Supplement of Atmos. Chem. Phys., 20, 4193–4207, 2020
https://doi.org/10.5194/acp-20-4193-2020-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

Shipborne measurements of Antarctic submicron organic aerosols: an NMR perspective linking multiple sources and bioregions

Stefano Decesari et al.

Correspondence to: Stefano Decesari (s.decesari@isac.cnr.it)

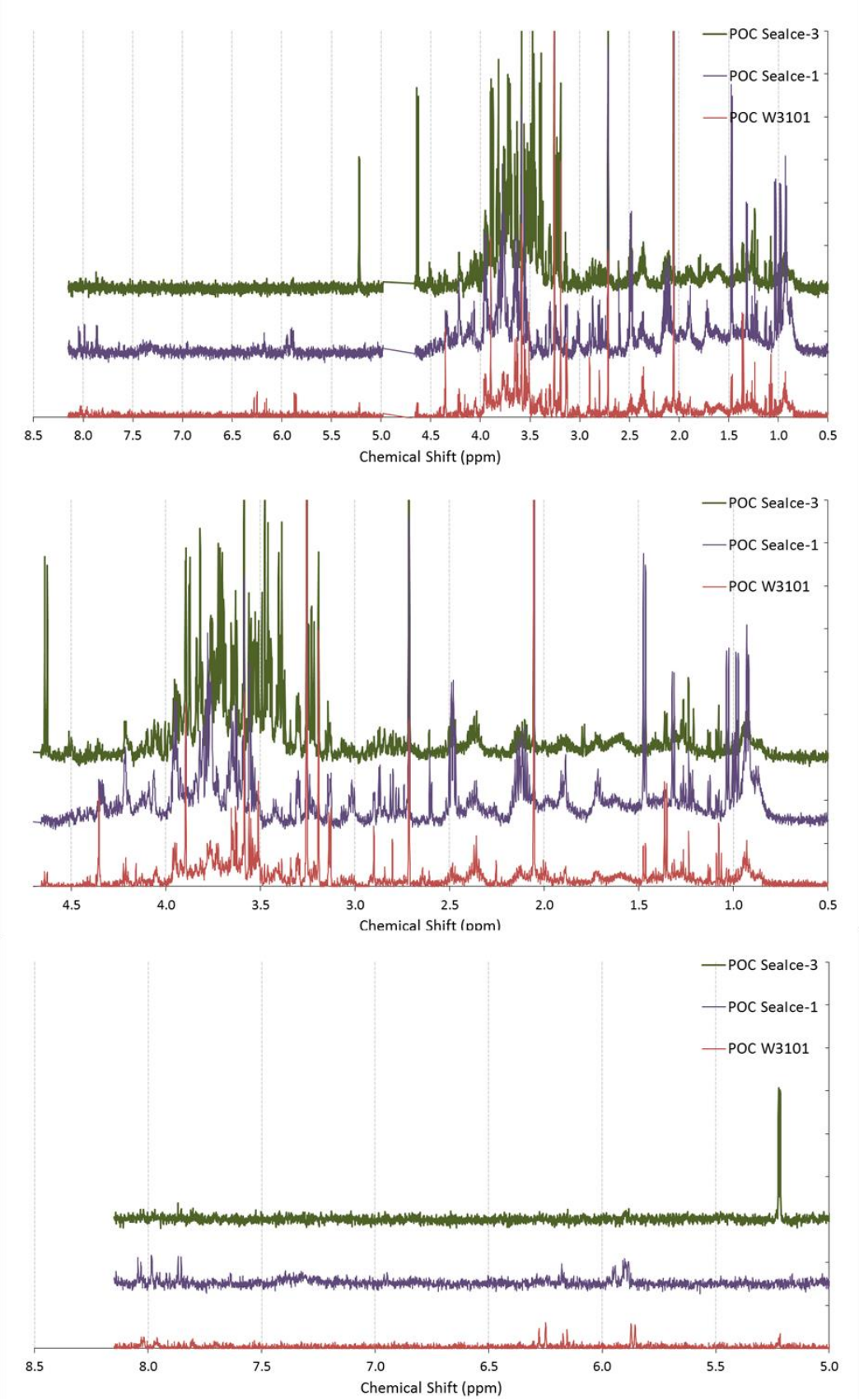

Figure S1. ^{1}H NMR spectra of POC samples. The middle and bottom panels provide a focus on the aliphatic and aromatic regions of the spectra, respectively. The area between 4.7 and 5.0 ppm, containing the disturbance from the suppression of the HDO peak, was omitted from the figure.

