Supplementary Information.

Table S1 – The molecular formulae (MF) and associated errors of the identified SOA compounds in experiment MC_{high} using FTICR-MS and HPLC-QTOFMS in negative ionisation mode.

t_R	MW [g mol^{-1}]	FTICR-MS MF	Error [ppm]	Score [%]	HPLC-QTOFMS MF	Error [ppm]	Score [%]
14.3	138				$C_7H_6O_3$	-9.7	100
30.1	152	$C_8H_8O_3$	0.3	100	$C_8H_8O_3$	-1.4	100
28.1	166	$C_9H_{10}O_3$	0.8	100	$C_9H_{10}O_3$	1.2	100
33	168	$C_8H_8O_4$	1.2	100	$C_8H_8O_4$	0.2	100
12.5	180	$C_9H_8O_4$	0.9	100	$C_9H_8O_4$	2.6	100
16.1	182	$C_9H_{10}O_4$	0.8	100	$C_9H_{10}O_4$	-0.3	100
17.6	191	$C_{10}H_9NO_3$	0.7	100	$C_{10}H_9NO_3$	-3.2	100
33.7	194	$C_{11}H_{14}O_3$	0	100	$C_{11}H_{14}O_3$	-0.9	0
25.2	196	$C_{10}H_{12}O_4$	1	100	$C_{10}H_{12}O_4$	2.5	100
20.2	198	$C_{10}H_{14}O_4$	0.9	100	$C_{10}H_{14}O_4$	2.4	100
20.7	199	$C_8H_9NO_5$	0.2	100	$C_8H_9NO_5$	-0.2	100
39.6	209	$C_{10}H_{11}NO_4$	0	100	$C_{10}H_{11}NO_4$	4.3	100
27.8	210	$C_{11}H_{14}O_4$	0.9	100	$C_{11}H_{14}O_4$	1.4	100
21.3	213	$C_9H_{11}NO_5$	0.7	100	$C_9H_{11}NO_5$	0.5	100
21	214	$C_{11}H_{18}O_4$	0.4	100	$C_{11}H_{18}O_4$	2	100
18.6	236	$C_8H_{12}O_8$	-2.9	100	$C_8H_{12}O_8$	36.6	0.13
31.8	238	$C_{12}H_{14}O_5$	0.9	100	$C_{12}H_{14}O_5$	9.9	100
22.2	243	$C_{10}H_{13}NO_6$	0.6	100	$C_{10}H_{13}NO_6$	-0.7	100
35.9	252	$C_{13}H_{16}O_5$	1.6	100	$C_{13}H_{16}O_5$	18.6	30.3
12.8	277	$C_9H_{11}NO_9$	0.2	100	$C_9H_{11}NO_9$	0.9	100
28.8	292	$C_{15}H_{16}O_6$	1.2	100			
23.3	296	$C_{18}H_{16}O_4$	-6.8	100	$C_{18}H_{16}O_4$	3.5	100
36.1	317	$C_{16}H_{15}NO_6$	-0.3	100	$C_{16}H_{15}NO_6$	1.8	100
36.2	428	$C_{18}H_{20}O_{12}$	-0.1	100	$C_{18}H_{20}O_{12}$	-0.8	100

