



Supplement of

Modeling daytime and nighttime secondary organic aerosol formation via multiphase reactions of biogenic hydrocarbons

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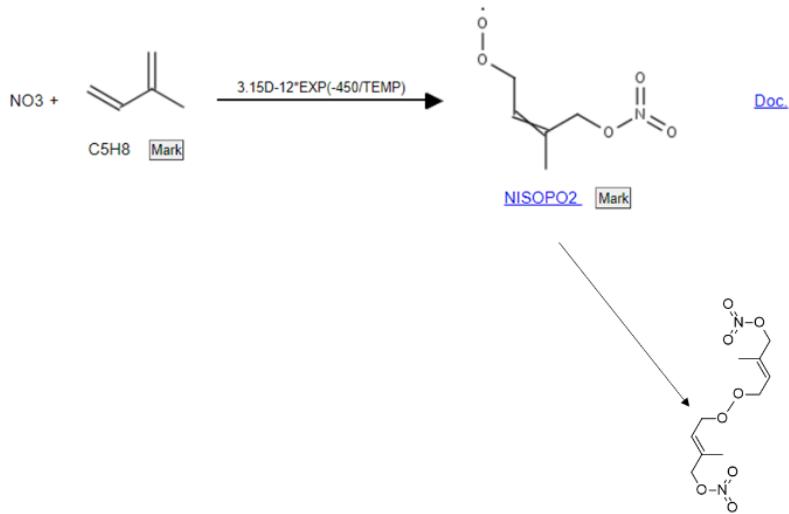
Section S1. The oxidation process of biogenic hydrocarbons.

The model parameters and the predetermined mathematical equations for stoichiometric coefficients for lumping bins were derived by using the products predicted from the semi-explicit mechanisms for the atmospheric oxidation of biogenic HCs. In this study, semi-explicit gas mechanisms were improved to predict low volatility products by the addition of autoxidation mechanisms and the combination of nitrate-originating peroxy radicals to the preexisting explicit gas mechanisms. Those additional mechanisms were illustrated in Schemes S1-S3 of Section S1.1. The model parameter and the equations are integrated to the predicted hydrocarbon consumption from any gas mechanisms. In order to support SOA formation in complex ambient air, model parameters and equations for stoichiometric coefficients were integrated with SAPRAC07TC (Table S4 in Section S1.2).

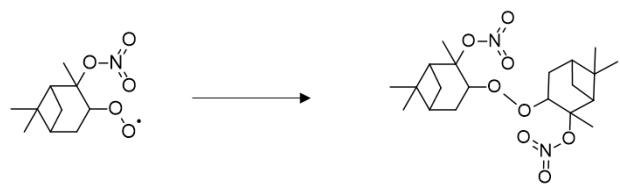
Section S1.1 Additional gas oxidation paths to the preexisting explicit gas mechanism

The gas-phase oxidation of three biogenic HCs (isoprene, α -pinene, and β -caryophyllene) of this study was explicitly processed by using the Master Chemical Mechanism (MCM v3.3.1) (Saunders et al., 2003;Jenkin et al., 2012;Jenkin et al., 2015) to generate lumping species and their model parameters. The recently identified oxidation mechanisms that can yield low volatile products were also integrated with MCM. For example, the Peroxy Radical Autoxidation Mechanism (PRAM) (Roldin et al., 2019) that forms the highly oxygenated organic molecule (HOM) (Molteni et al., 2019) and the accretion reaction to form ROOR from the RO₂ (Bates et al., 2022;Zhao et al., 2021) were added. Furthermore, the oxidation process of biogenic HCs by O(³P) (Paulson et al., 1992;Alvarado et al., 1998) was included in gas mechanisms to fulfill the oxidation mechanism used in the current regional model.

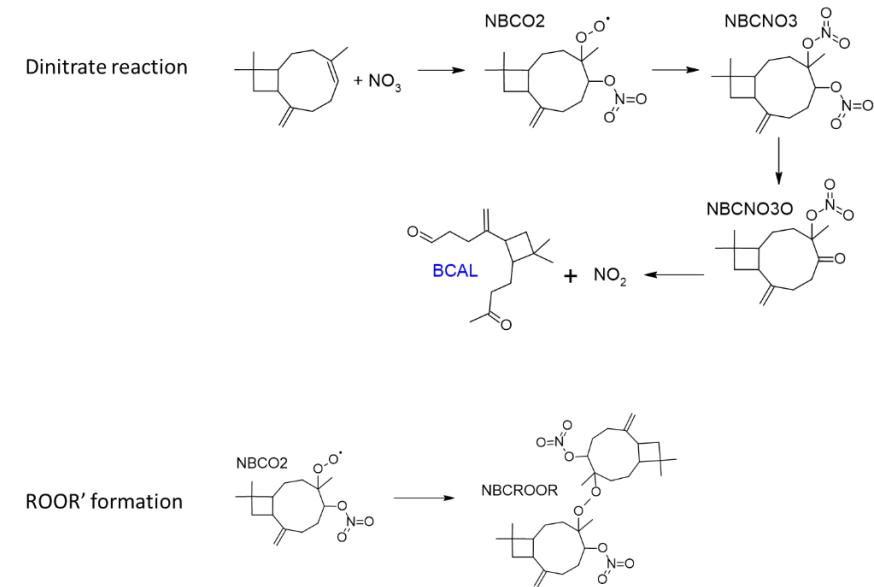
The accretion reaction to form ROOR from the NO₃-originated RO₂ from α -pinene has been reported by (Bates et al., 2022;Zhao et al., 2021). Thus, the ROOR formation of NO₃-originated RO₂ from all three HCs were applied as presented in Schemes S1-S3. The oxidation of isoprene with O(³P) is shown in Scheme S4 as an example.



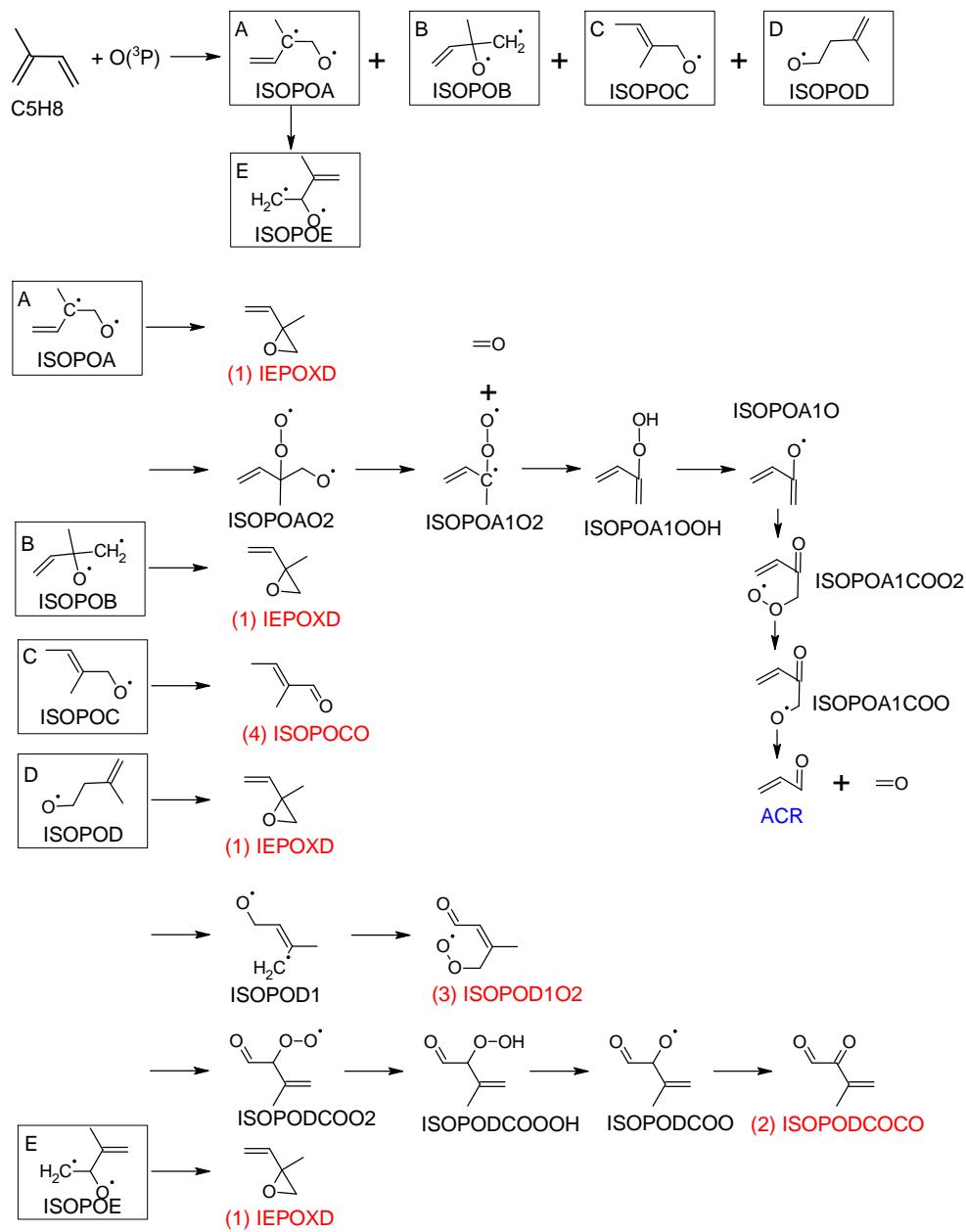
Scheme S1. The ROOR formation process of the NO₃-originated RO₂ from isoprene.



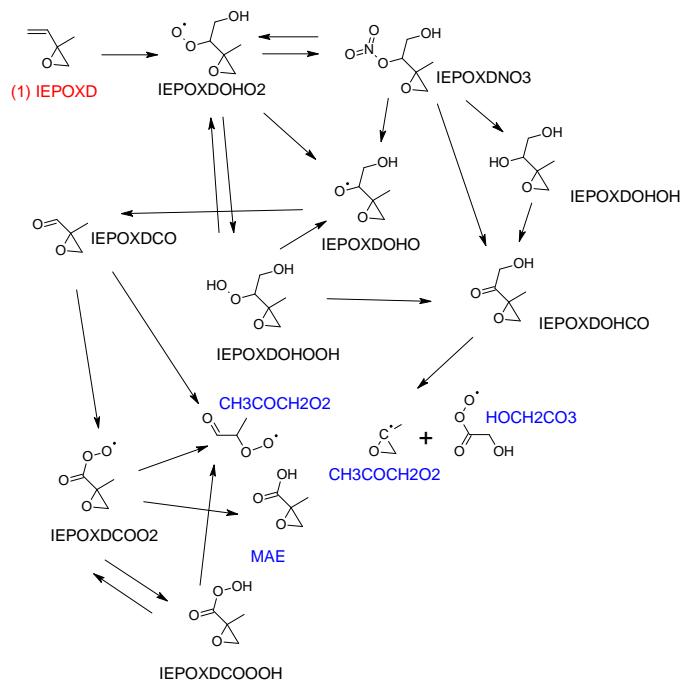
Scheme S2. The ROOR formation process of the NO_3 -originated RO_2 from α -pinene.



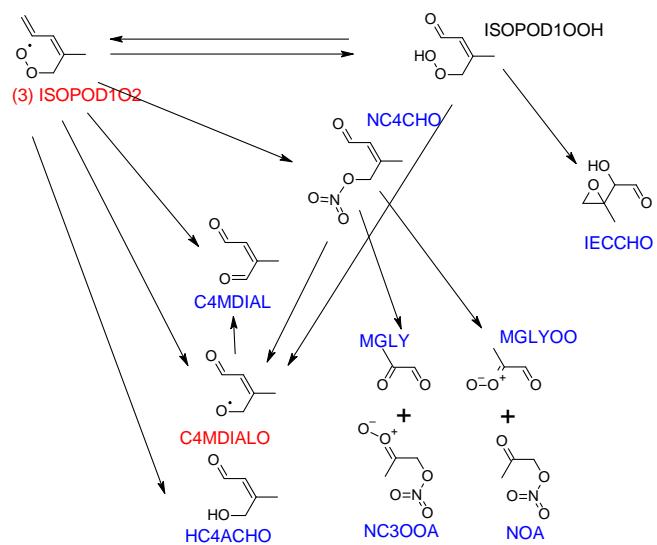
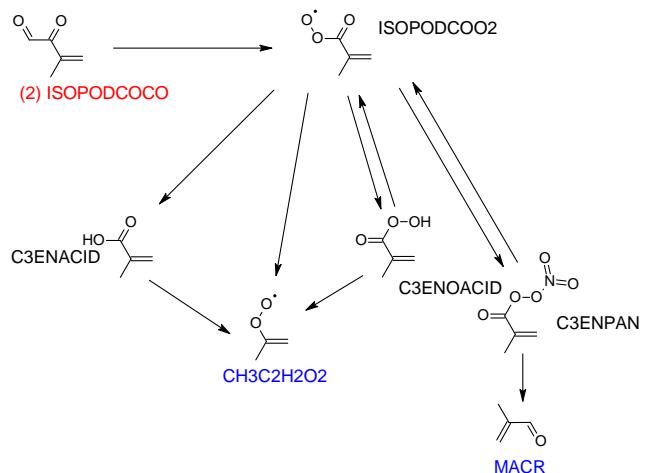
Scheme S3. The dinitrate formation in β -caryophyllene and the further reaction to form ROOR.



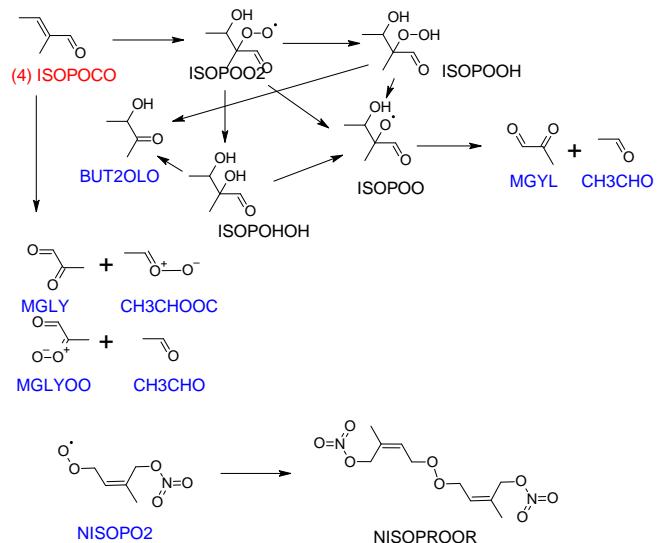
Scheme S4. Isoprene oxidation path by $\text{O}(\text{P}^3)$ (continue).



50 Scheme S4. Isoprene oxidation path by $\text{O}^{\cdot}(3\text{P})$ (continue).



Scheme S4. Isoprene oxidation path by O(³P) (continue).



Scheme S4. Isoprene oxidation path by O(³P).

55 The mechanisms associated with Schemes S1-S4 were summarized in Table S1-S3. The format of mechanisms follows in those in the MCM.

Table S1. Additional mechanisms in oxidation reaction of isoprene.

ROOR formation from RO₂ compounds produced by nitrate radical reaction	
Reactions	Rate constant
NISOPPO ₂ = NISOPPROR	1.30D-12*RO ₂ *0.18
The oxidation of isoprene by O(3P)	
Reactions	Rate constant
C5H ₈ + O = ISOPOA + ISOPOE	3.0000D-11*0.185
C5H ₈ + O = ISOPOB	3.0000D-11*0.37
C5H ₈ + O = ISOPOC	3.0000D-11*0.13
C5H ₈ + O = ISOPOD	3.0000D-11*0.26
ISOPOA + OH = IEPOXD	5.00D-11*0.92
ISOPOA + OH = ISOPAO ₂	5.00D-11*0.08
ISOPAO ₂ = ISOPOA1O ₂ + HCHO	KDEC
ISOPOA1O ₂ + HO ₂ = ISOPOA1OOH	KRO2HO ₂ *0.64
ISOPOA1OOH + OH = ISOPOA1COO ₂	1.90D-12*EXP(190/TEMP)
ISOPOA1COO + NO = ISOPOA1COO	KRO2NO* 0.916
ISOPOA1COO ₂ + NO ₃ = ISOPOA1COO	KRO2NO ₃
ISOPOA1COO = ACR + HCHO	KDEC
ISOPOB + OH = IEPOXD	5.00D-11*0.92
ISOPOD + OH = IEPOXD	5.00D-11*0.92
ISOPOD + OH = ISOPOD1	2.70D-11*EXP(390/TEMP)*0.288
ISOPOD1 = ISOPOD1O ₂	2.50D-12*EXP(-480/TEMP)*O ₂
ISOPOD + OH = ISOPODCOO ₂	2.70D-11*EXP(390/TEMP)*0.712
ISOPODCOO ₂ + HO ₂ = ISOPODCOOOH	KRO2HO ₂ *0.706
ISOPODCOOOH = ISOPODCOO ₂	J(41)
ISOPODCOO ₂ = ISOPODCOCO	KDEC
ISOPODCOOOH + OH = ISOPODCOCO	1.54D-10*0.05
ISOPOC = ISOPOCO	KDEC
IEPOXD + OH = IEPOXDOHO ₂ + HNO ₃	6.6D-12*EXP(465/TEMP)
IEPOXDOHO ₂ + HO ₂ = IEPOXDOHOOH	KRO2HO ₂ *0.625
IEPOXDOHO ₂ + NO = IEPOXDOHO + NO ₂	KRO2NO*0.936
IEPOXDOHO ₂ + NO = IEPOXDNO ₃	KRO2NO*0.064
IEPOXDOHO ₂ + NO ₃ = IEPOXDOHO + NO ₂	KRO2NO ₃
IEPOXDOHO ₂ = IEPOXDOHO	8.8D-13*0.6*RO ₂
IEPOXDOHO ₂ = IEPOXDOHCO	8.8D-13*0.2*RO ₂
IEPOXDOHO ₂ = IEPOXDOHOH	8.8D-13*0.2*RO ₂
IEPOXDOHOH + OH = IEPOXDOHCO + HO ₂	1.73D-11
IEPOXDOHCO = CH ₃ COCH ₂ O ₂ + HOCH ₂ CO ₃	J(22)
IEPOXDOHOH + OH = IEPOXDOHCO + OH	3.15D-11
IEPOXDOHOH + OH = IEPOXDOHO ₂	1.90D-12*EXP(190/TEMP)
IEPOXDOHOH = IEPOXDOHO	J(41)
IEPOXDOHO = IEPOXDCO	2.00D+14*EXP(-6382/TEMP)
IEPOXDCO + OH = IEPOXDCOO ₂	2.22D-11
IEPOXDCO + NO ₃ = IEPOXDCOO ₂ + HNO ₃	KNO3AL*8.5
IEPOXDCO = CH ₃ COCH ₂ O ₂	J(22)
IEPOXDCOO ₂ + HO ₂ = MAE	KAPHO ₂ *0.15

IEPOXDCOO2 + HO2 = CH3COCH2O2	KAPHO2*0.44
IEPOXDCOO2 + HO2 = IEPOXDCOOOH	KAPHO2*0.41
IEPOXDCOOOH + OH = IEPOXDCOO2	5.17D-12
IEPOXDCOOOH = CH3COCH2O2 + OH	J(41)
IEPOXDCOOOH = CH3COCH2O2 + OH	J(22)
ISOPODCOCO + OH = ISOPODCOO2 + CO	1.67D-11
ISOPODCOCO + NO3 = ISOPODCOO2 + HNO3	KNO3AL*0.55
ISOPODCOCO = ISOPODCOO2 + HO2 + CO	J(34)
ISOPODCOO2 + HO2 = C3ENOACID	KAPHO2*0.41
ISOPODCOO2 + HO2 = CH3C2H2O2 + OH	KRO2HO2*0.44
ISOPODCOO2 + HO2 = C3ENACID + O3	KAPHO2*0.15
ISOPODCOO2 + NO = CH3C2H2O2 + NO2	KAPNO
ISOPODCOO2 + NO3 = CH3C2H2O2 + NO2	KRO2NO3*1.74
ISOPODCOO2 + NO2 = C3ENPAN	KFPAN
ISOPODCOO2 = C3ENACID	1.00D-11*0.3*RO2
ISOPODCOO2 = CH3C2H2O2	1.00D-11*0.7*RO2
C3ENOACID = CH3C2H2O2	J(41)
C3ENOACID + OH = ISOPODCOO2	1.82D-11
C3ENACID + OH = CH3C2H2O2	1.46D-11
C3ENPAN = ISOPODCOO2	KBPAN
C3ENPAN + OH = MACR + CO + NO2	1.45D-11
ISOPOD1O2 + HO2 = ISOPOD1OOH	KRO2HO2*0.770
ISOPOD1O2 + NO = NC4CHO	KRO2NO*0.087
ISOPOD1O2 + NO = C4MDIALO	KRO2NO*0.913
ISOPOD1O2 + NO3 = C4MDIALO	KRO2NO3
ISOPOD1O2 = C4MDIAL	2.00D-12*0.2*RO2
ISOPOD1O2 = HC4ACHO	2.00D-12*0.2*RO2
ISOPOD1O2 = C4MDIALO	2.00D-12*0.6*RO2
ISOPOD1OOH = C4MDIALO	J(41)
ISOPOD1OOH + OH = IECCHO	1.54D-10*0.93
ISOPOD1OOH + OH = C4MDIALO	1.54D-10*0.07
ISOPOCO + OH = ISOPOO2	3.23D-12
ISOPOCO + O3 = MGLYOX + CH3CHOOC	6.51D-15*EXP(-829/TEMP)*0.5
ISOPOCO + O3 = MGLYOO + CH3CHO	6.51D-15*EXP(-829/TEMP)*0.5
ISOPOO2 + HO2 = ISOPOOH	KRO2HO2*0.706
ISOPOO2 + NO = ISOPOO	KRO2NO
ISOPOO2 + NO3 = ISOPOO	KRO2NO3
ISOPOO2 = ISOPOHOH	9.2D-14*RO2*0.3
ISOPOO2 = ISOPOO	9.2D-14*RO2*0.7
ISOPOOH = ISOPOO	J(41)
ISOPOOH = BUT2OLO + CO + OH	4.58D-11
ISOPOOH = BUT2OLO + CO + OH + HO2	J(17)*2
ISOPOHOH + OH = ISOPOO	5.7D-11
ISOPOHOH = BUT2OLO + HO2 + HO2	J(17)*2
ISOPOO = MGLYOX + CH3CHO	KDEC
C4MDIALO = C4MDIAL + HO2	8.9D-14*EXP(-550/TEMP)*O2
BUT2OLO + OH = BIACET + HO2	5.86D-12
BUT2OLO = CH3CO3 + CH3CHO + HO2	J(22)
BIACET = CH3CO3 + CH3CO3	J(35)
OH + BIACET = BIACETO2	1.40D-18*TEMP**2*EXP(194/TEMP)

<chem>CH3CHOOC = CH3CHOO</chem>	KDEC*0.11
<chem>CH3CHOOC = CH3O2 + CO + OH</chem>	KDEC*0.89

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Table S2. Additional mechanisms in oxidation reaction of α -pinene.

