Supplement of Atmos. Chem. Phys., 21, 7845–7862, 2021
https://doi.org/10.5194/acp-21-7845-2021-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

On the similarities and differences between the products of oxidation of hydrocarbons under simulated atmospheric conditions and cool flames

Roland Benoit et al.

Correspondence to: Roland Benoit (roland.benoit@cnrs-orleans.fr)

Fig. S1, CH_2- Kendrick mass defect plots, DBE: 1-4.

Fig. S2, CH_2- Kendrick mass defect plots, DBE: 5-8.

Fig. S3, CH_2- Kendrick mass defect plots, DBE: 9-11.

Fig. S4, examples of reaction mechanisms for the formation of KHPs from limonene and all the reaction sites of limonene that can give KHPs (18 isomers in total).

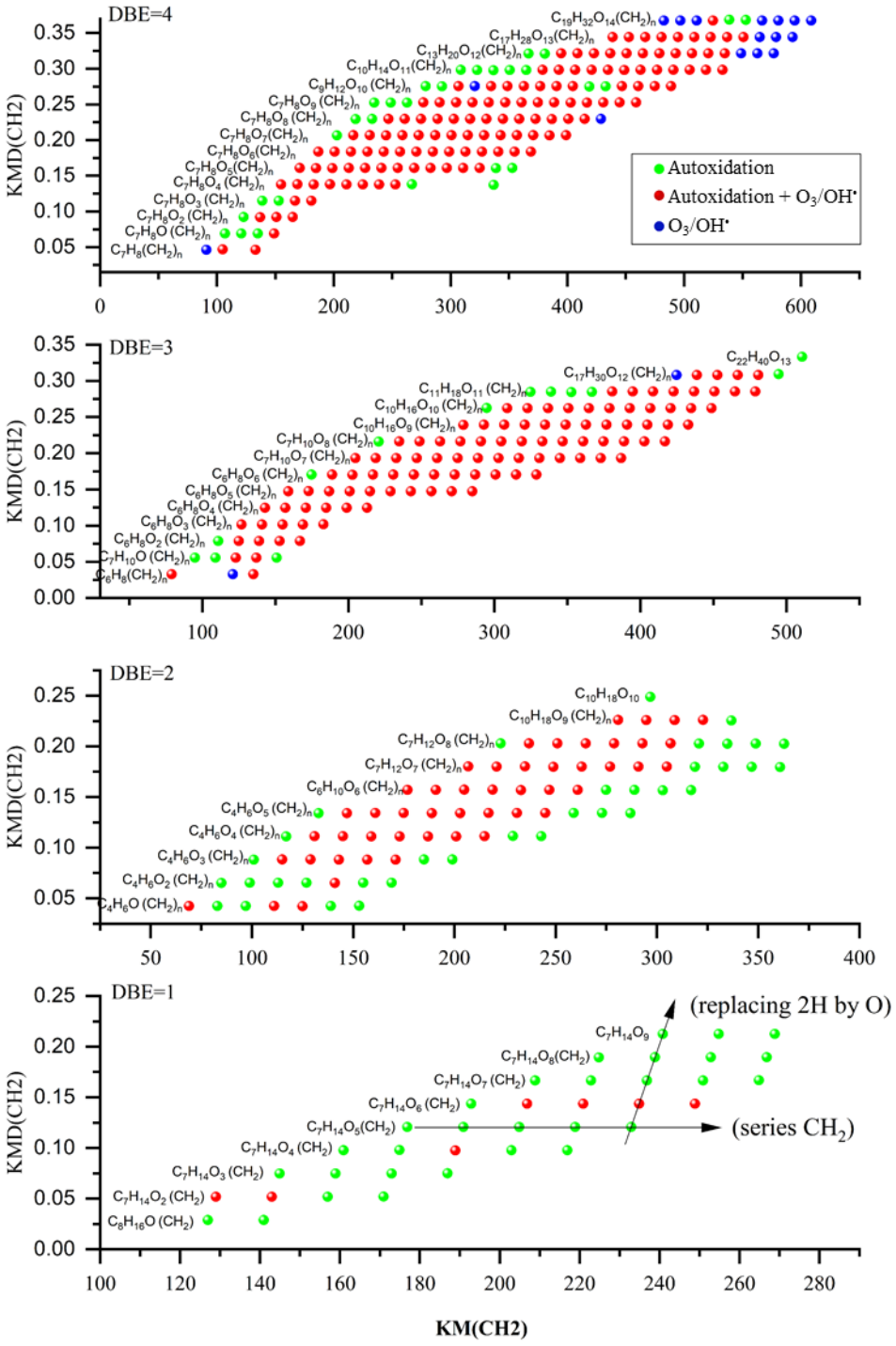
Fig. S5, all 18 isomers potentially formed by oxidation from the radical $OH^{\cdot}$.

