

Supporting information - Synthetic cannabinoids consumed via e-cigarettes in English schools

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Table S1. Results summary for all samples in R1

R1S1	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
1	RF	Vaporesso	Orange	NDD	-
2	RF	Vaporesso	Yellow	MDMB-4en-PINACA 4F-MDMB-BINACA MDMB-INACA	0.63
3	LB	'Elux Mr Blue', Yellow Liquid	Yellow	NDD	-
4	LB	'Elux Lemon and Lime', Yellow Liquid	Yellow	NDD	-
5	RF	-	-	MDMB-4en-PINACA	IM
6	RF	Vaporesso	Brown	NDD	-
7	RF	Vaporesso	Green	MDMB-4en-PINACA 4F-MDMB-BINACA MDMB-INACA	0.14
8	RF	Vaporesso	Yellow	MDMB-4en-PINACA 4F-MDMB-BINACA MDMB-INACA	IM
9	UB	-	Yellow	MDMB-4en-PINACA 4F-MDMB-BINACA MDMB-INACA	0.89
R1S2	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
10	RF	Vaporesso	Clear	MDMB-4en-PINACA MDMB-INACA	0.11
11	SU	-	-	NT	-
12	SU	Gold bar	Yellow	NDD	-
13	LB	'Elux Mr Blue', Yellow Liquid	Blue	MDMB-4en-PINACA MDMB-PINACA	2.69
14	RF	Vaporesso	Green	MDMB-4en-PINACA MDMB-INACA	1.32
R1S3	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
15	SU	Crystal bar, Cherry fizz	-	NT	-
R1S4	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
16	SU	Enjoy Ultra	-	NT	-
17	SU	OXAV	-	NT	-
18	RF	Vaporesso, orange liquid	Yellow	MDMB-4en-PINACA MDMB-INACA 4F-MDMB-BINACA	0.56
19	SU	Hit Fusion, Pink Lemonade	-	NT	-
20	SU	Elf Bar	-	NDD	-
R1S5	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
21	SU	Crystal Bar, Pineapple peach mango	-	NT	-
22	SU	Crystal Bar, Cola ice	-	NT	-
23	SU	Crystal bar, Cola ice	-	NT	-
R1S6	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
24	SU	Random Tornado	-	NT	-
25	SU	Sky Hunter	-	NT	-
26	RF	Vaporesso	Brown	MDMB-4en-PINACA	0.29
27	UB	-	Yellow	MDMB-4en-PINACA	0.51

4F-MDMB-BINACA

R1S7	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
28	SU	Lost Mary, Blue Razz Cherry	-	NDD	-
29	SU	Crystal Bar, Blueberry sour raspberry	-	NT	-
30	SU	Crystal Bar, Blueberry peach ice	-	NDD	-
31	SU	Twister bar, Strawberry raspberry cherry	-	NDD	-
32	SU	Elfbar	-	NDD	-
33	SU	Lost Mary, Pineapple ice	-	NDD	-
34	SU	Lost Mary, Cherry ice	-	NT	-
35	SU	Lost Mary, Cherry ice	-	NDD	-
36	SU	Elfbar, Cola	-	NDD	-
37	SU	Brand unknown	-	NT	-
38	SU	Crystal Bar, Lemon and Lime	-	NDD	-
39	SU	Elfbar	-	NDD	-
40	SU	Lost Mary, Pineapple ice	-	NT	-
41	SU	Crystal Bar, Tiger blood	-	NDD	-
42	SU	Crystal bar, Lemon and Lime	-	NDD	-
43	SU	Lost Mary, Pineapple ice	-	NDD	-
44	SU	Elfbar	-	NDD	-
45	SU	Lost Mary, Double Apple	-	NT	-
46	SU	Lost Mary, Blue Razz ice	-	NT	-
47	SU	Lost Mary, Kiwi passion fruit guava	-	NDD	-
48	SU	Bloody Mary Crystal, Strawberry ice	-	NT	-
49	SU	Crystal Bar, Lemon and Lime	-	NT	-
50	RF	Vaporesso	Yellow	MDMB-4en-PINACA	IM
51	SU	Crystal Bar, Lemon and Lime	-	NT	-
52	RF	Vaporesso	Green	ADB-BUTINACA MDMB-4en-PINACA	2.04
53	RF	Vaporesso	Yellow	MDMB-4en-PINACA	'low'
R1S8	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
54	SU	Unknown brand, Cherry ice	Yellow	NDD	-
55	LB	Labelled bottle, Elux, Blueberry raspberry, yellow liquid	Yellow	NDD	-
56	RF	Vaporesso, yellow liquid	Yellow	MDMB-4en-PINACA	'low'
57	RF	Vaporesso, yellow liquid	Yellow	NDD	-
58	RF	Vaporesso, Brown liquid	Brown	NDD	-
59	LB	Labelled bottle, Frunk, Pineapple express, Clear liquid	Clear	NDD	-
60	LB	Labelled bottle, Elux, MR Blue, Green liquid	Green	MDMB-4en-PINACA	'low'
61	LB	Labelled bottle, Elux, Cherry ice, yellow liquid	Yellow	NDD	-
62	UB	-	Clear	MDMB-4en-PINACA	3.52
63	RF	Vaporesso, orange liquid	Yellow	MDMB-4en-PINACA	'low'
64	LB	Labelled bottle, Elux, Blueberry cherry cranberry, orange liquid	Yellow	MDMB-4en-PINACA	'low'
65	RF	Vaporesso, green liquid	Green	MDMB-4en-PINACA	1.31
66	SU	Crystal bar, Cherry ice	-	NT	-
67	SU	Crystal bar, Watermelon strawberry	-	NT	-

68	SU	Crystal bar, Lemon and Lime	-	NT	-
69	SU	Crystal bar, Cherry ice	Yellow	NDD	-
70	RF	Vaporesso, yellow liquid	Yellow	MDMB-4en-PINACA	0.37
71	RF	Vaporesso, green liquid	Green	MDMB-4en-PINACA ADB-4en-PINACA	0.39
72	SU	Randm tornado	Yellow	MDMB-4en-PINACA	IM
73	RF	Vaporesso, green liquid	Green	NDD	-
74	SU	R and M, Magic mint	-	NDD	-
75	RF	Arc Mini	-	NT	-
76	SU	Vuse Go	-	NT	-
77	SU	Crystal Bar, Sour apple blueberry	-	NDD	-
78	SU	Crystal Bar, Fizzy cherry	-	NDD	-
79	RF	Vaporesso	Yellow	MDMB-4en-PINACA	'low'
80	SU	Bloody Mary, triple berry	Yellow	NDD	-
81	SU	Crystal bar, Lemon and Lime	-	NT	-
82	SU	Crystal bar, Lemon and Lime	Yellow	NDD	-
83	LB	Labelled bottle, Elflic, strawberry ice cream, yellow liquid	Yellow	NDD	-
84	SU	Elfbar, Strawberry raspberry cherry ice	Yellow	NDD	-
85	UB	Unlabelled bottle, clear liquid	Clear	NDD	-
86	SU	Zillion	Yellow	NDD	-
87	SU	Elfbar, watermelon	Yellow	NDD	-
88	LB	Zeus, clear liquid	Clear	NDD	-
89	LB	Zeus, clear liquid	Clear	NDD	-

R1S9	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
90	RF	Vaporesso	Green	MDMB-4en-PINACA	0.42
91	RF	Vaporesso	Yellow	NDD	-
92	RF	Vaporesso	Green	MDMB-4en-PINACA	0.36
93	UB	-	Blue	MDMB-4en-PINACA	2.6
94	UB	-	Blue	MDMB-4en-PINACA MDMB-PINACA	1.24
95	SU	Enjoy Ultra, peach watermelon strawberry	-	NDD	-

R1S10	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
96	SU	Crystal bar	Yellow	NDD	-
97	SU	Elfbar	Yellow	NDD	-
98	SU	Gold bar	Yellow	NDD	-
99	SU	Crystal bar	Yellow	NDD	-
100	SU	Crystal bar	Yellow	NDD	-
101	SU	Ene Legend	Yellow	NT	-
102	SU	Hyati pro	Yellow	NDD	-
103	SU	Elux legend pro	Yellow	NDD	-
104	SU	Elfbar	Brown	NDD	-
105	SU	Crystal bar	Yellow	NT	-
106	SU	Crystal bar	Yellow	NT	-
107	SU	Elfbar	Brown	NDD	-
108	SU	Randm Tornado	Yellow	NDD	-
109	SU	Elfbar	Yellow	NDD	-

