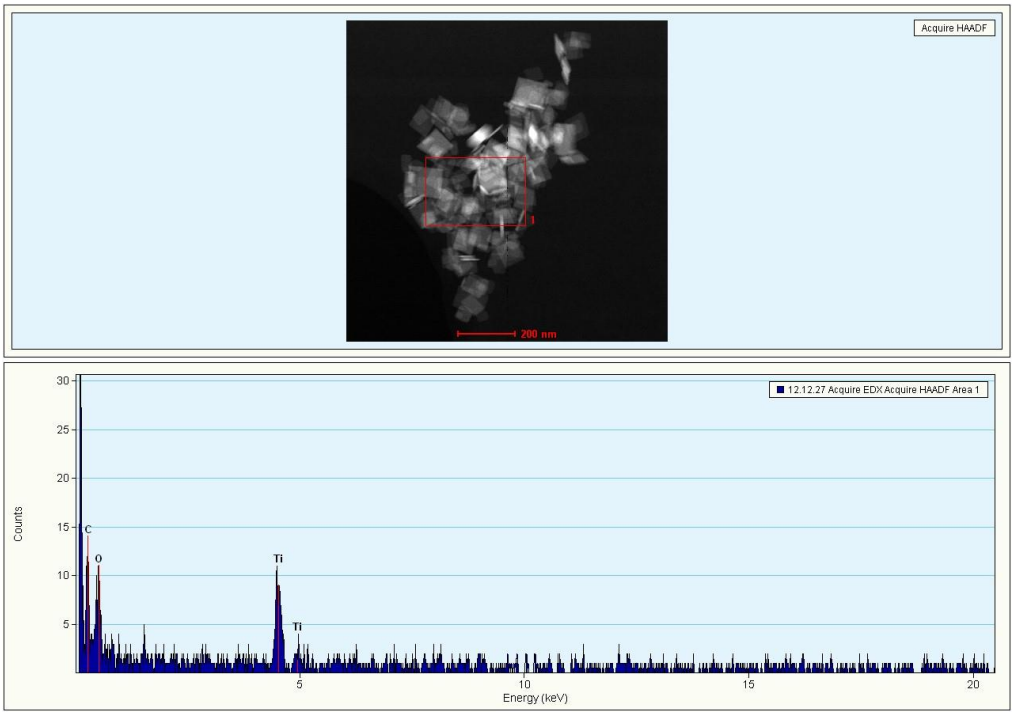
Supplementary information

Levofloxacin Degradation, Antimicrobial Activity Decrease, and Potential for Water Disinfection Using Peroxydisulfate Activation by Ag/TiO_2 under Sunlight

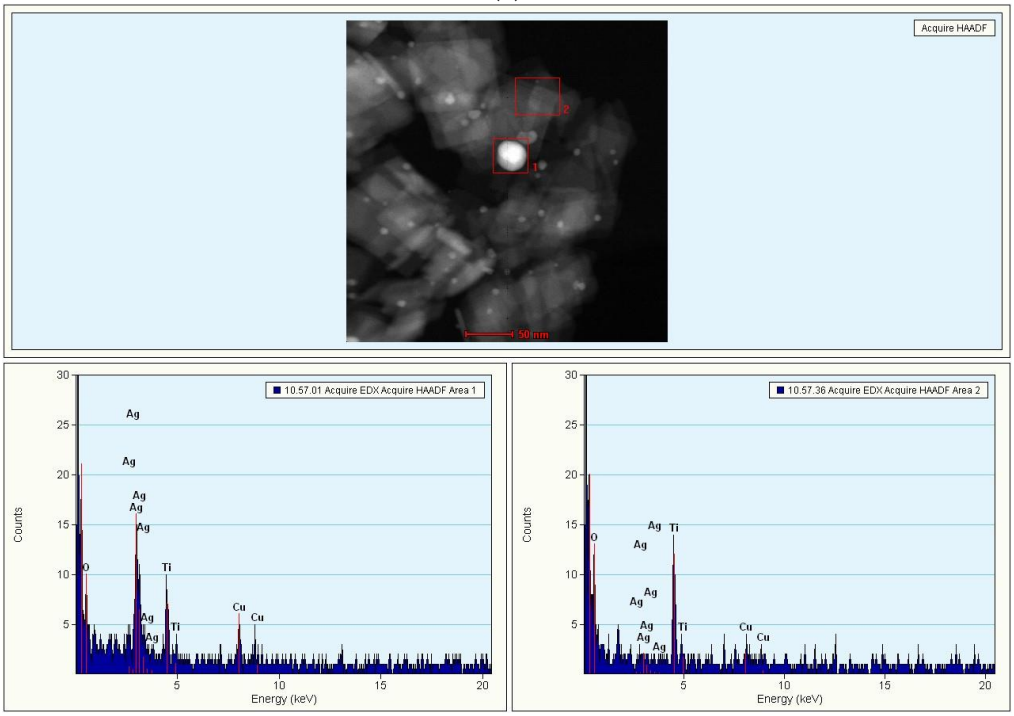
Sindy D. Jojoa-Sierra [1,2], Cesar Jaramillo-Paez [3], Efraím A. Serna-Galvis [2,4], Inés García-Rubio [5,6], María C. Hidalgo [7], José A. Navío [7], María P. Ormad [1], Ricardo A. Torres-Palma [2,*] and Rosa Mosteo [1,*]

