

# Discovery of novel biphenyl-substituted diarylpyrimidines with a cyanomethyl linker as HIV-1 NNRTIs by a molecular hybridization strategy Design of Biphenyl-Substituted Diarylpyrimidines with a Cyanomethyl Linker as HIV-1 NNRTIs via a Molecular Hybridization Strategy

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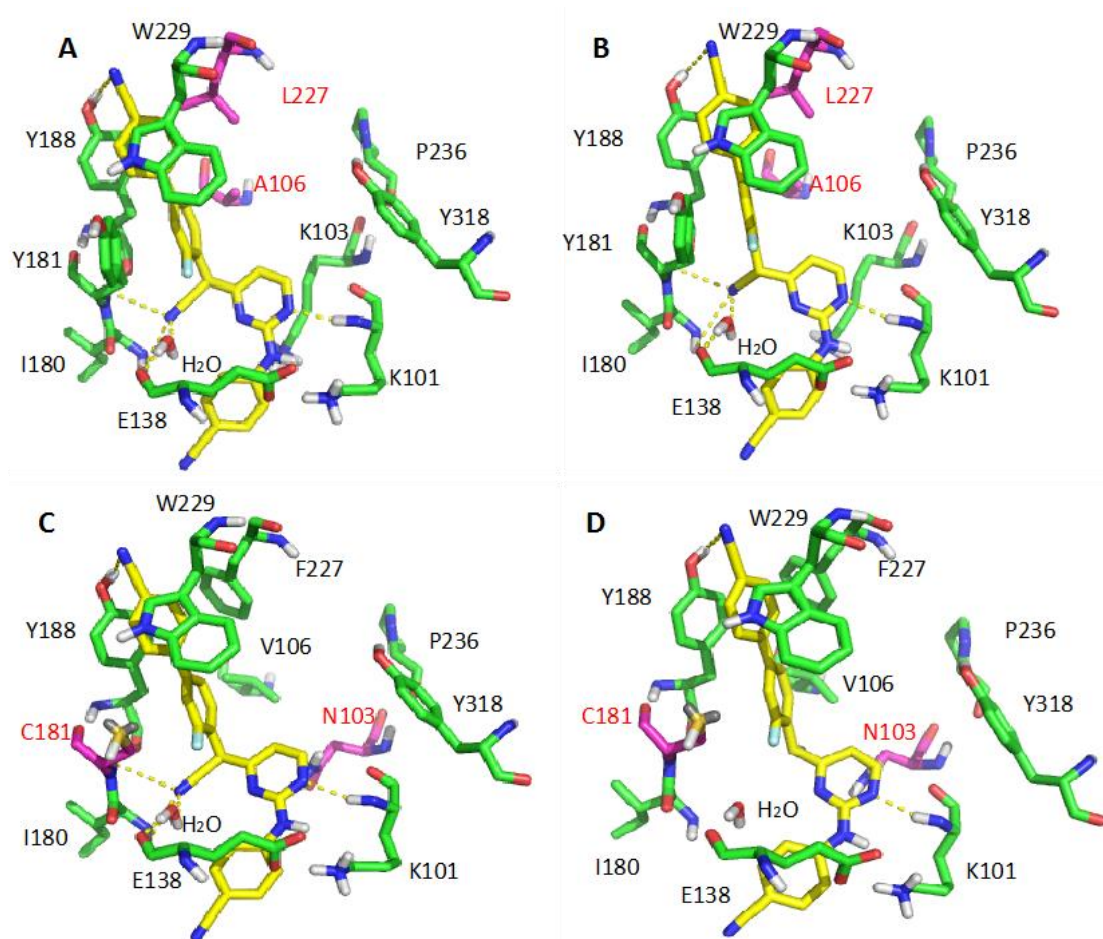
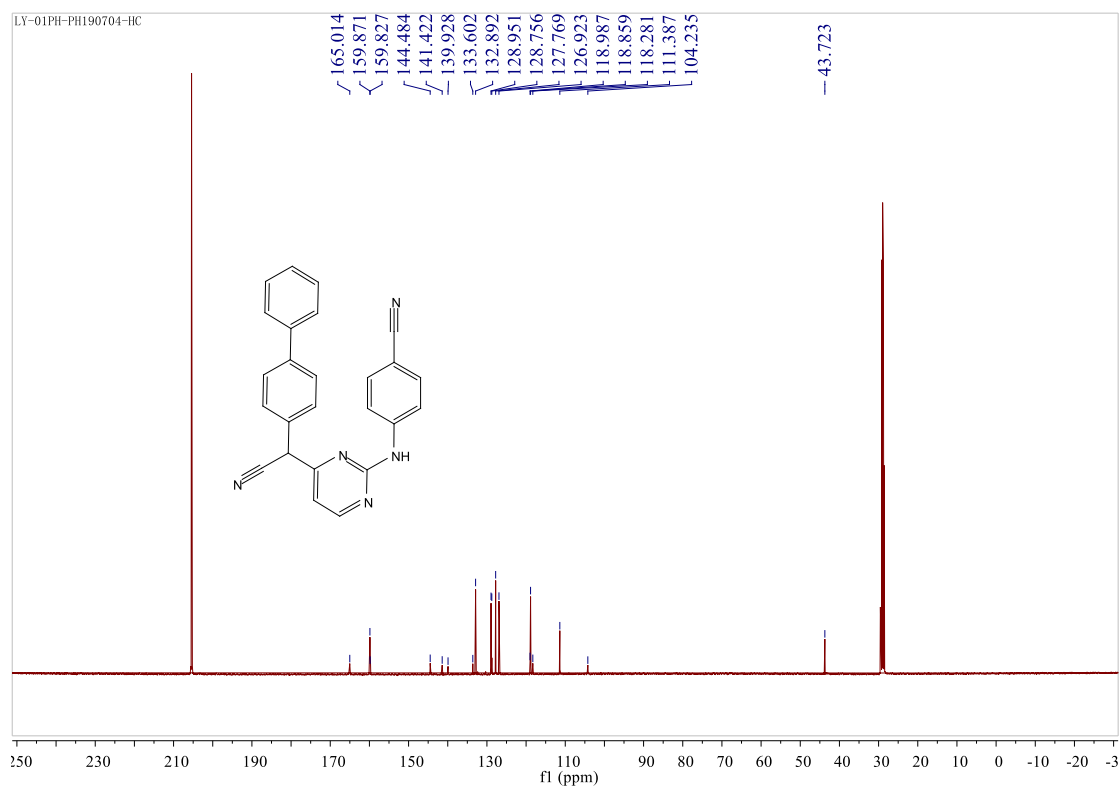
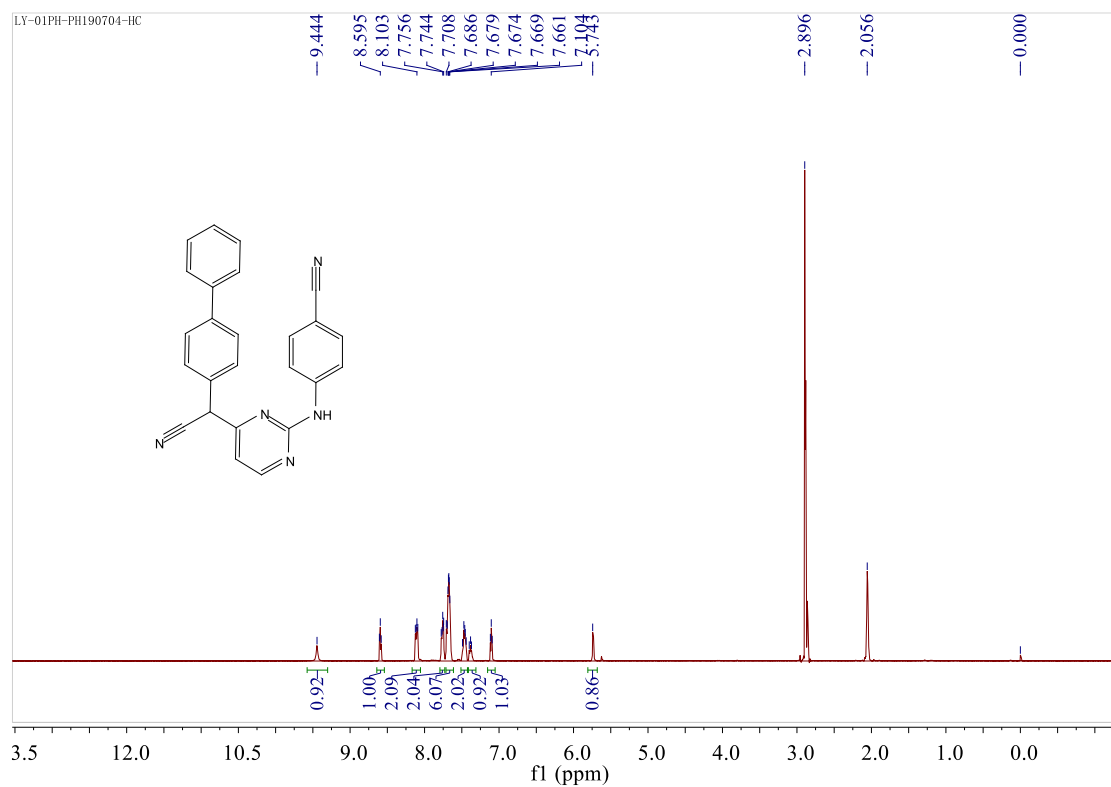


Figure S1 Predicted binding modes of **10p** with double mutant (F227L + V106A, K103N + Y181C) RT (PDB: 2ZD1). (A) F227L + V106A mutant RT with **10p-S**; (B) F227L + V106A mutant RT with **10p-R**; (C) K103N + Y181C mutant RT with **10p-S**; (D) K103N + Y181C mutant RT with **10p-R**.

# $^1\text{H}$ -NMR, $^{13}\text{C}$ -NMR and MS spectra of compounds

## 1. Spectra of compound 10a



# Display Report

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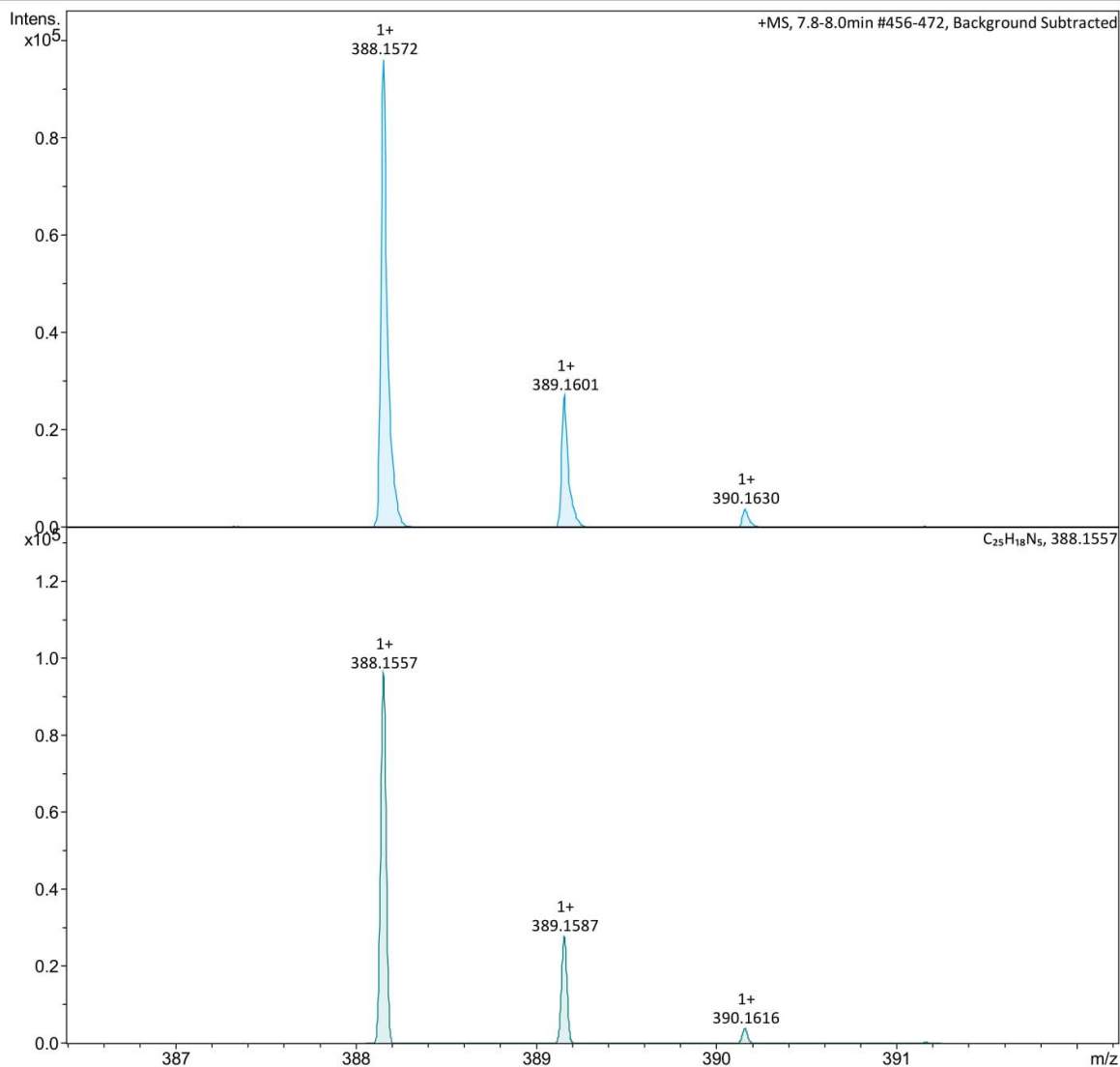
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Operator BDAL@DE  
Instrument compact 8255754.20127

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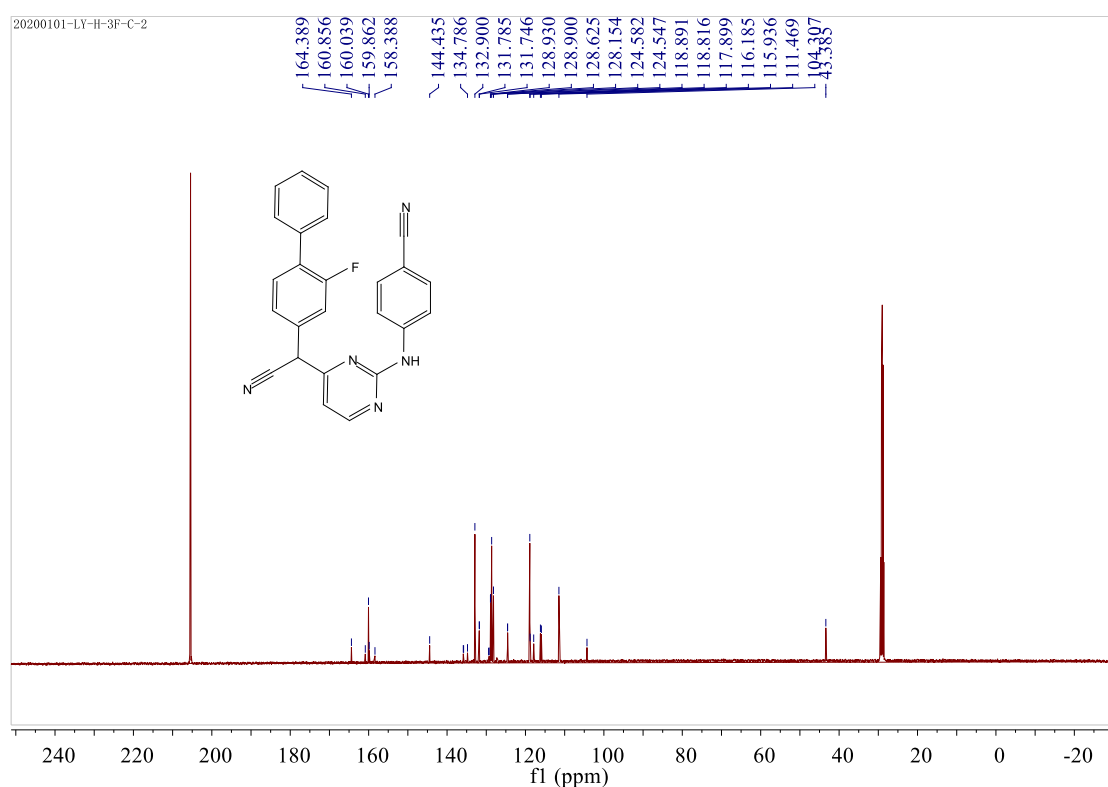
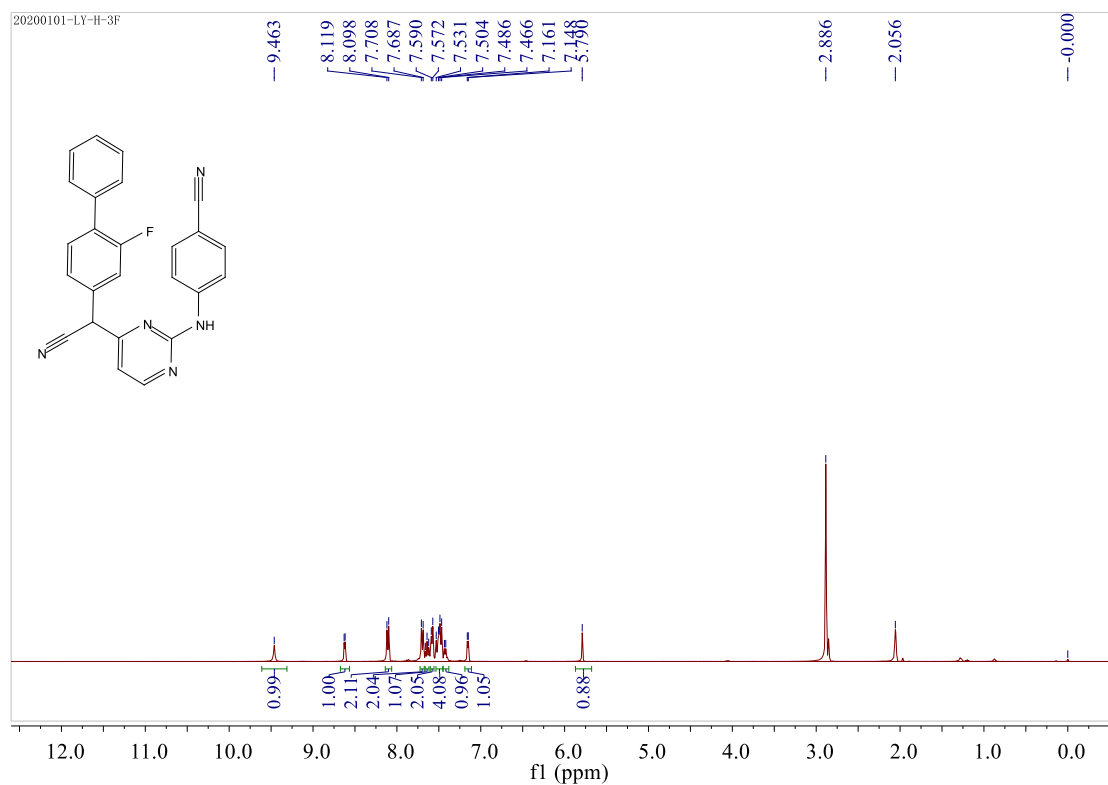
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## 2. Spectra of compound 10b



