

## Supporting Information

### Synthesis of Hydantoin androgen Receptor Antagonists and Study on Their Antagonistic Activity

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<sup>b</sup> Shanghai Engineering Research Center of Molecular Therapeutics and New Drug Development, School of Chemistry and Molecular Engineering, East China Normal University, 3663 North Zhongshan Road, Shanghai 200062, China

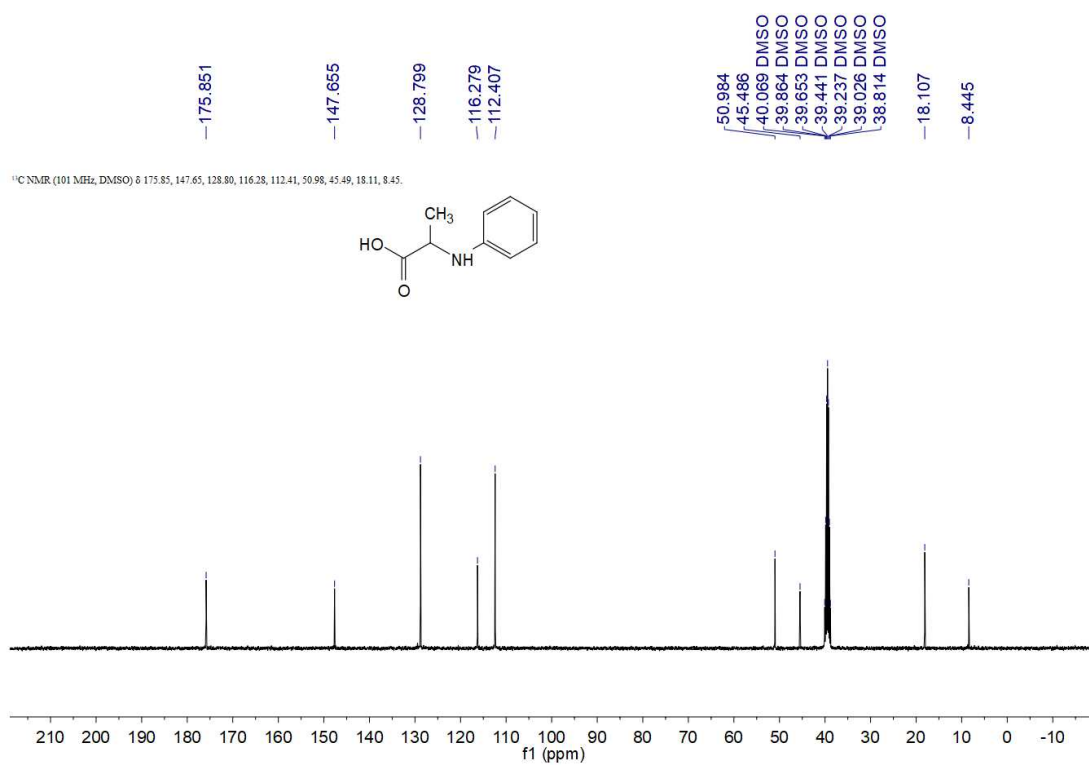
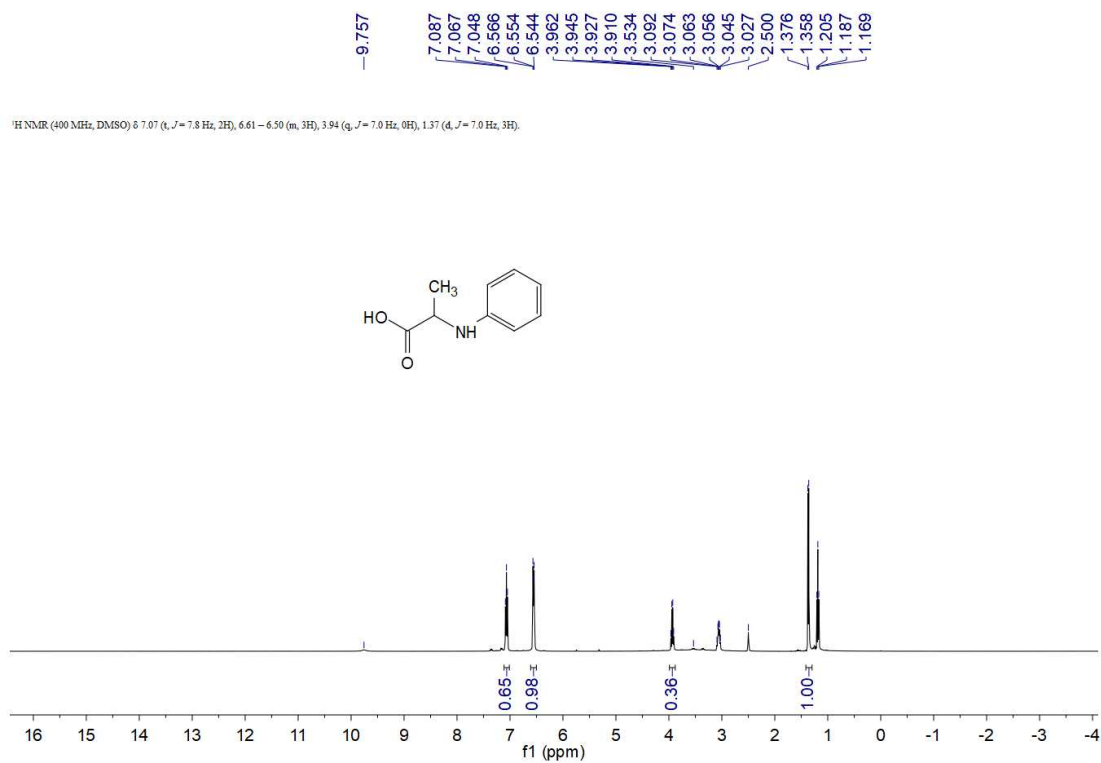
<sup>c</sup> The National Center for Drug Screening and the CAS Key Laboratory of Receptor Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences (CAS), 189 Guo Shou Jing Road, Shanghai 200031, China

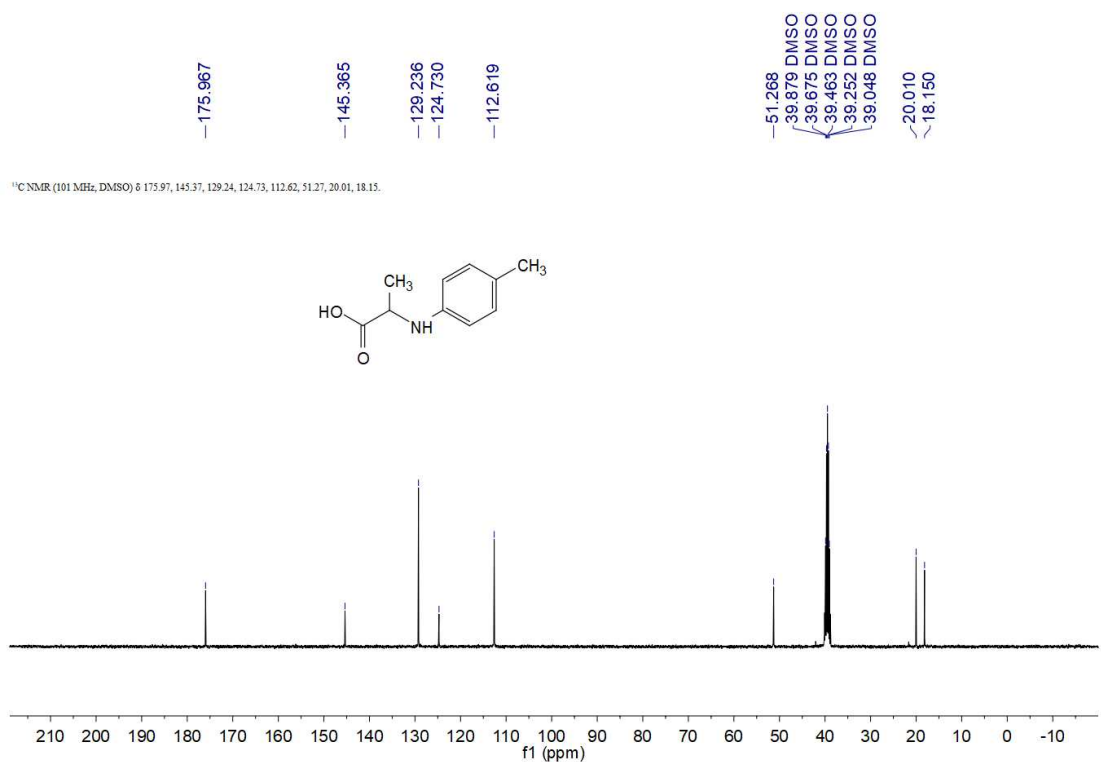
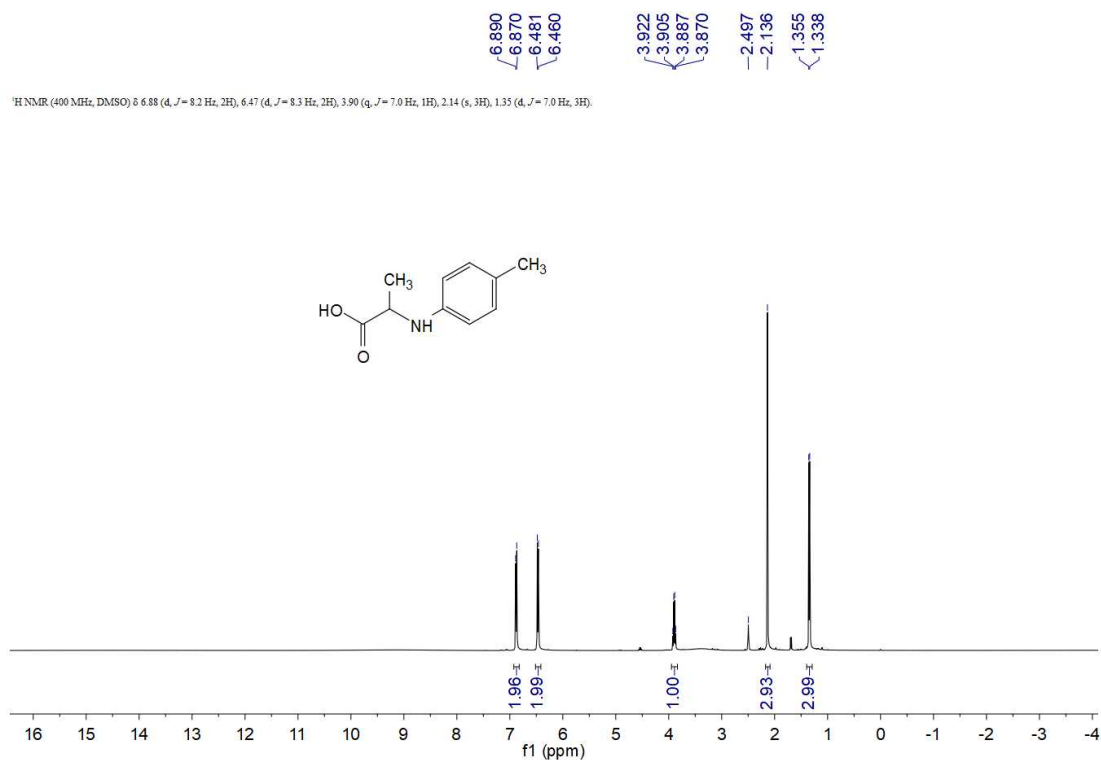
\*Corresponding authors:

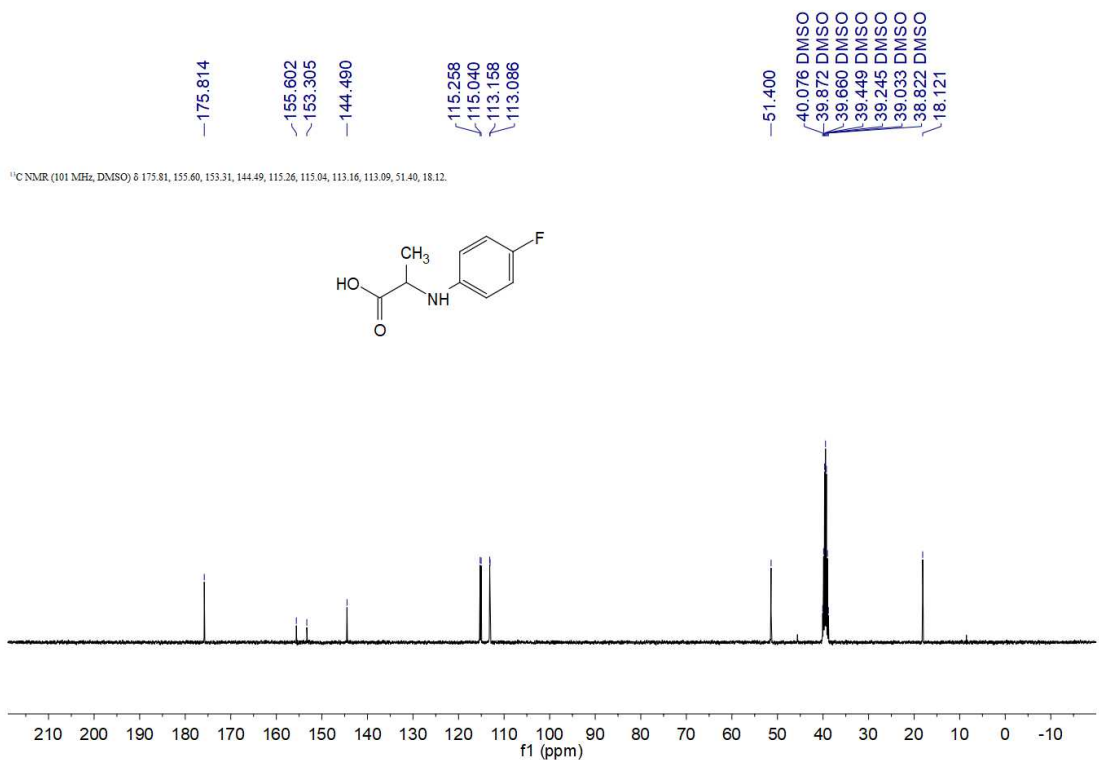
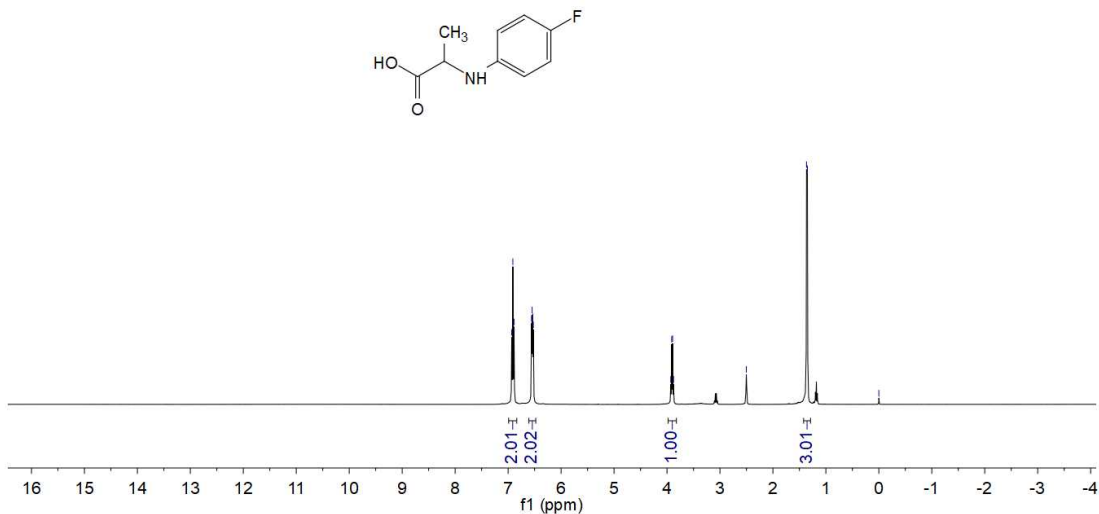
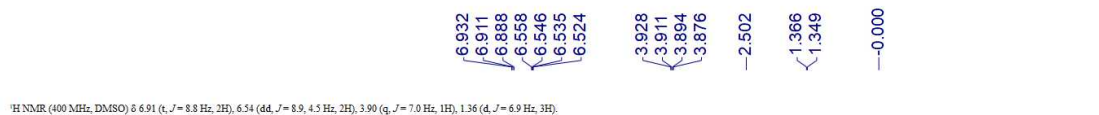
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jyjin@chem.ecnu.edu.cn (J.J.)

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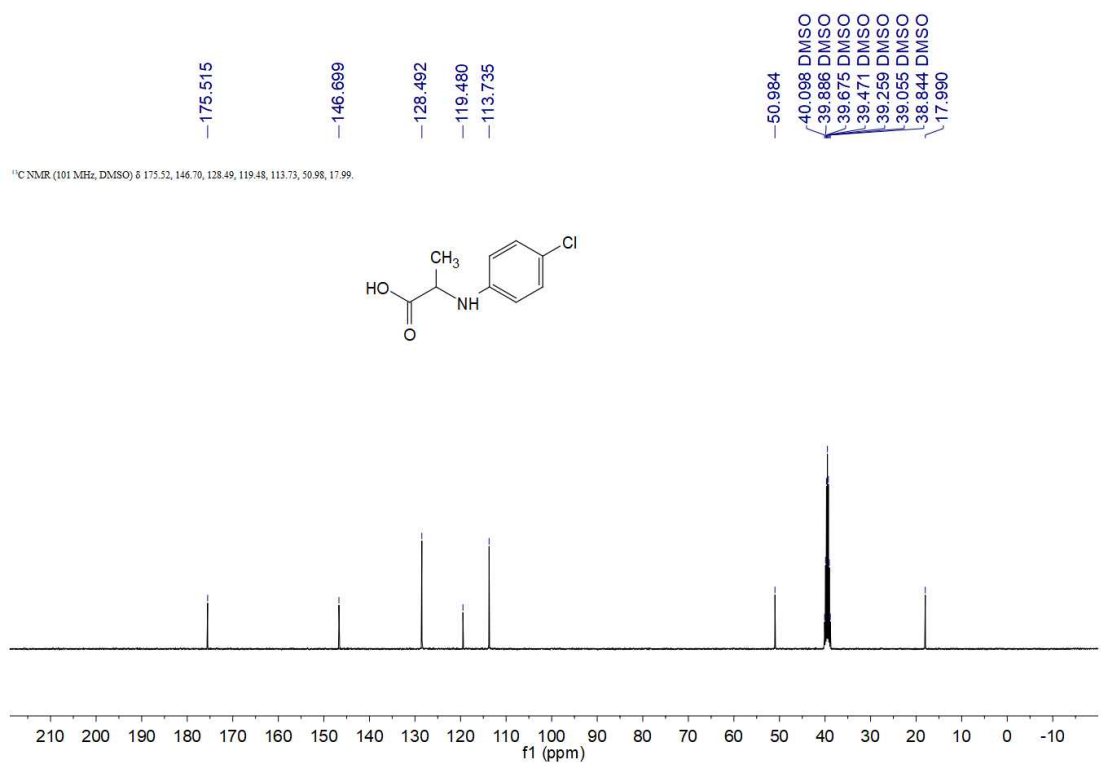
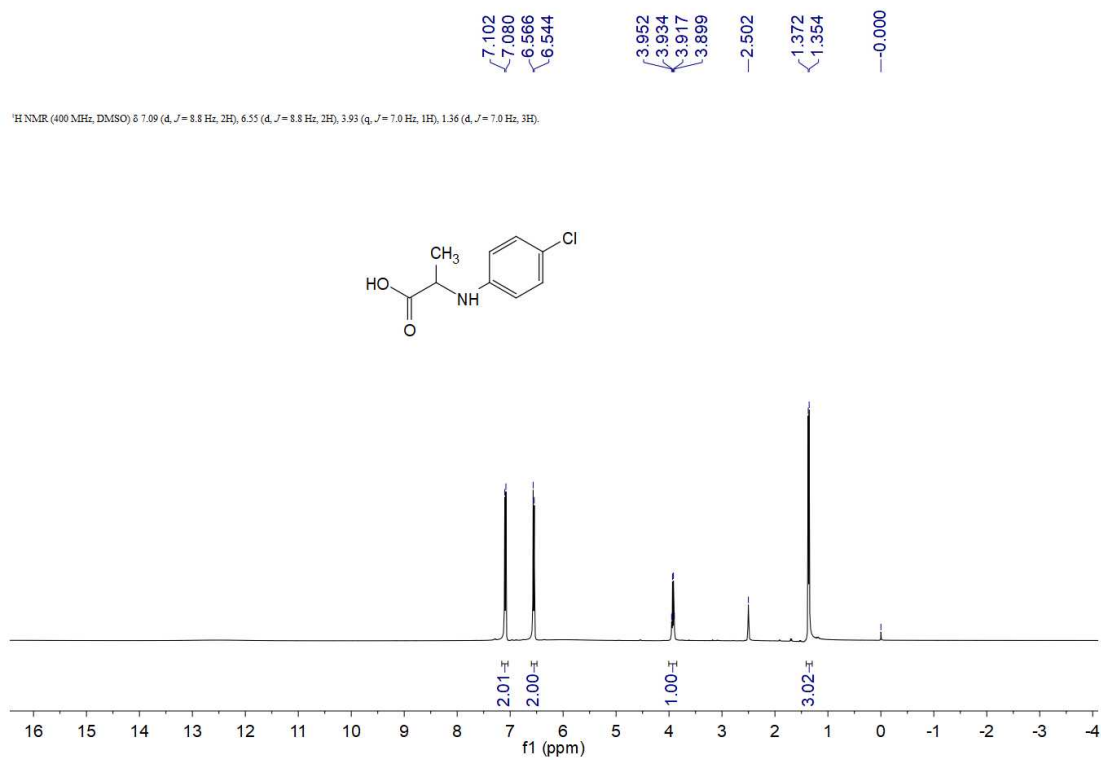
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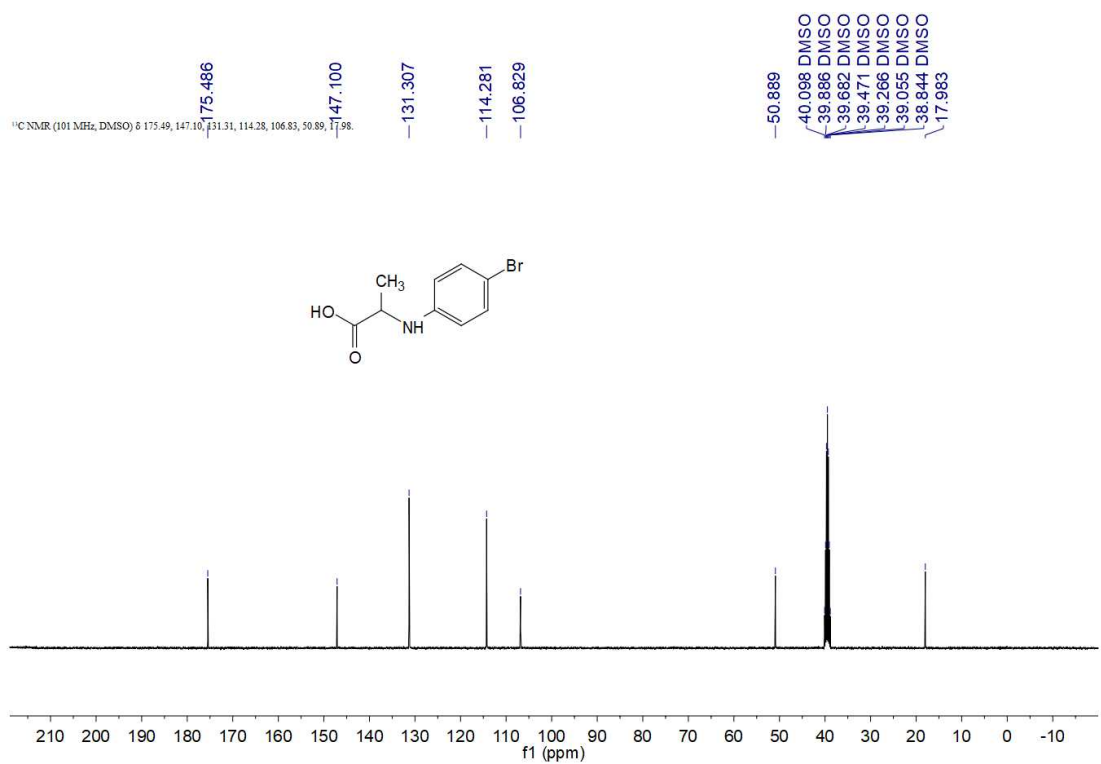
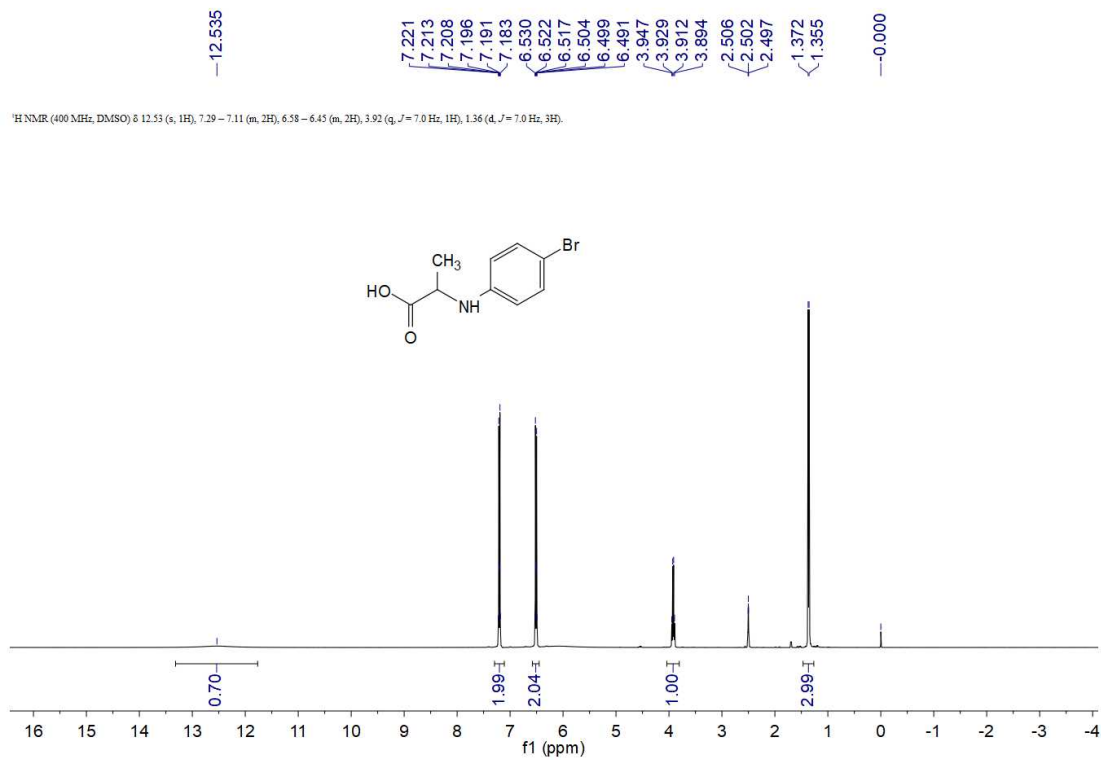


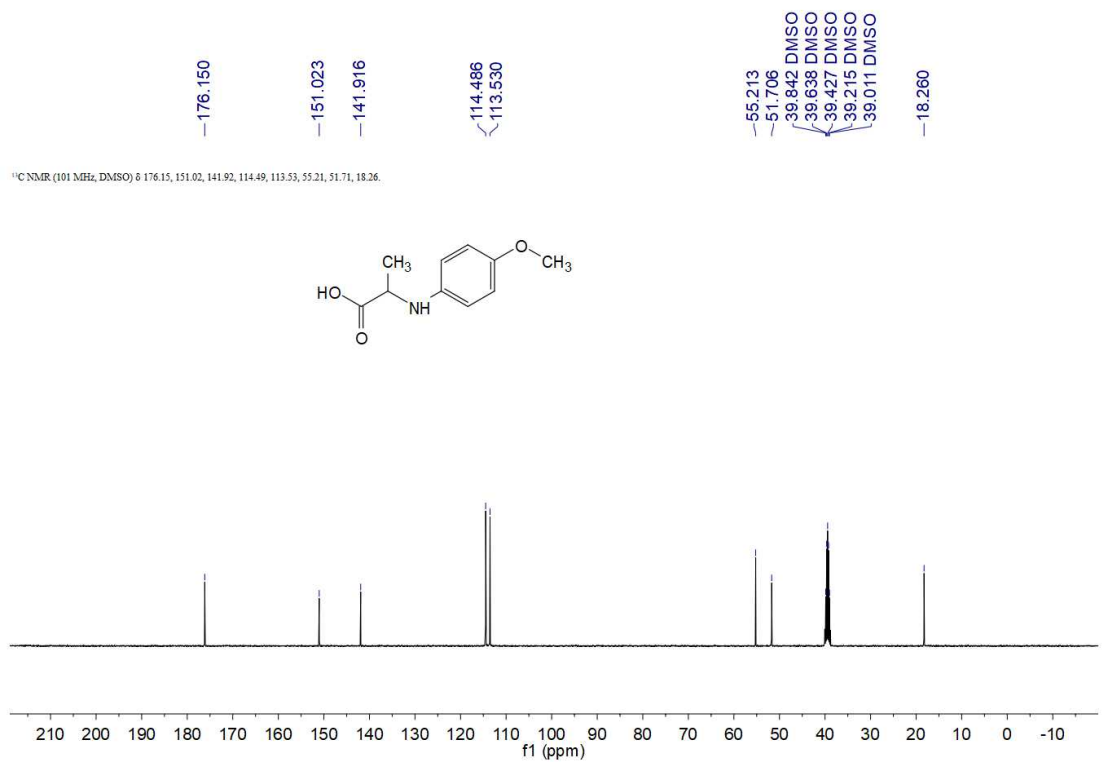
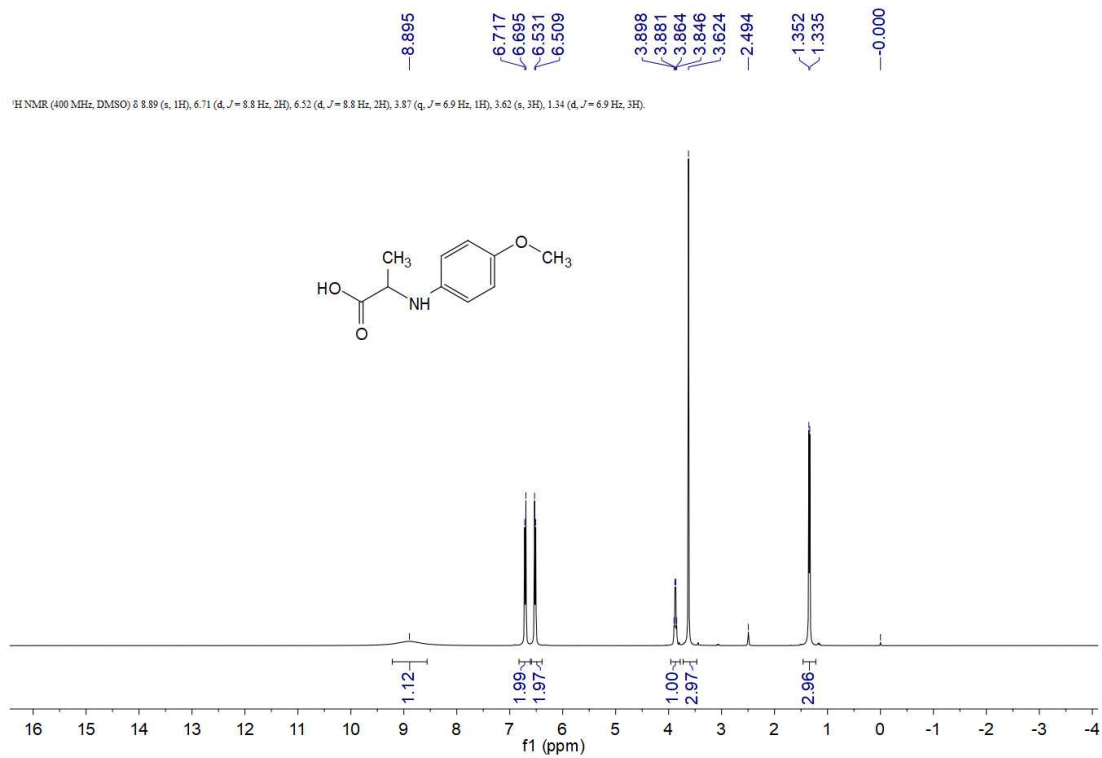


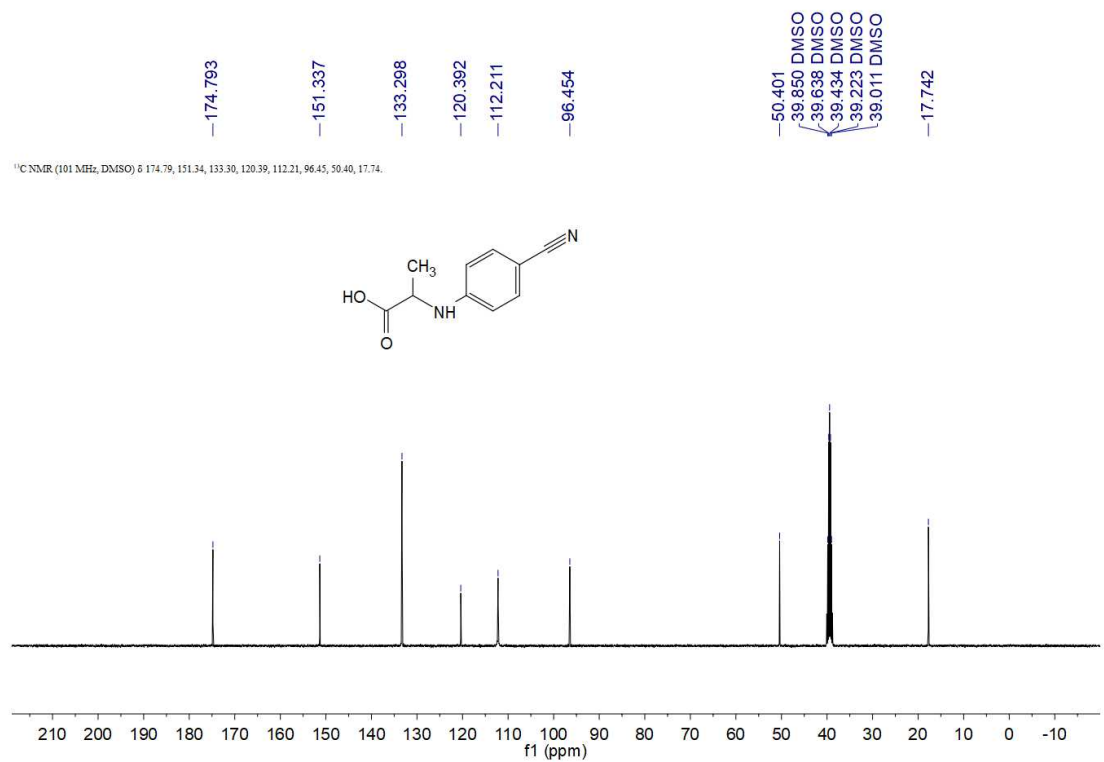
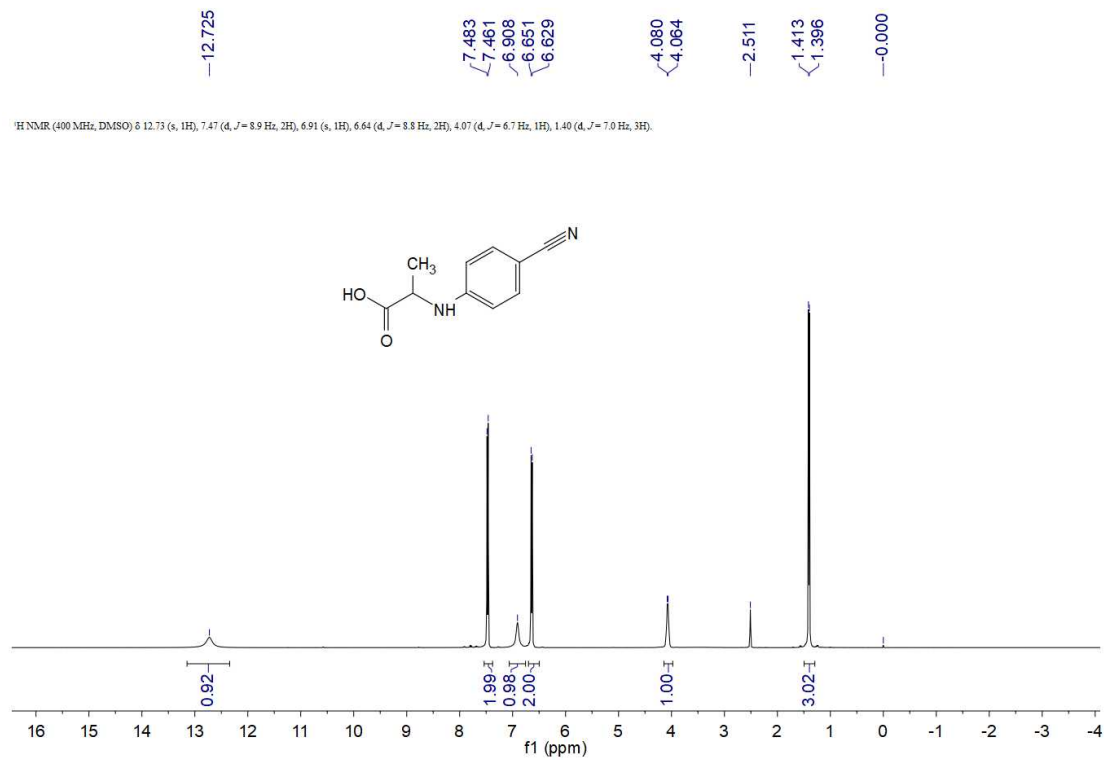


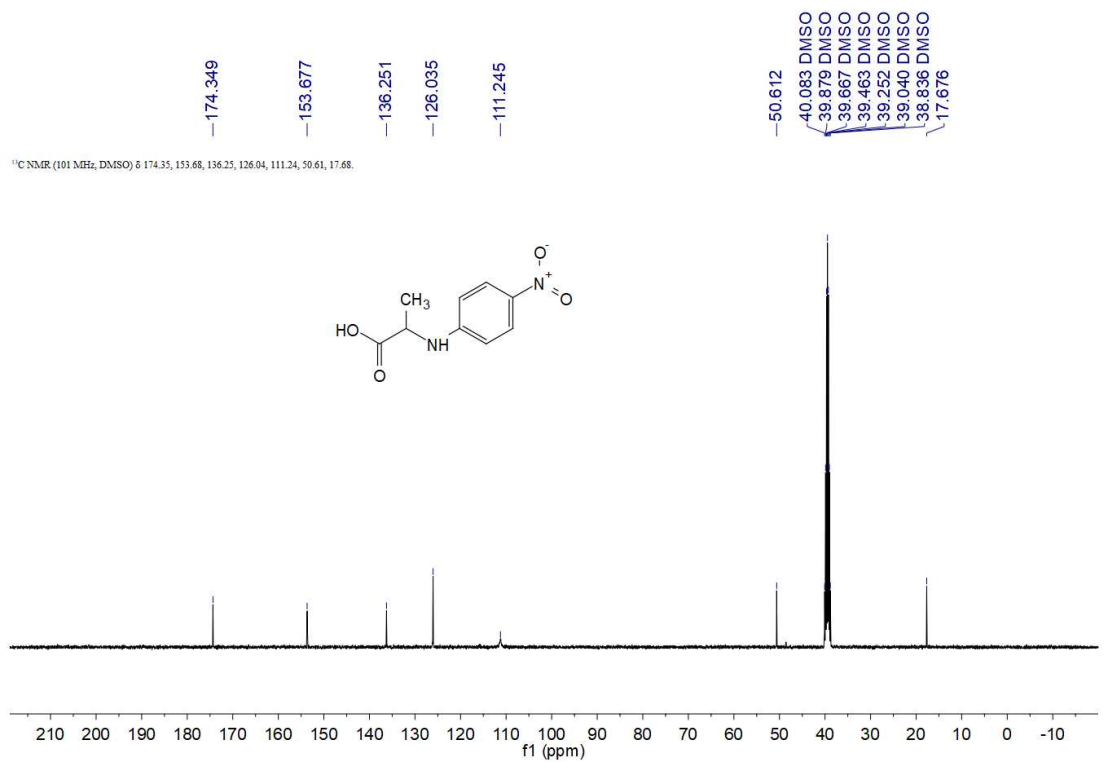
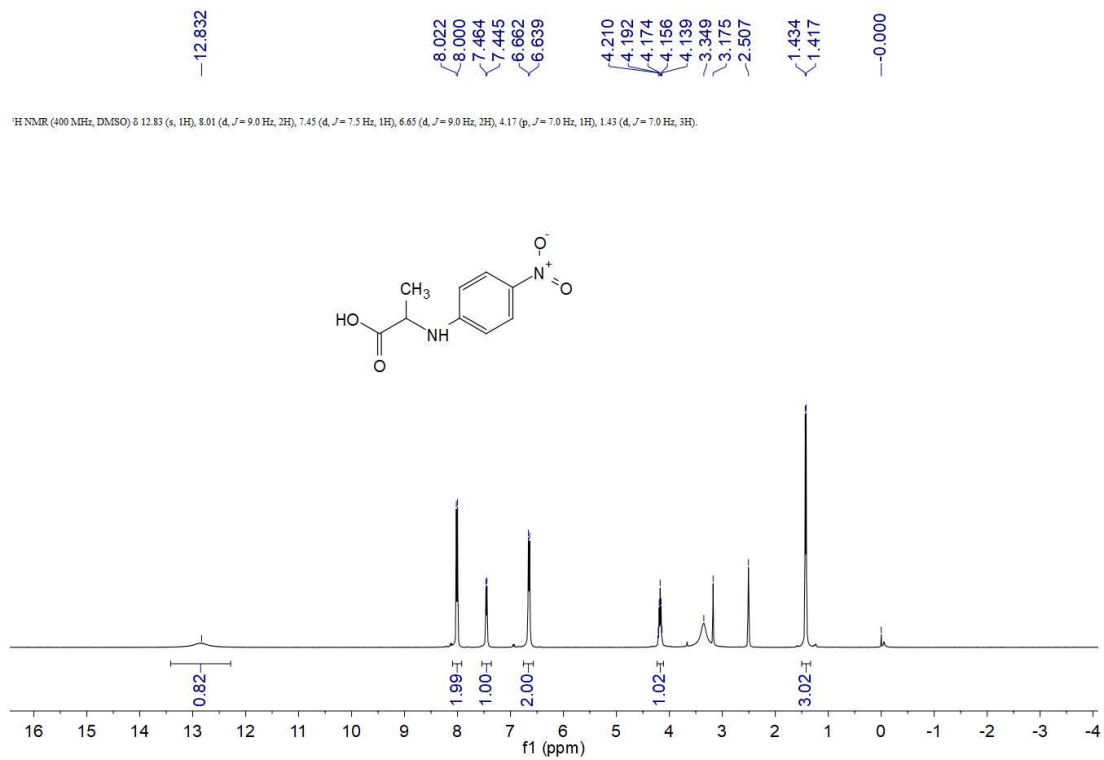


