



*Supplement of*

## **Effects of storage conditions on the molecular-level composition of organic aerosol particles**

**Julian Resch et al.**

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## S1 Sample collection and preparation

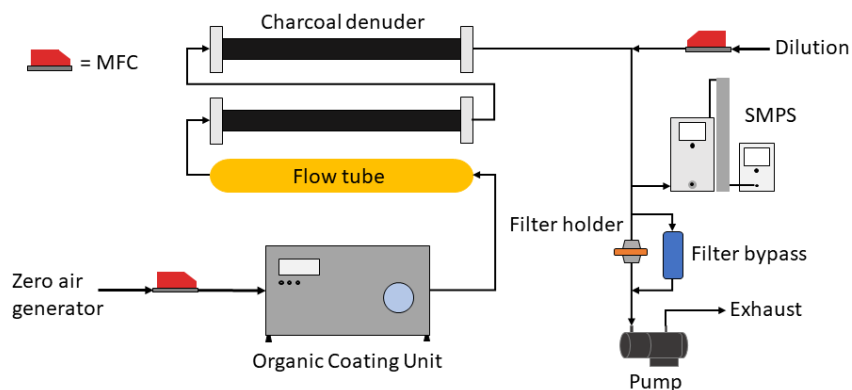


Figure S1: Setup used for the collection of laboratory-generated secondary organic aerosol samples.

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Table S1: Table of all SOA filters collected displaying the collection time for each filter, the sum of collected mass per filter quarter and the average SOA mass concentration in the OCU measured by the SMPS.

SOA sample	Filter number	Collection time [hh:mm:ss]	Sum of collected mass per filter quarter [ $\mu\text{g}$ ]	Average concentration in OCU/SMPS [ $\mu\text{g m}^{-3}$ ]
$\beta$ -pinene	Filter 1	00:30:41	319.9	6582.8
$\beta$ -pinene	Filter 2	00:30:36	315.5	6511.8
$\beta$ -pinene	Filter 3	00:30:43	313.7	6445.8
$\beta$ -pinene	Filter 4	00:30:44	315.8	6490.8
$\beta$ -pinene	Filter 5	00:30:40	311.6	6418.4
$\beta$ -pinene	Filter 6	00:30:37	314.4	6485.4
$\beta$ -pinene	Filter 7	00:30:40	317.3	6536.1
$\beta$ -pinene	Filter 8	00:28:59	304.3	6604.4
$\beta$ -pinene	Filter 9	00:30:41	309.9	6379.0
$\beta$ -pinene	Filter 10	00:30:44	312.0	6410.6

$\beta$ -pinene	Filter 11	00:30:42	310.9	6396.4
$\beta$ -pinene	Filter 12	00:30:41	319.8	6583.4
$\beta$ -pinene	Filter 13	00:30:44	318.4	6543.5
$\beta$ -pinene	Filter 14	00:30:39	315.7	6506.9
$\beta$ -pinene	Filter 15	00:30:36	315.0	6502.4
$\beta$ -pinene	Filter 16	00:34:05	303.7	5658.5
$\beta$ -pinene	Filter 17	00:34:07	291.3	5421.6
$\beta$ -pinene	Filter 18	00:29:02	256.6	5565.5
$\beta$ -pinene	Filter 19	00:34:05	299.7	5583.3
$\beta$ -pinene	Filter 20	00:34:11	301.3	5597.3
$\beta$ -pinene	Filter 21	00:34:02	291.7	5443.0
$\beta$ -pinene	Filter 22	00:34:13	288.4	5352.9
$\beta$ -pinene	Filter 23	00:34:05	302.6	5641.2
$\beta$ -pinene	Filter 24	00:34:01	299.2	5587.2
$\beta$ -pinene	Filter 25	00:34:14	303.5	5630.8
Naphthalene	Filter 1	00:42:37	306.0	4605.4
Naphthalene	Filter 2	00:39:10	306.9	5004.4
Naphthalene	Filter 3	00:39:16	309.8	5042.3
Naphthalene	Filter 4	00:39:35	309.6	4990.5
Naphthalene	Filter 5	00:42:39	299.3	4528.3
Naphthalene	Filter 6	00:34:12	288.5	5360.0
Naphthalene	Filter 7	00:34:10	296.5	5511.5
Naphthalene	Filter 8	00:37:30	306.7	5216.3
Naphthalene	Filter 9	00:34:07	292.4	5439.2
Naphthalene	Filter 10	00:37:30	310.6	5283.5
Naphthalene	Filter 11	00:41:14	293.2	4553.3
Naphthalene	Filter 12	00:42:50	304.9	4563.8
Naphthalene	Filter 13	00:37:37	297.0	5034.3

Naphthalene	Filter 14	00:37:40	309.0	5230.3
Naphthalene	Filter 15	00:37:40	300.5	5087.1
Naphthalene	Filter 16	00:46:04	334.0	4659.3
Naphthalene	Filter 17	00:37:30	338.8	5763.2
Naphthalene	Filter 18	00:37:34	298.0	5055.0
Naphthalene	Filter 19	00:37:26	297.9	5075.4
Naphthalene	Filter 20	00:37:26	302.0	5144.8
Naphthalene	Filter 21	00:39:08	315.3	5147.3
Naphthalene	Filter 22	00:37:27	290.1	4939.3
Naphthalene	Filter 23	00:39:07	308.9	5044.9
Naphthalene	Filter 24	00:37:35	311.3	5282.9
Naphthalene	Filter 25	00:37:31	304.1	5169.8