110	SU	Hyati pro	Yellow	NDD	-
111	SU	Lost mary	Yellow	NT	-
112	SU	Gold bar	Yellow	NDD	-
113	SU	Crystal bar	Yellow	NT	-
114	SU	-	Yellow	NDD	-
115	SU	Ene Legend	Brown	NDD	-
116	SU	-	Brown	NDD	-
R1S11	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
117	UB	-	Pink	MDMB-4en-PINACA MDMB-PINACA	1.5
R1S12	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
118	RF	Vaporesso	Red	MDMB-4en-PINACA	'low'
119	UB	-	Purple	ADB-BUTINACA	2.16
120	UB	-	Yellow	ADB-BUTINACA	1.19
121	UB	-	Yellow	ADB-BUTINACA	1.28
122	UB	-	Green	MDMB-4en-PINACA 4F-MDMB-BINACA MDMB-INACA	1.28
123	UB	-	Green	MDMB-4en-PINACA 4F-MDMB-BINACA MDMB-INACA	0.34
124	SU	-	Brown resin	THC	508.15
125	SU	Crystal bar	-	NT	-
126	SU	Crystal bar	-	NT	-
127	SU	Enjoy ultra	-	NT	-
128	SU	Twins maxfel	-	NT	-
129	SU	Lost mary	-	NT	-
130	SU	Enjoy ultra	-	NT	-
131	SU	88. vapes	-	NT	-
132	SU	Hayati pro ultra	-	NT	-
133	SU	Crystal bar	-	NT	-
134	SU	Randm tornado	-	NT	-
135	SU	Randm tornado	-	NT	-
136	SU	Randm tornado	-	NT	-
137	SU	88 vapes	-	NT	-
138	SU	Crystal original	-	NT	-
139	SU	Lost mary	-	NT	-
140	SU	Lost mary	-	NT	-
141	SU	Randm tornado	-	NT	-
142	SU	Insta bar	-	NT	-
143	SU	88. vapes	-	NT	-
144	SU	-	-	NT	-
145	SU	-	-	NT	-
146	SU	-	-	NT	-
147	SU	-	-	NT	-
148	SU	-	-	NT	-
149	SU	-	-	NT	-

150	SU	-	-	NT	-
R1S13	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
151	SU	Twister bar	-	NT	-
152	SU	Crystal bar	Yellow	NDD	-
153	SU	Crystal bar	Yellow	NDD	-
154	SU	Crystal bar	-	NT	-
155	SU	Crystal bar	-	NT	-
156	SU	-	-	NT	-

NDD, no drug detected; 'low', concentration below level of NMR measurement; IM, insufficient material; NT, not tested; SU, single use; RF, refillable; UB, unlabelled bottle; LB, labelled bottle.

Table S2. Results summary for all samples in R2

R2S1	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
1	UB	-	Purple	MDMB-4en-PINACA MDMB-PINACA	1.71
2	UB	-	Clear	MDMB-4en-PINACA	IM
3	UB	-	Purple	MDMB-4en-PINACA MDMB-PINACA	1.56
4	UB	-	Blue	MDMB-4en-PINACA	2.92
5	RF	Vapresso	Clear	MDMB-4en-PINACA	IM
6	UB	-	Yellow	MDMB-4en-PINACA	IM
7	LB	Elux, Mr Blue	Yellow	NDD	-
8a	SU	Hyati (2 nd pad)	Green	MDMB-4en-PINACA	0.17
8b	SU	Hyati (main pad)	Yellow	MDMB-4en-PINACA	0.05
9	SU	-	Yellow	NDD	-
10	SU	-	Yellow	NDD	-
11	SU	-	Yellow	NDD	-
12	SU	-	Yellow	NDD	-
13	SU	-	Yellow	NDD	-
14	SU	-	Yellow	NDD	-
15	SU	-	Yellow	NDD	-
16	SU	-	Yellow	NDD	-
17a	SU	Hyati (2 nd pad)	Purple	MDMB-4en-PINACA	0.4
17b	SU	Hyati (main pad)	Brown	MDMB-4en-PINACA	IM
18	SU	-	Brown	NDD	-
19	SU	-	-	NT	-
20	SU	-	-	NT	-
21	SU	-	-	NT	-
22	SU	Randm Tornado	Yellow	MDMB-4en-PINACA MDMB-INACA	IM
23	SU	Randm tornado	Green	MDMB-4en-PINACA	0.3
24	SU	-	Clear	NDD	-
25	SU	Quoa	Yellow	MDMB-4en-PINACA	0.14
26	SU	-	Yellow	NDD	-
27	SU	-	-	NT	-
28	SU	-	-	NT	-
29	SU	Hyati pro ultra	Yellow	MDMB-4en-PINACA	0.15
30	SU	-	Yellow	NDD	-
31	SU	-	Yellow	NDD	-
32	SU	-	Yellow	NDD	-
33	SU	-	Yellow	NDD	-
R2S2	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
34	RF	-	-	NT	-
35	RF	Elfbar	Yellow	NDD	-
36	UB	-	Pink	Heroin MDMB-4en-PINACA ADB-BUTINACA	0.1 (heroin), 0.28 (SC)
37	RF	88 Vapes	Blue	MDMB-4en-PINACA	0.4

38	RF	Elfbar	Yellow	NDD	-
39	RF	Caliburn	Clear	NDD	-
40	LB	IVG salt, Cherry bubblegum breeze	Clear	NDD	-
41	UB	-	Clear	NDD	-
42	LB	Bar juice, watermelon	Yellow	NDD	-
43	LB	Elux	Yellow	NDD	-
44	RF	Vaporesso	Yellow	NDD	-
45	RF	RPM	Brown	MDMB-4en-PINACA MDMB-INACA	'low'
46	SU	Elux legend pro	Brown	NDD	-
47	SU	Elux legend pro	Brown	NDD	-
48	SU	Elux legend pro	Brown	NDD	-
49	SU	Elux legend pro	Brown	NDD	-
50	SU	Randm tornado	Brown	NDD	-
51	SU	Randm tornado	Yellow	NDD	-
52	SU	Randm tornado	Yellow	NDD	-
53	SU	Ene legend	Yellow	NDD	-
54	SU	Hyati pro ultra	Yellow	NDD	-
55	SU	Ene legend	Yellow	NDD	-
56	SU	Elfbar	Yellow	NDD	-
57	SU	Elfbar	Brown	NDD	-
58	SU	Elfbar	Brown	NDD	-
59	SU	Elfbar	Brown	NDD	-
60	SU	Elfbar	Yellow	NDD	-
61	SU	-	Brown	NDD	-
62	SU	Hyati	Yellow	NDD	-
63	SU	Hyati pro ultra	Yellow	NDD	-
64	SU	Lost Mary	Yellow	NDD	-
65	SU	Lost MArY	Brown	NDD	-
R2S3	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
66	UB	-	Yellow	NDD	-
67	UB	-	Red	MDMB-4en-PINACA MDMB-INACA	0.54
68	UB	-	Clear	MDMB-4en-PINACA	IM
69	UB	-	Yellow opaque	NDD	-
70	UB	-	Yellow	MDMB-BUTINACA MDMB-4en-PINACA MDMB-PINACA	1.12
71	UB	-	Yellow	MDMB-BUTINACA MDMB-INACA	0.97
72	UB	-	Clear	MDMB-4en-PINACA MDMB-INACA	0.38
73	UB	-	Clear	MDMB-4en-PINACA	IM
74	UB	-	Clear	MDMB-4en-PINACA	IM
75	RF	88 Vapes	-	NT	-
76	RF	88 Vapes	Yellow	MDMB-4en-PINACA	'low'
77	SU			NT	-

78	RF	Vaporesso	Yellow	MDMB-4en-PINACA ADB-4en-PINACA MDMB-INACA	1.26
79	SU	WGA pro	-	NT	-
80	LB	-	Clear	NDD	-
81	LB	-	Yellow	NDD	-
82	LB	-	Yellow	NDD	-
83	LB	-	Yellow	NDD	-
84	LB	-	Yellow	NDD	-
85	LB	-	Yellow	NDD	-
86	LB	-	Yellow	NDD	-
87	RF	Vaporesso	Yellow	NDD	-
88	RF	Solus	Clear	MDMB-4en-PINACA	IM
89	RF	KRT	-	NDD	-
90	RF	Caliburn	Clear	NDD	-
91	RF	OXVA	Brown	MDMB-4en-PINACA MDMB-BUTINACA MDMB-INACA	0.27
92	RF	Vaporesso	Brown	MDMB-4en-PINACA	'low'
93	RF	Just	-	NDD	-
94	RF	-	Brown	NDD	-
95	SU	Hyati pro	Yellow	NDD	-
96	SU	Hyati pro	Yellow	NDD	-
97	SU	Hyati pro	Yellow	NDD	-
98	SU	Hyati pro	Yellow	NDD	-
99	SU	Hyati pro	Yellow	NDD	-
100	SU	Hyati pro	Yellow	NDD	-
101	SU	Hyati pro	Yellow	NDD	-
102	SU	Hyati pro	Brown	NDD	-
103	SU	Hyati pro	Yellow	NDD	-
104	SU	Hyati pro	Yellow	NDD	-
105	SU	Hyati pro	Yellow	NDD	-
106	SU	Hyati pro	Yellow	NDD	-
107	SU	Hyati pro	Yellow	NDD	-
108	SU	Hyati pro	Yellow	NDD	-
109	SU	Hyati pro	Yellow	NDD	-
110	SU	Hyati pro	Yellow	NDD	-
111	SU	Hyati pro	Yellow	NDD	-
112	SU	Hyati pro	Yellow	NDD	-
113	SU	Hyati pro	Brown	NDD	-
114	SU	Hyati pro	Yellow	NDD	-
115	SU	Crystal pro	-	NT	-
116	SU	Crystal pro	Yellow	NDD	-
117	SU	Crystal pro	-	NT	-
118	SU	WGA	Brown	NDD	-
119	SU	Hyati pro ultra	Clear	NDD	-
120	SU	Crystal bar	-	NT	-

