Open Characterization of vaping liquids in Canada: chemical profiles and trends

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Supplementary Material

Table S1: Chemical compounds of analytical grade or higher purchased from Sigma Aldrich Canada.

| CASRN     | Common Name               | Chemical Name                                      |
|-----------|---------------------------|---------------------------------------------------|
| 928-96-1  | (3Z)-3-Hexen-1-ol         | Leaf alcohol                                      |
| 115-95-7  | 1,6-octadien-3-ol, 3,7-dimethyl-, acetate | 1,6-octadien-3-ol, 3,7-dimethyl-, acetate         |
| 71-41-0   | 1-amylalcohol             | 1-amylalcohol                                     |
| 123-92-2  | 1-butanol, 3-methyl-, acetate | 1-butanol, 3-methyl-, acetate                     |
| 23726-92-3| 1-Damascone               | 1-Damascone                                       |
| 111-27-3  | 1-hexanol                 | 1-hexanol                                         |
| 108-48-5  | 2,6 ethylpyridine         | 2,6 ethylpyridine                                |
| 1124-11-4 | 2356-Tetramethylpyrazine  | 2356-Tetramethylpyrazine                         |
| 1072-83-9 | 2-acetylpyrrole           | 2-acetylpyrrole                                  |
| Number      | Compound                          | Compound                          |
|-------------|-----------------------------------|-----------------------------------|
| 15679-19-3 | 2-isopropyl-4-methylthiazole      | 2-isopropyl-4-methylthiazole      |
| 35158-25-9 | 2-isopropyl-5-methyl-2-hexenal    | 2-isopropyl-5-methyl-2-hexenal    |
| 119-84-6   | 3,4-dihydrocoumarin               | 3,4-dihydrocoumarin               |
| 93-18-5    | 3-methyl-3-phenylglycidate        | 3-methyl-3-phenylglycidate        |
| 122-00-9   | 4-methylacetophenone              | 4-methylacetophenone              |
| 620-02-0   | 5-methylfurfural                  | 5-methylfurfural                  |
| 24851-98-7 | Methyl dihydrojasmonate           | methyl 2-(3-oxo-2-pentylcyclopentyl)acetate |
| 10094-34-5 | a,a-dimethylphenethyl butyrate    | a,a-dimethylphenethyl butyrate    |
| 22047-25-2 | acetylpyrazine                    | acetylpyrazine                    |
| 127-41-3   | a-ionone                          | Alpha-ionone                      |
| 104-21-2   | Anisyl acetate                   | Anisyl acetate                   |
| 98-55-5    | a-terpineol                       | a-terpineol                       |
| 80450-69-7 | cis-Hedione                       | cis-Hedione                       |
| 100-52-7   | Benzaldehyde                      | Benzaldehyde                      |
| 2568-25-4  | Benzaldehyde PG acetal            | Benzaldehyde PG acetal            |
| 101-97-3   | benzeneacetic acid, ethyl ester   | benzeneacetic acid, ethyl ester   |
| 140-11-4   | Benzyl acetate                   | Benzyl acetate                   |
| 100-51-6   | Benzyl alcohol                    | Benzyl alcohol                    |
| 106-27-4   | butanoic acid, 3-methylbutyl ester| butanoic acid, 3-methylbutyl ester|
| 3681-71-8  | Cis-3-hexenyl acetate            | Cis-3-hexenyl acetate            |
| Number     | Compound                        | Compound                        |
|------------|---------------------------------|---------------------------------|
| 35852-46-1 | cis-3-hexenyli-valerate         | cis-3-hexenyli-valerate         |
| 106-22-9   | Citronellol                     | Citronellol                     |
| 21834-92-4 | Cocal                           | Cocal                           |
