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Molecular insights into new particle formation in Barcelona, Spain

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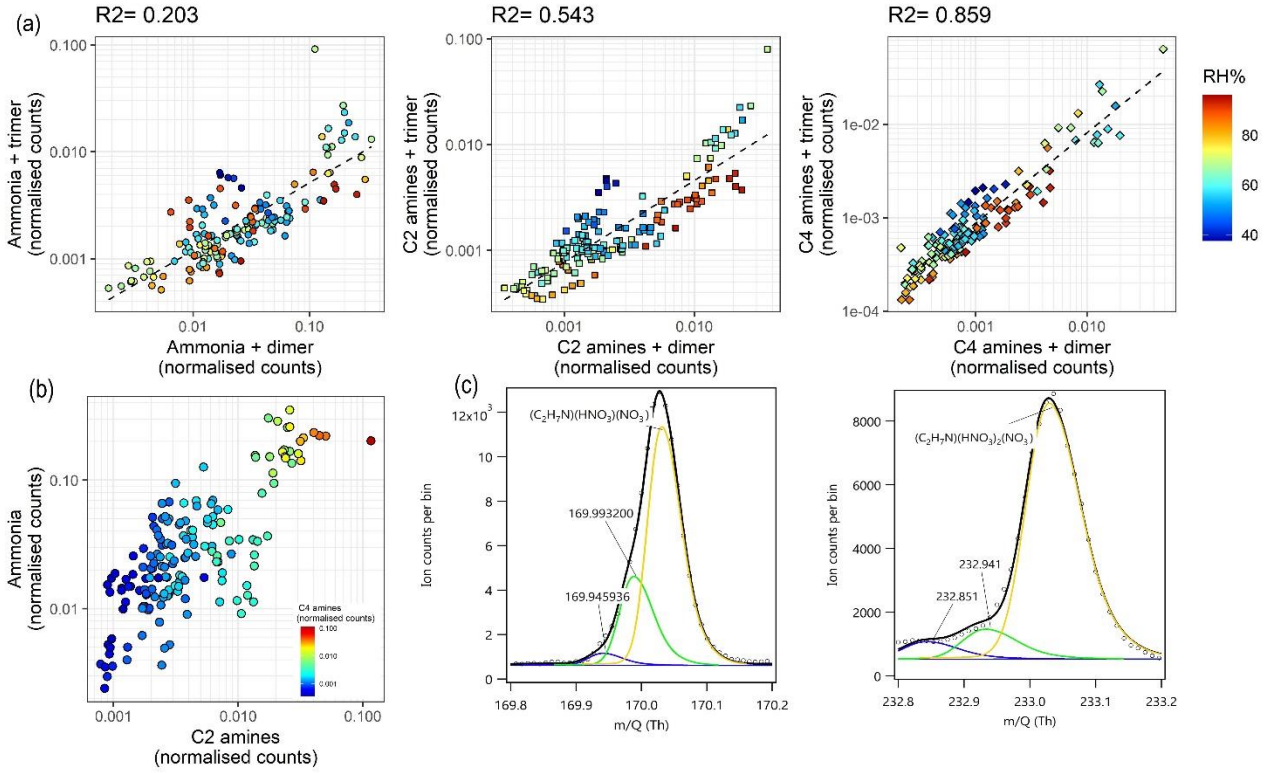


9

10 **Figure S1:** Ammonia and amine measurements via CI-APi-ToF, showing (a) ammonia, C_2 and C_4
11 amines as measured clustered with the nitrate dimer and trimer. Colour scale shows an RH dependence. (b)

Ammonia plotted against C_2 amines, coloured by C_4 amine concentration, and (c) peak fits for the C_2 amine ion as clustered with the nitrate dimer and trimer.

