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Supplement of

Formation of highly oxygenated organic molecules from the oxidation of limonene by OH radical: significant contribution of H-abstraction pathway

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This supplement expounds the calibration coefficient of NO_3^--CIMS for H_2SO_4 and the distribution and possible formation pathway of monomers with carbon number less than 10 and dimers. Moreover, additional schemes, figures and tables are presented beside those in the main text.

S1 Calibration coefficient of NO_3^--CIMS for H_2SO_4

The calibration coefficient of H_2SO_4 was used to convert peak intensity measured by CIMS to concentrations. The concentrations of H_2SO_4 can be described as follows:

$$[H_2SO_4] = C \times I \qquad \text{(Eq. S1)}$$

where C is the calibration coefficient of H_2SO_4, I is the peak intensity of H_2SO_4 determined by normalized peak area of H_2SO_4 at time t, i.e., the peak area divided by total signal of mass spectrum (termed as normalized count (nc)).

In this study, the concentration of HOM was calculated according the calibration coefficient of H_2SO_4 and peak intensity of HOM. It relies on the premises that the charging efficiency of HOM and H_2SO_4 by NO_3^- are about the same and close to the collision limit (Ehn et al., 2014; Jokinen et al., 2015). In the SAPHIR chamber, H_2SO_4 was generated from oxidation of SO_2 by OH radical (Zhao et al., 2016). OH radicals and SO_2 were characterized by using laser induced fluorescence (LIF) and SO_2 analyzer (Thermo Systems 43i), respectively (Zhao et al., 2021). The concentration of H_2SO_4 in the chamber can be described by the following equation.

$$\frac{d[H_2SO_4]}{dt} = k[SO_2][OH] - (k_{wl} + k_{dil})[H_2SO_4] \qquad \text{(Eq. S2)}$$

where $[H_2SO_4]$, $[SO_2]$, [OH] represent the respective concentration, k is the rate constant for the reaction of SO_2 with OH, k_{wl} and k_{dil} are the wall loss rate of H_2SO_4 (~2.2×10^{-3} s^{-1} in fan-on condition; ~6.0×10^{-4} s^{-1} in fan-off condition) and the dilution rate of H_2SO_4 (~1×10^{-5} s^{-1}) (Zhao et al., 2018; Guo et al., 2022), respectively. Substituting Eq. S1 to Eq. S2 and integrating, one can get

$$C = \frac{k[SO_2][OH]}{\frac{I-I_0}{t}+(k_{wl}+k_{dil})I} \qquad \text{(Eq. S3)}$$

where I_0 is the peak intensity at the initial time. C was determined to be 2.5×10^{10} molecules cm^{-3} nc^{-1} (Zhao et al., 2021). The second term of denominator in Eq. S3 is much smaller than the first term and can omitted. The uncertainty of C was estimated to -52%/+101% from the uncertainty of SO_2 concentration (~7 %), OH concentration (~ 10 %), I (~ 10%) and k (Δlogk=±0.3) using error propagation, which have been used in our previous calibration (Zhao et al., 2021).

S2 Importance of secondary-generation chemistry in HOM formation

When we focus on the early stages of the experiments (first 15 min), secondary chemistry is not important in this study. This can be quantified by the following comparison of the chemistry of the limonene and limonaldehyde, which is the dominant first-generation C_{10} product. To quantify the relative importance of these two pathways, the relative reaction rates of hydrogen abstraction from limonene+OH to that from limonaldehyde+OH were calculated as below:

$$\frac{R[LIM+OH]_{H\ abstraction}}{R[LIMAL+OH]_{H\ abstraction}} = \frac{k[LIM+OH]\times[LIM]\times[OH]\times BR_{LIM}[H\ abstraction]}{k[LIMAL+OH]\times[LIMAL]\times[OH]\times BR_{LIMAL}[H\ abstraction]}$$

$$= \frac{k[LIM+OH]\times[LIM]\times BR_{LIM}[H\ abstraction]}{k[LIMAL+OH]\times[LIM]_r\times Y[LIMAL]\times BR_{LIMAL}[H\ abstraction]} \qquad \text{(Eq. S4)}$$

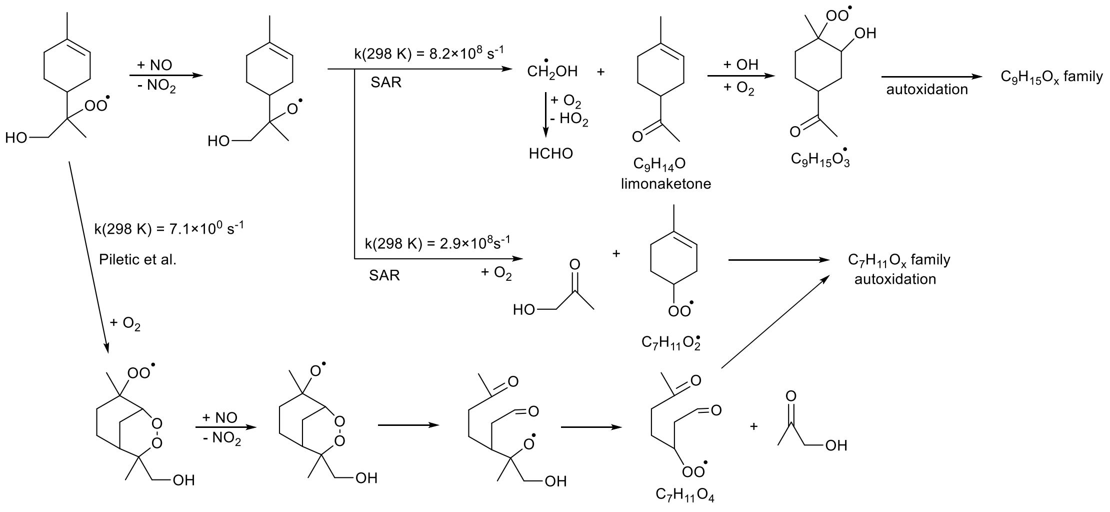
where k[LIM+OH] and k[LIMAL+OH] are reaction rate constants based on MCM v3.3.1 (Atkinson, 1997). [LIM], [LIMAL], and [OH] are the concentrations of limonene, limonaldehyde, and OH radicals, while limonene and OH radicals concentrations were measured and concentrations of limonaldehyde were estimated on the basis of their NO-dependent yields (0.29 at low NO and 0.28 at high NO) (Y[LIMAL] in Equation S4) (Hakola et al., 1994). BR_{LIM}[H abstraction] and BR_{LIMAL}[H abstraction] are the branching ratio of H-abstraction channel from limonene + OH and limonaldehyde + OH, respectively. The branching ratio is 0.34 for the reaction limonene + OH (Rio et al., 2010) and 0.29 for limonaldehyde + OH based on MCM v3.3.1 (http://mcm.york.ac.uk/). The uncertainties of the relative reaction rates were estimated to be -41%/+141% at low NO and high NO, from the uncertainty of limonene concentration (~15%), k[LIM+OH] (Δlogk=±0.08), and Y[LIMAL] (±0.06 at low NO and high NO) using error propagation. As a result, hydrogen abstraction from limonene is 19-1600 times faster than that from limonaldehyde at low NO and 29-87 times at high NO (Fig. S9). Note that the concentrations of limonaldehyde were estimated from consumed limonene, which only reflect the production and neglect consumption. Therefore, the relative importance of limonaldehyde was even overestimated using this method. Based on this evidence, the contribution of limonaldehyde to HOM formation was likely negligible at early stages of the experiments. Therefore, the second-generation reactions are unlikely to contribute the $C_{10}H_{15}O_x$-related HOM observed in our study.

S3 Formation mechanism of $C_{<10}$ monomers

$C_7H_8O_x$ (x=5-7, 9, 14) and $C_9H_{15}NO_x$ (x=6-14) were the most abundant $C_{<10}$ monomers at low and high NO, respectively, with $C_9H_{15}NO_x$ the second most abundant $C_{<10}$ monomers family in low NO condition. In addition, $C_7H_9O_x\bullet$ (x=5,10) and $C_7H_{11}O_x\bullet$ (x=10,11) were also observed at high NO.

Given the smaller carbon backbone, these monomers are likely formed from fragmentation reactions of an alkoxy intermediate formed in the reaction of RO_2 with NO, the dominant bimolecular RO_2 loss process in our reaction system. Within the first 15 min of the experiments, at low and high NO the ratios of $\frac{C_{6-9}\ monomers}{total\ HOM\ products}$ are 0.24 and 0.46, respectively. This is consistent with the ratios of $\frac{C_{10}H_{15}NO_x+C_{10}H_{17}NO_x}{C_{10}\ monomers}$ (0.28 and 0.55 at low and high NO, respectively), which indicated that high NO concentration is conducive to the generation of organic nitrates and fragment products.

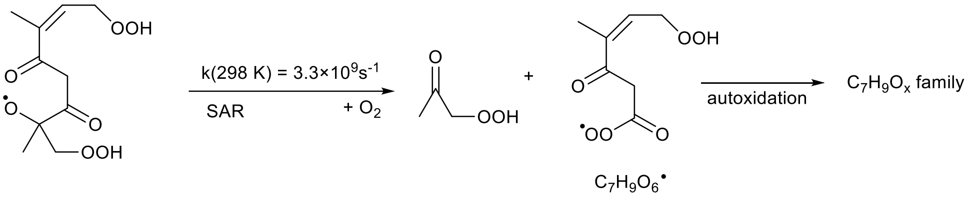
For $C_9H_{15}NO_x$, a formation pathway based on the OH addition step on the exocyclic double bond seems most likely (see below), though other pathways may exist. This mechanism of single carbon loss in monoterpene oxidation was already discussed in previous work (Bianchi et al., 2019; Fry et al., 2011). It initially forms limonaketone which is oxidized further after reaction with OH; this compound is known to form SOA (e.g. Donahue et al. (2007)). The $C_9H_{15}NO_x$ product family was also observed in the NO_3 initiated oxidation of limonene, however it gained its nitrogen by the NO_3 radical addition (Guo et al., 2022). In field observations, the $C_9H_{15}NO_x$ nitrate family was found to reach a maximum during daytime between 9:00 and 12:00, highly correlated with the NO_x maximum concentration (Massoli et al., 2018).



Scheme S1. Example reaction scheme for $C_7H_{11}O_x$• and $C_9H_{15}O_x$•family formation

Formation of C_7 HOM is more pronounced at low NO conditions where autoxidation of RO_2 has less competition by reaction with NO, suggesting that C_7 HOM are likely formed by fragmentation of oxygenated intermediates, e.g., alkoxy formed from the reaction of RO_2 with NO. Furthermore, for e.g., $C_7H_8O_x$ (x=5-7, 9, 14) not all members of the family where observed, which suggests they are likely not formed from their own autoxidation chains as most C_{10} monomers, but from fragmentation of C_{10} monomers.

The OH addition channel (see above) readily produces $C_7H_{11}O_x$•, which can autoxidize (possibly involving further alkoxy-peroxy steps) to generate the corresponding family of HOM. For $C_7H_9O_x$• we show an example pathway from an intermediate proposed in the C_{10} autoxidation chain after H-abstraction (see scheme 2 in the main text). The latter RO_2 family also gives rise to the observed termination $C_7H_8O_x$, products, which was also observed in limonene+O_3 oxidation (Tomaz et al., 2021).



Scheme S2. Example reaction scheme for $C_7H_9O_x$• family formation

We could not find an apparent pathway to $C_8H_{11}O_x$• which is analogously to the example mechanisms proposed in this work. However, alkoxy fragmentation in other autoxidation pathways of the ring-opened intermediates, or in intermediates formed in secondary chemistry, are likely to offer pathways to these radicals.

It seems likely that many of these $C_{<10}$ HOM families are not necessarily formed from one parent molecule that undergoes autoxidation, but rather that a fraction of the C_{10} HOM autoxidation intermediates decomposes after reaction with NO throughout the entire C_{10} autoxidation chain. The probability of decomposition then depends on the lifetime of the RO_2 intermediate, in competition with the NO reaction, and the competition between fragmentation and H-migration in the resulting alkoxy radical. Given the highly branched mechanism, it is outside the scope of this work to try and create a full model to describe this, and such a diffuse set of $C_{<10}$ HOM sources would make a simplified model analysis of the HOM yields meaningless.

S4 Formation mechanism of dimers

The formation pathways of all dimer families were considered as accretion reaction of two monomers RO_2, which followed the Reaction S1 (R. S1). Similar to monomers, several dimer families were observable in HOM dimer spectrum. Among the dimers, compounds with 20 carbons are the dominant families. We take $C_{20}H_{30-34}O_x$ families as examples to further discuss the formation pathway of dimers observed in our experiments. Based on reaction R. S1, $C_{20}H_{30}O_x$ families are likely formed by two RO_2 radicals $C_{10}H_{15}O_x\bullet$ (R. S2). As x in the monomers is above 7, the oxygen number of $C_{20}H_{30}O_x$ is expected to be above 12, with an O_2 eliminated in the dimerization reaction. This is generally in accord with the relatively higher intensity of $C_{20}H_{30}O_x$ with $x \geq 12$ in this families at both low and high NO (Table S8 and Table S9). However, at low NO, there are still very small amounts $C_{20}H_{30}O_{10}$ (1.3%) observed. Based on reaction R. S2, $C_{10}H_{15}O_x\bullet$ radicals with $x \leq 6$ were required to participate in dimer formation to explain the observed $C_{20}H_{30}O_{10}$. However, we did not observe them because of their low concentration or the lower sensitivity of NO_3^--CIMS to less oxygenated organics.

$$\text{Monomer } RO_2\ 1 + \text{Monomer } RO_2\ 2 \rightarrow \text{Dimer} + O_2 \qquad \text{(R. S1)}$$

$$C_{10}H_{15}O_{x1}\bullet + C_{10}H_{15}O_{x2}\bullet \rightarrow C_{20}H_{30}O_{x1+x2-2} + O_2 \qquad \text{(R. S2)}$$

Similarly, $C_{20}H_{34}O_x$ families were likely formed by two $C_{10}H_{17}O_x\bullet$ radicals, as reaction R. S3 shows. As x in the monomers are above 8 in low NO condition and above 5 at high NO condition, the oxygen number of $C_{20}H_{34}O_x$ is expected to be above 14 and 8, respectively. However, we still observed $C_{20}H_{34}O_x$ with x=10-13 in this study (Table S8 and Table S9). $C_{20}H_{34}O_x$ families in low NO condition may be attributed to the participation some other less oxygenated RO_2 radicals in dimer formation, which cannot be detected by NO_3^--CIMS as mentioned above. This method-specific phenomenon of dimers products has also been described in our previous studies (Shen et al., 2021; Guo et al., 2022).

$$C_{10}H_{17}O_{x1}\bullet + C_{10}H_{17}O_{x2}\bullet \rightarrow C_{20}H_{34}O_{x1+x2-2} + O_2 \qquad \text{(R. S3)}$$

Moreover, $C_{20}H_{32}O_x$ may be formed by the cross-accretion reaction of one $C_{10}H_{15}O_x\bullet$ RO_2 radical and one $C_{10}H_{17}O_x\bullet$ RO_2 radical (R. S4). Due to the monomer oxygen number being above 7 and 8 in low NO condition and above 7 and 5 in high NO condition, the oxygen number of $C_{20}H_{32}O_x$ is expected to be above 13 and 10, respectively. The expected oxygen atom number in $C_{20}H_{32}O_x$ is consistent with the observation of $C_{20}H_{32}O_{x(x\geq10)}$ in high NO condition (Table S9), but not consistent with the observed $C_{20}H_{32}O_{x(x\geq9)}$ in low NO condition. This again suggests that less oxygenated RO_2 participated in dimer formation $C_{20}H_{32}O_x$. The ratios of $C_{20}H_{30}O_x/C_{20}H_{32}O_x/C_{20}H_{34}O_x$ at low and high NO in the first 15 min were found to be 0.64: 1.6: 1 at low NO, and 1.12: 1.6: 1 at high NO. Based on R. S2-R. S4, these ratios can also confirm that $C_{10}H_{15}O_x\bullet$ radical related chemistry plays an important role in dimers formation from limonene+OH oxidation.

$$C_{10}H_{15}O_{x1}\bullet + C_{10}H_{17}O_{x2}\bullet \rightarrow C_{20}H_{32}O_{x1+x2-2} + O_2 \qquad \text{(R. S4)}$$

There are two more families $C_{19}H_{30}O_x$ (x=10-17) and $C_{19}H_{32}O_x$ (x=10-15) families besides the dominant C_{20} dimers families in low NO condition. Considering that $C_{10}H_{15}O_x\bullet$ and $C_{10}H_{17}O_x\bullet$ were the most abundant RO_2 radicals in this study, and based on the above reaction pathway (R. S1), $C_9H_{15}O_x\bullet$ RO_2 radicals were expected. The $C_{19}H_{30}O_x$ and $C_{19}H_{32}O_x$ families with oxygen numbers<10 were not observed during the experiments. It is likely that the sensitivity to $C_9H_{15}O_x\bullet$ RO_2 radicals with lower oxygen numbers was too low to allow detection by the NO_3^--CIMS. Meanwhile, C_{17} or C_{18} dimers were likely formed by C_7 and C_8 monomers RO_2 radical through the reaction pathway (R. S1). Possible formation pathways of dominant oligomer families are illustrated in Table S10. Even though the concentrations of C_7 and C_8 monomers RO_2 radical were low and the concentrations of their dimer products were less than C_{20} dimers, as extremely low volatility organic compounds (ELVOCs), dimer are expected to be easily condensed in the particle phase (Tröstl et al., 2016) and thus still play an important role in the new particle formation or growth.

