

Supplementary Material

Headspace Analysis for Screening of Volatile Organic Compound Profiles of Electronic Juice Bulk Material

Analytical and Bioanalytical Chemistry

Ryan F. LeBouf*, Dru A. Burns, Anand Ranpara, Kathleen Attfield, Leonard Zwack, Aleksandr B. Stefaniak

*(304) 285-6287; rlebouf@cdc.gov, 1095 Willowdale Rd, Morgantown, WV, USA 26505;

Headspace concentrations of different analytes varied by flavor type: 2,3-hexanedione and acetone (Figure S1); acetonitrile and alpha-pinene (Figure S2); chloroform and ethylbenzene (Figure S3); isopropyl alcohol and m,p-xylene (Figure S4); methyl methacrylate and methylene chloride (Figure S5); n-hexane and o-xylene (Figure S6); and styrene and toluene (Figure S7).

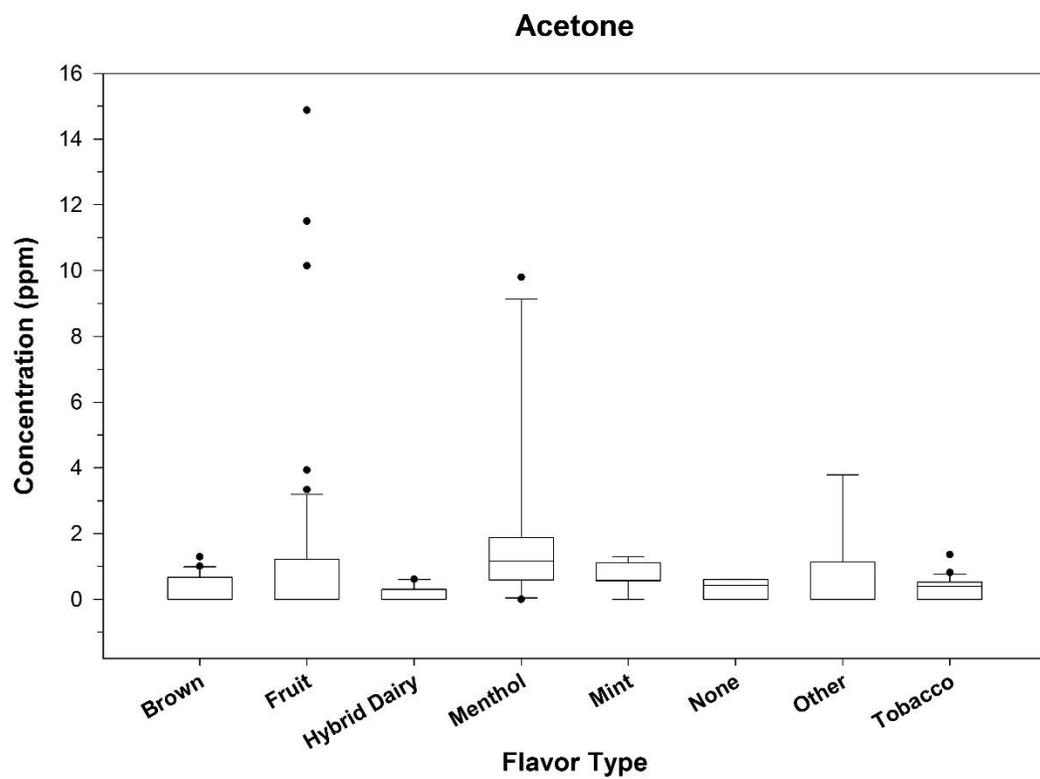
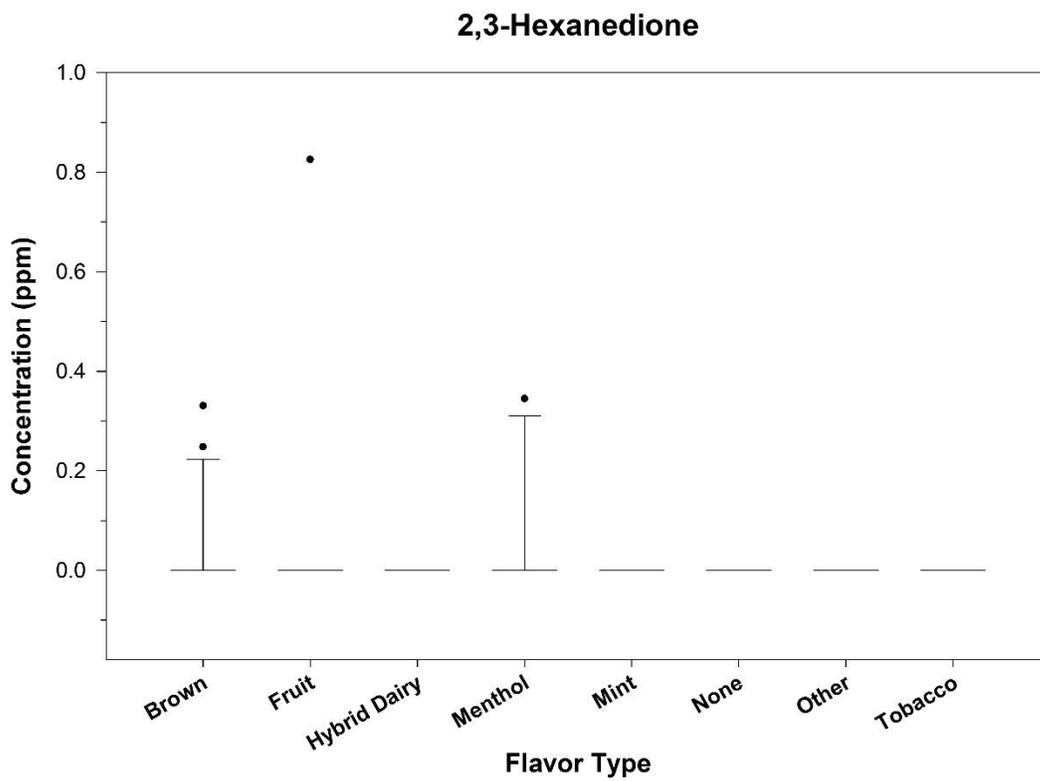