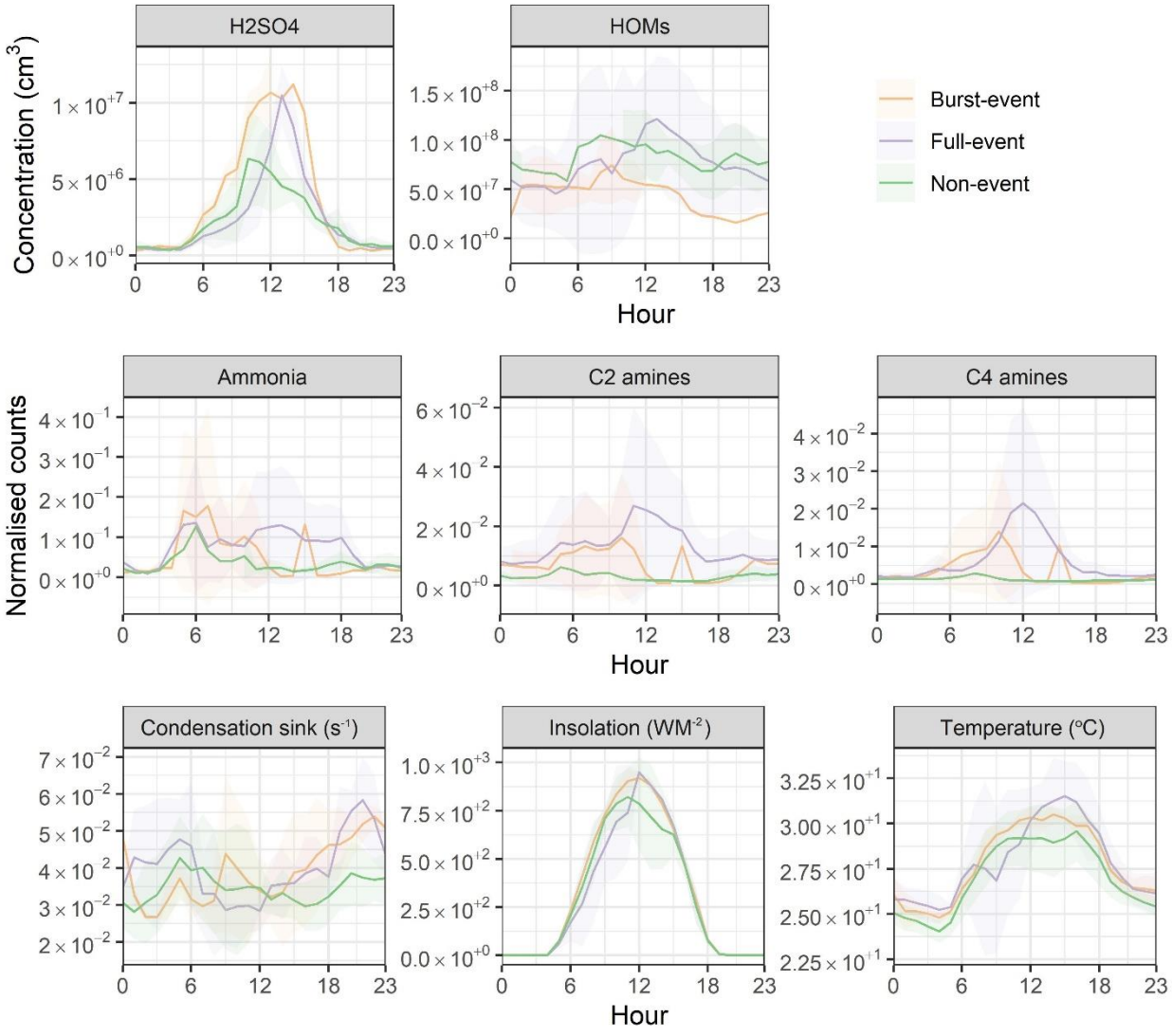


Figure S2: Diurnal profiles of (from top left through bottom right), H_2SO_4, HOMs, NH_3, C_2 amines, C_4 amines, condensation sink, insolation and temperature. Shaded regions show 1 standard deviation on the mean.

