

Supplemental Information for

BAERLIN2014 – stationary measurements and source apportionment at an urban background station in Berlin, Germany

Erika von Schneidemesser, Boris Bonn, Tim M. Butler, Christian Ehlers, Holger Gerwig, Hannele Hakola, Heidi Hellén, Andreas Kerschbaumer, Dieter Klemp, Claudia Kofahl, Jürgen Kura, Anja Lüdecke, Rainer Nothard, Axel Pietsch, Jörn Quedenau, Klaus Schäfer, James J. Schauer, Ashish Singh, Ana-Maria Villalobos, Matthias Wiegner, Mark G. Lawrence

NMVOC data:

As stated in the main text of the paper, to be able to make reasonable comparisons with previous work regarding the contribution of different compound classes to the measured mixing ratios of NMVOCs, as well as the OH reactivity attributed to these NMVOCs, a subset of the compounds was selected and used in the analysis. This subset was based on a number of different papers in the literature, and those compounds that were regularly included in OH reactivity calculations (e.g., (Dolgorouky et al., 2012; Gilman et al., 2009; Goldan et al., 2004; Liu et al., 2008)). This includes 57 NMVOCs, and while this does not capture the complete OH reactivity, it allows for more equal comparisons with other studies. The 57 NMVOCs included, are as follows:

Alkanes: cyclohexane, cyclopentane/2,3-dimethylbutane, ethane, heptane, methylcyclohexane, methylcyclopentane, n-decane, n-hexane, n-octane, n-pentane, propane, 2-methylbutane, 2-methylheptane, 2-methylhexane, 2-methylpentane, 2-methylpropane, 2,2-dimethylbutane, 2,3-dimethylpentane, 3-methylpentane

Alkenes and alkynes: cis-2-butene, cis-2-pentene, ethyne, i-butene, 1-butene, propene, trans-2-butene, trans-2-pentene, 1-pentene, 1,3-butadiene, 2-methyl-1-butene, 2-methyl-2-butene, 3-methyl-1-butene

Aromatics: benzene, ethylbenzene, i-propylbenzene, m-ethyltoluene, m-/p-xylene, n-propylbenzene, o-ethyltoluene, o-xylene, p-ethyltoluene, styrene, toluene, 1,2,3-trimethylbenzene, 1,2,4-trimethylbenzene/t-butylbenzene, 1,3,5-trimethylbenzene

Oxygenated: acetaldehyde, acetone, ethanol, MEK, methanol, 2-propanol

Biogenics and their oxidation products: α -pinene, β -pinene, isoprene, methacrolein, methylvinylketon

For information on individual mixing ratios by location, see Bonn et al. 2016.

Table S1. Details of the NMVOC measurements.

Instrument	Compounds or m/z measured	Detection limits	Sampling interval
PTR-MS	28, 29, 31, 33, 34, 35, 38, 39, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 53, 55, 56, 57, 59, 60, 61, 63, 65, 67, 69, 71, 73, 75, 77, 79, 81, 83, 85, 86, 87, 89, 91, 93, 95, 97, 99, 101, 103, 105, 107, 109, 113, 115, 117, 119, 121, 127, 129, 132, 135, 137, 143, 147, 149, 151, 155, 157, 181, 205	varies (10s of pptv), see Bourtsoukidis et al., 2012	4.5 minutes
AMA Instruments GC5000 BTX	benzene, toluene	30 pptv	30 min data
Canister samples	Ethene, Ethyne, Ethane, Propene, Propane, Propyne, Acetaldehyde, 2-Methylpropane, Methanol, 1-Butene/i-butene, 1,3-Butadiene, n-Butane, trans-2-Butene, cis-2-Butene, 1,2-Butadiene, Ethanol, 3-Methyl-1-butene, 2-Methylbutane, Acetone, 1-Pentene, 2-Propanol, 2-Methyl-1-butene, n-Pentane, Isoprene, trans-2-Pentene, cis-2-Pentene, Propanal, 2-Methyl-2-butene, Acetic acid methyl ester, 1,3-Pentadiene, Cyclopentadiene, 2,2-Dimethylbutane, 2-Butanol, 1-Propanol, Cyclopentene, Methacrolein, Cyclopentane/2,3-dimethylbutane, 2-Methylpentane, Methyl vinyl ketone, Butanal, 1-Hexene, 3-Methylpentane, 2-Methyl-1-pentene, n-Hexane, trans-2-Hexene, cis-2-Hexene, 1,3-Hexadiene, Methylcyclopentane, 2,4-Dimethylpentane, Methylcyclopentene, Benzene, 1-Butanol, Cyclohexane, 2-Methylhexane, 2,3-Dimethylpentane, 3-Methylhexane, Pentanal, Cyclohexene, 1,3-Dimethylcyclopentane, 1-Heptene, 2,2,4-Trimethylpentane, Heptane, 2,3-Dimethyl-2-pentene, Octene, Methylcyclohexane, 2,3,4-Trimethylpentane, Toluene, 2-Methylheptane, 4-Methylheptane, 3-Methylheptane, Hexanal, Acetic acid butyl ester, n-Octane, Dimethylcyclohexane isomer, Ethylbenzene, m/p-Xylene, Heptanal, Styrene, 1-Nonene, o-Xylene, n-Nonane, i-Propylbenzene, α -Pinene, n-Propylbenzene, m-Ethyltoluene, p-Ethyltoluene, 1,3,5-Trimethylbenzene, Sabinene, o-Ethyltoluene, Octanal, β -Pinene, 1,2,4-Trimethylbenzene/t-butylbenzene, n-Decane, 1,2,3-Trimethylbenzene, Limonene, Eucalyptol, Indane, 1,3-Diethylbenzene, 1,4-Diethylbenzene, Butylbenzene, n-Undecane, n-Dodecane, n-Tridecane	5-20 ppt (see Urban 2010, Table 3.3 for individual LOD)	Intermittent (non-continuous) samples
Cartridge samples	Isoprene, 2-methyl-3-butanol, α -pinene, camphene, β -pinene, 3 Δ -carene, p-cymene, 1,8-cineol, limonene, terpinolene, 4-acetyl-1-methylcyclohexene, nopinone, bornylacetate, longicycline, iso-longifolene, β -caryophyllene, aromadendrene, α -humulene, Benzene, Toluene, Ethylbenzene, p/m-xylene, styrene, o-xylene, propylbenzene, 3-ethyltoluene, 4-ethyltoluene, 1,3,5-trimethylbenzene, 2-ethyltoluene, 1,2,4-trimethylbenzene, 1,2,3-trimethylbenzene, hexane, heptane, octane, nonane, decane	3-60 ng/m ³ (see main text and Mäki et al. (2017) for more details)	Intermittent (non-continuous) samples

Table S2. Pearson correlation coefficients (r) with 95% confidence intervals for hourly data.

	RH (%)	O ₃ ($\mu\text{g m}^{-3}$)	NO ($\mu\text{g m}^{-3}$)	NO ₂ ($\mu\text{g m}^{-3}$)	CO (mg m^{-3})	Benzene ($\mu\text{g m}^{-3}$)	Toluene ($\mu\text{g m}^{-3}$)	PM ₁₀ ($\mu\text{g m}^{-3}$)	MLH (m)	PKW at MC220 (count)	PKW at MC143 (count)
Temp (°C)	-0.71 [-0.72, -0.70]	0.82 [0.81, 0.83]	-0.28 [-0.31, -0.26]	-0.38 [-0.40, -0.35]	-0.26 [-0.28, -0.23]	-0.14 [-0.17, -0.11]	-0.15 [-0.18, -0.13]	0.36 [0.34, 0.38]	0.50 [0.47, 0.53]	0.60 [0.58, 0.63]	0.55 [0.52, 0.57]
RH (%)	1 [-0.77, -0.74]	-0.76 [0.15, 0.20]	0.17 [0.14, 0.20]	0.17 [0.10, 0.15]	0.13 [0.06, 0.11]	0.08 [0.13, 0.18]	0.15 [-0.21, -0.15]	-0.18 [-0.69, -0.64]	-0.66 [-0.75, -0.72]	-0.74 [-0.72, -0.68]	-0.70 [-0.72, -0.68]
O ₃ ($\mu\text{g m}^{-3}$)	1 [-0.41, -0.36]	-0.39 [-0.58, -0.55]	-0.57 [-0.45, -0.41]	-0.43 [-0.35, -0.30]	-0.33 [-0.36, -0.31]	-0.34 [0.22, 0.27]	0.24 [0.57, 0.62]	0.59 [0.52, 0.58]	0.55 [0.47, 0.53]	0.50 [0.47, 0.53]	
NO ($\mu\text{g m}^{-3}$)		1 [0.56, 0.59]	0.58 [0.70, 0.73]	0.72 [0.51, 0.55]	0.53 [0.47, 0.51]	0.49 [0.06, 0.11]	0.09 [0.22, 0.27]	-0.20 [0.57, 0.62]	-0.06 [0.52, 0.58]	0.00 [0.47, 0.53]	
NO ₂ ($\mu\text{g m}^{-3}$)			1 [0.81, 0.83]	0.82 [0.62, 0.65]	0.63 [0.49, 0.53]	0.51 [0.08, 0.14]	0.11 [0.22, 0.27]	-0.29 [0.57, 0.62]	-0.06 [0.52, 0.58]	-0.05 [0.47, 0.53]	
CO (mg m^{-3})				1 [0.70, 0.72]	0.71 [0.57, 0.60]	0.59 [0.14, 0.19]	0.16 [0.22, 0.27]	-0.22 [0.57, 0.62]	0.01 [0.52, 0.58]	0.02 [0.47, 0.53]	
Benzene ($\mu\text{g m}^{-3}$)					1 [0.78, 0.80]	0.79 [0.21, 0.26]	0.23 [0.22, 0.27]	-0.15 [0.57, 0.62]	0.02 [0.52, 0.58]	0.02 [0.47, 0.53]	
Toluene ($\mu\text{g m}^{-3}$)						1 [0.14, 0.20]	0.17 [0.22, 0.27]	-0.15 [0.57, 0.62]	-0.06 [0.52, 0.58]	-0.07 [0.47, 0.53]	
PM ₁₀ ($\mu\text{g m}^{-3}$)							1 [-0.00, 0.08]	0.04 [0.15, 0.23]	0.19 [0.15, 0.23]	0.12 [0.08, 0.16]	
MLH (m)								1 [0.48, 0.57]	0.53 [0.48, 0.57]	0.48 [0.43, 0.52]	
PKW at MC220 (count)									1 [0.93, 0.94]	0.94 [0.93, 0.94]	