| 80-71-7    | Corylone                        | Corylone                        |
| 112-31-2   | Decanal                         | Decanal                         |
| 105-53-3   | Diethyl malonate                | Diethyl malonate                |
| 123-25-1   | Diethyl succinate               | butanedioic acid, diethyl ester |
| 89-78-1    | DL-Menthol                      | DL-Menthol                      |
| 1122-62-9  | ethanone, 1-(2-pyridinyl)-      | ethanone, 1-(2-pyridinyl)-      |
| 13327-56-5 | Ethyl 3-(methylthio)propionate  | Ethyl 3-(methylthio)propionate  |
| 141-97-9   | Ethyl acetoacetate              | Ethyl acetoacetate              |
| 103-36-6   | Ethyl cinnamate                 | Ethyl cinnamate                 |
| 106-30-9   | Ethyl heptanoate                | Ethyl heptanoate                |
| 123-66-0   | Ethyl hexanoate                 | Ethyl hexanoate                 |
| 97-64-3    | Ethyl lactate                   | Ethyl lactate                   |
| 4940-11-8  | Ethyl maltol                    | 2-Ethyl-3-hydroxy-4-pyrene      |
| 121-32-4   | Ethyl vanillin                  | Ethyl vanillin                  |
| 7452-79-1  | Ethyl-2-methylbutyrate          | butanoic acid, 2-methyl-, ethyl ester |
| 97-53-0    | Eugenol                         | Eugenol                         |
| 3658-77-3  | Furaneol                        | Furaneol                        |
| CAS Number | Chemical Name          | Chemical Name          |
|------------|------------------------|------------------------|
| 98-00-0    | Furfuryl alcohol       | Furfuryl alcohol       |
| 96-48-0    | gamma-butyrolactone    | gamma-butyrolactone    |
| 2305-05-7  | g-dodecalactone        | g-dodecalactone        |
| 105-90-8   | Geranyl propionate     | Geranyl propionate     |
| 695-06-7   | g-hexalactone          | g-hexalactone          |
| 56-81-5    | Glycerol               | Propane-1,2,3-triol    |
| 108-29-2   | g-valeroactone         | g-valeroactone         |
| 142-92-7   | Hexyl acetate          | Hexyl acetate          |
| 6378-65-0  | Hexyl hexanoate        | Hexyl hexanoate        |
| 659-70-1   | Isoamyl isovalerate    | Isoamyl isovalerate    |
| 6728-26-3  | Leaf aldehyde          | Leaf aldehyde          |
| 138-86-3   | Limonene               | Limonene               |
| 78-70-6    | Linalool               | Linalool               |
| 60047-17-8 | Linalool oxide         | Linalool oxide         |
| 79-20-9    | L-menthyl acetate      | L-menthyl acetate/menthyl acetate |
| 118-71-8   | Maltol                 | Maltol                 |
| 106-72-9   | Melonal                | Melonal                |
| 1490-04-6  | Menthol                | Menthol                |
| 89-80-5    | Menthone               | Menthone               |
| 103-26-4   | Methyl cinnamate       | Methyl cinnamate       |
| Code     | Compound                      | Code     | Compound                      |
|----------|-------------------------------|----------|-------------------------------|
| 110-93-0 | Methyl heptenone              | 110-93-0 | Methyl heptenone              |
| 119-36-8 | Methyl salicylate             | 119-36-8 | Methyl salicylate             |
| 106-25-2 | Nerol + geraniol              | 106-25-2 | Nerol + geraniol              |
| 54-11-5  | Nicotine                      | 54-11-5  | Nicotine                      |
| 487-19-4 | Nicotyrine                    | 487-19-4 | 3-(1-methylpyrrol-2-yl)pyridine |
| 140-26-1 | Phenethyl isovalerate         | 140-26-1 | Phenethyl isovalerate         |
| 57-55-6  | Propane-1,2-diol              | 57-55-6  | Propylene Glycol              |
| 123-32-0 | Pyrazine, 2,5-dimethyl-       | 123-32-0 | Pyrazine, 2,5-dimethyl-       |
