Fluoroquinolones as potential photochemotherapeutic agents: covalent addition to guanosine monophosphate.

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Electronic Supplementary Information:

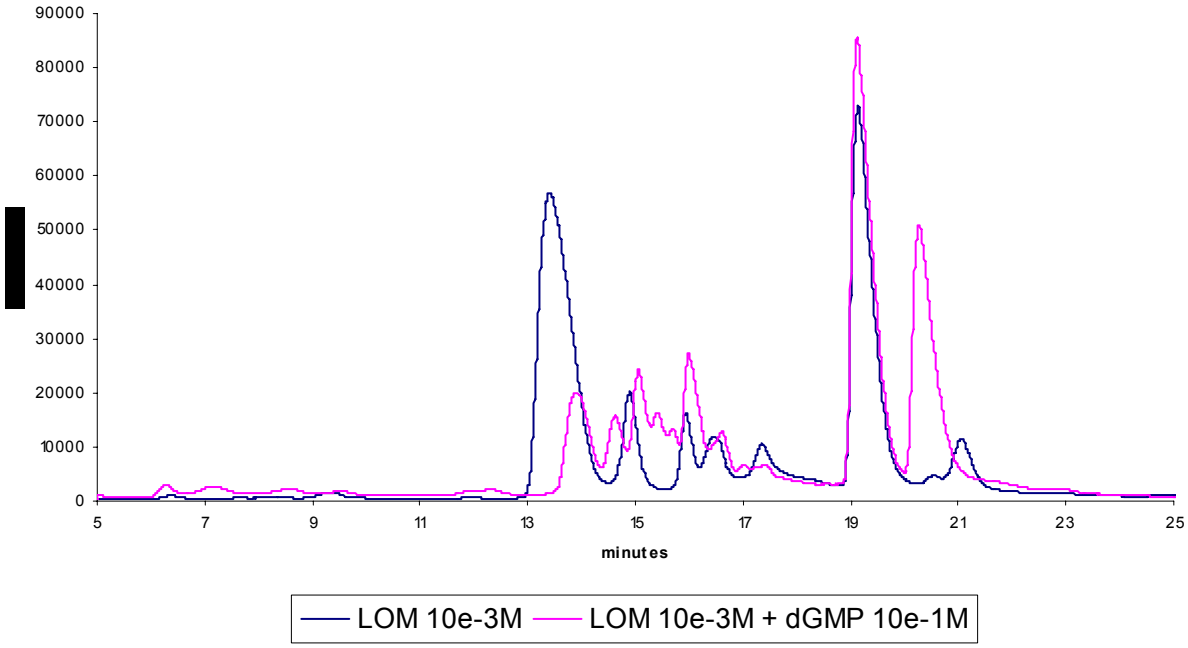
Chemicals.

Lomefloxacin (LOM), Fleroxacin (FLX), 2'-deoxyguanosine 5'-monophosphate (dGMP) and sodium bicarbonate were supplied by Fluka-Sigma Aldrich (Milan, Italy). All of the solvents were reagent grade or higher in quality and were purchased from Carlo Erba Reagenti SpA(Milan, Italy)

