Quantification of Terpenes by 1DGC-MS and 2DGC-TOF-MS

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I. INTRODUCTION

On a global scale, biogenic emissions account for 95% of the natural carbon emitted to the atmosphere (C1850t/1850 GtG). Biogenic emissions of organic compounds mostly occur in the gas phase, however, partitioning between the gas and particle phases is also possible. The use of novel tools, such as ozone- and light-oxidant gas chromatography (O3-GC) has demonstrated that a substantial fraction of organic species in the gas and particle-mixed phases have not been identified and quantified. This study focused on terpenes and aromatics, which are major contributors to the atmospheric production of secondary organic aerosols (SOA) with 1,000 years. The SOA are hygroscopic and occur in the particle phase and lead to a net increase in aerosol concentration. In addition, both monoterpenes and sesquiterpenes are effective cloud condensation nuclei leading to an increase in the particle number concentration and to the formation of clouds that also increase aerosol. The objective of this study was to identify and characterize the complex mixture of terpenes in essential oils of plants by GC-MS. The motivation for this work was to develop analytical methodologies to investigate pathways of biogenic SOA formation.

II. METHODS

Sesquiterpene standards (β-sesquiphellandrene, β-Caryophyllene, β-Santalene, β-Techneol, β-Aubriol, β-Phellandrene, β-Terpinene, β-Patchoulene, α-Terpinene, β-Patchoulene, β-Santalene, γ-Santalene, α-Terpinene, β-Caryophyllene, carvacrol, carvone, carvone, caryophyllene, geraniol, terpinolene, and pulegone) were isolated and purified by gas chromatography. Terpenes and aromatics were identified by comparison of the retention times and mass spectra obtained by 1DGC-MS and 2DGC-TOF-MS.

Essential oils were isolated from leaves and needles of Picea mariana (Black Spruce), Picea mariana (South Pine) and Pinus contorta (Cedar) by steam distillation. Samples of the oils were analyzed by GC-MS.

III. RESULTS

Black Spruce

Scots Pine

Cedar

Table 1: Comparison of terpenes identified by 2DGC-MS and 2DGC-TOF-MS.

Table 2: Comparison of terpenes identified by 2DGC-MS and 2DGC-TOF-MS.

Table 3: Comparison of terpenes identified by 2DGC-MS and 2DGC-TOF-MS.

IV. Findings

1. Quantification: Better resolution of terpene stereoisomers by 2DGC-MS compared to 1DGC-MS is attributed to the length of the columns in the 2DGC-MS.

2. Identification of terpenes: Identification of the complex mixture of terpenes in essential oils was achieved by the combination of retention time analysis of authentic standards, desorption integration, 1DGC-MS, and 2DGC-TOF-MS. The 2DGC-TOF-MS allowed identification of 76 terpenes in Black Spruce, 53 in Scots Pine and 41 in Cedar, in comparison, 7, 12 and 17 terpenes, respectively, were identified by 1DGC-MS.

3. Essential oil composition: The composition of Black Spruce, Scots Pine and Cedar, was investigated. The monoterpenes in all three comprise 66% of terpenes, 11% of Black Spruce, and 36% of Cedar, whereas sesquiterpenes (C15) comprise less than 5% of the studied terpenes. Other than monoterpenes, the most abundant compounds were terpinolene for Black Spruce and camphene for Cedar.

4. Possible alteration of the terpene distribution by steam distillation is unknown and requires further investigation.

References

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