S5 Supplement figures and tables

Figure S1-S9

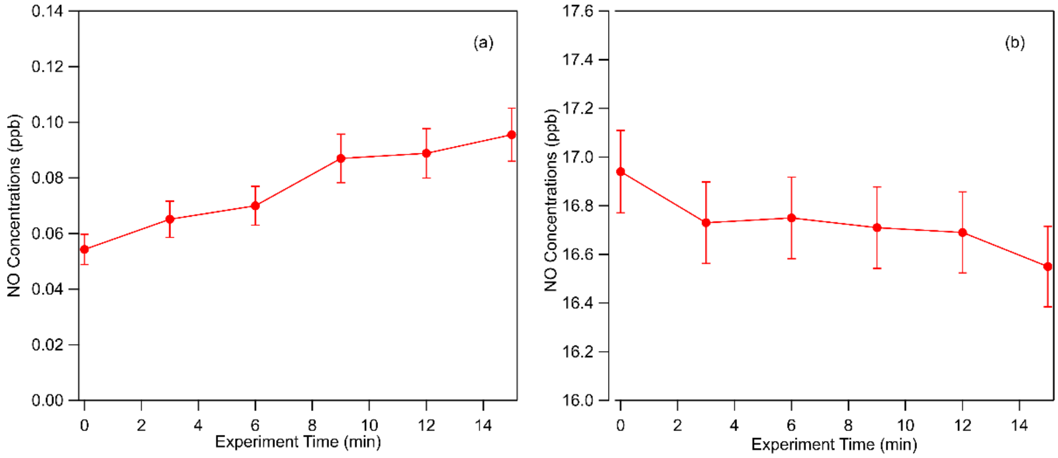


Figure S1. The concentrations of NO at (a) low and (b) high NO in the first 15 min experiments of this study

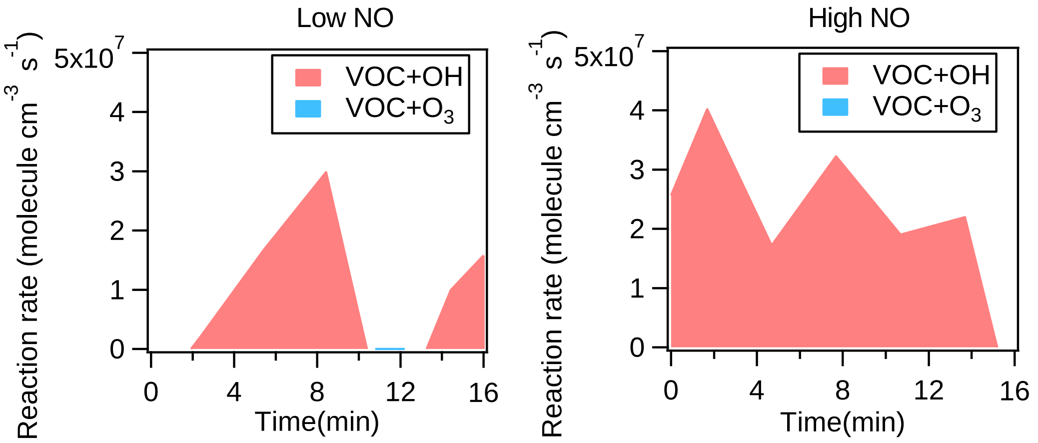


Figure S2. The reaction rate k[VOC][oxidant] for VOC+OH and VOC+O_3 at low and high NO of the first 15 min in this study. The VOC+OH rate is stacked on the VOC+O_3 rate. Noted that VOC+OH rate is close to zero when clouds pass by.

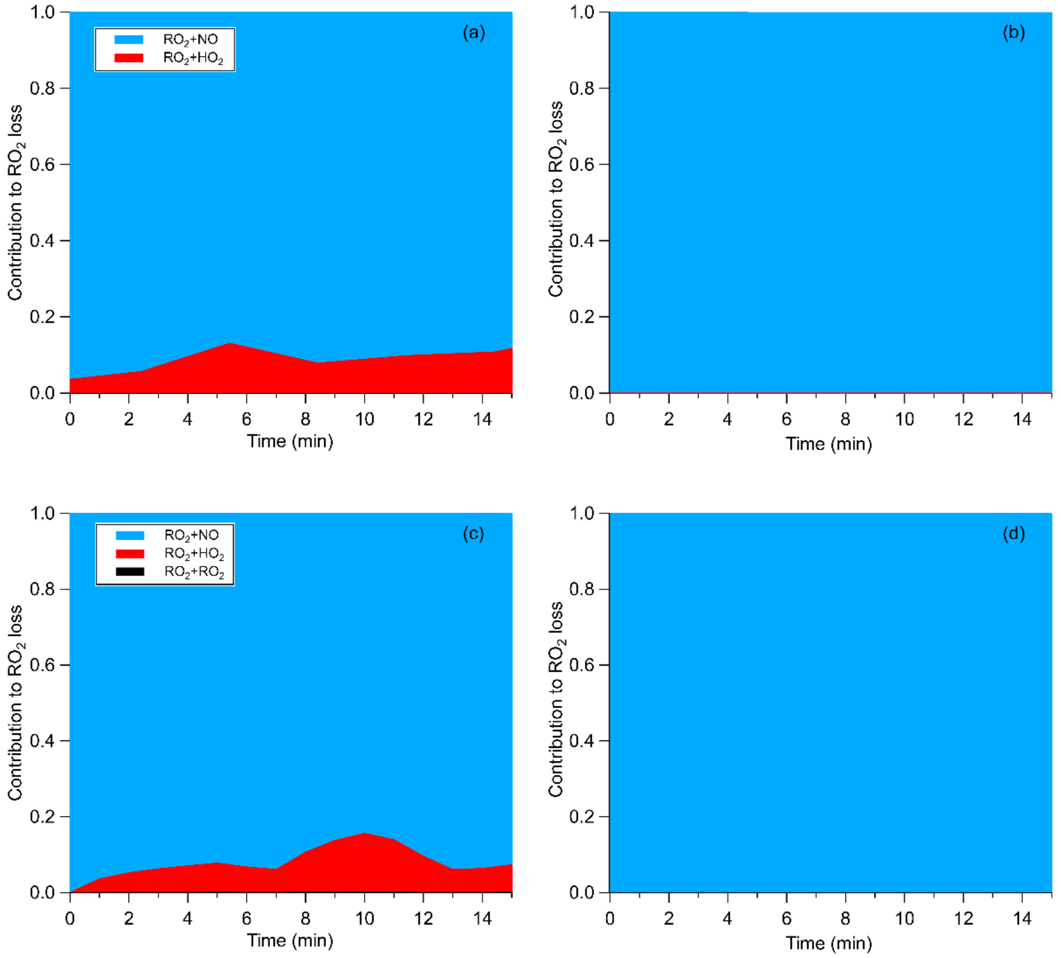


Figure S3. The contribution of RO_2 loss by RO_2+NO and RO_2+HO_2 at low NO (a, c) and high NO (b, d) in this study. The contribution of RO_2 loss by RO_2+NO and RO_2+HO_2 in panel (a) and (b) were obtained using measured RO_2, HO_2, and NO concentrations. An average reactive rate constants for the reaction RO_2 with NO ($k = 7.5*10^{-12}*Exp(290/T)$), HO_2 ($k = 5.2*10^{-13}*Exp(980/T)$), and RO_2 ($k = 9.2*10^{-14}$) were used mainly based MCM v3.3.1 and the reference therein. And the data in panel (c) and (d) were obtained using box model with MCM according to the initial conditions in this study.

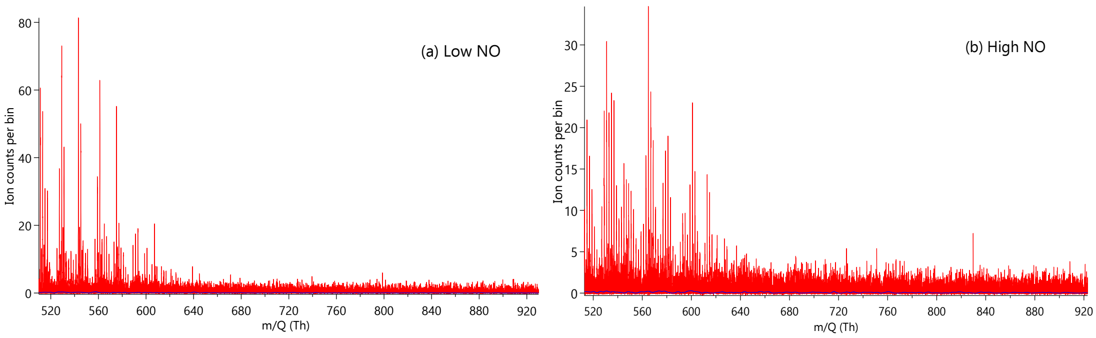


Figure S4. The average mass spectrum in the range of 520-920 Th at low and high NO over the first 15 min.

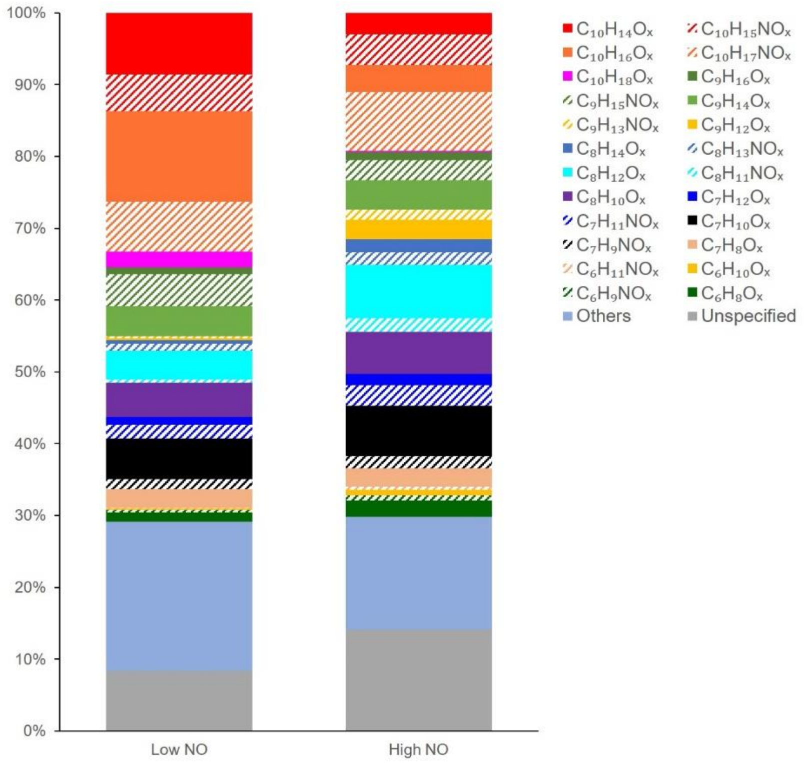


Figure S5. The contributions of different monomers formed in the oxidation of limonene by OH at 15 mins after the start of the experiments. Others: identified compounds not being C_6-C_{10} monomers; Unspecified: compounds to which specific elemental formula could not be attributed.

