

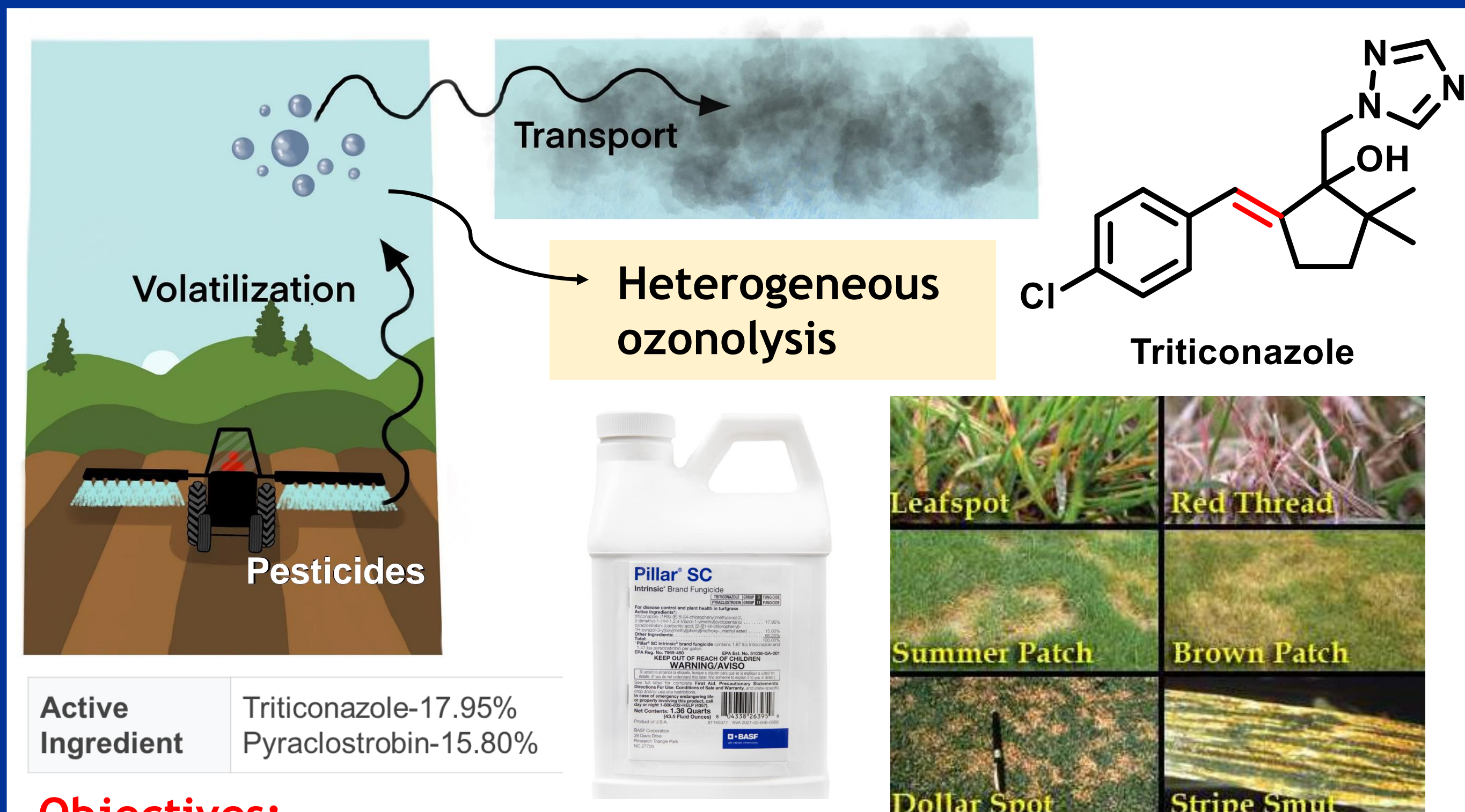


Pesticides in the Atmosphere: The Heterogeneous Ozonolysis of Triticonazole