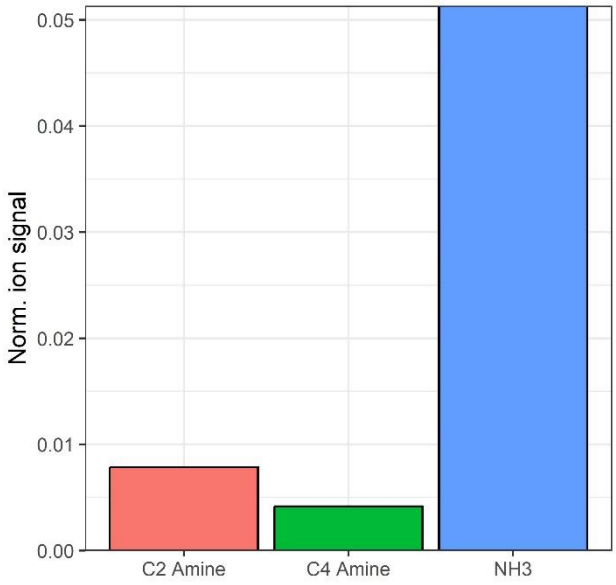
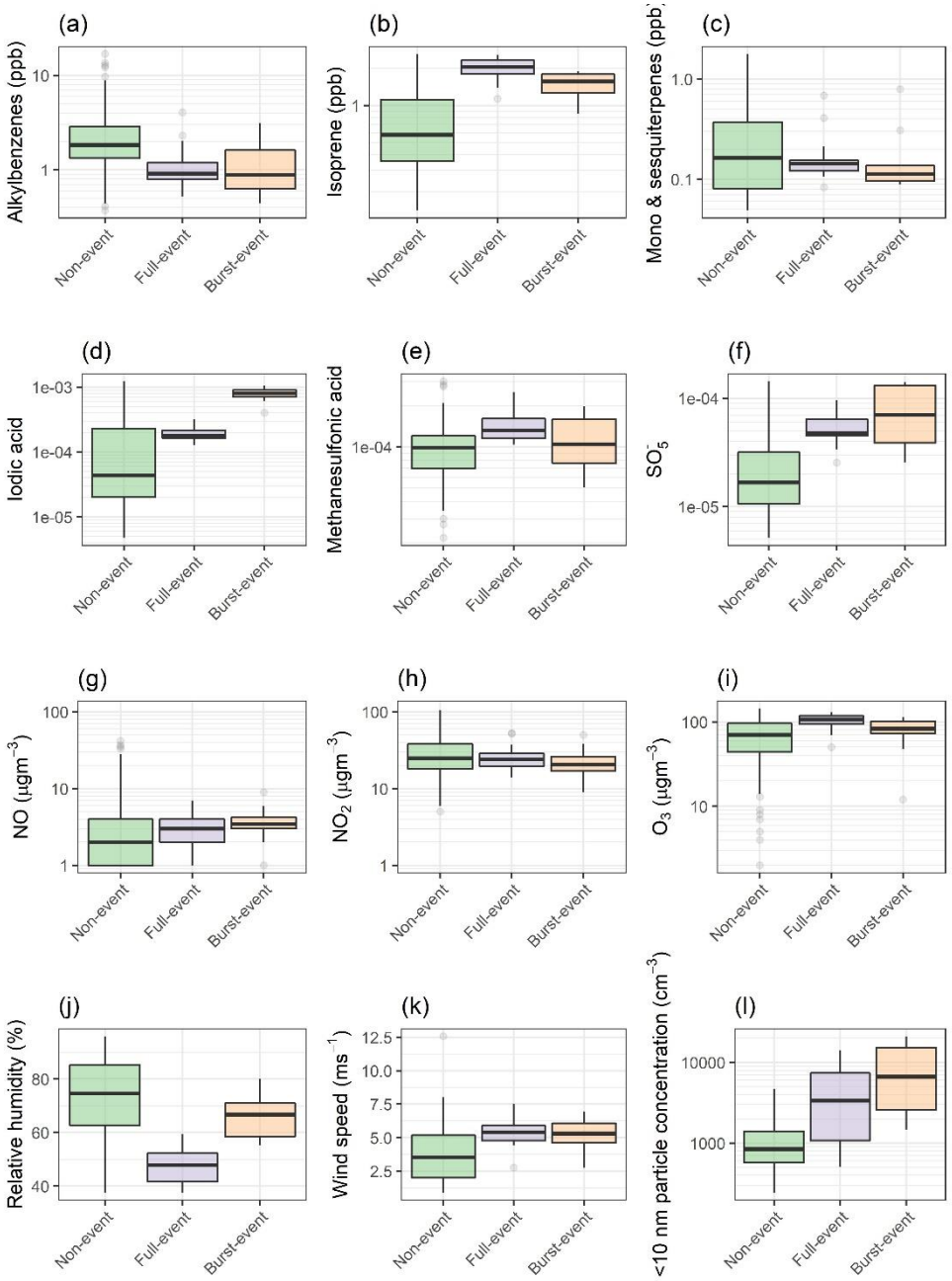


Figure S3: Mean ammonia and amine signals across the campaign as measured by CI-APi-ToF. Units of normalised ion counts.



21

22 **Figure S4:** Box plots as figures 2 & 3 for (a-c) VOCs as measured by PTR-ToF-MS, (d-f) other ions
23 as measured by CI-APi-ToF (units of norm. counts) (g-i) trace gases, and (j-l) meteorological and
24 <10 nm particle count parameters.

