

Supplementary Materials

A Comprehensive Study on the Acidic Compounds in Gas and Particle Phases of Mainstream Cigarette Smoke

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Table S1. Contents of the identified acids in the particulate phase ($\mu\text{g}/\text{mg}$ tar).

Compounds	L1	L2	L3	L4	L5	M1	M2	M3	M4	<i>p</i>
formic acid	5.21E+00	3.80E+00	3.67E+00	3.51E+00	3.44E+00	3.93E+00	3.77E+00	3.78E+00	3.16E+00	5.28E-01
acetic acid	9.20E+00	6.04E+00	6.80E+00	7.23E+00	6.50E+00	7.45E+00	6.92E+00	6.15E+00	5.26E+00	3.75E-01
acrylic acid	1.04E+00	7.54E-01	8.15E-01	6.97E-01	7.75E-01	1.06E+00	1.00E+00	9.30E-01	7.70E-01	1.89E-01
propionic acid	7.77E-01	5.55E-01	6.24E-01	5.97E-01	6.72E-01	7.37E-01	6.69E-01	6.43E-01	5.14E-01	9.47E-01
2-methyl-propionic acid	7.68E-02	6.59E-02	6.73E-02	7.90E-02	7.18E-02	1.12E-01	1.01E-01	1.02E-01	7.99E-02	4.92E-03 **
2-methyl-butyric acid	6.59E-02	5.93E-02	6.08E-02	7.71E-02	5.91E-02	1.58E-01	1.46E-01	1.53E-01	1.19E-01	3.12E-05 ***
2-ene-butyric acid	1.84E-01	1.32E-01	1.55E-01	1.92E-01	1.67E-01	2.14E-01	1.99E-01	2.00E-01	1.66E-01	9.79E-02
3-methyl-butyric acid	1.56E-01	1.38E-01	1.38E-01	1.68E-01	1.34E-01	2.44E-01	2.28E-01	2.43E-01	1.84E-01	1.02E-03 **
valeric acid	5.89E-02	4.82E-02	4.85E-02	5.63E-02	5.18E-02	7.18E-02	6.53E-02	6.84E-02	5.42E-02	2.16E-02 *
2-methyl-2-ene-butyric acid	4.73E-02	3.73E-02	4.02E-02	4.62E-02	4.05E-02	4.98E-02	4.53E-02	4.67E-02	3.64E-02	5.24E-01
2-pentenoic acid	4.33E-02	3.16E-02	3.55E-02	4.03E-02	3.48E-02	4.27E-02	3.98E-02	4.11E-02	3.21E-02	5.77E-01
3-methyl-pentanoic acid	6.16E-02	3.24E-02	3.52E-02	3.22E-02	3.80E-02	3.94E-01	3.63E-01	4.03E-01	2.77E-01	5.39E-06 ***
4-methyl-pentanoic acid	4.46E-02	3.93E-02	3.16E-02	4.99E-02	3.60E-02	7.38E-02	6.87E-02	7.29E-02	5.68E-02	8.61E-04 ***
phenol	9.60E-01	8.16E-01	7.83E-01	1.01E+00	8.47E-01	1.06E+00	9.86E-01	1.02E+00	8.41E-01	1.98E-01
lactic acid	2.49E+00	1.82E+00	1.91E+00	3.27E+00	2.77E+00	1.45E+00	1.40E+00	1.38E+00	1.19E+00	9.49E-03 **
caproic acid	8.66E-02	8.06E-02	7.00E-02	7.95E-02	6.91E-02	1.07E-01	9.29E-02	1.03E-01	8.14E-02	1.99E-02 *
glycolic acid	1.21E+00	9.56E-01	8.63E-01	9.44E-01	6.92E-01	4.47E-01	4.19E-01	4.40E-01	4.18E-01	1.18E-03 **
2-carbonyl-propionic acid	9.56E-01	5.61E-01	6.96E-01	7.17E-01	6.00E-01	1.30E-01	1.25E-01	1.16E-01	9.47E-02	1.36E-04 ***
2-hydroxy-butyric acid	1.59E-01	1.10E-01	1.16E-01	1.47E-01	1.31E-01	1.33E-01	1.29E-01	1.31E-01	1.03E-01	5.05E-01
levulinic acid	5.23E-01	3.38E-01	3.63E-01	4.40E-01	3.83E-01	3.52E-01	3.19E-01	3.20E-01	2.50E-01	4.96E-02 *
o-cresol	2.28E-01	1.97E-01	1.87E-01	2.32E-01	2.13E-01	3.03E-01	2.78E-01	3.01E-01	2.41E-01	3.56E-03 **
2-furancarboxylic acid	1.38E+00	8.98E-01	9.32E-01	1.14E+00	8.89E-01	8.97E-01	8.09E-01	8.07E-01	6.68E-01	6.43E-02
3-hydroxy-propionic acid	1.98E+00	1.55E+00	1.72E+00	1.91E+00	1.77E+00	3.36E+00	3.51E+00	3.81E+00	3.12E+00	1.21E-05 ***
p-cresol	4.65E-01	3.84E-01	3.86E-01	4.87E-01	4.22E-01	6.12E-01	5.68E-01	5.73E-01	4.70E-01	8.81E-03 **
3-hydroxy-butyric acid	5.32E-02	3.43E-02	3.54E-02	4.44E-02	4.00E-02	7.47E-02	7.26E-02	7.68E-02	6.00E-02	6.83E-04 ***
furanacetic acid	2.62E-02	1.46E-01	1.46E-01	4.44E-02	2.58E-02	1.75E-01	3.28E-02	2.39E-02	3.22E-02	8.02E-01
2-hydroxymethyl-butyric acid	3.80E-01	2.68E-01	1.76E-01	3.49E-01	2.97E-01	2.99E+00	3.37E+00	3.79E+00	3.48E+00	1.58E-07 ***

