

## *Supporting Information*

# **Synthesis of Difluoromethylated Spiropyrazolones via [3+2] Cycloaddition of Difluoroacetohydrazoneyl Bromides with Alkylidene Pyrazolones**

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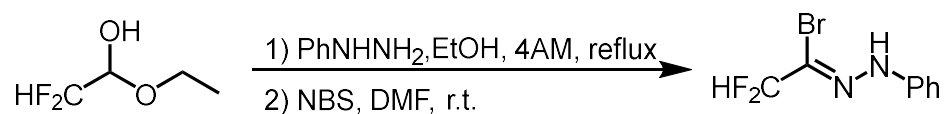
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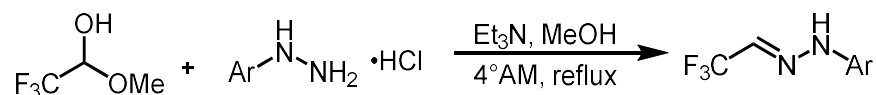
## Synthesis of Difluoroacetohydrazoneyl Bromide 1a<sup>1</sup>



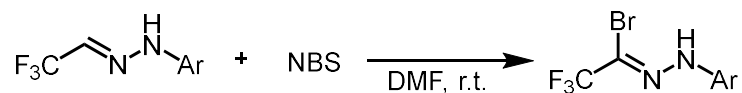
**Step 1:** A mixture of hydrazines (1.0 mmol, 1.0 equiv.), difluoroacetaldehyde ethyl hemiacetal (1.5 mmol, 1.5 equiv.), and freshly activated molecular sieves 4Å in EtOH (8 mL) was stirred at 75 °C in a round-bottom in an oil bath, and the reaction was monitored by TLC. After the reaction was completed, the solvent was removed in vacuo to afford intermediate product, which was used directly for the next step.

**Step 2:** To a solution of crude mixture from step 1 in DMF (8 mL) was added NBS. The resulting solution was stirred at room temperature, and the reaction was monitored by TLC. After the reaction was completed, the reaction was quenched with sat. NaCl aq., and the mixture was extracted with ethyl acetate (3 × 15 mL), dried over MgSO<sub>4</sub>, filtered, and concentrated in vacuo. The resulting products were purified by column chromatography on silica gel (EA)/petroleum ether (PE) (1:10–1:20) to afford difluoroacetohydrazoneyl bromide (76% yields).

## General procedure for the synthesis of trifluoroacetohydrazoneyl bromides 5<sup>2,3</sup>



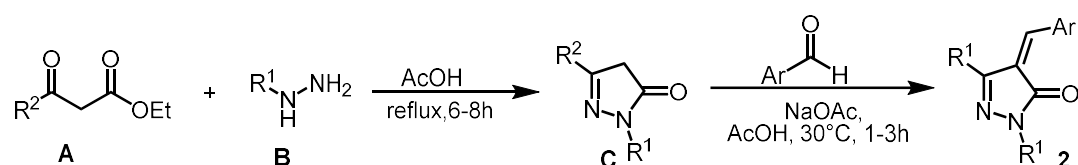
**Step 1:** A mixture of hydrazine hydrochlorides (2.0 mmol, 1.0 equiv.), triethylamine (1.0 mmol, 1.0 equiv.), trifluoroacetaldehyde ethyl hemiacetal (1.5 mmol, 1.5 equiv.), and freshly activated molecular sieves 4 Å in EtOH (8 mL) was stirred at 75 °C in a round-bottom in an oil bath, and the reaction was monitored by TLC. After the reaction was completed, the solvent was removed in vacuo to afford intermediate products, which was used directly for the next step.



**Step 2:** To a solution of crude mixture from step 1 in DMF (8 mL) was added NBS (2.2 mmol, 1.1 equiv.). The resulting solution was stirred at room temperature, and the reaction was monitored by TLC. After the reaction was completed, the reaction was quenched with sat. NaCl aq., and the mixture was extracted with ethyl acetate (3 x 15 mL), dried over MgSO<sub>4</sub>, filtered, and concentrated in vacuo. The resulting products was purified by column chromatography on silica gel (EA)/petroleum ether (PE) (1:8–1:20) to afford trifluoroacetohydrazoneyl bromides 5.



## Synthesis of 4-arylidene pyrazolone derivatives **2** <sup>4</sup>



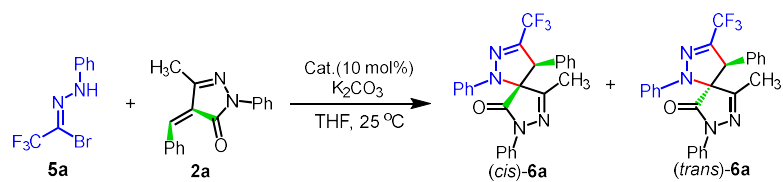
**Step 1:** The solution of corresponding ethyl ester **A** (10 mmol, 1.0 equiv.), hydrazine **B** (11 mmol, 1.1 equiv.) in acetic acid (20 mL) was refluxed in oil bath for 6-8 h, and left to cool. The crude product **C** could be obtained by recrystallization by using acetic acid as a yellow solid, which could be used directly in next step without further purification.

**Step 2:** To a solution of above product **C** (8.0 mmol, 1.0 equiv.) in acetic acid (20 mL) was added aldehyde (8.8 mmol, 1.1 equiv.) and sodium acetate (8.8 mmol, 1.1 equiv.). The mixture was stirred at 30 °C for 1-3 h after completion, H<sub>2</sub>O (50 mL) was added to reaction mixture. The aqueous phase was extracted with EtOAc (3 × 20 mL), dried over sodium sulfate, and concentrated in *vacuo*. The crude residue was subjected to column chromatography (silica gel) using Hexanes/EtOAc (100:1) as eluent.

## References

- [1] Kaneko, S.; Yamazaki, T.; Kitazume, T. A remarkably simple route to versatile difluoromethylated molecules. *J. Org. Chem.* **1993**, *58*, 2302.
- [2] Tanaka, K.; Maeno, S.; Mitsunashi, K. Cycloadditions of *N*-Aryl-C (Trifluoromethyl)nitrilimines with Dimethyl Fumarate and Maleate. *J. Heterocyclic Chem.* **1985**, *22*, 565.
- [3] Mloston, G.; Urbaniak, K.; Utecht, G.; Lentz, D.; Jasinski, M. Trifluoromethylated 2,3-dihydro-1,3,4-thiadiazoles via the regioselective [3+2]-cycloadditions of fluorinated nitrile imines with aryl, hetaryl, and ferrocenyl thioketones. *J. Fluor. Chem.* **2016**, *192*, 147.
- [4]. Khairnar, P. V.; Su, Y.-H.; Chen, Y.-C.; Edukondalu, A.; Chen, Y.-R.; Lin, W. Organophosphane-Catalyzed Direct  $\beta$ -Acylation of 4-Arylidene Pyrazolones and 5-Arylidene Thiazolones with Acyl Chlorides. *Org. Lett.* **2020**, *22*, 6868.

## Optimization of asymmetric reaction conditions <sup>a</sup>

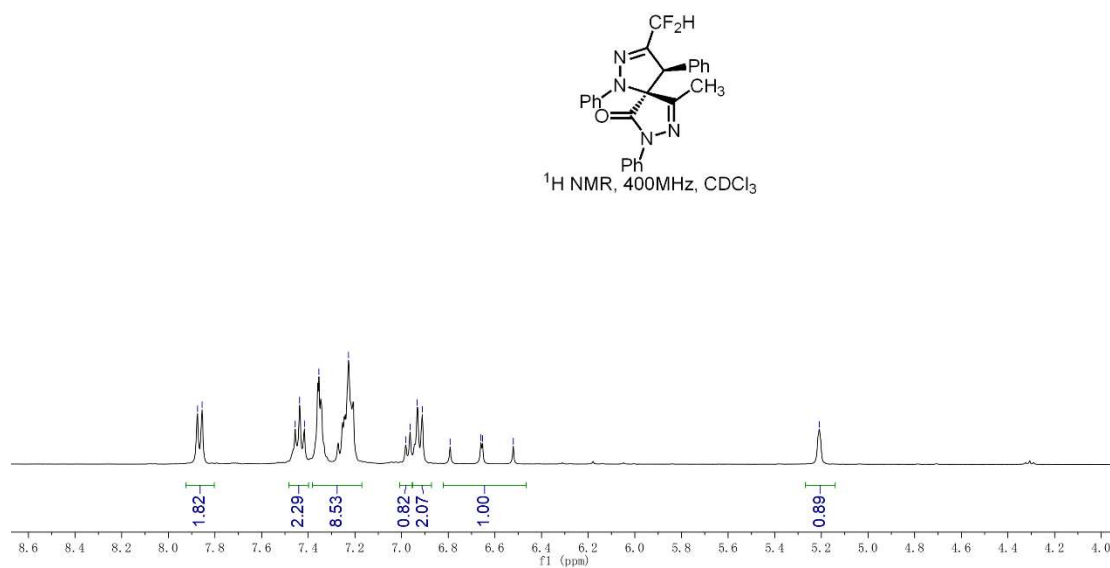
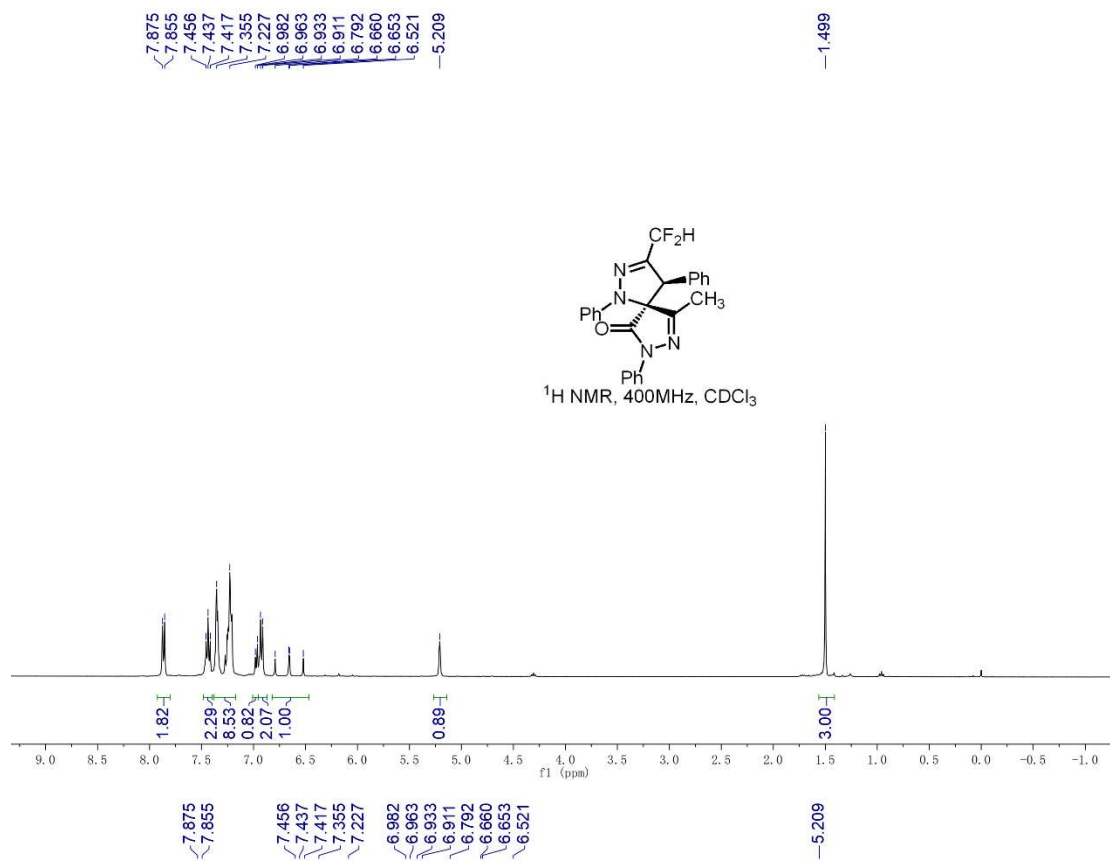


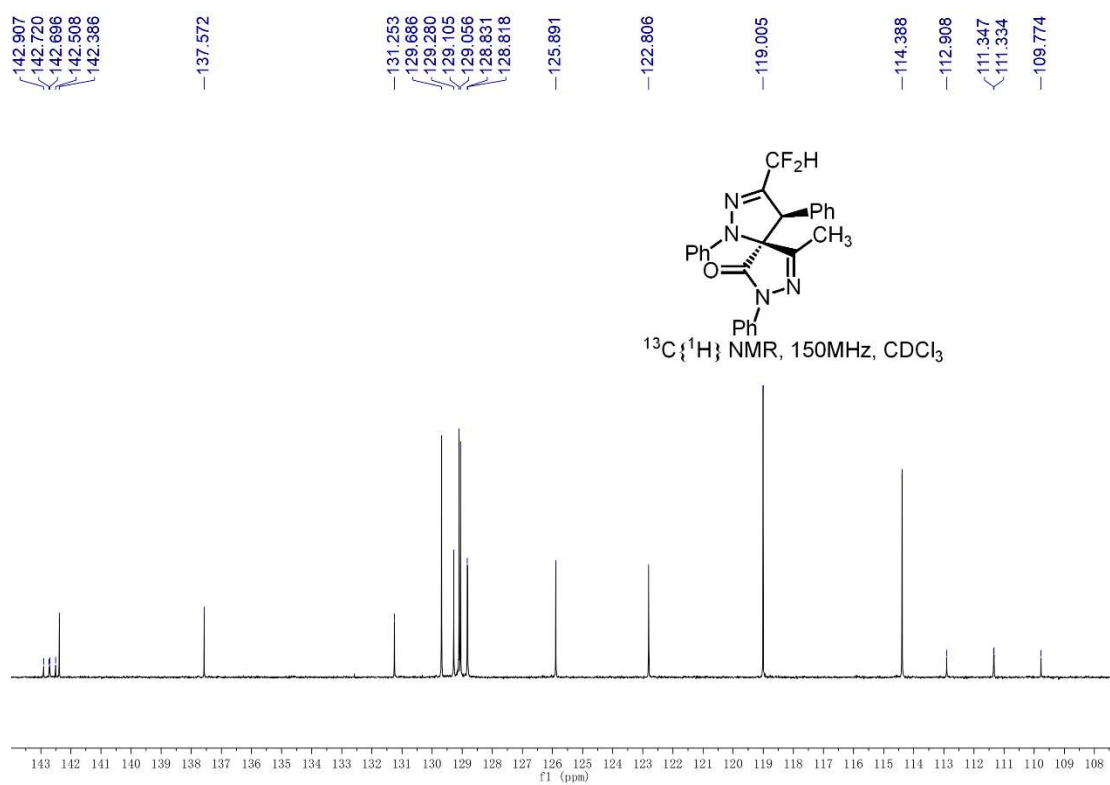
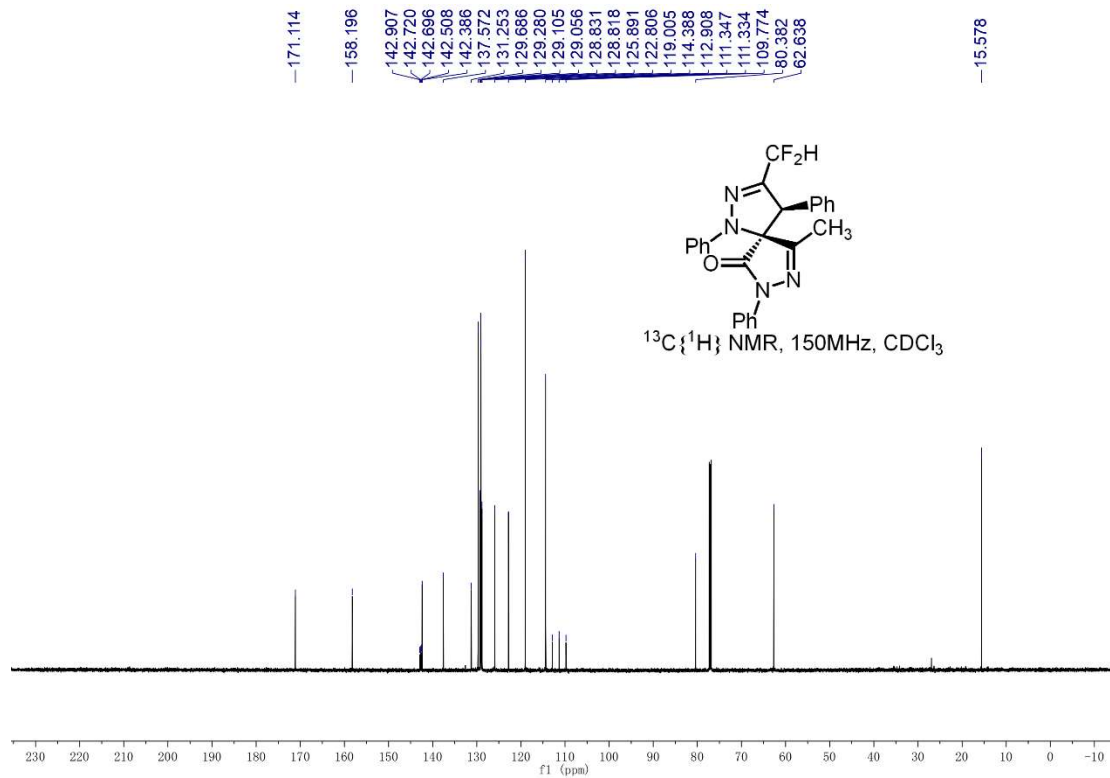
Entry	Cat	Total Yield <sup>b</sup> (%)	(cis)-6a/(trans)-6a
<b>1</b>		77	2.3:1.0
<b>2</b>		20	4.0:1.0
<b>3</b>		95	2.0:1.0
<b>4</b>		49	2.8:1.0
<b>5</b>		81	1.0:1.4

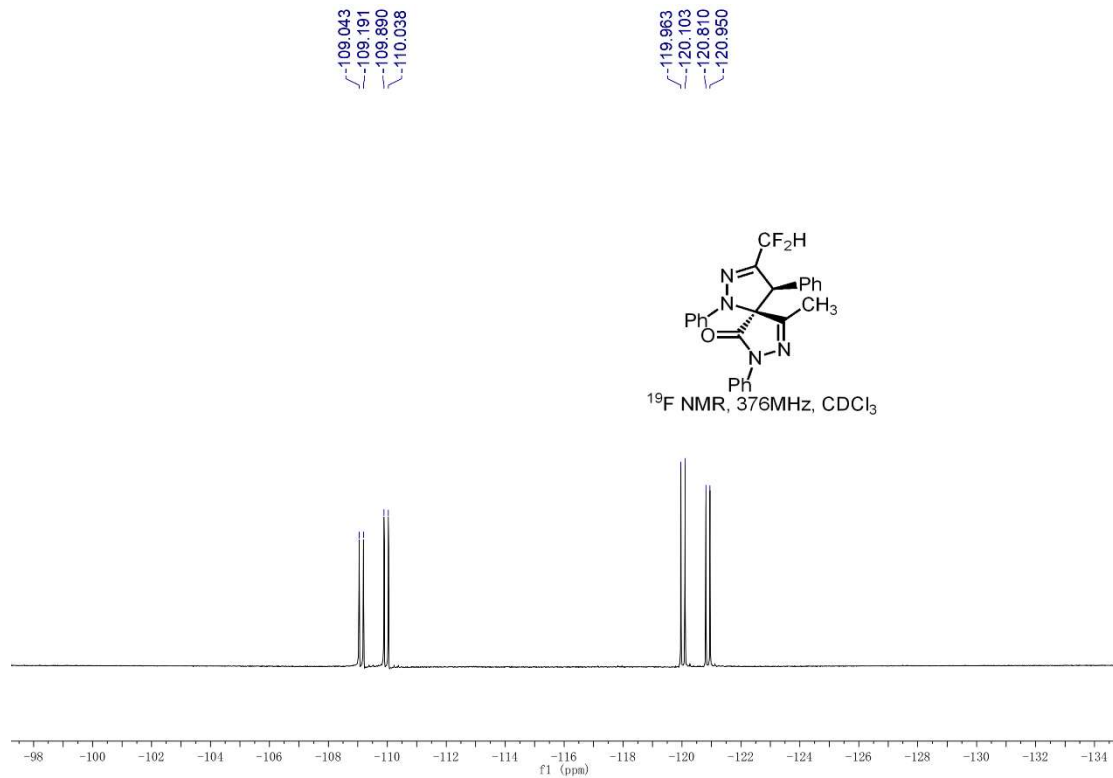
<sup>a</sup>Reactions were performed with **1a** (0.12 mmol, 1.2 equiv.), **2a** (0.1 mmol, 1.0 equiv.), and  $K_2CO_3$  (0.12 mmol, 1.2 equiv.) in solvent (3.0 mL) at 25 °C in metal bath for 12 h. <sup>b</sup>Isolated yield.

# NMR and HRMS spectra copies of compounds 3a–3m, 4a–4m ,4l–4p and 6a–6l

NMR copies of compound (*trans*)-3a:







HRMS (ESI) copy of compound ((*trans*)-**3a**):

### Mass Spectrum SmartFormula Report

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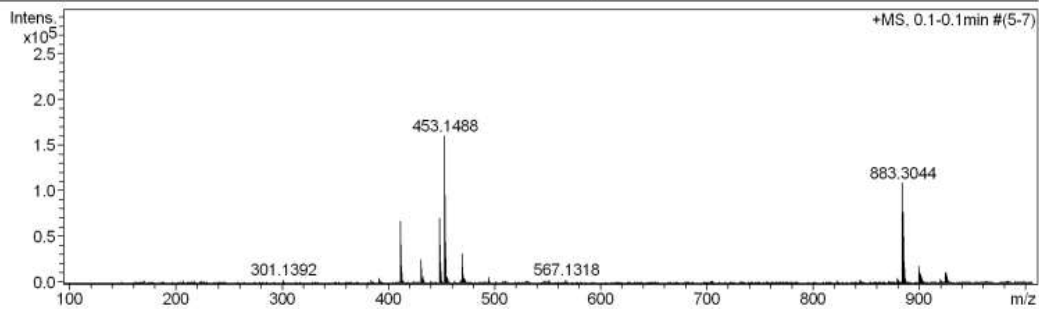
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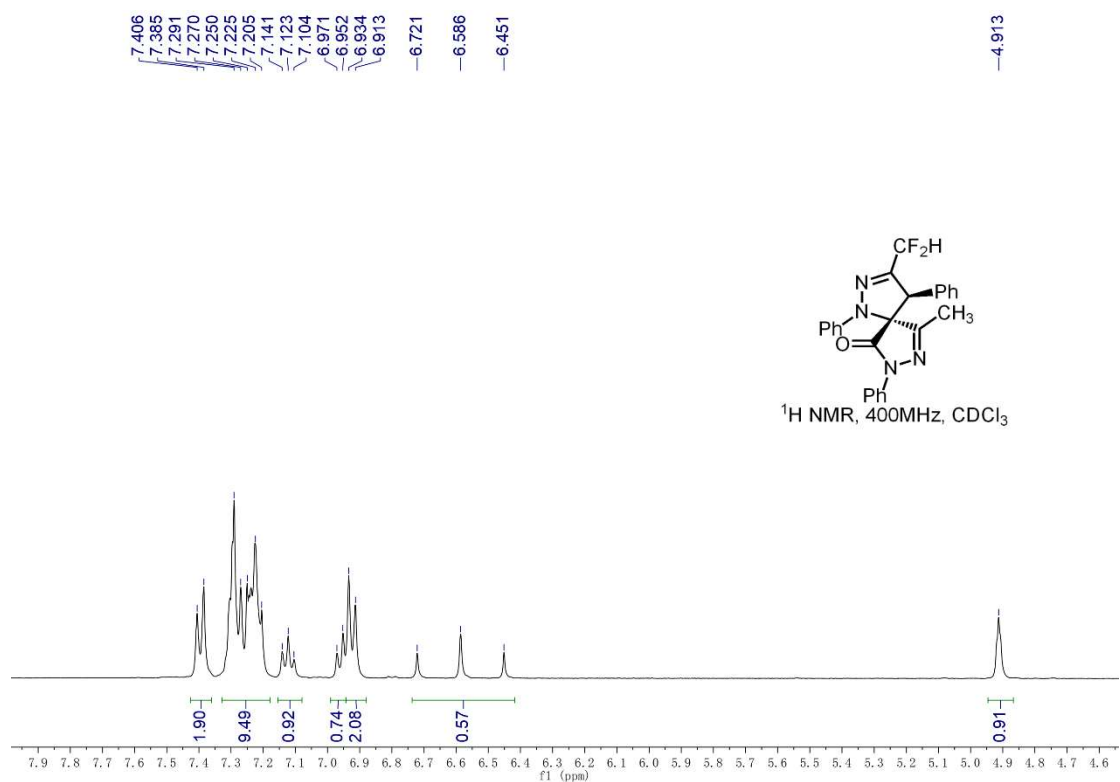
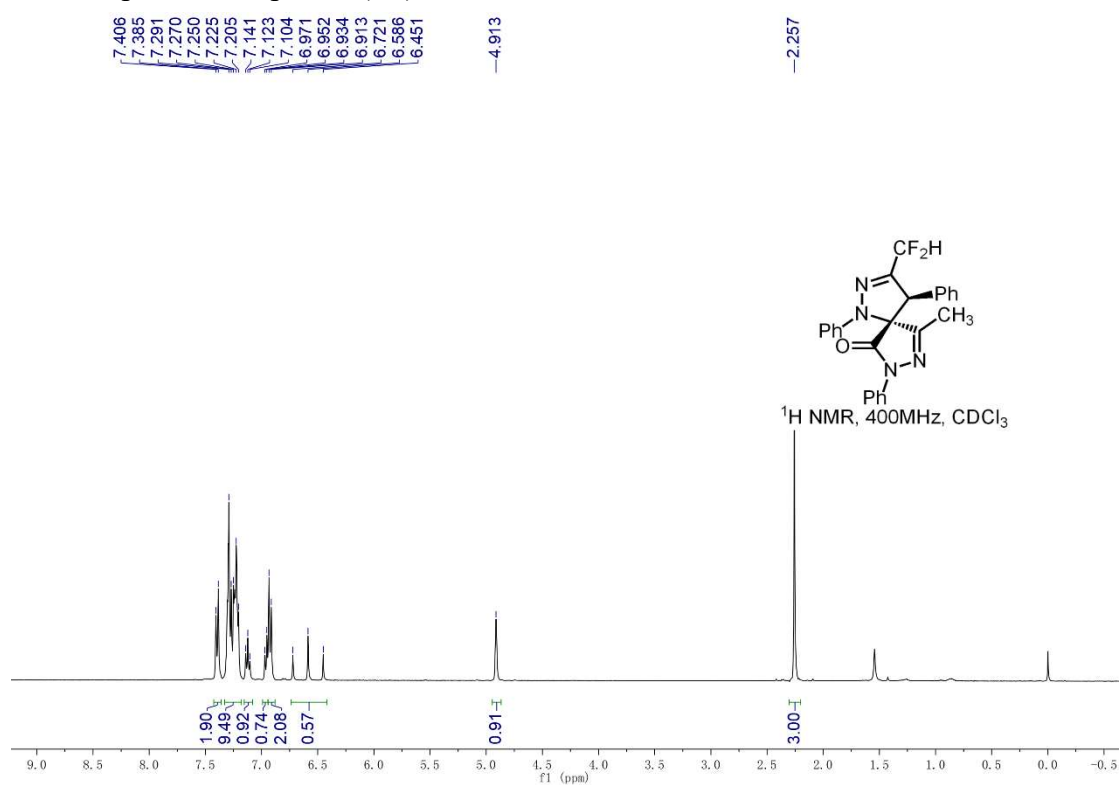
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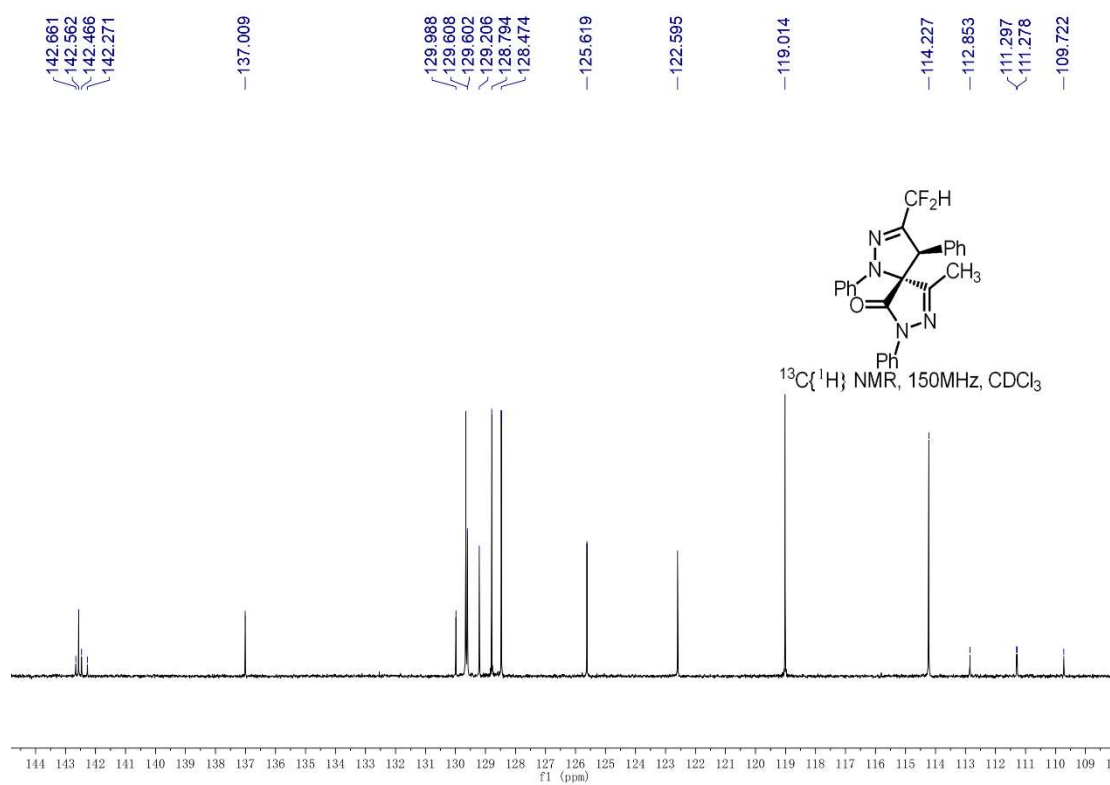
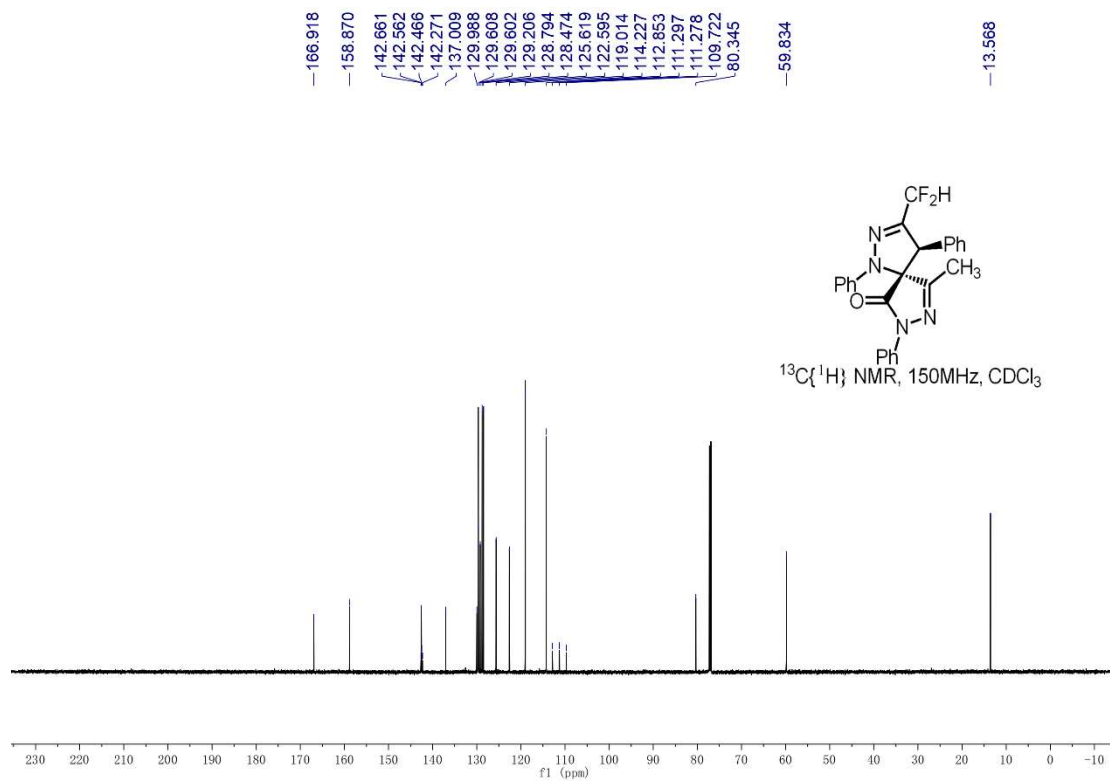
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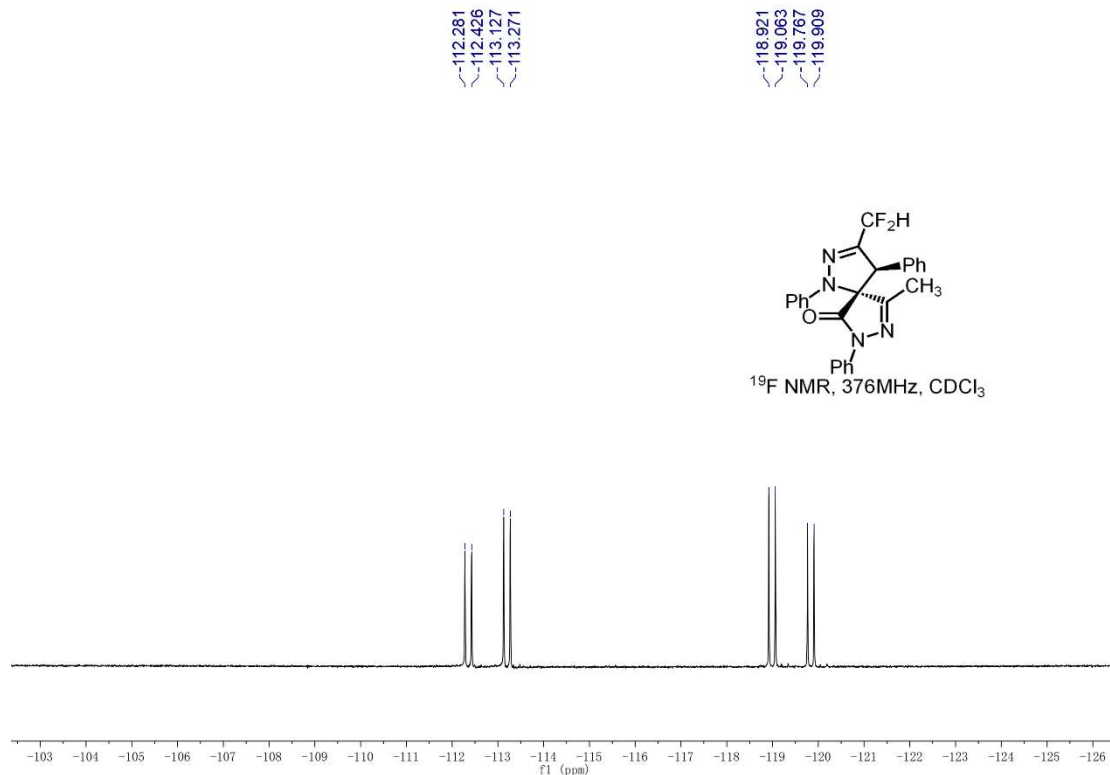


Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-R	e j ≠ Conf	mS	Std	Std	Std	Std	Std	Std
453.1488	1	C <sub>25</sub> H <sub>20</sub> F <sub>2</sub> N <sub>4</sub> NaO	453.1497	2.1	2.1	16.5	ok	even	3.1	4.3	1.1	1.9	0.3	842.7	

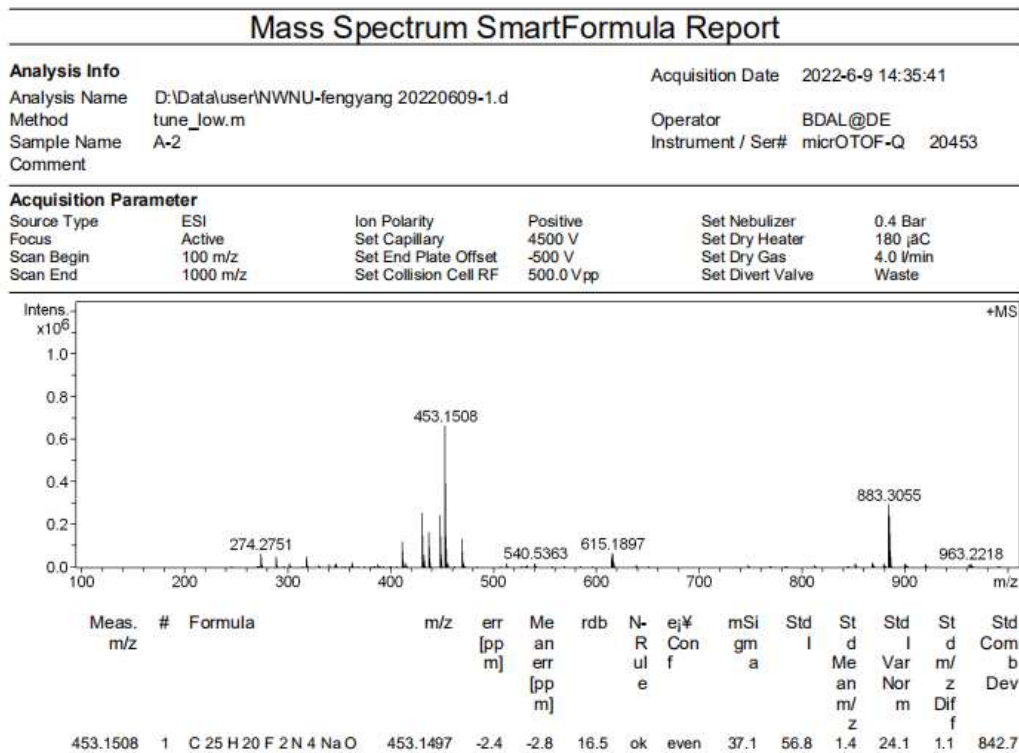
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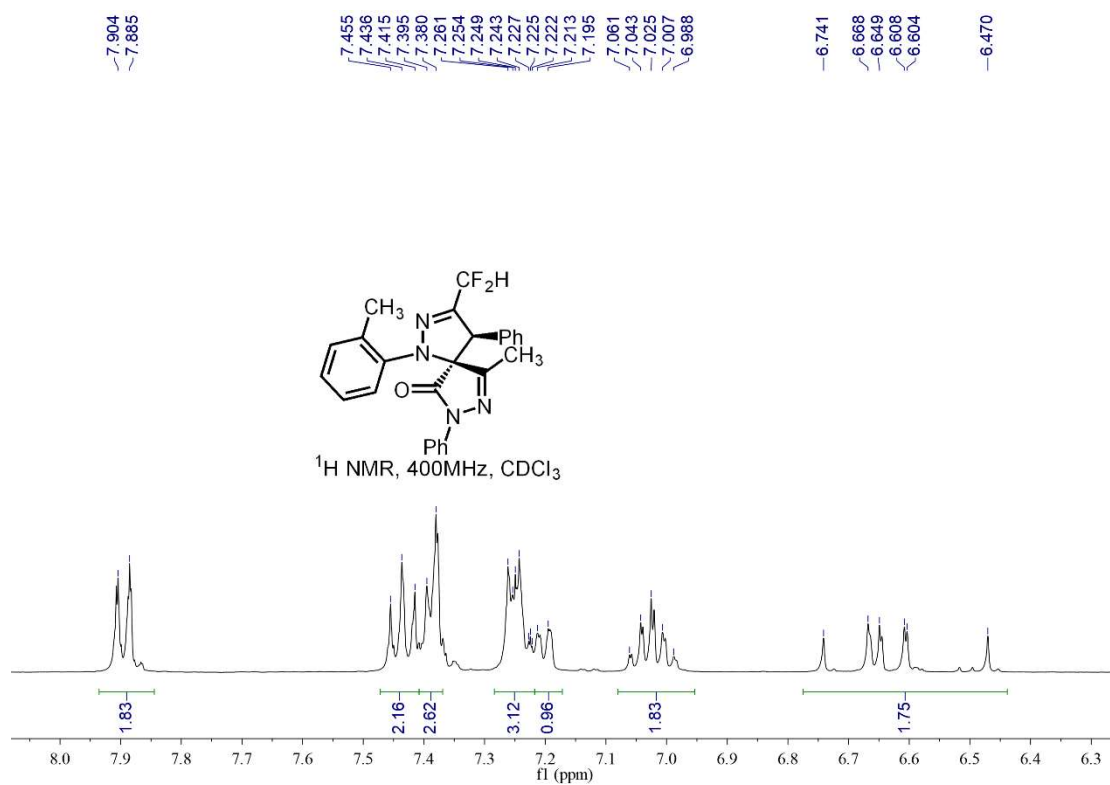
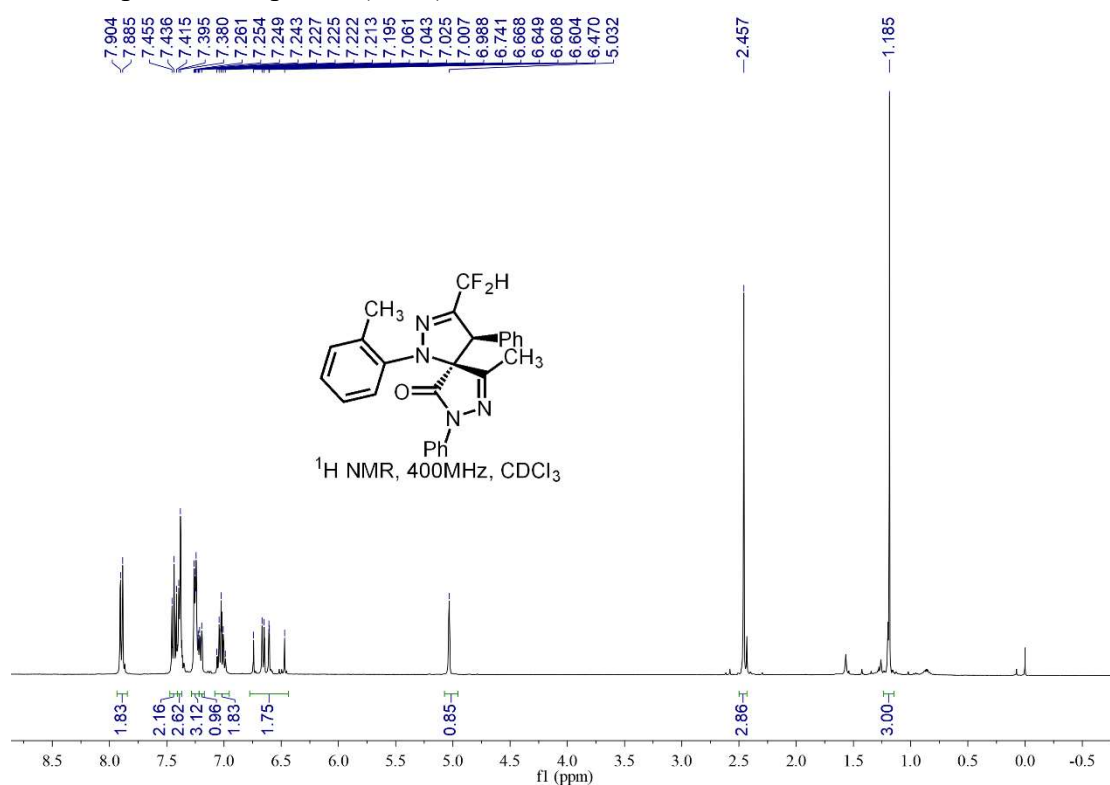


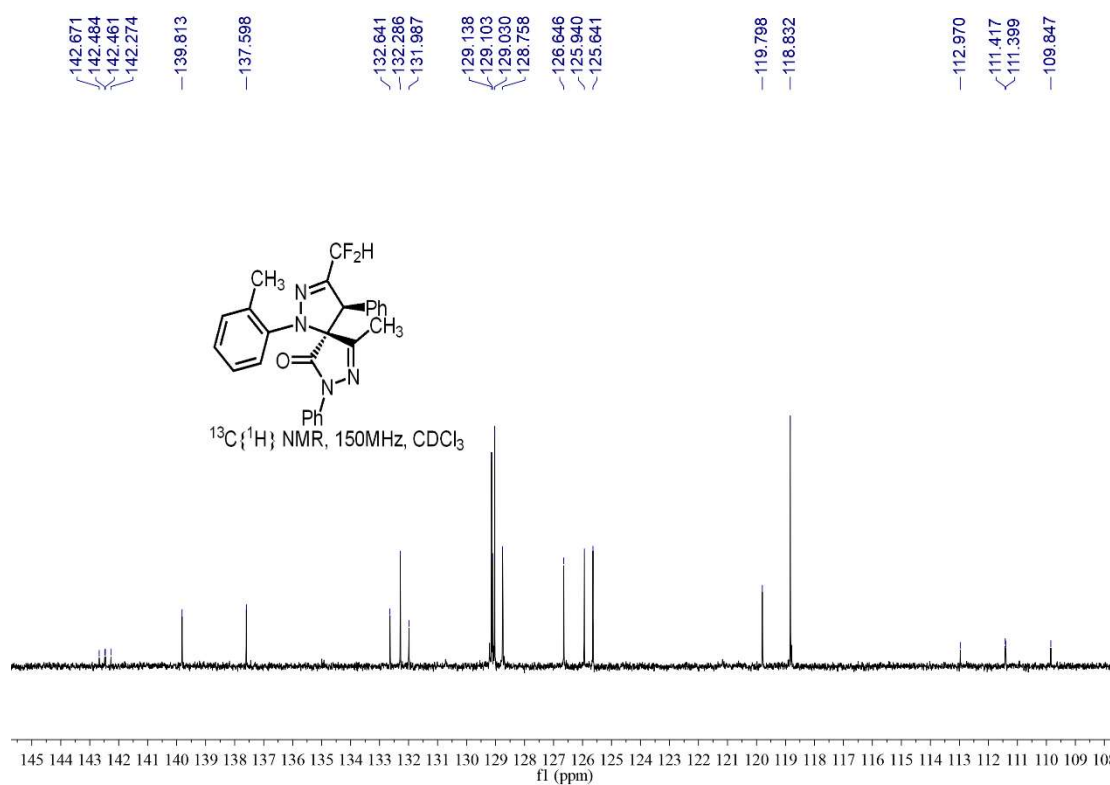
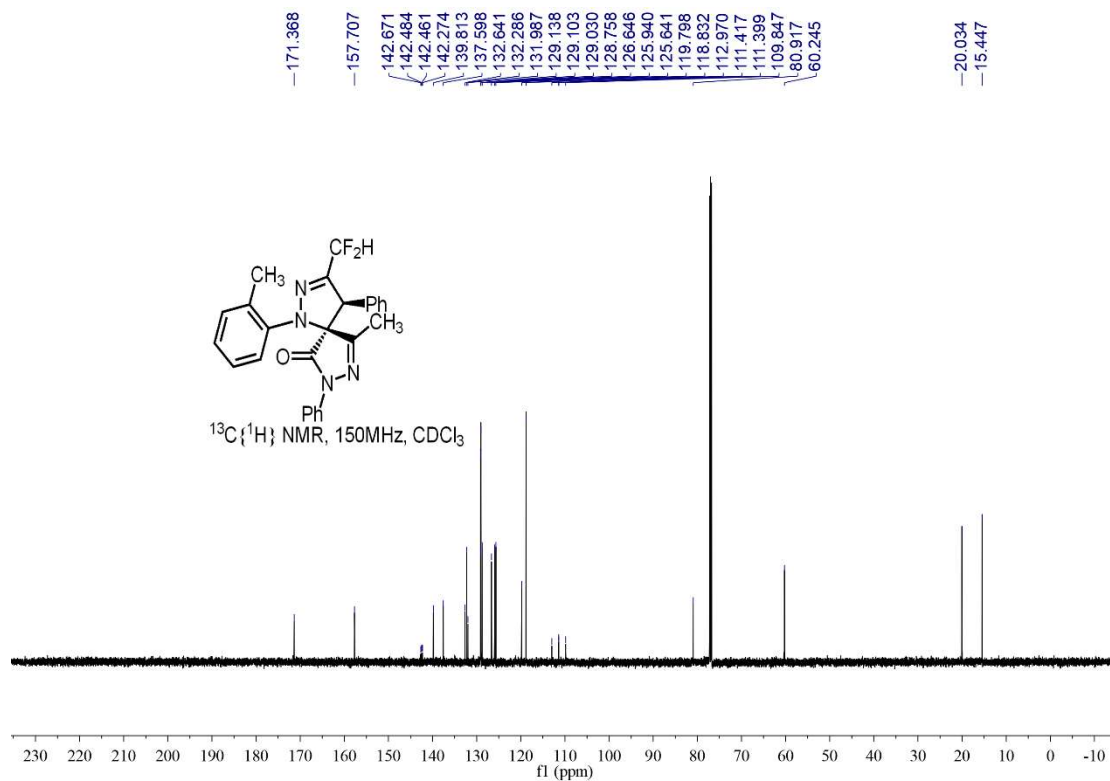
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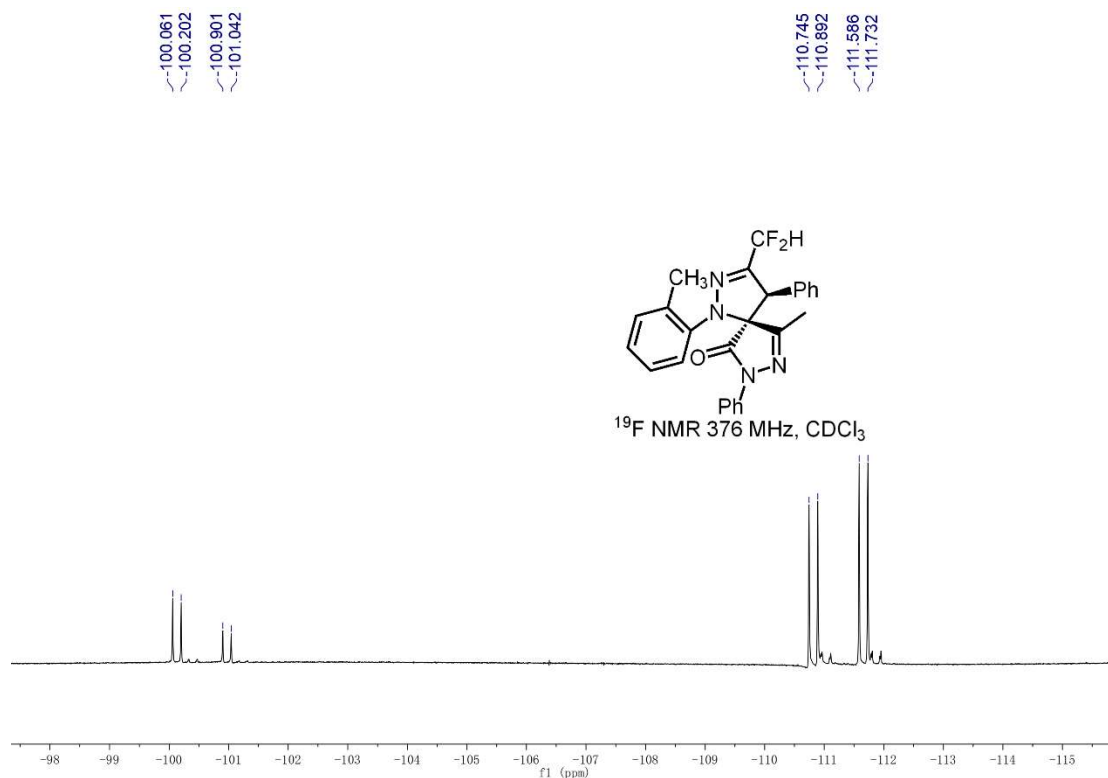




NMR copies of compound (*trans*)-**3b**:







HRMS (ESI) copy of compound (*trans*)-**3b**:

### Mass Spectrum SmartFormula Report

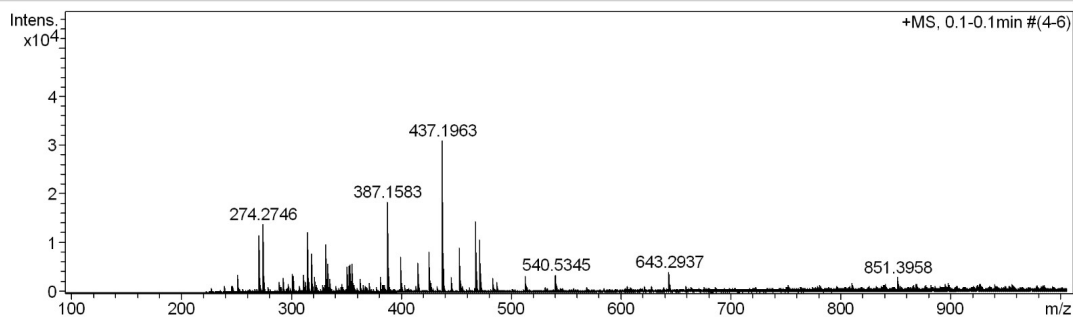
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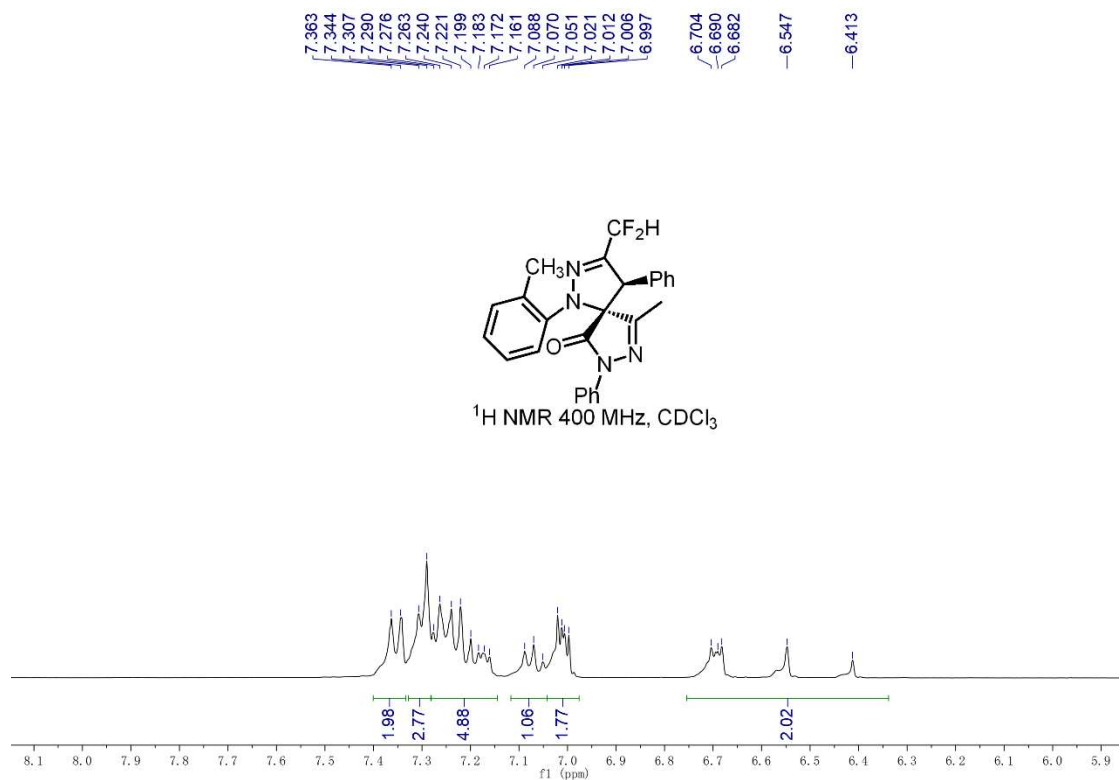
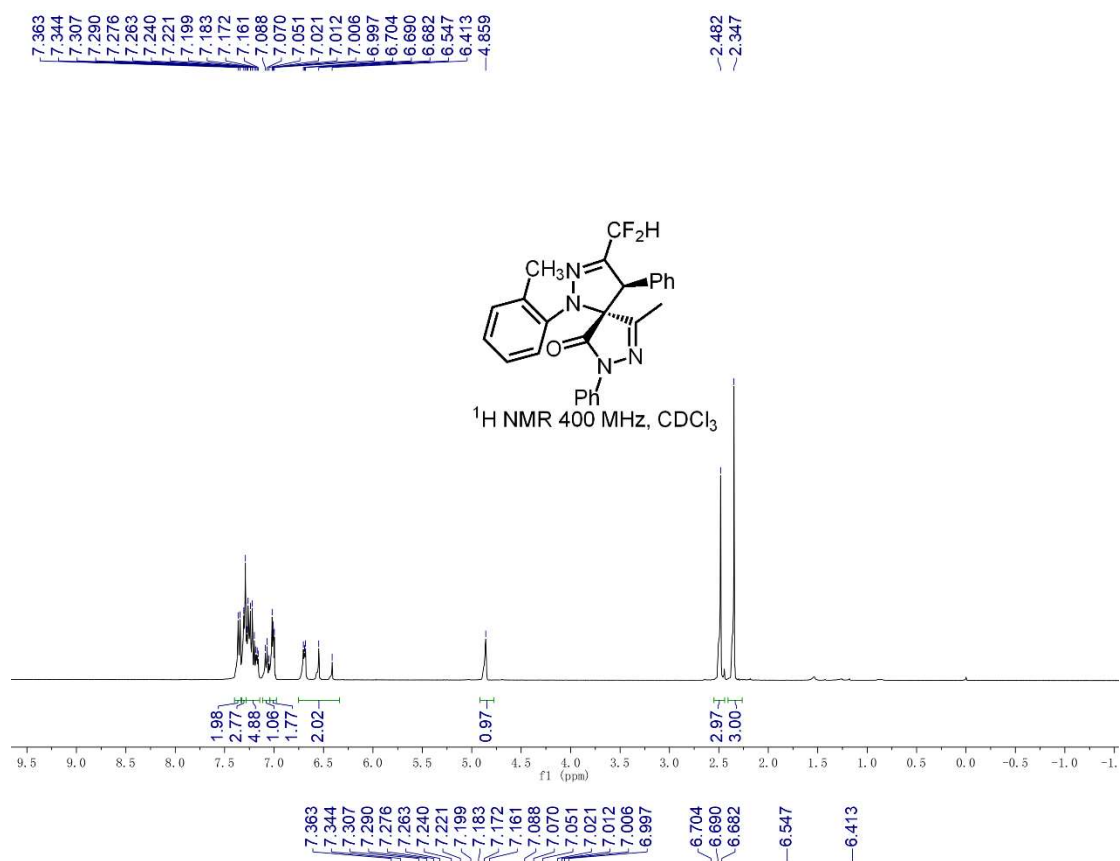
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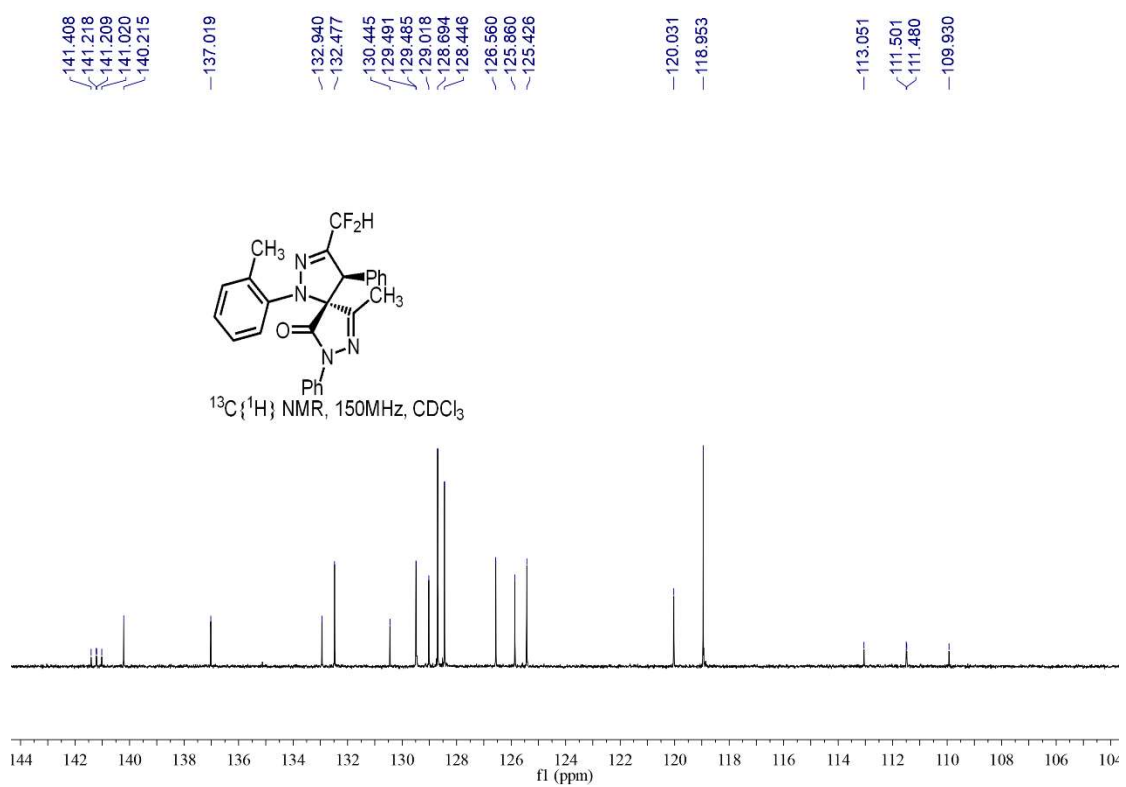
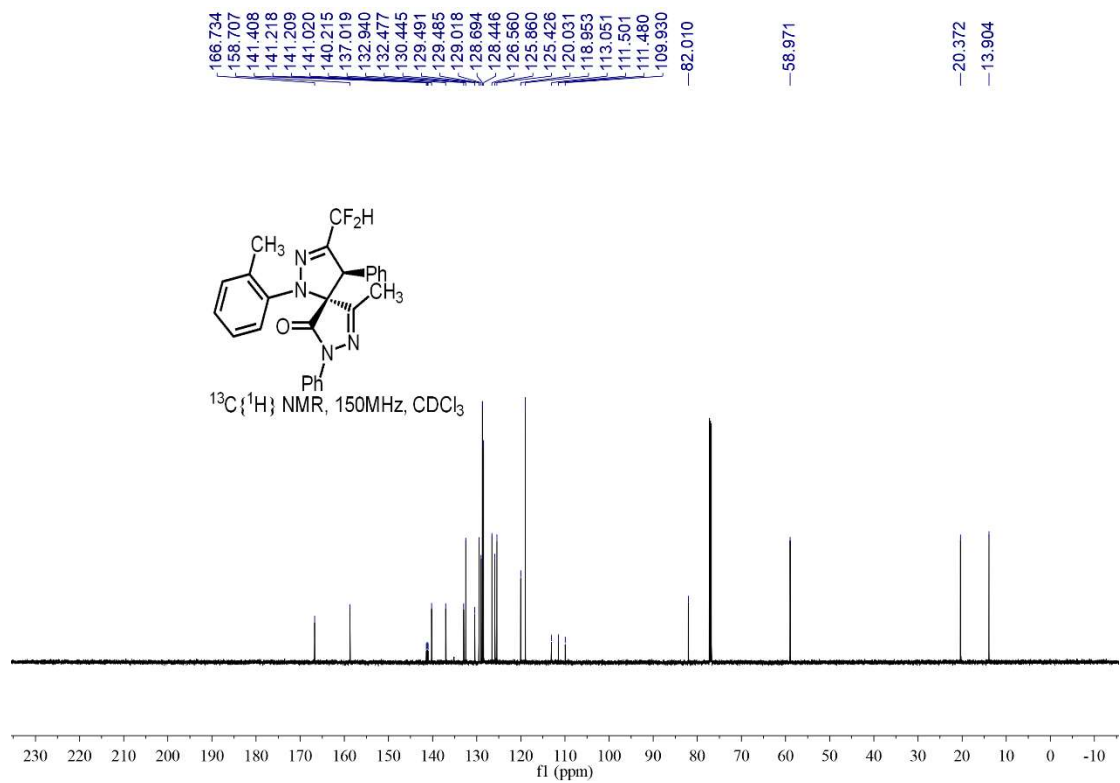
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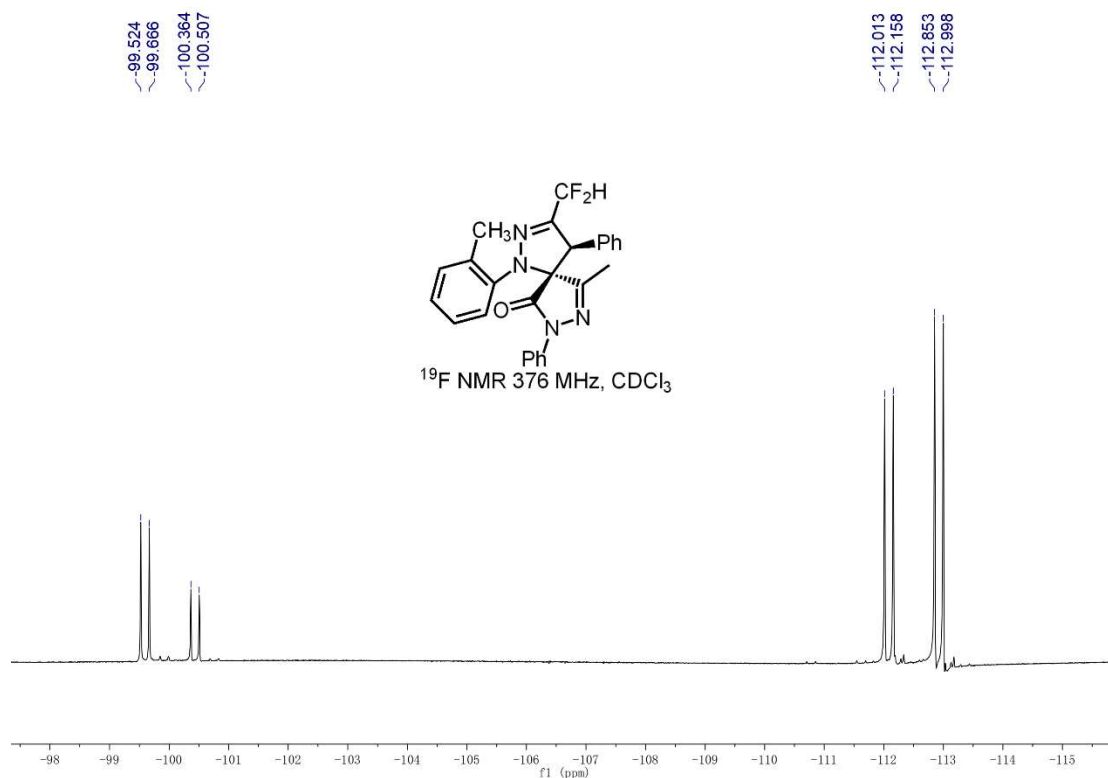


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m/z						ul	f	a		Me an m/z	Var Nor m	Dif z	b Dev
467.1660	C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	-1.2	-1.7	16.5	ok	even	24.7	33.1	0.9	26.0	0.9	842.7

NMR copies of compound (*cis*)-**3b**:







HRMS (ESI) copy of compound (*cis*)-**3b**:

### Mass Spectrum SmartFormula Report

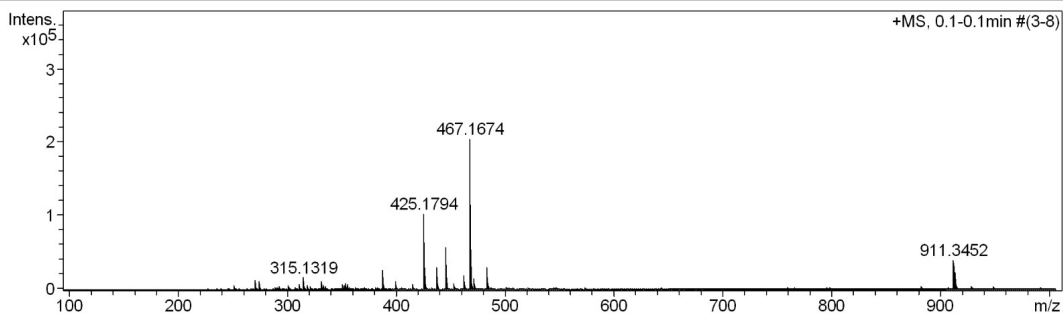
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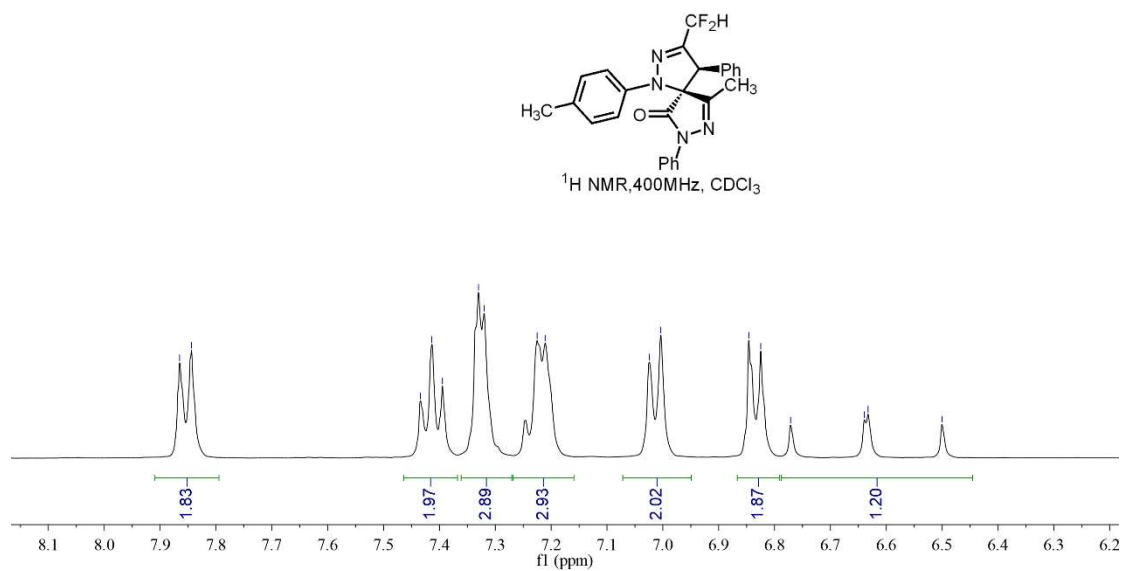
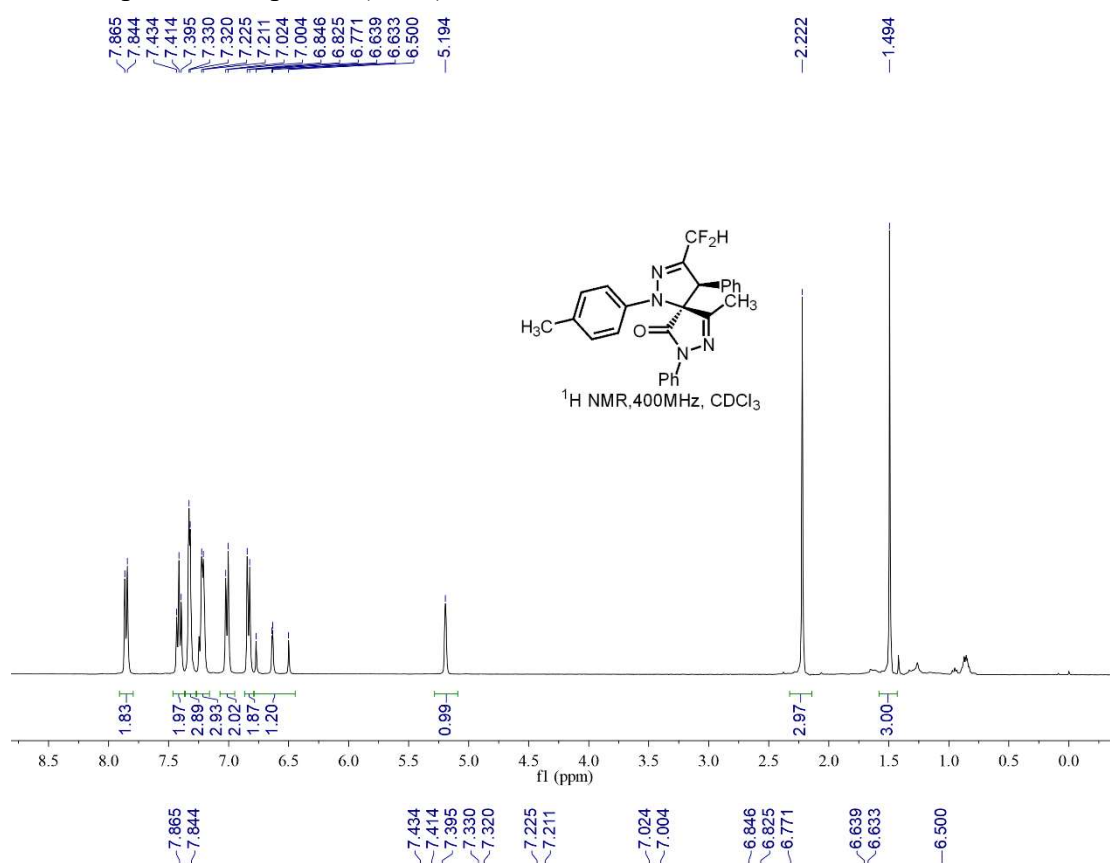
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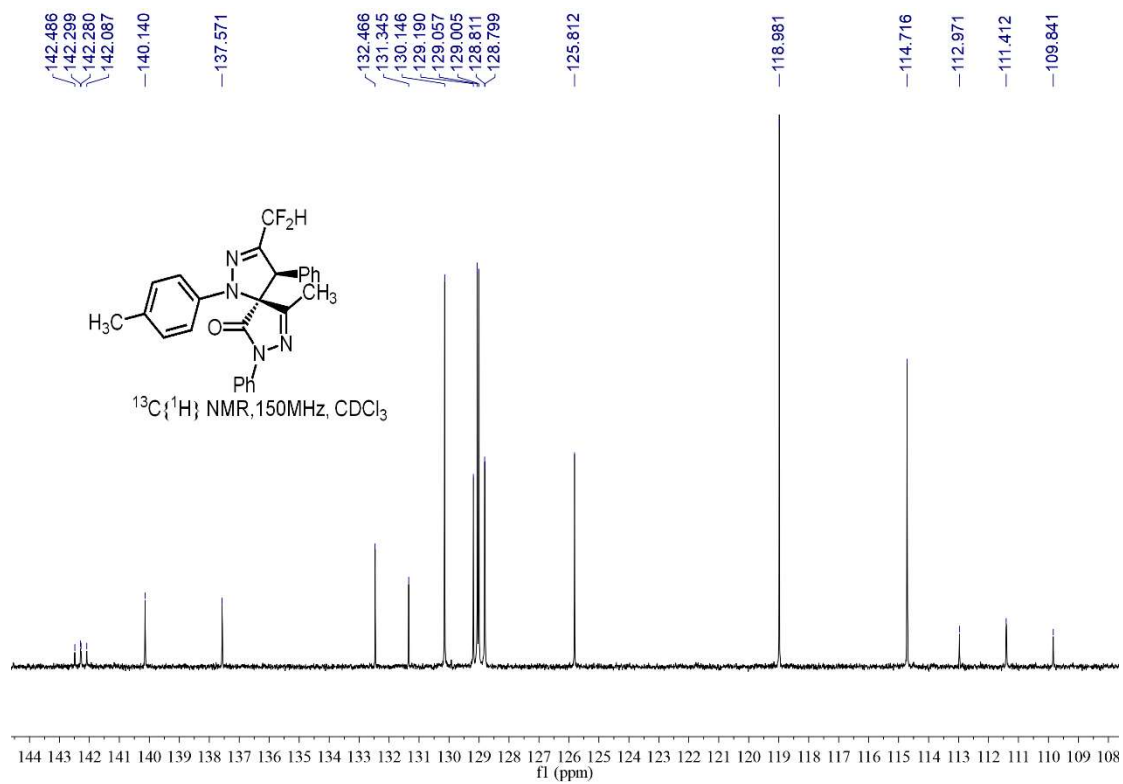
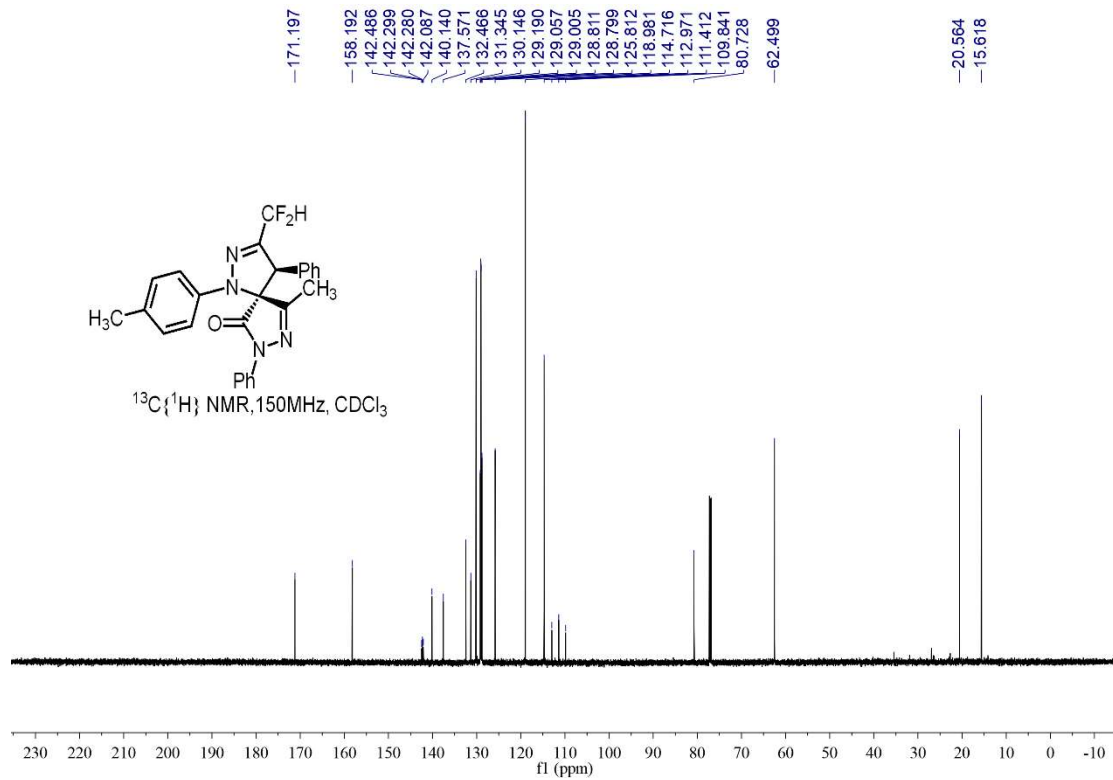
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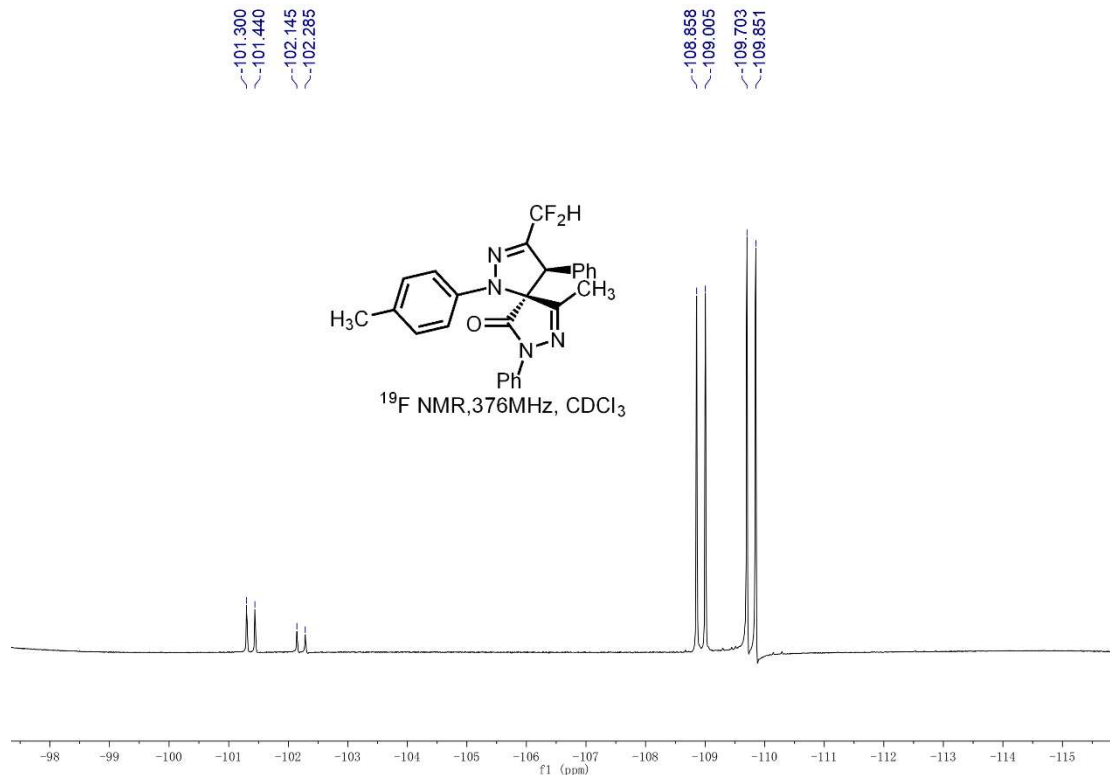
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467.1674	1 C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	-4.4	-4.5	16.5	ok	even		17.3	25.6	2.1	10.9	0.4	842.7

NMR copies of compound (*trans*)-3c:









HRMS (ESI) copy of compound (*trans*)-**3c**:

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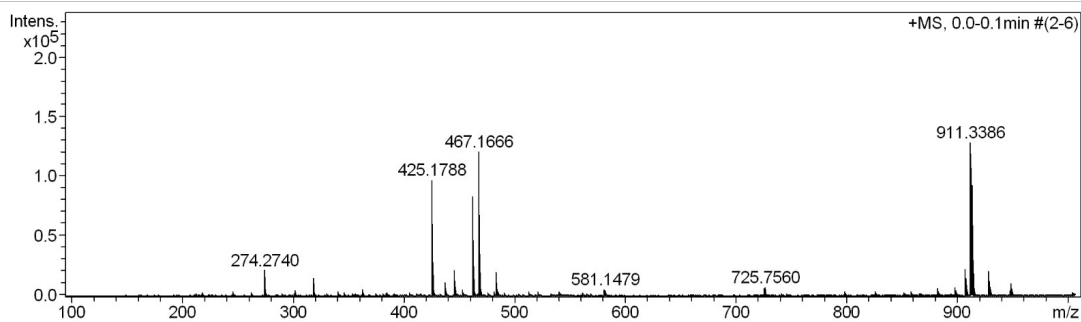
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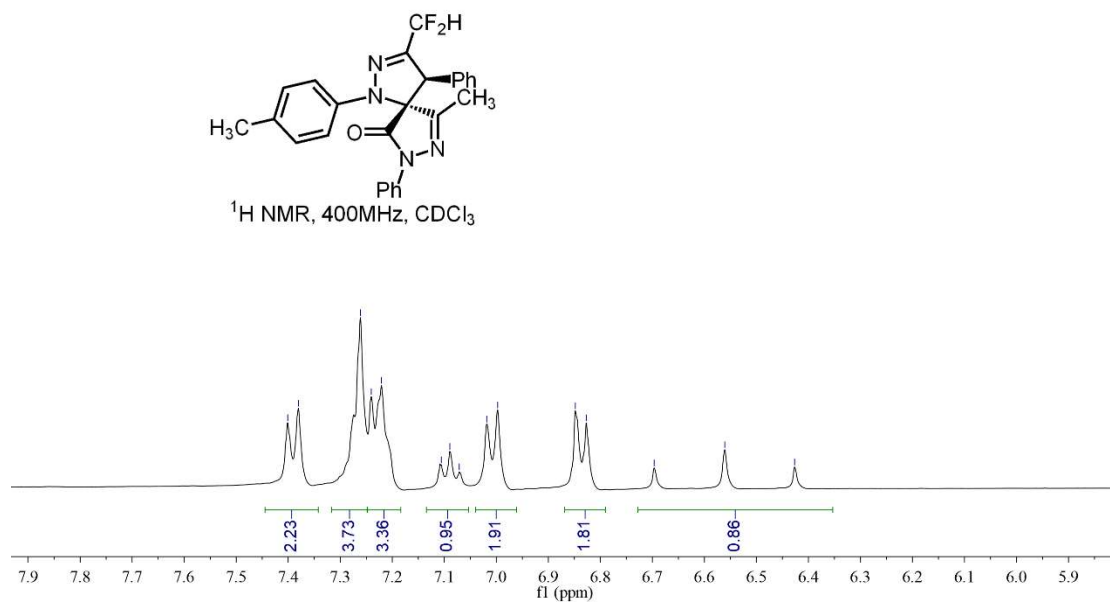
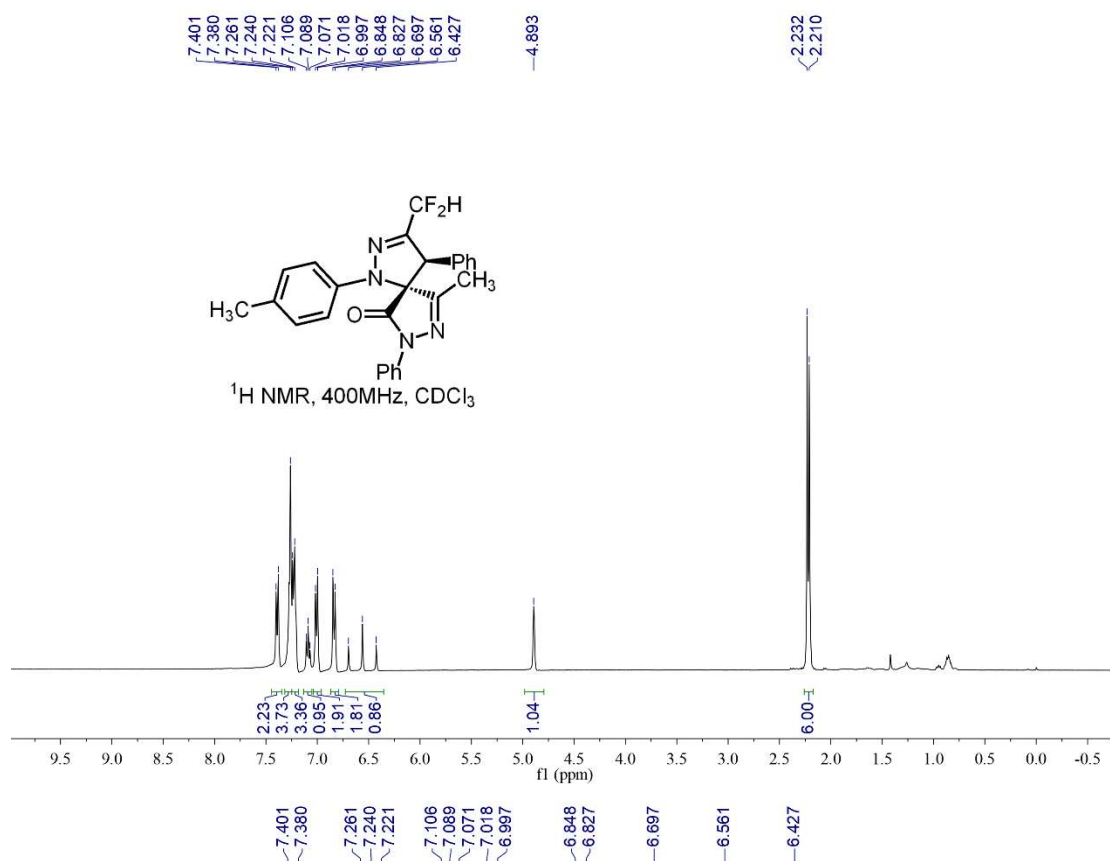
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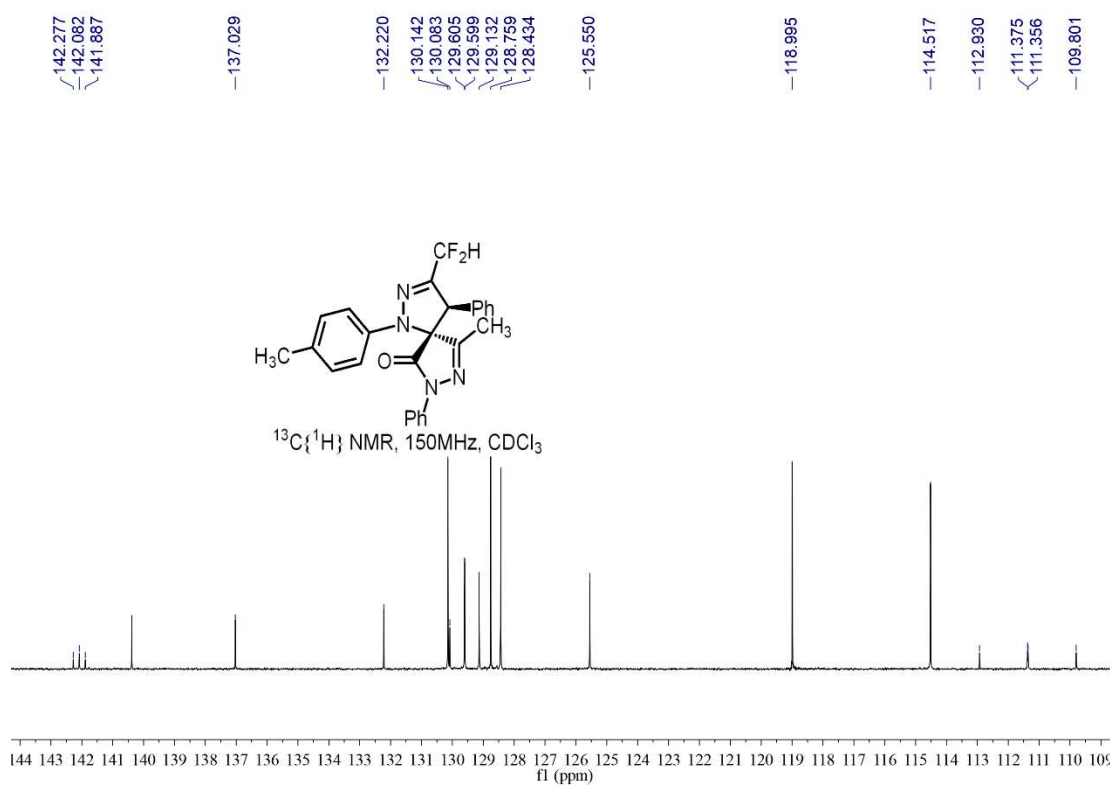
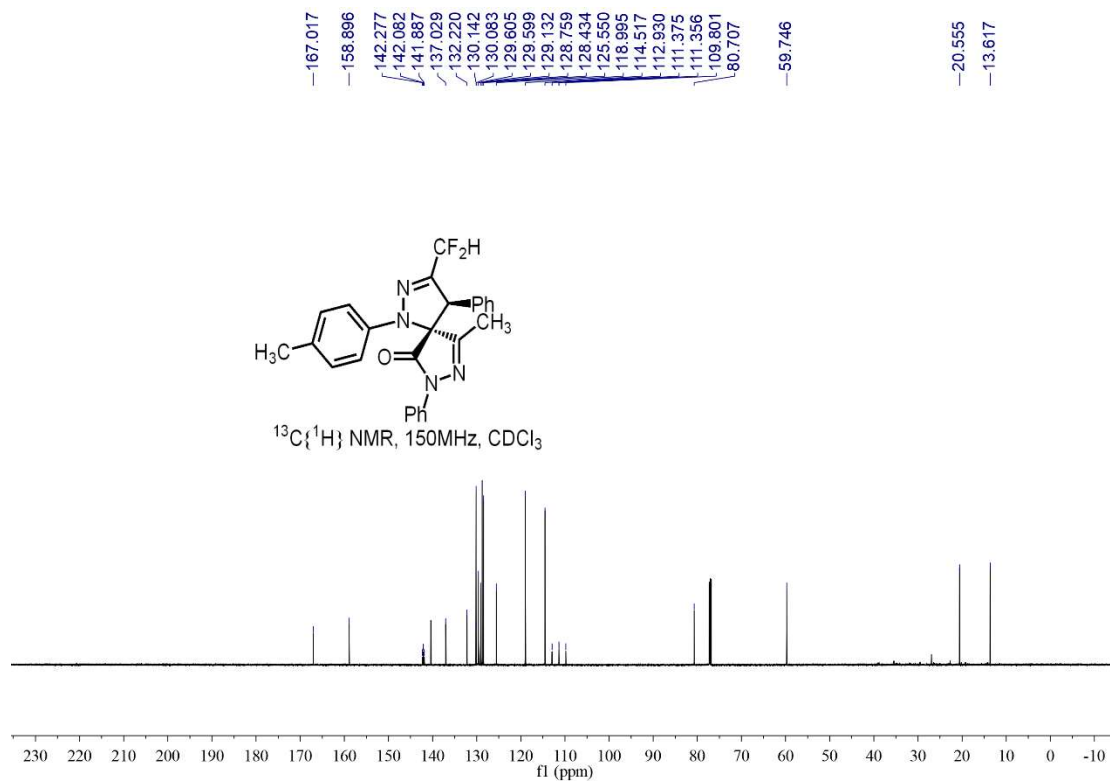
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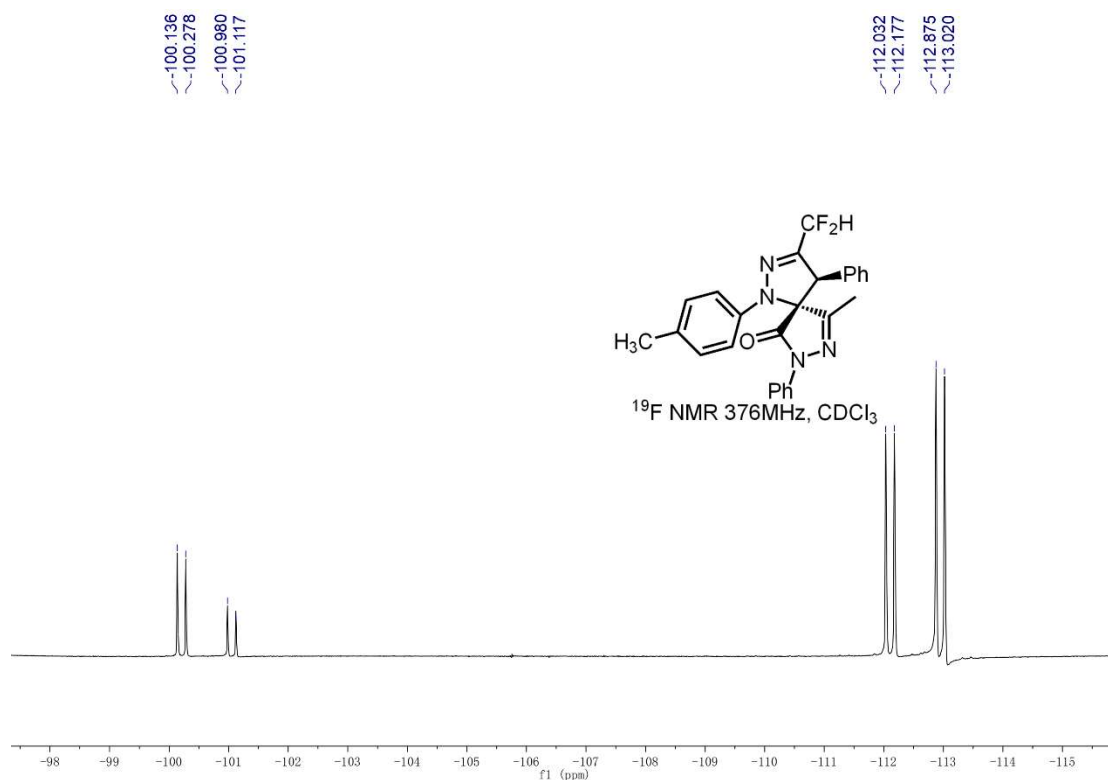


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R	e; % Conf	mS ig ma	Std l	Std Me an Va z or m	Std l m/ z Diff	Std Com b Dev	
467.1666	1 C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	-2.5	-2.8	16.5	ok	even	3.8	4.9	1.5	2.7	1.0	842.7

NMR copies of compound (*cis*)-**3c**:







HRMS (ESI) copy of compound (*cis*)-**3c**:

### Mass Spectrum SmartFormula Report

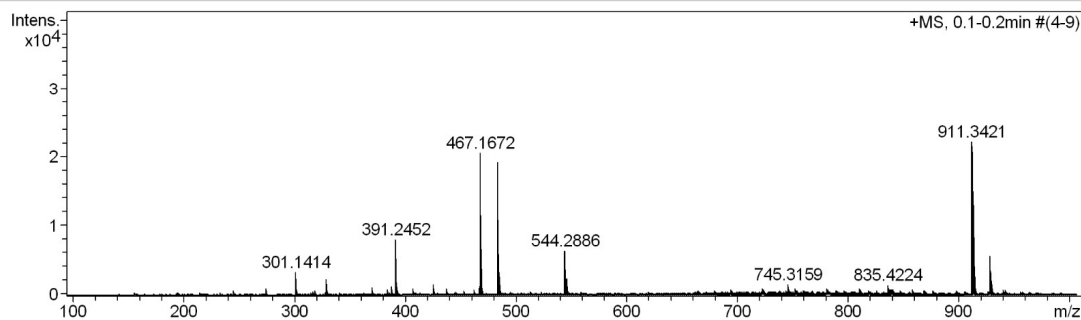
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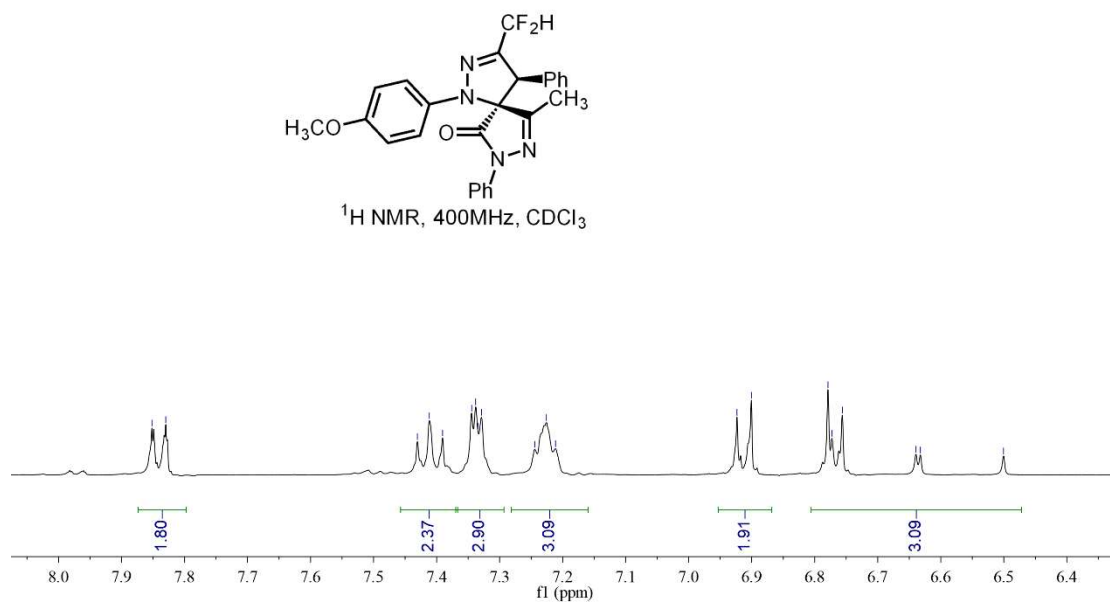
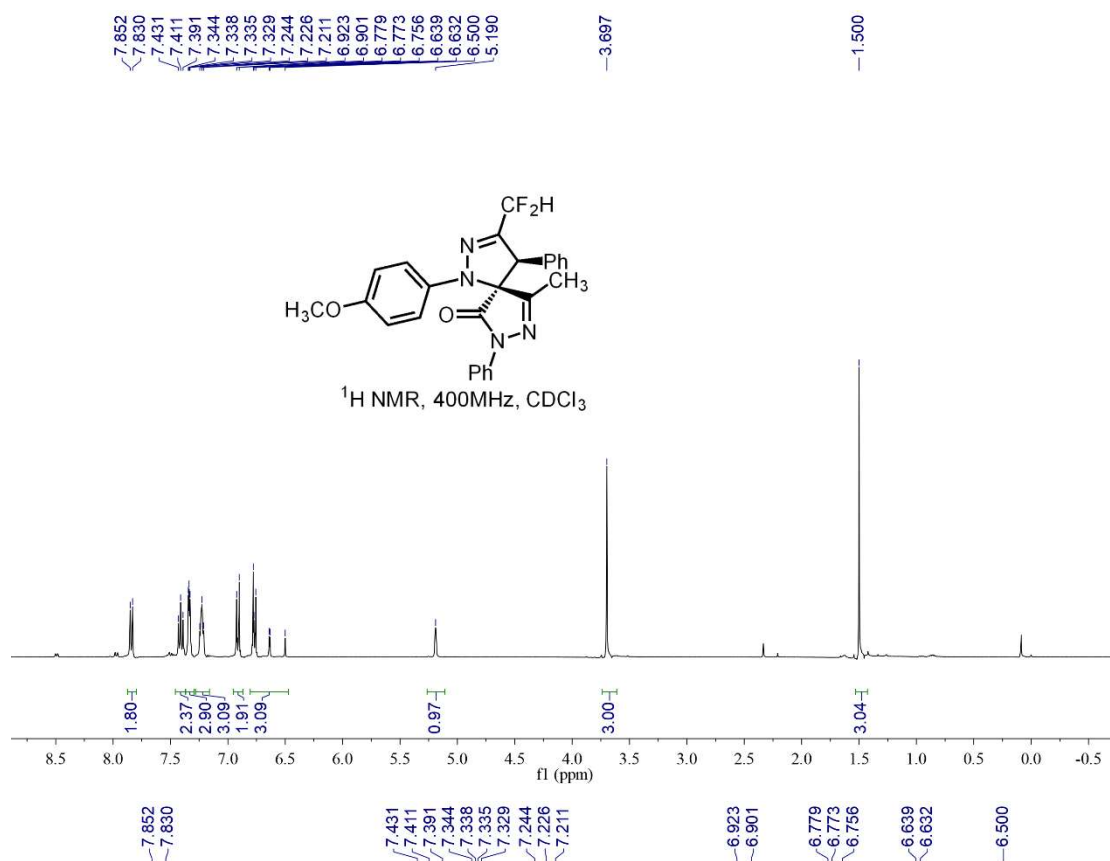
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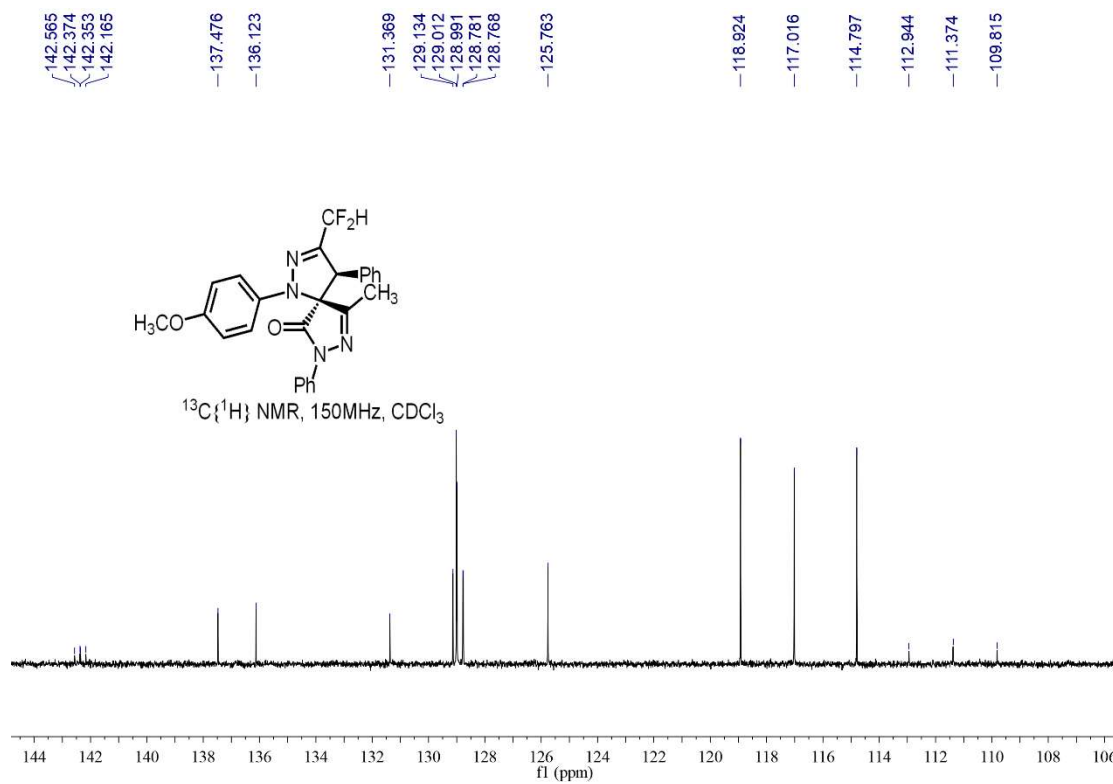
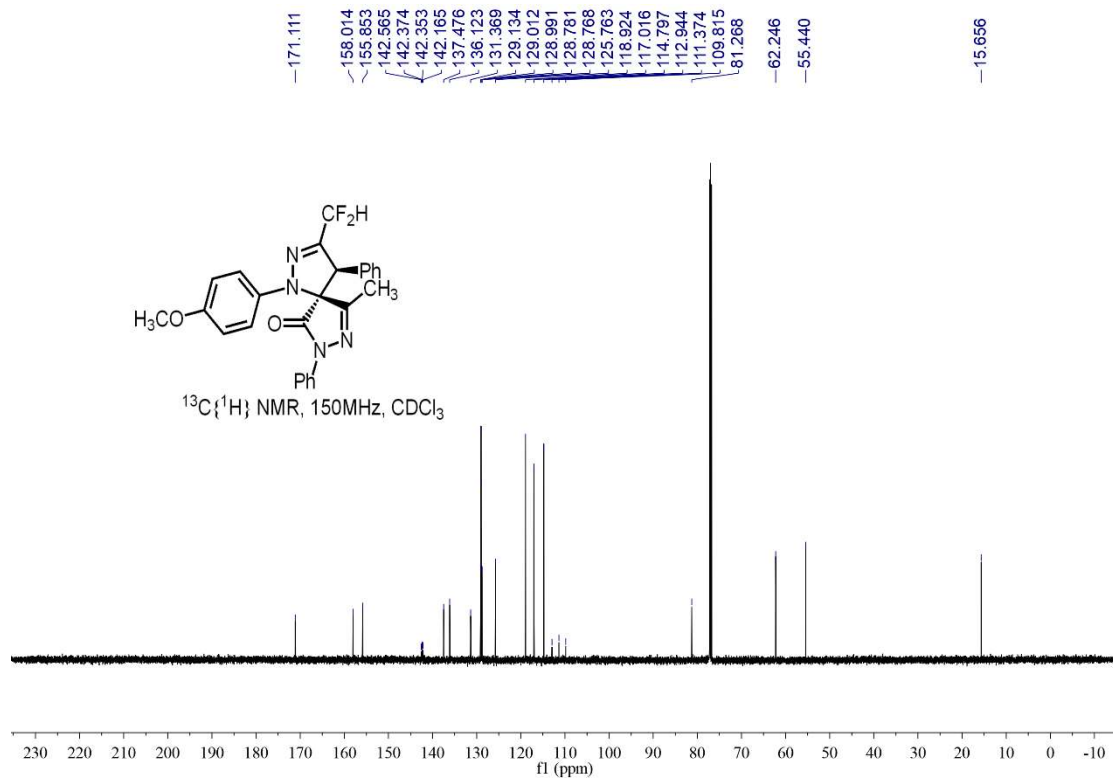
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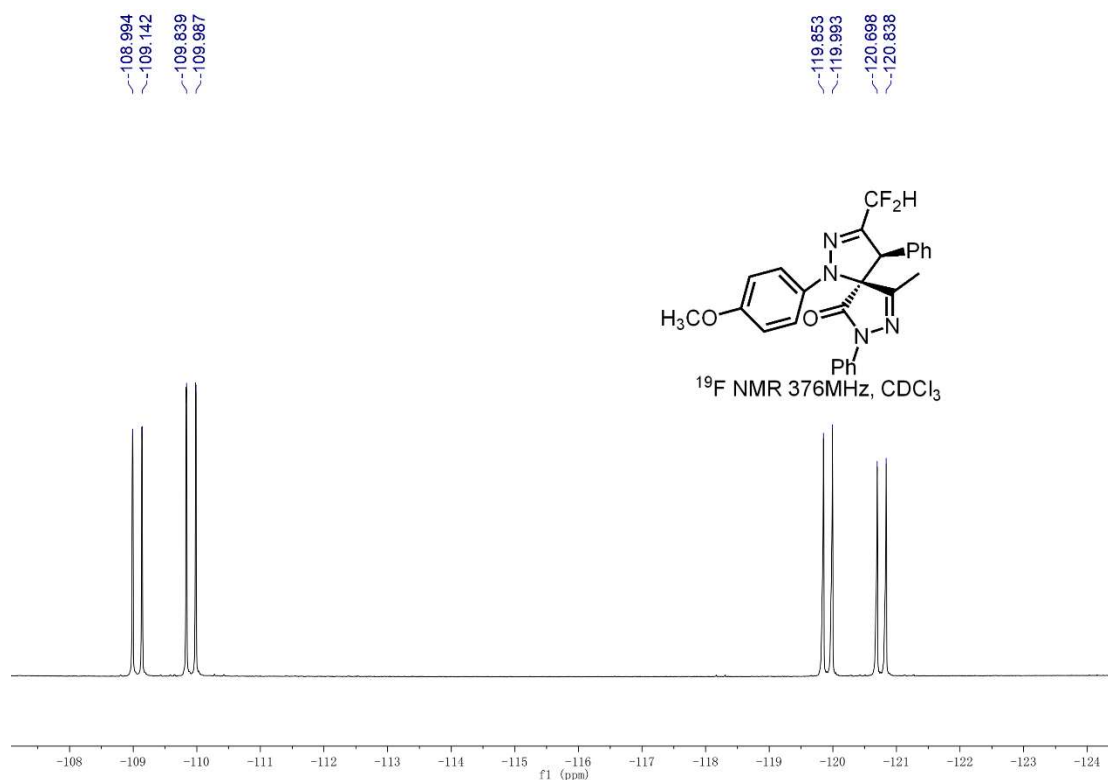


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467.1672	1 C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	-3.9	-3.4	16.5	ok	even	14.3	21.6	2.1	9.5	0.2	842.7

NMR copies of compound (*trans*)-**3d**:







HRMS (ESI) copy of compound (*trans*)-**3d**:

### Mass Spectrum SmartFormula Report

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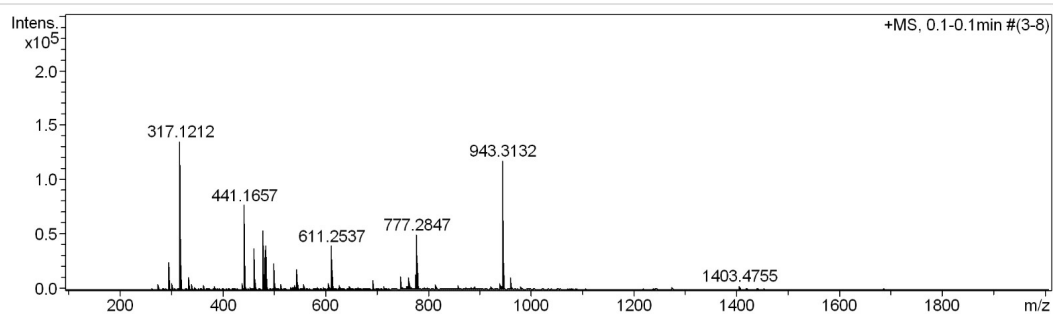
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 Instrument / Ser# micrOTOF-Q 20453

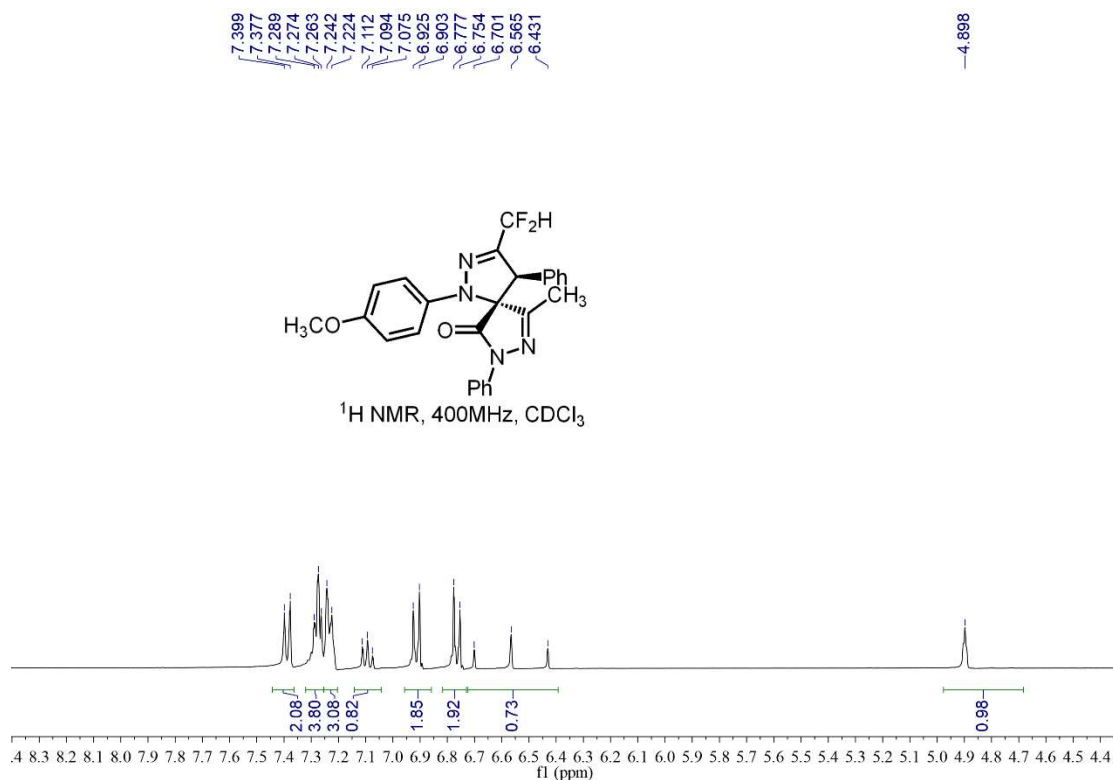
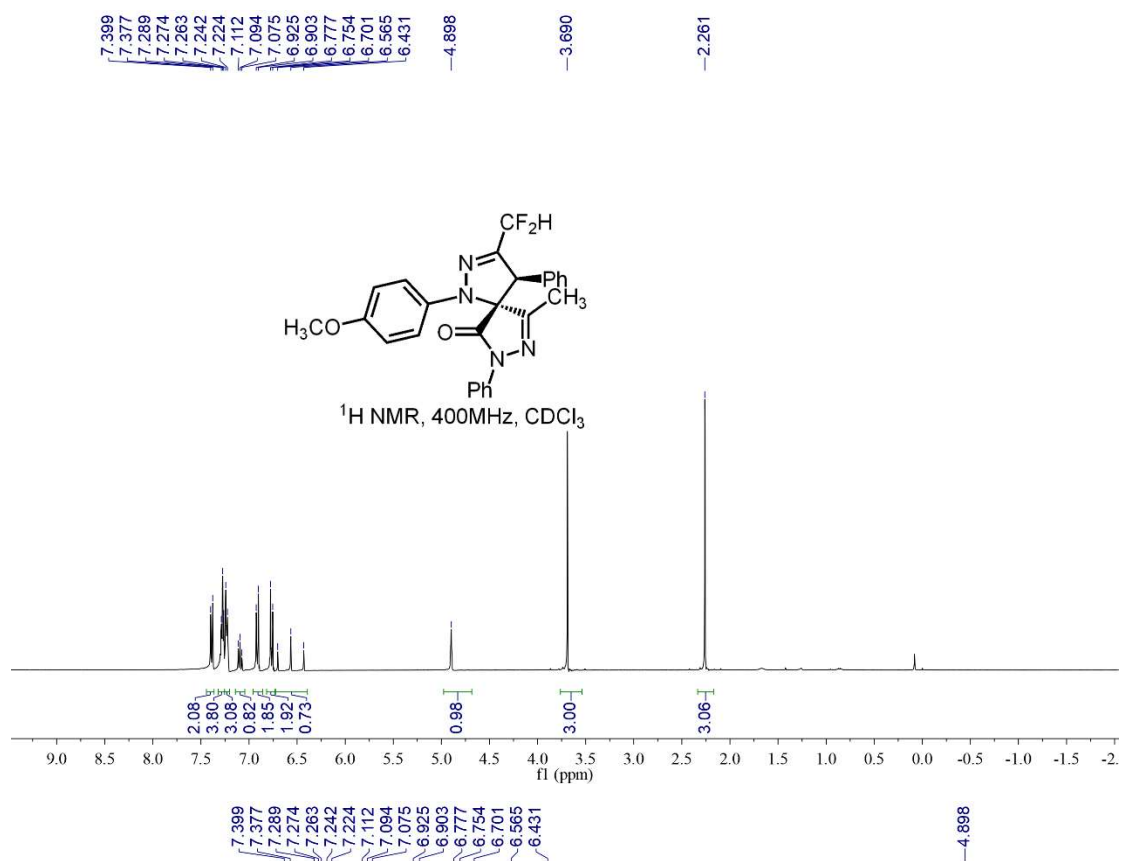
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
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Scan End	2000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

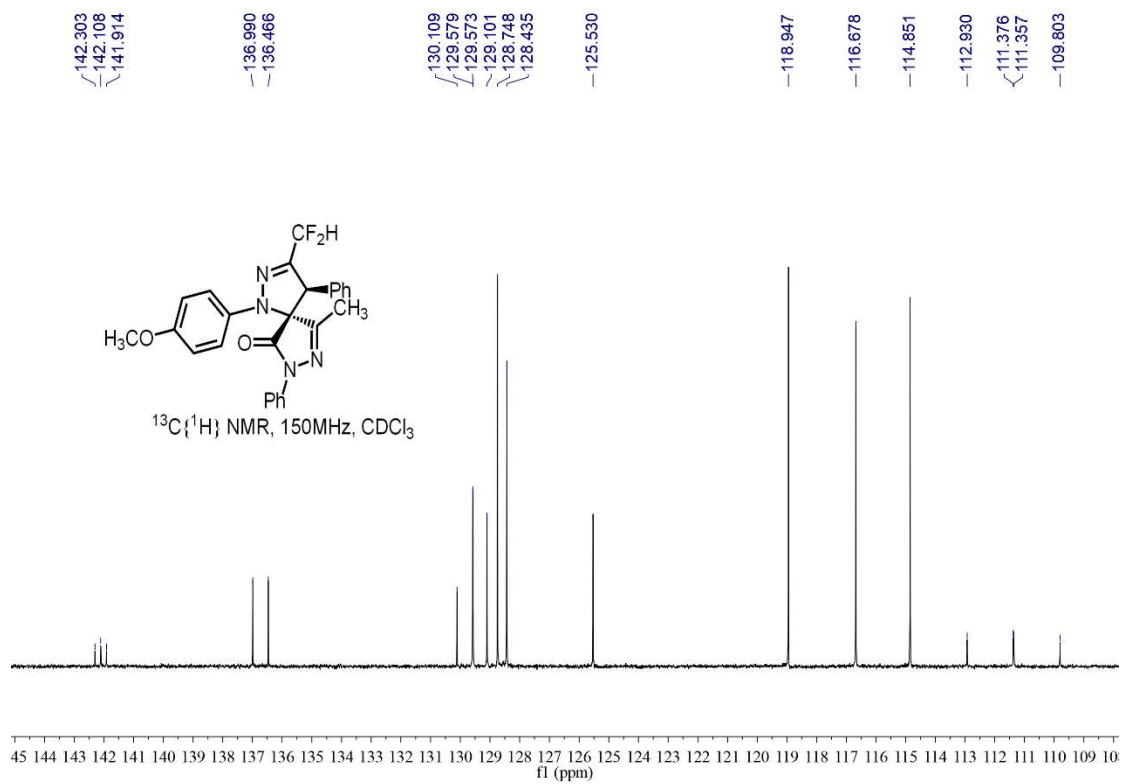
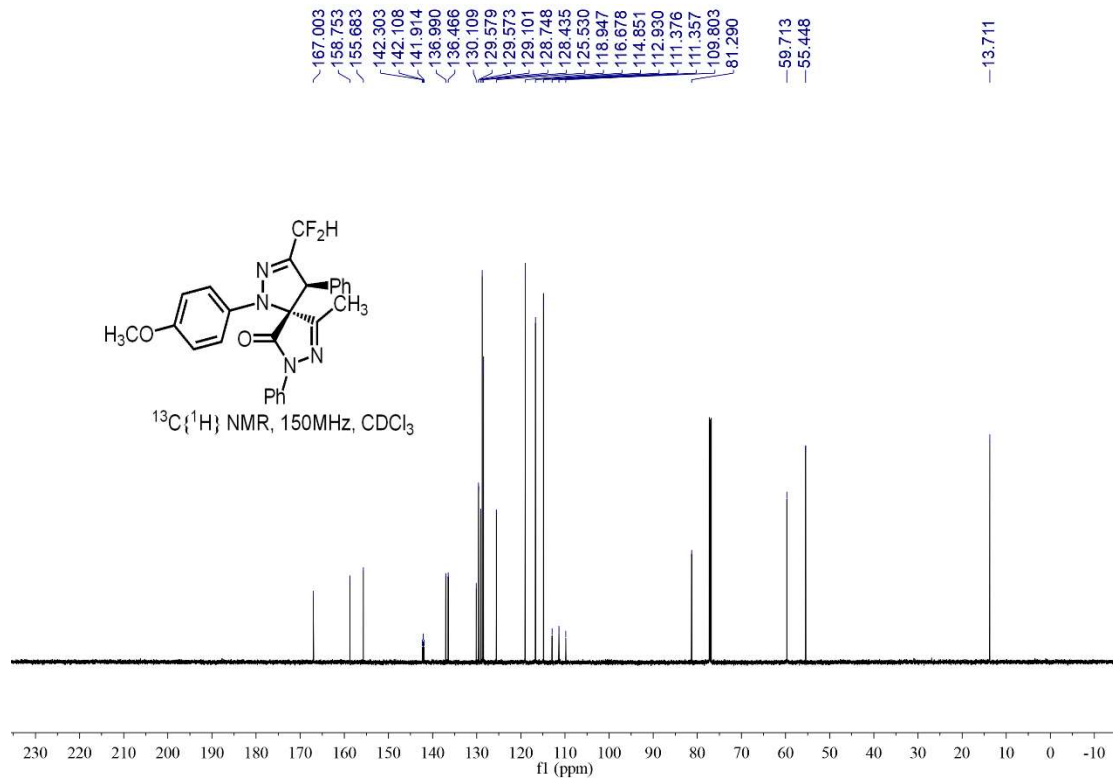


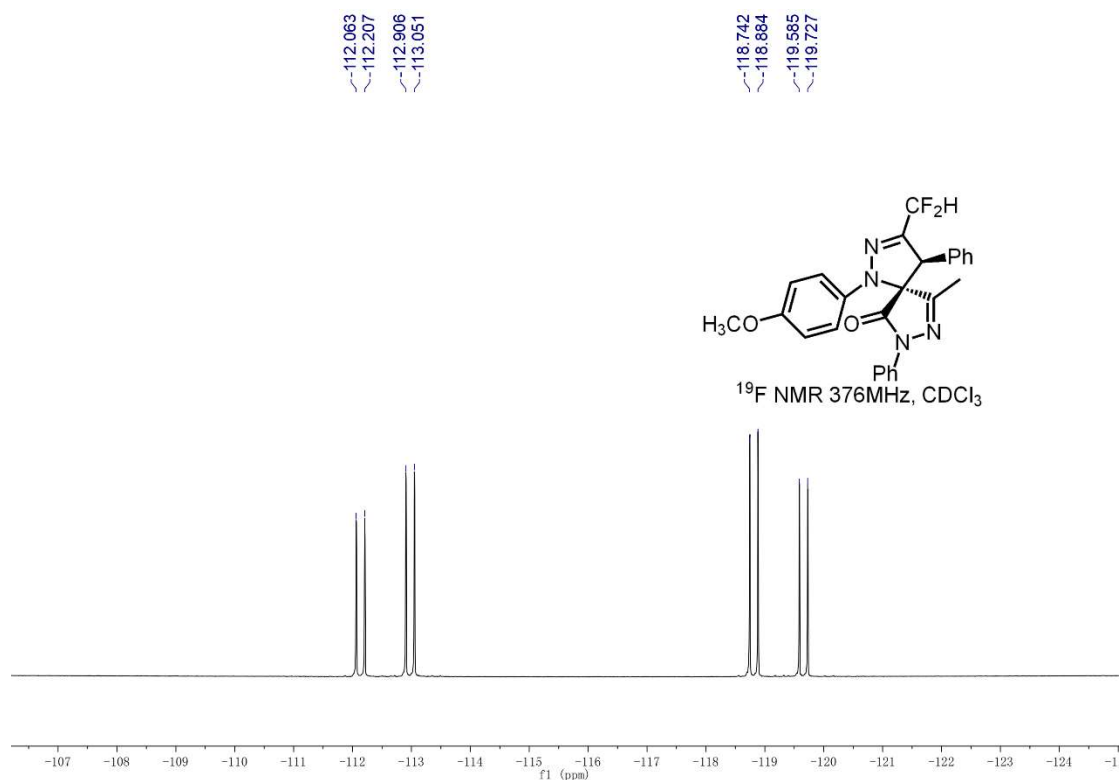
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdB	N-R	ej# Conf	mSi gma	Std l	St d Me an m/z	Std l Var m	Std l Dif f	Std Com b Dev
461.1788	1 C <sub>26</sub> H <sub>23</sub> F <sub>2</sub> N <sub>4</sub> O <sub>2</sub>	461.1784	-0.9	0.2	16.5	ok	even	42.9	66.5	1.2	28.7	1.8	842.7

NMR copies of compound (*cis*)-**3d**:









HRMS (ESI) copy of compound (*cis*)-**3d**:

### Mass Spectrum SmartFormula Report

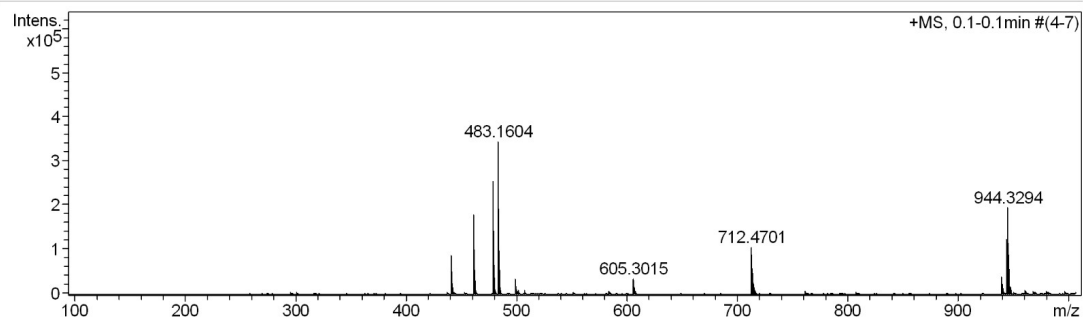
#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20220707---2.d  
 Method tune\_low.m  
 Sample Name A221  
 Comment

Acquisition Date 2022-7-7 11:25:15  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

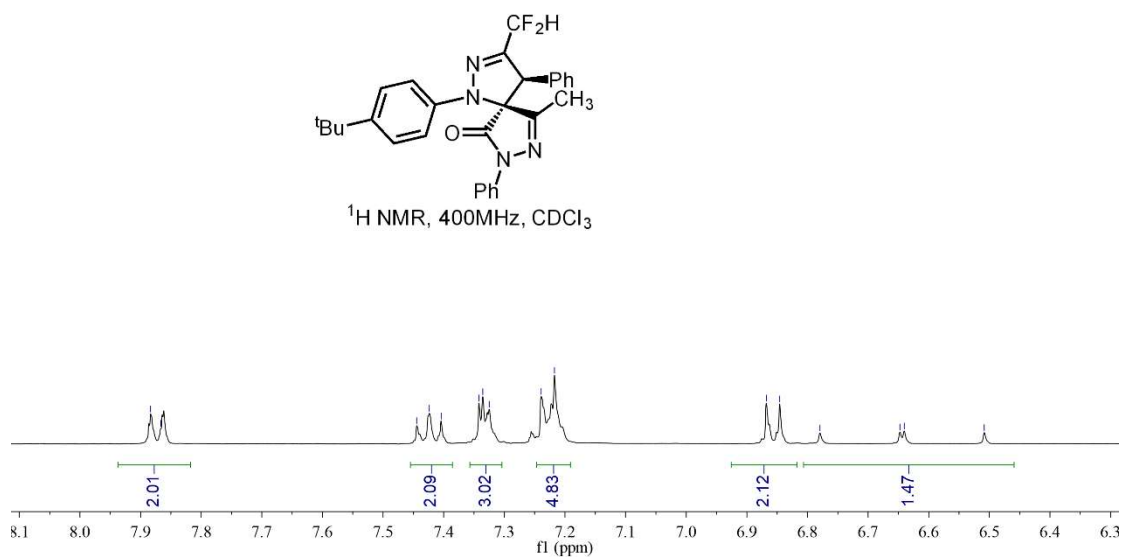
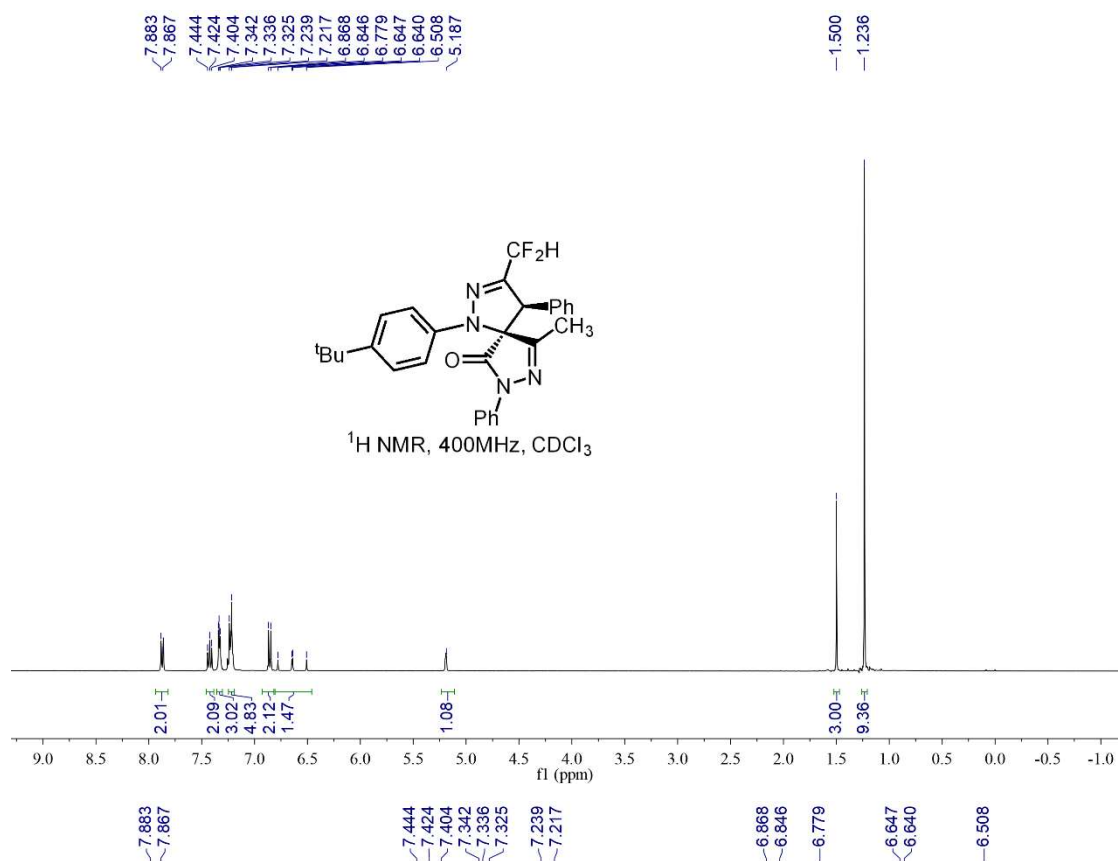
#### Acquisition Parameter

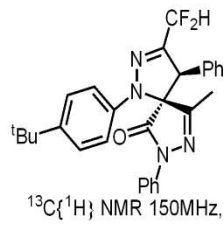
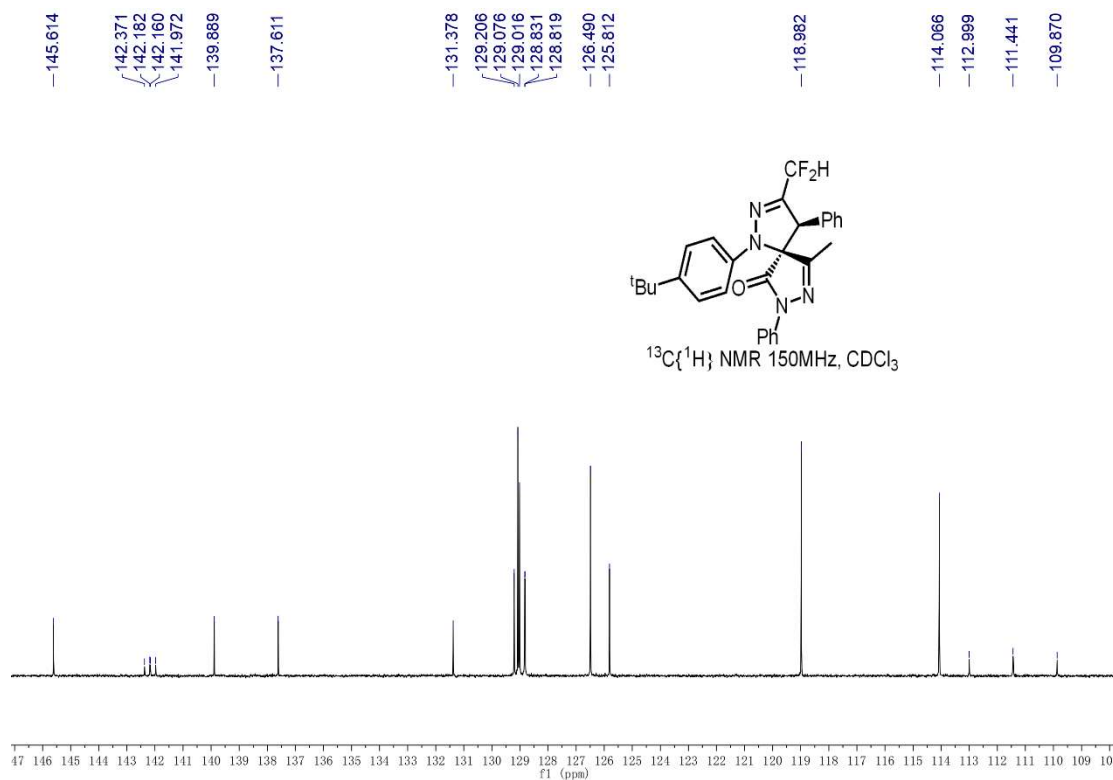
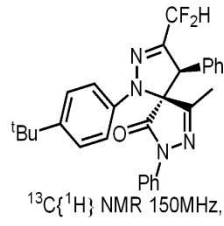
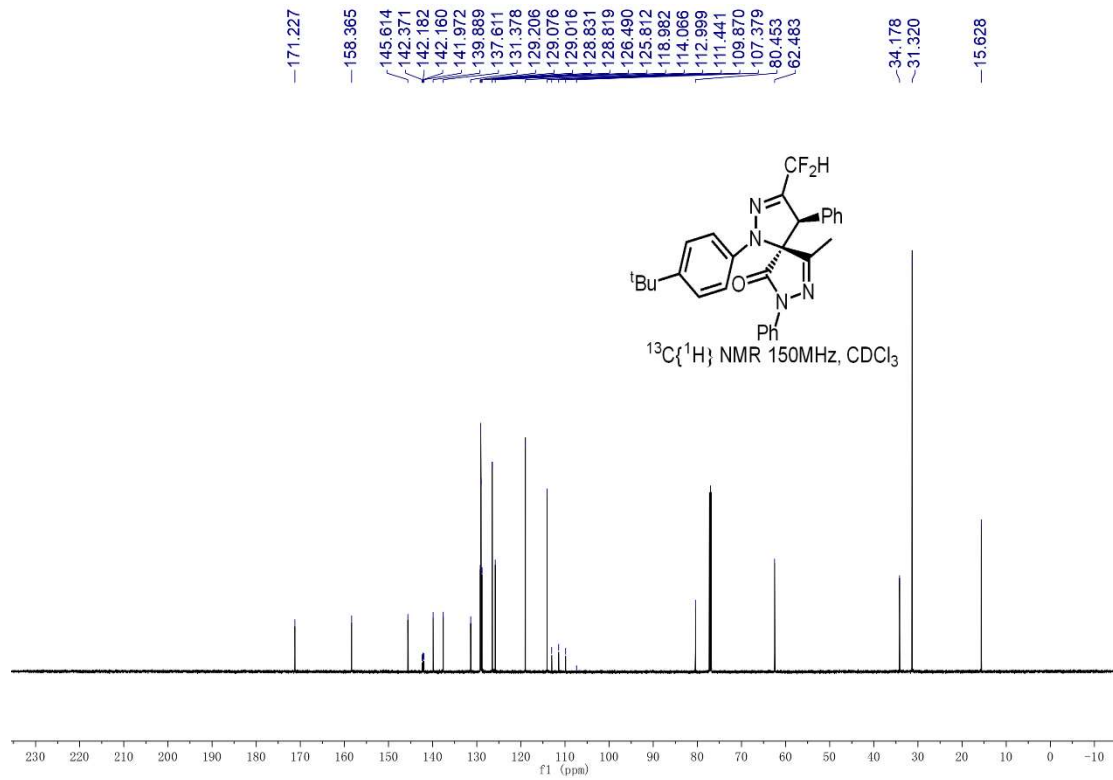
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-R	e <sub>i</sub> ≠ Conf	m Sigma	St d l	St d l	St d l	St d l	Std Com b Dev
483.1604	1 C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO <sub>2</sub>	483.1603	-0.3	-0.8	16.5	ok	even	4.5	6.5	0.7	2.8	0.7	842.7

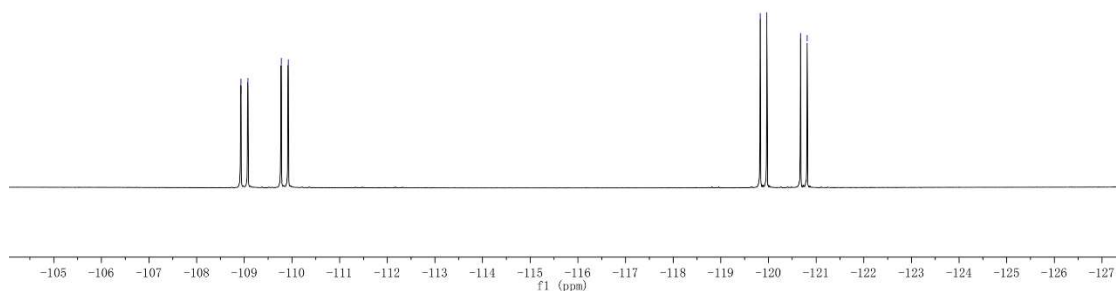
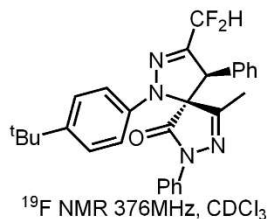
NMR copies of compound (*trans*)-**3e**:





-108.930  
-109.077  
-109.775  
-109.923

-119.828  
-119.968  
-120.673  
-120.813



HRMS (ESI) copy of compound (*trans*)-3e:

### Mass Spectrum SmartFormula Report

#### Analysis Info

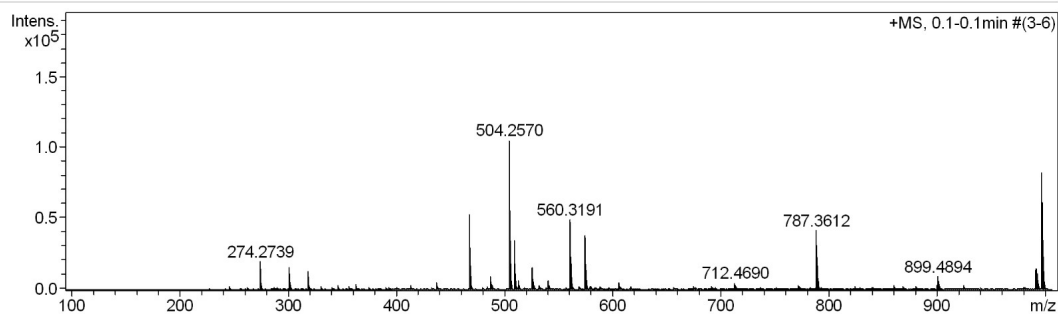
Analysis Name D:\Data\user\NWNWU-fengyang 20220707-5.d  
Method tune\_low.m  
Sample Name A-25  
Comment

Acquisition Date 2022-7-7 11:29:58

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

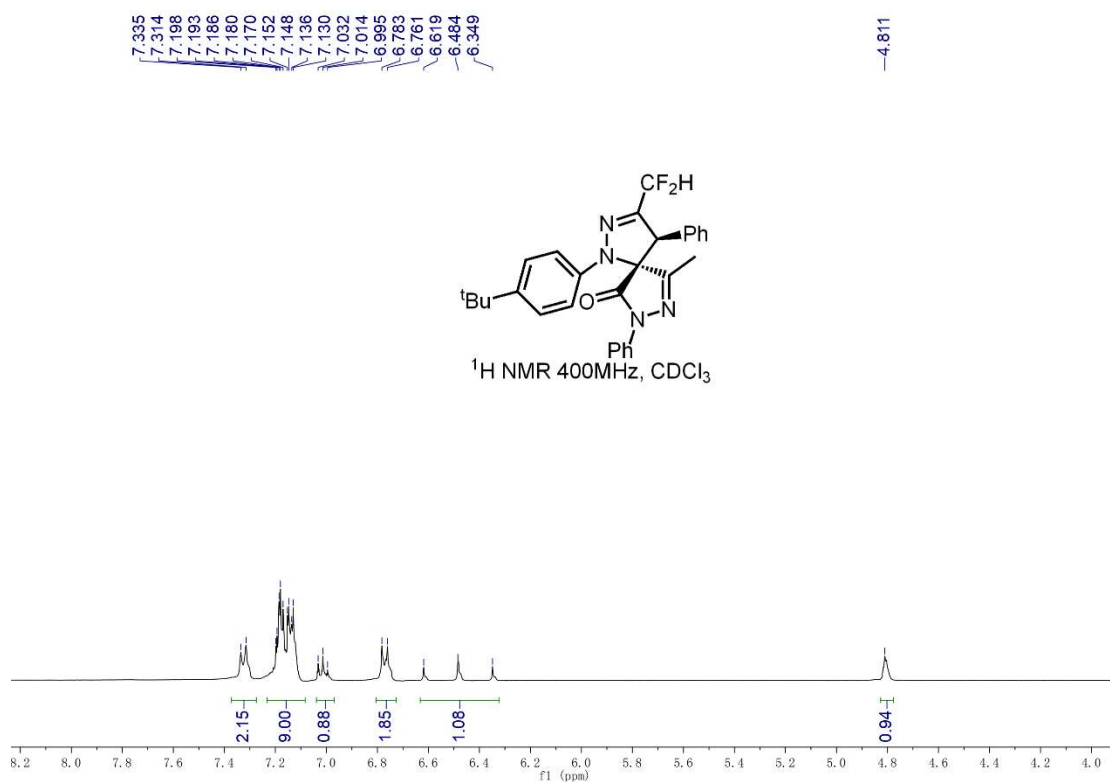
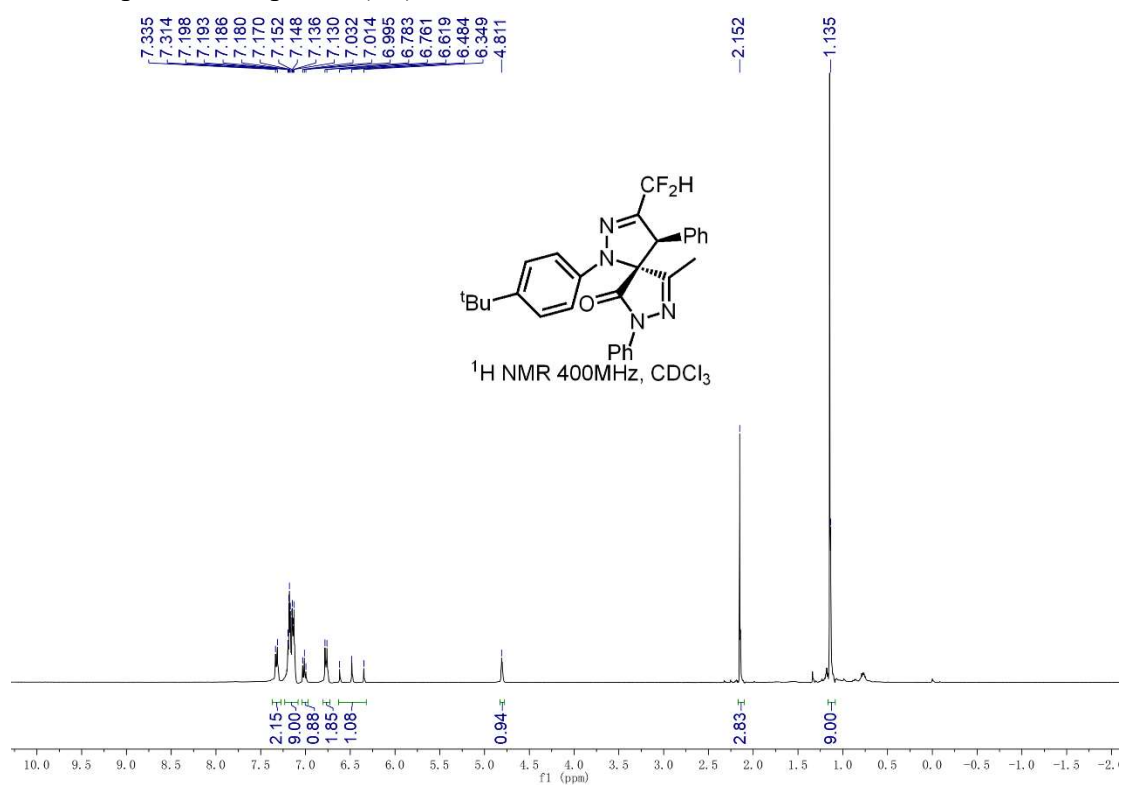
#### Acquisition Parameter

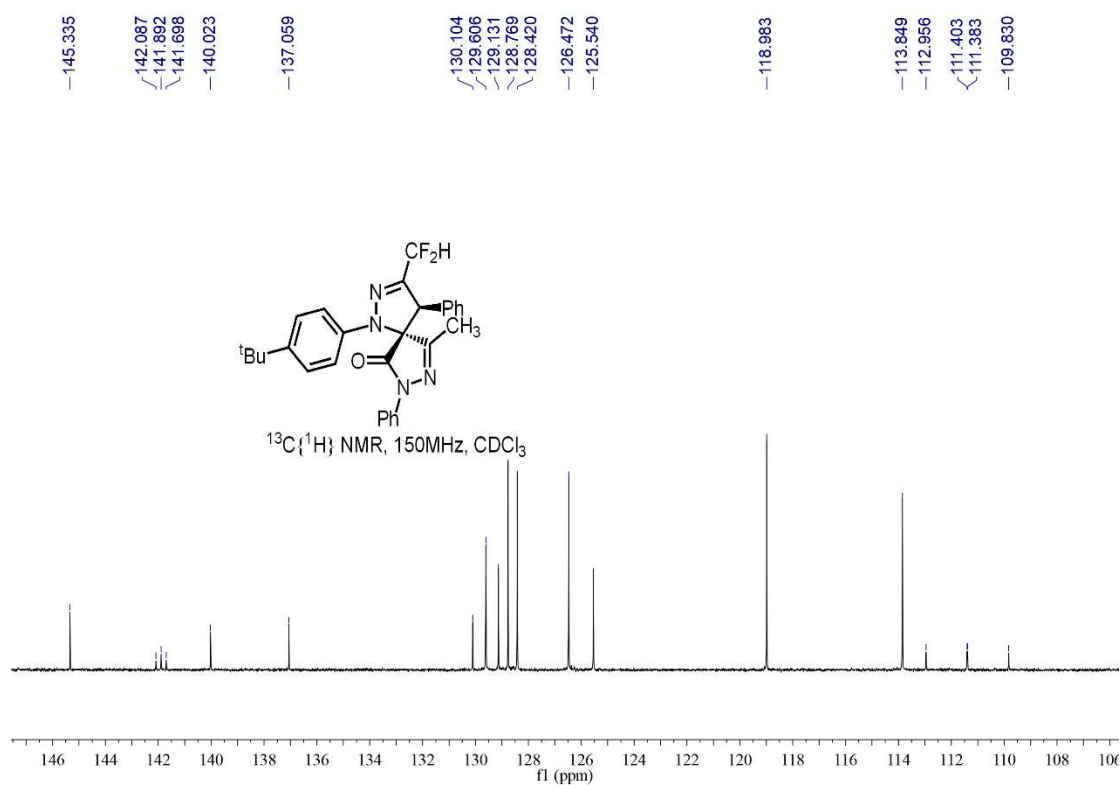
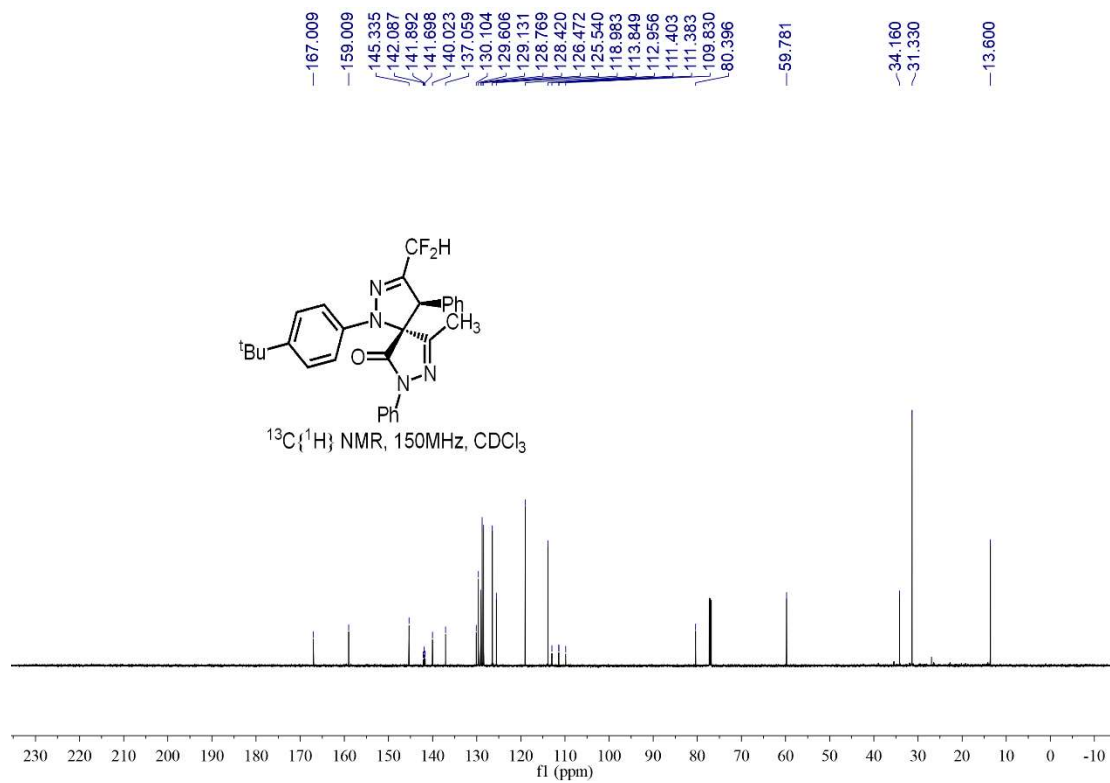
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

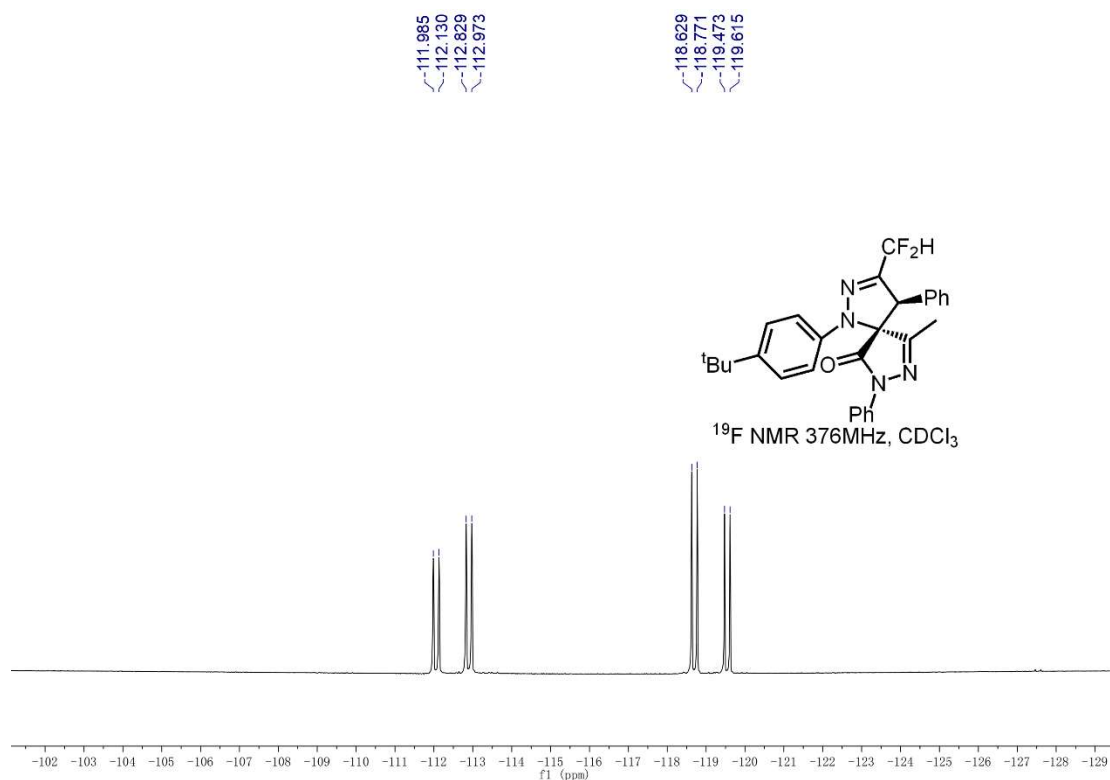


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>i</sub> ≠	mS Conf	Std	Std	Std	Std	Std
m/z									l	l	l	l	l
509.2129	1 C <sub>29</sub> H <sub>28</sub> F <sub>2</sub> N <sub>4</sub> NaO	509.2123	-1.0	-1.0	16.5	ok	even	6.3	9.1	0.5	4.0	0.5	842.7

NMR copies of compound (*cis*)-**3e**:







HRMS (ESI) copy of compound (*cis*)-**3e**:

### Mass Spectrum SmartFormula Report

#### Analysis Info

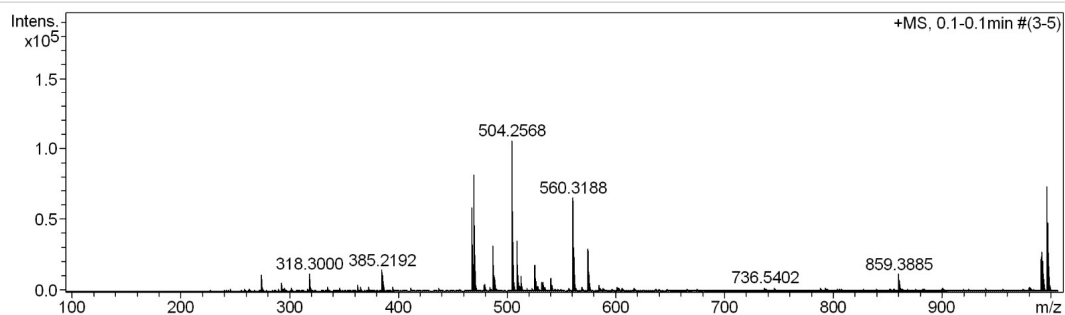
Analysis Name D:\Data\user\NWNNU-fengyang 20220707-6.d  
 Method tune\_low.m  
 Sample Name A-251  
 Comment