Figure S1: Box plots of headspace concentrations (ppm) for 2,3-hexanedione and acetone

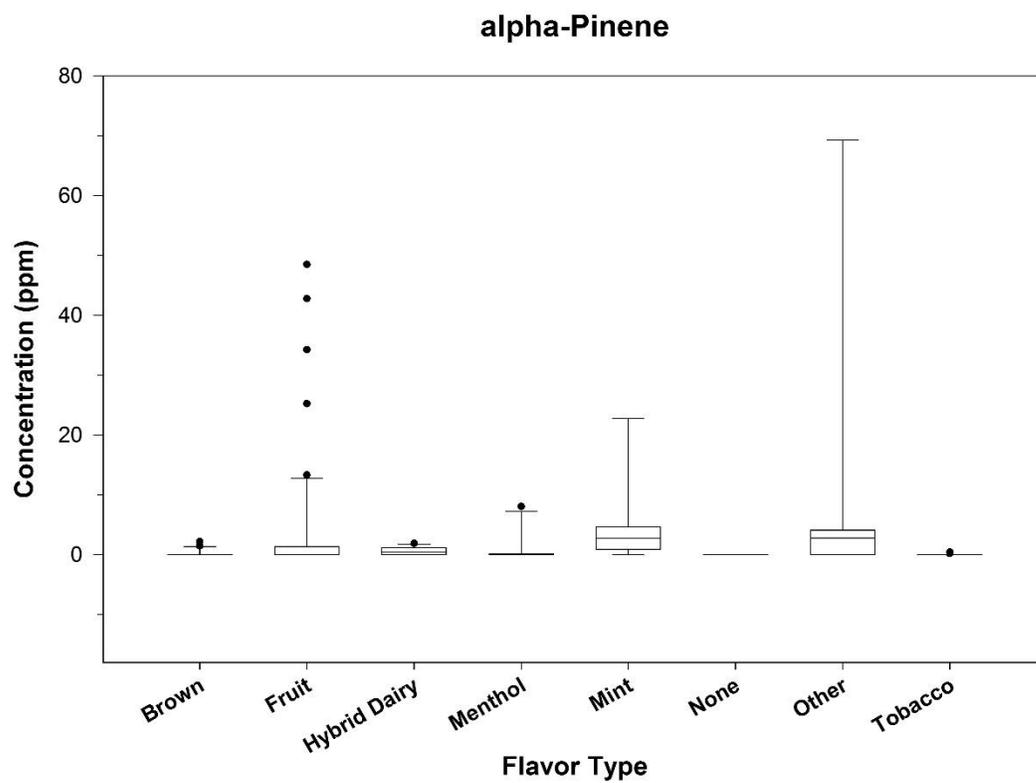
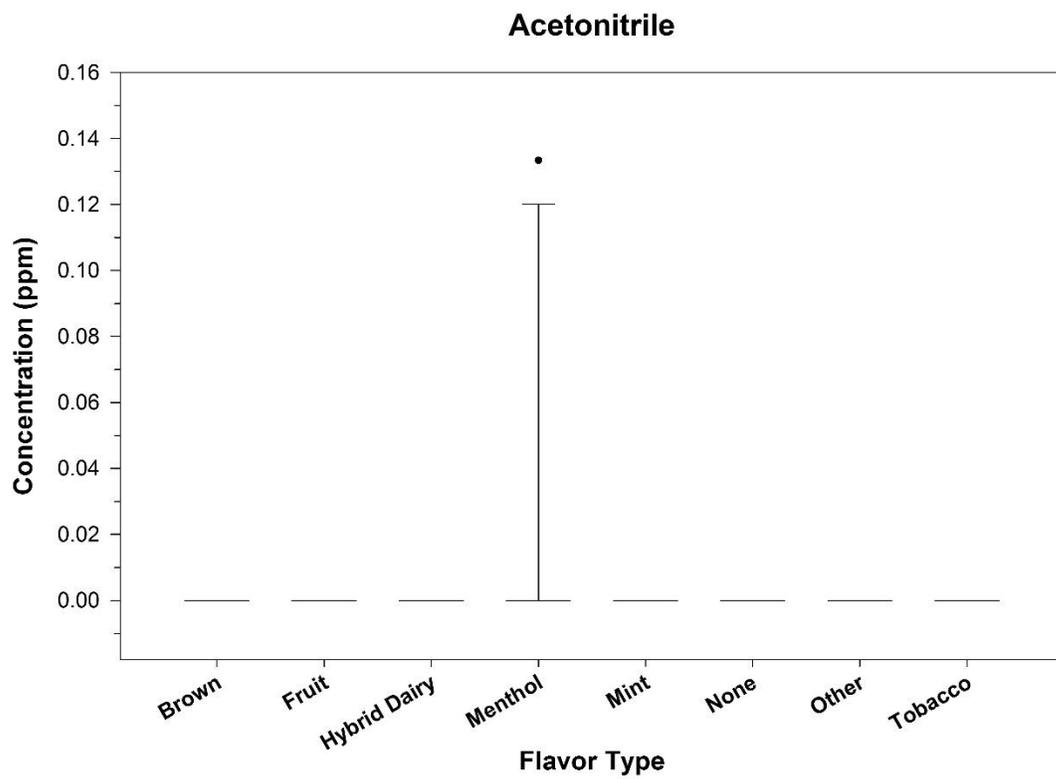


