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Supplemental Material

Effect of Atmospheric Aging on Soot Particle Toxicity in Lung Cell Models at the Air–Liquid Interface: Differential Toxicological Impacts of Biogenic and Anthropogenic Secondary Organic Aerosols (SOAs)

Svenja Offer, Elena Hartner, Sebastiano Di Bucchianico, Christoph Bisig, Stefanie Bauer, Jana Pantzke, Elias J. Zimmermann, Xin Cao, Stefanie Binder, Evelyn Kuhn, Anja Huber, Seongho Jeong, Uwe Käfer, Patrick Martens, Arunas Meseriacovas, Jan Bendl, Ramona Brejcha, Angela Buchholz, Daniella Gat, Thorsten Hohaus, Narges Rastak, Gert Jakobi, Markus Kalberer, Tamara Kanashova, Yue Hu, Christoph Ogris, Annalisa Marsico, Fabian Theis, Michal Pardo, Thomas Gröger, Sebastian Öder, Jürgen Orasche, Andreas Paul, Till Ziehm, Zhi-Hui Zhang, Thomas Adam, Olli Sippula, Martin Sklorz, Jürgen Schnelle-Kreis, Hendryk Czech, Astrid Kiendler-Scharr, Yinon Rudich, and Ralf Zimmermann

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Figure S1. Stability of β -pinene and naphthalene aging, respectively over 4 h exposure time measured with different methods and on different days (A) organic content measured by AMS (B) black carbon (BC) measured by Aethalometer (C) d9-butanol measured by PTR-MS (D) ozone measured by an ozone monitor (E) PN and (F) size distribution measured by SMPS. (A-E) Results are shown of one representative exposure with either SOA β PIN-SP, SOA β NAP-SP or with SP (E-F), respectively. All exposures were conducted on different days. Corresponding numeric data are found in Excel Tables S1-S6, respectively. Note: SOA β NAP-SP/SOA β PIN-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with either naphthalene or β -pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor, SP; pure SP (CAST soot; 1 mg m⁻³) were fed into the potential aerosol mass reactor without aging; AMS, high-resolution time-of-flight aerosol mass spectrometer; PTR-MS, quadrupole proton-transfer reaction mass spectrometer; SMPS, scanning mobility particle sizer.

Figure S2. TEM micrographs of SP, SOA β NAP-SP and SOA β PIN-SP. Representative TEM micrographs of 1 mg m⁻³ SP (A), photochemically-aged SP (1 mg m⁻³) coated by naphthalene (4 mg m⁻³, SOA β NAP-SP) (B) and β -pinene (4 mg m⁻³, SOA β PIN-SP) (C) aging products, scale bar 200 nm. Note: TEM, Transmission electron microscopy; SP; pure SP (CAST soot; 1 mg m⁻³) were fed into the potential aerosol mass reactor without aging; SOA β NAP-SP/SOA β PIN-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with either naphthalene or β -pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor.

Figure S3. GC \times GC-TOFMS contour plots for SOA β PIN-SP (A) and SOA β NAP-SP (B). Note: GC \times GC-TOFMS, comprehensive two-dimensional gas chromatography - time-of-flight mass spectrometer; SOA β NAP-SP/SOA β PIN-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with either naphthalene or β -pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor.

Figure S4. Relative cumulative abundance of the 100 peaks with the highest intensities in GC \times GC-TOFMS (ranked from compounds with highest to lowest areas). Compounds were identified via NIST mass spectral library match and retention indices for (A) SOA β NAP-SP and (B) SOA β PIN-SP. Processing was done with a minimum peak S/N of 1000. Compounds marked in red were detected in both aerosol types. The numeric data corresponding to this figure is shown in the column cumulative abundance [%] of Table S1 for SOA β NAP-SP and of Table S2 for SOA β PIN-SP. Note: SOA β NAP-SP/SOA β PIN-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with either naphthalene or β -pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor; GC \times GC-TOFMS, comprehensive two-dimensional gas chromatography - time-of-flight mass spectrometer.

Figure S5. Diagram of the relative AMS intensity fraction of m/z 43 vs m/z 44 (f_{44} vs. f_{43}) for $\text{SOA}_{\beta\text{PIN}}\text{-SP}$ and $\text{SOA}_{\text{NAP}}\text{-SP}$. Corresponding numeric data are shown in Table S5. Note: AMS, high-resolution time-of-flight aerosol mass spectrometer; $\text{SOA}_{\text{NAP}}\text{-SP}/\text{SOA}_{\beta\text{PIN}}\text{-SP}$, soot particles (SP, CAST soot; 1 mg m^{-3}) together with either naphthalene or β -pinene (4 mg m^{-3}) photochemically aged with OH radicals in a potential aerosol mass reactor.

Additional File- Excel Document

Table S1. GC×GC-TOFMS peak table for the 100 peaks with the highest signal intensities found in SOA_{NAP}-SP.

	Name	Formula	Similarity	Area	1st Dimension Time [s]	2nd Dimension Time [s]	Cumulative Abundance [%]	Substance class	CxHx	Aldehyde	Ketone	Alcohol	Ether	Carboxylic acid ester	Carboxylic acid	Epoxy	Furan
1	Cyclopenten, 1-ethenyl-3-methylene-	C8H10	867	3.3E+10	2080	2.237	5.7	Unsaturated cyclic compounds	x								
2	1(3H)-Isobenzofuranone	C8H6O2	937	2.67E+10	4384.85	3.411	10.3	Aromatics, Heterocyclic compounds						x			
3	Phenylglyoxal	C8H6O2	817	1.6E+10	2609.96	2.689	13.0	Aromatics		x	x						
4	Phthalic anhydride	C8H4O3	808	1.33E+10	4244.86	3.596	15.3	Aromatics, Heterocyclic compounds			x			x			
5	Ethanone, 2-(formyloxy)-1-phenyl-	C9H8O3	904	1.29E+10	4384.85	3.405	17.5	Aromatics		x	x		x				
6	Cyclobutene, 2-propenylidene-	C7H8	894	1.2E+10	2075	1.931	19.6	Unsaturated cyclic compounds	x								
7	Naphthalene	C10H8	916	1.01E+10	3689.89	2.767	21.3	Aromatics	x								
8	Ninhydri	C9H6O4	813	9.98E+09	5024.81	3.52	23.0	Aromatics			x	x					
9	Vinyl trans-cinnamate	C11H10O2	848	9.91E+09	5089.8	3.22	24.7	Aromatics						x			
10	Benzenecethanol, α,β-dimethyl-	C10H14O	858	9.57E+09	2075	2.256	26.4	Aromatics				x					
11	Peak 1118			9.28E+09	5094.8	3.737	28.0	Unidentified									
12	Benzoic acid, 2-(hydroxymethyl)-	C8H8O3	709	8.59E+09	4389.85	3.481	29.4	Aromatics				x			x		
13	Coumarin	C9H6O2	841	8.58E+09	4604.84	3.272	30.9	Aromatics, Heterocyclic compounds						x	x		
14	Peak 28			7.94E+09	2080	2.243	32.3	Unidentified									
15	Phenacylidene diacetate	C12H12O5	758	7.46E+09	2609.96	2.704	33.6	Aromatics			x			x			
16	Peak 470			7.26E+09	3694.89	3.18	34.8	Unidentified									
17	1,2-Benzenedicarboxylic acid	C8H6O4	927	7.15E+09	4244.86	3.166	36.0	Aromatics							x		
18	Peak 700			6.99E+09	4239.86	3.196	37.2	Unidentified									
19	1H-Indene-1,3(2H)-dione	C9H6O2	916	6.73E+09	4349.85	3.066	38.4	Aromatics			x						
20	1,2-Dihydroxynaphthalene	C10H8O2	826	6.07E+09	5709.76	3.538	39.4	Aromatics				x					
21	1H-2-benzopyran-1,4(3H)-dione	C9H6O3	842	5.96E+09	5094.8	3.44	40.5	Aromatics, Heterocyclic compounds			x			x			
22	Phenacylidene diacetate	C12H12O5	839	5.89E+09	3954.88	3.05	41.5	Aromatics			x			x			
23	2,3-Naphthalenediol	C10H8O2	915	5.85E+09	5884.75	3.588	42.5	Aromatics				x					
24	Coumarin-6-carboxaldehyde	C10H6O3	724	5.81E+09	5509.78	3.621	43.5	Aromatics, Heterocyclic compounds		x				x			
25	Spiro[isobenzofuran-1(3H)-one-3,2'-tetrahydrofuran-5'-one]	C11H8O4	845	5.51E+09	4924.81	3.393	44.4	Aromatics			x						x
26	3-Butenoic acid, 2-oxo-4-phenyl-	C10H8O3	816	5.48E+09	5099.8	3.217	45.4	Aromatics			x				x		
27	Benzene, (1-ethoxyethenyl)-	C10H12O	761	5.41E+09	4299.85	3.048	46.3	Aromatics					x				
28	Peak 1259			4.77E+09	5409.78	3.653	47.1	Unidentified									
29	4-Isopropoxybenzaldehyde	C10H12O2	749	4.69E+09	3024.94	2.696	47.9	Aromatics		x			x				
30	1,2-Benzenedicarboxaldehyde	C8H6O2	922	4.64E+09	3949.88	3.058	48.7	Aromatics		x							
31	Peak 1116			4.58E+09	5094.8	3.364	49.5	Unidentified									
32	Peak 24			4.57E+09	2075	2.681	50.3	Unidentified									