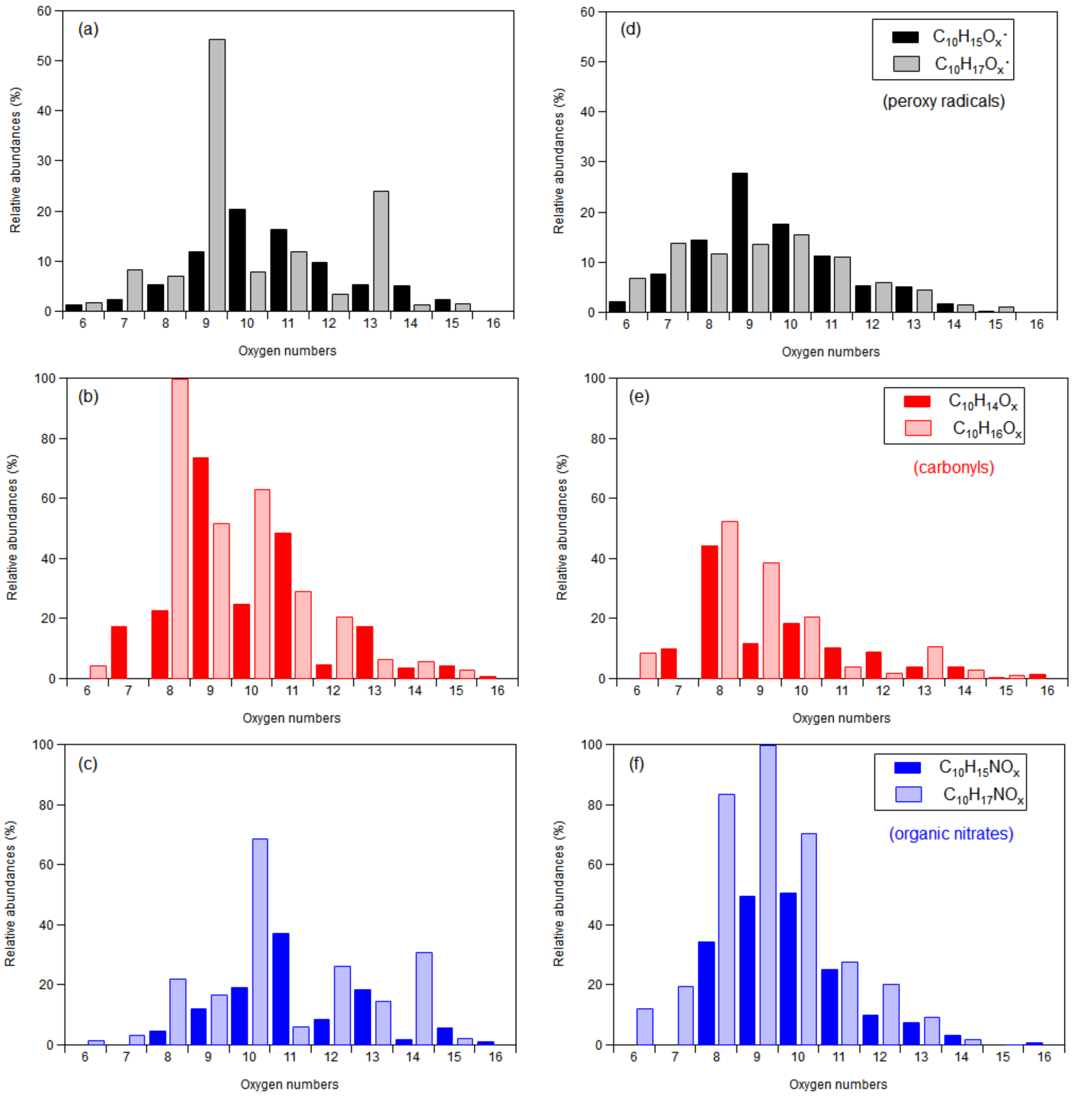


Figure S6. Relative abundances of individual products at low NO (0.06 - 0.1 ppb, panel a-c) and high NO (~17 ppb, panel d-f) at the first 15 min with the panels (a, d) showing $C_{10}H_{15}O_x\bullet$ (peroxy radicals, x=6-15) and $C_{10}H_{17}O_x\bullet$ (peroxy radicals, x=6-15) in black, the panels (b, e) showing $C_{10}H_{14}O_x$ (carbonyls, x=7-16) and $C_{10}H_{16}O_x$ (carbonyls, x=6, 8-15) in red, and the panels (c, f) showing $C_{10}H_{15}NO_x$ (organic nitrates, x=8-16) and $C_{10}H_{17}NO_x$ (organic nitrates, x=6-15) in blue. $C_{10}H_{15}O_x\bullet$ and their related products are in solid bars and $C_{10}H_{17}O_x\bullet$ and their related products are in transparent bars. The individual products are normalized to the signals the most abundant individual product respectively ($C_{10}H_{16}O_8$ at low NO and $C_{10}H_{17}NO_9$ at high NO).

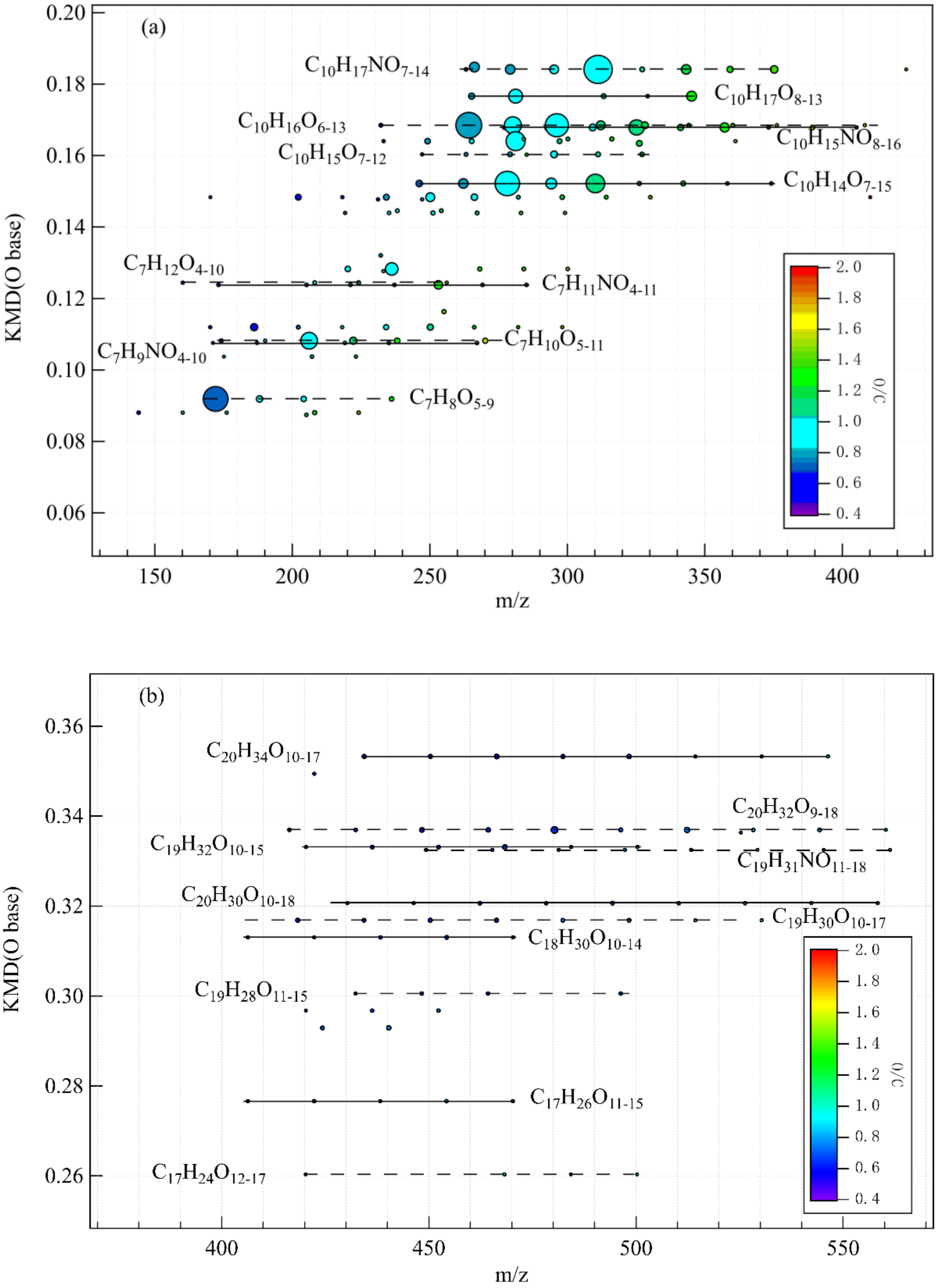


Figure S7. O-based Kendrick mass defect plot of **(a)** monomers and **(b)** dimers products at low NO. The area of the circles is proportional to the average signal intensity of each peak during 15 min after the louvres opening. Dashed lines mark the product families with organic nitrates; solid line mark the product families without nitrogen.

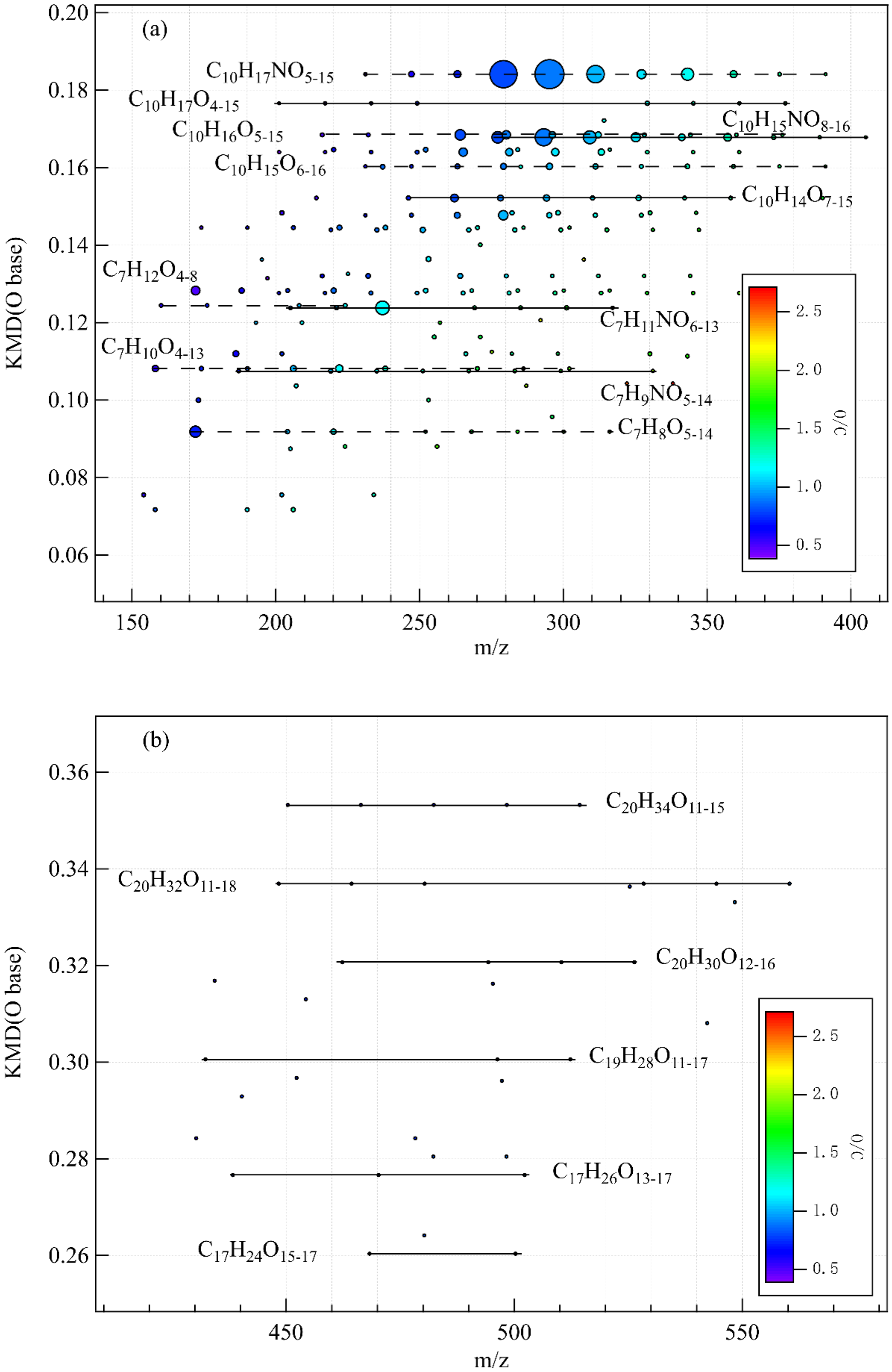


Figure S8. O-based Kendrick mass defect plot of **(a)** monomers and **(b)** dimers products at high NO. The area of the circles is proportional to the average signal intensity of each peak during 15 min after the louvres opening. Solid lines mark the products families.

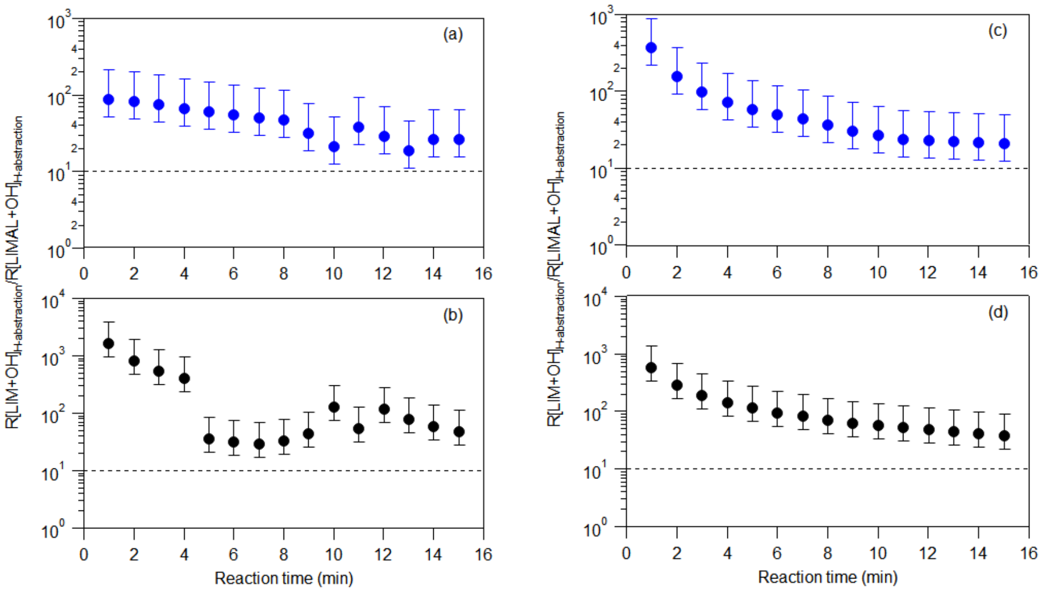


Figure S9. The relative ratio of hydrogen abstraction rate of the reaction limonene+OH to that of the reaction limonaldehyde+OH within the first 15 min reaction time obtained from measured at low NO (a, c) and high NO (b, d). Panels a-b and c-d show the results obtained from measured limonene concentration and limonaldehyde yield and from MCM modeling, respectively. The dashed lines are at the value of 10 (i.e., ~10% contribution of secondary chemistry). Note that different scales of y axes between panel (a, c) and (b, d). The large change in panel (b) results from the large measurement uncertainty of low accumulated limonene consumption measured by PTR-ToF-MS in the first few minutes.

Table S1-S10

Table S1. The experimental conditions in this study

Exp.	**Limonene added (ppb)**	**NO added (ppb)**	**OH (cm^{-3})**	**RH**
Low NO	**7**	**none**	**5.3*10^5**	**75%**
High NO	**7**	**17**	**2.2*10^5**	**75%**

Table S2. Relative average signal of $C_{10}H_{15}O_x$• radicals and their termination products in low NO conditions. The signal is each peak's average signal within the first 15 min of the experiment, normalized to that of $C_{10}H_{16}O_8$ as the highest peak. "M", "M-17", "M-15" and "M+1" represent the molecular weight of the RO_2 and their termination products with RO_2, HO_2 and NO, respectively.