benzoic acid	5.11E-01	3.58E-01	3.58E-01	4.50E-01	3.66E-01	5.04E-01	4.61E-01	4.87E-01	3.69E-01	3.23E-01	
phenylacetic acid	1.41E-01	1.01E-01	1.99E-01	1.20E-01	1.36E-01	3.82E-02	7.37E-02	1.19E-01	1.17E-01	7.70E-02	
3-methyl-2-furancarboxylic acid	1.70E-01	1.33E-01	1.56E-01	2.03E-01	1.70E-01	2.43E-01	2.41E-01	2.04E-01	1.85E-01	2.35E-02	*
catechol	4.68E+00	3.10E+00	3.13E+00	4.07E+00	3.27E+00	3.51E+00	3.35E+00	3.44E+00	2.75E+00	3.47E-01	
2,3-dihydroxy-propionic acid	3.59E-01	2.84E-01	2.48E-01	2.74E-01	1.84E-01	1.78E-01	1.65E-01	1.84E-01	1.73E-01	2.18E-02	*
quinol/resorcinol	1.16E-01	8.83E-02	8.28E-02	1.13E-01	8.84E-02	7.41E-02	6.83E-02	6.57E-02	5.46E-02	7.61E-03	**
2-isopropyl-3-carbonyl-butyric acid	4.77E+00	3.02E+00	2.91E+00	3.54E+00	2.68E+00	1.62E+00	1.44E+00	1.46E+00	1.26E+00	2.74E-03	**
malic acid	1.56E-01	1.13E-01	8.20E-02	8.16E-02	7.61E-02	4.67E-02	2.67E-02	3.02E-02	4.77E-02	8.77E-03	**
1,2,3-glycinol	6.01E-01	4.48E-01	3.87E-01	5.19E-01	3.80E-01	2.80E-01	2.63E-01	2.56E-01	2.29E-01	3.37E-03	**
threonic acid	1.56E+01	8.20E+00	2.59E+00	2.18E+00	1.79E+00	5.59E+00	5.37E+00	5.11E+00	4.31E+00	7.54E-01	
m-hydroxy-benzoic acid	7.43E-01	5.09E-01	4.79E-01	6.52E-01	4.66E-01	3.93E-01	3.52E-01	3.43E-01	3.01E-01	1.04E-02	*
vanillic acid	2.72E-01	2.01E-01	1.69E-01	2.61E-01	2.10E-01	2.05E-01	1.83E-01	1.83E-01	1.43E-01	1.18E-01	
tetradecanoic acid	6.40E-01	4.23E-01	3.17E-01	5.12E-01	3.89E-01	7.22E-01	7.39E-01	7.21E-01	5.44E-01	1.96E-02	*
palmitic acid	4.25E+01	2.81E+01	2.55E+01	3.58E+01	2.88E+01	2.81E+01	2.57E+01	2.69E+01	2.05E+01	1.16E-01	
linoleic acid	1.96E+01	1.30E+01	1.39E+01	1.74E+01	1.44E+01	1.43E+01	1.32E+01	1.38E+01	1.04E+01	1.30E-01	
linolenic acid	1.49E+01	1.01E+01	1.03E+01	1.28E+01	1.04E+01	7.95E+00	6.90E+00	7.07E+00	5.50E+00	4.13E-03	**
oleic acid	1.08E+01	7.32E+00	7.54E+00	9.71E+00	7.99E+00	7.92E+00	7.29E+00	7.66E+00	5.81E+00	1.29E-01	
octadecanoic acid	1.07E+01	7.14E+00	7.42E+00	9.01E+00	7.40E+00	8.75E+00	7.47E+00	7.80E+00	5.83E+00	3.84E-01	
eicosanic acid	3.72E+00	2.73E+00	3.06E+00	3.84E+00	3.15E+00	4.62E+00	4.23E+00	4.62E+00	3.46E+00	2.75E-02	*