33	Benzocyclobuten-1(2H)-one	C8H6O	726	4.54E+09	3949.88	3.079	51.1	Aromatics			x					
34	Benzylidenemalonaldhyde	C10H8O2	790	4.38E+09	4909.82	3.359	51.8	Aromatics		x						
35	Benzofuran-2-carboxaldehyde	C9H6O2	887	4.25E+09	4539.84	3.205	52.6	Aromatics, Heterocyclic compounds		x			x			
36	Peak 1083			4.1E+09	5024.81	3.575	53.3	Unidentified								
37	4,4-Dimethyl-1-phenylpent-1-en-3-one	C13H16O	719	4.03E+09	4924.81	3.36	53.9	Aromatics						x		
38	Peak 565			3.94E+09	3949.88	2.087	54.6	Unidentified								
39	Peak 1292			3.9E+09	5479.78	3.63	55.3	Unidentified								
40	Benzocyclobuten-1(2H)-one	C8H6O	868	3.75E+09	4804.82	3.446	55.9	Aromatics			x					
41	Peak 245			3.61E+09	2954.94	2.714	56.6	Unidentified								
42	3-Methylidene-2-benzofuran-1-one	C9H6O2	830	3.46E+09	4429.85	3.226	57.2	Aromatics, Heterocyclic compounds			x					x
43	Peak 8			3.4E+09	2045	2.268	57.7	Unidentified								
44	Peak 23			3.39E+09	2075	2.575	58.3	Unidentified								
45	Ethanone, 1-(2,5-dimethylphenyl)-	C10H12O	799	3.38E+09	4429.85	3.16	58.9	Aromatics			x					
46	1-Penten-3-one, 1-phenyl-	C11H12O	867	3.38E+09	5234.79	3.527	59.5	Aromatics			x					
47	Formic acid phenyl ester	C7H6O2	732	3.36E+09	2644.96	2.583	60.1	Aromatics		x			x			
48	2,4-Octadiyne	C8H10	820	3.2E+09	2204.99	2.294	60.6	Unsaturated non-cyclic compounds	x							
49	2-Propyl-1-pentanol	C8H18O	898	3.17E+09	2874.95	2.173	61.2	Saturated non-cyclic compounds				x				
50	Bicyclo[4.2.0]octa-1,3,5-triene	C8H8	850	3.08E+09	2204.99	2.378	61.7	Aromatics	x							
51	1,4-Benzenedicarboxaldehyde	C8H6O2	842	3.05E+09	5314.79	3.667	62.2	Aromatics		x						
52	1H-Inden-1-one, 2,3-dihydro-	C9H8O	933	2.91E+09	4104.87	3.04	62.7	Aromatics			x					
53	Peak 727			2.88E+09	4299.85	3.101	63.2	Unidentified								
54	4-Methylphthalic anhydride	C9H6O3	780	2.8E+09	2764.95	2.587	63.7	Aromatics, Heterocyclic compounds			x			x		
55	Peak 15			2.77E+09	2065	2.452	64.2	Unidentified								
56	Coumarin, 8-methyl-	C10H8O2	782	2.73E+09	4764.82	3.019	64.6	Aromatics, Heterocyclic compounds						x		
57	Indan, epoxide	C9H8O	707	2.68E+09	3869.88	3.185	65.1	Aromatics								x
58	Peak 581			2.45E+09	3959.88	3.266	65.5	Unidentified								
59	2H-Inden-2-one, 1,3-dihydro-	C9H8O	925	2.45E+09	3869.88	2.867	65.9	Aromatics			x					
60	Peak 701			2.32E+09	4239.86	3.406	66.3	Unidentified								
61	Peak 1022			2.25E+09	4919.82	3.417	66.7	Unidentified								
62	2-Decen-1-ol	C10H20O	830	2.23E+09	3249.92	2.218	67.1	Unsaturated non-cyclic compounds				x				
63	Peak 967			2.23E+09	4799.82	2.537	67.5	Unidentified								
64	Peak 892			2.22E+09	4654.83	3.166	67.9	Unidentified								
65	Bicyclo[4.2.0]octa-1,3,5-triene-7-carboxylic acid	C9H8O2	851	2.12E+09	4819.82	3.377	68.2	Aromatics							x	
66	2-Coumaranone	C8H6O2	917	2.09E+09	3904.88	3.012	68.6	Aromatics						x		
67	1,2-Naphthalenedione	C10H6O2	930	2.09E+09	3704.89	2.91	68.9	Aromatics			x					
68	Peak 1293			1.96E+09	5479.78	3.652	69.3	Unidentified								
69	Peak 1129			1.95E+09	5109.8	3.539	69.6	Unidentified								