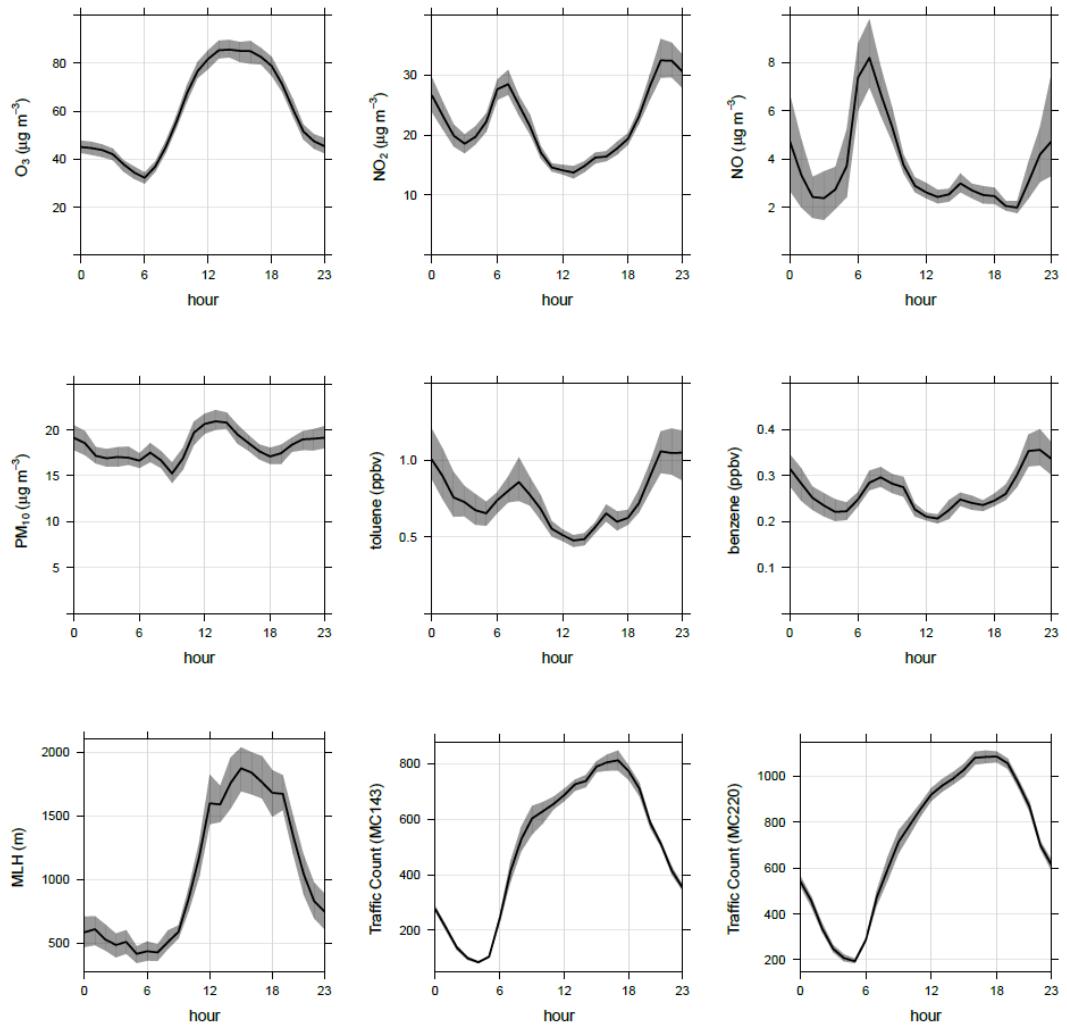


Figure S1. Diurnal variation in air pollutants and MLH measured in Neukölln, and traffic counts from the MC143 and MC220 locations.

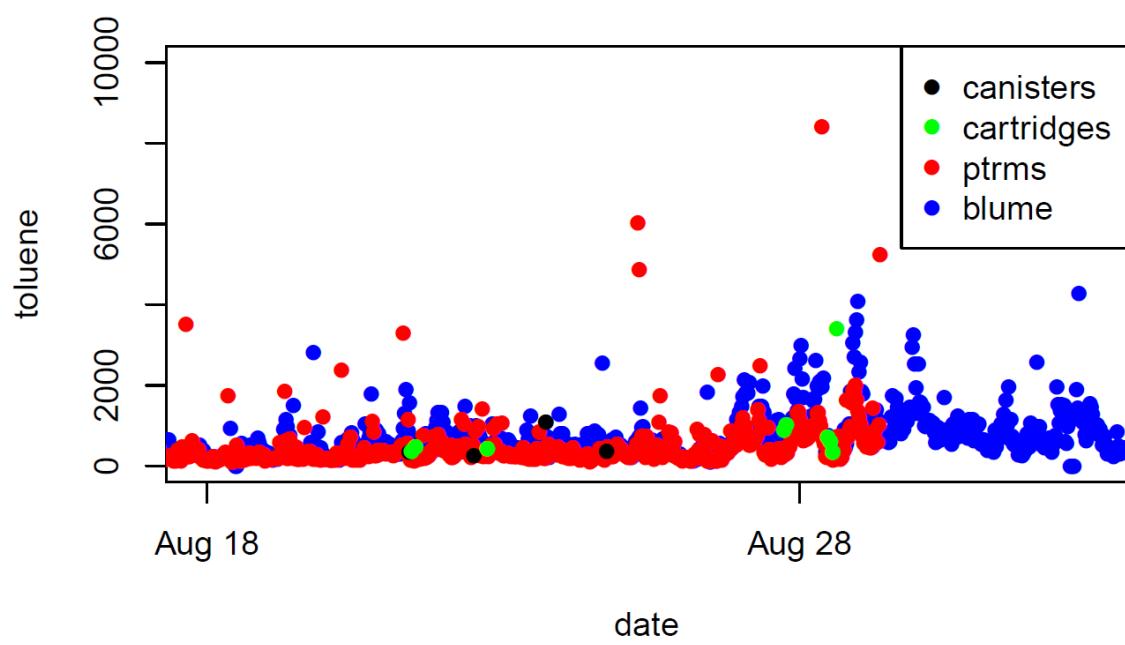
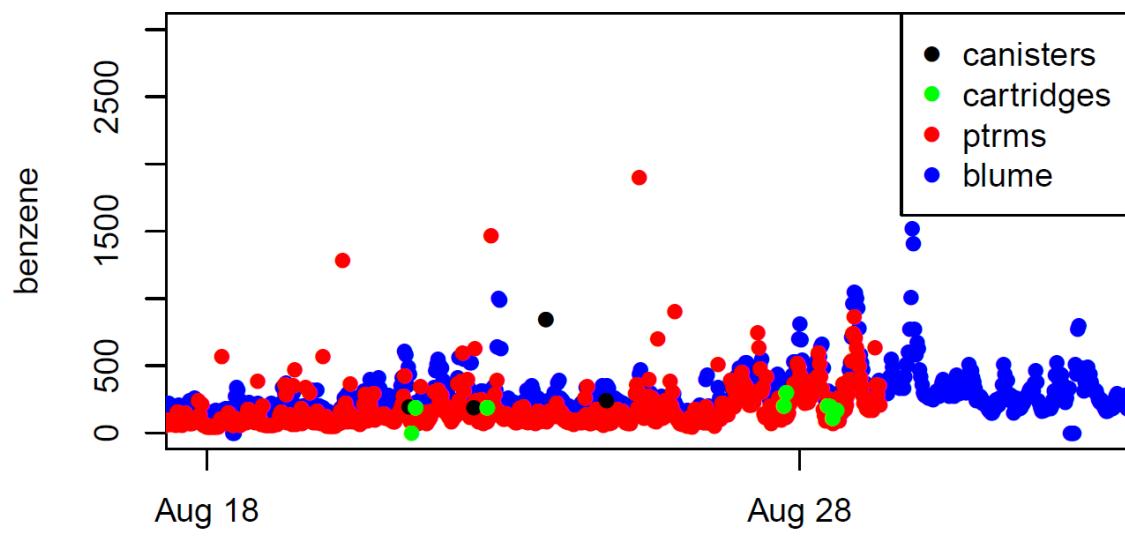


Figure S2. Mixing ratios measured for benzene (top) and toluene (bottom) by the individual cartridge and canister samples, and the continuous PTR-MS and BLUME network. Units are pptv.