| 109-08-0 | Pyrazine, methyl-             | 109-08-0 | Pyrazine, methyl-             |
| 110-86-1 | pyridine                      | 110-86-1 | pyridine                      |
| 5471-51-2| Raspberry ketone              | 5471-51-2| Raspberry ketone              |
| 93-92-5  | Styralyl acetate              | 93-92-5  | Styralyl acetate              |
| 78-69-3  | Tetrahydrolinalol             | 78-69-3  | Tetrahydrolinalol             |
| 36431-72-8| Theaspirane                   | 36431-72-8| Theaspirane                   |
| 928-95-0 | trans-2-hexenol               | 928-95-0 | (E)-2-Hexen-1-ol              |
| 14667-55-1| Trimethyl-pyrazine            | 14667-55-1| pyrazine, trimethyl-          |
| 121-33-5 | Vanillin                      | 121-33-5 | Vanillin                      |
| 706-14-9 | γ-Decalactone                 | 706-14-9 | γ-Decalactone                 |
| 104-61-0 | γ-Nonalactone                 | 104-61-0 | γ-Nonalactone                 |
| 705-86-2 | δ-decalactone                 | 705-86-2 | δ-decalactone                 |
| Ref ID | Reference Type | Authors, Primary | Periodical Abbrev | Pub Year | Volume | Issue | Start Page |
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| 3     | Journal Article | Barrington-Trimis, J. L.; et al. | JAMA | 2014 | 312 | 23 | 249/3 |
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| 5     | Journal Article | Behar, R. Z. et al. | Toxicol. In Vitro | 2014 | 28 | 2 | 198 |
| 6     | Journal Article | Bekki, K. et al. | Int. J. Environ. Res. Public. Health. | 2014 | 11 | 11 | 111/92 |
| 7     | Journal Article | Benowitz, N. L. et al. | JAMA | 2013 | 310 | 7 | 685 |
| 8     | Journal Article | Bertholon, J. F. et al. | Respiration | 2013 | 86 | 5 | 433 |
| 9     | Journal Article | Bhatnagar, A. et al. | Circulation | 2014 | 130 | 16 | 141/8 |
| 10    | Journal Article | Burstyn, I. | BMC Public Health | 2014 | 14 | | 18 |
| 11    | Journal Article | Cahn, Z. et al. | J. Public Health Policy | 2011 | 32 | 1 | 16 |
|   | Journal Article | Callahan-Lyon, P. | Tob. Control | 2014 | ii36 |
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| 13 | Journal Article | Cervellati, F. et al. | Toxicol. In. Vitro. | 2014 | 28 5 999 |
| 14 | Journal Article | Chatham-Stephens, K. et al. | MMWR Morb. Mortal. Wkly. Rep. | 2014 | 63 13 292 |
| 15 | Journal Article | Chen, I. L. | Nicotine Tob. Res. | 2013 | 15 2 615 |
| 16 | Journal Article | Cheng, T. | Tob. Control | 2014 | ii11 |
| 17 | Journal Article | Czogala, J. et al. | Nicotine Tob. Res. | 2014 | 16 6 655 |
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| 32  | Journal Article | Goniewicz, M. L. et al. | Addiction | 2014 | 109 | 3 | 500 |
| 33  | Journal Article | Goniewicz, M. L. et al. | Tob.Control | 2014 | 23 | 2 | 133 |
| 34  | Journal Article | Goniewicz, M. L. et al. | Nicotine Tob.Res. | 2013 | 15 | 1 | 158 |
| 35  | Journal Article | Goniewicz, M. L. et al. | Nicotine Tob.Res. | 2015 | 17 | 2 | 256 |
| 36  | Journal Article | Grana, R. et al. | Circulation | 2014 | 129 | 19 | 197 |
| 37  | Journal Article | Hahn, J. et al. | Tob Induc Dis. | 2014 | 12 | 1 | 23 |
| 38  | Journal Article | Hajek, P. et al. | Addiction | 2014 | 109 | 11 | 180 |
| 39  | Journal Article | Hajek, P. et al. | Nicotine Tob.Res. | 2015 | 17 | 2 | 175 |
| 40  | Journal Article | Ingebrethsen, B. J. et al. | Inhal.Toxicol. | 2012 | 24 | 14 | 976 |
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| 42  | Journal Article | Laugesen, M. | | 2008 | | | |
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| 44 | Journal Article | Manigrasso, M. et al. | Environ.Pollut. | 2015 | 196  | 257    |