121	SU	Crystal bar	-	NT	-
122	SU	Crystal bar	Clear	NDD	-
123	SU	Crystal bar	Yellow	NDD	-
124	SU	Crystal bar	-	NT	-
125	SU	Elux legend	Yellow	NDD	-
126	SU	Elux legend	Brown	NDD	-
127	SU	Elux legend	Yellow	NDD	-
128	SU	Elux legend	Yellow	NDD	-
129	SU	Elux legend	Yellow	NDD	-
130	SU	Elux legend	Brown	NDD	-
131	SU	Elux legend	Yellow	NDD	-
132	SU	Elux legend	Brown	NDD	-
133	SU	Ene Legend	Yellow	NDD	-
134	SU	Ene Legend	Yellow	NDD	-
135	SU	Randm Tornado	Yellow	NDD	-
136	SU	Randm Tornado	Yellow	NDD	-
137	SU	Randm Tornado	Yellow	NDD	-
138	SU	Randm Tornado	Yellow	NDD	-
139	SU	Randm Tornado	Yellow	NDD	-
140	SU	Randm Tornado	Brown	NDD	-
141	SU	Randm Tornado	Brown	NDD	-
142	SU	Randm Tornado	Brown	NDD	-
143	SU	Ene Legend	Yellow	NDD	-
144	SU	Elux legend	Yellow	NDD	-
145	SU	Elux legend	Yellow	NDD	-
146	SU	Crystal bar	Yellow	NDD	-
147	SU	Crystal bar	-	NT	-
148	SU	Crystal bar	Yellow	NDD	-
149	SU	Crystal bar	Yellow	NDD	-
150	SU	Elfbar	Yellow	NDD	-
151	SU	Elfbar	Yellow	NDD	-
152	SU	Elfbar	Clear	NDD	-
153	SU	Elfbar	Yellow	NDD	-
154	SU	Elfbar	Yellow	NDD	-
155	SU	Elfbar	Brown	NDD	-
156	SU	Elfbar	Yellow	NT	-
157	SU	Elfbar	Yellow	NDD	-
158	SU	Elfbar	Yellow	NDD	-
159	SU	Veev	Clear	NDD	-
160	SU	Lost mary	Yellow	NT	-
161	SU	-	Yellow	NDD	-
162	SU	-	Yellow	NDD	-
163	SU	Geek	Yellow	NDD	-
164	SU	-	Yellow	NDD	-
R2S4	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
165	UB	-	Yellow	MDMB-4en-PINACA	IM
166	RF	Vaporesso	Yellow	MDMB-4en-PINACA	IM

167	-	-	Yellow	NDD	-
R2S5	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
168	RF	Bear+ Aspire	Yellow	NDD	-
169	LB	-	Yellow	NDD	-
170	RF	Smok Fortis	-	NDD	-
171	RF	OXVA	Brown	NDD	-
172	RF	Tri Box	Yellow	MDMB-4en-PINACA	IM
173	SU	Hyati pro ultra	Yellow	NDD	-
174	SU	Hyati pro	Yellow	NDD	-
175	SU	Hyati pro	Yellow	NDD	-
176	SU	Randm Tornado	Yellow	NDD	-
177	SU	Randm Tornado	Yellow	NDD	-
178	SU	Hyati pro	Yellow	NDD	-
179	SU	-	Yellow	NDD	-
180	SU	-	Yellow	NDD	-
181	SU	Hyati pro ultra	Yellow	NDD	-
182	SU	-	Yellow	NDD	-
183	SU	Elux legend pro	Yellow	NDD	-
184	SU	Crystal bar	Yellow	NDD	-
185	SU	Elux legend pro	Brown	NDD	-
186	SU	Crystal bar	Yellow	NDD	-
187	SU	Crystal bar	Yellow	NDD	-
188	SU	Crystal bar	Yellow	NDD	-
189	SU	Crystal bar	-	NT	-
190	SU	Crystal bar	Yellow	NDD	-
191	SU	Crystal bar	Yellow	NDD	-
192	SU			NT	-
R2S6	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
193	UB	-	Pink	MDMB-4en-PINACA MDMB-PINACA	2.45
194	RF	Gotek cart	Pink	MDMB-4en-PINACA MDMB-PINACA	2.08
195	RF	Gotek cart	Green	MDMB-4en-PINACA MDMB-PINACA	1.04
196	SU	Hyati pro	Yellow	NDD	-
197	SU	Hyati pro	Yellow	NDD	-
198	SU	Elux legend	Brown	NDD	-
R2S7	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
199	LB	Elux Banana ice	Yellow	NDD	-
200	LB	Elux, gummy bear	Yellow	NDD	-
201	LB	Elux, gummy bear	Yellow	NDD	-
202	SU	Randm Tornado	Yellow	NDD	-
203	SU	Hyati duo mesh	Yellow	NDD	-
204	SU	-	Yellow	NDD	-
205	SU	Lost Mary	Yellow	NDD	-
R2S8	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
206	RF	Vapresso	Yellow	NDD	-

207	SU	Randm Tornado	Yellow	NDD	-
208	SU	Randm Tornado	Clear	NDD	-
209	SU	Randm Tornado	Yellow	NDD	-
210	SU	Hyati pro ultra	Yellow	NDD	-
211	SU	Hyati pro ultra	Yellow	NDD	-
212	SU	Crystal bar	Yellow	NDD	-
213	SU	Crystal bar	Yellow	NDD	-
214	SU	Crystal bar	Yellow	NDD	-
215	SU	Hyati pro max	Yellow	NDD	-
216	SU	Crystal bar	Yellow	NDD	-
217	SU	88 vapes	Yellow	NDD	-
218	SU	-	Yellow	NDD	-
R2S9	Sample type	Detail	Liquid colour	LC-MS result	Quant (mg / mL)
219	RF	X-Priv	Yellow	MDMB-4en-PINACA	IM
220	UB	-	Yellow opaque	MDMB-4en-PINACA MDMB-INACA	0.82
221	RF	-	Brown	MDMB-4en-PINACA MDMB-INACA	0.55
222	LB	Heizen blue	Yellow	NDD	-
223	LB	EPIQ	Yellow	NDD	-
224	LB	Sense by vapearts	Clear	NDD	-
225	LB	Sense by vapearts	Clear	NDD	-
226	LB	Vape district, Pineapple mango	Clear	NDD	-
227	RF	Smok	Clear	NDD	-
228	SU	Randm Tornado	Clear	NDD	-
229	RF	-	Brown	4F-MDMB-BINACA	IM
230	RF	-	Green	MDMB-4en-PINACA 4F-MDMB-BINACA	IM
231	RF	-	Brown	NDD	-
232	SU	Hyati pro	Yellow	NDD	-
233	SU	Hyati pro	Yellow	NDD	-
234	SU	Hyati pro	Yellow	NDD	-
235	SU	Hyati pro	Yellow	NDD	-
236	SU	Hyati pro	Yellow	NDD	-
237	SU	Hyati pro	Yellow	NDD	-
238	SU	Hyati pro	Yellow	NDD	-
239	SU	Hyati pro	Yellow	NDD	-
240	SU	Hyati pro	Yellow	NDD	-
241	SU	Hyati pro	Yellow	NDD	-
242	SU	Hyati pro	Yellow	NDD	-
243	SU	Hyati pro	Yellow	NDD	-
244	SU	Hyati pro	Yellow	NDD	-
245	SU	Hyati pro	Yellow	NDD	-
246	SU	Hyati pro	Yellow	NDD	-
247	SU	Ene Legend	Brown	NDD	-
248	SU	Ene Legend	Yellow	NDD	-
249	SU	Elux Legend	Brown	NDD	-

250	SU	Elux Legend	Brown	NDD	-
251	SU	Elux Legend	Brown	NDD	-
252	SU	Crystal bar	Yellow	NDD	-
253	SU	Crystal bar	-	NT	-
254	SU	Crystal prime	Yellow	NDD	-
255	SU	Randm Tornado	-	NT	-
256	SU	Randm Tornado	Brown	MDMB-4en-PINACA	0.05
257	SU	Elfbar	Brown	NDD	-
258	SU	Elfbar	Yellow	NDD	-
259	SU	Elfbar	Brown	NDD	-
260	SU	Elfbar	Brown	NDD	-
261	SU	Elfbar	Brown	NDD	-
262	SU	Crystal bar	Yellow	NDD	-
263	SU	Crystal bar	Yellow	NDD	-
264	SU	Crystal bar	Yellow	NDD	-
265	SU	-	-	NT	-
266	SU	-	Brown	NDD	-
267	SU	Crystal pro	Brown	NDD	-
268	SU	WGA	Yellow	NDD	-
269	SU	WGA	-	NT	-
270	SU	Hyati pro ultra	Yellow	NDD	-
271	SU	Lost mary	Green	NDD	-
272	SU	Lost mary	Yellow	NDD	-

NDD, no drug detected; 'low', concentration below level of NMR measurement; IM, insufficient material; NT, not tested; SU, single use; RF, refillable; UB, unlabelled bottle; LB, labelled bottle.