RO_2	RC=O	ROH	ROOH	$RONO_2$
$C_{10}H_{15}O_6$ 1.4%			$C_{10}H_{16}O_6$ 4.6%	
$C_{10}H_{15}O_7$ 2.5%		$C_{10}H_{16}O_6$ 4.6%		$C_{10}H_{15}NO_8$ 5.0%
$C_{10}H_{15}O_8$ 5.5%	$C_{10}H_{14}O_7$ 17.7%		$C_{10}H_{16}O_8$ 100%	$C_{10}H_{15}NO_9$ 12.3%
$C_{10}H_{15}O_9$ 12.1%	$C_{10}H_{14}O_8$ 22.8%	$C_{10}H_{16}O_8$ 100%	$C_{10}H_{16}O_9$ 51.9%	$C_{10}H_{15}NO_{10}$ 19.5%
$C_{10}H_{15}O_{10}$ 20.3%	$C_{10}H_{14}O_9$ 73.4%	$C_{10}H_{16}O_9$ 51.9%	$C_{10}H_{16}O_{10}$ 63.3%	$C_{10}H_{15}NO_{11}$ 37.6%
$C_{10}H_{15}O_{11}$ 16.5%	$C_{10}H_{14}O_{10}$ 24.9%	$C_{10}H_{16}O_{10}$ 63.3%	$C_{10}H_{16}O_{11}$ 29.4%	$C_{10}H_{15}NO_{12}$ 8.8%
$C_{10}H_{15}O_{12}$ 9.9%	$C_{10}H_{14}O_{11}$ 48.8%	$C_{10}H_{16}O_{11}$ 29.4%	$C_{10}H_{16}O_{12}$ 21.0%	$C_{10}H_{15}NO_{13}$ 18.7%
$C_{10}H_{15}O_{13}$ 5.6%	$C_{10}H_{14}O_{12}$ 4.9%	$C_{10}H_{16}O_{12}$ 21.0%	$C_{10}H_{16}O_{13}$ 6.7%	$C_{10}H_{15}NO_{14}$ 2.2%
$C_{10}H_{15}O_{14}$ 5.4%	$C_{10}H_{14}O_{13}$ 17.84%	$C_{10}H_{16}O_{13}$ 6.7%	$C_{10}H_{16}O_{14}$ 5.9%	$C_{10}H_{15}NO_{15}$ 5.9%
$C_{10}H_{15}O_{15}$ 2.5%	$C_{10}H_{14}O_{14}$ 3.8%	$C_{10}H_{16}O_{14}$ 5.9%	$C_{10}H_{16}O_{15}$ 3.1%	$C_{10}H_{15}NO_{16}$ 1.4%

Table S3. Relative average signal of $C_{10}H_{17}O_x$• radicals and their termination products in low NO conditions. The percentage value is the peak's average signal within the first 15 min of the experiment, relative to that of $C_{10}H_{16}O_8$. "M", "M-17", "M-15" and "M+1" represent the molecular weight of the RO_2 and their termination products with RO_2, HO_2 and NO, respectively.

RO_2	RC=O	ROH	ROOH	$RONO_2$
$C_{10}H_{17}O_6$ 1.9%				$C_{10}H_{17}NO_7$ 3.6%
$C_{10}H_{17}O_7$ 8.6%	$C_{10}H_{16}O_6$ 4.6%			$C_{10}H_{17}NO_8$ 22.2%
$C_{10}H_{17}O_8$ 7.2%			$C_{10}H_{18}O_8$ 34.2%	$C_{10}H_{17}NO_9$ 16.9%
$C_{10}H_{17}O_9$ 54.4%	$C_{10}H_{16}O_8$ 100%	$C_{10}H_{18}O_8$ 34.2%		$C_{10}H_{17}NO_{10}$ 69.1%
$C_{10}H_{17}O_{10}$ 8.1%	$C_{10}H_{16}O_9$ 51.9%			$C_{10}H_{17}NO_{11}$ 6.3%
$C_{10}H_{17}O_{11}$ 12.0%	$C_{10}H_{16}O_{10}$ 63.3%			$C_{10}H_{17}NO_{12}$ 26.3%
$C_{10}H_{17}O_{12}$ 3.7%	$C_{10}H_{16}O_{11}$ 29.4%		$C_{10}H_{18}O_{12}$ 17.0%	$C_{10}H_{17}NO_{13}$ 14.7%
$C_{10}H_{17}O_{13}$ 24.2%	$C_{10}H_{16}O_{12}$ 21.0%	$C_{10}H_{18}O_{12}$ 17.0%		$C_{10}H_{17}NO_{14}$ 31.0%
$C_{10}H_{17}O_{14}$ 1.6%	$C_{10}H_{16}O_{13}$ 6.7%			$C_{10}H_{17}NO_{15}$ 2.6%
$C_{10}H_{17}O_{15}$ 1.7%	$C_{10}H_{16}O_{14}$ 5.9%			

Table S4. Identification of HOM monomers and dimers species at low NO.

m/z	Detected ion formula	Target molecule formula
324.0186	$C_5H_{11}NO_{14}[^{15}N]-$	$C_5H_{11}NO_{11}$
387.0143	$C_5H_{12}N_2O_{17}[^{15}N]-$	$C_5H_{12}N_2O_{14}$
237.9971	$C_5H_5NO_9[^{15}N]-$	$C_5H_5NO_6$
253.0080	$C_5H_6N_2O_9[^{15}N]-$	$C_5H_6N_2O_6$
209.0069	$C_5H_6O_8[^{15}N]-$	$C_5H_6O_5$
225.0018	$C_5H_6O_9[^{15}N]-$	$C_5H_6O_6$
319.9873	$C_5H_7NO_{14}[^{15}N]-$	$C_5H_7NO_{11}$
211.0226	$C_5H_8O_8[^{15}N]-$	$C_5H_8O_5$
209.0433	$C_6H_{10}O_7[^{15}N]-$	$C_6H_{10}O_4$
320.0237	$C_6H_{11}NO_{13}[^{15}N]-$	$C_6H_{11}NO_{10}$
354.0292	$C_6H_{13}NO_{15}[^{15}N]-$	$C_6H_{13}NO_{12}$
202.0123	$C_6H_5NO_6[^{15}N]-$	$C_6H_5NO_3$
218.0073	$C_6H_5NO_7[^{15}N]-$	$C_6H_5NO_4$
249.9971	$C_6H_5NO_9[^{15}N]-$	$C_6H_5NO_6$
376.9724	$C_6H_6N_2O_{16}[^{15}N]-$	$C_6H_6N_2O_{13}$
284.9866	$C_6H_6O_{12}[^{15}N]-$	$C_6H_6O_9$
237.0018	$C_6H_6O_9[^{15}N]-$	$C_6H_6O_6$
268.0077	$C_6H_7NO_{10}[^{15}N]-$	$C_6H_7NO_7$
284.0026	$C_6H_7NO_{11}[^{15}N]-$	$C_6H_7NO_8$
252.0127	$C_6H_7NO_9[^{15}N]-$	$C_6H_7NO_6$
283.0186	$C_6H_8N_2O_{10}[^{15}N]-$	$C_6H_8N_2O_7$
299.0135	$C_6H_8N_2O_{11}[^{15}N]-$	$C_6H_8N_2O_8$
207.0277	$C_6H_8O_7[^{15}N]-$	$C_6H_8O_4$
223.0226	$C_6H_8O_8[^{15}N]-$	$C_6H_8O_5$
239.0175	$C_6H_8O_9[^{15}N]-$	$C_6H_8O_6$
271.0073	$C_6H_8O_{11}[^{15}N]-$	$C_6H_8O_8$
287.0022	$C_6H_8O_{12}[^{15}N]-$	$C_6H_8O_9$
238.0335	$C_6H_9NO_8[^{15}N]-$	$C_6H_9NO_5$
270.0233	$C_6H_9NO_{10}[^{15}N]-$	$C_6H_9NO_7$
286.0182	$C_6H_9NO_{11}[^{15}N]-$	$C_6H_9NO_8$
345.0189	$C_7H_{10}N_2O_{13}[^{15}N]-$	$C_7H_{10}N_2O_{10}$
408.9986	$C_7H_{10}N_2O_{17}[^{15}N]-$	$C_7H_{10}N_2O_{14}$
237.0382	$C_7H_{10}O_8[^{15}N]-$	$C_7H_{10}O_5$
253.0331	$C_7H_{10}O_9[^{15}N]-$	$C_7H_{10}O_6$
269.0281	$C_7H_{10}O_{10}[^{15}N]-$	$C_7H_{10}O_7$
285.0230	$C_7H_{10}O_{11}[^{15}N]-$	$C_7H_{10}O_8$
301.0179	$C_7H_{10}O_{12}[^{15}N]-$	$C_7H_{10}O_9$
317.0128	$C_7H_{10}O_{13}[^{15}N]-$	$C_7H_{10}O_{10}$
333.0077	$C_7H_{10}O_{14}[^{15}N]-$	$C_7H_{10}O_{11}$
284.0390	$C_7H_{11}NO_{10}[^{15}N]-$	$C_7H_{11}NO_7$
300.0339	$C_7H_{11}NO_{11}[^{15}N]-$	$C_7H_{11}NO_8$

316.0288	$C_7H_{11}NO_{12}[^{15}N]$-	$C_7H_{11}NO_9$
332.0237	$C_7H_{11}NO_{13}[^{15}N]$-	$C_7H_{11}NO_{10}$
348.0186	$C_7H_{11}NO_{14}[^{15}N]$-	$C_7H_{11}NO_{11}$
268.0440	$C_7H_{11}NO_9[^{15}N]$-	$C_7H_{11}NO_6$
333.0315	$C_7H_{12}NO_{13}[^{15}N]$-	$C_7H_{12}NO_{10}$
223.0590	$C_7H_{12}O_7[^{15}N]$-	$C_7H_{12}O_4$
239.0539	$C_7H_{12}O_8[^{15}N]$-	$C_7H_{12}O_5$
271.0437	$C_7H_{12}O_{10}[^{15}N]$-	$C_7H_{12}O_7$
287.0386	$C_7H_{12}O_{11}[^{15}N]$-	$C_7H_{12}O_8$
319.0284	$C_7H_{12}O_{13}[^{15}N]$-	$C_7H_{12}O_{10}$
217.0120	$C_7H_6O_7[^{15}N]$-	$C_7H_6O_4$
233.0069	$C_7H_6O_8[^{15}N]$-	$C_7H_6O_5$
235.0226	$C_7H_8O_8[^{15}N]$-	$C_7H_8O_5$
251.0175	$C_7H_8O_9[^{15}N]$-	$C_7H_8O_6$
267.0124	$C_7H_8O_{10}[^{15}N]$-	$C_7H_8O_7$
299.0022	$C_7H_8O_{12}[^{15}N]$-	$C_7H_8O_9$
378.9768	$C_7H_8O_{17}[^{15}N]$-	$C_7H_8O_{14}$
218.0436	$C_7H_9NO_6[^{15}N]$-	$C_7H_9NO_3$
234.0386	$C_7H_9NO_7[^{15}N]$-	$C_7H_9NO_4$
250.0335	$C_7H_9NO_8[^{15}N]$-	$C_7H_9NO_5$
282.0233	$C_7H_9NO_{10}[^{15}N]$-	$C_7H_9NO_7$
298.0182	$C_7H_9NO_{11}[^{15}N]$-	$C_7H_9NO_8$
314.0131	$C_7H_9NO_{12}[^{15}N]$-	$C_7H_9NO_9$
330.0080	$C_7H_9NO_{13}[^{15}N]$-	$C_7H_9NO_{10}$
452.9884	$C_8H_{10}N_2O_{19}[^{15}N]$-	$C_8H_{10}N_2O_{16}$
233.0433	$C_8H_{10}O_7[^{15}N]$-	$C_8H_{10}O_4$
249.0382	$C_8H_{10}O_8[^{15}N]$-	$C_8H_{10}O_5$
265.0331	$C_8H_{10}O_9[^{15}N]$-	$C_8H_{10}O_6$
281.0281	$C_8H_{10}O_{10}[^{15}N]$-	$C_8H_{10}O_7$
297.0230	$C_8H_{10}O_{11}[^{15}N]$-	$C_8H_{10}O_8$
313.0179	$C_8H_{10}O_{12}[^{15}N]$-	$C_8H_{10}O_9$
329.0128	$C_8H_{10}O_{13}[^{15}N]$-	$C_8H_{10}O_{10}$
361.0026	$C_8H_{10}O_{15}[^{15}N]$-	$C_8H_{10}O_{12}$
296.0390	$C_8H_{11}NO_{10}[^{15}N]$-	$C_8H_{11}NO_7$
312.0339	$C_8H_{11}NO_{11}[^{15}N]$-	$C_8H_{11}NO_8$
376.0135	$C_8H_{11}NO_{15}[^{15}N]$-	$C_8H_{11}NO_{12}$
378.0054	$C_8H_{11}O_{16}[^{15}N]$-	$C_8H_{11}O_{13}$
343.0397	$C_8H_{12}N_2O_{12}[^{15}N]$-	$C_8H_{12}N_2O_9$
267.0488	$C_8H_{12}O_9[^{15}N]$-	$C_8H_{12}O_6$
283.0437	$C_8H_{12}O_{10}[^{15}N]$-	$C_8H_{12}O_7$
299.0386	$C_8H_{12}O_{11}[^{15}N]$-	$C_8H_{12}O_8$
331.0284	$C_8H_{12}O_{13}[^{15}N]$-	$C_8H_{12}O_{10}$
347.0234	$C_8H_{12}O_{14}[^{15}N]$-	$C_8H_{12}O_{11}$

363.0183	$C_8H_{12}O_{15}[^{15}N]-$	$C_8H_{12}O_{12}$
282.0597	$C_8H_{13}NO_9[^{15}N]-$	$C_8H_{13}NO_6$
298.0546	$C_8H_{13}NO_{10}[^{15}N]-$	$C_8H_{13}NO_7$
314.0495	$C_8H_{13}NO_{11}[^{15}N]-$	$C_8H_{13}NO_8$
330.0444	$C_8H_{13}NO_{12}[^{15}N]-$	$C_8H_{13}NO_9$
346.0393	$C_8H_{13}NO_{13}[^{15}N]-$	$C_8H_{13}NO_{10}$
362.0343	$C_8H_{13}NO_{14}[^{15}N]-$	$C_8H_{13}NO_{11}$
301.0543	$C_8H_{14}O_{11}[^{15}N]-$	$C_8H_{14}O_8$
317.0492	$C_8H_{14}O_{12}[^{15}N]-$	$C_8H_{14}O_9$
316.0652	$C_8H_{15}NO_{11}[^{15}N]-$	$C_8H_{15}NO_8$
340.0288	$C_9H_{11}NO_{12}[^{15}N]-$	$C_9H_{11}NO_9$
355.0397	$C_9H_{12}N_2O_{12}[^{15}N]-$	$C_9H_{12}N_2O_9$
295.0437	$C_9H_{12}O_{10}[^{15}N]-$	$C_9H_{12}O_7$
454.9929	$C_9H_{12}O_{20}[^{15}N]-$	$C_9H_{12}O_{17}$
310.0546	$C_9H_{13}NO_{10}[^{15}N]-$	$C_9H_{13}NO_7$
294.0597	$C_9H_{13}NO_9[^{15}N]-$	$C_9H_{13}NO_6$
389.0452	$C_9H_{14}N_2O_{14}[^{15}N]-$	$C_9H_{14}N_2O_{11}$
405.0401	$C_9H_{14}N_2O_{15}[^{15}N]-$	$C_9H_{14}N_2O_{12}$
437.0299	$C_9H_{14}N_2O_{17}[^{15}N]-$	$C_9H_{14}N_2O_{14}$
233.0797	$C_9H_{14}O_6[^{15}N]-$	$C_9H_{14}O_3$
265.0695	$C_9H_{14}O_8[^{15}N]-$	$C_9H_{14}O_5$
281.0644	$C_9H_{14}O_9[^{15}N]-$	$C_9H_{14}O_6$
297.0594	$C_9H_{14}O_{10}[^{15}N]-$	$C_9H_{14}O_7$
313.0543	$C_9H_{14}O_{11}[^{15}N]-$	$C_9H_{14}O_8$
329.0492	$C_9H_{14}O_{12}[^{15}N]-$	$C_9H_{14}O_9$
361.0390	$C_9H_{14}O_{14}[^{15}N]-$	$C_9H_{14}O_{11}$
377.0339	$C_9H_{14}O_{15}[^{15}N]-$	$C_9H_{14}O_{12}$
473.0034	$C_9H_{14}O_{21}[^{15}N]-$	$C_9H_{14}O_{18}$
296.0753	$C_9H_{15}NO_9[^{15}N]-$	$C_9H_{15}NO_6$
312.0703	$C_9H_{15}NO_{10}[^{15}N]-$	$C_9H_{15}NO_7$
328.0652	$C_9H_{15}NO_{11}[^{15}N]-$	$C_9H_{15}NO_8$
344.0601	$C_9H_{15}NO_{12}[^{15}N]-$	$C_9H_{15}NO_9$
360.0550	$C_9H_{15}NO_{13}[^{15}N]-$	$C_9H_{15}NO_{10}$
424.0347	$C_9H_{15}NO_{17}[^{15}N]-$	$C_9H_{15}NO_{14}$
407.0557	$C_9H_{16}N_2O_{15}[^{15}N]-$	$C_9H_{16}N_2O_{12}$
331.0648	$C_9H_{16}O_{12}[^{15}N]-$	$C_9H_{16}O_9$
347.0597	$C_9H_{16}O_{13}[^{15}N]-$	$C_9H_{16}O_{10}$
363.0547	$C_9H_{16}O_{14}[^{15}N]-$	$C_9H_{16}O_{11}$
379.0496	$C_9H_{16}O_{15}[^{15}N]-$	$C_9H_{16}O_{12}$
362.0706	$C_9H_{17}NO_{13}[^{15}N]-$	$C_9H_{17}NO_{10}$
361.0866	$C_9H_{18}N_2O_{12}[^{15}N]-$	$C_9H_{18}N_2O_9$
377.0815	$C_9H_{18}N_2O_{13}[^{15}N]-$	$C_9H_{18}N_2O_{10}$
409.0714	$C_9H_{18}N_2O_{15}[^{15}N]-$	$C_9H_{18}N_2O_{12}$

