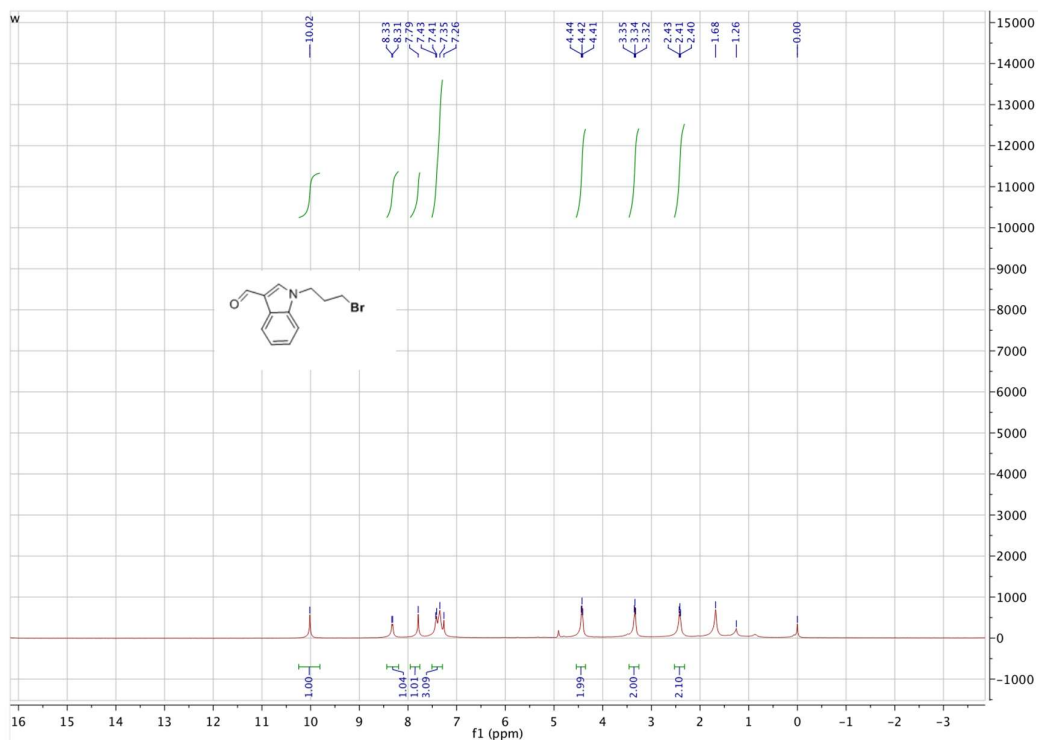
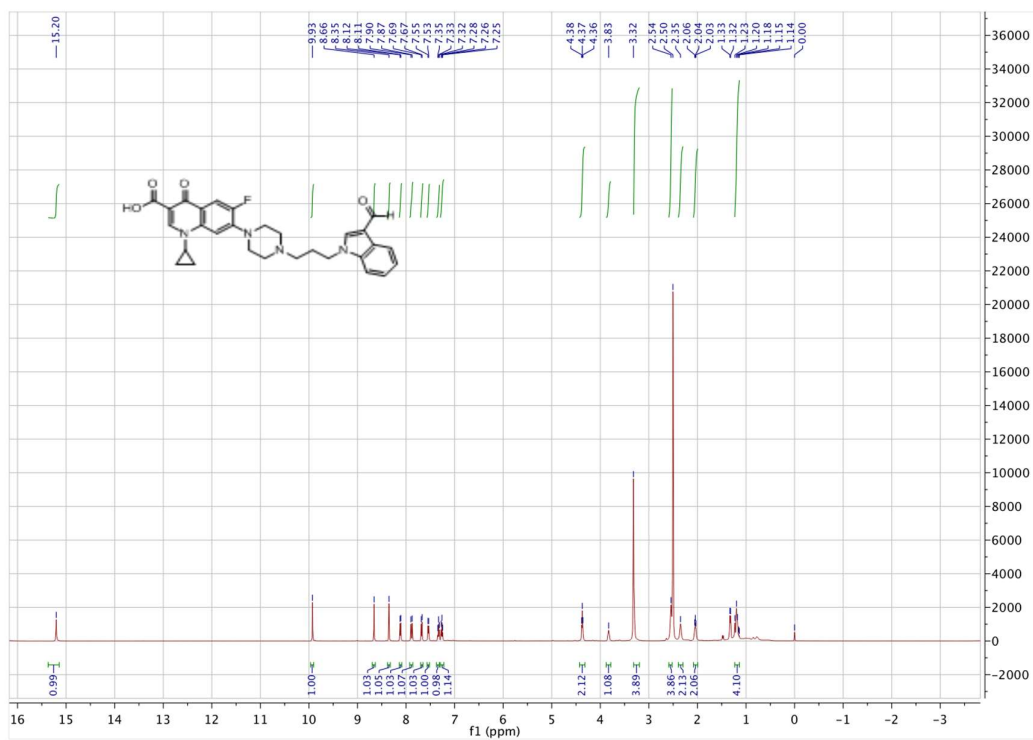