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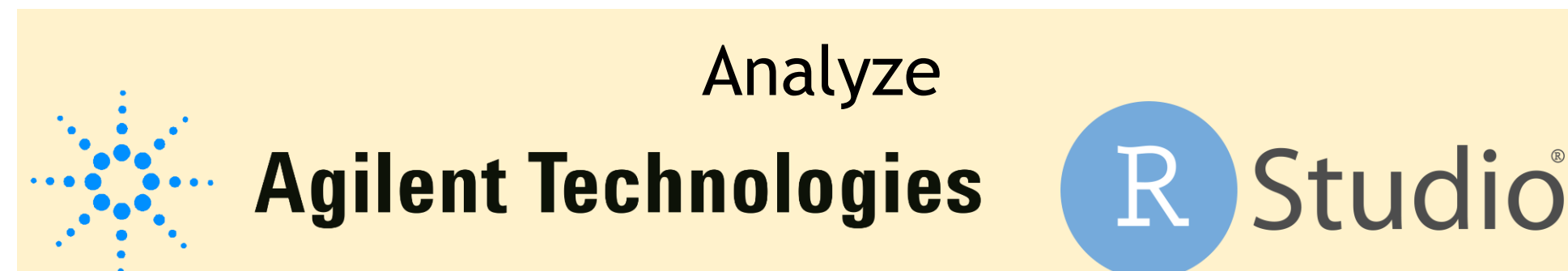
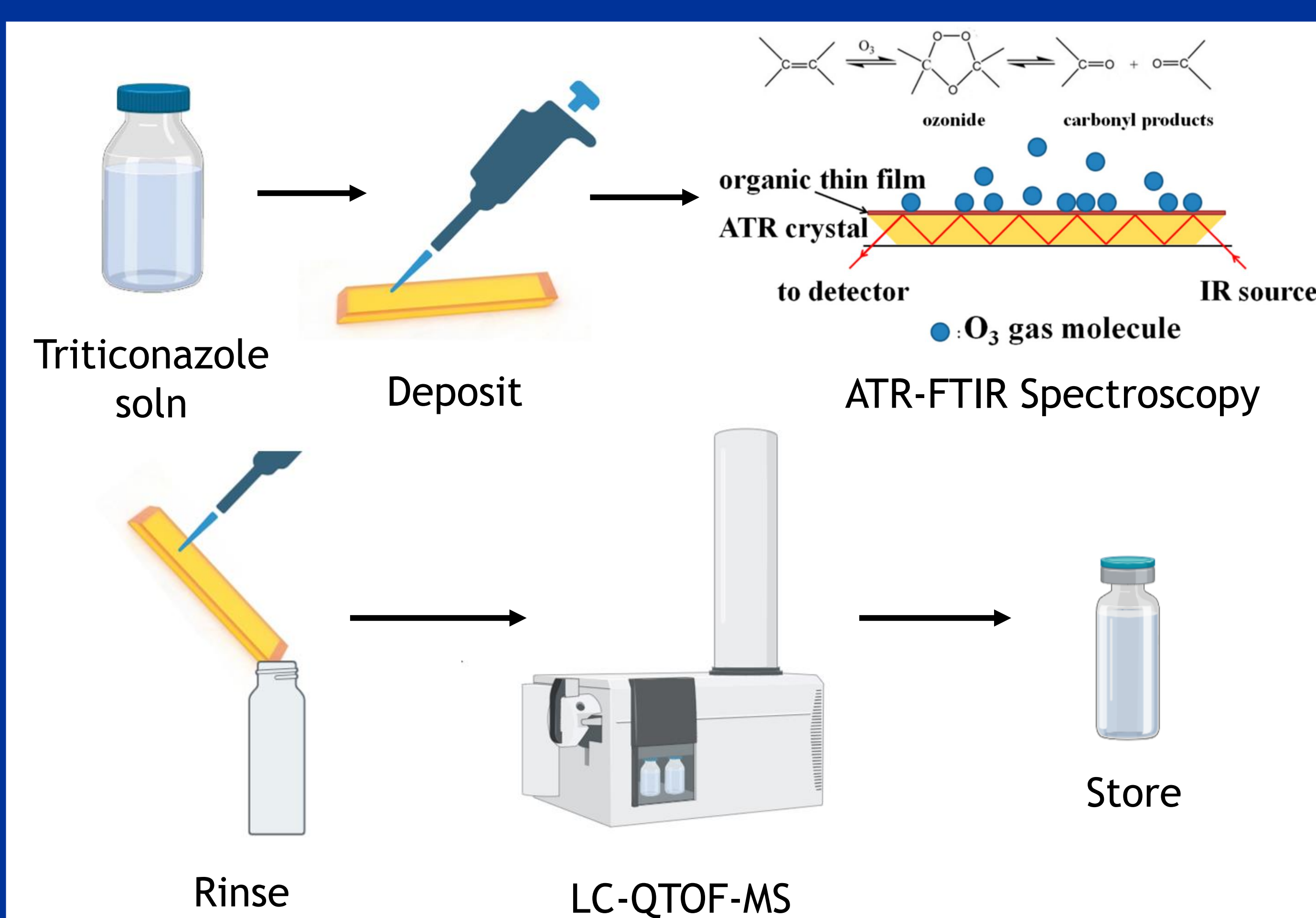
Motivation