Figure S2: Box plots of headspace concentrations (ppm) for acetonitrile and alpha-pinene

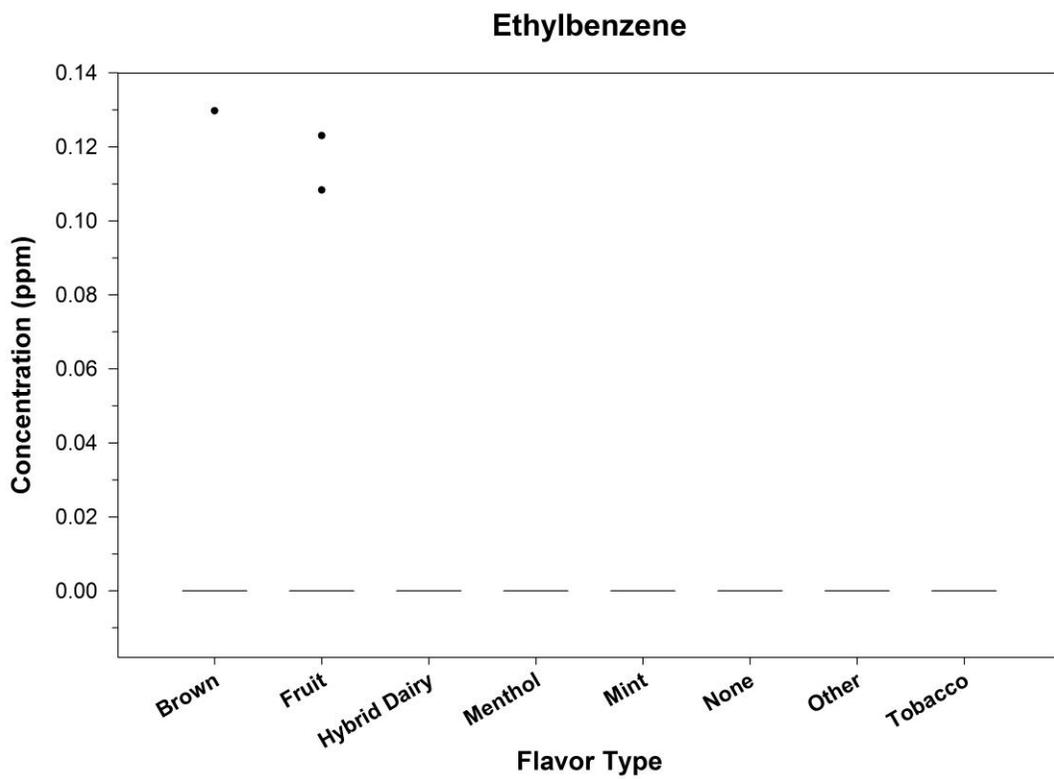
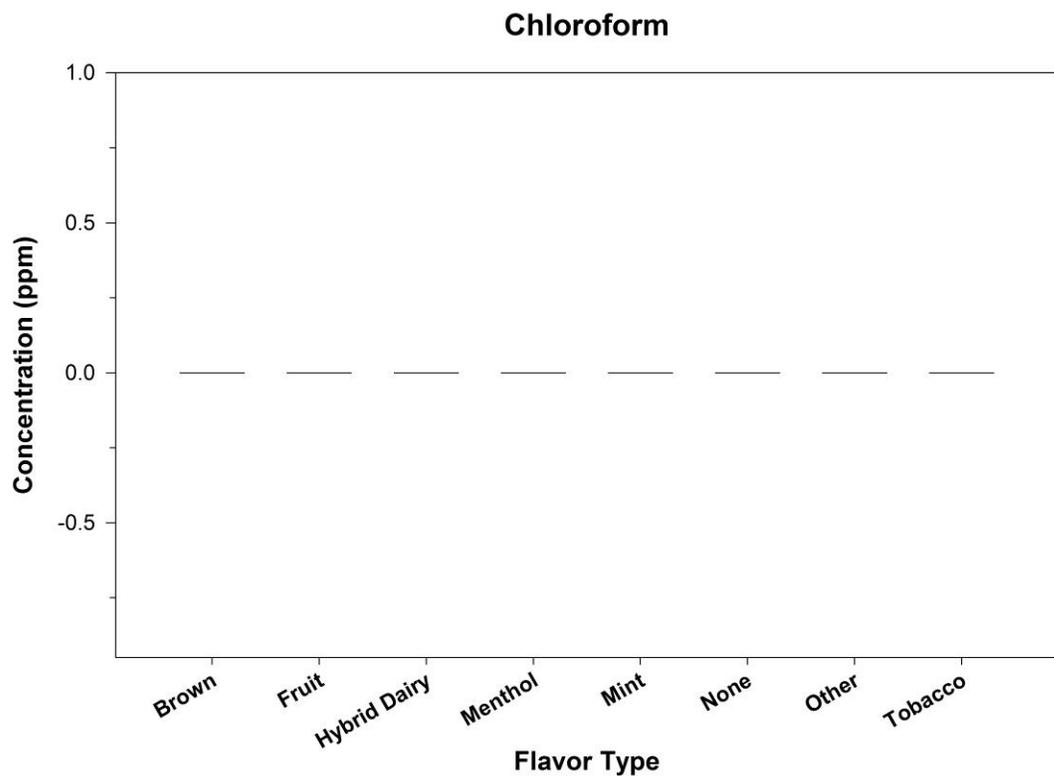


