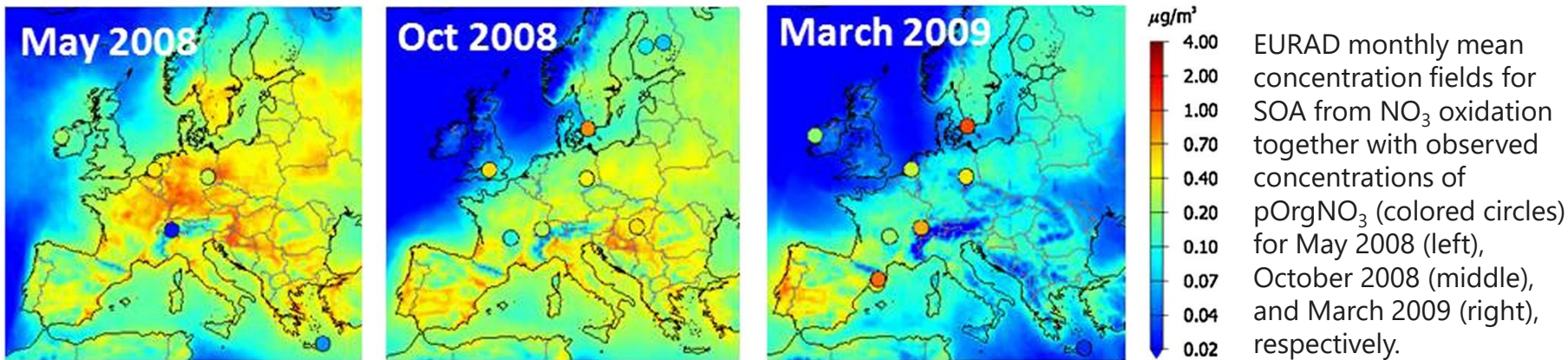


Molecular characterization and volatility of organonitrates: Latest observations from field and laboratory

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Organonitrates



34% to 44% of submicron aerosol nitrate measured by AMS
(Kiendler-Scharr et al., GRL, 2016)

EURAD: EUROpean Air pollution and Dispersion-Inverse Model (EURAD-IM) chemistry transport model (Elbern et al, 2007).

Organonitrates – why do we care?

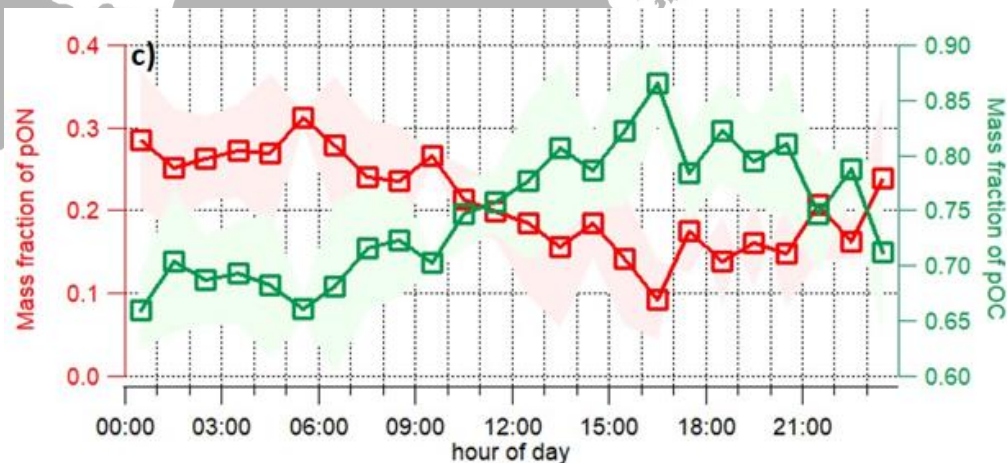
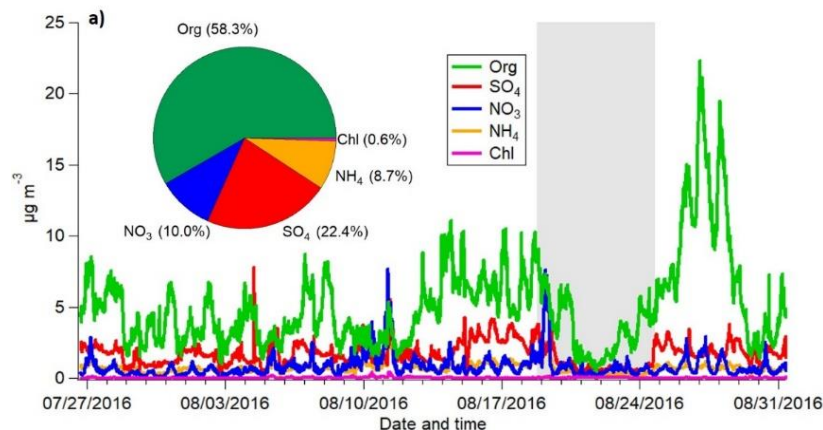
- Reservoir or sink (temporary or permanent) of NO_x
- Impact on tropospheric O_3 levels
- Influence on SOA yields
- Influence new particle formation rates
- Nighttime chemistry: Formation via NO_3 -oxidation of VOCs
- Daytime chemistry: Formation via peroxyradical reactions with NO_x

