Supplementary Material

Non-Targeted Analysis Using Gas Chromatography Mass Spectrometry for Evaluation of Chemical Composition of E-Vapor Products

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Accuracy

A summary of the percent relative standard deviation (%RSD) accuracy results for the 2ppm, 5ppm, and 10ppm fortified matrices are presented for each analyte in Table 1 below.

Table 1. Summary of accuracy results: 2ppm, 5ppm and 10 ppm

| %RSD at 2PPM | Hydroxyacetone | 2,3,5-trimethylpyrazine | Menthone | (E)-Beta-Damascone | Cinnamic acid methyl ester | Myosmine | Piperonal | Cotinine |
|--------------|-----------------|------------------------|---------|-------------------|---------------------------|----------|-----------|----------|
| F1           | NA*             | 21.08                  | 18.81   | 19.15             | 23.17                     | 26.95    | 24.33     | 22.72    |
| F2           | 1.78            | 6.47                   | 4.87    | 1.57              | 2.01                      | 0.43     | 1.88      | 3.00     |
| F3           | 9.05            | 9.55                   | 7.50    | 6.74              | 6.33                      | 7.75     | 7.12      | 78.89**  |
| F4           | 4.98            | 1.12                   | 3.34    | 2.24              | 3.69                      | 4.37     | 2.77      | 7.13     |
| F5           | 10.52           | 7.12                   | 8.27    | 4.60              | 11.52                     | 7.77     | 6.35      | 8.88     |
| %RSD at 5PPM | Hydroxyacetone | 2,3,5-trimethylpyrazine | Menthone | (E)-Beta-Damascone | Cinnamic acid methyl ester | Myosmine | Piperonal | Cotinine |
| F1           | 7.43            | 7.58                   | 9.56    | 6.60              | 6.91                      | 5.83     | 9.03      | 4.70     |
| F2           | 8.68            | 0.17                   | 2.42    | 2.87              | 2.08                      | 2.10     | 4.12      | 2.47     |
| F3           | 9.41            | 7.55                   | 8.40    | 11.68             | 14.12                     | 10.61    | 13.54     | 5.30     |
| F4           | 4.19            | 1.26                   | 3.07    | 2.73              | 1.80                      | 2.31     | 2.57      | 5.84     |
| F5           | 1.91            | 3.74                   | 6.01    | 3.36              | 6.66                      | 3.52     | 8.67      | 2.51     |
| %RSD at 10PPM| Hydroxyacetone | 2,3,5-trimethylpyrazine | Menthone | (E)-Beta-Damascone | Cinnamic acid methyl ester | Myosmine | Piperonal | Cotinine |
| F1           | 9.90            | 2.78                   | 2.26    | 0.40              | 1.66                      | 1.90     | 1.83      | 1.69     |
| F2           | 1.85            | 1.23                   | 3.12    | 2.47              | 0.10                      | 1.02     | 1.77      | 3.06     |
| F3           | 3.48            | 0.84                   | 4.44    | 2.16              | 1.42                      | 1.34     | 3.79      | 1.83     |
| F4           | 5.59            | 4.31                   | 3.32    | 4.67              | 4.36                      | 2.38     | 4.46      | 6.39     |
| F5           | 3.35            | 2.47                   | 4.27    | 1.67              | 2.82                      | 3.97     | 5.52      | 3.22     |
* %RSD could not be calculated because two of the three replicates were below LOD/not detected.
** Highest or lowest of the result set.

### Selectivity

Summary of selectivity data (Table 2 and Table 3) for Product A and Product B e-vapor prototype products that were aged ~2 years.

