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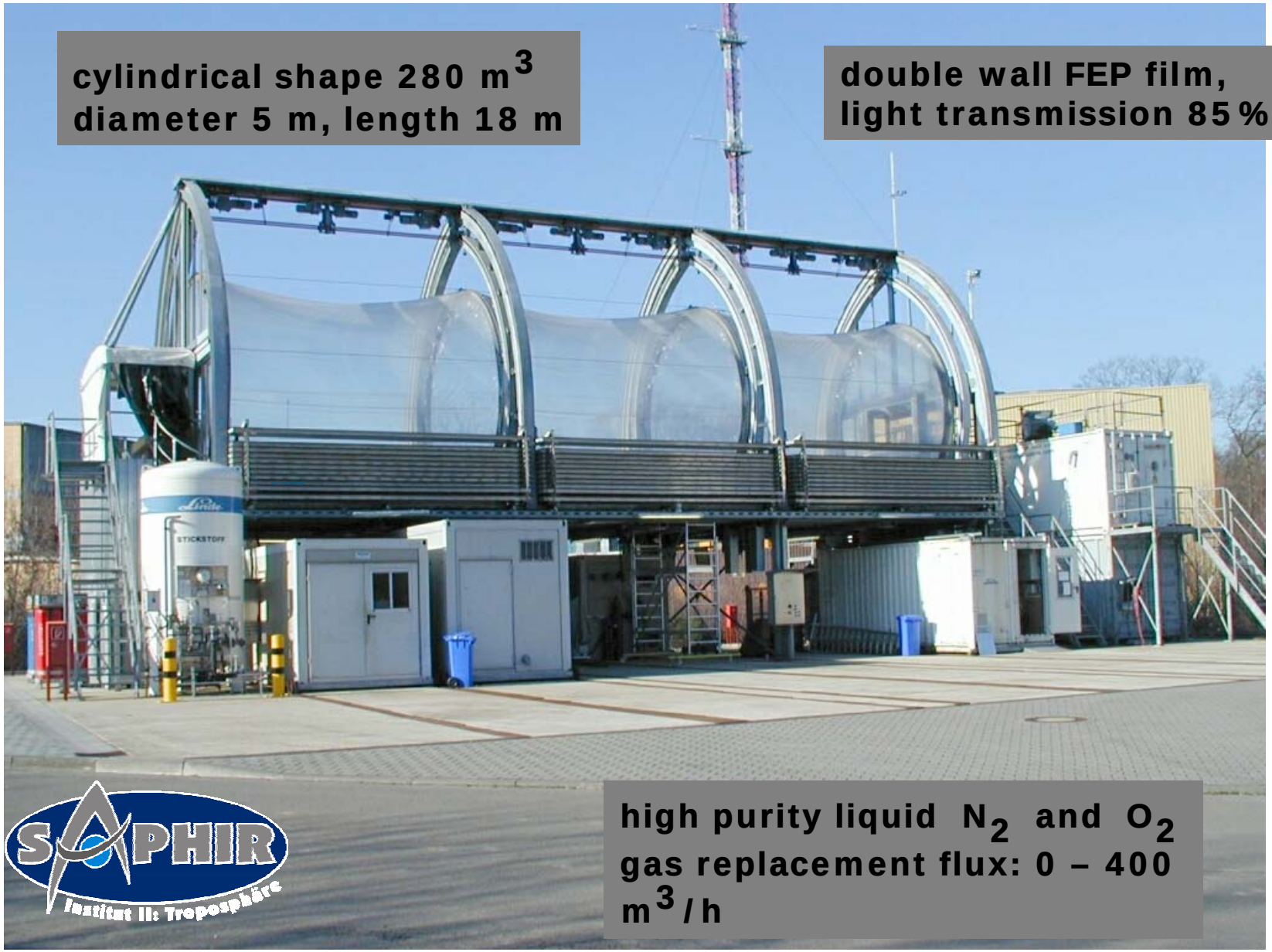
JÜLICH
FORSCHUNGSZENTRUM

ToF-AMS characterisation of SOA from NO3 oxidation of β - Pinene

AMS Users Meeting 2008 | Astrid Kiendler-Scharr

Secondary Organic Particles

- Current estimates of global biogenic SOA sources: 12 – 910 TgC/yr
- Comparisons field observation – model show large discrepancies
- C14 measurements in OA show large contribution of „modern“ C
- NO3 as anthropogenic oxidant
- SOA and organic nitrate yields from NO3 + monoterpene
- Measurements during the international NO3/N2O5 Intercomparison at SAPHIR summer 2007


cylindrical shape 280 m3
diameter 5 m, length 18 m
double wall FEP film,
light transmission 85 %
high purity liquid N2 and O2
gas replacement flux: 0 – 400
m3/h
SAPHIR
Institut II: Troposphäre

- Two experiments β-Pinene+NO3 under dry/wet conditions
- Measured Parameters:

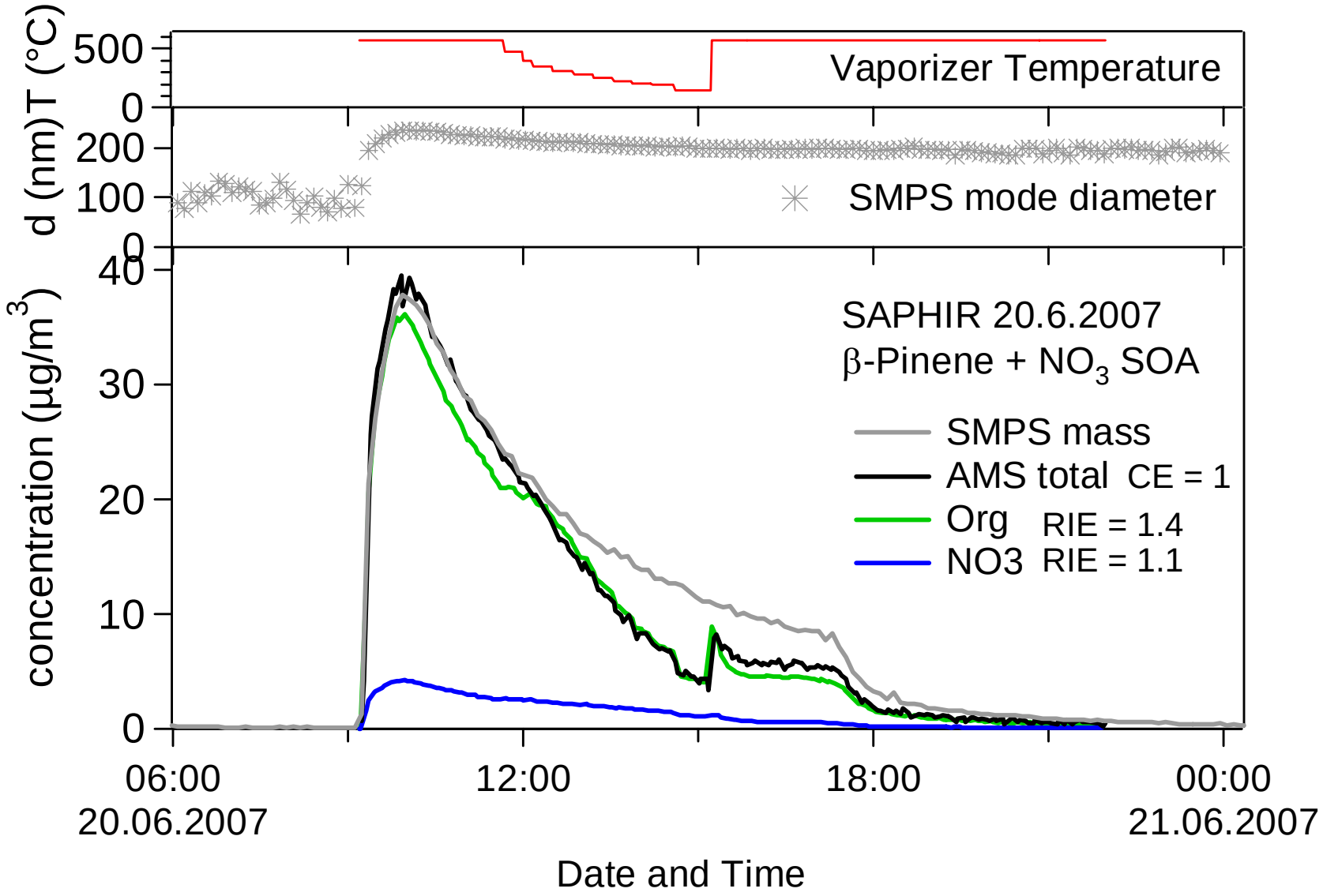
- RH, T, O3, NOx
- VOCs, NO3, N2O5
- organic nitrates (NO2-TD-LIF)
- SOA number density (CPC) and size distribution (SMPS)
- SOA composition (AMS)