Quantification of these processes requires a better understanding of the fundamental properties of organonitrates in the gas and particle phases based on laboratory and field observations

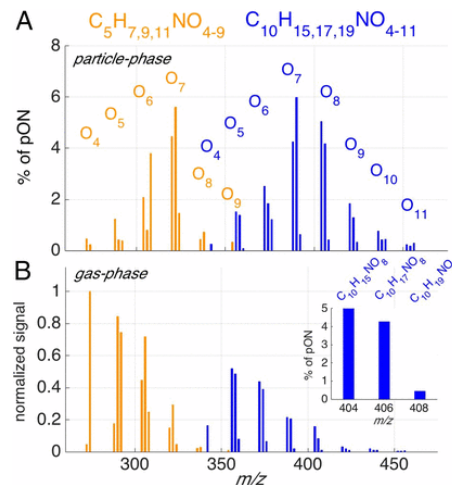
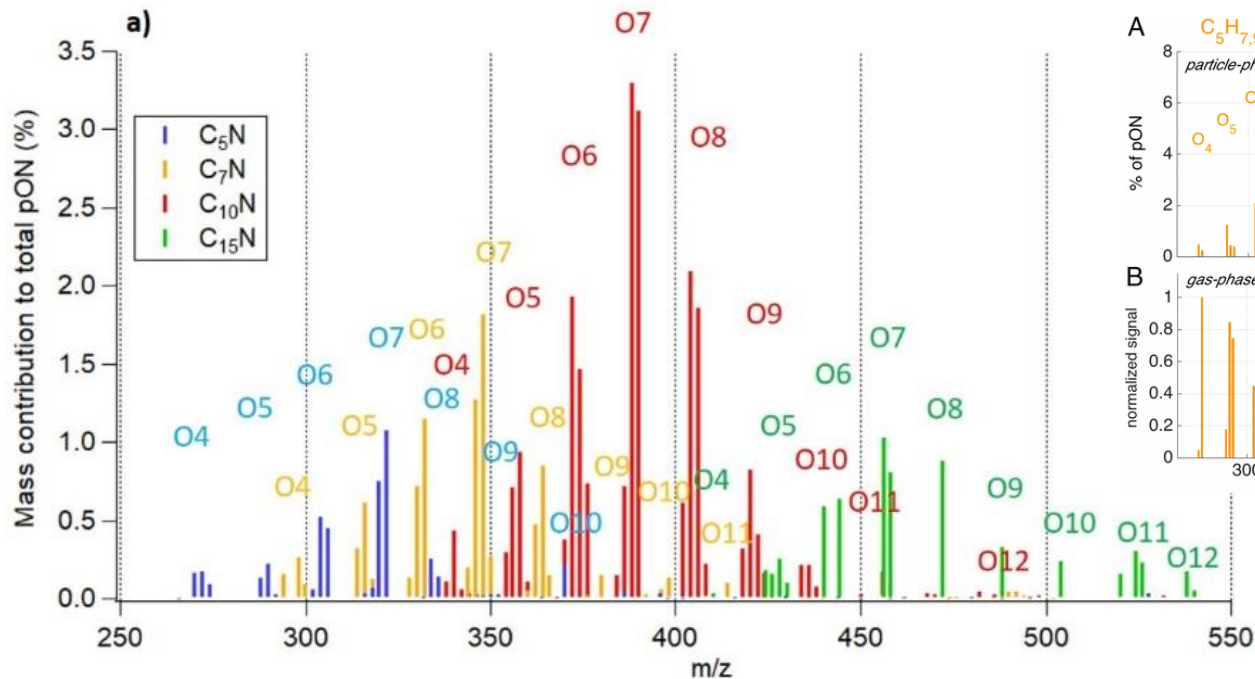
Karlsruhe, Germany: Higher fraction of organics and organonitrates during the night