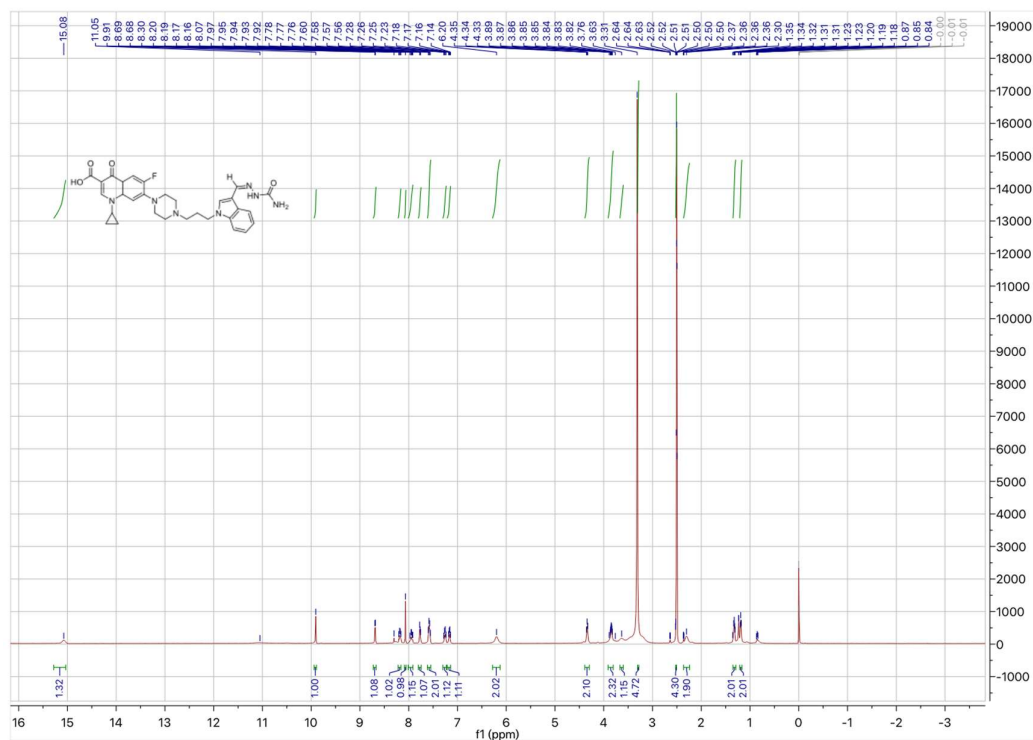
## Supporting Information

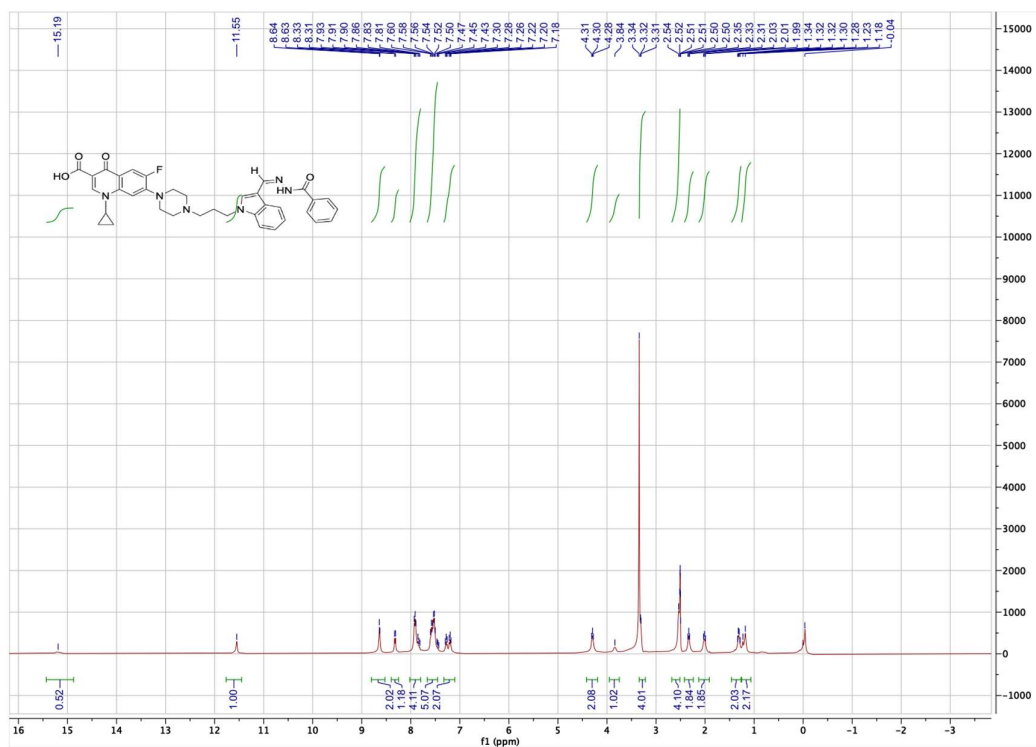


<sup>1</sup>H NMR of compound 1

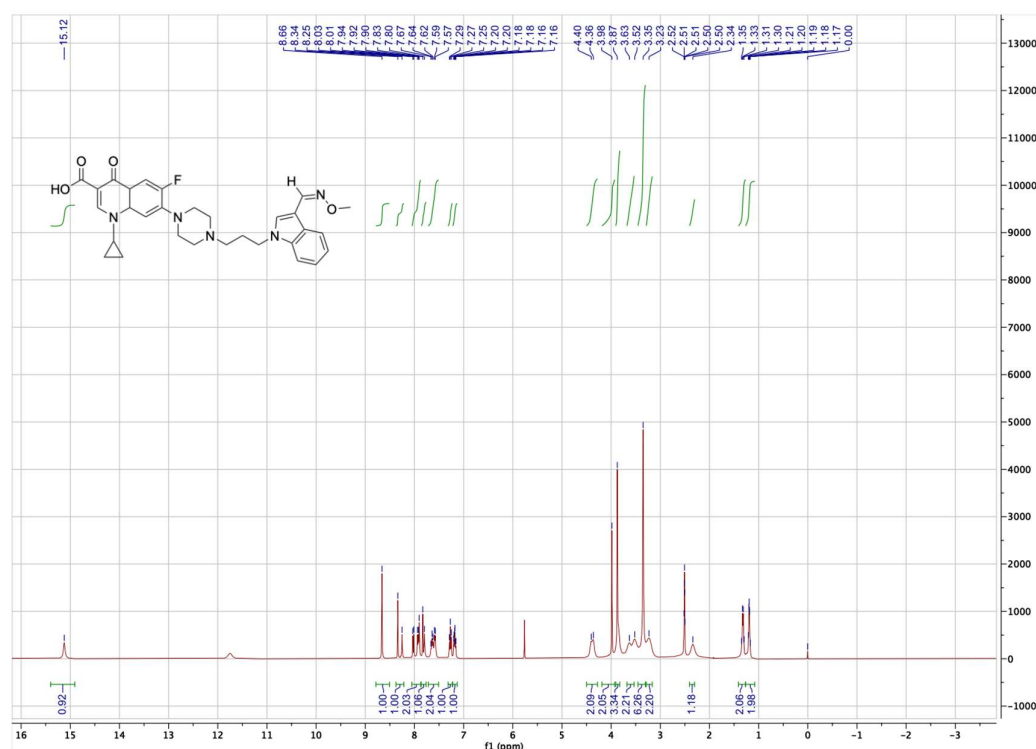


<sup>1</sup>H NMR of compound 2

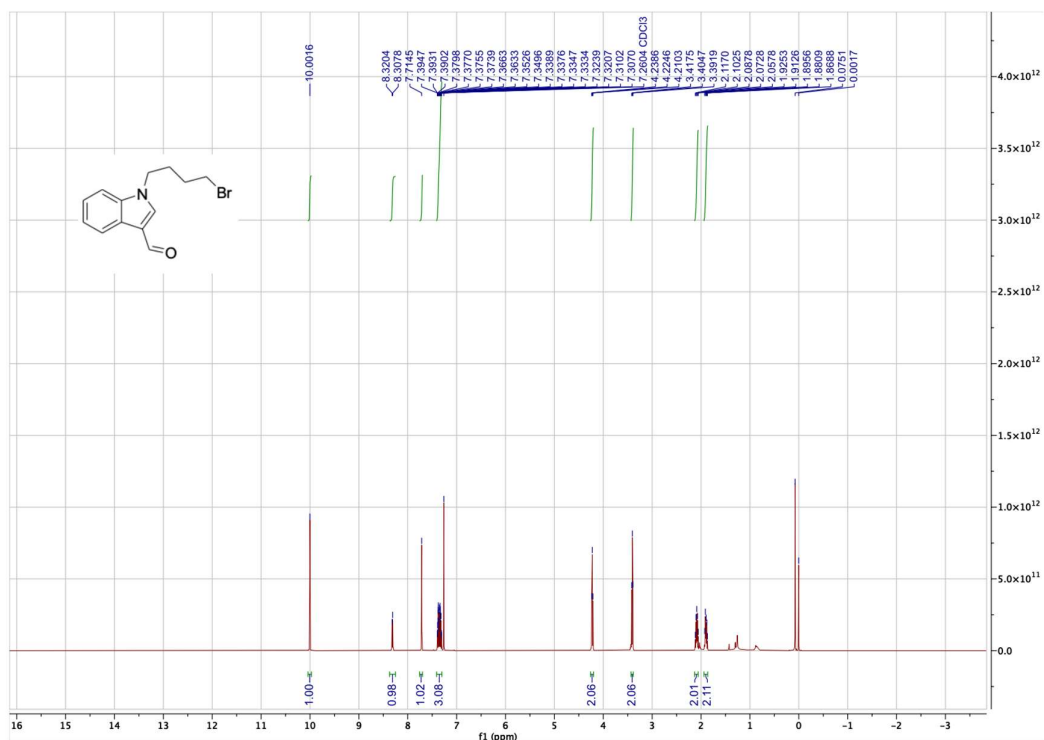




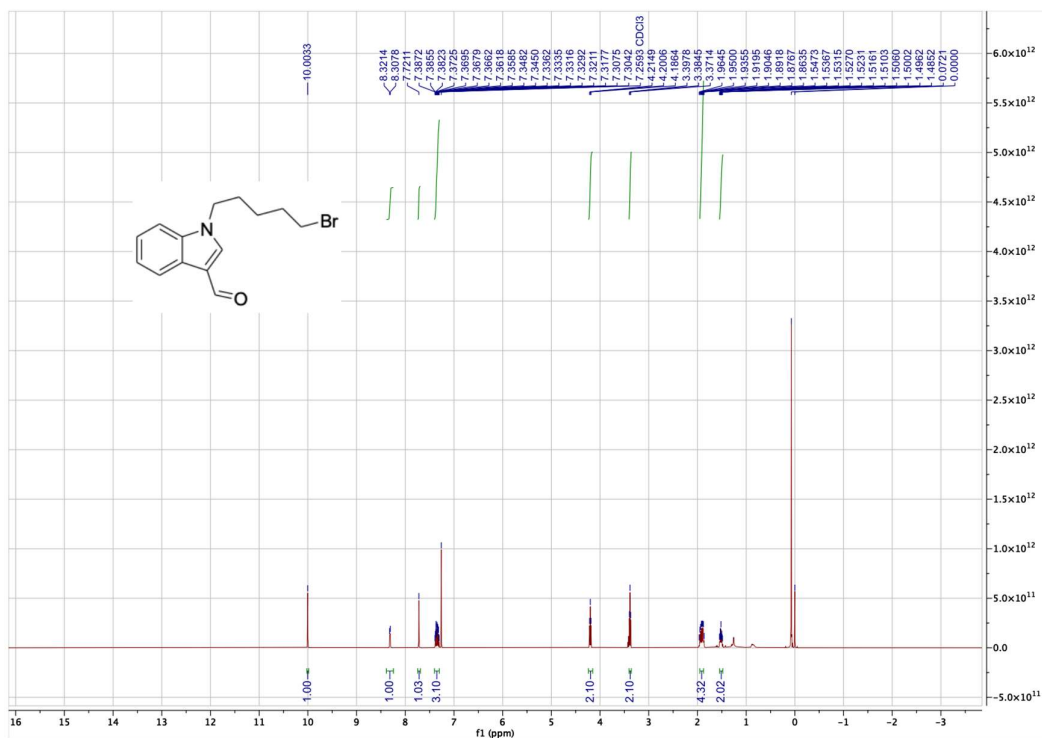
<sup>1</sup>H NMR of compound 3c



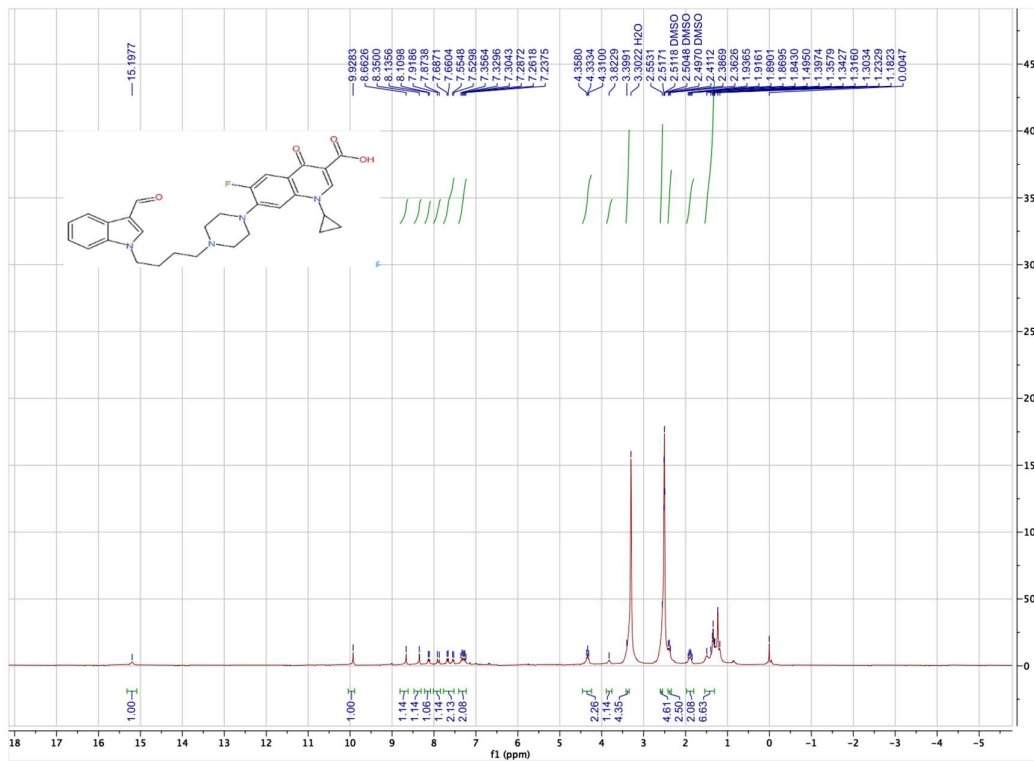