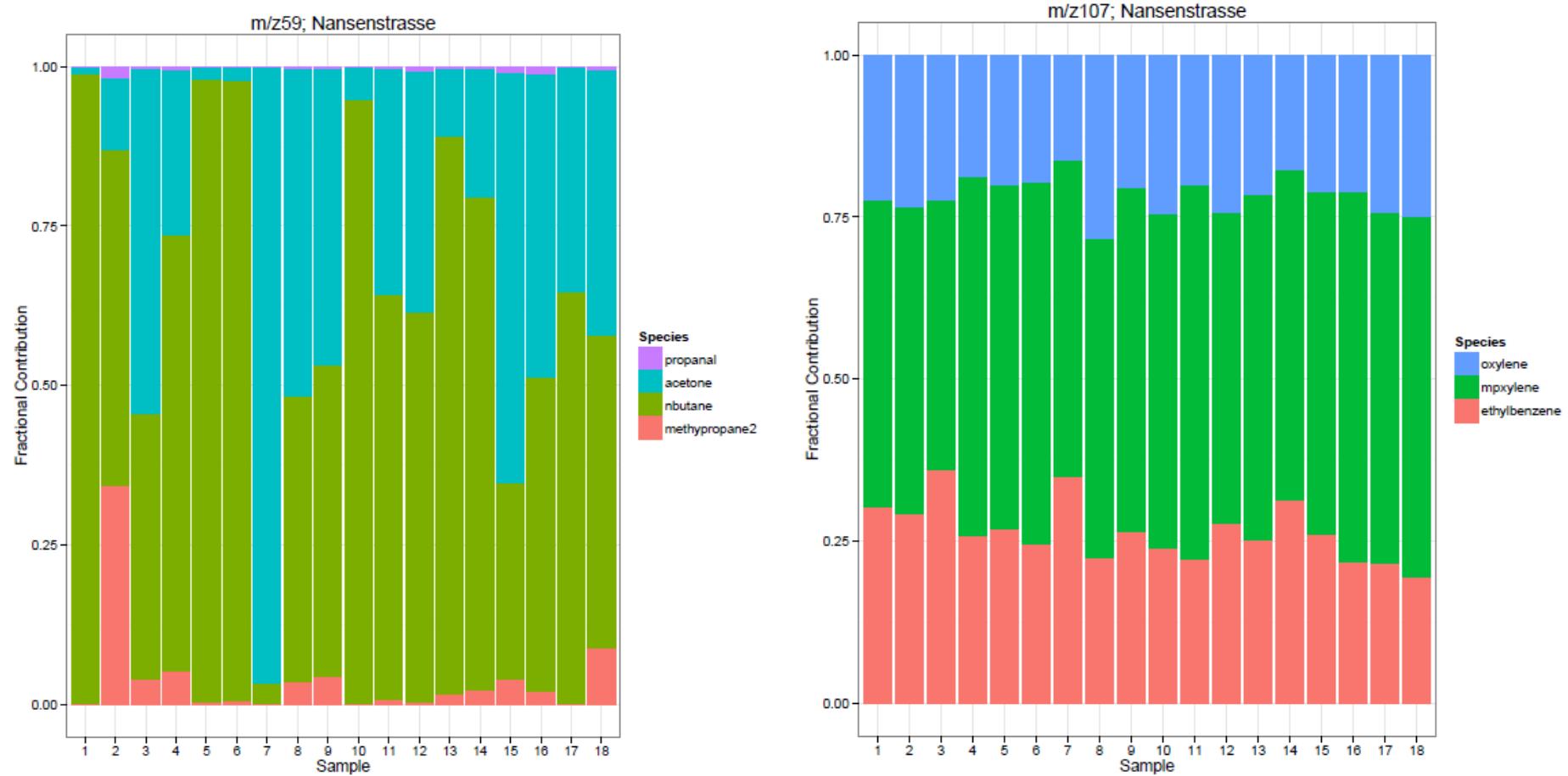
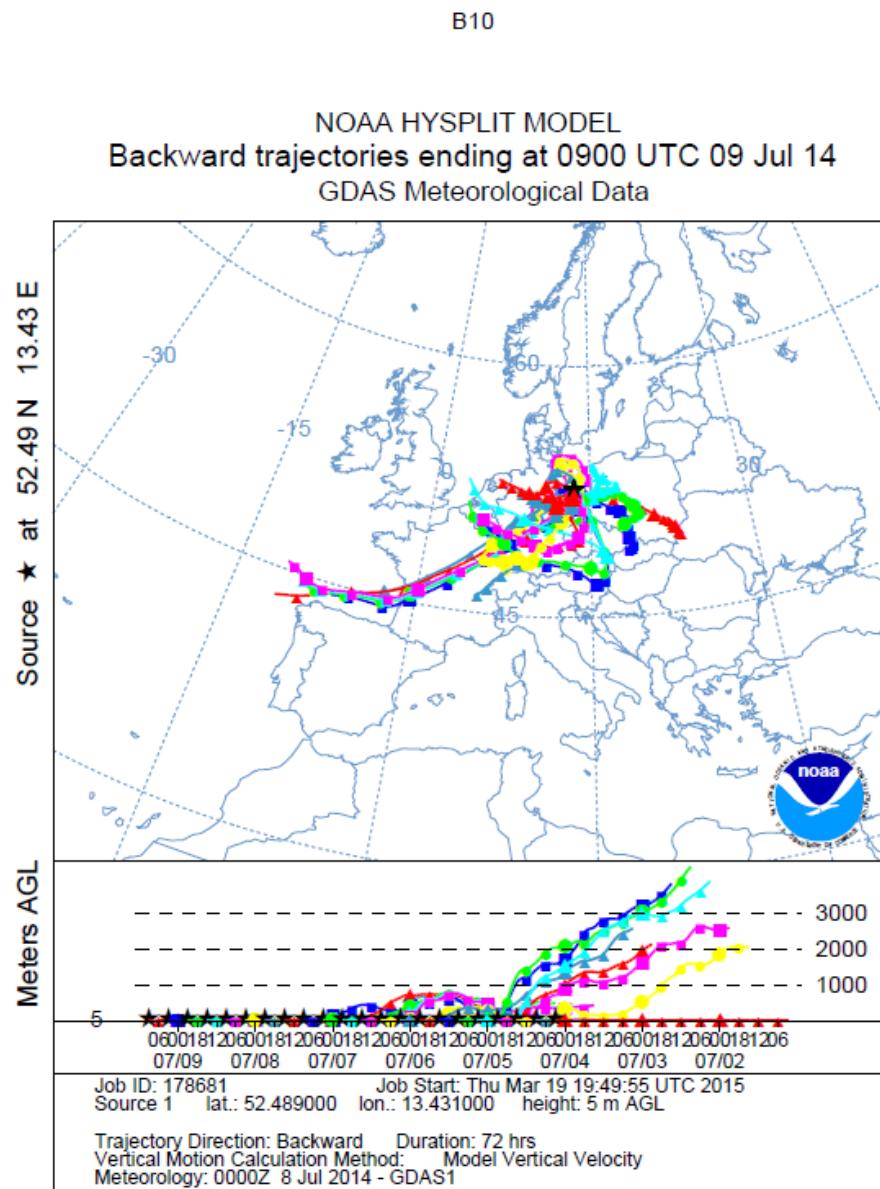


Figure S3. Fractional contribution of the individual NMVOCs measured by canister sample (GC-MS) to m/z 59 (left) and m/z 107 (right) for the 18 individual samples taken in Neukölln during the campaign.