Table S3. Results summary for all samples in R3

R3S1	Sample type	Detail	Liquid colour	Presumptive result
1	SU	Boutiq, French Toast	Yellow resin	THC
2	SU	CCELL	Yellow resin	THC
3	SU	Bubbglegum Runtz	Yellow resin	THC
4	RF	Argus	Yellow	SC
5	SU	Crystal bar	-	NDD
6	RF	Gotek	-	NDD
7	RF	Sonder	-	NDD
8	RF	Vapresso	-	NDD
9	RF	Vapresso	-	NDD
10	RF	Vapresso	-	NDD
11	SU	Crystal prime	-	NDD
12	SU	Crystal prime	-	NDD
13	SU	Hyati pro, blue razz cherry	-	NDD
14	LB	Hyati, berry lemonade	-	NDD
15	LB	Hyati, strawberry watermelon	-	NDD
R3S2	Sample type	Detail	Liquid colour	Presumptive result
16	RF	Vapresso	Yellow	SC
17	RF	Vapresso	Blue	SC
18	UB	-	Blue	SC
19	UB	-	Blue	SC
20	UB	-	Blue	SC
21	RF	Gotek	-	NDD
22	SU	Elfbar	-	NDD
23	RF	Sonder	-	NDD
24	RF	Vapresso	-	NDD
25	RF	Vapresso	-	NDD
26	LB	Hit Liquid	-	NDD
27	LB	Elux, berry lemonade	-	NDD
28	LB	Elux, gummy bear	-	NDD
29	SU	Hyati, Cherry cola	-	NDD
30	SU	Hyati, blue soure raspberry	-	NDD
31	SU	Hyati, triple mango	-	NDD
32	SU	Lux pro, Mr blue	-	NDD
33	SU	Hyati, strawberry raspberry ice	-	NDD
34	SU	Hyati	-	NDD
35	SU	Crystal prime	-	NDD
36	SU	Crystal prime	-	NDD
37	SU	Hyati ultra, blue razz gummy bear	-	NDD
38	SU	Hyati duo, rainbow sherbert	-	NDD
39	SU	Crystal, juicy peach	-	NDD
40	SU	Crystal pro plus	-	NDD
41	SU	Hyati, mad blue	-	NDD
R3S3	Sample type	Detail	Liquid colour	Presumptive result
42	UB	-	Clear	SC

43	UB	-	Clear	SC
44	UB	-	Pink	SC
45	UB	-	Yellow	SC
46	UB	-	Yellow	SC
47	UB	-	Yellow	SC
48	LB	Elux, gummy bear	-	NDD
R3S4	Sample type	Detail	Liquid colour	Presumptive result
49	RF	Gotek	Green	SC
R3S5	Sample type	Detail	Liquid colour	Presumptive result
50	RF	Backpackboyz	Yellow resin	THC
51	RF	CCELL	Yellow	THC
52	RF	Gotek	Green	SC
53	SU	Elfbar	-	NDD
54	RF	Vaporesso	-	NDD
55	LB	Gost red	-	NDD
56	LB	Elux, Gummey bear	-	NDD
57	LB	Bar juice, blueberry soure raspberry	-	NDD
58	LB	Pod salt nexus	-	NDD
59	RF	Vaporesso	-	NDD
60	RF	Vaporesso	-	NDD
61	RF	Gotek	-	NDD
62	RF	Gotek	-	NDD
63	RF	Powtop	-	NDD
64	RF	Vaporesso	-	NDD
65	RF	Vaporesso	-	NDD
66	RF	Gotek	-	NDD
67	RF	Gotek	-	NDD
68	RF	Gotek	-	NDD
69	RF	Gotek	-	NDD
70	SU	Randm Tornado	-	NDD
71	SU	Randm Tornado	-	NDD
72	SU	Randm Tornado	-	NDD
73	SU	Crystal bar	-	NDD
74	SU	Crystal bar	-	NDD
75	SU	Crystal bar	-	NDD
76	SU	Crystal bar	-	NDD
77	SU	Crystal prime	-	NDD
78	SU	Hyati pro, blue razz cherry	-	NDD
79	SU	Hyati pro, blue razz cherry	-	NDD
80	SU	Hyati pro ultra	-	NDD
81	SU	Hyati	-	NDD
82	SU	Hyati	-	NDD
83	SU	Hyati	-	NDD
84	SU	Elux	-	NDD

NDD, no drug detected; SC, synthetic cannabinoid; THC, tetrahydrocannabinol; SU, single use; RF, refillable; UB, unlabelled bottle; LB, labelled bottle.

Table S4. Data summary for R1, R2 and R3 for SC positives.

School	SC de- tected	Total sub- mission	Total sin- gle use	Total liquid/re- fillable	Total alarm	Alarm sin- gle use	Alarm liq- uid/refillable	[Average] (mg / mL)	Alarm rate total	Alarm rate single use	Alarm rate liq- uid/refillable
R1S1	Yes	9	0	9	5	0	5	0.55	0.56	0.00	0.56
R1S2	Yes	5	2	3	3	0	3	1.37	0.60	0.00	0.60
R1S3	No	1	1	0	0	0	0	0.00	0.00	0.00	0.00
R1S4	Yes	5	4	1	1	0	1	0.56	0.20	0.00	0.20
R1S5	No	3	3	0	0	0	0	0.00	0.00	0.00	0.00
R1S6	Yes	4	2	2	2	0	2	0.40	0.50	0.00	0.50
R1S7	Yes	26	23	3	3	0	3	2.04	0.12	0.00	0.12
R1S8	Yes	36	16	20	10	1	9	1.40	0.28	0.03	0.25
R1S9	Yes	6	1	5	4	0	4	1.16	0.67	0.00	0.67
R1S10	No	21	21	0	0	0	0	0.00	0.00	0.00	0.00
R1S11	Yes	1	0	1	1	0	1	1.50	1.00	0.00	1.00
R1S12	Yes	33	27	6	6	0	6	1.25	0.18	0.00	0.18
R1S13	No	6	6	0	0	0	0	0.00	0.00	0.00	0.00
		156	106	50	35	1	34	0.00	0.224	0.01	0.22
R2S1	Yes	31	24	7	12	6	6	0.88	0.39	0.19	0.19
R2S2	Yes	32	20	12	3	0	3	0.34	0.09	0.00	0.09
R2S3	Yes	99	71	28	13	0	13	0.76	0.13	0.00	0.13
R2S4	Yes	3	0	3	2	0	2	0	0.67	0.00	0.67
R2S5	Yes	25	20	5	1	0	1	0	0.04	0.00	0.04
R2S6	Yes	6	3	3	3	0	3	1.86	0.50	0.00	0.50
R2S7	No	7	4	3	0	0	0	0	0.00	0.00	0.00
R2S8	No	13	12	1	0	0	0	0	0.00	0.00	0.00
R2S9	Yes	54	42	12	6	1	5	0.47	0.11	0.02	0.09
		270	196	74	40	7	33	0	0.148	0.03	0.12

School	SC de- tected	Total sub- mission	Total sin- gle use	Total liquid/re- fillable	Total alarm	Alarm sin- gle use	Alarm liq- uid/refillable	[Average] (mg / mL)	Alarm rate total	Alarm rate single use	Alarm rate liquid/re- fillable
R3S1	Yes	15	7	8	1	0	1	NA	0.07	0.00	0.07
R3S2	Yes	26	14	12	5	0	5	NA	0.19	0.00	0.19
R3S3	Yes	7	0	7	6	0	6	NA	0.86	0.00	0.86
R3S4	Yes	1	0	1	1	0	1	NA	1.00	0.00	1.00
R3S5	Yes	35	16	19	1	0	1	NA	0.03	0.00	0.03
		84	37	47	14	0	14	NA	0.167	0.00	0.167
	0.75	510	339	171	89	8	81	1.03	0.1745	0.0157	0.159

Table S5. Results summary for all samples in R4.

