Supporting Information

Gas-Phase Esterification within a Miniature Ion Trap Mass Spectrometer: Mechanistic Insight and Diagnostic Markers for Quinolone Screening

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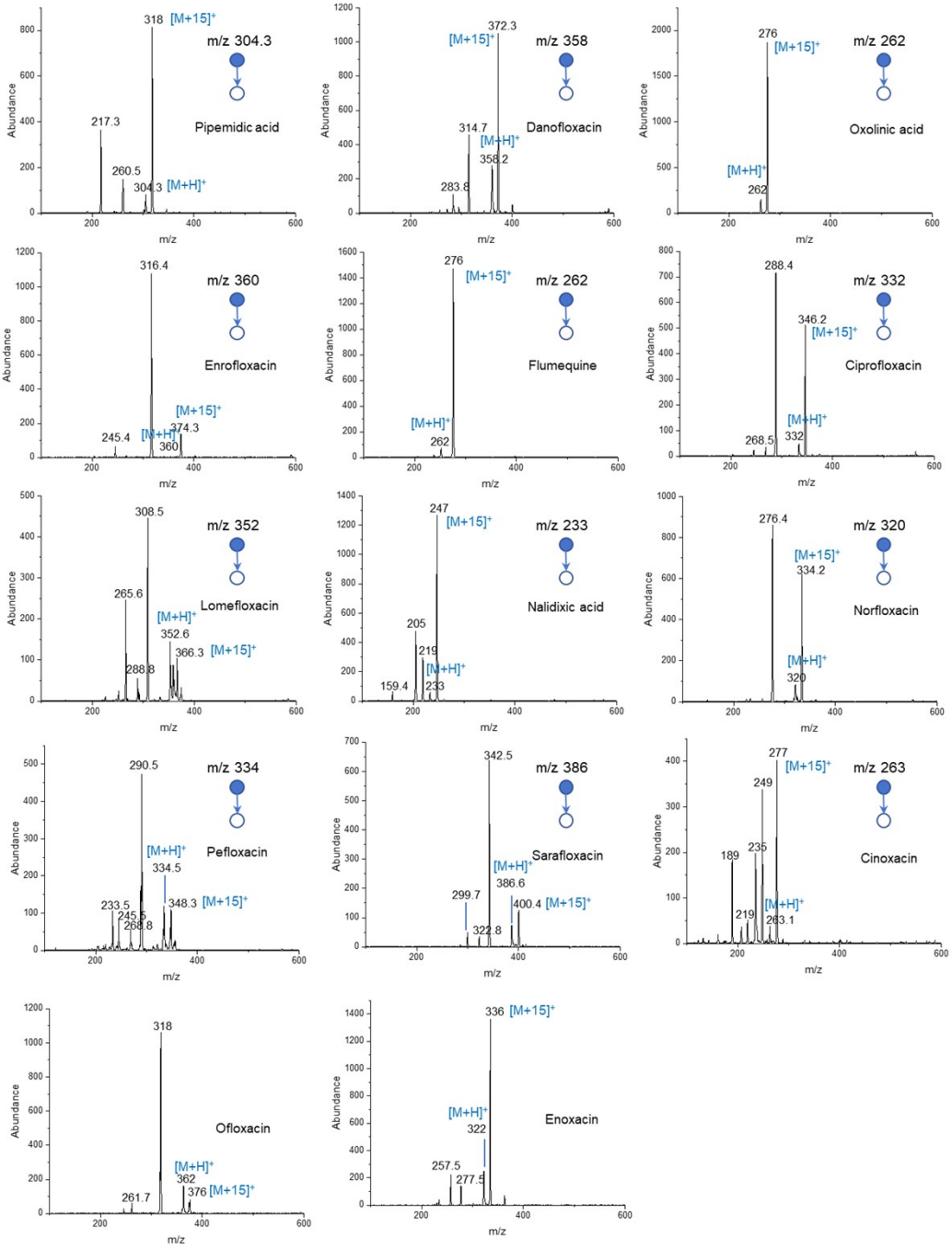


Figure S1. MS^2 tandem mass spectra of 14 all quinolones where adduct products were observed.