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**Table S2: List of all the samples analyzed and exact days between collection and analysis. Each condition was analyzed for samples stored at +20° C, -20° C and -80° C. \*Due to technical problems during the filter extraction for these samples they were excluded from the analysis.**

Sample	Immediately		24 hours		1 week		2 weeks		4 weeks	
	Extract [days]	Filter [days]	Extract [days]	Filter [days]	Extract [days]	Filter [days]	Extract [days]	Filter [days]	Extract [days]	Filter [days]
β-pinene-SOA	0		2	2	6	7	16	15	33	28
naphthalene-SOA	0		1	2	7	8	14	14	27	33
HVAS 1 11.-12.05.2022	0		2	1	7	7	/*	/*	44	44
HVAS 2 17.-18.05.2022	0		1	1	10	7	19	18	33	32
HVAS 3 25.-26.05.2022	0		1	1	10	9	20	19	28	29

HVAS 4 29.-30.05.2022	0	2	1	8	7	18	18	28	28
HVAS 5 30.-31.05.2022	0	2	2	8	8	18	18	28	28

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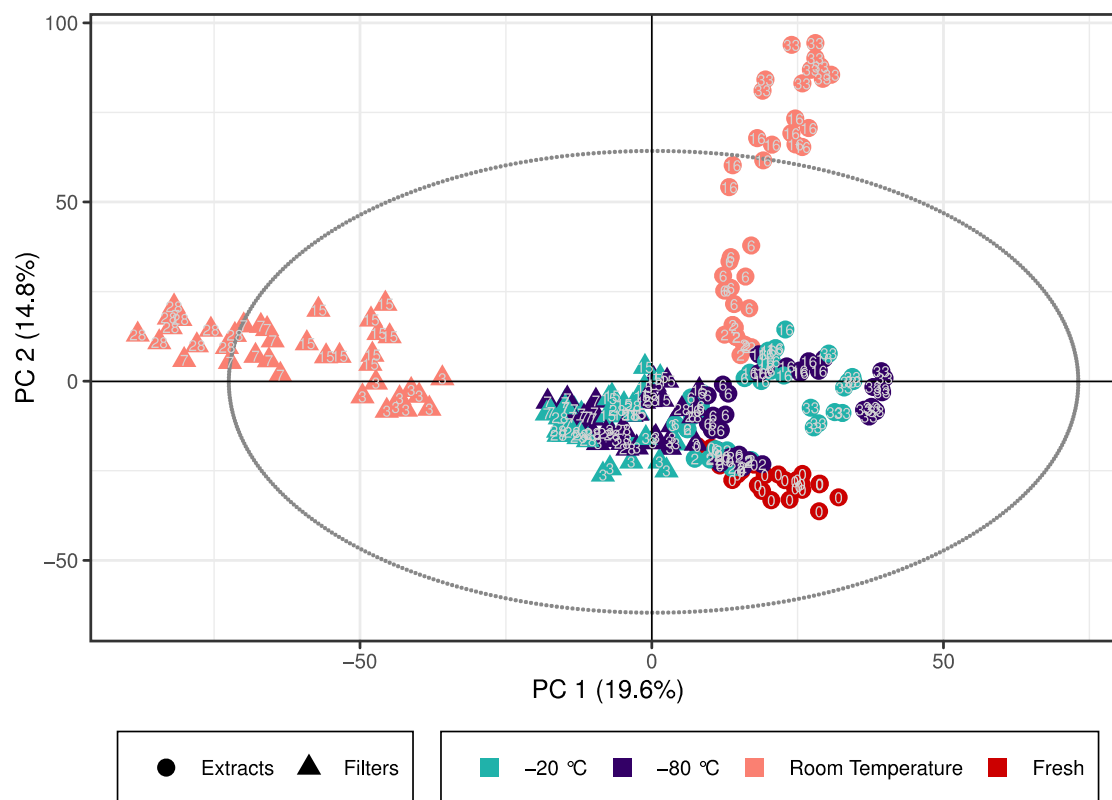
## S2 Preparation of standards used for calibration

Stock solutions of 1 mg mL<sup>-1</sup> were prepared for each chemical. Cis-pinonic acid and 4-hydroxy benzoic acid were dissolved in the standard diluent (SD) of 1:10 ACN:H<sub>2</sub>O, pimelic acid and camphoric acid in a 1:10 mixture of Dimethyl Sulfoxide (DMSO):SD and 1,2-naphthoquinone in 1:5 DMSO:SD. The addition of DMSO was necessary to completely dissolve the standards in the mixture. The concentrations used are given in Table S3. Dilution (Dil) 1 was made up of 100 μL of each of the 5 standards used and 500 μL SD in order to have 1 mL total volume. The standards dilution series 1-4 were then run twice in the LC-MS in reversed order starting with the least concentrated. Peak area was obtained for each compound in the chromatogram and then averaged between the two runs and then used for comparison between different measurement days.