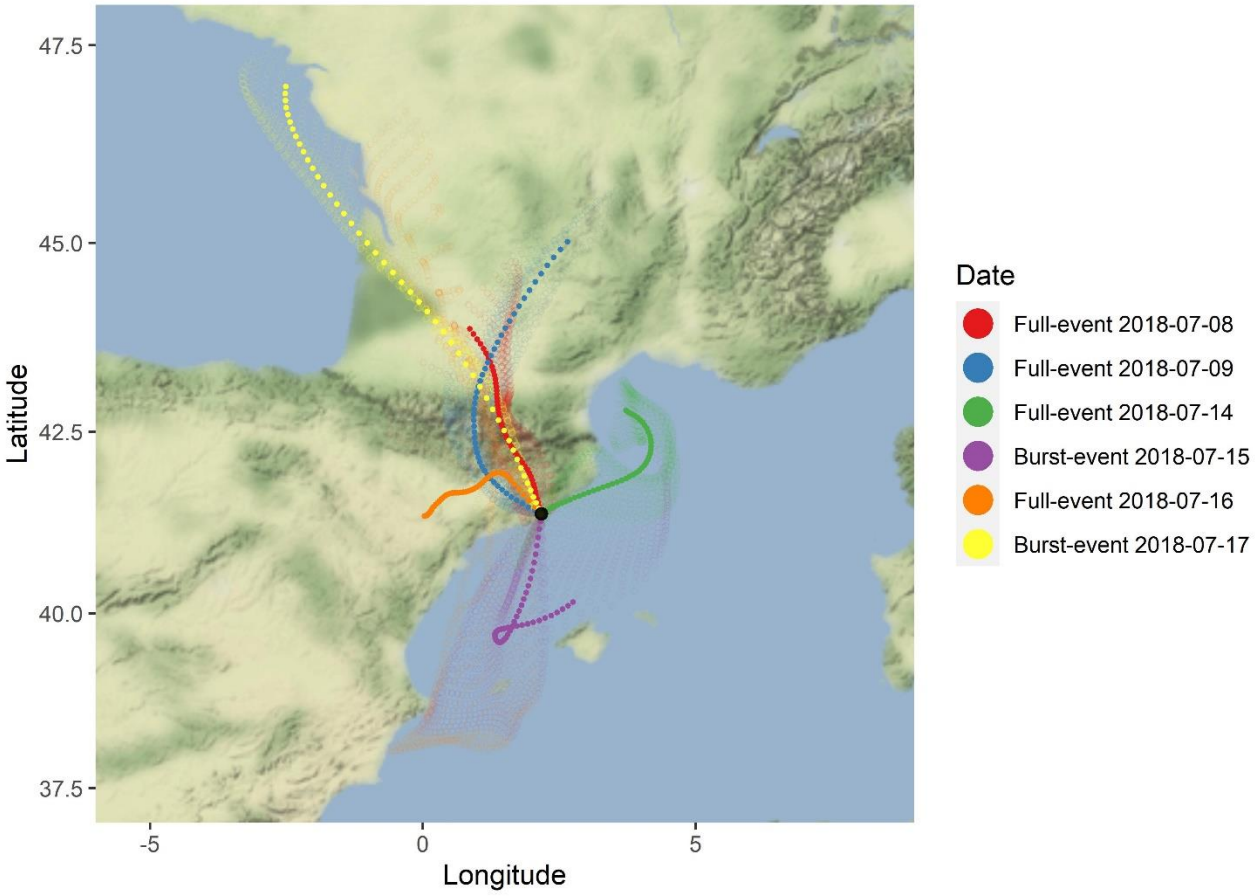


Figure S5: HYSPLIT 96 hour back trajectories per nucleation event. Dark dashed lines show mean trajectory per event, light dashed lines show hourly trajectories from which mean is calculated. Base map from OpenStreetMap (© OpenStreetMap contributors 2019, distributed under a Creative Commons BY-SA License).

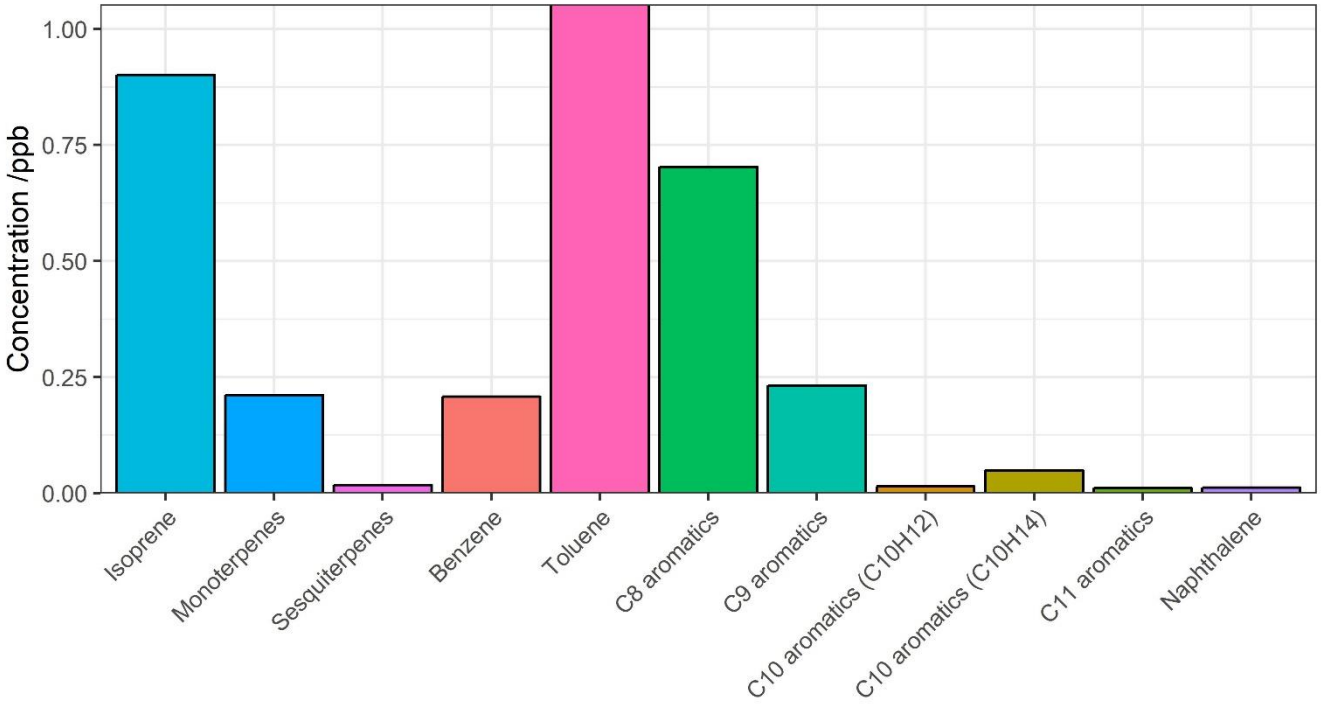


Figure S6: Mean selected VOC concentrations across the campaign as measured by PTR-ToF-MS.