<sup>1</sup>H NMR of compound 3d



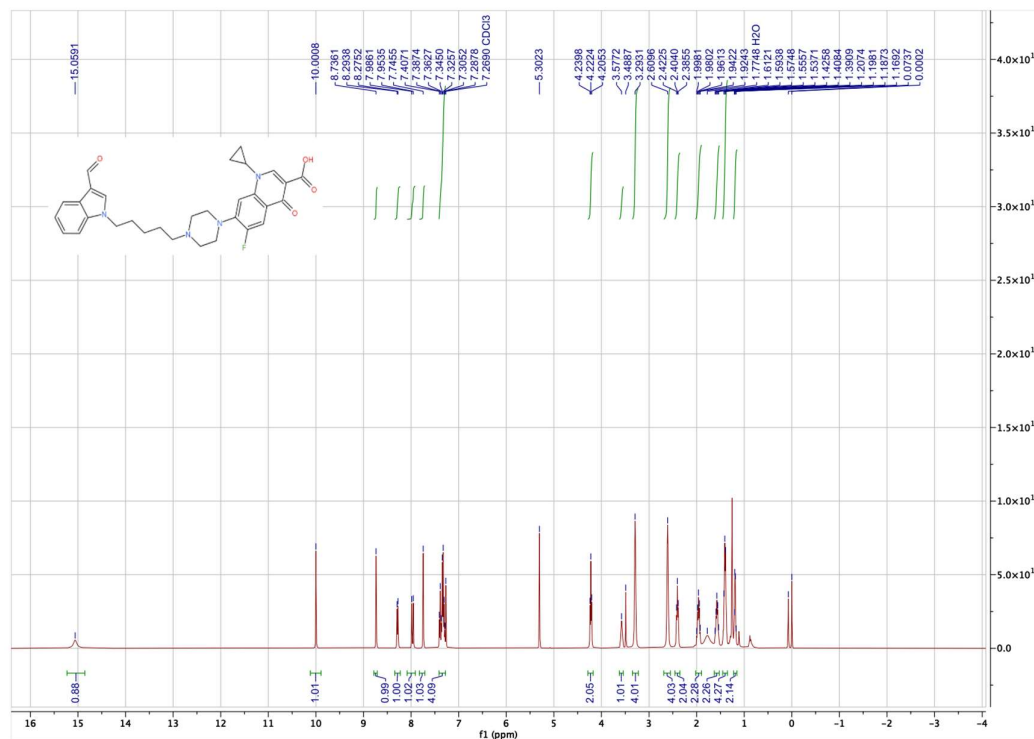
<sup>1</sup>H NMR of compound 4a



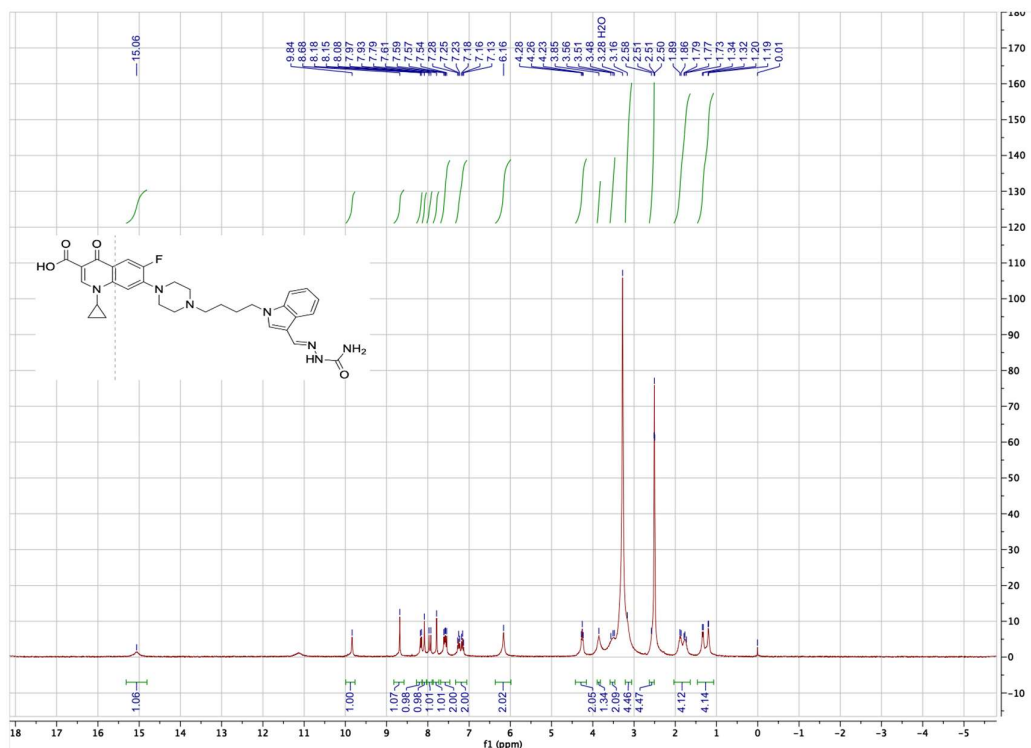
<sup>1</sup>H NMR of compound 4b



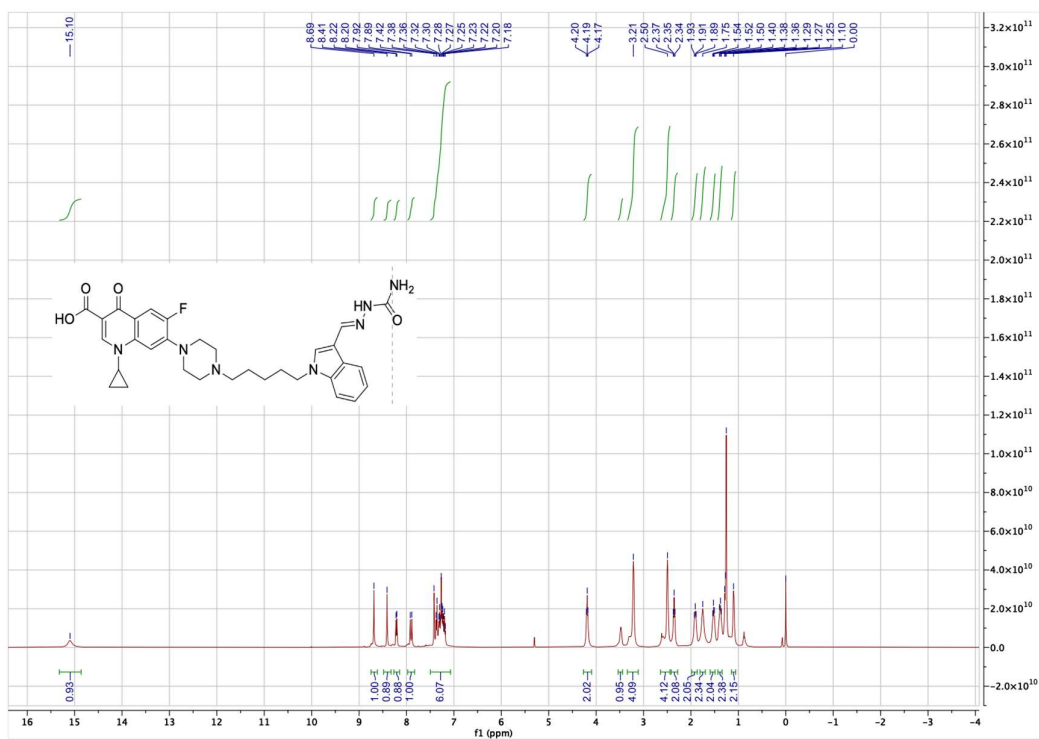
<sup>1</sup>H NMR of compound 5a



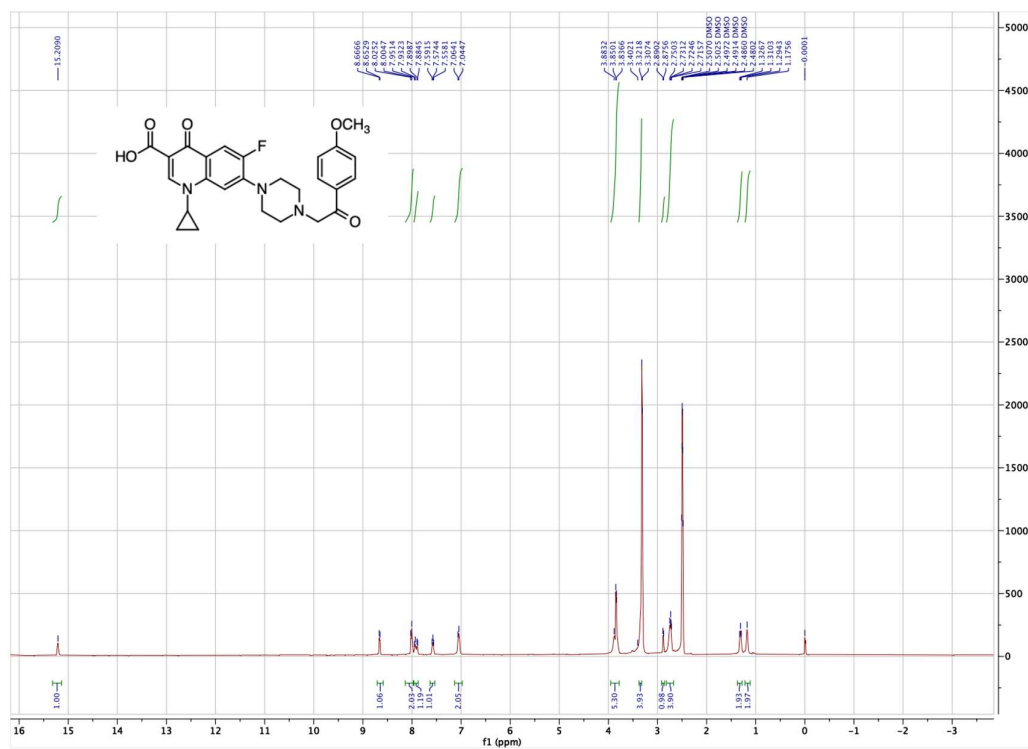
<sup>1</sup>H NMR of compound 5b



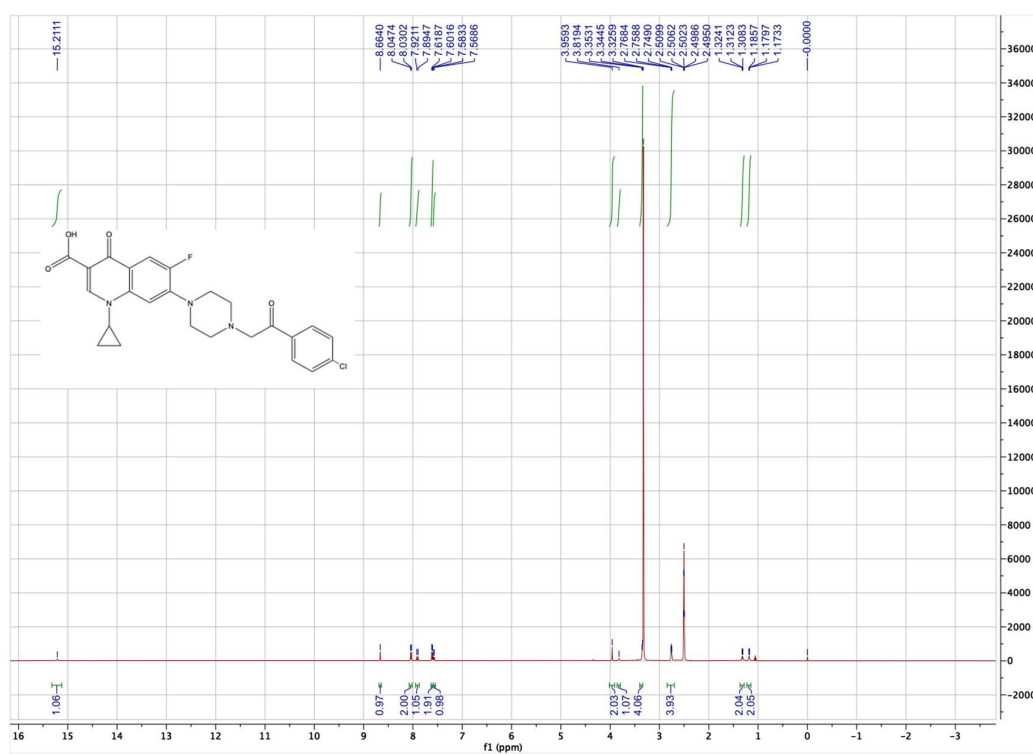
