

# Comprehensive profiling of terpenes and terpenoids in different cannabis strains using GC×GC-TOFMS

Jasmeen Kaur <sup>1</sup>, Ning Sun <sup>2</sup> and Jane E. Hill <sup>1,2,\*</sup>

<sup>1</sup>Department of Chemical and Biological Engineering, University of British Columbia, 2360 E Mall, Vancouver, BC V6T 1Z3, Canada.

<sup>2</sup>School of Biomedical Engineering, University of British Columbia, 251 - 2222 Health Sciences Mall, Vancouver, BC V6T 1Z3, Canada.

\* Correspondence: jane.hill@ubc.ca; Tel.: +1 604-822-3238

**Table S1.** List of terpenes in the standard mixtures.

S. No. *	Standard mixture	Standard name	Chemical formula	Chemical class
1	Can-Terp Mix 2H	$\alpha$ -Pinene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
2	Can-Terp Mix 1H	Camphene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
3	Can-Terp Mix 2H	Sabinene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
4	Can-Terp Mix 1H	$\beta$ -Myrcene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
5	Can-Terp Mix 2H	$\beta$ -Pinene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
6	Can-Terp Mix 1H	$\alpha$ -Phellandrene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
7	Can-Terp Mix 1H	3-Carene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
8	Can-Terp Mix 2H	$\alpha$ -Terpinene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
9	Can-Terp Mix 2H	D-Limonene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
10	Can-Terp Mix 1H	Eucalyptol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
11	Can-Terp Mix 1H	Ocimene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
12	Can-Terp Mix 2H	$\gamma$ -Terpinene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
13	Can-Terp Mix 2H	Sabinene hydrate	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
14	Can-Terp Mix 2H	Terpinolene	C <sub>10</sub> H <sub>16</sub>	Monoterpene
15	Can-Terp Mix 1H	Linalool	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
16	Can-Terp Mix 1H	(+)-Fenchone	C <sub>10</sub> H <sub>16</sub> O	Monoterpenoid
17	Can-Terp Mix 2H	L-(-)-Fenchone	C <sub>10</sub> H <sub>16</sub> O	Monoterpenoid
18	Can-Terp Mix 2H	(1R)-Endo-(+)-Fenchyl alcohol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
19	Can-Terp Mix 2H	$\beta$ -Terpineol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
20	Can-Terp Mix 1H	Isopulegol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
21	Can-Terp Mix 1H	Camphor	C <sub>10</sub> H <sub>16</sub> O	Monoterpenoid
22	Can-Terp Mix 2H	(1S)-(-)-Camphor	C <sub>10</sub> H <sub>16</sub> O	Monoterpenoid
23	Can-Terp Mix 2H	(1R)-(+)-Camphor	C <sub>10</sub> H <sub>16</sub> O	Monoterpenoid
24	Can-Terp Mix 1H	Isoborneol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
25	Can-Terp Mix 2H	(+)-Borneol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
26	Can-Terp Mix 1H	Hexahydrothymol	C <sub>10</sub> H <sub>20</sub> O	Monoterpenoid
27	Can-Terp Mix 2H	(-)-Borneol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
28	Can-Terp Mix 2H	$\alpha$ -Terpineol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
29	Can-Terp Mix 1H	Nerol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid

30	Can-Terp Mix 2H	Geraniol	C <sub>10</sub> H <sub>18</sub> O	Monoterpenoid
31	Can-Terp Mix 2H	(+)-Pulegone	C <sub>10</sub> H <sub>16</sub> O	Monoterpenoid
32	Can-Terp Mix 1H	Geranyl acetate	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	Monoterpenoid
33	Can-Terp Mix 1H	Farnesene (isomer1)	C <sub>15</sub> H <sub>24</sub>	Sesquiterpene
34	Can-Terp Mix 2H	$\alpha$ -Cedrene	C <sub>15</sub> H <sub>24</sub>	Sesquiterpene
35	Can-Terp Mix 1H	<i>trans</i> -Caryophyllene	C <sub>15</sub> H <sub>24</sub>	Sesquiterpene
36	Can-Terp Mix 1H	Farnesene (isomer2)	C <sub>15</sub> H <sub>24</sub>	Sesquiterpene
37	Can-Terp Mix 2H	Humulene	C <sub>15</sub> H <sub>24</sub>	Sesquiterpene
38	Can-Terp Mix 1H	Valencene	C <sub>15</sub> H <sub>24</sub>	Sesquiterpene
39	Can-Terp Mix 1H	<i>cis</i> -Nerolidol	C <sub>15</sub> H <sub>26</sub> O	Sesquiterpenoid
40	Can-Terp Mix 2H	<i>trans</i> -Nerolidol	C <sub>15</sub> H <sub>26</sub> O	Sesquiterpenoid
41	Can-Terp Mix 1H	Caryophyllene oxide	C <sub>15</sub> H <sub>26</sub> O	Sesquiterpenoid
42	Can-Terp Mix 2H	Guaiol	C <sub>15</sub> H <sub>26</sub> O	Sesquiterpenoid
43	Can-Terp Mix 1H	Cedrol	C <sub>15</sub> H <sub>26</sub> O	Sesquiterpenoid
44	Can-Terp Mix 1H	$\alpha$ -Bisabolol	C <sub>15</sub> H <sub>26</sub> O	Sesquiterpenoid

\* The compounds are listed as they appear in the GC×GC-TOFMS chromatogram of the standard mixture in Figure 1a.

**Table S2.** List of contaminants removed during data analysis.

Contaminant name
Benzaldehyde
Benzaldehyde, 3-benzyloxy-2-fluoro-4-methoxy-
Benzene, 1,3-dimethyl-
Benzene, [3-(2-cyclohexylethyl)-6-cyclopentylhexyl]-
Benzyl oxy tridecanoic acid
Cyclohexane, 1,3-dimethyl-, cis-
Cyclohexane, ethyl-
Cyclohexane, 1,2,3-trimethyl-
Cyclohexane, 1,2,4-trimethyl-
Cyclopropane, 1-butyl-1-methyl-2-propyl-
Dodecane, 1-fluoro-
1-Dodecanol, 3,7,11-trimethyl-
Ethylbenzene
2-Methylthiolane, S,S-dioxide
Octane, 1,1'-oxybis-
1-Octanol, 2-butyl-
Pentalene, octahydro-, cis-
1-Tetradecanol
Toluene
2-Undecanethiol, 2-methyl-
p-Xylene
Sil