

## Supplementary Material

for

**Influence of transition metal-based activating agent on the properties and catalytic activity of sewage sludge-derived catalysts. Insights on mechanism, DFT calculation and degradation pathways.**

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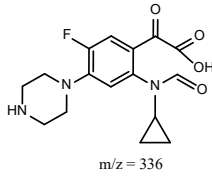
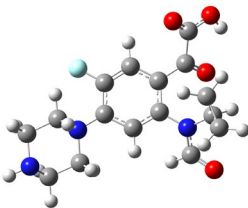
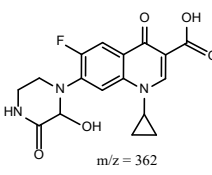
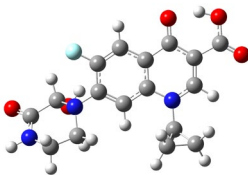
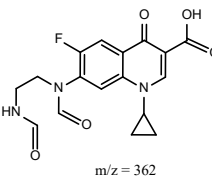
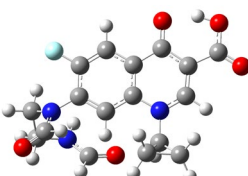
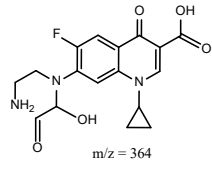
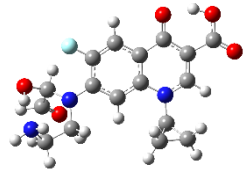
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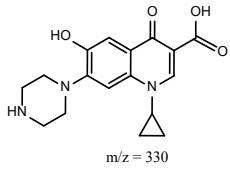
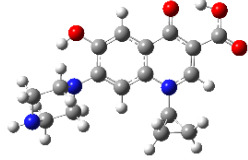
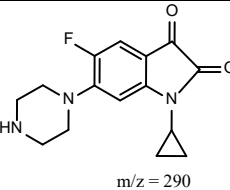
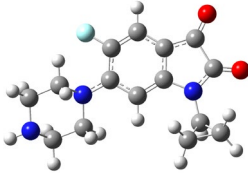
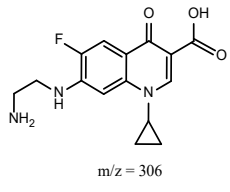
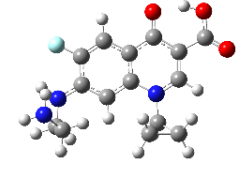
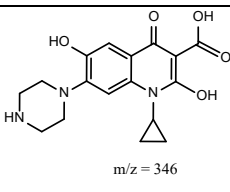
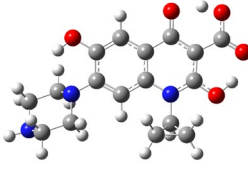
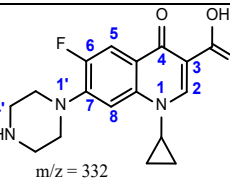
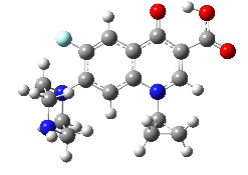
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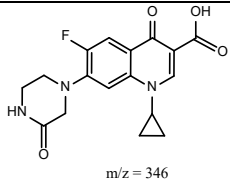
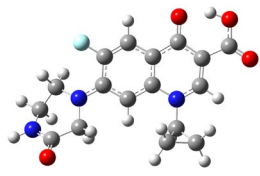
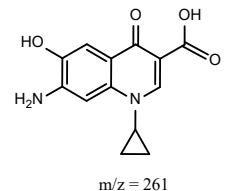
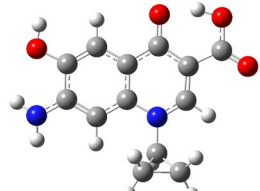
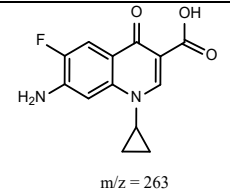
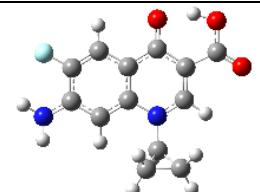
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**Figures: 6**

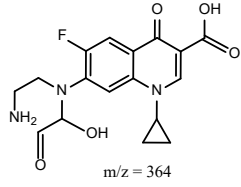
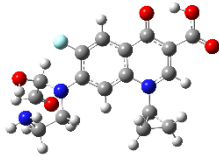
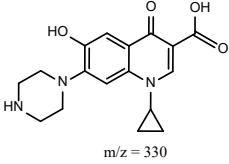
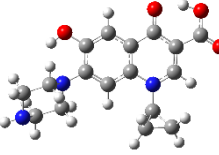
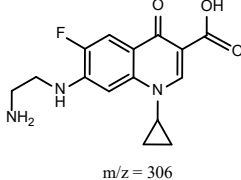
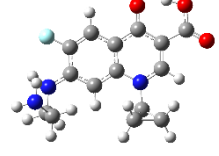
**Table S1.** Retention Time, Relative Intensity at 4.5 kV Interface Voltage, Mass Spectra, Molecular Formula, Name and Proposed Structure of CPF Products in Degradation Pathway (T1), Homo and Lumo Energies, Optimised structure. Urban-Fe Catalyst.

Compound	t <sub>R</sub> (min)	[M+H] <sup>+</sup> (m/z)	Molecular Formula	Name	Structure	E <sub>HOMO</sub> (eV)	E <sub>LUMO</sub> (eV)	Optimization
1		336	C <sub>16</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>4</sub>	2-[2-(N-cyclopropylformamido)-5-fluoro-4-(piperazin-1-yl)phenyl]-2-oxoacetic acid		-7,44232	-1,75078	
2		362	C <sub>17</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>5</sub>	1-cyclopropyl-6-fluoro-7-(2-hydroxy-3-oxopiperazin-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,88858	-1,10505	
3	1.4	362	C <sub>17</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>5</sub>	1-cyclopropyl-6-fluoro-7-[N-(2-formamidoethyl)formamido]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,97321	-1,28030	
4 (T2-1, T3-4, T4-4)		364	C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>5</sub>	7-[(2-aminoethyl)(1-hydroxy-2-oxoethyl)amino]-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,56640	-1,02016	

5 (T2-2, T3-6)	6.6	330	C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>	1-cyclopropyl-6-hydroxy-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid	 m/z = 330	-7,46109	-0,97145	
6 (T3-7)	7.3	290	C <sub>15</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>2</sub>	1-cyclopropyl-5-fluoro-6-(piperazin-1-yl)indoline-2,3-dione	 m/z = 290	-7,30490	-1,95323	
7 (T2-3, T3-8)	8.0	306	C <sub>15</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>3</sub>	7-[(2-aminoethyl)amino]-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	 m/z = 306	-7,28885	-0,89526	
8	8.3	346	C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub>	1-cyclopropyl-2,6-dihydroxy-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid	 m/z = 346	-7,38735	-0,91675	
Ciprofloxacin	8.9	332	C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>	ciprofloxacin	 m/z = 332	-7,21619	-0,98070	

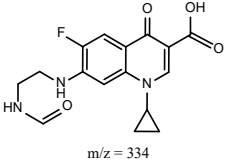
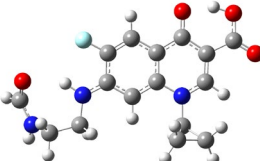
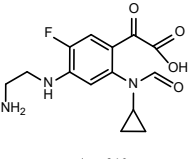

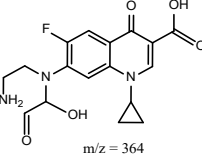
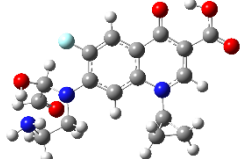
9	9.7	346	C <sub>17</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>4</sub>	1-cyclopropyl-6-fluoro-4-oxo-7-(3-oxopiperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid	 m/z = 346	-7,33102	-0,96192	
10	9.9	261	C <sub>13</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>	7-amino-1-cyclopropyl-6-hydroxy-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	 m/z = 261	-7,28068	-0,83267	
11 (T2-4)	10.5	263	C <sub>13</sub> H <sub>11</sub> FN <sub>2</sub> O <sub>3</sub>	7-amino-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	 m/z = 263	-7,55633	-0,93662	

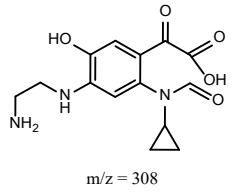
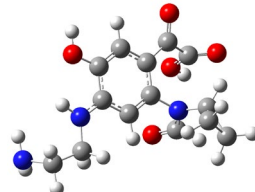
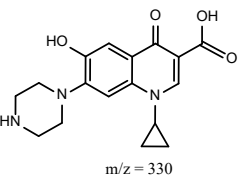
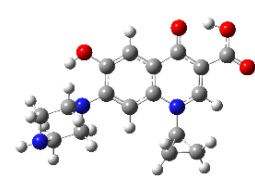
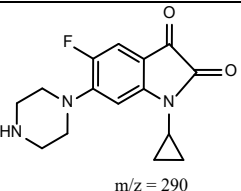
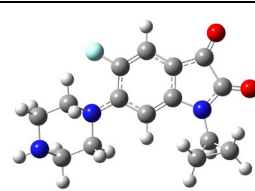
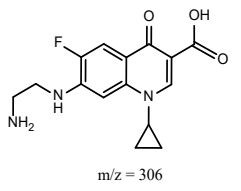
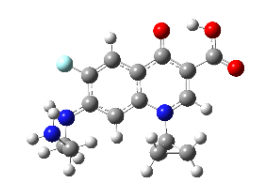
**Table S2.** Retention Time, Relative Intensity at 4.5 kV Interface Voltage, Mass Spectra, Molecular Formula, Name and Proposed Structure of CPF Products in Degradation Pathway (T2), Homo and Lumo Energies, Optimised structure. Industrial-Fe Catalyst.