**Table 2. Product A and Product B e-liquid and aerosol fortification results.**

| Compound                        | Product A – Liquid* | Product B – Liquid* | Product A – Aerosol* | Product B – Aerosol* |
|--------------------------------|---------------------|---------------------|----------------------|----------------------|
| Hydroxyacetone Unfortified (PPM) | ND                  | 10.97               | 23.26                | 14.88                |
| Hydroxyacetone Fortified (PPM)  | 6.22                | 13.85               | 29.07                | 21.15                |
| **Difference (PPM)**            | **6.22**            | **2.89**            | **5.80**             | **6.28**             |
| Trimethylpyrazine Unfortified (PPM) | ND                  | ND                  | ND                   | ND                   |
| Trimethylpyrazine Fortified (PPM) | 16.09               | 13.97               | 24.37                | 21.51                |
| **Difference (PPM)**            | **16.09**           | **13.97**           | **24.37**            | **21.51**            |
| Menthone Unfortified (PPM)      | ND                  | 304.63              | ND                   | 266.63               |
| Menthone Fortified (PPM)        | 7.20                | 309.86              | ND                   | 290.88               |
| **Difference (PPM)**            | **7.20**            | **5.23**            | **11.62**            | **24.25**            |
| (E)-Beta-Damascone Unfortified (PPM) | ND                  | ND                  | ND                   | ND                   |
| (E)-Beta-Damascone Fortified (PPM) | 12.37               | 20.74               | 18.38                | 21.68                |
| **Difference (PPM)**            | **12.37**           | **20.74**           | **18.38**            | **21.68**            |
| Cinnamic acid methyl ester Unfortified (PPM) | ND                  | ND                  | ND                   | ND                   |
| Cinnamic acid methyl ester Fortified (PPM) | 15.44               | 14.92               | 23.84                | 21.84                |
| **Difference (PPM)**            | **15.44**           | **14.92**           | **23.84**            | **21.84**            |
| Myosmine Unfortified (PPM)      | 7.08                | 16.48               | 10.85                | 22.01                |
| Myosmine Fortified (PPM)        | 17.41               | 28.50               | 27.35                | 37.16                |
| **Difference (PPM)**            | **10.33**           | **12.02**           | **16.49**            | **15.15**            |
| Piperonal Unfortified (PPM)     | ND                  | ND                  | ND                   | ND                   |
| Piperonal Fortified (PPM)       | 16.58               | 17.12               | 24.32                | 23.12                |
| **Difference (PPM)**            | **16.58**           | **17.12**           | **24.32**            | **23.12**            |
| Cotinine Unfortified (PPM)      | 4.88                | 4.53                | 8.68                 | 8.50                 |
| Cotinine Fortified (PPM)        | 16.25               | 17.17               | 24.80                | 24.21                |
| **Difference (PPM)**            | **11.37**           | **12.64**           | **16.12**            | **15.70**            |

(* The average estimated concentration results for 3 replicates, n=3.*)
Table 3. Product A and Product B e-liquid and aerosol average match factor scores and correct identification

| Selectivity samples                  | Average Match Factor Score | Correct/Incorrect | % Identified correctly |
|--------------------------------------|----------------------------|-------------------|------------------------|
| Product A Unfortified (E-liquid)     | 95.0                       | NA                | NA                     |
| Product A Fortified (E-liquid)       | 90.1                       | 23/24             | 95.8                   |
| Product B Unfortified (E-liquid)     | 94.6                       | NA                | NA                     |
| Product B Fortified (E-liquid)       | 91.6                       | 24/24             | 100.0                  |
| Product A Unfortified (Aerosol)      | 92.6                       | NA                | NA                     |
| Product A Fortified (Aerosol)        | 92.8                       | 24/24             | 100.0                  |
| Product B Unfortified (Aerosol)      | 92.4                       | NA                | NA                     |
| Product B Fortified (Aerosol)        | 91.6                       | 24/24             | 100.0                  |
| Overall Average                      | 92.6                       | 95/96             | 99.0                   |

Limit of Detection

Summary of the match factor score and S/N for each analyte for 0.7 ppm fortified F1-matrix analysis.

