Supporting Information for

An Overlooked Kinetic Relaxation in the Formation of Sesquiterpene-Derived Criegee Intermediates

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Text S1. Derivation of the formation rate constant of CIs

This section describes the detailed derivation for the formation rate constant of CIs. For simplicity in the derivation, we firstly consider one CI from the ozonolysis of the sesquiterpene (SQT) molecule, wherein only one SPC and one POZ connect the reaction chain (Scheme II in the manuscript). For atmospheric chemistry models, the formation rate of CIs (R_f) is typically given by Eq. (S1).

$$R_f = k_{CI} \cdot C_{SQT} \cdot C_{O_3} \tag{S1}$$

Here k_{CI} is the formation rate constant of CIs generated from the reactions between sesquiterpene (SQT) and O_3, while C_{SQT} and C_{O3} represent the concentrations of SQT and O_3. If we change the perspective and start to think about the basic principle of elementary reactions, R_f is actually determined by the rate of POZ decomposition (Scheme II in the manuscript), and its expression is given by Eq. (S2).

$$R_f = k_3 \cdot C_{POZ} \tag{S2}$$

If we try to compare Eq. (S2) with Eq. (S1), we will find it necessary to express the concentration of POZ (C_{POZ}) as a function of C_{SQT} and C_{O3}. Based on Scheme II in the manuscript, the kinetics regarding the change of C_{POZ} along with ozonolysis time (t) can be analytically expressed as Eq. (S3).

$$\frac{dC_{POZ}}{dt} = k_2 \cdot C_{SPC} - (k_{-2} + k_3) \cdot C_{POZ} \tag{S3}$$

The quantity C_{SPC} represents the concentration of SPC and k_2 is the rate constant of POZ formation from the SPC. The generated POZ can either reversely produce SPC again or decompose into the CI, with the rate constants represented by k_{-2} and k_3, respectively. As supported by experimental studies(Talukdar et al., 2003; Davis et al., 2005; Ou and Chen, 2025), C_{SPC} can be approximated by its steady-state concentration (Eq. (S4)).

$$\frac{dC_{SPC}}{dt} = 0 \quad \text{(S4)}$$

Eq. (S4) means that, at any time during the SQT ozonolysis, the concentration of the SPC is assumed to be constant. The left-hand side of Eq. (S4), based on Scheme II in the manuscript, can be expressed as Eq. (S5).

$$\frac{dC_{SPC}}{dt} = k_1 \cdot p \cdot C_{SQT} \cdot C_{O_3} - (k_{-1} + k_2) \cdot C_{SPC} \quad \text{(S5)}$$

Here k_1 is the rate constant of effective collisions between the SQT and O_3, p is the branching ratio that the effective collisions can produce this SPC (as the SQT and O_3 indeed yield multiple SPCs), k_{-1} is the dissociation rate constant of the SPC, k_2 is the formation rate constant of the POZ from the SPC. Combining Eqs. (S4) and (S5), the steady-state concentration of SPC, denoted as $C_{SPC,ss}$, is given by Eq. (S6).

$$C_{SPC,ss} = k_1 \cdot p \cdot \left(\frac{1}{k_{-1}+k_2}\right) \cdot C_{SQT} \cdot C_{O_3} \quad \text{(S6)}$$

Eq. (S6) suggests that, within the modeling timescale, both the concentrations of SQT and O_3 are stable enough, so C_{SQT} and C_{O3} remain constant. It is noted that $C_{SPC,ss}$ is a function of temperature since k_1, k_{-1} and k_2 may change during the temperature variations. Substituting Eq. (S6) into Eq. (S3), we obtain Eq. (S7).

$$\frac{dC_{POZ}}{dt} = k_1 \cdot p \cdot \left(\frac{k_2}{k_{-1}+k_2}\right) \cdot C_{SQT} \cdot C_{O_3} - (k_{-2} + k_3) \cdot C_{POZ} \quad \text{(S7)}$$

For convenience, if we denote C_{POZ} as y, the first term on the right-hand side of Eq. (S7) as b, and $(k_{-2} + k_3)$ in Eq. (S7) as a, the Eq. (S7) then becomes a classical ordinary differential equation as shown in Eq. (S8).

$$\frac{dy}{dt} = b - ay \quad \text{(S8)}$$

After rearranging the Eq. (S8), we can conduct the indefinite integral as Eq. (S9), and then obtain the expression of y as a function of t with a constant c' for integration (Eq. (S10)).

$$\frac{1}{a} \cdot \int \frac{d(ay)}{b-ay} = \int dt \tag{S9}$$

$$y = \frac{b}{a} \cdot (1 - c'e^{-at}) \tag{S10}$$

Notably, in the experimental measurements of CI formation from ozonolysis, there is typically no pre-existing POZ (i.e., $y = 0$) when the ozonolysis starts (i.e., $t = 0$). In this case, we can obtain the value of c' by solving Eq. (S10), which provides $c' = 1$.

By transforming a and b back to their original symbols, the analytical expression of C_{POZ} is given by Eq. (S11).

$$C_{POZ} = k_1 \cdot p \cdot \left(\frac{1}{k_{-2}+k_3}\right) \cdot \left(\frac{k_2}{k_{-1}+k_2}\right) \cdot \left[1 - e^{-(k_{-2}+k_3)t}\right] \tag{S11}$$

Substituting Eq. (S11) into Eq. (S2), the analytical expression of R_f is given by Eq. (S12).

$$R_f = k_1 \cdot p \cdot \left(\frac{k_3}{k_{-2}+k_3}\right) \cdot \left(\frac{k_2}{k_{-1}+k_2}\right) \cdot \left[1 - e^{-(k_{-2}+k_3)t}\right] \cdot C_{SQT} \cdot C_{O_3} \tag{S12}$$