Compound	$t_R$ (min)	$[M+H]^+$ (m/z)	Molecular Formula	Name	Structure	$E_{HOMO}$ (eV)	$E_{LUMO}$ (eV)	Optimization
1	1.4	364	$C_{17}H_{18}FN_3O_5$	7-[(2-aminoethyl)(1-hydroxy-2-oxoethyl)amino]-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinolin e-3-carboxylic acid		-7,56640	1,02016	
2	6.7	330	$C_{17}H_{19}N_3O_4$	1-cyclopropyl-6-hydroxy-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid		-7,46109	0,97145	
3	8.0	306	$C_{15}H_{16}FN_3O_3$	7-[(2-aminoethyl)amino]-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinolin e-3-carboxylic acid		-7,28885	0,89526	

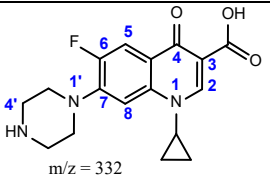
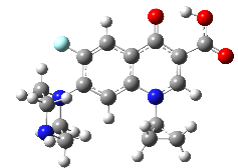
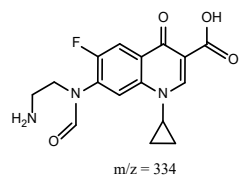
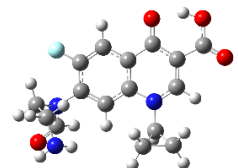
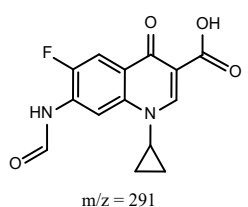
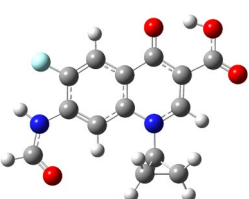
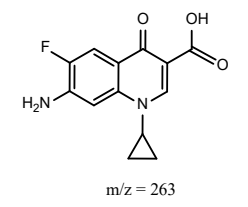
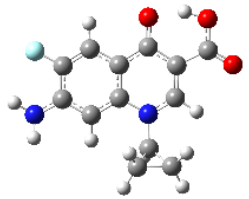
<b>Ciprofloxacin</b>	8.9	332	$C_{17}H_{18}FN_3O_3$	Ciprofloxacin	 <chem>C1CN2CCN(C1)CC2C3=C(F)C(=O)N(C3)C(=O)O</chem> $m/z = 332$	-7,21619	0,98070	
<b>4</b>	10.5	263	$C_{13}H_{11}FN_2O_3$	7-amino-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	 <chem>C1CCN2C(=O)C(=O)N(C2)C(=O)O</chem> $m/z = 263$	-7,55633	0,93662	

**Table S3.** Retention Time, Relative Intensity at 4.5 kV Interface Voltage, Mass Spectra, Molecular Formula, Name and Proposed Structure of CPF Products in Degradation Pathway (T3), Homo and Lumo Energies, Optimised structure. Industrial-Ni Catalyst.

Compound	t <sub>R</sub> (min)	[M+H] <sup>+</sup> (m/z)	Molecular Formula	Name	Structure	E <sub>HOMO</sub> (eV)	E <sub>LUMO</sub> (eV)	Optimization
<b>2 (T4-2)</b>	0.9	334	C <sub>16</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>4</sub>	1-cyclopropyl-6-fluoro-7-[(2-formamidoethyl)amino]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,26327	-0,85389	
<b>3 (T4-3)</b>		310	C <sub>14</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>4</sub>	2-{4-[(2-aminoethyl)amino]-2-(N-cyclopropylformamido)-5-fluorophenyl}-2-oxoacetic acid		-7,23687	-1,66452	
<b>4 (T4-4, T2-1, T1-4)</b>	1.4	364	C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>5</sub>	7-[(2-aminoethyl)(1-hydroxy-2-oxoethyl)amino]-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,56640	-1,02016	

5	1.5	308	C <sub>14</sub> H <sub>17</sub> N <sub>3</sub> O <sub>5</sub>	2-{4-[(2-aminoethyl)amino]-2-(N-cyclopropylformamido)-5-hydroxyphenyl}-2-oxoacetic acid		-7,01592	-1,24002	
6 (T2-2, T1-5)	6.7	330	C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub>	1-cyclopropyl-6-hydroxy-4-oxo-7-(piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylic acid		-7,46109	-0,97145	
7 (T1-6)	7.3	290	C <sub>15</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>2</sub>	1-cyclopropyl-5-fluoro-6-(piperazin-1-yl)indoline-2,3-dione		-7,30490	-1,95323	
8 (T2-3, T1-7)	7.9	306	C <sub>15</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>3</sub>	7-[(2-aminoethyl)amino]-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,28885	-0,89526	



<b>Ciprofloxacin</b>	8.7	332	C <sub>17</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>3</sub>	Ciprofloxacin		-7,21619	-0,98070	
<b>9</b>	10.4	334	C <sub>16</sub> H <sub>16</sub> FN <sub>3</sub> O <sub>4</sub>	7-[N-(2-aminoethyl)formamido]-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,98301	-1,29118	
<b>10</b>	10.5	291	C <sub>14</sub> H <sub>11</sub> FN <sub>2</sub> O <sub>4</sub>	1-cyclopropyl-6-fluoro-7-formamido-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,95226	-1,23757	
<b>11 (T2-4 y T1-11)</b>	10.5	263	C <sub>13</sub> H <sub>11</sub> FN <sub>2</sub> O <sub>3</sub>	7-amino-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,55633	-0,93662	

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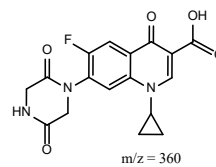
12

10.7

360

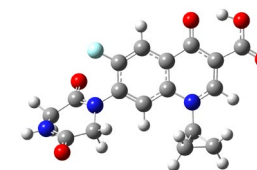
C<sub>17</sub>H<sub>14</sub>FN<sub>3</sub>O<sub>5</sub>

1-cyclopropyl-  
7-(2,5-  
dioxopiperazin-  
1-yl)-6-fluoro-4-  
oxo-1,4-  
dihydroquinolin-  
e-3-carboxylic  
acid

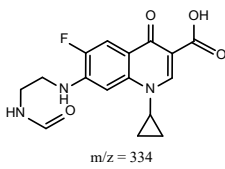
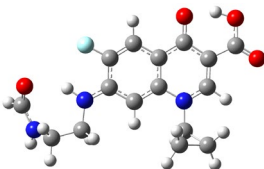
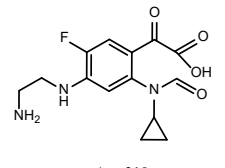
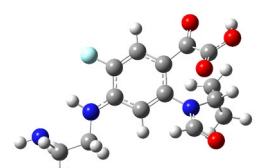
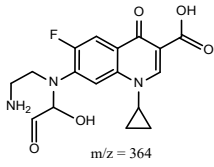
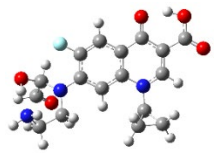


-7,96940

-1,29907

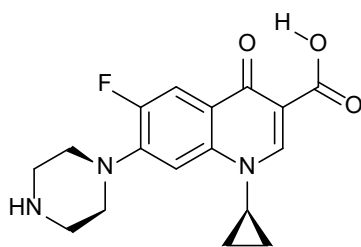


**Table S4.** Retention Time, Relative Intensity at 4.5 kV Interface Voltage, Mass Spectra, Molecular Formula, Name and Proposed Structure of CPF Products in Degradation Pathway (T4), Homo and Lumo Energies, Optimised structure. Industrial-FeNi Catalyst.

Compound	$t_R$ (min)	$[M+H]^+$ (m/z)	Molecular Formula	Name	Structure	$E_{HOMO}$ (eV)	$E_{LUMO}$ (eV)	Optimization
2	0.9	334	$C_{16}H_{16}FN_3O_4$	1-cyclopropyl-6-fluoro-7-[(2-formamidoethyl)amino]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,26327	0,85389	
3		310	$C_{14}H_{16}FN_3O_4$	2-{4-[(2-aminoethyl)amino]-2-(N-cyclopropylformamido)-5-fluorophenyl}-2-oxoacetic acid		-7,23687	1,66452	
4	1.3	364	$C_{17}H_{18}FN_3O_5$	7-[(2-aminoethyl)(1-hydroxy-2-oxoethyl)amino]-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid		-7,56640	1,02016	

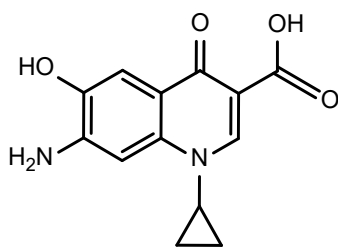
**Table S5.** Energetic data of organic compounds involved in the reactions.

