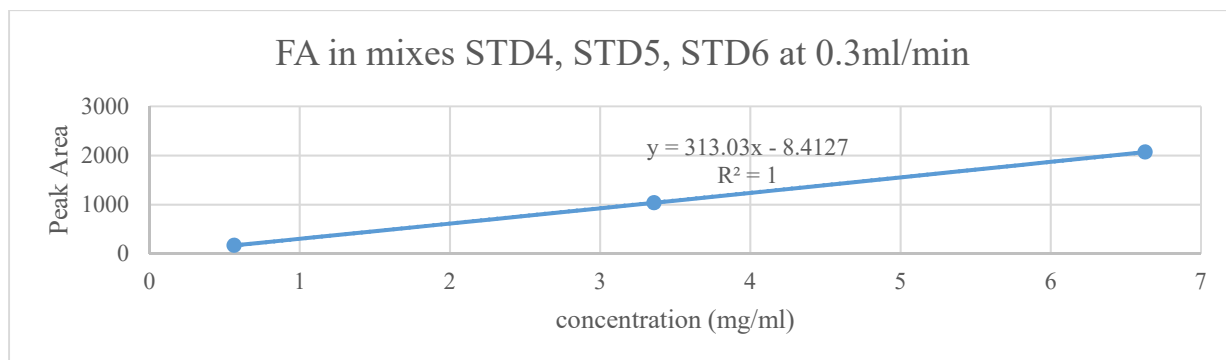


Figure S12. Formic acid (FA) in mix standard solutions STD4, STD5, & STD6 calibration curve at mobile phase flow rate 0.3 ml/min.

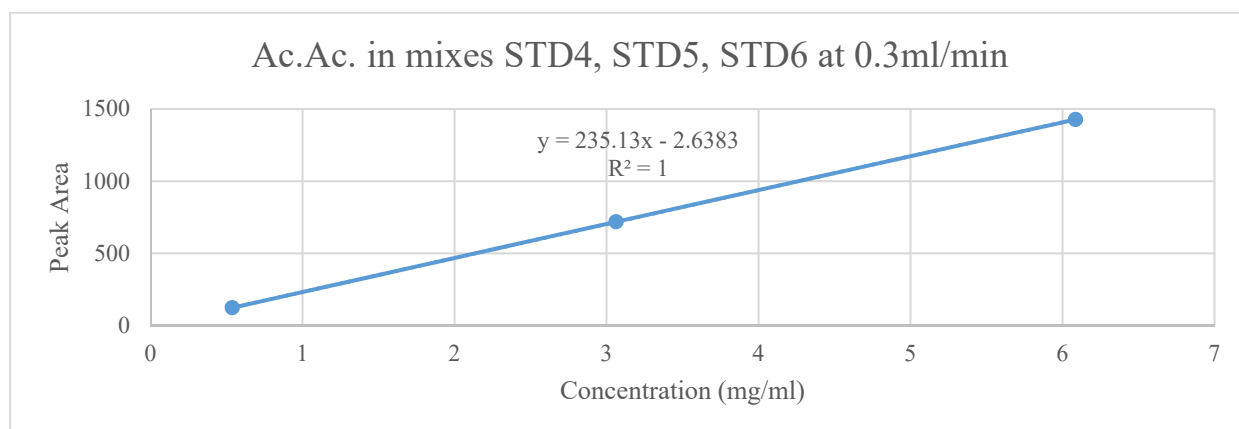


Figure S13. Acetic acid (Ac. Ac.) in mix standard solutions STD4, STD5, & STD6 calibration curve at mobile phase flow rate 0.3 ml/min.