Addition of mechanism (α-pinene + O(3P))	
Reaction	Reaction rate
<chem>APINENE + O = APINEPOX</chem>	0.77*3.6D-11
<chem>APINEPOX + OH = APINEPO2</chem>	1.16D-11
<chem>APINEPO2 + HO2 = APINEPOOH</chem>	KRO2HO2*0.706
<chem>APINEPO2 = APINEBCO</chem>	0.4*9.2D-14*RO2
<chem>APINEPO2 = APINEBOCO</chem>	0.6*9.2D-14*RO2
<chem>APINEPO2 + NO = APINEPNO3</chem>	0.23*KRO2NO
<chem>APINEPO2 + NO = APINBO</chem>	0.77*KRO2NO
<chem>APINEPNO3 + OH = APINEBCO</chem>	3.64D-12
<chem>APINEPOOH = APINEBOCO + OH</chem>	J(41)
<chem>APINEBOCO = C96CO3</chem>	KDEC
<chem>APINEBCO + OH = C96CO3</chem>	8.18D-12
<chem>APINO+OH = APINOO2</chem>	1.2D-11*EXP(440/TEMP)*0.075
<chem>APINOO2 + NO = APINOO</chem>	KRO2NO *0.875
<chem>APINOO2 + NO = APINONO3</chem>	KRO2NO*0.125
<chem>APINOO = CH3COCH3 + APINOHOO2</chem>	KDEC
<chem>APINOHOO2 + NO = APINOHOO</chem>	KRO2NO*0.875
<chem>APINOHOO2 + NO = APINOHNO3</chem>	KRO2NO*0.125
further oxidation pathway from dinitrate product (NAPINANO3) from NO3 radical reation	
Reaction	Reaction rate
<chem>NAPINANO3 + OH = NAPINACO + NO2</chem>	3.64D-12
<chem>NAPINACO + OH = NAPINACOO2</chem>	1.2D-11*EXP(440/TEMP)*0.075
<chem>NAPINACOO2 = NAPINACOO</chem>	6.70D-15*RO2*0.7
<chem>NAPINACOO = C719NO3O2 + CH3COCH3</chem>	KDEC
<chem>C719NO3O2 = C751CO + NO2</chem>	KDEC
<chem>C751CO + OH = C717O2</chem>	6.34D-12*EXP(448/TEMP)*0.19
<chem>C751CO + OH = C751COO2</chem>	6.34D-12*EXP(448/TEMP)*0.19
<chem>C751CO + NO3 = C751COO2</chem>	KNO3AL*5.5
<chem>C751CO = C751O2</chem>	J(15)
<chem>C751COO2 + HO2 = C751O2 + OH</chem>	KAPHO2*0.44
<chem>C751COO2 + HO2 = C751COOH + O3</chem>	KAPHO2*0.15
<chem>C751COO2 + HO2 = C751COOOH</chem>	KAPHO2*0.41
<chem>C751COO2 + NO = C751O2 + NO2</chem>	KAPNO
<chem>C751COO2 + NO2 = C751PPEN</chem>	KFPAN
<chem>C751COO2 + NO3 = C751O2 + NO2</chem>	KRO2NO3*1.74
<chem>C751COO2 = C751O2</chem>	1.00D-11*0.7*RO2
<chem>C751COO2 = C751COOH</chem>	1.00D-11*0.3*RO2
<chem>C751PPEN + OH = C651CO + NO2</chem>	6.85D-12
<chem>C751PPEN = C651COO2</chem>	KBPAN
<chem>C751COOOH + OH = C651COO2</chem>	1.04D-11
<chem>C751COOOH = C651O2 + OH</chem>	J(41)
<chem>C751COOH + OH = C651O2</chem>	6.88D-12
<chem>C751O2 + HO2 = C651COOH</chem>	KRO2HO2*0.625
<chem>C751O2 + NO = C651CNO3</chem>	KRO2NO*0.033
<chem>C751O2 + NO = C651O + NO2</chem>	KRO2NO*0.967
<chem>C751O2 + NO3 = C651CO + NO2</chem>	KRO2NO3
<chem>C751O2 = C651CO</chem>	1.30D-12*0.2*RO2
<chem>C751O2 = C651COH</chem>	1.30D-12*0.2*RO2

C751O2 = C651O	1.30D-12*0.6*RO2
C651CNO3 = C651O + NO2	J(53)
C651CNO3 + OH = C651CO + NO2	1.6D-12
C651COOH = C651O + OH	J(41)
C651COOH + OH = C651CO + OH	1.24D-11
C651COOH + OH = C651O2	1.90D-12*EXP(190/TEMP)
C651CO + NO3 = HNO3 + C551COO2	1.7D-12*EXP(-1500/TEMP)
C651CO + OH = C551COO2	6.0D-12*EXP(410/TEMP)
C651CO = BIACET + CH3COCH3	J(16)
C651CO = C551O2 + CO + HO2	J(15)
C651COH + OH = C651CO + HO2	5.3D-12*EXP(140/TEMP)
C651O = C651CO + HO2	8.9D-14*EXP(-550/TEMP)*O2
C651COO2 + HO2 = C551O2 + OH	KAPHO2*0.44
C651COO2 + HO2 = C651CCOOH + O3	KAPHO2*0.15
C651COO2 + HO2 = C651COOOH	KAPHO2*0.41
C651COO2 + NO = C551O2 + NO2	KAPNO
C651COO2 + NO2 = C551PAN	KFPAN
C651COO2 + NO3 = C651O2	KRO2NO3 * 1.74
C651COO2 = C651O2	1.00D-11*0.7*RO2
C651COO2 = C651CCOOH	1.00D-11*0.3*RO2
C651O2 + HO2 = C651COOH	KRO2HO2*0.625
C651O2 + NO = C651CNO3	KRO2NO*0.033
C651O2 + NO = C651O	KRO2NO *0.967
C651O2 + NO3 = C651O	KRO2NO3
C651O2 = C651CO	1.30D-12*0.2*RO2
C651O2 = C651COH	1.30D-12*0.2*RO2
C651O2 = C651O	1.30D-12*0.6*RO2
C651CCOOH + OH = C651O2	6.88D-12
C651COOOH + OH = C651COO2	1.04D-11
C651COOOH = C651O2 + OH	J(41)
C551PAN + OH = CO23C4CHO + CO + NO2	6.85D-12
C551PAN = C551COO2 + NO2	KBPAN
C551O2 + HO2 = C551OOH	KRO2HO2*0.625
C551O2 + NO = C551NO3	KRO2NO*0.033
C551O2 + NO = C551O + NO2	KRO2NO*0.967
C551O2 + NO3 = C551O + NO2	KRO2NO3
C551O2 = CO23C4CHO	1.30D-12*0.2*RO2
C551O2 = C551OH	1.30D-12*0.2*RO2
C551O2 = C551O	1.30D-12*0.6*RO2
C551COO2 + HO2 = C551O2 + OH	KAPHO2*0.44
C551COO2 + HO2 = C551COOOH + O3	KAPHO2*0.15
C551COO2 + HO2 = C551O2	KAPHO2*0.41
C551COO2 + NO = C551O2 + NO2	KAPNO
C551COO2 + NO2 = C551PAN	KFPAN
C551COO2 + NO3 = C551O2	KRO2NO3*1.74
C551COO2 = C551O2	1.00D-11*0.7*RO2
C551COO2 = C551ACID	1.00D-11*0.3*RO2
C551ACID + OH = BIACETO2	6.88D-12
C551OOH = C551O + OH	J(41)
C551OOH + OH = CO23C4CHO + OH	1.24D-11
C551OOH + OH = C551O2	1.90D-12*EXP(190/TEMP)
C551O = CO23C4CHO + HO2	8.9D-14*EXP(-550/TEMP)*O2
C551OH + OH = CO23C4CHO + HO2	5.3D-12*EXP(140/TEMP)

C551COOOH + OH = C551COO2	1.04D-11
C551COOOH = C551O2 + OH	J(41)
C551NO3 = C551O + NO2	J(53)
C551NO3 + OH = CO23C4CHO + NO2	1.6D-12
BIACET = CH3CO3 + CH3CO3	J(35)
OH + BIACET = BIACETO2	1.40D-18*TEMP**2*EXP(194/TEMP)

Table S3. Additional mechanisms in oxidation reaction of β -caryophyllene.

Addition of dinitrate formation and ROOR' from nitrate radical reaction with BCARY	
Reaction	Reaction rate
NBCO2 + NO = NBCNO3	KRO2NO*0.3
NBCNO3 + OH = NBCNO3O	3.64D-12
NBCNO3O + OH = BCAL + NO2	6.20D-11
NBCO2 = NBCROOR	9.20D-14*RO2*0.18

Section S1.2 Prediction of HC consumption by using SAPRC07TC

65 In this study, the oxidation of biogenic hydrocarbons (isoprene, α -pinene, and β -caryophyllene) was simulated by using SAPRC07tc. In the mechanism, the biogenic hydrocarbons are oxidized by 4 major oxidants (OH radicals, O₃, NO₃ radicals, and O(³P)). The reaction rate constants of β -caryophyllene were determined based on the MCM v3.3.1 (Jenkin et al., 2012) and reduced to simulate the oxidation of β -caryophyllene in the chamber.

Table S4. The oxidation mechanisms of isoprene, α -pinene, and β -caryophyllene in this study.

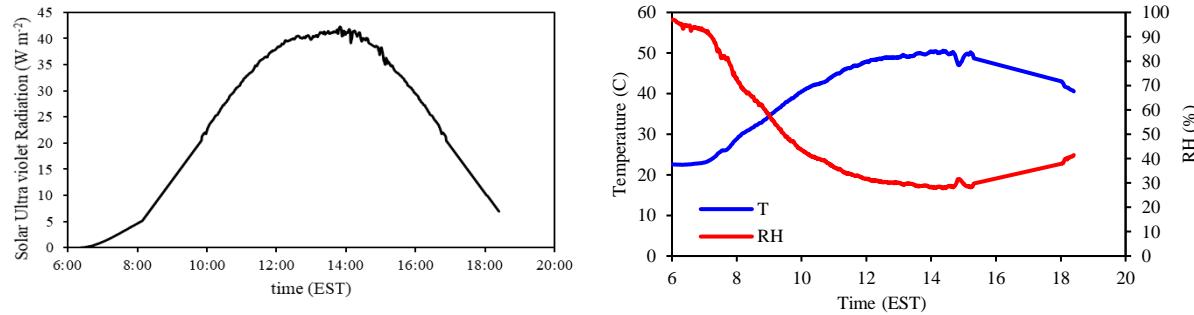
ID	Reaction	Rate constant (molecule s ⁻¹)
ISOP1	ISOP + O3P = 0.25*MEO2 + 0.24*XMA3 + 0.24*RO2C + 0.01*RO2X + 0.01*ZRN3 + 0.24*XHCH + 0.75*PRD2 + 0.25*Y6PX - 1.01*XC	3.5×10^{-11}
ISOP2	ISOP + OH = 0.907*XHO2 + 0.986*RO2C + 0.093*RO2X + 0.093*ZRN3 + 0.624*XHCH + 0.23*XMAC + 0.32*XMVK + 0.357*XIPR + Y6PX - 0.167*X	$2.54 \times 10^{-11} \times e^{\frac{410}{T}}$
ISOP3	ISOP + O3 = 0.066*HO2 + 0.266*OH + 0.192*XMA3 + 0.192*RO2C + 0.008*RO2X + 0.008*ZRN3 + 0.275*CO + 0.122*CO2 + 0.4*HCHO + 0.192*XHCH + 0.204*FACD + 0.39*MACR + 0.16*MVK + 0.15*IPRD + 0.1*PRD2 + 0.2*Y6PX - 0.559*XC	$7.86 \times 10^{-15} \times e^{\frac{-1912}{T}}$
ISOP4	ISOP + NO3 = 0.749*XHO2 + 0.187*XNO2 + 0.936*RO2C + 0.064*RO2X + 0.064*ZRN3 + 0.936*XIPR + Y6PX + 0.813*XN - 0.064*XC	$3.03 \times 10^{-12} \times e^{\frac{-448}{T}}$
APIN1	APIN + O3P = PRD2 + 4*XC	3.20×10^{-11}
APIN2	APIN + OH = 0.799*XHO2 + 0.004*XRC3 + 1.042*RO2C + 0.197*RO2X + 0.197*ZRN3 + 0.002*XCO + 0.022*XHCH + 0.776*XRCH + 0.034*XACE + 0.02*XMGL + 0.023*XBAC + Y6PX + 6.2*XC	$1.21 \times 10^{-11} \times e^{\frac{436}{T}}$
APIN3	APIN + O3 = 0.009*HO2 + 0.102*XHO2 + 0.728*OH + 0.001*XMC3 + 0.297*XRC3 + 1.511*RO2C + 0.337*RO2X + 0.337*ZRN3 + 0.029*CO + 0.051*XCO + 0.017*CO2 + 0.344*XHCH + 0.24*XRCH + 0.345*XACE + 0.008*MEK + 0.002*XGLY + 0.081*XBAC + 0.255*PRD2 + 0.737*Y6PX + 2.999*XC	$5.00 \times 10^{-16} \times e^{\frac{-530}{T}}$
APIN4	APIN + NO3 = 0.056*XHO2 + 0.643*XNO2 + 0.007*XRC3 + 1.05*RO2C + 0.293*RO2X + 0.293*ZRN3 + 0.005*XCO + 0.007*XHCH + 0.684*XRCH + 0.069*XACE + 0.002*XMGL + 0.056*XRN3 + Y6PX + 0.301*XN + 5.608*XC	$1.19 \times 10^{-12} \times e^{\frac{490}{T}}$
SESQ1	SESQ + O3P = 0.237*RCHO + 0.763*PRD2 + 9.711*XC	4.02×10^{-11}
SESQ2	SESQ + OH = 0.734*XHO2 + 0.064*XRC3 + 1.211*RO2C + 0.201*RO2X + 0.201*ZRN3 + 0.001*XCO + 0.411*XHCH + 0.385*XRCH + 0.037*XACE + 0.007*XMEK + 0.003*XGLY + 0.009*XBAC + 0.003*XMVK + 0.002*XIPR + 0.409*XPD2 + Y6PX + 9.375*XC	1.97×10^{-12}
SESQ3	SESQ + O3 = 0.078*HO2 + 0.046*XHO2 + 0.499*OH + 0.202*XMC3 + 0.059*XRC3 + 0.49*RO2C + 0.121*RO2X + 0.121*ZRN3 + 0.249*CO + 0.063*CO2 + 0.127*HCHO + 0.033*XHCH + 0.208*XRCH + 0.057*XACE + 0.002*MEK + 0.172*FACD + 0.068*PACD + 0.003*XGLY + 0.039*XBAC + 0.002*XMAC + 0.001*XIPR + 0.502*PRD2 + 0.428*Y6PX + 8.852*XC	1.8×10^{-15}
SESQ4	SESQ + NO3 = 0.227*XHO2 + 0.287*XNO2 + 0.026*XRC3 + 1.786*RO2C + 0.46*RO2X + 0.46*ZRN3 + 0.012*XCO + 0.023*XHCH + 0.002*XCCH + 0.403*XRCH + 0.239*XACE + 0.005*XMAC + 0.001*XMVK + 0.004*XIPR + 0.228*XRN3 + Y6PX + 0.485*XN + 8.785*XC	1.90×10^{-11}
BENZ	BENZ + OH = 0.57*HO2 + 0.29*XHO2 + 0.116*OH + 0.29*RO2C + 0.024*RO2X + 0.024*ZRN3 + 0.29*XGLY + 0.57*CRES + 0.029*XAF1 + 0.261*XAF2 + 0.116*AFG3 + 0.314*YAPX - 0.976*XC	$2.33 \times 10^{-12} \times e^{\frac{193}{T}}$
TOLU	TOLU + OH = 0.181*HO2 + 0.454*XHO2 + 0.312*OH + 0.454*RO2C + 0.054*RO2X + 0.054*ZRN3 + 0.238*XGLY + 0.151*XGLY + 0.181*CRES + 0.065*XBAL + 0.195*XAF1 + 0.195*XAF2 + 0.312*AFG3 + 0.073*Y6PX + 0.435*YAPX - 0.109*XC	$1.81 \times 10^{-12} \times e^{\frac{338}{T}}$

MXYL	$\text{MXYL} + \text{OH} = 0.159*\text{HO}_2 + 0.52*\text{XHO}_2 + 0.239*\text{OH} + 0.52*\text{RO}_2\text{C} + 0.082*\text{RO}_2\text{X} + 0.082*\text{ZRN}_3 + 0.1*\text{XGLY} + 0.38*\text{XMGL} + 0.159*\text{CRES} + 0.041*\text{XBAL} + 0.336*\text{XAF}_1 + 0.144*\text{XAF}_2 + 0.239*\text{AFG}_3 + 0.047*\text{Y}_6\text{PX} + 0.555*\text{YAPX} + 0.695*\text{XC}$	2.31×10^{-11}
OXYL	$\text{OXYL} + \text{OH} = 0.161*\text{HO}_2 + 0.554*\text{XHO}_2 + 0.198*\text{OH} + 0.554*\text{RO}_2\text{C} + 0.087*\text{RO}_2\text{X} + 0.087*\text{ZRN}_3 + 0.084*\text{XGLY} + 0.238*\text{XMGL} + 0.185*\text{XBAC} + 0.161*\text{CRES} + 0.047*\text{XBAL} + 0.253*\text{XAF}_1 + 0.253*\text{XAF}_2 + 0.198*\text{AFG}_3 + 0.055*\text{Y}_6\text{PX} + 0.586*\text{YAPX} + 0.484*\text{XC}$	1.36×10^{-11}
PXYL	$\text{PXYL} + \text{OH} = 0.159*\text{HO}_2 + 0.487*\text{XHO}_2 + 0.278*\text{OH} + 0.487*\text{RO}_2\text{C} + 0.076*\text{RO}_2\text{X} + 0.076*\text{ZRN}_3 + 0.286*\text{XGLY} + 0.112*\text{XMGL} + 0.159*\text{CRES} + 0.088*\text{XBAL} + 0.045*\text{XAF}_1 + 0.067*\text{XAF}_2 + 0.278*\text{AFG}_3 + 0.286*\text{XAF}_3 + 0.102*\text{Y}_6\text{PX} + 0.461*\text{YAPX} + 0.399*\text{XC}$	1.43×10^{-11}
B124	$\text{B124} + \text{OH} = 0.022*\text{HO}_2 + 0.627*\text{XHO}_2 + 0.23*\text{OH} + 0.627*\text{RO}_2\text{C} + 0.121*\text{RO}_2\text{X} + 0.121*\text{ZRN}_3 + 0.074*\text{XGLY} + 0.405*\text{XMGL} + 0.112*\text{XBAC} + 0.022*\text{CRES} + 0.036*\text{XBAL} + 0.088*\text{XAF}_1 + 0.352*\text{XAF}_2 + 0.23*\text{AFG}_3 + 0.151*\text{XAF}_3 + 0.043*\text{Y}_6\text{PX} + 0.705*\text{YAPX} + 1.19*\text{XC}$	3.25×10^{-11}

Section S2. Reference conditions for the simulation.

The sunlight intensity, temperature, and RH illustrated in Fig. S1 was measured on 06/19/2015 in the UF-APHOR. The sunlight intensity in Fig. S1 is applied as a reference sunlight intensity for the sensitivity and uncertainty tests.

- 75 The daytime SOA formation in Figs. 5 and 6 were simulated at a given reference condition, to investigate the diurnal variations in biogenic SOA and the sensitivity of temperature and the NO_x levels to the biogenic SOA from each oxidation path.



80 Figure S1. Time profiles of reference sunlight radiance (left) measured by using Total Ultra-Violet Radiation (TUVR) and temperature and humidity (right) in the UF-APHOR on 06/19/2015.