Submitted to ACP:

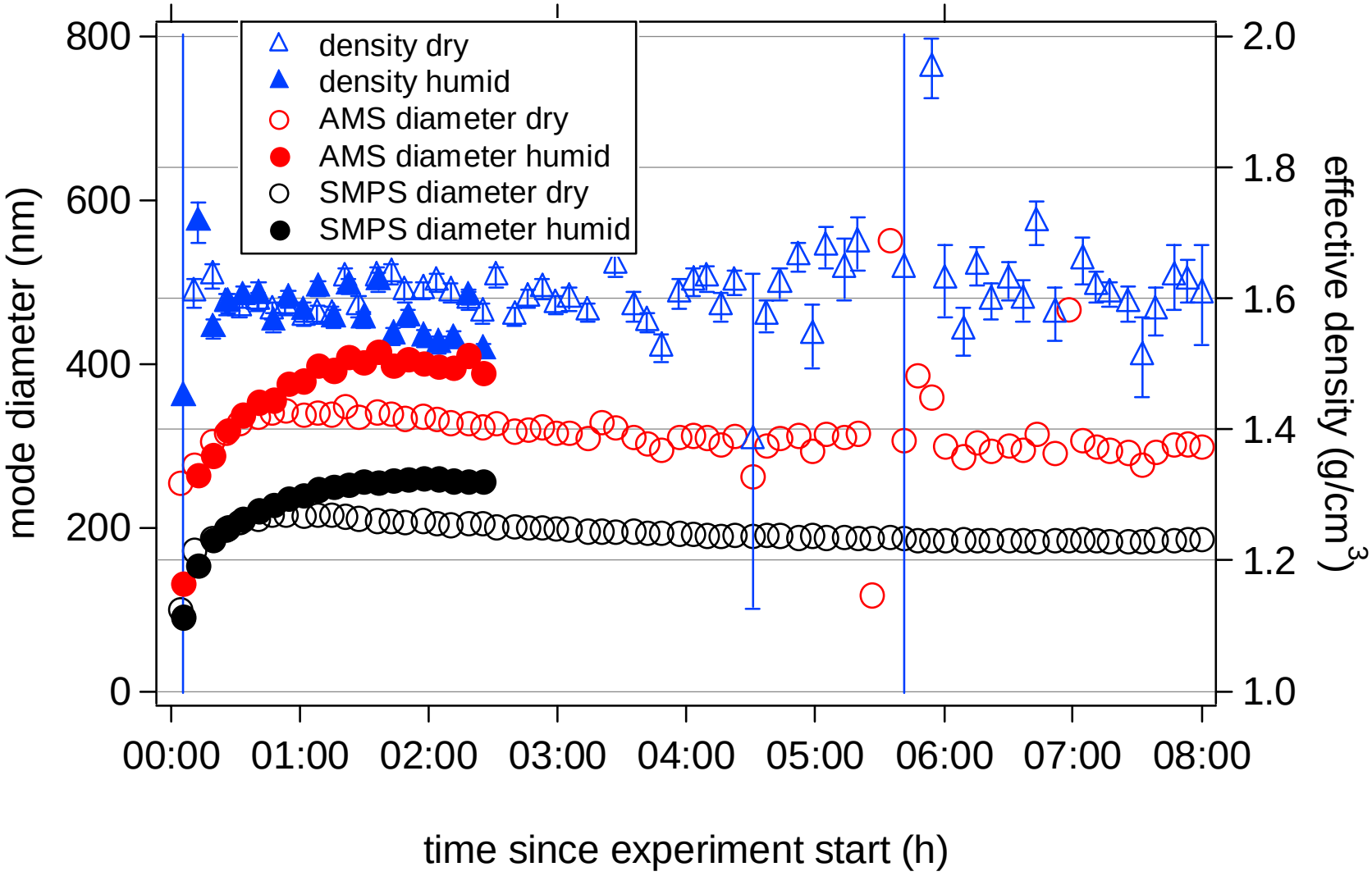
Organic nitrate and secondary organic aerosol yield from NO3 oxidation of β-pinene evaluated using a gas-phase kinetics/aerosol partitioning model