Fig. S6, UHPLC spectrum of the compound $C_{16}H_{18}O_6N_4$ from the reaction of KHPs with 2,4-DNPH, inset: increase of the line intensity to 9.71 min depending on the reaction time with DNPH.

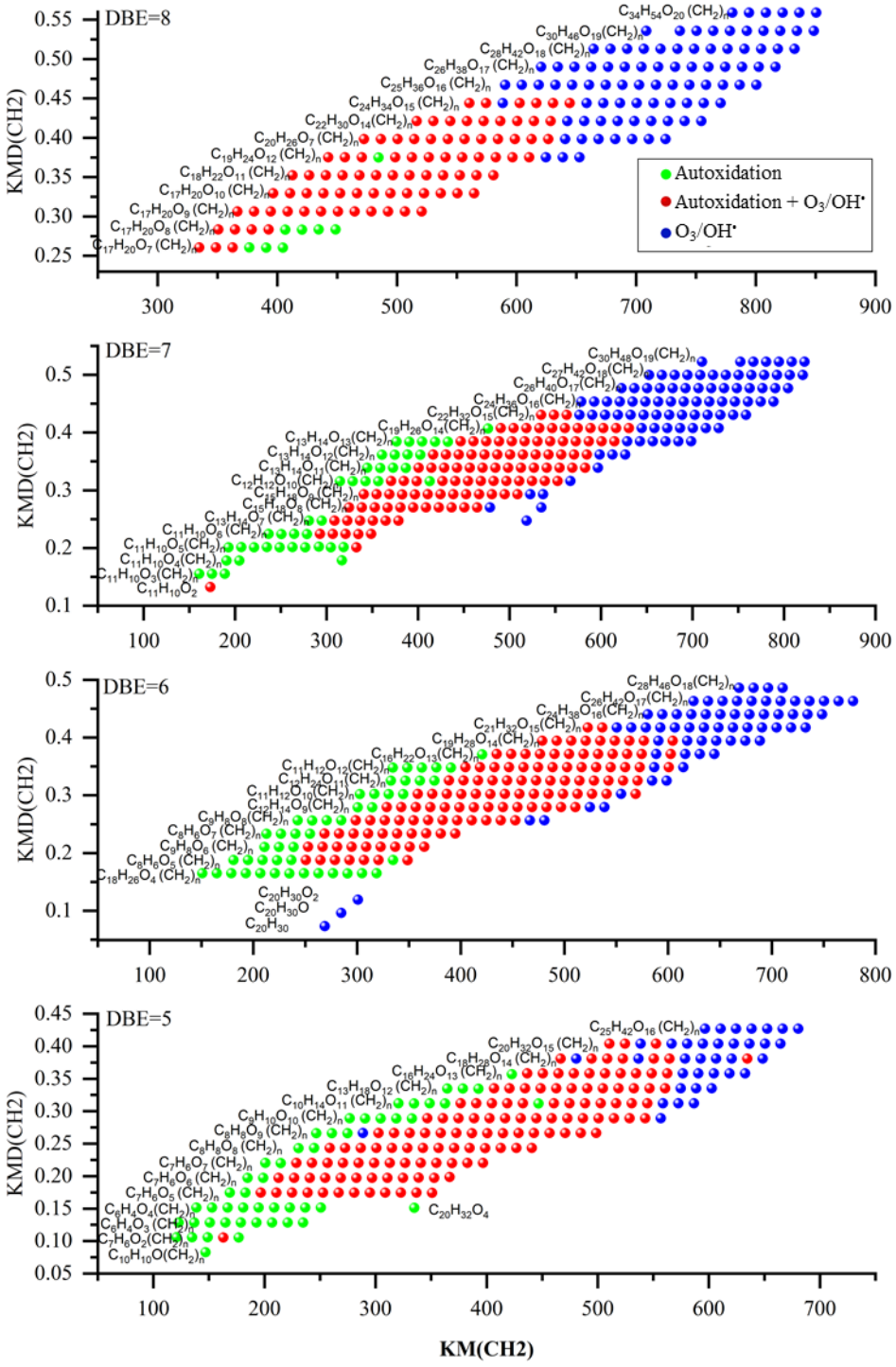
Fig. S7, comparison of UHPLC profiles of diketones and KHPs. a) UHPLC KHPs with diketones extracted from the MS/MS of the KHP, b) diketones UHPLC profile.