| 45 | Journal Article | Manigrasso, M. et al. | Environ.Pollut. | 2015 | 202  | 24     |
| 46 | Journal Article | McAuley, T. R. et al. | Inhal.Toxicol. | 2012 | 24   | 12     | 850    |
| 47 | Journal Article | McAuley, L. et al. | Chest | 2012 | 141  | 4      | 1110   |
| 48 | Journal Article | Misra, M. et al. | Int.J.Environ.Res.Public.Health. | 2014 | 11   | 11     | 11325  |
| 49 | Journal Article | Oh, A. Y. et al. | Laryngoscope | 2014 | 124  | 12     | 2702   |
| 50 | Journal Article | Orr, M. S. | Tob.Control | 2014 |      | ii18   |
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| 52 | Journal Article | Paradise, J. | Yale J.Health.Policy. Law.Ethics | 2013 | 13   | 2      | 326    |
| 53 | Journal Article | Pellegrino, R. M. et al. | Ann.Ig. | 2012 | 24   | 4      | 279    |
| 54 | Journal Article | Romagna, G. et al. | Inhal.Toxicol. | 2013 | 25   | 6      | 354    |
| 55 | Journal Article | Schober, W. et al. | Int.J.Hyg.Environ.Health | 2014 | 217  | 6      | 628    |
| 56 | Journal Article | Schraufnagel, D. E. | Pediatr.Allergy Immunol.Pulmonol. | 2015 | 28   | 1      | 2      |
| 57 | Journal Article | Schroeder, M. J. et al. | Tob.Control | 2014 | ii30 |
| 58 | Journal Article | Trtchounian, A. et al. | Nicotine Tob.Res. | 2010 | 12 | 9 | 905 |
| 59 | Journal Article | Vansickel, A. R. et al. | Cancer Epidemiol. Biomarkers Prev. | 2010 | 19 | 8 | 1945 |
| 60 | Journal Article | Vansickel, A. R. et al. | Nicotine Tob.Res. | 2013 | 15 | 1 | 267 |
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| 62 | Journal Article | Williams, M. et al. | PLoS One | 2013 | 8 | 3 | e57987 |
| 63 | Journal Article | Yan, X. S. et al. | Regul.Toxicol.Pharmacol. | 2015 | 71 | 1 | 24 |
| 64 | Journal Article | Hureaux, J. et al. | Thorax | 2014 | 69 | 6 | 596 |
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| 66 | Journal Article | Westenberger, B., J. | | 2009 | |
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| 68 | Journal Article | Farsalinos, K. E. et al. | Int.J.Environ.Res.Publ.Health. | 2015 | 12 | 4 | 3439 |
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| 72 | Journal Article | Lerner, C. A. et al. | PLoS One      | 2015 | 10   | 2 | e01 167 32 |
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| 76 | Journal Article | Talih, S. et al.       | Nicotine Tob.Res. | 2015 | 17   | 2 | 150 |
| 77 | Journal Article | Hutzler, C. et al.     | Arch.Toxicol. | 2014 | 88   | 7 | 129 5 |
| 78 | Journal Article | Marini, S. et al.      | Toxicol.Appl.Pharmacol. | 2014 | 278  | 1 | 9 |
| 79 | Journal Article | Ruprecht, A. A. et al. | Tumori        | 2014 | 100  | 1 | e24 |
| 80 | Journal Article | Kim, H. J. et al.      | J.Chromatogr.A | 2013 | 1291 |    | 48 |
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| 103| Journal Article | Lerner, C. A. et al. | Environ. Pollut. | 2015 | 198 | 100 |
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| 129 | Web Page        | ABC News        | 2015 | 2015 | 4215 | 6 |
| 130 | Web Page        | The Jerusalem Post | 2013 | 2015 | 4215 | 6 |
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| 133 | Journal Article | Fowles, J. R. et al. | Crit. Rev. Toxicol. | 2013 | 43 | 4 | 363 |
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| 141 | Journal Article | Farsalinos, K. E. et al. | Sci. Rep. | 2015 | 5 |   | 112 69 |
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| 143 | Journal Article | Rubenstein, D. A. et al. | Mol. Immunol. | 2015 |        |       |       |
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Section 1: Open Characterization Project- Assigning roles to detected chemicals in vaping liquids

