Evolution of the chemical fingerprint of biomass burning organic aerosol during aging

Amelie Bertrand1,2,*, Giulia Stefenelli3, Coty N. Jen4, Simone M. Pieber3, Emily A. Bruns3, Brice Temime-Roussel1, Jay G. Slowik3, Allen H. Goldstein4, Imad El Haddad3, Urs Baltensperger3, André S.H. Prévôt3, Henri Wortham1 and Nicolas Marchand1

1Aix Marseille Univ, CNRS, LCE, Marseille France
2Agence de l’environnement et de la Maîtrise de l’Energie, 20, avenue du Grössilé – BP 90406 49004 Angers cedex 01 France
3Laboratory of Atmospheric Chemistry, Paul Schererrer Institute, 5232, Villigen, Switzerland
Department of Environmental Sciences, Policy, and Management, University of California at Berkeley, California, United States
4Now at Laboratory of Atmospheric Chemistry, Paul Scherrer Institute, 5232, Villigen, Switzerland

Correspondence to: Nicolas Marchand (nicolas.marchand@univ-amu.fr)
1. TAG-AMS Analysis

Figure S1: Chromatograms of biomass burning organic aerosol by TAG-AMS.
### Table S1: Quantified compounds. In bold font are highlighted the compounds for which the authentic standards were available, as well the m/z used to quantify the compounds.

| Compounds         | m/z         | Compounds         | m/z         |
|-------------------|-------------|-------------------|-------------|
| **Anhydrosugars** |             | **Alkanes**       |             |
| Levoglucosan      | 217, 204, 191, 333 | Octadecane | 43, 57, 71, 85 |
| Mannosan          | 204, 217, 191, 333 | Nonadecane | 43, 57, 71, 86 |
| Galactosan        | 204, 217, 191, 333 | Eicosane | 43, 57, 71, 87 |
|                   |             | Heneicosane | 43, 57, 71, 88 |
|                   |             | Docosane | 43, 57, 71, 89 |
|                   |             | Tricosane | 43, 57, 71, 90 |
|                   |             | Tetracosane | 43, 57, 71, 91 |
|                   |             | Pentacosane | 43, 57, 71, 92 |
|                   |             | Hexacosane | 43, 57, 71, 93 |
|                   |             | Heptacosane | 43, 57, 71, 94 |
| **PAHs**          |             |                   |             |
| Acenaphthene*     | 154         | Vanillic Acid | 267, 297, 282, 312, 223 |
| Acenaphthylene*   | 152         | 3-Guanacylpropanol | 206, 236, 326, 179 |
| Fluorene*         | 166         | Vanillic Aldehyde | 220, 219, 250, 192, 235 |
| Phenanthrene      | 178         |                   |             |
| Anthracene        | 178         |                   |             |
| Fluoranthenes*    | 202         |                   |             |
| Aacenphanthenes*  | 202         |                   |             |
| Pyrene            | 202         |                   |             |
| Benzo[a]anthracene | 228     |                   |             |
| Chrycene          | 228         |                   |             |
| Benzo[b]fluoranthene | 252    |                   |             |
| Benzo[k]fluoranthene | 252     |                   |             |
| Benzo[j]fluoranthene | 252    |                   |             |
| Benzo[e]pyrene*   | 252         |                   |             |
| Benzo[a]pyrene    | 252         |                   |             |
| Perylene*         | 252         |                   |             |
| **Oxogenated PAHs** |            |                   |             |
| 1,2-Acenaphthylenone | 188, 139   |                   |             |
| Benzo[b]naptho[1,2-d]fluoran* | 218, 203, 189 | Syringyl Acetone | 239, 209, 267, 252 |
| Benzo[b]naptho[2,3-d]fluoran* | 218, 203, 189 | Propionyl Syringol | 223, 253, 267, 282, 297 |
| 2,3-5,6-Dibenzo[a]xanthene* | 218, 203, 189 | Syringe Acid | 297, 312, 327, 253, 342 |
| Benzo[k,l]xanthene* | 218, 203, 189 | Synapyl Aldehyde | 222, 250, 280, 265 |
| 4-Oxapyrene-5-one* | 220, 163, 192 | Palmotoleic Acid | 75, 177 |
| 9H-Fluoren-9-one* | 180, 152 | Palmitic Acid | 117, 129, 227, 313 |
| 9,10-Anthraquinone* | 152, 180, 208 | Oleic Acid | 117, 129, 357 |
| Xanthene*         | 196, 138, 139 | Stearic Acid | 117, 129, 341, 359, 257 |
| Cyclopentad[e,f]phenanthrene-4-one* | 204, 176 | **Nitrocatechols** |             |
| **Methylated PAHs** |            | 4-Nitrocatechol | 284, 299, 73 |
| 3-methylphenanthrene | 192      | 5-Methyl-5-Nitrocatechol | 296, 313, 180, 73 |
| 2-methylphenanthrene | 192      | 3-Methyl-5-Nitrocatechol | 298, 313, 73 |
| 2-methylantracene | 192         | **Others**        |             |
| 4,9-methylphenanthrene | 192    | Pyrogallol | 239, 342, 73 |
| 1-methylphenanthrene | 192      | Nonanonic Acid | 215, 117, 129, 73, 75 |
|                   |             | Vanillic Acid | 297, 298, 371 |
|                   |             | Methylglutaric Acid | 261, 199, 171, 143, 99 |
|                   |             | Tyrosol* | 179, 193, 267 |

The following surrogates were used:

- *Phenanthrene,  Benzo[b]fluoranthene,  Benzo[a]pyrene,  Eicosane,  Docosane,  Tetracosane,  Hexacosane
- *Acetosyringone,  **Vanillic Acid,  *Syringol,  Syringaldehyde,  *Coniferyl Aldehyde,  *Palmitic Acid,  Vanillin
Table S2: TAG-AMS detection limit of the compounds (determined on the basis of a 10 minute sampling at 2 L min\(^{-1}\)).

| Compounds                  | LD (ng.m\(^{-3}\)) | Compounds                  | LD (ng.m\(^{-3}\)) |
|----------------------------|--------------------|----------------------------|--------------------|
| Levoglucosan               | 0.99               | Nonadecane                 | 1.40               |
| Mannosan                   | 0.99               | Eicosane                   | 0.68               |
| Galactosan                 | 0.99               | Heneicosane                | 1.03               |
| Acenaphtene                | 0.84               | Docosane                   | 1.05               |
| Acenaphthylene             | 0.69               | Tricosane                  | 0.85               |
| Fluorene                   | 0.64               | Tetracosane                | 0.83               |
| Phenanthrene               | 0.63               | Pentacosane                | 1.63               |
| Anthracene                 | 0.77               | Hexacosane                 | 1.63               |
| Fluoranthenhene            | 0.44               | Heptacosane                | 2.48               |
| Acenaphanthenhene          | 0.22               | Vanline                    | 1.07               |
| Pyrene                     | 0.23               | Acetovanilone              | 0.98               |
| Benzo[a]anthracene         | 0.12               | Vanilnic Acid              | 0.80               |
| Chrysene                   | 0.11               | 3-Guaiacylpropanol         | 1.26               |
| Benzo[b]fluoranthene       | 0.37               | Coniferyl Aldehyde         | 1.22               |
| Benzo[k]fluoranthene       | 0.69               | Syringaldehyde             | 1.10               |
| Benzo[j]fluoranthene       | 0.09               | Syringol                   | 1.75               |
| Benzo[e]pyrene             | 0.75               | Acetosyringone             | 1.84               |
| Benzo[a]pyrene             | 0.38               | Isoeugenol                 | 1.00               |
| Perylene                   | 0.76               | Syringyl Acetone           | 0.90               |
| 1,2-Aacenaphthyleneone     | 0.42               | Propionyl Syringol         | 0.96               |
| Benzo[b]naptho[1,2-d]furan | 0.17               | Syringic Acid              | 0.38               |
| Benzo[b]naptho[2,3-d]furan | 0.17               | Synapyl Aldehyde           | 1.05               |
| 2,3,5,6-Dibenzoxyalene     | 0.17               | Palmitoleic Acid           | 5.15               |
| Benzo[k,1]xanthene         | 0.17               | Palmitic Acid              | 5.40               |
| 4-Oxyprene-5-one           | 0.14               | Oleic Acid                 | 0.15               |
| 9H-Fluoren-9-one           | 1.12               | Stearic Acid               | 1.06               |
| 9,10-Anthraquinone         | 1.62               | 4-Nitrocatechol             | 1.55               |
| Xanthone                   | 0.26               | Pyrogallol                 | 1.56               |
| Cyclopenta[d,e,f]phenanthrene-4one | 0.14 | Methylsyringol         | 0.09               |
| 3-methylphenanthrene       | 0.75               | Nonanoic Acid              | 0.12               |
| 2-methylphenanthrene       | 0.76               | Vanillylmandelic acid      | 0.23               |
| 2-methylanthracene         | 0.55               | Methylglutaric acid        | 0.42               |
| 4,9-methylphenanthrene     | 0.58               | Tyrosol                    | 1.00               |
| 1-methylphenanthrene       | 0.77               | 5-Methyl-5-Nitrocatechol    | 1.51               |
| Octadecane                 | 1.55               | 3-Methyl-5-Nitrocatechol    | 0.89               |

*calculated on the basis of a 10 minutes sampling at 2 L.min\(^{-1}\)

2. Off line samples and 2D-GC analysis

Two samples were collected on quartz fiber filter for each experiment - before and during photo-oxidation - in parallel with the TAG (Figure 2). Sampling lasted for 20 minutes at a flow rate of 20 L min\(^{-1}\). The sampling line was equipped with a parallel plate charcoal denuder to remove all organic gases. Prior to their use, the filters were baked at 550 °C for 4 hours to prevent any trace contamination and stored after collection at – 4 °C.