Fig S8, Comparison of the UHPLC profile (negative APCI mode) of $C_{10}H_{16}O_2$ isomers from the Waddington mechanism with that obtained by the addition of DNPH.

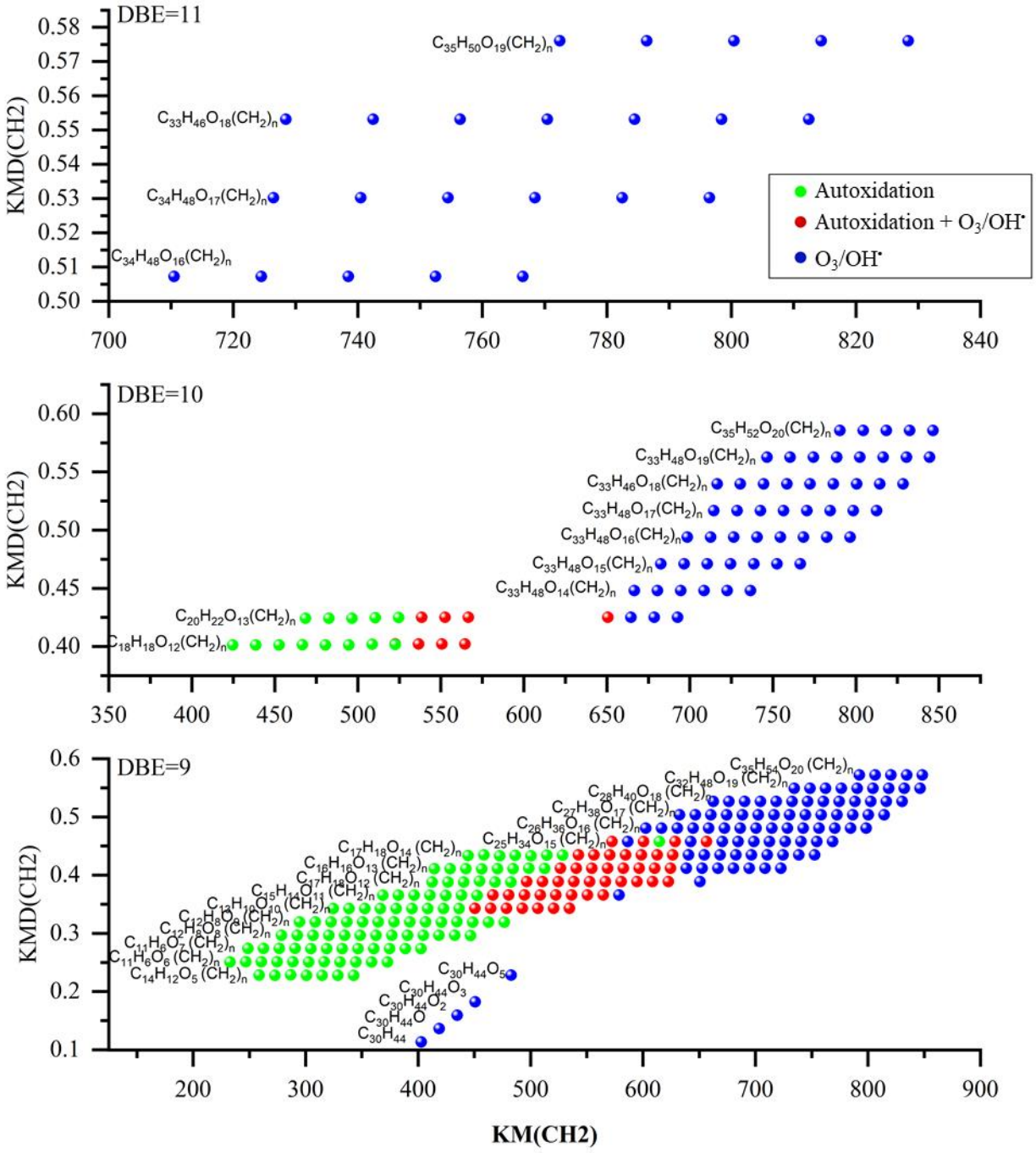
Fig. S9, Comparison of limonene oxidation spectra sample analyzed by FIA and HESI (negative mode, sheath 12, aux gas 0, voltage 3.8kV, Tcapillary 300°C, vaporizer temperature120°C, Hamilton syringe at a flow rate of 3 μL min−1) (a) mass range 50-750 amu, b) 150-750 amu; insets: zoom on the 300-600 amu range.