<sup>1</sup>H NMR of compound 6a



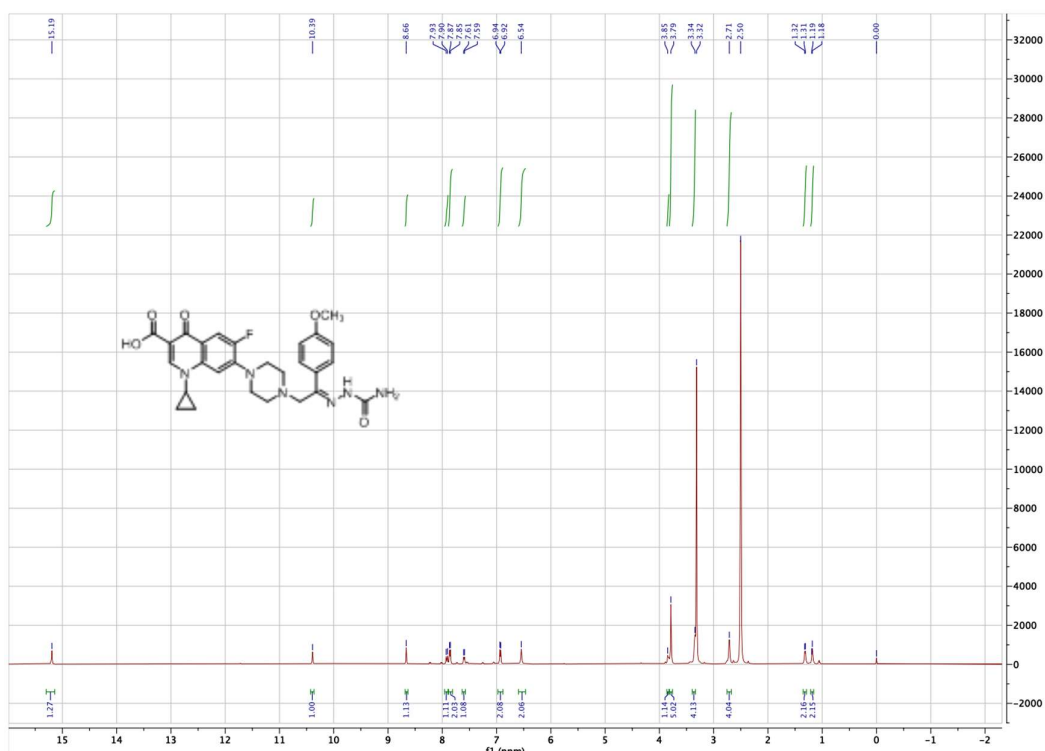
<sup>1</sup>H NMR of compound 6b



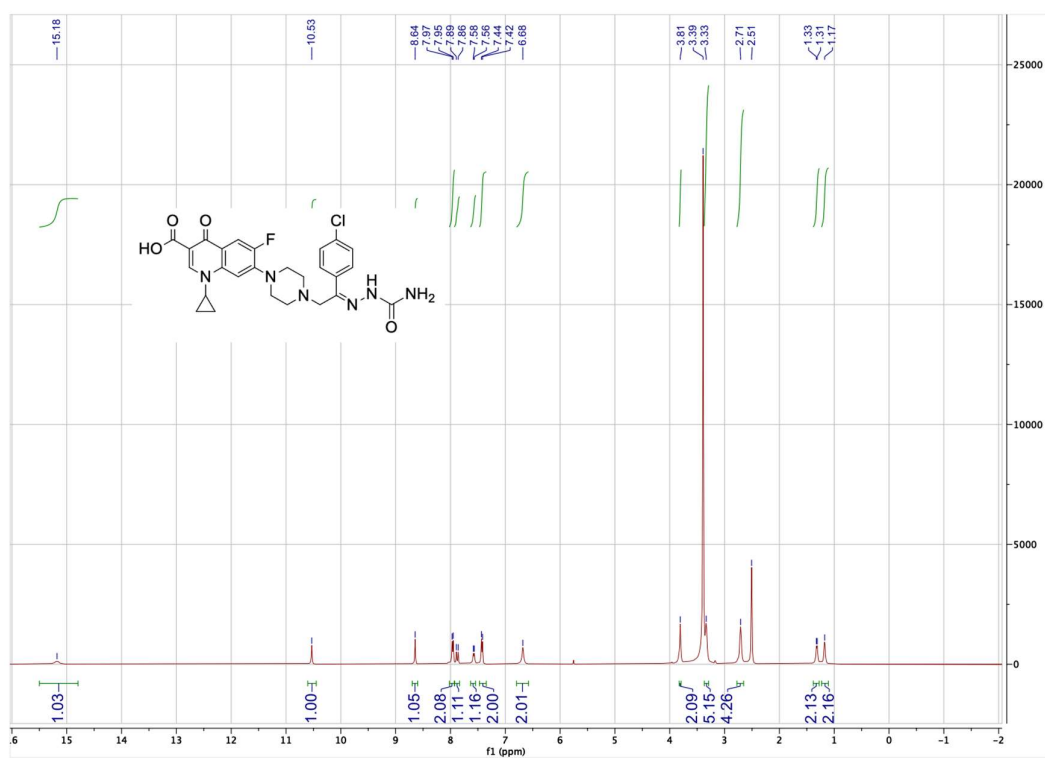
*<sup>1</sup>H NMR of compound 7a*



*<sup>1</sup>H NMR of compound 7b*

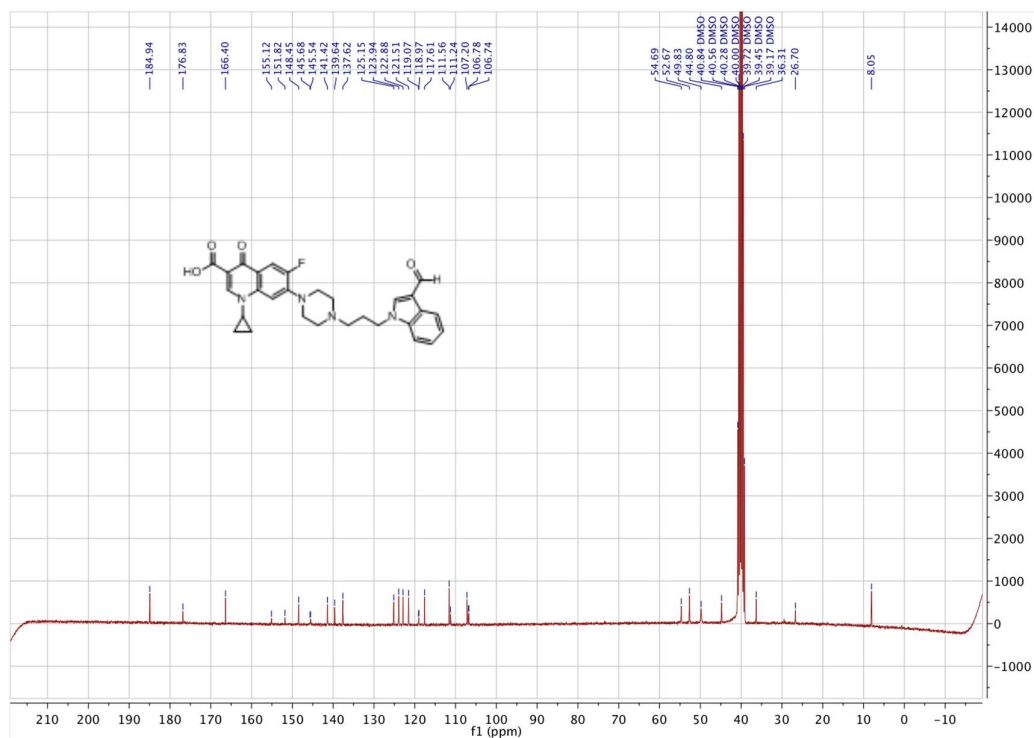


<sup>1</sup>H NMR of compound 8a

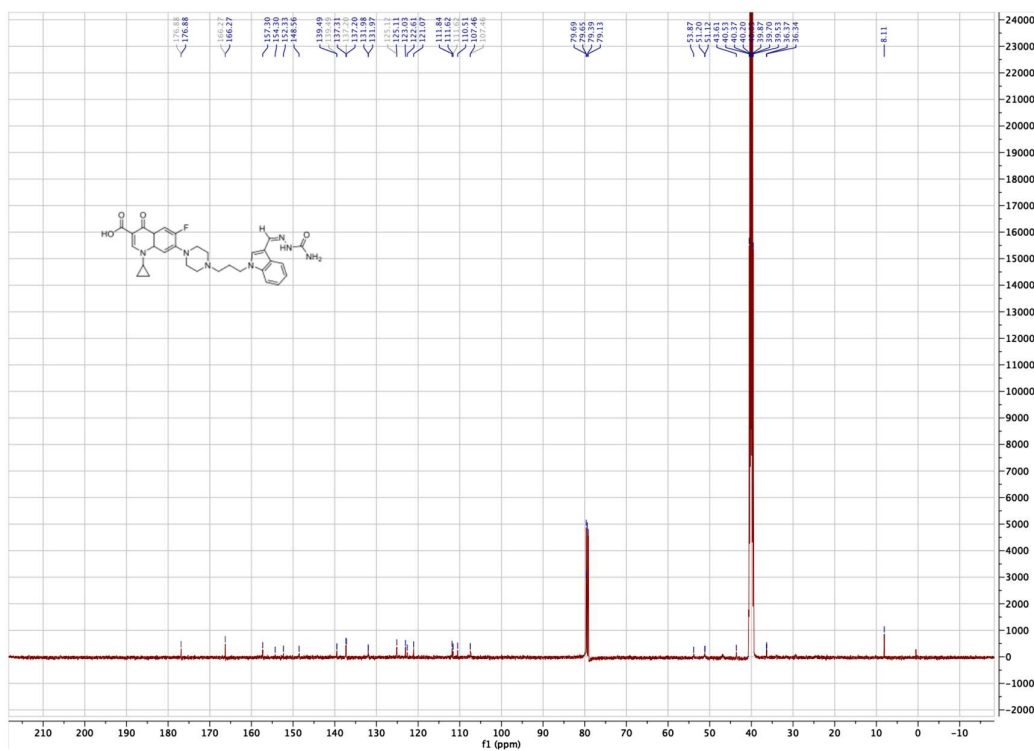