Section S3. Wall-free biogenic SOA formation

The chamber-generated SOA mass is influenced by the deposition of organic vapor to the chamber wall. The simulation of SOA yields in Fig. 4 is performed with the model parameters obtained in the presence of the chamber wall. To investigate the SOA formation in the ambient air, the wall-free SOA model parameter has recently been derived by (Han and Jang, 2022). Figure S2 displays the potential SOA yield without the chamber wall bias simulated by the UNIPAR-SAPRC model from each oxidation path, which is calculated with the same amount of HC consumption at two different NO_x levels ((a) high NO_x: HC/NO_x = 3 ppbC/ppb and (b) low NO_x: HC/NO_x = 10 ppbC/ppb). For this calculation, the consumptions of biogenic HCs are set to 50 ppb (138 µg m⁻³), 30 ppb (162 µg m⁻³), and 20 ppb (167 µg m⁻³) for isoprene, α-pinene, and β-caryophyllene, respectively. The temperature is set to 298 K at two different relative humidity (RH) levels (45% and 80%) and three different seed conditions (no seed, wet-AS, and wet ammonium bisulfate (AHS)) with 10 µg m⁻³ of OM₀. For the inorganic seeded simulation, the seed concentration is 20 µg m⁻³ (dry mass). The α-pinene SOA is the most influenced biogenic SOA by gas-wall partitioning, especially in the OH- and NO₃-initiated oxidation paths. The acidic seed effects on biogenic SOA formation reduce by correction of model parameters.

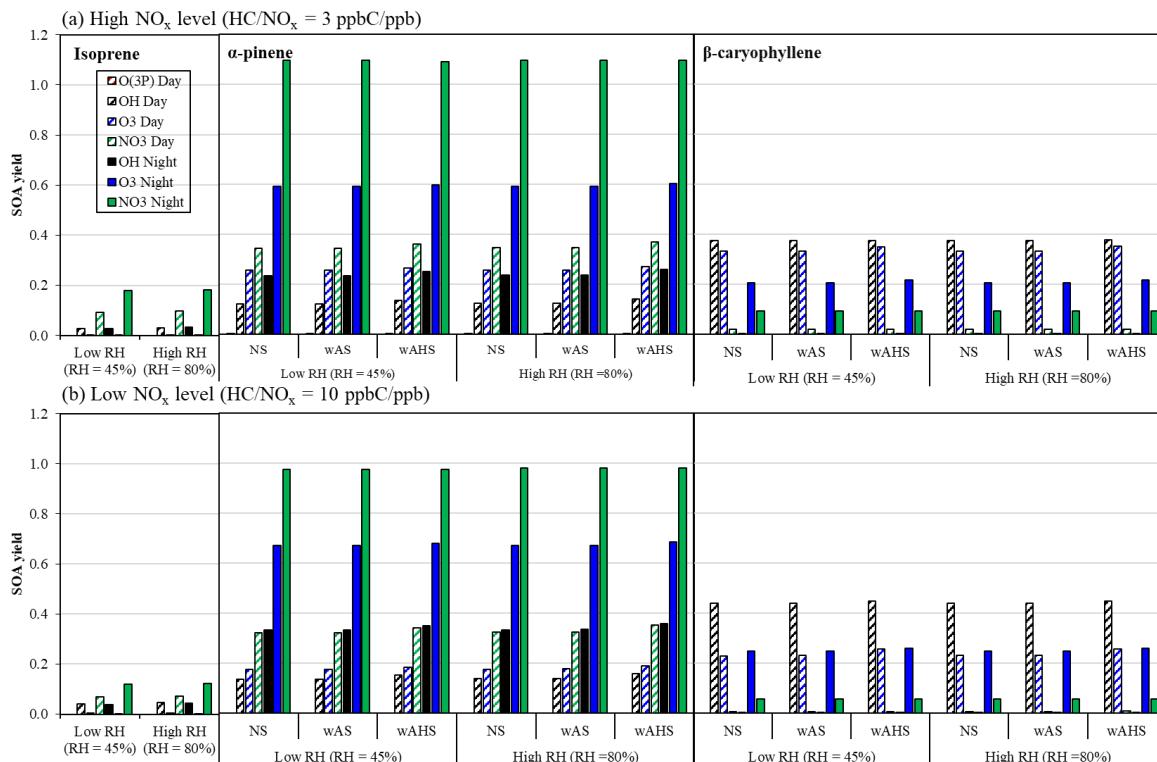
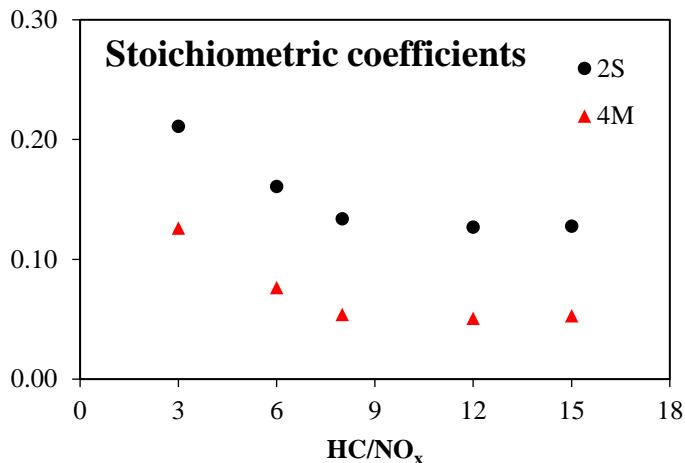


Figure S2. The potential SOA yield from each oxidation path from the given HC consumption under (a) high NO_x level (HC/NO_x = 3 ppbC/ppb) and (b) low NO_x level (HC/NO_x = 10 ppbC/ppb) in the absence of gas-wall partitioning bias. The consumption of biogenic HC was set to 50 ppb (138 µg m⁻³), 30 ppb (162 µg m⁻³), and 20 ppb (167 µg m⁻³) for isoprene, α-pinene, and β-caryophyllene, respectively. The SOA formation was simulated at 298K under two different RH (45% and 80%) with 10 µg m⁻³ of OM₀. For the α-pinene and β-caryophyllene, the SOA formed at 3 different seed conditions (NS, wAS, wAHS). The wall-free model parameters were applied to simulate SOA formation (Han and Jang, 2022).

105 Figure S3 illustrates the stoichiometric coefficients of 2S and 4M, which increase with increasing NO_x and can significantly contribute to SOA mass. These two species originate from the reaction of a nitrate radical with the ozonolysis products.



110 Figure S3. Stoichiometric coefficients of group 2S and 4M from β -caryophyllene ozonolysis products under various
NO_x levels.

Section S4. The sensitivity of the biogenic SOA to the initial HC concentration.

To investigate the influence of the initial concentration of biogenic HCs on SOA formation at a given NO_x level (high NO_x condition), Fig. S4 illustrates the simulated SOA yield from (a) isoprene, (b) α -pinene, and (c) β -caryophyllene in both daytime (solid line) and nighttime (dashed line) with various initial HC concentrations, ranging from 2 ppb to 50 ppb. For the nighttime simulation, the initial concentration of O₃ was set to 30 ppb.

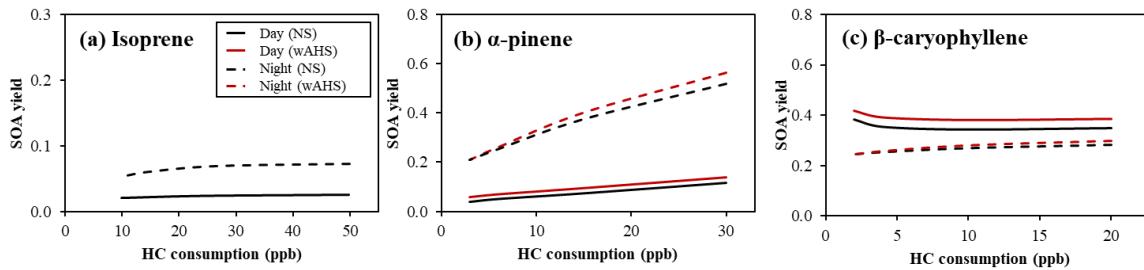


Figure S4. The biogenic SOA yield from (a) isoprene, (b) α -pinene, and (c) β -caryophyllene in both daytime (solid line) and nighttime (dashed line) under the various HC consumption, ranging from 2 ppb to 50 ppb. The HC/NO_x level was set to 3 ppbC/ppb. The SOA formation was simulated with 10 $\mu\text{g m}^{-3}$ of OM₀ at the 50% of RH. The daytime SOA formation was simulated under the reference sunlight intensity (Fig. S1), which was measured on 06/19/2015 at the UF-APHOR. The wall-free model parameters were applied to simulate SOA formation (Han and Jang, 2022).

Section S5. Uncertainties in biogenic SOA associated with the model parameters

- 125 The uncertainty test of SOA mass was performed for two major processes associated with partitioning (P_L) and aerosol phase reactions in both the organic phase and the aqueous phase (k_o , and k_{AC}) The uncertainty in SOA mass in Fig. S5 was performed by increasing/decreasing P_L , k_o , and k_{AC} as a factor of 1.5/0.5, at the high NO_x level (HC/NO_x = 3 ppbC/ppb) with 10 $\mu\text{g m}^{-3}$ of OM₀. The daytime SOA mass was simulated with the sunlight profile on 06/19/2015 near summer solstice. Temperature and RH set as 298K and 50%, respectively. The amount of both neutral (wet-AS) 130 and acidic (wet-AHS) seed was fixed to 20 $\mu\text{g m}^{-3}$ (dry mass).

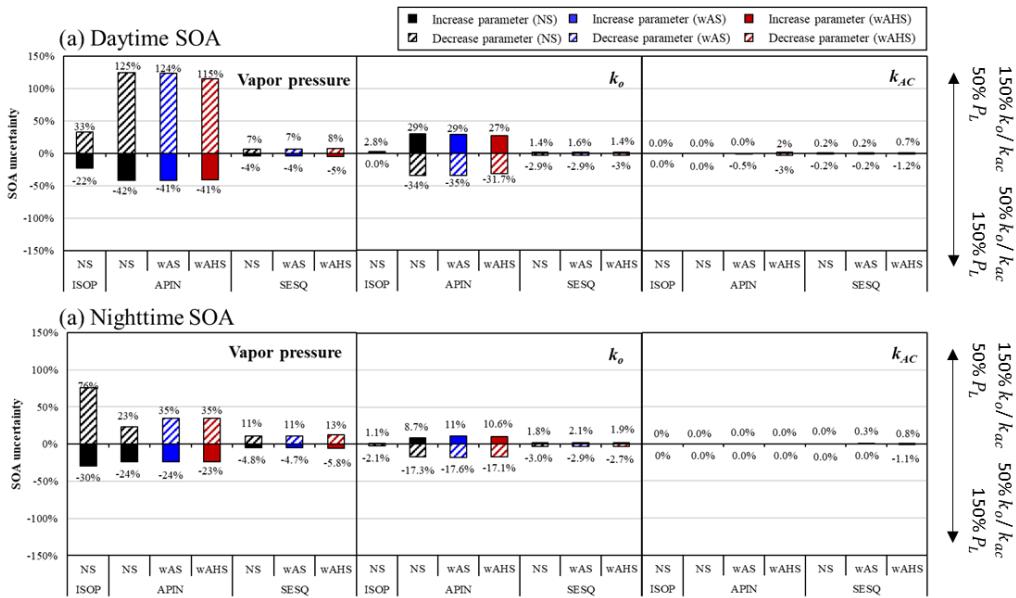
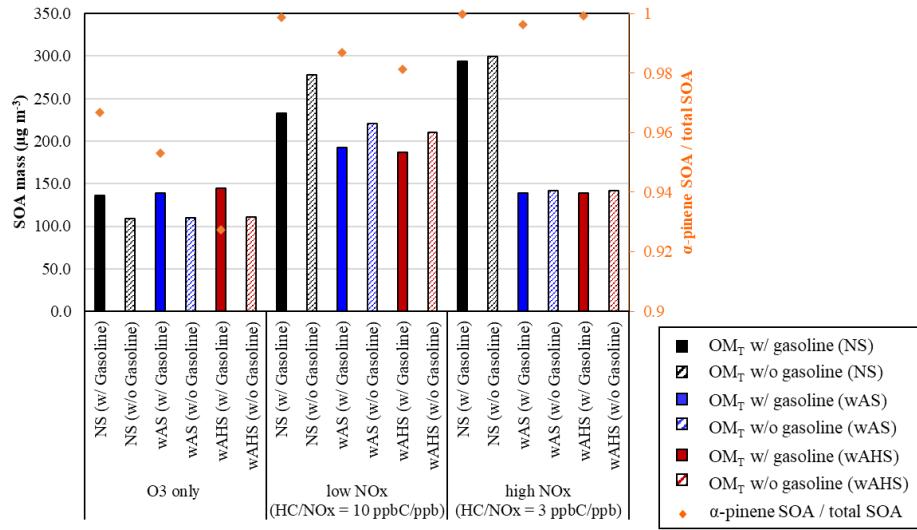


Figure S5. Uncertainties in the prediction of SOA formation associated with vapor pressure (P_L), reaction rate constant in the organic phase (k_o), and reaction rate constant in the inorganic phase (k_{AC}) in (a) day and (b) night. The simulation performed at the high NO_x level (HC/NO_x = 3 ppbC/ppb) with 10 $\mu\text{g m}^{-3}$ of OM₀. The daytime SOA mass was simulated with the sunlight profile on 06/19/2015 near summer solstice (Fig. S1). Temperature and RH are set as 298K and 50%, respectively. The amount of both wAS and wAHS was fixed to 20 $\mu\text{g m}^{-3}$ (dry mass). The wall-free model parameters were applied to simulate SOA mass (Han and Jang, 2022).

Section S6. Nighttime Biogenic SOA formation in the presence of gasoline fuel

140 To investigate the SOA formation in urban area, α -pinene SOA formation was simulated in the presence of gasoline fuel under three different NO_x levels (O_3 only, low NO_x ($\text{HC}/\text{NO}_x = 10 \text{ ppbC/ppb}$), and high NO_x ($\text{HC}/\text{NO}_x = 3 \text{ ppbC/ppb}$)) and seed conditions (NS, wAS, and wAHS). Fig. S6 illustrates the simulated total SOA mass (bar) and the contribution of α -pinene SOA to the total SOA. Overall, the nighttime SOA was dominantly generated from the α -pinene with the high contributions (> 90%).

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Figure S6. The α -pinene SOA mass under three different seed conditions (NS, wAS, and wAHS) and three different NO_x conditions: O_3 only, low NO_x ($\text{HC}/\text{NO}_x = 10 \text{ ppbC/ppb}$), and high NO_x ($\text{HC}/\text{NO}_x = 3 \text{ ppbC/ppb}$) with $10 \mu\text{g m}^{-3}$ of OM_0 . To investigate the impact of the anthropogenic HCs on the oxidation and SOA formation of α -pinene, the α -pinene SOA formation was simulated with and without gasoline fuel in the system. The symbols denote the contribution of α -pinene SOA to the total SOA. The wall-free model parameters were applied to simulate SOA mass (Han and Jang, 2022).

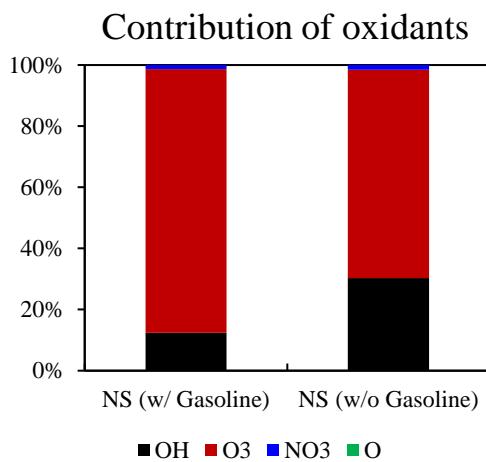


Figure S7. The simulated contribution of each oxidation path on the consumption of α -pinene in the presence of gasoline (Fig. 8 (a)).

155 **Section S7. Model parameters used in this study****Section S7.1 Lumping structures and their parameters**

Reactivity scales of the oxidation products are determined according to the number of reactive functional groups in their chemical structure. The reactivity bins used in UNIPAR are very fast (VF, α -hydroxybicarbonyls and tricarbonyls), fast (F, 2 epoxides or aldehydes,), medium (M, 1 epoxide or aldehyde), slow (S, ketones), partitioning

160 only (P) and multi-alcohol (MA, 3 or more alcohols) (Beardsley and Jang, 2016; Yu et al., 2021; Zhou et al., 2019). The explicit chemical structures of oxidation products from isoprene, α -pinene, and β -caryophyllene are summarized in Table S5-S7 as examples.

165 Table S5. The example of the oxidation product from isoprene in lumping bins. Empty bins represent lumping groups for which isoprene has no oxidation products.

$\backslash VP$ R_i	n = 1 (10 ⁻⁸ mmHg)	n = 2 (10 ⁻⁶ mmHg)	n = 3 (10 ⁻⁵ mmHg)	n = 4 (10 ⁻⁴ mmHg)	n = 5 (10 ⁻³ mmHg)	n = 6 (10 ⁻² mmHg)	n = 7 (10 ⁻¹ mmHg)	n = 8 (10 ⁰ mmHg)
VF								
F								
M								
S								
P								
MA								

Table S6. The example of the oxidation product from α - pinene in lumping bins. Empty bins represent lumping groups for which α - pinene has no oxidation products.

$\frac{\text{VP}}{R_i}$	n = 1 (10^{-8}mmHg)	n = 2 (10^{-6}mmHg)	n = 3 (10^{-5}mmHg)	n = 4 (10^{-4}mmHg)	n = 5 (10^{-3}mmHg)	n = 6 (10^{-2}mmHg)	n = 7 (10^{-1}mmHg)	n = 8 (10^0mmHg)
VF								
F								
M								
S								
P								
MA								

170

Table S7. The example of the oxidation product from β -caryophyllene in lumping bins. Empty bins represent lumping groups for which β -caryophyllene has no oxidation products.

$\frac{\text{VP}}{R_i}$	n = 1 (10^{-8}mmHg)	n = 2 (10^{-6}mmHg)	n = 3 (10^{-5}mmHg)	n = 4 (10^{-4}mmHg)	n = 5 (10^{-3}mmHg)	n = 6 (10^{-2}mmHg)	n = 7 (10^{-1}mmHg)	n = 8 (10^0mmHg)
VF								
F								
M								
S								
P								
MA								

Section S7.2. physicochemical parameters

Table S8. Unified physicochemical parameters of lumping species from oxidation of isoprene, α -pinene and β -caryopyllene.

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Lumped species	Isoprene			α -Pinene			β -Caryopyllene		
	MW ($g mol^{-1}$)	O:C	H-Bonding	MW ($g mol^{-1}$)	O:C	H-Bonding	MW ($g mol^{-1}$)	O:C	H-Bonding
1VF	0.0	0.0	0.0	210.6	0.8	2.0	0.0	0.0	0.0
2VF	0.0	0.0	0.0	162.1	1.2	2.6	176.1	1.0	2.0
3VF	0.0	0.0	0.0	207.1	1.6	1.0	0.0	0.0	0.0
4VF	118.1	1.0	2.0	134.1	1.3	2.0	132.1	0.8	2.0
5VF	0.0	0.0	0.0	156.4	0.6	0.5	130.1	0.8	1.0
6VF	116.1	1.0	1.0	142.1	0.7	0.0	142.1	0.7	0.0
7VF	100.4	0.8	1.0	100.6	0.8	0.3	0.0	0.0	0.0
8VF	100.1	0.8	0.0	99.1	0.8	0.0	0.0	0.0	0.0
1F	0.0	0.0	0.0	0.0	0.0	0.0	254.9	0.4	2.0
2F	0.0	0.0	0.0	0.0	0.0	0.0	249.7	0.3	1.0
3F	0.0	0.0	0.0	0.0	0.0	0.0	245.5	0.3	0.3
4F	177.1	1.2	2.0	184.2	0.3	1.0	223.0	0.2	0.0
5F	0.0	0.0	0.0	163.5	0.4	1.0	206.1	0.2	0.0
6F	102.1	0.8	1.0	116.8	0.6	1.0	181.3	0.2	0.0
7F	121.7	1.0	1.0	114.1	0.6	0.0	0.0	0.0	0.0
8F	97.7	0.3	0.0	72.1	0.7	0.0	72.1	0.7	0.0
1M	239.3	1.8	4.0	475.1	0.6	1.5	261.9	0.4	1.7
2M	253.1	2.0	2.0	261.0	0.7	0.7	256.7	0.3	1.1
3M	189.4	1.4	3.0	216.1	0.5	1.0	246.2	0.2	1.0
4M	167.8	1.5	2.0	179.1	0.5	1.0	238.4	0.2	0.0
5M	179.1	1.7	1.0	169.4	0.6	0.4	211.3	0.2	0.3
6M	121.1	1.1	2.0	168.1	0.2	0.0	156.0	0.4	0.5
7M	137.5	0.8	1.0	127.7	0.7	0.1	92.3	1.0	1.5
8M	74.9	0.7	0.7	195.2	0.4	0.2	92.4	0.5	0.3
1S	0.0	0.0	0.0	362.1	1.0	3.3	342.5	0.4	1.4
2S	298.7	2.4	2.0	312.2	1.1	3.7	253.8	0.3	1.4
3S	224.1	1.6	2.0	219.4	0.8	1.8	232.2	0.2	1.1
4S	179.1	1.8	1.0	211.6	0.5	1.0	252.8	0.3	0.0
5S	171.1	1.1	1.7	204.4	0.6	1.1	188.4	0.3	0.6
6S	139.3	1.2	2.0	170.5	0.2	0.7	176.5	1.0	0.1
7S	100.5	1.0	1.4	236.3	0.6	1.5	163.1	1.5	0.0
8S	103.8	0.9	1.3	200.0	0.4	1.0	123.2	0.9	0.3
1P	260.7	2.0	3.3	321.2	1.1	2.9	295.4	0.4	2.1
2P	226.0	1.6	4.0	316.4	0.8	1.6	234.6	0.3	2.6
3P	165.1	1.5	3.6	265.7	0.9	2.5	328.0	0.4	0.0
4P	192.8	1.6	2.5	224.9	0.6	2.0	185.9	0.5	1.9
5P	222.1	1.6	1.0	213.5	0.2	1.3	252.3	0.2	0.0