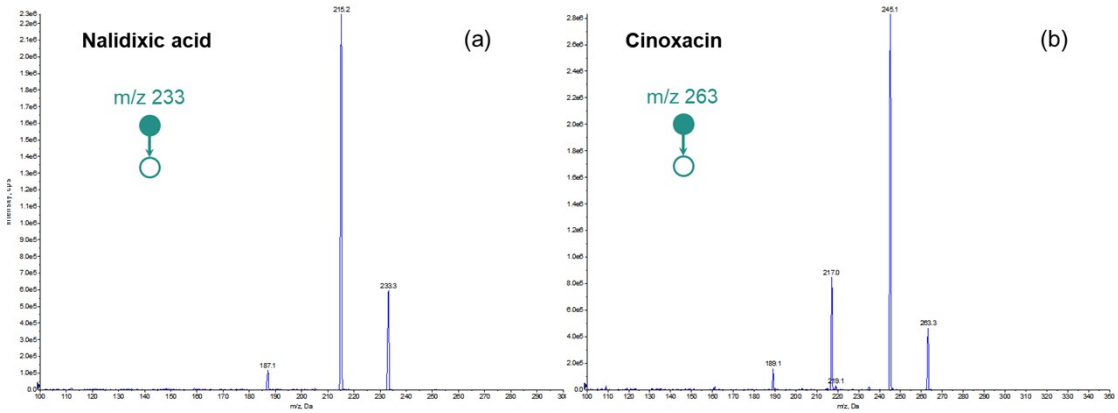


Figure S2. MS^2 tandem mass spectra of (a) nalidixic acid and (b) cinoxacin using QqQ mass spectrometer (AB4500 Triple Quad™, AB SCIEX). No adduct ions were generated for both analytes.

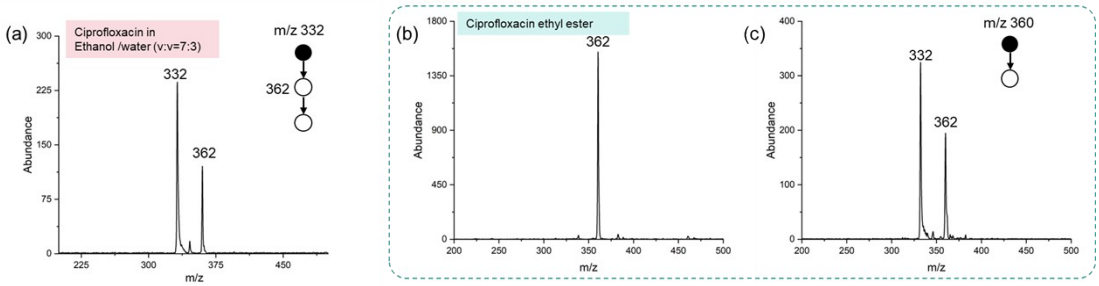


Figure S3. (a) MS3 spectrum of ciprofloxacin adduct (m/z 362); and full-MS spectrum (b), and MS2 spectrum of ciprofloxacin ethyl ester (m/z 362).