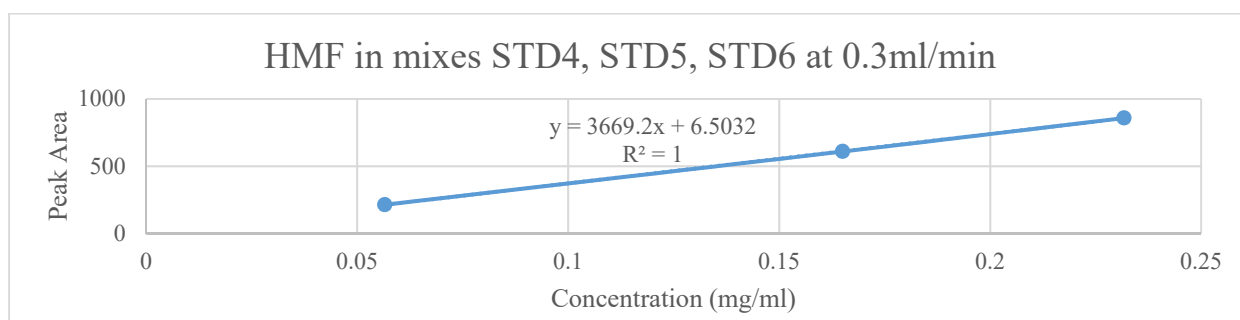


Figure S14. HMF in mix standard solutions STD4, STD5, & STD6 calibration curve at mobile phase flow rate 0.3 ml/min.

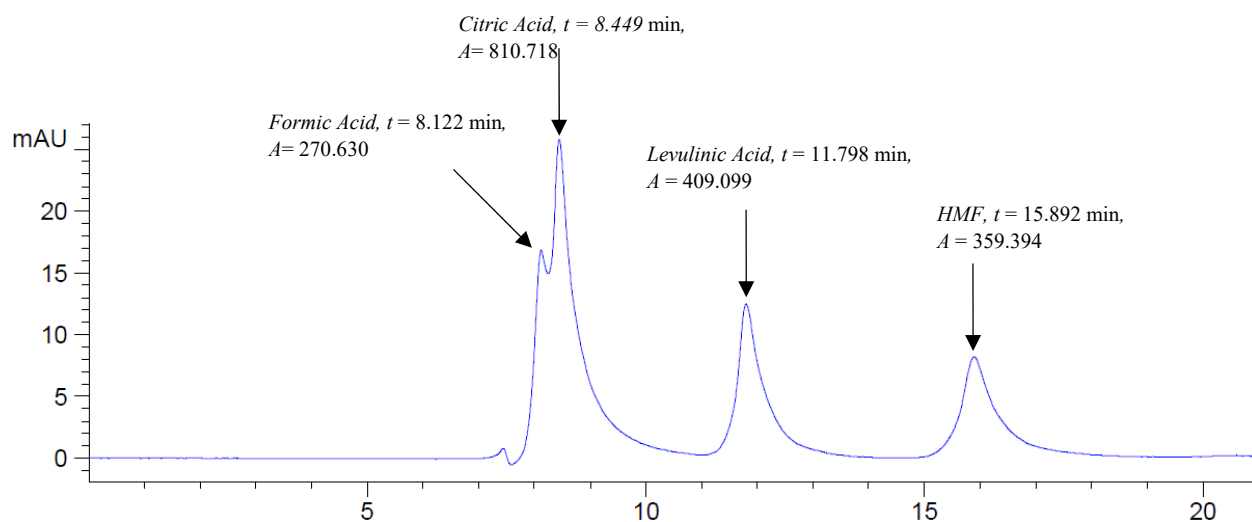


Figure S15. Mix standard solution STD1 chromatogram run at UV-210 nm at conditions: flow rate: 0.3ml/min., column temperature: 30°C, run time: 20 min.