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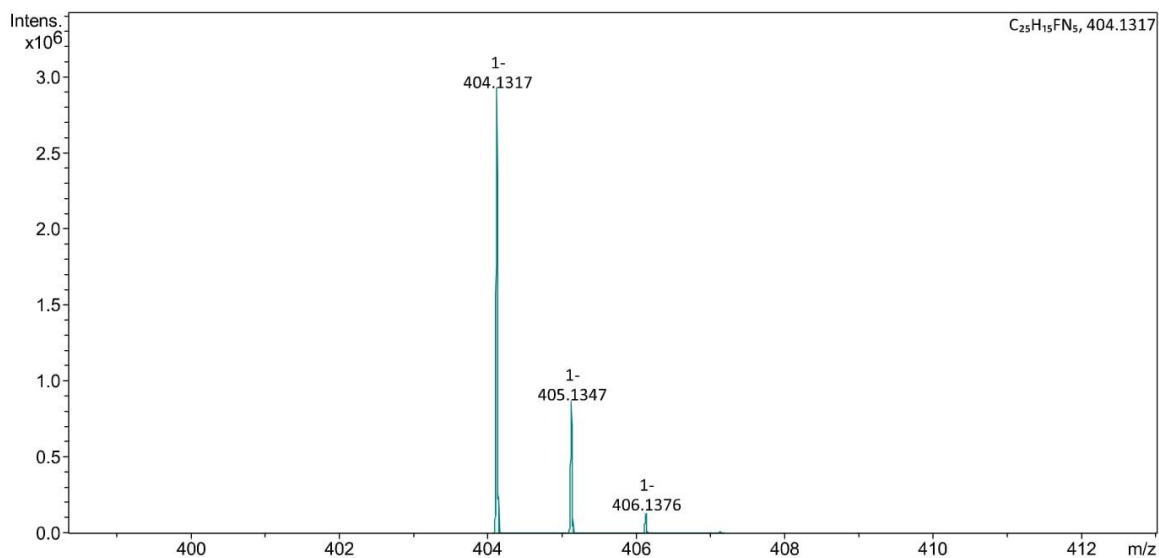
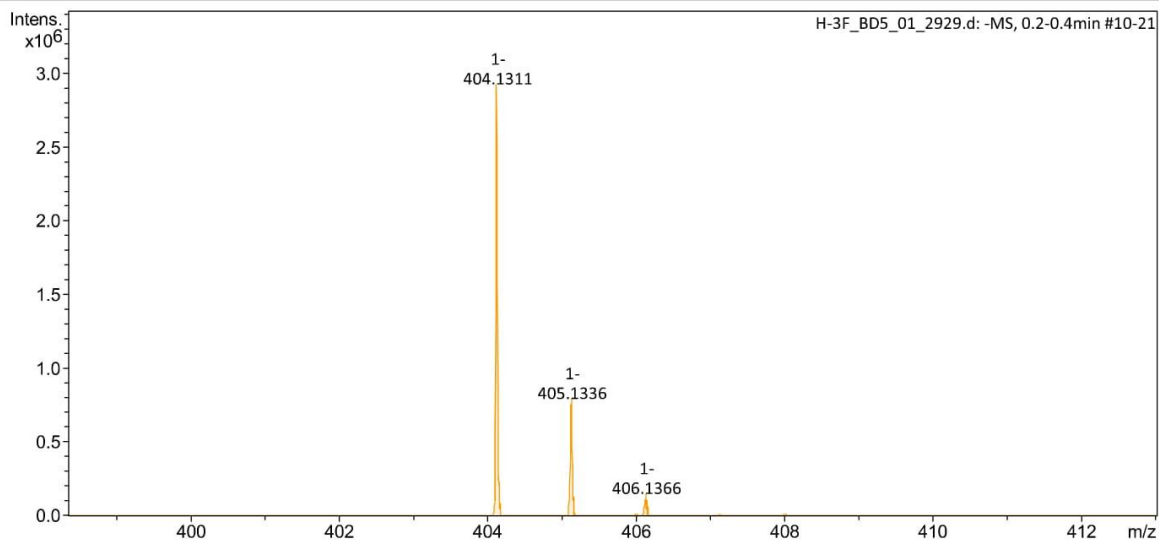
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Instrument compact 8255754.20127

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H-3F\_BD5\_01\_2929.d

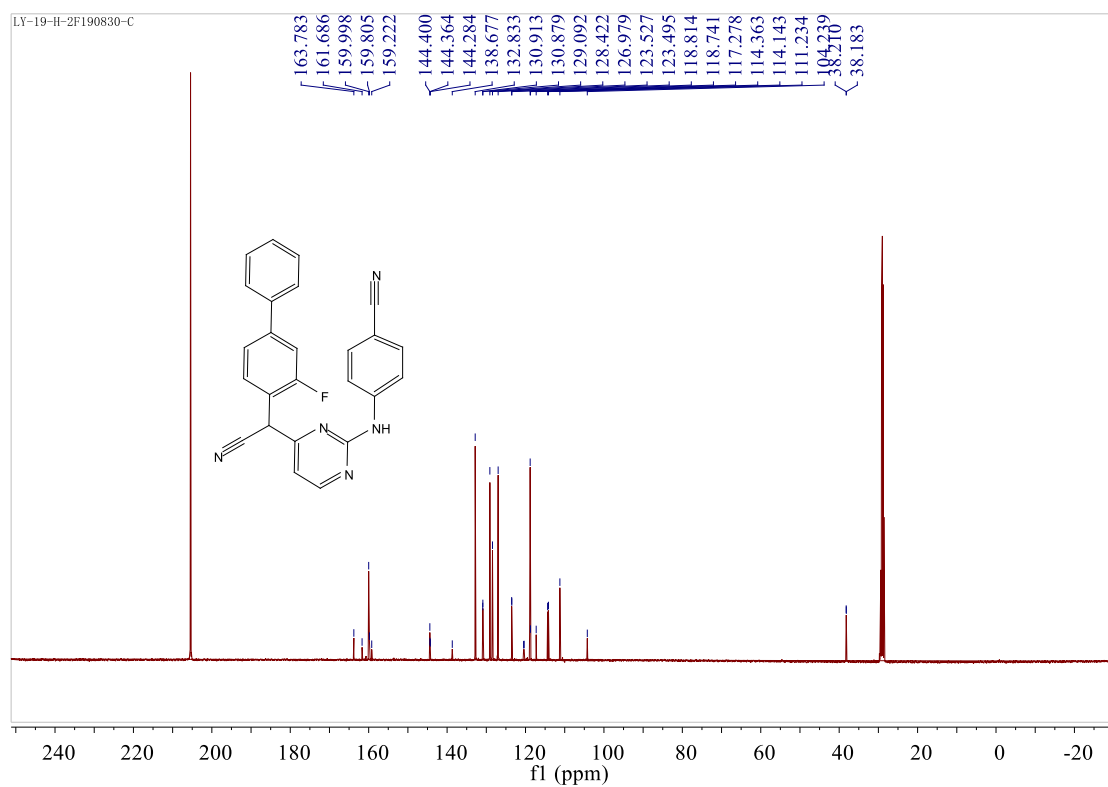
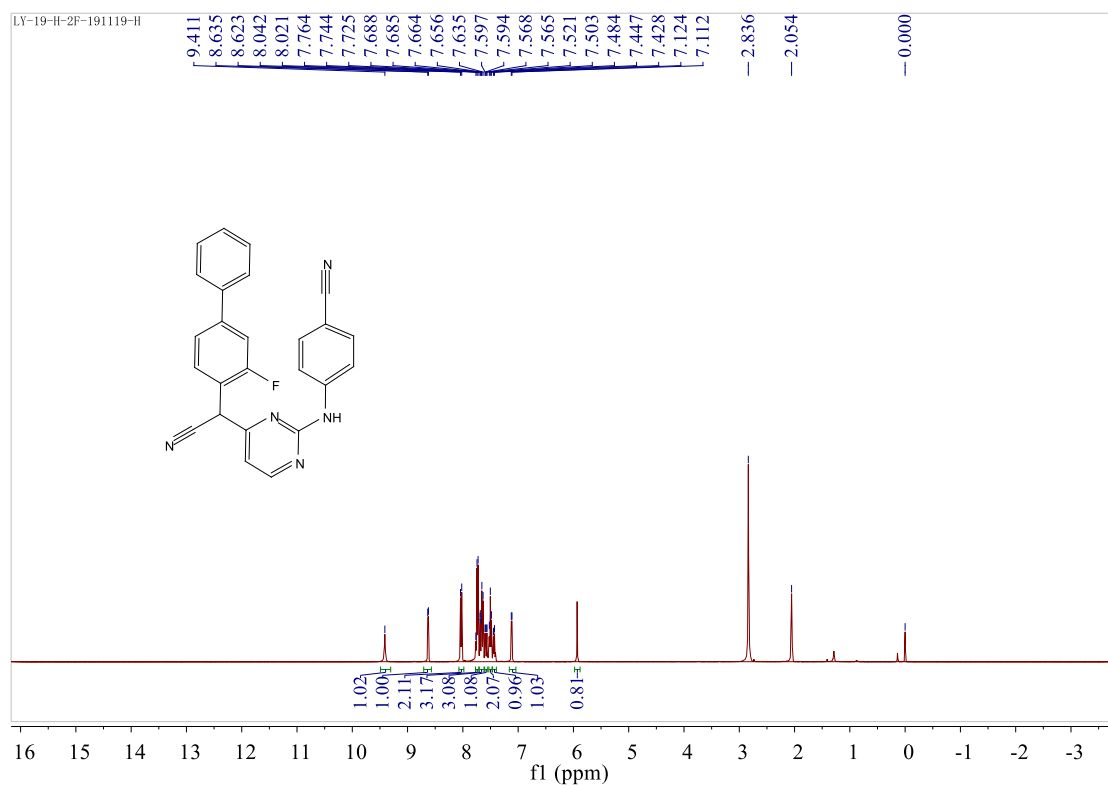
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### 3. Spectra of compound 10c



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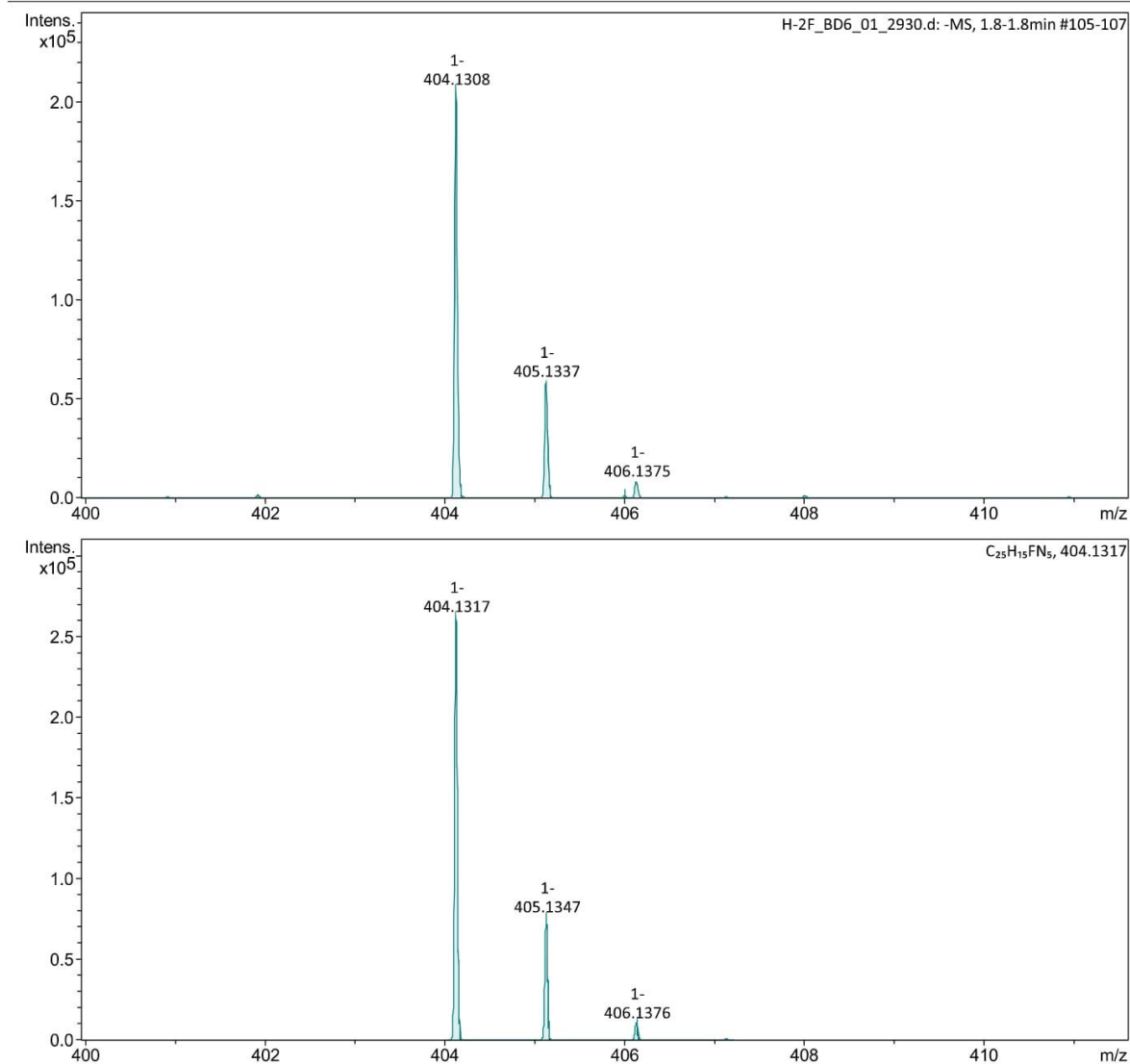
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Instrument compact 8255754.20127

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H-2F\_BD6\_01\_2930.d

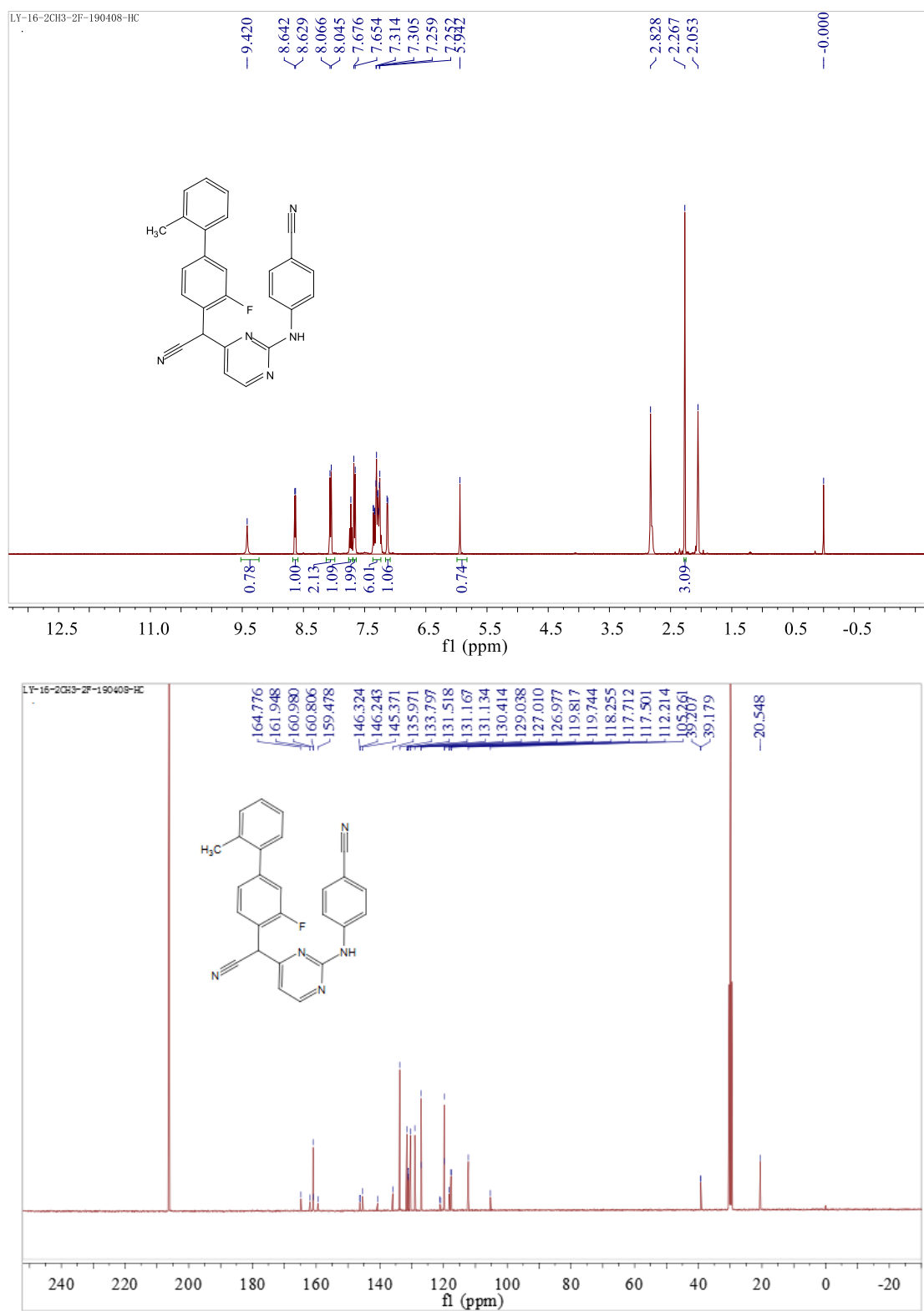
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#### 4. Spectra of compound 10d





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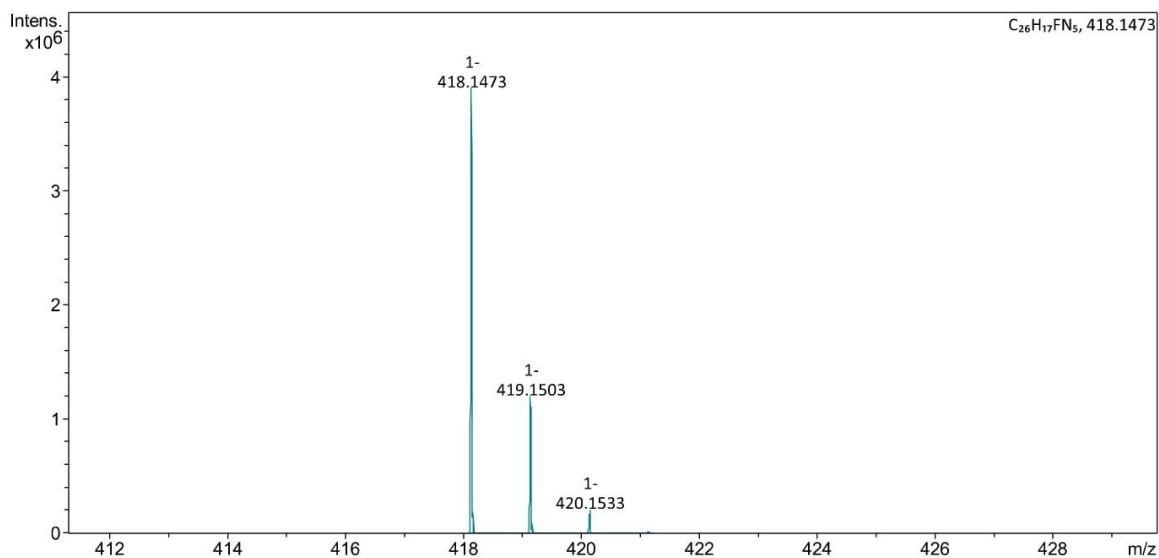
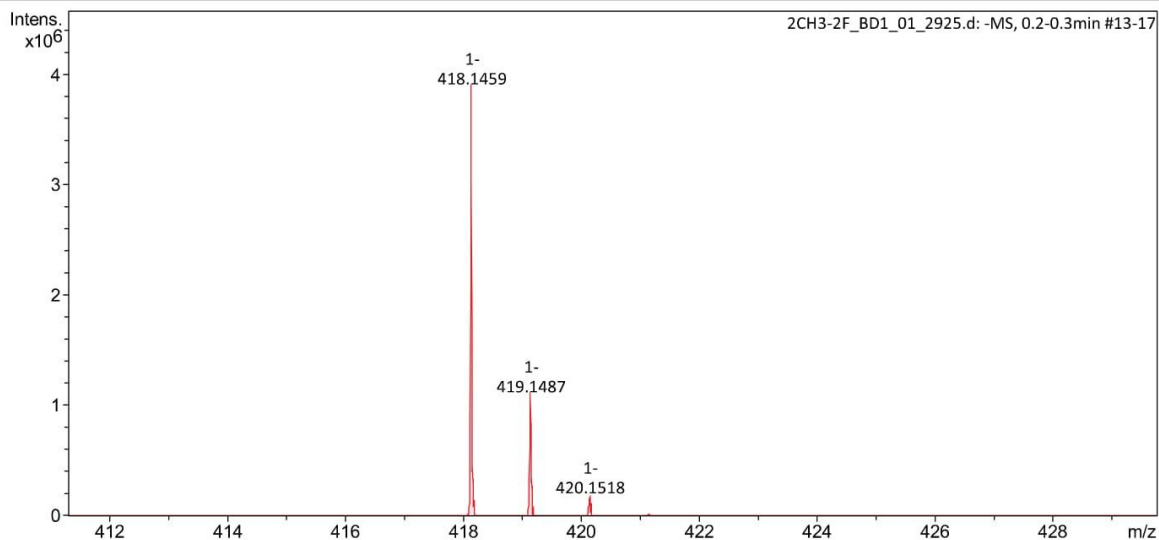
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Operator BDAL@DE  
Instrument compact 8255754.20127