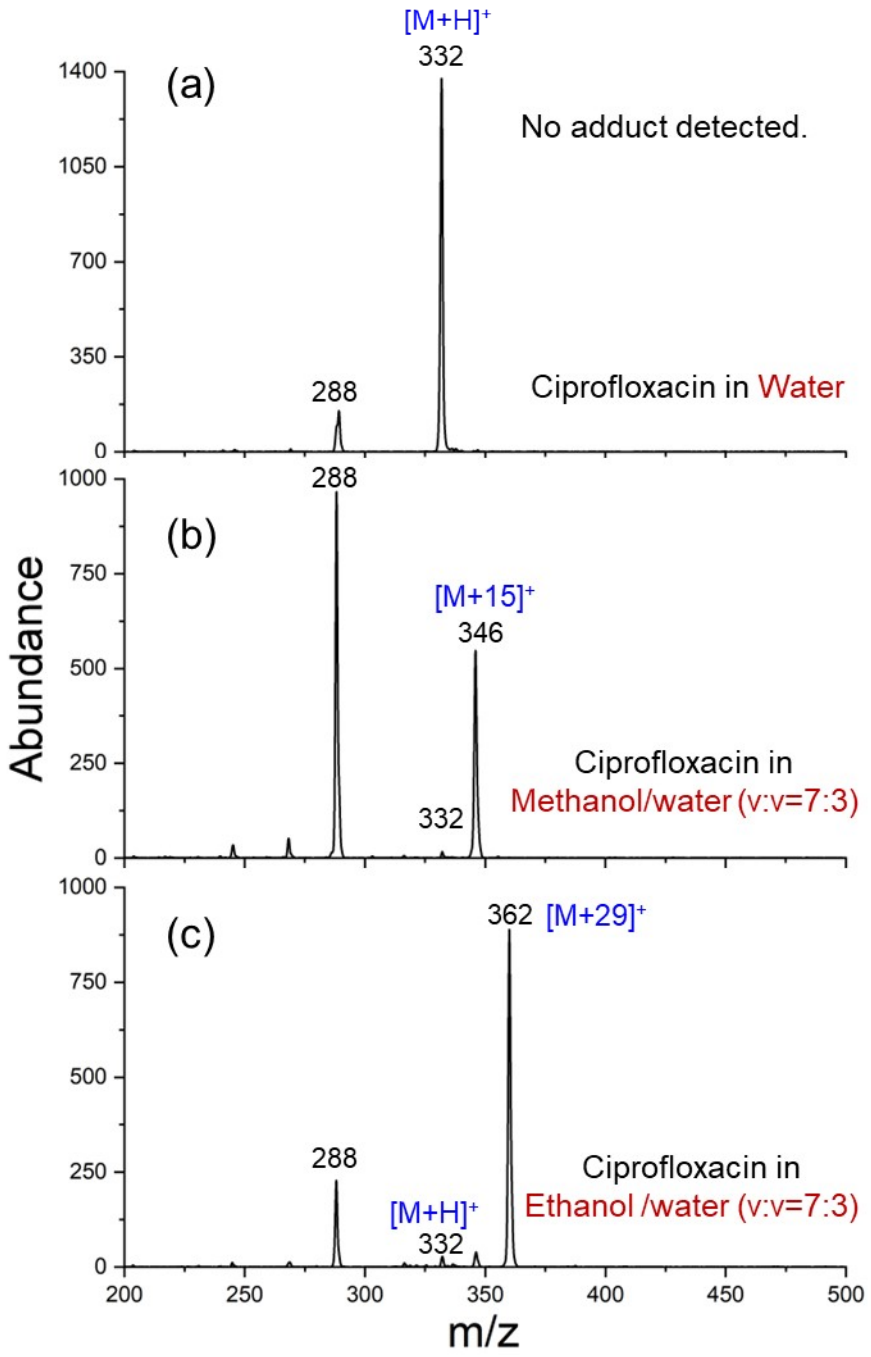


Figure S4. Tandem mass spectra of ciprofloxacin diluted in (a) water, (b) Methanol/water, and (c) Ethanol /water.