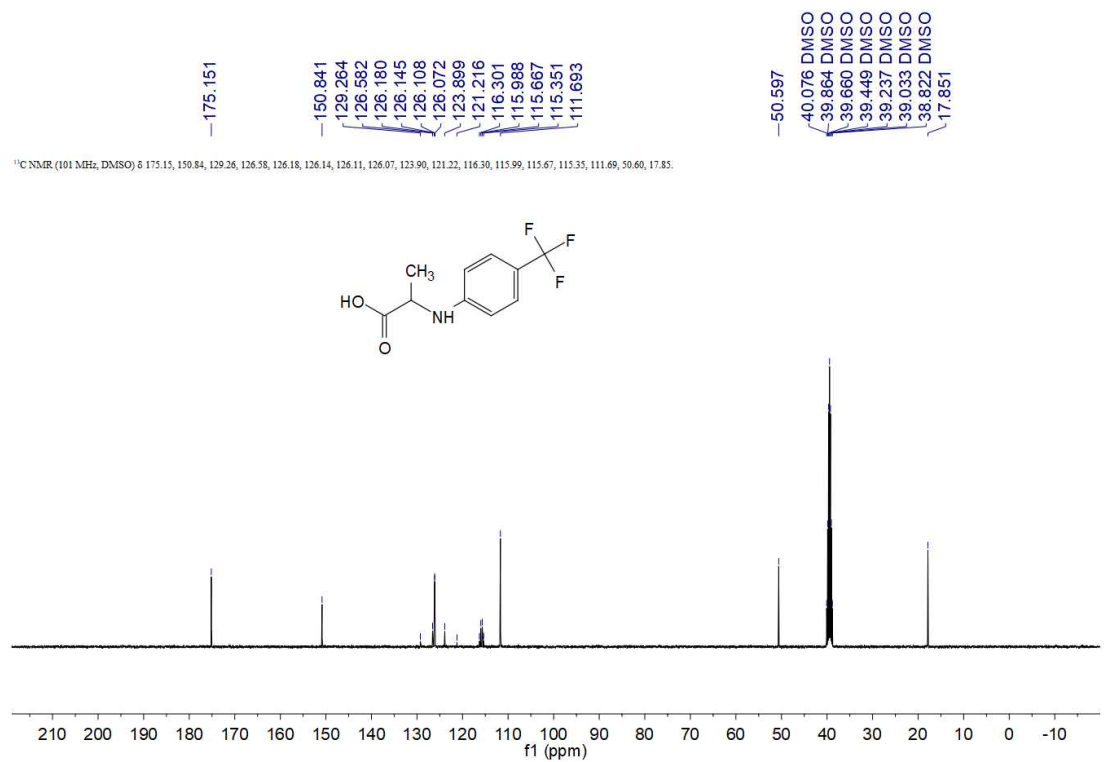
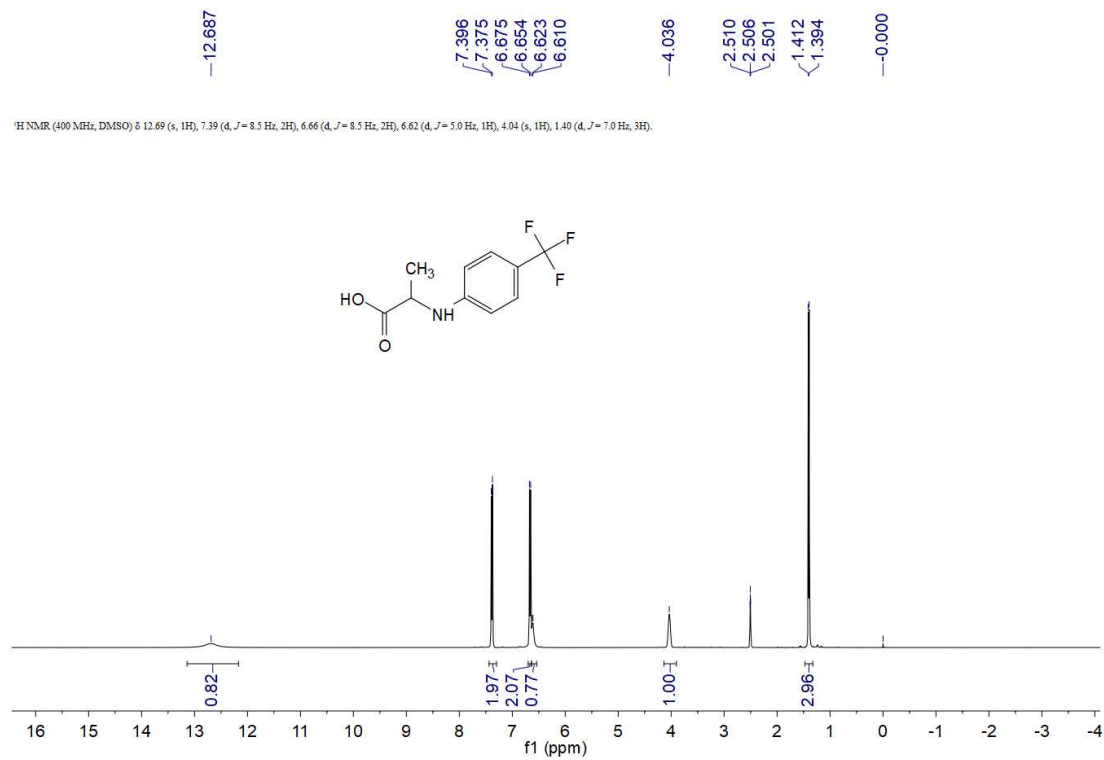


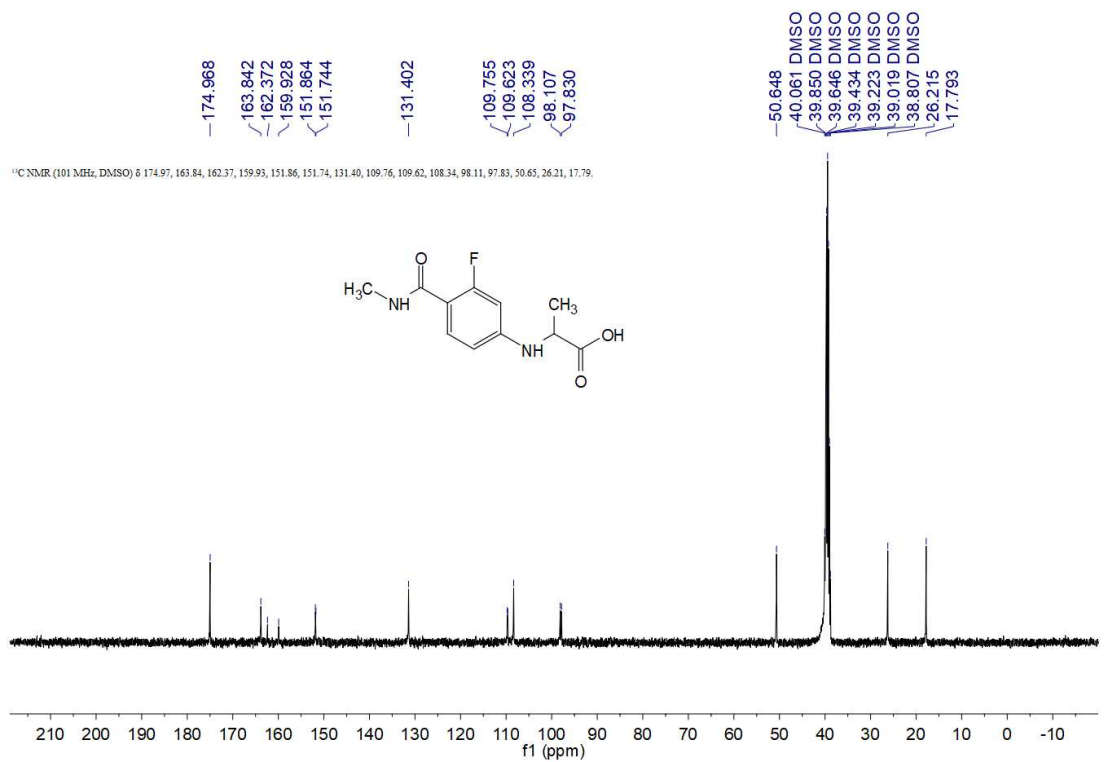
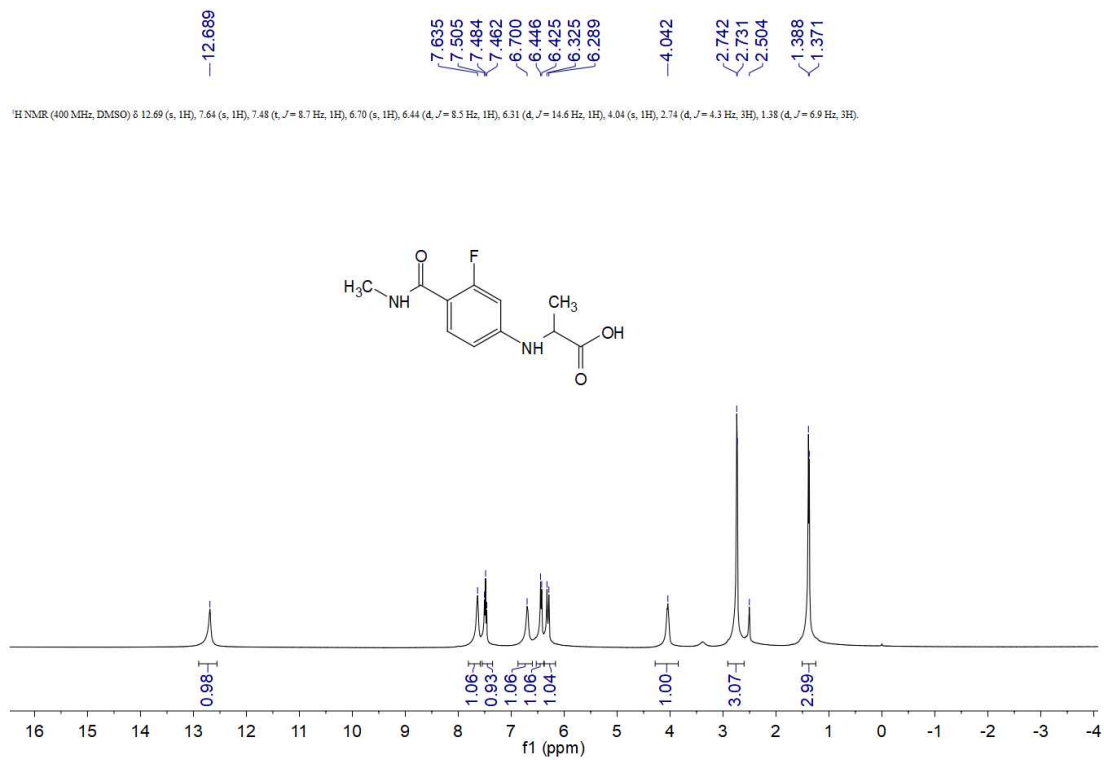




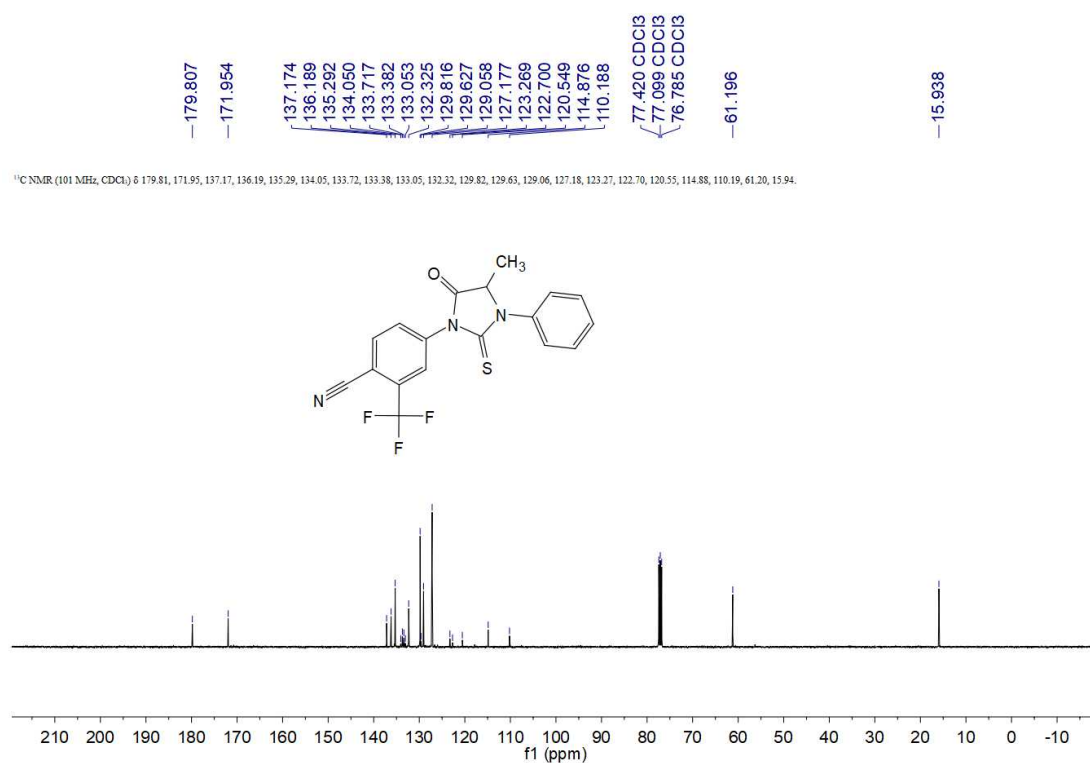
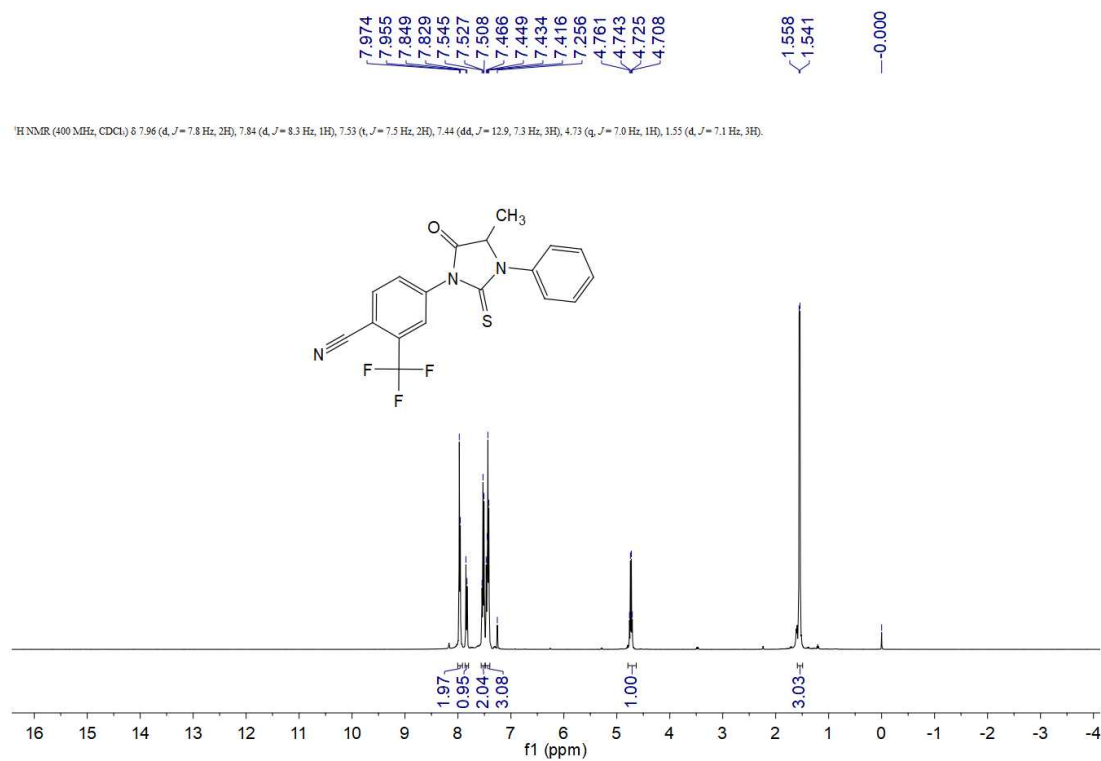




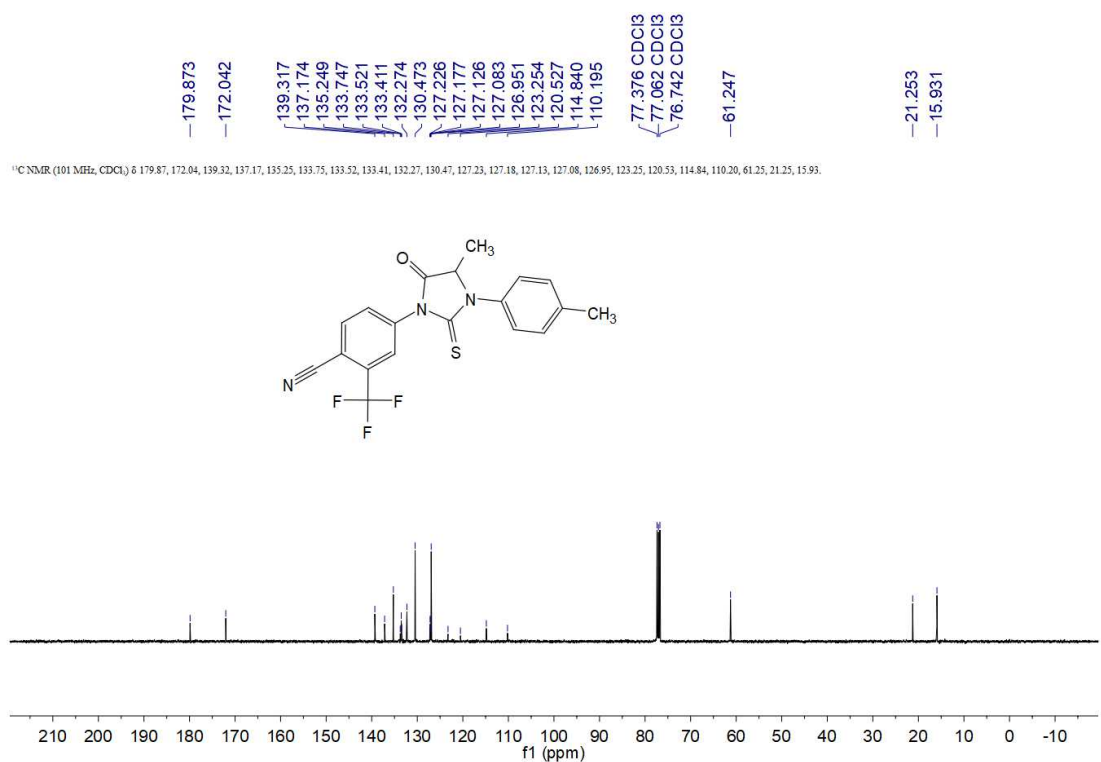
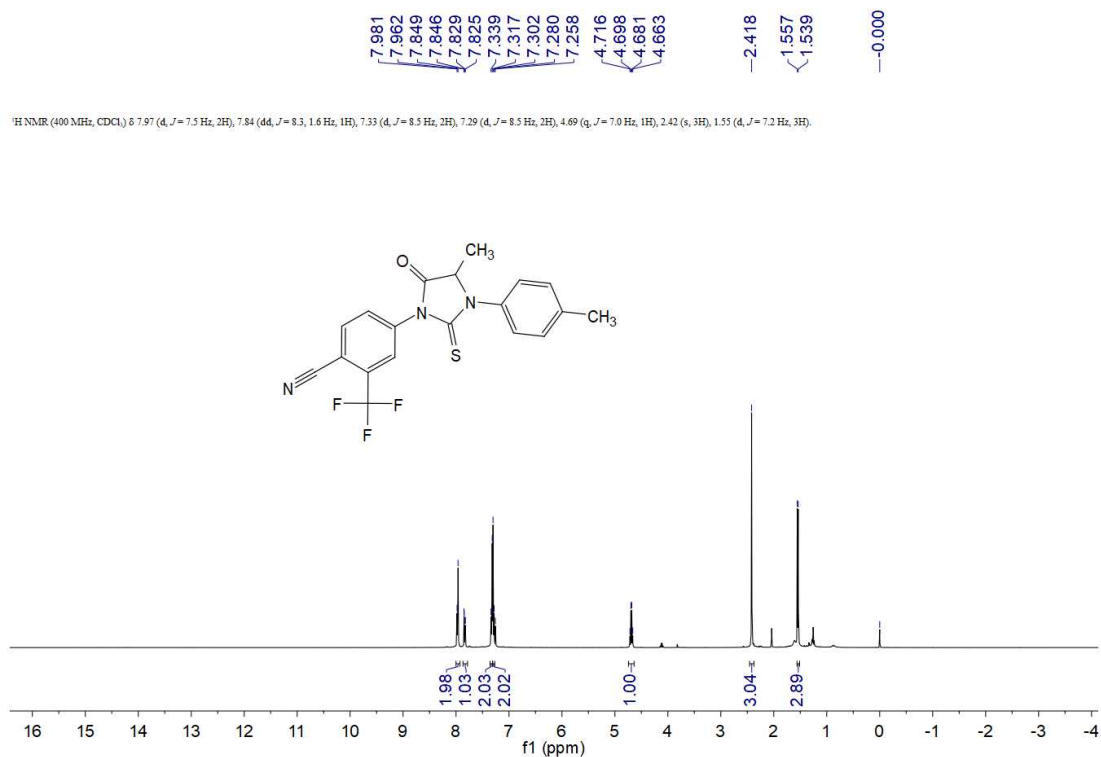


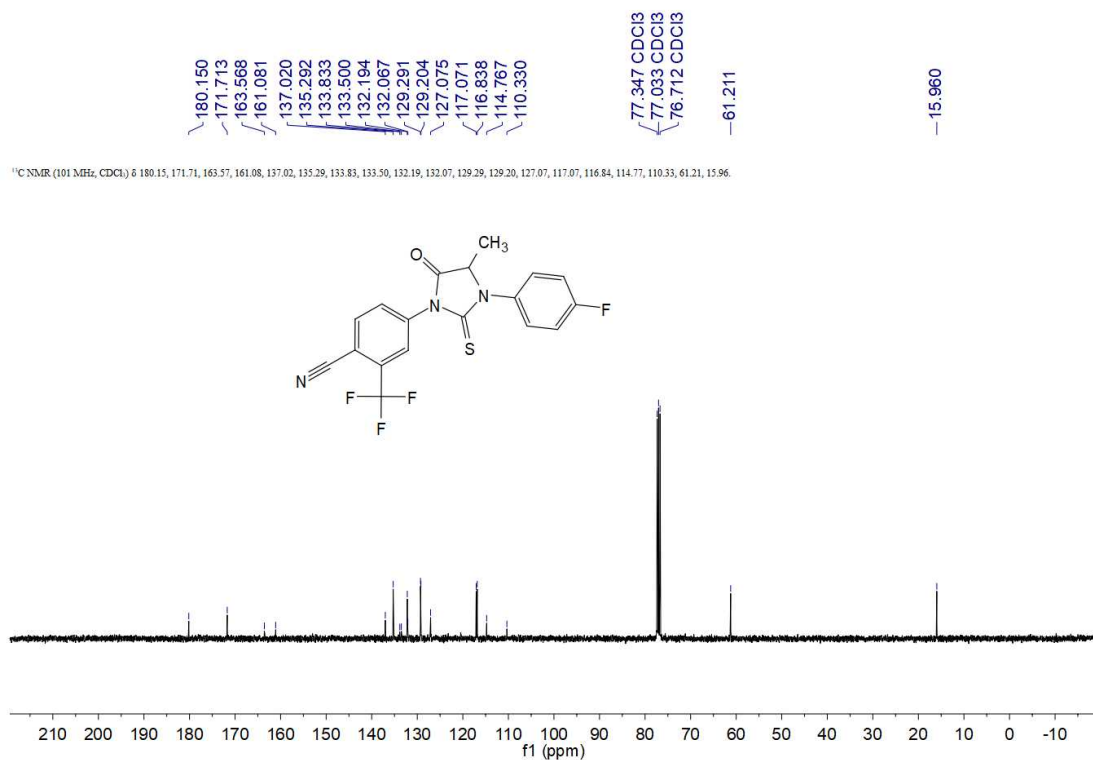
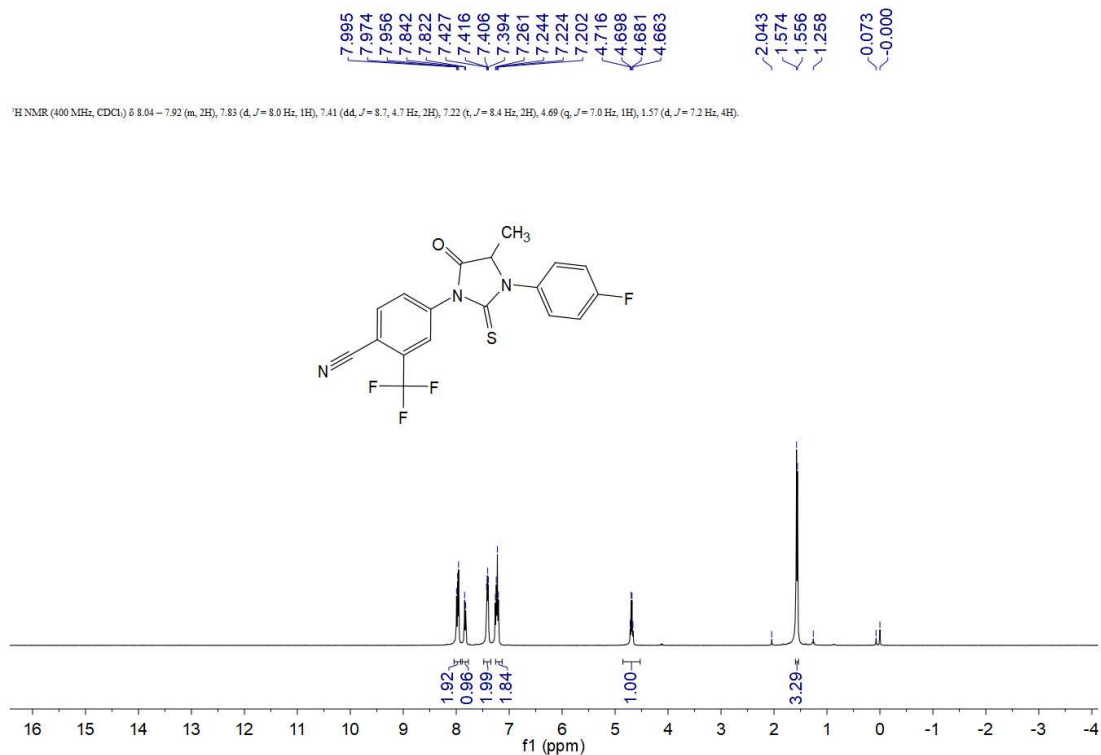


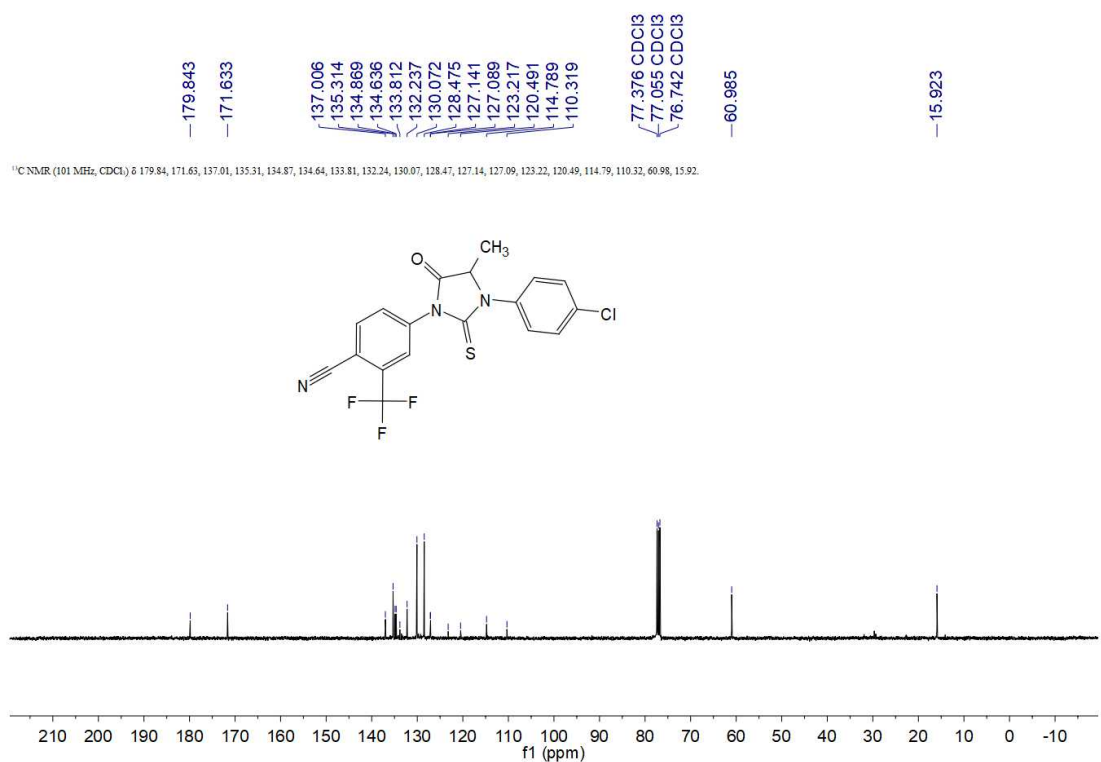
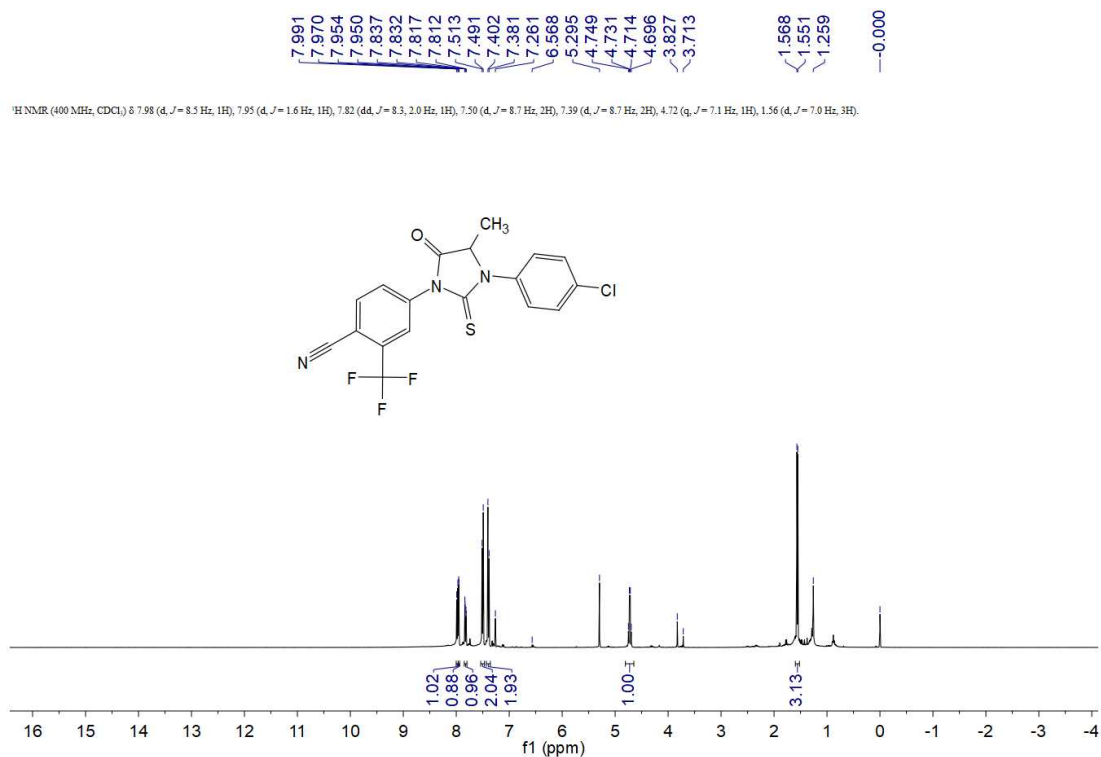
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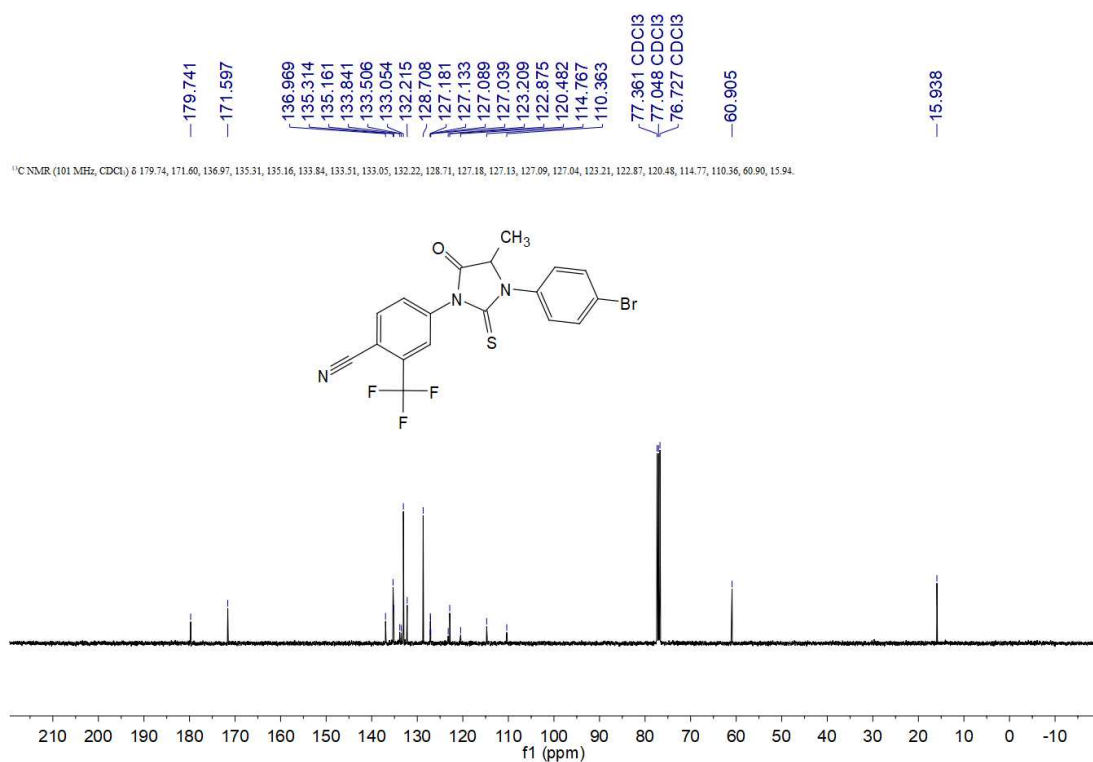
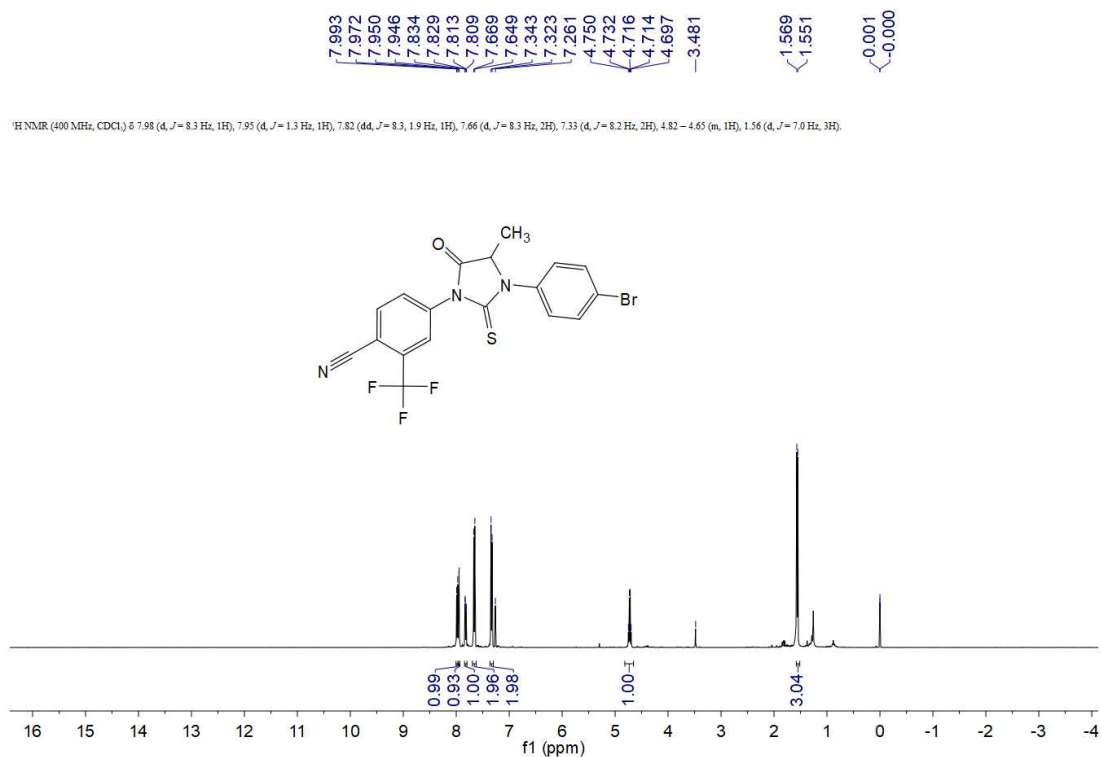


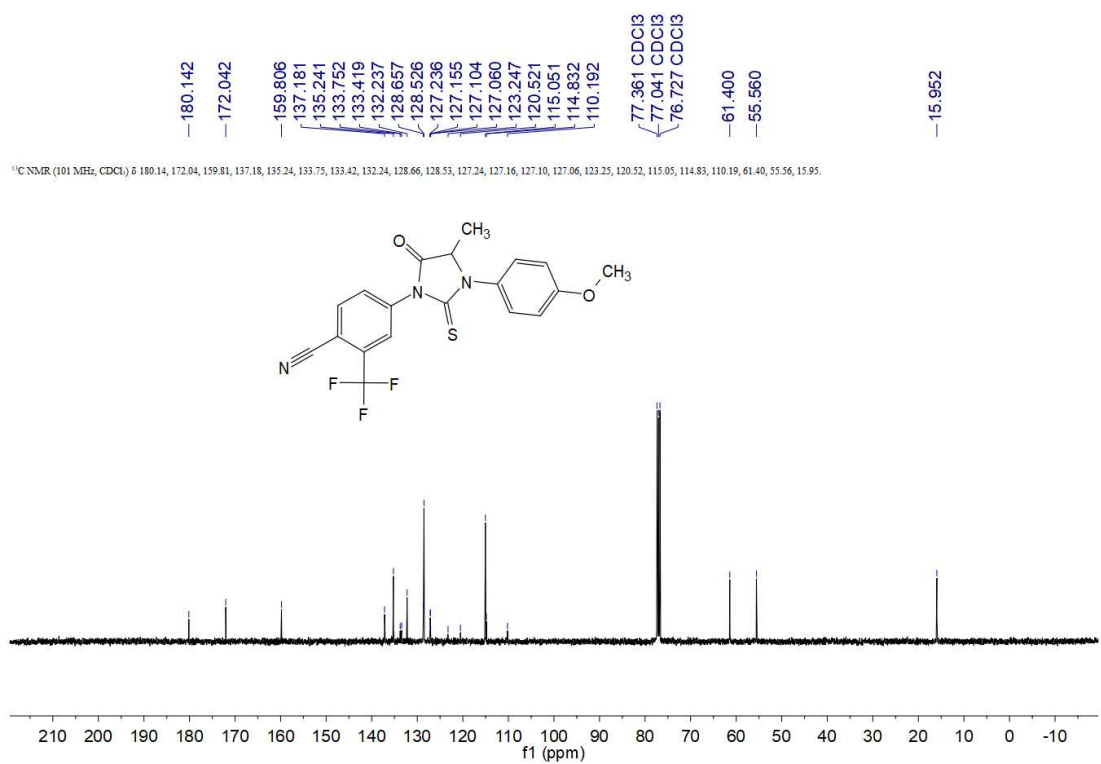
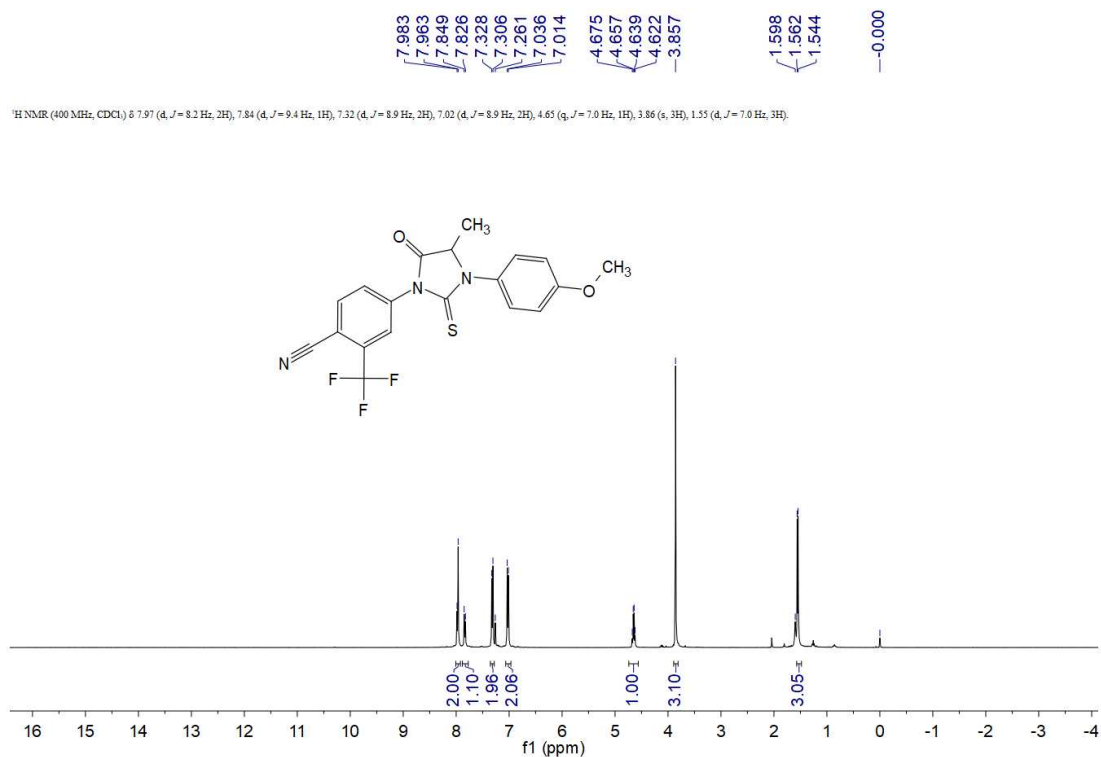