Mass fractions of particulate organonitrates (pON) and particulate organic compounds (pOC) measured by FIGAERO-CIMS (Huang et al., EST, 2019)



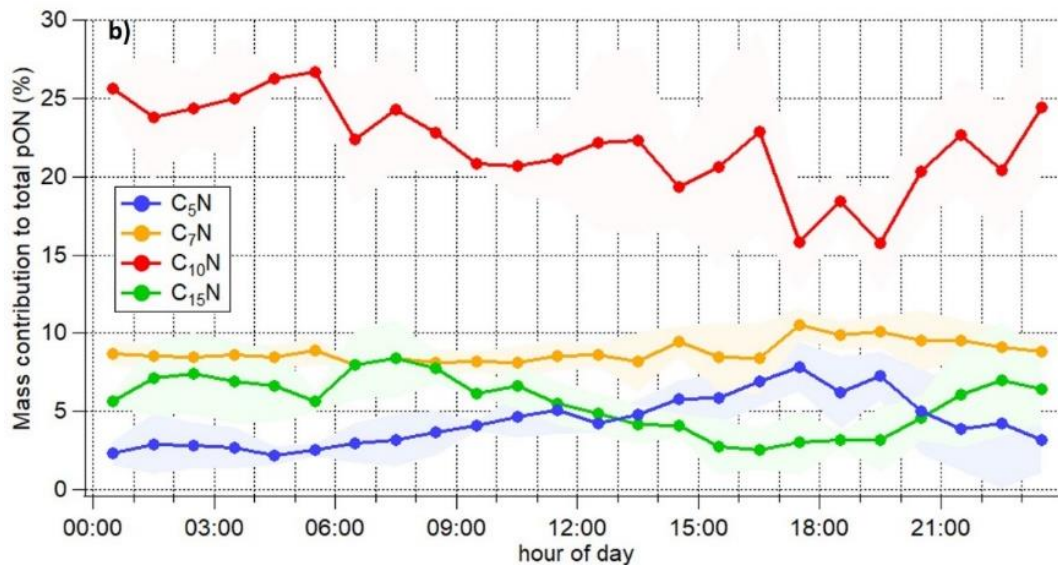
Organonitrates are highly functionalized



Similar observations in the SE US (Lee, Mohr, et al., PNAS, 2016)

Mass contribution to total pON of individual pON as a function of m/z ratio. Different colors indicate carbon numbers of the molecules, the labels the number of oxygen atoms per molecule (Huang et al., EST, 2019).⁵

Differences in diel patterns are indicative of different precursors and/or formation mechanisms



