



Supplement of

Identification of highly oxygenated organic molecules and their role in aerosol formation in the reaction of limonene with nitrate radical

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11 S1 Determination of the calibration coefficient

12 A calibration coefficient was determined and used to convert peak intensity in CIMS to 13 concentrations. The calibration coefficient of H_2SO_4 can be applied to HOM because the ionization 14 efficiency of HOM and H_2SO_4 are close (Ehn et al., 2014; Pullinen et al., 2020). The concentration 15 of H_2SO_4 is given by:

16

$$[H_2SO_4] = C \times I \tag{Eq. S1}$$

17 where C is the calibration coefficient of H_2SO_4 , I is the normalized count (nc, the peak area of an 18 ion divided by total ion signal of mass spectrum) of peak intensity. The detailed description of the 19 derivation of the calibration coefficient for H₂SO₄ in SAPHIR chamber can be found elsewhere 20 (Ehn et al., 2014; Pullinen et al., 2020; Zhao et al., 2021). In brief, H₂SO₄ was produced in the 21 chamber by OH•-initiated oxidation of SO₂. OH• were mainly generated from photolysis of HONO. 22 Concentrations of SO₂ and OH• were measured by laser induced fluorescence (LIF) (Fuchs et al., 23 2012) and an SO₂ analyzer (Thermo System 43i). The concentration of H₂SO₄ is given by: 24 $d[H_2SO_4]/dt = k[SO_2][OH\bullet] - (k_{wall}+k_{dil})[H_2SO_4]$ (Eq. S2) 25 where $[H_2SO_4]$, $[SO_2]$, and $[OH^{\bullet}]$ are concentrations, k is the rate constant of the reaction of SO₂ w

26 ith OH•, k_{wall} is the wall loss rate (6×10⁻⁴ s⁻¹) (Zhao et al., 2018), and k_{dil} is the dilution rate (1×10⁻⁵ 27 s⁻¹).

C was determined to be 2.5×10^{10} molecule cm⁻³ nc⁻¹ for H₂SO₄. The uncertainty of C is -52 % /+101 % from the uncertainty of SO₂ concentration (~7 %), OH• concentration (~10 %), I (~ 10 %) and k (Δ logk = ±0.3) using error propagation (Zhao et al., 2021).

A relative transmission efficiency curve of the ${}^{15}NO_{3}$ -CIMS was measured with perfluoropentanoic acid (C₄F₉COOH) in our previous study (Pullinen et al., 2020). A monotonous decrease of the transmission function from 100 % to 86 % was determined within an m/z range of 62-791 Th. Thus, the uncertainty of the mass-independent transmission efficiency used when applying the calibration coefficient of H₂SO₄ to HOM is determined to be -0 %/+14 %.

36 When the chamber was actively mixed, the wall loss is determined to be $(2.2\pm0.2) \times 10^{-3} \text{ s}^{-1}$. 37 We examined the decay of nitrated compounds such as $C_{10}H_{15}NO_{9-12}$ (volatility in the 38 LVOC/ELVOC range) and non-nitrated compounds such as $C_{10}H_{14}O_{8-11}$ in the reaction of limonene 39 with OH in the presence of NO, which all showed similar decay rates as shown below (Fig. S16).

40 The wall loss rate in SAPHIR chamber during active mixing is comparable to the chambers 41 such as those reported by Peräkylä et al. (2020) (lifetime ~400 s) and Krechmer et al. (2016) 42 (lifetime \sim 7 to 13 min). The time for complete mixing is \sim 1 min (Fuchs et al., 2013) when the fan 43 was on, which was further confirmed using measured VOC concentrations. We would like to note 44 that the SAPHIR chamber is much larger than the chambers in the cited studies above (270 m³ vs a few m³) and also the chamber is running in batch mode instead of the continuous flow mode used 45 46 for many other chambers for HOM studies such as the COALA chamber (Peräkylä et al., 2020) or 47 our JPAC chamber (Ehn et al., 2014; Pullinen et al., 2020). The large volume and batch running

- 48 mode may result in a thicker boundary layer of the chamber wall, which delays vapor wall
- 49 deposition.
- 50
- 51

52 S2 HOM condensation on SOA

53 Estimation of HOM condensation on SOA was based on measurement of HOM concentration and 54 particle surface concentration, and the assumption that all HOM colliding with the surface of 55 particles led to a net and irreversible uptake. Collision rate of a gas phase HOM species with 56 particles of all size is given by:

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$$K = \gamma \frac{\pi}{4} (d_p + d_v)^2 (\overline{c_p}^2 + \overline{c_v}^2)^{\frac{1}{2}} \cdot C_v$$
 (Eq. S3)

where d_p and d_v are the diameters of the particle and molecule, and \overline{c}_p and \overline{c}_v are the average thermal speeds of the particle and the HOM species, respectively. C_v represents measured HOM molecule concentration. The coefficient γ is given by:

61
$$\gamma = \frac{4}{3} K n \beta_m$$
 (Eq. S4)

where Kn is the Knudsen number and β_m is the correction factor in the transition regime according to the Fuchs-Sutugin approach (Seinfeld and Pandis, 2006). Then, particle growth rate as represented in mass concentration (GR_m) can be described as:

65

66
$$GR_m = \frac{dM}{dt} = \rho_p \frac{dV_p}{dt} = \rho_p K \frac{m_v}{\rho_v} = \frac{\pi}{4} \gamma \frac{\rho_p}{\rho_v} (d_p + d_v)^2 (\overline{c_p}^2 + \overline{c_v}^2)^{\frac{1}{2}} \cdot m_v C_v$$

67
$$= \frac{\pi}{4} \gamma \frac{\rho_p}{\rho_v} \left(d_p + d_v \right)^2 \left(\frac{8kT}{\pi} \right)^{\frac{1}{2}} \left(\frac{1}{m_p} + \frac{1}{m_v} \right)^{\frac{1}{2}} \cdot m_v C_v$$
(Eq. S5)

68

69 where *M* is the particle mass concentration (μ g/m³), *t* is time, *V_p* is the particle volume, *T* is 70 temperature, m_p and m_v are the exact mass of particle and vapour, respectively. Omitting the $\frac{1}{m_p}$ 71 term (much smaller than $\frac{1}{m_v}$) (Ehn et al., 2014) and the d_v term (small compared to d_p) in Eq. 4, 72 one can get

$$GR_m = \frac{1}{4} \gamma \frac{\rho_p}{\rho_v} S_p \left(\frac{8kT}{\pi m_v}\right)^{\frac{1}{2}} \cdot m_v C_v$$
(Eq. S6)

where S_p is the particle surface concentration measured by SMPS. The calculation of γ using Eq. S4 was taken from previous studies (Lehtinen and Kulmala, 2003; Seinfeld and Pandis, 2006). Multiplying the calculated particle mass growth rate by time interval gives the particle growth in each time interval.

The wall loss and dilution loss rates of the particles are obtained from a later period of the experiment when particle mass ceased to grow and the change in particle mass was only due to the wall loss and dilution. During this period the loss rate of the total particle mass concentration (TM) was obtained through linear fit of ln(TM) to t when:

82
$$ln(TM_{t_n}) = ln(TM_{t_0}) - (k_{wall} + k_{dil})(t_n - t_0)$$
(Eq. S7)

- Herein ln(TM) decreased linearly over time at constant geometric mean of the particle diameter, which suggests no noticeable evaporation loss. The wall loss was independently determined from the particle number concentration, which showed values consistent with method using mass concentration. The value of particle wall loss rate in this experiment k_{wall} was determined to be 3.6×10^{-5} s⁻¹.
- 88
- 89

90 S3 Simulations based on the Master Chemical Mechanism (MCM)

91 Besides simulations of the RO_2^{\bullet} loss pathway (Sect. 2.5), we conducted several simulations 92 including concentrations of NO₃, N₂O₅, limonene and RO₂• (Fig. S4) based on MCM v3.3.1 93 (http://mcm.york.ac.uk/) iChamber, using an open-source program 94 (https://sites.google.com/view/wangsiyuan/models?authuser=0) (Wang and Pratt, 2017). 95 The modeled concentration of NO3, N2O5 and limonene by MCM generally match the behavior of measured concentrations (Fig. S4 a~c). The overestimated limonene concentrations can be 96 97 attributed to the absence of a temperature-dependence of the rate constant for the reaction of 98 limonene with NO₃. RO₂• concentrations showed 1st-generation trend (Fig. S4d). The reaction rate 99 (k×limonene×NO₃) was highest at every injection of limonene (Fig. S4e). As for oxidation products, 100 the second time of NO₃ attack to organic nitrate with a C=C double bond is not included in MCM, so the simulation of the closed-shell products does not present 1st or 2nd generation product patterns 101 as we have observed in CIMS. But we are able to observe several good simulation of 1st and 2nd 102 103 generation RO2• (Fig. S4f,g). For example, the "NLIMALO2" (Fig. S4g) showed a typical time 104 series of 2nd generation RO₂•, which is formed via NO₃ attack of a 1st-generation carbonyl product 105 which does not contain N atom according to the MCM mechanism. 106

107 S4 Supplement figures, reaction schemes, and tables



108 Figures S1 - S16

109

110 Figure S1. Contribution of NO₃ and O₃ oxidation pathways of limonene to chemical loss of

111 limonene presented as fractions during the experiment. Black vertical lines indicate time for six

112 limonene additions into the chamber.