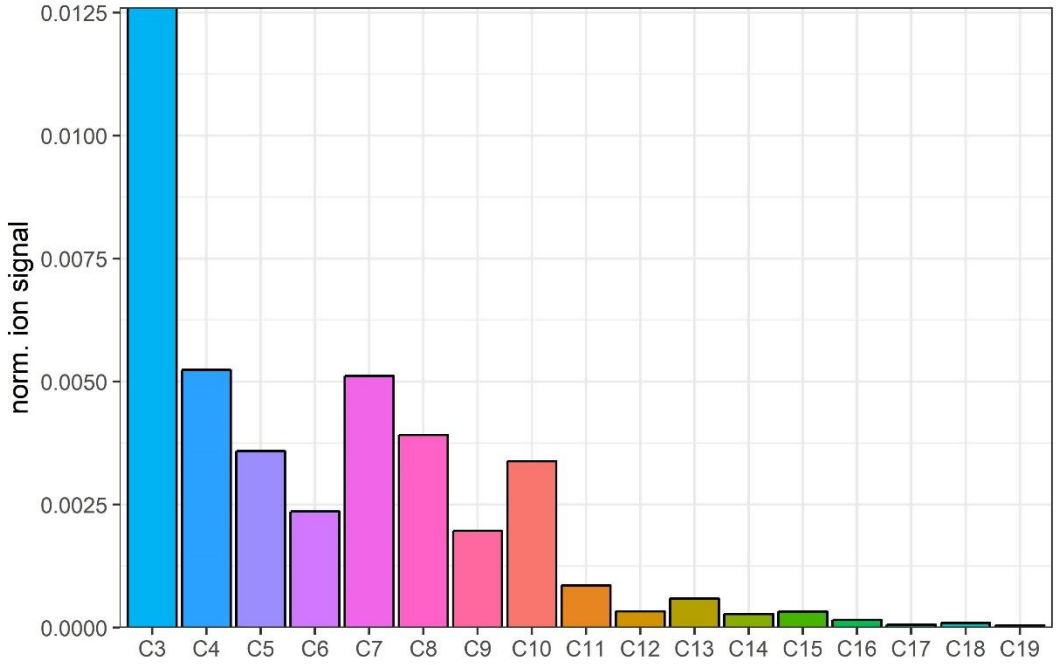


Figure S7: Mean ion signals per carbon number across the campaign as measured by CI-APi-ToF. Units of normalised ion counts.