6P	155.5	1.8	1.4	230.6	1.5	1.0	157.1	1.2	0.5
7P	114.8	1.6	2.0	0.0	0.0	0.0	111.7	1.6	1.1
8P	103.5	2.3	0.4	112.2	1.9	0.0	85.0	2.1	0.9
1MA	212.5	1.5	4.5	0.0	0.0	0.0	0.0	0.0	0.0
2MA	181.1	1.2	4.0	160.2	0.6	3.0	0.0	0.0	0.0
3MA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4MA	118.1	0.6	3.0	238.6	0.6	1.0	0.0	0.0	0.0
5MA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6MA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7MA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8MA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MGLY	58.0	1.0	0.0	72.1	0.7	0.0	72.1	0.7	0.0
GLY	118.1	0.6	2.0	58.0	1.0	0.0	58.0	1.0	0.0

Section S7.3. Stoichiometric coefficients

(a) Isoprene

180 Table S9. Stoichiometric coefficient array of oxygenated products from the oxidation of isoprene under the sunlight for UNIPAR model

Oxidation path: isoprene + OH (day)				Oxidation path: isoprene + OH (day)				
NOx level: Low NOx				NOx level: High NOx				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	3.02E-12	-2.93E-10	8.20E-09	-4.34E-08	4.04E-12	1.75E-10	-1.51E-09	2.46E-09
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	1.75E-07	-1.55E-05	3.13E-04	3.74E-03	-4.53E-06	8.52E-05	8.08E-05	6.42E-05
8VF	4.95E-09	-4.58E-07	1.05E-05	7.87E-05	-2.28E-07	4.86E-06	-1.45E-05	1.43E-05
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	1.06E-08	-1.05E-06	2.94E-05	4.46E-04	-2.16E-07	7.63E-07	8.12E-05	-4.63E-05
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	-1.27E-07	1.65E-05	-7.51E-04	1.33E-02	-6.30E-06	4.24E-05	1.12E-03	-2.20E-03
7F	7.61E-08	-8.27E-06	2.83E-04	5.56E-04	-1.33E-07	-1.15E-05	4.50E-04	-6.27E-04
8F	-4.03E-09	6.90E-08	1.44E-05	7.07E-04	-4.36E-06	1.55E-04	-1.79E-03	7.66E-03
1M	8.03E-10	-8.17E-08	2.42E-06	-6.46E-06	-4.66E-09	1.33E-07	-7.00E-08	1.74E-06
2M	1.00E-08	-9.53E-07	2.39E-05	4.98E-05	-3.04E-07	6.71E-06	-2.05E-05	1.82E-05
3M	7.53E-09	8.64E-07	-1.60E-04	9.73E-03	1.73E-06	-8.52E-05	1.17E-03	3.20E-03
4M	-7.36E-10	8.88E-08	-3.73E-06	6.19E-05	8.71E-09	-6.16E-07	8.62E-06	-1.05E-06
5M	4.64E-08	-4.78E-06	1.40E-04	7.42E-04	-4.53E-07	5.26E-06	1.23E-04	3.59E-04
6M	1.91E-07	-2.82E-05	1.69E-03	1.26E-02	3.47E-05	-9.27E-04	8.83E-03	-3.53E-03
7M	-1.04E-07	3.46E-06	5.72E-04	9.88E-03	-1.22E-04	3.38E-03	-2.98E-02	9.95E-02
8M	-1.59E-06	2.14E-04	-1.07E-02	3.13E-01	2.74E-05	-1.52E-03	1.79E-02	1.70E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	-1.10E-13	1.18E-11	-4.04E-10	4.57E-09	-1.93E-12	4.53E-12	3.99E-10	-7.93E-10
3S	-2.99E-10	3.47E-08	-1.37E-06	2.05E-05	6.70E-09	-2.83E-07	3.11E-06	3.69E-07
4S	3.51E-09	-1.36E-07	-9.82E-06	4.49E-04	-3.19E-07	5.65E-06	5.22E-06	-1.50E-05
5S	2.33E-08	-1.69E-06	-1.08E-05	4.22E-03	3.51E-07	-3.74E-05	6.97E-04	2.91E-04
6S	3.56E-07	-2.74E-05	1.41E-04	4.98E-02	1.04E-05	-5.44E-04	8.54E-03	5.93E-03
7S	-3.06E-07	3.92E-05	-1.78E-03	3.38E-02	3.89E-06	-3.95E-04	6.50E-03	-1.03E-02
8S	2.14E-07	-2.17E-05	6.18E-04	1.18E-02	5.59E-06	-1.68E-04	2.01E-03	6.77E-03
1P	3.23E-07	-3.27E-05	9.59E-04	-2.34E-03	-6.44E-06	1.67E-04	-7.39E-04	9.21E-04
2P	-7.97E-08	1.24E-05	-7.16E-04	2.11E-02	5.32E-06	-2.25E-04	2.65E-03	5.45E-03
3P	6.17E-09	-5.63E-07	1.24E-05	9.29E-05	-1.51E-07	2.76E-06	3.64E-06	-1.13E-05

4P	-4.50E-10	-2.46E-07	3.49E-05	1.19E-03	-4.67E-06	1.37E-04	-1.31E-03	5.58E-03
5P	-2.81E-08	3.51E-06	-1.59E-04	3.27E-03	9.84E-06	-2.51E-04	1.86E-03	-1.40E-03
6P	-1.48E-07	2.29E-06	8.85E-04	1.01E-01	-2.56E-05	9.94E-04	-1.23E-02	1.60E-01
7P	2.89E-08	-2.83E-05	3.13E-03	-1.96E-02	-9.08E-07	1.71E-04	-1.45E-03	8.35E-03
8P	-1.62E-06	2.28E-04	-1.17E-02	2.71E-01	3.99E-05	-3.27E-03	5.26E-02	-6.78E-02
1MA	6.78E-09	-6.37E-07	1.49E-05	1.51E-04	-1.27E-07	2.93E-06	-8.82E-06	1.50E-04
2MA	2.16E-09	-2.25E-07	7.07E-06	-3.12E-05	-2.67E-08	7.86E-07	-3.98E-06	5.17E-06
3MA	0.00E+00							
4MA	-2.11E-11	-3.88E-09	6.46E-07	-4.82E-06	-3.38E-10	3.09E-08	-1.35E-07	1.53E-07
5MA	0.00E+00							
6MA	0.00E+00							
7MA	0.00E+00							
8MA	0.00E+00							
MGLY	-3.44E-07	4.32E-05	-1.98E-03	4.80E-02	1.72E-05	-6.79E-04	7.58E-03	7.17E-03
GLY	-1.47E-07	1.79E-05	-7.94E-04	2.05E-02	-3.20E-06	1.11E-04	-1.77E-03	2.41E-02
IEPOX	7.81E-07	-9.01E-05	3.46E-03	-1.95E-02	-7.34E-06	2.60E-04	-1.35E-03	1.77E-03

Table S9. (continued)

Oxidation path: isoprene + O ₃ (day)					Oxidation path: isoprene + O ₃ (day)				
NO _x level: Low NO _x					NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹	
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-3.96E-13	5.76E-11	-1.15E-09	6.74E-09	6.97E-13	-7.08E-12	2.62E-11	-2.94E-11	
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	-5.00E-15	4.91E-13	-8.98E-12	4.87E-11	5.72E-15	-6.97E-14	2.79E-13	-3.35E-13	
7VF	-2.27E-08	9.72E-07	6.61E-05	-5.49E-04	-1.08E-07	5.47E-06	-2.45E-05	5.01E-05	
8VF	-2.67E-10	1.09E-08	5.95E-07	-6.22E-06	7.07E-10	1.25E-08	-8.51E-08	1.95E-07	
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	3.01E-08	-2.52E-06	1.30E-05	3.53E-03	-4.68E-06	6.23E-05	2.40E-04	-3.18E-04	
7F	-2.52E-09	1.21E-07	6.48E-06	-4.47E-05	-1.44E-08	7.04E-07	-4.27E-06	2.23E-05	
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-2.93E-13	2.52E-11	-3.74E-10	1.72E-09	3.21E-13	-1.65E-12	4.82E-12	-5.79E-12	
3M	-3.14E-12	5.10E-10	-9.31E-09	5.24E-08	7.01E-12	-3.74E-11	1.39E-10	-1.46E-10	
4M	-1.75E-14	3.19E-11	6.74E-11	-7.74E-10	-7.93E-13	5.45E-11	-1.68E-10	1.53E-10	
5M	-2.63E-09	2.72E-07	-9.89E-06	2.11E-04	-4.09E-07	1.20E-05	-1.23E-04	5.85E-04	
6M	-3.41E-09	1.90E-08	3.19E-05	1.86E-05	-1.02E-07	3.37E-06	-1.03E-05	2.15E-04	
7M	1.56E-08	-1.39E-06	1.75E-05	1.32E-03	-1.83E-06	2.53E-05	8.27E-05	-7.86E-05	
8M	9.71E-07	-1.06E-04	3.35E-03	6.94E-02	-3.35E-05	8.95E-04	-5.56E-03	9.19E-02	
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	4.71E-09	-7.76E-07	3.61E-05	-2.19E-04	-5.80E-08	1.69E-06	-2.66E-06	3.47E-06	
5S	-1.37E-10	6.02E-09	2.94E-07	5.60E-07	-4.77E-09	1.02E-07	-1.38E-07	5.35E-08	
6S	4.44E-08	-7.33E-06	4.50E-04	2.43E-03	-2.76E-06	7.22E-05	-3.04E-04	4.88E-03	
7S	-2.30E-09	2.23E-07	-2.07E-06	1.31E-03	8.20E-07	-3.09E-05	3.75E-04	-1.59E-04	
8S	-6.91E-07	7.34E-05	-2.22E-03	7.91E-02	3.66E-05	-8.38E-04	4.11E-03	6.96E-02	
1P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3P	-9.23E-11	8.72E-09	-2.37E-07	6.65E-06	1.00E-10	-7.39E-08	1.38E-06	-1.11E-06	
4P	1.08E-09	-9.72E-08	1.84E-06	3.32E-05	-3.43E-08	3.73E-07	4.63E-06	-6.67E-06	
5P	-1.15E-21	2.16E-19	-5.46E-18	3.72E-17	5.63E-22	-8.99E-21	4.21E-20	-5.48E-20	
6P	-3.15E-07	4.12E-05	-2.01E-03	4.15E-02	1.20E-05	-7.71E-04	1.05E-02	-1.30E-02	
7P	1.70E-08	-2.22E-06	8.77E-05	6.06E-04	-6.23E-07	1.20E-05	2.51E-06	6.97E-04	

8P	-1.21E-06	1.46E-04	-6.43E-03	2.43E-01	1.13E-04	-4.37E-03	4.82E-02	4.03E-02
1MA	0.00E+00	0.00E+00						
2MA	0.00E+00	0.00E+00						
3MA	0.00E+00	0.00E+00						
4MA	0.00E+00	0.00E+00						
5MA	0.00E+00	0.00E+00						
6MA	0.00E+00	0.00E+00						
7MA	0.00E+00	0.00E+00						
8MA	0.00E+00	0.00E+00						
MGLY	2.97E-07	-3.34E-05	1.23E-03	3.05E-03	1.56E-06	-1.77E-05	5.95E-04	6.13E-03
GLY	4.25E-08	-4.54E-06	1.41E-04	-6.22E-05	-8.17E-07	2.14E-05	-1.09E-04	6.82E-04
IEPOX	0.00E+00	0.00E+00						

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Table S9. (continued)

Oxidation path: isoprene + NO ₃ (day)				Oxidation path: isoprene + NO ₃ (day)				
NO _x level: Low NO _x				NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	2.09E-19	-7.63E-17	8.29E-15	-4.52E-14	-2.03E-17	7.09E-16	-2.09E-15	2.00E-15
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-3.73E-18	6.05E-17	3.79E-14	-2.49E-13	-6.32E-17	3.07E-15	-1.12E-14	1.22E-14
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	-3.17E-07	4.26E-05	-2.21E-03	6.91E-02	-1.44E-06	5.41E-05	-2.10E-03	6.80E-02
8F	-3.56E-15	8.66E-14	3.20E-11	-1.73E-10	-5.01E-14	2.24E-12	-1.68E-12	2.79E-12
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-4.11E-18	3.18E-16	9.74E-15	-8.41E-14	-5.97E-18	8.83E-16	-4.12E-15	5.05E-15
3M	1.04E-09	-1.46E-07	7.97E-06	-1.90E-05	-1.79E-08	4.08E-07	2.73E-06	-3.05E-06
4M	2.88E-16	-2.87E-14	7.92E-13	1.84E-11	1.72E-15	-2.11E-13	4.59E-12	-3.51E-12
5M	-3.28E-08	3.83E-06	-1.54E-04	2.46E-03	2.14E-06	-5.63E-05	3.67E-04	1.10E-03
6M	-8.04E-14	3.84E-12	5.91E-10	-3.14E-09	-1.04E-12	4.56E-11	-3.19E-11	2.19E-11
7M	1.59E-06	-1.89E-04	7.57E-03	1.20E-01	4.60E-05	-1.51E-03	2.11E-02	7.07E-02
8M	3.90E-07	-3.95E-05	6.17E-04	3.17E-01	-4.12E-05	1.10E-03	-9.28E-03	3.44E-01
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	2.90E-17	-3.27E-15	1.18E-13	1.80E-13	-3.90E-16	4.75E-15	1.07E-13	-1.24E-13
5S	8.56E-17	-8.32E-15	2.02E-13	3.02E-12	-6.17E-16	-1.70E-14	7.28E-13	-8.38E-13
6S	-4.78E-18	6.64E-16	-8.18E-15	3.49E-14	1.21E-17	4.28E-17	-3.00E-16	4.17E-16
7S	-5.72E-19	1.47E-17	5.92E-15	-3.70E-14	-1.25E-17	5.37E-16	-1.86E-15	1.91E-15
8S	-1.44E-06	1.82E-04	-8.63E-03	2.73E-01	-2.66E-05	9.90E-04	-1.78E-02	3.11E-01
1P	3.78E-17	-2.74E-15	-1.09E-14	5.03E-12	4.91E-16	-5.63E-14	1.08E-12	-1.20E-12
2P	1.02E-11	-1.50E-09	8.78E-08	-1.94E-07	-1.61E-10	3.69E-09	3.56E-08	-1.93E-08
3P	7.64E-12	-1.60E-08	2.46E-06	-8.02E-06	-3.07E-17	2.21E-15	-7.58E-15	8.59E-15
4P	2.11E-17	-2.00E-15	6.33E-14	3.64E-12	1.30E-15	-6.38E-14	1.01E-12	-9.81E-13
5P	-9.84E-09	1.52E-06	-8.92E-05	2.82E-03	2.41E-06	-7.26E-05	6.74E-04	1.45E-04
6P	4.13E-07	-5.15E-05	2.29E-03	2.49E-02	-3.17E-06	5.13E-05	1.43E-03	2.66E-02
7P	-7.50E-16	-9.68E-13	1.45E-10	-6.03E-10	-2.38E-13	8.36E-12	1.76E-11	1.99E-12

8P	-2.94E-08	3.71E-06	-1.78E-04	7.21E-03	5.16E-06	-1.36E-04	1.01E-03	4.09E-03
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	-3.27E-15	3.15E-13	1.14E-12	-2.08E-11	2.65E-15	2.88E-13	-1.21E-12	1.46E-12
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-4.69E-08	6.06E-06	-3.20E-04	2.56E-02	3.33E-06	-9.16E-05	5.88E-04	2.29E-02
GLY	-1.22E-07	1.66E-05	-8.96E-04	3.85E-02	7.24E-06	-1.91E-04	1.00E-03	3.29E-02
IEPOX	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

Table S9. (continued)

Oxidation path: isoprene + O(³ P) (day)				Oxidation path: isoprene + O(³ P) (day)				
NO _x level: Low NO _x				NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	-5.72E-20	4.73E-18	3.37E-16	-1.14E-15	-6.05E-19	2.49E-17	7.28E-17	7.94E-17
8VF	-1.44E-33	1.74E-31	1.46E-30	-1.02E-29	-4.15E-33	3.04E-31	-6.39E-31	1.25E-30
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-1.84E-19	1.22E-17	1.53E-15	-5.28E-15	-3.10E-18	1.15E-16	2.57E-16	3.16E-16
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	1.56E-27	-1.14E-25	-4.47E-24	1.15E-21	-6.48E-24	1.71E-22	-1.43E-21	4.83E-21
7F	-4.51E-14	5.39E-12	-2.37E-10	6.86E-09	-1.77E-11	4.85E-10	-4.43E-09	1.87E-08
8F	-4.81E-11	5.95E-09	-2.77E-07	8.90E-06	-1.50E-08	4.07E-07	-3.69E-06	1.71E-05
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-1.43E-24	5.04E-22	-7.95E-21	4.12E-20	1.03E-23	-1.37E-23	-2.58E-23	7.72E-23
3M	-1.81E-19	1.14E-17	1.55E-15	-5.30E-15	-3.15E-18	1.15E-16	2.66E-16	3.58E-16
4M	-1.04E-34	2.69E-32	-3.09E-31	1.50E-30	3.58E-34	7.27E-33	-1.87E-32	4.21E-32
5M	1.71E-19	-1.92E-17	6.85E-16	1.80E-14	-3.56E-17	8.89E-16	-6.27E-15	3.27E-14
6M	-1.01E-12	1.22E-10	-5.51E-09	1.93E-07	-1.99E-11	4.83E-10	-3.01E-09	1.90E-08
7M	-2.25E-11	2.78E-09	-1.29E-07	4.15E-06	-8.52E-09	2.33E-07	-2.12E-06	9.72E-06
8M	-3.31E-08	4.13E-06	-1.96E-04	6.74E-03	-4.63E-09	1.27E-07	-1.16E-06	5.18E-06
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	2.50E-17	-2.81E-15	9.88E-14	2.00E-12	-3.64E-15	8.96E-14	-5.97E-13	3.40E-12
5S	1.15E-18	-1.30E-16	4.56E-15	1.22E-13	-2.46E-16	6.14E-15	-4.37E-14	2.26E-13
6S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7S	-1.69E-19	1.10E-17	1.36E-15	-1.75E-15	-8.08E-18	2.39E-16	-8.65E-16	5.83E-15
8S	-1.56E-13	1.86E-11	-8.32E-10	2.85E-08	-7.40E-11	2.02E-09	-1.83E-08	7.77E-08
1P	8.34E-28	-1.10E-25	5.80E-24	3.71E-24	-5.41E-26	1.33E-24	-5.79E-24	3.10E-23
2P	-5.53E-20	3.17E-18	4.96E-16	-1.72E-15	-1.00E-18	3.64E-17	8.35E-17	1.00E-16
3P	-8.32E-19	4.80E-17	7.44E-15	-2.58E-14	-1.50E-17	5.45E-16	1.26E-15	1.44E-15
4P	-3.34E-20	3.73E-18	-1.78E-17	3.52E-17	-2.09E-20	3.46E-18	-1.96E-17	7.58E-17
5P	5.55E-17	-6.17E-15	2.12E-13	4.26E-12	-7.42E-15	1.80E-13	-1.16E-12	6.83E-12
6P	-1.34E-10	1.64E-08	-7.49E-07	2.43E-05	-5.32E-08	1.46E-06	-1.34E-05	5.99E-05
7P	-1.20E-10	1.46E-08	-6.68E-07	2.17E-05	-4.75E-08	1.30E-06	-1.19E-05	5.35E-05

8P	4.72E-11	-5.57E-09	2.18E-07	2.57E-06	-4.44E-09	1.09E-07	-6.74E-07	4.49E-06
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	4.24E-10	-4.90E-08	1.82E-06	2.75E-05	-4.54E-08	1.13E-06	-7.26E-06	4.69E-05
GLY	-1.16E-11	1.42E-09	-6.54E-08	2.11E-06	-4.44E-09	1.21E-07	-1.11E-06	5.05E-06
IEPOX	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

¹ The stoichiometric coefficient is calculated by $\alpha = A \times (\text{HC: NO}_x)^3 + B \times (\text{HC: NO}_x)^2 + C \times (\text{HC: NO}_x) + D$, where HC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

Table S10. Stoichiometric coefficient array of oxygenated products from the oxidation of isoprene in nighttime for UNIPAR model.