Juliane L. Fry, Astrid Kiendler-Scharr, et al. 2008

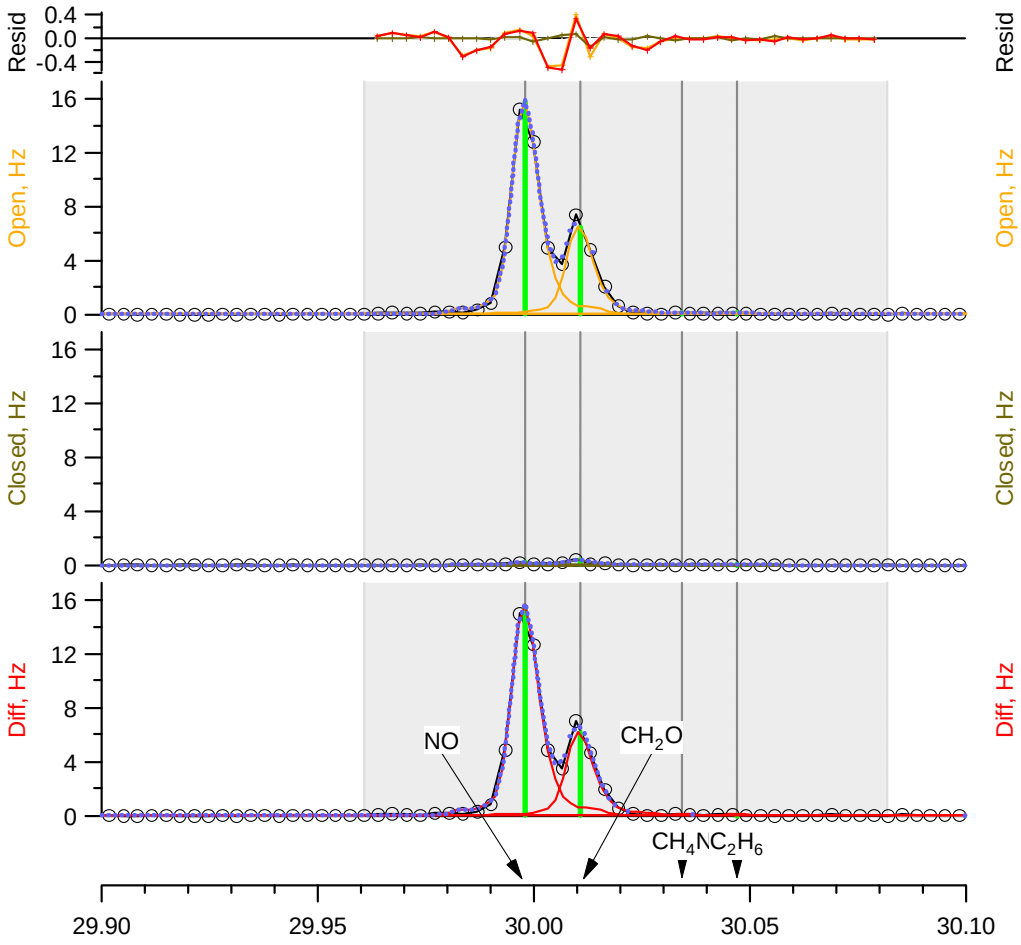
Comparison SMPS and AMS: β-Pinene + NO3, dry