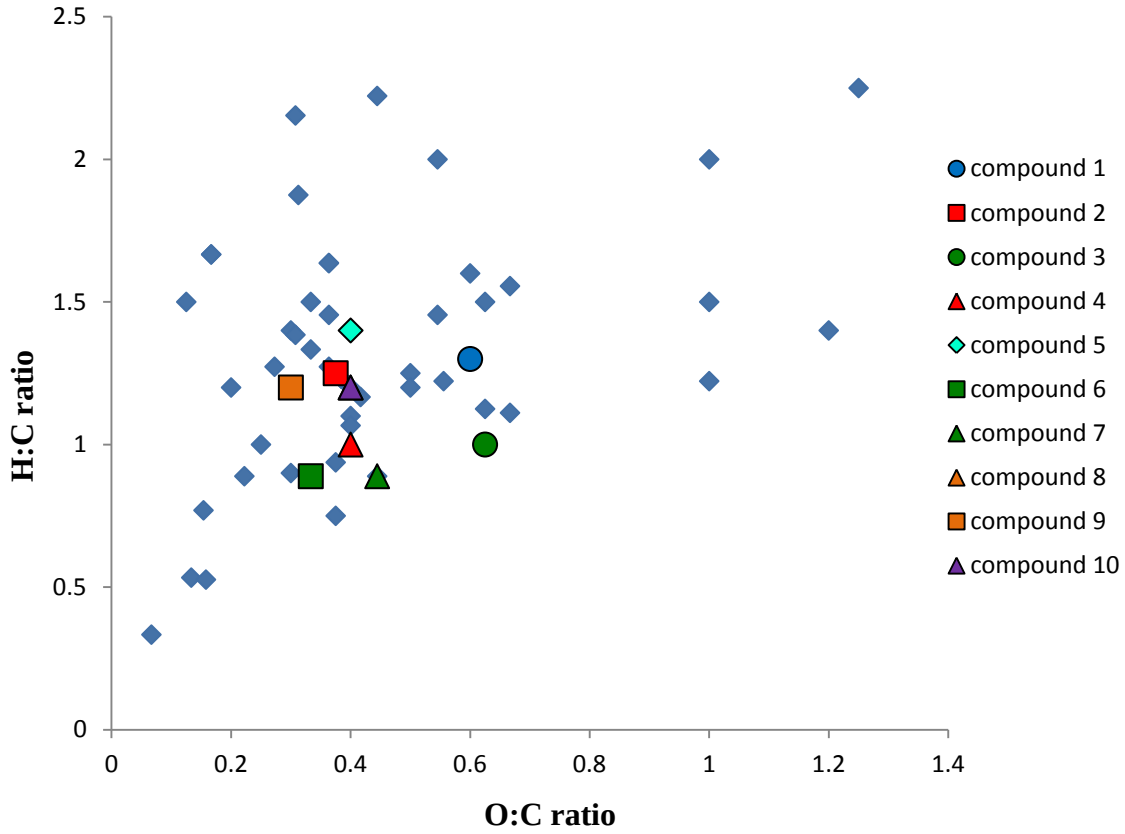
Error = displayed in ppm and calculated by taking the difference between the exact and measured mass for the assigned molecular formula; dividing the difference by the exact mass and multiplying by 10^6. MF score = the fit of the theoretical and measured isotopic distribution and abundance for the assigned molecular formula (displayed in percent).

Table S2 – The molecular formulae (MF) and associated errors of the identified SOA compounds in experiment MC_{high} using FTICR-MS and HPLC-QTOFMS in positive ionisation mode.

t_R	MW [g mol^{-1}]	FTICR-MS MF	Error [ppm]	Score [%]	HPLC-QTOFMS MF	Error [ppm]	Score [%]
34.3	98				$C_6H_{10}O$*	18	100
36.4	98				$C_6H_{10}O$*	14	100
33.7	120				$C_4H_8O_4$	-88.2	0
28.2	146	$C_7H_{14}O_3$	-1.9	100	$C_8H_{12}O$*	30.1	100
18.5	151				$C_4H_9NO_5$	-21.2	100
27.3	164				$C_{10}H_{12}O_2$	16.6	100
12.1	168	$C_9H_{12}O_3$*	4.7	100	$C_9H_{12}O_2$†	3.1	100
27.9	170	$C_8H_{10}O_4$*	4.4	100	$C_{11}H_{12}O_3$	-2.6	100
14.5	177				$C_5H_7NO_6$	-26.2	100
27.6	180				$C_{10}H_{12}O_3$	-7.8	100
22.5	180	$C_{10}H_{12}O_3$*	5	85.11	$C_{10}H_{12}O_3$*	8.9	100
36	180	$C_{10}H_{12}O_3$*	4.6	100	$C_{10}H_{12}O_3$*	-39.1	0.63
33.5	182	$C_{10}H_{14}O_3$*	4.7	100	$C_{10}H_{14}O_3$*	-54.5	0.02
10.2	184				$C_8H_8O_5$	48	0.02
15.7	188	$C_8H_{12}O_5$*	4.6	100	$C_8H_{12}O_5$*	-59.2	0
41.2	192	$C_9H_{20}O_4$*	3.9	100	$C_9H_{20}O_4$*	37.7	100
20.5	196				$C_{10}H_{12}O_4$	9.9	100