One pair of samples (primary and aged OA, experiment 5) was analyzed following the method by Isaacman et al. (2012) using a 2D-GC coupled to an Electron Impact/Vacuum Ultra Violet (VUV) light - High Resolution - Time of Flight - Mass Spectrometer (GCxGC.
EI/VUV HR-ToF-MS). The parent mass of the compounds and structural information were obtained respectively via ionization with VUV light (-10.5 eV) and EI (-70 eV).

For analysis, 0.41 cm$^2$ punches of the filters were desorbed in a helium environment at 320 °C. The desorbed content was derivatized under a stream of MSTFA enriched helium and trapped in a Cooled Injection System (CIS) maintained at 30 °C prior to injection onto the GC columns. Compounds are first separated by volatility with a Rxi-5Sil MS Restek column then by polarity with a Rtx-200 MS Restek column. The intensity signals from each pair of filters are normalized to that of the internal standard. The normalized signal from the fresh emissions sample is then subtracted from that of the aged emissions sample. Figure 5 illustrates compounds that significantly decrease in concentration during aging (shown in green), i.e., compounds lost to the walls or reacted away. In addition, the 2D-GC analysis served to check for potential co-elution of the compounds examined in this study.

**REFERENCES:**

Isaacman, G., Wilson, K.R., Chan, A.W.H., Worton, D.R., Kimmel, J.R., Nah, T., Hohaus, T., Gonin, M., Kroll, J.H., Worsnop, D.R., Goldstein, A.H., 2012. Improved Resolution of Hydrocarbon Structures and Constitutional Isomers in Complex Mixtures Using Gas Chromatography-Vacuum Ultraviolet-Mass Spectrometry. Anal. Chem. 84, 2335–2342.

**Figure S2:** Results of the 2D-GC analysis of the quartz fiber filters. (a) Chromatogram of a sample collected before lights on. (b) Chromatogram of a sample collected during aging.
3. Emission Factors and Contributions to OA
**Table S3**: Emission factor (in µg kg\(^{-1}\)) for primary and aged emissions

| Experiment I - Stove A | Fresh          | Aged           |
|------------------------|----------------|----------------|
| **Integrated OH exposure (molecule cm\(^{-3}\) hour)** | 0              | 5.25 × 10\(^6\) |
| **OA (mg kg\(^{-1}\))** | 1336           | 4076           |
| **OM/OC**              | 1.8            | 2              |
| **EF Compounds (µg kg\(^{-1}\))** |                  |                |

| Compound                              | Fresh            | Aged             |
|----------------------------------------|------------------|------------------|
| Levoglucosan                           | 249 × 10\(^3\)   | 219 × 10\(^3\)   |
| Mannosan                               | 13 × 10\(^3\)    | 10 × 10\(^3\)    |
| Galactosan                             | 1 × 10\(^3\)     | 720              |
| Acenaphtene                            | 660              | 83 | 818 |
| Acenaphthylene                         | 1 × 10\(^3\)     | 1 × 10\(^3\)    |
| Fluorene                               | 4 × 10\(^3\)     | 3 × 10\(^3\)    |
| Phenanthrene                           | 1 × 10\(^3\)     | 752              |
| Anthracene                             | 519              | 1 × 10\(^3\)    |
| Acenaphthylene                         | 1.8              | 83              |
| Pyrene                                 | 82               | 37              |
| Benzo[a]anthracene                     | 88               | 69              |
| Benzo[b]fluoranthrene                  | 68               | 68              |
| Benzo[k]fluoranthrene                  | < LD             | < LD            |
| Benzo[j]fluoranthene                   | 6                | 4              |
| Benzo[e]pyrene                         | < LD             | < LD            |
| Benzo[a]pyrene                         | < LD             | < LD            |
| Perylene                               | < LD             | < LD            |
| 1.2-Acenaphthlenone                    | 2 × 10\(^3\)    | 1 × 10\(^3\)    |
| Benzo[b]naphto[1.2-d]furan             | 54               | 135             |
| Benzo[b]naphto[2.3-d]furan             | 17               | 29              |
| Benzo[k]xanthene                       | 6                | 6              |
| 4-Oxapyrene-5-one                     | < LD             | < LD            |
| 9H-Fluoren-9-one                       | 190              | 205             |
| 9,10-Anthraquinone                     | < LD             | < LD            |
| Xanthone                               | < LD             | < LD            |
| Cyclo pent[a.d.e.f]phenanthrene        | 158              | 195             |
| 3-methylphenanthrene                   | 336              | 308             |
| 2-methylphenanthrene                   | 408              | 407             |
| 2-methylanthracene                     | 112              | 101             |
| 4,9-methylphenanthrene                 | 208              | 222             |
| 1-methylphenanthrene                   | 192              | 188             |
| Octadecane                             | 371              | 398             |
| Nonadecane                             | 672              | 932             |
| Eicosane                               | 218              | 312             |
| Heneicosane                            | 114              | 46              |
| Docosane                               | 216              | 258             |
| Tricosane                              | 82               | 25              |
| Tetracosane                            | 53               | 32              |
| Pentacosane                            | 103              | 112             |
| Hexacosane                             | 45               | 33              |
| Heptacosane                            | 66               | 52              |
| Vanillin                               | 5 × 10\(^3\)    | 11 × 10\(^3\)  |
| Acetovanillone                         | 1 × 10\(^3\)    | 3 × 10\(^3\)    |
| Vanillic Acid                          | 3 × 10\(^3\)    | 3 × 10\(^3\)    |
| 3-Guaiaacylpropanol                    | 1 × 10\(^3\)    | 1 × 10\(^3\)    |
| Conyeryl Aldehyde                      | 4 × 10\(^3\)    | 1 × 10\(^3\)    |
| Syringaldehyde                         | 34 × 10\(^3\)   | 34 × 10\(^3\)  |
| Syringol                               | 19 × 10\(^3\)   | 6 × 10\(^3\)    |
| Acetylsyringone                        | 5 × 10\(^3\)    | 4 × 10\(^3\)    |
| Isoeugenol                             | 11 × 10\(^3\)   | 3 × 10\(^3\)    |
| Syringyl Acetone                       | 65 × 10\(^3\)   | 19 × 10\(^3\)   |
| Propionyl Syringol                     | 7 × 10\(^3\)    | 4 × 10\(^3\)    |
| Syringic Acid                          | 1 × 10\(^3\)    | 2 × 10\(^3\)    |
| Synapyl Aldehyde                       | 17 × 10\(^3\)   | 3 × 10\(^3\)    |
| Palmitoleic Acid                       | 3 × 10\(^3\)    | 112             |
| Palmitic Acid                          | 828              | 614             |
| Oleic Acid                             | < LD             | < LD            |
| Stearic Acid                           | 363              | 306             |
| 4-Nitrocanthol                         | 751              | 55 × 10\(^3\)  |
| Pyrogallol                             | < LD             | 159             |
| Methylysyringol                        | 516              | 331             |
| Vanillylmandelic acid                  | 168              | 1 × 10\(^3\)    |
| 2-methyl-2-pentanecidoic Acid          | < LD             | 2 × 10\(^3\)    |
| Tyrosol                                | 2 × 10\(^3\)    | 4 × 10\(^3\)    |
| 5-Methyl-5-nitrocatechol               | < LD             | 6 × 10\(^3\)    |
| 3-Methyl-5-nitrocatechol               | 687              | 11 × 10\(^3\)  |
### Table S3: (Continued)