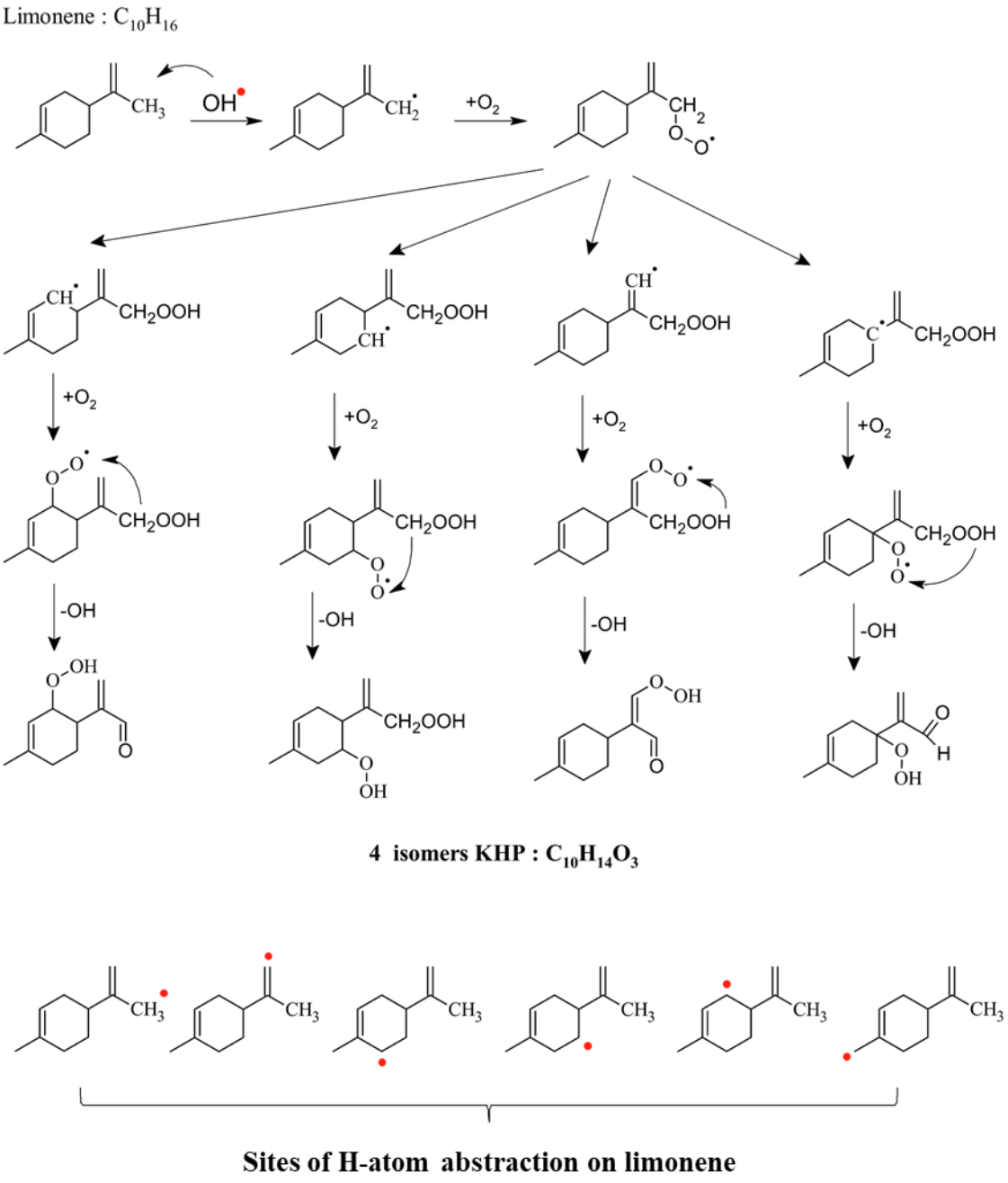
25 **SI Figure 1.** CH_2- Kendrick mass defect plots, DBE: 1-4