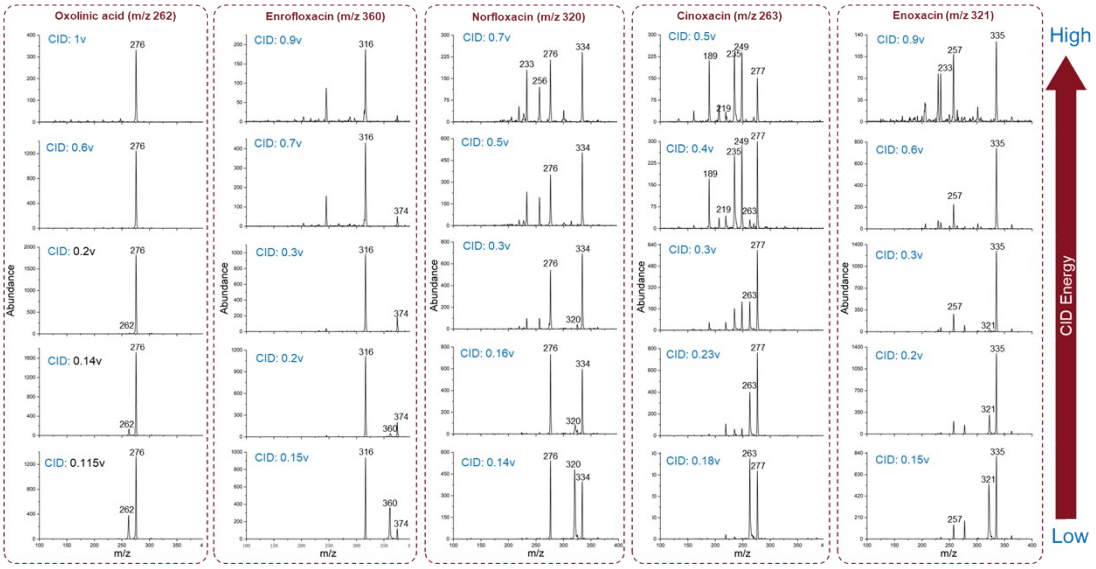
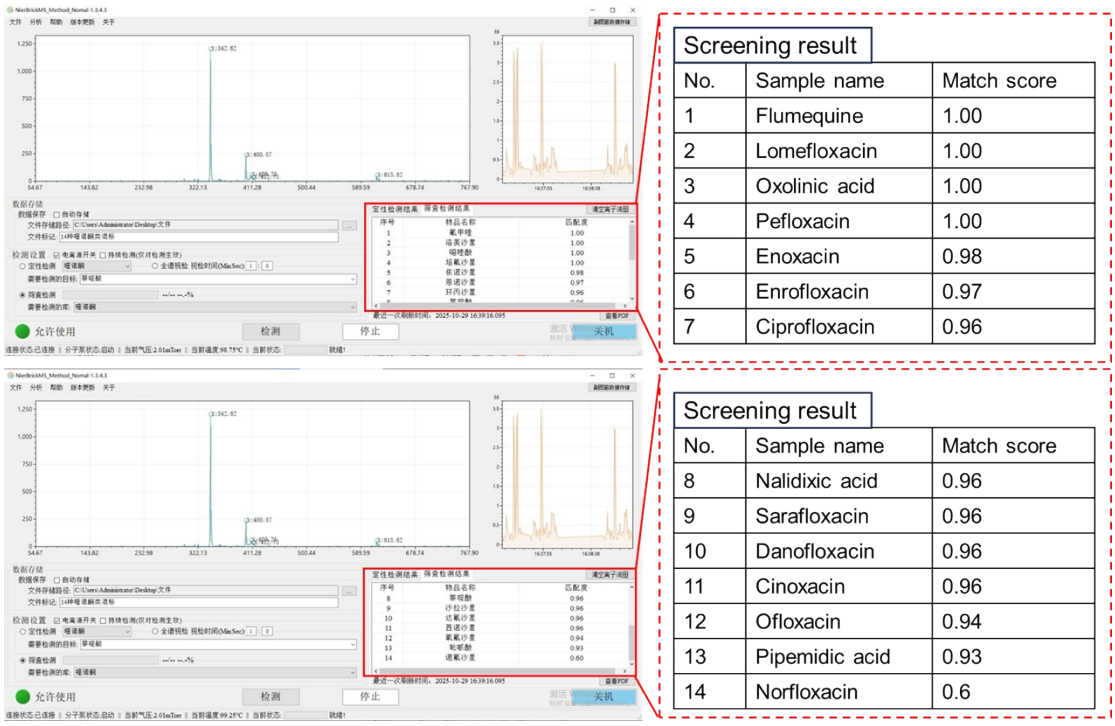


Figure S5. MS2 spectra of quinolones under different CID voltages.