| Experiment 2 - Stove A | Fresh | Aged |
|------------------------|-------|------|
| **Integrated OH exposure (molecule cm⁻³ hour)** | 0 | 4.83 × 10⁶ |
| **OA (mg kg⁻¹)** | 1205 | 4145 |
| **OM/OC** | 1.7 | 1.9 |
| **EF Compounds (µg kg⁻¹)** | | |
| Levoglucosan | 152 × 10³ | 98 × 10³ |
| Mannosan | 13 × 10³ | 10 × 10³ |
| Galactosan | 10 × 10³ | 778 |
| Acenaphthene | 851 | 1 × 10⁹ |
| Acenaphthylene | 2 × 10⁹ | 583 |
| Fluorene | 1 × 10⁹ | 997 |
| Phenanthrene | 4 × 10⁹ | 3 × 10⁹ |
| Anthracene | 694 | 533 |
| Fluoranthenes | 425 | 742 |
| Acenaphtene | 54 | 48 |
| Pyrene | 160 | 246 |
| Benzo[a]anthracene | 99 | 28 |
| Chrysene | 105 | 68 |
| Benzo[b]fluoranthene | 82 | 23 |
| Benzo[k]fluoranthene | < LD | 42 |
| Benzo[j]fluoranthene | 8 | < LD |
| Benzo[e]pyrene | 28 | 1 |
| Benzo[a]pyrene | 5 | < LD |
| Perylene | < LD | < LD |
| 1,2-Acenaphthylene | 2 × 10⁹ | 2 × 10⁹ |
| Benzo[b]napthol[1,2-d]furan | 55 | 93 |
| Benzo[b]napthol[2,3-d]furan | 28 | 44 |
| 2,3,5,6-Dibenzoalene | 22 | 31 |
| Benzo[k,l]xanthene | 12 | < LD |
| 4-Oxapyrene-5-one | 20 | 20 |
| 9H-Fluoren-9-one | 127 | 182 |
| 9,10-Anthraquinone | 53 | 2 |
| Xanthone | < LD | < LD |
| Cyclopenta[d,e,f]phenanthrene | 76 | 91 |
| 3-methylphenanthrene | 105 | 92 |
| 2-methylphenanthrene | 137 | 161 |
| 2-methylantracene | 62 | 49 |
| 4,9-methylphenanthrene | 70 | 89 |
| 1-methylphenanthrene | 60 | 74 |
| Octadecane | 114 | 122 |
| Nonadecane | 260 | 285 |
| Eicosane | 127 | 146 |
| Henicosane | 67 | 117 |
| Docosane | 166 | 52 |
| Tricosane | 120 | 42 |
| Tetracosane | 105 | 31 |
| Pentacosane | 182 | 180 |
| Hexacosane | 120 | 112 |
| Heptacosane | 161 | 85 |
| Vanillin | 4 × 10³ | 12 × 10³ |
| Acetovanillone | 920 | 3 × 10³ |
| Vanillic Acid | 1 × 10³ | 3 × 10³ |
| 3-Guaiaacylpropanol | 4 × 10³ | 1 × 10³ |
| Conyferyl Aldehyde | 4 × 10⁹ | 586 |
| Syringaldehyde | 25 × 10³ | 26 × 10³ |
| Syringol | 12 × 10³ | 5 × 10³ |
| Acetosyringone | 5 × 10³ | 4 × 10³ |
| Isoegenol | 7 × 10³ | 2 × 10³ |
| Syringyl Acetone | 79 × 10³ | 12 × 10³ |
| Propionyl Syringol | 6 × 10³ | 3 × 10³ |
| Syringic Acid | 725 | 1 × 10³ |
| Synapyl Aldehyde | 13 × 10³ | 921 |
| Palmitoleic Acid | < LD | < LD |
| Palmitic Acid | < LD | 401 |
| Oleic Acid | 137 | 5 |
| Stearic Acid | 255 | 212 |
| 4-Nitrocatechol | 244 | 48 × 10³ |
| Pyrogallol | < LD | 143 |
| Methylysinigol | 888 | 551 |
| Vanillylmandelic acid | 192 | 908 |
| 2-methyl-2-pentanedioc Acid | < LD | 1 × 10³ |
| Tyrosol | 2 × 10³ | 7 × 10³ |
| 5-Methyl-5-Nitrocatechol | 84 | 4 × 10³ |
| 3-Methyl-5-Nitrocatechol | < LD | 8 × 10³ |
| EF Compounds (µg kg⁻¹) | Fresh | Aged |
|------------------------|-------|------|
| Levoglucosan           | 248 × 10³ | 101 × 10³ |
| Mannosan               | 20 × 10⁹ | 9 × 10⁹ |
| Galactosan             | 4 × 10⁹ | 3 × 10⁹ |
| Acenaphthene           | 956    | 1 × 10⁹ |
| Acenaphthylene         | 2 × 10⁹ | 559   |
| Fluorene               | 462    | 545   |
| Phenanthrene           | 3 × 10⁹ | 2 × 10⁹ |
| Anthracene             | 685    | 491   |
| Fluoranthene           | < LD   | < LD  |
| Acephenanthrene        | < LD   | < LD  |
| Pyrene                 | < LD   | < LD  |
| Benzo[a]anthracene     | < LD   | < LD  |
| Chrysene               | < LD   | < LD  |
| Benzo[b]fluoranthrene  | < LD   | < LD  |
| Benzo[k]fluoranthene   | < LD   | < LD  |
| Benzo[j]fluoranthene   | < LD   | < LD  |
| Benzo[e]pyrene         | < LD   | < LD  |
| Benzo[a]pyrene         | < LD   | < LD  |
| Perylene               | < LD   | < LD  |
| 1,2-Acenaphthylene     | 2 × 10⁹ | 543   |
| Benzo[b]naphthalene    | < LD   | < LD  |
| Benzo[b]naphthalene    | < LD   | < LD  |
| 2,3,5,6-Dibenzoxalene  | < LD   | < LD  |
| Benzo[k,l]xanthene     | NaN    | NaN   |
| 4-Oxapyrene-5-one      | < LD   | < LD  |
| 9H-Fluoren-9-one       | 102    | 225   |
| 9,10-Anthraquinone     | < LD   | < LD  |
| Xanthone               | < LD   | < LD  |
| Cyclopenta[d,e,f]phenanthrene | 69    | 157   |
| 3-methylphenanthrene   | 48     | 86    |
| 2-methylphenanthrene   | 64     | 152   |
| 2-methylanthracene     | 9      | 28    |
| 4,9-methylphenanthrene | 41     | 70    |
| 1-methylphenanthrene   | 47     | 94    |
| Octadecane             | 212    | 159   |
| Nonadecane             | 51     | 142   |
| Eicosane               | 90     | 253   |
| Henecosane             | < LD   | < LD  |
| Docosane               | < LD   | < LD  |
| Tricosane              | < LD   | < LD  |
| Tetracosane            | < LD   | < LD  |
| Pentacosane            | < LD   | < LD  |
| Hexacosane             | < LD   | < LD  |
| Heptacosane            | < LD   | < LD  |
| Vanillin               | 6 × 10⁹ | 1.3 × 10¹ |
| Acetovanillone         | 1 × 10⁹ | 2 × 10⁹ |
| Vanillic Acid          | 1 × 10⁹ | 3 × 10⁹ |
| 3-Guaiaicypropanol     | 4 × 10⁹ | 770   |
| Coniferyl Aldehyde     | 4 × 10⁹ | 577   |
| Syringaldehyde         | 29 × 10⁹ | 19 × 10⁹ |
| Syringol               | 16 × 10³ | 10 × 10³ |
| Acetosyringone         | 5 × 10⁹ | 2 × 10⁹ |
| Isoeugenol             | 11 × 10⁹ | 4 × 10⁹ |
| Syringyl Acetone       | 69 × 10⁹ | 8 × 10⁹ |
| Propionyl Syringol     | 7 × 10⁹ | 3 × 10⁹ |
| Syringic Acid          | 656    | 1 × 10⁹ |
| Synapyl Aldehyde       | 9 × 10⁹ | 723   |
| Palmitoleic Acid       | < LD   | < LD  |
| Palmitic Acid          | 1 × 10⁹ | 896   |
| Oleic Acid             | < LD   | < LD  |
| Stearic Acid           | 446    | 432   |
| 4-Nitrocatechol        | 118    | 30 × 10³ |
| Pyrogallol             | 136    | 255   |
| Methylosyringol        | 676    | 670   |
| Vanillylmandelic acid  | < LD   | 789   |
| 2-methyl-2-pentanedioc Acid | < LD | 1 × 10⁹ |
| Tyrosol                | 1 × 10⁹ | 3 × 10⁹ |
| 5-Methyl-5-Nitrocatechol | < LD | 3 × 10⁹ |
| 3-Methyl-5-Nitrocatechol | 151 | 6 × 10⁹ |
| EF Compounds (µg kg⁻¹) | Fresh | Aged |
|------------------------|-------|------|
| Levoglucosan           | 59 × 10³ | 50 × 10³ |
| Mannosan               | 5 × 10³  | 4 × 10³  |
| Galactosan             | 1 × 10⁶  | 543   |
| Acenaphthene           | 342   | < LD  |
| Acenaphthyline         | 838   | 221   |
| Fluorene               | 254   | 352   |
| Phenanthrene           | 1 × 10⁹ | 1 × 10⁹ |
| Anthracene             | 243   | 232   |
| Fluoranthenecarbon     | 470   | 2 × 10³ |
| Acephenanthrene        | 15    | 34    |
| Pyrene                 | 151   | 709   |
| Benz[a]anthracene      | 6     | 10    |
| Chrysene               | 11    | 13    |
| Benz[b]fluoranthene    | < LD  | < LD  |
| Benz[k]fluoranthene    | < LD  | < LD  |
| Benz[j]fluoranthene    | < LD  | < LD  |
| Benz[e]pyrene          | < LD  | < LD  |
| Benz[a]pyrene          | < LD  | < LD  |
| Perylene               | < LD  | < LD  |
| 1,2-Acenaphthylenone   | 701   | 1 × 10⁹ |
| Benzo[b]naphtho[1,2-d]furan | 32   | 174   |
| Benzo[b]naphtho[2,3-d]furan | 15   | 71    |
| 2,3-5,6-Dibenzoazulene | 8     | 50    |
| Benzo[k,l]xanthene     | < LD  | < LD  |
| 4-Oxapyrene-5-one      | < LD  | < LD  |
| 9H-Fluoren-9-one       | 70    | 198   |
| 9,10-Anthraquinone     | < LD  | < LD  |
| Xanthone               | < LD  | < LD  |
| Cyclopenta[d,e,f]phenanthrene | 67   | 138   |
| 3-methylphenanthrene   | 46    | 69    |
| 2-methylphenanthrene   | 59    | 104   |
| 2-methylantracene      | 13    | 19    |
| 4,9-methylenaphthrene  | 41    | 62    |
| 1-methylenaphthrene    | 43    | 65    |
| Octadecane             | 95    | 262   |
| Nonadecane             | 53    | 153   |
| Eicosane               | 13    | 41    |
| Henecicosane           | 65    | 307   |
| Docosane               | 127   | 379   |
| Tricosane              | 49    | 157   |
| Tetracosane            | 43    | 93    |
| Pentacosane            | 80    | 180   |
| Hexacosane             | 38    | 86    |
| Heptacosane            | < LD  | < LD  |
| Vanillin               | 4 × 10⁶ | 1.0 × 10⁹ |
| Acetovanillone         | 695   | 1 × 10⁹ |
| Vanillic Acid          | 398   | 1 × 10⁹ |
| 3-Guaiacylpropanol     | 627   | 280   |
| Coniferyl Aldehyde     | 542   | 193   |
| Syringaldehyde         | 4 × 10⁹ | 5 × 10³ |
| Syringol               | 5 × 10⁹ | 2 × 10⁹ |
| Acetosyringone         | 866   | 418   |
| Isoeugenol             | 3 × 10⁹ | 1 × 10⁹ |
| Syringyl Acetone       | 10 × 10⁹ | 2 × 10⁹ |
| Propionyl Syringol     | 2 × 10⁹ | 272   |
| Syringic Acid          | 295   | 737   |
| Synapyl Aldehyde       | 2 × 10⁹ | 226   |
| Palmitoleic Acid       | < LD  | < LD  |
| Palmitic Acid          | 611   | 908   |
| Oleic Acid             | < LD  | < LD  |
| Stearic Acid           | 283   | 447   |
| 4-Nitrocatechol        | 276   | 19 × 10³ |
| Pyrogallol             | 60    | 241   |
| Methylsyringol         | 162   | 116   |
| Vanillylmandelic acid  | 81    | 679   |
| 2-methyl-2-pentanediioic Acid | < LD | < LD |
| Tyrosol                | 926   | 1 × 10⁹ |
| 5-Methyl-5-Nitrocatechol | < LD | 2 × 10³ |
| 3-Methyl-5-Nitrocatechol | 467 | 3 × 10³ |
Table S3: (Continued)