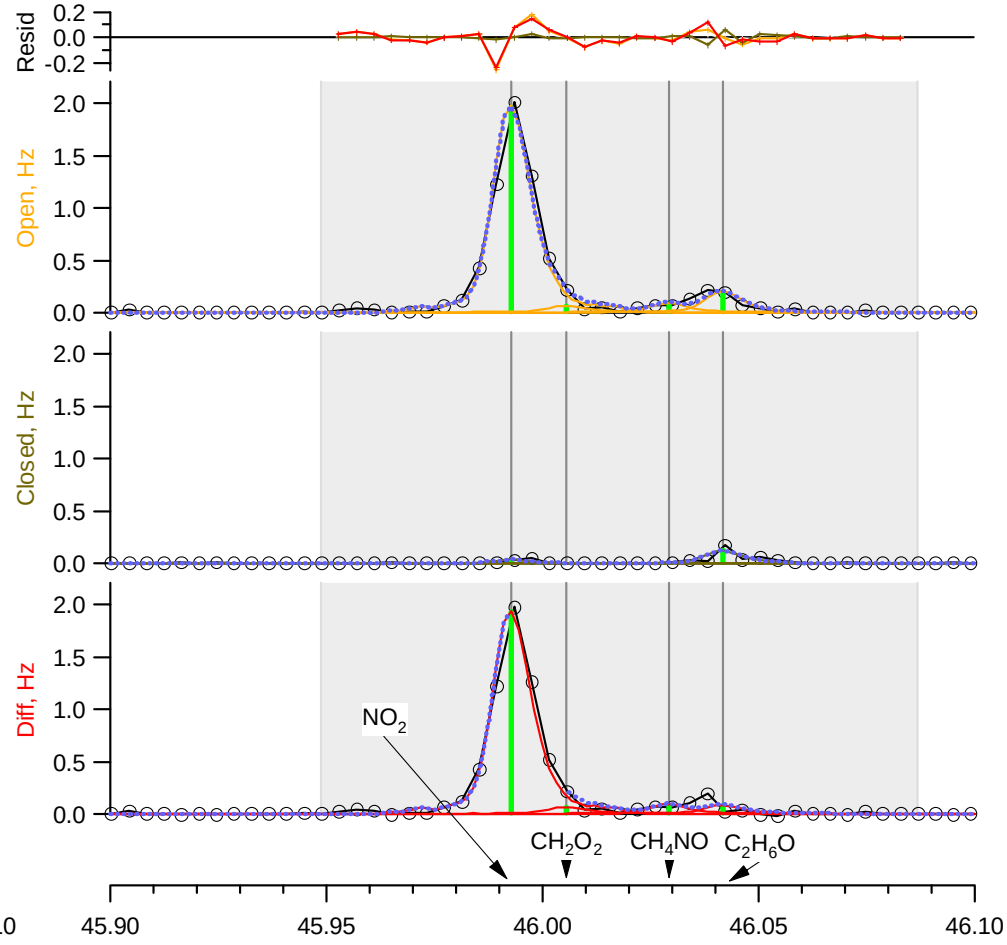


Comparison SMPS and AMS: β-Pinene + NO3, dry



Nitrate Diagnostics





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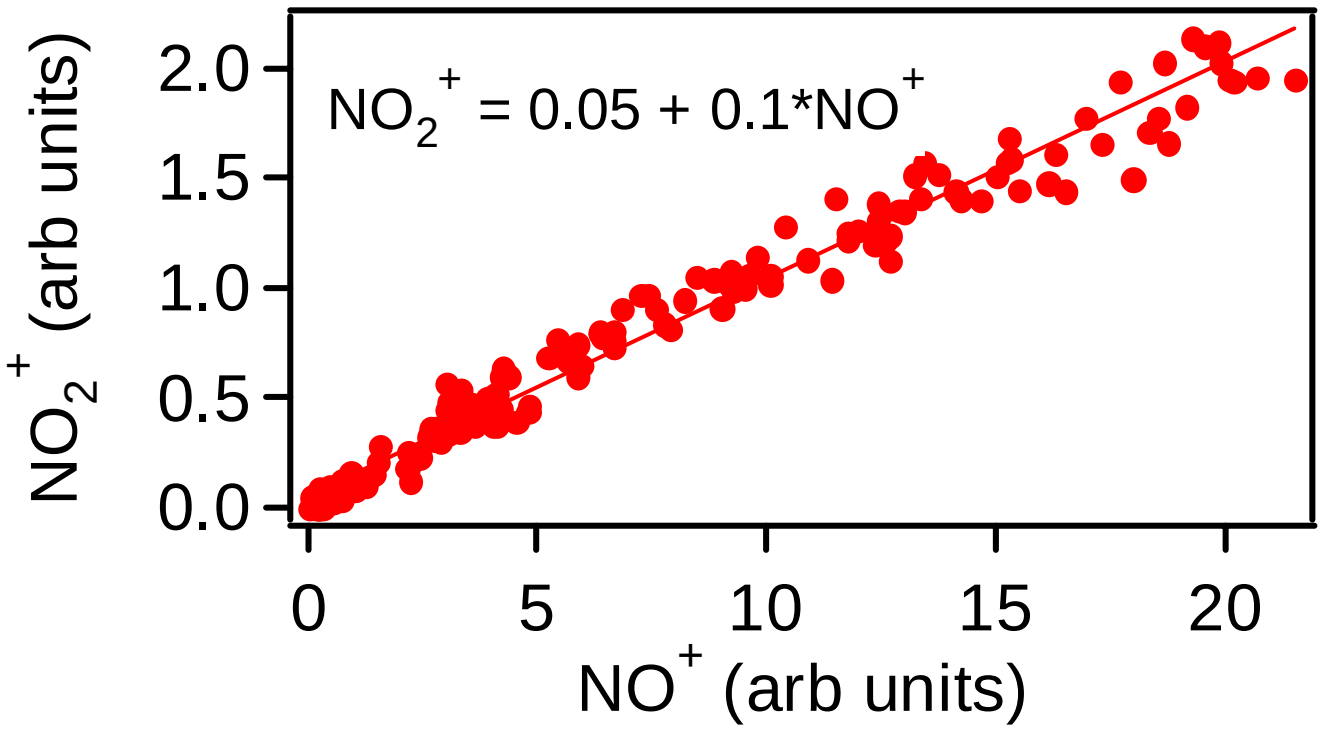

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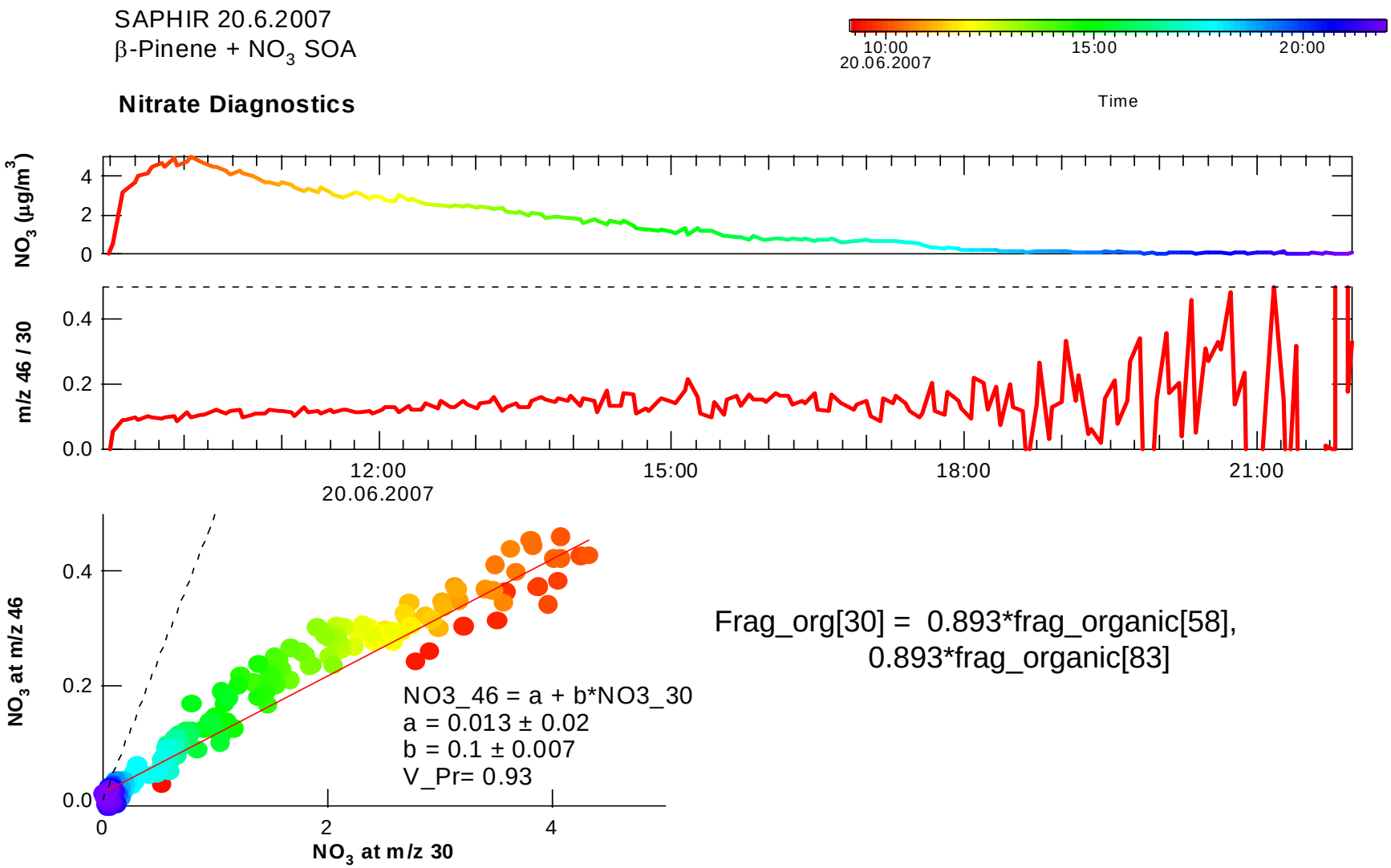
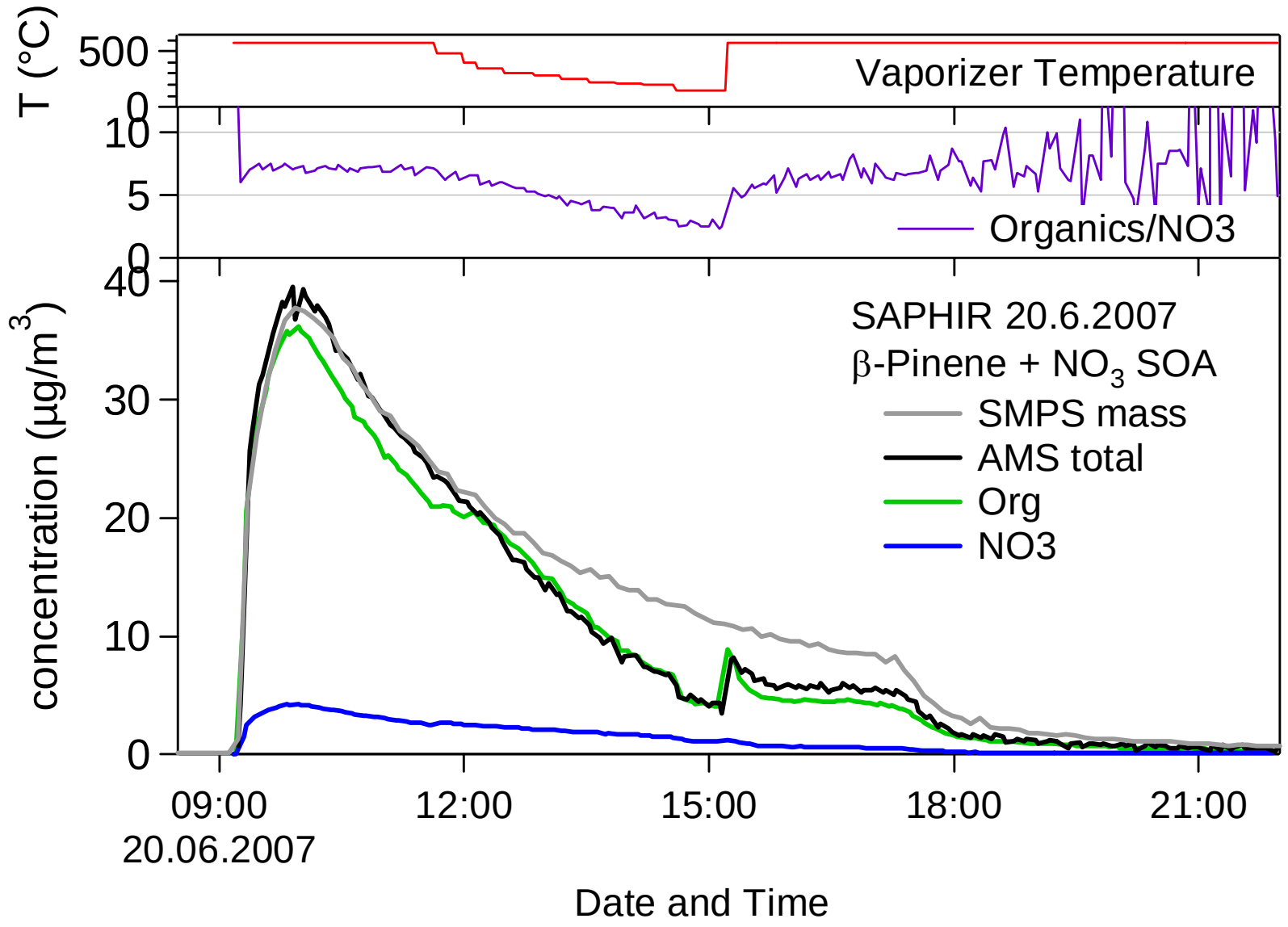