Lumped species	Oxidation path: isoprene + OH (night)				Oxidation path: isoprene + OH (night)			
	NOx level: Low NOx				NOx level: High NOx			
	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	3.40E-19	-4.91E-17	2.15E-15	-1.74E-14	-9.64E-22	2.16E-20	3.91E-20	-1.16E-19
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	5.52E-10	-7.88E-08	3.36E-06	-2.40E-05	2.22E-09	-5.99E-08	4.87E-07	1.40E-06
8VF	3.64E-11	-5.22E-09	2.24E-07	-1.73E-06	2.42E-11	-7.98E-10	1.05E-08	5.79E-11
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	2.81E-09	-4.02E-07	1.72E-05	-1.12E-04	1.59E-08	-4.58E-07	4.45E-06	9.28E-06
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	5.08E-12	-7.24E-10	3.07E-08	-2.32E-07	4.15E-12	-1.12E-10	9.40E-10	5.38E-09
7F	2.49E-09	-3.56E-07	1.53E-05	-9.57E-05	1.52E-08	-4.42E-07	4.43E-06	9.86E-06
8F	7.59E-09	-1.05E-06	4.11E-05	-1.79E-04	5.41E-09	7.61E-07	-2.57E-05	3.11E-04
1M	2.05E-11	-2.92E-09	1.25E-07	-9.51E-07	1.89E-11	-6.60E-10	8.29E-09	-7.25E-09
2M	4.29E-11	-6.10E-09	2.59E-07	-1.98E-06	3.03E-11	-9.55E-10	1.08E-08	-4.22E-09
3M	1.19E-08	-1.71E-06	7.49E-05	-2.33E-04	1.23E-07	-4.61E-06	7.08E-05	-3.54E-05
4M	3.66E-13	-5.32E-11	2.37E-09	-1.91E-08	7.45E-14	-3.30E-12	5.51E-11	-4.98E-11
5M	2.94E-09	-4.23E-07	1.84E-05	-6.03E-05	6.69E-08	-1.83E-06	1.54E-05	5.03E-05
6M	-1.05E-07	1.45E-05	-5.72E-04	6.20E-02	1.77E-05	-5.03E-04	4.75E-03	4.25E-02
7M	-2.59E-07	3.63E-05	-1.48E-03	9.10E-02	2.81E-05	-7.87E-04	7.18E-03	5.84E-02
8M	3.85E-08	-5.63E-06	2.53E-04	6.87E-03	3.44E-06	-9.85E-05	9.49E-04	5.77E-03
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	5.00E-28	-6.55E-26	2.30E-24	-1.31E-23	-2.48E-27	7.06E-26	-6.67E-25	2.21E-24
3S	3.15E-20	-4.08E-18	1.40E-16	-6.71E-16	-7.98E-18	2.18E-16	-1.93E-15	5.64E-15
4S	9.75E-13	-1.38E-10	5.83E-09	-4.44E-08	3.75E-13	-8.33E-12	3.10E-11	1.01E-09
5S	1.87E-09	-2.68E-07	1.16E-05	-8.23E-05	4.19E-09	-1.49E-07	2.05E-06	-1.04E-06
6S	6.01E-08	-8.78E-06	3.94E-04	2.97E-02	1.27E-05	-3.49E-04	2.99E-03	2.53E-02
7S	8.12E-09	-1.16E-06	4.95E-05	-3.16E-04	2.52E-08	-7.06E-07	6.46E-06	5.42E-05
8S	3.27E-08	-4.68E-06	2.00E-04	-1.10E-03	3.85E-08	-1.08E-06	9.78E-06	4.48E-04
1P	5.58E-12	-7.50E-10	2.76E-08	-1.42E-07	5.09E-11	-1.17E-09	4.91E-09	6.21E-08
2P	2.40E-12	-3.23E-10	1.19E-08	-6.23E-08	6.86E-12	-8.26E-11	-1.74E-09	3.71E-08
3P	4.05E-13	-5.35E-11	1.88E-09	-5.40E-09	-7.06E-11	2.01E-09	-1.92E-08	7.01E-08
4P	9.10E-09	-1.31E-06	5.64E-05	-7.55E-05	2.13E-07	-7.09E-06	8.69E-05	-1.93E-05
5P	2.93E-10	-4.13E-08	1.69E-06	-1.07E-05	-1.16E-09	3.82E-08	-4.77E-07	4.32E-06
6P	4.27E-08	-6.18E-06	2.71E-04	7.75E-04	-7.12E-07	1.28E-05	4.54E-05	1.78E-03

7P	1.90E-06	-2.75E-04	1.21E-02	1.52E-02	4.78E-05	-1.66E-03	2.26E-02	-3.41E-03
8P	8.42E-08	-1.20E-05	5.16E-04	-3.07E-03	3.83E-07	-1.12E-05	1.10E-04	6.35E-04
1MA	5.59E-13	-7.50E-11	2.73E-09	-1.24E-08	-2.59E-11	7.96E-10	-8.66E-09	3.96E-08
2MA	1.90E-13	-2.54E-11	9.15E-10	-3.53E-09	-9.74E-12	3.06E-10	-3.43E-09	1.65E-08
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	5.93E-10	-8.56E-08	3.75E-06	4.75E-05	6.42E-08	-1.72E-06	1.35E-05	5.24E-05
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	1.01E-07	-1.45E-05	6.18E-04	-3.76E-03	3.25E-07	-9.04E-06	8.08E-05	8.71E-04
GLY	6.54E-08	-9.35E-06	4.00E-04	-2.34E-03	2.52E-07	-7.09E-06	6.55E-05	6.07E-04
IEPOX	3.79E-08	-5.46E-06	2.38E-04	-1.75E-03	2.92E-08	-1.35E-06	2.71E-05	-2.19E-05

Table S10. (continued)

Oxidation path: isoprene + O ₃ (night)				Oxidation path: isoprene + O ₃ (night)				
NO _x level: Low NO _x				NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-2.11E-13	3.30E-11	-1.57E-09	7.25E-08	4.94E-11	-1.29E-09	6.35E-09	8.21E-08
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	-4.85E-17	7.66E-15	-3.76E-13	1.43E-11	1.63E-14	-4.77E-13	3.61E-12	7.73E-12
7VF	-2.92E-11	4.45E-09	-1.93E-07	2.44E-05	8.02E-09	-2.17E-07	1.26E-06	2.47E-05
8VF	1.25E-17	-2.31E-14	4.88E-12	1.59E-09	1.08E-12	-3.47E-11	3.50E-10	5.47E-10
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	2.65E-13	-3.78E-11	1.15E-09	9.55E-07	2.45E-13	-3.89E-10	1.19E-08	8.73E-07
7F	9.71E-13	-1.83E-10	1.39E-08	1.86E-06	7.57E-10	-2.33E-08	2.25E-07	1.33E-06
8F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-7.10E-16	1.12E-13	-5.62E-12	1.80E-10	-8.22E-14	3.58E-12	-5.68E-11	4.42E-10
3M	-1.05E-11	1.69E-09	-8.82E-08	4.49E-06	4.58E-09	-1.45E-07	1.32E-06	5.93E-07
4M	-5.67E-12	9.00E-10	-4.55E-08	1.93E-06	5.12E-10	-1.11E-08	-2.21E-08	2.50E-06
5M	-3.51E-15	3.93E-13	2.28E-12	1.30E-08	6.52E-12	-2.06E-10	1.98E-09	7.46E-09
6M	1.47E-10	-2.32E-08	1.19E-06	1.04E-04	4.98E-08	-1.81E-06	2.27E-05	1.46E-05
7M	9.74E-14	-1.39E-11	4.18E-10	3.52E-07	9.69E-14	-1.44E-10	4.39E-09	3.22E-07
8M	-4.12E-09	6.36E-07	-2.98E-05	2.55E-03	3.55E-07	-5.92E-06	-6.36E-05	3.29E-03
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	-4.76E-14	7.27E-12	-3.41E-10	3.01E-08	-1.43E-11	5.34E-10	-6.92E-09	5.86E-08
5S	4.97E-18	3.49E-15	1.81E-12	1.24E-12	-6.69E-15	2.02E-13	3.25E-13	1.72E-12
6S	9.75E-10	-1.52E-07	7.57E-06	6.73E-04	3.44E-07	-1.26E-05	1.59E-04	3.56E-05
7S	7.17E-11	-1.15E-08	6.17E-07	3.43E-04	3.16E-08	-1.10E-06	1.29E-05	2.96E-04
8S	5.41E-08	-8.56E-06	4.40E-04	1.01E-01	2.21E-05	-7.84E-04	9.48E-03	6.50E-02
1P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3P	-1.83E-18	2.97E-16	-1.60E-14	3.75E-13	-2.79E-16	1.08E-14	-1.53E-13	1.01E-12
4P	-2.14E-16	3.40E-14	-1.78E-12	3.60E-11	-8.08E-14	2.91E-12	-3.61E-11	1.76E-10
5P	6.18E-34	-4.74E-32	1.81E-29	5.89E-31	-1.11E-31	3.24E-30	-6.27E-30	9.61E-30
6P	-2.96E-11	4.68E-09	-2.38E-07	9.85E-06	1.13E-09	-6.84E-09	-6.51E-07	1.46E-05
7P	-2.74E-10	4.41E-08	-2.36E-06	4.83E-05	-2.99E-08	1.30E-06	-2.09E-05	1.44E-04

8P	1.49E-08	-2.53E-06	1.29E-04	1.73E-01	3.84E-06	-1.33E-04	1.59E-03	1.67E-01
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	5.61E-10	-9.05E-08	4.89E-06	2.92E-03	2.43E-07	-8.41E-06	9.84E-05	2.56E-03
GLY	-1.81E-14	2.85E-12	-1.42E-10	7.09E-09	2.20E-13	1.72E-11	-7.20E-10	1.16E-08
IEPOX	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

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Table S10. (continued)

Oxidation path: isoprene + NO ₃ (night)				Oxidation path: isoprene + NO ₃ (night)				
NO _x level: Low NO _x				NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7VF	-3.00E-19	4.63E-17	-2.28E-15	3.71E-14	-7.20E-16	2.01E-14	-1.84E-13	5.82E-13
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	-4.13E-17	6.54E-15	-3.37E-13	6.02E-12	-2.29E-14	6.83E-13	-7.09E-12	2.94E-11
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	-3.87E-13	6.29E-11	-3.46E-09	7.72E-08	-2.89E-10	8.34E-09	-8.22E-08	3.33E-07
8F	-7.23E-15	1.21E-12	-6.93E-11	1.50E-09	3.15E-14	2.38E-12	-1.20E-10	1.89E-09
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	-5.60E-19	9.23E-17	-5.24E-15	1.27E-13	-3.53E-16	1.03E-14	-1.04E-13	4.53E-13
3M	-4.12E-08	6.73E-06	-3.74E-04	8.46E-03	-2.08E-05	6.22E-04	-6.49E-03	2.95E-02
4M	-4.65E-12	7.39E-10	-3.87E-08	7.61E-07	-7.52E-09	2.12E-07	-1.98E-06	6.68E-06
5M	-8.24E-15	1.30E-12	-6.76E-11	1.31E-09	-1.90E-11	5.27E-10	-4.80E-09	1.53E-08
6M	-1.00E-14	1.77E-12	-1.15E-10	3.61E-09	-5.07E-13	1.76E-11	-2.88E-10	4.29E-09
7M	-1.69E-06	2.94E-04	-1.86E-02	5.69E-01	-6.54E-05	2.68E-03	-4.94E-02	7.09E-01
8M	-4.25E-08	7.51E-06	-4.88E-04	1.53E-02	-7.43E-07	4.19E-05	-1.01E-03	1.79E-02
1S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3S	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4S	-2.50E-21	3.80E-19	-1.81E-17	2.77E-16	-2.82E-17	7.56E-16	-6.46E-15	1.77E-14
5S	-7.66E-23	1.15E-20	-5.31E-19	7.65E-18	-2.15E-18	5.68E-17	-4.75E-16	1.24E-15
6S	2.05E-19	-3.53E-17	1.90E-15	2.53E-15	-5.51E-18	9.87E-17	1.43E-15	-1.76E-15
7S	-3.53E-21	5.81E-19	-3.22E-17	6.87E-16	-5.24E-19	1.69E-17	-2.11E-16	1.39E-15
8S	-3.30E-07	5.78E-05	-3.72E-03	1.16E-01	-6.28E-06	3.17E-04	-7.37E-03	1.33E-01
1P	-2.76E-18	4.25E-16	-2.08E-14	3.44E-13	-4.12E-14	1.09E-12	-9.20E-12	2.45E-11
2P	-1.06E-08	1.72E-06	-9.48E-05	2.20E-03	-7.61E-06	2.19E-04	-2.15E-03	8.78E-03
3P	-1.03E-06	1.82E-04	-1.19E-02	3.81E-01	8.11E-05	-1.75E-03	4.56E-04	3.70E-01
4P	-2.13E-14	3.32E-12	-1.67E-10	2.97E-09	-9.26E-11	2.53E-09	-2.23E-08	6.58E-08
5P	-6.33E-08	1.02E-05	-5.52E-04	1.19E-02	-8.36E-05	2.33E-03	-2.16E-02	7.54E-02
6P	-2.03E-06	3.56E-04	-2.29E-02	7.66E-01	1.34E-04	-2.87E-03	-1.73E-03	7.44E-01
7P	-7.28E-14	1.20E-11	-7.18E-10	2.64E-08	-2.95E-11	8.79E-10	-9.22E-09	5.49E-08

8P	-2.91E-09	4.70E-07	-2.56E-05	5.53E-04	-3.06E-06	8.63E-05	-8.15E-04	2.99E-03
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	-3.22E-09	5.27E-07	-2.96E-05	6.85E-04	-1.04E-06	3.29E-05	-3.72E-04	1.95E-03
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-1.44E-07	2.55E-05	-1.67E-03	5.34E-02	4.92E-06	-8.87E-05	-1.08E-03	5.41E-02
GLY	-1.36E-07	2.40E-05	-1.56E-03	4.90E-02	9.99E-07	2.34E-05	-2.00E-03	5.26E-02
IEPOX	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

¹ The stoichiometric coefficient is calculated by $\alpha = A \times (\text{HC: NO}_x)^3 + B \times (\text{HC: NO}_x)^2 + C \times (\text{HC: NO}_x) + D$, where HC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

(b) α -pinene

Table S11. Stoichiometric coefficient array of oxygenated products from the oxidation of α -pinene under the sunlight for UNIPAR model

Oxidation path: α -pinene + OH (day)					Oxidation path: α -pinene + OH (day)			
Lumped species	NOx level: Low NOx				NOx level: High NOx			
	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	2.31E-08	-2.37E-06	7.04E-05	-3.40E-04	-5.18E-08	2.66E-06	-1.16E-05	2.12E-05
6VF	2.48E-08	-2.66E-06	7.97E-05	-2.95E-04	-1.97E-07	7.65E-06	-6.03E-05	2.52E-04
7VF	5.66E-08	-6.39E-06	2.15E-04	-9.51E-04	-2.56E-07	1.04E-05	-3.25E-05	7.85E-05
8VF	-7.40E-09	3.87E-07	3.27E-06	-4.22E-05	4.94E-08	-6.41E-07	3.00E-06	-3.38E-06
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	-1.87E-07	2.36E-05	-8.80E-04	1.66E-02	2.33E-06	-1.01E-04	8.63E-04	9.74E-03
8F	1.28E-08	-1.76E-06	6.58E-05	-1.84E-04	-1.07E-07	5.45E-06	-4.54E-05	2.81E-04
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	-1.02E-07	8.07E-06	-7.49E-05	1.50E-04	3.65E-07	-4.47E-06	1.79E-05	-2.06E-05
4M	-6.68E-07	6.94E-05	-1.89E-03	2.72E-02	6.80E-06	-2.39E-04	1.95E-03	1.32E-02
5M	6.39E-07	-7.62E-05	2.56E-03	1.37E-02	-7.18E-06	2.32E-04	-1.10E-03	2.64E-02
6M	-7.47E-06	8.80E-04	-2.92E-02	4.78E-01	1.15E-04	-3.95E-03	2.83E-02	2.79E-01
7M	-8.89E-08	2.65E-05	-1.61E-03	7.34E-02	2.61E-06	-2.15E-04	2.68E-03	5.40E-02
8M	-3.89E-08	2.99E-06	-3.22E-05	8.73E-05	1.26E-07	-1.75E-06	7.80E-06	-9.81E-06
1S	-1.10E-08	1.03E-06	-1.29E-05	4.49E-05	2.93E-08	-3.21E-07	1.32E-06	-1.57E-06
2S	7.31E-08	-6.57E-06	1.95E-04	-3.83E-05	-2.49E-07	-2.17E-06	2.31E-04	-4.49E-04
3S	-3.78E-07	2.72E-05	-1.61E-04	1.46E-02	3.10E-06	-8.73E-05	9.94E-04	1.11E-02
4S	1.40E-06	-1.73E-04	6.41E-03	3.94E-02	-8.97E-06	2.91E-04	4.05E-04	6.13E-02
5S	2.10E-06	-2.08E-04	5.63E-03	2.18E-02	-1.14E-05	3.35E-04	-9.39E-04	4.52E-02
6S	-9.09E-07	7.73E-05	-1.32E-03	9.71E-03	6.07E-06	-1.47E-04	8.50E-04	3.62E-03
7S	-2.39E-07	1.70E-05	-1.87E-04	2.80E-03	8.82E-07	-1.14E-05	-8.43E-06	2.64E-03
8S	-1.92E-09	1.27E-07	-1.02E-06	8.39E-07	8.42E-09	-1.36E-07	6.73E-07	-9.09E-07
1P	1.40E-08	-1.54E-06	6.58E-05	2.71E-03	4.09E-07	-1.55E-05	2.19E-04	2.20E-03
2P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3P	-4.79E-09	5.95E-07	-8.49E-06	3.44E-05	1.05E-08	-5.80E-08	1.73E-07	-1.73E-07
4P	-3.94E-08	4.76E-06	-1.63E-04	6.09E-03	-4.26E-07	1.60E-05	-2.70E-04	6.44E-03

5P	-9.42E-07	1.17E-04	-3.96E-03	2.29E-01	1.99E-05	-7.08E-04	5.95E-03	1.94E-01
6P	-4.29E-09	5.03E-07	-2.52E-05	1.35E-03	-1.54E-08	1.13E-06	-3.55E-05	1.40E-03
7P	0.00E+00							
8P	9.72E-07	-9.50E-05	2.61E-03	-7.72E-03	-4.83E-07	-1.00E-05	1.34E-03	-2.53E-03
1MA	0.00E+00							
2MA	-3.35E-09	4.39E-07	-1.68E-05	1.60E-03	-1.07E-08	-1.61E-06	3.27E-05	1.34E-03
3MA	0.00E+00							
4MA	-2.88E-10	4.25E-08	-8.50E-08	-1.08E-07	-1.11E-10	3.96E-08	-9.69E-08	7.90E-08
5MA	0.00E+00							
6MA	0.00E+00							
7MA	0.00E+00							
8MA	0.00E+00							
MGLY	6.00E-08	-5.26E-06	1.11E-04	8.91E-04	-1.71E-06	4.70E-05	-3.44E-04	2.01E-03
GLY	3.07E-08	-3.53E-06	1.19E-04	-5.43E-04	-2.57E-08	2.86E-06	-4.32E-07	1.33E-05

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Table S11. (Continued)

Oxidation path: α -pinene + O ₃ (day)					Oxidation path: α -pinene + O ₃ (day)				
NO _x level: Low NO _x					NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹	
1VF	1.53E-07	-1.45E-05	4.66E-04	-2.67E-03	4.67E-07	-1.63E-06	8.79E-06	-1.01E-05	
2VF	1.79E-08	-1.91E-06	6.63E-05	-2.97E-04	-3.00E-07	8.90E-06	-4.65E-05	6.20E-05	
3VF	2.30E-07	-1.77E-05	2.66E-04	2.69E-03	1.46E-06	-5.90E-05	7.39E-04	6.93E-04	
4VF	6.33E-08	-6.45E-06	2.11E-04	-9.61E-04	-8.19E-07	2.46E-05	-1.26E-04	1.67E-04	
5VF	4.10E-07	-3.19E-05	5.18E-04	5.27E-03	-1.67E-05	6.24E-04	-7.37E-03	3.36E-02	
6VF	1.38E-08	-1.43E-06	3.55E-05	1.18E-03	1.88E-08	-1.36E-05	3.30E-04	-4.52E-04	
7VF	1.74E-07	-1.57E-05	4.19E-04	-1.21E-03	-9.41E-08	1.35E-05	-1.40E-04	1.40E-03	
8VF	1.05E-07	-9.80E-06	2.64E-04	-9.67E-04	-7.65E-07	2.03E-05	-5.84E-05	7.64E-05	
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
4F	2.42E-08	-2.06E-06	4.29E-05	1.72E-05	-6.34E-07	2.57E-05	-3.23E-04	1.46E-03	
5F	3.23E-08	-2.79E-06	6.81E-05	-2.62E-04	-2.02E-06	6.97E-05	-7.42E-04	2.50E-03	
6F	1.74E-08	-1.47E-06	3.29E-05	-4.31E-05	-1.66E-06	5.74E-05	-6.20E-04	2.16E-03	
7F	7.73E-08	-6.53E-06	1.38E-04	3.25E-05	-1.40E-05	4.69E-04	-4.86E-03	1.59E-02	
8F	7.52E-08	-5.82E-06	1.52E-04	1.99E-03	3.29E-06	-1.10E-04	1.21E-03	-1.49E-03	
1M	6.82E-07	-8.32E-05	3.98E-03	-1.44E-02	-4.63E-06	1.52E-04	8.05E-04	-2.05E-03	
2M	6.13E-08	-4.58E-06	1.66E-04	-9.02E-04	-3.71E-07	1.66E-05	-1.53E-04	4.71E-04	
3M	2.70E-07	-2.45E-05	7.18E-04	-4.00E-03	4.71E-07	9.05E-07	-1.12E-05	1.03E-04	
4M	1.77E-06	-1.47E-04	3.19E-03	-1.66E-03	-4.85E-05	1.86E-03	-2.22E-02	9.41E-02	
5M	9.87E-07	-8.32E-05	2.02E-03	3.59E-02	-6.70E-05	2.40E-03	-2.62E-02	1.31E-01	
6M	6.60E-07	-5.40E-05	1.04E-03	5.61E-03	-9.98E-05	3.50E-03	-3.86E-02	1.40E-01	
7M	1.70E-06	-1.40E-04	3.00E-03	7.40E-03	-5.35E-05	1.87E-03	-2.00E-02	8.61E-02	
8M	1.52E-07	-1.41E-05	4.54E-04	-2.34E-03	1.18E-08	7.71E-06	-8.31E-06	-5.24E-06	
1S	3.32E-07	-3.10E-05	7.00E-04	2.37E-02	1.87E-05	-6.27E-04	6.89E-03	2.41E-03	
2S	-2.07E-07	1.93E-05	-5.81E-04	2.96E-02	2.03E-05	-6.56E-04	6.56E-03	4.83E-03	
3S	2.40E-06	-1.98E-04	4.16E-03	1.42E-02	-1.11E-06	1.17E-04	-1.50E-03	3.83E-02	
4S	2.18E-06	-1.64E-04	2.77E-03	8.94E-02	5.92E-05	-1.55E-03	1.12E-02	7.79E-02	
5S	4.34E-06	-3.51E-04	6.76E-03	3.32E-02	2.91E-06	-1.43E-04	3.00E-03	4.62E-02	
6S	1.09E-06	-9.72E-05	2.94E-03	-1.05E-02	1.13E-06	3.02E-05	-1.19E-04	5.41E-03	
7S	1.22E-06	-1.16E-04	3.47E-03	-1.41E-02	-7.70E-06	2.56E-04	-1.34E-03	4.56E-03	
8S	-4.36E-08	3.15E-06	-4.19E-05	2.22E-04	-2.29E-07	6.45E-06	-3.52E-05	4.84E-05	
1P	5.26E-07	-4.95E-05	1.51E-03	-7.65E-03	1.00E-10	2.28E-05	3.52E-06	-9.72E-05	
2P	5.16E-07	-4.48E-05	1.25E-03	-5.72E-03	-4.95E-06	1.77E-04	-1.60E-03	5.15E-03	
3P	1.80E-07	-1.56E-05	3.77E-04	-2.20E-04	-6.00E-07	3.71E-06	2.79E-04	-3.90E-04	
4P	2.94E-07	-2.23E-05	5.04E-04	1.14E-02	6.28E-06	-1.17E-04	1.93E-04	1.63E-02	
5P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
6P	1.57E-07	-1.17E-05	1.57E-04	3.31E-03	5.79E-07	-3.54E-05	5.69E-04	1.08E-03	
7P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	