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2CH3-2F\_BD1\_01\_2925.d

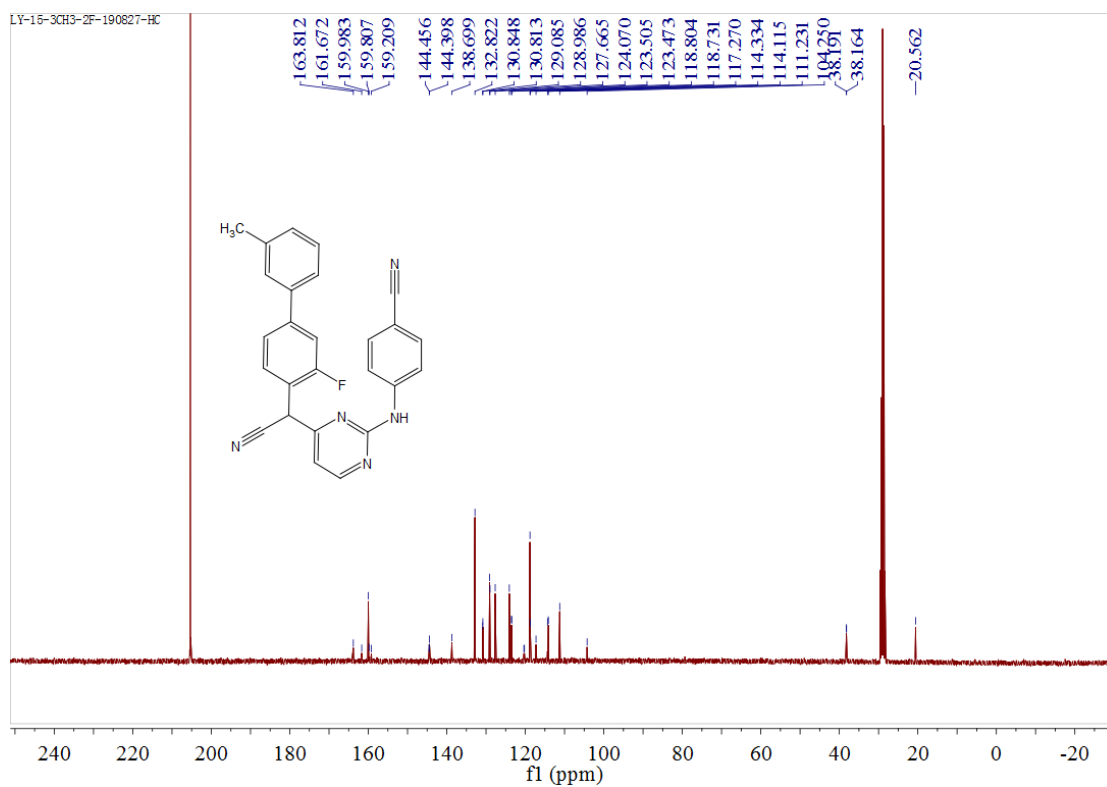
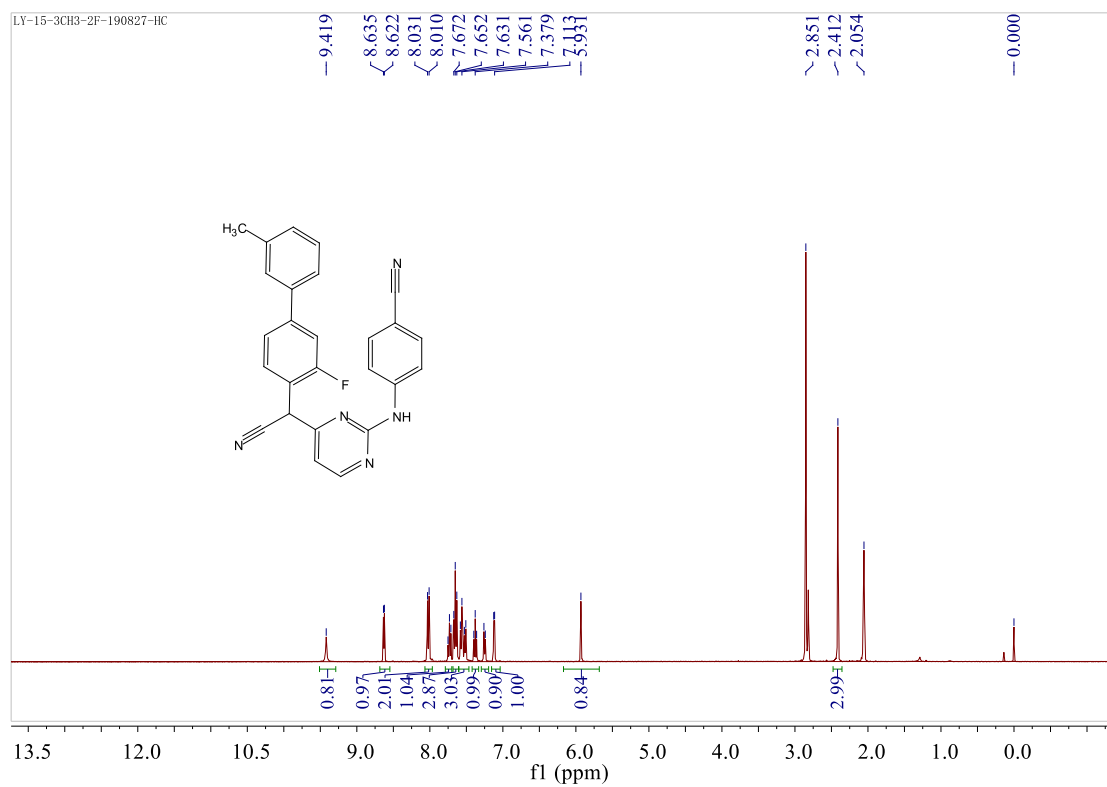
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## 5. Spectra of compound 10e



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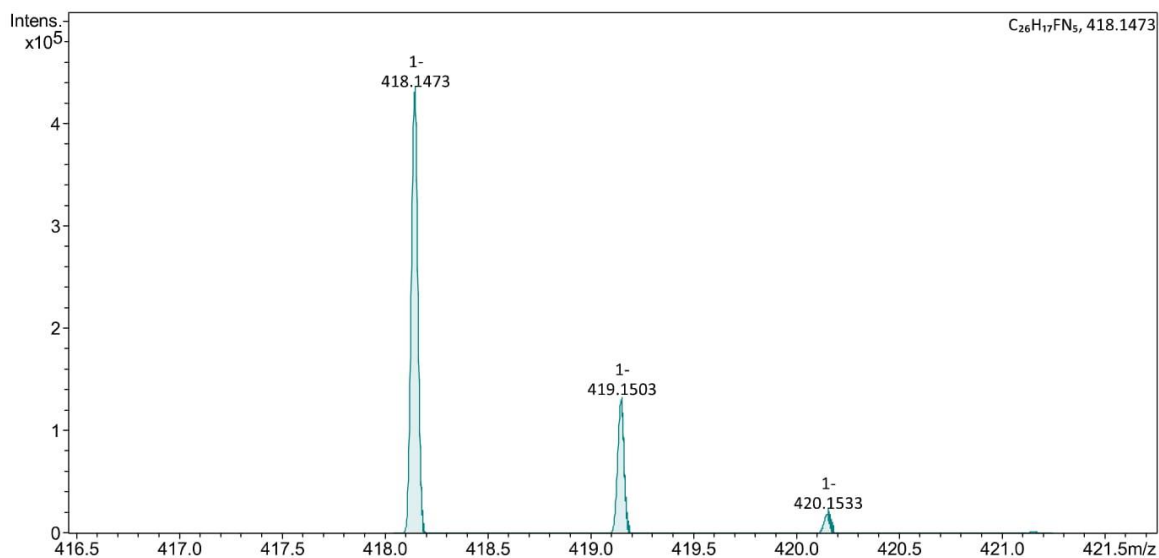
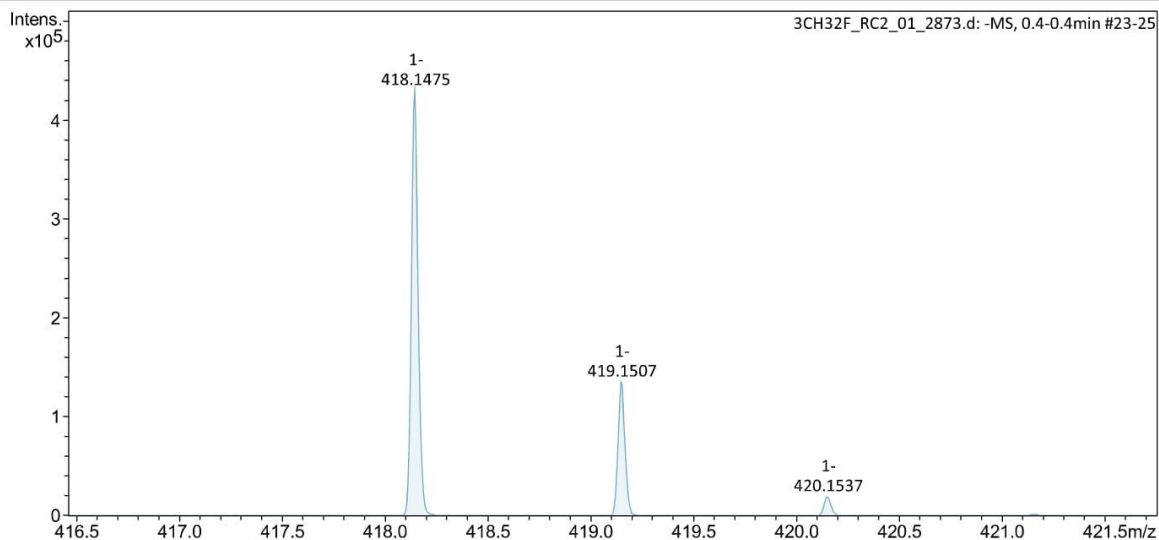
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Operator BDAL@DE  
Instrument compact 8255754.20127

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3CH32F\_RC2\_01\_2873.d

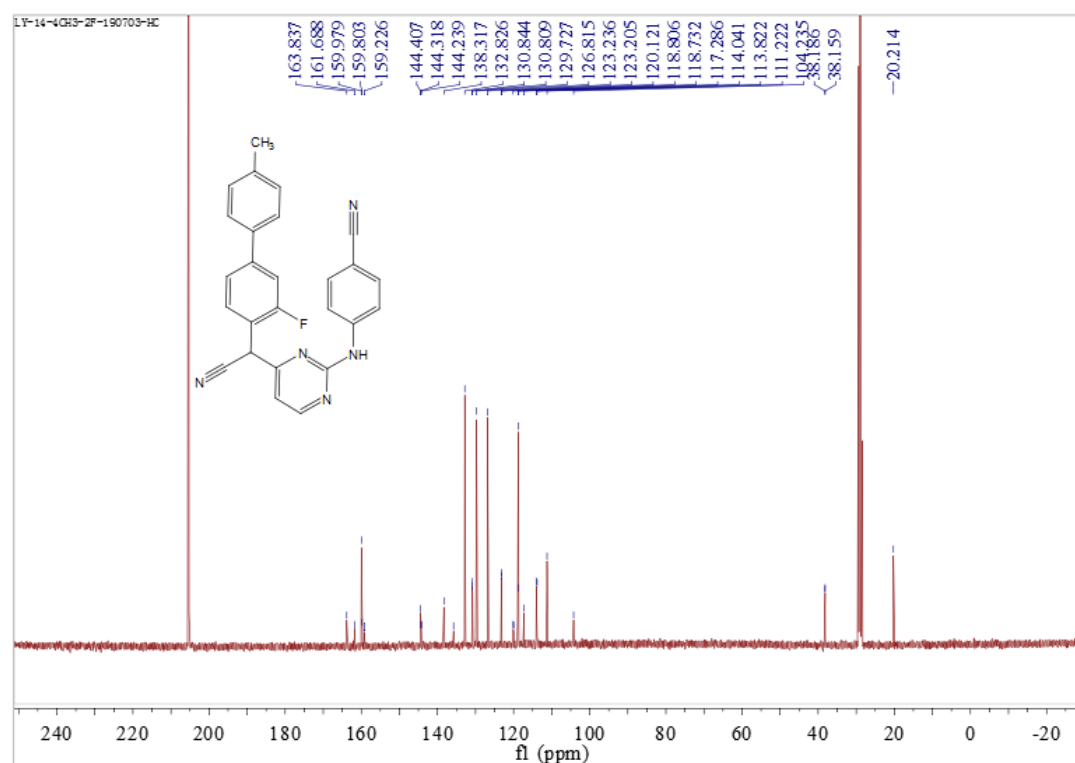
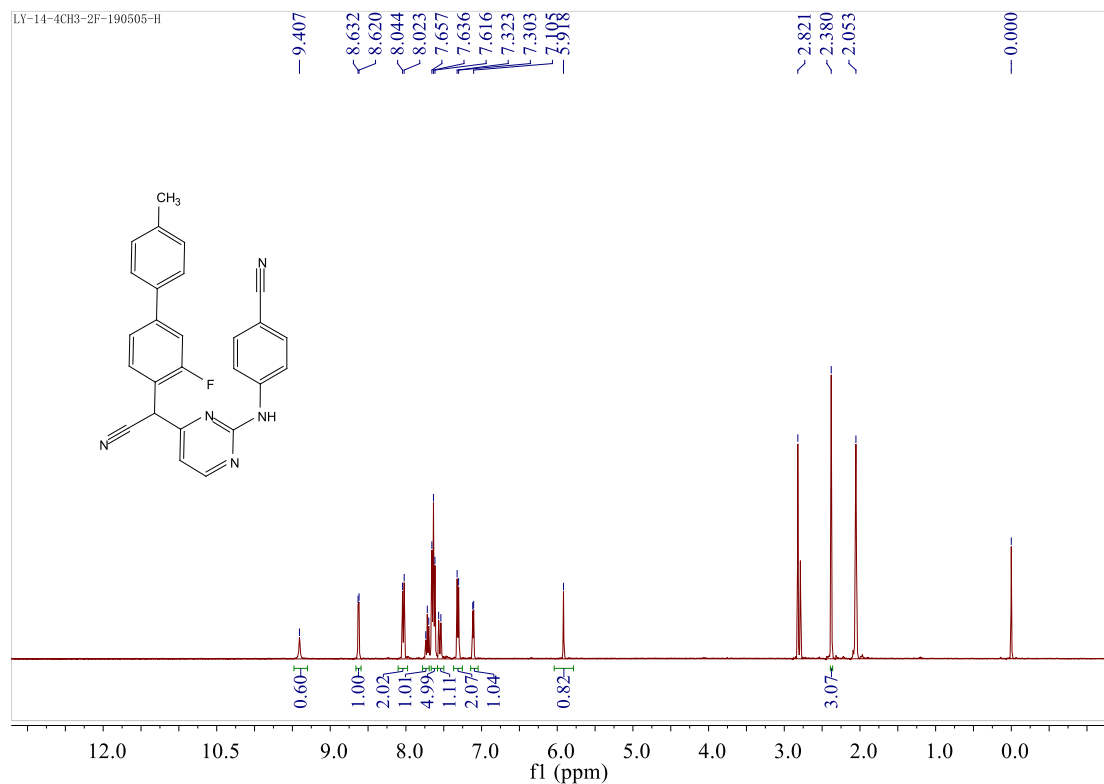
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## 6. Spectra of compound 10 f



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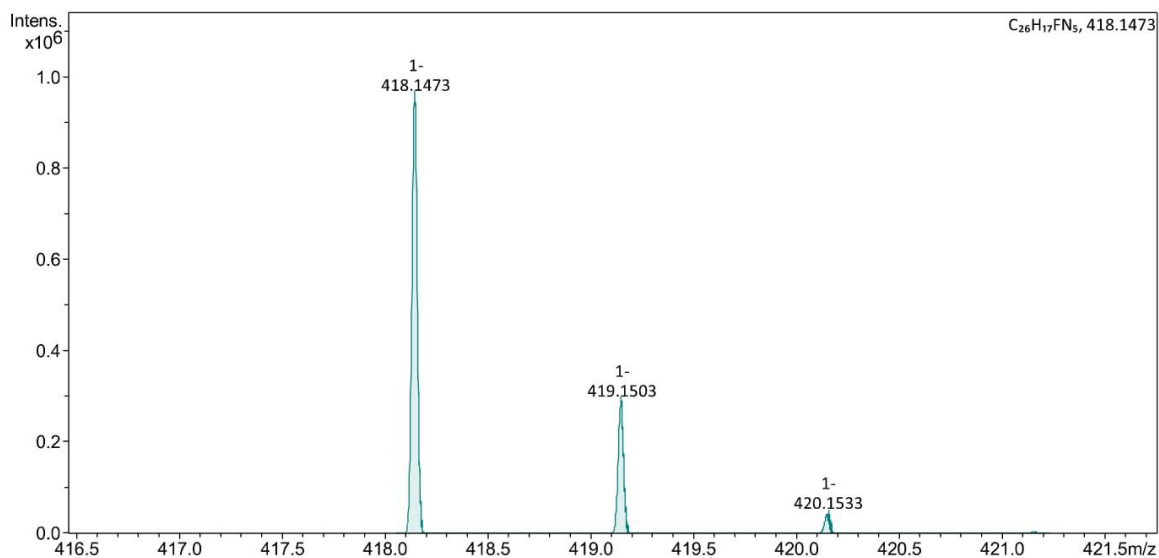
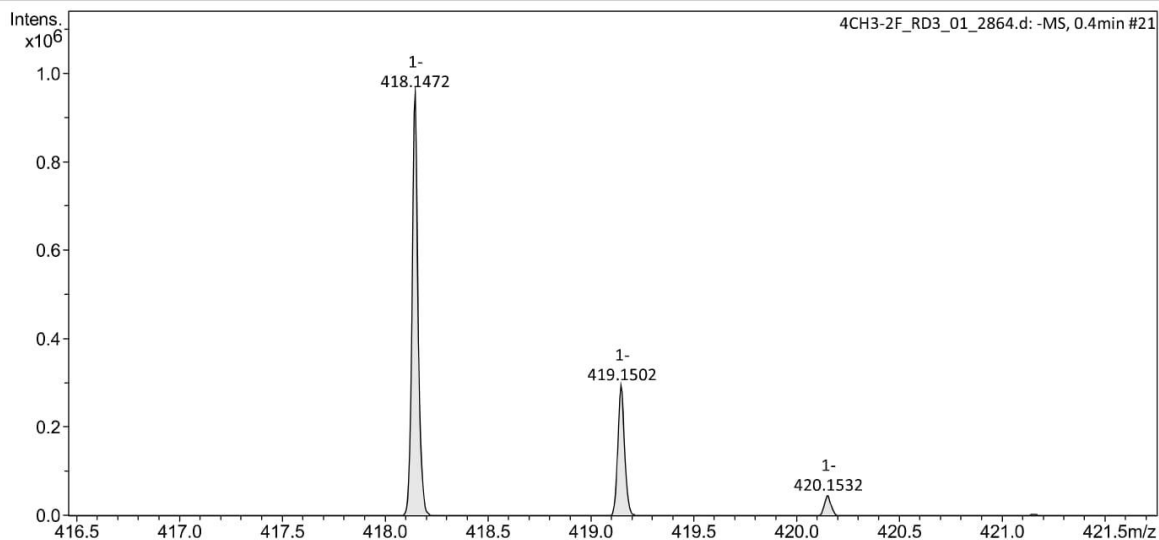
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Operator BDAL@DE  
Instrument compact 8255754.20127

