Supporting information

Photo-oxidation of 11-nor-9-carboxy-Δ^9-tetrahydrocannabinol using medium-pressure UV and UV/H_2O_2 – A kinetic study

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SI- Text-1. Kinetic models for THC-COOH in UV

The mechanisms of oxidation by UV photolysis have been investigated extensively, and kinetic rates of THC-COOH under both UV and UV/H_2O_2 are described presently. The kinetic model for the degradation of PPCPs by UV and UV/H_2O_2 was described by Sharpless and Linden (2003)[1] and the model is here applied to THC-COOH:

$$-\frac{d[THC-COOH]}{dt}=k_{UV}[THC-COOH] \qquad \text{Eq. (1)}$$

Where, k_{UV} can be either time-based pseudo first-order rate constant (min^{-1}) from the slope of the plot of ln([THC-COOH$_0$]/[THC-COOH]) versus reaction time (min) or fluence-based pseudo first-order rate constant (cm^2 mJ^{-1}), by using the plot of ln([THC-COOH$_0$]/[THC-COOH]) versus UV dose (mJ cm^{-2}). In this study, k_{UV} was estimated from the slope of the plot of ln[THC-COOH$_0$]/[THC-COOH] versus UV dose (mJ cm^{-2}).

SI- Text-2. Kinetic models for THC-COOH in UV/H_2O_2

With the addition of H_2O_2, two main pathways contribute to the overall degradation of THC-COOH: UV photolysis (k_{UV}) and hydroxyl radical attack ($k_{\cdot OH}$)[2,3] and based on this approach, the expression is represented as:

$$-\frac{d[THC-COOH]}{dt} = k_{UV}[THC-COOH] + k_{\cdot OH}[\cdot OH][THC-COOH] \qquad \text{Eq. (1)}$$

Where $k_{\cdot OH}$ is the second-order rate constant for the reaction between ·OH and THC-COOH. Because the hydroxyl radical concentration can be assumed to be constant over the range of the reaction[3] and this results in $k_{\cdot OH}$ converting into a pseudo first-order rate constant $k'_{\cdot OH}$. Thus, the following equation may be used to describe the degradation of THC-COOH during UV/H_2O_2 process:

$$-\frac{d[THC-COOH]}{dt} = (k_{UV} + k'_{\cdot OH})[THC-COOH] = k_T[THC-COOH] \qquad \text{Eq. (2)}$$

Where k_T is the pseudo first-order rate constant for overall oxidation of THC-COOH by UV/H_2O_2 process and it can be determined from the slope of a plot between ln([THC-$COOH_0$]/[THC-COOH]) versus UV fluences (mJ cm^{-2}). Once the reaction constant k_T is known, the rate constant for the radical reaction $k'_{\cdot OH}$ can be deduced by subtracting the previous known value of k_{UV} (the fluence based pseudo first-order rate constant for the degradation of THC-COOH by UV photolysis).

Table S1: Optimized compound-specific parameters and retention time for LC-MS/MS

Analytes	Precursor Ion (m1/z)	Product Ion (m/z)	Dwell	Fragmentor (V)	Collision energy (V)	Cell accelerator voltage (V)
THC-COOH	345.2	327.1 (299.1)	200	120	14 (18)	4
THC-COOH-d_3	348	330	200	120	18	4

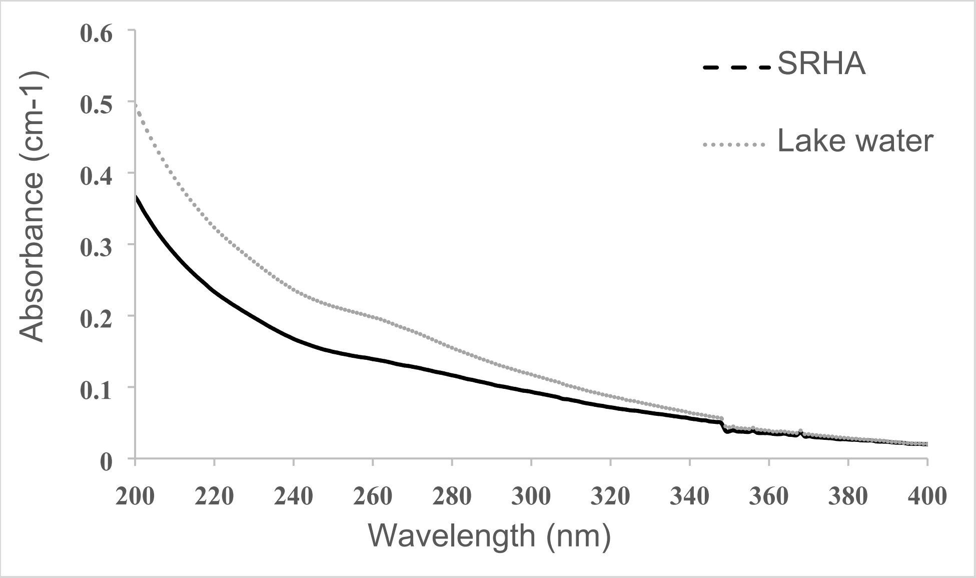

Figure S1. Absorption spectra of three different water types using a Cary 50 UV spectrophotometer (Agilent Technology, Canada). 4 mg L^{-1} of Suwannee river humic acid (SRHA) and lake water from the Lake Major drinking water treatment plant, Halifax, NS, Canada.

References

[1] Sharpless C. M. and Linden, K.G., 2003. Experimental and model comparisons of low- and medium-pressure Hg lamps for the direct and H_2O_2 assisted UV photodegradation of *N*-Nitrosodimethylamine in simulated drinking water. Environmental. Science & Technology 37(9), 1933-1940.

[2] Chelme-Ayala, P., El-Din, M. G., Smith, D.W., 2010. Degradation of bromoxynil and trifluralin in natural water by direct photolysis and UV plus H_2O_2 advanced oxidation process. Water research 44(7), 2221-2228.

[3] Benitez, F. J., Acero, J. L., Real, F. J., Roldan, G., Casas, F., 2011. Comparison of different chemical oxidation treatments for the removal of selected pharmaceuticals in water matrices. Chemical Engineering Journal 168(3), 1149-1156.