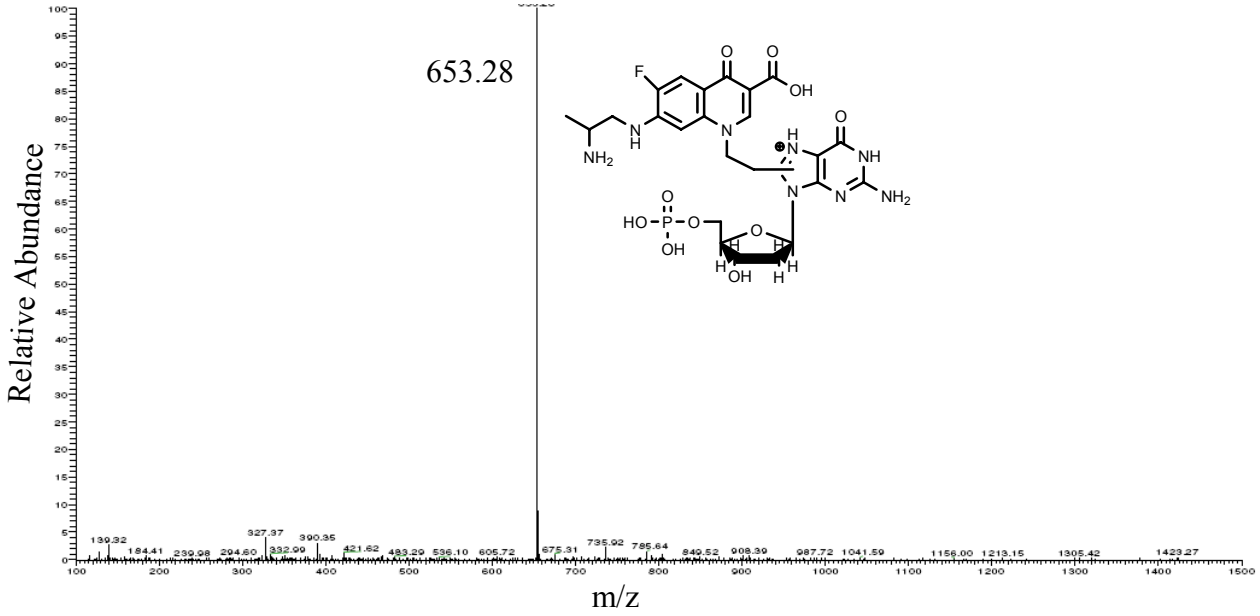
General experimental details and procedures.

A $5x10^{-4}$ M, nitrogen flushed, aqueous solution of **LOM** containing $2x10^{-3}$ moles per liter of **dGMP** was irradiate in quartz tube (10 ml) for 5 min by a merry-go-round multi lamp reactor equipped with ten 15 W lamps, with maximum emission centred at 310 nm.
HPLC-MS experiments were performed with a LXQ Thermo system on a Synergi, 5 µm hydro-RP 80A, 150mm x 4.6mm, Phenomenex column equipped with a similar guard-column. Mobile phase was A: H_2O(0.5%v/v formic acid) – B: ACN (%A: 90 for 10 min – 86 till 13 minutes – 85 till 20 minute plus 5 min equilibration) at a flow rate of 1.2 mL min^{-1}.

