

Supplementary Information for

Photochemical degradation of antibiotics: real-time investigation by aerodynamic thermal breakup droplet ionization mass spectrometry

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Text S1

The ATBDI method gist is based on two well-known formulas:

The Young–Laplace equation, (Rusanov, A.I., 1967. Phase Equilibria and Surface Phenomena. Khimiya, Leningrad [in Russian]):

$$P_d = P_0 + \frac{2\sigma}{r} \quad (1s)$$

where P_d is pressure inside a droplet of radius r , P_0 is ambient pressure, and σ is surface tension of the liquid;

and the van der Waals equation (Straub, J., Rosner, N., Grigull, U., 1980. Oberflächenspannung von leichtem und schwerem Wasser, Wärme- und Stoffübertragung. 13, 241-252):

$$\sigma \approx (T_c - T)^{3/2} \quad (2s)$$

where T_c is critical temperature.

The pressure inside a micron-sized drop can reach several atmospheres (eq. 1s), and it is controlled by surface tension (σ). As σ decreases (it heats up to a temperature close to T_c , eq. 2s), this pressure leads to the explosive breakup of the drop. According to the Dodd interpretation, the small droplets obtained are statistically charged (if there are charged particles in the initial solution).

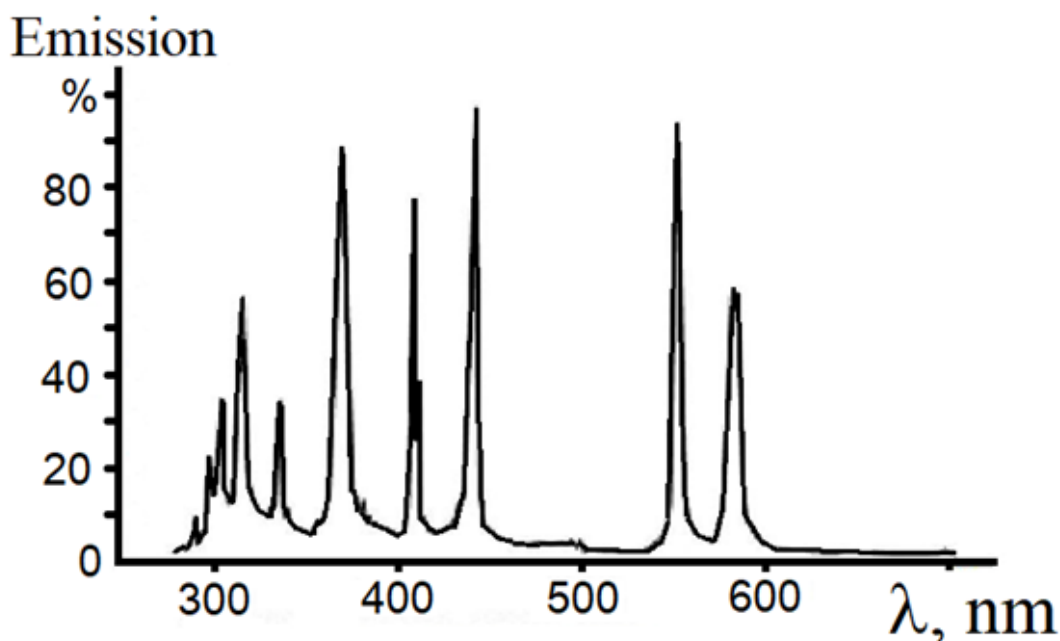


Figure S1. The emission spectrum of a mercury lamp DRK-120 (an arc mercury-quartz lamp) in the UV-vis region.

