**Supplementary Material to**

# Mass-spectrometric identification of primary biological particle markers and application to pristine submicron aerosol measurements in Amazonia

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## Details on the evaluation of AMS data from the AMAZE field campaign

### 1 Modifications made to fragmentation table (SQUIRREL v1.49)

<u>Gas phase correction derived from blank measurements:</u>

frag_air[29] = 0.845* 0.00736 * frag_air[28]

frag_CO2[44] = 0.83 * 0.00037 * 1.36 * 1.28 * 1.14 * frag_air[28]

frag_RH[18] = 0.8 * 0.01 * frag_air[28]

frag_O16[16] = 1.10 * 0.353 * frag_air[14]

Changes to account for the high contribution of organic nitrates:

frag_nitrate[46] = 46,

frag_nitrate[30] = 2* frag_nitrate[46],

frag_organic[30] = 30,-frag_nitrate[30],-frag_air[30]

This is based on the following assumptions: *m/z* 46 is only due to $NO_2^+$ from inorganic nitrate, the ratio of *m/z* 30 to *m/z* 46 is 2:1 for inorganic ammonium nitrate (Allan et al., 2003; Hogrefe et al., 2004), and therefore the rest of *m/z* 30 is due to organic nitrate or other organic ions (as $CH_4N^+$ and $CH_2O^+$). The high-resolution data (12 h averages) show that between 20 and 60 % (on average 35 %) of *m/z* 30 is due to $NO^+$ (see Figure S1, lower panel).

For the calculation of the mass concentration standard relative ionization efficiencies were used (nitrate: 1.1; sulfate: 1.2; organics: 1.4, ammonium: 4; chloride: 1.3). The applied collection efficiency (CE) was 1.0, which is consistent with the intercomparisons with other instruments and the liquid character of the submicron particles (see Chen et al., (2009)

## 2 Contributions of the marker *m/z* to the UMR mass peaks:

Figure S1 shows the ratios of the marker peak intensities to the respective UMR (unit mass resolution) peak (*m/z* 30 and 42 for amino acids, upper panel (a); *m/z* 60, 61, and 73 for carbohydrates, middle panel, (b)). The lower panel (c) shows the ratio of $NO^+$ to the UMR peak at *m/z* 30.

Mean values and standard deviations of the respective fractions:

$CH_4N^+$ (to *m/z* 30): 0.086 ± 0.030

$C_2H_4N^+$ (to *m/z* 42): 0.098 ± 0.036

$C_2H_4O_2^+$ (to *m/z* 60) 0.800 ± 0.061

$C_2H_5O_2^+$ (to *m/z* 61) 0.0681 ± 0.070

$C_3H_5O_2^+$ (to *m/z* 73): 0.669 ± 0.123

$NO^+$ (to *m/z* 30): 0.353 ± 0.087

Figure S2 shows the high resolution peak fitting for *m/z* 30 and 42 for the examples for March 05, 12 h (local time), when the amino acid markers showed maximum values.