8P	1.80E-06	-1.43E-04	2.49E-03	2.74E-02	-1.05E-05	1.48E-04	1.37E-03	2.09E-02
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-4.06E-09	2.73E-07	-2.68E-06	1.44E-05	-3.07E-08	8.84E-07	-5.04E-06	7.17E-06
GLY	4.33E-07	-3.46E-05	6.26E-04	4.28E-03	3.21E-06	-1.38E-04	1.90E-03	-9.79E-04

Table S11. (Continued)

Oxidation path: α -pinene + NO ₃ (day)					Oxidation path: α -pinene + NO ₃ (day)				
NO _x level: Low NO _x					NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹	
1VF	-2.03E-11	2.12E-09	-7.25E-08	8.86E-07	-2.03E-11	2.12E-09	-7.25E-08	8.86E-07	
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
5VF	-6.52E-11	6.52E-09	-2.04E-07	2.03E-06	-6.52E-11	6.52E-09	-2.04E-07	2.03E-06	
6VF	-8.91E-10	9.36E-08	-3.28E-06	4.24E-05	-8.91E-10	9.36E-08	-3.28E-06	4.24E-05	
7VF	-2.55E-09	2.67E-07	-9.08E-06	1.07E-04	-2.55E-09	2.67E-07	-9.08E-06	1.07E-04	
8VF	-2.86E-11	2.98E-09	-1.01E-07	1.21E-06	-2.86E-11	2.98E-09	-1.01E-07	1.21E-06	
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
7F	-6.49E-08	7.27E-06	-4.10E-04	1.73E-02	-6.49E-08	7.27E-06	-4.10E-04	1.73E-02	
8F	-1.25E-09	1.29E-07	-4.33E-06	5.39E-05	-1.25E-09	1.29E-07	-4.33E-06	5.39E-05	
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
3M	3.77E-11	-4.34E-09	1.72E-07	6.76E-07	3.77E-11	-4.34E-09	1.72E-07	6.76E-07	
4M	-4.26E-08	4.64E-06	-2.11E-04	6.22E-03	-4.26E-08	4.64E-06	-2.11E-04	6.22E-03	
5M	-2.18E-07	2.31E-05	-8.70E-04	1.50E-02	-2.18E-07	2.31E-05	-8.70E-04	1.50E-02	
6M	4.02E-06	-3.56E-04	9.46E-03	5.13E-01	4.02E-06	-3.56E-04	9.46E-03	5.13E-01	
7M	-5.14E-07	5.39E-05	-2.37E-03	7.73E-02	-5.14E-07	5.39E-05	-2.37E-03	7.73E-02	
8M	-1.17E-13	-1.10E-10	4.91E-09	3.43E-07	-1.17E-13	-1.10E-10	4.91E-09	3.43E-07	
1S	2.37E-15	-2.11E-13	3.66E-13	3.45E-10	2.37E-15	-2.11E-13	3.66E-13	3.45E-10	
2S	1.59E-12	-1.90E-10	7.15E-09	6.34E-08	1.59E-12	-1.90E-10	7.15E-09	6.34E-08	
3S	-6.48E-08	6.76E-06	-3.01E-04	1.03E-02	-6.48E-08	6.76E-06	-3.01E-04	1.03E-02	
4S	-6.49E-07	6.87E-05	-2.74E-03	6.29E-02	-6.49E-07	6.87E-05	-2.74E-03	6.29E-02	
5S	-2.54E-07	3.01E-05	-1.42E-03	6.75E-02	-2.54E-07	3.01E-05	-1.42E-03	6.75E-02	
6S	-7.85E-07	8.30E-05	-3.23E-03	6.52E-02	-7.85E-07	8.30E-05	-3.23E-03	6.52E-02	
7S	1.02E-11	-1.15E-09	2.87E-08	6.67E-07	1.02E-11	-1.15E-09	2.87E-08	6.67E-07	
8S	1.69E-14	-1.77E-12	2.23E-11	2.19E-09	1.69E-14	-1.77E-12	2.23E-11	2.19E-09	
1P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
2P	1.03E-11	-1.11E-09	6.47E-08	6.56E-08	1.03E-11	-1.11E-09	6.47E-08	6.56E-08	
3P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
4P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
5P	6.71E-07	-3.63E-05	-1.11E-03	4.30E-01	6.71E-07	-3.63E-05	-1.11E-03	4.30E-01	
6P	-5.86E-11	6.03E-09	-2.03E-07	2.52E-06	-5.86E-11	6.03E-09	-2.03E-07	2.52E-06	
7P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	

8P	-6.33E-08	6.91E-06	-2.58E-04	3.89E-03	-6.33E-08	6.91E-06	-2.58E-04	3.89E-03
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-7.76E-14	8.52E-12	-3.46E-10	7.32E-09	-7.76E-14	8.52E-12	-3.46E-10	7.32E-09
GLY	-1.83E-09	1.88E-07	-6.31E-06	7.53E-05	-1.83E-09	1.88E-07	-6.31E-06	7.53E-05

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Table S11. (Continued)

Oxidation path: α -pinene + O(³ P) (day)				Oxidation path: α -pinene + O(³ P) (day)				
NOx level: Low NOx				NOx level: High NOx				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	-2.80E-25	1.90E-23	-1.84E-22	1.55E-20	-1.92E-21	6.10E-20	-5.93E-19	1.71E-18
6VF	-7.56E-17	7.52E-15	-2.42E-13	3.49E-12	-6.49E-14	2.09E-12	-2.07E-11	6.30E-11
7VF	-1.20E-19	1.10E-17	-3.19E-16	6.99E-15	-3.13E-16	9.99E-15	-9.77E-14	2.87E-13
8VF	-3.51E-21	3.19E-19	-8.23E-18	2.08E-16	-6.81E-18	2.18E-16	-2.13E-15	6.35E-15
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	-9.61E-12	9.66E-10	-3.19E-08	4.97E-07	-4.62E-09	1.50E-07	-1.50E-06	4.84E-06
8F	-8.70E-16	8.71E-14	-2.83E-12	4.18E-11	-4.21E-13	1.36E-11	-1.37E-10	4.37E-10
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	-3.54E-18	3.23E-16	7.18E-15	-5.42E-15	-5.11E-17	2.00E-15	-1.14E-14	5.73E-14
4M	-2.49E-12	2.50E-10	-8.23E-09	1.28E-07	-1.20E-09	3.89E-08	-3.91E-07	1.26E-06
5M	-1.50E-12	1.51E-10	-4.95E-09	7.63E-08	-7.49E-10	2.43E-08	-2.44E-07	7.80E-07
6M	-5.89E-09	5.98E-07	-2.01E-05	3.35E-04	-1.93E-06	6.29E-05	-6.42E-04	2.19E-03
7M	-1.33E-10	1.35E-08	-4.50E-07	7.35E-06	-4.46E-08	1.46E-06	-1.48E-05	5.03E-05
8M	-1.27E-18	1.22E-16	2.59E-15	-2.01E-15	-1.02E-17	4.53E-16	-1.29E-15	1.18E-14
1S	1.43E-30	1.31E-28	-1.99E-27	8.50E-27	4.61E-30	-1.46E-29	5.03E-29	7.31E-29
2S	-2.68E-27	2.66E-25	2.05E-25	2.58E-24	-7.40E-26	2.61E-24	-2.35E-23	7.46E-23
3S	-1.88E-11	1.90E-09	-6.34E-08	1.04E-06	-6.28E-09	2.05E-07	-2.09E-06	7.08E-06
4S	-6.55E-11	6.62E-09	-2.21E-07	3.59E-06	-2.19E-08	7.13E-07	-7.27E-06	2.46E-05
5S	-3.21E-11	3.25E-09	-1.08E-07	1.77E-06	-1.09E-08	3.55E-07	-3.62E-06	1.22E-05
6S	-6.15E-17	5.77E-15	1.27E-13	-1.33E-13	-5.24E-16	2.29E-14	-7.25E-14	5.80E-13
7S	-7.89E-19	7.47E-17	1.58E-15	-1.15E-15	-8.43E-18	3.49E-16	-1.52E-15	9.60E-15
8S	-5.53E-22	5.10E-20	1.07E-18	-4.08E-19	-9.32E-21	3.55E-19	-2.24E-18	1.06E-17
1P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6P	-6.05E-19	5.55E-17	-1.62E-15	4.43E-14	-7.17E-16	2.31E-14	-2.28E-13	7.05E-13
7P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

8P	-1.31E-06	1.35E-04	-4.69E-03	8.21E-02	-3.06E-05	1.31E-03	-1.97E-02	1.42E-01
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-1.16E-24	1.02E-22	2.20E-21	-8.43E-23	-4.39E-23	1.53E-21	-1.26E-20	4.63E-20
GLY	-4.65E-18	4.22E-16	-1.21E-14	3.40E-13	-6.00E-15	1.93E-13	-1.90E-12	5.85E-12

¹ The stoichiometric coefficient is calculated by $\alpha = A \times (\text{HC: NO}_x)^3 + B \times (\text{HC: NO}_x)^2 + C \times (\text{HC: NO}_x) + D$, where HC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

Table S12. Stoichiometric coefficient array of oxygenated products from the oxidation of α -pinene in nighttime for UNIPAR model

Oxidation path: α -pinene + OH (night)				Oxidation path: α -pinene + OH (night)				
NOx level: Low NOx				NOx level: High NOx				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	1.90E-09	-2.36E-07	1.02E-05	-2.52E-05	-2.32E-08	5.71E-07	2.19E-06	-6.22E-07
6VF	3.92E-12	-3.49E-10	7.33E-09	1.11E-07	8.12E-11	-3.36E-09	4.44E-08	-2.94E-08
7VF	3.40E-09	-4.35E-07	2.21E-05	-1.12E-05	-1.24E-08	-6.47E-08	2.03E-05	-1.32E-05
8VF	2.31E-10	-3.59E-08	1.90E-06	-6.67E-06	-5.26E-09	1.54E-07	-1.65E-07	3.26E-07
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	-3.00E-08	3.34E-06	-1.51E-04	1.49E-02	6.67E-07	-1.91E-05	7.05E-05	1.43E-02
8F	2.79E-10	-3.88E-08	1.97E-06	2.62E-07	9.85E-10	-6.79E-08	2.35E-06	-1.26E-06
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	-4.63E-11	8.28E-08	-9.62E-07	3.17E-06	2.25E-09	2.35E-09	-7.49E-08	1.51E-07
4M	-6.04E-08	6.32E-06	-2.14E-04	3.07E-02	1.01E-06	-2.61E-05	7.80E-05	2.99E-02
5M	3.62E-08	-2.43E-06	-1.98E-05	1.07E-02	-9.53E-09	-6.54E-06	9.42E-05	1.01E-02
6M	6.90E-07	-6.79E-05	2.20E-03	5.56E-01	-3.59E-05	1.05E-03	-7.93E-03	5.83E-01
7M	9.38E-08	-9.33E-06	2.84E-04	-7.88E-05	-6.02E-07	5.53E-06	2.39E-04	-3.57E-04
8M	4.54E-10	-1.53E-07	1.57E-05	-4.72E-05	-3.41E-08	1.06E-06	2.25E-06	-1.26E-06
1S	6.51E-08	-7.74E-06	3.57E-04	-4.82E-04	-4.44E-07	7.18E-06	2.28E-04	-1.74E-04
2S	7.54E-08	-7.36E-06	2.22E-04	-2.15E-04	-6.67E-07	1.09E-05	1.15E-04	-1.88E-04
3S	8.82E-10	3.76E-07	-4.80E-05	5.43E-03	-3.31E-08	1.54E-07	-2.83E-05	5.31E-03
4S	1.03E-06	-1.05E-04	3.40E-03	-6.87E-03	-1.03E-05	2.16E-04	8.06E-04	-1.35E-03
5S	6.85E-09	-1.15E-06	1.68E-04	1.03E-02	-3.69E-07	1.08E-05	5.17E-05	1.06E-02
6S	8.12E-08	-8.41E-06	3.00E-04	2.19E-02	-2.58E-06	7.25E-05	-4.38E-04	2.38E-02
7S	6.86E-10	-1.30E-07	8.66E-06	3.13E-03	-8.36E-09	1.46E-07	6.12E-06	3.13E-03
8S	8.96E-09	-1.08E-06	4.97E-05	-9.98E-05	-9.15E-08	2.06E-06	1.98E-05	-1.43E-05
1P	-1.41E-08	1.64E-06	-7.09E-05	2.72E-03	6.60E-08	-4.81E-07	-5.60E-05	2.70E-03
2P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3P	1.06E-08	-1.22E-06	5.47E-05	-4.19E-05	-3.92E-08	5.64E-08	4.65E-05	-3.56E-05
4P	1.25E-08	-1.10E-06	3.66E-05	9.99E-03	-1.16E-08	-1.02E-06	4.47E-05	9.93E-03
5P	3.66E-08	-2.50E-06	8.21E-05	2.66E-01	-9.15E-07	2.62E-05	-1.75E-04	2.67E-01
6P	1.55E-08	-1.89E-06	9.19E-05	1.44E-03	-1.58E-07	3.52E-06	4.03E-05	1.59E-03

7P	0.00E+00							
8P	1.34E-07	-1.27E-05	3.58E-04	-2.68E-05	-1.09E-06	1.38E-05	2.67E-04	-4.35E-04
1MA	0.00E+00							
2MA	-5.65E-09	5.69E-07	-1.68E-05	1.73E-03	1.65E-07	-4.59E-06	2.97E-05	1.62E-03
3MA	0.00E+00							
4MA	3.12E-08	-3.56E-06	1.51E-04	-2.12E-04	-2.10E-07	3.45E-06	9.20E-05	-7.31E-05
5MA	0.00E+00							
6MA	0.00E+00							
7MA	0.00E+00							
8MA	0.00E+00							
MGLY	-2.38E-08	2.30E-06	-7.09E-05	1.06E-03	3.31E-07	-5.96E-06	-3.18E-05	1.12E-03
GLY	1.90E-09	-2.72E-07	1.49E-05	-2.48E-05	-2.00E-08	4.23E-07	8.11E-06	-4.88E-06

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Table S12. (Continued)

Oxidation path: α -pinene + O ₃ (night)					Oxidation path: α -pinene + O ₃ (night)				
NO _x level: Low NO _x					NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹	
1VF	-5.18E-10	3.46E-08	2.28E-05	-2.09E-05	-1.16E-08	4.12E-07	1.88E-05	-7.80E-06	
2VF	1.39E-16	1.23E-12	-7.92E-12	2.12E-11	9.48E-15	8.63E-13	-3.30E-12	3.67E-12	
3VF	-1.30E-10	-4.77E-09	2.39E-06	-6.29E-06	-3.79E-09	1.22E-07	1.01E-06	-1.65E-06	
4VF	1.11E-15	9.65E-12	-6.19E-11	1.66E-10	7.40E-14	6.76E-12	-2.58E-11	2.87E-11	
5VF	1.13E-08	-1.15E-06	7.20E-05	1.28E-02	1.33E-06	-4.48E-05	5.21E-04	1.14E-02	
6VF	6.00E-10	-6.35E-08	2.19E-06	1.01E-05	1.02E-08	-4.17E-07	6.29E-06	-4.49E-06	
7VF	6.18E-09	-6.10E-07	2.30E-05	-1.86E-05	-7.74E-09	-4.50E-07	2.54E-05	-4.17E-05	
8VF	-5.77E-12	5.99E-08	5.69E-07	-1.34E-06	-9.91E-10	9.04E-08	2.85E-07	-5.67E-07	
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
4F	2.70E-09	-2.24E-07	-2.24E-07	1.27E-02	1.09E-06	-3.58E-05	3.59E-04	1.16E-02	
5F	-3.08E-10	1.99E-08	1.70E-05	-1.15E-05	-5.07E-09	1.80E-07	1.53E-05	-6.17E-06	
6F	-4.40E-11	3.03E-09	2.60E-06	-5.45E-07	-4.88E-10	1.76E-08	2.45E-06	-9.00E-08	
7F	1.01E-07	-1.04E-05	3.19E-04	4.66E-03	3.80E-06	-1.39E-04	1.72E-03	-6.07E-06	
8F	-9.09E-11	1.24E-08	1.79E-06	-4.07E-06	-2.36E-09	9.05E-08	9.51E-07	-1.29E-06	
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
2M	7.74E-08	-7.49E-06	-5.56E-05	6.69E-02	7.17E-06	-2.43E-04	2.38E-03	5.93E-02	
3M	1.14E-07	-1.16E-05	3.88E-04	4.51E-02	5.45E-06	-1.93E-04	2.32E-03	3.88E-02	
4M	4.54E-08	-4.77E-06	4.46E-04	5.70E-02	6.82E-06	-2.29E-04	2.75E-03	4.98E-02	
5M	1.29E-07	-1.05E-05	-9.76E-04	3.78E-01	2.37E-05	-7.84E-04	6.88E-03	3.54E-01	
6M	-1.10E-07	1.20E-05	-4.13E-04	1.62E-01	1.00E-05	-3.08E-04	2.69E-03	1.53E-01	
7M	-3.67E-09	3.32E-07	2.78E-05	4.81E-02	1.81E-06	-5.88E-05	6.22E-04	4.64E-02	
8M	5.02E-08	-5.12E-06	1.74E-04	1.18E-02	3.23E-06	-1.12E-04	1.30E-03	8.15E-03	
1S	-1.54E-08	1.90E-06	-5.07E-05	3.22E-03	-1.19E-06	4.13E-05	-4.61E-04	4.52E-03	
2S	-2.17E-08	2.21E-06	-7.45E-05	5.92E-03	-1.53E-06	5.31E-05	-6.08E-04	7.62E-03	
3S	2.24E-07	-2.34E-05	7.32E-04	3.79E-02	5.44E-06	-2.10E-04	2.83E-03	3.06E-02	
4S	5.85E-07	-6.05E-05	1.92E-03	1.02E-01	2.52E-05	-9.04E-04	1.10E-02	7.25E-02	
5S	1.11E-07	-1.21E-05	4.41E-04	1.39E-02	4.01E-06	-1.47E-04	1.92E-03	8.98E-03	
6S	5.39E-08	-5.46E-06	1.98E-04	4.46E-02	5.24E-06	-1.78E-04	1.98E-03	3.90E-02	
7S	3.51E-08	-3.58E-06	1.19E-04	1.58E-02	2.77E-06	-9.50E-05	1.07E-03	1.28E-02	
8S	1.10E-13	-1.16E-11	4.13E-10	2.63E-09	2.15E-12	-8.52E-11	1.25E-09	-3.11E-10	
1P	-6.66E-11	4.17E-08	-1.65E-07	4.45E-07	1.01E-10	3.45E-08	-6.85E-08	5.87E-08	
2P	-1.76E-08	-2.10E-06	8.08E-04	-7.19E-04	-2.61E-07	6.19E-06	7.20E-04	-4.30E-04	
3P	-3.57E-10	4.87E-08	5.29E-07	-2.27E-06	-1.92E-09	1.05E-07	-1.02E-07	-8.37E-08	
4P	-7.12E-10	4.74E-07	-1.75E-06	4.79E-06	9.69E-10	3.99E-07	-7.10E-07	5.51E-07	
5P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	
6P	-5.83E-11	1.17E-08	-7.42E-08	1.97E-07	2.84E-11	8.22E-09	-3.15E-08	3.48E-08	
7P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	

