Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.


Supporting Information

# Photochemical Degradation of the UV Filter Octylmethoxycinnamate in Solution and in Aggregates

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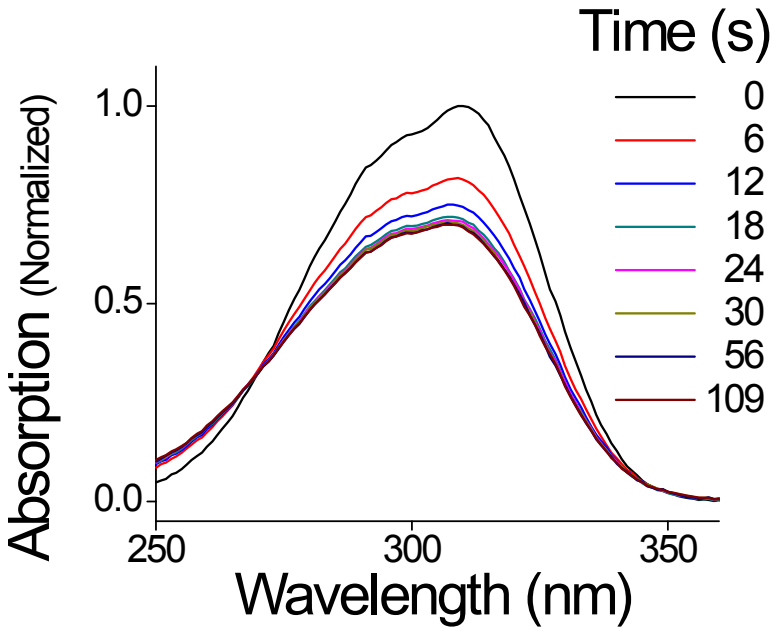


Figure S1. Absorption spectra of *trans*-OMC in methanol under solar simulated UV irradiation. Only one isosbestic point is obvious because of the red-shift in the absorption spectrum compared to that in cyclohexane. The photostationary state between the two OMC isomers is achieved quickly and further photodegradation is negligible.