Table 4: Analysis of 0.7ppm fortified F1 matrix

| F1 Matrix | Compound       | PPM (Estimated Conc)* | Match Factor | S/N  |
|-----------|----------------|-----------------------|--------------|------|
| Blank     | Hydroxyacetone | ND                    | NA           | NA   |
| Replicate 1 |              | ND                    | NA           | NA   |
| Replicate 2 |              | ND                    | NA           | NA   |
| Replicate 3 |              | ND                    | NA           | NA   |
| Replicate 4 |              | ND                    | NA           | NA   |
| Replicate 5 |              | ND                    | NA           | NA   |
| Replicate 6 |              | ND                    | NA           | NA   |
| Blank     | Trimethylpyrazine | ND                  | NA           | NA   |
| Replicate 1 |              | ND                    | NA           | NA   |
| Replicate 2 |              | ND                    | NA           | NA   |
| Replicate 3 |              | ND                    | NA           | NA   |
| Replicate 4 |              | ND                    | NA           | NA   |
| Replicate 5 |              | ND                    | NA           | NA   |
| Replicate 6 |              | ND                    | NA           | NA   |
| Blank     | Menthone      | 0.41                  | 78.8         | 17.61|
| Replicate 1 |              | 0.45                  | 89.6         | 18.66|
| Replicate 2 |              | 0.43                  | 78.7         | 15.54|
| Replicate 3 |              | 0.38                  | 78.8         | 16.31|
| Replicate 4 |              | 0.41                  | 78.7         | 19.27|
| Replicate 5 |              | 0.43                  | 78.8         | 17.93|
| Blank     | (E)-Beta-Damascone | ND                  | NA           | NA   |
| Replicate 1 |              | ND                    | NA           | NA   |
| F1 Matrix | Compound | PPM (Estimated Conc)* | Match Factor | S/N |
|-----------|----------|----------------------|--------------|-----|
| Replicate 2 | ND | NA | NA |
| Replicate 3 | ND | NA | NA |
| Replicate 4 | ND | NA | NA |
| Replicate 5 | ND | NA | NA |
| Replicate 6 | ND | NA | NA |
| Blank | ND | NA | NA |
| Replicate 1 | 0.97 | 88 | 8.59 |
| Replicate 2 | 0.89 | 88 | 8.45 |
| Replicate 3 | ND | NA | NA |
| Replicate 4 | ND | NA | NA |
| Replicate 5 | ND | NA | NA |
| Replicate 6 | ND | NA | NA |

Cinnamic acid methyl ester

| Blank | ND | NA | NA |
| Replicate 1 | 3.91 | 93.9 | 81.09 |
| Replicate 2 | 4.54 | 93.9 | 94.1 |
| Replicate 3 | 5.03 | 92.9 | 118.79 |
| Replicate 4 | 4.68 | 93.3 | 69.84 |
| Replicate 5 | 4.97 | 92.2 | 100.4 |
| Replicate 6 | 5.07 | 92.2 | 106.52 |

| Blank | ND | NA | NA |
| Replicate 1 | 0.99 | 71.9 | 45.8 |
| Replicate 2 | 1.02 | 71.9 | 29.96 |
| Replicate 3 | 0.91 | 72 | 30.5 |
| Replicate 4 | 0.92 | 71.9 | 27.79 |
| Replicate 5 | 1.00 | 71.9 | 38.99 |
| Replicate 6 | 1.00 | 72 | 35.02 |

| Blank | ND | NA | NA |
| Replicate 1 | 4.97 | 92.4 | 121.71 |
| Replicate 2 | 5.36 | 93.2 | 131.85 |
| Replicate 3 | 6.03 | 94.2 | 145.55 |
| Replicate 4 | 6.26 | 92.8 | 132.91 |
| Replicate 5 | 5.43 | 86.8 | 113.54 |
| Replicate 6 | 5.87 | 92.8 | 97.43 |

| Blank | ND | NA | NA |
| Replicate 1 | 6.01 | 91.6 | 126.7 |

(ND - Not detected; NA - Not applicable)

**Threshold of significant change**

Individual replicate data for determination of threshold for significant change for all matrices is summarized in Table 5. Fold increase was calculated as (Xt) divided by (Xc), where, Xc is the grand mean of the three day intermediate precision value for each analyte and Xt is the calculated value for a measurable increase, (Xc+6S.D.).
Table 5. Determination of fold increase used for identification of changes for all matrices

