

## *Supporting Information*

# **Substituent-controllable regioselective annulation of $\beta$ -enaminones with *N*-sulfonyl triazoles for modular access to imidazoles and pyrroles**

Hua Wang,<sup>1</sup> Tongtong Zhou,<sup>1</sup> Mengdi Wu,<sup>1</sup> Qingqing Ye,<sup>2,\*</sup> and Xinwei He,<sup>1,\*</sup>

<sup>1</sup> Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials (State Key Laboratory Cultivation Base), College of Chemistry and Materials Science, Anhui Normal University, Wuhu 241000, P.R. China

<sup>2</sup> Department of Medicine, Chuzhou City Vocation College, Chuzhou 239000, P.R. China

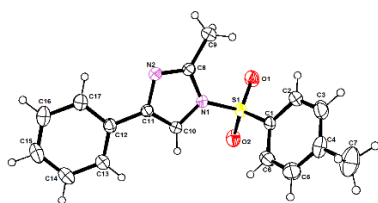
\*Corresponding authors: yeqingqing1983@sohu.com; xinweihe@mail.ahnu.edu.cn

### **Table of contents**

1. X-ray crystallographic data of compound <b>3a</b> -----	S2
2. X-ray crystallographic data of compound <b>5a</b> -----	S2
3. NMR spectra for all compounds-----	S3
4. GC-MS spectra for mechanistic investigations-----	S56



## 1. X-ray crystallographic data of compound 3a



**Figure S1.** ORTEP drawing of compound **3a** (30% probability for the thermal ellipsoid).

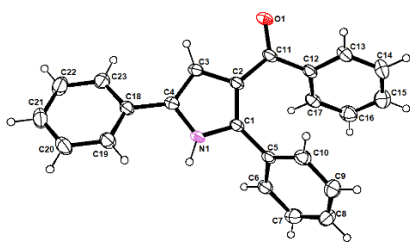
The purified compound **3a** is dissolved in a mixed solvent of ethyl acetate and petroleum ether, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal was obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCD APEX-2 diffractometer (graphite- monochromated Mo  $K\alpha$  radiation,  $\lambda=0.71073$  nm) at 298 K.

**Table S1.** Crystal data and structure refinement for compound **3a**.

CCDC number	2260879
Identification code	20191014c
Empirical formula	C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> S
Formula weight	312.38
Temperature	298.15 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c
Unit cell dimensions	a = 12.6175(5) Å $\alpha$ = 90°. b = 12.5587(5) Å $\beta$ = 99.2860(10). c = 10.4154(4) Å $\gamma$ = 90°.
Volume	1628.79(11) Å <sup>3</sup>
Z	4
Density (calculated)	1.274 g/cm <sup>3</sup>
$\mu$	0.207 mm <sup>-1</sup>
F(000)	656.0
Crystal size	0.21 × 0.2 × 0.19 mm <sup>3</sup>
2 $\theta$ range for data collection	5.722 to 55.072°
Index ranges	-16 ≤ h ≤ 16, -16 ≤ k ≤ 16, -13 ≤ l ≤ 13
Reflections collected	42190
Independent reflections	3738 [R(int) = 0.0258, R(sigma) = 0.0119]
Data / restraints / parameters	3738 / 0 / 201
Goodness-of-fit on F <sup>2</sup>	1.088
Final R indices [I>2sigma(I)]	R <sub>1</sub> = 0.0429, wR <sub>2</sub> = 0.1112
Final R indices (all data)	R <sub>1</sub> = 0.0511, wR <sub>2</sub> = 0.1204
Largest diff. peak and hole	0.21 and -0.43 eÅ <sup>-3</sup>



## 1. X-ray crystallographic data of compound 5a



**Figure S2.** ORTEP drawing of compound **5a** (30% probability for the thermal ellipsoid).

The purified compound **5a** is dissolved in a mixed solvent of ethyl acetate and petroleum ether, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal was obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCD APEX-2 diffractometer (graphite-monochromated Mo  $K\alpha$  radiation,  $\lambda=0.71073$  nm) at 298 K.