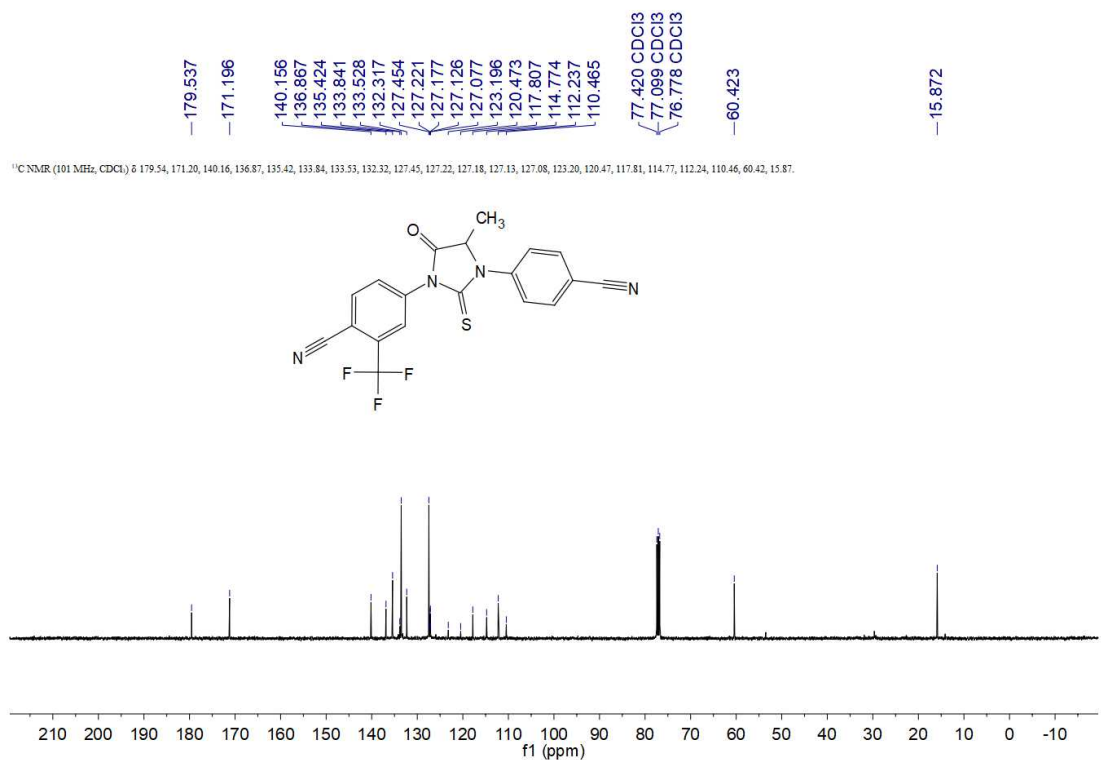
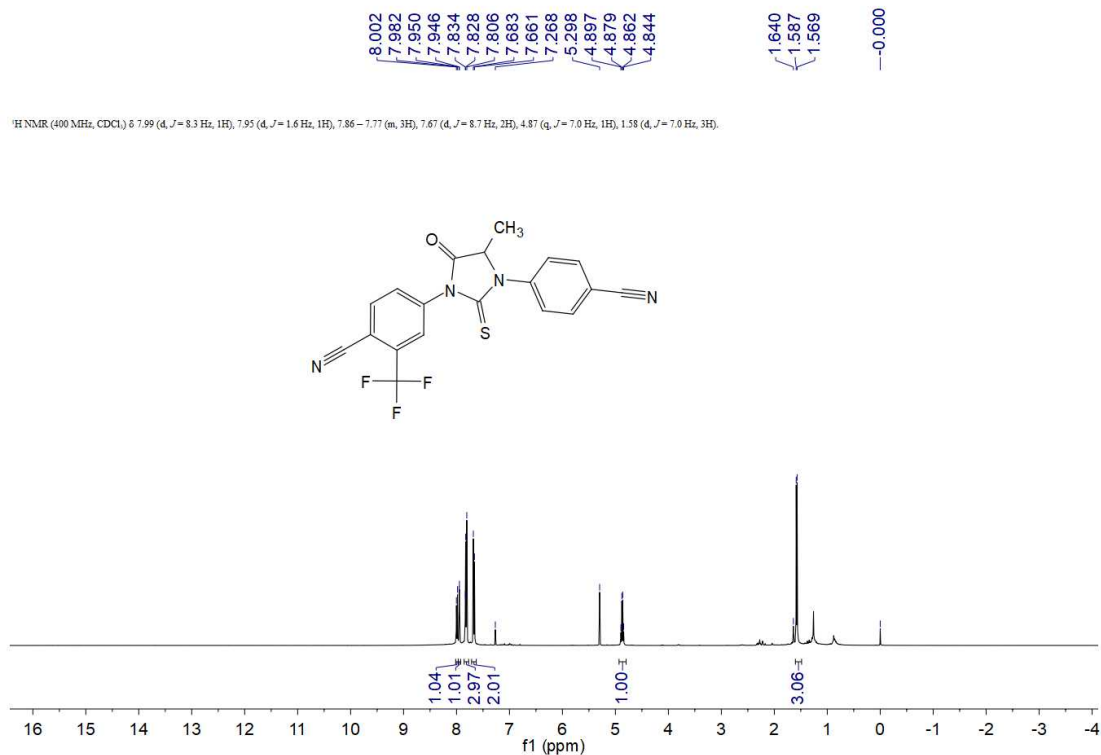


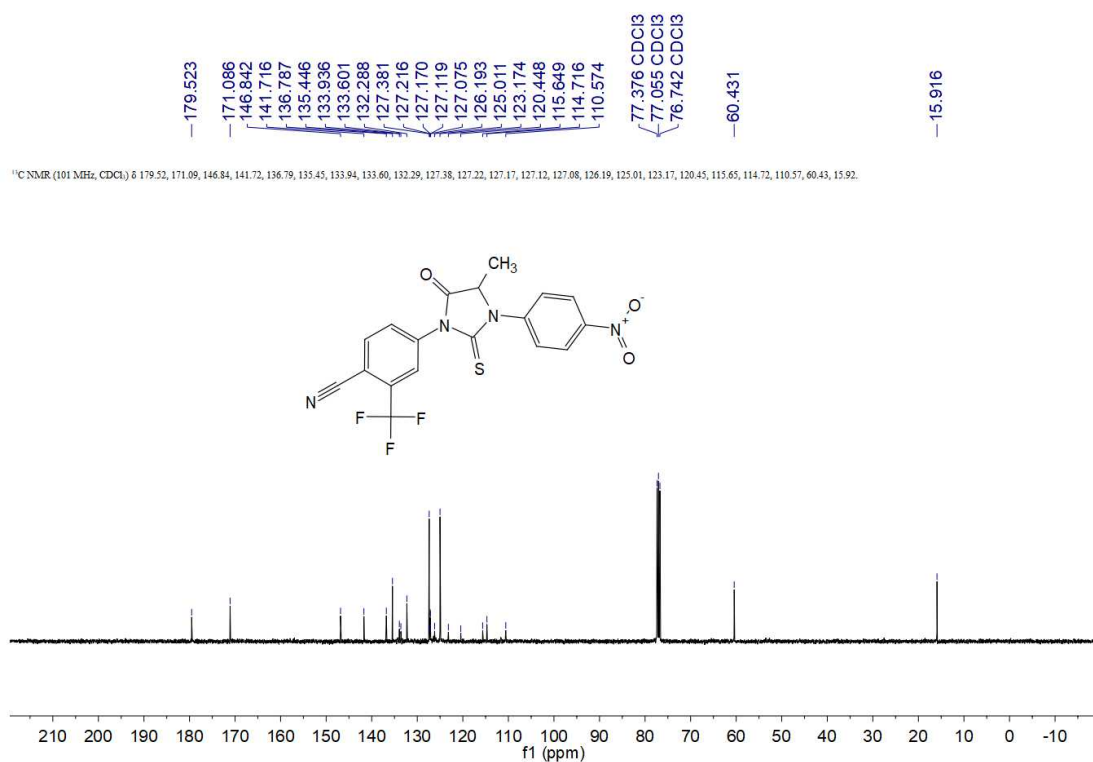
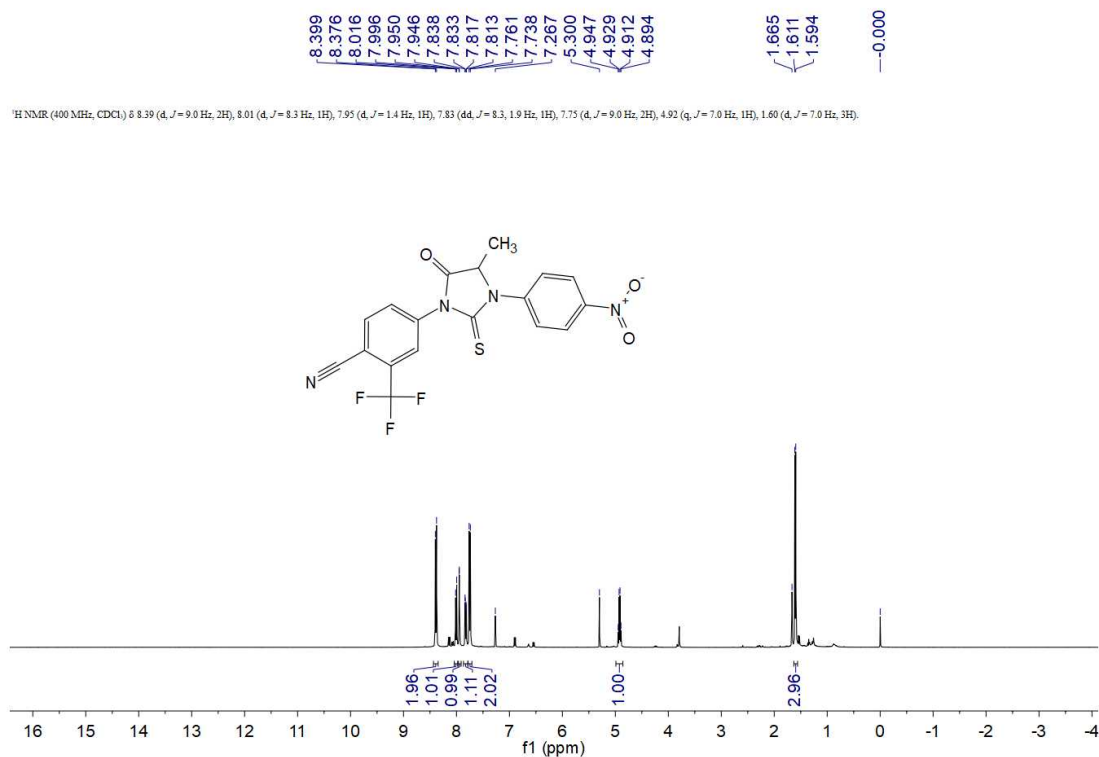


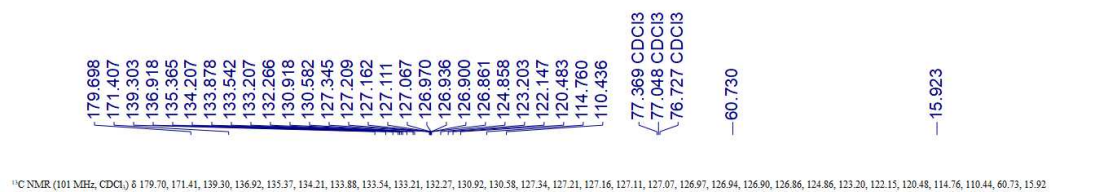
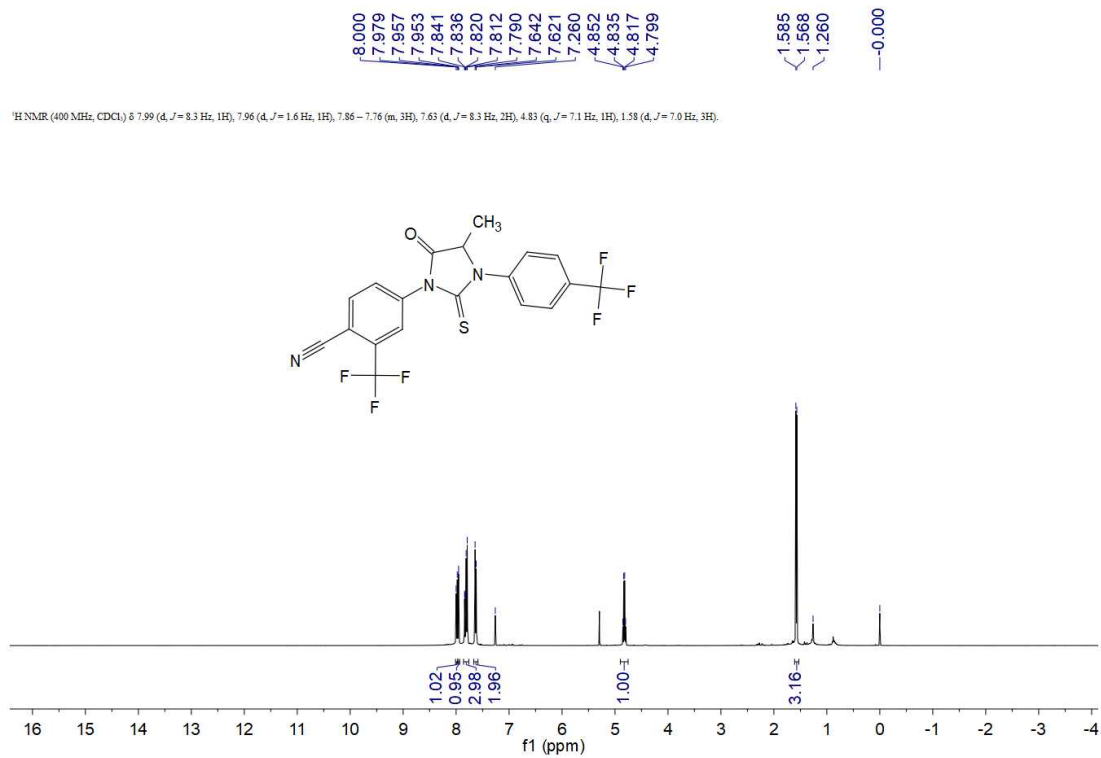




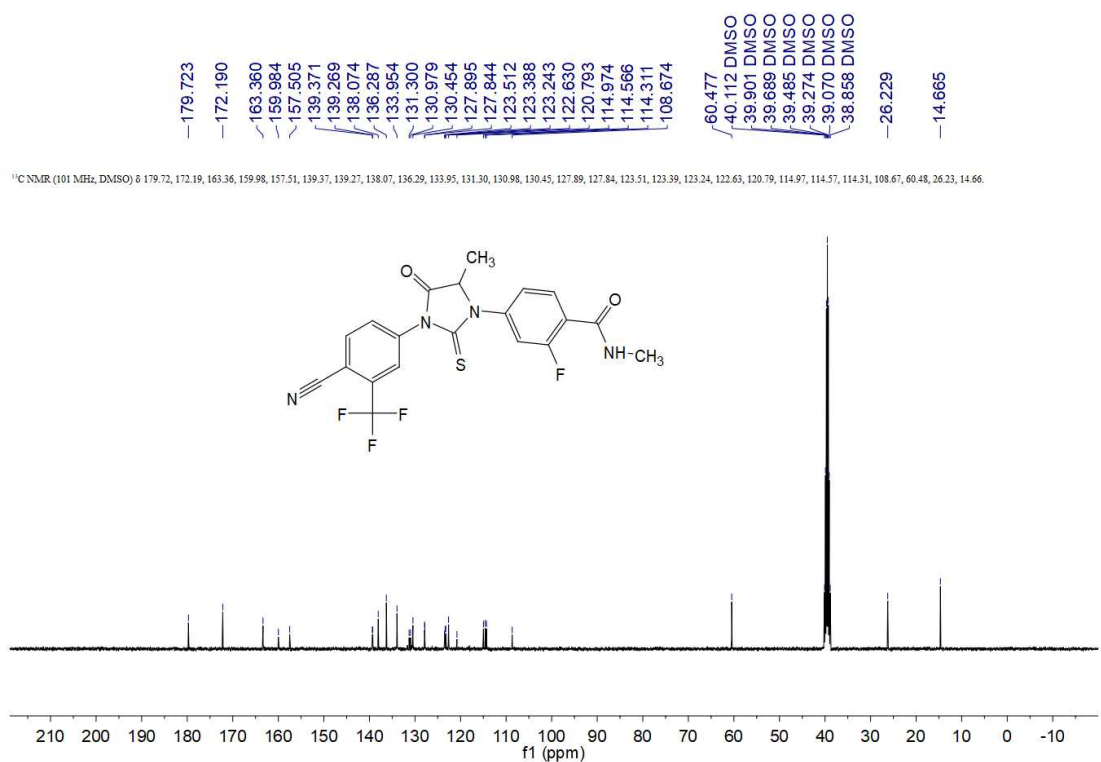
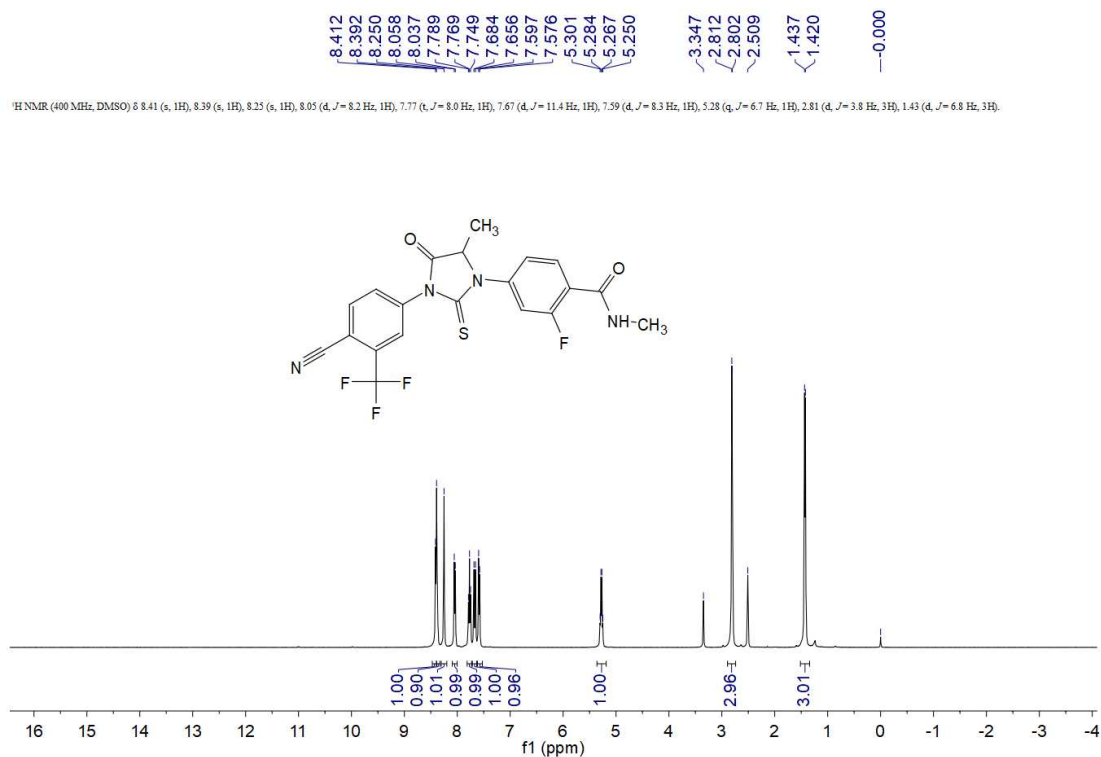


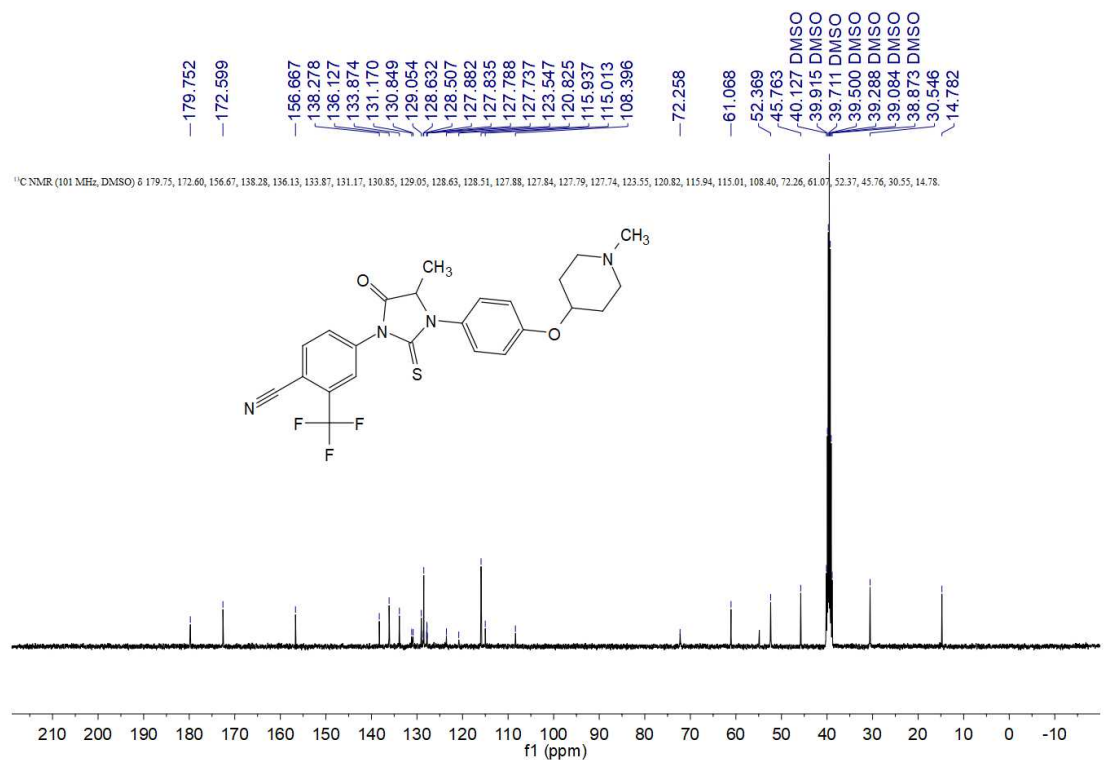
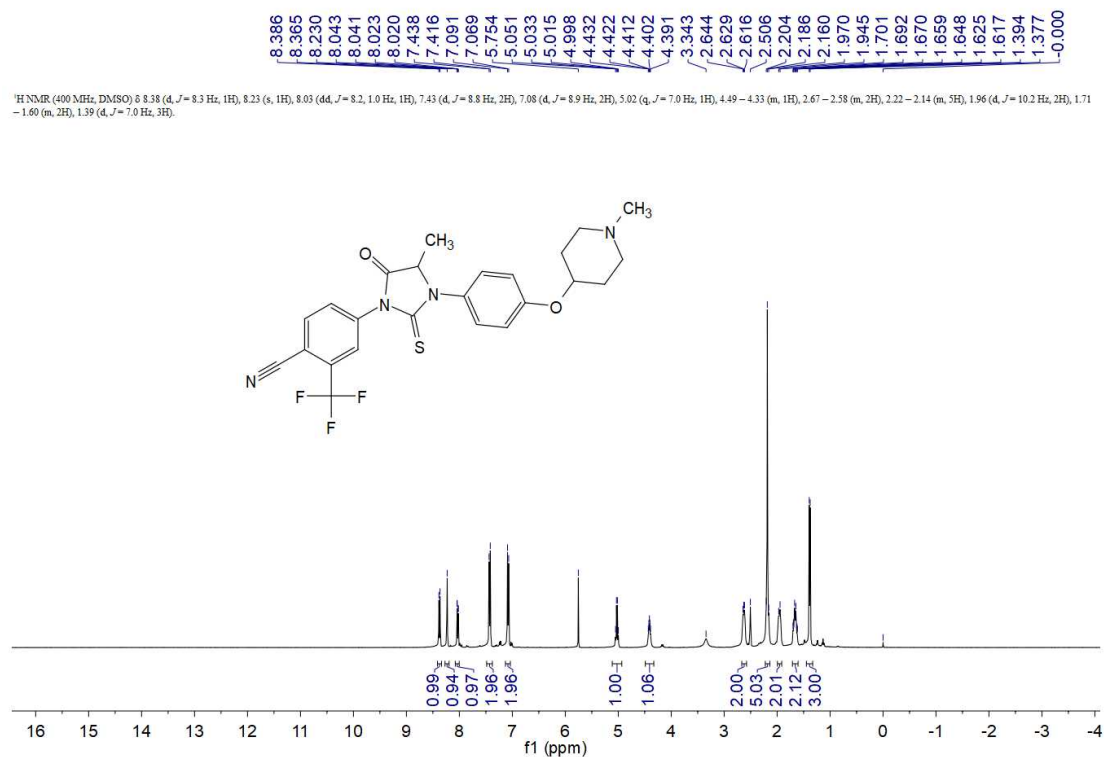




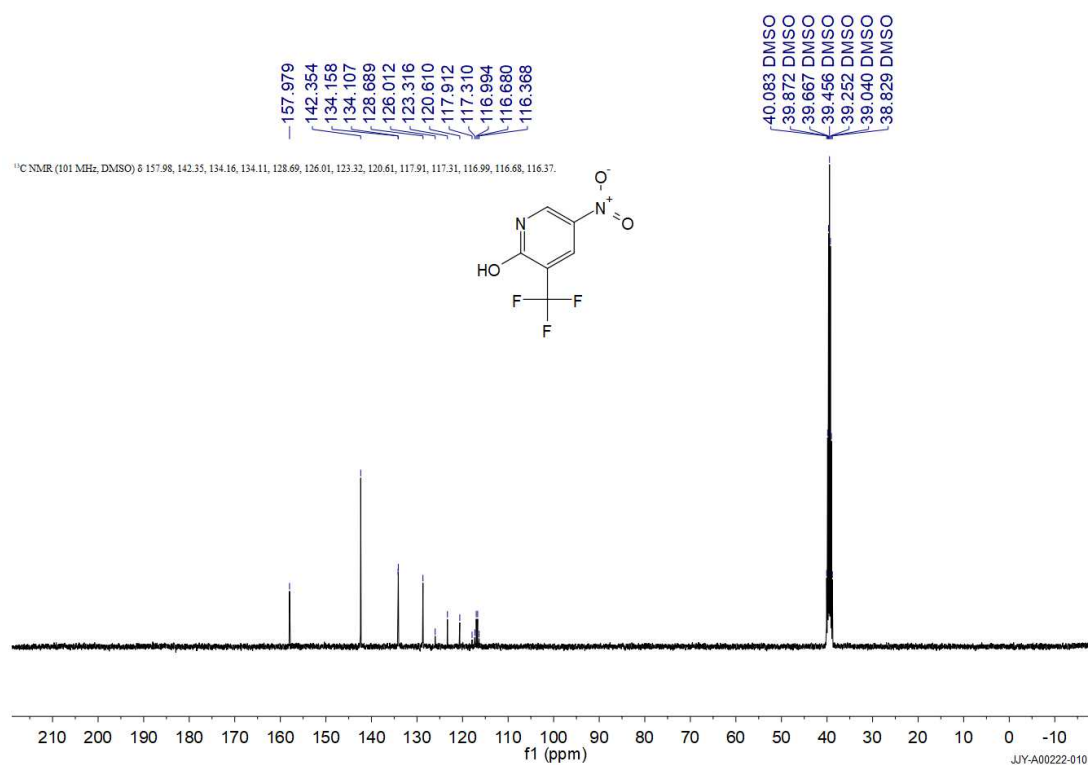
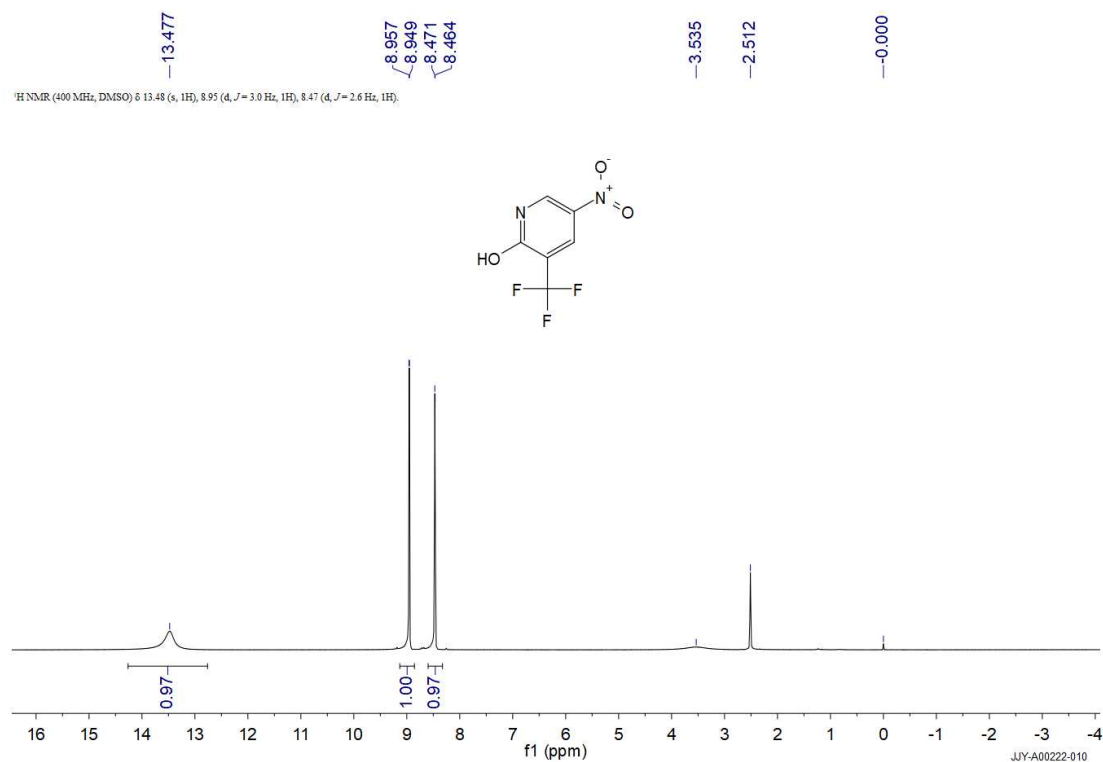


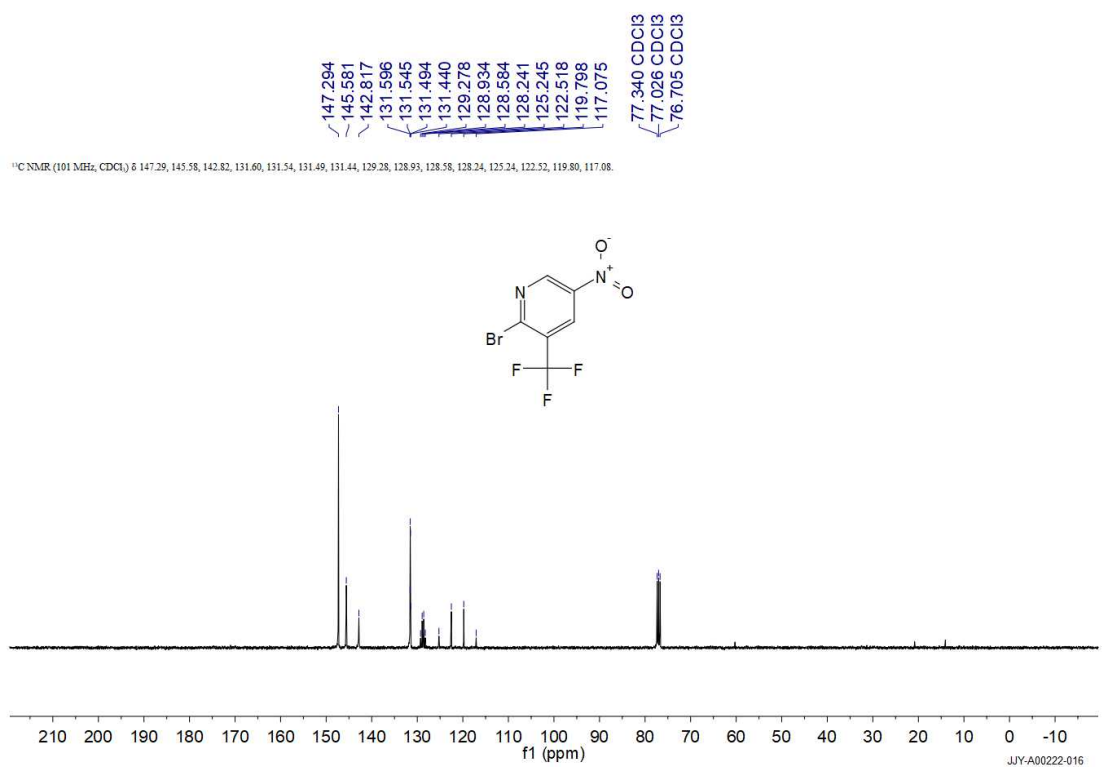
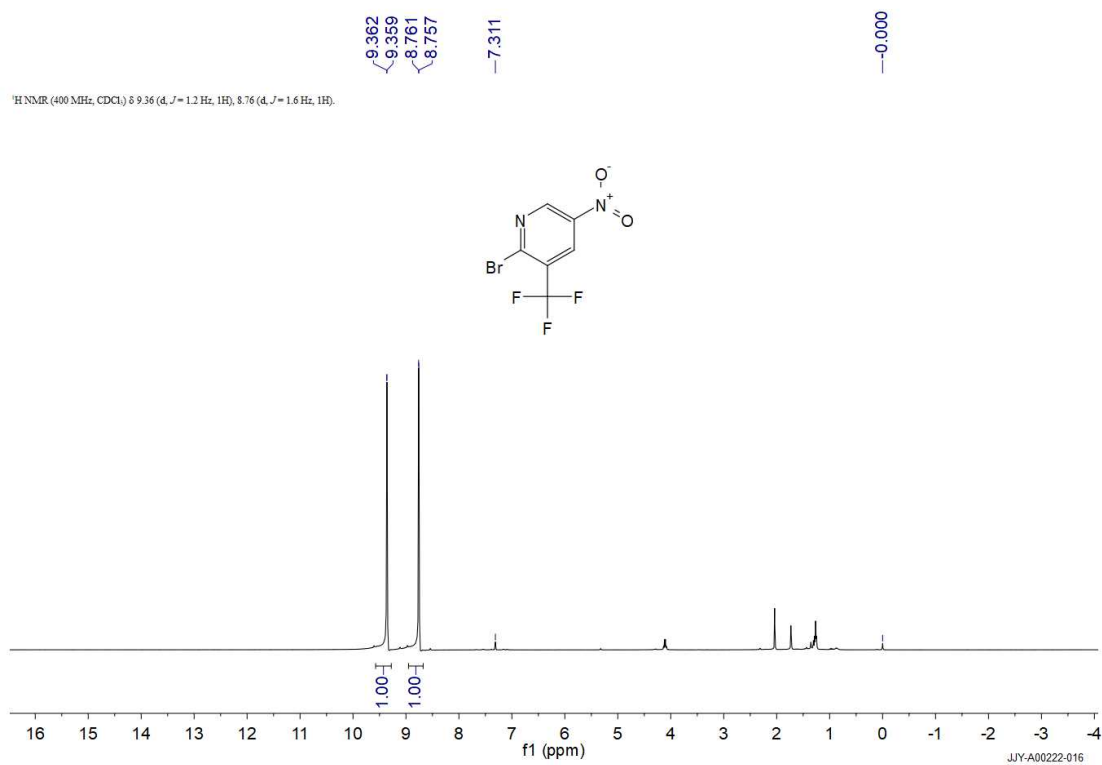


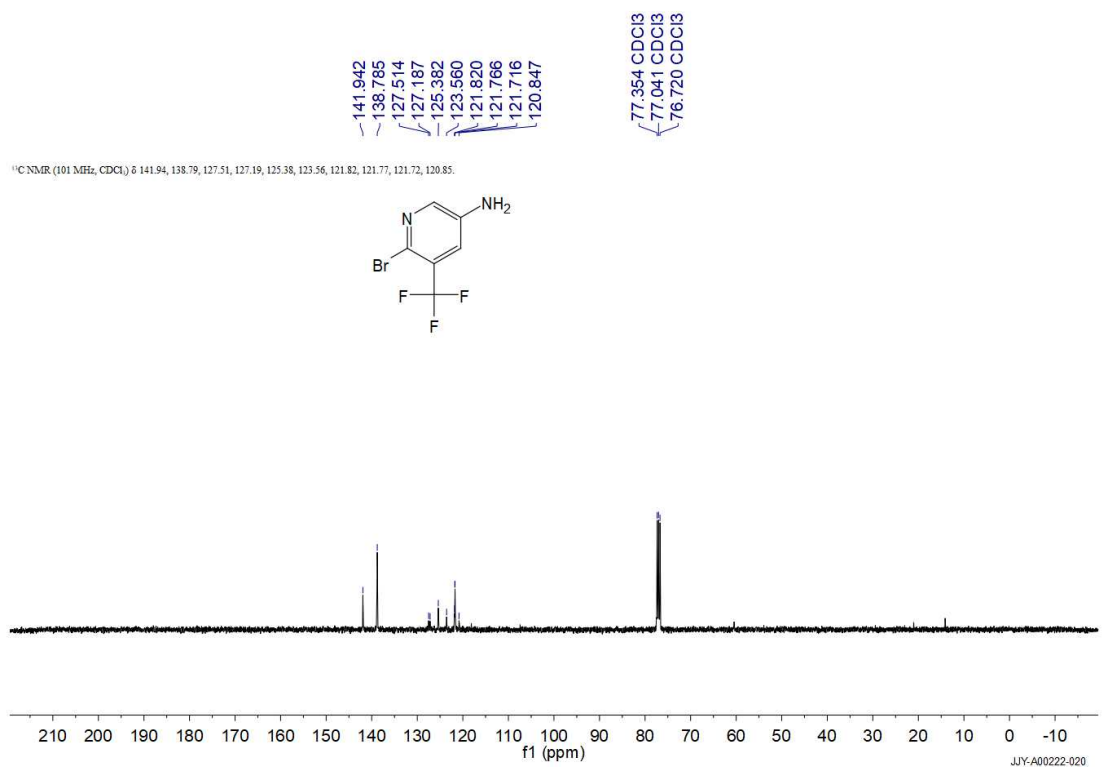
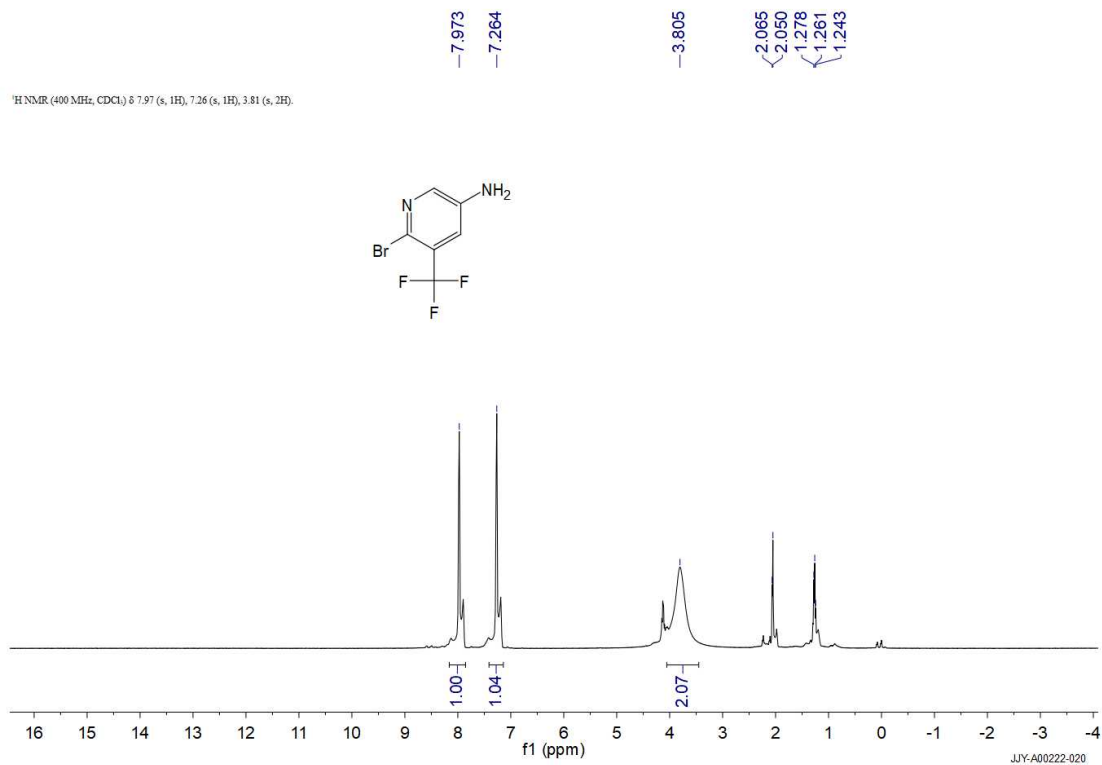