113



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Figure S2. Examples of high-resolution peak fitting of HOM containing 1 N atom (left panel) and 5 N atoms (right panel). Red lines are the mass spectrum, blue and orange lines show the sum of the isotopic contributions and the fitted peaks, and the residuals, respectively. The black vertical lines denote the exact mass of the fitted peaks.



121 Figure S3. RO₂• loss rate based on bimolecular reactions with RO₂•, NO₃, NO₂, NO and HO₂• (color

bars) during the first limonene addition period (P1). Blue rectangle denotes the first 10 min of the

123 reaction time (P1a), which is the time period used for peak fitting.

124





126 Figure S4. Simulation results of limonene + NO₃ gas-phase chemistry based on MCM v3.3.1 using 127 iChamber model. The whole period of experiment was simulated, at measured T and RH, and 128 additions of limonene, NO2 and O3 were included as initial conditions according to the experimental 129 procedure. (a) \sim (c): Comparison of simulated (blue trace) and measured (red trace) concentrations 130 of (a) NO₃, (b) N₂O₅ and (c) limonene. (d)~(g): Simulated concentrations of (d) total RO₂• included 131 in the limonene + NO_3 gas-phase chemistry in MCM v3.3.1, (e) reaction rate of limonene with NO_3 132 (coefficient k×limonene×NO₃), compared with a measured 1st-generation HOM product 133 C₂₀H₃₁NO₁₃; (f) "NLIMO2", an example of 1st-generation C₁₀ RO₂•, and (g) "NLIMALO2", an

134 example of 2^{nd} -generation C_{10} RO₂•, compared with a measured 2^{nd} -generation HOM RO₂•, 135 $C_{10}H_{15}N_2O_{12}\bullet$.



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138 Figure S5. Kendrick mass defect plot (O atom-based) of major dimer products. The area of the

139 circles is proportional to the average intensity of each compound during the P1a period. The color

140 denotes O/C ratio. Dashed lines indicate major product families that were identified.

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Figure S6. Kendrick mass defect plot (O-atom-based) of trimers. The area of the circles is
proportional to the average intensity of each compound during the P1a period. The color denotes
O/C ratio. Dashed lines indicate major product families that were identified.

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Figure S7. Time series of peak intensity of the $C_{10}H_{16}NO_x$ • family during the whole experimental period. The vertical black, red and blue lines represent the time of limonene, NO₂ and O₃ additions, respectively.

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Figure S8. Time series of peak intensity of two representatives of the $C_{10}H_{14}O_x$ family during the whole experimental period. The vertical black, red and blue lines represent the time of limonene, NO₂ and O₃ additions, respectively.



Figure S9. Time series of peak intensity of the C₉H₁₅NO_x family during the whole experimental
period. The vertical black, red and blue lines represent the time of limonene, NO₂ and O₃ additions,
respectively.



Figure S10. Time series of peak intensity of the C₈H₁₁NO_x family during the whole experimental
period. The vertical black, red and blue lines represent the time of limonene, NO₂ and O₃ additions,
respectively.



Figure S11. Time series of peak intensity of the C₇H₉NO_x family during the whole experimental
period. The vertical black, red and blue lines represent the time of limonene, NO₂ and O₃ additions,
respectively.



Figure S12. Time series of peak intensity of the C₂₀H₃₁NO_x family during the whole experimental
period. The vertical black, red and blue lines represent the time of limonene, NO₂ and O₃ additions,
respectively.



178Figure S13. Time series of peak intensity of the $C_{20}H_{33}N_3O_x$ family during the whole experimental179period. The vertical black, red and blue lines represent the time of limonene, NO2 and O3 additions,180respectively.

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Figure S14. Time series of peak intensity of the $C_{20}H_{34}N_4O_x$ family during the whole experimental period. The vertical black, red and blue lines represent the time of limonene, NO₂ and O₃ additions, respectively.

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Figure S15. HOM concentration over time in the first limonene addition period (P1). The HOM concentration underwent a period of rapid increase (first-production phase), followed by an intermediate phase where it remained constant and a second phase of increase afterwards (secondproduction phase). In the first-production phase, primary HOM production contributed most to the HOM increase, while in the intermediate phase and the second-production phase, wall loss and secondary HOM production increased in importance.

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195

196Figure S16. Decay of HOM $C_{10}H_{14}O_{8-11}$ (a) and $C_{10}H_{15}NO_{9-12}$ (b) due to wall loss during active197mixing in SAPHIR chamber. The lifetimes (tau) of wall loss of each species are listed in the legend198(s).

200

201 Reaction schemes S1 to S3



203 Scheme S1. The possible formation pathways towards the production of $1N-C_{10}$ HOM RO₂ radicals 204 ($C_{10}H_{16}NO_x$ •) and stable products $C_{10}H_{15}NO_x$ initiated by O₃ oxidation of limonene (Mentel et al., 205 2015).



208 Scheme S2. Possible formation pathways of C_{10} monomers without nitrogen atoms.



211 Scheme S3. Example scheme for C₉H₁₃NO_x and C₉H₁₅NO_x formation from limonene; the depicted

212 reactions may not be the dominant pathways.

Tables S1 to S3

I. I can hot hot	in millionene + 1003 experiment:	
m/z	Detected ion formula	Parent molecule formula
268.0077	C ₆ H ₇ NO ₇ [¹⁵ N]O ₃ ⁻	C ₆ H ₇ NO ₇
284.0026	C ₆ H ₇ NO ₈ [¹⁵ N]O ₃ ⁻	C ₆ H ₇ NO ₈
284.9866	C ₆ H ₆ O ₉ [¹⁵ N]O ₃ ⁻	C ₆ H ₆ O ₉
302.0131	C ₆ H ₉ NO ₉ [¹⁵ N]O ₃ ⁻	C ₆ H ₉ NO ₉
312.9927	$C_6H_6N_2O_9[^{15}N]O_3^-$	C ₆ H ₆ N ₂ O ₉
333.0189	$C_6H_{10}N_2O_{10}[^{15}N]O_3^-$	C ₆ H ₁₀ N ₂ O ₁₀
280.0077	C ₇ H ₇ NO ₇ [¹⁵ N]O ₃ ⁻	C ₇ H ₇ NO ₇
282.0233	C ₇ H ₉ NO ₇ [¹⁵ N]O ₃ ⁻	C7H9NO7
283.0073	$C_7H_8O_8[^{15}N]O_3^{-1}$	C ₇ H ₈ O ₈
284.0390	C ₇ H ₁₁ NO ₇ [¹⁵ N]O ₃ ⁻	C ₇ H ₁₁ NO ₇
297.0104	C ₇ H ₈ NO ₈ [¹⁵ N]O ₃ ⁻	C ₇ H ₈ NO ₈
311.0135	$C_7H_8N_2O_8[^{15}N]O_3^-$	C7H8N2O8
314.0131	C ₇ H ₉ NO ₉ [¹⁵ N]O ₃ ⁻	C7H9NO9
315.0210	$C_7H_{10}NO_9[^{15}N]O_3^-$	C ₇ H ₁₀ NO ₉
316.0288	C ₇ H ₁₁ NO ₉ [¹⁵ N]O ₃ ⁻	C ₇ H ₁₁ NO ₉
330.0080	C7H9NO10[¹⁵ N]O3 ⁻	C ₇ H ₉ NO ₁₀
332.0237	$C_7H_{11}NO_{10}[^{15}N]O_3^{-1}$	C ₇ H ₁₁ NO ₁₀
343.0033	$C_7H_8N_2O_{10}[^{15}N]O_3^{-1}$	$C_7H_8N_2O_{10}$
346.0030	C ₇ H ₉ NO ₁₁ [¹⁵ N]O ₃ ⁻	C ₇ H ₉ NO ₁₁
347.0108	$C_7H_{10}NO_{11}[^{15}N]O_3^-$	C ₇ H ₁₀ NO ₁₁
358.9982	$C_7H_8N_2O_{11}[^{15}N]O_3^-$	C ₇ H ₈ N ₂ O ₁₁
374.9931	$C_7H_8N_2O_{12}[^{15}N]O_3^-$	C7H8N2O12
390.9880	$C_7H_8N_2O_{13}[^{15}N]O_3^{-1}$	C ₇ H ₈ N ₂ O ₁₃
406.9830	$C_7H_8N_2O_{14}[^{15}N]O_3^-$	$C_7H_8N_2O_{14}$
408.9986	$C_7H_{10}N_2O_{14}[^{15}N]O_3^-$	C ₇ H ₁₀ N ₂ O ₁₄
280.0440	$C_8H_{11}NO_6[^{15}N]O_3^{-1}$	C ₈ H ₁₁ NO ₆
283.0437	$C_8H_{12}O_7[^{15}N]O_3^-$	C ₈ H ₁₂ O ₇
296.0390	$C_8H_{11}NO_7[^{15}N]O_3^-$	C ₈ H ₁₁ NO ₇
297.0468	$C_8H_{12}NO_7[^{15}N]O_3^-$	C ₈ H ₁₂ NO ₇
312.0339	$C_8H_{11}NO_8[^{15}N]O_3^{-1}$	C ₈ H ₁₁ NO ₈
313.0417	$C_8H_{12}NO_8[^{15}N]O_3^{-1}$	C ₈ H ₁₂ NO ₈
314.0495	$C_8H_{13}NO_8[^{15}N]O_3^{-1}$	C ₈ H ₁₃ NO ₈
316.0652	$C_8H_{15}NO_8[^{15}N]O_3^{-1}$	C ₈ H ₁₅ NO ₈
325.0291	$C_8H_{10}N_2O_8[^{15}N]O_3^-$	$C_8H_{10}N_2O_8$
328.0288	$C_8H_{11}NO_9[^{15}N]O_3^{-1}$	$C_8H_{11}NO_9$
329.0366	$C_8H_{12}NO_9[^{15}N]O_3$	C ₈ H ₁₂ NO ₉
330.0444	C ₈ H ₁₃ NO ₉ [¹⁵ N]O ₃	C ₈ H ₁₃ NO ₉
344.0237	$C_8H_{11}NO_{10}[^{15}N]O_3^{-1}$	C ₈ H ₁₁ NO ₁₀
345.0315	$C_8H_{12}NO_{10}[^{15}N]O_3^{-1}$	C ₈ H ₁₂ NO ₁₀
346.0393	C ₈ H ₁₃ NO ₁₀ [¹⁵ N]O ₃	C ₈ H ₁₃ NO ₁₀
360.0186	$C_8H_{11}NO_{11}[^{15}N]O_3^{-1}$	C ₈ H ₁₁ NO ₁₁