Table S2. Contents of the identified acids in the gaseous phase ($\mu\text{g}/\text{mg}$ tar).

Compounds	L1	L2	L3	L4	L5	M1	M2	M3	M4	<i>p</i>	
formic acid	3.15E-01	3.03E-01	2.76E-01	3.28E-01	2.06E-01	3.24E-01	5.23E-01	4.31E-01	5.22E-01	1.12E-02	*
acetic acid	1.19E+00	9.92E-01	7.18E-01	9.84E-01	9.27E-01	7.52E-01	7.43E-01	1.30E+00	6.43E-01	5.28E-01	
acrylic acid	1.19E-02	1.58E-02	9.80E-03	7.87E-03	5.43E-03	6.12E-03	9.38E-03	1.81E-02	7.34E-03	9.82E-01	
propionic acid	5.68E-02	5.39E-02	1.00E-01	5.29E-02	9.10E-02	3.53E-02	4.64E-01	2.95E-01	4.38E-02	1.76E-01	
2-methyl-propionic acid	6.79E-03	7.04E-03	7.45E-03	6.68E-03	8.86E-03	9.55E-03	1.69E-02	1.80E-02	8.93E-03	2.69E-02	*
2-methyl-butyric acid	5.90E-04	1.30E-03	5.35E-04	4.94E-03	3.88E-03	3.08E-03	6.03E-03	3.61E-03	5.76E-03	9.37E-02	
2-ene-butyric acid	1.57E-02	1.90E-02	2.57E-02	1.97E-02	2.14E-02	9.29E-03	3.18E-03	1.10E-02	3.85E-03	1.11E-03	***
3-methyl-butyric acid	6.60E-03	6.52E-03	4.08E-03	5.99E-03	5.14E-03	6.69E-03	8.15E-03	8.42E-03	7.87E-03	1.24E-02	*
valeric acid	2.53E-03	3.02E-03	1.16E-02	2.19E-03	1.04E-02	1.38E-02	3.08E-02	3.05E-02	2.45E-03	7.76E-02	