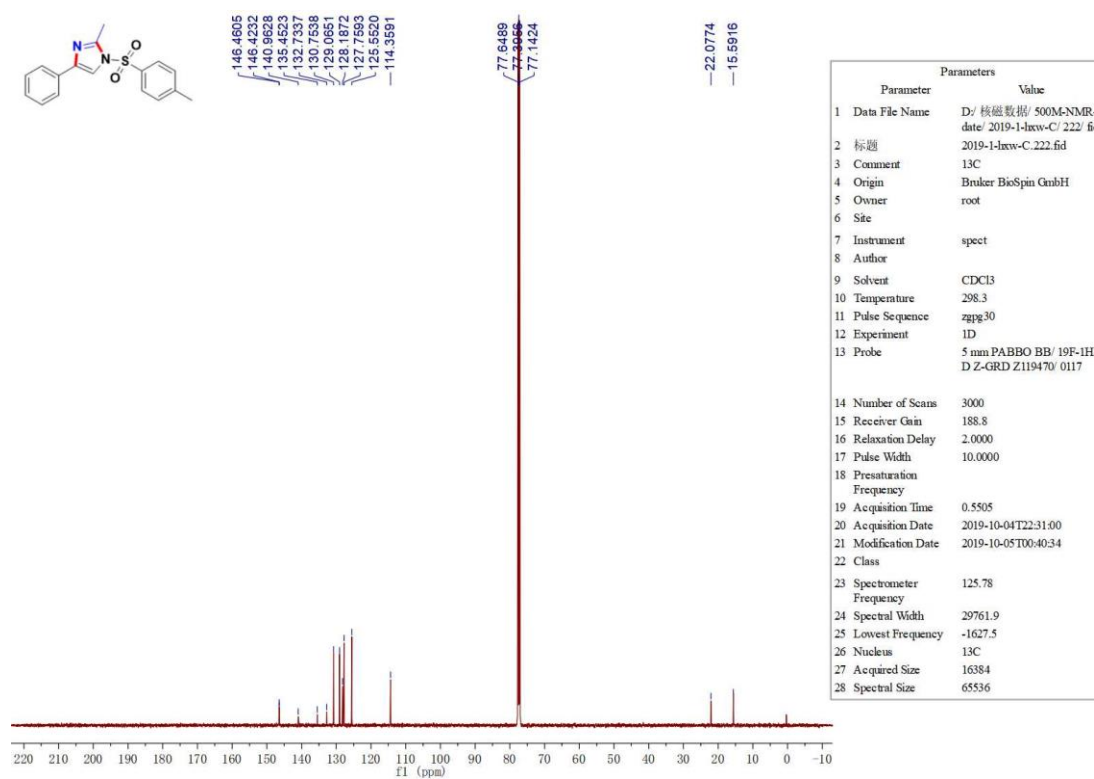
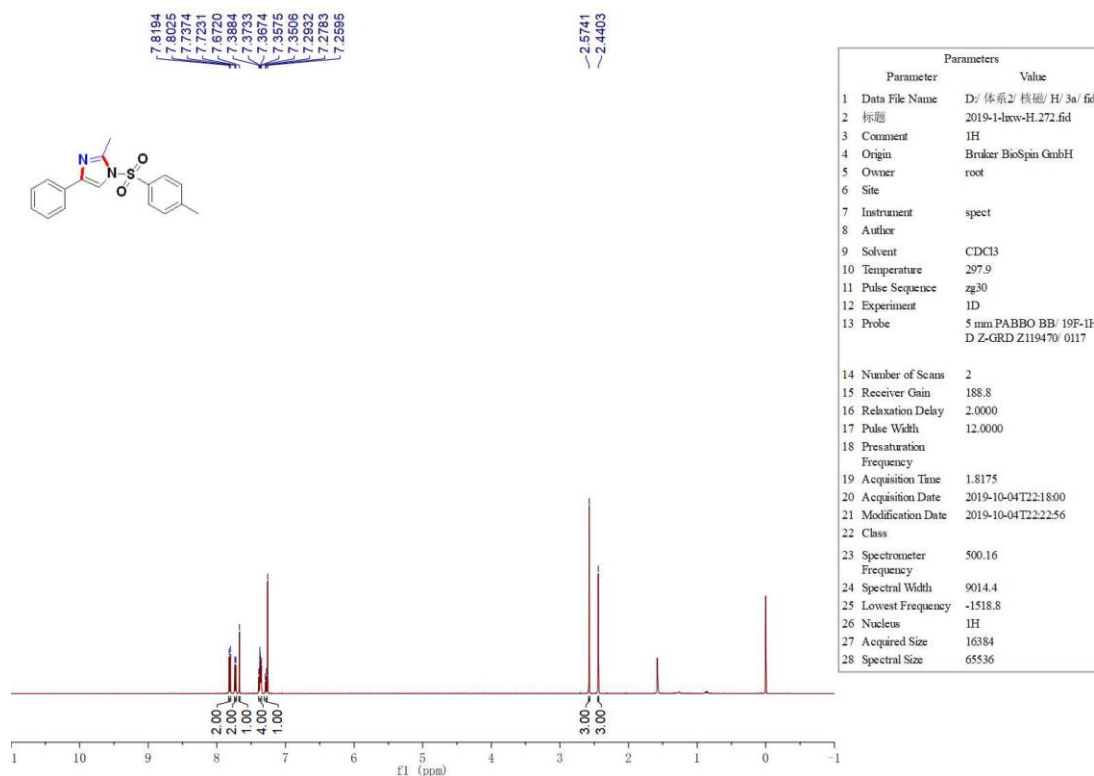
**Table S2.** Crystal data and structure refinement for compound **5a**.