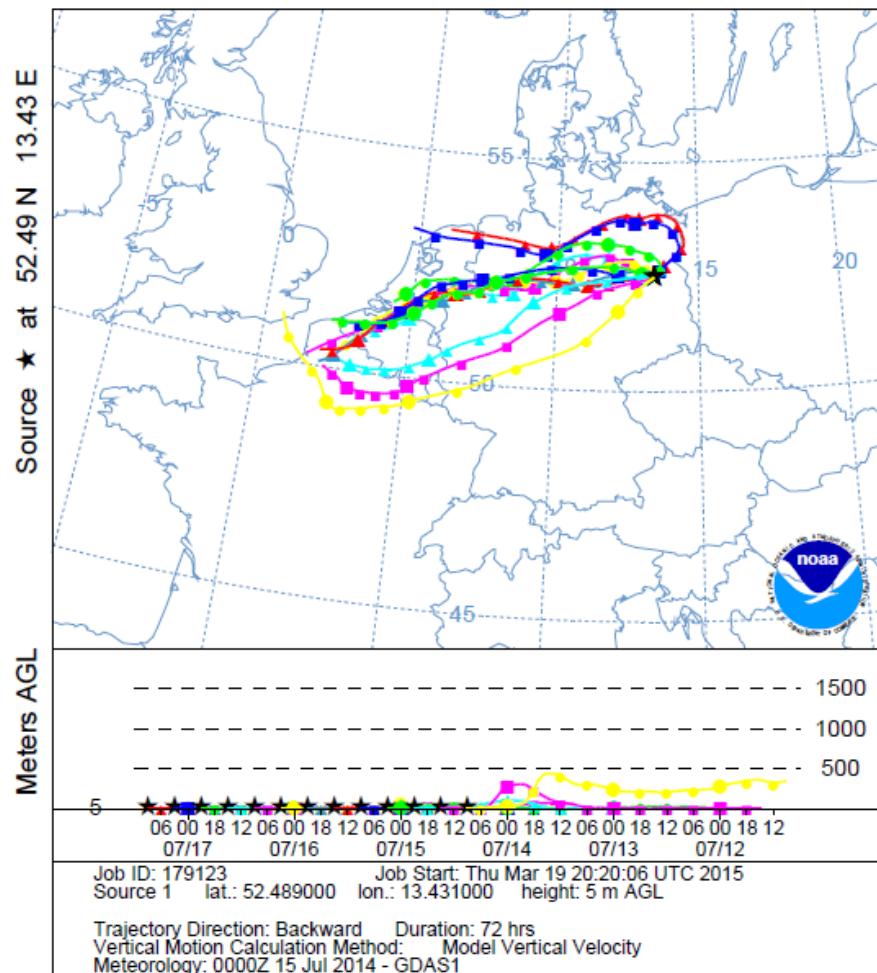
Figure S4. Back trajectories calculated by filter, organized by filter group.

(a) **Group A**

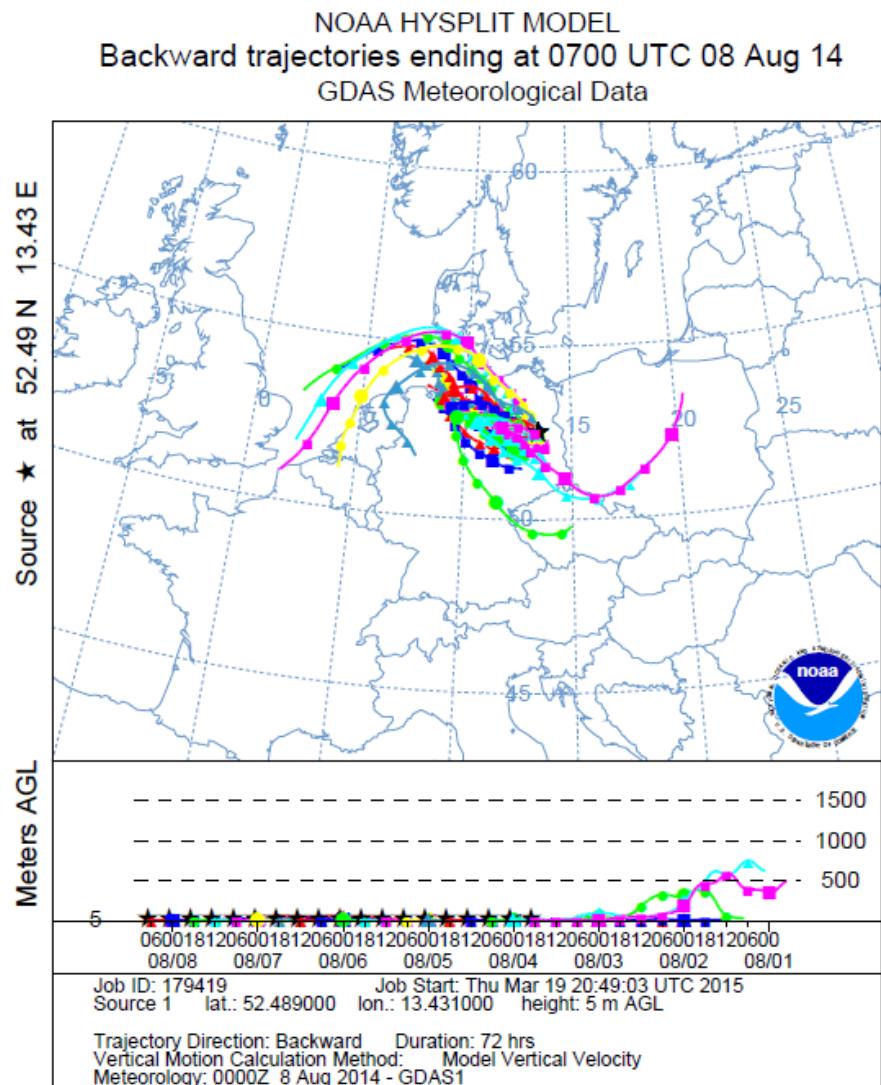


B13

NOAA HYSPLIT MODEL
Backward trajectories ending at 0900 UTC 17 Jul 14
GDAS Meteorological Data