2-methyl-2-ene-butyric acid	6.68E-03	7.62E-03	1.75E-02	8.08E-03	1.33E-02	2.92E-02	1.85E-02	1.76E-02	2.94E-03	2.65E-01	
2-pentenoic acid	1.12E-01	1.76E-01	9.14E-02	5.89E-02	1.42E-03	3.17E-02	1.56E-03	9.31E-04	1.00E-03	4.96E-02	*
3-methyl-pentanoic acid	7.18E-04	8.93E-04	6.46E-04	5.05E-04	4.92E-04	2.14E-03	2.60E-03	2.39E-03	2.15E-03	3.58E-06	***
4-methyl-pentanoic acid	6.16E-04	4.45E-04	5.43E-04	6.66E-04	4.31E-04	1.51E-03	7.62E-04	1.46E-03	1.49E-03	2.59E-03	**
phenol	5.83E-03	7.91E-03	5.46E-03	5.11E-03	6.62E-03	6.91E-03	2.06E-02	1.65E-02	6.50E-03	7.96E-02	
lactic acid	7.73E-03	1.20E-02	4.39E-02	4.90E-03	1.26E-02	1.57E-02	2.11E-02	1.70E-02	9.58E-03	9.63E-01	
caproic acid	1.22E-02	1.41E-02	1.54E-02	1.11E-02	1.46E-02	3.01E-02	3.38E-02	3.33E-02	1.41E-02	1.10E-02	*
glycolic acid	4.36E-03	3.32E-03	3.90E-03	2.26E-03	2.61E-03	5.55E-03	4.74E-03	4.60E-03	3.17E-03	8.92E-02	
2-carbonyl-propionic acid	2.30E-03	5.90E-03	1.85E-03	9.04E-04	1.87E-03	3.11E-03	5.43E-04	1.77E-03	2.93E-04	3.49E-01	
2-hydroxy-butyric acid	1.50E-03	1.36E-03	1.71E-03	8.86E-04	1.99E-03	9.59E-04	1.78E-03	1.43E-03	1.64E-03	8.96E-01	
levulinic acid	1.76E-03	1.44E-03	3.26E-03	1.49E-03	3.11E-03	3.38E-03	4.13E-03	5.00E-03	3.13E-03	2.30E-02	*
o-cresol	1.23E-03	1.37E-03	3.61E-04	1.22E-03	5.34E-04	1.00E-03	1.01E-03	6.09E-04	1.69E-03	6.74E-01	
2-furancarboxylic acid	6.69E-04	2.85E-04	1.29E-03	5.96E-04	1.35E-03	1.18E-03	1.70E-03	7.62E-04	1.10E-03	2.70E-01	
3-hydroxy-propionic acid	6.34E-02	1.64E-01	1.57E-02	1.14E-01	3.98E-02	2.46E-02	1.16E-01	9.21E-02	3.79E-02	7.54E-01	
p-cresol	1.13E-03	1.52E-03	4.32E-04	9.73E-04	8.72E-04	9.07E-04	1.12E-03	1.02E-03	1.30E-03	6.48E-01	
3-hydroxy-butyric acid	8.11E-03	1.01E-02	2.13E-03	1.17E-02	5.69E-03	5.55E-03	1.03E-02	7.66E-03	5.87E-03	9.26E-01	
furanacetic acid	1.60E-03	1.77E-03	5.25E-03	9.47E-03	9.49E-03	5.31E-03	1.13E-02	9.95E-03	2.77E-03	5.15E-01	
2-hydroxymethyl-butyric acid	1.63E-04	7.97E-05	2.26E-04	2.15E-05	3.54E-04	9.91E-04	6.96E-04	7.41E-04	1.27E-04	3.01E-02	*
benzoic acid	7.56E-03	9.08E-03	2.21E-01	6.77E-03	5.86E-01	7.55E-01	2.27E-01	2.64E-01	7.93E-03	4.61E-01	
phenylacetic acid	1.45E-02	4.91E-02	5.25E-03	7.57E-03	2.22E-02	6.76E-03	8.61E-03	1.52E-02	3.48E-02	7.60E-01	
3-methyl-2-furancarboxylic acid	7.99E-03	8.00E-03	3.94E-03	9.47E-03	5.25E-02	2.39E-02	9.89E-03	1.91E-02	1.24E-02	9.97E-01	
catechol	2.39E-05	3.02E-04	4.53E-04	1.15E-04	2.23E-04	1.81E-04	1.97E-04	1.98E-04	2.77E-04	9.14E-01	
2,3-dihydroxy-propionic acid	6.72E-04	8.59E-04	6.26E-04	6.77E-04	8.99E-04	1.38E-03	1.17E-03	4.75E-03	9.91E-04	1.37E-01	
quinol/resorcinol	7.52E-05	2.12E-05	1.36E-05	7.88E-05	6.82E-05	8.28E-05	1.93E-04	1.03E-04	1.00E-04	3.87E-02	*
2-isopropyl-3-carbonyl-butyric acid	6.79E-03	9.89E-03	3.94E-03	1.89E-03	9.49E-03	2.66E-03	6.91E-03	2.82E-03	2.77E-03	2.30E-01	
malic acid	5.86E-04	8.88E-04	3.08E-04	2.96E-04	2.91E-04	2.08E-03	4.90E-04	6.74E-04	9.37E-04	1.37E-01	
1,2,3-glycinol	5.87E-05	9.49E-05	3.62E-05	5.22E-05	3.51E-05	4.65E-05	7.75E-05	8.98E-05	1.39E-04	1.61E-01	
threonic acid	1.04E-02	3.89E-02	2.10E-02	2.27E-02	2.33E-02	5.79E-03	2.70E-02	1.79E-02	2.52E-02	5.41E-01	
m-hydroxy-benzoic acid	3.52E-04	4.55E-04	2.67E-04	6.10E-04	5.40E-04	2.78E-04	4.50E-04	7.92E-04	3.69E-04	8.27E-01	
vanillic acid	5.29E-04	4.14E-04	5.11E-05	7.38E-04	2.52E-04	2.35E-04	5.48E-04	5.56E-04	7.52E-04	4.65E-01	
tetradecanoic acid	1.64E-02	2.43E-02	8.59E-03	2.29E-02	1.10E-02	1.11E-02	8.53E-03	1.35E-02	1.51E-02	2.61E-01	