Objectives:

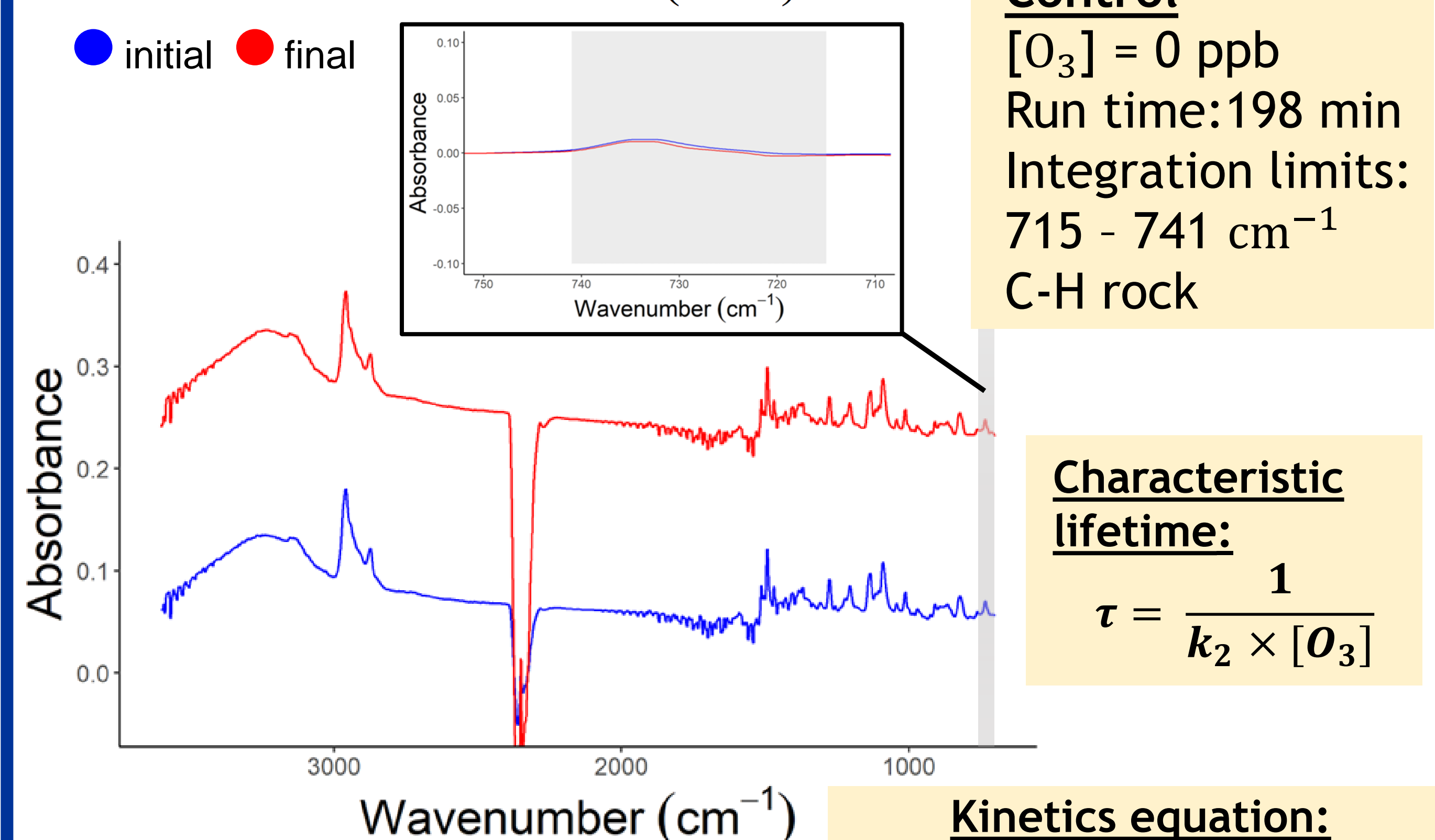
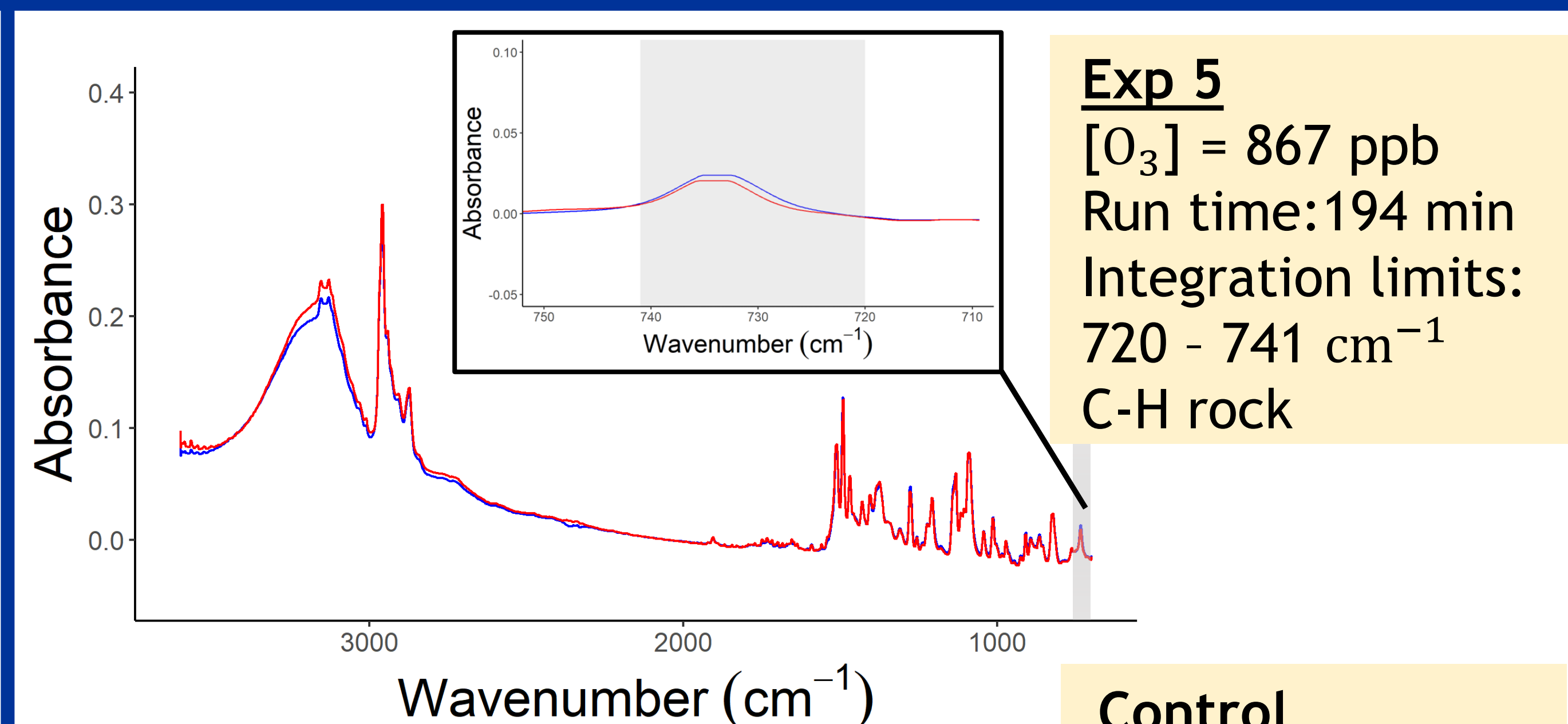
1. Conduct ozonolysis degradation of triticonazole and monitor using ATR-FTIR spectroscopy.
2. Determine rate constant.
3. Characterize products using LC-QTOF-MS