Acquisition Date 2022-7-7 11:31:21

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

#### Acquisition Parameter

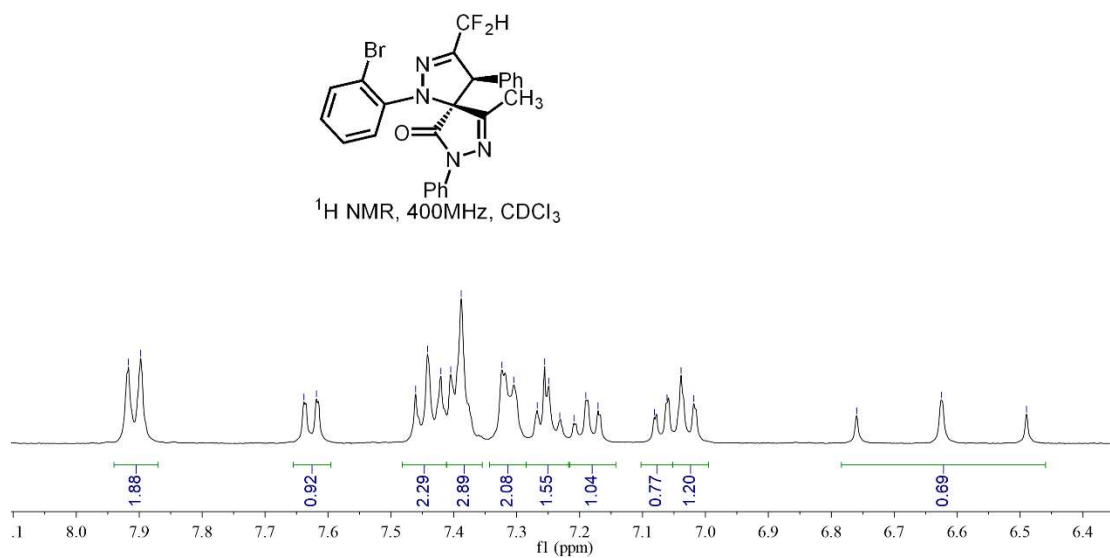
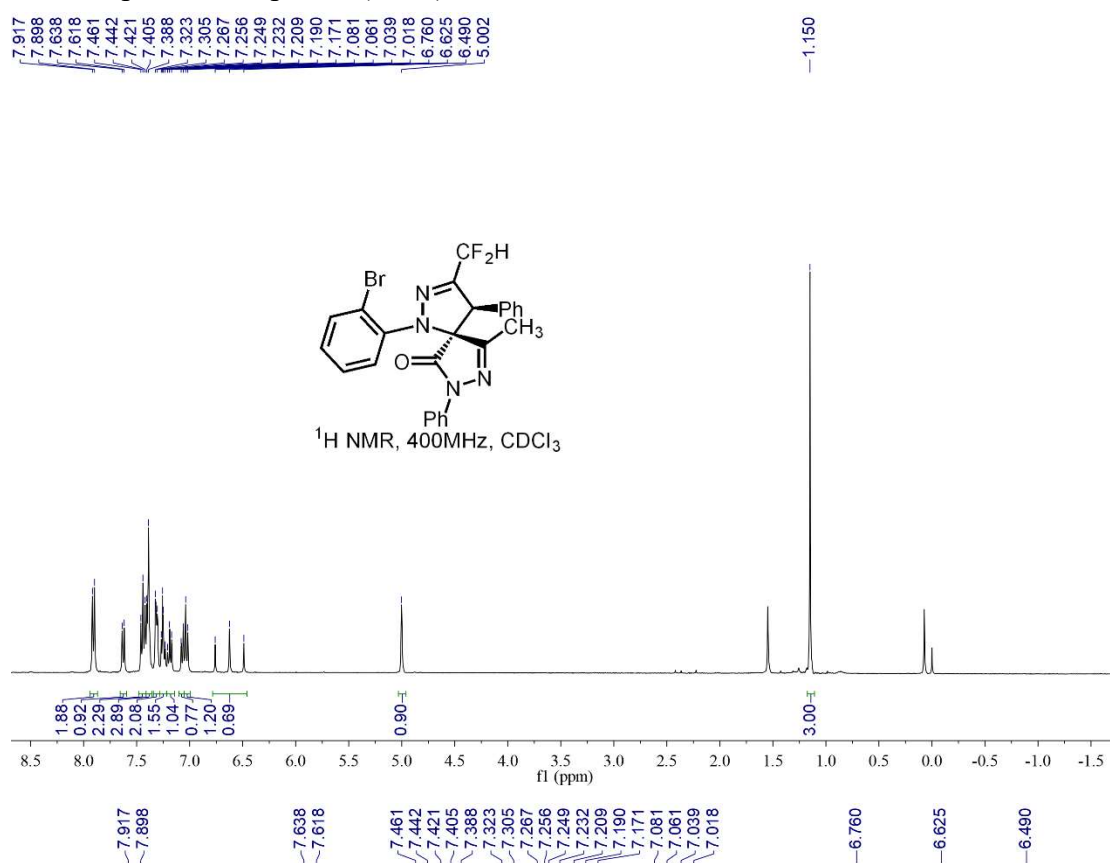
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

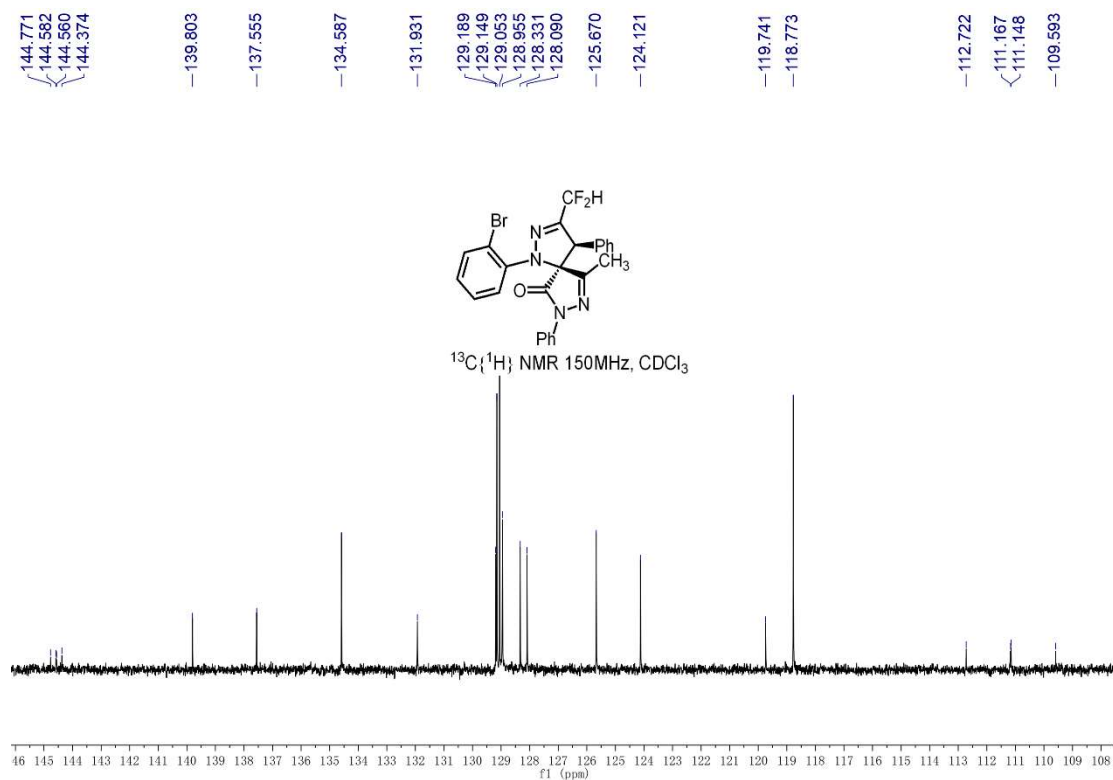
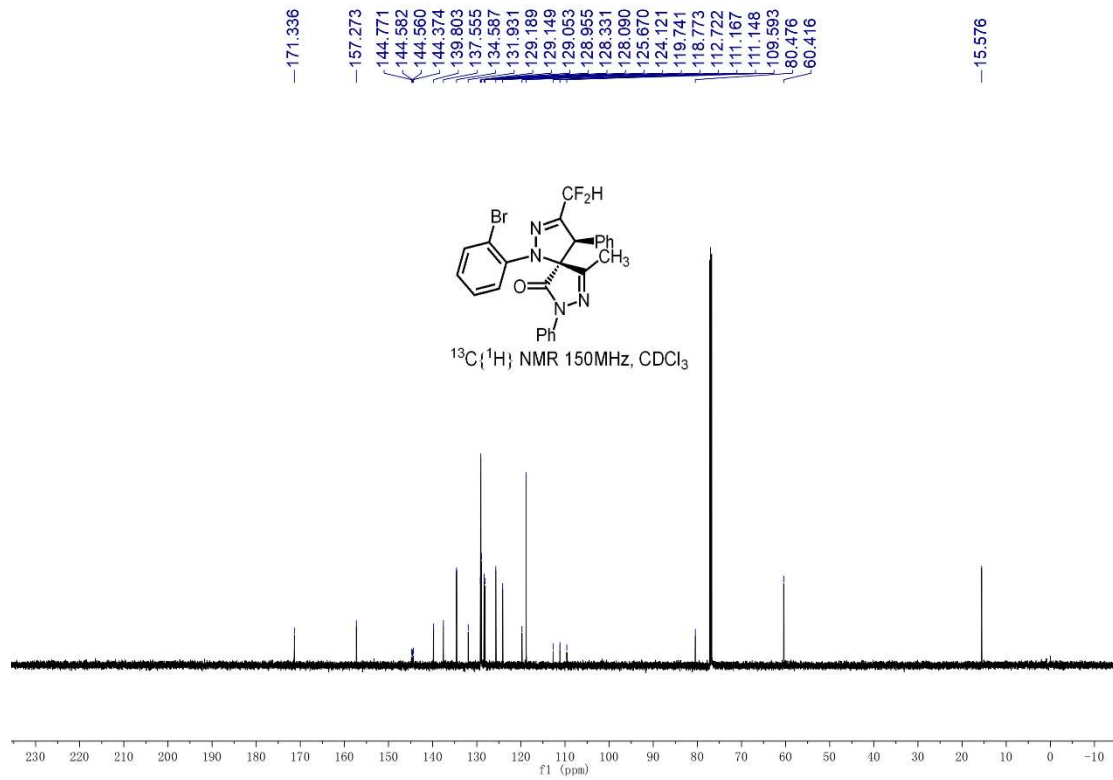


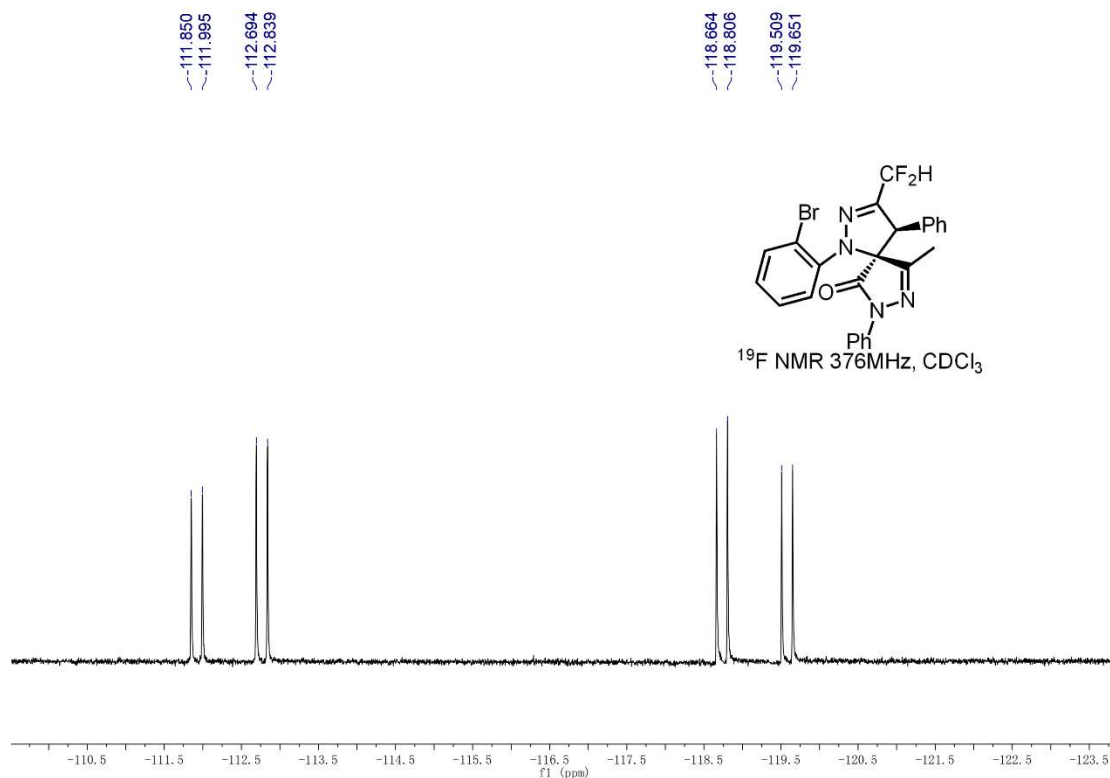
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j% Con f	mSi gm a	Std l	St d Me m/z	Std l Var Nor m	Std m/z Diff	Std Com b Dev
509.2131	1 C <sub>29</sub> H <sub>28</sub> F <sub>2</sub> N <sub>4</sub> NaO	509.2123	-1.4	-5.9	16.5	ok	even	20.0	31.6	9.1	15.6	23.7	842.7



NMR copies of compound (*trans*)-**3f**:







HRMS (ESI) copy of compound (*trans*)-3f:

### Mass Spectrum SmartFormula Report

**Analysis Info**

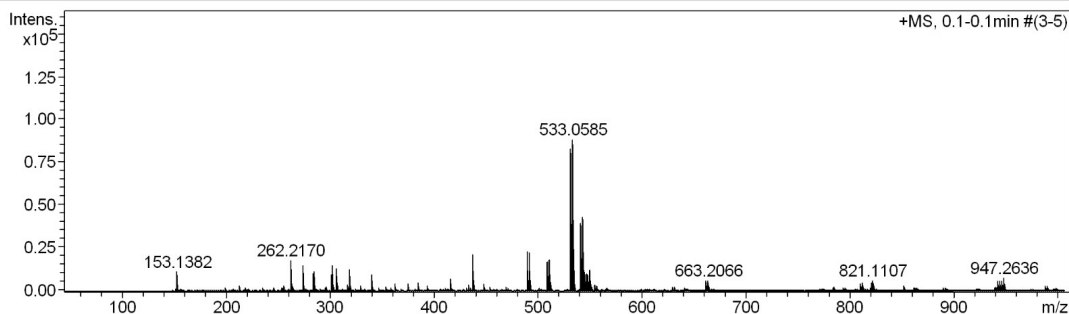
Analysis Name D:\Data\user\NWNNU-fengyang 20230321--1.d  
 Method tune\_low.m  
 Sample Name A-18  
 Comment

Acquisition Date 2023-3-21 15:30:09

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

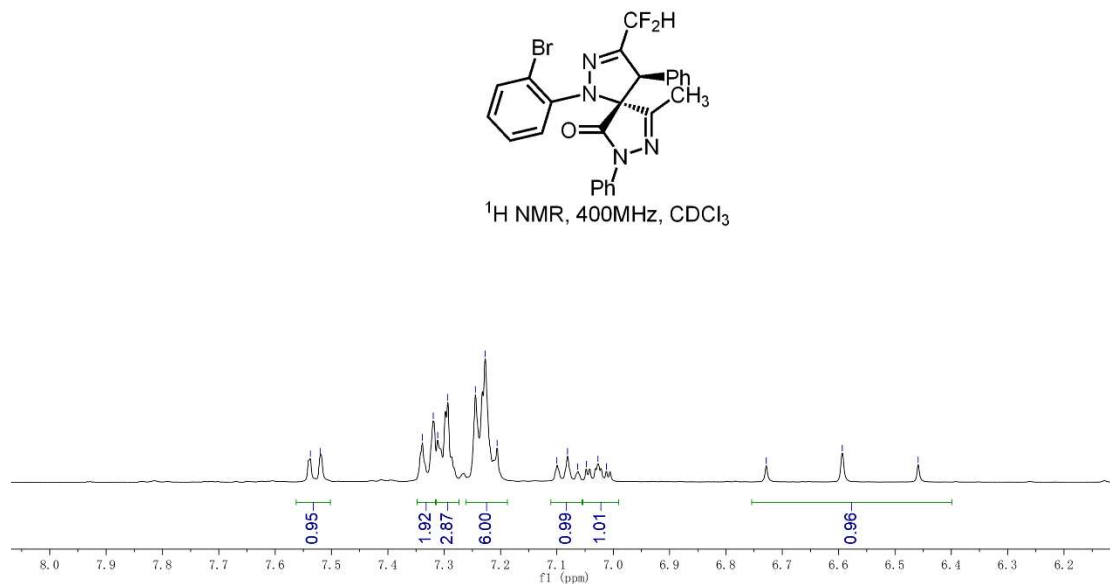
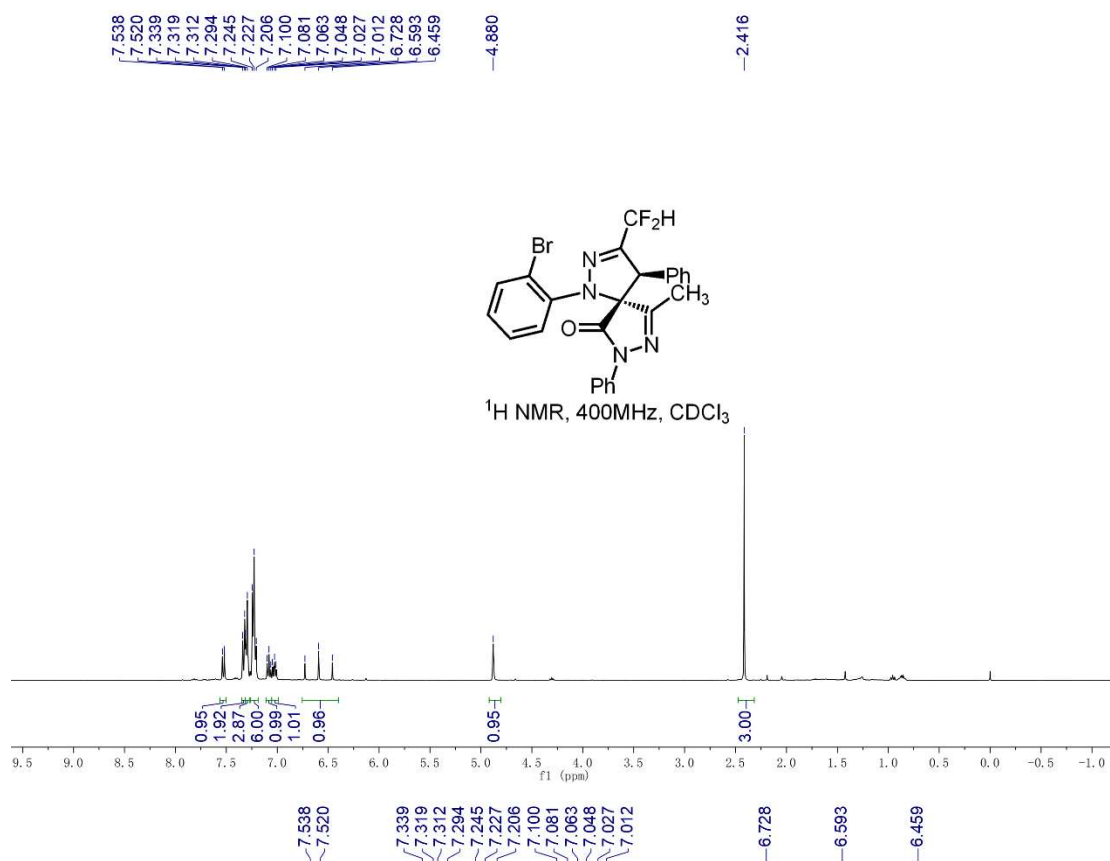
**Acquisition Parameter**

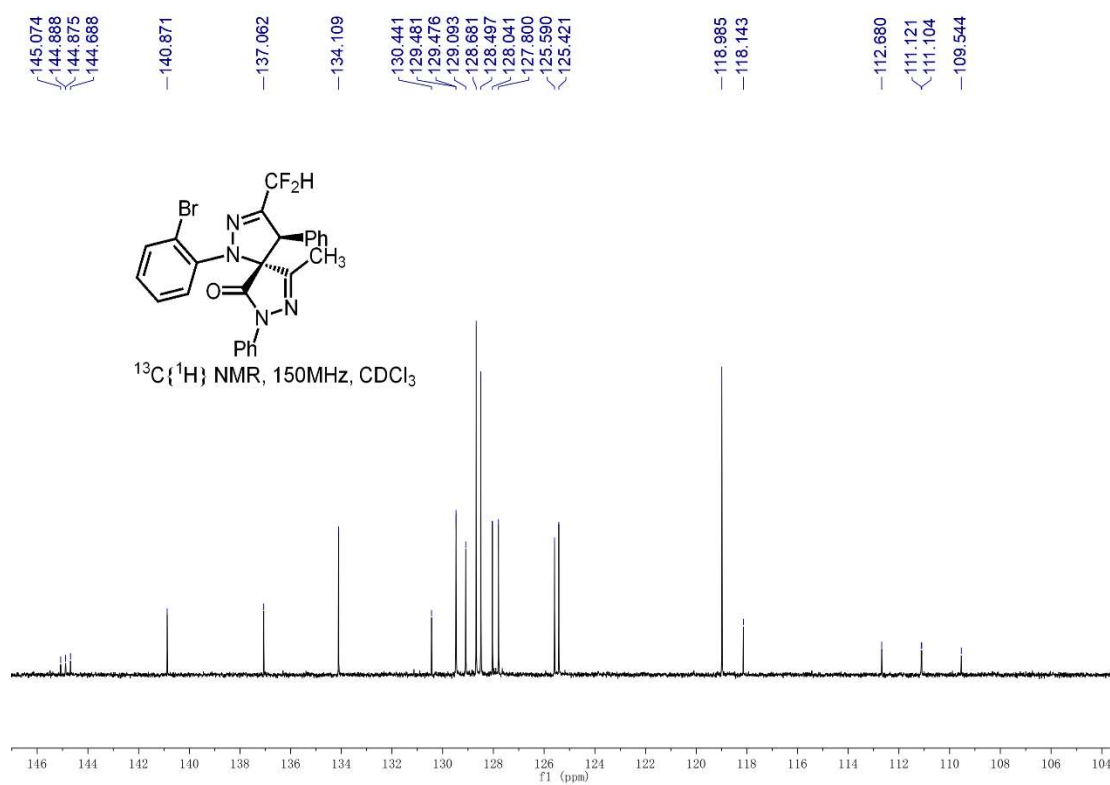
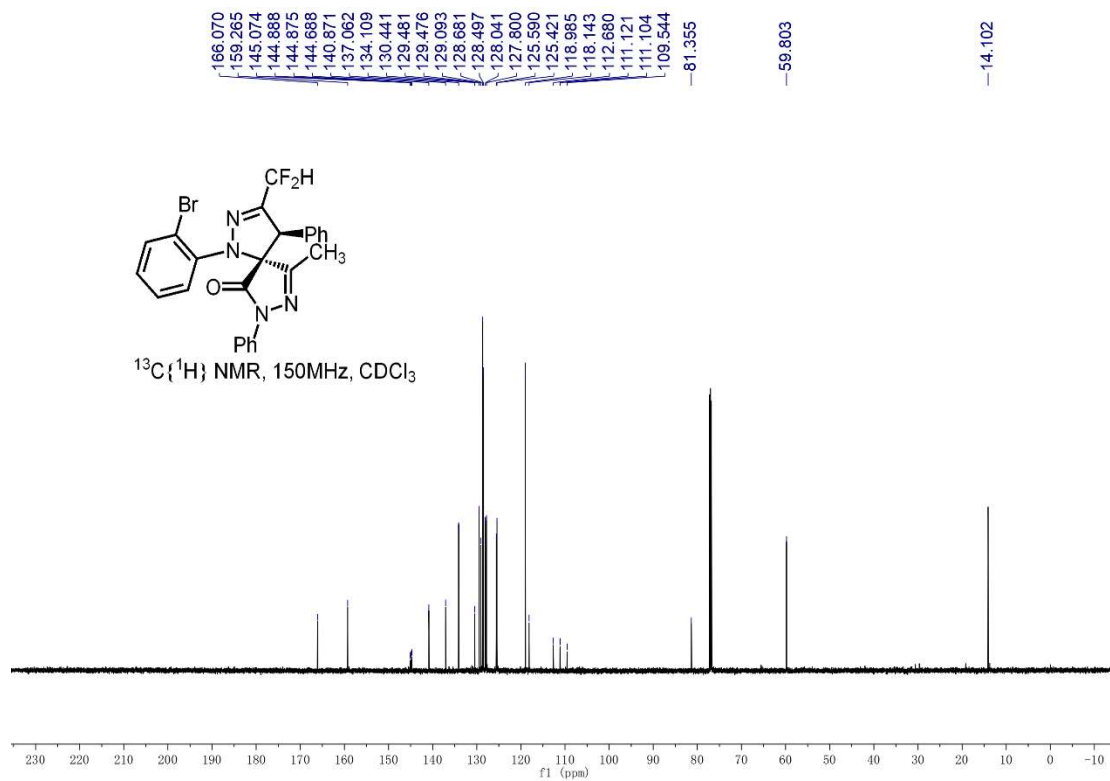
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

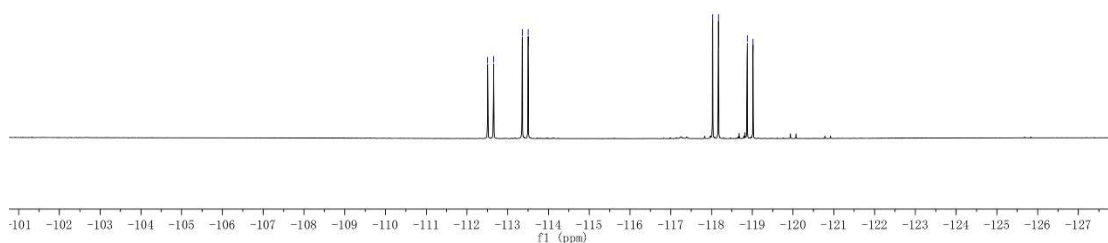
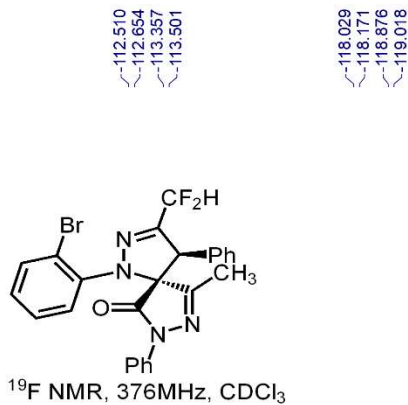


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej% Conf	mSi gm a	Std l	St d l	St d l	St d l	Std Com b
531.0600	1 C <sub>25</sub> H <sub>19</sub> BrF <sub>2</sub> N <sub>4</sub> NaO	531.0603	0.6	0.4	16.5	ok	even	22.2	17.7	0.5	5.9	0.7	842.7

NMR copies of compound (*cis*)-**3f**:







HRMS (ESI) copy of compound (*cis*)-**3f**:

### Mass Spectrum SmartFormula Report

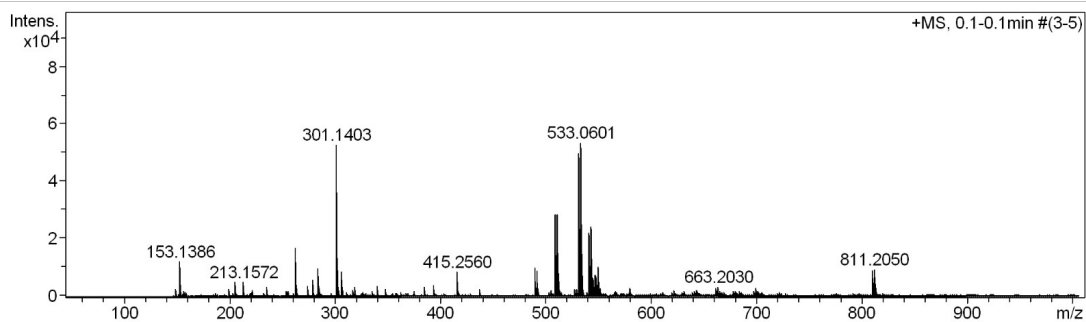
**Analysis Info**

Analysis Name D:\Data\user\NWNNU-fengyang 20230321-2.d  
 Method tune\_low.m  
 Sample Name A-181  
 Comment

Acquisition Date 2023-3-21 15:31:47  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

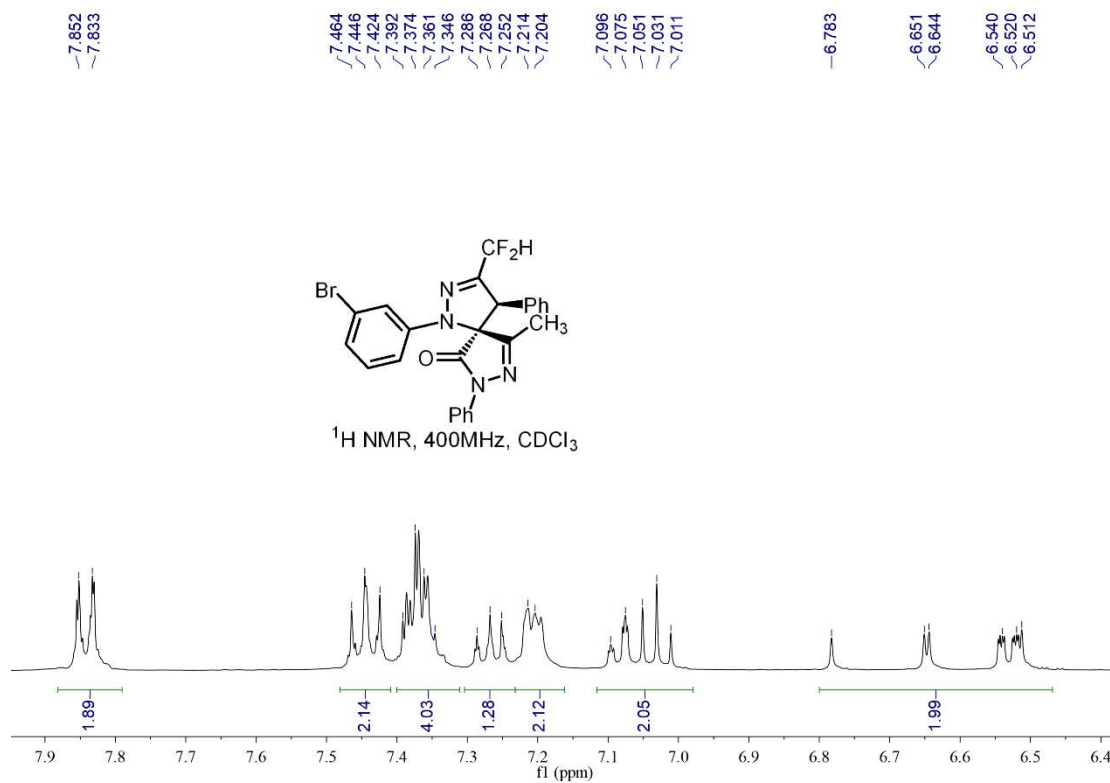
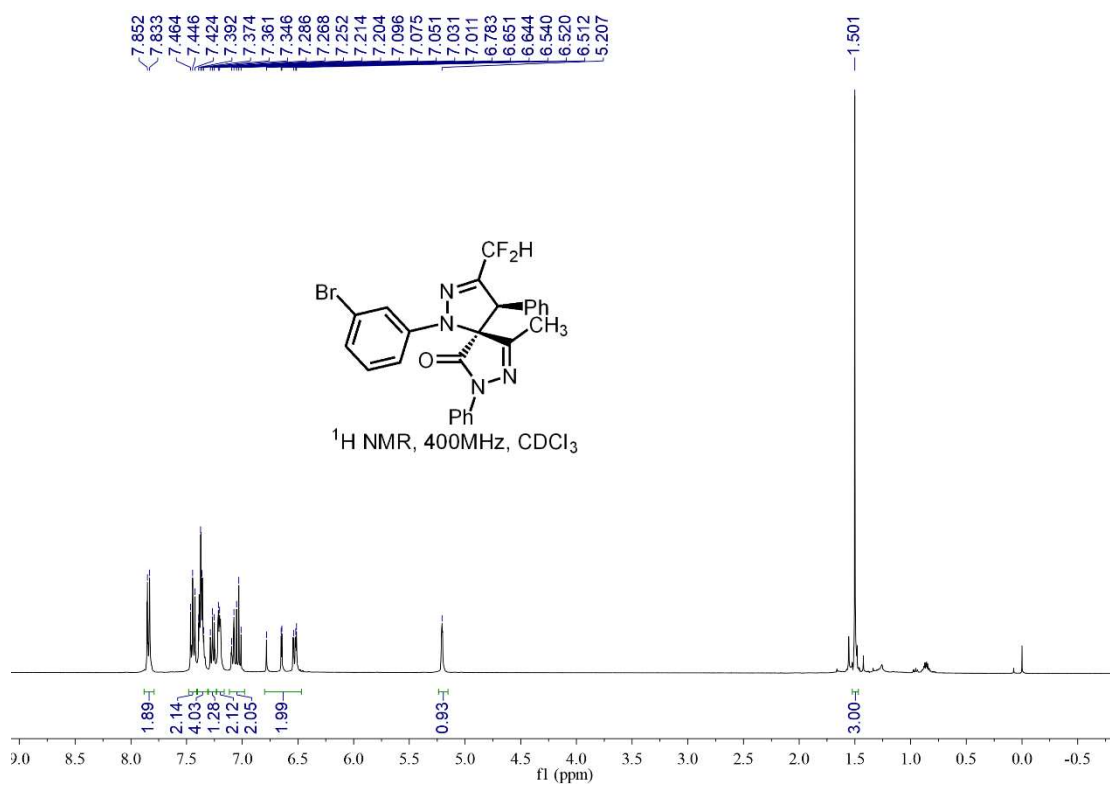
**Acquisition Parameter**

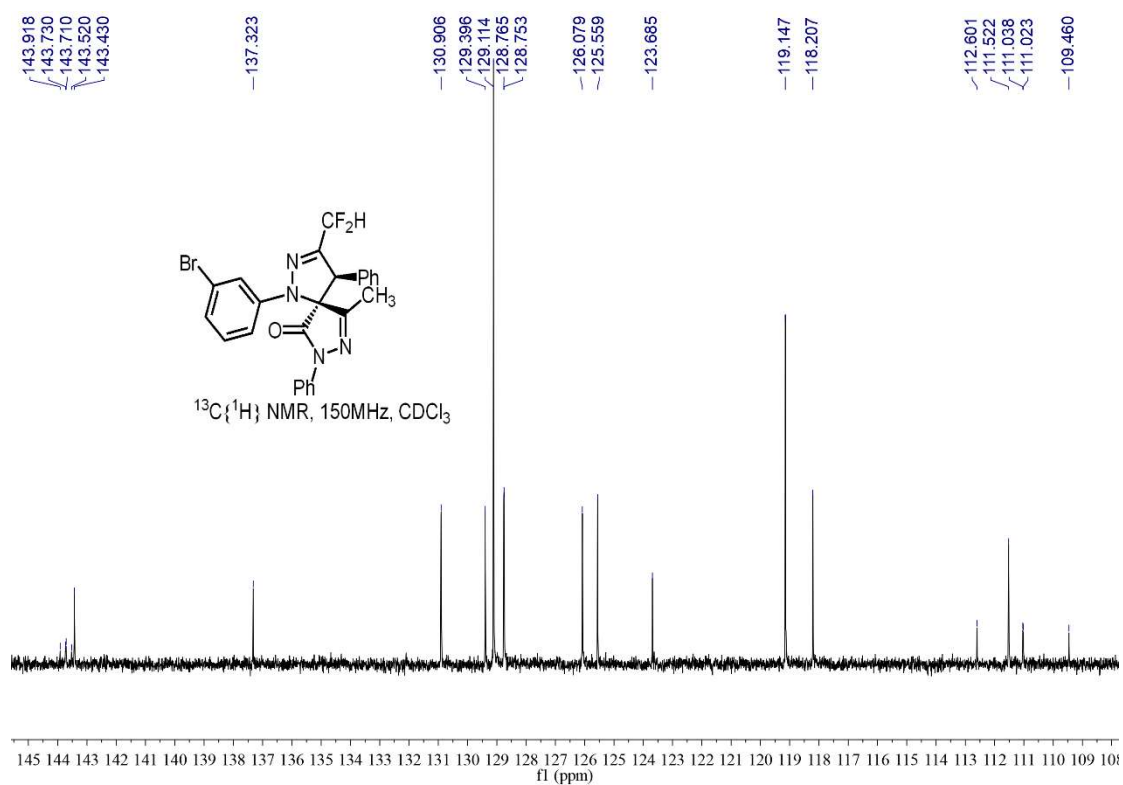
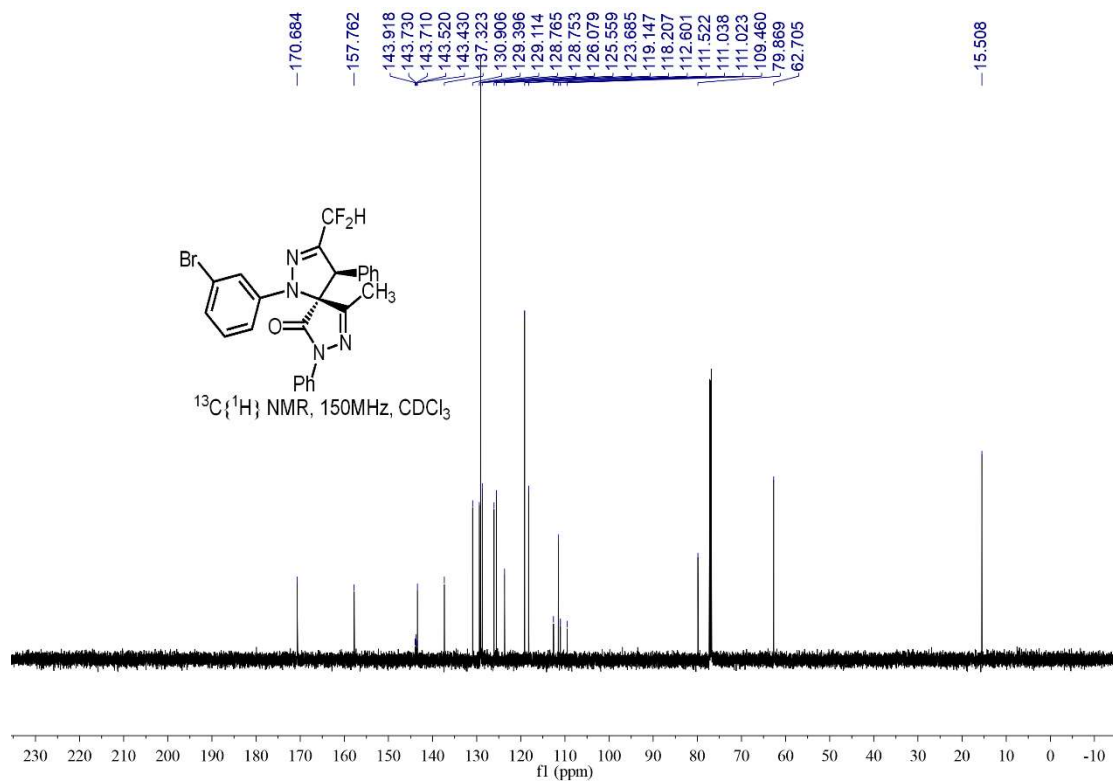
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{A}$ C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e;f	Con	mSi gm	Std l	St d	St d l	St d m/	Std Com b
531.0612	1 C <sub>25</sub> H <sub>19</sub> BrF <sub>2</sub> N <sub>4</sub> NaO	531.0603	-1.7	-1.6	16.5	ok	even	28.0	23.9	1.3	8.3	1.8	842.7	

NMR copies of compound (*trans*)-**3g**:

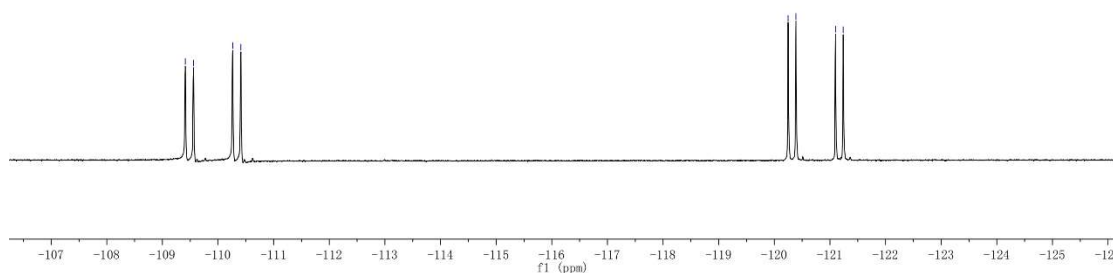
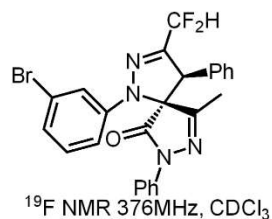






-109.412  
-109.560  
-110.263  
-110.410

-120.248  
-120.388  
-121.098  
-121.238



HRMS (ESI) copy of compound (*trans*)-**3g**:

### Mass Spectrum SmartFormula Report

#### Analysis Info

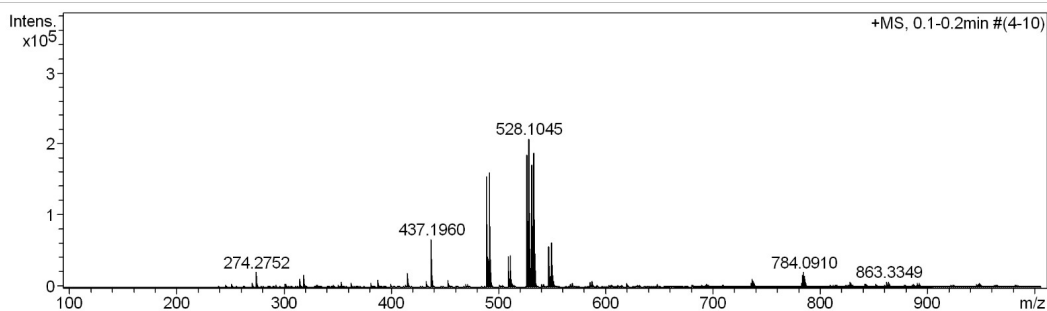
Analysis Name D:\Data\user\NWNU-fengyang 20220609-4.d  
Method tune\_low.m  
Sample Name A-19  
Comment

Acquisition Date 2022-6-9 14:42:26

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

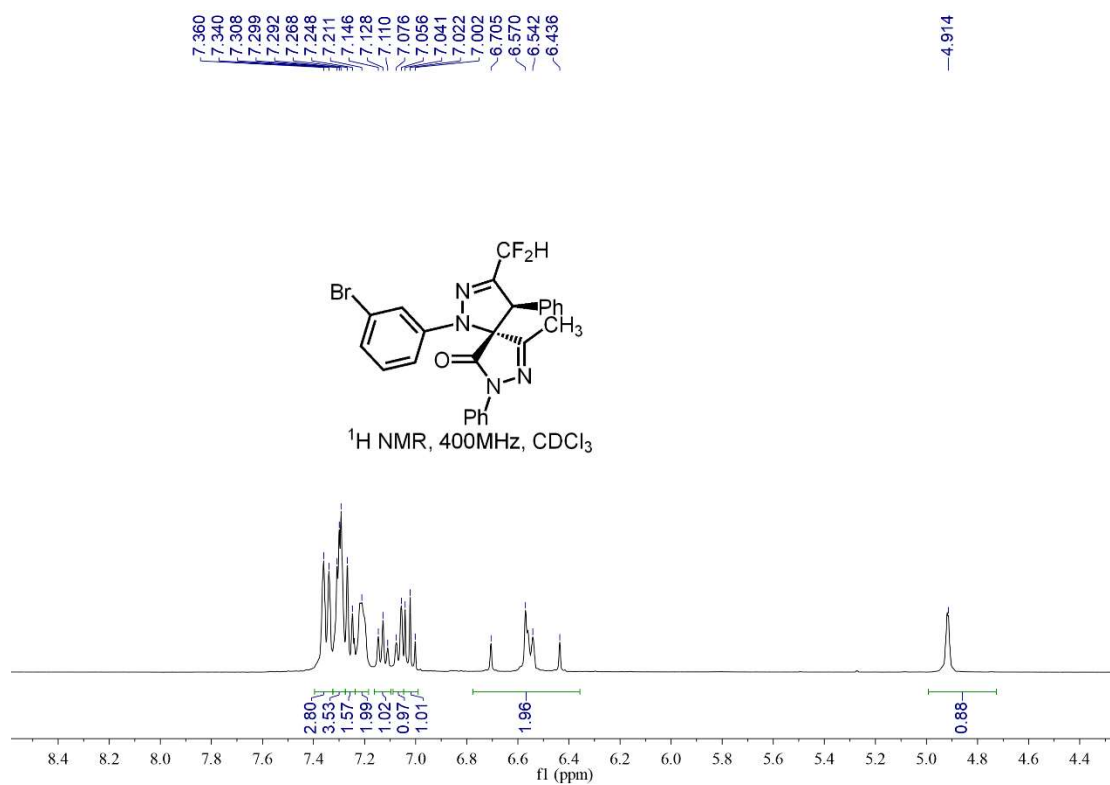
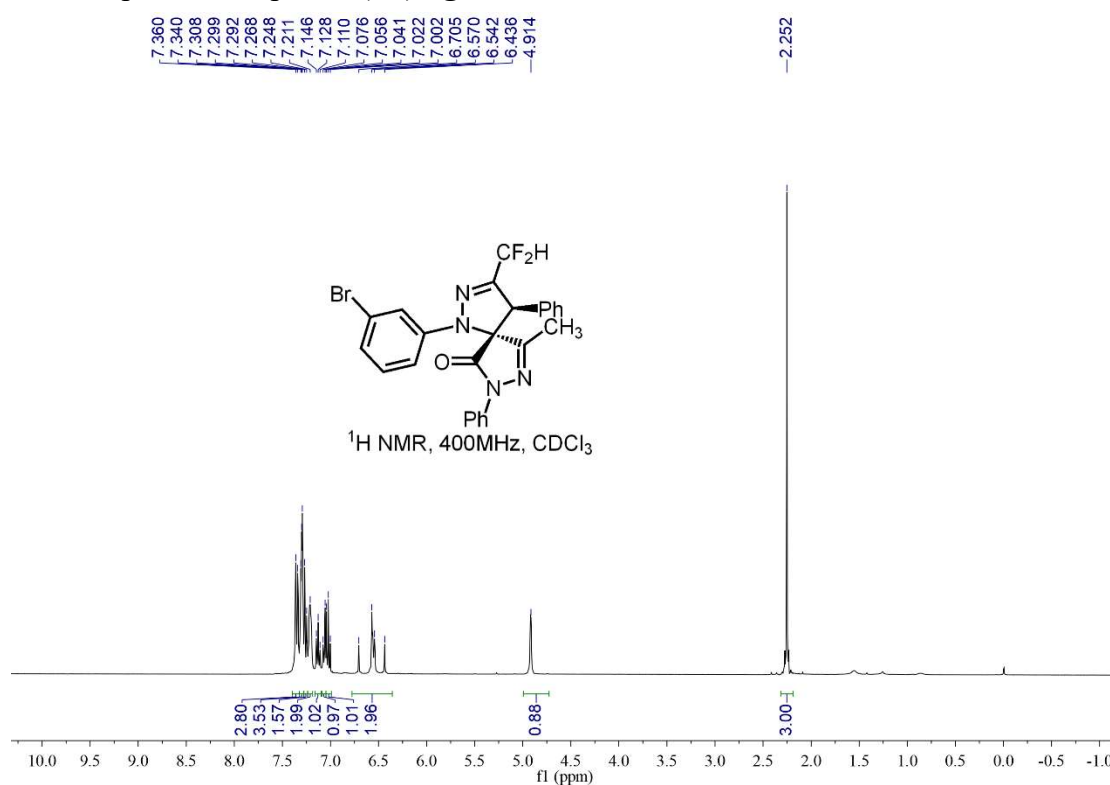
#### Acquisition Parameter

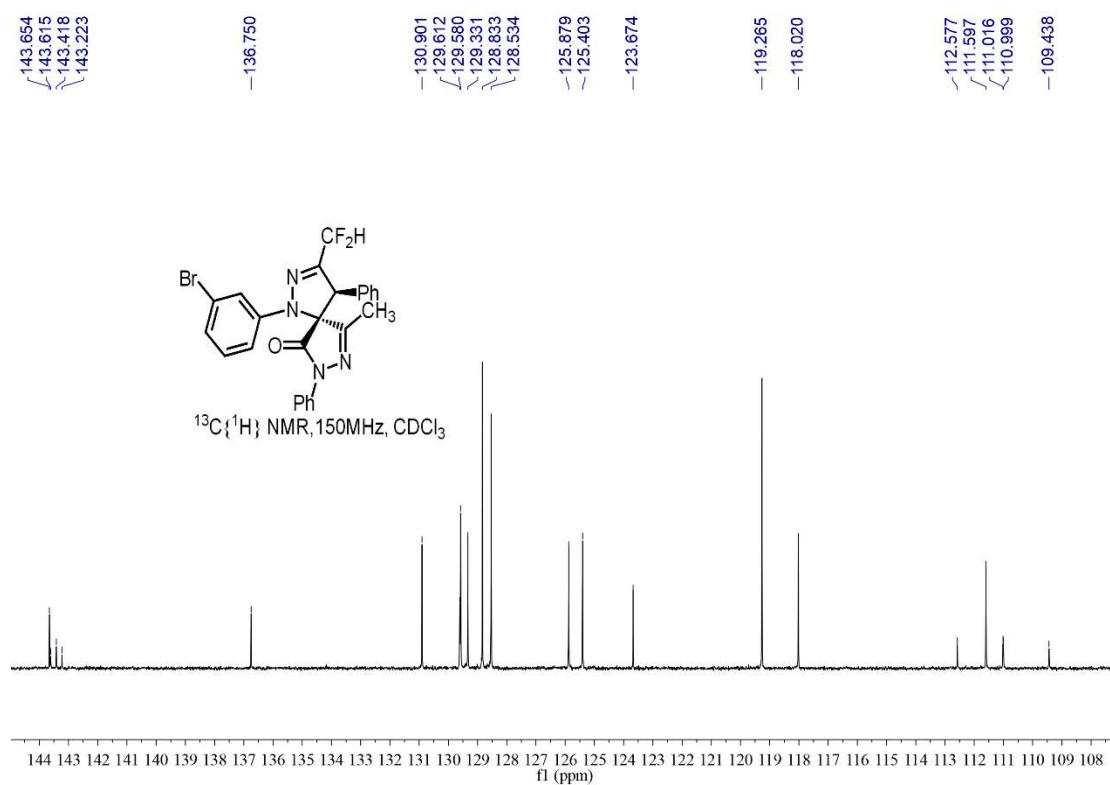
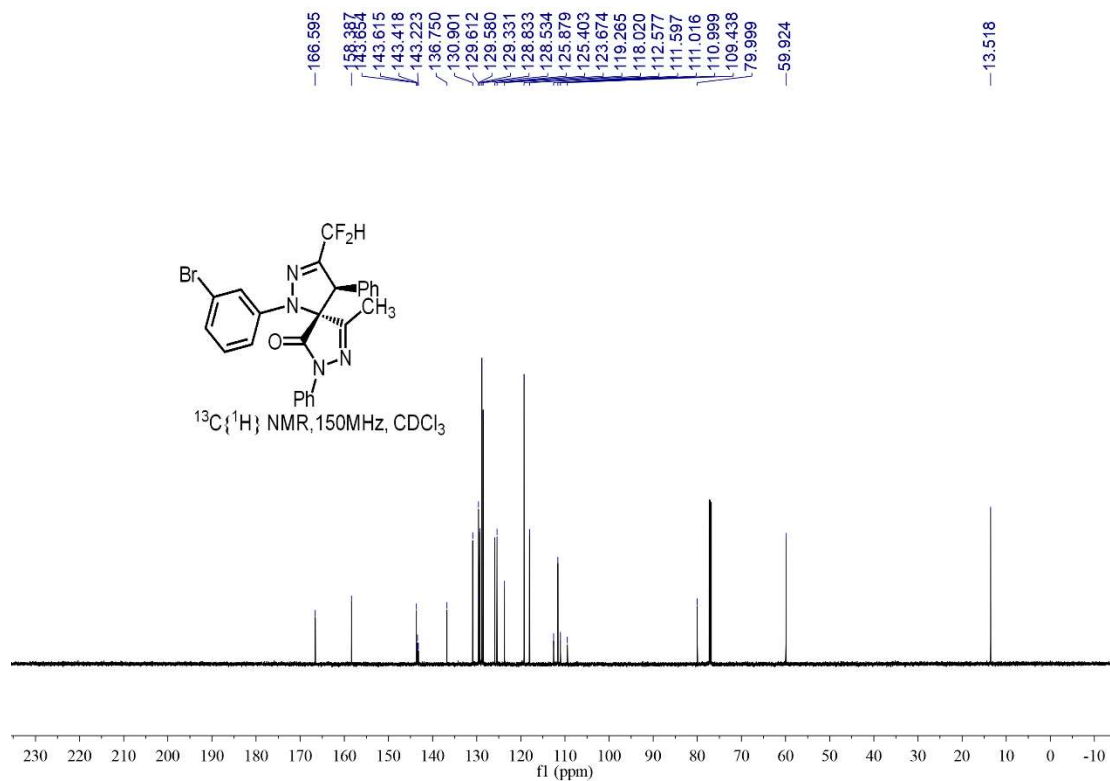
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $^{\circ}\text{C}$
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



Meas. # m/z	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R ul e	e j Con f	mSi gm a	Std l	St d M ea n m/ z	St d l Va r i a n c e	St d m/ z	Std Com b Dev
531.0621	1 C <sub>25</sub> H <sub>19</sub> BrF <sub>2</sub> N <sub>4</sub> NaO	531.0603	-3.5	-3.1	16.5	ok	even	36.9	23.4	1.7	7.3	0.7	842.7

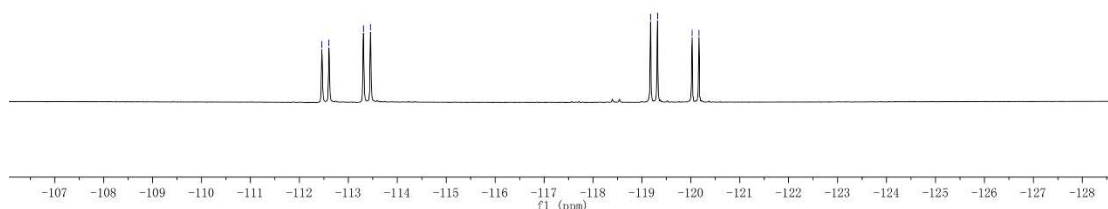
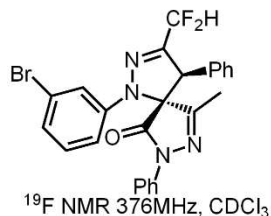
NMR copies of compound (*cis*)-**3g**:





-112.459  
-112.603  
-113.307  
-113.452

-119.177  
-119.319  
-120.026  
-120.168



HRMS (ESI) copy of compound (*cis*)-**3g**:

### Mass Spectrum SmartFormula Report

#### Analysis Info

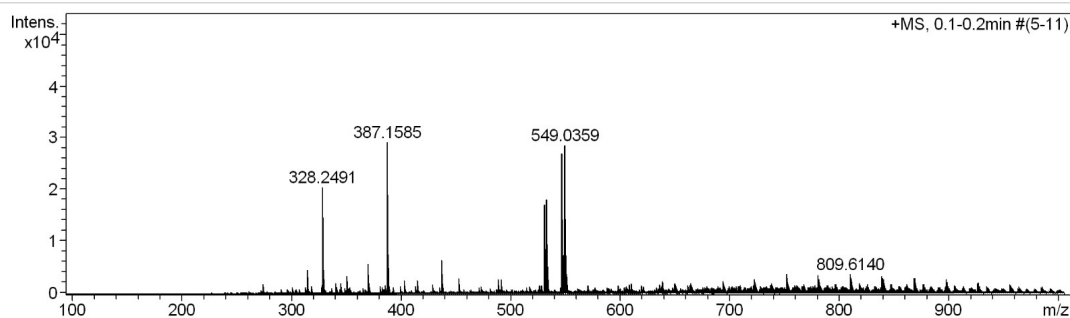
Analysis Name D:\Data\user\NWNW-fengyang 20220609-5.d  
Method tune\_low.m  
Sample Name A-191  
Comment

Acquisition Date 2022-6-9 14:43:53

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

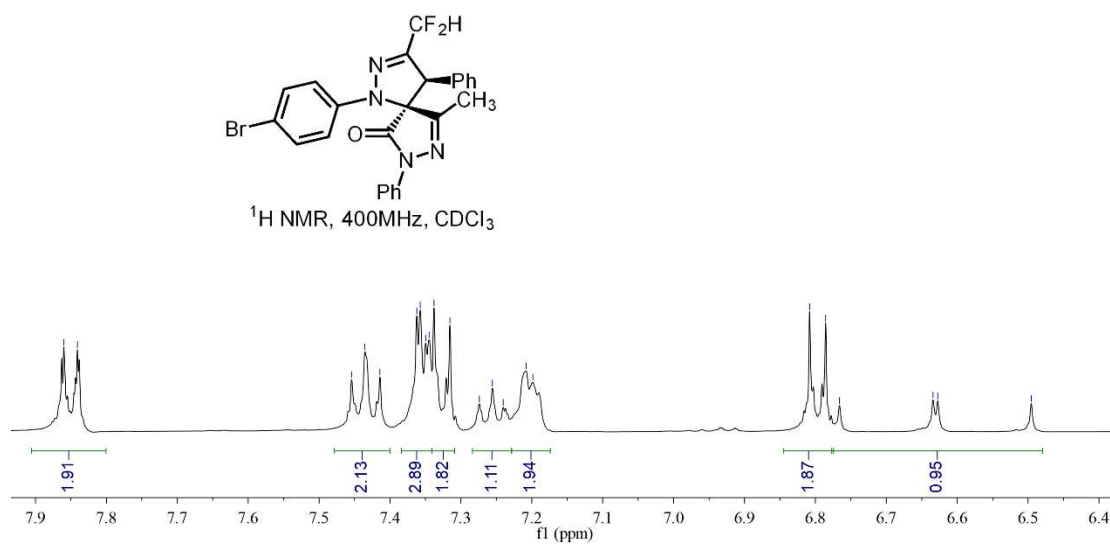
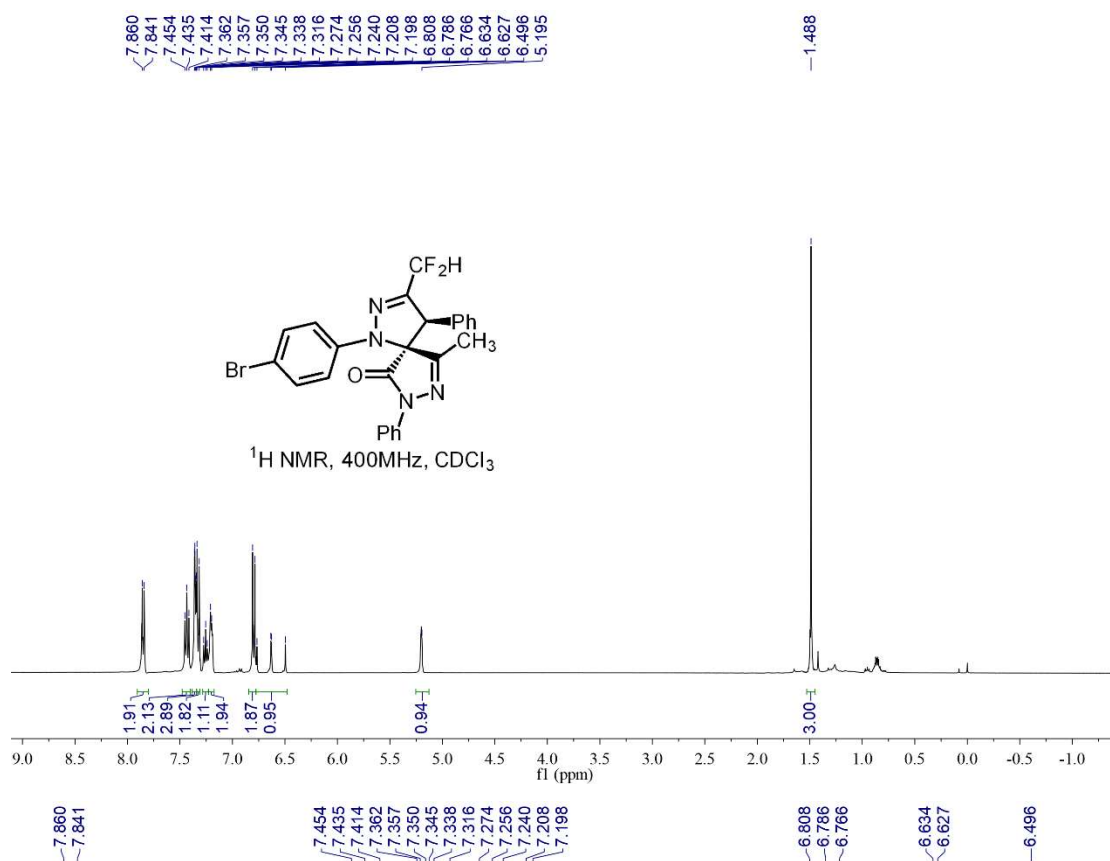
#### Acquisition Parameter

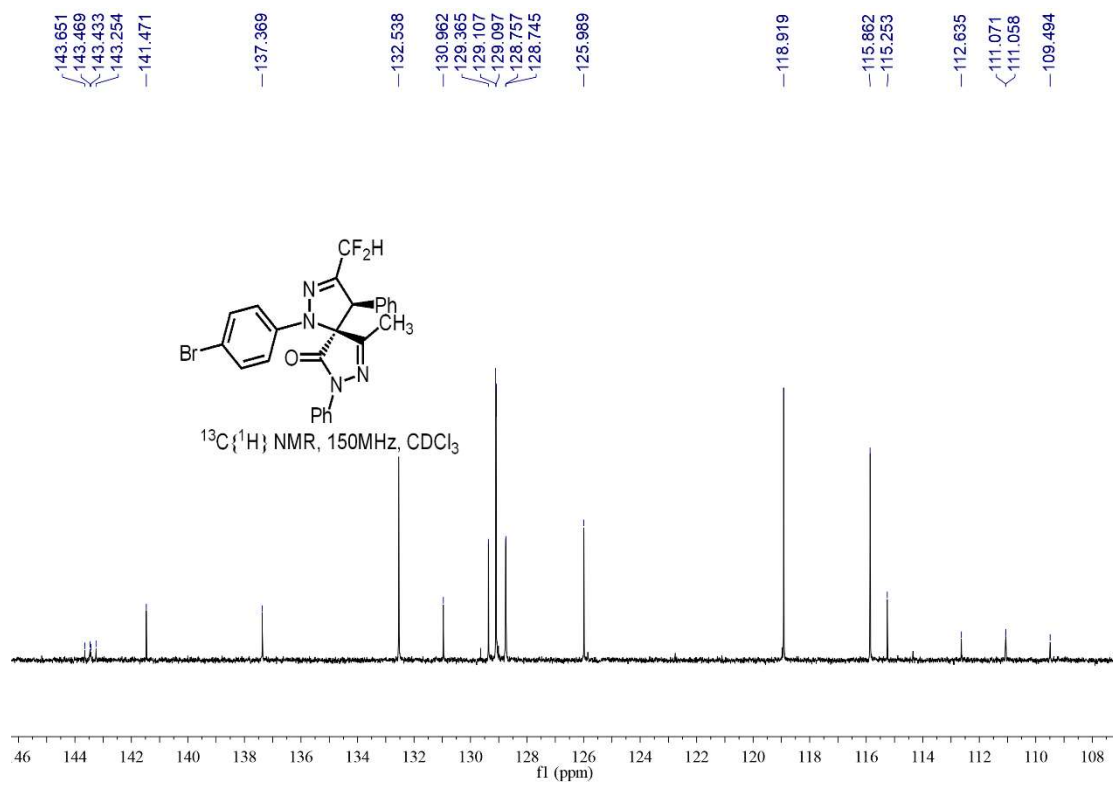
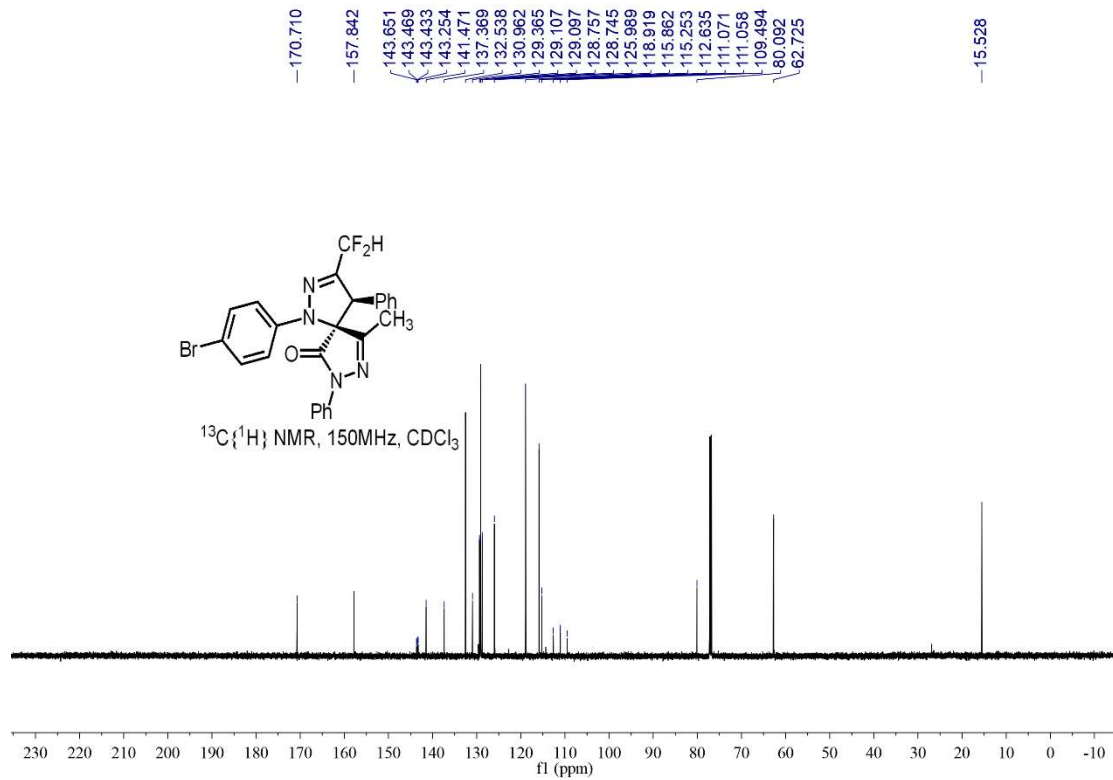
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

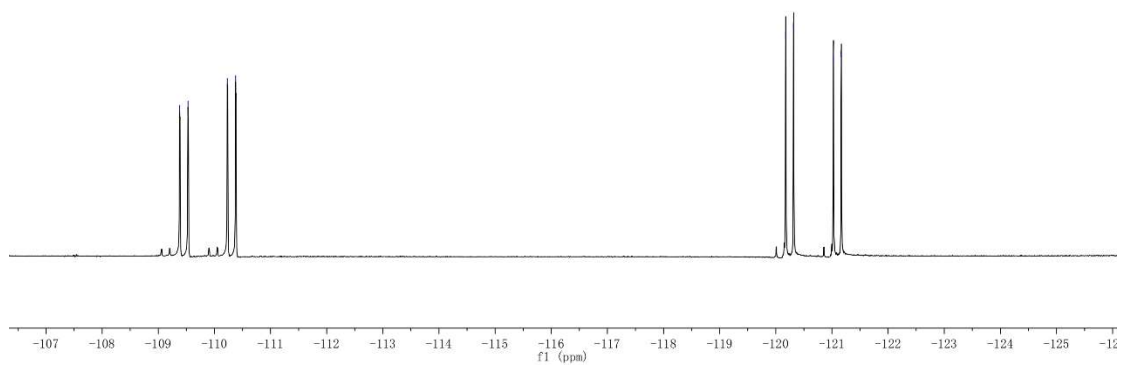
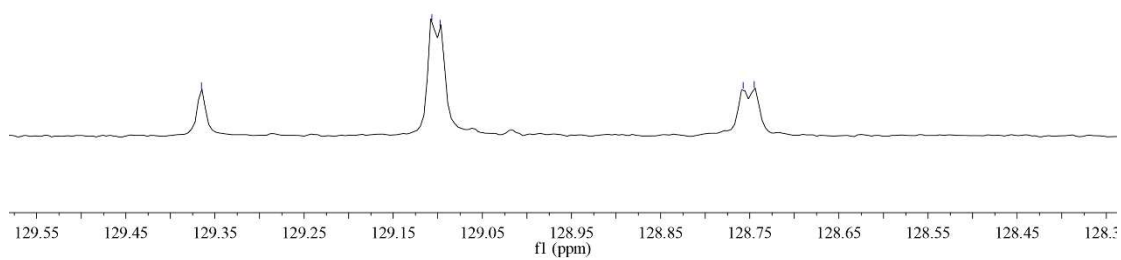
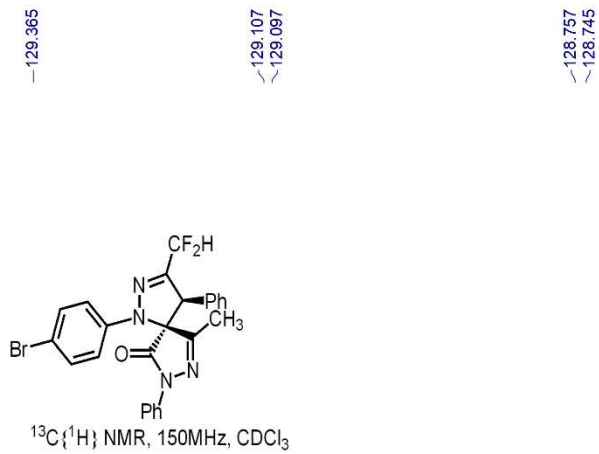


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N	e <sub>i</sub> %	mSi	Std	St	Std	St	Std
m/z						R	Con	gm	l	d	Var	m/	d
						ul	e	a		M	Nor	m/	z
										ea	m	Dif	f
										n			
										m/			
										z			
531.0625	1 C <sub>25</sub> H <sub>19</sub> BrF <sub>2</sub> N <sub>4</sub> NaO	531.0603	-4.2	-3.8	16.5	ok	even	29.5	26.0	2.1	12.5	0.5	842.7

NMR copies of compound (*trans*)-**3h**:







HRMS (ESI) copy of compound (*trans*)-3h:

Mass Spectrum SmartFormula Report

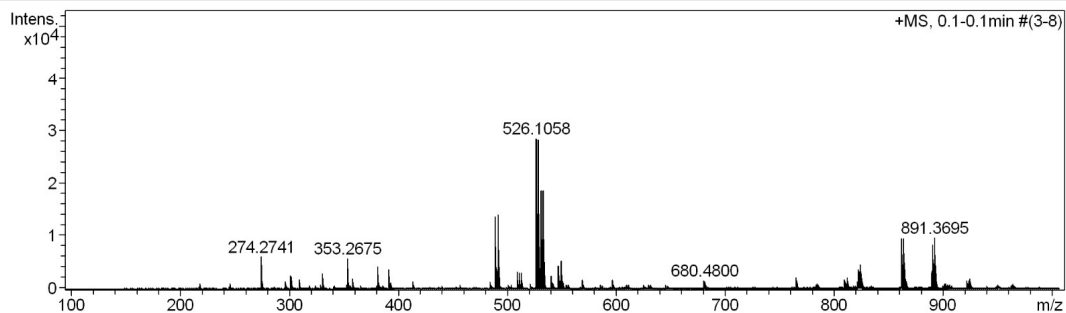
Analysis Info

Analysis Name D:\Data\user\fengyang 20220616-16.d  
 Method tune\_low.m  
 Sample Name A-16  
 Comment

Acquisition Date 2022-6-16 11:00:38  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

Acquisition Parameter

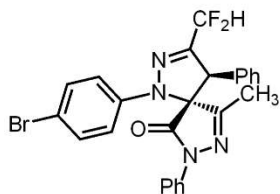
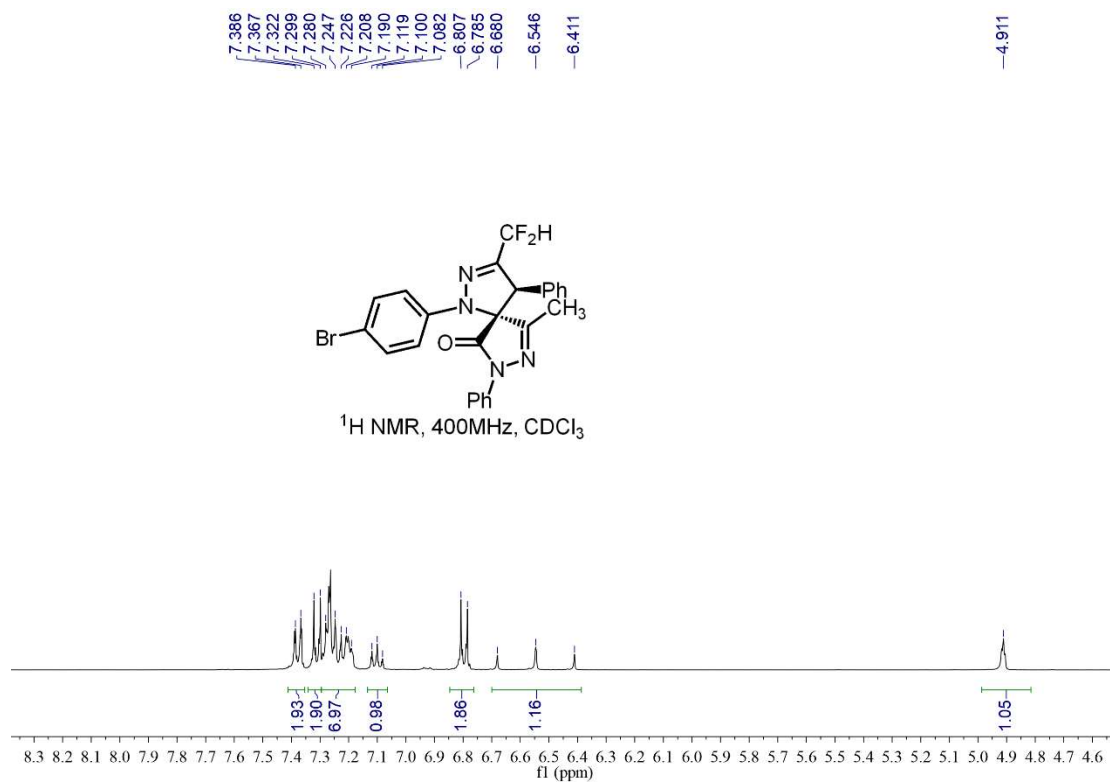
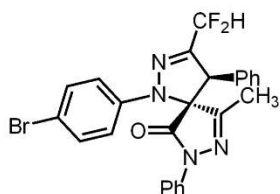
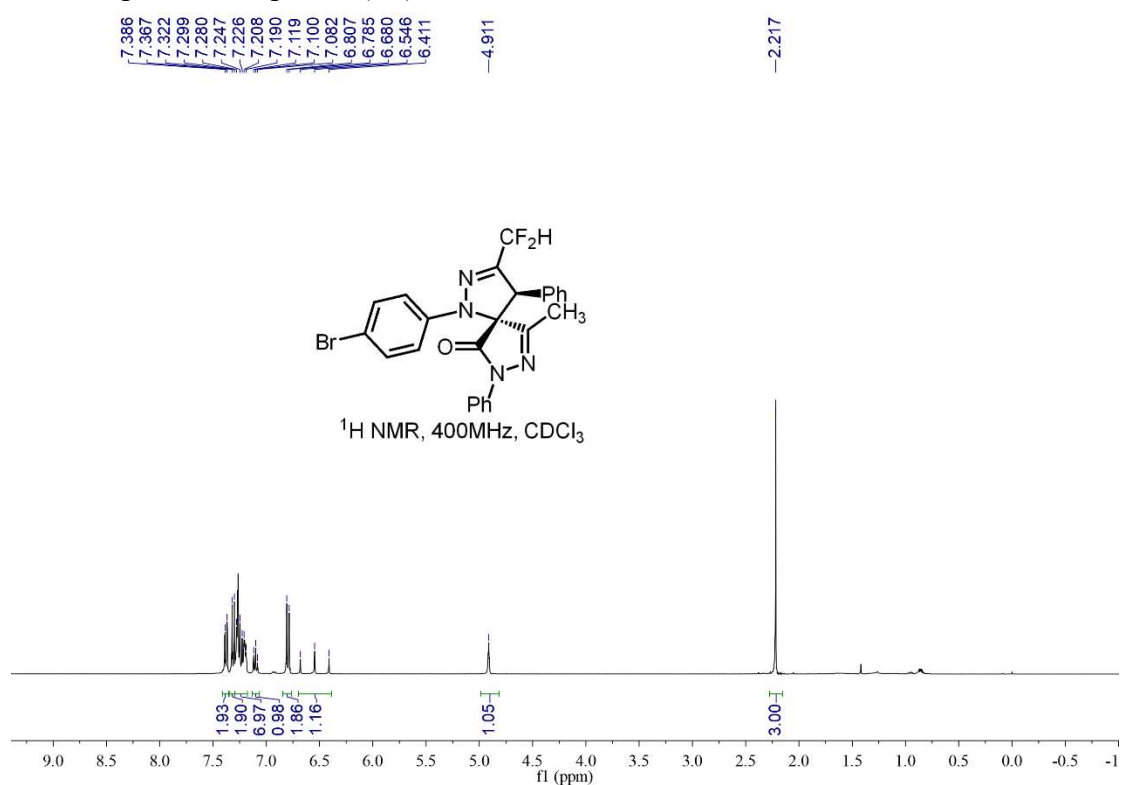
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

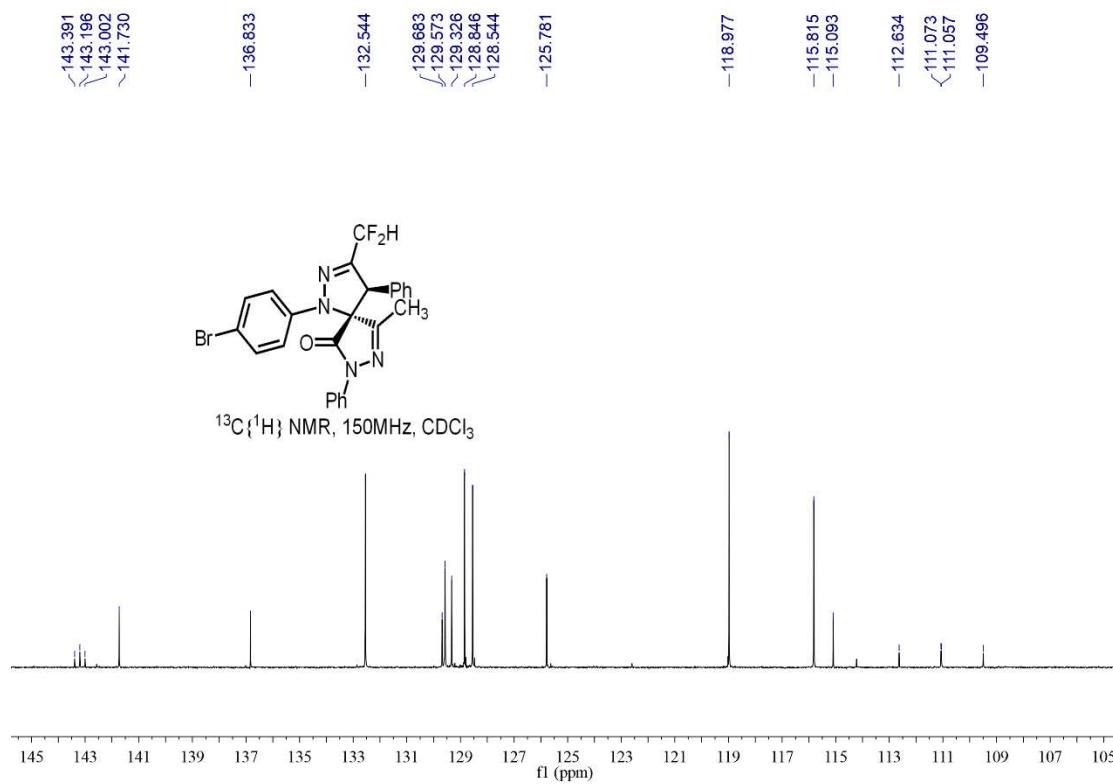
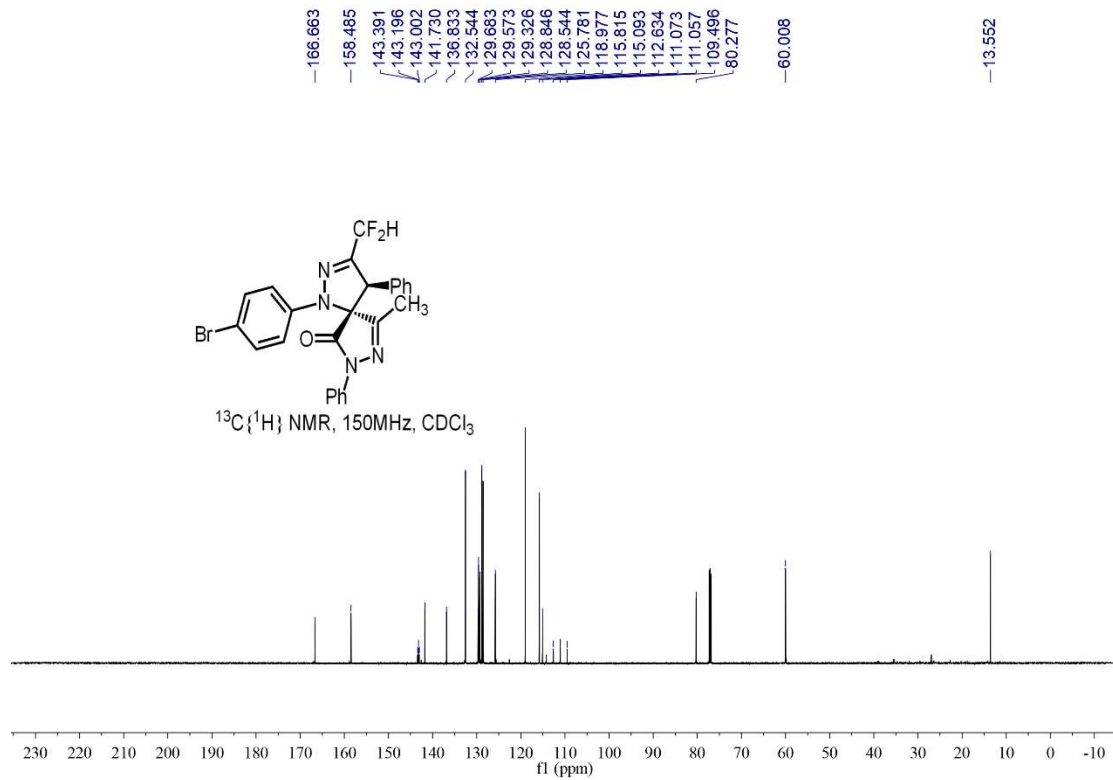


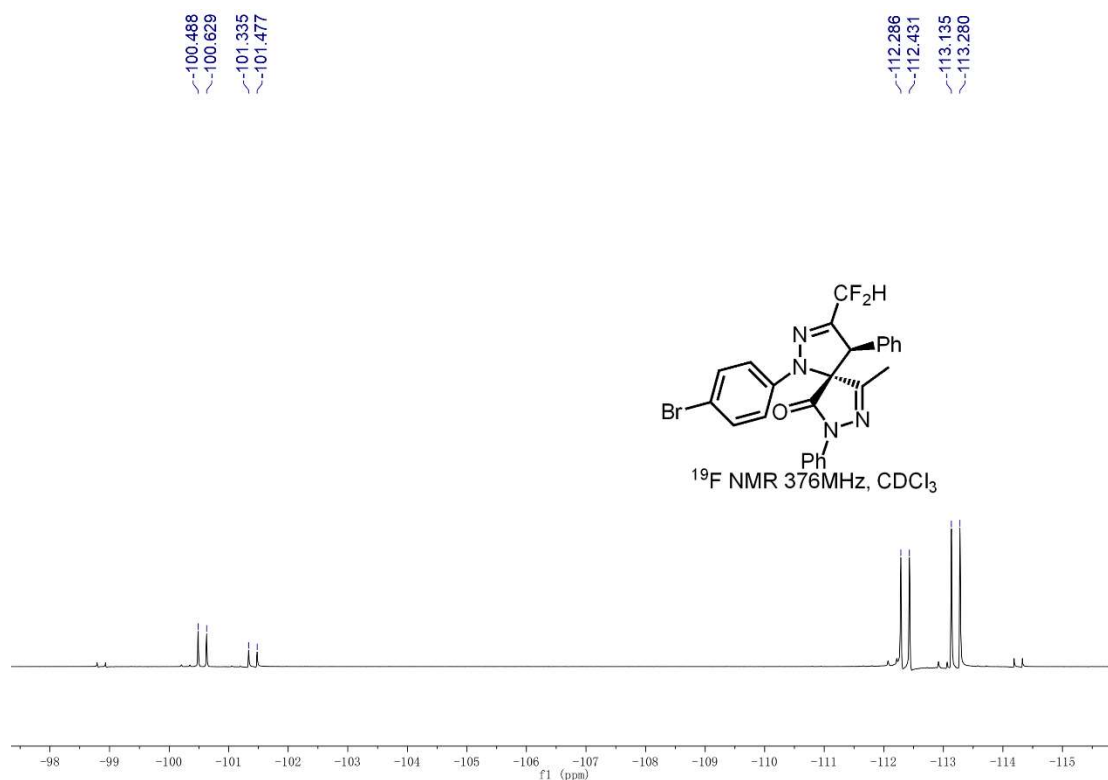
Meas. #	m/z	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e	Conf	mSig	Std I	Std Mean m/z	Std VarN	Std m/z	Std Comb Dev
526.1058	1	C <sub>25</sub> H <sub>23</sub> BrF <sub>2</sub> N <sub>5</sub> O	526.1049	-1.8	-2.3	15.5	ok		even	8.5	6.9	1.3	2.4	0.4	842.7



NMR copies of compound (*cis*)-**3h**:







HRMS (ESI) copy of compound (*cis*)-**3h**:

### Mass Spectrum SmartFormula Report

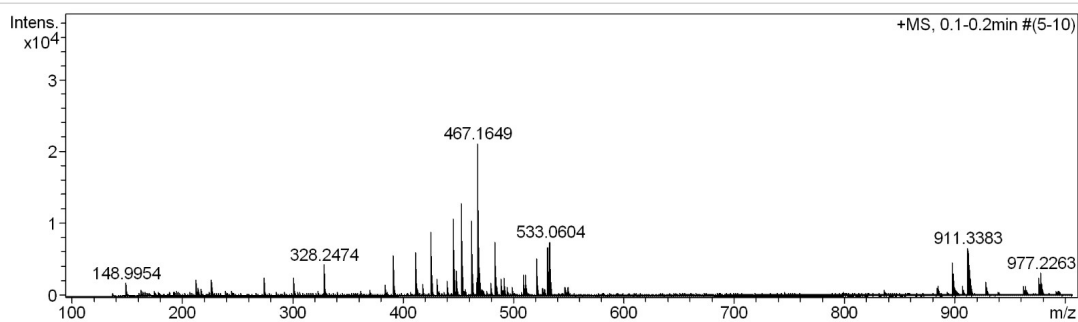
#### Analysis Info

Analysis Name D:\Data\user\fengyang 20220616--17.d  
 Method tune\_low.m  
 Sample Name A-161  
 Comment

Acquisition Date 2022-6-16 11:05:13  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

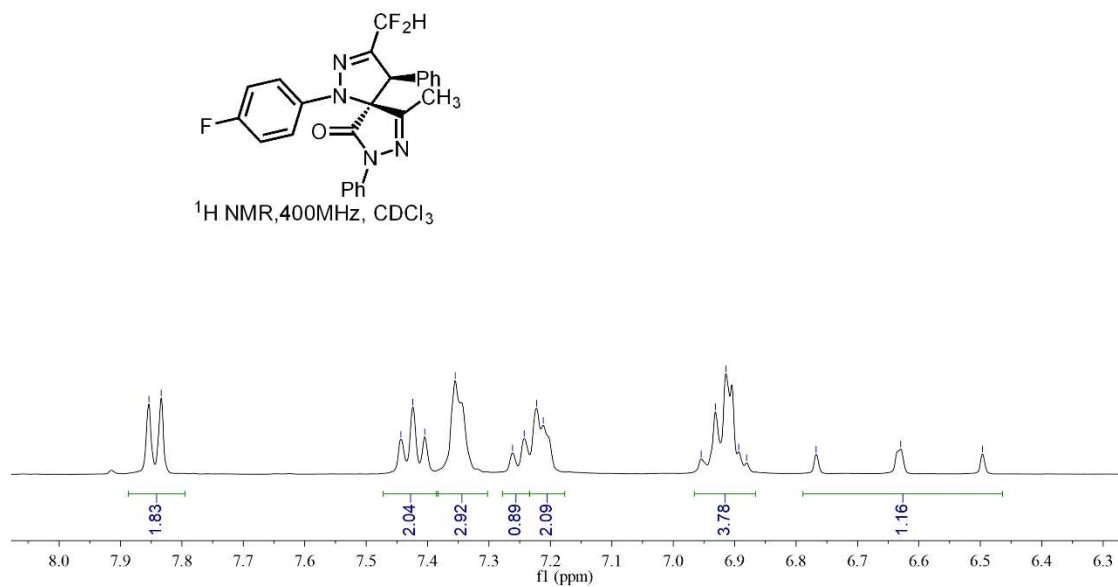
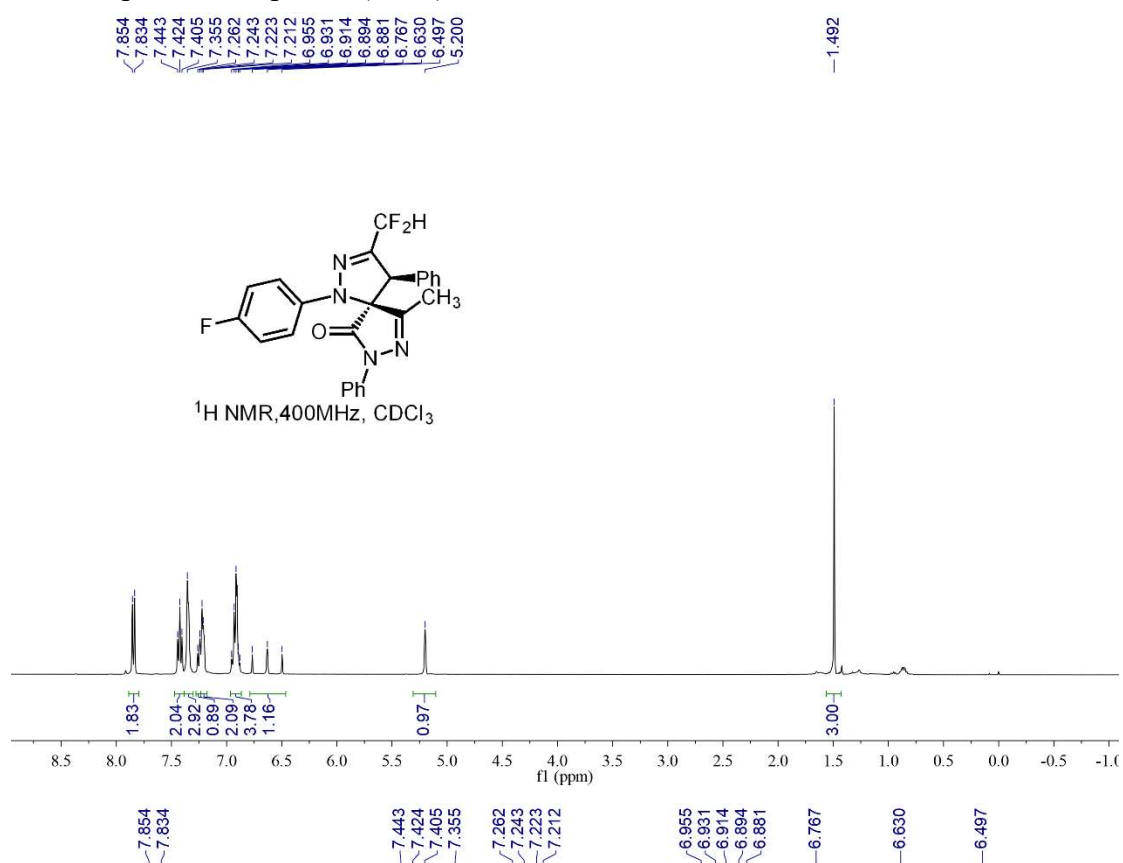
#### Acquisition Parameter

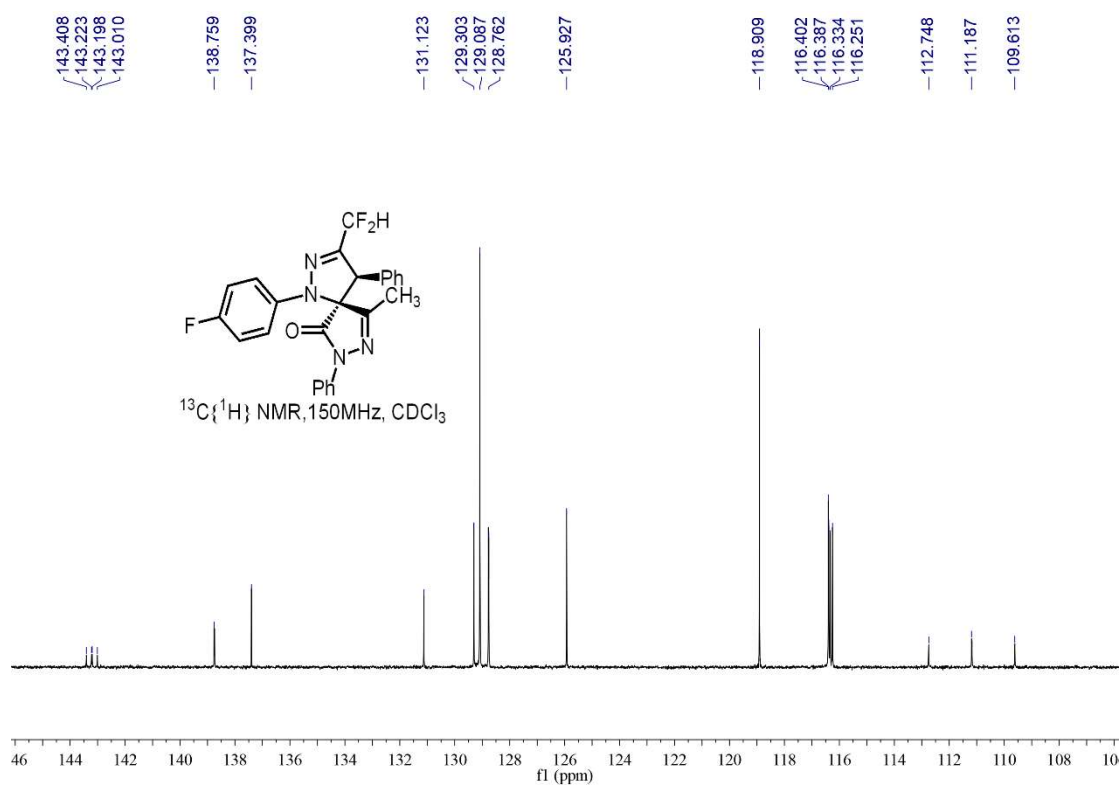
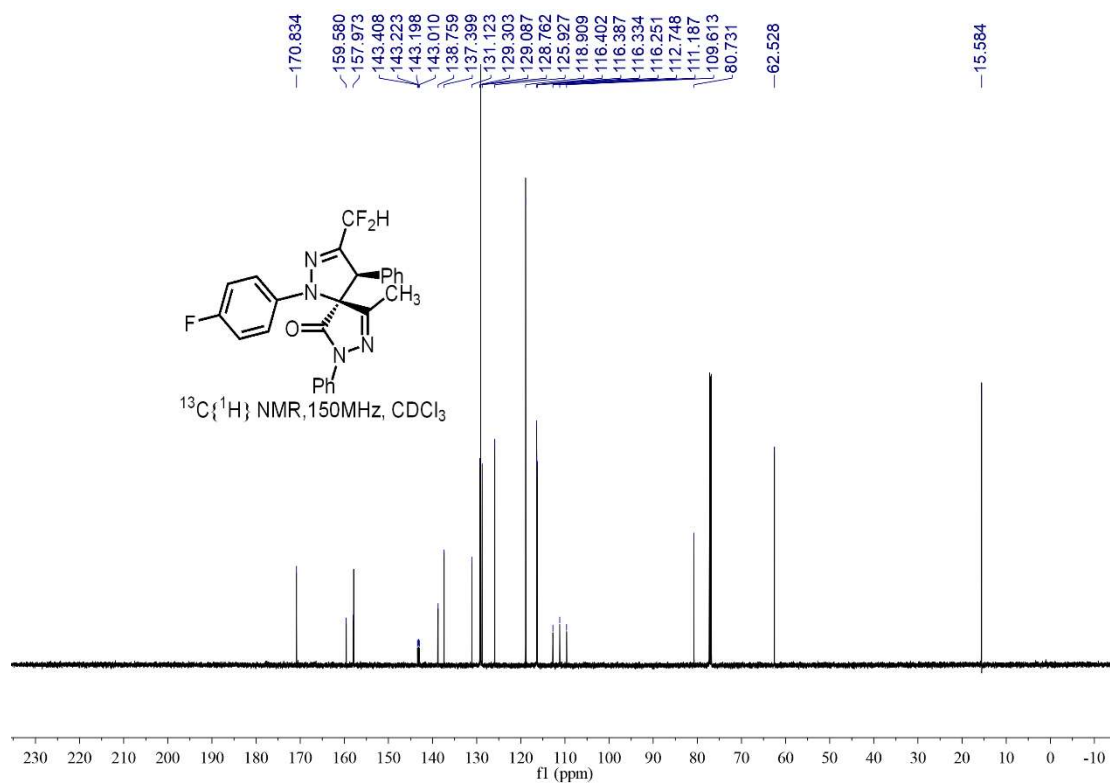
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j̇C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

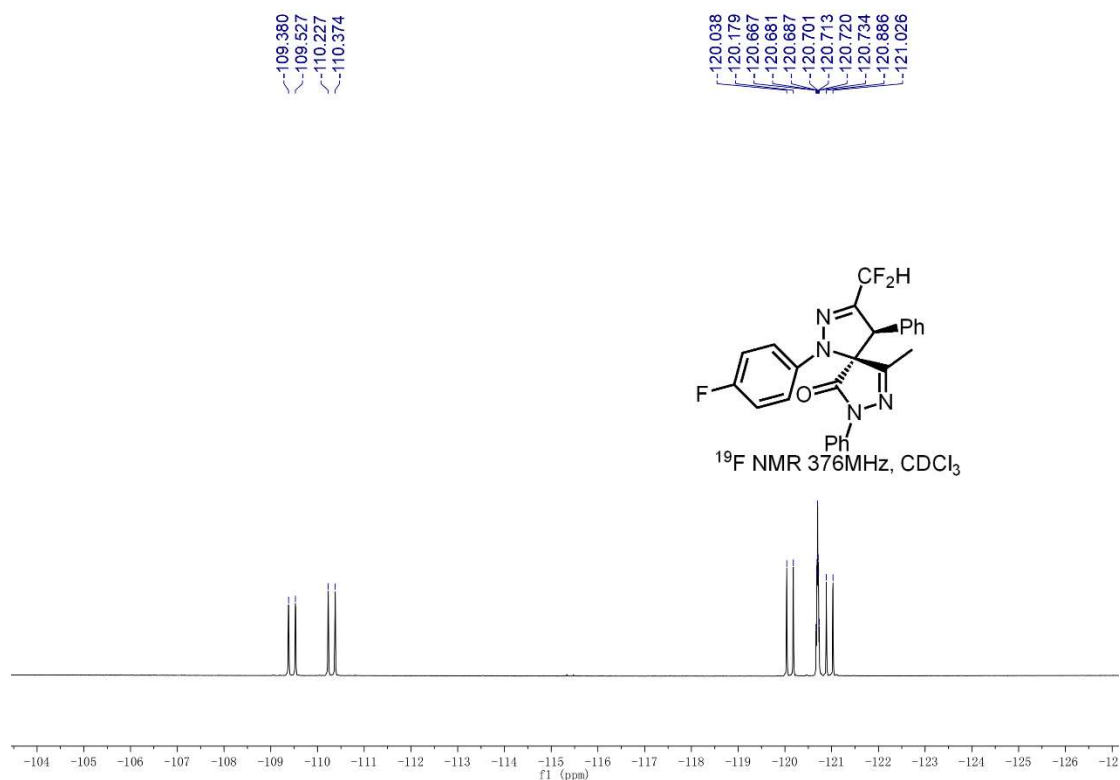


Meas. #	Formula	m/z	err	Me	rdb	N-	e	mSi	Std	St	Std	St	Std
m/z			[p	an		R	Con	gm	l	d	l	d	Com
			p	err		ul	f	a	Me	Var	m/	z	b
			m]	[p		e			an	Nor	m	Dif	Dev
			m]						m/	m	f		
531.0591	1 C 25 H 19 Br F 2 N 4 Na O	531.0603	2.2	0.8	16.5	ok	even	41.4	28.3	2.4	12.5	4.3	842.7

NMR copies of compound (*trans*)-**3i**:







HRMS (ESI) copy of compound (*trans*)-3i:

### Mass Spectrum SmartFormula Report

#### Analysis Info

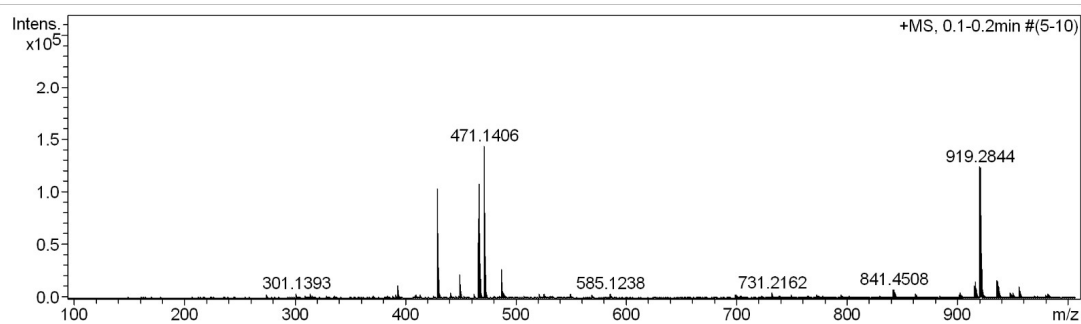
Analysis Name D:\Data\user\fangyang 20220616-19.d  
 Method tune\_low.m  
 Sample Name A-26  
 Comment

Acquisition Date 2022-6-16 11:09:50

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

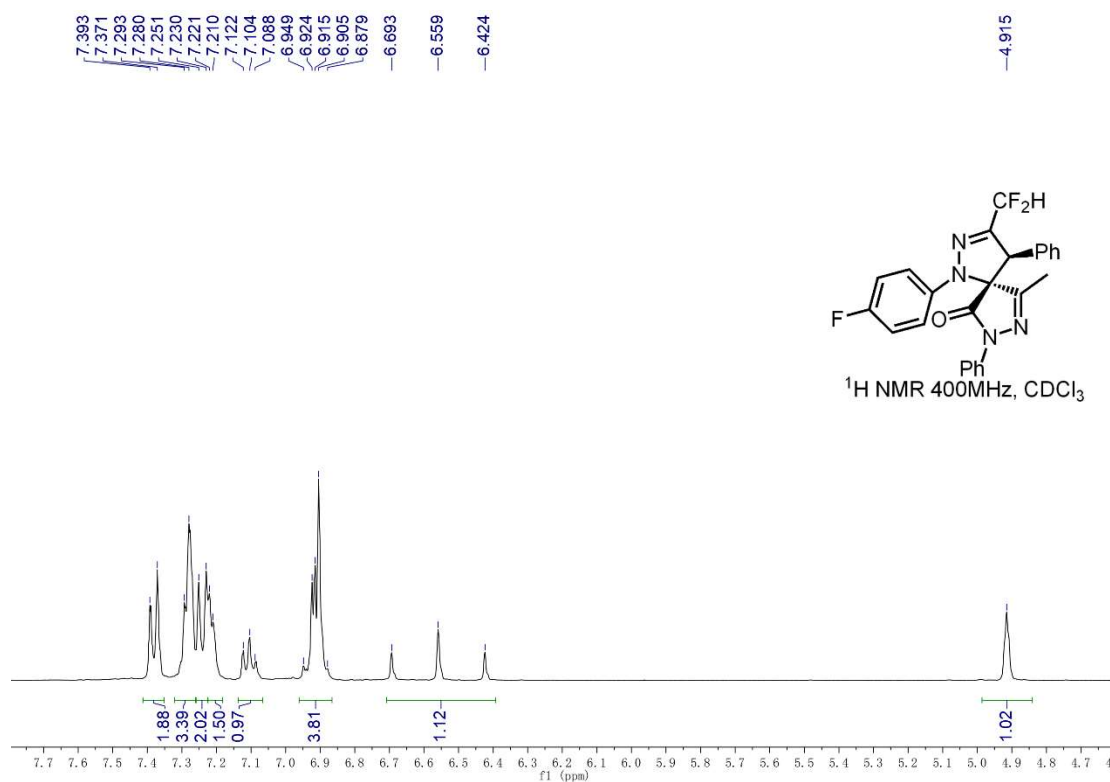
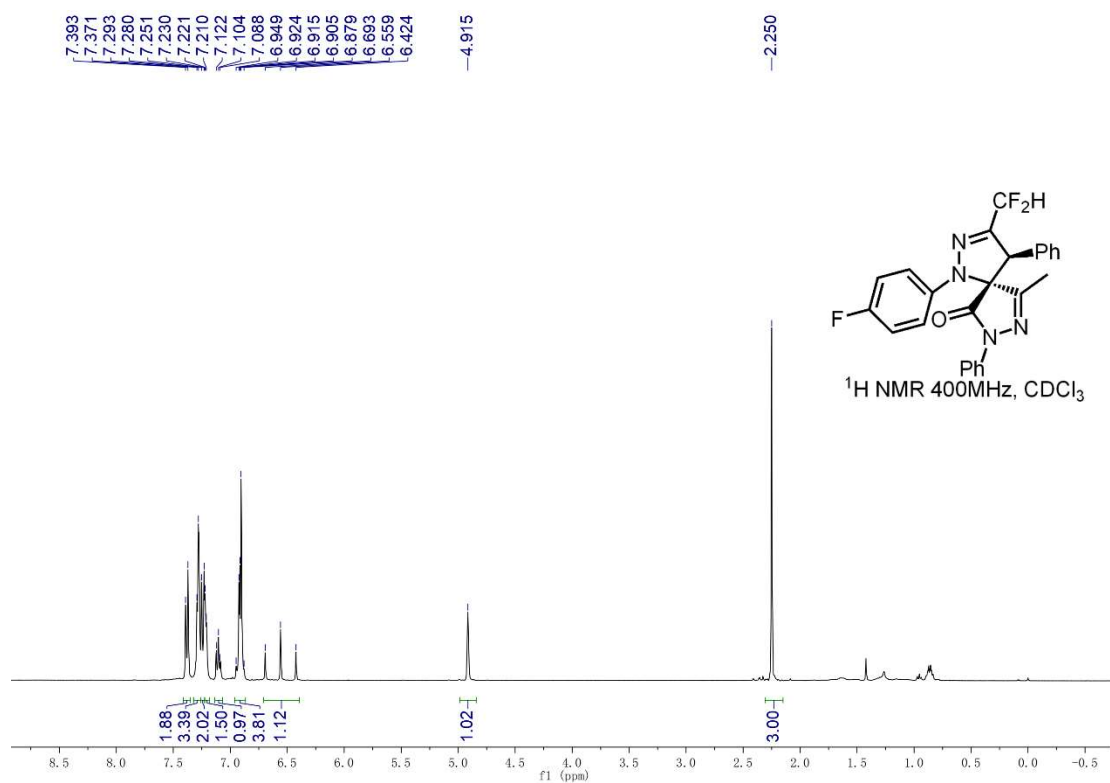
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{C}$
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

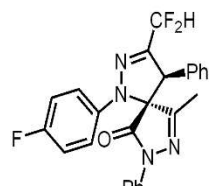
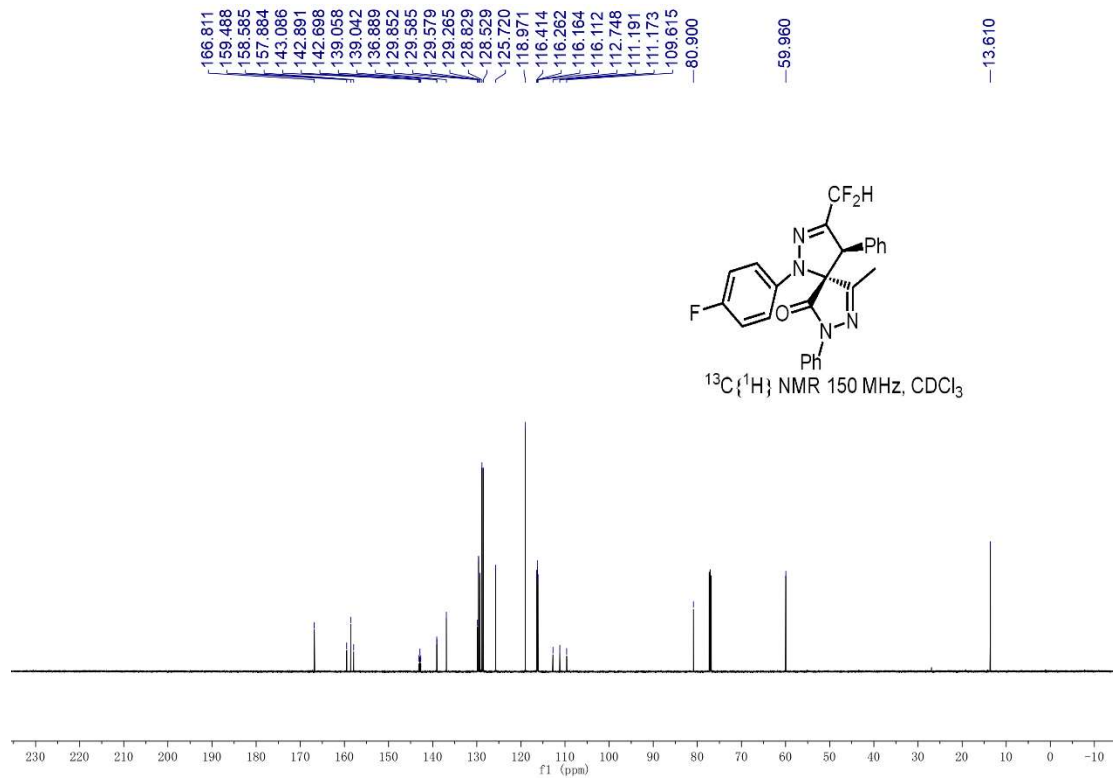


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>i</sub> ¥ Conf	mS ig ma	Std l	Std Me an m/z	Std l Va r or m	Std m/ rN Diff	Std Com b Dev
471.1406	1 C <sub>25</sub> H <sub>19</sub> F <sub>3</sub> N <sub>4</sub> NaO	471.1403	-0.6	-1.2	16.5	ok	even	6.1	8.4	0.8	3.8	1.4	842.7

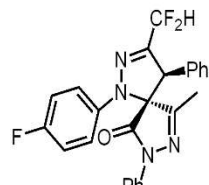
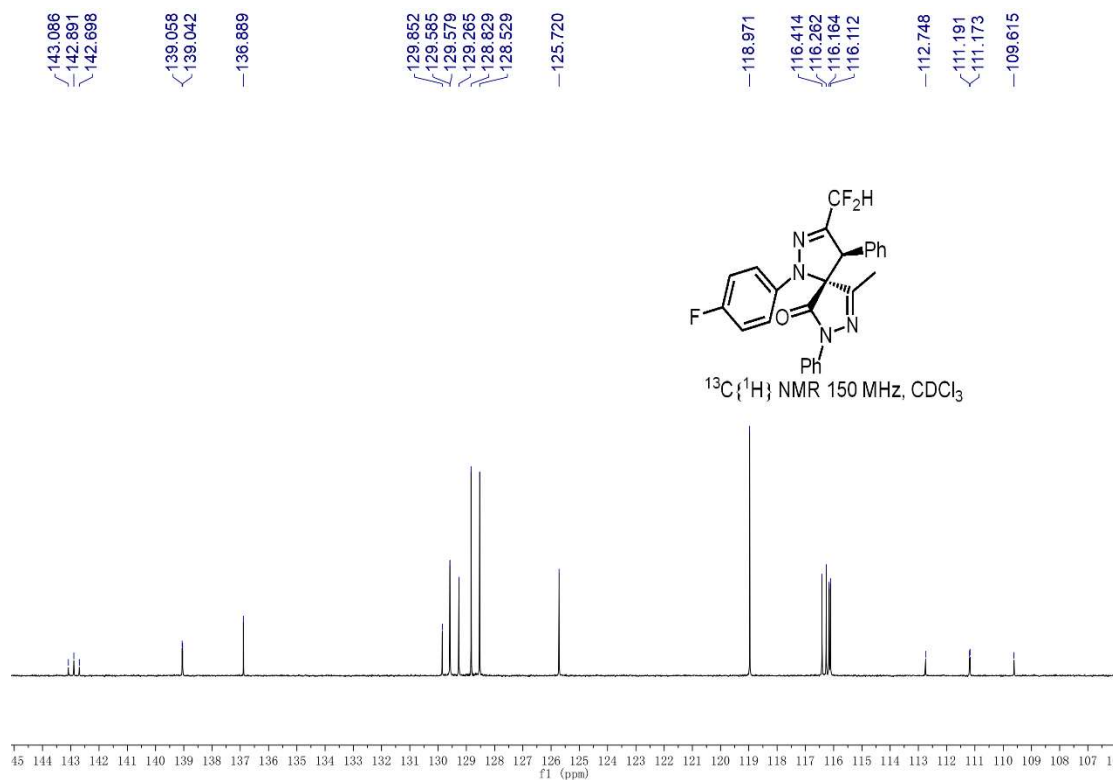
NMR copies of compound (*cis*)-**3i**:



L

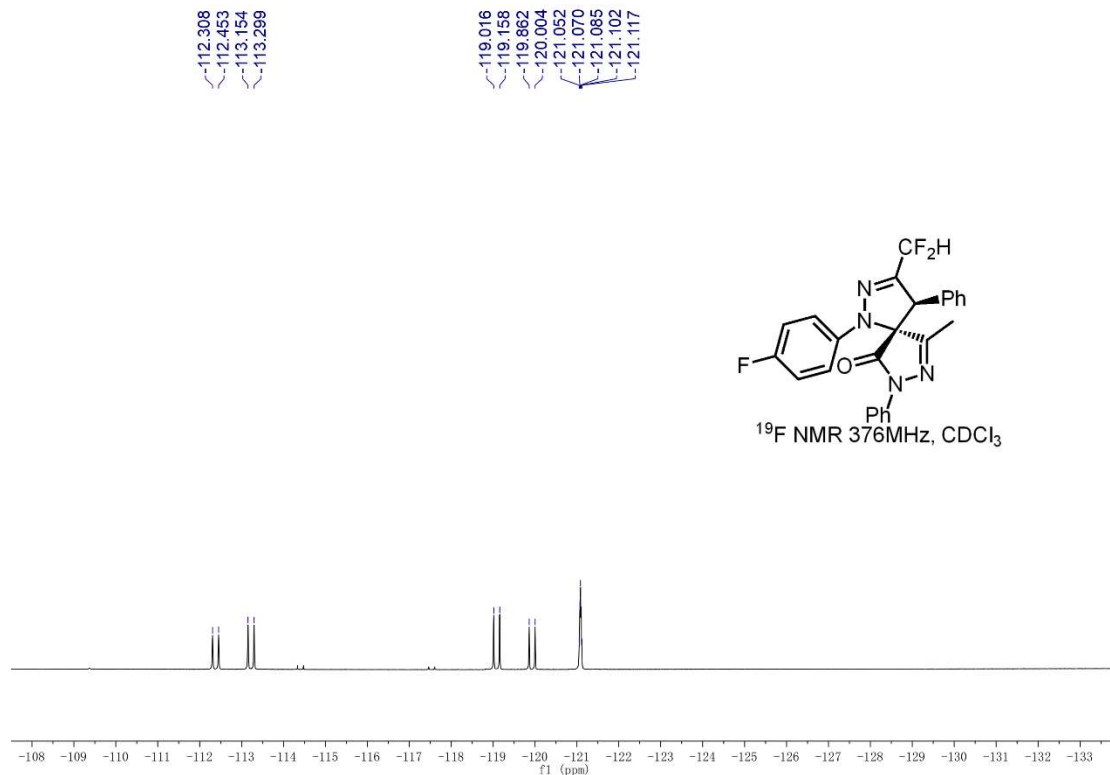


<sup>13</sup>C{<sup>1</sup>H}; NMR 150 MHz, CDCl<sub>3</sub>



<sup>13</sup>C{<sup>1</sup>H}; NMR 150 MHz, CDCl<sub>3</sub>





HRMS (ESI) copy of compound (*cis*)-**3i**:

### Mass Spectrum SmartFormula Report

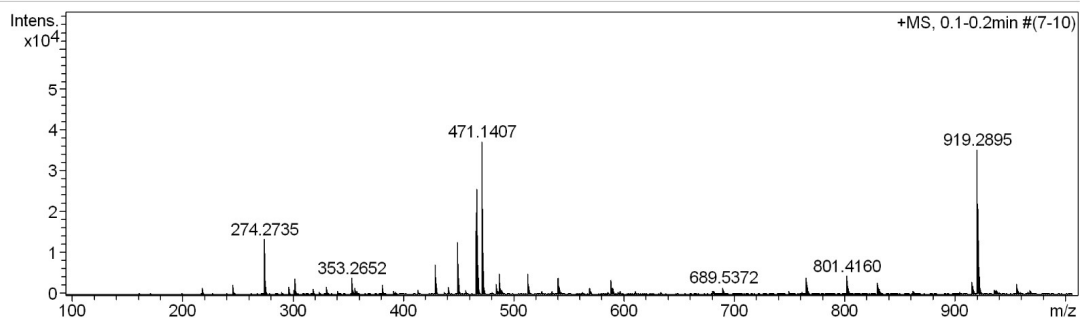
**Analysis Info**

Analysis Name D:\Data\user\fengyang 20220616-20.d  
 Method tune\_low.m  
 Sample Name A-261  
 Comment

Acquisition Date 2022-6-16 11:11:14  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

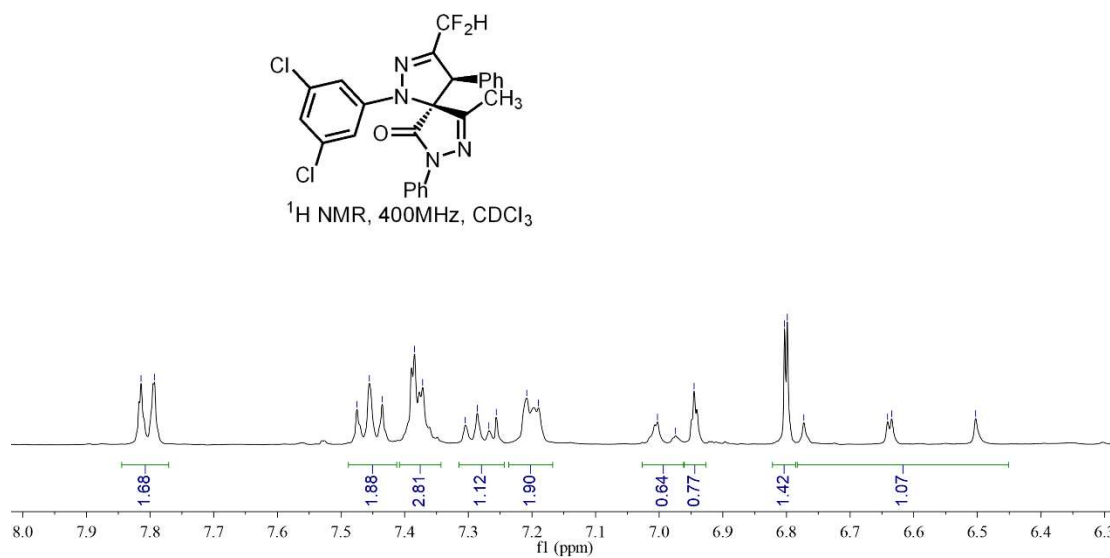
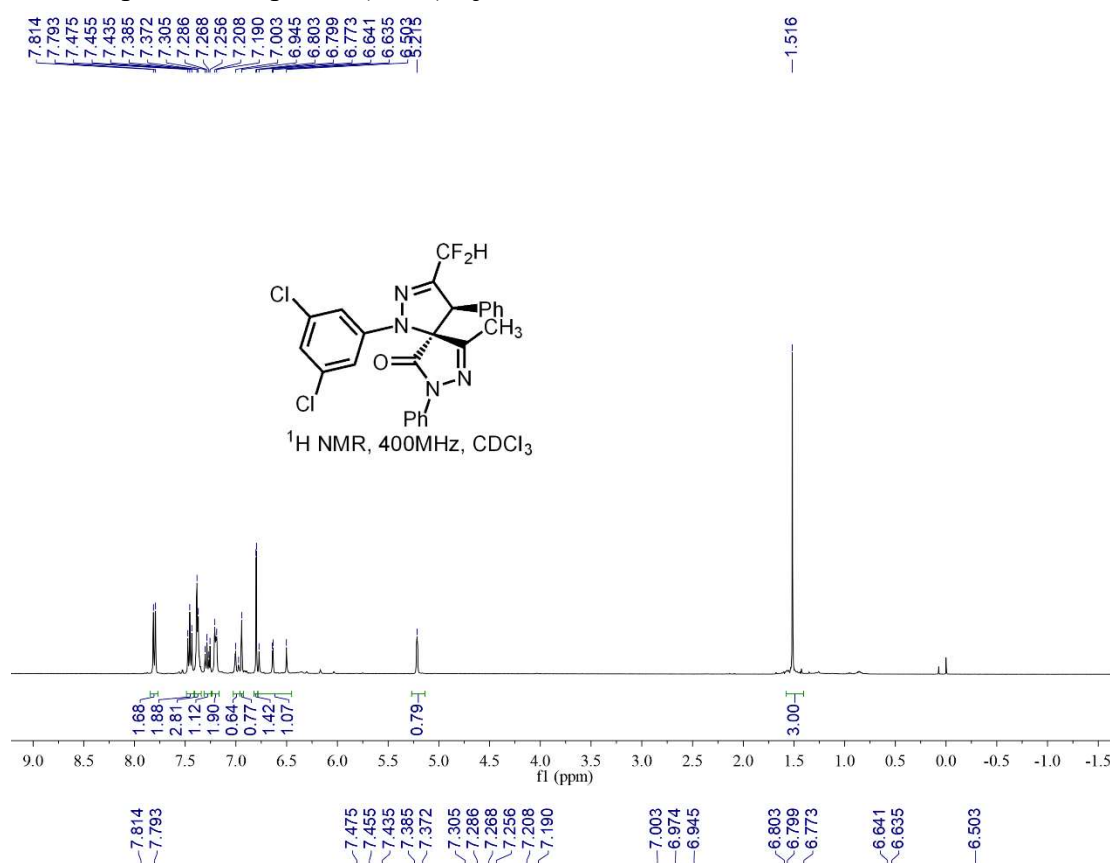
**Acquisition Parameter**

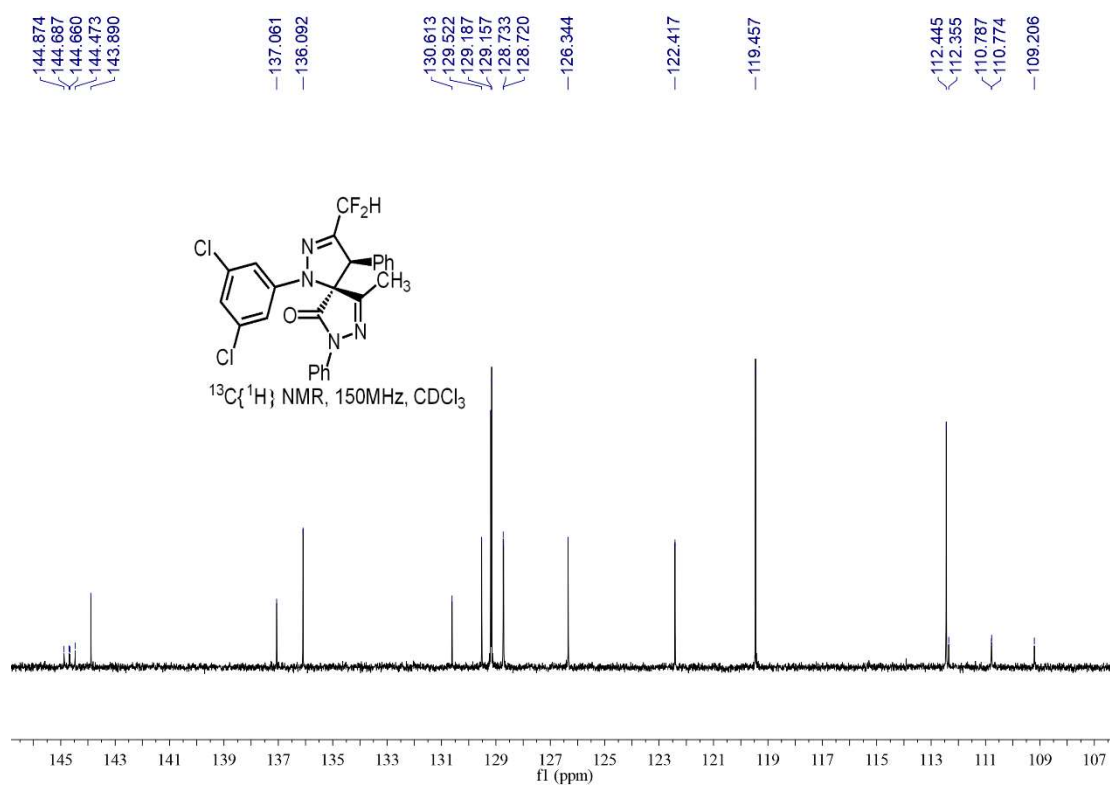
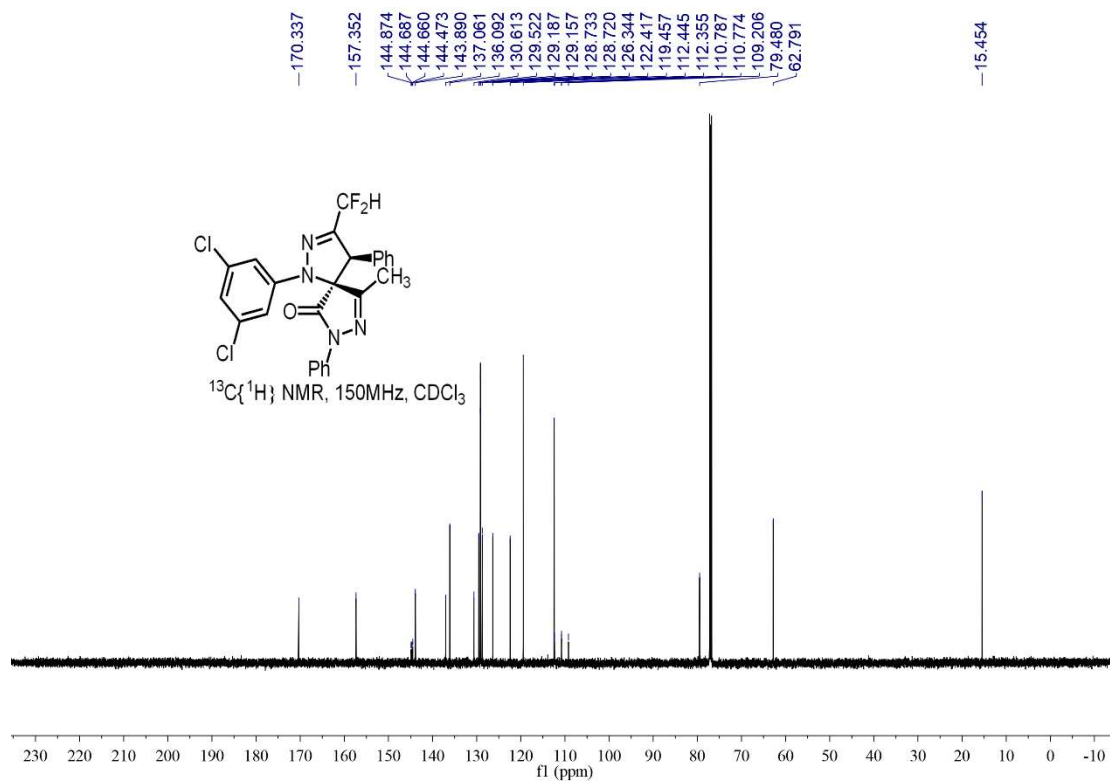
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

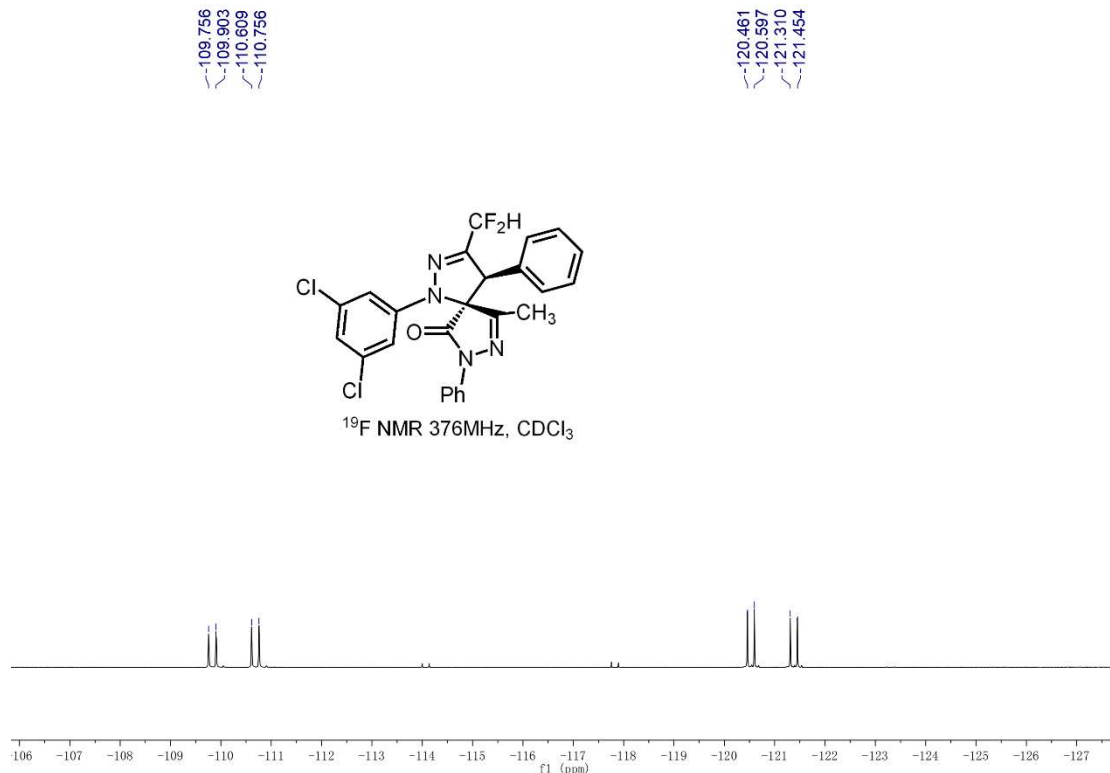


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ei% Conf	mS	Std	Std	Std	Std	Std
m/z						ul		ig	l	Me	l	m/	Com
						e		ma		m/	rN	Diff	Dev
471.1407	1 C <sub>25</sub> H <sub>19</sub> F <sub>3</sub> N <sub>4</sub> NaO	471.1403	-0.9	-0.9	16.5	ok	even	6.5	8.4	0.5	4.5	0.3	842.7

NMR copies of compound (*trans*)-**3j**:







HRMS (ESI) copy of compound (*trans*)-3j:

### Mass Spectrum SmartFormula Report

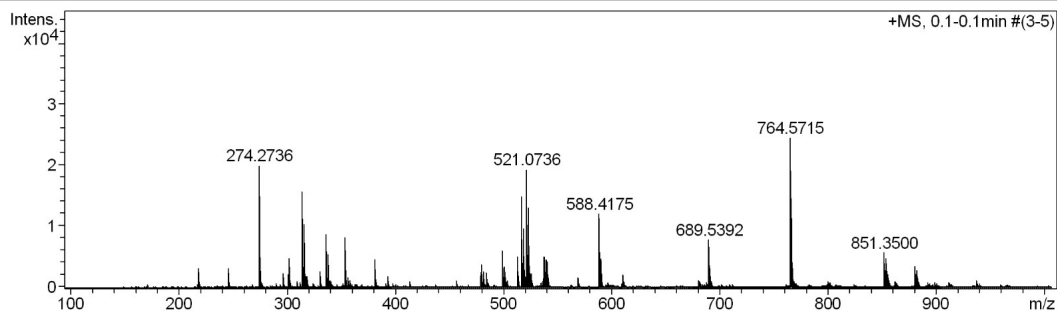
**Analysis Info**

Analysis Name D:\Data\user\fengyang 20220616-18.d  
 Method tune\_low.m  
 Sample Name A-21  
 Comment

Acquisition Date 2022-6-16 11:06:59  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

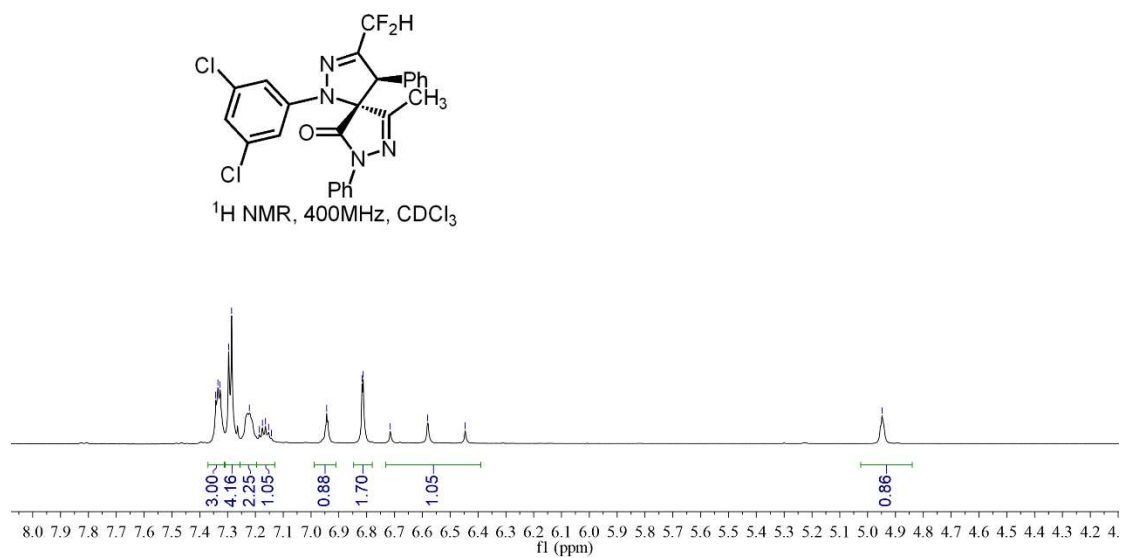
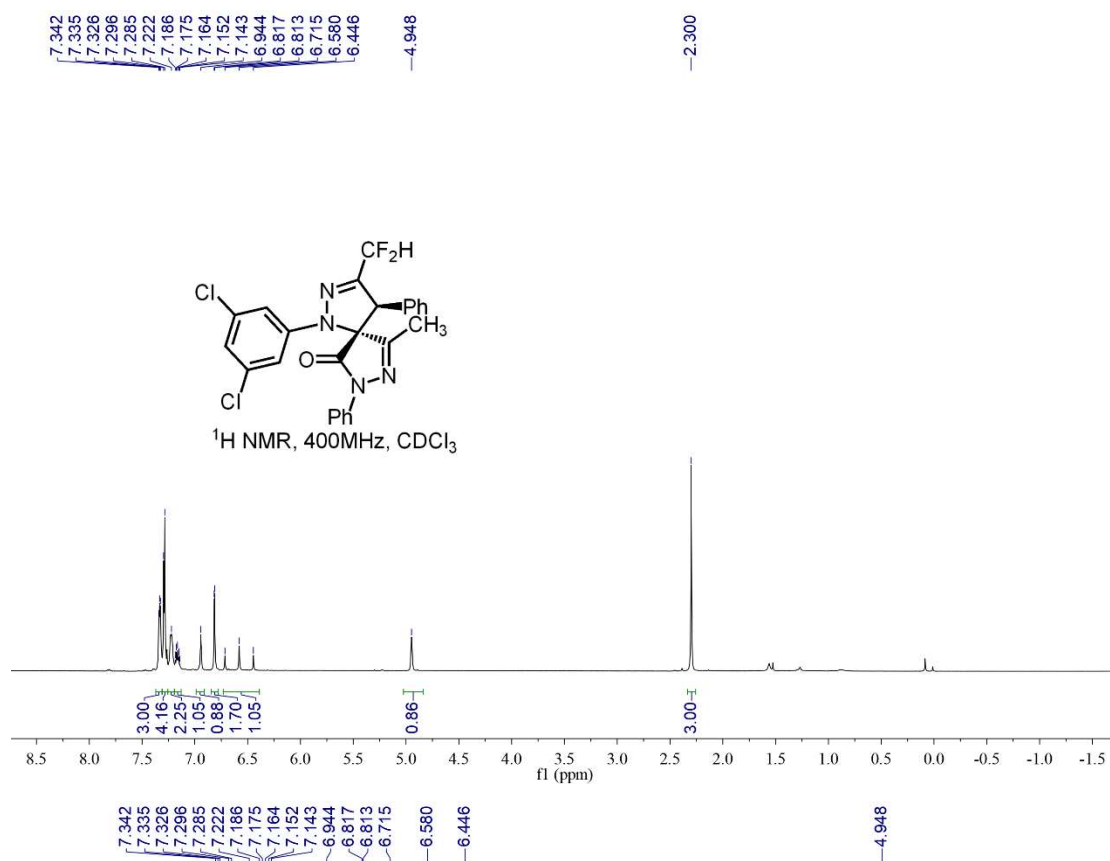
**Acquisition Parameter**

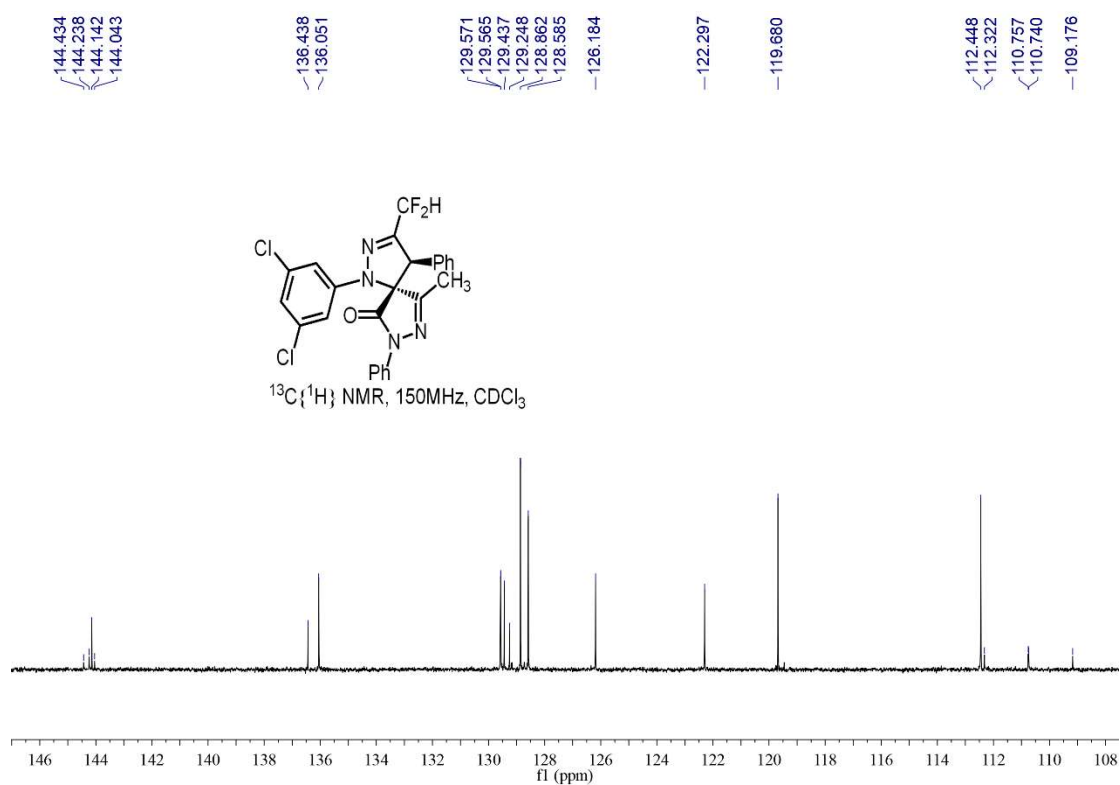
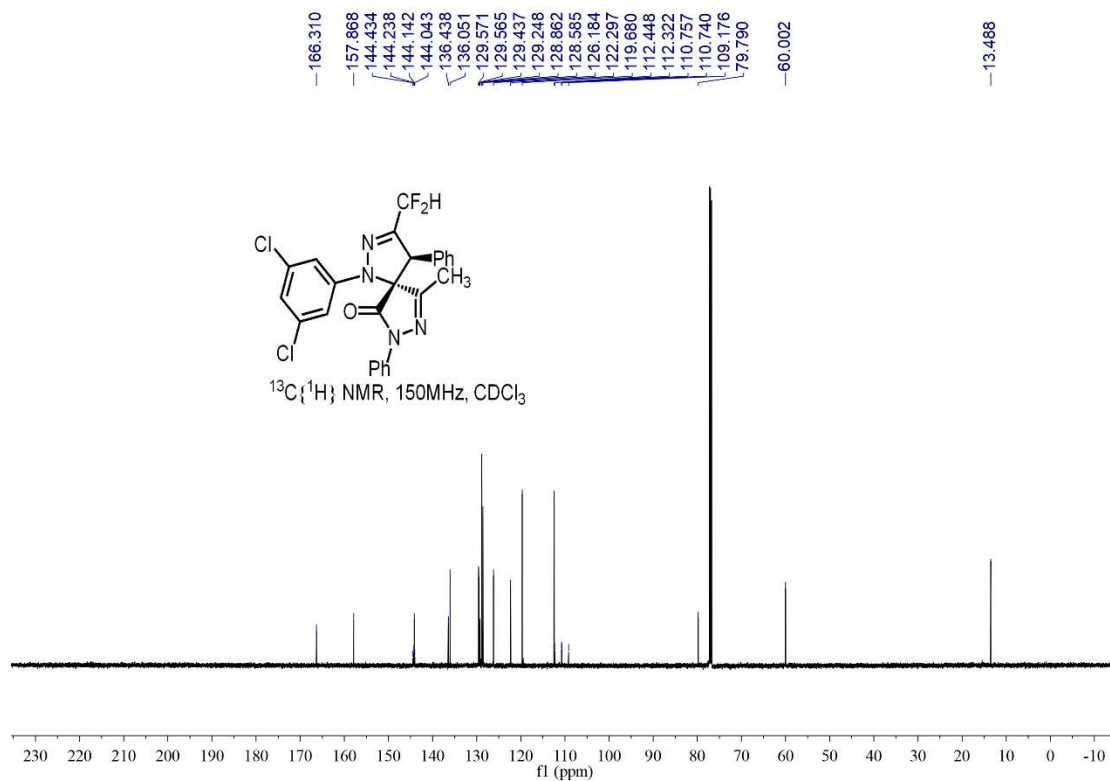
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j̄aC
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R ul e	e j % Con	m Si g a	St d l	St d l	St d l	St d l	Std Com b Dev
521.0736	1 C <sub>25</sub> H <sub>18</sub> Cl <sub>2</sub> F <sub>2</sub> N <sub>4</sub> NaO	521.0718	-3.5	-2.7	16.5	ok	even	6.0	6.8	1.8	2.5	2.0	842.7

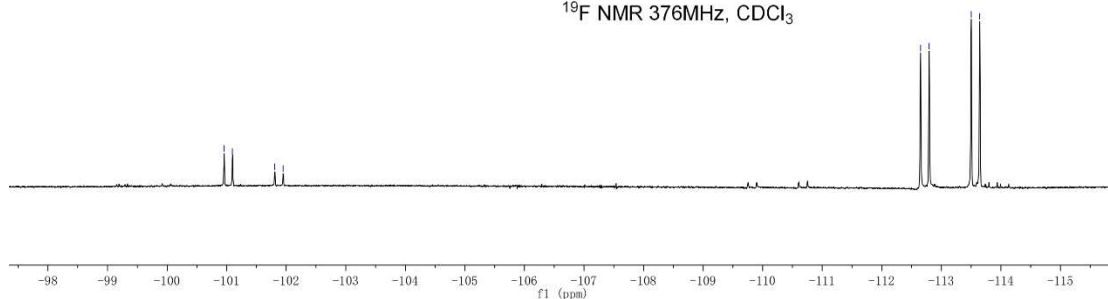
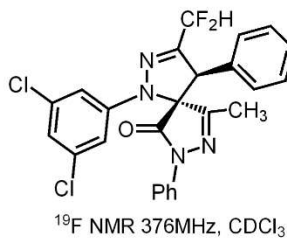
NMR copies of compound (*cis*)-**3j**:





~100.959  
~101.096  
~101.806  
~101.947

~112.651  
~112.796  
~113.502  
~113.646



HRMS (ESI) copy of compound (*cis*)-3j:

### Mass Spectrum SmartFormula Report

#### Analysis Info

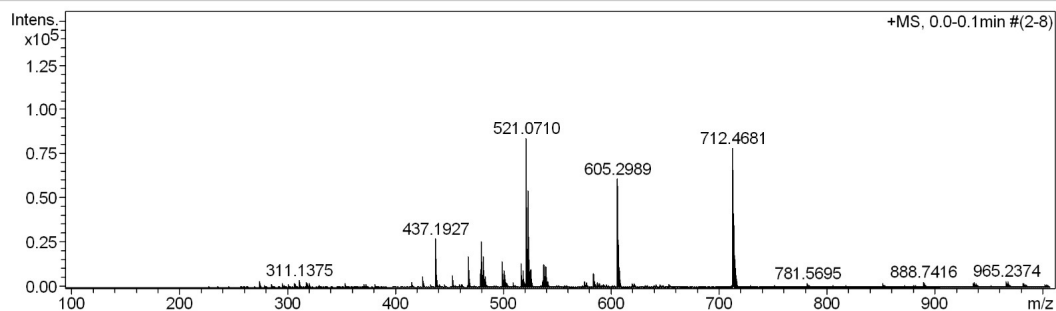
Analysis Name D:\Data\user\NWNNU-fengyang 20220707-13.d  
Method tune\_low.m  
Sample Name A-211  
Comment

Acquisition Date 2022-7-7 11:41:25

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

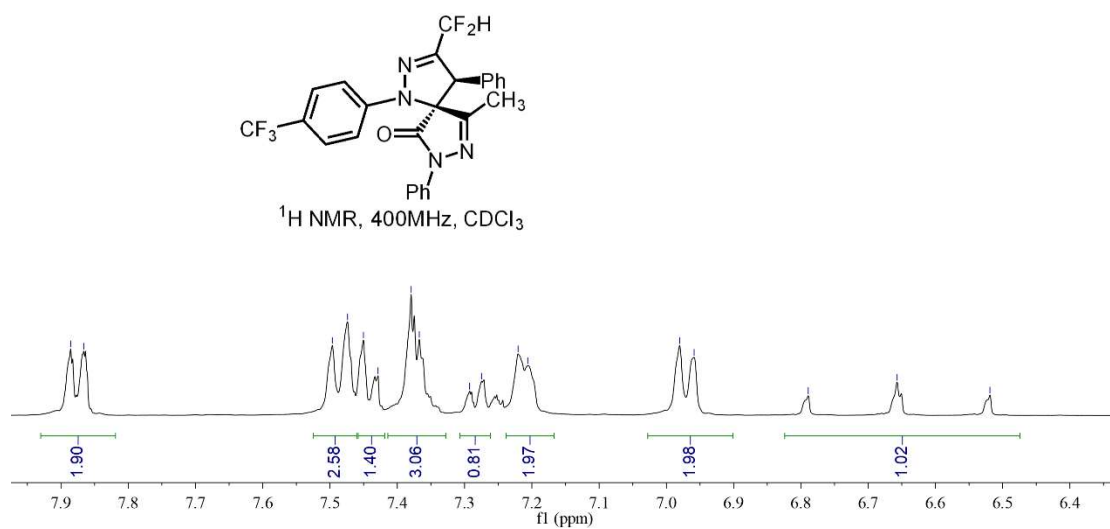
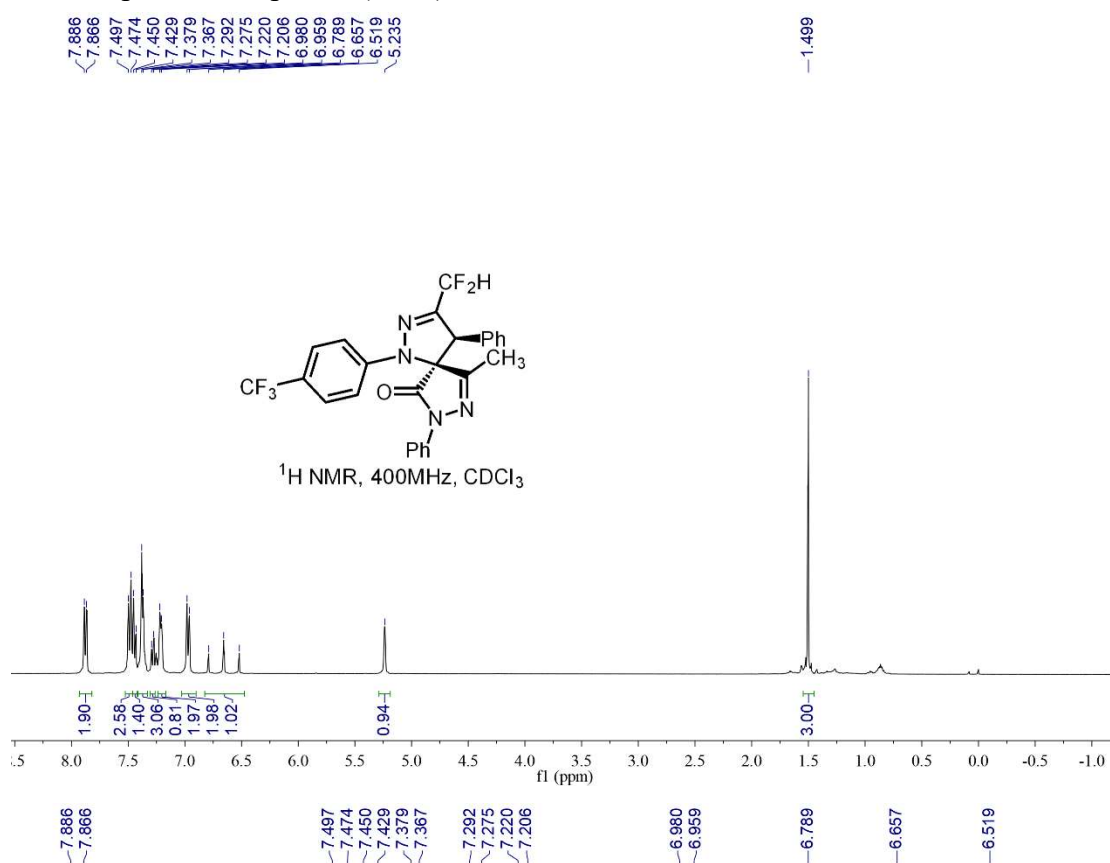
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j̄C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

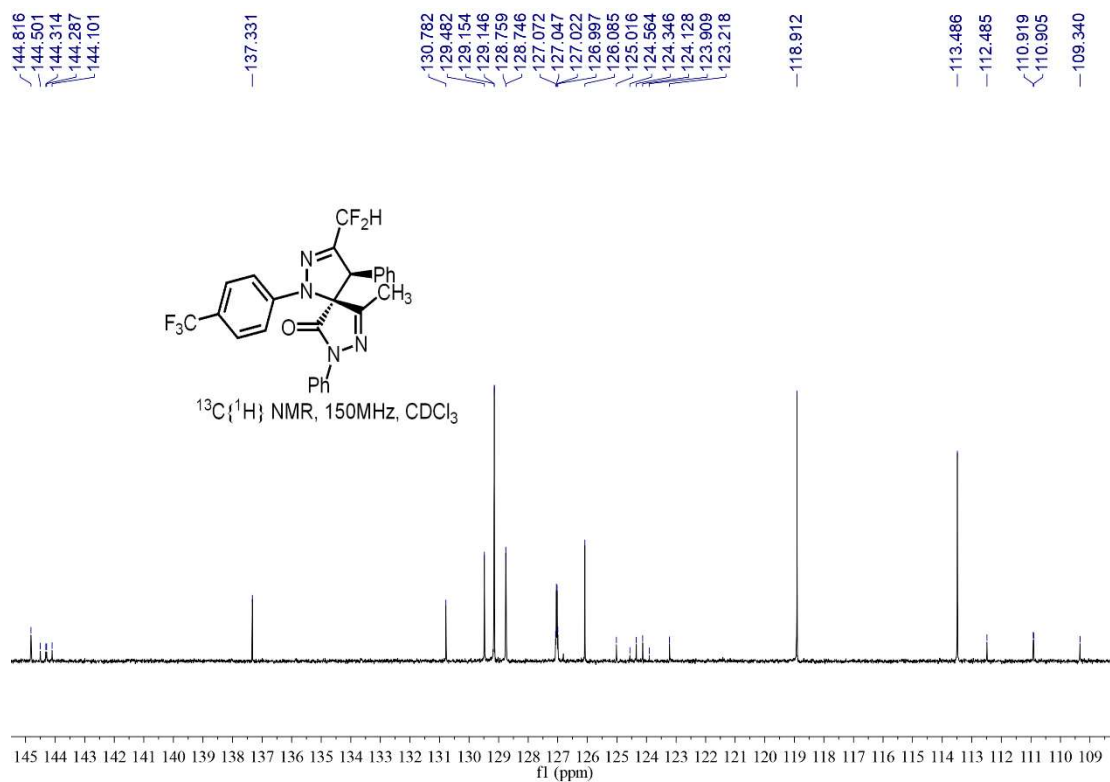
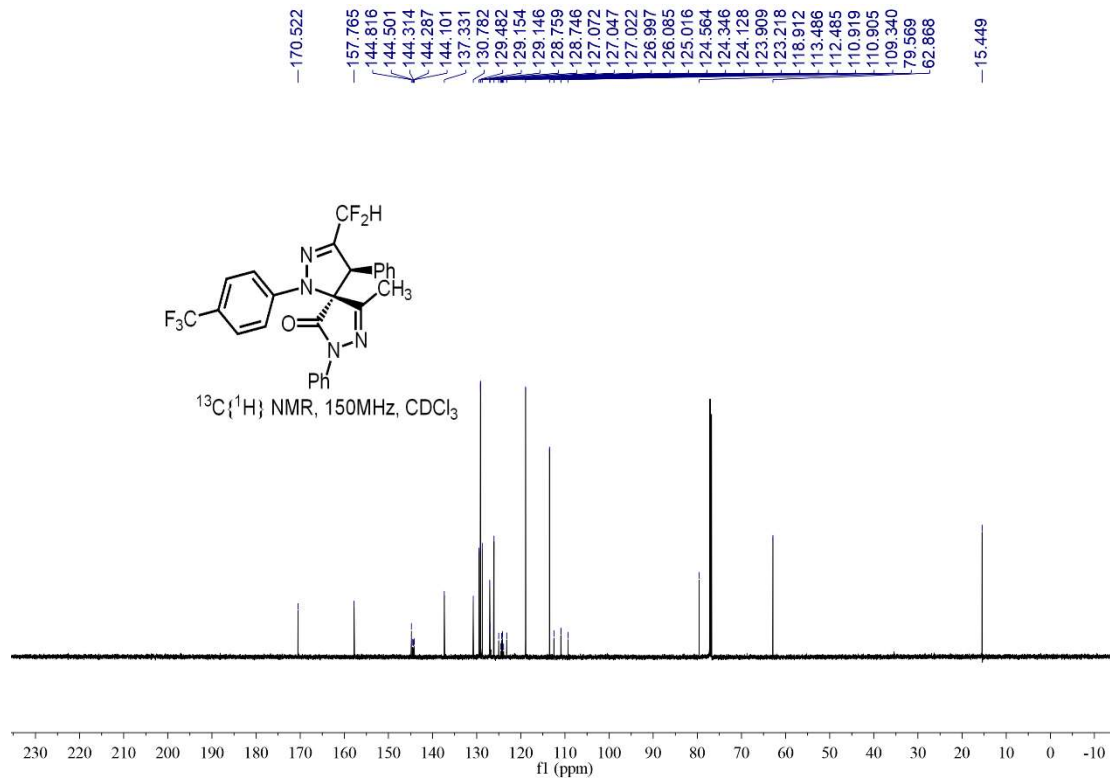