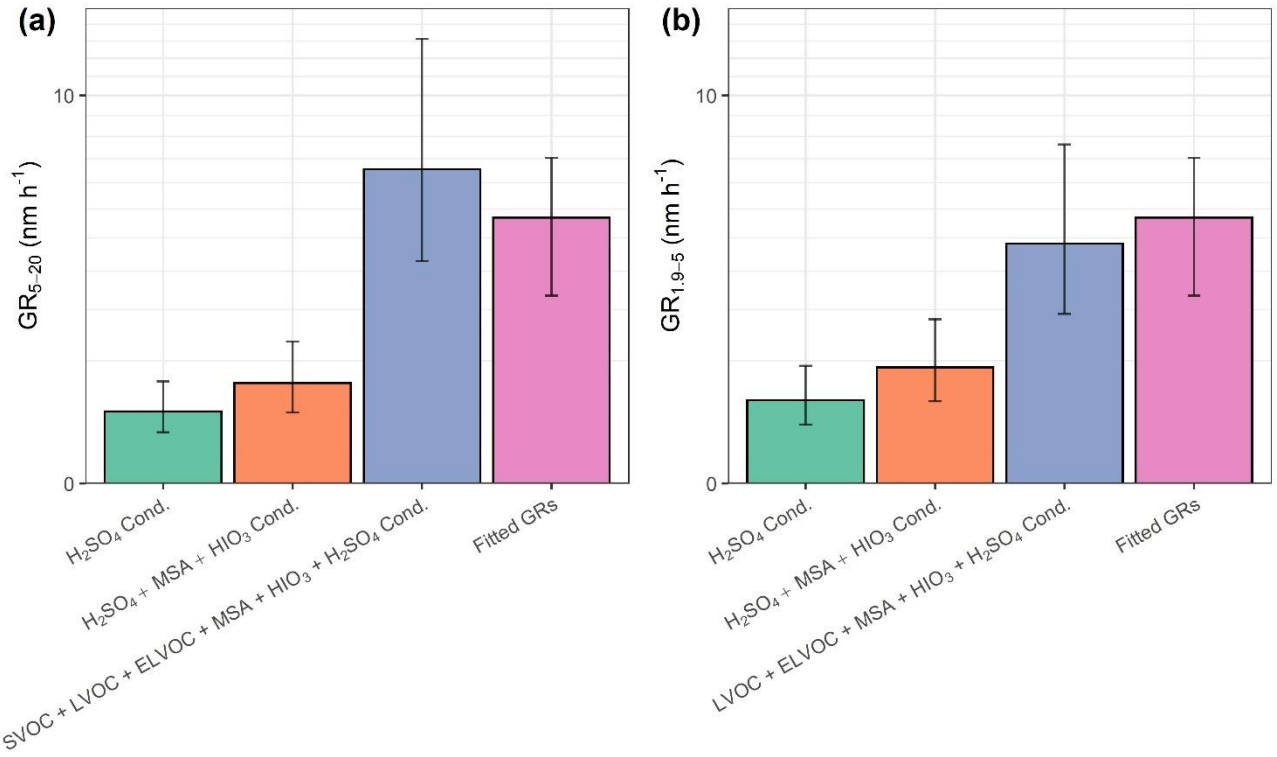


Figure S8: Condensational growth rates between (a) 5 - 20 nm and (b) 1.9 – 5 nm, calculated from H_2SO_4 condensation, H_2SO_4, MSA, and HIO_3 condensation, and SVOC, LVOC, ELVOC, H_2SO_4, MSA and HIO_3 in (a), and LVOC, ELVOC, H_2SO_4, MSA and HIO_3 in (b). Also presented are growth rates from particle count data. Error bars represent uncertainties on the concentration of species measured by CI-APi-ToF, and the uncertainties from GR calculations. Systematic uncertainties from the methods of Nieminen et al. (2010) are not included.

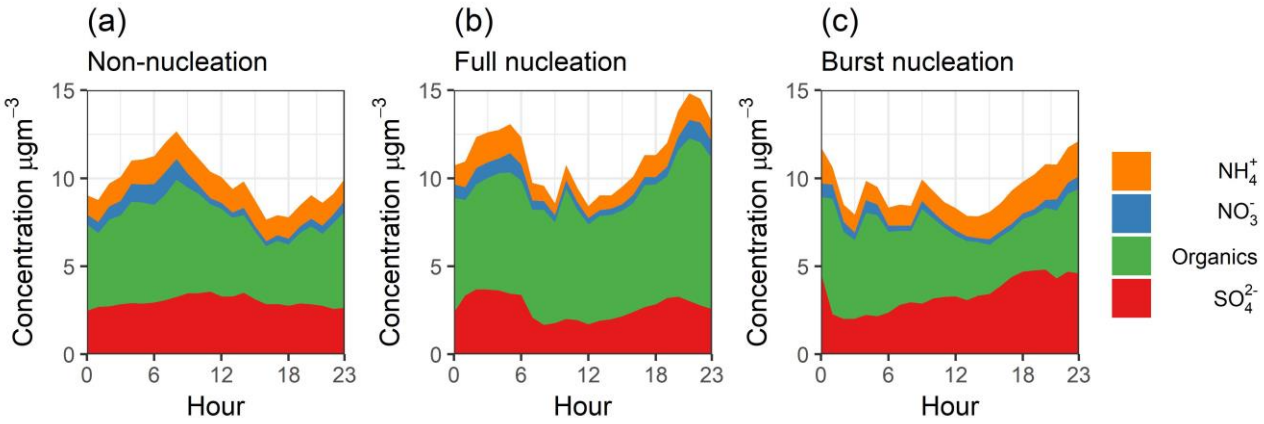


Figure S9: Average diurnals of particle composition as measured by ACSM on (a) non-nucleation, (b) full-nucleation and (c) burst-nucleation days.