|       | Hydroxyaceton | 2,3,5-trimethylpyrazine | Menthone | (E)-Beta-Damascone | Cinnamic acid methyl ester | Myosmine | Piperonal | Cotinine |
|-------|---------------|--------------------------|----------|-------------------|---------------------------|----------|-----------|----------|
| F1    |               |                          |          |                   |                           |          |           |          |
| Day 1 | Mean          | 3.10                     | 5.45     | 2.60              | 4.32                      | 5.55     | 7.63      | 6.24     | 9.45     |
| Day 2 | Mean          | 2.49                     | 4.74     | 2.37              | ND                        | 5.04     | 7.38      | 5.91     | 8.11     |
| Day 3 | Mean          | 3.27                     | 5.08     | 2.44              | 4.17                      | 5.00     | 8.15      | 6.19     | 9.20     |
|       | x_c           | 2.95                     | 5.09     | 2.47              | 4.24                      | 5.19     | 7.72      | 6.11     | 8.92     |
|       | S.D.          | 0.41                     | 0.35     | 0.12              | 0.10                      | 0.31     | 0.39      | 0.18     | 0.71     |
|       |               | x_t                       | 3.17     | 4.85              | 7.04                      | 10.09    | 7.19      | 13.20    |          |
| Fold  | Increase      | 1.84                     | 1.42     | 1.28              | 1.14                      | 1.35     | 1.31      | 1.18     | 1.48     |
| F2    |               |                          |          |                   |                           |          |           |          |
| Day 1 | Mean          | 2.91                     | 5.06     | 2.47              | 3.94                      | 4.98     | 6.41      | 5.78     | 8.80     |
| Day 2 | Mean          | 3.13                     | 5.36     | 2.71              | ND                        | 5.69     | 7.41      | 6.60     | 8.83     |
| Day 3 | Mean          | 3.51                     | 5.19     | 2.63              | 4.23                      | 5.34     | 6.98      | 5.74     | 7.38     |
|       | x_c           | 3.19                     | 5.20     | 2.60              | 4.08                      | 5.34     | 6.93      | 6.04     | 8.33     |
|       | S.D.          | 0.30                     | 0.15     | 0.12              | 0.20                      | 0.36     | 0.50      | 0.49     | 0.83     |
|       |               | x_t                       | 5.01     | 6.11              | 3.31                      | 5.31     | 7.47      | 9.93     | 13.29    |
| Fold  | Increase      | 1.57                     | 1.17     | 1.27              | 1.30                      | 1.40     | 1.43      | 1.48     | 1.59     |
| F3    |               |                          |          |                   |                           |          |           |          |
| Day 1 | Mean          | 5.50                     | 5.23     | 2.53              | 4.13                      | 5.37     | 4.11      | 6.07     | 4.84     |
| Day 2 | Mean          | 4.29                     | 5.08     | 2.51              | ND                        | 5.27     | 4.23      | 6.25     | 4.60     |
| Day 3 | Mean          | 6.09                     | 5.48     | 2.79              | 4.38                      | 5.66     | 4.28      | 6.35     | 5.44     |
|       | x_c           | 5.29                     | 5.26     | 2.61              | 4.26                      | 5.43     | 4.20      | 6.22     | 4.96     |
|       | S.D.          | 0.92                     | 0.20     | 0.16              | 0.18                      | 0.20     | 0.08      | 0.14     | 0.43     |
|       |               | x_t                       | 10.81    | 6.46              | 3.54                      | 5.32     | 6.64      | 4.71     | 7.06     | 7.53    |
| Fold  | Increase      | 2.04                     | 1.23     | 1.36              | 1.25                      | 1.22     | 1.12      | 1.13     | 1.52     |
| F4    |               |                          |          |                   |                           |          |           |          |
| Day 1 | Mean          | 4.26                     | 4.90     | 2.40              | 3.90                      | 5.12     | 3.76      | 5.44     | 4.79     |
| Day 2 | Mean          | 4.21                     | 4.86     | 2.48              | ND                        | 5.19     | 4.07      | 5.91     | 4.34     |
| Day 3 | Mean          | 4.66                     | 5.32     | 2.76              | 4.27                      | 5.19     | 4.23      | 6.20     | 5.52     |
|       | x_c           | 4.38                     | 5.03     | 2.55              | 4.09                      | 5.16     | 4.02      | 5.85     | 4.88     |
|       | S.D.          | 0.25                     | 0.25     | 0.19              | 0.26                      | 0.04     | 0.24      | 0.38     | 0.60     |
|       |               | x_t                       | 5.88     | 6.55              | 3.66                      | 5.64     | 5.41      | 5.44     | 8.15     | 8.47    |
| Fold  | Increase      | 1.34                     | 1.30     | 1.44              | 1.38                      | 1.05     | 1.35      | 1.39     | 1.74     |
| F5    |               |                          |          |                   |                           |          |           |          |
| Day 1 | Mean          | 13.86                    | 5.41     | 2.55              | 4.10                      | 5.47     | 3.96      | 5.97     | 5.02     |
| Day 2 | Mean          | 11.47                    | 5.45     | 2.70              | ND                        | 5.77     | 4.44      | 6.66     | 4.66     |
| Day 3 | Mean          | 13.49                    | 6.04     | 2.81              | 4.69                      | 6.13     | 4.95      | 6.76     | 7.03     |
|       | x_c           | 12.94                    | 5.63     | 2.69              | 4.40                      | 5.79     | 4.45      | 6.46     | 5.57     |
|       | S.D.          | 1.28                     | 0.35     | 0.13              | 0.42                      | 0.33     | 0.50      | 0.43     | 1.28     |
|       |               | x_t                       | 20.64    | 7.74              | 3.46                      | 6.89     | 7.79      | 7.44     | 9.04     | 13.23   |
| Fold Increase | 1.60 | 1.37 | 1.29 | 1.57 | 1.35 | 1.67 | 1.40 | 2.38 |
|---------------|------|------|------|------|------|------|------|------|