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4CH3-2F\_RD3\_01\_2864.d

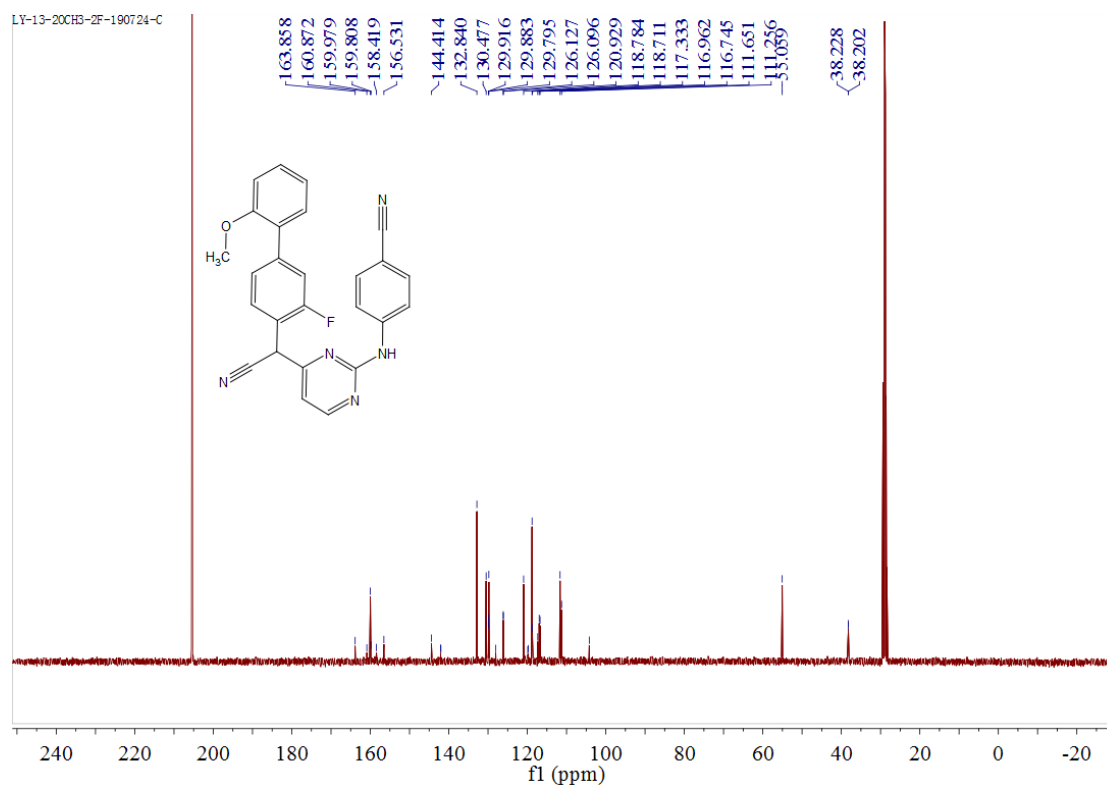
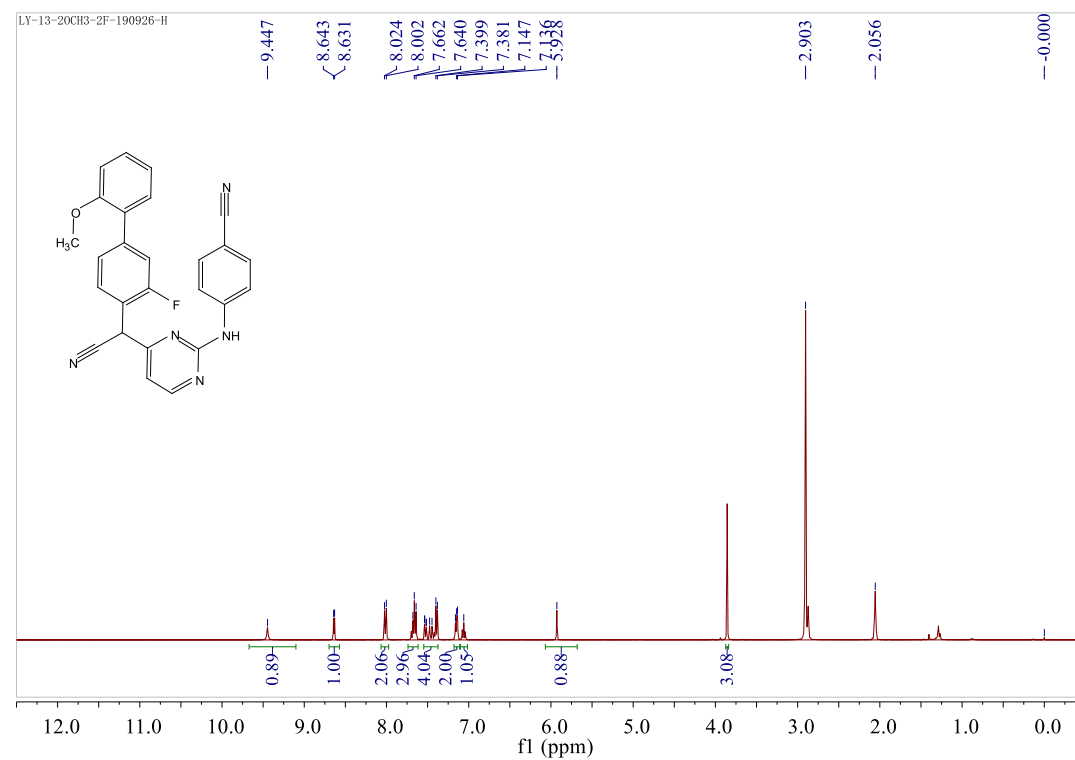
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## 7. Spectra of compound 10g



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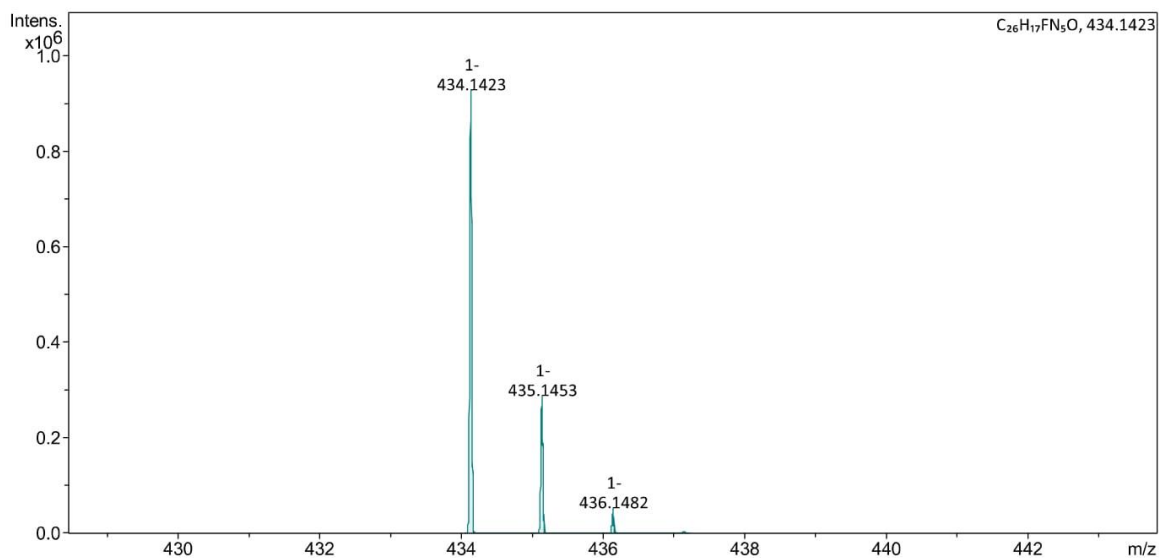
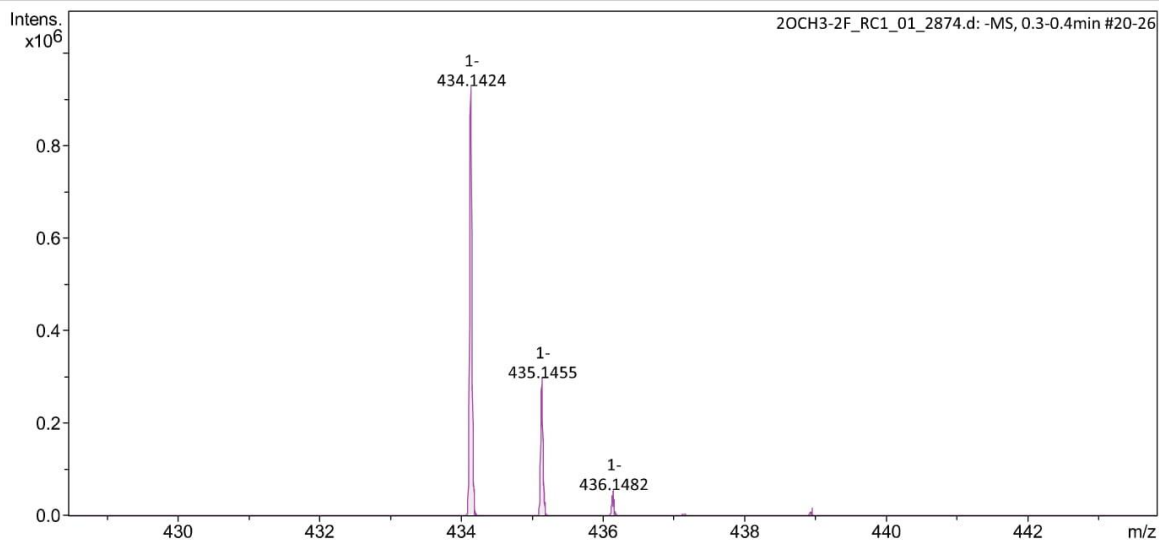
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Operator BDAL@DE  
Instrument compact 8255754.20127

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2OCH3-2F\_RC1\_01\_2874.d

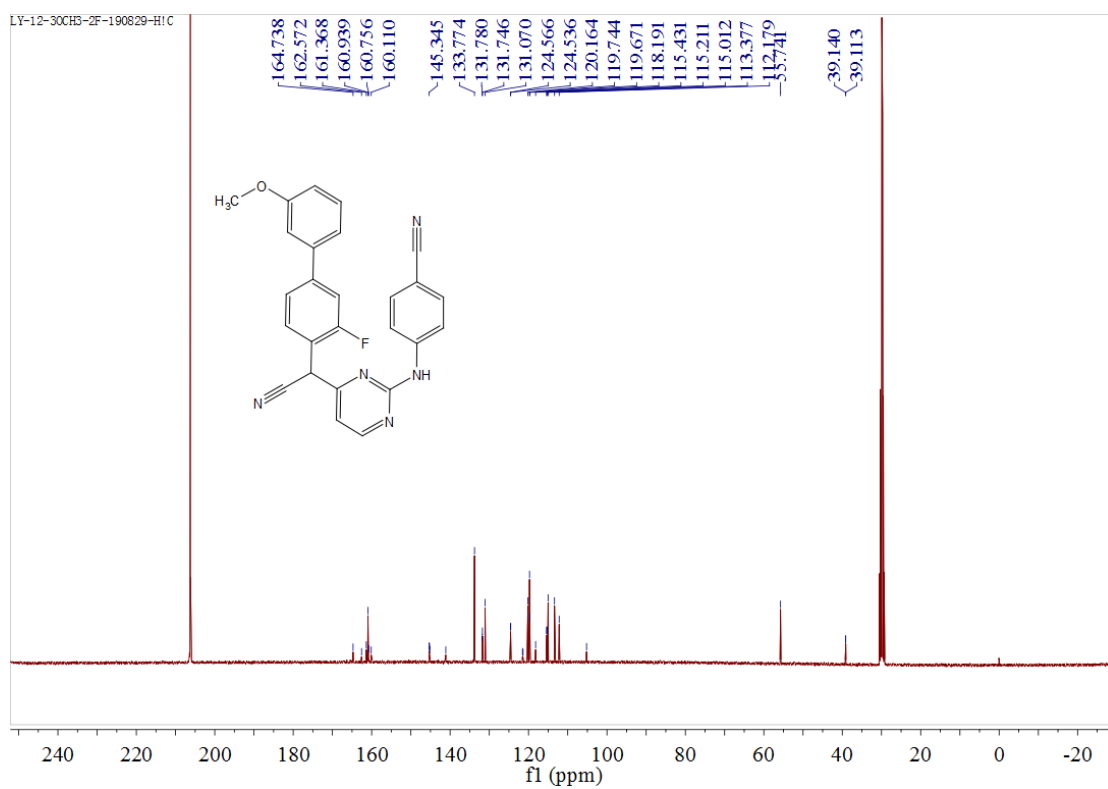
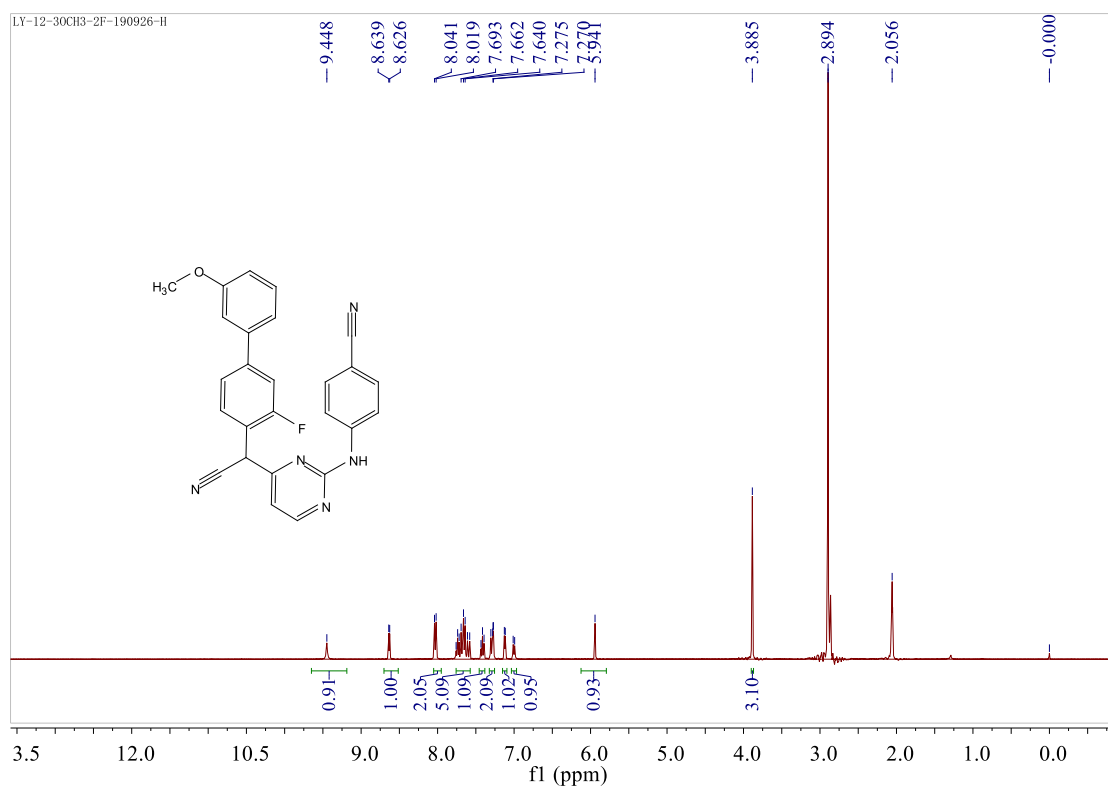
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## 8. Spectra of compound 10h





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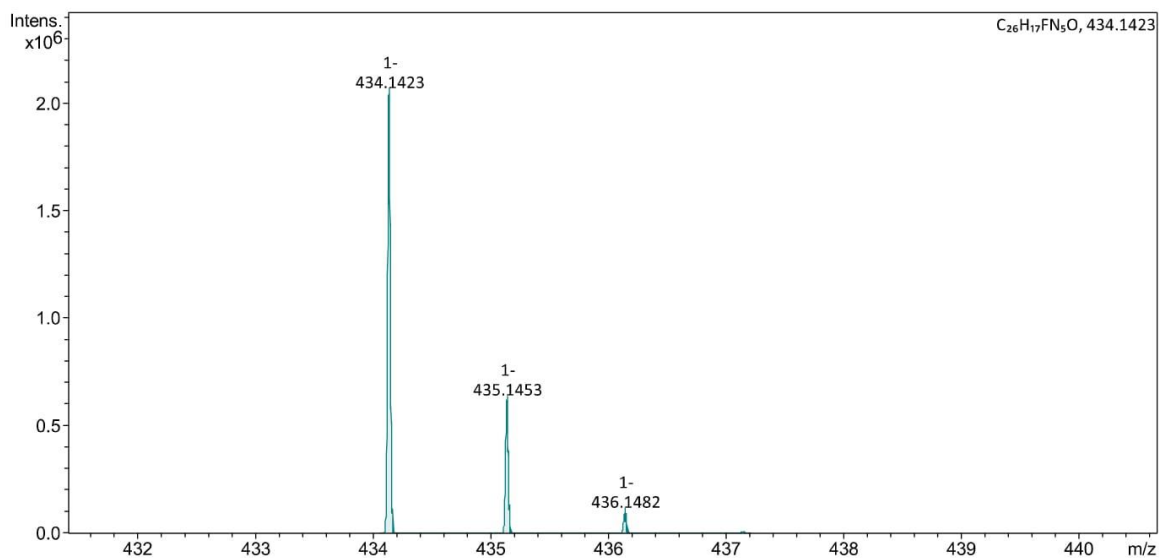
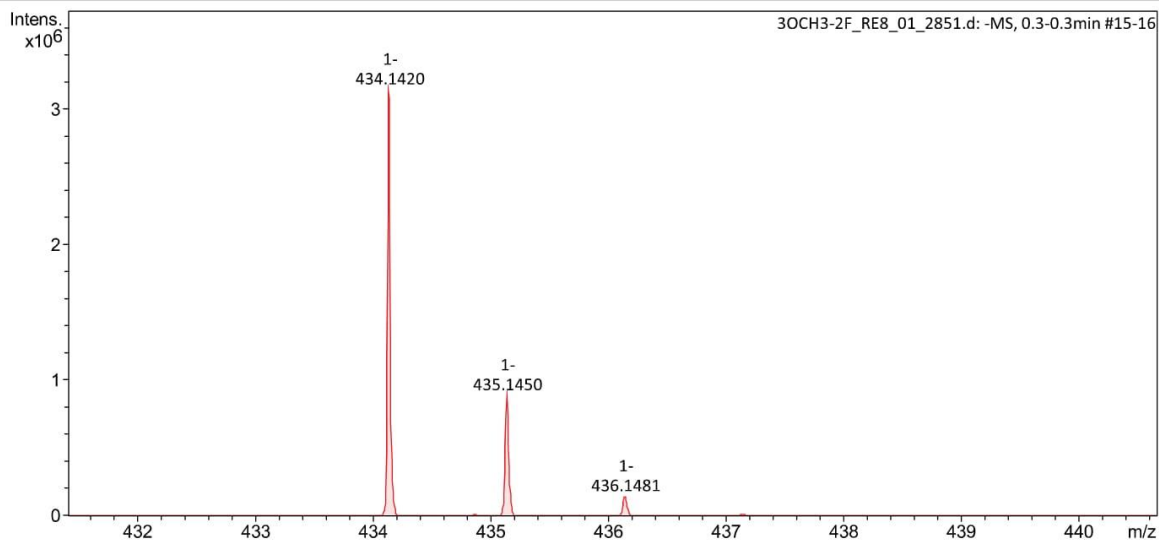
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Operator BDAL@DE  
Instrument compact 8255754.20127

