

Flavor-Toxicant Correlation in E-cigarettes: A Meta-Analysis

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Table S1. A List of chemical compounds identified in the meta-analysis with structural information.

Chemical	FG*1	FG2	FG3	FG4
1,4-Cineole	Ether			
1-Amyl alcohol	Alcohol			
1-Ethenyloxy pentane	Alkene	Ether		
1-Pentanol	Alcohol			
2,3,5,6-Tetramethylpyrazine	Pyrazine			
2,3,5-Trimethylpyrazine	Pyrazine			
2,3-Butanedione	Diketone			
2,3-Pentanedione	Diketone			
2,5-Dimethylpyrazine	Pyrazine			
2,6-Dimethyl-1,8-naphthyridine	Pyridine			
2,6-Dimethyl-4-propyl pyridine	Pyridine			
2,6-Dimethylpyridine	Pyridine			
2-Acetylpyridine	Ketone	Pyridine		
2-Ethoxy-1-(3' pyridyl) ethylene	Alkene	Ether	Pyridine	
2-Isopropyl-4-methylthiazole	Thiazole			
2-Isopropyl-5-methylhex-2-enal	Aldehyde	Alkene		
2-Methoxy-4-propylphenol	Ether	Phenol		
2-Methylbutyl acetate	Ester			
2-Methylbutyrate	Ester			
2-Methylpyrazine	Pyrazine			
3-Methyl-1-phenyl-1H-pyrazole	Aryl	Pyrazole		
3-Methylcoumarin	Alkene	Aryl	Ester	
3-Methylcyclopentane-1,2-dione	Diketone			
4-(4-Hydroxyphenyl)butan-2-one	Ketone	Phenol		
4,4-Dimethyloxolan-2-one	Lactone			
4-Methoxy benzaldehyde	Aldehyde	Aryl	Ether	
4-Methylacetophenone	Aryl	Ketone		
5-Methylfurfural	Aldehyde	Furan		
6-Methyl-5-hepten-2-one	Alkene	Ketone		
6-Methylcoumarin	Alkene	Aryl	Ester	
7-Methylcoumarin	Alkene	Aryl	Ester	
Acetaldehyde hexamethylenediazone	Hydrazone			
Acetoin	Alcohol	Ketone		
Acetophenone	Aryl	Ketone		
Acetylpyrazine	Ketone	Pyrazine		
Acetylpyrrole	Ketone	Pyrrole		
Allyl cyclohexanepropionate	Alkene	Ester		
Allyl hexanoate	Alkene	Ester		
Amyl acetate	Ester			

Amyl butyrate	Ester		
Anethole	Alkene	Aryl	Ether
Anisyl acetate	Aryl	Ester	Ether
Benzaldehyde	Aldehyde	Aryl	
Benzyl acetate	Aryl	Ester	
Benzyl Alcohol	Alcohol	Aryl	
Benzyl Benzoate	Aryl	Ester	
Benzyl butyrate	Aryl	Ester	
Benzyl cinnamate	Alkene	Aryl	Ester
Benzyl propanoate	Aryl	Ester	
Butyl butyrate	Ester		
Butyl butyrolactate	Ester		
Caffeine	Pyrimidinedione	Imidazole	
Camfor	Ketone		
Carvone	Ketone	Alkene	
Cinnamaldehyde	Aldehyde	Alkene	Aryl
Cinnamyl alcohol	Alcohol	Alkene	Aryl
Cinnamyl isovalerate	Alkene	Aryl	Ester
Cis-3-Hexenal	Aldehyde	Alkene	
Cis-3-Hexenol	Alcohol	Alkene	
Cis-3-Hexenylacetate	Alkene	Ester	
Cis-3-Hexenylvalerate	Alkene	Ester	
Cis-Limonene oxide	Alkene	Epoxide	
Citral	Aldehyde	Alkene	
Citronellol	Alcohol	Alkene	
Cocal	Aldehyde	Alkene	Aryl
Corylone	Diketone		
Coumarin	Alkene	Aryl	Lactone
Decanal	Aldehyde		
Diethyl succinate	Ester		
Estragole	Alkene	Aryl	Ether
Ethanol	Alcohol		
Ethyl 2-methyl butanoate	Ester		
Ethyl 3-methyl-3-phenyloxirane-2-carboxylate	Aryl	Epoxide	Ester
Ethyl acetate	Ester		
Ethyl acetoacetate	Ester	Ketone	
Ethyl anthranilate	Aryl	Ester	Amine
Ethyl butanoate	Ester		
Ethyl caproate	Ester		
Ethyl caprylate	Ester		
Ethyl cinnamate	Alkene	Aryl	Ester
Ethyl heptanoate	Ester		
Ethyl hexanoate	Ester		