Frag_org[30] = 0.893*frag_organic[58], 0.893*frag_organic[83]

Organics Composition AMS



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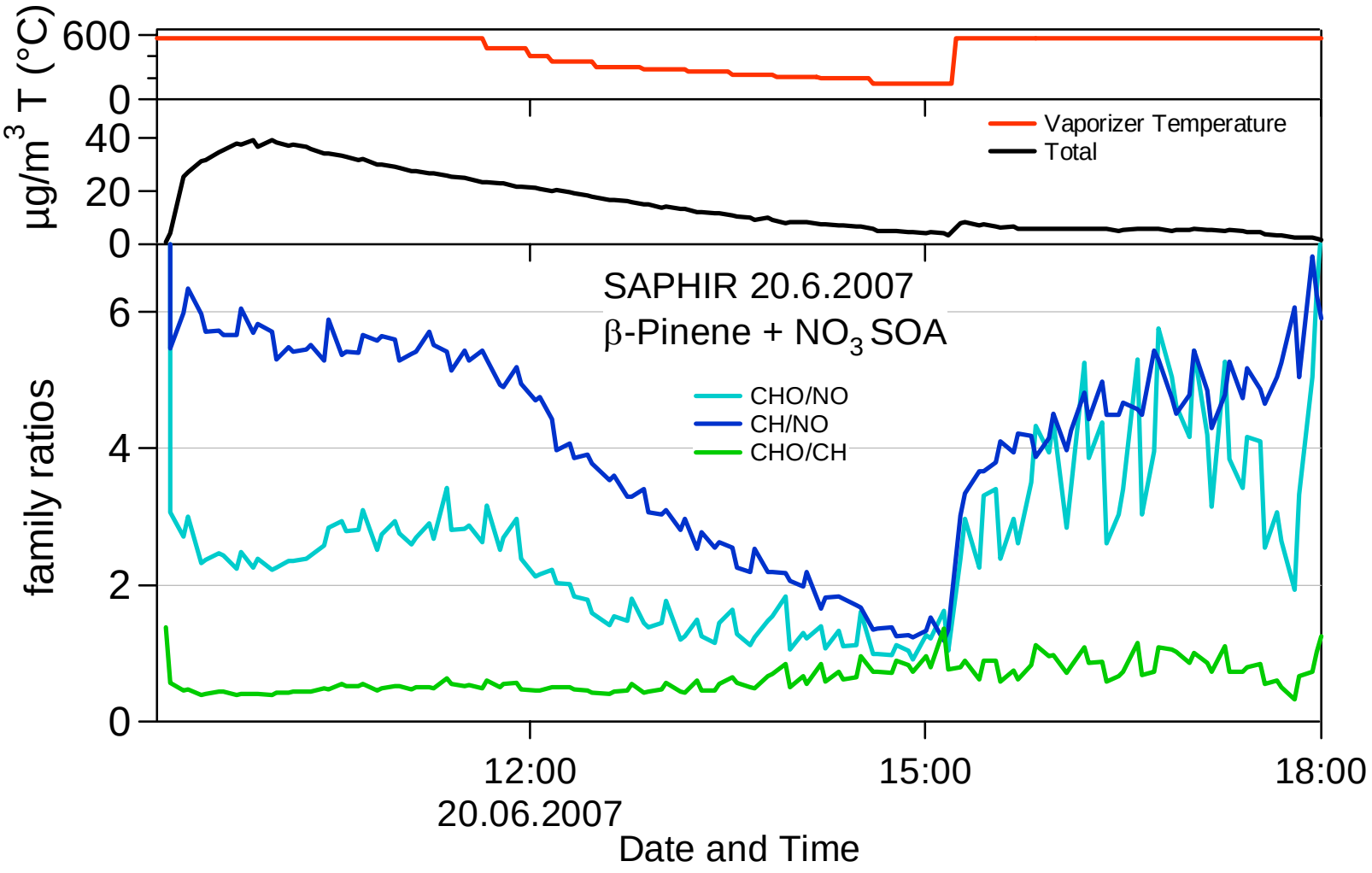