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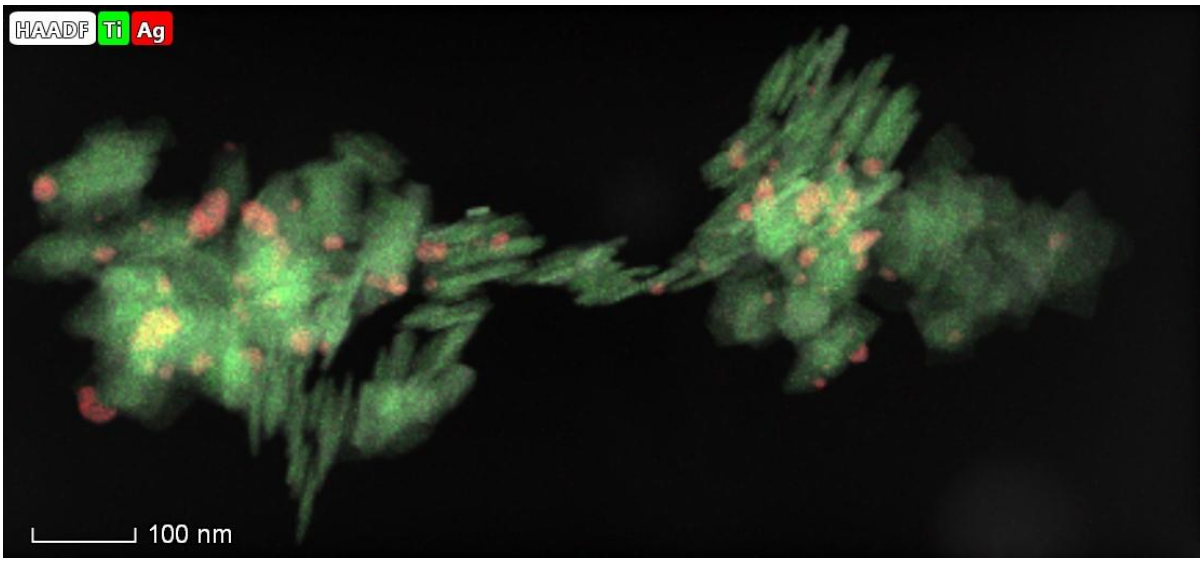
Supplementary Figures