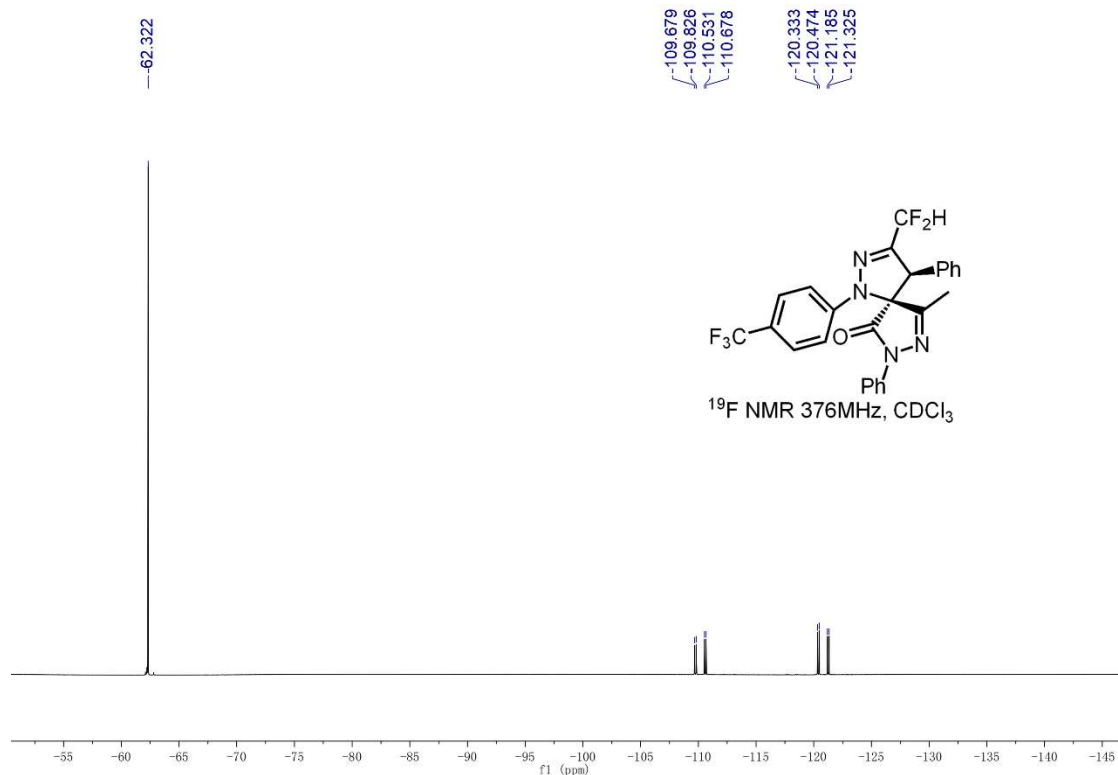
Meas. #	Formula	m/z	err	M	rdb	N-	e	mSi	Std	St	St	St	Std	
m/z			[p	ea		R	Con	gm	l	d	d	d	Com	
			p	n		ul	f	a		M	Va	m/	b	
			m]	err		e				ea	rN	z	Dev	
				[p						n	or	Dif		
				p						m/	m/	f		
				m]						z				
521.0710	1	C 25 H 18 Cl 2 F 2 N 4 Na O	521.0718	1.6	1.0	16.5	ok	even	16.7	17.4	1.3	4.4	2.1	842.7

NMR copies of compound (*trans*)-3k:









HRMS (ESI) copy of compound (*trans*)-3k:

### Mass Spectrum SmartFormula Report

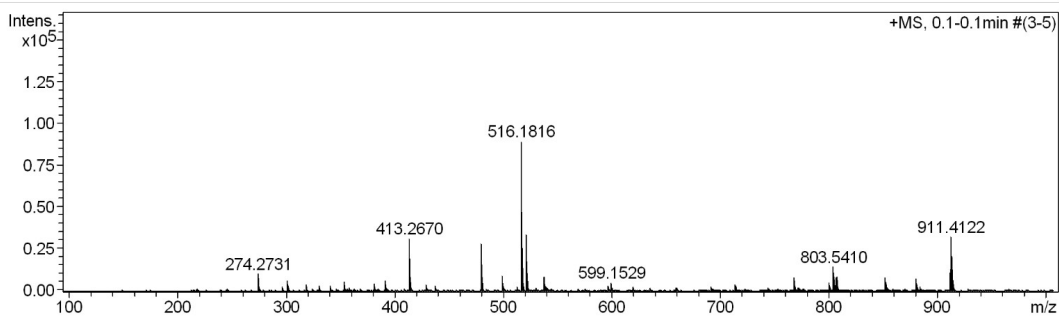
**Analysis Info**

Analysis Name D:\Data\user\fengyang 20220616-14.d  
 Method tune\_low.m  
 Sample Name A-15  
 Comment

Acquisition Date 2022-6-16 10:54:39  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

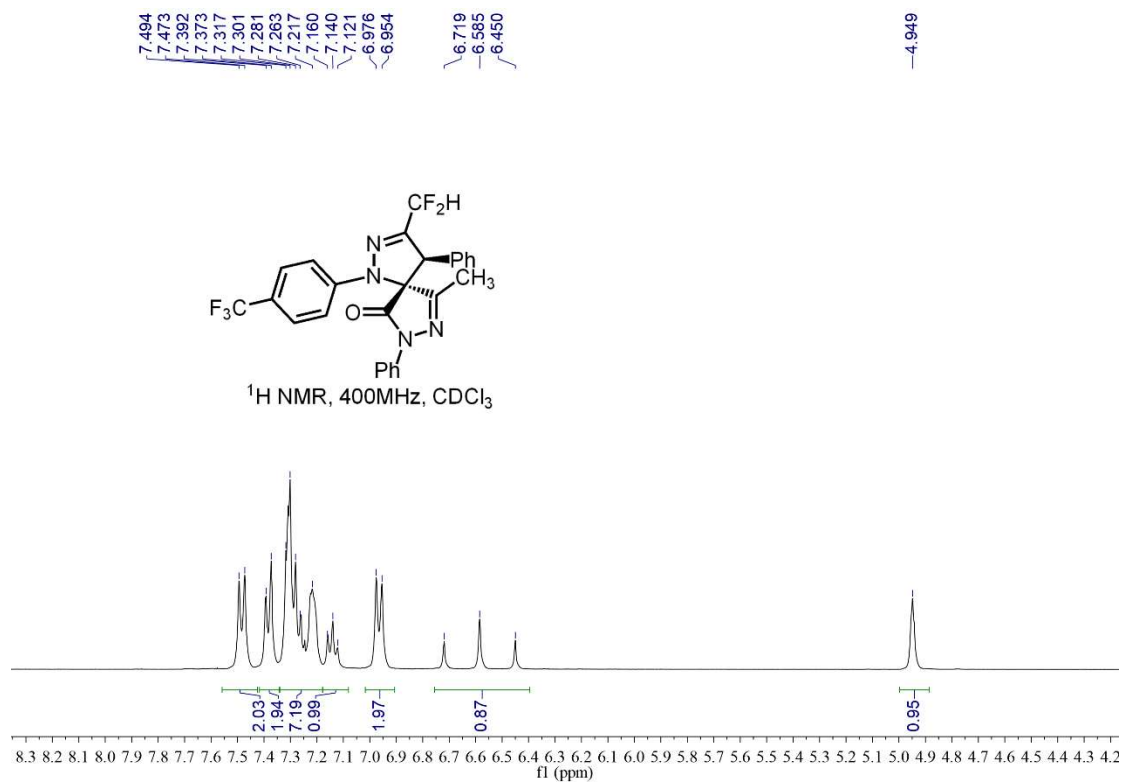
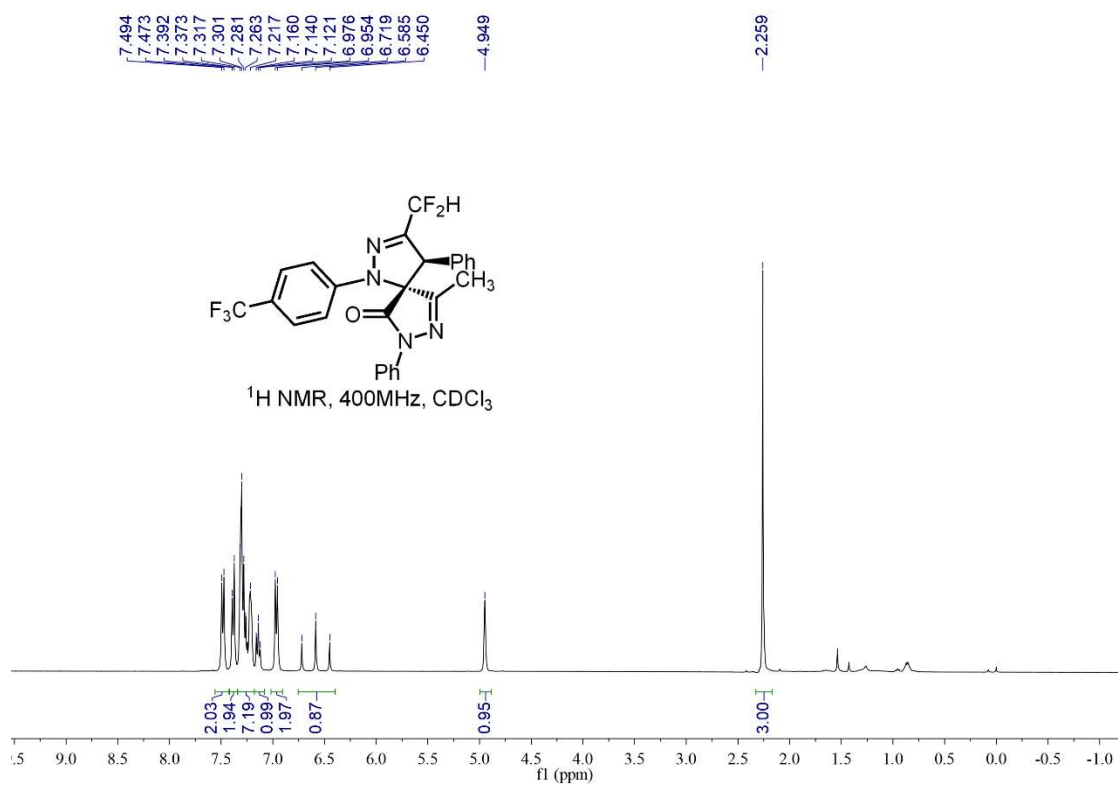
**Acquisition Parameter**

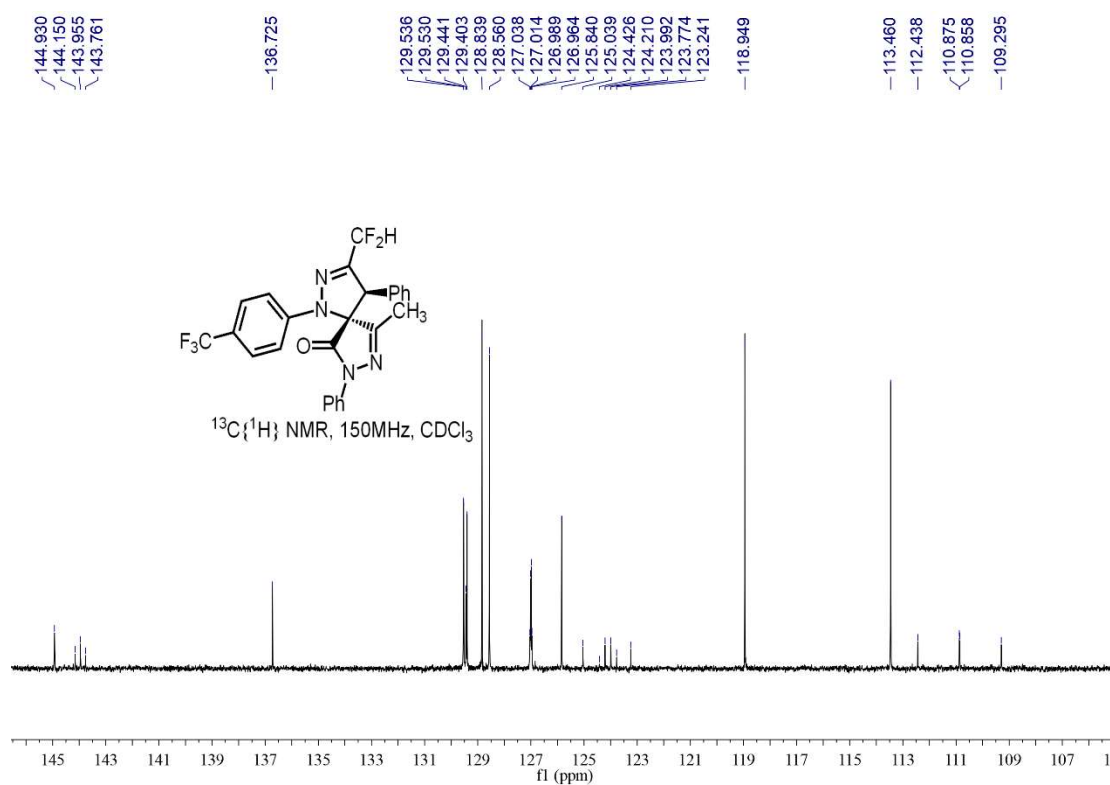
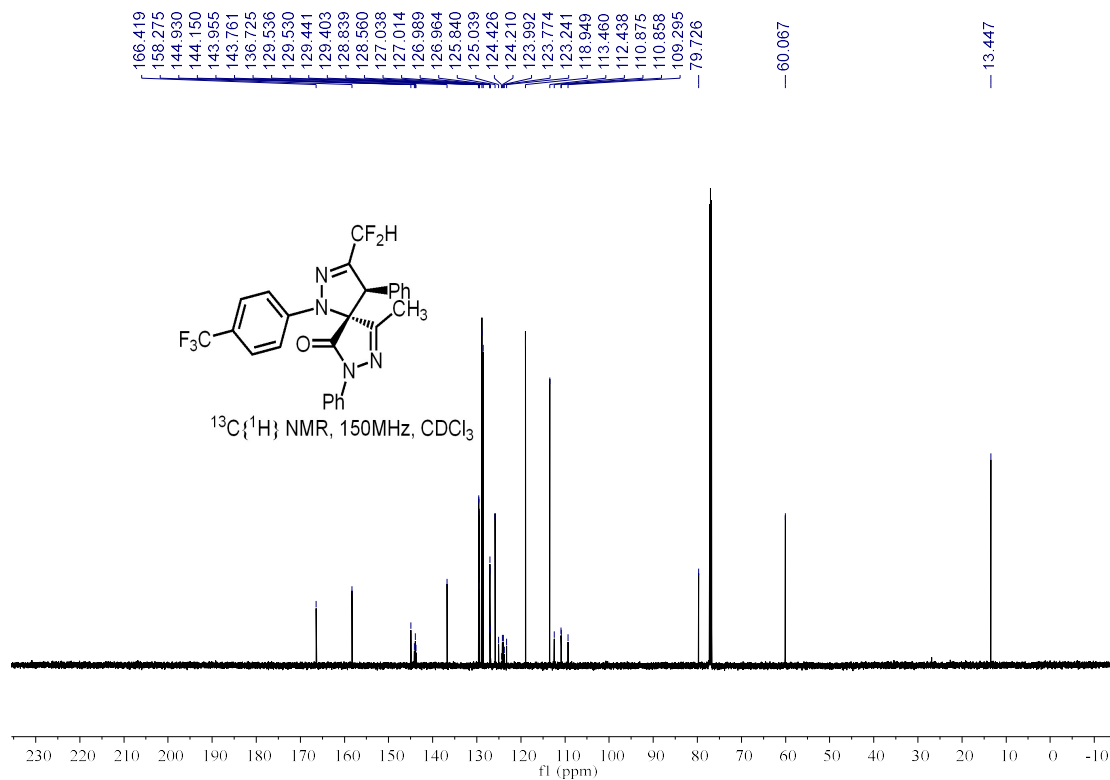
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{A}$ C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

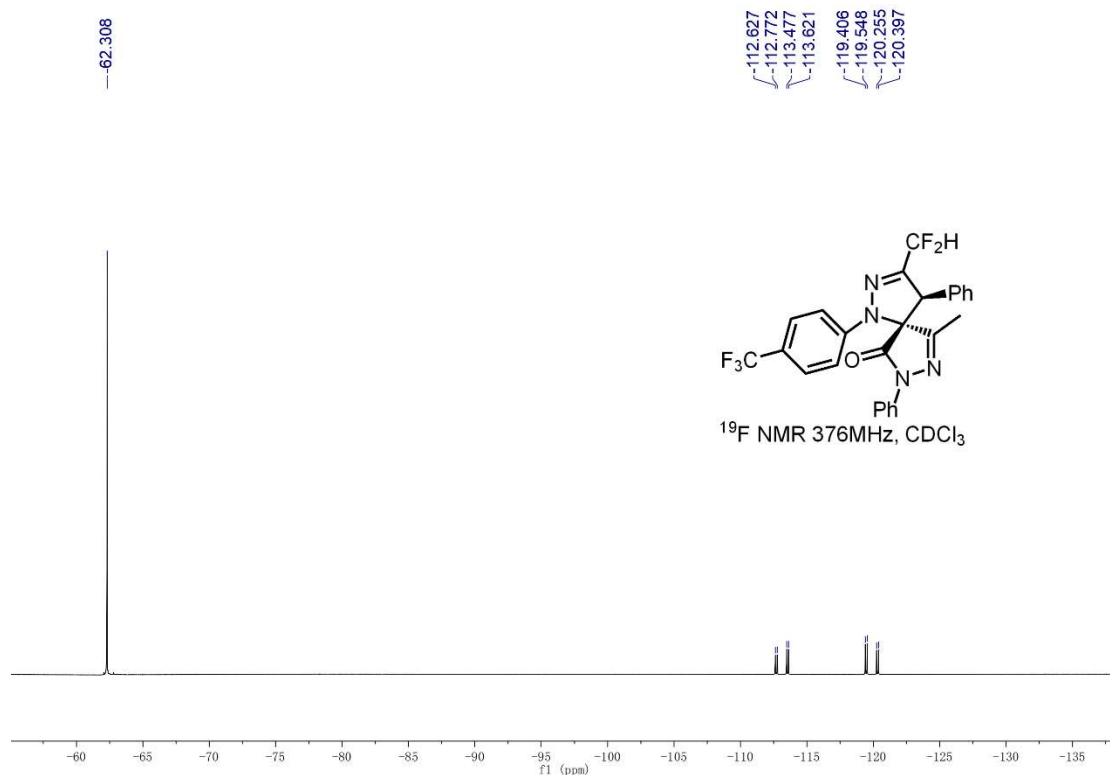


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N	e <sub>i</sub> %	mSi gm	Std l	St d m/z	Std Var m	Std Nor m	Std Dif f	Std Com b Dev
516.1816	1 C <sub>26</sub> H <sub>25</sub> F <sub>2</sub> N <sub>5</sub> NaO <sub>3</sub>	516.1818	0.3	0.8	15.5	ok	even	7.2	10.3	0.7	4.5	1.2	646.6	
	2 C <sub>23</sub> H <sub>26</sub> F <sub>3</sub> N <sub>5</sub> NaO <sub>4</sub>	516.1829	2.5	3.0	11.5	ok	even	12.1	19.0	1.6	8.3	1.2	833.3	
	3 C <sub>21</sub> H <sub>27</sub> F <sub>3</sub> N <sub>5</sub> Na <sub>2</sub> O <sub>4</sub>	516.1805	-2.1	-1.7	8.5	ok	even	24.9	39.7	1.0	17.0	1.2	839.3	
	4 C <sub>19</sub> H <sub>22</sub> F <sub>3</sub> N <sub>11</sub> NaO <sub>2</sub>	516.1802	-2.7	-2.2	12.5	ok	even	25.5	41.9	1.3	18.2	1.1	868.6	
	5 C <sub>21</sub> H <sub>25</sub> F <sub>6</sub> N <sub>5</sub> NaO <sub>2</sub>	516.1805	-2.2	-1.7	8.5	ok	even	25.7	42.0	1.0	18.2	1.2	849.5	
	6 C <sub>19</sub> H <sub>24</sub> F <sub>4</sub> N <sub>9</sub> Na <sub>2</sub> O	516.1830	2.7	3.1	9.5	ok	even	30.7	51.5	1.7	22.3	1.2	913.1	
521.1371	1 C <sub>26</sub> H <sub>19</sub> F <sub>5</sub> N <sub>4</sub> NaO	521.1371	0.1	-0.1	16.5	ok	even	8.5	13.5	0.2	6.3	0.4	842.7	

NMR copies of compound (*cis*)-**3k**:







HRMS (ESI) copy of compound (*cis*)-3k:

### Mass Spectrum SmartFormula Report

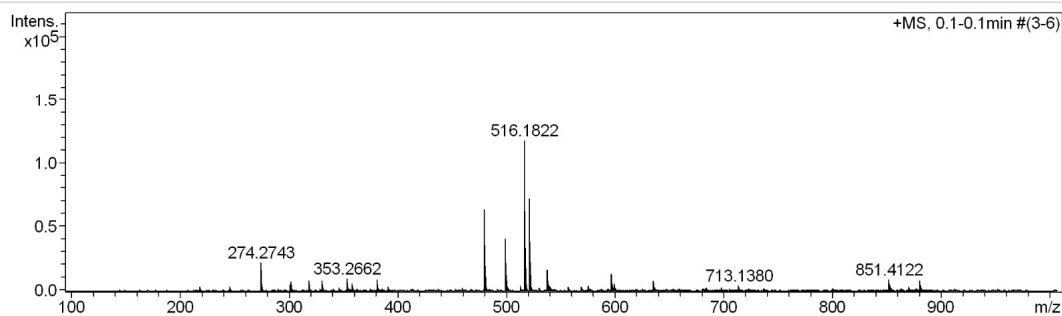
#### Analysis Info

Analysis Name D:\Data\user\fengyang 20220616-15.d  
 Method tune\_low.m  
 Sample Name A-151  
 Comment

Acquisition Date 2022-6-16 10:56:48  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

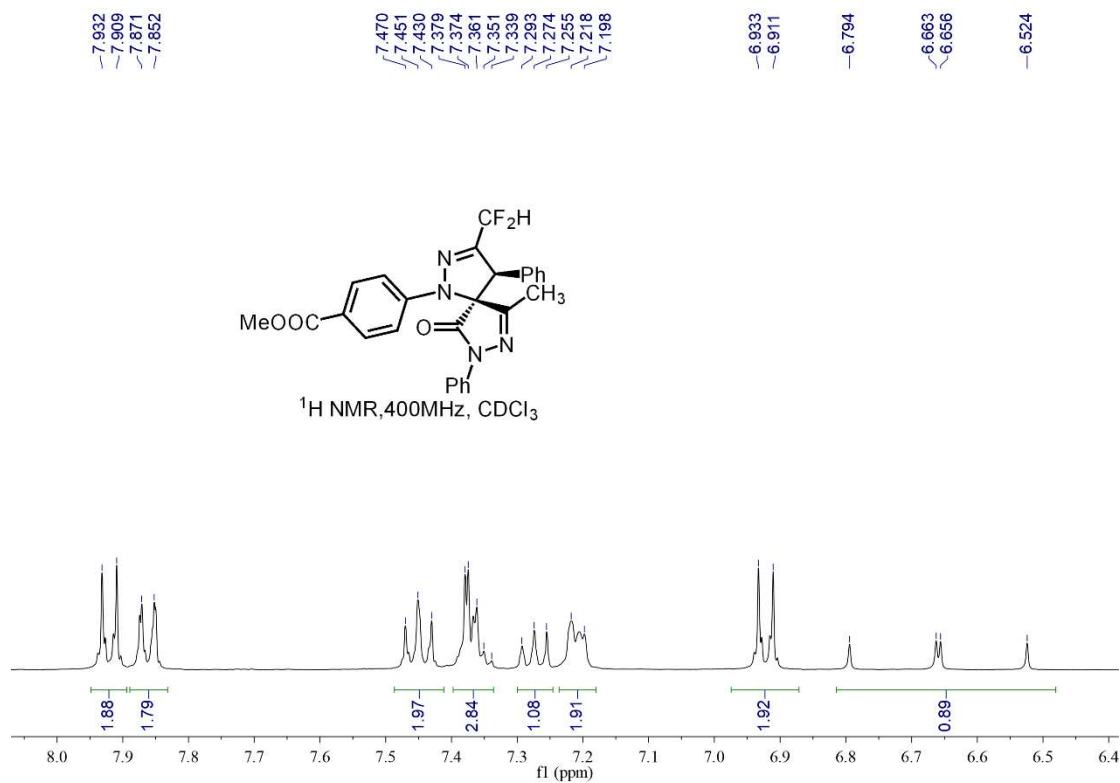
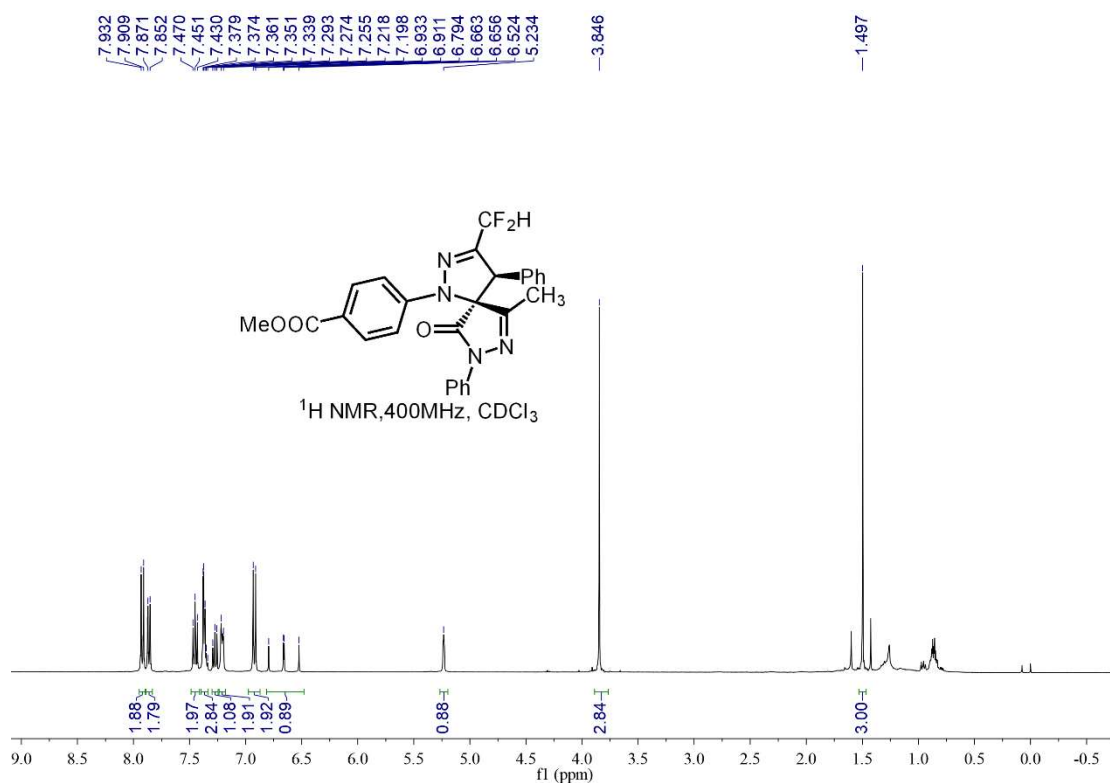
#### Acquisition Parameter

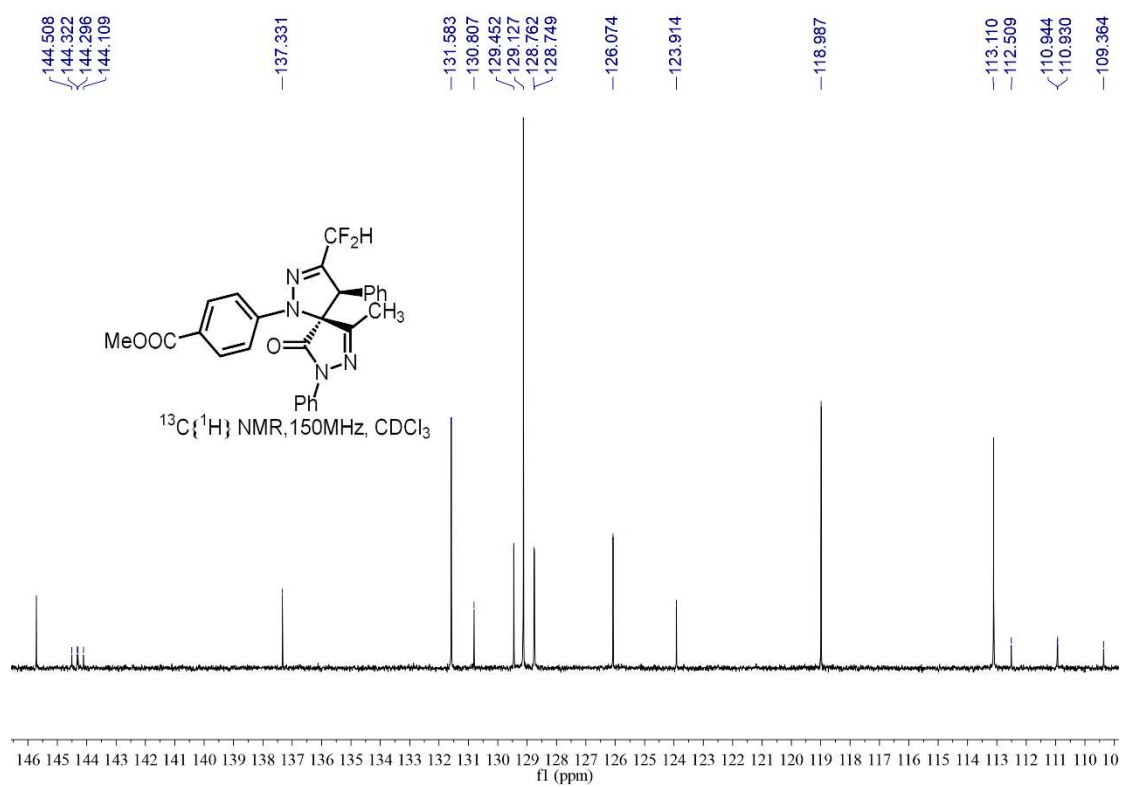
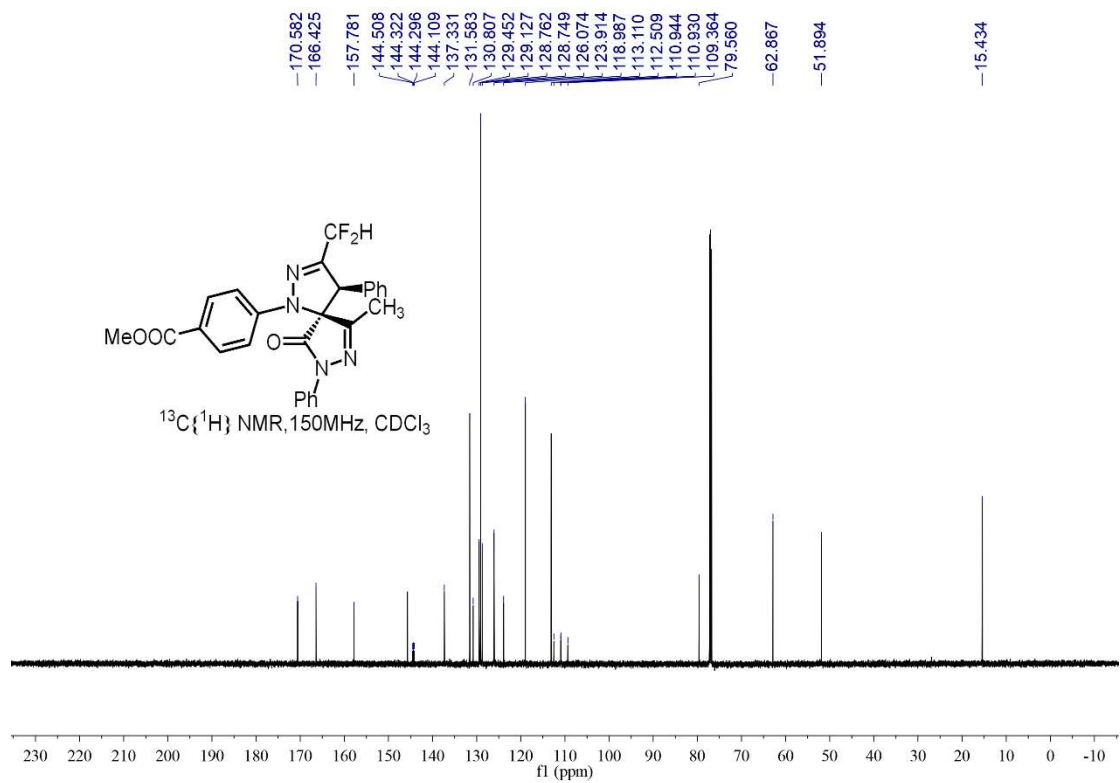
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{C}$
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

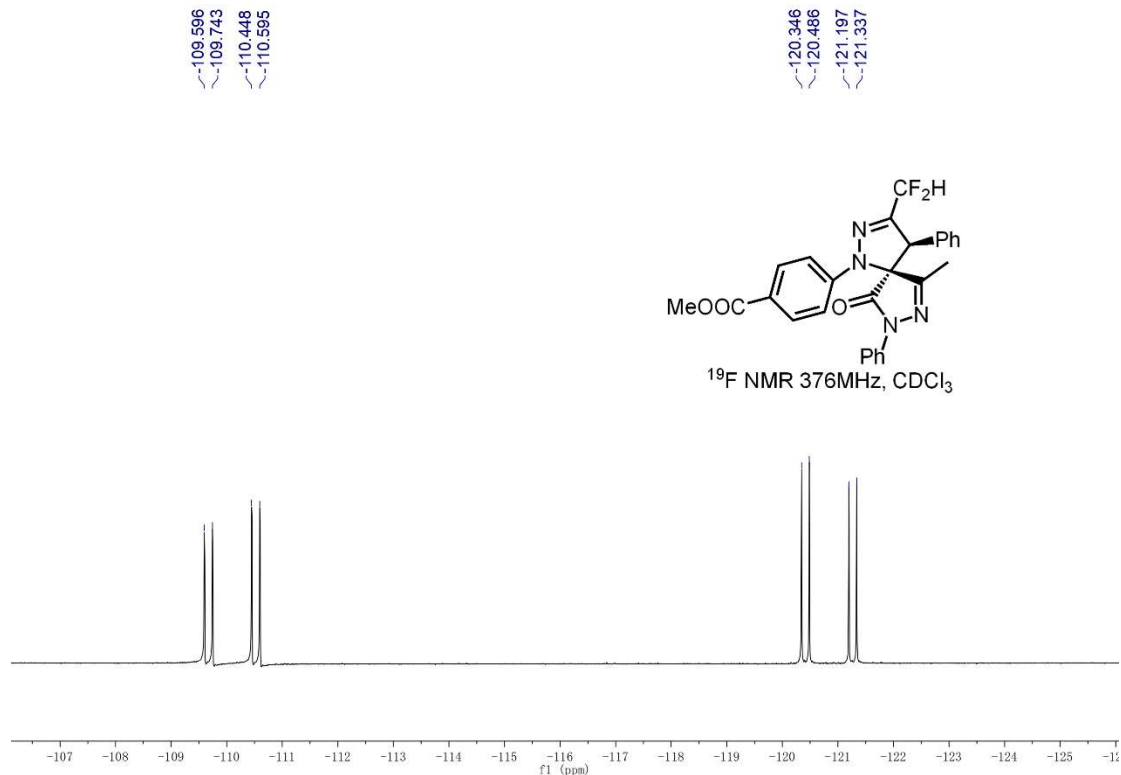


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R	ei % Conf	mSi gm	Std l	St d	St d l	St d	Std Com b
521.1379	1 C <sub>26</sub> H <sub>19</sub> F <sub>5</sub> N <sub>4</sub> NaO	521.1371	-1.5	-1.4	16.5	ok	even	10.2	14.9	0.7	6.4	0.2	842.7

NMR copies of compound (*trans*)-**31**:







HRMS (ESI) copy of compound (*trans*)-3I:

Mass Spectrum SmartFormula Report

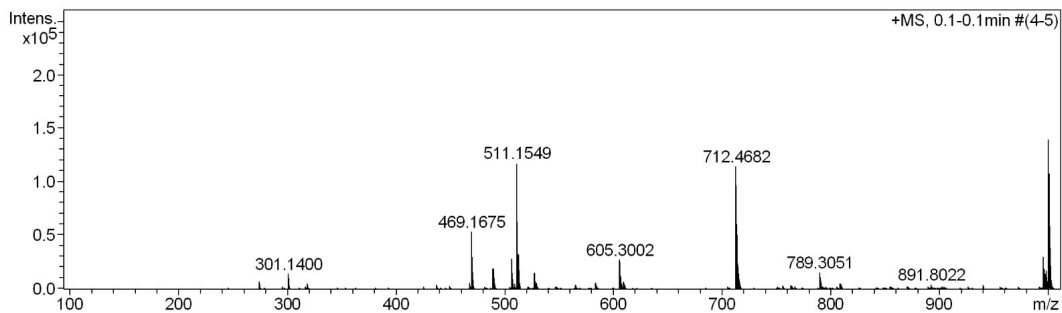
Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20220707-7.d  
 Method tune\_low.m  
 Sample Name A-27  
 Comment

Acquisition Date 2022-7-7 11:32:35  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

Acquisition Parameter

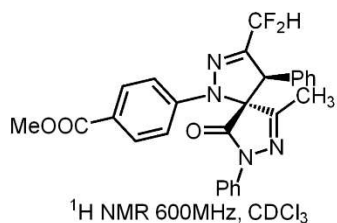
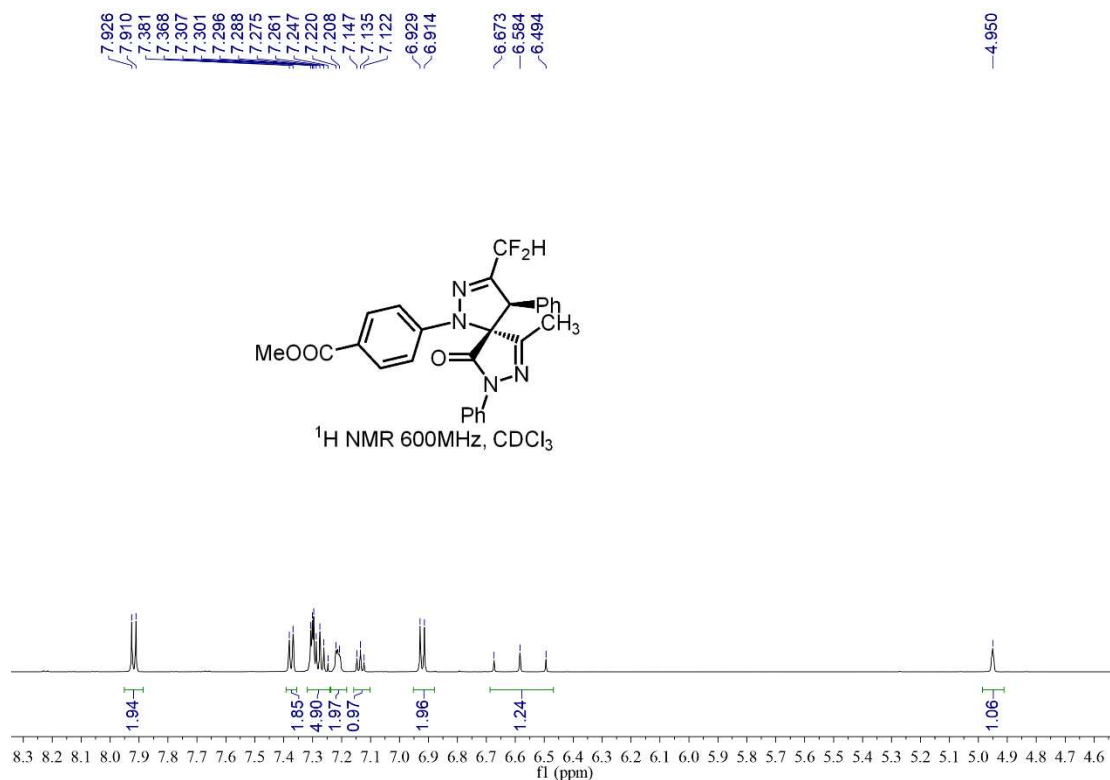
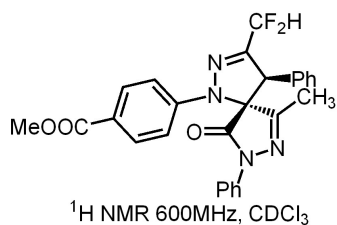
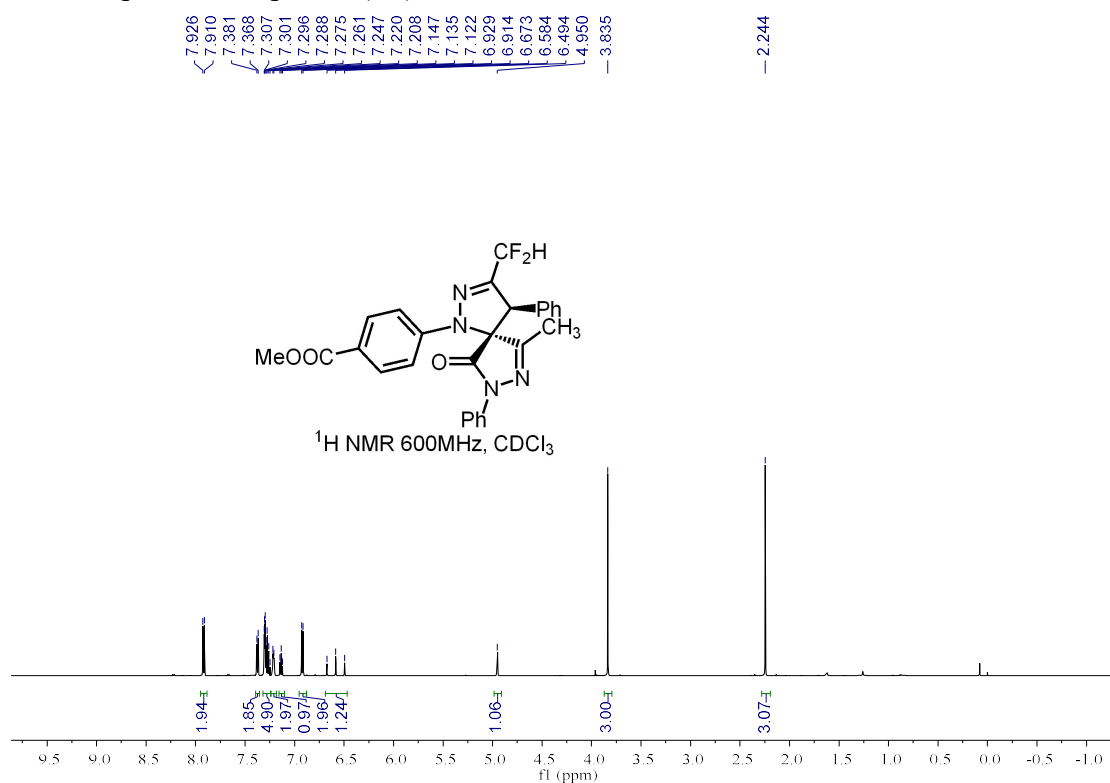
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

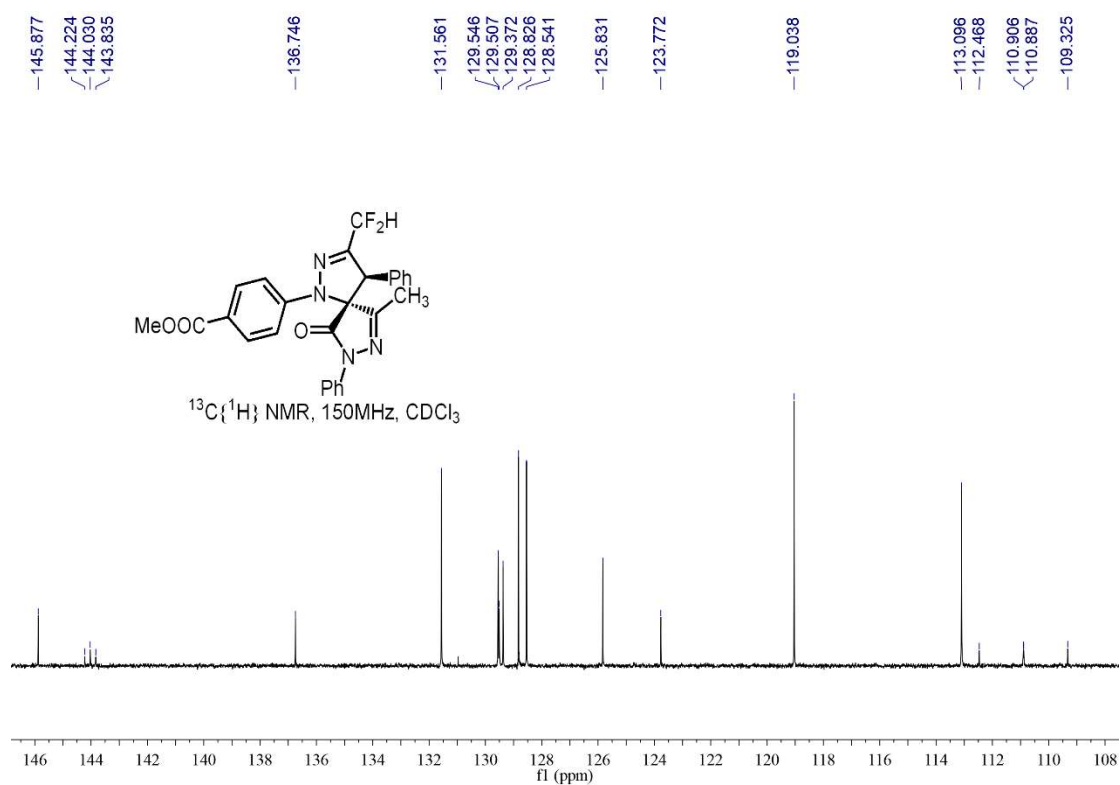
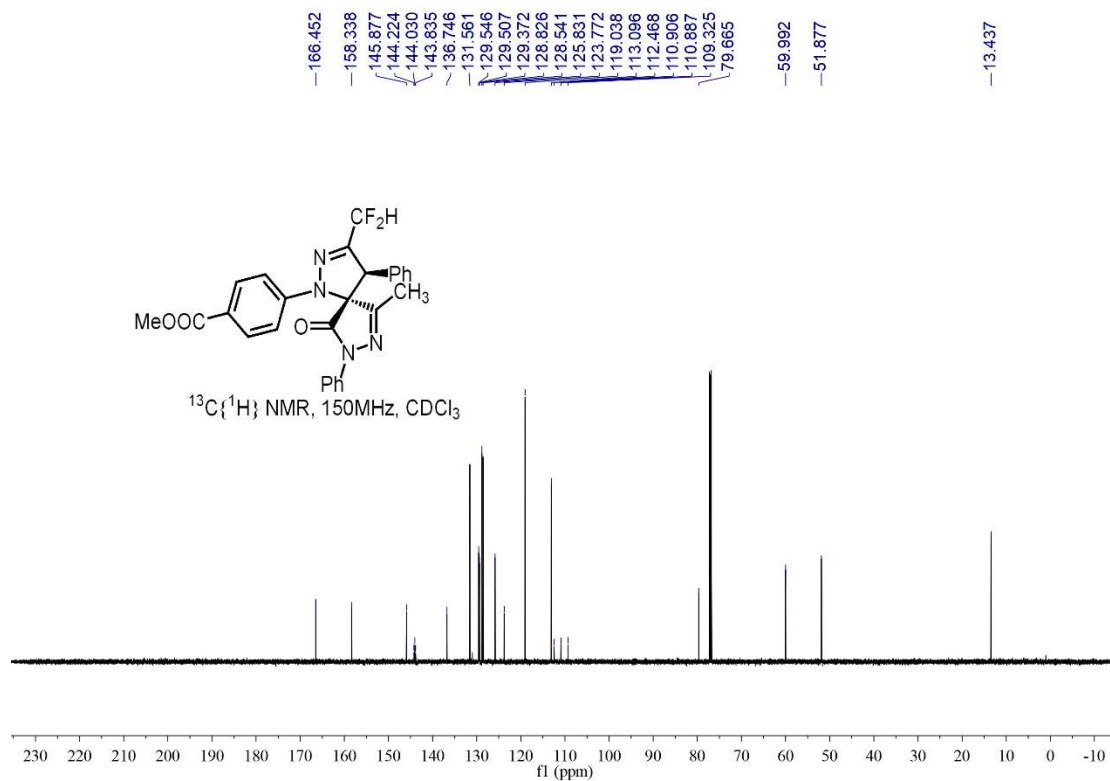


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j ≠ Conf	mSi gm	Std l	St d	St d l	St d m/	Std Com b
511.1549	1 C 27 H 22 F 2 N 4 Na O 3	511.1552	0.5	0.5	17.5	ok	even	14.1	23.0	0.6	7.7	1.9	842.7



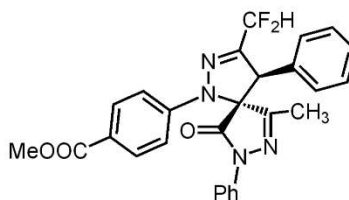
NMR copies of compound (*cis*)-**3l**:



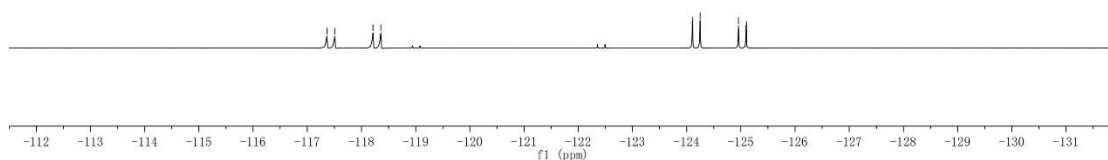


~117.362  
~117.507  
~118.212  
~118.356

~124.112  
~124.248  
~124.956  
~125.103



<sup>19</sup>F NMR 376MHz, CDCl<sub>3</sub>



HRMS (ESI) copy of compound (*cis*)-3I:

### Mass Spectrum SmartFormula Report

#### Analysis Info

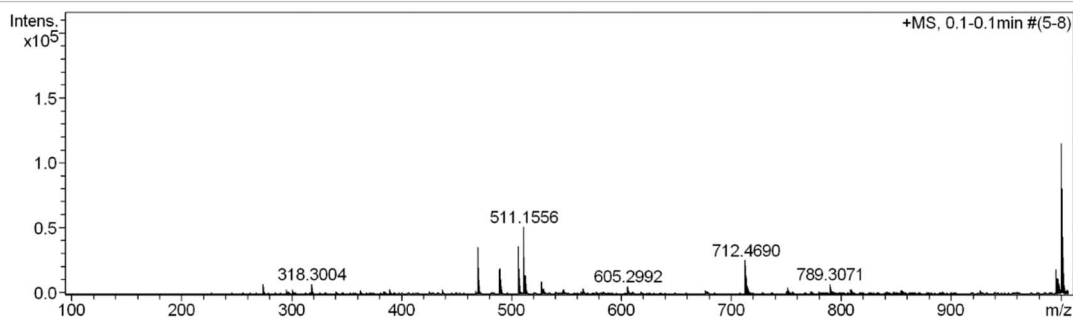
Analysis Name D:\Data\user\NWNNU-fengyang 20220707-8.d  
Method tune\_low.m  
Sample Name A-271  
Comment

Acquisition Date 2022-7-7 11:34:04

Operator BDAL@DE  
Instrument / Ser# microTOF-Q 20453

#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 i°C
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Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

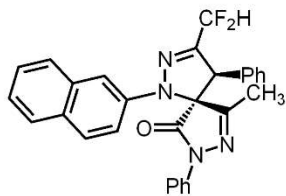


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e_j Con	mSi gm	Std l	St d	St d l	St d m/	Std Com b
511.1556	1 C <sub>27</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO <sub>3</sub>	511.1552	-0.7	-0.6	17.5	ok	even	17.5	28.0	0.7	9.4	2.0	842.7

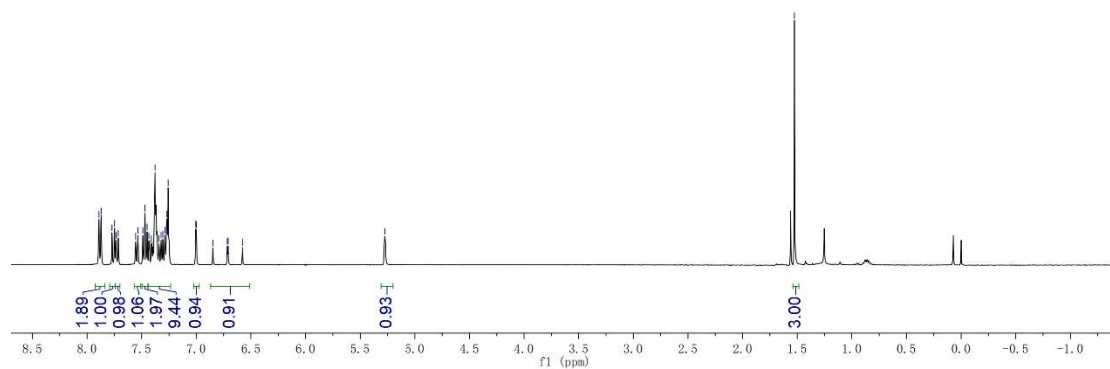
NMR copies of compound (*trans*)-3m:

7.891  
7.871  
7.771  
7.748  
7.735  
7.715  
7.555  
7.489  
7.470  
7.450  
7.434  
7.412  
7.378  
7.342  
7.322  
7.306  
7.288  
7.269  
7.258  
7.005  
6.999  
6.848  
6.716  
6.709  
6.577  
5.274

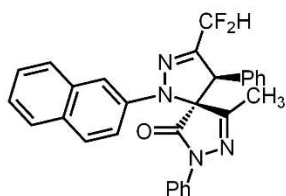
-1.526



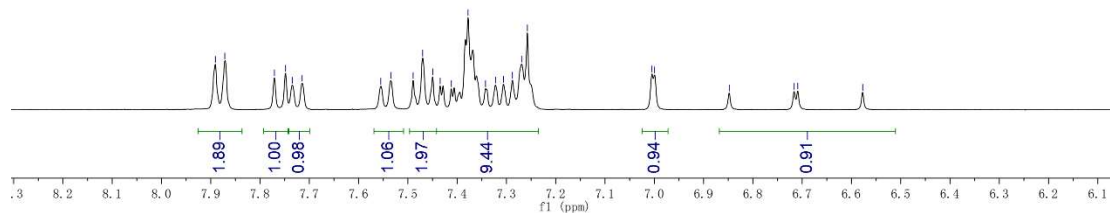
<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>

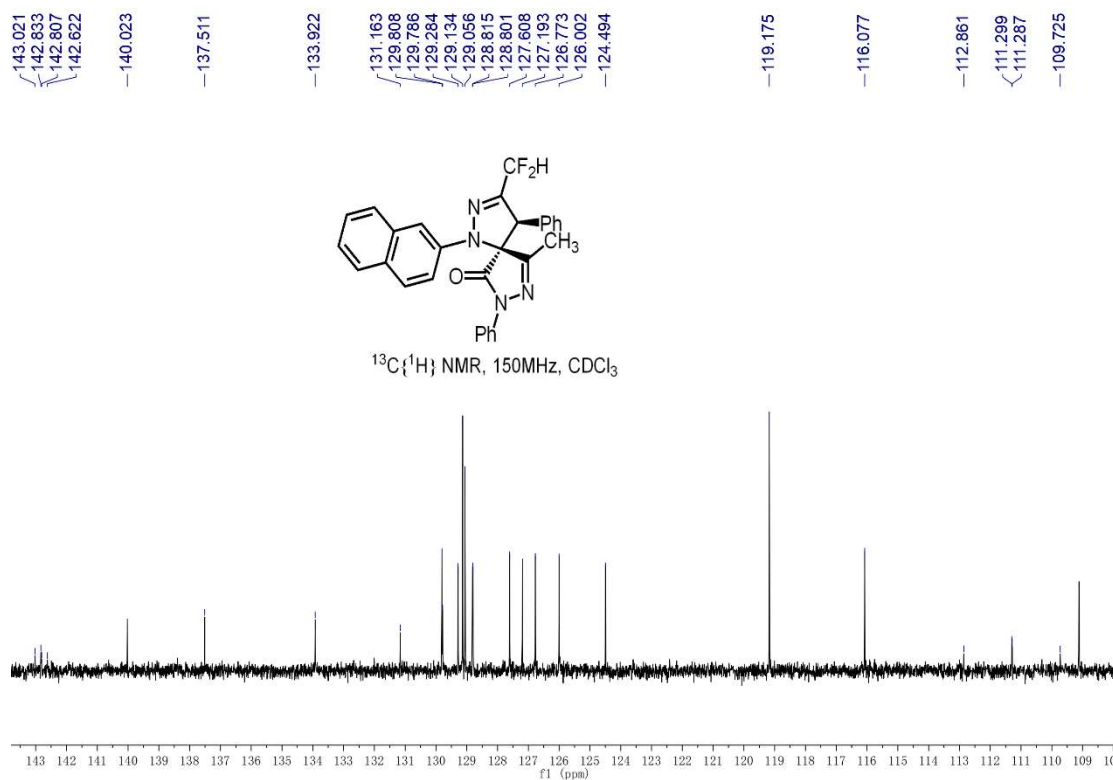
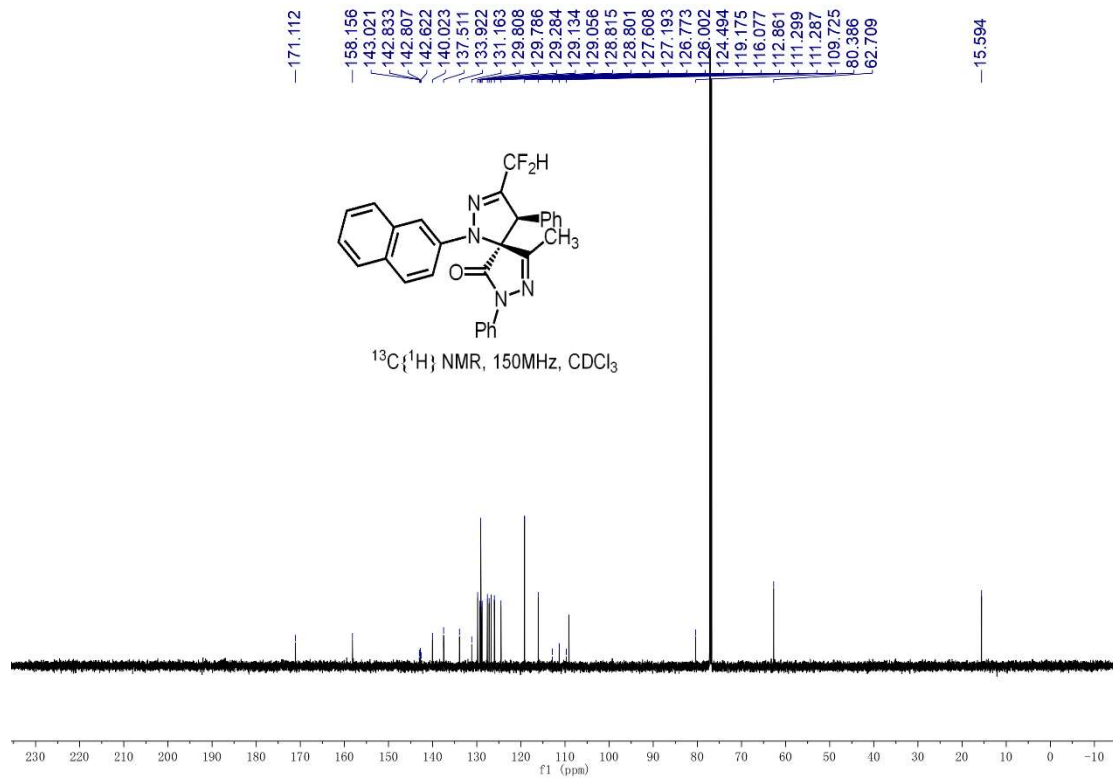


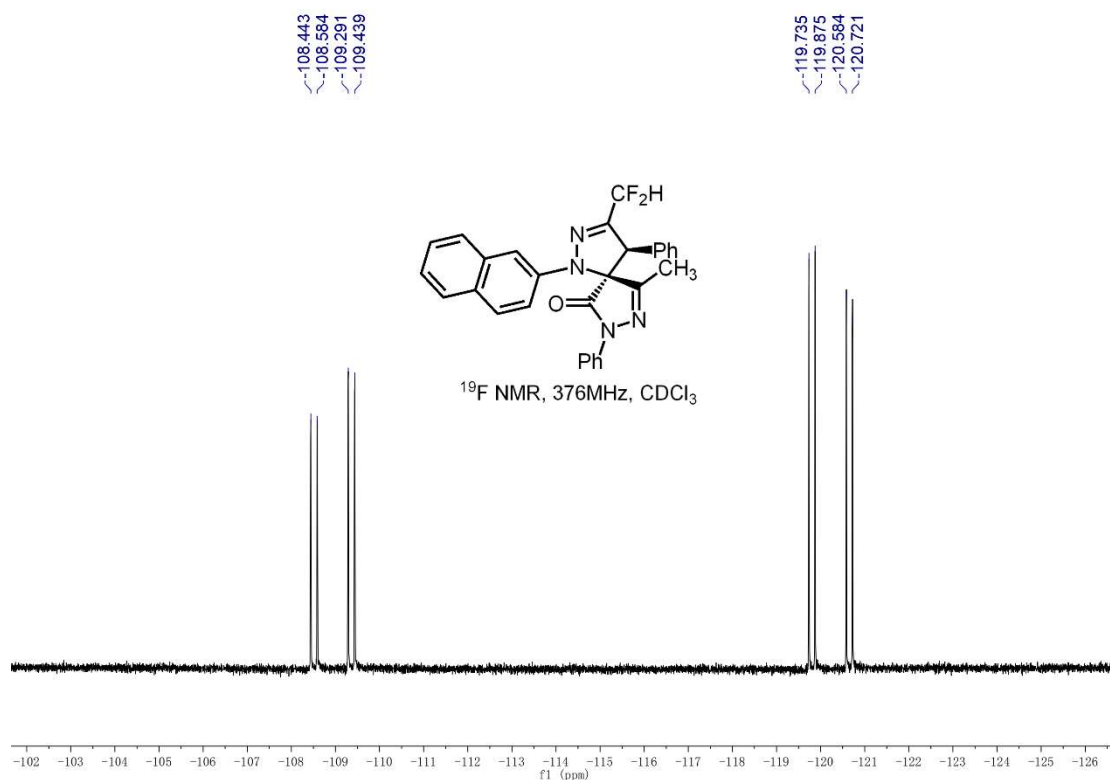
7.891  
7.871  
7.771  
7.748  
7.735  
7.715  
7.555  
7.489  
7.470  
7.450  
7.434  
7.412  
7.378  
7.342  
7.322  
7.306  
7.288  
7.269  
7.258  
7.005  
6.999  
6.848  
6.716  
6.709  
6.577



<sup>1</sup>H NMR, 400MHz, CDCl<sub>3</sub>







HRMS (ESI) copy of compound (*trans*)-**3m**:

### Mass Spectrum SmartFormula Report

**Analysis Info**

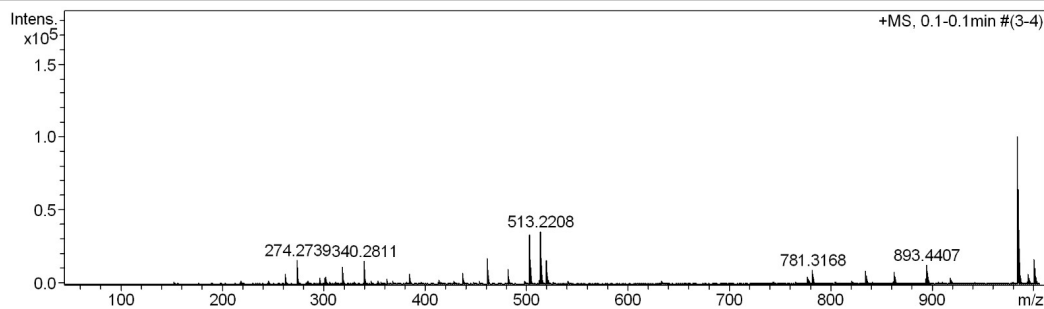
Analysis Name D:\Data\user\NWNNU-fengyang 20230321-3.d  
 Method tune\_low.m  
 Sample Name A-23  
 Comment

Acquisition Date 2023-3-21 15:33:32

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

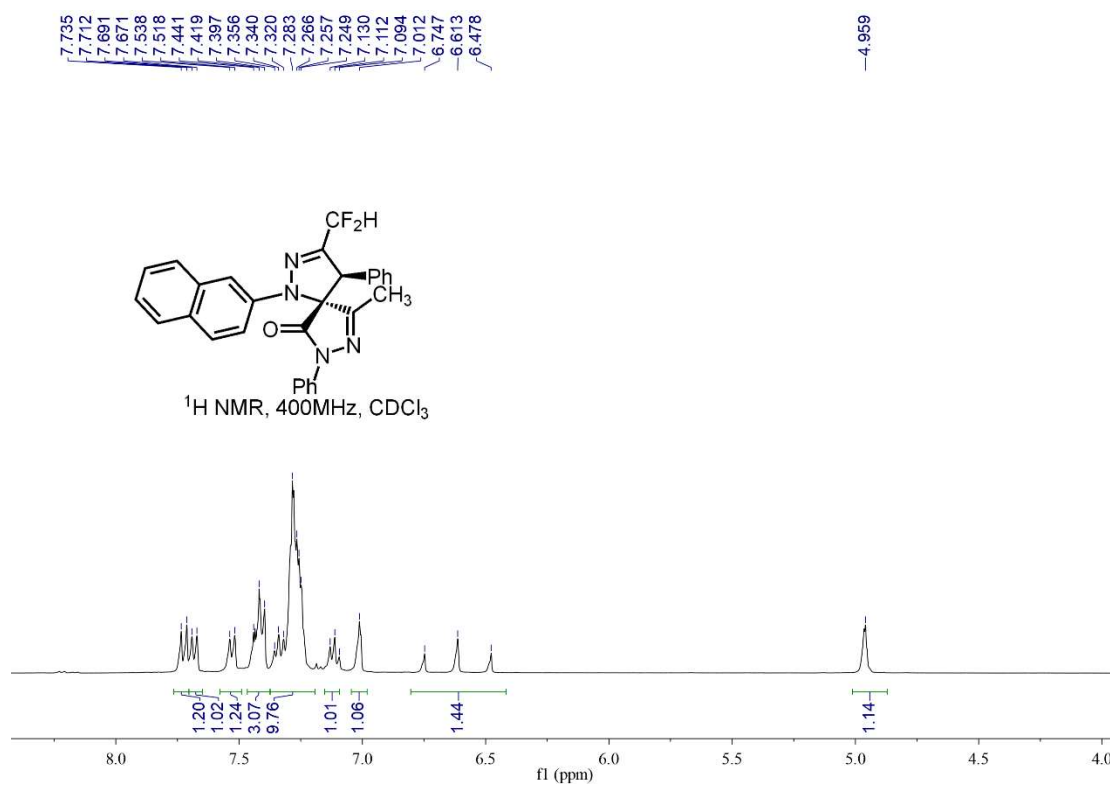
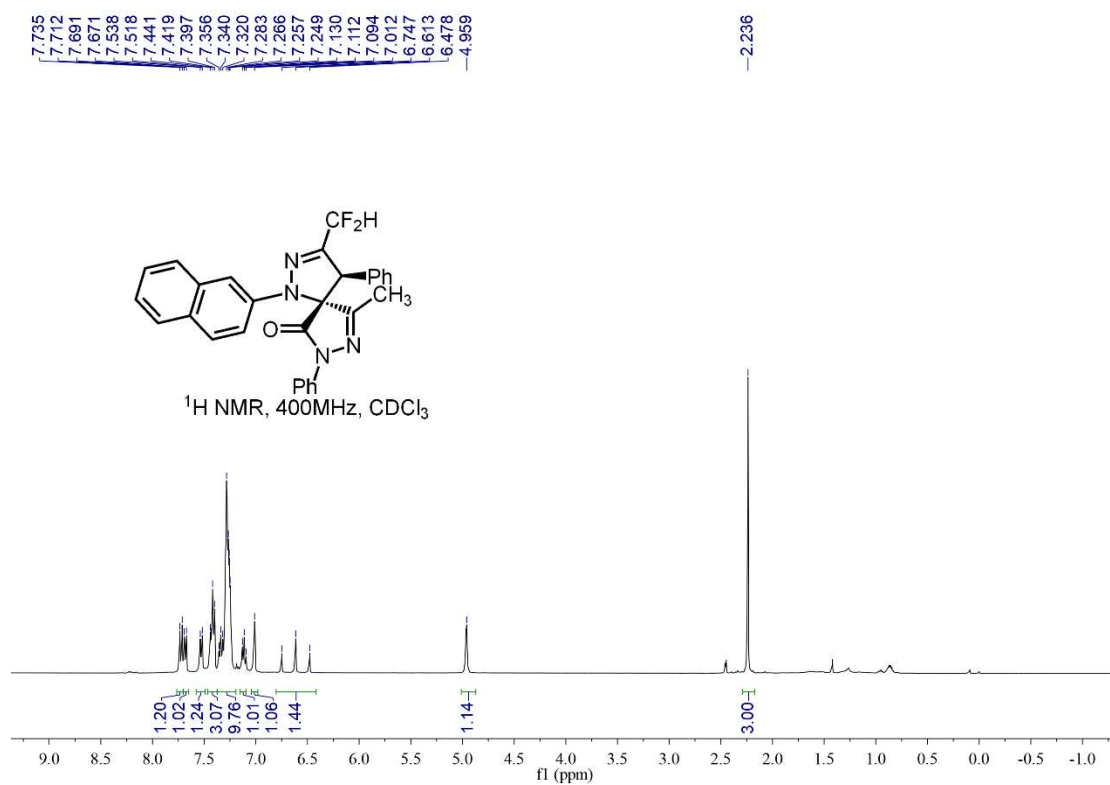
**Acquisition Parameter**

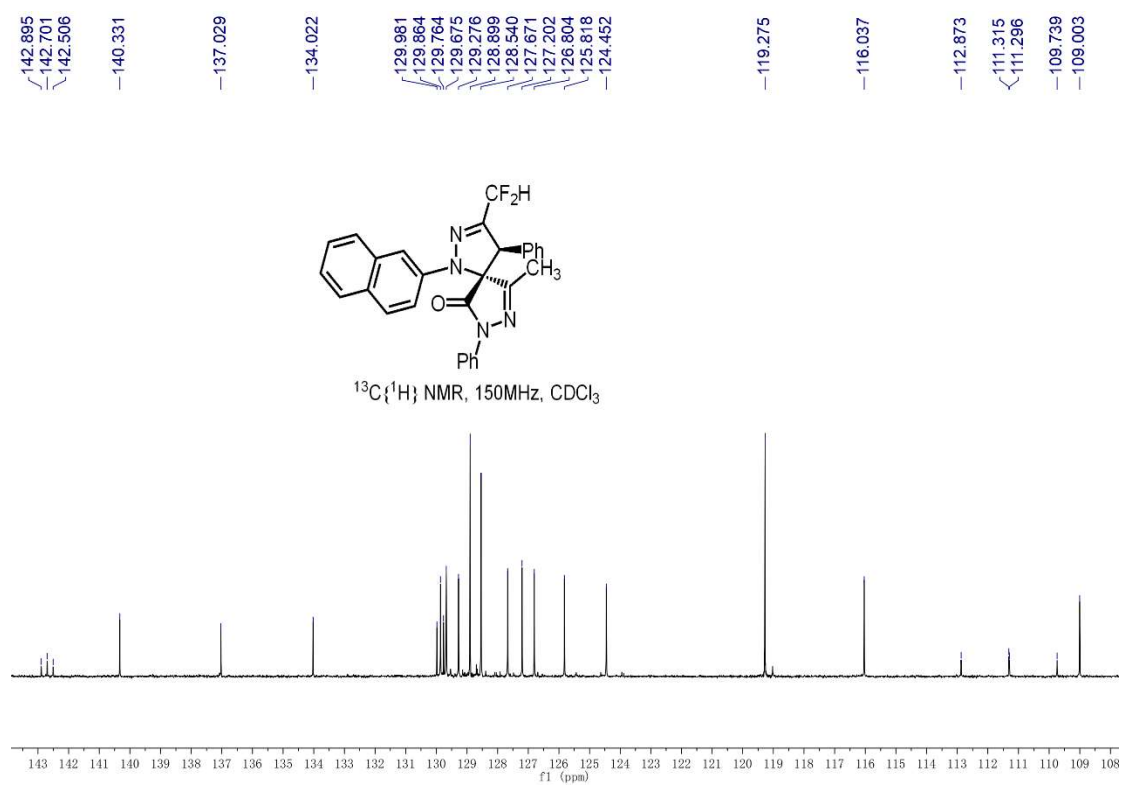
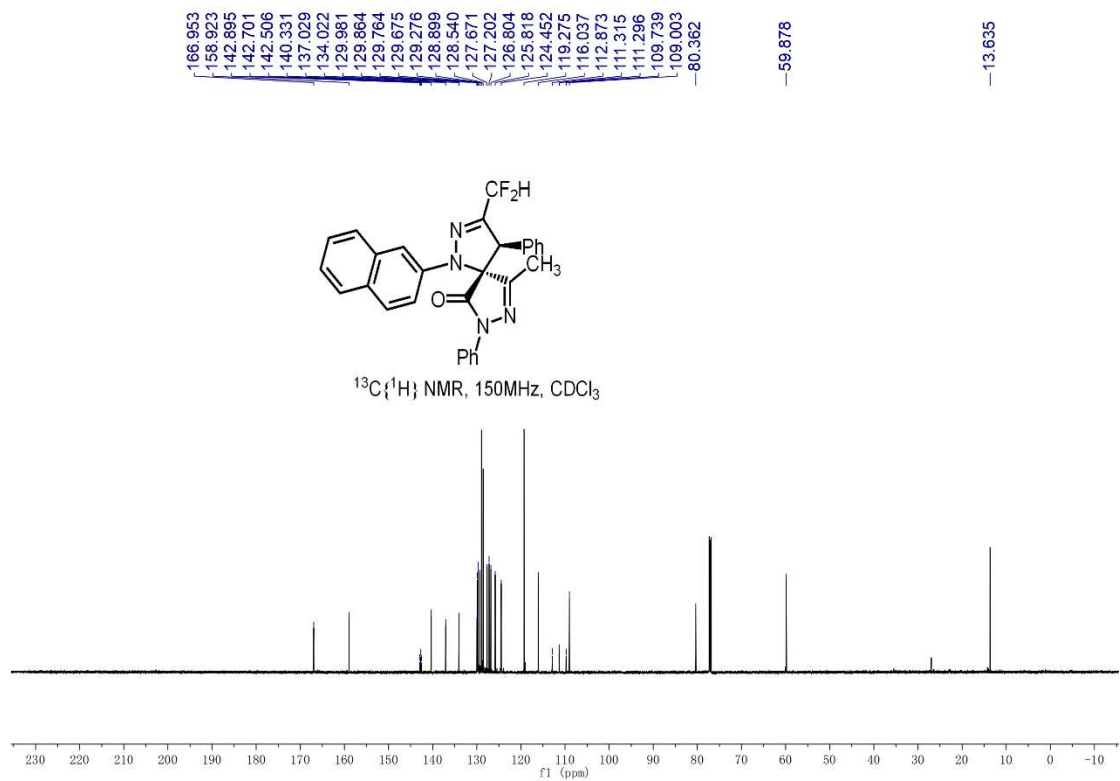
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{C}$
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



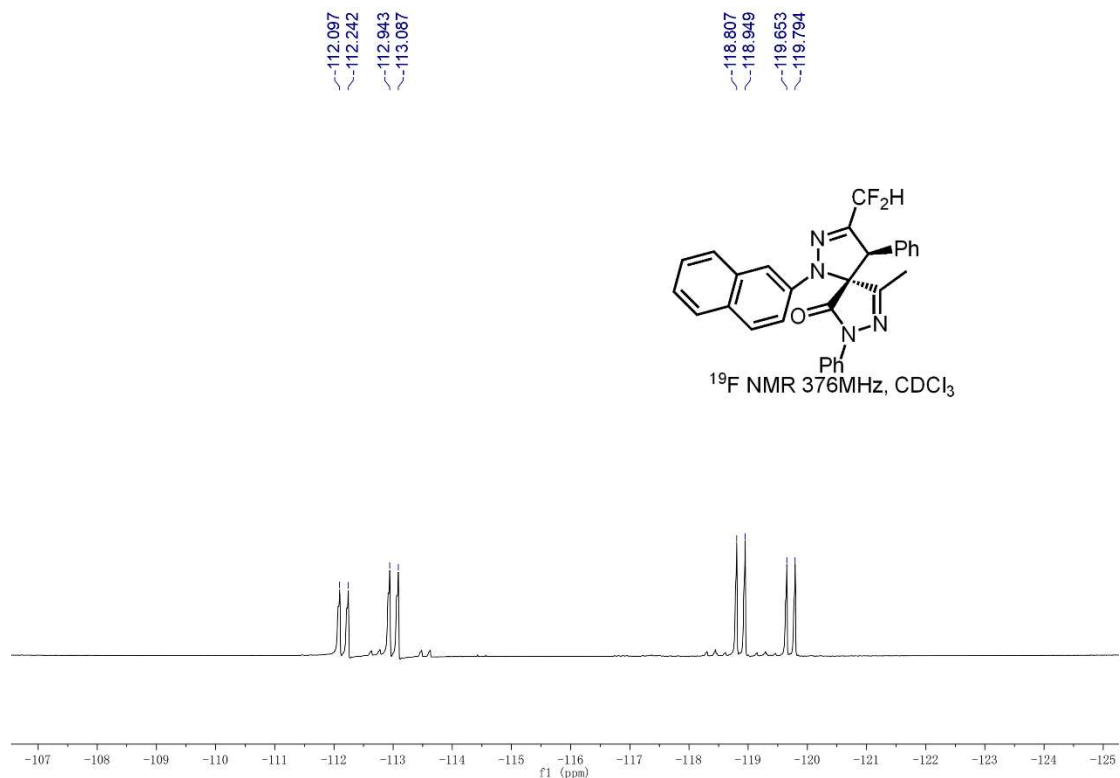
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>j</sub> Conf	mS	Std	Std	Std	Std	Std
m/z						ul		ig	l	Me	l	m/	Com
								ma		an	Va	z	Dev
										m/	rN	Diff	
										z	or	m	
503.1654	1 C <sub>29</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	503.1654	-0.1	0.1	19.5	ok	even	7.7	12.7	0.5	4.7	1.7	842.7

NMR copies of compound (*cis*)-**3m**:









HRMS (ESI) copy of compound (*cis*)-**3m**:

### Mass Spectrum SmartFormula Report

#### Analysis Info

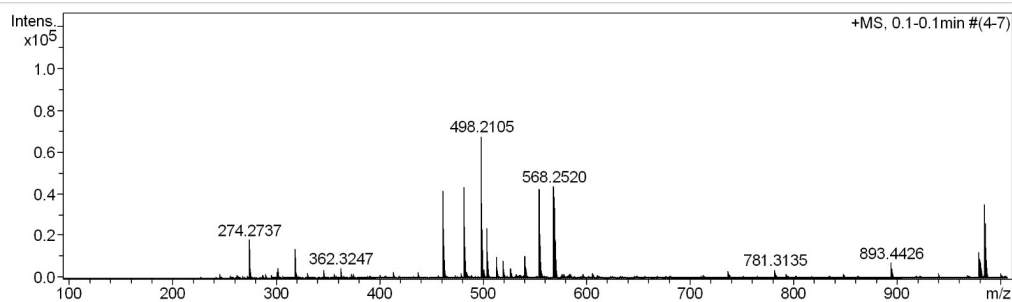
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 Method tune\_low.m  
 Sample Name A-231  
 Comment

Acquisition Date 2022-7-7 11:26:47

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

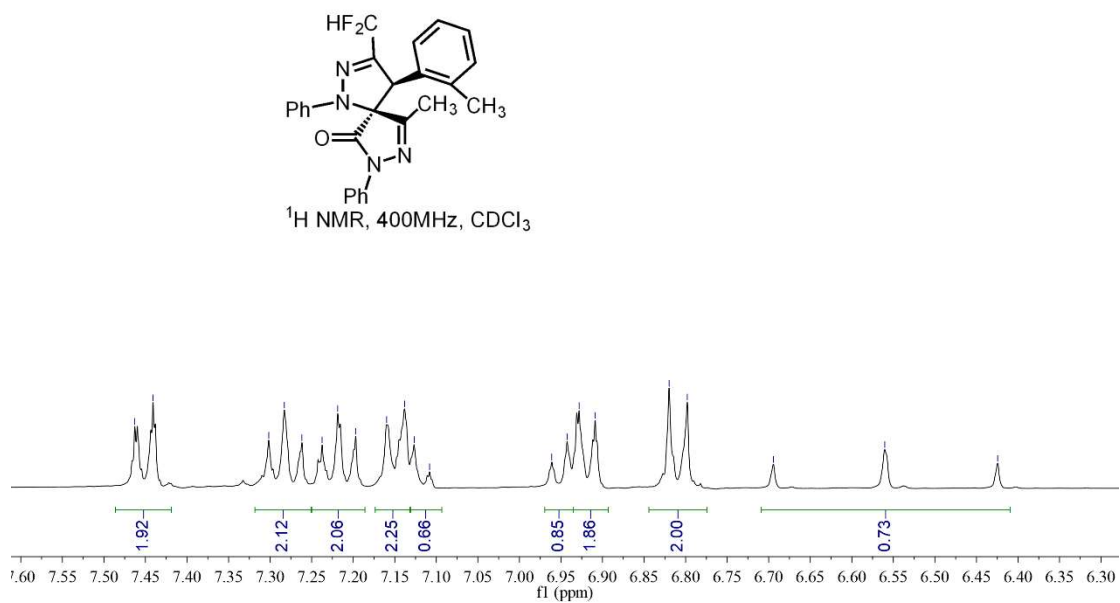
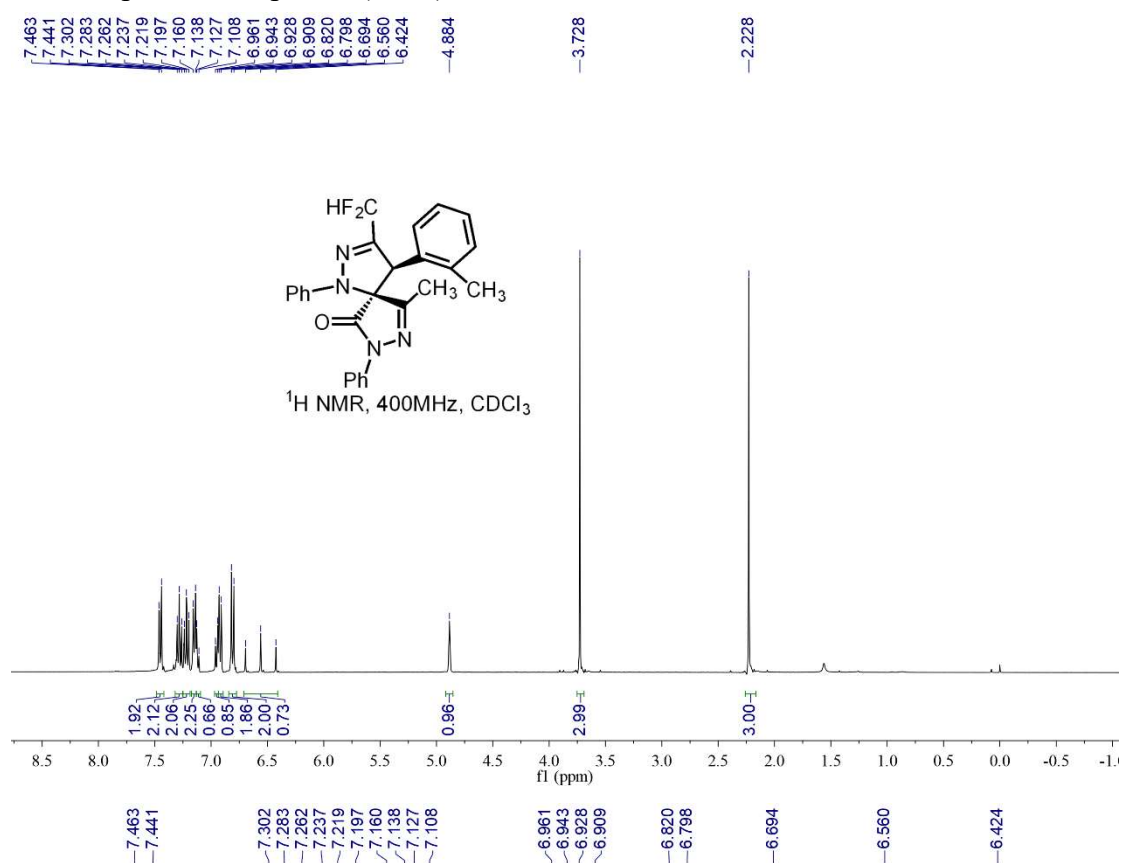
#### Acquisition Parameter

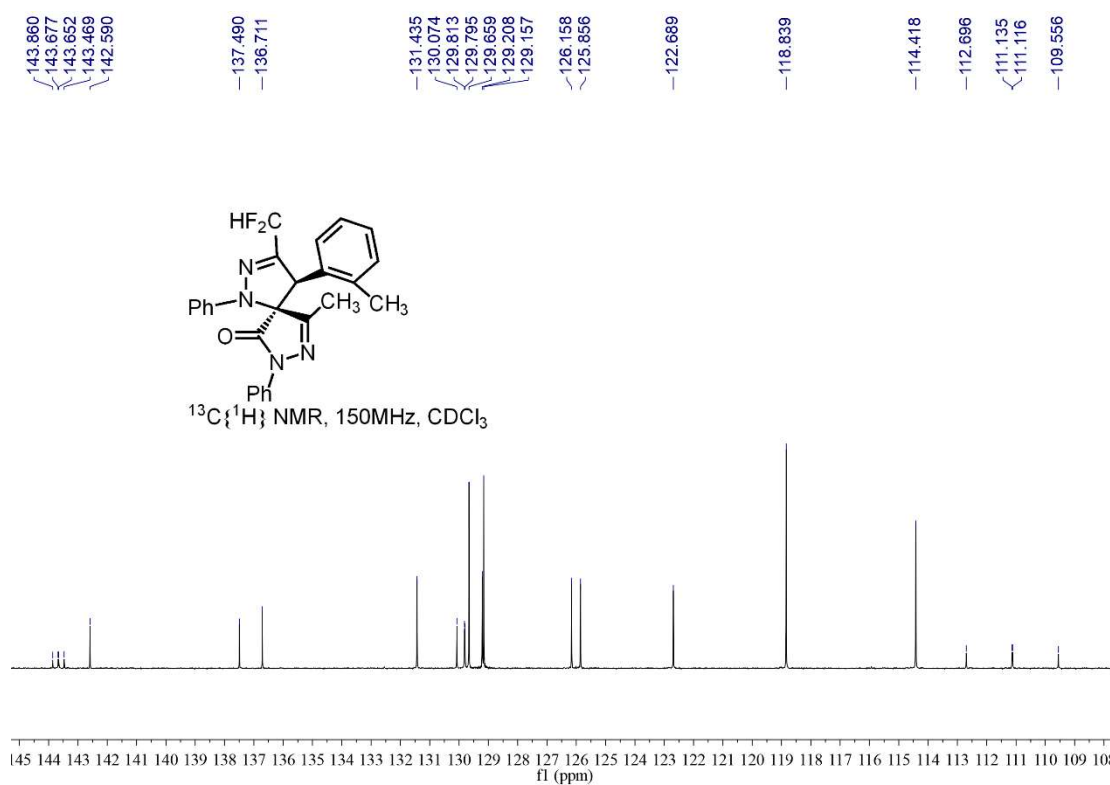
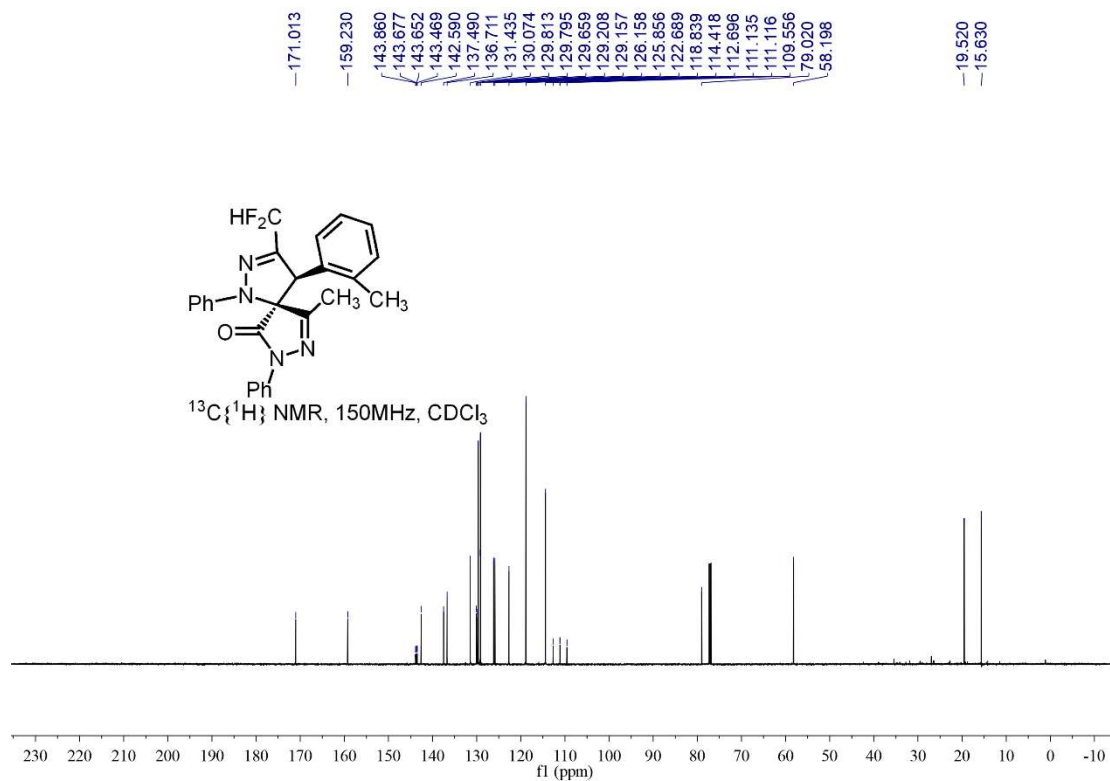
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

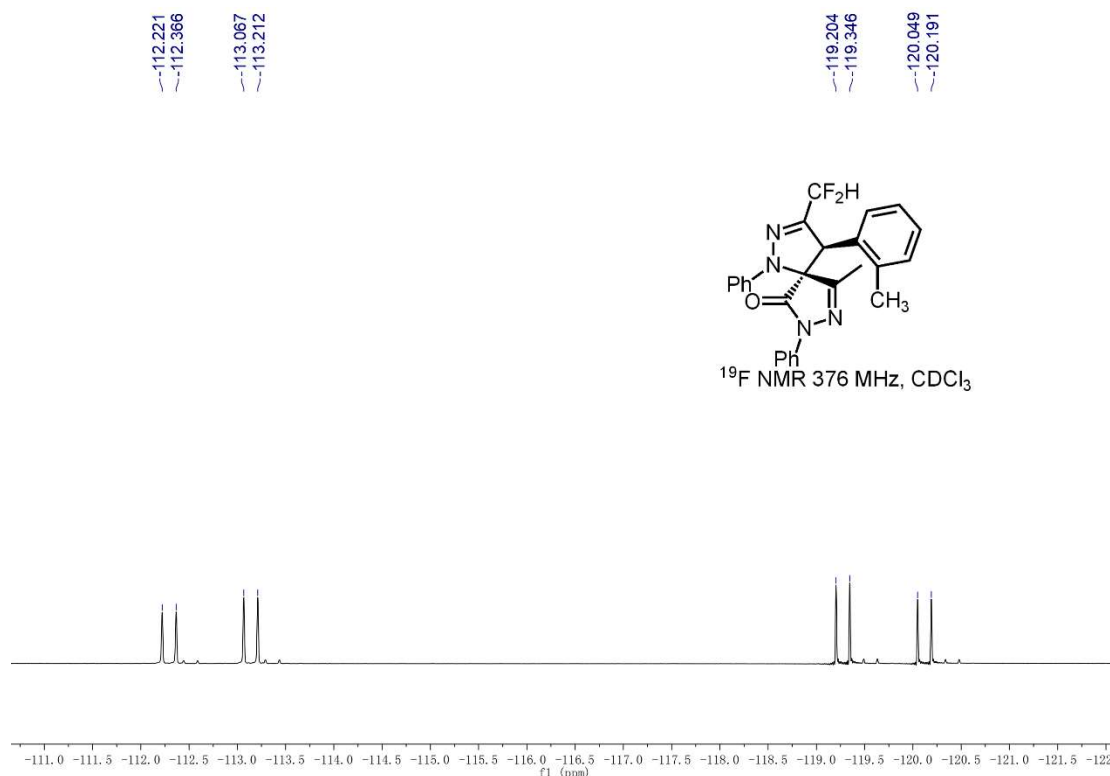


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej% Conf	mSi gma	Std l	Std Me an z	Std l Va rN or m	Std m/ rN Diff	Std z	Std Com b Dev
481.1835	1 C <sub>29</sub> H <sub>23</sub> F <sub>2</sub> N <sub>4</sub> O	481.1834	-0.0	0.8	19.5	ok	even	10.0	18.0	1.0	7.3	2.6	842.7	

NMR copies of compound (*trans*)-4a:







HRMS (ESI) copy of compound (*trans*)-4a:

### Mass Spectrum SmartFormula Report

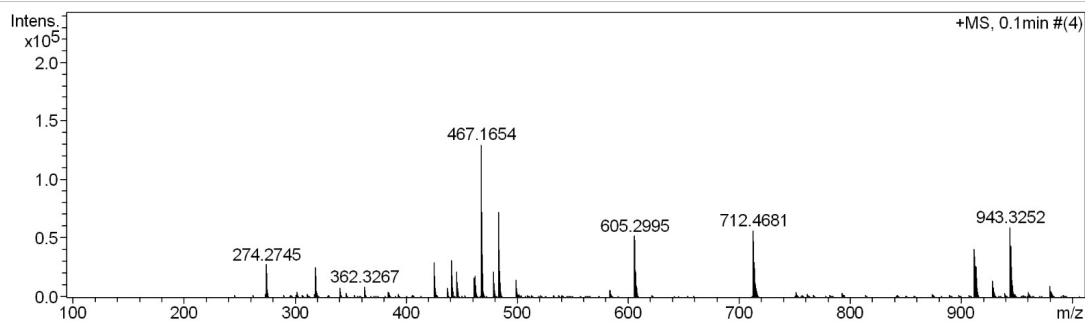
#### Analysis Info

Analysis Name D:\Data\user\NWN-ufengyang 20220707-11.d  
 Method tune\_low.m  
 Sample Name A-30  
 Comment

Acquisition Date 2022-7-7 11:37:22  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

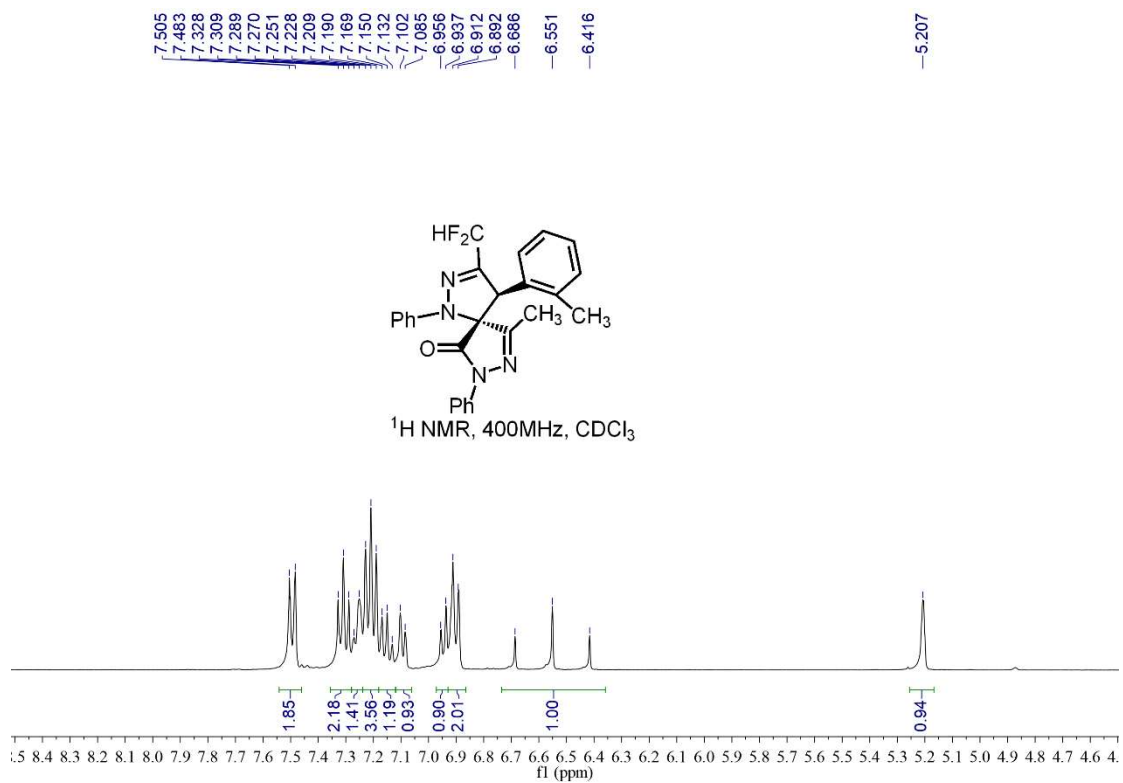
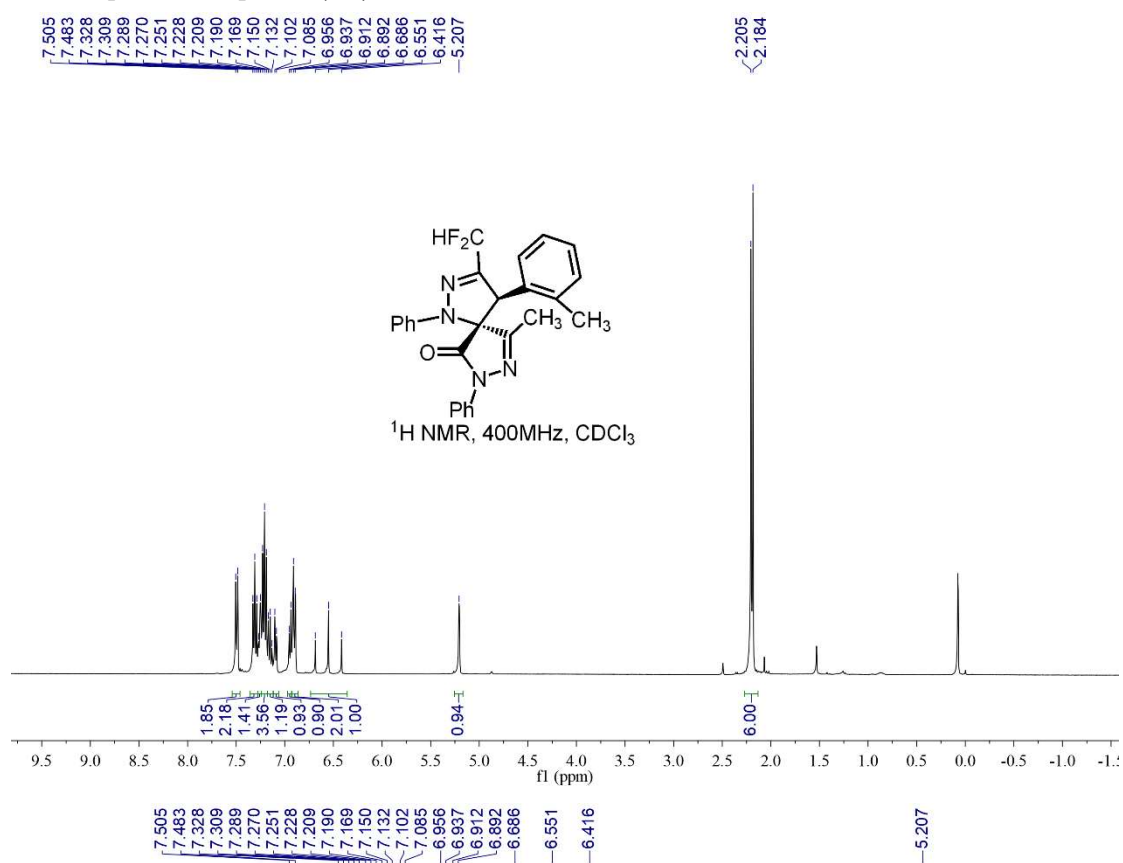
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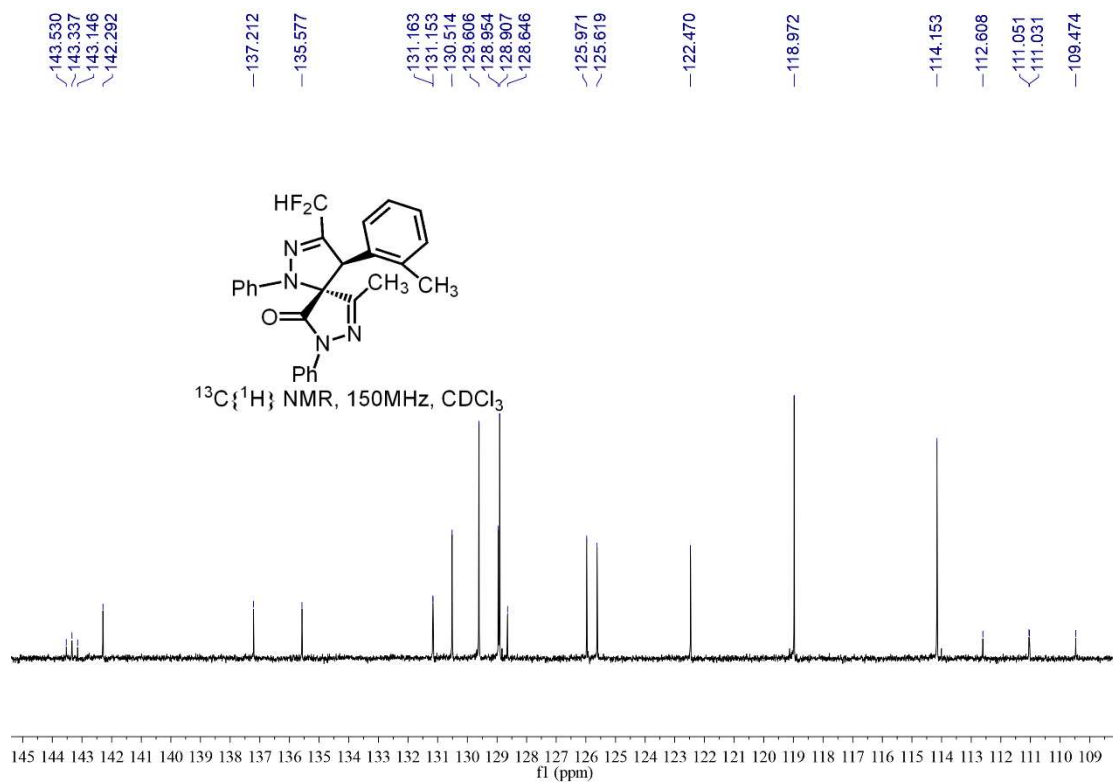
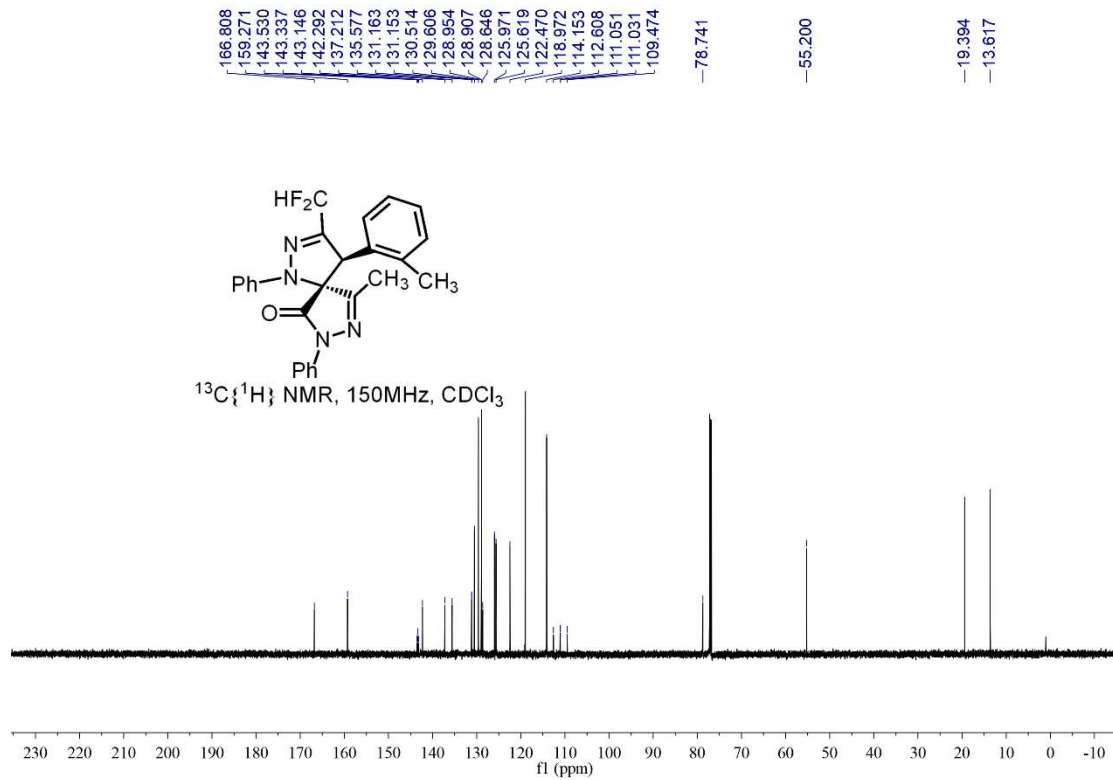
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

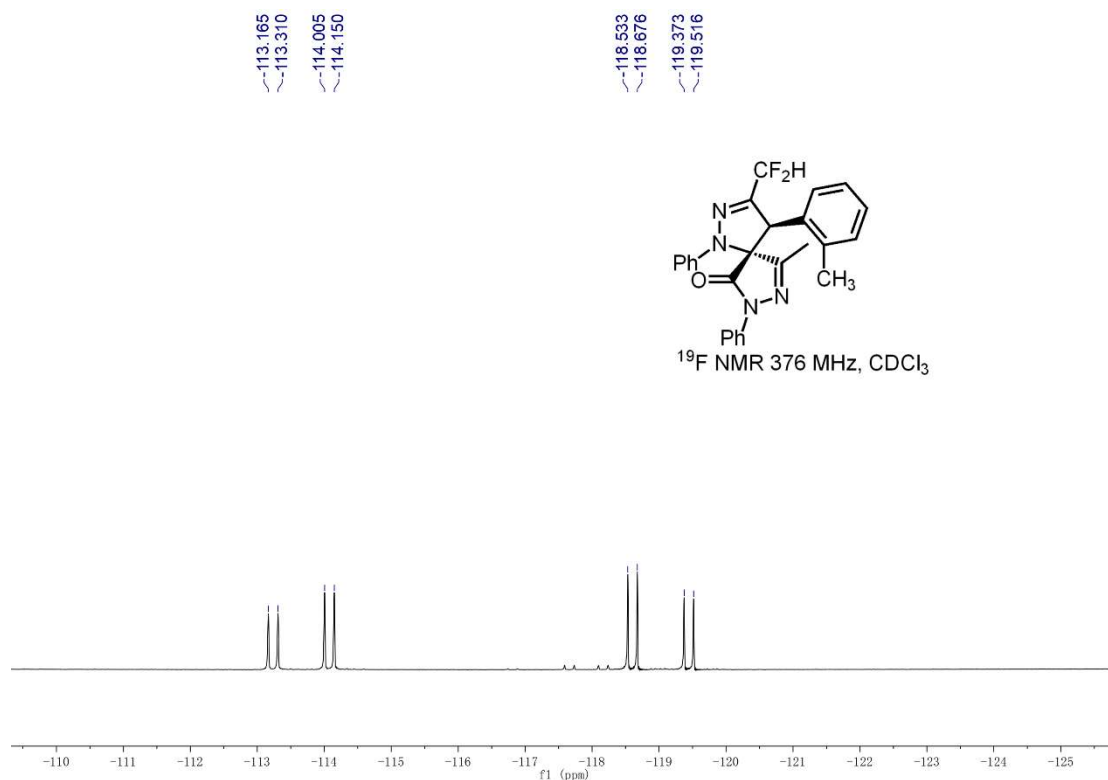


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j ≠ Conf	m Sigma	Std l	St d l	St d l	St d l	Std Com b Dev
467.1654	1 C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	-0.1	-0.3	16.5	ok	even	8.5	12.4	0.3	5.3	0.6	842.7

NMR copies of compound (*cis*)-4a:







HRMS (ESI) copy of compound (*cis*)-4a:

### Mass Spectrum SmartFormula Report

#### Analysis Info

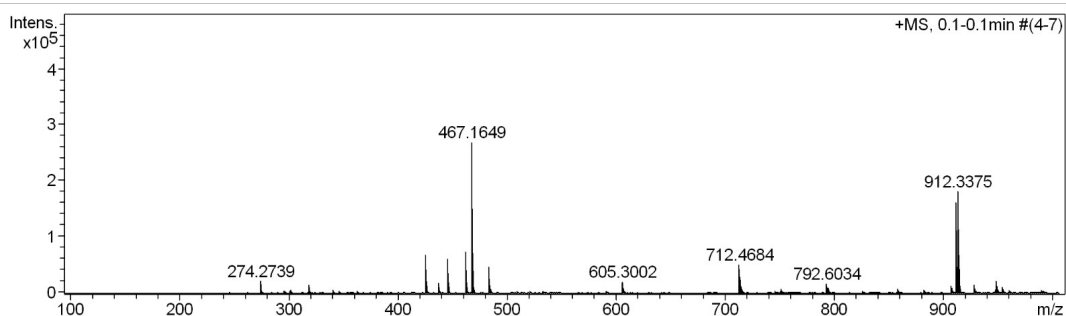
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 Method tune\_low.m  
 Sample Name A-301  
 Comment

Acquisition Date 2022-7-7 11:39:22

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

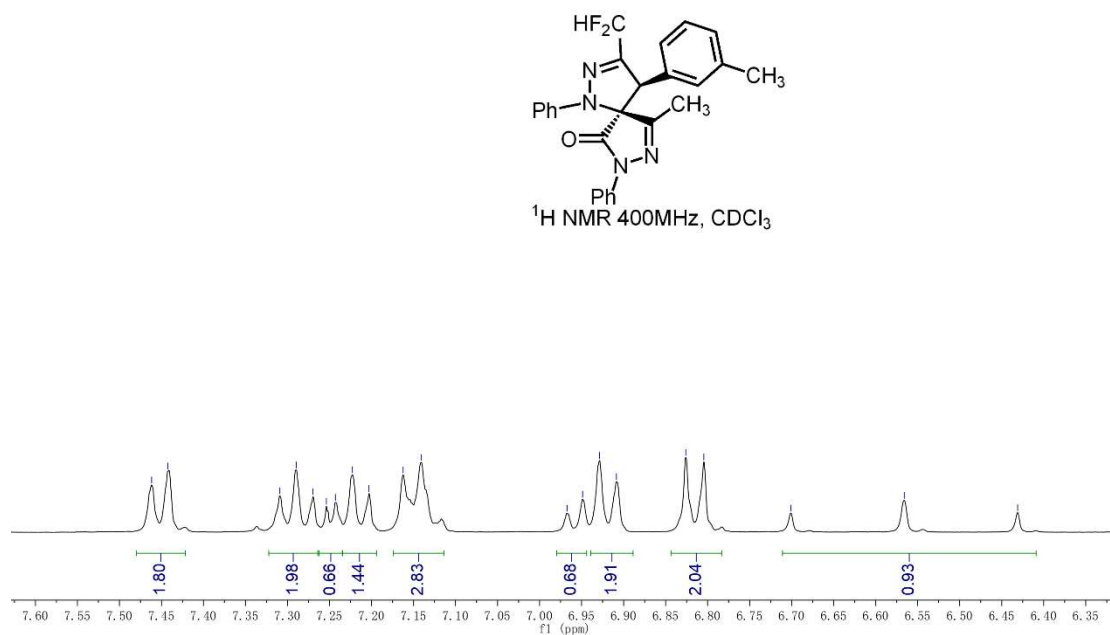
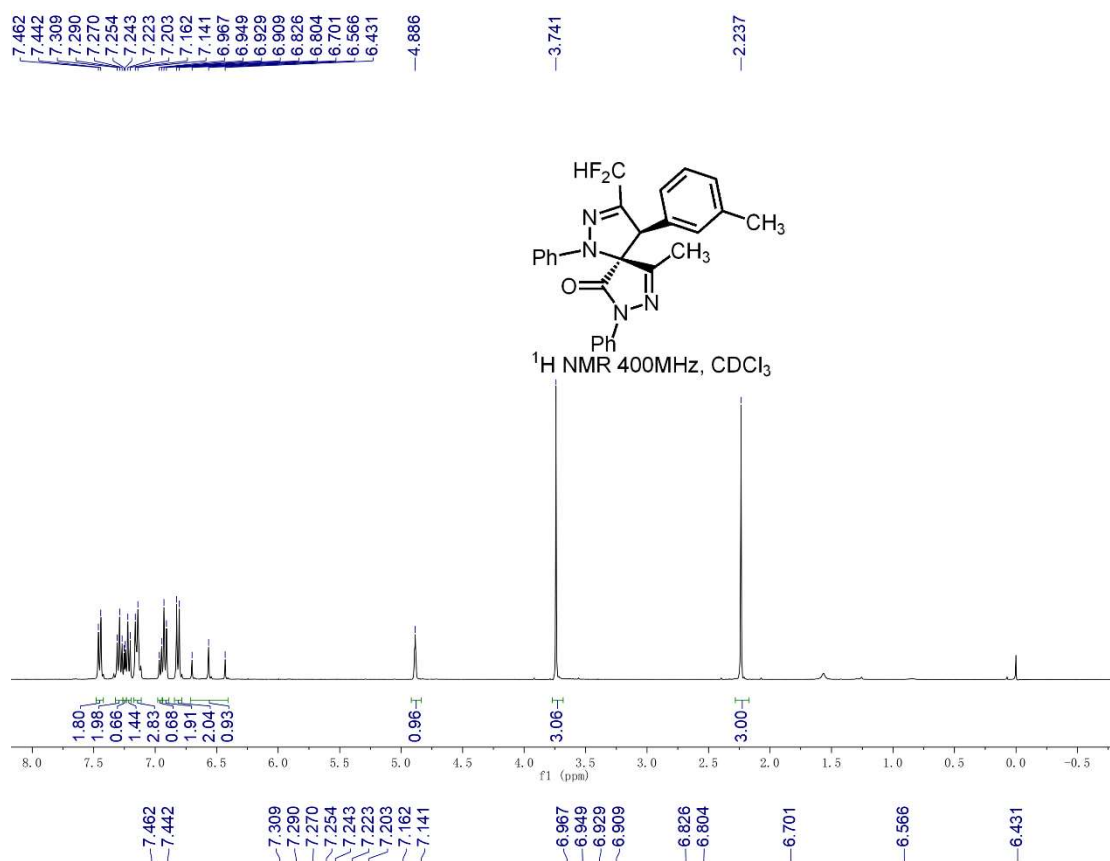
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

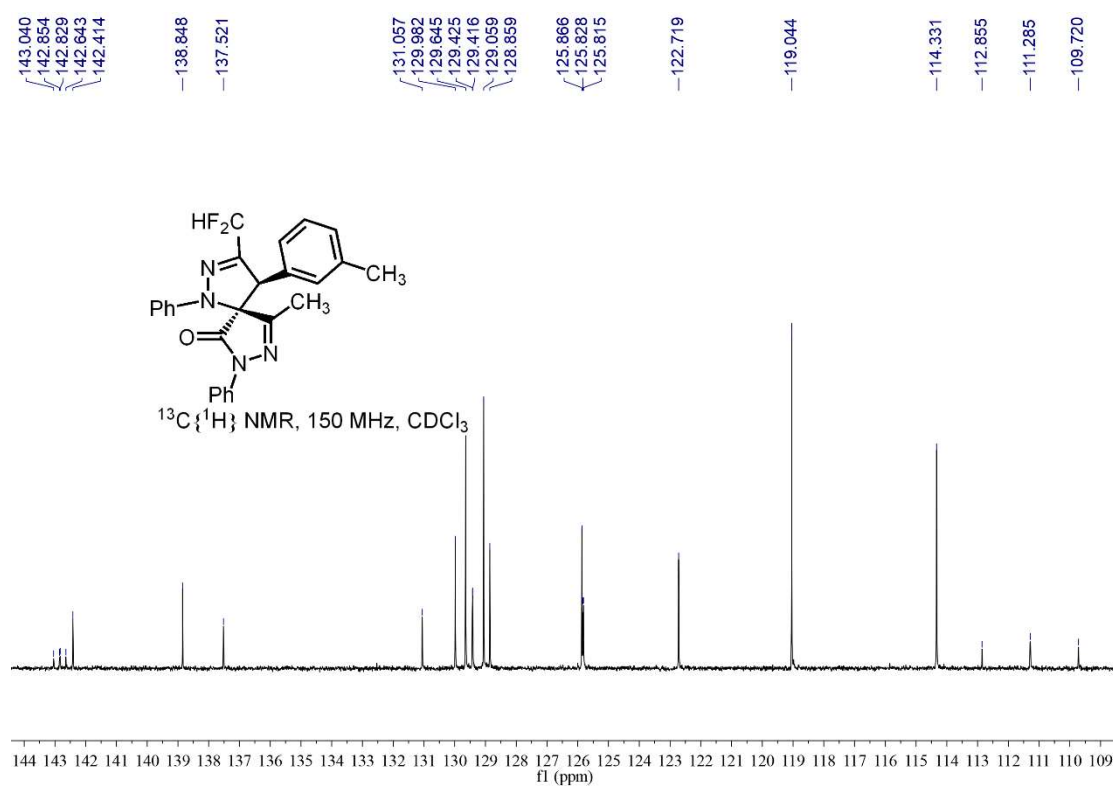
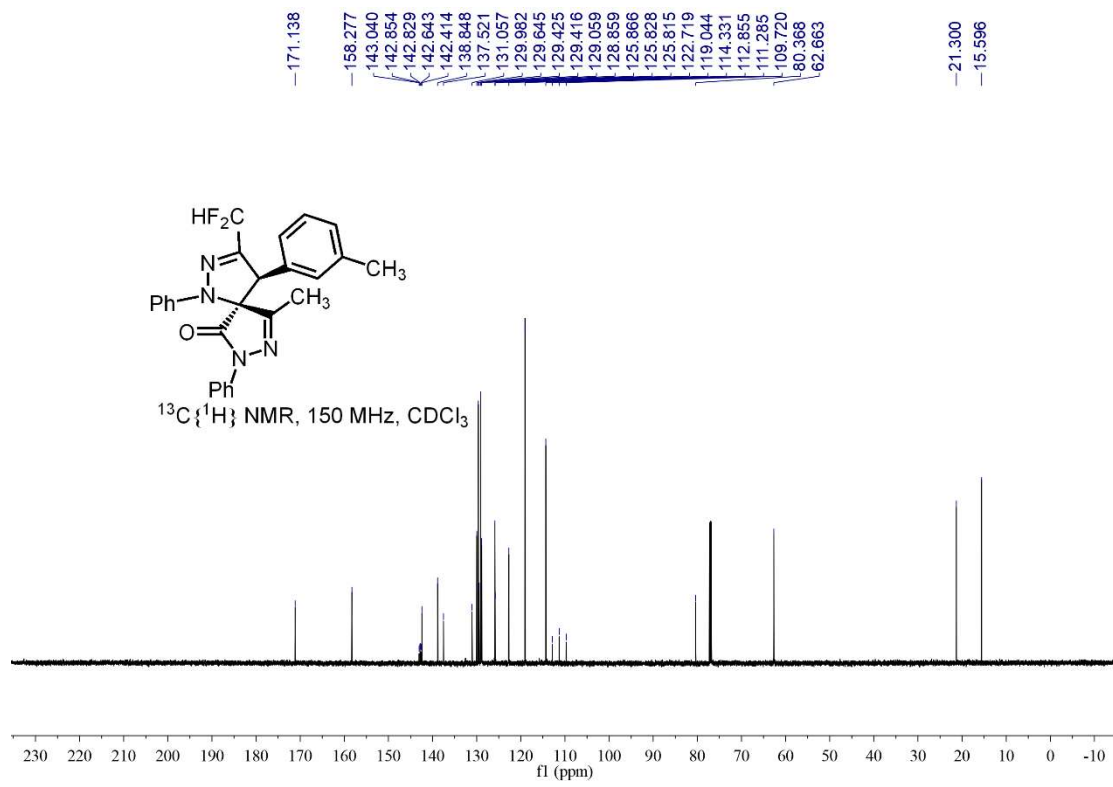


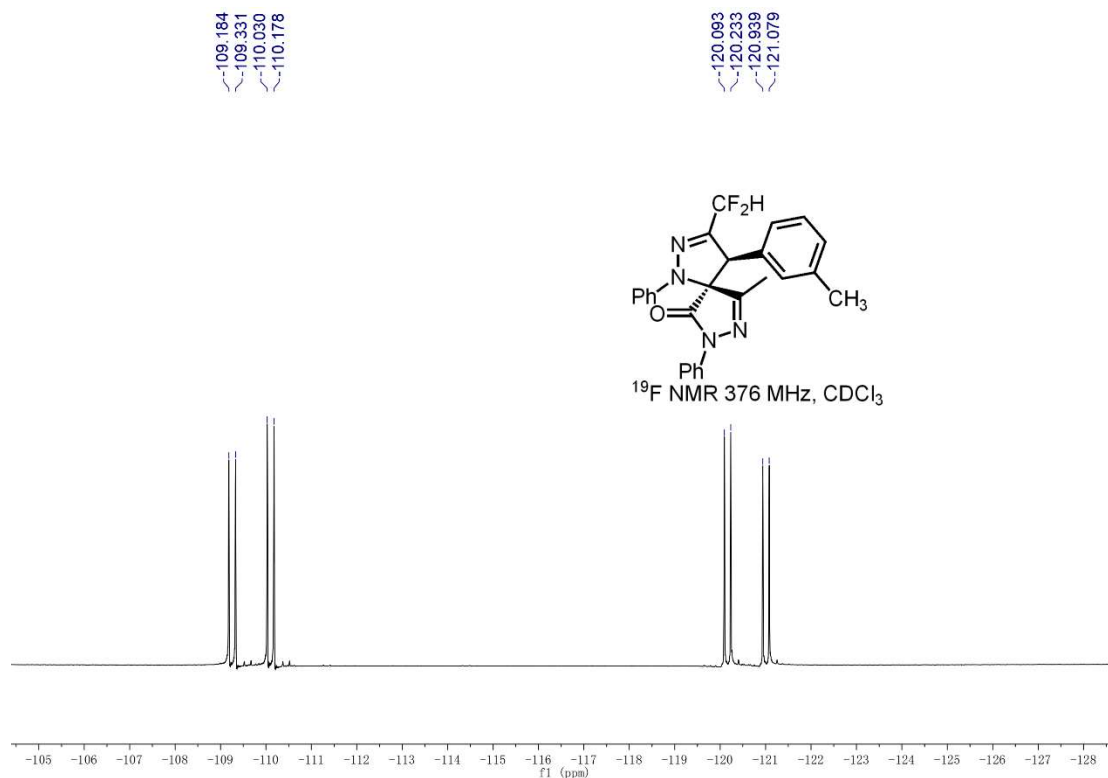
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R Conf	ej% Conf	mSi gma	Std l	St d Me an m/z	Std l Var Nor m	St d m/z Dif f	Std Com b Dev
467.1649	1 C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	0.9	0.3	16.5	ok	even	16.4	24.7	0.6	10.5	1.3	842.7

NMR copies of compound (*trans*)-4b:









HRMS (ESI) copy of compound (*trans*)-4b:

### Mass Spectrum SmartFormula Report

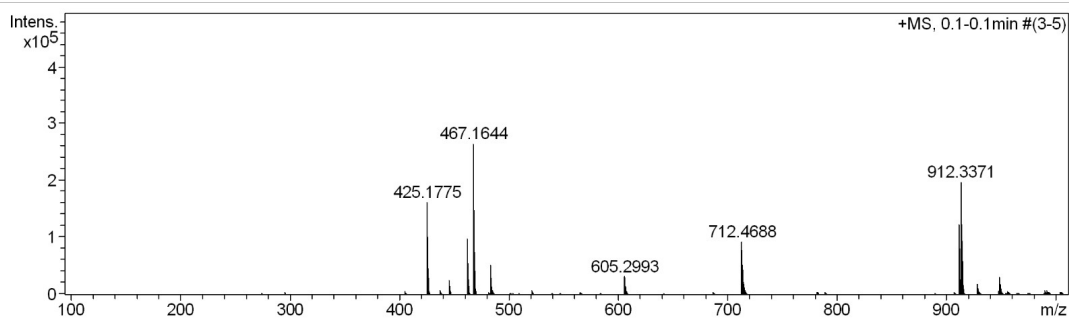
#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20220707-9.d  
 Method tune\_low.m  
 Sample Name A-29  
 Comment

Acquisition Date 2022-7-7 11:35:20  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

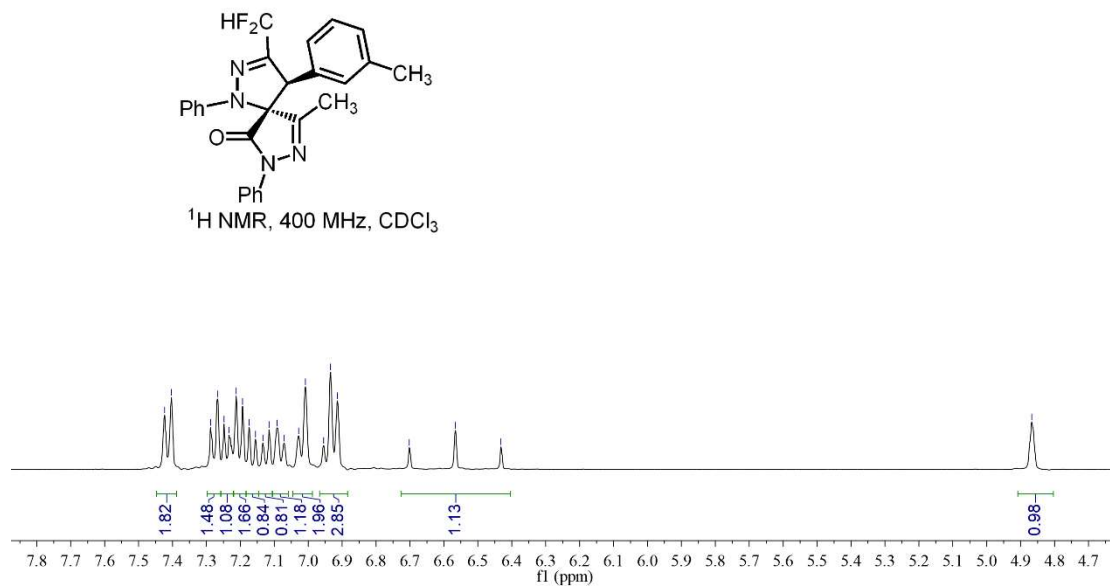
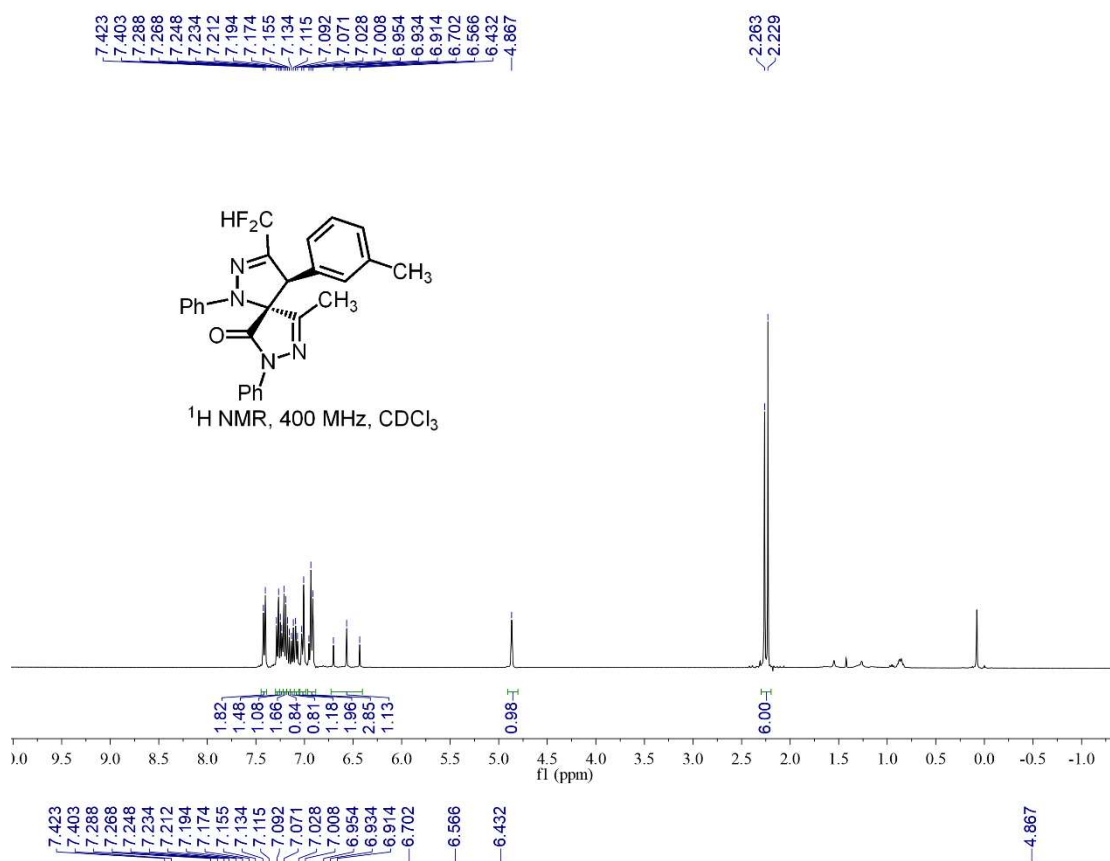
#### Acquisition Parameter

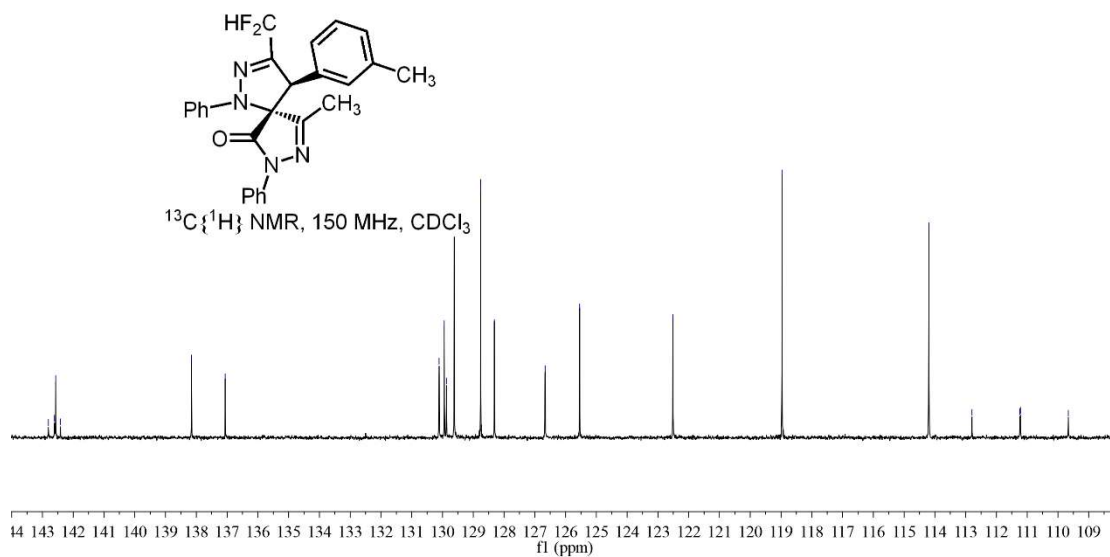
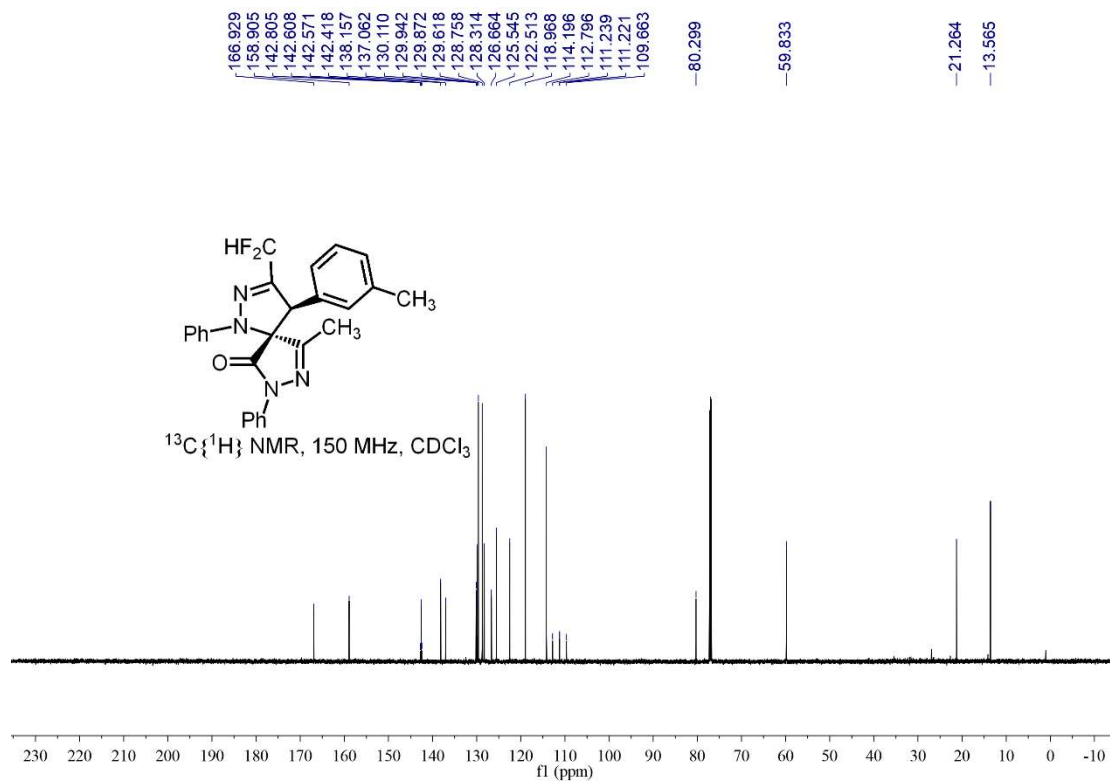
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{C}$
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

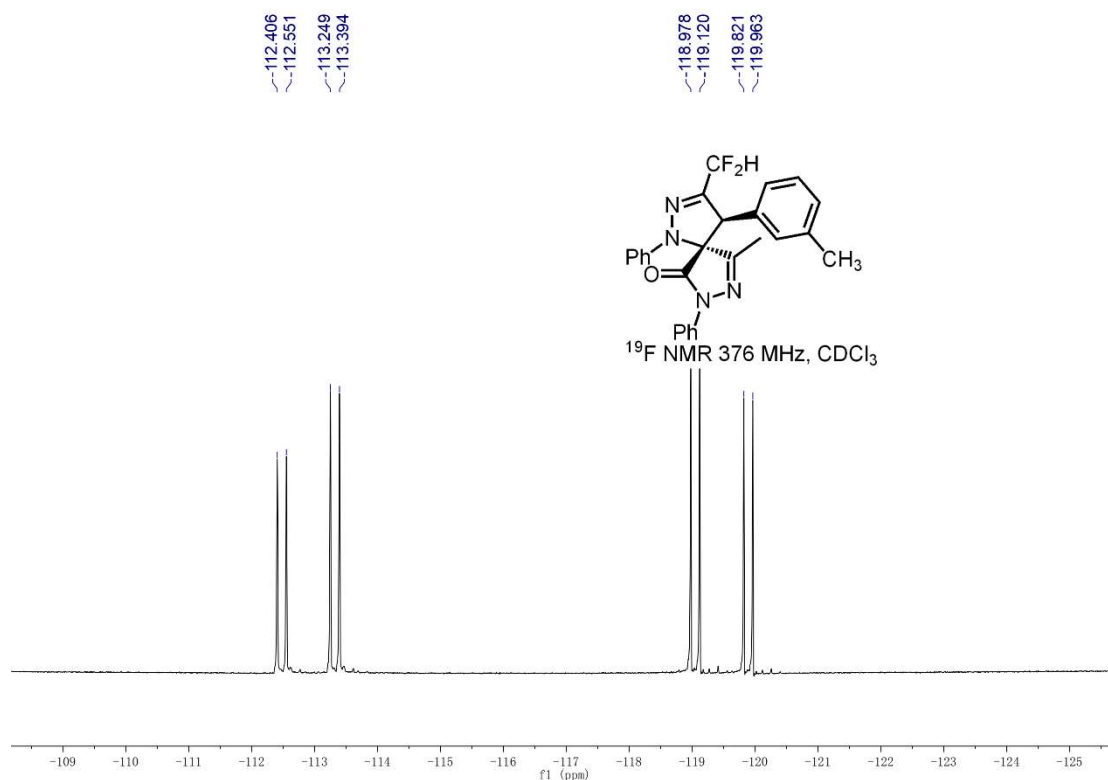


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j %	Conf	mS	ig	ma	Std l	Std Me an m/z	Std l Va rN or m	Std m/z Diff	Std Com b Dev
467.1644	1 C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	2.1	1.2	16.5	ok	even	8.2	11.9	1.0	5.1	1.9	842.7			

NMR copies of compound (*cis*)-**4b**:







HRMS (ESI) copy of compound (*cis*)-4b:

### Mass Spectrum SmartFormula Report

#### Analysis Info

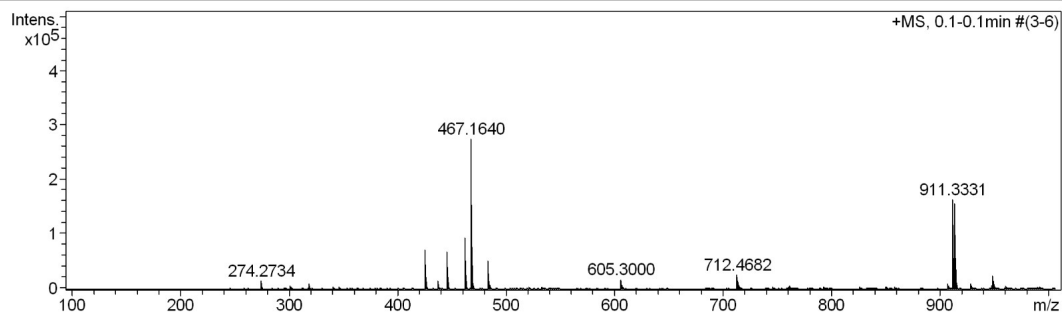
Analysis Name D:\Data\user\NWNWU-fengyang 20220707-10.d  
 Method tune\_low.m  
 Sample Name A-291  
 Comment

Acquisition Date 2022-7-7 11:36:24

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

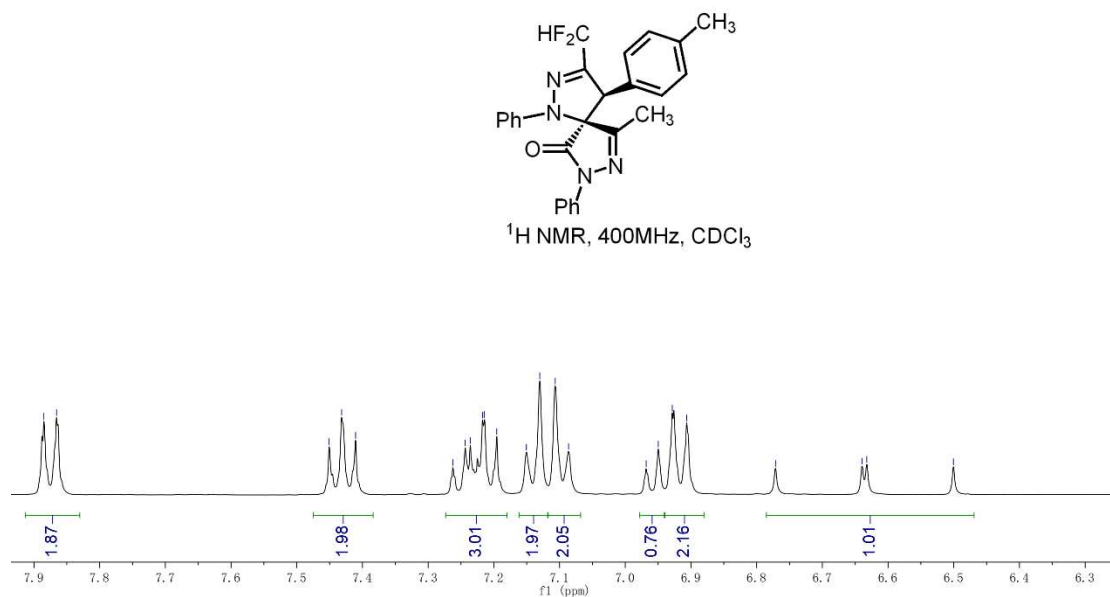
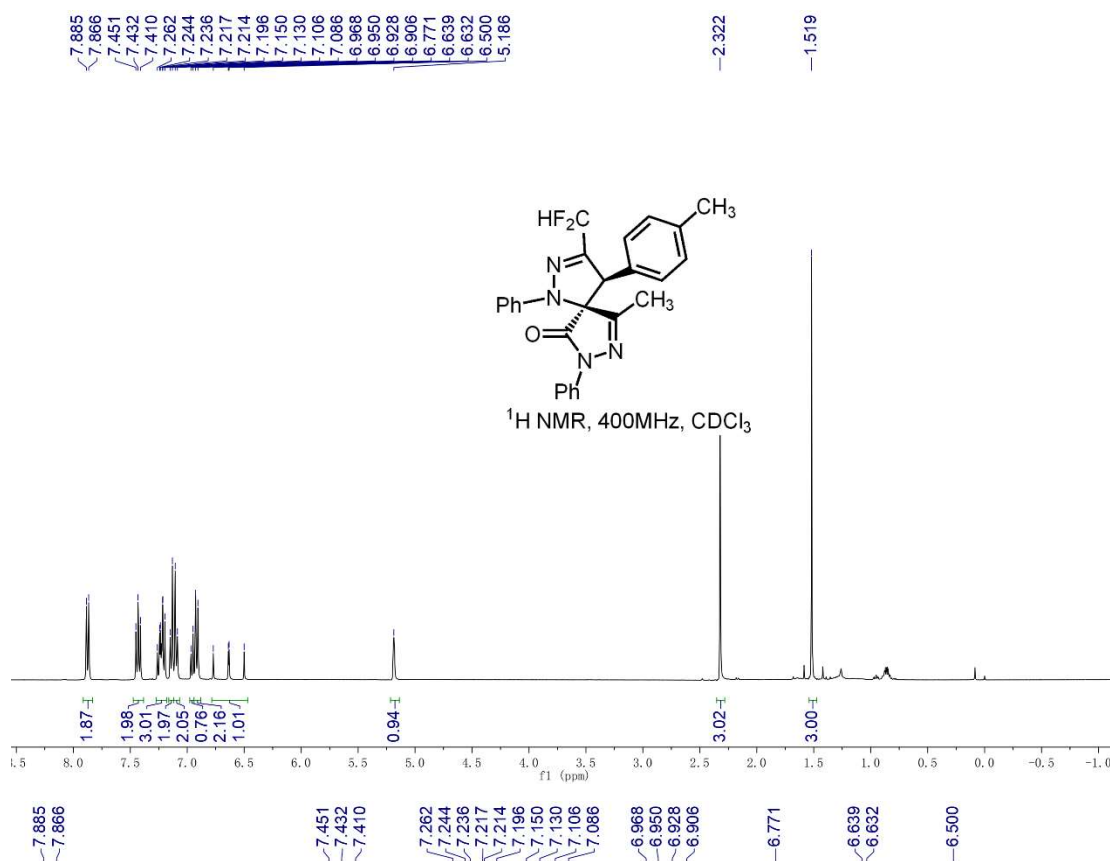
#### Acquisition Parameter

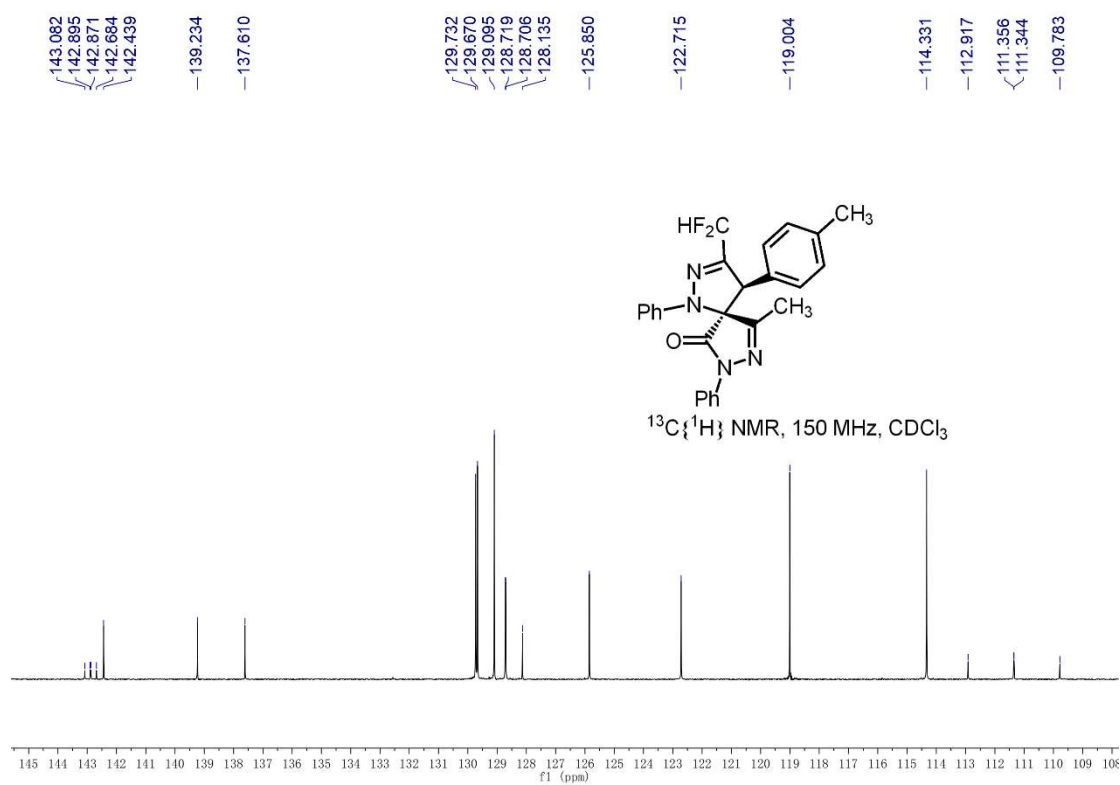
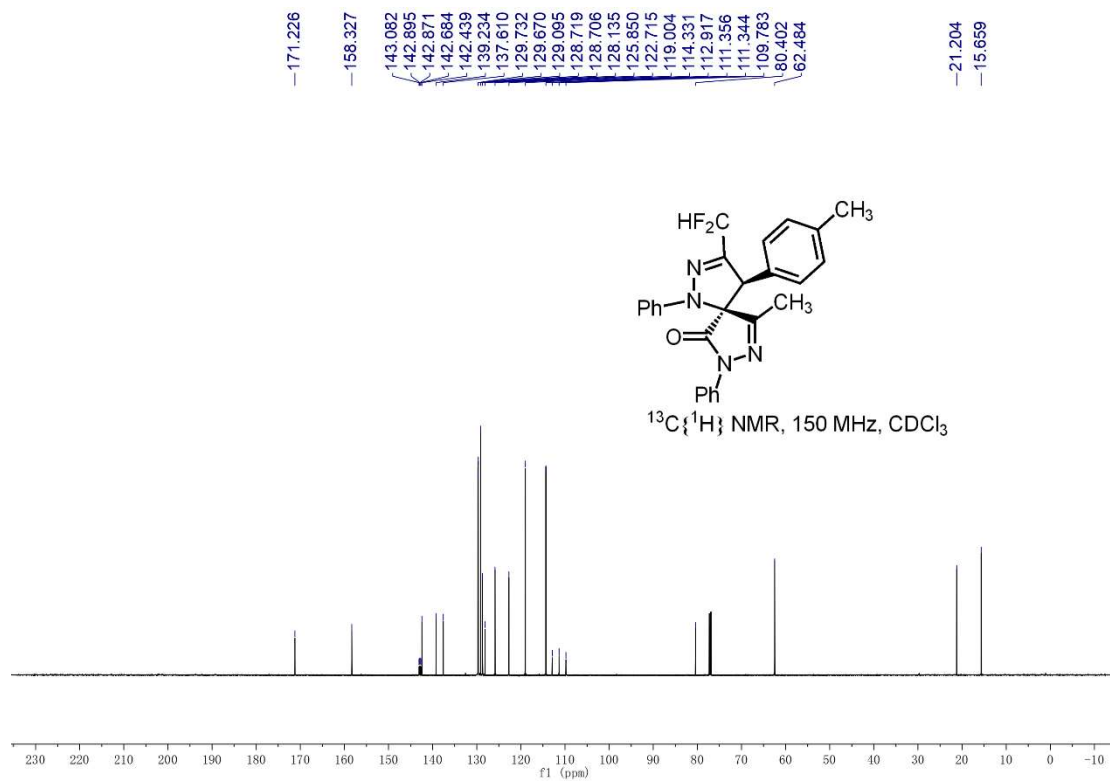
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

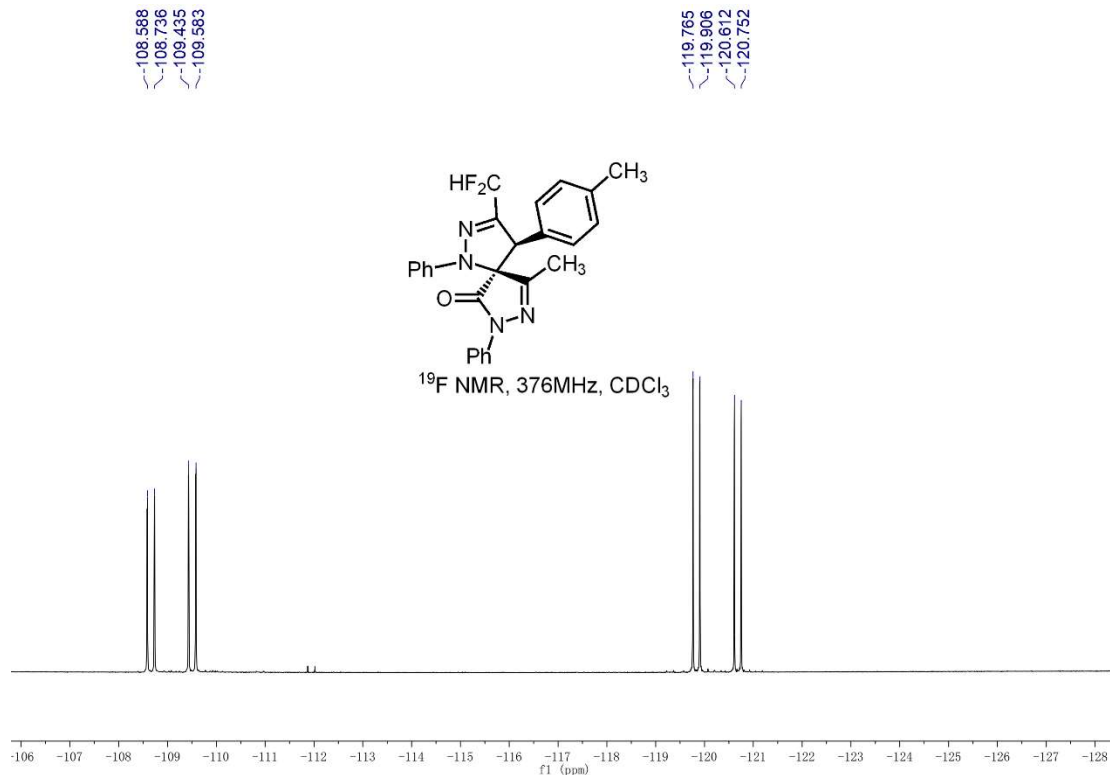


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdB	N-R	ej% Conf	mSi gma	Std l	St d	St d l	St d	Std Com b
m/z						ul	e			Me an z	Val or m	m/ Dif f	Dev
467.1640	1 C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	2.9	2.2	16.5	ok	even	10.7	15.8	1.2	6.7	1.6	842.7

NMR copies of compound (*trans*)-4c:







HRMS (ESI) copy of compound (*trans*)-4c:

### Mass Spectrum SmartFormula Report

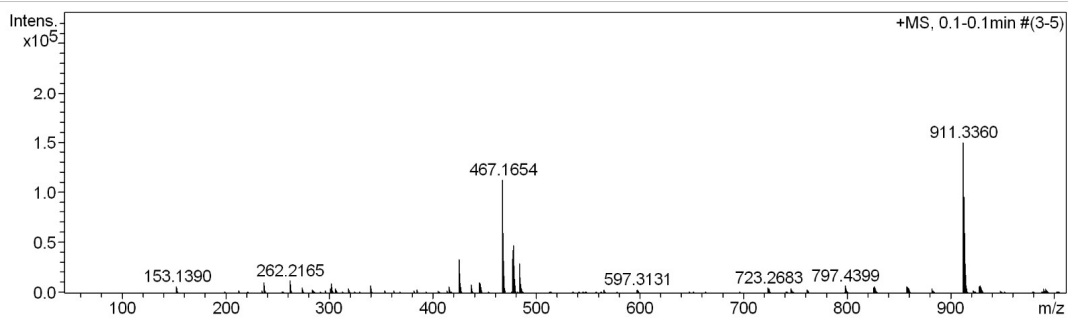
**Analysis Info**

Analysis Name D:\Data\user\NWN\U-fengyang 20230321-4.d  
 Method tune\_low.m  
 Sample Name A-28  
 Comment

Acquisition Date 2023-3-21 15:35:55  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

**Acquisition Parameter**

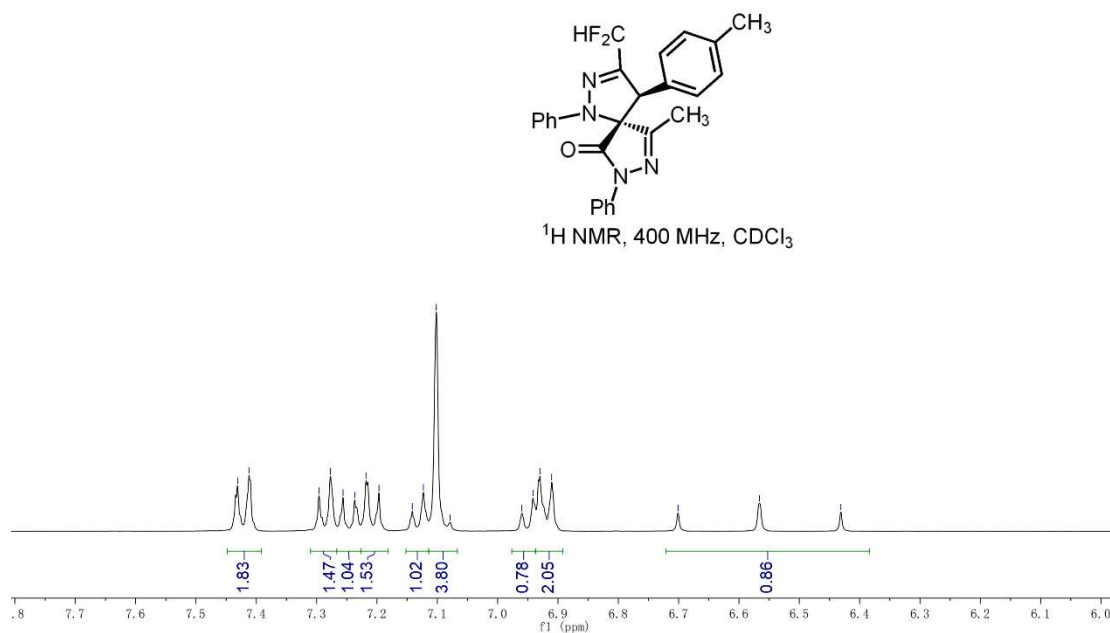
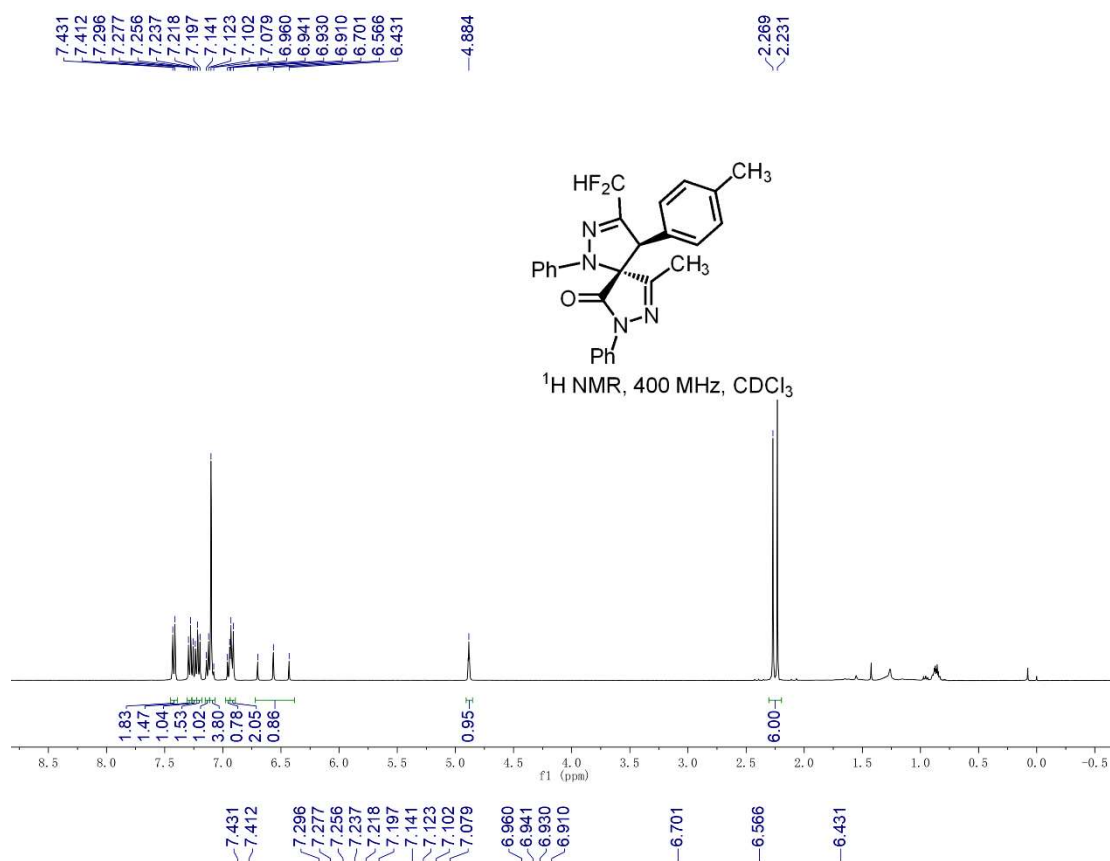
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