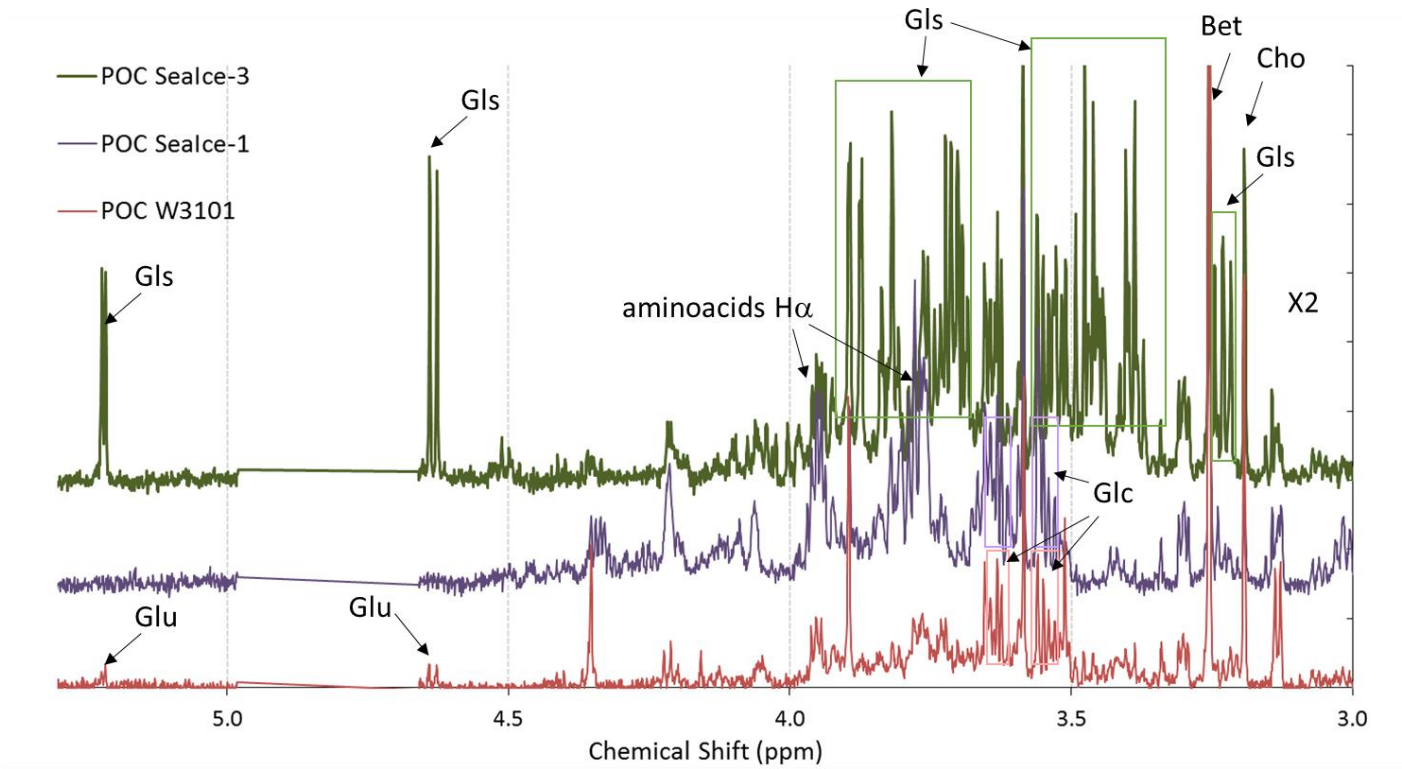

Figure S2. ^{1}H NMR spectra of POC samples. Focus on the region between 3.0 and 5.3 ppm. Specific NMR resonances were assigned to alpha hydrogen atoms of aminoacids, N-osmolytes (Bet: betaine; Cho: choline), glycerol (Glc) and to glucose (Gls).