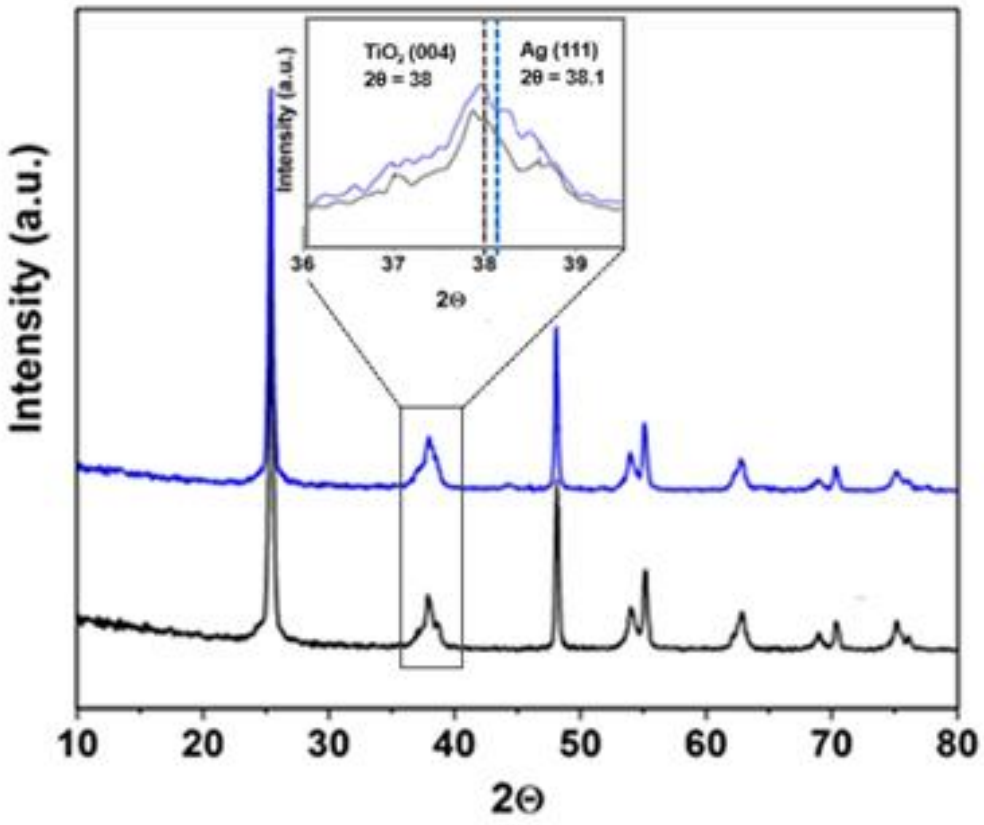
(**a**)



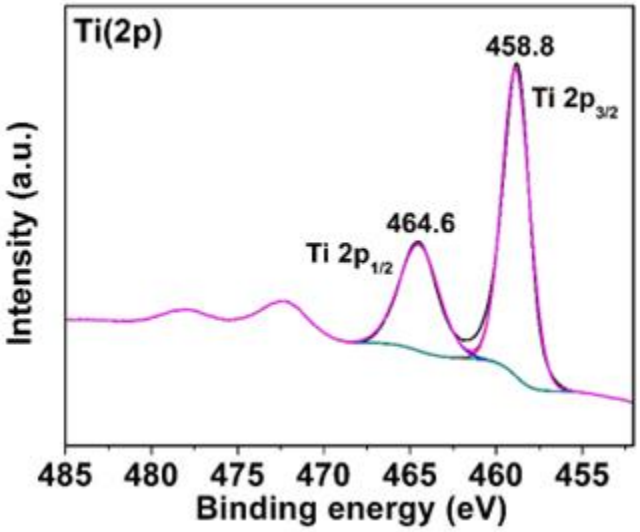
(b)


HAADF
Ti
Ag
100 nm

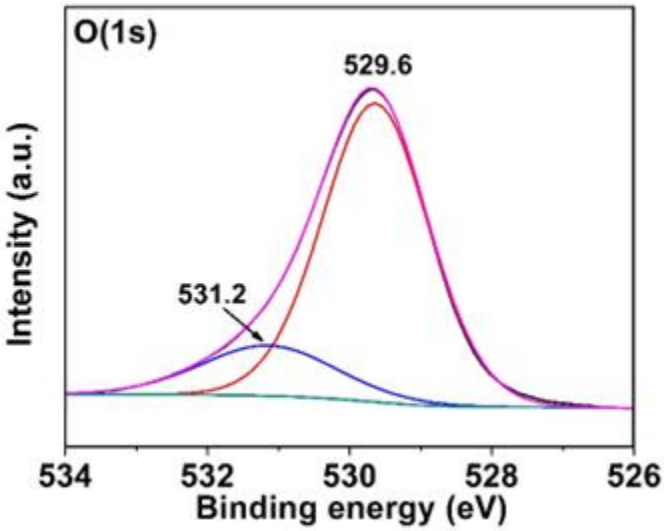
(c)


Intensity (a.u.)
TiO2 (004)
2θ = 38
Ag (111)
2θ = 38.1
36
37
38
39
2Θ
10
20
30
40
50
60
70
80
2Θ