CCDC number	2260880
Identification code	mo_20200109b_0m_a
Empirical formula	C <sub>23</sub> H <sub>17</sub> N O
Formula weight	323.38
Temperature	298.15 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.9209(10) Å $\alpha$ = 113.914(4)°. b = 13.3600(16) Å $\beta$ = 91.364(4)°. c = 14.6495(16) Å $\gamma$ = 102.145(5)°.
Volume	1722.3(3) Å <sup>3</sup>
Z	4
Density (calculated)	1.247 g/cm <sup>3</sup>
$\mu$	0.076 mm <sup>-1</sup>
F(000)	680.0
Crystal size	0.23 × 0.21 × 0.2 mm <sup>3</sup>
2 $\theta$ range for data collection	5.84 to 55.168°
Index ranges	-12 ≤ h ≤ 12, -17 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected	68223
Independent reflections	7947 [R(int) = 0.0439, R(sigma) = 0.0241]
Data / restraints / parameters	7947 / 0 / 451
Goodness-of-fit on F <sup>2</sup>	1.046
Final R indices [I > 2sigma(I)]	R <sub>1</sub> = 0.0547, wR <sub>2</sub> = 0.1552
Final R indices (all data)	R <sub>1</sub> = 0.0784, wR <sub>2</sub> = 0.1779
Largest diff. peak and hole	0.26 and -0.29 eÅ <sup>-3</sup>