Now we obtain the formation rate of a single CI as a function of all the related rate constants of elemental reactions as well as the concentrations of SQT and O_3. Considering all the SPCs and their corresponding POZs generated from the ozonolysis and all the CIs generated from POZ decomposition, Eq. (S12) can be rewritten into a comprehensive expression given by Eq. (S13).

$$R_f = k_1 \cdot \sum_i \sum_j \left\{p_i \cdot \left(\frac{k_{3,i,j}}{k_{-2,i}+k_{3,i,j}}\right) \cdot \left(\frac{k_{1,i} \cdot k_{2,i}}{k_{-1,i}+k_{2,i}}\right) \cdot \left[1 - e^{-(k_{-2,i}+k_{3,i,j})t}\right]\right\} \cdot C_{SQT} \cdot C_{O_3} \tag{S13}$$

The subscript i in Eq. (S13) indicates the i-th SPC and the i-th POZ, and the subscript j indicates the j-th CI from the i-th POZ decomposition. Both i and j are positive integers. The value of i ranges from 1 to the total number of CIs, while the value of j is either 1 or 2, since each POZ can decompose into two possible CIs. Comparing Eq. (S13) with Eq. (S1), we can directly obtain the expression of k_{CI}, which shows the rate constant of total CI formation (Eq. (S14)).

$$k_{CI} = k_1 \cdot \sum_i \sum_j \left\{p_i \cdot \left(\frac{k_{3,i,j}}{k_{-2,i}+k_{3,i,j}}\right) \cdot \left(\frac{k_{1,i} \cdot k_{2,i}}{k_{-1,i}+k_{2,i}}\right) \cdot \left[1 - e^{-(k_{-2,i}+k_{3,i,j})t}\right]\right\} \tag{S14}$$

Eq. (S14) handles all the kinetic details at the "double-well" potential energy surface of the CI formation mechanism, and we indicate that Eq. (S14) can be simplified by two approximations. The first approximation is that k_{-2} may vanish, as it is negligibly small compared to $k_{3,i,j}$. This is because the energy barriers for the decomposition of POZs into SPCs are significantly higher than those for the CI formation(Donahue et al., 2011; Vereecken and Francisco, 2012; Taatjes et al., 2014). In this case, k_{CI} can be approximated by Eq. (S15).

$$k_{CI} \approx k_1 \cdot \sum_i \sum_j \left[p_i \cdot \frac{k_{3,i,j}}{k_{3,i,j}} \cdot \left(\frac{k_{2,i}}{k_{-1,i}+k_{2,i}} \right) \cdot \left(1 - e^{-k_{3,i,j} t} \right) \right]$$

$$= k_1 \cdot \sum_i \sum_j \left[p_i \cdot \left(\frac{k_{2,i}}{k_{-1,i}+k_{2,i}} \right) \cdot \left(1 - e^{-k_{3,i,j} t} \right) \right] \quad \text{(S15)}$$

The second approximation is that the decomposition of each POZ produces only one major CI. Although there should be two CIs generated from the one POZ, one of the CIs has a faster formation rate, wherein its k_3 is typically ~1−10 orders of magnitude higher than that of the other (Fig. 3). In this case, the summation based on j vanishes so that k_{CI} can be further approximated by Eq. (S16).

$$k_{CI} \approx k_1 \cdot \sum_i \left[p_i \cdot \left(\frac{k_{2,i}}{k_{-1,i}+k_{2,i}} \right) \cdot \left(1 - e^{-k_{3,i} t} \right) \right] \quad \text{(S16)}$$

The expression of k_{CI} in Eq. (S16) is very similar to the expression of k_{oz} (Eq. (1) in the manuscript). Their relationship can be clearly illustrated if we denote the branching ratio of the i-th ozonolysis channel (i.e., the reaction pathway that generates the i-th CI through the i-th SPC and the i-th POZ) as r_i, which is given by Eq. (S17).

$$r_i = p_i \cdot \left(\frac{k_{2,i}}{k_{-1,i}+k_{2,i}} \right) \Big/ \sum_i \left[p_i \cdot \left(\frac{k_{2,i}}{k_{-1,i}+k_{2,i}} \right) \right] \quad \text{(S17)}$$

Eq. (S17) reveals that $\sum_i r_i = 1$. Substituting Eq. (S17) into Eq. (S16), the relationship between k_{CI} and k_{oz} can be derived as Eq. (S18).

$$k_{CI} \approx k_1 \cdot \sum_i \left\{ r_i \cdot \sum_i \left[p_i \cdot \left(\frac{k_{2,i}}{k_{-1,i}+k_{2,i}} \right) \right] \cdot (1 - e^{-k_{3,i}t}) \right\}$$

$$= k_1 \cdot \sum_i \left[p_i \cdot \left(\frac{k_{2,i}}{k_{-1,i}+k_{2,i}} \right) \right] \cdot \sum_i [r_i \cdot (1 - e^{-k_{3,i}t})]$$

$$= k_{oz} \cdot \sum_i [r_i \cdot (1 - e^{-k_{3,i}t})] \quad \text{(S18)}$$

Eq. (S18) provides a clear physical sense that, for the i-th CI, its formation rate constant can be estimated by the product of the ozonolysis rate constant and the time-dependent branching ratio projecting of this CI ($f_{CI,i}$), which is given by Eq. (S19).

$$f_{CI,i} = r_i \cdot (1 - e^{-k_{3,i}t}) \quad \text{(S19)}$$

Thus, the relationship between k_{CI} and k_{oz} can be written as Eq. (S20).

$$k_{CI} \approx k_{oz} \cdot \sum_i f_{CI,i} \quad \text{(S20)}$$

The time dependence of $f_{CI,i}$ shows the kinetic relaxation of k_{CI}. Eqs. (S19) and (S20) reveal that, when the ozonolysis begins (i.e., $t = 0$), the value of $f_{CI,i}$ is zero, which means that if the i-th POZ does not pre-exist, the initial formation rate constant of the i-th CI is zero, even though the ozonolysis rate constant of the SQT is the positive number k_{oz}. It is also noted that the value of $f_{CI,i}$ will unlimitedly approach r_i if the t is infinitely large (Eq. (S21)).