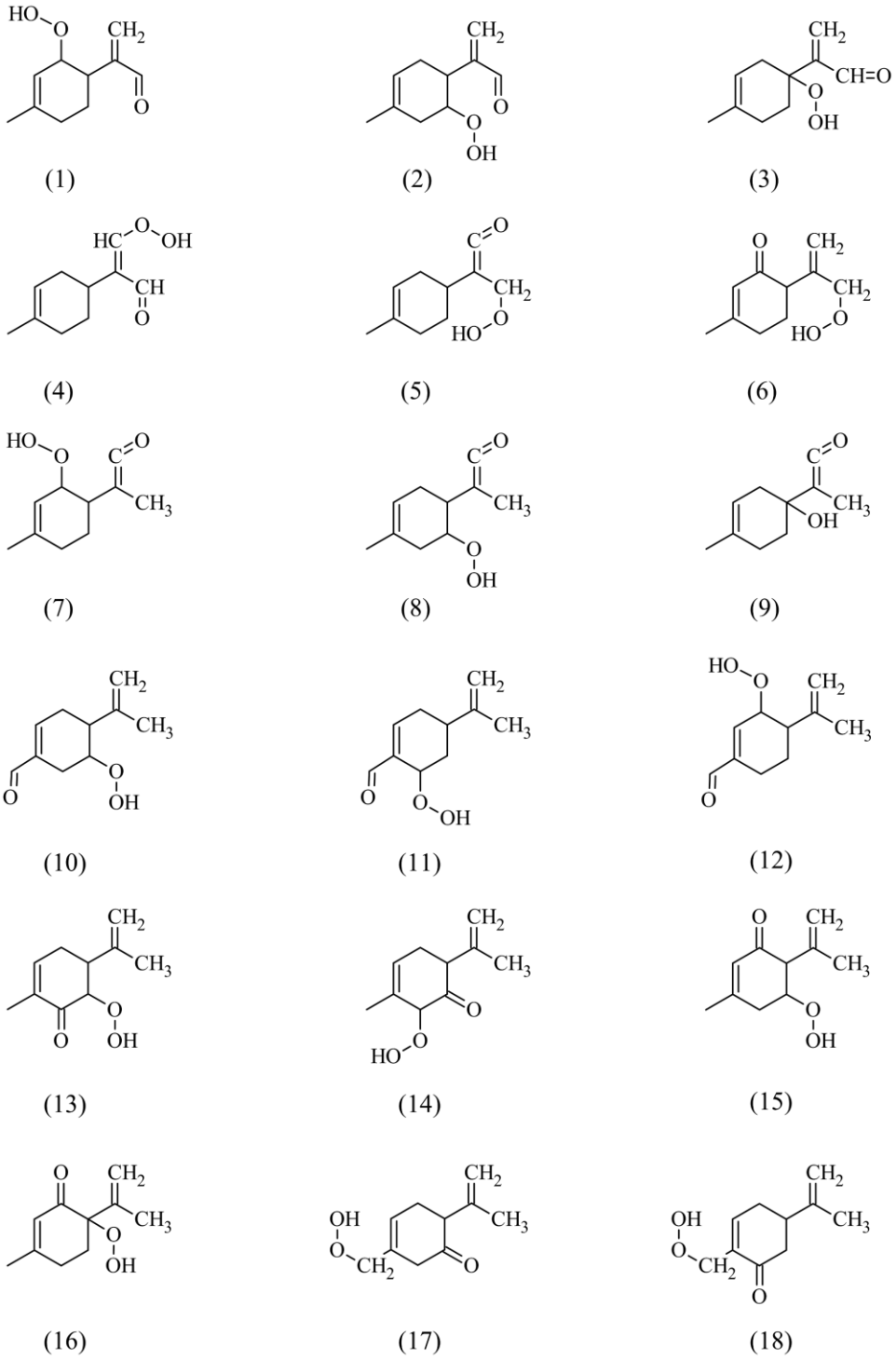
SI Figure 2. CH_2- Kendrick mass defect plots, DBE: 5-8