**MassHunter Unknowns Analysis parameters for data processing method**

Following parameters were optimized specifically for NTA method workflow discussed in the manuscript. Peak detection: “Deconvolution”, Peak filter – exclude m/z 28, S/N – 6, Absolute area ≥ 8000 counts, Absolute height ≥ 1000 counts; Deconvolution: RT window size factor – 45, Left and Right m/z Δ = 0.5, m/z Δ units – AMU, Do not select “Use integer m/z values”. Component shape: Sharpness Threshold = 25%; Ion peaks: Min number of ion peaks – 1, Max number of ion peak shapes to store: 6; Library search: Select all relevant libraries, Pre-search type – Normal, Match factor (only applicable to custom library) – Use RT match, RT penalty – Trapezoidal, RT range – 20 sec, Penalty free range 18 sec, mismatch penalty – Additive, Max RT penalty 20; Compound Identification: Max Hit count - 1, Min match factor - 55, Min m/z - 30, Library search type - Spectral search, Multi-Library Search type - Stop when found;

Target match: Select – Qualifier ion ratios, Hit ion - Target ion and qualifier ion(s), Hit RT – Within target RT window, Additional target hit match – select “Use compound name”;

Estimation response factor (RF): Select Manual RF, Manual response factor – Enter the calculate manual response factor; Blank subtraction: Perform blank subtraction – de-select, Retention time window – FWHM – “5” times, Peak threshold – Select component area, 10%.
| Retention time (min) | Compound                        | CAS#      | Identification | Avg (µg/gm) | Count (# of Times Identified) |
|----------------------|---------------------------------|-----------|----------------|-------------|------------------------------|
| 3.33                 | Hexanal*                         | 66-25-1   | HIGH           | 1.62        | 3                            |
| 4.08                 | Pyridine                         | 110-86-1  | CONFIRMED      | 5.80        | 3                            |
| 4.75                 | Dimethoxydimethylsilane*         | 1112-39-6 | CONFIRMED      | 28.86       | 3                            |
| 5.04                 | Hydroxycetone*                   | 116-09-6  | CONFIRMED      | 13.28       | 3                            |
| 5.61                 | 1,4-diethyl-benzene*             | 105-05-5  | MEDIUM         | 1.49        | 3                            |
| 6.00                 | Trimethylpyrazine                | 14667-55-1| CONFIRMED      | 47.50       | 3                            |
| 6.50                 | Acetic acid                      | 64-19-7   | CONFIRMED      | 588.60      | 3                            |
| 7.72                 | 1-Dodecanamine, N,N-dimethyl-     | 112-18-5  | CONFIRMED      | 12.78       | 3                            |
| 7.95                 | Menthol                          | 89-78-1   | CONFIRMED      | 5.30        | 3                            |
| 8.14                 | Acetylpyrazine                   | 22047-25-2| CONFIRMED      | 7.85        | 3                            |
| 8.45                 | Diethoxydimethylsilane           | 78-62-6   | CONFIRMED      | 25.46       | 3                            |
| 8.50                 | Unknown*                         | 0-00-0    | NA             | 3.77        | 3                            |
| 8.55                 | 2(3H)-Furanone, 5-ethylidihydro- | 695-06-7  | CONFIRMED      | 15.06       | 3                            |
| 8.66                 | Unknown                          | 0-00-0    | NA             | 2.25        | 3                            |
| 8.88                 | .beta.-Citronellol*              | 106-22-9  | CONFIRMED      | 0.74        | 2                            |
| 9.16                 | N,N-Dimethyltetradecanamine*     | 112-75-4  | CONFIRMED      | 6.24        | 2                            |
| 9.31                 | gamma-Heptalactone               | 105-21-5  | CONFIRMED      | 18.95       | 3                            |
| 9.36                 | Dipropylene glycol               | 110-98-5  | CONFIRMED      | 24.29       | 3                            |
| 9.40                 | beta-Damascenone                 | 23726-93-4| CONFIRMED      | 1.71        | 3                            |
| 9.50                 | Ethanone, 1-(3-pyridinyl)-*      | 350-03-8  | CONFIRMED      | 1.02        | 3                            |