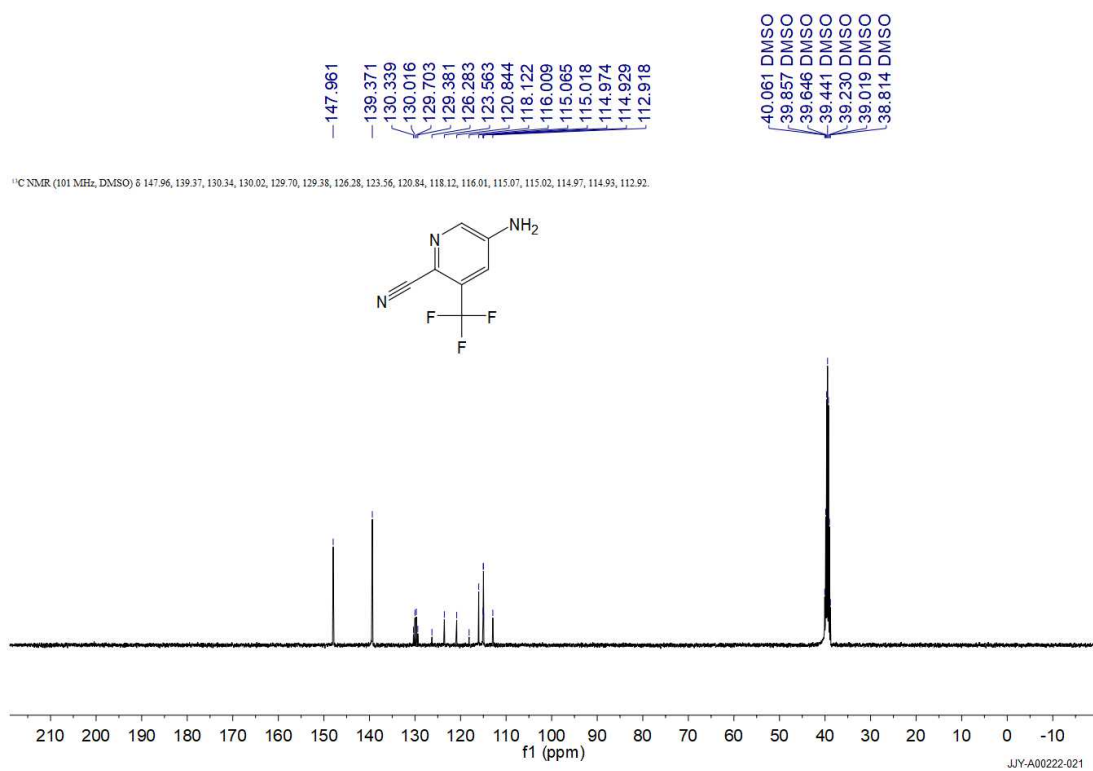
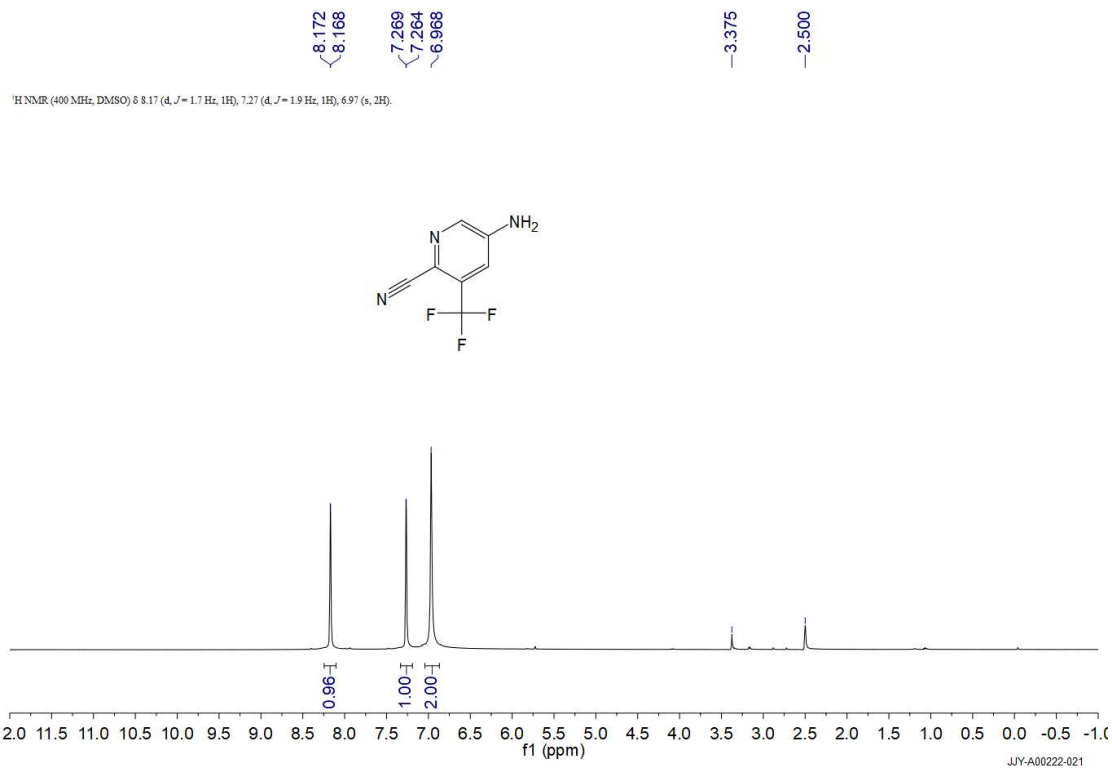


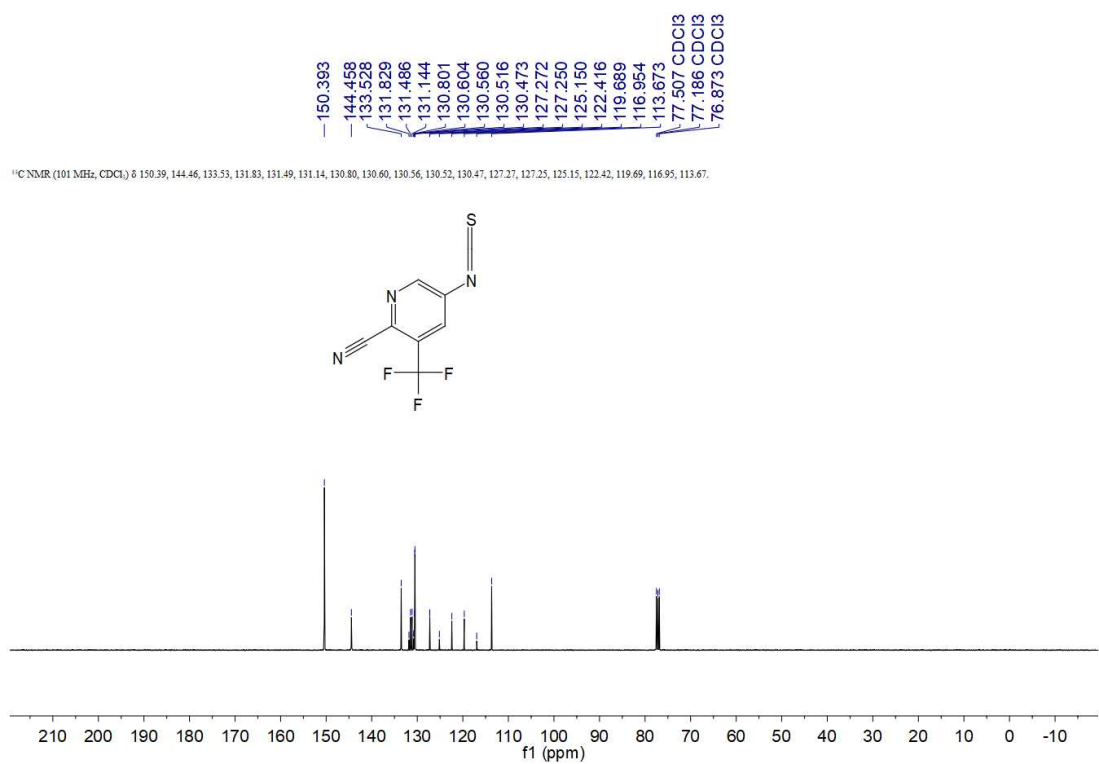
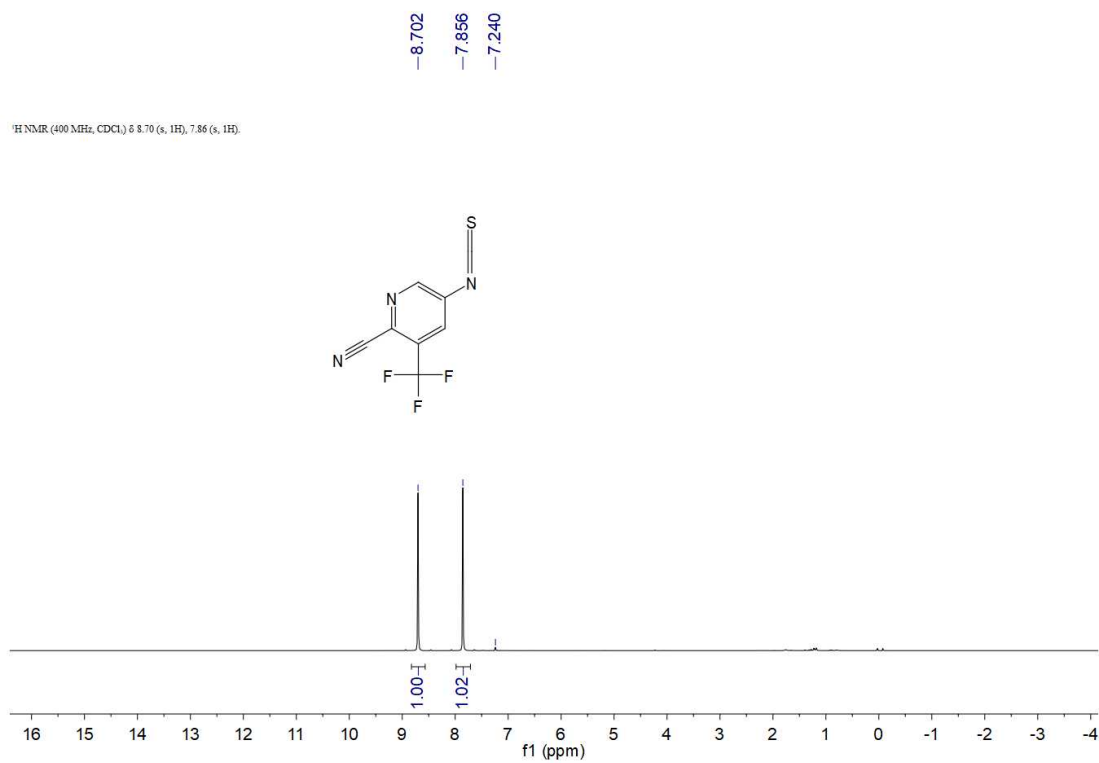
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of compound **13-17**



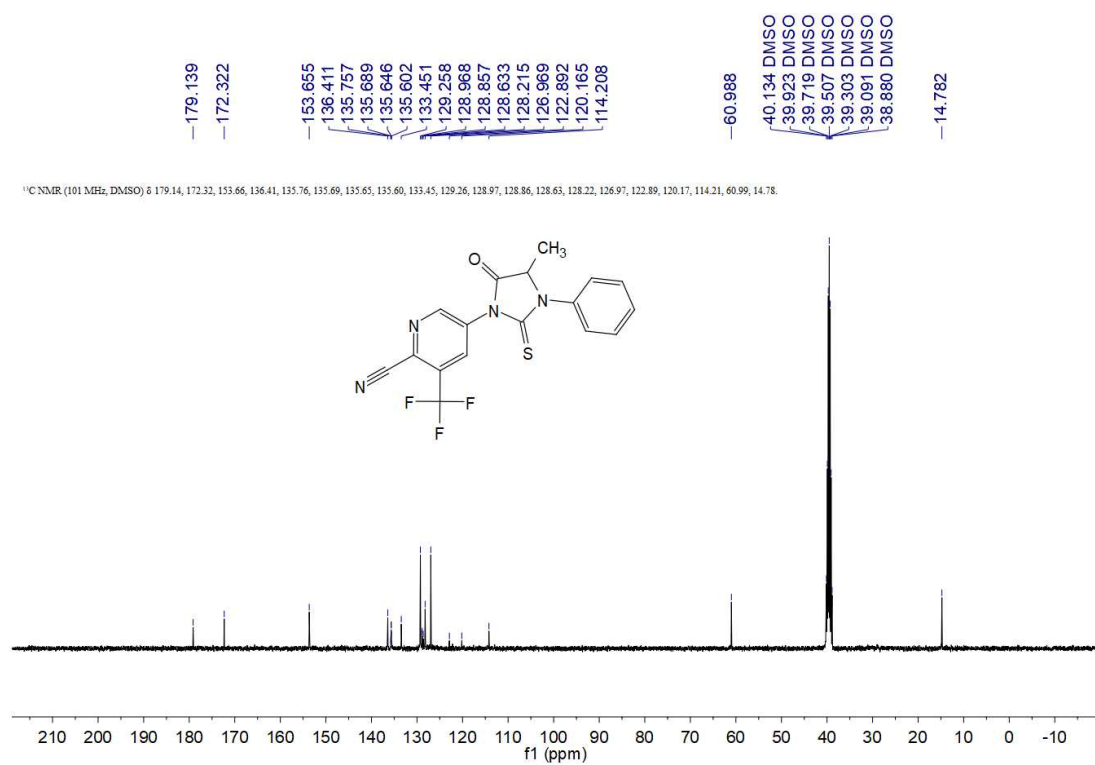
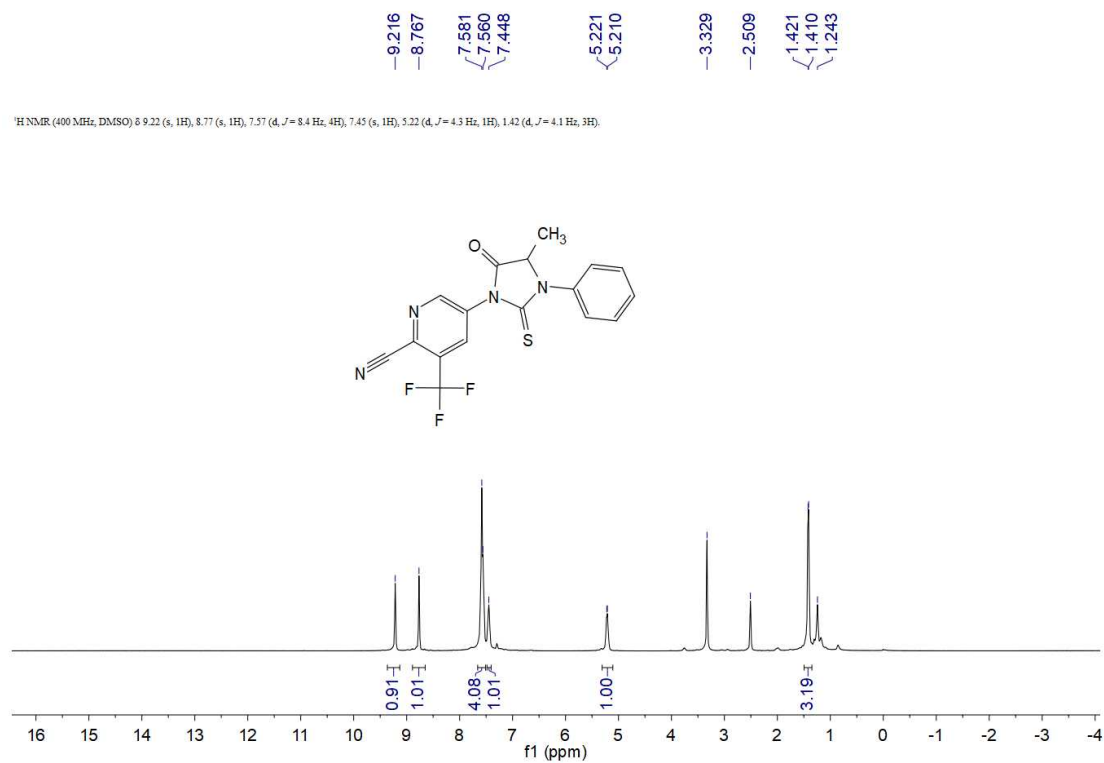




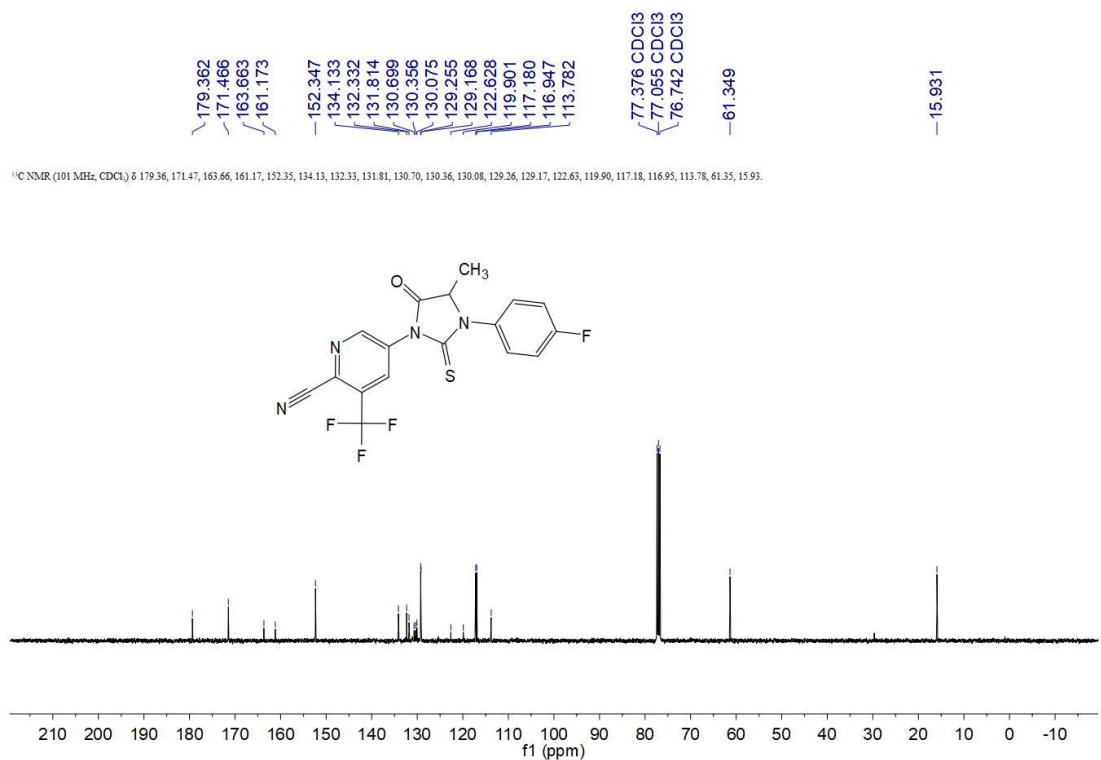
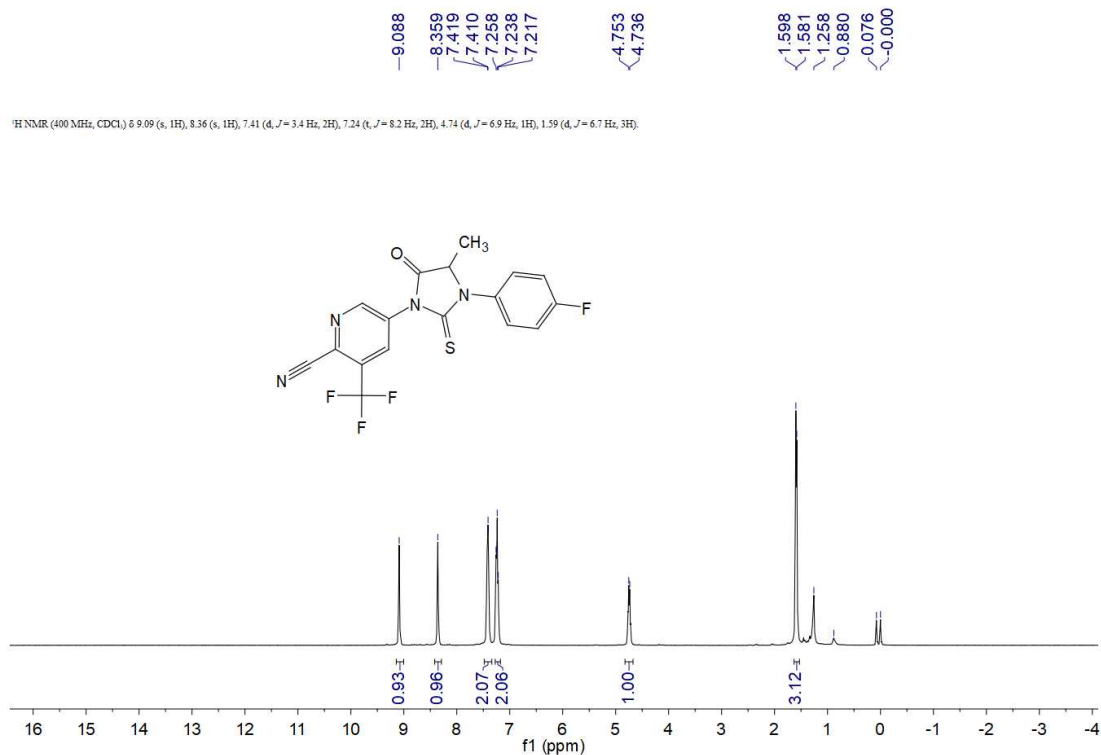


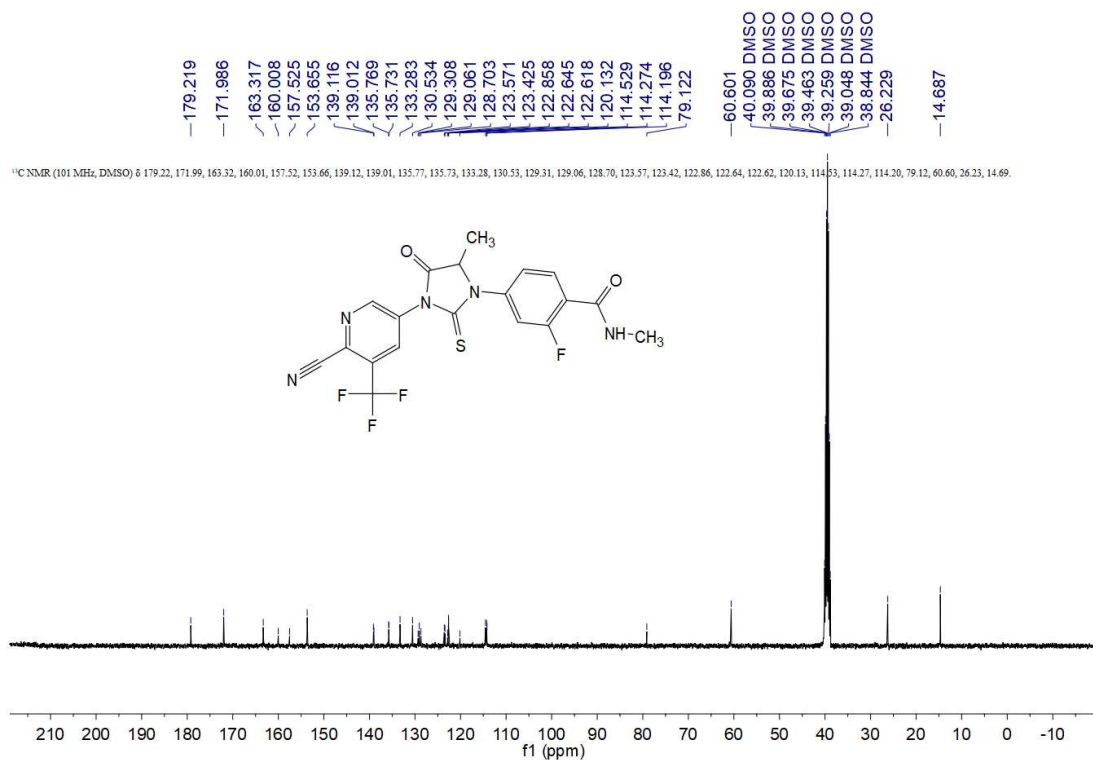
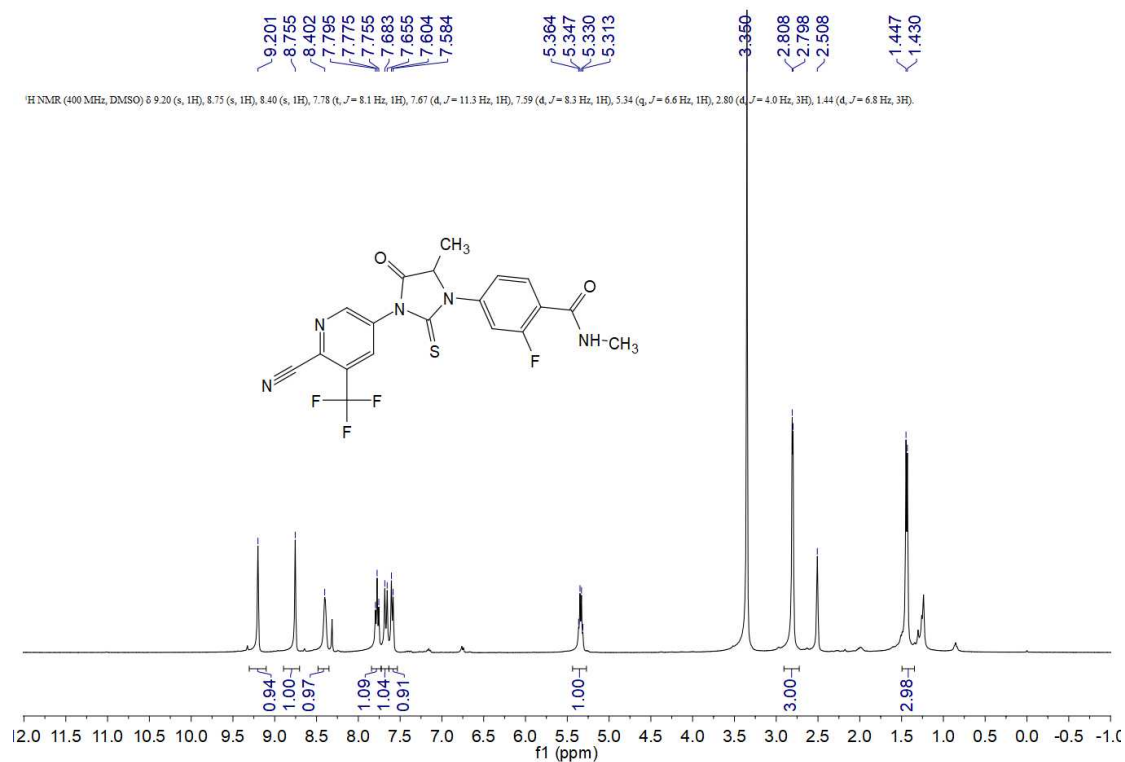


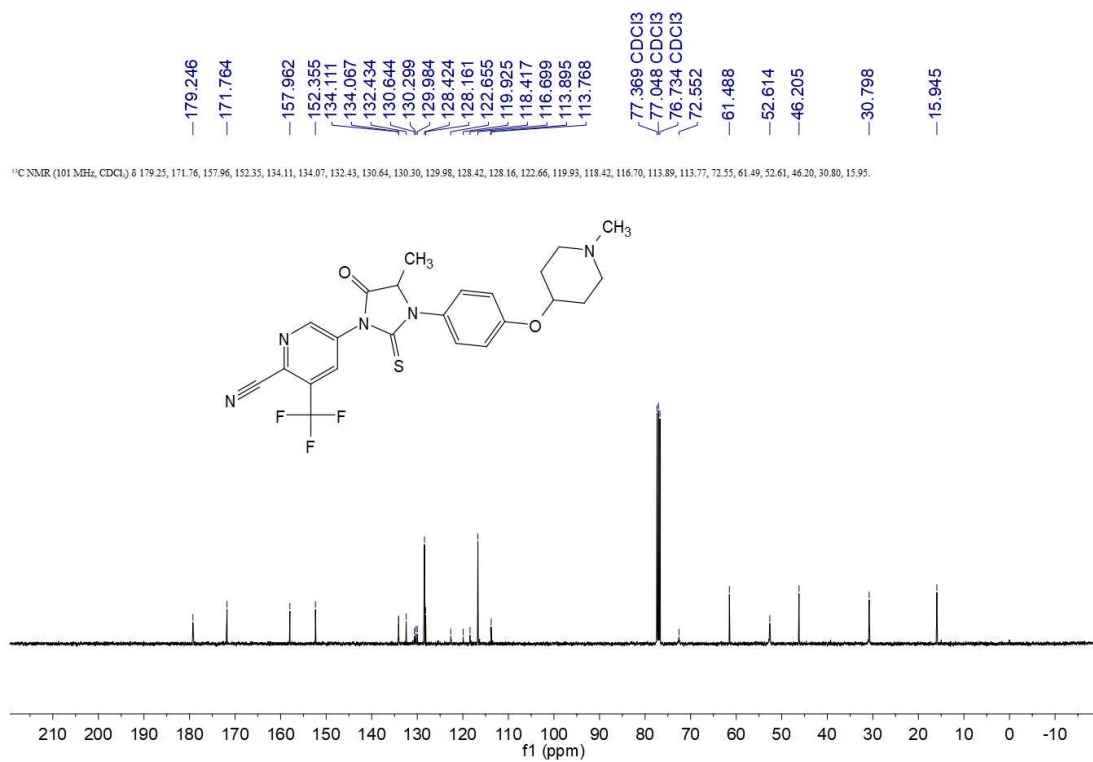
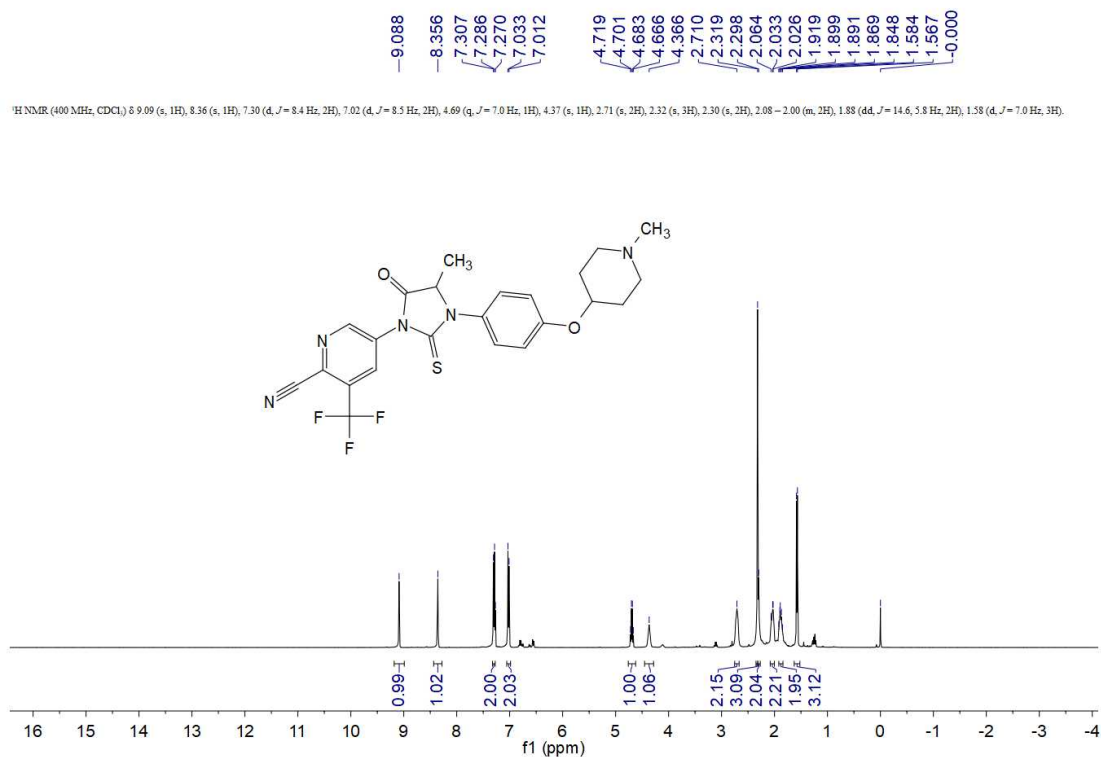
$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of *compound 18a-d*



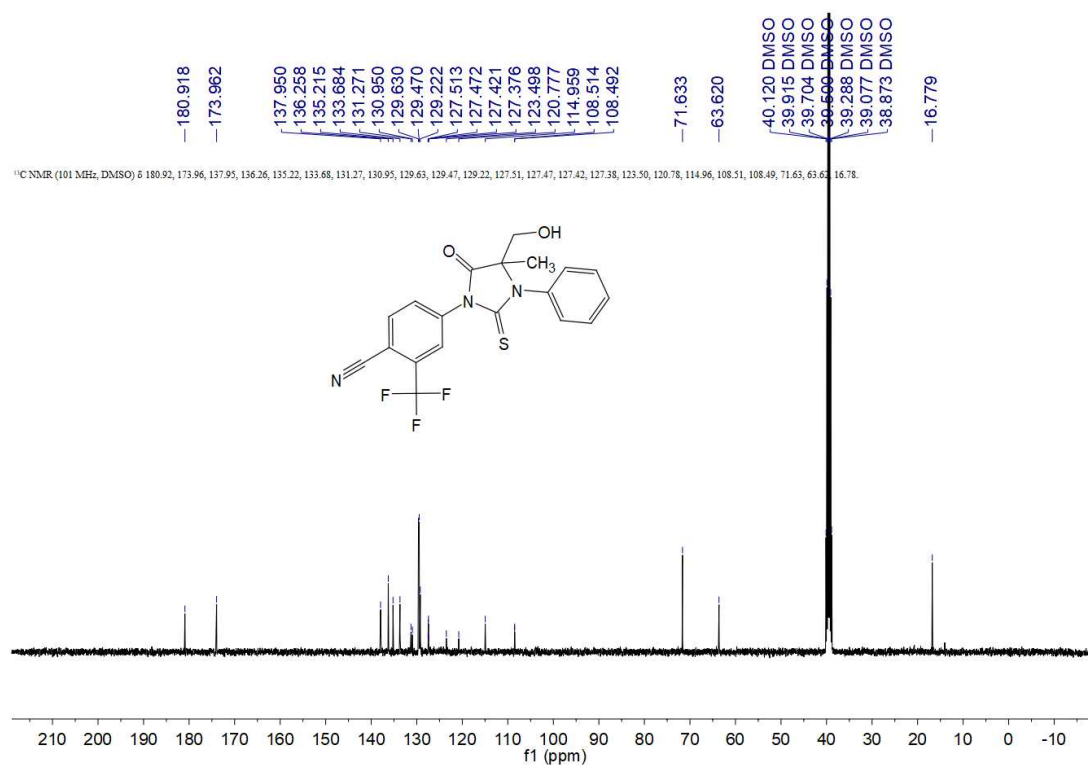
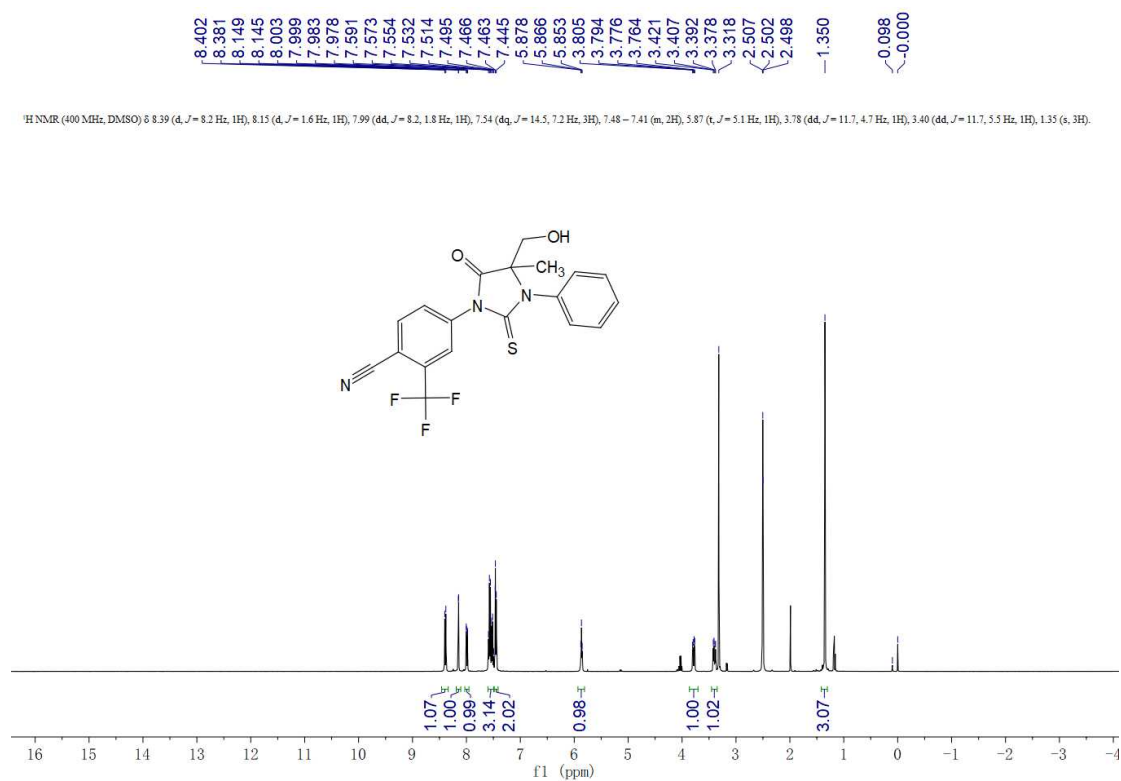








$^1\text{H}$   $^{13}\text{C}$ , NMR and HRMS spectra of *compound 6a-l*



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

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

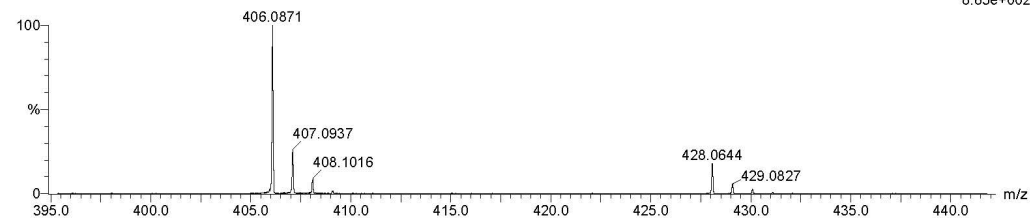
Elements Used:

C: 19-19 H: 14-15 N: 3-3 O: 2-2 F: 3-3 Na: 0-1 S: 1-1

JJY-A00193-062 28 (0.571)

1: TOF MS ES+

8.65e+002



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

406.0871

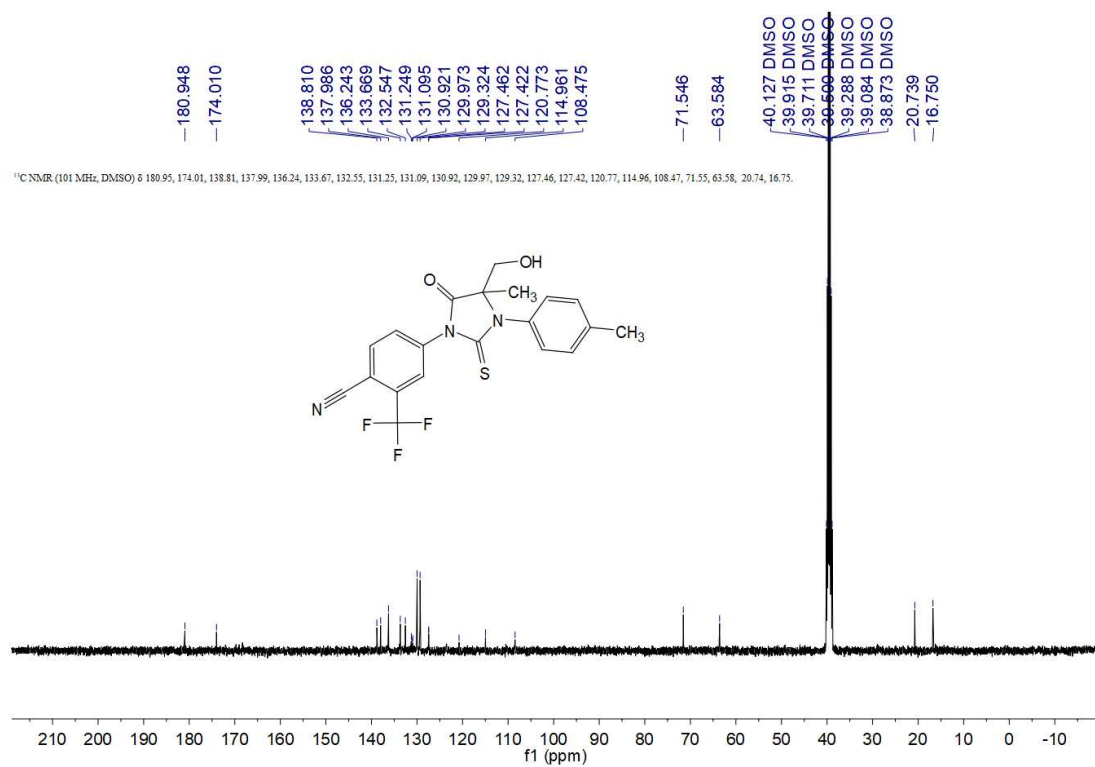
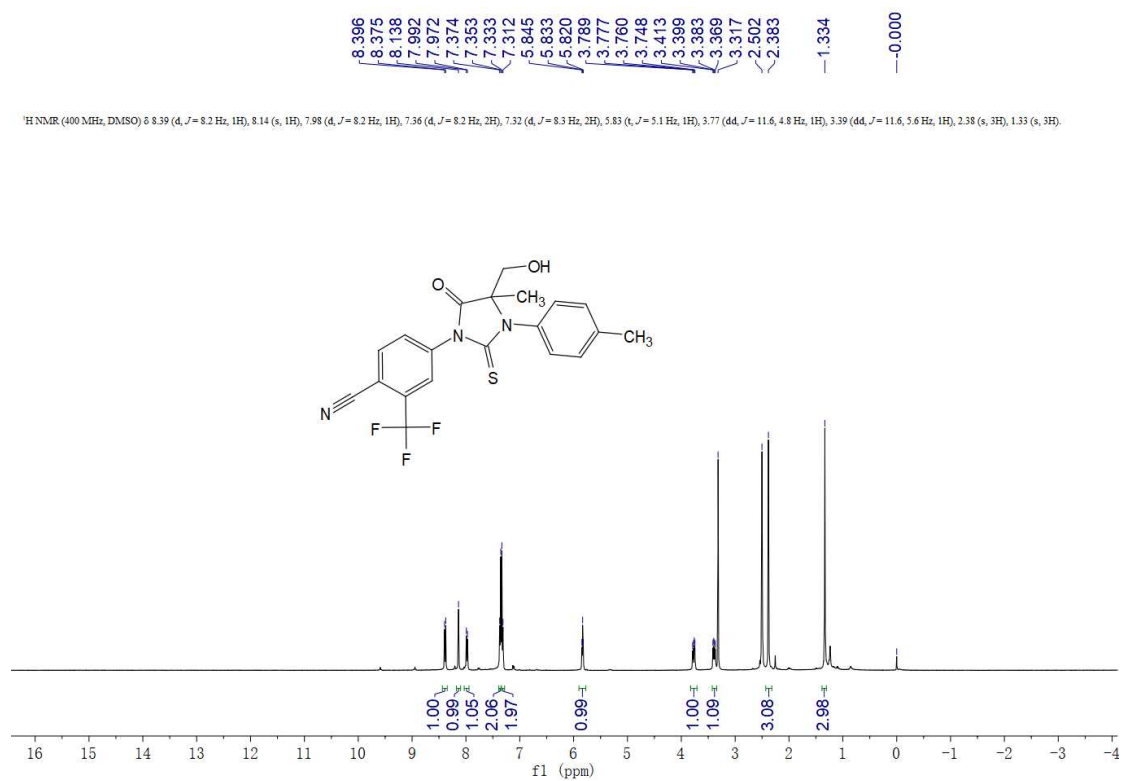
406.0837