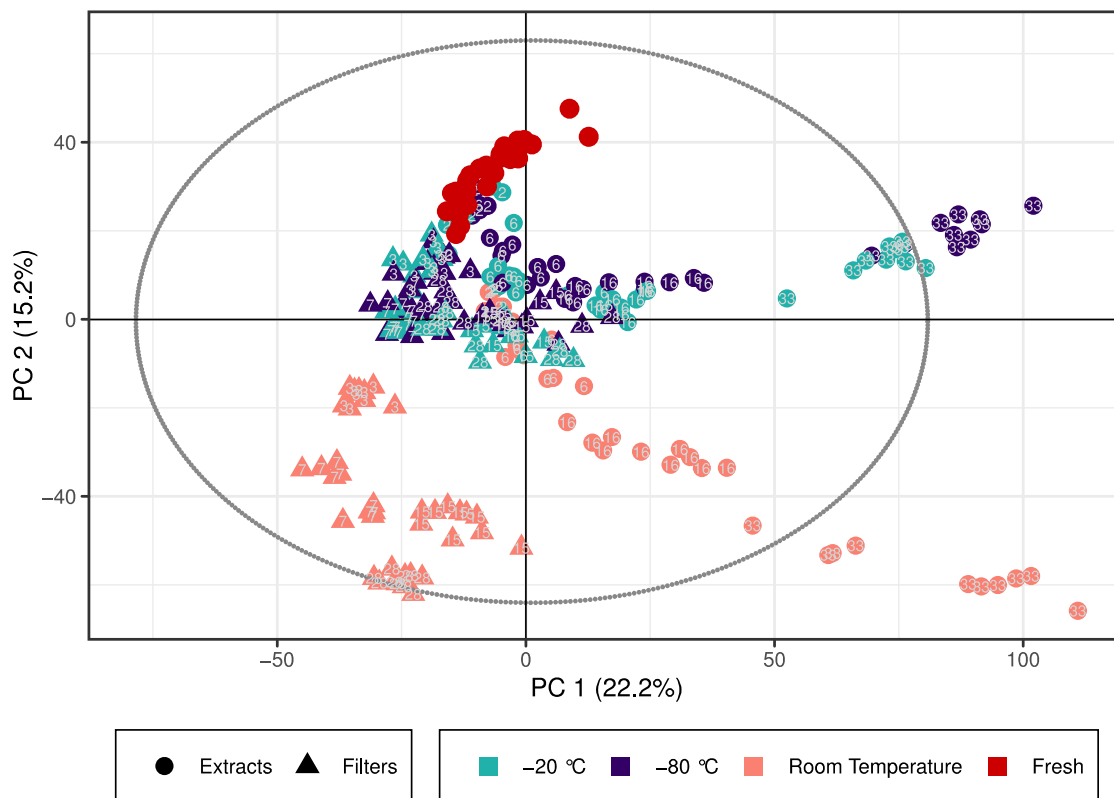
25 **Table S3: Concentration, mixture, solution and diluent of the standards used for calibration.**

Standard Dilution	Concentration [mg mL <sup>-1</sup> ]	Mixture	Solution [μL]	Standard Diluent [μL]
Stock 1	1			
Stock 2	0.1	1:10; stock 1:SD	100	900
Dil 1	0.01	1:10; stock 2:SD	5*100	500
Dil 2	0.001	1:10; dilution 1:SD	100	900
Dil 3	0.0001	1:10; dilution 2:SD	100	900
Dil 4	0.00001	1:10; dilution 3:SD	100	900