$$\lim_{t\to\infty} k_{CI}(t,T) \approx \lim_{t\to\infty} \left[k_{oz}(T) \cdot \sum_i f_{CI,i}(t,T) \right]$$

$$= k_{oz}(T) \cdot \lim_{t\to\infty} \sum_i f_{CI,i}(t,T)$$

$$= k_{oz}(T) \cdot \lim_{t\to\infty} \sum_i [r_i \cdot (1 - e^{-k_{3,i}t})]$$

$$= k_{oz}(T) \cdot \sum_i r_i$$

$$= k_{oz}(T) \quad \text{(S21)}$$

Eq. (S21) indicates that k_{oz} represents the plateau value of k_{CI} if ozonolysis could proceed indefinitely. In the real atmosphere, k_{CI} is always in a state of deviation from k_{oz}, though it continuously tends toward this value.

Text S2. Formation rate constant of CIs with scale factors accounting for the pre-existing POZs

This section derives the analytical expression of k_{CI} if POZs pre-exist before the SQT ozonolysis starts. For convenience, we still start by considering only one CI produced from its corresponding POZ. The analytical expression of k_{CI} in Text S1 is derived based on the absence of pre-existing POZs, so that in Eq. (S10) the value of c' equals 1. If the initial concentration of this POZ is not zero, we may denote the value of its initial concentration as y_0 ($y_0 > 0$), and the value of c' can be obtained by solving Eq. (S10), which gives $c' = 1 - (y_0 \cdot a / b)$.

In the meantime, we also notice that, when t is infinitely large, the concentration of POZ unlimitedly approaches a constant, which is denoted as y_∞ in Eq. (S22).

$$y_\infty = \lim_{t\to\infty}\left[\frac{b}{a}\cdot(1-c'e^{-at})\right] = \frac{b}{a} \tag{S22}$$

We find it more convenient to express c' as $c' = 1 - (y_0 / y_\infty)$, so Eq. (S10) transforms into a general expression of y, as shown in Eq. (S23).

$$y = y_\infty \cdot [1 - (1 - \frac{y_0}{y_\infty}) \cdot e^{-at}] \tag{S23}$$

In this case, if we define the scale factor (s) as the ratio of the initial POZ concentration to its ultimate value at an infinite t (i.e., $s = y_0 / y_\infty$ and $s > 0$), and transform y_∞, a and b back to their original symbols, the analytical expression of C_{POZ} incorporating the scale factor will be given by Eq. (S24).

$$C_{POZ} = k_1 \cdot p \cdot \left(\frac{1}{k_{-2}+k_3}\right) \cdot \left(\frac{k_2}{k_{-1}+k_2}\right) \cdot \left[1 - (1-s) \cdot e^{-(k_{-2}+k_3)t}\right] \tag{S24}$$

Considering the formation of all the POZs and their CIs, along with the approximations discussed in Text S1, we further obtain the analytical expression of k_{CI} that accounts for the pre-existing POZs, as given by Eq. (S25).

$$k_{CI} \approx k_{oz} \cdot \sum_i \{r_i \cdot [1 - (1 - s_i) \cdot e^{-k_{3,i}t}]\} \tag{S25}$$

Thus, the analytical expression of $f_{CI,i}$ becomes Eq. (S26).

$$f_{CI,i} = r_i \cdot [1 - (1 - s_i) \cdot e^{-k_{3,i}t}] \quad \text{(S26)}$$

Eqs. (S25) and (S26) show that, when the ozonolysis begins (i.e., t = 0), the value of $f_{CI,i}$ is no longer zero but $r_i \cdot s_i$. Such a difference reveals that, if the i-th POZ pre-exists, the initial formation rate constant of the i-th CI is not yet zero. As s_i in Eq. (S26) is not considered as a time-independent quantity in this kinetic study, the value of k_{CI} with pre-existing POZs will unlimitedly approach k_{oz} if the t is infinitely large (Eq. (S27)).

$$\begin{aligned} \lim_{t\to\infty} k_{CI}(t,T) &\approx \lim_{t\to\infty}\left[k_{oz}(T) \cdot \textstyle\sum_i f_{CI,i}(t,T)\right] \\ &= k_{oz}(T) \cdot \lim_{t\to\infty} \textstyle\sum_i f_{CI,i}(t,T) \\ &= k_{oz}(T) \cdot \lim_{t\to\infty} \textstyle\sum_i \{r_i \cdot [1 - (1 - s_i) \cdot e^{-k_{3,i}t}]\} \\ &= k_{oz}(T) \cdot \textstyle\sum_i r_i \\ &= k_{oz}(T) \end{aligned} \quad \text{(S27)}$$

Eqs. (S26) and (S27) indicate that, although pre-existing POZs may help reduce the gap between k_{CI} and k_{oz}, k_{CI} is still deviated from k_{oz}. We should be cautious about using k_{oz} to represent k_{CI} in the modeling of CI formation.

Table S1. Fitted pre-exponential factors (*A*) of the Arrhenius equation based on the computational results of k_{-1} and k_2 for each SPC generated from the ozonolysis of α-cedrene and α-copaene.

SPC	α-cedrene		α-copaene	
	k_{-1}	k_2	k_{-1}	k_2
SPC1-1	1.6×10^{13}	4.2×10^{10}	1.6×10^{13}	9.3×10^{9}
SPC1-2	1.6×10^{13}	2.1×10^{10}	1.6×10^{13}	7.9×10^{9}
SPC2-1	1.6×10^{13}	2.1×10^{10}	1.6×10^{13}	5.7×10^{13}
SPC2-2	1.6×10^{13}	1.7×10^{10}	1.6×10^{13}	1.5×10^{13}

Table S2. Branching ratio of the ozonolysis channels of α-cedrene and α-copaene corresponding to different SPCs across the studied temperatures.

