

On the formation of highly oxidized pollutants by autoxidation of terpenes under low temperature combustion conditions: the case of limonene and α -pinene.

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Fig. S1: AP and LM mass Spectra acquired with a HESI source in negative mode

Tab. S1: APCI source +/-, α -Pinene, limonene and APCI source α -Pinene/limonene

Tab. S2: HESI source +/-, α -Pinene, limonene and HESI source α -Pinene/limonene

Fig. S2: 3-D representation of all limonene oxidation data where DBE is used as third dimension

Fig. S3: Autoxidation reaction mechanism for limononic acid

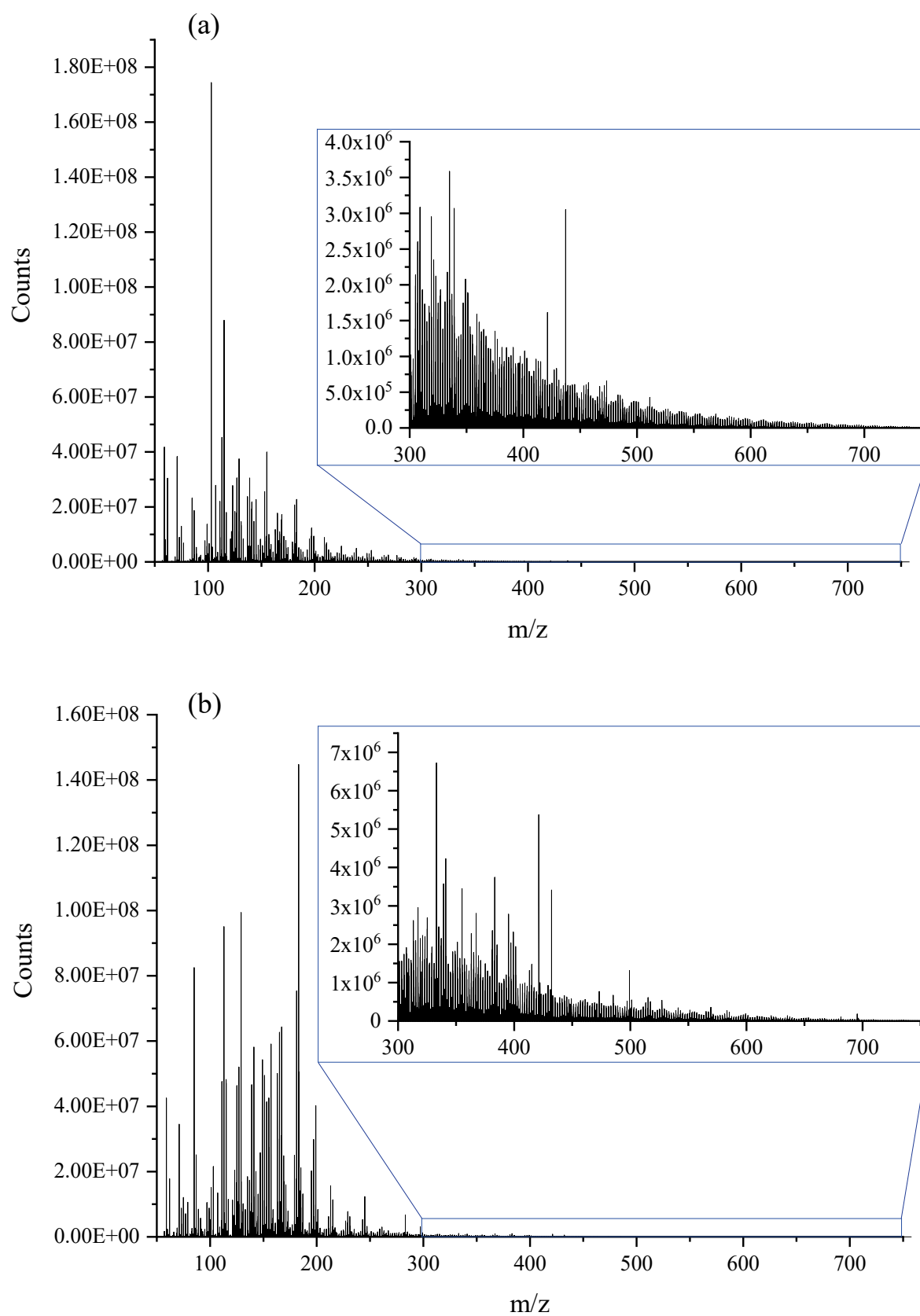


Fig. S1: α -pinene and limonene mass Spectra acquired with a HESI source in negative mode

Table S1. Representation of the mass spectrometry data characterizing the oxidation of α -pinene and limonene (ionization source: APCI positive and negative mode, JSR experiments).