216 Table S1. Peak list from limonene + NO₃ experiment.

361.0264	C ₈ H ₁₂ NO ₁₁ [¹⁵ N]O ₃ ⁻	$C_8H_{12}NO_{11}$
376.0135	C ₈ H ₁₁ NO ₁₂ [¹⁵ N]O ₃ ⁻	$C_8H_{11}NO_{12}$
377.0214	C ₈ H ₁₂ NO ₁₂ [¹⁵ N]O ₃ ⁻	$C_8H_{12}NO_{12}$
392.0084	C ₈ H ₁₁ NO ₁₃ [¹⁵ N]O ₃ ⁻	C ₈ H ₁₁ NO ₁₃
420.9986	$C_8H_{10}N_2O_{14}[^{15}N]O_3^-$	$C_8H_{10}N_2O_{14}$
297.0832	$C_9H_{16}NO_6[^{15}N]O_3^{-1}$	C ₉ H ₁₆ NO ₆
311.0624	$C_9H_{14}NO_7[^{15}N]O_3^{-1}$	C9H14NO7
312.0703	C ₉ H ₁₅ NO ₇ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₅ NO ₇
324.0577	$C_9H_{13}N_2O_7[^{15}N]O_3^{-1}$	$C_9H_{13}N_2O_7$
326.0495	C ₉ H ₁₃ NO ₈ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₃ NO ₈
327.0573	C ₉ H ₁₄ NO ₈ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₄ NO ₈
328.0652	C ₉ H ₁₅ NO ₈ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₅ NO ₈
329.0730	C ₉ H ₁₆ NO ₈ [¹⁵ N]O ₃ ⁻	C9H16NO8
342.0444	C ₉ H ₁₃ NO ₉ [¹⁵ N]O ₃ ⁻	C9H13NO9
343.0523	C ₉ H ₁₄ NO ₉ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₄ NO ₉
344.0601	C ₉ H ₁₅ NO ₉ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₅ NO ₉
358.0393	C ₉ H ₁₃ NO ₁₀ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₃ NO ₁₀
359.0472	C ₉ H ₁₄ NO ₁₀ [¹⁵ N]O ₃ ⁻	$C_9H_{14}NO_{10}$
360.0550	C ₉ H ₁₅ NO ₁₀ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₅ NO ₁₀
370.0268	$C_9H_{11}N_2O_{10}[^{15}N]O_3^-$	$C_9H_{11}N_2O_{10}$
371.0346	$C_9H_{12}N_2O_{10}[^{15}N]O_3^-$	$C_9H_{12}N_2O_{10}$
374.0343	C ₉ H ₁₃ NO ₁₁ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₃ NO ₁₁
375.0421	C ₉ H ₁₄ NO ₁₁ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₄ NO ₁₁
376.0499	C ₉ H ₁₅ NO ₁₁ [¹⁵ N]O ₃ ⁻	$C_9H_{15}NO_{11}$
390.0292	C ₉ H ₁₃ NO ₁₂ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₃ NO ₁₂
391.0370	C ₉ H ₁₄ NO ₁₂ [¹⁵ N]O ₃ ⁻	$C_9H_{14}NO_{12}$
392.0448	C ₉ H ₁₅ NO ₁₂ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₅ NO ₁₂
403.0244	$C_9H_{12}N_2O_{12}[^{15}N]O_3^-$	$C_9H_{12}N_2O_{12}$
405.0401	$C_9H_{14}N_2O_{12}[^{15}N]O_3^-$	$C_9H_{14}N_2O_{12}$
406.0241	C ₉ H ₁₃ NO ₁₃ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₃ NO ₁₃
407.0319	$C_9H_{14}NO_{13}[^{15}N]O_3^{-1}$	$C_9H_{14}NO_{13}$
408.0397	C ₉ H ₁₅ NO ₁₃ [¹⁵ N]O ₃ ⁻	C ₉ H ₁₅ NO ₁₃
422.0190	C ₉ H ₁₃ NO ₁₄ [¹⁵ N]O ₃ ⁻	$C_9H_{13}NO_{14}$
423.0268	$C_9H_{14}NO_{14}[^{15}N]O_3^{-1}$	$C_9H_{14}NO_{14}$
309.0594	$C_{10}H_{14}O_7[^{15}N]O_3^{-1}$	$C_{10}H_{14}O_7$
309.0832	$C_{10}H_{16}NO_6[^{15}N]O_3^{-1}$	$C_{10}H_{16}NO_6$
311.0750	$C_{10}H_{16}O_7[^{15}N]O_3^-$	$C_{10}H_{16}O_7$
324.0703	$C_{10}H_{15}NO_7[^{15}N]O_3^{-1}$	$C_{10}H_{15}NO_{7}$
325.0543	$C_{10}H_{14}O_8[^{15}N]O_3^{-1}$	$C_{10}H_{14}O_8$
325.0781	C ₁₀ H ₁₆ NO ₇ [¹⁵ N]O ₃ ⁻	$C_{10}H_{16}NO_7$
327.0699	$C_{10}H_{16}O_8[^{15}N]O_3^-$	$C_{10}H_{16}O_8$
340.0652	$C_{10}H_{15}NO_8[^{15}N]O_3^{-1}$	$C_{10}H_{15}NO_8$
341.0492	$C_{10}H_{14}O_9[^{15}N]O_3^{-1}$	$C_{10}H_{14}O_9$
341.0730	$C_{10}H_{16}NO_8[^{15}N]O_3^{-1}$	$C_{10}H_{16}NO_8$
342.0570	$C_{10}H_{15}O_9[^{15}N]O_3^{-1}$	$C_{10}H_{15}O_9$
343.0648	$C_{10}H_{16}O_9[^{15}N]O_3$	$C_{10}H_{16}O_9$