3.4

8.4

12.5

C19 H15 N3 O2 F3 S



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

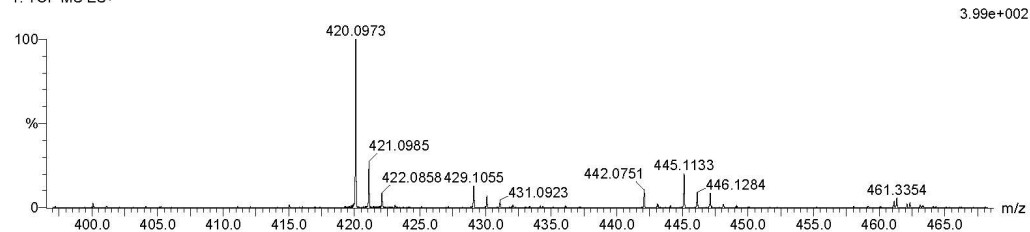
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-20 H: 17-17 N: 3-3 O: 2-2 F: 3-3 S: 1-1

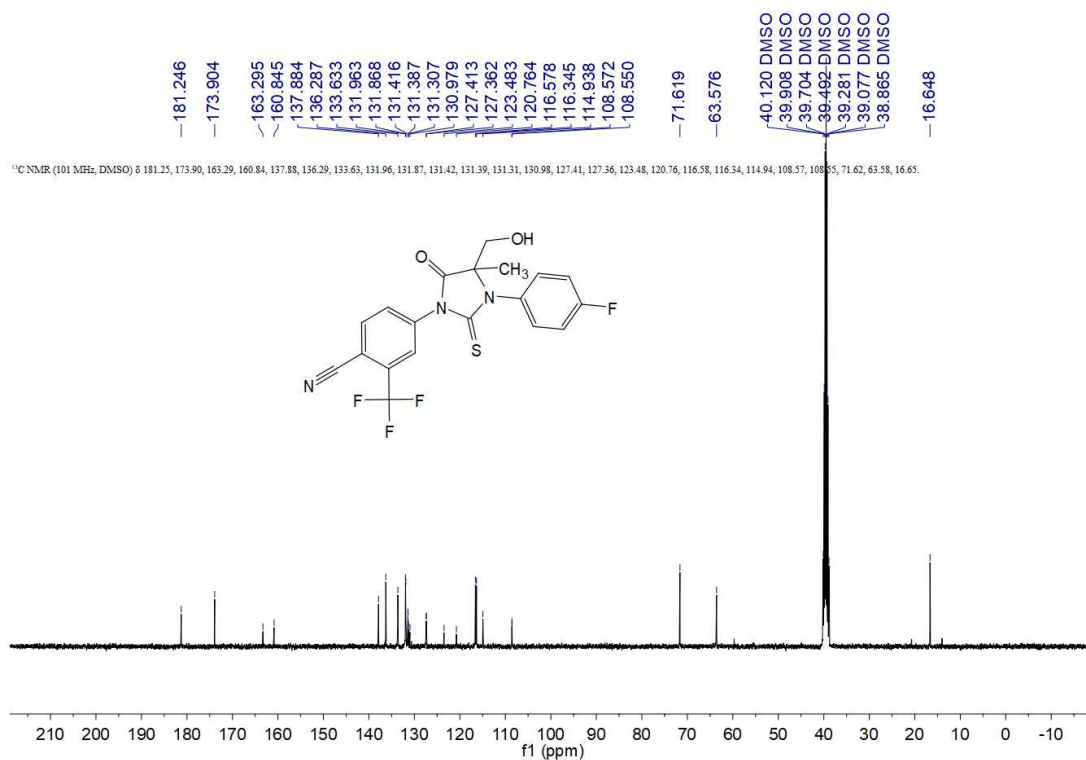
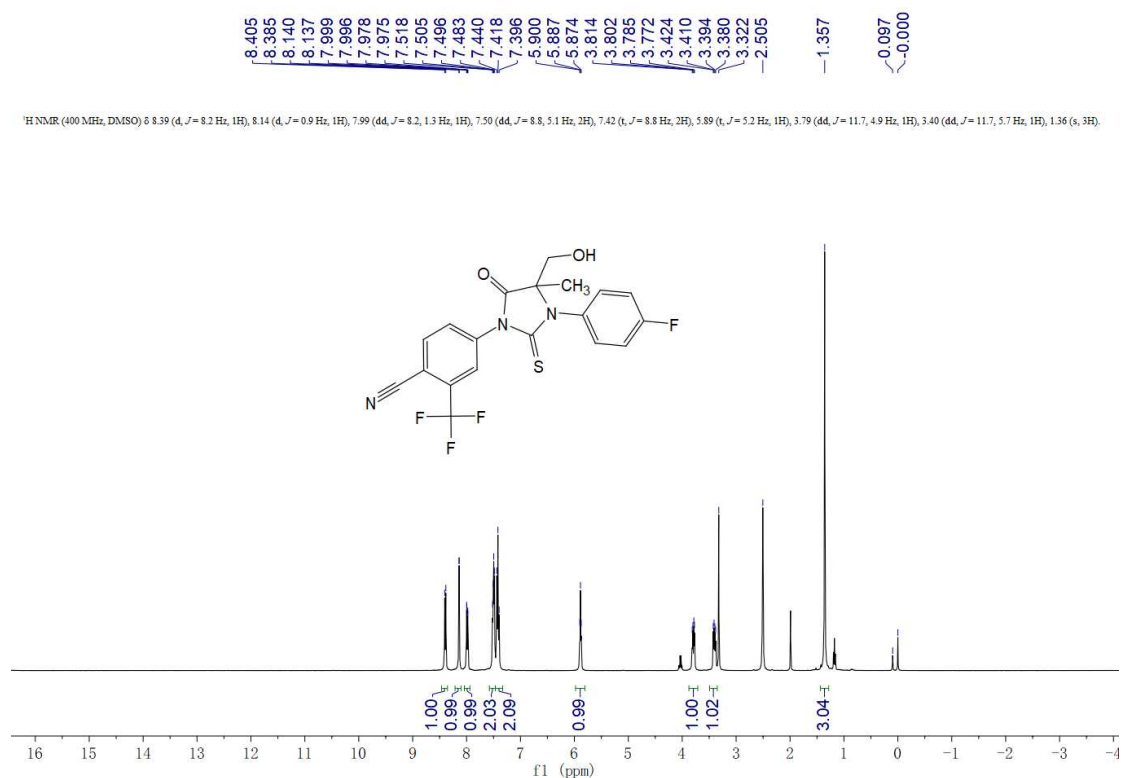
JJY-A00193-014 27 (0.554)

1: TOF MS ES+



Minimum: -1.5  
Maximum: 5.0 500.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
420.0973	420.0994	-2.1	-5.0	12.5	C20 H17 N3 O2 F3 S





## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

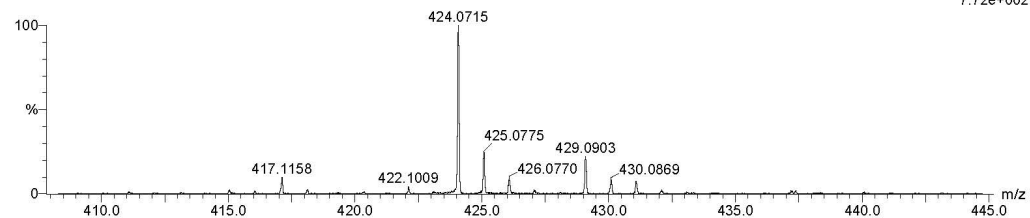
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 14-14 N: 3-3 O: 2-2 F: 4-4 S: 1-1

JJY-A00193-039 25 (0.520) Cm (24:25)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

424.0715

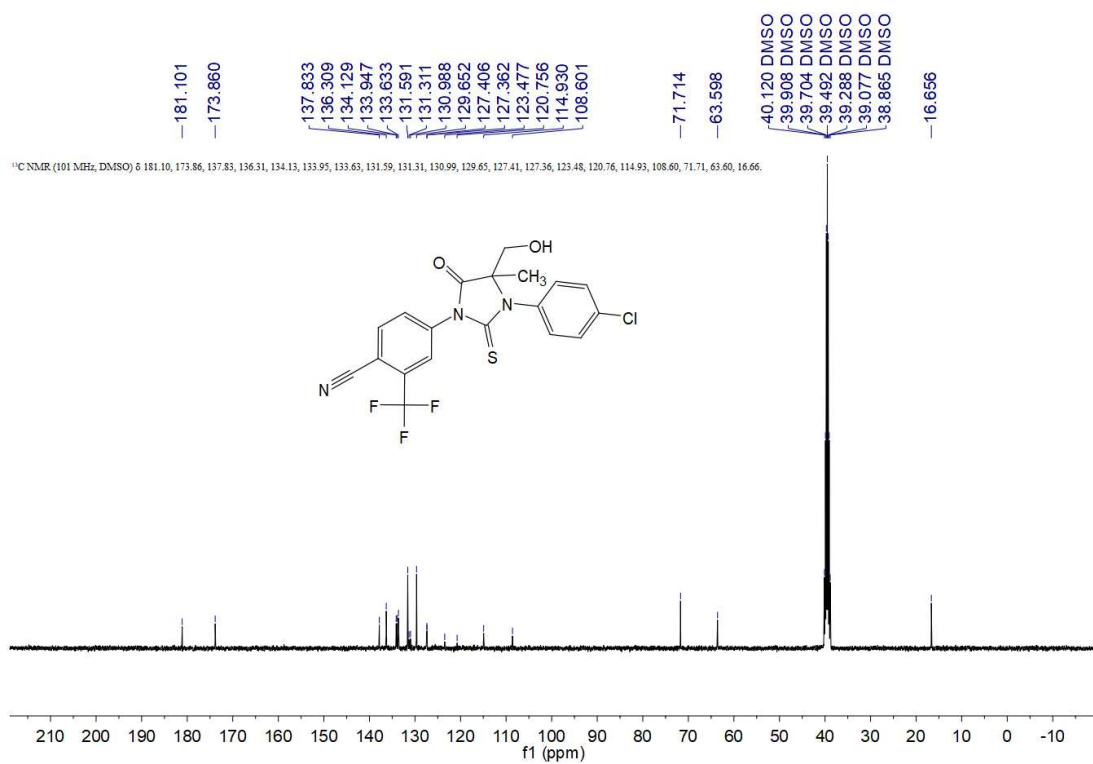
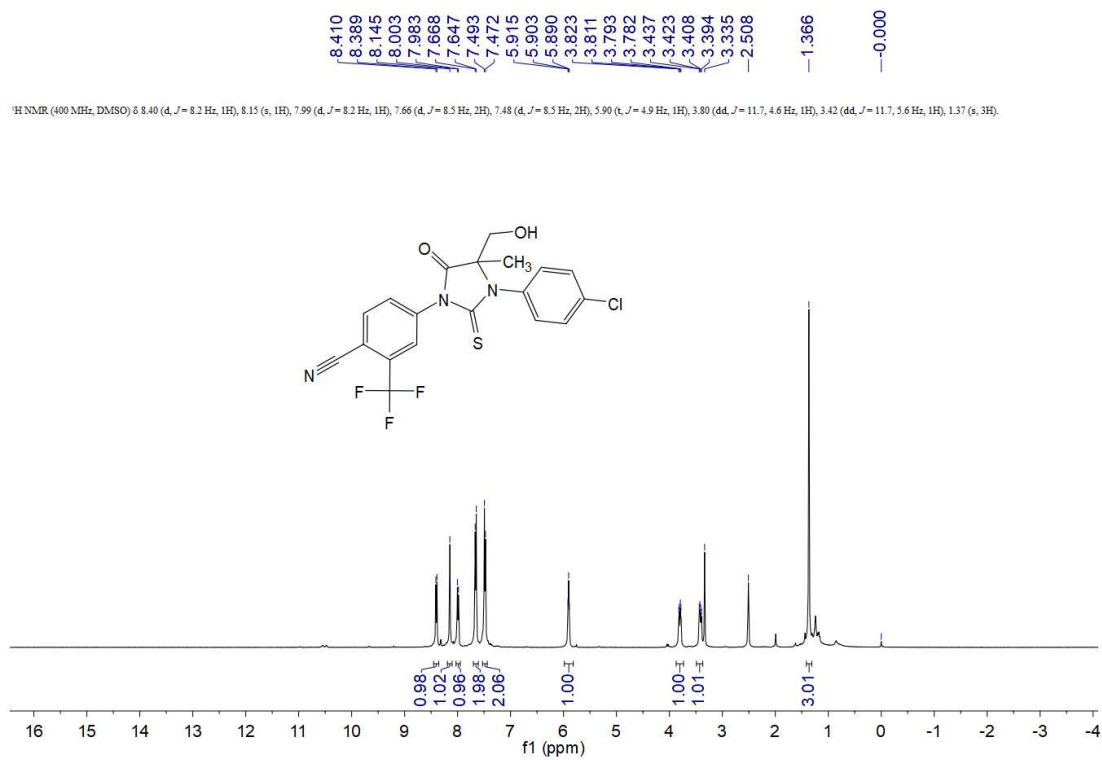
424.0743

-2.8

-6.6

12.5

C19 H14 N3 O2 F4 S



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

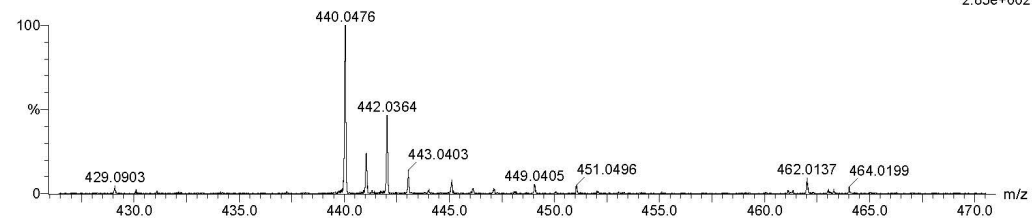
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 14-14 N: 3-3 O: 2-2 F: 3-3 S: 1-1 Cl: 1-1

JJY-A00193-056 30 (0.605)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

440.0476

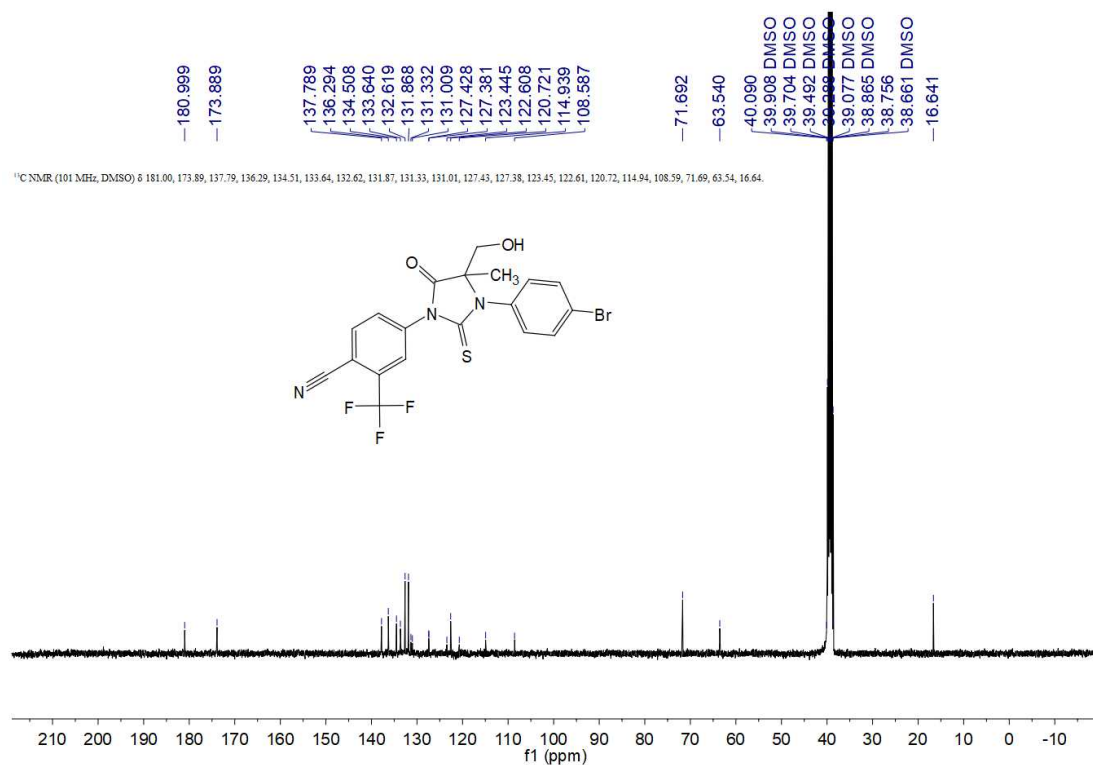
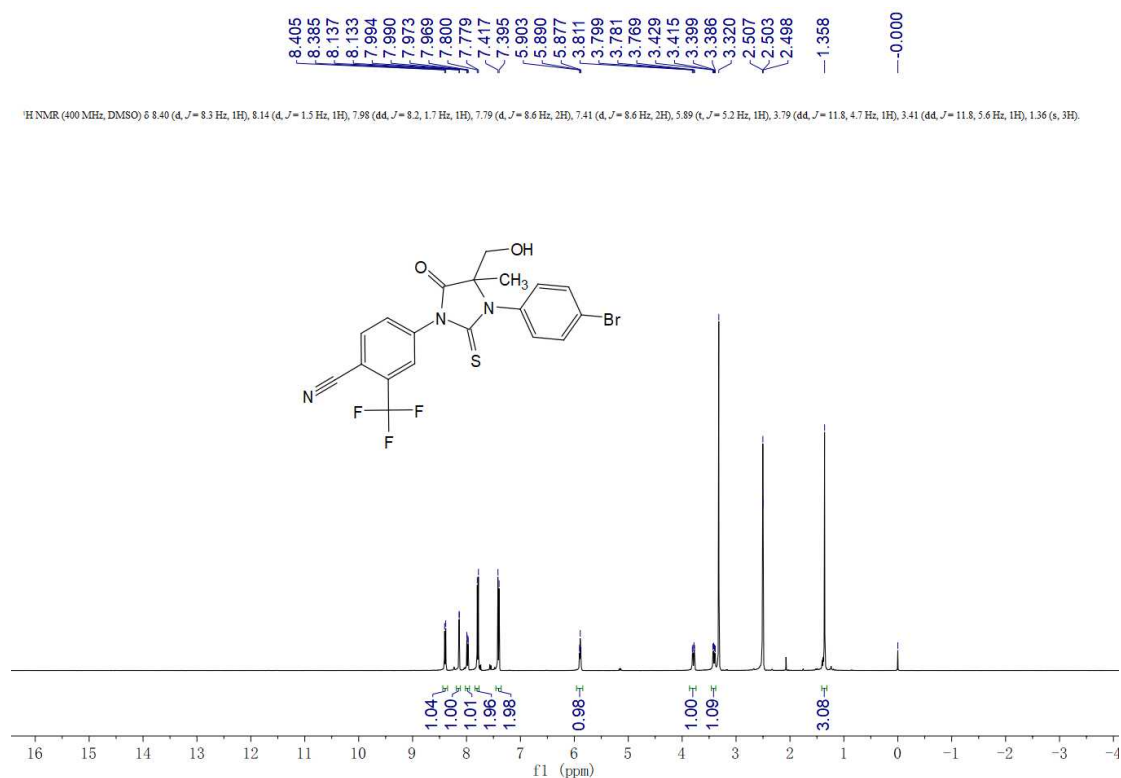
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2.9

6.6

12.5

C19 H14 N3 O2 F3 S Cl



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

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

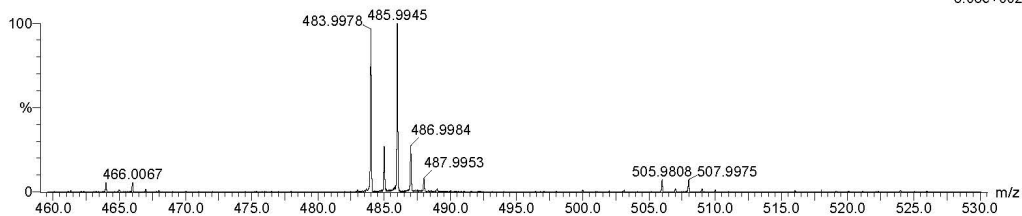
Elements Used:

C: 19-19 H: 14-14 N: 3-3 O: 2-2 F: 3-3 S: 1-1 Br: 1-1

JJY-A00193-060 23 (0.467)

1: TOF MS ES+

6.06e+002



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

483.9978

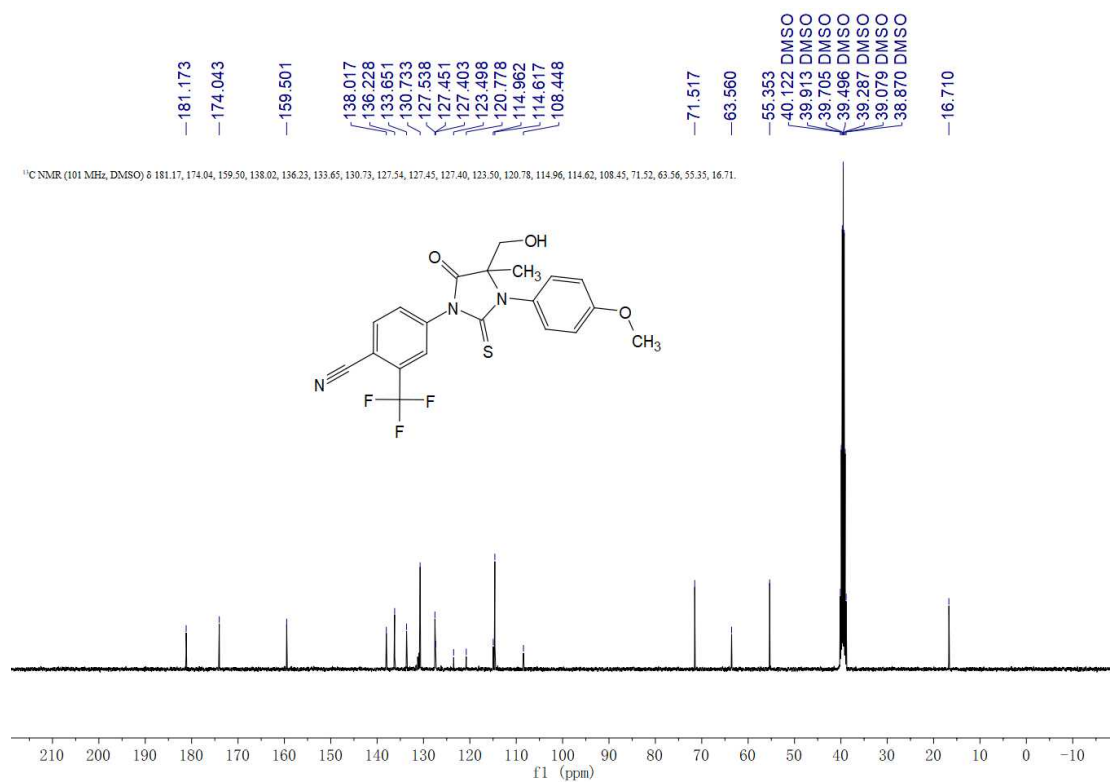
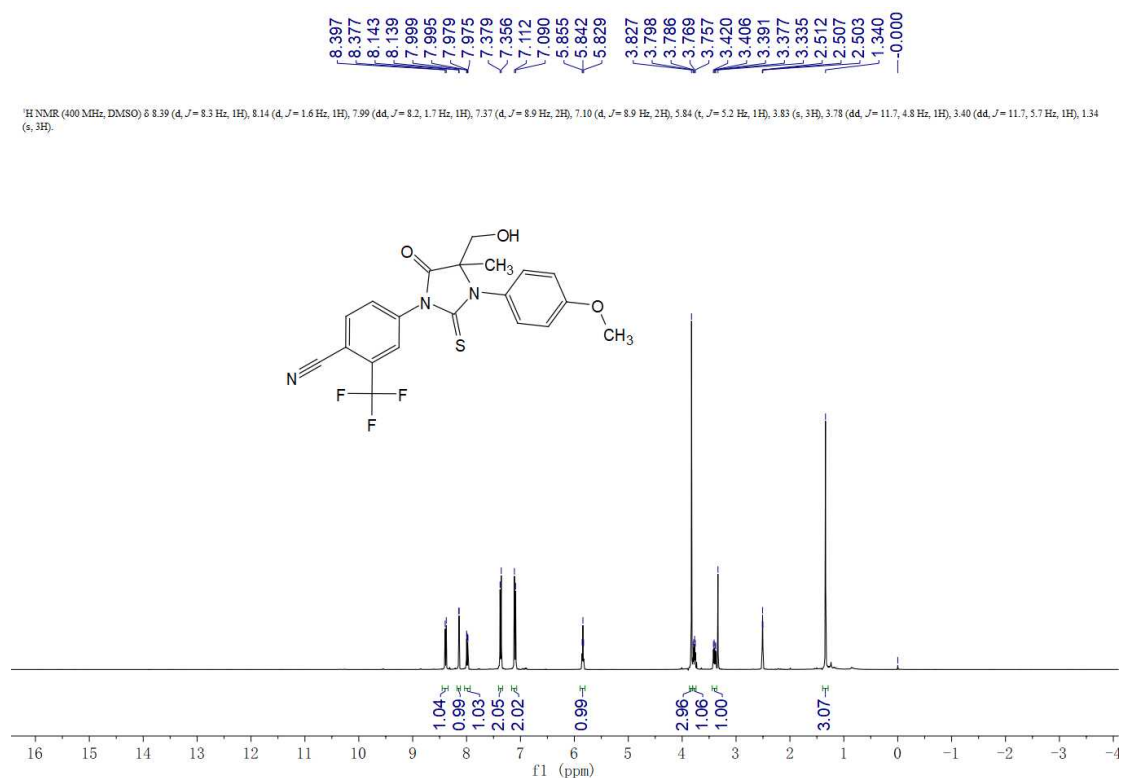
483.9942

3.6

7.4

12.5

C19 H14 N3 O2 F3 S Br



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

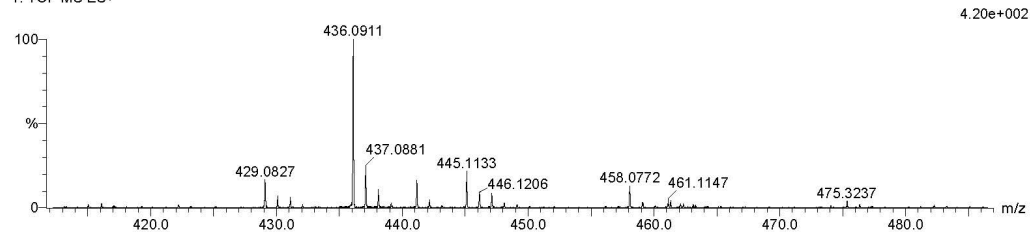
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-20 H: 17-17 N: 3-3 O: 3-3 F: 3-3 S: 1-1

JJY-A00193-043 43 (0.866)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

436.0911

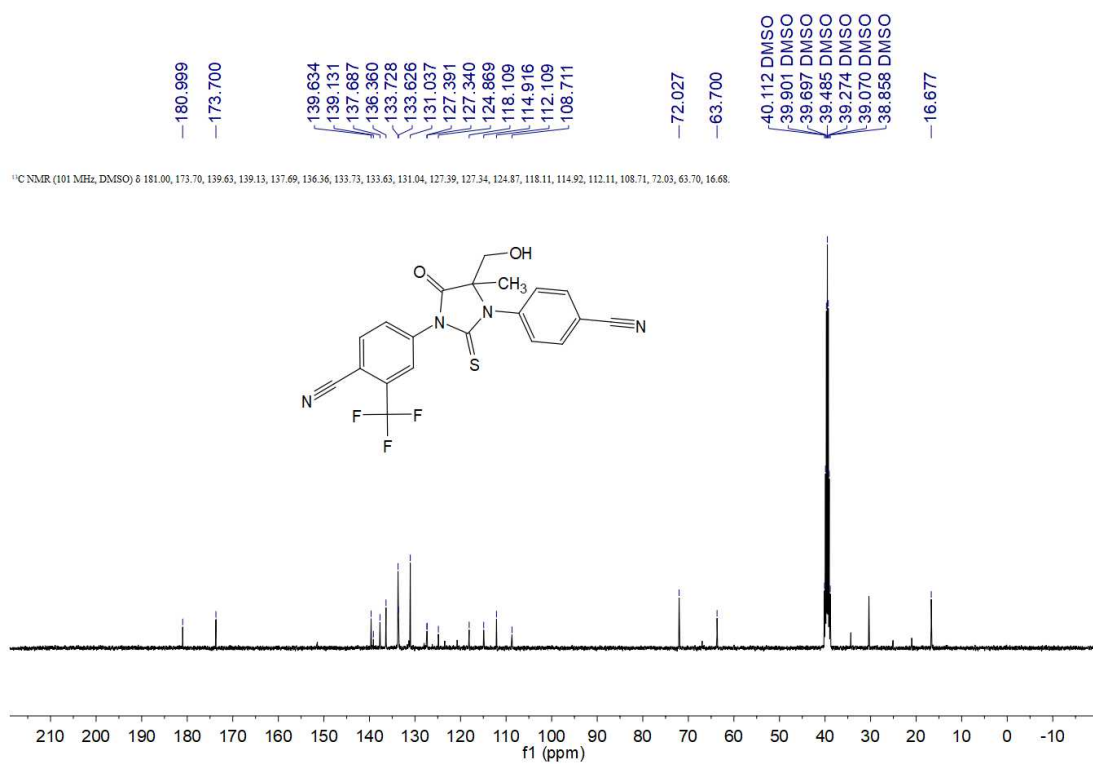
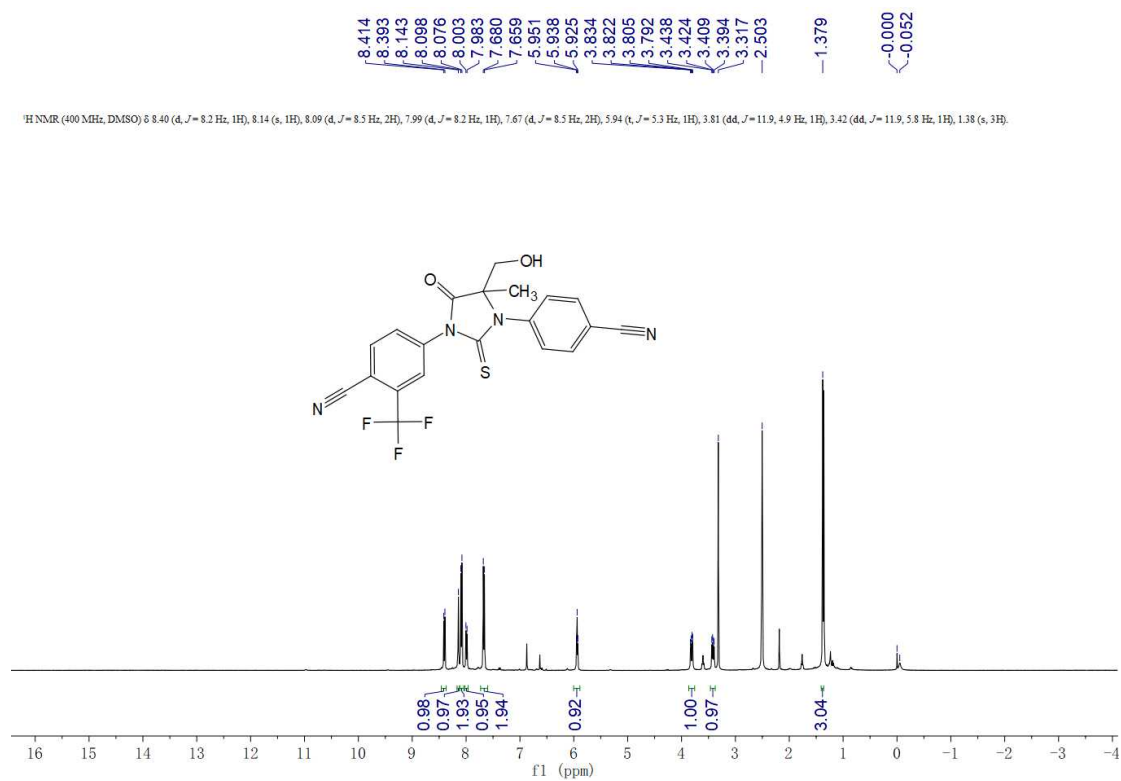
436.0943

-3.2

-7.3

12.5

C20 H17 N3 O3 F3 S





## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

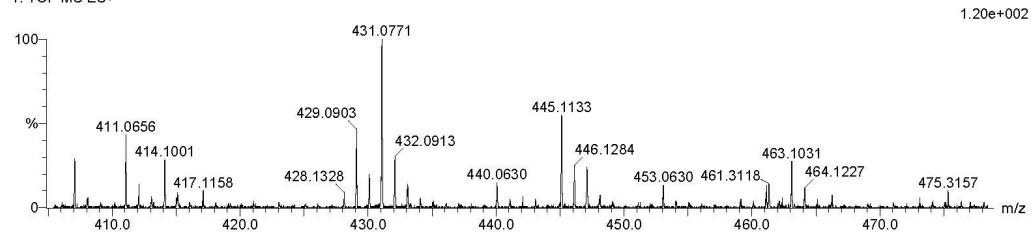
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-20 H: 13-14 N: 4-4 O: 2-2 F: 3-3 Na: 0-1 S: 1-1

JJY-A00193-076 22 (0.450)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

431.0771

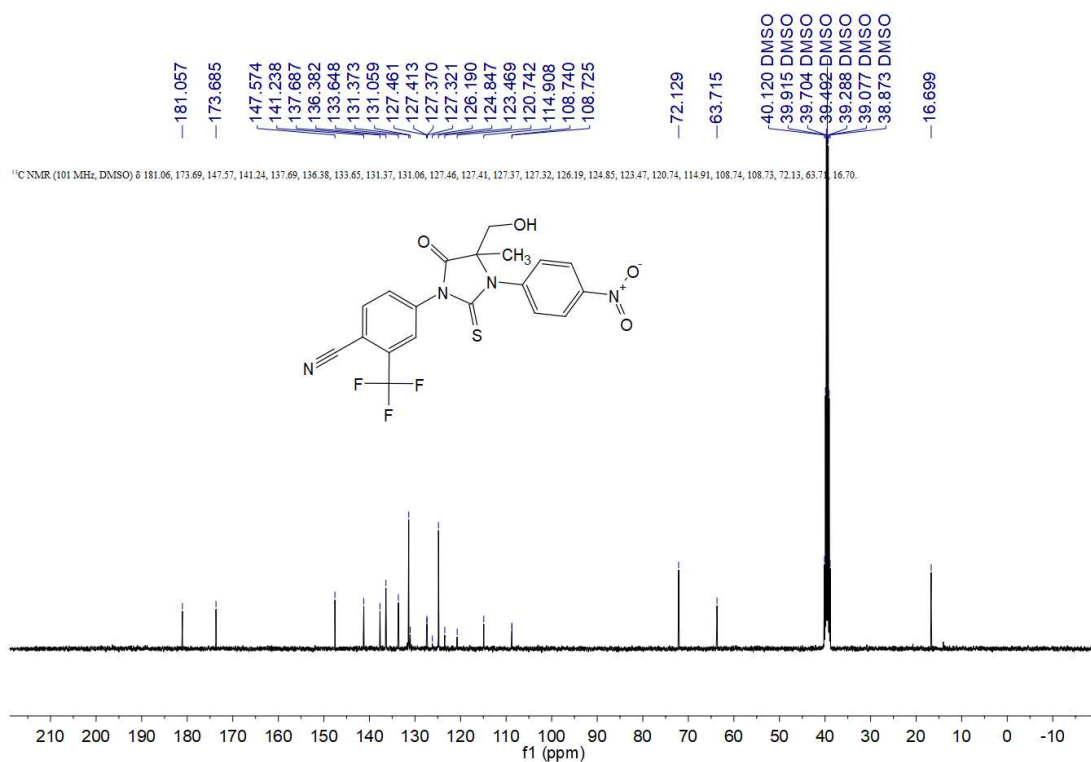
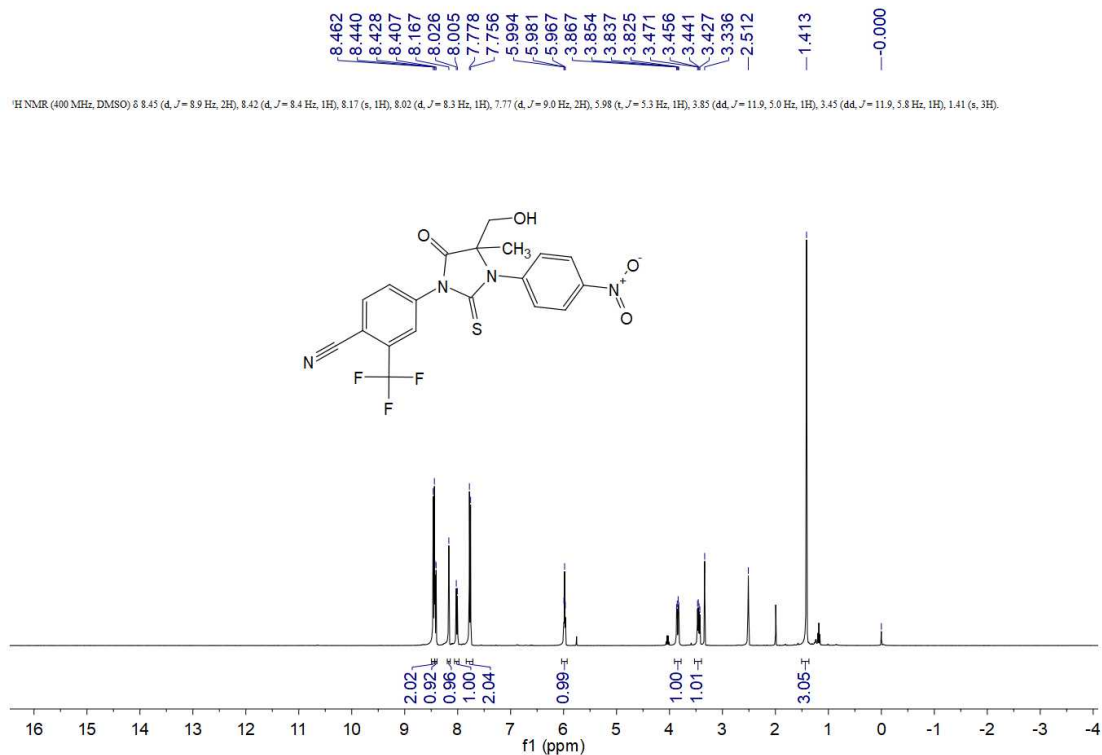
431.0790

-1.9

-4.4

14.5

C20 H14 N4 O2 F3 S



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

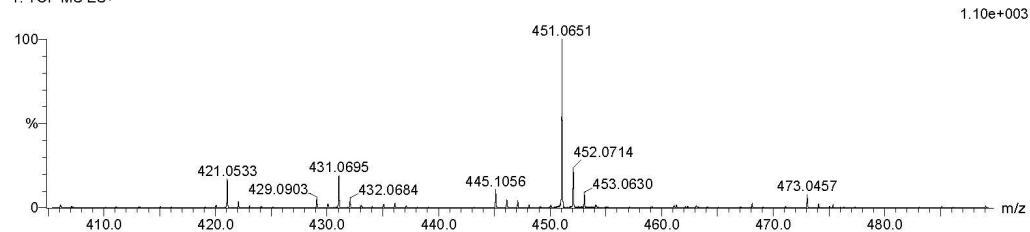
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 14-14 N: 4-4 O: 4-4 F: 3-3 S: 1-1

JJY-A00193-082 20 (0.416) Cm (20:22)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

