Supporting information

Photo-oxidation of 11-nor-9-carboxy-Δ⁹-tetrahydrocannabinol using medium-pressure UV and UV/H₂O₂ – A kinetic study

Yuri Park, Allison L. Mackie, Sean A. MacIsaac, Graham A. Gagnon*

*Centre for Water Resources Studies, Faculty of Civil and Resource Engineering, Dalhousie University, Halifax, NS, CA

* Corresponding Author: Graham A. Gagnon
Email: graham.gagnon@dal.ca
Address: Department of Civil and Resource Engineering, Dalhousie University, 1360 Barrington Street, Halifax NS, Canada (B3H 4R2)
Phone: +1 902 494 6070
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\textsubscript{2}O\textsubscript{2} are described presently. The kinetic model for the degradation of PPCPs by UV and UV/H\textsubscript{2}O\textsubscript{2} was described by Sharpless and Linden (2003)\textsuperscript{1} and the model is here applied to THC-COOH:

\[
-\frac{d[THC-COOH]}{dt} = k_{UV}[THC-COOH]
\]

Eq. (1)

Where, \(k_{UV}\) can be either time-based pseudo first-order rate constant (min\textsuperscript{-1}) from the slope of the plot of ln([THC-COOH\textsubscript{0}]/[THC-COOH]) versus reaction time (min) or fluence-based pseudo first-order rate constant (cm\textsuperscript{2} mJ\textsuperscript{-1}), by using the plot of ln([THC-COOH\textsubscript{0}]/[THC-COOH]) versus UV dose (mJ cm\textsuperscript{-2}). In this study, \(k_{UV}\) was estimated from the slope of the plot of ln([THC-COOH\textsubscript{0}]/[THC-COOH]) versus UV dose (mJ cm\textsuperscript{-2}).
SI- Text-2. Kinetic models for THC-COOH in UV/H\textsubscript{2}O\textsubscript{2}

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

$$-\frac{d[THC-COOH]}{dt} = k_{UV} [THC-COOH] + k_{·OH} [·OH][THC-COOH]$$

Eq. (1)

Where $k_{·OH}$ 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\textsuperscript{3} and this results in $k_{·OH}$ converting into a pseudo first-order rate constant $k'_{·OH}$. Thus, the following equation may be used to describe the degradation of THC-COOH during UV/H\textsubscript{2}O\textsubscript{2} process:

$$-\frac{d[THC-COOH]}{dt} = (k_{UV} + k'_{·OH})[THC-COOH] = k_{T}[THC-COOH]$$

Eq. (2)

Where $k_{T}$ is the pseudo first-order rate constant for overall oxidation of THC-COOH by UV/H\textsubscript{2}O\textsubscript{2} process and it can be determined from the slope of a plot between ln([THC-COOH\textsubscript{0}]/[THC-COOH]) versus UV fluences (mJ cm\textsuperscript{-2}). Once the reaction constant $k_{T}$ is known, the rate constant for the radical reaction $k'_{·OH}$ 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

<table>
<thead>
<tr>
<th>Analytes</th>
<th>Precursor Ion (m/z)</th>
<th>Product Ion (m/z)</th>
<th>Dwell</th>
<th>Fragmentor (V)</th>
<th>Collision energy (V)</th>
<th>Cell accelerator voltage (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>THC-COOH</td>
<td>345.2</td>
<td>327.1 (299.1)</td>
<td>200</td>
<td>120</td>
<td>14 (18)</td>
<td>4</td>
</tr>
<tr>
<td>THC-COOH-d₃</td>
<td>348</td>
<td>330</td>
<td>200</td>
<td>120</td>
<td>18</td>
<td>4</td>
</tr>
</tbody>
</table>
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