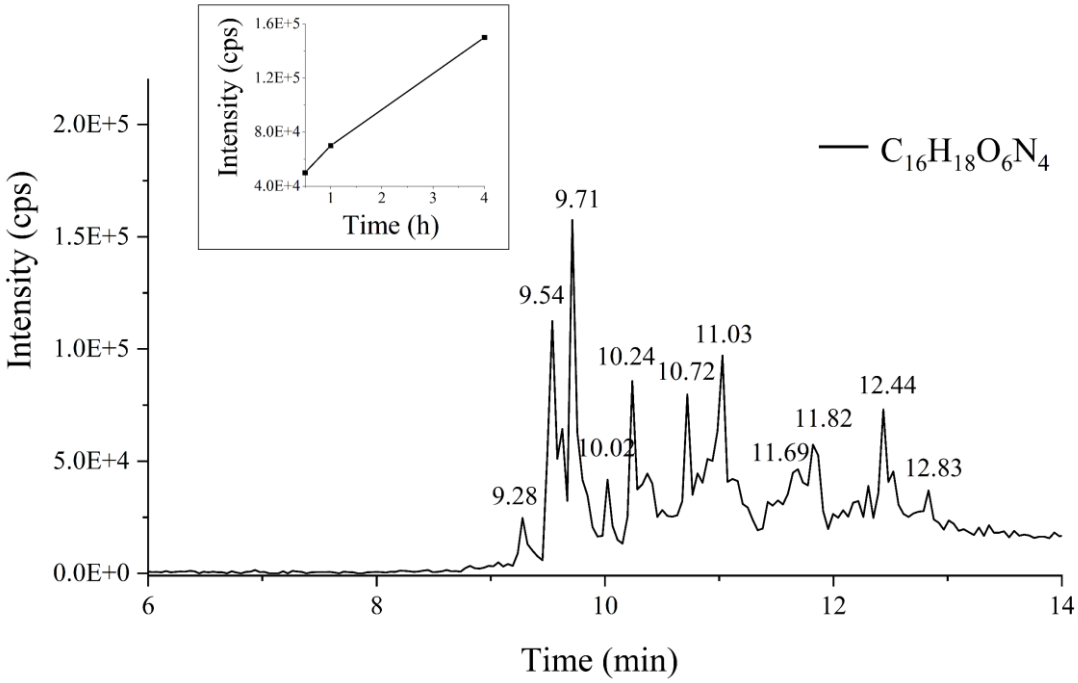
SI Figure 3. CH_2- Kendrick mass defect plots, DBE: 9-11



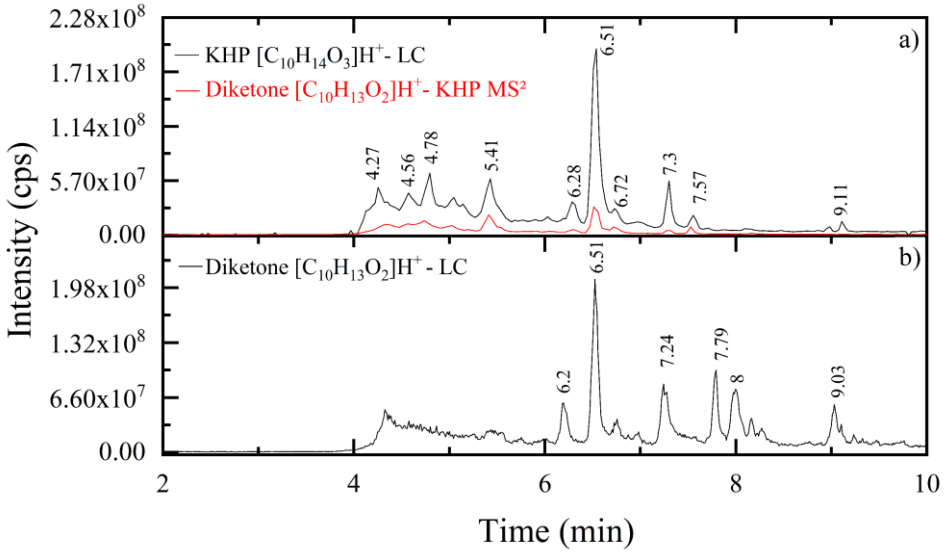
SI Figure 4. Examples of reaction mechanisms for the formation of KHPs from limonene and all the sites of H-atom abstraction on limonene that can give KHPs (18 isomers in total).