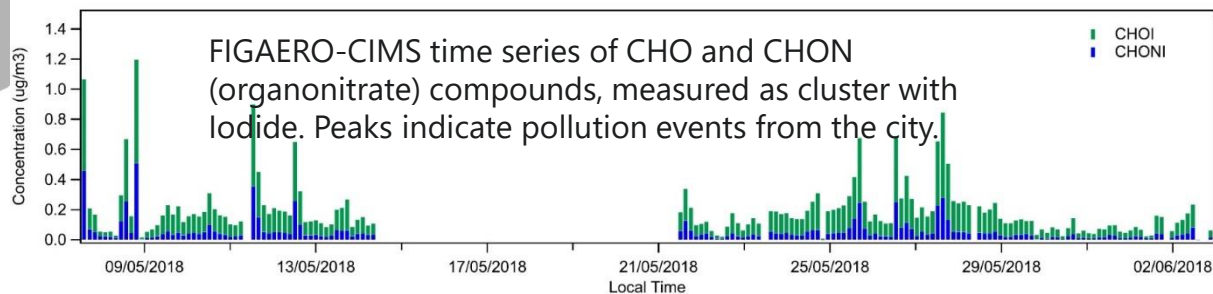
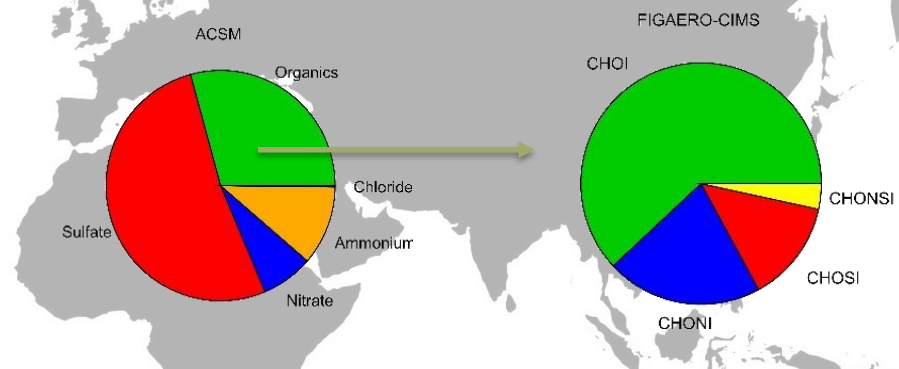
Mean diel patterns of the mass contribution of the C_xN (x = 5, 7, 10, 15) groups to total pON (Huang et al., EST, 2019). C₅ can be indicative of isoprene as a precursor, C₇ of anthropogenic VOCs, C₁₀ of monoterpenes, and C₁₅ of sesquiterpenes.

Chacaltaya, Bolivia: Observations of highly functionalized organic nitrates at 5240 m a.s.l.)



Research station

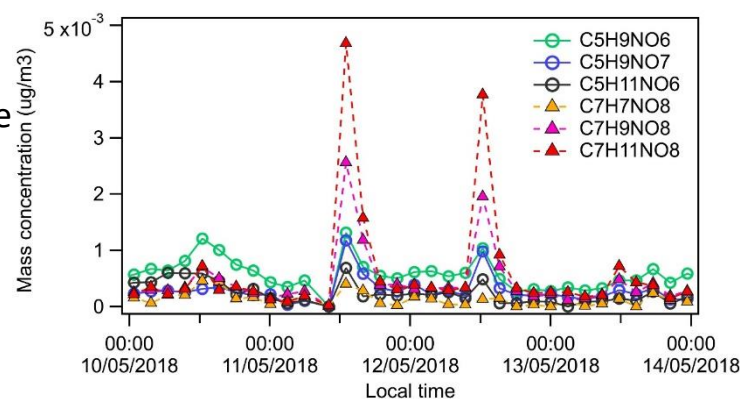
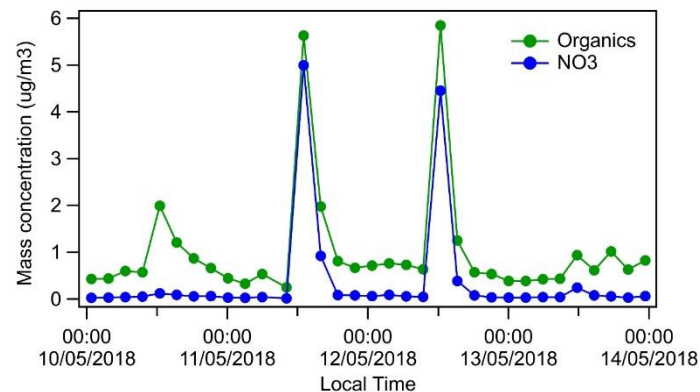
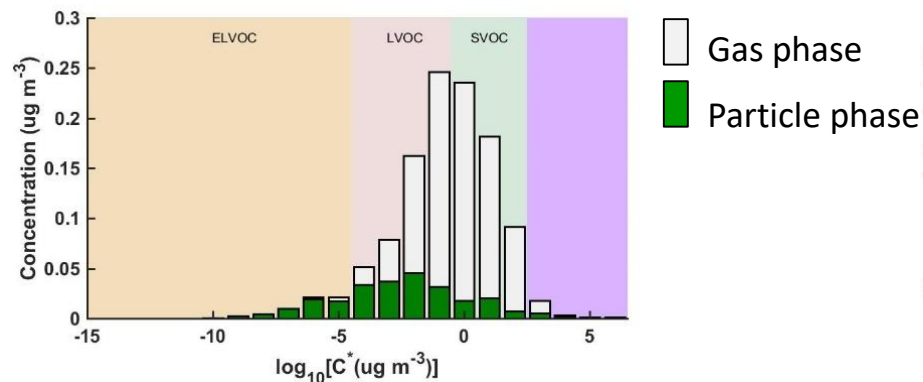
City of El Alto/La Paz