R4S7	Sample type	Detail	Liquid colour	GC-MS result
1	SU	crystal prime	-	NDD
2	SU	Jeeter	-	THC
3	RF	ox	-	4F-MDMB-BINACA
4	SU	novo	-	4F-MDMB-BINACA
5	SU	non refillable firerose	-	NDD
6	RF	red oxva	-	4F-MDMB-BINACA
7	RF	blue oxva	-	4F-MDMB-BINACA
8	SU	happy vibes	-	NDD
9	SU	green crystal prime	-	NDD
10	LB	elux vape refill blueberry	-	NDD
11	LB	jucce candy black jack	-	NDD
12	UB	unknown -in small vial no ID	Clear	MDMB-4en-PINACA
13	LB	pukka juice lime lemonade	-	NDD
14	LB	soda king lemon lime	-	NDD
15	LB	crystal clear blueberry sour raspberry	-	NDD
16	RF	-	-	MDMB-4en-PINACA
17	RF	OXVA gold/green with refill top	-	NDD
18	LB	elux vape refill strawberry ice cream	-	NDD
19	LB	elux vape refill kiwi passion fruit	-	NDD
20	LB	elux vape refill cherry cola	-	NDD
21	RF	unknown	-	NDD
22	RF	black and gold	-	MDMB-4en-PINACA
23	SU	pale green KLAK	-	NDD
24	RF	lime green and green OXVA	-	NDD
25	LB	elux tiger blood	-	NDD
26	RF	blue and black OXVA	-	NDD
27	LB	elflio - cherry	-	NDD
28	RF	silver oxva	-	MDMB-4en-PINACA
29	SU	-	-	NDD
30	RF	-	-	MDMB-4en-PINACA
31	RF	-	-	NDD
32	RF	-	-	NDD
33	RF	-	-	MDMB-4en-PINACA
34	UB	-	Pink	MDMB-4en-PINACA
35	RF	-	-	MDMB-4en-PINACA
36	RF	-	-	NDD
37	RF	-	-	MDMB-4en-PINACA
38	RF	-	-	NDD
39	RF	-	-	MDMB-4en-PINACA
40	RF	-	-	MDMB-4en-PINACA
41	LB	mango	-	NDD
42	LB	watermelon	-	NDD
43	LB	blueberry	-	NDD
44	UB	-	green	MDMB-4en-PINACA

45	SU	yellow with white top	-	THC
46	SU	crystal fire blue and yellow	-	NDD
47	LB	lemon and lime nearly full	-	NDD
48	LB	lemon and lime nearly empty	-	NDD
49	SU	lost mary red/yellow	-	NDD
50	SU	Hayati pro max	-	NDD

NDD, no drug detected; THC, tetrahydrocannabinol; SU, single use; RF, refillable; UB, unlabelled bottle; LB, labelled bottle.

Table S6. LC-MS parent molecule and fragment ion mass to charge (m/z) ratios used to confirm compounds found in the e-cigarettes/liquids.

Compound	Parent	F1	F2	F3	F4	F5	F6
MDMB-4en-PINACA	358.2125	213.1022	298.1914	145.0396	86.0964	171.089	163.0502
ADB-BUTINACA	331.2128	201.1022	286.1914	314.1863	163.0502	145.0396	219.1128
4F-MDMB-BINACA	364.2031	219.0928	304.1819	145.0396	237.1034	237.1022	236.1193
MDMB-PINACA	360.2281	215.1179	145.0396	300.207			
ADB-4en-PINACA	343.2128	213.1022	298.1914	326.1863	365.1948		
MDMB-INACA	290.1499	145.0396	230.1288	86.0964			
Δ^9 -THC	315.2131	193.1223	123.0441	259.1693	235.1693	233.1536	221.1536

R1S1.2

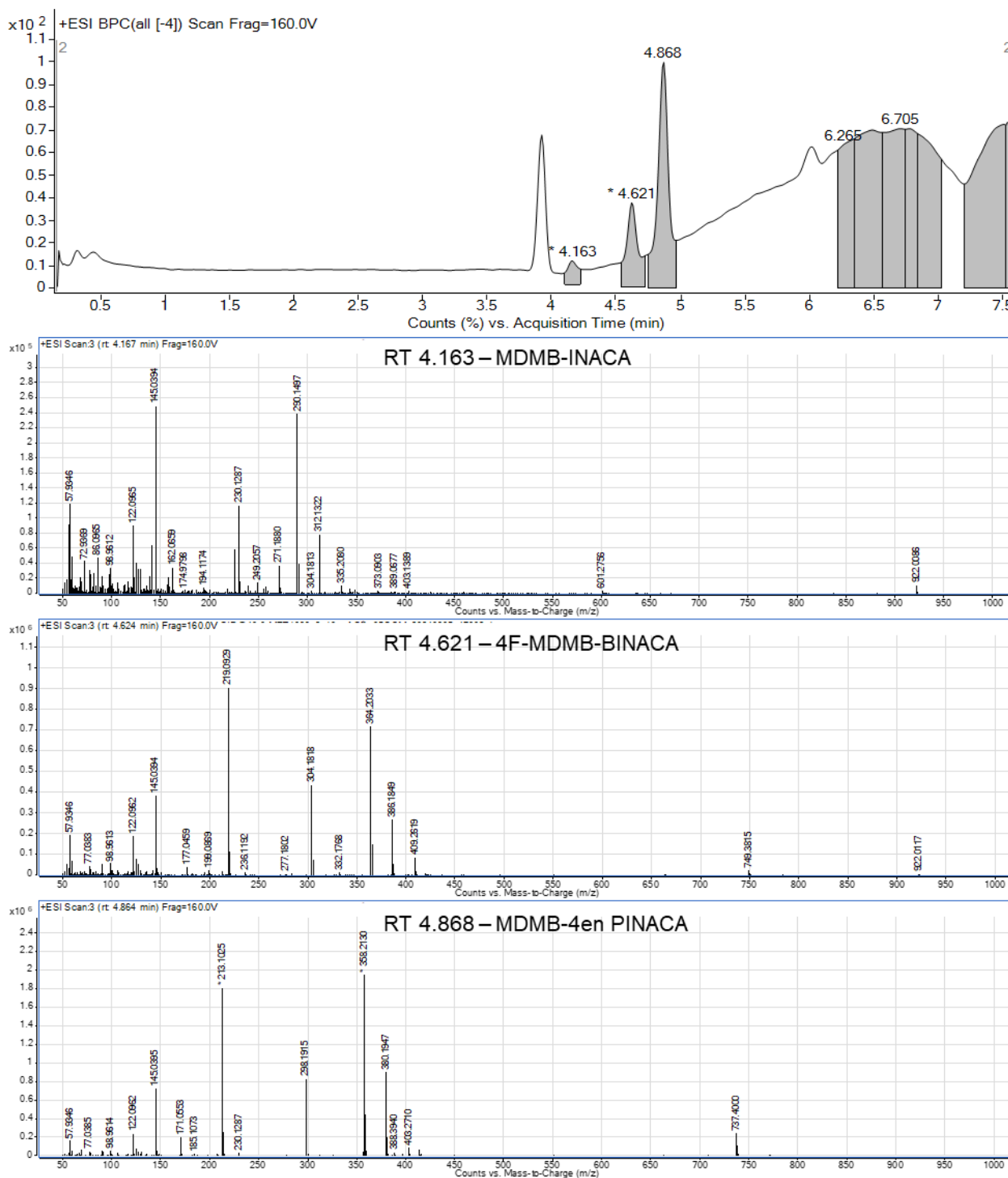


Figure S1. Example LC-MS chromatogram and spectra for sample R1S1.2 with MDMB-4en-PINACA, 4F-MDMB-BINACA and MDMB-INACA SCs identified. Molecular weights of compounds: MDMB-INACA – 289.330 g mol⁻¹, 4F-MDMB-BINACA – 363.433 g mol⁻¹, MDMB-4en-PINACA - 357.454 g mol⁻¹.