<b>Compound</b>	<b>Electronic energy (kcal/mol)</b>	<b>Free energy (kcal/mol)</b>	<b>Entropy (cal/(mol·K))</b>	<b>Enthalpy (kcal/mol)</b>	<b>E<sub>HOMO</sub> (eV)</b>	<b>E<sub>LUMO</sub> (eV)</b>
Ciprofloxacin	-720626,1580	-720458,3633	168,549	-720388,7273	-7,21619	-0,98070
MZ-261	-572933,3070	-572823,3736	144,238	-572763,7822	-7,28068	-0,83267
MZ-263	-587998,3775	-587896,0157	142,956	-587836,9532	-7,55633	-0,93662
MZ-290	-624815,3143	-624669,9436	155,211	-624605,8184	-7,30490	-1,95323
MZ-291	-659117,5457	-659010,9940	153,614	-658947,5283	-7,95226	-1,23757
MZ-306	-672060,7186	-671916,6587	167,219	-671847,5724	-7,28885	-0,89526
MZ-308	-680265,8094	-680120,6671	182,498	-680045,2680	-7,01592	-1,24002
MZ-310	-695331,8425	-695193,4917	179,015	-695119,5315	-7,23687	-1,66452
MZ-330	-705561,2815	-705385,9904	169,911	-705315,7916	-7,46109	-0,97145
MZ-334A	-743189,7223	-743042,8701	179,860	-742968,5610	-7,26327	-0,85389
MZ-334B	-743178,6913	-743030,1209	176,186	-742957,3298	-7,98301	-1,29118
MZ-336	-743898,6029	-743736,2091	179,840	-743661,9082	-7,44232	-1,75078
MZ-346A	-752778,2388	-752601,0477	173,136	-752529,5166	-7,38735	-0,91675
MZ-346B	-767095,0557	-766941,6340	175,516	-766869,1196	-7,33102	-0,96192
MZ-360	-813559,8444	-813420,1463	180,819	-813345,4407	-7,96940	-1,29907
MZ-362A	-814305,3771	-814149,9361	181,615	-814074,9017	-7,88858	-1,10505
MZ-362B	-814307,5439	-814155,4293	187,446	-814077,9859	-7,97321	-1,28030
MZ-364	-815035,2077	-814868,3893	187,753	-814790,8185	-7,56640	-1,02016

**Table S6.** Cartesian coordinates for optimized structure of ciprofloxacin.

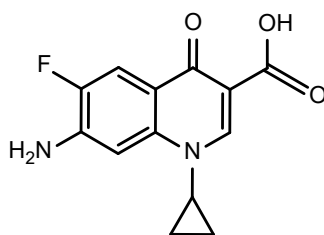
<u>ATOM TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	1.16925600	-2.03831100	-0.26296700
C	1.75749000	-0.76374200	-0.47890100
C	0.87998700	0.31577300	-0.51864800
C	-0.49212900	0.15086700	-0.31653400
C	-1.03204200	-1.12043400	-0.07685900
C	-0.16029100	-2.22005900	-0.06067400
N	-1.34375100	1.25777000	-0.33905500
C	-2.65729100	1.09457900	-0.18713000
C	-3.25161800	-0.12269300	0.03177100
C	-2.45308500	-1.30839200	0.11247600
F	1.95403100	-3.12726200	-0.33012100
C	-0.79725400	2.58229400	-0.57850700
C	0.03892900	3.21753500	0.48298700
C	-1.33521100	3.74142800	0.18790700
O	-2.95126500	-2.44343900	0.32749200
C	-4.71699500	-0.17185700	0.19026300
O	-5.22297900	-1.37802100	0.41269800
O	-5.43846600	0.80595300	0.12587300
N	3.11448300	-0.65341600	-0.72171600
C	4.04515700	-1.28070100	0.23641900
C	4.32906400	-0.34967600	1.40247400
N	4.90591400	0.90404800	0.91601500
C	3.95024300	1.56535400	0.02455700
C	3.64441200	0.64523800	-1.14729400
H	1.26456800	1.30477900	-0.69267400
H	-0.54831100	-3.21933300	0.07844000
H	-3.25844300	1.99067100	-0.24377100
H	-0.50883200	2.73477400	-1.60879300
H	0.90045200	3.78059200	0.15683600
H	0.16300100	2.66027500	1.40063000
H	-2.10061500	3.54878400	0.92511900
H	-1.43473600	4.67144200	-0.34983500
H	-4.45300900	-2.03276400	0.42691900
H	3.64037700	-2.21481200	0.60500500
H	4.97108600	-1.49576300	-0.29842100
H	3.39091100	-0.17993800	1.94947200
H	5.03065200	-0.83263600	2.08067700
H	5.07192900	1.50957800	1.71114500
H	4.38359600	2.48992900	-0.35314200
H	3.02215000	1.81907400	0.55234400
H	4.57353300	0.44161100	-1.68183000
H	2.95883800	1.11110400	-1.85028500

**Table S7.** Cartesian coordinates for optimized structure of MZ-261.



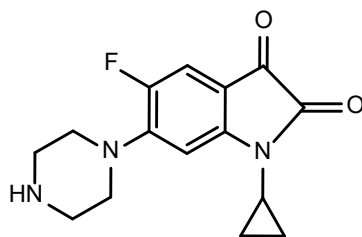
<u>ATOM TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	-3.44391500	-0.85362000	-0.06290700
C	-2.01958200	-0.47336300	-0.07707500
C	-1.69615700	0.85228000	-0.22488700
N	-0.44367200	1.30359300	-0.24163000
C	-0.18186500	2.72115300	-0.41626600
C	0.35656300	3.49965900	0.73775000
C	-1.05400200	3.71276900	0.27319000
C	0.62796100	0.41314800	-0.14468900
C	0.36813500	-0.95776900	0.01625800
C	1.45472000	-1.84681300	0.11512500
C	2.73841200	-1.39177000	0.05277600
O	3.83940000	-2.19259200	0.14096700
C	3.00592000	-0.00690400	-0.12051100
N	4.30294600	0.41624900	-0.13926300
C	1.94285700	0.87581000	-0.21901000
C	-0.98549600	-1.45409100	0.06522500
O	-1.24339900	-2.68048700	0.21662900
O	-4.35981100	-0.06048900	-0.18622200
O	-3.68237600	-2.14850500	0.09794400
H	-2.47183100	1.59567600	-0.33627400
H	0.18795300	2.95876200	-1.40356500
H	0.48876400	2.96163600	1.66544700
H	1.10272400	4.24851400	0.51978500
H	-1.84075000	3.33658100	0.91025800
H	-1.29306500	4.61059500	-0.27532200
H	1.26479900	-2.90490300	0.23882100
H	3.57332900	-3.11435200	0.24556300
H	5.00994800	-0.27127700	-0.34677700
H	4.47835100	1.34192500	-0.49781800
H	2.15704900	1.92457700	-0.35674800
H	-2.78401300	-2.61298300	0.17845000

**Table S8.** Cartesian coordinates for optimized structure of MZ-263.



ATOM TYPE	x	y	z
C	2.70226700	-1.41067100	0.05050300
C	3.01535100	-0.04551300	-0.12659700
C	1.95833900	0.84982200	-0.21872000
C	0.64048300	0.39816700	-0.14474500
C	0.35810900	-0.96994700	0.01865800
C	1.43062900	-1.87306200	0.12130500
N	-0.42092100	1.30052400	-0.24036200
C	-1.67948600	0.86245000	-0.22341400
C	-2.02279300	-0.45694500	-0.07526700
C	-1.00232100	-1.45221900	0.06895700
F	3.74046000	-2.26015700	0.14405200
C	-0.14487600	2.71523500	-0.41861500
C	-1.00494100	3.71666400	0.27197000
C	0.40483000	3.49080700	0.73222400
O	-1.27192100	-2.67274500	0.22084000
C	-3.45323300	-0.81561400	-0.06232400
O	-3.71257800	-2.10680800	0.09832500
O	-4.35590000	-0.00866300	-0.18662800
N	4.31523100	0.33812100	-0.24624000
H	2.18237600	1.89674200	-0.35331800
H	1.24267500	-2.92926700	0.25236200
H	-2.44549000	1.61586000	-0.33547700
H	0.22378000	2.94694300	-1.40774700
H	-1.23778600	4.61543200	-0.27765500
H	-1.79268300	3.34931200	0.91299500
H	0.53463000	2.95366900	1.66075000
H	1.15759500	4.23161400	0.50971300
H	-2.82660200	-2.58706300	0.17996700
H	4.51894500	1.32012900	-0.14381700
H	5.02728900	-0.29180100	0.08805700

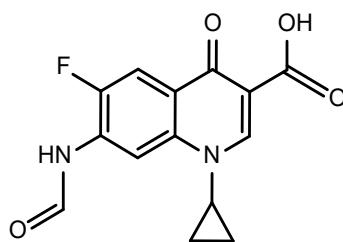
**Table S9.** Cartesian coordinates for optimized structure of MZ-290.



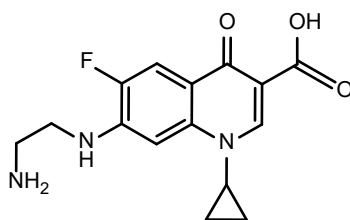
ATOM TYPE	x	y	z
N	2.46331500	0.65793300	0.20877100
C	2.52671600	2.08226100	0.34786100
C	1.91661900	2.91992100	-0.73341800
C	3.40512300	2.84055000	-0.59461000
C	1.26367200	-0.08849000	0.15607400
C	1.52790700	-1.45407500	0.02889600
C	0.47712200	-2.36310100	-0.03485400
C	-0.79655800	-1.86947000	0.02050500
F	-1.81477900	-2.75073500	0.04328200
C	-1.09749800	-0.49045000	0.12977100
N	-2.41019300	-0.06905000	0.20378600
C	-2.64075100	1.33304500	0.55661300
C	-4.10052500	1.55453900	0.89678500
N	-4.94682000	1.18095000	-0.23399000
C	-4.75168700	-0.23776700	-0.52471700
C	-3.30623300	-0.49394900	-0.88962000
C	-0.01612400	0.40933600	0.21315000
C	2.96207300	-1.61944200	0.02461700
O	3.66851900	-2.59645300	-0.06138900
C	3.53335500	-0.17892600	0.17309300
O	4.70830500	0.10234200	0.24949600
H	2.44568000	2.43490200	1.36669500
H	1.41192100	3.82262300	-0.42518500
H	1.46659000	2.39139800	-1.56130700
H	3.94201700	2.26401500	-1.33278300
H	3.93408700	3.68960700	-0.19033100
H	0.64422300	-3.43003900	-0.09600200
H	-2.03375800	1.58389300	1.42405500
H	-2.35048300	1.99011300	-0.27270500
H	-4.34402900	0.97266200	1.79476900
H	-4.24636700	2.60763600	1.12909800
H	-5.91478800	1.32648500	0.02746400
H	-5.37947000	-0.52746600	-1.36525200
H	-5.01766600	-0.86938700	0.33244700
H	-3.04960300	0.07671500	-1.79007000
H	-3.16442100	-1.54639200	-1.10293700
H	-0.18889400	1.47001500	0.29679600