356.0601	$C_{10}H_{15}NO_9[^{15}N]O_3^{-1}$	$C_{10}H_{15}NO_{9}$
357.0441	$C_{10}H_{14}O_{10}[^{15}N]O_3^-$	$C_{10}H_{14}O_{10}$
357.0679	$C_{10}H_{16}NO_9[^{15}N]O_3^{-1}$	$C_{10}H_{16}NO_9$
358.0519	$C_{10}H_{15}O_{10}[^{15}N]O_3^-$	$C_{10}H_{15}O_{10}$
358.0757	$C_{10}H_{17}NO_9[^{15}N]O_3^{-1}$	$C_{10}H_{17}NO_9$
359.0597	$C_{10}H_{16}O_{10}[^{15}N]O_{3}^{-1}$	$C_{10}H_{16}O_{10}$
371.0710	$C_{10}H_{16}N_2O_9[^{15}N]O_3^-$	$C_{10}H_{16}N_2O_9$
372.0550	$C_{10}H_{15}NO_{10}[^{15}N]O_{3}^{-}$	C ₁₀ H ₁₅ NO ₁₀
373.0390	$C_{10}H_{14}O_{11}[^{15}N]O_3^-$	$C_{10}H_{14}O_{11}$
373.0628	$C_{10}H_{16}NO_{10}[^{15}N]O_{3}^{-}$	$C_{10}H_{16}NO_{10}$
374.0468	$C_{10}H_{15}O_{11}[^{15}N]O_3^-$	$C_{10}H_{15}O_{11}$
374.0706	$C_{10}H_{17}NO_{10}[^{15}N]O_{3}^{-1}$	$C_{10}H_{17}NO_{10}$
375.0547	$C_{10}H_{16}O_{11}[^{15}N]O_{3}$	$C_{10}H_{16}O_{11}$
385.0502	$C_{10}H_{14}N_2O_{10}[^{15}N]O_3^-$	$C_{10}H_{14}N_2O_{10}$
386.0581	$C_{10}H_{15}N_2O_{10}[^{15}N]O_3^{-1}$	$C_{10}H_{15}N_2O_{10}$
387.0659	$C_{10}H_{16}N_2O_{10}[^{15}N]O_3^-$	$C_{10}H_{16}N_2O_{10}$
388.0499	$C_{10}H_{15}NO_{11}[^{15}N]O_{3}^{-1}$	$C_{10}H_{15}NO_{11}$
389.0339	$C_{10}H_{14}O_{12}[^{15}N]O_{3}^{-1}$	$C_{10}H_{14}O_{12}$
389.0577	$C_{10}H_{16}NO_{11}[^{15}N]O_{3}^{-}$	C ₁₀ H ₁₆ NO ₁₁
390.0418	$C_{10}H_{15}O_{12}[^{15}N]O_3^-$	$C_{10}H_{15}O_{12}$
390.0656	$C_{10}H_{17}NO_{11}[^{15}N]O_3^-$	C ₁₀ H ₁₇ NO ₁₁
391.0734	$C_{10}H_{18}NO_{11}[^{15}N]O_3^-$	$C_{10}H_{18}NO_{11}$
402.0530	$C_{10}H_{15}N_2O_{11}[^{15}N]O_3^-$	$C_{10}H_{15}N_2O_{11}$
403.0608	$C_{10}H_{16}N_2O_{11}[^{15}N]O_3^-$	$C_{10}H_{16}N_2O_{11}$
404.0448	$C_{10}H_{15}NO_{12}[^{15}N]O_{3}^{-}$	$C_{10}H_{15}NO_{12}$
405.0527	$C_{10}H_{16}NO_{12}[^{15}N]O_{3}^{-1}$	$C_{10}H_{16}NO_{12}$
406.0605	$C_{10}H_{17}NO_{12}[^{15}N]O_{3}^{-1}$	$C_{10}H_{17}NO_{12}$
417.0401	$C_{10}H_{14}N_2O_{12}[^{15}N]O_3^-$	$C_{10}H_{14}N_2O_{12}$
418.0479	$C_{10}H_{15}N_2O_{12}[^{15}N]O_3^-$	$C_{10}H_{15}N_2O_{12}$
420.0397	$C_{10}H_{15}NO_{13}[^{15}N]O_{3}^{-1}$	$C_{10}H_{15}NO_{13}$
420.0636	$C_{10}H_{17}N_2O_{12}[^{15}N]O_3^-$	$C_{10}H_{17}N_2O_{12}$
422.0554	$C_{10}H_{17}NO_{13}[^{15}N]O_{3}^{-1}$	$C_{10}H_{17}NO_{13}$
433.0350	$C_{10}H_{14}N_2O_{13}[^{15}N]O_3^-$	$C_{10}H_{14}N_2O_{13}$
434.0666	$C_{10}H_{17}N_3O_{12}[^{15}N]O_3^-$	$C_{10}H_{17}N_3O_{12}$
435.0506	$C_{10}H_{16}N_2O_{13}[^{15}N]O_3^-$	$C_{10}H_{16}N_2O_{13}$
437.0425	$C_{10}H_{16}NO_{14}[^{15}N]O_{3}^{-1}$	$C_{10}H_{16}NO_{14}$
437.0663	$C_{10}H_{18}N_2O_{13}[^{15}N]O_3^-$	$C_{10}H_{18}N_2O_{13}$
438.0503	$C_{10}H_{17}NO_{14}[^{15}N]O_{3}^{-1}$	C ₁₀ H ₁₇ NO ₁₄
451.0456	$C_{10}H_{16}N_2O_{14}[^{15}N]O_3^-$	$C_{10}H_{16}N_2O_{14}$
453.0612	$C_{10}H_{18}N_2O_{14}[^{15}N]O_3^-$	$C_{10}H_{18}N_2O_{14}$
466.0565	$C_{10}H_{17}N_3O_{14}[^{15}N]O_3^-$	$C_{10}H_{17}N_3O_{14}$
467.0405	$C_{10}H_{16}N_2O_{15}[^{15}N]O_3^-$	$C_{10}H_{16}N_2O_{15}$
482.0514	$C_{10}H_{17}N_3O_{15}[^{15}N]O_3^-$	$C_{10}H_{17}N_3O_{15}$
498.0463	$C_{10}H_{17}N_3O_{16}[^{15}N]O_3^{-1}$	$C_{10}H_{17}N_3O_{16}$
453.1618	$C_{17}H_{28}NO_9[^{15}N]O_3^{-1}$	$C_{17}H_{28}NO_9$
467.1649	$C_{17}H_{28}N_2O_9[^{15}N]O_3^{-1}$	$C_{17}H_{28}N_2O_9$

500.1387	$C_{17}H_{27}NO_{12}[^{15}N]O_3^{-1}$	C ₁₇ H ₂₇ NO ₁₂
513.1340	$C_{17}H_{26}N_2O_{12}[^{15}N]O_3^{-1}$	$C_{17}H_{26}N_2O_{12}$
531.1445	$C_{17}H_{28}N_2O_{13}[^{15}N]O_3^{-1}$	$C_{17}H_{28}N_2O_{13}$
545.1238	$C_{17}H_{26}N_2O_{14}[^{15}N]O_3^-$	$C_{17}H_{26}N_2O_{14}$
548.1235	$C_{17}H_{27}NO_{15}[^{15}N]O_3^{-1}$	C ₁₇ H ₂₇ NO ₁₅
449.1907	$C_{18}H_{30}N_2O_7[^{15}N]O_3^-$	$C_{18}H_{30}N_2O_7$
480.1489	$C_{18}H_{27}NO_{10}[^{15}N]O_3^{-1}$	C ₁₈ H ₂₇ NO ₁₀
511.1547	$C_{18}H_{28}N_2O_{11}[^{15}N]O_3^{-1}$	$C_{18}H_{28}N_2O_{11}$
527.1496	$C_{18}H_{28}N_2O_{12}[^{15}N]O_3^{-1}$	$C_{18}H_{28}N_2O_{12}$
529.1415	$C_{18}H_{28}NO_{13}[^{15}N]O_3^{-1}$	$C_{18}H_{28}NO_{13}$
558.1554	$C_{18}H_{29}N_3O_{13}[^{15}N]O_3^{-1}$	$C_{18}H_{29}N_3O_{13}$
562.1391	$C_{18}H_{29}NO_{15}[^{15}N]O_{3}^{-1}$	$C_{18}H_{29}NO_{15}$
574.1504	$C_{18}H_{29}N_3O_{14}[^{15}N]O_3^-$	$C_{18}H_{29}N_3O_{14}$
494.1645	$C_{19}H_{29}NO_{10}[^{15}N]O_{3}$	$C_{19}H_{29}NO_{10}$
496.1802	$C_{19}H_{31}NO_{10}[^{15}N]O_{3}^{-1}$	$C_{19}H_{31}NO_{10}$
509.1754	$C_{19}H_{30}N_2O_{10}[^{15}N]O_3^{-1}$	$C_{19}H_{30}N_2O_{10}$
510.1595	$C_{19}H_{29}NO_{11}[^{15}N]O_3^{-1}$	C ₁₉ H ₂₉ NO ₁₁
512.1751	$C_{19}H_{31}NO_{11}[^{15}N]O_{3}^{-1}$	$C_{19}H_{31}NO_{11}$
525.1704	$C_{19}H_{30}N_2O_{11}[^{15}N]O_3^-$	$C_{19}H_{30}N_2O_{11}$
526.1544	$C_{19}H_{29}NO_{12}[^{15}N]O_{3}^{-1}$	$C_{19}H_{29}NO_{12}$
528.1700	$C_{19}H_{31}NO_{12}[^{15}N]O_{3}$	$C_{19}H_{31}NO_{12}$
541.1653	$C_{19}H_{30}N_2O_{12}[^{15}N]O_3^-$	$C_{19}H_{30}N_2O_{12}$
542.1493	$C_{19}H_{29}NO_{13}[^{15}N]O_{3}^{-1}$	$C_{19}H_{29}NO_{13}$
544.1649	$C_{19}H_{31}NO_{13}[^{15}N]O_{3}^{-1}$	$C_{19}H_{31}NO_{13}$
557.1602	$C_{19}H_{30}N_2O_{13}[^{15}N]O_3^-$	$C_{19}H_{30}N_2O_{13}$
560.1599	$C_{19}H_{31}NO_{14}[^{15}N]O_{3}^{-1}$	$C_{19}H_{31}NO_{14}$
573.1551	$C_{19}H_{30}N_2O_{14}[^{15}N]O_3^-$	$C_{19}H_{30}N_2O_{14}$
575.1708	$C_{19}H_{32}N_2O_{14}[^{15}N]O_3^-$	$C_{19}H_{32}N_2O_{14}$
576.1548	$C_{19}H_{31}NO_{15}[^{15}N]O_{3}^{-1}$	$C_{19}H_{31}NO_{15}$
577.1388	$C_{19}H_{30}O_{16}[^{15}N]O_{3}^{-1}$	$C_{19}H_{30}O_{16}$
585.1663	$C_{19}H_{30}N_4O_{13}[^{15}N]O_3^{-1}$	$C_{19}H_{30}N_4O_{13}$
589.1500	$C_{19}H_{30}N_2O_{15}[^{15}N]O_3^{-1}$	$C_{19}H_{30}N_2O_{15}$
604.1609	$C_{19}H_{31}N_3O_{15}[^{15}N]O_3^{-1}$	$C_{19}H_{31}N_3O_{15}$
605.1449	$C_{19}H_{30}N_2O_{16}[^{15}N]O_3^{-1}$	$C_{19}H_{30}N_2O_{16}$
607.1368	$C_{19}H_{30}NO_{17}[^{15}N]O_{3}^{-1}$	C ₁₉ H ₃₀ NO ₁₇
617.1562	$C_{19}H_{30}N_4O_{15}[^{15}N]O_3^{-1}$	$C_{19}H_{30}N_4O_{15}$
620.1558	$C_{19}H_{31}N_3O_{16}[^{15}N]O_3^{-1}$	$C_{19}H_{31}N_3O_{16}$
621.1398	$C_{19}H_{30}N_2O_{17}[^{15}N]O_3^{-1}$	$C_{19}H_{30}N_2O_{17}$
636.1507	$C_{19}H_{31}N_3O_{17}[^{15}N]O_3^{-1}$	$C_{19}H_{31}N_3O_{17}$
637.1348	$C_{19}H_{30}N_2O_{18}[^{15}N]O_3^{-1}$	$C_{19}H_{30}N_2O_{18}$
652.1457	$C_{19}H_{31}N_3O_{18}[^{15}N]O_3^{-1}$	$C_{19}H_{31}N_3O_{18}$
664.1569	$C_{19}H_{31}N_5O_{17}[^{15}N]O_3^{-1}$	C ₁₉ H ₃₁ N ₅ O ₁₇
668.1406	$C_{19}H_{31}N_3O_{19}[^{15}N]O_3^{-1}$	$C_{19}H_{31}N_3O_{19}$
680.1518	$C_{19}H_{31}N_5O_{18}[^{15}N]O_3^{-1}$	$C_{19}H_{31}N_5O_{18}$
696.1467	$C_{19}H_{31}N_5O_{19}[^{15}N]O_3^{-1}$	C ₁₉ H ₃₁ N ₅ O ₁₉
507.1962	$C_{20}H_{32}N_2O_9[^{15}N]O_3^{-1}$	$C_{20}H_{32}N_2O_9$