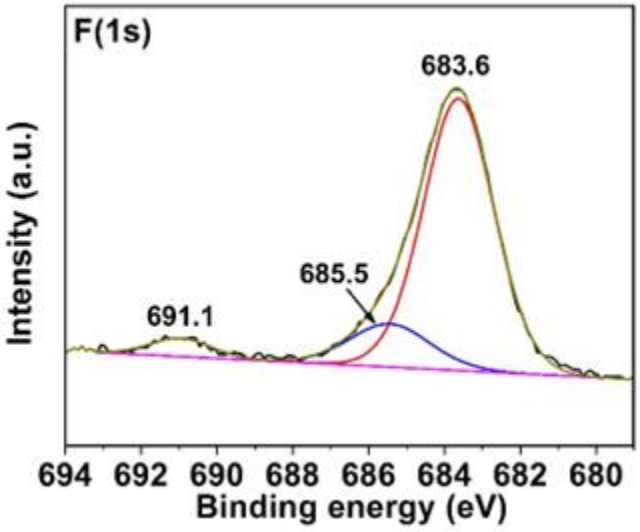
(d)


Ti(2p)
458.8
Ti 2p3/2
464.6
Ti 2p1/2
Intensity (a.u.)
485 480 475 470 465 460 455
Binding energy (eV)

(e)


O(1s)
529.6
531.2
Intensity (a.u.)
534 532 530 528 526
Binding energy (eV)

(f)



(g)

Figure. S1. EDS analyses for (**a**) TiO_2, (**b**) Ag/ TiO_2, (**c**) Elemental distribution mapping of Ag/TiO_2, zoomed-in version of Fig. 1e (**d**), high-resolution XPS for Titanium (**e**), Oxygen (**f**), and Fluorine (g) in Ag/TiO_2.

Text S1.

-The XPS spectra of Ti(2p), O(1s) and F(1s) regions are shown in **Figure S1e-g**. In the Ti(2p) region, characteristic signals from the Ti $2p_{3/2}$ and Ti $2p_{1/2}$ doublet appear at 458.8 and 464.6 eV, respectively, assigned to Ti^{4+} species present in the TiO_2 network. The O(1s) region shows one peak at 529.6 eV attributed to oxygen (O_2^-) in the crystal lattice, with a shoulder at 531.2 eV attributed to hydroxyl groups, evidencing that the sample was hydroxylated.

-The F (1s) region shows a well-defined peak at 683.6 eV, ascribed to fluoride in the form of surface (< Ti^{4+}—F−) species [1], evidencing the presence of superficial F ions coming from the synthetic media. This peak has also a small shoulder at higher binding energies (685.5 eV) which could be attributed to interactions between the surface F and superficial silver species [2]. The second small peak appearing at 691.1 eV could be assigned to substitutional F in solid solution TiO_2-xFx [1].