Organics Composition AMS

- Estimated molar mass of organic nitrates

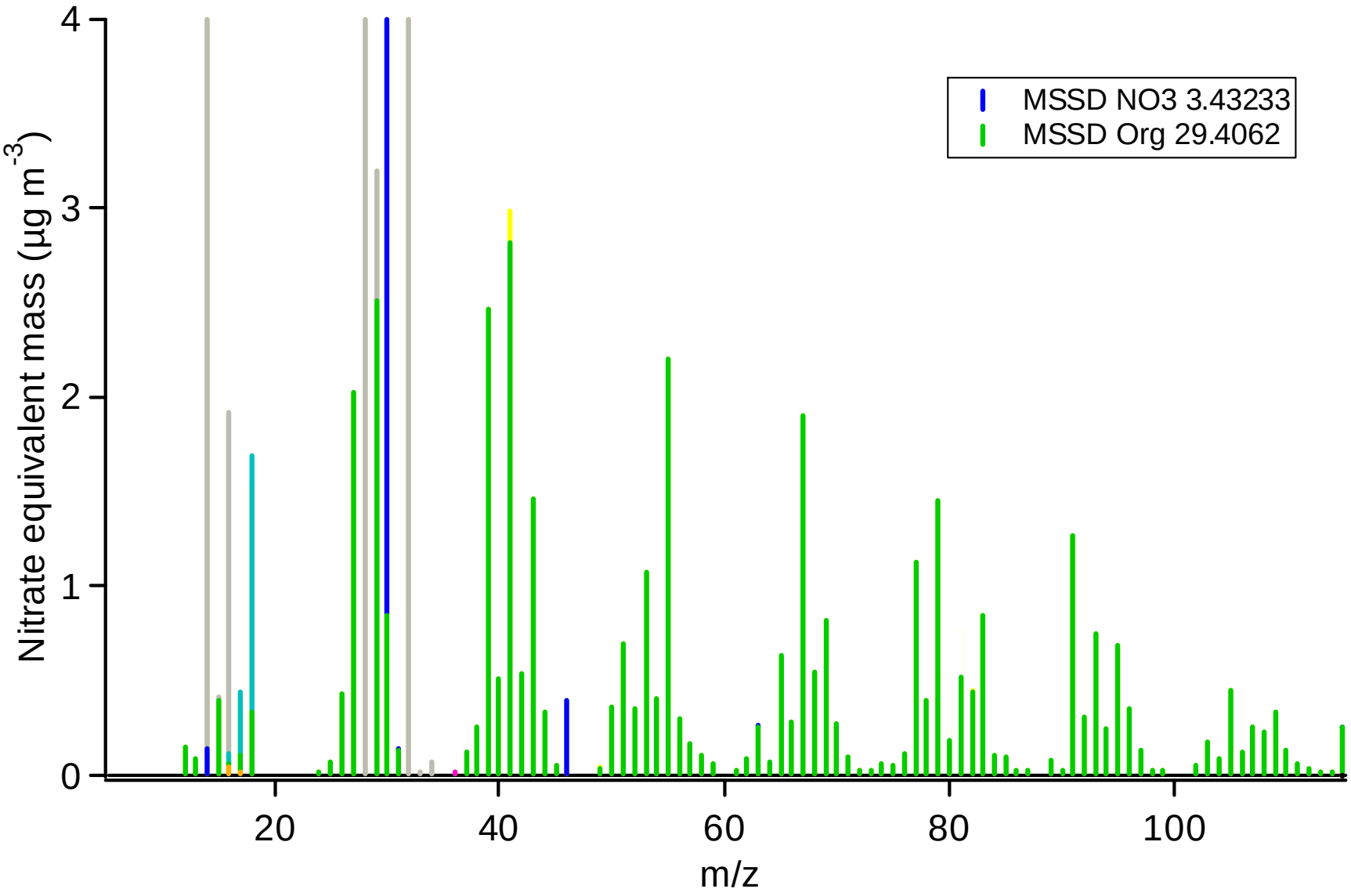
  Organic/Nitrate ratio R at T = 145°C
  assuming all signal at this temperature from organic nitrates
  → R = 2.7 +/- 0.2 results in MW = 229 +/- 12 g/mole

- Fraction of SOA consisting of organic nitrates

  Two approaches:
  Organic/Nitrate ratio R = 9 +/- 1 throughout the experiment
  With MW of organic nitrate = 215-231 g/mole this corresponds to 32-41% of total aerosol mass is organic nitrate

  At T = 145 °C the ratio of AMS mass (4.5 µg/m^3) to SMPS mass (11.6 µg/m^3) corresponds to 39% of total aerosol mass is organic nitrate.

Organics Composition AMS



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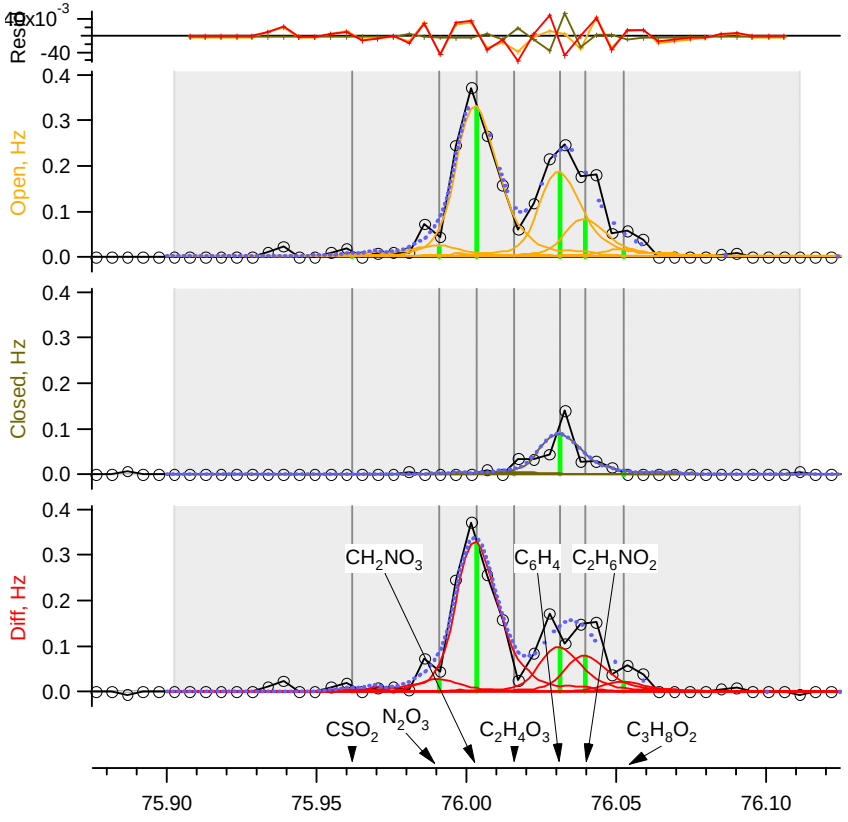