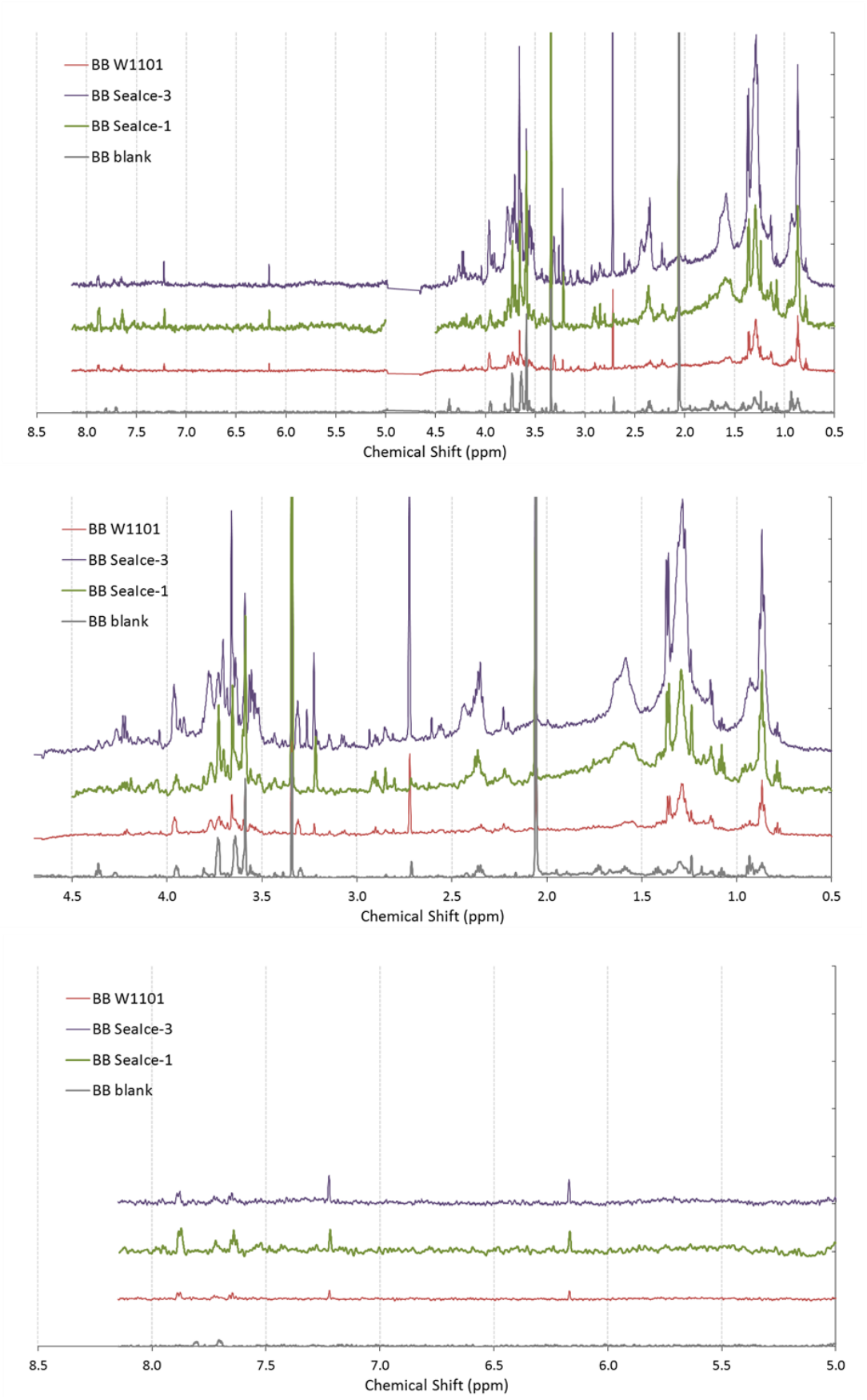

Figure S3. Same as Figure S1 but for the three samples of aerosolized seawater contrasted to the spectrum of a blank filter used in the tank filter holder.

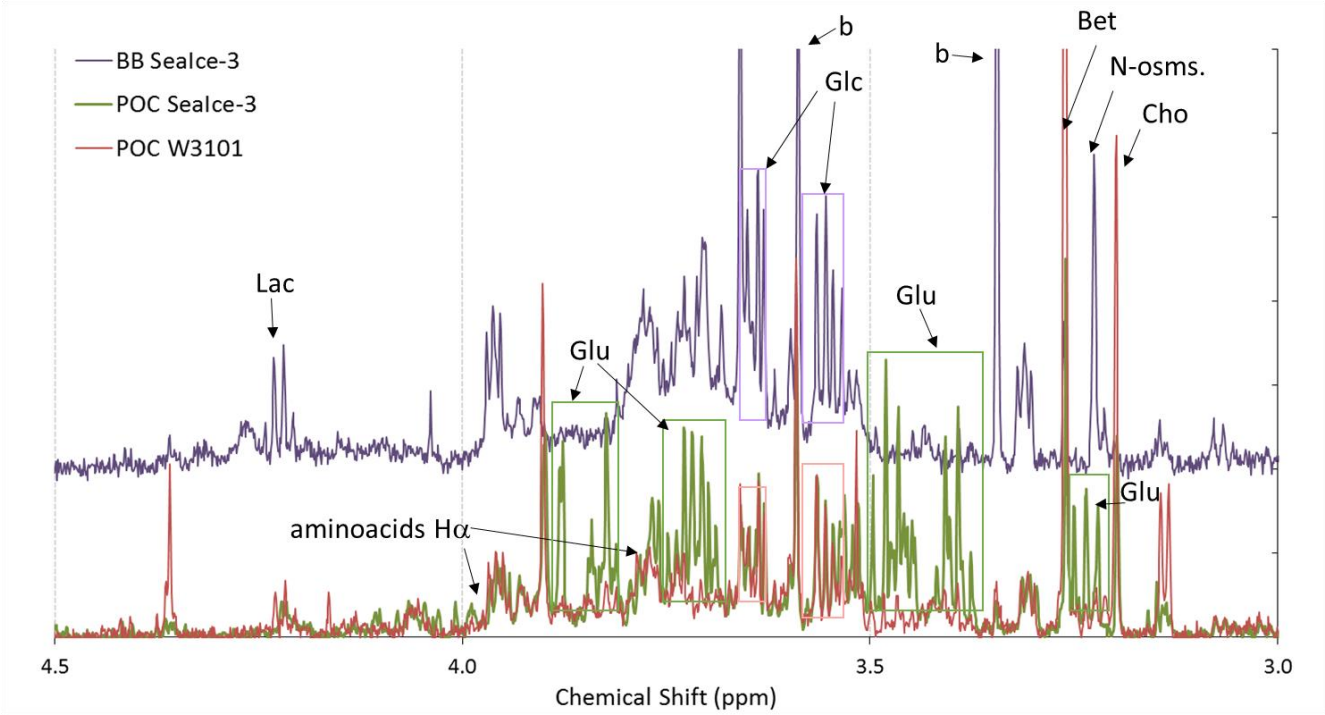

Figure S4. ^{1}H NMR spectra of the aerosolized sea ice sample #3 (BB SeaIce-3) (on top), with comparison with the spectra of POC in seawater (POC W3101) and in sea ice (POC SeaIce-1) (at the bottom): focus on the region between 3.0 and 4.5 ppm. Specific resonances were assigned to lactic acid (Lac), glycerol (Glc), N-osmolytes (Bet: betaine; "N-ozms": unidentified, possibly phosphocholine; Cho: choline) and to blank contaminations (b).