**Table S10.** Cartesian coordinates for optimized structure of MZ-291.

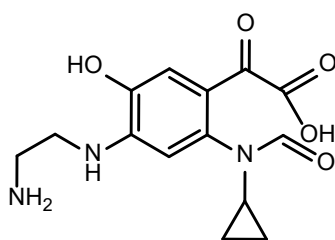


ATOM TYPE	x	y	z
C	-4.01444200	-0.20537200	-0.08771500
C	-2.53964000	-0.14806300	-0.08427000
C	-1.93386600	1.07642500	-0.22028300
N	-0.61395000	1.25113400	-0.22304500
C	-0.05401400	2.58217000	-0.38801900
C	0.64640900	3.21384800	0.76901400
C	-0.68843300	3.72956800	0.31901300
C	0.23793800	0.15118800	-0.12117900
C	-0.30916500	-1.13009300	0.02439100
C	0.55244100	-2.23187800	0.12640500
C	1.89359200	-2.02997000	0.08069600
F	2.73636100	-3.06906000	0.17535600
C	2.46607800	-0.75257200	-0.06945700
N	3.85495600	-0.68671100	-0.10582300
C	1.62501600	0.33705300	-0.17558100
C	-1.74818300	-1.33052600	0.05739200
O	-2.25041300	-2.47174200	0.19396200
O	-4.72766000	0.77167200	-0.21159200
O	-4.53747300	-1.41630800	0.05564800
C	4.64018900	0.42050700	-0.13994500
O	4.24288900	1.57033700	-0.15553900
H	-2.53190000	1.96912600	-0.33277900
H	0.35026500	2.74408600	-1.37698000
H	0.66607400	2.64897600	1.69001100
H	1.53591600	3.78503200	0.55013000
H	-0.73277000	4.66300700	-0.22013200
H	-1.53373700	3.52367000	0.95889200
H	0.15447300	-3.23016700	0.23876200
H	4.34853200	-1.56904000	-0.07107000
H	2.04040100	1.31831500	-0.30522200
H	-3.77804600	-2.07171000	0.13956300
H	5.70422300	0.16390400	-0.14991900

**Table S11.** Cartesian coordinates for optimized structure of MZ-306.

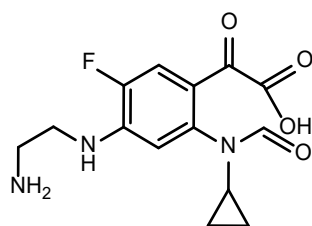
ATOM TYPE	x	y	z
C	1.49934500	-2.10716800	-0.20355500
C	2.10192100	-0.85685200	-0.48903100
C	1.26489800	0.25234700	-0.54897900
C	-0.10767900	0.11636700	-0.33330900
C	-0.67740900	-1.14074700	-0.06936700
C	0.17044000	-2.26327500	-0.00521100
N	-0.93722800	1.23867300	-0.37818900
C	-2.25493600	1.10773600	-0.22422000
C	-2.87377600	-0.09090400	0.02045900
C	-2.09839700	-1.29167800	0.12412700
F	2.32401700	-3.16816400	-0.14225300
C	-0.36060300	2.54560000	-0.64028500
C	-0.87338700	3.73134000	0.10219900
C	0.48621000	3.17902800	0.41350700
O	-2.62547300	-2.41125200	0.36256300
C	-4.33948200	-0.10743400	0.18109900
O	-4.86860400	-1.29870100	0.42690600
O	-5.04142700	0.88360200	0.09886100
N	3.43810000	-0.80926200	-0.72665700
H	1.68458600	1.22024900	-0.76398600
H	-0.23781800	-3.24267900	0.20057700
H	-2.83570000	2.01560800	-0.30146400
H	-0.06395700	2.67252500	-1.67174300
H	-0.94747800	4.65344600	-0.45301200
H	-1.64671500	3.57117500	0.83887400
H	0.59131200	2.63518900	1.34149200
H	1.36334900	3.71460800	0.08270200
H	-4.10856600	-1.96782400	0.45308200
H	3.95826700	-1.62894600	-0.45164500
C	4.18115900	0.44164000	-0.75006500
C	4.27494500	1.12620000	0.61010300
H	3.72979300	1.11522600	-1.47965100
H	5.18339200	0.20615600	-1.10512000
H	4.82636500	2.05654100	0.47635200
H	3.27853800	1.39602300	0.96097100
N	4.92665300	0.33262300	1.64904700
H	4.39897900	-0.52215700	1.79415900
H	5.84136100	0.04169900	1.31781700

**Table S12.** Cartesian coordinates for optimized structure of MZ-308.

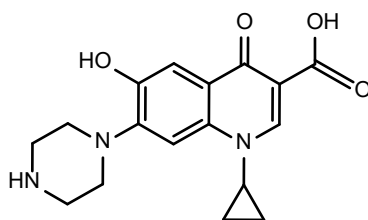


ATOM TYPE	x	y	z
C	3.29939700	0.86123200	-0.60705900
C	1.61375700	-1.75428100	-1.32215600
N	1.43437100	-1.14652100	-0.12961800
C	2.09288400	-1.62402700	1.06956100
C	2.17229100	-3.09537200	1.32280500
C	1.25413600	-2.24002400	2.14342800
C	0.46711900	-0.09839800	0.01262000
C	0.86976800	1.22207200	0.22927800
C	-0.11967300	2.18813600	0.50026100
C	-1.44310900	1.85729600	0.50052200
O	-2.45045900	2.75197400	0.72406000
C	-1.86069700	0.52279600	0.24891700
N	-3.17559400	0.23623500	0.24222400
C	-3.70448800	-1.09650500	0.02395400
C	-5.22214300	-1.07814600	-0.00347300
N	-5.82353600	-0.33924800	-1.11117100
C	-0.87073100	-0.44451300	0.02768600
C	2.25339600	1.66801000	0.17332400
O	2.66023500	2.70821900	0.65894200
O	1.02683100	-1.45405300	-2.35196100
O	4.30293700	0.42700800	-0.10507000
O	3.00416100	0.80751100	-1.89606800
H	2.36320300	-2.55194900	-1.28901100
H	2.93026600	-1.01862800	1.38731300
H	3.08154600	-3.46551400	1.77095100
H	1.71329500	-3.75116400	0.59794600
H	0.19573900	-2.32831500	1.94493800
H	1.52206200	-2.01716100	3.16462400
H	0.17353600	3.21521500	0.67716600
H	-2.08222400	3.63161200	0.87193700
H	-3.81925400	0.98121500	0.46433800
H	-3.32842700	-1.48751300	-0.92577000
H	-3.36224000	-1.77014100	0.81508500
H	-5.59361800	-0.66046000	0.93298000
H	-5.56149800	-2.11145500	-0.04798600
H	-5.57188400	0.64106900	-1.04754600
H	-5.42912600	-0.67417600	-1.98439100
H	-1.14463900	-1.47892400	-0.12101700
H	3.70548700	0.33809200	-2.37884500

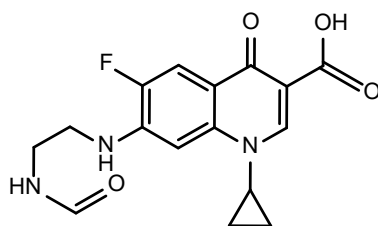
**Table S13.** Cartesian coordinates for optimized structure of MZ-310.



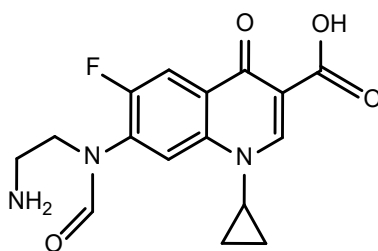
ATOM TYPE	x	y	z
C	3.05018000	-0.88432100	-1.12164000
C	1.14784900	2.25272700	-0.98599000
N	1.27364200	1.29321200	-0.04075500
C	2.46389000	1.31545100	0.77924500
C	2.48752200	2.18524800	1.99870700
C	2.43043500	0.69292500	2.13495800
C	0.33212800	0.22925600	0.01418500
C	0.74462000	-1.10880000	0.05583500
C	-0.22765300	-2.10444000	0.24133600
C	-1.54305000	-1.76558800	0.29549500
F	-2.48217200	-2.72164600	0.42869100
C	-1.99617800	-0.43599000	0.21423400
N	-3.31640900	-0.16501100	0.30089700
C	-3.86467200	1.14531700	-0.00039600
C	-5.37395600	1.11148800	0.10576200
N	-5.93412700	0.12740800	-0.82193100
C	-1.01098100	0.55638200	0.10214000
C	2.12827700	-1.55954400	-0.07940800
O	2.58749800	-2.52632300	0.49255800
O	1.93874400	3.17485200	-1.12034100
O	2.63814800	-0.23619300	-2.04469400
O	4.33576300	-1.14845300	-0.95911700
H	0.27869700	2.12619200	-1.63933100
H	3.38359100	1.26173700	0.21178600
H	3.41263600	2.69448200	2.22177300
H	1.58273900	2.73284100	2.21846200
H	1.49404200	0.26190200	2.45927800
H	3.31702900	0.16343900	2.44979300
H	0.06058500	-3.14553600	0.29486900
H	-3.95269700	-0.93943300	0.17225300
H	-3.47209900	1.88054500	0.70256700
H	-3.56806800	1.45891500	-1.00760500
H	-5.74269000	2.12577300	-0.06388700
H	-5.65601200	0.82590100	1.11911700
H	-6.93535100	0.06500400	-0.68156000
H	-5.79867700	0.45571600	-1.77255700
H	-1.29720300	1.59777800	0.12224200
H	4.45959500	-1.75143600	-0.20691300