**Supplementary Figures**

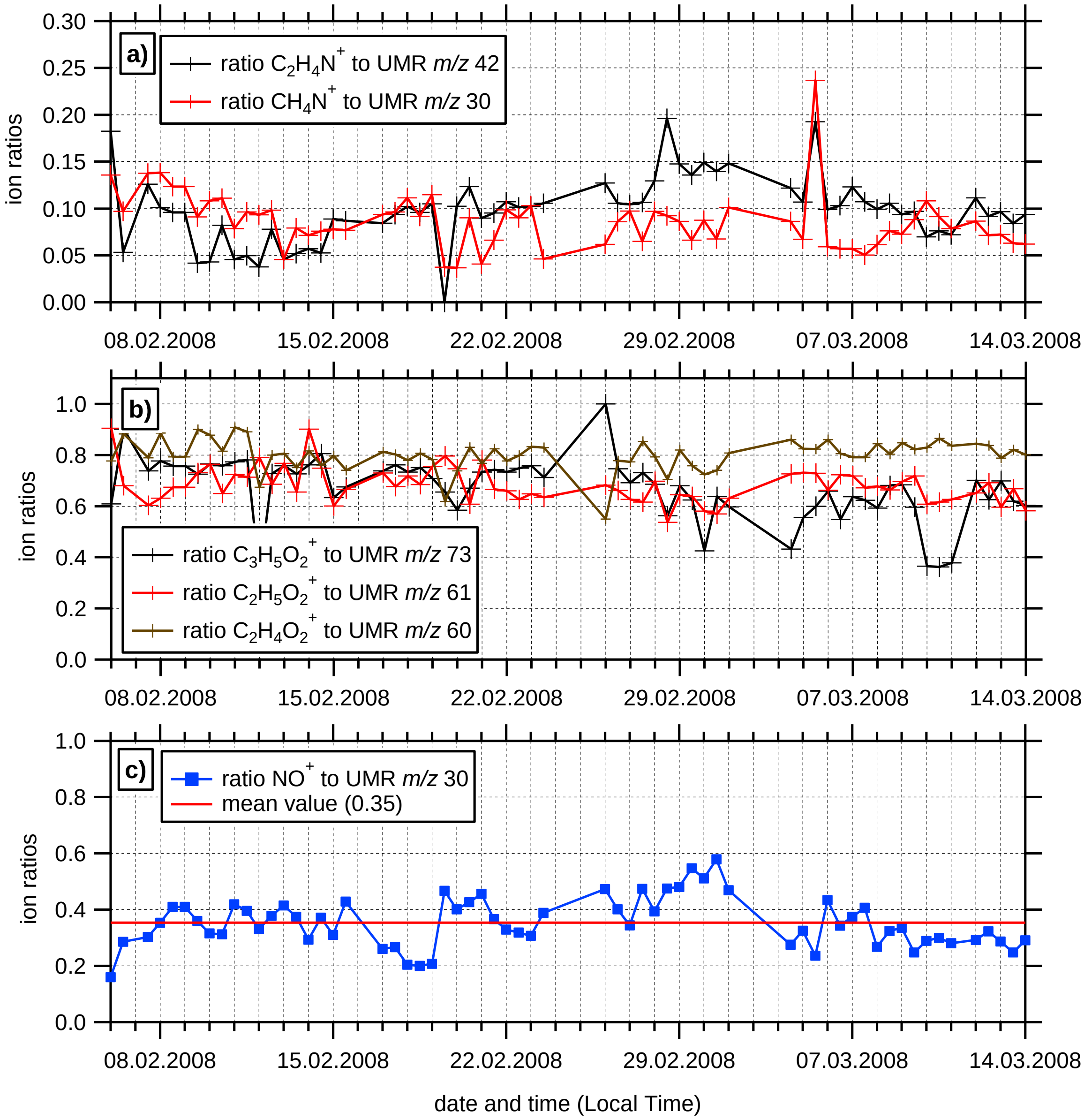


Figure S1. Fraction of marker peaks to the total UMR peak at the nominal *m/z* ratio measured during AMAZE-08. a) amino acid markers, b) carbohydrate markers, c) fraction of $NO^+$ to UMR *m/z* 30.

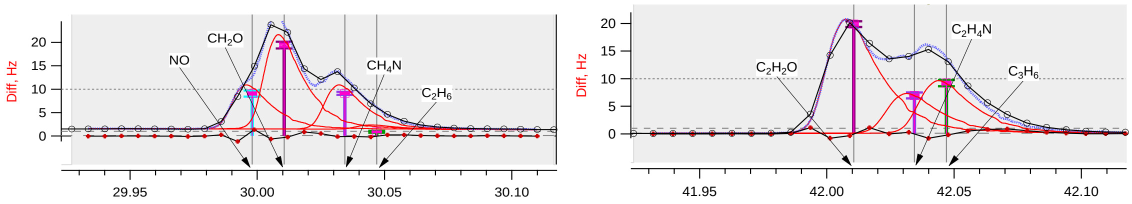


Figure S2. High resolution peak at *m/z* 30 and *m/z* 42 from March 05, 2008, 12 h (local time). During this time period $CH_4N^+$ and $C_2H_4N^+$ contribute significantly more to the respective UMR peak than during other times.