

## Supplemental Information

Functional characterization of flavorings in electronic cigarette refill  
liquids by nuclear magnetic resonance spectroscopy

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Table S1. The manufacturer, flavor and nicotine content of the refill e-liquids and, nicotine, propylene glycol, glycerol and non-exchangeable hydrogen types concentrations measured in this study

Brand	Flavor	Nicotine content (mg/ml)	Cluster	This study								
				Nicotine	Propylene glycol mg/ml	Glycerol	H-C	H-C-C=	H-C-O	O-CH-O and H-C=C	Ar-H	H-C=O
1	Blueberry cobbler	12	I	15	482	846	1210	918	3,987	97	741	94
1	Blueberry cobbler	24	I	25	456	628	1345	1,183	1,260	75	779	153
1	Blueberry	24	I	22	606	453	1370	494	2,516	21	216	19
1	Blueberry	12	I	13	669	509	1035	646	2,100	39	214	13
1	Cherry	12	I	15	336	857	588	599	824	24	271	42
1	Caramel cafe	24	I	21	347	594	763	1,012	1,520	59	572	80
1	Caramel cafe	12	I	13	487	700	1,306	647	928	70	734	134
1	Cherry	24	I	31	352	903	514	1,054	707	16	306	40
1	Carolina bold	12	I	10	512	499	394	407	429	0	22	12
1	Carolina bold	24	I	21	463	528	352	35	430	2	29	4
1	Glacier mint	24	II	22	586	450	2,427	198	525	0	56	17
1	Glacier mint	12	II	14	708	573	2,226	640	450	5	73	31
1	Gold leaf	12	II	13	428	440	727	813	372	2	89	0
1	Gold leaf	0	II	4	516	553	774	512	554	4	95	5
1	Gold leaf	24	II	26	497	516	848	470	376	1	99	2
1	Menthol	24	II	25	318	728	1,847	309	483	11	340	40
1	Menthol	12	II	13	454	731	1,675	673	722	12	303	32
1	Mint chocolate	12	II	12	684	392	1,038	497	870	12	44	9
1	Menthol	0	II	1	620	614	1,552	129	523	19	226	28
1	Mint chocolate	24	II	25	798	432	1,098	368	658	3	76	1
1	Strawberry mint	12	III	14	529	740	1,712	817	1187	27	183	6
1	Strawberry mint	24	III	27	472	767	1,533	245	795	23	193	21

Brand	Flavor	Nicotine content (mg/ml)	Cluster	This study								
				Nicotine	Propylene glycol mg/ml	Glycerol	H-C	H-C-C=	H-C-O	O-CH-O and H-C=C	Ar-H	H-C=O
1	Tobacco	12	III	15	367	959	299	705	669	22	125	28
1	Tobacco	24	III	28	476	757	259	264	531	22	127	24
1	Vanilla	0	III	0	426	643	359	62	238	14	93	24
1	Vanilla	24	III	19	352	516	403	735	617	14	214	35
2	Berry mint	6	III	5	551	576	1292	388	444	7	75	11
1	Vanilla	12	III	9	381	549	281	439	480	12	102	16
2	Cherry	6	III	6	602	595	397	229	446	9	53	0
3	Blood orange	10	IV	10	633	698	2834	363	604	0	4	0
2	Gourmet crème	6	IV	5	526	525	684	254	443	4	53	20
2	Tobacco	6	IV	4	460	477	272	177	571	10	20	11
2	Watermelon	6	IV	5	570	565	416	255	407	57	87	11
3	Peach tea	15	V	13	561	487	589	580	334	57	340	8
3	Single malt scotch	15	V	15	662	625	1455	316	517	0	39	4
3	Blood orange	15	V	13	516	590	2422	448	425	0	7	0
3	Single malt scotch	10	V	9	636	595	1359	381	410	0	36	0
3	Pomegranate	15	V	13	535	523	604	677	335	7	155	0
3	Peach tea	10	V	9	554	509	693	440	374	61	345	0
3	Vanilla bean	15	V	14	615	578	454	542	741	44	310	79
3	Pomegranate	10	V	14	939	860	921	732	697	17	261	4
3	Vanilla bean	10	V	10	664	601	420	399	598	36	304	53