Figure S3: Box plots of headspace concentrations (ppm) for chloroform and ethylbenzene

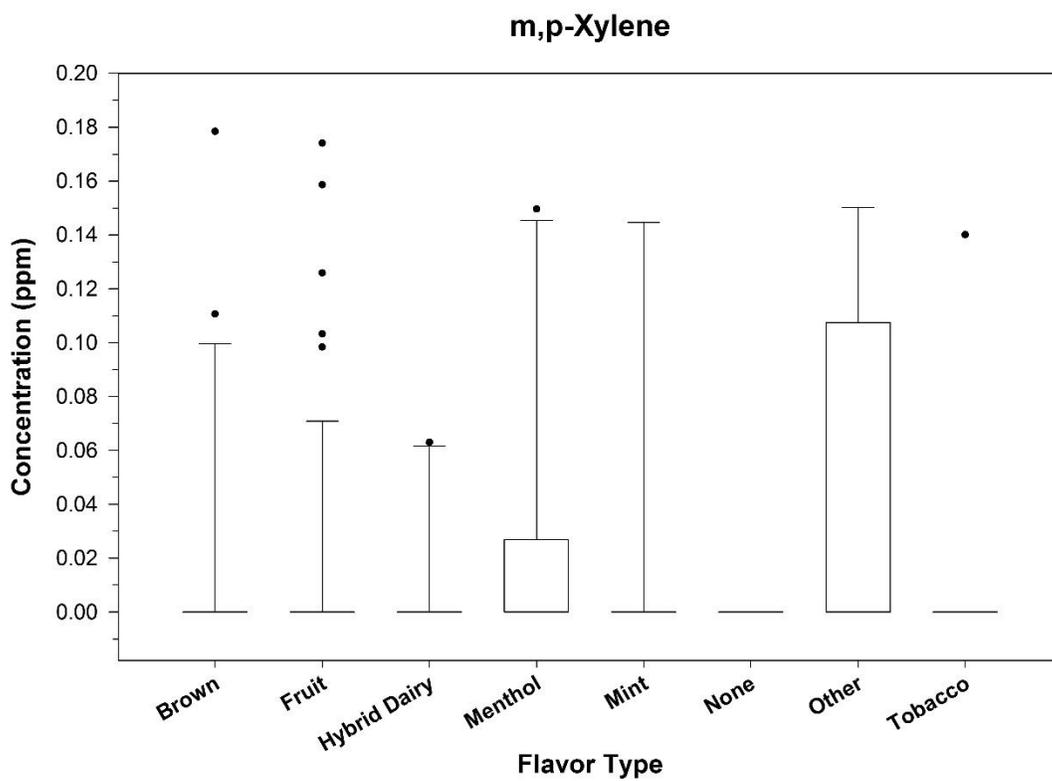
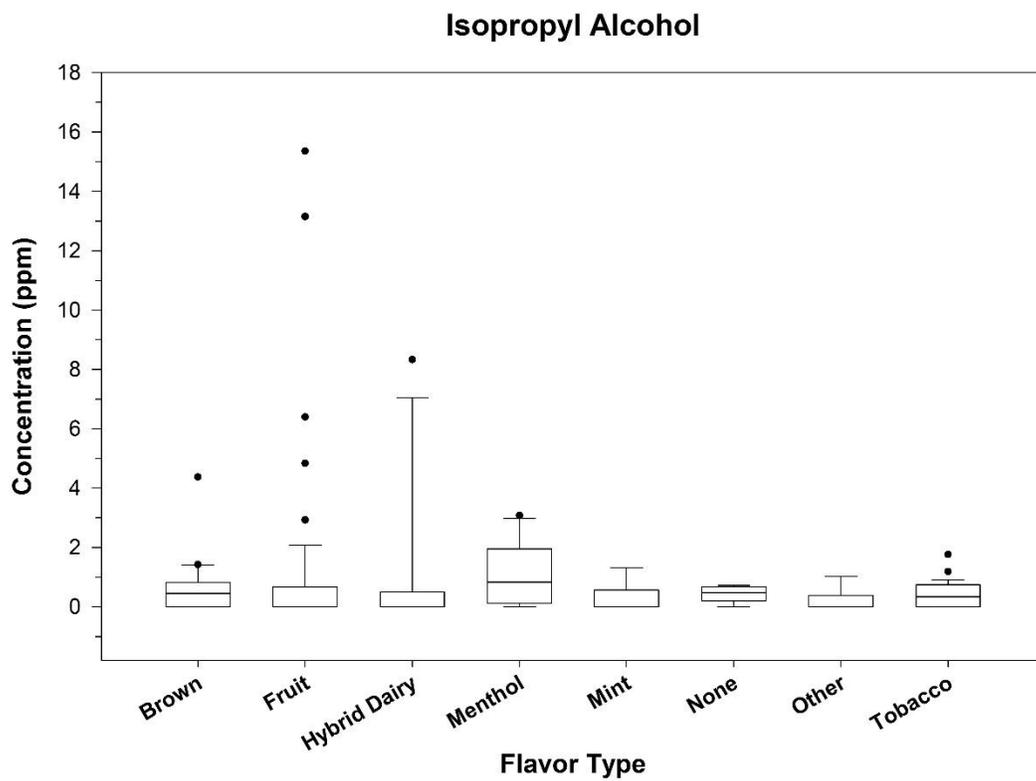


