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Identification of characteristic mass spectrometric markers for primary biological aerosol particles and comparison with field data from submicron pristine aerosol particles

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The contribution of primary biological aerosol (PBA) to the total aerosol particle concentration is estimated to range between 25 and 80%, depending on location and season. Especially in the tropical rain forest it is expected that PBA is a major source of particles in the supermicron range, and is also an important fraction of the submicron aerosol. PBA particles like plant fragments, pollen, spores, fungi, viruses etc. contain chemical compounds as proteins, sugars, amino acids, chlorophyll, and cellular material as cellulose. For this reason we have performed mass spectrometric laboratory measurements (Aerodyne C-ToF and W-ToF AMS, single particle laser ablation instrument SPLAT) on pure submicron aerosol particles containing typical PBA compounds in order to identify typical mass spectral patterns of these compounds and to explain the observed fragmentation patterns on the basis of molecular structures. These laboratory data were compared to submicron particle mass spectra obtained during AMAZE-08 (Amazonian Aerosol CharacteriZation Experiment, Brazil, February/March 2008). The results indicate that characteristic m/z ratios for carbohydrates (e.g., glucose, saccharose, levoglucosan, mannitol) can be identified, for example m/z = 60($C_2H_4O_2^+$) or m/z = 61($C_2H_5O_2^+$). Certain characteristic peaks for amino acids were also identified in the laboratory experiments. In the field data from AMAZE-08, these characteristic peaks for carbohydrates and amino acids were found, and their contribution to the total organic mass was estimated to about 5%. Fragment ions from peptides and small proteins were also identified in laboratory experiments. Larger proteins, however, seem to become oxidized to CO_2^+ to a large extend in the vaporizing process of the AMS. Thus, detection of proteins in atmospheric aerosol particles with the AMS appears to be difficult.