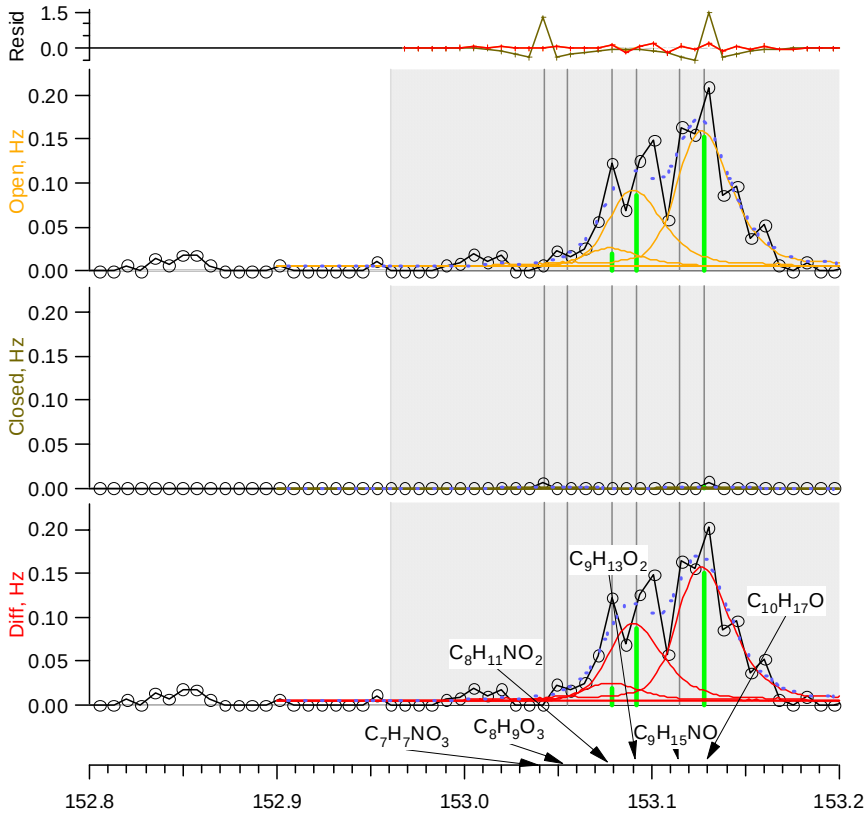

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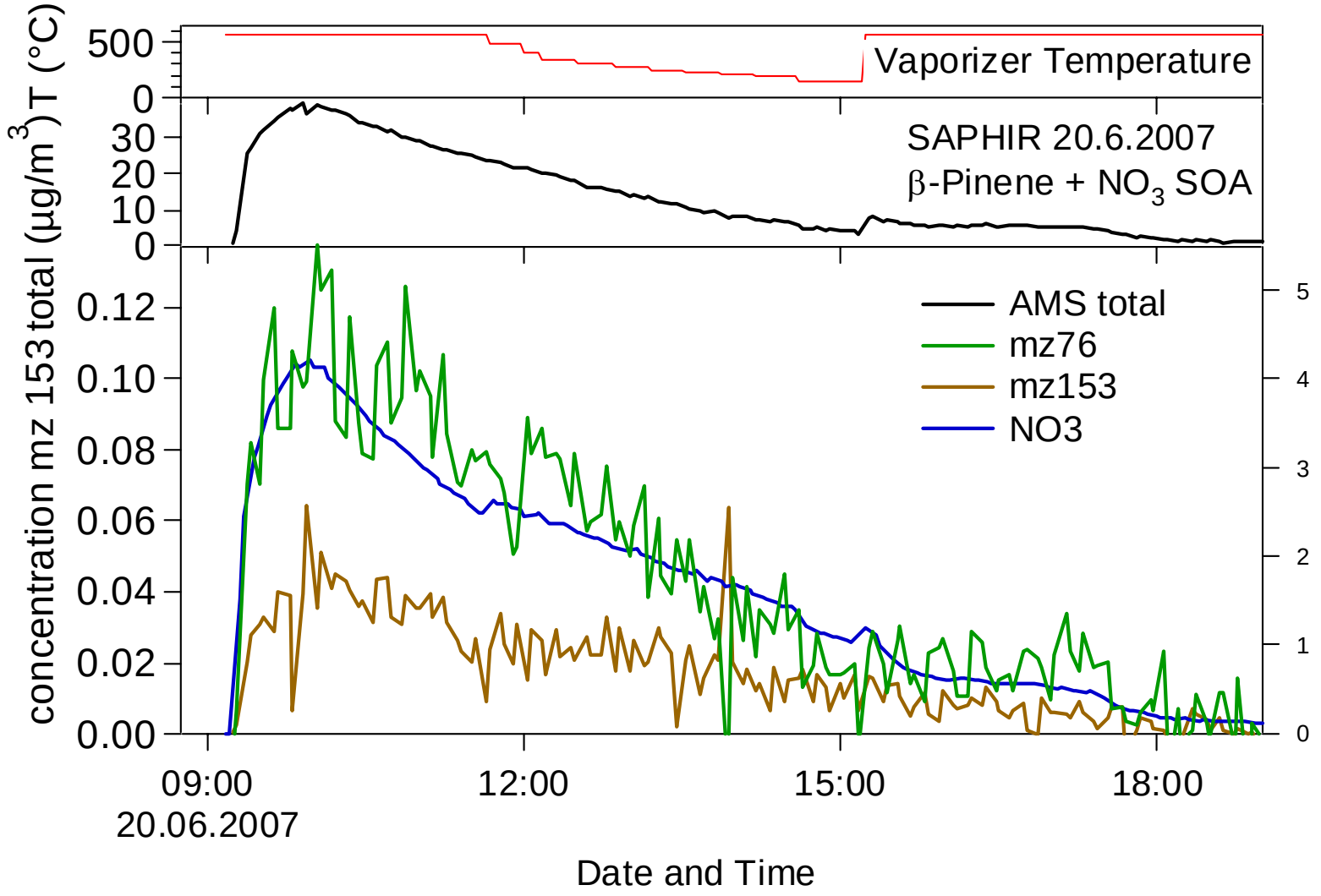