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3OCH3-2F\_RE8\_01\_2851.d

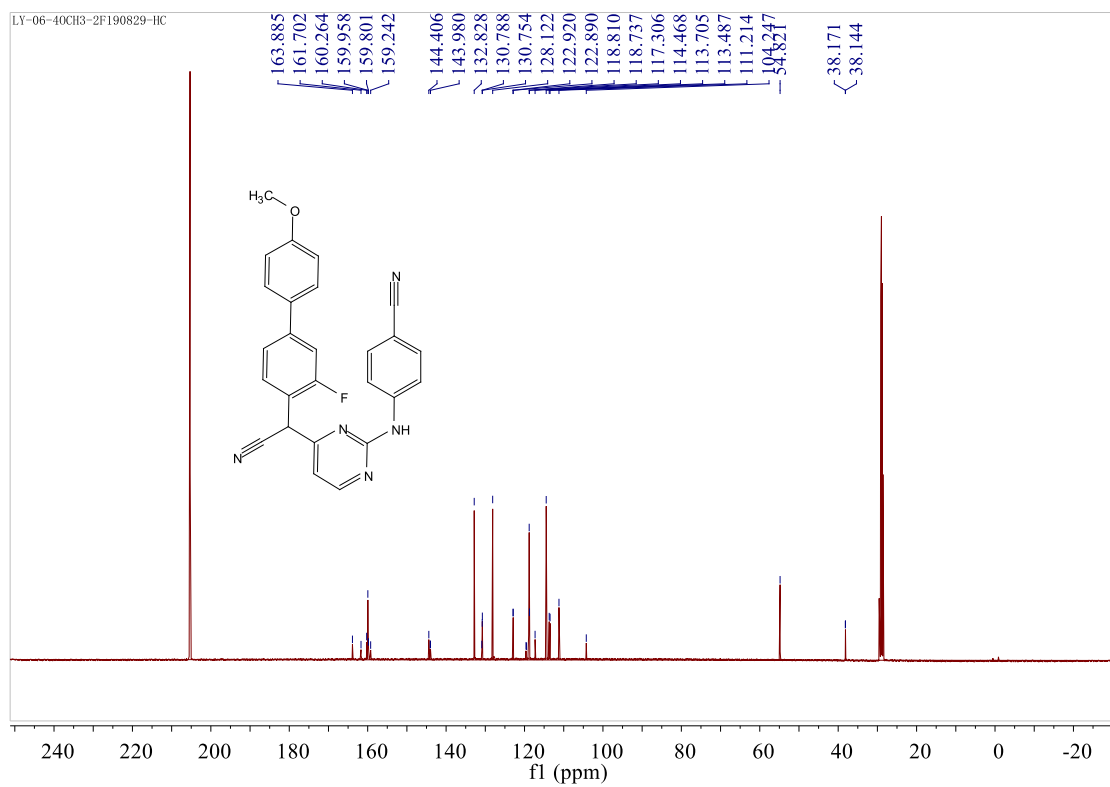
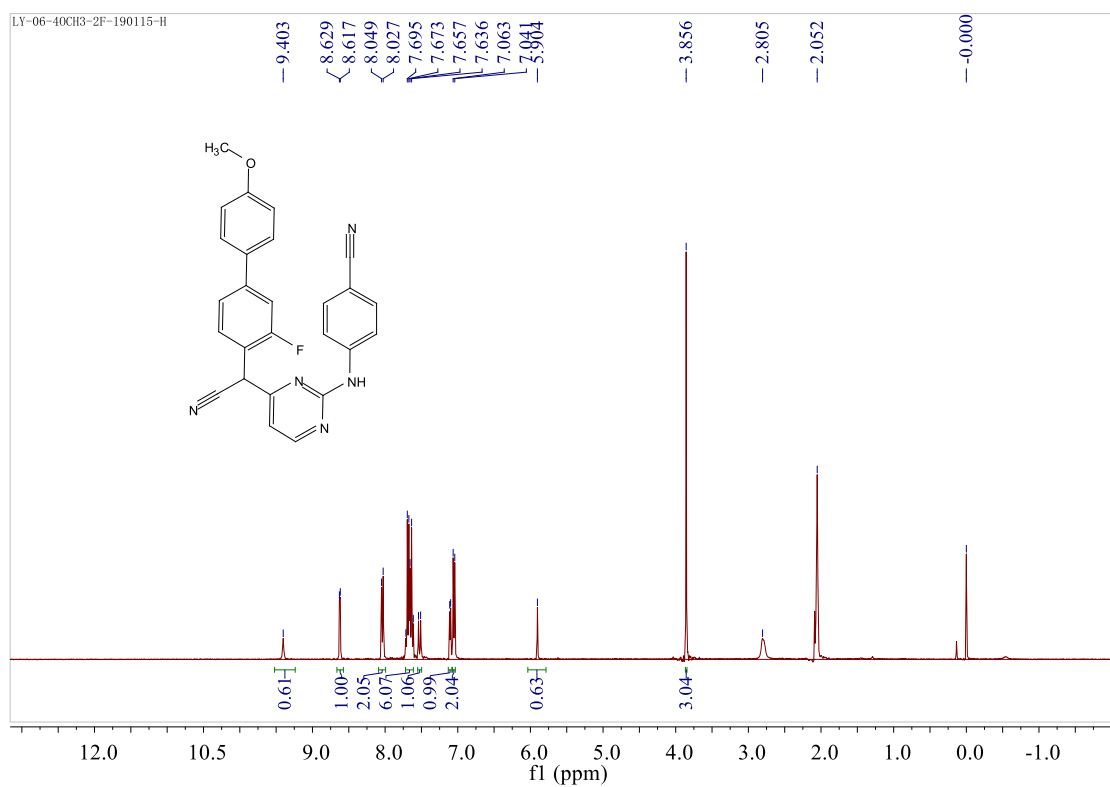
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## 9. Spectra of compound 10i



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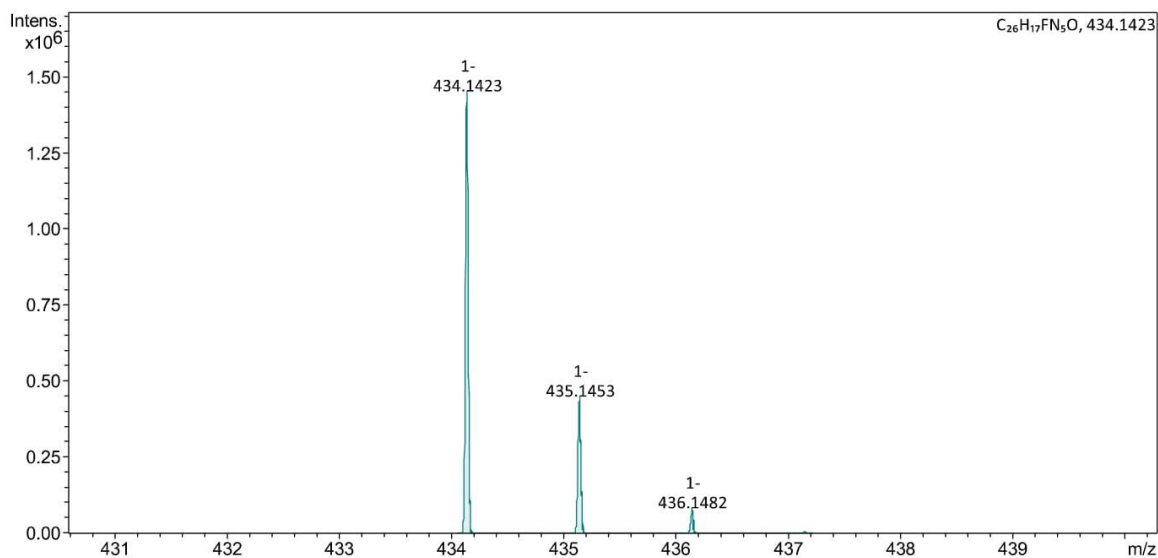
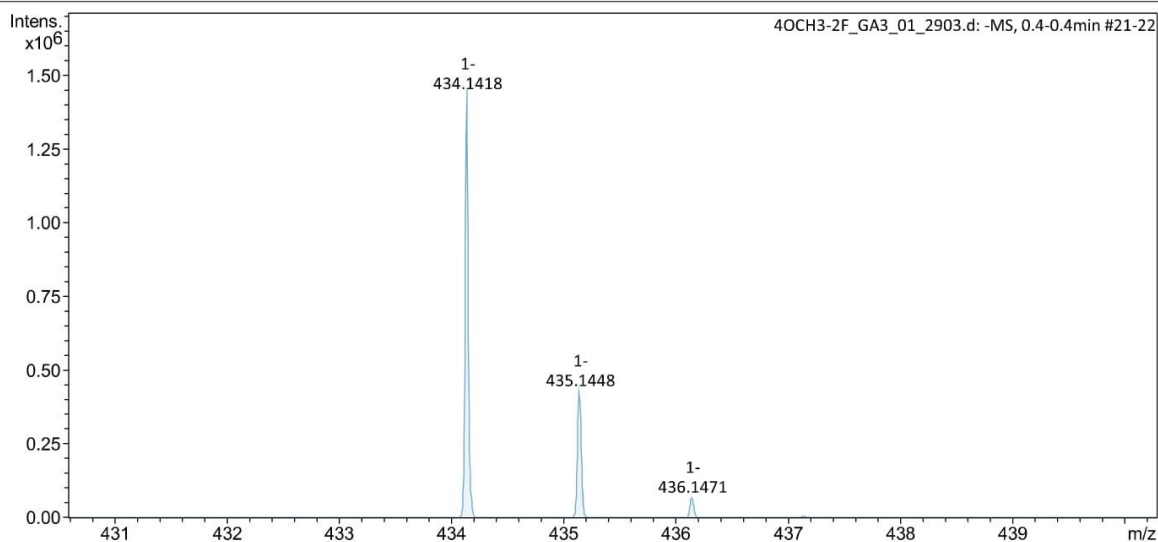
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Operator BDAL@DE  
Instrument compact 8255754.20127

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4OCH3-2F\_GA3\_01\_2903.d

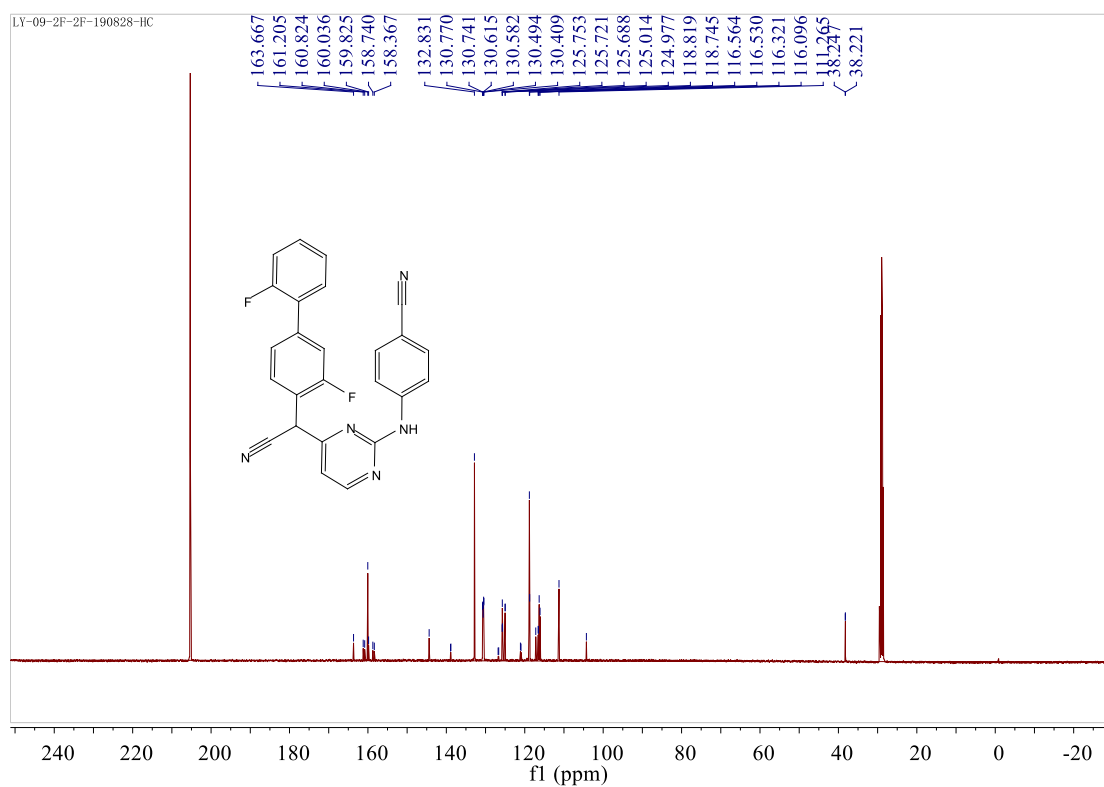
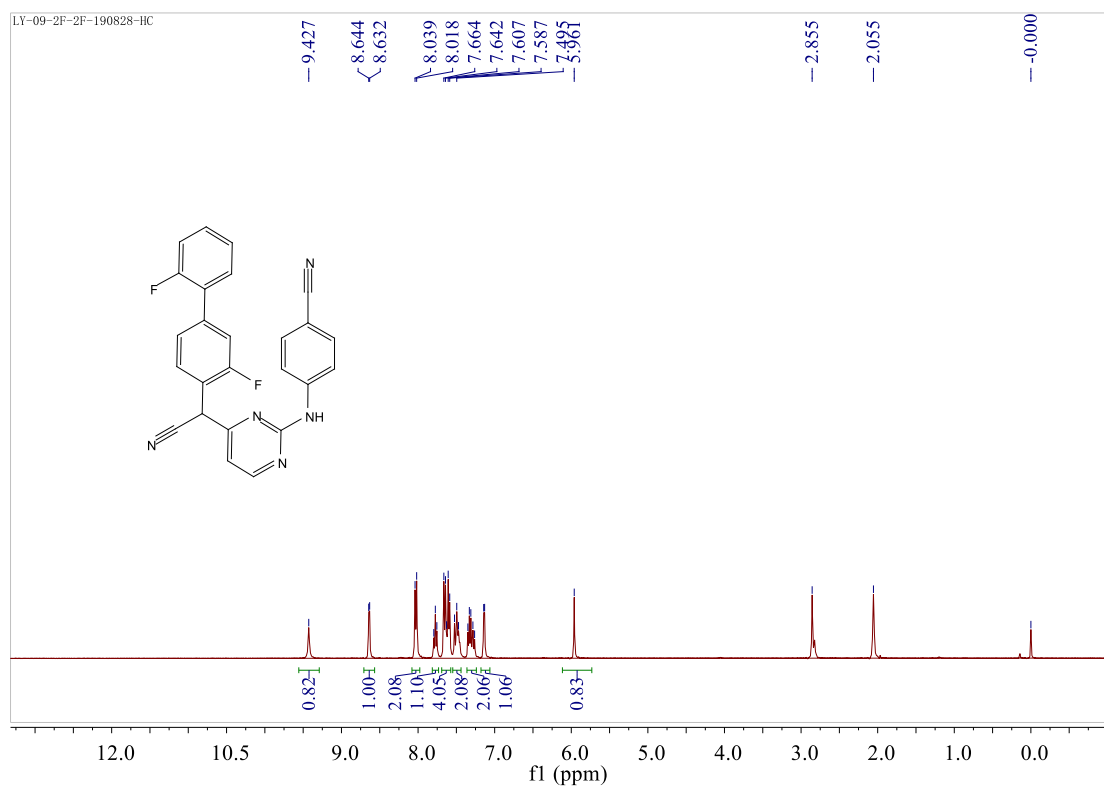
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## 10. Spectra of compound 10j



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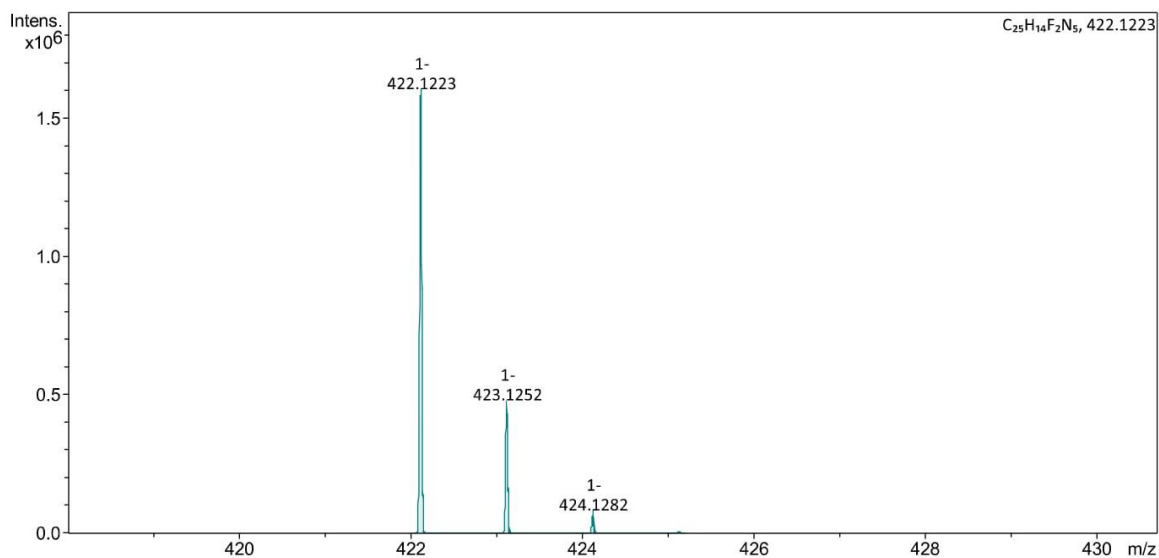
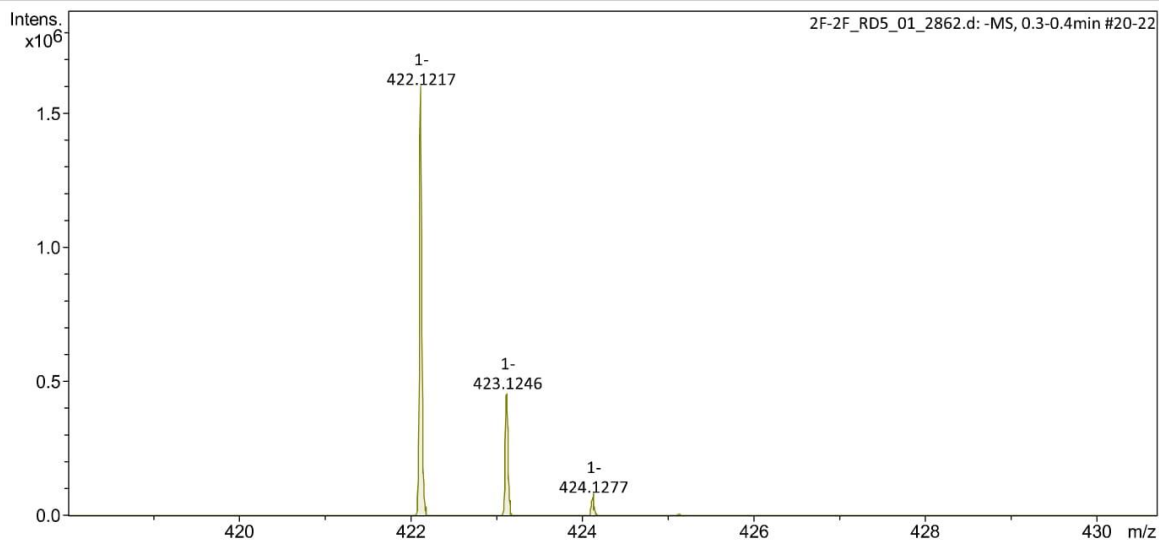
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### Acquisition Parameter