**Table S14.** Cartesian coordinates for optimized structure of MZ-330.

ATOM TYPE	x	y	z
C	-1.16598000	-1.87473400	0.08235400
C	-1.64541200	-0.54043700	0.17378900
C	-0.73518300	0.49640600	0.22752400
C	0.64037600	0.24199800	0.15419700
C	1.10260200	-1.07460000	0.03310900
C	0.17594500	-2.12645600	0.00292400
N	1.55919500	1.29330800	0.19887500
C	2.86438300	1.04202300	0.16927700
C	3.39037400	-0.22352000	0.06387400
C	2.52528300	-1.35804300	-0.02041500
C	1.08016000	2.65858300	0.32839000
C	0.40768400	3.29786500	-0.84107800
C	1.77388000	3.74740600	-0.41455100
O	2.96108200	-2.53311100	-0.12732800
C	4.85715200	-0.37377900	0.03653600
O	5.29863900	-1.62044400	-0.07147100
O	5.63563000	0.55928800	0.10635700
N	-3.03613800	-0.35746100	0.25210400
C	-3.48954000	0.92484500	0.79269100
C	-4.98859900	0.88291300	1.01053200
N	-5.66921700	0.62169700	-0.25740600
C	-5.22751600	-0.66350700	-0.79691700
C	-3.73144700	-0.63599500	-1.02225100
H	-1.08760300	1.51078100	0.31579400
H	0.52874400	-3.14670500	-0.04852800
H	3.51860300	1.89921800	0.23384700
H	0.69351200	2.87221700	1.31461800
H	-0.44412200	3.92751800	-0.63335800
H	0.34765400	2.71005300	-1.74578400
H	2.60061200	3.47579900	-1.05398000
H	1.87626400	4.69163300	0.09725900
H	4.49099100	-2.22593300	-0.11539000
H	-2.98057900	1.10844800	1.73783200
H	-3.24967400	1.74554400	0.10453600
H	-5.21470300	0.11421300	1.76006800
H	-5.31579400	1.84334900	1.40417300
H	-6.66611000	0.57312200	-0.08356000
H	-5.72715700	-0.84933600	-1.74585300
H	-5.46317500	-1.49498200	-0.11971800
H	-3.47648800	0.14645500	-1.74810200
H	-3.39703600	-1.58849600	-1.42733100
O	-2.03413000	-2.92298600	0.10918700
H	-2.90554200	-2.60347100	0.38459400

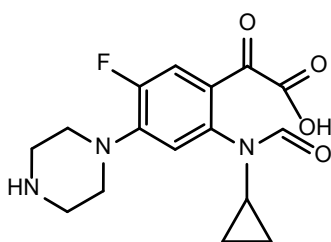
**Table S15.** Cartesian coordinates for optimized structure of MZ-334A.

ATOM TYPE	x	y	z
C	4.90241200	-0.63256300	0.31694100
C	3.45671600	-0.37057300	0.19013400
C	3.01155300	0.92101000	0.29762700
N	1.72862900	1.26968700	0.19136200
C	1.33976400	2.66130200	0.33621600
C	0.84688200	3.39921900	-0.86427100
C	2.18834100	3.72192900	-0.27578900
C	0.74668900	0.29614600	-0.00207900
C	1.13906800	-1.04779900	-0.12873300
C	0.14330100	-2.02610800	-0.32838900
C	-1.15402700	-1.65394700	-0.38679900
F	-2.12150200	-2.57005000	-0.57183400
C	-1.58218100	-0.30823800	-0.25241900
N	-2.89807800	-0.03036100	-0.32397300
C	-3.43349800	1.30072700	-0.12062100
C	-4.94786600	1.27745600	-0.17815600
N	-5.56060600	0.51550600	0.90101900
C	-0.60070100	0.66039600	-0.05701600
C	2.52384100	-1.43377100	-0.04206800
O	2.89267200	-2.63467600	-0.15500100
O	5.73424300	0.23379400	0.51619600
O	5.25849300	-1.90467400	0.19897900
C	-5.79688500	-0.79393100	0.83746900
O	-5.48004500	-1.51764500	-0.10855800
H	3.70945300	1.72516500	0.47946300
H	0.86504600	2.86537200	1.28550300
H	0.02666000	4.08521400	-0.71622500
H	0.84153100	2.85572500	-1.79813600
H	3.05647200	3.41271600	-0.83889500
H	2.30465200	4.63362000	0.28930900
H	0.41646800	-3.06697200	-0.42890100
H	-3.55350700	-0.79490800	-0.42016300
H	-3.06811700	1.97796900	-0.89667500
H	-3.10406700	1.69650800	0.84416600
H	-5.27906100	0.85539700	-1.12623900
H	-5.31512100	2.29765600	-0.11522700
H	-5.84942300	1.00140900	1.73659100
H	-0.89117700	1.69210000	0.05041600
H	4.41286200	-2.44131500	0.03949000
H	-6.31211400	-1.19095900	1.71795800

**Table S16.** Cartesian coordinates for optimized structure of MZ-334B.

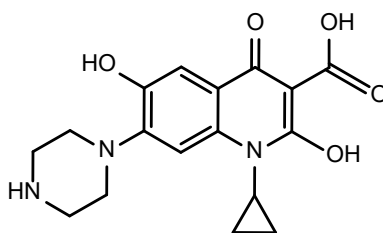
ATOM TYPE	x	y	z
C	-4.68858000	-0.20462100	0.04016900
C	-3.21601200	-0.14389600	-0.04606800
C	-2.62644100	1.07956800	-0.25246300
N	-1.31111300	1.25823000	-0.34670500
C	-0.76381200	2.58647900	-0.56847200
C	0.02685500	3.22463700	0.52586200
C	-1.33781100	3.74070200	0.17835700
C	-0.45199700	0.16343100	-0.27301900
C	-0.97444800	-1.11518800	-0.03933300
C	-0.10659500	-2.20939100	0.05687500
C	1.23453500	-2.01524500	-0.08811600
F	2.06513700	-3.06078100	-0.02401700
C	1.77768600	-0.74537200	-0.33386000
N	3.17698000	-0.58571700	-0.47203400
C	4.01810600	-0.85529900	0.70173900
C	3.75012500	0.14395800	1.82154800
N	3.94545300	1.54558700	1.46402900
C	0.92937500	0.33616600	-0.42036000
C	-2.41303700	-1.31853000	0.08862600
O	-2.89631200	-2.45478800	0.29477500
O	-5.41078900	0.76672300	-0.07106100
O	-5.19859100	-1.41166000	0.24963600
C	3.66173000	0.11229400	-1.52713700
O	4.82532500	0.46089300	-1.65408000
H	-3.23547800	1.96728800	-0.34666800
H	-0.43866800	2.73859900	-1.58764900
H	0.11832900	2.66653100	1.44693500
H	0.89751400	3.79214700	0.23372100
H	-1.42200100	4.67039000	-0.36246800
H	-2.13080400	3.54153500	0.88405800
H	-0.49814500	-3.20205200	0.22739300
H	3.82710500	-1.86936600	1.04838800
H	5.05208500	-0.79427300	0.37192100
H	2.72919800	0.02041100	2.18446600
H	4.41199400	-0.11157600	2.64827900
H	4.85729000	1.65543300	1.03142300
H	3.26838900	1.81227100	0.75537800
H	1.35061000	1.31531200	-0.59094200
H	-4.43607300	-2.06323200	0.31143400
H	2.90804000	0.31341800	-2.29677600

**Table S17.** Cartesian coordinates for optimized structure of MZ-336.

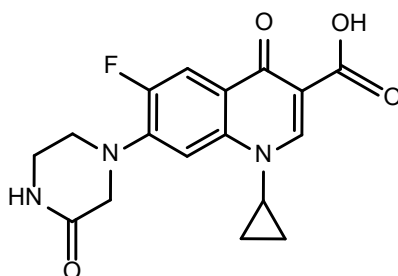


ATOM TYPE	x	y	z
O	-2.85473800	-2.74016100	0.99543600
C	-3.36561600	-2.13515000	0.09280100
C	-1.22667100	2.82557500	-0.96976600
N	-1.53141100	1.72363200	-0.24334200
C	-0.70908200	0.56913900	-0.32165600
C	-1.26145700	-0.71406800	-0.40239300
C	-0.40027900	-1.81543000	-0.38253800
C	0.95299600	-1.62884400	-0.34231800
F	1.74221300	-2.71318800	-0.43382500
C	1.54551200	-0.35934600	-0.25592300
N	2.92531400	-0.21720500	-0.21933800
C	3.61680900	-0.93566200	0.86828500
C	5.11236000	-0.93241500	0.63895500
N	5.60000300	0.44261200	0.55082400
C	4.94419200	1.11043300	-0.57152100
C	3.44522800	1.14420800	-0.35486300
C	0.66566200	0.72884100	-0.22736500
C	-2.69373400	-0.93960800	-0.62474500
O	-3.40694700	-0.25643700	-1.32317000
O	-1.86788700	3.86478800	-0.92496100
C	-2.70732600	1.77028600	0.59683000
C	-2.63062100	2.50319100	1.89779900
C	-2.71534700	1.00308100	1.87540500
O	-4.58452900	-2.39790300	-0.34285500
H	-0.36064600	2.70305300	-1.62786100
H	-0.78078400	-2.82350600	-0.46823100
H	3.39031300	-0.43856800	1.81951900
H	3.25952100	-1.95749000	0.92549600
H	5.59502500	-1.43700200	1.47382500
H	5.33096400	-1.50070100	-0.27411500
H	6.59713300	0.42018100	0.37260700
H	5.15117400	0.60326000	-1.52241200
H	5.30840400	2.13294000	-0.64974800
H	2.97056000	1.62052100	-1.21082000
H	3.21859700	1.73609100	0.54102300
H	1.05695300	1.72390200	-0.08046900
H	-3.63323600	1.83851300	0.04447700
H	-3.49953700	3.06996000	2.19588400
H	-1.67559200	2.93544200	2.15868500
H	-3.64405400	0.52781600	2.15469800
H	-1.82048100	0.45704100	2.13801800
H	-4.82452200	-1.76372800	-1.04067500