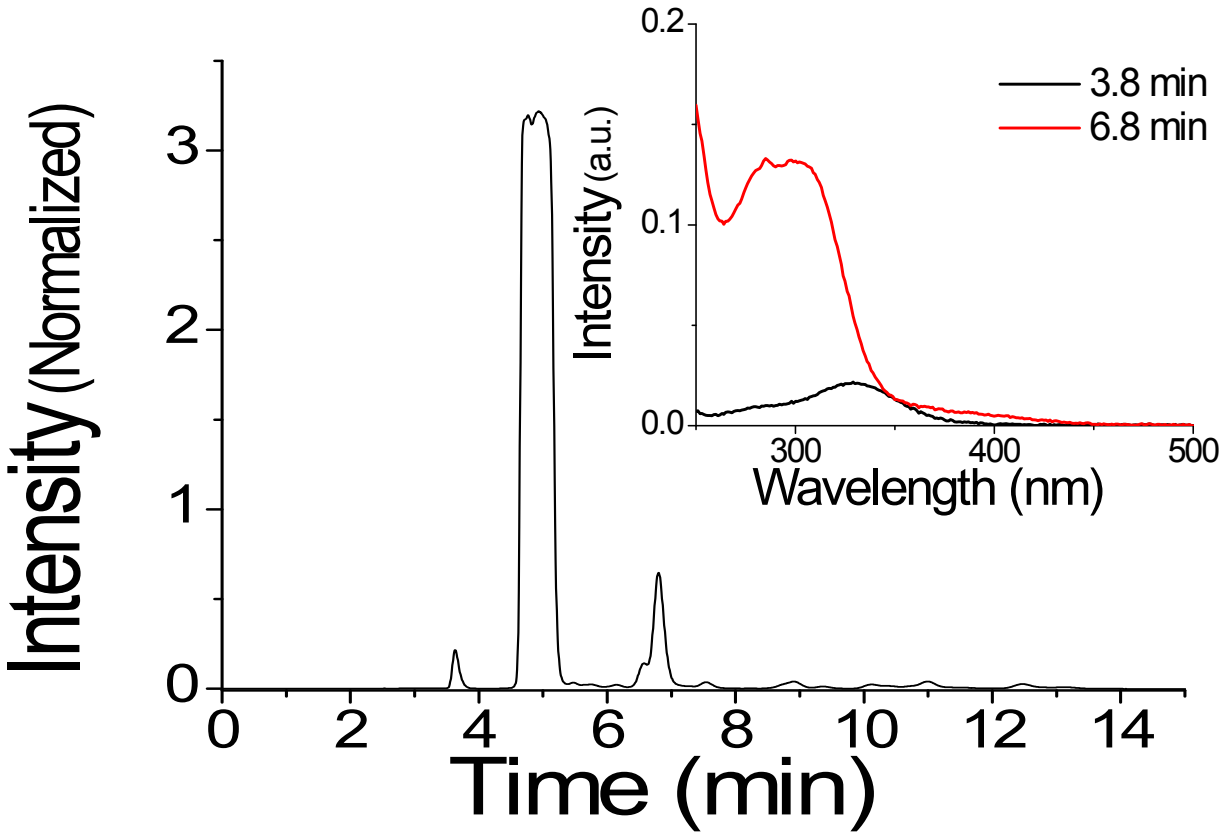


Figure S2. HPLC chromatograph of post-UV irradiated OMC thin film detected at 310 nm. The peak at 3.8 minutes is a solvent impurity. The chromatogram shows intense peaks at 5 minutes corresponding to the cis and trans isomers. The peaks between 6 and 8 minutes correspond to the photodimers [Ref. MacManus). The absorption spectrum of the 6.8 minute eluent peak is shown in the inset. Note that there are no distinguishable peaks after 8 minutes.