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2F-2F\_RD5\_01\_2862.d

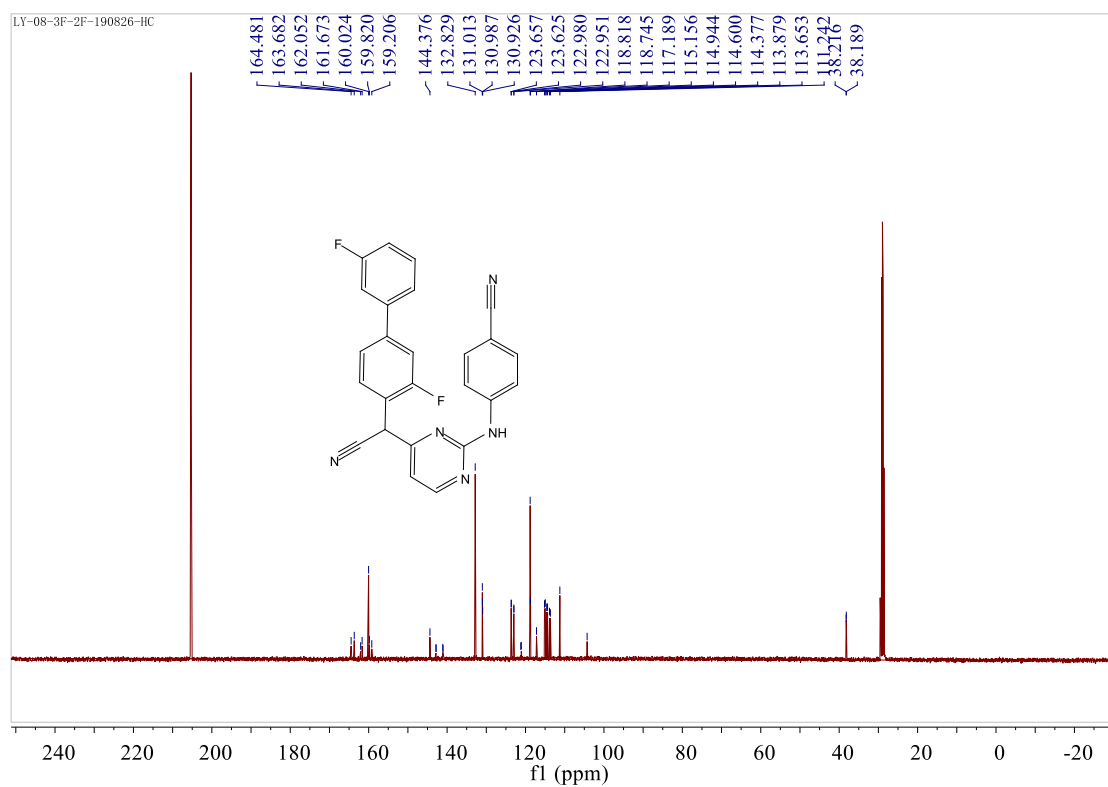
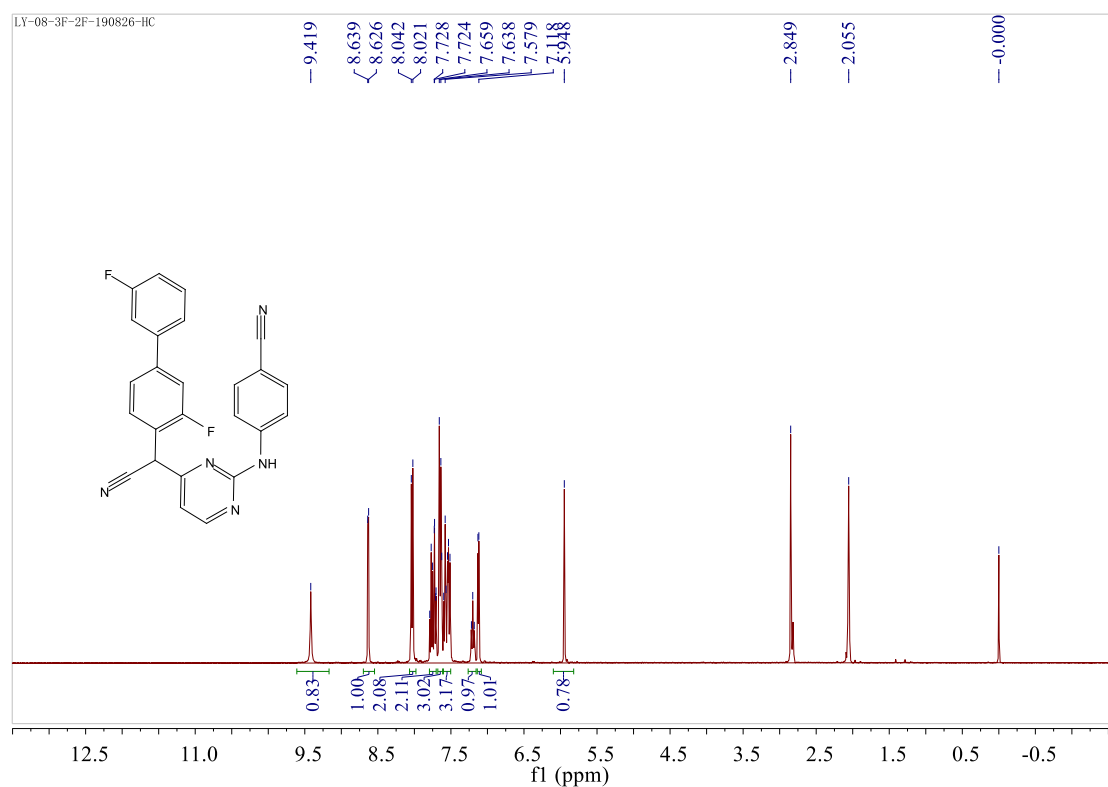
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## 11. Spectra of compound 10k



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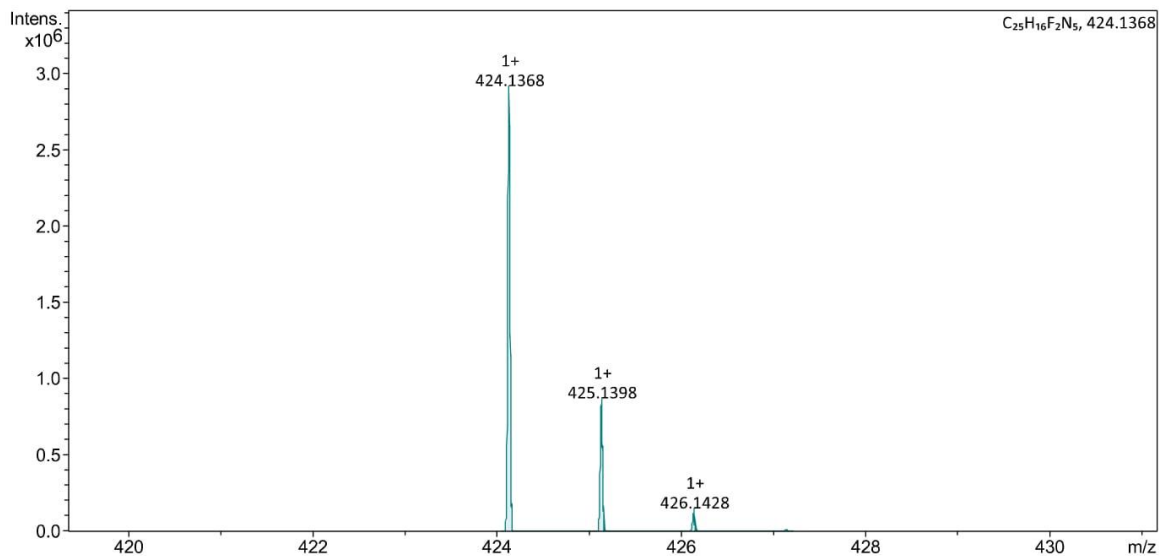
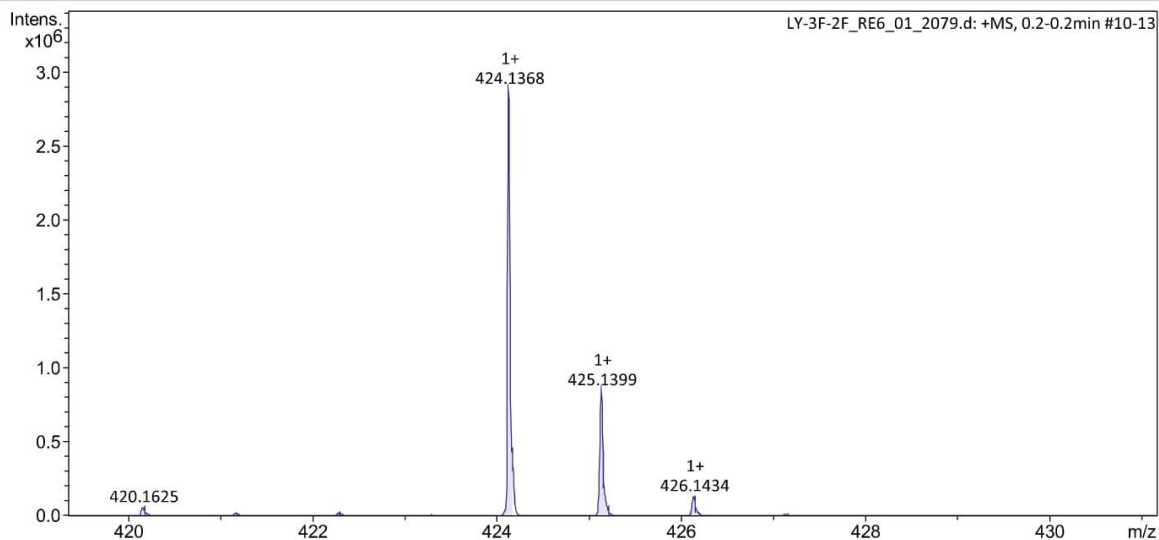
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Comment

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Operator BDAL@DE  
Instrument compact 8255754.20127

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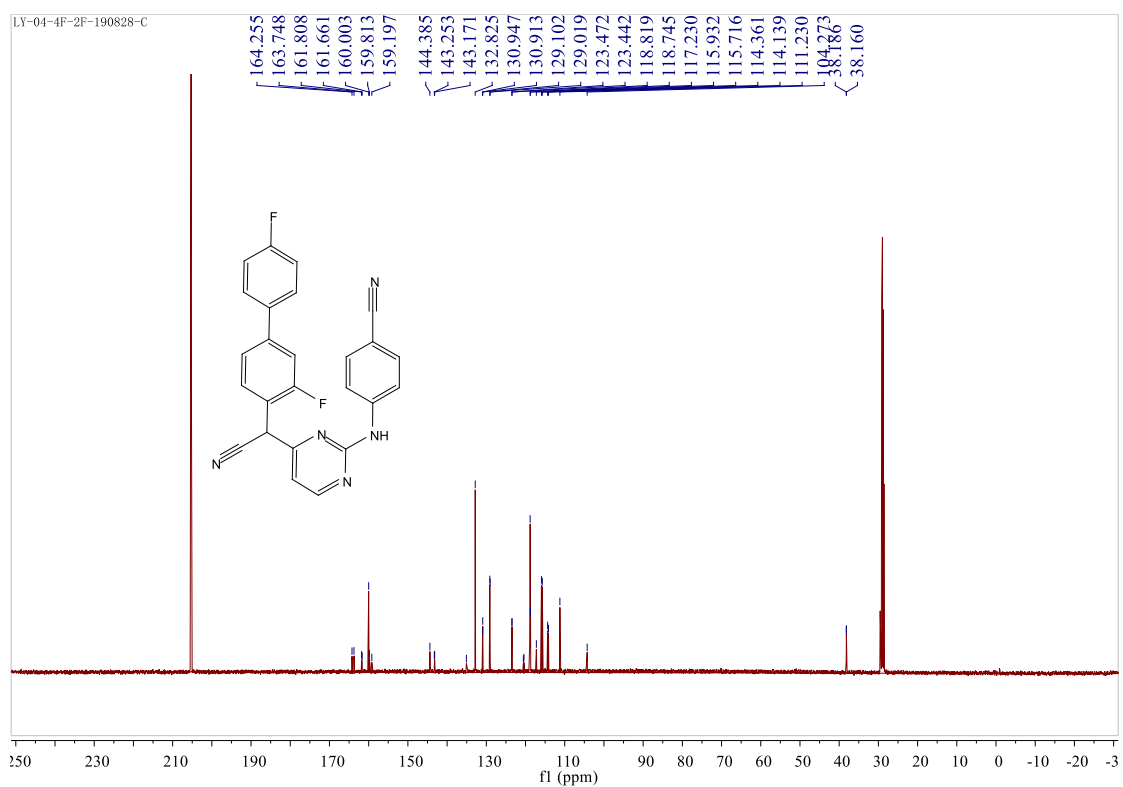
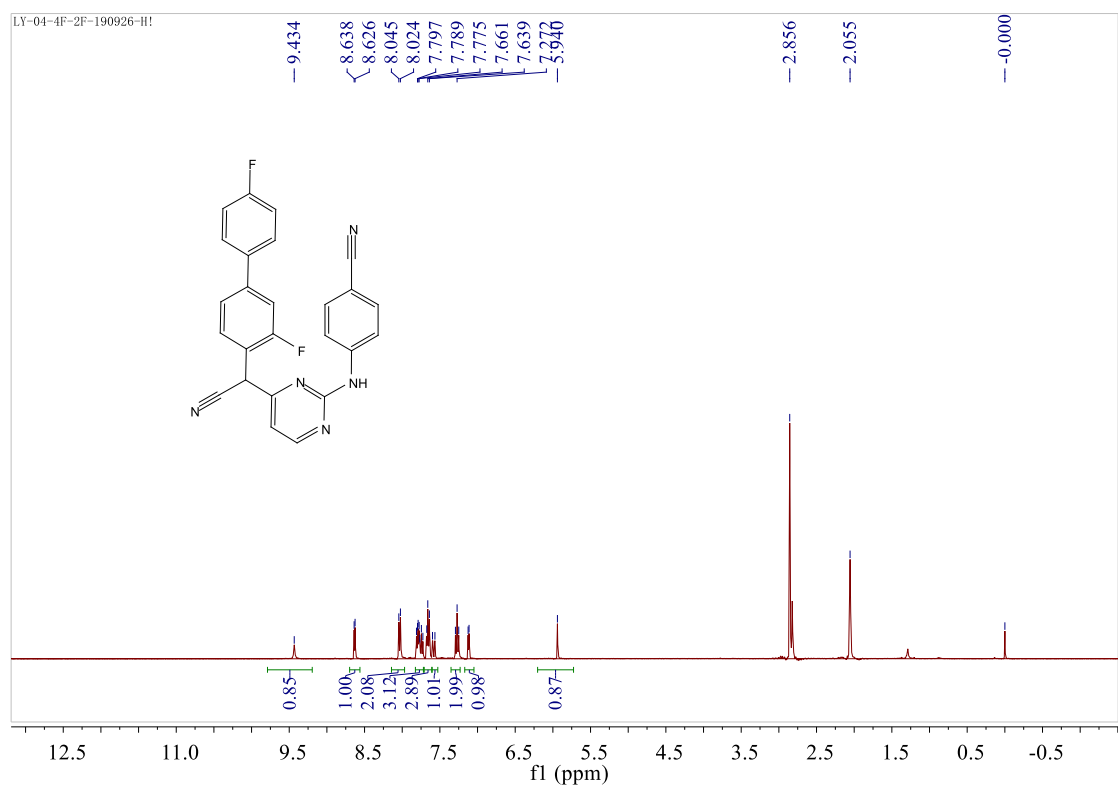
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## 12. Spectra of compound 10k





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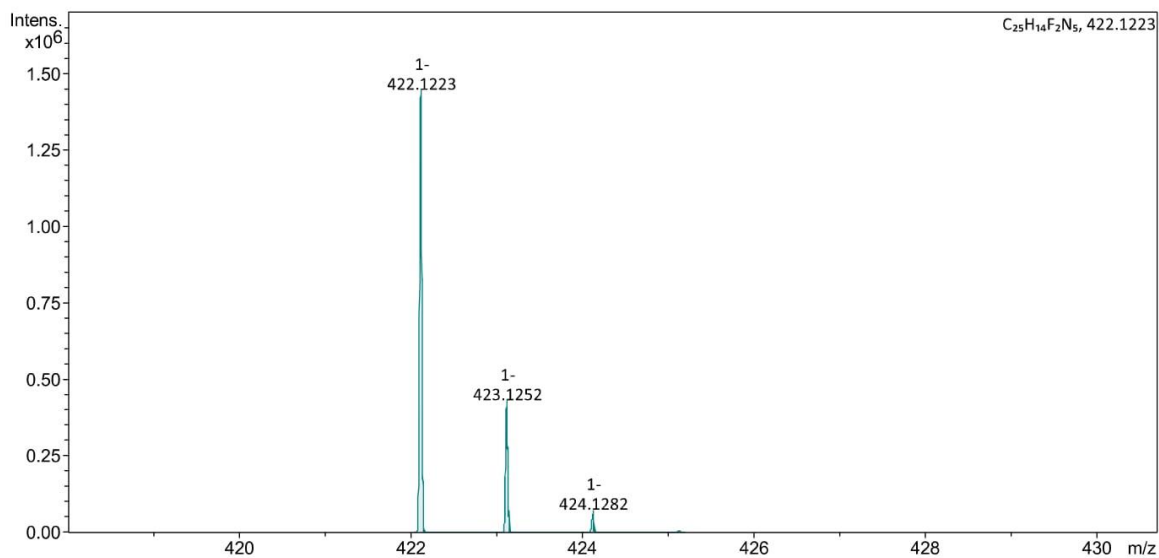
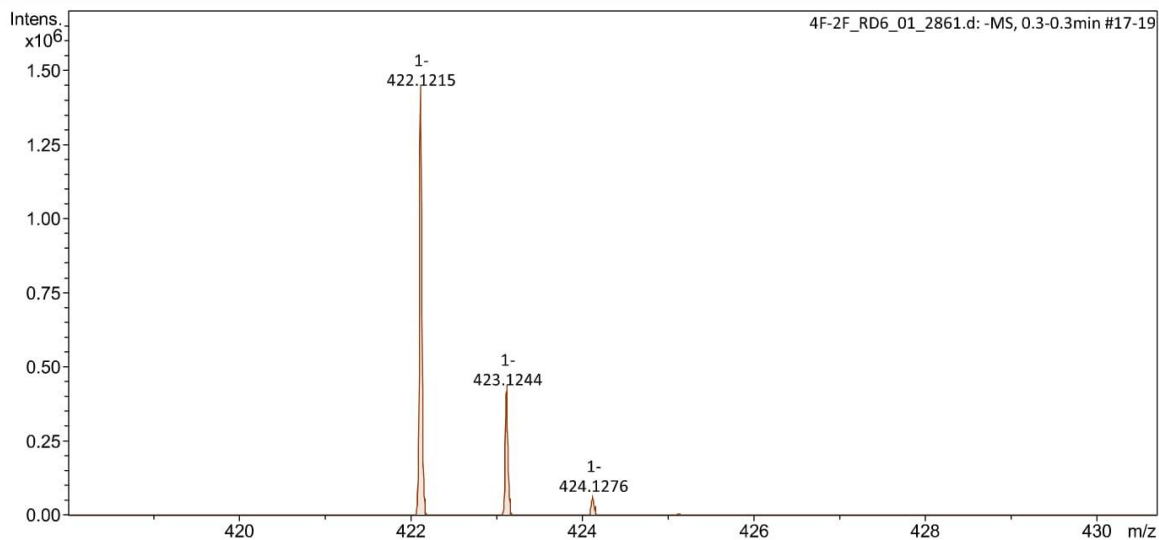
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Operator BDAL@DE  
Instrument compact 8255754.20127

