

SUPPORTING INFORMATION:**Nicotine in Tobacco Product Aerosols:****"It's Déjà Vu All Over Again"[§]**

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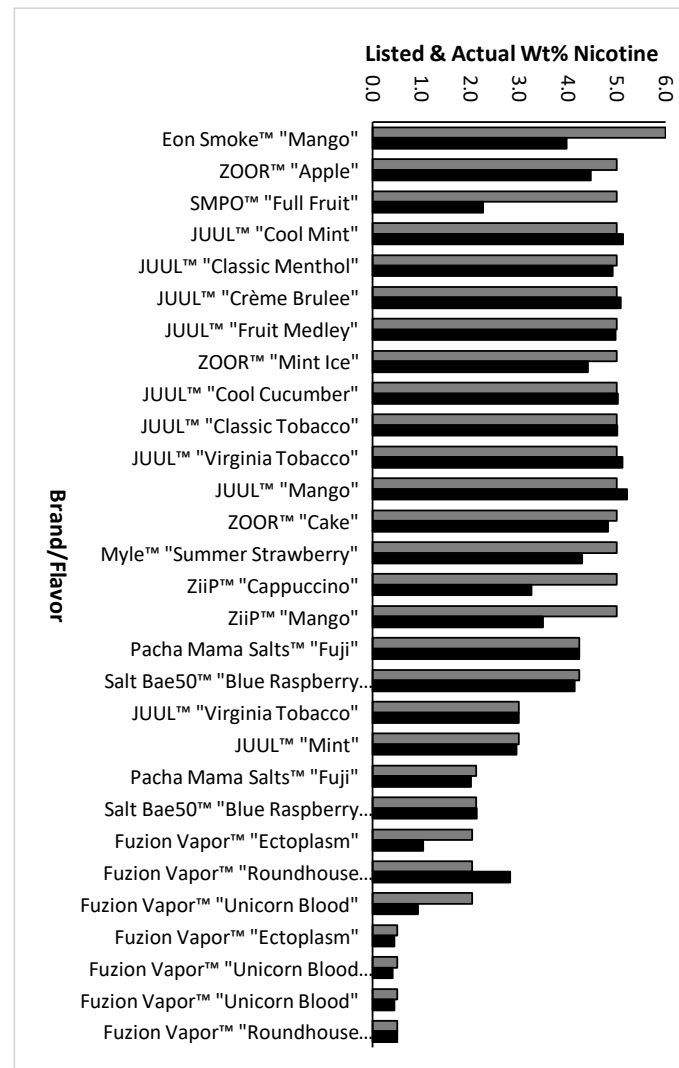


Figure S-1. Comparisons between listed and actual nicotine weight-% contents for a selection of e-liquids. The listed amounts are shown by grey bars, while the actual amounts (as assessed by ¹H NMR integrations converted to weight-% values) are shown by black bars.