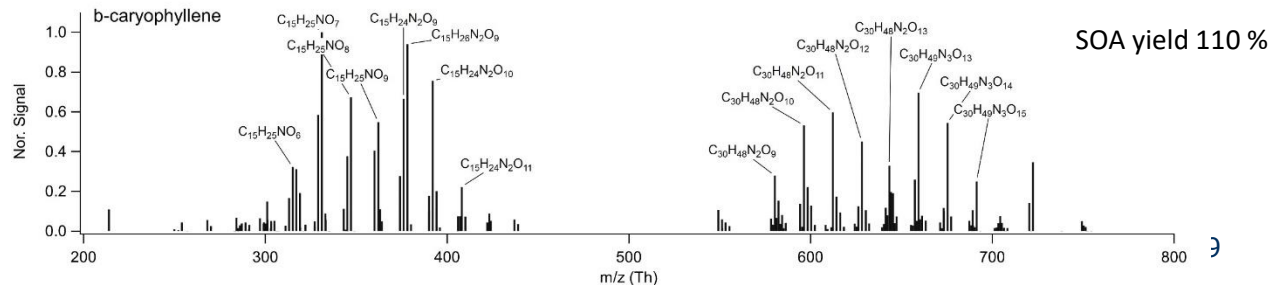
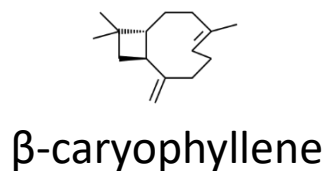
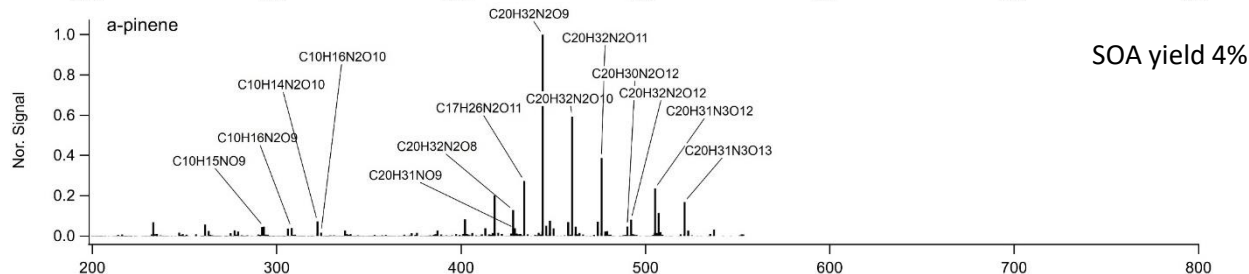
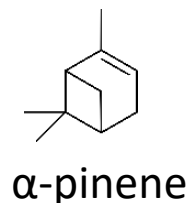
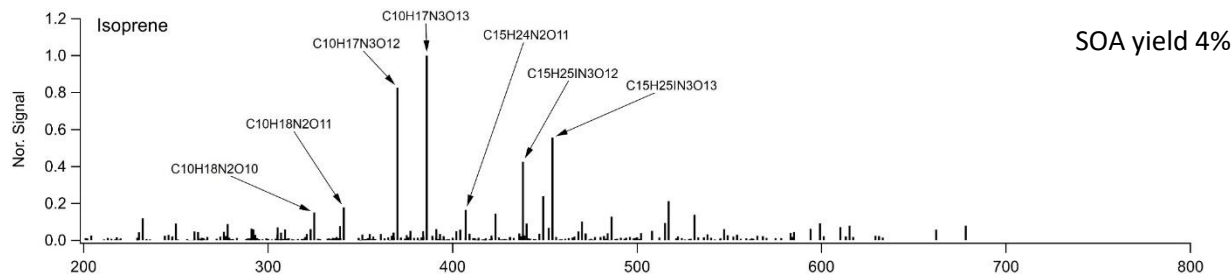
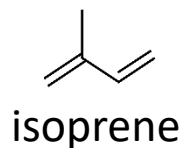
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Organonitrates related to city pollution: Chemical formulae and volatility