T (K)	α-cedrene ozonolysis				α-copaene ozonolysis			
	1-1	1-2	2-1	2-2	1-1	1-2	2-1	2-2
243	0.00	0.00	0.94	0.06	0.00	0.00	0.66	0.34
248	0.00	0.00	0.94	0.06	0.00	0.00	0.65	0.35
253	0.00	0.00	0.93	0.07	0.00	0.00	0.65	0.35
258	0.00	0.00	0.93	0.07	0.00	0.00	0.64	0.36
263	0.00	0.00	0.93	0.07	0.00	0.00	0.63	0.37
268	0.00	0.00	0.93	0.07	0.00	0.00	0.63	0.37
273	0.00	0.00	0.92	0.08	0.00	0.00	0.62	0.38
278	0.00	0.00	0.92	0.08	0.00	0.00	0.62	0.38
283	0.00	0.00	0.92	0.08	0.00	0.00	0.61	0.39
288	0.00	0.00	0.91	0.09	0.00	0.00	0.60	0.40
293	0.00	0.00	0.91	0.09	0.00	0.00	0.60	0.40
298	0.00	0.00	0.91	0.09	0.00	0.00	0.59	0.41
303	0.00	0.00	0.90	0.10	0.00	0.00	0.59	0.41
308	0.00	0.00	0.90	0.10	0.00	0.00	0.59	0.41
313	0.00	0.00	0.90	0.10	0.00	0.00	0.58	0.42
318	0.00	0.00	0.90	0.10	0.00	0.00	0.58	0.42
323	0.00	0.00	0.89	0.11	0.00	0.00	0.57	0.43

Table S3. Relaxation timescale of CI formation from the ozonolysis of α-farnesene and β-farnesene.

T (K)	α-farnesene (unit: minutes)		β-farnesene (unit: minutes)	
	CI1	CI2	CI1	CI2
243	0.4	7.1	556.3	483.9
248	0.2	3.5	276.1	210.7
253	0.1	1.8	140.8	94.7
258	0.1	0.9	73.7	43.9
263	0.0	0.5	39.5	20.9
268	0.0	0.3	21.7	10.3
273	0.0	0.2	12.1	5.2
278	0.0	0.1	7.0	2.7
283	0.0	0.1	4.1	1.4
288	0.0	0.0	2.4	0.8
293	0.0	0.0	1.5	0.4
298	0.0	0.0	0.9	0.2
303	0.0	0.0	0.6	0.1
308	0.0	0.0	0.4	0.1
313	0.0	0.0	0.2	0.0
318	0.0	0.0	0.1	0.0
323	0.0	0.0	0.1	0.0

Table S4. Comparison of computed POZ decomposition energy barriers between DLPNO-CCSD(T)/def2-TZVPP and DLPNO-CCSD(T)/cc-pVTZ (unit: kcal mol^{-1}).

Sesquiterpenes	DLPNO-CCSD(T)/def2-TZVPP		DLPNO-CCSD(T)/cc-pVTZ	
	CI1	CI2	CI1	CI2
α-cedrene	15.2	18.3	15.6	18.7
α-copaene	21.4	22.9	21.8	23.2
β-caryophyllene	27.6	25.8	28.1	26.3
α-farnesene	15.6	16.2	15.9	16.5
β-farnesene	16.4	19.2	16.9	19.5

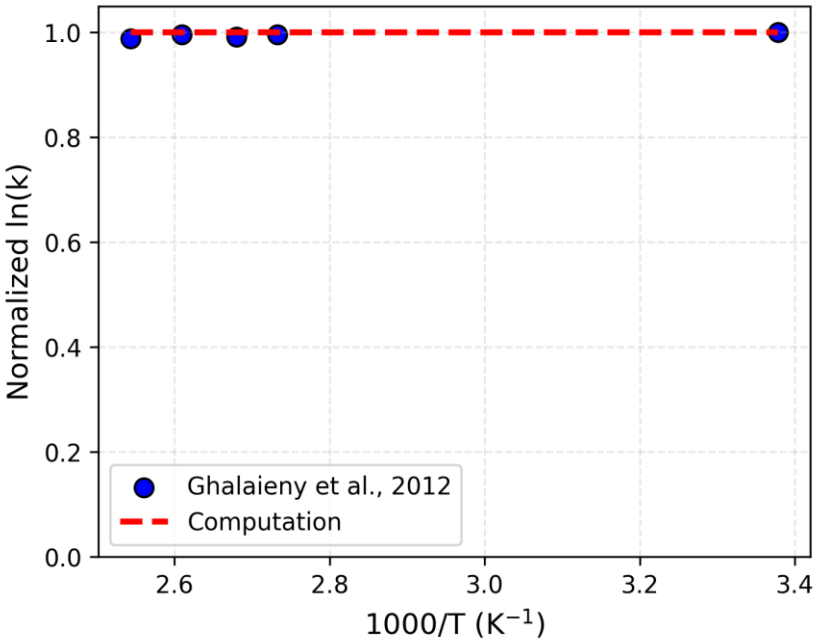


Figure S1. The experimental and computed ozonolysis rate constant of α-cedrene at different temperatures. The experimental data is reproduced with permission (Ghalaieny et al., 2012). Copyright 2012 Royal Society of Chemistry.