### Acquisition Parameter

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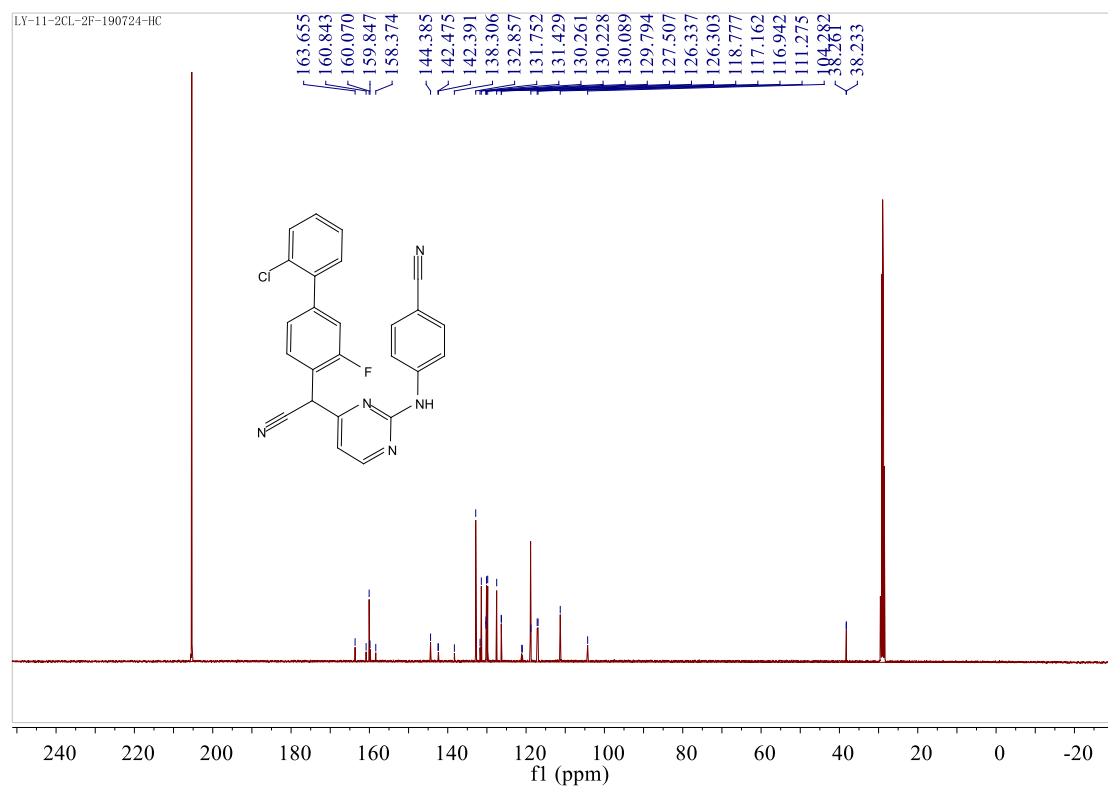
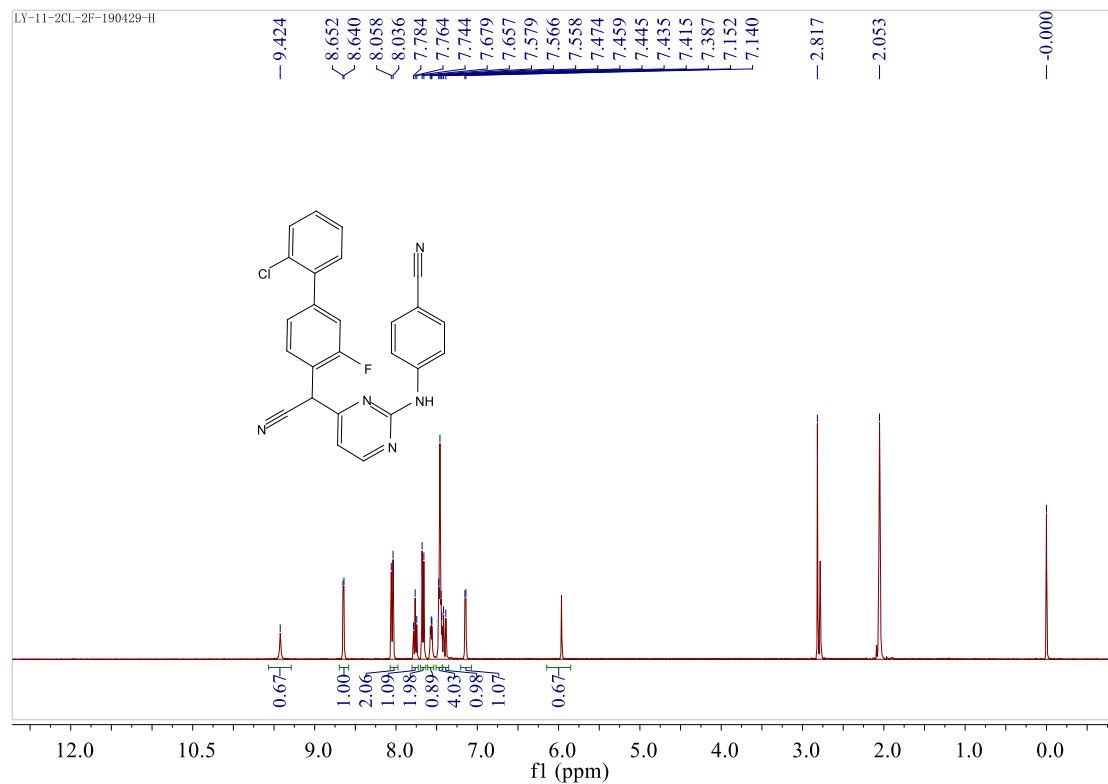
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### 13. Spectra of compound 10m



## Display Report

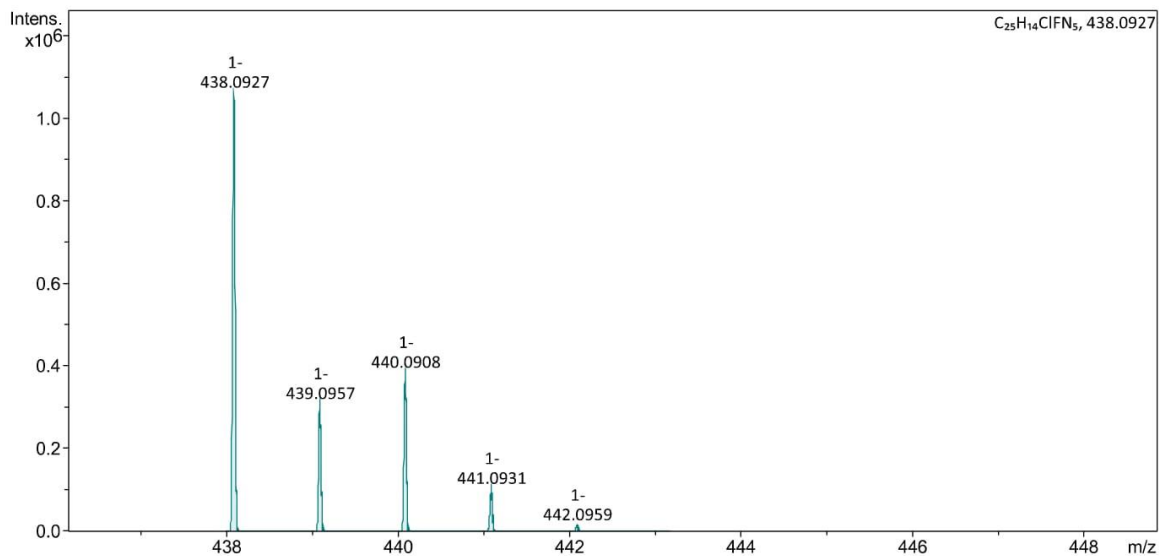
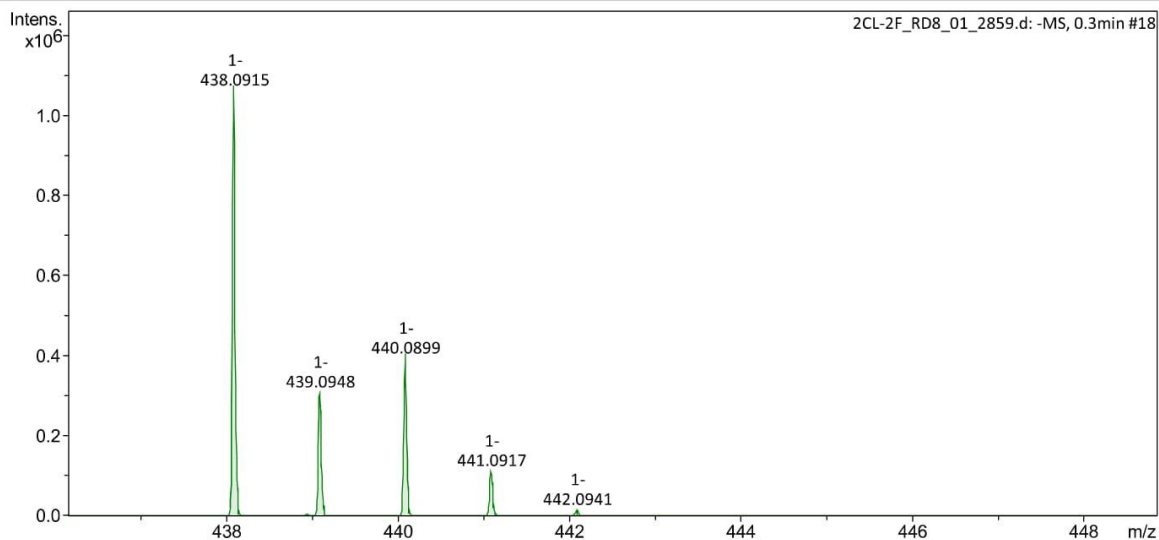
### Analysis Info

Analysis Name D:\Data\data\2019\2CL-2F\_RD8\_01\_2859.d  
Method MS-2MIN-NEG.m  
Sample Name 2CL-2F  
Comment

Acquisition Date 12/18/2019 17:00:20 PM  
Operator BDAL@DE  
Instrument compact 8255754.20127

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



2CL-2F\_RD8\_01\_2859.d

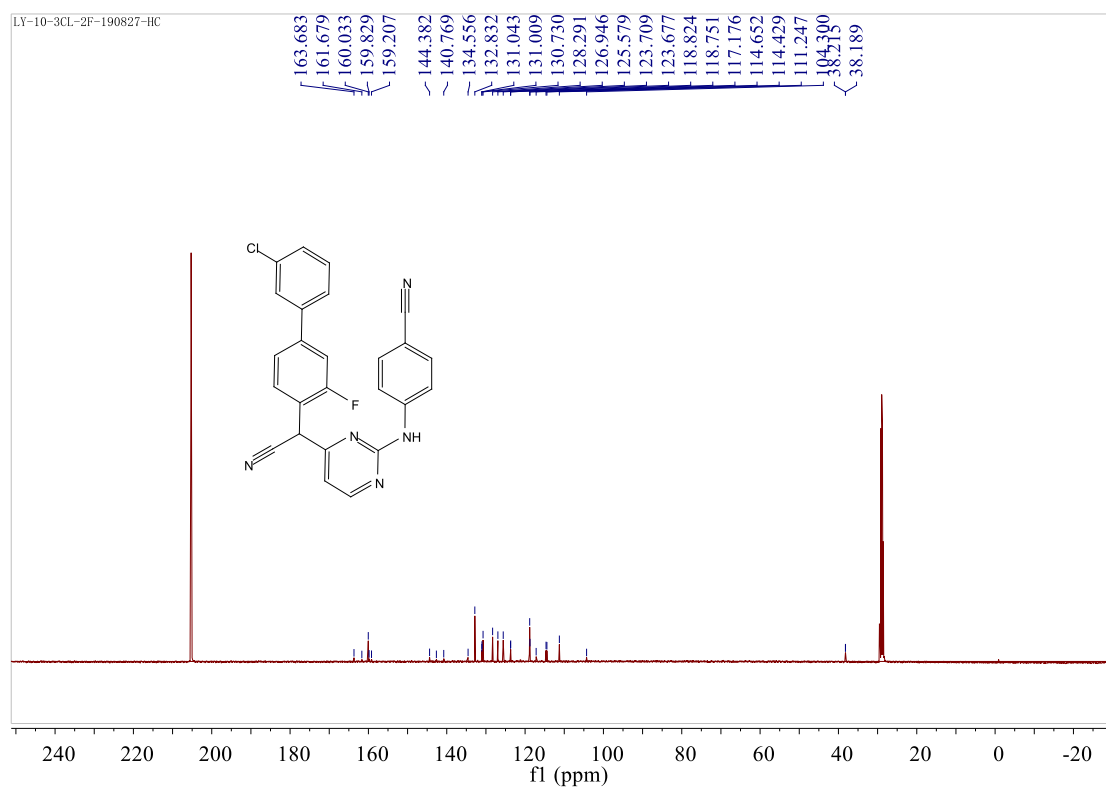
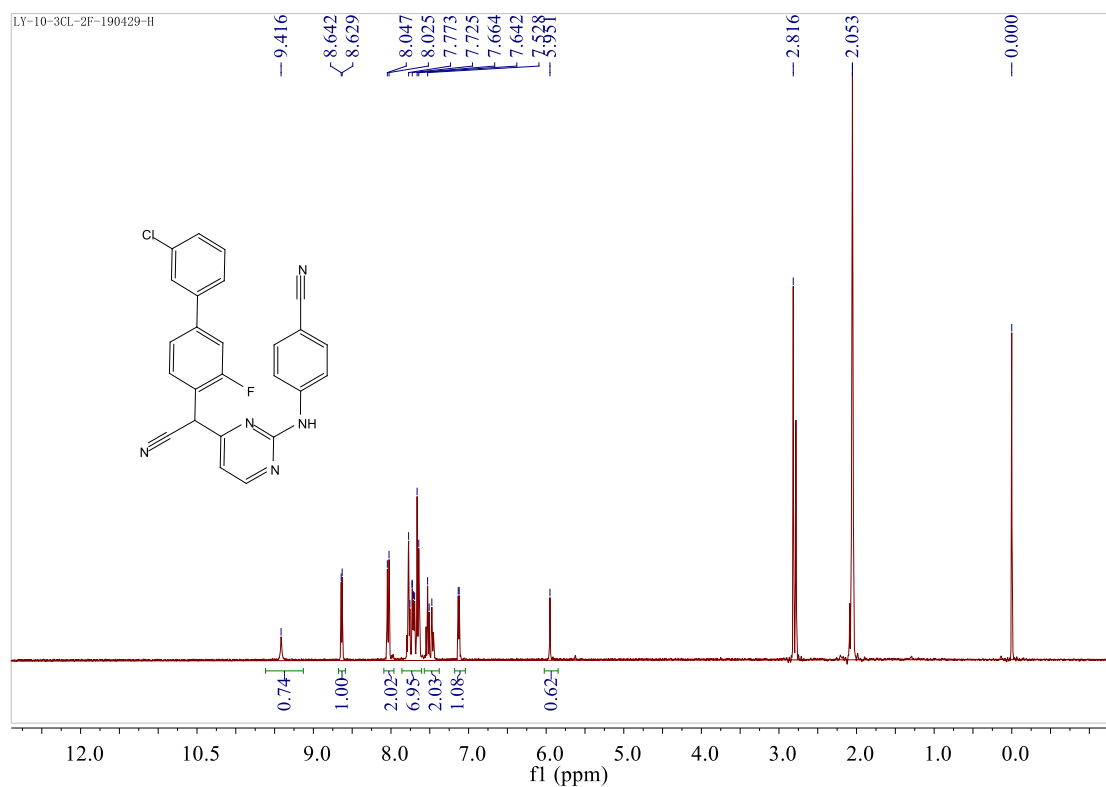
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## 14. Spectra of compound 10n



## Display Report

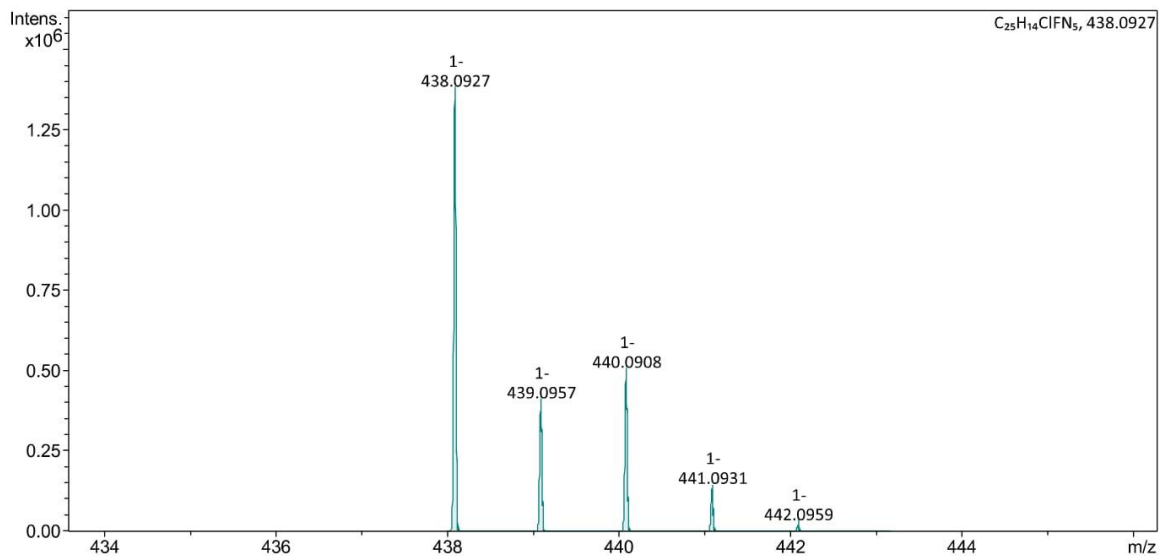
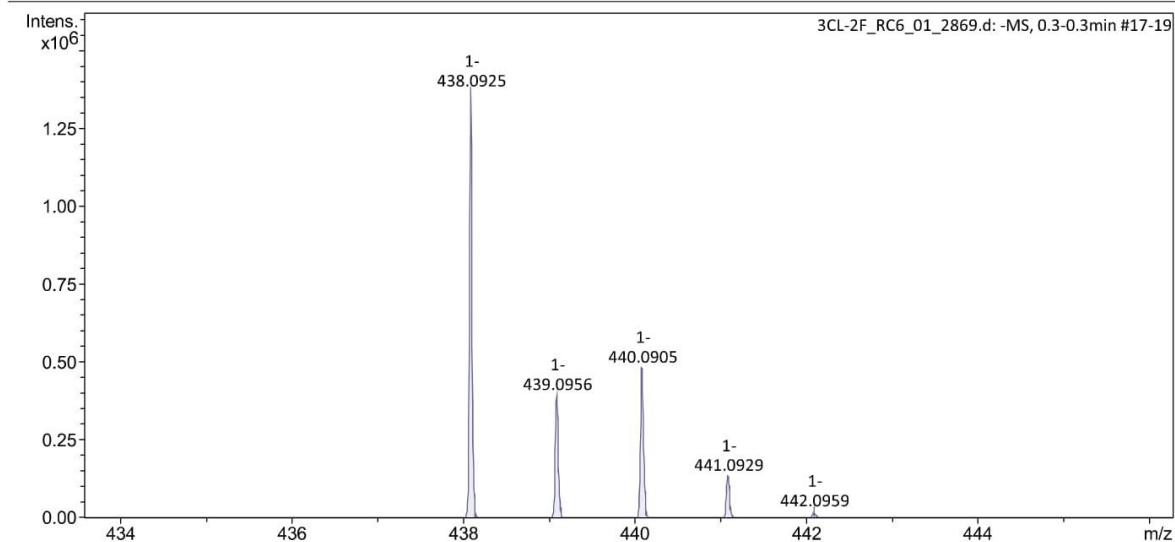
### Analysis Info

Analysis Name D:\Data\data\2019\3CL-2F\_RC6\_01\_2869.d  
Method MS-2MIN-NEG.m  
Sample Name 3CL-2F  
Comment

Acquisition Date 12/18/2019 17:27:57 PM  
Operator BDAL@DE  
Instrument compact 8255754.20127