| 9.66                 | 2-Methoxyphenol                  | 90-05-1   | CONFIRMED      | 43.27       | 3                            |
| 10.11                | Unknown                          | 0-00-0    | NA             | 1.11        | 3                            |
| 11.08                | Ethyl Maltol                     | 4940-11-8 | HIGH           | 124.89      | 3                            |
| 11.50                | Unknown*                         | 0-00-0    | NA             | 1.31        | 1                            |
| 12.00                | Eugenol                          | 97-53-0   | CONFIRMED      | 5.24        | 3                            |
| 12.04                | Myosmine                         | 532-12-7  | CONFIRMED      | 4.25        | 3                            |
| 12.38                | delta-Decalactone*               | 705-86-2  | CONFIRMED      | 4.04        | 3                            |
| 13.10                | beta nicotyline                  | 487-19-4  | CONFIRMED      | 10.54       | 3                            |
| 13.90                | Bisabolol oxide A                | 22567-36-8| MEDIUM         | 2.12        | 3                            |
| 14.05                | Benzoic Acid                     | 65-85-0   | CONFIRMED      | 1896.10     | 1                            |
| 14.60                | Unknown                          | 0-00-0    | NA             | 1.98        | 2                            |
| 14.70                | Unknown*                         | 0-00-0    | NA             | 24.78       | 3                            |
| 14.75                | p-Dioxane-2,5-dimethanol         | 14236-12-5| CONFIRMED      | 12.23       | 3                            |
| 14.86                | Vanillin                         | 121-33-5  | CONFIRMED      | 44.01       | 3                            |
| 14.92                | Bis(2,6-hydroxymethyl) dioxane   | 54120-69-3| CONFIRMED      | 21.40       | 3                            |
| 15.14                | Bis(2,6-hydroxymethyl) dioxane - Iso2 | 0-00-0 | HIGH          | 3.28        | 1                            |
| 15.15                | Bis(2,6-hydroxymethyl) dioxane - Iso3 | 0-00-0 | HIGH          | 27.92       | 3                            |
| 15.26                | Bis(2,6-hydroxymethyl) dioxane - Iso4 | 0-00-0 | HIGH          | 8.84        | 3                            |
| Retention time (min) | Compound                              | CAS#         | Identification Confidence | Avg (µg/gm) | Count (# of Times Identified) |
|---------------------|---------------------------------------|--------------|---------------------------|-------------|-------------------------------|
| 15.30               | Guaiacyl acetone                      | 2503-46-0    | CONFIRMED                 | 7.24        | 3                             |
| 15.40               | Bis(2,6-hydroxymethyl) dioxane - Iso5 | 0-00-0       | HIGH                      | 46.05       | 3                             |
| 15.88               | N-Methyl nicotinamide*                | 114-33-0     | CONFIRMED                 | 0.86        | 3                             |
| 16.30               | 3,4-Dipyridyl Ketone*                 | 0-00-0       | CONFIRMED                 | 1.11        | 3                             |
| 16.70               | Cotinine                              | 486-56-6     | CONFIRMED                 | 3.19        | 3                             |
| 16.96               | Unknown Long Chain Alkane             | 0-00-0       | NA                        | 3.80        | 2                             |
| 17.60               | Unknown Long Chain Alkane             | 0-00-0       | NA                        | 4.74        | 2                             |
| 18.64               | Unknown Long Chain Alkane             | 0-00-0       | NA                        | 6.07        | 2                             |
| 19.58               | Unknown Long Chain Alkane             | 0-00-0       | NA                        | 6.69        | 2                             |
| 21.19               | Unknown Long Chain Alkane*            | 0-00-0       | NA                        | 3.17        | 1                             |