451.0651

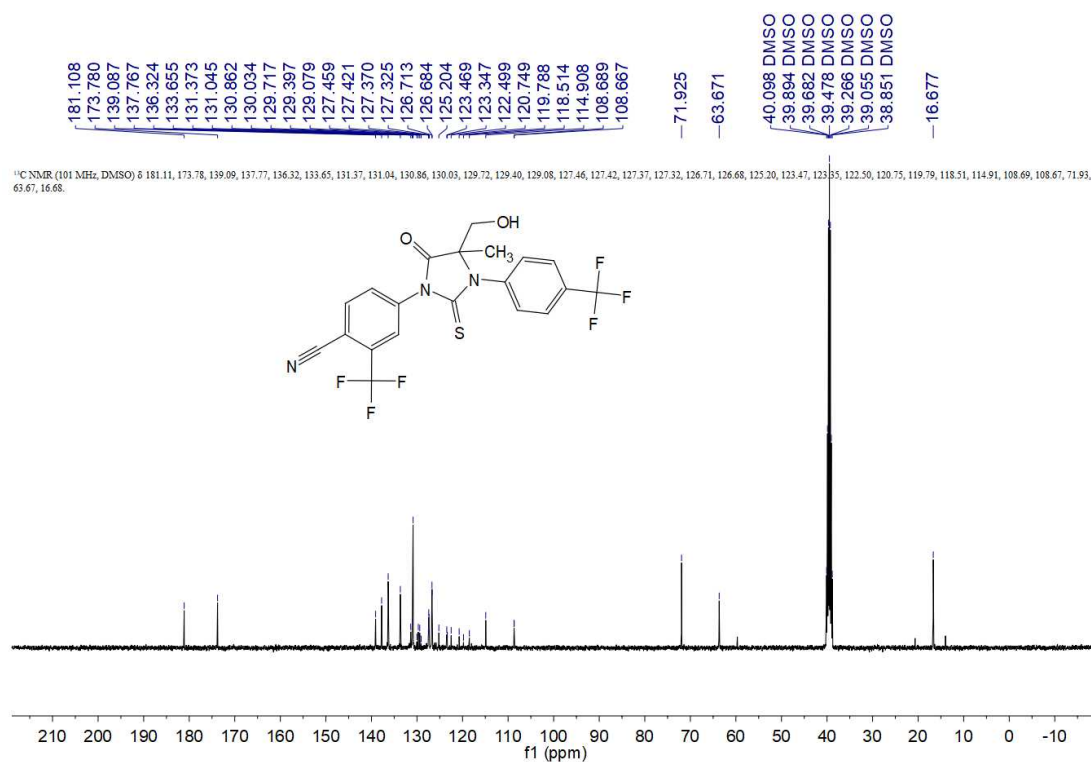
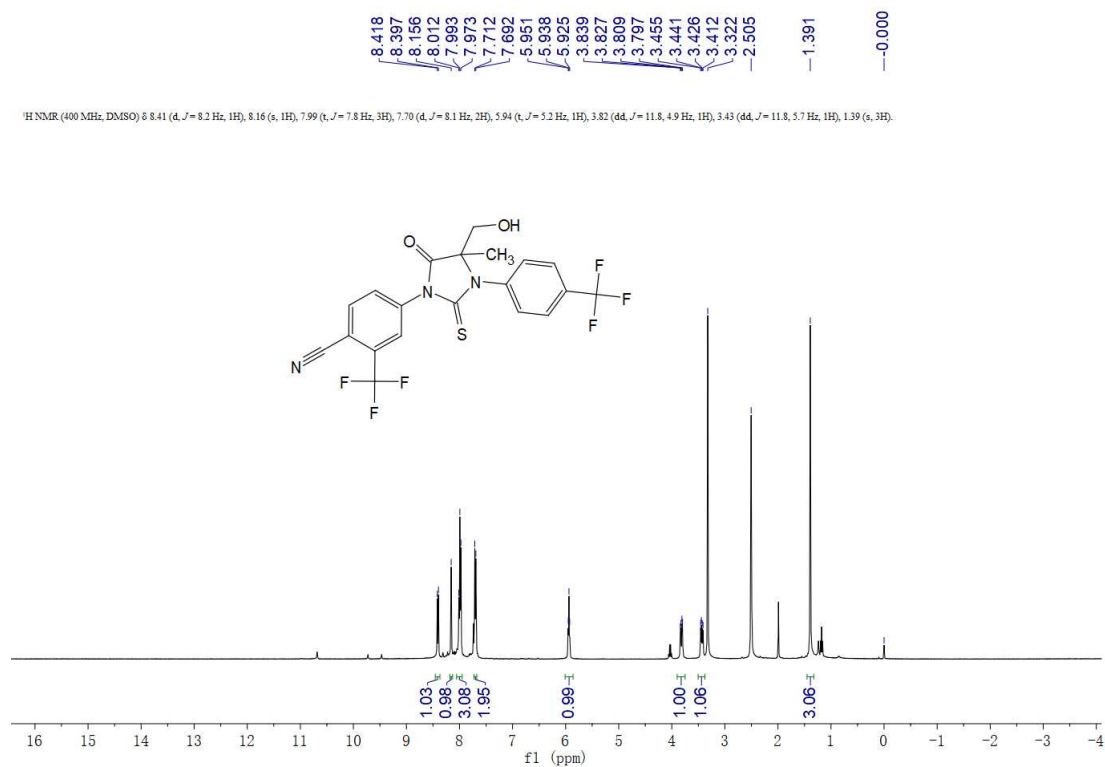
451.0688

-3.7

-8.2

13.5

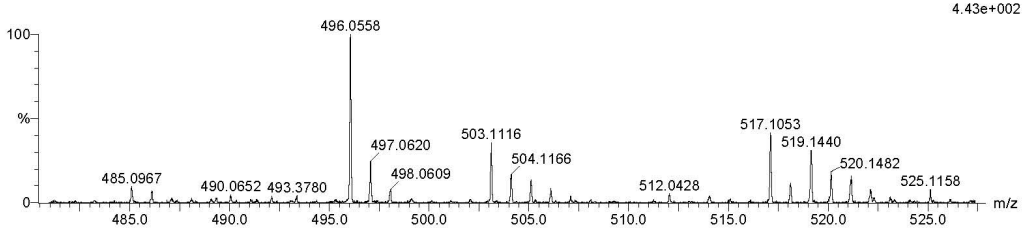
C19 H14 N4 O4 F3 S



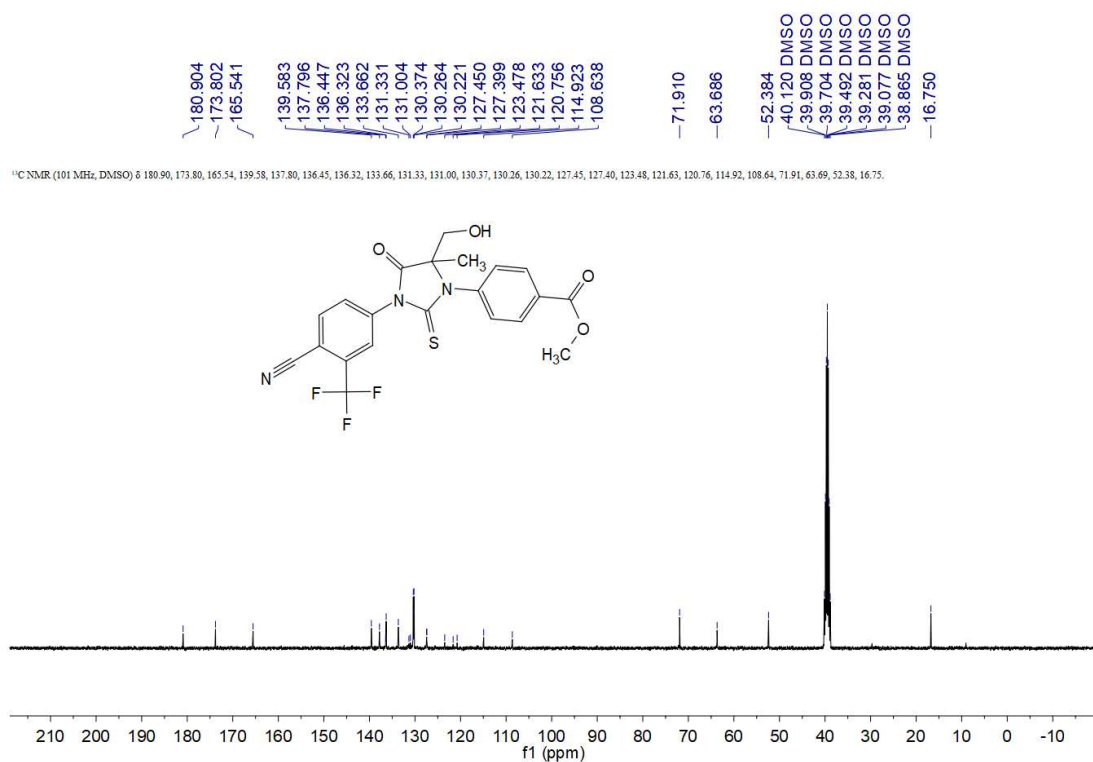
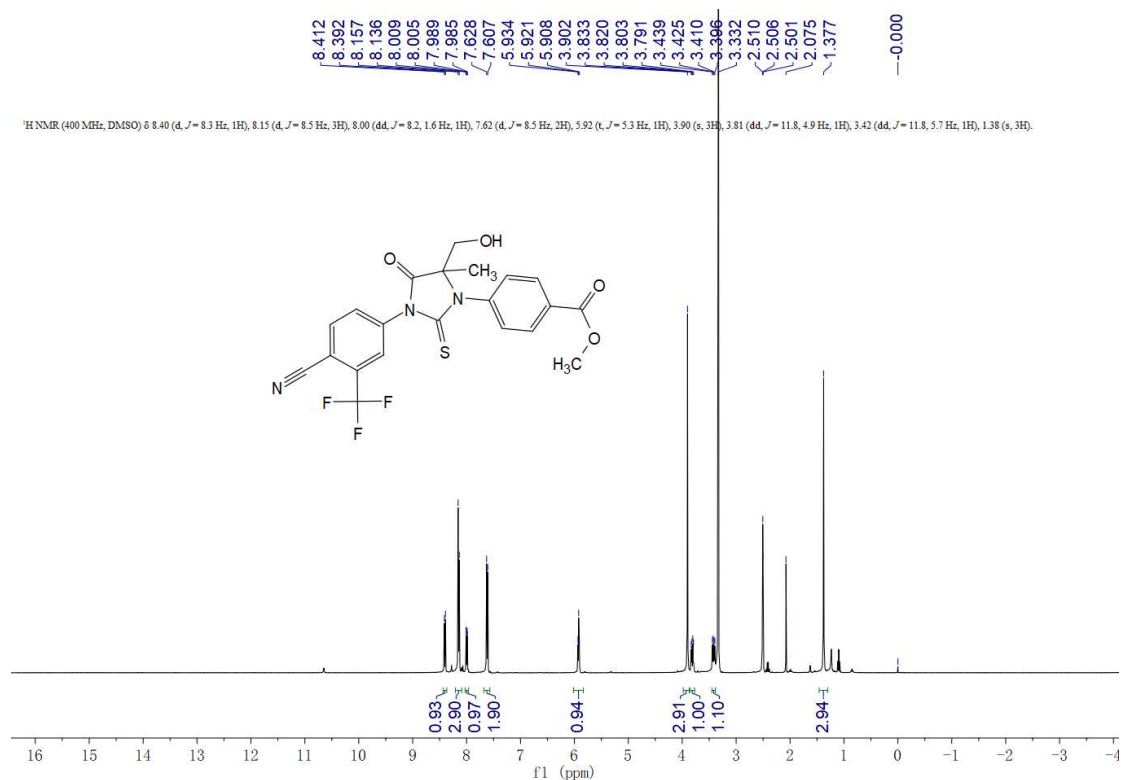
Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0  
Element prediction: Off

Monoisotopic Mass, Even Electron Ions  
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)  
Elements Used:  
C: 20-20 H: 13-14 N: 3-3 O: 2-2 F: 6-6 Na: 0-1 S: 1-1  
JJY-A00193-086 30 (0.605) Cm (25:33)  
1: TOF MS ES+



Minimum:				-1.5	
Maximum:		5.0	500.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
496.0558	496.0530	2.8	5.6	12.5	C20 H13 N3 O2 F6 Na S



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

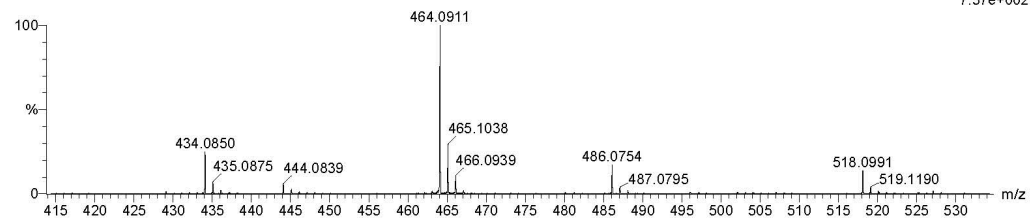
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 21-21 H: 17-17 N: 3-3 O: 4-4 F: 3-3 S: 1-1

JJY-A00193-080 24 (0.484)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

464.0911

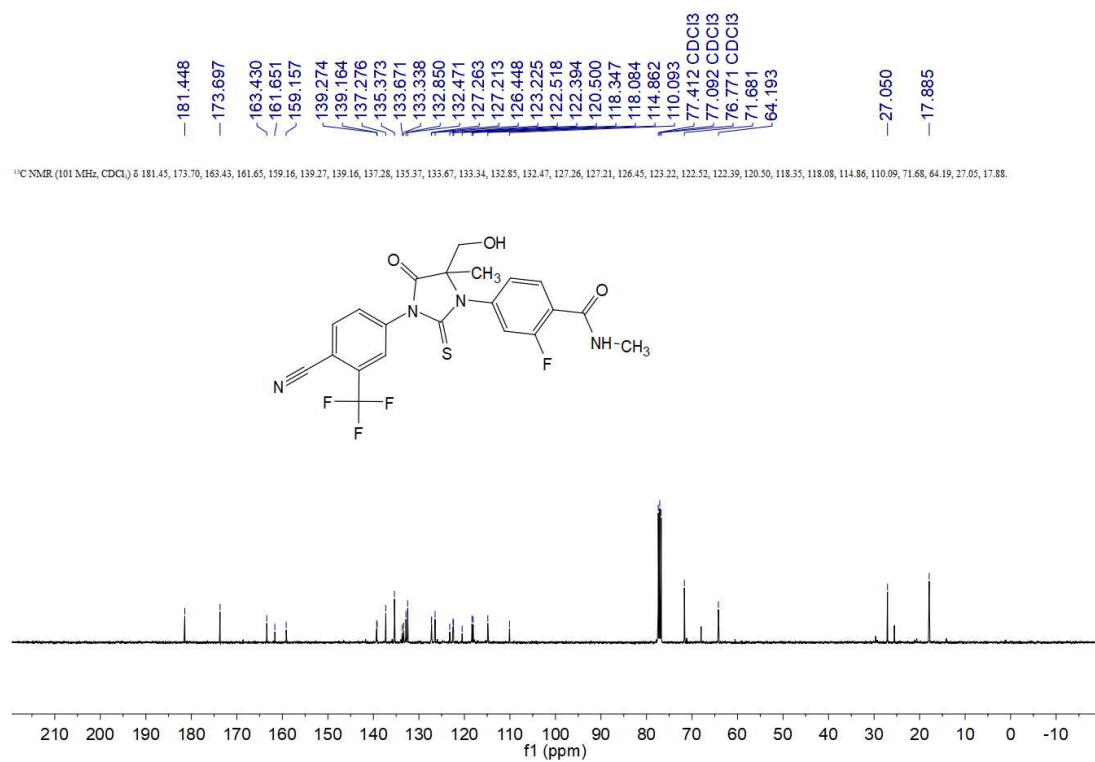
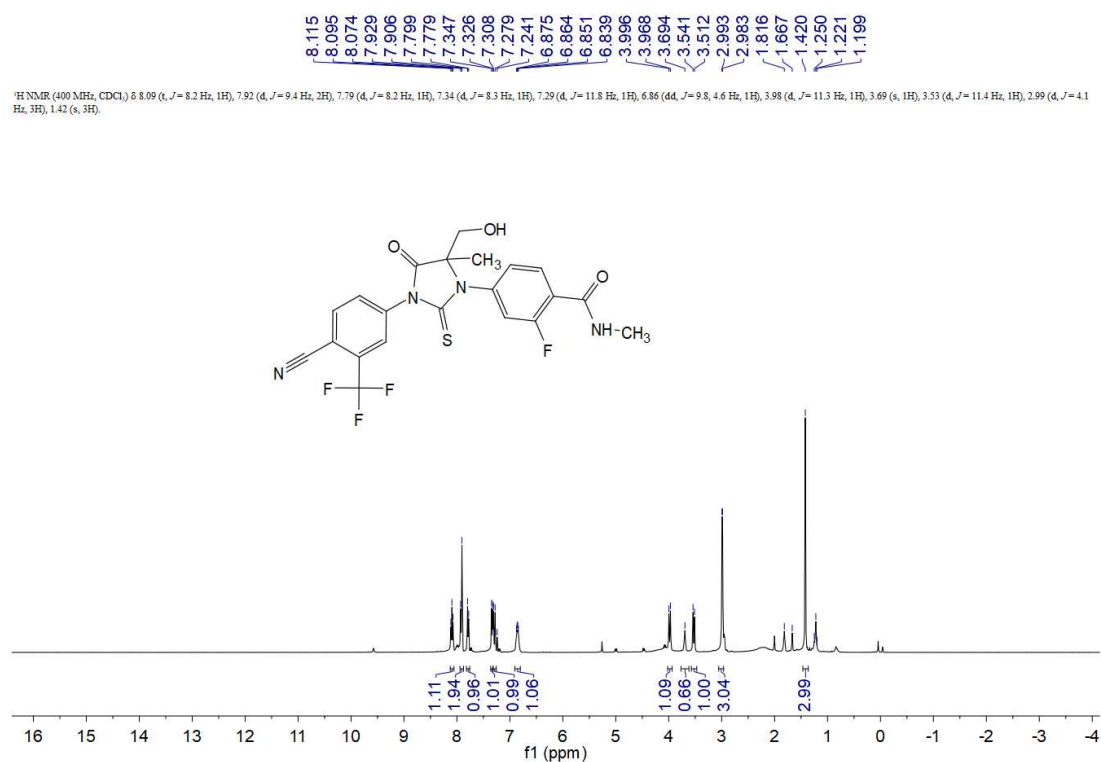
464.0892

1.9

4.1

13.5

C21 H17 N3 O4 F3 S





## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

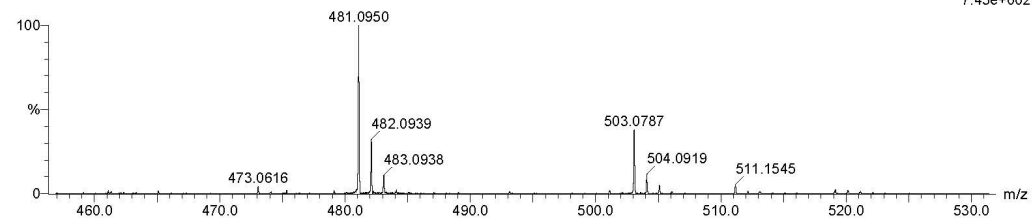
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 21-21 H: 17-17 N: 4-4 O: 3-3 F: 4-4 S: 1-1

JJY-A00222-065 29 (0.588)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

481.0950

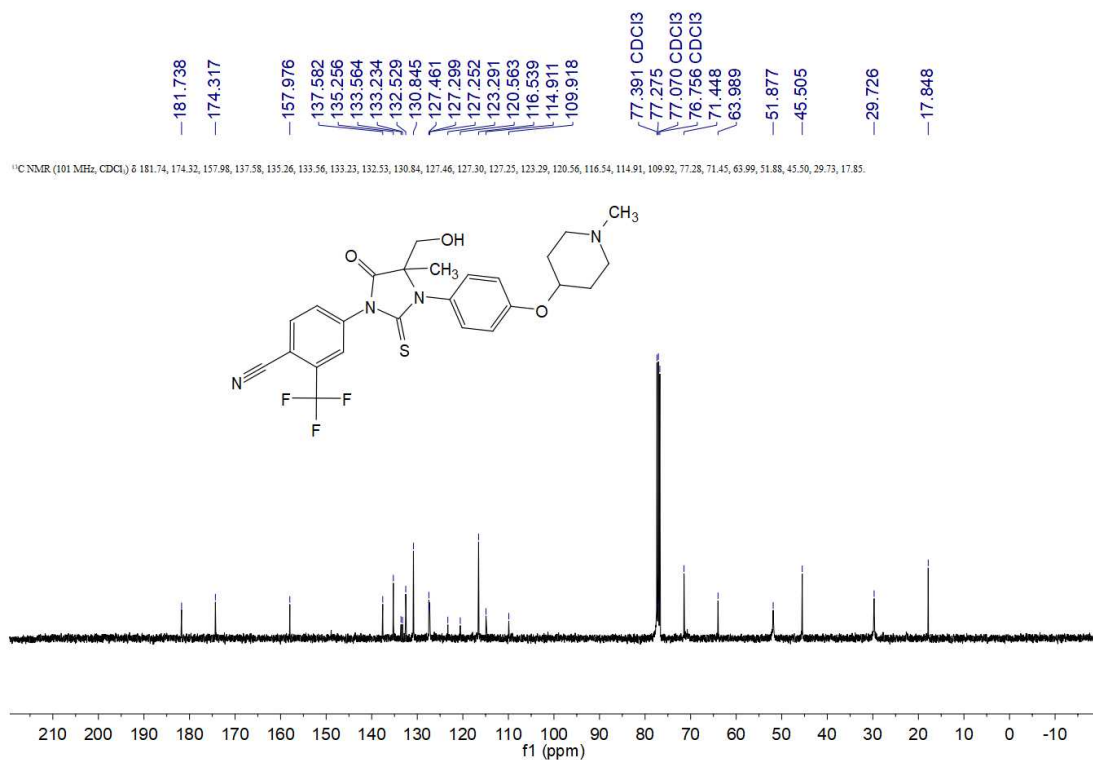
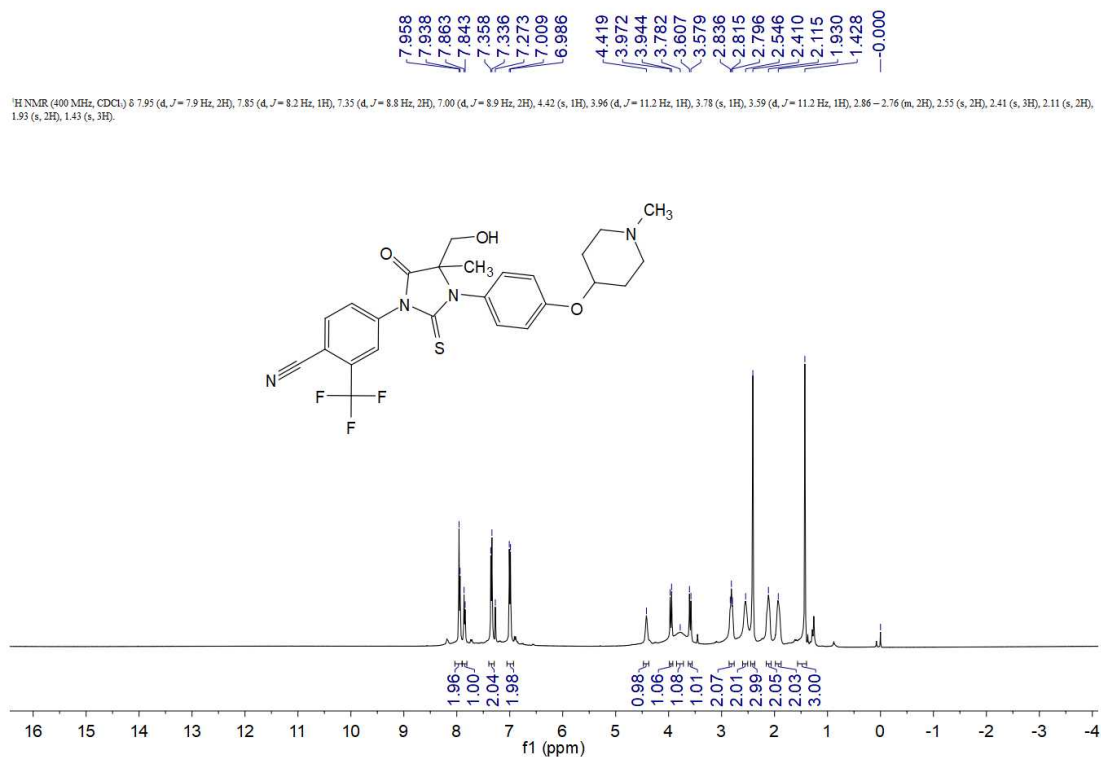
481.0958

-0.8

-1.7

13.5

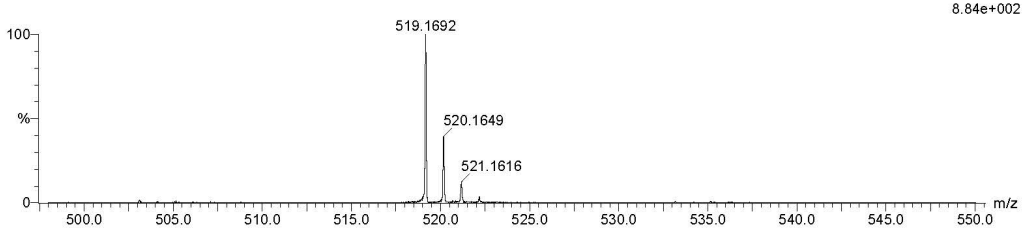
C21 H17 N4 O3 F4 S



Single Mass Analysis

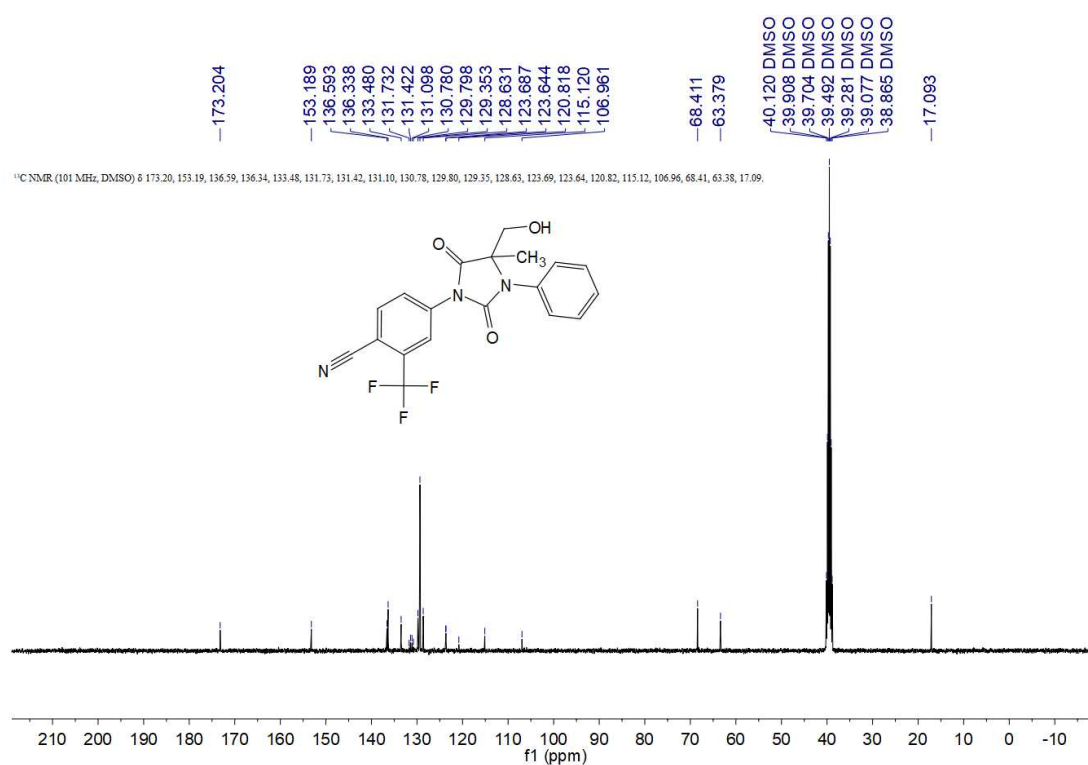
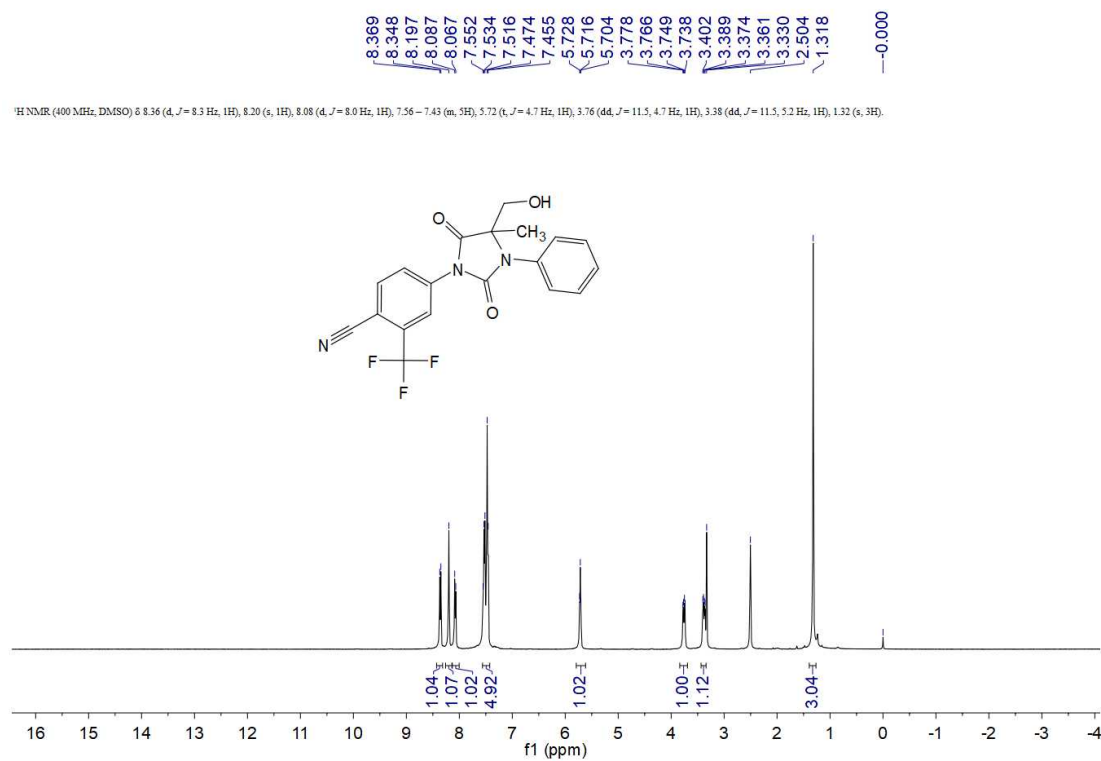
Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0  
Element prediction: Off

Monoisotopic Mass, Even Electron Ions  
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)  
Elements Used:  
C: 25-25 H: 26-26 N: 4-4 O: 3-3 F: 3-3 S: 1-1  
JJY-A00222-066 44 (0.883)  
1: TOF MS ES+



Minimum:				-1.5	
Maximum:	5.0	500.0		50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
519.1692	519.1678	1.4	2.7	13.5	C25 H26 N4 O3 F3 S

$^1\text{H}$ ,  $^{13}\text{C}$ , NMR and HRMS spectra of *compound 7a-j*



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

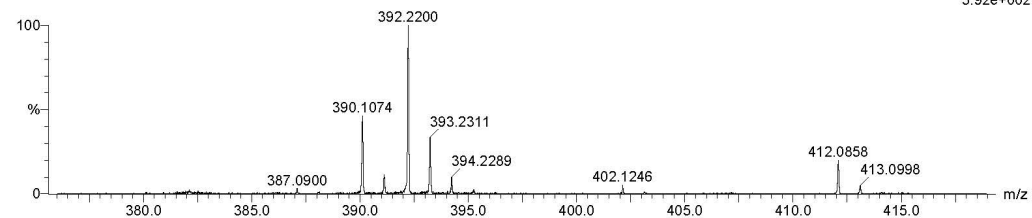
2 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 14-15 N: 3-3 O: 3-3 F: 3-3 Na: 0-1

JJY-A00193-061 26 (0.537)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

390.1074

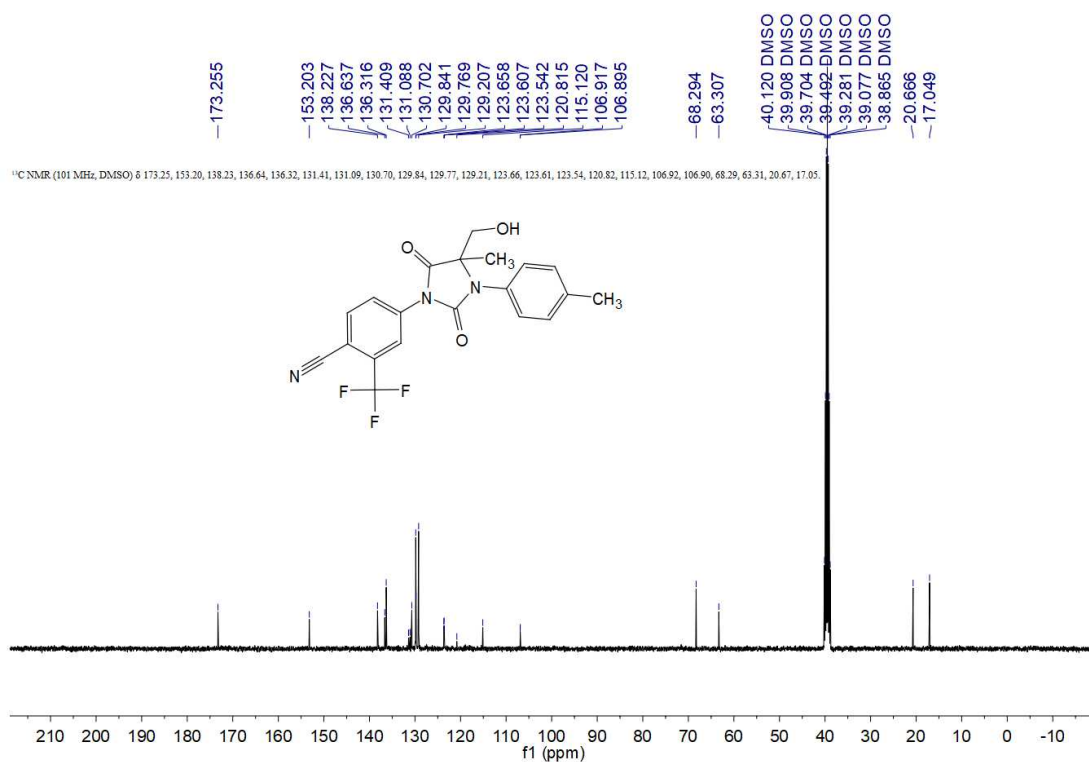
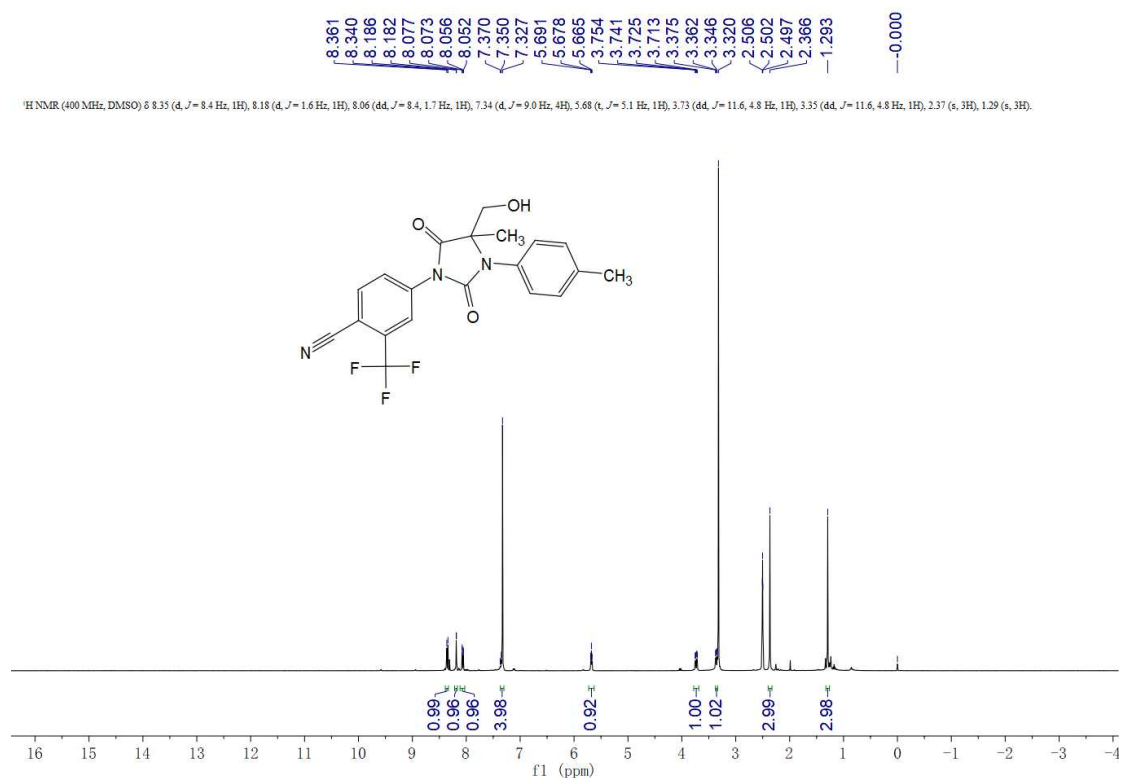
390.1066

0.8

2.1

12.5

C19 H15 N3 O3 F3



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

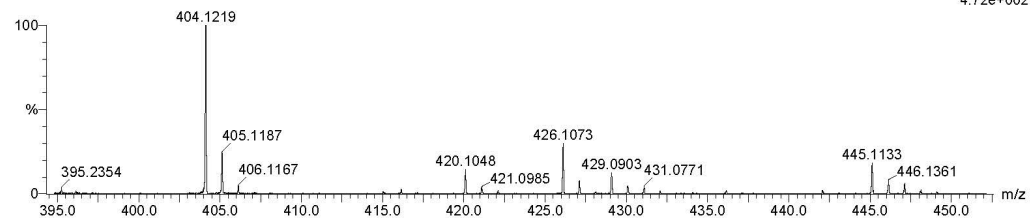
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-20 H: 17-17 N: 3-3 O: 3-3 F: 3-3

JJY-A00193-013 26 (0.537)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

404.1219

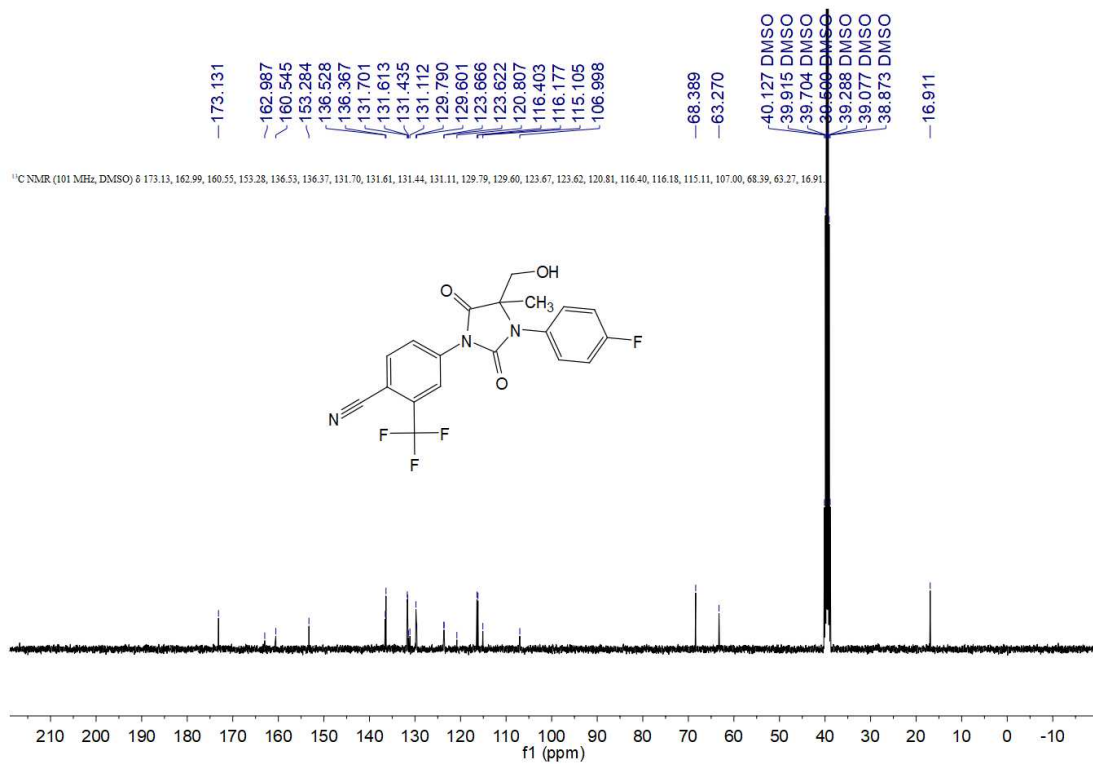
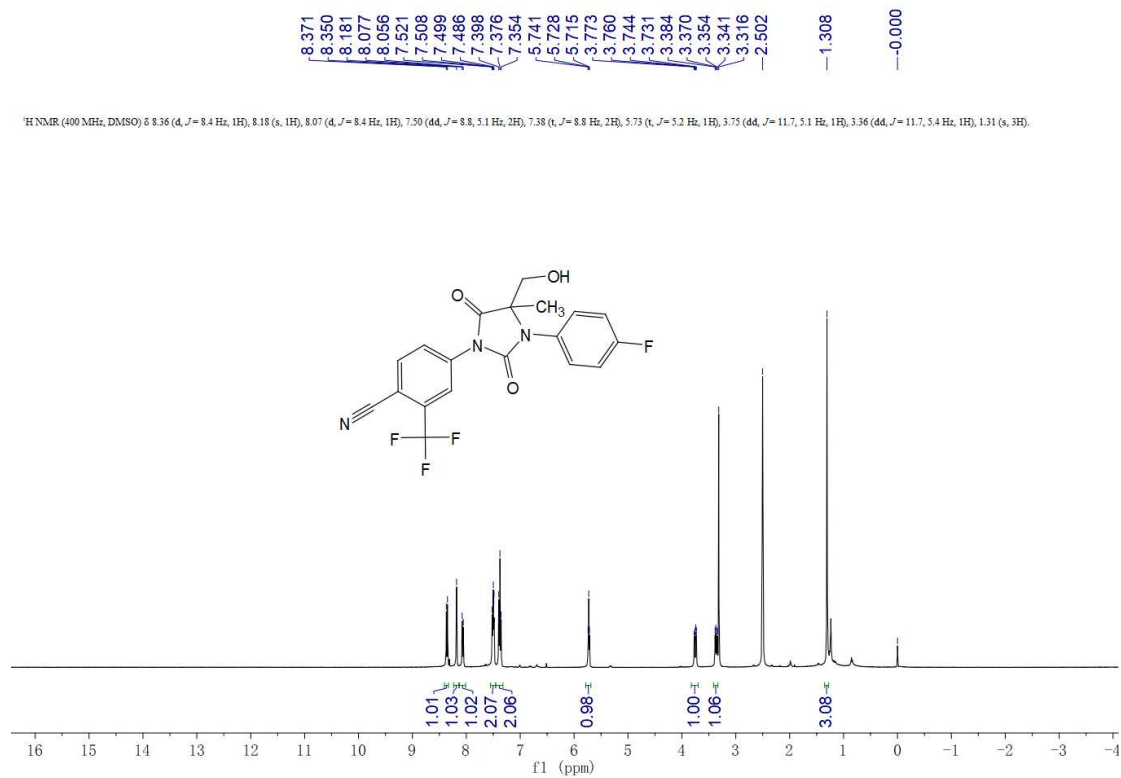
404.1222