|                          | Fresh       | Aged        |
|--------------------------|-------------|-------------|
| **Integrated OH exposure (molecule cm\(^{-3}\) hour)** |             |             |
| OA (mg kg\(^{-1}\))      |             |             |
|                          | 806         | 2033        |
| OM/OC                    | 1.7         | 2           |
| **EF Compounds (µg kg\(^{-1}\))** |             |             |
| Levoglucosan             | 110 × 10\(^3\) | 58 × 10\(^3\) |
| Mannosan                 | 7 × 10\(^3\)  | 5 × 10\(^3\)  |
| Galactosan               | 2 × 10\(^3\)  | 1 × 10\(^3\)  |
| Acenaphthene             | 304         | 4 × 10\(^4\)  |
| Acenaphthylene           | 4 × 10\(^9\) | 2 × 10\(^9\)  |
| Fluorene                 | 720         | 1 × 10\(^9\)  |
| Phenanthrene             | 888         | 3 × 10\(^9\)  |
| Anthracene               | 207         | 514         |
| Fluoranthrene            | 648         | 2 × 10\(^9\)  |
| Acephenanthrene          | 110         | 58 × 10\(^3\) |
| Pyrene                   | 259         | 691         |
| Benzo[a]anthracene       | 48          | 26          |
| Chrysene                 | 66          | 40          |
| Benzo[b]fluoranthene     | < LD        | < LD        |
| Benzo[k]fluoranthene     | < LD        | < LD        |
| Benzo[jj]fluoranthene    | < LD        | < LD        |
| Benzo[e]pyrene           | < LD        | < LD        |
| Benzo[a]pyrene           | < LD        | < LD        |
| Perylene                 | < LD        | < LD        |
| 1,2-Acenaphthylene| 1 × 10\(^9\) | 2 × 10\(^9\)  |
| Benzo[b]naptho[1,2-d]furan | 52       | 178         |
| Benzo[b]naptho[2,3-d]furan | 24   | 83          |
| 2,3-5,6-Dibenzoalene     | 17          | 58          |
| Benzo[k,j]xanthenne      | < LD        | < LD        |
| 4-Oxapyrene-5-one        | < LD        | < LD        |
| 9H-Fluoren-9-one         | 96          | 264         |
| 9,10-Anthraquinone       | < LD        | < LD        |
| Xanthone                 | < LD        | < LD        |
| Cyclopenta[d,e,f]phenanthrene | 56      | 124         |
| 3-methylphenanthrene     | 30          | 77          |
| 2-methylphenanthrene     | 39          | 114         |
| 2-methylanthracene       | < LD        | < LD        |
| 4,9-methylphenanthrene   | 26          | 72          |
| 1-methylphenanthrene     | 32          | 79          |
| Octadecane               | 182         | 390         |
| Nonadecane               | 89          | 204         |
| Eicosane                 | 165         | 324         |
| Henecicosane             | 116         | 381         |
| Docosane                 | 266         | 591         |
| Tricosane                | 145         | 262         |
| Tetracosane              | 154         | 241         |
| Pentacosane              | 287         | 447         |
| Hexacosane               | 170         | 275         |
| Heptacosane              | 75          | 87          |
| Vanillin                 | 7 × 10\(^9\) | 12 × 10\(^9\) |
| Acetovanilone            | 1 × 10\(^9\) | 2 × 10\(^9\)  |
| Vanillic Acid            | 830         | 2 × 10\(^9\)  |
| 3-Guaiacylpropanol       | 2 × 10\(^9\) | 710         |
| Confyeryl Aldehyde       | 2 × 10\(^9\) | 515         |
| Syringaldehyde           | 17 × 10\(^9\) | 1.1 × 10\(^9\) |
| Syringol                 | 4 × 10\(^9\) | 3 × 10\(^9\)  |
| Acetosyringone           | 3 × 10\(^9\) | 1 × 10\(^9\)  |
| Isoeugenol               | 5 × 10\(^9\) | 2 × 10\(^9\)  |
| Syringyl Acetone         | 23 × 10\(^9\) | 5 × 10\(^9\)  |
| Propionyl Syringol       | 3 × 10\(^9\) | 1 × 10\(^9\)  |
| Syringic Acid            | 577         | 1 × 10\(^9\)  |
| Synapyl Aldehyde         | 5 × 10\(^9\) | 757         |
| Palmitoleic Acid         | < LD        | < LD        |
| Palmitic Acid            | 1 × 10\(^9\) | 1 × 10\(^9\)  |
| Oleic Acid               | < LD        | < LD        |
| Stearic Acid             | 557         | 710         |
| 4-Nitrocatechol          | 2 × 10\(^9\) | 29 × 10\(^9\) |
| Pyrogallol               | 113         | 331         |
| Methylsyringol           | 157         | 210         |
| Vanillylmandelic acid    | 48          | 373         |
| 2-methyl-2-pentanedioic Acid | < LD | 436 |
| Tyrosol                  | 1 × 10\(^9\) | 2 × 10\(^9\)  |
| 5-Methyl-5-Nitrocatechol | < LD | 3 × 10\(^9\)  |
| 3-Methyl-5-Nitrocatechol | 900 | 6 × 10\(^9\)  |
Table S3: (Continued)