70	4-Methylene-3,4-dihydroisocoumarin	C10H8O2	786	1.88E+09	4979.81	3.273	69.9	Aromatics, Heterocyclic compounds						x			
71	1-(2-Vinylphenyl)propan-1-one	C11H12O	808	1.87E+09	4964.81	3.262	70.3	Aromatics			x						
72	Peak 1371			1.87E+09	5629.77	3.38	70.6	Unidentified									
73	Peak 1197			1.78E+09	5264.79	3.382	70.9	Unidentified									
74	Benzene, 1-ethynyl-4-methyl-	C9H8	868	1.77E+09	4104.87	3.059	71.2	Aromatics	x								
75	Peak 763			1.73E+09	4384.85	2.62	71.5	Unidentified									
76	Peak 944			1.71E+09	4764.82	3.003	71.8	Unidentified									
77	Peak 1288			1.67E+09	5469.78	3.66	72.1	Unidentified									
78	Peak 1114			1.67E+09	5089.8	3.238	72.4	Unidentified									
79	2-Butenal, 2-methyl-, (E)-	C5H8O	730	1.64E+09	2349.98	3.365	72.6	Unsaturated non-cyclic compounds		x							
80	Peak 720			1.58E+09	4294.86	3.075	72.9	Unidentified									
81	Peak 603			1.52E+09	4014.87	3.16	73.2	Unidentified									
82	o-Toluic acid, phenyl ester	C14H12O2	820	1.45E+09	4294.86	3.163	73.4	Aromatics						x			
83	Vinyl trans-cinnamate	C11H10O2	813	1.45E+09	4919.82	3.192	73.7	Aromatics						x			
84	Benzoic acid, 2-(hydroxymethyl)-	C8H8O3	716	1.44E+09	4544.84	3.146	73.9	Aromatics				x			x		
85	4H-1-Benzopyran-4-one	C9H6O2	928	1.43E+09	4574.84	3.313	74.2	Aromatics, Heterocyclic compounds			x		x				
86	1,3,5-Cycloheptatriene, 3,7,7-trimethyl-	C10H14	867	1.39E+09	2874.95	2.239	74.4	Unsaturated cyclic compounds	x								
87	2-Propenoic acid, 3-(2-hydroxyphenyl)-, (E)-	C9H8O3	896	1.39E+09	4744.83	3.37	74.6	Aromatics				x			x		
88	Decanal	C10H20O	918	1.36E+09	3699.89	2.214	74.9	Saturated non-cyclic compounds		x							
89	1,3-Phenylene, bis(3-phenylpropenoate)	C24H18O4	846	1.36E+09	4329.85	2.953	75.1	Aromatics						x			
90	Naphth[2,3-b]oxirene-2,7-dione, 1a,7a-dihydro-	C10H6O3	901	1.33E+09	5004.81	3.313	75.3	Aromatics			x					x	
91	Benzocyclobuten-1(2H)-one	C8H6O	882	1.31E+09	2774.95	2.588	75.6	Aromatics			x						
92	Peak 102			1.3E+09	2349.98	2.674	75.8	Unidentified									
93	Benzoic acid, 2-(hydroxymethyl)-	C8H8O3	723	1.2E+09	5849.76	3.758	76.0	Aromatics				x			x		
94	Peak 1060			1.18E+09	4989.81	2.355	76.2	Unidentified									
95	Peak 792			1.18E+09	4434.85	3.027	76.4	Unidentified									
96	Peak 918			1.15E+09	4704.83	3.24	76.6	Unidentified									
97	1,4-Naphthalenediol	C10H8O2	771	1.15E+09	4734.83	3.1	76.8	Aromatics				x					
98	Peak 927			1.12E+09	4729.83	3.193	77.0	Unidentified									
99	Peak 946			1.11E+09	4764.82	3.121	77.2	Unidentified									
100	Pentanedioic acid, 2-oxo-, dimethyl ester	C7H10O5	717	1.1E+09	2904.94	2.635	77.4	Saturated non-cyclic compounds			x			x			

This table corresponds to Figure 2A, S3B and S4A. Note: GC×GC-TOFMS, comprehensive two-dimensional gas chromatography - time-of-flight mass spectrometer; SOA_{NAP}-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with naphthalene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor.

Table S2. GC×GC-TOFMS peak table for the 100 peaks with the highest signal intensities found in SOA_βPIN-SP.

	Name	Formula	Similarity	Area	1st Dimension Time [s]	2nd Dimension Time [s]	Cumulative Abundance [%]	Substance class	CxHx	Aldehyde	Ketone	Alcohol	Ether	Carboxylic acid ester	Carboxylic acid	Epox y	Furan
1	Bicyclo[3.1.1]hepta n-2-one, 6,6- dimethyl-	C9H14O	914	4.8E+10	3484.9	2.6	4.9	Saturated cyclic compounds			x						
2	Phenylglyoxal	C8H6O2	827	2.6E+10	2599.96	2.664	7.6	Aromatics		x	x						
3	Cyclopentene, 1- ethenyl-3- methylene-	C8H10	744	1.9E+10	2044.99	2.268	9.5	Unsaturated cyclic compounds	x								
4	Peak 908			1.8E+10	3484.9	2.6	11.4	Unidentified									
5	Peak 909			1.8E+10	3484.9	2.611	13.2	Unidentified									
6	Cyclopentane, 1- acetyl-1,2-epoxy-	C7H10O2	753	1.7E+10	2054.99	2.288	14.9	Saturated cyclic compounds									
7	Peak 1974			1.3E+10	4749.82	2.892	16.3	Unidentified									
8	Peak 998			1.1E+10	3589.89	2.566	17.4	Unidentified									
9	2-Propenoic acid, 2-methyl-, oxiranylmethyl ester	C7H10O3	678	1.0E+10	3499.9	2.534	18.5	Unsaturated non-cyclic compounds						x		x	
10	Bicyclo[3.2.1]oct- 2-ene, 3-methyl-4- methylene-	C10H14	780	1.0E+10	2884.94	2.211	19.5	Unsaturated cyclic compounds	x								
11	1-Pentyn-3-ol	C5H8O	801	9.8E+09	2494.96	2.493	20.5	Unsaturated non-cyclic compounds				x					
12	Benzene, 1-methyl- 3-(1- methylene-phenyl)-	C10H12	910	9.7E+09	3214.92	2.321	21.5	Aromatics	x								
13	Peak 999			9.5E+09	3589.89	2.643	22.5	Unidentified									
14	α-Thujenal	C10H14O	816	7.9E+09	3734.88	2.496	23.3	Unsaturated cyclic compounds		x							
15	Peak 1700			7.9E+09	4384.84	3.137	24.1	Unidentified									
16	Peak 815			7.7E+09	3384.9	2.545	24.9	Unidentified									
17	Bicyclo[2.2.1]hepta ne-2,5-diol, 1,7,7- trimethyl-, (2- endo,5-exo)-	C10H18O2	804	7.4E+09	3679.89	2.447	25.7	Saturated cyclic compounds				x					
18	1-Cyclohexene-1- carboxaldehyde, 4- (1-methylene-phenyl)-	C10H14O	844	7.2E+09	4079.86	2.508	26.4	Unsaturated cyclic compounds		x							
19	Benzene, 1-(1,5- dimethylhexyl)-4- methyl-	C15H24	730	6.7E+09	2889.94	2.226	27.1	Aromatics	x								
20	4-Pentenoic acid, 2-formyl-2-methyl- ethyl ester	C9H14O3	715	6.6E+09	4169.85	2.746	27.8	Unsaturated non-cyclic compounds		x				x			
21	Bicyclo[3.1.1]hepta ne-2- carboxaldehyde, 6,6-dimethyl-	C10H16O	785	6.5E+09	3734.88	2.449	28.5	Saturated cyclic compounds		x							
22	3-Methyl-2- butenoic acid, cyclobutyl ester	C9H14O2	744	6.5E+09	3494.9	2.556	29.1	Saturated cyclic compounds						x			
23	Ethandione, bis(p- tolyl)-	C16H14O2	789	6.3E+09	2874.94	2.239	29.8	Aromatics			x						
24	3-Cyclohexene-1- carboxaldehyde, 1,3,4-trimethyl- 6,6-	C10H16O	792	6.3E+09	3634.89	2.428	30.4	Unsaturated cyclic compounds		x							
25	Dimethylcycloocta- 2,4-dienone	C10H14O	730	6.1E+09	3689.89	2.476	31.1	Unsaturated cyclic compounds			x						
26	3,4-Dihydro-6- methyl-2H-pyran- 2-one	C6H8O2	808	6.1E+09	2324.97	2.47	31.7	Heterocyclic compounds			x		x				