8P	2.43E-09	-1.90E-07	1.79E-05	1.65E-04	1.02E-07	-3.71E-06	5.70E-05	3.18E-05
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	6.21E-11	-6.46E-09	2.29E-07	1.48E-06	1.42E-09	-5.49E-08	7.76E-07	-4.14E-07
GLY	-6.00E-11	1.19E-08	1.44E-07	-7.78E-07	-6.05E-10	3.21E-08	-9.10E-08	6.69E-08

Table S12. (Continued)

Oxidation path: α -pinene + NO ₃ (night)				Oxidation path: α -pinene + NO ₃ (night)				
NO _x level: Low NO _x				NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	-2.15E-20	2.42E-18	-9.24E-17	1.29E-15	1.03E-18	-3.16E-17	2.47E-16	2.67E-16
2VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5VF	-8.05E-19	8.12E-17	-2.58E-15	2.69E-14	-8.03E-19	1.54E-16	-4.32E-15	3.63E-14
6VF	-1.18E-18	1.18E-16	-3.69E-15	3.72E-14	-5.65E-18	3.74E-16	-7.79E-15	5.59E-14
7VF	-1.79E-17	1.75E-15	-5.23E-14	4.84E-13	-1.15E-15	4.07E-14	-4.72E-13	1.87E-12
8VF	-1.75E-17	1.71E-15	-5.12E-14	4.74E-13	-1.13E-15	3.98E-14	-4.62E-13	1.83E-12
1F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7F	-1.67E-12	1.79E-10	-6.35E-09	8.06E-08	2.50E-11	-5.99E-10	2.64E-10	6.56E-08
8F	-1.06E-16	1.03E-14	-3.08E-13	2.85E-12	-7.05E-15	2.48E-13	-2.87E-12	1.13E-11
1M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2M	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3M	-2.33E-13	2.52E-11	-9.07E-10	1.22E-08	4.46E-12	-1.16E-10	3.42E-10	9.12E-09
4M	-2.91E-12	3.17E-10	-1.16E-08	1.60E-07	6.28E-11	-1.69E-09	6.70E-09	1.12E-07
5M	-1.10E-11	1.15E-09	-3.99E-08	5.08E-07	-1.48E-10	6.37E-09	-1.03E-07	7.41E-07
6M	-6.10E-06	7.94E-04	-4.04E-02	1.06E+00	1.08E-04	-2.84E-03	-5.07E-03	9.58E-01
7M	-8.05E-11	8.43E-09	-2.90E-07	3.66E-06	-1.17E-09	4.99E-08	-7.86E-07	5.49E-06
8M	-1.32E-19	1.37E-17	-4.59E-16	5.24E-15	1.69E-18	-3.69E-17	-7.10E-17	4.56E-15
1S	-4.98E-23	5.08E-21	-1.65E-19	1.81E-18	1.21E-22	3.81E-21	-2.11E-19	2.19E-18
2S	-1.71E-14	1.95E-12	-7.79E-11	1.24E-09	5.61E-13	-1.64E-11	9.99E-11	7.30E-10
3S	-3.01E-11	3.02E-09	-9.48E-08	9.65E-07	-9.58E-10	3.60E-08	-4.63E-07	2.23E-06
4S	-3.45E-08	3.47E-06	-1.10E-04	1.17E-03	-2.45E-06	8.49E-05	-9.66E-04	3.91E-03
5S	-1.80E-07	3.05E-05	-2.19E-03	9.30E-02	1.28E-05	-3.98E-04	2.22E-03	7.93E-02
6S	-6.38E-11	6.77E-09	-2.39E-07	3.17E-06	-5.16E-10	2.57E-08	-4.88E-07	4.16E-06
7S	-8.43E-21	8.23E-19	-2.47E-17	2.29E-16	-5.69E-19	2.00E-17	-2.31E-16	9.09E-16
8S	-5.41E-24	5.47E-22	-1.74E-20	1.84E-19	-1.03E-23	1.20E-21	-3.06E-20	2.52E-19
1P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2P	-2.73E-06	3.69E-04	-1.97E-02	5.52E-01	7.42E-05	-2.12E-03	5.13E-03	4.78E-01
3P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5P	-1.44E-06	1.78E-04	-8.51E-03	2.21E-01	-1.53E-06	2.26E-04	-9.61E-03	2.27E-01
6P	-1.47E-19	1.45E-17	-4.46E-16	4.34E-15	-8.40E-18	2.97E-16	-3.48E-15	1.43E-14
7P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

8P	-1.77E-12	1.89E-10	-6.65E-09	8.37E-08	2.49E-11	-5.82E-10	-2.12E-10	6.96E-08
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	-4.30E-20	4.41E-18	-1.45E-16	1.59E-15	3.55E-19	-5.24E-18	-9.28E-17	1.62E-15
GLY	-9.38E-20	9.85E-18	-3.36E-16	3.94E-15	1.65E-18	-4.13E-17	1.02E-16	2.93E-15

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¹ The stoichiometric coefficient is calculated by $\alpha = A \times (\text{HC: NO}_x)^3 + B \times (\text{HC: NO}_x)^2 + C \times (\text{HC: NO}_x) + D$, where HC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

(c) β -caryophyllene235 Table S13. Stoichiometric coefficient array of oxygenated products from the oxidation of β -caryophyllene under the sunlight for UNIPAR model

Oxidation path: β -caryophyllene + OH (day)					Oxidation path: β -caryophyllene + OH (day)			
Lumped species	NOx level: Low NOx				NOx level: High NOx			
	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	3.41E-12	3.13E-10	-9.50E-09	7.05E-08	7.99E-12	-9.07E-11	4.09E-10	-5.03E-10
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	1.83E-10	3.06E-09	-1.76E-07	1.52E-06	1.88E-10	-2.31E-09	9.65E-09	-1.18E-08
5VF	-4.26E-09	4.08E-07	-6.27E-06	1.71E-04	1.33E-07	-2.83E-06	2.55E-05	9.93E-06
6VF	-1.41E-11	-1.14E-09	2.18E-07	5.14E-06	6.10E-09	-1.40E-07	1.17E-06	3.21E-06
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	6.58E-13	2.61E-09	-6.39E-08	4.37E-07	5.69E-11	-6.43E-10	2.64E-09	-3.20E-09
2F	5.02E-12	9.53E-10	-2.63E-08	1.87E-07	2.19E-11	-2.68E-10	1.16E-09	-1.44E-09
3F	1.60E-11	4.71E-10	-1.96E-08	1.58E-07	1.71E-11	-1.77E-10	8.29E-10	-1.04E-09
4F	1.25E-08	-1.69E-06	6.52E-05	4.59E-03	2.32E-06	-5.77E-05	5.14E-04	3.29E-03
5F	2.98E-09	-1.05E-07	-1.14E-05	1.01E-03	1.77E-08	-2.21E-06	-3.02E-05	1.54E-03
6F	-7.35E-10	6.27E-08	-7.10E-07	8.37E-05	6.45E-08	-1.48E-06	1.43E-05	9.81E-06
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	7.66E-08	-1.02E-05	4.41E-04	6.25E-03	3.39E-06	-7.85E-05	1.05E-03	2.89E-03
1M	1.44E-09	2.96E-07	-7.36E-06	2.17E-04	1.29E-07	-3.09E-06	2.77E-05	5.88E-05
2M	-9.17E-09	1.29E-06	-2.81E-05	7.98E-04	4.61E-07	-1.04E-05	1.01E-04	1.00E-04
3M	1.22E-09	2.97E-09	-6.65E-07	2.29E-05	1.56E-08	-3.72E-07	3.15E-06	5.77E-06
4M	2.04E-06	-2.19E-04	5.99E-03	2.21E-01	4.52E-05	-1.21E-03	9.79E-03	2.46E-01
5M	7.04E-07	-5.50E-05	3.72E-05	7.89E-02	-1.79E-04	4.20E-03	-3.81E-02	2.38E-01
6M	-7.85E-08	6.71E-06	-3.26E-05	9.81E-03	3.98E-06	-9.08E-05	1.02E-03	3.96E-03
7M	-6.75E-08	6.09E-06	-7.79E-05	5.43E-03	3.67E-06	-8.44E-05	8.00E-04	1.33E-03
8M	-4.48E-07	4.19E-05	-8.56E-04	8.49E-02	4.99E-05	-1.18E-03	1.04E-02	3.77E-02
1S	-1.61E-07	1.74E-05	-2.59E-04	2.05E-02	1.36E-05	-3.25E-04	3.13E-03	4.91E-03
2S	3.17E-07	-3.35E-05	8.82E-04	7.54E-02	1.66E-05	-4.64E-04	4.00E-03	7.24E-02
3S	1.53E-07	-1.39E-05	3.24E-04	1.57E-02	6.14E-06	-1.60E-04	1.14E-03	1.69E-02
4S	6.49E-07	-6.59E-05	1.61E-03	4.41E-02	-1.43E-05	2.67E-04	-2.36E-03	7.09E-02
5S	4.82E-09	1.61E-07	-1.18E-05	2.90E-04	-2.36E-05	5.82E-04	-4.61E-03	1.24E-02
6S	-8.15E-08	7.39E-06	-7.24E-05	1.05E-03	5.49E-07	-3.10E-06	3.95E-05	6.32E-06
7S	-1.88E-08	1.73E-06	-2.15E-05	2.23E-04	9.40E-08	-2.02E-07	2.01E-06	-1.19E-06
8S	-2.71E-08	2.97E-06	-7.20E-05	1.73E-03	9.76E-07	-2.14E-05	1.99E-04	1.97E-04
1P	1.09E-11	1.40E-09	-1.79E-08	1.22E-07	1.85E-11	5.32E-10	1.62E-09	-2.14E-09
2P	6.17E-11	-3.82E-09	2.53E-07	-1.98E-06	-2.55E-10	7.83E-09	1.81E-09	-5.26E-09
3P	2.43E-13	-1.09E-11	9.91E-10	-7.76E-09	-9.87E-13	3.47E-11	7.46E-12	-1.89E-11
4P	3.97E-11	4.39E-09	-1.27E-07	9.34E-07	1.24E-10	-1.41E-09	5.94E-09	-7.22E-09

5P	-1.21E-08	1.06E-06	-2.28E-06	1.02E-04	7.30E-08	3.02E-07	1.41E-06	4.73E-07
6P	-1.32E-07	1.07E-05	-1.08E-05	1.45E-03	9.16E-07	-6.70E-07	7.50E-05	2.64E-05
7P	-9.90E-09	1.05E-06	-2.62E-05	8.95E-04	5.14E-07	-1.18E-05	1.06E-04	2.35E-04
8P	-4.95E-09	1.69E-07	5.49E-05	5.13E-04	3.00E-08	3.04E-06	4.41E-05	1.18E-04
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	-3.86E-09	3.91E-07	-6.62E-06	1.23E-04	6.39E-08	-1.25E-06	1.26E-05	4.94E-06

Table S13. (Continued)

Oxidation path: β -caryophyllene + O ₃ (day)				Oxidation path: β -caryophyllene + O ₃ (day)				
NO _x level: Low NO _x				NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	5.59E-12	-8.81E-10	4.41E-08	-2.73E-07	1.10E-10	-9.63E-11	-3.80E-09	7.89E-09
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	8.14E-09	-1.19E-06	5.54E-05	-4.00E-04	1.67E-07	-1.62E-06	4.73E-06	-4.25E-06
5VF	1.81E-08	-1.81E-06	4.05E-05	3.67E-04	-6.28E-07	1.35E-05	-2.64E-05	7.60E-05
6VF	3.59E-12	-3.76E-10	7.97E-09	1.67E-07	-1.56E-10	2.12E-09	1.41E-08	9.32E-09
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	6.01E-10	7.71E-08	-2.19E-06	1.59E-05	-6.86E-10	2.89E-08	-1.36E-07	1.65E-07
2F	1.05E-09	-5.23E-09	-1.58E-07	2.21E-06	-2.34E-10	2.09E-08	-1.20E-07	1.65E-07
3F	1.44E-10	-1.58E-08	6.67E-07	-4.48E-06	2.27E-09	-2.17E-08	6.15E-08	-5.32E-08
4F	-1.08E-07	1.16E-05	-2.65E-04	3.27E-03	1.01E-05	-2.21E-04	1.07E-03	3.09E-03
5F	1.07E-08	-1.46E-06	5.77E-05	3.76E-04	-1.19E-05	3.02E-04	-2.37E-03	6.38E-03
6F	-1.84E-08	1.83E-06	-3.62E-05	4.31E-04	1.11E-06	-2.65E-05	1.67E-04	1.25E-04
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	-2.24E-07	2.24E-05	-5.27E-04	1.26E-02	2.18E-05	-5.94E-04	4.65E-03	1.17E-03
1M	-2.57E-08	3.90E-06	5.37E-05	-5.88E-04	6.88E-07	-5.10E-06	9.97E-06	-3.42E-06
2M	1.51E-08	-1.09E-06	1.66E-04	-1.86E-05	-1.67E-08	1.42E-05	-1.27E-04	1.35E-03
3M	-6.49E-08	6.90E-06	-7.61E-05	1.16E-03	3.65E-06	-6.21E-05	2.60E-05	3.45E-03
4M	-1.95E-06	1.96E-04	-3.80E-03	8.10E-02	2.15E-04	-4.44E-03	1.78E-02	1.15E-01
5M	-1.21E-07	1.31E-05	-3.38E-04	9.98E-03	-2.59E-04	6.67E-03	-5.53E-02	1.58E-01
6M	2.17E-07	-2.46E-05	6.50E-04	2.61E-02	-9.25E-06	7.37E-05	1.95E-03	1.28E-02
7M	-4.71E-08	6.52E-06	-4.33E-04	3.48E-02	-5.41E-06	-1.94E-04	5.86E-03	-2.67E-03
8M	-4.68E-07	4.27E-05	-1.51E-03	9.35E-02	6.72E-05	-2.27E-03	2.34E-02	1.07E-02
1S	1.66E-06	-2.13E-04	8.98E-03	-2.73E-02	2.85E-05	-5.09E-04	5.85E-03	6.38E-03
2S	-2.29E-06	2.28E-04	-5.14E-03	1.74E-01	3.32E-05	5.05E-05	-1.75E-02	2.88E-01
3S	6.02E-07	-8.99E-05	4.58E-03	-3.31E-02	1.54E-05	-1.47E-04	4.23E-04	-3.73E-04
4S	-3.22E-06	3.37E-04	-7.22E-03	1.20E-01	3.97E-04	-8.88E-03	4.72E-02	1.03E-01
5S	5.16E-07	-6.10E-05	2.33E-03	-1.60E-02	7.26E-06	-8.06E-05	2.80E-04	-3.01E-04
6S	2.46E-07	-1.71E-05	-2.41E-04	2.63E-02	-5.60E-05	1.21E-03	-5.30E-03	6.66E-03
7S	5.49E-08	-3.66E-06	-4.86E-05	4.41E-03	-8.63E-06	1.92E-04	-8.67E-04	1.08E-03
8S	3.19E-07	-3.49E-05	1.05E-03	-3.08E-03	-1.45E-07	2.19E-05	1.61E-04	1.44E-04
1P	-4.80E-08	9.44E-06	-1.76E-04	1.06E-03	7.90E-08	1.10E-06	-8.43E-06	1.25E-05
2P	9.40E-09	-4.16E-07	6.22E-06	-3.09E-05	8.55E-11	-1.10E-09	1.60E-08	-2.42E-08
3P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4P	-2.01E-10	-1.11E-07	1.74E-05	-1.42E-04	7.10E-08	-6.29E-07	1.63E-06	-1.24E-06
5P	8.66E-08	-9.55E-06	3.24E-04	-4.10E-04	-3.94E-04	1.03E-02	-8.69E-02	2.37E-01
6P	1.53E-07	-4.52E-06	-8.59E-04	4.30E-02	-9.17E-05	1.87E-03	-7.31E-03	8.45E-03
7P	4.06E-08	-4.33E-06	1.15E-04	5.47E-04	1.61E-07	-6.32E-06	1.52E-04	1.75E-04

8P	3.31E-07	-3.73E-05	1.26E-03	-4.22E-05	-4.71E-06	8.01E-05	6.23E-04	-7.02E-04
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	5.89E-08	-6.02E-06	1.56E-04	1.32E-04	-1.27E-06	3.40E-05	-1.42E-04	2.18E-04

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Table S13. (Continued)

Oxidation path: β -caryophyllene + NO ₃ (day)				Oxidation path: β -caryophyllene + NO ₃ (day)				
NO _x level: Low NO _x				NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	-2.61E-17	3.63E-15	-6.94E-14	3.87E-13	4.94E-17	-5.34E-16	1.99E-15	-2.31E-15
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	1.38E-16	3.98E-14	-1.04E-12	6.81E-12	4.93E-16	-6.21E-15	2.51E-14	-3.04E-14
5VF	-1.21E-10	1.08E-08	-6.58E-08	-1.31E-07	3.86E-10	-2.11E-09	6.18E-09	-4.99E-09
6VF	-1.92E-13	1.54E-11	-2.48E-11	-8.74E-10	7.32E-13	-4.63E-12	1.30E-11	-1.12E-11
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	-4.42E-15	4.50E-13	-7.07E-12	3.31E-11	8.20E-15	-8.31E-14	2.98E-13	-3.38E-13
2F	-4.23E-17	4.60E-15	-6.78E-14	3.10E-13	8.86E-17	-6.09E-16	1.85E-15	-1.89E-15
3F	-3.01E-17	1.85E-14	-4.56E-13	2.96E-12	1.51E-16	-1.95E-15	7.98E-15	-9.74E-15
4F	2.08E-09	-3.32E-07	1.59E-05	-1.02E-04	-4.34E-09	4.73E-07	-1.44E-06	2.00E-06
5F	2.56E-09	-2.56E-07	6.23E-06	1.35E-05	-4.01E-08	7.11E-07	1.78E-06	9.19E-07
6F	-3.15E-11	-3.14E-10	2.22E-07	-1.89E-06	3.12E-10	1.53E-09	-6.56E-09	1.20E-08
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	1.47E-09	-2.67E-07	1.43E-05	-6.12E-05	-1.09E-08	3.88E-07	3.07E-06	1.11E-06
1M	-2.89E-12	2.66E-10	-2.27E-09	2.66E-09	8.16E-12	-4.53E-11	1.26E-10	-1.08E-10
2M	-2.42E-10	2.65E-08	-4.47E-07	2.30E-06	3.85E-10	-3.27E-09	1.26E-08	-1.40E-08
3M	1.78E-11	-2.55E-09	1.09E-07	-6.84E-07	-3.71E-11	3.19E-09	-9.94E-09	1.36E-08
4M	2.71E-07	-3.19E-05	1.07E-03	-3.08E-03	-2.87E-06	6.51E-05	8.49E-05	1.34E-04
5M	9.12E-09	-1.40E-06	6.68E-05	-3.52E-04	-7.61E-08	2.93E-06	-2.82E-06	8.94E-06
6M	-1.83E-09	1.26E-07	4.31E-06	-2.59E-05	9.18E-11	2.23E-07	6.82E-07	5.54E-07
7M	3.29E-11	-8.07E-09	5.32E-07	-2.41E-06	-3.52E-10	1.53E-08	1.03E-07	5.70E-08
8M	2.61E-08	-3.97E-06	1.89E-04	-7.11E-04	-2.27E-07	6.72E-06	3.56E-05	3.27E-05
1S	-3.45E-09	8.34E-08	2.10E-05	-1.53E-04	6.90E-09	7.36E-07	-1.19E-06	2.53E-06
2S	2.14E-08	-2.61E-06	9.08E-05	-3.15E-04	-1.34E-07	3.31E-06	1.47E-05	1.40E-05
3S	-1.16E-13	4.56E-11	-9.92E-10	5.97E-09	6.39E-13	-6.79E-12	2.56E-11	-2.99E-11
4S	8.44E-09	-1.17E-06	5.14E-05	-2.17E-04	-9.49E-08	2.74E-06	7.20E-07	6.66E-06
5S	9.96E-16	9.70E-12	-1.85E-10	1.06E-09	1.92E-13	-9.11E-13	2.94E-12	-3.13E-12
6S	-3.86E-11	3.56E-09	-1.43E-08	-8.38E-08	1.26E-10	-2.10E-10	3.92E-10	1.49E-09
7S	-1.73E-11	1.67E-09	-2.24E-08	8.71E-08	3.85E-11	-3.50E-10	1.23E-09	-1.33E-09
8S	-5.36E-10	4.19E-08	7.11E-07	-5.94E-06	8.61E-10	4.09E-08	2.09E-08	1.41E-07
1P	-3.06E-16	2.76E-14	-5.58E-14	-1.20E-12	1.07E-15	-1.28E-15	-6.31E-15	1.40E-14
2P	-2.75E-16	2.23E-14	4.06E-14	-1.75E-12	9.99E-16	-1.02E-15	-6.81E-15	1.43E-14
3P	1.91E-07	-2.26E-05	7.48E-04	4.63E-03	-5.16E-08	-4.00E-05	1.28E-03	1.15E-03
4P	-3.06E-15	2.61E-13	2.95E-13	-1.69E-11	9.33E-15	3.76E-14	-2.09E-13	2.89E-13
5P	-8.78E-12	5.15E-10	1.45E-08	-1.60E-07	4.72E-11	-3.53E-11	-1.55E-10	9.01E-10
6P	-2.36E-10	2.09E-08	1.00E-07	-1.46E-06	4.04E-10	1.34E-08	-2.85E-08	6.49E-08
7P	-7.87E-11	-2.41E-09	1.05E-06	-5.23E-06	-6.21E-10	4.23E-08	1.47E-07	1.93E-07

8P	2.12E-10	-2.65E-08	9.93E-07	-4.51E-07	-2.33E-09	3.50E-08	5.82E-07	-9.54E-10
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	-4.45E-11	4.03E-09	5.88E-09	-2.11E-07	9.94E-11	1.60E-09	-3.43E-09	7.06E-09