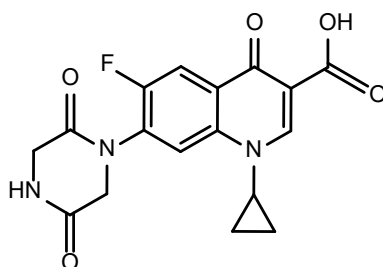


**Table S18.** Cartesian coordinates for optimized structure of MZ-346A.

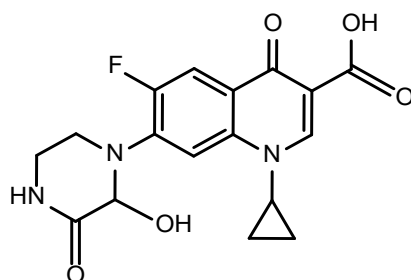
<u>ATOM TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	-4.63475500	-0.70341500	-0.28523200
C	-3.20899500	-0.44504700	-0.13711400
C	-2.74118000	0.86487800	-0.31222800
N	-1.44631600	1.18309000	-0.16524800
C	-1.03319000	2.57305400	-0.24309600
C	-0.27631700	3.15209300	0.90990100
C	-1.68830200	3.56887500	0.65638100
C	-0.49231300	0.16794000	0.02440200
C	-0.89956500	-1.15364600	0.22388900
C	0.06132500	-2.14648200	0.45464600
C	1.39472500	-1.83809400	0.45547400
O	2.30150400	-2.81381700	0.74644300
C	1.82200700	-0.51725800	0.17272600
N	3.20553900	-0.27256900	0.14629300
C	3.88352900	-0.87255800	-1.02200700
C	5.38415400	-0.78583000	-0.84772500
N	5.78448600	0.61279200	-0.70098700
C	5.12277000	1.19328800	0.46730400
C	3.61860800	1.12367300	0.29595500
C	0.87221100	0.46920600	-0.02104900
C	-2.30940100	-1.49955800	0.17401800
O	-2.70577900	-2.68015500	0.36389800
O	-5.44968600	0.17861400	-0.57494500
O	-5.03473700	-1.94096100	-0.09457400
O	-3.55878400	1.83788700	-0.63123700
H	-0.75844200	2.88592000	-1.24025100
H	0.52943700	3.82946500	0.66980100
H	-0.09944400	2.49962500	1.75280700
H	-1.88401000	4.54391200	0.23713200
H	-2.43972400	3.19524600	1.33547600
H	-0.25680600	-3.15975300	0.65552600
H	3.16037200	-2.40076900	0.91616800
H	3.58029800	-1.91113200	-1.13405800
H	3.58061300	-0.33379900	-1.92873600
H	5.66942500	-1.38703100	0.02556900
H	5.86943000	-1.21190900	-1.72385100
H	6.78618300	0.64785000	-0.55346100
H	5.41934200	2.23552500	0.56887700
H	5.39728700	0.67061900	1.39214400
H	3.33081200	1.71287700	-0.58419100
H	3.12368100	1.54642800	1.16943600
H	1.19140800	1.47495900	-0.23498400
H	-4.20298000	-2.48664800	0.12996800
H	-4.47485500	1.42616000	-0.68792300

**Table S19.** Cartesian coordinates for optimized structure of MZ-346B.

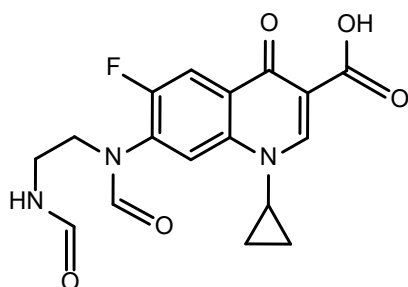
<u>ATOM TYPE</u>	<u>x</u>	<u>y</u>	<u>z</u>
C	-5.04572500	-0.23026800	-0.16975500
C	-3.57416500	-0.14521100	-0.12096800
C	-2.98406200	1.07909000	-0.30624100
N	-1.66674300	1.27649200	-0.27118300
C	-1.12534500	2.60731500	-0.48465700
C	-0.47758300	3.31011000	0.66208900
C	-1.80489700	3.77615800	0.14138000
C	-0.80032600	0.19884800	-0.07762400
C	-1.33796200	-1.08102200	0.12146200
C	-0.45247500	-2.14927400	0.33721700
C	0.88675800	-1.93550900	0.33230900
F	1.70312800	-2.96100100	0.62915300
C	1.46610900	-0.66347800	0.08404200
N	2.82758400	-0.49712700	0.08490800
C	3.70002600	-1.55852700	-0.45193900
C	4.86153300	-0.94760200	-1.20714700
N	5.53304600	0.02825300	-0.36349300
C	4.82302900	0.96750700	0.26090600
C	3.32863900	0.87352400	0.04757600
C	0.58200500	0.39564600	-0.10655100
C	-2.76621600	-1.30413400	0.11660400
O	-3.26278200	-2.44523800	0.30142000
O	-5.77282000	0.72330400	-0.37682800
O	-5.55155500	-1.44047800	0.03076900
O	5.31674900	1.87833800	0.92753000
H	-3.59092200	1.95335300	-0.49226500
H	-0.68938500	2.72902600	-1.46601900
H	-0.47931000	2.79264600	1.61068900
H	0.40744500	3.88909400	0.44558000
H	-1.84702600	4.68107700	-0.44459600
H	-2.66841100	3.58510900	0.76130300
H	-0.83488600	-3.14072300	0.53529200
H	4.08425400	-2.18026600	0.35567700
H	3.13548800	-2.18599200	-1.13785500
H	5.56840500	-1.72812300	-1.46894200
H	4.51445000	-0.47549400	-2.12762300
H	6.54113800	0.06406500	-0.30980100
H	2.85130800	1.45893200	0.82958600
H	3.12016300	1.35966200	-0.91526800
H	0.96814600	1.38046900	-0.30281000
H	-4.77899700	-2.07361600	0.17770400

**Table S20.** Cartesian coordinates for optimized structure of MZ-360.

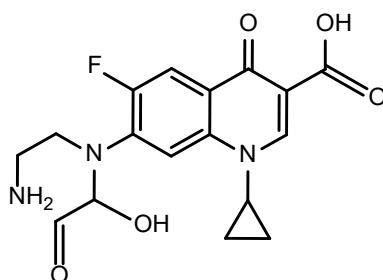
ATOM TYPE	x	y	z
C	-5.14140700	-0.39640200	0.01266200
C	-3.67457900	-0.23148700	-0.02152900
C	-3.16485200	1.00400600	-0.33815300
N	-1.86280200	1.27420800	-0.39140600
C	-1.40689300	2.61062900	-0.73613400
C	-0.72833800	3.42606700	0.31421400
C	-2.10874600	3.78603900	-0.14849300
C	-0.93006400	0.26445700	-0.15944600
C	-1.37180300	-1.02032500	0.18240100
C	-0.43373700	-2.02633100	0.43947700
C	0.89617100	-1.74631800	0.33974400
F	1.79206700	-2.68583500	0.64891500
C	1.35512600	-0.47813600	-0.04737000
N	2.74350700	-0.22862600	-0.14379400
C	3.50988700	-1.00890100	-0.95546900
C	4.97658000	-0.66936200	-1.00827500
N	5.43854300	0.07846500	0.14294900
C	4.69453900	0.99387300	0.76659300
C	3.24717000	1.05813000	0.34424000
C	0.43995400	0.52198600	-0.28602800
C	-2.79573100	-1.31863100	0.27608300
O	-3.20505700	-2.45988700	0.58934000
O	-5.92682000	0.49636900	-0.24012600
O	-5.57089500	-1.60764900	0.34303000
O	5.12643400	1.75587800	1.62789900
O	3.05764800	-1.91854000	-1.63047900
H	-3.83015700	1.82632500	-0.55928600
H	-1.04144300	2.67902600	-1.75067900
H	-0.64260300	2.97998900	1.29480800
H	0.10859900	4.03079700	-0.00044600
H	-2.23693000	4.64247600	-0.79188600
H	-2.92013300	3.59688100	0.53878700
H	-0.76072600	-3.01358200	0.73290000
H	5.14439900	-0.11992400	-1.93844600
H	5.52128200	-1.60638100	-1.07173000
H	6.42261500	0.04142100	0.37341500
H	2.66179500	1.35555800	1.20915200
H	3.15635200	1.83451300	-0.42057000
H	0.78954500	1.49828900	-0.58383200
H	-4.76607400	-2.18633200	0.50892700