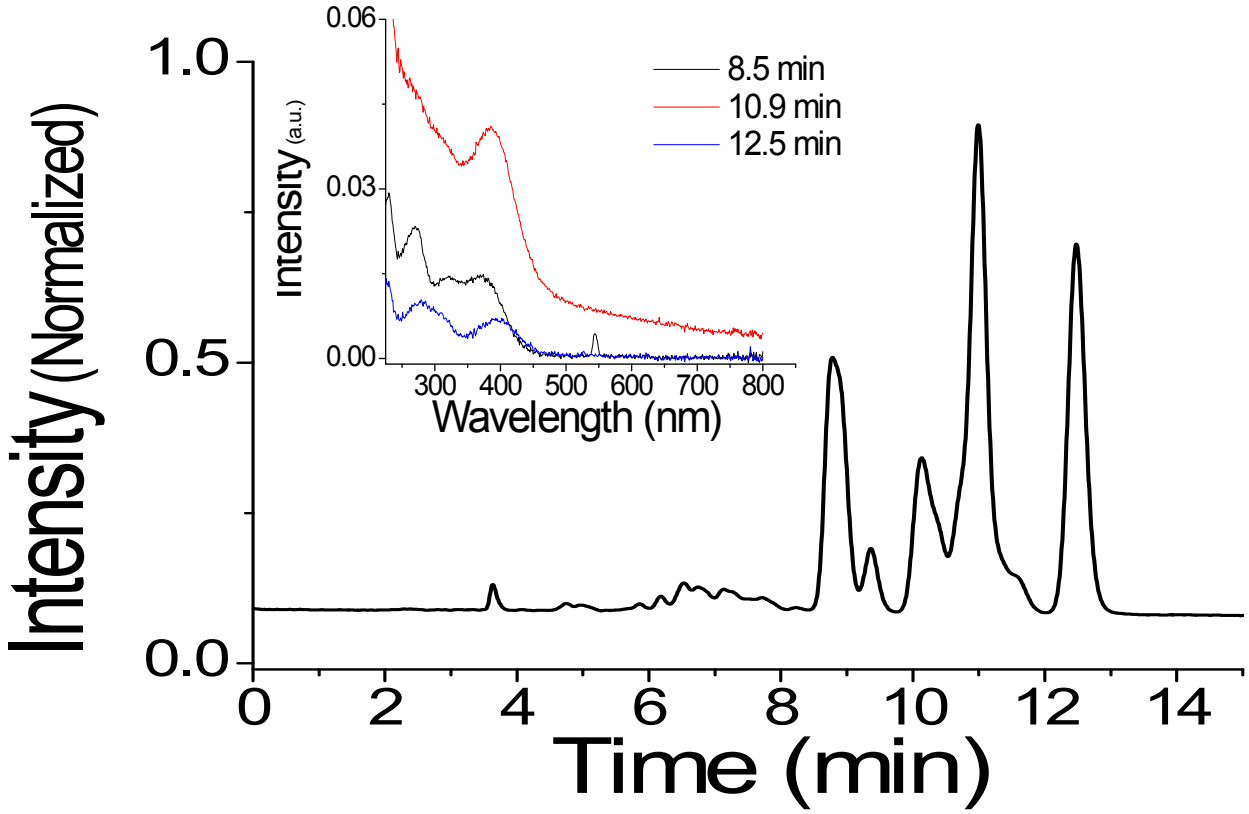


Figure S3. a) HPLC chromatograph of post-UV irradiated OMC thin film detected at 400 nm. The absorption spectra for the UVA absorbing fractions collected at 8.5 minutes, 10.9 minutes, and 12.5 minutes are shown in the inset. Each of these samples had < 0.1 mg once the solvent was evaporated, preventing further analysis by NMR. All these spectra show UVA absorption; we attribute the peaks near 280 nm to the presence of dimers based upon the mass spec of the sample at 12.5 min (Figure S4). The *cis* and *trans* photoisomers of OMC eluted at 5 minutes, and the photodimers between 6 and 8 minute (Figure S2).

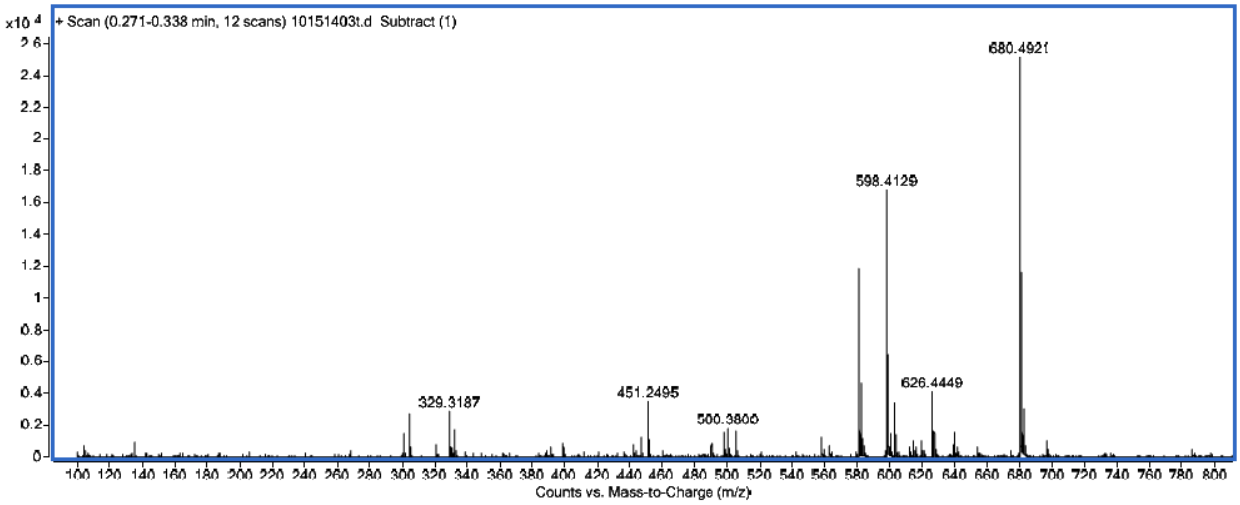


Figure S4. Mass spectrum of eluent at 12.5 min from the HPLC chromatograph.

The data shows that there is no monomeric peak at 281 m/z, which is consistent with the HPLC showing the monomeric forms elute at 5 min before the UVA-absorbing species at rf > 8 min. In addition to photodimer peaks at 451 m/z and 581 m/z, there are multiple unidentified peaks of large m/z including 598 m/z, 625 m/z and 680 m/z. The presence of these peaks suggests that larger oligomeric species have been formed in the neat film after solar UV irradiation.