Supplementary information

Photodegradation of methotrexate in aqueous solution: degradation kinetics and identification of transformation products

Anaïs Espinosa, Sylvie Nélieu*, Pascale Lieben, Charles Skarbek, Raphaël Labruère, Pierre Benoit

*sylvie.nelieu@inrae.fr; Université Paris-Saclay, INRAE, AgroParisTech, UMR ECOSYS, 78850, Thiverval-Grignon, France

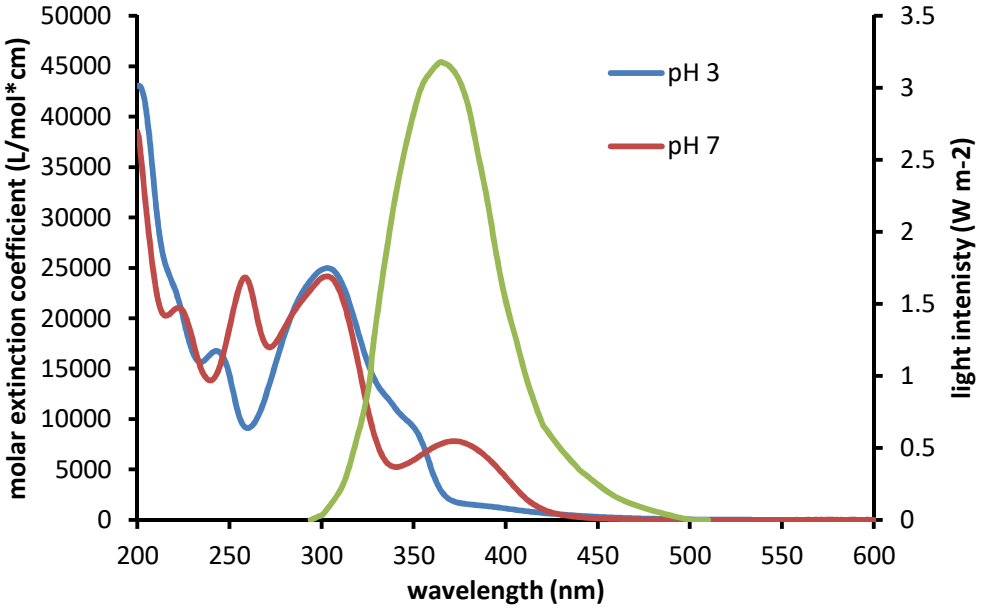

Fig. S1. Methotrexate absorption spectra at pH 7 and 3, and emission spectrum of the polychromatic lamps.

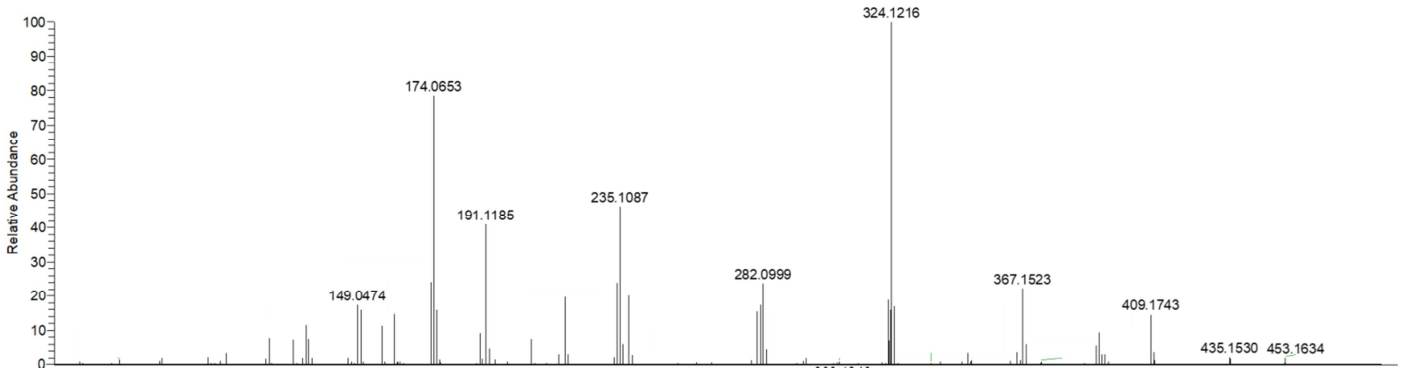

Fig. S2. Daughter ion spectrum (MS^2) of $[M - H]^-$ Methotrexate pseudo-molecular ion

Fig. S3. Negative mode for the identification of TP 408a:

a) Daughter ion spectrum (MS^2) of $[M - H]^-$ TP408a pseudo-molecular ion (m/z 407)

b) Fragmentation pattern from deprotonated parent ion

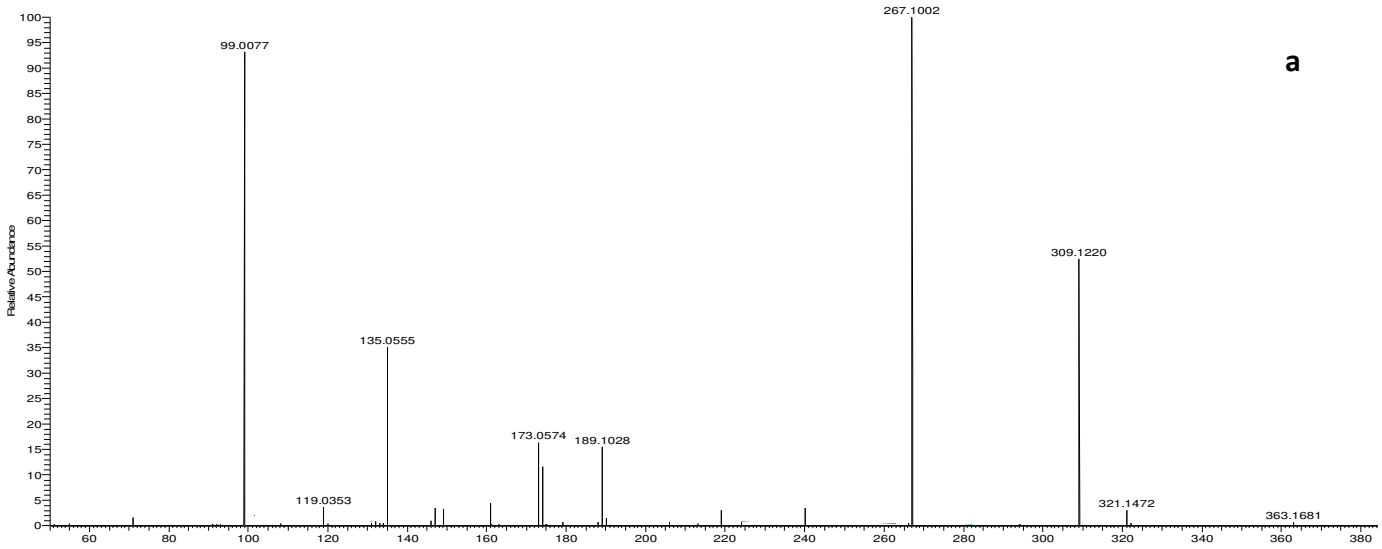

Fig. S4. Negative mode for the identification of TP 408b:

a) Daughter ion spectrum (MS^2) of $[M - H]^-$ TP408b pseudo-molecular ion (m/z 407)

b) Fragmentation pattern from deprotonated parent ion