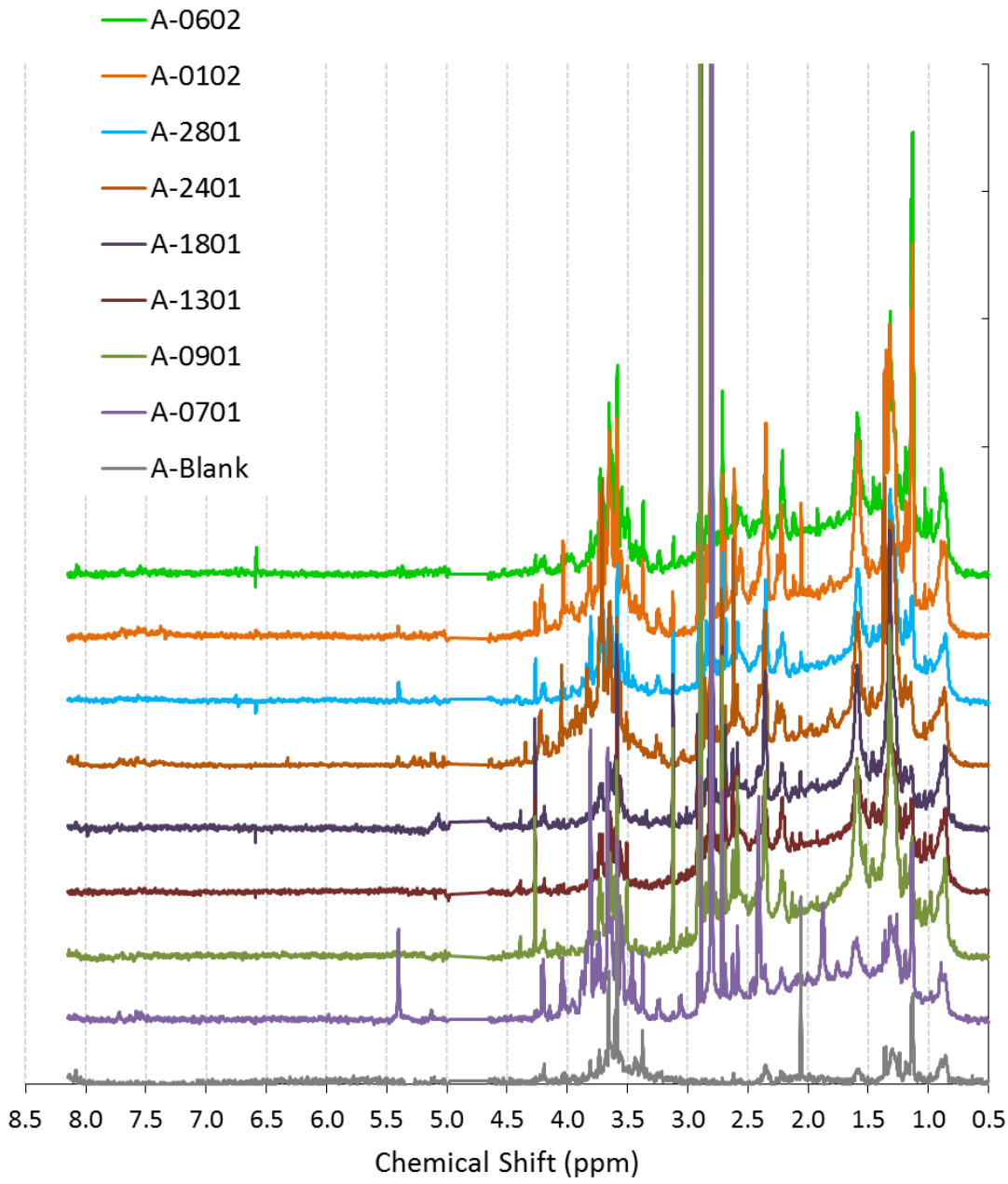

Figure S5. ^{1}H NMR spectra of the ambient PM1 WSOC aerosol samples. The area between 4.7 and 5.0 ppm, containing the disturbance from the suppression of the HDO peak, was omitted from the figure.