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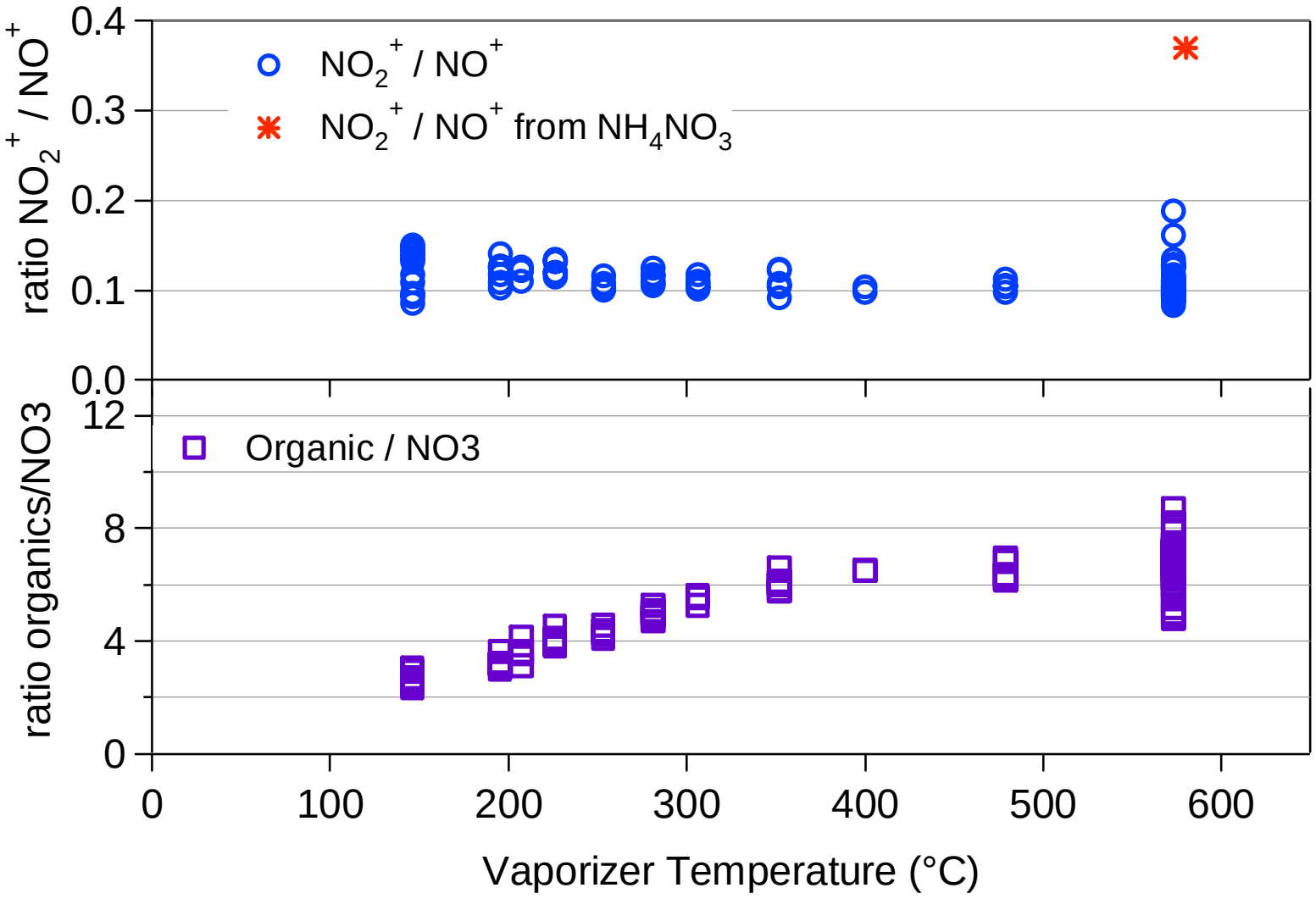
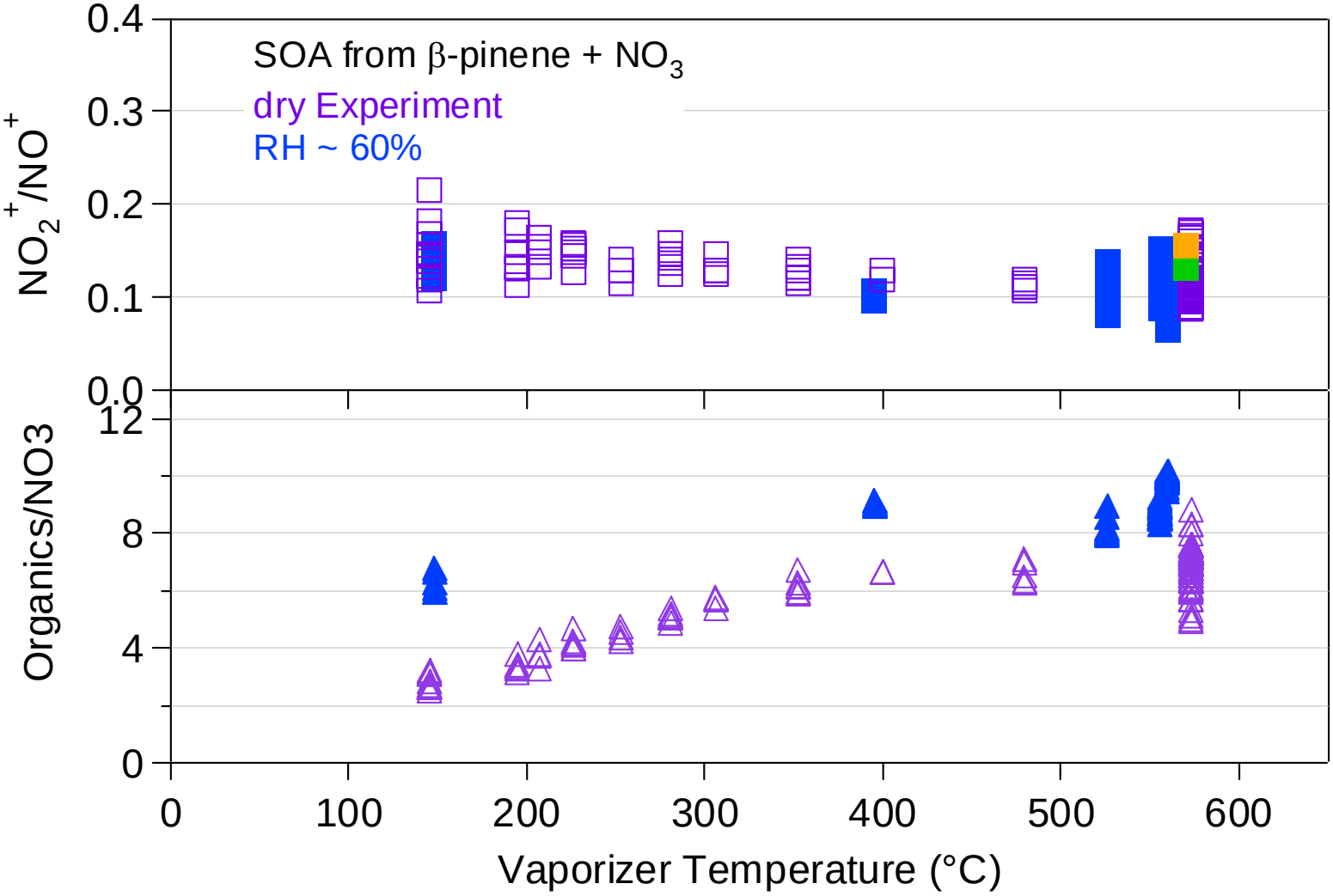


Comparison dry/humid experiment



Summary

SOA yield ~50% under both dry and humid conditions

SOA density 1.6 g/cm3

Organic to Nitrate ratio is ~ 9

Organic nitrates decompose in NO^+, NO_2^+ mostly

NO_2^+/NO^+ ratio ~ 0.1 for SOA studied < than from inorganic nitrate

Higher masses containing C, H, N, and O difficult to identify but
Peaks found at e.g. m/z 76, 153

Thank you!