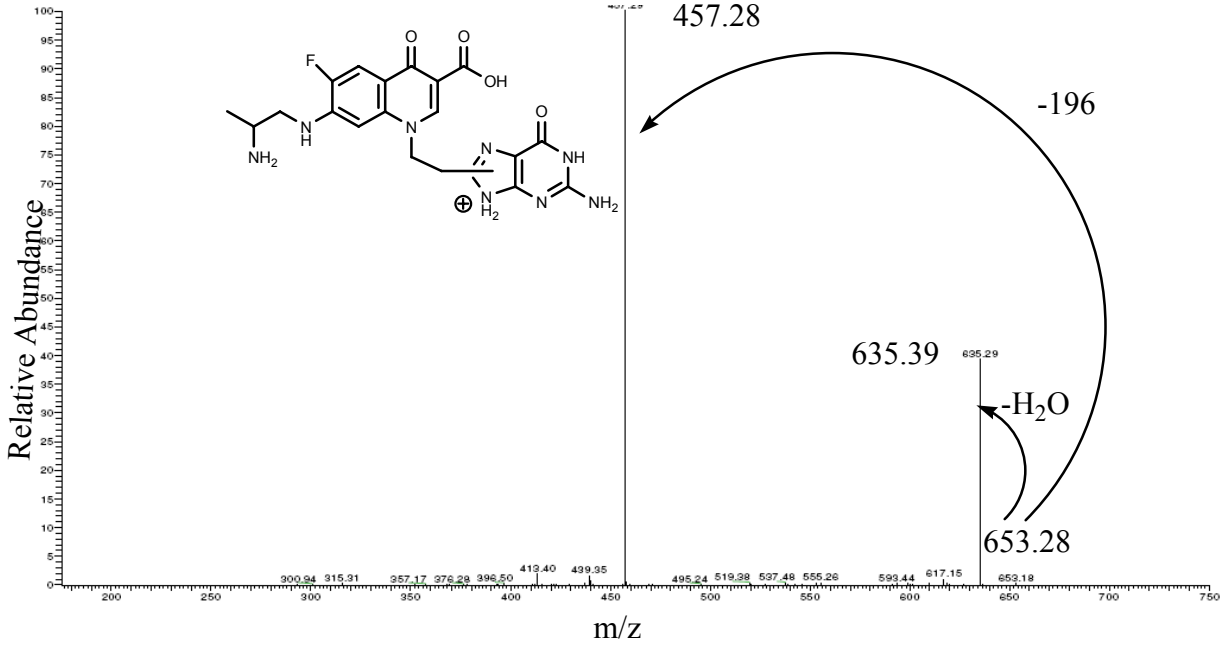
HPLC trace of irradiated **1** (blue); the same in the presence of dGMP (magenta)



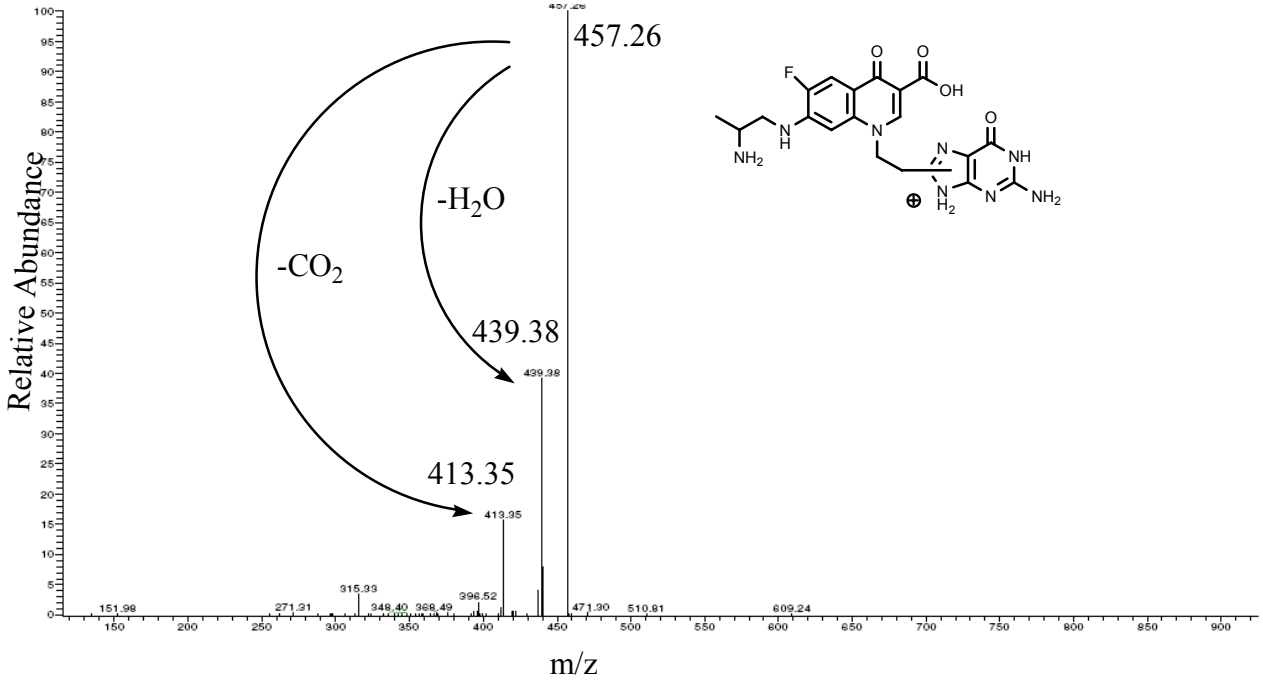
MS spectra peaks t_R 7-8 min:



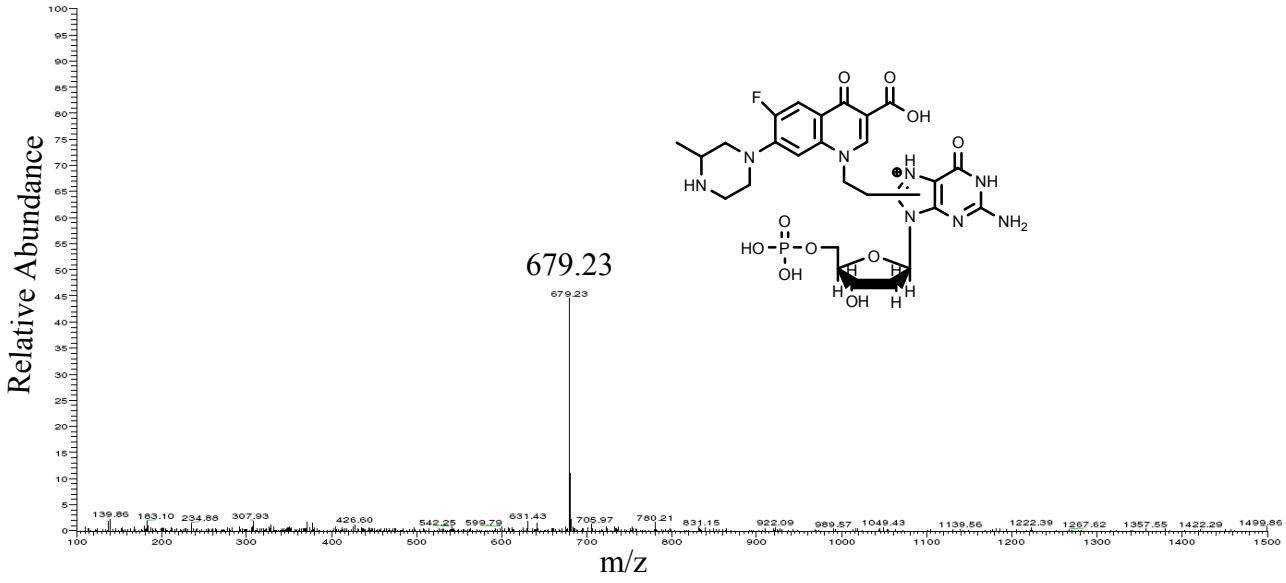
MS/MS spectra peaks t_R 7-8 min:



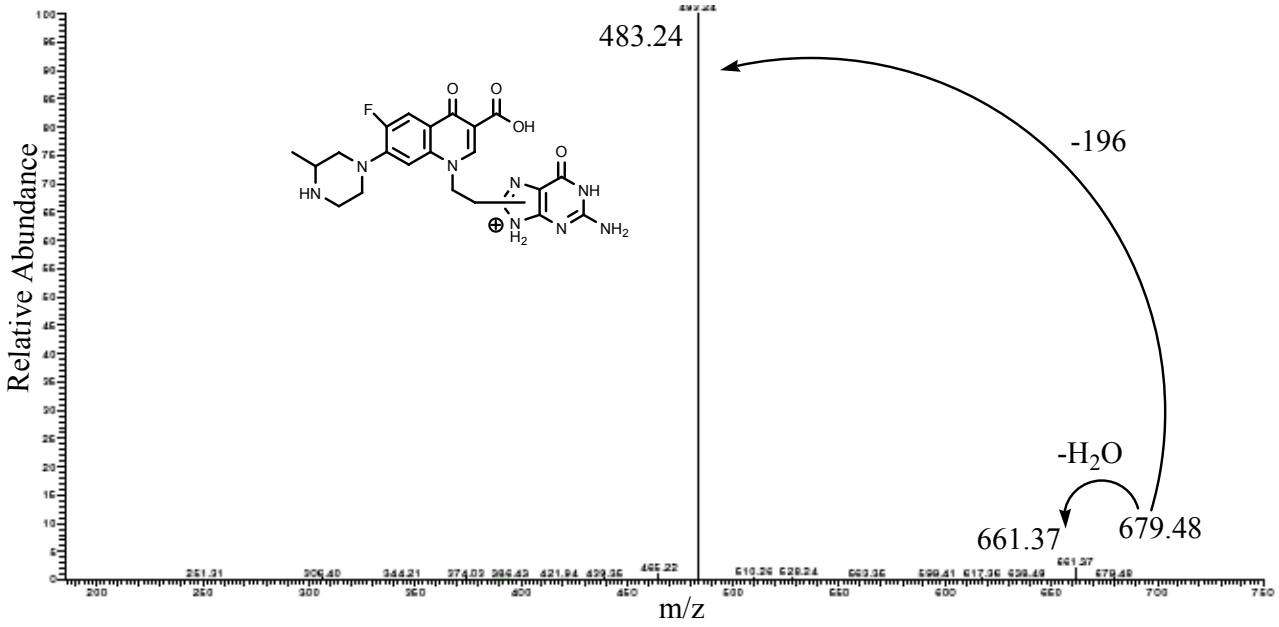
MS/MS/MS spectra peaks t_R 7-8 min (products **6**):



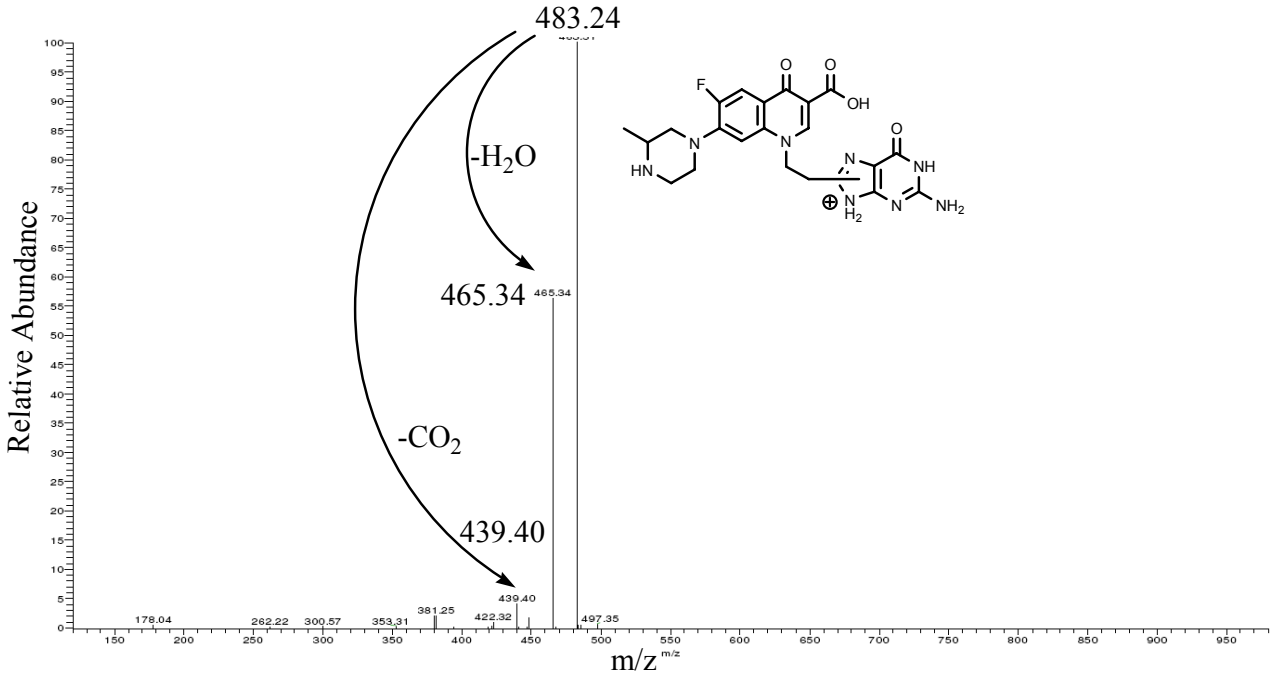
MS spectra peaks t_R 14-15 min (products **5**):