|                        | Fresh    | Aged     |
|------------------------|----------|----------|
| Integrated OH exposure (molecule cm\(^{-3}\) hour) | 0        | 5.25 \times 10^6 |
| OA (mg kg\(^{-1}\))    | 531      | 2317     |
| OM/OC                  | 1.8      | 2        |
| EF Compounds (µg kg\(^{-1}\)) |          |          |
| Levoglucosan           | 160 \times 10^9 | 101 \times 10^9 |
| Mannosan               | 11 \times 10^9  | 9 \times 10^9  |
| Galactosan             | 1 \times 10^9   | 1 \times 10^9   |
| Acenaphthene           | 709       | 2 \times 10^6  |
| Acenaphthylene         | 594       | 249       |
| Fluorene               | 292       | 484       |
| Phenanthrene           | 2 \times 10^9 | 2 \times 10^9 
| Anthracene             | 412       | 314       |
| Fluoranthene           | 495       | 1 \times 10^9 |
| Acephenanthrene        | 17        | 18        |
| Pyrene                 | 169       | 452       |
| Benzo[a]anthracene     | 20        | 16        |
| Chrysenene             | 28        | 23        |
| Benzo[b]fluoranthene   | < LD      | < LD      |
| Benzo[k]fluoranthene   | < LD      | < LD      |
| Benzo[j]fluoranthene   | < LD      | < LD      |
| Benzo[e]pyrene         | < LD      | < LD      |
| Benzo[a]pyrene         | < LD      | < LD      |
| Perylene               | < LD      | < LD      |
| 1,2-Acenaphthylene     | 1 \times 10^9 | 2 \times 10^9 |
| Benzo[b]napth[1,2-d]furan | 39    | 107       |
| Benzo[b]napth[2,3-d]furan | 19 | 50        |
| 2,3,5,6-Dibenzoalene   | 11        | 35        |
| Benzo[k,l]xanthene     | < LD      | < LD      |
| 4-Oxapyrene-5-one      | < LD      | < LD      |
| 9H-Fluoren-9-one       | 109       | 189       |
| 9,10-Anthraquinone     | < LD      | < LD      |
| Xanthone               | < LD      | < LD      |
| Cyclopenta[d,e,f]phenanthrene | 72 | 97        |
| 3-methylphenanthrene   | 67        | 74        |
| 2-methylphenanthrene   | 81        | 103       |
| 2-methylanthracene     | 19        | 22        |
| 4,9-methylphenanthrene | 45        | 65        |
| 1-methylphenanthrene   | 39        | 64        |
| Octadecane             | 139       | 299       |
| Nonadecane             | 72        | 121       |
| Eicosane               | 31        | 70        |
| Heneicosane            | 96        | 230       |
| Docosane               | 179       | 397       |
| Tricosane              | 106       | 171       |
| Tetracosane            | < LD      | < LD      |
| Pentacosane            | 187       | 251       |
| Hexacosane             | 116       | 140       |
| Heptacosane            | 51        | 60        |
| Vanillin               | 5 \times 10^9 | 1.1 \times 10^9 |
| Acetovanillone         | 961       | 2 \times 10^9 |
| Vanillic Acid          | 1 \times 10^9 | 2 \times 10^9 |
| 3-Guaiacylpropanol     | 2 \times 10^9 | 643 |
| Coniferyl Aldehyde     | 1 \times 10^9 | 347 |
| Syringaldehyde         | 14 \times 10^9 | 13 \times 10^9 |
| Syringol               | 7 \times 10^9  | 5 \times 10^9  |
| Acetosyringone         | 2 \times 10^9 | 2 \times 10^9 |
| Isoeugenol             | 6 \times 10^9  | 3 \times 10^9  |
| Syringyl Acetone       | 34 \times 10^9 | 6 \times 10^9 |
| Propionyl Syringol     | 4 \times 10^9  | 3 \times 10^9  |
| Syringic Acid          | 782       | 1 \times 10^9 |
| Synapyl Aldehyde       | 5 \times 10^9  | 575 |
| Palmitoleic Acid       | < LD      | < LD      |
| Palmitic Acid          | 713       | 822       |
| Oleic Acid             | < LD      | < LD      |
| Stearic Acid           | 348       | 469       |
| 4-Nitrocatechol        | < LD      | 44 \times 10^9 |
| Pyrogallol             | 70        | 339       |
| Methylsyringol         | 485       | 365       |
| Vanillylmandelic acid  | 54        | 1 \times 10^9 |
| 2-methyl-2-pentanediolic Acid | < LD | 529 |
| Tyrosol                | 2 \times 10^9 | 2 \times 10^9 |
| 5-Methyl-5-Nitrocatechol | 130 | 4 \times 10^9 |
| 3-Methyl-5-Nitrocatechol | 507 | 8 \times 10^9 |
| Table S3: (Continued) | Fresh | Aged |
|------------------------|-------|------|
| **Integrated OH exposure (molecule cm\(^{-3}\) hour)** | 0 | 5.60 × 10\(^6\) |
| **OA (mg kg\(^{-1}\))** | 651 | 3562 |
| **OM/OC** | 1.8 | 2 |
| **EF Compounds (µg kg\(^{-1}\))** | | |
| Levoglucosan | 202 × 10\(^3\) | 121 × 10\(^3\) |
| Mannosan | 16 × 10\(^3\) | 10 × 10\(^3\) |
| Galactosan | 3 × 10\(^3\) | 2 × 10\(^3\) |
| Acenaphthene | 1 × 10\(^3\) | 2 × 10\(^3\) |
| Acenaphthylene | 2 × 10\(^3\) | 489 |
| Fluorene | 535 | 582 |
| Phenanthrene | 1 × 10\(^3\) | 2 × 10\(^3\) |
| Anthracene | 229 | 188 |
| Fluoranthene | 301 | 1 × 10\(^3\) |
| Acephenanthrene | 9 | 15 |
| Pyrene | 113 | 349 |
| Benzo[a]anthracene | 15 | 13 |
| Chrysene | 25 | 26 |
| Benzo[b]fluoranthene | < LD | < LD |
| Benzo[k]fluoranthene | < LD | < LD |
| Benzo[j]fluoranthene | < LD | < LD |
| Benzo[e]pyrene | < LD | < LD |
| Benzo[a]pyrene | < LD | < LD |
| Perylene | < LD | < LD |
| 1,2-Acenaphthylene | 2 × 10\(^9\) | 2 × 10\(^9\) |
| Benzo[b]naptho[1,2-d]furan | 28 | 75 |
| Benzo[b]naptho[2,3-d]furan | 9 | 43 |
| 2,3,5,6-Dibenzo[c,e]pyrene | 9 | 29 |
| Benzo[k,l]xanthene | < LD | < LD |
| 4-Oxapyrene-5-one | < LD | < LD |
| 9H-Fluoren-9-one | 95 | 177 |
| 9,10-Anthraquinone | < LD | < LD |
| Xanthone | < LD | < LD |
| Cyclopenta[d,e,f]phenanthrene | 54 | 80 |
| 3-methylphenanthrene | 44 | 69 |
| 2-methylphenanthrene | 54 | 97 |
| 2-methylanthracene | 25 | 57 |
| 4,9-methylphenanthrene | 30 | 58 |
| 1-methylphenanthrene | 33 | 60 |
| Octadecane | 203 | 272 |
| Nonadecane | 79 | 131 |
| Eicosane | 162 | 244 |
| Heneicosane | 73 | 246 |
| Docosane | 181 | 418 |
| Tricosane | 75 | 158 |
| Tetracosane | 93 | 120 |
| Pentacosane | 183 | 222 |
| Hexacosane | 65 | 81 |
| Heptacosane | 48 | 50 |
| Vanillin | 7 × 10\(^3\) | 14 × 10\(^3\) |
| Acetovanillone | 934 | 2 × 10\(^9\) |
| Vanillic Acid | 1 × 10\(^3\) | 3 × 10\(^3\) |
| 3-Guaiacylpropanol | 3 × 10\(^3\) | 931 |
| Coniferyl Aldehyde | 2 × 10\(^3\) | 687 |
| Syringaldehyde | 20 × 10\(^3\) | 17 × 10\(^3\) |
| Syringol | 12 × 10\(^3\) | 6 × 10\(^3\) |
| Acetosyringone | 4 × 10\(^3\) | 2 × 10\(^3\) |
| Isoeugenol | 15 × 10\(^3\) | 5 × 10\(^3\) |
| Syringyl Acetone | 52 × 10\(^3\) | 9 × 10\(^3\) |
| Propionyl Syringol | 6 × 10\(^3\) | 3 × 10\(^3\) |
| Syringic Acid | 994 | 188 |
| Synapyl Aldehyde | 9 × 10\(^3\) | 905 |
| Palmitoleic Acid | < LD | < LD |
| Palmitic Acid | 1 × 10\(^3\) | 843 |
| Oleic Acid | < LD | < LD |
| Stearic Acid | 506 | 416 |
| 4-Nitrocatechol | 509 | 65 × 10\(^3\) |
| Pyrogallol | 112 | 430 |
| Methylsyringol | 274 | 557 |
| Vanillylmandelic acid | 110 | 1 × 10\(^3\) |
| 2-methyl-2-pentanedic acid | 88 | 1 × 10\(^3\) |
| Tyrosol | 1 × 10\(^3\) | 3 × 10\(^3\) |
| 5-Methyl-5-Nitrocatechol | < LD | 4 × 10\(^3\) |
| 3-Methyl-5-Nitrocatechol | 830 | 10 × 10\(^3\) |
### Table S3: (Continued)

| EF Compounds (µg kg⁻¹) | Fresh | Aged |
|------------------------|-------|------|
| Levoglucosan           | 4.9 × 10⁹ | 2.2 × 10⁹ |
| Mannosan               | 6 × 10⁹    | 3 × 10⁹   |
| Galactosan             | 582      | 175    |
| Acenaphthene           | 619      | 940    |
| Acenaphylene           | 924      | 173    |
| Fluorene               | 783      | 729    |
| Phenanthrene           | 981      | 792    |
| Anthracene             | 219      | 115    |
| Fluoranthrene          | 1 × 10⁹  | 2 × 10⁹ |
| Acaenophanthenone      | 783      | 729    |
| Pyrene                 | 381      | 543    |
| Benzo[a]anthracene     | 8        | 5      |
| Chrysene               | 15       | 10     |
| Benzo[b]fluoranthenone | < LD     | < LD   |
| Benzo[k]fluoranthenene | < LD     | < LD   |
| Benzo[j]fluoranthenene | < LD     | < LD   |
| Benzo[e]pyrene         | < LD     | < LD   |
| Benzo[a]pyrene         | < LD     | < LD   |
| Perylene               | < LD     | < LD   |
| 1,2-Acenaphthylene     | 783      | 729    |
| Benzo[b]napthal[1,2-d]furan | 74 | 121    |
| Benzo[b]napthal[2,3-d]furan | 28 | 50     |
| 2,3-5,6-Dibenzoazalene | 17      | 33     |
| Benzo[k,l]anthracene   | < LD     | < LD   |
| 4-Oxapyrene-5-one      | < LD     | < LD   |
| 9H-Fluoren-9-one       | 122      | 132    |
| 9,10-Anthraquinone     | < LD     | < LD   |
| Xanthone               | < LD     | < LD   |
| Cyclopenta[d,e,f]phenanthrene | 161 | 125     |
| 3-methylphenanthrene   | 93       | 47     |
| 2-methylphenanthrene   | 139      | 77     |
| 2-methylanthracene     | 31       | 16     |
| 4,9-methylphenanthrene | 83       | 44     |
| 1-methylphenanthrene   | 115      | 53     |
| Octadecane             | 96       | 140    |
| Nonadecane             | 69       | 74     |
| Eicosane               | 142      | 189    |
| Heneicosane            | 110      | 183    |
| Docosane               | 179      | 242    |
| Tricosane              | 93       | 100    |
| Tetracosane            | 46       | 47     |
| Pentacosane            | 85       | 87     |
| Hexacosane             | 35       | 29     |
| Heptacosane            | < LD     | < LD   |
| Vanillin               | 5 × 10⁶  | 6 × 10⁶ |
| Acetovanillnone        | 1 × 10⁹  | 954    |
| Vanillic Acid          | 476      | 737    |
| 3-Guaiacylpropanol     | 625      | 185    |
| Conyferly Aldehyde     | 344      | 120    |
| Syringaldehyde         | 7 × 10⁹  | 5 × 10⁹ |
| Syringol               | 2 × 10⁹  | 1 × 10⁹ |
| Acetosyringone         | 741      | 260    |
| Isoeugenol             | 3 × 10⁹  | 684    |
| Syringyl Acetone       | 6 × 10⁹  | 1 × 10⁹ |
| Propionyl Syringol     | 2 × 10⁹  | 890    |
| Syringic Acid          | 382      | 444    |
| Synapyl Aldehyde       | 2 × 10⁹  | 123    |
| Palmitoleic Acid       | < LD     | < LD   |
| Palmitic Acid          | 326      | 396    |
| Oleic Acid             | < LD     | < LD   |
| Stearic Acid           | 211      | 196    |
| 4-Nitrocatechol        | 2 × 10⁹  | 9 × 10⁹ |
| Pyrogallol             | 65       | 133    |
| Methylsyringol         | 543      | 133    |
| Vanillylmandelic acid  | 38       | 129    |
| 2-methyl-2-pentanedioic Acid | 5 | 91 |
| Tyrosol                | 2 × 10⁹  | 1 × 10⁹ |
| 5-Methyl-5-Nitrocatechol | 424 | 1 × 10⁹ |
| 3-Methyl-5-Nitrocatechol | 693 | 2 × 10⁹ |