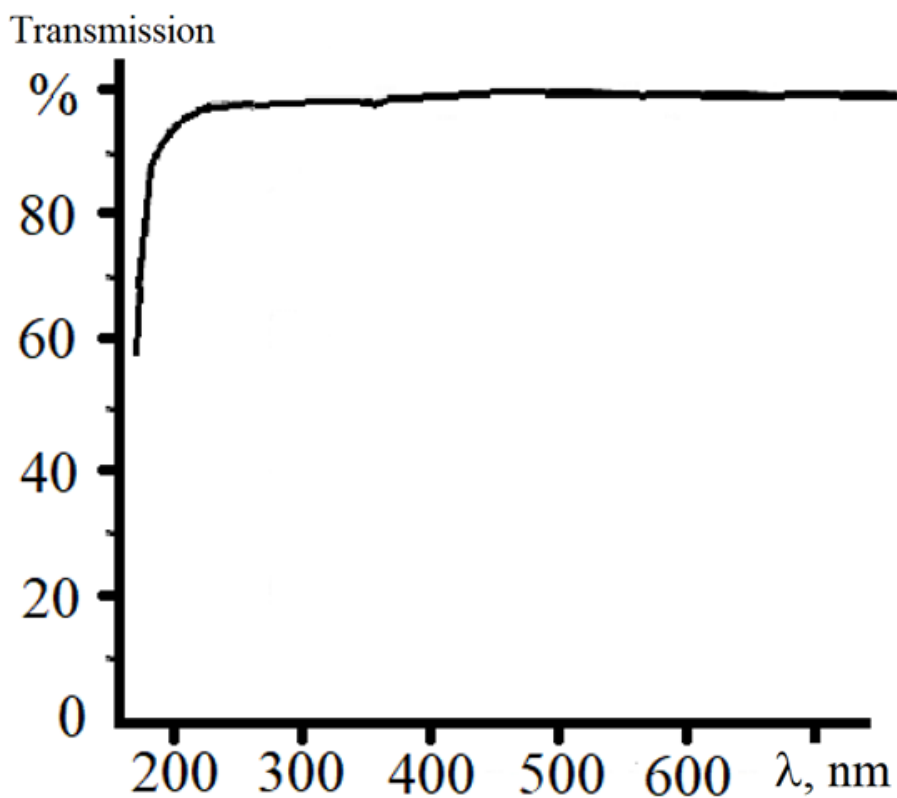
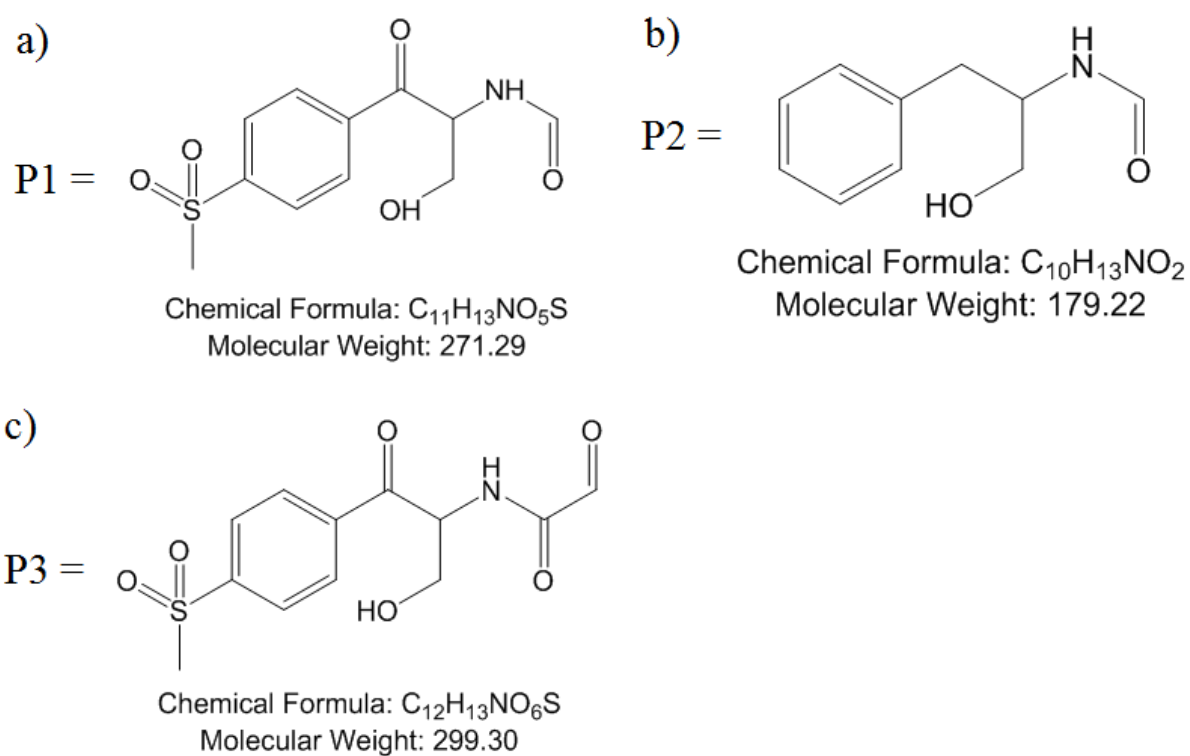
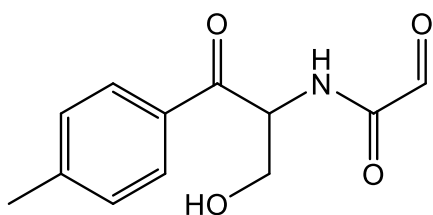


Figure S2. The transmission spectrum of quartz glass in the UV-vis region.