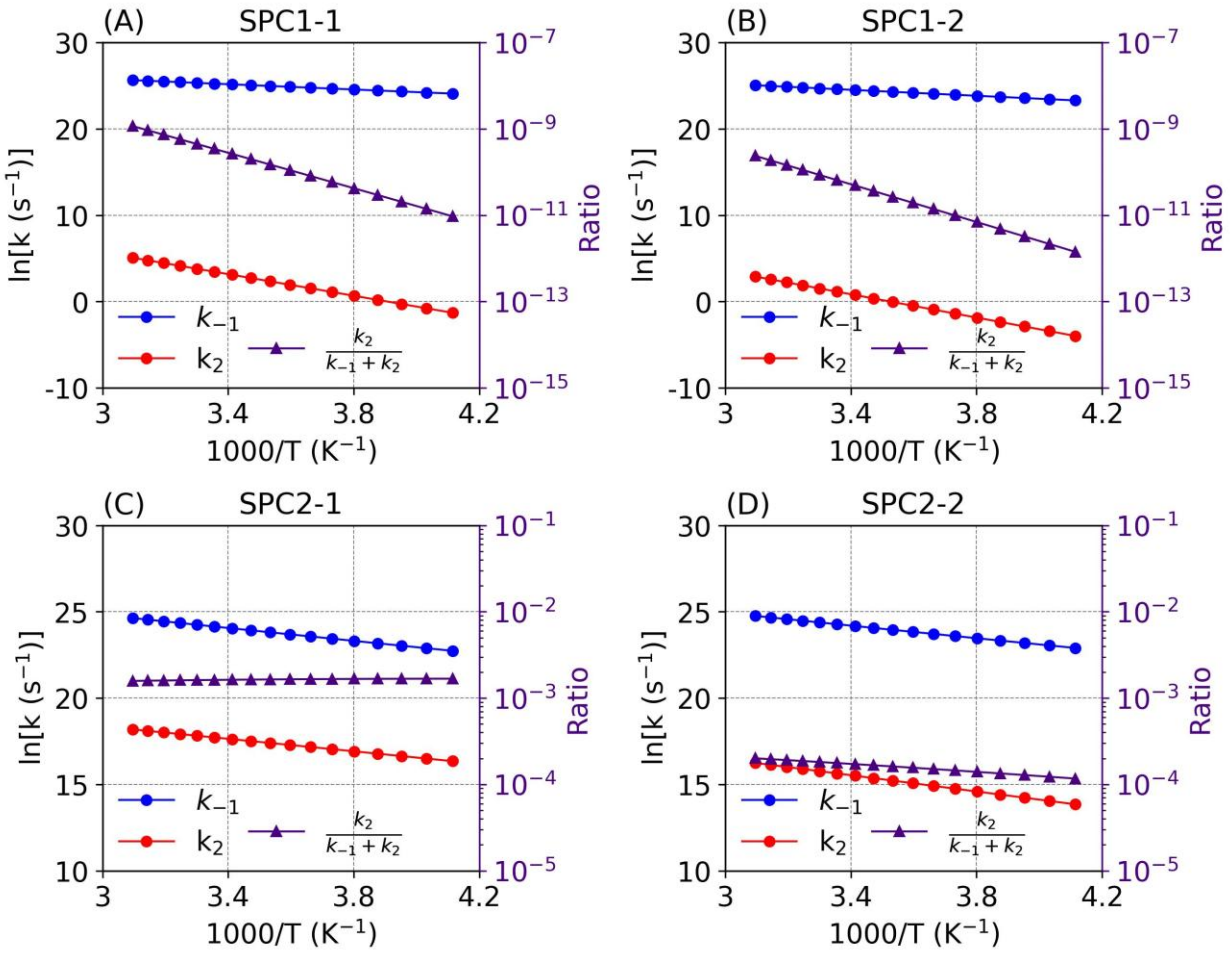
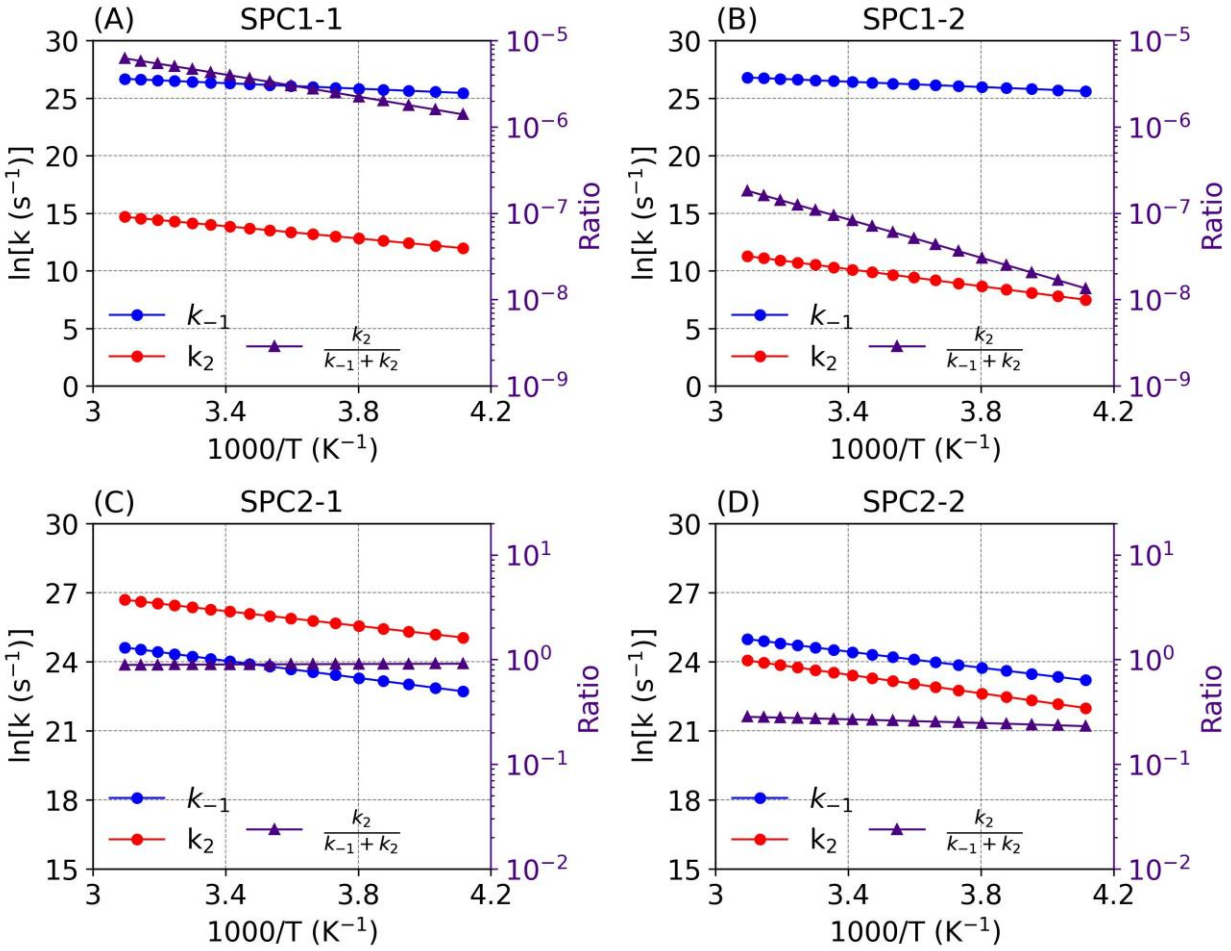