Ethyl isovalerate	Ester			
Ethyl lactate	Alcohol	Ester		
Ethyl maltol	Alcohol	Alkene	Ether	Ketone
Ethyl phenylacetate	Aryl	Ester		
Ethyl propanoate	Ester			
Ethyl Salicylate	Ester	Phenol		
Ethyl vanillin	Aldehyde	Ether	Phenol	
Ethyl-methyl-hydroxymethyl amine	Alcohol	Amine		
Eucalyptol	Ether			
Eugenol	Alkene	Ether	Phenol	
Fenchol	Alcohol			
Furaneol	Alcohol	Alkene	Ether	Ketone
Furfural	Aldehyde	Furan		
Furfuryl alcohol	Alcohol	Furan		
Geranyl propanoate	Alkene	Ester		
Guaiacol	Ether	Phenol		
Hedione	Ester	Ketone		
Heliotropine	Aldehyde	Aryl	Ether	
Hemineurine	Thiazole	Alcohol		
Hexanol	Alcohol			
Hexyl 2-methylbutyrate	Ester			
Hexyl acetate	Ester			
Hexyl hexanoate	Ester			
Hydrocoumarin	Aryl	Lactone		
Hydroxyacetone	Alcohol	Ketone		
hydroxydihydrocarvone	Alcohol	Alkene	Ketone	
Isoamyl butyrate	Ester			
Isoamyl isovalerate	Ester			
Isoamyl phenylacetate	Aryl	Ester		
Isobutyl acetate	Ester			
Isopentyl acetate	Ester			
Isopentyl alcohol	Alcohol			
Isopulegol	Alcohol	Alkene		
Isosafroeugenol	Alkene	Ether	Phenol	
Limonene	Alkene			
Linalool	Alcohol	Alkene		
Linalool oxide	Alcohol	Alkene	Ether	
Linalyl acetate	Alkene	Ester		
L-menthyl acetate	Ester			
Luminol	Aryl	Amine	Amide	
Maltol	Alcohol	Alkene	Ether	Ketone
Melonal	Aldehyde	Alkene		
Menthol	Alcohol			

Menthone	Ketone		
Methyl 3-hydroxyhexanoate	Alcohol	Ester	
Methyl anthranilate	Aryl	Ester	Amine
Methyl cinnamate	Alkene	Aryl	Ester
Methyl cyclopentenolone	Alcohol	Alkene	Ketone
Methyl heptenone	Alkene	Ketone	
Methyl salicylate	Ester	Phenol	
Neomenthol	Alcohol		
Nerol	Alcohol	Alkene	
Nerol acetate	Alkene	Ester	
p-Anisaldehyde	Aldehyde	Aryl	Ether
p-Cymene	Aryl		
Phenethyl alcohol	Alcohol	Aryl	
Phenethyl isovalerate	Aryl	Ester	
Piperitone	Alkene	Ketone	
Piperonal	Aldehyde	Aryl	Ether
p-Tolualdehyde	Aldehyde	Aryl	
Pulegone	Alkene	Ketone	
Pyridine	Pyridine		
Styralyl acetate	Aryl	Ester	
Tetrahydrolinalool	Alcohol		
Theaspirane	Alkene	Ether	
Thymol	Phenol		
Trans-2-Hexenol	Alcohol	Alkene	
Triacetin	Ester		
Vanillin	Aldehyde	Ether	Phenol
α,α -Dimethylphenethyl butyrate	Aryl	Ester	
α -Ionone	Alkene	Ketone	
α -Pinene	Alkene		
α -Terpineol	Alcohol	Alkene	
β -Damascone	Alkene	Ketone	
β -Ionone	Alkene	Ketone	
β -Myrcene	Alkene		
β -Pinene	Alkene		
γ -Butyrolactone	Lactone		
γ -Decalactone	Lactone		
γ -Dodecalactone	Lactone		
γ -Hexalactone	Lactone		
γ -Ionone	Alkene	Ketone	
γ -Nonalactone	Lactone		
γ -Octalactone	Lactone		
γ -Terpinene	Alkene		
γ -Undecalactone	Lactone		

γ -Valerolactone	Lactone
δ -Decalactone	Lactone
δ -Dodecalactone	Lactone
δ -Tetradecalactone	Lactone
δ -undecalactone	Lactone

* FG: functional group.