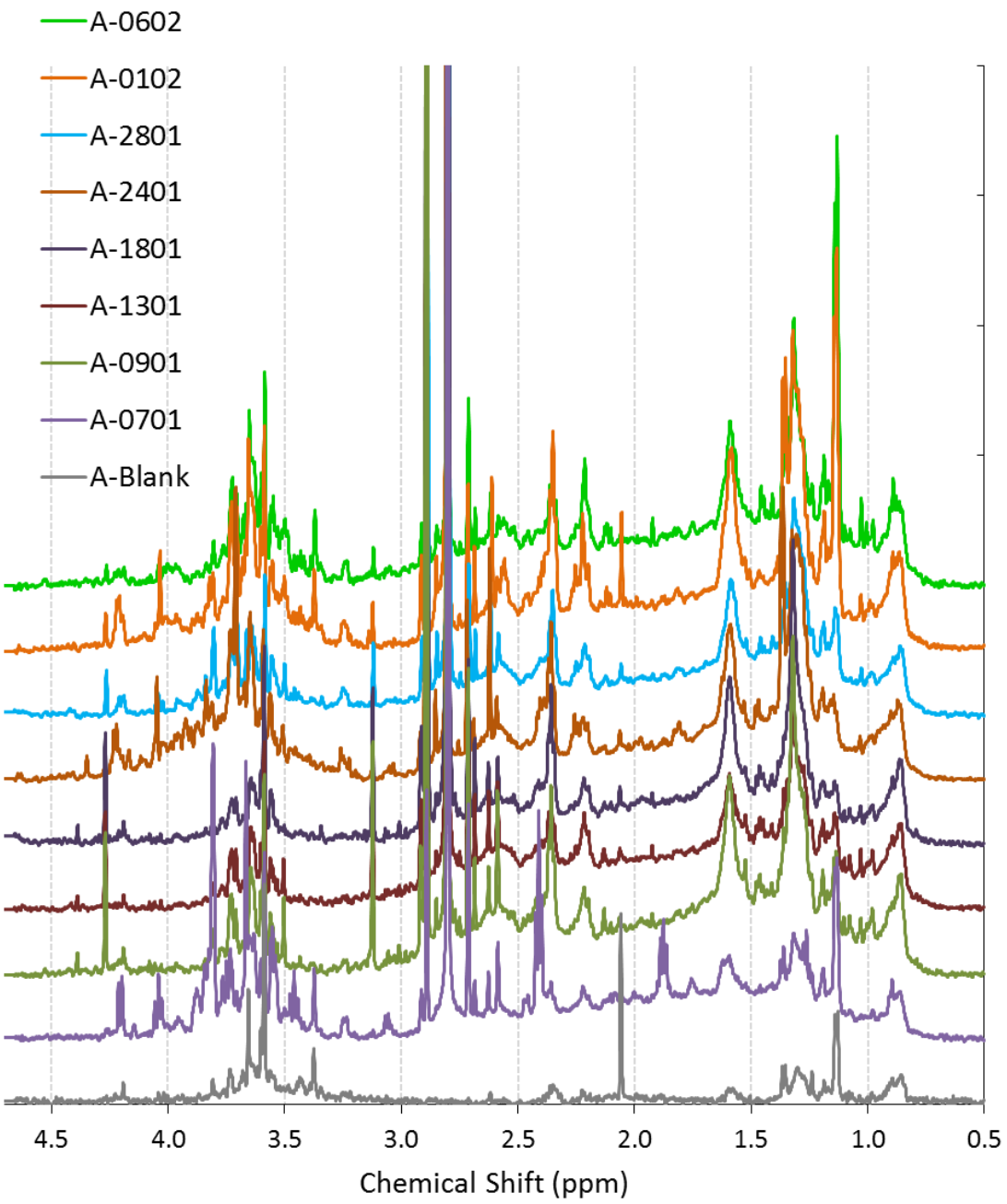

Figure S6. ^{1}H NMR spectra of the ambient PM1 WSOC aerosol samples: focus on the aliphatic region.

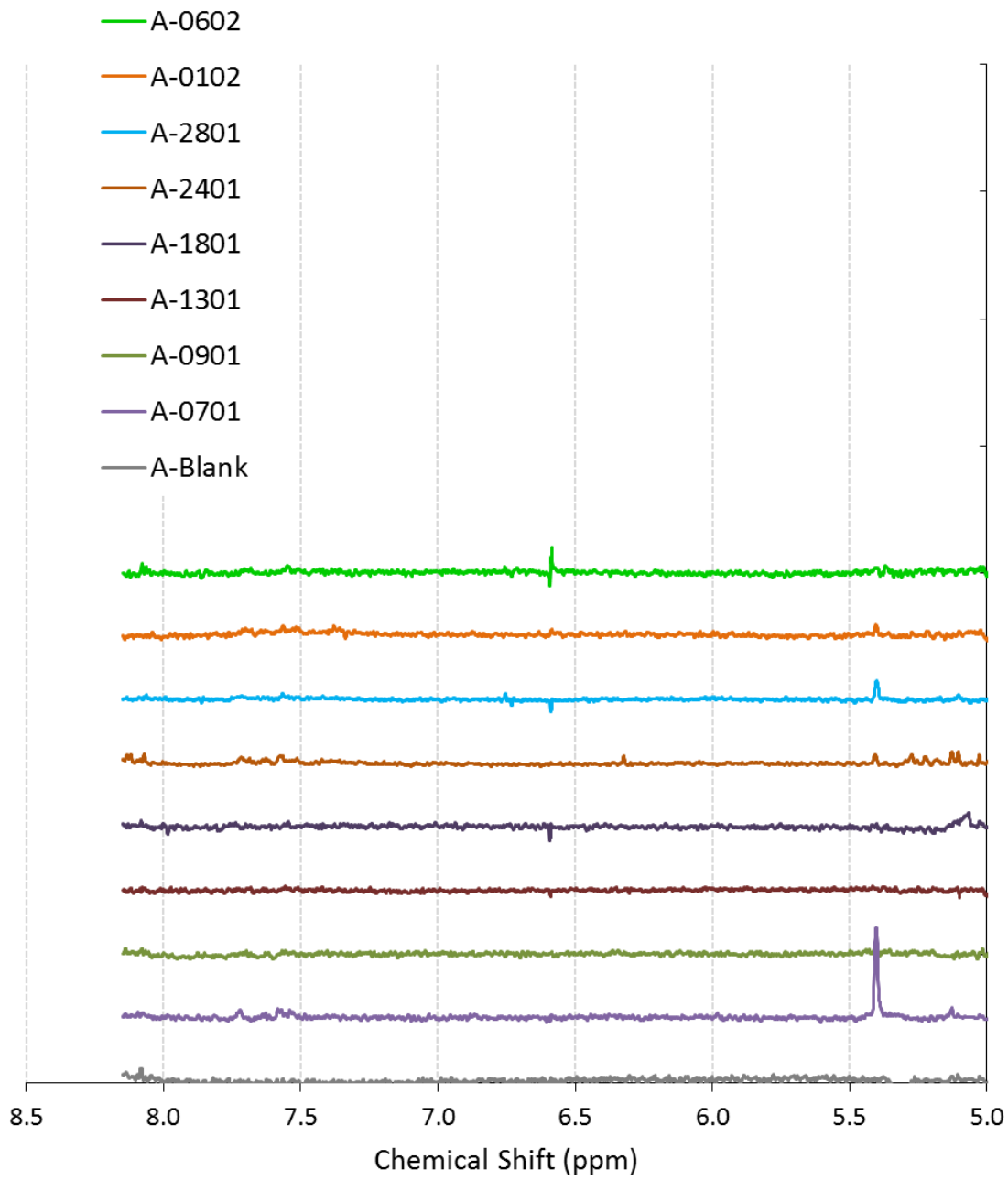

Figure S7. ^{1}H NMR spectra of the ambient PM1 WSOC aerosol samples: focus on the aromatic region.