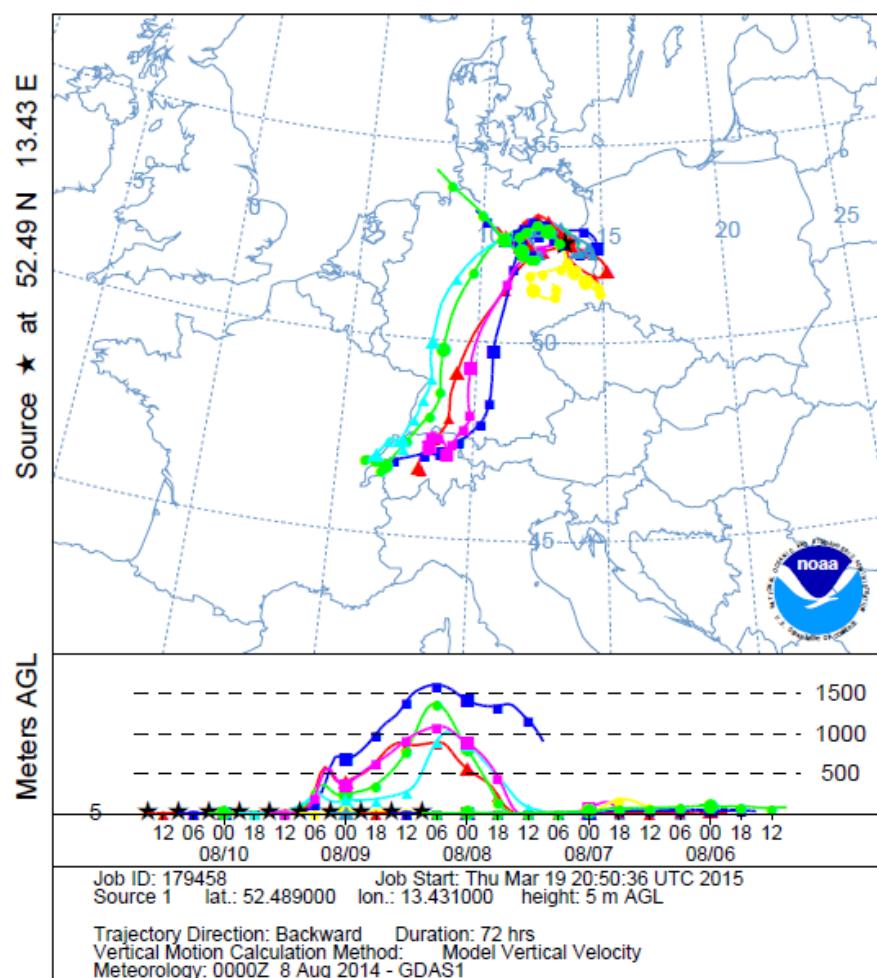


b20



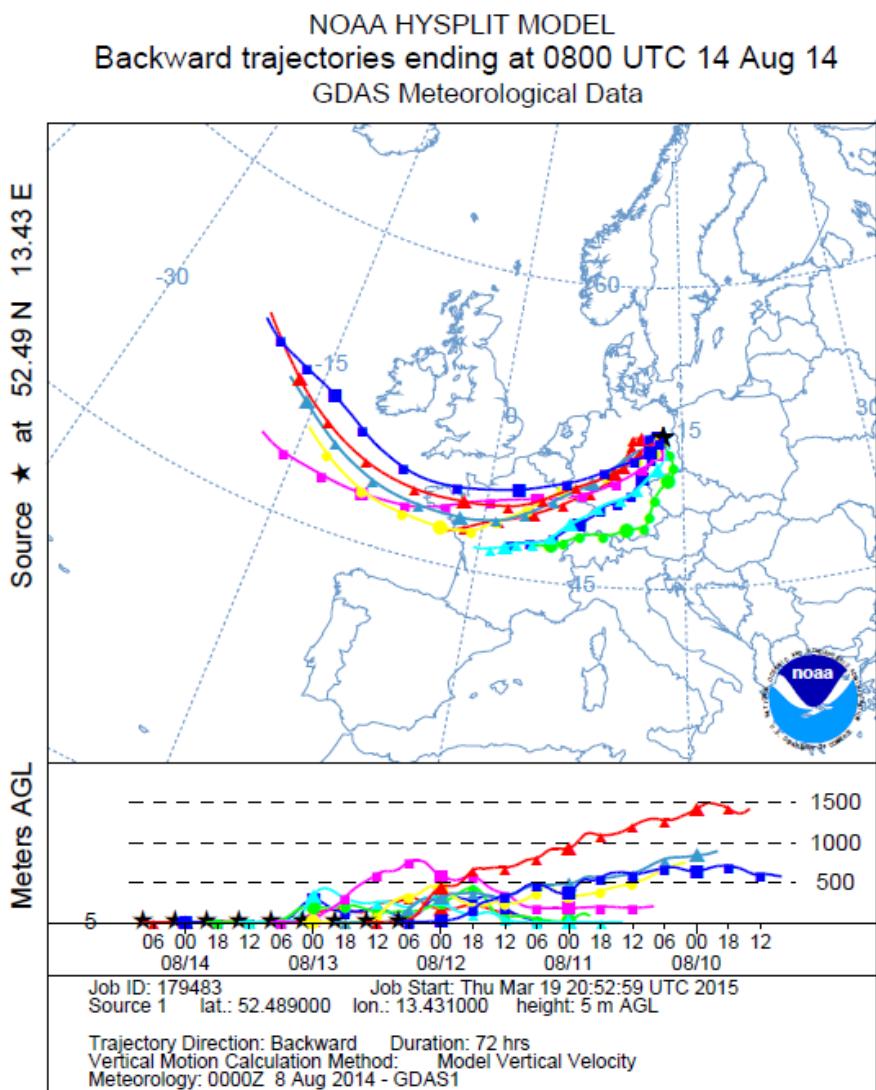
B21

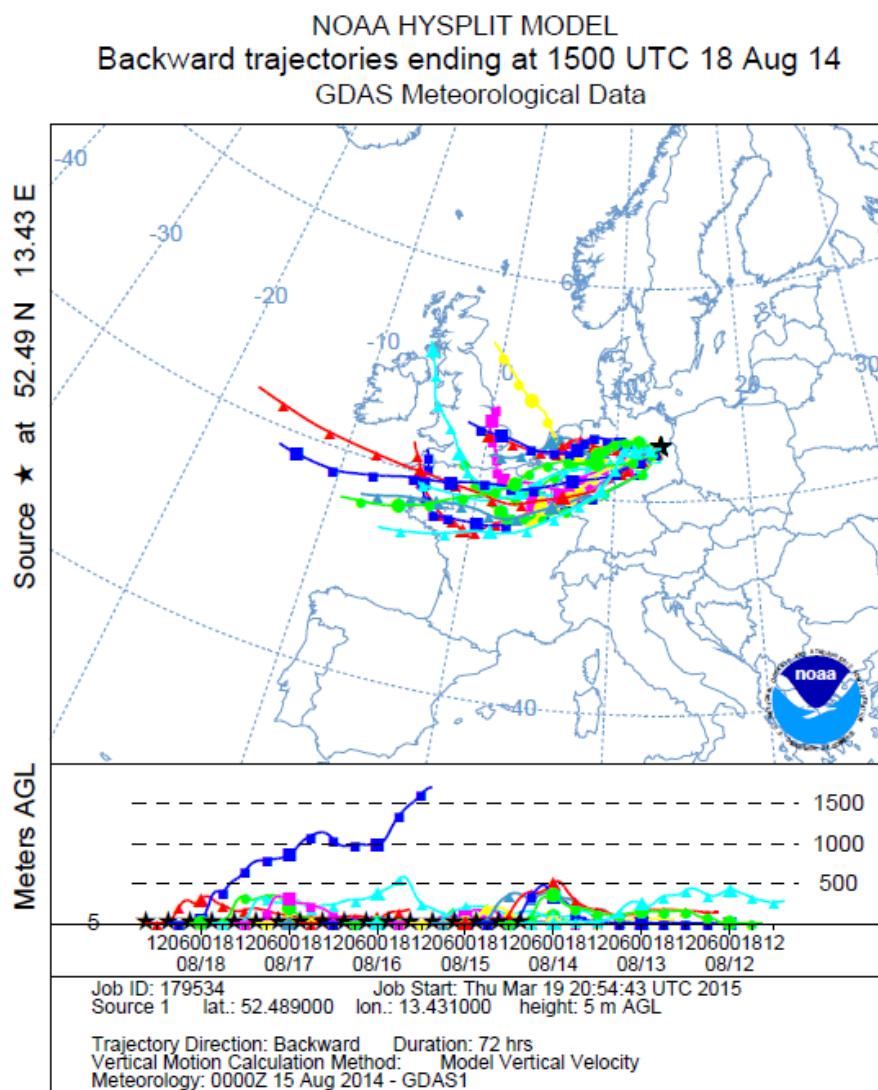
NOAA HYSPLIT MODEL
Backward trajectories ending at 1500 UTC 10 Aug 14
GDAS Meteorological Data