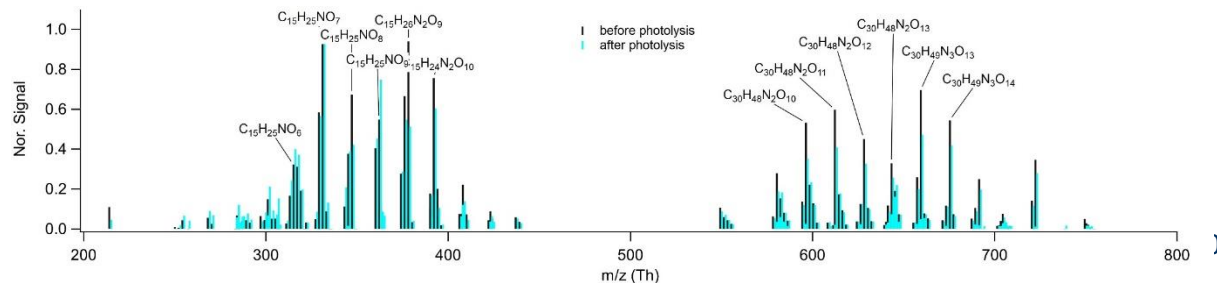
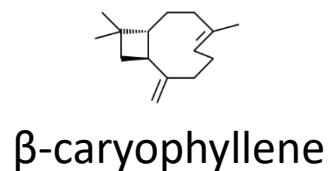
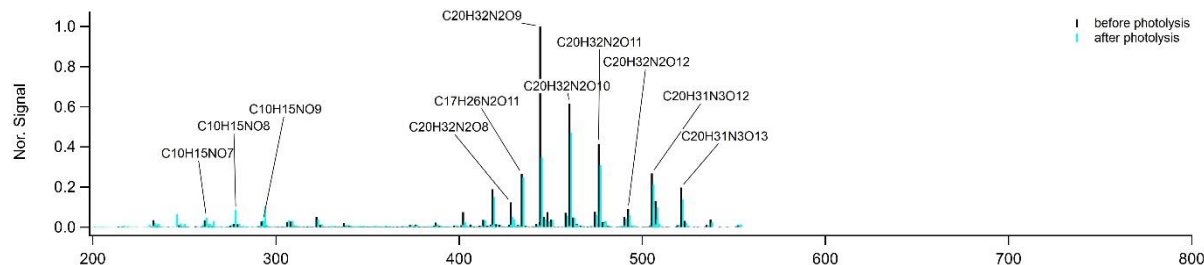
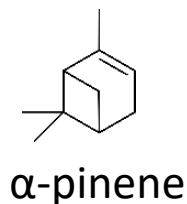
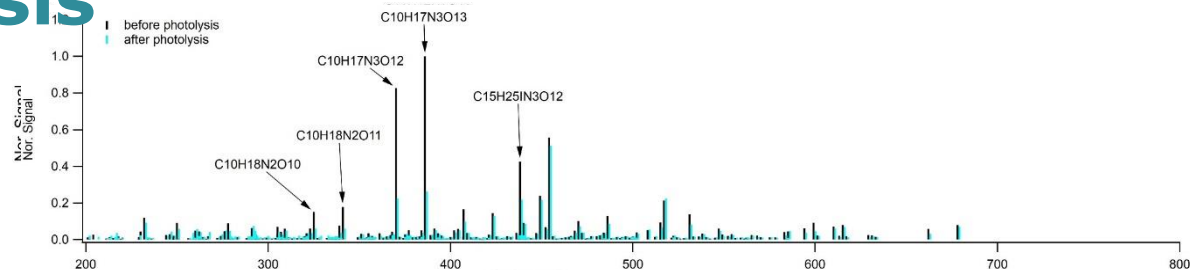
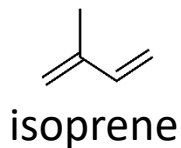
Volatility Basis Set
(based on Li et al. ACP 2016)