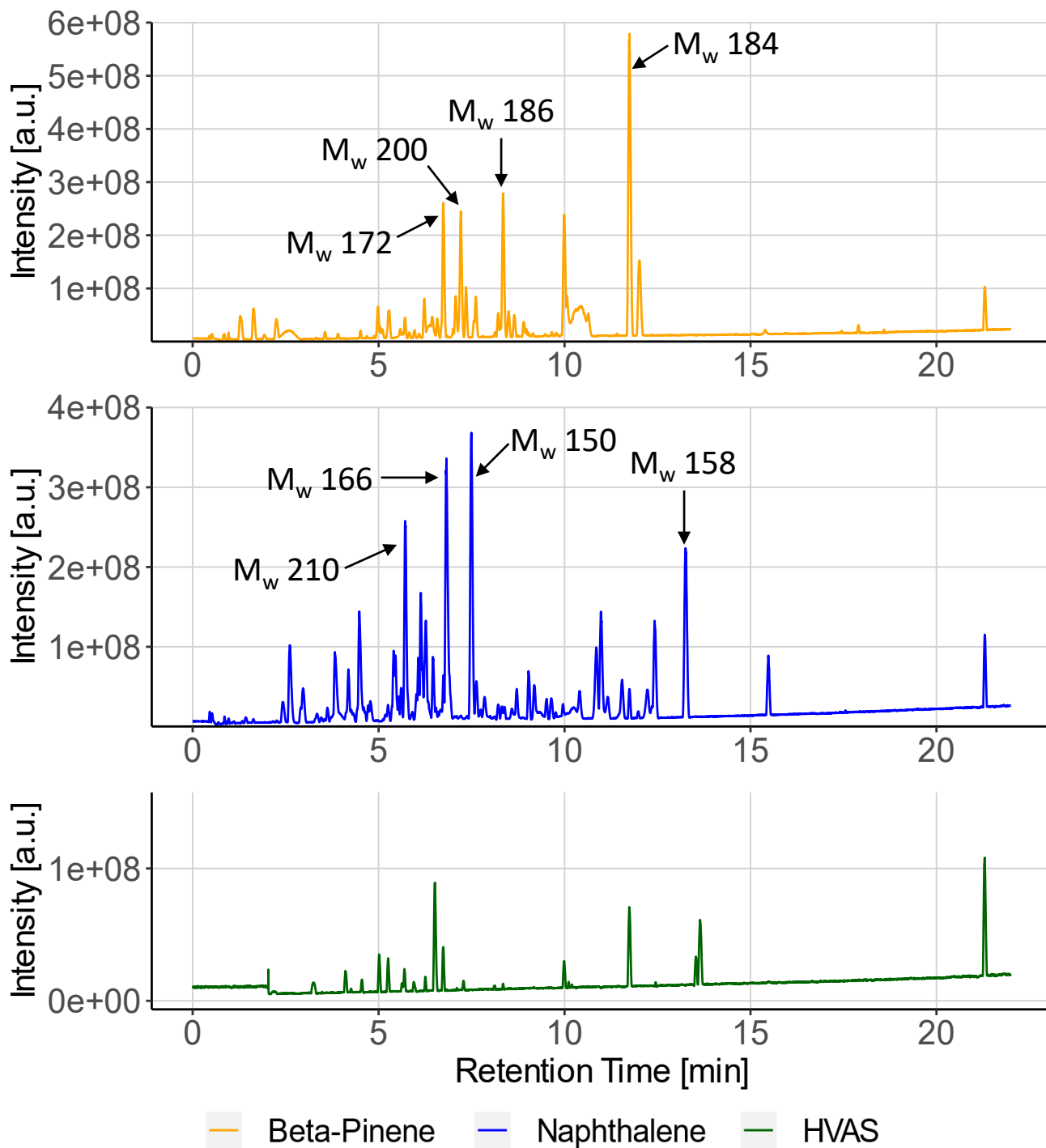
### S3 Results



30 **Figure S2:** Same PCA scores plot as shown in Fig. 1 but with the storage time [days] of each sample represented by the numbers inside the icons.



**Figure S3:  $\text{Log}_{10}(x)$  normalized PCA scores plot of the  $\beta$ -pinene SOA samples with the storage time [days] of each sample represented by the numbers inside the icons.**