(b) Group B

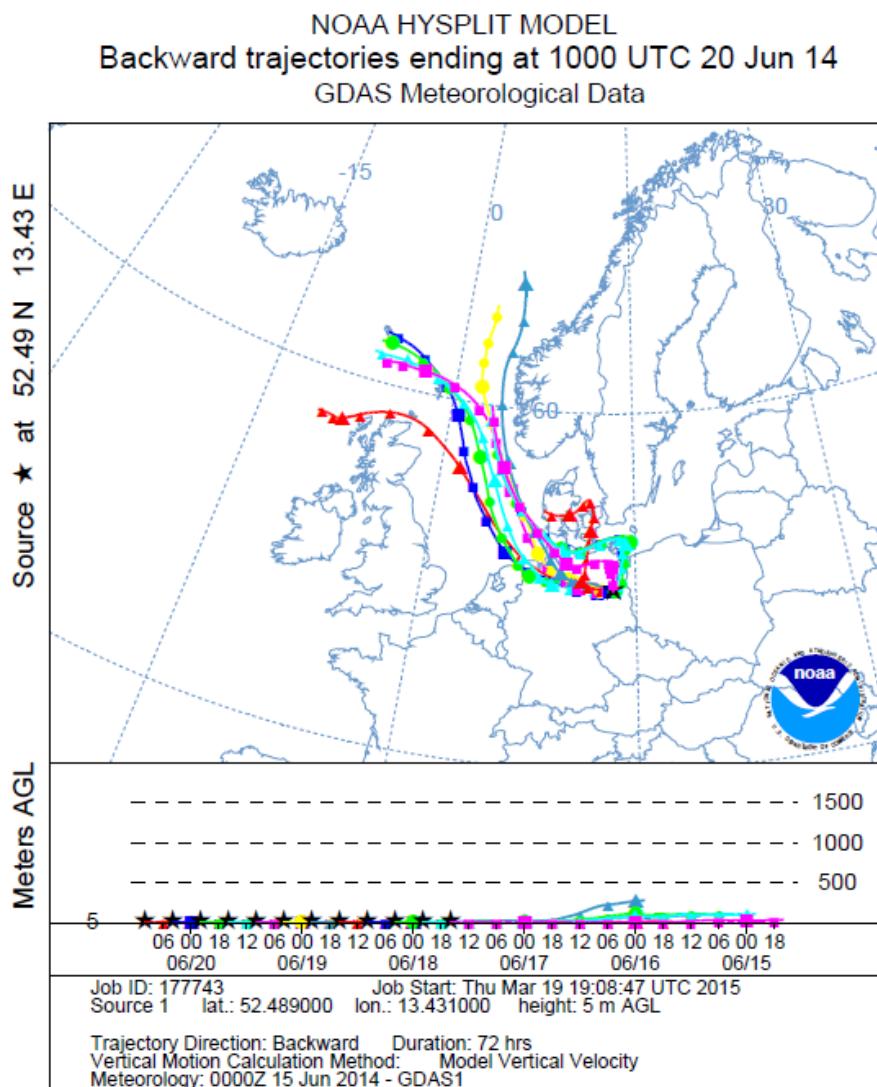
B23

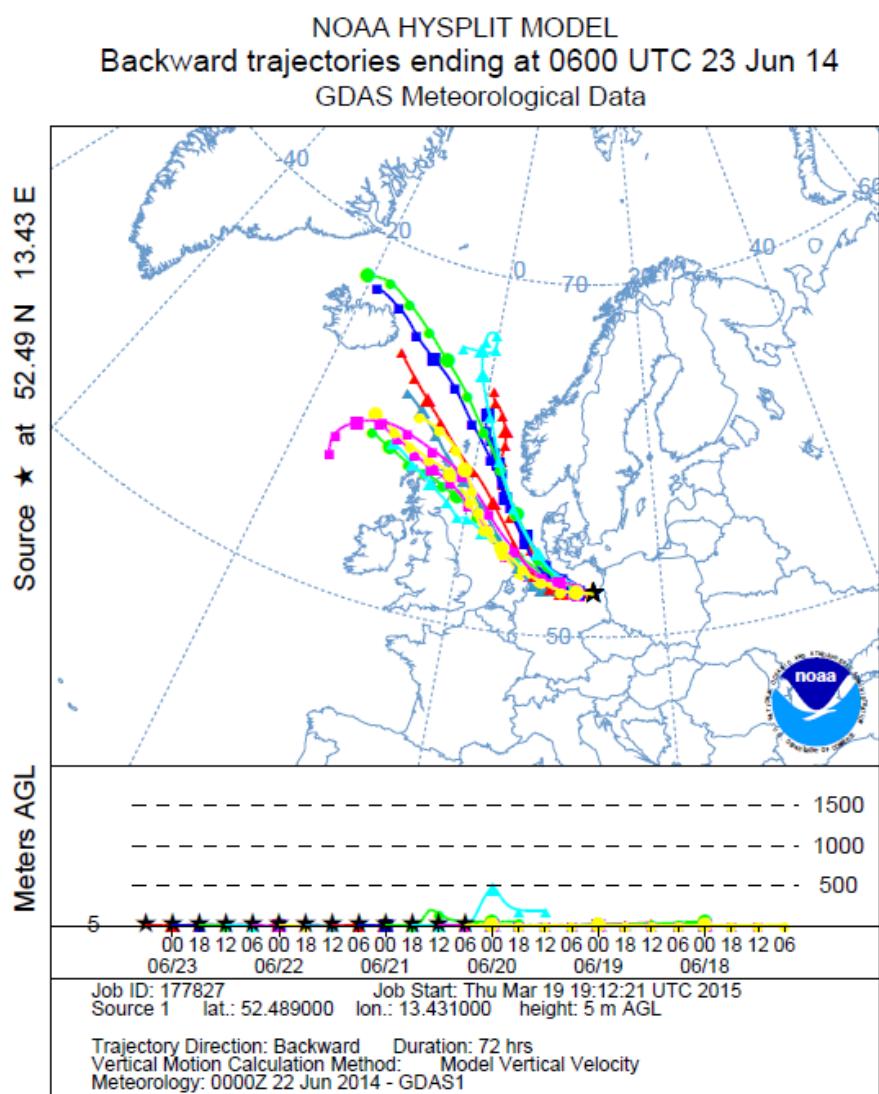


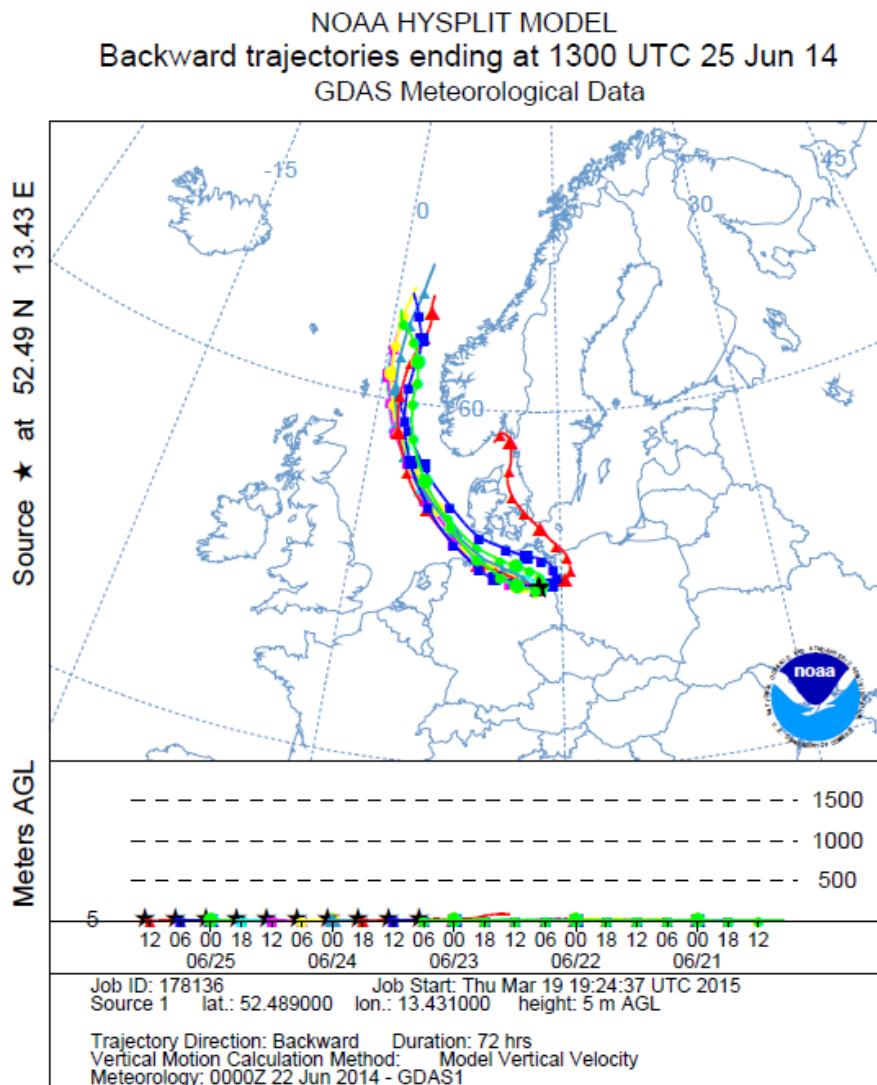


(c) Group C

B4

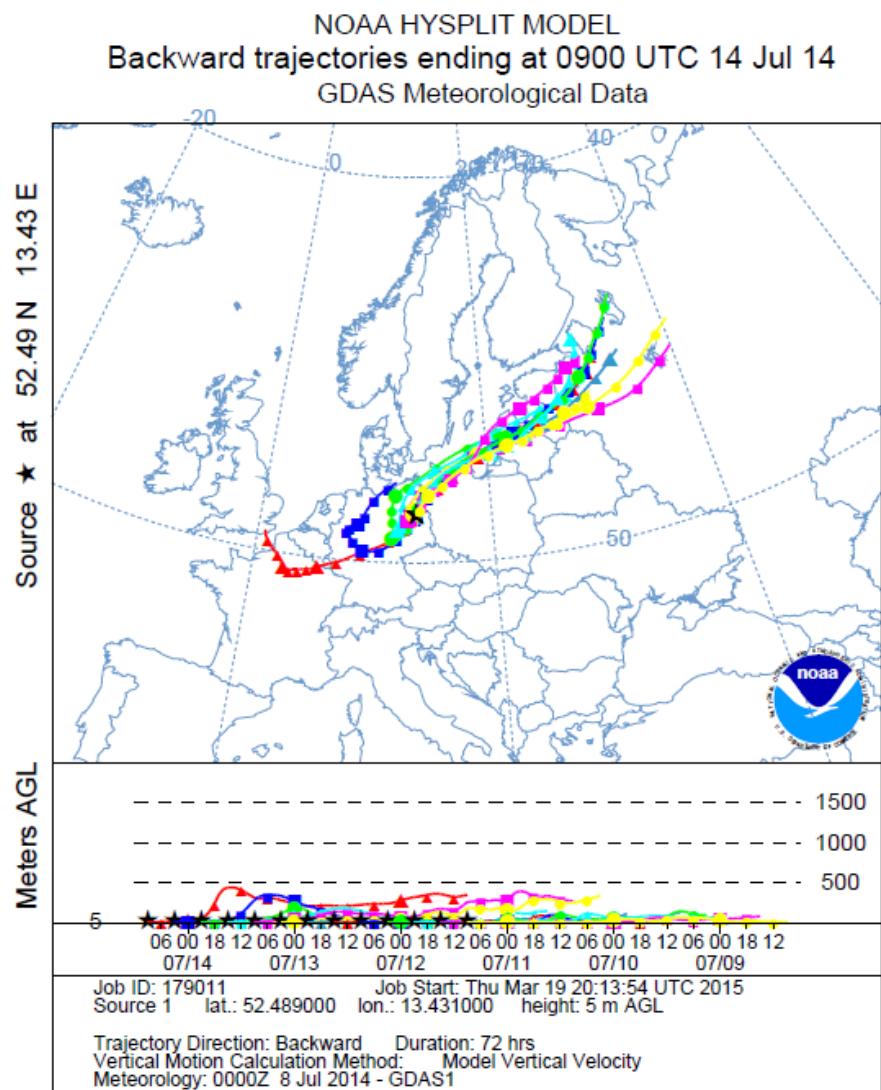




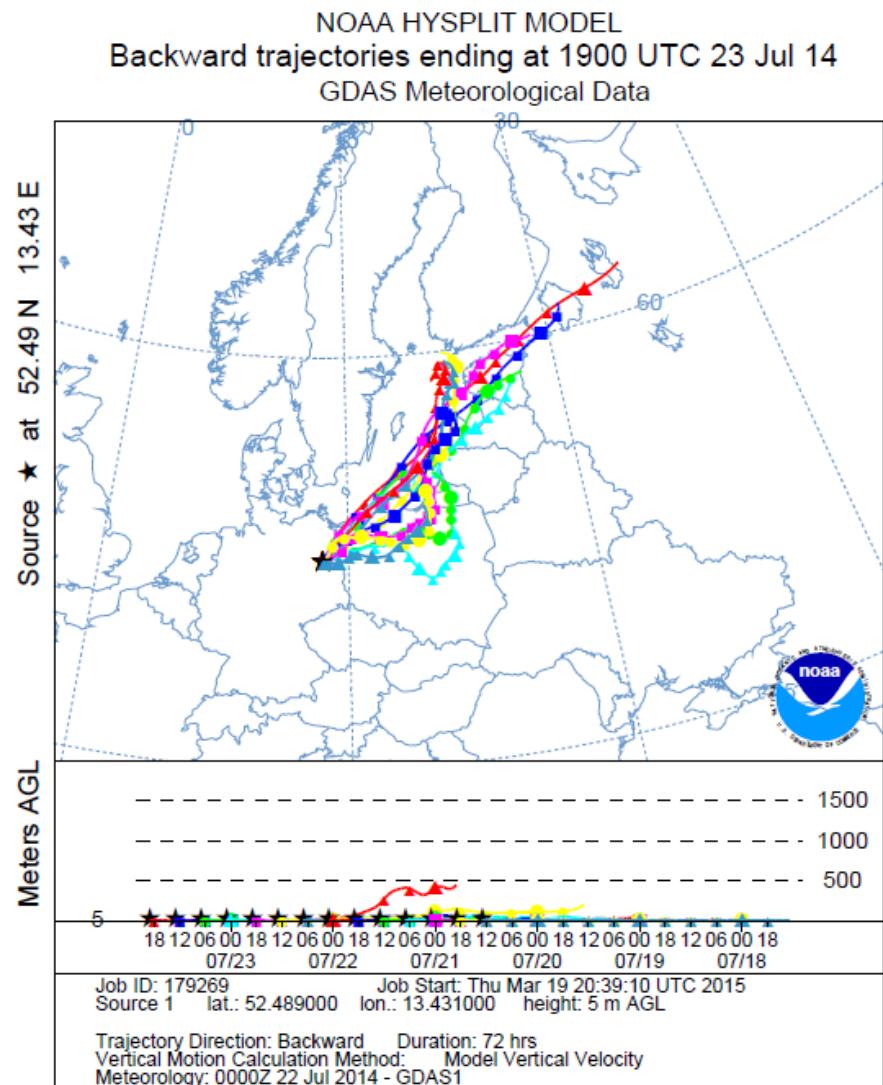