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



3CL-2F\_RC6\_01\_2869.d

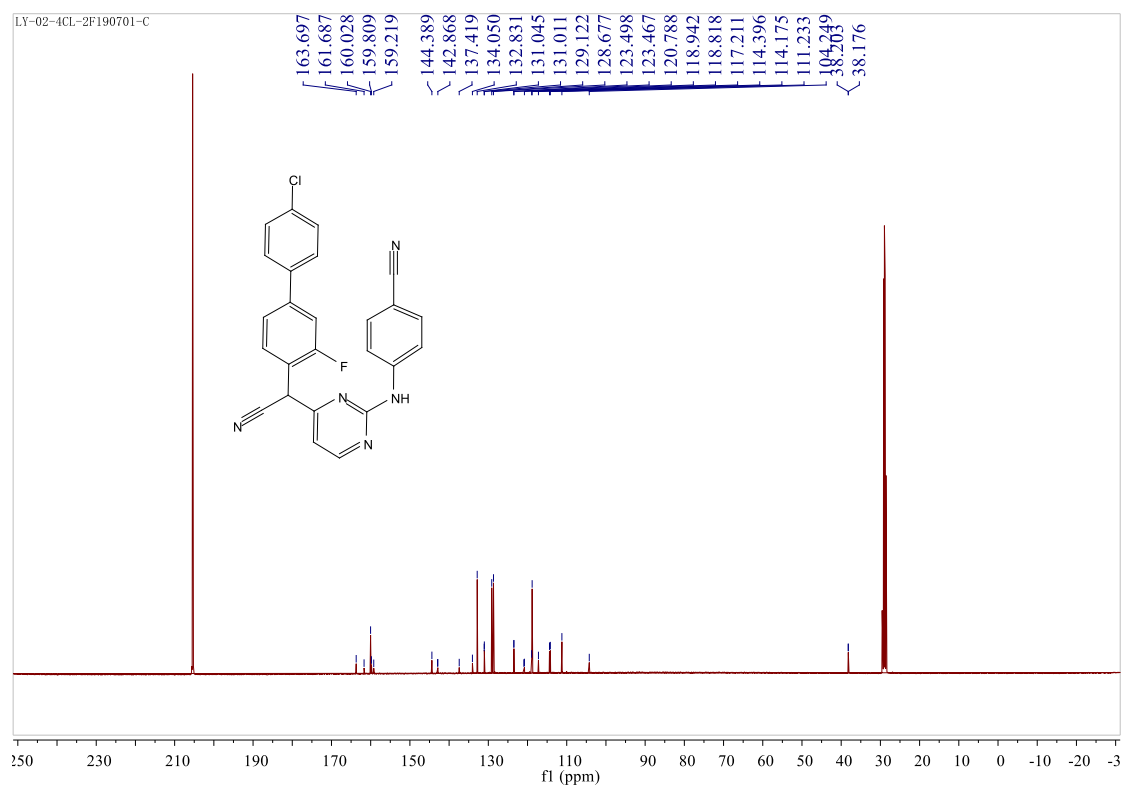
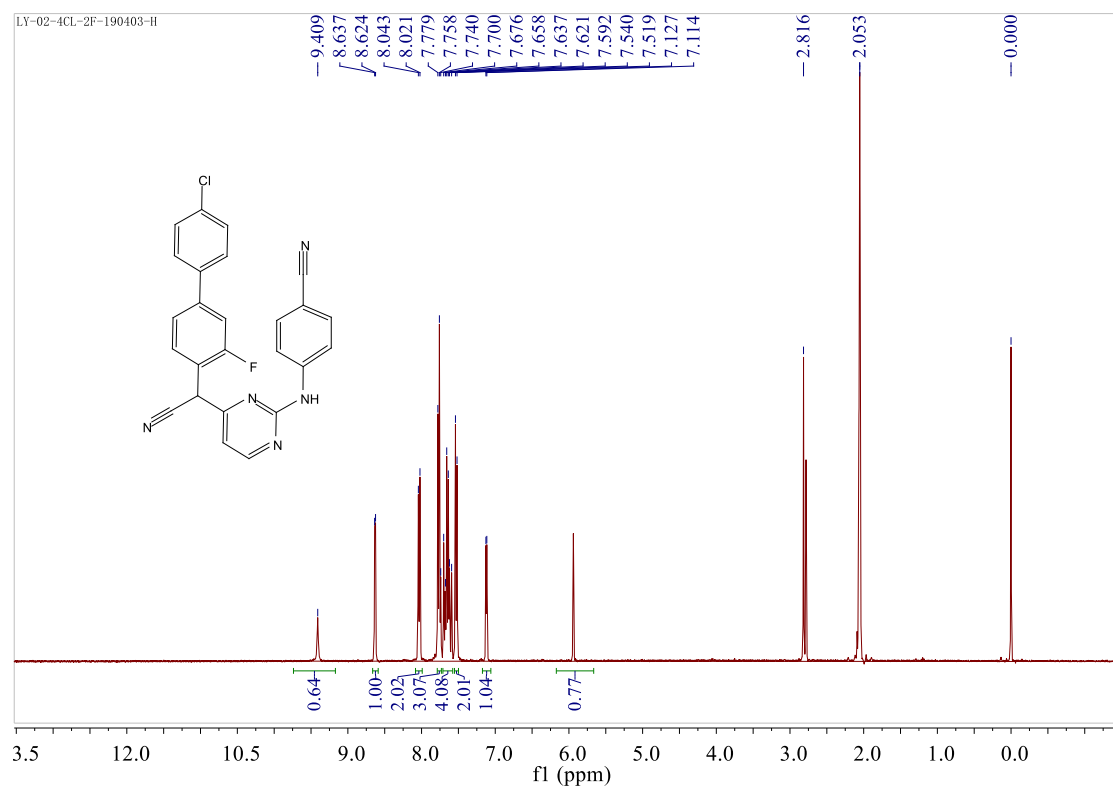
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## 15. Spectra of compound 10o



# Display Report

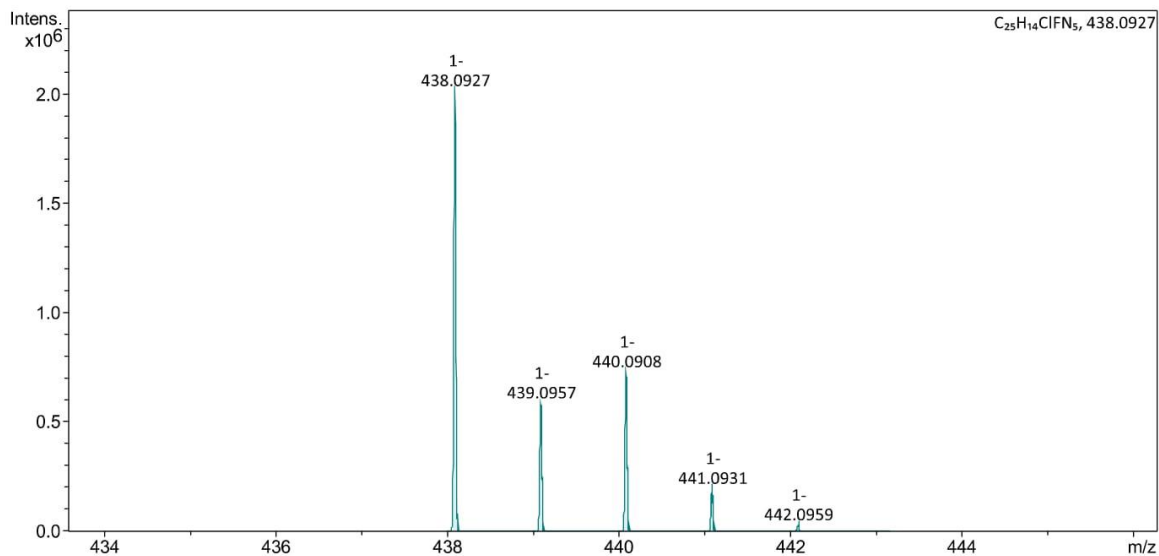
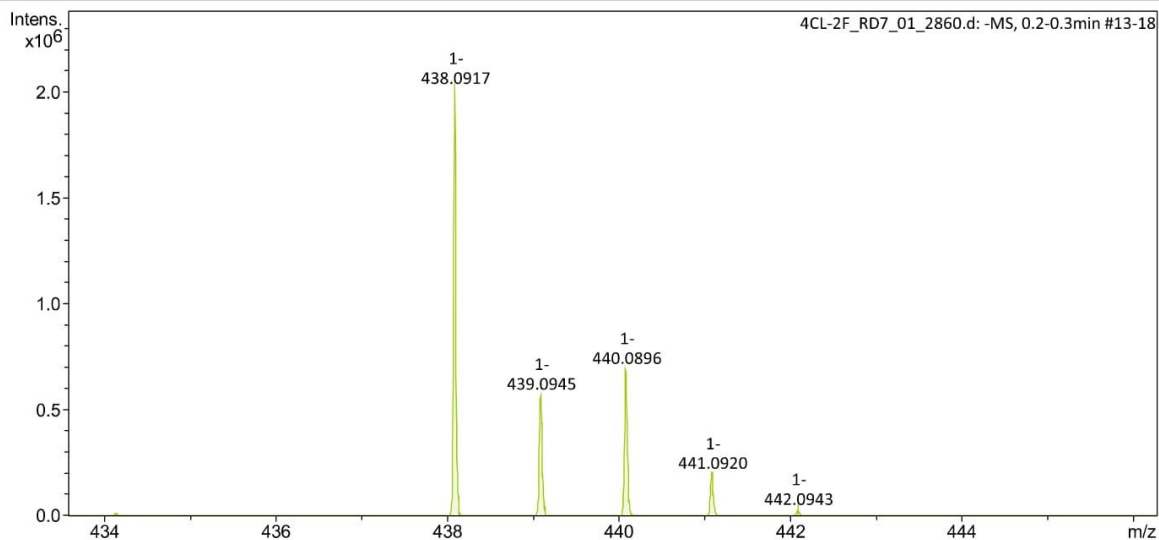
## Analysis Info

Analysis Name D:\Data\data\2019\4CL-2F\_RD7\_01\_2860.d  
Method MS-2MIN-NEG.m  
Sample Name 4CL-2F  
Comment

Acquisition Date 12/18/2019 17:03:06 PM  
Operator BDAL@DE  
Instrument compact 8255754.20127

## Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



4CL-2F\_RD7\_01\_2860.d

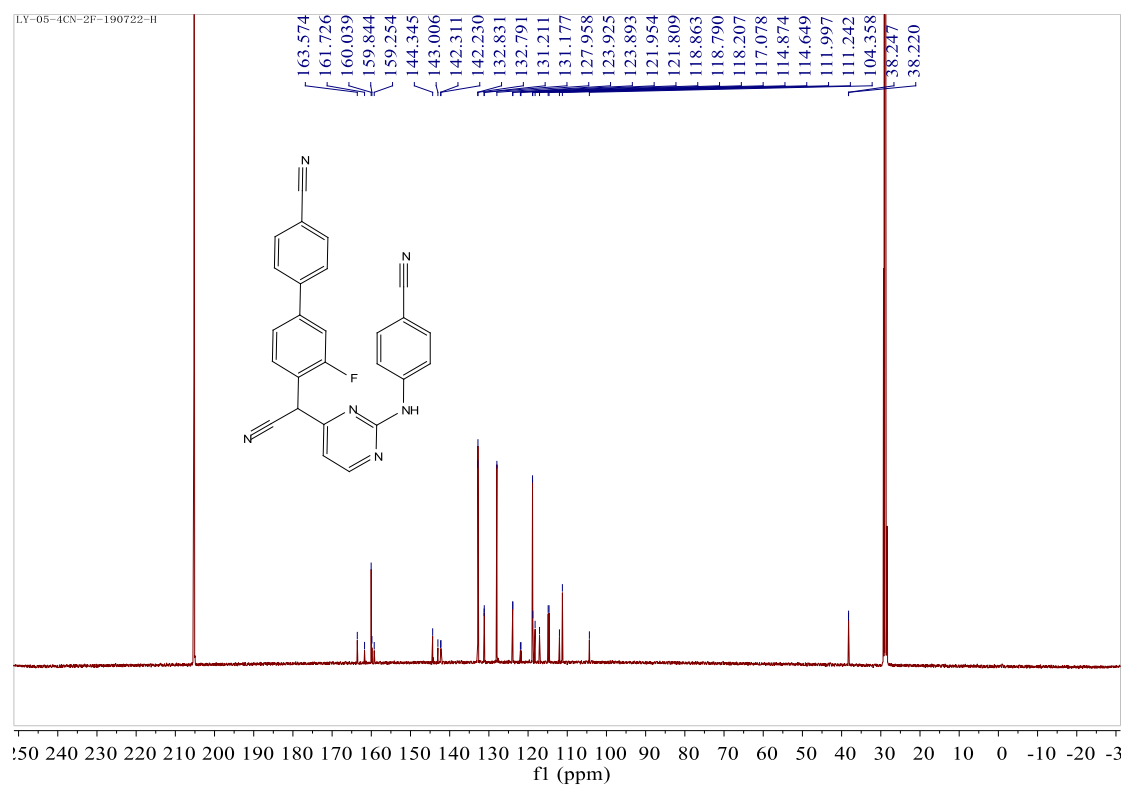
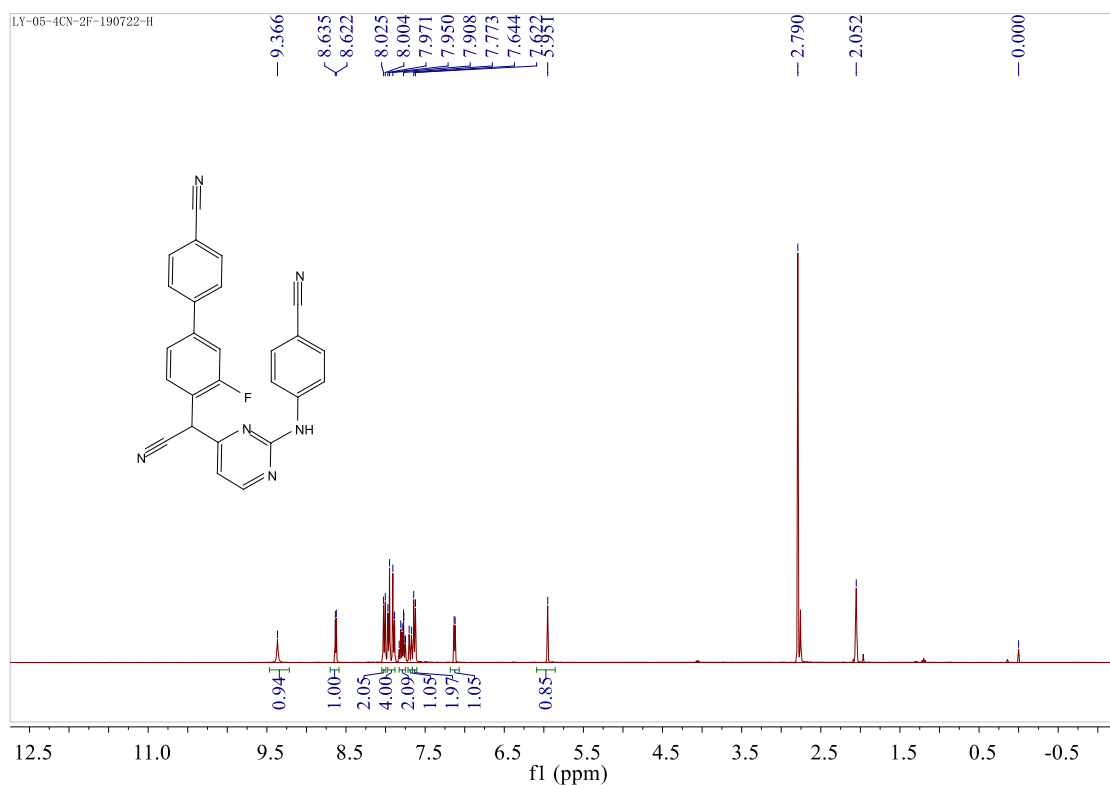
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## 16. Spectra of compound 10p





## Display Report

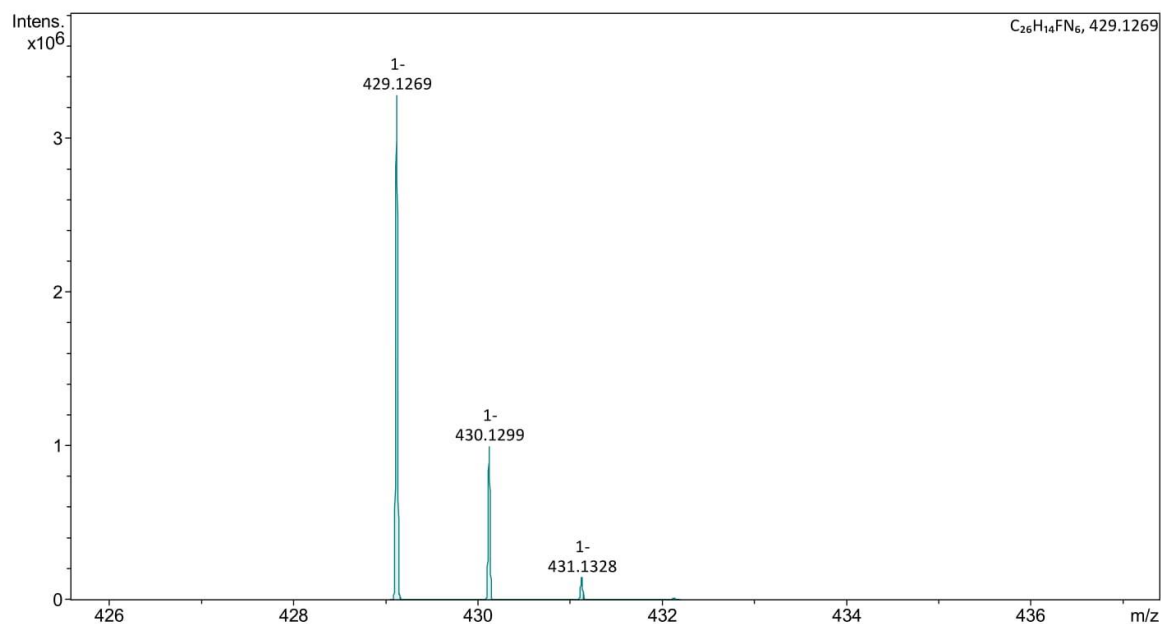
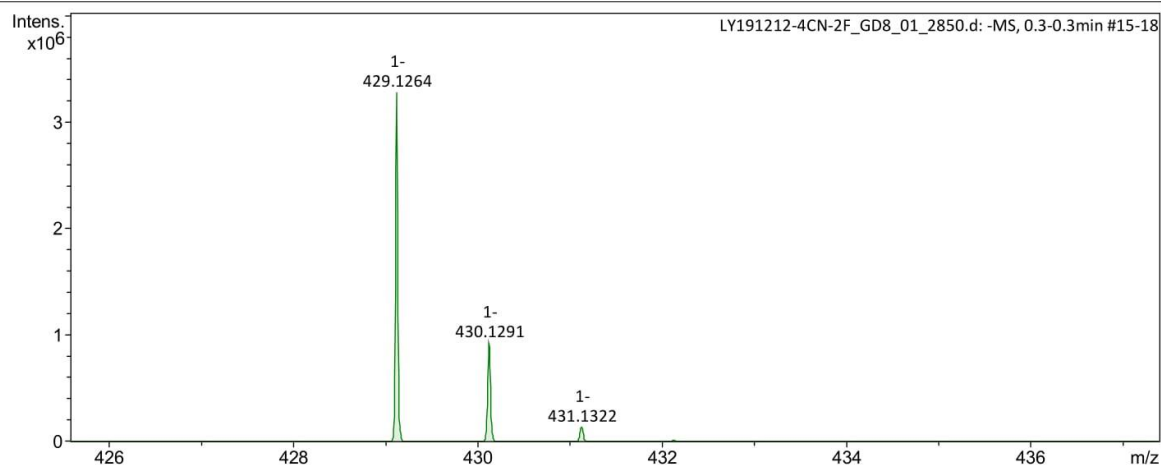
### Analysis Info

Analysis Name D:\Data\data\2019\LY191212-4CN-2F\_GD8\_01\_2850.d  
Method MS-2MIN-NEG.m  
Sample Name LY191212-4CN-2F  
Comment

Acquisition Date 12/18/2019 12:26:12 PM  
Operator BDAL@DE  
Instrument compact 8255754.20127

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



LY191212-4CN-2F\_GD8\_01\_2850.d  
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