<sup>1</sup>H NMR of compound 8b

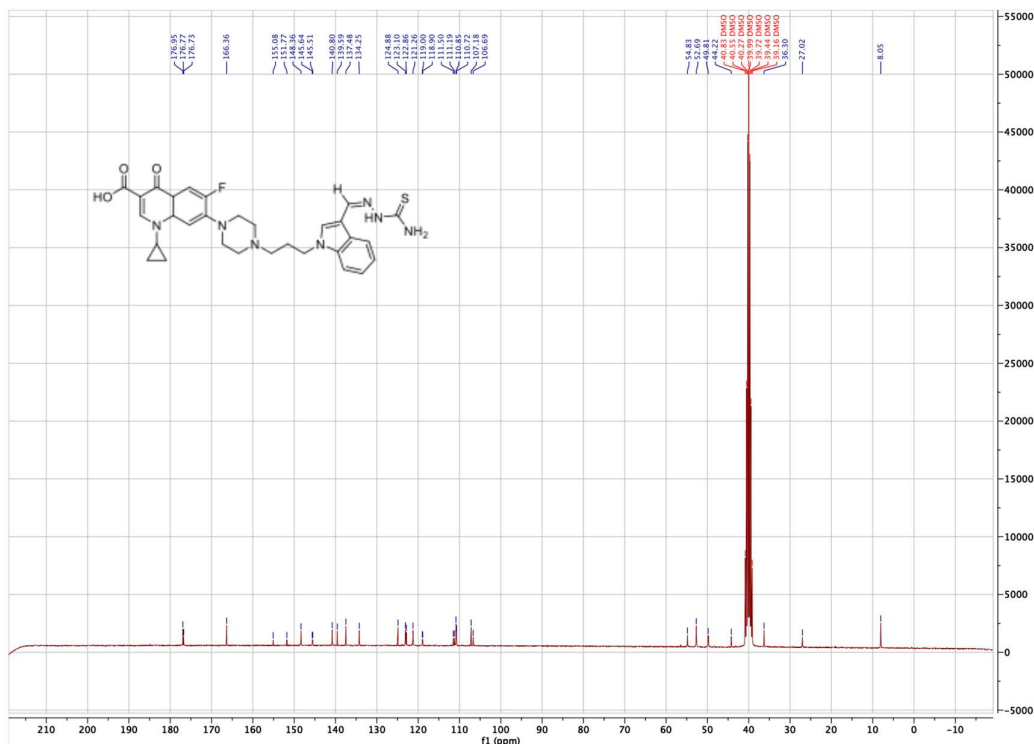




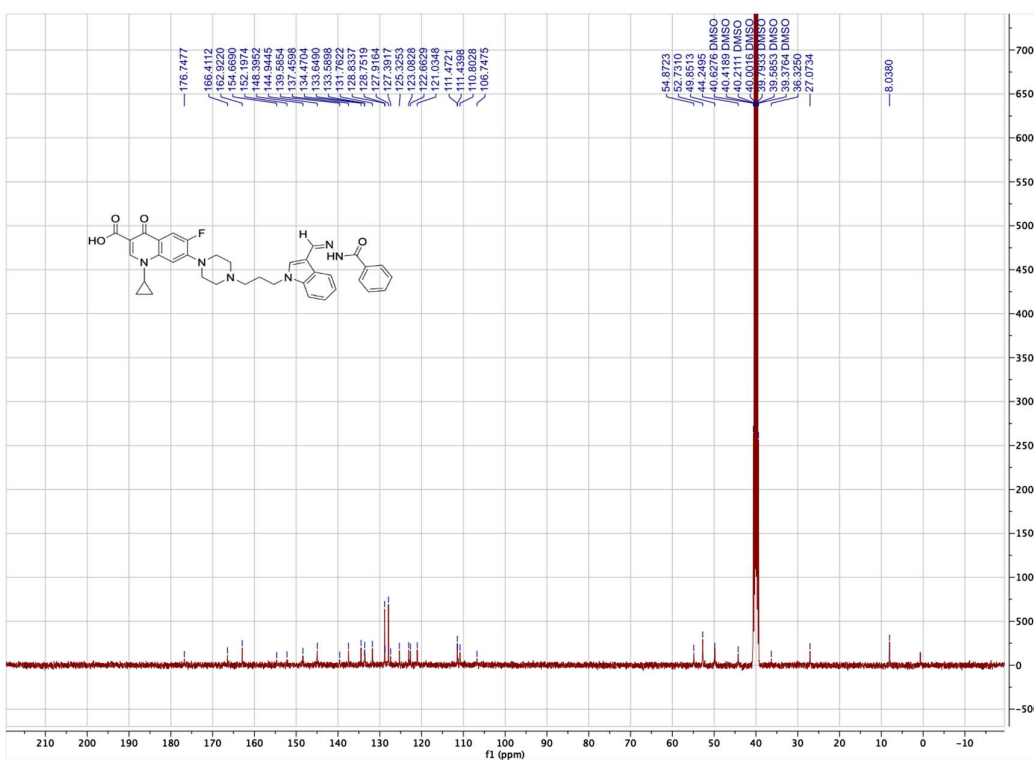
$^{13}\text{C}$  NMR of compound 2



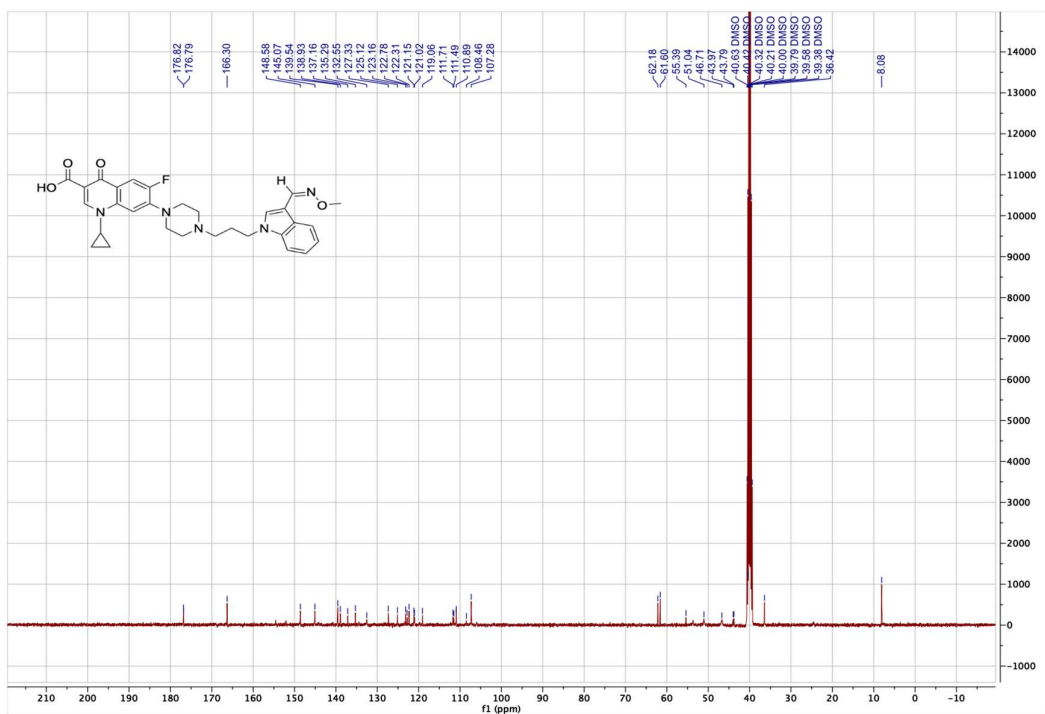
$^{13}\text{C}$  NMR of compound 3a



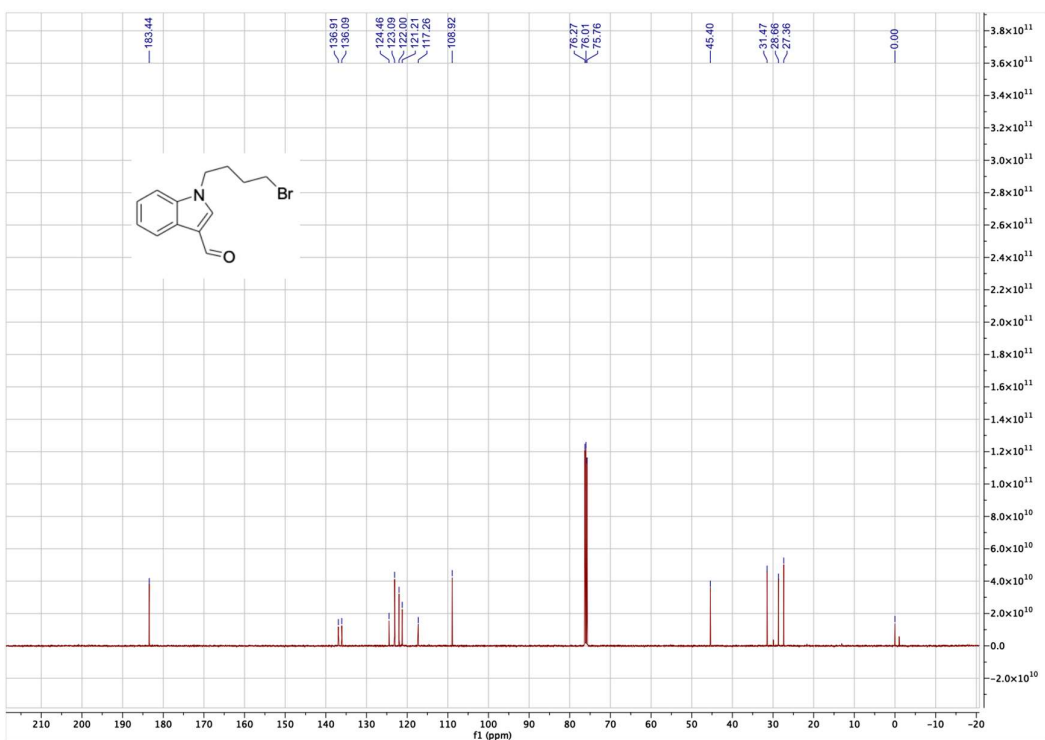
<sup>13</sup>C NMR of compound 3b



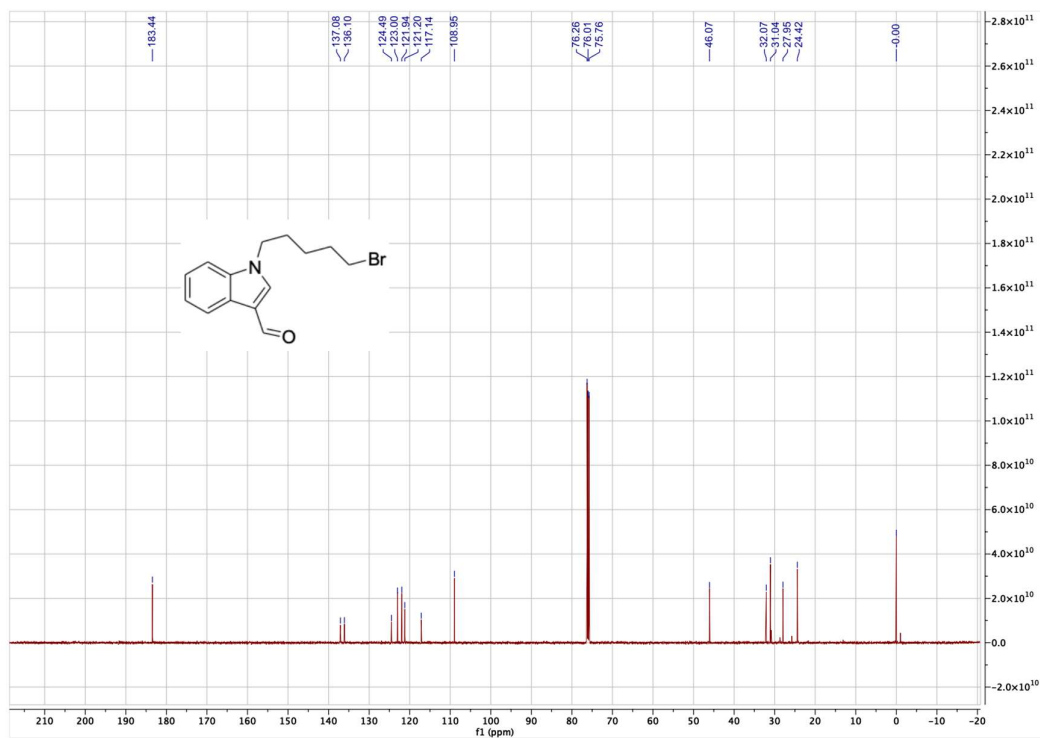
<sup>13</sup>C NMR of compound 3c