	Name	Formula	Similarity	Area	1st Dimension Time [s]	2nd Dimension Time [s]	Cumulative Abundance [%]	Substance class	CxHx	Aldehyde	Ketone	Alcohol	Ether	Carboxylic acid ester	Carboxylic acid	Epox y	Furan
27	4-Hexen-2-one, 3-methyl-	C7H12O	858	6.1E+09	2184.98	2.332	32.3	Unsaturated non-cyclic compounds			x						
28	1,1,3,3,5-Pentamethylcyclohexane	C11H22	750	5.8E+09	4084.86	2.555	32.9	Saturated cyclic compounds	x								
29	4-Methyl-2,3-hexadien-1-ol	C7H12O	789	5.7E+09	2794.94	2.408	33.5	Unsaturated non-cyclic compounds				x					
30	Bicyclo[3.2.0]hept-2-en-6-one, 7,7-dimethyl-	C9H12O	825	5.4E+09	3394.9	2.575	34.1	Unsaturated cyclic compounds			x						
31	Bicyclo[3.1.1]heptan-2-one, 3,6,6-trimethyl-	C10H16O	739	5.3E+09	3884.87	2.631	34.6	Saturated cyclic compounds			x						
32	1,3-Propanediol, 2,2-diethyl-	C7H16O2	705	5.3E+09	3859.87	2.688	35.2	Saturated non-cyclic compounds				x					
33	Peak 1073			5.3E+09	3689.89	2.402	35.7	Unidentified									
34	Cyclobutene, 2-propenylidene-	C7H8	799	5.2E+09	3229.91	2.374	36.2	Unsaturated cyclic compounds	x								
35	Cyclohexanone, 2-methyl-5-(1-methylethenyl)-	C10H16O	784	5.1E+09	4049.86	2.905	36.8	Saturated cyclic compounds			x						
36	1,2-Cyclopentanedione	C5H6O2	772	4.9E+09	2059.99	2.689	37.3	Saturated cyclic compounds			x						
37	1,4-Cyclohexanedione	C6H8O2	940	4.9E+09	3274.91	3.119	37.8	Saturated cyclic compounds			x						
38	3-Ethenyl-3-methylcyclopentanone	C8H12O	898	4.6E+09	3044.93	2.462	38.2	Saturated cyclic compounds			x						
39	Peak 2080			4.5E+09	4924.81	3.005	38.7	Unidentified									
40	p-Mentha-1,8-dien-7-ol	C10H16O	926	4.5E+09	4154.86	2.457	39.2	Unsaturated cyclic compounds				x					
41	Peak 1743			4.5E+09	4439.84	2.835	39.6	Unidentified									
42	Furan, 2,3-dihydro-4-(1-methylpropyl)-, (S)-	C8H14O	798	4.4E+09	2104.99	2.348	40.1	Heterocyclic compounds									x
43	Ethanone, 1-(1,2,2,3-tetramethylcyclopentyl)-, (1R-cis)-	C11H20O	737	4.4E+09	4544.83	2.924	40.5	Saturated cyclic compounds			x						
44	3-Hexene-2,5-dione	C6H8O2	804	4.3E+09	2524.96	2.743	41.0	Unsaturated non-cyclic compounds			x						
45	Peak 1548			4.3E+09	4194.85	2.868	41.4	Unidentified									
46	Bicyclo[4.2.0]octa-1,3,5-triene, 3-methyl-	C9H10	843	4.3E+09	2684.95	2.36	41.9	Aromatics	x								
47	Formic acid phenyl ester	C7H6O2	820	4.3E+09	2649.95	2.559	42.3	Aromatics						x			
48	3,5-Octadiene, 4,5-diethyl-	C12H22	776	4.3E+09	4459.84	2.755	42.7	Unsaturated non-cyclic compounds	x								
49	Peak 1979			4.1E+09	4759.82	2.808	43.2	Unidentified									
50	6,11-Dimethyl-2,6,10-dodecatrien-1-ol	C14H24O	749	4.1E+09	4224.85	2.728	43.6	Unsaturated non-cyclic compounds				x					
51	2-[2-(5-Norbornenyl)oxy]-tetrahydropyran	C12H18O2	732	4.1E+09	3824.88	2.605	44.0	Heterocyclic compounds, Unsaturated cyclic compounds					x				
52	1,4-Cyclohexadiene, 3-ethenyl-1,2-dimethyl-	C10H14	884	4.1E+09	2774.94	2.182	44.4	Unsaturated cyclic compounds	x								

	Name	Formula	Similarity	Area	1st Dimension Time [s]	2nd Dimension Time [s]	Cumulative Abundance [%]	Substance class	CxHx	Aldehyde	Ketone	Alcohol	Ether	Carboxylic acid ester	Carboxylic acid	Epox y	Furan
82	2-Methoxyphenylacetone	C10H12O2	757	3.0E+09	3974.87	2.602	55.1	Aromatics			x		x				
83	Peak 1305			3.0E+09	3939.87	2.676	55.4	Unidentified									
84	1-Cyclohexene-1-carboxaldehyde, 5,5-dimethyl-3-oxo-	C9H12O2	729	3.0E+09	4414.84	2.944	55.7	Unsaturated cyclic compounds		x	x						
85	Cyclopentanol, 2,4,4-trimethyl-	C8H16O	748	3.0E+09	3799.88	2.604	56.1	Saturated cyclic compounds				x					
86	1,5,5-Trimethyl-6-methylene-cyclohexene	C10H16	755	3.0E+09	4124.86	2.746	56.4	Unsaturated non-cyclic compounds	x								
87	Cyclohexanol, 2-methylene-3-(1-methylethyl)-, cis-	C10H18O	728	3.0E+09	3899.87	2.649	56.7	Saturated cyclic compounds				x					
88	Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, [1S-(1 α ,2 β ,5 α)]-	C10H18	775	2.9E+09	4599.83	2.957	57.0	Saturated cyclic compounds	x								
89	2-Pentanone, 3-methylene-	C6H10O	757	2.9E+09	3504.9	2.877	57.3	Saturated non-cyclic compounds			x						
90	1,4-Methanonaphthalene-9-one, 1,2,3,4-tetrahydro-	C11H10O	809	2.9E+09	3519.9	2.518	57.6	Aromatics			x						
91	1,2-Cyclohexanedicarboxaldehyde	C8H12O2	710	2.8E+09	4239.85	2.641	57.8	Saturated cyclic compounds		x							
92	Hexanoic acid, 1,1-dimethylpropyl ester	C11H22O2	742	2.8E+09	2709.95	2.726	58.1	Saturated non-cyclic compounds						x			
93	Peak 1070			2.8E+09	3684.89	2.446	58.4	Unidentified									
94	3-Hepten-2-one, 4-methyl-	C8H14O	723	2.8E+09	2874.94	2.574	58.7	Unsaturated non-cyclic compounds			x						
95	Benzaldehyde, 4-(1-methylethyl)-	C10H12O	859	2.8E+09	3934.87	2.516	59.0	Aromatics		x							
96	3-Methyl-3-cyclohexen-1-one	C7H10O	767	2.8E+09	4164.86	2.881	59.3	Unsaturated cyclic compounds			x						
97	Benzaldehyde, 4-(1-methylethyl)-	C10H12O	851	2.8E+09	4024.86	2.489	59.6	Aromatics		x							
98	L-Fenchone	C10H16O	708	2.8E+09	4349.84	2.701	59.8	Saturated cyclic compounds			x						
99	3-Nonen-5-yne, 4-ethyl-, (Z)-	C11H18	790	2.7E+09	3269.91	2.323	60.1	Unsaturated non-cyclic compounds	x								
100	5-Cyclodecene, 1,2-epoxy-	C10H16O	756	2.7E+09	4299.85	3.027	60.4	Saturated cyclic compounds			x					x	

This table corresponds to Figure 2B, S3A and S4B. Note: GC×GC-TOFMS, comprehensive two-dimensional gas chromatography - time-of-flight mass spectrometer; SOA β PIN-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with β -pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor.

Table S3. Areas of the 100 peaks with the highest signal intensities from GC×GC-TOFMS classified by compound classes and functional groups for SOA_{NAP}-SP.