309.0594	$C_{10}H_{14}O_{10}[^{15}N]$-	$C_{10}H_{14}O_7$
325.0543	$C_{10}H_{14}O_{11}[^{15}N]$-	$C_{10}H_{14}O_8$
341.0492	$C_{10}H_{14}O_{12}[^{15}N]$-	$C_{10}H_{14}O_9$
357.0441	$C_{10}H_{14}O_{13}[^{15}N]$-	$C_{10}H_{14}O_{10}$
373.0390	$C_{10}H_{14}O_{14}[^{15}N]$-	$C_{10}H_{14}O_{11}$
389.0339	$C_{10}H_{14}O_{15}[^{15}N]$-	$C_{10}H_{14}O_{12}$
469.0085	$C_{10}H_{14}O_{20}[^{15}N]$-	$C_{10}H_{14}O_{17}$
324.0703	$C_{10}H_{15}NO_{10}[^{15}N]$-	$C_{10}H_{15}NO_7$
340.0652	$C_{10}H_{15}NO_{11}[^{15}N]$-	$C_{10}H_{15}NO_8$
356.0601	$C_{10}H_{15}NO_{12}[^{15}N]$-	$C_{10}H_{15}NO_9$
372.0550	$C_{10}H_{15}NO_{13}[^{15}N]$-	$C_{10}H_{15}NO_{10}$
388.0499	$C_{10}H_{15}NO_{14}[^{15}N]$-	$C_{10}H_{15}NO_{11}$
404.0448	$C_{10}H_{15}NO_{15}[^{15}N]$-	$C_{10}H_{15}NO_{12}$
420.0397	$C_{10}H_{15}NO_{16}[^{15}N]$-	$C_{10}H_{15}NO_{13}$
436.0347	$C_{10}H_{15}NO_{17}[^{15}N]$-	$C_{10}H_{15}NO_{14}$
452.0296	$C_{10}H_{15}NO_{18}[^{15}N]$-	$C_{10}H_{15}NO_{15}$
468.0245	$C_{10}H_{15}NO_{19}[^{15}N]$-	$C_{10}H_{15}NO_{16}$
310.0672	$C_{10}H_{15}O_{10}[^{15}N]$-	$C_{10}H_{15}O_7$
326.0621	$C_{10}H_{15}O_{11}[^{15}N]$-	$C_{10}H_{15}O_8$
342.0570	$C_{10}H_{15}O_{12}[^{15}N]$-	$C_{10}H_{15}O_9$
358.0519	$C_{10}H_{15}O_{13}[^{15}N]$-	$C_{10}H_{15}O_{10}$
374.0468	$C_{10}H_{15}O_{14}[^{15}N]$-	$C_{10}H_{15}O_{11}$
390.0418	$C_{10}H_{15}O_{15}[^{15}N]$-	$C_{10}H_{15}O_{12}$
435.0506	$C_{10}H_{16}N_2O_{16}[^{15}N]$-	$C_{10}H_{16}N_2O_{13}$
295.0801	$C_{10}H_{16}O_9[^{15}N]$-	$C_{10}H_{16}O_6$
327.0699	$C_{10}H_{16}O_{11}[^{15}N]$-	$C_{10}H_{16}O_8$
343.0648	$C_{10}H_{16}O_{12}[^{15}N]$-	$C_{10}H_{16}O_9$
359.0597	$C_{10}H_{16}O_{13}[^{15}N]$-	$C_{10}H_{16}O_{10}$
375.0547	$C_{10}H_{16}O_{14}[^{15}N]$-	$C_{10}H_{16}O_{11}$
391.0496	$C_{10}H_{16}O_{15}[^{15}N]$-	$C_{10}H_{16}O_{12}$
407.0445	$C_{10}H_{16}O_{16}[^{15}N]$-	$C_{10}H_{16}O_{13}$
423.0394	$C_{10}H_{16}O_{17}[^{15}N]$-	$C_{10}H_{16}O_{14}$
439.0343	$C_{10}H_{16}O_{18}[^{15}N]$-	$C_{10}H_{16}O_{15}$
326.0859	$C_{10}H_{17}NO_{10}[^{15}N]$-	$C_{10}H_{17}NO_7$
342.0808	$C_{10}H_{17}NO_{11}[^{15}N]$-	$C_{10}H_{17}NO_8$
358.0757	$C_{10}H_{17}NO_{12}[^{15}N]$-	$C_{10}H_{17}NO_9$
374.0706	$C_{10}H_{17}NO_{13}[^{15}N]$-	$C_{10}H_{17}NO_{10}$
390.0656	$C_{10}H_{17}NO_{14}[^{15}N]$-	$C_{10}H_{17}NO_{11}$
406.0605	$C_{10}H_{17}NO_{15}[^{15}N]$-	$C_{10}H_{17}NO_{12}$
422.0554	$C_{10}H_{17}NO_{16}[^{15}N]$-	$C_{10}H_{17}NO_{13}$
328.0777	$C_{10}H_{17}O_{11}[^{15}N]$-	$C_{10}H_{17}O_8$
344.0727	$C_{10}H_{17}O_{12}[^{15}N]$-	$C_{10}H_{17}O_9$
376.0625	$C_{10}H_{17}O_{14}[^{15}N]$-	$C_{10}H_{17}O_{11}$

392.0574	$C_{10}H_{17}O_{15}[^{15}N]$-	$C_{10}H_{17}O_{12}$
408.0523	$C_{10}H_{17}O_{16}[^{15}N]$-	$C_{10}H_{17}O_{13}$
357.0917	$C_{10}H_{18}N_2O_{11}[^{15}N]$-	$C_{10}H_{18}N_2O_8$
421.0714	$C_{10}H_{18}N_2O_{15}[^{15}N]$-	$C_{10}H_{18}N_2O_{12}$
453.0612	$C_{10}H_{18}N_2O_{17}[^{15}N]$-	$C_{10}H_{18}N_2O_{14}$
329.0856	$C_{10}H_{18}O_{11}[^{15}N]$-	$C_{10}H_{18}O_8$
393.0652	$C_{10}H_{18}O_{15}[^{15}N]$-	$C_{10}H_{18}O_{12}$
493.1177	$C_{15}H_{26}O_{17}[^{15}N]$-	$C_{15}H_{26}O_{14}$
479.1384	$C_{15}H_{28}O_{16}[^{15}N]$-	$C_{15}H_{28}O_{13}$
495.1333	$C_{15}H_{28}O_{17}[^{15}N]$-	$C_{15}H_{28}O_{14}$
486.1231	$C_{16}H_{25}NO_{15}[^{15}N]$-	$C_{16}H_{25}NO_{12}$
473.1278	$C_{16}H_{26}O_{15}[^{15}N]$-	$C_{16}H_{26}O_{12}$
525.1439	$C_{16}H_{30}O_{18}[^{15}N]$-	$C_{16}H_{30}O_{15}$
541.1388	$C_{16}H_{30}O_{19}[^{15}N]$-	$C_{16}H_{30}O_{16}$
572.1446	$C_{16}H_{31}NO_{20}[^{15}N]$-	$C_{16}H_{31}NO_{17}$
543.1544	$C_{16}H_{32}O_{19}[^{15}N]$-	$C_{16}H_{32}O_{16}$
591.1392	$C_{16}H_{32}O_{22}[^{15}N]$-	$C_{16}H_{32}O_{19}$
623.1290	$C_{16}H_{32}O_{24}[^{15}N]$-	$C_{16}H_{32}O_{21}$
574.1603	$C_{16}H_{33}NO_{20}[^{15}N]$-	$C_{16}H_{33}NO_{17}$
590.1552	$C_{16}H_{33}NO_{21}[^{15}N]$-	$C_{16}H_{33}NO_{18}$
606.1501	$C_{16}H_{33}NO_{22}[^{15}N]$-	$C_{16}H_{33}NO_{19}$
622.1450	$C_{16}H_{33}NO_{23}[^{15}N]$-	$C_{16}H_{33}NO_{20}$
483.1122	$C_{17}H_{24}O_{15}[^{15}N]$-	$C_{17}H_{24}O_{12}$
531.0969	$C_{17}H_{24}O_{18}[^{15}N]$-	$C_{17}H_{24}O_{15}$
547.0918	$C_{17}H_{24}O_{19}[^{15}N]$-	$C_{17}H_{24}O_{16}$
563.0868	$C_{17}H_{24}O_{20}[^{15}N]$-	$C_{17}H_{24}O_{17}$
469.1329	$C_{17}H_{26}O_{14}[^{15}N]$-	$C_{17}H_{26}O_{11}$
485.1278	$C_{17}H_{26}O_{15}[^{15}N]$-	$C_{17}H_{26}O_{12}$
501.1227	$C_{17}H_{26}O_{16}[^{15}N]$-	$C_{17}H_{26}O_{13}$
517.1177	$C_{17}H_{26}O_{17}[^{15}N]$-	$C_{17}H_{26}O_{14}$
533.1126	$C_{17}H_{26}O_{18}[^{15}N]$-	$C_{17}H_{26}O_{15}$
487.1435	$C_{17}H_{28}O_{15}[^{15}N]$-	$C_{17}H_{28}O_{12}$
503.1384	$C_{17}H_{28}O_{16}[^{15}N]$-	$C_{17}H_{28}O_{13}$
483.1486	$C_{18}H_{28}O_{14}[^{15}N]$-	$C_{18}H_{28}O_{11}$
499.1435	$C_{18}H_{28}O_{15}[^{15}N]$-	$C_{18}H_{28}O_{12}$
515.1384	$C_{18}H_{28}O_{16}[^{15}N]$-	$C_{18}H_{28}O_{13}$
609.1398	$C_{18}H_{30}N_2O_{20}[^{15}N]$-	$C_{18}H_{30}N_2O_{17}$
469.1693	$C_{18}H_{30}O_{13}[^{15}N]$-	$C_{18}H_{30}O_{10}$
485.1642	$C_{18}H_{30}O_{14}[^{15}N]$-	$C_{18}H_{30}O_{11}$
501.1591	$C_{18}H_{30}O_{15}[^{15}N]$-	$C_{18}H_{30}O_{12}$
517.1540	$C_{18}H_{30}O_{16}[^{15}N]$-	$C_{18}H_{30}O_{13}$
533.1490	$C_{18}H_{30}O_{17}[^{15}N]$-	$C_{18}H_{30}O_{14}$
495.1486	$C_{19}H_{28}O_{14}[^{15}N]$-	$C_{19}H_{28}O_{11}$

511.1435	$C_{19}H_{28}O_{15}[^{15}N]^-$	$C_{19}H_{28}O_{12}$
527.1384	$C_{19}H_{28}O_{16}[^{15}N]^-$	$C_{19}H_{28}O_{13}$
559.1282	$C_{19}H_{28}O_{18}[^{15}N]^-$	$C_{19}H_{28}O_{15}$
481.1693	$C_{19}H_{30}O_{13}[^{15}N]^-$	$C_{19}H_{30}O_{10}$
497.1642	$C_{19}H_{30}O_{14}[^{15}N]^-$	$C_{19}H_{30}O_{11}$
513.1591	$C_{19}H_{30}O_{15}[^{15}N]^-$	$C_{19}H_{30}O_{12}$
529.1540	$C_{19}H_{30}O_{16}[^{15}N]^-$	$C_{19}H_{30}O_{13}$
545.1490	$C_{19}H_{30}O_{17}[^{15}N]^-$	$C_{19}H_{30}O_{14}$
561.1439	$C_{19}H_{30}O_{18}[^{15}N]^-$	$C_{19}H_{30}O_{15}$
577.1388	$C_{19}H_{30}O_{19}[^{15}N]^-$	$C_{19}H_{30}O_{16}$
593.1337	$C_{19}H_{30}O_{20}[^{15}N]^-$	$C_{19}H_{30}O_{17}$
558.1680	$C_{19}H_{31}N_2O_{16}[^{15}N]^-$	$C_{19}H_{31}N_2O_{13}$
512.1751	$C_{19}H_{31}NO_{14}[^{15}N]^-$	$C_{19}H_{31}NO_{11}$
528.1700	$C_{19}H_{31}NO_{15}[^{15}N]^-$	$C_{19}H_{31}NO_{12}$
544.1649	$C_{19}H_{31}NO_{16}[^{15}N]^-$	$C_{19}H_{31}NO_{13}$
560.1599	$C_{19}H_{31}NO_{17}[^{15}N]^-$	$C_{19}H_{31}NO_{14}$
576.1548	$C_{19}H_{31}NO_{18}[^{15}N]^-$	$C_{19}H_{31}NO_{15}$
592.1497	$C_{19}H_{31}NO_{19}[^{15}N]^-$	$C_{19}H_{31}NO_{16}$
608.1446	$C_{19}H_{31}NO_{20}[^{15}N]^-$	$C_{19}H_{31}NO_{17}$
624.1395	$C_{19}H_{31}NO_{21}[^{15}N]^-$	$C_{19}H_{31}NO_{18}$
483.1849	$C_{19}H_{32}O_{13}[^{15}N]^-$	$C_{19}H_{32}O_{10}$
499.1799	$C_{19}H_{32}O_{14}[^{15}N]^-$	$C_{19}H_{32}O_{11}$
515.1748	$C_{19}H_{32}O_{15}[^{15}N]^-$	$C_{19}H_{32}O_{12}$
531.1697	$C_{19}H_{32}O_{16}[^{15}N]^-$	$C_{19}H_{32}O_{13}$
547.1646	$C_{19}H_{32}O_{17}[^{15}N]^-$	$C_{19}H_{32}O_{14}$
563.1595	$C_{19}H_{32}O_{18}[^{15}N]^-$	$C_{19}H_{32}O_{15}$
493.1693	$C_{20}H_{30}O_{13}[^{15}N]^-$	$C_{20}H_{30}O_{10}$
509.1642	$C_{20}H_{30}O_{14}[^{15}N]^-$	$C_{20}H_{30}O_{11}$
573.1439	$C_{20}H_{30}O_{18}[^{15}N]^-$	$C_{20}H_{30}O_{15}$
589.1388	$C_{20}H_{30}O_{19}[^{15}N]^-$	$C_{20}H_{30}O_{16}$
605.1337	$C_{20}H_{30}O_{20}[^{15}N]^-$	$C_{20}H_{30}O_{17}$
621.1286	$C_{20}H_{30}O_{21}[^{15}N]^-$	$C_{20}H_{30}O_{18}$
588.1548	$C_{20}H_{31}NO_{18}[^{15}N]^-$	$C_{20}H_{31}NO_{15}$
526.1670	$C_{20}H_{31}O_{15}[^{15}N]^-$	$C_{20}H_{31}O_{12}$
542.1619	$C_{20}H_{31}O_{16}[^{15}N]^-$	$C_{20}H_{31}O_{13}$
479.1900	$C_{20}H_{32}O_{12}[^{15}N]^-$	$C_{20}H_{32}O_9$
495.1849	$C_{20}H_{32}O_{13}[^{15}N]^-$	$C_{20}H_{32}O_{10}$
511.1799	$C_{20}H_{32}O_{14}[^{15}N]^-$	$C_{20}H_{32}O_{11}$
527.1748	$C_{20}H_{32}O_{15}[^{15}N]^-$	$C_{20}H_{32}O_{12}$
559.1646	$C_{20}H_{32}O_{17}[^{15}N]^-$	$C_{20}H_{32}O_{14}$
575.1595	$C_{20}H_{32}O_{18}[^{15}N]^-$	$C_{20}H_{32}O_{15}$
607.1494	$C_{20}H_{32}O_{20}[^{15}N]^-$	$C_{20}H_{32}O_{17}$
623.1443	$C_{20}H_{32}O_{21}[^{15}N]^-$	$C_{20}H_{32}O_{18}$

