

Supplementary Information for

“Detection of Low Molecular Weight Adulterants in Beverages by Direct Analysis in Real Time Mass Spectrometry”

Edward Sisco^{a*} and Jeffrey Dake

^aNational Institute of Standards and Technology, Materials Measurement Science Division,
Gaithersburg, MD, USA

^bUnited States Army Criminal Investigation Laboratory,
Gillem Enclave, GA 30297, United States

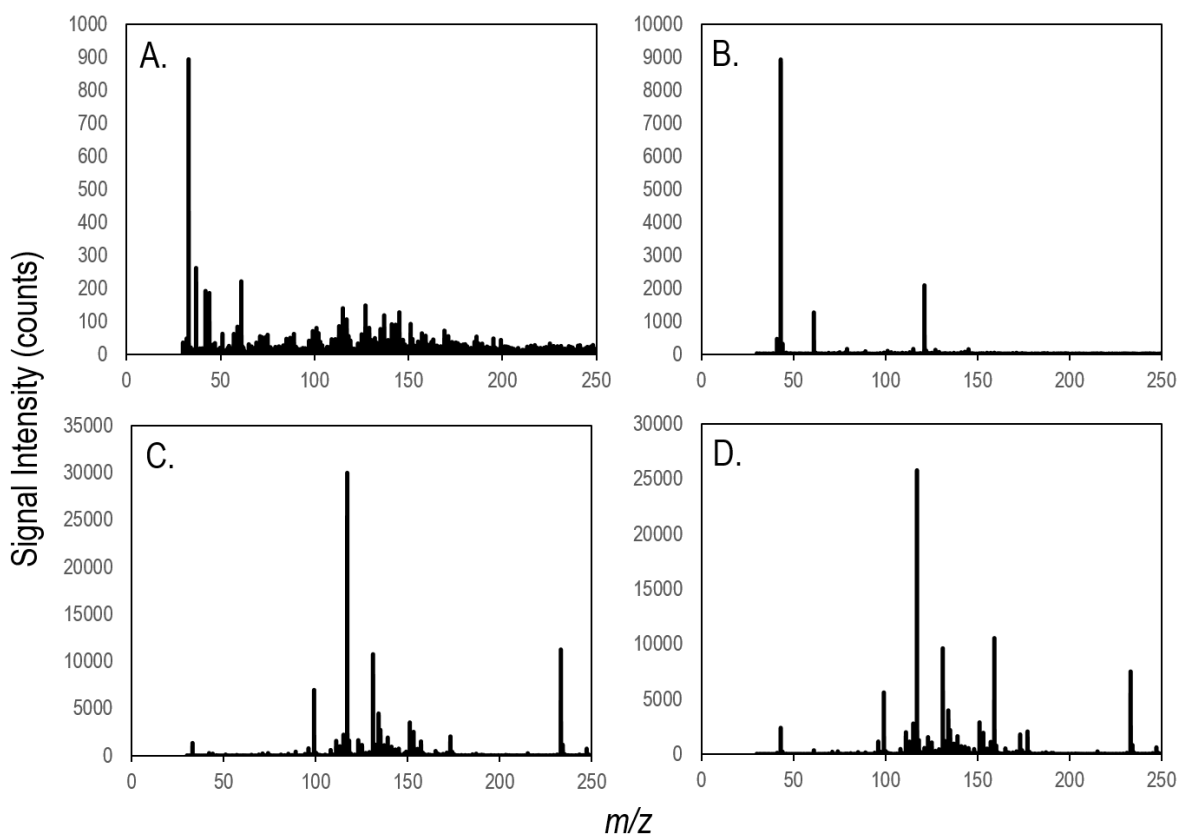


Figure S1. Positive ion mass spectra of methanol (A. & C.) and 1-propanol (B. & D.) both neat (A. & B.) and in the presence of hexanoic acid (C. & D.).