Figure S4: Box plots of headspace concentrations (ppm) for isopropyl alcohol and m,p-xylene

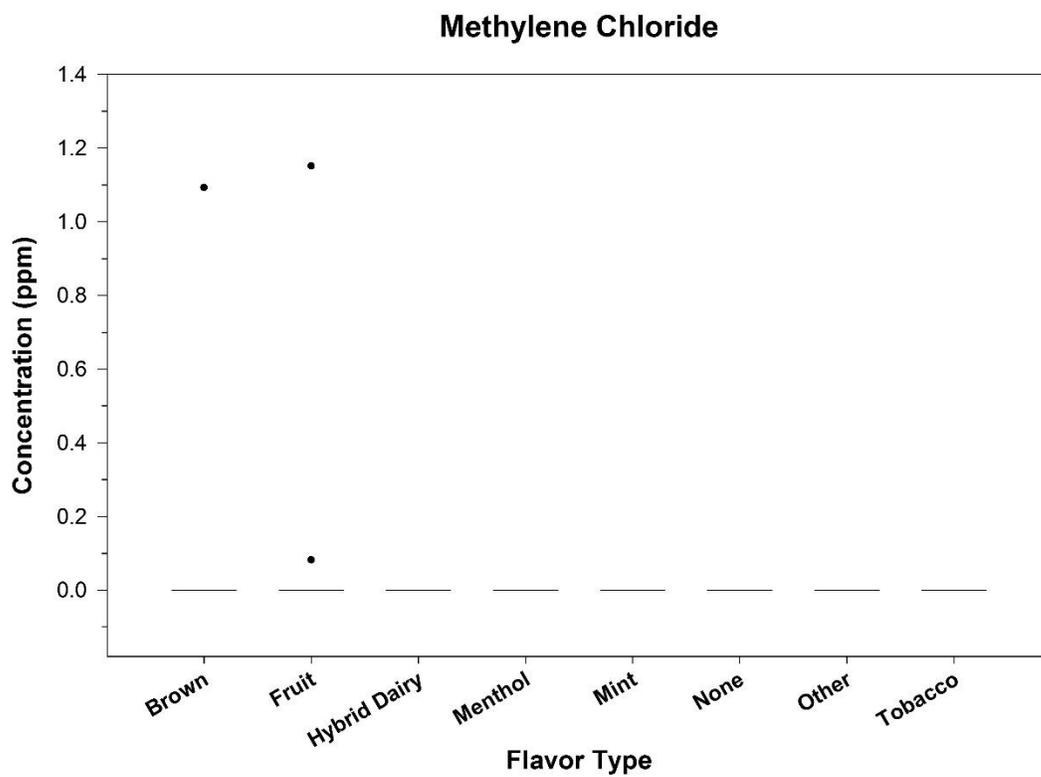
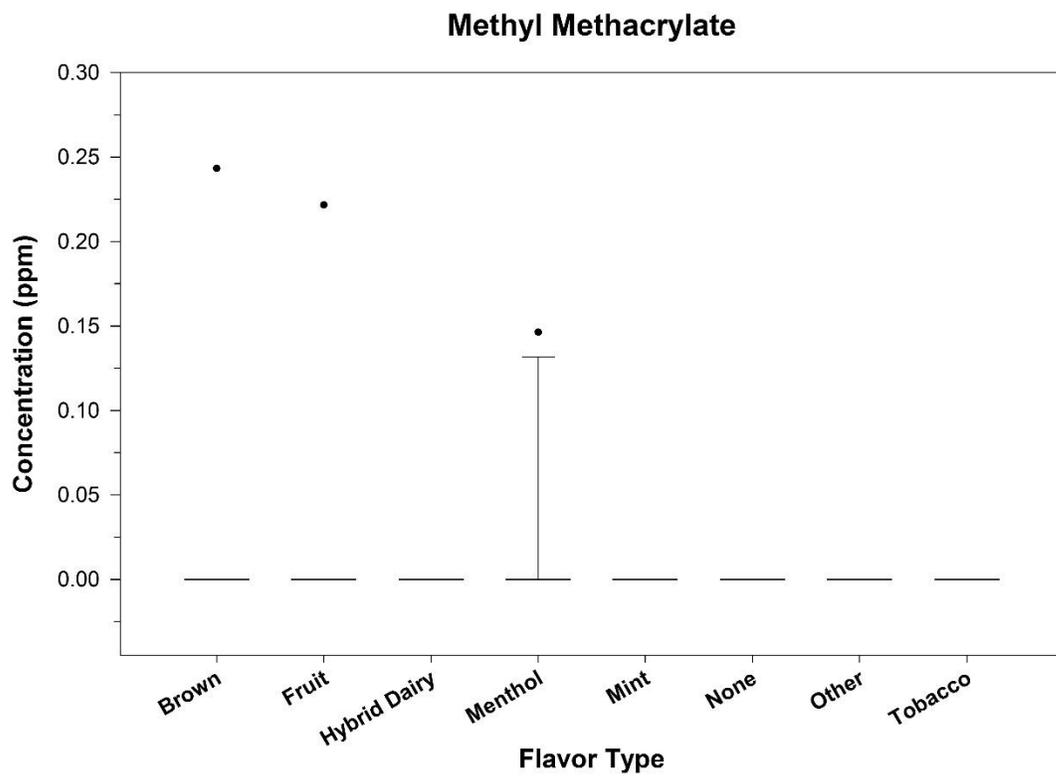