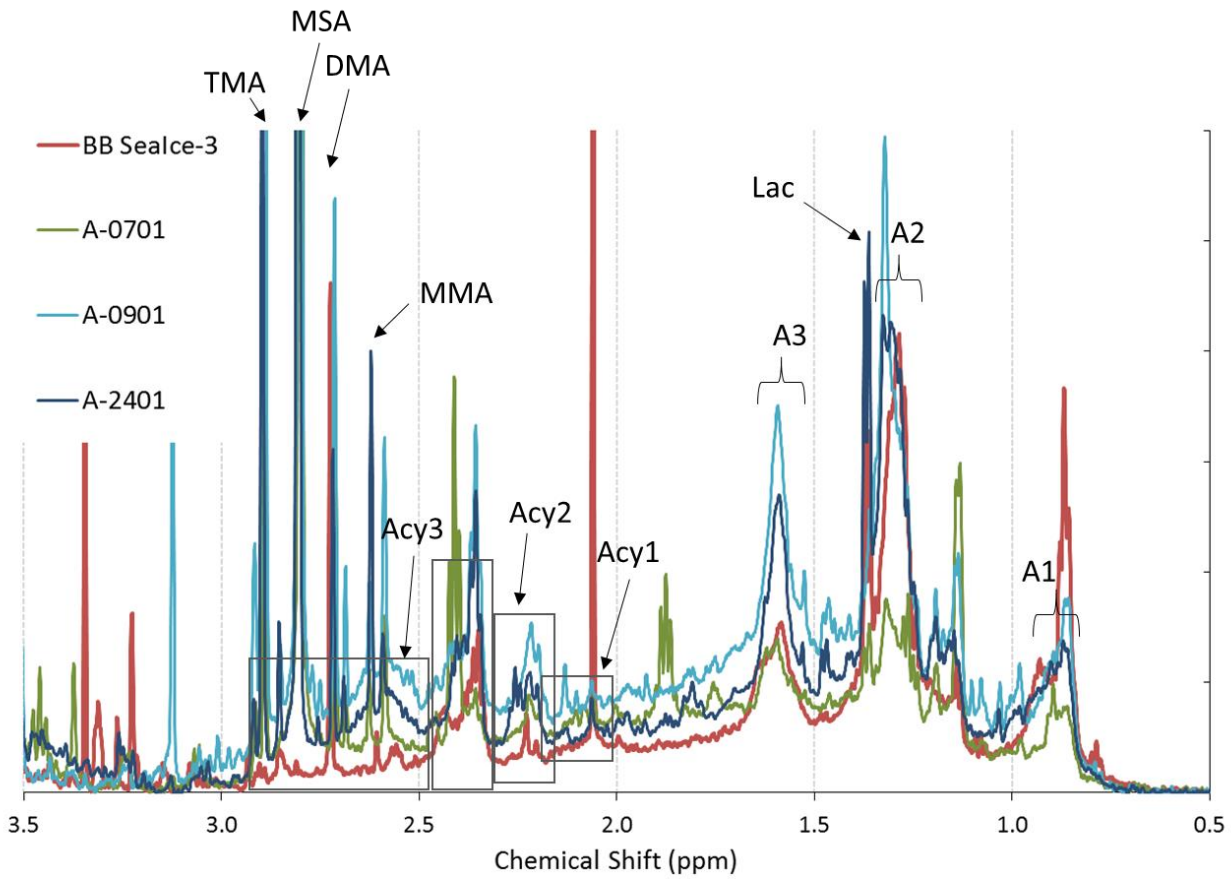

Figure S8. ^{1}H NMR spectra of one bubble bursting sample (BB SeaIce-3) and of three ambient PM1 WSOC aerosol samples (A-0701, A-0901, A-2401): focus on the region between 0.5 and 3.5 ppm of chemical shift. Specific spectral bands were assigned to lactic acid (Lac), monomethylamine (MMA), dimethylamine (DMA), trimethylamine (TMA), methanesulphonate (MSA), as well as to unresolved mixtures of compounds carrying linear alkylic structures (A1, A2, A3) and acyls (Acy1, Acy2, Acy3). Linear alkylic bands are split into resonances of terminal methyls (A1), methylenic chains (A2) and of methynes or methylenes in beta position to an ester/acid group (A3). A1, A2, A3 bands in the bubble bursting sample are attributed to lipids. The spectra of the ambient aerosol samples A-0901, A-2401 (showing abundant methylenic chains) are scaled to the spectrum of BB_SI3 based on the height of band A2. The spectrum of the ambient aerosol sample A-0701 is scaled to the spectrum of BB_SI3 based on the height of band A3. Acyl groups are split into acetate esters (Acy1), CH groups adjacent to a keto group (Acy2), CH groups adjacent to a carboxylic or ester group (Acy3), and acyls in multifunctionalized aliphatic structures (Acy3).