A wide variety of chemical compounds in vaping products have been detected in the Open Characterization Project. These chemicals have been assigned roles in order to have a better understanding of the part they may play within a vaping liquid. To identify the likely role(s) of each chemical compound, a literature synthesis was conducted which involved drawing from a variety of sources including published literature, open source websites (PubChem (National Institutes of Health (NIH) 2021a), Chem Spider ((Royal Society of Chemistry 2021)), The Human Metabolome Database (HMDB) (Wishart et al. 2018), Flavor DB (Garg et al. 2018), FooDB (Harrington et al. 2019)), manufacturer specifications, patents, Safety Data Sheets (SDS) and other. In addition, a number of chemical compounds are assigned roles based on an in-house database of chemicals which was developed between 2015 and 2017, namely eCigDB. This database of chemical compounds in vaping liquids was compiled from previously reported peer-reviewed studies and used to create a list of expected compounds in vaping products as well as increase confidence in the chemicals identified in the Open Characterization Project.

Chemicals are classified into at least one of the six (6) roles listed below. Each of the roles includes examples of supporting literature to help illustrate how roles were developed and assigned to the various chemicals.

Assigned roles for detected chemicals:

1.) Alkaloids - Class of organic compounds that contain a basic nitrogen atom. In vaping liquids, these most frequently include nicotine and nicotine-related minor alkaloids. Supporting literature used to
assign this role are published scientific studies from PubMed, data obtained from PubChem, and also the following data sources:
- The Chemical Components of Tobacco and Tobacco Smoke by Alan Rodgman, Thomas A. Perfetti (Second Edition)
- Chemistry of alkaloids by P.B. Saxena (2007)

2.) Processing - Various chemical compounds known to be used in the manufacture of vaping and tobacco products, flavours and food industry such as solvents, diluents, and processing agents. In addition to patents, PubChem, Chem Spider and other open sources the following resources were used:
- Good Scents website (Good Scents Company 2021)
- Leffingwell database (Leffingwell & Associates 2011)
- Manufacture’s web pages e.g. The Perfumer’s Apprentice (The Flavor and Perfumer’s Apprentice 2021)
- Substances Added to Food (formerly Everything Added to Foods in the United States (EAFUS))(U.S. Food and Drug Administration 2021)
- Directories for chemical suppliers, which often lists fine chemicals and describes type of chemical synthesis e.g. LookChem

3.) Natural Extracts - Natural extracts are generally complex mixtures of individual chemical compounds previously detected in extracts of living organisms (examples include plants and animals). These chemical compounds may have organoleptic properties and are most frequently searched for on PubChem, Good Scents, FooDB, and HMDB. PubMed searches with these names and CAS numbers often yield examples of non-targeted studies on extracts or essential oils of various plants and where these compounds might be present.

4.) Flavours and Fragrances - Chemical compounds that have organoleptic/sensory properties and are known to impart flavour and/or odour. In most cases data sources are Leffingwell Flavor-Base, Good Scent Company, The Flavor and Extract Manufacturers Association (FEMA)((FEMA) 2021), Joint FAO/WHO Expert Committee on Food Additives (JECFA)(Food and Agriculture Organization of United Nations 2021) and Fenaroli’s Handbook on Flavour Ingredients (Burdock 2016). In addition, online resources from suppliers of raw aromatic and flavour materials were used as well e.g. The Flavor and Perfumer’s Apprentice (The Flavor and Perfumer’s Apprentice 2021)

5.) Indirect Additive/Leaching/Degradation - Chemical compounds previously detected as indirect additives in food contact materials. This category also includes chemicals known to be associated with degradation of various other chemical compounds found to be present in the individual samples, for example, glycidol being a degradation product of glycerin. Sources of information include PubChem, Substances Added to Food (formerly EAFUS) and searching of published studies on degradation, indirect food contact additives and leaching of various components of vaping liquids.

6.) Unknown roles - Two types of chemical compounds are identified with unknown roles:
   (1) Chemicals whose identities are not known. Chemicals whose identities are unknown are those that are true unknowns, meaning upon use of spectral library and spectral matching no appropriate chemical match was found in any mass spectral library used; National Institute of Standards and Technology (NIST), Wiley or Flavors and Fragrances of Natural and Synthetic Compounds. Since no International Union of Pure and Applied Chemistry (IUPAC) chemical name or
Chemical Abstracts Service (CAS) number could be identified for these chemical compounds their roles could not be determined.

(2) Chemicals for which identities are tentatively identified. There are a number of chemical compounds detected in vaping liquids for which identification is tentatively assigned (chemical name and CAS known) but for which literature synthesis generated none or inconclusive data. For example, a proportion of these chemical compounds with unknown role in vaping liquids did have matches with chemical compounds previously detected in yeast extract. Data matching was accomplished through publicly available informatics platform and data repository Yeast Resource Centre (University of Washington 2018). Yeast extract is a mixture of individual chemical compounds that may be used as food flavouring or enhancer(U.S. Food and Drug Administration 2020). Although a number of yeast related compounds detected in the Open Characterization Project could be originating from the yeast extract used for flavouring, some could be present as a result of product ageing, fermentation or presence of other microbes.

*Chemicals with multiple roles*

According to literature pertaining to the detected chemicals some may play multiple roles in vaping liquids, therefore more than one role may be assigned to a particular chemical. For example, a chemical may be found in a natural extract as well as have organoleptic properties, thus this chemical would be assigned the roles of natural extract and flavour. Literature used for assigning multiple roles have been discussed under various roles listed above.