Figure S5: Box plots of headspace concentrations (ppm) for methyl methacrylate and methylene chloride

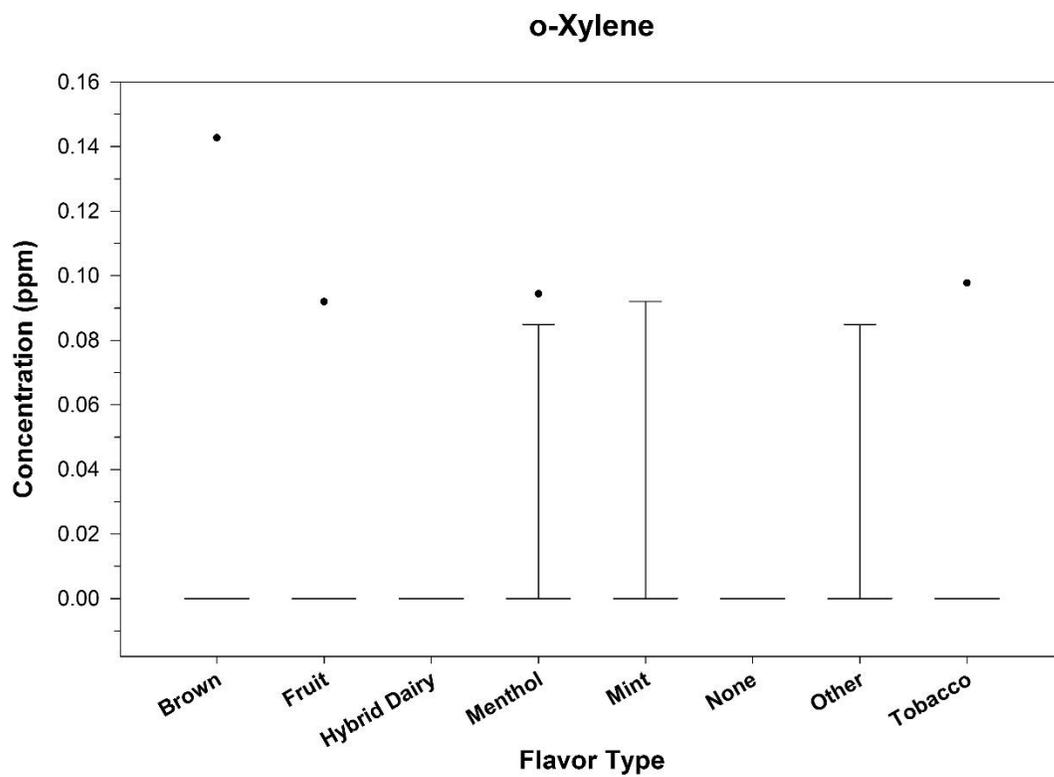
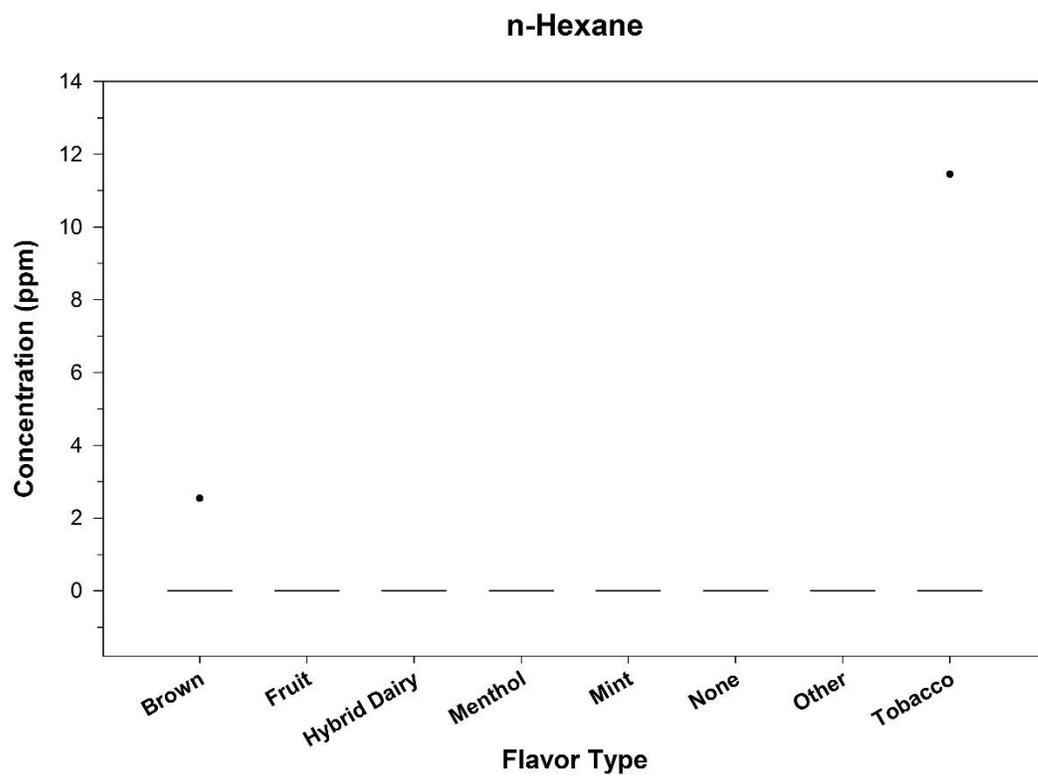