### Experiment 8 - Stove B

| Integrated OH exposure (molecule cm⁻³ hour) | Fresh | Aged |
|--------------------------------------------|-------|------|
| OA (mg kg⁻¹)                               | 117   | 550  |
| OM/OC                                      | 1.9   | 2.1  |

Experiment 8 - Stove B
Table S3: (Continued)

| Experiment 9 - Stove C | Fresh | Aged |
|------------------------|-------|------|
| **Integrated OH exposure (molecule cm\(^{-3}\) hour)** | 0 | 4.19 × 10\(^6\) |
| **OA (mg kg\(^{-1}\))** | 115 | 59 |
| **OM/OC** | 1.7 | 2 |
| **EF Compounds (µg kg\(^{-1}\))** | | |
| Levoglucosan | 51 x 10\(^3\) | 28 x 10\(^3\) |
| Mannosan | 8 x 10\(^3\) | 4 x 10\(^3\) |
| Galactosan | 742 | 239 |
| Acenaphthene | 74 | 465 |
| Acenaphthylene | 372 | 139 |
| Fluorene | 97 | 115 |
| Phenanthrene | 317 | 552 |
| Anthracene | 66 | 102 |
| Fluoranthene | 399 | 732 |
| Acephepanthrene | 11 | 15 |
| Pyrene | 138 | 295 |
| Benzo[a]anthracene | 14 | 13 |
| Chrysene | 26 | 23 |
| Benzo[b]fluoranthene | < LD | < LD |
| Benzo[k]fluoranthene | < LD | < LD |
| Benzo[j]fluoranthene | < LD | < LD |
| Benzo[e]pyrene | < LD | < LD |
| Benzo[a]pyrene | < LD | < LD |
| Perylene | < LD | < LD |
| 1,2-Acencapthylene | 296 | 362 |
| Benzo[b]naphto[1,2-d]furan | 29 | 66 |
| Benzo[b]naphto[2,3-d]furan | 14 | 28 |
| 2,3,5,6-Dibenzoalcohol | 10 | 20 |
| Benzo[k,l]xanthene | 3 | 4 |
| 4-Oxapyrene-5-one | < LD | < LD |
| 9H-Fluoren-9-one | 44 | 74 |
| 9,10-Anthraquinone | < LD | < LD |
| Xanthone | < LD | < LD |
| Cyclopenta[d,e,f]phenanthrene | 33 | 41 |
| 3-methylphenanthrene | 16 | 19 |
| 2-methylphenanthrene | 27 | 31 |
| 2-methylanthracene | 4 | 5 |
| 4,9-methylphenanthrene | 14 | 17 |
| 1-methylphenanthrene | 16 | 21 |
| Octadecane | 65 | 142 |
| Nonadecane | 44 | 66 |
| Eicosane | 79 | 161 |
| Heneicosane | 81 | 146 |
| Docosane | 102 | 188 |
| Tricosane | 66 | 85 |
| Tetracosane | 34 | 37 |
| Pentacosane | 67 | 84 |
| Hexacosane | 24 | 17 |
| Heptacosane | 26 | 14 |
| Vanillin | 3 x 10\(^3\) | 4 x 10\(^3\) |
| Acetovanillone | 488 | 538 |
| Vanillic Acid | 352 | 499 |
| 3-Guaiaicylpropanol | 116 | 68 |
| Coniferyl Aldehyde | 174 | 83 |
| Syringaldehyde | 2 x 10\(^3\) | 2 x 10\(^3\) |
| Syringol | 925 | 585 |
| Acetosyringone | 219 | 113 |
| Isoeugenol | 1 x 10\(^3\) | 249 |
| Syringyl Acetone | 1 x 10\(^3\) | 484 |
| Propionyl Syringol | 506 | 532 |
| Syringic Acid | 240 | 260 |
| Synapyl Aldehyde | 628 | 95 |
| Palmitoleic Acid | < LD | < LD |
| Palmitic Acid | 1 x 10\(^3\) | 502 |
| Oleic Acid | < LD | < LD |
| Stearic Acid | 267 | 180 |
| 4-Nitrocatechol | < LD | 7 x 10\(^3\) |
| Pyrogallol | 23 | 85 |
| Methylsyringol | 28 | 25 |
| Vanillylmandelic acid | 107 | 108 |
| 2-methyl-2-pentandioic Acid | < LD | 17 |
| Tyrosol | 362 | 281 |
| 5-Methyl-5-Nitrocatechol | < LD | 396 |
| 3-Methyl-5-Nitrocatechol | < LD | 685 |
Table S3: (Continued)

| EF Compounds (µg kg⁻¹) | Fresh | Aged |
|------------------------|-------|------|
| Levoglucosan           | 28×10³ | 16×10³ |
| Mannosan               | 4×10⁹  | 3×10⁹  |
| Galactosan             | 187    |      |
| Acenaphthene           | 265    | 248  |
| Acenaphthylene         | 408    | 89   |
| Fluorene               | 70     | 69   |
| Phenanthrene           | 374    | 535  |
| Anthracene             | 52     | 48   |
| Fluoranthenone         | 234    | 462  |
| Acephenanthrene        | 9.10   |      |
| Pyrene                 | 90     | 191  |
| Benzo[a]anthracene     | 19     | 16   |
| Chrysene               | 25     | 24   |
| Benzo[b]fluoranthene   | <LD    | <LD  |
| Benzo[k]fluoranthene   | <LD    | <LD  |
| Benzo[j]fluoranthene   | <LD    | <LD  |
| Benzo[e]pyrene         | <LD    | <LD  |
| Benzo[a]pyrene         | <LD    | <LD  |
| Perylene               | <LD    | <LD  |
| 1,2-Acenaphthyleneone  | 235    | 252  |
| Benzo[b]naphtho[1,2-d]furan | 22  | 43  |
| Benzo[b]naphtho[2,3-d]furan | 11  | 21  |
| 2,3,5,6-Dibenzo[a]pyrene | 9   | 14   |
| Benzo[k,l]xanthene     | 4      |      |
| 4-Oxapyrene-5-one      | <LD    | <LD  |
| 9H-Fluoren-9-one       | 34     | 56   |
| 9,10-Anthraquinone     | <LD    | <LD  |
| Xanthone               | <LD    | <LD  |
| Cyclopenta[d,e,f]phenanthrene | 19  | 26  |
| 3-methylphenanthrene   | 12     | 15   |
| 2-methylphenanthrene   | 17     | 23   |
| 2-methylanthracene     | 5      | 3    |
| 4,9-methylphenanthrene | 13     | 15   |
| 1-methylphenanthrene   | 11     | 15   |
| Octadecane             | 56     | 95   |
| Nonadecane             | 28     | 40   |
| Eicosane               | 55     | 77   |
| Henecicosane           | 50     | 100  |
| Docosane               | 94     | 146  |
| Tricosane              | 60     | 60   |
| Tetracosane            | 27     | 25   |
| Pentacosane            | 62     | 56   |
| Hexacosane             | 14     | 12   |
| Heptacosane            | 16     | 14   |
| Vanillin               | 2×10⁹  | 1×10⁹ |
| Acetovanillone         | 314    | 349  |
| Vanillic Acid          | 316    | 421  |
| 3-Guaiaicypropanol     | <LD    | 67   |
| Coniferyl Aldehyde     | 144    | 70   |
| Syringaldehyde         | 2×10⁹  | 1×10⁹ |
| Syringol               | 658    | 323  |
| Acetosyringone         | 167    | 90   |
| Isoeugenol             | 335    | 17   |
| Syringyl Acetone       | 547    | 301  |
| Propionyl Syringol     | 643    | 392  |
| Syringic Acid          | 207    | 240  |
| Synapyl Aldehyde       | 300    | 128  |
| Palmitoleic Acid       | <LD    | <LD  |
| Palmitic Acid          | 314    | 241  |
| Oleic Acid             | <LD    | <LD  |
| Stearic Acid           | 168    | 105  |
| 4-Nitrocatechol        | <LD    | 7×10³ |
| Pyrogallol             | 30     | 64   |
| Methylsyringol         | 21     | 14   |
| Vanillymendelic acid   | 23     | 39   |
| 2-methyl-2-pentanedioc Acid | <LD | 7   |
| Tyrosol                | 153    | 157  |
| 5-Methyl-5-Nitrocatechol | 62   | 327  |
| 3-Methyl-5-Nitrocatechol | 19   | 428  |
| EF Compounds (µg kg⁻¹) | Fresh | Aged |
|------------------------|-------|------|
| Levoglucosan           | 26 × 10³ | 22 × 10³ |
| Mannosan               | 5 × 10⁹  | 4 × 10⁹  |
| Galactosan             | 754    | 323   |
| Acenaphthene           | 314    | 431   |
| Acenaphylene           | 1 × 10⁹ | 183   |
| Fluorene               | 130    | 96    |
| Phenanthrene           | 484    | 631   |
| Anthracene             | 77     | 93    |
| Fluoranthene           | 248    | 360   |
| Acenaphanthenre        | 12     | 11    |
| Pyrene                 | 108    | 152   |
| Benz[a]anthracene      | 27     | 22    |
| Chrysene               | 36     | 31    |
| Benzo[b]fluoranthrene  | < LD   | < LD  |
| Benzo[k]fluoranthene   | < LD   | < LD  |
| Benzo[j]fluoranthene   | < LD   | < LD  |
| Benzo[e]pyrene         | < LD   | < LD  |
| Benzo[a]pyrene         | < LD   | < LD  |
| Perylene               | < LD   | < LD  |
| 1,2-Acenaphthylene     | 470    | 373   |
| Benzo[b]naphtho[1,2-d]furan | 26  | 37  |
| Benzo[b]naphtho[2,3-d]furan | 13 | 18  |
| 2,3-5,6-Dibenzo[a]pyrene | 10 | 13  |
| Benzo[k,l]anthracene   | < LD   | < LD  |
| 4-Oxapyrene-5-one      | < LD   | < LD  |
| 9H-Fluoren-9-one       | 43     | 56    |
| 9,10-Anthraquinone     | < LD   | < LD  |
| Xanthenone             | < LD   | < LD  |
| Cyclopenta[d,e,f]phenanthrene | 20  | 23  |
| 3-methylphenanthrene   | 12     | 15    |
| 2-methylphenanthrene   | 18     | 22    |
| 2-methylyanthracene    | 3      | 1     |
| 4,9-methylphenanthrene | 10     | 13    |
| 1-methylphenanthrene   | 11     | 13    |
| Octadecane             | 83     | 91    |
| Nonadecane             | 35     | 40    |
| Eicosane               | 93     | 101   |
| Heneicosane            | 83     | 99    |
| Docosane               | 133    | 141   |
| Tricosane              | 65     | 65    |
| Tetracosane            | 38     | 29    |
| Pentacosane            | 73     | 60    |
| Hexacosane             | 18     | 13    |
| Heptacosane            | < LD   | < LD  |
| Vanillin               | 2 × 10⁶ | 3 × 10⁶ |
| Acetovanillone         | 295    | 469   |
| Vanillic Acid          | 404    | 627   |
| 3-Guaiacylpropanol     | 70     | 98    |
| Coniferyl Aldehyde     | 158    | 108   |
| Syringaldehyde         | 2 × 10⁹ | 2 × 10⁹ |
| Syringol               | 913    | 433   |
| Acetosyringone         | 160    | 123   |
| Isoeugenol             | 404    | 95    |
| Syringyl Acetone       | 366    | 404   |
| Propionyl Syringol     | 411    | 479   |
| Syringic Acid          | 233    | 335   |
| Synapyl Aldehyde       | 305    | 209   |
| Palmitoleic Acid       | < LD   | < LD  |
| Palmitic Acid          | 383    | 351   |
| Oleic Acid             | < LD   | < LD  |
| Stearic Acid           | 131    | 149   |
| 4-Nitrocatechol        | 180    | 11 × 10³ |
| Pyrogallol             | 40     | 89    |
| Methylsyringol         | 19     | 14    |
| Vanillylmandelic acid  | < LD   | 59    |
| 2-methyl-2-pentanedioc Acid | < LD | 8  |
| Tyrosol                | 93     | 115   |
| 5-Methyl-5-Nitrocatechol | 61 | 508  |
| 3-Methyl-5-Nitrocatechol | 261 | 790  |
Table S4: pWLC contribution of the compounds to the total OA mass concentration at different times of the photo-oxidative process.