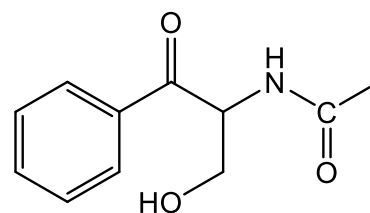
Scheme S1.

P4



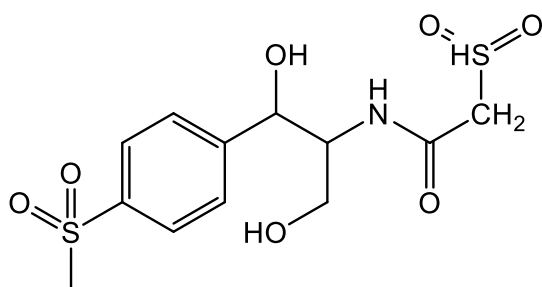
Chemical Formula: $C_{12}H_{13}NO_4$
Molecular Weight: 235.24

P5



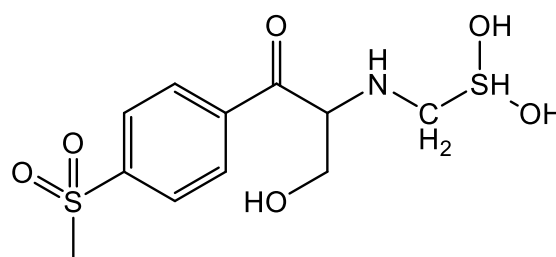
Chemical Formula: $C_{11}H_{13}NO_3$
Molecular Weight: 207.23

P6



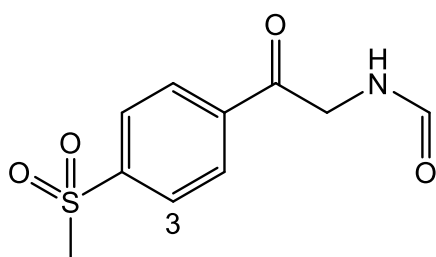
Chemical Formula: $C_{12}H_{17}NO_7S_2$
Molecular Weight: 351.39

P7



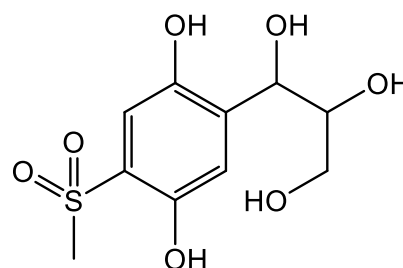
Chemical Formula: $C_{11}H_{17}NO_6S_2$
Molecular Weight: 323.38

P8



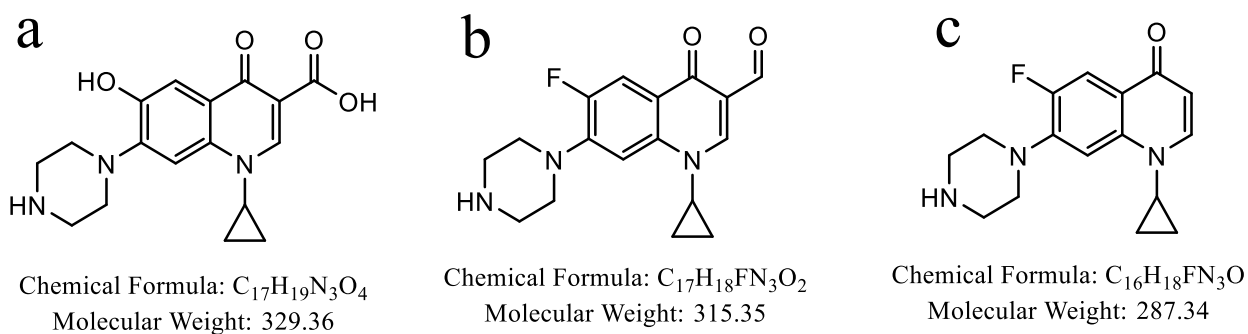
Chemical Formula: $C_{10}H_{11}NO_4S$
Molecular Weight: 241.26

P9



Chemical Formula: $C_{10}H_{14}O_7S$
Molecular Weight: 278.28

Scheme S2.



a - 1-cyclopropyl-6-hydroxy-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid

b - 1-cyclopropyl-6-fluoro-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carbaldehyde

c - 1-cyclopropyl-6-fluoro-7-(piperazin-1-yl)quinolin-4(1H)-one

Scheme S3.