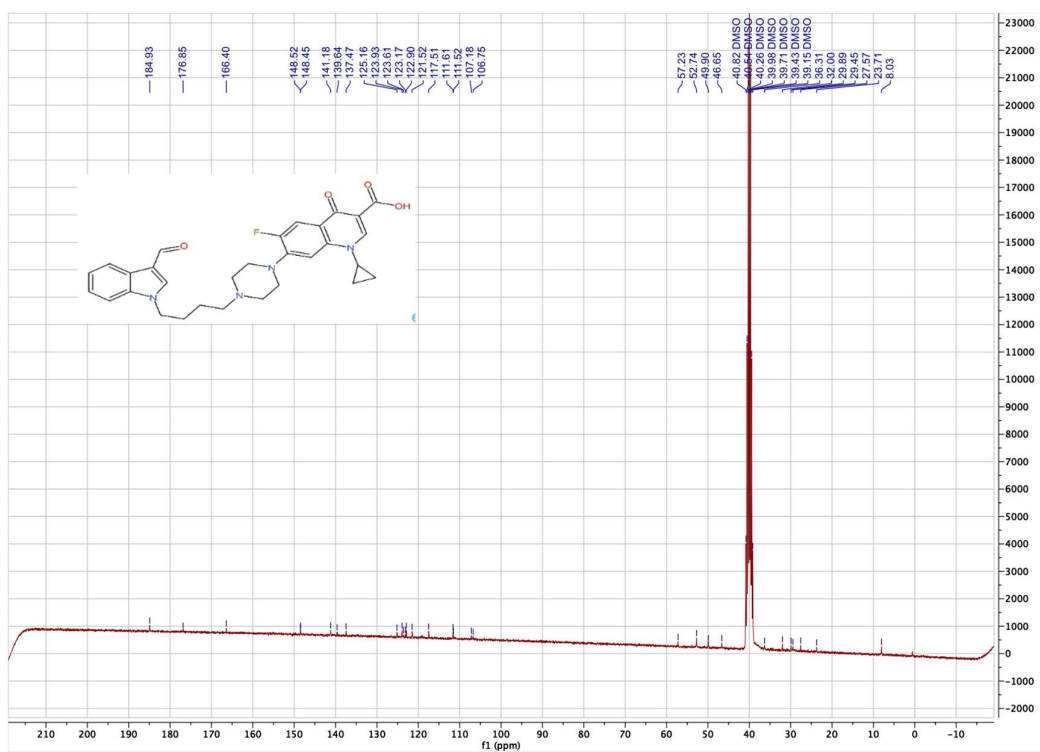
<sup>13</sup>C NMR of compound **3d**



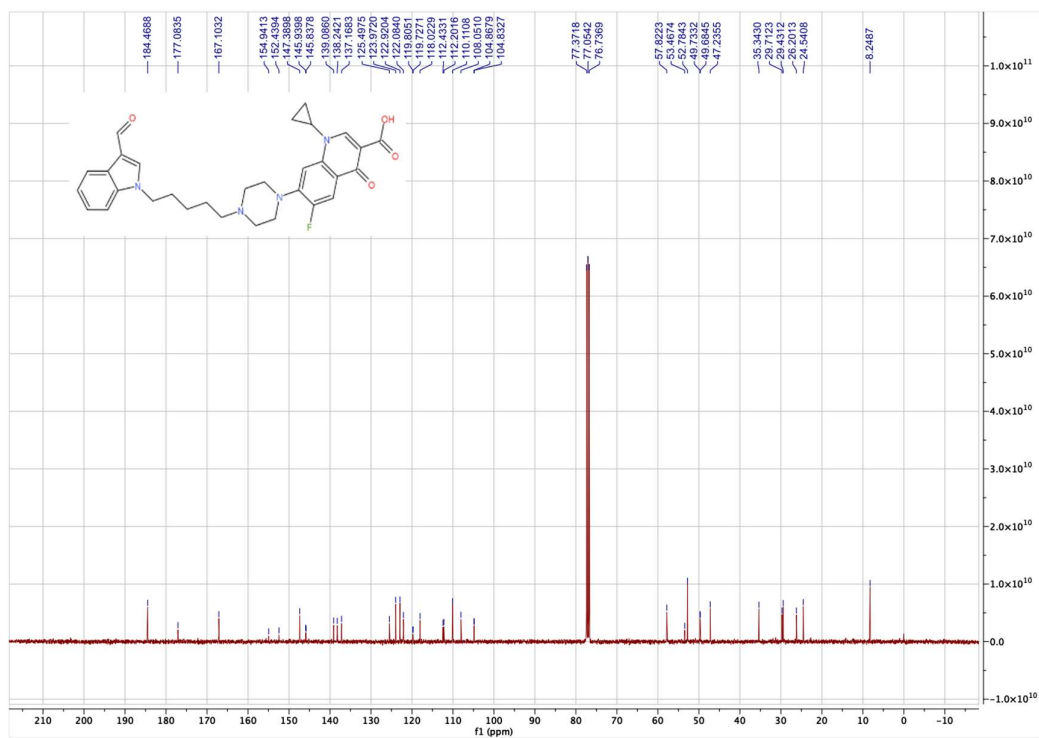
<sup>13</sup>C NMR of compound **4a**



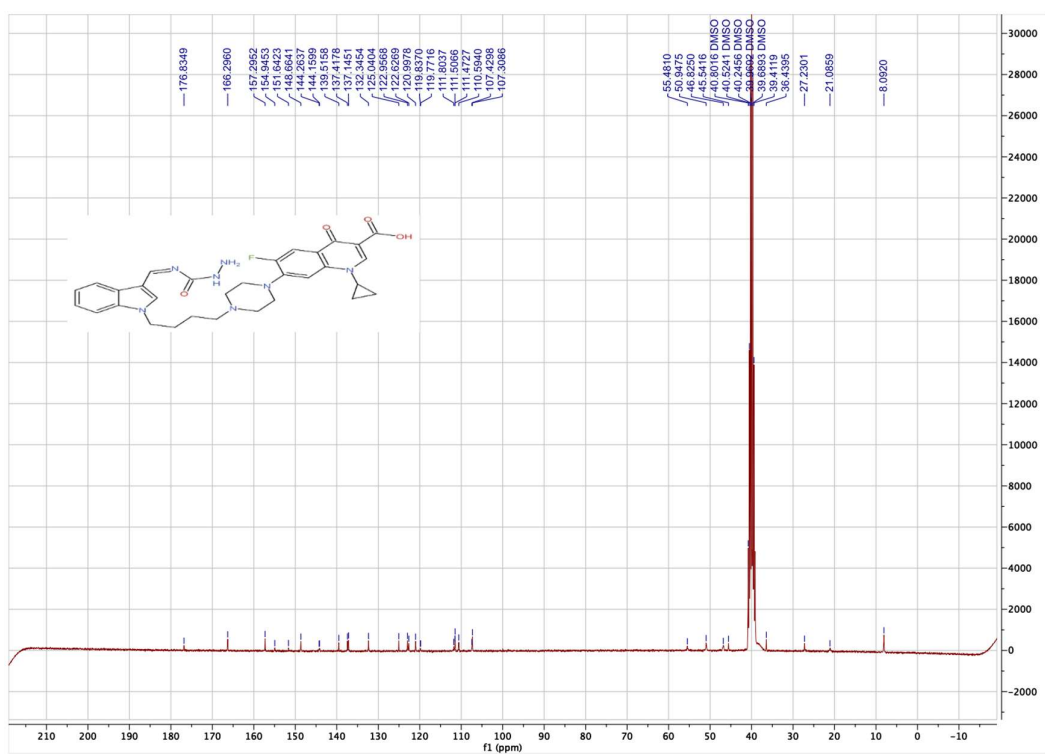
$^{13}\text{C}$  NMR of compound **4b**



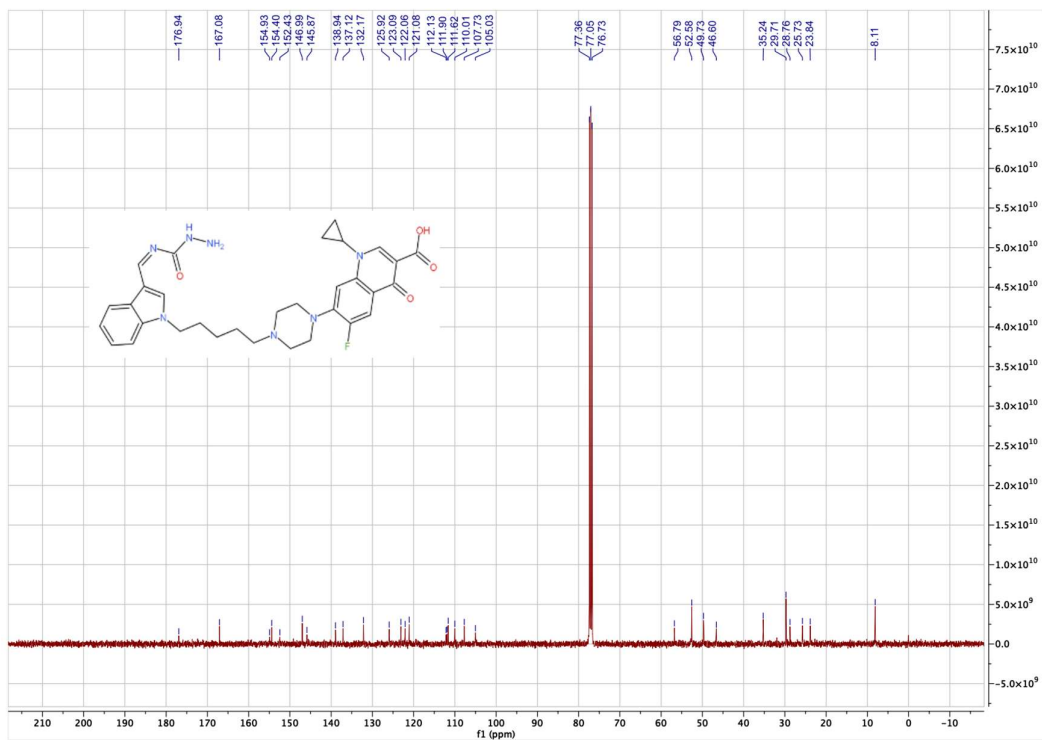
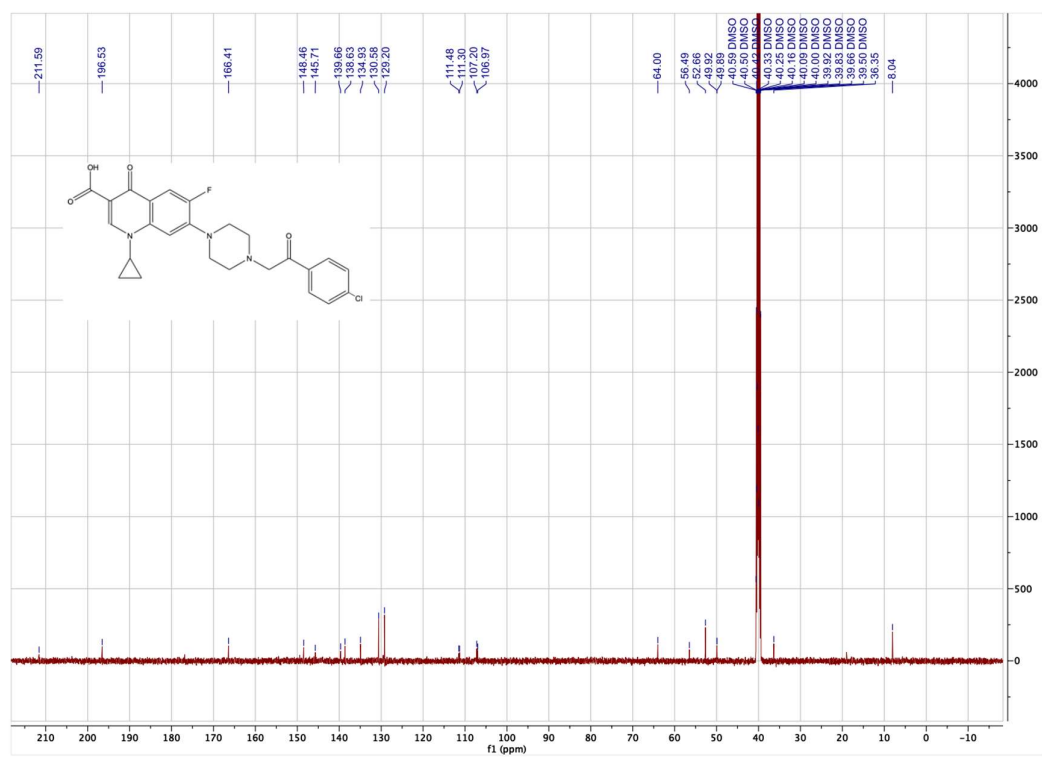
$^{13}\text{C}$  NMR of compound **5a**