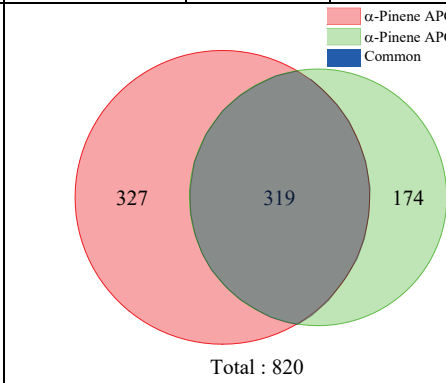
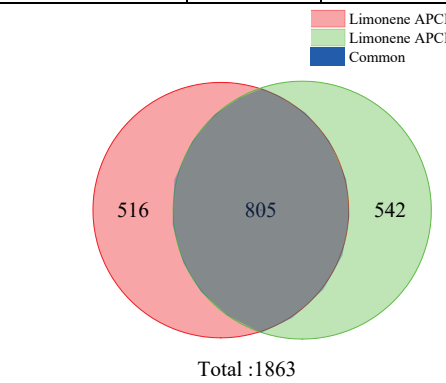
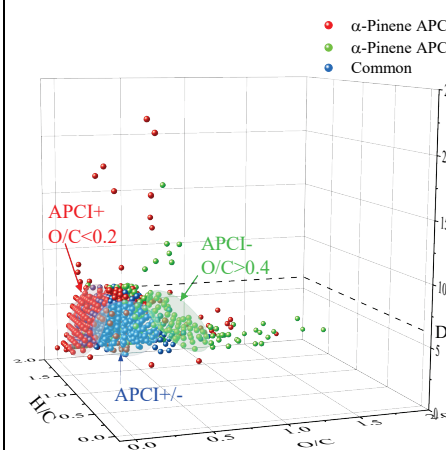
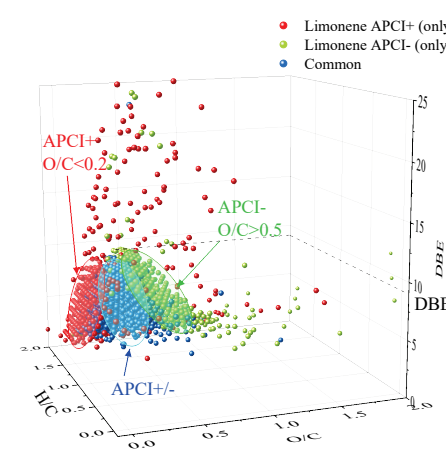
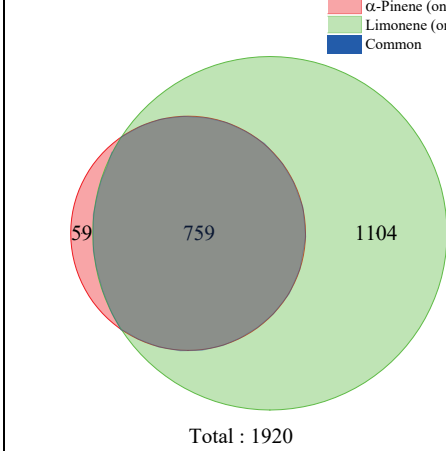
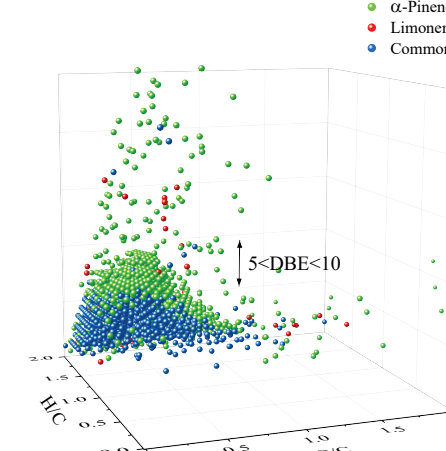
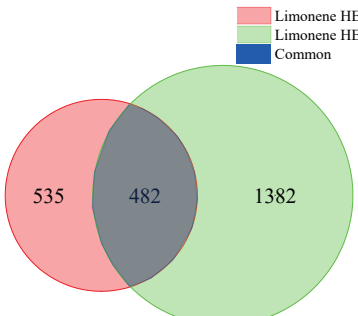
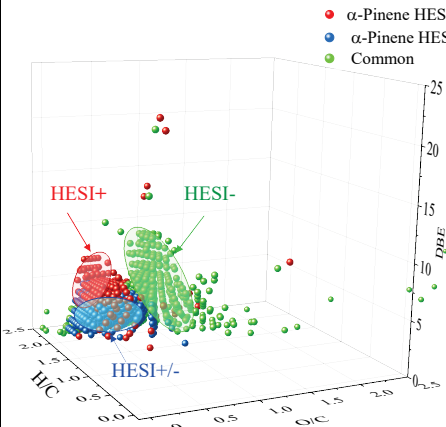
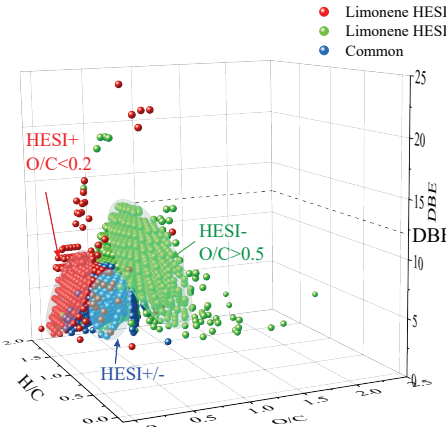
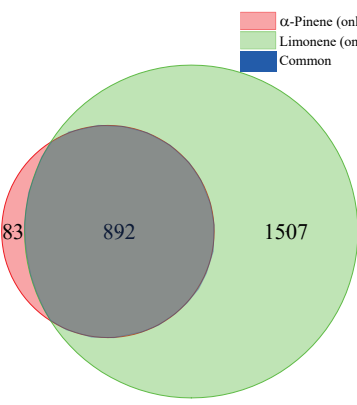
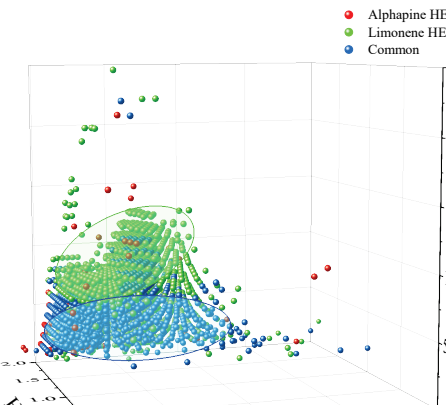
	α-Pinene			Limonene		
Source and mode	APCI⁺		APCI⁻	APCI⁺		APCI⁻
Number of compounds	646		503	1321		1346
Distribution	specific to positive mode 327	common 319	specific to negative mode 174	specific to positive mode 516	common 805	specific to negative mode 542
Venn graph	 ■ α-Pinene APCI⁺ ■ α-Pinene APCI⁻ ■ Common Total : 820			 ■ Limonene APCI⁺ ■ Limonene APCI⁻ ■ Common Total : 1863		
VK vs DBE	 ● α-Pinene APCI⁺ (only) ● α-Pinene APCI⁻ (only) ● Common APCI⁺ O/C<0.2 APCI⁻ O/C>0.4 APCI⁺/⁻			 ● Limonene APCI⁺ (only) ● Limonene APCI⁻ (only) ● Common APCI⁺ O/C<0.2 APCI⁻ O/C>0.5 APCI⁺/⁻		
	 ■ α-Pinene (only) ■ Limonene (only) ■ Common Total : 1920			 ● α-Pinene (only) ● Limonene (only) ● Common 5 < DBE < 10		