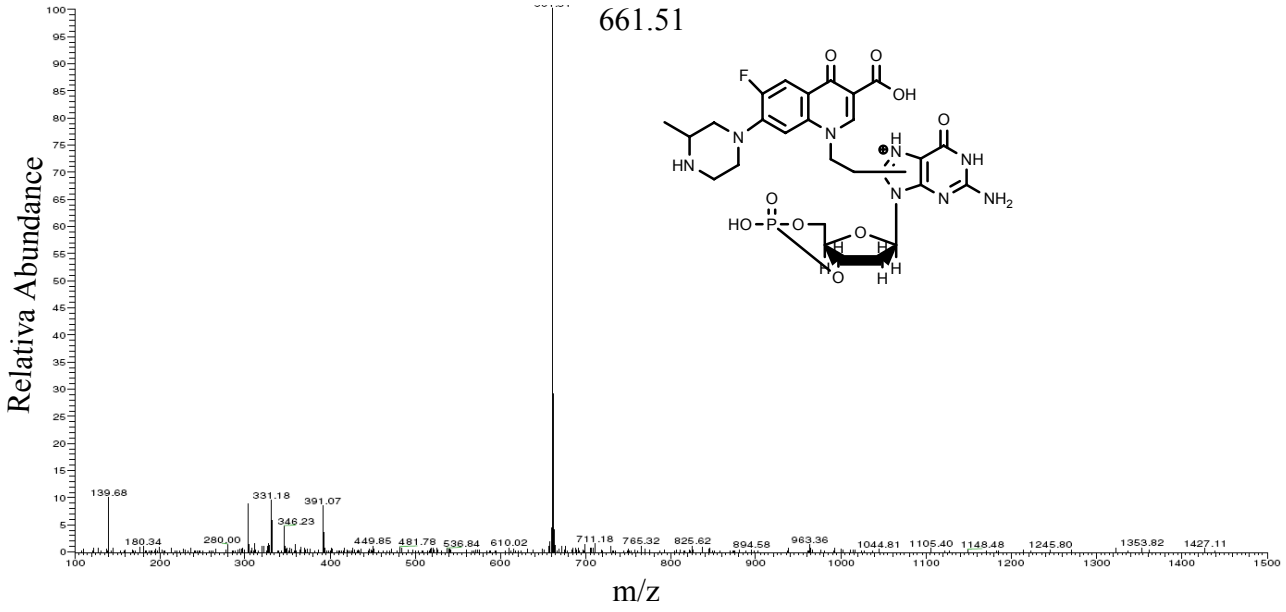
MS/MS spectra peaks t_R 14-15 min:



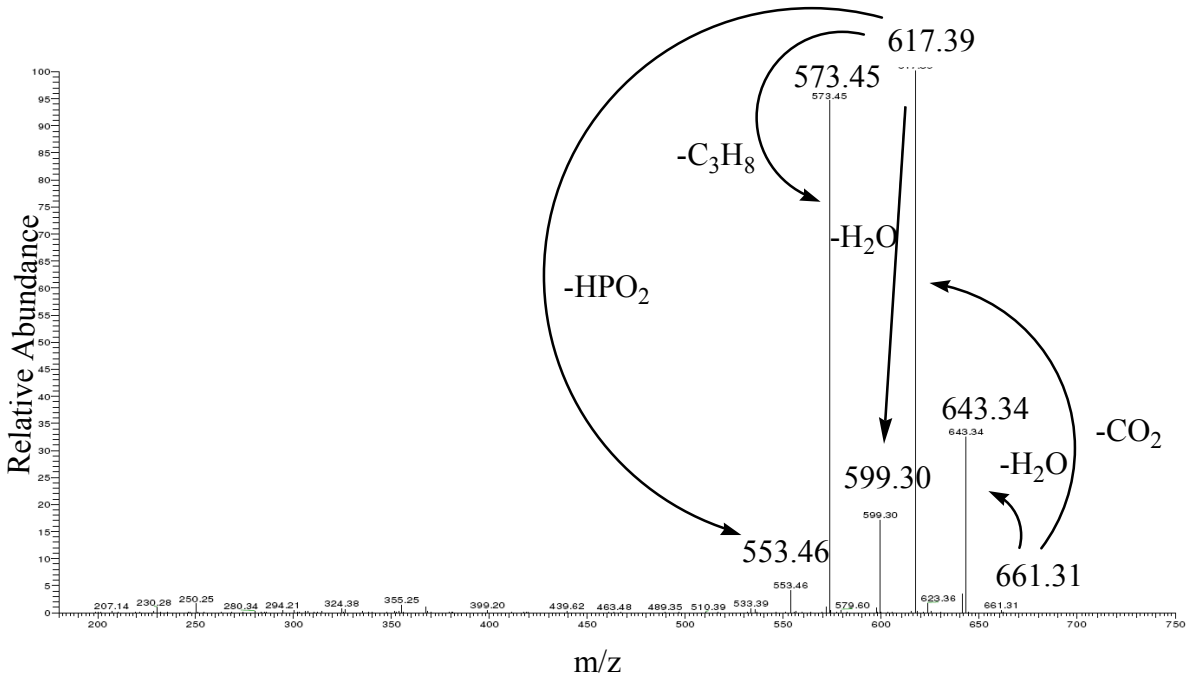
MS/MS/MS spectra peaks t_R 14-15 min:



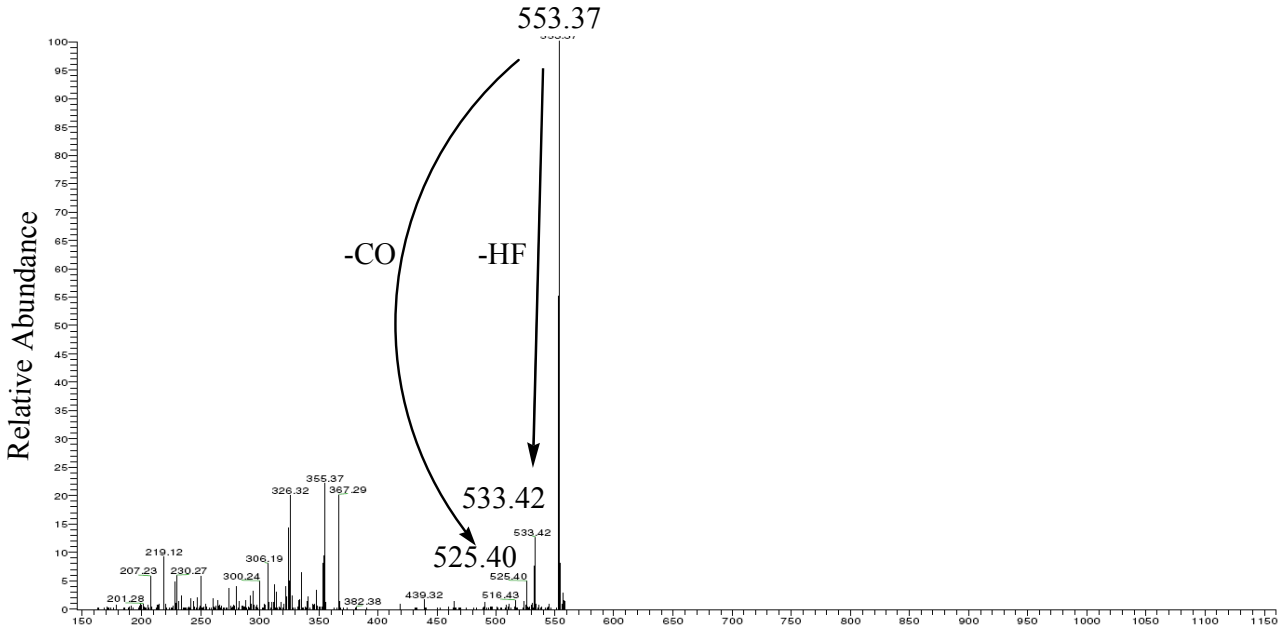
MS spectra peaks t_R 19-25 min (products **5'**:



MS/MS spectra peaks t_R 19-25 min:



MS/MS/MS spectra peaks t_R 19-25 min:



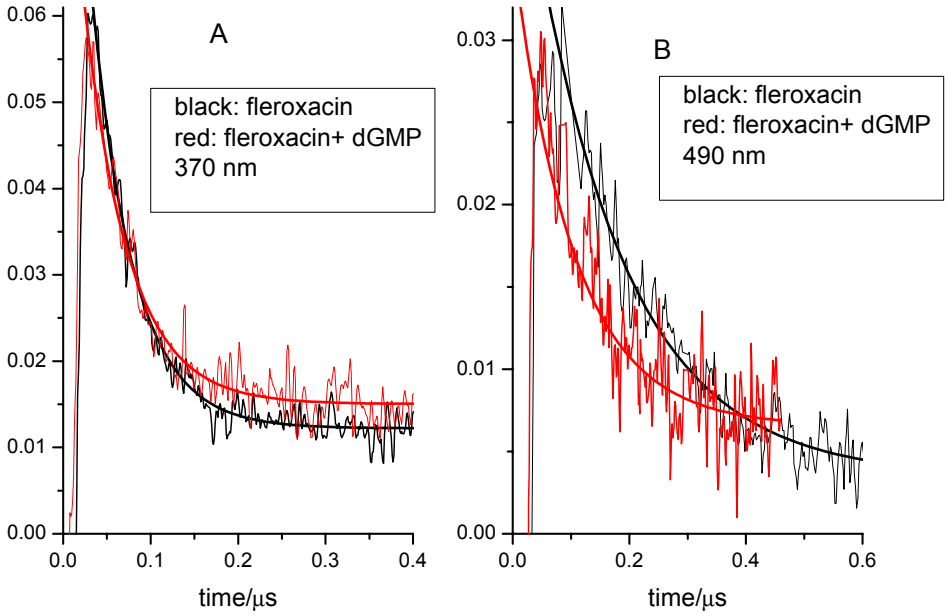


Figure S1. Absorbance changes following excitation at 355 nm of a N_2O saturated 1.4×10^{-4} M solution of fleroxacin in 1.0×10^{-3} M HCO_3 buffer of pH 7.2 at 25 °C at (A) 370 nm and (B) 490 nm: black lines, fleroxacin red lines, fleroxacin + 1×10^{-2} M dGMP.

Fluorescence spectra of 10^{-5}M water solution of **LOM** in the presence of increasing quantity of dGMP (from 0 to 10^{-3} M).