508.1802	$C_{20}H_{31}NO_{10}[^{15}N]O_3^{-1}$	$C_{20}H_{31}NO_{10}$
523.1911	$C_{20}H_{32}N_2O_{10}[^{15}N]O_3^-$	$C_{20}H_{32}N_2O_{10}$
524.1751	$C_{20}H_{31}NO_{11}[^{15}N]O_{3}^{-1}$	C ₂₀ H ₃₁ NO ₁₁
539.1860	$C_{20}H_{32}N_2O_{11}[^{15}N]O_3^-$	$C_{20}H_{32}N_2O_{11}$
540.1700	$C_{20}H_{31}NO_{12}[^{15}N]O_{3}^{-1}$	C ₂₀ H ₃₁ NO ₁₂
542.1857	$C_{20}H_{33}NO_{12}[^{15}N]O_{3}$	C ₂₀ H ₃₃ NO ₁₂
543.1697	C ₂₀ H ₃₂ O ₁₃ [¹⁵ N]O ₃ ⁻	$C_{20}H_{32}O_{13}$
553.1653	$C_{20}H_{30}N_2O_{12}[^{15}N]O_3^-$	$C_{20}H_{30}N_2O_{12}$
555.1809	$C_{20}H_{32}N_2O_{12}[^{15}N]O_3^-$	$C_{20}H_{32}N_2O_{12}$
556.1649	$C_{20}H_{31}NO_{13}[^{15}N]O_{3}^{-1}$	C ₂₀ H ₃₁ NO ₁₃
557.1490	$C_{20}H_{30}O_{14}[^{15}N]O_{3}$	$C_{20}H_{30}O_{14}$
559.1646	$C_{20}H_{32}O_{14}[^{15}N]O_{3}$	$C_{20}H_{32}O_{14}$
569.1602	$C_{20}H_{30}N_2O_{13}[^{15}N]O_3^-$	$C_{20}H_{30}N_2O_{13}$
570.1680	$C_{20}H_{31}N_2O_{13}[^{15}N]O_3^-$	$C_{20}H_{31}N_2O_{13}$
570.1918	$C_{20}H_{33}N_3O_{12}[^{15}N]O_3^-$	$C_{20}H_{33}N_3O_{12}$
571.1758	$C_{20}H_{32}N_2O_{13}[^{15}N]O_3^{-1}$	$C_{20}H_{32}N_2O_{13}$
572.1599	$C_{20}H_{31}NO_{14}[^{15}N]O_{3}^{-1}$	C ₂₀ H ₃₁ NO ₁₄
575.1595	$C_{20}H_{32}O_{15}[^{15}N]O_{3}$	$C_{20}H_{32}O_{15}$
585.1551	$C_{20}H_{30}N_2O_{14}[^{15}N]O_3^-$	$C_{20}H_{30}N_2O_{14}$
586.1629	$C_{20}H_{31}N_2O_{14}[^{15}N]O_3^-$	$C_{20}H_{31}N_2O_{14}$
586.1867	$C_{20}H_{33}N_3O_{13}[^{15}N]O_3^-$	C ₂₀ H ₃₃ N ₃ O ₁₃
587.1708	$C_{20}H_{32}N_2O_{14}[^{15}N]O_3^-$	C ₂₀ H ₃₂ N ₂ O ₁₄
588.1548	$C_{20}H_{31}NO_{15}[^{15}N]O_{3}^{-1}$	C ₂₀ H ₃₁ NO ₁₅
590.1704	$C_{20}H_{33}NO_{15}[^{15}N]O_{3}$	C ₂₀ H ₃₃ NO ₁₅
591.1544	$C_{20}H_{32}O_{16}[^{15}N]O_{3}^{-1}$	$C_{20}H_{32}O_{16}$
600.1660	$C_{20}H_{31}N_3O_{14}[^{15}N]O_3^-$	$C_{20}H_{31}N_3O_{14}$
601.1500	$C_{20}H_{30}N_2O_{15}[^{15}N]O_3^-$	$C_{20}H_{30}N_2O_{15}$
602.1578	$C_{20}H_{31}N_2O_{15}[^{15}N]O_3^{-1}$	$C_{20}H_{31}N_2O_{15}$
602.1817	$C_{20}H_{33}N_3O_{14}[^{15}N]O_3^-$	$C_{20}H_{33}N_3O_{14}$
603.1657	$C_{20}H_{32}N_2O_{15}[^{15}N]O_3^-$	$C_{20}H_{32}N_2O_{15}$
606.1653	$C_{20}H_{33}NO_{16}[^{15}N]O_{3}$	C ₂₀ H ₃₃ NO ₁₆
616.1609	$C_{20}H_{31}N_3O_{15}[^{15}N]O_3^{-1}$	$C_{20}H_{31}N_3O_{15}$
617.1449	$C_{20}H_{30}N_2O_{16}[^{15}N]O_3^-$	$C_{20}H_{30}N_2O_{16}$
618.1528	$C_{20}H_{31}N_2O_{16}[^{15}N]O_3^-$	$C_{20}H_{31}N_2O_{16}$
618.1766	$C_{20}H_{33}N_3O_{15}[^{15}N]O_3^-$	$C_{20}H_{33}N_3O_{15}$
619.1606	$C_{20}H_{32}N_2O_{16}[^{15}N]O_3^-$	$C_{20}H_{32}N_2O_{16}$
632.1558	$C_{20}H_{31}N_3O_{16}[^{15}N]O_3^-$	$C_{20}H_{31}N_3O_{16}$
633.1398	$C_{20}H_{30}N_2O_{17}[^{15}N]O_3^-$	$C_{20}H_{30}N_2O_{17}$
633.1637	$C_{20}H_{32}N_3O_{16}[^{15}N]O_3^-$	$C_{20}H_{32}N_3O_{16}$
633.1875	$C_{20}H_{34}N_4O_{15}[^{15}N]O_3^-$	$C_{20}H_{34}N_4O_{15}$
634.1715	$C_{20}H_{33}N_{3}O_{16}[^{15}N]O_{3}$	$C_{20}H_{33}N_3O_{16}$
635.1555	$C_{20}H_{32}N_2O_{17}[^{15}N]O_3^{-1}$	$C_{20}H_{32}N_2O_{17}$
648.1507	$C_{20}H_{31}N_{3}O_{17}[^{15}N]O_{3}$	$C_{20}H_{31}N_3O_{17}$
649.1586	$C_{20}H_{32}N_3O_{17}[^{15}N]O_3^{-1}$	$C_{20}H_{32}N_3O_{17}$
649.1824	$C_{20}H_{34}N_4O_{16}[^{15}N]O_3$	$C_{20}H_{34}N_4O_{16}$
650.1664	$C_{20}H_{33}N_3O_{17}[^{15}N]O_3^{-1}$	$C_{20}H_{33}N_3O_{17}$