	CxHx	Aldehyde	Ketone	Alcohol	Ether	Carboxylic acid ester	Carboxylic acid	Epoxy	Furan	Unidentified
Aromatics	1.5E+10	5.9E+10	1.2E+11	4.5E+10	3.2E+10	1.0E+11	3.6E+10	4.0E+09	9.0E+09	0
Heterocyclic compounds	0	1.0E+10	2.7E+10	0	5.7E+09	6.8E+10	8.6E+09	0	3.5E+09	0
Saturated non-cyclic compounds	0	1.4E+09	1.1E+09	3.2E+09	0	1.1E+09	0	0	0	0
Unsaturated non-cyclic compounds	3.2E+09	1.6E+09	0	2.2E+09	0	0	0	0	0	0
Saturated cyclic compounds	0	0	0	0	0	0	0	0	0	0
Unsaturated cyclic compounds	4.7E+10	0	0	0	0	0	0	0	0	0
Unidentified	0	0	0	0	0	0	0	0	0	1.1E+11

This table corresponds to Figure 2E. Note: GC×GC-TOFMS, comprehensive two-dimensional gas chromatography - time-of-flight mass spectrometer; SOA_{NAP}-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with naphthalene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor.

Table S4. Areas of the 100 peaks with the highest signal intensities from GC×GC-TOFMS classified by compound classes and functional groups for SOA_{βPIN-SP}.

	CxHx	Aldehyde	Ketone	Alcohol	Ether	Carboxylic acid ester	Carboxylic acid	Epoxy	Furan	Unidentified
Aromatics	2.7E+10	3.1E+10	3.8E+10	0	3.0E+09	4.3E+09	0	0	0	0
Heterocyclic compounds	0	0	9.8E+09	0	1.4E+10	0	0	0	8.1E+09	0
Saturated non-cyclic compounds	0	0	6.0E+09	5.3E+09	0	6.3E+09	3.5E+09	3.5E+09	0	0
Unsaturated non-cyclic compounds	1.0E+10	6.6E+09	1.7E+10	3.1E+10	3.8E+09	2.1E+10	0	1.0E+10	0	0
Saturated cyclic compounds	1.2E+10	9.3E+09	9.6E+10	2.0E+10	0	6.5E+09	0	5.8E+09	0	0
Unsaturated cyclic compounds	4.2E+10	2.8E+10	1.7E+10	4.5E+09	4.1E+09	0	0	0	0	0
Unidentified	0	0	0	0	0	0	0	0	0	1.4E+11

This table corresponds to Figure 2F. Note: GC×GC-TOFMS, comprehensive two-dimensional gas chromatography - time-of-flight mass spectrometer; SOA_{βPIN-SP}, soot particles (SP, CAST soot; 1 mg m⁻³) together with β-pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor.

Table S5. Relative AMS intensity fraction of m/z 43 vs m/z 44 (f_{44} vs. f_{43}) for SOA _{β PIN-SP} and SOA_{NAP-SP}.

SOA _{βPIN-SP}		SOA _{NAP-SP}		SOA _{βPIN-SP}		SOA _{NAP-SP}	
F43	F44	F43	F44	F43	F44	F43	F44
0.12552084	0.088352814	0.011312465	0.10256327	0.12594332	0.087701477	0.011332938	0.10178624
0.12536591	0.088149071	0.011249838	0.10097587	0.1264039	0.087834068	0.011354873	0.10064898
0.12541899	0.088585526	0.011187937	0.10279159	0.12613066	0.087467514	0.011244824	0.10213763
0.12548135	0.088090517	0.011832626	0.10070522	0.12606567	0.088270627	0.011338827	0.10219531
0.12516919	0.088310793	0.011222817	0.10412512	0.12541714	0.088482991	0.011302163	0.10133233
0.12526931	0.088368803	0.011247191	0.10191435	0.12557203	0.08821284	0.011403976	0.10023145
0.12540846	0.088367589	0.011859154	0.10056046	0.12540454	0.087974891	0.01129391	0.10075324
0.12531169	0.088729419	0.011264383	0.10057431	0.12545131	0.087659098	0.011300722	0.10132349
0.12538216	0.08770667	0.01119424	0.099763617	0.1257403	0.087902136	0.0112585	0.10082649
0.12526491	0.08811345	0.01128626	0.10012679	0.12562746	0.088394217	0.011359434	0.10207463
0.12511815	0.088749781	0.0113118	0.09941972	0.12543252	0.087536201	0.011353889	0.10307538
0.12537508	0.088008769	0.01121917	0.099280685	0.1255922	0.08769878	0.011296742	0.10228642
0.12534848	0.088258438	0.011322094	0.1003483	0.12543675	0.088263929	0.011280274	0.1029937
0.12519021	0.087688886	0.01126293	0.10013687	0.12576877	0.087383755	0.011319958	0.10316098
0.12504336	0.088177182	0.011336234	0.10053151	0.12592293	0.087639816	0.011380685	0.10222198
0.12483092	0.088007897	0.011481197	0.098817974	0.1254985	0.087916322	0.011302773	0.10195565
0.124584	0.087724231	0.011302772	0.098075628	0.12539251	0.08792872	0.011596603	0.10156846
0.1247077	0.087932594	0.011241195	0.099830985	0.12522769	0.088039055	0.011427742	0.10319555
0.1252542	0.087579869	0.011235936	0.10071564	0.12554468	0.087471567	0.011459501	0.1030727
0.12498266	0.087415002	0.011278965	0.099999882	0.12514246	0.088181995	0.011368616	0.10245007
0.12492536	0.087405182	0.011644157	0.099485718	0.12571456	0.088001207	0.011411589	0.10275534
0.12478599	0.087241009	0.011341893	0.099419713	0.12535606	0.087820061	0.011623018	0.10159773
0.12516491	0.087463133	0.01127617	0.10060116	0.12532039	0.088137433	0.011330169	0.10199314
0.12525791	0.087014593	0.011211312	0.10091677	0.12540892	0.087602101	0.011671931	0.10119675
0.12534384	0.087241799	0.01128221	0.10173059	0.12558746	0.087706313	0.01142396	0.10161284
0.12583394	0.087177254	0.011360032	0.10260754	0.12581566	0.087708972	0.012513304	0.096633919
0.12539339	0.08719828	0.011334266	0.10213055	0.12544288	0.087878764	0.011659699	0.10051109
0.12536545	0.087796271	0.011237731	0.10213131	0.12576553	0.087434366	0.012208143	0.1007293
0.12541506	0.087405182	0.011342216	0.10204857			0.011419251	0.10137048

This table corresponds to Figure S5. Note: AMS, high-resolution time-of-flight aerosol mass spectrometer; SOA_{NAP-SP}/SOA _{β PIN-SP}, soot particles (SP, CAST soot; 1 mg m⁻³) together with either naphthalene or β -pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor.

Table S6. Toxicity results of monoculture exposed to SP, SOA_{βPIN}-SP and SOA_{NAP}-SP.

	Ctrl	SP	SOA _{NAP} -SP				SOA _{βPIN} -SP			
dilution		undiluted (1:1)	undiluted (1:1)	1:3	1:10	1:30	undiluted (1:1)	1:3	1:10	1:30
% cell viability	100 ± 6	78 ± 6	40 ± 2	54 ± 3	65 ± 4	65 ± 4	75 ± 3	79 ± 5	91 ± 4	87 ± 5
MDA ng ml ⁻¹	4 ± 0.4	12 ± 4	53 ± 8	24 ± 6	14 ± 2	10 ± 3	23 ± 7	16 ± 4	4 ± 2	7 ± 4
% DNA breaks	4 ± 0.1	8 ± 0.3	16 ± 0.8	16 ± 0.7	14 ± 0.5	13 ± 0.4	11 ± 0.4	10 ± 0.4	9 ± 0.5	5 ± 0.7
IL8 pg ml ⁻¹	360 ± 148	360 ± 80	601 ± 41	503 ± 37	427 ± 22	407 ± 30	383 ± 26	336 ± 12	348 ± 48	363 ± 13
Angiogenic potential	3.5 ± 0.2	3.5 ± 0.3	3.9 ± 0.2	-	-	-	3.6 ± 0.3	-	-	-