Figure S6: Box plots of headspace concentrations (ppm) for n-hexane and o-xylene

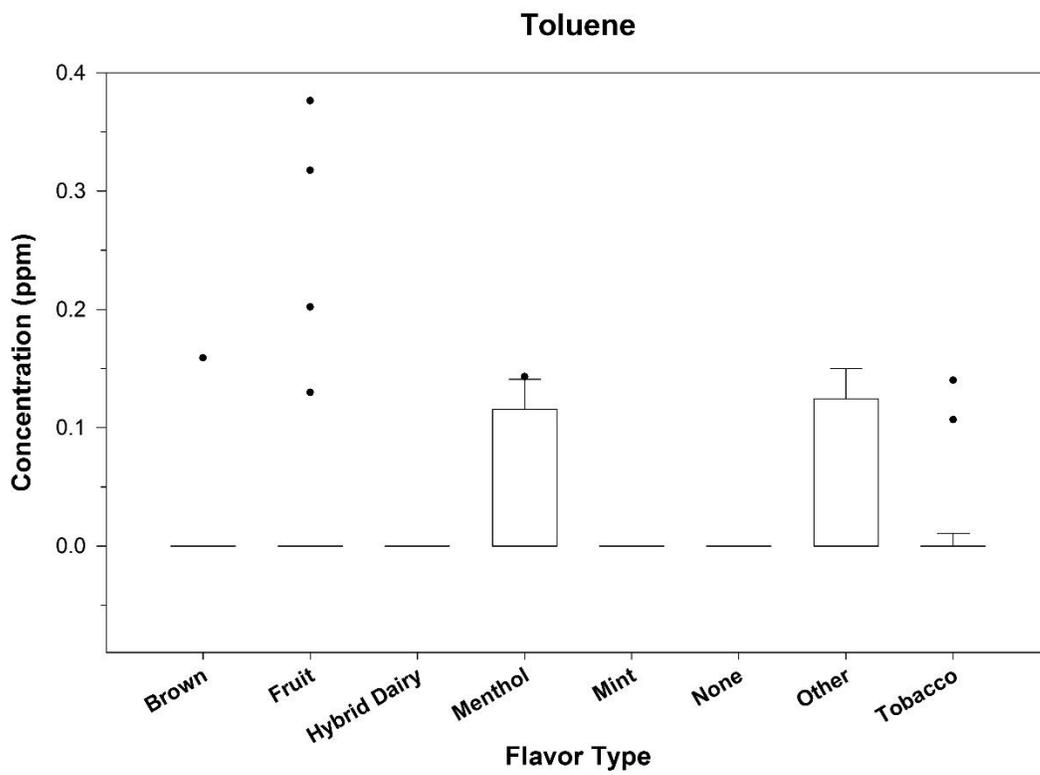
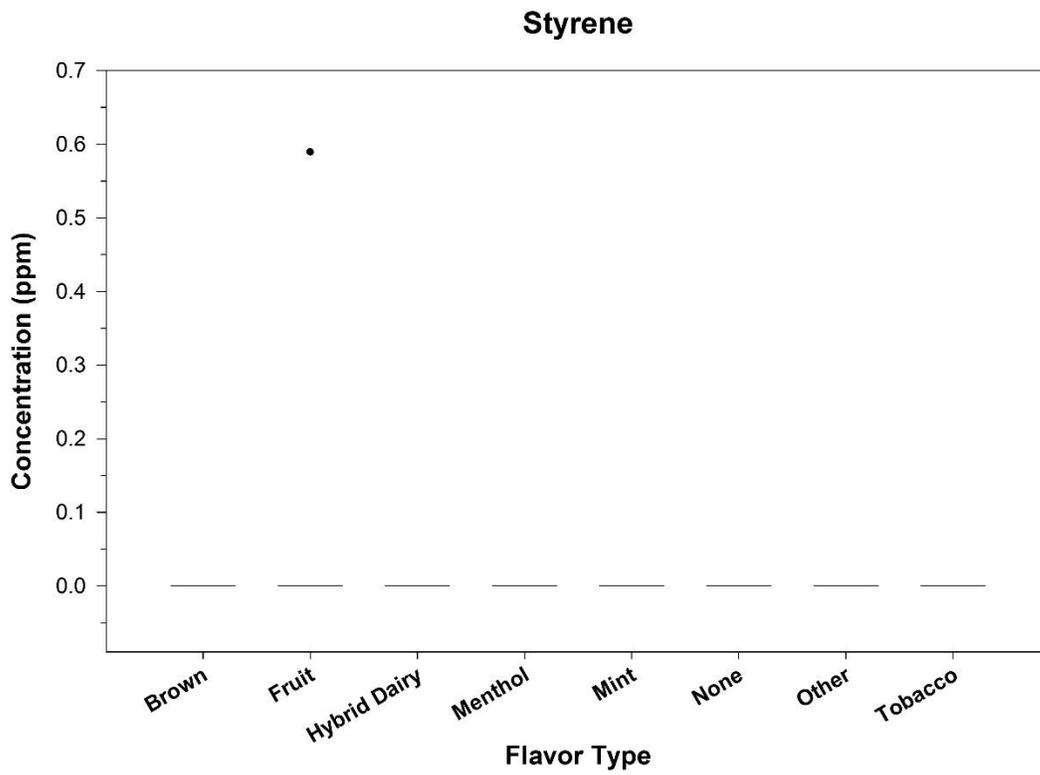