**Table S21.** Cartesian coordinates for optimized structure of MZ-362A.

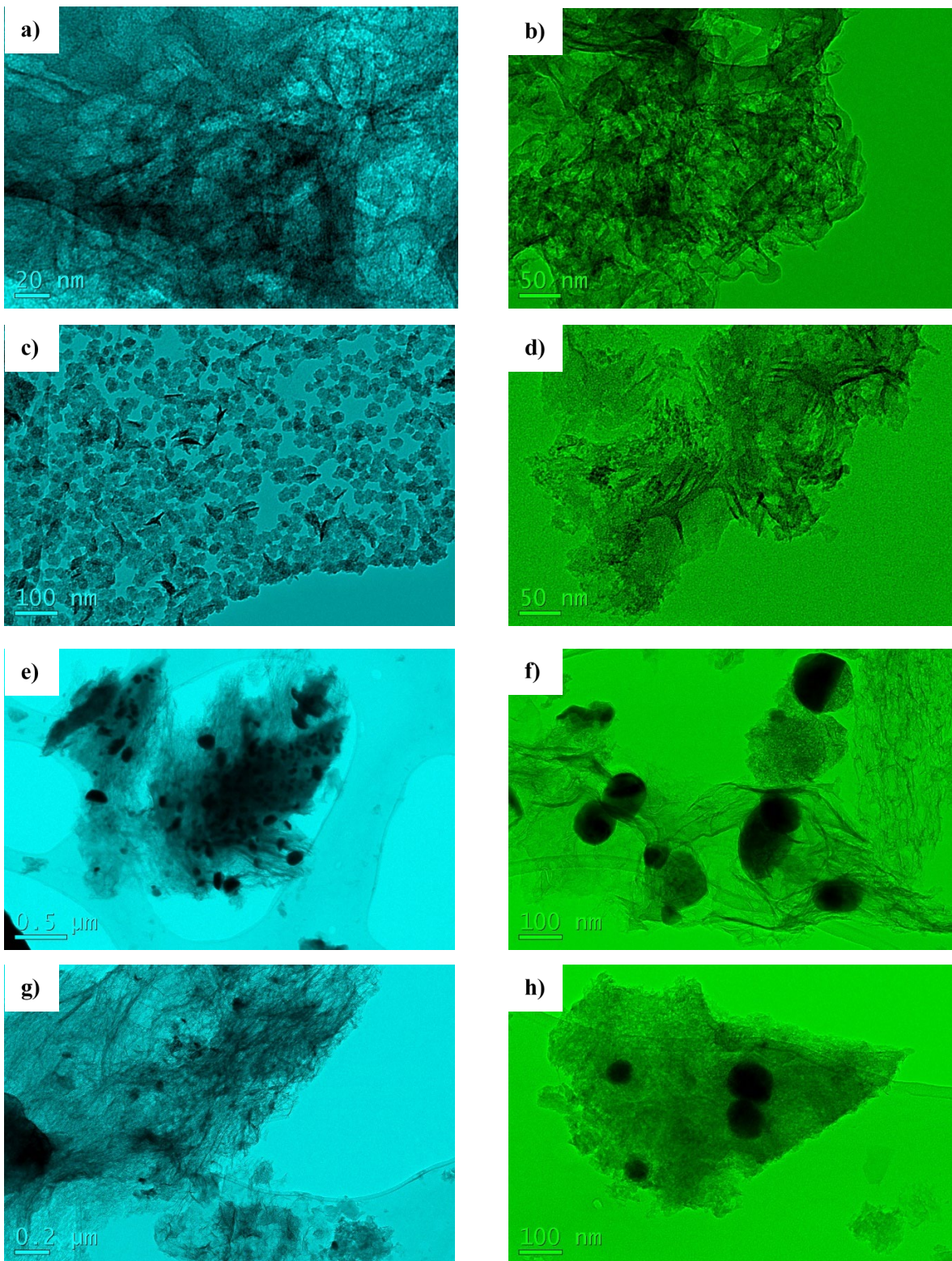
ATOM TYPE	x	y	z
C	5.15476100	-0.57160500	0.26999300
C	3.70281100	-0.33765600	0.14661700
C	3.22674500	0.93428500	0.34786700
N	1.93985500	1.26359500	0.25565000
C	1.51769400	2.63362100	0.49350100
C	0.99747500	3.43250600	-0.65540200
C	2.33533800	3.75080300	-0.05655300
C	0.98523400	0.28495400	-0.02166100
C	1.39822300	-1.03442700	-0.24419100
C	0.43151800	-2.00679000	-0.53558700
C	-0.88092700	-1.65682600	-0.58851400
F	-1.78732500	-2.58843300	-0.91985600
C	-1.33066000	-0.34251800	-0.33933300
N	-2.70202900	-0.04920400	-0.41841800
C	-3.06521800	1.36786000	-0.46450700
C	-4.47065400	1.48548500	-1.00022000
N	-5.36869400	0.59722500	-0.27427600
C	-4.99839800	-0.47015100	0.42609300
C	-3.50719300	-0.77271000	0.55748500
C	-0.37517300	0.61445500	-0.05330100
C	2.80200000	-1.40061300	-0.17620400
O	3.18650500	-2.57770600	-0.38010300
O	5.95846700	0.29828000	0.54657700
O	5.54926400	-1.82008700	0.05588100
O	-3.17187400	-0.44771200	1.89265400
O	-5.79512900	-1.21615000	0.99780700
H	3.90699300	1.73602200	0.59637900
H	1.04695000	2.76392200	1.45742800
H	0.99749700	2.94895900	-1.62177500
H	0.16168000	4.08662100	-0.45823100
H	2.43369900	4.62760900	0.56433000
H	3.20667300	3.49762800	-0.64227700
H	0.72755300	-3.02637800	-0.73742900
H	-2.39475100	1.88721400	-1.14403700
H	-2.98665700	1.83262900	0.52312500
H	-4.48984200	1.23705900	-2.06145700
H	-4.82271700	2.50711600	-0.88051800
H	-6.36557000	0.74315000	-0.36789300
H	-3.39563200	-1.84110300	0.39576000
H	-0.68383600	1.62315600	0.16331500
H	4.73060800	-2.36804000	-0.15627400
H	-2.42997200	-0.99802500	2.16853400

**Table S22.** Cartesian coordinates for optimized structure of MZ-362B.

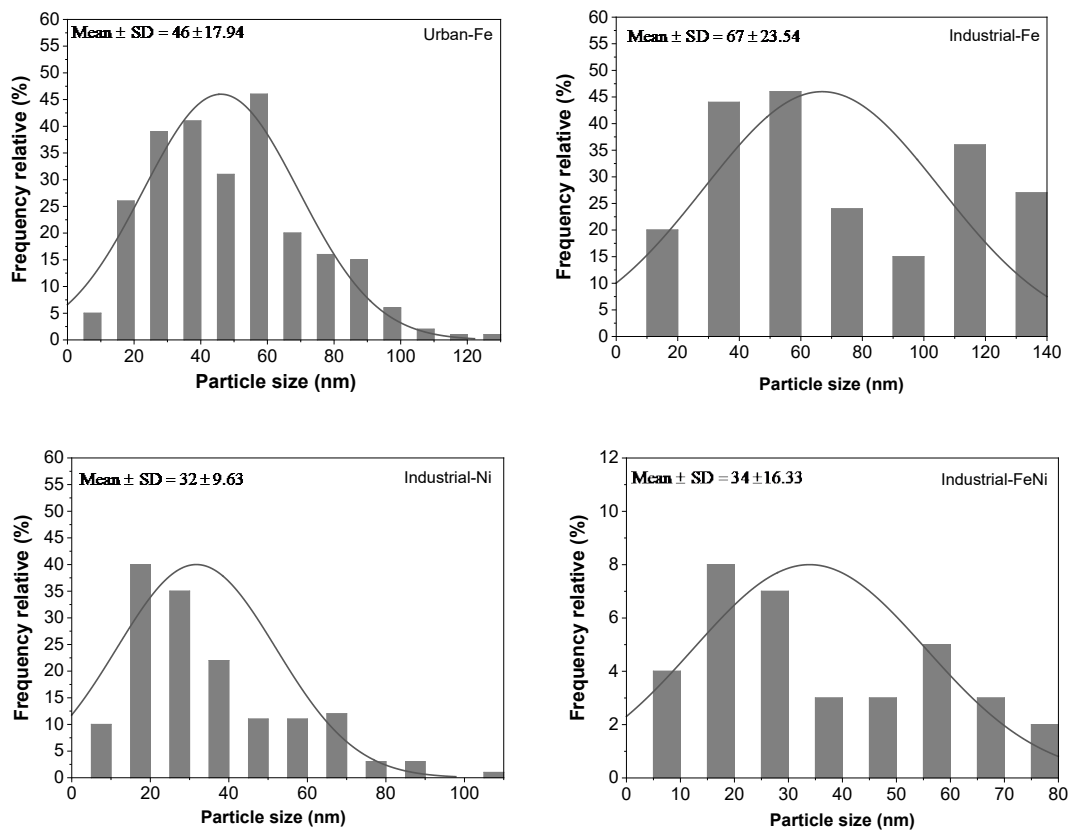
ATOM TYPE	x	y	z
C	4.79292400	-0.32861500	0.37342100
C	3.33989700	-0.23768200	0.12745500
C	2.76762300	1.00910000	0.06077200
N	1.47136800	1.21537100	-0.16023400
C	0.93873800	2.56760100	-0.19651400
C	0.43364100	3.10085900	-1.49623000
C	1.70723000	3.62862000	-0.90536200
C	0.60653900	0.13155800	-0.29933700
C	1.11476500	-1.17275100	-0.24623600
C	0.24198200	-2.25848500	-0.38570100
C	-1.08983200	-2.03045100	-0.55692200
F	-1.91992900	-3.06423900	-0.73529100
C	-1.62610800	-0.73246400	-0.57328500
N	-3.01707700	-0.53993300	-0.72454200
C	-3.95898400	-1.17012900	0.20840400
C	-4.34983400	-0.22005300	1.33353100
N	-3.20898900	0.17192100	2.13917000
C	-2.55241400	1.32022100	1.96533800
C	-3.47867600	0.39131900	-1.59596300
C	-0.76908300	0.33969300	-0.45119700
C	2.53772400	-1.40947000	-0.03840500
O	3.00896800	-2.56901500	0.00050100
O	5.51267900	0.63868700	0.52789400
O	5.28739100	-1.55927700	0.41945000
O	-4.65521800	0.69939600	-1.69251500
O	-1.50139600	1.61796900	2.52962500
H	3.37458400	1.89373400	0.19015000
H	0.40253500	2.82785300	0.70521000
H	0.52569700	2.45210300	-2.35566700
H	-0.45654800	3.71044700	-1.46228800
H	2.62763500	3.34433000	-1.39378900
H	1.70625900	4.60831300	-0.45367000
H	0.62343600	-3.26942400	-0.37181600
H	-3.49287700	-2.05920900	0.62274100
H	-4.84724300	-1.47042600	-0.34322200
H	-5.08680400	-0.71314500	1.96428100
H	-4.80287300	0.68196100	0.92729100
H	-2.77134000	-0.52715500	2.72739800
H	-3.04621600	2.00875300	1.26665100
H	-2.70217900	0.82770400	-2.23355800
H	-1.17828200	1.33832200	-0.44384400
H	4.53029200	-2.20282800	0.26874200