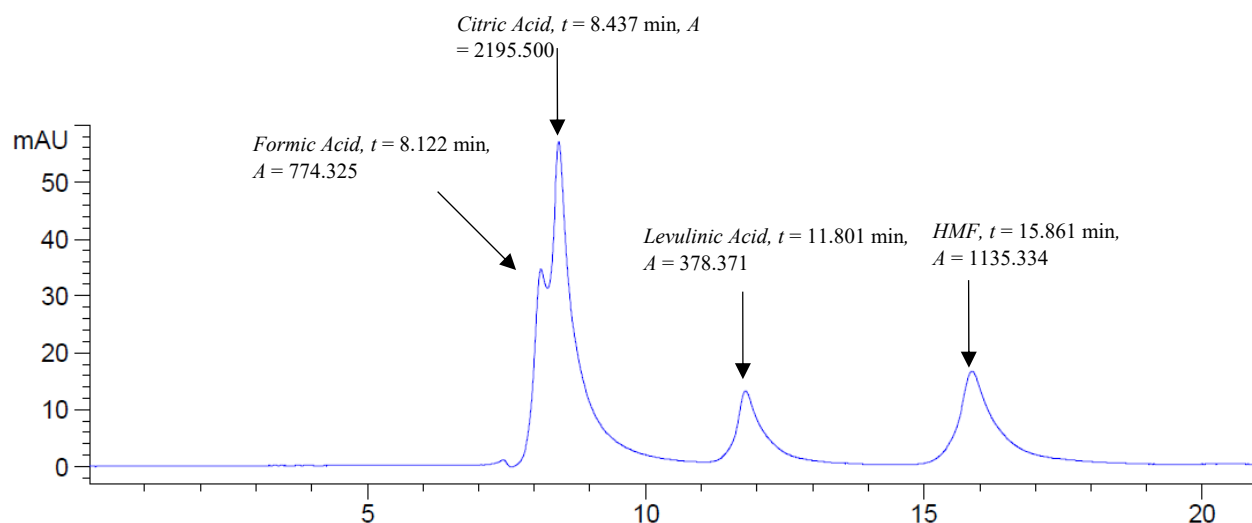


Figure S16. Mix standard solution STD3 chromatogram run at UV-210 nm at conditions: flow rate: 0.3ml/min., column temperature: 30°C, run time: 20 min.

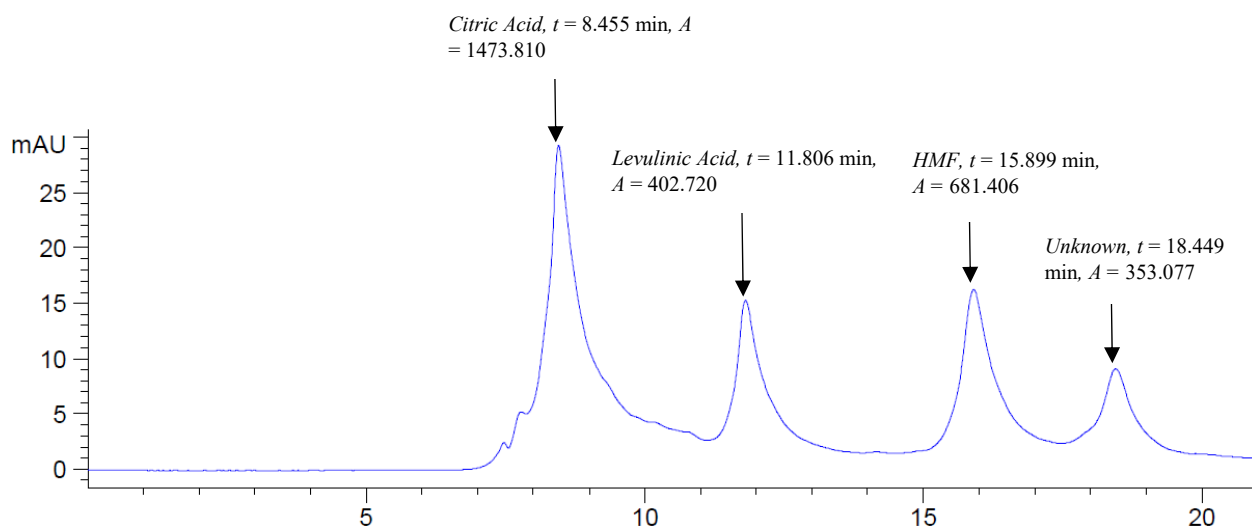


Figure S17. Pomegranate molasses (Pom.B) sample chromatogram run at UV-210 nm at conditions: flow rate: 0.3ml/min., column temperature: 30°C, run time: 20 min.