palmitic acid	3.93E+00	5.57E+00	3.39E+00	5.48E+00	3.95E+00	1.52E+00	1.19E+00	4.49E+00	4.29E+00	1.28E-01	
linoleic acid	1.51E-02	1.37E-02	1.18E-02	7.57E-03	7.44E-03	6.27E-03	1.26E-02	1.28E-02	9.74E-03	7.38E-01	
linolenic acid	5.00E-03	9.33E-03	8.22E-03	5.93E-03	1.81E-02	6.79E-03	1.33E-02	1.02E-02	1.15E-02	7.10E-01	
oleic acid	4.55E-02	2.72E-02	2.82E-02	4.22E-02	2.67E-02	1.68E-02	3.50E-02	3.35E-02	2.89E-02	3.86E-01	
octadecanoic acid	2.38E+00	3.13E+00	2.44E+00	2.86E+00	2.33E+00	8.90E-01	7.42E-01	1.89E+00	2.15E+00	1.14E-02	*
eicosanic acid	2.29E-02	3.44E-02	1.79E-02	5.10E-02	2.56E-02	2.55E-02	2.62E-02	5.83E-02	4.26E-02	4.37E-01	

Table S3. VIP values of individual acid.

Var ID (Primary)	M10.VIP[1+1+0]	2.44693 * M10.VIP[1]cvSE
3-methyl-pentanoic acid	1.27029	0.22596
2-methyl-butyric acid	1.26227	0.307044
3-hydroxy-propionic acid	1.25293	0.242651
2-hydroxymethyl-butyric acid	1.2416	0.316905
2-carbonyl-propionic acid	1.22251	0.242543
3-hydroxy-butyric acid	1.21667	0.335142
3-methyl-butyric acid	1.21605	0.358808
4-methyl-pentanoic acid	1.20864	0.434382
glycolic acid	1.19307	0.349361
o-cresol	1.17788	0.390014
2-isopropyl-3-carbonyl-butyric acid	1.16794	0.435098
2-methyl-propionic acid	1.16763	0.495594
1,2,3-glycinol	1.14422	0.38421
malic acid	1.13427	0.750753
p-cresol	1.13007	0.487997
linolenic acid	1.114	0.33429
tetradecanoic acid	1.0961	0.591086
valeric acid	1.09425	0.46804
caproic acid	1.08899	0.677116
m-hydroxy-benzoic acid	1.08861	0.456993
2,3-dihydroxy-propionic acid	1.07676	0.559148
quinol/resorcinol	1.0578	0.351918
eicosanic acid	1.0549	0.32148
3-methyl-2-furancarboxylic acid	1.01631	0.740374
2-furancarboxylic acid	0.970357	0.661947
lactic acid	0.968582	0.475798
levulinic acid	0.955007	0.505668
palmitic acid	0.899147	0.650947
2-ene-butyric acid	0.89363	0.570761
acrylic acid	0.862408	0.940461

phenylacetic acid	0.850113	1.08538
linoleic acid	0.846137	0.496376
oleic acid	0.846094	0.517931
benzoic acid	0.83886	0.542979
phenol	0.821893	0.506262
vanillic acid	0.815894	0.586388
formic acid	0.797337	1.11156
catechol	0.777314	0.804984
acetic acid	0.750705	0.698727
octadecanoic acid	0.742762	0.632192
threonic acid	0.728659	0.974063
2-pentenoic acid	0.693931	0.447611
2-methyl-2-ene-butyric acid	0.674098	0.460869
2-hydroxy-butyric acid	0.636833	0.580799
propionic acid	0.561501	0.318195
furanacetic acid	0.190775	0.866551