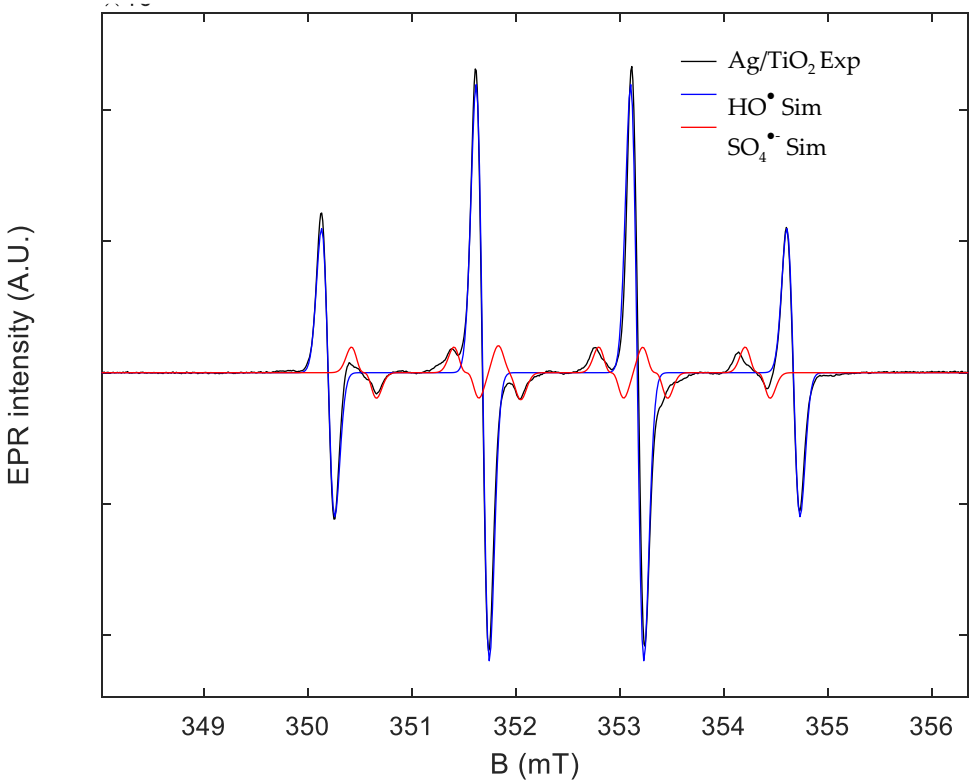


Figure. S2. EPR spectrum of radicals generated by the Ag/TiO_2-sunlight system, captured using DMPO. Signals: Black: experimental results, blue: simulated DMPO-•OH, and red: simulated DMPO-SO_4. Test conditions: DMPO = 5 mM; PDS = 100 mM. Simulation software: EasySpin in the MATLAB. (Exp. = in the experiment; Sim. = in the simulation).

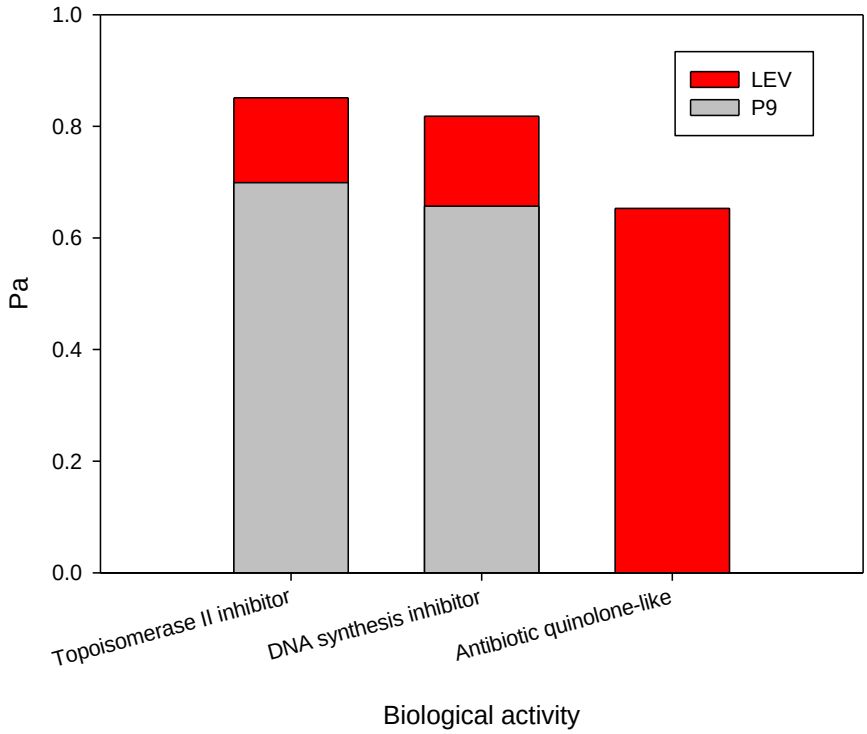
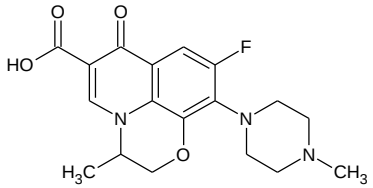
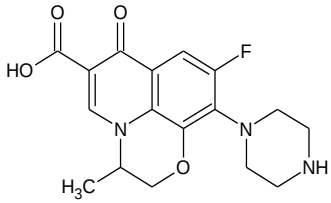
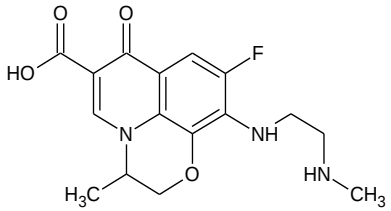
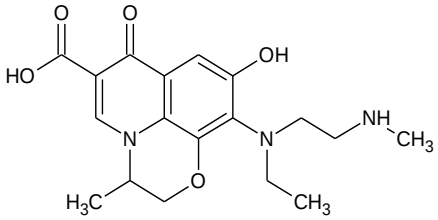
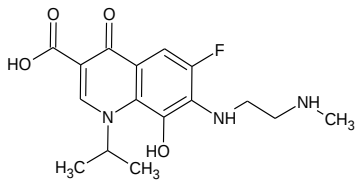
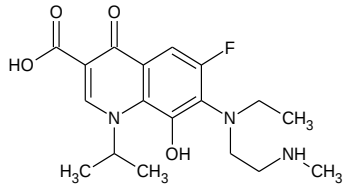
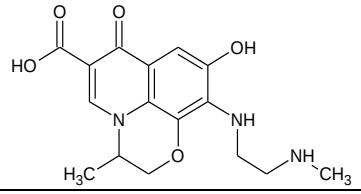
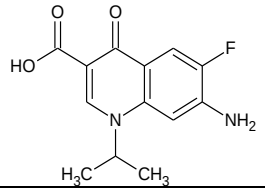
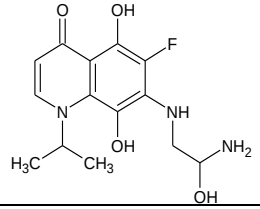