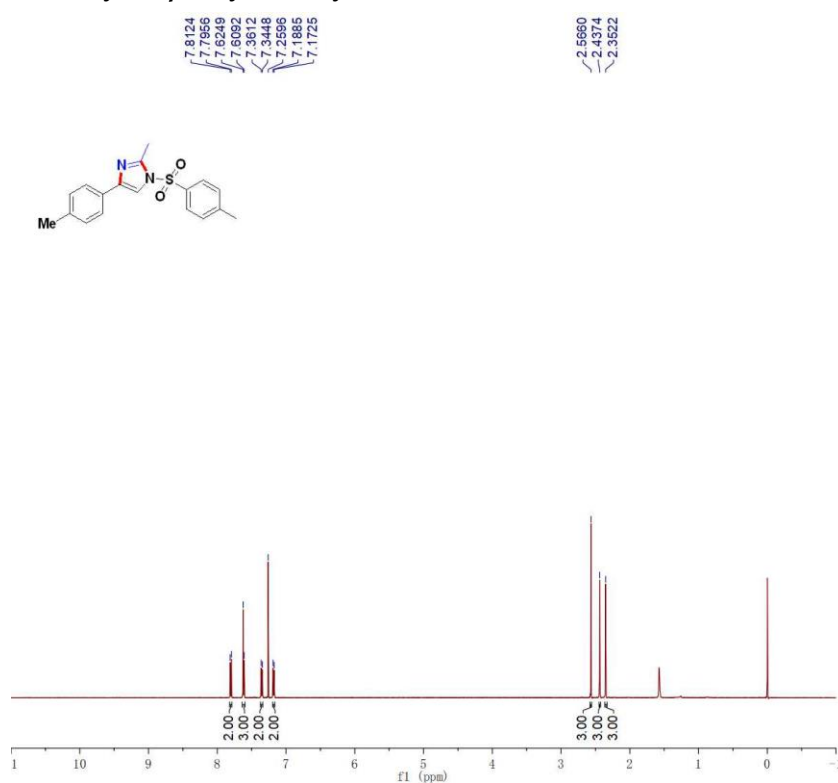
### 3. NMR spectra for all compounds

#### 2-Methyl-4-phenyl-1-tosyl-1H-imidazole (3a)

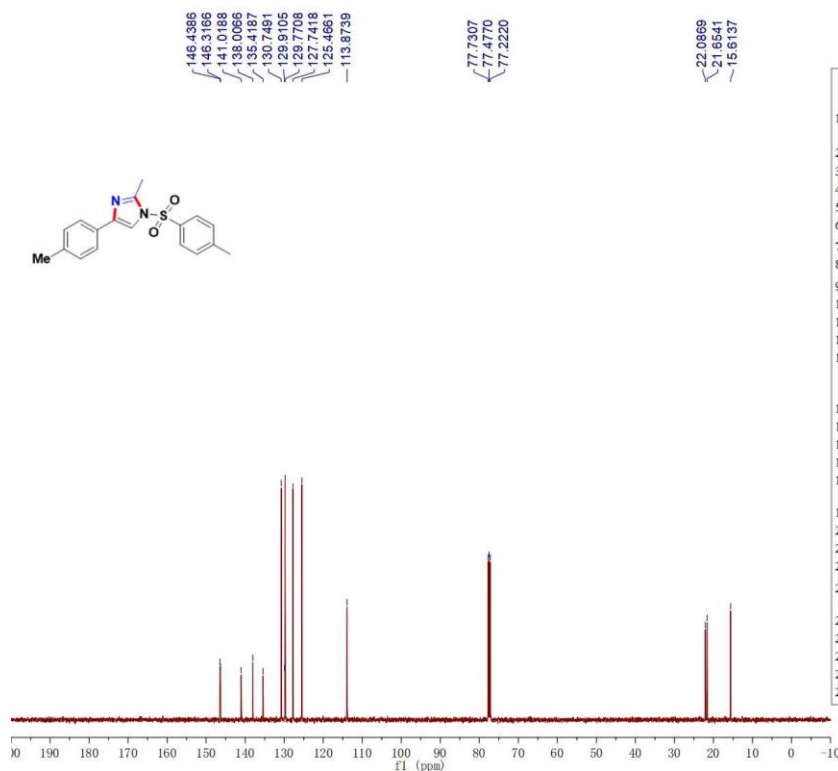




## 2-Methyl-4-(*p*-tolyl)-1-tosyl-1*H*-imidazole (3b)



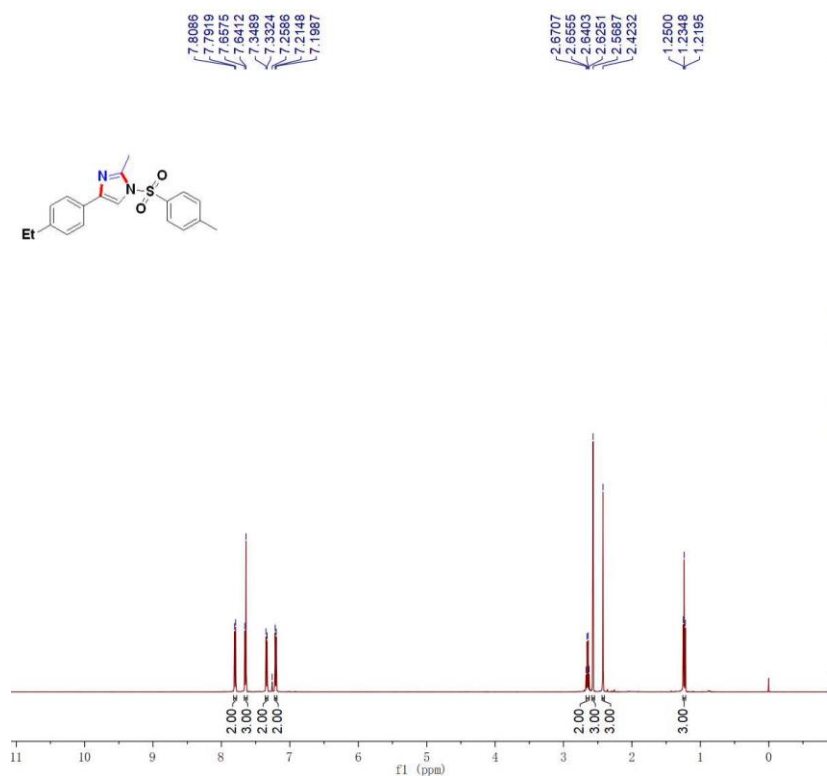
Parameters	
Parameter	Value
1 Data File Name	D:/体系2/核磁/H/ 4-甲 基.fid
2 标题	2019-1-hxxw-H.275.fid
3 Comment	1H
