

Table S1. The peak volume of the flavor profile, as characterized by GC-IMS in ciba pepper samples with varying salt concentrations, was determined (mean  $\pm$  sd).

Count	Compound	CAS	Molecule	MW	RI	Rt(s)	Dt(ms)	LJA	LJB	LJC	LJD	LJE
			Formula									
Alcohol	2-furanmethanol	98-00-0	C <sub>5</sub> H <sub>6</sub> O <sub>2</sub>	98.1	894.7	244.055	1.3702	119.1 $\pm$ 15.54 <sup>c</sup>	361.6 $\pm$ 12.47 <sup>a</sup>	243.25 $\pm$ 32.05 <sup>b</sup>	185.44 $\pm$ 11.43 <sup>b</sup>	207.76 $\pm$ 32.39 <sup>b</sup>
	(Z)-2-Penten1ol	1576-95-0	C <sub>5</sub> H <sub>10</sub> O	86.1	772.6	176.859	1.42855	406.23 $\pm$ 19.35 <sup>a</sup>	378.28 $\pm$ 13.25 <sup>a</sup>	443.61 $\pm$ 22.63 <sup>a</sup>	436.04 $\pm$ 43.5 <sup>a</sup>	403.99 $\pm$ 34.47 <sup>a</sup>
	1-propanethiol	107-03-9	C <sub>3</sub> H <sub>8</sub> S	76.2	842.7	213.477	1.16314	139.63 $\pm$ 4.85 <sup>c</sup>	195.62 $\pm$ 2.69 <sup>a</sup>	144.36 $\pm$ 9.65 <sup>c</sup>	102.67 $\pm$ 9.86 <sup>d</sup>	170.57 $\pm$ 6.93 <sup>b</sup>
	propanol	71-23-8	C <sub>3</sub> H <sub>8</sub> O	60.1	1008.3	353.786	1.10306	1124.73 $\pm$ 19.78 <sup>b</sup>	1155.14 $\pm$ 15.68 <sup>b</sup>	1390.39 $\pm$ 25.4 <sup>a</sup>	1353.62 $\pm$ 24.75 <sup>a</sup>	1350.24 $\pm$ 9.42 <sup>a</sup>
	1-Decanol	112-30-1	C <sub>10</sub> H <sub>22</sub> O	158.3	1217.4	743.761	1.62597	2006.1 $\pm$ 72.03 <sup>b</sup>	1871.41 $\pm$ 52.21 <sup>bc</sup>	2520.1 $\pm$ 403.99 <sup>a</sup>	1608.3 $\pm$ 178.59 <sup>c</sup>	1774.37 $\pm$ 28.12 <sup>bc</sup>
	2,3-Butanediol	513-85-9	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	90.1	782.7	179.437	1.36415	117.33 $\pm$ 9.23 <sup>c</sup>	179.04 $\pm$ 0.67 <sup>bc</sup>	177.25 $\pm$ 33.52 <sup>bc</sup>	303.8 $\pm$ 29.91 <sup>a</sup>	245.12 $\pm$ 45.03 <sup>ab</sup>
	2-Butanol	78-92-2	C <sub>4</sub> H <sub>10</sub> O	74.1	635	128.589	1.15062	1261.85 $\pm$ 50.69 <sup>a</sup>	1151.36 $\pm$ 42.65 <sup>a</sup>	635.77 $\pm$ 42.79 <sup>b</sup>	548.76 $\pm$ 29.94 <sup>bc</sup>	441.85 $\pm$ 31.08 <sup>c</sup>
	pent-1-en-3-ol-M	616-25-1	C <sub>5</sub> H <sub>10</sub> O	86.1	684.3	153.057	0.94634	191.24 $\pm$ 3.62 <sup>d</sup>	245.47 $\pm$ 6.26 <sup>c</sup>	509.59 $\pm$ 15.98 <sup>a</sup>	540.03 $\pm$ 35.27 <sup>a</sup>	416.74 $\pm$ 25.99 <sup>b</sup>
	(E)-3-Hexen-1-ol	928-97-2	C <sub>6</sub> H <sub>12</sub> O	100.2	893.9	243.418	1.55739	72.35 $\pm$ 5.58 <sup>d</sup>	355.79 $\pm$ 10.55 <sup>ab</sup>	388.32 $\pm$ 71.43 <sup>a</sup>	195.72 $\pm$ 39.86 <sup>c</sup>	257.6 $\pm$ 47.84 <sup>bc</sup>
	1-Propanol, 2-methyl-	78-83-1	C <sub>4</sub> H <sub>10</sub> O	74.1	1078.7	485.171	1.17003	78.48 $\pm$ 11.62 <sup>b</sup>	99.08 $\pm$ 1.06 <sup>b</sup>	158.72 $\pm$ 11.45 <sup>a</sup>	144.69 $\pm$ 9.76 <sup>a</sup>	149.56 $\pm$ 5.8 <sup>a</sup>