651 1504	C II N O [¹⁵ N] O -	CUNO
664 1457	$\frac{C_{20}H_{32}N_2O_{18}[-1N]O_3}{C_{10}H_{10}N_{10}}$	$C_{20}H_{32}N_{2}O_{18}$
665 1525	$\frac{C_{20}H_{31}N_{3}O_{18}[-N]O_{3}}{C_{10}H_{10}N_{10}}$	C H NO
003.1333	$C_{20}H_{32}N_{3}O_{18}[-N]O_{3}$	$C_{20}H_{32}N_{3}O_{18}$
003.1773	$C_{20}H_{34}N_4O_{17}[^{-5}N]O_3$	$C_{20}H_{34}N_4O_{17}$
666.1613	$C_{20}H_{33}N_3O_{18}[^{15}N]O_3$	$C_{20}H_{33}N_{3}O_{18}$
667.1453	$C_{20}H_{32}N_2O_{19}[{}^{15}N]O_3^{-1}$	$C_{20}H_{32}N_2O_{19}$
680.1406	$C_{20}H_{31}N_3O_{19}[{}^{15}N]O_3^{-1}$	$C_{20}H_{31}N_{3}O_{19}$
681.1484	$C_{20}H_{32}N_3O_{19}[^{15}N]O_3^{-1}$	$C_{20}H_{32}N_3O_{19}$
681.1722	$C_{20}H_{34}N_4O_{18}[^{15}N]O_3^{-1}$	C ₂₀ H ₃₄ N ₄ O ₁₈
682.1562	$C_{20}H_{33}N_3O_{19}[^{15}N]O_3^{-1}$	C ₂₀ H ₃₃ N ₃ O ₁₉
683.1402	$C_{20}H_{32}N_2O_{20}[^{15}N]O_3^{-1}$	$C_{20}H_{32}N_2O_{20}$
696.1355	$C_{20}H_{31}N_3O_{20}[^{15}N]O_3^{-1}$	$C_{20}H_{31}N_3O_{20}$
697.1671	$C_{20}H_{34}N_4O_{19}[^{15}N]O_3^{-1}$	C ₂₀ H ₃₄ N ₄ O ₁₉
698.1511	$C_{20}H_{33}N_3O_{20}[^{15}N]O_3^-$	C ₂₀ H ₃₃ N ₃ O ₂₀
713.1620	$C_{20}H_{34}N_4O_{20}[^{15}N]O_3^-$	$C_{20}H_{34}N_4O_{20}$
784.2607	$C_{26}H_{47}N_3O_{20}[^{15}N]O_3^-$	$C_{26}H_{47}N_3O_{20}$
892.2414	$C_{26}H_{47}N_5O_{25}[^{15}N]O_3^-$	$C_{26}H_{47}N_5O_{25}$
771.2668	$C_{27}H_{44}N_6O_{16}[^{15}N]O_3^-$	C ₂₇ H ₄₄ N ₆ O ₁₆
727.2545	$C_{28}H_{44}N_2O_{16}[^{15}N]O_3^-$	C ₂₈ H ₄₄ N ₂ O ₁₆
744.2334	$C_{28}H_{43}NO_{18}[^{15}N]O_{3}^{-1}$	C ₂₈ H ₄₃ NO ₁₈
770.2715	C ₂₈ H ₄₅ N ₅ O ₁₆ [¹⁵ N]O ₃ ⁻	C ₂₈ H ₄₅ N ₅ O ₁₆
786.2664	$C_{28}H_{45}N_5O_{17}[^{15}N]O_3^{-1}$	C ₂₈ H ₄₅ N ₅ O ₁₇
864.2254	$C_{28}H_{43}N_5O_{22}[^{15}N]O_3^{-1}$	C ₂₈ H ₄₃ N ₅ O ₂₂
803.2818	C ₂₉ H ₄₈ N ₄ O ₁₈ [¹⁵ N]O ₃	C ₂₉ H ₄₈ N ₄ O ₁₈
804.2658	$C_{29}H_{47}N_3O_{19}[^{15}N]O_3^{-1}$	C ₂₉ H ₄₇ N ₃ O ₁₉
817.2610	$C_{29}H_{46}N_4O_{19}[^{15}N]O_3^{-1}$	C ₂₉ H ₄₆ N ₄ O ₁₉
818.2450	$C_{29}H_{45}N_3O_{20}[^{15}N]O_3^{-1}$	C ₂₉ H ₄₅ N ₃ O ₂₀
833.2559	C ₂₉ H ₄₆ N ₄ O ₂₀ [¹⁵ N]O ₃	C ₂₉ H ₄₆ N ₄ O ₂₀
835.2240	$C_{29}H_{44}N_2O_{22}[^{15}N]O_3^{-1}$	C ₂₉ H ₄₄ N ₂ O ₂₂
836.2556	$C_{29}H_{47}N_3O_{21}[^{15}N]O_3^{-1}$	C ₂₉ H ₄₇ N ₃ O ₂₁
865.2458	$C_{29}H_{46}N_4O_{22}[^{15}N]O_3^{-1}$	C ₂₉ H ₄₆ N ₄ O ₂₂
881.2407	$C_{29}H_{46}N_4O_{23}[^{15}N]O_3^{-1}$	C ₂₉ H ₄₆ N ₄ O ₂₃
897.2356	C ₂₉ H ₄₆ N ₄ O ₂₄ [¹⁵ N]O ₃ ⁻	C29H46N4O24
772.2647	$C_{30}H_{47}NO_{18}[^{15}N]O_{3}^{-1}$	C ₃₀ H ₄₇ NO ₁₈
783.2919	$C_{30}H_{48}N_4O_{16}[^{15}N]O_3^{-1}$	C30H48N4O16
787.2756	$C_{30}H_{48}N_2O_{18}[^{15}N]O_3^{-1}$	C30H48N2O18
788.2596	$C_{30}H_{47}NO_{19}[^{15}N]O_{3}^{-1}$	C30H47NO19
799.2868	$C_{30}H_{48}N_4O_{17}[^{15}N]O_3^-$	C ₃₀ H ₄₈ N ₄ O ₁₇
800.2709	$\frac{C_{30}H_{47}N_{3}O_{18}[^{15}N]O_{3}}{C_{30}H_{47}N_{3}O_{18}[^{15}N]O_{3}}$	$C_{30}H_{47}N_3O_{18}$
802.2865	$\frac{C_{30}H_{49}N_3O_{18}[^{15}N]O_3}{C_{30}H_{49}N_3O_{18}[^{15}N]O_3}$	$\frac{C_{30}H_{40}N_3O_{18}}{C_{30}H_{40}N_3O_{18}}$
815.2818	$C_{30}H_{48}N_4O_{18}[^{15}N]O_2^{-1}$	C30H48N4O19
816.2658	$C_{30}H_{47}N_{2}O_{10}[^{15}N]O_{2}^{-1}$	C30H47N2O10
831.2767	$C_{30}H_{48}N_4O_{10}[^{15}N]O_2^{-1}$	C30H48N4O10
834 2763	$C_{20}H_{40}N_2O_{20}[^{15}N]O_2^{-1}$	C20H40N2O20
847 2716	$C_{20}H_{49}N_4O_{20}[^{15}N]O_2^{-1}$	$C_{20}H_{49}N_{4}O_{20}$
848 2556	$C_{20}H_{47}N_2O_{21}[^{15}N]O_{27}$	$C_{20}H_{48}V_{4}O_{20}$
0-0.2330	$\bigcirc 30114/13021[$ 11] $\bigcirc 3$	○ 30114/1 1 3 ○ 21