A549 monoculture were exposed 4 h in an ALI exposure system to unaged pure SP (CAST soot; 1mg m⁻³) or atmospheric photooxidation (aging) by OH radicals in a potential aerosol mass reactor of SP (CAST soot; 1mg m⁻³) together with either naphthalene (4 mg m⁻³) or β-pinene (4 mg m⁻³), forming SOA_{NAP}-SP and SOA_{βPIN}-SP, respectively. Results are presented as mean values ± SEM of n independent experiments (Ctrl: n = 8, SP: n =4, SOA_{βPIN}-SP: n = 4 and SOA_{NAP}-SP: n = 5 for all dilutions). Angiogenic potential was calculated using the following equation $Angiogenic\ score = \left(\frac{(No.of\ sprouting\ cells)*1 + (No.of\ connected\ cells)*2 + (no.of\ polygons)*3}{Total\ number\ of\ cells} \right) + (0, 1\ or\ 2)$. The addition of 0, 1 or 2 to the total value is depending on the presence of a complex mesh. No complex mesh is represented by the addition of 0 points, for the existence of luminal structures consisting of 2-3 cell layers an addition of 1 point is necessary and for luminal structures greater than 3 cell layers an additional value of 2 is added. This table corresponds to Figure 4B, D, F and Figure 5A, B, C, D and Figure 6A, B, D. Note: SP, soot particle; MDA, malondialdehyde; IL8, interleukin 8; -, no data available.

Table S7. Toxicity results of co-culture exposed to SP, SOA_{βPIN}-SP and SOA_{NAP}-SP.

	Ctrl	SP	SOA _{NAP} -SP				SOA _{βPIN} -SP			
dilution		undiluted (1:1)	undiluted (1:1)	1:3	1:10	1:30	undiluted (1:1)	1:3	1:10	1:30
MDA ng ml ⁻¹	6 ± 1	11 ± 5	53 ± 8	27 ± 3	14 ± 2	10 ± 1	18 ± 6	12 ± 3	4 ± 2	7 ± 4
% DNA breaks	4 ± 0.1 (A549) 4 ± 0.1 (EA.hy926)	8 ± 0.2 (A549) 4 ± 0.1 (EA.hy926)	17 ± 0.8 (A549) 8 ± 0.3 (EA.hy926)	19 ± 0.6 (A549) 7 ± 0.4 (EA.hy926)	11 ± 1.5 (A549) 5 ± 0.2 (EA.hy926)	15 ± 1.6 (A549) 5 ± 0.2 (EA.hy926)	12 ± 1.6 (A549) 4 ± 0.3 (EA.hy926)	9 ± 0.3 (A549) 4 ± 0.1 (EA.hy926)	9 ± 1.2 (A549) 4 ± 0.1 (EA.hy926)	6 ± 0.5 (A549) 4 ± 0.05 (EA.hy926)
IL8 pg ml ⁻¹	340 ± 28	520 ± 41	1199 ± 271	934 ± 47	824 ± 26	881 ± 26	878 ± 287	666 ± 22	651 ± 22	569 ± 32
Angiogenic potential	3.3 ± 0.3	3.4 ± 0.1	3.8 ± 0.2	-	-	-	3.0 ± 0.3	-	-	-

Co-culture (A549/EA.hy926) were exposed 4 h in an ALI exposure system to unaged pure SP (CAST soot; 1 mg m⁻³) or atmospheric photooxidation (aging) by OH radicals in a potential aerosol mass reactor of SP (CAST soot; 1 mg m⁻³) together with either naphthalene (4 mg m⁻³) or β-pinene (4 mg m⁻³), forming SOA_{NAP}-SP and SOA_{βPIN}-SP, respectively. Results are presented as mean values ± SEM of n independent experiments (Ctrl: n = 8, SP: n = 4, SOA_{βPIN}-SP: n = 4 and SOA_{NAP}-SP: n = 5 for all dilutions). Angiogenic potential was calculated using the following equation
$$\text{Angiogenic score} = \left(\frac{(\text{No. of sprouting cells}) \times 1 + (\text{No. of connected cells}) \times 2 + (\text{no. of polygons}) \times 3}{\text{Total number of cells}} \right) + (0, 1 \text{ or } 2).$$
 The addition of 0, 1 or 2 to the total value is depending on the presence of a complex mesh. No complex mesh is represented by the addition of 0 points, for the existence of luminal structures consisting of 2-3 cell layers an addition of 1 point is necessary and for luminal structures greater than 3 cell layers an additional value of 2 is added. This table corresponds to Figure 4B, D, F and Figure 5A, B, C, D and Figure 6A, B, D. Note: SP, soot particle; MDA, malondialdehyde; IL8, interleukin 8; -, no data available.