Table S1. (continued).

Count	Compound	CAS	Molecule Formula	MW	RI	Rt (s)	Dt (ms)	LJA	LJB	LJC	LJD	LJE
	1,2-Propanediol	57-55-6	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	76.1	735.4	167.265	1.29365	60.34±1.7 <sup>b</sup>	125.53±8.37 <sup>a</sup>	47.71±2.18 <sup>b</sup>	53.65±7.04 <sup>b</sup>	44.45±8.3 <sup>b</sup>
	1-hexanol	111-27-3	C <sub>6</sub> H <sub>14</sub> O	102.2	853.1	219.466	1.32533	25.35±1.25 <sup>d</sup>	21.4±1.35 <sup>d</sup>	104.92±9.81 <sup>c</sup>	332.34±1.02 <sup>a</sup>	142.27±11.99 <sup>b</sup>
Alcohol	4-Methyl-1-pentanol	626-89-1	C <sub>6</sub> H <sub>14</sub> O	102.2	844.8	214.674	1.32443	4.11±2.15 <sup>d</sup>	15.09±1.92 <sup>c</sup>	44.49±7.23 <sup>c</sup>	165.74±20.21 <sup>a</sup>	79.64±8.89 <sup>b</sup>
	3-Methyl-1-pentanol	589-35-5	C <sub>6</sub> H <sub>14</sub> O	102.2	819.3	200.025	1.32424	143.79±7.43 <sup>d</sup>	95.62±6.02 <sup>c</sup>	659.73±73.38 <sup>c</sup>	2137.01±122.57 <sup>a</sup>	932.74±45.45 <sup>b</sup>
	pent-1-en-3-ol-D	616-25-1	C <sub>5</sub> H <sub>10</sub> O	86.1	685.8	153.849	1.33038	2140.34±51.88 <sup>a</sup>	1651±68.72 <sup>b</sup>	347.15±34.88 <sup>c</sup>	354.57±50.71 <sup>c</sup>	448.23±81.91 <sup>c</sup>
	(E)-2-hexenal	6728-26-3	C <sub>6</sub> H <sub>10</sub> O	98.1	1217.7	744.341	1.19728	6461.57±91.01 <sup>b</sup>	6352.18±86.78 <sup>b</sup>	7071.7±190.49 <sup>a</sup>	6017.15±294.41 <sup>c</sup>	6294.62±41.03 <sup>b</sup>
	2-hydroxybenzaldehyde	90-02-8	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	122.1	1047.8	427.59	1.1479	272.17±25.06 <sup>b</sup>	368.48±9.62 <sup>a</sup>	215.44±3.59 <sup>c</sup>	292.96±24.86 <sup>b</sup>	197.6±2.18 <sup>c</sup>
Aldehyde	3-methylbutanal	590-86-3	C <sub>5</sub> H <sub>10</sub> O	86.1	638.3	130.253	1.18838	2007.77±157.78 <sup>a</sup>	1600.86±20.61 <sup>b</sup>	934.56±53.83 <sup>d</sup>	1276±112.05 <sup>c</sup>	714.09±63.75 <sup>d</sup>
	2-methylbutanal	96-17-3	C <sub>5</sub> H <sub>10</sub> O	86.1	672.8	147.385	1.1758	258.24±16.97 <sup>a</sup>	242.35±4.45 <sup>a</sup>	100.92±15.27 <sup>c</sup>	189.29±3.92 <sup>b</sup>	118.04±7.96 <sup>c</sup>
	3-Methyl-2-butenal	107-86-8	C <sub>5</sub> H <sub>8</sub> O	84.1	786	180.867	1.08255	59.32±4.07 <sup>c</sup>	91.27±1.2 <sup>bc</sup>	63.51±10.94 <sup>c</sup>	131.04±14.46 <sup>a</sup>	97.39±17.34 <sup>ab</sup>