35 Figure S4: Base peak chromatogram of the different immediately extracted aerosol samples in this study.



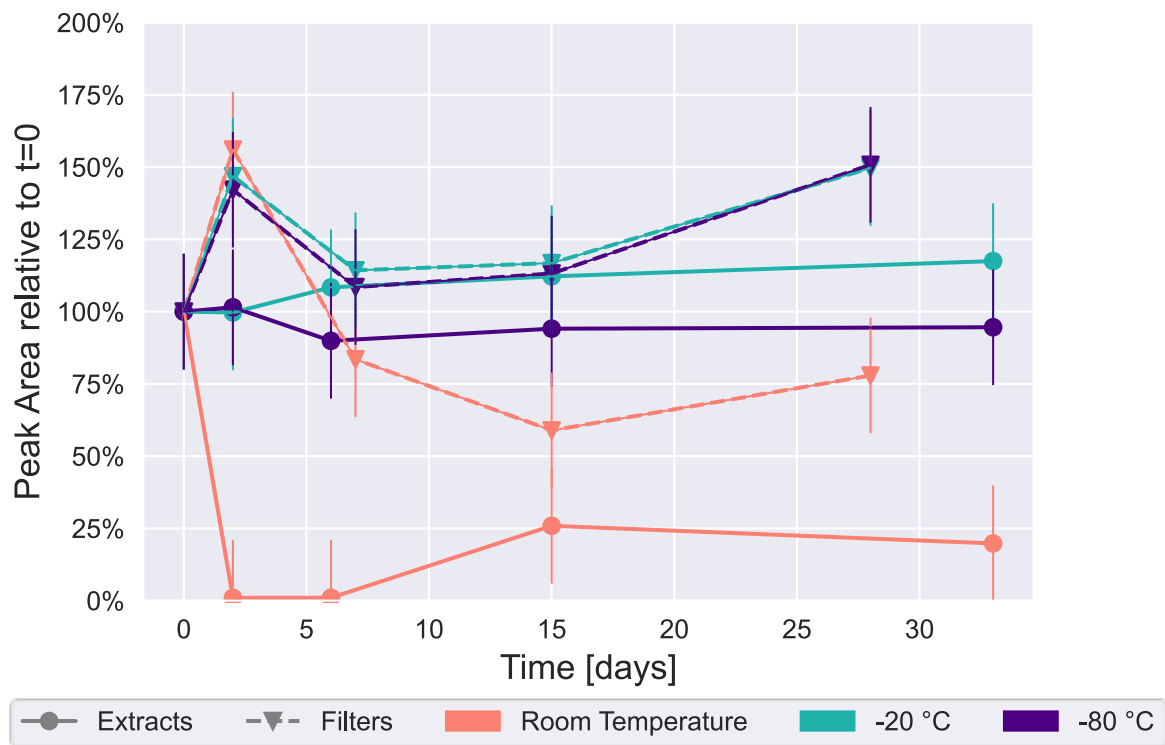
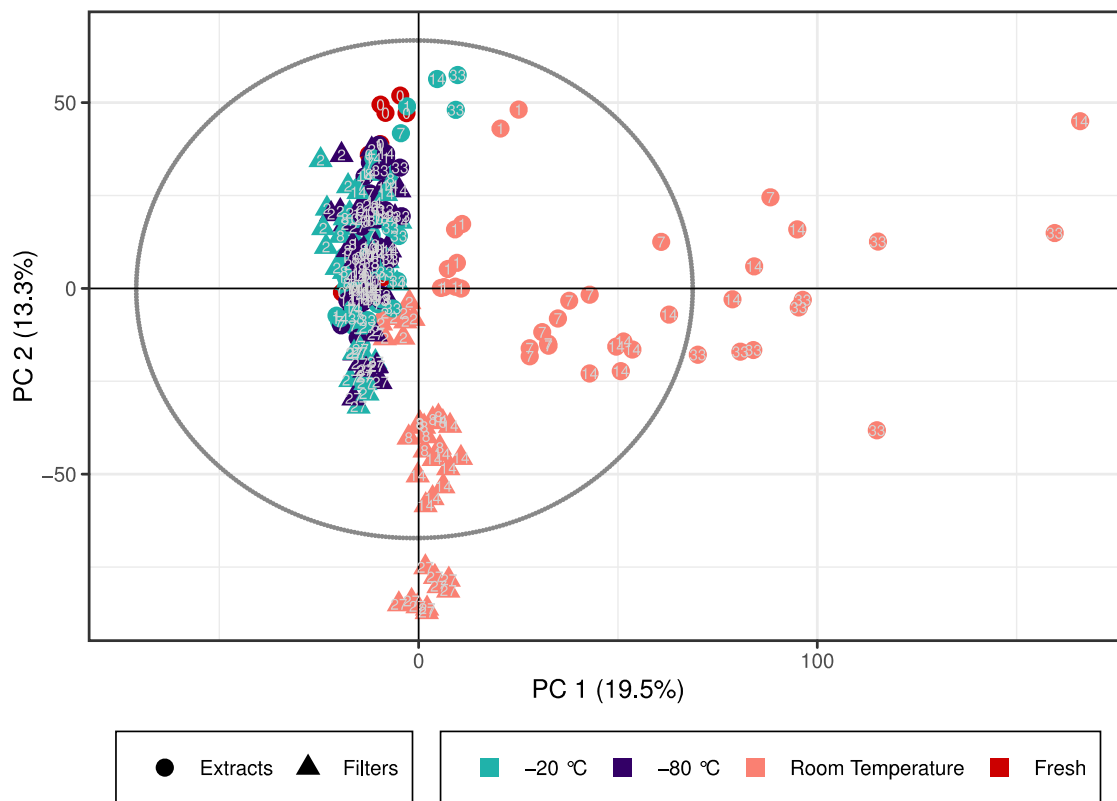
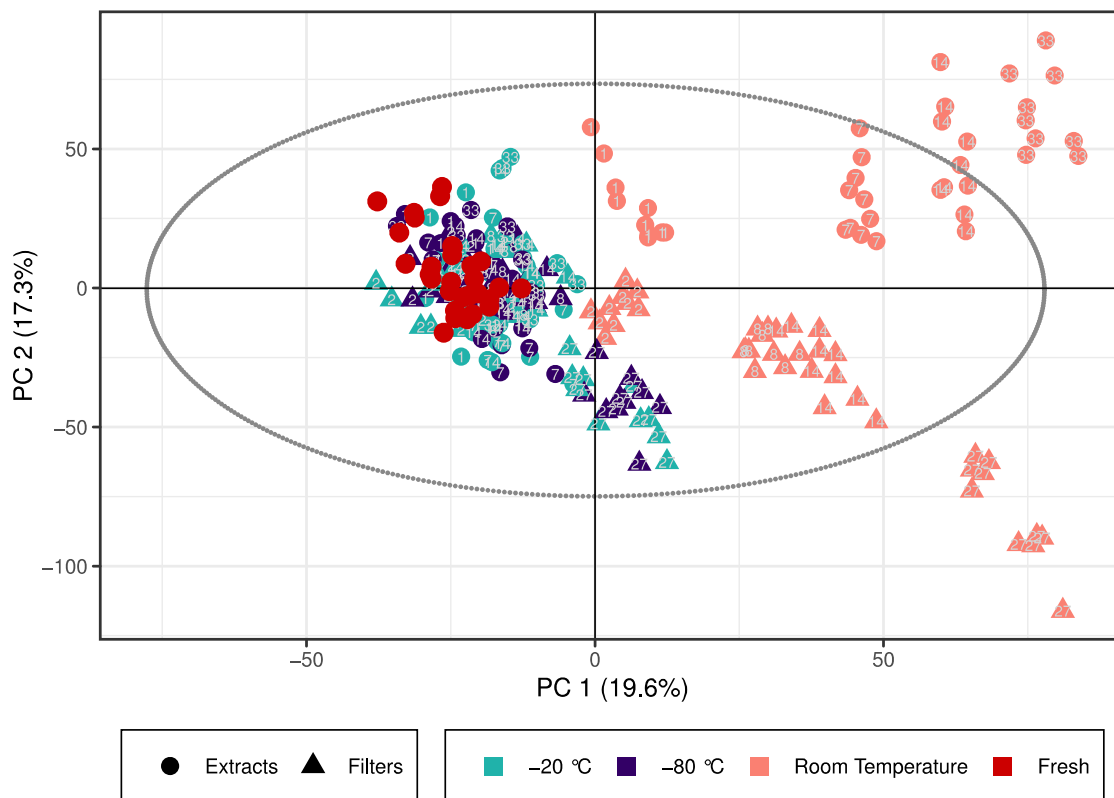