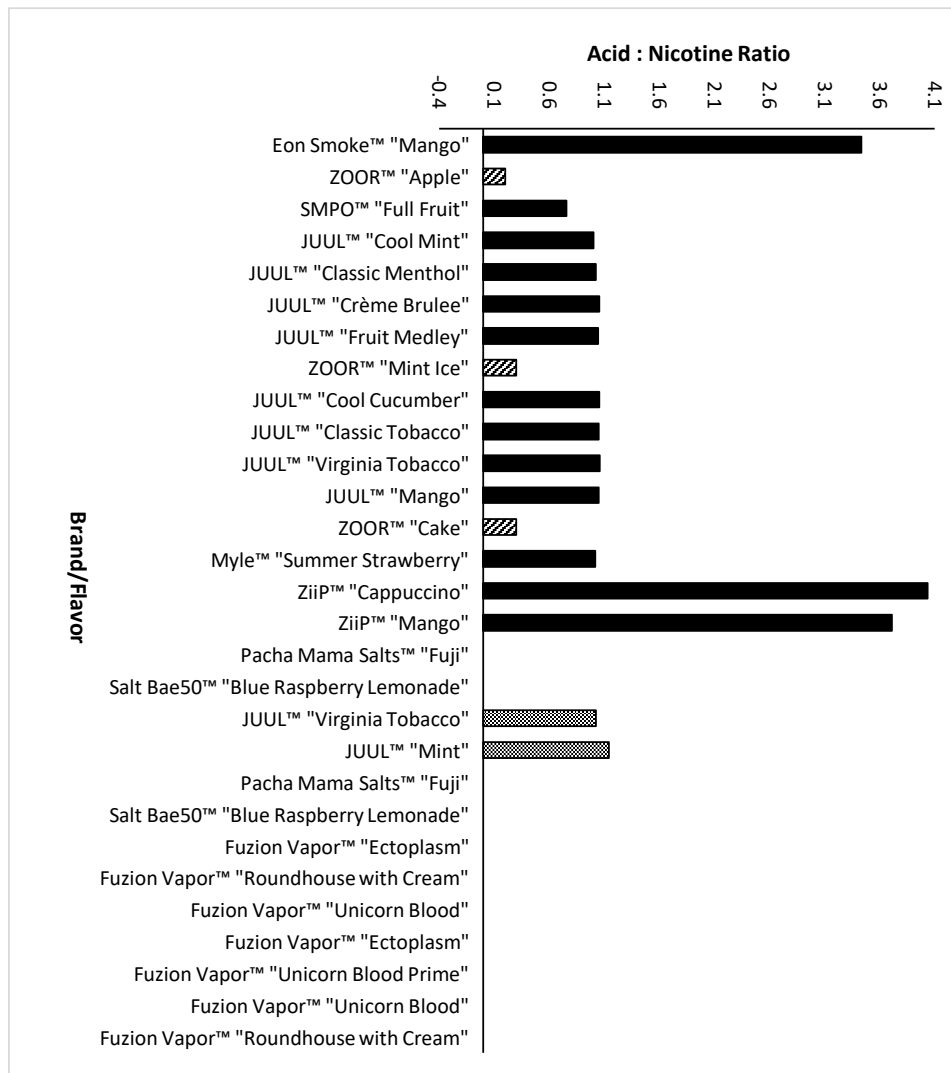


Figure S-2. The ratio of mol-% acid / mol-% nicotine for e-liquids containing benzoic acid or levulinic acid. Note that the ZOOR™ product was found not contain any benzoic acid (but did contain levulinic acid; indicated as striped bar), all other products with a positive acid/nicotine ratio contained benzoic acid, and the JUUL™ products are all essentially 1:1 benzoic acid/nicotine. JUUL™ 3 weight% e-liquids are shown as checkered bars.