Table S1. (continued).

Count	Compound	CAS	Molecule Formula	MW	RI	Rt (s)	Dt (ms)	LJA	LJB	LJC	LJD	LJE
Aldehyde	2-methylpropanal	78-84-2	C <sub>4</sub> H <sub>8</sub> O	72.1	783.4	179.62	1.30507	51.13±4.1 <sup>b</sup>	177.94±4.95 <sup>a</sup>	55.96±5.56 <sup>b</sup>	177.63±20.92 <sup>a</sup>	69.21±12.43 <sup>b</sup>
	Butanal	123-72-8	C <sub>4</sub> H <sub>8</sub> O	72.1	857.6	222.038	1.27537	32.69±1.26 <sup>b</sup>	61.7±1.19 <sup>a</sup>	14.75±1.57 <sup>c</sup>	19.12±1.95 <sup>c</sup>	16.5±2.28 <sup>c</sup>
	Furfural	98-01-1	C <sub>5</sub> H <sub>4</sub> O <sub>2</sub>	96.1	835.3	209.188	1.32463	106.3±3.51 <sup>d</sup>	61.59±3.33 <sup>c</sup>	225.35±23.33 <sup>c</sup>	1011.44±54.08 <sup>a</sup>	348.55±36.84 <sup>b</sup>
	trans-2-pentenal	1576-87-0	C <sub>5</sub> H <sub>8</sub> O	84.1	741.6	168.875	1.37037	14.94±1.28 <sup>cd</sup>	12.95±0.56 <sup>d</sup>	29.59±2.7 <sup>a</sup>	19.03±3.46 <sup>bc</sup>	21.88±2.51 <sup>ab</sup>
Acid	2-methylbutanoic acid-D	116-53-0	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.1	840.8	212.352	1.46864	172.97±5.8 <sup>b</sup>	277.79±11.45 <sup>a</sup>	164.19±6.89 <sup>c</sup>	136.75±6.91 <sup>d</sup>	164.26±5.92 <sup>bc</sup>
	acetic acid	64-19-7	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	60.1	611.8	117.085	1.04722	2031.95±19.5 <sup>c</sup>	2129.27±54.41 <sup>c</sup>	3496.21±43 <sup>a</sup>	2458.79±85.02 <sup>b</sup>	3429.99±43.62 <sup>a</sup>
	2-Methylbutanoic acid-M	116-53-0	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.1	852.9	219.354	1.20229	208.31±22.49 <sup>c</sup>	122.03±3.83 <sup>d</sup>	329.05±17.82 <sup>b</sup>	360.36±5.16 <sup>ab</sup>	394.43±6.43 <sup>a</sup>
	3-methylbutyric acid	503-74-2	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.1	817.5	199.003	1.47341	83.69±1.75 <sup>b</sup>	303.19±21.93 <sup>a</sup>	65.75±2.32 <sup>c</sup>	27.97±1.44 <sup>d</sup>	60.09±3.27 <sup>c</sup>
Ester	Propanoic acid	79-09-4	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.1	654.6	138.341	1.26372	113.23±11.81 <sup>d</sup>	179.27±8.62 <sup>cd</sup>	338.42±50.88 <sup>a</sup>	244.51±23.92 <sup>bc</sup>	325.7±29.56 <sup>ab</sup>
	Acetic acid 2-propyl ester	108-21-4	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.1	909.4	256.773	1.47796	531.5±30.38 <sup>a</sup>	405.94±21.59 <sup>b</sup>	327.68±23.45 <sup>c</sup>	296.87±28.2 <sup>c</sup>	337.65±34.91 <sup>bc</sup>

Table S1. (continued).