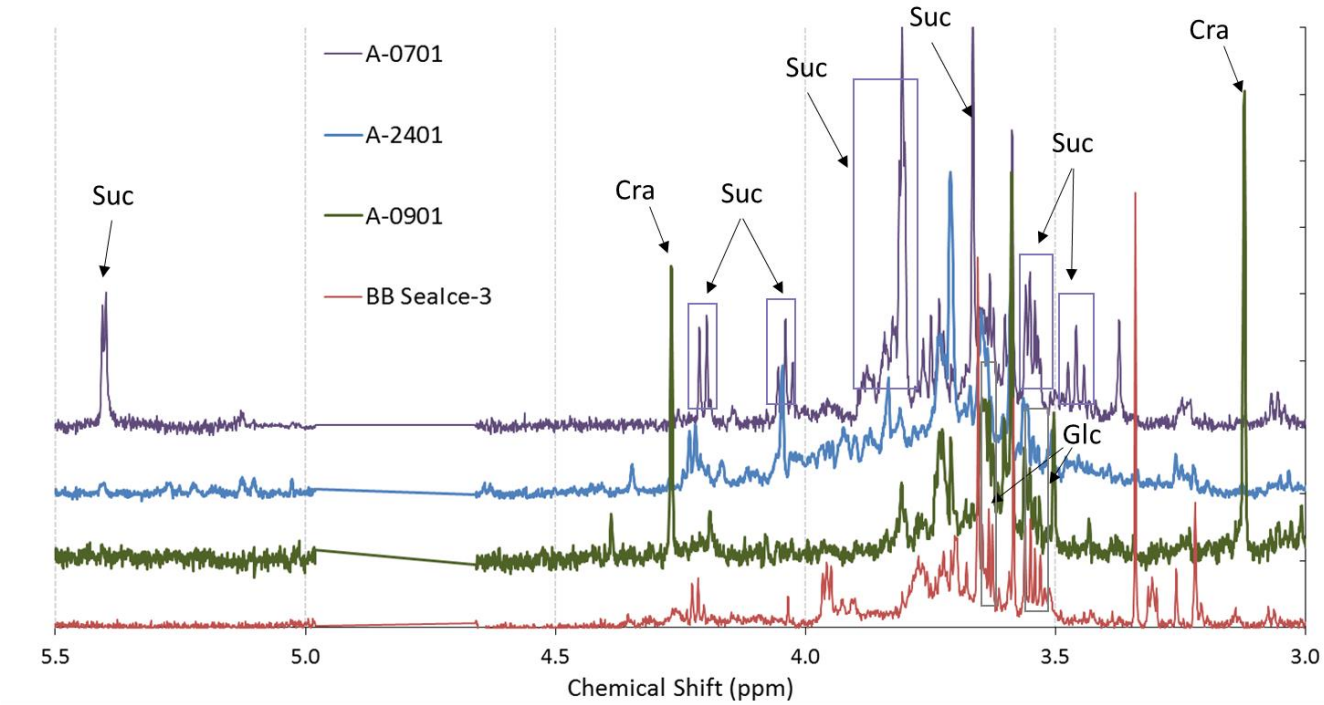

Figure S9: Same as Figure S8, but with a focus on the spectral region between 3.0 and 5.5 ppm. Resonances of sucrose (Suc), creatinine (Cra), glycerol (Glc) are highlighted.

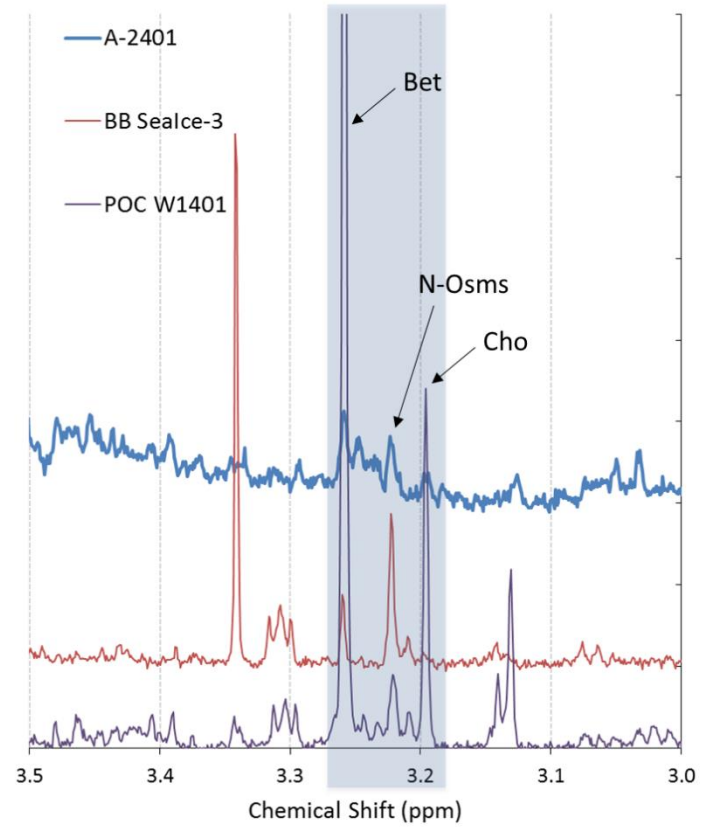

Figure S10: ^{1}H NMR spectra of on POC sample (POC W1401), one bubble bursting sample (BB Sealce-3) and of the ambient sample A-2401. Focus on the spectral region containing the resonances of small N-osmolytes (region highlighted): Bet: betaine; "N-Osms": unidentified, possibly phosphocholine; Cho: choline.