497.2006	$C_{20}H_{34}O_{13}[^{15}N]^-$	$C_{20}H_{34}O_{10}$
513.1955	$C_{20}H_{34}O_{14}[^{15}N]^-$	$C_{20}H_{34}O_{11}$
529.1904	$C_{20}H_{34}O_{15}[^{15}N]^-$	$C_{20}H_{34}O_{12}$
545.1853	$C_{20}H_{34}O_{16}[^{15}N]^-$	$C_{20}H_{34}O_{13}$
561.1803	$C_{20}H_{34}O_{17}[^{15}N]^-$	$C_{20}H_{34}O_{14}$
577.1752	$C_{20}H_{34}O_{18}[^{15}N]^-$	$C_{20}H_{34}O_{15}$
593.1701	$C_{20}H_{34}O_{19}[^{15}N]^-$	$C_{20}H_{34}O_{16}$
609.1650	$C_{20}H_{34}O_{20}[^{15}N]^-$	$C_{20}H_{34}O_{17}$

Table S5. Identification of HOM monomers and dimers species at high NO.

m/z	Detected ion formula	Target molecule formula
277.0179	$C_5H_{10}O_{12}[^{15}N]-$	$C_5H_{10}O_9$
309.0077	$C_5H_{10}O_{14}[^{15}N]-$	$C_5H_{10}O_{11}$
340.9975	$C_5H_{10}O_{16}[^{15}N]-$	$C_5H_{10}O_{13}$
225.0018	$C_5H_6O_9[^{15}N]-$	$C_5H_6O_6$
256.0077	$C_5H_7NO_{10}[^{15}N]-$	$C_5H_7NO_7$
272.0026	$C_5H_7NO_{11}[^{15}N]-$	$C_5H_7NO_8$
287.9975	$C_5H_7NO_{12}[^{15}N]-$	$C_5H_7NO_9$
319.9873	$C_5H_7NO_{14}[^{15}N]-$	$C_5H_7NO_{11}$
303.0084	$C_5H_8N_2O_{12}[^{15}N]-$	$C_5H_8N_2O_9$
338.9819	$C_5H_8O_{16}[^{15}N]-$	$C_5H_8O_{13}$
242.0284	$C_5H_9NO_9[^{15}N]-$	$C_5H_9NO_6$
258.0233	$C_5H_9NO_{10}[^{15}N]-$	$C_5H_9NO_7$
274.0182	$C_5H_9NO_{11}[^{15}N]-$	$C_5H_9NO_8$
306.0080	$C_5H_9NO_{13}[^{15}N]-$	$C_5H_9NO_{10}$
353.9928	$C_5H_9NO_{16}[^{15}N]-$	$C_5H_9NO_{13}$
317.0240	$C_6H_{10}N_2O_{12}[^{15}N]-$	$C_6H_{10}N_2O_9$
305.0128	$C_6H_{10}O_{13}[^{15}N]-$	$C_6H_{10}O_{10}$
256.0440	$C_6H_{11}NO_9[^{15}N]-$	$C_6H_{11}NO_6$
272.0390	$C_6H_{11}NO_{10}[^{15}N]-$	$C_6H_{11}NO_7$
320.0237	$C_6H_{11}NO_{13}[^{15}N]-$	$C_6H_{11}NO_{10}$
303.0448	$C_6H_{12}N_2O_{11}[^{15}N]-$	$C_6H_{12}N_2O_8$
319.0397	$C_6H_{12}N_2O_{12}[^{15}N]-$	$C_6H_{12}N_2O_9$
274.0546	$C_6H_{13}NO_{10}[^{15}N]-$	$C_6H_{13}NO_7$
370.0241	$C_6H_{13}NO_{16}[^{15}N]-$	$C_6H_{13}NO_{13}$
281.0029	$C_6H_6N_2O_{10}[^{15}N]-$	$C_6H_6N_2O_7$
221.0069	$C_6H_6O_8[^{15}N]-$	$C_6H_6O_5$
237.0018	$C_6H_6O_9[^{15}N]-$	$C_6H_6O_6$
252.9968	$C_6H_6O_{10}[^{15}N]-$	$C_6H_6O_7$
268.9917	$C_6H_6O_{11}[^{15}N]-$	$C_6H_6O_8$
316.9764	$C_6H_6O_{14}[^{15}N]-$	$C_6H_6O_{11}$
268.0077	$C_6H_7NO_{10}[^{15}N]-$	$C_6H_7NO_7$
299.0135	$C_6H_8N_2O_{11}[^{15}N]-$	$C_6H_8N_2O_8$
223.0226	$C_6H_8O_8[^{15}N]-$	$C_6H_8O_5$
239.0175	$C_6H_8O_9[^{15}N]-$	$C_6H_8O_6$
271.0073	$C_6H_8O_{11}[^{15}N]-$	$C_6H_8O_8$
287.0022	$C_6H_8O_{12}[^{15}N]-$	$C_6H_8O_9$
318.9921	$C_6H_8O_{14}[^{15}N]-$	$C_6H_8O_{11}$
270.0233	$C_6H_9NO_{10}[^{15}N]-$	$C_6H_9NO_7$
286.0182	$C_6H_9NO_{11}[^{15}N]-$	$C_6H_9NO_8$
297.0342	$C_7H_{10}N_2O_{10}[^{15}N]-$	$C_7H_{10}N_2O_7$
329.0240	$C_7H_{10}N_2O_{12}[^{15}N]-$	$C_7H_{10}N_2O_9$

377.0088	$C_7H_{10}N_2O_{15}[^{15}N]-$	$C_7H_{10}N_2O_{12}$
221.0433	$C_7H_{10}O_7[^{15}N]-$	$C_7H_{10}O_4$
237.0382	$C_7H_{10}O_8[^{15}N]-$	$C_7H_{10}O_5$
253.0331	$C_7H_{10}O_9[^{15}N]-$	$C_7H_{10}O_6$
269.0281	$C_7H_{10}O_{10}[^{15}N]-$	$C_7H_{10}O_7$
285.0230	$C_7H_{10}O_{11}[^{15}N]-$	$C_7H_{10}O_8$
301.0179	$C_7H_{10}O_{12}[^{15}N]-$	$C_7H_{10}O_9$
333.0077	$C_7H_{10}O_{14}[^{15}N]-$	$C_7H_{10}O_{11}$
349.0026	$C_7H_{10}O_{15}[^{15}N]-$	$C_7H_{10}O_{12}$
364.9975	$C_7H_{10}O_{16}[^{15}N]-$	$C_7H_{10}O_{13}$
268.0440	$C_7H_{11}NO_9[^{15}N]-$	$C_7H_{11}NO_6$
284.0390	$C_7H_{11}NO_{10}[^{15}N]-$	$C_7H_{11}NO_7$
300.0339	$C_7H_{11}NO_{11}[^{15}N]-$	$C_7H_{11}NO_8$
332.0237	$C_7H_{11}NO_{13}[^{15}N]-$	$C_7H_{11}NO_{10}$
348.0186	$C_7H_{11}NO_{14}[^{15}N]-$	$C_7H_{11}NO_{11}$
364.0135	$C_7H_{11}NO_{15}[^{15}N]-$	$C_7H_{11}NO_{12}$
380.0084	$C_7H_{11}NO_{16}[^{15}N]-$	$C_7H_{11}NO_{13}$
299.0499	$C_7H_{12}N_2O_{10}[^{15}N]-$	$C_7H_{12}N_2O_7$
223.0590	$C_7H_{12}O_7[^{15}N]-$	$C_7H_{12}O_4$
239.0539	$C_7H_{12}O_8[^{15}N]-$	$C_7H_{12}O_5$
271.0437	$C_7H_{12}O_{10}[^{15}N]-$	$C_7H_{12}O_7$
287.0386	$C_7H_{12}O_{11}[^{15}N]-$	$C_7H_{12}O_8$
286.0546	$C_7H_{13}NO_{10}[^{15}N]-$	$C_7H_{13}NO_7$
334.0393	$C_7H_{13}NO_{13}[^{15}N]-$	$C_7H_{13}NO_{10}$
317.0604	$C_7H_{14}N_2O_{11}[^{15}N]-$	$C_7H_{14}N_2O_8$
480.0092	$C_7H_{15}NO_{22}[^{15}N]-$	$C_7H_{15}NO_{19}$
339.0547	$C_7H_{16}O_{14}[^{15}N]-$	$C_7H_{16}O_{11}$
217.0120	$C_7H_6O_7[^{15}N]-$	$C_7H_6O_4$
249.0018	$C_7H_6O_9[^{15}N]-$	$C_7H_6O_6$
296.0026	$C_7H_7NO_{11}[^{15}N]-$	$C_7H_7NO_8$
235.0226	$C_7H_8O_8[^{15}N]-$	$C_7H_8O_5$
267.0124	$C_7H_8O_{10}[^{15}N]-$	$C_7H_8O_7$
283.0073	$C_7H_8O_{11}[^{15}N]-$	$C_7H_8O_8$
314.9971	$C_7H_8O_{13}[^{15}N]-$	$C_7H_8O_{10}$
330.9921	$C_7H_8O_{14}[^{15}N]-$	$C_7H_8O_{11}$
346.9870	$C_7H_8O_{15}[^{15}N]-$	$C_7H_8O_{12}$
362.9819	$C_7H_8O_{16}[^{15}N]-$	$C_7H_8O_{13}$
378.9768	$C_7H_8O_{17}[^{15}N]-$	$C_7H_8O_{14}$
250.0335	$C_7H_9NO_8[^{15}N]-$	$C_7H_9NO_5$
282.0233	$C_7H_9NO_{10}[^{15}N]-$	$C_7H_9NO_7$
298.0182	$C_7H_9NO_{11}[^{15}N]-$	$C_7H_9NO_8$
314.0131	$C_7H_9NO_{12}[^{15}N]-$	$C_7H_9NO_9$
330.0080	$C_7H_9NO_{13}[^{15}N]-$	$C_7H_9NO_{10}$

346.0030	$C_7H_9NO_{14}[^{15}N]-$	$C_7H_9NO_{11}$
361.9979	$C_7H_9NO_{15}[^{15}N]-$	$C_7H_9NO_{12}$
393.9877	$C_7H_9NO_{17}[^{15}N]-$	$C_7H_9NO_{14}$
436.9935	$C_8H_{10}N_2O_{18}[^{15}N]-$	$C_8H_{10}N_2O_{15}$
249.0382	$C_8H_{10}O_8[^{15}N]-$	$C_8H_{10}O_5$
265.0331	$C_8H_{10}O_9[^{15}N]-$	$C_8H_{10}O_6$
281.0281	$C_8H_{10}O_{10}[^{15}N]-$	$C_8H_{10}O_7$
313.0179	$C_8H_{10}O_{12}[^{15}N]-$	$C_8H_{10}O_9$
329.0128	$C_8H_{10}O_{13}[^{15}N]-$	$C_8H_{10}O_{10}$
345.0077	$C_8H_{10}O_{14}[^{15}N]-$	$C_8H_{10}O_{11}$
361.0026	$C_8H_{10}O_{15}[^{15}N]-$	$C_8H_{10}O_{12}$
392.9925	$C_8H_{10}O_{17}[^{15}N]-$	$C_8H_{10}O_{14}$
264.0491	$C_8H_{11}NO_8[^{15}N]-$	$C_8H_{11}NO_5$
280.0440	$C_8H_{11}NO_9[^{15}N]-$	$C_8H_{11}NO_6$
296.0390	$C_8H_{11}NO_{10}[^{15}N]-$	$C_8H_{11}NO_7$
312.0339	$C_8H_{11}NO_{11}[^{15}N]-$	$C_8H_{11}NO_8$
328.0288	$C_8H_{11}NO_{12}[^{15}N]-$	$C_8H_{11}NO_9$
344.0237	$C_8H_{11}NO_{13}[^{15}N]-$	$C_8H_{11}NO_{10}$
360.0186	$C_8H_{11}NO_{14}[^{15}N]-$	$C_8H_{11}NO_{11}$
376.0135	$C_8H_{11}NO_{15}[^{15}N]-$	$C_8H_{11}NO_{12}$
392.0084	$C_8H_{11}NO_{16}[^{15}N]-$	$C_8H_{11}NO_{13}$
408.0034	$C_8H_{11}NO_{17}[^{15}N]-$	$C_8H_{11}NO_{14}$
423.9983	$C_8H_{11}NO_{18}[^{15}N]-$	$C_8H_{11}NO_{15}$
439.9932	$C_8H_{11}NO_{19}[^{15}N]-$	$C_8H_{11}NO_{16}$
235.0590	$C_8H_{12}O_7[^{15}N]-$	$C_8H_{12}O_4$
251.0539	$C_8H_{12}O_8[^{15}N]-$	$C_8H_{12}O_5$
267.0488	$C_8H_{12}O_9[^{15}N]-$	$C_8H_{12}O_6$
283.0437	$C_8H_{12}O_{10}[^{15}N]-$	$C_8H_{12}O_7$
315.0335	$C_8H_{12}O_{12}[^{15}N]-$	$C_8H_{12}O_9$
331.0284	$C_8H_{12}O_{13}[^{15}N]-$	$C_8H_{12}O_{10}$
347.0234	$C_8H_{12}O_{14}[^{15}N]-$	$C_8H_{12}O_{11}$
363.0183	$C_8H_{12}O_{15}[^{15}N]-$	$C_8H_{12}O_{12}$
379.0132	$C_8H_{12}O_{16}[^{15}N]-$	$C_8H_{12}O_{13}$
282.0597	$C_8H_{13}NO_9[^{15}N]-$	$C_8H_{13}NO_6$
298.0546	$C_8H_{13}NO_{10}[^{15}N]-$	$C_8H_{13}NO_7$
314.0495	$C_8H_{13}NO_{11}[^{15}N]-$	$C_8H_{13}NO_8$
330.0444	$C_8H_{13}NO_{12}[^{15}N]-$	$C_8H_{13}NO_9$
346.0393	$C_8H_{13}NO_{13}[^{15}N]-$	$C_8H_{13}NO_{10}$
362.0343	$C_8H_{13}NO_{14}[^{15}N]-$	$C_8H_{13}NO_{11}$
378.0292	$C_8H_{13}NO_{15}[^{15}N]-$	$C_8H_{13}NO_{12}$
394.0241	$C_8H_{13}NO_{16}[^{15}N]-$	$C_8H_{13}NO_{13}$
410.0190	$C_8H_{13}NO_{17}[^{15}N]-$	$C_8H_{13}NO_{14}$
329.0604	$C_8H_{14}N_2O_{11}[^{15}N]-$	$C_8H_{14}N_2O_8$