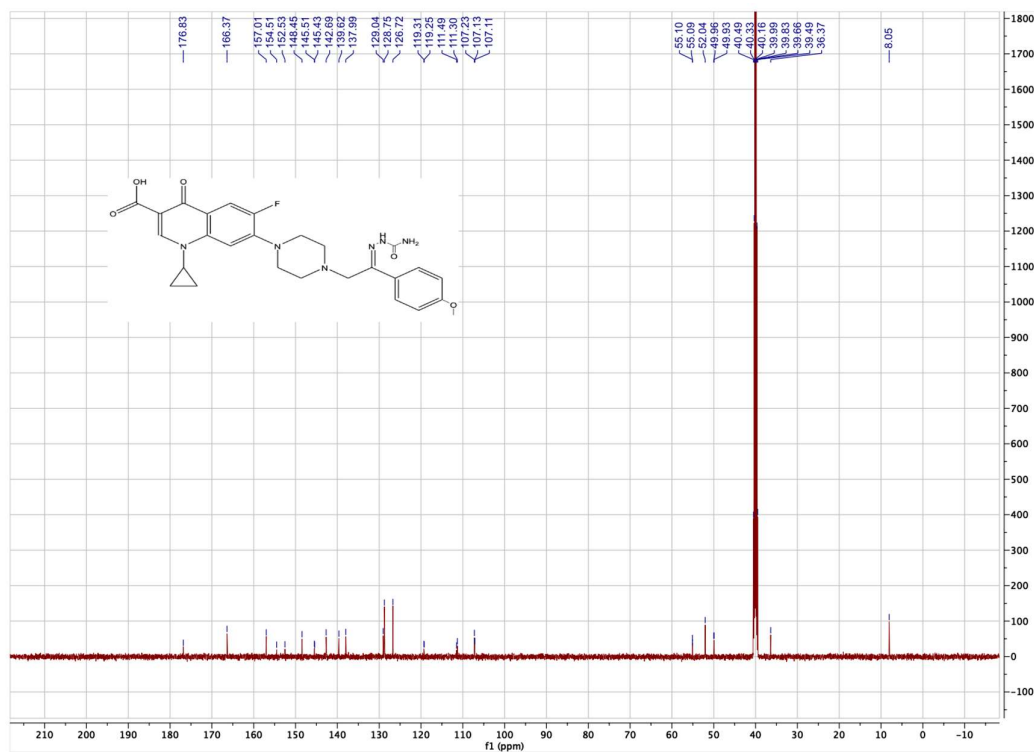


<sup>13</sup>C NMR of compound **5b**

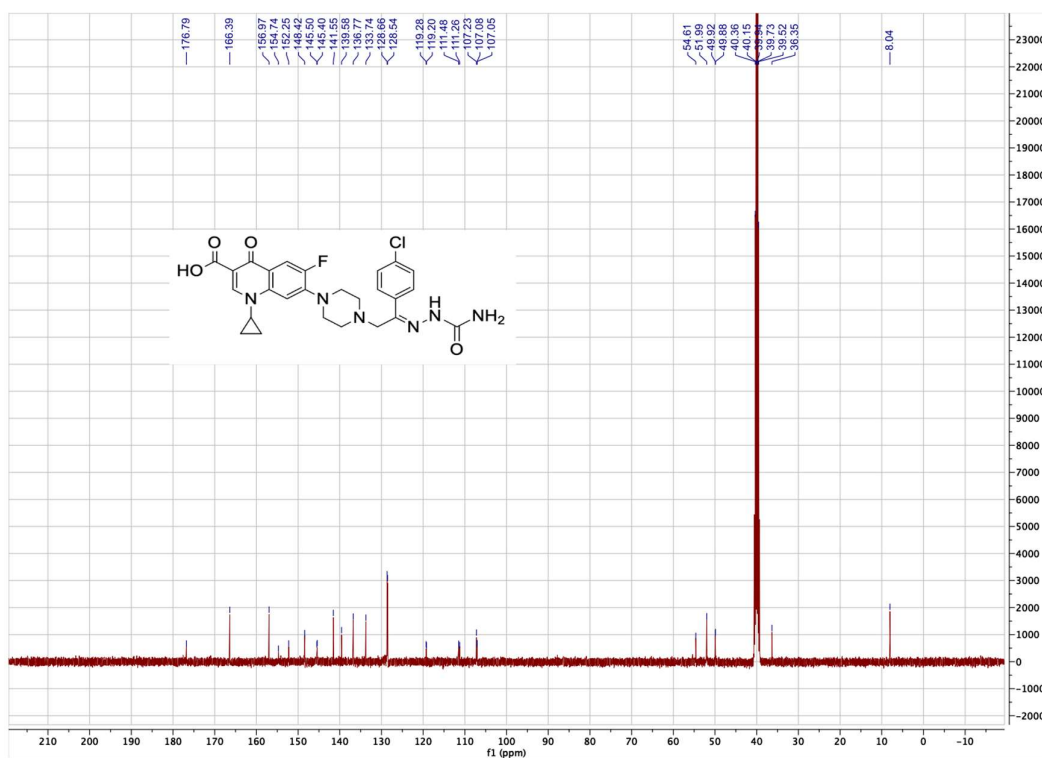


<sup>13</sup>C NMR of compound **6a**

 $^{13}\text{C}$  NMR of compound **6b** $^{13}\text{C}$  NMR of compound **7b**



$^{13}\text{C}$  NMR of compound **8a**



$^{13}\text{C}$  NMR of compound **8b**

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

30 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

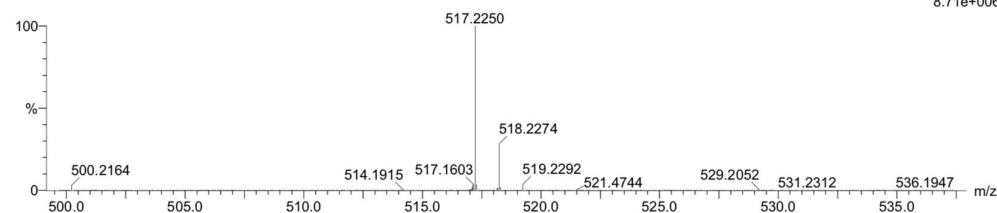
Elements Used:

C: 29-29 H: 10-35 N: 0-5 O: 0-7 F: 1-1

e

0502-4-M-2 24 (0.151)

1: TOF MS ES+  
8.71e+006



Minimum:  
Maximum:

5.0 20.0 -1.5  
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
517.2250	517.2251	-0.1	-0.2	16.5	1035.2	n/a	n/a	C <sub>29</sub> H <sub>30</sub> N <sub>4</sub> O <sub>4</sub> F

## HR-MS of compound 2

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

50 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

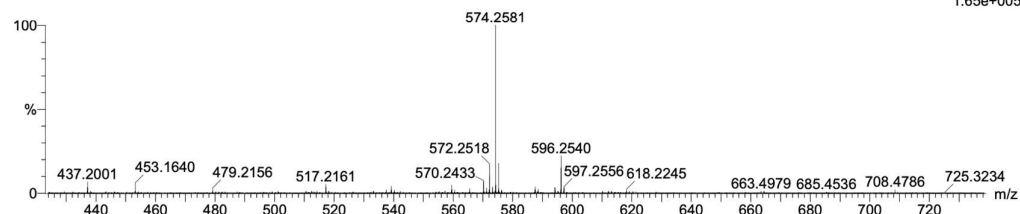
Elements Used:

C: 29-30 H: 10-35 N: 0-7 O: 0-7 F: 1-1

e

0502-4-M-3A 46 (0.274)

1: TOF MS ES+  
1.65e+005



Minimum:  
Maximum:

5.0 20.0 -1.5  
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
574.2581	574.2578	0.3	0.5	17.5	817.6	n/a	n/a	C <sub>30</sub> H <sub>33</sub> N <sub>7</sub> O <sub>4</sub> F

## HR-MS of compound 3a



## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

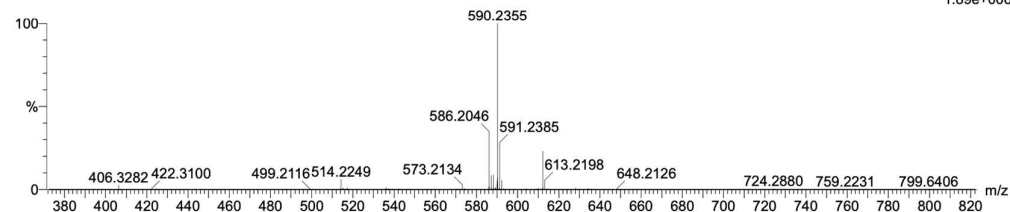
46 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 29-30 H: 10-35 N: 0-7 O: 0-7 F: 1-1 S: 1-1

e

0502-4-M-3B 24 (0.151)

1: TOF MS ES+  
1.89e+006Minimum:  
Maximum:5.0 20.0 -1.5  
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
590.2355	590.2350	0.5	0.8	17.5	822.5	n/a	n/a	C30 H33 N7 O3 F S

*HR-MS of compound 3b*

## Elemental Composition Report

Page 1

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

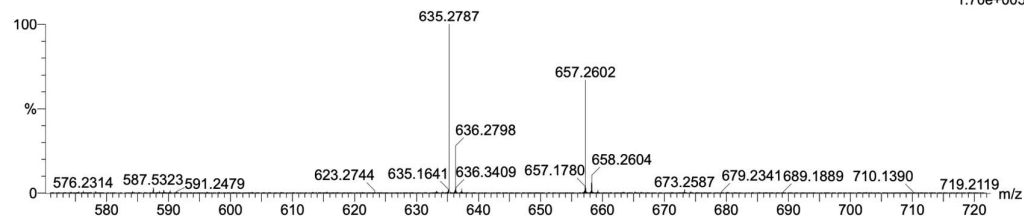
26 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 36-36 H: 30-40 N: 0-7 O: 0-7 F: 1-1

e

0502-4-M-3C 39 (0.238)

1: TOF MS ES+  
1.70e+005Minimum:  
Maximum:5.0 20.0 -1.5  
50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
635.2787	635.2782	0.5	0.8	21.5	703.7	n/a	n/a	C36 H36 N6 O4 F