NA is not applicable; * New compounds at T=6

Table 7: Analysis of commercial product 3.5% NBW (T=6), aerosol, Average Conc.(n=3)

| Retention time (min) | Compound                              | CAS#         | Identification Confidence | Avg (µg/gm) | Count (# of Times Identified) |
|---------------------|---------------------------------------|--------------|---------------------------|-------------|-------------------------------|
| 3.33                | Hexanal*                              | 66-25-1      | HIGH                      | 1.21        | 2                             |
| 3.72                | Decamethylcyclopentasiloxane          | 541-02-6     | CONFIRMED                 | 15.03       | 3                             |
| 4.08                | Pyridine*                             | 110-86-1     | CONFIRMED                 | 9.97        | 3                             |
| 5.04                | Hydroxyacetone                        | 116-09-6     | CONFIRMED                 | 25.38       | 3                             |
| 5.61                | 1,4-diethyl-benzene*                  | 105-05-5     | MEDIUM                    | 0.79        | 3                             |
| 6.00                | Trimethylpyrazine                     | 14667-55-1   | CONFIRMED                 | 36.46       | 3                             |
| 6.50                | Acetic acid                           | 64-19-7      | CONFIRMED                 | 566.17      | 3                             |
| 7.95                | Menthol                               | 89-78-1      | CONFIRMED                 | 6.72        | 3                             |
| 8.14                | Acetylpyrazine                        | 22047-25-2   | CONFIRMED                 | 6.26        | 3                             |
| 8.45                | Diethoxymethylsilane*                 | 78-62-6      | CONFIRMED                 | 18.30       | 3                             |
| 8.55                | 2(3H)-Furanone, 5-ethylidihydro-      | 695-06-7     | CONFIRMED                 | 14.37       | 3                             |
| 8.66                | Unknown                               | 0-00-0       | NA                        | 2.20        | 3                             |
| 9.16                | N,N-Dimethyltetradecanamine           | 112-75-4     | CONFIRMED                 | 6.14        | 1                             |
| 9.31                | gamma-Heptalactone                    | 105-21-5     | CONFIRMED                 | 19.38       | 3                             |
| 9.36                | Dipropylene glycol                    | 110-98-5     | CONFIRMED                 | 23.58       | 3                             |
| 9.40                | beta-Damascenone                      | 23726-93-4   | CONFIRMED                 | 2.28        | 3                             |
| 9.50                | Ethanone, 1-(3-pyridinyl)-*           | 350-03-8     | CONFIRMED                 | 0.92        | 3                             |
| 9.66                | 2-Methoxyphenol                       | 90-05-1      | CONFIRMED                 | 38.30       | 3                             |
| 10.10               | Phenethyl alcohol*                    | 60-12-8      | CONFIRMED                 | 0.97        | 2                             |
| 10.11               | Unknown                               | 0-00-0       | NA                        | 0.97        | 3                             |
| 10.55               | Phenol*                               | 108-95-2     | CONFIRMED                 | 2.05        | 2                             |
| 11.08               | Ethyl Maltol                          | 4940-11-8    | HIGH                      | 111.81      | 3                             |
| 12.00               | Eugenol                               | 97-53-0      | CONFIRMED                 | 4.36        | 3                             |
| Retention time (min) | Compound                                      | CAS#    | Identification Confidence | Avg (µg/gm) | Count (# of Times Identified) |
|---------------------|-----------------------------------------------|---------|---------------------------|-------------|-------------------------------|
| 12.04               | Myosmine                                      | 532-12-7| CONFIRMED                 | 5.40        | 3                             |
| 12.38               | delta-Decalactone*                            | 705-86-2| CONFIRMED                 | 5.40        | 3                             |
