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Chemical characterisation and comparison of Isoprene Organosulphates in simulation chamber experiments and ambient aerosol samples in the Amazon rainforest

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In tropical forests, organic material accounts for a large fraction of particulate matter and the contribution can be as high as 90 % at the submicrometer scale, mainly through the formation of secondary organic aerosols (SOA) from the oxidation of biogenically released volatile organic compounds (VOCs). Despite the abundance of organic material and the important role these particles play in the rainforest boundary layer, the composition of submicrometer organic aerosols is poorly understood (Andreae et al., 2015; Hallquist et al., 2009).

Several different biogenic VOCs are released in tropical regions, but it is undisputed that isoprene is emitted in such large global quantities (600 Tg year^{-1}) that the formation of SOA results in significant production of atmospheric particulate matter even at small yields (Chen et al., 2015; Liu et al., 2016). NOx concentrations have a strong influence on SOA production, but SO_2 also affects SOA composition. Reactions of acidic sulphate aerosol with Isoprene derived oxidation products leads to the formation of organosulphates (OS) that provide information about mixtures of biogenic gases and anthropogenic pollutants. Due to the large variety of formation processes, the composition of SOA is very complex and varies constantly. To understand the formation and transformation processes, specific molecular marker compounds must be identified and quantified. Methyltetrol sulphates and methyltetrols are isoprene SOA markers that are formed from isoprene-derived epoxydiols (IEPOX). However, organosulphates have proved analytically challenging to quantify, due to lack of authentic standards and the complex sample matrix in which they are observed.

This study provides a suitable analytical tool for chemical characterisation of such isoprene derived organosulphates by combining high performance liquid chromatography (HPLC) with electrospray ionisation ultra-high resolution orbitrap mass spectrometry (ESI-UHR-Orbitrap-MS). Chamber simulation experiments were performed to investigate isoprene OS formation by comparing different atmospheric reaction pathways and authentic standards were synthesised to enable complete identification of individual OS compounds. Marker compounds for aged isoprene derived organic aerosols could be assigned and quantified in ambient aerosol samples of the

Amazon rainforest. Moreover, it could be shown that the lack of authentic standards has led to significant underestimation of isoprene derived OS concentrations in the past.

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