Count	Compound	CAS	Molecule	MW	RI	Rt(s)	Dt(ms)	LJA	LJB	LJC	LJD	LJE
			Formula									
Ester	isoamyl acetate	123-92-2	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	130.2	1135.1	590.369	1.30748	5571.87±68 <sup>bc</sup>	5895.82±175.63 <sup>ab</sup>	5576.43±196.39 <sup>c</sup>	6057.23±211.71 <sup>d</sup>	5575.6±195.86 <sup>bc</sup>
	Butyl 2-methylbutanoate	15706-73-7	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	158.2	1218.6	746.061	1.38933	639.19±22.04 <sup>b</sup>	598.87±17.57 <sup>c</sup>	825.66±45.63 <sup>a</sup>	512.38±64.36 <sup>d</sup>	578.46±10.03 <sup>c</sup>
	isobutyl butyrate	539-90-2	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	144.2	955.8	296.774	1.32179	468.8±6.44 <sup>c</sup>	480.22±9.62 <sup>c</sup>	559.55±5.04 <sup>b</sup>	663.91±10.97 <sup>a</sup>	553.65±26.87 <sup>b</sup>
	Acetic acid, hexyl ester	142-92-7	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	144.2	1008.1	353.405	1.39124	108.39±4.73 <sup>ab</sup>	103.68±10.84 <sup>b</sup>	131.81±15.56 <sup>a</sup>	95.19±6.59 <sup>b</sup>	103.16±7.69 <sup>b</sup>
	Ethyl 2-methylbutanoate	7452-79-1	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	130.2	1052	435.316	1.64048	583.36±103.75 <sup>a</sup>	294.73±3.94 <sup>b</sup>	137.78±21.31 <sup>c</sup>	192.22±20.23 <sup>bc</sup>	256.94±86.36 <sup>b</sup>
	Methyl 2-methylbutanoate-M	868-57-5	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.2	1008.5	354.218	1.19047	336.81±4.61 <sup>b</sup>	303.6±13.13 <sup>c</sup>	374.78±9.94 <sup>ab</sup>	379.78±2.73 <sup>a</sup>	366.21±6.08 <sup>ab</sup>
	Butyl formate	592-84-7	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.1	1033.8	401.336	1.21029	1976.12±113.77 <sup>b</sup>	2044.31±145.18 <sup>b</sup>	2076.83±217.15 <sup>b</sup>	2336.33±155.54 <sup>a</sup>	2269.21±16.14 <sup>a</sup>
	methyl 3-methylbutanoate	556-24-1	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.2	783.4	179.632	1.20558	483.09±11.04 <sup>c</sup>	499.19±11.52 <sup>c</sup>	672.84±28.88 <sup>b</sup>	801.81±22.46 <sup>a</sup>	764.03±32.16 <sup>a</sup>
	Formic acid, 3-methylbutyl ester	110-45-2	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.2	782.6	179.416	1.27869	149.44±0.11 <sup>a</sup>	120.09±3.36 <sup>b</sup>	76.6±5.93 <sup>c</sup>	61.98±9.11 <sup>c</sup>	65.71±6.47 <sup>c</sup>

Table S1. (continued).