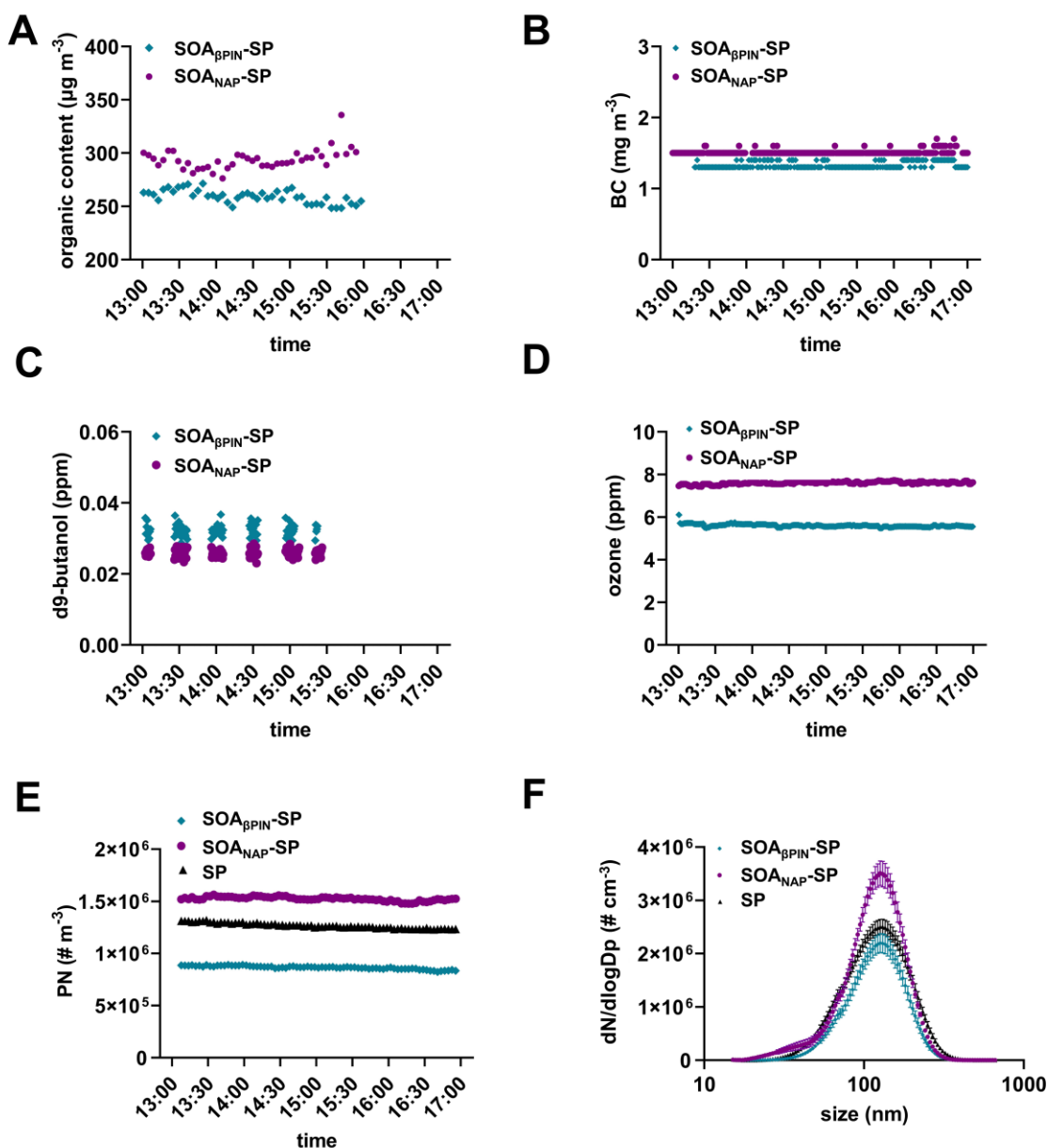


Figure S1. Stability of β -pinene and naphthalene aging, respectively over 4 h exposure time measured with different methods and on different days (A) organic content measured by AMS (B) black carbon (BC) measured by Aethalometer (C) d9-butanol measured by PTR-MS (D) ozone measured by an ozone monitor (E) PN and (F) size distribution measured by SMPS. (A-E) Results are shown of one representative exposure with either $\text{SOA}_{\beta\text{PIN}}\text{-SP}$, $\text{SOA}_{\text{NAP}}\text{-SP}$ or with SP (E-F), respectively. All exposures were conducted on different days. Corresponding numeric data are found in Excel Tables S1-S6, respectively. Note: $\text{SOA}_{\text{NAP}}\text{-SP}/\text{SOA}_{\beta\text{PIN}}\text{-SP}$, soot particles (SP, CAST soot; 1 mg m^{-3}) together with either naphthalene or β -pinene (4 mg m^{-3}) photochemically aged with OH radicals in a potential aerosol mass reactor, SP; pure SP (CAST soot; 1 mg m^{-3}) were fed into the potential aerosol mass reactor without aging; AMS, high-resolution time-of-flight aerosol mass spectrometer; PTR-MS, quadrupole proton-transfer reaction mass spectrometer; SMPS, scanning mobility particle sizer.

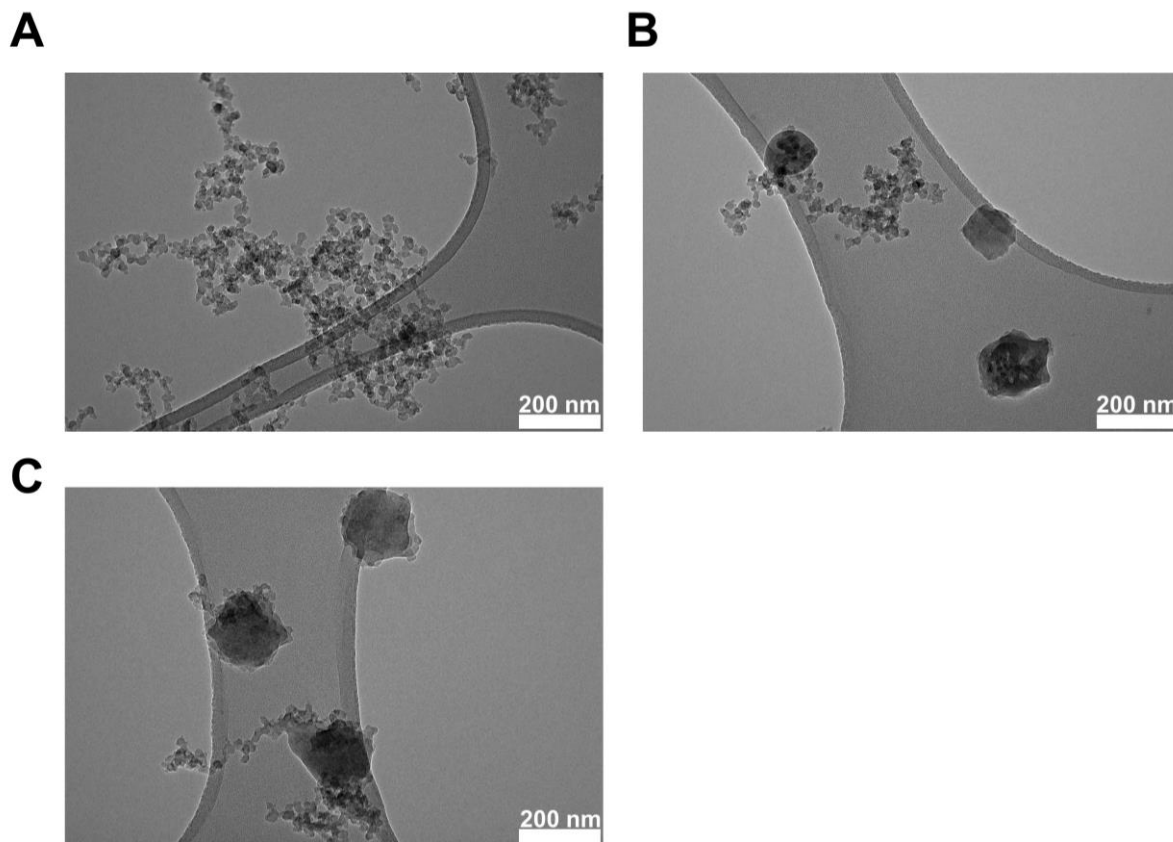


Figure S2. TEM micrographs of SP, SOA_{NAP}-SP and SOA_{βPIN}-SP. Representative TEM micrographs of 1 mg m⁻³ SP (A), photochemically-aged SP (1 mg m⁻³) coated by naphthalene (4 mg m⁻³, SOA_{NAP}-SP) (B) and β-pinene (4 mg m⁻³, SOA_{βPIN}-SP) (C) aging products, scale bar 200 nm. Note: TEM, Transmission electron microscopy; SP; pure SP (CAST soot; 1 mg m⁻³) were fed into the potential aerosol mass reactor without aging; SOA_{NAP}-SP/SOA_{βPIN}-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with either naphthalene or β-pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor.

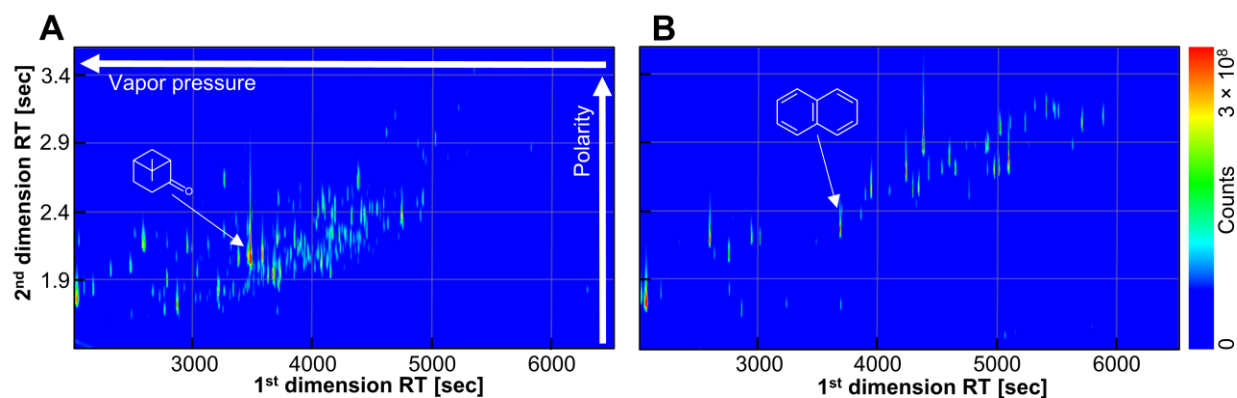


Figure S3. GC×GC-TOFMS contour plots for SOA_{βPIN}-SP (A) and SOA_{NAP}-SP (B). Note: GC×GC-TOFMS, comprehensive two-dimensional gas chromatography - time-of-flight mass spectrometer; SOA_{NAP}-SP/SOA_{βPIN}-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with either naphthalene or β-pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor.