849.2396	$C_{30}H_{46}N_2O_{22}[^{15}N]O_3^-$	$C_{30}H_{46}N_2O_{22}$
862.2825	$C_{30}H_{49}N_5O_{20}[^{15}N]O_3^-$	$C_{30}H_{49}N_5O_{20}$
863.2665	$C_{30}H_{48}N_4O_{21}[^{15}N]O_3^-$	$C_{30}H_{48}N_4O_{21}$
866.2662	$C_{30}H_{49}N_3O_{22}[^{15}N]O_3^-$	$C_{30}H_{49}N_3O_{22}$
867.2502	$C_{30}H_{48}N_2O_{23}[^{15}N]O_3^-$	$C_{30}H_{48}N_2O_{23}$
879.2614	$C_{30}H_{48}N_4O_{22}[^{15}N]O_3^-$	$C_{30}H_{48}N_4O_{22}$
880.2454	$C_{30}H_{47}N_3O_{23}[^{15}N]O_3^-$	$C_{30}H_{47}N_3O_{23}$
895.2563	$C_{30}H_{48}N_4O_{23}[^{15}N]O_3^-$	$C_{30}H_{48}N_4O_{23}$
896.2404	$C_{30}H_{47}N_3O_{24}[^{15}N]O_3^{-1}$	$C_{30}H_{47}N_3O_{24}$
911.2513	$C_{30}H_{48}N_4O_{24}[^{15}N]O_3^-$	$C_{30}H_{48}N_4O_{24}$
926.2621	$C_{30}H_{49}N_5O_{24}[^{15}N]O_3^-$	$C_{30}H_{49}N_5O_{24}$

Table S2. Observed $C_9H_{14}NO_x$ • radicals (m) and their termination products, including carbonyl compounds (m-17), hydroxyl compounds (m-15), and hydroperoxy compounds (m+1). Their concentrations during P1a period are normalized to that of $C_9H_{15}NO_8$, which had the highest concentration among the families of 1N-C₉ monomers. Their relative intensities during the P1a period are shown on the second line in each cell.

Peroxy radical m	Carbonyl m-17	Hydroxy m-15	Hydroperoxy m+1
C ₉ H ₁₄ NO ₇ •			C ₉ H ₁₅ NO ₇
18.8 %			19.3 %
$C_9H_{14}NO_8\bullet$		C ₉ H ₁₅ NO ₇	C ₉ H ₁₅ NO ₈
27.9 %		19.3 %	100.0 %
$C_9H_{14}NO_9\bullet$	C ₉ H ₁₃ NO ₈	C ₉ H ₁₅ NO ₈	$C_9H_{15}NO_9$
20.7 %	98.6 %	100.0 %	66.2 %
$C_9H_{14}NO_{10}\bullet$	C ₉ H ₁₃ NO ₉	C ₉ H ₁₅ NO ₉	C ₉ H ₁₅ NO ₁₀
46.2 %	56.9 %	66.2 %	30.9 %
$C_9H_{14}NO_{11}\bullet$	C ₉ H ₁₃ NO ₁₀	C ₉ H ₁₅ NO ₁₀	C ₉ H ₁₅ NO ₁₁
12.4 %	38.3 %	30.9 %	3.6 %
$C_9H_{14}NO_{12}\bullet$	C9H13NO11	C9H15NO11	C9H15NO12
12.2 %	14.5 %	3.6 %	23.9 %
$C_9H_{14}NO_{13}\bullet$	C ₉ H ₁₃ NO ₁₂	C ₉ H ₁₅ NO ₁₂	C ₉ H ₁₅ NO ₁₃
9.7 %	13.9 %	23.9 %	10.4 %
$C_9H_{14}NO_{14}\bullet$	C9H13NO13	C9H15NO13	
20.1 %	10.0 %	10.4 %	
	C9H13NO14		
	8.9 %		

Table S3. Reaction rate constants (code named in the MCM) of every individual RO₂• bimolecular

227 reaction used for estimating RO₂• fate according to MCM.

RO ₂ • species	R	ate constant with the	reactant below (cm ³ n	nolecule ⁻¹ s ⁻¹)	
	HO ₂ •	NO	NO ₃ •	RO ₂ •	NO ₂
C732CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C622CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
MACRO2	KRO2HO2*0.625	KRO2NO	KRO2NO3	9.20E-14	
NC826O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	9.20E-14	
MMALANHYO2	KRO2HO2*0.706	KRO2NO	KRO2NO3	9.20E-14	
NORLIMO2	KRO2HO2*0.890	KRO2NO	KRO2NO3	9.20E-14	
C312COCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
NLMKAO2	KRO2HO2*0.914	KRO2NO*0.760	KRO2NO3	9.20E-14	
C629O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	9.20E-14	
C624CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C622O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	1.30E-12	
C537O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	8.80E-13	
NLIMALO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	9.20E-14	
C531O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	2.00E-12	
LMKAO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	9.20E-14	
C533O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	8.80E-13	
C816O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	2.50E-13	
C517CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C626O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	1.30E-12	
C535O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	9.20E-14	
C731CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C626CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
HMVKBO2	KRO2HO2*0.625	KRO2NO	KRO2NO3	8.80E-13	
C31CO3	КАРНО2	KAPNO	KRO2NO3*1.6	1.00E-11	KFPAN
C3MCODBCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
IECCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C732O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	1.30E-12	
INCO2	KRO2HO2*0.706	KRO2NO	KRO2NO3	2.90E-12	
HPC52CO3	КАРНО2	KAPNO	KRO2NO3*1.6	1.00E-11	KFPAN
INCNCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C519CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C823CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C735O2	KRO2HO2*0.820	KRO2NO	KRO2NO3	9.20E-14	
MMALNACO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
HCOCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
HCOCH2O2	KRO2HO2*0.387	KRO2NO	KRO2NO3	2.00E-12	
C923CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
CONM2CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C518CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C822CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
HOCH2CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
CHOC3COCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN

C926O2	KRO2HO2*0.890	KRO2NO	KRO2NO3	9.20E-14	
C511CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C924O2	KRO2HO2*0.890	KRO2NO	KRO2NO3	8.80E-13	
C47CO3	КАРНО2	KAPNO	KRO2NO3*1.6	1.00E-11	KFPAN
C520O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	9.20E-14	
C733O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	8.80E-12	
LMKBO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	8.80E-13	
MEKAO2	KRO2HO2*0.625	KRO2NO	KRO2NO3	2.00E-12	
C731O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	1.30E-12	
INDHPCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
CO23C4CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C823O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	1.30E-12	
C730O2	KRO2HO2*0.820	KRO2NO	KRO2NO3	9.20E-14	
C734O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	8.80E-12	
C527O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	8.80E-13	
CH3COCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C57O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	9.20E-14	
C824O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	8.80E-12	
NC623O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	8.80E-13	
HOCH2CH2O2	1.53D- 13*EXP(1300/TEMP)	KRO2NO	KRO2NO3	2*(KCH3O2*7.8 D- 14*EXP(1000/T EMP))@0.5	
INDO2	KRO2HO2*0.706	KRO2NO	KRO2NO3	8.80E-13	
INDO2 CH3CO3	KRO2HO2*0.706 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP)	KRO2NO3 4.00E-12	8.80E-13 1.00E-11	KFPAN
INDO2 CH3CO3 CH3COCH2O2	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP)	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO	KRO2NO3 4.00E-12 kRO2NO3	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5	KFPAN
INDO2 CH3CO3 CH3COCH2O2 MACROHO2	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12	KFPAN
INDO2 CH3CO3 CH3COCH2O2 MACROHO2 COHM2CO3	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3*1.74	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11	KFPAN
INDO2 CH3CO3 CH3COCH2O2 CH3COCH2O2 MACROHO2 COHM2CO3	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KRO2HO2*0.859	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 8.80E-13	KFPAN
INDO2 CH3CO3 CH3COCH2O2 CH3COCH2O2 MACROHO2 COHM2CO3 C821O2 C58NO3CO3	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KRO2HO2*0.859 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 8.80E-13 1.00E-11	KFPAN KFPAN KFPAN
INDO2 CH3CO3 CH3COCH2O2 CH3COCH2O2 MACROHO2 COHM2CO3 COHM2CO3 C57NO3CO3	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KAPHO2 KAPHO2 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO KAPNO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 8.80E-13 1.00E-11 1.00E-11	KFPAN KFPAN KFPAN KFPAN
INDO2 CH3CO3 CH3COCH2O2 MACROHO2 COHM2CO3 C821O2 C58NO3CO3 C57NO3CO3 ISOPCO2	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KAPHO2 KAPHO2 KAPHO2 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO KAPNO KAPNO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 8.80E-13 1.00E-11 1.00E-11 2.00E-12	KFPAN KFPAN KFPAN KFPAN
INDO2 CH3CO3 CH3COCH2O2 CH3COCH2O2 MACROHO2 COHM2CO3 C57NO3CO3 ISOPCO2 MACRNCO3	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KRO2HO2*0.859 KAPHO2 KAPHO2 KRO2HO2*0.706 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO KAPNO KAPNO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 1.00E-11 1.00E-11 2.00E-12 1.00E-11	KFPAN KFPAN KFPAN KFPAN KFPAN
INDO2 CH3CO3 CH3COCH2O2 CH3COCH2O2 MACROHO2 COHM2CO3 C58NO3CO3 C57NO3CO3 ISOPCO2 MACRNCO3 C925O2	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.706 KAPHO2 KRO2HO2*0.890	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO KAPNO KAPNO KAPNO KAPNO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 kRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 8.80E-13 1.00E-11 1.00E-11 2.00E-12 1.00E-11 9.20E-14	KFPAN KFPAN KFPAN KFPAN KFPAN
IND02 CH3CO3 CH3COCH2O2 MACROHO2 COHM2CO3 C82102 C58N03CO3 C57N03CO3 ISOPCO2 MACRNCO3 C92502 C92302	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KRO2HO2*0.859 KAPHO2 KAPHO2 KRO2HO2*0.706 KAPHO2 KRO2HO2*0.890 KRO2HO2*0.890	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO KAPNO KAPNO KAPNO KAPNO KRO2NO KAPNO KRO2NO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 1.00E-11 1.00E-11 2.00E-12 1.00E-11 9.20E-14 1.32E-12	KFPAN KFPAN KFPAN KFPAN KFPAN
INDO2 CH3CO3 CH3COCH2O2 MACROHO2 COHM2CO3 C82102 C58N03CO3 C57N03CO3 ISOPCO2 MACRNCO3 C92502 C92302 C817CO3	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.706 KRO2HO2*0.890 KRO2HO2*0.890 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO KAPNO KAPNO KRO2NO KAPNO KRO2NO KAPNO KRO2NO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3 KRO2NO3*1.74 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 1.00E-11 1.00E-11 2.00E-12 1.00E-11 9.20E-14 1.32E-12 1.00E-11	KFPAN KFPAN KFPAN KFPAN KFPAN
IND02 CH3CO3 CH3COCH2O2 MACROHO2 COHM2CO3 C82102 C58N03CO3 C57N03CO3 ISOPCO2 MACRNCO3 C92502 C92302 C817CO3 HC4CCO3	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KRO2HO2*0.859 KAPHO2 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.859 KAPHO2 KAPHO2 KRO2HO2*0.859 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO KAPNO KAPNO KAPNO KAPNO KAPNO KAPNO KRO2NO KAPNO KAPNO KAPNO KAPNO KAPNO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 1.00E-11 1.00E-11 2.00E-12 1.00E-11 9.20E-14 1.32E-12 1.00E-11 1.00E-11 1.00E-11 1.00E-11	KFPAN KFPAN KFPAN KFPAN KFPAN KFPAN
IND02 CH3CO3 CH3COCH2O2 MACROHO2 COHM2CO3 C82102 C58N03CO3 C57N03CO3 ISOPCO2 MACRNCO3 C92502 C92302 C817CO3 HC4CCO3 LIMA02	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.890 KRO2HO2*0.890 KRO2HO2*0.890 KAPHO2 KRO2HO2*0.890 KRO2HO2*0.890 KAPHO2 KAPHO2 KAPHO2 KRO2HO2*0.890 KRO2HO2*0.890 KAPHO2 KAPHO2 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO KAPNO KAPNO KRO2NO KAPNO KRO2NO KAPNO KRO2NO KAPNO KRO2NO KAPNO KRO2NO KAPNO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3 KRO2NO3*1.74 KRO2NO3 KRO2NO3*1.74 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 1.00E-11 2.00E-12 1.00E-11 9.20E-14 1.32E-12 1.00E-11 1.00E-11 9.20E-14	KFPAN KFPAN KFPAN KFPAN KFPAN KFPAN KFPAN
IND02 CH3CO3 CH3COCH2O2 MACROHO2 COHM2CO3 C82102 C58N03CO3 C57N03CO3 ISOPCO2 MACRNCO3 C92502 C92302 C817CO3 HC4CCO3 LIMA02 HC4ACO3	KRO2HO2*0.706 KAPHO2 1.36D- 13*EXP(1250/TEMP) KRO2HO2*0.625 KAPHO2 KRO2HO2*0.859 KAPHO2 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.859 KAPHO2 KAPHO2 KRO2HO2*0.859 KAPHO2 KRO2HO2*0.890 KRO2HO2*0.890 KRO2HO2*0.890 KAPHO2 KRO2HO2*0.914 KAPHO2	KRO2NO 7.5D- 12*EXP(290/TE MP) kRO2NO KRO2NO KAPNO KAPNO KAPNO KAPNO KAPNO KRO2NO KAPNO KRO2NO KAPNO KRO2NO KAPNO KRO2NO KAPNO KRO2NO KAPNO KRO2NO KAPNO KAPNO KAPNO KAPNO	KRO2NO3 4.00E-12 kRO2NO3 kRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74 KRO2NO3*1.74	8.80E-13 1.00E-11 2*(K298CH3O2* 8.0D-12)@0.5 1.40E-12 1.00E-11 1.00E-11 2.00E-12 1.00E-11 9.20E-14 1.32E-12 1.00E-11 9.20E-14 1.00E-11 9.20E-14 1.00E-11	KFPAN KFPAN KFPAN KFPAN KFPAN KFPAN KFPAN

C822O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	1.30E-12	
C820O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	9.20E-14	
INB1NBCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C826O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	9.20E-14	
LIMALBO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	8.80E-13	
C57AO2	KRO2HO2*0.706	KRO2NO	KRO2NO3	8.80E-13	
LIMCO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	9.20E-14	
C817O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	1.30E-12	
NLIMO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	9.20E-14	
NC728O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	9.20E-14	
CHOC3COO2	KRO2HO2*0.625	KRO2NO	KRO2NO3	2.00E-12	
NC730O2	KRO2HO2*0.820	KRO2NO	KRO2NO3	9.20E-14	
C728O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	9.20E-14	
LIMALO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	9.20E-14	
C4M2ALOHO2	KRO2HO2*0.706	KRO2NO	KRO2NO3	9.20E-14	
MACRNBCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
HCOCH2CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C727O2	KRO2HO2*0.820	KRO2NO	KRO2NO3	8.80E-13	
C58O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	9.20E-14	
С729СО3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
MC3CODBCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
HPC52O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	9.20E-14	
HMVKBCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
ISOPDO2	KRO2HO2*0.706	KRO2NO	KRO2NO3	2.90E-12	
C624O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	2.50E-13	
C727CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
INDHCO3	KAPHO2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
BIACETO2	KRO2HO2*0.625	KRO2NO	KRO2NO3	2.00E-12	
CISOPCO2	KRO2HO2*0.706	KRO2NO	KRO2NO3	2.00E-12	
LMLKAO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	8.80E-13	
CO2H3CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
LIMBO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	8.80E-13	
CH3O2	3.8D- 13*EXP(780/TEMP)* (1-1/(1+498*EXP(- 1160/TEMP)))	2.3D- 12*EXP(360/TE MP)	1.2E-12	2*KCH3O2*RO 2*7.18*EXP(- 885/TEMP) 2*KCH3O2*RO 2*(1-7.18*EXP(- 885/TEMP))	KMT13
LIMALAO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	8.80E-13	
C825O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	8.80E-12	
CO2N3CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
MACO3	КАРНО2	8.70D- 12*EXP(290/TE MP)	KRO2NO3*1.74	1.00E-11	KFPAN
INB1NACO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN

C58AO2	KRO2HO2*0.706	KRO2NO	KRO2NO3	8.80E-13	
C59O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	9.20E-14	
CHOMOHCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C729O2	KRO2HO2*0.820	KRO2NO	KRO2NO3	1.30E-12	
CO25C6CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
CO2C3CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
H01C03C402	KRO2HO2*0.625	KRO2NO	KRO2NO3	2.00E-12	
MMALNBCO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
CHOCOCH2O2	KRO2HO2*0.520	KRO2NO	KRO2NO3	2.00E-12	
HOC2H4CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C628O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	9.20E-14	
C623O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	8.00E-13	
C625O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	9.20E-14	
LMLKBO2	KRO2HO2*0.914	KRO2NO	KRO2NO3	8.80E-13	
C627O2	KRO2HO2*0.770	KRO2NO	KRO2NO3	2.50E-12	
C517O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	1.30E-12	
C3MDIALO2	KRO2HO2*0.625	KRO2NO	KRO2NO3	9.20E-14	
C819O2	KRO2HO2	KRO2NO	KRO2NO3	9.20E-14	
CO2C4CO3	КАРНО2	KAPNO	KRO2NO3*1.74	1.00E-11	KFPAN
C534O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	9.20E-14	
C818O2	KRO2HO2*0.859	KRO2NO	KRO2NO3	1.30E-12	
C511O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	8.80E-13	
C519O2	KRO2HO2*0.706	KRO2NO	KRO2NO3	8.80E-13	

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