Figure S7: Box plots of headspace concentrations (ppm) for styrene and toluene

Flavor type affected the composition of tentatively identified compounds from a comparison with the NIST11 mass spectral library (Table S1). Ethyl acetate was the most frequently identified chemical for most flavor types with the exception of Fruit and Mint. The most commonly identified compounds in Mint flavor type were terpenes: γ -terpinene (86%) and β -pinene 71%.

Table S1. Most frequently identified compounds for each flavor type

Flavor Type	Identified Compound	Frequency (%)
Brown (n=20)	ethyl acetate	70
	ethyl butanoate	65
	ethyl propionate	50
	isopentyl isovalerate	30
	ethyl 2-methylbutanoate	15
Fruit (n=57)	paraldehyde	15
	ethyl butanoate	88
	ethyl acetate	86
	ethyl 2-methylbutanoate	70
	isoamyl acetate	46
	ethyl propionate	42
	ethyl 3-methylbutanoate	33
	isobutyl acetate	32
Hybrid Dairy (n=11)	2-methylbutyl acetate	28
	ethyl acetate	91
	isopentyl isovalerate	73
	ethyl butanoate	64
	isoamyl acetate	55
	2-methylbutyl acetate	46
	2-heptanone	46
	ethyl propionate	46
	1,3-dioxolane, 2,2,4-trimethyl	36
	pentyl acetate	36
	ethyl 2-methylbutanoate	36
	γ -terpinene	36
	β -pinene	27
	p-cymene	27
Mint (n=7)	γ -terpinene	86
	β -pinene	71
	ethyl acetate	71
	1,3-dioxolane, 2,2,4-trimethyl	57
	p-cymene	57
	cyclohexanone, 5-methyl-2-(1-methylethyl)-, (2R-cis)-	43
	camphene	43
	β -ocimene	43
Menthol (n=10)	ethyl acetate	50
	ethyl butanoate	50
	cyclohexanone, 5-methyl-2-(1-methylethyl)-, (2R-cis)-	30
	β -pinene	30
	1,8-cineole	30
	ethyl propionate	30
Tobacco (n=28)	ethyl acetate	68
	ethyl propionate	46
	ethyl butanoate	29
	cyclohexanone, 5-methyl-2-(1-methylethyl)-, (2R-cis)-	18
Other (n=7)	ethyl acetate	100
	benzaldehyde	86
	β -pinene	43
	ethyl butanoate	43
None (n=5)	ethyl acetate	80
	ethyl butanoate	20
	isobutyl acetate	20