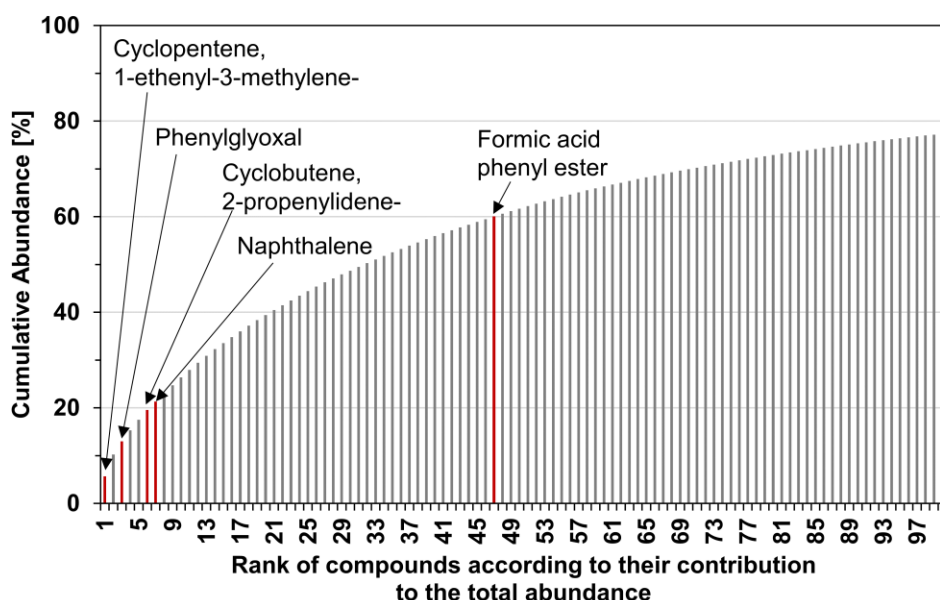
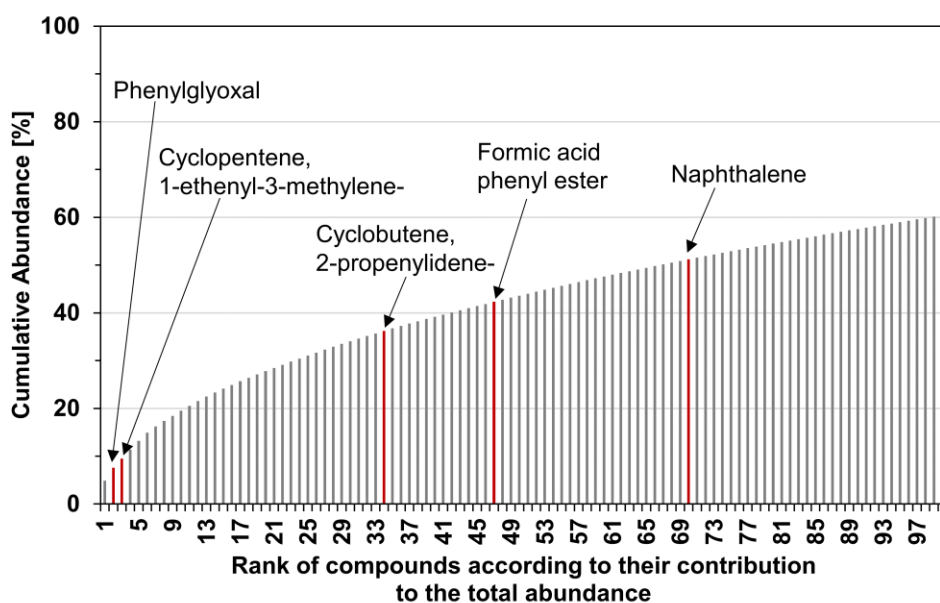
A**B**

Figure S4. Relative cumulative abundance of the 100 peaks with the highest intensities in GCxGC-TOFMS (ranked from compounds with highest to lowest areas). Compounds were identified via NIST mass spectral library match and retention indices for (A) SOA_{NAP}-SP and (B) SOA_{βPIN}-SP. Processing was done with a minimum peak S/N of 1000. Compounds marked in red were detected in both aerosol types. The numeric data corresponding to this figure is shown in the column cumulative abundance [%] of Table S1 for SOA_{NAP}-SP and of Table S2 for SOA_{βPIN}-SP. Note: SOA_{NAP}-SP/SOA_{βPIN}-SP, soot particles (SP, CAST soot; 1 mg m⁻³) together with either naphthalene or β-pinene (4 mg m⁻³) photochemically aged with OH radicals in a potential aerosol mass reactor; GCxGC-TOFMS, comprehensive two-dimensional gas chromatography - time-of-flight mass spectrometer.

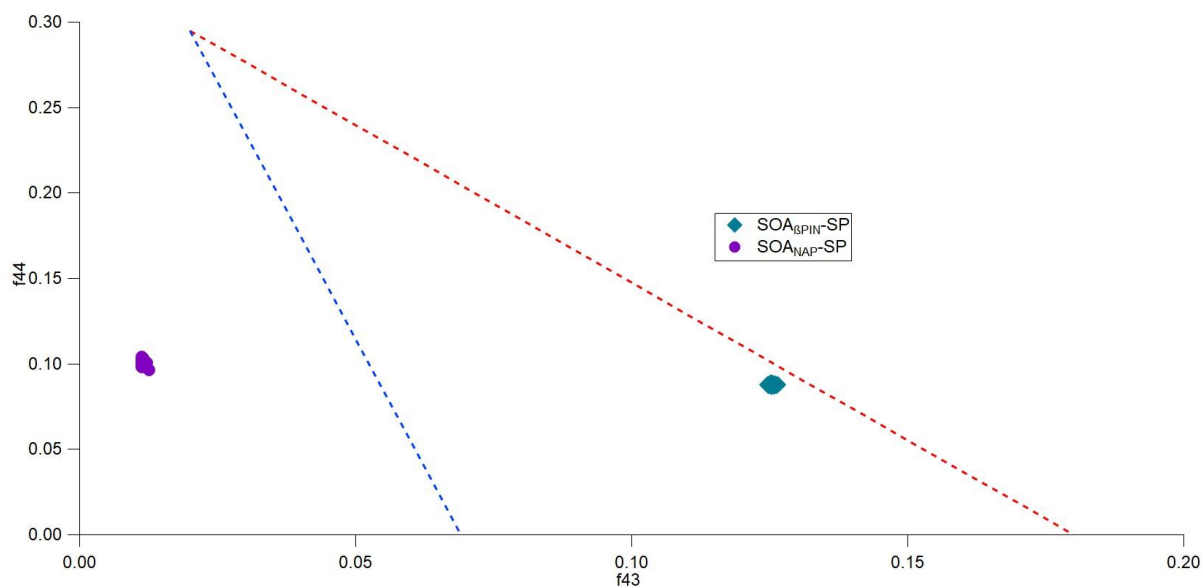


Figure S5. Diagram of the relative AMS intensity fraction of m/z 43 vs m/z 44 (f_{44} vs. f_{43}) for $\text{SOA}_{\beta\text{PIN-SP}}$ and $\text{SOA}_{\text{NAP-SP}}$. Corresponding numeric data are shown in Table S5. Note: AMS, high-resolution time-of-flight aerosol mass spectrometer; $\text{SOA}_{\text{NAP-SP}}/\text{SOA}_{\beta\text{PIN-SP}}$, soot particles (SP, CAST soot; 1 mg m^{-3}) together with either naphthalene or β -pinene (4 mg m^{-3}) photochemically aged with OH radicals in a potential aerosol mass reactor.