Figure S2. Temperature dependence of $ln(k_{-1})$, $ln(k_2)$ and $k_2 / (k_{-1} + k_2)$ of α-cedrene ozonolysis.



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194 **Figure S3.** Temperature dependence of $ln(k_{-1})$, $ln(k_2)$ and $k_2 / (k_{-1} + k_2)$ of α-copaene ozonolysis.

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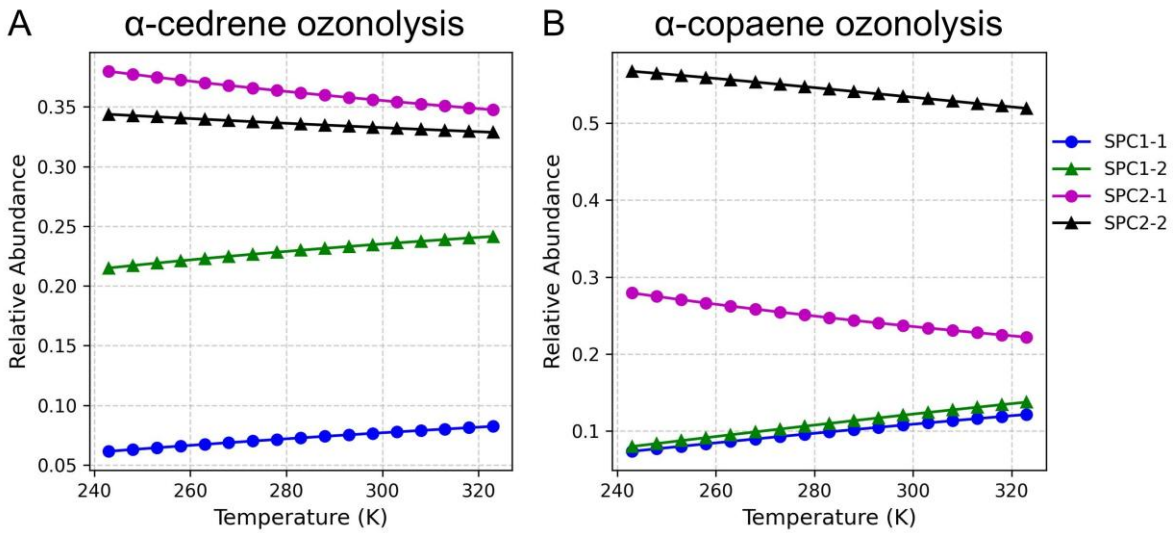
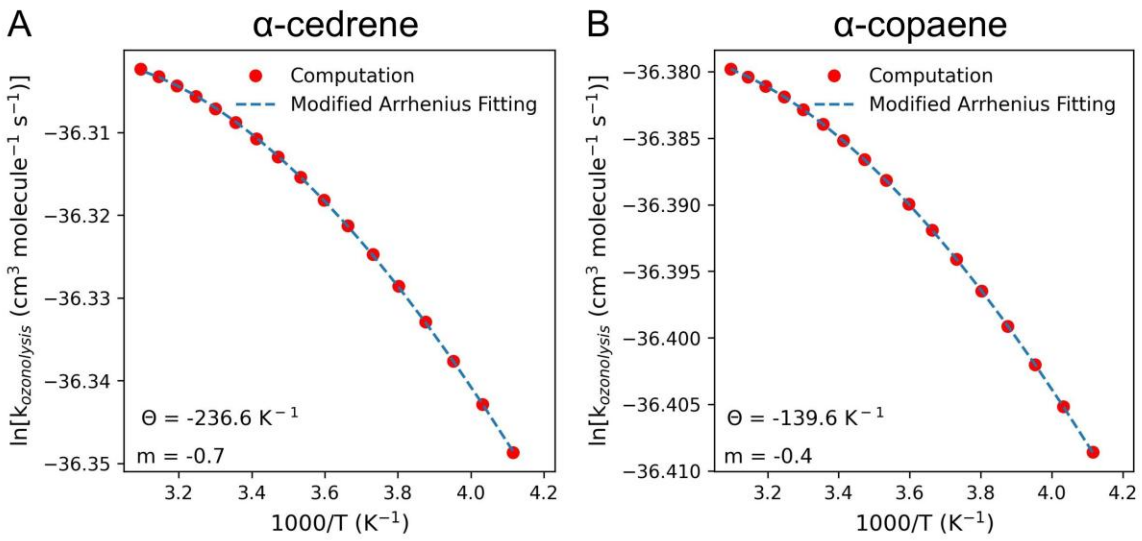


Figure S4. The relative abundance of SPCs in the ozonolysis of (A) α-cedrene and (B) α-copaene across the studied temperatures.