-0.3

-0.7

12.5

C20 H17 N3 O3 F3





## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

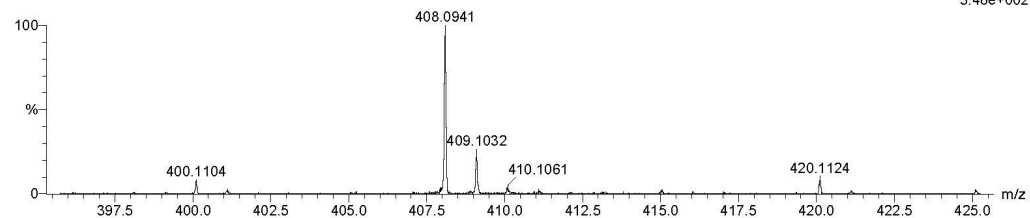
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 14-14 N: 3-3 O: 3-3 F: 4-4

JJY-A00193-038 26 (0.537)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

408.0941

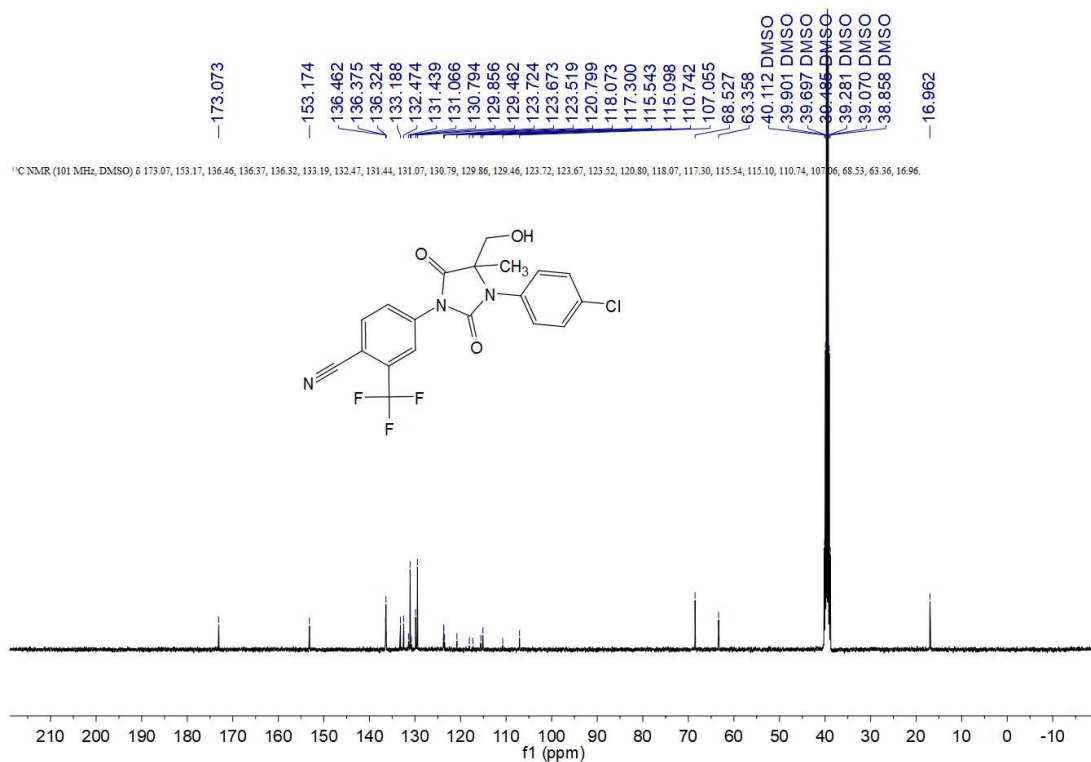
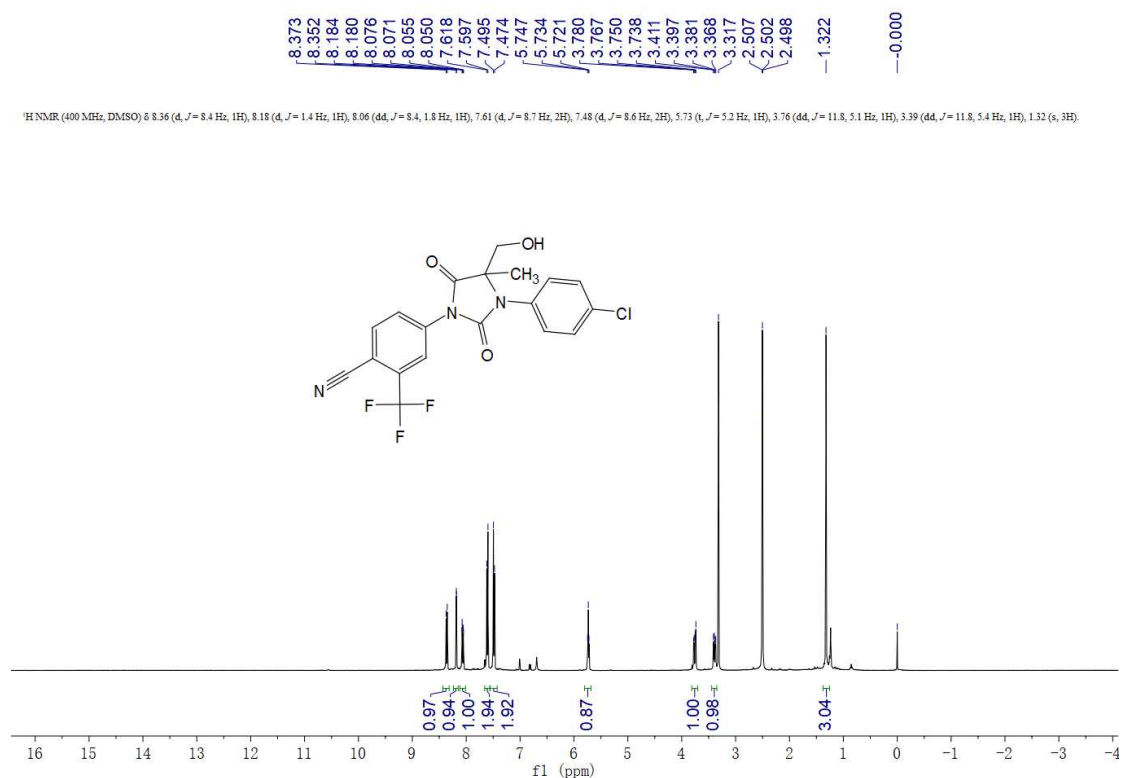
408.0971

-3.0

-7.4

12.5

C19 H14 N3 O3 F4



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

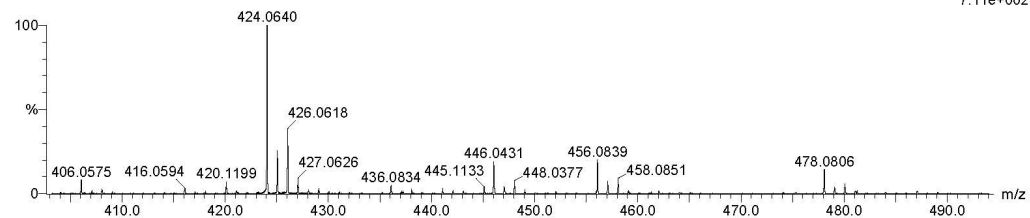
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 14-14 N: 3-3 O: 3-3 F: 3-3 Cl: 1-1

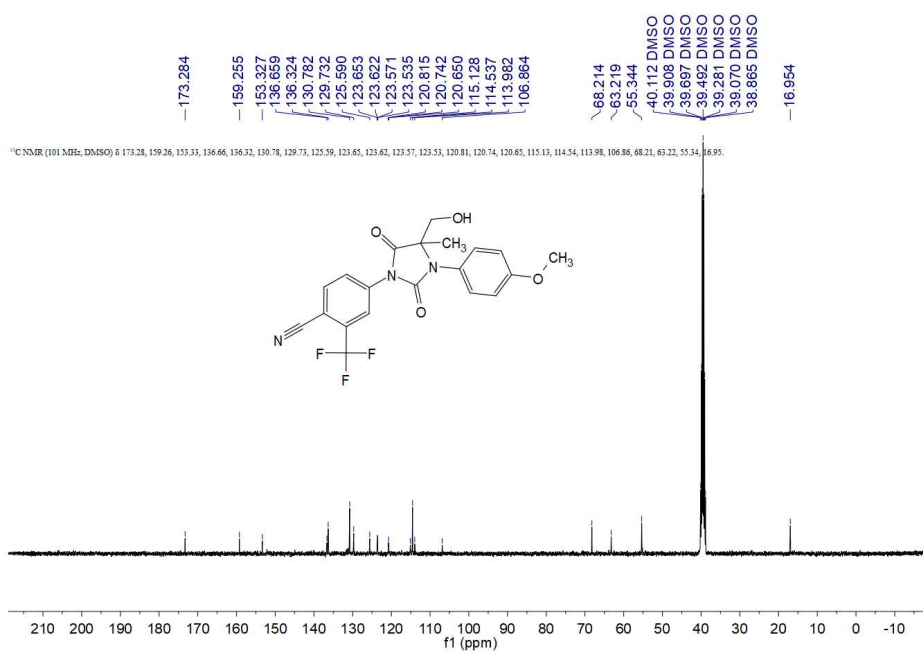
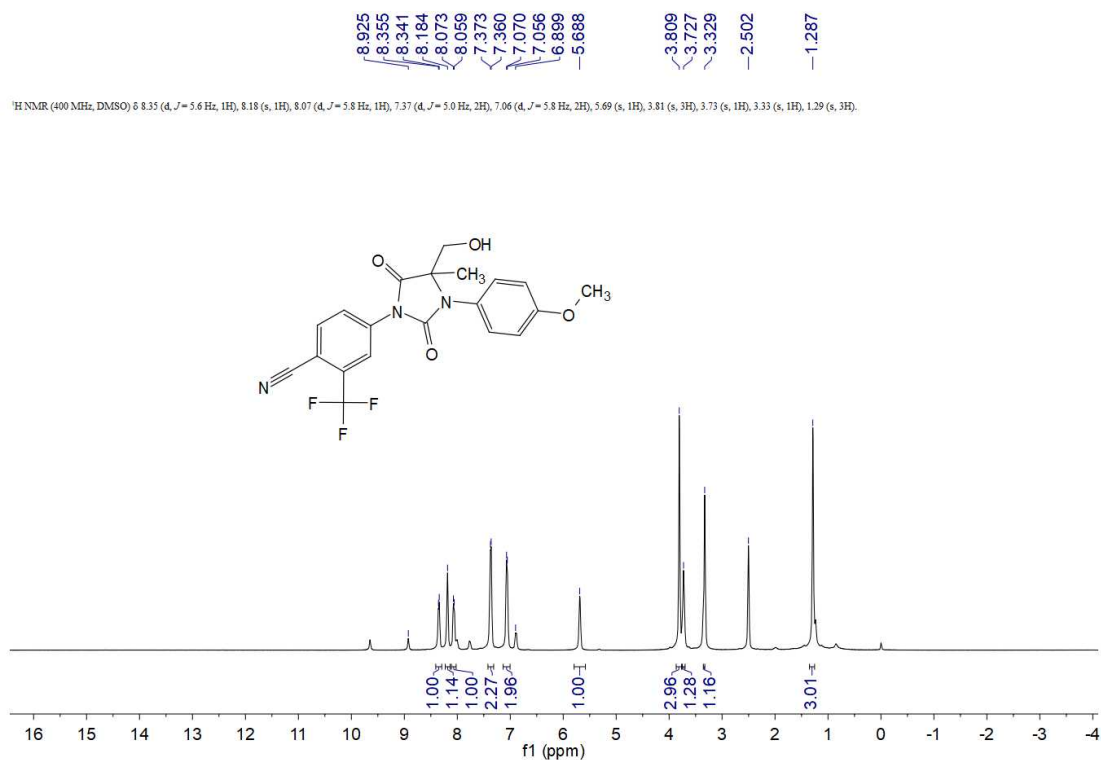
JJY-A00193-055 27 (0.554)

1: TOF MS ES+



Minimum: -1.5  
Maximum: 5.0 500.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
424.0640	424.0676	-3.6	-8.5	12.5	C19 H14 N3 O3 F3 Cl



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

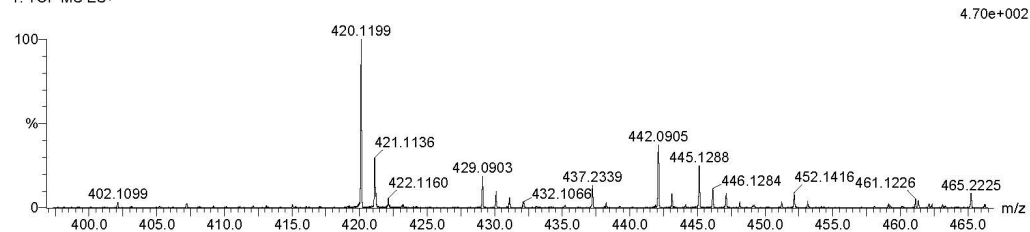
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-20 H: 17-17 N: 3-3 O: 4-4 F: 3-3

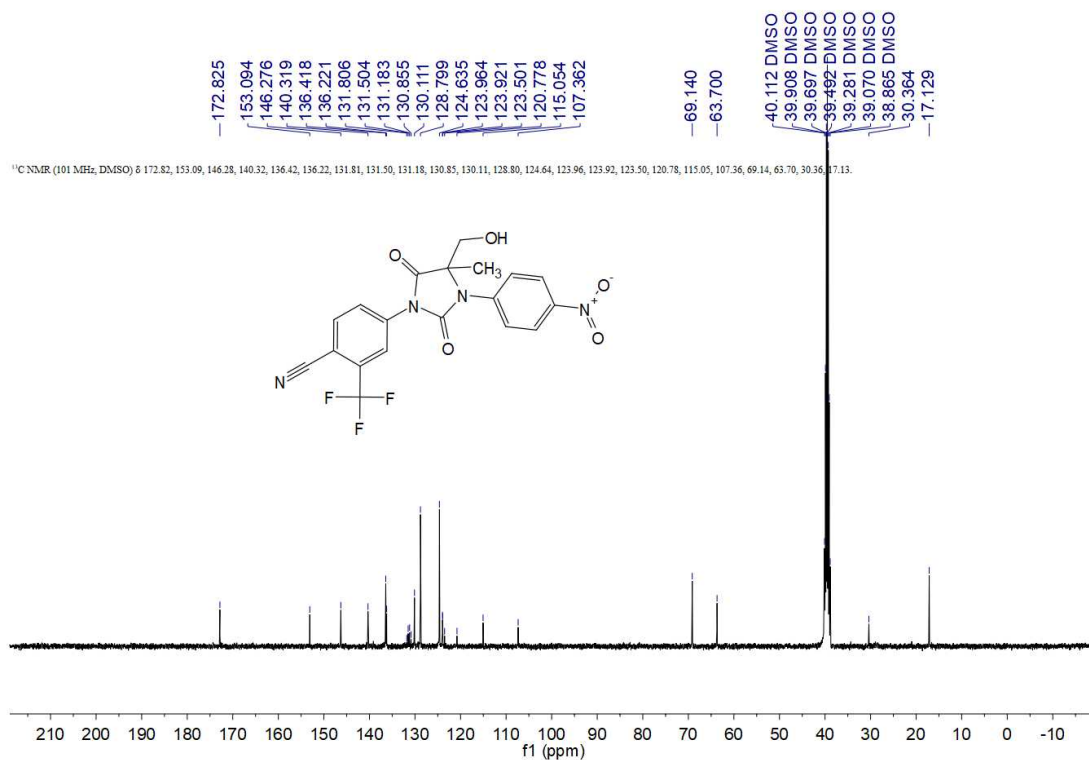
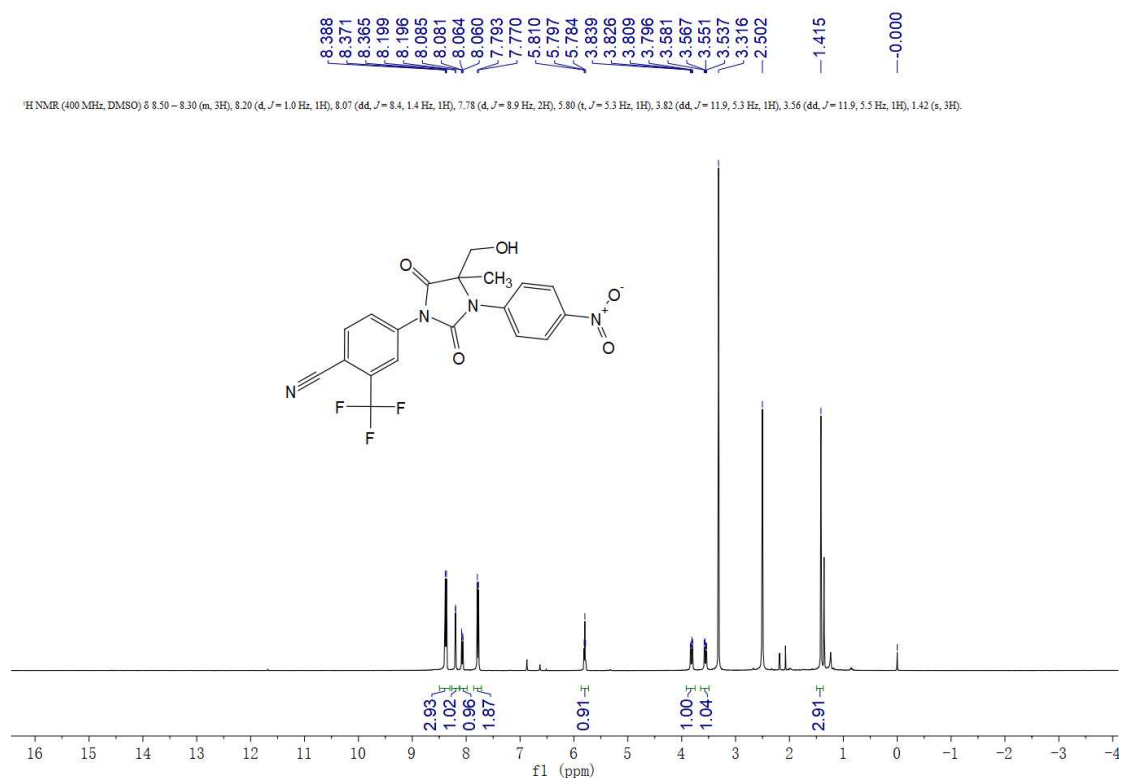
JJY-A00193-042 18 (0.382)

1: TOF MS ES+



Minimum: -1.5  
Maximum: 500.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
420.1199	420.1171	2.8	6.7	12.5	C20 H17 N3 O4 F3



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

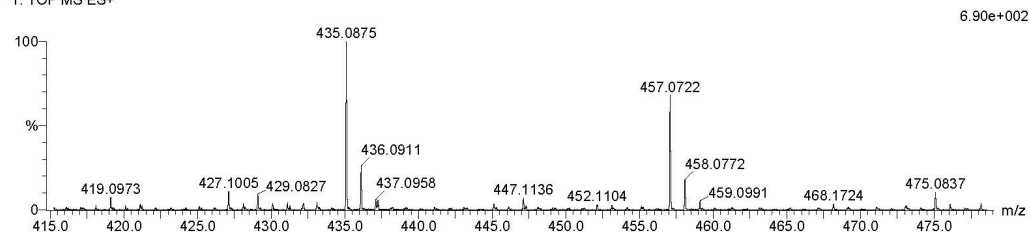
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 13-13 N: 4-4 O: 5-5 F: 3-3 Na: 0-1

JJY-A00193-085-2 29 (0.588)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

457.0722

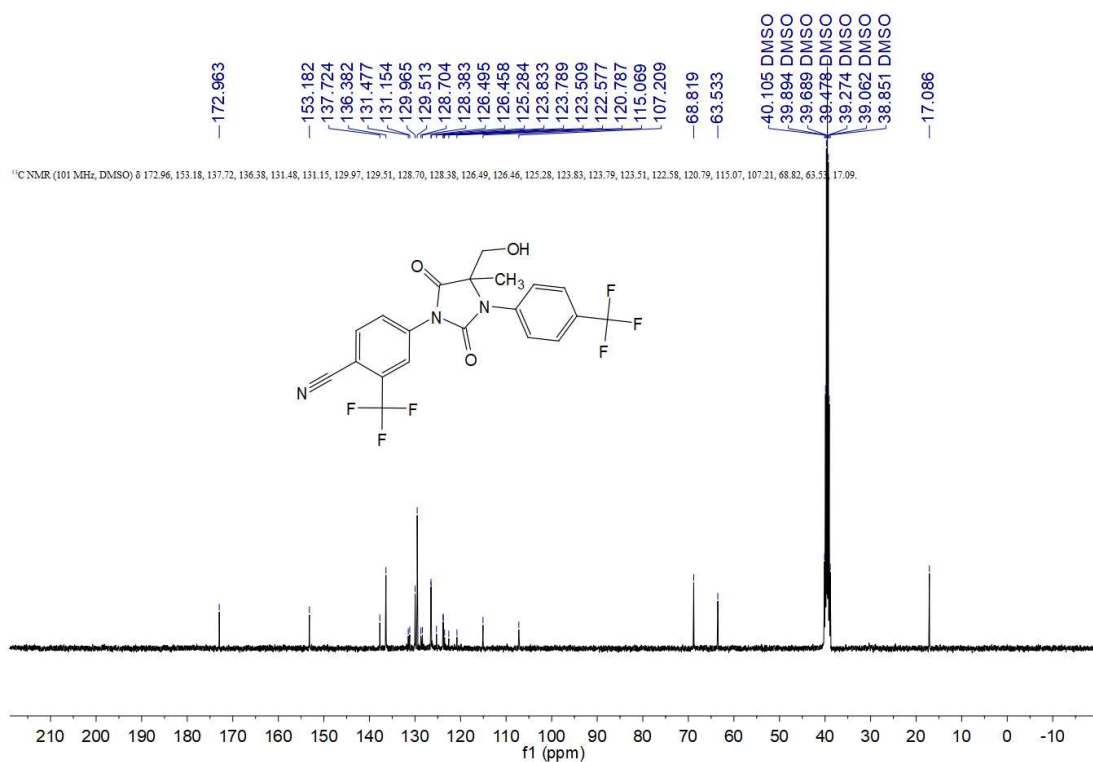
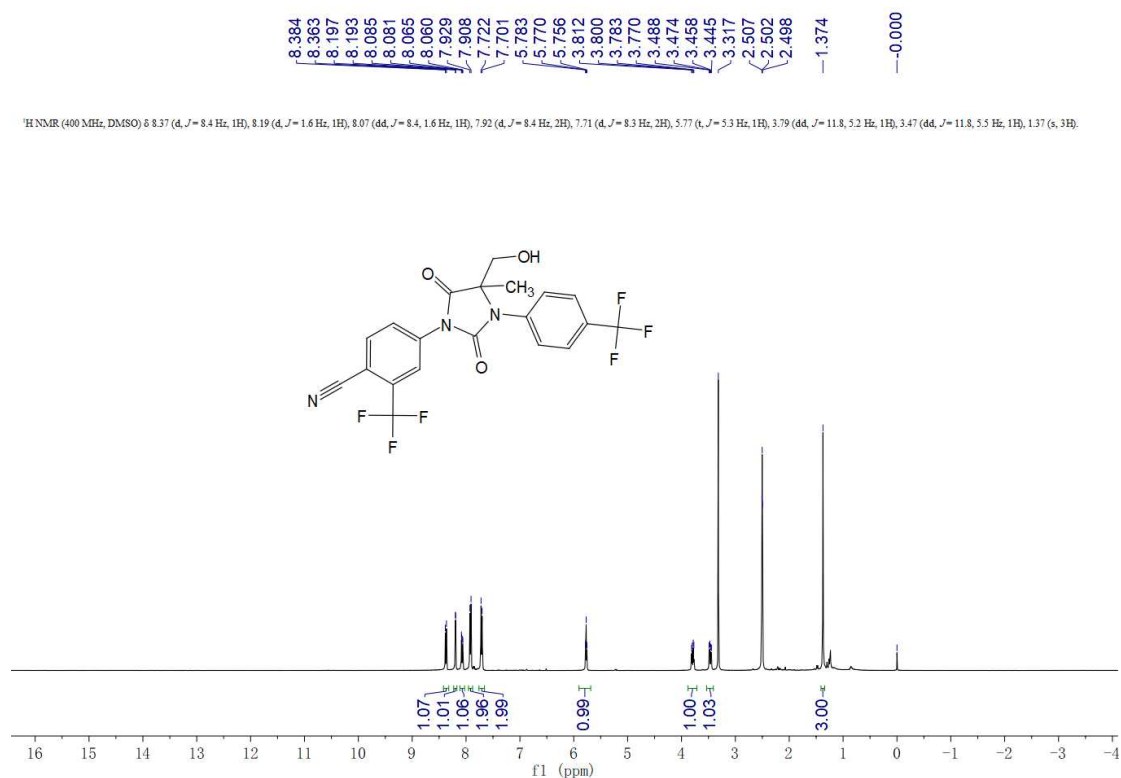
457.0736

-1.4

-3.1

13.5

C19 H13 N4 O5 F3 Na





## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

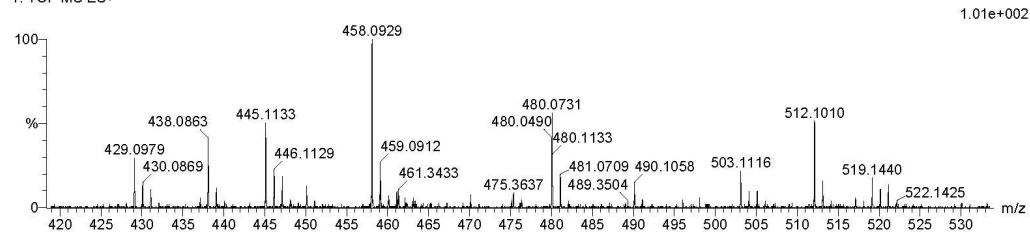
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-20 H: 14-14 N: 3-3 O: 3-3 F: 6-6

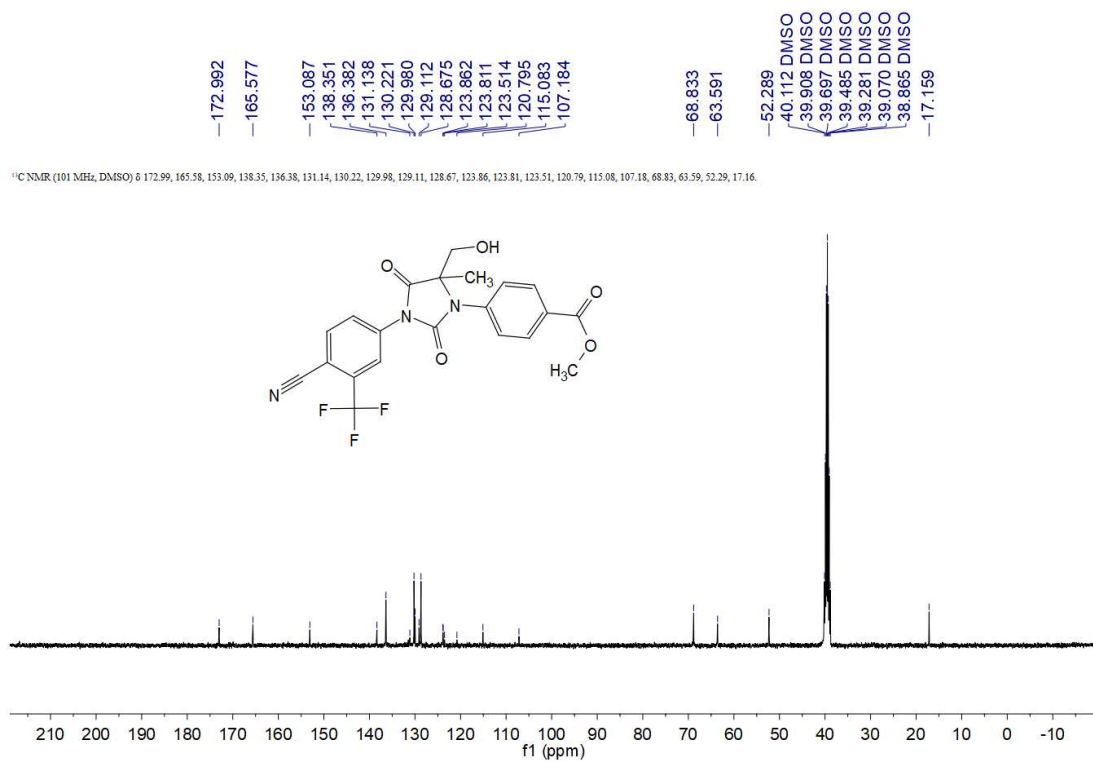
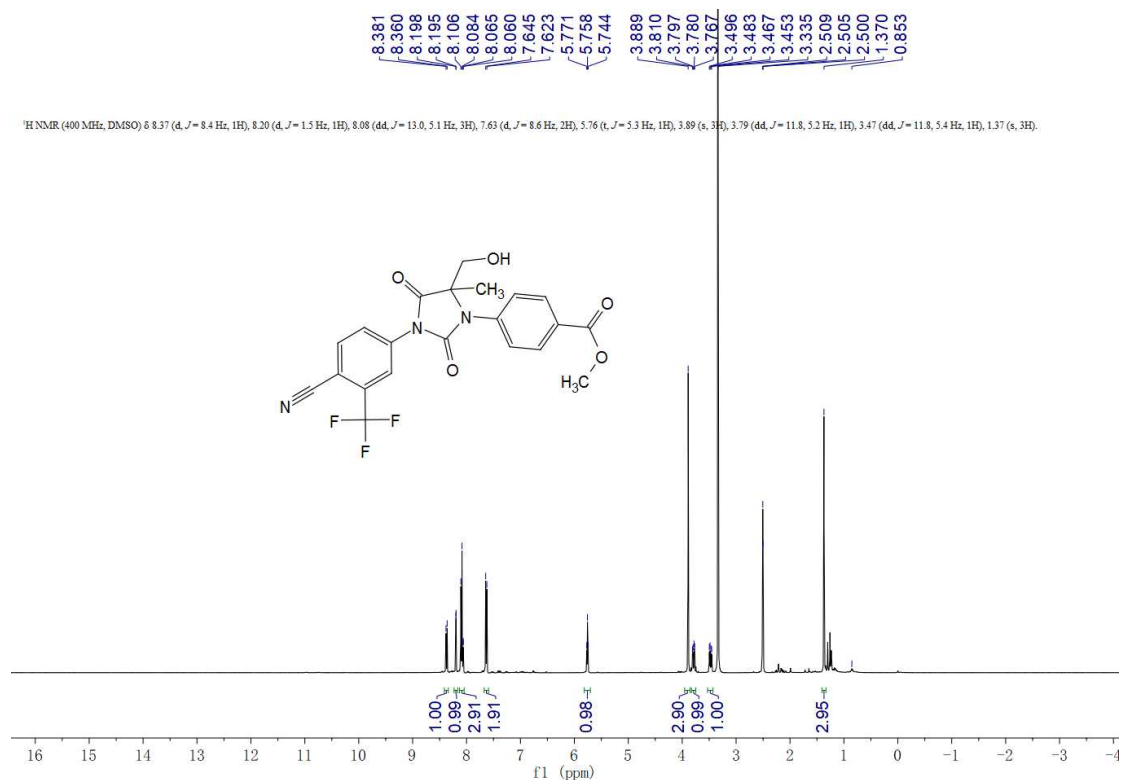
JJY-A00193-089 28 (0.571)

1: TOF MS ES+



Minimum: -1.5  
Maximum: 500.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
458.0929	458.0939	-1.0	-2.2	12.5	C20 H14 N3 O3 F6



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

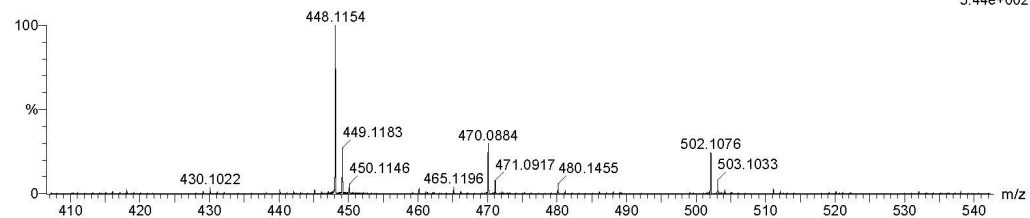
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 21-21 H: 17-17 N: 3-3 O: 5-5 F: 3-3

JJY-A00193-092 18 (0.382)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

448.1154

448.1120

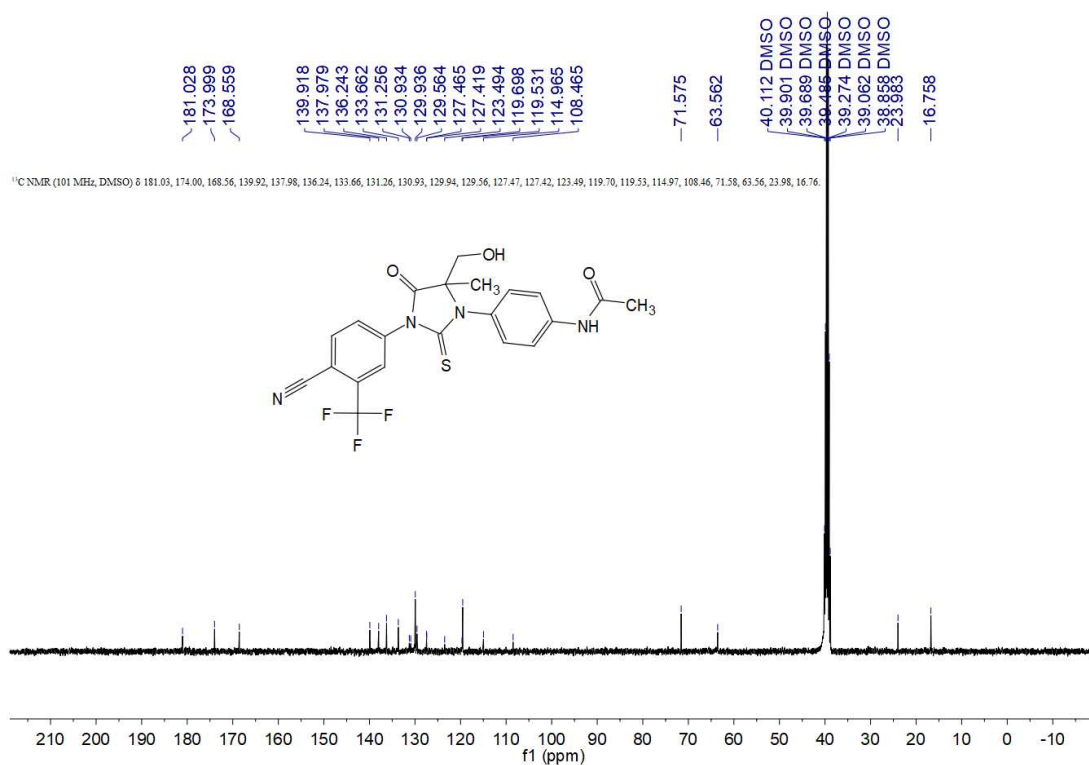
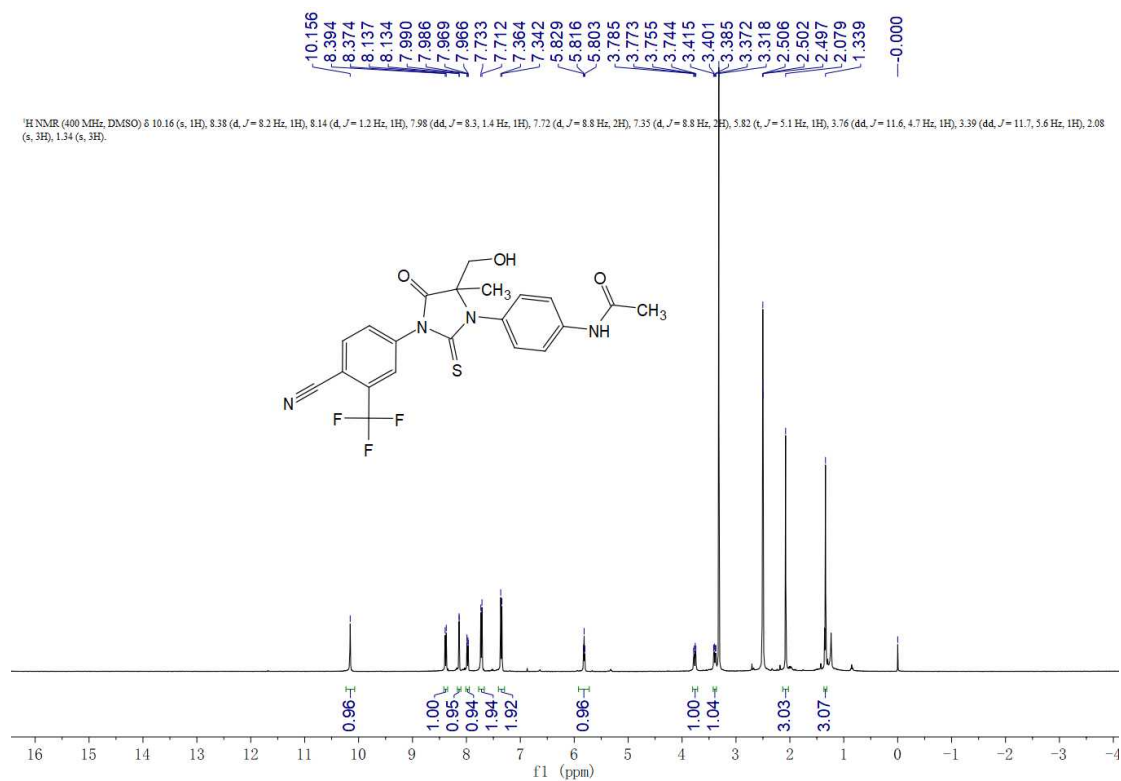
3.4

7.6

13.5

C21 H17 N3 O5 F3

$^1\text{H}$ ,  $^{13}\text{C}$ , NMR and HRMS spectra of *compound 9*



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

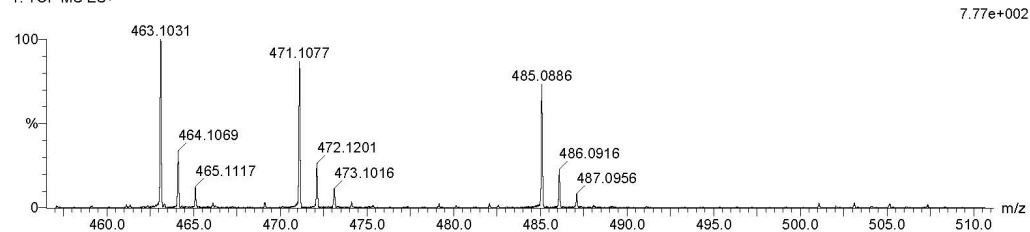
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 21-21 H: 17-17 N: 4-4 O: 3-3 F: 3-3 Na: 0-1 S: 1-1

JJY-A00193-088 35 (0.710)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

485.0886

485.0871

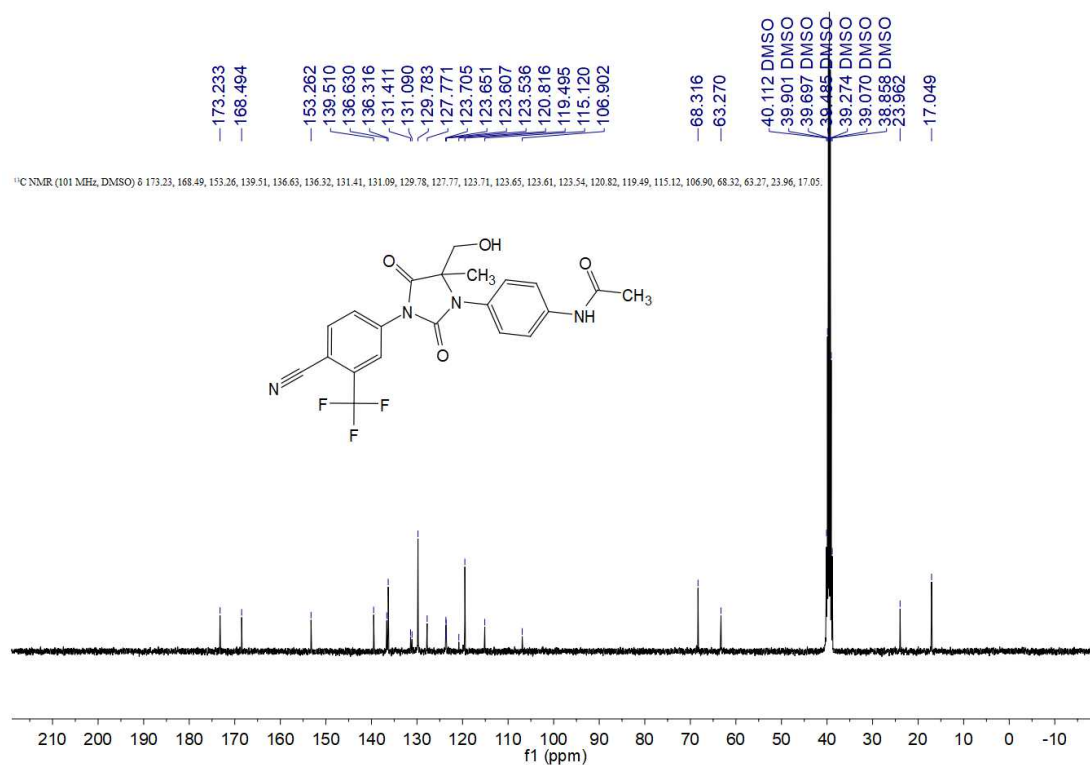
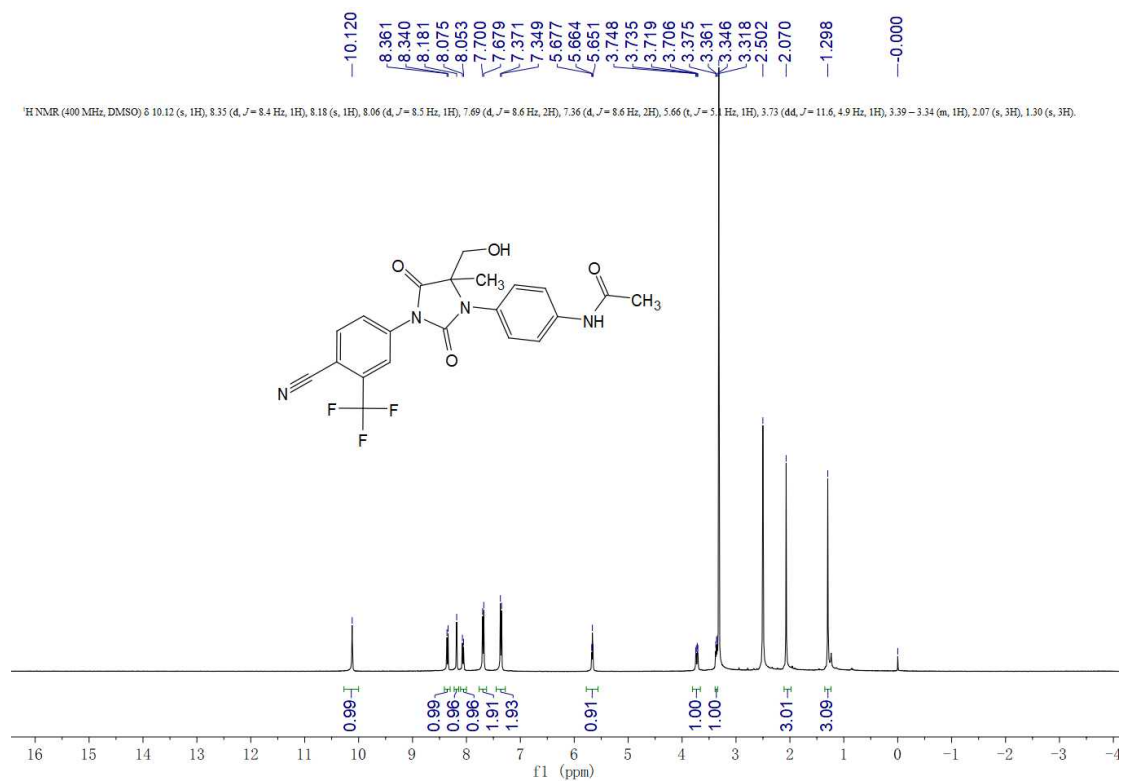
1.5