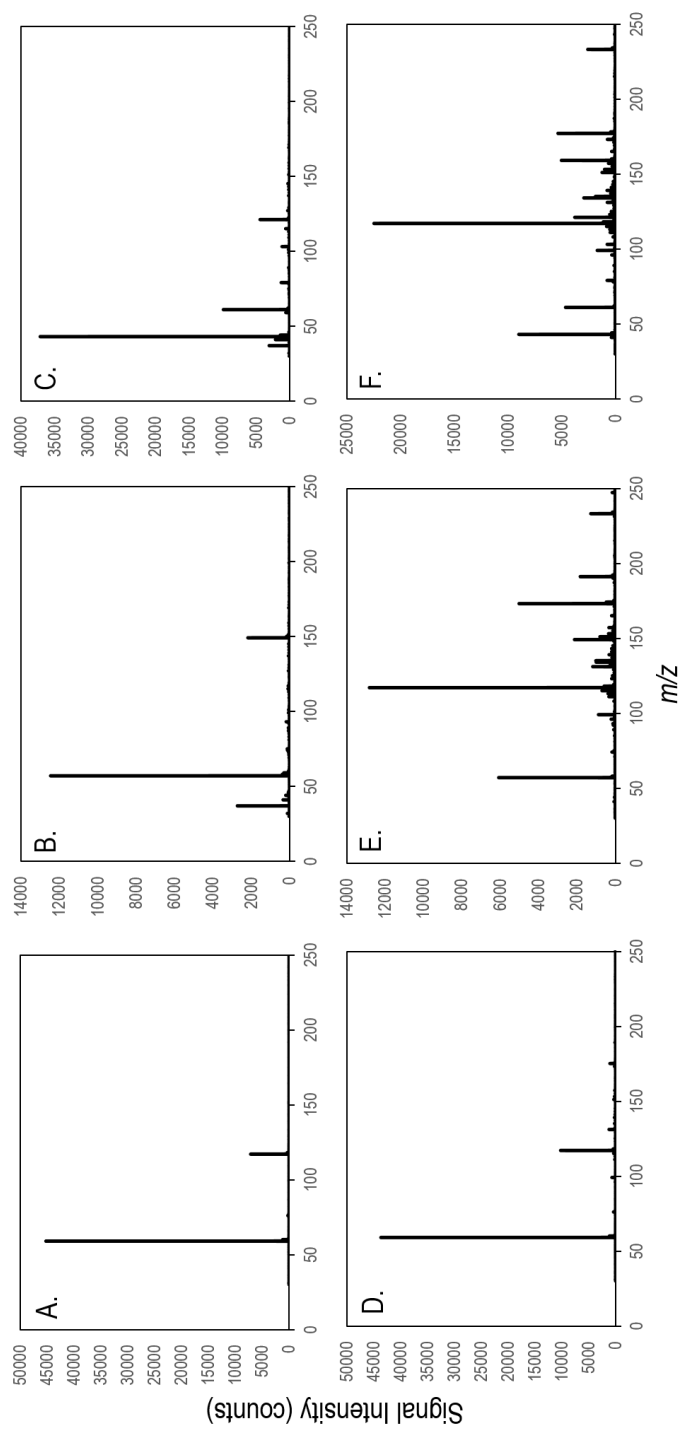


Figure S2. Positive ion mass spectra of acetone (A. & D.), 1-butanol (B. & E.), and 2-propanol (C. & F.) both neat (A., B., & C.) and in the presence of hexanoic acid (D., E., & F.).

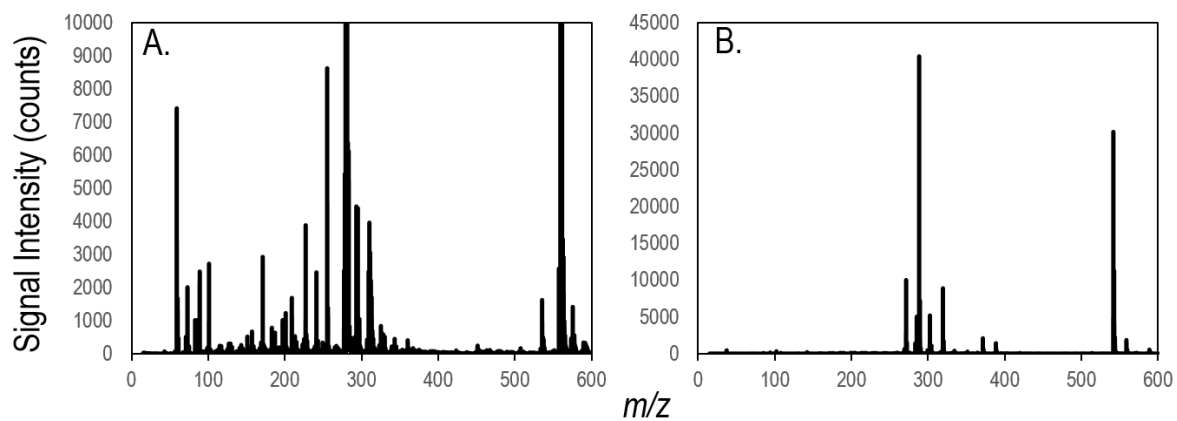


Figure S3. Representative mass spectra of NaClO in negative mode with the presence of linoleic acid (A.) and NH_4OH in positive mode in the presence of methyl palmitate (B.).