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201 **Figure S5.** Fitting of the computed temperature-dependent ozonolysis rate constants with the
202 modified Arrhenius equation.

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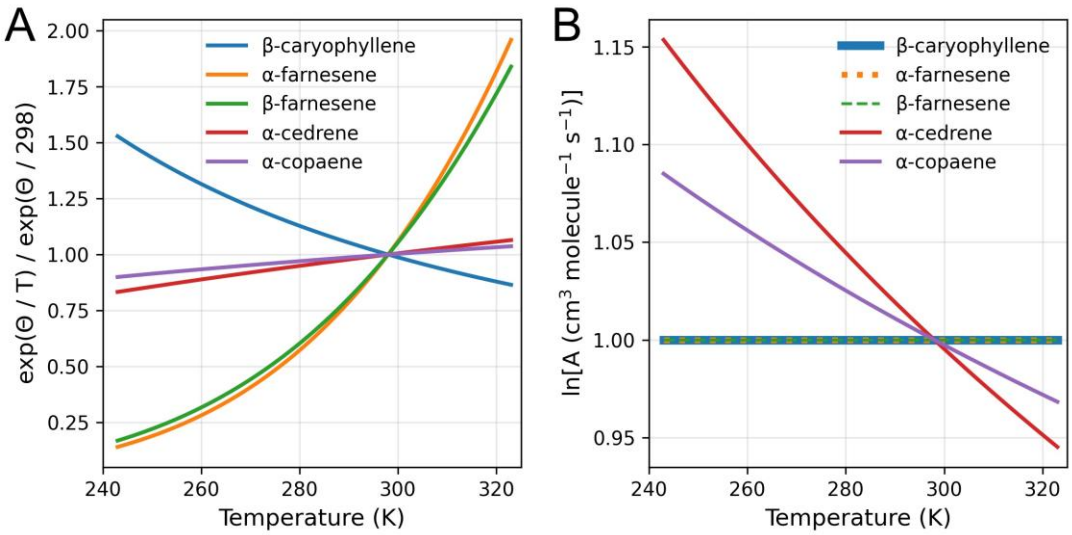

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205 **Figure S6.** Comparison of Arrhenius equation components among β-caryophyllene (Gao et al.,
206 2022), α-farnesene (Kim et al., 2011), β-farnesene (Kim et al., 2011), α-cedrene, and α-copaene:
207 (A) relative exponential factor, and (B) pre-exponential factor (natural logarithm).

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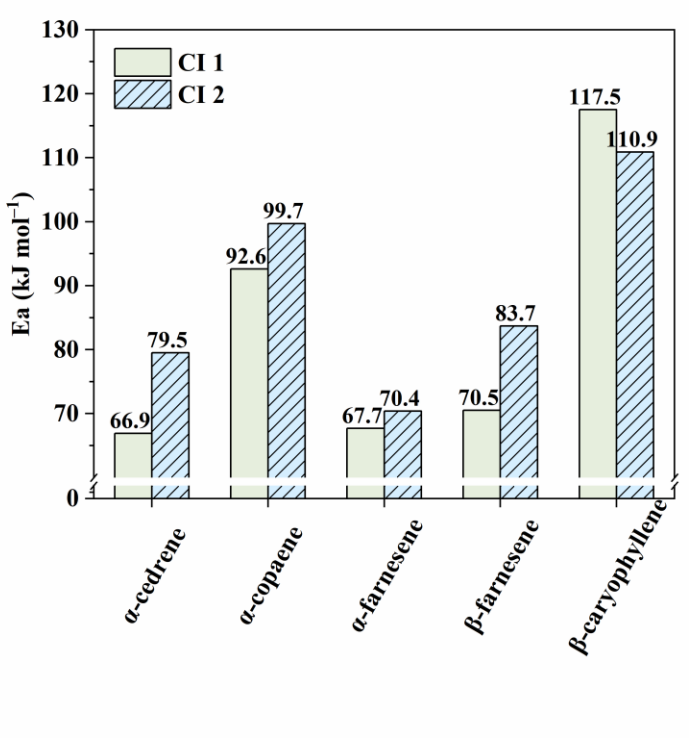

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210 **Figure S7.** Activation energy of POZ decomposition rate constants (k_3) corresponding to CI1 and
211 CI2 of all the studied sesquiterpenes.