Methods



Roberts et al., J. Chem. Educ. 2016, 93(4), 733-737.

Reaction Kinetics

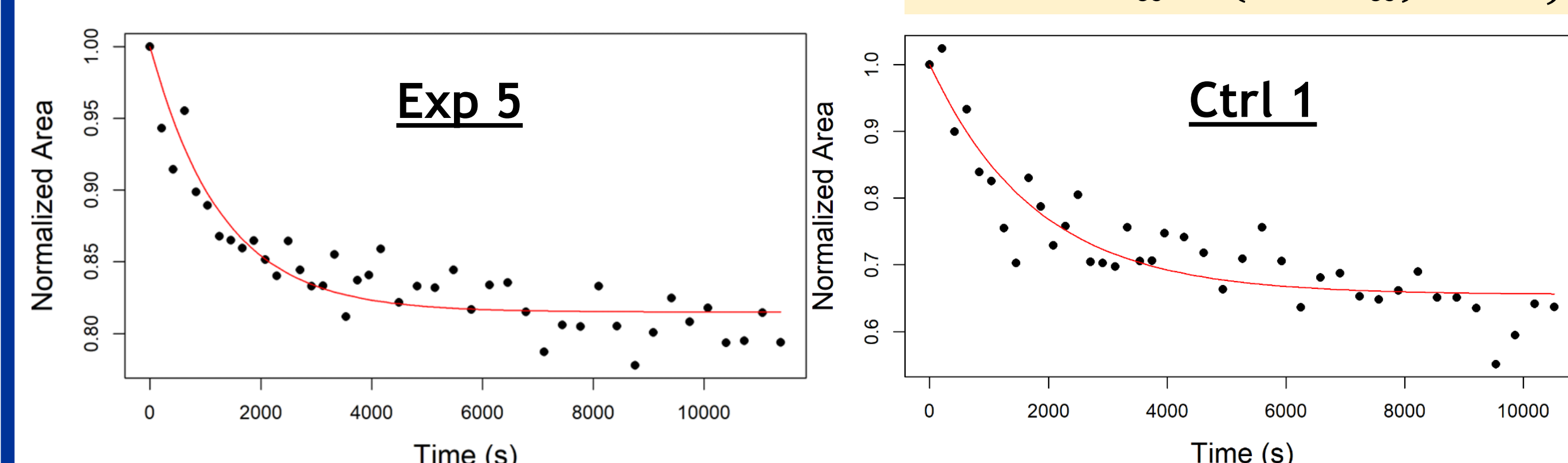


Characteristic lifetime:

$$\tau = \frac{1}{k_2 \times [O_3]}$$

Kinetics equation:

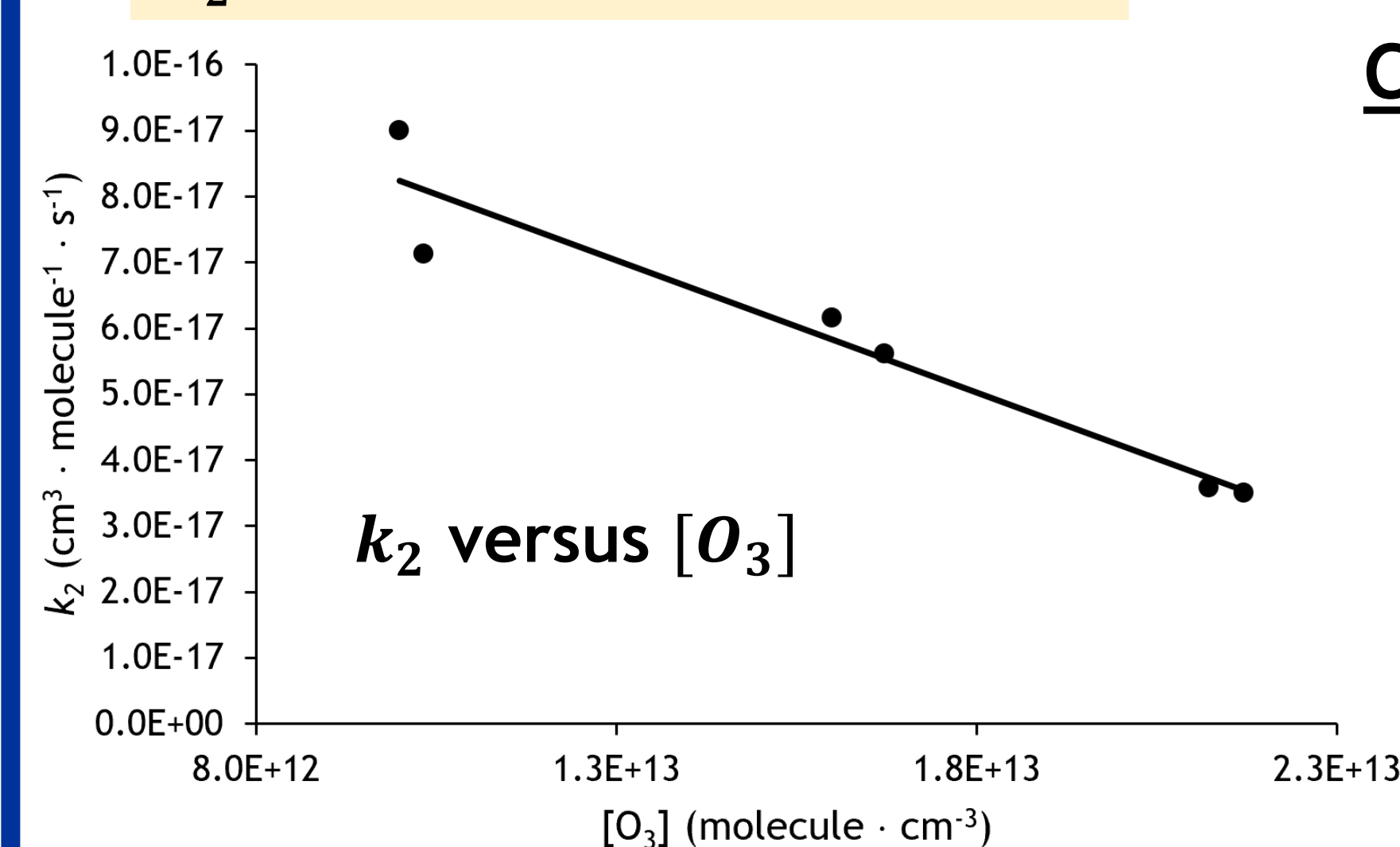
$$\text{Area} = A_{\infty} + (1 - A_{\infty})e^{-k_1 t}$$