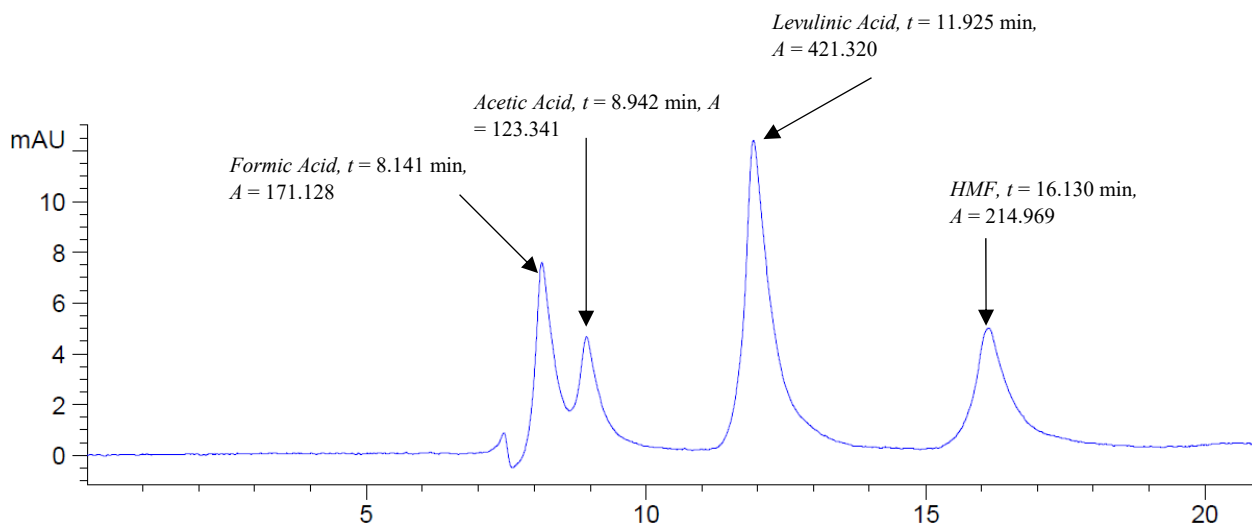


Figure S18. Standard mix solution STD4 chromatogram run at UV-210 nm at conditions: flow rate: 0.3ml/min., column temperature: 30°C, run time: 20 min.

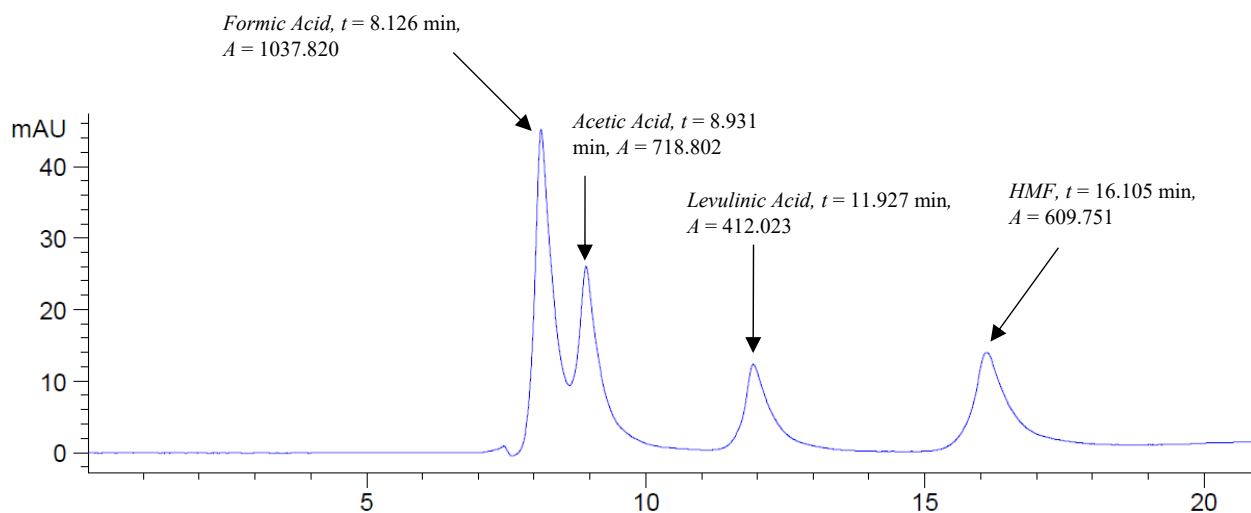


Figure S19. Standard mix solution STD5 chromatogram run at UV-210 nm at conditions: flow rate: 0.3ml/min., column temperature: 30°C, run time: 20 min.