Screening result

No.	Sample name	Match score
1	Flumequine	1.00
2	Lomefloxacin	1.00
3	Oxolinic acid	1.00
4	Pefloxacin	1.00
5	Enoxacin	0.98
6	Enrofloxacin	0.97
7	Ciprofloxacin	0.96

Screening result

No.	Sample name	Match score
8	Nalidixic acid	0.96
9	Sarafloxacin	0.96
10	Danofloxacin	0.96
11	Cinoxacin	0.96
12	Ofloxacin	0.94
13	Pipemidic acid	0.93
14	Norfloxacin	0.6

Figure S6. The screen capture of the screening results of quinolones on MS software.

Table S1. Summary of screening results for the 14 quinolone standards using the conventional approaches without adduct peaks.

No.	Name	Chemical formula	MW	Confidence score
1	Nalidixic acid	$C_{12}H_{12}N_2O_3$	232.2	0.65
2	Oxolinic acid	$C_{13}H_{11}NO_5$	261.2	0.20
3	Flumequine	$C_{14}H_{12}FNO_3$	261.2	0.54
4	Cinoxacin	$C_{12}H_{10}N_2O_5$	262.2	0.68
5	Pipemidic acid	$C_{14}H_{17}N_5O_3$	303.3	0.56
6	Norfloxacin	$C_{16}H_{18}FN_3O_3$	319.3	0.39
7	Enoxacin	$C_{15}H_{17}FN_4O_3$	320.3	0.58
8	Ciprofloxacin	$C_{17}H_{18}FN_3O_3$	331.3	0.36
9	Pefloxacin	$C_{17}H_{20}FN_3O_3$	333.3	0.55
10	Lomefloxacin	$C_{17}H_{19}F_2N_3O_3$	351.3	0.74
11	Danofloxacin	$C_{19}H_{20}FN_3O_3$	357.3	0.41
12	Enrofloxacin	$C_{19}H_{22}FN_3O_3$	359.4	0.74
13	Ofloxacin	$C_{18}H_{20}FN_3O_4$	361.3	0.36
14	Sarafloxacin	$C_{20}H_{17}F_2N_3O_3$	385.3	0.73

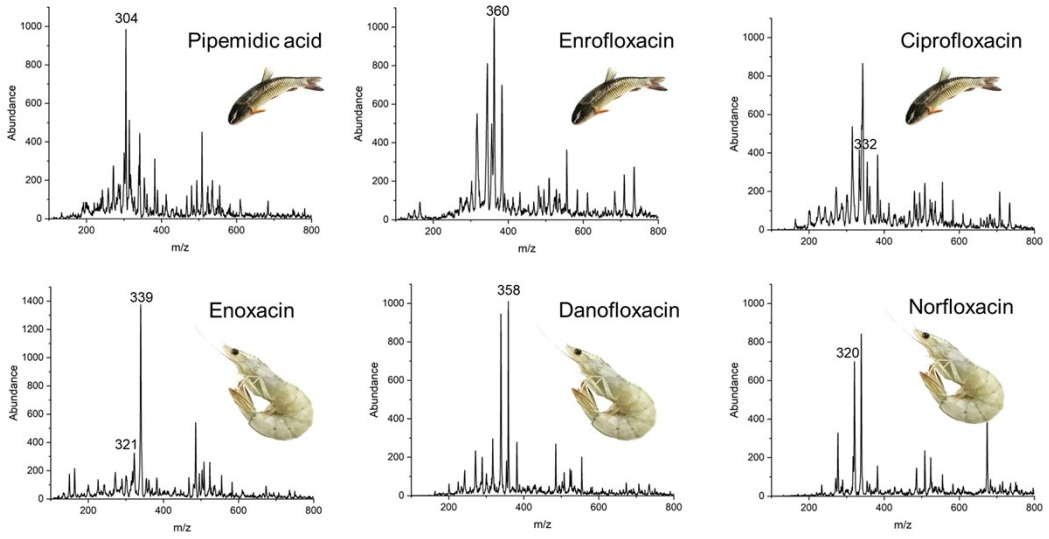


Figure S7. Full-scan mass spectra of (a) pipemidic acid, (b) enrofloxacin, and (c) ciprofloxacin detected in grass fish; and (d) enoxacin, (e) danofloxacin, and (f) norfloxacin detected in shrimper.