R1S12.119

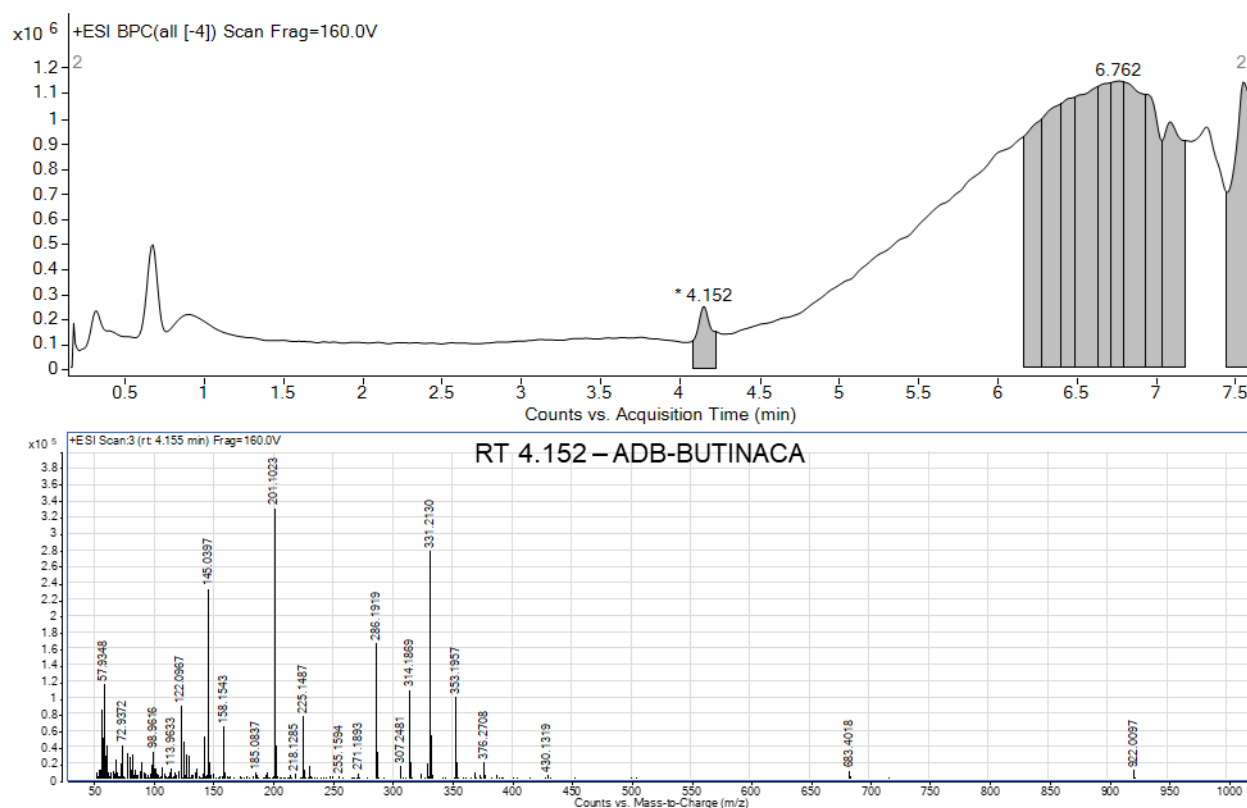


Figure S2. Example LC-MS chromatogram and spectra for sample R1S12.119 with ADB-BUTINACA identified. Molecular weight of ADB-BUTINACA is 330.432 g mol⁻¹.

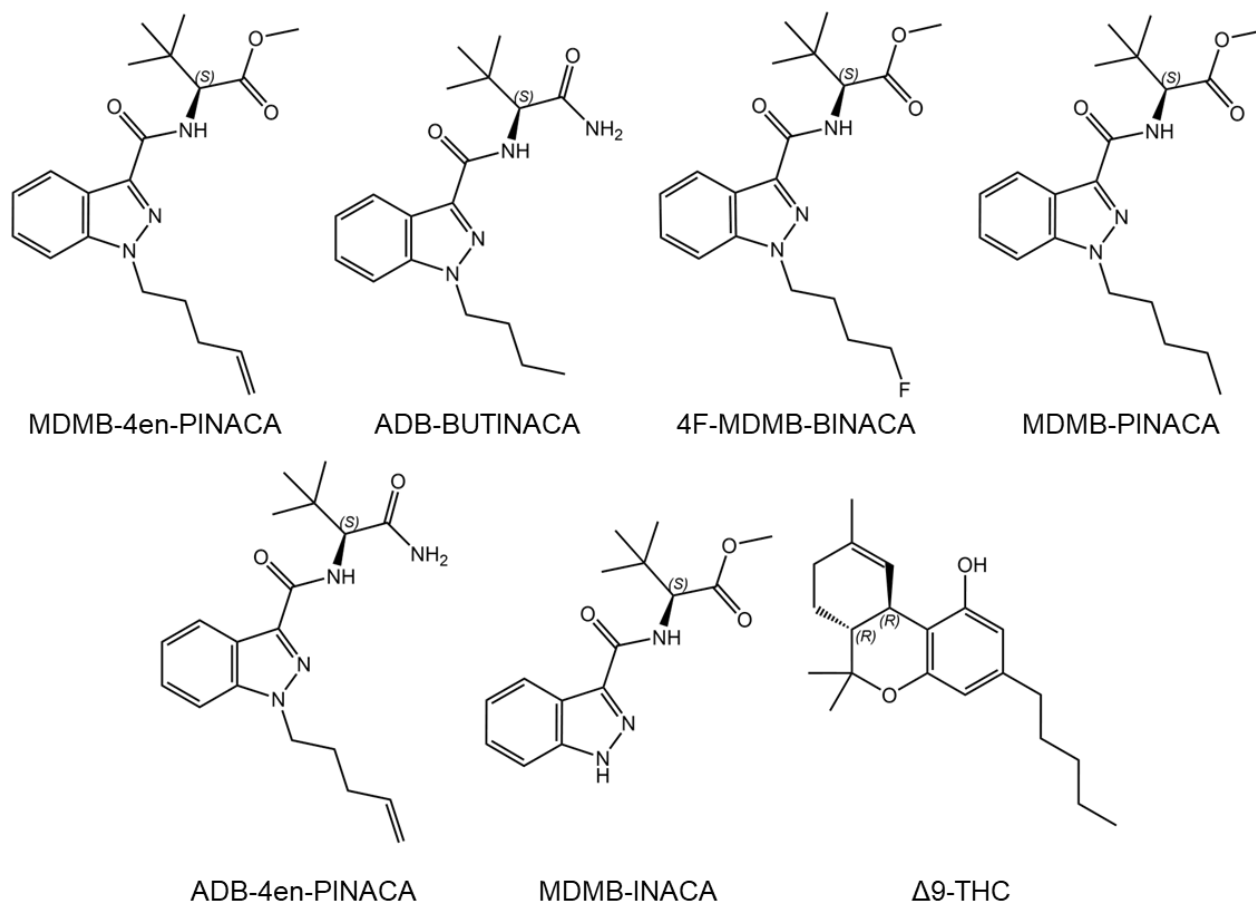


Figure S3. Structures of illicit drugs identified.