19.8	196	$C_{10}H_{12}O_4$*	5	100	$C_{10}H_{12}O_4$*	9.4	100
10.8	198	$C_{13}H_{10}O_2$*	4.2	100	$C_{13}H_{10}O_2$*	-35.7	0
14.1	198	$C_{30}H_{10}O_2$*	4.2	100	$C_{13}H_{10}O_2$*	22.9	3.11
14.8	204	$C_{12}H_{12}O_3$*	16.6	100			
19.1	212	$C_{10}H_{12}O_5$*	4.2	88.4			
33	212	$C_{11}H_{16}O_4$*	5.1	100	$C_{10}H_{18}O_6$	23.4	0.5
21.4	214	$C_{11}H_{18}O_4$*	5	100			
41.5	218	$C_9H_{14}O_6$*	5	100	$C_9H_{20}O_7$	-1.9	100
16.3	220	$C_{15}H_8O_2$	15.1	8.62	$C_8H_{12}O_7$	1.5	100
20.9	226	$C_{12}H_{18}O_4$*	5.4	100	$C_{12}H_{18}O_4$*	48	0
30.4	232	$C_{10}H_{16}O_6$	5.3	100	$C_{10}H_{16}O_6$	-10.7	100
43.2	234	$C_{13}H_{16}O_5$*	5.6	100	$C_{13}H_{20}O_5$	-9.7	100
33.8	238	$C_{13}H_{18}O_4$*	5.4	100	$C_{13}H_{18}O_4$*	33.1	0
17.1	244	$C_{11}H_{16}O_6$*	5.6	100			
47.4	248	$C_{13}H_{28}O_4$*	9.3	100	$C_{13}H_{28}O_4$*	-54.2	0
37.7	250	$C_{11}H_{22}O_6$*	6.2	100	$C_{11}H_{22}O_6$*	-17.4	4.07
8.9	286	$C_{19}H_{10}O_3$	5.2	100	$C_{19}H_{10}O_3$	43.7	0
44	302	$C_{16}H_{30}O_5$*	6.2	100	$C_{16}H_{30}O_5$*	49.4	0

* Identified as $[M+Na]^+$, the Na adduct has been removed from molecular formula and molecular weight corrected. † Identified as $[M+K]^+$, the K adduct has been removed from molecular formula and molecular weight corrected. Error = displayed in ppm and calculated by taking the difference between the exact and measured mass for the assigned molecular formula; dividing the difference by the exact mass and multiplying by 10^6. MF score = the fit of the theoretical and measured isotopic distribution and abundance for the assigned molecular formula (displayed in percent)



SI Figure 1 – Van Krevelen plot of the 59 SOA compounds observed in MC_{high}. Blue diamond's represent structurally unidentified compounds. Legend shows the structurally identified compounds 1 to 10, refer to Table 2 for compound identification. For the structurally identified compounds only; related generations of compounds are shown in the same colour. The change of shape but use of the same colour indicates a

change in the SOA compound structure through the reaction with $^{\bullet}OH$ radicals or NO_2. Compounds 8 and 10 are structural isomers; compound 8 is hidden by compound 10.