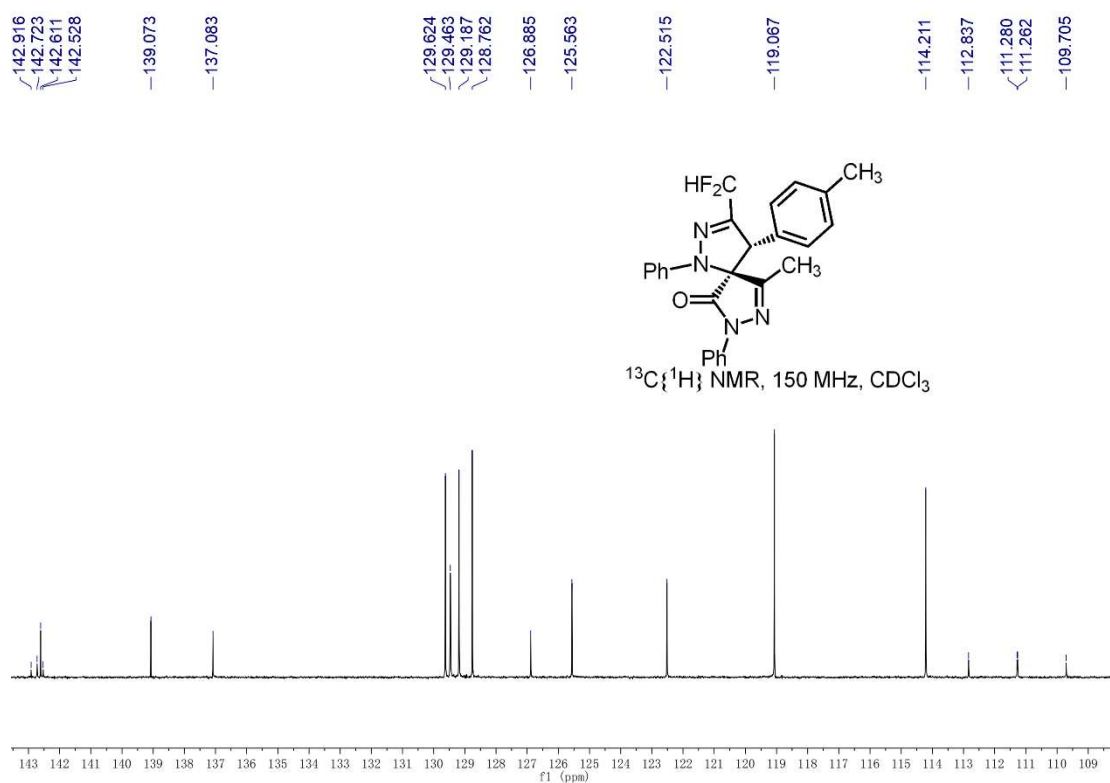
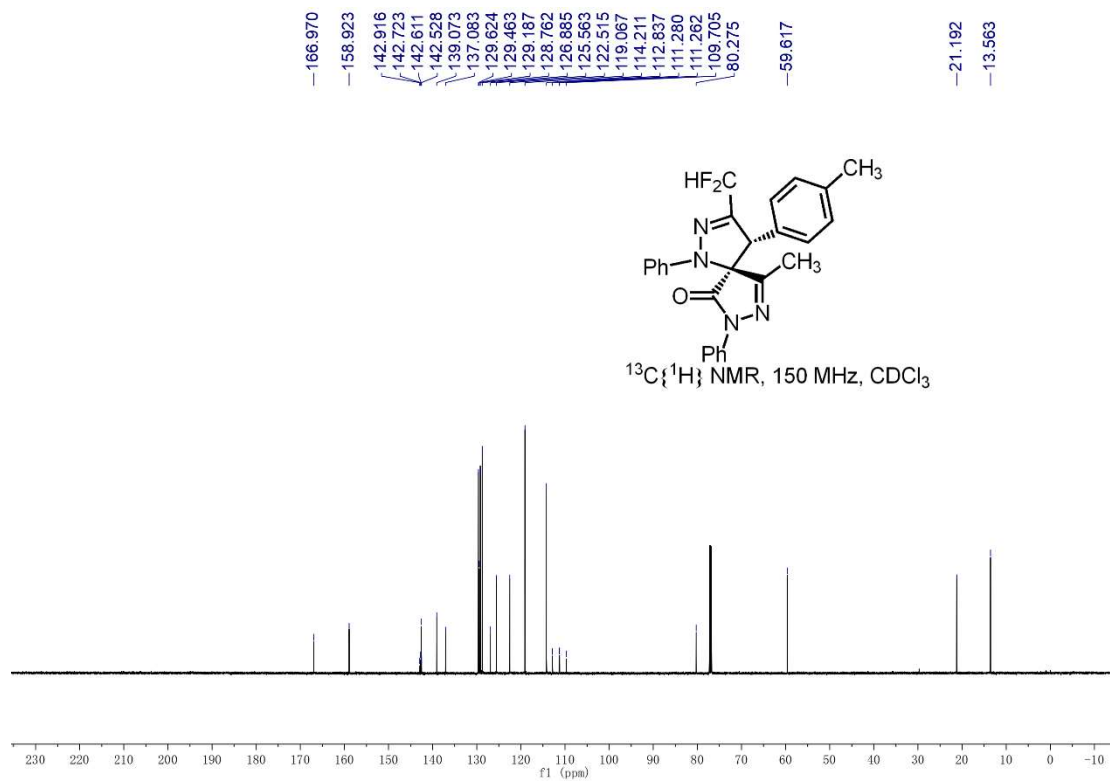


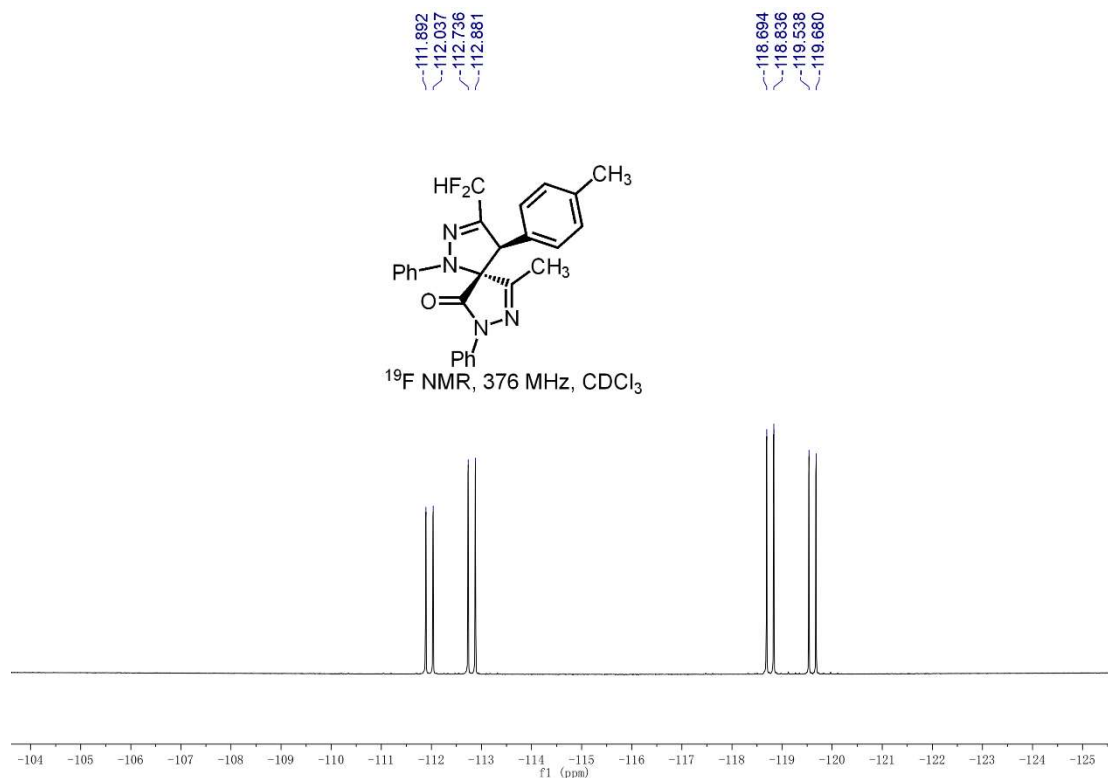
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej% Conf	mS	Std	Std	Std	Std	Std	
m/z									l	Me	l	m/	Com	
										an	Val	z	Dev	
										m/	rN	Diff		
										z	or			
										m				
467.1654	1	C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	0.0	0.0	16.5	ok	even	4.9	6.2	0.1	3.9	0.1	842.7



NMR copies of compound (*cis*)-4c:







HRMS (ESI) copy of compound (*cis*)-4c:

### Mass Spectrum SmartFormula Report

**Analysis Info**

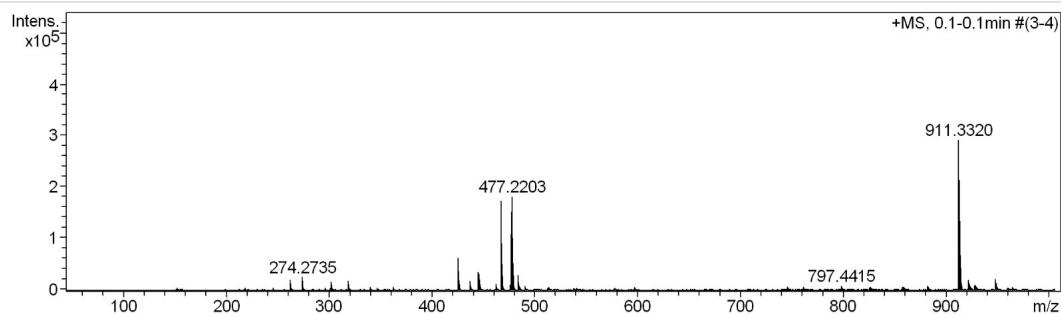
Analysis Name D:\Data\user\NWNWU-fengyang 20230321-5.d  
 Method tune\_low.m  
 Sample Name A-281  
 Comment

Acquisition Date 2023-3-21 15:37:20

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

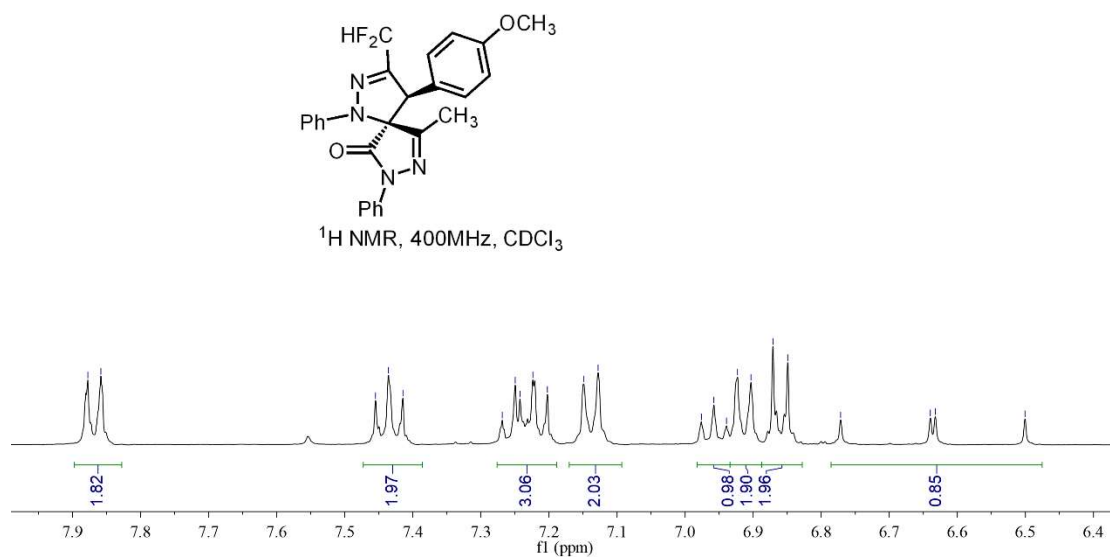
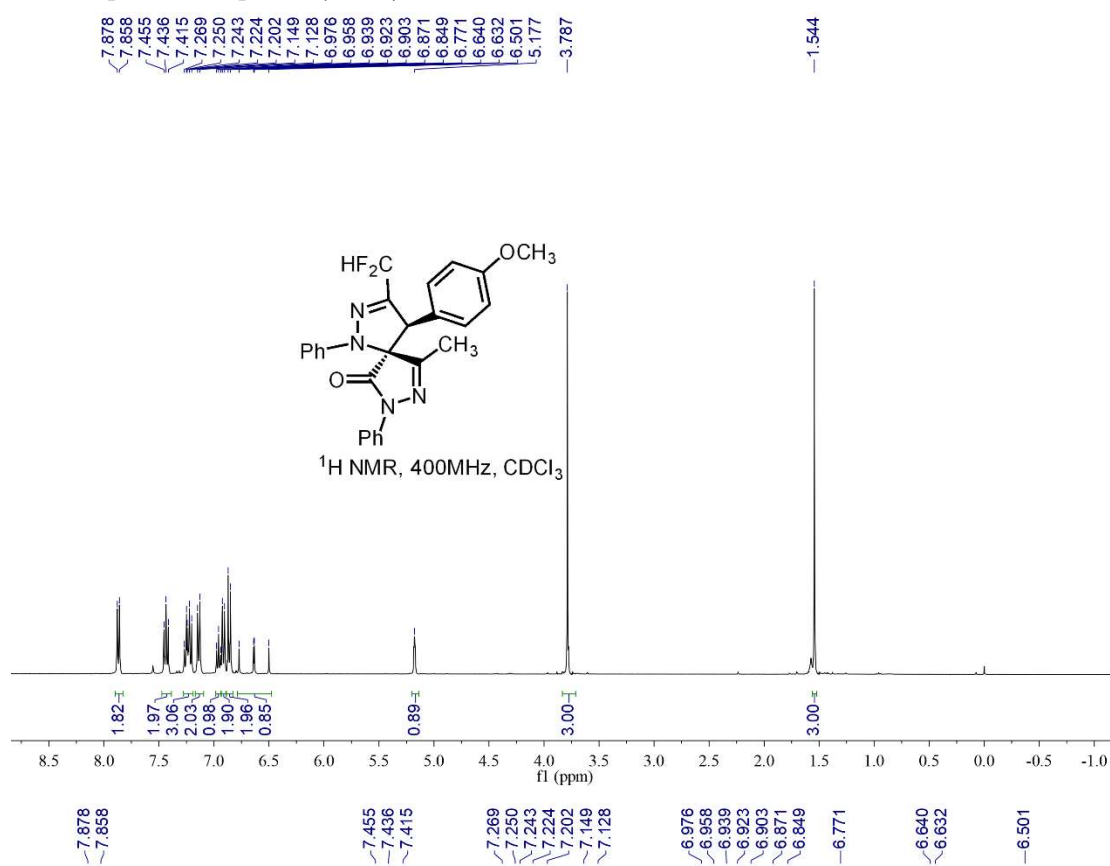
**Acquisition Parameter**

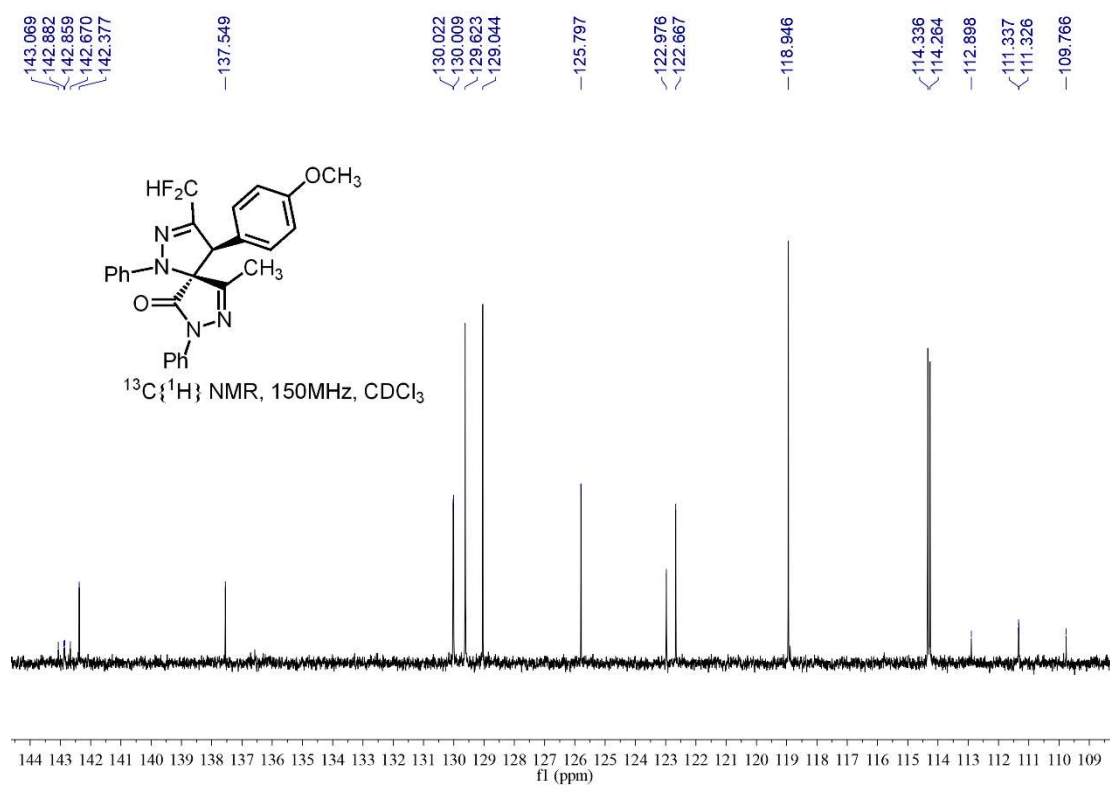
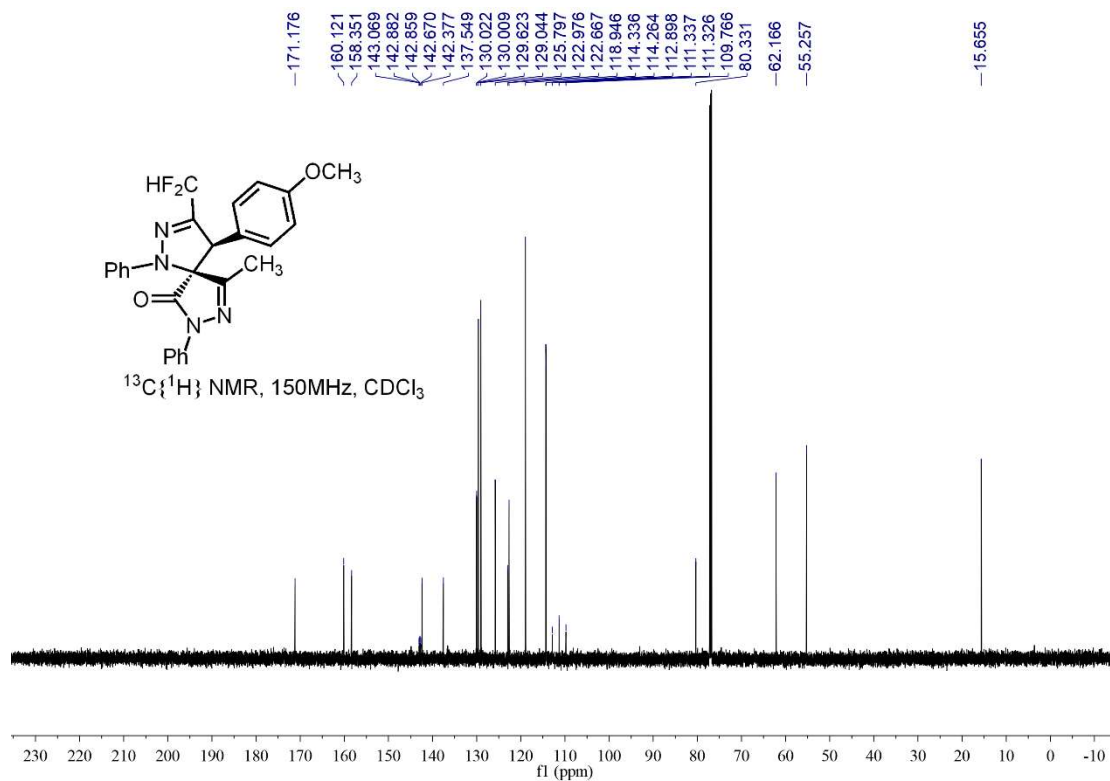
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



Meas. m/z	#	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R	e;# Conf	mS ig ma	Std l	Std Me an z	Std l Va rN or m	Std m/ z Diff	Std Com b Dev
467.1648	1	C 26 H 22 F 2 N 4 Na O	467.1654	1.2	0.7	16.5	ok	even	4.5	5.7	0.5	3.2	1.1	842.7

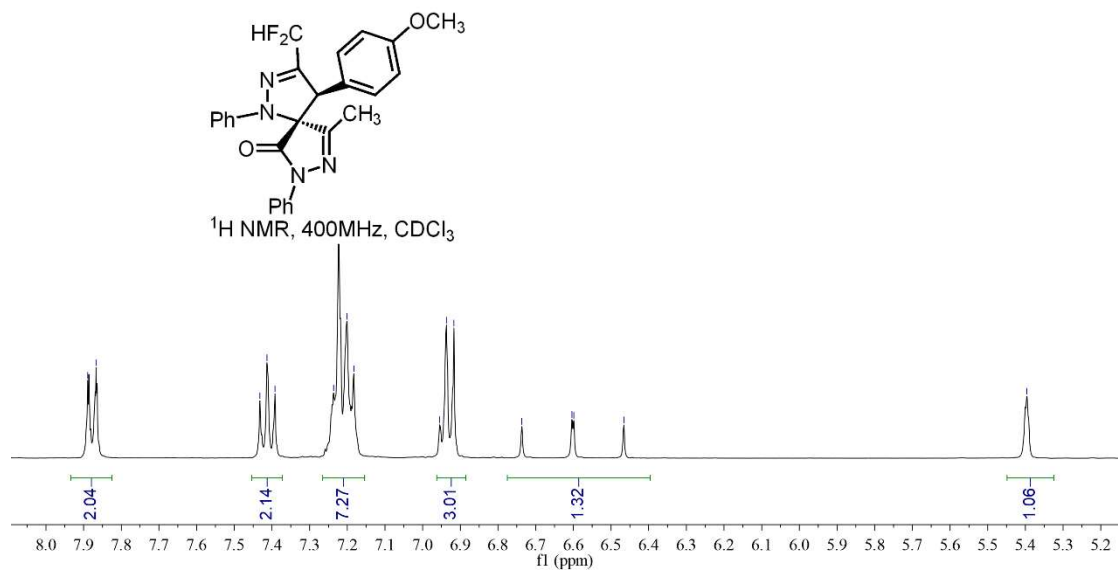
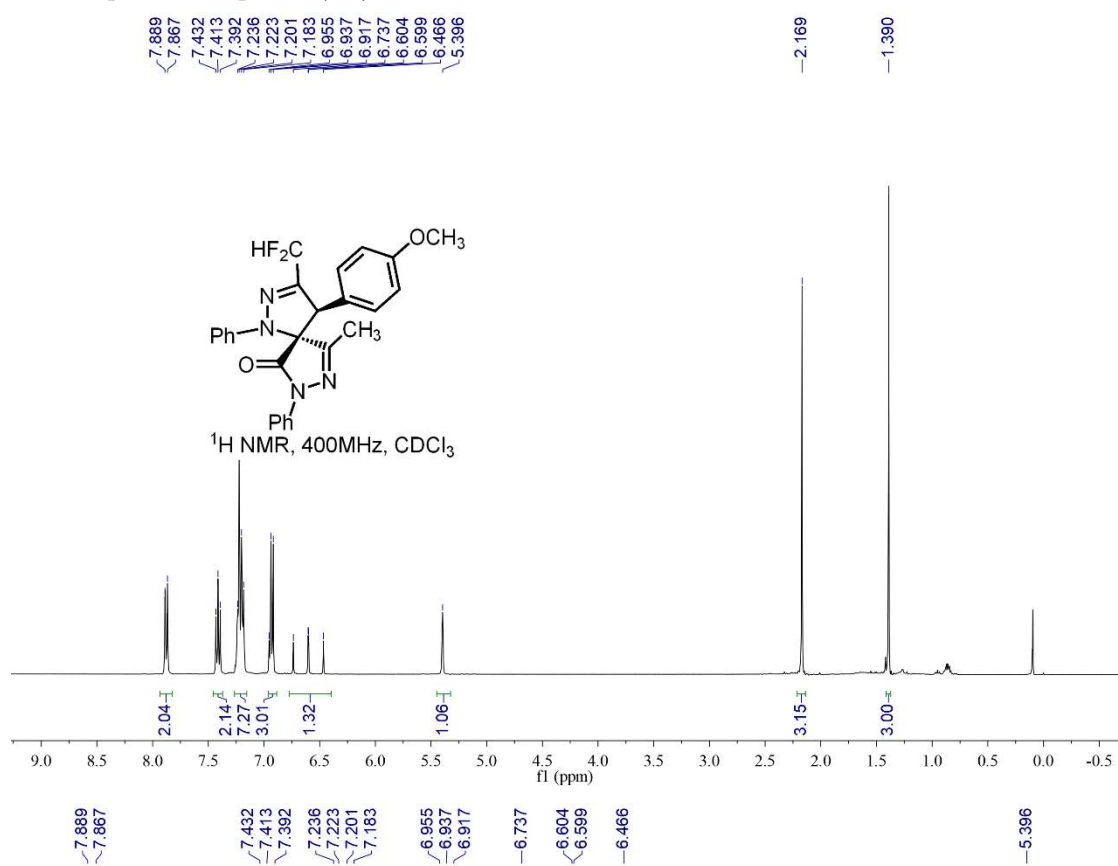
NMR copies of compound (*trans*)-4d:

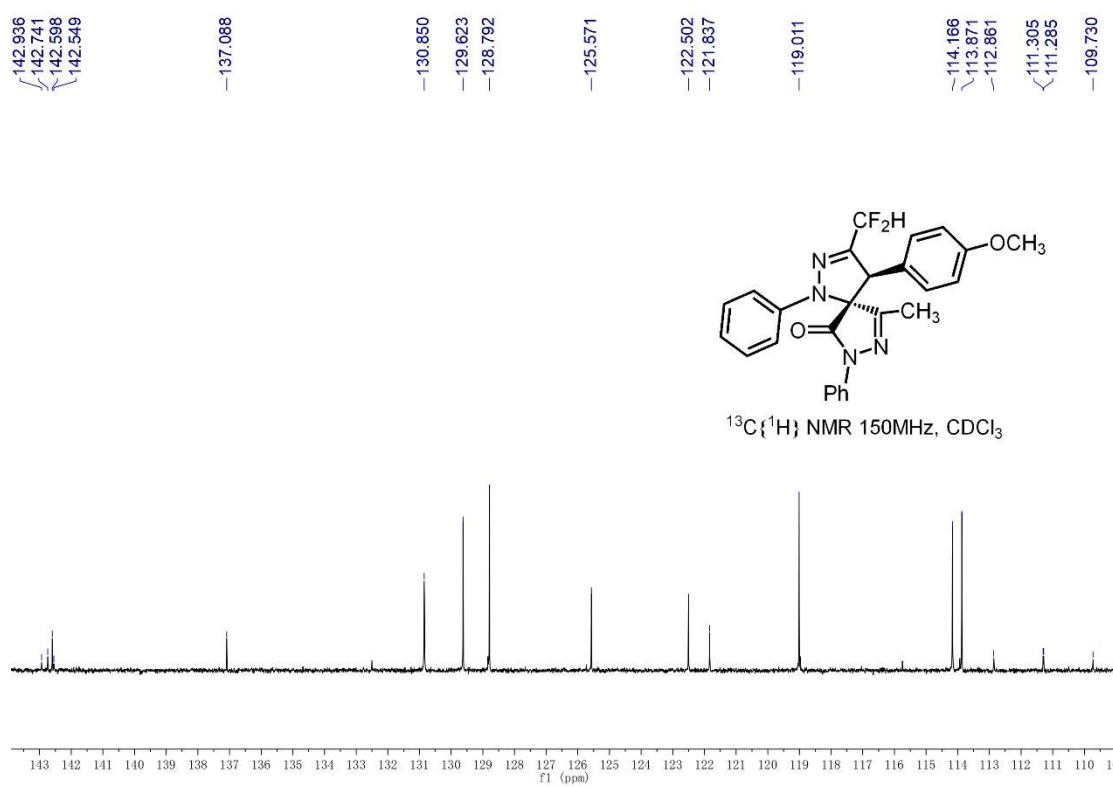
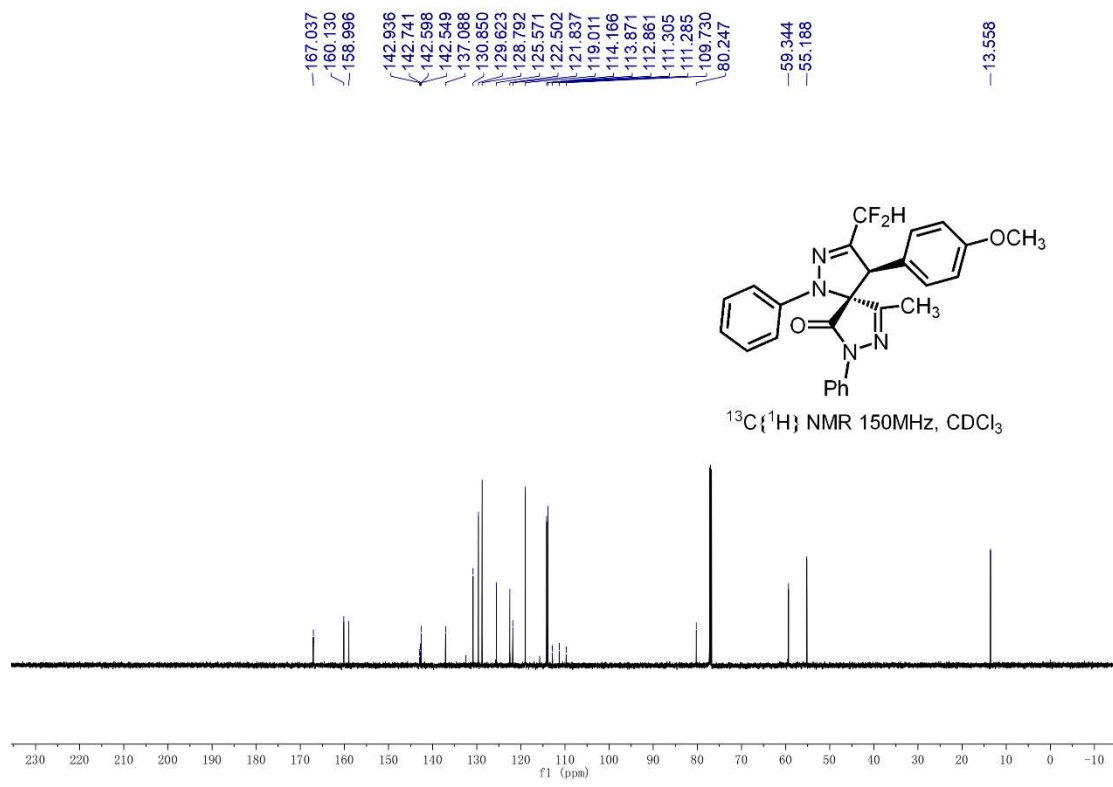






NMR copies of compound (*cis*)-4d:

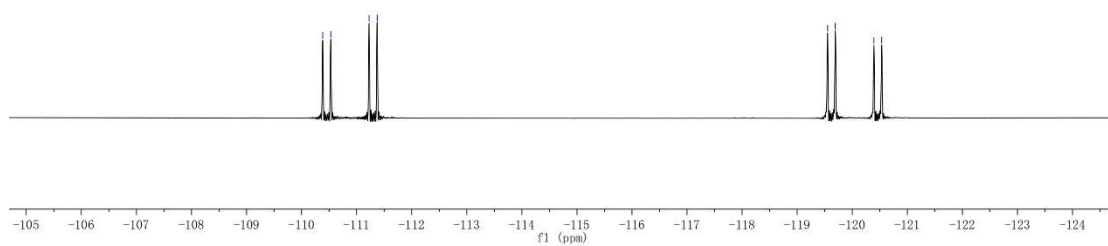
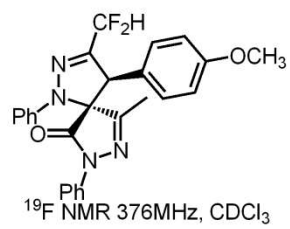






~110.383  
~110.529  
~111.225  
~111.371

~119.553  
~119.693  
~120.394  
~120.535



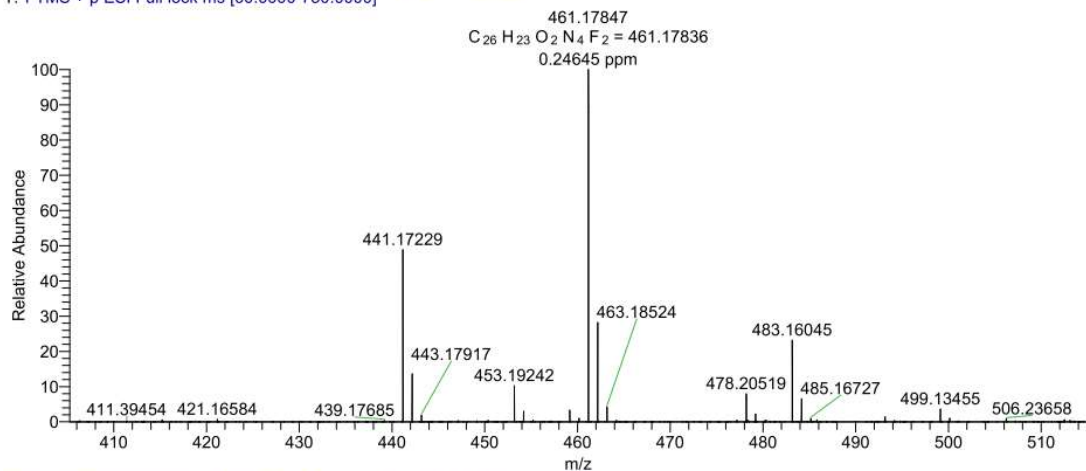
# HRMS (ESI) copy of compound (*cis*)-4d:

G:\HYL-FENGYANG-A-241

03/29/23 17:07:05

HYL-FENGYANG-A-241#36-88 RT: 0.16-0.39 AV: 53 NL: 3.04E8

T: FTMS + p ESI Full lock ms [60.0000-750.0000]

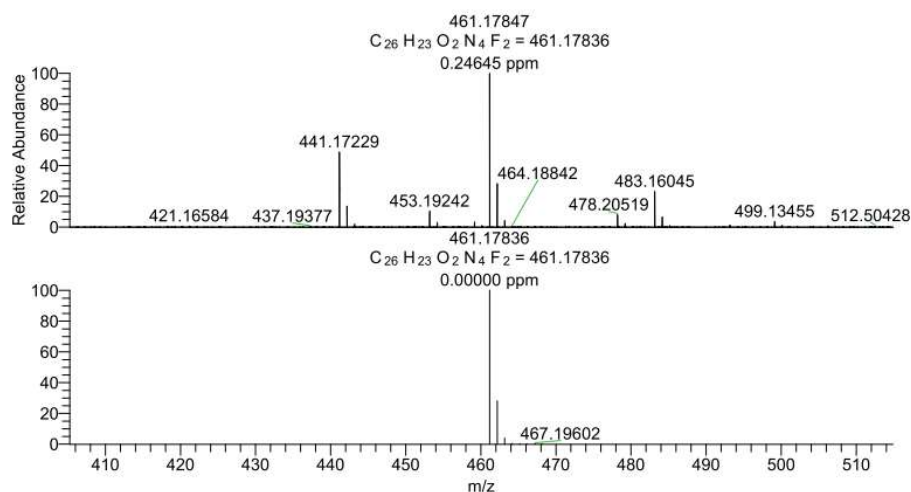


HYL-FENGYANG-A-241#36-88 RT: 0.16-0.39 AV: 53

T: FTMS + p ESI Full lock ms [60.0000-750.0000]

m/z = 405.24017-514.89430

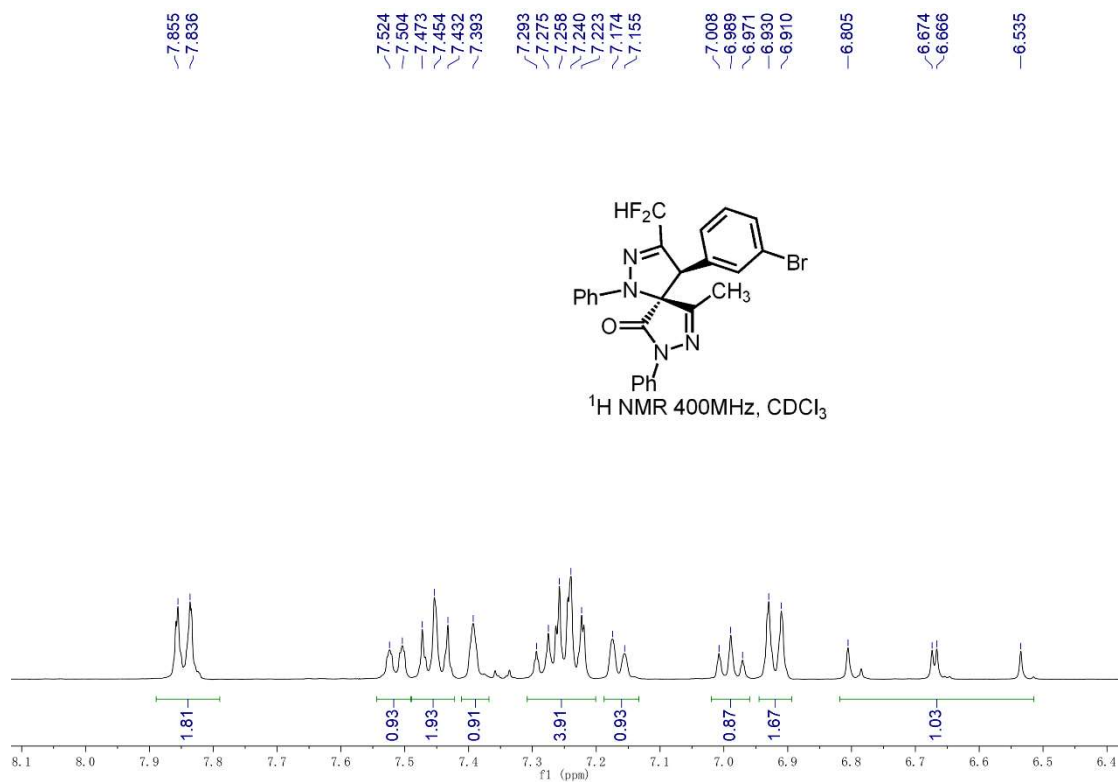
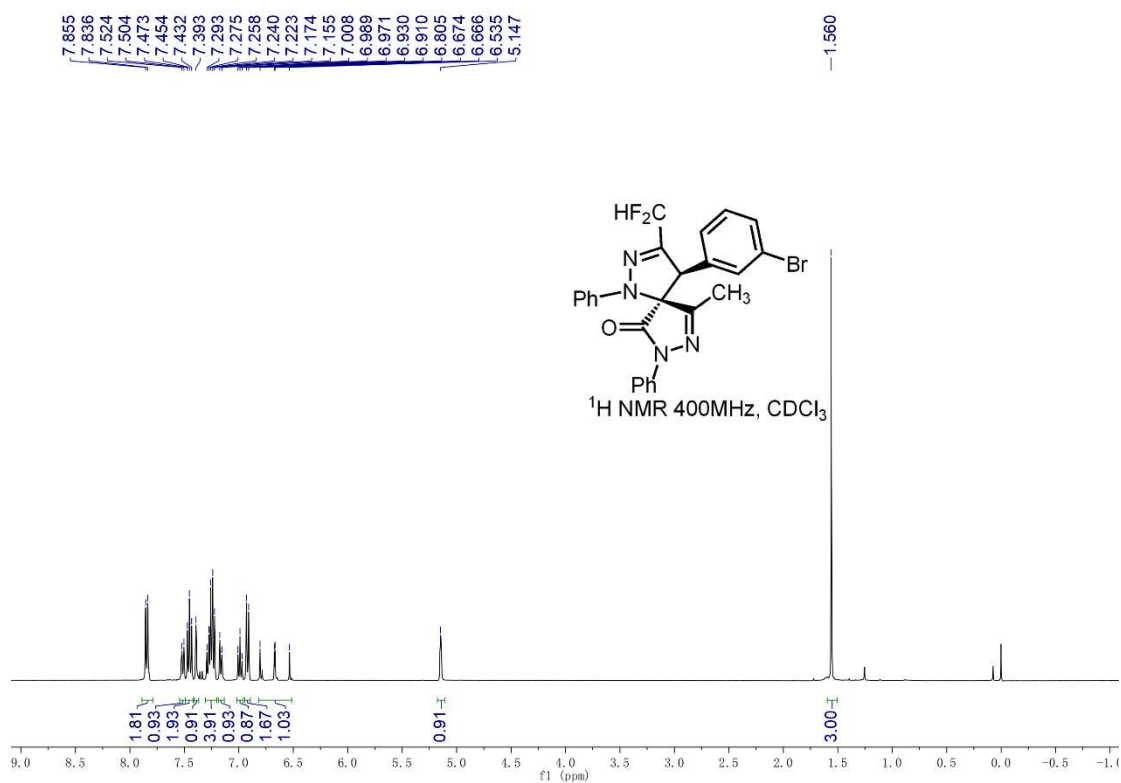
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
441.17229	149043664.0	48.68			
442.17581	41409804.0	13.52			
461.17847	306196384.0	100.00	461.17836	0.11	C <sub>26</sub> H <sub>23</sub> O <sub>2</sub> N <sub>4</sub> F <sub>2</sub>
462.18201	86076024.0	28.11			
483.16045	70750096.0	23.11			

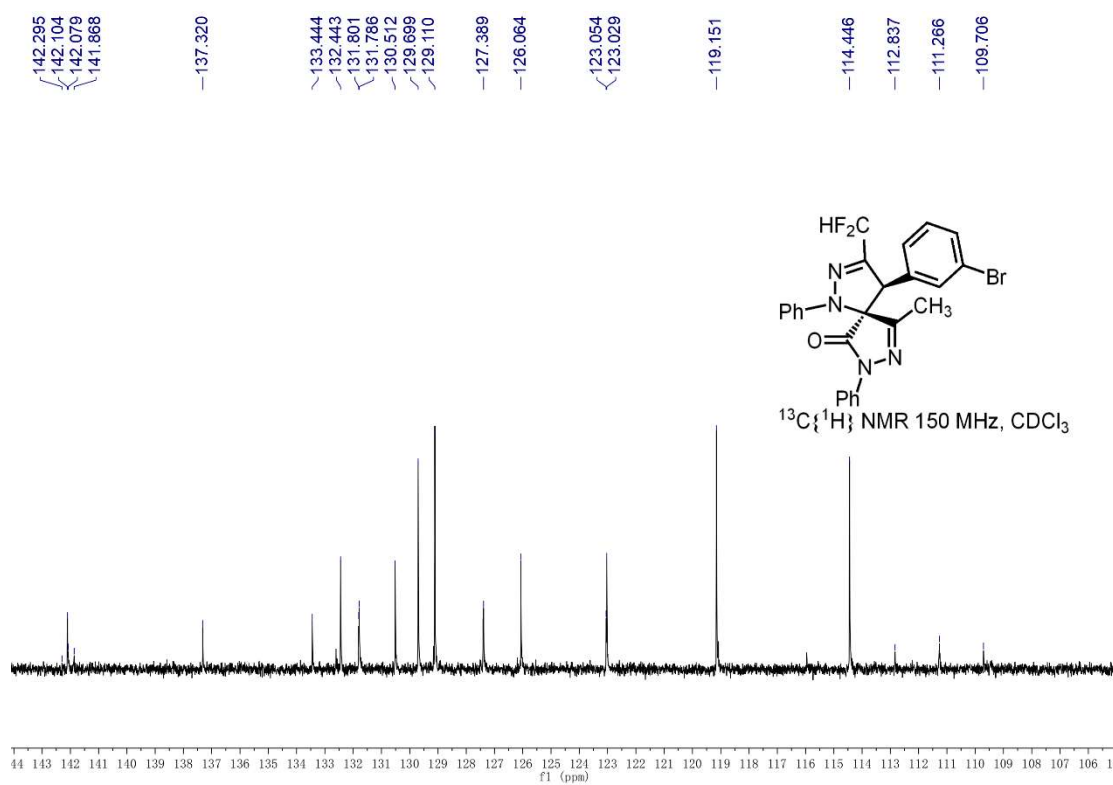
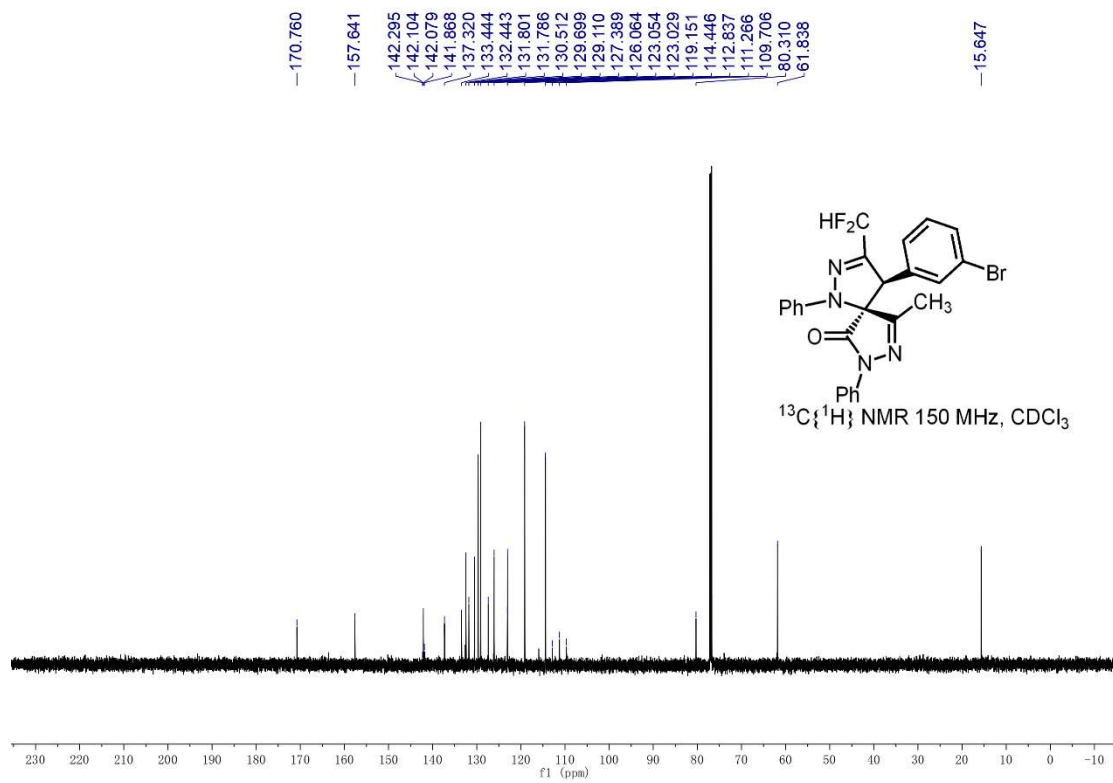


NL:  
3.04E8  
HYL-FENGYANG-A-  
241#36-88 RT:  
0.16-0.39 AV: 53 T:  
FTMS + p ESI Full lock  
ms [60.0000-750.0000]

NL:  
7.39E5  
C<sub>26</sub>H<sub>23</sub>F<sub>2</sub>N<sub>4</sub>O<sub>2</sub>:  
C<sub>26</sub>H<sub>23</sub>F<sub>2</sub>N<sub>4</sub>O<sub>2</sub>  
pa Chrg 1

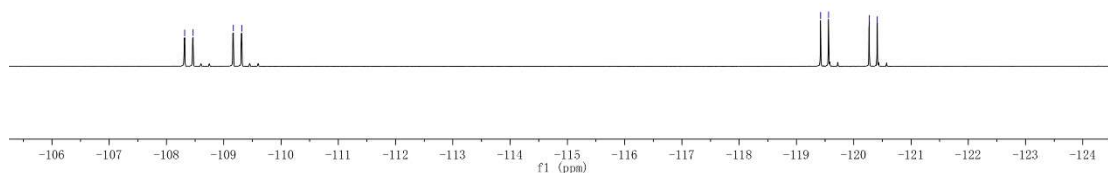
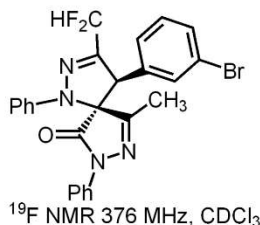
NMR copies of compound (*trans*)-4e:





-108.317  
-108.465  
-109.167  
-109.315

-119.422  
-119.561  
-120.272  
-120.411



HRMS (ESI) copy of compound (*trans*)-4e:

### Mass Spectrum SmartFormula Report

#### Analysis Info

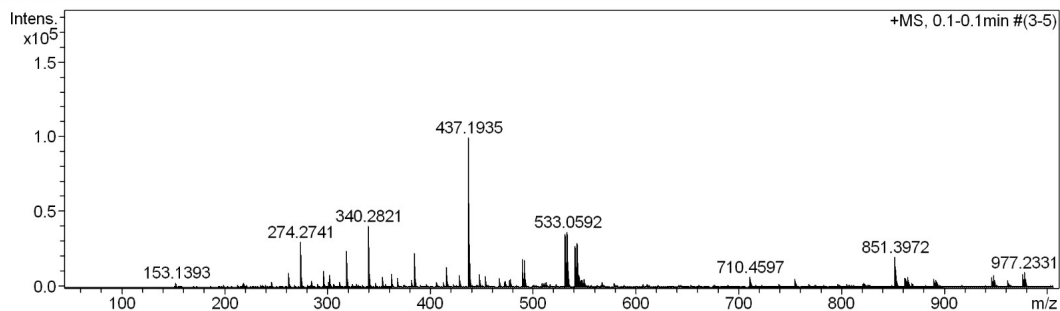
Analysis Name D:\Data\user\NWNWU-fengyang 20230321-6.d  
Method tune\_low.m  
Sample Name A-52  
Comment

Acquisition Date 2023-3-21 15:38:53

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

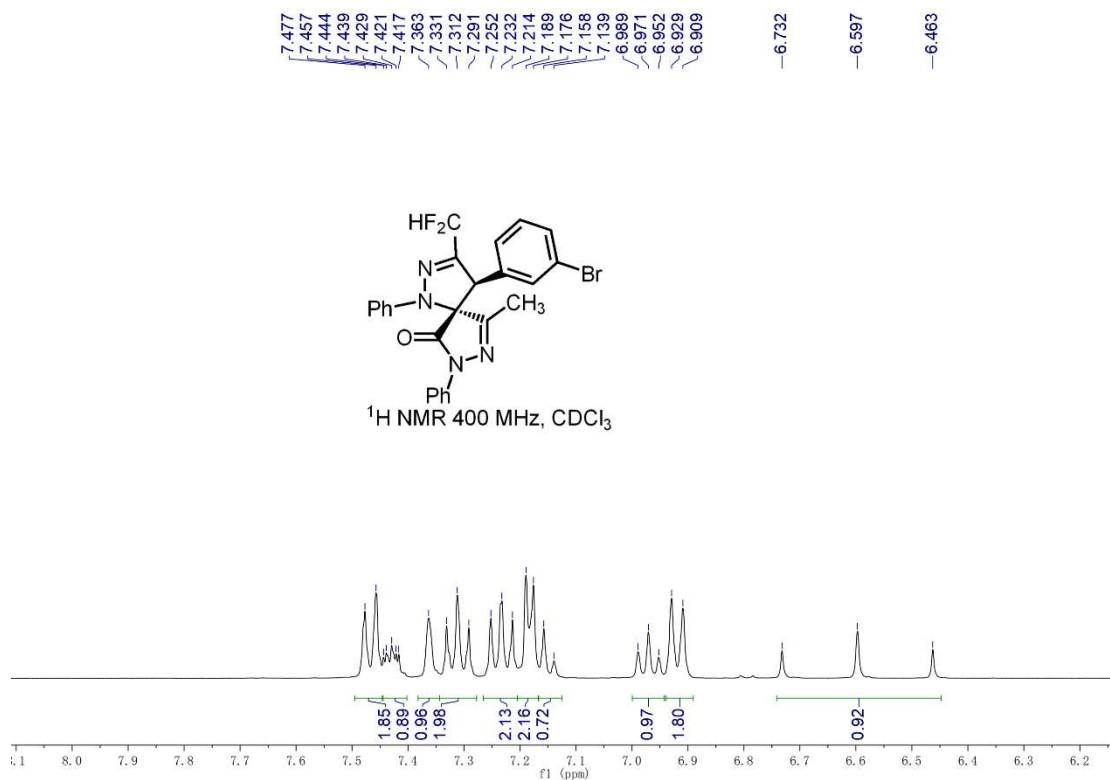
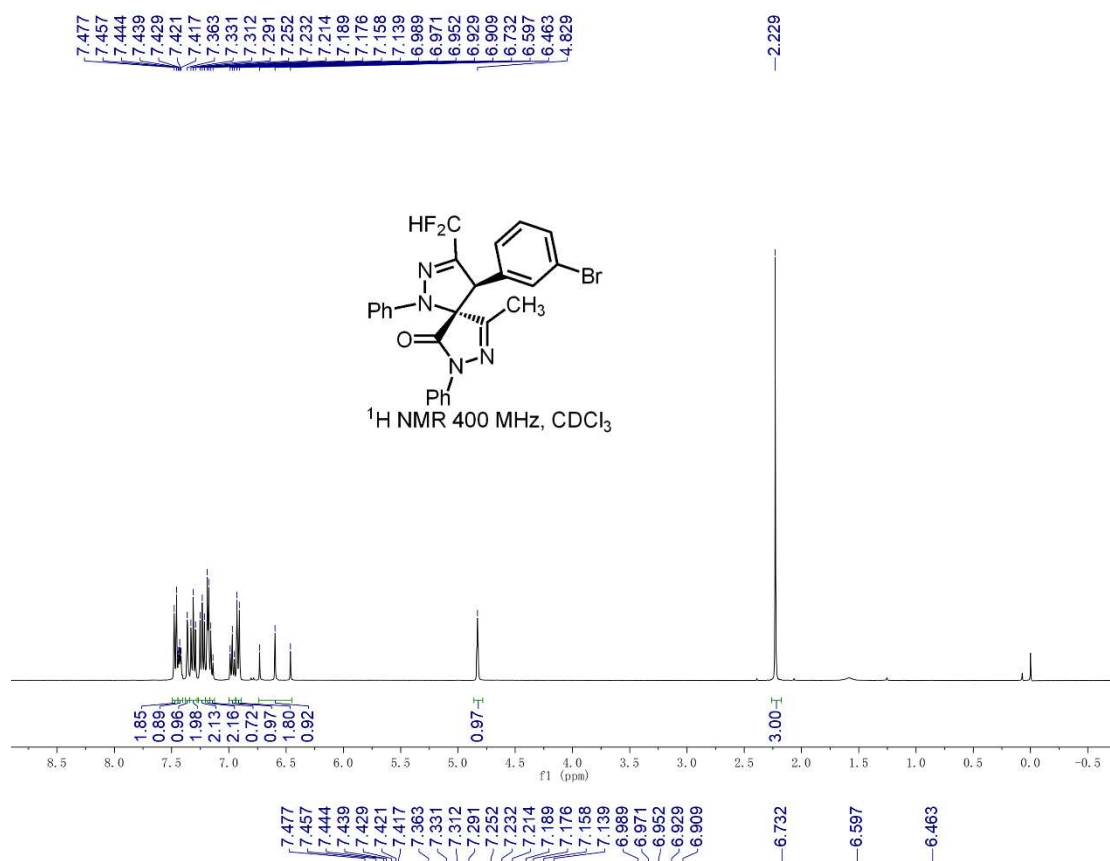
#### Acquisition Parameter

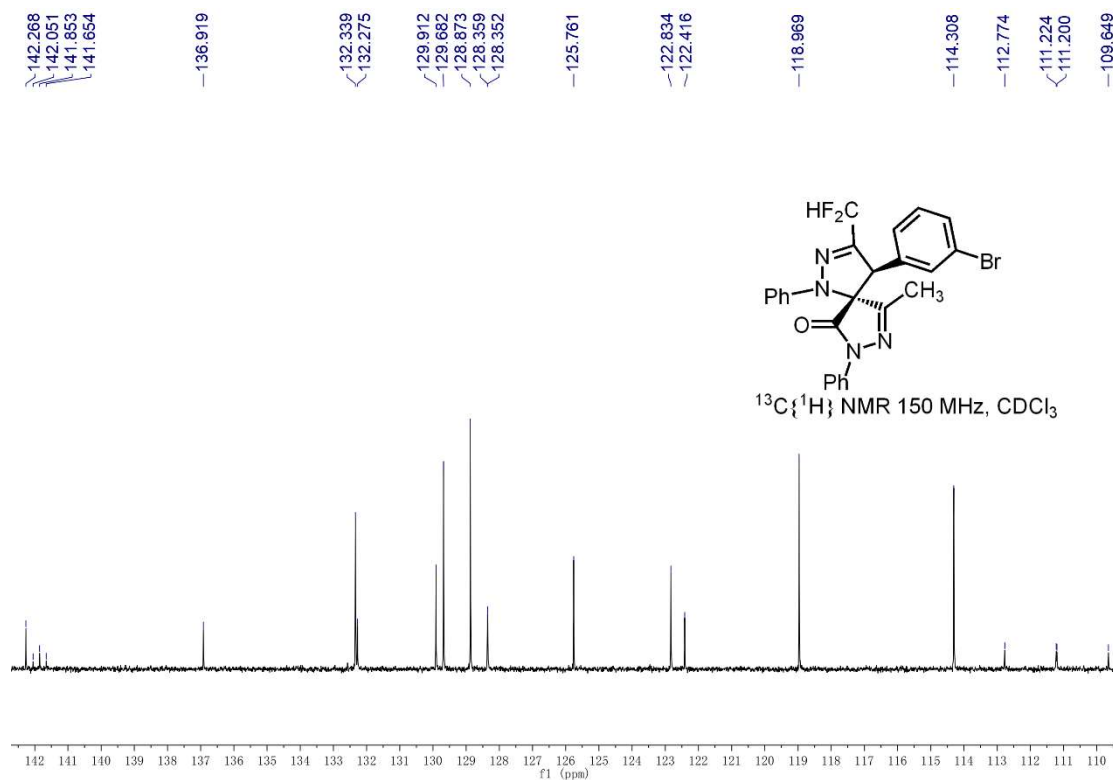
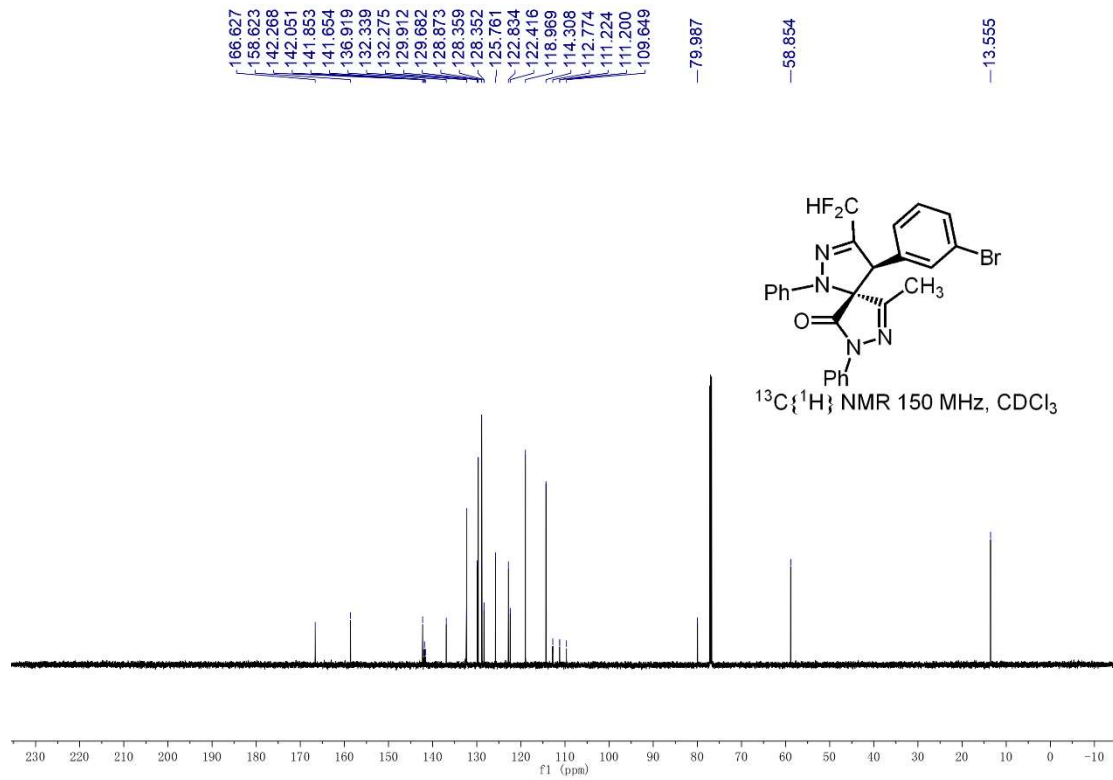
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j̄C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



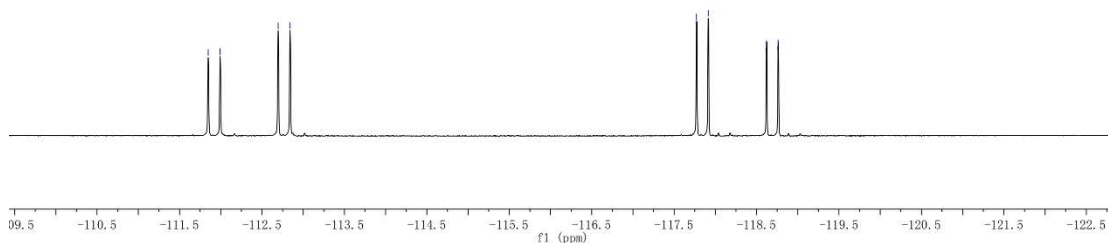
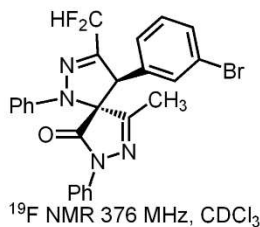
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- ul e	e; Con f	mSi gm a	Std l	St d M ea n m/z	St d Va r m	St d m/ z	Std Com b Dev
531.0603	1 C <sub>25</sub> H <sub>19</sub> BrF <sub>2</sub> N <sub>4</sub> NaO	531.0603	-0.1	-0.9	16.5	ok	even	17.7	17.2	1.1	6.4	1.0	842.7

NMR copies of compound (*cis*)-4e:





~111.848  
~111.992  
~112.696  
~112.841  
~117.771  
~117.913  
~118.619  
~118.761



HRMS (ESI) copy of compound (*cis*)-4e:

## Mass Spectrum SmartFormula Report

### Analysis Info

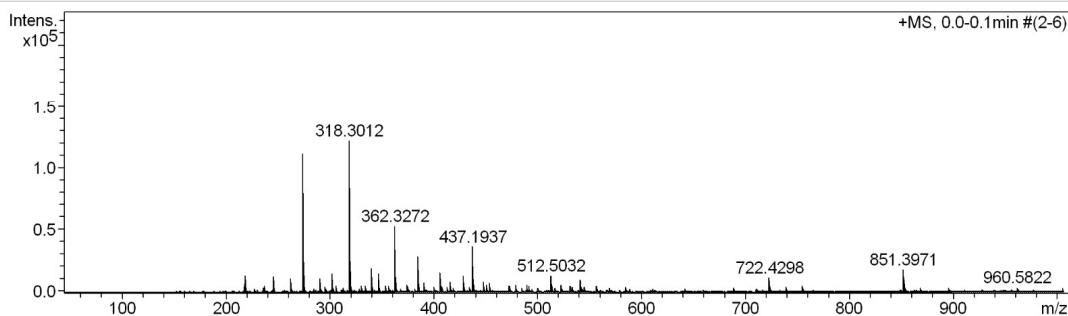
Analysis Name D:\Data\user\NWNWU-fengyang 20230321-7.d  
Method tune\_low.m  
Sample Name A-521  
Comment

Acquisition Date 2023-3-21 15:40:46

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

### Acquisition Parameter

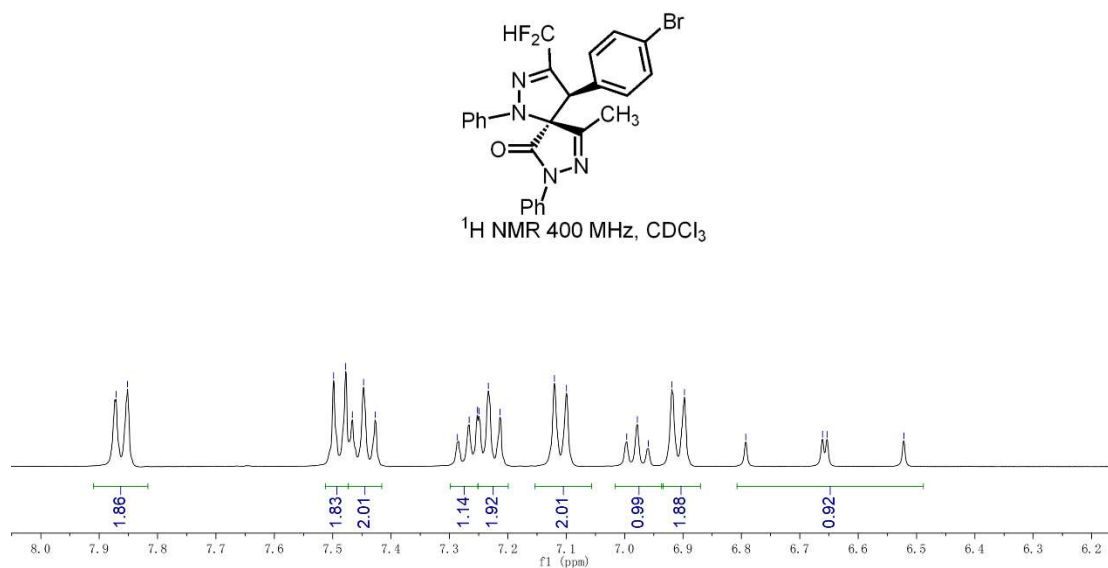
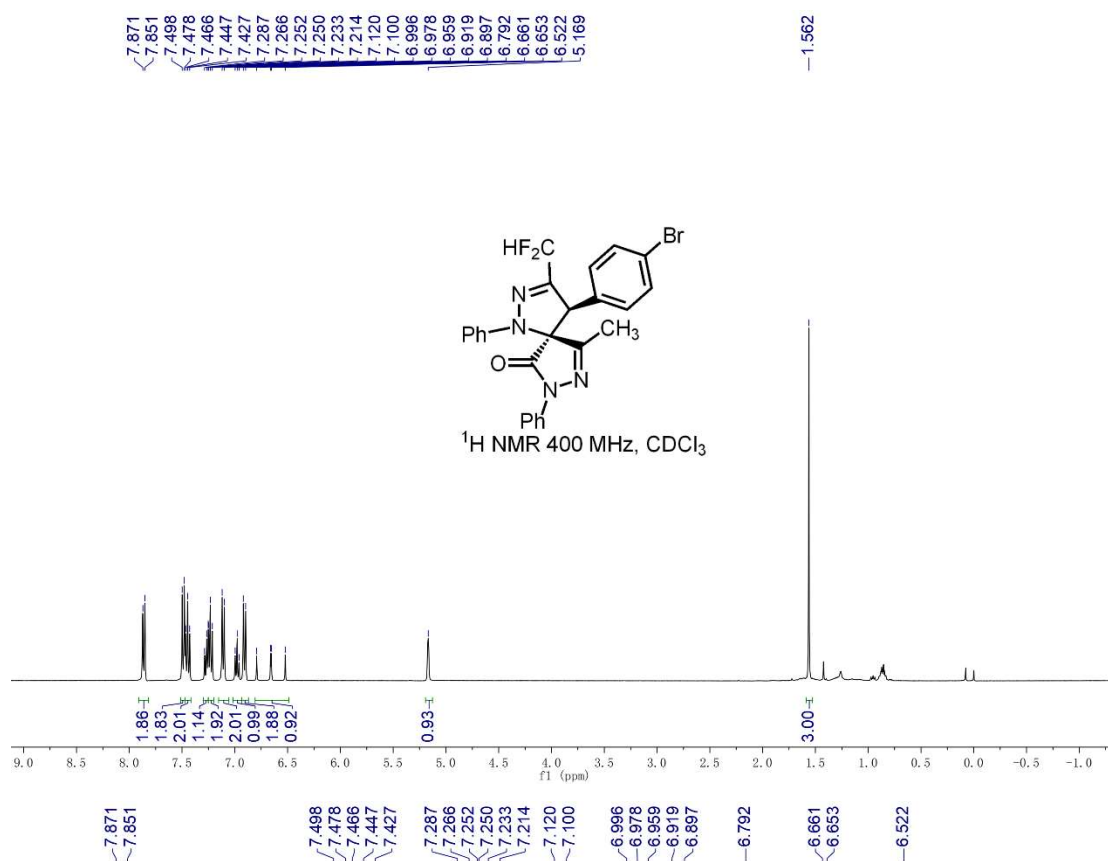
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Me an [ppm]	rdb	N	ej% Con	mSi gma	Std I	St d M ea n/z	Std l Var m	St d Nor m	St d Dif f	Std Com b Dev
531.0613	1 C <sub>25</sub> H <sub>19</sub> BrF <sub>2</sub> N <sub>4</sub> NaO	531.0603	-2.0	-0.9	16.5	ok	even	129.2	127.7	0.7	53.5	0.8	842.7	



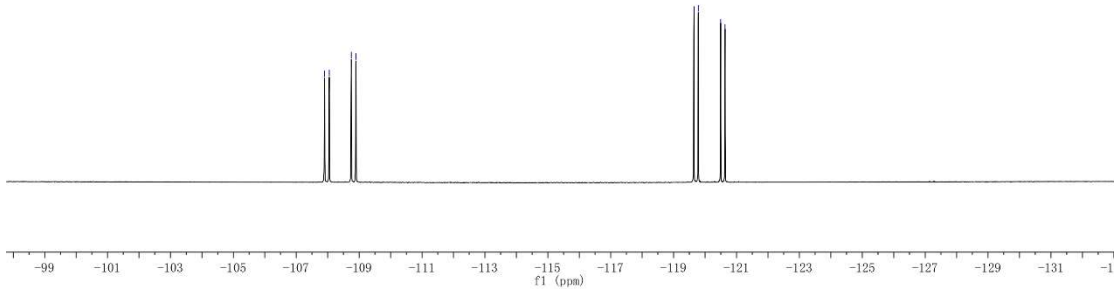
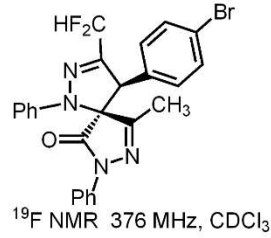
NMR copies of compound (*trans*)-4f:





-107.903  
-108.051  
-108.753  
-108.901

-119.647  
-119.786  
-120.497  
-120.636



HRMS (ESI) copy of compound (*trans*)-4f:

### Mass Spectrum SmartFormula Report

#### Analysis Info

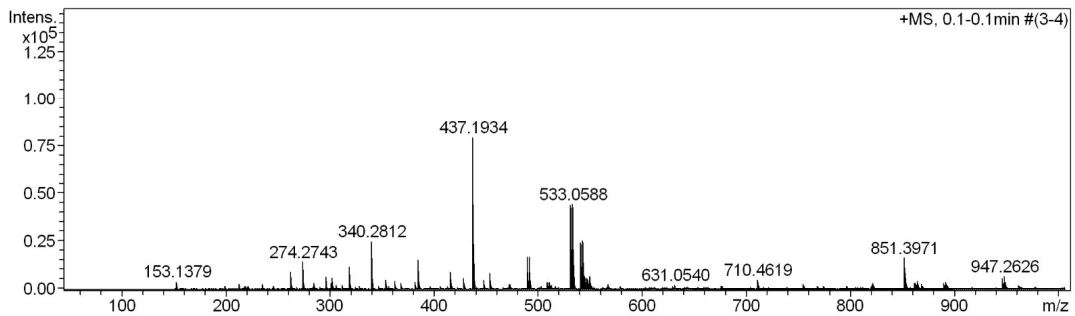
Analysis Name D:\Data\user\NWNNU-fengyang 20230321-8.d  
Method tune\_low.m  
Sample Name A-51  
Comment

Acquisition Date 2023-3-21 15:42:30

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

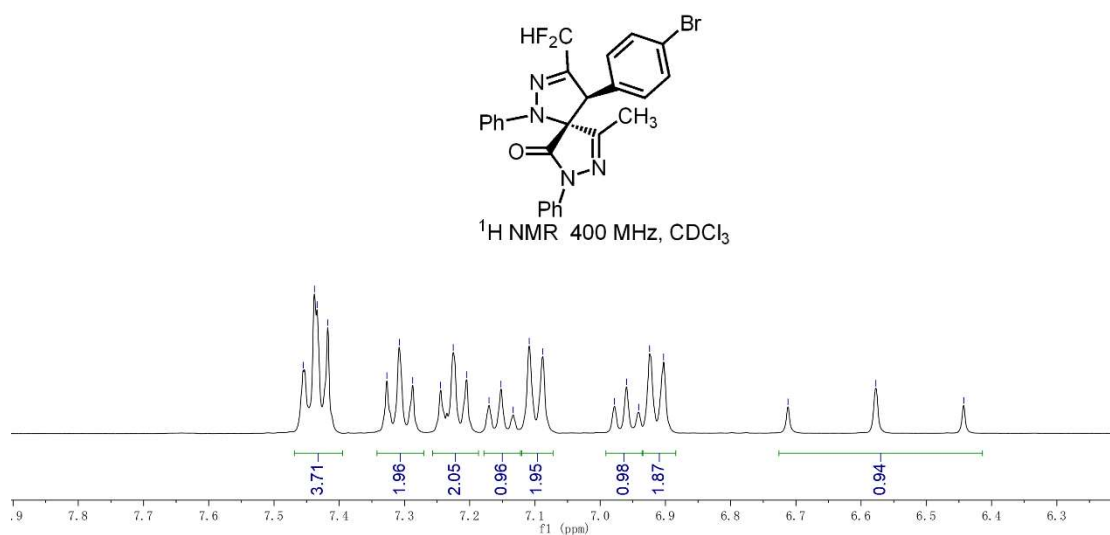
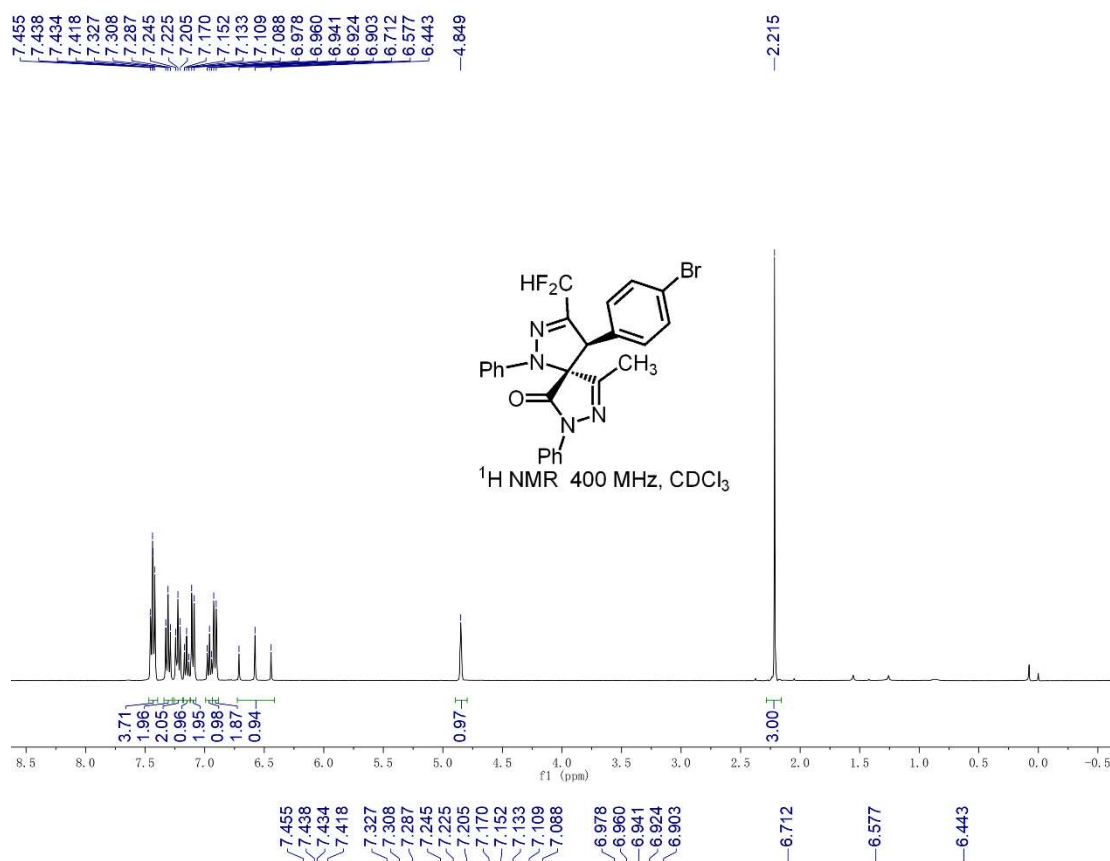
#### Acquisition Parameter

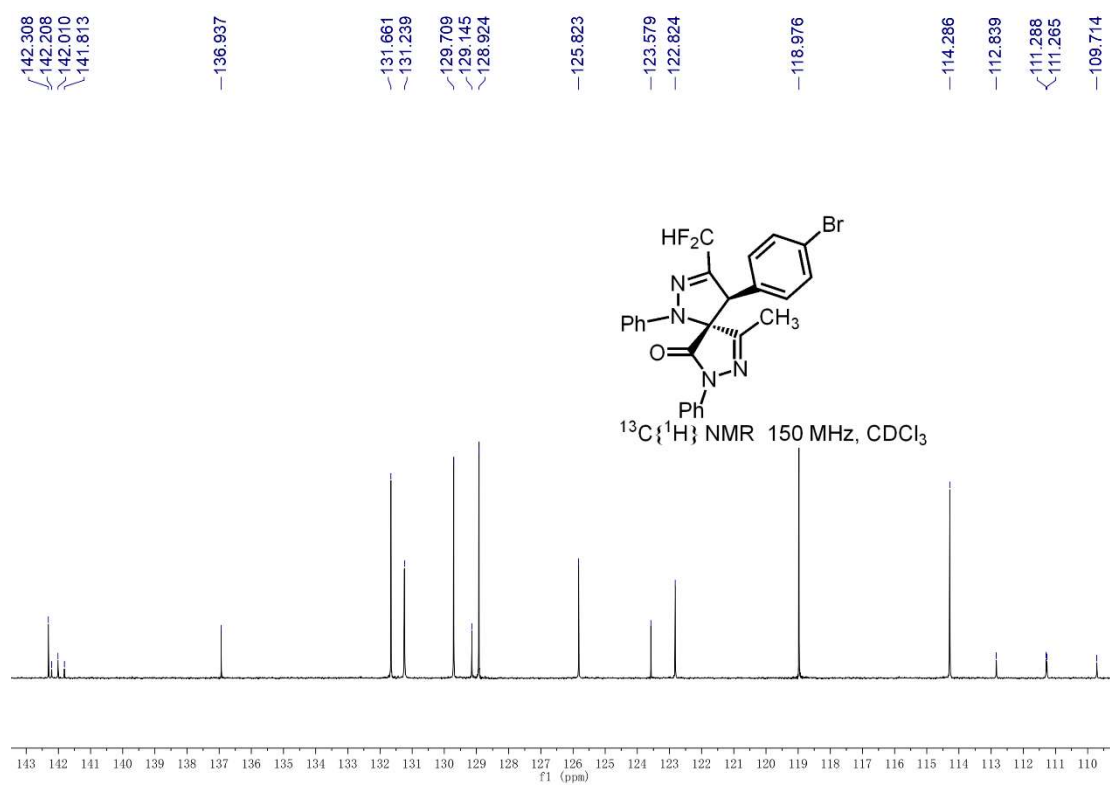
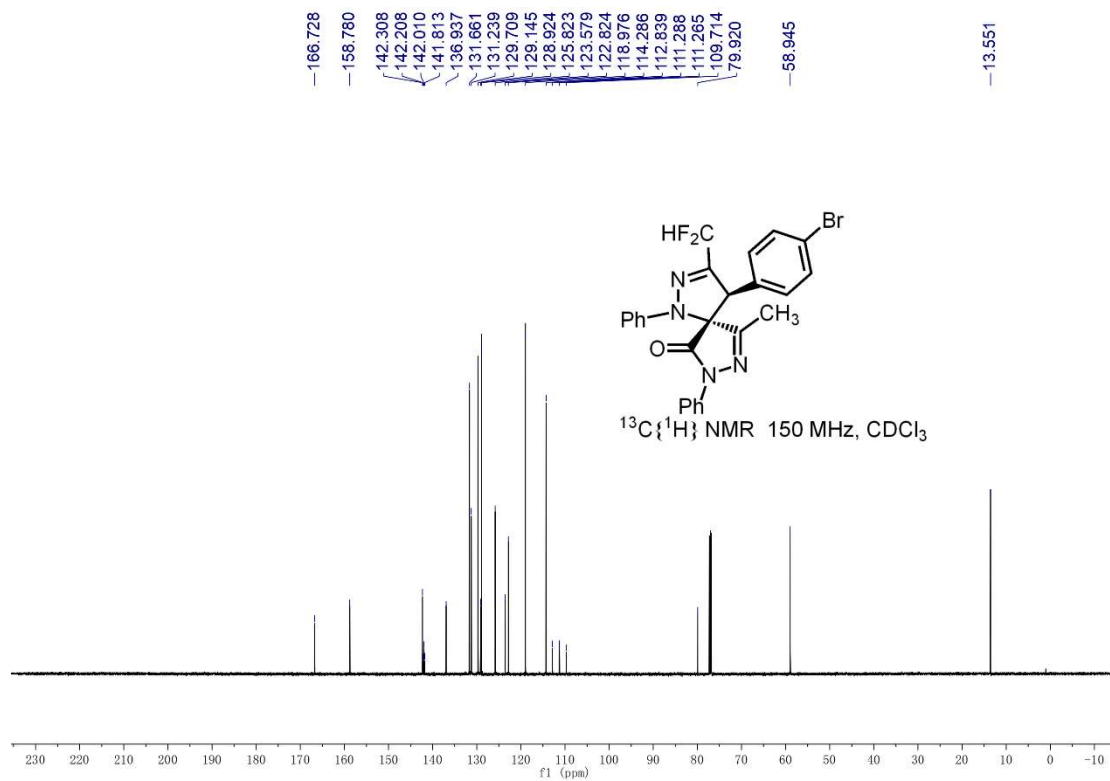
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



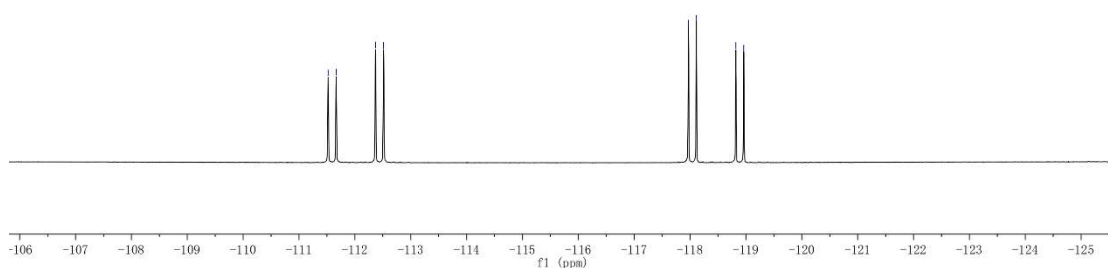
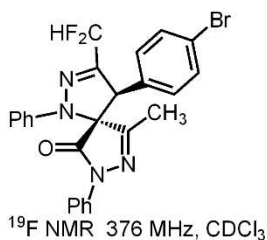
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R ul e	e j % Con f	mSi gm a	Std l	St d M ea n m/z	St d Va rN or m	St d m/ z	Std Com b Dev
531.0609	1 C <sub>25</sub> H <sub>19</sub> BrF <sub>2</sub> N <sub>4</sub> NaO	531.0603	-1.3	-0.6	16.5	ok	even	15.0	13.9	0.7	5.0	1.0	842.7

NMR copies of compound (*cis*)-4f:





~-111.520  
 ~-111.665  
 ~-112.369  
 ~-112.513  
 ~-117.970  
 ~-118.112  
 ~-118.819  
 ~-118.960



HRMS (ESI) copy of compound (*cis*)-4f:

### Mass Spectrum SmartFormula Report

#### Analysis Info

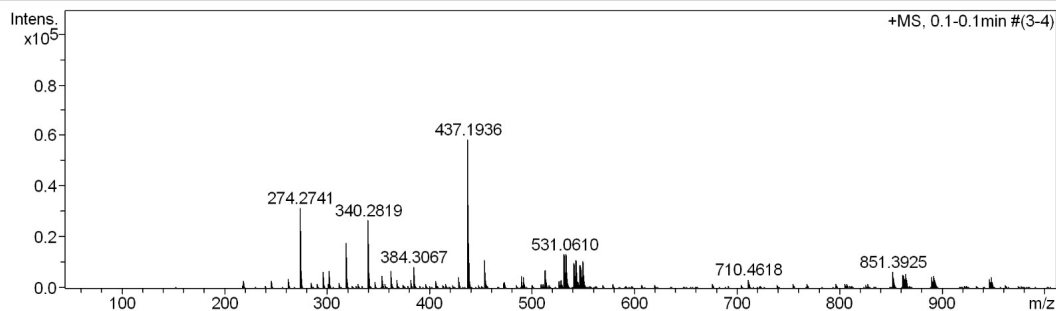
Analysis Name D:\Data\user\NWNNU-fengyang 20230321-9.d  
 Method tune\_low.m  
 Sample Name A-511  
 Comment

Acquisition Date 2023-3-21 15:44:10

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

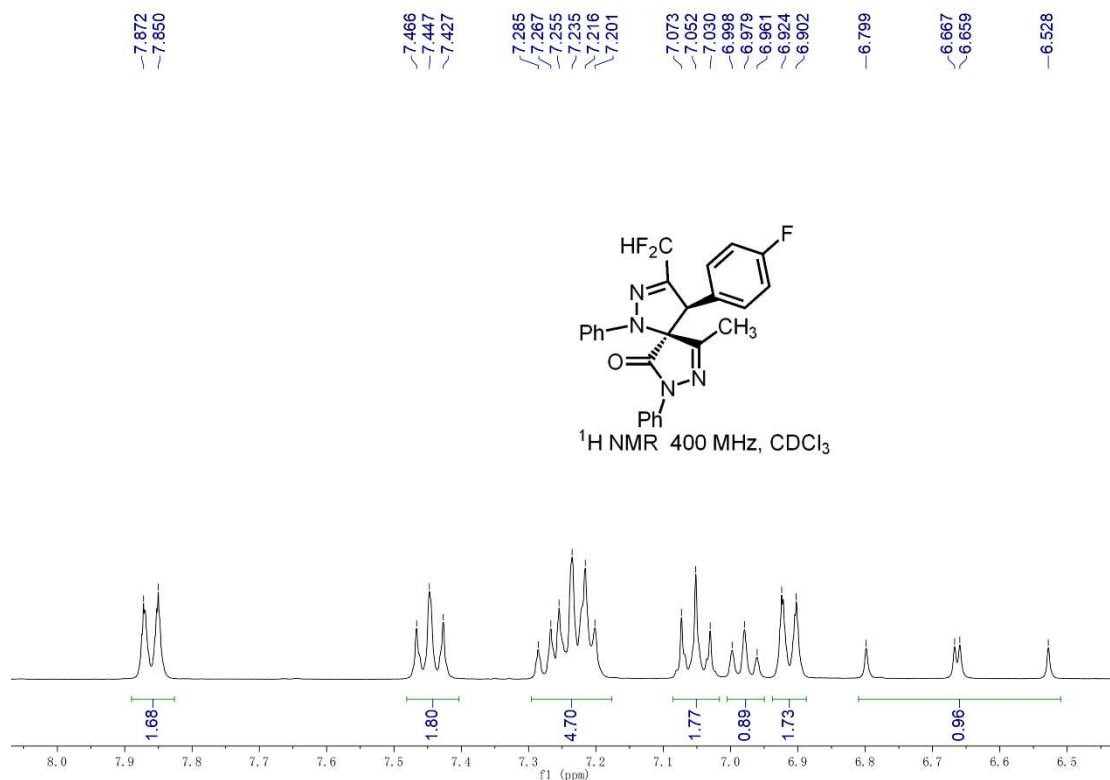
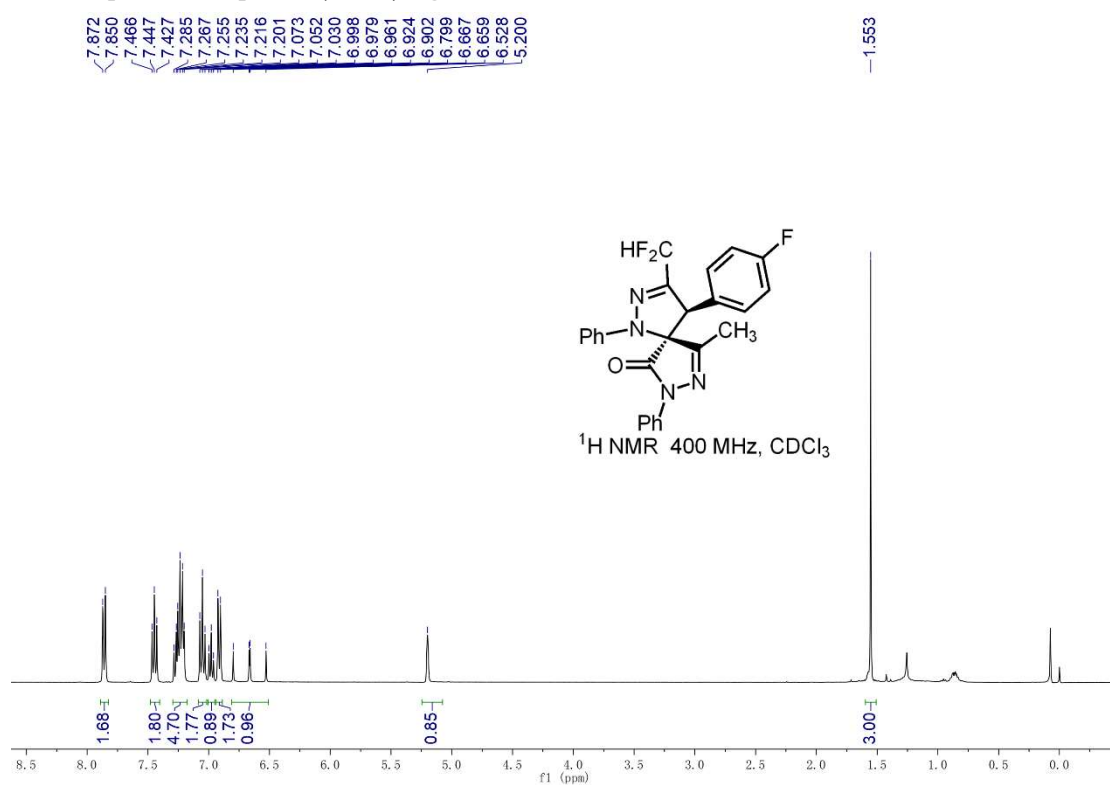
#### Acquisition Parameter

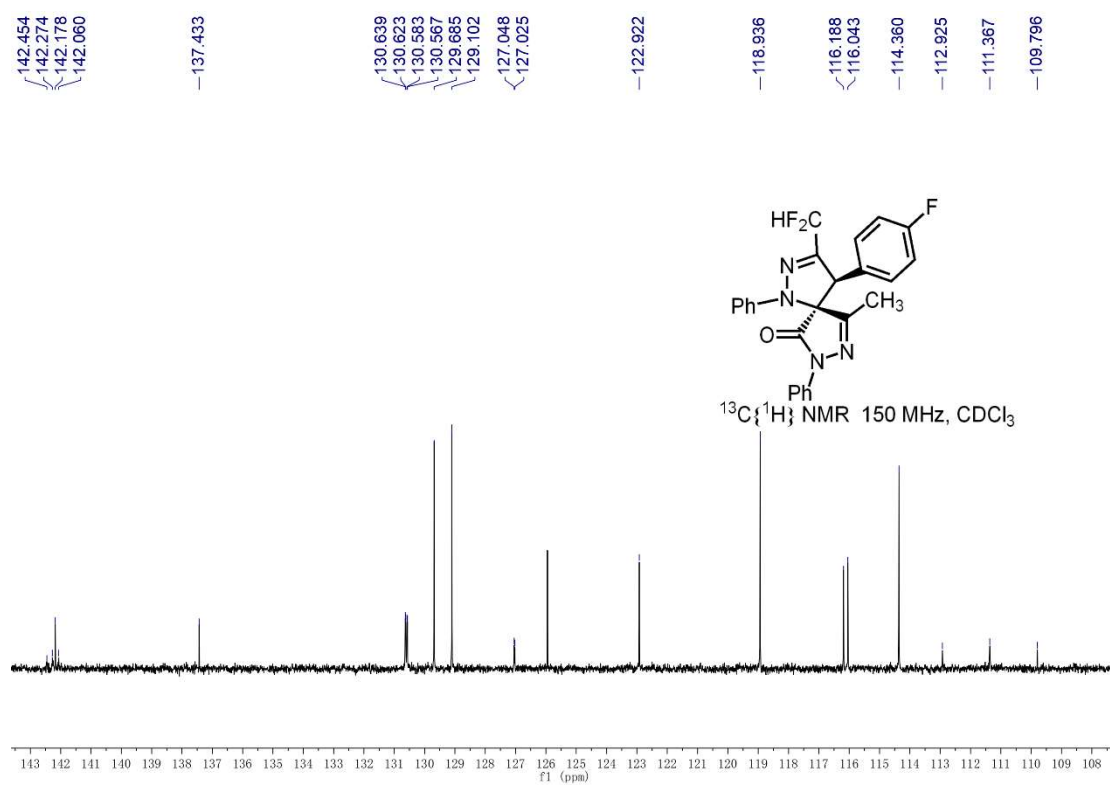
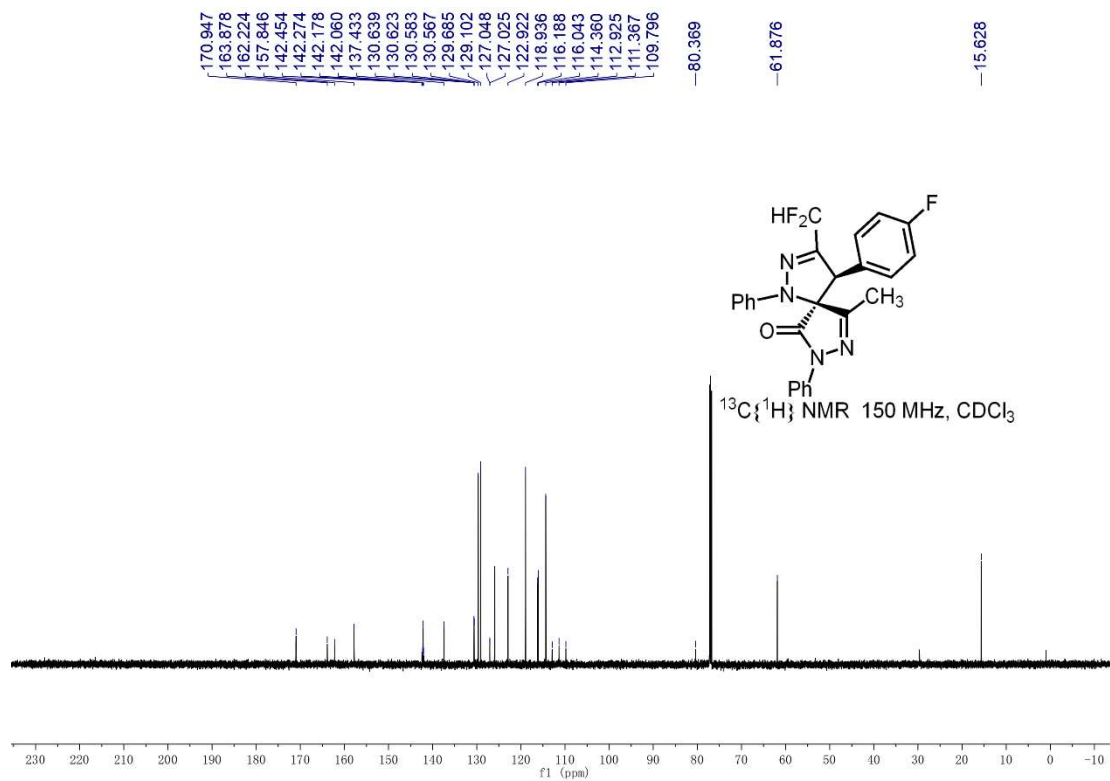
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



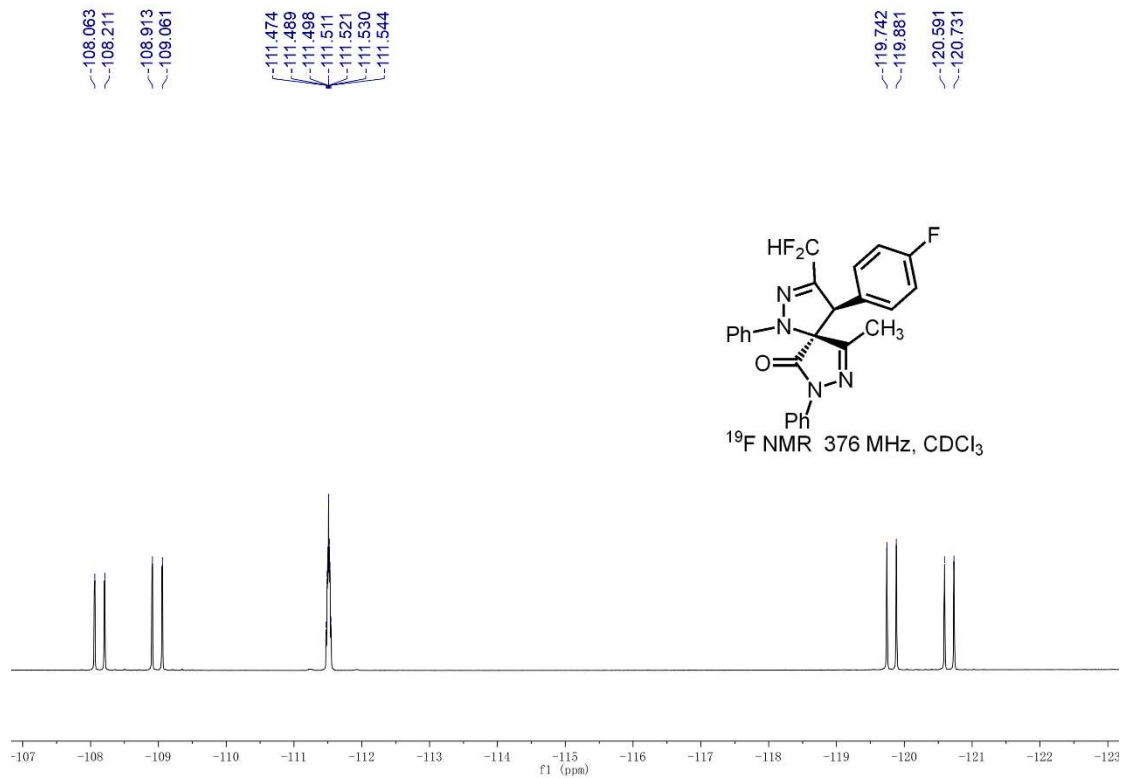
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N	e j %	mSi gm	Std l	St d l	Std Var m	St d l	Std Com b
531.0610	1 C <sub>25</sub> H <sub>19</sub> BrF <sub>2</sub> N <sub>4</sub> NaO	531.0603	-1.3	-0.1	16.5	ok	even	22.6	19.8	0.7	11.2	0.9	842.7

NMR copies of compound (*trans*)-4g:









HRMS (ESI) copy of compound (*trans*)-4g:

### Mass Spectrum SmartFormula Report

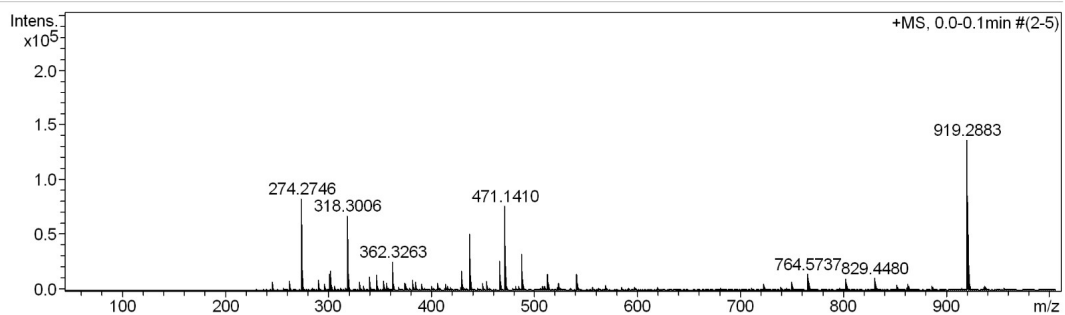
#### Analysis Info

Analysis Name D:\Data\user\NWNW-fengyang 20230321-10.d  
 Method tune\_low.m  
 Sample Name A-50  
 Comment

Acquisition Date 2023-3-21 16:37:42  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

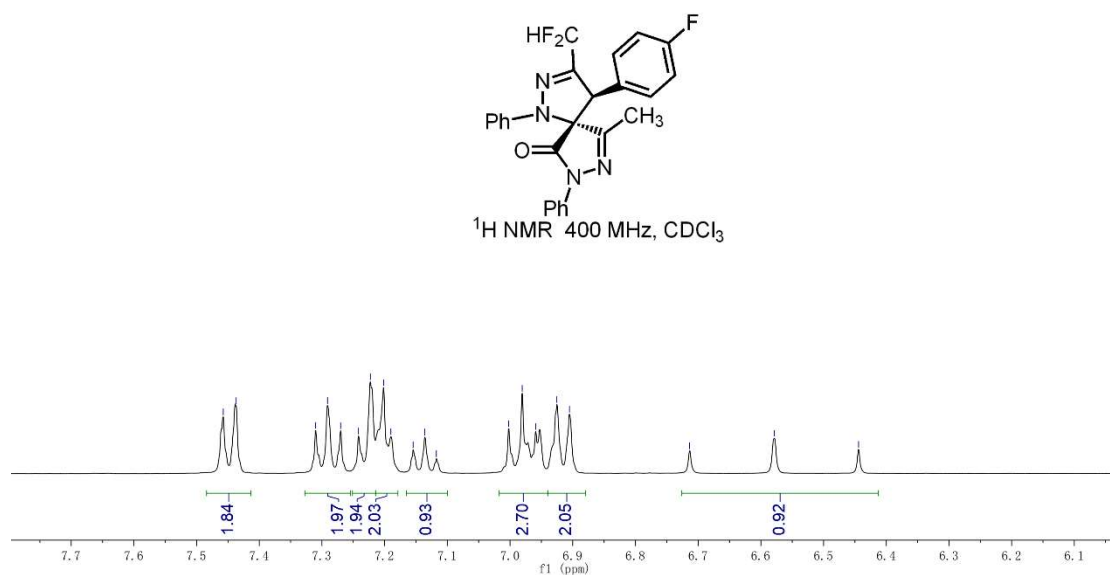
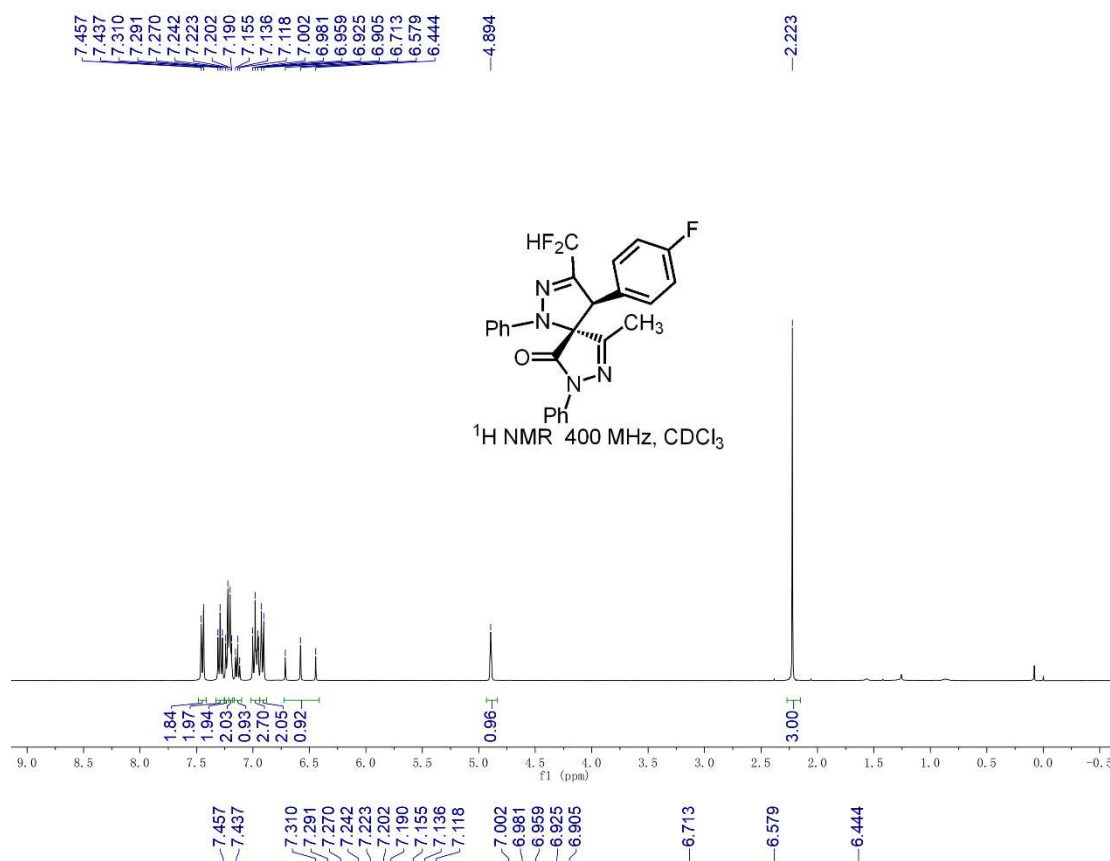
#### Acquisition Parameter

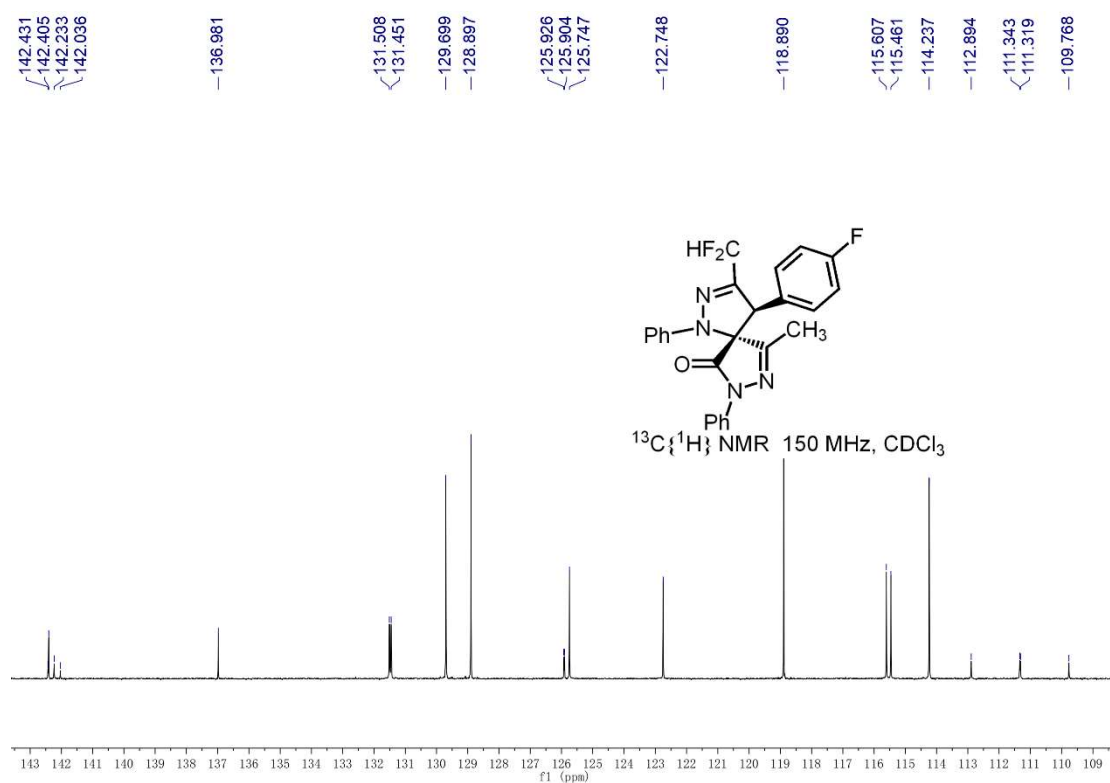
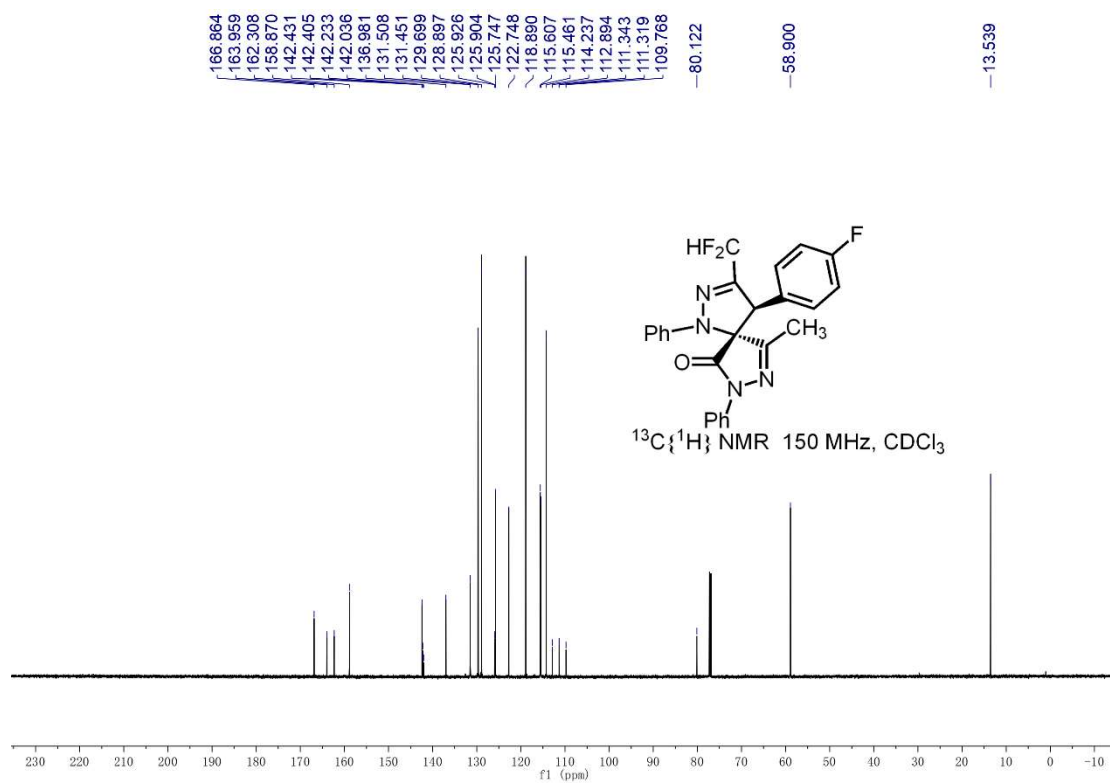
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

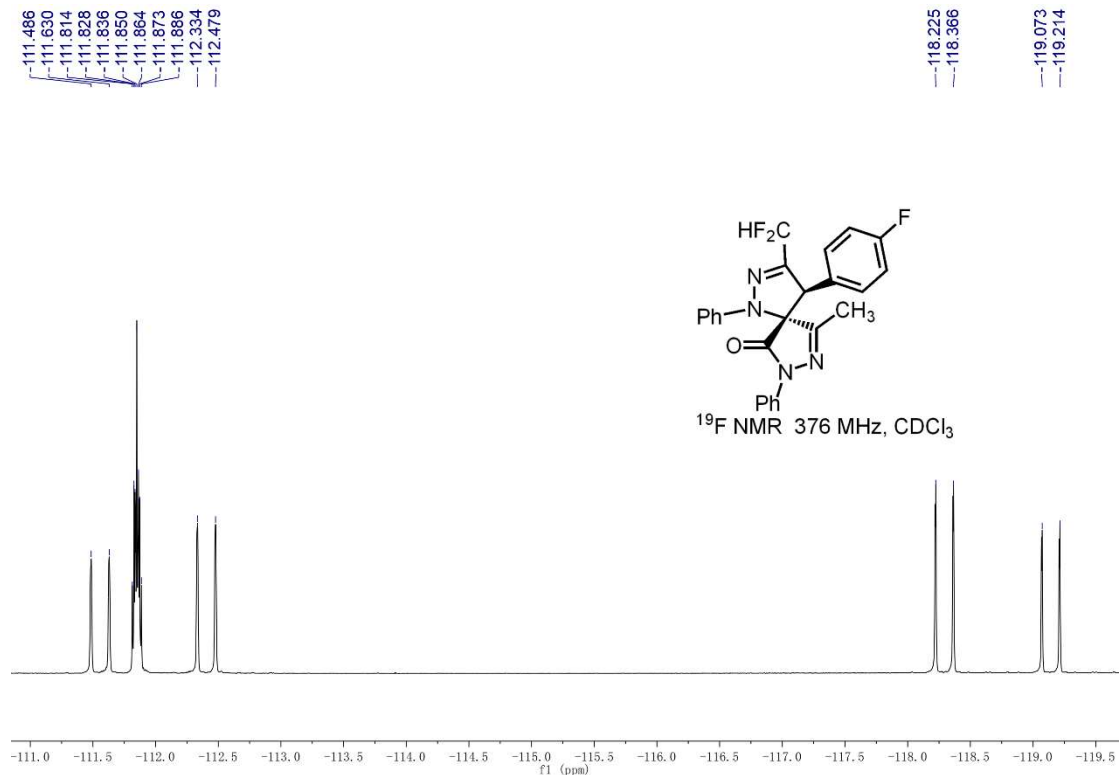


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej¥ Conf	mS ig ma	Std l	Std Me an z	Std l Va rN or m	Std m/ z Diff	Std Com b Dev
471.1410	1 C <sub>25</sub> H <sub>19</sub> F <sub>3</sub> N <sub>4</sub> NaO	471.1403	-1.4	-1.5	16.5	ok	even	4.0	6.1	0.8	4.2	0.1	842.7

NMR copies of compound (*cis*)-4g:







HRMS (ESI) copy of compound (*cis*)-4g:

### Mass Spectrum SmartFormula Report

#### Analysis Info

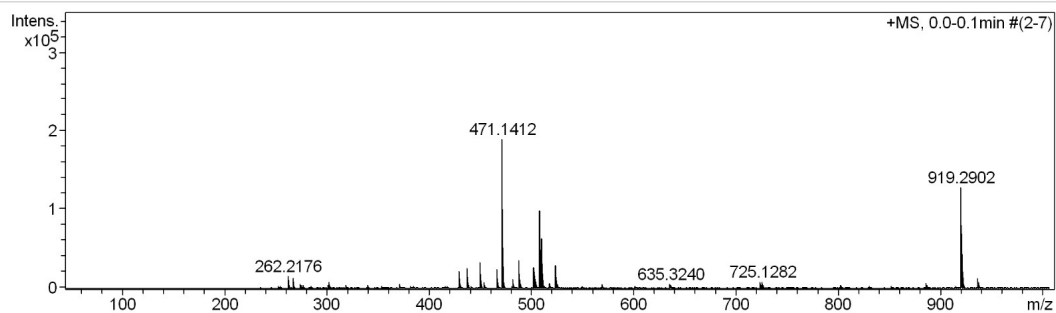
Analysis Name D:\Data\user\NWNW-fengyang 20230321--11.d  
 Method tune\_low.m  
 Sample Name A-501  
 Comment

Acquisition Date 2023-3-21 16:41:00

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

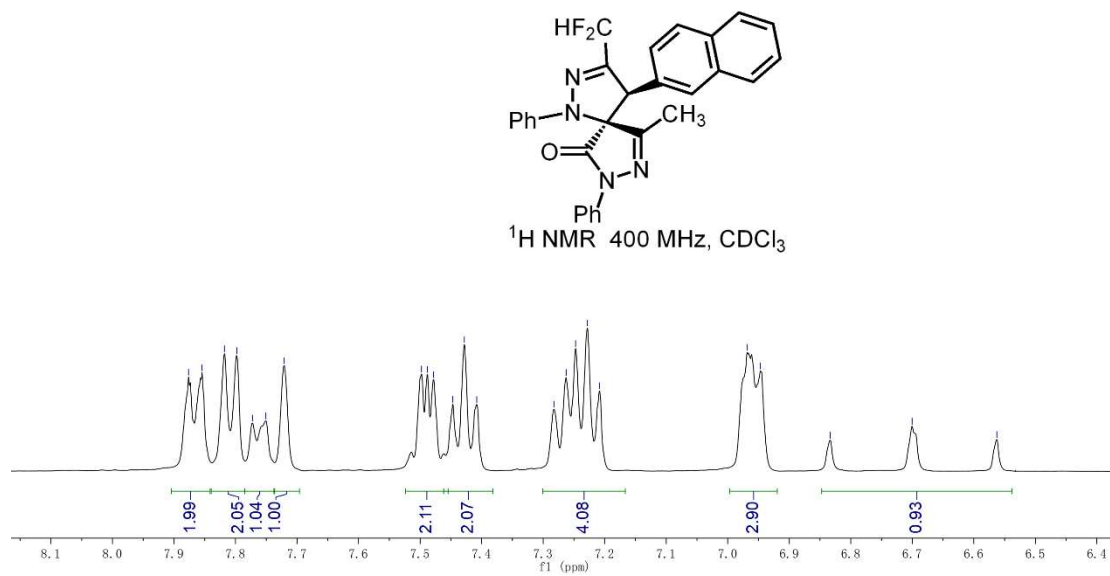
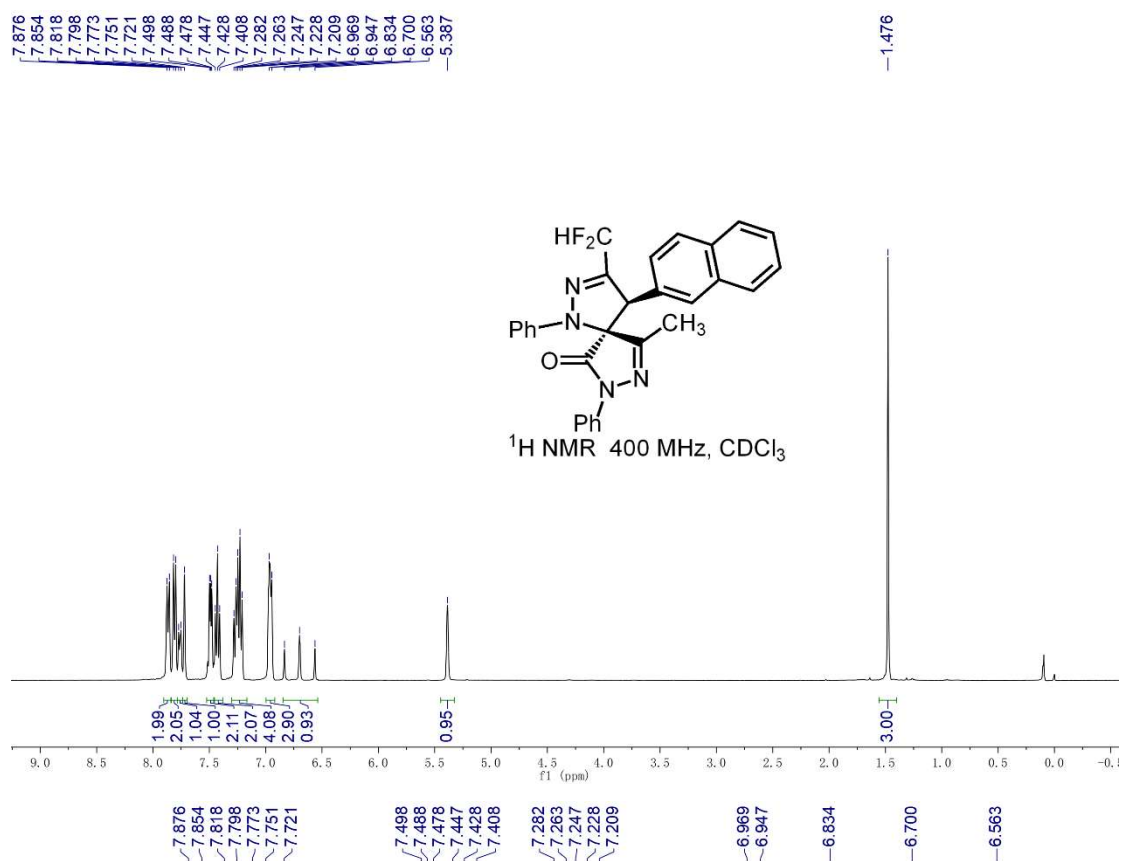
#### Acquisition Parameter

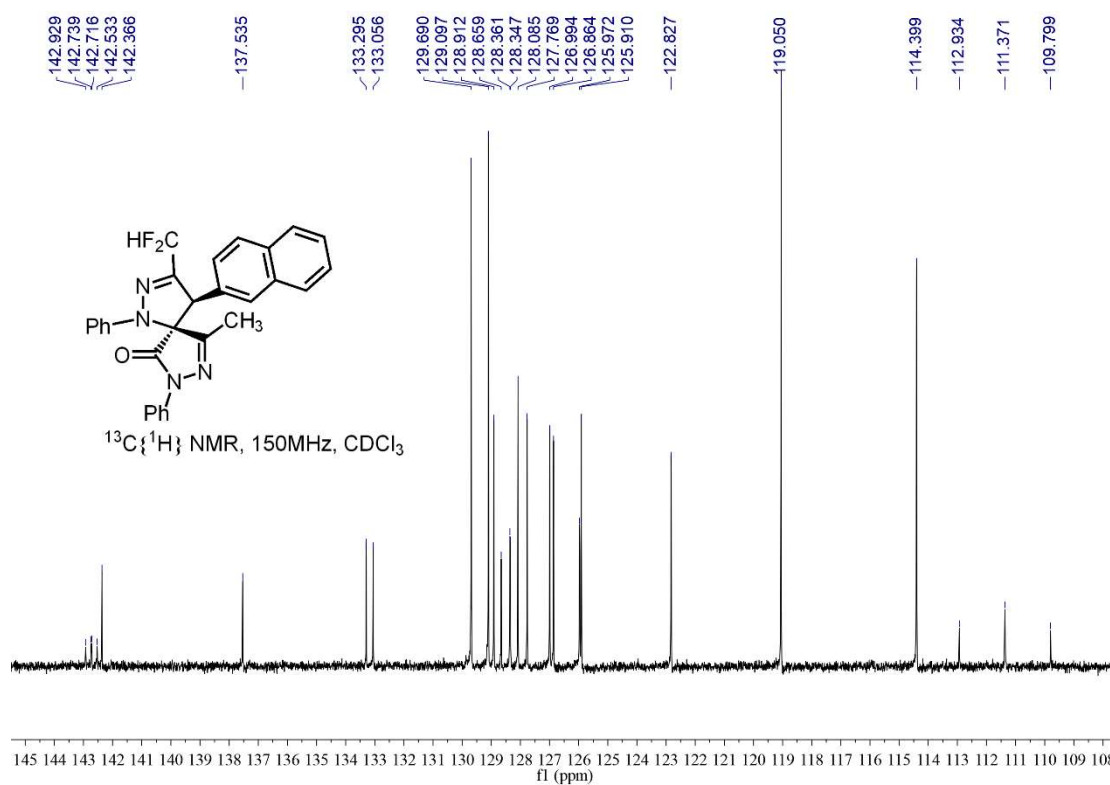
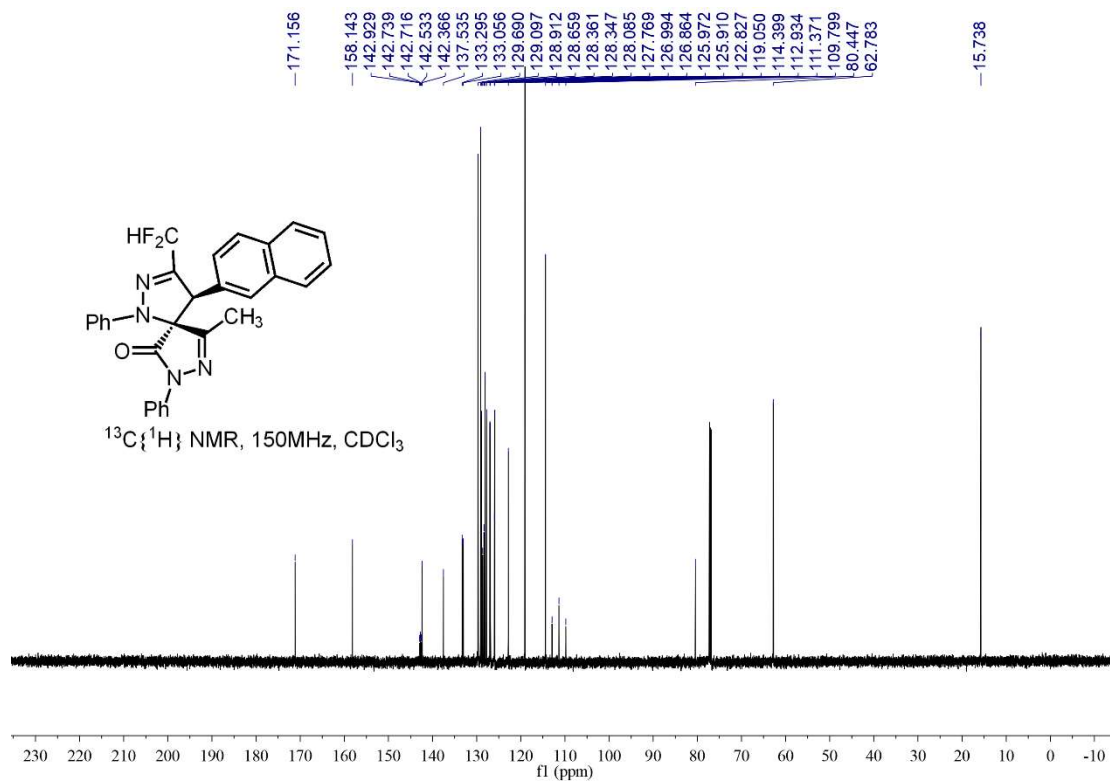
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{C}$
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>j</sub> Conf	m Sig	Std l	St d	St d l	St d	Std Com
m/z										Me an z	Va rN z	m/ or Dif	b Dev
471.1412	1 C <sub>25</sub> H <sub>19</sub> F <sub>3</sub> N <sub>4</sub> NaO	471.1403	-2.0	-2.1	16.5	ok	even	8.6	11.9	1.0	5.4	0.3	842.7

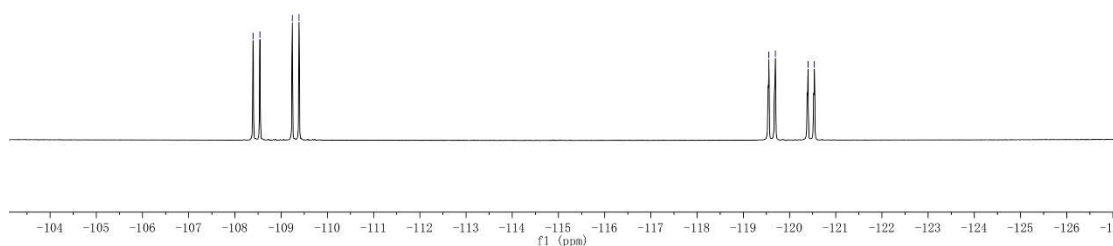
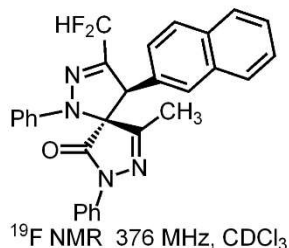
NMR copies of compound (*trans*)-4h:





-108.391  
-108.539  
-109.238  
-109.386

-119.554  
-119.694  
-120.401  
-120.541



HRMS (ESI) copy of compound (*trans*)-4h:

### Mass Spectrum SmartFormula Report

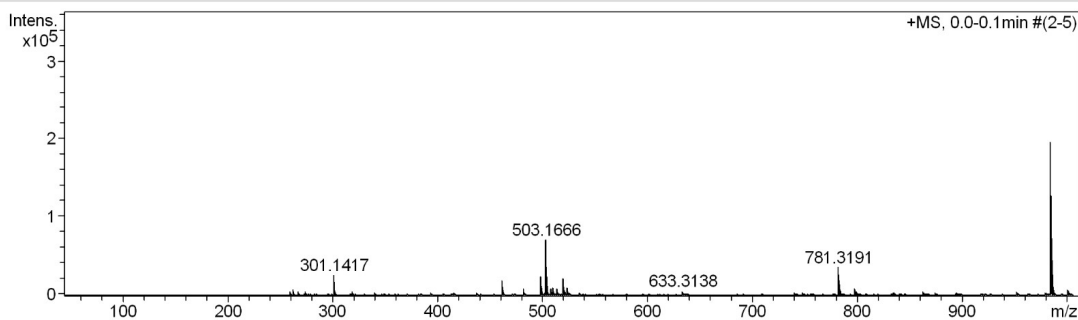
#### Analysis Info

Analysis Name D:\Data\user\NWN\U-fengyang 20230321-12.d  
Method tune\_low.m  
Sample Name A-34  
Comment

Acquisition Date 2023-3-21 16:43:38  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

#### Acquisition Parameter

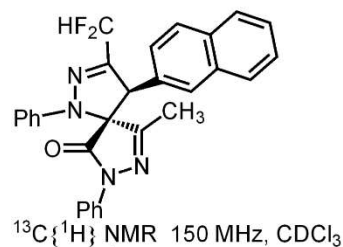
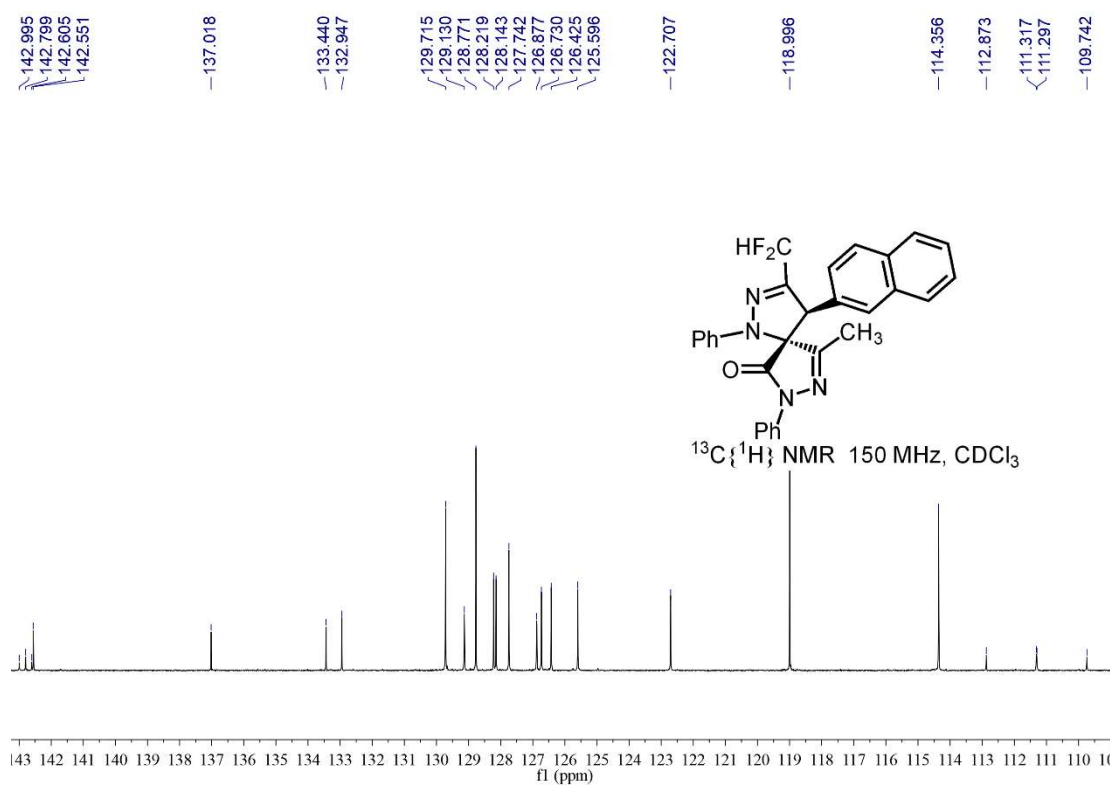
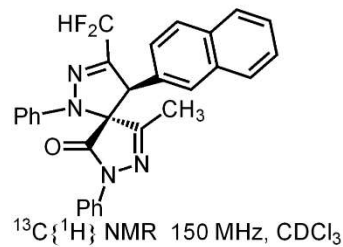
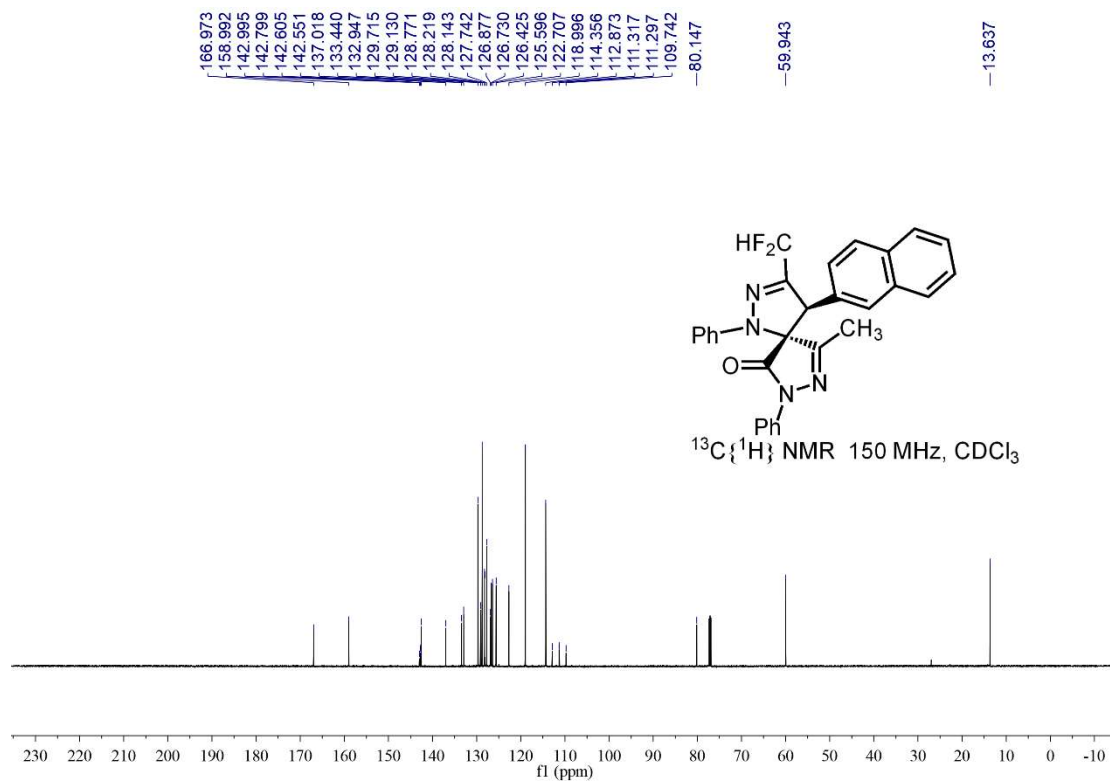
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej% Conf	m Sigma	Std l	St d	St d l	St d	Std Com b
503.1666	C <sub>29</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	503.1654	-2.5	-2.3	19.5	ok	even	6.0	10.2	1.2	4.2	0.9	842.7

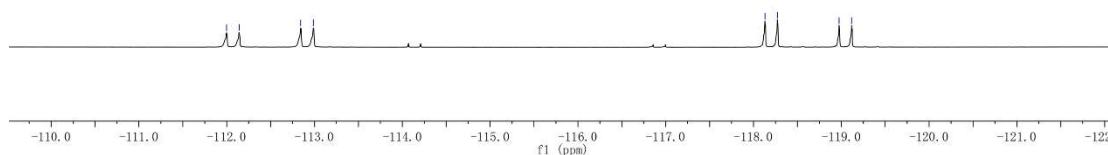
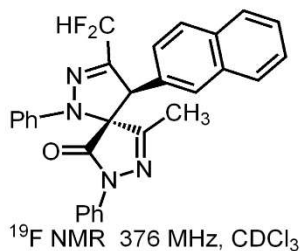






~111.997  
~112.142  
~112.843  
~112.987

~118.130  
~118.272  
~118.975  
~119.117



HRMS (ESI) copy of compound (*cis*)-4h:

### Mass Spectrum SmartFormula Report

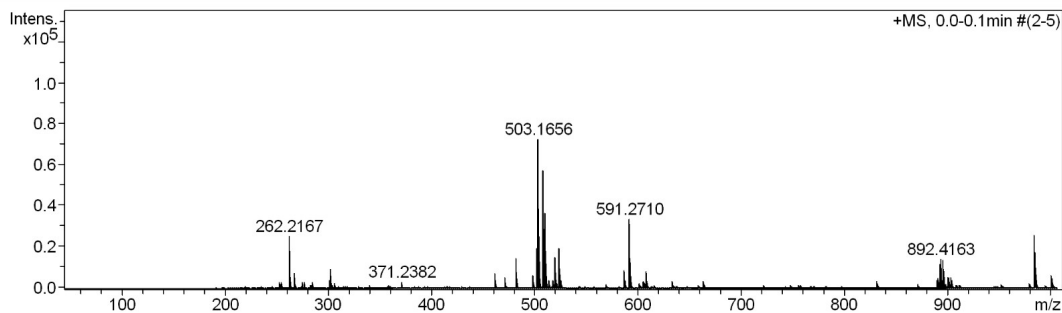
#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20230321--13.d  
Method tune\_low.m  
Sample Name A-341  
Comment

Acquisition Date 2023-3-21 17:05:28  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

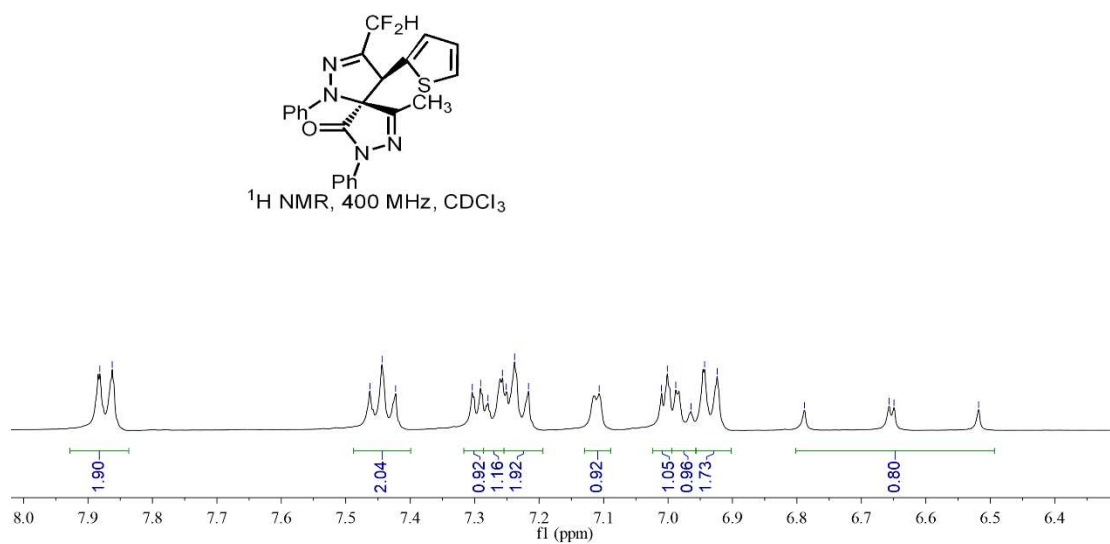
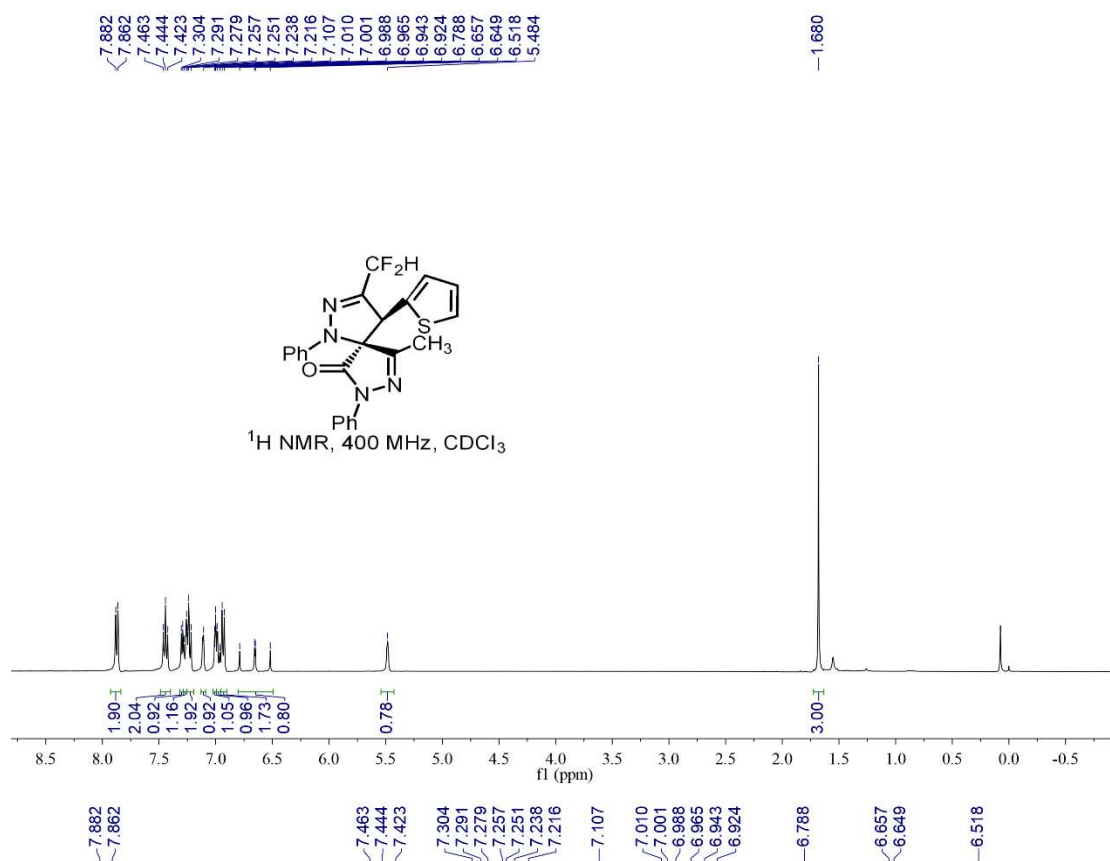
#### Acquisition Parameter

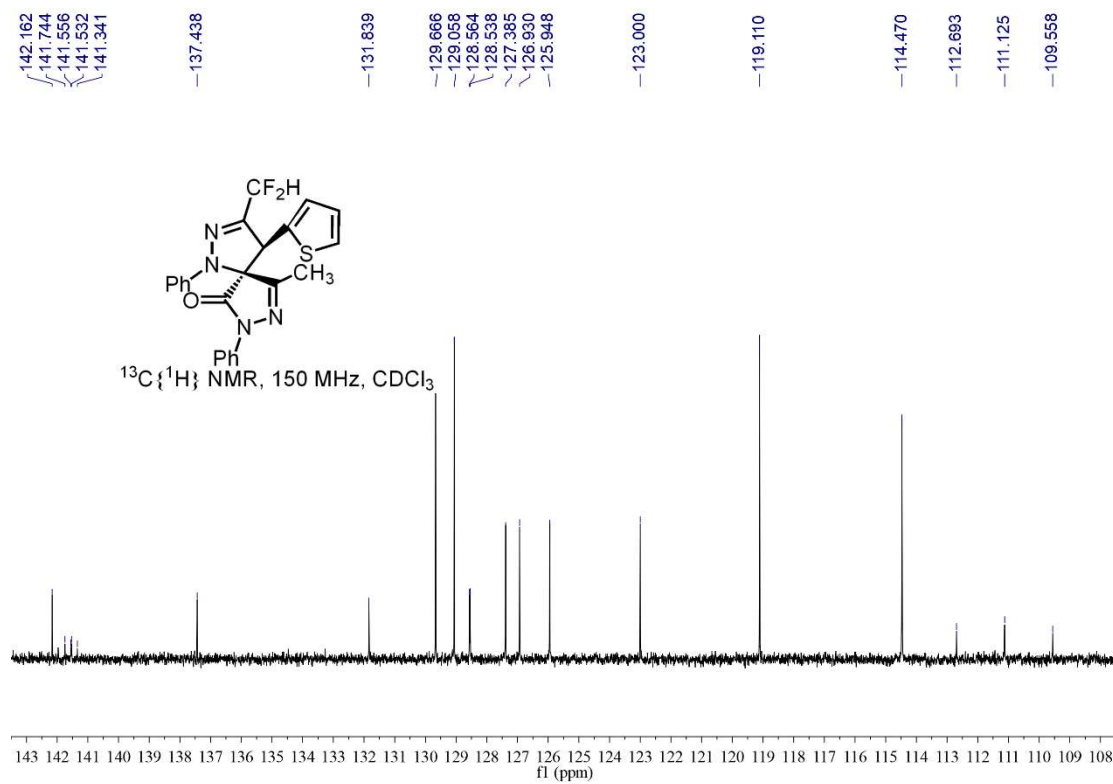
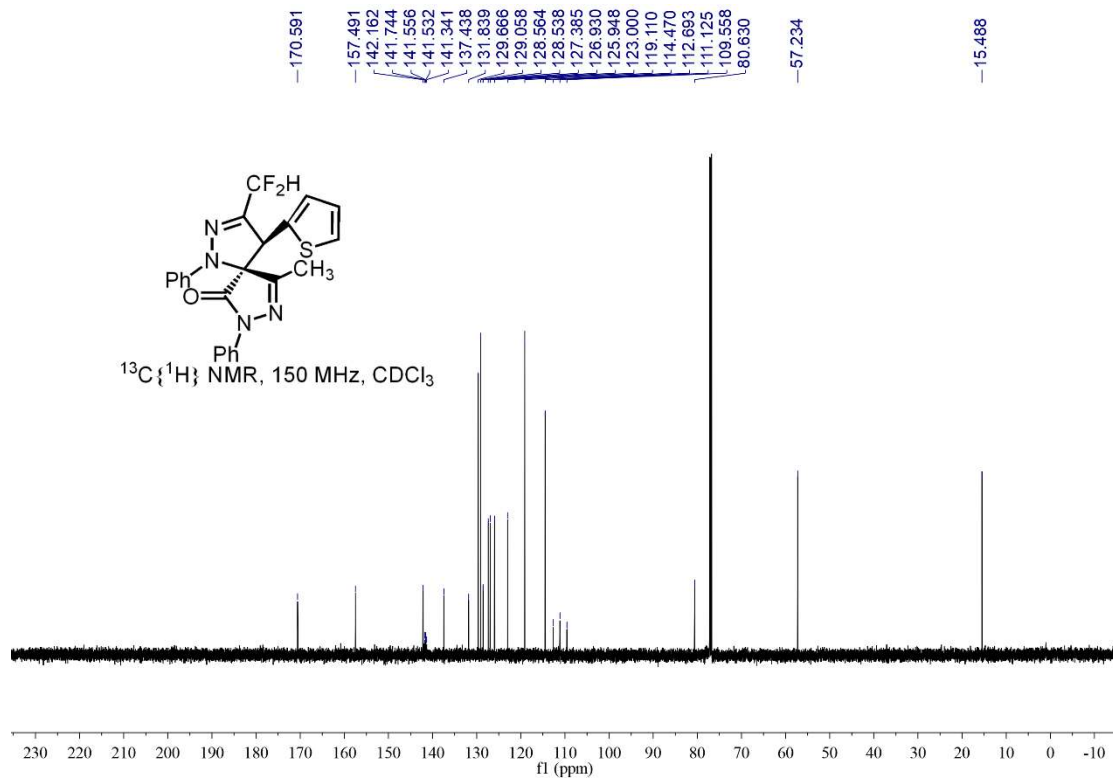
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j % Conf	mSi gma	Std l	St d	St d l	St d	St d	Std Com b Dev
503.1656	1 C <sub>29</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	503.1654	-0.3	0.3	19.5	ok	even	12.2	20.9	0.6	7.5	1.5	842.7	

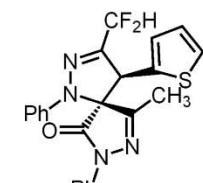
NMR copies of compound (*trans*)-4i:



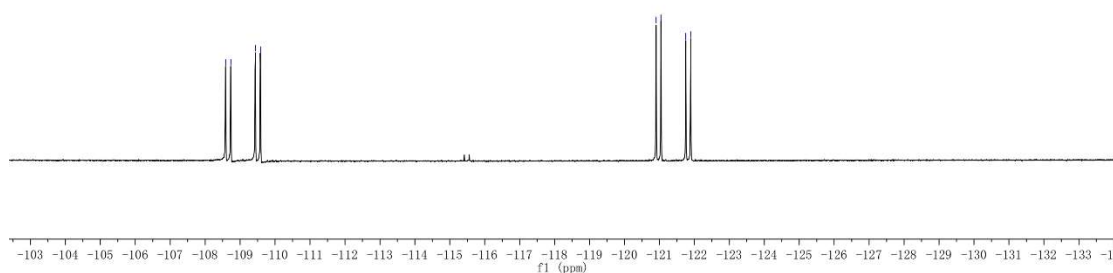


-108.588  
-108.736  
-109.438  
-109.585

-120.904  
-121.043  
-121.753  
-121.893



<sup>19</sup>F NMR 376 MHz, CDCl<sub>3</sub>



HRMS (ESI) copy of compound (*trans*)-4i:

### Mass Spectrum SmartFormula Report

#### Analysis Info

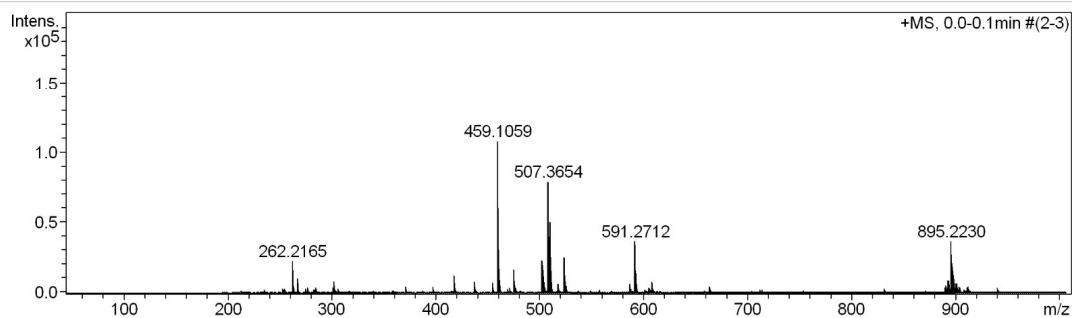
Analysis Name D:\Data\user\NWNNU-fengyang 20230321--14.d  
Method tune\_low.m  
Sample Name A-32  
Comment

Acquisition Date 2023-3-21 17:08:29

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

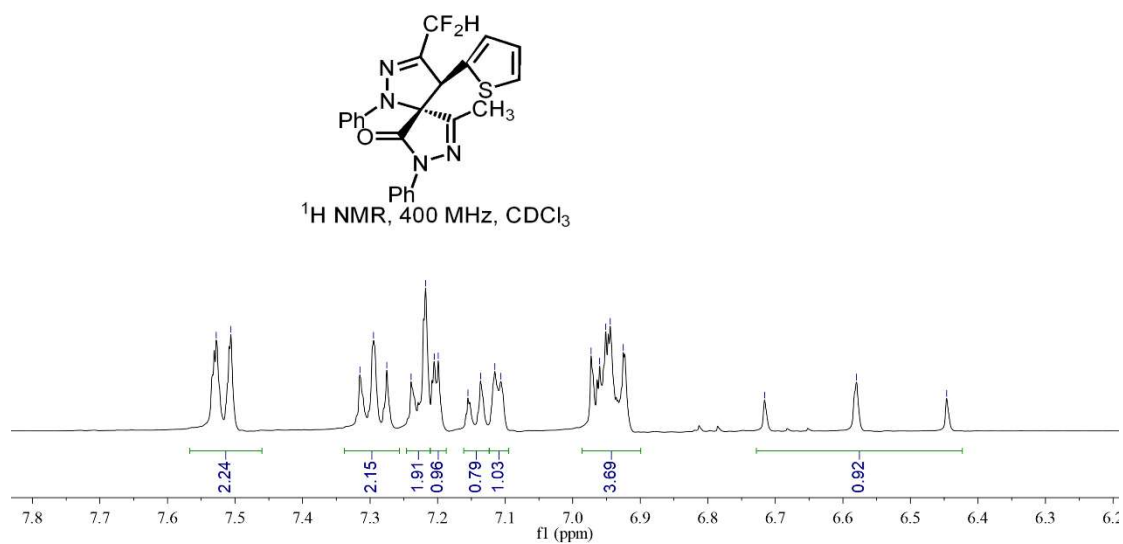
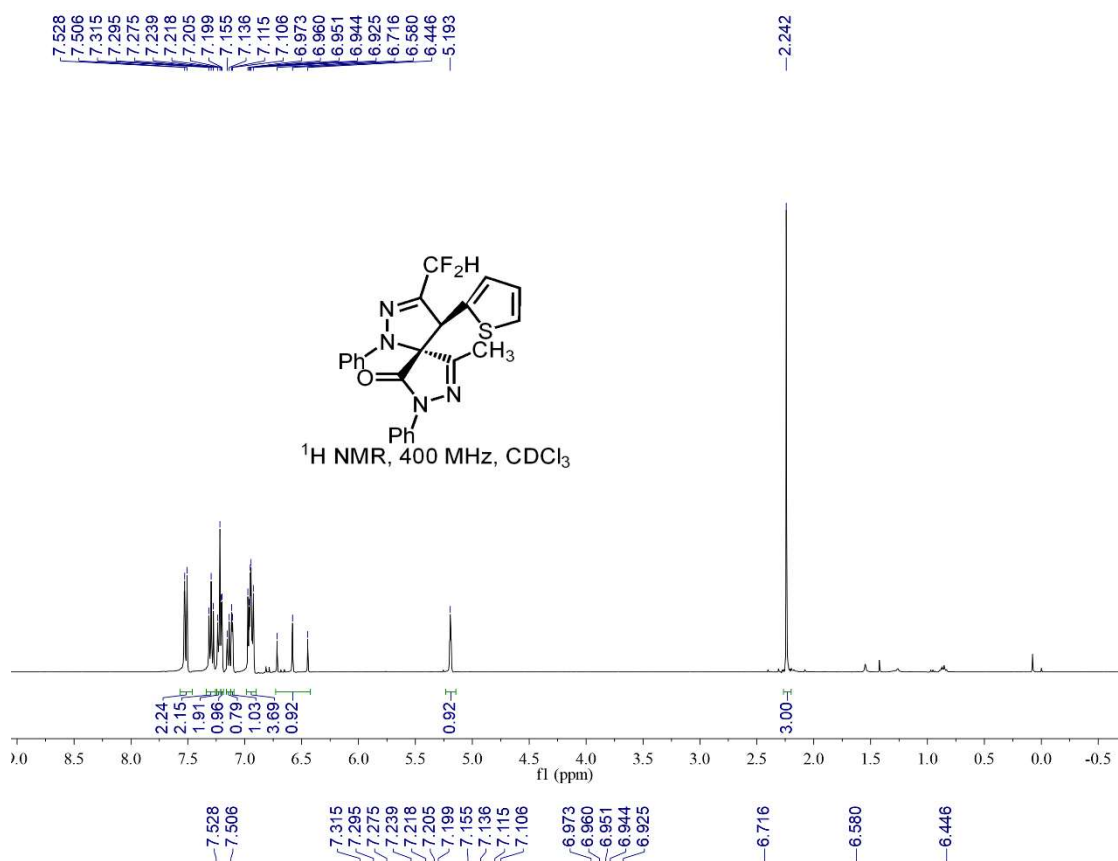
#### Acquisition Parameter