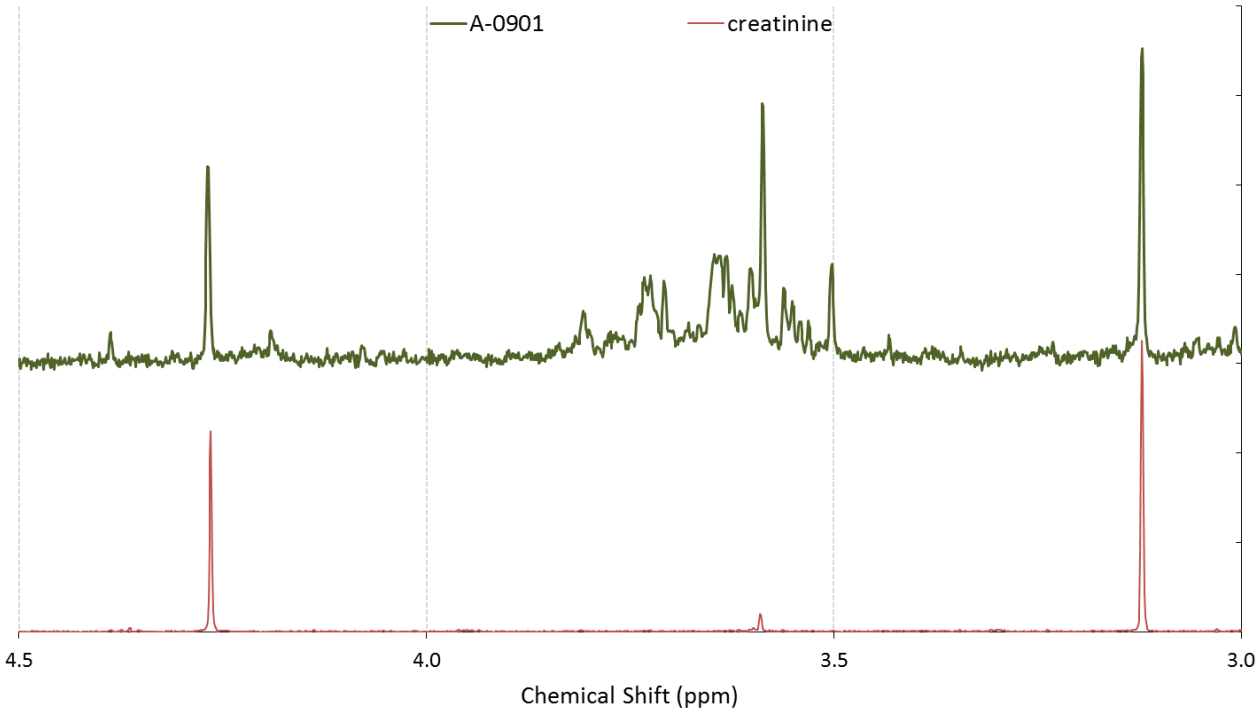

Figure S11: Comparison between the ^{1}H NMR spectra of an ambient sample from the Weddell Sea area (A-0901) and of a standard of creatinine (conc: 0.1 mM]).

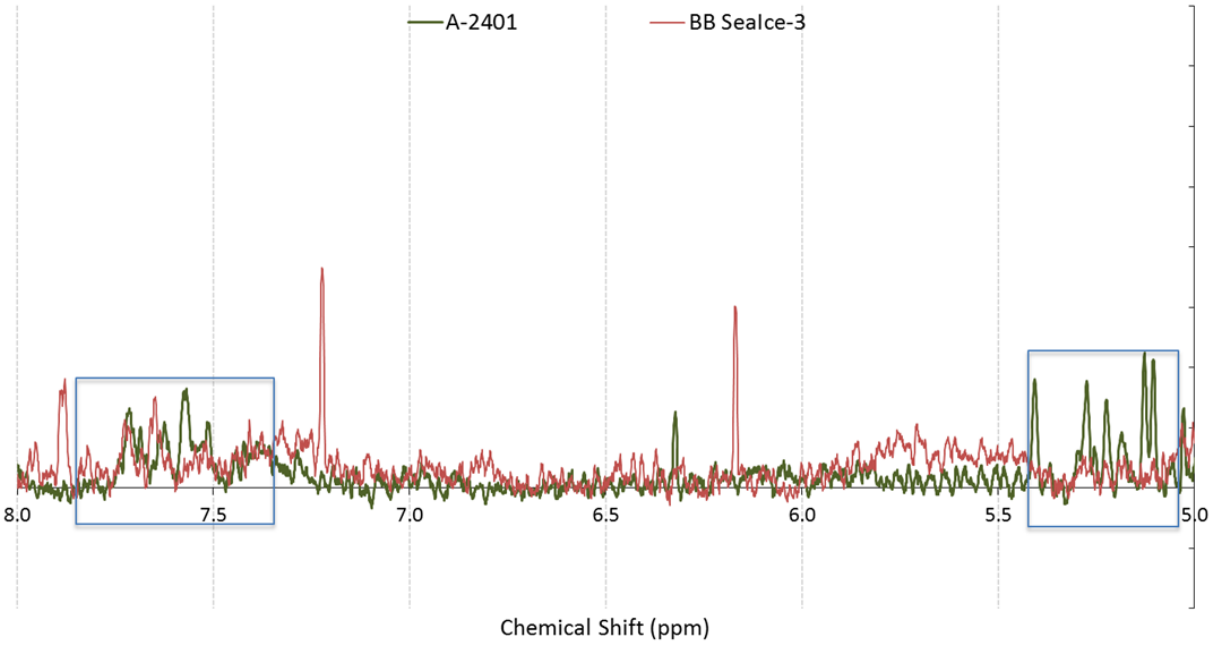

Figure S12: ^{1}H NMR spectra of one bubble bursting sample (BB_SI3) and of the ambient WSOC aerosol sample 240115: Focus on the aromatic region. The main areas of overlap are highlighted.

Table S1. UHPLC-HESI-HRMS creatinine quantification results

sample ID:	**0104**	**0106**	**0111D**	**0112N**	**0115N**	**0119N**	**0120N**	**0129D**
sampling times:	04 Jan 16:11 – 16:25	06 Jan 17:12 – 16:05	10 Jan 04:55 – 11 Jan 10:28	11 Jan 12:53 – 12 Jan 02:17	14 Jan 16:17 – 15 Jan 01:45	18 Jan 10:35 – 19 Jan 10:29	19 Jan 10:41 – 20 Jan 13:15	29 Jan 09:40 – 21:49
Creatinine* (ng/m^3)	0.030	0.018	0.044	0.009	0.052	0.012	0.033	0.036

*Based on a three-point calibration using neat creatinine in concentrations of 1.2, 12, and 120 ng/mL. Experimental conditions for the UHPLC-MS analysis are reported in Section 2.4.

Table S2. Creatinine calibration results by UHPLC-HESI-HRMS

Calibration std.	**Conc. (ng/mL)**	**Peak area (a.u.)**	**RT (min)**
1	1.2	6302965	0.33
2	12	56953602	0.33
3	120	440017098	0.33
Calib. Function*	(3.61E6±0.009E6)x	+(7.53E6±6.21E6)	
R^2	0.999		

*Linear least squares fit in MS Excel 2010.