| Integrated molecule (molecule cm⁻³) | OH exposure hour | Bin 0 | Bin 1 | Bin 2 | Bin 3 | Bin 4 | Bin 5 | Bin 6 |
|-----------------------------------|------------------|-------|-------|-------|-------|-------|-------|-------|
| Levoglucosan (min - max)          |                  | 29.18 | 20    | 20    | 14    | 10    | 13    | 9     |
| Mannosan (min - max)              |                  | 3.19  | 0.5   | 0.18  | 0.5   | 0.18  | 0.5   | 0.18  |
| Galactosan (min - max)            |                  | 0.19  | 0.44  | 0.16  | 0.11  | 0.14  | 0.04  | 0.03  |
| Aacenaphthylene (min - max)       |                  | 0.15  | 0.06  | 0.07  | 0.07  | 0.05  | 0.03  | 0.05  |
| Anthracene (min - max)            |                  | 0.08  | 0.04  | 0.03  | 0.03  | 0.02  | 0.02  | 0.02  |
| Fluoranthen (min - max)           |                  | 0.22  | 0.07  | 0.14  | 0.13  | 0.12  | 0.16  | 0.16  |
| Aacenaphthene (min - max)         |                  | 0.08  | 0.04  | 0.03  | 0.03  | 0.02  | 0.02  | 0.02  |
| Pyrene (min - max)                |                  | 0.08  | 0.02  | 0.05  | 0.05  | 0.04  | 0.07  | 0.05  |
| Benzo[a]anthracene (min - max)    |                  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  |
| Chrysene (min - max)              |                  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  |
| Benzo[b]fluoranthene (min - max)  |                  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  |

*Primary Compounds (% OA)*

| Integrated molecule (molecule cm⁻³) | OH exposure hour | Bin 0 | Bin 1 | Bin 2 | Bin 3 | Bin 4 | Bin 5 | Bin 6 |
|-----------------------------------|------------------|-------|-------|-------|-------|-------|-------|-------|
| Levoglucosan (min - max)          |                  | 29.18 | 20    | 20    | 14    | 10    | 13    | 9     |
| Mannosan (min - max)              |                  | 3.19  | 0.5   | 0.18  | 0.5   | 0.18  | 0.5   | 0.18  |
| Galactosan (min - max)            |                  | 0.19  | 0.44  | 0.16  | 0.11  | 0.14  | 0.04  | 0.03  |
| Aacenaphthylene (min - max)       |                  | 0.15  | 0.06  | 0.07  | 0.07  | 0.05  | 0.03  | 0.05  |
| Anthracene (min - max)            |                  | 0.08  | 0.04  | 0.03  | 0.03  | 0.02  | 0.02  | 0.02  |
| Fluoranthen (min - max)           |                  | 0.22  | 0.07  | 0.14  | 0.13  | 0.12  | 0.16  | 0.16  |
| Aacenaphthene (min - max)         |                  | 0.08  | 0.04  | 0.03  | 0.03  | 0.02  | 0.02  | 0.02  |
| Pyrene (min - max)                |                  | 0.08  | 0.02  | 0.05  | 0.05  | 0.04  | 0.07  | 0.05  |
| Benzo[a]anthracene (min - max)    |                  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  |
| Chrysene (min - max)              |                  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  |
| Benzo[b]fluoranthene (min - max)  |                  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  | 0.01  |
Table S4: (Continued)

| Integrated OH exposure (molecule cm\(^{-3}\) hour) | 0 n = 11 | > 0 - 0.5 \(\times\) 10\(^6\) n = 6 | 0.5 - 2 \(\times\) 10\(^6\) n = 11 | 2 - 4 \(\times\) 10\(^6\) n = 17 | 4 - 6 \(\times\) 10\(^6\) n = 15 | 6 - 7.5 \(\times\) 10\(^6\) n = 8 | 7.5 - 9 \(\times\) 10\(^6\) n = 2 |
|--------------------------------------------------|-----------|----------------|----------------|----------------|----------------|----------------|----------------|
| Benzo[k]fluoranthene | BDL | < 0.01 | < 0.01 | < 0.01 | < 0.01 | BDL | BDL | BDL |
| Benzo[j]fluoranthene | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | BDL | BDL | BDL |
| Benzo[e]pyrene | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | BDL | BDL | BDL |
| Benzo[a]pyrene | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | BDL | BDL | BDL |
| Perylene | BDL | BDL | BDL | BDL | BDL | BDL | BDL |
| 1,2-Acenaphthylene | 0.31 | 0.14 | 0.15 | 0.10 | 0.08 | 0.11 | 0.08 |
| Benzo[b]naphtho[1,2-d]furan | 0.02 | < 0.01 | 0.01 | 0.01 | < 0.01 | 0.02 | 0.01 |
| Benzo[b]naphtho[2,3-d]furan | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 |
| 2,3-5,6-Dibenzoxalene | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 |
| Benzo[k,l]xanthene | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 |
| 4-Oxapyrene-5-one | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | BDL | BDL | BDL |
| 9H-Fluoren-9-one | 0.03 | 0.01 | 0.02 | 0.02 | 0.01 | 0.02 | 0.02 |
| 9,10-Anthraquinone | < 0.01 | < 0.01 | < 0.01 | < 0.01 | < 0.01 | BDL | BDL | BDL |
| Xanthone | BDL | BDL | BDL | BDL | BDL | BDL | BDL |
| Integrated OH exposure (molecule cm$^3$ hour) | 0 n = 11 | n = 6 | 0.5 - 2 x 10$^6$ | n = 11 | 0.5 - 4 x 10$^6$ | n = 17 | 2 - 4 x 10$^6$ | n = 15 | 4 - 6 x 10$^6$ | n = 8 | 6 - 7.5 x 10$^6$ | n = 2 | 7.5 - 9 x 10$^6$ | n = 4 |
|---------------------------------------------|---------|------|-----------------|-------|-----------------|------|----------------|-------|-----------------|------|-----------------|------|-----------------|------|
| Cyclopenta[e,f]phenanthrene-4-one            | 0.03    | < 0.01 | 0.01            |       | 0.01            | < 0.01 | 0.01          |       | 0.01            | < 0.01 | 0.01          | < 0.01 | 0.01          | < 0.01 |
| 3-methylphenanthrene                         | 0.02    | < 0.01 | < 0.01          | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01 | < 0.01        | < 0.01 |
| 2-methylphenanthrene                         | 0.03    | 0.01   | 0.01            | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01| 0.01            | < 0.01 | < 0.01        | < 0.01 | < 0.01        | < 0.01 |
| 2-methylnaphthalene                          | < 0.01  | < 0.01 | < 0.01          | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01 | < 0.01        | < 0.01 |
| 4,9-dimethylphenanthrene                     | 0.02    | < 0.01 | < 0.01          | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01 | < 0.01        | < 0.01 |
| 1-methylphenanthrene                         | 0.02    | < 0.01 | < 0.01          | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01 | < 0.01        | < 0.01 |
| Octadecane                                   | 0.05    | 0.02   | 0.03            |       | 0.03            |       | 0.02          |       | 0.03            |       | 0.02          |       | 0.02          |       |
| Nonadecane                                   | 0.03    | 0.01   | 0.01            | < 0.01| < 0.01          | < 0.01| 0.01          |       | 0.01            |       | 0.02          |       | 0.02          |       |
| Eicosane                                     | 0.04    | 0.01   | 0.03            | 0.02  | 0.02            | 0.03  | 0.03          |       | 0.02            |       | 0.02          |       | 0.02          |       |
| Heneicosane                                  | 0.04    | 0.01   | 0.03            | 0.02  | 0.02            | 0.03  | 0.03          |       | 0.02            |       | 0.02          |       | 0.02          |       |
| Docosane                                     | 0.06    | 0.02   | 0.04            | 0.04  | 0.03            | 0.05  | 0.03          |       | 0.05            |       | 0.03          |       | 0.03          |       |
| Aceenaphthene                                | 0.03    | 0.09   | 0.14            | 0.12  | 0.09            | 0.14  | 0.09          |       | 0.14            |       | 0.09          |       | 0.09          |       |
| Tetracosane                                  | 0.02    | < 0.01 | 0.01            | < 0.01| < 0.01          | < 0.01| < 0.01        | < 0.01| < 0.01          | < 0.01 | < 0.01        | < 0.01 | < 0.01        | < 0.01 |
| Pentacosane                                  | 0.04    | 0.01   | 0.02            | 0.02  | 0.01            | 0.02  | 0.02          | < 0.01| 0.02            | < 0.01 | 0.02          | < 0.01 | 0.02          | < 0.01 |