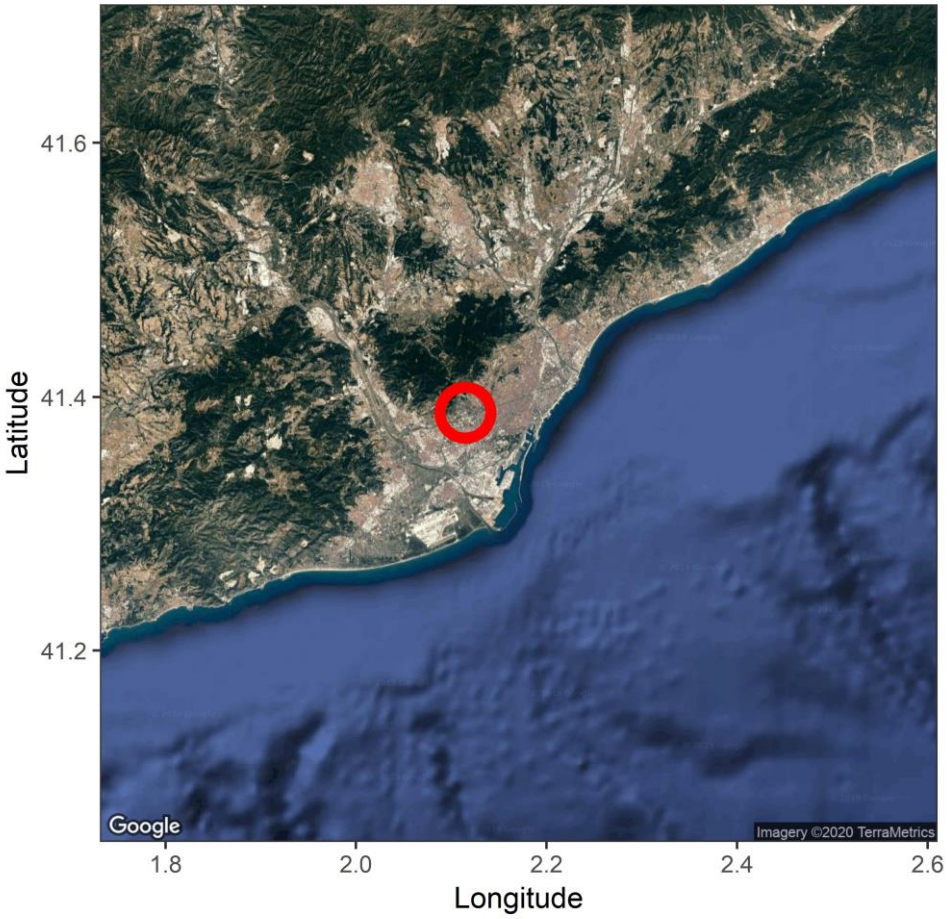


Figure S10: Location of sampling site. Map data: Google, TerraMetrics 2020.

54

Table S1: Ions identified by CI-APi-ToF

Ion	m/Q
Cl^-	34.97
NO_2^-	45.99
$C_3H_3O^-$	55.02
$(NO_3)^-$	61.99
$C_3H_3O_2^-$	71.01
$C_3H_5O_2^-$	73.03
Br^-	78.92
$H_2O(NO_3)^-$	80.00
$C_4H_5O_2^-$	85.03
$C_3H_3O_3^-$	87.01
$CH_3SO_3^-$	94.98
$CFH_3(NO3)^-$	96.01
HSO_4^-	96.96
$HCl(NO3)^-$	97.97
$H_4O_2(NO3)^-$	98.01
$C_4H_5O_3^-$	101.02
$C_3H_3O_4^-$	103.00
SO_5^-	111.95
$C_4H_3O_4^-$	115.00
$C_4H_5O_4^-$	117.02
$C_3H_4O(NO_3)^-$	118.01
$C_3H_3O_5^-$	119.00
$HNO_3NO_3^-$	124.98
I^-	126.91
$C_4H_3O_5^-$	131.00
$C_5H_7O_4^-$	131.03
$C_4H_5O_5^-$	133.01
$NH_3(HNO_3)(NO_3)^-$	142.01
$C_5H_5O_5^-$	145.01
$C_5H_7O_5^-$	147.03
$C_3H_6O_3(NO_3)^-$	152.02
$C_6H_7O_5^-$	159.03
$C_4H_6O_3(NO_3)^-$	164.02
$C_3H_5NO_3(NO_3)^-$	165.02

$C_3H_4O_4(NO_3)^-$	166.00
$C_6H_5NO(NO_3)^-$	169.03
$C_2H_7N(HNO_3)(NO_3)^-$	170.04
$C_7H_7O_5^-$	171.03
$C_7H_9O_5^-$	173.05
IO_3^-	174.89
$C_4H_5NO_3(NO_3)^-$	177.02
$C_4H_4O_4(NO_3)^-$	178.00
$C_5H_7O_7^-$	179.02
$C_4H_6O_4(NO_3)^-$	180.01
$C_5H_9O_7^-$	181.04
$C_4H_8O_4(NO_3)^-$	182.03
$C_8H_{11}O_5^-$	187.06
$(HNO_3)_2(NO_3)^-$	187.98
$C_7H_9O_6^-$	189.04
$C_5H_7NO_3(NO_3)^-$	191.03
$C_4H_6N_2O_3(NO_3)^-$	192.03
$C_4H_5NO_4(NO_3)^-$	193.01
$C_5H_8O_4(NO_3)^-$	194.03
$H_2SO_4HSO_4^-$	194.93
$C_5H_7O_8^-$	195.01
$C_3H_6N_2O_4(NO_3)^-$	196.02
$C_4H_8O_5(NO_3)^-$	198.03
$C_4H_{11}N(HNO_3)(NO_3)^-$	198.07
$C_7H_7NO_2(NO_3)^-$	199.04
$C_6H_5NO_3(NO_3)^-$	201.02
$C_8H_{11}O_6^-$	203.06
$C_6H_6O_4(NO_3)^-$	204.01
$NH_3(HNO3)_2(NO_3)^-$	205.01
$C_6H_8O_4(NO_3)^-$	206.03
$C_5H_7NO_4(NO_3)^-$	207.03
$C_4H_6N_2O_4(NO_3)^-$	208.02
$C_5H_8O_5(NO_3)^-$	210.03
$C_4H_7NO_5(NO_3)^-$	211.02
$C_8H_6O_3(NO_3)^-$	212.02
$C_3H_5NO_6(NO_3)^-$	213.00