Table S2. Representation of the mass spectrometry data characterizing the oxidation of α -pinene and limonene (ionization source: HESI positive and negative modes, JSR experiments).

	α -Pinene			Limonene		
Source and mode	HESI ⁺		HESI ⁻	HESI ⁺		HESI ⁻
Number of compounds	594		693	1017		1864
Distribution	specific to positive mode 282	common 312	specific to negative mode 381	specific to positive mode 353	common 482	specific to negative mode 1342
Venn Graph	 Total : 975			 Total : 2399		
VK vs DBE						
	 Total : 2482					

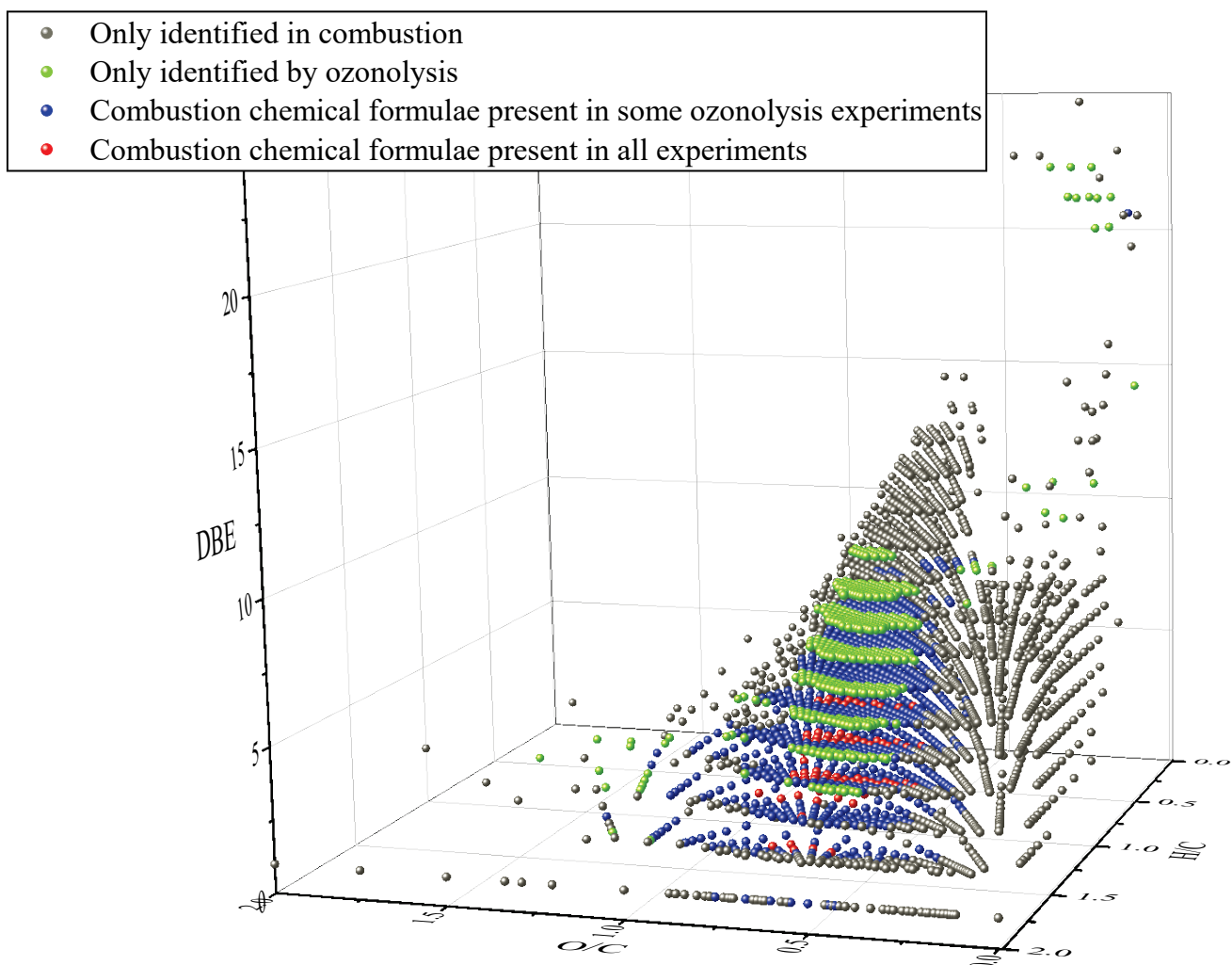


Fig. S2: 3-D representation of all limonene oxidation data where DBE is used as third dimension