| 12.70               | Unknown Nicotine Related Compound             | 0-00-0  | NA                        | 2.10        | 3                             |
| 13.10               | beta nicotyamine                              | 487-19-4| CONFIRMED                 | 14.32       | 3                             |
| 13.90               | Bisabolol oxide A                             | 22567-36-8| MEDIUM                    | 2.01        | 3                             |
| 13.90               | Unknown Nicotine Related Compound             | 0-00-0  | NA                        | 3.38        | 3                             |
| 14.05               | Benzoic Acid                                  | 65-85-0 | CONFIRMED                 | 1811.81     | 3                             |
| 14.75               | p-Dioxane-2,5-dimethanol                      | 14236-12-5| CONFIRMED                | 17.27       | 3                             |
| 14.86               | Vanillin                                      | 121-33-5| CONFIRMED                 | 45.24       | 3                             |
| 14.92               | Bis(2,6-hydroxymethyl) dioxane               | 54120-69-3| CONFIRMED              | 31.36       | 3                             |
| 15.01               | Unknown*                                      | 0-00-0  | NA                        | 26.69       | 3                             |
| 15.14               | Bis(2,6-hydroxymethyl) dioxane - Iso2         | 0-00-0  | HIGH                      | 4.08        | 3                             |
| 15.15               | Bis(2,6-hydroxymethyl) dioxane - Iso3         | 0-00-0  | HIGH                      | 40.64       | 3                             |
| 15.20               | Unknown                                      | 0-00-0  | NA                        | 2.41        | 2                             |
| 15.26               | Bis(2,6-hydroxymethyl) dioxane - Iso4         | 0-00-0  | HIGH                      | 12.12       | 3                             |
| 15.30               | Guaiacyl acetone                              | 2503-46-0| CONFIRMED                | 5.52        | 3                             |
| 15.40               | Bis(2,6-hydroxymethyl) dioxane - Iso5         | 0-00-0  | HIGH                      | 70.15       | 3                             |
| 15.88               | N-Methylnicotinamide*                         | 114-33-0| CONFIRMED                 | 1.46        | 3                             |
| 16.30               | 3,4-Dipyridyl Ketone*                        | 0-00-0  | CONFIRMED                 | 1.86        | 3                             |
| 16.70               | Cotinine                                      | 486-56-6| CONFIRMED                 | 4.89        | 3                             |
| 16.80               | Hexadecanoic Acid*                            | 57-10-3 | CONFIRMED                 | 11.83       | 3                             |
| 16.96               | Unknown Long Chain Alkane*                   | 0-00-0  | NA                        | 7.57        | 1                             |
| 17.00               | Unknown Nicotine Related Compound             | 0-00-0  | NA                        | 1.71        | 3                             |
| 17.60               | Unknown Long Chain Alkane                     | 0-00-0  | NA                        | 6.88        | 2                             |
| 18.64               | Unknown Long Chain Alkane*                   | 0-00-0  | NA                        | 14.18       | 1                             |
| 18.94               | Octadecanoic acid*                           | 57-11-4 | CONFIRMED                 | 9.70        | 2                             |
| 19.48               | Unknown*                                      | 0-00-0  | NA                        | 1.78        | 1                             |
| 19.58               | Unknown Long Chain Alkane                     | 0-00-0  | NA                        | 17.36       | 1                             |
| 20.13               | Unknown Nicotine Related Compound*           | 0-00-0  | NA                        | 3.68        | 3                             |
| 20.22               | Unknown*                                      | 0-00-0  | NA                        | 1.93        | 3                             |
| 21.19               | Unknown Long Chain Alkane*                   | 0-00-0  | NA                        | 14.41       | 1                             |

NA is not applicable; * New compounds at T=6