Count	Compound	CAS	Molecule	MW	RI	Rt(s)	Dt(ms)	LJA	LJB	LJC	LJD	LJE
			Formula									
Ester	Isobutyl isobutyrate	97-85-8	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	144.2	1080.8	489.107	1.29028	152.18±13.78 <sup>a</sup>	155.42±21.96 <sup>a</sup>	163.11±16.78 <sup>a</sup>	154.31±13.64 <sup>a</sup>	164.98±3.72 <sup>a</sup>
	Linalyl acetate	115-95-7	C <sub>12</sub> H <sub>20</sub> O <sub>2</sub>	196.3	1248.7	802.071	1.19953	631.32±17.25 <sup>ab</sup>	619.64±25.34 <sup>b</sup>	574.01±67.49 <sup>c</sup>	659.01±30.02 <sup>a</sup>	654.08±3.19 <sup>a</sup>
	Ethyl isovalerate	108-64-5	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	130.2	1068	465.201	1.67191	1000.21±9.24 <sup>a</sup>	977.13±16.27 <sup>ab</sup>	955.59±12.2 <sup>ab</sup>	891.95±15.75 <sup>b</sup>	907.78±2.04 <sup>b</sup>
	Methyl 2-methylbutanoate-D	868-57-5	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.2	1008.2	353.692	1.55135	223.9±11.47 <sup>b</sup>	213.76±12.09 <sup>b</sup>	305.26±34.24 <sup>a</sup>	224.8±19.86 <sup>b</sup>	221.85±6.13 <sup>b</sup>
	propyl acetate	109-60-4	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.1	932.6	276.726	1.47554	883.93±37.43 <sup>c</sup>	884.41±3.12 <sup>c</sup>	1083.24±41.69 <sup>b</sup>	1485.68±8.4 <sup>a</sup>	1122.22±31.82 <sup>b</sup>
	acetic acid ethyl ester	141-78-6	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	88.1	624.3	123.299	1.11267	4893.64±86.94 <sup>ab</sup>	5032.11±66.16 <sup>a</sup>	4647.97±158.01 <sup>c</sup>	4125.46±104.43 <sup>d</sup>	4568.07±118.22 <sup>bc</sup>
	2(3H)-Furanone, dihydro-5-methyl-	108-29-2	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	100.1	947.6	289.657	1.41396	46.02±4.58 <sup>b</sup>	44.04±3.52 <sup>bc</sup>	35.92±1.94 <sup>c</sup>	97.01±3.03 <sup>a</sup>	3.78±5.53 <sup>bc</sup>
	(Z)-3-hexenyl acetate	3681-71-8	C <sub>8</sub> H <sub>14</sub> O <sub>2</sub>	142.2	1008.1	353.388	1.31726	185.61±11.87 <sup>c</sup>	186.69±7.76 <sup>c</sup>	219.58±12.24 <sup>ab</sup>	227.69±5.02 <sup>a</sup>	197.5±7.1 <sup>bc</sup>
	Ethyl butanoate	105-54-4	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	116.2	799.5	188.63	1.20525	211.66±11.58 <sup>c</sup>	259.3±7.7 <sup>b</sup>	249.04±5.15 <sup>bc</sup>	314.67±3.56 <sup>a</sup>	311.59±9.88 <sup>a</sup>

Table S1. (continued).