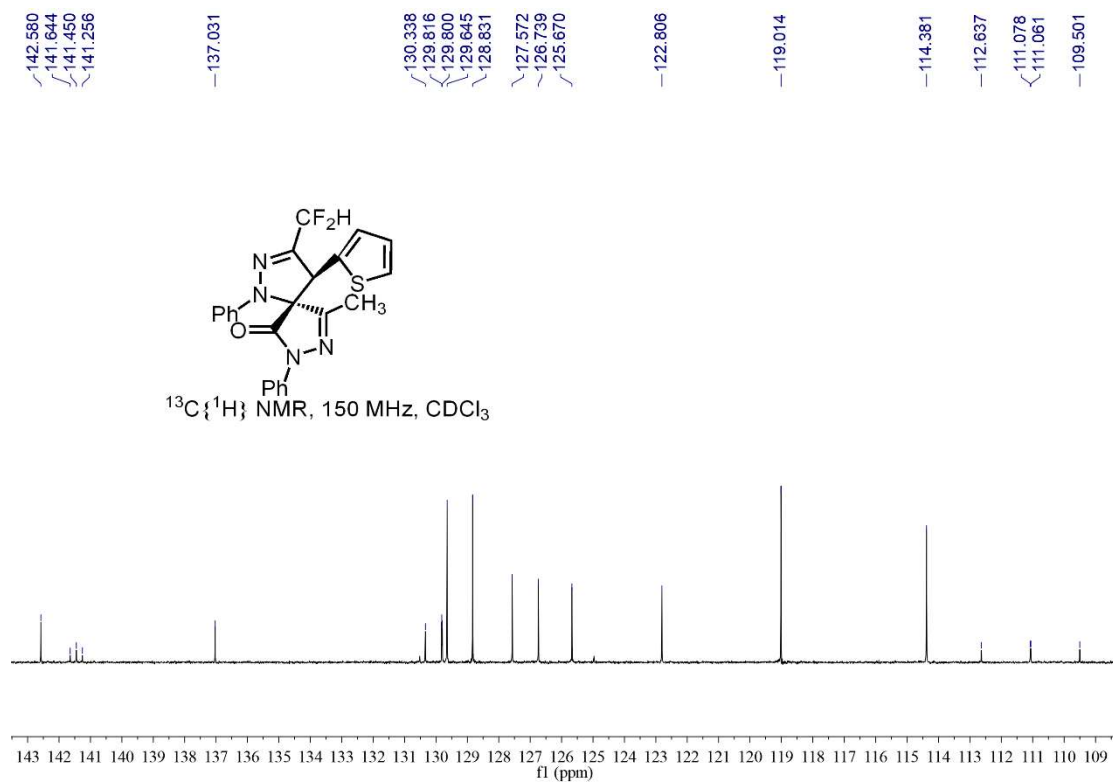
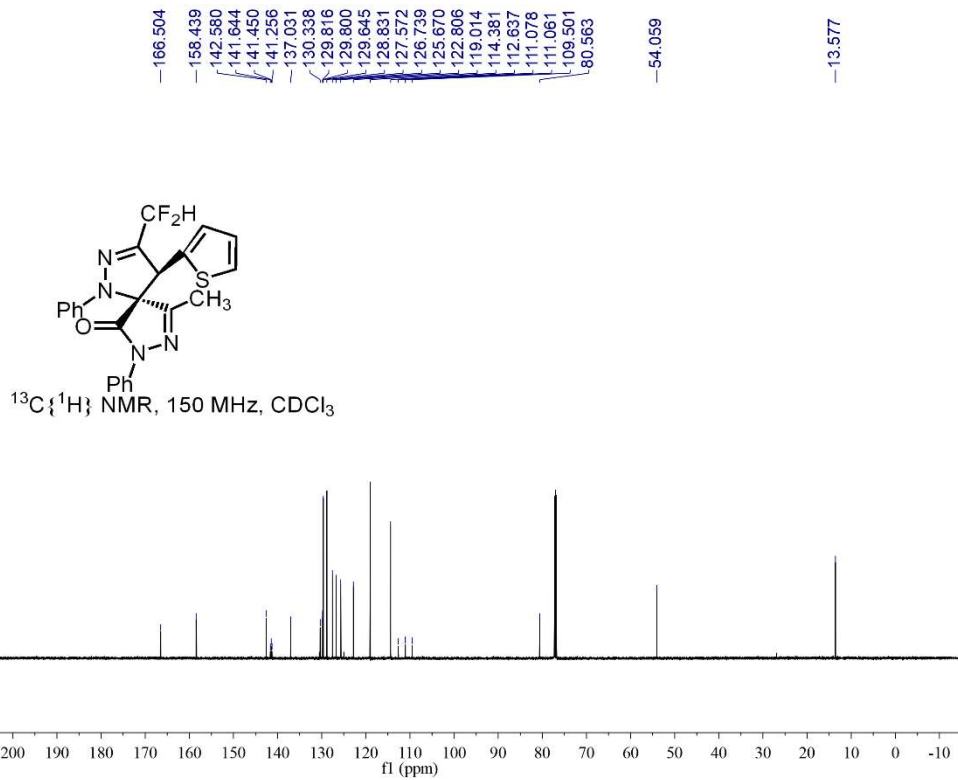
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 i°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



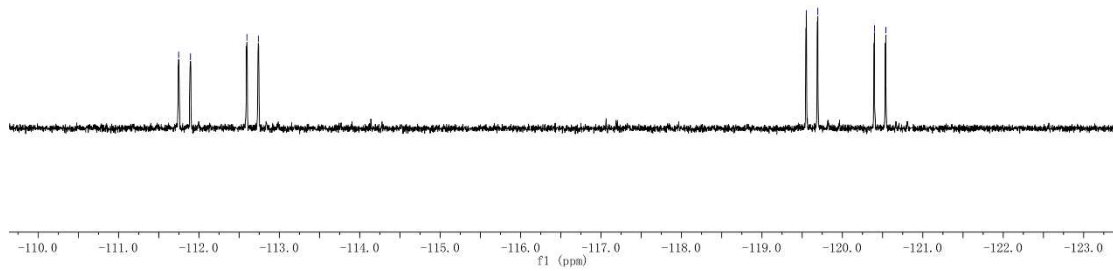
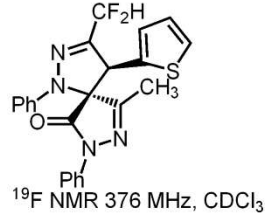
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>i</sub> Conf	m Si gm a	Std l	St d	St d l	St d	Std Com b
459.1059	C <sub>23</sub> H <sub>18</sub> F <sub>2</sub> N <sub>4</sub> NaOS	459.1062	0.5	-0.1	15.5	ok	even	6.5	11.7	1.0	3.9	2.6	842.7

NMR copies of compound (*cis*)-4i:





$\sim$ -111.748  
 $\sim$ -111.897  
 $\sim$ -112.596  
 $\sim$ -112.740  
 $\sim$ -119.552  
 $\sim$ -119.693  
 $\sim$ -120.398  
 $\sim$ -120.539



HRMS (ESI) copy of compound (*cis*)-4i:

### Mass Spectrum SmartFormula Report

#### Analysis Info

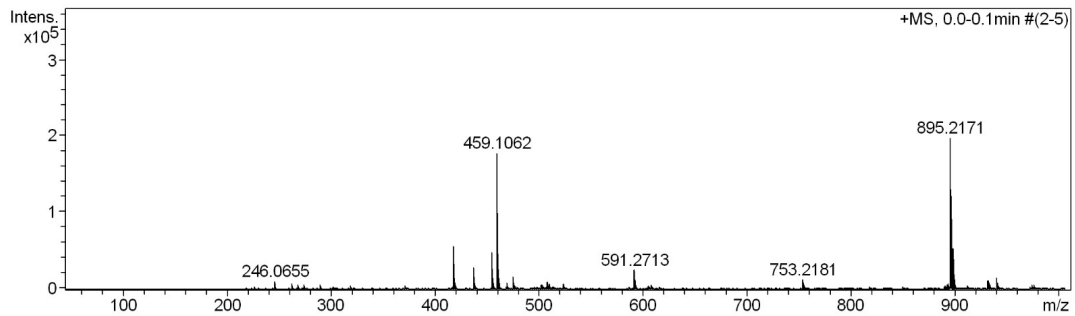
Analysis Name D:\Data\user\NWNW-fengyang 20230321-15.d  
 Method tune\_low.m  
 Sample Name A-321  
 Comment

Acquisition Date 2023-3-21 17:10:46

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

#### Acquisition Parameter

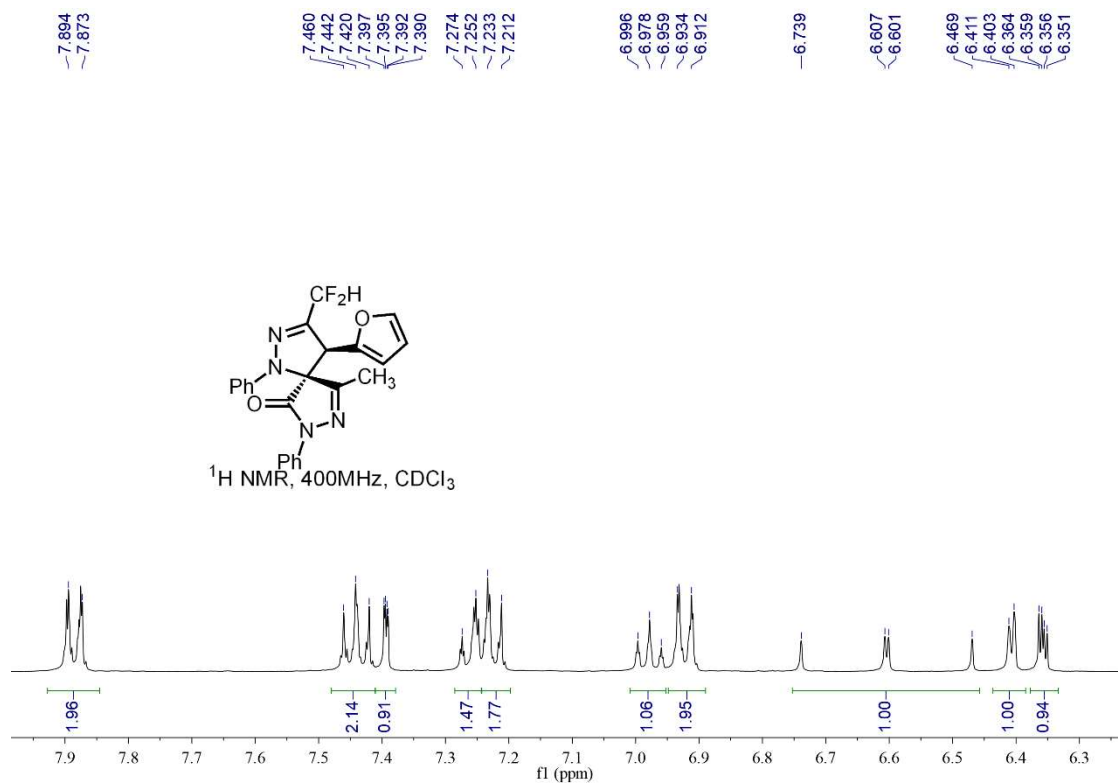
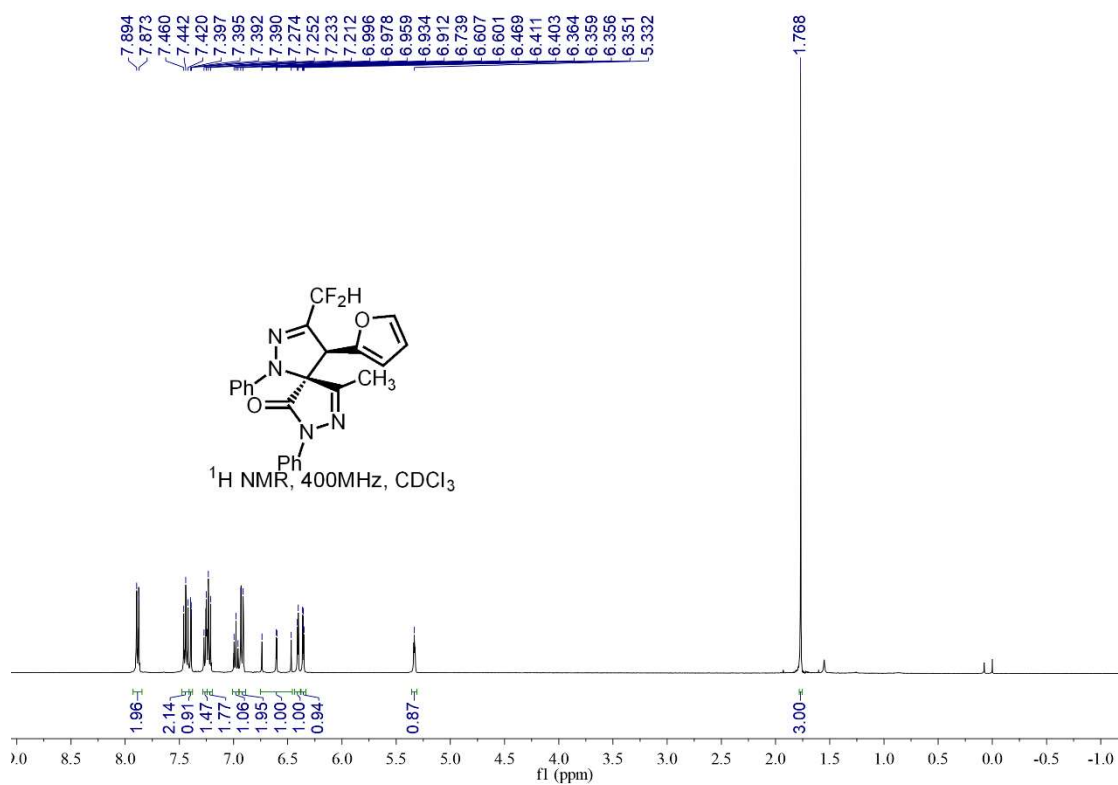
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 jnC
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

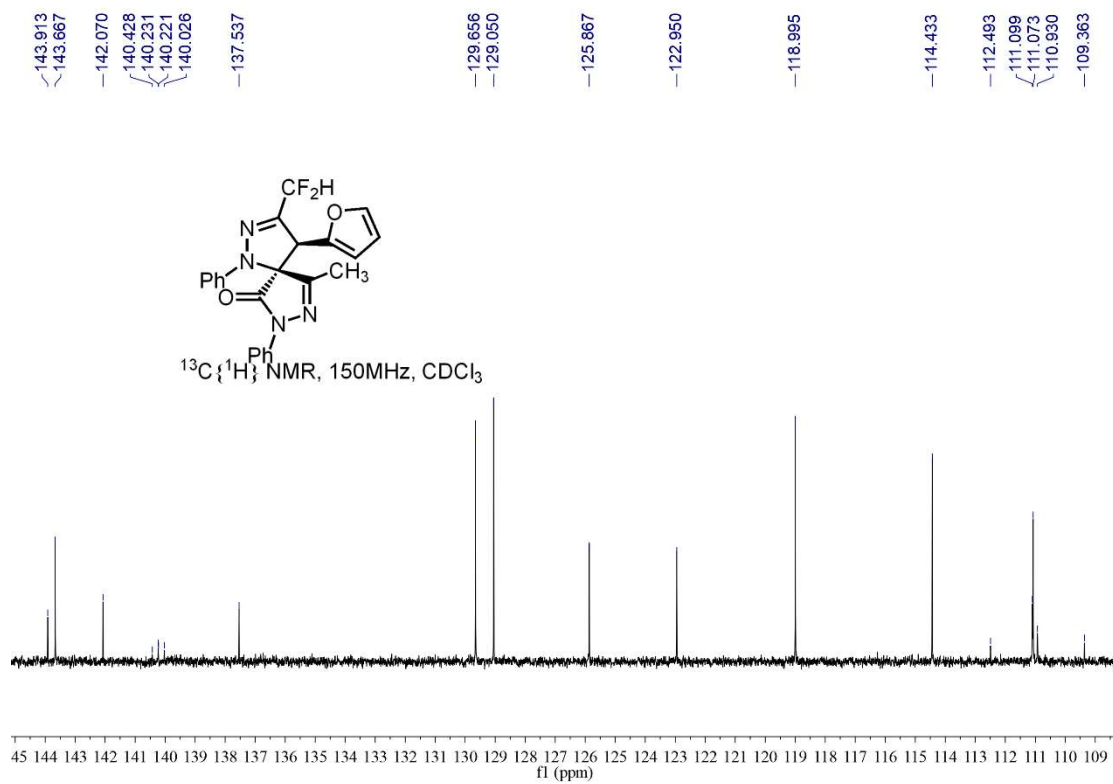
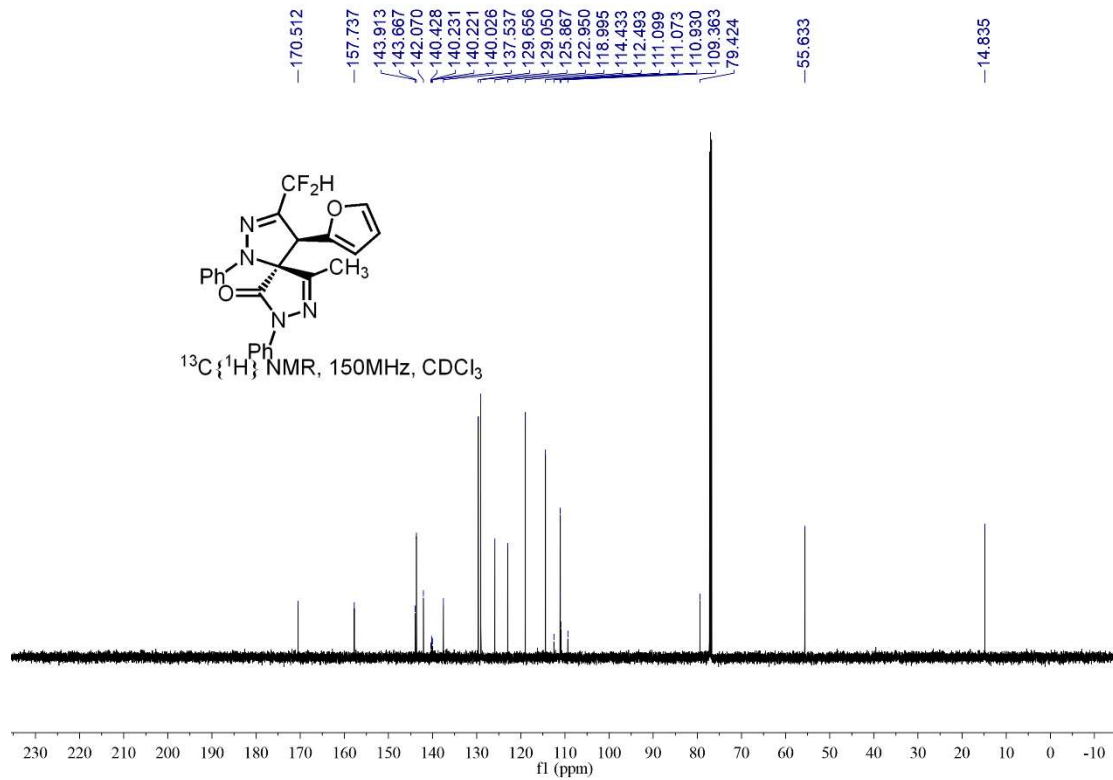


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>i</sub> ≠ Con	m Si gm a	Std l	St d	St d l	St d	Std Com b Dev
459.1062	1 C <sub>23</sub> H <sub>18</sub> F <sub>2</sub> N <sub>4</sub> NaOS	459.1062	-0.2	-1.1	15.5	ok	even	8.1	13.2	1.5	4.5	3.9	842.7



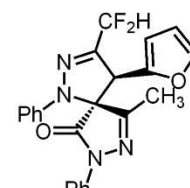
NMR copies of compound (*trans*)-4j:



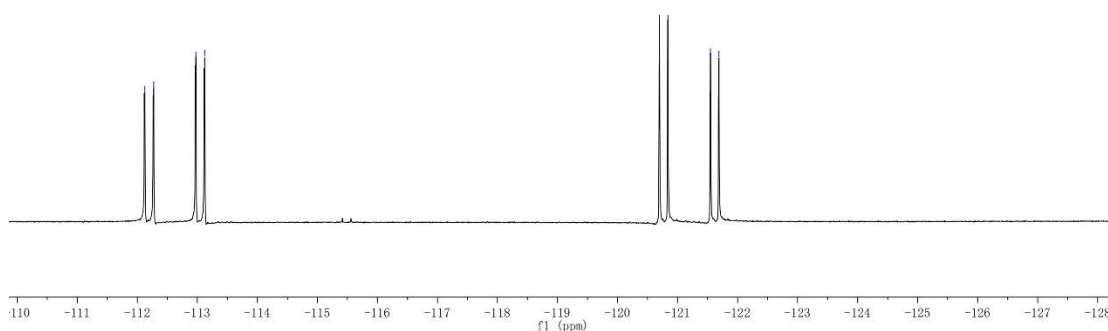


~112.126  
~112.272  
~112.976  
~113.122

~120.699  
~120.839  
~121.549  
~121.689



<sup>19</sup>F NMR 376 MHz, CDCl<sub>3</sub>



HRMS (ESI) copy of compound (*trans*)-4j:

### Mass Spectrum SmartFormula Report

#### Analysis Info

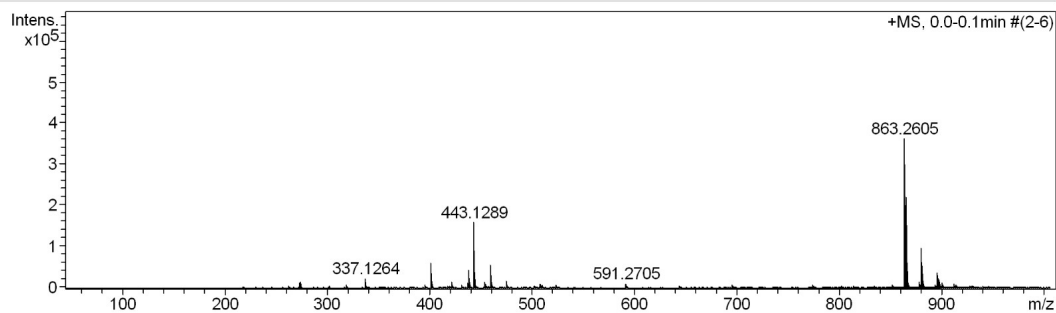
Analysis Name D:\Data\user\NWNNU-fengyang 20230321-16.d  
Method tune\_low.m  
Sample Name A-33  
Comment

Acquisition Date 2023-3-21 17:13:40

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

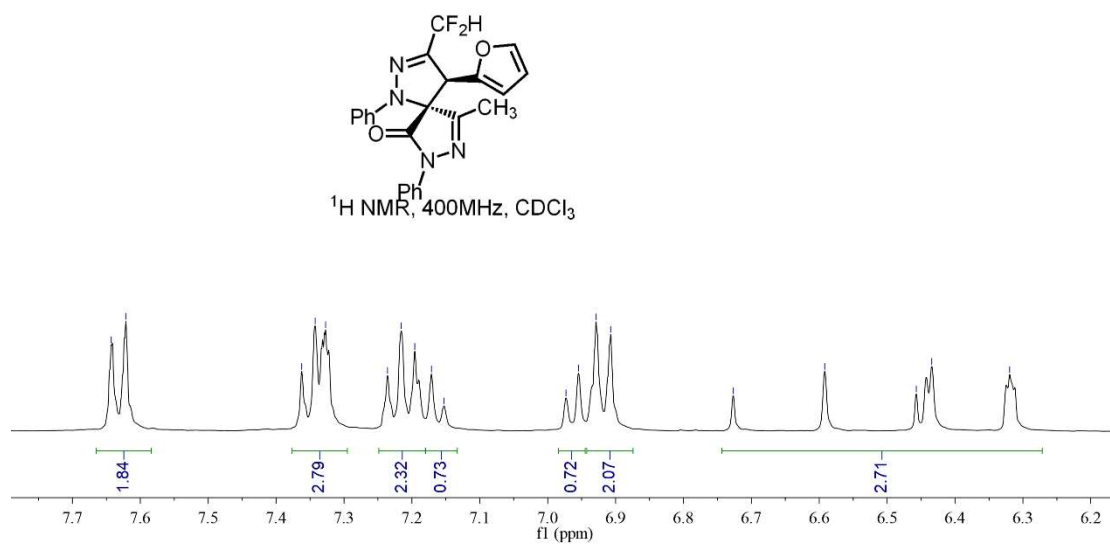
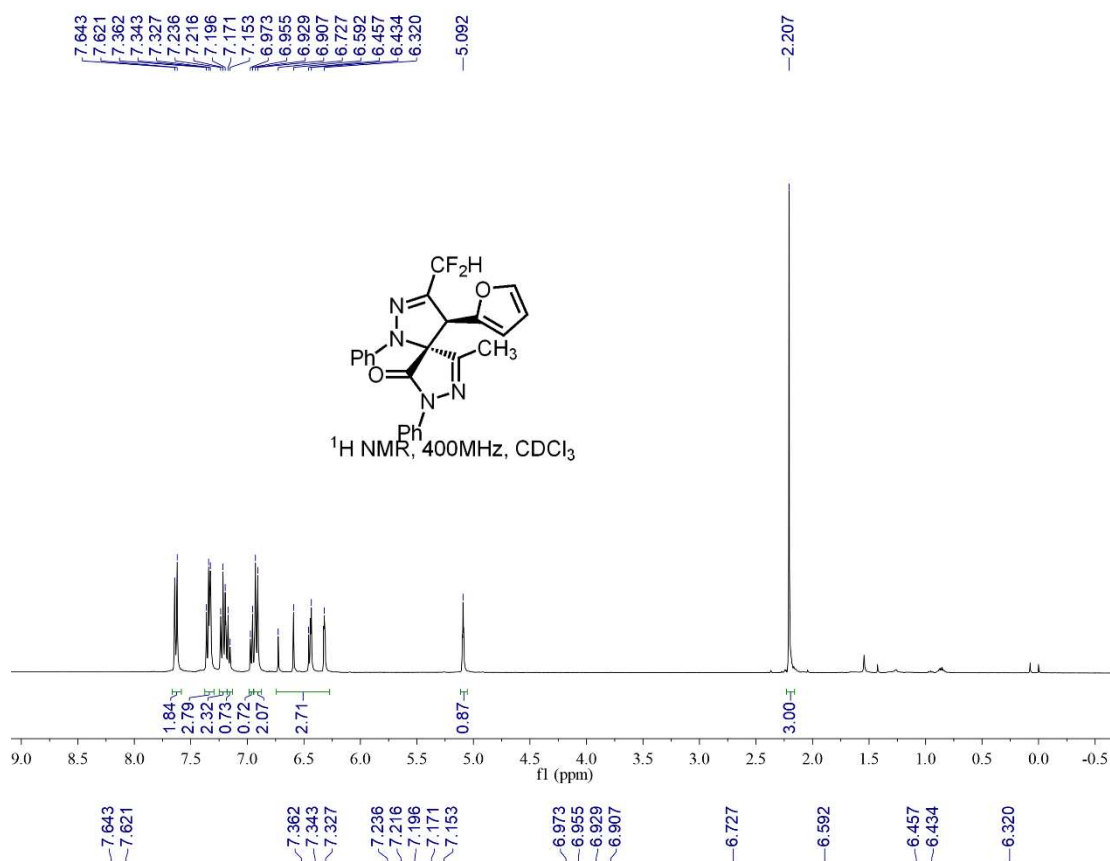
#### Acquisition Parameter

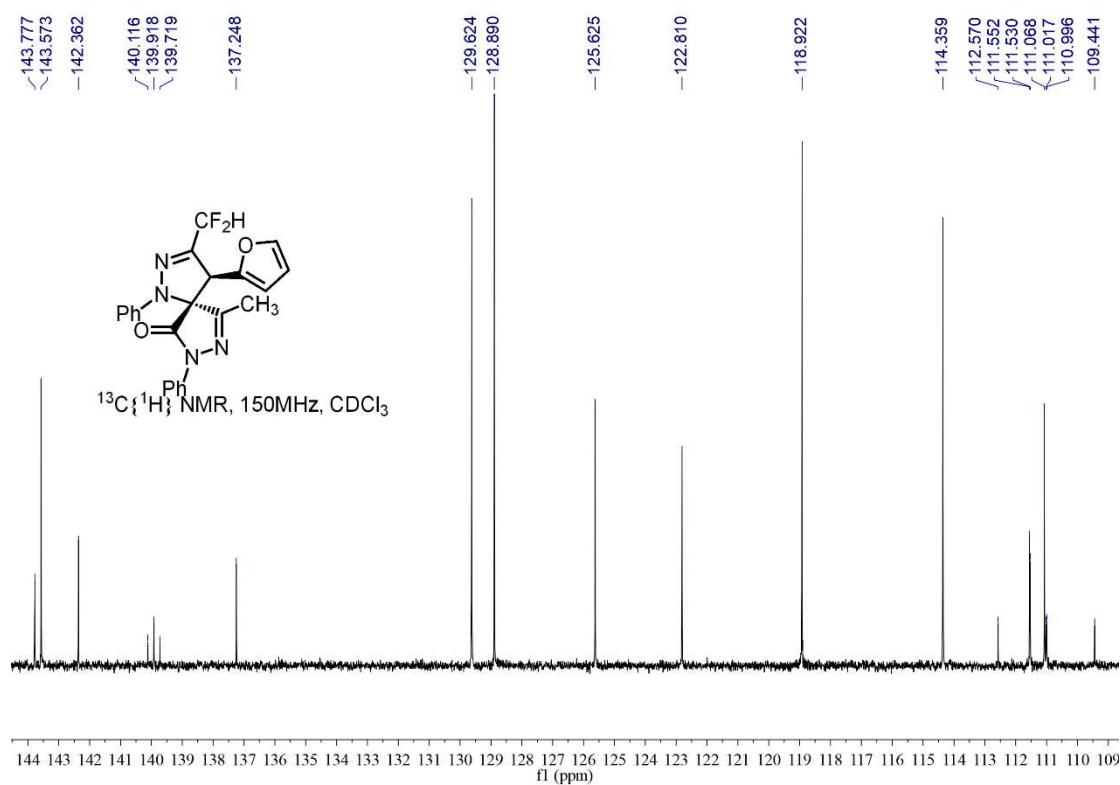
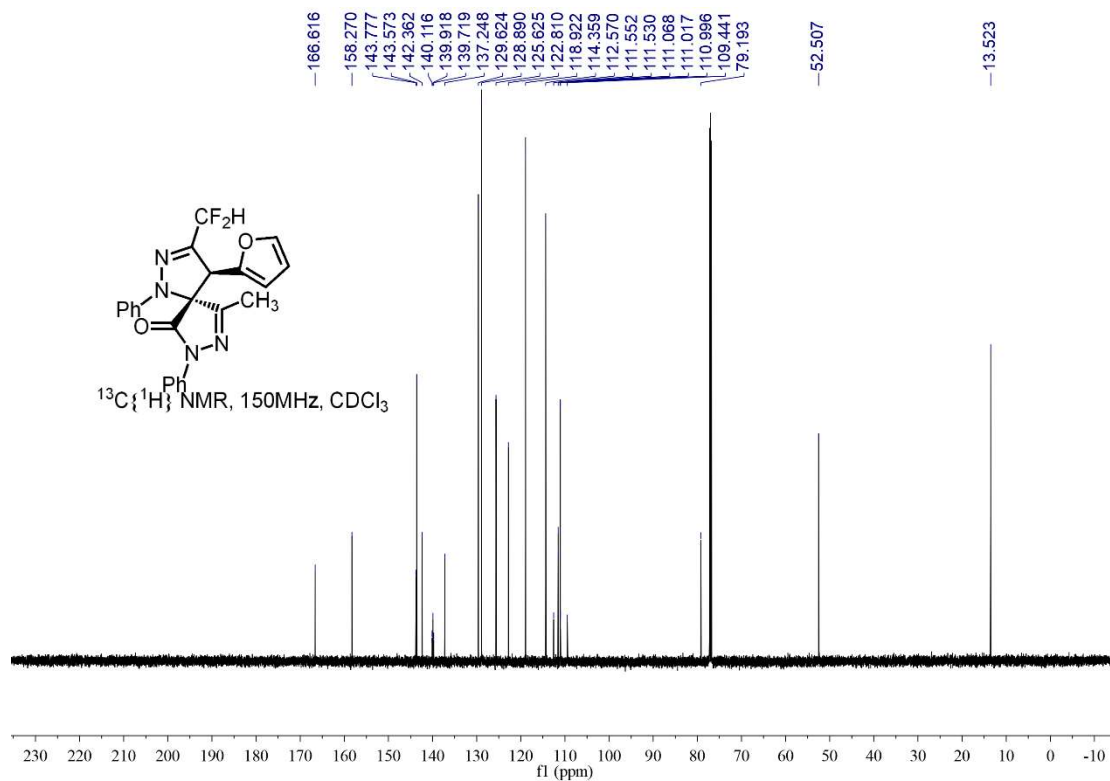
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

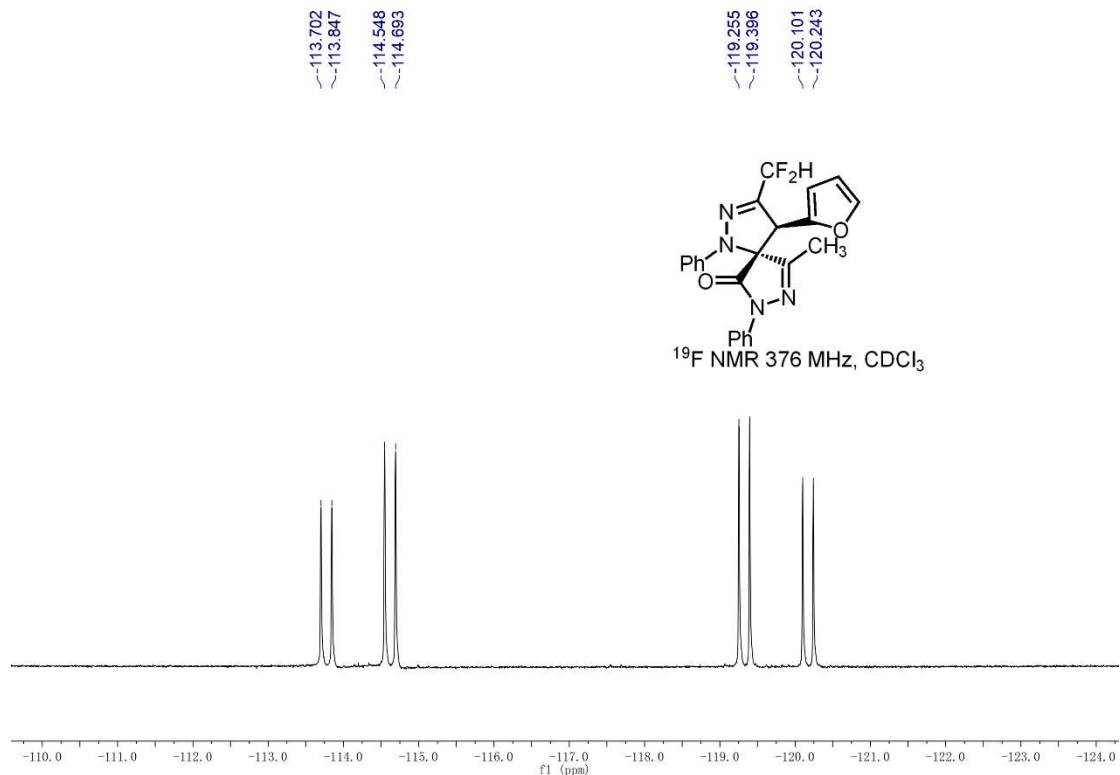


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>i</sub> ≠ Conf	m Sig	Std I	St d	St d I	St d	Std Com
443.1289	1 C <sub>23</sub> H <sub>18</sub> F <sub>2</sub> N <sub>4</sub> NaO <sub>2</sub>	443.1290	0.2	-0.1	15.5	ok	even	9.4	14.5	0.6	6.1	1.1	842.7

NMR copies of compound (*cis*)-4j:







HRMS (ESI) copy of compound (*cis*)-4j:

### Mass Spectrum SmartFormula Report

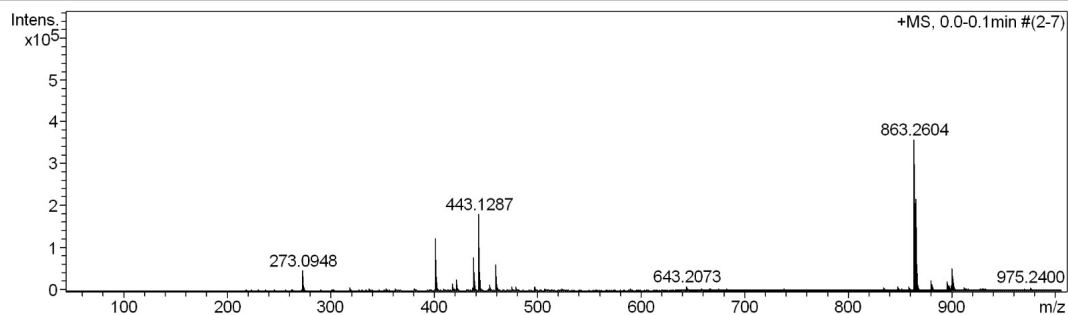
#### Analysis Info

Analysis Name D:\Data\user\NWN\U-fengyang 20230321-17.d  
 Method tune\_low.m  
 Sample Name A-331  
 Comment

Acquisition Date 2023-3-21 17:15:42  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

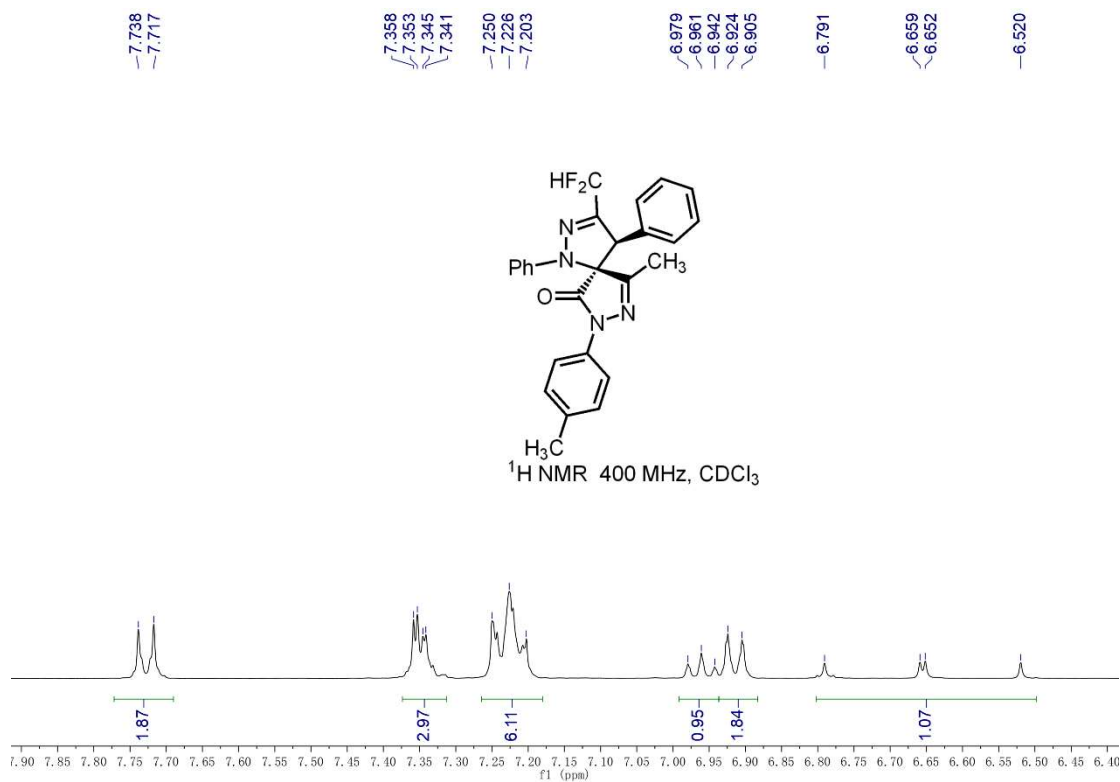
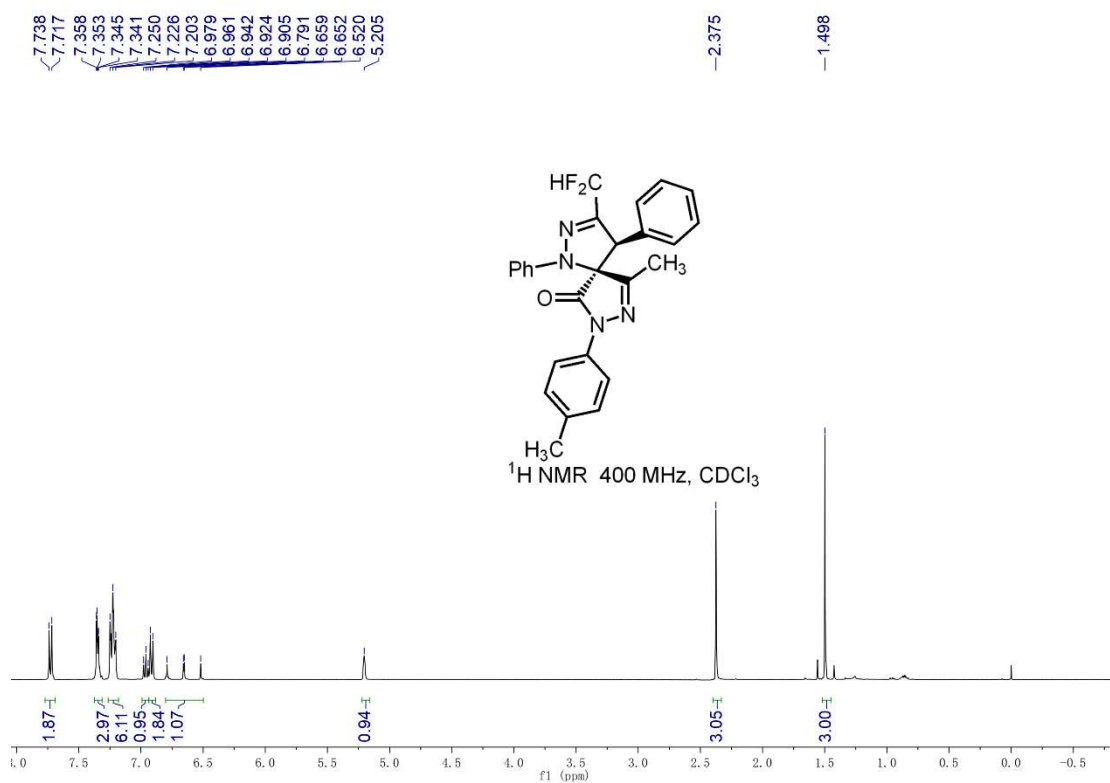
#### Acquisition Parameter

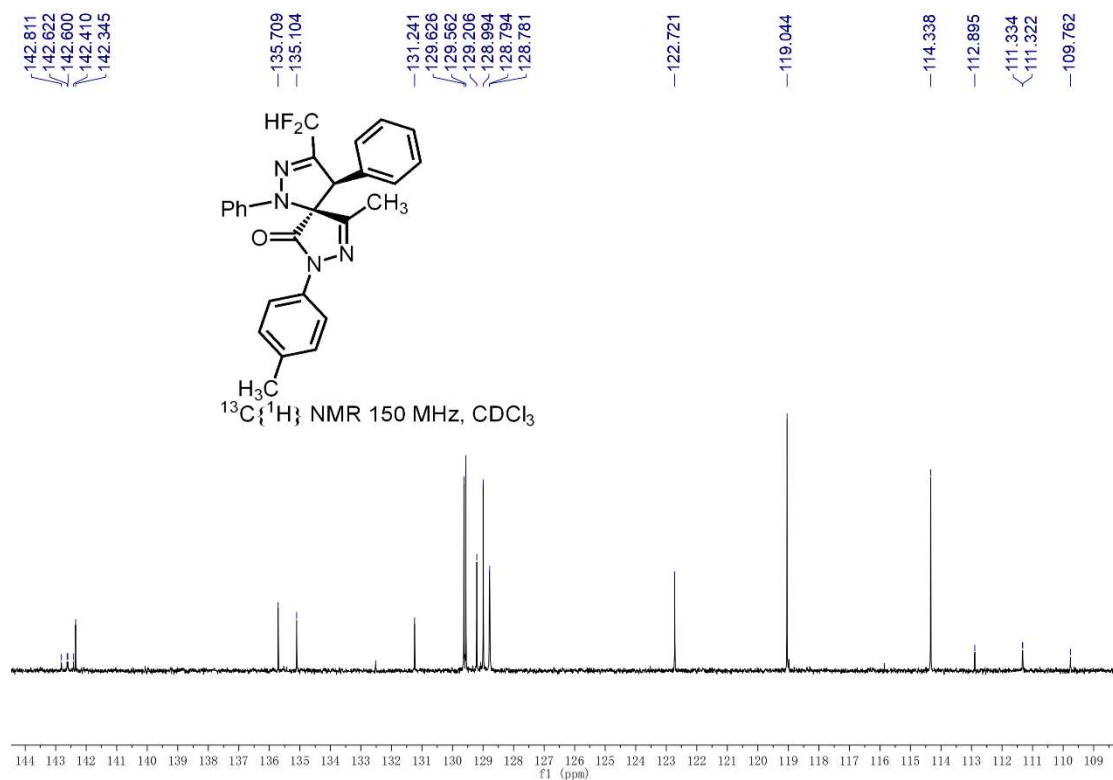
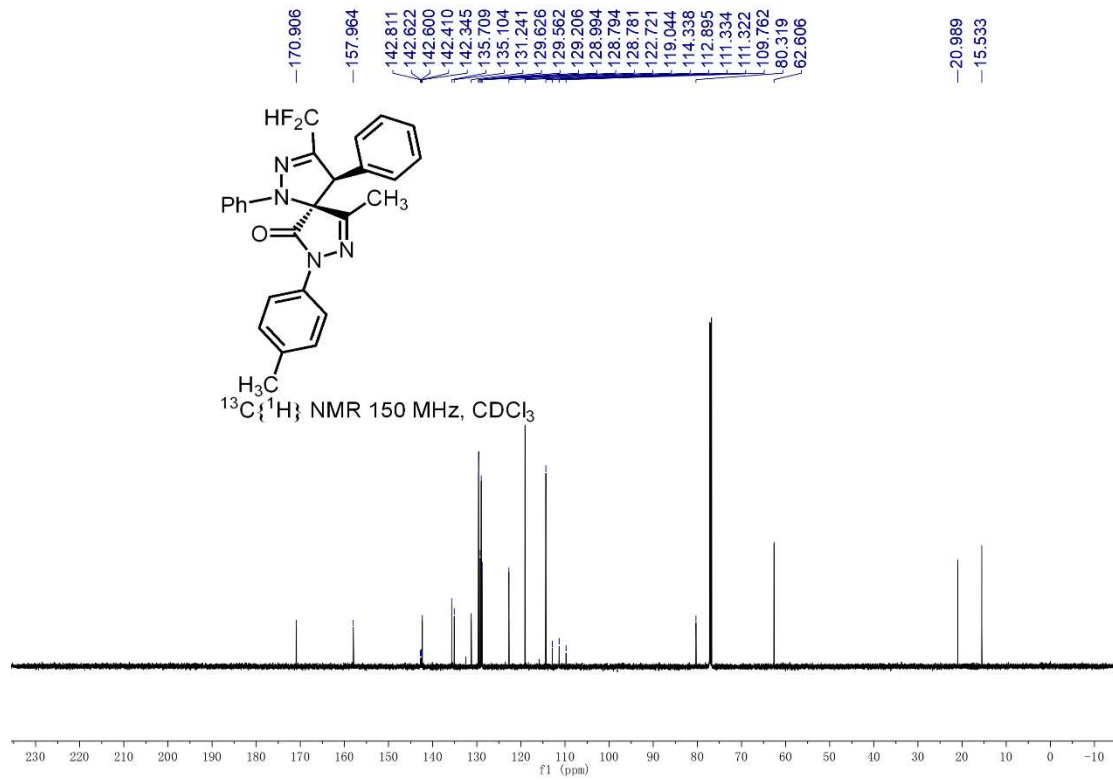
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



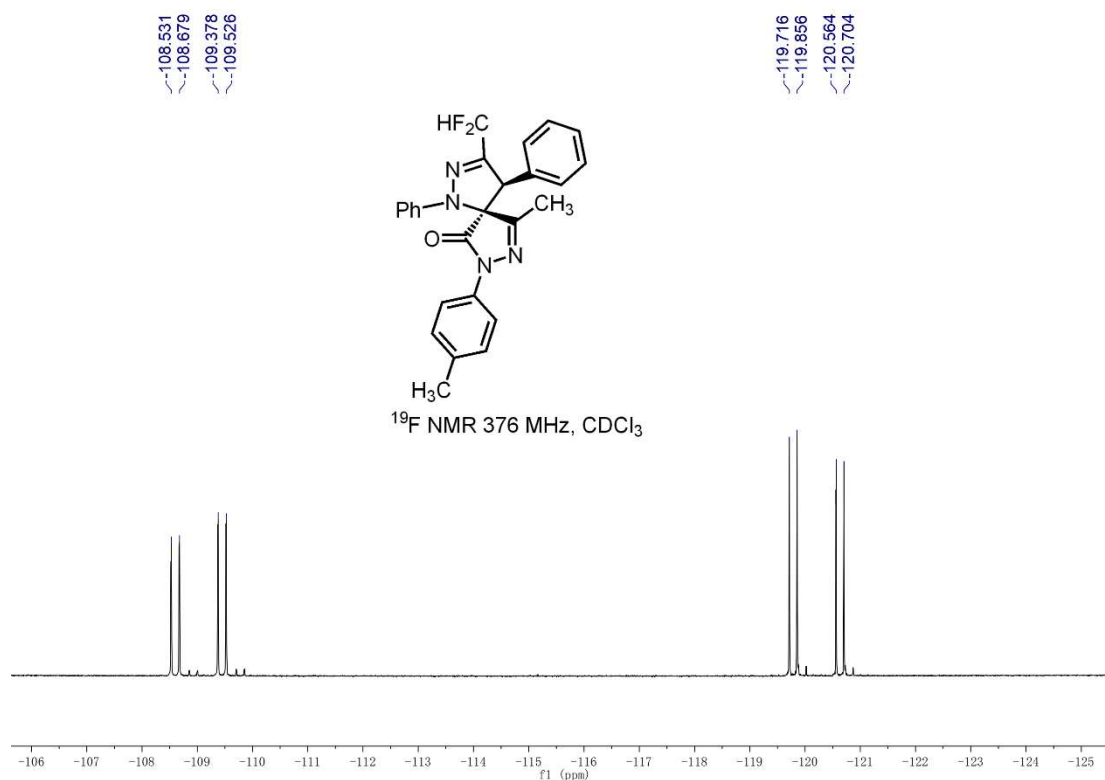
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j ≠ Conf	mSi gm a	Std l	St d Me an z	St d l rN or m	St d m/ Dif f	Std Com b Dev
443.1287	1 C <sub>23</sub> H <sub>18</sub> F <sub>2</sub> N <sub>4</sub> NaO <sub>2</sub>	443.1290	0.8	0.4	15.5	ok	even	12.7	19.0	0.5	8.2	1.0	842.7

NMR copies of compound (*trans*)-4I:









HRMS (ESI) copy of compound (*trans*)-4l:

### Mass Spectrum SmartFormula Report

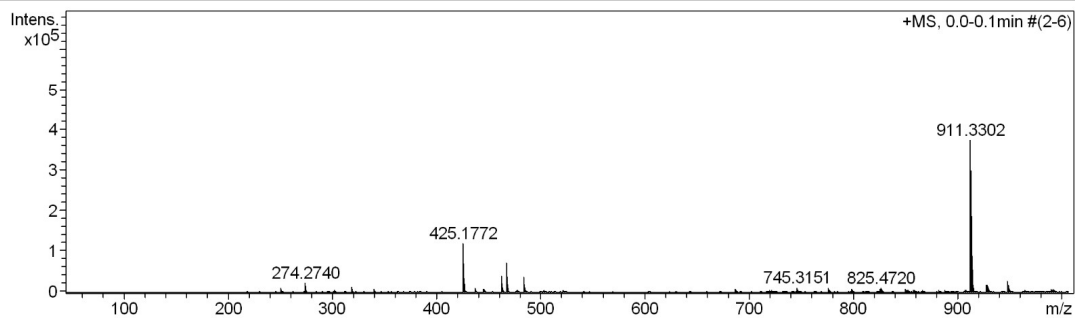
**Analysis Info**

Analysis Name D:\Data\user\NWN\U-fengyang 20230321-18.d  
 Method tune\_low.m  
 Sample Name A-53  
 Comment

Acquisition Date 2023-3-21 17:18:49  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

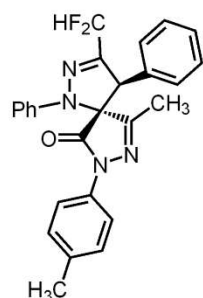
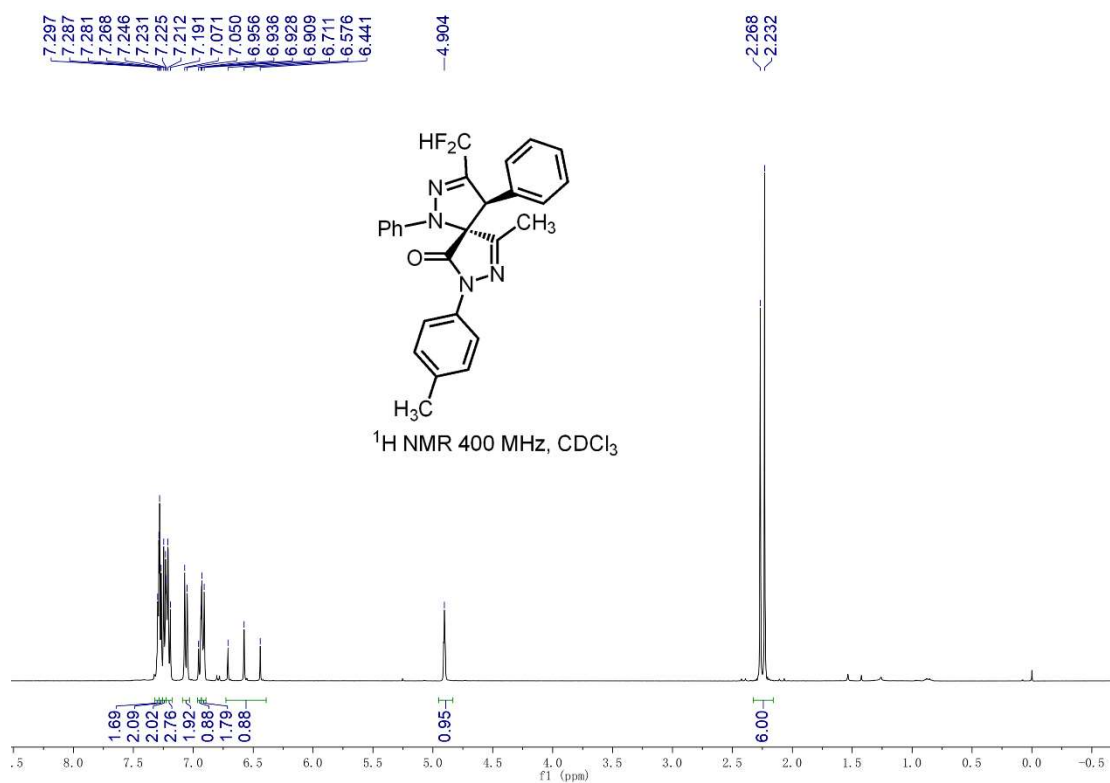
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

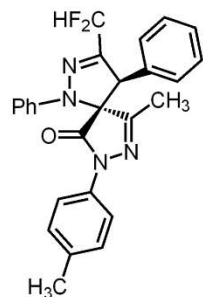
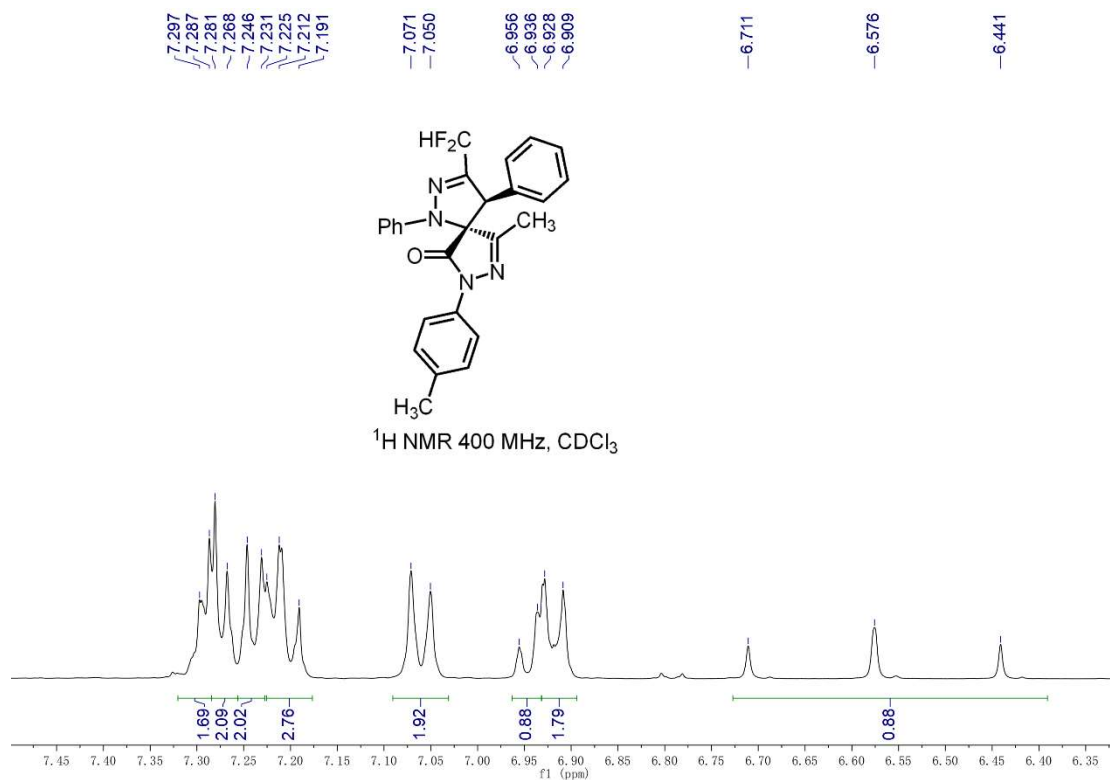


Meas. m/z	#	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej#	Conf	mS	Std	Std	Std	Std	Std
											l	Me	l	m/	Std
												an	Val	z	Dev
												m/	rN	Diff	
467.1651	1	C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	0.7	0.6	16.5	ok	even		5.7	8.3	0.3	3.5	0.2	842.7

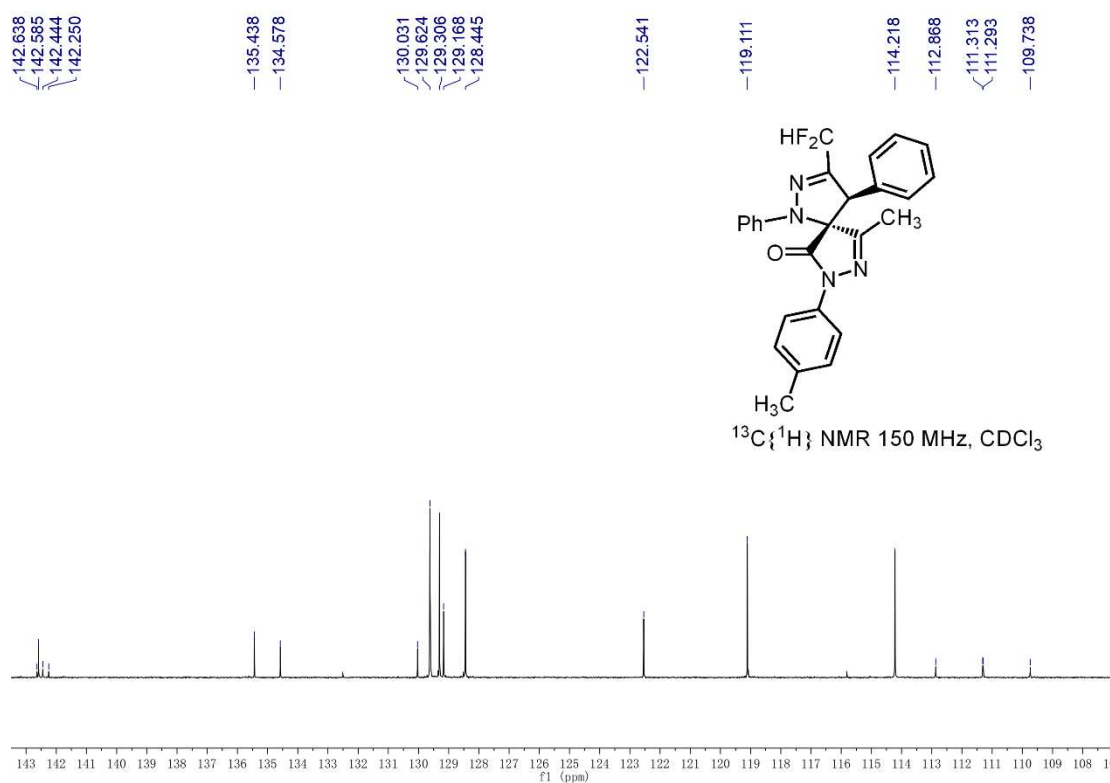
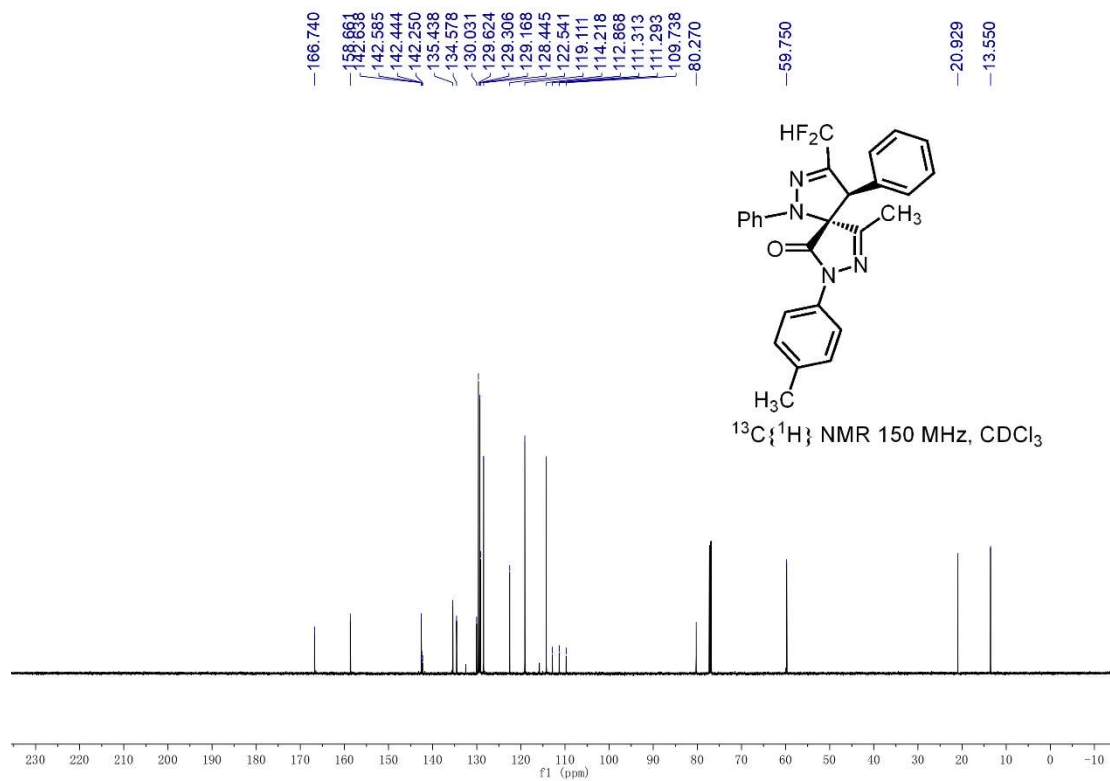
NMR copies of compound (*cis*)-41:

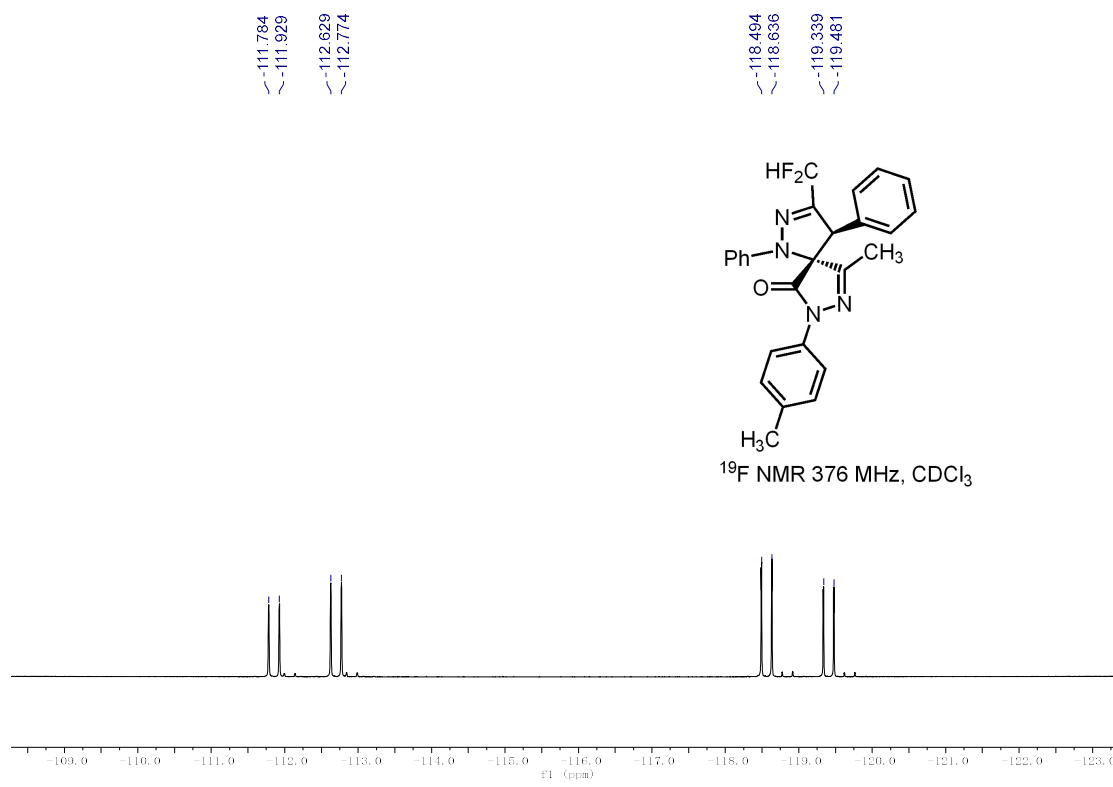


<sup>1</sup>H NMR 400 MHz, CDCl<sub>3</sub>



<sup>1</sup>H NMR 400 MHz, CDCl<sub>3</sub>





HRMS (ESI) copy of compound (*cis*)-4l:

### Mass Spectrum SmartFormula Report

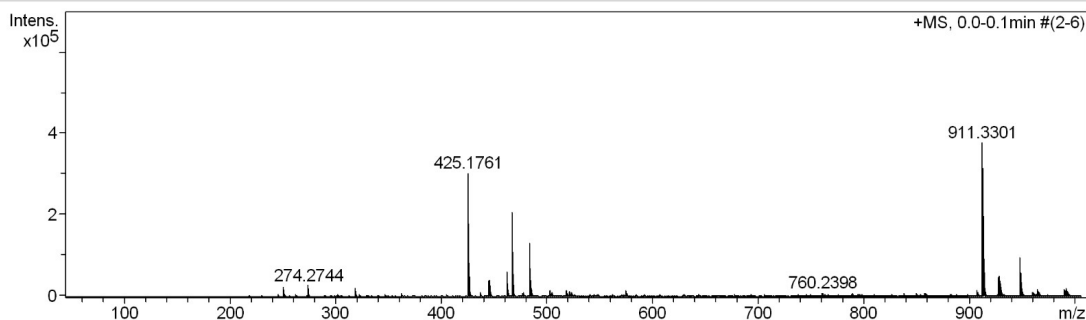
**Analysis Info**

Analysis Name D:\Data\user\NWNW-fengyang 20230321-19.d  
 Method tune\_low.m  
 Sample Name A-531  
 Comment

Acquisition Date 2023-3-21 17:20:51  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

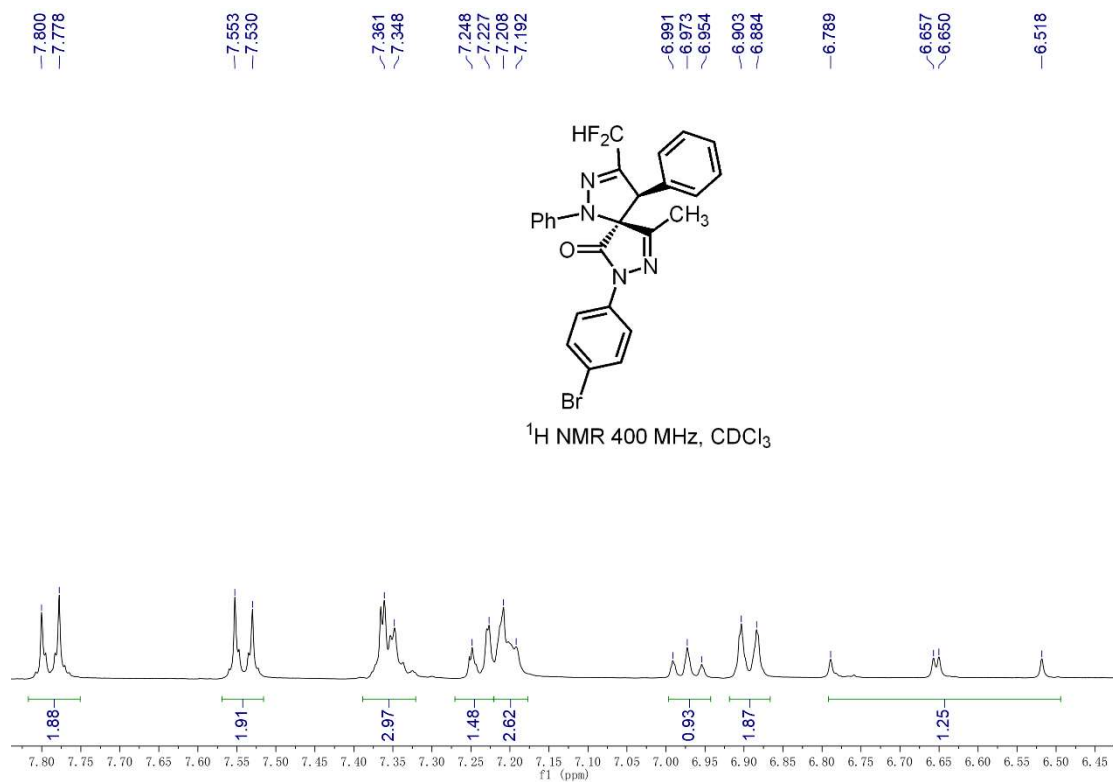
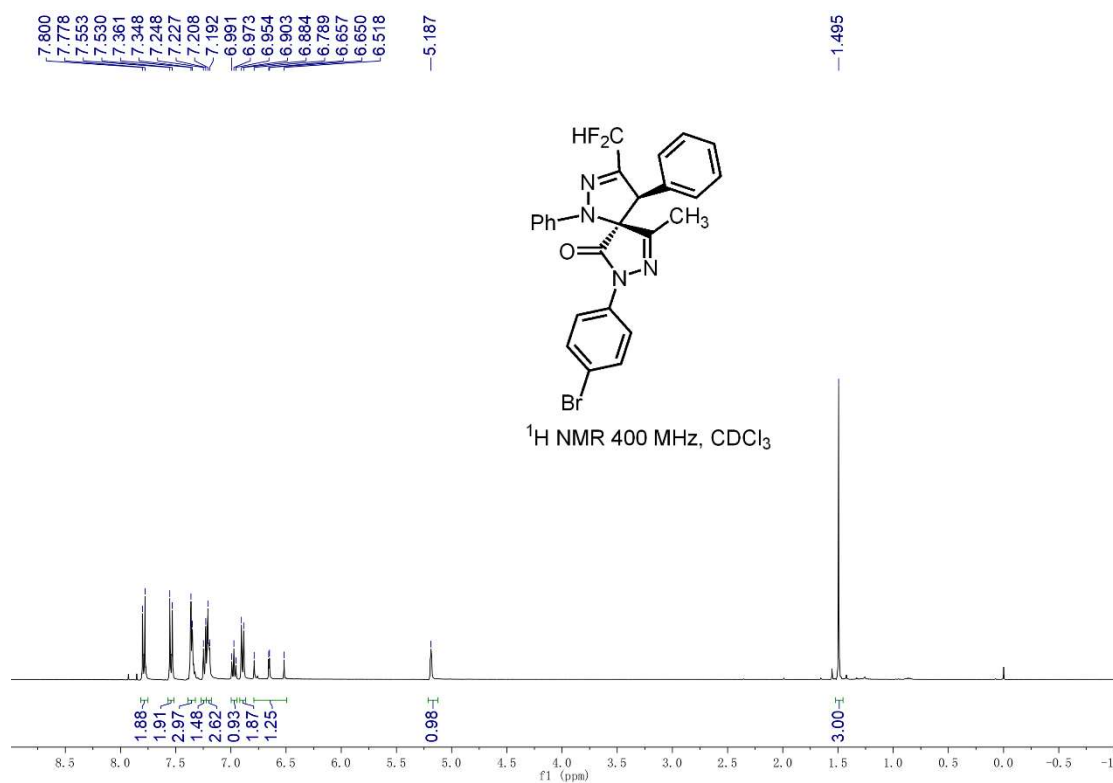
**Acquisition Parameter**

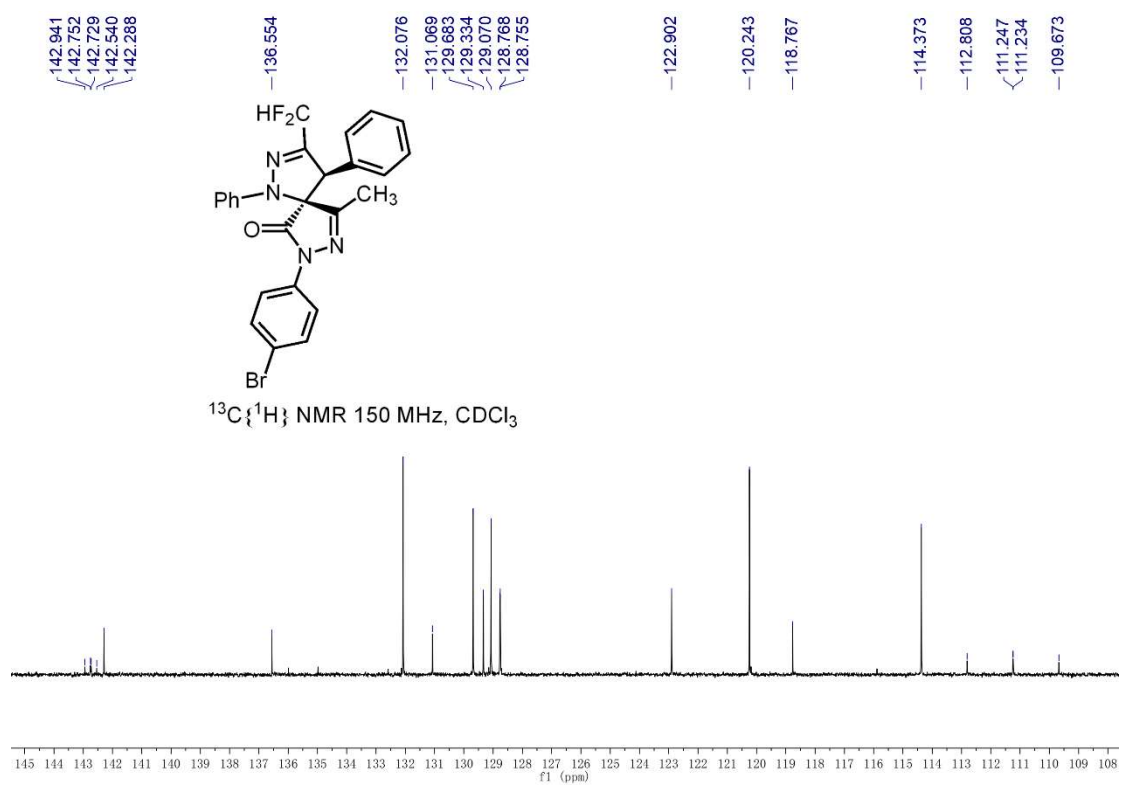
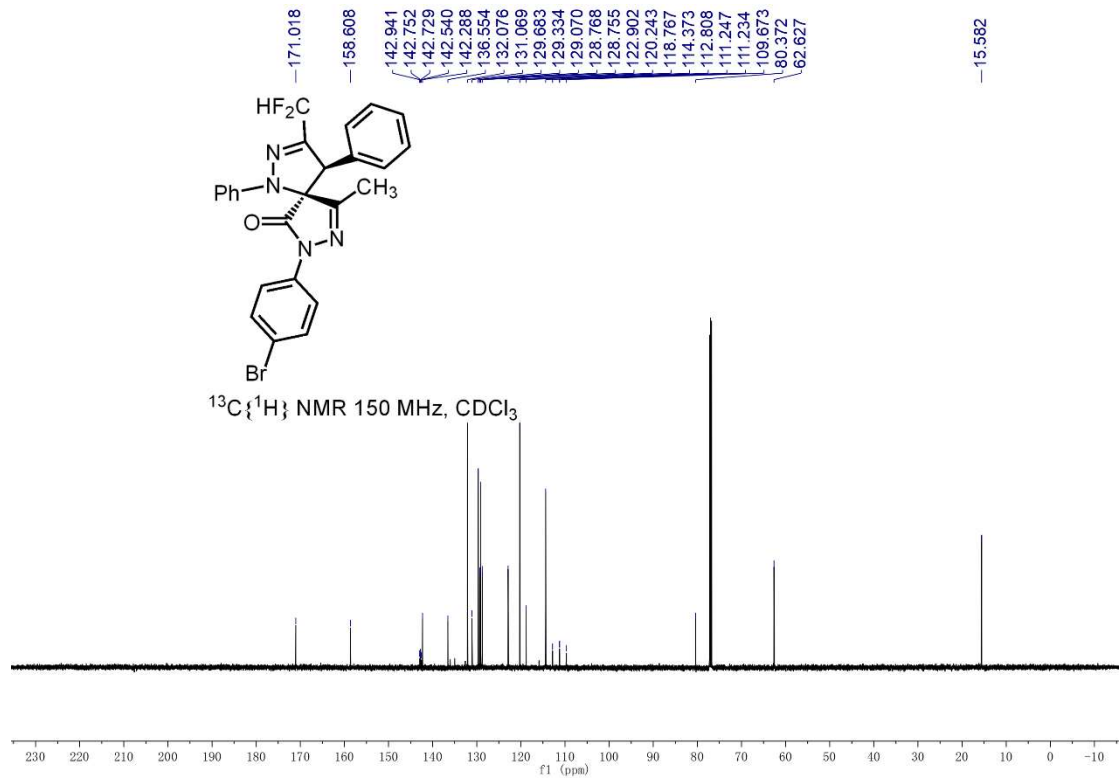
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{A}$ C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

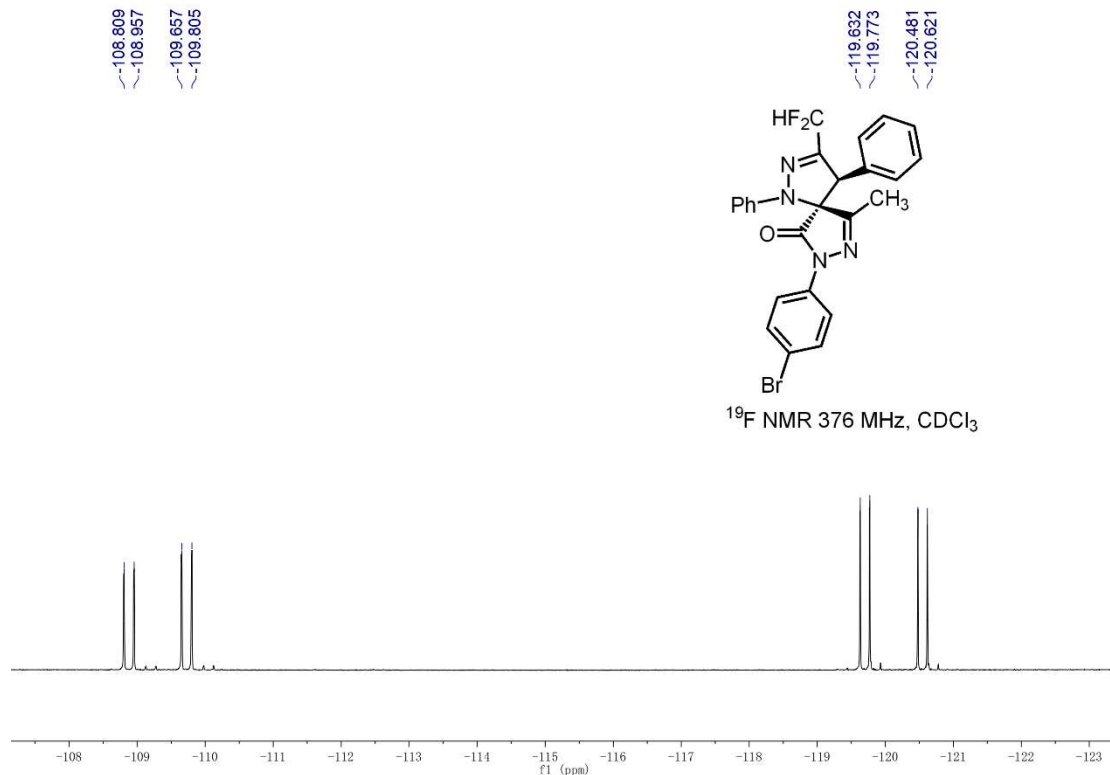


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>i</sub> ≠ Conf	mSi gma	Std l	St d Me an z	Std l Var m/ m/	St d Nor m/ m/	St d Dif f	Std Com b Dev
467.1650	1 C <sub>26</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	467.1654	0.9	0.7	16.5	ok	even	20.0	29.8	0.4	12.7	0.6	842.7	

NMR copies of compound (*trans*)-4m:







HRMS (ESI) copy of compound (*trans*)-4m:

### Mass Spectrum SmartFormula Report

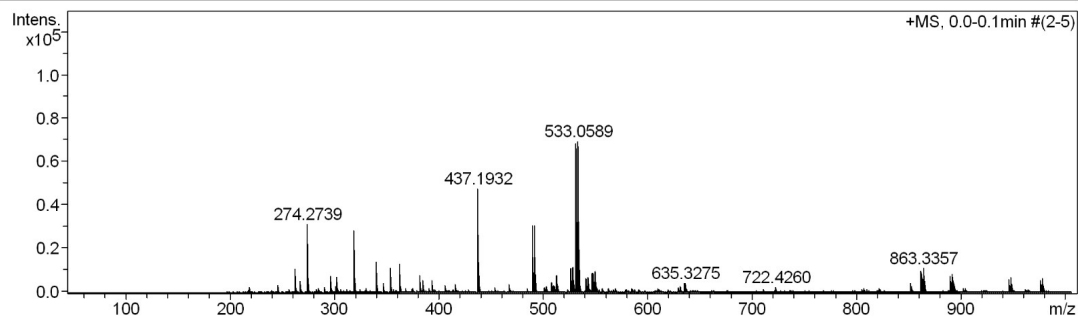
**Analysis Info**

Analysis Name D:\Data\user\NWNNU-fengyang 20230321-20.d  
 Method tune\_low.m  
 Sample Name A-56  
 Comment

Acquisition Date 2023-3-21 17:24:25  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

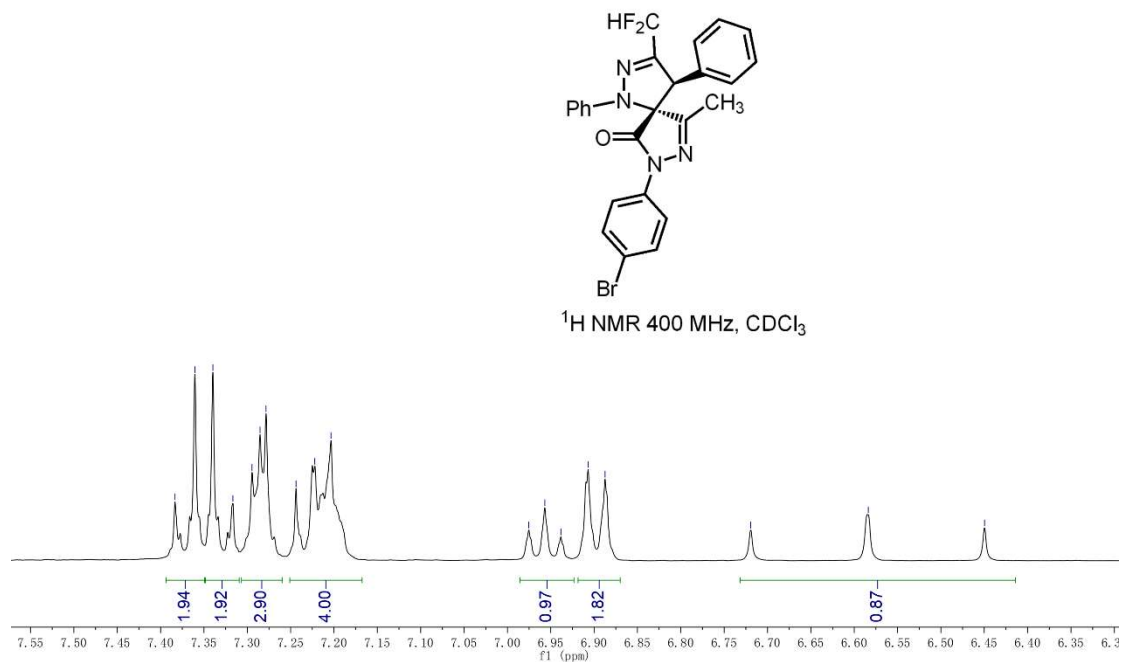
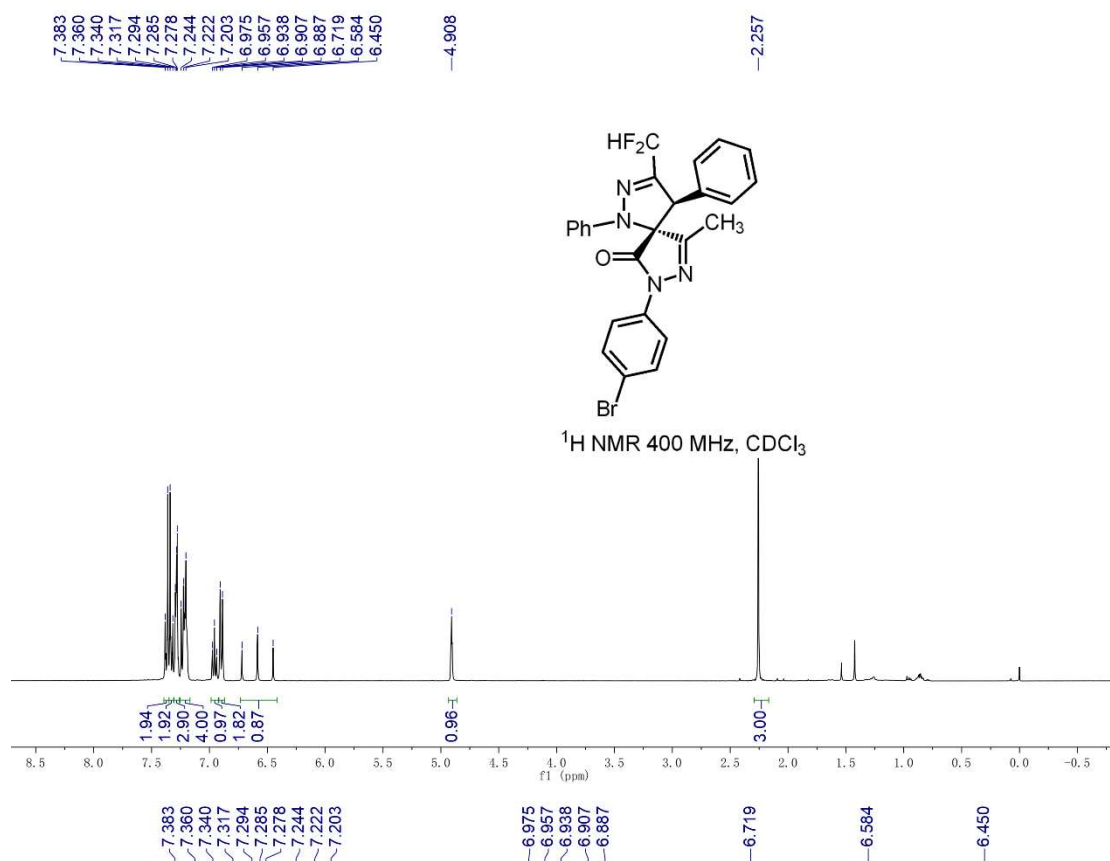
**Acquisition Parameter**

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

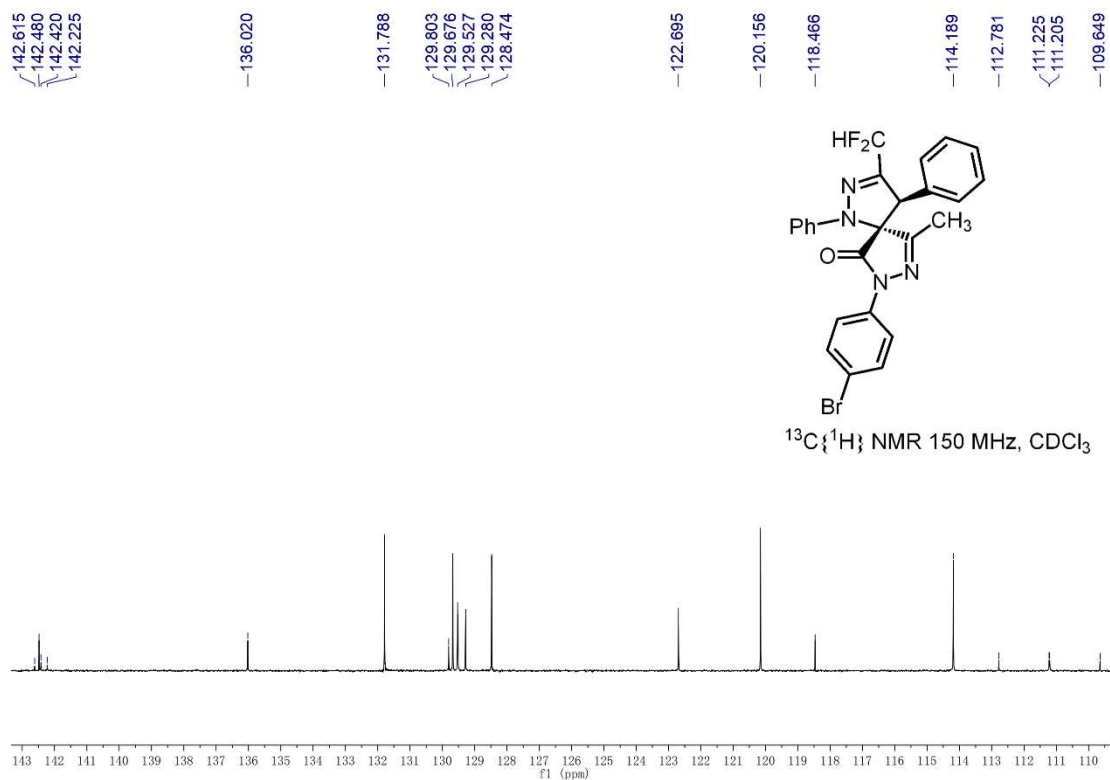
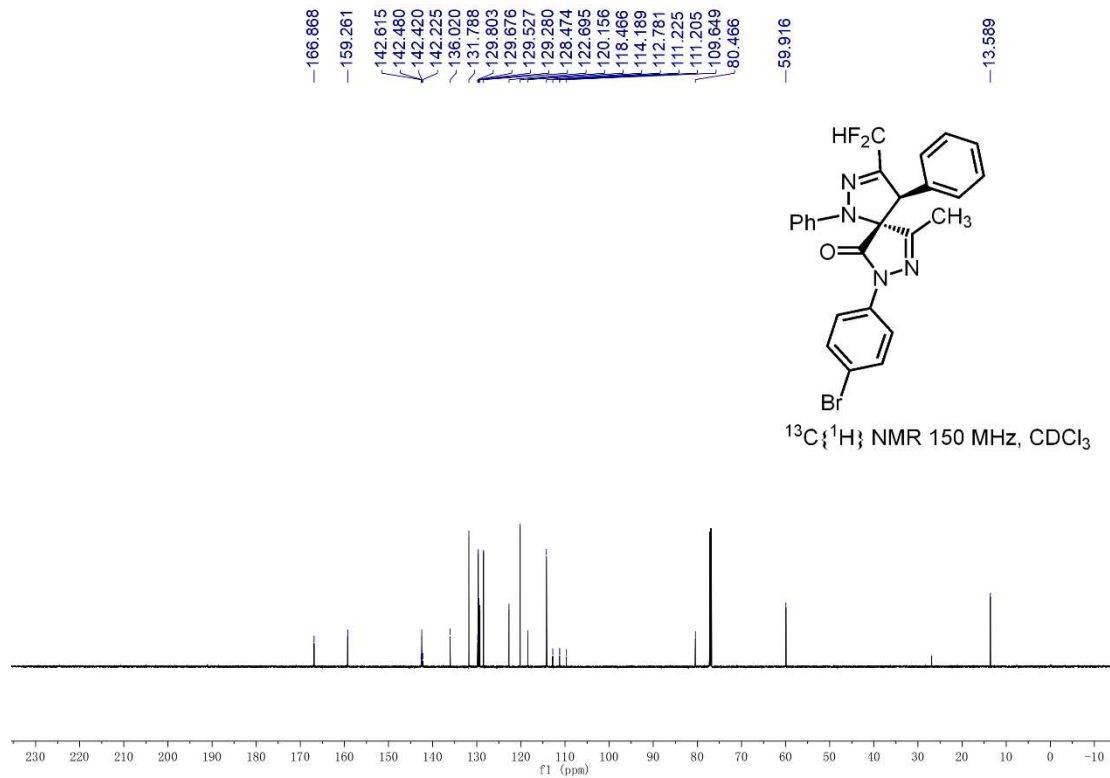


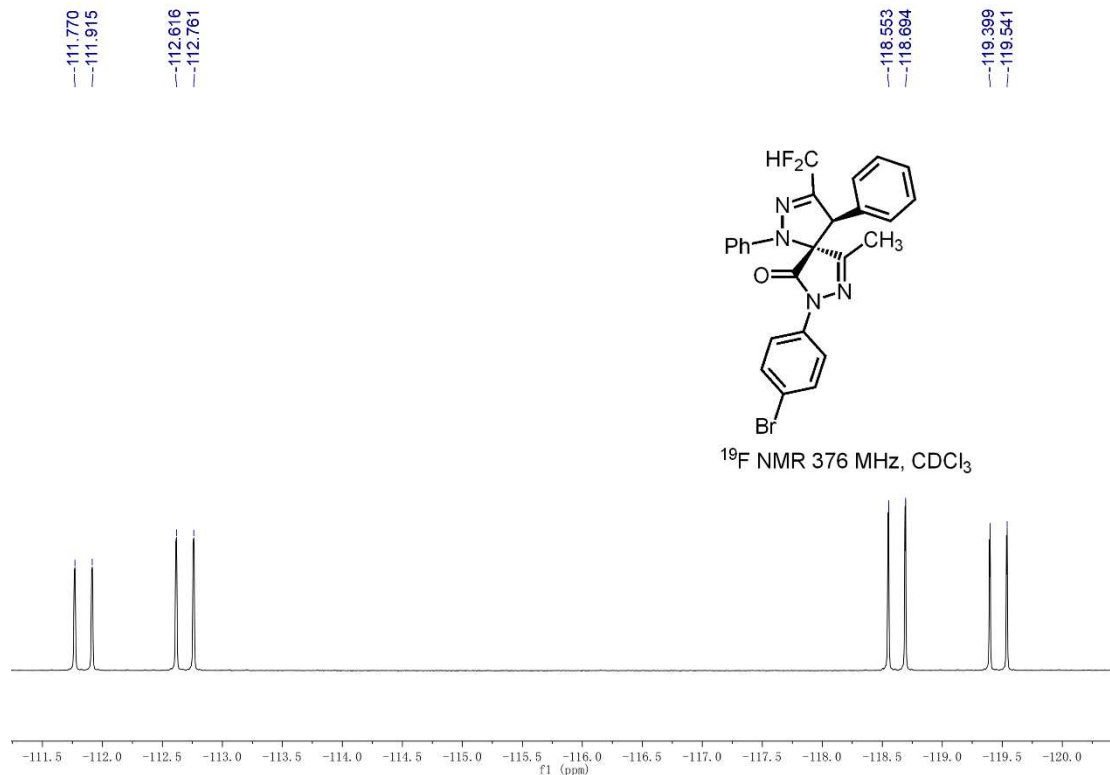
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej% Conf	mSi gm a	Std l	St d	St d l	St d	Std Com b Dev
531.0599	1 C <sub>25</sub> H <sub>19</sub> BrF <sub>2</sub> N <sub>4</sub> NaO	531.0603	0.6	0.2	16.5	ok	even	11.7	11.7	0.8	4.3	1.3	842.7

NMR copies of compound (*cis*)-4m:









HRMS (ESI) copy of compound (*cis*)-4m:

### Mass Spectrum SmartFormula Report

#### Analysis Info

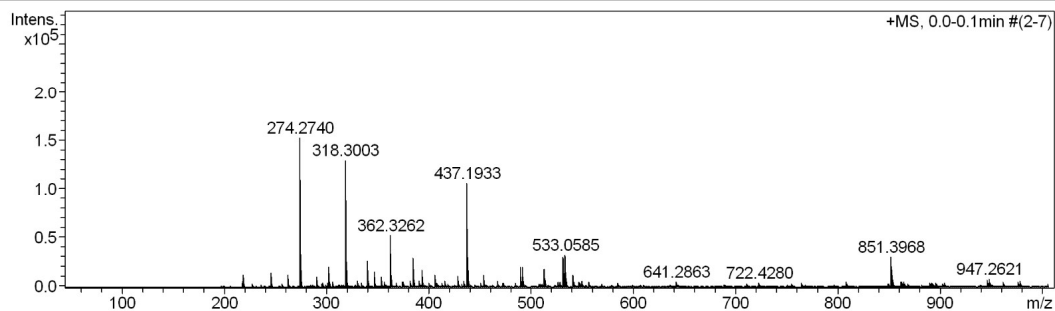
Analysis Name D:\Data\user\NWNNU-fengyang 20230321-21.d  
 Method tune\_low.m  
 Sample Name A-561  
 Comment

Acquisition Date 2023-3-21 17:26:16

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

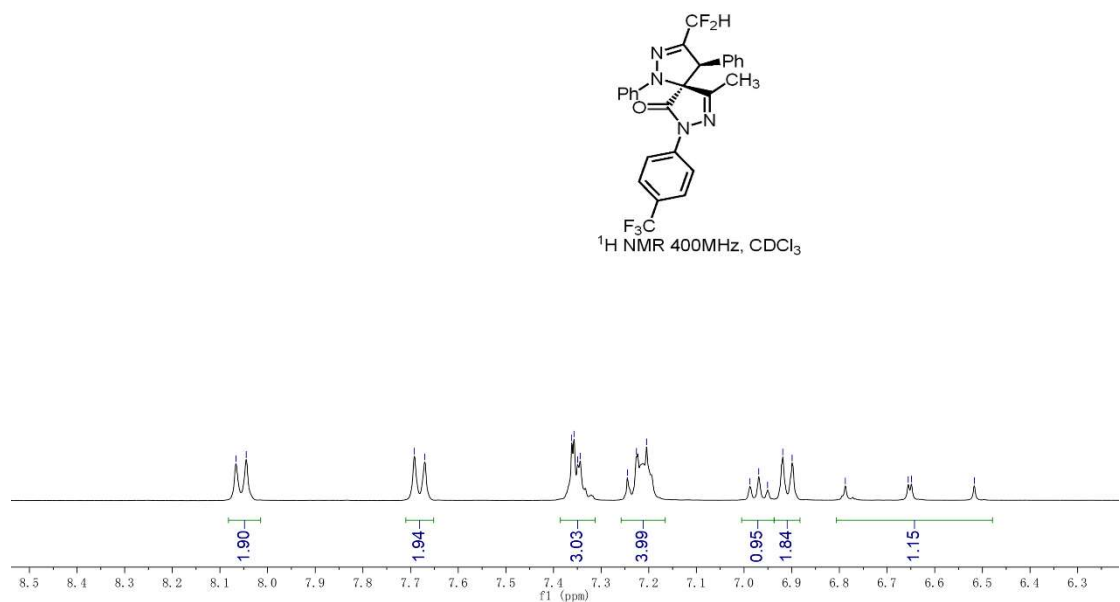
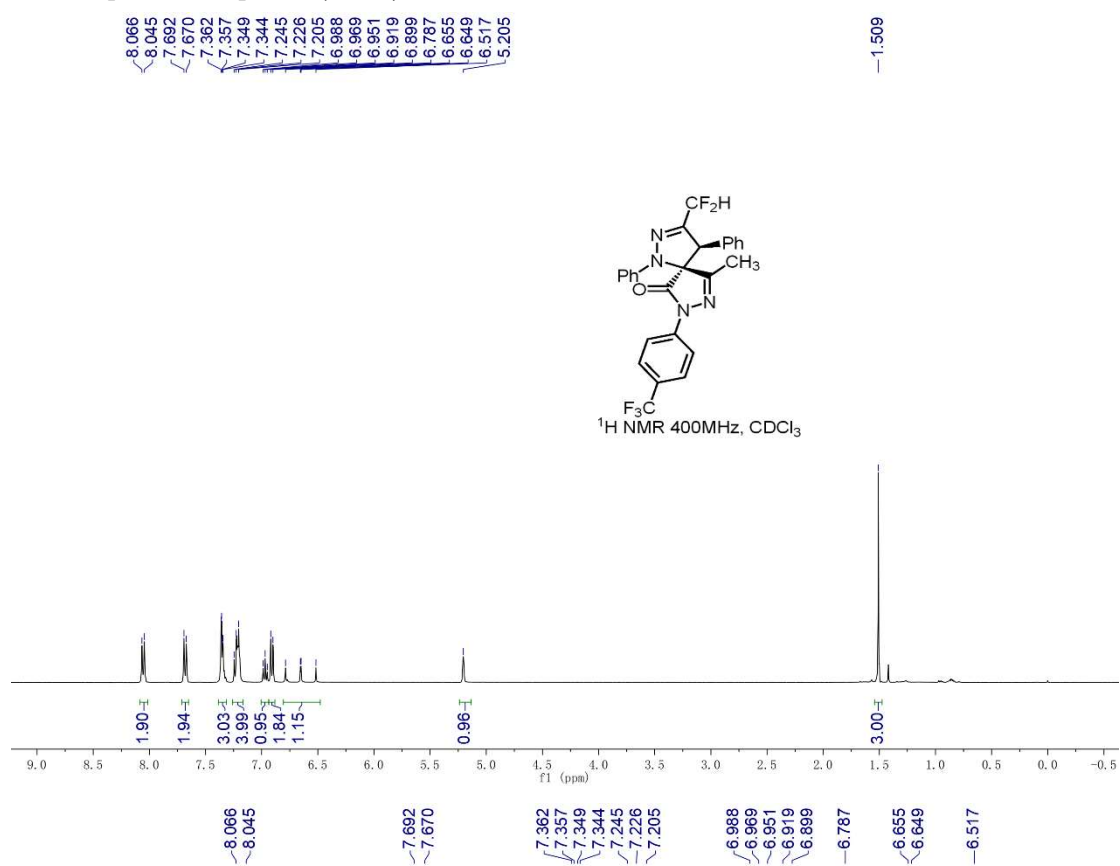
#### Acquisition Parameter

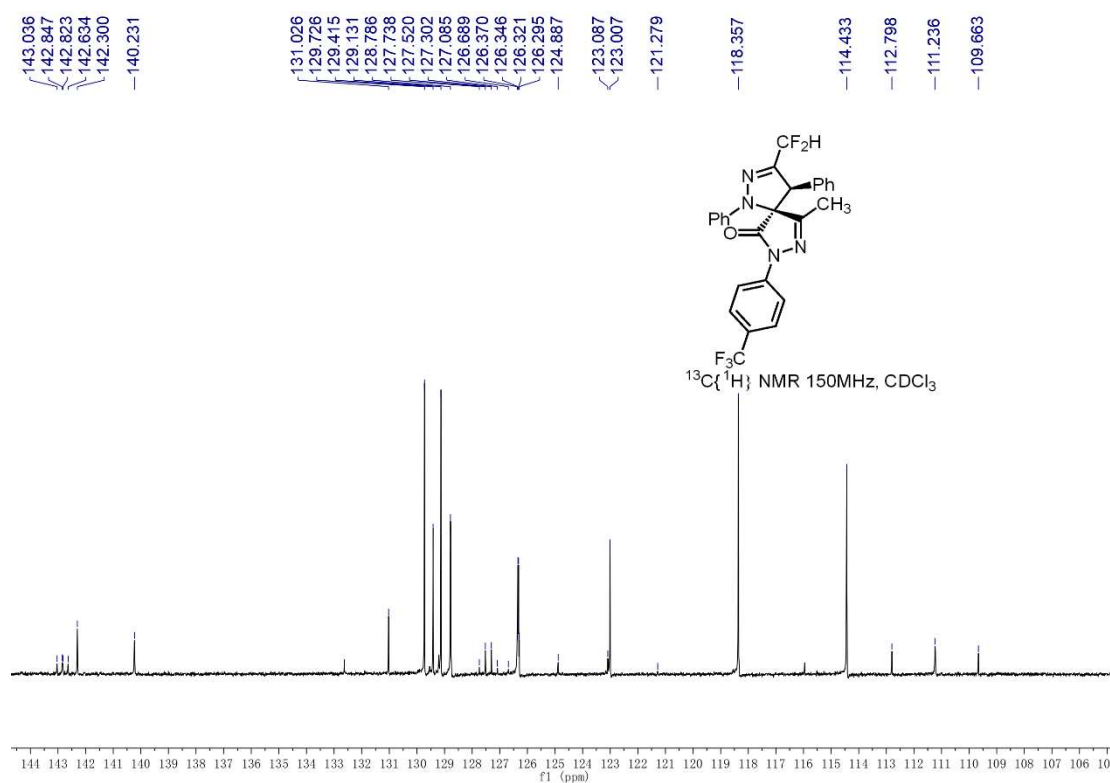
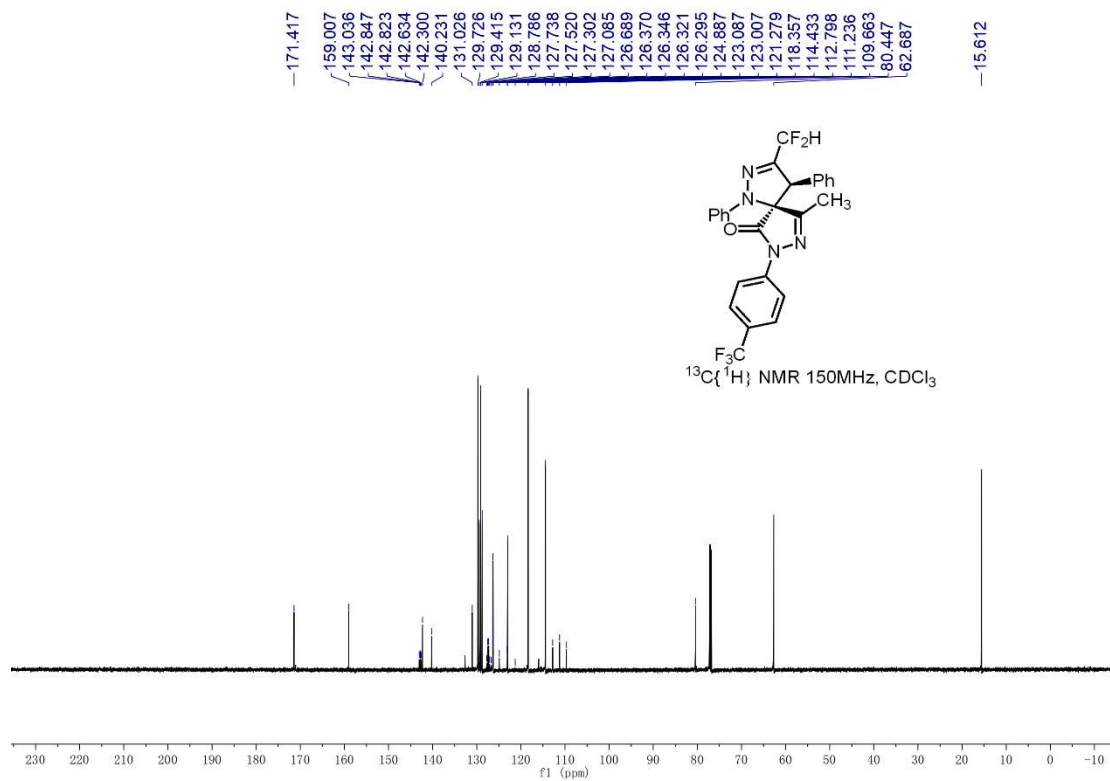
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

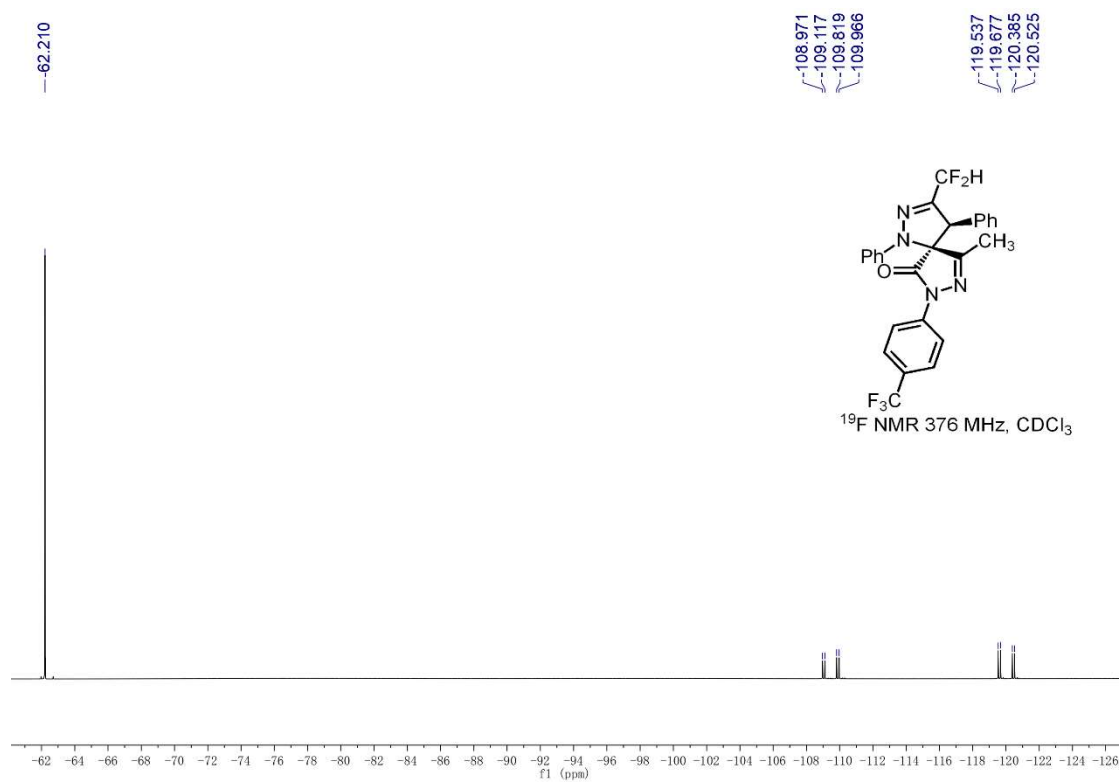
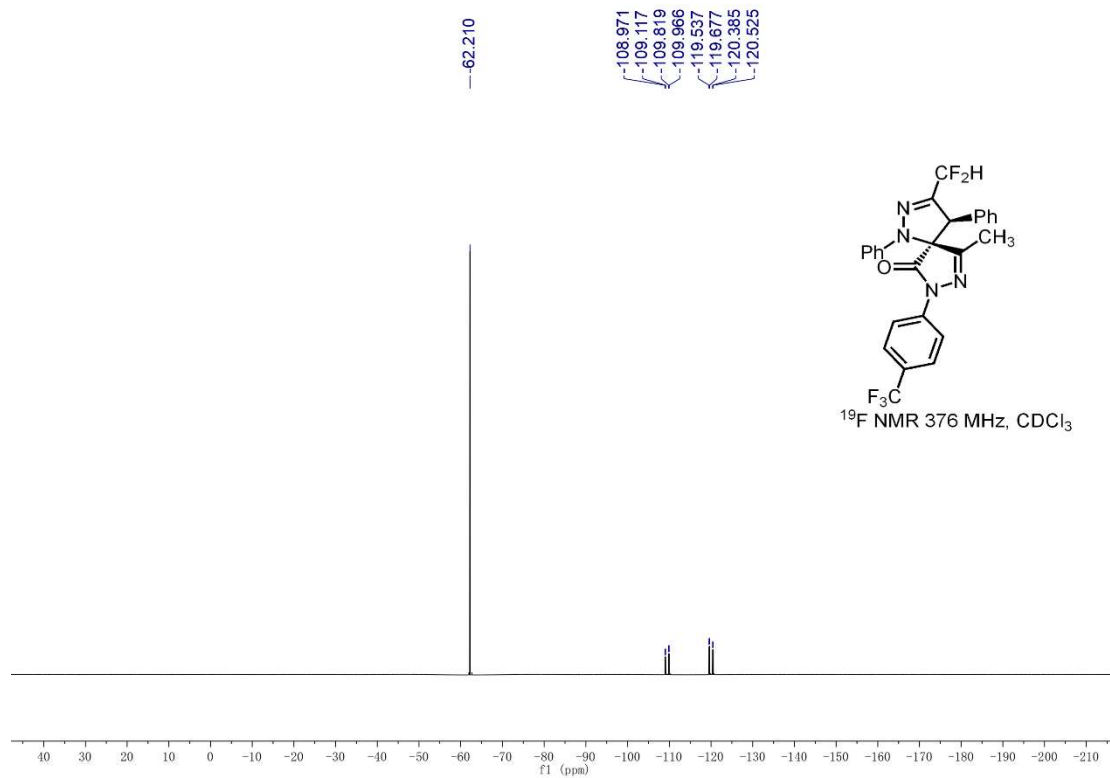


Meas. #	Formula	m/z	err [p]	Me an [p]	rdb	N-R	ej%	mSi gm	Std l	St d	Std l	St d	Std Com b
531.0601	1 C 25 H 19 Br F 2 N 4 Na O	531.0603	0.3	0.4	16.5	ok	even	28.9	23.8	0.6	11.9	0.9	842.7

NMR copies of compound (*trans*)-4n:

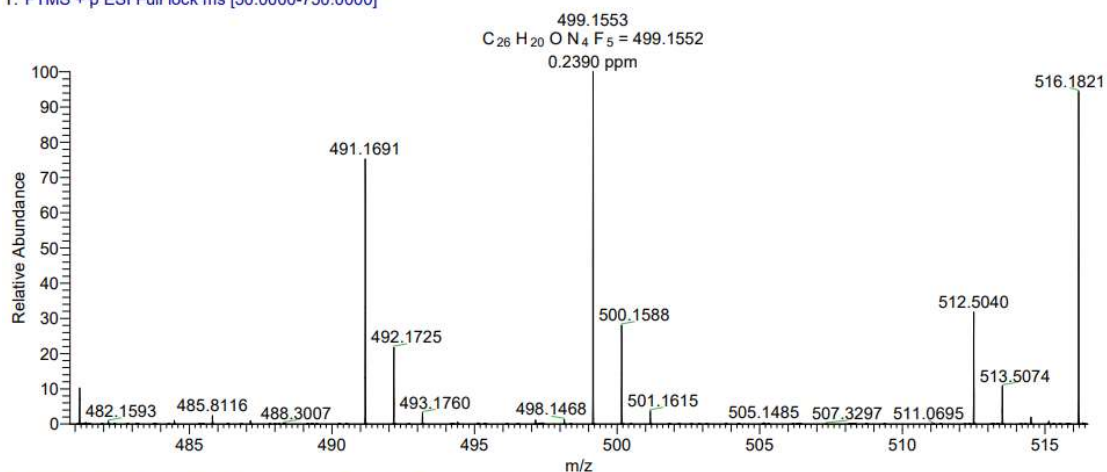






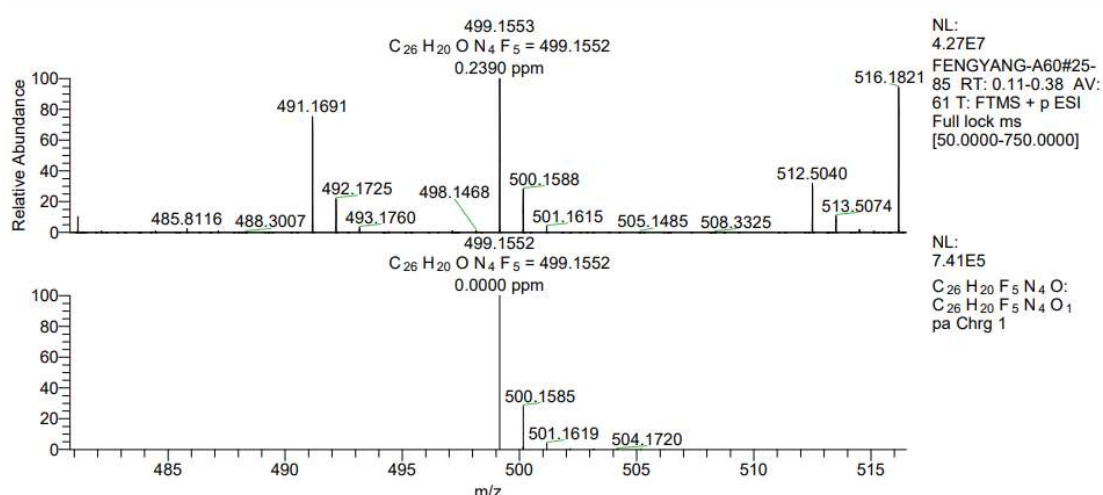
# HRMS (ESI) copy of compound (*trans*)-4n:

FENGYANG-A60#25-85 RT: 0.11-0.38 AV: 61 NL: 4.27E7  
 T: FTMS + p ESI Full lock ms [50.0000-750.0000]



FENGYANG-A60#25-85 RT: 0.11-0.38 AV: 61  
 T: FTMS + p ESI Full lock ms [50.0000-750.0000]  
 m/z = 480.8124-516.5004

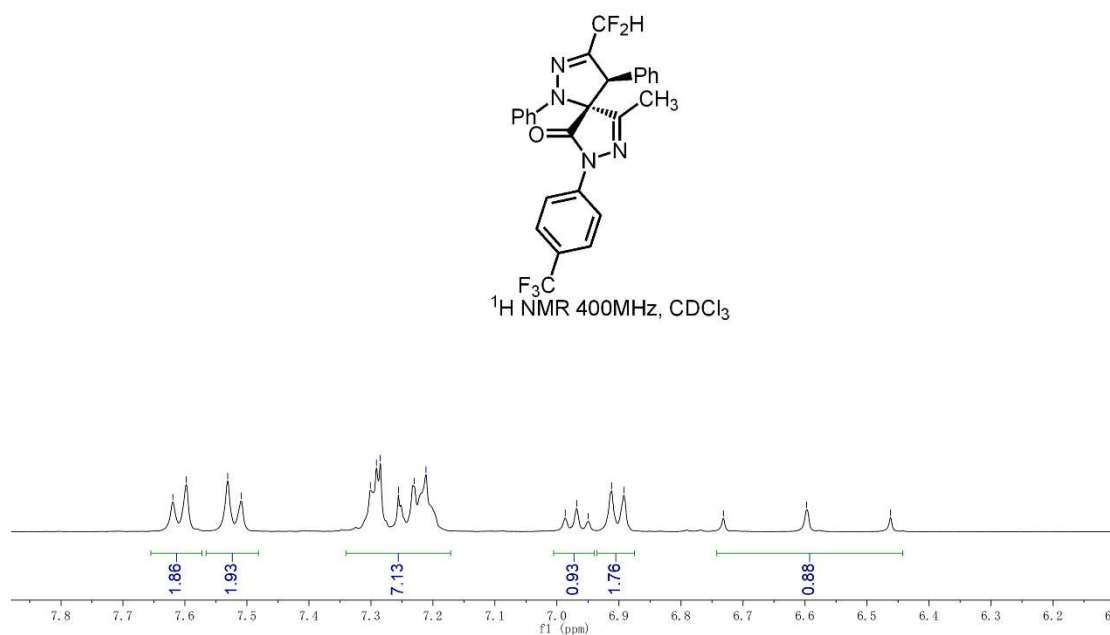
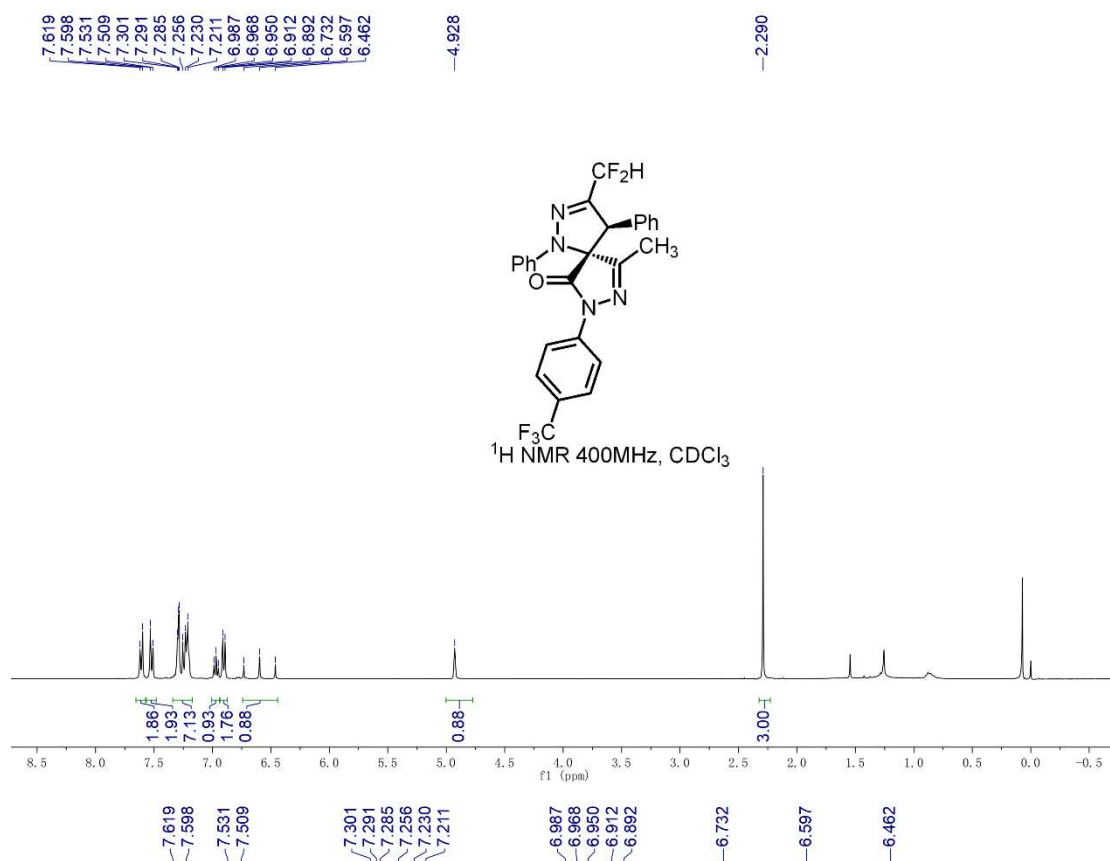
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
491.1691	32232198.0	75.39			
499.1553	42752016.0	100.00	499.1552	0.12	C <sub>26</sub> H <sub>20</sub> O N <sub>4</sub> F <sub>5</sub>
512.5040	13690603.0	32.02			
516.1821	40365292.0	94.42			

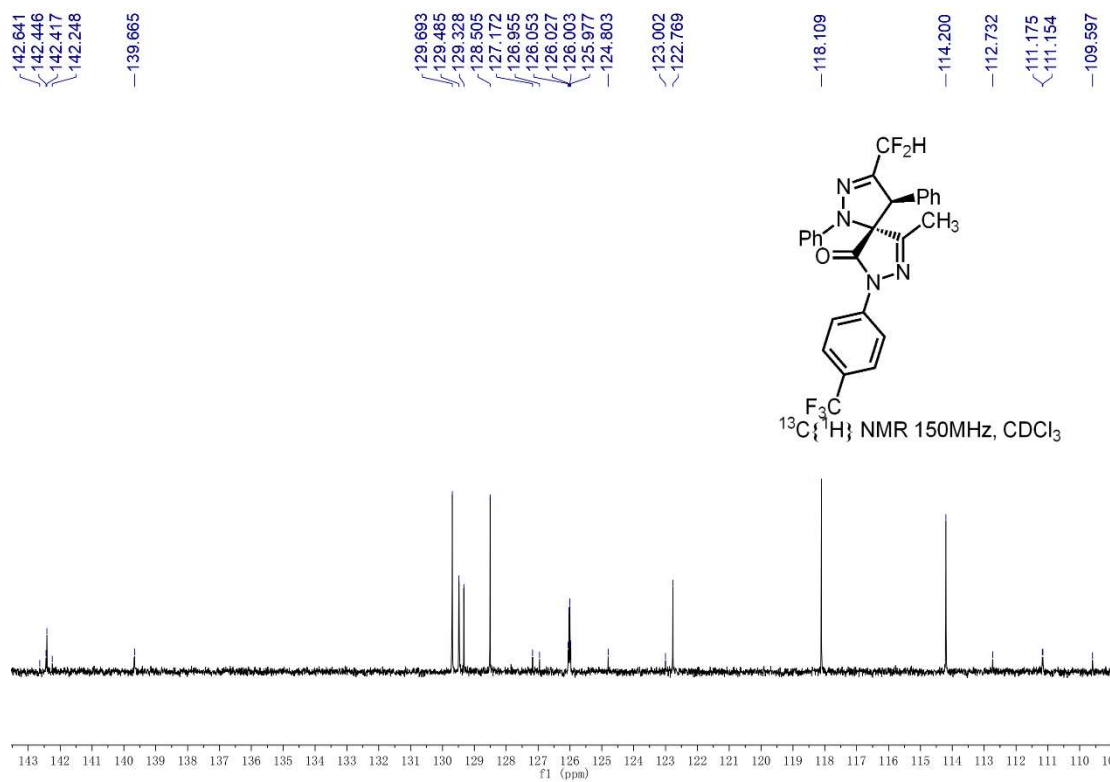
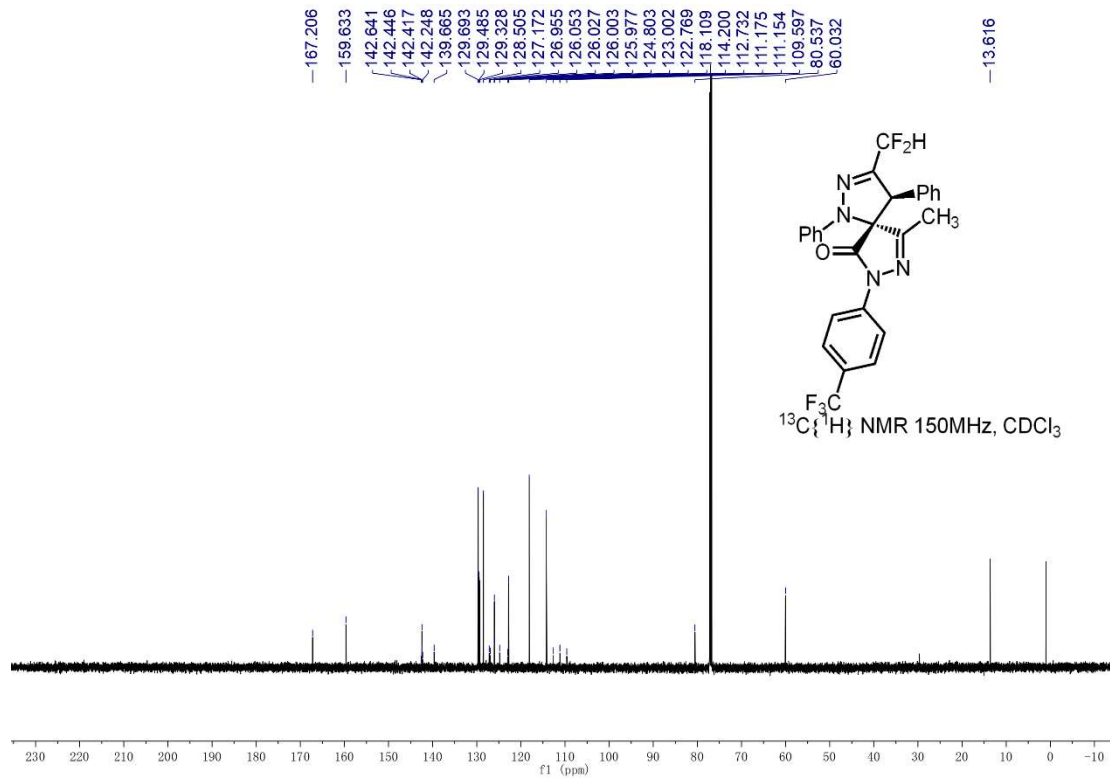


NL:  
 4.27E7  
 FENGYANG-A60#25-  
 85 RT: 0.11-0.38 AV:  
 61 T: FTMS + p ESI  
 Full lock ms  
 [50.0000-750.0000]

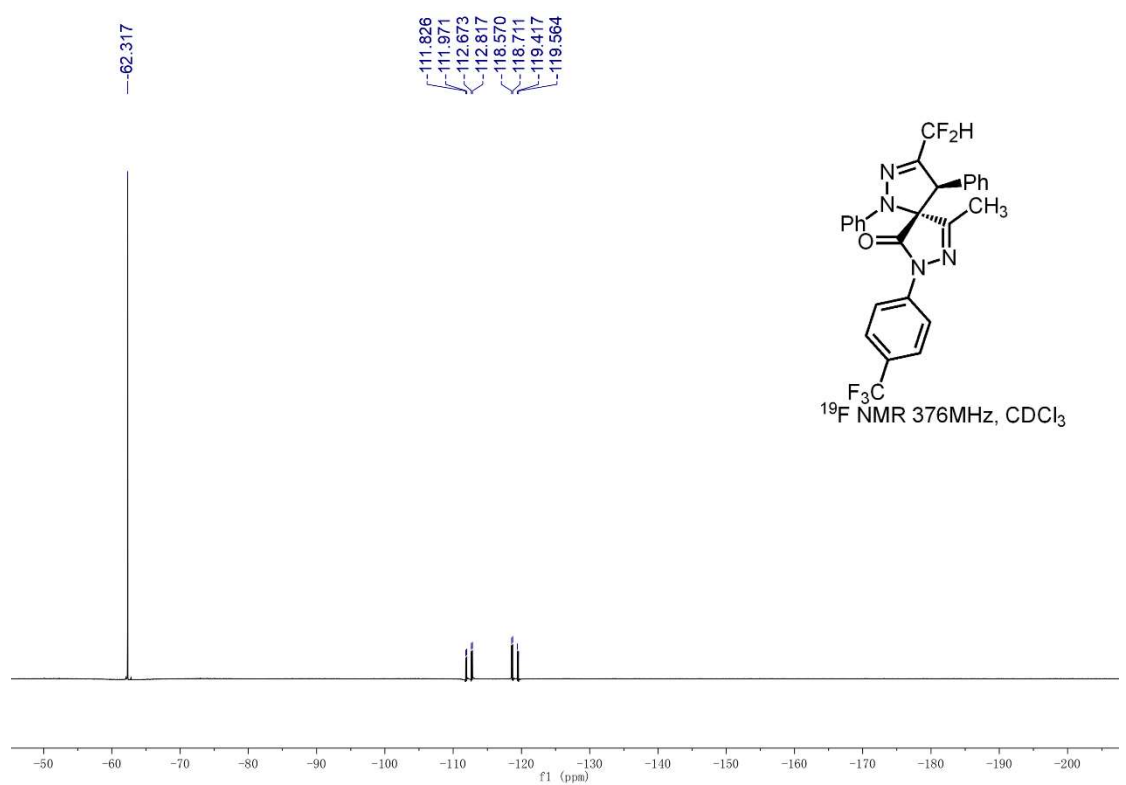
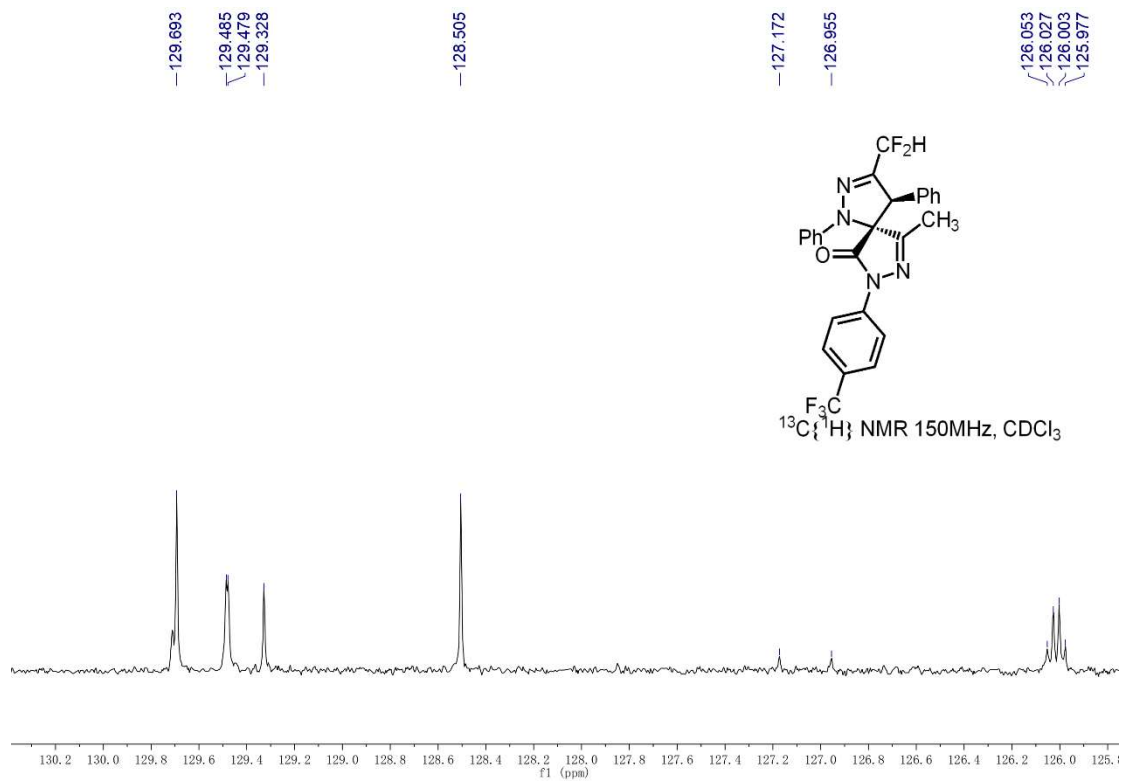
NL:  
 7.41E5  
 C<sub>26</sub>H<sub>20</sub>F<sub>5</sub>N<sub>4</sub>O:  
 C<sub>26</sub>H<sub>20</sub>F<sub>5</sub>N<sub>4</sub>O<sub>1</sub>  
 pa Chrg 1

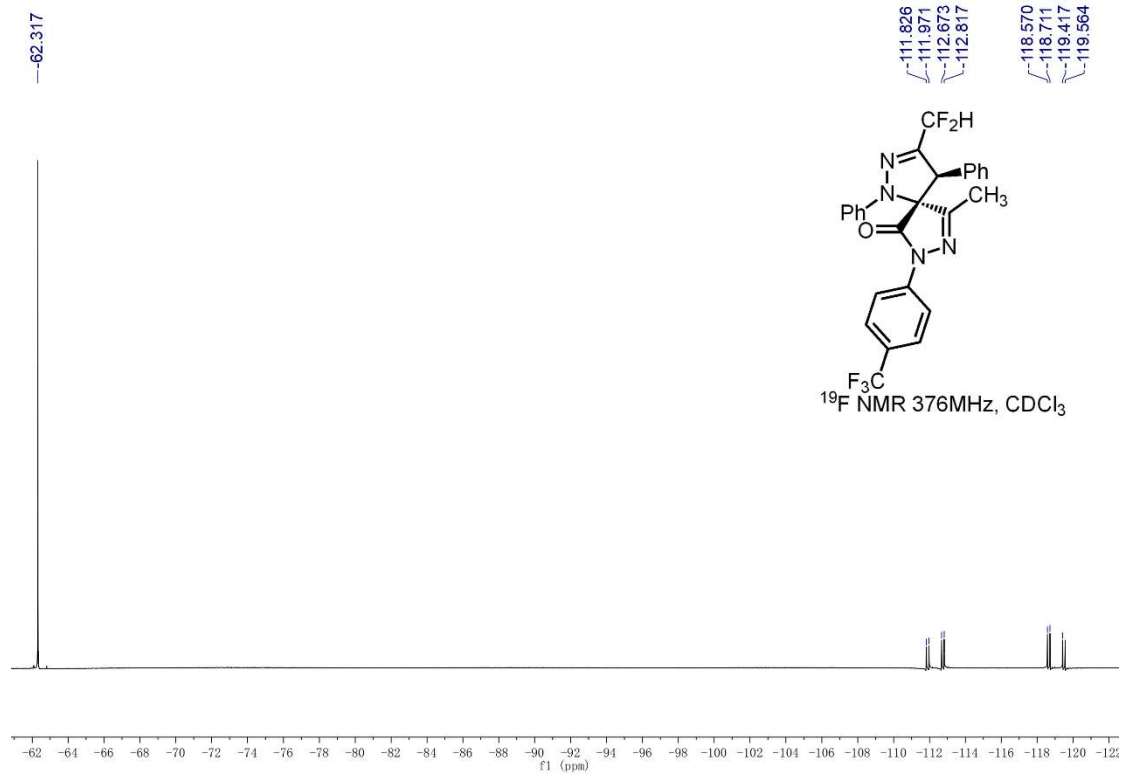
NMR copies of compound **4n**:





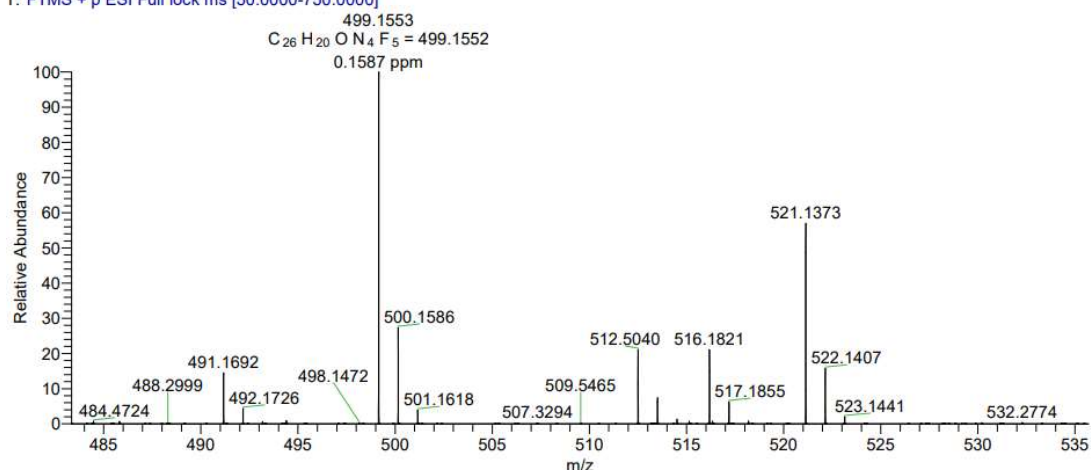






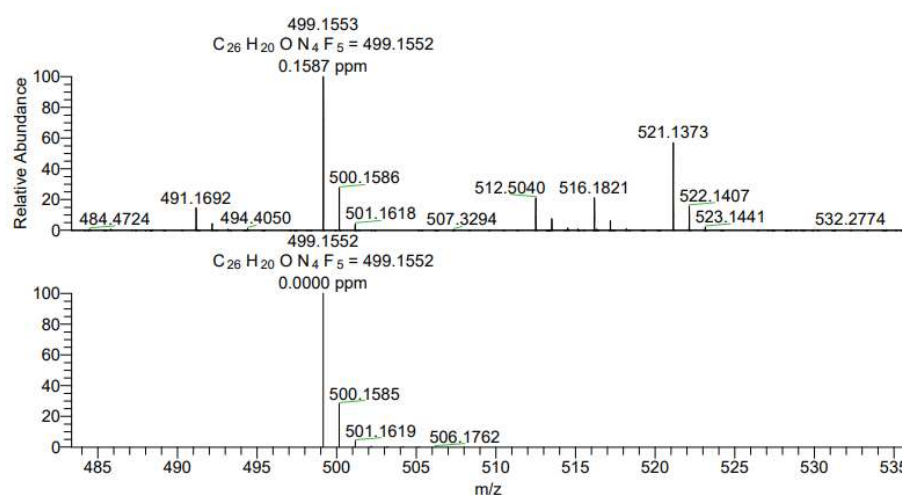
# HRMS (ESI) copy of compound (*cis*)-4n:

FENGYANG-A601#27-68 RT: 0.12-0.30 AV: 42 NL: 3.74E7  
 T: FTMS + p ESI Full lock ms [50.0000-750.0000]



FENGYANG-A601#27-68 RT: 0.12-0.30 AV: 42  
 T: FTMS + p ESI Full lock ms [50.0000-750.0000]  
 m/z = 483.3411-535.6811

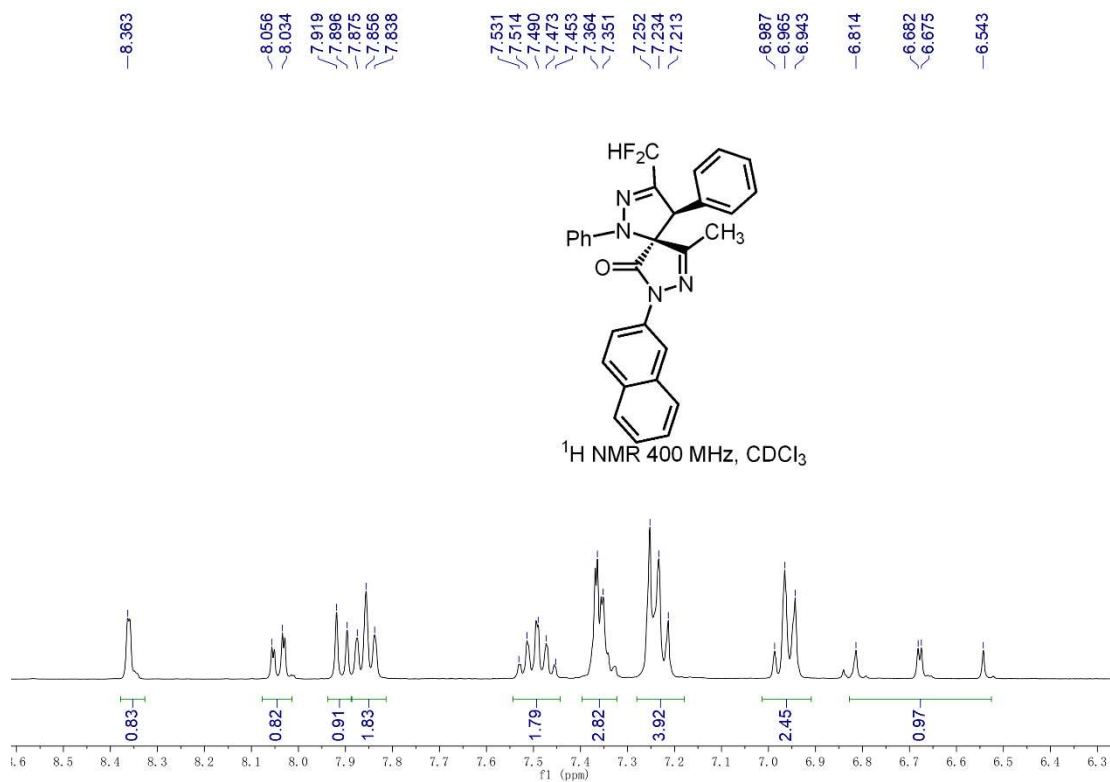
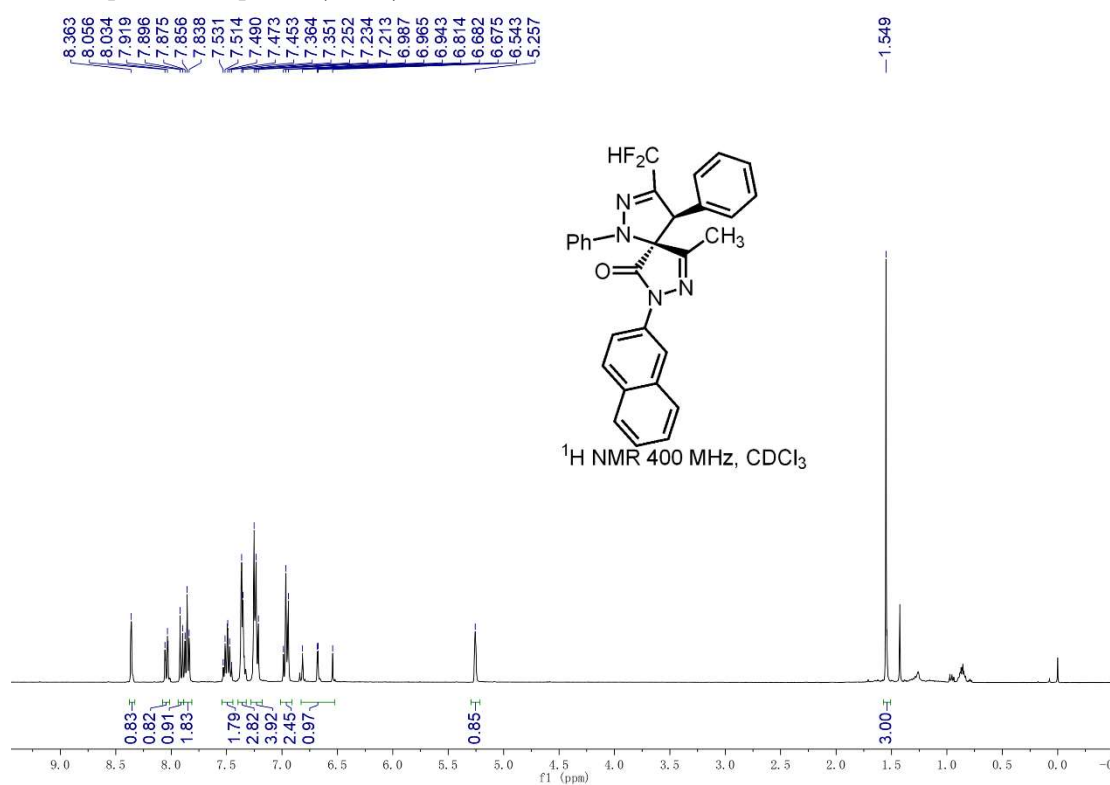
m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	Composition
499.1553	38434080.0	100.00	499.1552	0.08	C <sub>26</sub> H <sub>20</sub> O N <sub>4</sub> F <sub>5</sub>
500.1586	10593993.0	27.56			
516.1821	8098729.0	21.07			
521.1373	21384144.0	55.64			

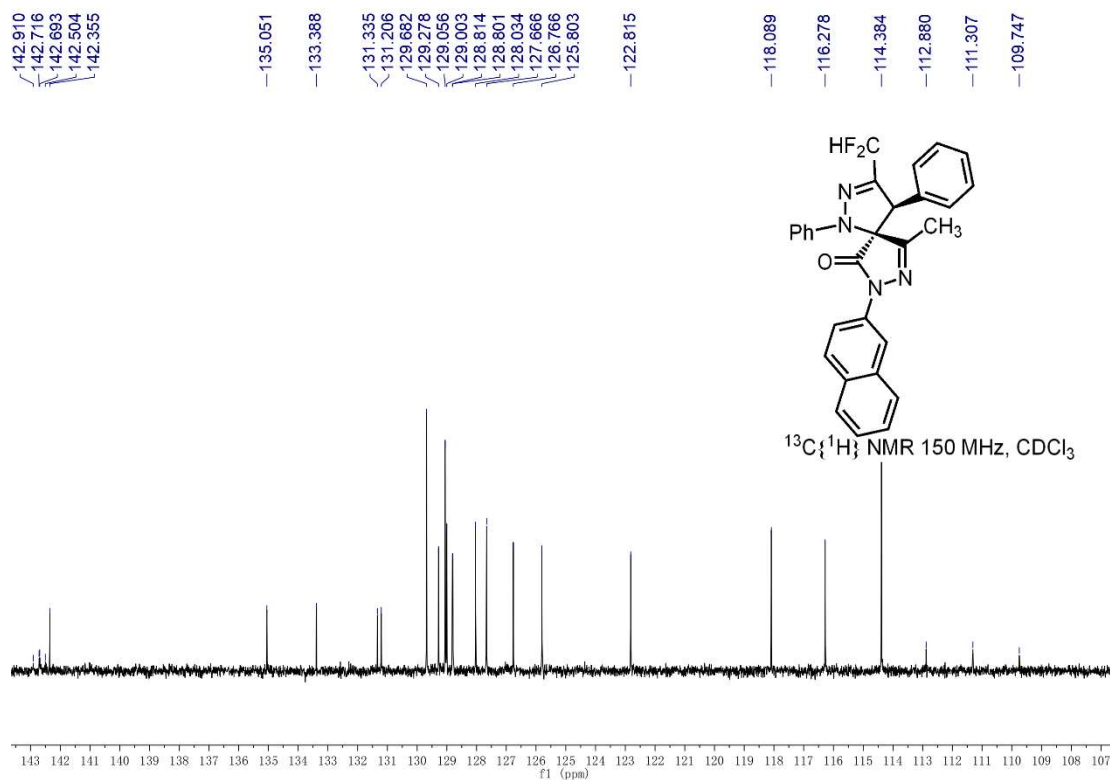
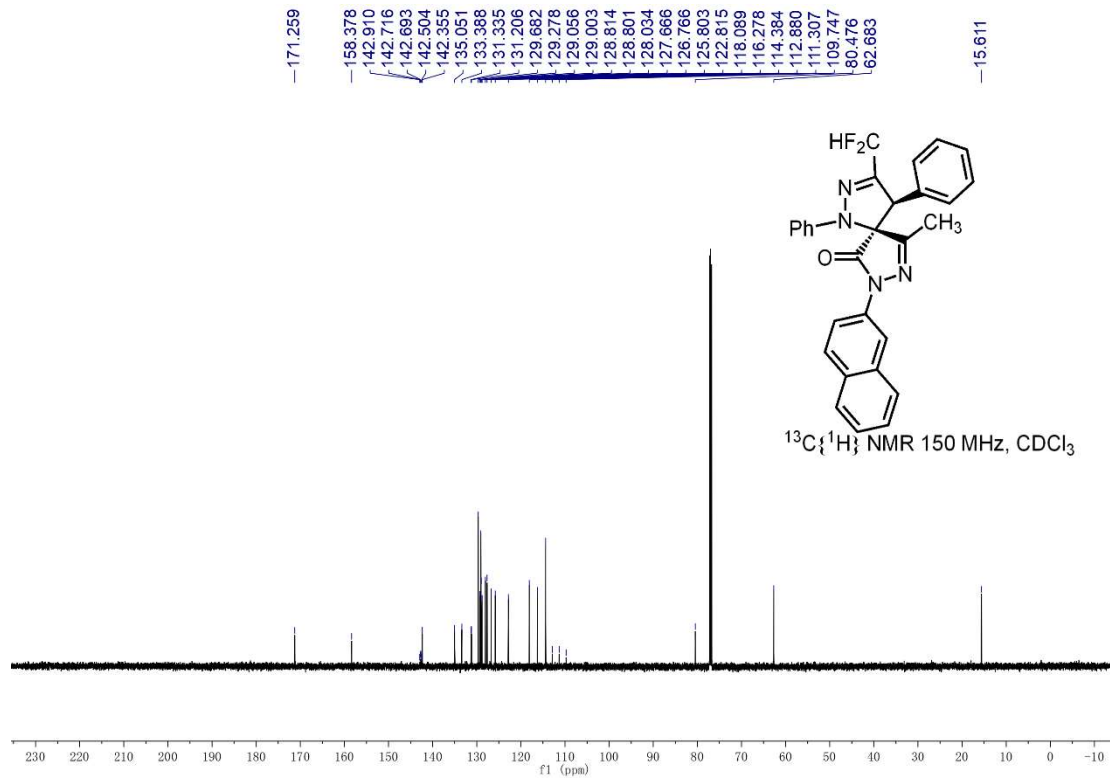


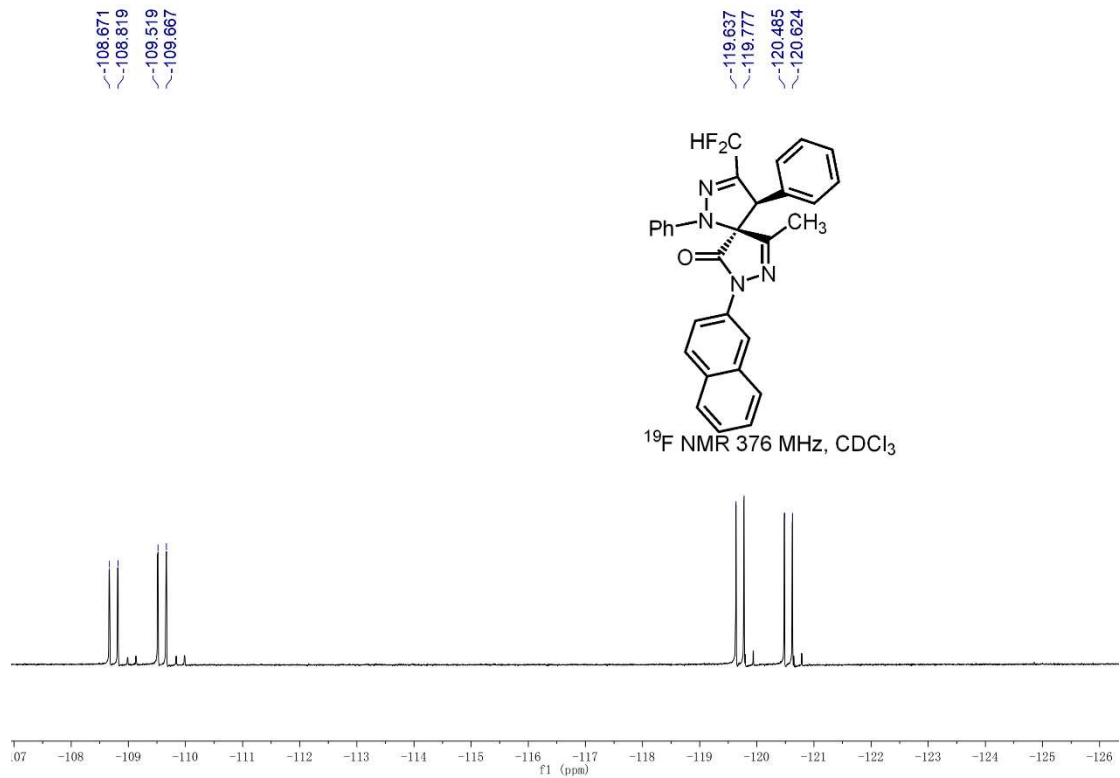
NL:  
 3.74E7  
 FENGYANG-A601#27-68 RT: 0.12-0.30 AV: 42 T: FTMS + p ESI Full lock ms [50.0000-750.0000]

NL:  
 7.41E5  
 C<sub>26</sub>H<sub>20</sub>F<sub>5</sub>N<sub>4</sub>O:  
 C<sub>26</sub>H<sub>20</sub>F<sub>5</sub>N<sub>4</sub>O<sub>1</sub>  
 pa Chrg 1

NMR copies of compound (*trans*)-4o:







HRMS (ESI) copy of compound (*trans*)-4o:

### Mass Spectrum SmartFormula Report

#### Analysis Info

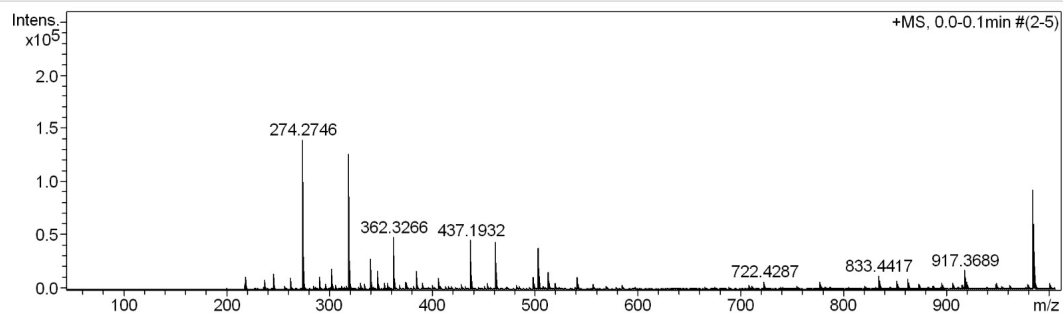
Analysis Name D:\Data\user\NWN\U-fengyang 20230321-22.d  
Method tune\_low.m  
Sample Name A-58  
Comment