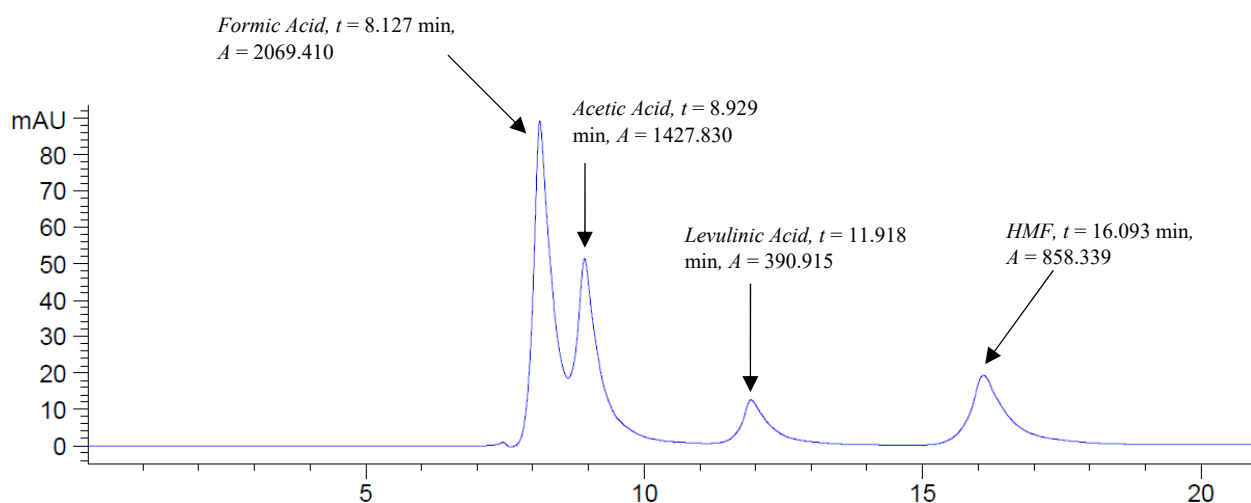


Figure S20. Standard mix solution STD6 chromatogram run at UV-210 nm at conditions: flow rate: 0.3ml/min., column temperature: 30°C, run time: 20 min.

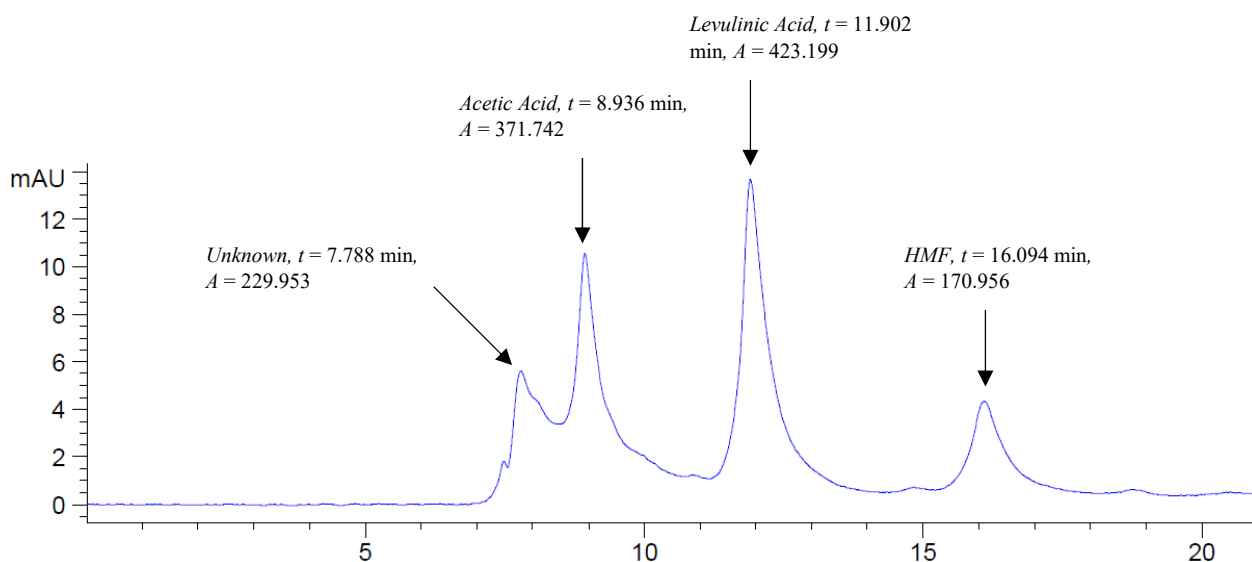


Figure S21. Balsamic vinegar B.VIN (B) chromatogram run at UV-210 nm at conditions: flow rate: 0.3ml/min., column temperature: 30°C, run time: 20 min.