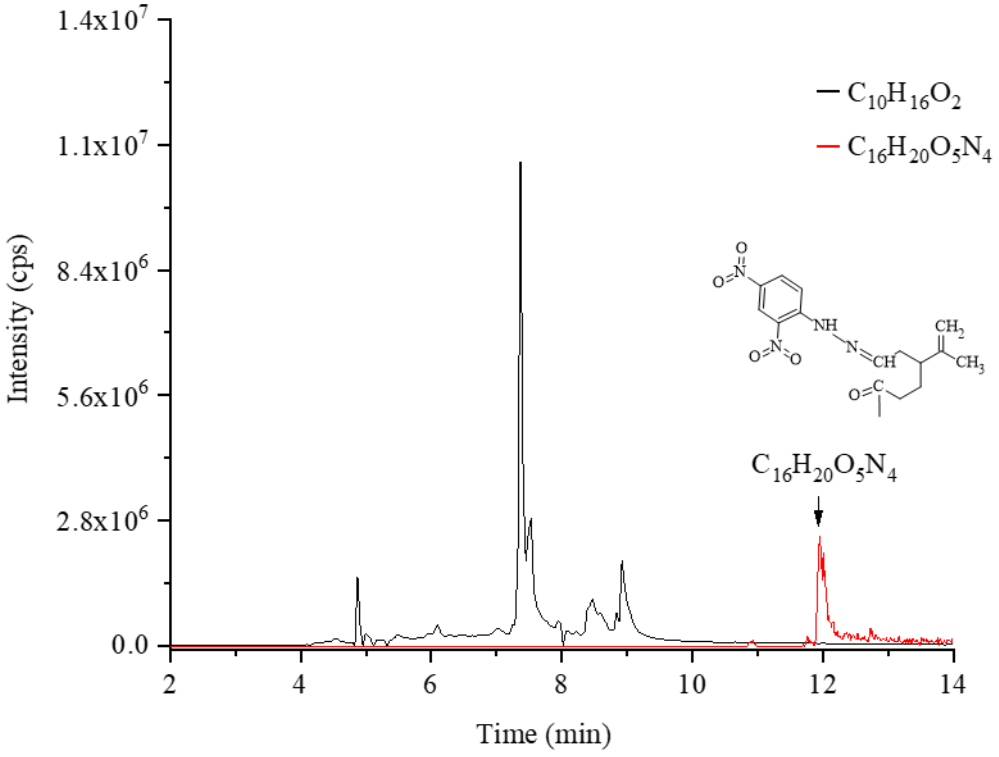
35 **SI Figure 5.** 18 isomers of KHP potentially formed by oxidation initiated by the radical OH˙