*HR-MS of compound 3c*

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

25 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

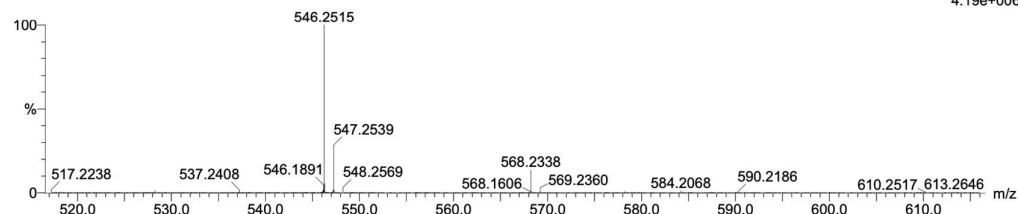
Elements Used:

C: 30-30 H: 30-40 N: 0-7 O: 0-7 F: 1-1

e

0502-4-M-3D 21 (0.135)

1: TOF MS ES+  
4.19e+006



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
546.2515	546.2517	-0.2	-0.4	16.5	958.2	n/a	n/a	C30 H33 N5 O4 F

*HR-MS of compound 3d*

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

26 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

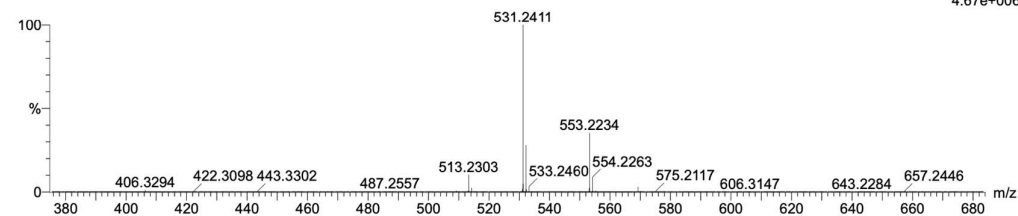
Elements Used:

C: 30-30 H: 30-40 N: 0-7 O: 0-7 F: 1-1

e

0502-4-M-5A 23 (0.146)

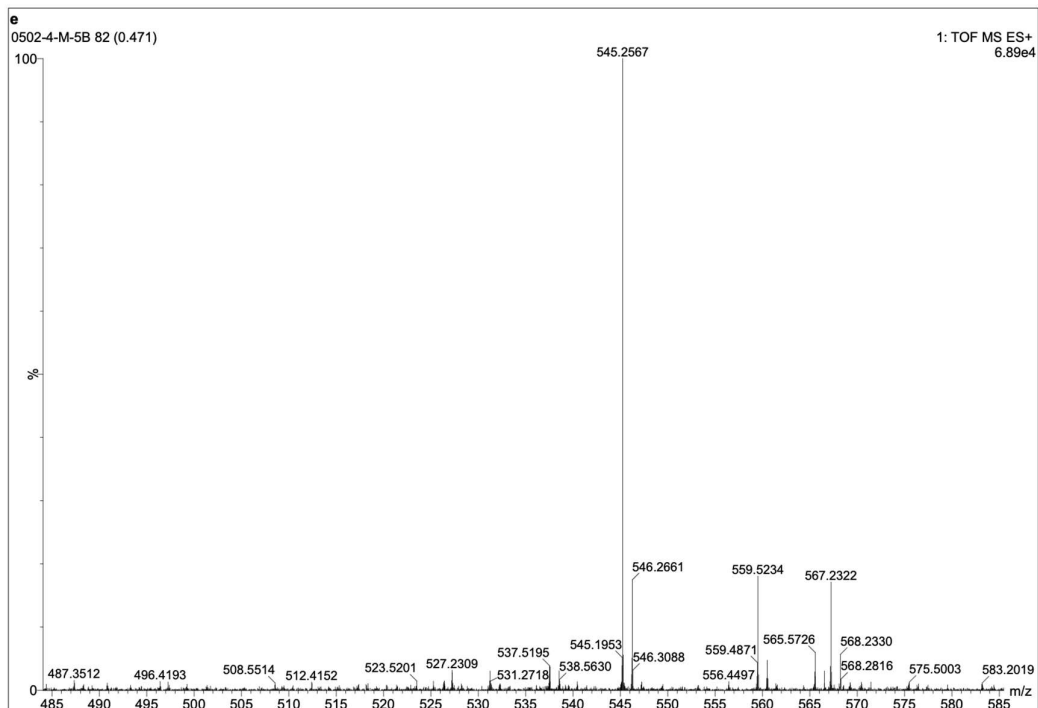
1: TOF MS ES+  
4.67e+006



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
531.2411	531.2408	0.3	0.6	16.5	941.8	n/a	n/a	C30 H32 N4 O4 F

*HR-MS of compound 5a*



*HR-MS of compound 5b*

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

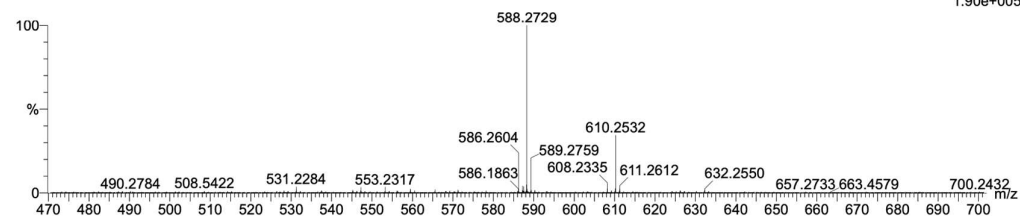
Elements Used:

C: 31-32 H: 30-40 N: 7-7 O: 0-7 F: 1-1

**e**

0502-4-M-6A 35 (0.217)

1: TOF MS ES+  
1.90e+005



Minimum: -1.5  
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
588.2729	588.2735	-0.6	-1.0	17.5	701.8	n/a	n/a	C31 H35 N7 O4 F

*HR-MS of compound 6a*

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

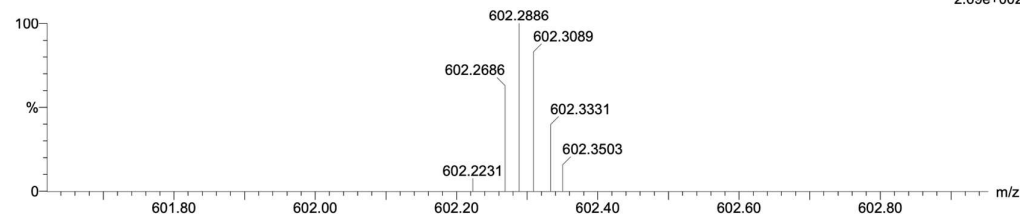
Elements Used:

C: 31-32 H: 30-40 N: 7-7 O: 0-7 F: 1-1

e

0502-4-M-6B 81 (0.466)

1: TOF MS ES+  
2.69e+002



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
602.2886	602.2891	-0.5	-0.8	17.5	49.0	n/a	n/a	C32 H37 N7 O4 F

*HR-MS of compound 6b*

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

43 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

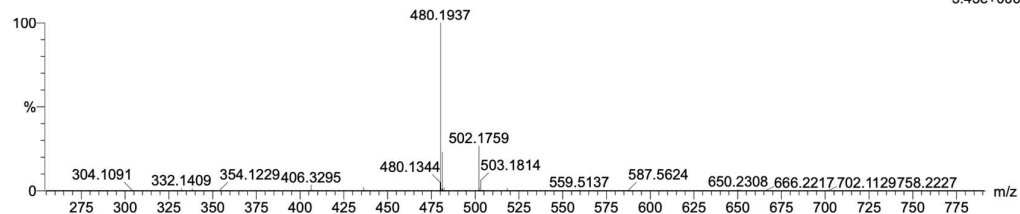
Elements Used:

C: 26-30 H: 27-40 N: 0-7 O: 0-7 F: 1-1

2

0502-4-M-10A 29 (0.177)

1: TOF MS ES+  
3.43e+006



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
480.1937	480.1935	0.2	0.4	14.5	1091.4	n/a	n/a	C26 H27 N3 O5 F

*HR-MS of compound 7a*

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

52 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

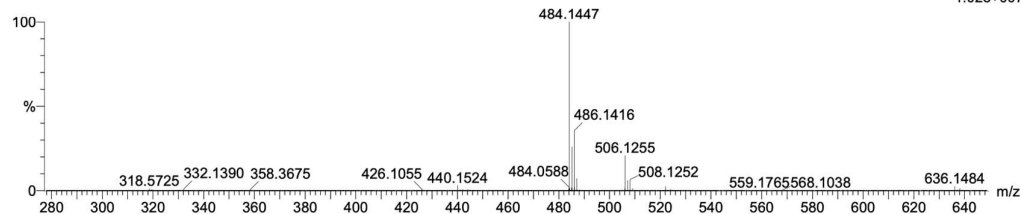
Elements Used:

C: 25-29 H: 24-40 N: 0-7 O: 0-7 F: 1-1 Cl: 1-1

2

0502-4-M-10B 25 (0.156)

1: TOF MS ES+  
1.02e+007



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
484.1447	484.1439	0.8	1.7	14.5	1214.7	n/a	n/a	C25 H24 N3 O4 F Cl

*HR-MS of compound 7b*

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

40 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

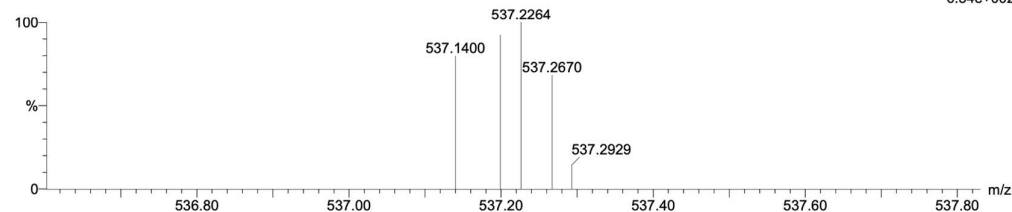
Elements Used:

C: 27-27 H: 24-40 N: 0-7 O: 0-7 F: 1-1

2

0502-4-M-11A 113 (0.641)

1: TOF MS ES+  
6.34e+002



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
537.2264	537.2262	0.2	0.4	15.5	44.4	n/a	n/a	C27 H30 N6 O5 F

*HR-MS of compound 8a*

## Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

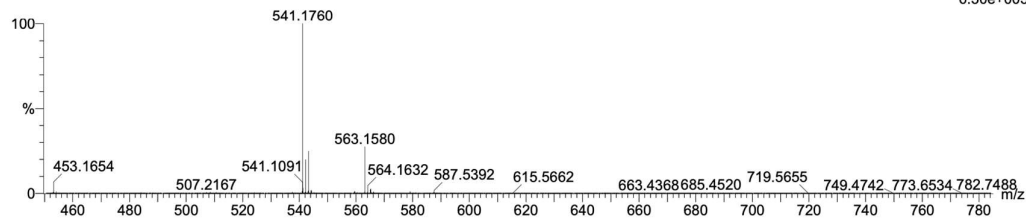
11 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 26-27 H: 24-40 N: 5-7 O: 0-7 F: 1-1 Cl: 1-1

2

0502-4-M-11B 40 (0.243)

1: TOF MS ES+  
6.30e+005

Minimum:

Maximum:

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
541.1760	541.1766	-0.6	-1.1	15.5	853.2	n/a	n/a	C <sub>26</sub> H <sub>27</sub> N <sub>6</sub> O <sub>4</sub> FCl

*HR-MS of compound 8b*