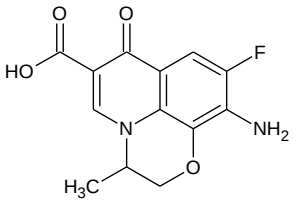
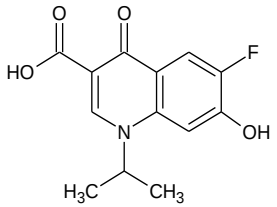
Figure S3. Prediction of biological activity for LEV and P9 using the PASS software (https://www.way2drug.com/passonline/predict.php).

Supplementary Tables

Table S1. Characteristics of the identified by-products of Levofloxacin (LEV).

Compound	Structure Proposed	Chemical Name	$[M+H]^+$	Main Fragments $[M+H]^+$	Also found By
LEV		9-fluoro-3-methyl-10-(4-methylpiperazin-1-yl)-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid	**[362]**	279, 183	-
P1		9-fluoro-3-methyl-7-oxo-10-(piperazin-1-yl)-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid	**[348]**	336, 313, 298, 279, 241, 195, 182	[3,4]
P2		9-fluoro-3-methyl-10-{[2-(methylamino)ethyl]amino}-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid	**[336]**	314, 279, 255, 223, 210, 201, 182	-
P3		10-{ethyl[2-(methylamino)ethyl]amino}-9-hydroxy-3-methyl-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid	**[362]**	343, 34, 282, 256, 224, 201, 182	-

Compound	Structure Proposed	Chemical Name	$[M+H]^+$	Main Fragments $[M+H]^+$	Also found By
P4		6-fluoro-8-hydroxy-7-{[2-(methyl-amino)ethyl]amino}-4-oxo-1-(pro-pan-2-yl)-1,4-dihydroquinoline-3-carboxylic acid	**[338]**	312, 266, 279, 256, 245, 224, 200, 182	-
P5		7-[(2-aminoethyl)(ethyl)amino]-6-fluoro-8-hydroxy-4-oxo-1-(pro-pan-2-yl)-1,4-dihydroquinoline-3-carboxylic acid	**[366]**	334, 312, 279, 256, 194	-
P6		9-hydroxy-3-methyl-10-{[2-(me-thylamino)ethyl]amino}-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid	**[334]**	312, 279, 256, 194	-
P7		7-amino-6-fluoro-4-oxo-1-(propan-2-yl)-1,4-dihydroquinoline-3-car-boxylic acid	**[265]**	222, 183	-
P8		7-[(2-amino-2-hydro-xyethyl)amino]-6-fluoro-5,8-dihydroxy-1-(propan-2-yl)quino-lin-4(1H)-one	**[312]**	279, 267, 235	-

Compound	Structure Proposed	Chemical Name	$[M+H]^+$	Main Fragments $[M+H]^+$	Also found By
P9		10-amino-9-fluoro-3-methyl-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid	**[279]**	270, 255, 235, 229, 201, 182	[3] [5]
P10		6-fluoro-7-hydroxy-4-oxo-1-(propan-2-yl)-1,4-dihydroquinoline-3-carboxylic acid	**[266]**	242, 201, 182	[6]

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