**Table S23.** Cartesian coordinates for optimized structure of MZ-364.

ATOM TYPE	x	y	z
C	-5.17847700	-0.47774700	-0.11758400
C	-3.71632700	-0.28441700	-0.07616800
C	-3.21928600	0.98356800	-0.24453800
N	-1.91999700	1.27643900	-0.21662300
C	-1.47640200	2.64452200	-0.42263800
C	-0.86748200	3.38098900	0.72412400
C	-2.22963600	3.75688500	0.22121700
C	-0.97610800	0.26311300	-0.04303500
C	-1.41386500	-1.05586700	0.13660200
C	-0.45508300	-2.06219300	0.33070200
C	0.86499900	-1.74784700	0.32583600
F	1.76269700	-2.71120700	0.58988200
C	1.34212400	-0.43354300	0.09940000
N	2.70093300	-0.16260400	0.12379100
C	3.10569400	1.23751400	0.30137200
C	4.57956800	1.40880100	0.62146600
N	4.99775700	0.57470600	1.75241200
C	4.18462000	-0.34776600	-1.83393600
C	3.60141800	-1.04175300	-0.60356000
C	0.39009800	0.56065900	-0.07207600
C	-2.82435300	-1.38451800	0.13141300
O	-3.23052300	-2.56301700	0.29179000
O	-5.97589000	0.42434000	-0.29197800
O	-5.59084900	-1.72754500	0.05095400
O	4.61483400	-1.59229000	0.19302500
O	3.51414500	0.33266500	-2.56715700
H	-3.89129000	1.81291200	-0.41164300
H	-1.06033600	2.80426600	-1.40713900
H	-0.02764000	4.02247900	0.50379800
H	-0.82247800	2.85644400	1.66778800
H	-3.07083300	3.49906300	0.84751700
H	-2.34179300	4.66166600	-0.35561600
H	-0.76540700	-3.08156900	0.51174100
H	2.51911700	1.63448200	1.13083700
H	2.87961800	1.83966000	-0.58309000
H	5.20509300	1.14640200	-0.23555600
H	4.73426000	2.47470200	0.79820800
H	5.94229500	0.82117100	2.02517800
H	4.39960100	0.75648300	2.55199200
H	5.24804100	-0.55292000	-2.03706900
H	3.02558900	-1.86427500	-1.02983000
H	0.70997700	1.57278100	-0.25040500
H	-4.77277400	-2.30469200	0.17596900
H	4.85110300	-0.91358900	0.88666100

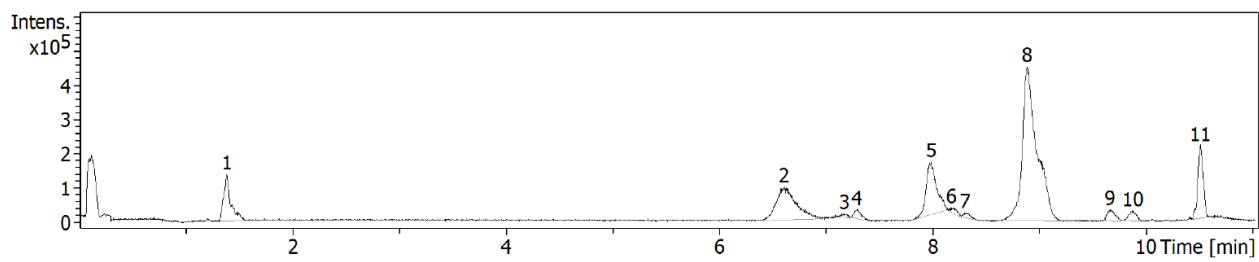


**Figure S1.** HR-TEM images of the metal dispersion of the active phase on the catalyst surface. (a,b) Urban-Fe catalyst, (c,d) Industrial-Fe Catalyst, (e,f) Industrial-Ni catalyst, (g,h) Industrial FeNi catalyst. Metallic particles are seen as dark spots.

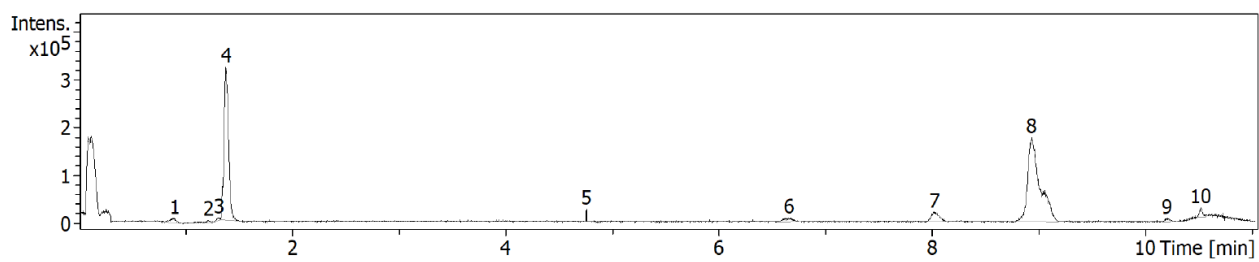


**Figure S2.** The histograms of iron and nickel particle size distributions.

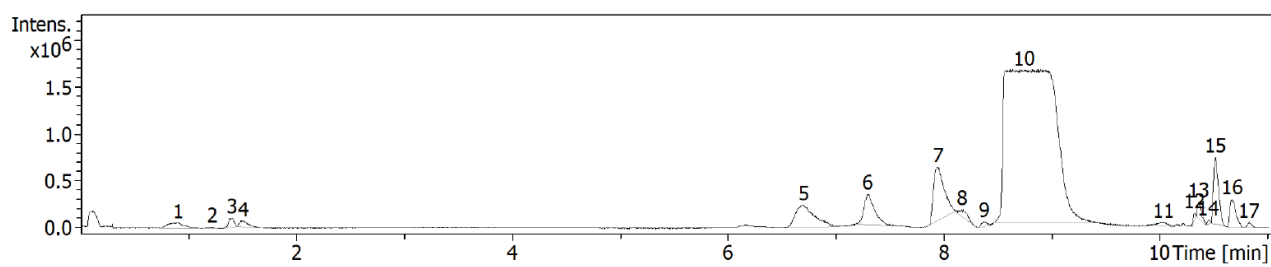




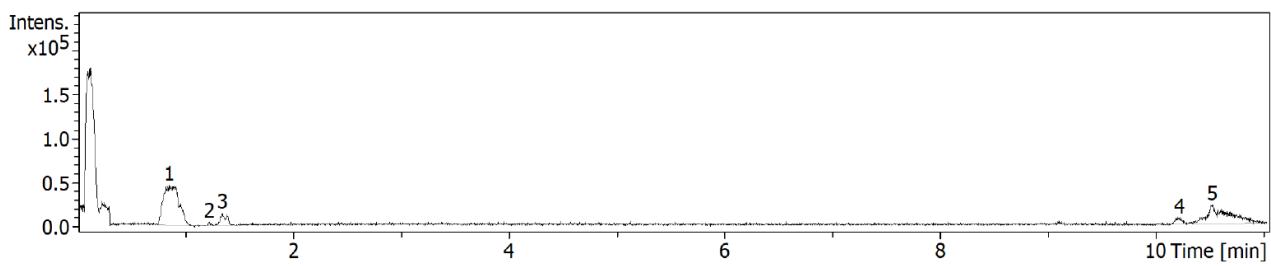
**Figure S3.** LC-MS chromatogram for the liquid sample of Urban-Fe catalyst.



**Figure S4.** LC-MS chromatogram for the liquid sample of Industrial-Fe catalyst.



**Figure S5.** LC-MS chromatogram for the liquid sample of Industrial-Ni catalyst.



**Figure S6.** LC-MS chromatogram for the liquid sample of Industrial-FeNi catalyst.

**References:**

- [1] Z.-j. Liu, J-q. Wan, Z-C. Yan, Y. Wang, Y.W. Ma, Efficient removal of ciprofloxacin by heterogeneous electro-Fenton using natural air–cathode, *Chem, Eng. J.* 433 (2022) 133767.
- [2] S. Li, T. Huang, P. Du, W. Liu, J. Hu, Photocatalytic transformation fate and toxicity of ciprofloxacin related to dissociation species: Experimental and theoretical evidences, *Water Res.* 185 (2020) 116286.