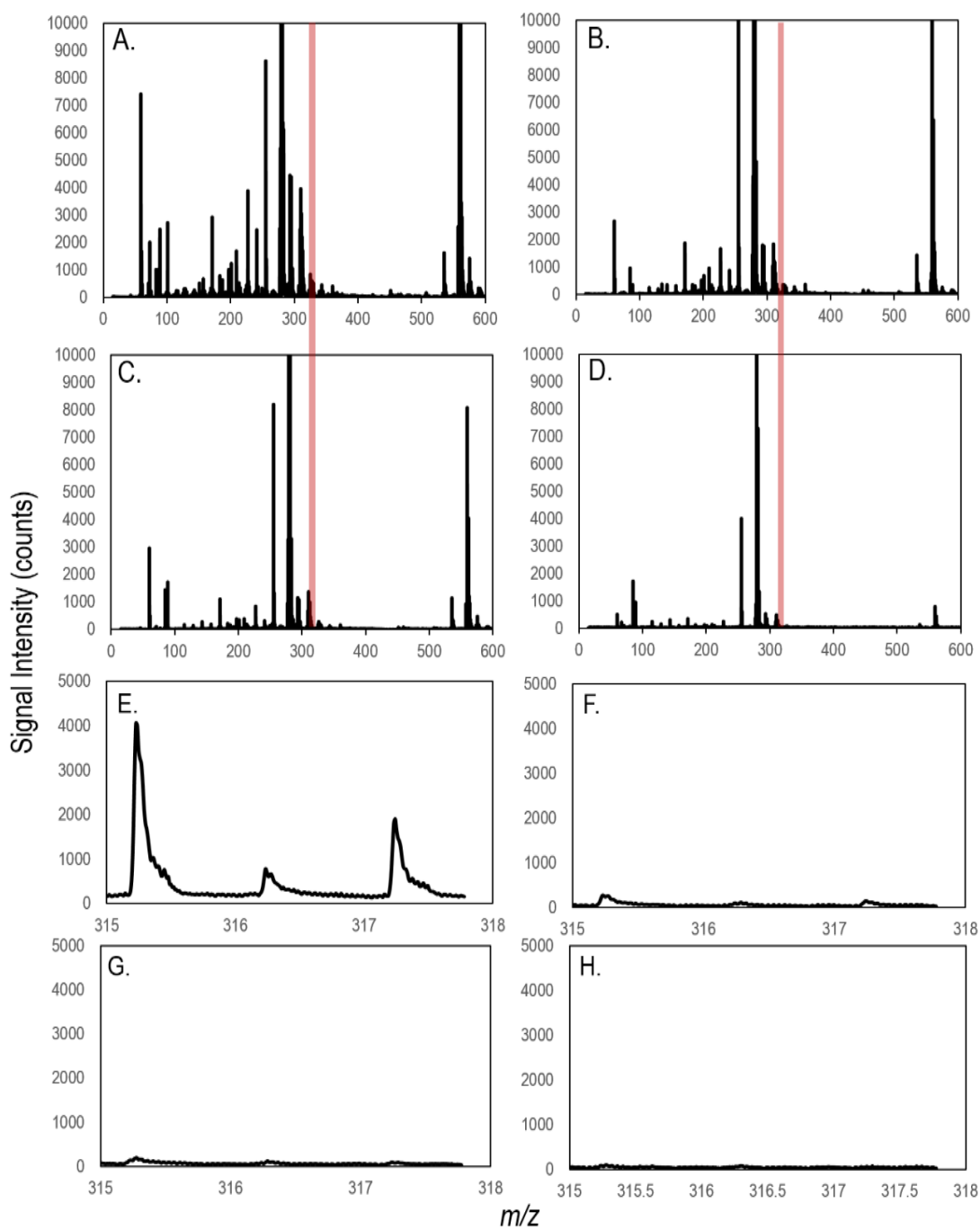


Figure S4. Representative mass spectra of NaClO (A.), NaCl (B.), KClO₃ (C.) and KClO₄ (D.) in the presence of linoleic acid. Location of the [Linoleic Acid+ClO-O]⁻ adduct, specific to ClO⁻, identified with red bar. Expanded mass spectra of the adduct ion (315 *m/z* and 317 *m/z*) for NaClO (E.), NaCl (F.), KClO₃ (G.), and KClO₄ (H.) are also shown.