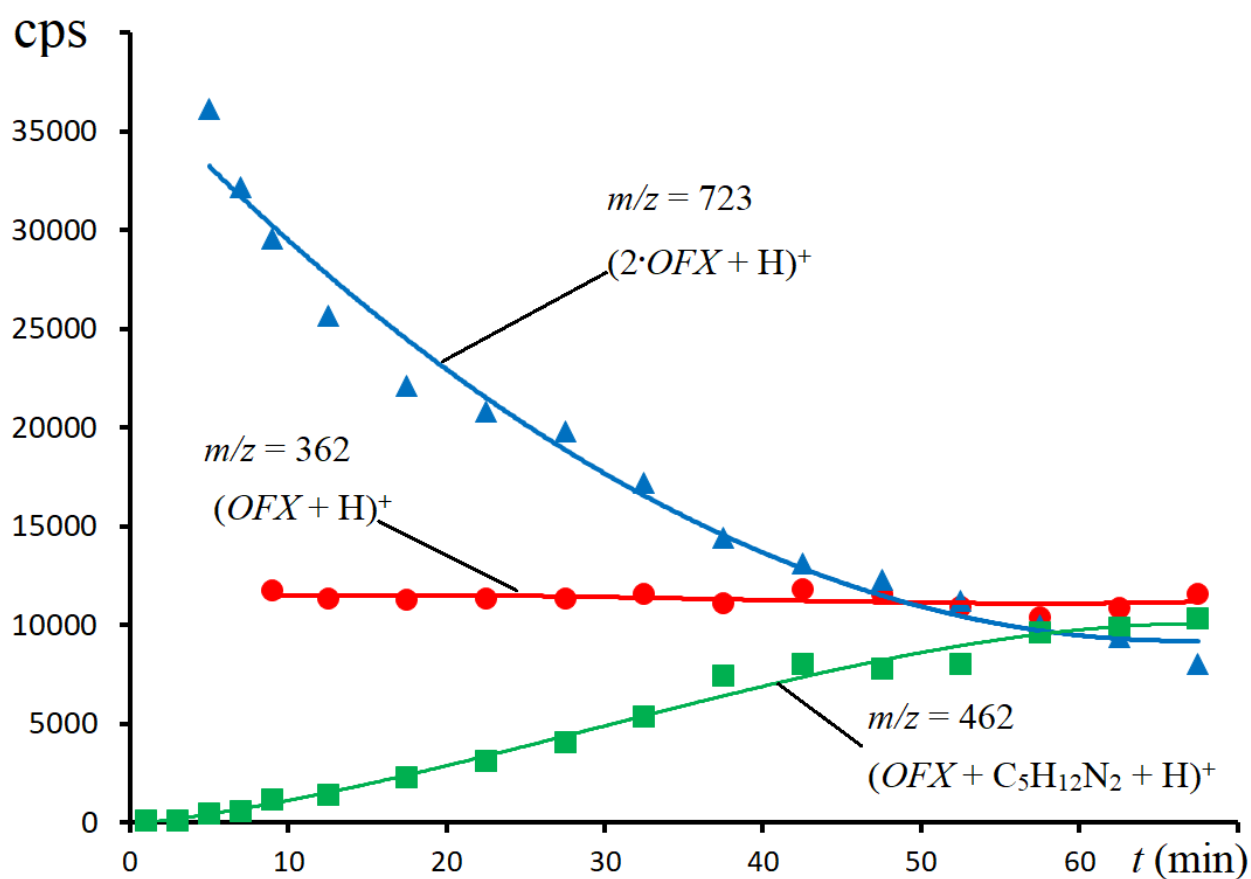
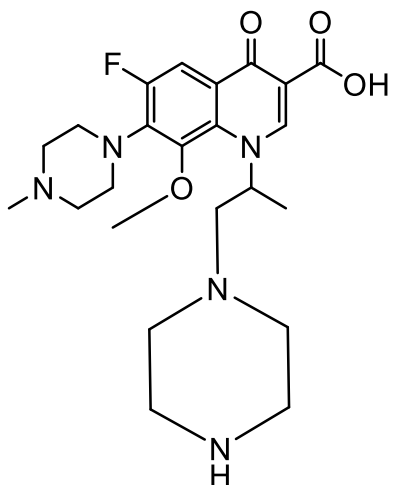


Figure S3. Kinetics of changes in peak intensities in the ATBDI mass spectra upon photolysis of the OFX aqueous solution. Experimental conditions: OFX concentration – 10^{-4} ; quartz tank; full light quartz lamp DRK-120.



6-fluoro-8-methoxy-7-(4-methylpiperazin-1-yl)-4-oxo-1-(1-(piperazin-1-yl)propan-2-yl)-1,4-dihydroquinoline-3-carboxylic acid

Chemical Formula: $C_{23}H_{32}FN_5O_4$

Molecular Weight: 461.54

Scheme S4.