$C_{10}H_{13}O_5^-$	213.08
$C_4H_8O_6(NO_3)^-$	214.02
$C_7H_7NO_3(NO_3)^-$	215.03
$C_7H_6O_4(NO_3)^-$	216.01
$C_7H_9NO_3(NO_3)^-$	217.05
$C_7H_8O_4(NO_3)^-$	218.03
$C_7H_{10}O_4(NO_3)^-$	220.05
$C_6H_9NO_4(NO_3)^-$	221.04
$C_5H_8N_2O_4(NO_3)^-$	222.04
$C_{10}H_7O_6^-$	223.02
$C_5H_8O_6(NO_3)^-$	226.02
$C_4H_7NO_6(NO_3)^-$	227.02
$C_4H_6O_7(NO_3)^-$	228.00
$C_8H_9NO_3(NO_3)^-$	229.05
$C_7H_7NO_4(NO_3)^-$	231.03
$C_2H_7N(HNO3)_2(NO_3)^-$	233.04
$C_7H_{10}O_5(NO_3)^-$	236.04
$C_7H_{12}O_5(NO_3)^-$	238.06
$C_{10}H_7O_7^-$	239.02
$C_4H_6N_2O_6(NO_3)^-$	240.01
$C_5H_8O_7(NO_3)^-$	242.02
$C_5H_{11}NO_6(NO_3)^-$	243.05
$C_5H_{10}O_7(NO_3)^-$	244.03
$C_9H_{12}O_4(NO_3)^-$	246.06
$C_7H_7NO_5(NO_3)^-$	247.02
$C_8H_{10}O_5(NO_3)^-$	248.04
$C_7H_9NO_5(NO_3)^-$	249.04
$C_8H_{12}O_5(NO_3)^-$	250.06
$C_7H_{11}NO_5(NO_3)^-$	251.05
$C_7H_{10}O_6(NO_3)^-$	252.04
$C_7H_{12}O_6(NO_3)^-$	254.05
$C_6H_{11}NO_6(NO_3)^-$	255.05
$C_6H_{10}O_7(NO_3)^-$	256.03
$C_5H_8O_8(NO_3)^-$	258.01
$C_8H_7NO_5(NO_3)^-$	259.02
$C_9H_{10}O_5(NO_3)^-$	260.04

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$C_9H_{12}O_5(NO_3)^-$	262.06
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$C_9H_{14}O_5(NO_3)^-$	264.07
$C_7H_9NO_6^-(NO_3)^-$	265.03
$C_7H_8O_7(NO_3)^-$	266.01
$C_8H_{12}O_6(NO_3)^-$	266.05
$C_7H_{11}NO_6(NO_3)^-$	267.05
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$C_6H_{11}NO_7(NO_3)^-$	271.04
$C_6H_{10}O_8(NO_3)^-$	272.03
$C_5H_9NO_8(NO_3)^-$	273.02
$C_5H_8O_9(NO_3)^-$	274.01
$C_{10}H_{12}O_5(NO_3)^-$	274.06
$C_{10}H_{14}O_5(NO_3)^-$	276.07
$C_9H_{13}NO_5(NO_3)^-$	277.07
$C_9H_{12}O_6(NO_3)^-$	278.05
$C_{10}H_{16}O_5(NO_3)^-$	278.09
$C_8H_{11}NO_6^-(NO_3)^-$	279.05
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$C_8H_{14}O_7(NO_3)^-$	284.06
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$C_{10}H_{15}NO_5(NO_3)^-$	291.08
$C_{10}H_{14}O_6(NO_3)^-$	292.07

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$C_{14}H_{14}O_8(NO_3)^-$	372.06
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$C_{15}H_{16}O_8(NO_3)^-$	386.07
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$C_{18}H_{21}N(NO_3)O_5^-$	393.13
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$C_{16}H_{19}N(NO_3)O_7^-$	399.10
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$C_{15}H_{17}N(NO_3)O_8^-$	401.08
$C_{12}H_{20}(NO_3)O_{11}^-$	402.09
$C_{10}H_{15}N(NO_3)O_{12}^-$	403.05
$C_{15}H_{18}(NO_3)O_9^-$	404.08
$C_{18}H_{17}N(NO_3)O_6^-$	405.09
$C_{19}H_{23}N(NO_3)O_5^-$	407.15
$C_{19}H_{22}(NO_3)O_6^-$	408.13