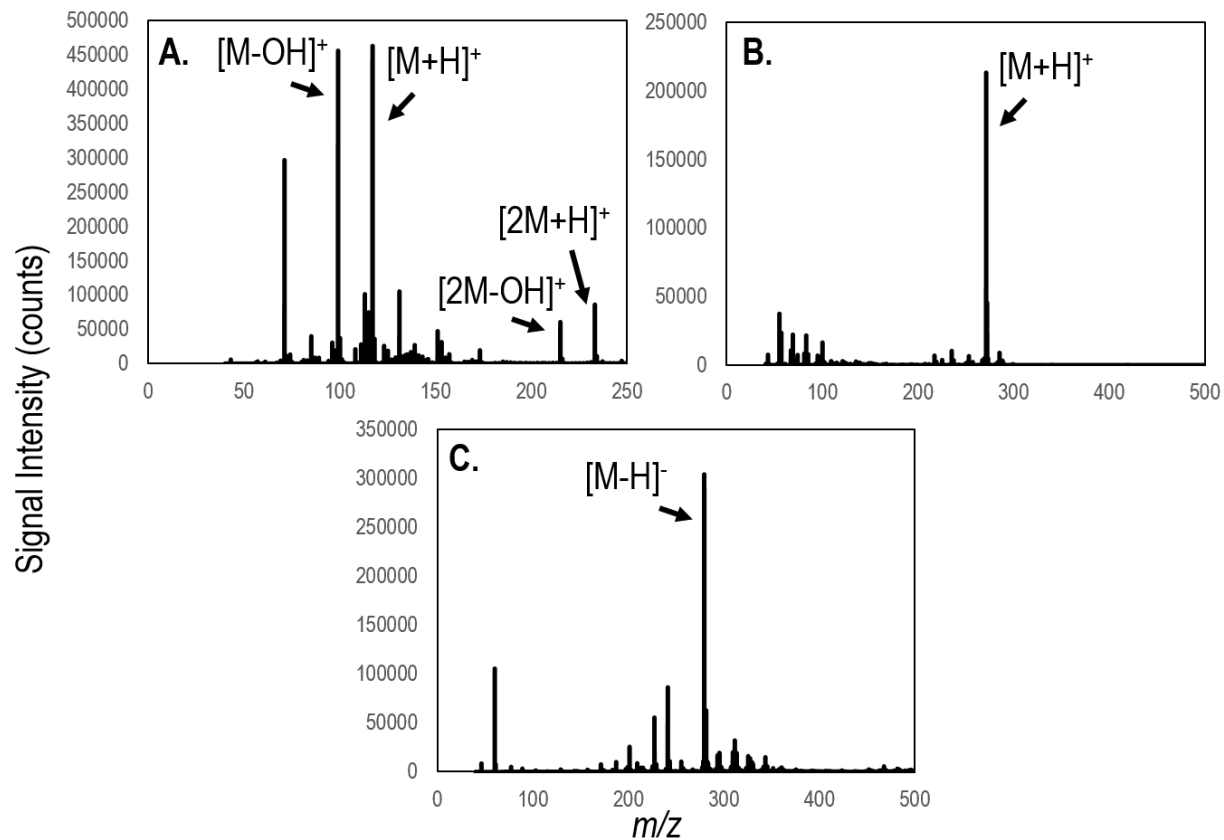


Figure S5. Representative mass spectra of the dopants (hexanoic acid (A.), methyl palmitate (B.), and linoleic acid (C.)) analyzed without an adulterants present. Select peaks of interest are also highlighted. Hexanoic acid and methyl palmitate were analyzed in positive mode while linoleic acid was analyzed in negative mode.

	MeOH	EtOH	PrOH	IPA	BuOH	Ace	EG	NH ₄ OH	NaClO
Coca-Cola®	Green	Green	Green	Green	Green	Green	Green	Green	Green
Mountain Dew®	Green	Green	Green	Green	Green	Green	Green	Green	Green
2 % Milk	Green	Green	Green	Green	Green	Green	Green	Yellow	Yellow
Cranberry Juice	Green	Green	Green	Green	Green	Green	Green	Green	Green
Orange Juice	Green	Green	Green	Green	Green	Green	Green	Green	Green
Pineapple Juice	Green	Green	Green	Green	Green	Green	Green	Green	Green
Unsweetened Tea	Green	Green	Green	Green	Green	Green	Green	Green	Green
Red Bull®	Yellow	Yellow	Green	Green	Green	Green	Green	Green	Green
Gatorade®	Green	Green	Green	Green	Green	Green	Green	Green	Green
Coors®	Red	Black	Yellow	Red	Green	Green	Green	Green	Green
Hard Cider	Red	Black	Yellow	Red	Green	Green	Green	Green	Green
Pinot Noir	Red	Black	Yellow	Red	Green	Green	Green	Green	Green
Vodka	Red	Black	Red	Red	Yellow	Green	Yellow	Green	Green
Rum	Red	Black	Red	Red	Yellow	Green	Yellow	Green	Green
Whiskey	Red	Black	Red	Red	Yellow	Green	Yellow	Green	Green

Table S1. Detection of adulterants out of the fifteen beverages examined. A green cell indicates detection was possible at at least 0.1 % v/v. A yellow cell indicates detection was possible at 1.0 % v/v but not at 0.1% v/v. A red cell indicates that detection was not possible at or below a level of 1.0 % v/v. Black shaded cells were not tested because the beverage contained the adulterant.