Count	Compound	CAS	Molecule	MW	RI	Rt(s)	Dt(ms)	LJA	LJB	LJC	LJD	LJE
			Formula									
Ester	Isobutyl formate	542-55-2	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.1	684.7	153.256	1.20011	174.02±1.28 <sup>bc</sup>	143.94±5.66 <sup>c</sup>	169.59±26.55 <sup>c</sup>	274.99±41.8 <sup>a</sup>	253±33.01 <sup>ab</sup>
	Methyl hexanoate	106-70-7	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	130.2	910.6	257.811	1.67521	290.56±11.67 <sup>bc</sup>	242.65±14 <sup>c</sup>	371.89±41.5 <sup>b</sup>	570.93±44.37 <sup>a</sup>	385.52±46.08 <sup>b</sup>
	ethyl 2-hydroxypropanoate	97-64-3	C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>	118.1	820	200.429	1.1353	300.73±39.02 <sup>b</sup>	825.23±14.01 <sup>a</sup>	185.12±15.83 <sup>c</sup>	62.41±8.71 <sup>d</sup>	93.5±6.75 <sup>d</sup>
	3-Hepten-2-one	1119-44-4	C <sub>7</sub> H <sub>12</sub> O	112.2	935.4	279.146	1.63823	240.77±18.3 <sup>b</sup>	252.3±9.37 <sup>b</sup>	258.11±8.37 <sup>b</sup>	282.15±12.29 <sup>a</sup>	225.35±6.46 <sup>b</sup>
	4-Methyl-2-pentanone	108-10-1	C <sub>6</sub> H <sub>12</sub> O	100.2	1008.2	353.692	1.45582	1315.64±31.07 <sup>cd</sup>	1286.75±70.72 <sup>d</sup>	1639.48±71.86 <sup>a</sup>	1358.11±70.62 <sup>c</sup>	1391.36±8.2 <sup>b</sup>
Ketone	2-butanone	78-93-3	C <sub>4</sub> H <sub>8</sub> O	72.1	867.4	227.641	1.24852	273.38±14.24 <sup>a</sup>	270.57±4.53 <sup>a</sup>	276.31±11.27 <sup>a</sup>	168.6±5.56 <sup>c</sup>	236.82±10.6 <sup>b</sup>
	cyclopentanone-D	120-92-3	C <sub>5</sub> H <sub>8</sub> O	84.1	793	184.895	1.34483	515.83±21.36 <sup>b</sup>	486.05±10.29 <sup>bc</sup>	767.06±53.23 <sup>a</sup>	462.25±18.46 <sup>bc</sup>	438.38±31.73 <sup>c</sup>
	2-Propanone, 1-hydroxy-	116-09-6	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	74.1	672.8	147.382	1.2431	763.44±58.77 <sup>a</sup>	850.37±24.06 <sup>a</sup>	806.89±62.45 <sup>a</sup>	750.6±46.07 <sup>ab</sup>	638.45±45.88 <sup>b</sup>
	1-Penten-3-one	1629-58-9	C <sub>5</sub> H <sub>8</sub> O	84.1	675.5	148.706	1.28415	454.22±18.89 <sup>a</sup>	439.32±17.02 <sup>a</sup>	270.65±16.96 <sup>b</sup>	286.79±18.42 <sup>b</sup>	283.55±20.73 <sup>b</sup>
	cyclopentanone-M	120-92-3	C <sub>5</sub> H <sub>8</sub> O	84.1	792.6	184.688	1.11323	270.1±13.3 <sup>b</sup>	174.13±3.24 <sup>c</sup>	418.57±17.15 <sup>a</sup>	185.44±0.29 <sup>c</sup>	247.87±9.89 <sup>b</sup>

Table S1. (continued).