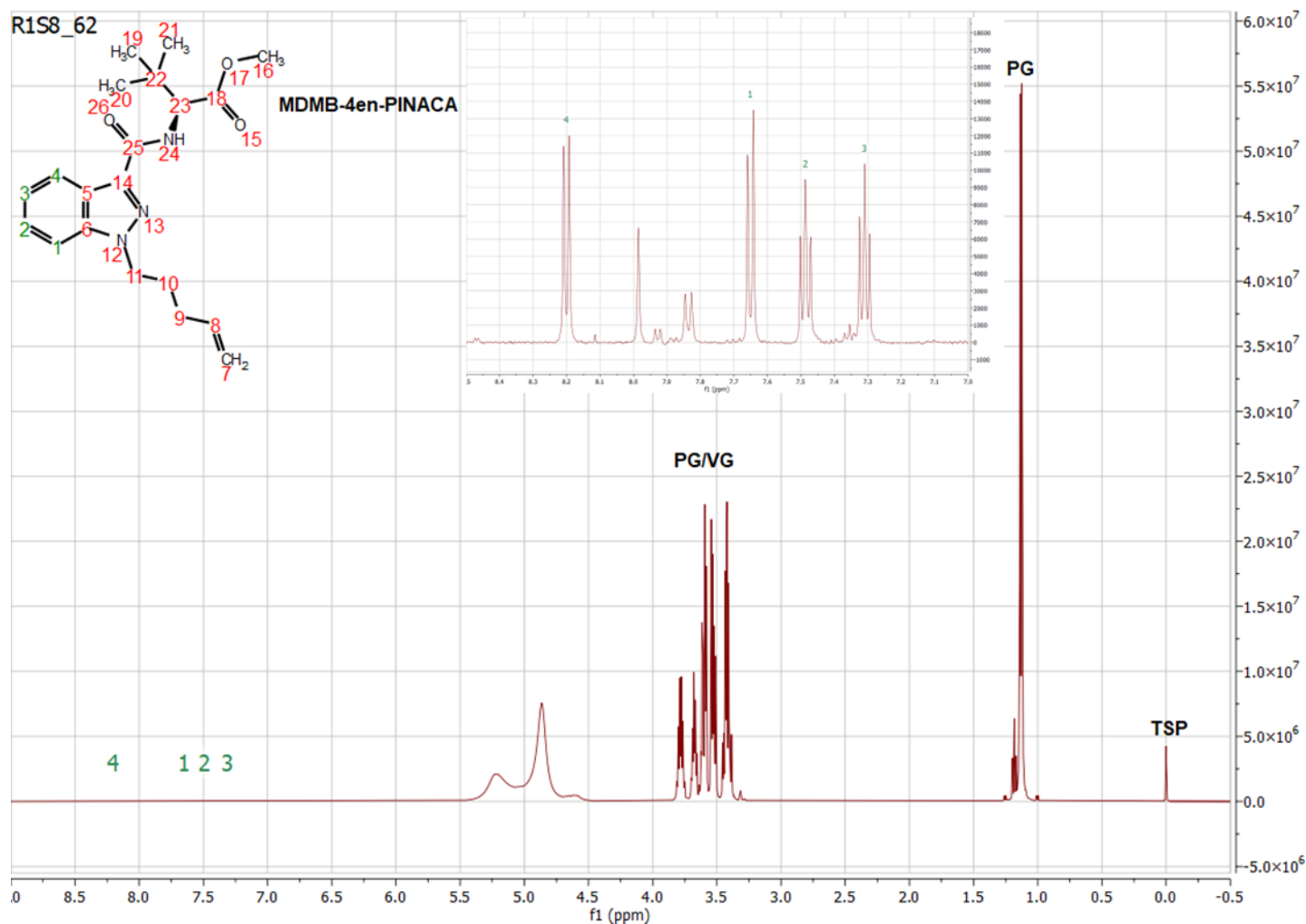


Figure S4. Example ¹H NMR spectra used for qNMR on sample R1S8.62 containing MDMB-4en-PINACA. Main spectra shows the sample is dominated by polyethylene glycol (PG) and vegetable glycerin (VG) that form the basis of e-cigarette liquid. Insert is of the 8.5 – 7.0 ppm region which shows the aromatic indazole peaks for hydrogens 1-4 used for the quantification. The internal standard 3-(trimethylsilyl)propionic-2,2,3,3-d₄ acid sodium salt (TSP) is shown at 0.0 ppm (3 mg added). The qNMR method used a 20 s delay, 128 scans and processing techniques (as described in materials and methods) such that ratio of the integration of the sample to TSP peaks can be used to calculate the concentration of the sample, 3.53 mg/mL in this case.

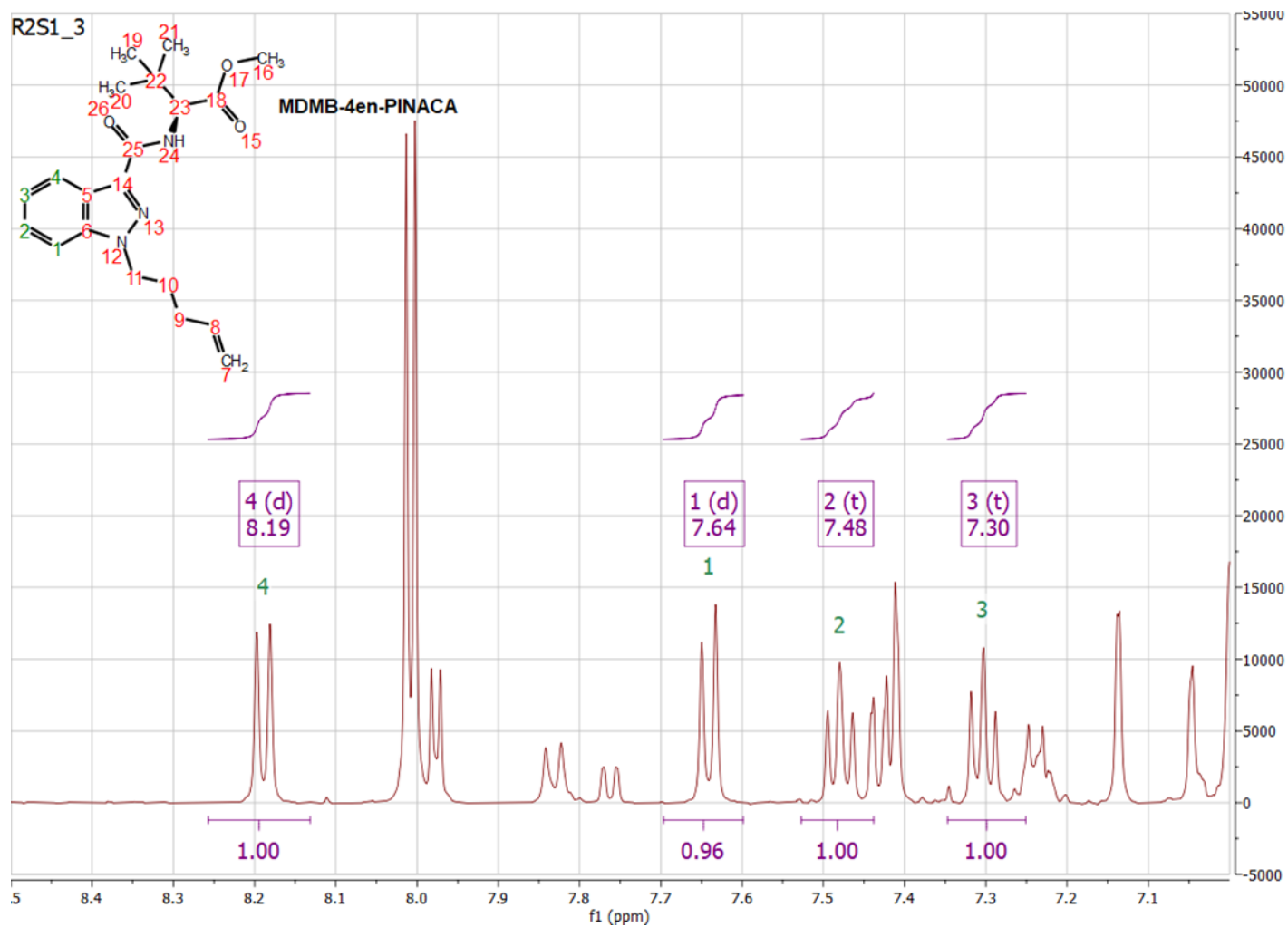


Figure S5. Example ^1H NMR spectra used for qNMR on sample R2S1.3 containing MDMB-4en-PINACA. The aromatic indazole 8.5 – 7.0 ppm region is shown with the multiplets and integration of hydrogens 1-4 used for the quantification.

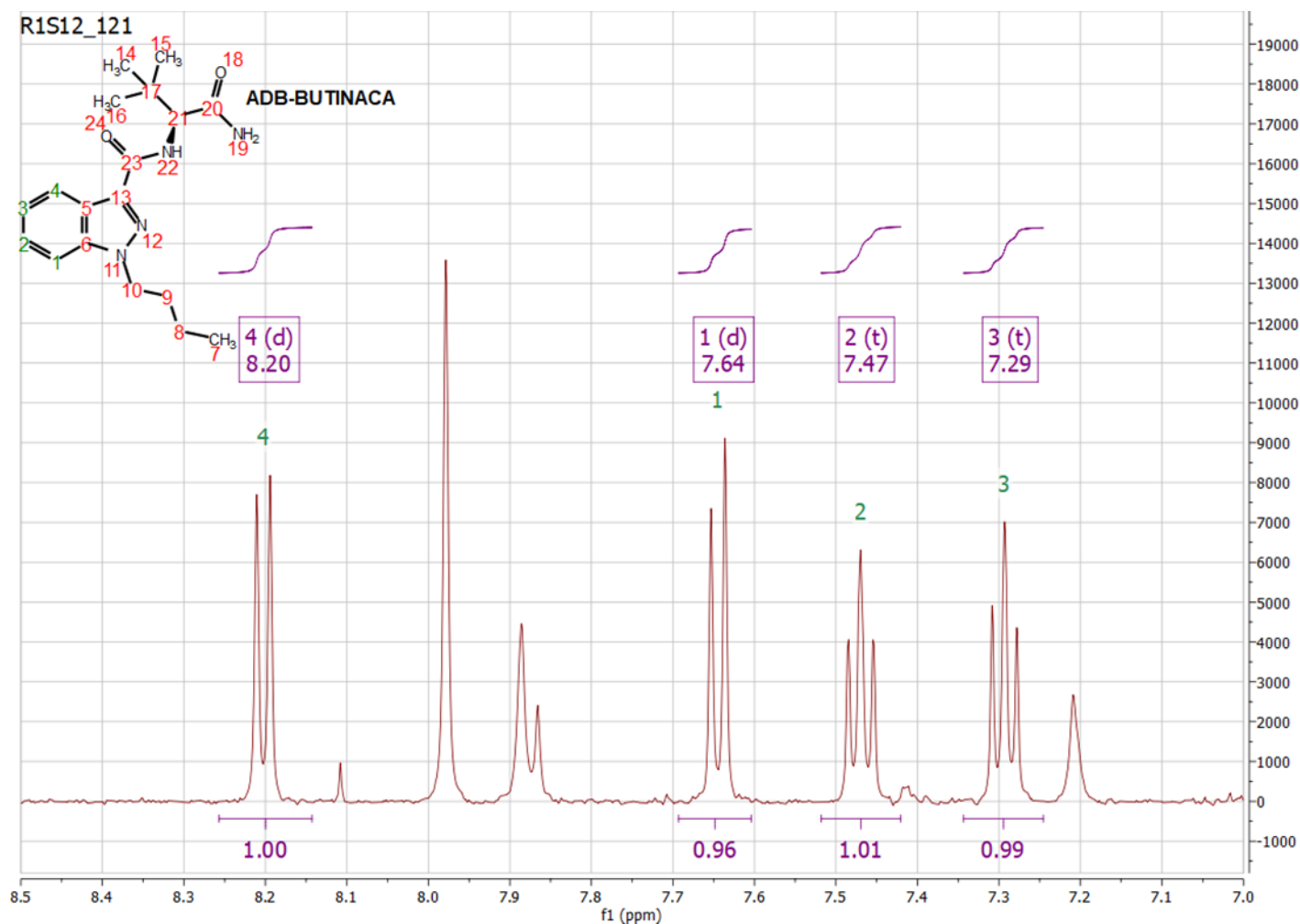


Figure S6. Example ^1H NMR spectra used for qNMR on sample R1S12.121 containing ADB-BUTINACA. The aromatic indazole 8.5 – 7.0 ppm region is shown with the multiplets and integration of hydrogens 1-4 used for the quantification.