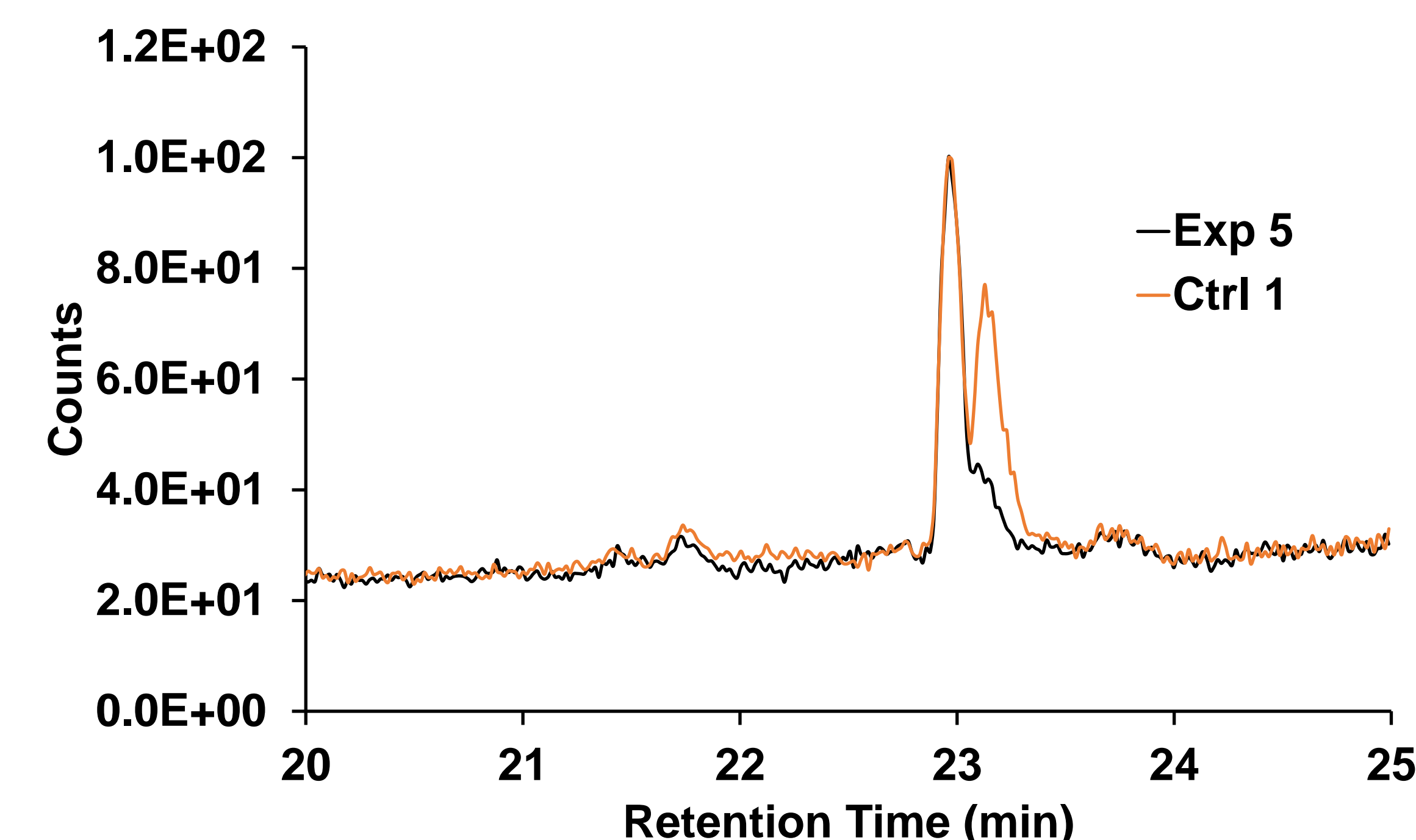
Characteristic lifetime:

Pristine conditions (20 ppb)
 $\tau = 6.9 - 9.5 \text{ hours}$

Polluted conditions (200 ppb)
 $\tau = 41-57 \text{ min}$



Product Identification



Compound (CAS #)	Molecular formula	[M+H] ⁺ (m/z)
Triticonazole (131983-72-7)	C ₁₇ H ₁₈ ClN ₃ O ₂	318.1368

Table of features found in 3 or more Exp

Compound #	Name (CAS #)	# of Exp	Avg Retention time (min)	Avg m/z	Formula	Formula difference (ppm)
2	Prednisolamate (5626-34-6)	4	23.15	474.2855	C ₂₇ H ₃₉ NO ₆	--
5	--	5	23.15	256.2999	C ₁₇ H ₃₇ N	0.15
7	--	4	21.73	158.1541	C ₉ H ₁₉ NO	1.00
9	--	3	23.85	332.3312	C ₂₃ H ₄₁ N	-0.33
17	--	3	23.15	488.3012	--	--

Conclusions

1. The reaction mechanism and pathway change when exposed to different amounts of ozone.
2. Features were identified via LC-QTOF-MS however, in silico analysis methods such as SIRIUS and CSI:FingerID should be performed to generate molecular formulas and structures.
3. Characterization of degradation products becomes ever more crucial as ozone increases in the atmosphere.

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