237.0746	$C_8H_{14}O_7[^{15}N]-$	$C_8H_{14}O_4$
253.0695	$C_8H_{14}O_8[^{15}N]-$	$C_8H_{14}O_5$
269.0644	$C_8H_{14}O_9[^{15}N]-$	$C_8H_{14}O_6$
301.0543	$C_8H_{14}O_{11}[^{15}N]-$	$C_8H_{14}O_8$
333.0441	$C_8H_{14}O_{13}[^{15}N]-$	$C_8H_{14}O_{10}$
349.0390	$C_8H_{14}O_{14}[^{15}N]-$	$C_8H_{14}O_{11}$
365.0339	$C_8H_{14}O_{15}[^{15}N]-$	$C_8H_{14}O_{12}$
300.0703	$C_8H_{15}NO_{10}[^{15}N]-$	$C_8H_{15}NO_7$
332.0601	$C_8H_{15}NO_{12}[^{15}N]-$	$C_8H_{15}NO_9$
380.0448	$C_8H_{15}NO_{15}[^{15}N]-$	$C_8H_{15}NO_{12}$
331.0761	$C_8H_{16}N_2O_{11}[^{15}N]-$	$C_8H_{16}N_2O_8$
342.9921	$C_8H_8O_{14}[^{15}N]-$	$C_8H_8O_{11}$
358.9870	$C_8H_8O_{15}[^{15}N]-$	$C_8H_8O_{12}$
422.9666	$C_8H_8O_{19}[^{15}N]-$	$C_8H_8O_{16}$
438.9616	$C_8H_8O_{20}[^{15}N]-$	$C_8H_8O_{17}$
453.9724	$C_8H_9NO_{20}[^{15}N]-$	$C_8H_9NO_{17}$
260.0542	$C_9H_{11}NO_7[^{15}N]-$	$C_9H_{11}NO_4$
355.0397	$C_9H_{12}N_2O_{12}[^{15}N]-$	$C_9H_{12}N_2O_9$
387.0295	$C_9H_{12}N_2O_{14}[^{15}N]-$	$C_9H_{12}N_2O_{11}$
231.0640	$C_9H_{12}O_6[^{15}N]-$	$C_9H_{12}O_3$
279.0488	$C_9H_{12}O_9[^{15}N]-$	$C_9H_{12}O_6$
295.0437	$C_9H_{12}O_{10}[^{15}N]-$	$C_9H_{12}O_7$
327.0335	$C_9H_{12}O_{12}[^{15}N]-$	$C_9H_{12}O_9$
343.0284	$C_9H_{12}O_{13}[^{15}N]-$	$C_9H_{12}O_{10}$
359.0234	$C_9H_{12}O_{14}[^{15}N]-$	$C_9H_{12}O_{11}$
375.0183	$C_9H_{12}O_{15}[^{15}N]-$	$C_9H_{12}O_{12}$
391.0132	$C_9H_{12}O_{16}[^{15}N]-$	$C_9H_{12}O_{13}$
294.0597	$C_9H_{13}NO_9[^{15}N]-$	$C_9H_{13}NO_6$
310.0546	$C_9H_{13}NO_{10}[^{15}N]-$	$C_9H_{13}NO_7$
326.0495	$C_9H_{13}NO_{11}[^{15}N]-$	$C_9H_{13}NO_8$
342.0444	$C_9H_{13}NO_{12}[^{15}N]-$	$C_9H_{13}NO_9$
358.0393	$C_9H_{13}NO_{13}[^{15}N]-$	$C_9H_{13}NO_{10}$
374.0343	$C_9H_{13}NO_{14}[^{15}N]-$	$C_9H_{13}NO_{11}$
390.0292	$C_9H_{13}NO_{15}[^{15}N]-$	$C_9H_{13}NO_{12}$
406.0241	$C_9H_{13}NO_{16}[^{15}N]-$	$C_9H_{13}NO_{13}$
341.0604	$C_9H_{14}N_2O_{11}[^{15}N]-$	$C_9H_{14}N_2O_8$
405.0401	$C_9H_{14}N_2O_{15}[^{15}N]-$	$C_9H_{14}N_2O_{12}$
249.0746	$C_9H_{14}O_7[^{15}N]-$	$C_9H_{14}O_4$
265.0695	$C_9H_{14}O_8[^{15}N]-$	$C_9H_{14}O_5$
281.0644	$C_9H_{14}O_9[^{15}N]-$	$C_9H_{14}O_6$
297.0594	$C_9H_{14}O_{10}[^{15}N]-$	$C_9H_{14}O_7$
313.0543	$C_9H_{14}O_{11}[^{15}N]-$	$C_9H_{14}O_8$
345.0441	$C_9H_{14}O_{13}[^{15}N]-$	$C_9H_{14}O_{10}$

361.0390	$C_9H_{14}O_{14}[^{15}N]-$	$C_9H_{14}O_{11}$
393.0288	$C_9H_{14}O_{16}[^{15}N]-$	$C_9H_{14}O_{13}$
409.0238	$C_9H_{14}O_{17}[^{15}N]-$	$C_9H_{14}O_{14}$
264.0855	$C_9H_{15}NO_7[^{15}N]-$	$C_9H_{15}NO_4$
280.0804	$C_9H_{15}NO_8[^{15}N]-$	$C_9H_{15}NO_5$
296.0753	$C_9H_{15}NO_9[^{15}N]-$	$C_9H_{15}NO_6$
312.0703	$C_9H_{15}NO_{10}[^{15}N]-$	$C_9H_{15}NO_7$
328.0652	$C_9H_{15}NO_{11}[^{15}N]-$	$C_9H_{15}NO_8$
344.0601	$C_9H_{15}NO_{12}[^{15}N]-$	$C_9H_{15}NO_9$
360.0550	$C_9H_{15}NO_{13}[^{15}N]-$	$C_9H_{15}NO_{10}$
376.0499	$C_9H_{15}NO_{14}[^{15}N]-$	$C_9H_{15}NO_{11}$
392.0448	$C_9H_{15}NO_{15}[^{15}N]-$	$C_9H_{15}NO_{12}$
408.0397	$C_9H_{15}NO_{16}[^{15}N]-$	$C_9H_{15}NO_{13}$
424.0347	$C_9H_{15}NO_{17}[^{15}N]-$	$C_9H_{15}NO_{14}$
375.0659	$C_9H_{16}N_2O_{13}[^{15}N]-$	$C_9H_{16}N_2O_{10}$
391.0608	$C_9H_{16}N_2O_{14}[^{15}N]-$	$C_9H_{16}N_2O_{11}$
283.0801	$C_9H_{16}O_9[^{15}N]-$	$C_9H_{16}O_6$
315.0699	$C_9H_{16}O_{11}[^{15}N]-$	$C_9H_{16}O_8$
347.0597	$C_9H_{16}O_{13}[^{15}N]-$	$C_9H_{16}O_{10}$
363.0547	$C_9H_{16}O_{14}[^{15}N]-$	$C_9H_{16}O_{11}$
379.0496	$C_9H_{16}O_{15}[^{15}N]-$	$C_9H_{16}O_{12}$
314.0859	$C_9H_{17}NO_{10}[^{15}N]-$	$C_9H_{17}NO_7$
330.0808	$C_9H_{17}NO_{11}[^{15}N]-$	$C_9H_{17}NO_8$
338.0495	$C_{10}H_{13}NO_{11}[^{15}N]-$	$C_{10}H_{13}NO_8$
386.0343	$C_{10}H_{13}NO_{14}[^{15}N]-$	$C_{10}H_{13}NO_{11}$
418.0241	$C_{10}H_{13}NO_{16}[^{15}N]-$	$C_{10}H_{13}NO_{13}$
369.0553	$C_{10}H_{14}N_2O_{12}[^{15}N]-$	$C_{10}H_{14}N_2O_9$
385.0502	$C_{10}H_{14}N_2O_{13}[^{15}N]-$	$C_{10}H_{14}N_2O_{10}$
401.0452	$C_{10}H_{14}N_2O_{14}[^{15}N]-$	$C_{10}H_{14}N_2O_{11}$
417.0401	$C_{10}H_{14}N_2O_{15}[^{15}N]-$	$C_{10}H_{14}N_2O_{12}$
465.0248	$C_{10}H_{14}N_2O_{18}[^{15}N]-$	$C_{10}H_{14}N_2O_{15}$
277.0695	$C_{10}H_{14}O_8[^{15}N]-$	$C_{10}H_{14}O_5$
309.0594	$C_{10}H_{14}O_{10}[^{15}N]-$	$C_{10}H_{14}O_7$
325.0543	$C_{10}H_{14}O_{11}[^{15}N]-$	$C_{10}H_{14}O_8$
341.0492	$C_{10}H_{14}O_{12}[^{15}N]-$	$C_{10}H_{14}O_9$
357.0441	$C_{10}H_{14}O_{13}[^{15}N]-$	$C_{10}H_{14}O_{10}$
373.0390	$C_{10}H_{14}O_{14}[^{15}N]-$	$C_{10}H_{14}O_{11}$
389.0339	$C_{10}H_{14}O_{15}[^{15}N]-$	$C_{10}H_{14}O_{12}$
405.0288	$C_{10}H_{14}O_{16}[^{15}N]-$	$C_{10}H_{14}O_{13}$
421.0238	$C_{10}H_{14}O_{17}[^{15}N]-$	$C_{10}H_{14}O_{14}$
453.0136	$C_{10}H_{14}O_{19}[^{15}N]-$	$C_{10}H_{14}O_{16}$
340.0652	$C_{10}H_{15}NO_{11}[^{15}N]-$	$C_{10}H_{15}NO_8$
356.0601	$C_{10}H_{15}NO_{12}[^{15}N]-$	$C_{10}H_{15}NO_9$

372.0550	$C_{10}H_{15}NO_{13}[^{15}N]-$	$C_{10}H_{15}NO_{10}$
388.0499	$C_{10}H_{15}NO_{14}[^{15}N]-$	$C_{10}H_{15}NO_{11}$
404.0448	$C_{10}H_{15}NO_{15}[^{15}N]-$	$C_{10}H_{15}NO_{12}$
420.0397	$C_{10}H_{15}NO_{16}[^{15}N]-$	$C_{10}H_{15}NO_{13}$
436.0347	$C_{10}H_{15}NO_{17}[^{15}N]-$	$C_{10}H_{15}NO_{14}$
468.0245	$C_{10}H_{15}NO_{19}[^{15}N]-$	$C_{10}H_{15}NO_{16}$
294.0723	$C_{10}H_{15}O_{9}[^{15}N]-$	$C_{10}H_{15}O_{6}$
310.0672	$C_{10}H_{15}O_{10}[^{15}N]-$	$C_{10}H_{15}O_{7}$
326.0621	$C_{10}H_{15}O_{11}[^{15}N]-$	$C_{10}H_{15}O_{8}$
342.0570	$C_{10}H_{15}O_{12}[^{15}N]-$	$C_{10}H_{15}O_{9}$
358.0519	$C_{10}H_{15}O_{13}[^{15}N]-$	$C_{10}H_{15}O_{10}$
374.0468	$C_{10}H_{15}O_{14}[^{15}N]-$	$C_{10}H_{15}O_{11}$
390.0418	$C_{10}H_{15}O_{15}[^{15}N]-$	$C_{10}H_{15}O_{12}$
422.0316	$C_{10}H_{15}O_{17}[^{15}N]-$	$C_{10}H_{15}O_{14}$
438.0265	$C_{10}H_{15}O_{18}[^{15}N]-$	$C_{10}H_{15}O_{15}$
454.0214	$C_{10}H_{15}O_{19}[^{15}N]-$	$C_{10}H_{15}O_{16}$
279.0852	$C_{10}H_{16}O_{8}[^{15}N]-$	$C_{10}H_{16}O_{5}$
295.0801	$C_{10}H_{16}O_{9}[^{15}N]-$	$C_{10}H_{16}O_{6}$
327.0699	$C_{10}H_{16}O_{11}[^{15}N]-$	$C_{10}H_{16}O_{8}$
343.0648	$C_{10}H_{16}O_{12}[^{15}N]-$	$C_{10}H_{16}O_{9}$
359.0597	$C_{10}H_{16}O_{13}[^{15}N]-$	$C_{10}H_{16}O_{10}$
375.0547	$C_{10}H_{16}O_{14}[^{15}N]-$	$C_{10}H_{16}O_{11}$
391.0496	$C_{10}H_{16}O_{15}[^{15}N]-$	$C_{10}H_{16}O_{12}$
407.0445	$C_{10}H_{16}O_{16}[^{15}N]-$	$C_{10}H_{16}O_{13}$
423.0394	$C_{10}H_{16}O_{17}[^{15}N]-$	$C_{10}H_{16}O_{14}$
439.0343	$C_{10}H_{16}O_{18}[^{15}N]-$	$C_{10}H_{16}O_{15}$
294.0961	$C_{10}H_{17}NO_{8}[^{15}N]-$	$C_{10}H_{17}NO_{5}$
310.0910	$C_{10}H_{17}NO_{9}[^{15}N]-$	$C_{10}H_{17}NO_{6}$
326.0859	$C_{10}H_{17}NO_{10}[^{15}N]-$	$C_{10}H_{17}NO_{7}$
342.0808	$C_{10}H_{17}NO_{11}[^{15}N]-$	$C_{10}H_{17}NO_{8}$
358.0757	$C_{10}H_{17}NO_{12}[^{15}N]-$	$C_{10}H_{17}NO_{9}$
374.0706	$C_{10}H_{17}NO_{13}[^{15}N]-$	$C_{10}H_{17}NO_{10}$
390.0656	$C_{10}H_{17}NO_{14}[^{15}N]-$	$C_{10}H_{17}NO_{11}$
406.0605	$C_{10}H_{17}NO_{15}[^{15}N]-$	$C_{10}H_{17}NO_{12}$
422.0554	$C_{10}H_{17}NO_{16}[^{15}N]-$	$C_{10}H_{17}NO_{13}$
438.0503	$C_{10}H_{17}NO_{17}[^{15}N]-$	$C_{10}H_{17}NO_{14}$
454.0452	$C_{10}H_{17}NO_{18}[^{15}N]-$	$C_{10}H_{17}NO_{15}$
264.0981	$C_{10}H_{17}O_{7}[^{15}N]-$	$C_{10}H_{17}O_{4}$
280.0930	$C_{10}H_{17}O_{8}[^{15}N]-$	$C_{10}H_{17}O_{5}$
296.0879	$C_{10}H_{17}O_{9}[^{15}N]-$	$C_{10}H_{17}O_{6}$
312.0828	$C_{10}H_{17}O_{10}[^{15}N]-$	$C_{10}H_{17}O_{7}$
392.0574	$C_{10}H_{17}O_{15}[^{15}N]-$	$C_{10}H_{17}O_{12}$
408.0523	$C_{10}H_{17}O_{16}[^{15}N]-$	$C_{10}H_{17}O_{13}$