Count	Compound	CAS	Molecule	MW	RI	Rt(s)	Dt(ms)	LJA	LJB	LJC	LJD	LJE
			Formula									
Ketone	1-(acetyloxy)-2-propanone	592-20-1	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub>	116.1	870.8	229.641	1.2029	142.43±19.01 <sup>c</sup>	119.06±5.73 <sup>c</sup>	210.31±8.9 <sup>b</sup>	270.51±11.74 <sup>a</sup>	259.68±7.37 <sup>a</sup>
	Pentan-2-one	107-87-9	C <sub>5</sub> H <sub>10</sub> O	86.1	982.7	319.903	1.11619	85.25±3.87 <sup>b</sup>	80.99±4.61 <sup>b</sup>	94.17±9.47 <sup>ab</sup>	93.2±2.56 <sup>ab</sup>	100.74±7.84 <sup>a</sup>
	gamma-Terpinene	99-85-4	C <sub>10</sub> H <sub>16</sub>	136.2	1264.1	830.863	1.19778	1798.85±55.82 <sup>bc</sup>	1875.84±39.41 <sup>abc</sup>	1839.73±110.95 <sup>c</sup>	1929.89±97.91 <sup>a</sup>	1886.84±66.6 <sup>ab</sup>
Alkene	Styrene	100-42-5	C <sub>8</sub> H <sub>8</sub>	104.2	866.8	227.306	1.41231	126.66±16.32 <sup>c</sup>	153.06±3.42 <sup>c</sup>	376.57±26.61 <sup>b</sup>	633.07±3.2 <sup>a</sup>	378.83±28.28 <sup>b</sup>
	alpha-Terpinene	99-86-5	C <sub>10</sub> H <sub>16</sub>	136.2	1022.2	379.781	1.21375	554.71±32.52 <sup>d</sup>	585.09±46.65 <sup>cd</sup>	654.13±57.52 <sup>c</sup>	780.45±23.59 <sup>a</sup>	701.66±10.83 <sup>b</sup>
Ether	Diethyl trisulfide	3600-24-6	C <sub>4</sub> H <sub>10</sub> S <sub>3</sub>	154.3	1128.3	577.668	1.21466	2611.21±193.44 <sup>ab</sup>	2708.71±139.64 <sup>a</sup>	2435.15±161.09 <sup>b</sup>	2808.12±145.65 <sup>a</sup>	2847.51±112.6 <sup>a</sup>
Others	2-Ethyl-3,5-dimethylpyrazine	13925-07-0	C <sub>8</sub> H <sub>12</sub> N <sub>2</sub>	136.2	1080.2	487.961	1.2153	527.3±43.09 <sup>c</sup>	556.01±57.04 <sup>bc</sup>	592.66±63.57 <sup>bc</sup>	673.92±56.92 <sup>a</sup>	638.45±21.84 <sup>ab</sup>
	2-methyl-3-(methylthio)furan-M	63012-97-5	C <sub>6</sub> H <sub>8</sub> OS	128.2	949.6	291.381	1.11735	1254.15±53.96 <sup>b</sup>	978.61±26.45 <sup>c</sup>	1387.82±38.79 <sup>a</sup>	935.04±65.44 <sup>c</sup>	1188.2±9.44 <sup>b</sup>
	2-methyl-3-(methylthio)furan-D	63012-97-5	C <sub>6</sub> H <sub>8</sub> OS	128.2	949.2	291.096	1.17478	233.91±4.52 <sup>b</sup>	274.26±7.64 <sup>a</sup>	119.85±13.29 <sup>c</sup>	286±15.7 <sup>a</sup>	140.51±2.02 <sup>c</sup>
	1,3-Dioxolane, 2,4-dimethyl, cis	3390-12-3	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	102.1	703.9	159.171	1.25552	259.97±19.64 <sup>a</sup>	233.08±5.69 <sup>a</sup>	119.84±12.17 <sup>b</sup>	108.46±9.98 <sup>b</sup>	107.44±2.47 <sup>b</sup>

Table S1. (continued).

Count	Compound	CAS	Molecule	MW	RI	Rt(s)	Dt(ms)	LJA	LJB	LJC	LJD	LJE
			Formula									
Others	Methylpyrazine	109-08-0	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub>	94.1	840.7	212.306	1.3946	227.49±17.46 <sup>c</sup>	262.08±7.96 <sup>c</sup>	600.19±34.2 <sup>b</sup>	790.88±8.18 <sup>a</sup>	606.31±30.34 <sup>b</sup>
	(E)-3-Pentenitrile	16529-66-1	C <sub>5</sub> H <sub>7</sub> N	81.1	700.6	158.31	1.37004	46.12±3.03 <sup>b</sup>	57.7±1.86 <sup>b</sup>	100.37±9.04 <sup>a</sup>	93.38±15.09 <sup>a</sup>	82.06±9.85 <sup>a</sup>
	Acetal	105-57-7	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	118.2	719.2	163.095	1.13155	163.77±27.98 <sup>a</sup>	117.12±8.49 <sup>a</sup>	38.64±2.14 <sup>b</sup>	31.1±1.99 <sup>b</sup>	34.23±3.6 <sup>b</sup>
	2-Propenenitrile	107-13-1	C <sub>3</sub> H <sub>3</sub> N	53.1	649.8	135.951	1.0859	441.73±13.74 <sup>d</sup>	457.37±4.87 <sup>d</sup>	758.75±17.9 <sup>c</sup>	1466.19±16.04 <sup>a</sup>	1079.95±18.62 <sup>b</sup>