(d) Group D

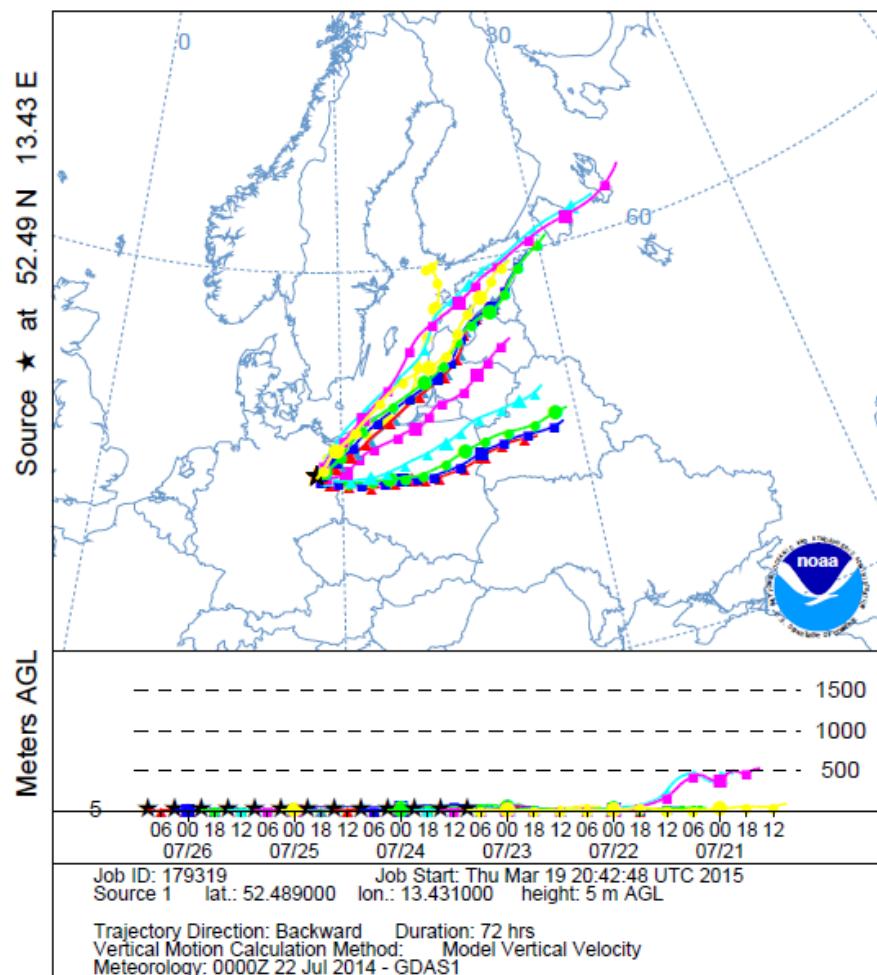
B12



B15

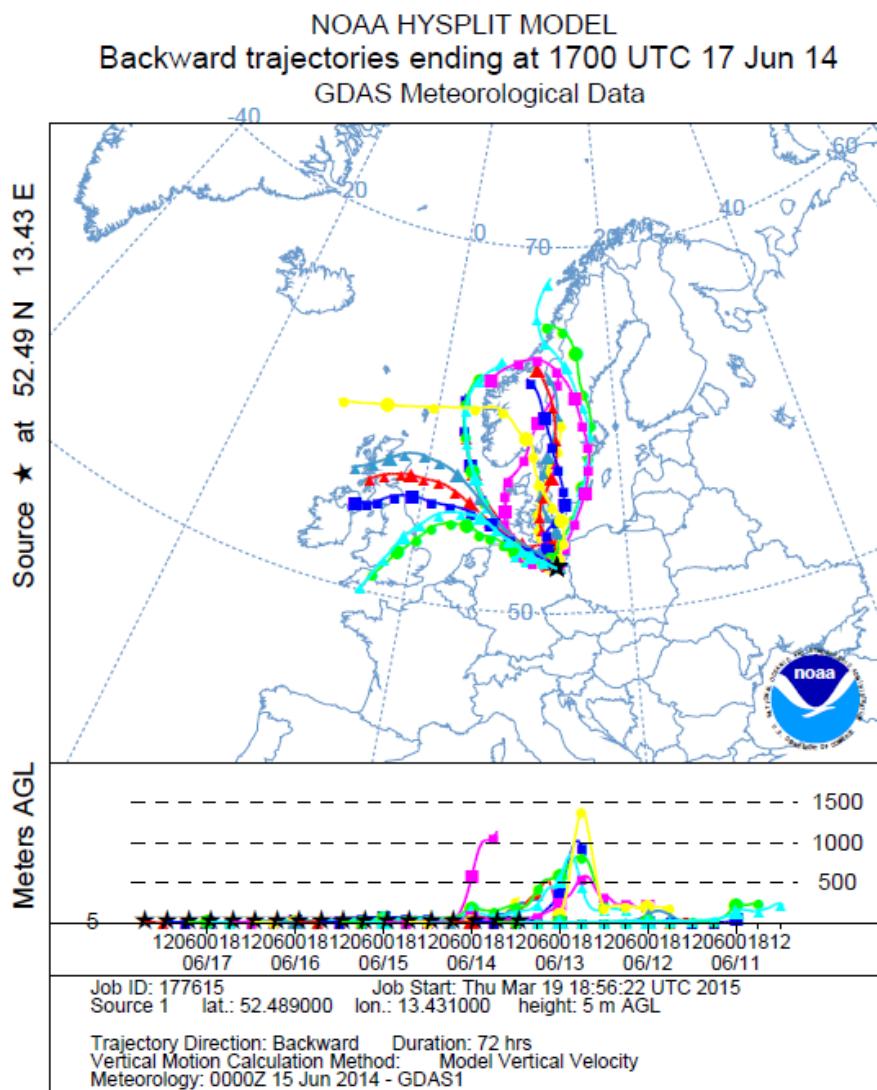


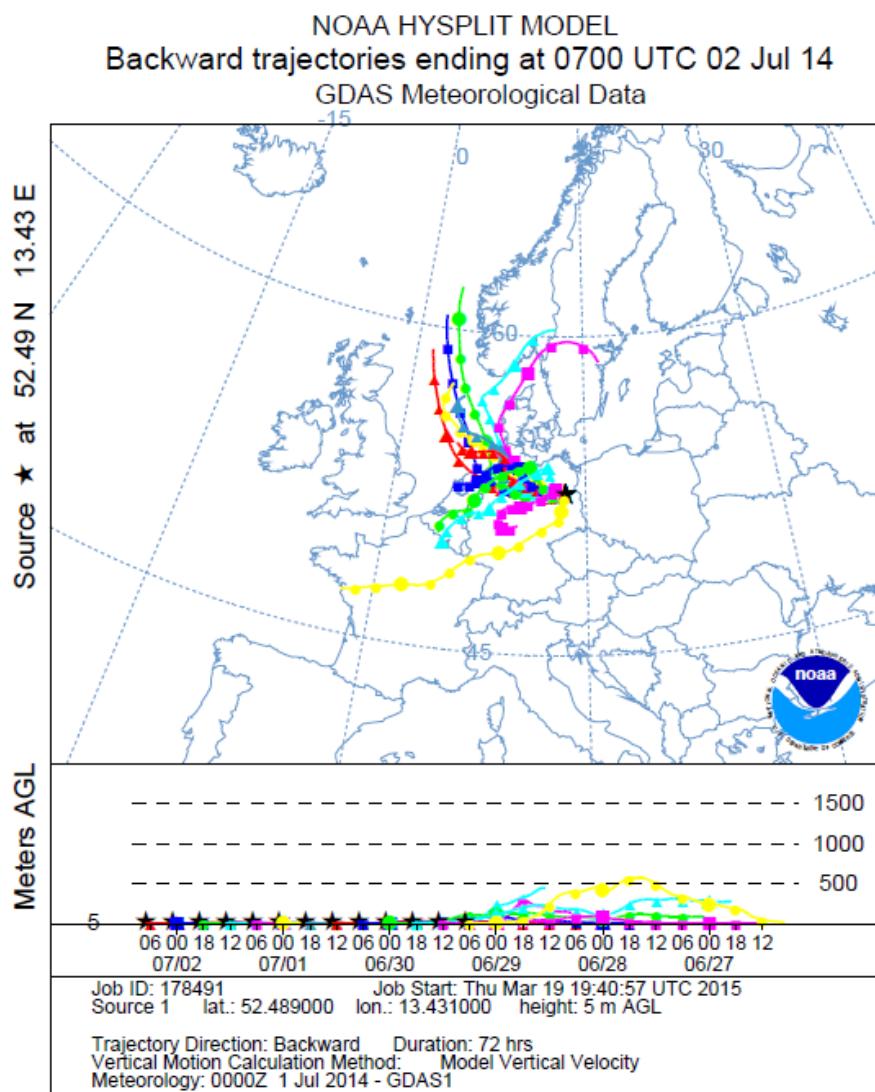
NOAA HYSPLIT MODEL
Backward trajectories ending at 0900 UTC 26 Jul 14