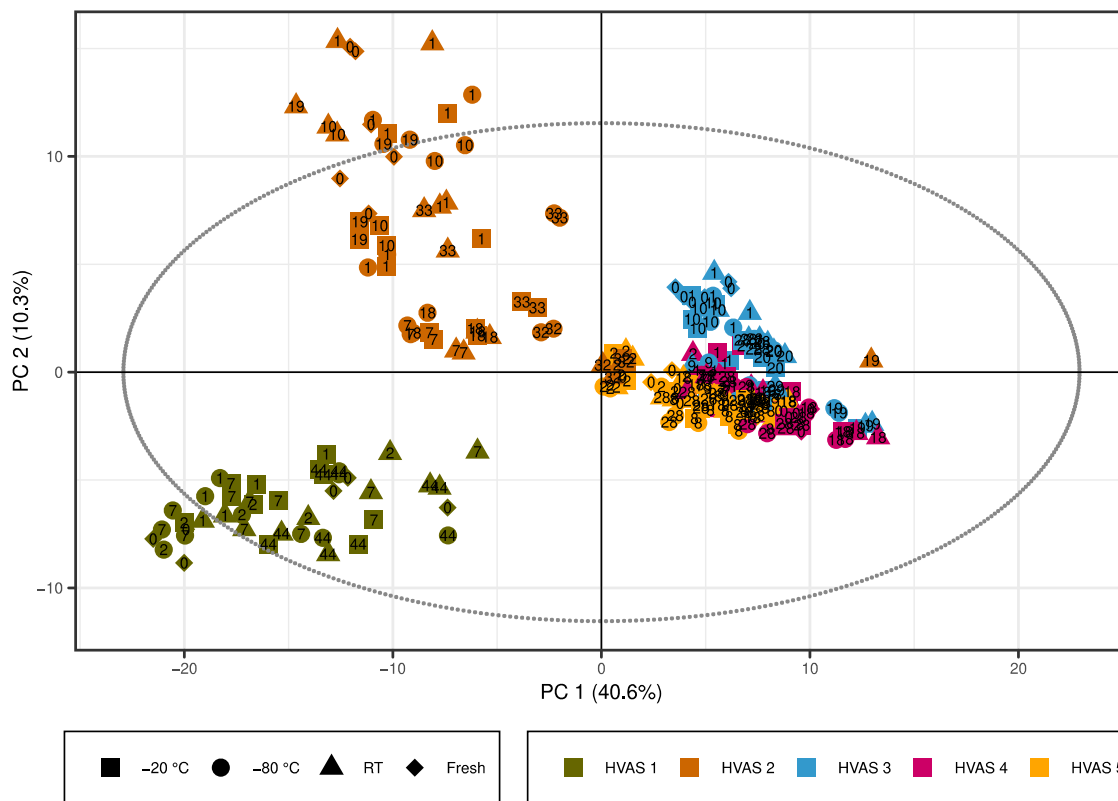
Figure S5: Time series of the  $M_w$  388 ( $m/z$  387.1659,  $C_{18}H_{28}O_9$ ) compound detected at 18.59 min in  $\beta$ -pinene SOA.



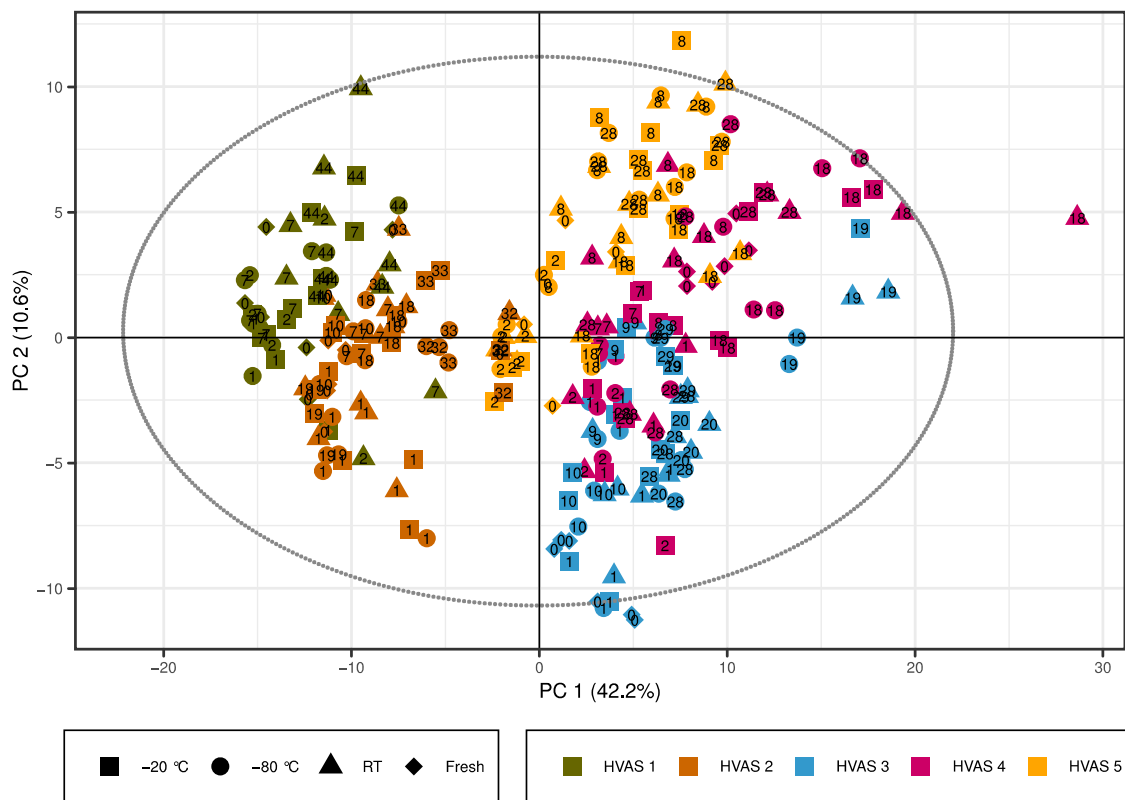
40 **Figure S6:** Same PCA scores plot as shown in Fig. 3, but with storage time [days] of each sample represented by the numbers inside the icons.