(Continued)
Table S4: (Continued)

| Integrated OH exposure (molecule cm⁻³) | 0   | > 0 - 0.5 x 10⁶ | 0.5 - 2 x 10⁶ | 2 - 4 x 10⁶ | 4 - 6 x 10⁶ | 6 - 7.5 x 10⁶ | 7.5 - 9 x 10⁶ |
|---------------------------------------|-----|----------------|--------------|------------|------------|-------------|-------------|
| n = 11                                |     | (< 0.01        | < 0.01       | < 0.01     | < 0.01     | < 0.01      | < 0.01      |
| Hexacosane                            | 0.02| (< BDL         | (< BDL       | (< BDL     | (< BDL     | (< BDL      | (< BDL      |
| Heptacosane                           |     | (< 0.01       | < 0.01       | < 0.01     | < 0.01     | < 0.01      | < 0.01      |
| 3-Guaiacylpropanol                    |     | (0.04 - 0.14  | (0.02 - 0.11 | (0.02 - 0.08| (0.02 - 0.04| (0.02 - 0.03)| (0.02 - 0.03)|
| Coniferyl Aldehyde                    |     | (0.05 - 0.12  | (0.02 - 0.08  | (0.01 - 0.07| (0.01 - 0.04| (0.01 - 0.04)| (0.01 - 0.04)|
| Syringaldehyde                        |     | (0.04 - 0.46  | (0.01 - 0.14  | (0.01 - 0.14| (0.01 - 0.05| (0.01 - 0.02)| (0.01 - 0.02)|
| Syringol                              |     | (0.24 - 2.42  | (0.10 - 1.21  | (0.09 - 0.48| (0.09 - 0.30| (0.10 - 0.29)| (0.09 - 0.17)|
| Methylsyringol                        |     | (0.13 - 0.55  | (0.05 - 0.12  | (0.02 - 0.08| (0.01 - 0.07| (0.01 - 0.04| (0.01 - 0.04)|
| Acetosyringone                        |     | (0.18 - 0.66  | (0.06 - 0.29  | (0.04 - 0.17| (0.04 - 0.08| (0.02 - 0.09| (0.03 - 0.06)| (0.04 - 0.06)|
| Isoeugenol                            |     | (0.09 - 0.29  | (0.01 - 0.18  | (0.01 - 0.16| (0.01 - 0.12| (0.01 - 0.12| (0.05 - 0.12)|
| Syringyl Acetone                      |     | (0.13 - 2.65  | (0.01 - 0.76  | (0.01 - 0.18| (0.01 - 0.12| (0.01 - 0.12| (0.06 - 0.12)|
| Propionyl Syringol                    |     | (0.29 - 2.71  | (0.18 - 0.69  | (0.16 - 0.33| (0.14 - 0.41| (0.15 - 0.35| (0.15 - 0.34)|
| Synapyl Aldehyde                      |     | (0.04 - 0.45  | (0.16 - 0.47  | (0.05 - 0.35| (0.02 - 0.26| (0.02 - 0.26| (0.06 - 0.14)|
| Palmitoleic Acid                      |     | (0.02 - 9.02  | < 0.01        | BDL         | BDL         | < 0.01      | < 0.01      |
| Palmitic Acid                         |     | (0.02 - 1.06  | (0.01 - 0.63  | (0.01 - 0.31| (0.01 - 0.26| (0.01 - 0.25| (0.01 - 0.27)|
**Table S4: (Continued)**

| Integrated (molecule) | OH cm⁻³ | exposure hour | 0 (n = 11) | > 0 - 0.5 x 10⁶ (n = 6) | 0.5 - 2 x 10⁶ (n = 11) | 2 - 4 x 10⁶ (n = 17) | 4 - 6 x 10⁶ (n = 15) | 6 - 7.5 x 10⁶ (n = 8) | 7.5 - 9 x 10⁶ (n = 2) |
|----------------------|---------|---------------|-------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| Oleic Acid           |         |               |             | < 0.01 (BDL - 0.01)    | < 0.01 (BDL - 0.01)    | < 0.01 (BDL - 0.01)    | < 0.01 (BDL - 0.01)    | BDL                    | BDL                    |
| Stearic Acid         |         |               |             | 0.11                   | 0.05                   | 0.06                   | 0.04                   | 0.03                   | 0.05                   | 0.02                   |

**Non-conventional Primary Compounds (% OA)**

|                  |         |               |             |             |             |             |             |             |             |
|------------------|---------|---------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| Vanillin         | 1.66    | 0.8           | 1.06        | 0.86        | 0.62        | 1.01        | 0.7         |
|                  | (0.34 - 4.22) | (0.33 - 1.69) | (0.27 - 2.46) | (0.23 - 1.86) | (0.20 - 1.51) | (0.20 - 2.05) | (0.20 - 1.19) |
| Acetovanillone   | 0.29    | 0.13          | 0.17        | 0.14        | 0.14        | 0.14        | 0.1         |
|                  | (0.04 - 0.07) | (0.06 - 0.25) | (0.05 - 0.40) | (0.05 - 0.26) | (0.04 - 0.86) | (0.05 - 0.26) | (0.05 - 0.16) |
| Vanillic Acid    | 0.24    | 0.12          | 0.16        | 0.14        | 0.1        | 0.14        | 0.09        |
|                  | (0.09 - 0.46) | (0.06 - 0.18) | (0.05 - 0.37) | (0.05 - 0.26) | (0.06 - 0.26) | (0.07 - 0.12) |
| Syringic Acid    | 0.17    | 0.09          | 0.11        | 0.08        | 0.06        | 0.08        | 0.05        |
|                  | (0.05 - 0.53) | (0.04 - 0.13) | (0.03 - 0.20) | (0.03 - 0.19) | (0.02 - 0.15) | (0.04 - 0.14) | (0.06 - 0.07) |
| Pyrogallol       | 0.02    | 0.02          | 0.03        | 0.02        | 0.02        | 0.02        | 0.01        |
|                  | (BDL - 0.06) | (BDL - 0.04) | (< 0.01 - 0.05) | (< 0.01 - 0.09) | (< 0.01 - 0.06) | (< 0.01 - 0.04) | (< 0.01 - 0.02) |
| Tyrosol          | 0.36    | 0.16          | 0.17        | 0.12        | 0.09        | 0.12        | 0.15        |
|                  | (0.11 - 1.29) | (0.09 - 0.28) | (0.07 - 0.70) | (0.06 - 0.31) | (0.05 - 0.19) | (0.07 - 0.20) | (0.07 - 0.12) |

**Secondary Compounds (% OA)**

|                  |         |               |             |             |             |             |             |             |             |
|------------------|---------|---------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 4 Nitroctecoh    | 0.19    | 0.81          | 1.68        | 2.43        | 1.77        | 1.92        | 1.05        |
|                  | (BDL - 1.37) | (0.40 - 1.41) | (0.84 - 1.83) | (0.71 - 6.27) | (0.70 - 4.11) | (0.97 - 5.85) | (0.96 - 1.14) |
| 4-Methyl-5-Nitroctechol | 0.05  | 0.15          | 0.2         | 0.18        | 0.14        | 0.15        | 0.11        |
|                  | (BDL - 0.36) | (0.07 - 0.26) | (0.05 - 0.30) | (0.07 - 0.28) | (0.06 - 0.23) | (0.10 - 0.19) | (0.08 - 0.13) |
| 3-Methyl-5-Nitroctechol | 0.15  | 0.48          | 0.45        | 0.32        | 0.25        | 0.24        | 0.19        |
|                  | (BDL - 0.59) | (0.30 - 0.57) | (0.17 - 0.94) | (0.14 - 0.95) | (0.12 - 0.42) | (0.20 - 0.34) | (0.18 - 0.20) |
| Vanillylmandelic acid | 0.02  | 0.08          | 0.06        | 0.04        | 0.03        | 0.03        | 0.02        |
|                  | (BDL - 0.09) | (0.03 - 0.16) | (0.02 - 0.17) | (0.02 - 0.16) | (0.03 - 0.05) | (0.02 - 0.05) | (0.02 - 0.02) |
| Methylglutaric acid | < 0.01 | 0.02          | 0.02        | 0.02        | 0.02        | 0.02        | 0.02        |
|                  | (BDL - 0.01) | (< 0.01 - 0.02) | (< 0.01 - 0.08) | (< 0.01 - 0.07) | (< 0.01 - 0.06) | (< 0.01 - 0.04) | (< 0.01 - 0.02) |

*Sum from the contribution of all compounds averaged within the bins*