424.0472	$C_{10}H_{17}O_{17}[^{15}N]-$	$C_{10}H_{17}O_{14}$
440.0421	$C_{10}H_{17}O_{18}[^{15}N]-$	$C_{10}H_{17}O_{15}$
357.0917	$C_{10}H_{18}N_2O_{11}[^{15}N]-$	$C_{10}H_{18}N_2O_8$
389.0815	$C_{10}H_{18}N_2O_{13}[^{15}N]-$	$C_{10}H_{18}N_2O_{10}$
405.0765	$C_{10}H_{18}N_2O_{14}[^{15}N]-$	$C_{10}H_{18}N_2O_{11}$
421.0714	$C_{10}H_{18}N_2O_{15}[^{15}N]-$	$C_{10}H_{18}N_2O_{12}$
453.0612	$C_{10}H_{18}N_2O_{17}[^{15}N]-$	$C_{10}H_{18}N_2O_{14}$
517.0409	$C_{10}H_{18}N_2O_{21}[^{15}N]-$	$C_{10}H_{18}N_2O_{18}$
621.0770	$C_{15}H_{26}O_{25}[^{15}N]-$	$C_{15}H_{26}O_{22}$
620.0930	$C_{15}H_{27}NO_{24}[^{15}N]-$	$C_{15}H_{27}NO_{21}$
638.1035	$C_{15}H_{29}NO_{25}[^{15}N]-$	$C_{15}H_{29}NO_{22}$
653.1144	$C_{15}H_{30}N_2O_{25}[^{15}N]-$	$C_{15}H_{30}N_2O_{22}$
480.1700	$C_{15}H_{31}NO_{15}[^{15}N]-$	$C_{15}H_{31}NO_{12}$
652.1192	$C_{16}H_{31}NO_{25}[^{15}N]-$	$C_{16}H_{31}NO_{22}$
531.0969	$C_{17}H_{24}O_{18}[^{15}N]-$	$C_{17}H_{24}O_{15}$
563.0868	$C_{17}H_{24}O_{20}[^{15}N]-$	$C_{17}H_{24}O_{17}$
501.1227	$C_{17}H_{26}O_{16}[^{15}N]-$	$C_{17}H_{26}O_{13}$
533.1126	$C_{17}H_{26}O_{18}[^{15}N]-$	$C_{17}H_{26}O_{15}$
565.1024	$C_{17}H_{26}O_{20}[^{15}N]-$	$C_{17}H_{26}O_{17}$
503.1384	$C_{17}H_{28}O_{16}[^{15}N]-$	$C_{17}H_{28}O_{13}$
651.1239	$C_{17}H_{32}O_{25}[^{15}N]-$	$C_{17}H_{32}O_{22}$
543.0969	$C_{18}H_{24}O_{18}[^{15}N]-$	$C_{18}H_{24}O_{15}$
545.1126	$C_{18}H_{26}O_{18}[^{15}N]-$	$C_{18}H_{26}O_{15}$
561.1075	$C_{18}H_{26}O_{19}[^{15}N]-$	$C_{18}H_{26}O_{16}$
560.1235	$C_{18}H_{27}NO_{18}[^{15}N]-$	$C_{18}H_{27}NO_{15}$
515.1384	$C_{18}H_{28}O_{16}[^{15}N]-$	$C_{18}H_{28}O_{13}$
517.1540	$C_{18}H_{30}O_{16}[^{15}N]-$	$C_{18}H_{30}O_{13}$
493.1329	$C_{19}H_{26}O_{14}[^{15}N]-$	$C_{19}H_{26}O_{11}$
541.1177	$C_{19}H_{26}O_{17}[^{15}N]-$	$C_{19}H_{26}O_{14}$
495.1486	$C_{19}H_{28}O_{14}[^{15}N]-$	$C_{19}H_{28}O_{11}$
559.1282	$C_{19}H_{28}O_{18}[^{15}N]-$	$C_{19}H_{28}O_{15}$
575.1231	$C_{19}H_{28}O_{19}[^{15}N]-$	$C_{19}H_{28}O_{16}$
591.1181	$C_{19}H_{28}O_{20}[^{15}N]-$	$C_{19}H_{28}O_{17}$
558.1442	$C_{19}H_{29}NO_{17}[^{15}N]-$	$C_{19}H_{29}NO_{14}$
497.1642	$C_{19}H_{30}O_{14}[^{15}N]-$	$C_{19}H_{30}O_{11}$
611.1443	$C_{19}H_{32}O_{21}[^{15}N]-$	$C_{19}H_{32}O_{18}$
525.1591	$C_{20}H_{30}O_{15}[^{15}N]-$	$C_{20}H_{30}O_{12}$
557.1490	$C_{20}H_{30}O_{17}[^{15}N]-$	$C_{20}H_{30}O_{14}$
573.1439	$C_{20}H_{30}O_{18}[^{15}N]-$	$C_{20}H_{30}O_{15}$
589.1388	$C_{20}H_{30}O_{19}[^{15}N]-$	$C_{20}H_{30}O_{16}$
588.1548	$C_{20}H_{31}NO_{18}[^{15}N]-$	$C_{20}H_{31}NO_{15}$
511.1799	$C_{20}H_{32}O_{14}[^{15}N]-$	$C_{20}H_{32}O_{11}$
527.1748	$C_{20}H_{32}O_{15}[^{15}N]-$	$C_{20}H_{32}O_{12}$

543.1697	$C_{20}H_{32}O_{16}[^{15}N]-$	$C_{20}H_{32}O_{13}$
591.1544	$C_{20}H_{32}O_{19}[^{15}N]-$	$C_{20}H_{32}O_{16}$
607.1494	$C_{20}H_{32}O_{20}[^{15}N]-$	$C_{20}H_{32}O_{17}$
623.1443	$C_{20}H_{32}O_{21}[^{15}N]-$	$C_{20}H_{32}O_{18}$
621.1762	$C_{20}H_{34}N_2O_{19}[^{15}N]-$	$C_{20}H_{34}N_2O_{16}$
637.1711	$C_{20}H_{34}N_2O_{20}[^{15}N]-$	$C_{20}H_{34}N_2O_{17}$
513.1955	$C_{20}H_{34}O_{14}[^{15}N]-$	$C_{20}H_{34}O_{11}$
529.1904	$C_{20}H_{34}O_{15}[^{15}N]-$	$C_{20}H_{34}O_{12}$
545.1853	$C_{20}H_{34}O_{16}[^{15}N]-$	$C_{20}H_{34}O_{13}$
561.1803	$C_{20}H_{34}O_{17}[^{15}N]-$	$C_{20}H_{34}O_{14}$
577.1752	$C_{20}H_{34}O_{18}[^{15}N]-$	$C_{20}H_{34}O_{15}$

Table S6. Normalized average signal of $C_{10}H_{15}O_x$• radical and their termination products in high NO conditions. The percentage value is the average signal of each peak normalized to that of $C_{10}H_{17}NO_9$ in 15 mins after the louvres opening. “M”, “M-17”, “M-15” and “M+1” represent the molecular weight of the RO_2 and their respective termination products with RO_2, HO_2 and NO.

RO_2	RC=O	ROH	ROOH	$RONO_2$
$C_{10}H_{15}O_6$ 2.4%		$C_{10}H_{16}O_5$ 15.7%	$C_{10}H_{16}O_6$ 9.0%	
$C_{10}H_{15}O_7$ 7.8%		$C_{10}H_{16}O_6$ 9.0%		$C_{10}H_{15}NO_8$ 34.6%
$C_{10}H_{15}O_8$ 14.7%	$C_{10}H_{14}O_7$ 10.2%		$C_{10}H_{16}O_8$ 52.7%	$C_{10}H_{15}NO_9$ 49.7%
$C_{10}H_{15}O_9$ 27.9%	$C_{10}H_{14}O_8$ 44.4%	$C_{10}H_{16}O_8$ 52.7%	$C_{10}H_{16}O_9$ 38.8%	$C_{10}H_{15}NO_{10}$ 51.0%
$C_{10}H_{15}O_{10}$ 17.8%	$C_{10}H_{14}O_9$ 11.9%	$C_{10}H_{16}O_9$ 38.8%	$C_{10}H_{16}O_{10}$ 21.0%	$C_{10}H_{15}NO_{11}$ 25.6%
$C_{10}H_{15}O_{11}$ 11.4%	$C_{10}H_{14}O_{10}$ 18.8%	$C_{10}H_{16}O_{10}$ 21.0%	$C_{10}H_{16}O_{11}$ 4.3%	$C_{10}H_{15}NO_{12}$ 10.3%
$C_{10}H_{15}O_{12}$ 5.5%	$C_{10}H_{14}O_{11}$ 10.7%	$C_{10}H_{16}O_{11}$ 4.3%	$C_{10}H_{16}O_{12}$ 2.0%	$C_{10}H_{15}NO_{13}$ 7.8%
$C_{10}H_{15}O_{13}$ 5.3%	$C_{10}H_{14}O_{12}$ 9.1%	$C_{10}H_{16}O_{12}$ 2.0%	$C_{10}H_{16}O_{13}$ 10.8%	$C_{10}H_{15}NO_{14}$ 3.4%
$C_{10}H_{15}O_{14}$ 1.8%	$C_{10}H_{14}O_{13}$ 4.4%	$C_{10}H_{16}O_{13}$ 10.8%	$C_{10}H_{16}O_{14}$ 3.3%	
$C_{10}H_{15}O_{15}$ 0.5%	$C_{10}H_{14}O_{14}$ 4.3%	$C_{10}H_{16}O_{14}$ 3.3%	$C_{10}H_{16}O_{15}$ 1.6%	$C_{10}H_{15}NO_{16}$ 1.0%
		$C_{10}H_{16}O_{15}$ 1.6%		

Table S7. Normalized average signal of $C_{10}H_{17}O_x$• radical and their termination products in high NO conditions. The percentage value is the average signal of each peak normalized to that of $C_{10}H_{17}NO_9$ in 15 mins after the louvres opening. “M”, “M-17”, “M-15” and “M+1” represent the molecular weight of the RO_2 and their respective termination products with RO_2, HO_2 and NO.

RO_2	RC=O	ROH	ROOH	$RONO_2$
$C_{10}H_{17}O_5$ 2.2%				$C_{10}H_{17}NO_6$ 12.4%
$C_{10}H_{17}O_6$ 7.0%	$C_{10}H_{16}O_5$ 15.7%			$C_{10}H_{17}NO_7$ 19.8%
$C_{10}H_{17}O_7$ 14.0%	$C_{10}H_{16}O_6$ 9.0%			$C_{10}H_{17}NO_8$ 93.6%
$C_{10}H_{17}O_8$ 11.8%				$C_{10}H_{17}NO_9$ 100.0%
$C_{10}H_{17}O_9$ 13.8%	$C_{10}H_{16}O_8$ 52.7%			$C_{10}H_{17}NO_{10}$ 70.8%
$C_{10}H_{17}O_{10}$ 15.7%	$C_{10}H_{16}O_9$ 38.8%		$C_{10}H_{18}O_{10}$ 9.3%	$C_{10}H_{17}NO_{11}$ 27.8%
$C_{10}H_{17}O_{11}$ 11.3%	$C_{10}H_{16}O_{10}$ 21.0%	$C_{10}H_{18}O_{10}$ 9.3%		$C_{10}H_{17}NO_{12}$ 20.3%
$C_{10}H_{17}O_{12}$ 6.1%	$C_{10}H_{16}O_{11}$ 4.3%			$C_{10}H_{17}NO_{13}$ 9.7%
$C_{10}H_{17}O_{13}$ 4.6%	$C_{10}H_{16}O_{12}$ 2.0%			$C_{10}H_{17}NO_{14}$ 2.0%
$C_{10}H_{17}O_{14}$ 1.6%	$C_{10}H_{16}O_{13}$ 10.8%			$C_{10}H_{17}NO_{15}$ 0.5%

Table S8. Normalized average signal of dimer products in low NO conditions. The percentage value is the average signal of each peak normalized to that of $C_{10}H_{16}O_8$ in 15 mins after the louvres opening.

C20 dimer families		
$C_{20}H_{30}O_x$	$C_{20}H_{32}O_x$	$C_{20}H_{34}O_x$
$C_{20}H_{30}O_{10}$ 1.1%	$C_{20}H_{32}O_9$ 2.7%	$C_{20}H_{34}O_{10}$ 7.9%
$C_{20}H_{30}O_{11}$ 1.2%	$C_{20}H_{32}O_{10}$ 3.7%	$C_{20}H_{34}O_{11}$ 4.9%
	$C_{20}H_{32}O_{11}$ 8.1%	$C_{20}H_{34}O_{12}$ 9.0%
	$C_{20}H_{32}O_{12}$ 4.2%	$C_{20}H_{34}O_{13}$ 5.9%
		$C_{20}H_{34}O_{14}$ 9.1%
$C_{20}H_{30}O_{15}$ 2.5%	$C_{20}H_{32}O_{14}$ 4.6%	$C_{20}H_{34}O_{15}$ 2.3%
$C_{20}H_{30}O_{16}$ 2.7%	$C_{20}H_{32}O_{15}$ 11.8%	$C_{20}H_{34}O_{16}$ 2.8%
$C_{20}H_{30}O_{17}$ 1.4%		
	$C_{20}H_{32}O_{17}$ 4.6%	

Table S9. Normalized average signal of dimer products in high NO conditions. The percentage value is the average signal of each peak normalized to that of $C_{10}H_{17}NO_9$ in 15 mins after the louvres opening.

$C_{20}H_{30}O_x$	$C_{20}H_{32}O_x$	$C_{20}H_{34}O_x$
		$C_{20}H_{34}O_{11}$ 0.2%
$C_{20}H_{30}O_{12}$ 0.3%	$C_{20}H_{32}O_{11}$ 0.4%	$C_{20}H_{34}O_{12}$ 0.7%
	$C_{20}H_{32}O_{12}$ 0.5%	$C_{20}H_{34}O_{13}$ 0.2%
$C_{20}H_{30}O_{14}$ 0.6%	$C_{20}H_{32}O_{13}$ 0.1%	$C_{20}H_{34}O_{14}$ 0.2%
$C_{20}H_{30}O_{15}$ 0.7%		$C_{20}H_{34}O_{15}$ 0.3%
$C_{20}H_{30}O_{16}$ 0.4%		
	$C_{20}H_{32}O_{16}$ 0.2%	
	$C_{20}H_{32}O_{17}$ 0.6%	

Table S10. Major dimer families and their possible formation pathways.

Dimer family	**Possible formation pathways**
$C_{20}H_{34}O_x$	$C_{10}H_{17}O_x\bullet + C_{10}H_{17}O_x\bullet$
$C_{20}H_{32}O_x$	$C_{10}H_{15}O_x\bullet + C_{10}H_{17}O_x\bullet$
$C_{20}H_{30}O_x$	$C_{10}H_{15}O_x\bullet + C_{10}H_{15}O_x\bullet$
$C_{19}H_{30}O_x$	$C_9H_{15}O_x\bullet + C_{10}H_{15}O_x\bullet$
	/ $C_9H_{13}O_x\bullet + C_{10}H_{17}O_x\bullet$
$C_{19}H_{28}O_x$	$C_9H_{13}O_x\bullet + C_{10}H_{15}O_x\bullet$
$C_{19}H_{26}O_x$	$C_9H_{11}O_x\bullet + C_{10}H_{15}O_x\bullet$

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