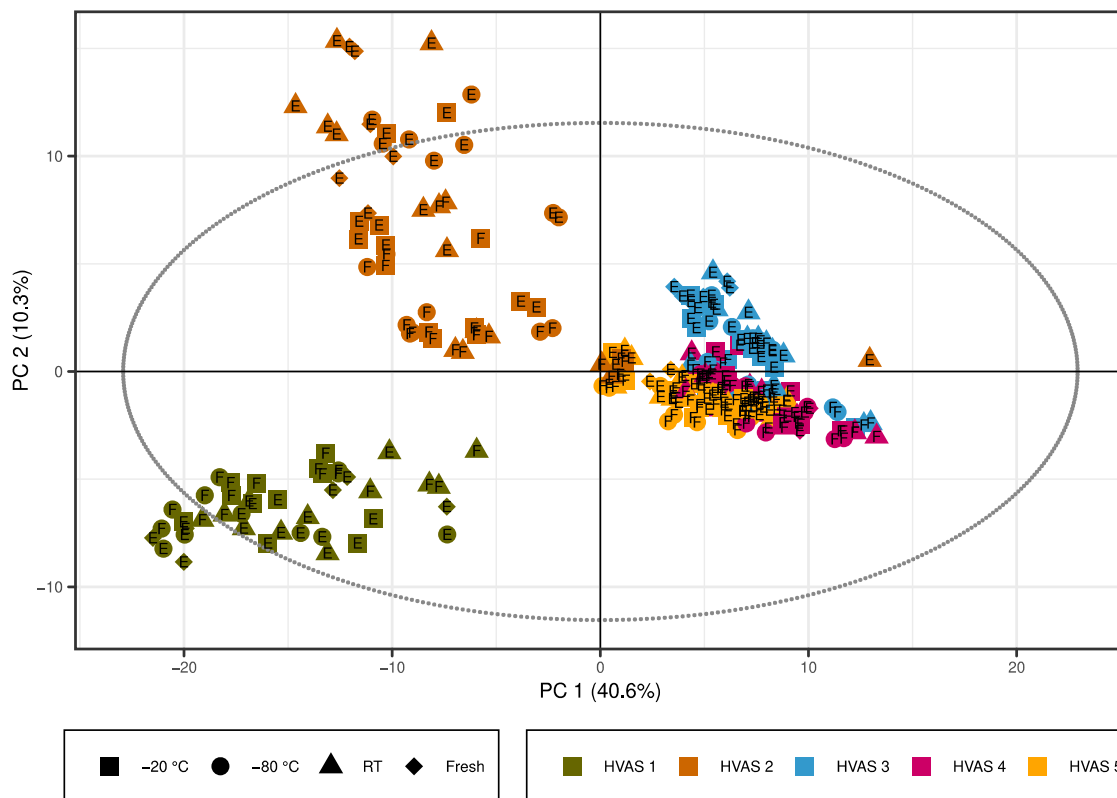
**Figure S7:  $\text{Log}_{10}(x)$  normalized PCA scores plot of the naphthalene SOA samples with the storage time [days] of each sample represented by the numbers inside the icons.**