3.1

13.5

C21 H17 N4 O3 F3 Na S

$^1\text{H}$ ,  $^{13}\text{C}$ , NMR and HRMS spectra of *compound 10*



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

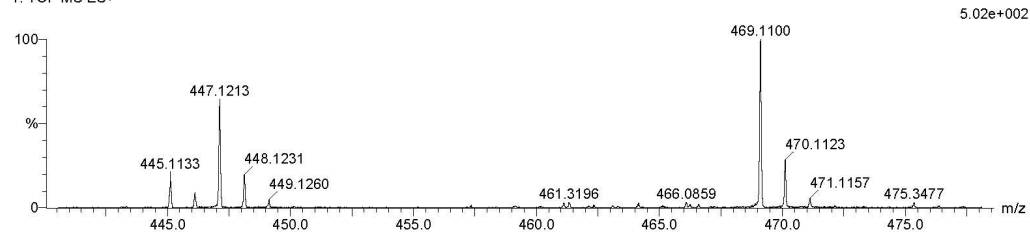
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 21-21 H: 17-17 N: 4-4 O: 4-4 F: 3-3 Na: 0-1

JJY-A00193-101 42 (0.849)

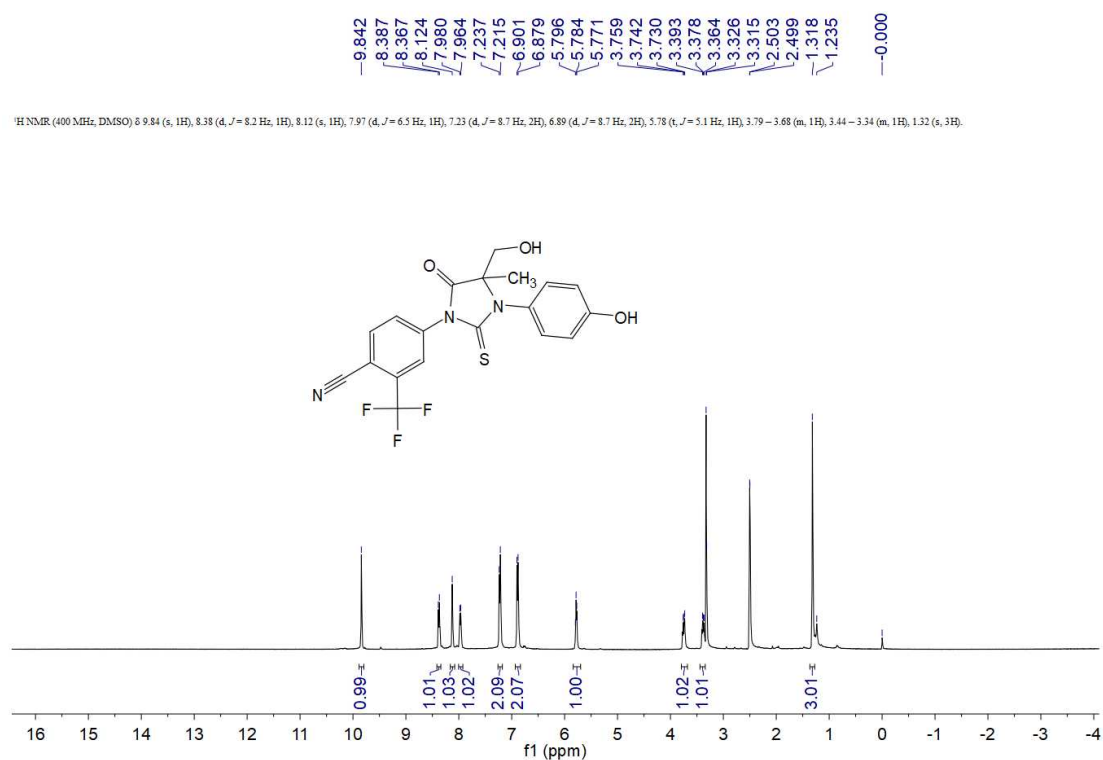
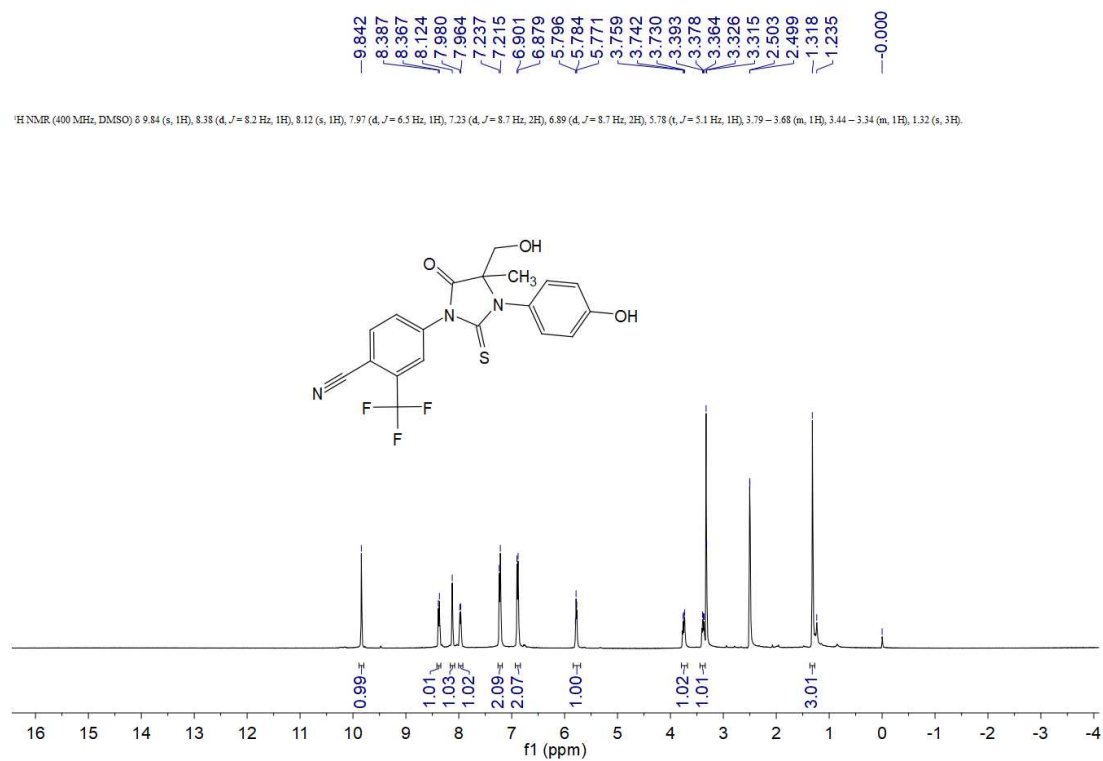
1: TOF MS ES+



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
469.1100	469.1100	0.0	0.0	13.5	C21 H17 N4 O4 F3 Na

$^1\text{H}$ ,  $^{13}\text{C}$ , NMR and HRMS spectra of *compound 11a-b*





## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

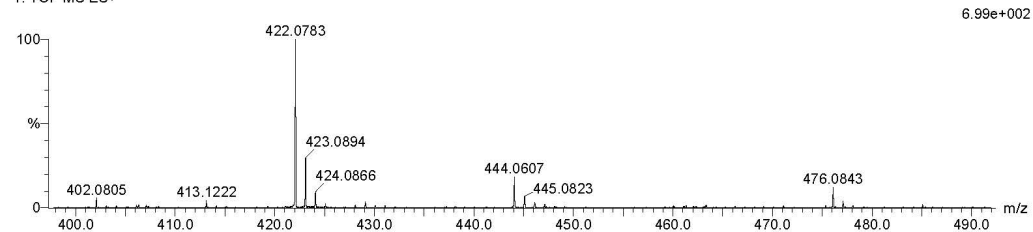
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 15-15 N: 3-3 O: 3-3 F: 3-3 S: 1-1

JJY-A00193-095 31 (0.622)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

422.0783

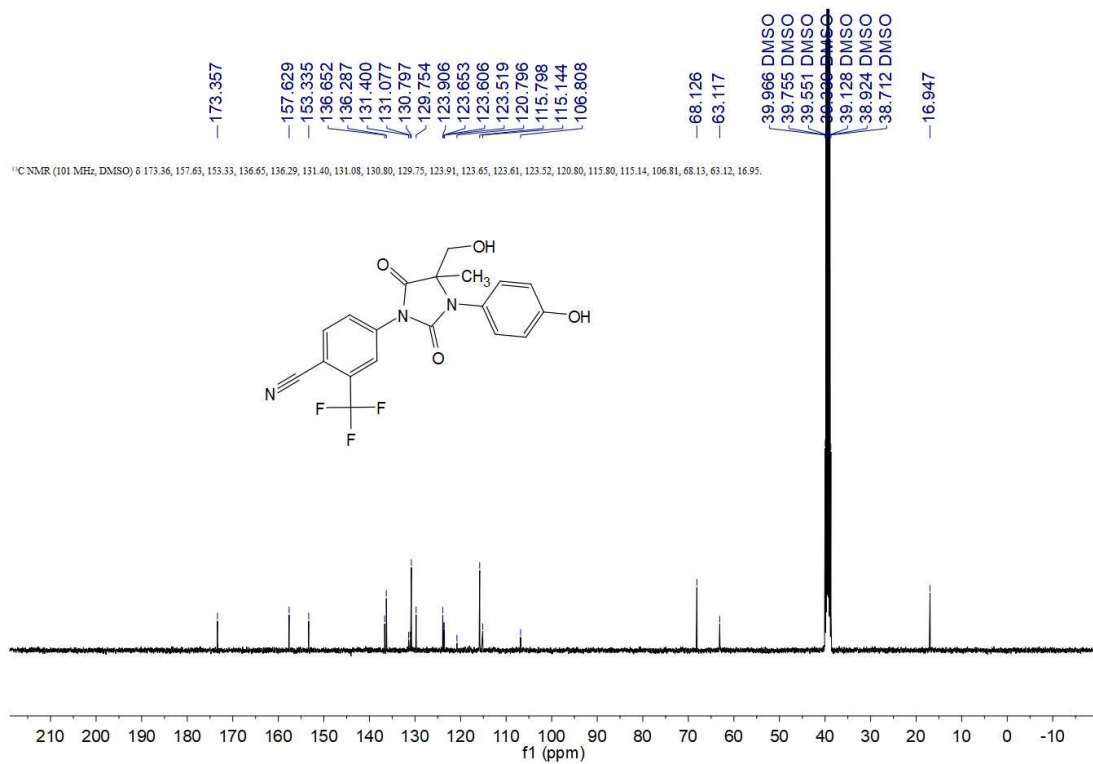
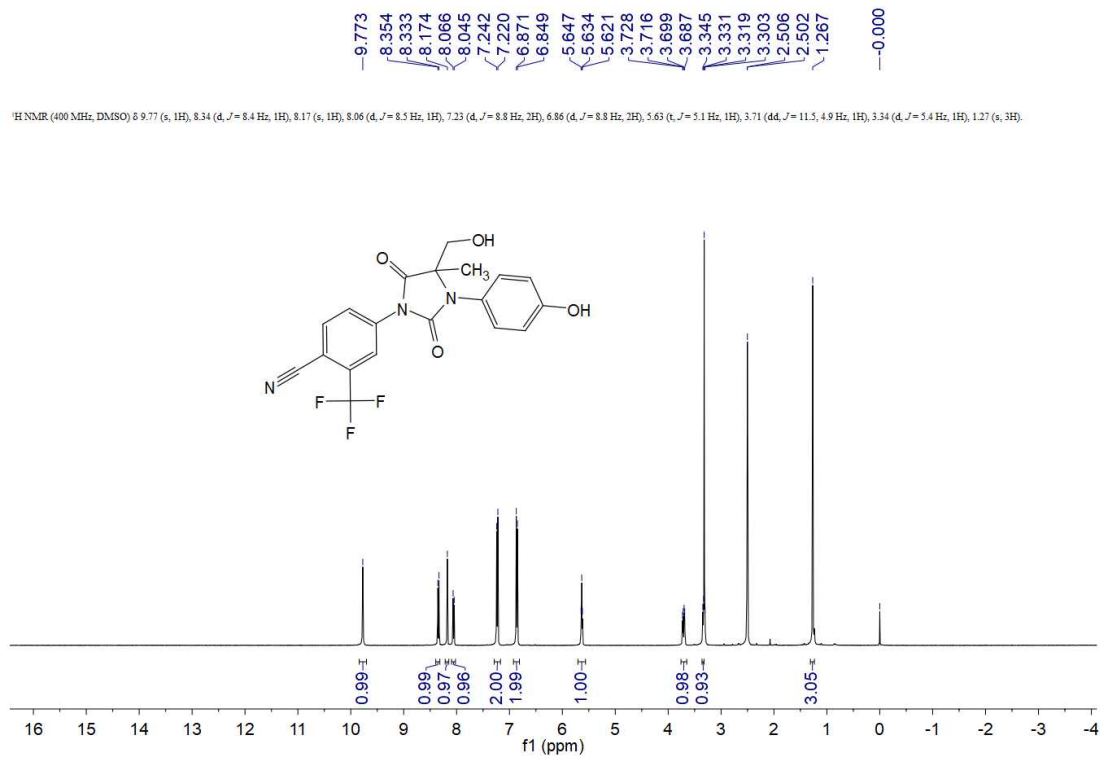
422.0786

-0.3

-0.7

12.5

C19 H15 N3 O3 F3 S



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

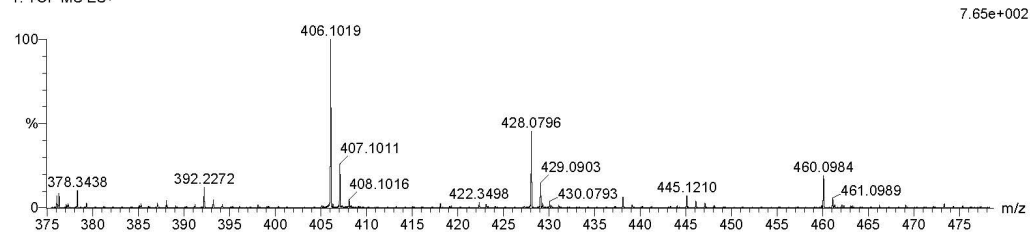
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 19-19 H: 15-15 N: 3-3 O: 4-4 F: 3-3

JJY-A00193-100 36 (0.727)

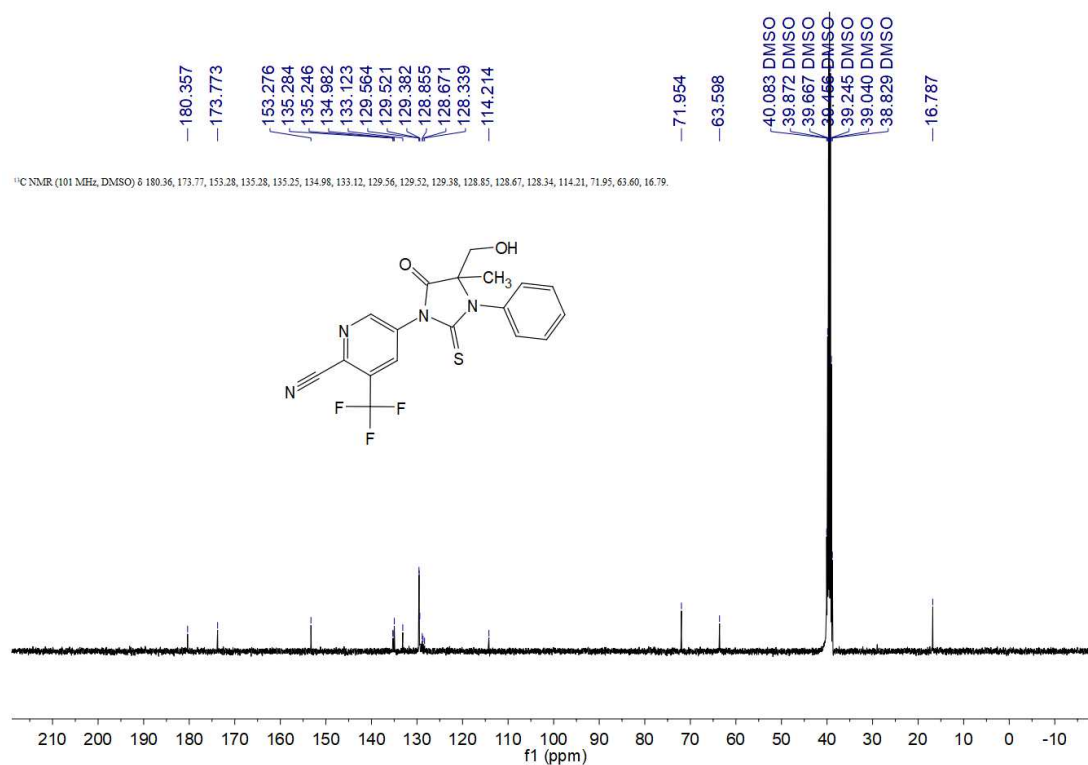
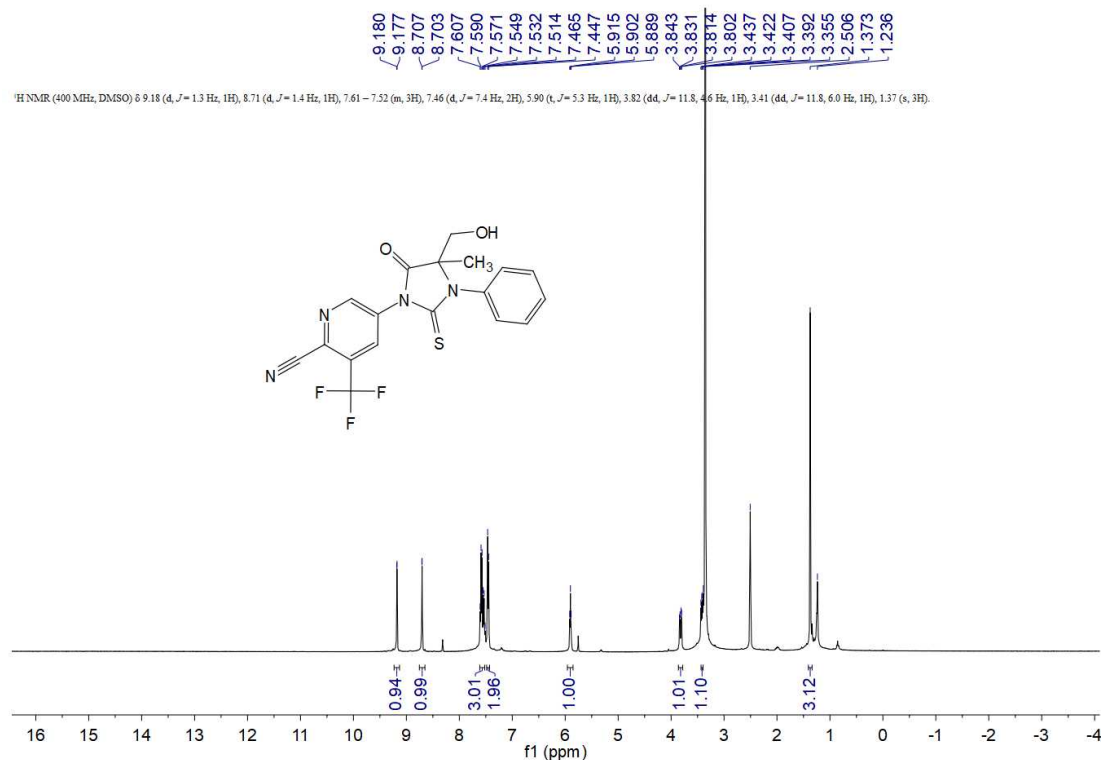
1: TOF MS ES+



Minimum: -1.5  
Maximum: 500.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
406.1019	406.1015	0.4	1.0	12.5	C19 H15 N3 O4 F3

$^1\text{H}$   $^{13}\text{C}$ , NMR and HRMS spectra spectra of compound **19a-d**



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

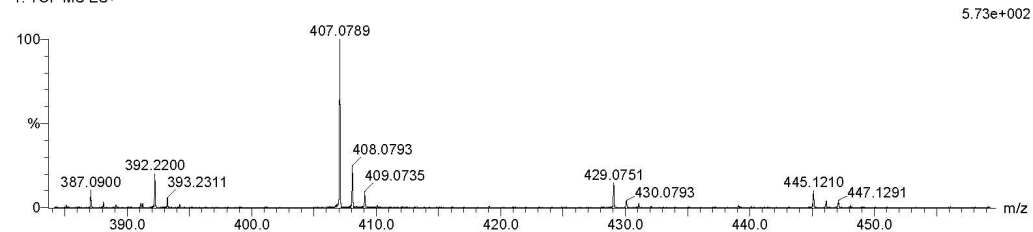
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 18-18 H: 14-14 N: 4-4 O: 2-2 F: 3-3 S: 1-1

JJY-A00222-062 35 (0.710)

1: TOF MS ES+

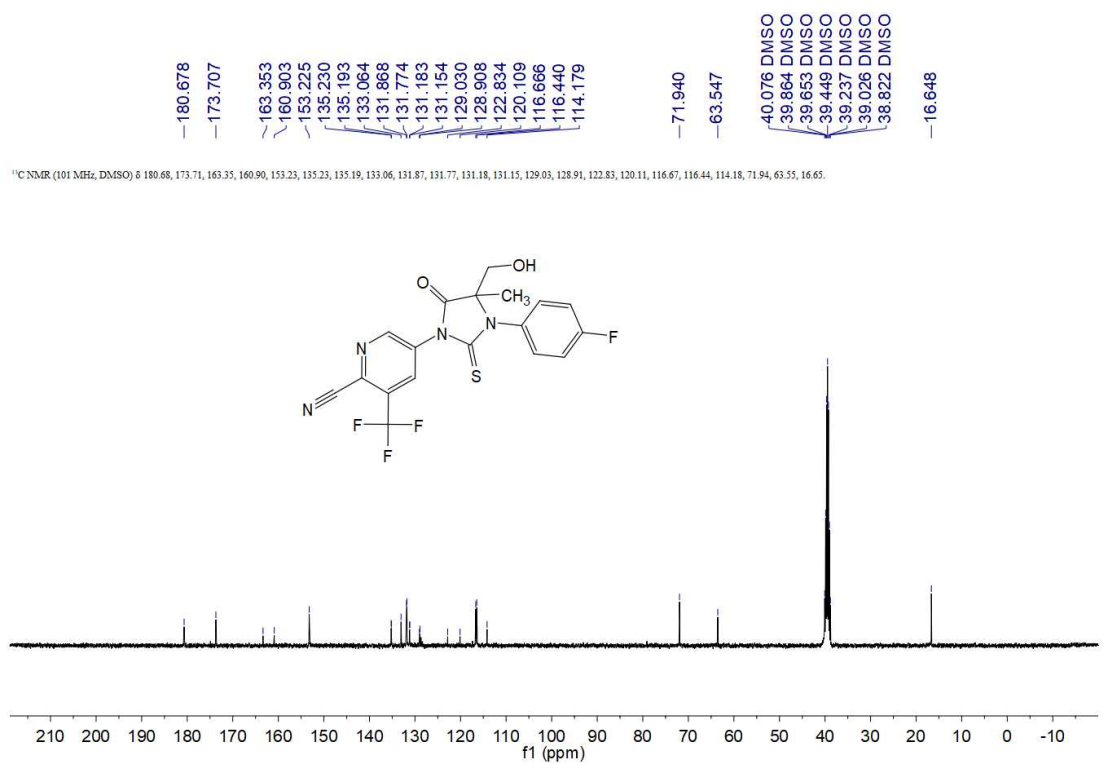
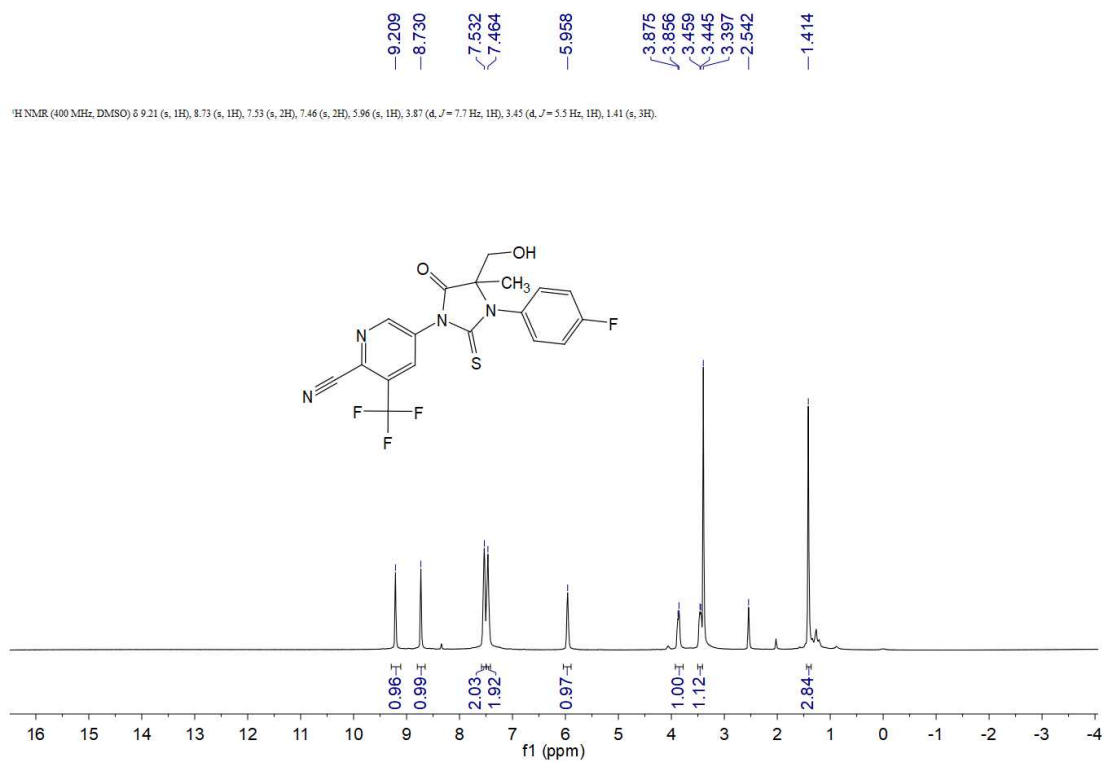


Minimum:

Maximum:

5.0 500.0 -1.5  
50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
407.0789	407.0790	-0.1	-0.2	12.5	C18 H14 N4 O2 F3 S



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

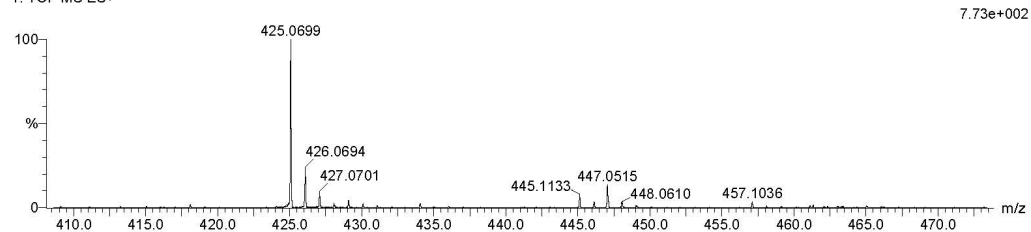
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 18-18 H: 13-13 N: 4-4 O: 2-2 F: 4-4 S: 1-1

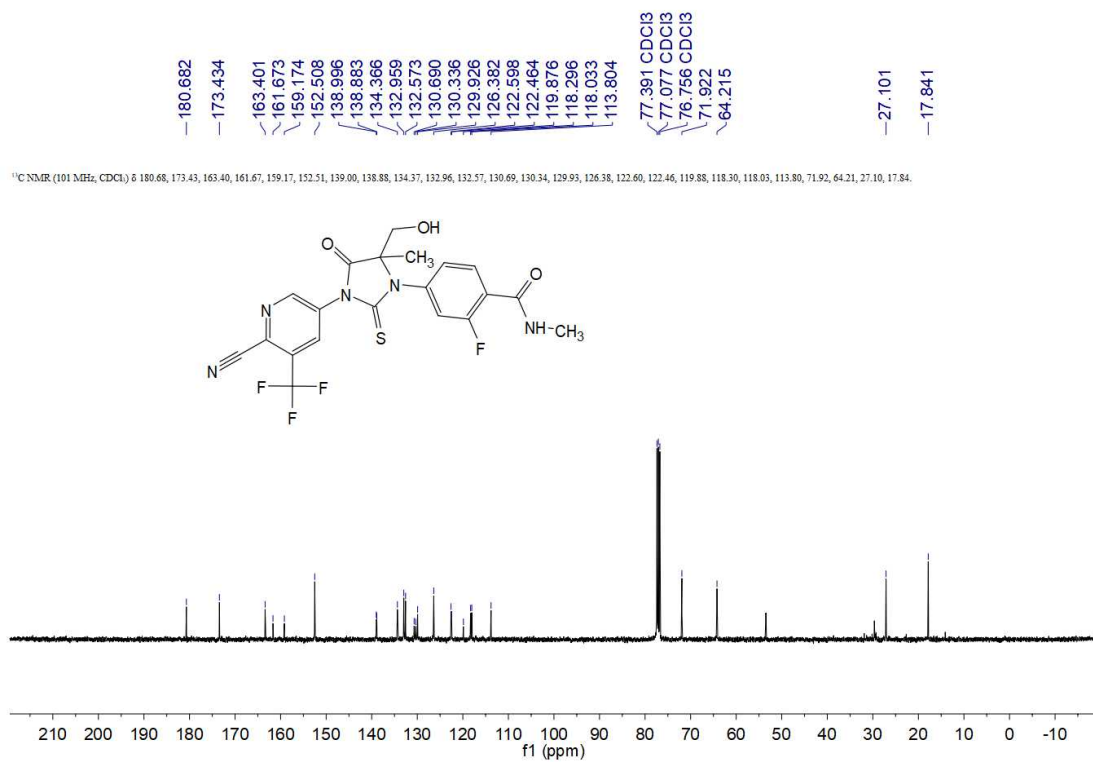
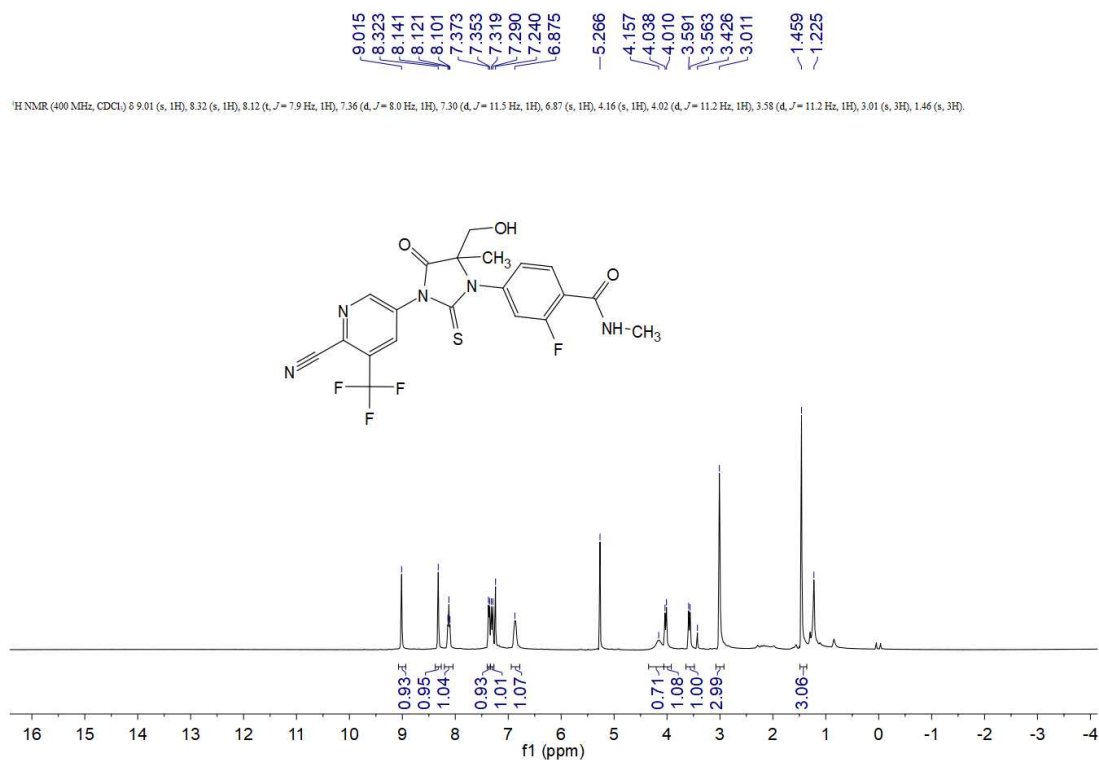
JJY-A00222-061 31 (0.622)

1: TOF MS ES+



Minimum: -1.5  
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula
425.0699	425.0695	0.4	0.9	12.5	C18 H13 N4 O2 F4 S





## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

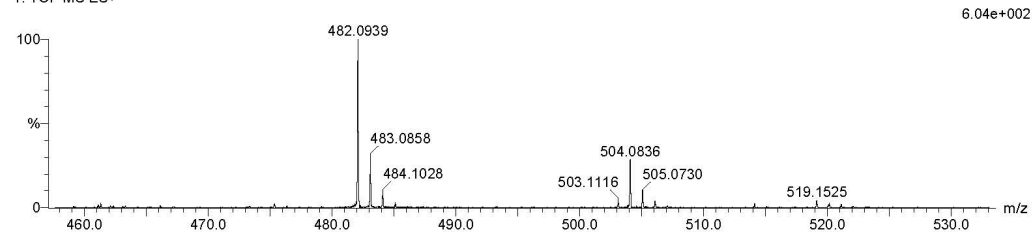
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 20-20 H: 16-16 N: 5-5 O: 3-3 F: 4-4 S: 1-1

JJY-A00222-063 35 (0.710)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

482.0939

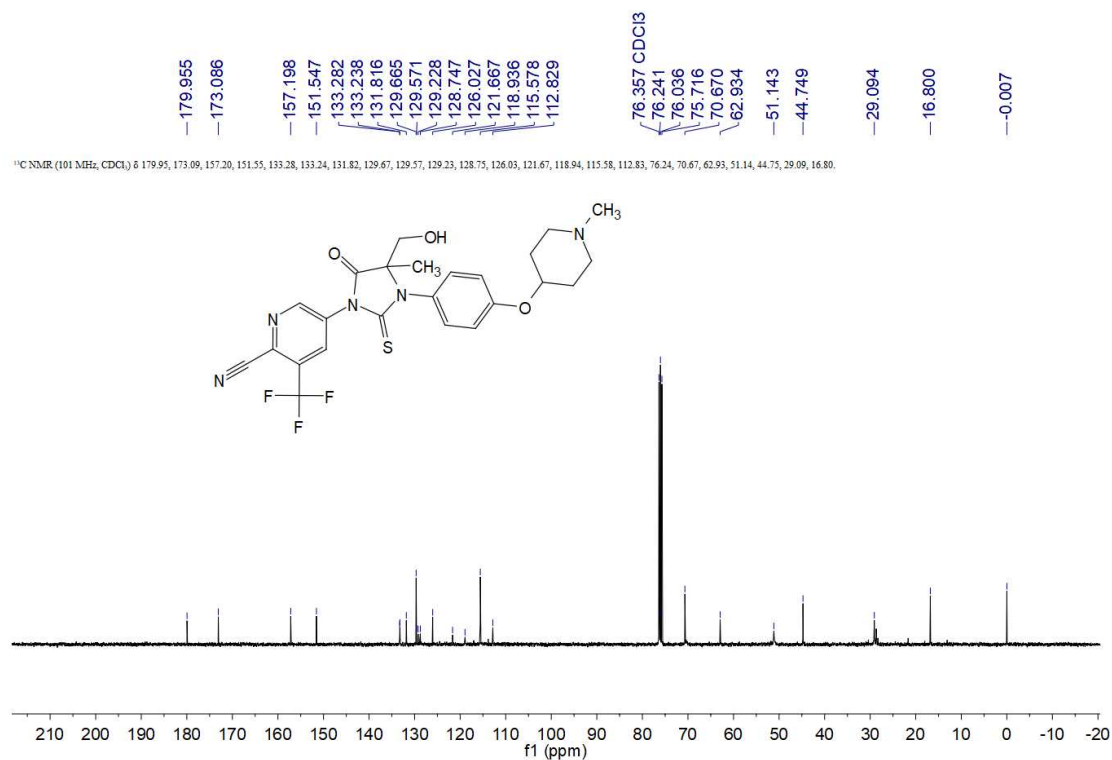
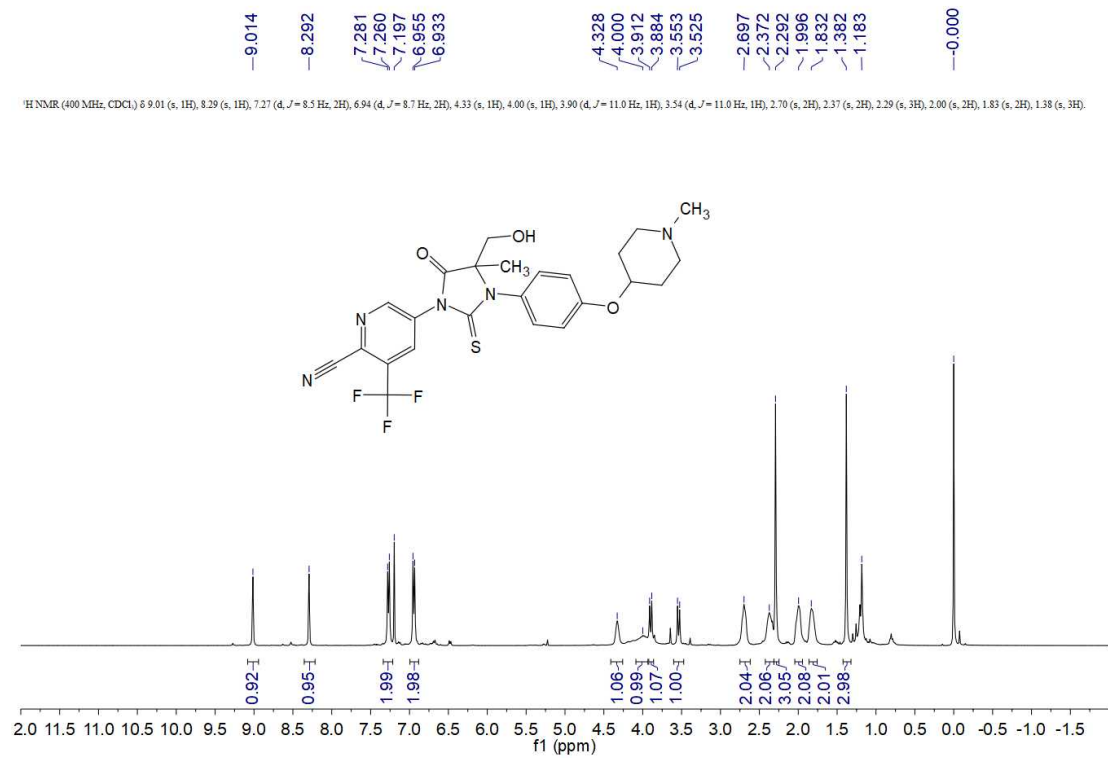
482.0910

2.9

6.0

13.5

C20 H16 N5 O3 F4 S



## Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Even Electron Ions

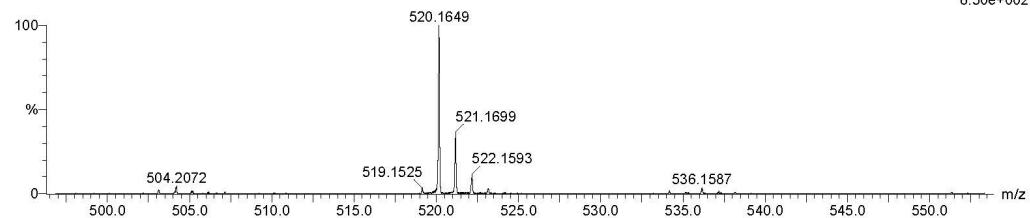
1 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 24-24 H: 25-25 N: 5-5 O: 3-3 F: 3-3 S: 1-1

JJY-A00222-064 41 (0.832)

1: TOF MS ES+



Minimum:

Maximum:

5.0

500.0

-1.5

50.0

Mass

Calc. Mass

mDa

PPM

DBE

Formula

520.1649

520.1630

1.9

3.7

13.5

C24 H25 N5 O3 F3 S