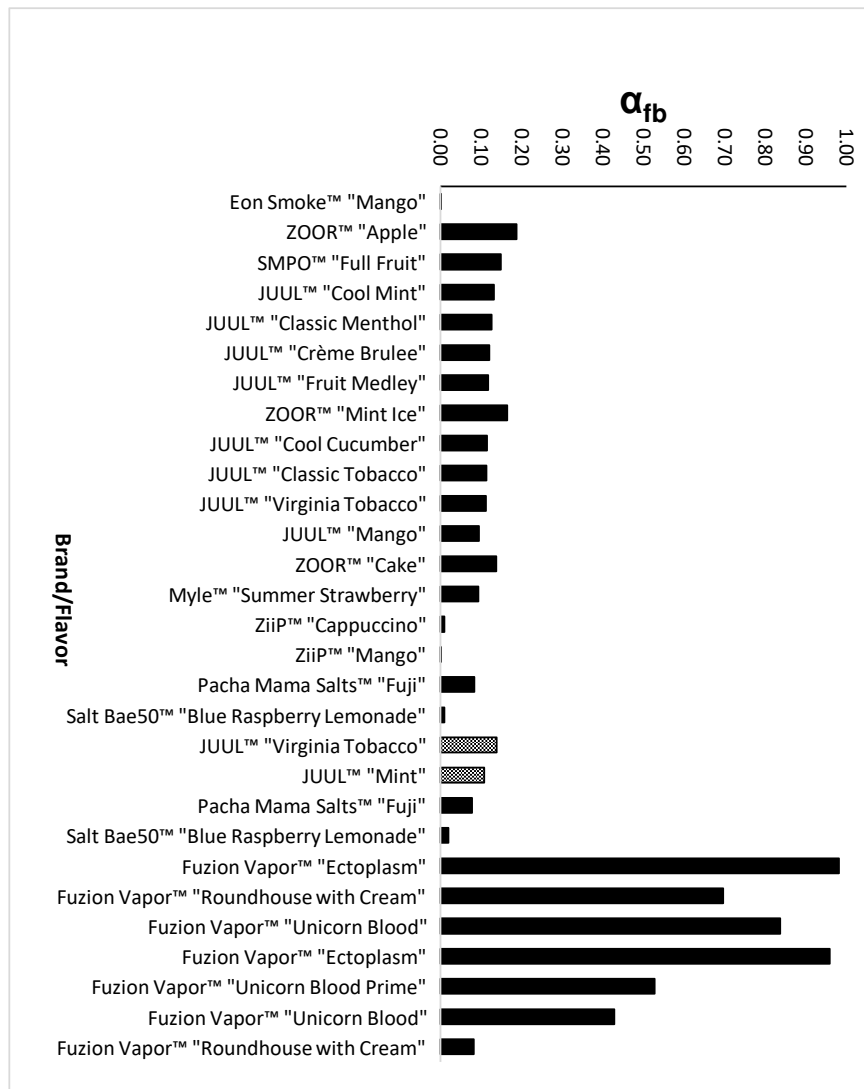


Figure S-3. The α_{fb} values for the selection of e-liquids sampled. The two products from JUUL™ with 3 weight-% nicotine, as opposed to with 5 weight-% in the rest of the JUUL™ products are shown as checkered bars. These values are the averages (when possible) of the determinations available from the multiple aromatic resonances from the nicotine molecules, as explained in Materials and Methods. For some products, only one, rather than two, α_{fb} value was able to be calculated (See Table S-1). Note how these values correlate strongly with the inverse of the benzoic acid / nicotine ratios shown in Figure 2.

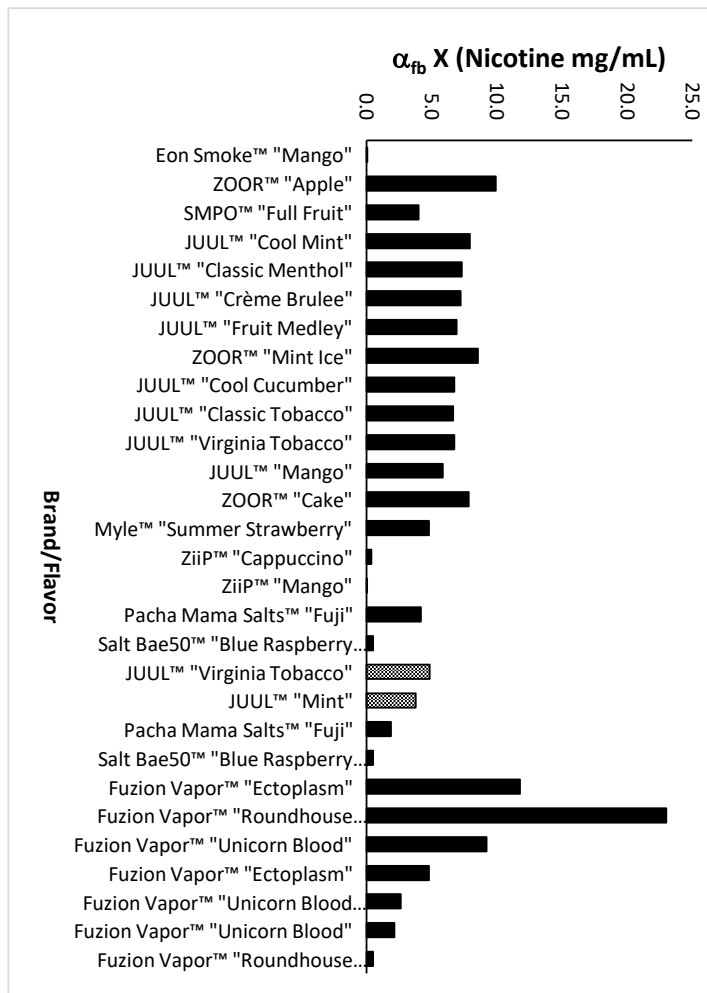


Figure S-4. The α_{fb} values from Figure 3, multiplied by the nicotine mg/mL values. The resulting numbers permit a rough comparison of the *total free-base nicotine exposure* that a user would obtain from vaping the same weight of aerosol from each product. Note that the benzoic acid variation across these pods has a strong influence on the total exposure to free-base nicotine. The two products from JUUL™ with 5 weight-% nicotine, as opposed to with 3 weight-% in the rest of the JUUL™ products are shown as checkered bars.