Acquisition Date 2023-3-21 17:29:38

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

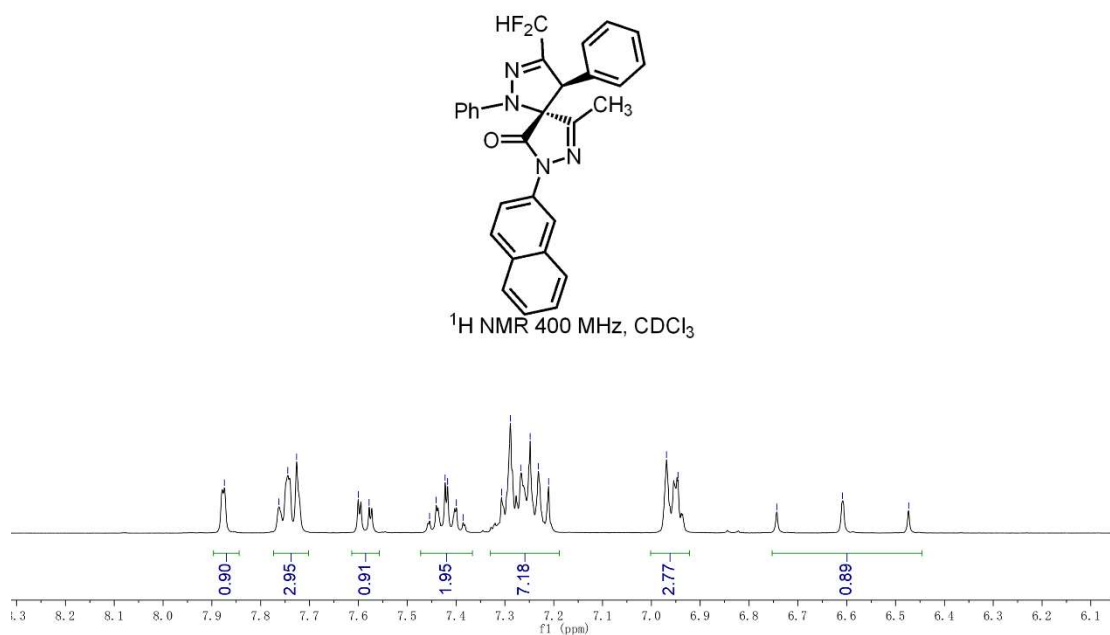
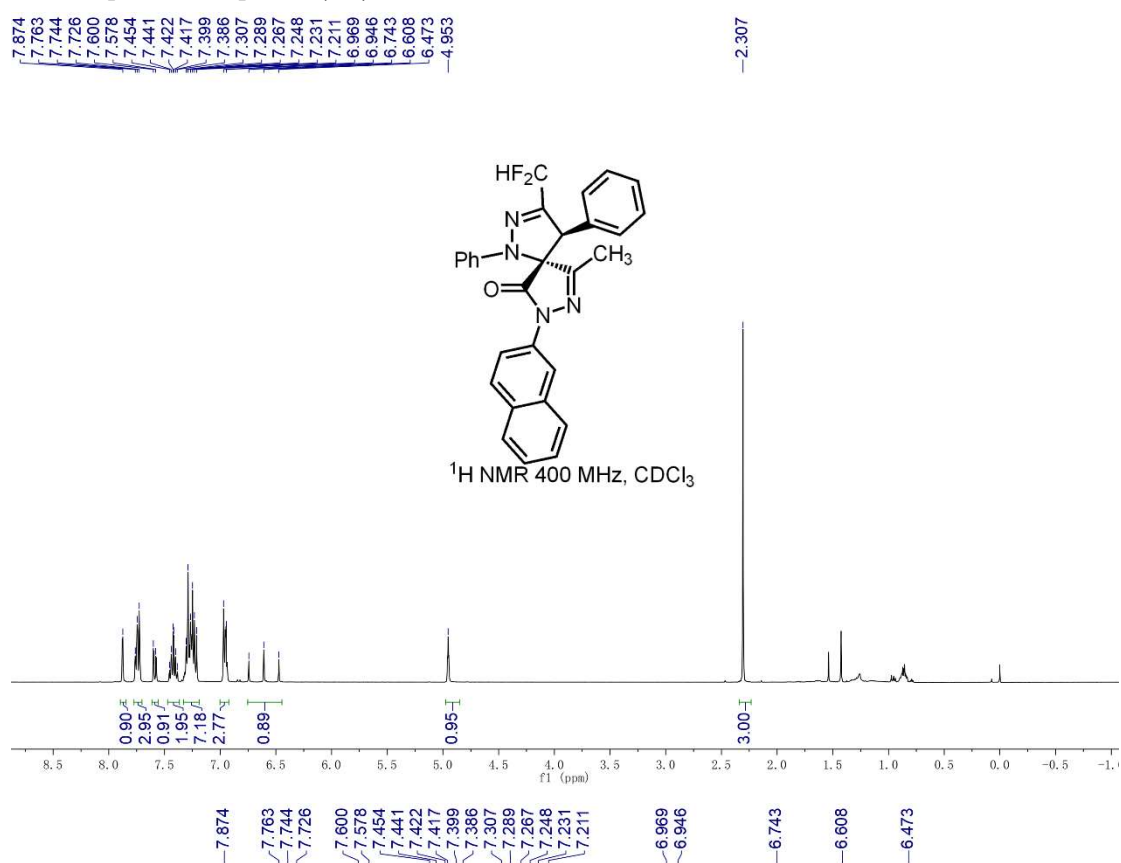
#### Acquisition Parameter

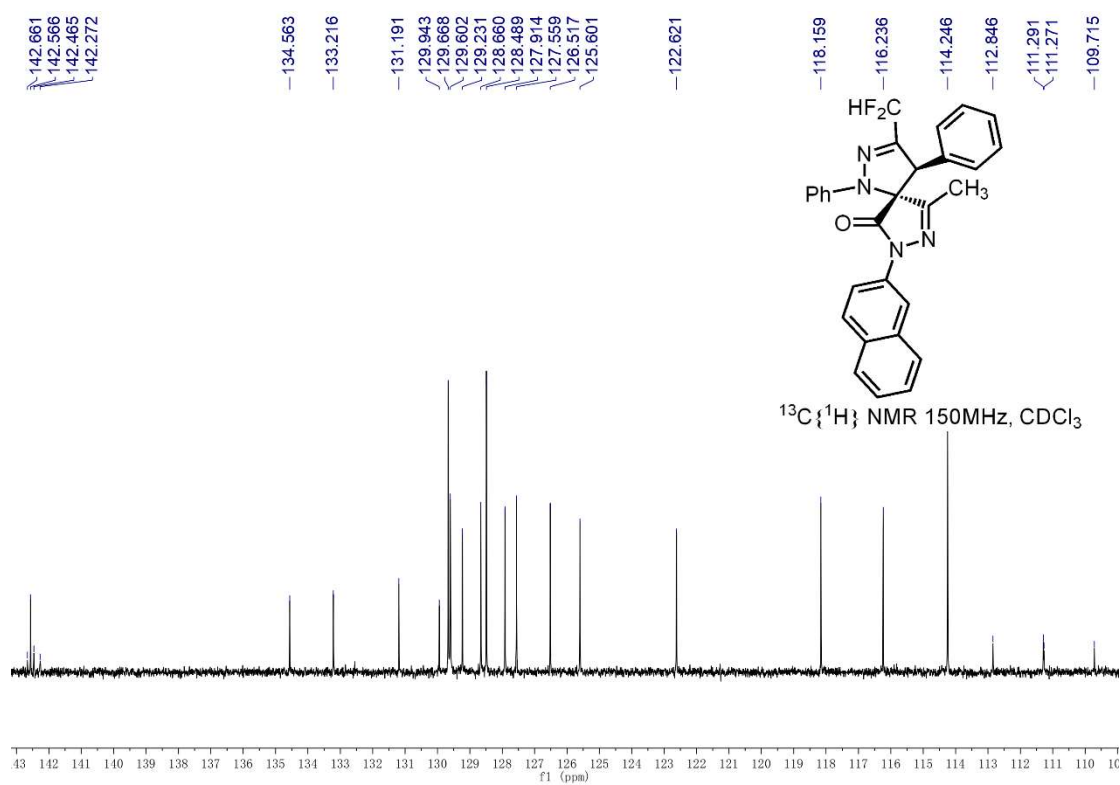
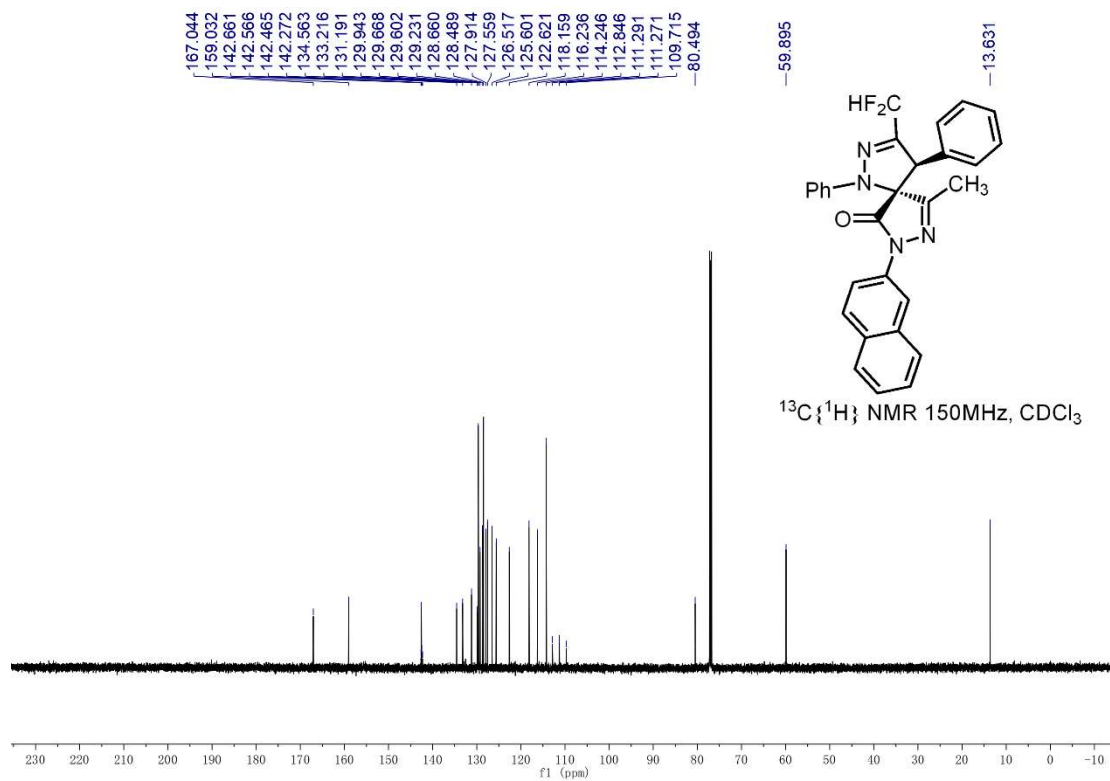
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j̄aC
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



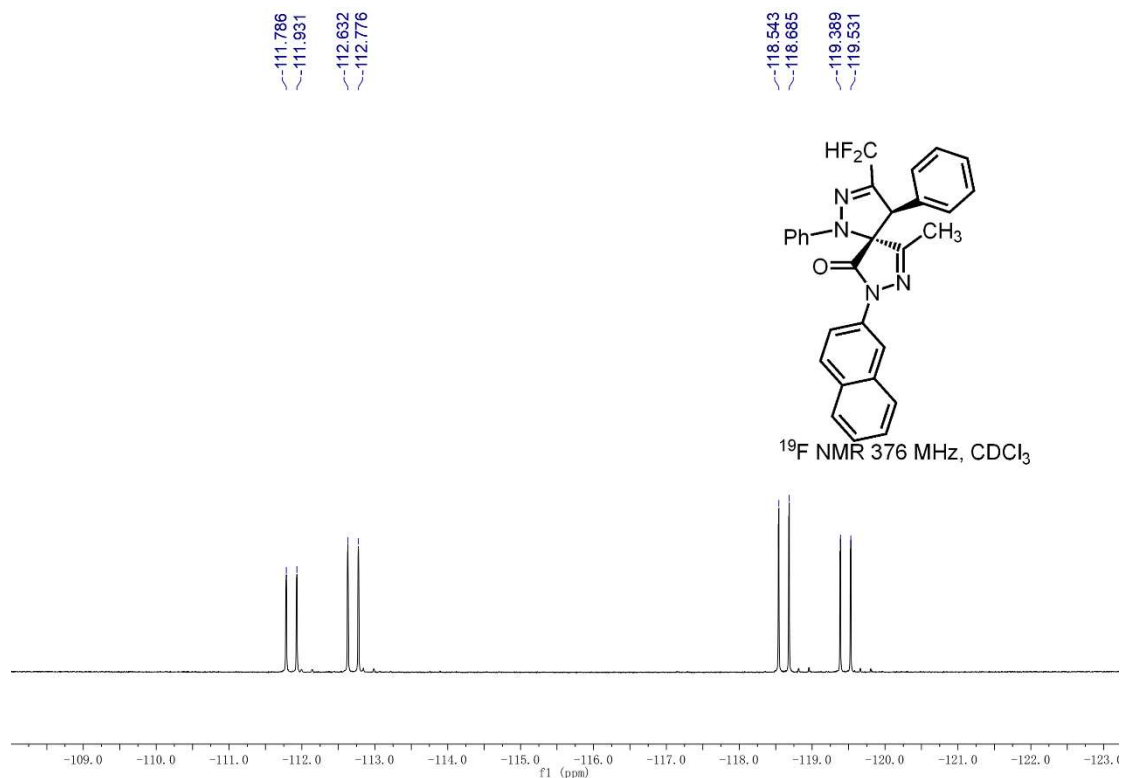
Meas. m/z	#	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j % Conf	mS	Std	Std	Std	Std	Std
503.1665	1	C <sub>29</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	503.1654	-2.3	-1.3	19.5	ok	even	5.7	8.7	1.0	3.6	1.9	842.7

NMR copies of compound (*cis*)-40:









HRMS (ESI) copy of compound (*cis*)-40:

### Mass Spectrum SmartFormula Report

#### Analysis Info

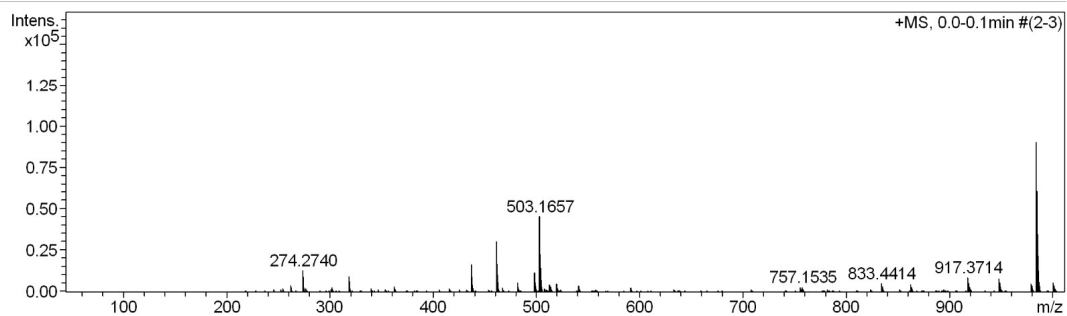
Analysis Name D:\Data\user\NWNNU-fengyang 20230321-23.d  
 Method tune\_low.m  
 Sample Name A-581  
 Comment

Acquisition Date 2023-3-21 17:32:06

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

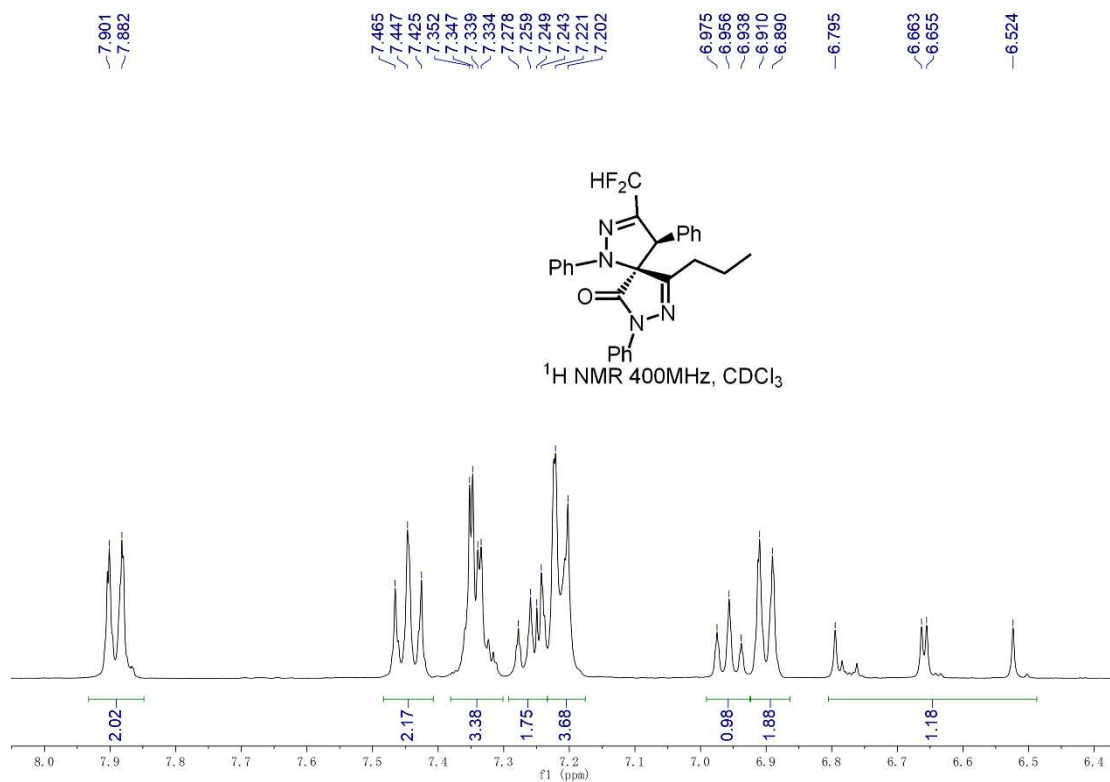
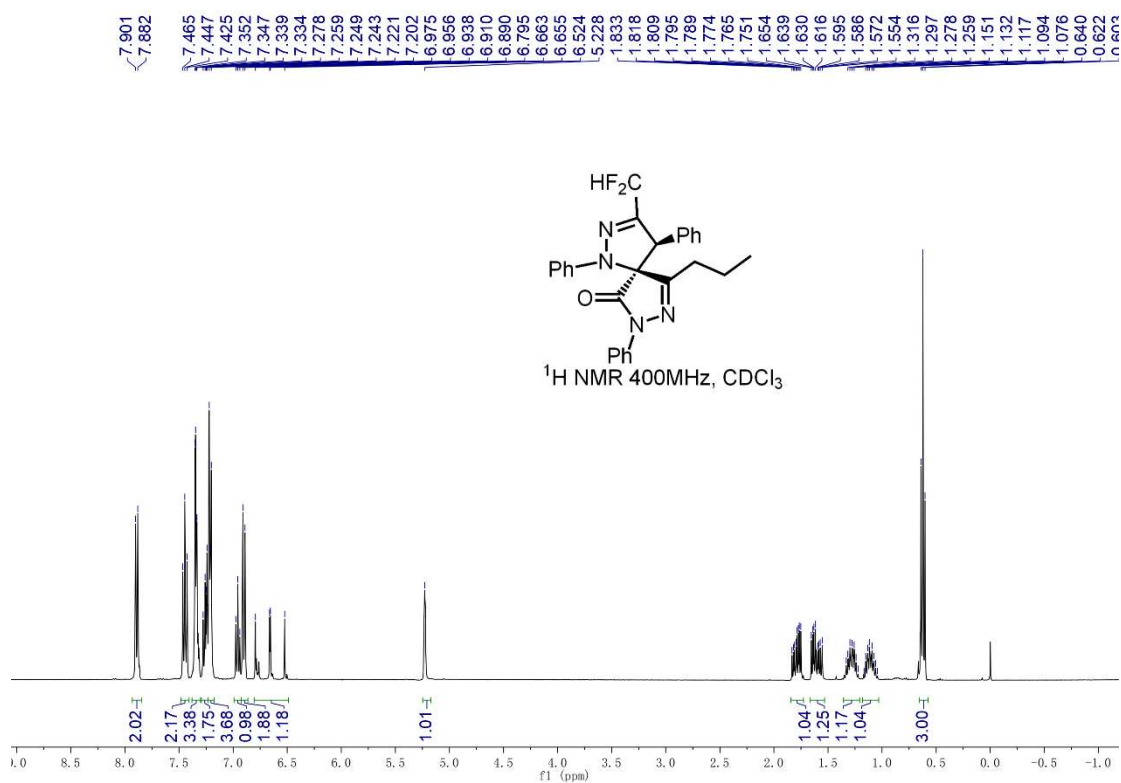
#### Acquisition Parameter

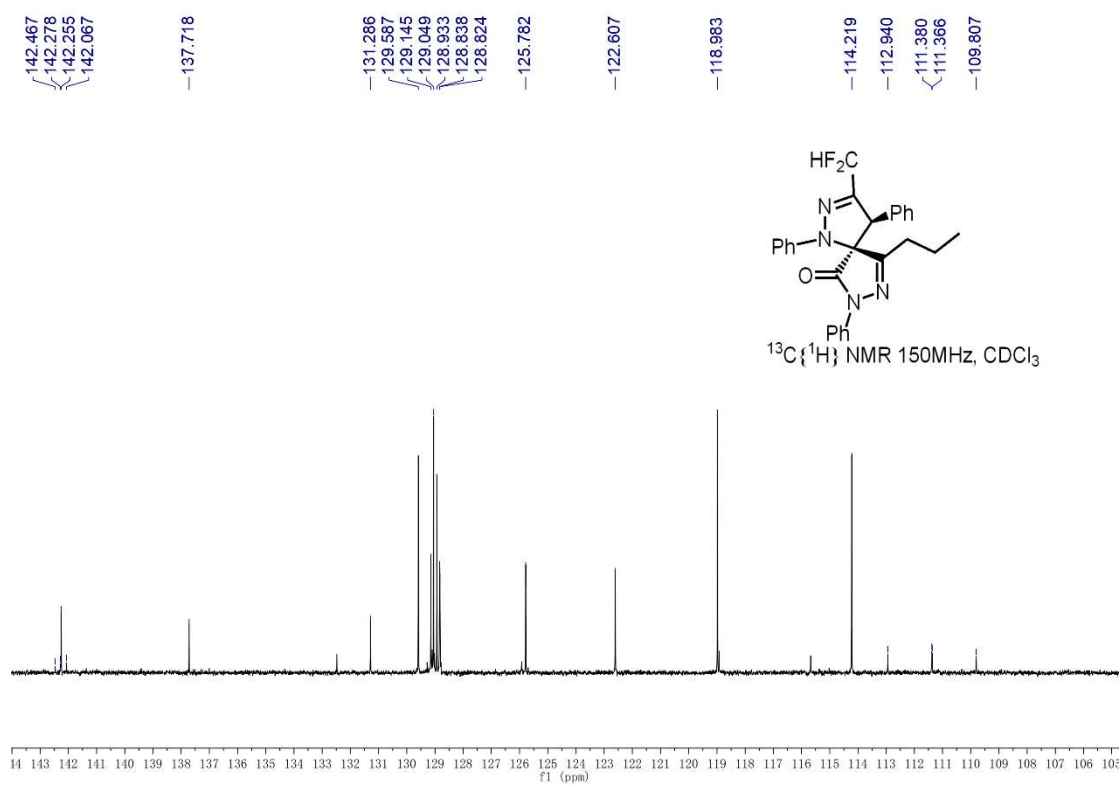
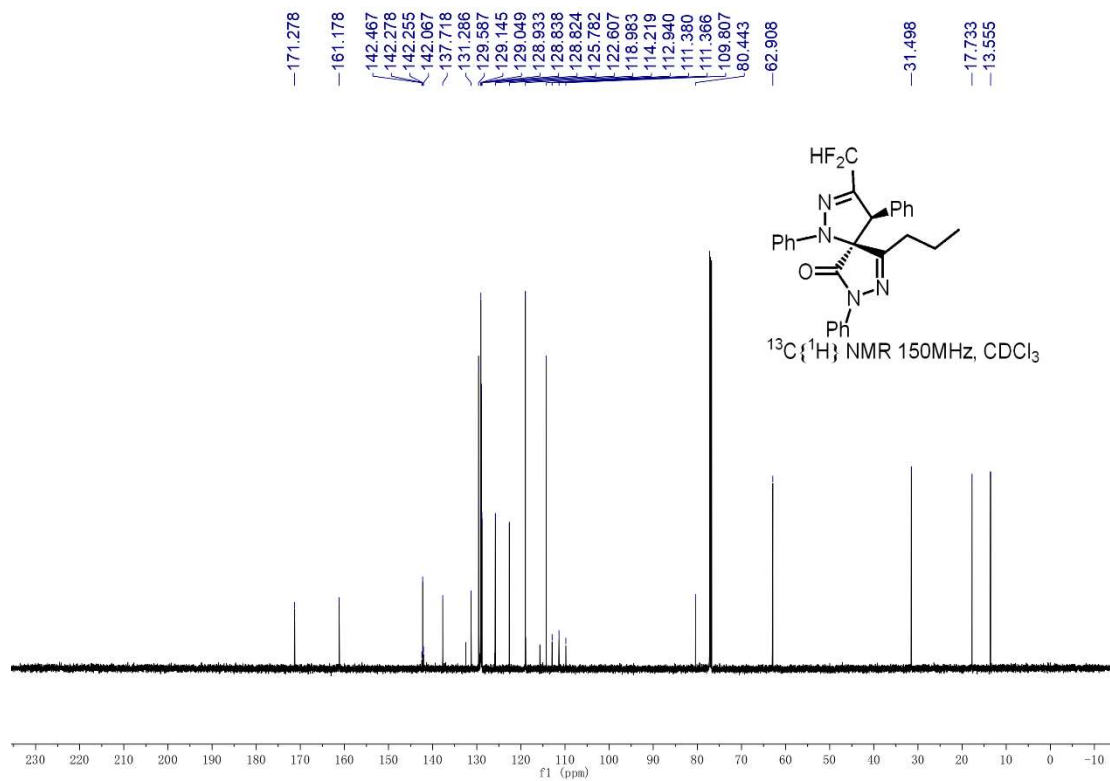
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu$ C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

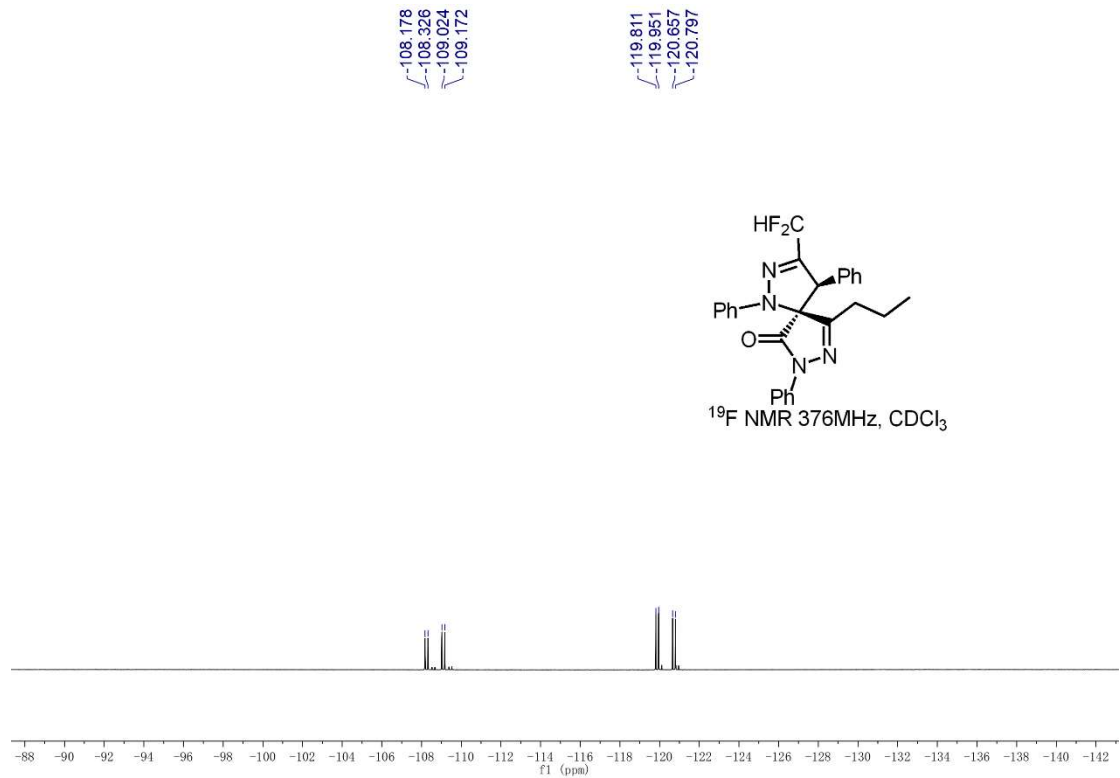


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej% Conf	m Sig	Std l	St d	St d l	St d	Std Com b Dev
503.1657	1 C <sub>29</sub> H <sub>22</sub> F <sub>2</sub> N <sub>4</sub> NaO	503.1654	-0.7	-0.6	19.5	ok	even	7.6	12.0	0.7	6.2	1.9	842.7

NMR copies of compound (*trans*)-4p:







HRMS (ESI) copy of compound (*trans*)-4p:

### Mass Spectrum SmartFormula Report

#### Analysis Info

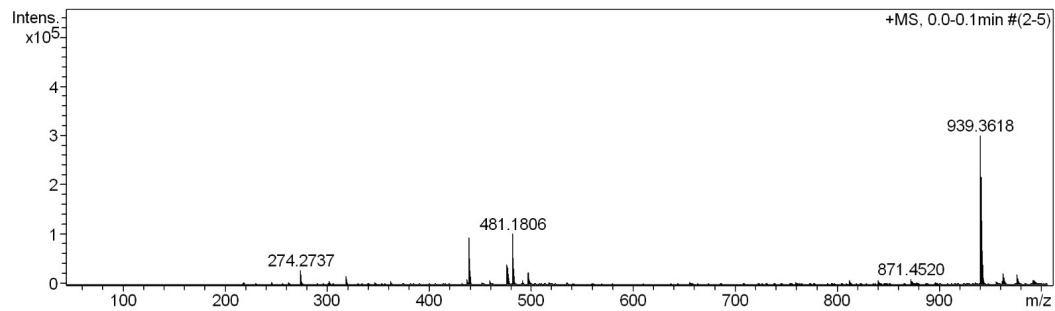
Analysis Name D:\Data\user\NWNW-fengyang 20230321-24.d  
 Method tune\_low.m  
 Sample Name A-55  
 Comment

Acquisition Date 2023-3-21 17:34:17

Operator BDAL@DE  
 Instrument / Ser# microTOF-Q 20453

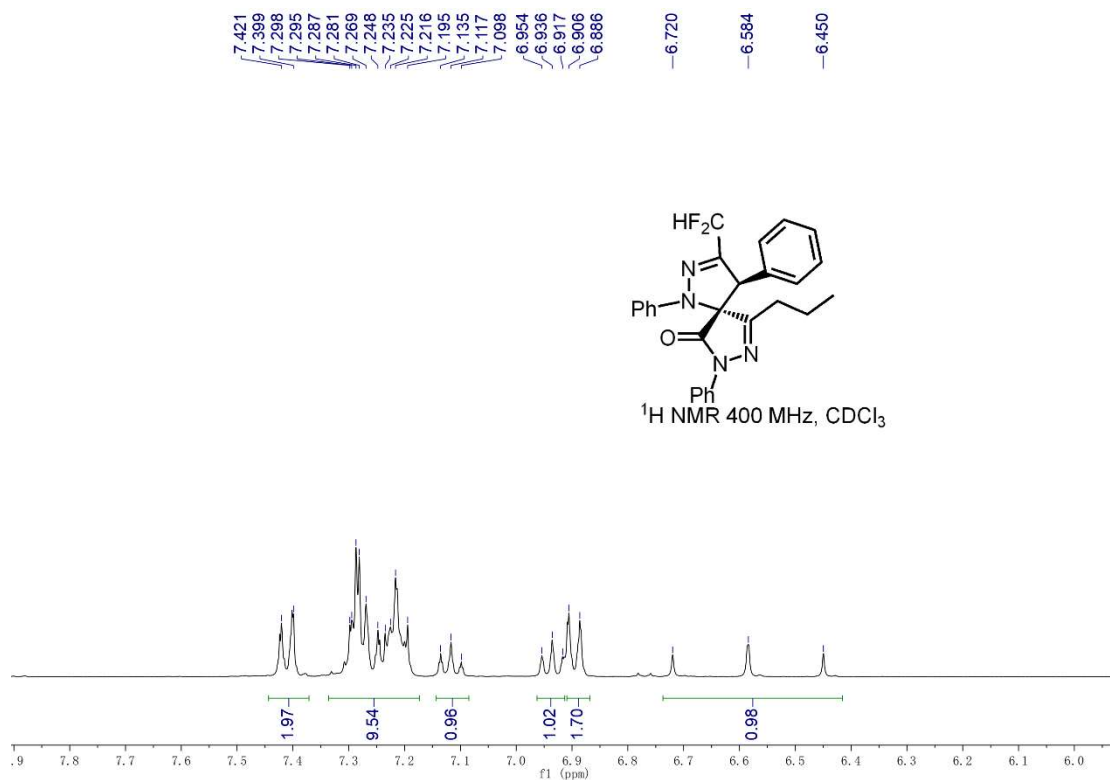
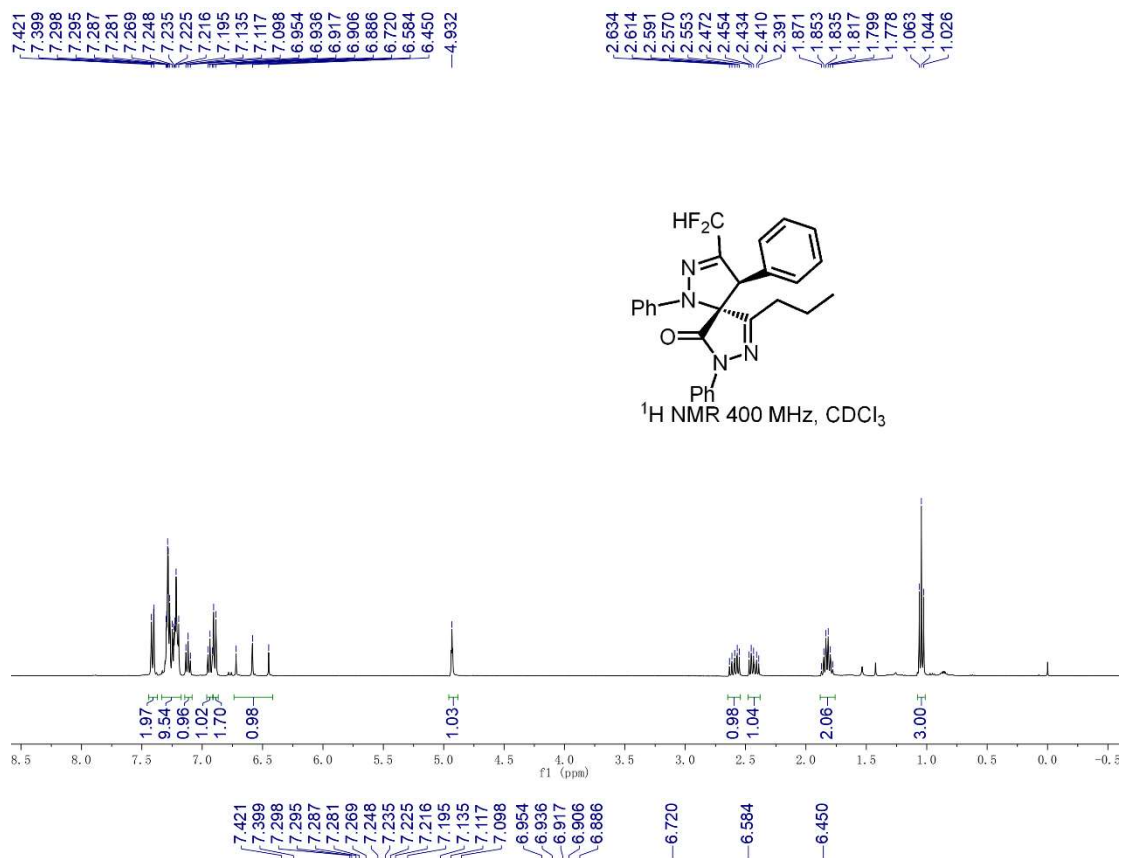
#### Acquisition Parameter

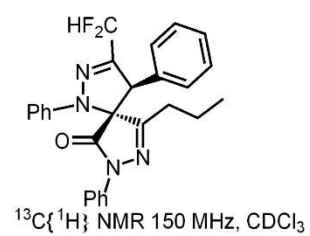
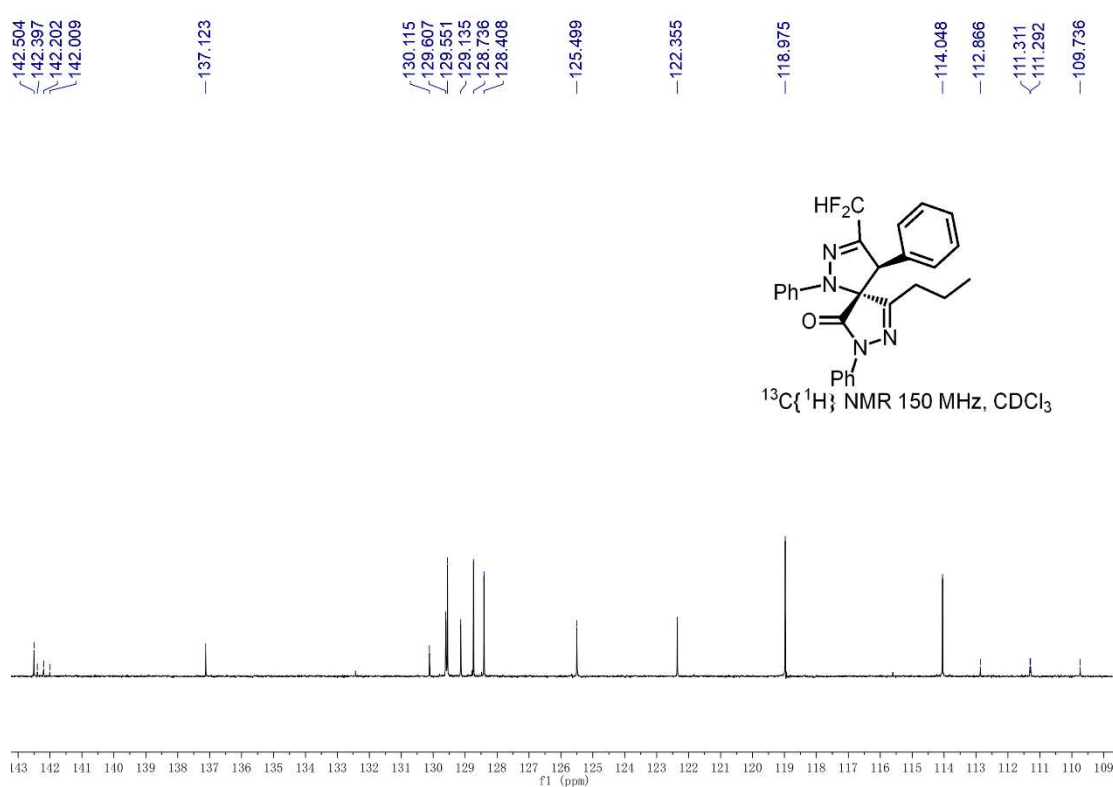
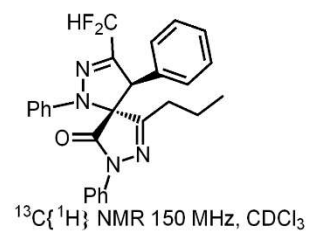
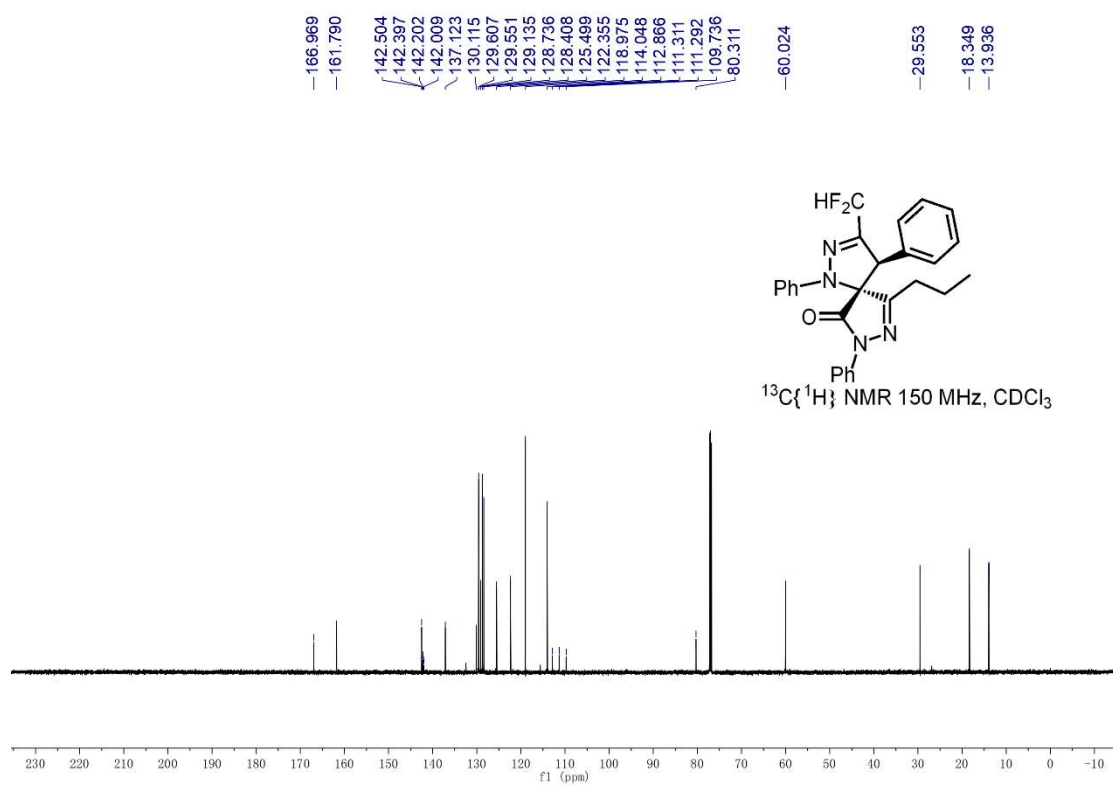
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej	Conf	mS	Std	Std	Std	Std	Std
m/z														
481.1806	1 C <sub>27</sub> H <sub>24</sub> F <sub>2</sub> N <sub>4</sub> NaO	481.1810	0.9	1.9	16.5	ok	even	3.7	6.0	1.2	3.3	1.9	842.7	

NMR copies of compound (*cis*)-4p:



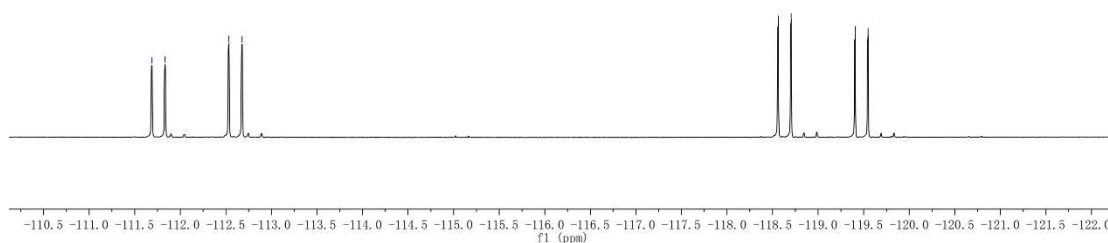
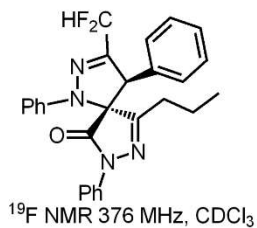


~111.689  
~111.833

~112.533  
~112.678

~118.563  
~118.704

~119.407  
~119.549



HRMS (ESI) copy of compound (*cis*)-4p:

### Mass Spectrum SmartFormula Report

#### Analysis Info

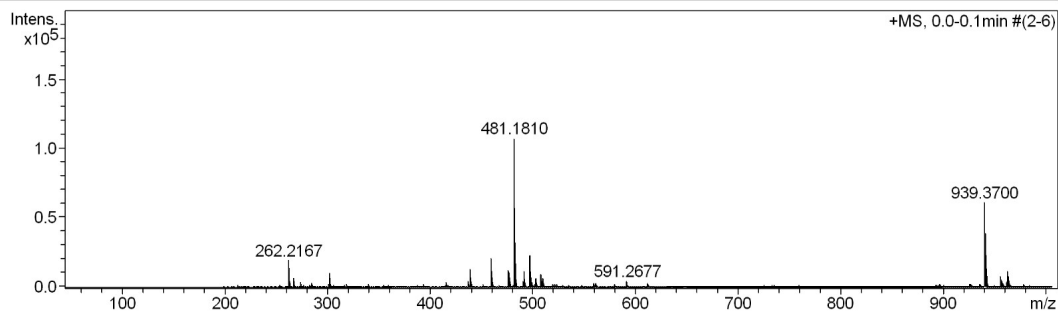
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Method tune\_low.m  
Sample Name A-551  
Comment

Acquisition Date 2023-3-21 17:37:43

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

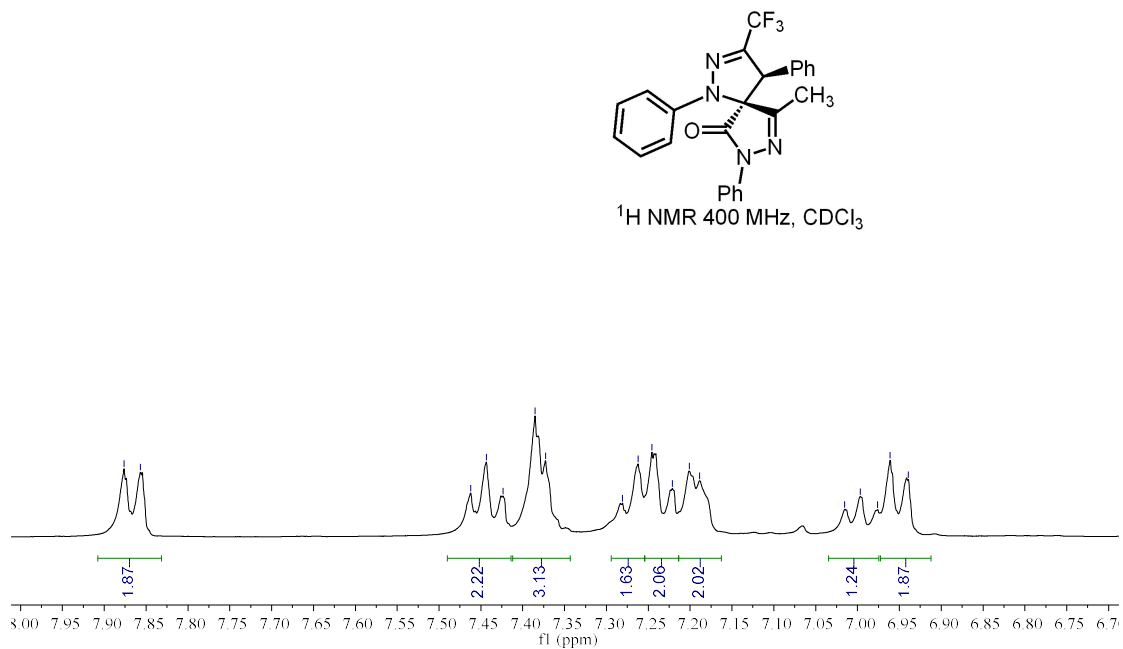
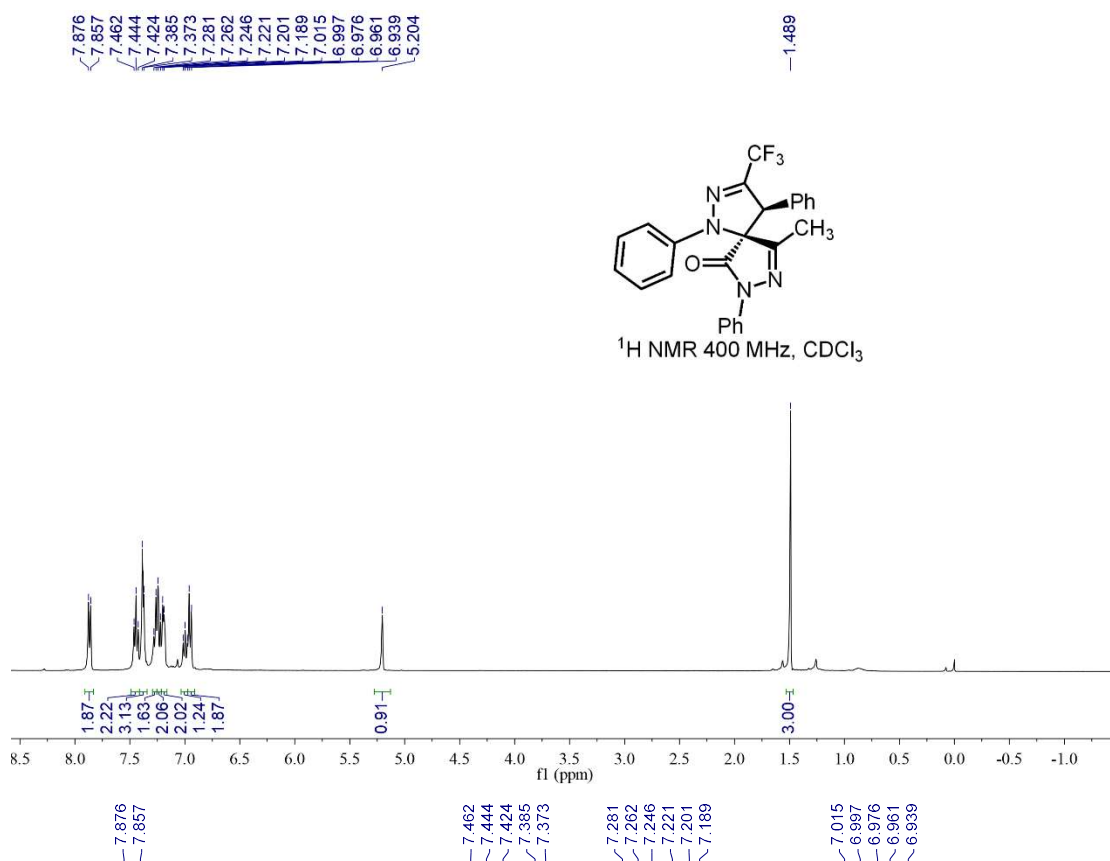
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

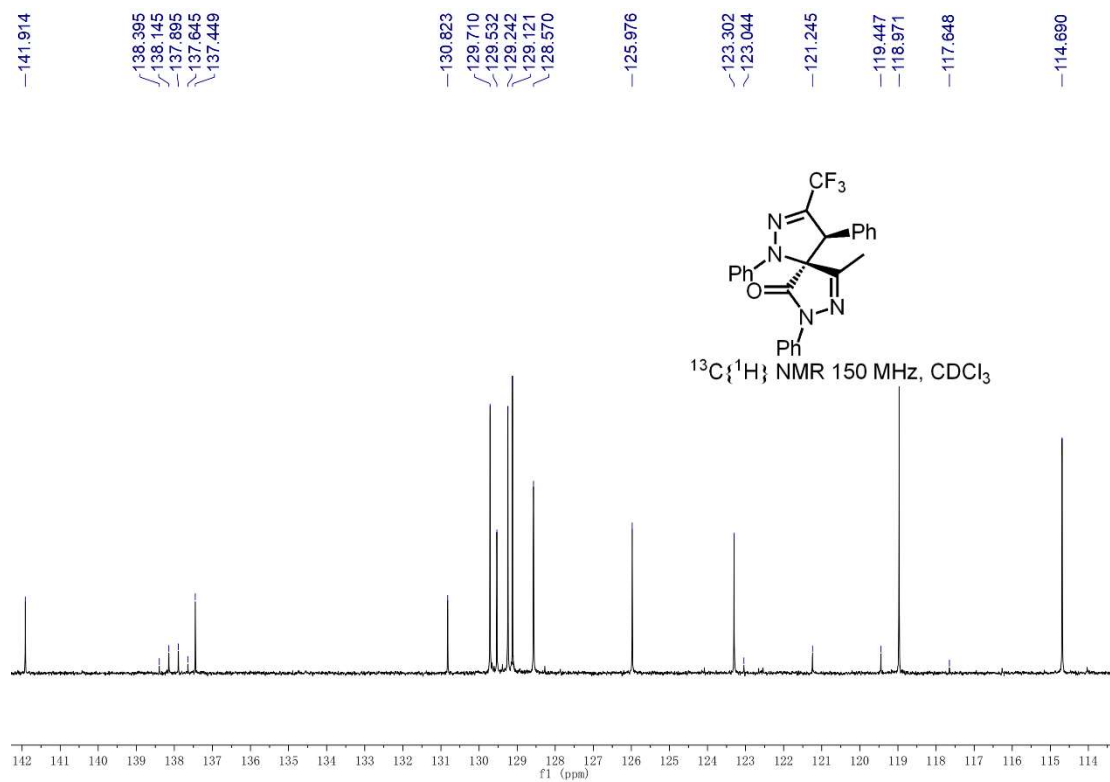
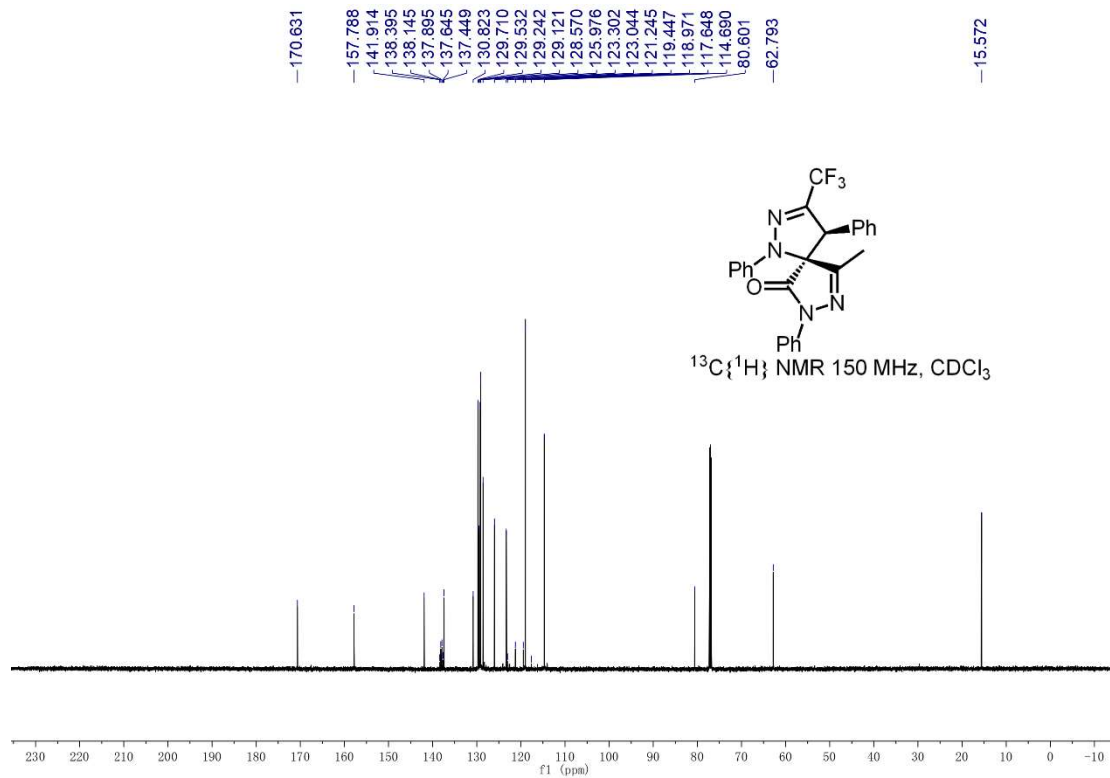


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej% Conf	mS	Std	Std	Std	Std	Std
m/z									l	Me	l	m/	Com
										an	Va	rN	z
										m/	rN	Diff	Dev
										z	or		
										m			
481.1810	1 C <sub>27</sub> H <sub>24</sub> F <sub>2</sub> N <sub>4</sub> NaO	481.1810	0.1	0.9	16.5	ok	even	4.4	6.4	1.1	3.3	3.0	842.7

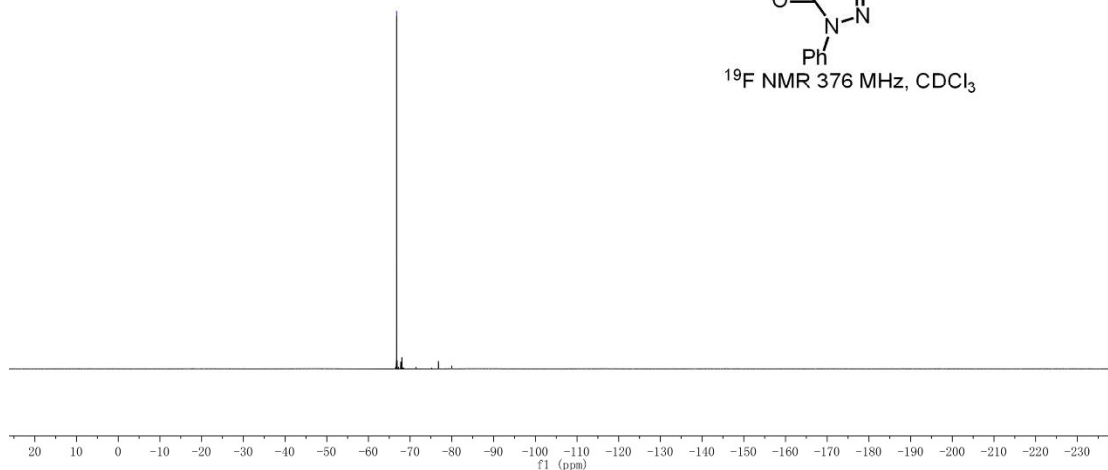
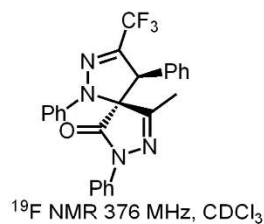
NMR copies of compound (*trans*)-6a:







-86.742



HRMS (ESI) copy of compound (*trans*)-6a:

### Mass Spectrum SmartFormula Report

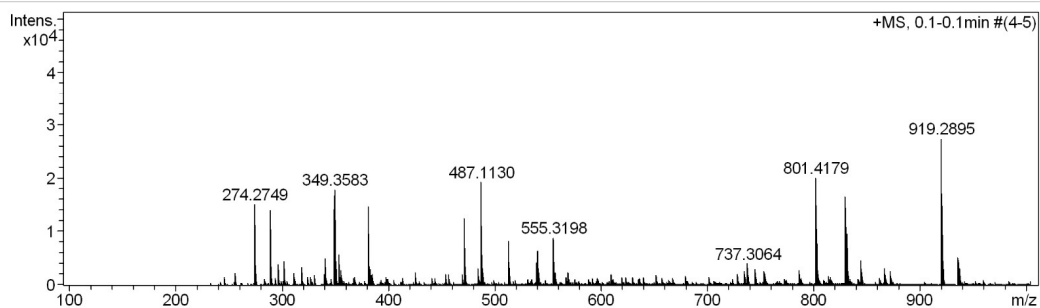
#### Analysis Info

Analysis Name D:\Data\user\maransong20211202-1.d  
Method tune\_low.m  
Sample Name 2-01  
Comment

Acquisition Date 2021-12-2 17:39:19  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

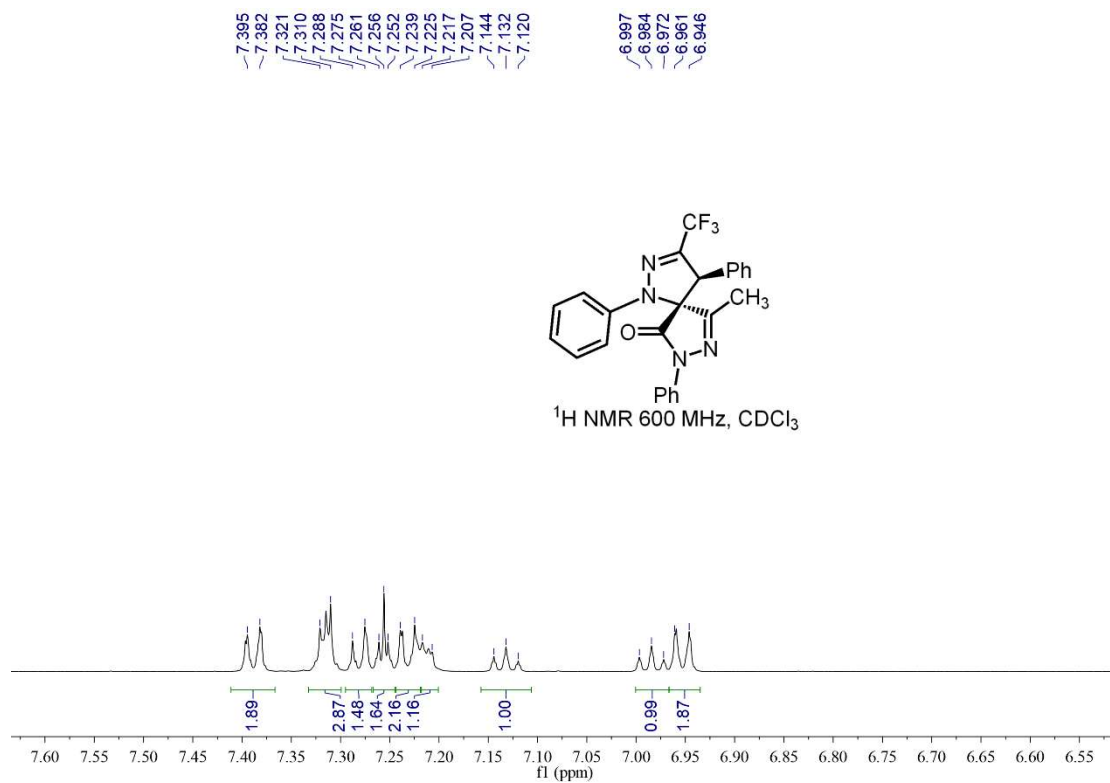
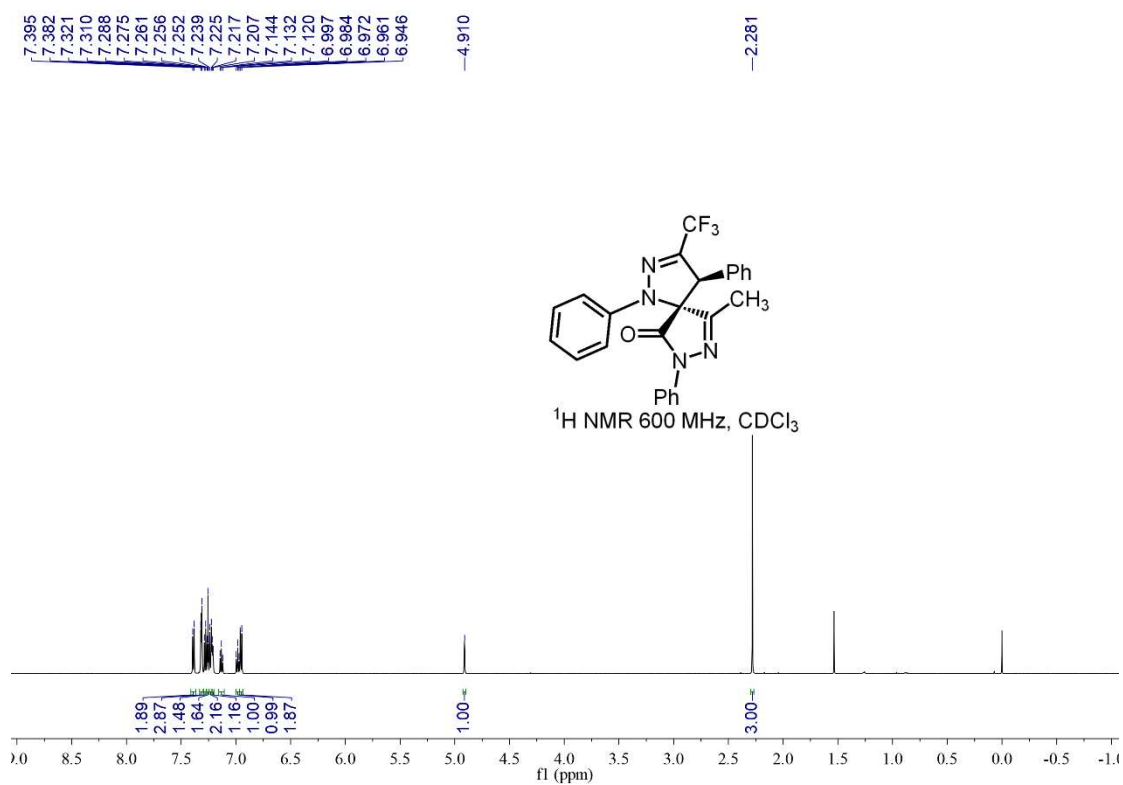
#### Acquisition Parameter

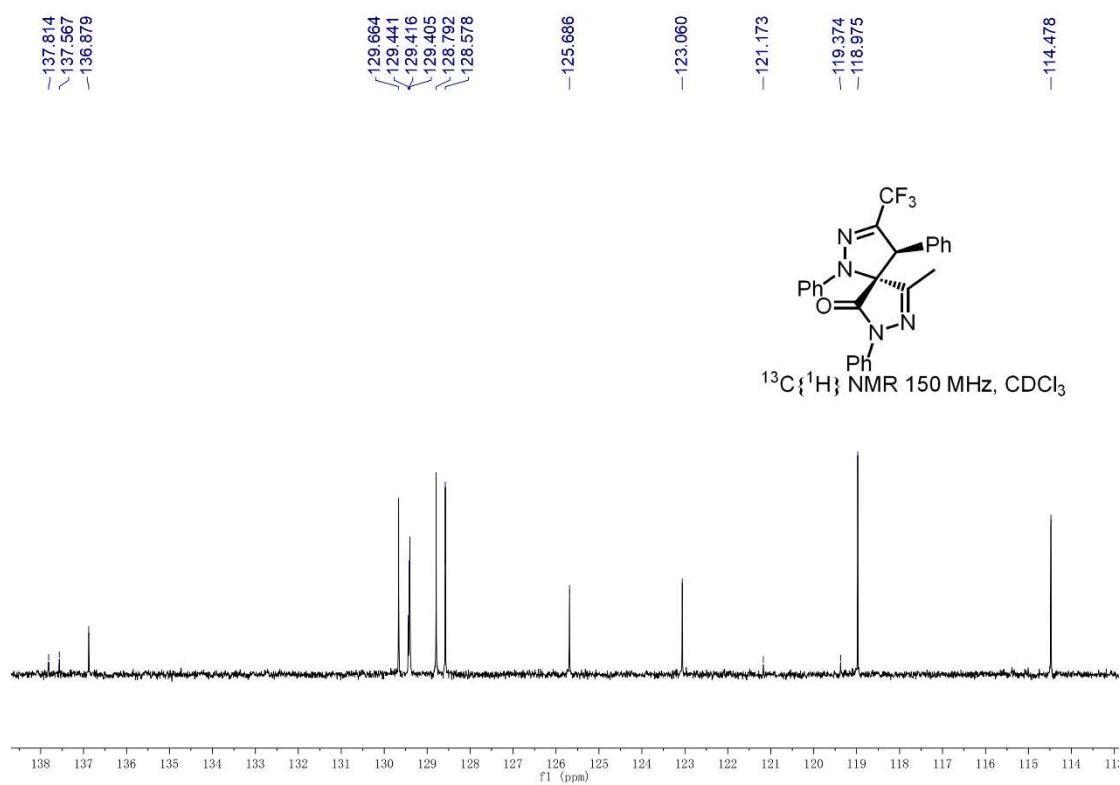
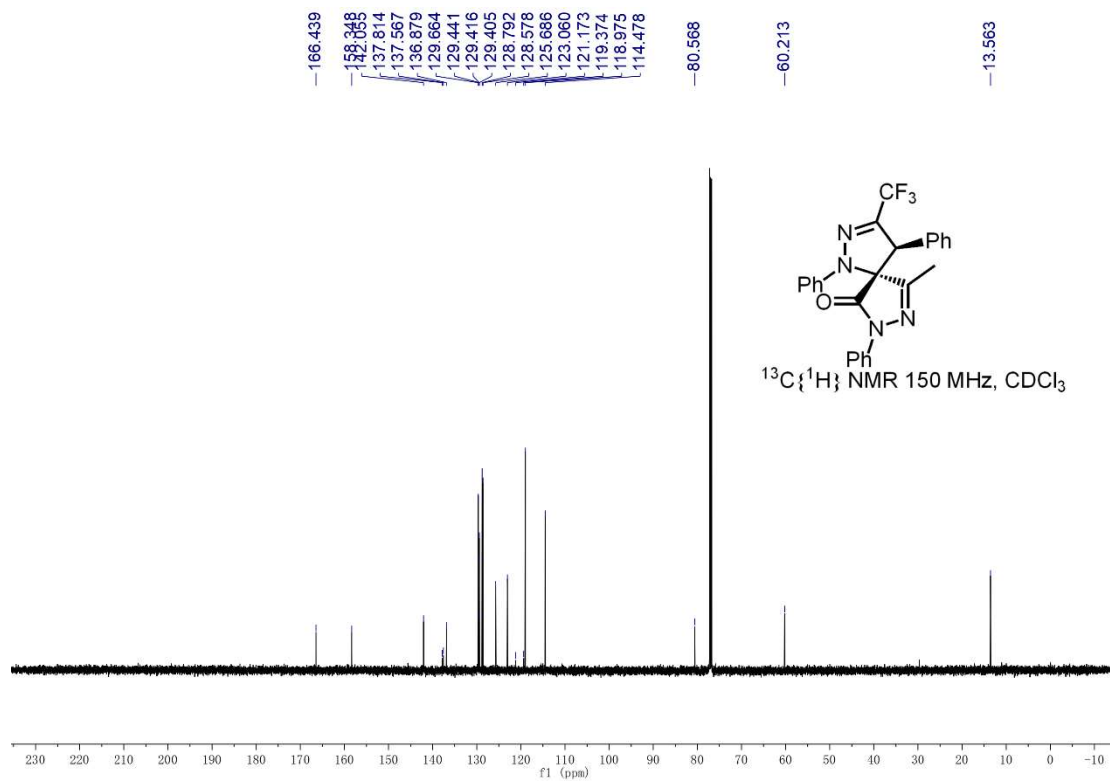
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



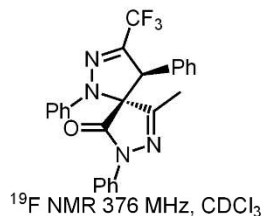
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- ul e	e; f	mSi gm a	Std l	St d Me an m/z	Std Var m	St d Nor m	St d Dif f	Std Com b Dev
471.1404	1 C <sub>25</sub> H <sub>19</sub> F <sub>3</sub> N <sub>4</sub> NaO	471.1403	-0.2	-0.6	16.5	ok	even	23.4	31.8	0.4	24.6	0.8	842.7	

NMR copies of compound (*cis*)-**6a**:





--62.479



HRMS (ESI) copy of compound (*cis*)-**6a**:

### Mass Spectrum SmartFormula Report

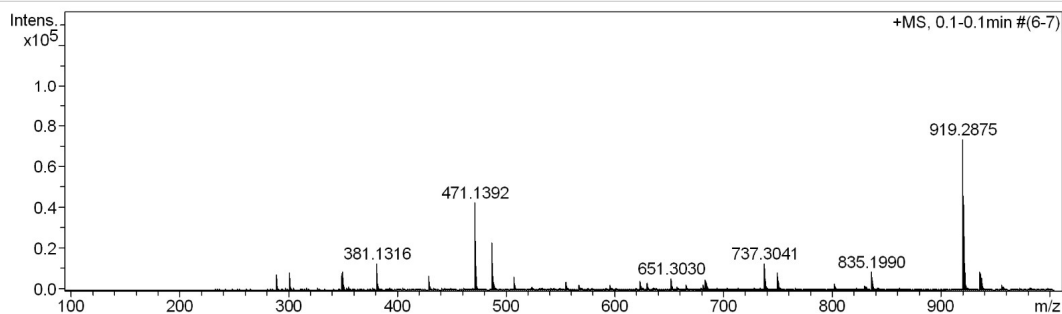
#### Analysis Info

Analysis Name D:\Data\user\maransong20211202-2.d  
Method tune\_low.m  
Sample Name 2-02  
Comment

Acquisition Date 2021-12-2 17:41:54  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

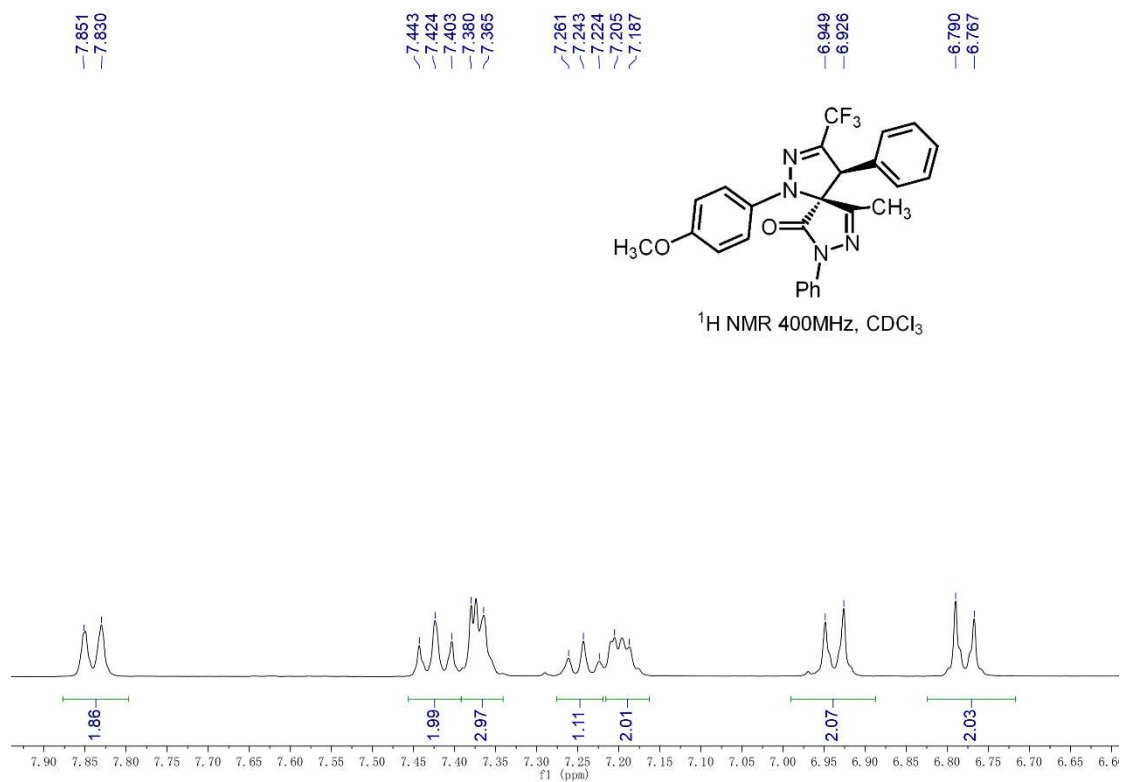
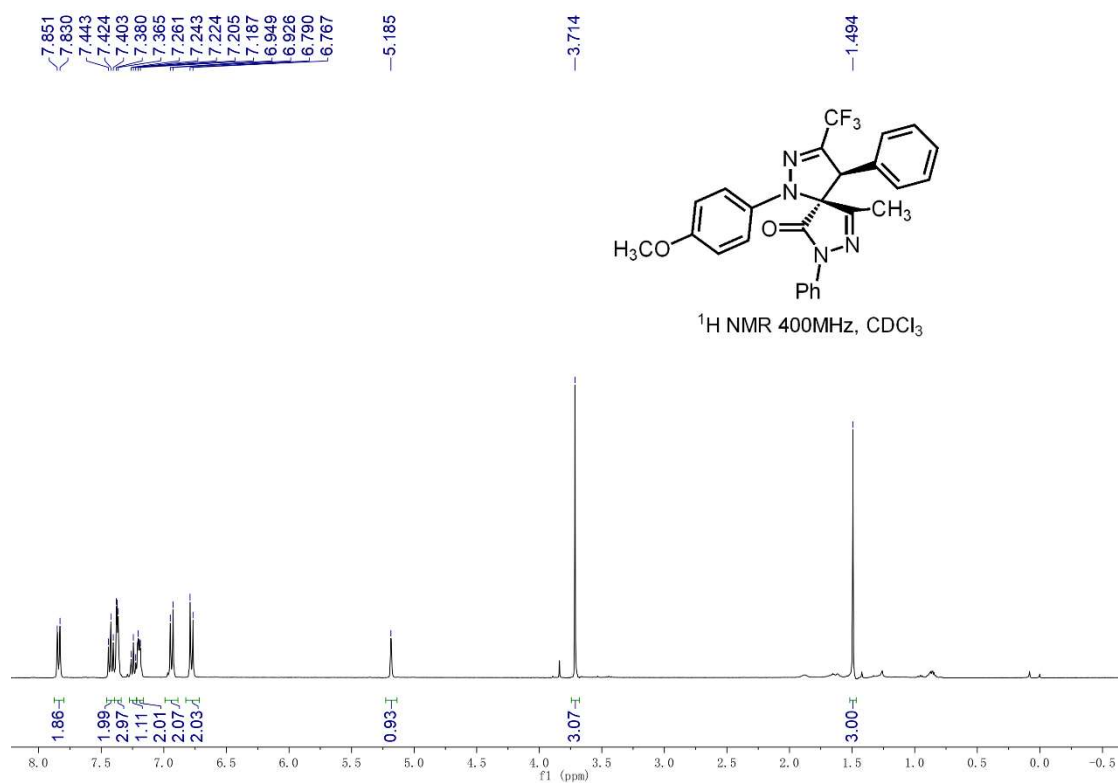
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste

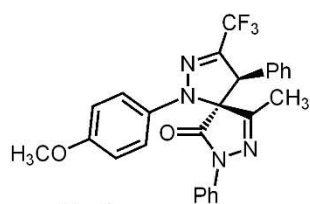


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R ul e	ej% Conf	mS ig ma	Std l	Std Me an m/z	Std l Va rN	Std m/ z Diff	Std Com b Dev
471.1392	1 C <sub>25</sub> H <sub>19</sub> F <sub>3</sub> N <sub>4</sub> NaO	471.1403	2.3	2.6	16.5	ok	even	5.2	6.9	1.2	3.4	0.6	842.7

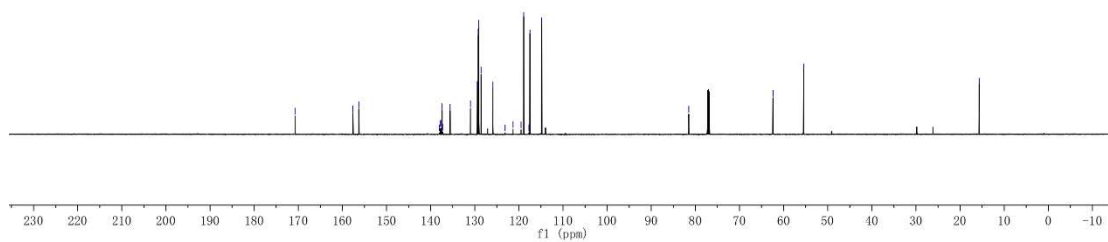
NMR copies of compound (*trans*)-**6b**:



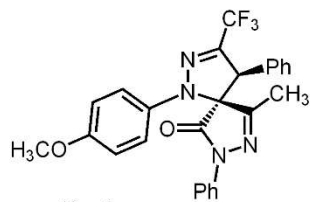
-170.661  
 -157.605  
 -156.272  
 -138.043  
 -137.793  
 -137.544  
 -137.407  
 -137.295  
 -135.594  
 -130.984  
 -129.425  
 -129.214  
 -129.068  
 -128.565  
 -125.879  
 -123.111  
 -121.314  
 -119.517  
 -118.906  
 -117.719  
 -117.502  
 -114.833  
 -81.501  
 -62.411  
 -55.436  
 -15.657



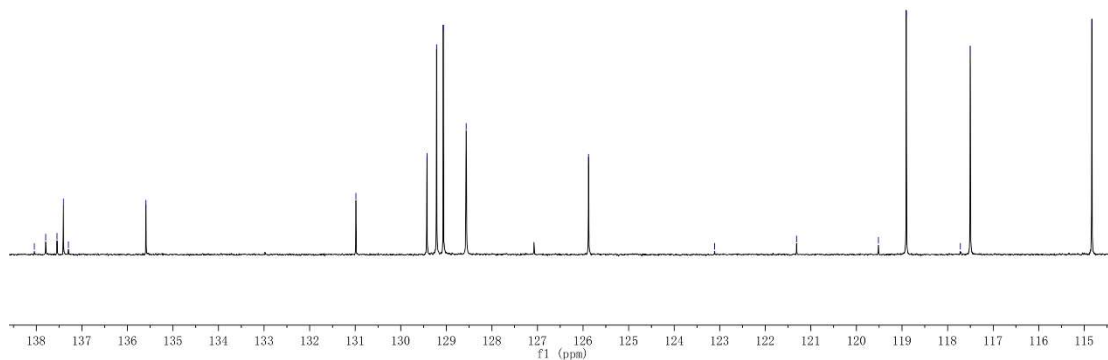
$^{13}\text{C}\{^1\text{H}\}$  NMR 150 MHz,  $\text{CDCl}_3$



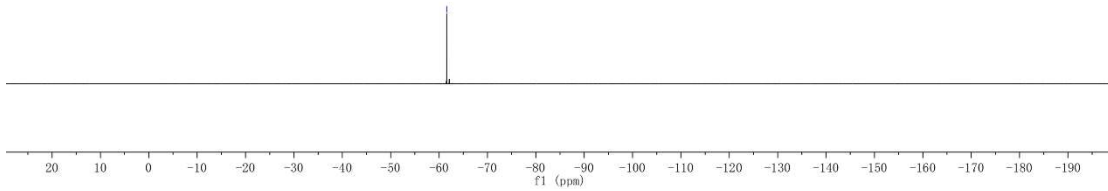
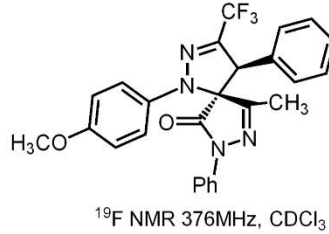
-138.043  
 -137.793  
 -137.544  
 -137.407  
 -137.295  
 -135.594  
 -130.984  
 -129.425  
 -129.214  
 -129.068  
 -128.565  
 -125.879  
 -123.111  
 -121.314  
 -119.517  
 -118.906  
 -117.719  
 -117.502  
 -114.833



$^{13}\text{C}\{^1\text{H}\}$  NMR 150 MHz,  $\text{CDCl}_3$



---61.559



HRMS (ESI) copy of compound (*trans*)-**6b**:

### Mass Spectrum SmartFormula Report

#### Analysis Info

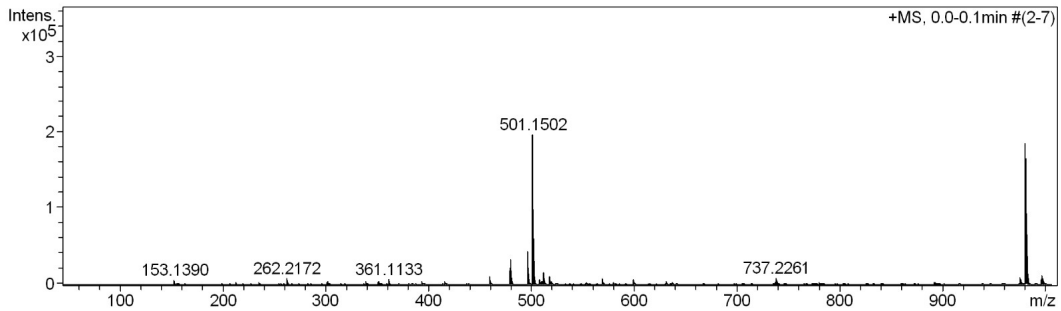
Analysis Name D:\Data\user\NWNNU-fengyang 20230322-1.d  
Method tune\_low.m  
Sample Name A-38  
Comment

Acquisition Date 2023-3-22 9:15:09

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

#### Acquisition Parameter

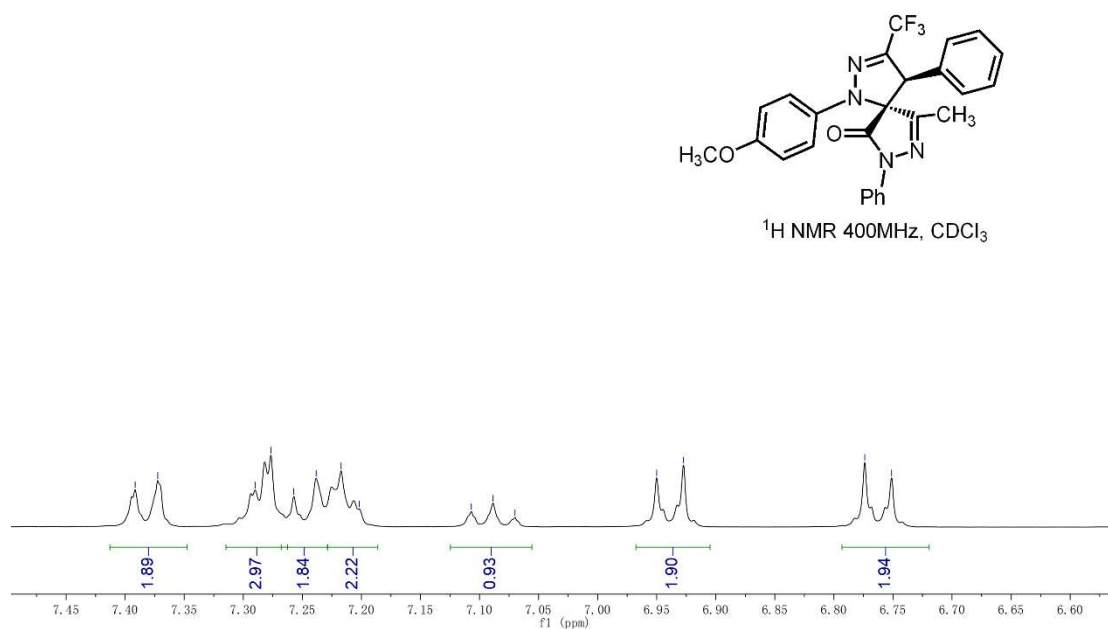
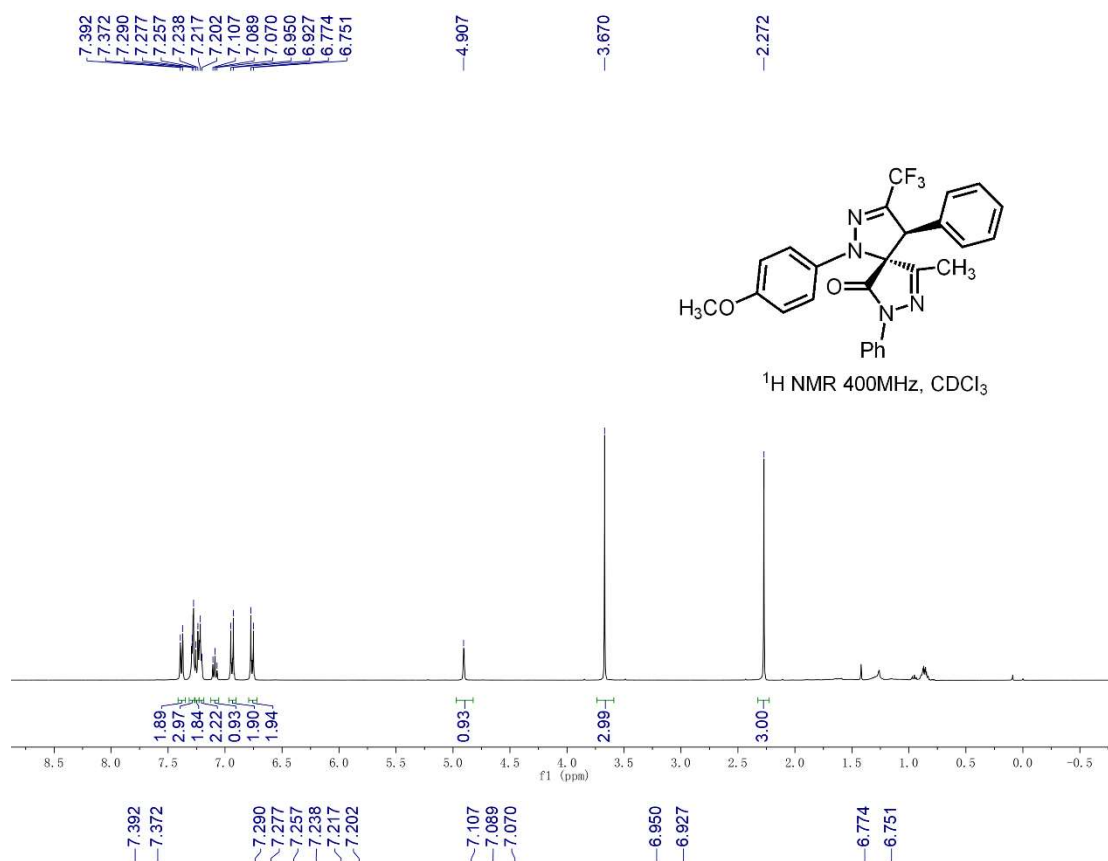
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j̄aC
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste

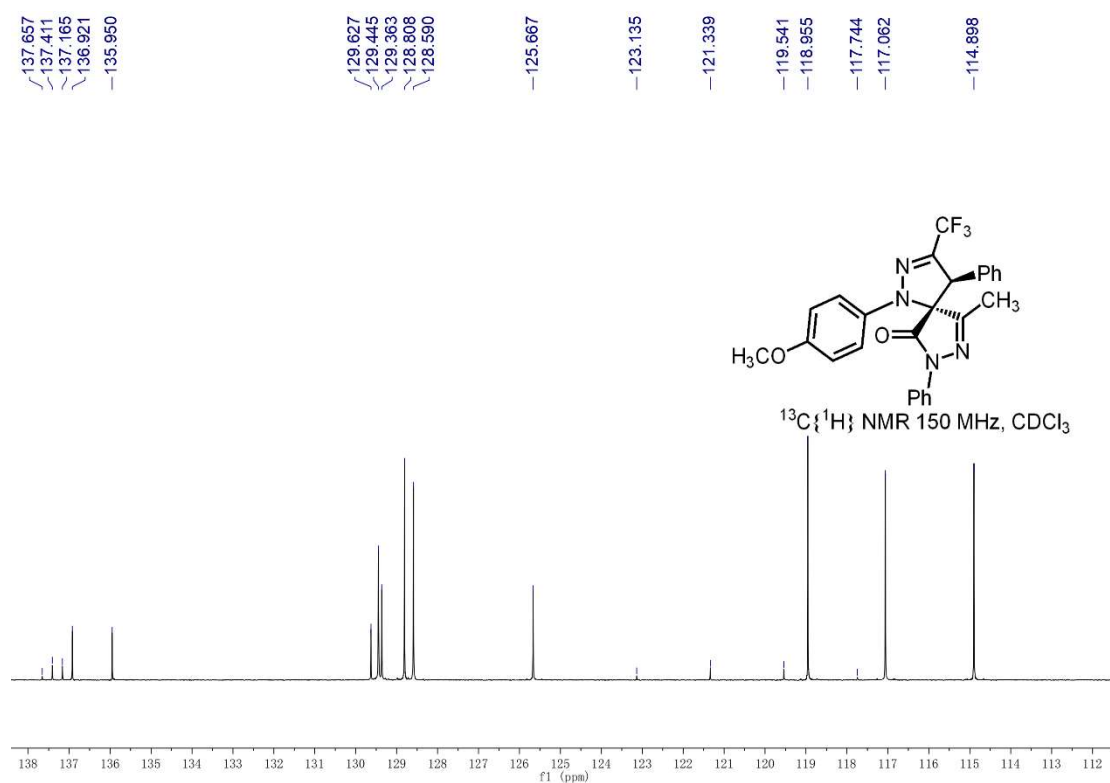
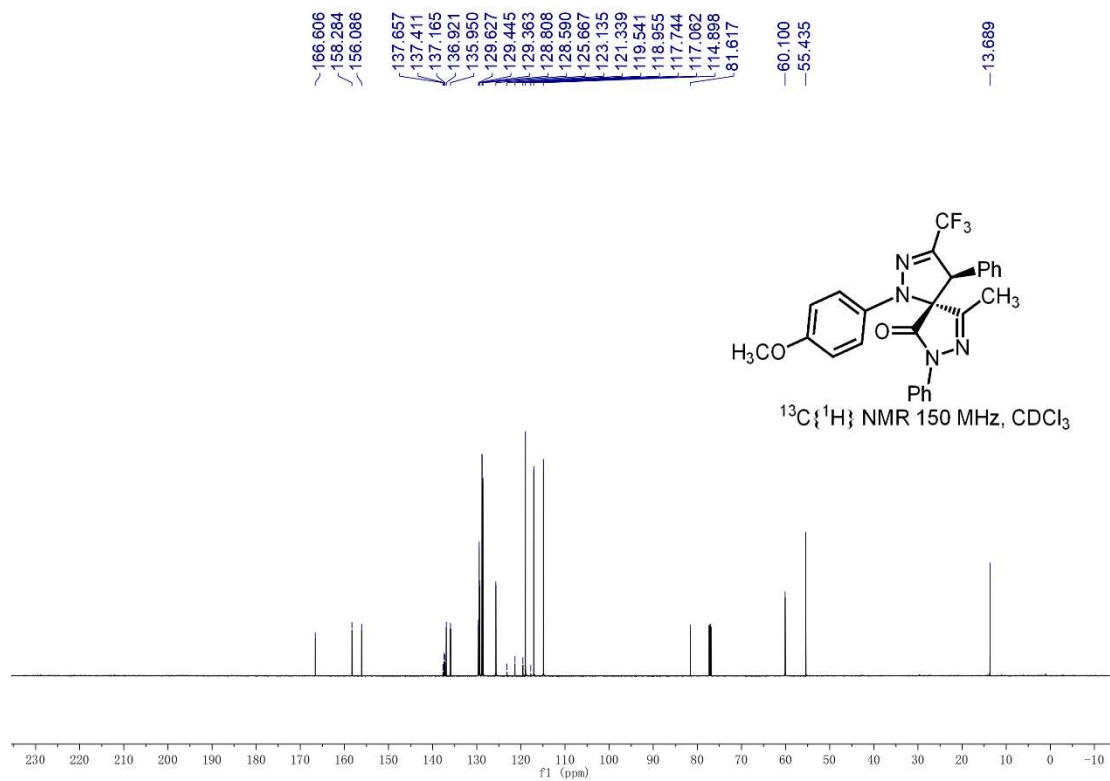


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>i</sub> ¥ Conf	mS ig ma	Std l	Std Me an m/z	Std l Va rN or m	Std m/z Diff	Std Com b Dev
501.1502	1 C <sub>26</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO <sub>2</sub>	501.1509	1.4	0.8	16.5	ok	even	5.2	8.1	0.7	3.7	1.2	842.7

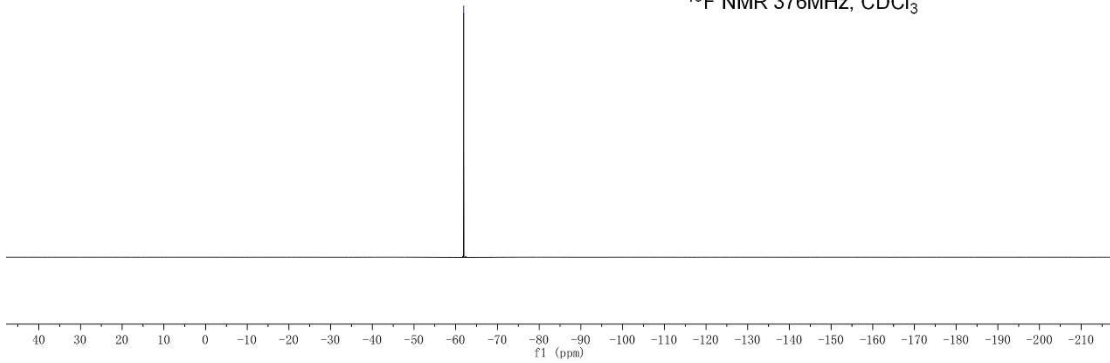
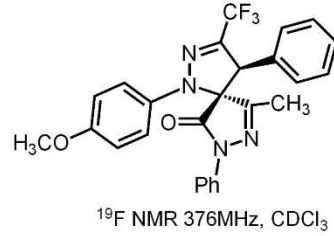


NMR copies of compound (*cis*)-**6b**:





61.909



HRMS (ESI) copy of compound (*cis*)-**6b**:

### Mass Spectrum SmartFormula Report

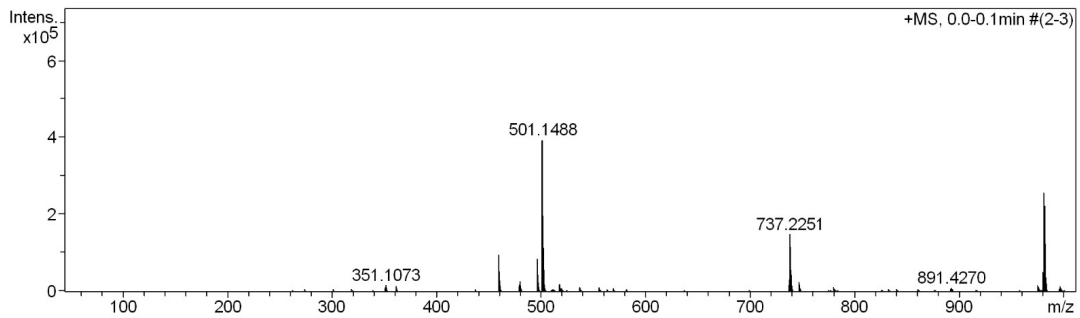
#### Analysis Info

Analysis Name D:\Data\user\NWNU-fengyang 20230322-2.d  
Method tune\_low.m  
Sample Name A-381  
Comment

Acquisition Date 2023-3-22 9:16:53  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

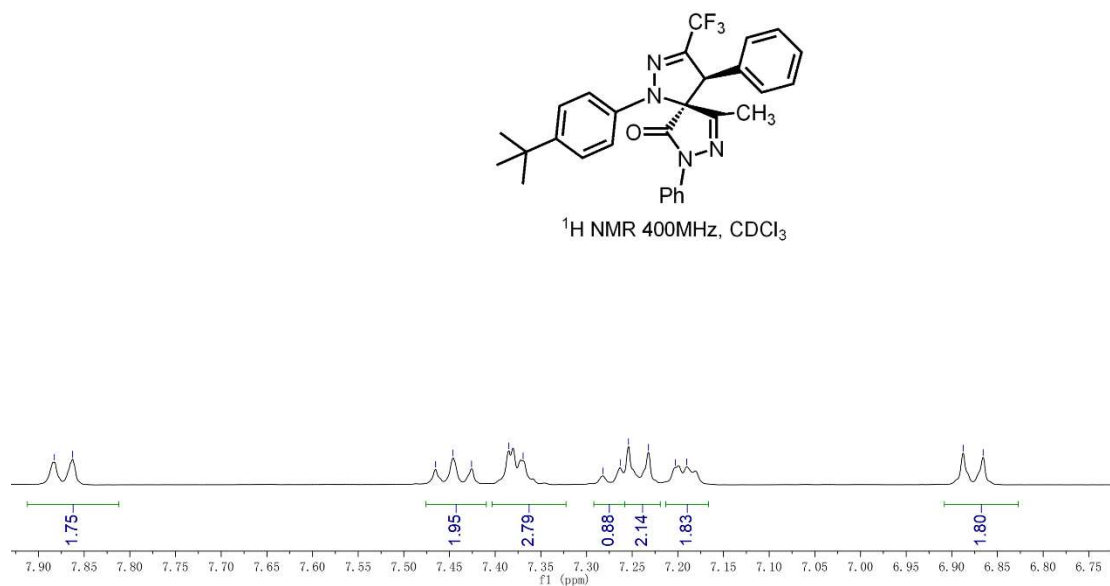
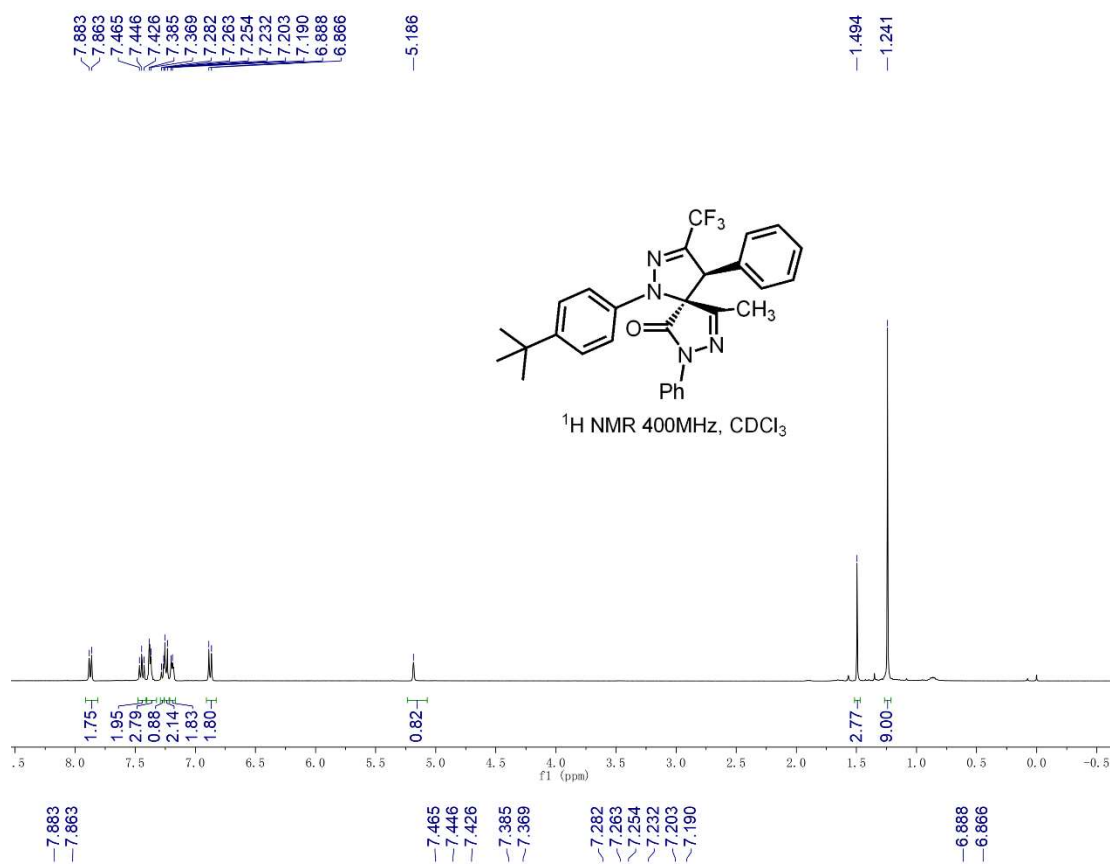
#### Acquisition Parameter

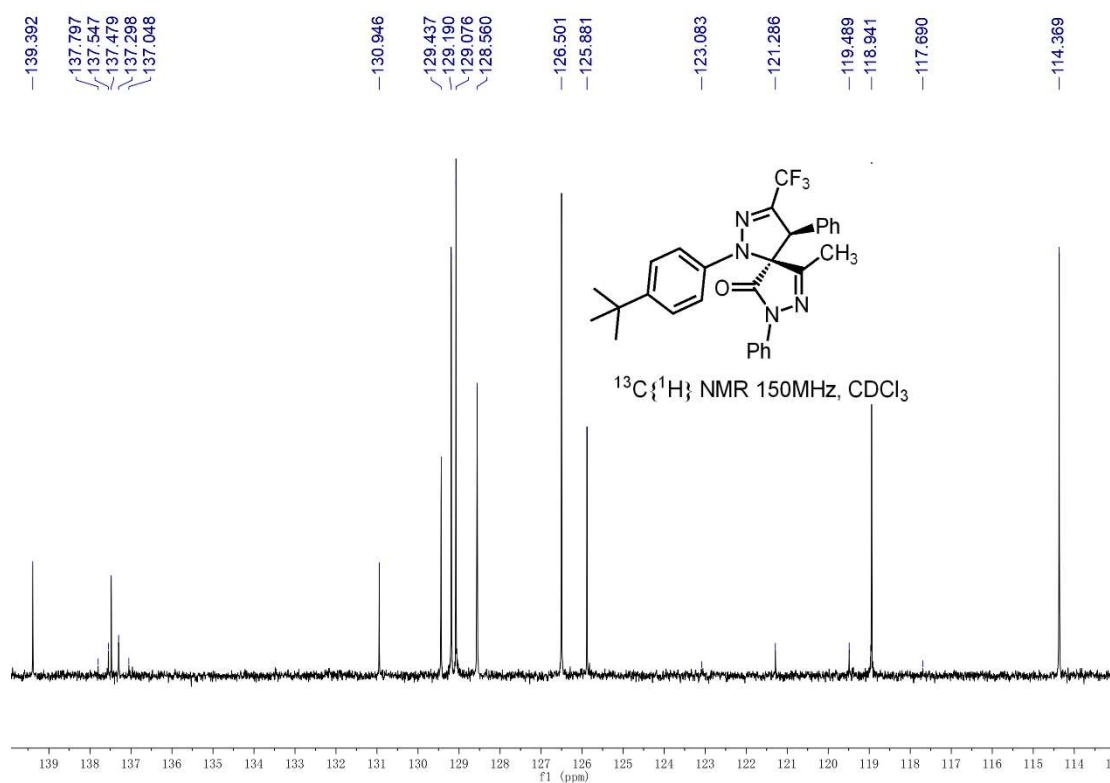
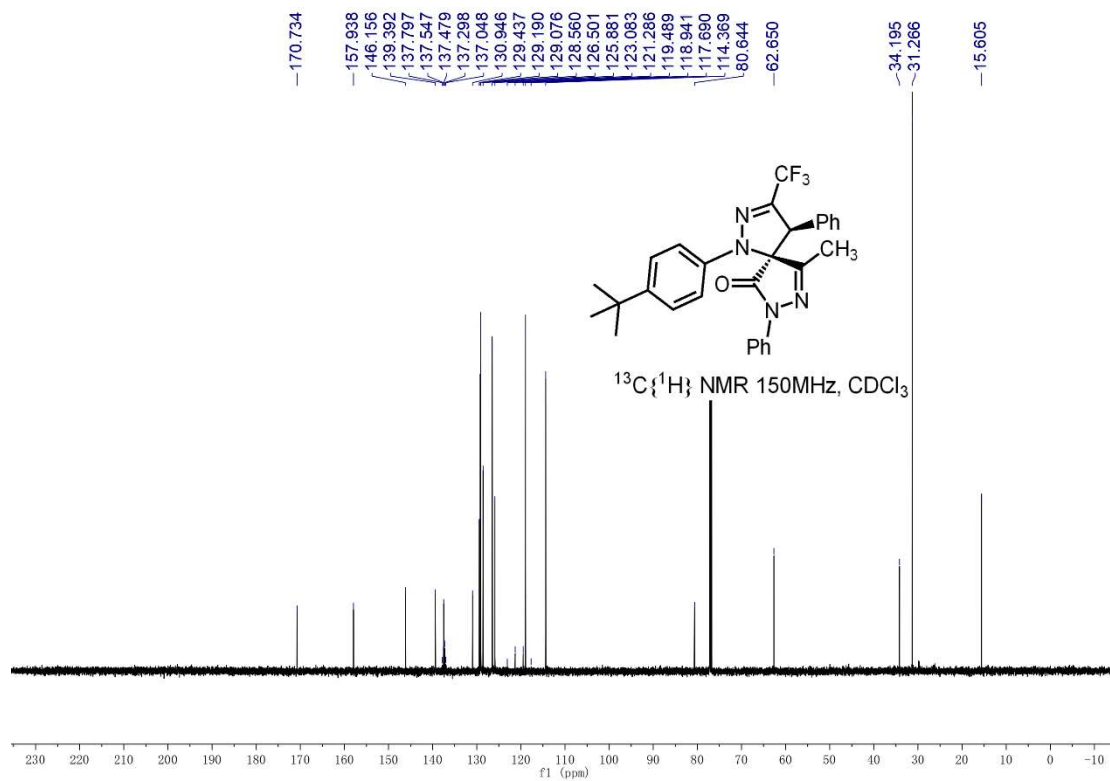
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



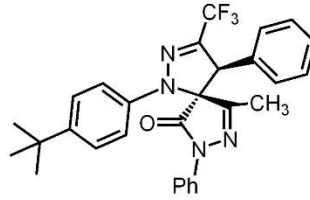
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R ul e	e;≠ Conf	mS ig ma	Std l	Std Me an m/z	Std l Va r or m	Std m/z Diff	Std Com b Dev
501.1488	1 C <sub>26</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO <sub>2</sub>	501.1509	4.1	3.0	16.5	ok	even	3.4	5.0	1.8	2.2	2.4	842.7

NMR copies of compound (*trans*)-6c:

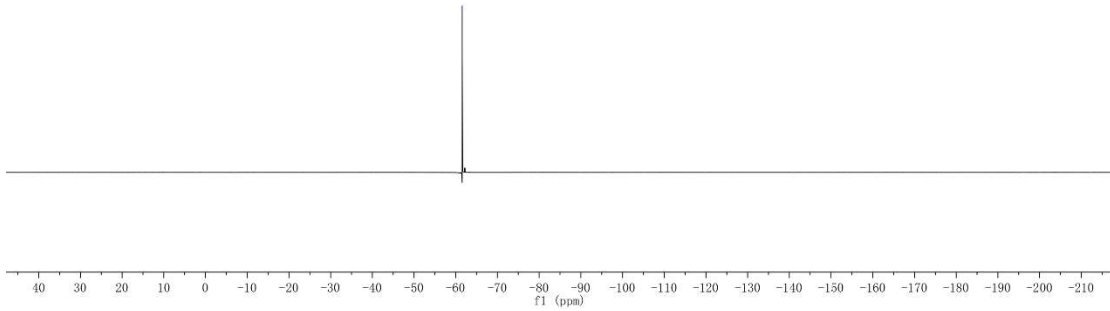




--61.555



<sup>19</sup>F NMR 376MHz, CDCl<sub>3</sub>



HRMS (ESI) copy of compound (*trans*)-6c:

### Mass Spectrum SmartFormula Report

#### Analysis Info

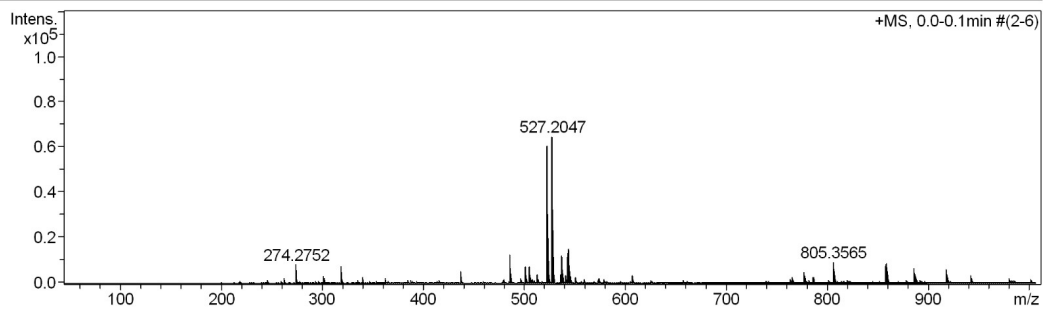
Analysis Name D:\Data\user\NWNW-fengyang 20230322-3.d  
Method tune\_low.m  
Sample Name A-39  
Comment

Acquisition Date 2023-3-22 9:20:19

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

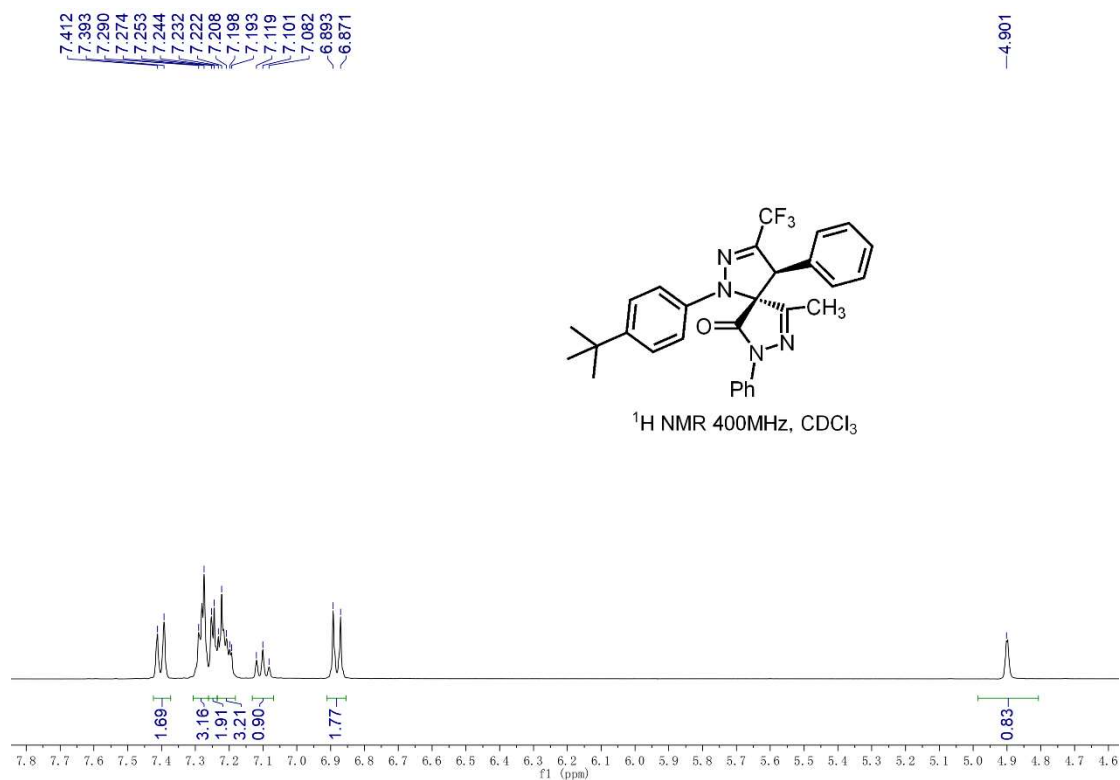
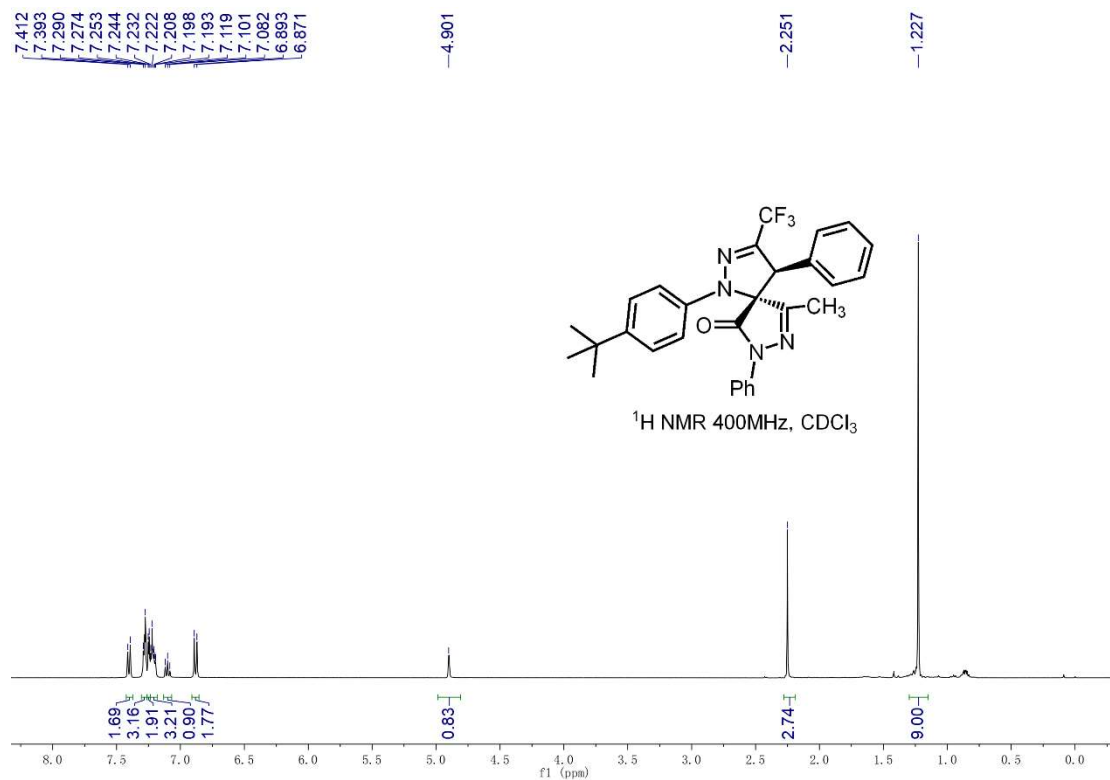
#### Acquisition Parameter

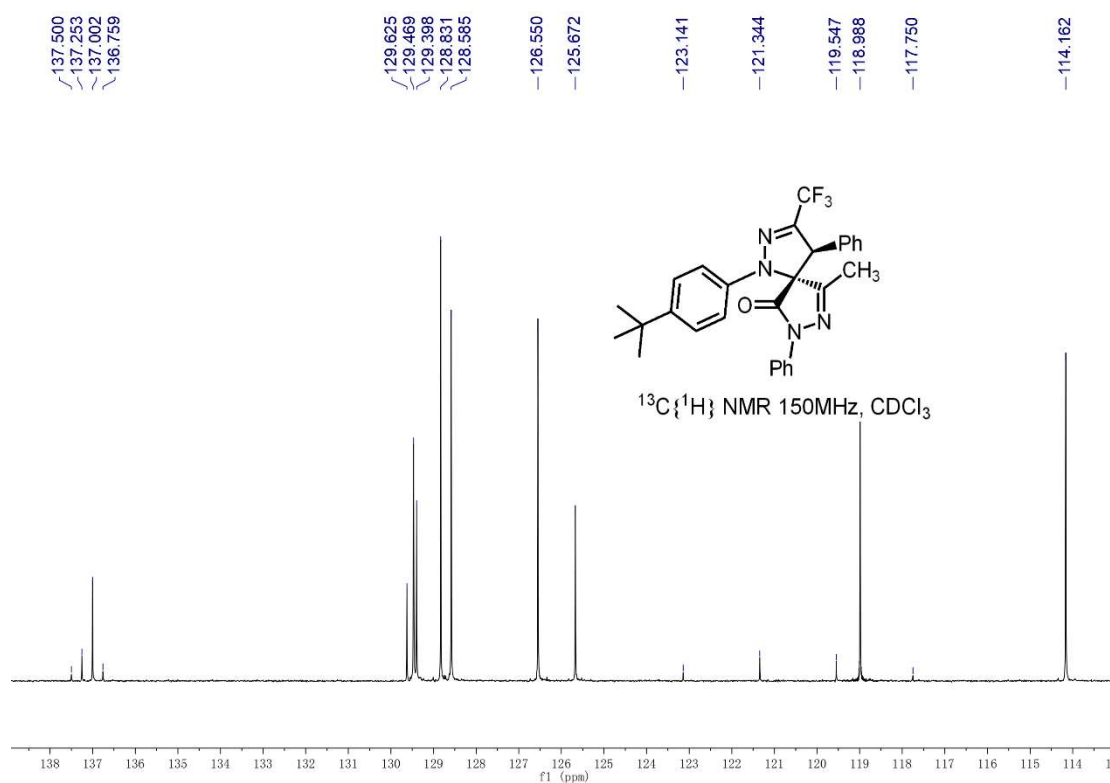
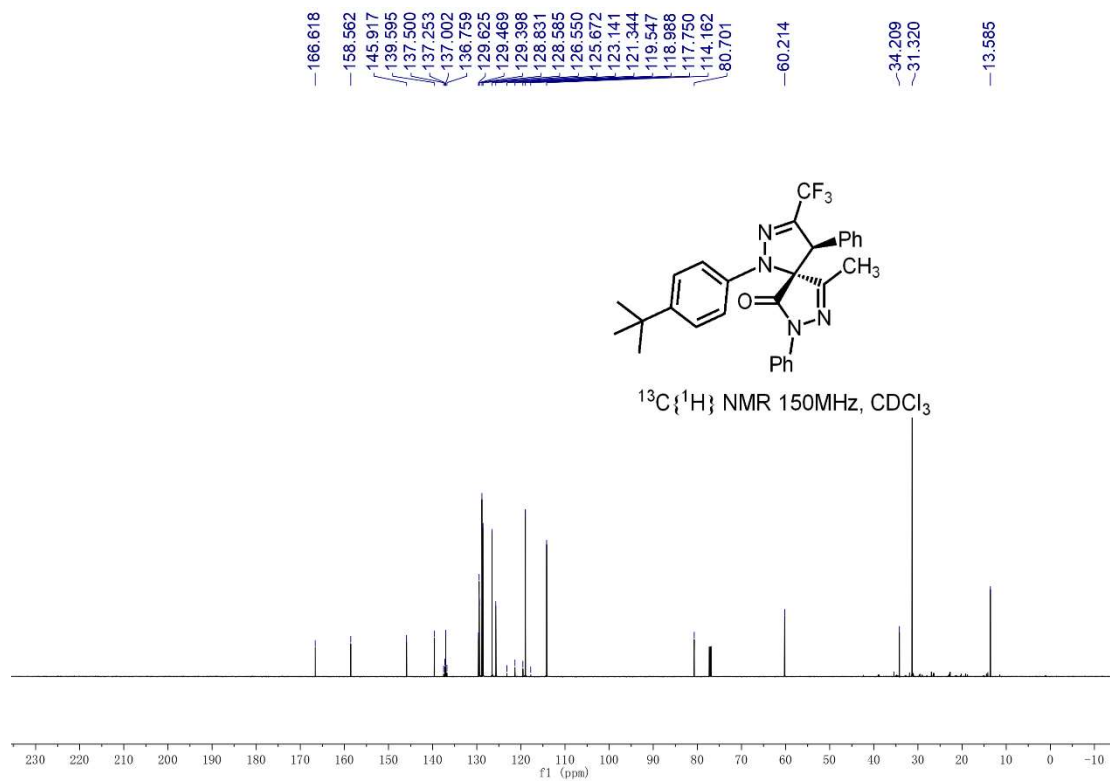
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu$ C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-R	ej $\neq$ Conf	mSi gm	Std l	Std d l	Std d l	Std d l	Std Com b
m/z										Me an z	Val rN z	m/ or Dif	Dev
527.2047	1 C <sub>29</sub> H <sub>27</sub> F <sub>3</sub> N <sub>4</sub> NaO	527.2029	-3.4	-3.0	16.5	ok	even	16.7	25.7	1.6	8.3	1.4	842.7

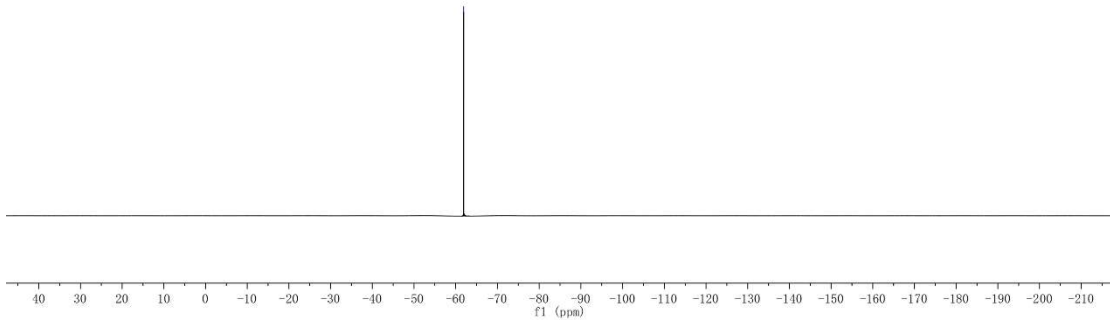
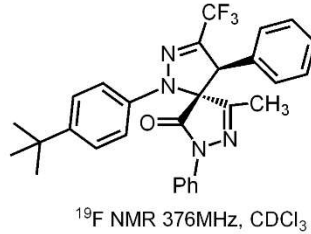
NMR copies of compound (*cis*)-**6c**:







61.887



HRMS (ESI) copy of compound (*cis*)-6c:

### Mass Spectrum SmartFormula Report

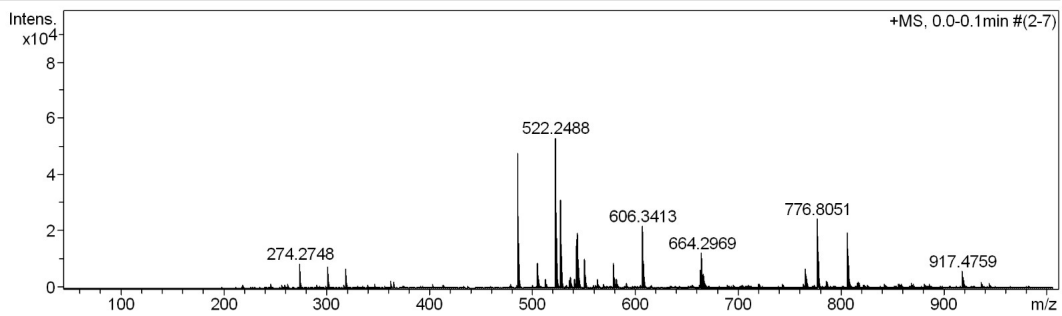
#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20230322-4.d  
Method tune\_low.m  
Sample Name A-391  
Comment

Acquisition Date 2023-3-22 9:22:37  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

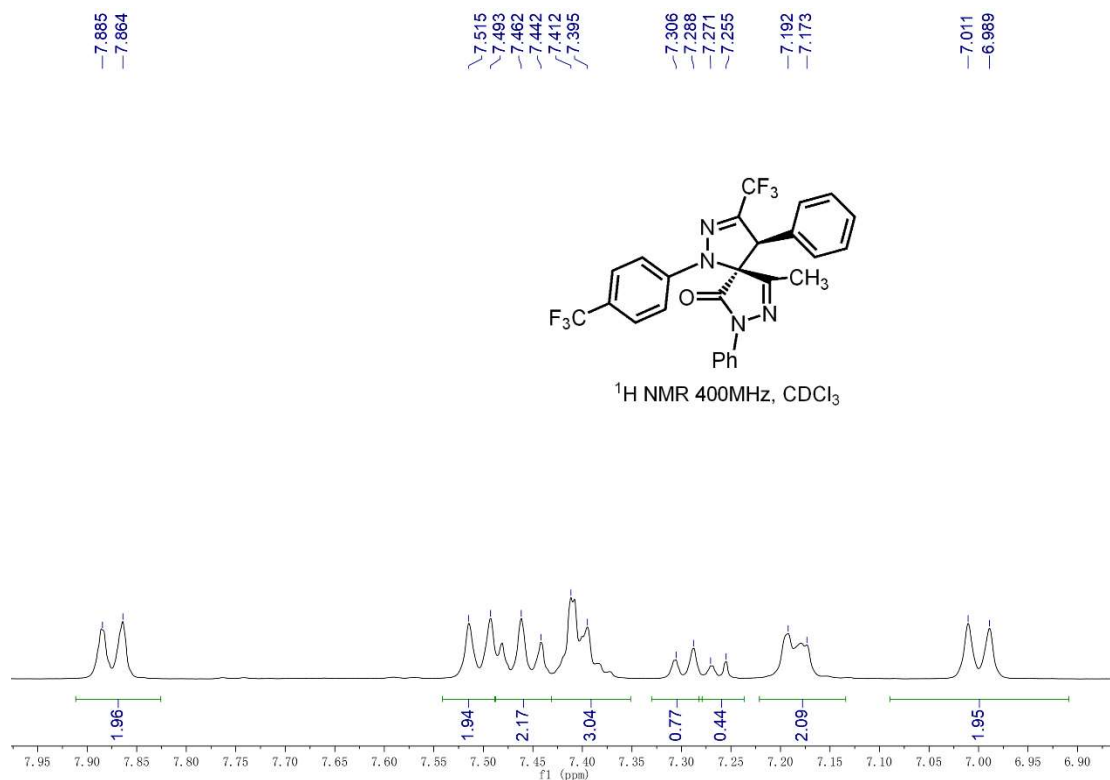
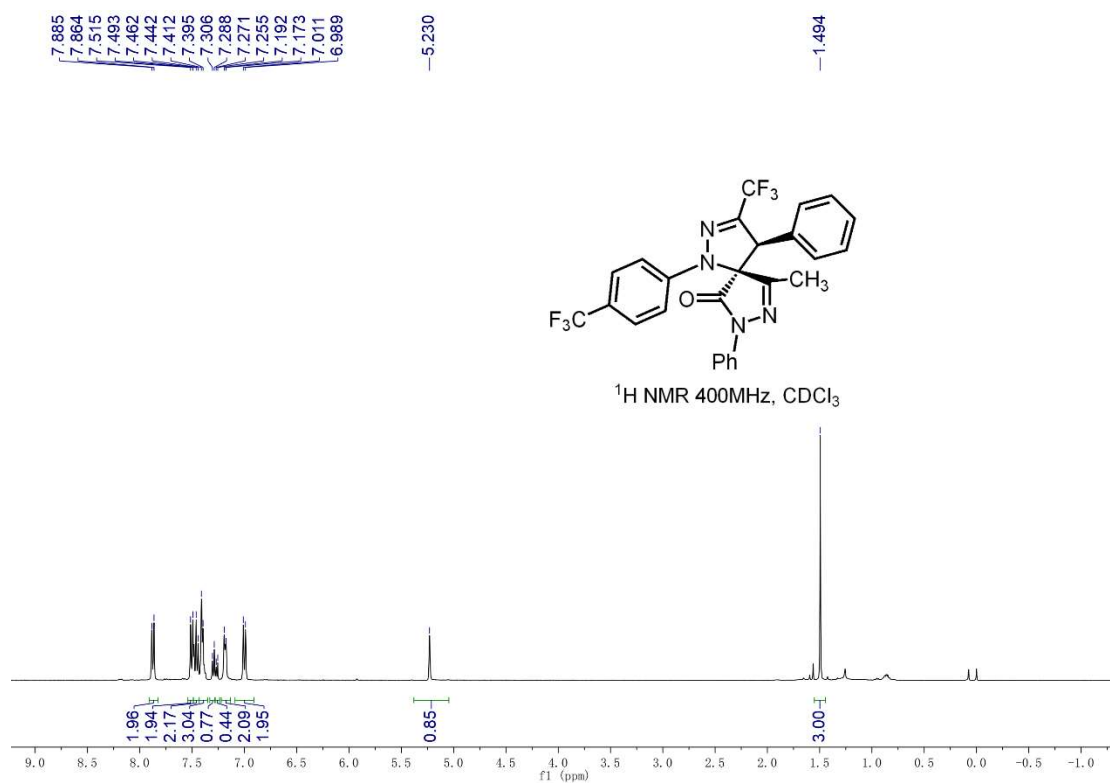
#### Acquisition Parameter

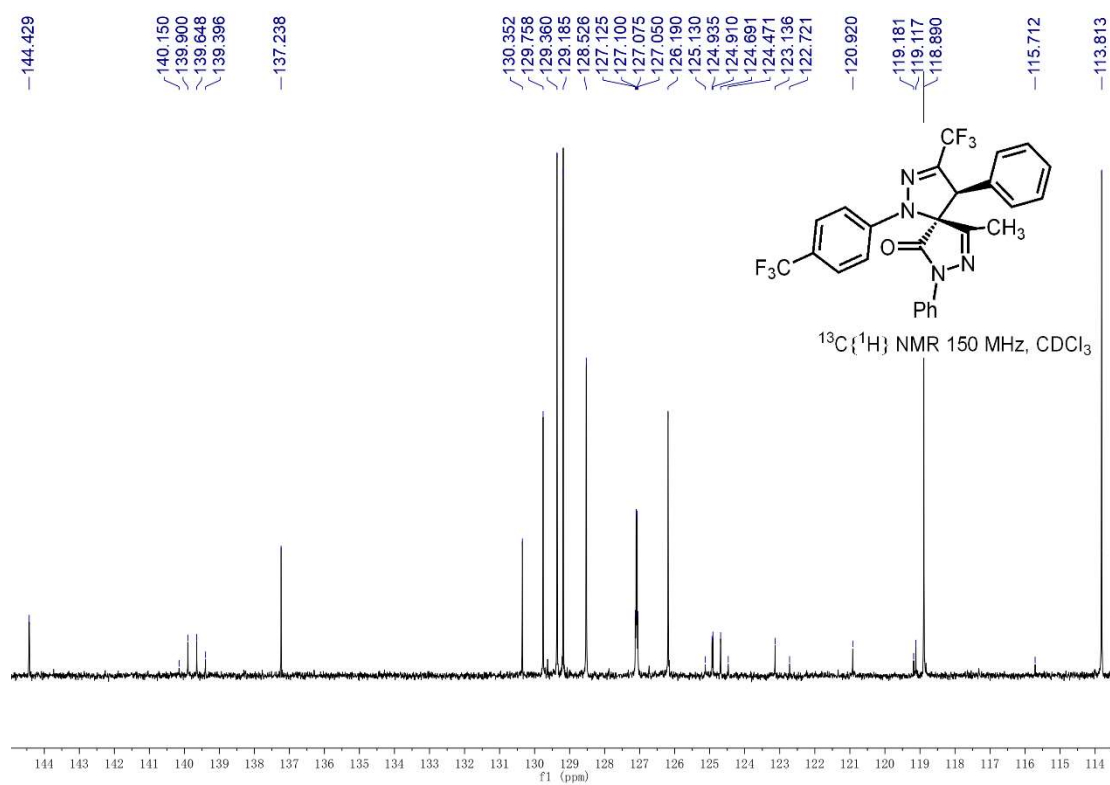
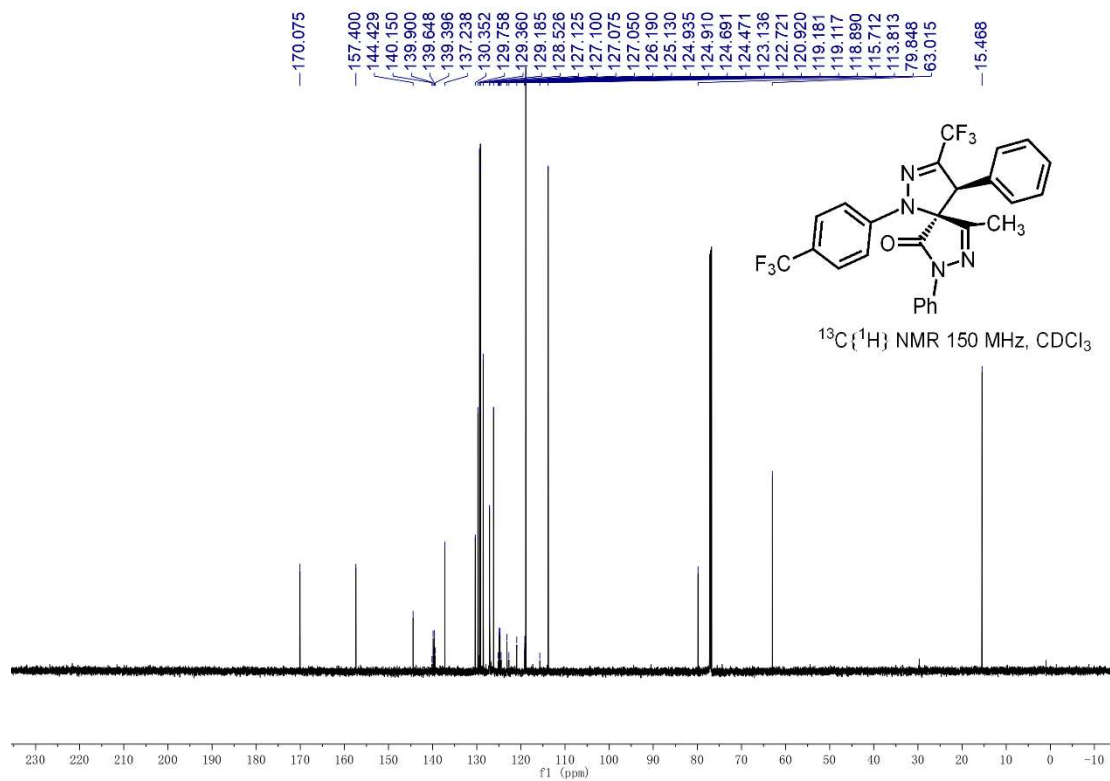
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

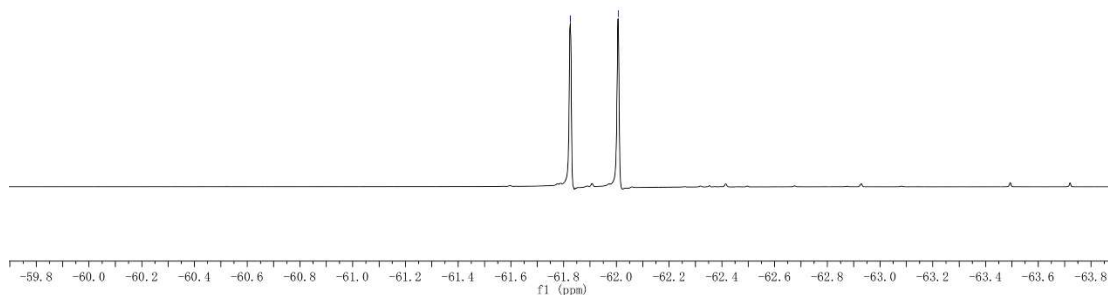
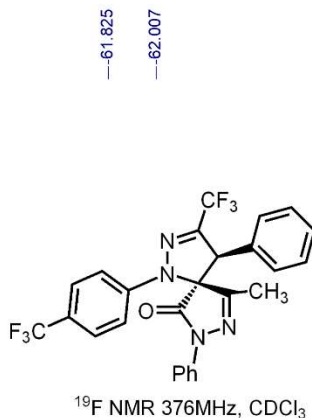


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>i</sub> ≠ Conf	mSi gm	Std l	St d Me an m/z	St d l Va rN or m/z	St d m/ Dif z m f	Std Com b Dev
527.2041	1 C <sub>29</sub> H <sub>27</sub> F <sub>3</sub> N <sub>4</sub> NaO	527.2029	-2.3	-1.9	16.5	ok	even	18.4	28.2	1.1	9.0	0.6	842.7

NMR copies of compound (*trans*)-6d:







HRMS (ESI) copy of compound (*trans*)-6d:

### Mass Spectrum SmartFormula Report

**Analysis Info**

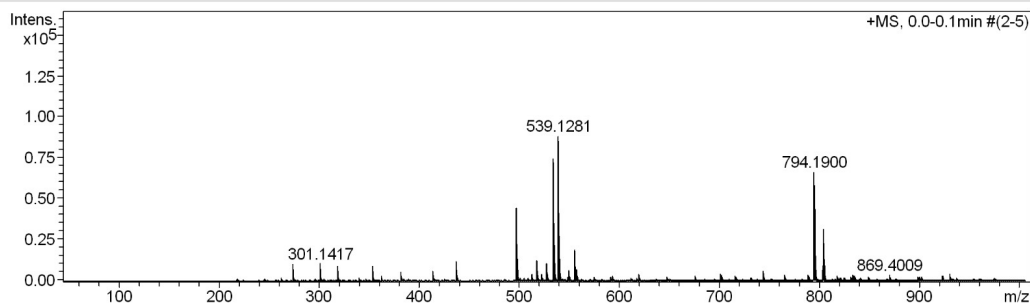
Analysis Name D:\Data\user\NWNNU-fengyang 20230322-5.d  
 Method tune\_low.m  
 Sample Name A-41  
 Comment

Acquisition Date 2023-3-22 9:25:35

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

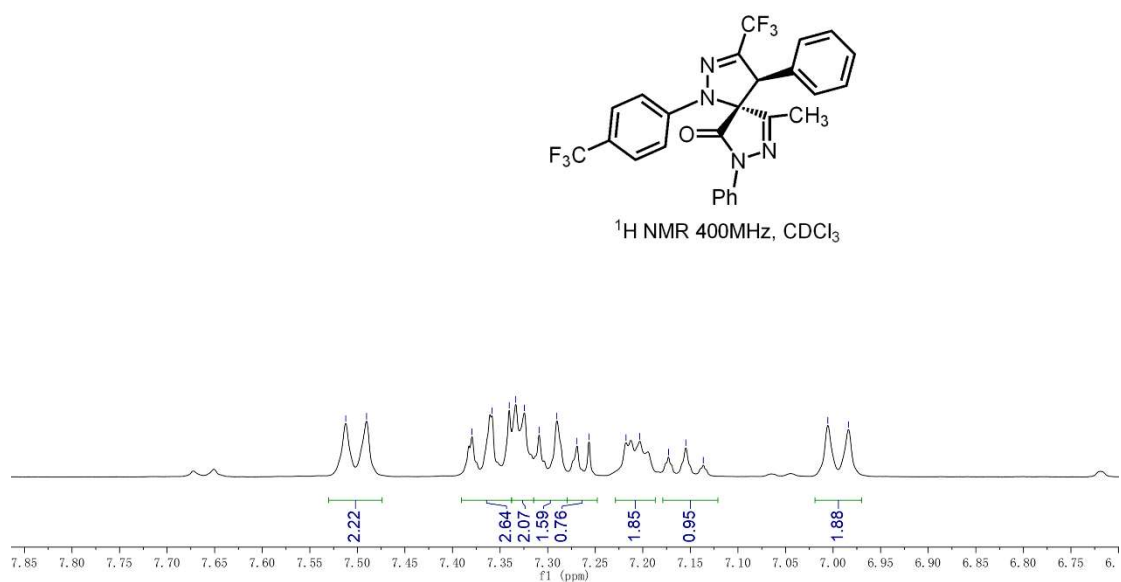
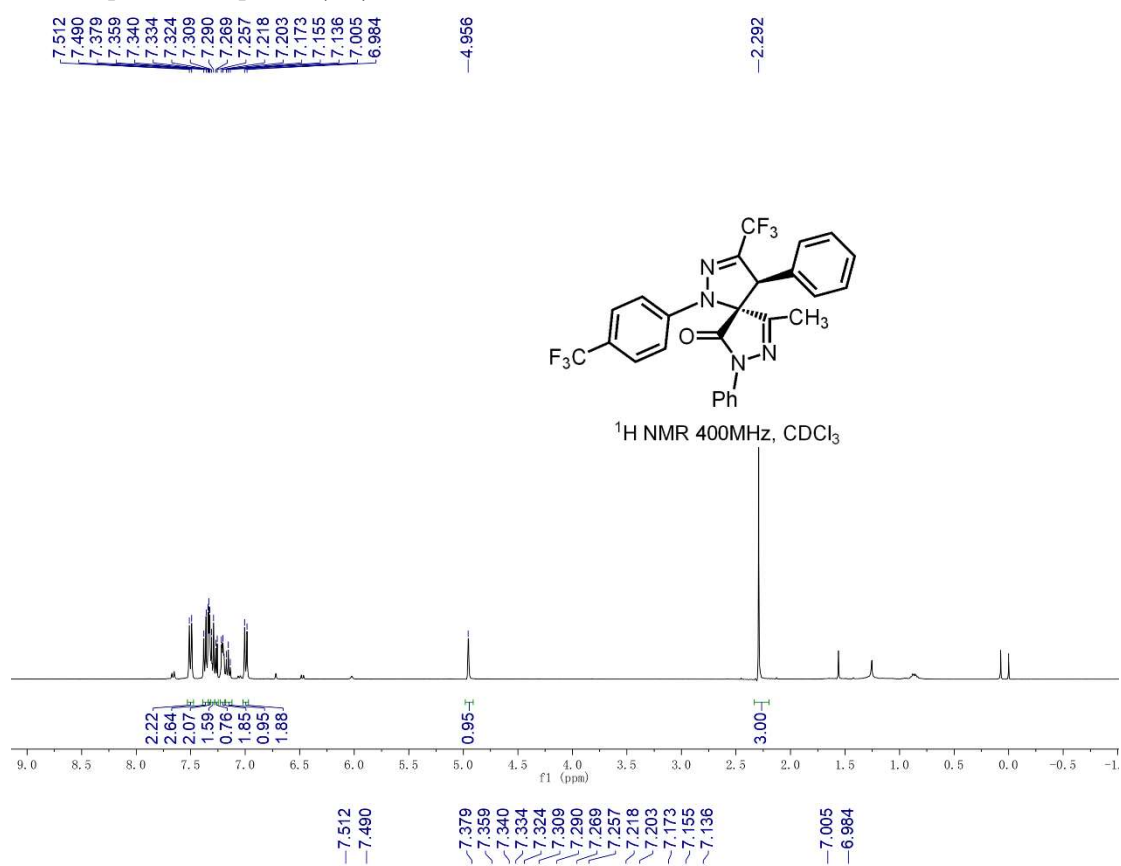
**Acquisition Parameter**

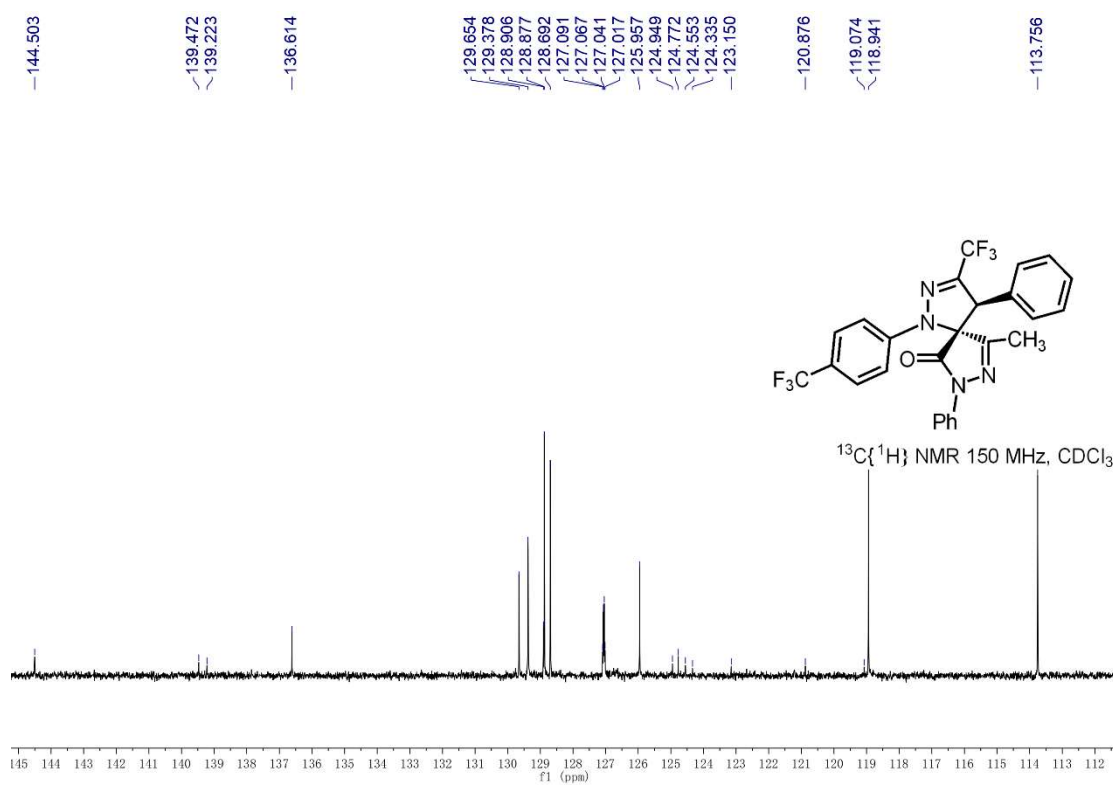
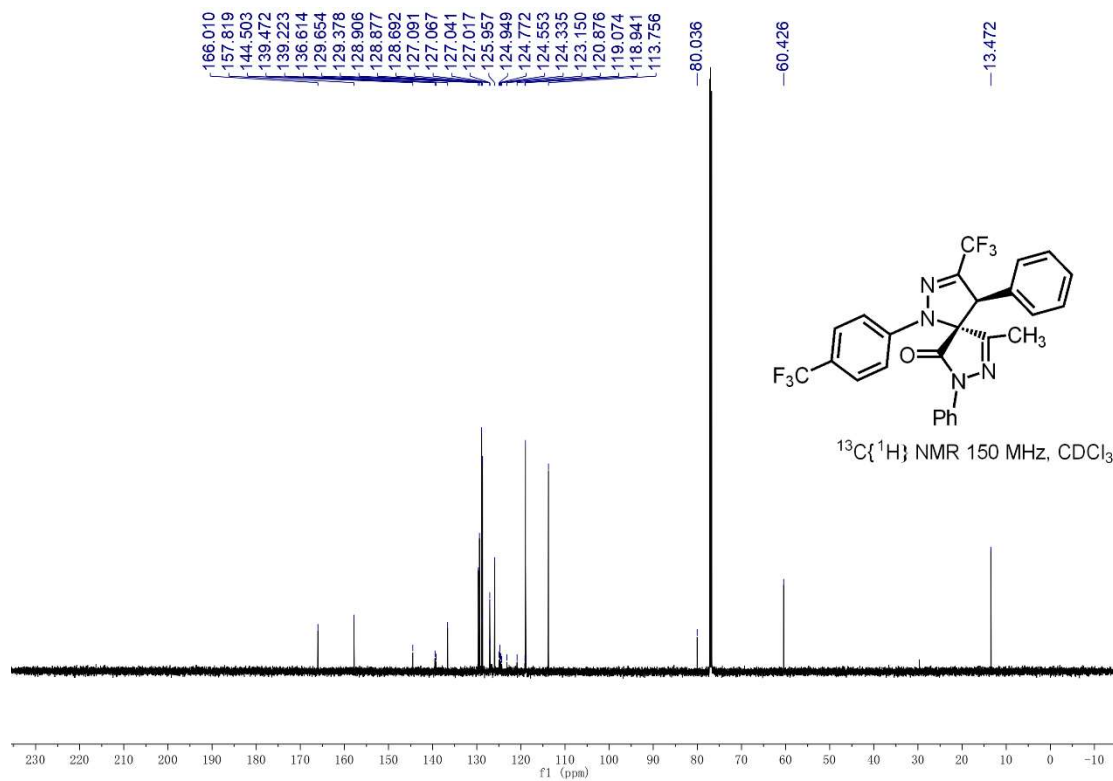
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



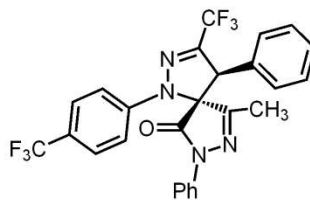
Meas. #	Formula	m/z	err [ppm]	Mass error [ppm]	rdB	N-R	ej%	mSi	Std	St	Std	St	Std
m/z						ul	Con	gm	l	d	l	d	Com
						e		a		Me	Var	m/	z
										an	Nor	m/	Dif
										z	m	f	Dev
539.1281	C <sub>26</sub> H <sub>18</sub> F <sub>6</sub> N <sub>4</sub> NaO	539.1277	-0.8	-0.5	16.5	ok	even	13.9	21.8	0.4	10.0	0.3	842.7

NMR copies of compound (*cis*)-**6d**:

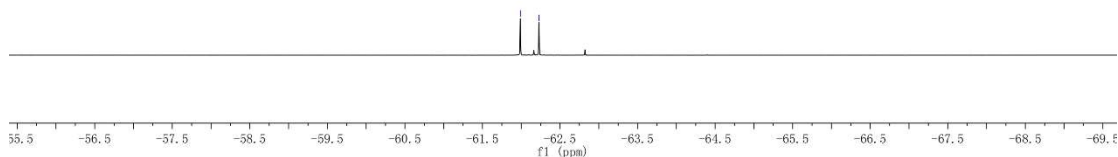




61.988  
62.230



<sup>19</sup>F NMR 376MHz, CDCl<sub>3</sub>



HRMS (ESI) copy of compound (*cis*)-6d:

### Mass Spectrum SmartFormula Report

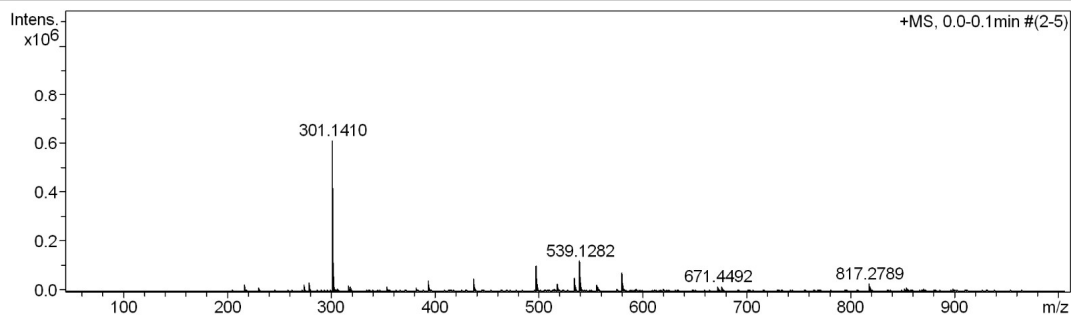
#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20230322-6.d  
Method tune\_low.m  
Sample Name A-411  
Comment

Acquisition Date 2023-3-22 9:27:42  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

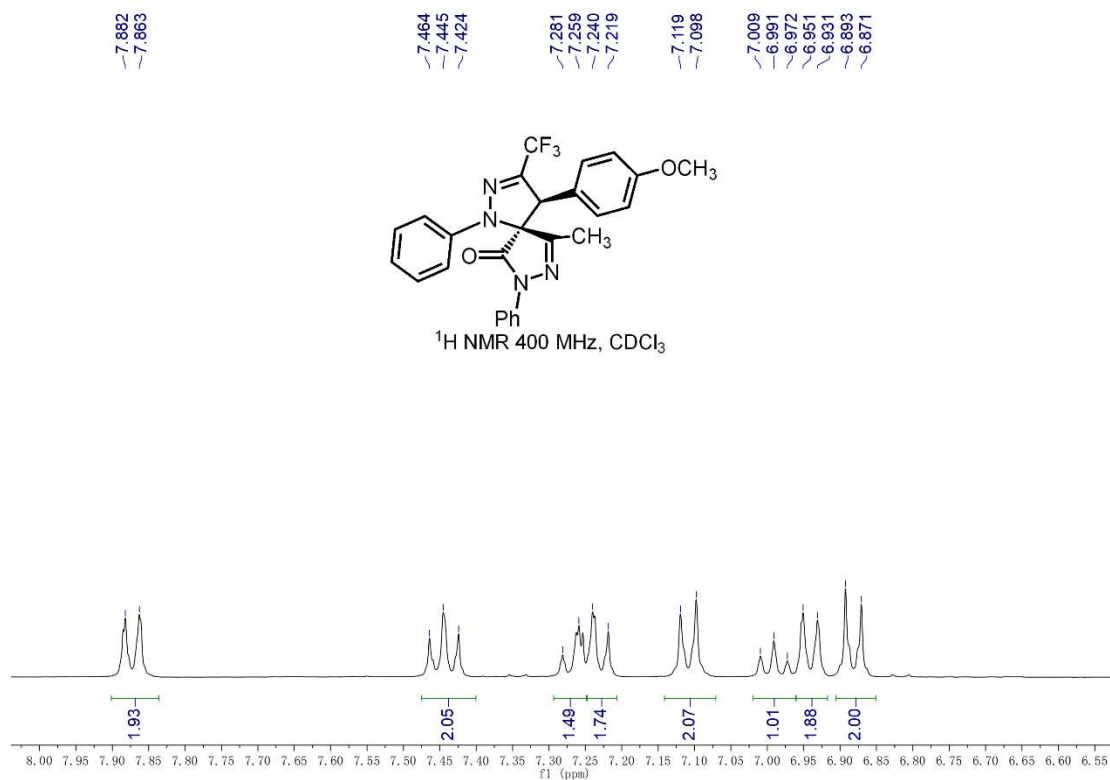
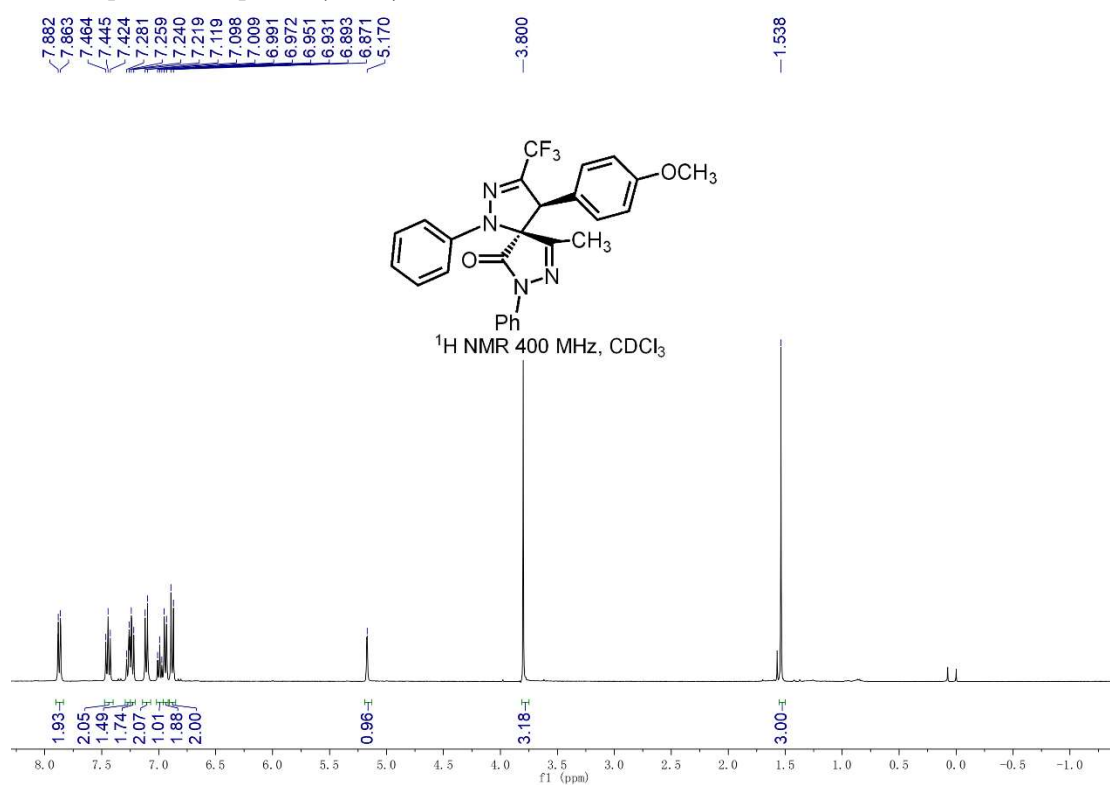
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