GDAS Meteorological Data



(e) Group E

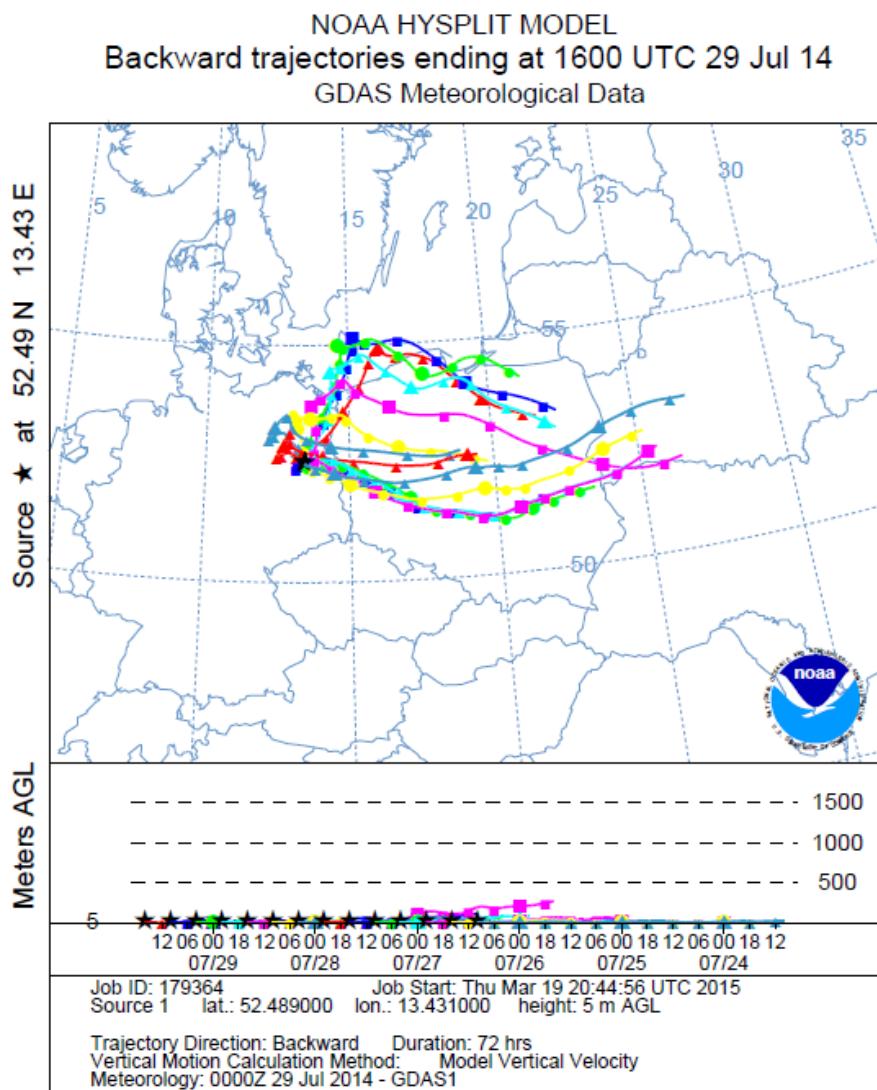
B3





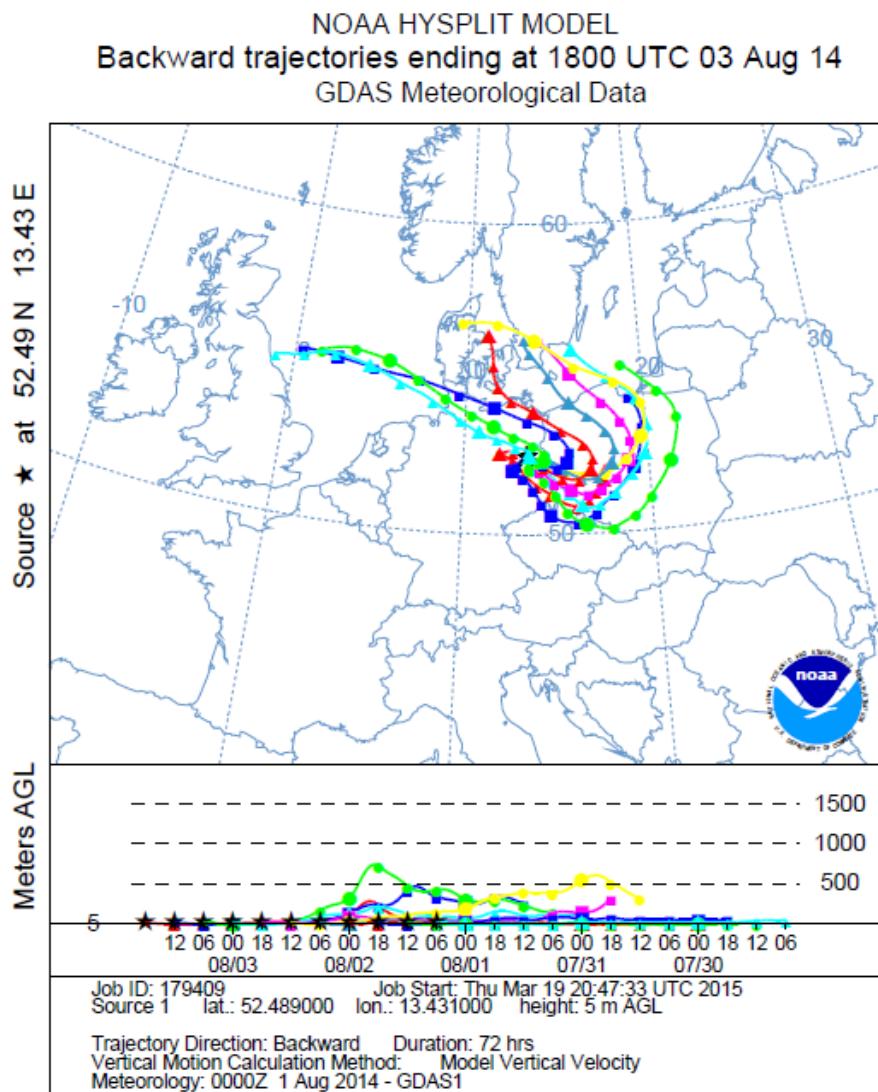
(f) Single filter B17

B17



(g) Single filter B19

B19



(h) Single filter B30

B30