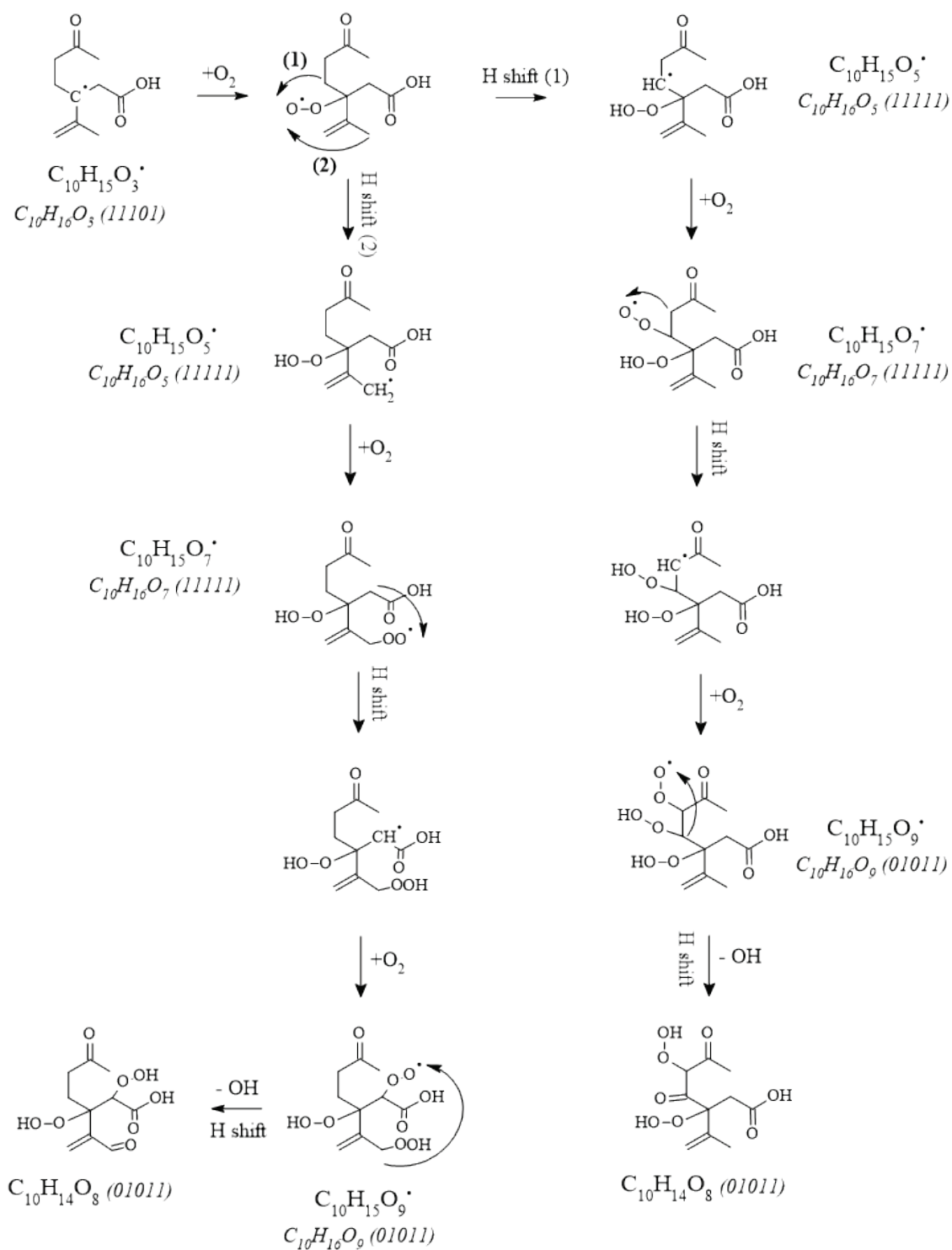


Fig. S3: Autoxidation radical reaction mechanism for limononic acid with examples of produced molecules