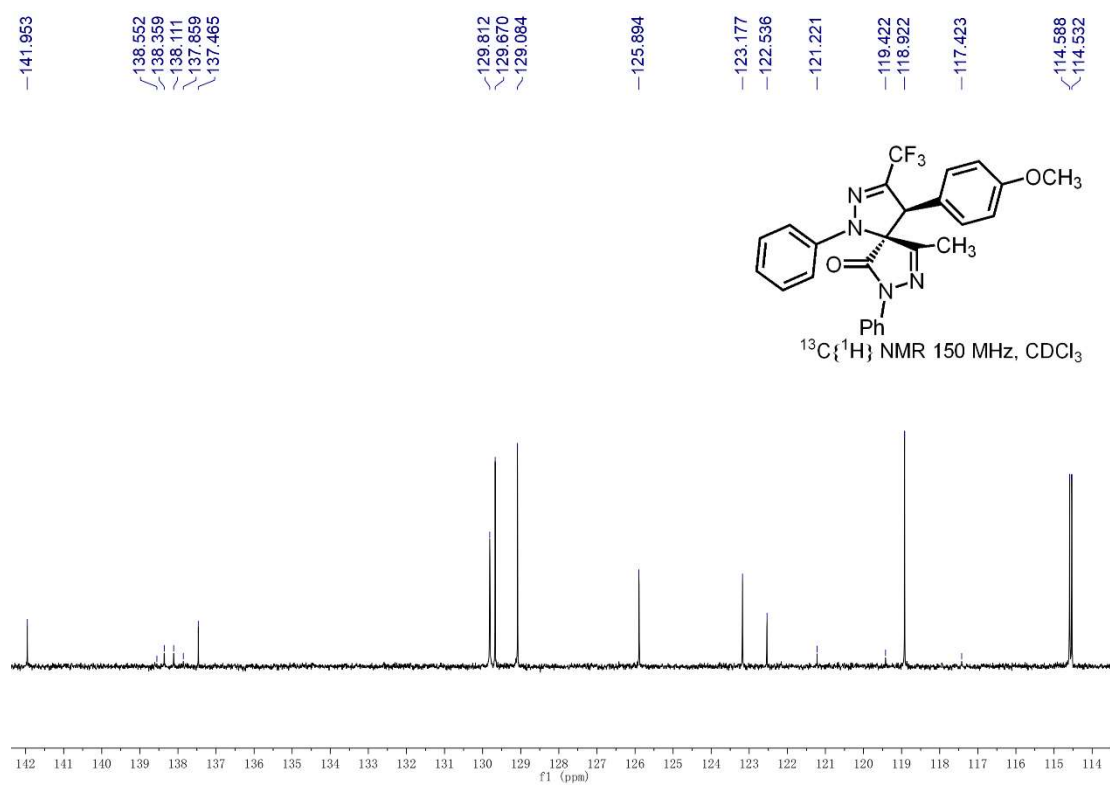
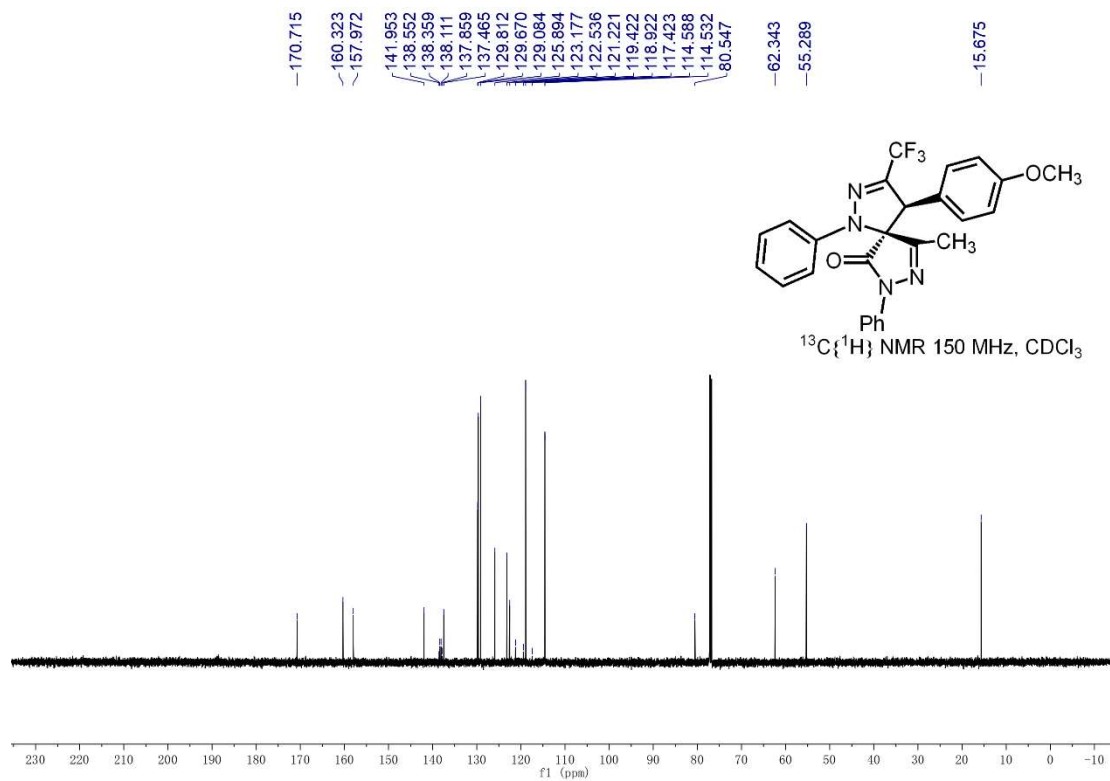


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R	e; % Conf	m Sigma	Std l	St d Me an z m	St d l rN or z m	St d m/ Dif f	Std Com b Dev
539.1282	1 C <sub>26</sub> H <sub>18</sub> F <sub>6</sub> N <sub>4</sub> NaO	539.1277	-0.9	-1.1	16.5	ok	even	7.0	11.9	0.6	6.8	0.4	842.7

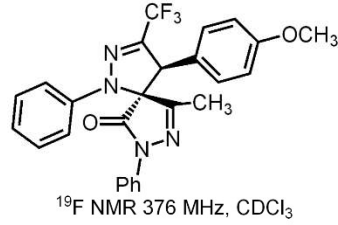
NMR copies of compound (*trans*)-6e:







61.679



HRMS (ESI) copy of compound (*trans*)-6e:

### Mass Spectrum SmartFormula Report

#### Analysis Info

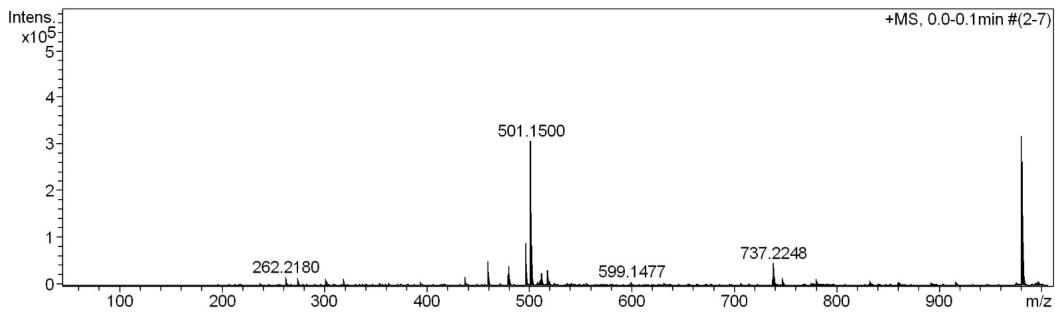
Analysis Name D:\Data\user\NWNNU-fengyang 20230322--7.d  
Method tune\_low.m  
Sample Name A-42  
Comment

Acquisition Date 2023-3-22 9:31:12

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

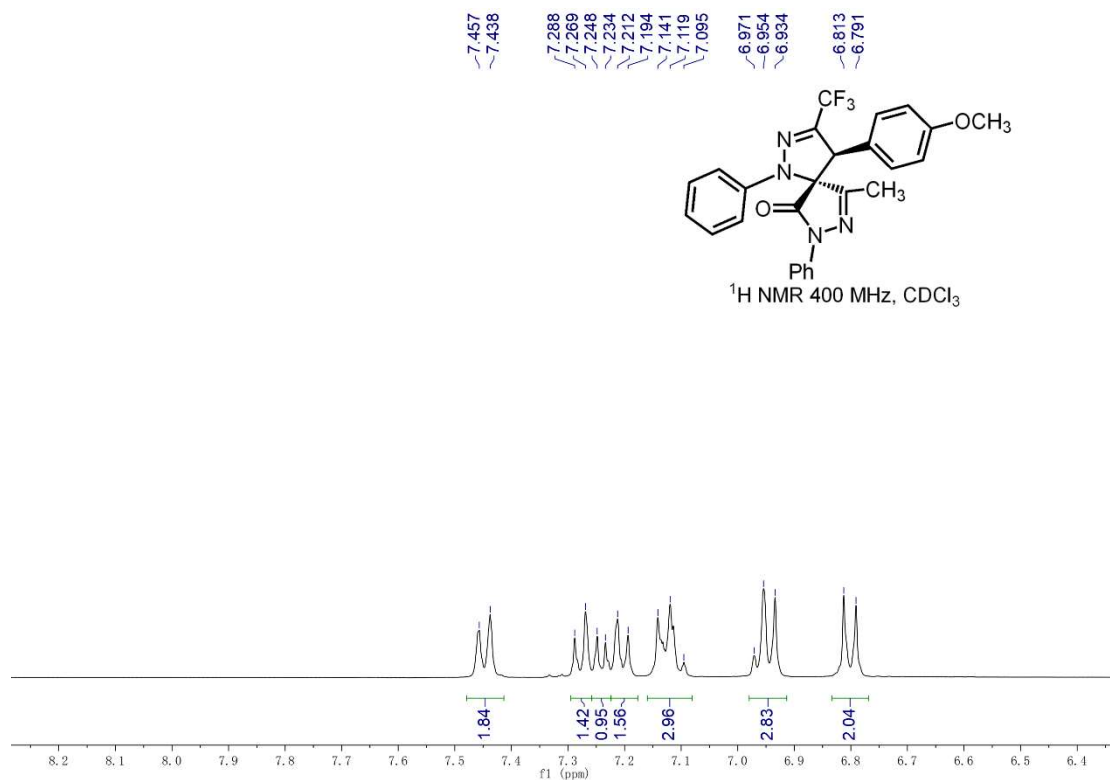
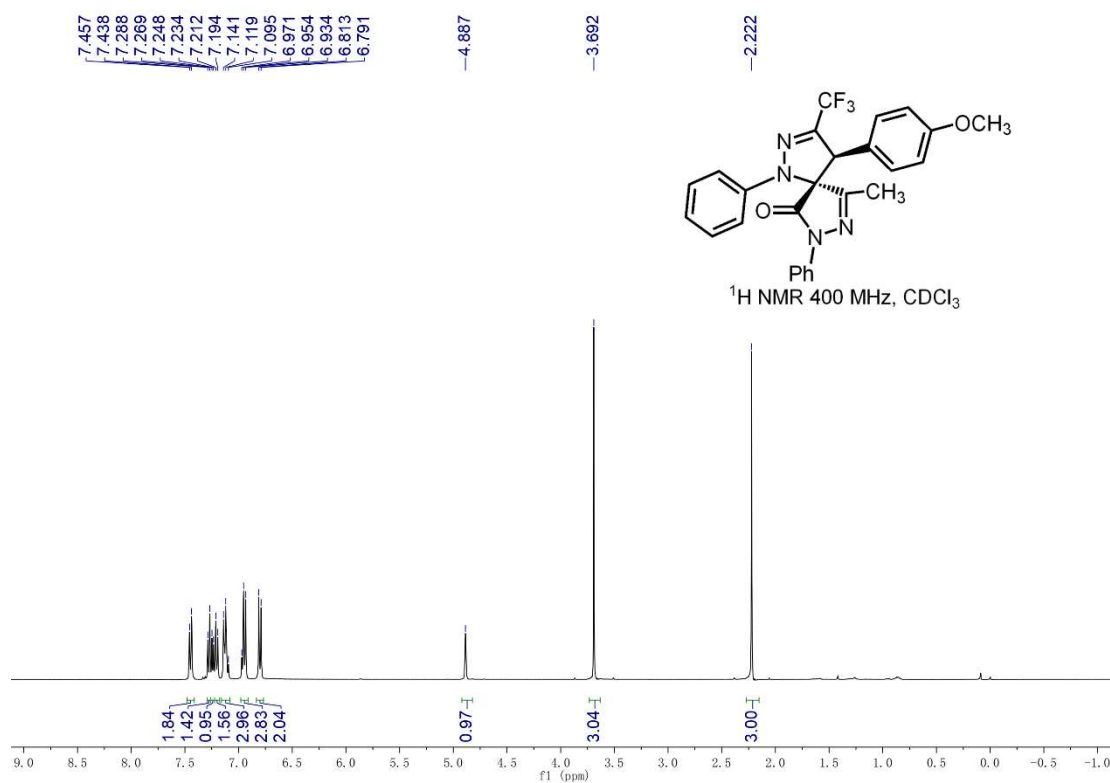
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j % Conf	mSi gm a	Std l	St d Me an z	St d l Va rN z m f	St d m/ Dif	Std Com b Dev
501.1500	1 C <sub>26</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO <sub>2</sub>	501.1509	1.8	1.1	16.5	ok	even	12.5	18.4	0.8	7.9	1.4	842.7

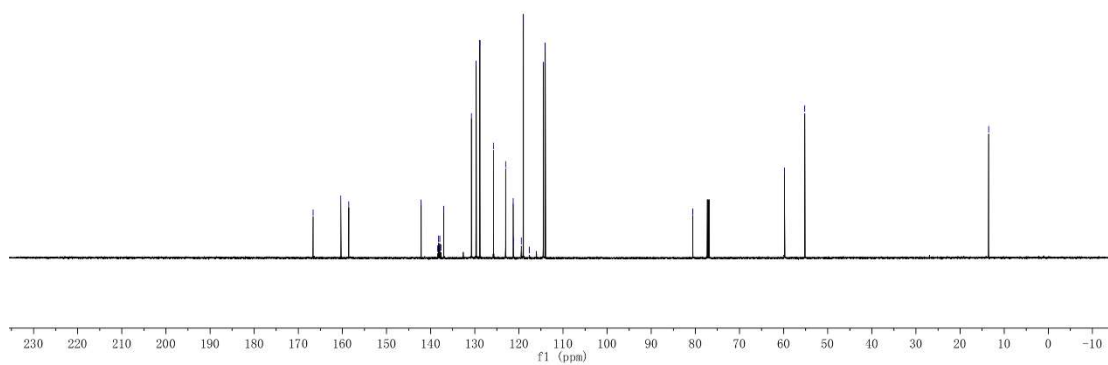
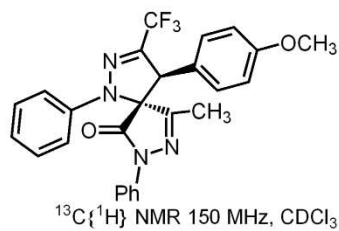
NMR copies of compound (*cis*)-**6e**:



166.649  
 160.337  
 158.560  
 142.175  
 138.414  
 138.168  
 137.922  
 137.676  
 137.023  
 130.759  
 129.691  
 128.848  
 125.700  
 123.027  
 121.290  
 121.248  
 119.450  
 119.006  
 117.653  
 114.454  
 114.012  
 80.557

59.761  
 55.191

13.540



138.414  
 138.168  
 137.922  
 137.676  
 137.023

130.759  
 129.691  
 128.848

125.700

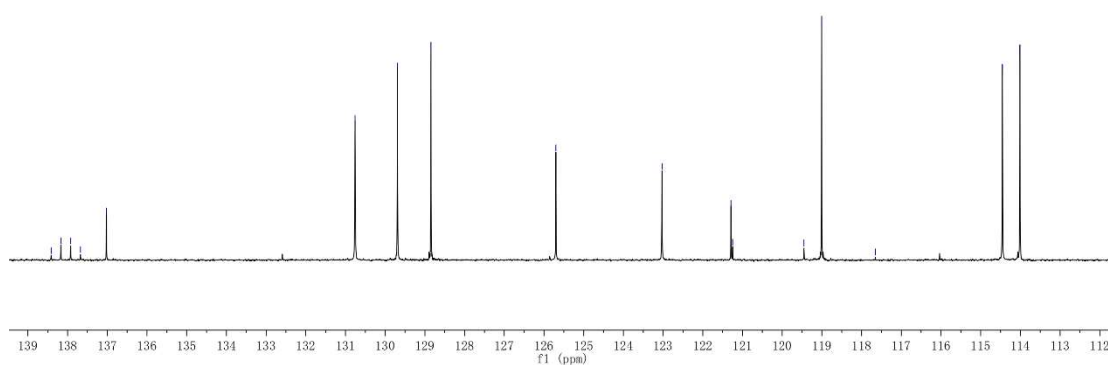
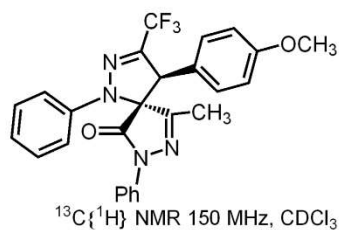
123.027

121.290  
 121.248

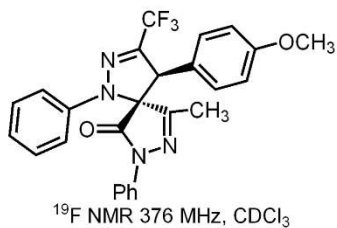
119.450  
 119.006

117.653

114.454  
 114.012



-62.083



HRMS (ESI) copy of compound (*cis*)-6e:

### Mass Spectrum SmartFormula Report

#### Analysis Info

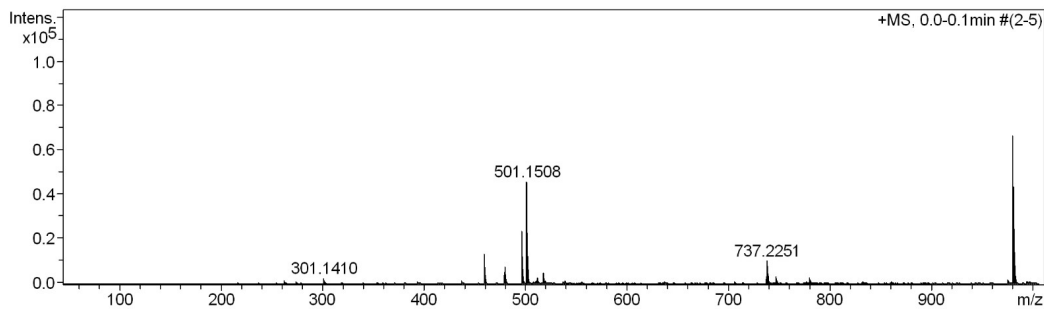
Analysis Name D:\Data\user\NWNW-fengyang 20230322-8.d  
Method tune\_low.m  
Sample Name A-421  
Comment

Acquisition Date 2023-3-22 9:33:02

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

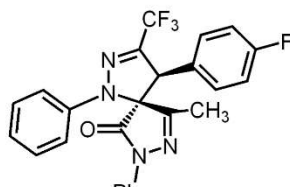
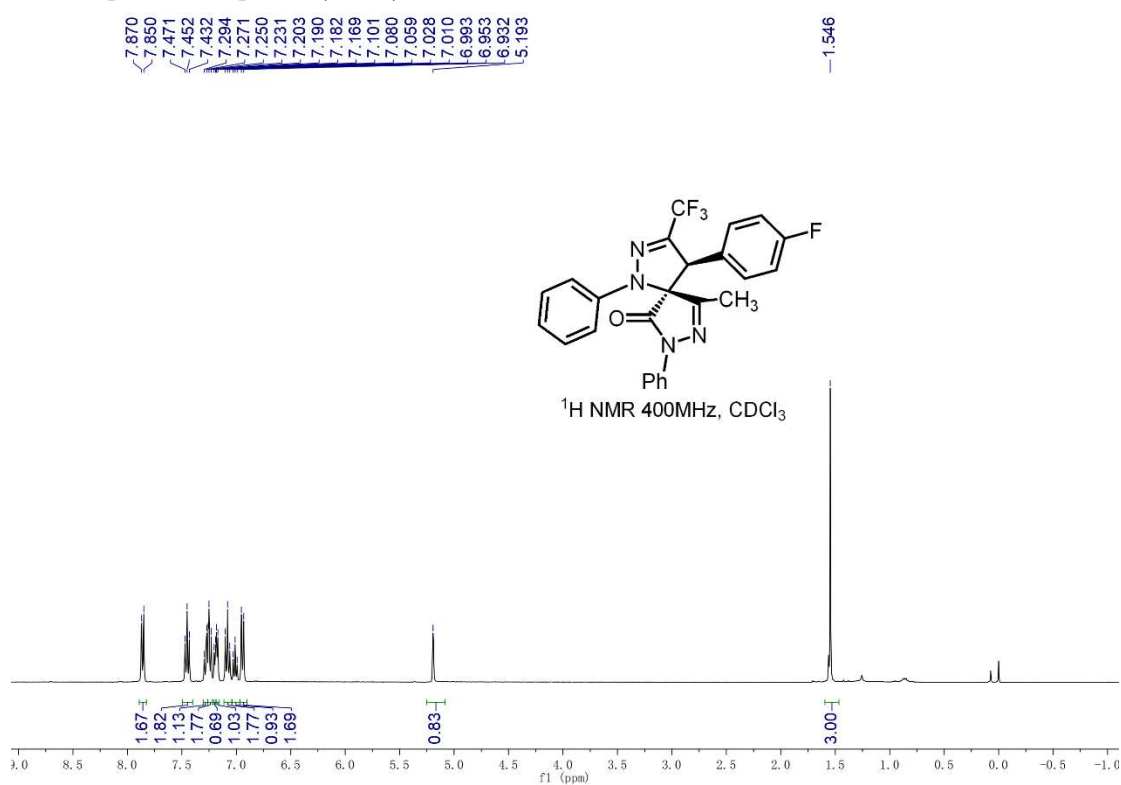
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{C}$
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

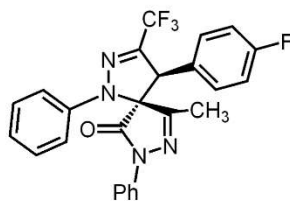
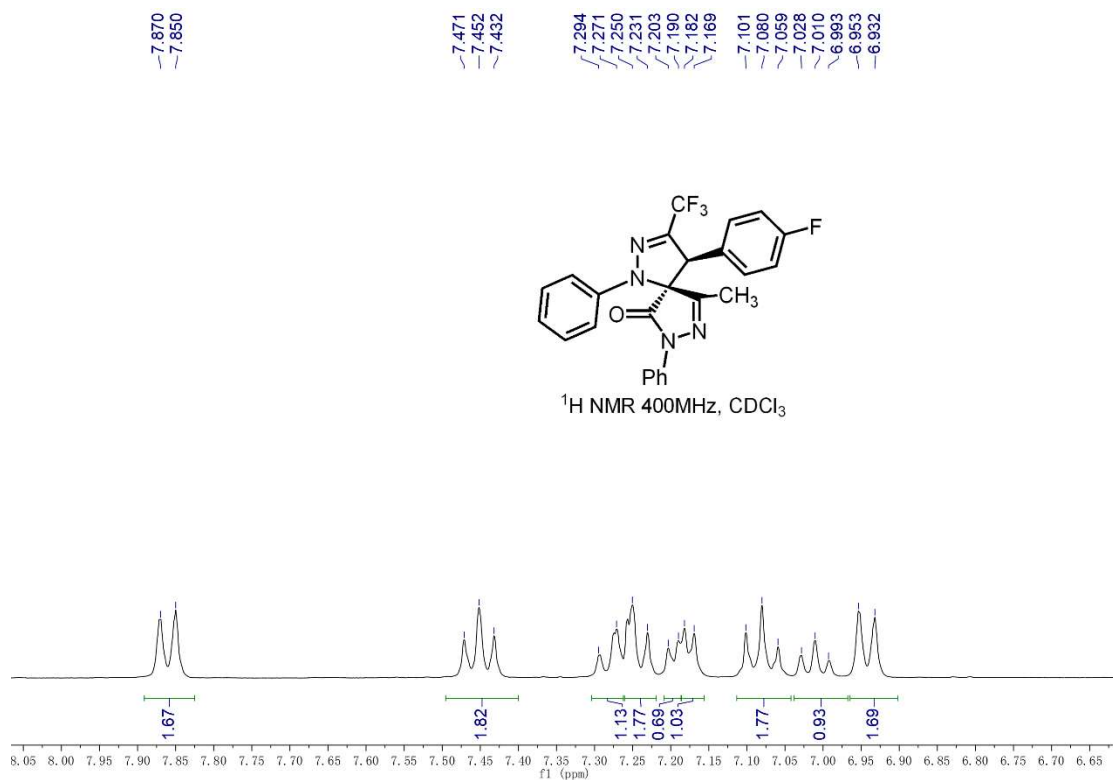


Meas. #	Formula	m/z	err [ppm]	Me an [ppm]	rdb	N- ul e	e j % Con f	mSi gm a	Std l	St d	St d l	St d	Std Com b
501.1508	1 C <sub>26</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO <sub>2</sub>	501.1509	0.3	-0.2	16.5	ok	even	14.9	21.9	0.5	9.4	1.2	842.7

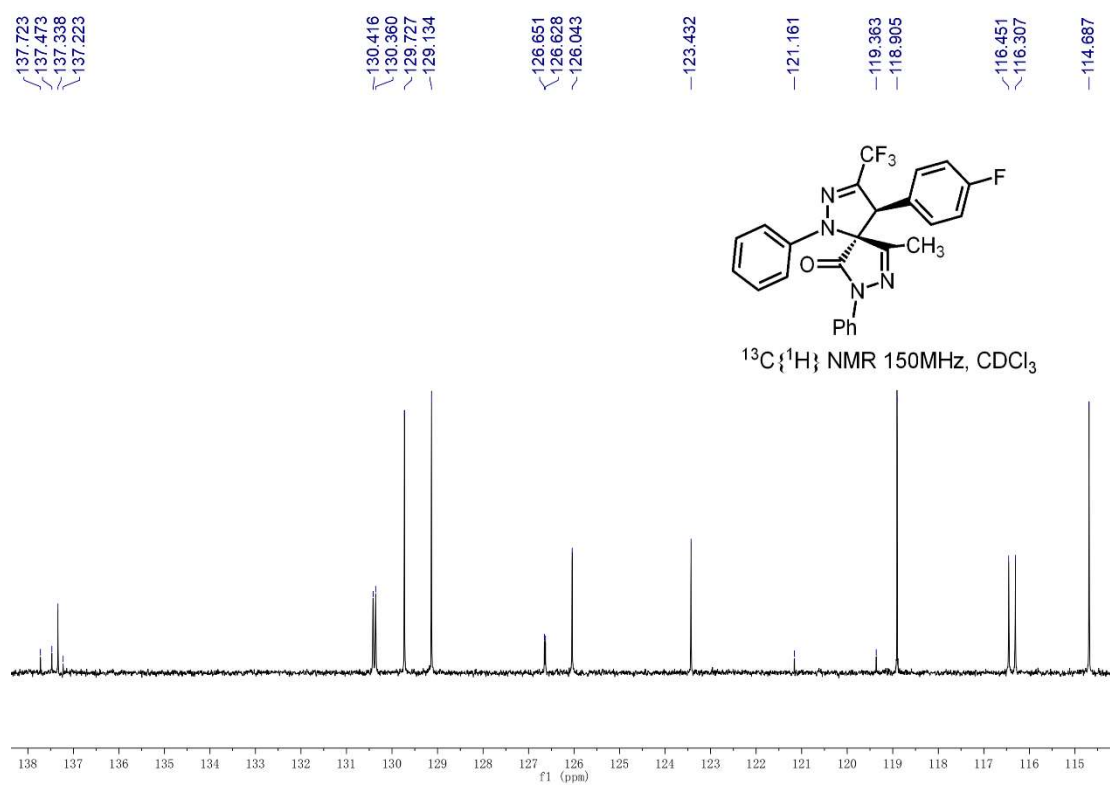
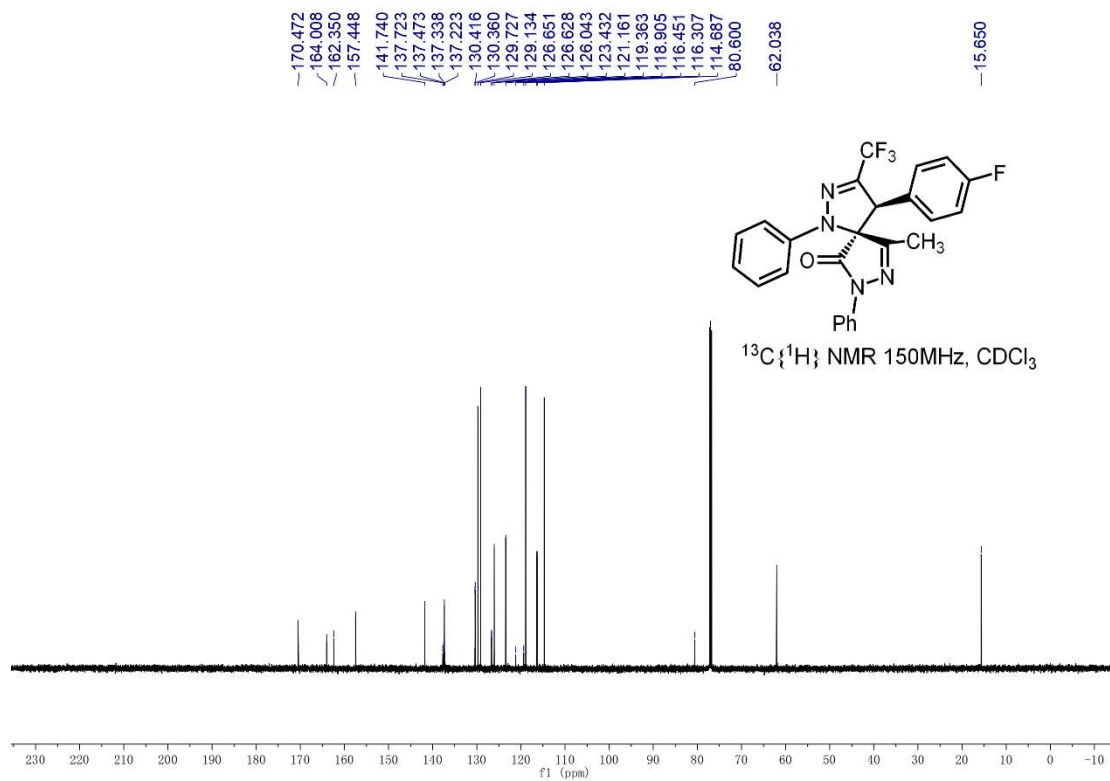
NMR copies of compound (*trans*)-6f:

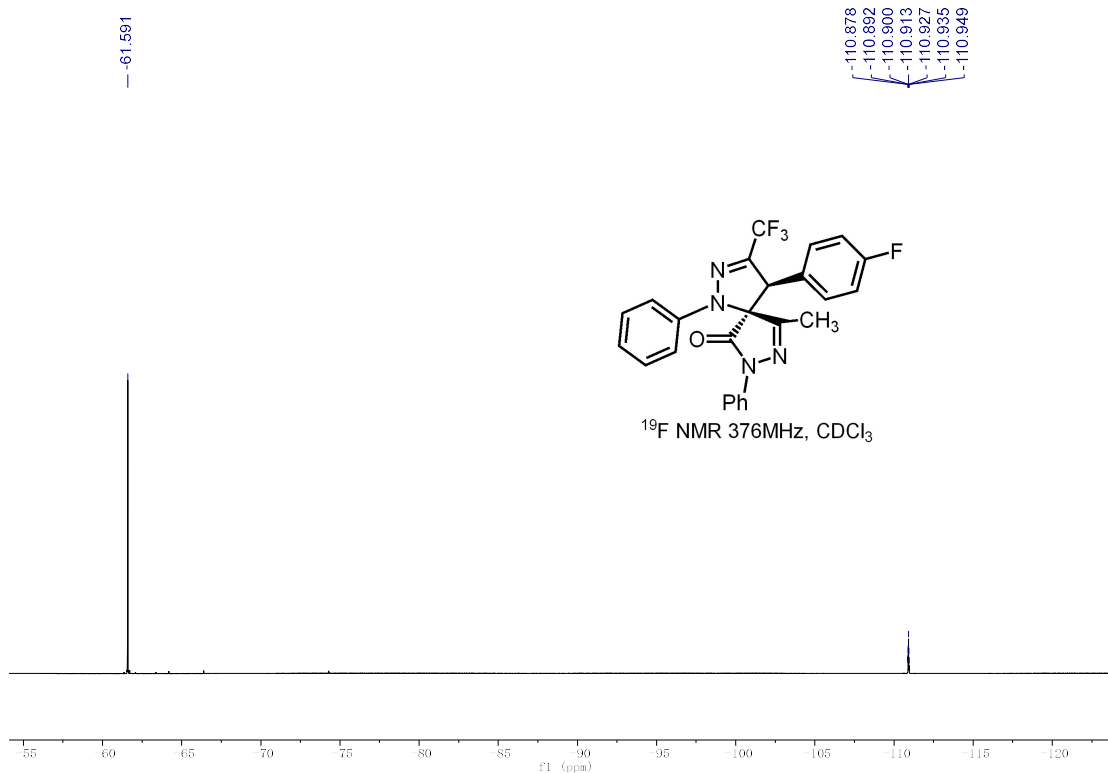


<sup>1</sup>H NMR 400MHz, CDCl<sub>3</sub>



<sup>1</sup>H NMR 400MHz, CDCl<sub>3</sub>





HRMS (ESI) copy of compound (*trans*)-6f:

### Mass Spectrum SmartFormula Report

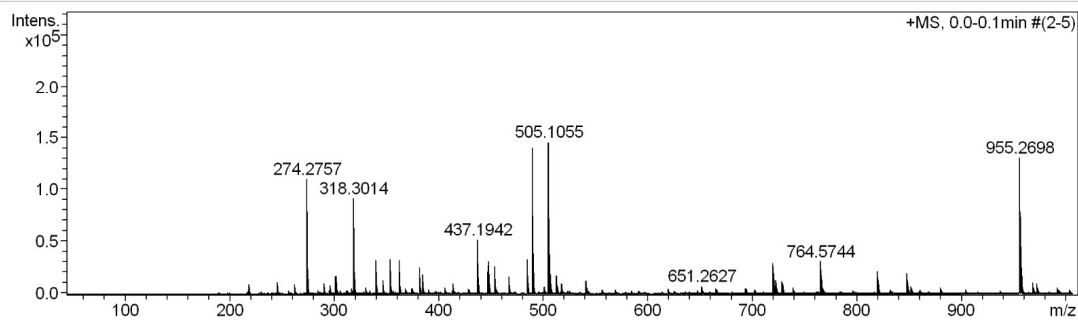
#### Analysis Info

Analysis Name D:\Data\user\NWNW-fengyang 20230322-9.d  
 Method tune\_low.m  
 Sample Name A-43  
 Comment

Acquisition Date 2023-3-22 9:36:11  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

#### Acquisition Parameter

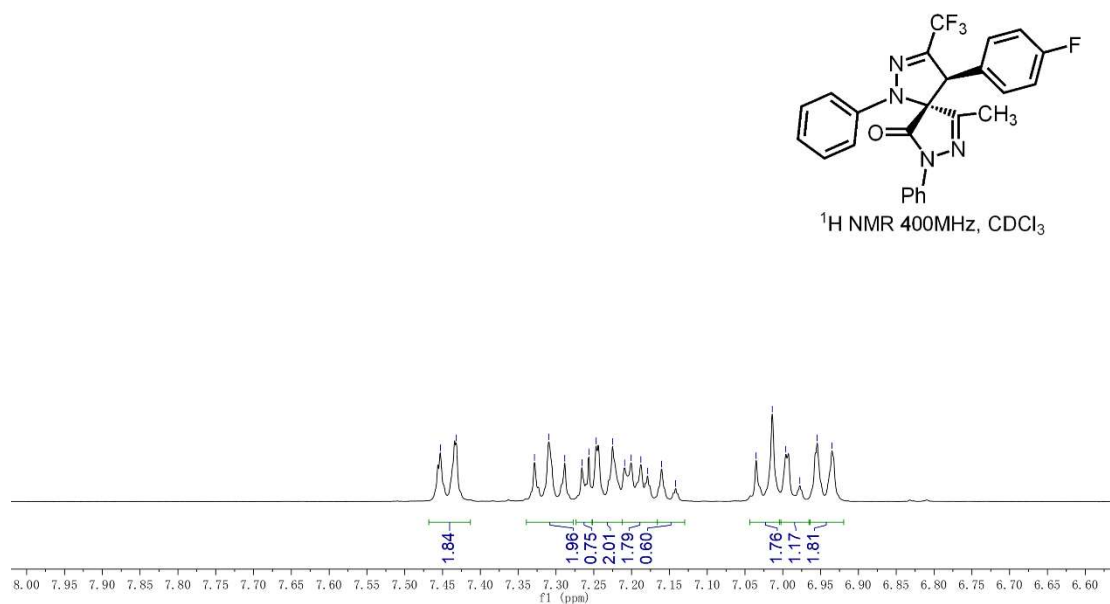
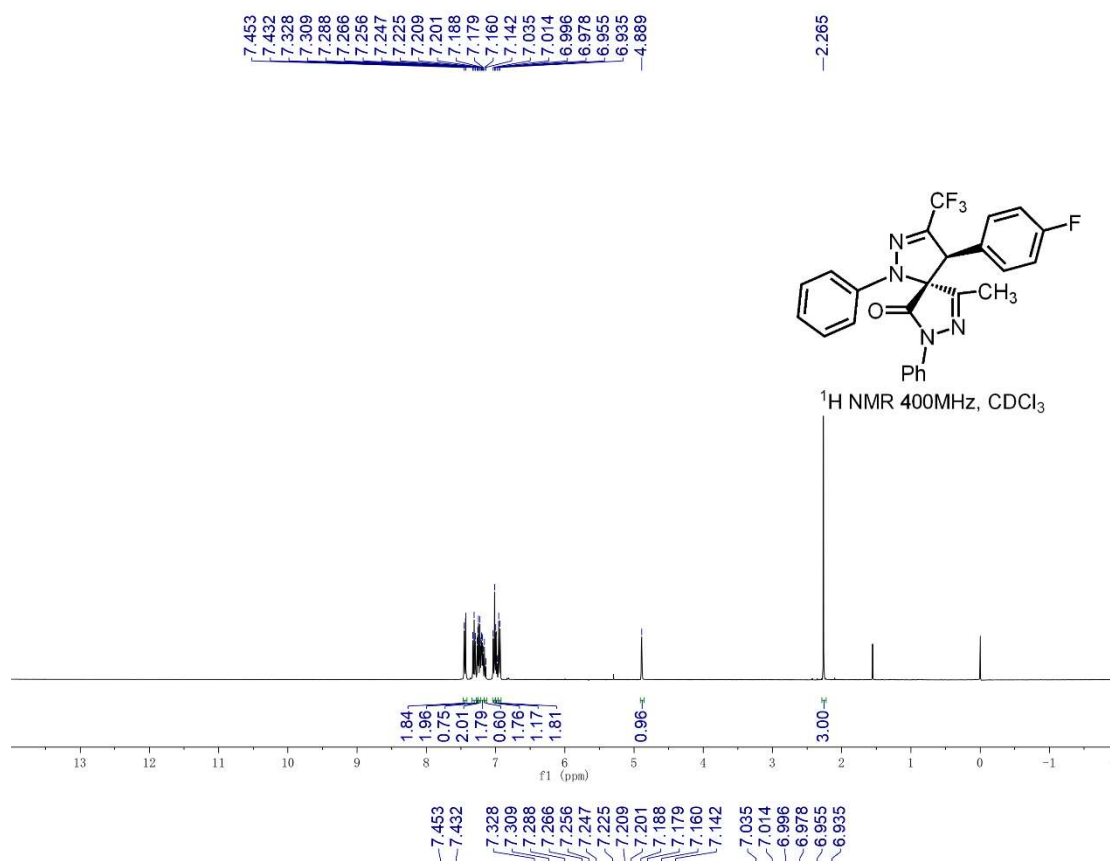
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

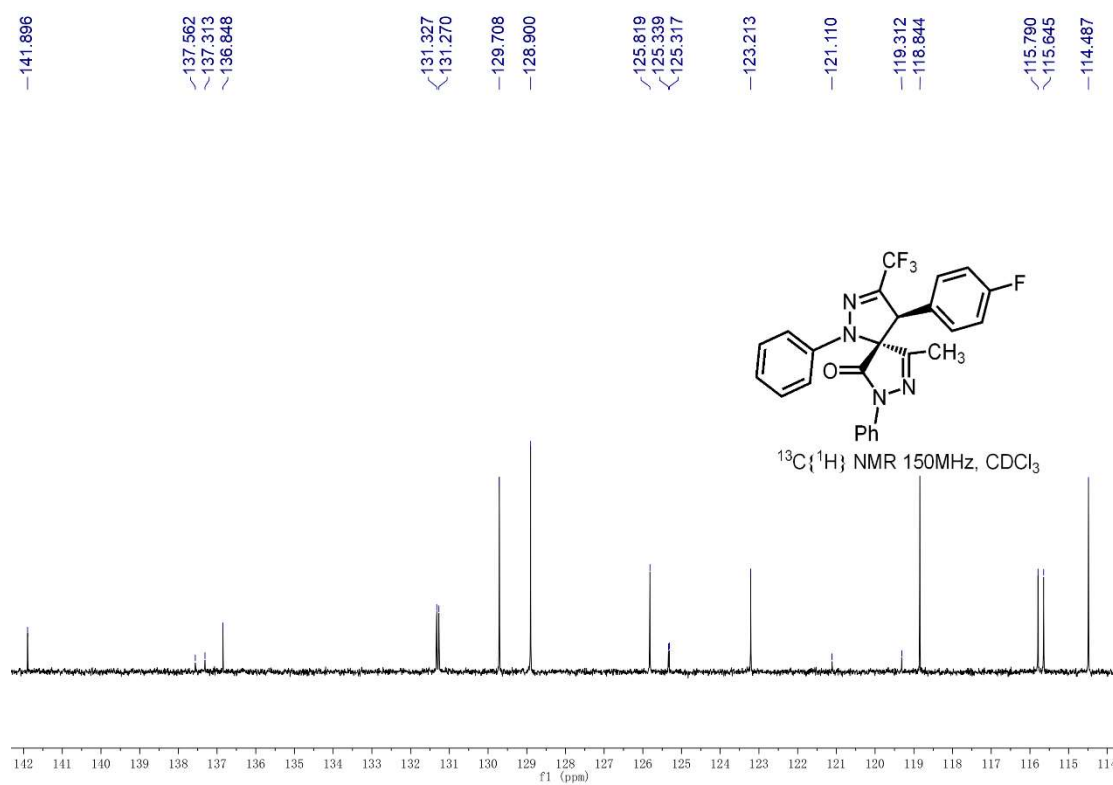
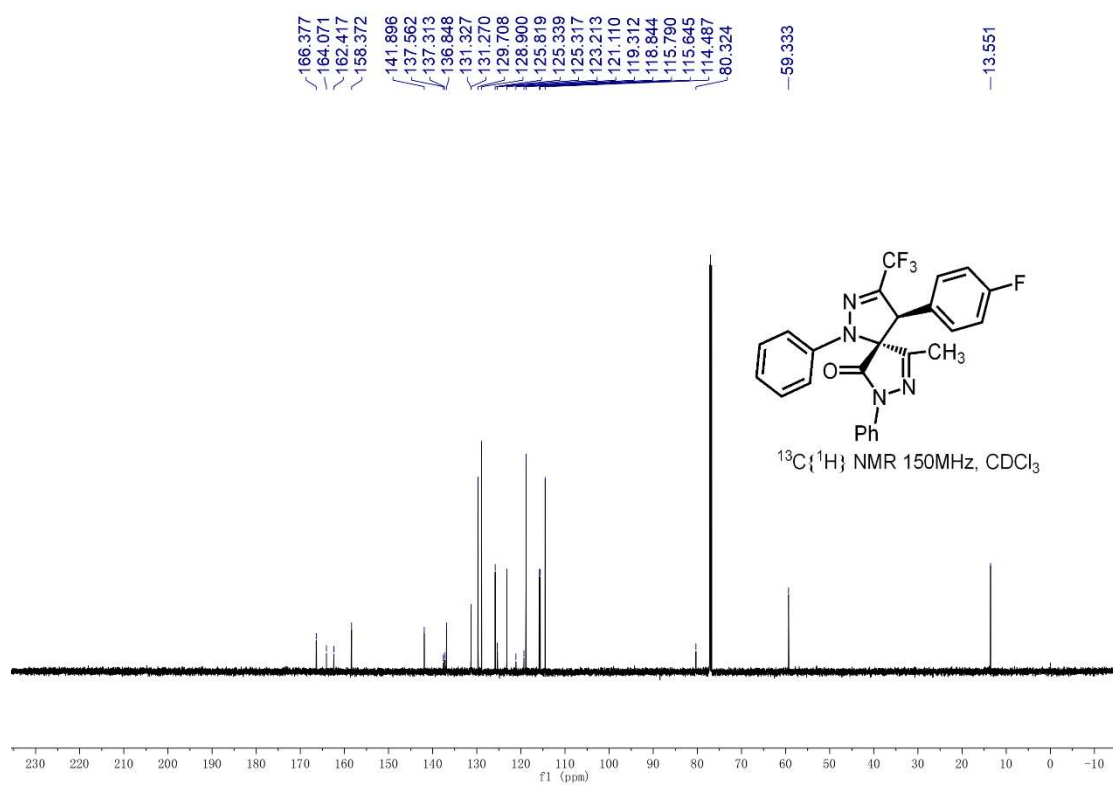


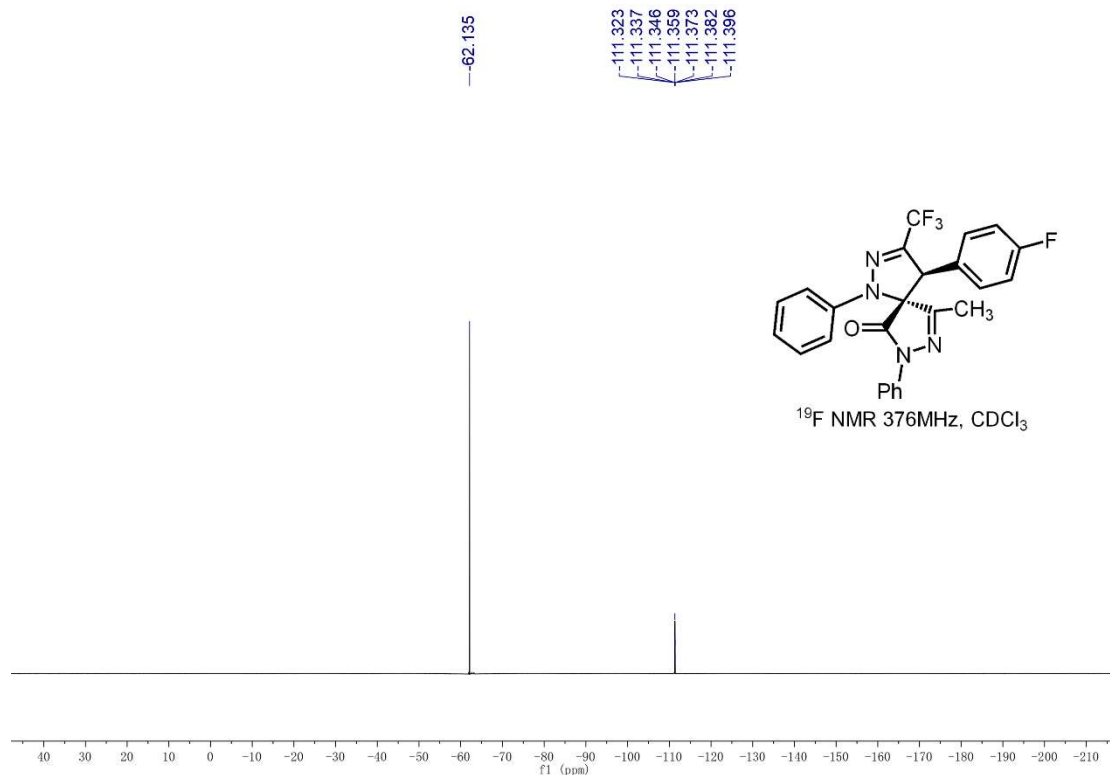
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ej%	mS	Std	Std	Std	Std	Std
m/z						ul	Conf	ig	l	Me	Std	Std	Std
						e		ma		m/	l	m/	Com
										z	rN	z	Dev
										or	Diff		
										m			
489.1315	1 C <sub>25</sub> H <sub>18</sub> F <sub>4</sub> N <sub>4</sub> NaO	489.1309	-1.1	-1.0	16.5	ok	even	7.4	9.8	0.5	4.8	0.1	842.7



NMR copies of compound (*cis*)-**6f**:







HRMS (ESI) copy of compound (*cis*)-6f:

### Mass Spectrum SmartFormula Report

**Analysis Info**

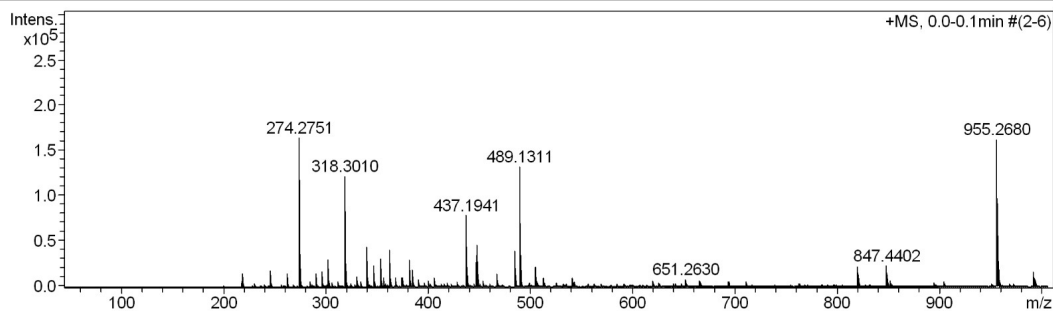
Analysis Name D:\Data\user\NWNNU-fengyang 20230322-10.d  
 Method tune\_low.m  
 Sample Name A-431  
 Comment

Acquisition Date 2023-3-22 9:38:19

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

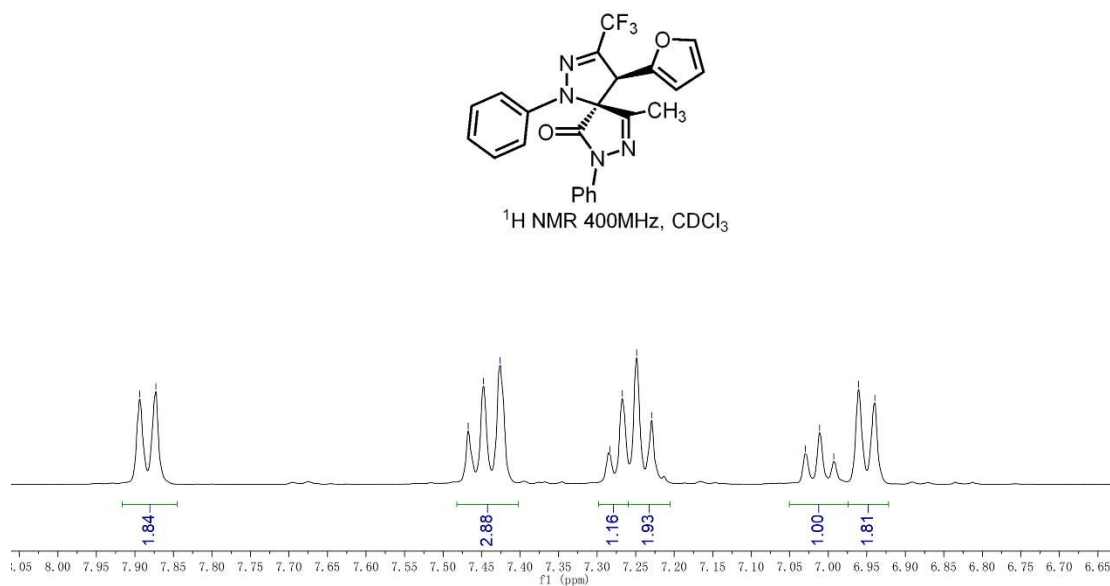
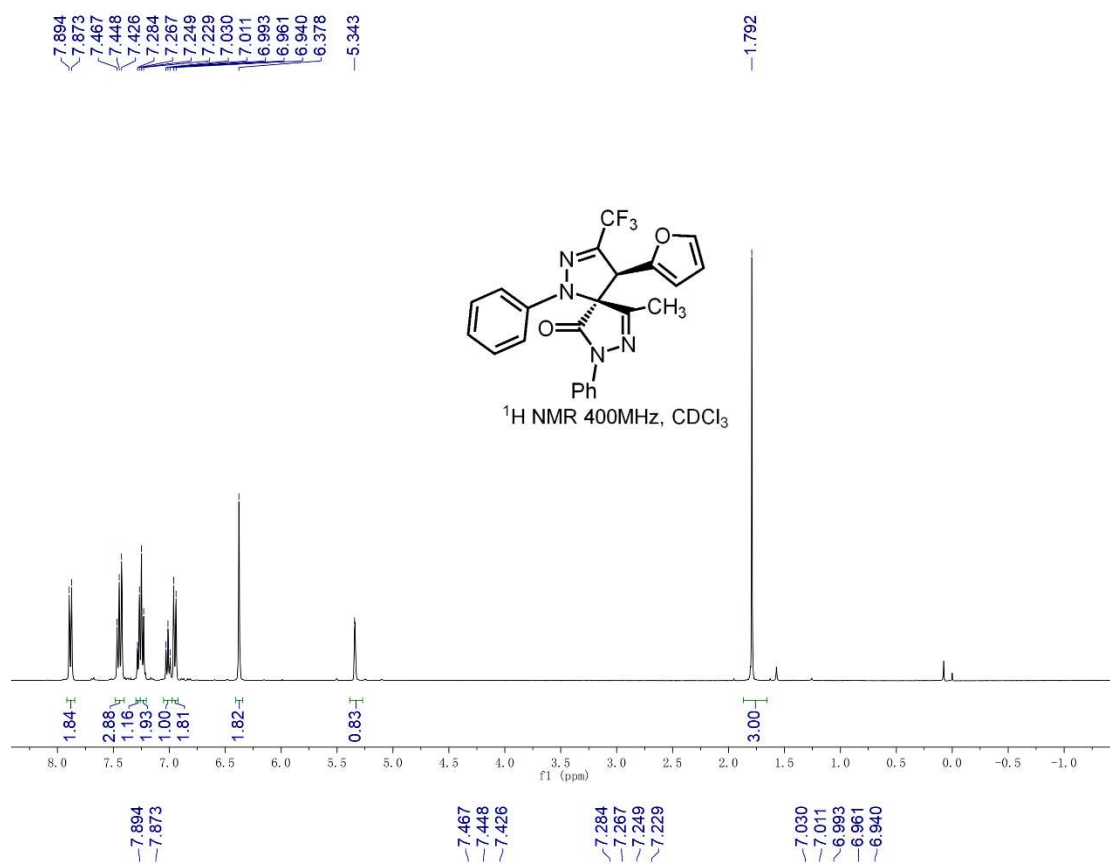
**Acquisition Parameter**

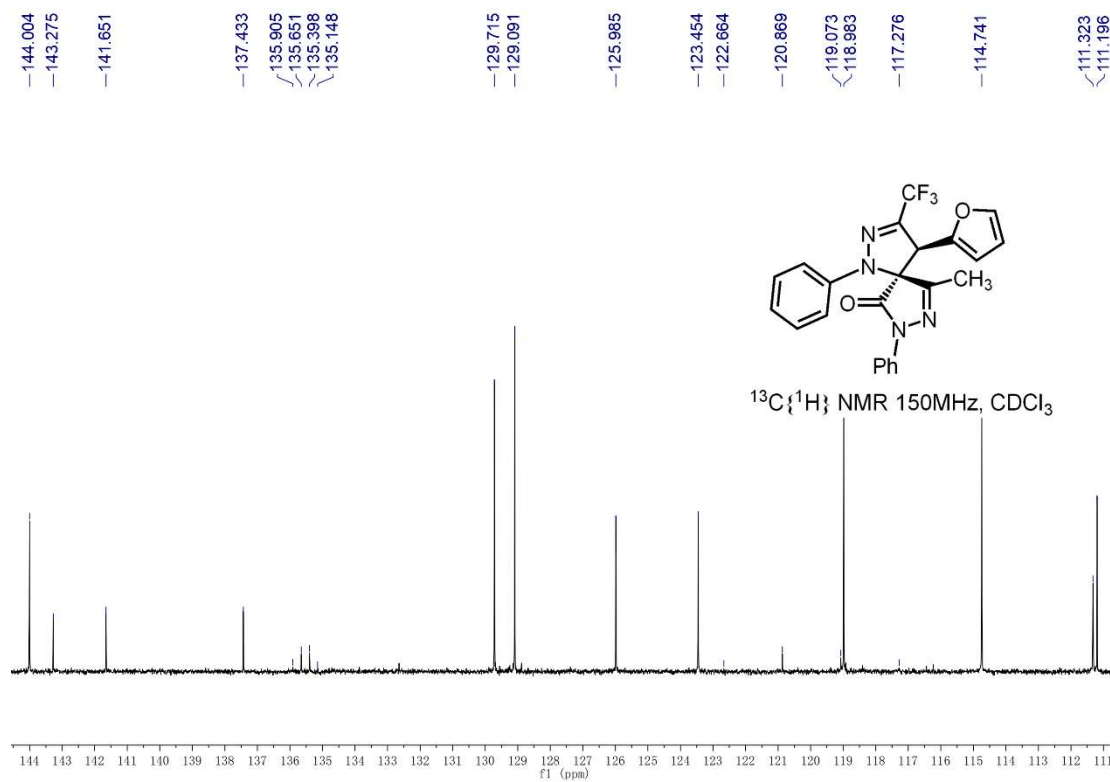
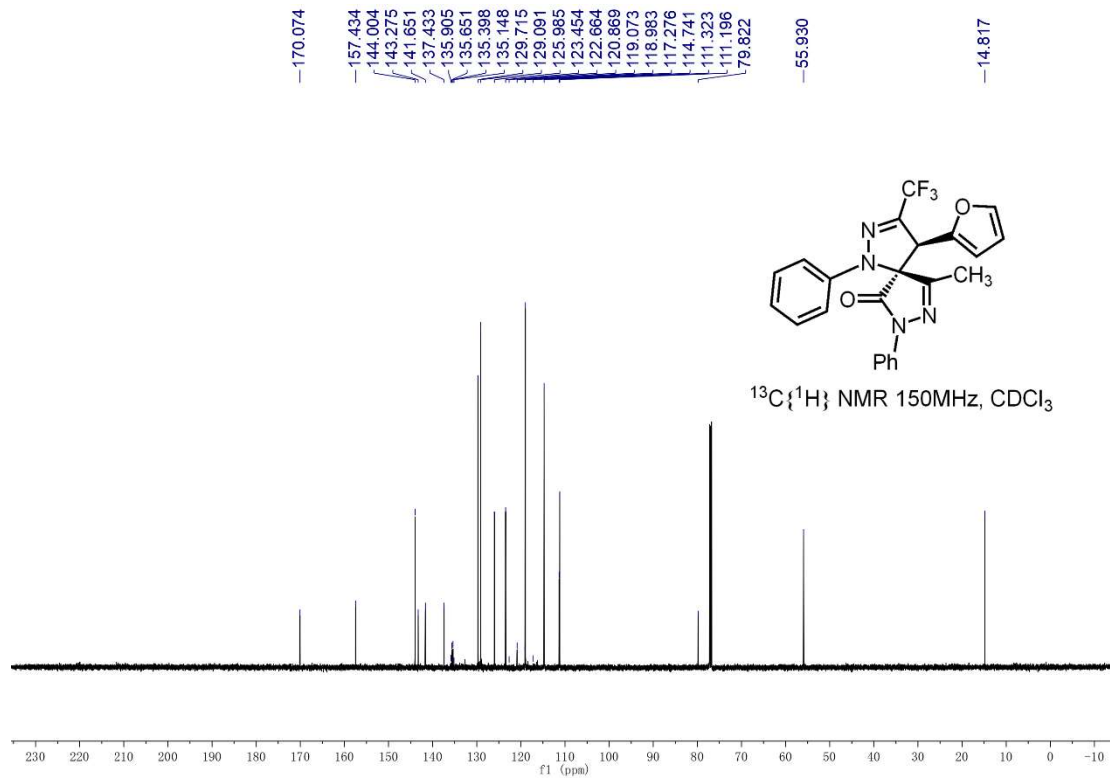
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



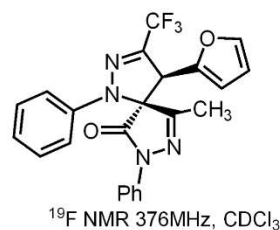
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j % Conf	mSi gm a	Std l	St d l	St d l	St d l	Std Com b Dev
489.1311	1 C <sub>25</sub> H <sub>18</sub> F <sub>4</sub> N <sub>4</sub> NaO	489.1309	-0.5	-0.7	16.5	ok	even	10.6	14.3	0.4	6.7	0.5	842.7

NMR copies of compound (*trans*)-6g:





--63.314



HRMS (ESI) copy of compound (*trans*)-6g:

### Mass Spectrum SmartFormula Report

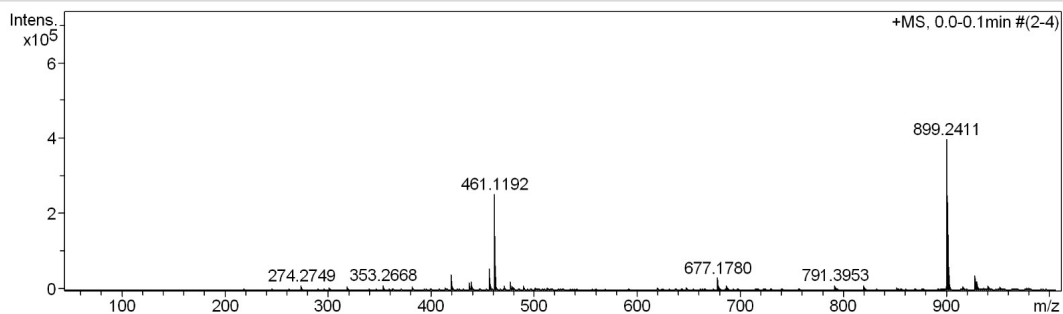
#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20230322-11.d  
Method tune\_low.m  
Sample Name A-44  
Comment

Acquisition Date 2023-3-22 9:58:47  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

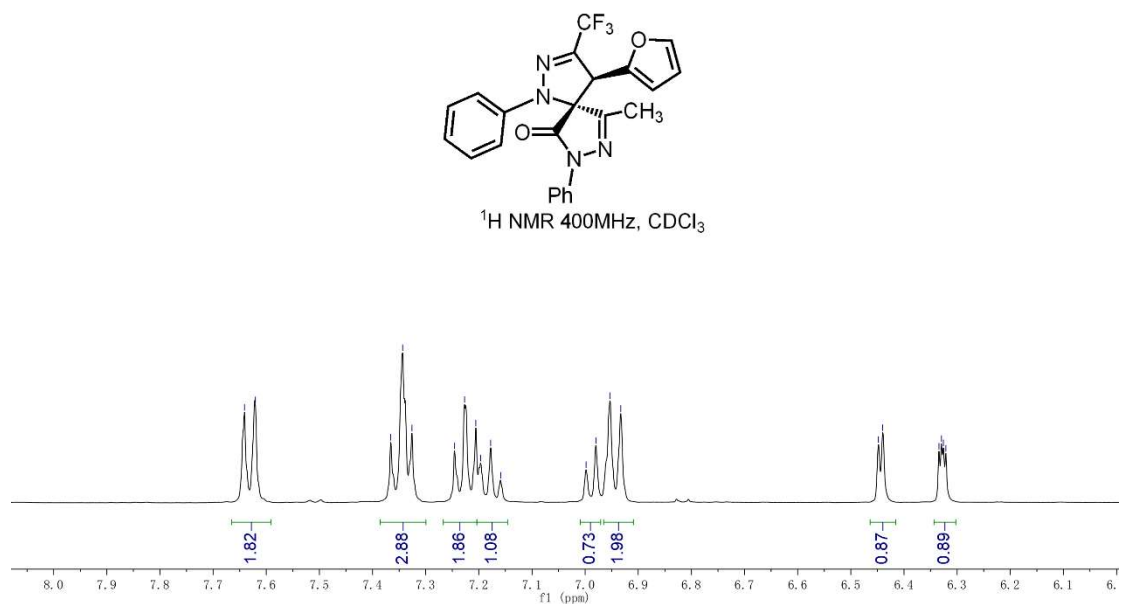
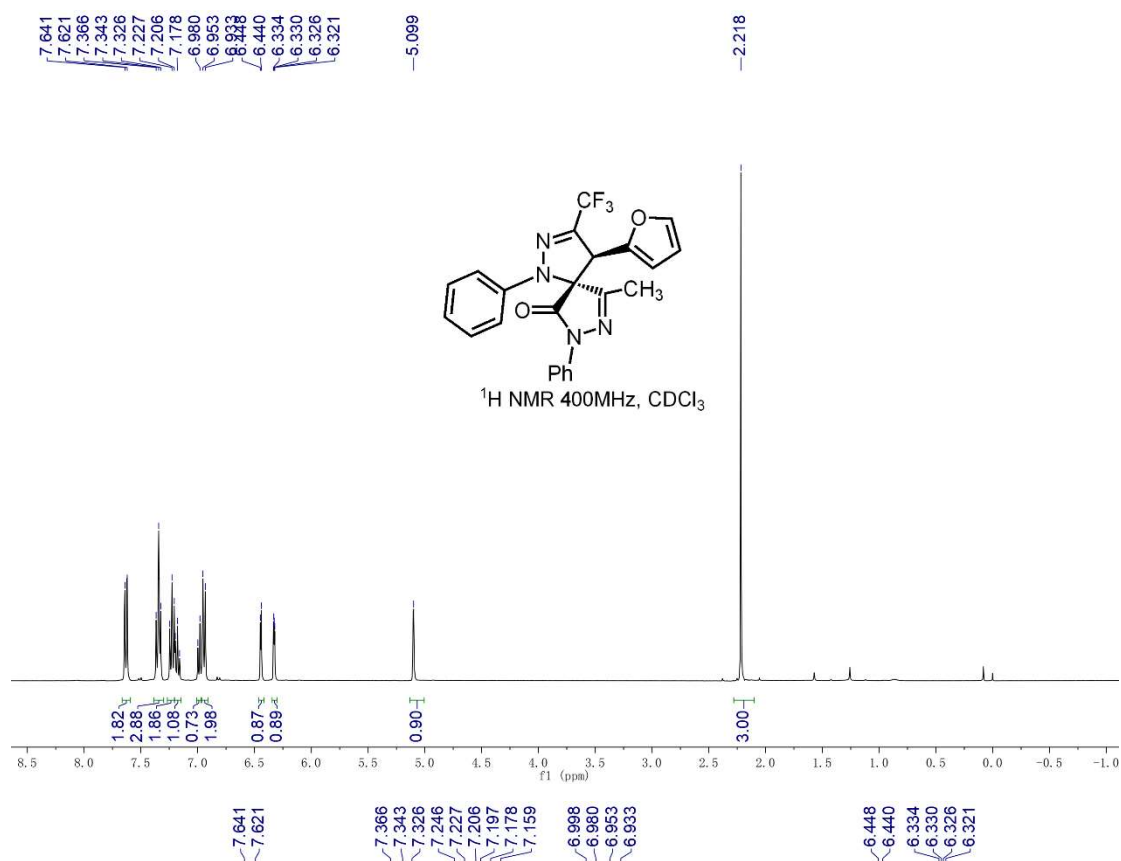
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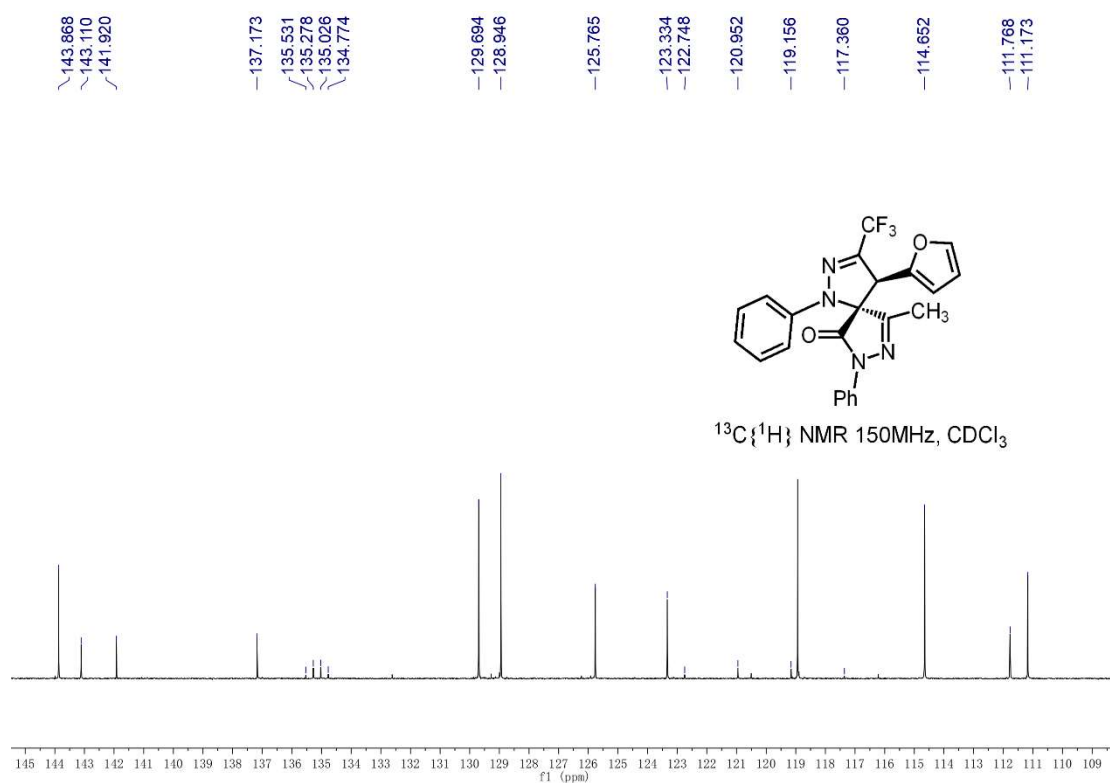
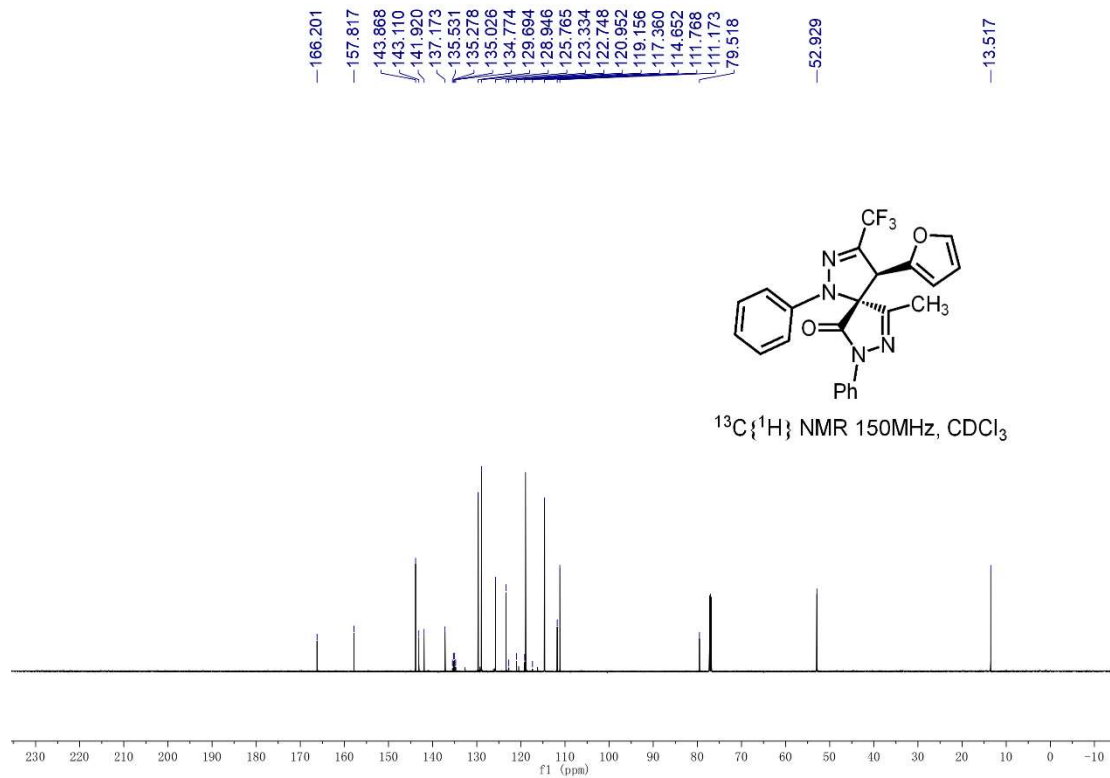
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	ei% Conf	m Sigma	Std l	St d l	St d l	St d l	Std Com b Dev
461.1192	1 C <sub>23</sub> H <sub>17</sub> F <sub>3</sub> N <sub>4</sub> O <sub>2</sub>	461.1196	0.8	1.1	15.5	ok	even	7.8	13.2	0.5	5.9	0.4	842.7

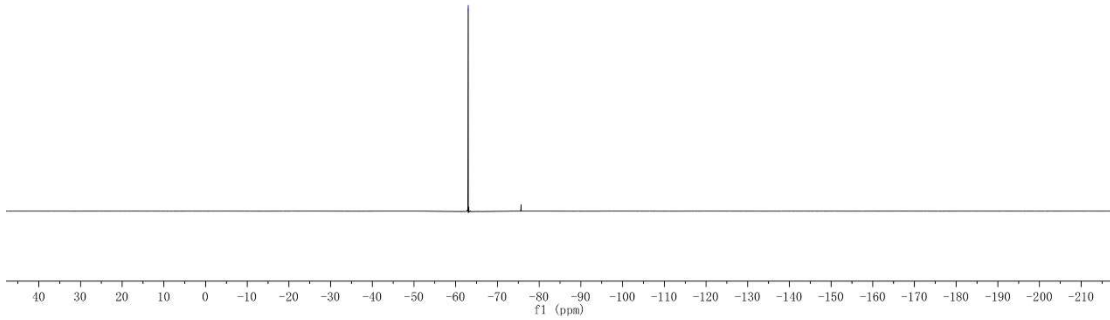
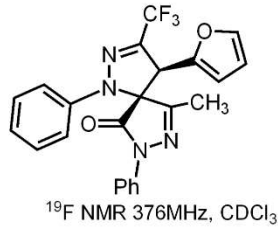
NMR copies of compound (*cis*)-**6g**:







62.988



HRMS (ESI) copy of compound (*cis*)-6g:

### Mass Spectrum SmartFormula Report

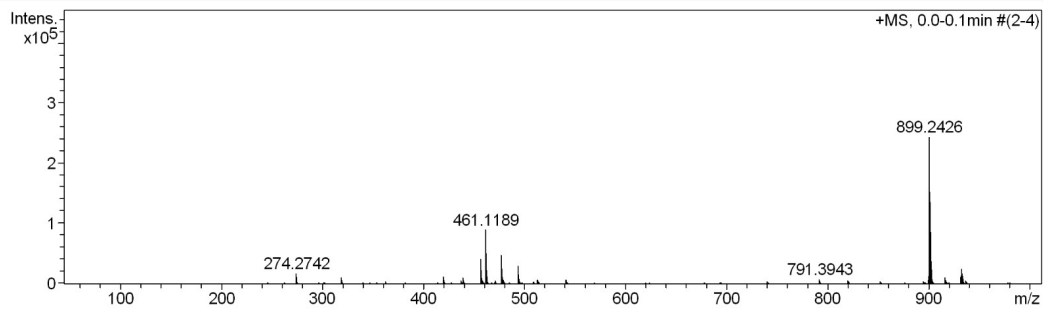
#### Analysis Info

Analysis Name D:\Data\user\NWNW-fengyang 20230322-12.d  
Method tune\_low.m  
Sample Name A-441  
Comment

Acquisition Date 2023-3-22 10:01:12  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

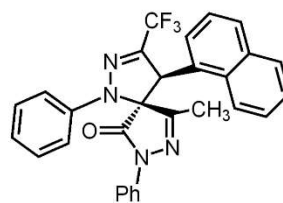
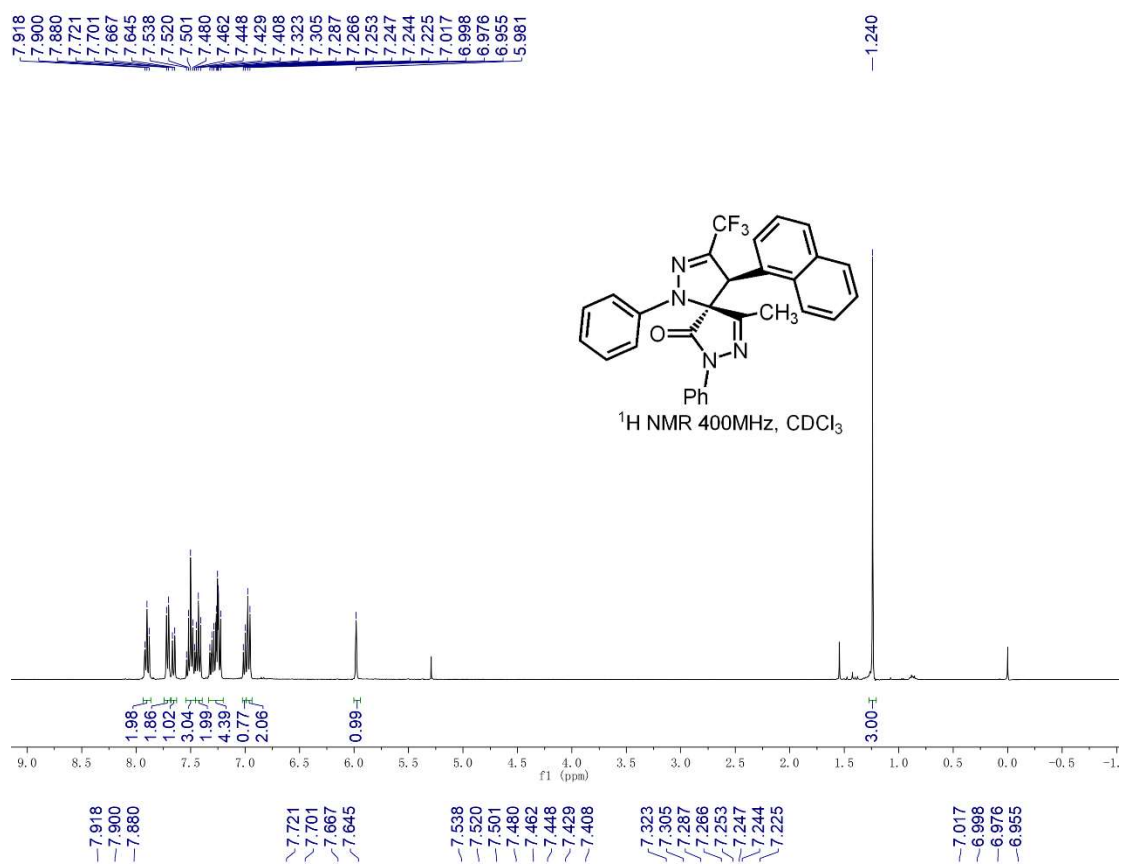
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

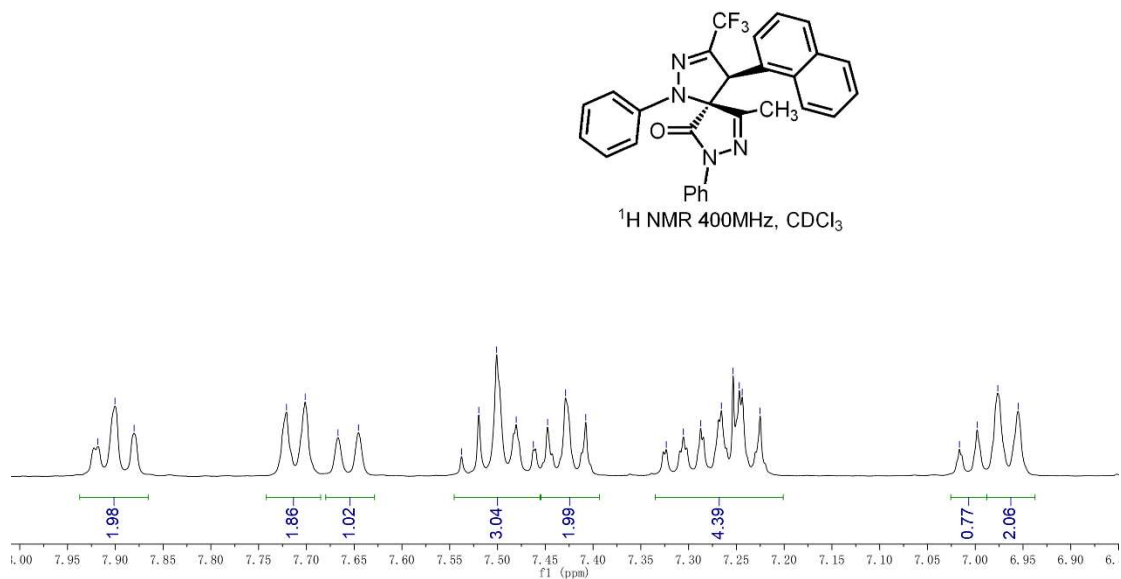


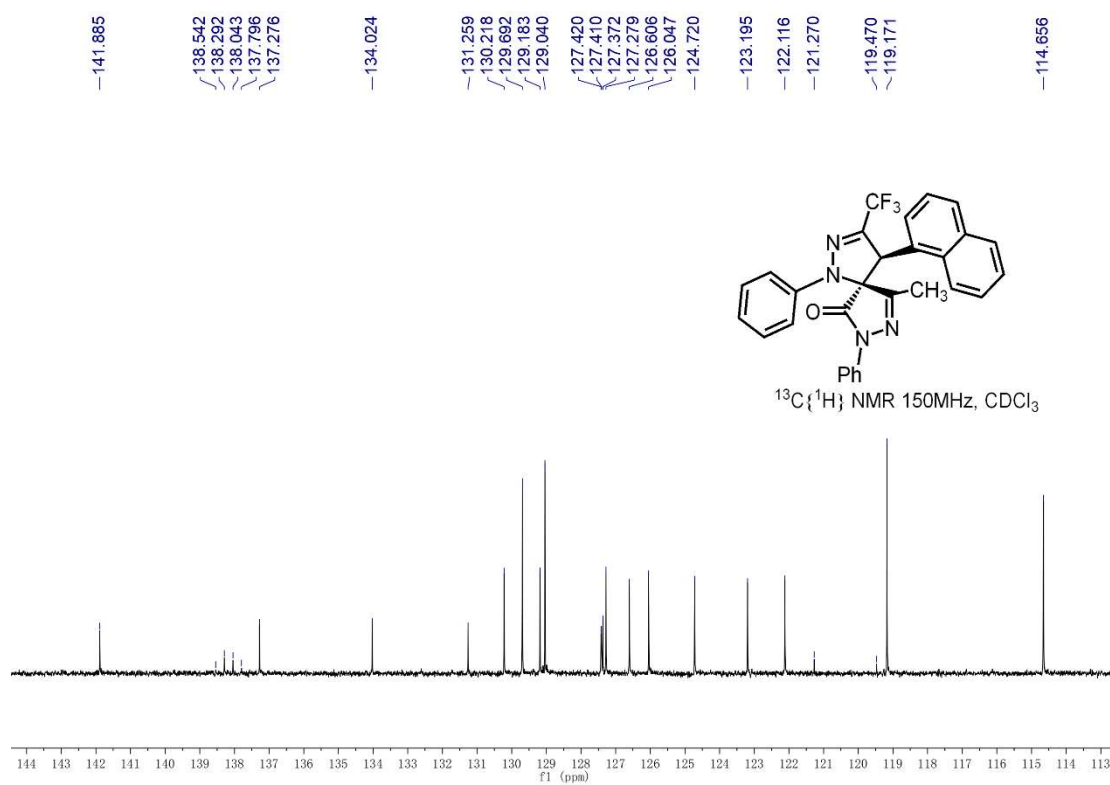
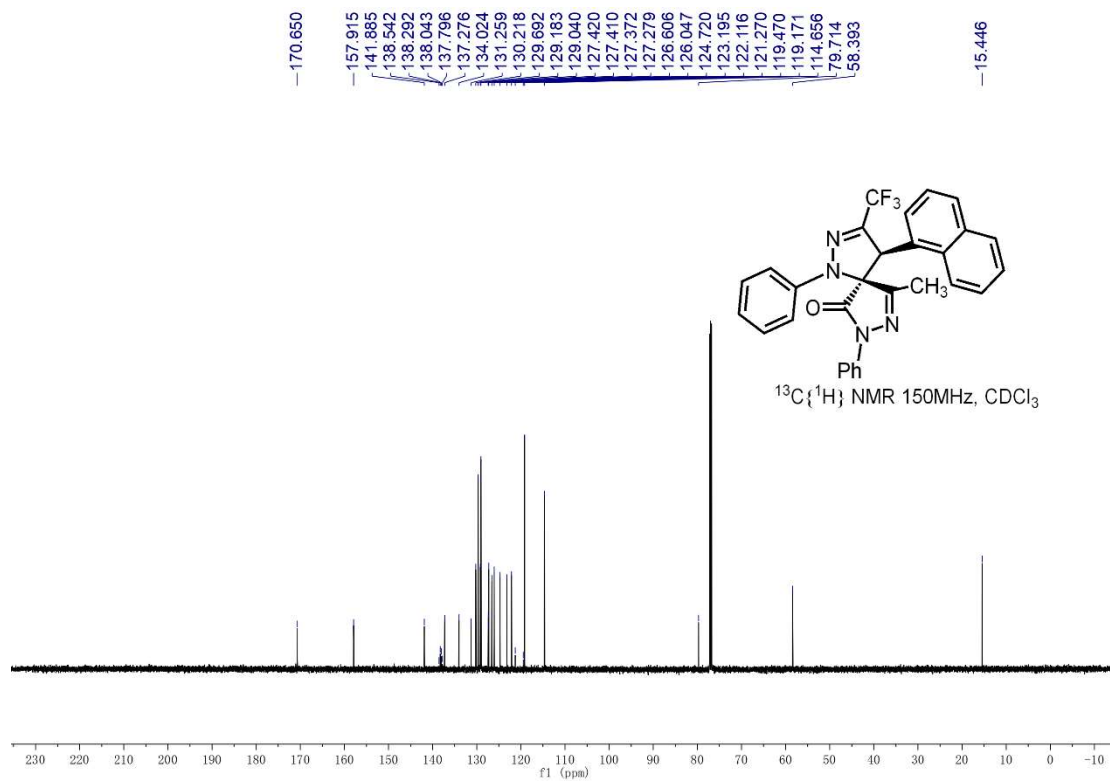
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>j</sub> ¥ Conf	mS ig ma	Std l	Std Me an m/z	Std l Va rN or m	Std m/z Diff	Std Com b Dev
461.1189	1 C <sub>23</sub> H <sub>17</sub> F <sub>3</sub> N <sub>4</sub> NaO <sub>2</sub>	461.1196	1.6	2.1	15.5	ok	even	1.4	2.4	1.1	1.6	1.0	842.7

NMR copies of compound (*trans*)-6h:

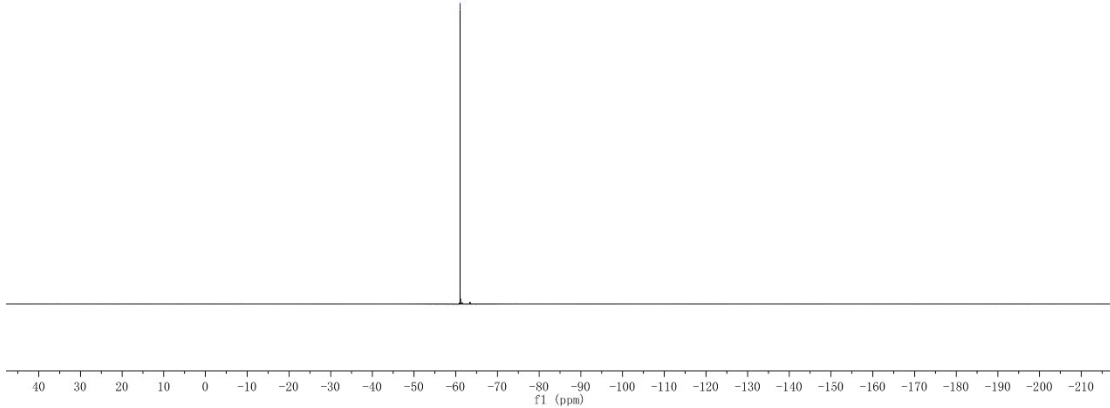
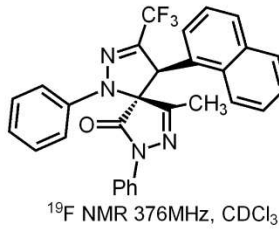


<sup>1</sup>H NMR 400MHz, CDCl<sub>3</sub>





-61.024



HRMS (ESI) copy of compound (*trans*)-6h:

### Mass Spectrum SmartFormula Report

#### Analysis Info

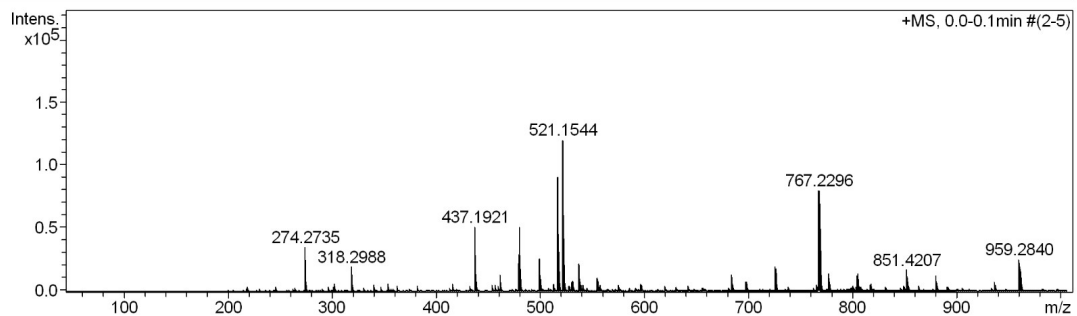
Analysis Name D:\Data\user\NWNNU-fengyang 20230322-13.d  
Method tune\_low.m  
Sample Name A-45  
Comment

Acquisition Date 2023-3-22 10:04:34

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

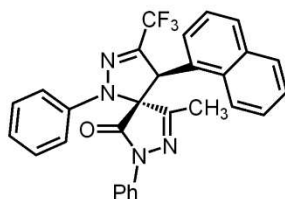
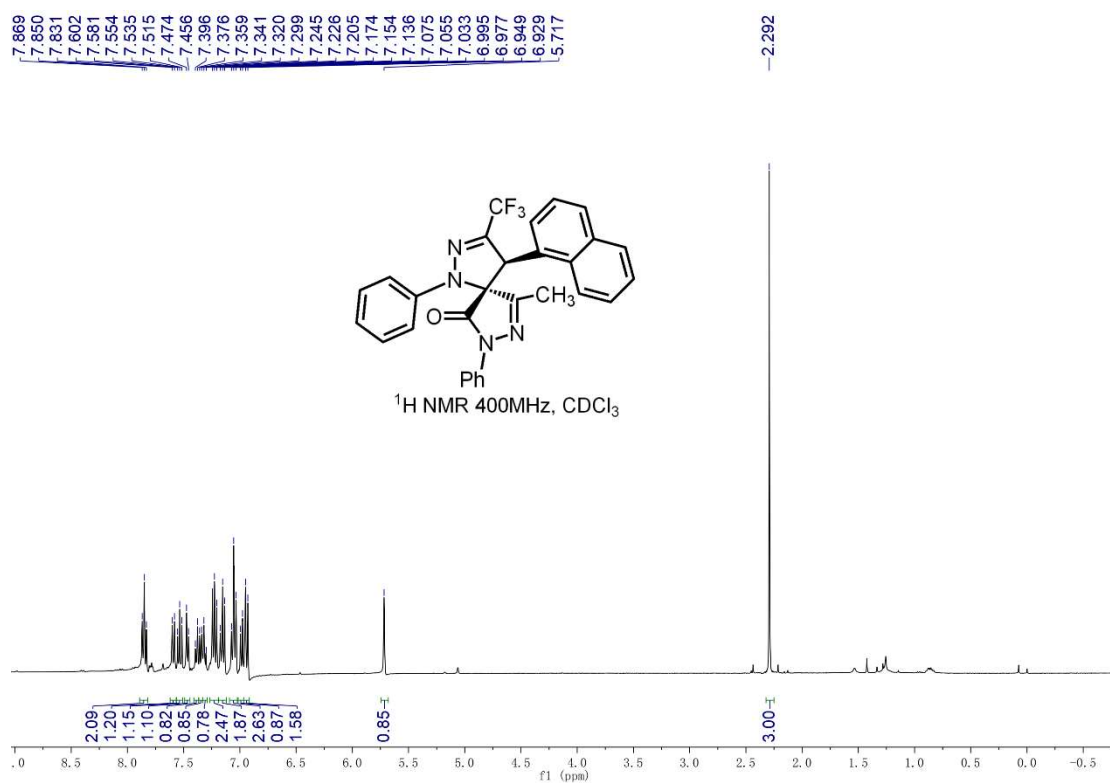
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 i°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

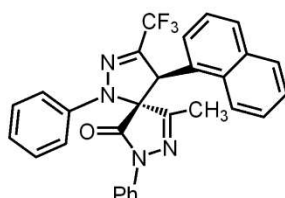


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>j</sub> Conf	mS	Std	Std	Std	Std	Std	
m/z						ul		ig	I	Me	I	m/	Com	
						e		ma		an	Va	z	b	
										m/	rN	Diff	Dev	
										z	or			
										m				
521.1544	1	C <sub>29</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO	521.1560	3.0	3.3	19.5	ok	even	8.5	13.3	1.7	4.8	0.5	842.7

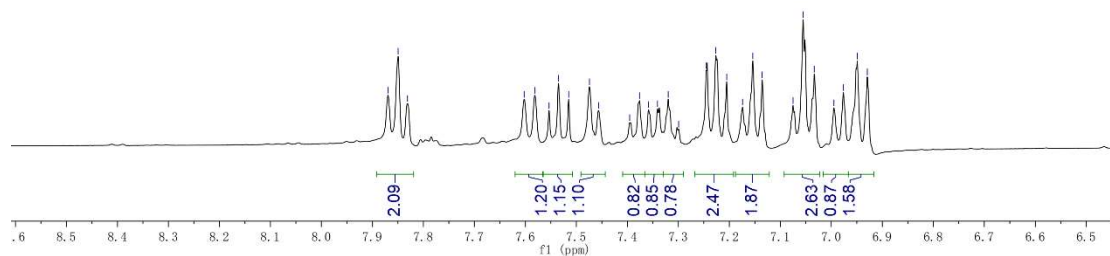
NMR copies of compound (*cis*)-**6h**:

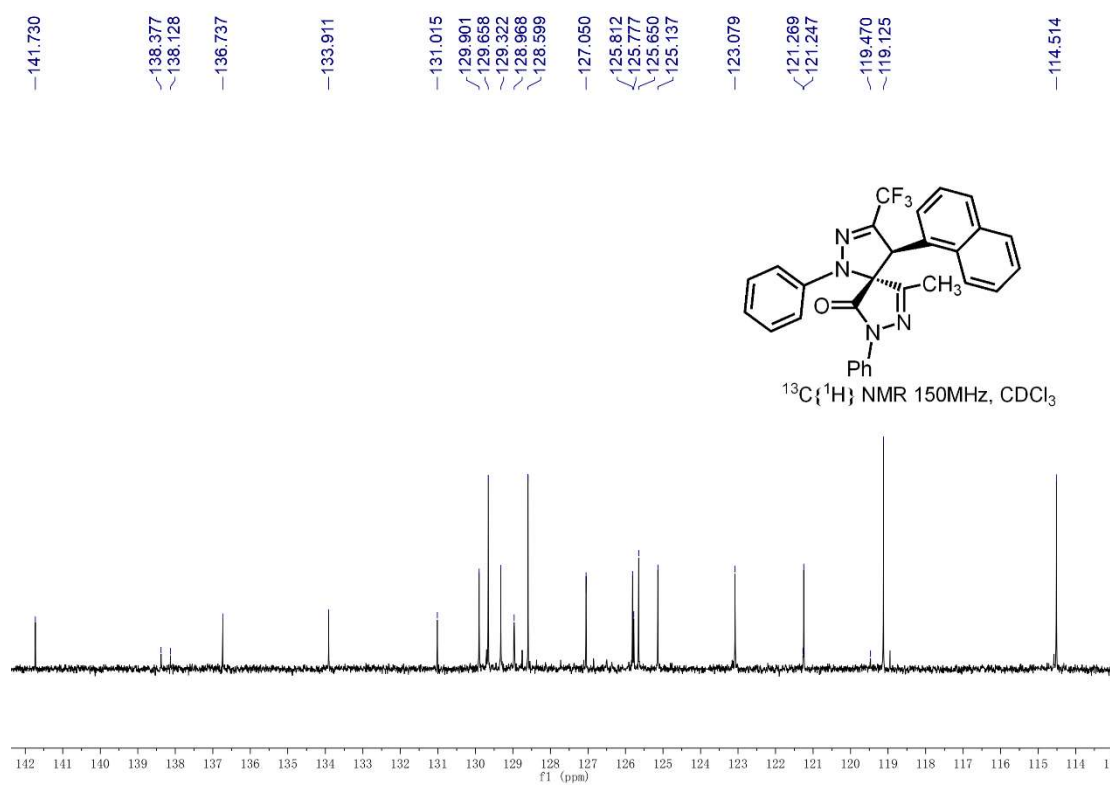
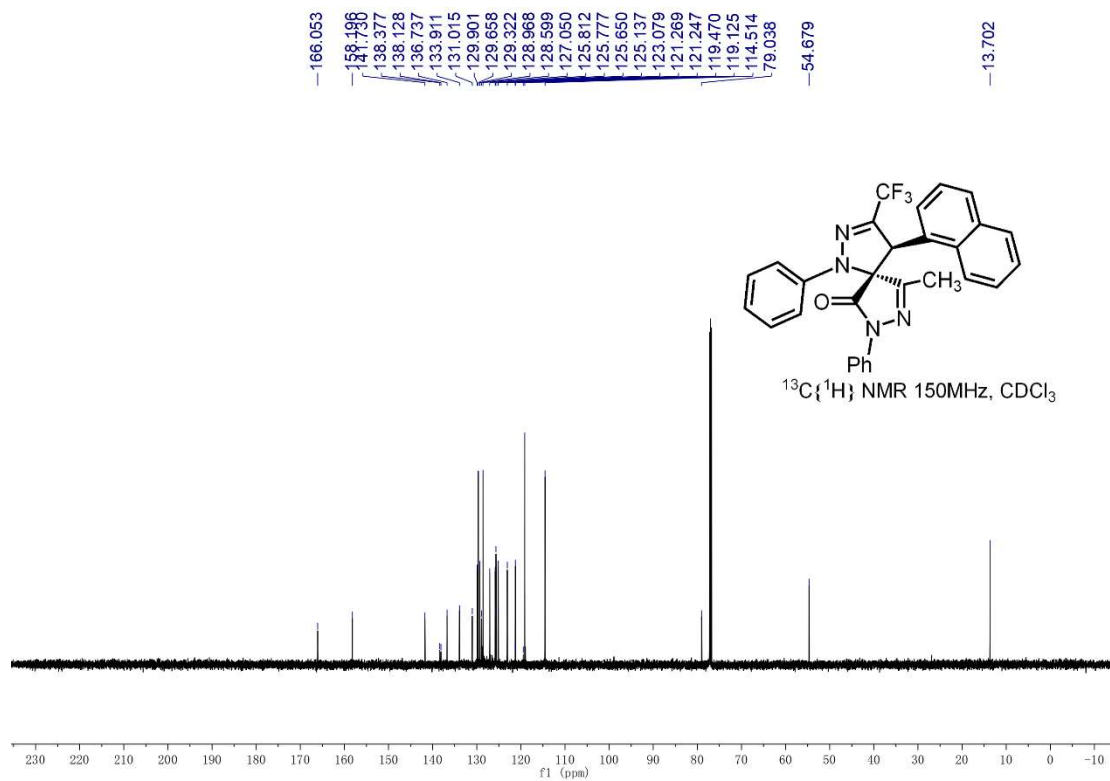


<sup>1</sup>H NMR 400MHz, CDCl<sub>3</sub>

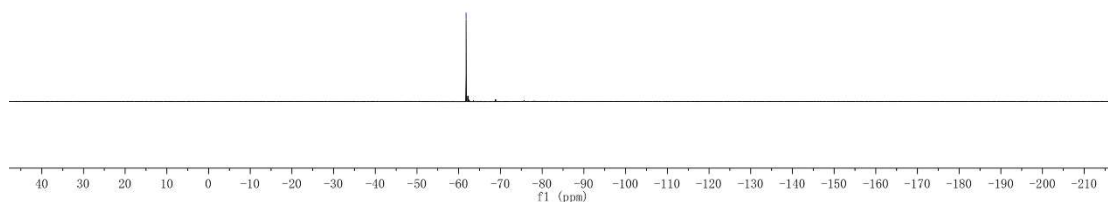
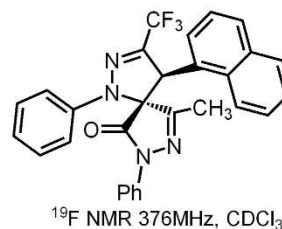


<sup>1</sup>H NMR 400MHz, CDCl<sub>3</sub>





---61.753



HRMS (ESI) copy of compound (*cis*)-**6h**:

### Mass Spectrum SmartFormula Report

#### Analysis Info

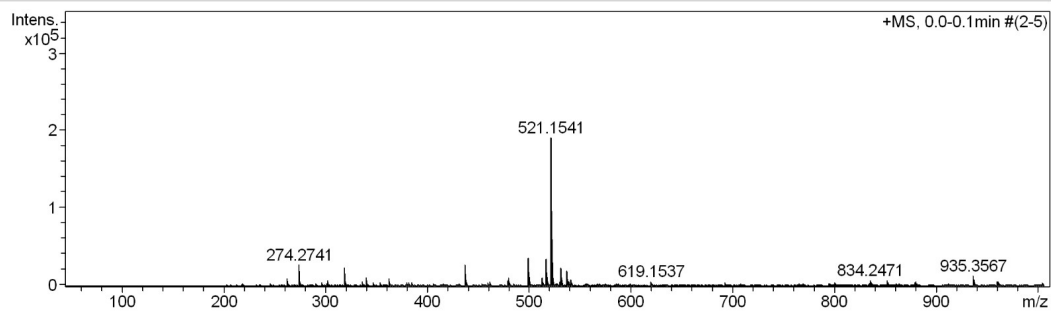
Analysis Name D:\Data\user\NWNU-fengyang 20230322-14.d  
Method tune\_low.m  
Sample Name A-451  
Comment

Acquisition Date 2023-3-22 10:07:10

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

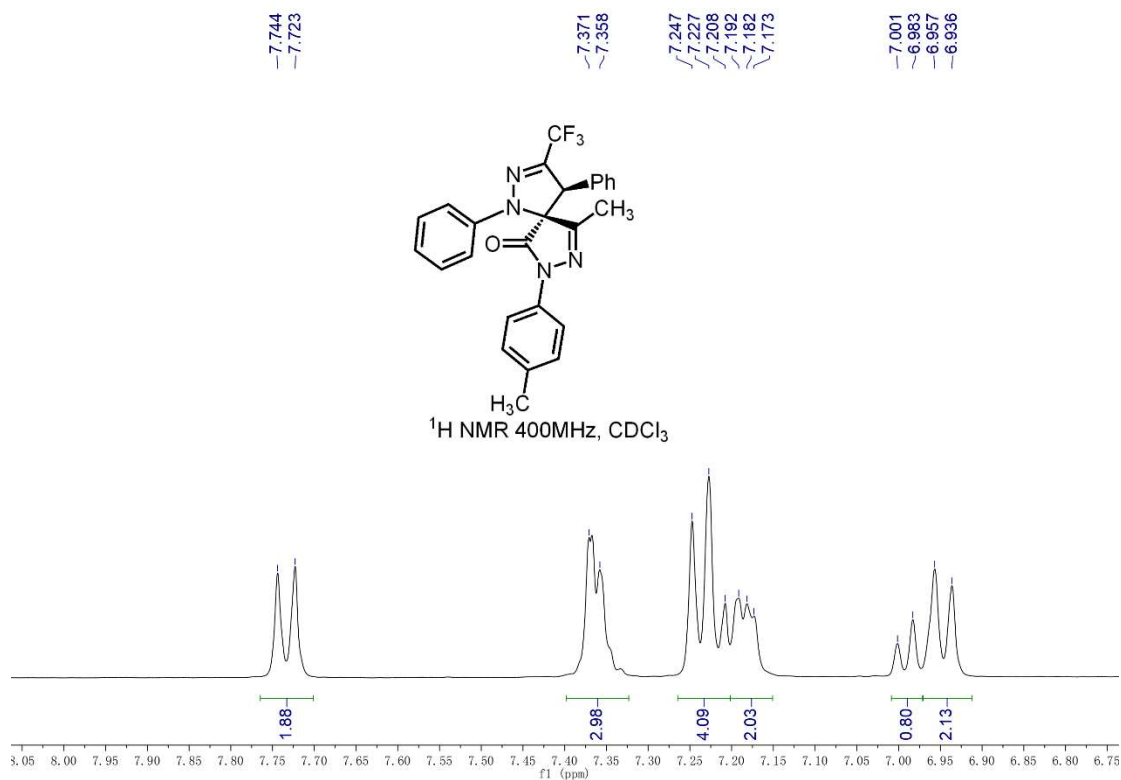
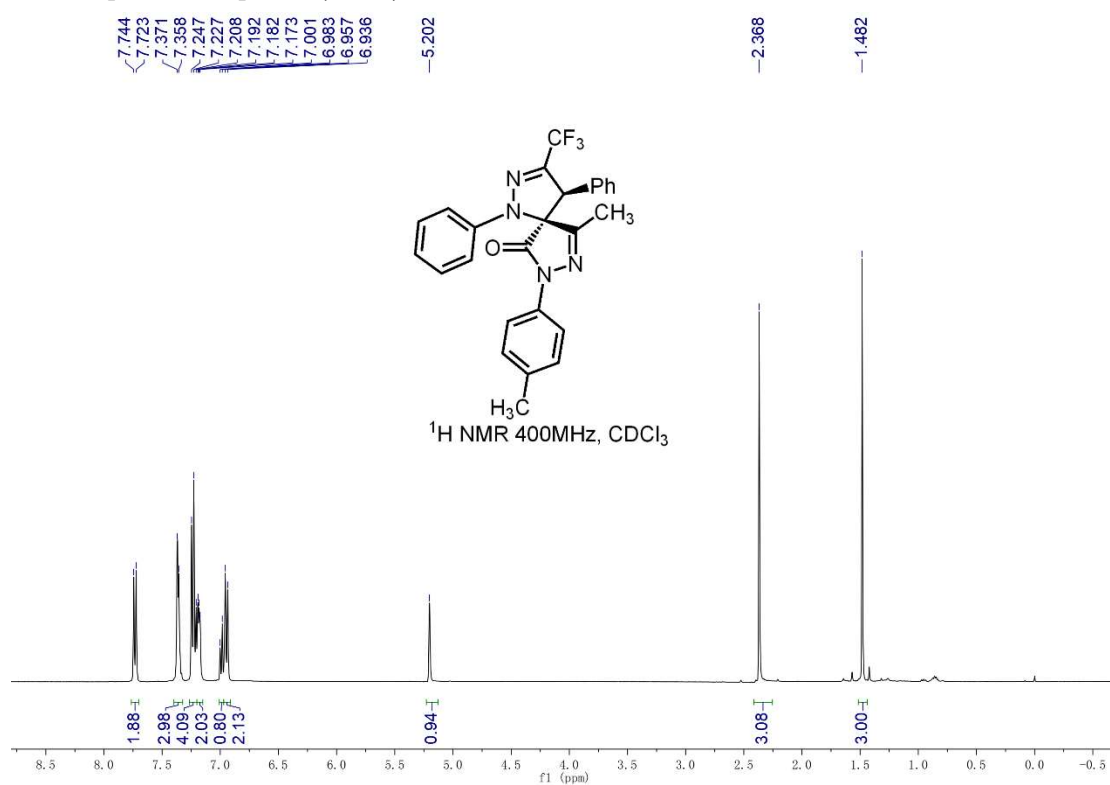
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

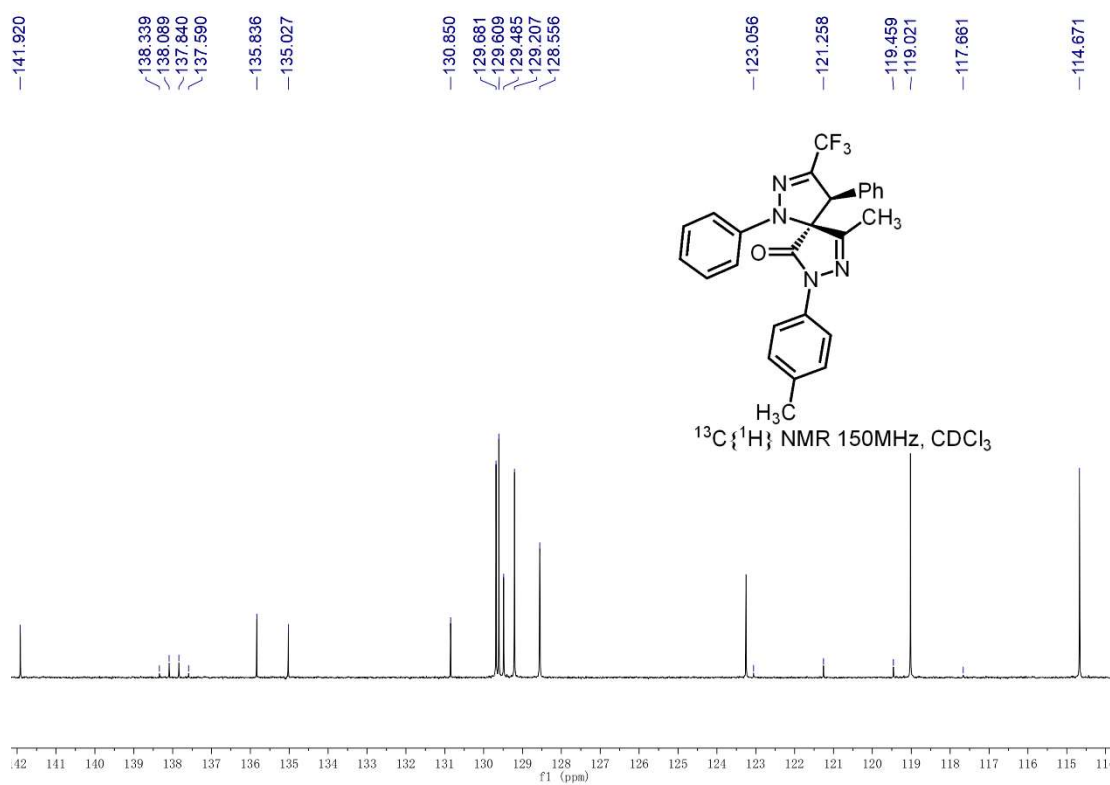
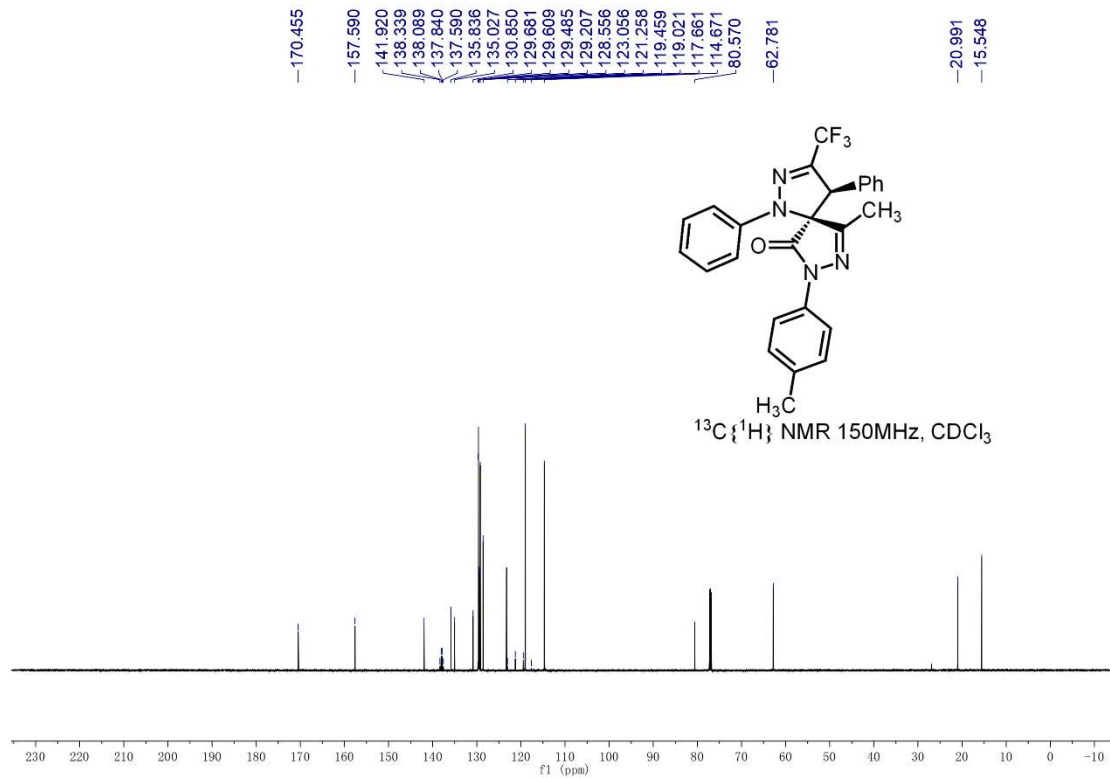


Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N- R	ei %	Conf	mS	Std	Std	Std	Std	Std
m/z						ul			ig	I	Me	I	m/	Com
						e			ma		an	Va	z	b
											rN	rN	Diff	Dev
											z	or		
											m			
521.1541	1	C <sub>29</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO	521.1560	3.5	3.2	19.5	ok	even	7.4	10.8	1.7	4.4	0.5	842.7

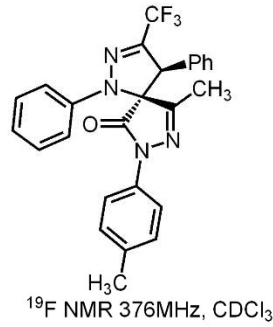
NMR copies of compound (*trans*)-6i:







--61.552



HRMS (ESI) copy of compound (*trans*)-6i:

### Mass Spectrum SmartFormula Report

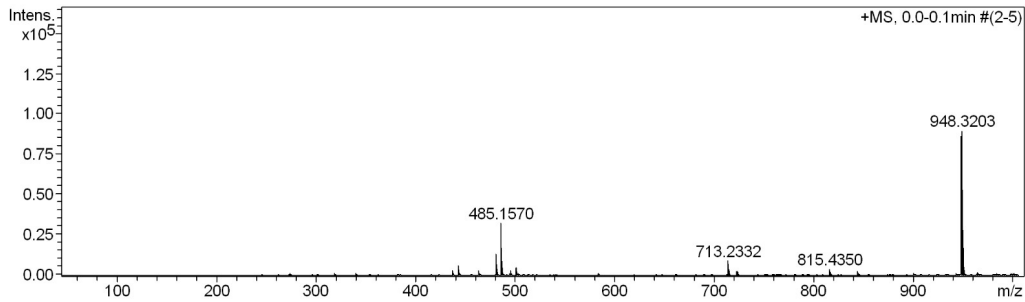
#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20230322-15.d  
Method tune\_low.m  
Sample Name A-46  
Comment

Acquisition Date 2023-3-22 10:09:32  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

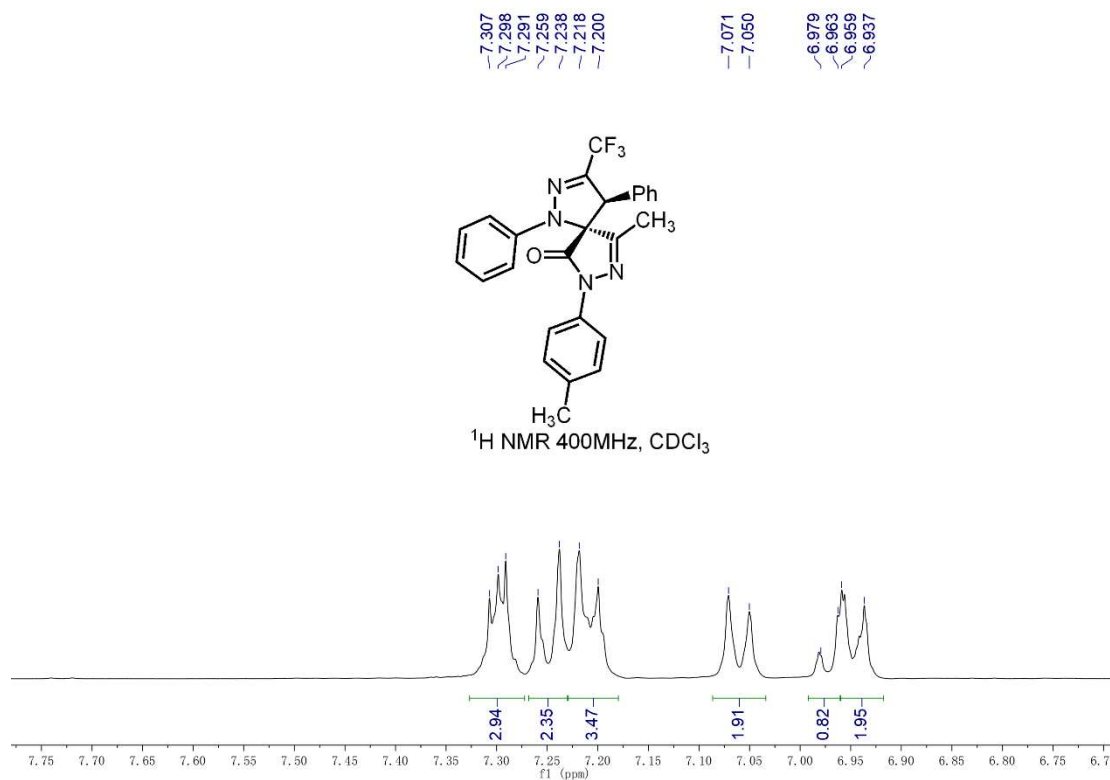
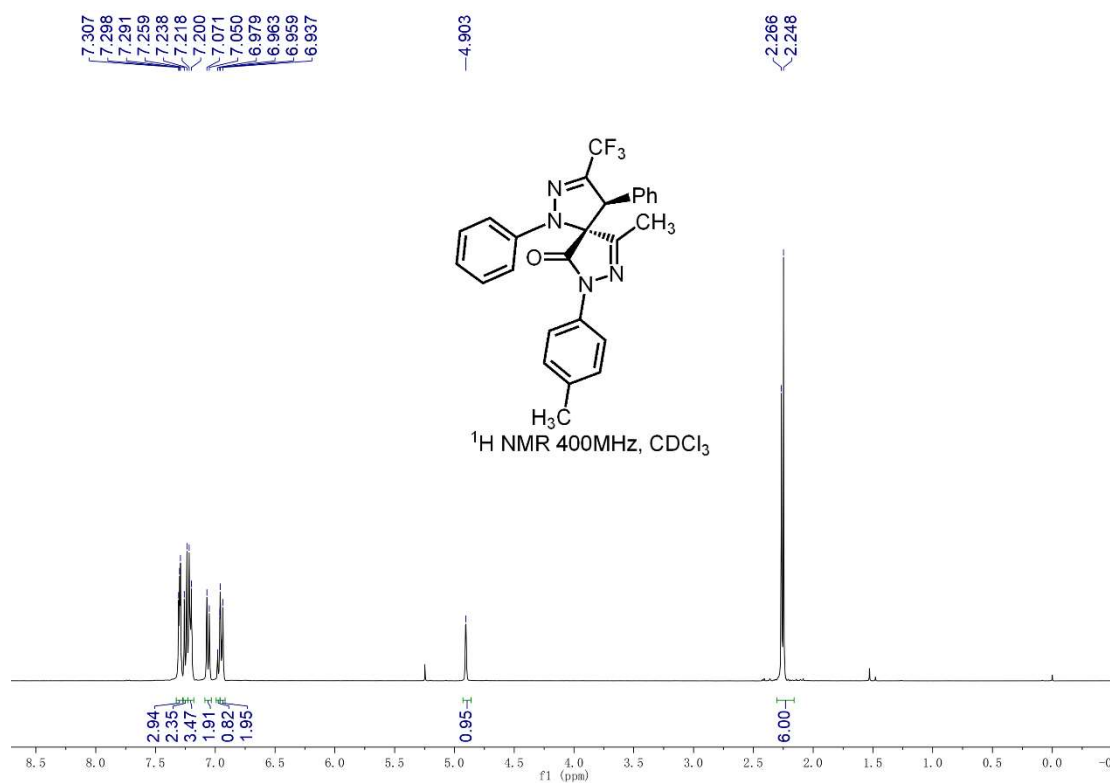
#### Acquisition Parameter

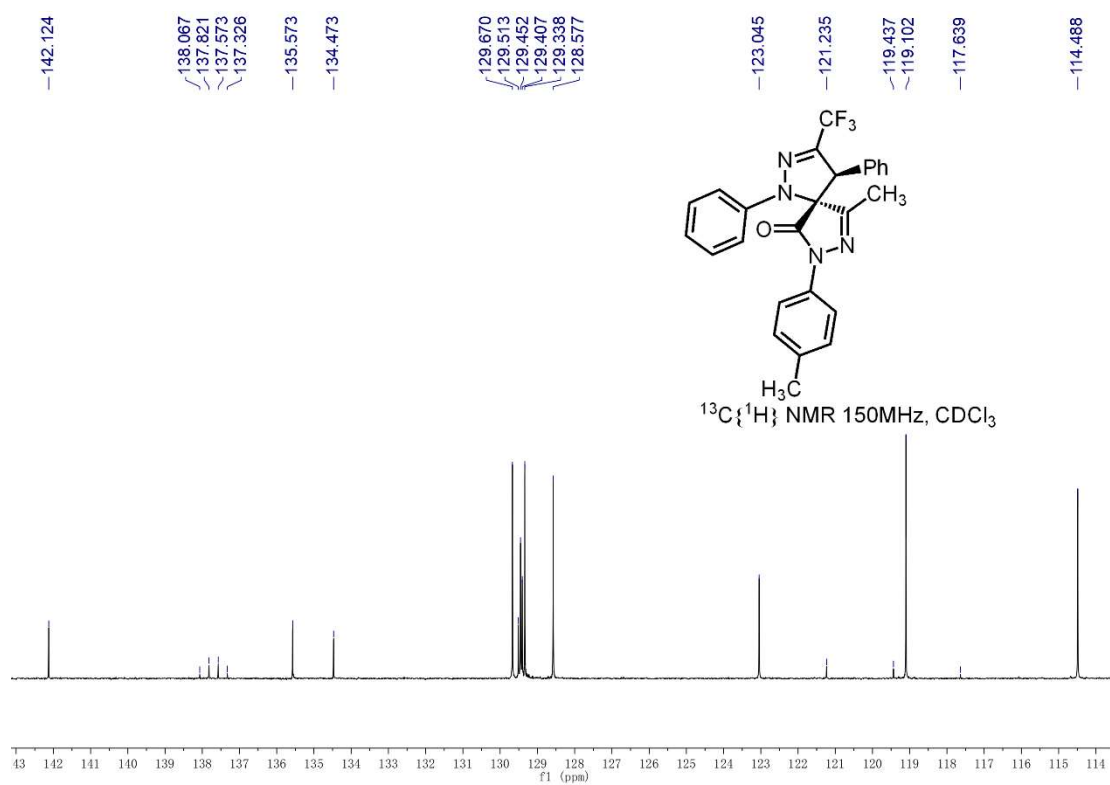
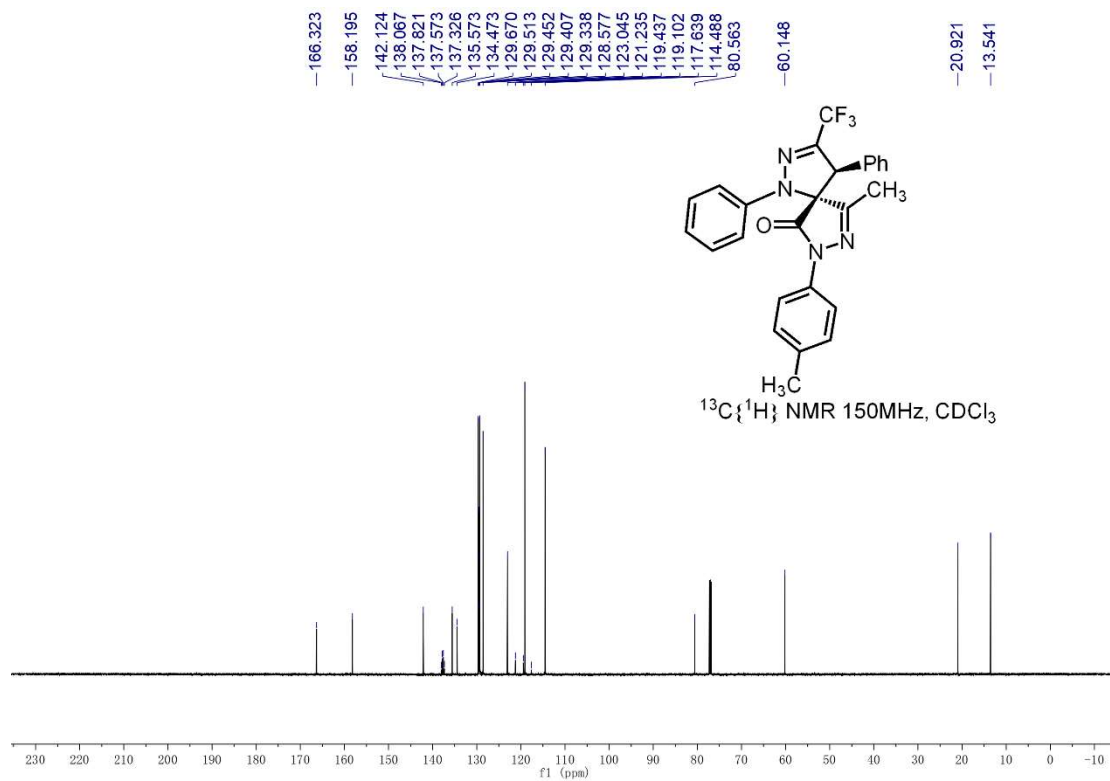
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



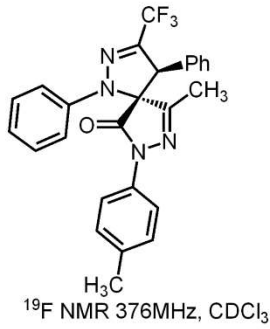
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e j %	Conf	m Sig	Std l	St d Me an m/z	St d Va rN or m	St d m/ z	St d Dif f	Std Com b Dev
485.1570	1 C <sub>26</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO	485.1560	-2.1	-1.8	16.5	ok	even	8.6	11.2	0.9	5.6	0.7	842.7		

NMR copies of compound (*cis*)-**6i**:





-62.033



HRMS (ESI) copy of compound (*cis*)-6i:

### Mass Spectrum SmartFormula Report

#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20230322-16.d  
Method tune\_low.m  
Sample Name A-461  
Comment

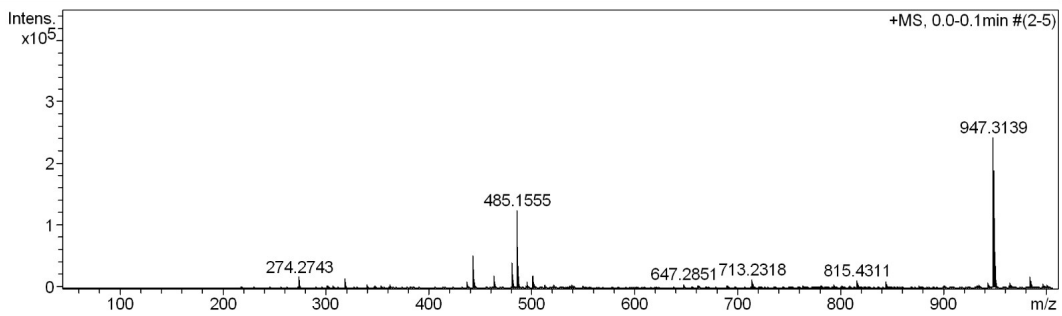
Acquisition Date 2023-3-22 10:11:44

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

#### Acquisition Parameter

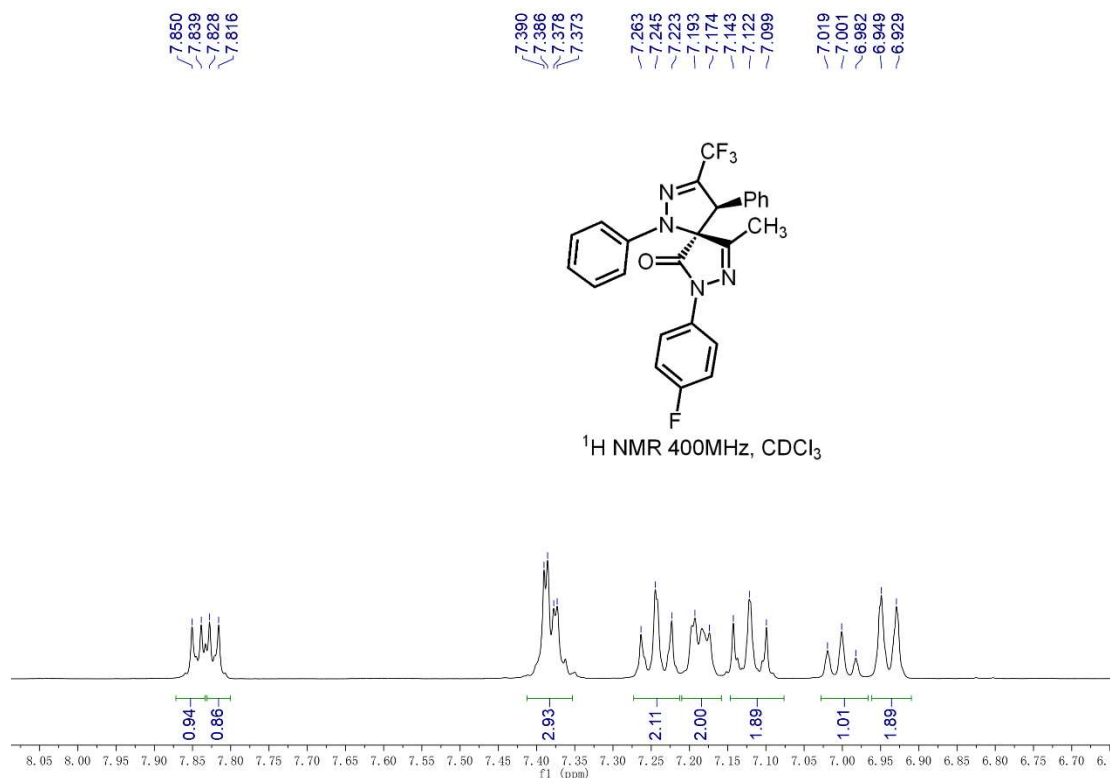
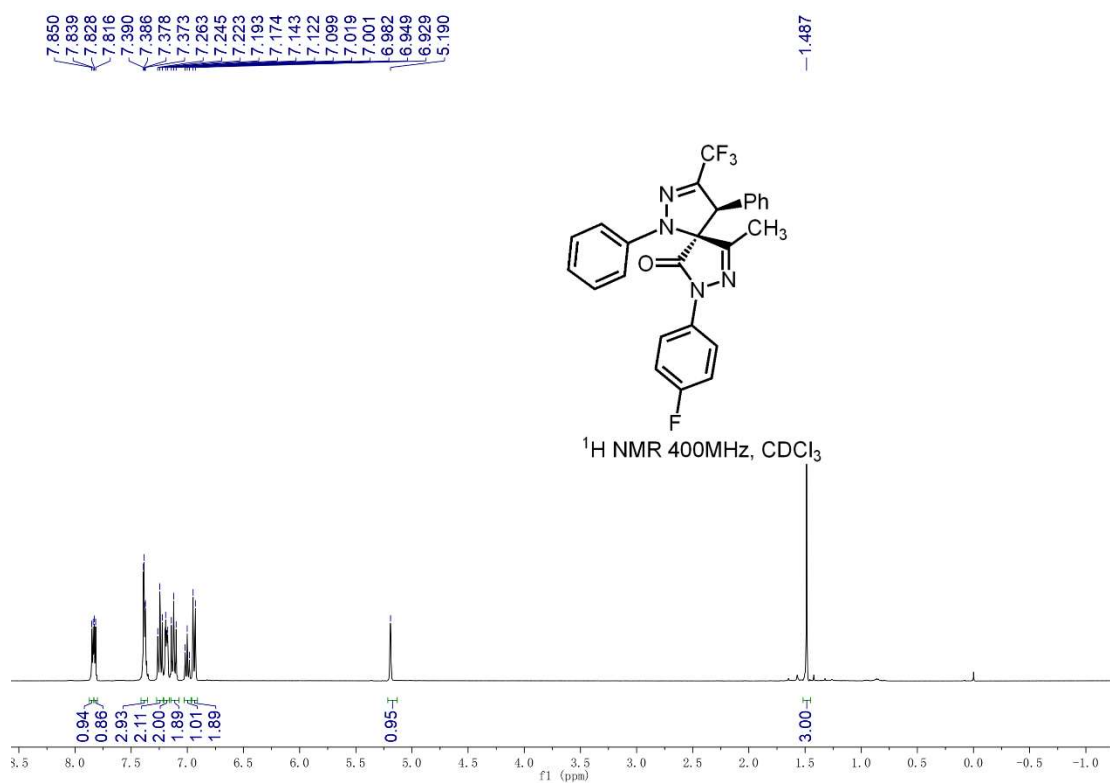
Source Type ESI  
Focus Active  
Scan Begin 50 m/z  
Scan End 1000 m/z  
Ion Polarity Positive  
Set Capillary 4500 V  
Set End Plate Offset -500 V  
Set Collision Cell RF 400.0 Vpp

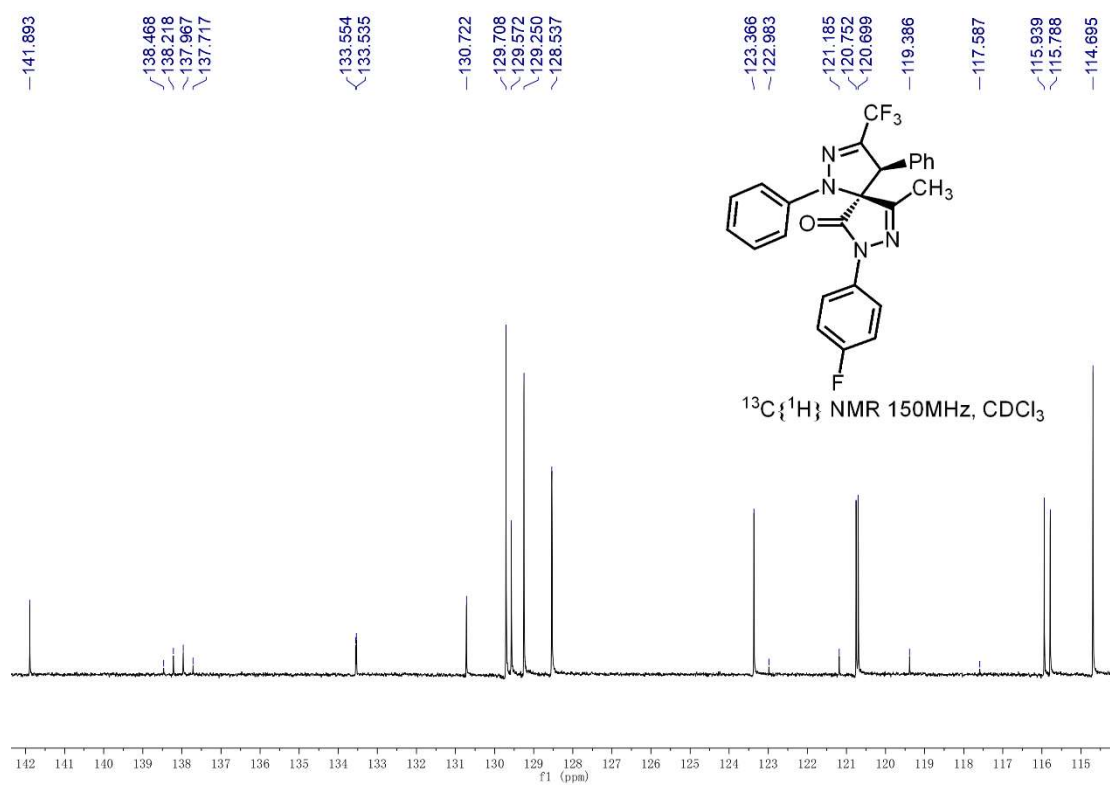
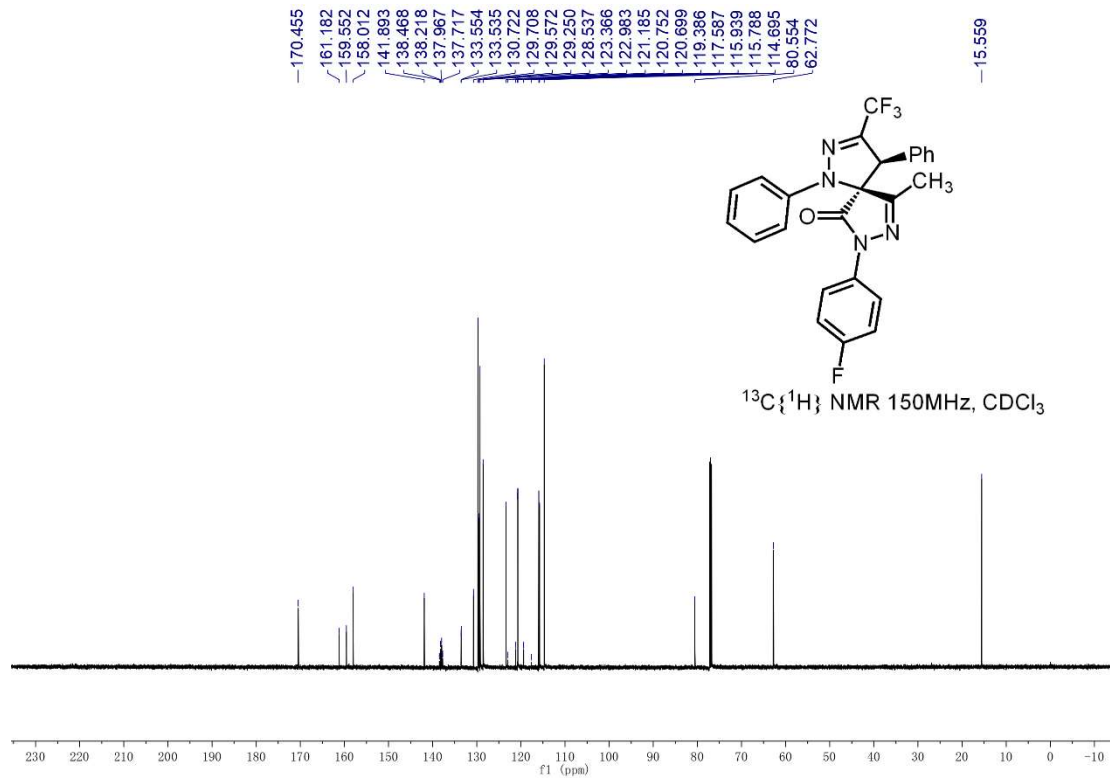
Set Nebulizer 0.4 Bar  
Set Dry Heater 180 j°C  
Set Dry Gas 4.0 l/min  
Set Divert Valve Waste

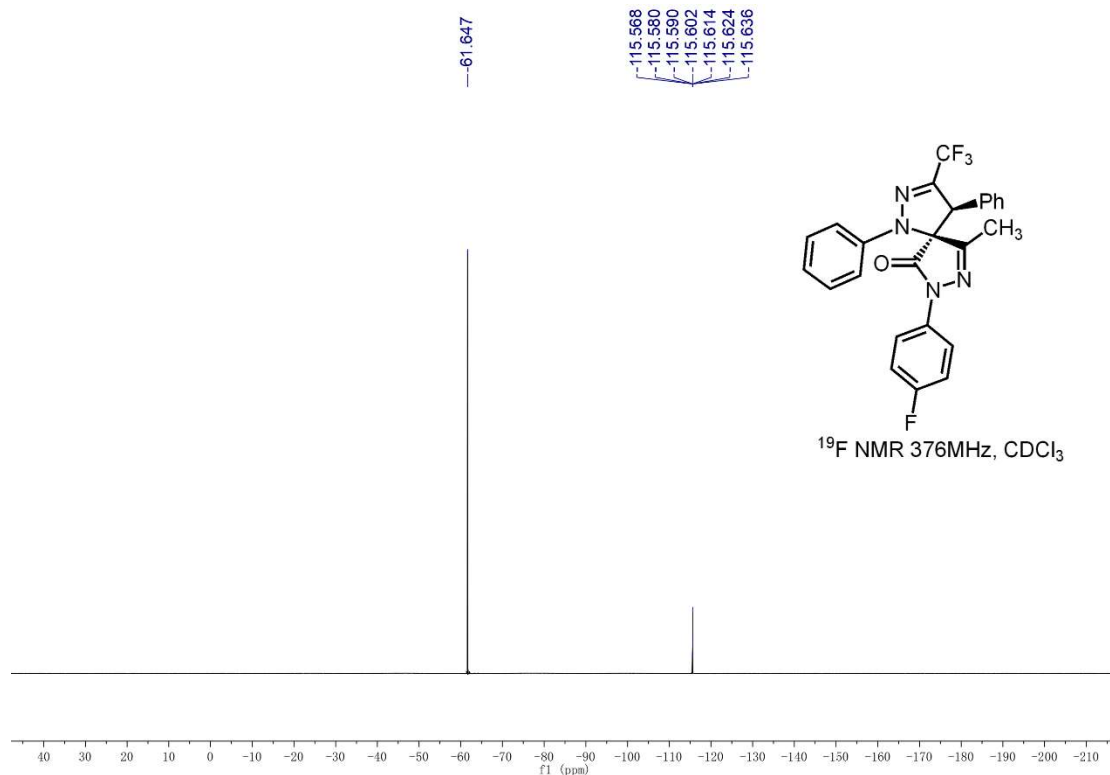


Meas. #	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N- R Conf	e <sub>i</sub> %	mS	Std I	Std Me	Std I	Std m/	Std rN	Std m/	Std Com
485.1555	1 C <sub>26</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO	485.1560	0.9	0.7	16.5	ok	even	8.8	11.6	0.4	5.6	0.5	842.7		

NMR copies of compound (*trans*)-6j:







HRMS (ESI) copy of compound (*trans*)-6j:

### Mass Spectrum SmartFormula Report

**Analysis Info**

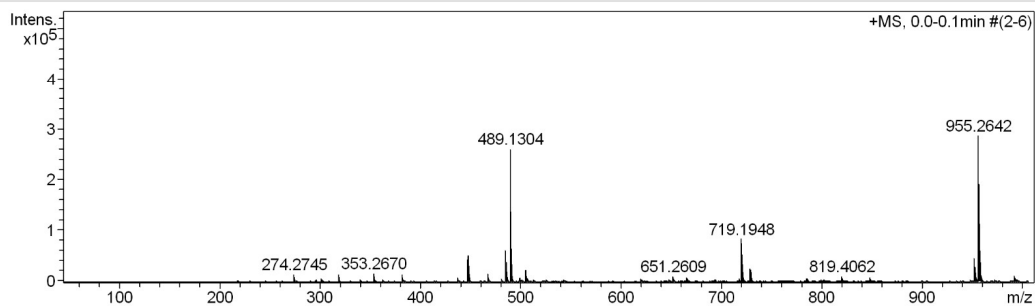
Analysis Name D:\Data\user\NWNNU-fengyang 20230322-17.d  
 Method tune\_low.m  
 Sample Name A-47  
 Comment

Acquisition Date 2023-3-22 10:13:53

Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

**Acquisition Parameter**

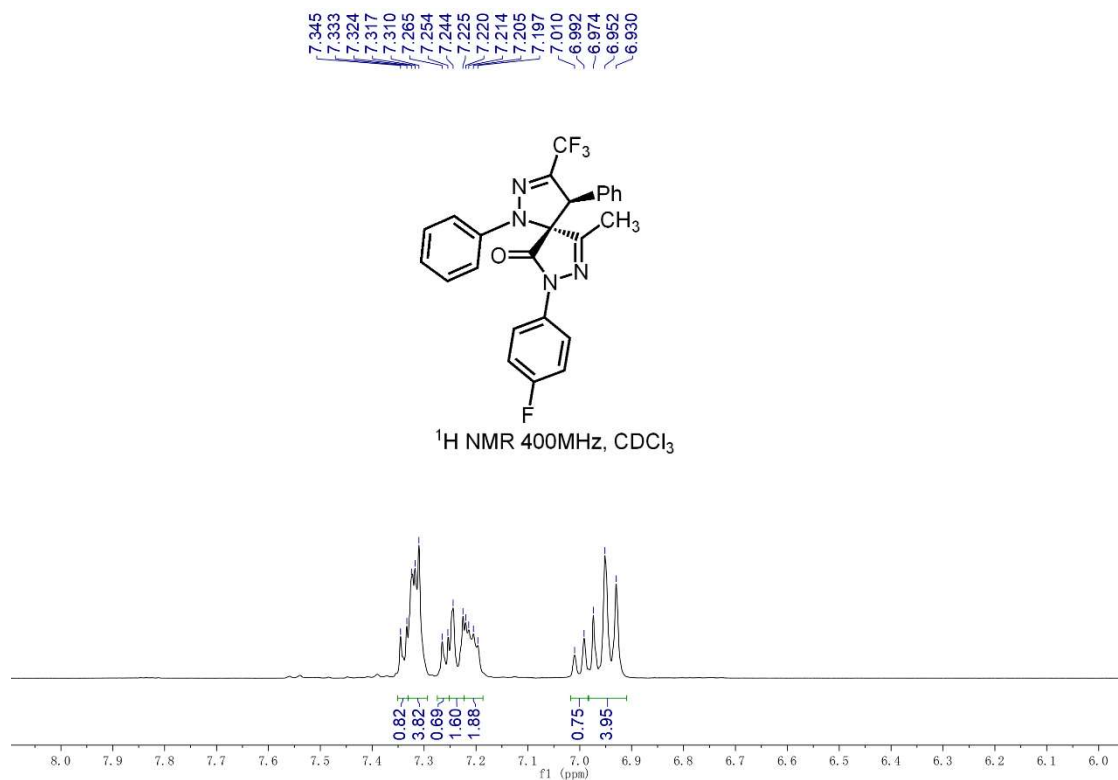
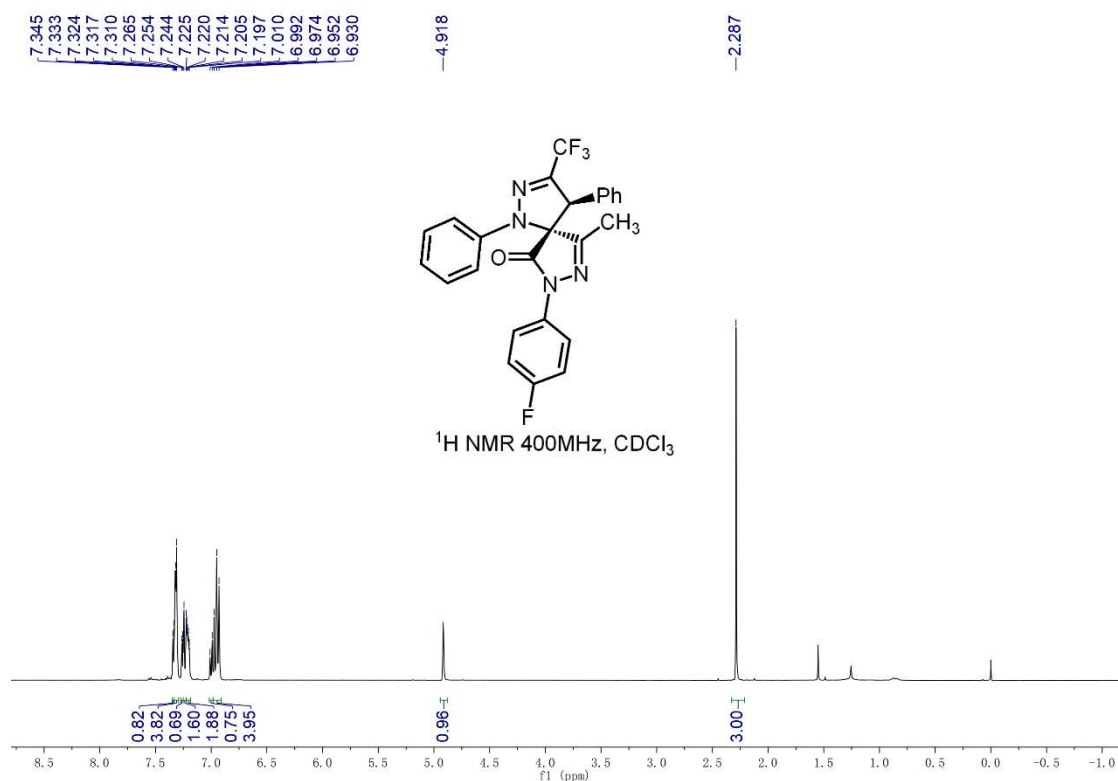
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j̄aC
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

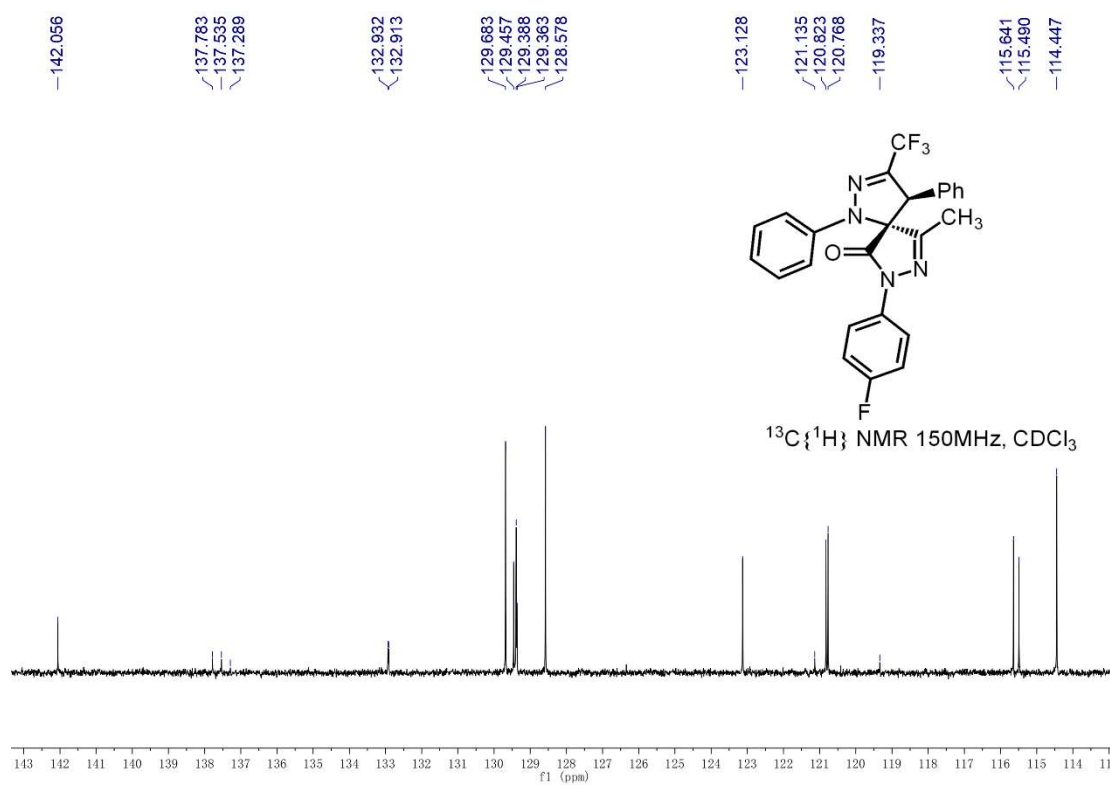
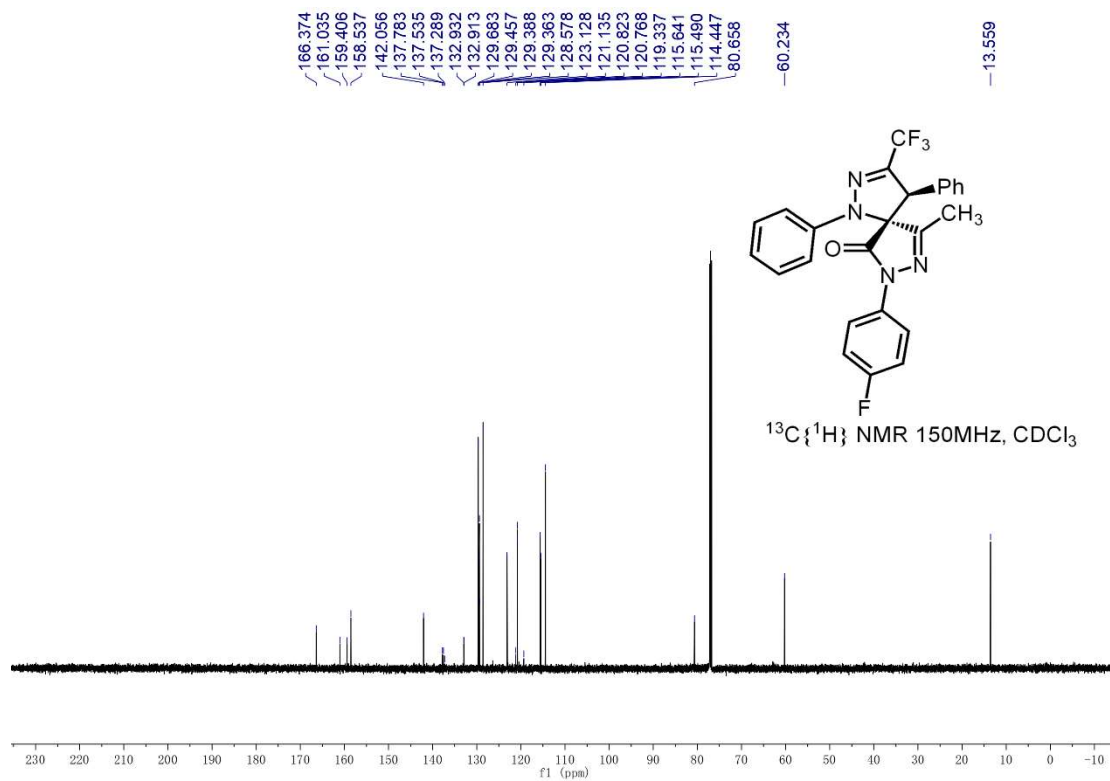


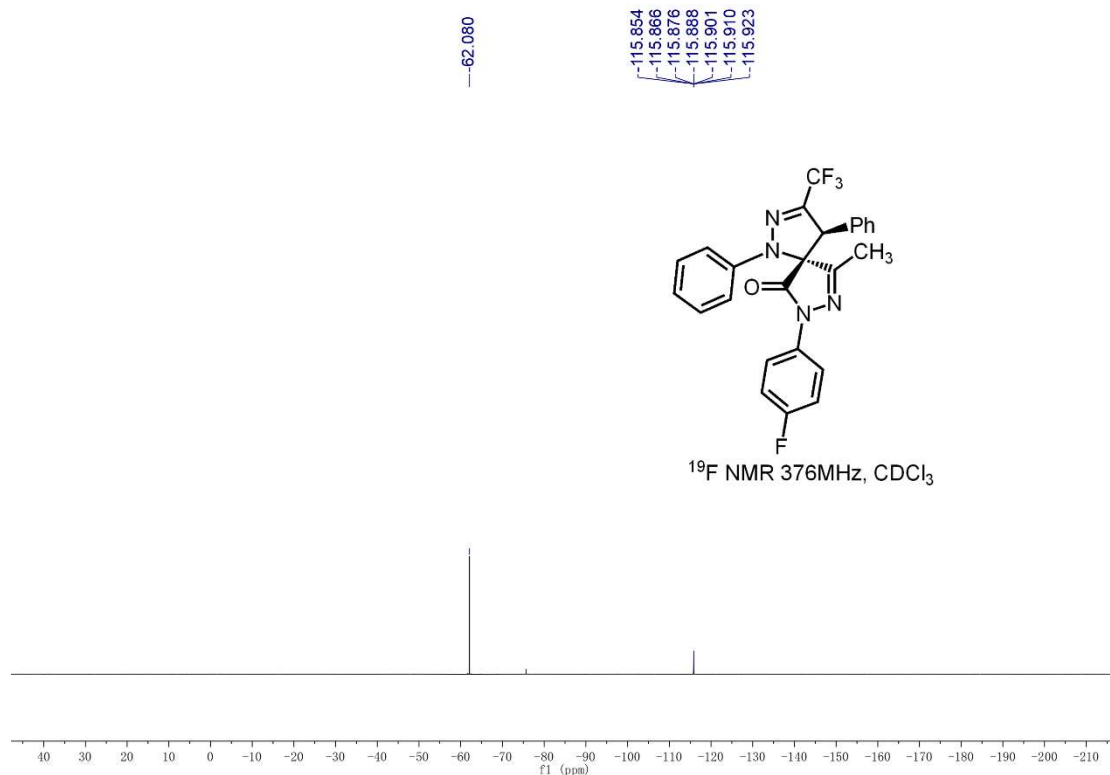
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdB	N-R Conf	e <sub>i</sub> %	mSi gma	Std l	St d Me an z	Std Var Nor m	St d m/ z Dif f	Std Com b Dev
489.1304	1 C <sub>25</sub> H <sub>18</sub> F <sub>4</sub> N <sub>4</sub> NaO	489.1309	1.1	0.8	16.5	ok	even	22.8	33.5	0.5	14.3	0.8	842.7



NMR copies of compound (*cis*)-**6j**:







HRMS (ESI) copy of compound (*cis*)-6j:

### Mass Spectrum SmartFormula Report

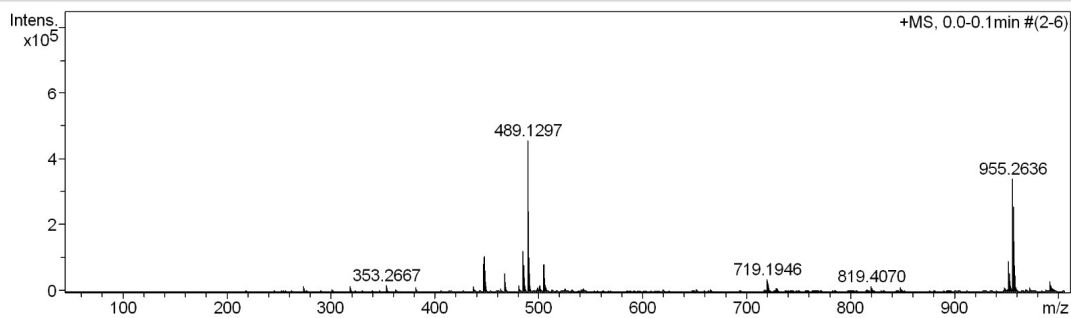
**Analysis Info**

Analysis Name D:\Data\user\NWNNU-fengyang 20230322-18.d  
 Method tune\_low.m  
 Sample Name A-471  
 Comment