**Section 2: Open Characterization Project- Analytical method validation and performance**

The analytical methods that employ the use of non-targeted analysis are most frequently full-scan methods that do not quantify but rather aim to identify chemical compounds present in the samples analyzed. In operating mass spectrometry detector in a full scan mode concentration levels are not determined, hence the limit of detection or ability to quantify a specific chemical at a prescribed concentration in a consistent manner is not an appropriate measure for method performance. Furthermore, the area under the detected peak for chemical generated in the full scan should not be relied upon to generate a corresponding calibrated concentration level. Instead validation can be performed using the repeated injection of the same sample over a period of time and checking for the detected compounds. In our case we have used laboratory prepared vaping liquid sample consisting of matrix (PG/VG in 50/50 w/w) and nicotine. This sample along with repeat analysis of previously analyzed sample was injected with processing batches or anytime maintenance was performed on the instruments. For example, rough estimates of signal to noise measurements while using full-scan were used for known, laboratory prepared nicotine concentration. Sample of laboratory-prepared vaping liquid containing nicotine, PG/VG and diluted 200 times with methanol were used to simulate and determine at which point nicotine would no longer be detected through varying added concentrations of nicotine and observing signal to noise after each injection. In case of nicotine, limit of detection using full scan was estimated using 3:1 signal to noise and determined at 0.03 mg/mL in this laboratory prepared vaping liquid sample. Such determination for all 1507 chemicals detected is not practical, needed, nor possible given the fact that genuine analytical standards for some infrequently detected chemicals are simply not available for commercial purchase. Further analytical efforts and investments in determining concentrations and limits of detection for non-prioritized compounds would not be justifiable.

Individual limits of detection for analytes of interest have been or will be determined employing the appropriate targeted methods which, depending on the compound, may include chemical extraction prior to analysis and use of labelled internal standards to correct for matrix effects. For example, targeted methodology for quantitation of nicotine has been already developed. Briefly this method employs use of single reaction monitoring (srn) mode while monitoring following ions: Nicotine (m/z) 84 and 162, quantifier and qualifier ions, respectively, Nicotine d7 (m/z) 87 and 169, quantifier and qualifier ions, respectively. Method
that An searched AMDIS Section well from trial, serum compared Characterization LC participating detected due instrumental. similar (Schymanski collaboration instrumental MS/MS limits calculated nicotine (appropriate and using performance of this method he the en same example, and silicone bands published participating laboratories as ENTACT trial’s preliminary results of 2.9% overlap when comparing GC, LC electro-spray ionization (ESI-), and LC ESI+, based methodologies. Higher overlap in Open Characterization study is likely due to a number of factors. First, vaping liquids are chemically less complex compared to the tested samples in both collaboration trials, raw river water (NORMAN), and, house dust, serum and silicone bands (ENTACT). Moreover, our comparison is between two GC MS/MS systems, run in the same laboratory environment with minimal sample pre-treatment, dilution with solvent only. For ENTACT trial, for example, sample extraction and pre-treatment, as well as analytical instruments differed significantly among participating laboratories. Finally, in our study the list of expected or “suspect” chemicals compiled from published literature was identical for two instruments used.

In the end, in order to complete the project of this magnitude in a timely manner, 810 vaping samples were analyzed using only one of the two available instruments. Samples for each instrument were assigned randomly. In order to account for bias in the subsequent targeted analysis, samples with positive detection as well as those with negative will be analyzed.

Section 3: Open Characterization Project- Automated Mass Spectral Deconvolution and Identification System (AMDIS)

AMDIS is an open source software used to aid in interpretation of complex GC/MS generated spectral data. The process is automated where the software detects background traces, calculates automatically noise levels and analyzes data and ion traces to detect peak maxima and unique traces to yield a clean spectra that can be searched in a spectral library (Stein 1999).

An example of a more complex sample of Creamy Custard with labeled 18mg/mL nicotine and 60/40 (PG/VG proportion) is illustrated in Figure S1. AMDIS has been especially useful in identifying detected compounds that co-elute with a very broad glycerol peak such as this one Figure S2.
Figure S1. Chromatogram of Creamy Custard sample with co-eluting unknown peak

Figure S2. Example of AMDIS workflow for Creamy Custard sample
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