SOA formation via NO_3 -oxidation of biogenic VOCs in the laboratory



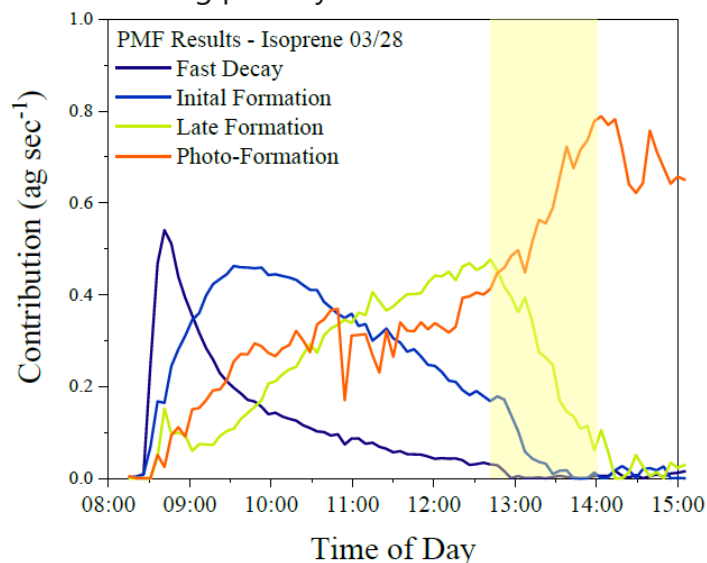
SOA formation via NO_3 -oxidation of biogenic VOCs in the laboratory - photolysis



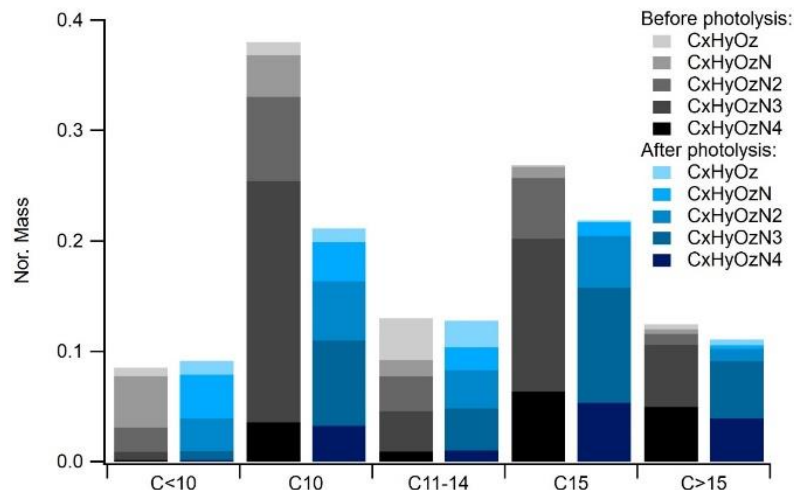
Department of Environmental Science

NO₃-isoprene SOA during dark aging and photolysis

PMF separates different compound groups measured by EESI-TOF during NO₃-SOA formation in the dark and their behavior during photolysis



Loss of oligomers with several nitrate groups during photolysis



3 main points:

- Organonitrates influence SOA properties and NO_x levels, knowledge of properties and fate contributes to understanding
- Recent ambient observations of organonitrates in different locations using state-of-the-art mass spectrometer techniques show they are highly functionalized and can have different organic precursors depending on environmental factors, and thus different volatilities
- Organonitrates formed during nighttime (NO_3 oxidation) may undergo photolysis during daytime, especially oligomers with several nitrate groups