Acquisition Date 2023-3-22 10:15:51  
 Operator BDAL@DE  
 Instrument / Ser# micrOTOF-Q 20453

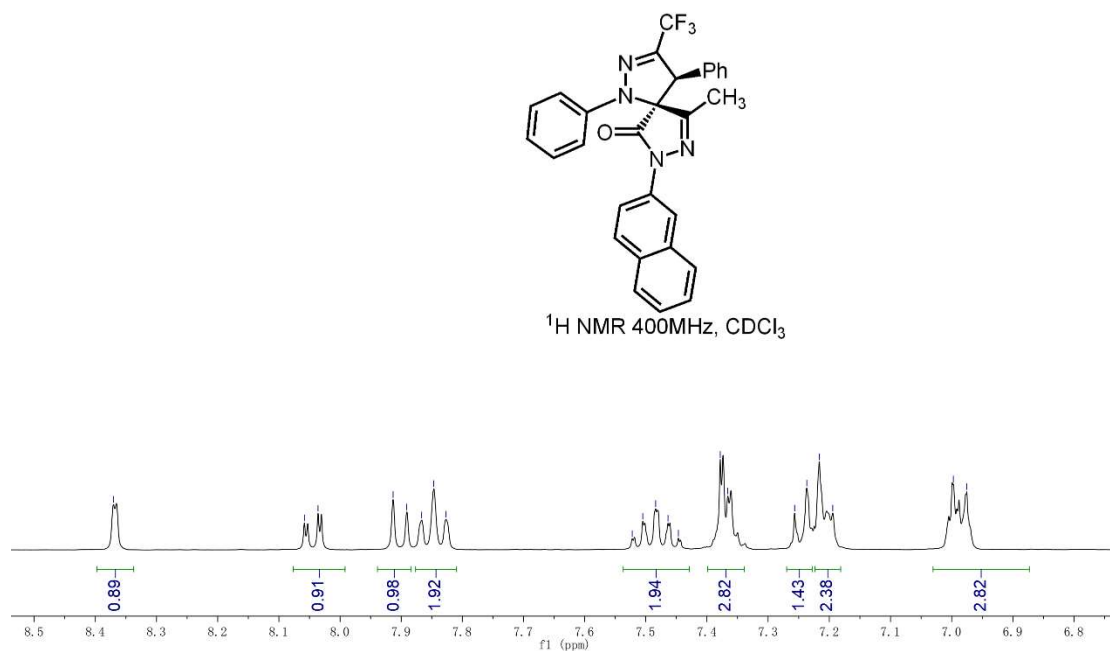
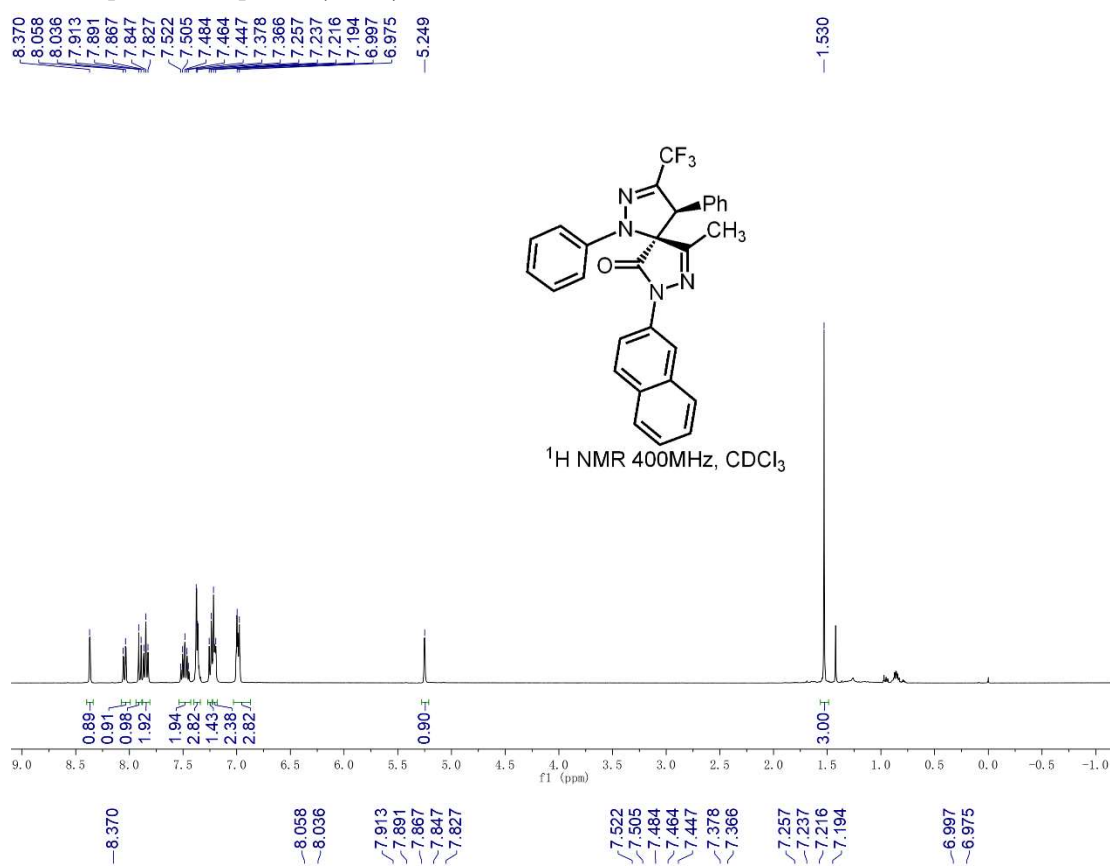
**Acquisition Parameter**

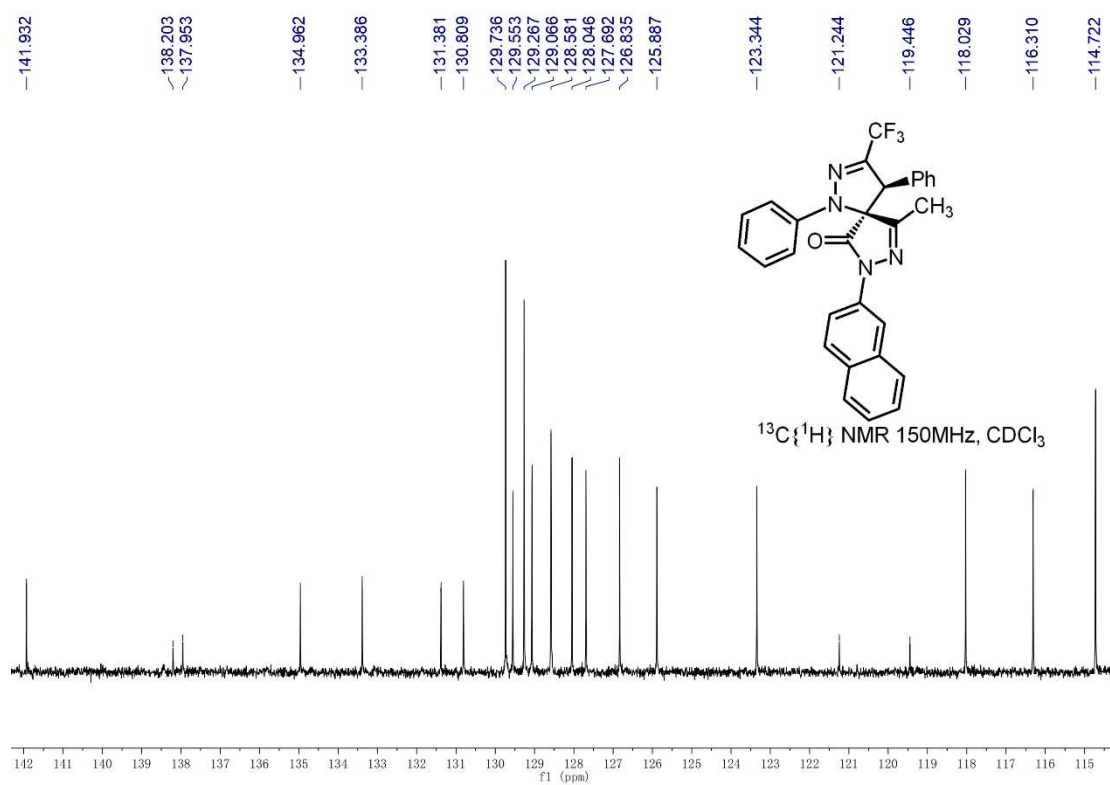
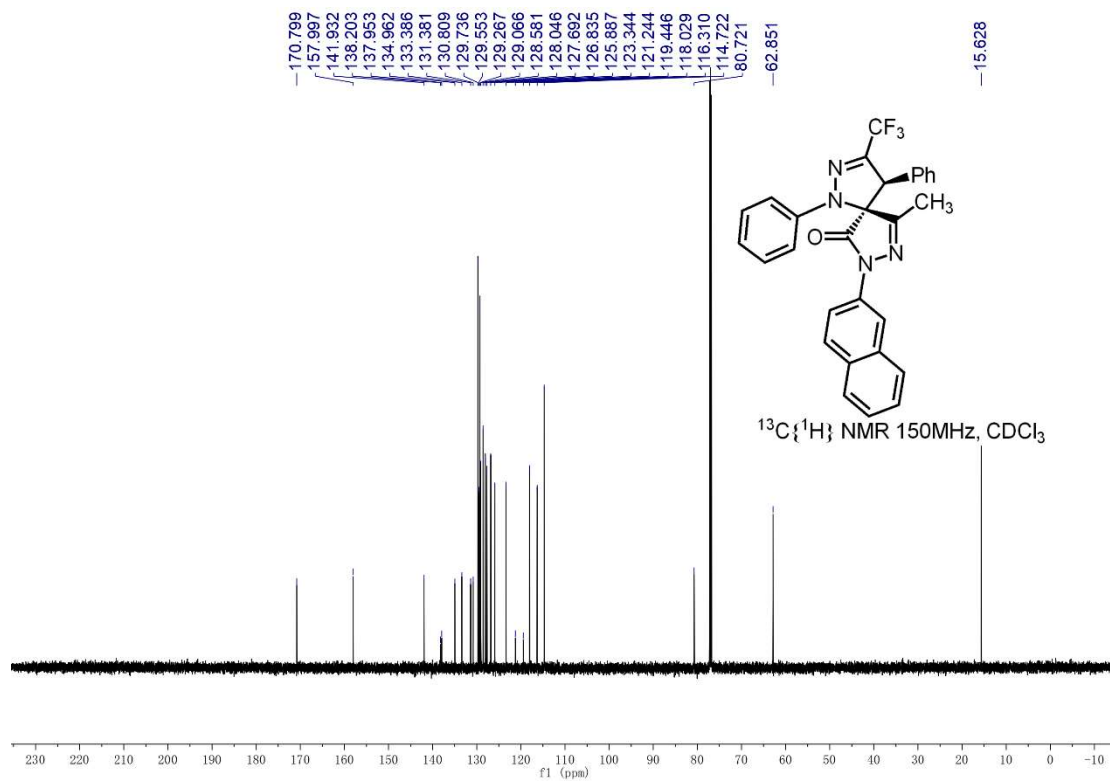
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



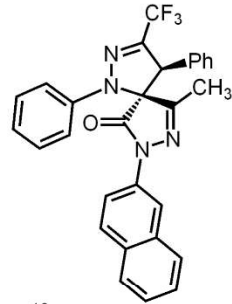
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R ul e	ej¥ Conf	mSi gma	Std l	St d Me an m/ z	Std l Var Nor m Dif f	St d m/ z	Std Com b Dev
489.1297	1 C <sub>25</sub> H <sub>18</sub> F <sub>4</sub> N <sub>4</sub> NaO	489.1309	2.4	1.7	16.5	ok	even	35.8	54.4	1.1	23.1	2.0	842.7

NMR copies of compound (*trans*)-6k:





--61.565



<sup>19</sup>F NMR 376MHz, CDCl<sub>3</sub>

HRMS (ESI) copy of compound (*trans*)-6k:

### Mass Spectrum SmartFormula Report

#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20230322-19.d  
Method tune\_low.m  
Sample Name A-59  
Comment

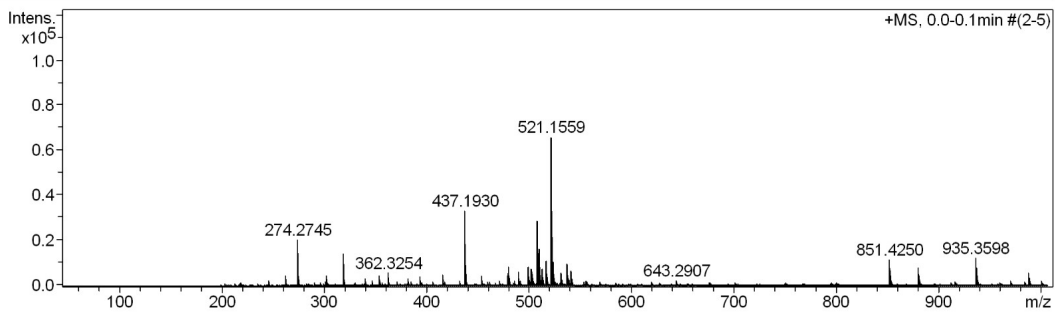
Acquisition Date 2023-3-22 10:19:17

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

#### Acquisition Parameter

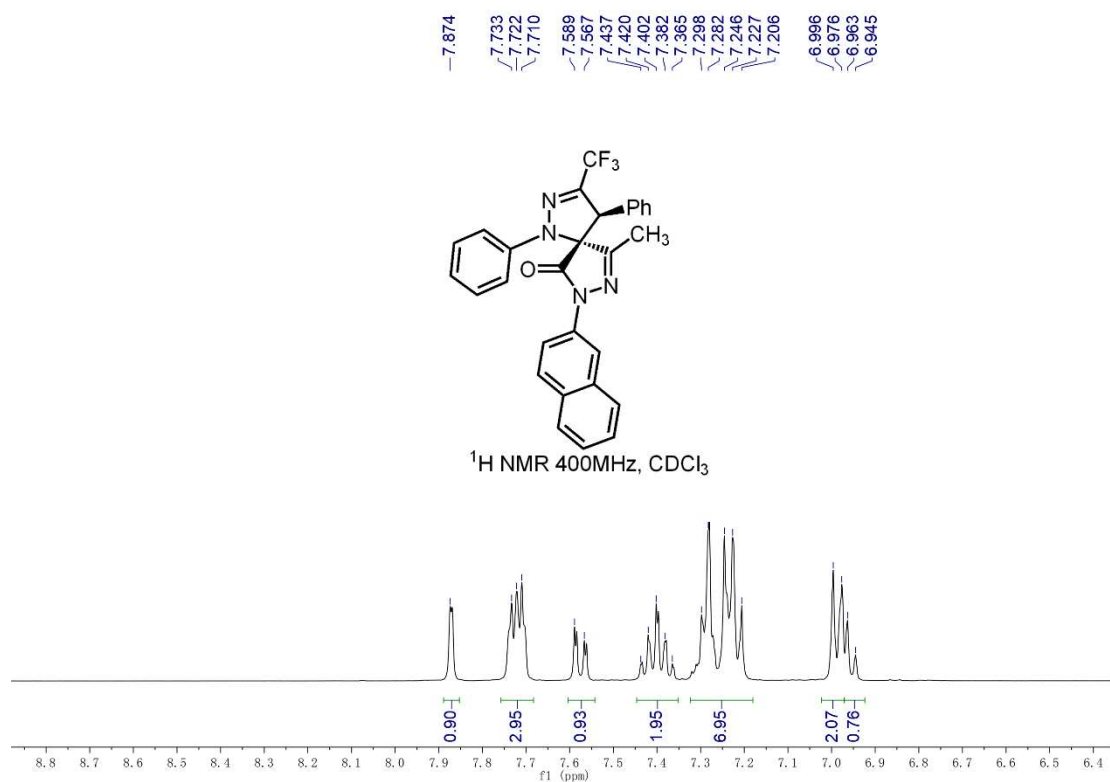
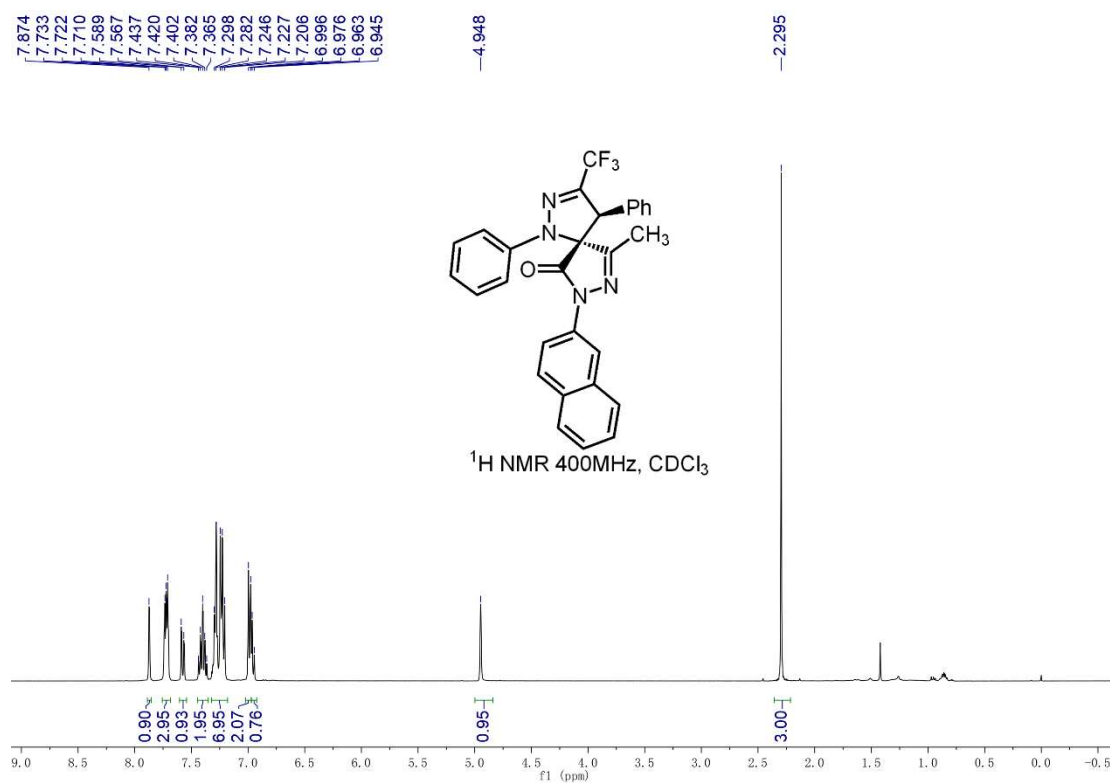
Source Type ESI Ion Polarity Positive  
Focus Active Set Capillary 4500 V  
Scan Begin 50 m/z Set End Plate Offset -500 V  
Scan End 1000 m/z Set Collision Cell RF 400.0 Vpp

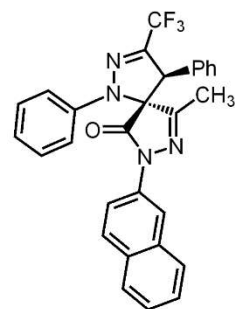
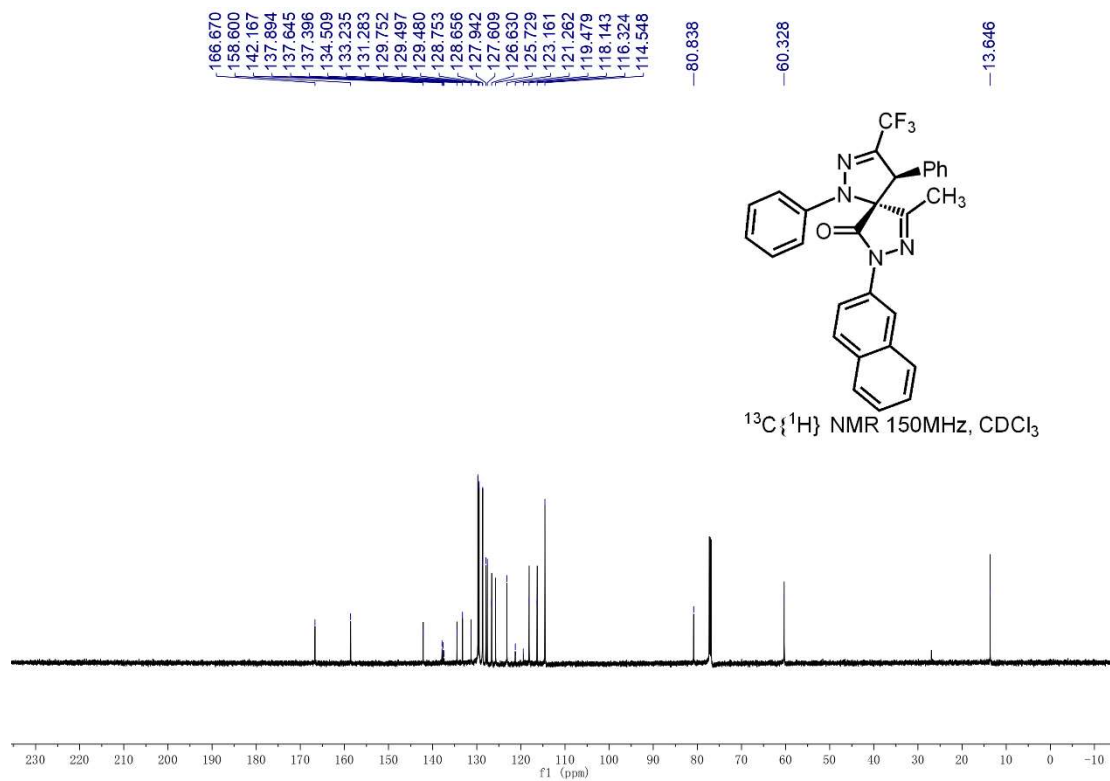
Set Nebulizer 0.4 Bar  
Set Dry Heater 180 j°C  
Set Dry Gas 4.0 l/min  
Set Divert Valve Waste



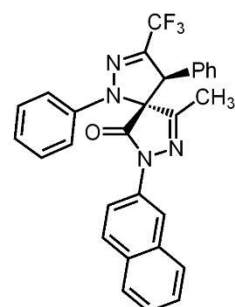
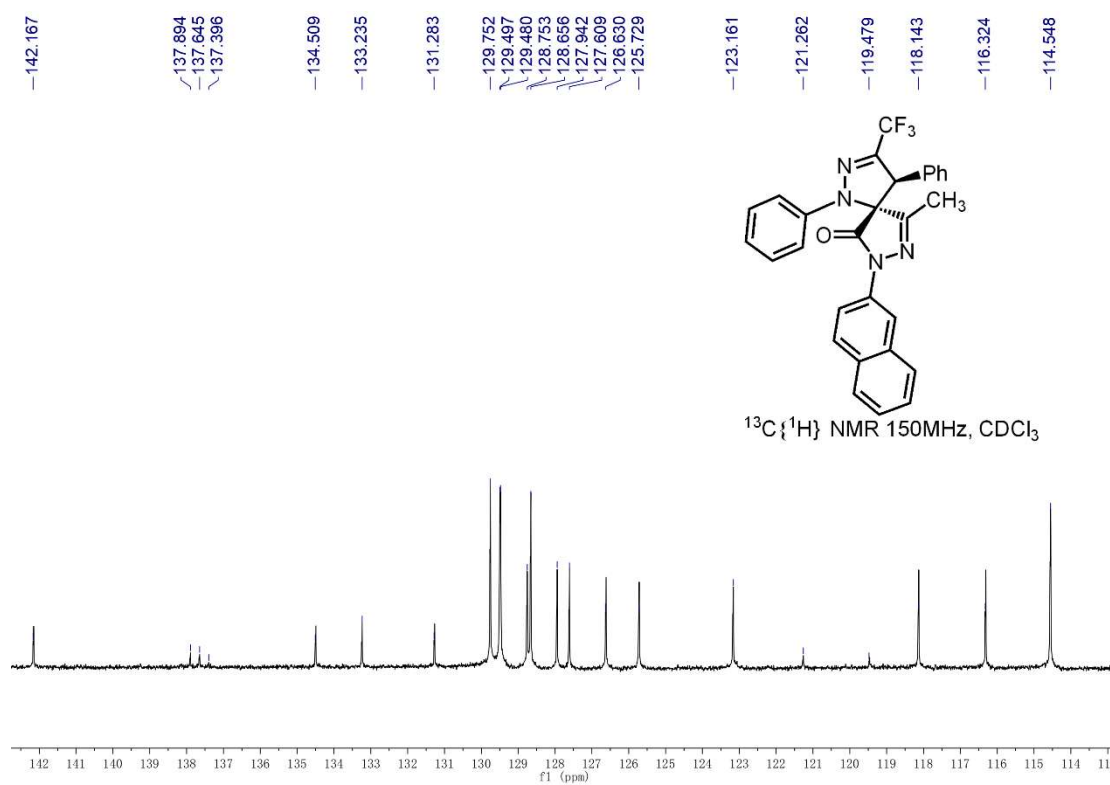
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>j</sub> Conf	mS	Std	Std	Std	Std	Std
m/z								ig ma	l	Me an	l Va	m/ z	Com b Dev
521.1559	1 C <sub>29</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO	521.1560	0.2	0.3	19.5	ok	even	6.0	9.5	0.6	5.0	1.6	842.7

NMR copies of compound (*cis*)-**6k**:





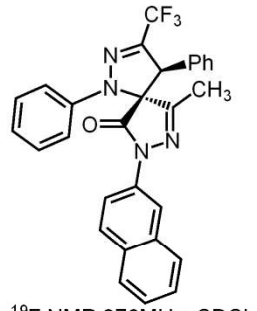
<sup>13</sup>C{<sup>1</sup>H} NMR 150MHz, CDCl<sub>3</sub>



<sup>13</sup>C{<sup>1</sup>H} NMR 150MHz, CDCl<sub>3</sub>



-61.959



HRMS (ESI) copy of compound (*cis*)-**6k**:

### Mass Spectrum SmartFormula Report

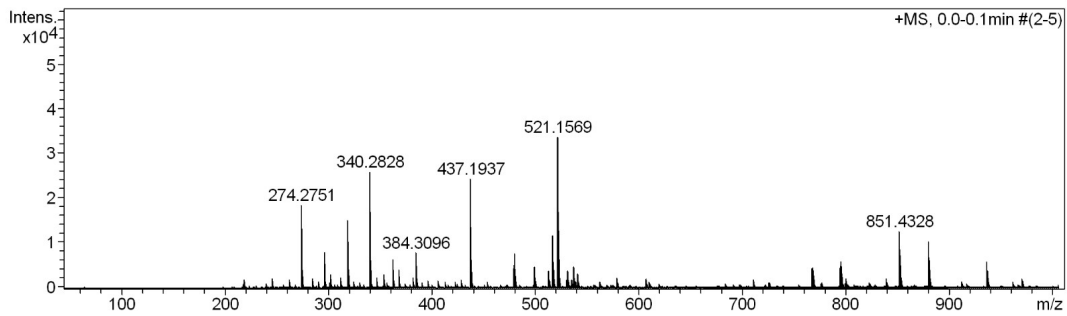
#### Analysis Info

Analysis Name D:\Data\user\NWNW-fengyang 20230322-20.d  
Method tune\_low.m  
Sample Name A-591  
Comment

Acquisition Date 2023-3-22 10:21:29  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

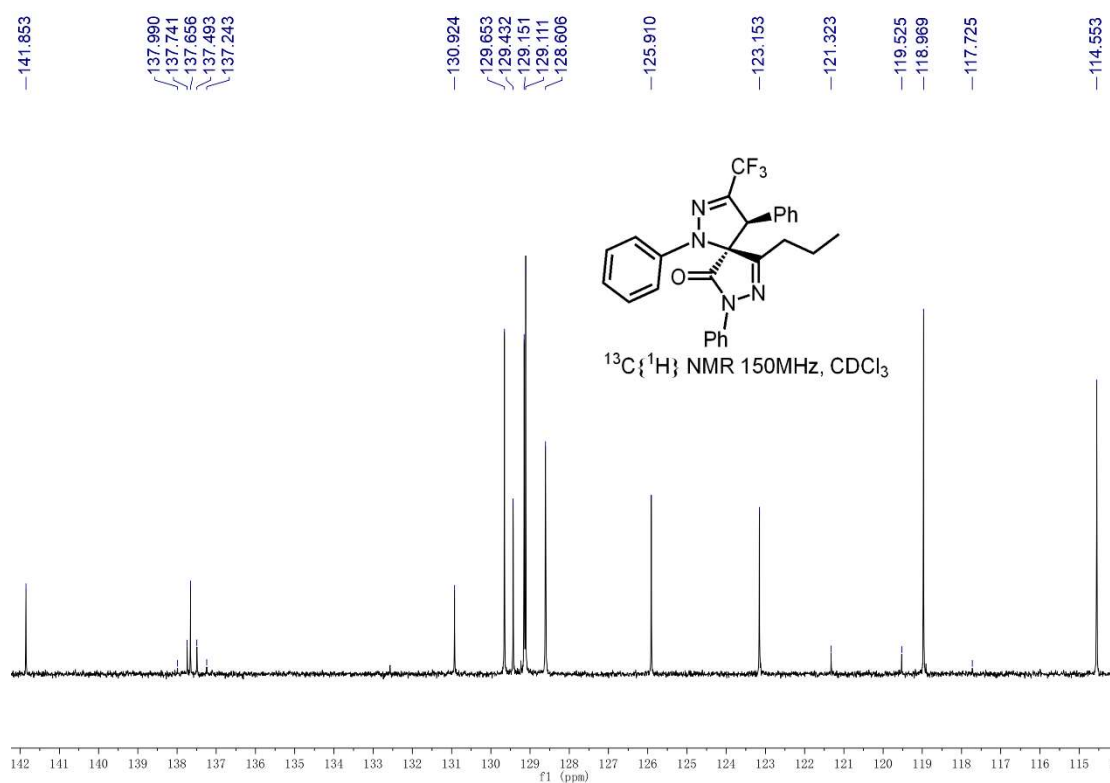
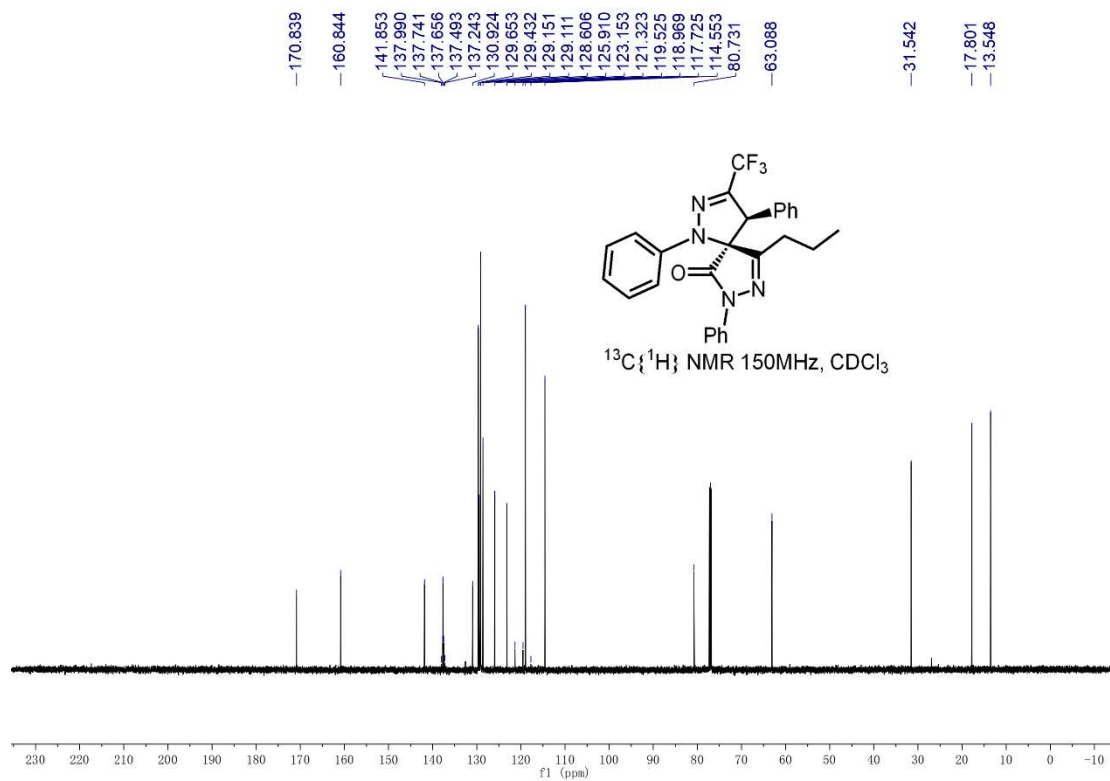
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 $\mu\text{C}$
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

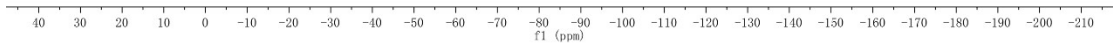
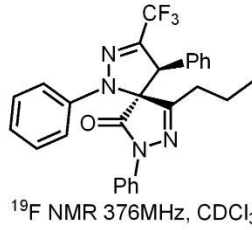


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N-R	e <sub>j</sub> Con	mSi gm a	Std l	St d Me an m/z	Std l Var m	Std l Nor m Dif	Std d Com b Dev
521.1569	1 C <sub>29</sub> H <sub>21</sub> F <sub>3</sub> N <sub>4</sub> NaO	521.1560	-1.9	-1.3	19.5	ok	even	25.0	39.3	0.9	12.5	1.2	842.7





-61.364



HRMS (ESI) copy of compound (*trans*)-**6l**:

### Mass Spectrum SmartFormula Report

#### Analysis Info

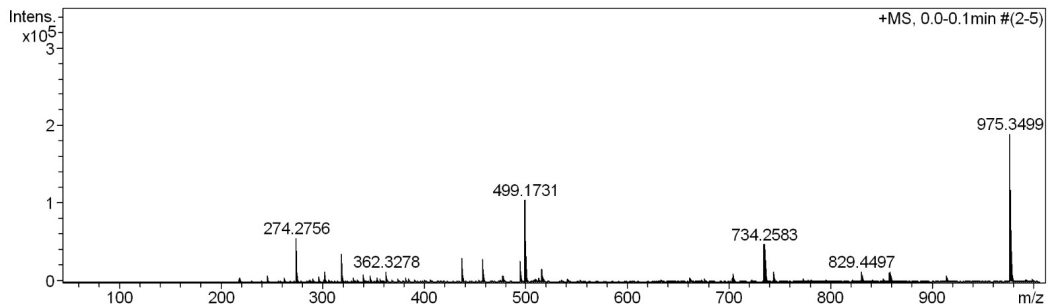
Analysis Name D:\Data\user\NWNW-fengyang 20230322-21.d  
Method tune\_low.m  
Sample Name A-48  
Comment

Acquisition Date 2023-3-22 10:24:09

Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

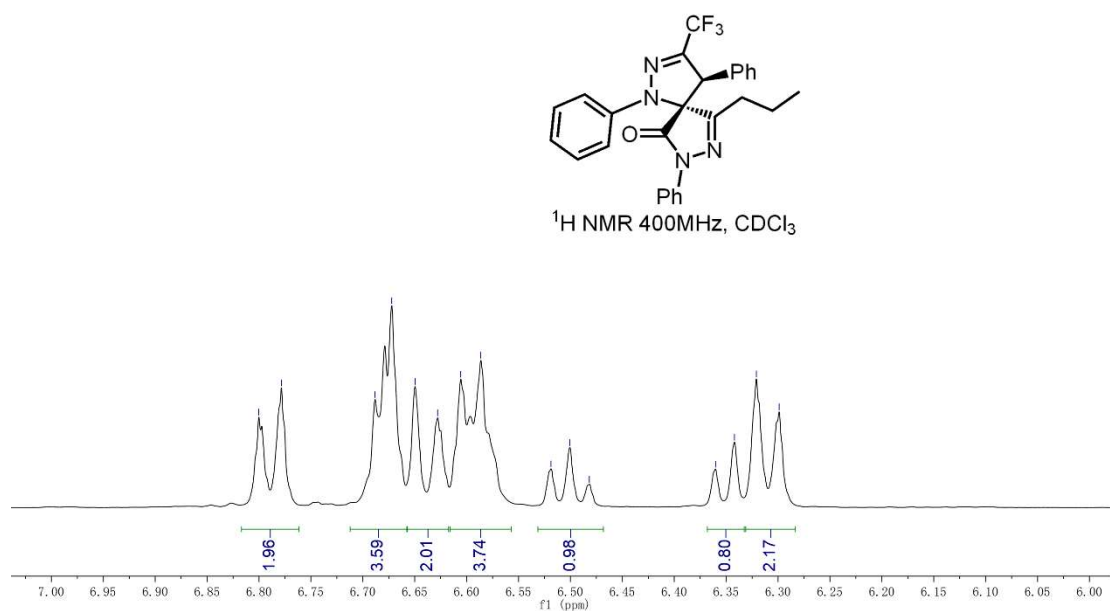
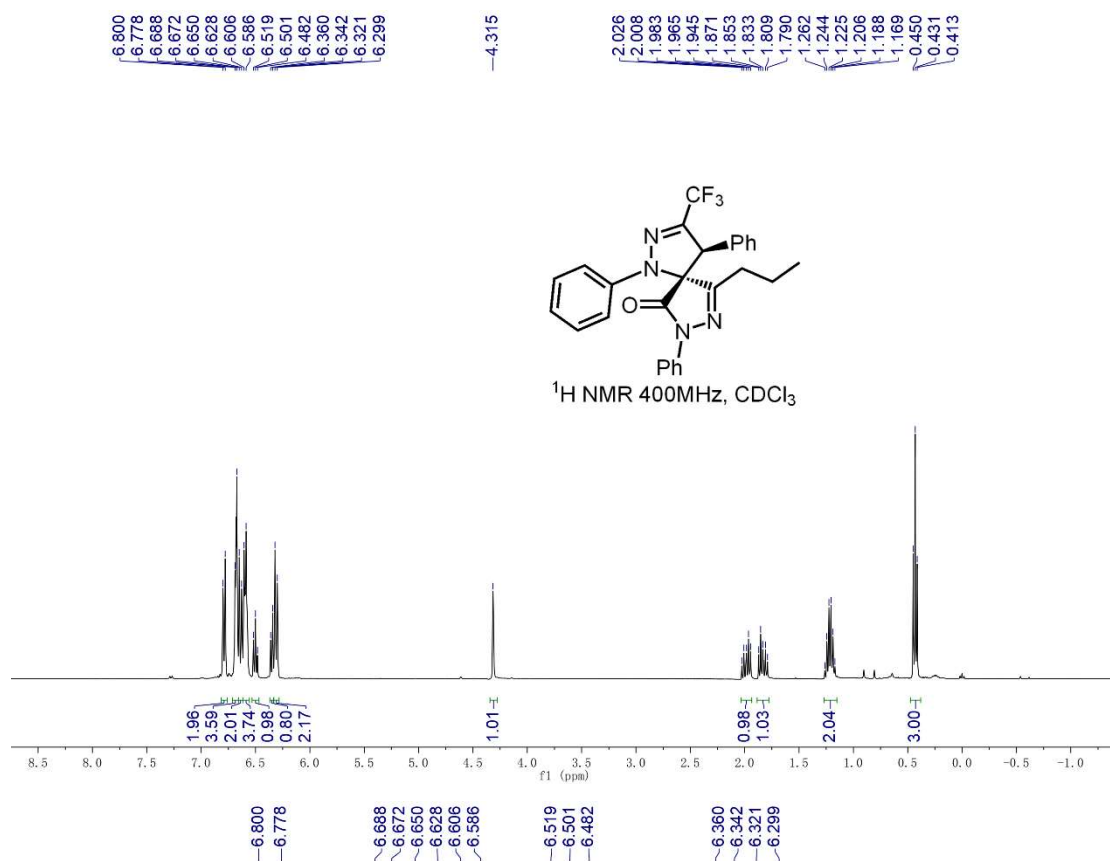
#### Acquisition Parameter

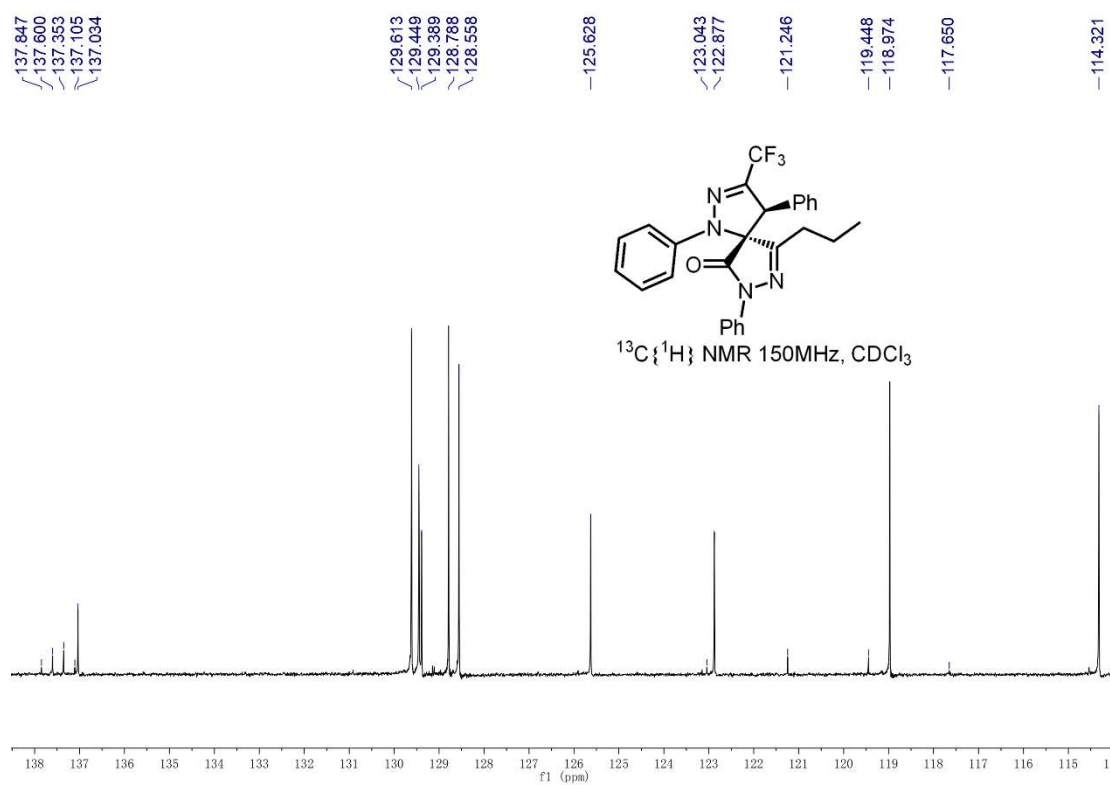
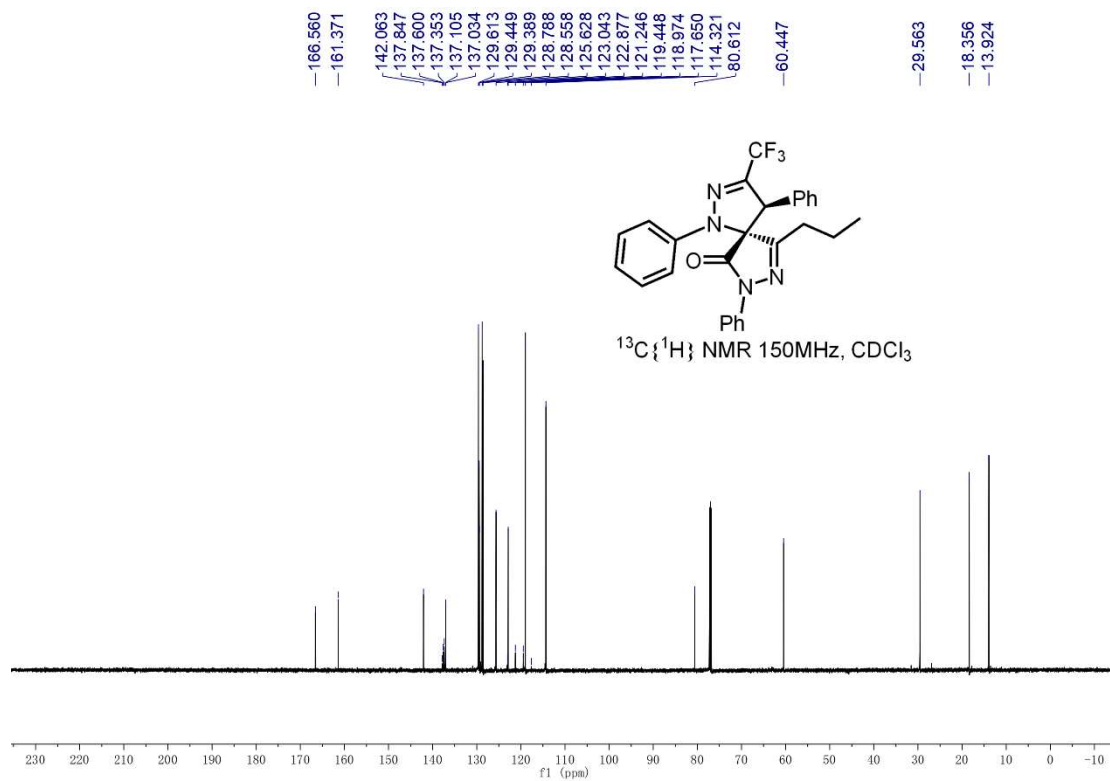
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste



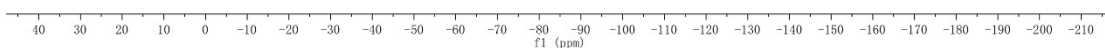
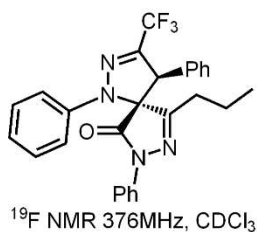
Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R Conf	e; %	mS	Std	Std	Std	Std	Std	Std
m/z														
499.1731	1 C <sub>27</sub> H <sub>23</sub> F <sub>3</sub> N <sub>4</sub> NaO	499.1716	-3.0	-2.6	16.5	ok	even	4.1	7.4	1.4	3.4	1.5	842.7	

NMR copies of compound (*cis*)-**6l**





---61.975



HRMS (ESI) copy of compound (*cis*)-**6l**:

### Mass Spectrum SmartFormula Report

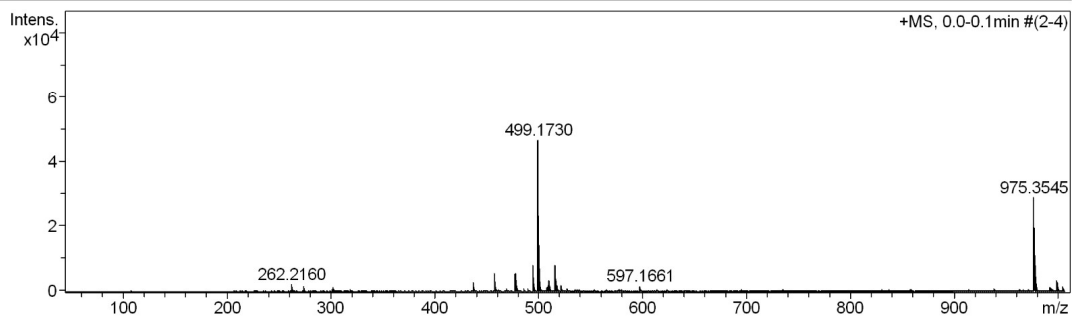
#### Analysis Info

Analysis Name D:\Data\user\NWNNU-fengyang 20230322-22.d  
Method tune\_low.m  
Sample Name A-481  
Comment

Acquisition Date 2023-3-22 10:26:23  
Operator BDAL@DE  
Instrument / Ser# micrOTOF-Q 20453

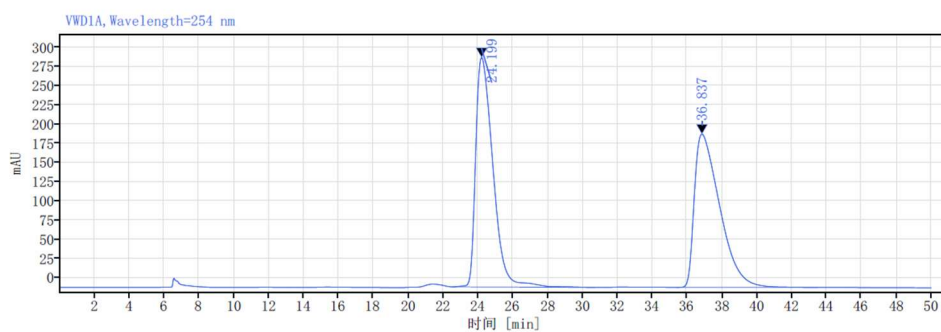
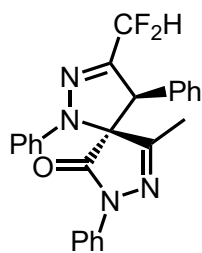
#### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 j°C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Waste

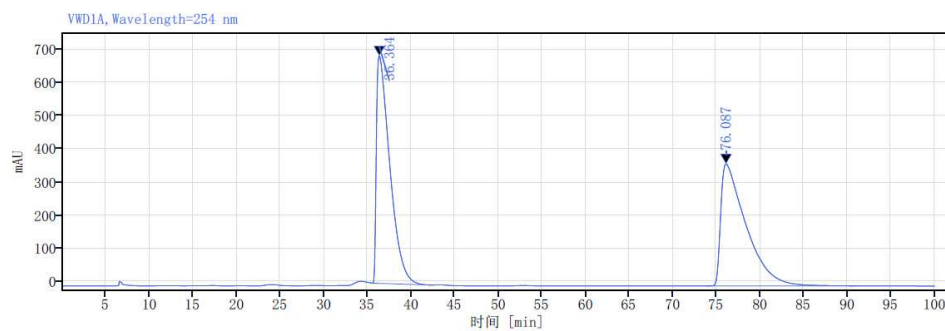
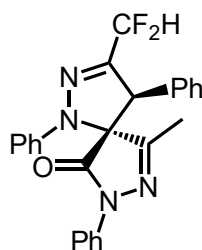


Meas. #	Formula	m/z	err [ppm]	Me an err [ppm]	rdb	N- R	e; % Conf	m Sig ma	Std l	St d Me an m/ z	St d Va rN or m	St d m/ Dif f	Std Com b Dev
499.1730	1 C 27 H 23 F 3 N 4 Na O	499.1716	-2.7	-1.5	16.5	ok	even	8.8	15.9	2.5	7.6	7.4	842.7

## HPLC chromatogram of compounds 3a, 4c, 4f, 4g:

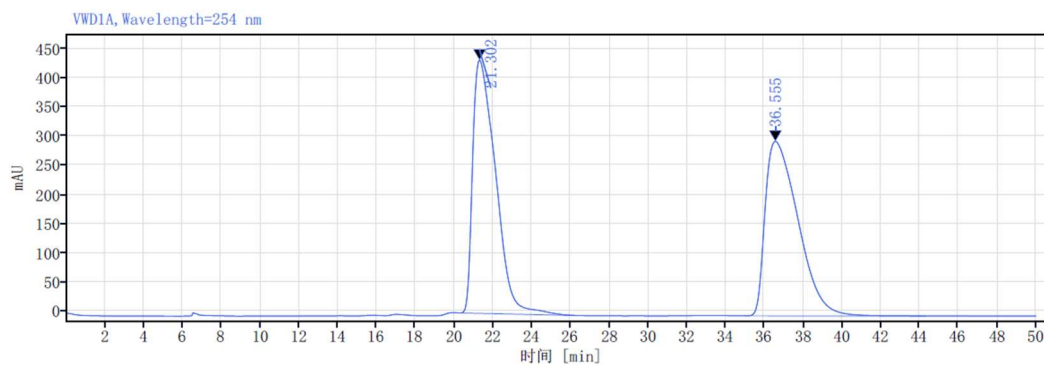
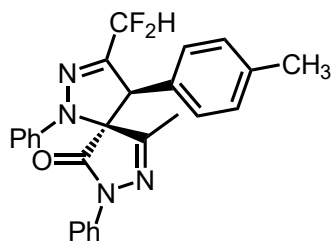


Single VWD1A, Wavelength=254 nm						
RetTime [min]	Type	Width [min]	Area	Height	Area%	Name
24.199	BB	8.15	20542.66	297.82	50.61	
36.837	BB	8.11	20049.18	198.95	49.39	
Total			40591.84			



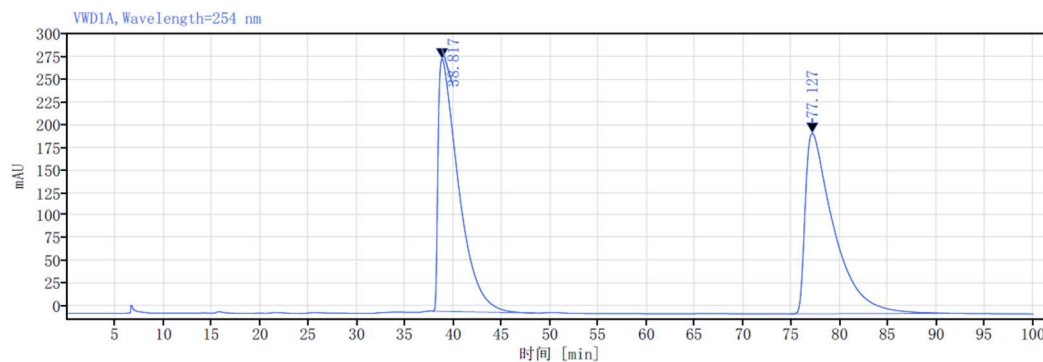
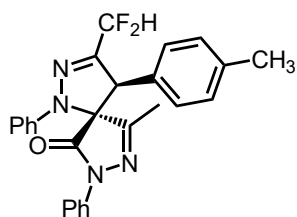
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RetTime [min]	Type	Width [min]	Area	Height	Area%	Name
36.364	BB	6.65	73577.04	688.46	49.79	
76.087	BB	17.27	74186.76	369.55	50.21	
Total			147763.80			





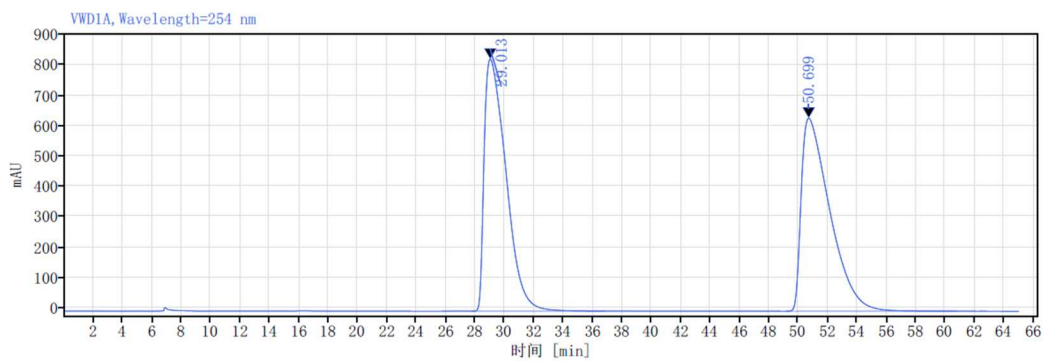
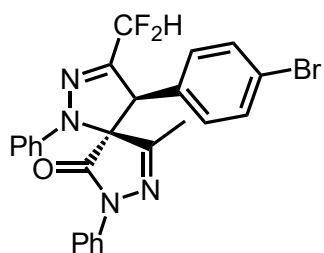
Single: VWD1A, Wavelength=254 nm

RetTime [min]	Type	Width [min]	Area	Height	Area%	Name
21.302	BB	6.18	35504.28	432.90	50.25	
36.555	BB	9.36	35145.20	298.38	49.75	
Total			70649.48			



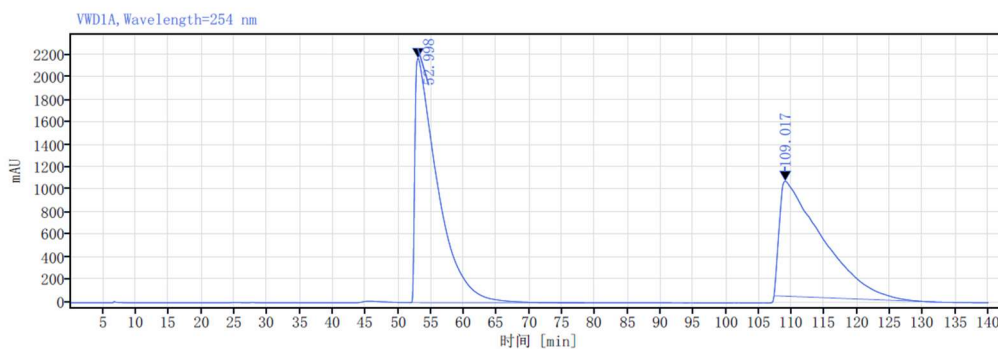
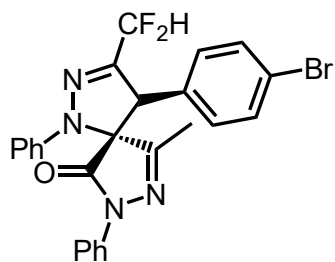
Single: VWD1A, Wavelength=254 nm

RetTime [min]	Type	Width [min]	Area	Height	Area%	Name
38.817	BB	10.44	40717.95	278.39	49.85	
77.127	BB	16.73	40956.83	199.06	50.15	
Total			81674.78			



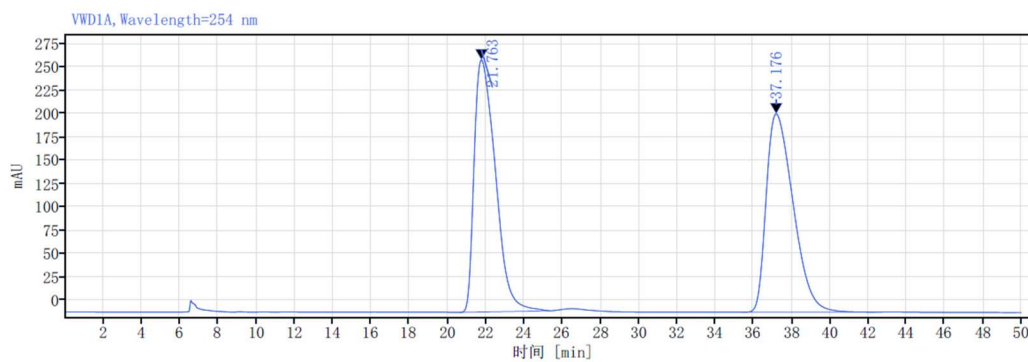
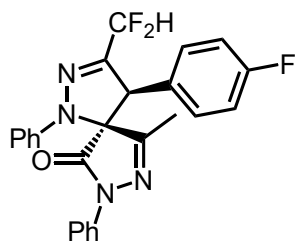
Single: VWD1A, Wavelength=254 nm

RetTime [min]	Type	Width [min]	Area	Height	Area%	Name
29.013	BB	9.06	85502.12	830.42	49.93	
50.699	BB	11.68	85739.51	636.02	50.07	
Total			171241.63			



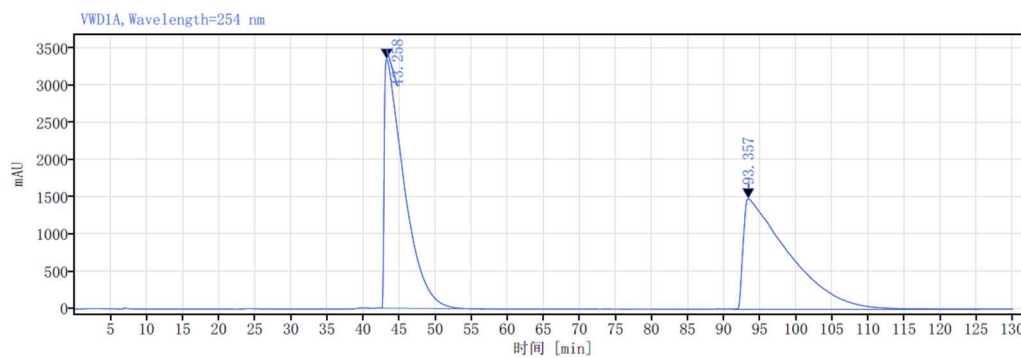
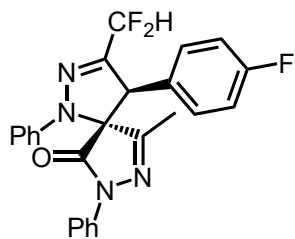
Single: VWD1A, Wavelength=254 nm

RetTime [min]	Type	Width [min]	Area	Height	Area%	Name
52.998	BB	26.61	520039.08	2168.05	52.60	
109.017	BBA	24.77	468587.69	1019.58	47.40	
Total			988626.77			



Single: VWD1A, Wavelength=254 nm

RetTime [min]	Type	Width [min]	Area	Height	Area%	Name
21.763	BB	4.76	20835.25	270.09	50.03	
37.176	BB	6.97	20812.05	212.49	49.97	
Total			41647.30			



Single: VWD1A, Wavelength=254 nm

RetTime [min]	Type	Width [min]	Area	Height	Area%	Name
43.258	BB	14.29	634003.70	3350.71	49.52	
93.357	BB	34.23	646412.38	1483.98	50.48	
Total			1280416.08			

## Crystallography data of compound (*cis*)-3a, (*cis*)-3j, (*trans*)-3j and (*cis*)-6a

### X-Ray Crystallographic Data of Compound (*cis*)-3a

Thermal ellipsoids are set at a 50% probability level. Crystal data have been deposited to CCDC, number 2178596.

#### Crystallization Details

The obtained compound (*cis*)-3a (35 mg) was dissolved in THF (0.2 mL) in a NMR tube at room temperature. Then petroleum ether (2 mL) was added to the solution slowly along the tube wall, resulting in a two-phase mixture. The colorless crystal of (*cis*)-3a was formed after the two-phase mixture has diffused.

#### Experimental

A suitable crystal was selected and placed on a ROD, Synergy Custom system, HyPix diffractometer. The crystal was kept at 301.78(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

#### Crystal structure determination

Crystal Data for C<sub>25</sub>H<sub>20</sub>F<sub>2</sub>N<sub>4</sub>O (*M* = 430.45 g/mol): monoclinic, space group P2<sub>1</sub>/c (no. 14), *a* = 8.9 855(2) Å, *b* = 19.7009(3) Å, *c* = 12.8893(2) Å, β = 102.475(2)°, *V* = 2227.82(7) Å<sup>3</sup>, *Z* = 4, *T* = 301.78(10) K, μ(Cu Kα) = 0.764 mm<sup>-1</sup>, *D*<sub>calc</sub> = 1.283 g/cm<sup>3</sup>, 15574 reflections measured (8.336° ≤ 2θ ≤ 155.024°), 4439 unique (*R*<sub>int</sub> = 0.0273, *R*<sub>sigma</sub> = 0.0273) which were used in all calculations. The final *R*<sub>1</sub> was 0.0621 (*I* > 2σ(*I*)) and *wR*<sub>2</sub> was 0.1944 (all data).

#### Refinement model description

Number of restraints - 26, number of constraints - unknown.

Details:

##### 1. Fixed Uiso

At 1.2 times of:

All C(H) groups, All C(H,H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Ternary CH refined with riding coordinates:

C2(H2), C22(H22A), C22(H22)

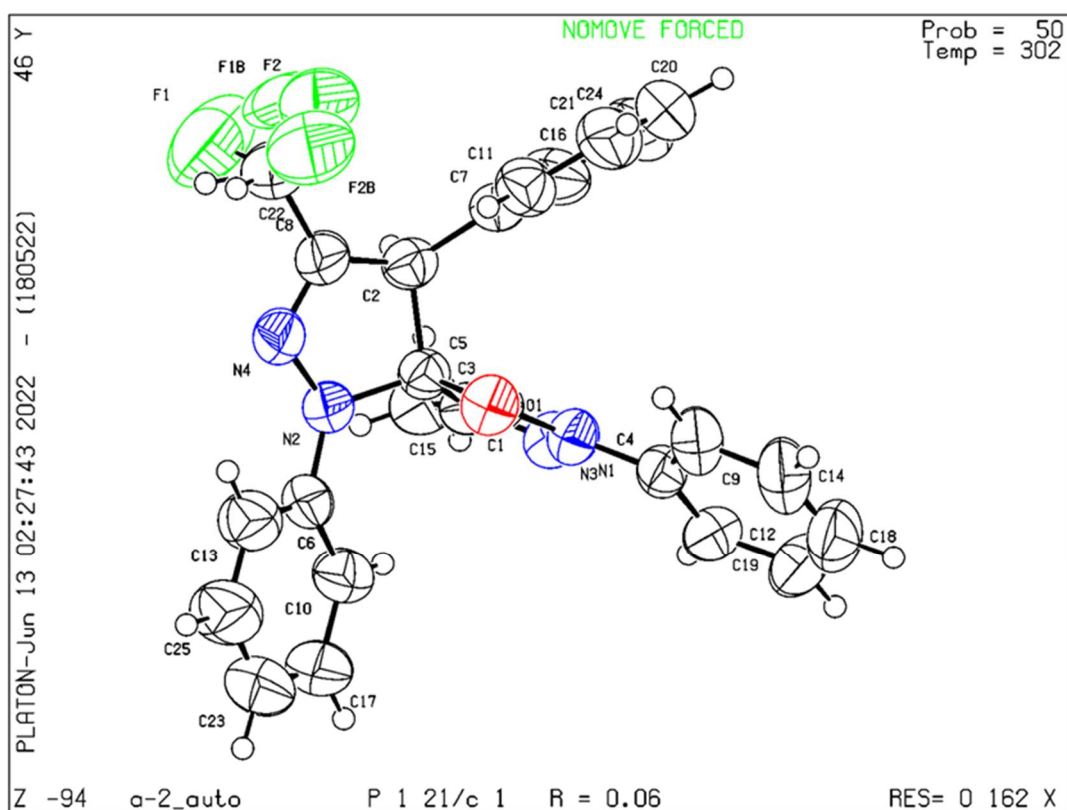
3.b Aromatic/amide H refined with riding coordinates:

C9(H9), C10(H10), C11(H11), C12(H12), C13(H13), C14(H14), C16(H16),  
C17(H17),

C18(H18), C19(H19), C20(H20), C21(H21), C23(H23), C24(H24), C25(H25)

4.c Idealised Me refined as rotating group:

C15(H15A,H15B,H15C)



**Table S1 Crystallographic Data of Compound (*cis*)-3a**

Identification code	A-2_auto
Empirical formula	C <sub>25</sub> H <sub>20</sub> F <sub>2</sub> N <sub>4</sub> O
Formula weight	430.45
Temperature/K	301.78(10)
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /c
a/Å	8.9855(2)
b/Å	19.7009(3)
c/Å	12.8893(2)
α/°	90
β/°	102.475(2)
γ/°	90
Volume/Å <sup>3</sup>	2227.82(7)
Z	4
ρ <sub>calc</sub> /g/cm <sup>3</sup>	1.283
μ/mm <sup>-1</sup>	0.764
F(000)	896.0
Crystal size/mm <sup>3</sup>	0.11 × 0.09 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	8.336 to 155.024
Index ranges	-11 ≤ h ≤ 11, -24 ≤ k ≤ 17, -15 ≤ l ≤ 16
Reflections collected	15574
Independent reflections	4439 [R <sub>int</sub> = 0.0273, R <sub>sigma</sub> = 0.0273]
Data/restraints/parameters	4439/26/308
Goodness-of-fit on F <sup>2</sup>	1.072
Final R indexes [I >= 2σ (I)]	R <sub>1</sub> = 0.0621, wR <sub>2</sub> = 0.1853
Final R indexes [all data]	R <sub>1</sub> = 0.0711, wR <sub>2</sub> = 0.1944
Largest diff. peak/hole / e Å <sup>-3</sup>	0.50/-0.41

**Table S2 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for Compound (*cis*)-3a.  $U_{eq}$  is defined as  $1/3$  of the trace of the orthogonalised UIJ tensor.**

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{eq}$
F1	7962(7)	1574(5)	6948(5)	190(2)
F1B	8383(6)	2140(3)	6932(4)	131.6(15)
F2	9029(6)	2235(3)	6149(7)	155.8(19)
F2B	9038(4)	1985(3)	5367(5)	135.7(15)
O1	5081.9(16)	2686.2(7)	2929.3(11)	65.1(4)
N1	3263.0(18)	3391.6(8)	3385.3(12)	58.5(4)
N2	4177.3(18)	1812.2(8)	4556.9(13)	62.1(4)
N3	2381.1(19)	3401.9(9)	4175.3(13)	64.2(4)
N4	5621(2)	1557.5(9)	4930.9(16)	70.9(5)
C1	4288(2)	2870.9(9)	3525.7(14)	53.4(4)
C2	5677(2)	2692.5(10)	5474.5(15)	60.3(5)
C3	2853(2)	2922.9(10)	4836.7(15)	60.0(5)
C4	2916(2)	3861.6(9)	2534.4(14)	60.6(5)
C5	4201(2)	2558.6(9)	4597.6(14)	54.8(4)
C6	3208(2)	1440.5(10)	3745.8(16)	63.2(5)
C7	6455(2)	3358.9(10)	5369.2(15)	61.0(5)
C8	6474(2)	2026.4(11)	5415.7(18)	69.7(5)
C9	4020(3)	4026.7(11)	1980.0(18)	76.6(6)
C10	1682(3)	1605.2(12)	3449(2)	77.8(6)
C11	7482(3)	3443.0(12)	4720.9(18)	74.3(6)
C12	1494(3)	4157.5(12)	2284(2)	79.9(6)
C13	3760(3)	896.3(13)	3264(2)	84.1(7)
C14	3663(4)	4488.4(12)	1147(2)	92.1(8)
C15	2173(3)	2790.3(15)	5768(2)	83.8(7)

**Table S3 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for Compound (*cis*)-3a.**

The Anisotropic displacement factor exponent takes the form: -  
 $2\pi^2[h^2a^2U_{11}+2hka^*b^*U_{12}+\dots]$ .

Atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>23</sub>	U <sub>13</sub>
F1	141(3)	231(4)	182(4)	95(4)	4(3)
F1B	104(2)	149(3)	112(3)	-10(2)	-45(2)
F2	104(3)	146(3)	193(4)	30(3)	-22(3)
F2B	66.0(18)	165(3)	174(3)	5(3)	20(2)
O1	71.3(8)	68.1(8)	59.7(7)	-2.2(6)	22.5(7)
N1	63.7(9)	57.8(8)	55.1(8)	1.5(6)	15.8(7)
N2	55.3(8)	57.1(9)	70.1(9)	6.5(7)	5.2(7)
N3	61.7(9)	70.0(10)	62.5(9)	-3.6(8)	16.7(7)
N4	59.6(9)	61.3(9)	87.8(12)	12.2(8)	7.0(8)
C1	53.9(9)	54.8(9)	50.9(9)	-2.8(7)	10.1(7)
C2	56.0(10)	69.7(11)	54.1(10)	3.2(8)	9.7(8)
C3	55.0(10)	69.5(11)	56.7(10)	-2.4(8)	14.7(8)
C4	76.4(12)	48.2(9)	53.0(9)	-5.4(7)	4.6(8)
C5	51.5(9)	57.3(10)	55.5(10)	1.7(7)	11.5(7)
C6	65.1(11)	57.4(10)	65.9(11)	6.0(8)	11.4(9)
C8	57.4(10)	67.4(12)	80.1(13)	11.0(10)	5.9(9)
C9	103.1(17)	56.8(11)	73.3(13)	4.9(9)	26.8(12)
C10	62.9(12)	74.6(13)	91.9(15)	-2.4(11)	8.0(11)
C11	75.7(13)	75.1(13)	72.9(13)	0.2(10)	17.7(10)
C12	77.6(13)	74.2(13)	77.2(14)	1.1(11)	-6.8(11)
C13	82.7(15)	80.0(14)	86.1(15)	-10.0(12)	10.6(12)
C14	144(3)	60.2(13)	75.9(14)	6.6(11)	31.7(15)
C15	71.0(13)	113.1(19)	73.2(14)	8.1(13)	28.8(11)
C16	77.1(14)	89.1(16)	90.1(16)	-29.3(13)	10.0(12)
C17	70.9(14)	94.6(18)	104.4(19)	3.3(15)	-0.8(13)
C18	162(3)	71.5(15)	73.9(16)	12.0(12)	0.5(18)
C19	111(2)	87.8(18)	93.9(19)	10.9(15)	-18.2(17)
C20	113(2)	69.9(16)	127(3)	7.9(16)	-20(2)
C21	94.8(18)	101(2)	90.6(17)	18.3(15)	10.2(14)
C22	65.2(14)	96.5(19)	131(3)	19.4(18)	-7.9(15)
C23	111(2)	90.9(18)	98.1(19)	-16.7(15)	-1.9(16)
C24	104(2)	72.0(16)	140(3)	-34.2(17)	-1(2)
C25	114(2)	91.7(19)	108(2)	-29.9(16)	1.7(18)



**Table S4 Bond Lengths for Compound (*cis*)-3a.**

<b>Atom</b>	<b>Atom</b>	<b>Length/Å</b>	<b>Atom</b>	<b>Atom</b>
F1	C22	1.327(6)	C4	C9
F1B	C22	1.321(6)	C4	C12
F2	C22	1.187(5)	C6	C10
F2B	C22	1.380(6)	C6	C13
O1	C1	1.212(2)	C7	C11
N1	N3	1.419(2)	C7	C16
N1	C1	1.364(2)	C8	C22
N1	C4	1.418(2)	C9	C14
N2	N4	1.377(2)	C10	C17
N2	C5	1.471(2)	C11	C21
N2	C6	1.412(3)	C12	C19
N3	C3	1.281(3)	C13	C25
N4	C8	1.274(3)	C14	C18
C1	C5	1.530(2)	C16	C24
C2	C5	1.568(3)	C17	C23
C2	C7	1.507(3)	C18	C19
C2	C8	1.505(3)	C20	C21
C3	C5	1.496(3)	C20	C24
C3	C15	1.483(3)	C23	C25

**Table S5 Bond Angles for Compound (*cis*)-3a.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom
C1	N1	N3	112.41(14)	C13	C6	N2
C1	N1	C4	128.54(16)	C11	C7	C2
C4	N1	N3	118.82(15)	C16	C7	C2
N4	N2	C5	110.26(14)	C16	C7	C11
N4	N2	C6	117.00(17)	N4	C8	C2
C6	N2	C5	123.13(15)	N4	C8	C22
C3	N3	N1	108.12(15)	C22	C8	C2
C8	N4	N2	109.19(17)	C4	C9	C14
O1	C1	N1	127.93(17)	C6	C10	C17
O1	C1	C5	127.14(16)	C7	C11	C21
N1	C1	C5	104.93(14)	C4	C12	C19
C7	C2	C5	114.72(16)	C25	C13	C6
C8	C2	C5	98.89(16)	C18	C14	C9
C8	C2	C7	121.32(17)	C24	C16	C7
N3	C3	C5	112.50(16)	C23	C17	C10
N3	C3	C15	122.23(19)	C14	C18	C19
C15	C3	C5	125.15(19)	C18	C19	C12
C9	C4	N1	119.45(19)	C24	C20	C21
C12	C4	N1	119.7(2)	C20	C21	C11
C12	C4	C9	120.8(2)	F1	C22	C8
N2	C5	C1	111.90(15)	F1B	C22	F2B
N2	C5	C2	101.39(14)	F1B	C22	C8
N2	C5	C3	118.72(15)	F2	C22	F1
C1	C5	C2	112.54(14)	F2	C22	C8
C3	C5	C1	101.22(15)	F2B	C22	C8
C3	C5	C2	111.53(15)	C25	C23	C17
C10	C6	N2	120.0(2)	C20	C24	C16
C10	C6	C13	119.2(2)	C23	C25	C13

**Table S6 Torsion Angles for Compound (*cis*)-3a.**

<b>A</b>	<b>B</b>	<b>C</b>	<b>D</b>	<b>Angle/°</b>	<b>A</b>	<b>B</b>	<b>C</b>	<b>D</b>	<b>Angle/°</b>
O1	C1	C5	N2	-42.9(2)	C4	C9	C14	C18	2.1(4)
O1	C1	C5	C2	70.5(2)	C4	C12	C19	C18	0.9(4)
O1	C1	C5	C3	-170.32(18)	C5	N2	N4	C8	14.4(2)
N1	N3	C3	C5	3.8(2)	C5	N2	C6	C10	-47.2(3)
C5	N2	C6	C10	-47.2(3)	C5	N2	C6	C13	134.8(2)
N1	C1	C5	N2	136.14(15)	C5	C2	C7	C11	-84.6(2)
N1	C1	C5	C2	-110.46(17)	C5	C2	C7	C16	92.7(2)
N1	C1	C5	C3	8.71(18)	C5	C2	C8	N4	-15.9(2)
N1	C4	C9	C14	179.99(19)	C5	C2	C8	C22	175.4(2)
N1	C4	C12	C19	178.6(2)	C6	N2	N4	C8	161.71(18)
N2	N4	C8	C2	2.1(3)	C6	N2	C5	C1	-48.0(2)
N2	N4	C8	C22	172.1(2)	C6	N2	C5	C2	-168.14(17)
N2	C6	C10	C17	-176.9(2)	C6	N2	C5	C3	69.4(2)
N2	C6	C13	C25	175.9(2)	C6	C10	C17	C23	0.8(4)
N3	N1	C1	O1	171.60(18)	C6	C13	C25	C23	1.3(5)
N3	N1	C1	C5	-7.43(19)	C7	C2	C5	N2	152.25(16)
N3	N1	C4	C9	157.70(18)	C7	C2	C5	C1	32.5(2)
N3	N1	C4	C12	-21.0(3)	C7	C2	C5	C3	-80.4(2)
N3	C3	C5	N2	-130.71(18)	C7	C2	C8	N4	-142.1(2)
N3	C3	C5	C1	-7.9(2)	C7	C2	C8	C22	49.2(3)
N3	C3	C5	C2	112.02(19)	C7	C11	C21	C20	-0.9(4)
N4	N2	C5	C1	96.97(18)	C7	C16	C24	C20	-0.9(5)
N4	N2	C5	C2	-23.19(19)	C8	C2	C5	N2	21.62(17)
N4	N2	C5	C3	-145.69(17)	C8	C2	C5	C1	-98.08(18)
N4	N2	C6	C10	170.01(19)	C8	C2	C5	C3	148.95(16)
N4	N2	C6	C13	-8.0(3)	C8	C2	C7	C11	34.0(3)
N4	C8	C22	F1	-81.8(5)	C8	C2	C7	C16	-148.6(2)
N4	C8	C22	F1B	-138.4(4)	C9	C4	C12	C19	-0.2(3)
N4	C8	C22	F2	154.0(7)	C9	C14	C18	C19	-1.4(4)
N4	C8	C22	F2B	99.2(4)	C10	C6	C13	C25	-2.1(4)
C1	N1	N3	C3	2.6(2)	C10	C17	C23	C25	-1.6(5)
C1	N1	C4	C9	-28.2(3)	C11	C7	C16	C24	1.1(4)
C1	N1	C4	C12	153.1(2)	C12	C4	C9	C14	-1.3(3)
C2	C7	C11	C21	177.2(2)	C13	C6	C10	C17	1.1(4)
C2	C7	C16	C24	-176.4(2)	C14	C18	C19	C12	-0.1(5)
C2	C8	C22	F1	86.7(5)	C15	C3	C5	N2	53.2(3)
C2	C8	C22	F1B	30.1(5)	C15	C3	C5	C1	176.1(2)
C2	C8	C22	F2	-37.5(8)	C15	C3	C5	C2	-64.0(3)
C2	C8	C22	F2B	-92.3(4)	C16	C7	C11	C21	-0.2(3)
C4	N1	N3	C3	177.64(17)	C17	C23	C25	C13	0.6(5)
C4	N1	C1	O1	-2.8(3)	C21	C20	C24	C16	-0.2(5)

C4	N1	C1	C5	178.13(17)	C24	C20	C21	C11	1.1(5)
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**Table S7 Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for Compound (*cis*)-3a.**

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H2	5367.68	2701.73	6158.55	72
H9	4984.71	3832.63	2160.46	92
H10	1300.09	1974.49	3758	93
H11	7751.32	3074.14	4350.43	89
H12	753.77	4043.64	2658.91	96
H13	4791.78	789.26	3439.47	101
H14	4385.71	4593.08	752.42	111
H15A	2844.66	2955.69	6399.56	126
H15B	2024.95	2310.85	5832.79	126
H15C	1208.9	3018.35	5673.21	126
H16	5409.18	3867.44	6358.39	104
H17	-306.83	1333.08	2481.07	112
H18	2056.74	5101.85	356.13	127
H19	233.72	4834.06	1298.09	124
H20	8110.59	5052.02	5079.07	132
H21	8812	4129.14	4192.14	116
H22A	8057.07	1335.01	6126.57	123
H22	8365.4	1454.56	5602.65	123
H23	620.33	403.32	1741.05	124
H24	6419.72	4912.93	6159.38	131
H25	3151.82	143.36	2212.81	130

## X-Ray Crystallographic Data of Compound (*trans*)-**3j**

Thermal ellipsoids are set at a 50% probability level. Crystal data have been deposited to CCDC, number 2253536.

### Crystallization Details

The obtained compound (*trans*)-**3j** (35 mg) was dissolved in THF (0.2 mL) in a NMR tube at room temperature. Then petroleum ether (2 mL) was added to the solution slowly along the tube wall, resulting in a two-phase mixture. The colorless crystal of (*trans*)-**3j** was formed after the two-phase mixture has diffused.

### Experimental

A suitable crystal was selected and placed on a ROD, Synergy Custom system, HyPix diffractometer. The crystal was kept at 301.71(10) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

### Crystal structure determination

Crystal Data for  $C_{50}H_{36}Cl_4F_4N_8O_2$  ( $M=998.67$  g/mol): monoclinic, space group  $I2/a$  (no. 15),  $a = 18.9993(2)$  Å,  $b = 11.37225(15)$  Å,  $c = 43.5762(5)$  Å,  $\beta = 96.9104(11)^\circ$ ,  $V = 9346.9(2)$  Å<sup>3</sup>,  $Z = 8$ ,  $T = 301.71(10)$  K,  $\mu(\text{Cu K}\alpha) = 2.864$  mm<sup>-1</sup>,  $D_{\text{calc}} = 1.419$  g/cm<sup>3</sup>, 30745 reflections measured ( $4.086^\circ \leq 2\theta \leq 154.802^\circ$ ), 9322 unique ( $R_{\text{int}} = 0.0332$ ,  $R_{\text{sigma}} = 0.0372$ ) which were used in all calculations. The final  $R_1$  was 0.0644 ( $I > 2\sigma(I)$ ) and  $wR_2$  was 0.2087 (all data).

### Refinement model description

Number of restraints - 42, number of constraints - unknown.

Details:

#### 1. Fixed Uiso

At 1.2 times of:

All C(H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Ternary CH refined with riding coordinates:

C4(H4), C48(H48), C2(H2), C44(H44)

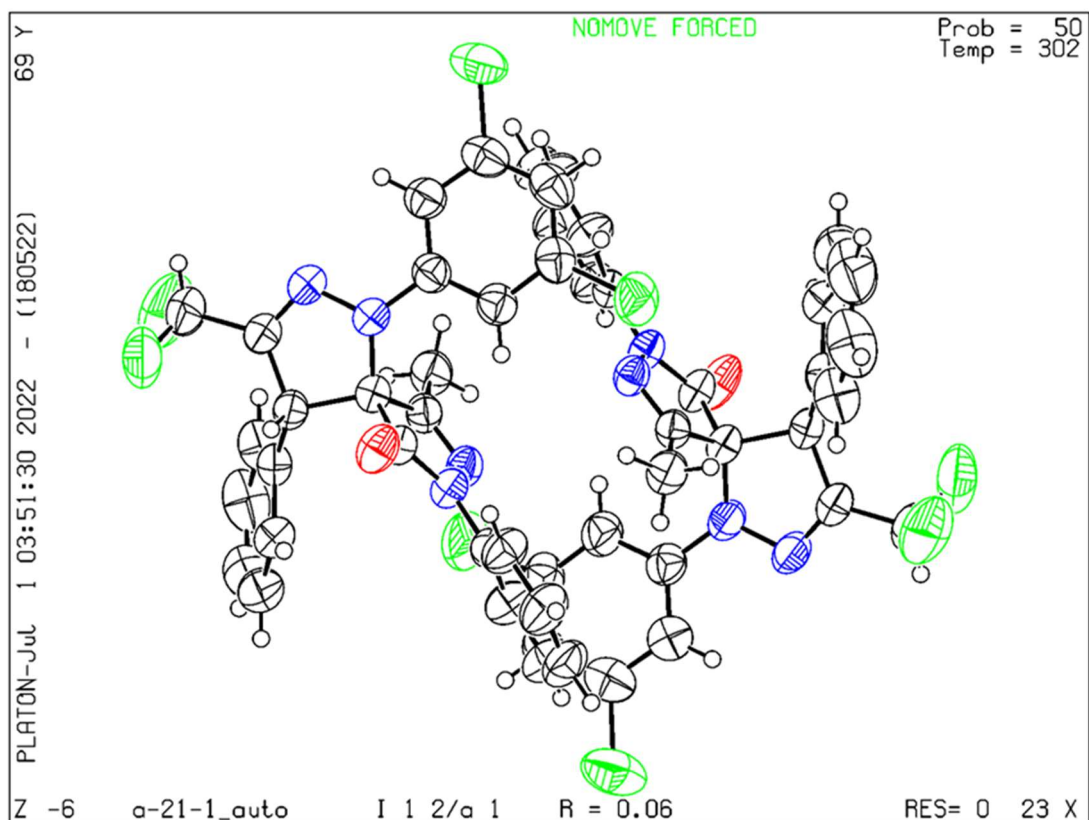
3.b Aromatic/amide H refined with riding coordinates:

C11(H11), C12(H12), C17(H17), C18(H18), C21(H21), C35(H35), C36(H36),  
C37(H37), C41(H41), C42(H42), C43(H43), C45(H45), C46(H46), C15(H15),  
C20(H20),

C23(H23), C25(H25), C29(H29), C30(H30), C33(H33), C38(H38), C39(H39),  
C40(H40), C47(H47), C49(H49), C50(H50)

4.c Idealised Me refined as rotating group:

C27(H27A,H27B,H27C), C28(H28A,H28B,H28C)



**Table S8 Crystal data and structure refinement for Compound (*trans*)-3j.**

Identification code	A-21-1_auto
Empirical formula	C <sub>50</sub> H <sub>36</sub> Cl <sub>4</sub> F <sub>4</sub> N <sub>8</sub> O <sub>2</sub>
Formula weight	998.67
Temperature/K	301.71(10)
Crystal system	monoclinic
Space group	I2/a
a/Å	18.9993(2)
b/Å	11.37225(15)
c/Å	43.5762(5)
$\alpha$ /°	90
$\beta$ /°	96.9104(11)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	9346.9(2)
Z	8
$\rho_{\text{calc}}$ /cm <sup>3</sup>	1.419
$\mu$ /mm <sup>-1</sup>	2.864
F(000)	4096.0
Crystal size/mm <sup>3</sup>	0.09 × 0.07 × 0.05
Radiation	Cu K $\alpha$ ( $\lambda$ = 1.54184)
2 $\Theta$ range for data collection/°	4.086 to 154.802
Index ranges	-23 ≤ h ≤ 23, -12 ≤ k ≤ 14, -54 ≤ l ≤ 39
Reflections collected	30745
Independent reflections	9322 [R <sub>int</sub> = 0.0332, R <sub>sigma</sub> = 0.0372]
Data/restraints/parameters	9322/42/615
Goodness-of-fit on F <sup>2</sup>	1.083
Final R indexes [I ≥ 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0644, wR <sub>2</sub> = 0.1957
Final R indexes [all data]	R <sub>1</sub> = 0.0760, wR <sub>2</sub> = 0.2087
Largest diff. peak/hole / e Å <sup>-3</sup>	0.80/-0.4

**Table S9 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for Compound (*trans*)-3j.  $U_{eq}$  is defined as 1/3 of the trace of the orthogonalised  $U_{ij}$  tensor.**

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{eq}$
C11	5481.6(4)	8115.4(8)	6281.8(2)	91.7(3)
C12	4703.7(5)	11241.2(6)	7096.2(2)	96.9(3)
F1	3393.5(13)	5307(2)	7977.5(4)	107.6(7)
F4	2535.8(15)	6359(3)	7803.5(6)	147.4(10)
O1	5038.9(9)	4619.5(17)	7129.4(4)	67.5(4)
N2	4287.1(9)	4522.5(16)	6671.9(4)	51.4(4)
N4	4137.7(12)	6875.8(17)	7173.9(4)	60.6(5)
N5	3658.1(10)	5080.1(17)	6538.8(4)	54.0(4)
N8	3830.7(12)	7142.9(18)	7434.1(4)	65.0(5)
C3	3917.8(11)	5729.6(18)	7045.0(4)	50.1(4)
C4	3580.5(12)	5158.4(19)	7322.6(4)	51.8(5)
C5	3451.1(11)	5777.9(19)	6739.1(5)	51.6(5)
C7	2949.4(12)	4366(2)	7233.2(5)	55.3(5)
C10	4613.1(11)	3691.8(19)	6491.0(4)	51.0(5)
C11	4192.6(14)	3030(2)	6278.1(6)	69.2(6)
C12	3073.0(16)	3197(2)	7168.3(5)	68.7(6)
C13	4438.1(12)	7784(2)	7016.1(5)	55.0(5)
C17	5061.0(13)	9578(2)	6704.0(6)	69.3(7)
C18	4424.4(13)	8930(2)	7125.6(5)	61.3(5)
C19	5073.7(12)	8434(2)	6606.0(5)	62.5(6)
C21	4765.3(12)	7528(2)	6753.9(5)	60.1(5)
C22	3503.6(14)	6239(2)	7515.7(5)	61.7(6)
C24	4513.1(11)	4907.7(19)	6963.6(4)	50.6(5)
C27	2842.4(14)	6589(2)	6664.1(5)	66.4(6)
C31	4732.3(14)	9802(2)	6966.5(6)	66.3(6)
C35	5643.2(16)	2758(3)	6338.6(7)	84.3(8)
C36	5226.6(17)	2103(3)	6125.5(6)	80.1(8)
C37	5339.3(13)	3556(3)	6524.7(6)	70.5(7)
C41	4499.9(17)	2238(3)	6095.4(6)	80.3(8)
C42	2255.5(14)	4762(3)	7213.4(7)	75.7(7)
C43	2520(2)	2430(3)	7082.2(7)	89.5(9)
C45	1700.8(17)	3955(4)	7124.6(8)	95.2(11)
C46	1849(2)	2807(4)	7059.3(8)	96.9(10)
C48	3211(2)	6286(3)	7820.1(7)	84.9(9)
C13	1806.0(7)	4356.7(11)	6176.2(2)	135.1(5)
C14	2813.7(6)	1205.1(8)	5436.6(3)	121.9(4)
F2	4097.2(14)	7168(2)	4523.6(5)	128.4(9)



F3	4893.7(12)	6017(3)	4712.5(5)	123.6(8)
O2	2405.3(8)	7925.5(19)	5381.6(3)	74.9(5)
N1	3165.2(9)	7904.1(16)	5835.8(3)	49.3(4)
N3	3783.0(9)	7288.3(16)	5960.7(4)	50.1(4)
N6	3227.6(11)	5608.3(18)	5312.5(4)	61.5(5)
N7	3537.8(11)	5335.4(19)	5049.8(4)	63.6(5)
C1	4473.3(12)	8058(2)	5262.3(5)	57.1(5)
C2	3830.7(11)	7292.8(19)	5172.9(4)	50.2(5)
C6	3491.1(11)	6719.8(19)	5449.6(4)	50.0(4)
C8	2875.9(10)	8763.1(18)	6019.6(4)	46.3(4)
C9	3965.6(11)	6605.7(19)	5752.3(4)	49.6(4)
C14	3884.8(12)	6221(2)	4975.3(5)	57.8(5)
C15	3323.7(13)	9408(2)	6229.3(5)	66.6(6)
C16	2953.9(12)	4689(2)	5474.6(5)	59.9(5)
C20	4366(2)	9232(3)	5324.8(6)	81.9(8)
C23	2353.5(15)	2883(3)	5793.0(7)	80.3(8)
C25	3030.4(13)	3527(2)	5385.6(6)	67.9(6)
C26	2924.9(11)	7570(2)	5541.6(4)	51.6(5)
C28	4557.9(14)	5758(2)	5816.5(5)	64.7(6)
C29	1881.6(14)	9796(3)	6171.3(6)	69.8(6)
C30	2583.3(15)	4946(3)	5723.8(6)	72.9(7)
C32	2726.5(15)	2655(3)	5544.5(7)	77.2(7)
C33	2153.0(12)	8953(2)	5989.8(5)	59.9(5)
C34	2286.6(15)	4041(3)	5874.4(6)	78.9(8)
C38	3044.2(16)	10243(3)	6408.1(6)	77.5(7)
C39	2322.5(16)	10443(3)	6379.5(6)	71.9(7)
C40	5154.5(14)	7636(3)	5280.1(7)	81.0(8)
C44	4196.4(16)	6162(3)	4674.7(6)	75.2(7)
C47	4925(3)	9983(4)	5407.1(8)	115.9(14)
C49	5724(2)	8399(5)	5363.0(9)	111.8(13)
C50	5593(3)	9556(5)	5424.0(9)	131.4(19)

**Table S10 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for Compound (*trans*)-  
3j. The Anisotropic displacement factor exponent takes the form: -  
 $2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$ .**

Atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>23</sub>	U <sub>13</sub>	U <sub>12</sub>
C11	82.8(5)	110.3(6)	88.6(5)	-5.5(4)	37.0(4)	-31.0(4)
Cl2	117.0(7)	55.2(4)	116.0(6)	-1.4(4)	3.7(5)	-5.8(4)
F4	124.9(18)	213(3)	114.1(16)	-8.7(16)	52.8(14)	47.7(18)
O1	58.9(9)	90.3(12)	51.3(8)	-5.6(8)	-0.9(7)	12.5(8)
N2	51.3(9)	58.5(10)	44.3(8)	-3.5(7)	5.1(7)	7.0(8)
N4	80.6(13)	53.4(11)	50.4(9)	-6.1(8)	18.1(9)	-5.5(9)
N5	55.5(10)	62.1(11)	43.9(8)	2.4(7)	4.3(7)	6.8(8)
N8	86.3(14)	59.1(11)	51.9(10)	-7.5(8)	17.3(9)	-0.1(10)
C3	54.4(11)	51.5(11)	45.0(10)	-0.7(8)	9.0(8)	0.0(9)
C4	57.1(11)	55.0(12)	44.4(10)	2.4(8)	10.7(8)	5.6(9)
C5	54.7(11)	53.6(11)	47.2(10)	4.6(8)	8.9(8)	3.5(9)
C7	58.6(12)	61.9(13)	46.6(10)	5.4(9)	11.6(9)	0.2(10)
C10	56.9(11)	54.5(12)	43.2(9)	1.3(8)	12.1(8)	2.9(9)
C11	65.1(14)	76.7(17)	64.0(13)	-14.4(12)	1.2(11)	5.0(12)
C12	84.1(17)	65.2(15)	58.8(12)	-8.5(11)	16.8(12)	-3.8(12)
C13	57.2(12)	56.0(12)	50.6(11)	2.2(9)	1.4(9)	-3.7(9)
C17	60.4(13)	70.4(16)	74.2(15)	13.2(12)	-3.6(12)	-14.8(12)
C18	64.7(13)	60.1(13)	57.2(12)	-0.3(10)	-0.4(10)	-2.4(10)
C19	48.9(11)	78.0(16)	59.6(12)	5.2(11)	2.9(9)	-11.4(11)
C21	57.3(12)	64.2(14)	58.9(12)	-0.7(10)	7.5(10)	-7.0(10)
C22	78.2(15)	58.7(13)	50.1(11)	-2.9(9)	15.0(10)	3.9(11)
C24	53.6(11)	55.6(12)	43.3(10)	-0.1(8)	8.6(8)	0.6(9)
C27	69.8(14)	68.1(15)	61.1(13)	8.1(11)	7.5(11)	18.1(12)
C31	64.1(14)	56.9(13)	72.8(14)	4.9(11)	-11.8(11)	-6.3(11)
C35	66.7(15)	105(2)	85.4(18)	-15.1(16)	26.5(14)	13.3(15)
C36	94(2)	84.8(19)	64.1(14)	-12.7(13)	21.0(14)	23.4(16)
C37	57.1(13)	84.8(18)	71.6(14)	-18.7(13)	15.6(11)	-1.0(12)
C41	89.5(19)	82.7(19)	67.1(15)	-22.8(13)	2.7(14)	8.1(15)
C42	61.8(14)	86.1(19)	80.0(16)	17.6(14)	12.7(12)	9.2(13)
C43	119(3)	81(2)	67.8(16)	-13.0(14)	10.5(17)	-24.5(19)
C45	60.6(15)	131(3)	91(2)	30(2)	0.0(14)	-10.3(18)
C46	99(3)	109(3)	78.2(18)	5.1(18)	-6.3(17)	-31(2)
C48	108(2)	85(2)	69.2(16)	-1.0(14)	39.3(16)	6.4(17)
Cl3	161.0(10)	147.7(9)	112.1(7)	-28.5(6)	79.8(7)	-74.2(8)
Cl4	129.2(8)	65.6(5)	173.0(10)	4.4(5)	27.4(7)	6.0(5)
F2	163(2)	150.4(19)	83.3(11)	38.2(12)	61.9(12)	56.9(16)
F3	98.9(14)	171(2)	109.3(14)	-13.3(13)	48.3(11)	36.5(14)

O2	51.8(8)	123.1(16)	47.2(8)	-17.9(9)	-4.4(7)	24.1(9)
N1	45.1(8)	62.7(11)	39.6(8)	-4.7(7)	3.0(6)	8.4(7)
N3	50.0(9)	59.0(10)	40.6(8)	1.4(7)	2.5(7)	7.7(7)
N6	71.1(12)	66.5(12)	49.2(9)	-11.4(8)	16.5(8)	-8.2(9)
N7	73.4(12)	70.3(13)	48.6(9)	-11.6(8)	13.7(9)	1.0(10)
C1	61.7(12)	68.9(14)	40.6(9)	5.1(9)	6.0(9)	-1.4(10)
C2	50.1(10)	61.3(12)	39.5(9)	0.8(8)	6.7(8)	9.5(9)
C6	49.4(10)	59.7(12)	41.6(9)	-4.4(8)	7.7(8)	3.9(9)
C8	48.9(10)	52.2(11)	38.1(8)	0.8(7)	7.2(7)	2.2(8)
C9	50.5(10)	53.5(11)	45.7(10)	3.4(8)	9.5(8)	4.9(9)
C14	60.0(12)	69.7(14)	44.7(10)	-4.8(9)	10.1(9)	8.0(10)
C15	58.7(13)	79.5(17)	58.5(12)	-16.7(11)	-6.0(10)	7.0(11)
C16	58.9(12)	67.8(14)	51.7(11)	-5.1(10)	1.5(9)	-7.6(10)
C20	112(2)	71.9(17)	64.2(14)	-8.9(12)	22.5(14)	-10.9(16)
C23	72.3(16)	86(2)	80.5(17)	11.7(14)	0.2(14)	-20.8(14)
C25	60.9(13)	71.8(16)	69.6(14)	-1.5(12)	2.6(11)	1.7(11)
C26	43.8(10)	70.8(13)	40.3(9)	-6.9(9)	4.9(8)	4.3(9)
C28	71.4(14)	66.4(14)	56.3(12)	4.9(10)	7.6(10)	22.0(12)
C29	56.2(13)	79.7(17)	76.8(15)	-16.0(13)	21.1(11)	5.5(12)
C30	75.7(16)	80.7(17)	65.0(14)	-10.4(12)	19.3(12)	-21.5(13)
C32	70.2(16)	67.0(16)	90.3(18)	6.6(13)	-7.9(14)	-3.9(12)
C33	49.6(11)	68.6(14)	63.3(12)	-15.3(10)	13.7(9)	-3.1(10)
C34	73.5(16)	101(2)	63.5(14)	-3.2(14)	13.0(12)	-29.9(15)
C38	83.8(18)	80.8(18)	64.1(14)	-23.9(13)	-6.1(13)	6.0(14)
C39	84.1(17)	74.5(16)	58.5(13)	-14.9(11)	14.3(12)	14.8(13)
C40	57.3(14)	105(2)	78.9(16)	19.1(15)	-1.3(12)	-1.9(14)
C44	83.9(18)	87.5(19)	58.3(13)	-6.7(13)	26.1(12)	12.3(14)
C47	163(4)	109(3)	77(2)	-17.1(18)	18(2)	-50(3)
C49	76(2)	157(4)	96(2)	35(2)	-12.0(17)	-31(2)
C50	147(4)	164(4)	76(2)	12(2)	-18(2)	-79(4)
F4	124.9(18)	213(3)	114.1(16)	-8.7(16)	52.8(14)	47.7(18)

**Table S11 Bond Lengths for Compound (*trans*)-3j.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C19	1.730(3)	C13	C34	1.727(3)
C12	C31	1.734(3)	C14	C32	1.728(3)
F1	C48	1.331(4)	F2	C44	1.322(4)
F4	C48	1.279(4)	F3	C44	1.325(4)
O1	C24	1.206(3)	O2	C26	1.208(3)
N2	N5	1.414(2)	N1	N3	1.418(2)
N2	C10	1.420(3)	N1	C8	1.416(2)
N2	C24	1.364(3)	N1	C26	1.362(2)
N4	N8	1.370(3)	N3	C9	1.274(3)
N4	C3	1.460(3)	N6	N7	1.384(3)
N4	C13	1.400(3)	N6	C6	1.461(3)
N5	C5	1.277(3)	N6	C16	1.397(3)
N8	C22	1.274(3)	N7	C14	1.267(3)
C3	C4	1.576(3)	C1	C2	1.512(3)
C3	C5	1.510(3)	C1	C20	1.383(4)
C3	C24	1.541(3)	C1	C40	1.374(4)
C4	C7	1.513(3)	C2	C6	1.575(3)
C4	C22	1.506(3)	C2	C14	1.503(3)
C5	C27	1.485(3)	C6	C9	1.511(3)
C7	C12	1.385(4)	C6	C26	1.535(3)
C7	C42	1.386(4)	C8	C15	1.382(3)
C10	C11	1.374(3)	C8	C33	1.381(3)
C10	C37	1.378(3)	C9	C28	1.482(3)
C11	C41	1.377(4)	C14	C44	1.503(3)
C12	C43	1.382(4)	C15	C38	1.376(4)
C13	C18	1.389(3)	C16	C25	1.389(4)
C13	C21	1.396(3)	C16	C30	1.394(3)
C17	C19	1.370(4)	C20	C47	1.377(5)
C17	C31	1.391(4)	C23	C32	1.388(4)
C18	C31	1.380(4)	C23	C34	1.373(4)
C19	C21	1.383(3)	C25	C32	1.376(4)
C22	C48	1.500(3)	C29	C33	1.382(3)
C35	C36	1.366(4)	C29	C39	1.372(4)
C35	C37	1.388(4)	C30	C34	1.378(4)
C36	C41	1.380(4)	C38	C39	1.380(4)
C42	C45	1.416(5)	C40	C49	1.401(5)
C43	C46	1.336(5)	C47	C50	1.353(7)
C45	C46	1.373(6)	C49	C50	1.371(7)

**Table S12 Bond Angles for Compound (*trans*)-3j.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N5	N2	C10	118.31(16)	C8	N1	N3	118.91(15)
C24	N2	N5	113.21(16)	C26	N1	N3	113.06(16)
C24	N2	C10	128.44(18)	C26	N1	C8	128.03(17)
N8	N4	C3	112.68(18)	C9	N3	N1	108.13(15)
N8	N4	C13	118.83(19)	N7	N6	C6	111.92(18)
C13	N4	C3	125.75(17)	N7	N6	C16	118.15(19)
C5	N5	N2	108.22(16)	C16	N6	C6	124.82(17)
C22	N8	N4	108.82(19)	C14	N7	N6	108.66(19)
N4	C3	C4	101.34(15)	C20	C1	C2	118.2(2)
N4	C3	C5	114.67(17)	C40	C1	C2	122.7(2)
N4	C3	C24	116.49(18)	C40	C1	C20	119.1(3)
C5	C3	C4	116.28(17)	C1	C2	C6	115.68(15)
C5	C3	C24	100.84(16)	C14	C2	C1	120.38(18)
C24	C3	C4	107.71(17)	C14	C2	C6	99.54(17)
C7	C4	C3	115.52(16)	N6	C6	C2	101.34(15)
C22	C4	C3	99.68(17)	N6	C6	C9	114.96(18)
C22	C4	C7	120.18(19)	N6	C6	C26	115.81(18)
N5	C5	C3	112.62(18)	C9	C6	C2	116.56(17)
N5	C5	C27	122.11(19)	C9	C6	C26	100.92(15)
C27	C5	C3	125.16(19)	C26	C6	C2	107.69(17)
C12	C7	C4	118.4(2)	C15	C8	N1	119.36(19)
C12	C7	C42	118.8(3)	C33	C8	N1	120.26(18)
C42	C7	C4	122.7(2)	C33	C8	C15	120.4(2)
C11	C10	N2	118.9(2)	N3	C9	C6	112.63(17)
C11	C10	C37	120.2(2)	N3	C9	C28	121.81(18)
C37	C10	N2	120.9(2)	C28	C9	C6	125.48(18)
C10	C11	C41	119.7(2)	N7	C14	C2	115.09(19)
C43	C12	C7	121.2(3)	N7	C14	C44	117.3(2)
C18	C13	N4	119.9(2)	C44	C14	C2	126.7(2)
C18	C13	C21	120.4(2)	C38	C15	C8	119.5(2)
C21	C13	N4	119.7(2)	C25	C16	N6	120.9(2)
C19	C17	C31	117.2(2)	C25	C16	C30	119.8(2)
C31	C18	C13	118.4(2)	C30	C16	N6	119.4(2)
C17	C19	C11	118.69(19)	C47	C20	C1	121.5(4)
C17	C19	C21	122.6(2)	C34	C23	C32	116.9(3)
C21	C19	C11	118.7(2)	C32	C25	C16	118.7(3)
C19	C21	C13	118.8(2)	O2	C26	N1	127.4(2)
N8	C22	C4	114.8(2)	O2	C26	C6	127.59(18)
N8	C22	C48	117.6(2)	N1	C26	C6	104.80(16)
C48	C22	C4	126.4(2)	C39	C29	C33	120.7(2)

O1	C24	N2	128.0(2)	C34	C30	C16	119.2(3)
O1	C24	C3	127.23(19)	C23	C32	C14	117.7(2)
N2	C24	C3	104.58(17)	C25	C32	C14	119.4(3)
C17	C31	C12	118.4(2)	C25	C32	C23	122.9(3)
C18	C31	C12	118.9(2)	C8	C33	C29	119.3(2)
C18	C31	C17	122.7(2)	C23	C34	C13	118.0(2)
C36	C35	C37	120.4(3)	C23	C34	C30	122.5(3)
C35	C36	C41	119.7(2)	C30	C34	C13	119.5(3)
C10	C37	C35	119.5(2)	C15	C38	C39	120.6(2)
C11	C41	C36	120.4(3)	C29	C39	C38	119.5(2)
C7	C42	C45	118.5(3)	C1	C40	C49	119.5(4)
C46	C43	C12	120.3(3)	F2	C44	F3	104.5(3)
C46	C45	C42	120.5(3)	F2	C44	C14	110.3(2)
C43	C46	C45	120.5(3)	F3	C44	C14	112.9(2)
F1	C48	C22	108.9(2)	C50	C47	C20	118.8(4)
F4	C48	F1	106.3(3)	C50	C49	C40	119.5(4)
F4	C48	C22	115.4(3)	C47	C50	C49	121.7(4)

**Table S13 Torsion Angles for Compound (*trans*)-3j.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C11	C19	C21	C13	179.79(17)	N1	N3	C9	C6	2.1(2)
N2	N5	C5	C3	-2.4(2)	N1	N3	C9	C28	-174.6(2)
N2	N5	C5	C27	173.9(2)	N1	C8	C15	C38	180.0(2)
N2	C10	C11	C41	178.5(2)	N1	C8	C33	C29	-179.9(2)
N2	C10	C37	C35	-178.3(3)	N3	N1	C8	C15	32.4(3)
N4	N8	C22	C4	3.4(3)	N3	N1	C8	C33	-147.5(2)
N4	N8	C22	C48	171.9(2)	N3	N1	C26	O2	178.4(2)
N4	C3	C4	C7	145.27(19)	N3	N1	C26	C6	-6.1(2)
N4	C3	C4	C22	15.0(2)	N6	N7	C14	C2	-3.2(3)
N4	C3	C5	N5	131.9(2)	N6	N7	C14	C44	-173.2(2)
N4	C3	C5	C27	-44.4(3)	N6	C6	C9	N3	-130.8(2)
N4	C3	C24	O1	52.3(3)	N6	C6	C9	C28	45.7(3)
N4	C3	C24	N2	-131.69(18)	N6	C6	C26	O2	-53.1(3)
N4	C13	C18	C31	179.3(2)	N6	C6	C26	N1	131.35(18)
N4	C13	C21	C19	-178.4(2)	N6	C16	C25	C32	-177.3(2)
N5	N2	C10	C11	-32.0(3)	N6	C16	C30	C34	177.1(2)
N5	N2	C10	C37	147.3(2)	N7	N6	C6	C2	17.4(2)
N5	N2	C24	O1	-177.7(2)	N7	N6	C6	C9	-109.2(2)
N5	N2	C24	C3	6.3(2)	N7	N6	C6	C26	133.62(19)
N8	N4	C3	C4	-15.3(2)	N7	N6	C16	C25	3.9(3)
N8	N4	C3	C5	110.8(2)	N7	N6	C16	C30	-174.4(2)
N8	N4	C3	C24	-131.8(2)	N7	C14	C44	F2	136.9(3)
N8	N4	C13	C18	0.4(3)	N7	C14	C44	F3	-106.6(3)
N8	N4	C13	C21	178.8(2)	C1	C2	C6	N6	-147.46(19)
N8	C22	C48	F1	-132.1(3)	C1	C2	C6	C9	-21.9(3)
N8	C22	C48	F4	108.4(4)	C1	C2	C6	C26	90.5(2)
C3	N4	N8	C22	8.4(3)	C1	C2	C14	N7	140.9(2)
C3	N4	C13	C18	160.2(2)	C1	C2	C14	C44	-50.3(3)
C3	N4	C13	C21	-21.4(3)	C1	C20	C47	C50	0.6(5)
C3	C4	C7	C12	85.6(2)	C1	C40	C49	C50	-0.2(5)
C3	C4	C7	C42	-94.3(3)	C2	C1	C20	C47	-179.9(3)
C3	C4	C22	N8	-12.2(3)	C2	C1	C40	C49	179.7(2)
C3	C4	C22	C48	-179.6(3)	C2	C6	C9	N3	110.8(2)
C4	C3	C5	N5	-110.2(2)	C2	C6	C9	C28	-72.6(3)
C4	C3	C5	C27	73.6(3)	C2	C6	C26	O2	59.4(3)
C4	C3	C24	O1	-60.6(3)	C2	C6	C26	N1	-116.11(19)
C4	C3	C24	N2	115.37(18)	C2	C14	C44	F2	-31.7(4)
C4	C7	C12	C43	-179.3(2)	C2	C14	C44	F3	84.8(3)
C4	C7	C42	C45	179.3(2)	C6	N6	N7	C14	-10.0(3)
C4	C22	C48	F1	34.9(4)	C6	N6	C16	C25	-148.7(2)

C4	C22	C48	F4	-84.6(4)	C6	N6	C16	C30	33.0(3)
C5	C3	C4	C7	20.3(3)	C6	C2	C14	N7	13.4(2)
C5	C3	C4	C22	-110.0(2)	C6	C2	C14	C44	-177.7(2)
C5	C3	C24	O1	177.1(2)	C8	N1	N3	C9	-177.09(18)
C5	C3	C24	N2	-6.9(2)	C8	N1	C26	O2	-1.8(4)
C7	C4	C22	N8	-139.4(2)	C8	N1	C26	C6	173.74(19)
C7	C4	C22	C48	53.2(4)	C8	C15	C38	C39	0.0(4)
C7	C12	C43	C46	0.1(4)	C9	C6	C26	O2	-177.9(3)
C7	C42	C45	C46	-0.1(4)	C9	C6	C26	N1	6.5(2)
C10	N2	N5	C5	179.41(19)	C14	C2	C6	N6	-16.93(19)
C10	N2	C24	O1	-0.1(4)	C14	C2	C6	C9	108.6(2)
C10	N2	C24	C3	-176.1(2)	C14	C2	C6	C26	-138.94(17)
C10	C11	C41	C36	0.2(5)	C15	C8	C33	C29	0.2(4)
C11	C10	C37	C35	1.0(4)	C15	C38	C39	C29	0.2(5)
C12	C7	C42	C45	-0.5(4)	C16	N6	N7	C14	-165.9(2)
C12	C43	C46	C45	-0.8(5)	C16	N6	C6	C2	171.5(2)
C13	N4	N8	C22	170.7(2)	C16	N6	C6	C9	44.9(3)
C13	N4	C3	C4	-176.2(2)	C16	N6	C6	C26	-72.3(3)
C13	N4	C3	C5	-50.1(3)	C16	C25	C32	C14	179.82(19)
C13	N4	C3	C24	67.3(3)	C16	C25	C32	C23	-0.9(4)
C13	C18	C31	C12	178.75(18)	C16	C30	C34	C13	-178.2(2)
C13	C18	C31	C17	-0.7(4)	C16	C30	C34	C23	1.4(4)
C17	C19	C21	C13	-1.1(4)	C20	C1	C2	C6	-87.1(2)
C18	C13	C21	C19	0.0(3)	C20	C1	C2	C14	153.2(2)
C19	C17	C31	C12	-179.78(18)	C20	C1	C40	C49	0.4(4)
C19	C17	C31	C18	-0.3(4)	C20	C47	C50	C49	-0.4(6)
C21	C13	C18	C31	0.9(3)	C25	C16	C30	C34	-1.2(4)
C22	C4	C7	C12	-154.8(2)	C26	N1	N3	C9	2.7(3)
C22	C4	C7	C42	25.3(3)	C26	N1	C8	C15	-147.4(2)
C24	N2	N5	C5	-2.8(3)	C26	N1	C8	C33	32.7(3)
C24	N2	C10	C11	150.6(2)	C26	C6	C9	N3	-5.5(2)
C24	N2	C10	C37	-30.1(3)	C26	C6	C9	C28	171.1(2)
C24	C3	C4	C7	-91.9(2)	C30	C16	C25	C32	0.9(4)
C24	C3	C4	C22	137.78(18)	C32	C23	C34	C13	178.4(2)
C24	C3	C5	N5	5.9(2)	C32	C23	C34	C30	-1.2(4)
C24	C3	C5	C27	-170.3(2)	C33	C8	C15	C38	-0.2(4)
C31	C17	C19	C11	-179.64(18)	C33	C29	C39	C38	-0.2(4)
C31	C17	C19	C21	1.2(4)	C34	C23	C32	C14	-179.7(2)
C35	C36	C41	C11	0.1(5)	C34	C23	C32	C25	1.0(4)
C36	C35	C37	C10	-0.7(5)	C39	C29	C33	C8	0.0(4)
C37	C10	C11	C41	-0.8(4)	C40	C1	C2	C6	93.6(3)
C37	C35	C36	C41	0.1(5)	C40	C1	C2	C14	-26.0(3)
C42	C7	C12	C43	0.6(4)	C40	C1	C20	C47	-0.6(4)



C42	C45	C46	C43	0.8(5)	C40	C49	C50	C47	0.2(6)
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**Table S14 Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for Compound (*trans*)-3j.**

Atom	x	y	z	U(eq)
H4	3949.34	4671.31	7436.52	62
H11	3702.44	3115.86	6257.34	83
H12	3536.98	2922.18	7182.8	82
H17	5263.56	10178.95	6599.41	83
H18	4212.98	9104.91	7301.78	74
H21	4775.69	6761.85	6679.94	72
H27A	2654.65	6496.28	6450.95	100
H27B	2998.56	7385.89	6700	100
H27C	2480.58	6410.9	6792.89	100
H35	6133.24	2669.47	6358.99	101
H36	5431.94	1568.42	6001.41	96
H37	5623.41	3995.48	6670.98	85
H41	4215.62	1791	5950.81	96
H42	2156.53	5540.43	7257.38	91
H43	2614.41	1648.26	7040.04	107
H45	1231.91	4205.09	7110.49	114
H46	1480.41	2287.8	6998.56	116
H48	3420.31	6959.95	7937.81	102
H2	3466.72	7799.02	5062.68	60
H15	3810.3	9277.35	6249.41	80
H20	3905.27	9521.26	5310.96	98
H23	2157.89	2279.99	5899.39	96
H25	3282.18	3342.71	5221.8	81
H28A	4930.85	5961.91	5695.88	97
H28B	4391.23	4979.34	5763.05	97
H28C	4735.19	5784.98	6032.2	97
H29	1395.12	9927.44	6152.12	84
H30	2536.95	5719.95	5787.47	88
H33	1851.75	8516.76	5849.04	72
H38	3344.14	10678.42	6549.58	93
H39	2136.58	11010.67	6500.53	86
H40	5236.62	6850.43	5237.5	97
H44	3973.13	5521.03	4547.72	90
H47	4845.28	10769.34	5450.35	139
H49	6187.94	8123.56	5376.53	134
H50	5973.48	10060.36	5478.34	158

## X-Ray Crystallographic Data of Compound (*cis*)-**3j**

Thermal ellipsoids are set at a 50% probability level. Crystal data have been deposited to CCDC, number 2253537.

### Crystallization Details

The obtained compound (*cis*)-**3j** (35 mg) was dissolved in THF (0.2 mL) in a NMR tube at room temperature. Then petroleum ether (2 mL) was added to the solution slowly along the tube wall, resulting in a two-phase mixture. The colorless crystal of (*cis*)-**3j** was formed after the two-phase mixture has diffused.

### Experimental

A suitable crystal was selected and placed on a ROD, Synergy Custom system, HyPix diffractometer. The crystal was kept at 274.7(3) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

### Crystal structure determination

Crystal Data for for for  $C_{25}H_{18}Cl_2F_2N_4O$  ( $M=499.33$  g/mol): monoclinic, space group  $P2_1/c$  (no. 14),  $a = 19.8243(4)$  Å,  $b = 7.18030(10)$  Å,  $c = 16.7155(3)$  Å,  $\beta = 104.020(2)^\circ$ ,  $V = 2308.48(7)$  Å<sup>3</sup>,  $Z = 4$ ,  $T = 274.7(3)$  K,  $\mu(\text{Cu K}\alpha) = 2.899$  mm<sup>-1</sup>,  $D_{\text{calc}} = 1.437$  g/cm<sup>3</sup>, 14610 reflections measured ( $10.764^\circ \leq 2\theta \leq 152.764^\circ$ ), 4553 unique ( $R_{\text{int}} = 0.0407$ ,  $R_{\text{sigma}} = 0.0266$ ) which were used in all calculations. The final  $R_1$  was 0.0533 ( $I > 2\sigma(I)$ ) and  $wR_2$  was 0.1410 (all data).

### Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

#### 1. Fixed Uiso

At 1.2 times of:

All C(H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Ternary CH refined with riding coordinates:

C8(H8), C17(H17)

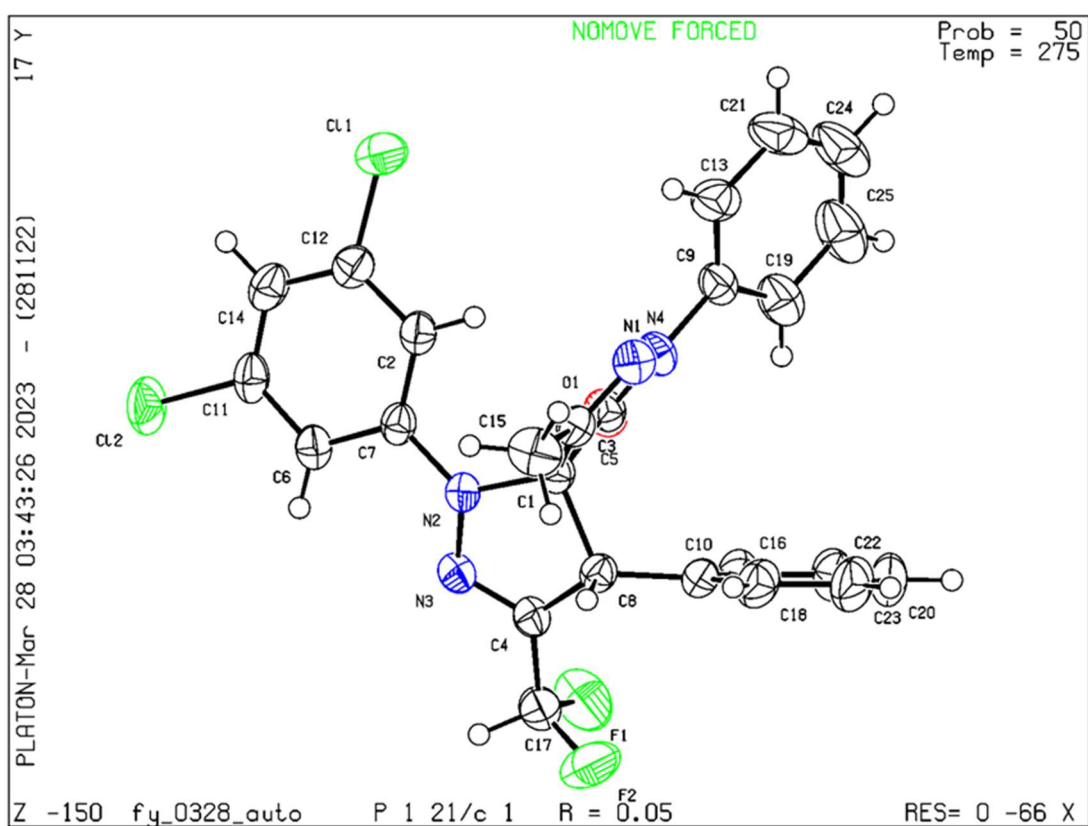
3.b Aromatic/amide H refined with riding coordinates:

C2(H2), C6(H6), C13(H13), C14(H14), C16(H16), C18(H18), C19(H19),  
C20(H20),

C21(H21), C22(H22), C23(H23), C24(H24), C25(H25)

4.c Idealised Me refined as rotating group:

C15(H15A,H15B,H15C)



**Table S15 Crystal data and structure refinement for Compound (*cis*)-3j.**

Identification code	FY_0328_auto
Empirical formula	C <sub>25</sub> H <sub>18</sub> Cl <sub>2</sub> F <sub>2</sub> N <sub>4</sub> O
Formula weight	499.33
Temperature/K	274.7(3)
Crystal system	monoclinic
Space group	P21/c
a/Å	19.8243(4)
b/Å	7.18030(10)
c/Å	16.7155(3)
α/°	90
β/°	104.020(2)
γ/°	90
Volume/Å <sup>3</sup>	2308.48(7)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.437
μ/mm <sup>-1</sup>	2.899
F(000)	1024.0
Crystal size/mm <sup>3</sup>	0.18 × 0.15 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	10.764 to 152.764
Index ranges	-25 ≤ h ≤ 22, -8 ≤ k ≤ 8, -16 ≤ l ≤ 20
Reflections collected	14610
Independent reflections	4553 [R <sub>int</sub> = 0.0407, R <sub>sigma</sub> = 0.0266]
Data/restraints/parameters	4553/0/308
Goodness-of-fit on F <sup>2</sup>	1.074
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0533, wR <sub>2</sub> = 0.1391
Final R indexes [all data]	R <sub>1</sub> = 0.0551, wR <sub>2</sub> = 0.1410
Largest diff. peak/hole / e Å <sup>-3</sup>	0.36/-0.56

**Table S16 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for Compound (*cis*)-3j.  $U_{eq}$  is defined as 1/3 of the trace of the orthogonalised UIJ tensor.**

Atom	x	y	z	U(eq)
C11	4963.4(3)	3795.5(8)	4033.3(3)	57.60(18)
C12	4580.3(3)	3939.5(8)	740.4(3)	58.70(18)
F1	787.6(8)	6250(2)	818.8(9)	76.7(5)
F2	816.0(8)	9263(3)	899.3(10)	81.3(5)
O1	2189.2(7)	4168.5(16)	2978.6(8)	40.9(3)
N1	2949.5(8)	7782(2)	4283.8(9)	37.4(3)
N2	2886.3(7)	7087(2)	2181.8(8)	33.7(3)
N3	2384.5(7)	7010(2)	1442.0(8)	34.7(3)
N4	2603.3(8)	6043.5(19)	4118.8(9)	35.8(3)
C1	2566.4(8)	7418(2)	2871.4(9)	29.8(3)
C2	3893.4(9)	5513(2)	3017.4(11)	36.3(4)
C3	2418.6(8)	5625(2)	3297.9(10)	31.7(3)
C4	1815.7(9)	7651(2)	1561.2(10)	34.9(3)
C5	2961.1(8)	8545(2)	3597.3(10)	33.6(3)
C6	3709.9(9)	5581(2)	1533.9(11)	36.3(4)
C7	3495.8(8)	6044(2)	2245.2(10)	32.5(3)
C8	1873.8(8)	8408(2)	2418.3(10)	32.8(3)
C9	2554.4(10)	4893(2)	4790.7(10)	37.6(4)
C10	1282.8(8)	8218(3)	2837.1(10)	37.1(4)
C11	4317.5(10)	4571(2)	1622.4(11)	40.1(4)
C12	4496.4(9)	4497(2)	3064.8(11)	39.4(4)
C13	3099.1(12)	4852(3)	5487.7(12)	50.0(5)
C14	4721.7(10)	4004(3)	2377.6(12)	43.0(4)
C15	3301.5(11)	10367(3)	3545.3(13)	50.1(5)
C16	860.0(10)	6649(3)	2743.4(12)	47.4(4)
C17	1200.0(10)	7752(3)	834.7(12)	46.2(4)
C18	1175.0(11)	9630(3)	3355.4(12)	50.7(5)
C19	1958.6(13)	3858(3)	4747.7(14)	52.6(5)
C20	245.5(11)	7922(5)	3687.9(14)	68.1(7)
C21	3032.5(17)	3787(3)	6154.6(14)	64.4(7)
C22	342.4(11)	6513(4)	3171.5(14)	61.2(6)
C23	657.5(13)	9477(4)	3782.4(14)	67.0(7)
C24	2441.3(19)	2766(3)	6122.5(15)	72.1(8)
C25	1912.9(17)	2785(3)	5422.3(17)	70.5(7)

**Table 17 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for Compound (*cis*)-3j. The Anisotropic displacement factor exponent takes the form:  $-2\pi^2[h^2a^2U_{11}+2hka*b*U_{12}+\dots]$**

Atom	U11	U22	U33	U23	U13	U12
C11	51.7(3)	64.3(3)	53.4(3)	7.1(2)	6.0(2)	15.5(2)
C12	67.0(3)	62.4(3)	57.9(3)	-9.4(2)	37.0(3)	10.3(2)
F1	62.8(8)	107.1(12)	55.6(8)	-1.0(7)	5.4(6)	-40.4(8)
F2	59.0(8)	102.7(12)	75.9(9)	7.6(8)	4.1(7)	35.2(8)
O1	53.9(7)	29.5(6)	41.8(6)	-5.8(5)	16.4(5)	-3.8(5)
N1	41.9(7)	32.0(7)	38.7(7)	-5.9(6)	10.4(6)	-2.3(6)
N2	33.2(7)	38.0(7)	31.9(7)	0.7(5)	12.2(5)	3.9(5)
N3	37.3(7)	35.9(7)	32.2(7)	2.4(5)	10.9(5)	-2.3(6)
N4	45.9(8)	31.5(7)	32.6(7)	-2.6(5)	14.4(6)	-3.6(6)
C1	30.7(7)	27.5(7)	33.4(8)	-1.9(6)	11.9(6)	1.6(6)
C2	36.9(8)	35.5(8)	40.3(8)	-0.5(7)	16.6(7)	1.1(7)
C3	34.7(8)	30.5(8)	32.7(8)	-2.1(6)	13.4(6)	2.2(6)
C4	35.7(8)	36.0(8)	34.7(8)	3.0(6)	12.1(6)	-1.8(6)
C5	32.8(8)	30.7(8)	37.8(8)	-4.4(6)	9.7(6)	0.4(6)
C6	39.7(8)	33.0(8)	40.5(8)	-0.5(7)	18.3(7)	-1.5(7)
C7	32.6(8)	27.9(7)	40.6(8)	0.1(6)	15.6(6)	-2.0(6)
C8	31.7(8)	30.6(7)	37.1(8)	0.5(6)	10.4(6)	1.8(6)
C9	50.9(10)	30.7(8)	35.0(8)	0.7(6)	17.9(7)	6.8(7)
C10	30.2(8)	47.1(9)	34.8(8)	0.7(7)	9.2(6)	6.2(7)
C11	45.1(9)	34.0(8)	48.7(10)	-6.2(7)	26.1(8)	-1.1(7)
C12	36.7(8)	34.4(8)	47.9(10)	1.8(7)	11.9(7)	0.3(7)
C13	60.7(12)	45.2(10)	43.3(10)	0.8(8)	10.8(8)	16.4(9)
C14	39.6(9)	35.1(9)	58.2(11)	-2.7(7)	19.4(8)	5.6(7)
C15	56.2(11)	36.2(9)	54.1(11)	-0.9(8)	6.3(9)	-12.6(8)
C16	38.6(9)	59.6(11)	46.1(10)	-3.2(9)	14.2(8)	-4.7(8)
C17	40.4(9)	59.5(11)	39.2(9)	4.4(8)	10.5(7)	-2.4(8)
C18	44.7(10)	60.6(12)	47.9(10)	-10.2(9)	13.7(8)	9.7(9)
C19	67.0(13)	45.5(11)	49.6(11)	2.9(8)	22.6(10)	-5.3(9)
C20	41.5(11)	120(2)	48.9(11)	4.5(13)	22.4(9)	8.1(13)
C21	99.7(19)	48.6(12)	42.0(11)	6.9(9)	11.9(11)	29.5(12)
C22	38.6(10)	93.1(18)	54.6(12)	6.5(12)	16.8(9)	-8.6(11)
C23	56.0(13)	99.1(19)	50.2(12)	-13.7(12)	21.6(10)	19.6(13)
C24	132(3)	40.7(11)	53.6(13)	16.2(10)	41.6(15)	20.2(14)
C25	106(2)	46.5(12)	71.1(16)	8.8(11)	45.6(15)	-9.1(12)

**Table S18 Bond Lengths for Compound (*cis*)-3j.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C12	1.7336(19)	C4	C17	1.500(2)
C12	C11	1.7386(17)	C5	C15	1.484(2)
F1	C17	1.350(2)	C6	C7	1.396(2)
F2	C17	1.345(3)	C6	C11	1.383(3)
O1	C3	1.211(2)	C8	C10	1.510(2)
N1	N4	1.4191(19)	C9	C13	1.384(3)
N1	C5	1.277(2)	C9	C19	1.382(3)
N2	N3	1.3878(19)	C10	C16	1.390(3)
N2	C1	1.4634(19)	C10	C18	1.384(3)
N2	C7	1.403(2)	C11	C14	1.382(3)
N3	C4	1.278(2)	C12	C14	1.376(3)
N4	C3	1.365(2)	C13	C21	1.385(3)
N4	C9	1.416(2)	C16	C22	1.389(3)
C1	C3	1.534(2)	C18	C23	1.389(3)
C1	C5	1.510(2)	C19	C25	1.387(3)
C1	C8	1.569(2)	C20	C22	1.373(4)
C2	C7	1.393(2)	C20	C23	1.370(4)
C2	C12	1.386(2)	C21	C24	1.372(4)
C4	C8	1.511(2)	C24	C25	1.369(4)

**Table S19 Bond Angles for Compound (*cis*)-3j.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C5	N1	N4	108.42(13)	C10	C8	C1	114.96(13)
N3	N2	C1	110.76(12)	C10	C8	C4	121.18(14)
N3	N2	C7	117.66(13)	C13	C9	N4	119.37(18)
C7	N2	C1	123.81(13)	C19	C9	N4	119.60(17)
C4	N3	N2	108.41(13)	C19	C9	C13	121.01(18)
C3	N4	N1	112.85(13)	C16	C10	C8	122.39(16)
C3	N4	C9	127.98(14)	C18	C10	C8	118.62(17)
C9	N4	N1	118.80(13)	C18	C10	C16	118.95(17)
N2	C1	C3	113.45(12)	C6	C11	C12	118.58(15)
N2	C1	C5	118.74(13)	C14	C11	C12	118.10(14)
N2	C1	C8	100.89(12)	C14	C11	C6	123.31(16)
C3	C1	C8	111.19(13)	C2	C12	C11	117.68(14)
C5	C1	C3	101.34(12)	C14	C12	C11	119.80(14)
C5	C1	C8	111.55(12)	C14	C12	C2	122.50(17)
C12	C2	C7	118.93(15)	C9	C13	C21	118.8(2)
O1	C3	N4	127.85(15)	C12	C14	C11	116.95(16)
O1	C3	C1	127.83(14)	C22	C16	C10	120.0(2)
N4	C3	C1	104.32(13)	F1	C17	C4	110.34(16)
N3	C4	C8	114.22(14)	F2	C17	F1	107.10(17)
N3	C4	C17	117.82(15)	F2	C17	C4	109.83(16)
C17	C4	C8	127.63(15)	C10	C18	C23	120.6(2)
N1	C5	C1	111.93(14)	C9	C19	C25	118.7(2)
N1	C5	C15	122.57(16)	C23	C20	C22	120.2(2)
C15	C5	C1	125.45(15)	C24	C21	C13	120.7(2)
C11	C6	C7	118.06(16)	C20	C22	C16	120.4(2)
C2	C7	N2	119.99(14)	C20	C23	C18	120.0(2)
C2	C7	C6	120.23(15)	C25	C24	C21	119.9(2)
C6	C7	N2	119.77(15)	C24	C25	C19	120.9(3)
C4	C8	C1	98.71(12)				



**Table S20 Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for Compound (*cis*)-3j.**

Atom	x	y	z	U(eq)
H2	3756.5	5834.46	3493.46	44
H6	3451.37	5941.31	1015.65	44
H8	1976.86	9740.74	2401.35	39
H13	3502.94	5528.89	5507.76	60
H14	5127.26	3321.27	2419.12	52
H15A	3507.36	10813.42	4091.16	75
H15B	2961.31	11246.37	3263.29	75
H15C	3655.85	10219.44	3247.67	75
H16	923.62	5691.47	2394.38	57
H17	1357.78	7814.89	323.18	55
H18	1451.57	10692.09	3418.46	61
H19	1595.79	3880.96	4275.77	63
H20	-100.69	7819.46	3974.34	82
H21	3392.39	3761.98	6629.39	77
H22	59.96	5462.95	3107.8	73
H23	590.72	10429.46	4132.29	80
H24	2399.7	2064.08	6575.55	87
H25	1517.82	2068.12	5398.61	85

## X-Ray Crystallographic Data of Compound (*cis*)-6a

Thermal ellipsoids are set at a 50% probability level. Crystal data have been deposited to CCDC, number 2253538.

### Crystallization Details

The obtained compound (*cis*)-6a (35 mg) was dissolved in THF (0.2 mL) in a NMR tube at room temperature. Then petroleum ether (2 mL) was added to the solution slowly along the tube wall, resulting in a two-phase mixture. The colorless crystal of (*cis*)-6a was formed after the two-phase mixture has diffused.

### Experimental

A suitable crystal was selected and placed on a ROD, Synergy Custom system, HyPix diffractometer. The crystal was kept at 287.3(2) K during data collection. Using Olex2 [1], the structure was solved with the SHELXT [2] structure solution program using Intrinsic Phasing and refined with the SHELXL [3] refinement package using Least Squares minimisation.

### Crystal structure determination

Crystal Data for C<sub>25</sub>H<sub>19</sub>F<sub>3</sub>N<sub>4</sub>O (M = 448.44 g/mol): monoclinic, space group P2<sub>1</sub>/c (no. 14), a = 9.01840(10) Å, b = 19.8009(3) Å, c = 12.6774(2) Å, β = 101.0820(10)°, V = 2221.62(5) Å<sup>3</sup>, Z = 4, T = 287.3(2) K, μ(Cu Kα) = 0.855 mm<sup>-1</sup>, D<sub>calc</sub> = 1.341 g/cm<sup>3</sup>, 17080 reflections measured (8.394° ≤ 2θ ≤ 154.578°), 4459 unique (R<sub>int</sub> = 0.0283, R<sub>sigma</sub> = 0.0235) which were used in all calculations. The final R<sub>1</sub> was 0.0531 (I > 2σ(I)) and wR<sub>2</sub> was 0.1555 (all data).

### Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

#### 1. Fixed Uiso

At 1.2 times of:

All C(H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Ternary CH refined with riding coordinates:

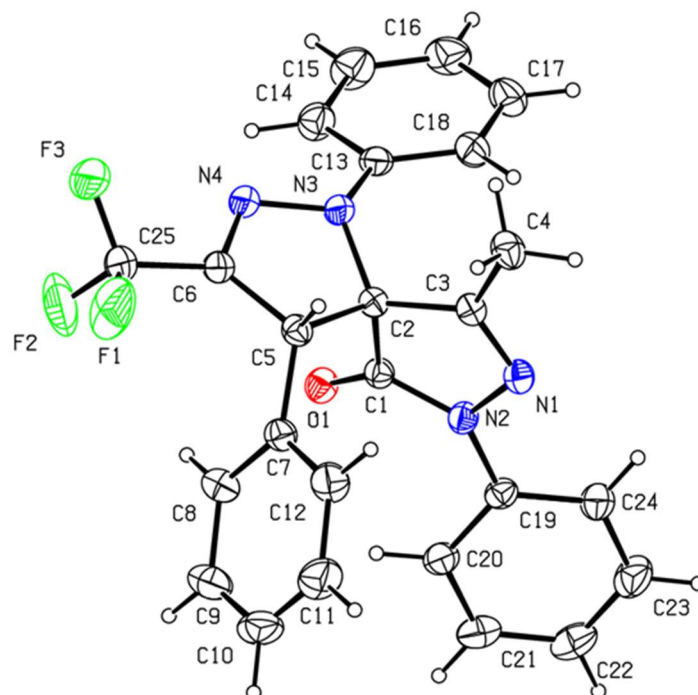
C5(H5)

3.b Aromatic/amide H refined with riding coordinates:

C8(H8), C9(H9), C10(H10), C11(H11), C12(H12), C14(H14), C15(H15), C16(H16),  
C17(H17), C18(H18), C20(H20), C21(H21), C22(H22), C23(H23), C24(H24)

4.c Idealised Me refined as rotating group:

C4(H4A,H4B,H4C)



**Table S21 Crystal data and structure refinement for Compound (*cis*)-6a.**

Identification code	Xray_1207_auto
Empirical formula	C <sub>25</sub> H <sub>19</sub> F <sub>3</sub> N <sub>4</sub> O
Formula weight	448.44
Temperature/K	287.3(2)
Crystal system	monoclinic
Space group	P21/c
a/Å	9.01840(10)
b/Å	19.8009(3)
c/Å	12.6774(2)
$\alpha$ /°	90
$\beta$ /°	101.0820(10)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	2221.62(5)
Z	4
$\rho$ calc/g/cm <sup>3</sup>	1.341
$\mu$ /mm <sup>-1</sup>	0.855
F(000)	928.0
Crystal size/mm <sup>3</sup>	0.19 × 0.11 × 0.09
Radiation	Cu K $\alpha$ ( $\lambda$ = 1.54184)
2 $\Theta$ range for data collection/°	8.394 to 154.578
Index ranges	-11 ≤ h ≤ 11, -23 ≤ k ≤ 24, -11 ≤ l ≤ 15
Reflections collected	17080
Independent reflections	4459 [Rint = 0.0283, Rsigma = 0.0235]
Data/restraints/parameters	4459/0/300
Goodness-of-fit on F <sup>2</sup>	1.085
Final R indexes [ $I \geq 2\sigma(I)$ ]	R1 = 0.0531, wR2 = 0.1510
Final R indexes [all data]	R1 = 0.0581, wR2 = 0.1555
Largest diff. peak/hole / e Å <sup>-3</sup>	0.52/-0.32

**Table S22 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for Compound (*cis*)-6a.  $U_{eq}$  is defined as 1/3 of of the trace of the orthogonalised UIJ tensor.**

Atom	x	y	z	$U_{eq}$
F(1)	1607(2)	7715.4(10)	3234.6(19)	154.6(10)
F(2)	1116.1(17)	8138.1(14)	4594(2)	155.6(9)
F(3)	2080.4(17)	8732.5(10)	3558(2)	144.2(9)
O(1)	4955.9(13)	7296.3(6)	7108.5(9)	55.1(3)
N(1)	7663.6(15)	6563.3(7)	5840.9(11)	52.1(3)
N(2)	6759.0(15)	6583.2(7)	6638.8(11)	48.8(3)
N(3)	5913.8(15)	8152.5(7)	5442.2(11)	51.0(3)
N(4)	4500.7(16)	8412.2(7)	5067.0(13)	57.7(4)
C(25)	2127(2)	8137.9(12)	3999(2)	77.4(6)
C(1)	5760.1(16)	7106.5(8)	6500.8(12)	44.7(3)
C(2)	5879.1(16)	7411.8(8)	5412.9(12)	45.1(4)
C(3)	7224.0(17)	7039.8(9)	5168.5(13)	48.6(4)
C(4)	7929(2)	7170.5(11)	4220.6(15)	65.3(5)
C(5)	4431.0(17)	7275.9(8)	4533.9(12)	48.3(4)
C(6)	3656.0(19)	7945.4(9)	4587.6(15)	56.0(4)
C(7)	3610.8(19)	6625.0(9)	4665.0(13)	51.5(4)
C(8)	2560(2)	6565.6(11)	5318.3(16)	64.8(5)
C(9)	1868(3)	5947.5(13)	5426(2)	83.8(7)
C(10)	2240(3)	5391.8(13)	4893(2)	92.7(8)
C(11)	3280(3)	5443.5(12)	4251(2)	95.6(8)
C(12)	3959(3)	6057.1(11)	4127.2(19)	73.9(6)
C(13)	6888.5(19)	8529.1(8)	6238.4(13)	52.1(4)
C(14)	6336(2)	9065.9(10)	6743.4(17)	69.5(5)
C(15)	7312(3)	9460.1(12)	7463(2)	87.3(7)
C(16)	8827(3)	9318.1(12)	7696(2)	85.4(7)
C(17)	9376(2)	8774.9(13)	7217.9(19)	78.0(6)
C(18)	8413(2)	8379.9(10)	6483.9(17)	65.2(5)
C(19)	7042.1(19)	6109.2(8)	7495.3(12)	49.3(4)
C(20)	5880(2)	5923.5(9)	8006.7(15)	60.6(4)
C(21)	6166(3)	5462.1(10)	8841.3(17)	73.7(6)
C(22)	7563(3)	5184.1(12)	9147.9(18)	83.4(7)
C(23)	8709(3)	5366.2(13)	8630(2)	84.5(7)
C(24)	8462(2)	5834.7(11)	7807.1(16)	66.1(5)

**Table S23 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for Compound (*cis*)-6a. The Anisotropic displacement factor exponent takes the form: - $2\pi^2[h_2a^*2U_{11}+2hka^*b^*U_{12}+\dots]$ .**

Atom	U11	U22	U33	U23	U13	U12
F(1)	110.3(13)	128.8(16)	181(2)	-31.6(14)	-81.2(13)	23.1(11)
F(2)	52.8(8)	232(3)	184(2)	50.5(18)	26.7(10)	26.5(11)
F(3)	71.4(9)	107.7(12)	227(2)	81.6(14)	-36.8(11)	-1.4(8)
O(1)	58.3(7)	57.7(7)	51.8(6)	-2.7(5)	17.0(5)	7.2(5)
N(1)	46.8(7)	56.1(8)	54.9(7)	-2.3(6)	13.3(6)	3.8(6)
N(2)	47.8(7)	49.5(7)	50.0(7)	2.5(5)	11.8(5)	5.6(5)
N(3)	44.2(7)	44.4(7)	61.1(8)	3.8(6)	2.1(6)	-0.9(5)
N(4)	46.6(7)	50.5(8)	72.8(9)	9.3(7)	3.4(6)	1.7(6)
C(25)	47.1(10)	69.0(13)	107.4(17)	14.6(12)	-6.7(10)	-2.3(9)
C(1)	42.8(7)	44.9(8)	45.4(8)	-3.1(6)	6.4(6)	-1.3(6)
C(2)	41.7(7)	45.1(8)	48.1(8)	-0.1(6)	8.0(6)	-1.1(6)
C(3)	42.6(8)	52.8(9)	50.7(8)	-2.2(7)	9.5(6)	-1.5(7)
C(4)	57.2(10)	82.0(13)	61.0(10)	3.0(9)	21.8(8)	0.6(9)
C(5)	44.5(8)	54.1(9)	45.4(8)	1.9(6)	6.6(6)	-2.2(7)
C(6)	46.9(9)	53.8(9)	64.5(10)	8.9(8)	3.2(7)	-1.6(7)
C(7)	48.4(8)	53.0(9)	49.8(8)	-1.6(7)	0.8(6)	-4.9(7)
C(8)	63.0(11)	66.3(12)	65.6(11)	0.2(9)	13.8(9)	-13.4(9)
C(9)	78.3(14)	88.8(17)	81.5(14)	16.8(12)	8.9(11)	-28.6(12)
C(10)	91.4(17)	63.1(14)	109.3(19)	12.1(13)	-16.5(14)	-25.3(12)
C(11)	96.7(18)	57.7(13)	122(2)	-25.6(13)	-4.5(16)	-6.2(12)
C(12)	69.1(12)	68.3(12)	82.5(13)	-21.7(10)	10.1(10)	-5.4(10)
C(13)	52.7(9)	46.0(8)	55.4(9)	5.1(7)	4.9(7)	-7.2(7)
C(14)	69.1(12)	61.2(11)	74.4(12)	-7.3(9)	4.7(9)	1.9(9)
C(15)	99.2(17)	67.7(14)	87.4(15)	-20.9(11)	-1.4(13)	-1.7(12)
C(16)	91.7(16)	70.4(14)	84.2(14)	-11.1(11)	-8.3(12)	-22.5(12)
C(17)	57.0(11)	82.3(15)	88.2(14)	0.1(12)	-2.4(10)	-16.7(10)
C(18)	53.1(10)	61.9(11)	78.0(12)	-4.4(9)	6.2(9)	-7.4(8)
C(19)	55.5(9)	41.7(8)	48.4(8)	-2.9(6)	4.2(7)	-0.2(7)
C(20)	67.8(11)	49.8(9)	66.1(10)	4.7(8)	17.6(8)	2.4(8)
C(21)	102.1(16)	52.6(11)	70.7(12)	6.3(9)	27.2(11)	-3.3(10)
C(22)	116.7(19)	60.9(12)	67.2(12)	15.7(10)	4.0(12)	6.5(12)
C(23)	81.2(14)	81.5(15)	81.0(14)	17.0(12)	-9.2(11)	15.8(12)
C(24)	57.4(10)	68.1(12)	67.2(11)	7.3(9)	-1.8(8)	2.0(9)

**Table S24 Bond Lengths for Compound (*cis*)-6a.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
F(1)	C(25)	1.298(3)	C(7)	C(8)	1.378(3)
F(2)	C(25)	1.291(3)	C(7)	C(12)	1.382(3)
F(3)	C(25)	1.300(3)	C(8)	C(9)	1.393(3)
O(1)	C(1)	1.2147(18)	C(9)	C(10)	1.366(4)
N(1)	N(2)	1.4169(18)	C(10)	C(11)	1.359(4)
N(1)	C(3)	1.282(2)	C(11)	C(12)	1.383(3)
N(2)	C(1)	1.362(2)	C(13)	C(14)	1.382(3)
N(2)	C(19)	1.421(2)	C(13)	C(18)	1.382(3)
N(3)	N(4)	1.3717(19)	C(14)	C(15)	1.381(3)
N(3)	C(2)	1.467(2)	C(15)	C(16)	1.370(4)
N(3)	C(13)	1.416(2)	C(16)	C(17)	1.372(4)
N(4)	C(6)	1.275(2)	C(17)	C(18)	1.386(3)
C(25)	C(6)	1.486(3)	C(19)	C(20)	1.384(2)
C(1)	C(2)	1.528(2)	C(19)	C(24)	1.377(3)
C(2)	C(3)	1.501(2)	C(20)	C(21)	1.384(3)
C(2)	C(5)	1.569(2)	C(21)	C(22)	1.361(4)
C(3)	C(4)	1.486(2)	C(22)	C(23)	1.375(4)
C(5)	C(6)	1.506(2)	C(23)	C(24)	1.382(3)
C(5)	C(7)	1.511(2)			

**Table S25 Bond Angles for Compound (*cis*)-6a.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(3)	N(1)	N(2)	107.89(13)	C(7)	C(5)	C(2)	115.25(13)
N(1)	N(2)	C(19)	118.92(13)	N(4)	C(6)	C(25)	117.72(17)
C(1)	N(2)	N(1)	112.76(12)	N(4)	C(6)	C(5)	114.81(15)
C(1)	N(2)	C(19)	128.17(13)	C(25)	C(6)	C(5)	126.65(17)
N(4)	N(3)	C(2)	110.62(12)	C(8)	C(7)	C(5)	123.12(16)
N(4)	N(3)	C(13)	117.24(14)	C(8)	C(7)	C(12)	118.36(18)
C(13)	N(3)	C(2)	123.47(13)	C(12)	C(7)	C(5)	118.50(17)
C(6)	N(4)	N(3)	108.88(14)	C(7)	C(8)	C(9)	120.4(2)
F(1)	C(25)	F(3)	106.6(2)	C(10)	C(9)	C(8)	120.1(2)
F(1)	C(25)	C(6)	112.2(2)	C(11)	C(10)	C(9)	119.9(2)
F(2)	C(25)	F(1)	104.0(2)	C(10)	C(11)	C(12)	120.4(2)
F(2)	C(25)	F(3)	106.4(2)	C(7)	C(12)	C(11)	120.7(2)
F(2)	C(25)	C(6)	113.4(2)	C(14)	C(13)	N(3)	120.35(16)
F(3)	C(25)	C(6)	113.47(17)	C(14)	C(13)	C(18)	119.45(17)
O(1)	C(1)	N(2)	127.93(14)	C(18)	C(13)	N(3)	120.15(16)
O(1)	C(1)	C(2)	127.15(14)	C(15)	C(14)	C(13)	120.0(2)
N(2)	C(1)	C(2)	104.91(12)	C(16)	C(15)	C(14)	120.6(2)
N(3)	C(2)	C(1)	112.17(12)	C(15)	C(16)	C(17)	119.6(2)
N(3)	C(2)	C(3)	118.78(13)	C(16)	C(17)	C(18)	120.4(2)
N(3)	C(2)	C(5)	101.55(12)	C(13)	C(18)	C(17)	119.9(2)
C(1)	C(2)	C(5)	112.33(12)	C(20)	C(19)	N(2)	119.51(15)
C(3)	C(2)	C(1)	101.06(12)	C(24)	C(19)	N(2)	120.05(16)
C(3)	C(2)	C(5)	111.38(13)	C(24)	C(19)	C(20)	120.44(17)
N(1)	C(3)	C(2)	112.50(14)	C(19)	C(20)	C(21)	119.15(19)
N(1)	C(3)	C(4)	122.68(15)	C(22)	C(21)	C(20)	120.8(2)
C(4)	C(3)	C(2)	124.72(15)	C(21)	C(22)	C(23)	119.8(2)
C(6)	C(5)	C(2)	98.46(13)	C(22)	C(23)	C(24)	120.6(2)
C(6)	C(5)	C(7)	120.30(14)	C(19)	C(24)	C(23)	119.2(2)



**Table S26 Torsion Angles for Compound (*cis*)-6a.**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
F(1)	C(25)	C(6)	N(4)	155.3(2)	C(2)	N(3)	C(13)	C(18)	49.4(2)
F(1)	C(25)	C(6)	C(5)	-13.7(3)	C(2)	C(5)	C(6)	N(4)	15.72(19)
F(2)	C(25)	C(6)	N(4)	-87.2(3)	C(2)	C(5)	C(6)	C(25)	-174.99(18)
F(2)	C(25)	C(6)	C(5)	103.8(3)	C(2)	C(5)	C(7)	C(8)	84.6(2)
F(3)	C(25)	C(6)	N(4)	34.4(3)	C(2)	C(5)	C(7)	C(12)	-93.54(19)
F(3)	C(25)	C(6)	C(5)	-134.6(2)	C(3)	N(1)	N(2)	C(1)	-2.96(18)
O(1)	C(1)	C(2)	N(3)	42.9(2)	C(3)	N(1)	N(2)	C(19)	-178.90(14)
O(1)	C(1)	C(2)	C(3)	170.44(16)	C(3)	C(2)	C(5)	C(6)	-148.79(14)
O(1)	C(1)	C(2)	C(5)	-70.8(2)	C(3)	C(2)	C(5)	C(7)	81.85(17)
N(1)	N(2)	C(1)	O(1)	-171.57(15)	C(5)	C(2)	C(3)	N(1)	-111.50(16)
N(1)	N(2)	C(1)	C(2)	7.87(17)	C(5)	C(2)	C(3)	C(4)	64.9(2)
N(1)	N(2)	C(19)	C(20)	-153.32(15)	C(5)	C(7)	C(8)	C(9)	-178.45(18)
N(1)	N(2)	C(19)	C(24)	26.3(2)	C(5)	C(7)	C(12)	C(11)	177.7(2)
N(2)	N(1)	C(3)	C(2)	-3.68(18)	C(6)	C(5)	C(7)	C(8)	-33.0(2)
N(2)	N(1)	C(3)	C(4)	179.86(15)	C(6)	C(5)	C(7)	C(12)	148.80(18)
N(2)	C(1)	C(2)	N(3)	-136.56(13)	C(7)	C(5)	C(6)	N(4)	141.63(16)
N(2)	C(1)	C(2)	C(3)	-9.01(15)	C(7)	C(5)	C(6)	C(25)	-49.1(3)
N(2)	C(1)	C(2)	C(5)	109.79(14)	C(7)	C(8)	C(9)	C(10)	0.8(3)
N(2)	C(19)	C(20)	C(21)	-179.91(16)	C(8)	C(7)	C(12)	C(11)	-0.6(3)
N(2)	C(19)	C(24)	C(23)	-178.94(18)	C(8)	C(9)	C(10)	C(11)	-0.5(4)
N(3)	N(4)	C(6)	C(25)	-172.44(17)	C(9)	C(10)	C(11)	C(12)	-0.4(4)
N(3)	N(4)	C(6)	C(5)	-2.1(2)	C(10)	C(11)	C(12)	C(7)	1.0(4)
N(3)	C(2)	C(3)	N(1)	131.08(15)	C(12)	C(7)	C(8)	C(9)	-0.3(3)
N(3)	C(2)	C(3)	C(4)	-52.5(2)	C(13)	N(3)	N(4)	C(6)	-163.14(15)
N(3)	C(2)	C(5)	C(6)	-21.36(14)	C(13)	N(3)	C(2)	C(1)	49.53(19)
N(3)	C(2)	C(5)	C(7)	-150.72(14)	C(13)	N(3)	C(2)	C(3)	-67.9(2)
N(3)	C(13)	C(14)	C(15)	-175.41(19)	C(13)	N(3)	C(2)	C(5)	169.66(14)
N(3)	C(13)	C(18)	C(17)	176.23(18)	C(13)	C(14)	C(15)	C(16)	-1.0(4)
N(4)	N(3)	C(2)	C(1)	-97.06(15)	C(14)	C(13)	C(18)	C(17)	-1.1(3)
N(4)	N(3)	C(2)	C(3)	145.54(14)	C(14)	C(15)	C(16)	C(17)	-0.7(4)
N(4)	N(3)	C(2)	C(5)	23.07(16)	C(15)	C(16)	C(17)	C(18)	1.5(4)
N(4)	N(3)	C(13)	C(14)	11.3(2)	C(16)	C(17)	C(18)	C(13)	-0.7(3)
N(4)	N(3)	C(13)	C(18)	-166.02(16)	C(18)	C(13)	C(14)	C(15)	1.9(3)
C(1)	N(2)	C(19)	C(20)	31.4(2)	C(19)	N(2)	C(1)	O(1)	3.9(3)
C(1)	N(2)	C(19)	C(24)	-148.97(18)	C(19)	N(2)	C(1)	C(2)	-176.66(14)
C(1)	C(2)	C(3)	N(1)	7.98(17)	C(19)	C(20)	C(21)	C(22)	-1.1(3)
C(1)	C(2)	C(3)	C(4)	-175.64(16)	C(20)	C(19)	C(24)	C(23)	0.6(3)
C(1)	C(2)	C(5)	C(6)	98.66(15)	C(20)	C(21)	C(22)	C(23)	0.5(4)
C(1)	C(2)	C(5)	C(7)	-30.70(19)	C(21)	C(22)	C(23)	C(24)	0.7(4)
C(2)	N(3)	N(4)	C(6)	-14.24(19)	C(22)	C(23)	C(24)	C(19)	-1.2(4)

C(2)	N(3)	C(13)	C(14)	-133.32(18)	C(24)	C(19)	C(20)	C(21)	0.5(3)
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**Table S27 Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for Compound (*cis*)-6a.**

Atom	x	y	z	U(eq)
H(4A)	8867.74	6929.62	4300.91	98
H(4B)	8113.31	7645.69	4168.17	98
H(4C)	7261	7020.64	3580.43	98
H(5)	4750.95	7254.79	3838.38	58
H(8)	2311.74	6940.94	5689.86	78
H(9)	1150.62	5912.88	5861.2	101
H(10)	1782.32	4978.62	4970.2	111
H(11)	3536.95	5064.07	3892.31	115
H(12)	4658.51	6087.98	3677.23	89
H(14)	5307.3	9161.62	6598.67	83
H(15)	6937.79	9825.02	7792.54	105
H(16)	9480.36	9588.5	8174.79	103
H(17)	10399.59	8671.22	7387.86	94
H(18)	8792.75	8015.13	6157.17	78
H(20)	4919.35	6106.25	7792.27	73
H(21)	5394.68	5340.73	9196.75	88
H(22)	7741.2	4871.83	9705.96	100
H(23)	9660.03	5172.26	8835.59	101
H(24)	9244.67	5963.14	7467.84	79