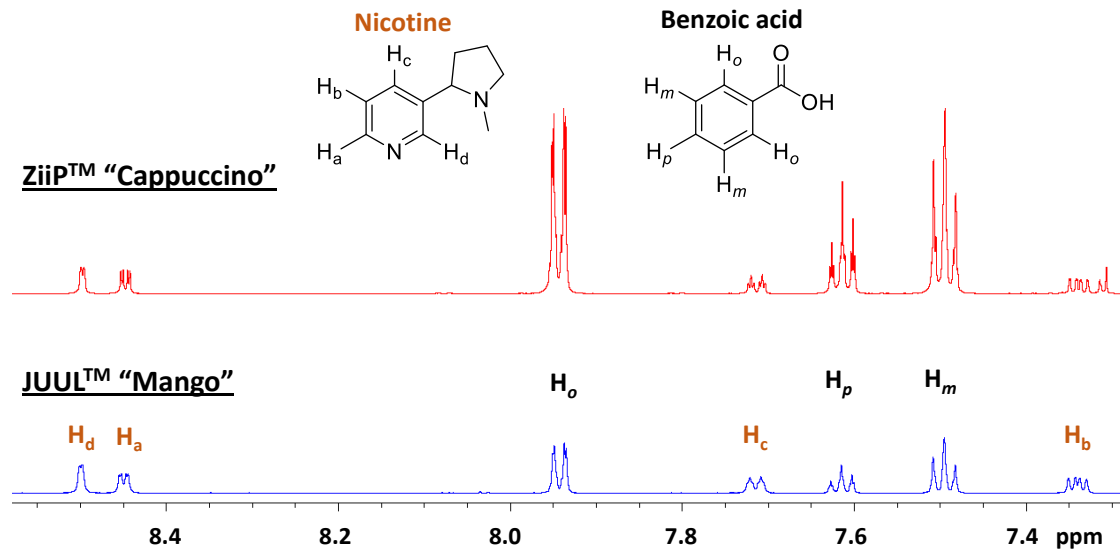


Figure S-5. Samples for composition analysis were prepared by adding a drop of each e-liquid to DMSO- d_6 and testing by 1H NMR. Spectra were normalized relative to the nicotine resonances because the e-liquids contained different ratios of propylene glycol:glycerol. Here, it can be seen that the ZiiP™ ‘Cappuccino’ e-liquid has a much higher benzoic acid:nicotine ratio (4:1) than the JUUL™ ‘Mango’ benzoic acid:nicotine ratio (1.1:1).

Table S-1. Full table of values for listed vs. measured nicotine contents, molar acid/nicotine ratios, and free-base fraction determinations (α_{fb}) for a selection JUUL™ pod liquids, “look-a-like/knockoff” pod liquids, and bottled e-liquids.