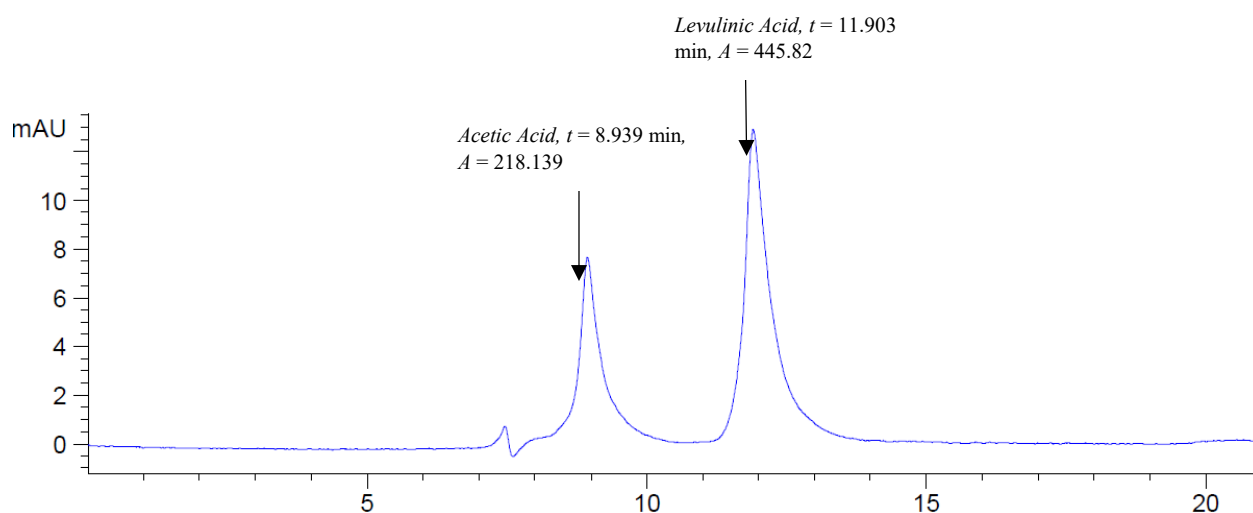


Figure S22. Apple cider vinegar ACV (B) chromatogram run at UV-210 nm at conditions: flow rate: 0.3ml/min., column temperature: 30°C, run time: 20 min.

Sample Calculations:

In order to quantify the commercial products' ingredients, a certain amount of pomegranate molasses, apple cider vinegar, and balsamic vinegar was weighed before was transferred into a 15 ml tube and diluted to volume. The calculation procedure of the concentrations of each species is as follows:

The weighed amount of pomegranate was $m_{\text{sample}} = m_{\text{POM}} = 0.3315 \text{ gr}$.

The density of pomegranate a density of $\rho_{\text{POM}} = 1.3803 \text{ gr/ml}$

Therefore, the volume of sample transferred into the 15 ml tube

$$V_{\text{POM}} = \frac{0.3315 \text{ gr}}{1.3803 \text{ gr/ml}} = 0.2402 \text{ ml}$$

The peak area of POM.A was 1441.2605, which was close to the area of STD2-inline-POM.A of a value of 1633.66931. The corresponding response factor RF= 739.931.

Thus, the concentration of citric acid in the vial $C_{cit, vial}$ is calculated as follows:

$$C_{cit, vial} = \frac{Cit. Area}{Cit. RF} = \frac{1441.2605}{739.9309} = 1.948 \text{ mg/ml}$$

Afterwards, the concentration of citric acid in the original sample of pomegranate before dilution $C_{cit, sample}$ was calculated using the below equation

$$C_{cit, sample} = \frac{C_{cit, vial} \times V_{total}}{V_{sample}} = \frac{(1.948 \text{ mg/ml}) \times (15 \text{ ml})}{0.2402 \text{ ml}} = 121.656 \text{ mg/ml}$$

The concentration of citric acid in POM.B is calculated in similar manner and its value was 125.1936 mg/ml. The standard deviation is calculated based on the values of the concentration of citric acid $C_{cit, vial}$ & $C_{cit, sample}$ of the samples duplicates.