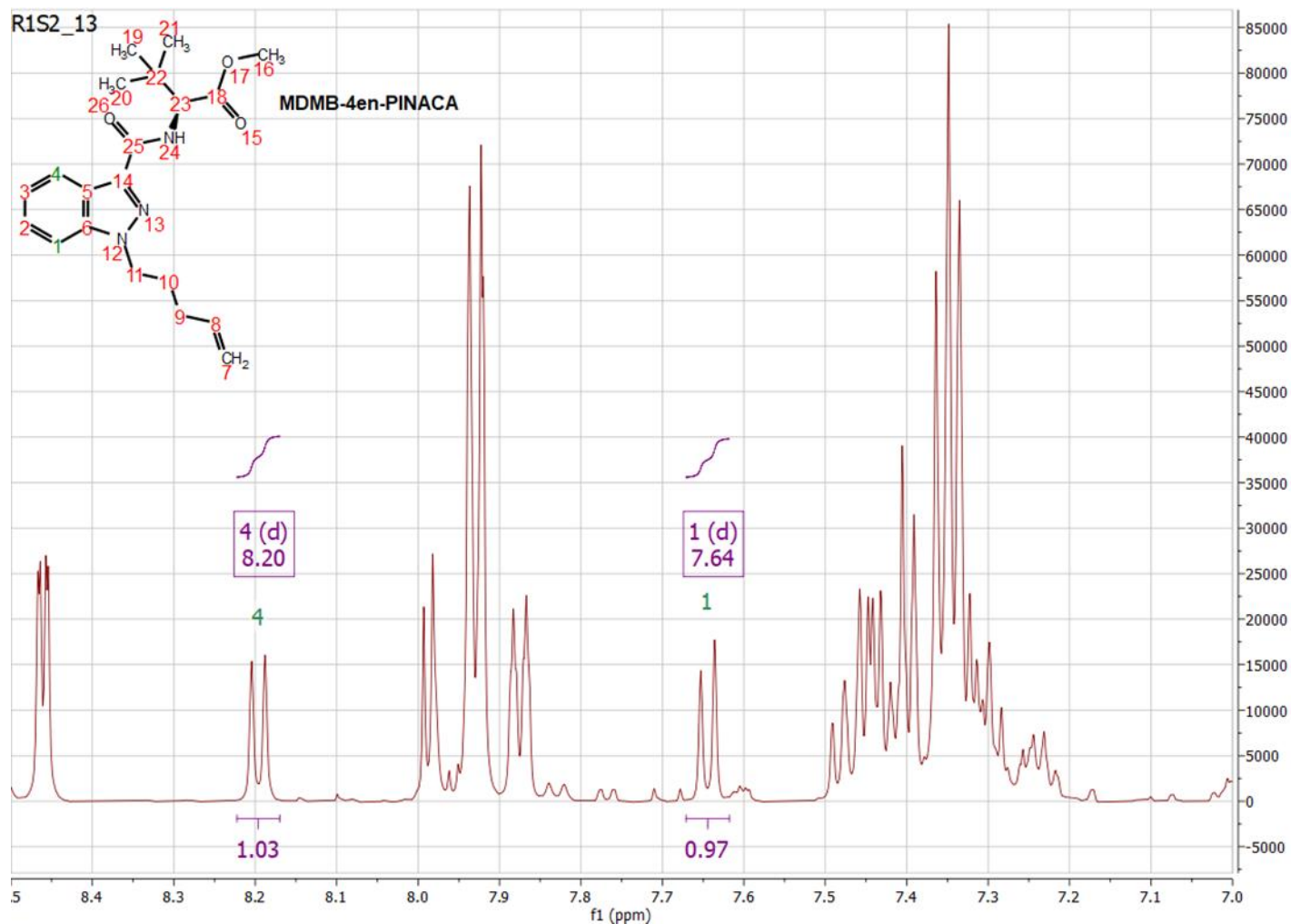


Figure S7. Example ^1H NMR spectra used for qNMR on sample R1S2.13 containing MDMB-4en-PINACA. The aromatic indazole 8.5 – 7.0 ppm region is shown highlighting that only the multiplets and integration of hydrogens 1 and 4 are able to be used for quantification due to additives in the e-cigarette liquid masking the other hydrogens.

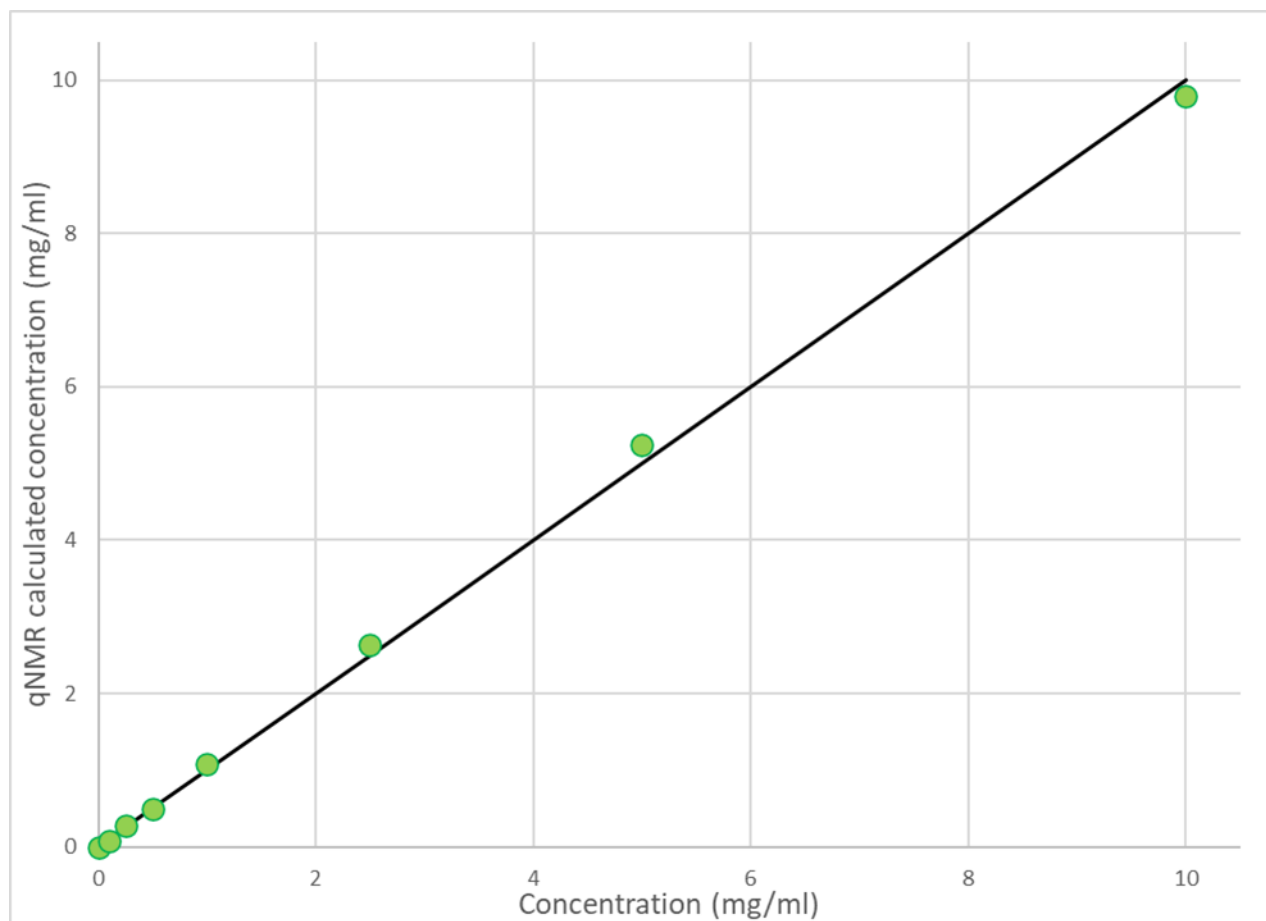


Figure S8. Plot showing the qNMR calculated values of a standard concentration range of MDMB-4en-PINACA in e-cigarette liquid. This shows good agreement with the true values (black line) highlighting the suitability of the qNMR technique for quantifying the e-cigarettes and liquids.



Figure S9. THC e-cigarettes from R3.

R4 SC e-cigarettes



R4 THC e-cigarettes



Figure S10. Positive samples (SC and THC) from R4.