Brand "Flavor"	Nicotine Content			Molar Ratio Acid/Nicotine	α_{fb} using H _a	α_{fb} using H _b	Average α_{fb}	E-liquid used to prepare proton-shift references for calculating α_{fb} [§]
	Listed (wt%)	Actual (wt%)	Actual (mol%)					
Eon Smoke™ "Mango"	6.0	4.0	2.1	3.4	0.00	U	N/A	JUUL™ "Mango"
ZOOR™ "Apple"	5.0	4.5	2.4	0.2*	ND	0.19	N/A	ZOOR™ "Apple"
SMPO™ "Full Fruit"	5.0	2.3	1.2	0.8	0.13	0.16	0.15 ± 0.02	JUUL™ "Mango"
JUUL™ "Cool Mint"	5.0	5.1	2.7	1.0	0.14	0.12	0.13 ± 0.01	JUUL™ "Mango"
JUUL™ "Classic Menthol"	5.0	4.9	2.7	1.0	0.14	0.11	0.13 ± 0.01	JUUL™ "Mango"
JUUL™ "Crème Brulee"	5.0	5.1	2.7	1.1	0.14	0.11	0.12 ± 0.01	JUUL™ "Mango"
JUUL™ "Fruit Medley"	5.0	5.0	2.7	1.0	0.13	0.11	0.12 ± 0.01	JUUL™ "Mango"
ZOOR™ "Mint Ice"	5.0	4.4	2.3	0.3*	0.16	0.17	0.17 ± 0	ZOOR™ "Cake"
JUUL™ "Cool Cucumber"	5.0	5.0	2.7	1.1	0.13	0.10	0.11 ± 0.01	JUUL™ "Mango"
JUUL™ "Classic Tobacco"	5.0	5.0	2.7	1.1	0.12	0.10	0.11 ± 0.01	JUUL™ "Mango"
JUUL™ "Virginia Tobacco"	5.0	5.1	2.8	1.1	0.12	0.10	0.11 ± 0.01	JUUL™ "Mango"
JUUL™ "Mango"	5.0	5.2	2.8	1.1	0.10	0.08	0.09 ± 0.01	JUUL™ "Mango"
ZOOR™ "Cake"	5.0	4.8	2.7	0.3*	0.14	0.14	0.14 ± 0	ZOOR™ "Cake"
Myle™ "Summer Strawberry"	5.0	4.3	2.3	1.0	0.09	0.09	0.09 ± 0	JUUL™ "Mango"
ZiiP™ "Cappuccino"	5.0	3.3	1.7	4.0	0.01	U	N/A	JUUL™ "Mango"
ZiiP™ "Mango"	5.0	3.5	1.8	3.7	0.00	U	N/A	JUUL™ "Mango"
Pacha Mama Salts™ "Fuji"	4.2	4.2	2.2	U	0.08	0.09	0.08 ± 0	PG+GL+Nicotine [‡]
Salt Bae ^{50™} "Blue Raspberry Lemonade"	4.2	4.1	2.1	U	0.01	0.01	0.01 ± 0.01	Salt Bae ^{50™} "Blue Raspberry Lemonade"
JUUL™ "Virginia Tobacco"	3.0	3.0	1.6	1.0	0.14	0.14	0.14 ± 0	JUUL™ "Mango"

Brand "Flavor"	Nicotine Content			Molar Ratio Acid/Nicotine	α_{fb} using H_a	α_{fb} using H_b	Average α_{fb}	E-liquid used to prepare proton-shift references for calculating α_{fb} [§]
	Listed (wt%)	Actual (wt%)	Actual (mol%)					
JUUL™ "Mint"	3.0	3.0	1.6	1.1	0.11	0.10	0.11 ± 0.01	JUUL™ "Mango"
Pacha Mama Salts™ "Fuji"	2.1	2.0	1.0	U	0.08	0.08	0.08 ± 0	PG+GL+Nicotine [‡]
Salt Bae ^{50™} "Blue Raspberry Lemonade"	2.1	2.1	1.1	U	0.02	0.01	0.02 ± 0.01	Salt Bae ^{50™} "Blue Raspberry Lemonade"
Fuzion Vapor™ "Ectoplasm"	2.0	1.0	0.5	U	U	0.98	N/A	PG+GL+Nicotine [‡]
Fuzion Vapor™ "Roundhouse with Cream"	2.0	2.8	1.6	U	0.68	0.71	0.70 ± 0.01	PG+GL+Nicotine [‡]
Fuzion Vapor™ "Unicorn Blood"	2.0	0.9	0.5	U	0.82	0.86	0.84 ± 0.02	PG+GL+Nicotine [‡]
Fuzion Vapor™ "Ectoplasm"	0.5	0.5	0.3	U	0.95	0.97	0.96 ± 0.01	PG+GL+Nicotine [‡]
Fuzion Vapor™ "Unicorn Blood Prime"	0.5	0.4	0.2	U	0.50	0.55	0.53 ± 0.02	PG+GL+Nicotine [‡]
Fuzion Vapor™ "Unicorn Blood"	0.5	0.4	0.2	U	0.42	0.44	0.43 ± 0.01	PG+GL+Nicotine [‡]
Fuzion Vapor™ "Roundhouse with Cream"	0.5	0.5	0.3	U	0.07	0.09	0.08 ± 0.01	PG+GL+Nicotine [‡]

* = Samples contained levulinic acid rather than benzoic acid (all other acids).

U = Undetected because the resonance(s) required for this calculation were not present, not resolved, or were too broad for analysis.

N/A = Not applicable because only one α_{fb} value was calculated.

§ = Acid and base references refer to the monoprotonated and free-base nicotine forms, respectively.

‡ = Lab-prepared propylene glycol (PG) + glycerol (GL) + 59 mg/mL nicotine mixture