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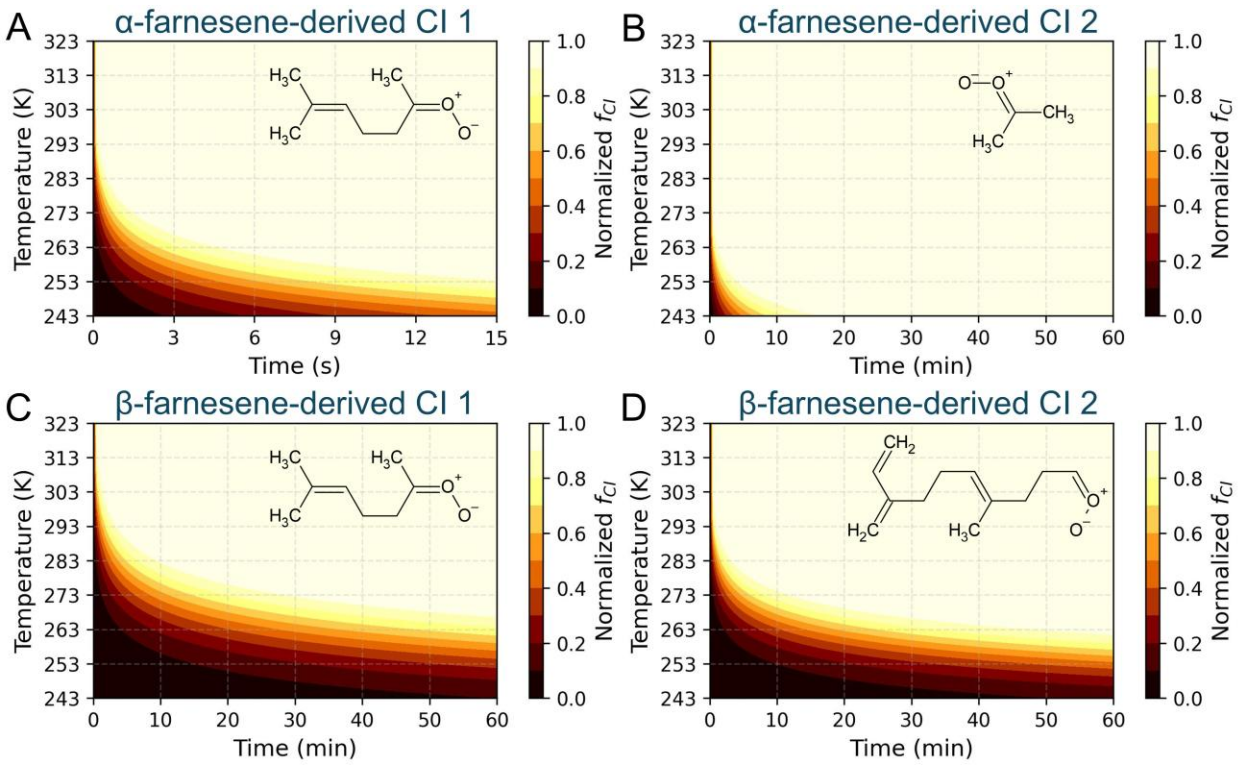

Figure S8. Kinetic relaxation of formation rate constant of (A) α-farnesene-derived CI1; (B) α-farnesene-derived CI2; (C) β-farnesene-derived CI1; (D) β-farnesene-derived CI2.

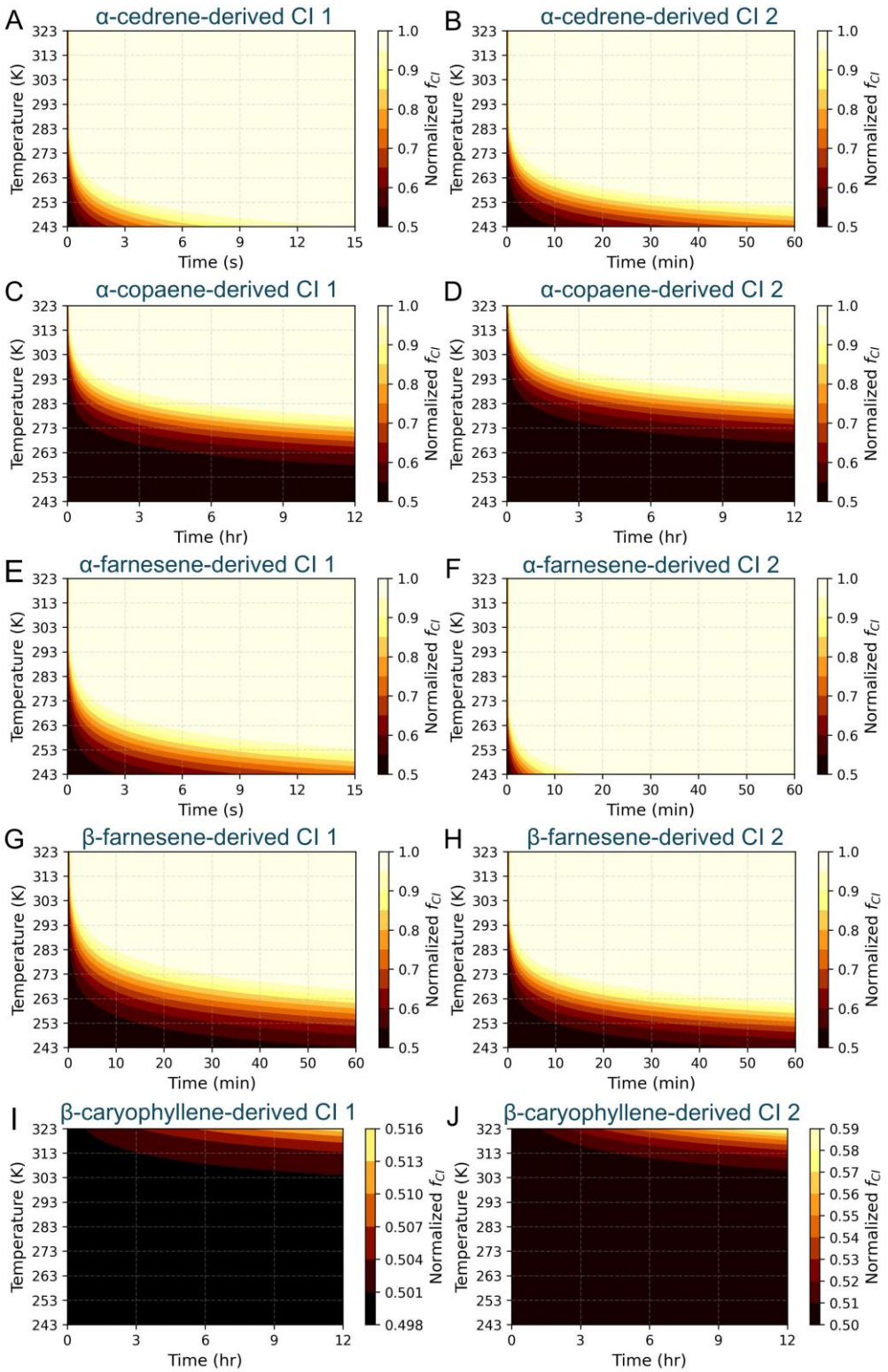

Figure S9. Kinetic relaxation of the modified k_{CI} with a scale factor of 0.5 for all the studied sesquiterpenes.

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