¹ The stoichiometric coefficient is calculated by $\alpha = A \times (\text{HC: NO}_x)^3 + B \times (\text{HC: NO}_x)^2 + C \times (\text{HC: NO}_x) + D$, where HC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

Table S14. Stoichiometric coefficient array of oxygenated products from the oxidation of β -caryophyllene in nighttime for UNIPAR model

Oxidation path: β -caryophyllene + OH (night)				Oxidation path: β -caryophyllene + OH (night)				
NOx level: Low NOx				NOx level: High NOx				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	-1.24E-11	1.24E-09	-2.34E-08	1.92E-06	4.13E-09	-7.99E-08	3.44E-07	2.05E-06
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	4.16E-12	-7.13E-10	5.16E-08	-6.22E-08	1.11E-10	-1.68E-10	3.26E-09	2.56E-07
5VF	4.01E-12	-6.95E-10	5.07E-08	-5.65E-08	1.13E-10	-2.71E-10	4.46E-09	2.51E-07
6VF	3.55E-13	-5.16E-11	2.80E-09	3.15E-08	8.87E-11	-2.32E-09	2.15E-08	-1.90E-08
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	1.48E-13	-2.02E-11	1.37E-09	-1.11E-09	-6.57E-12	1.25E-10	6.04E-10	-1.35E-09
2F	1.15E-09	-1.39E-07	5.98E-06	4.31E-04	1.16E-06	-2.71E-05	1.98E-04	1.91E-05
3F	7.51E-10	-1.00E-07	5.03E-06	4.43E-04	1.16E-06	-2.71E-05	1.99E-04	1.62E-05
4F	7.47E-10	-1.02E-07	5.36E-06	1.97E-04	6.23E-07	-1.44E-05	1.05E-04	-3.76E-06
5F	6.26E-12	-7.64E-10	3.05E-08	1.22E-07	2.23E-10	-7.13E-09	9.18E-08	-7.11E-08
6F	8.70E-14	-1.41E-11	8.46E-10	-1.61E-09	-1.93E-12	3.00E-11	5.48E-10	-8.90E-10
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	8.65E-09	-1.12E-06	5.69E-05	1.32E-03	4.02E-06	-9.30E-05	6.89E-04	3.44E-05
1M	4.18E-09	-5.24E-07	2.49E-05	2.10E-04	3.30E-07	-9.65E-06	1.14E-04	-1.12E-04
2M	-1.04E-08	1.37E-06	-4.20E-05	4.42E-03	1.16E-05	-2.84E-04	2.19E-03	-1.27E-03
3M	3.26E-09	-4.44E-07	2.70E-05	7.32E-04	2.15E-06	-5.06E-05	3.84E-04	-3.94E-05
4M	1.48E-07	-1.96E-05	9.29E-04	4.27E-02	1.27E-04	-2.91E-03	2.07E-02	2.99E-03
5M	2.79E-09	-2.92E-07	1.76E-05	6.83E-05	9.69E-07	-2.18E-05	1.57E-04	-1.77E-04
6M	-1.51E-11	-2.34E-09	1.11E-06	-3.52E-06	4.09E-10	1.01E-08	6.53E-07	-4.92E-07
7M	5.02E-09	-5.98E-07	1.92E-05	4.85E-04	3.19E-07	-9.29E-06	1.00E-04	2.18E-04
8M	2.93E-10	-4.21E-08	2.27E-06	1.02E-05	2.33E-08	-5.29E-07	5.06E-06	7.31E-06
1S	2.50E-09	-3.42E-07	1.71E-05	1.81E-04	4.38E-07	-1.12E-05	1.04E-04	-4.82E-05
2S	1.14E-08	-1.51E-06	7.37E-05	6.48E-03	1.67E-05	-3.89E-04	2.83E-03	5.42E-04
3S	5.55E-08	-7.05E-06	3.12E-04	8.50E-03	2.22E-05	-5.40E-04	4.36E-03	-1.46E-03
4S	3.71E-08	-4.74E-06	2.17E-04	1.86E-02	4.82E-05	-1.13E-03	8.15E-03	1.60E-03
5S	1.02E-10	-1.49E-08	1.50E-06	-1.44E-06	3.79E-09	-1.01E-07	2.11E-06	-2.72E-06
6S	7.44E-11	-9.96E-09	4.18E-07	1.13E-06	-2.32E-09	4.29E-08	8.48E-08	1.65E-06
7S	2.33E-15	-6.10E-13	4.72E-11	-2.18E-10	-1.63E-13	4.45E-12	-9.94E-12	2.61E-11
8S	-1.76E-14	1.02E-12	7.93E-11	-3.46E-10	2.57E-14	1.57E-12	3.95E-11	-1.76E-11
1P	1.98E-10	-2.55E-08	1.16E-06	3.45E-06	8.42E-09	-2.45E-07	3.17E-06	-3.38E-06
2P	1.03E-06	-1.23E-04	4.86E-03	9.98E-02	2.57E-04	-6.58E-03	5.77E-02	-4.68E-02
3P	9.75E-08	-1.19E-05	4.98E-04	1.86E-02	5.06E-05	-1.23E-03	9.71E-03	-3.84E-03
4P	-1.29E-13	1.38E-11	5.36E-10	-3.05E-09	-9.22E-13	5.08E-11	-4.40E-11	-2.83E-11
5P	-1.55E-13	1.35E-11	8.71E-10	-4.16E-09	-1.44E-12	6.52E-11	1.13E-10	-2.50E-10
6P	6.53E-10	-8.85E-08	4.04E-06	1.11E-05	4.92E-09	-1.74E-07	4.46E-06	1.11E-05

7P	7.28E-17	-4.90E-15	2.33E-13	1.08E-12	-2.24E-15	4.66E-14	-8.64E-14	1.49E-12
8P	1.83E-09	-2.30E-07	1.12E-05	5.31E-04	1.41E-06	-3.34E-05	2.52E-04	-1.16E-05
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	1.17E-11	-1.49E-09	6.19E-08	9.47E-08	1.18E-10	-5.56E-09	1.09E-07	-6.56E-08

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Table S14. (Continued)

Oxidation path: β -caryophyllene + O ₃ (night)				Oxidation path: β -caryophyllene + O ₃ (night)				
NO _x level: Low NO _x				NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	3.33E-14	-3.40E-12	8.20E-11	9.18E-10	-4.25E-12	7.68E-11	-2.06E-10	2.14E-10
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	3.98E-10	-3.86E-08	7.12E-07	3.69E-05	1.87E-08	-7.12E-07	9.01E-06	2.49E-06
5VF	3.55E-10	-3.35E-08	5.28E-07	3.86E-05	1.28E-08	-6.09E-07	8.61E-06	2.91E-06
6VF	4.26E-17	3.45E-15	1.88E-13	1.34E-11	-3.65E-14	6.32E-13	-1.01E-12	1.99E-13
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	5.64E-10	-9.84E-08	7.33E-06	6.40E-05	3.54E-07	-7.93E-06	5.86E-05	-3.32E-05
2F	3.61E-09	-5.33E-07	2.58E-05	7.49E-03	3.57E-05	-7.28E-04	3.91E-03	4.00E-03
3F	2.64E-10	-6.60E-08	6.50E-06	8.16E-05	4.48E-07	-9.33E-06	5.77E-05	2.74E-05
4F	9.60E-09	-1.78E-06	1.28E-04	1.12E-02	6.99E-05	-1.45E-03	8.33E-03	1.43E-03
5F	-1.58E-09	2.42E-07	-1.11E-05	2.46E-04	1.48E-06	-3.29E-05	2.07E-04	-1.61E-04
6F	-4.66E-10	6.58E-08	-2.99E-06	1.08E-04	-2.89E-07	5.24E-06	-2.09E-05	7.45E-05
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	1.33E-08	-2.47E-06	1.90E-04	9.87E-04	3.64E-05	-7.44E-04	4.18E-03	-2.76E-03
1M	3.34E-08	-4.72E-06	2.69E-04	4.39E-03	1.78E-05	-4.02E-04	2.92E-03	-9.33E-04
2M	4.52E-08	-6.51E-06	3.72E-04	1.49E-02	6.72E-05	-1.43E-03	8.85E-03	2.65E-03
3M	1.98E-08	-3.19E-06	2.61E-04	7.05E-03	2.99E-05	-6.35E-04	3.97E-03	1.93E-03
4M	1.77E-07	-3.46E-05	2.67E-03	2.05E-02	9.99E-04	-2.05E-02	1.14E-01	-9.24E-02
5M	1.75E-09	8.58E-08	-1.14E-05	7.83E-03	4.33E-05	-8.93E-04	4.93E-03	2.48E-03
6M	4.33E-09	-4.04E-07	1.81E-05	3.68E-04	-1.32E-06	2.29E-05	-4.87E-05	9.02E-05
7M	-2.60E-08	4.41E-06	-2.99E-04	1.71E-02	-4.08E-05	8.03E-04	-4.14E-03	1.84E-02
8M	-9.33E-09	1.52E-06	-8.44E-05	2.42E-03	-6.83E-06	1.21E-04	-4.32E-04	1.17E-03
1S	2.70E-08	-2.85E-06	1.36E-04	3.54E-02	3.24E-06	-2.93E-04	4.98E-03	1.35E-02
2S	-1.19E-08	1.72E-06	-9.26E-05	9.21E-02	4.24E-04	-8.72E-03	4.78E-02	4.15E-02
3S	2.00E-08	-2.01E-06	4.74E-05	4.59E-03	-1.35E-05	2.41E-04	-7.48E-04	2.53E-03
4S	1.79E-07	-2.14E-05	7.87E-04	3.43E-01	5.18E-04	-1.12E-02	6.99E-02	2.33E-01
5S	1.84E-09	-1.90E-07	2.70E-05	-4.81E-07	-3.11E-07	6.24E-06	-7.88E-06	3.14E-05
6S	-2.87E-08	3.55E-06	-1.44E-04	2.14E-03	-7.40E-06	1.31E-04	-5.17E-04	1.03E-03
7S	-4.14E-11	4.94E-09	-1.86E-07	2.44E-06	-3.66E-09	4.24E-08	1.15E-07	-3.41E-07
8S	7.55E-12	-3.03E-10	-3.06E-08	1.72E-06	-4.51E-09	7.54E-08	-1.55E-07	9.46E-08
1P	9.73E-08	-1.32E-05	7.36E-04	1.33E-02	4.81E-05	-1.10E-03	8.19E-03	-2.50E-03
2P	-1.17E-09	1.74E-07	1.81E-06	-9.86E-06	-6.63E-09	3.53E-07	-3.89E-07	2.90E-07
3P	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4P	1.28E-10	-6.04E-09	1.22E-06	-9.29E-07	1.12E-09	-2.32E-08	1.26E-06	-6.71E-07
5P	-1.34E-07	1.59E-05	-6.12E-04	1.72E-02	8.88E-04	-1.78E-02	9.01E-02	-4.39E-02
6P	-4.82E-08	6.19E-06	-2.61E-04	4.60E-03	-1.47E-05	2.60E-04	-1.00E-03	2.20E-03
7P	3.73E-14	1.08E-12	-2.30E-11	1.67E-09	-7.84E-12	1.47E-10	-5.89E-10	1.04E-09

8P	-1.44E-11	-3.54E-08	-2.94E-06	1.15E-02	2.19E-05	-4.69E-04	2.83E-03	7.26E-03
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	-4.29E-10	5.55E-08	-1.99E-06	5.35E-05	-1.56E-07	2.70E-06	-8.86E-06	2.36E-05

Table S14. (Continued)

Oxidation path: β -caryophyllene + NO ₃ (night)				Oxidation path: β -caryophyllene + NO ₃ (night)				
NO _x level: Low NO _x				NO _x level: High NO _x				
Lumped species	A ¹	B ¹	C ¹	D ¹	A ¹	B ¹	C ¹	D ¹
1VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2VF	-3.55E-22	4.45E-20	-1.87E-18	3.00E-17	8.73E-20	-2.32E-18	1.87E-17	-2.84E-17
3VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4VF	-6.06E-16	7.07E-14	-2.60E-12	3.25E-11	1.03E-13	-2.57E-12	1.82E-11	-1.54E-11
5VF	-5.96E-16	6.97E-14	-2.56E-12	3.20E-11	1.02E-13	-2.53E-12	1.79E-11	-1.51E-11
6VF	-1.89E-24	2.32E-22	-9.34E-21	1.38E-19	1.42E-21	-3.22E-20	2.12E-19	-2.88E-19
7VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8VF	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1F	4.49E-17	-3.79E-15	1.56E-14	3.89E-12	-3.78E-15	5.11E-14	2.05E-13	2.96E-13
2F	-4.94E-14	7.59E-12	-4.35E-10	1.11E-08	-1.10E-11	1.83E-10	-5.64E-10	6.29E-09
3F	-2.67E-15	5.41E-13	-3.85E-11	1.09E-09	-4.98E-13	1.49E-12	1.14E-10	-2.18E-11
4F	-8.10E-13	1.01E-10	-4.20E-09	6.99E-08	5.92E-10	-1.36E-08	8.97E-08	-1.12E-07
5F	-4.29E-12	5.44E-10	-2.39E-08	4.48E-07	3.15E-09	-7.12E-08	4.56E-07	-4.31E-07
6F	-2.68E-18	4.52E-16	-2.88E-14	8.19E-13	3.72E-15	-8.96E-14	6.57E-13	-8.75E-13
7F	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8F	-4.47E-09	5.49E-07	-2.26E-05	3.82E-04	2.57E-06	-5.71E-05	3.50E-04	-2.31E-04
1M	-1.03E-11	1.82E-09	-1.20E-07	3.41E-06	-8.60E-09	1.84E-07	-1.17E-06	4.52E-06
2M	-1.39E-09	1.95E-07	-9.95E-06	2.34E-04	-7.45E-07	1.64E-05	-1.11E-04	3.86E-04
3M	-1.38E-09	1.92E-07	-9.79E-06	2.29E-04	-7.40E-07	1.64E-05	-1.11E-04	3.84E-04
4M	-1.45E-07	1.75E-05	-6.91E-04	1.05E-02	7.72E-05	-1.70E-03	1.03E-02	-6.85E-03
5M	-6.32E-12	8.09E-10	-3.60E-08	6.90E-07	4.32E-09	-9.84E-08	6.39E-07	-5.99E-07
6M	-4.90E-13	7.59E-11	-4.87E-09	1.78E-07	3.75E-10	-8.71E-09	5.81E-08	3.82E-08
7M	-1.62E-11	2.03E-09	-8.53E-08	1.43E-06	1.20E-08	-2.74E-07	1.80E-06	-2.20E-06
8M	-3.76E-13	4.89E-11	-2.30E-09	5.37E-08	2.33E-10	-5.20E-09	3.21E-08	-7.28E-09
1S	-5.78E-07	7.14E-05	-2.98E-03	5.28E-02	-7.14E-04	1.68E-02	-1.23E-01	3.19E-01
2S	-1.14E-12	1.45E-10	-6.52E-09	1.57E-07	5.75E-10	-1.24E-08	7.09E-08	4.41E-08
3S	-1.46E-10	1.93E-08	-9.03E-07	1.84E-05	7.25E-08	-1.69E-06	1.14E-05	-8.10E-06
4S	-1.58E-12	2.30E-10	-1.33E-08	4.68E-07	8.02E-10	-1.94E-08	1.37E-07	1.00E-07
5S	1.38E-13	-1.19E-11	-1.65E-10	4.99E-08	-1.70E-10	3.69E-09	-2.28E-08	8.25E-08
6S	-1.51E-15	2.00E-13	-9.54E-12	2.01E-10	1.41E-12	-3.25E-11	2.19E-10	-2.69E-10
7S	2.71E-22	-1.99E-20	-6.09E-19	7.36E-17	4.51E-19	-1.06E-17	7.66E-17	-1.03E-16
8S	3.37E-20	-2.79E-18	-4.27E-17	1.00E-14	1.38E-17	-3.71E-16	3.34E-15	-1.16E-15
1P	8.94E-20	-1.30E-17	6.74E-16	1.59E-15	-7.32E-18	1.39E-16	-1.07E-16	1.82E-15
2P	3.48E-20	-5.04E-18	2.54E-16	6.30E-16	-2.87E-18	5.49E-17	-5.48E-17	7.28E-16
3P	-1.10E-07	1.36E-05	-5.69E-04	1.01E-02	-1.21E-04	2.87E-03	-2.14E-02	5.77E-02
4P	-3.67E-21	4.55E-19	-1.92E-17	3.42E-16	1.55E-18	-3.89E-17	2.93E-16	-4.30E-16
5P	-4.63E-17	6.03E-15	-2.71E-13	4.90E-12	2.13E-14	-5.01E-13	3.41E-12	-3.23E-12
6P	-2.46E-13	3.97E-11	-2.62E-09	9.81E-08	1.20E-10	-3.12E-09	2.45E-08	2.09E-08
7P	-1.23E-20	1.59E-18	-7.06E-17	1.22E-15	7.58E-18	-1.67E-16	1.03E-15	-8.14E-16

8P	-7.60E-10	9.66E-08	-4.25E-06	8.15E-05	2.81E-07	-6.30E-06	3.83E-05	5.63E-06
1MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
7MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
8MA	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
MGLY	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
GLY	-1.79E-14	2.55E-12	-1.32E-10	2.92E-09	-3.90E-12	7.50E-11	-3.95E-10	2.35E-09

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¹ The stoichiometric coefficient is calculated by $\alpha = A \times (\text{HC: NO}_x)^3 + B \times (\text{HC: NO}_x)^2 + C \times (\text{HC: NO}_x) + D$, where HC:NO_x is the ratio of total non-methane hydrocarbons to NO_x ratio (ppbC ppb⁻¹).

References

- 260 Alvarado, A., Tuazon, E. C., Aschmann, S. M., Atkinson, R., and Arey, J.: Products of the gas-phase reactions of O (3 P) atoms and O₃ with α -pinene and 1, 2-dimethyl-1-cyclohexene, *Journal of Geophysical Research: Atmospheres*, 103, 25541-25551, 1998.
- 265 Bates, K. H., Burke, G. J., Cope, J. D., and Nguyen, T. B.: Secondary organic aerosol and organic nitrogen yields from the nitrate radical (NO₃) oxidation of alpha-pinene from various RO₂ fates, *Atmospheric Chemistry and Physics*, 22, 1467-1482, 2022.
- 270 Beardsley, R., and Jang, M.: Simulating the SOA formation of isoprene from partitioning and aerosol phase reactions in the presence of inorganics, *Atmospheric Chemistry and Physics*, 16, 5993-6009, 10.5194/acp-16-5993-2016, 2016.
- 275 Han, S., and Jang, M.: Prediction of secondary organic aerosol from the multiphase reaction of gasoline vapor by using volatility-reactivity base lumping, *Atmospheric Chemistry and Physics*, 22, 625-639, 2022.
- Jenkin, M., Wyche, K., Evans, C., Carr, T., Monks, P., Alfarra, M., Barley, M., McFiggans, G., Young, J., and Rickard, A.: Development and chamber evaluation of the MCM v3.2 degradation scheme for beta-caryophyllene, *Atmospheric Chemistry and Physics*, 12, 5275-5308, 10.5194/acp-12-5275-2012, 2012.
- 280 Jenkin, M., Young, J., and Rickard, A.: The MCM v3.3.1 degradation scheme for isoprene, *Atmospheric Chemistry and Physics*, 15, 11433-11459, 2015.
- Molteni, U., Simon, M., Heinritzi, M., Hoyle, C. R., Bernhammer, A.-K., Bianchi, F., Breitenlechner, M., Brilke, S., Dias, A., and Duplissy, J.: Formation of highly oxygenated organic molecules from α -pinene ozonolysis: chemical characteristics, mechanism, and kinetic model development, *ACS Earth and Space Chemistry*, 3, 873-883, 2019.
- 285 Paulson, S. E., Flagan, R. C., and Seinfeld, J. H.: Atmospheric photooxidation of isoprene part I: The hydroxyl radical and ground state atomic oxygen reactions, *International Journal of Chemical Kinetics*, 24, 79-101, 1992.
- Roldin, P., Ehn, M., Kurtén, T., Olenius, T., Rissanen, M. P., Sarnela, N., Elm, J., Rantala, P., Hao, L., and Hyttinen, N.: The role of highly oxygenated organic molecules in the Boreal aerosol-cloud-climate system, *Nature communications*, 10, 1-15, 2019.
- 290 Saunders, S. M., Jenkin, M. E., Derwent, R., and Pilling, M.: Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part A): tropospheric degradation of non-aromatic volatile organic compounds, *Atmospheric Chemistry and Physics*, 3, 161-180, 2003.
- Yu, Z., Jang, M., Zhang, T., Madhu, A., and Han, S.: Simulation of Monoterpene SOA Formation by Multiphase Reactions Using Explicit Mechanisms, *ACS Earth and Space Chemistry*, 2021.
- Zhao, D., Pullinen, I., Fuchs, H., Schrade, S., Wu, R., Acir, I.-H., Tillmann, R., Rohrer, F., Wildt, J., and Guo, Y.: Highly oxygenated organic molecule (HOM) formation in the isoprene oxidation by NO₃ radical, *Atmospheric Chemistry and Physics*, 21, 9681-9704, 2021.
- 295 Zhou, C., Jang, M., and Yu, Z.: Simulation of SOA formation from the photooxidation of monoalkylbenzenes in the presence of aqueous aerosols containing electrolytes under various NO_x levels, *Atmospheric Chemistry and Physics*, 19, 5719-5735, 2019.