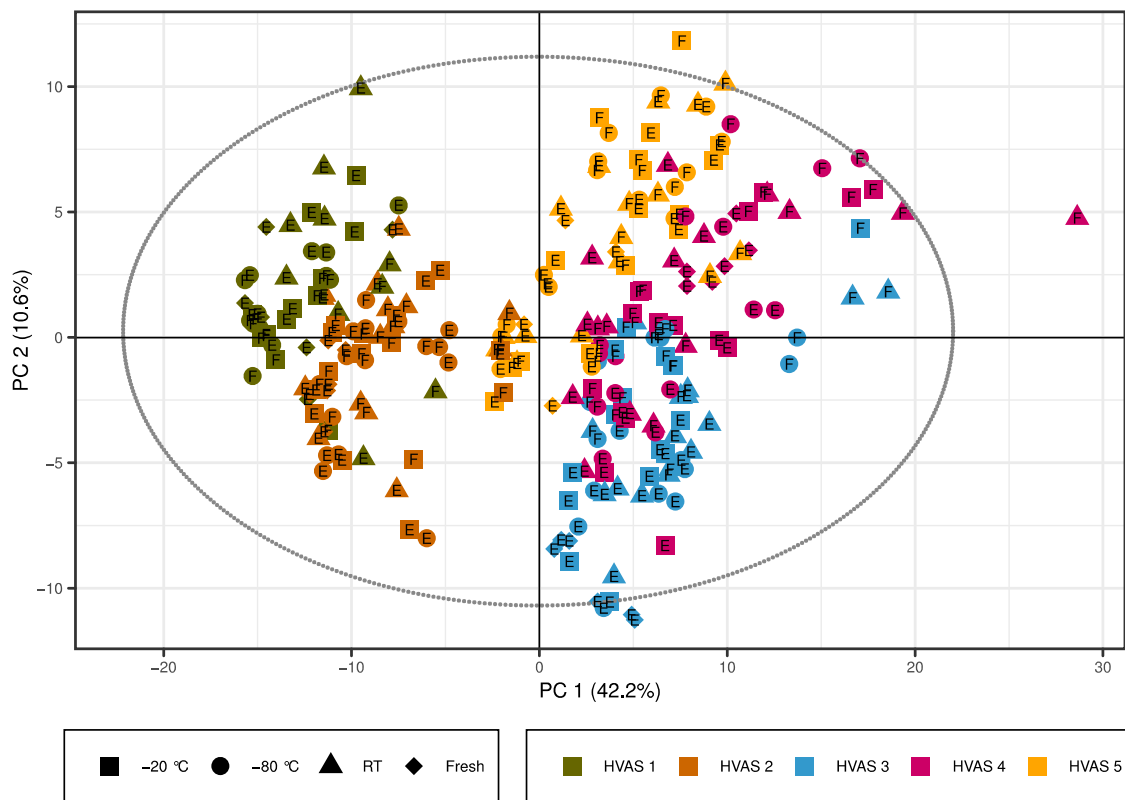
45 **Figure S8: Corrected PCA scores plots of all ambient samples and storage times [days] given as the numbers inside the icons.**



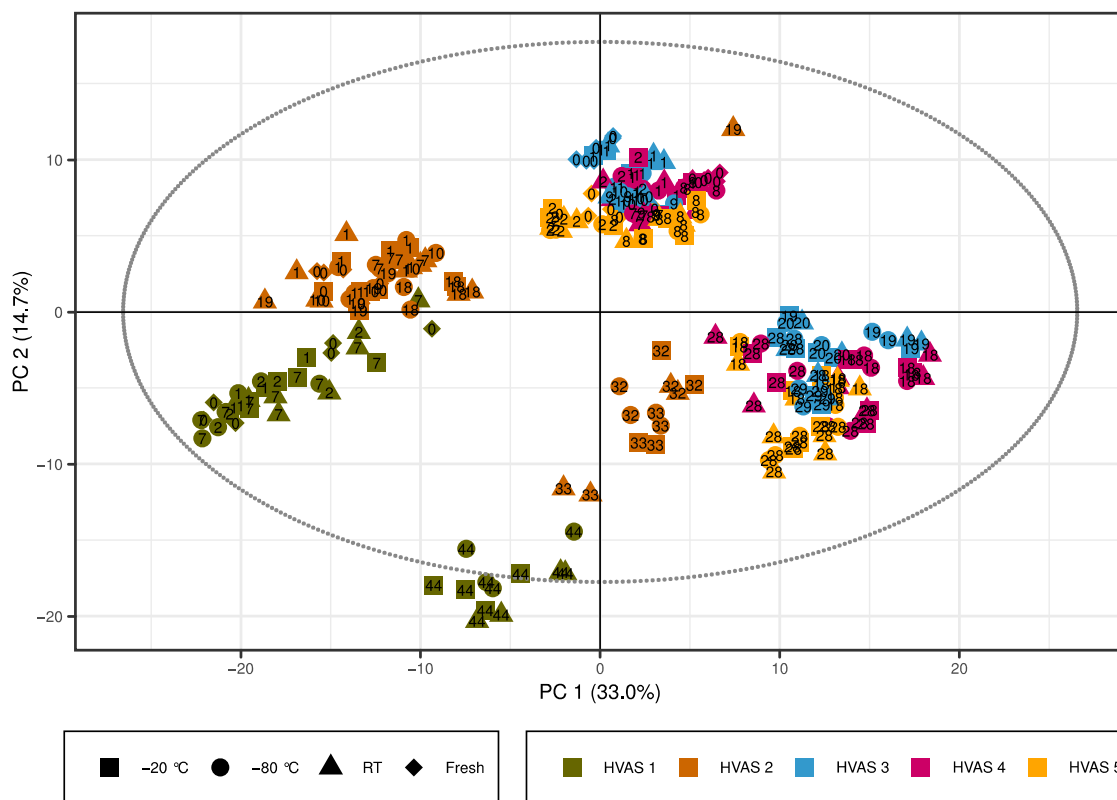
**Figure S9:  $\text{Log}_{10}(x)$  normalized PCA scores plot of the corrected ambient samples with the storage time [days] of each sample represented by the numbers inside the icons.**



50 **Figure S10: Corrected PCA scores plots of all ambient samples and the storage type given as labels inside the icons (E=Extracts and F=Filters).**



**Figure S11:  $\text{Log}_{10}(x)$  normalized PCA scores plot of the corrected ambient samples and the storage type given as labels inside the icons (E=Extract and F=Filter).**



**Figure S12: Non-corrected PCA scores plot of all ambient samples with storage time [days] given as numbers in the icons. A clear batch effect can be seen between samples which were analyzed before (top left) and after (bottom right) the switch of water as mobile phase A.**