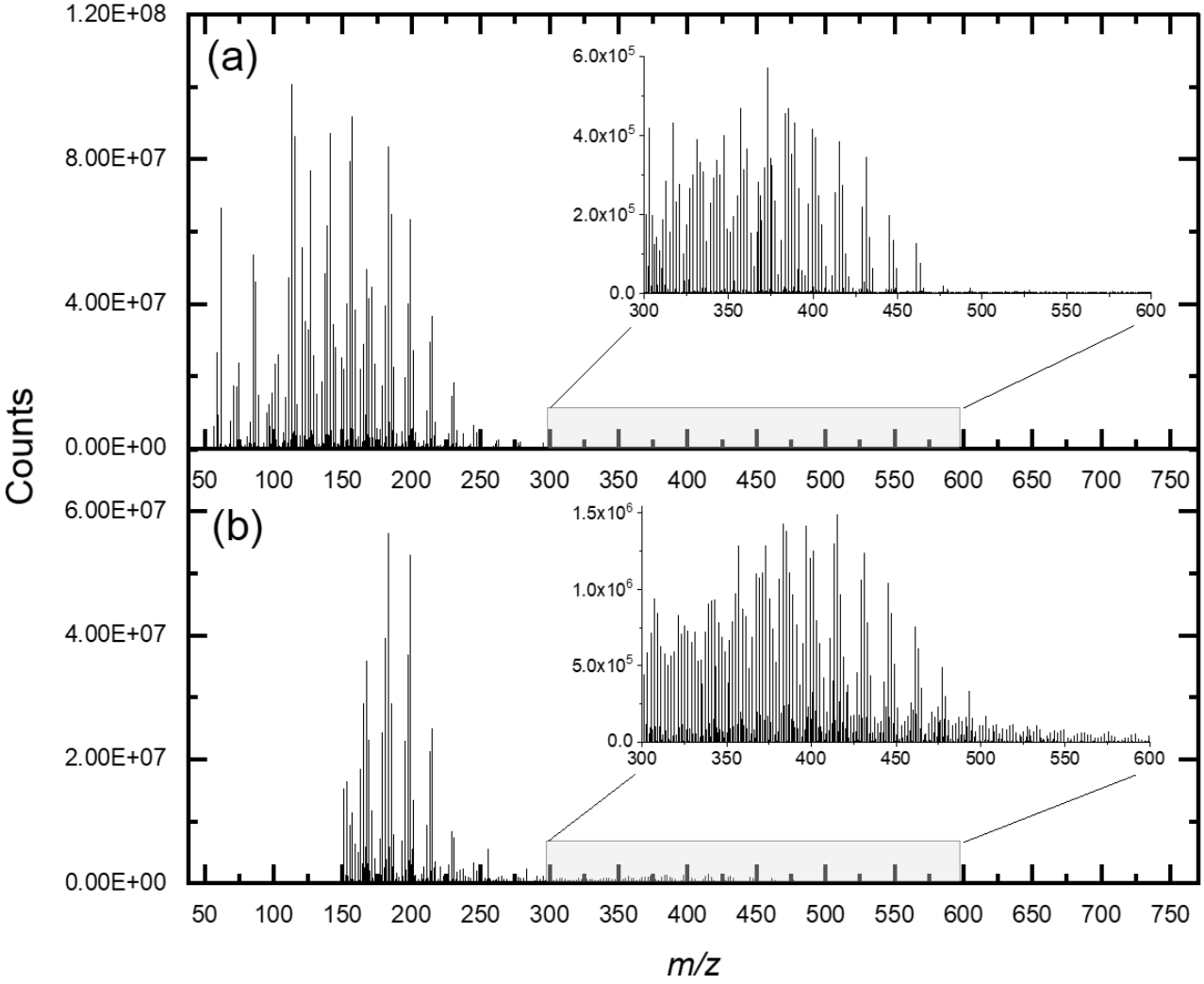
SI Figure 6. UHPLC-APCI neg (tSIM) spectrum of the compound $C_{16}H_{18}O_6N_4$ from the reaction of KHPs with 2,4-DNPH, inset: increase of the peak intensity at 9.71 min as a function of reaction time with DNPH.



SI Figure 7. comparison of UHPLC profiles of diketones and KHPs. a) UHPLC KHPs with diketones signal extracted from the MS/MS of the KHP, b) UHPLC profile of diketones.



45 **SI Figure 8.** Comparison of the UHPLC profile (APCI $^-$ mode) of $C_{10}H_{16}O_2$ (after adding DNPH) from the Waddington mechanism with that obtained by the addition of DNPH.



SI Figure 9. Comparison of limonene oxidation spectra sample analyzed by FIA and HESI (negative mode, sheath 12, aux gas 0, voltage 3.8kV, Tcapillary 300°C, vaporizer temperature120°C, sheath gas flow of 12 a.u., auxiliary gas flow of 6 a.u., sweep gas flow of 0 a.u., Hamilton syringe at a flow rate of 3 μL min−1), a) mass range 50-750 amu, b) 150-750 amu; insets: zoom on the 300-600 amu range.