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
14 Number of Scans	2
15 Receiver Gain	150.9
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2019-10-10T11:17:00
21 Modification Date	2019-10-10T11:17:38
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1518.8
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



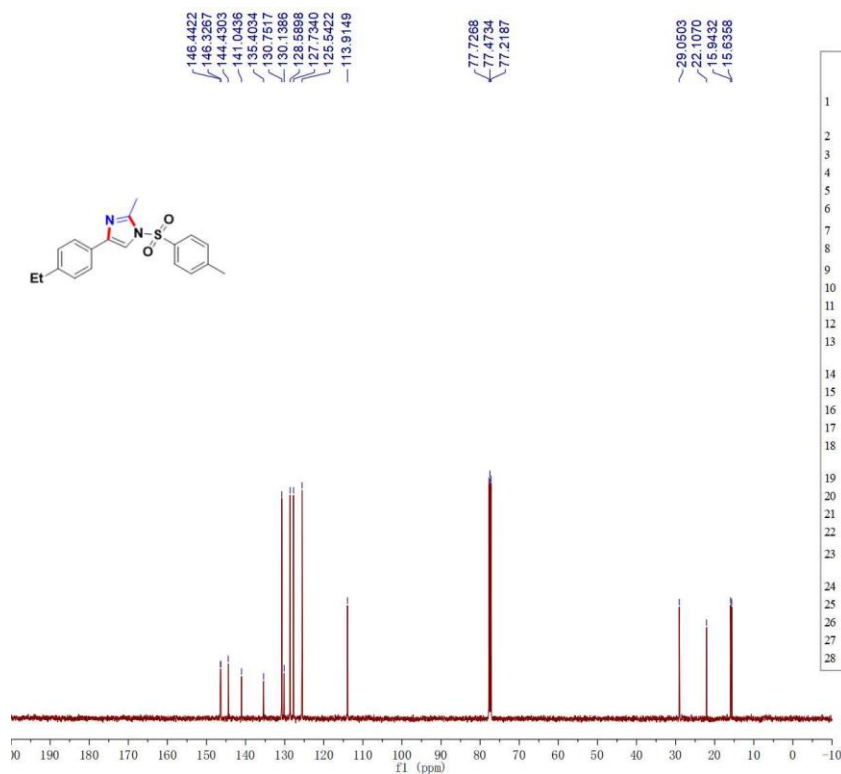
Parameters	
Parameter	Value
1 Data File Name	D:/核磁数据/ 500M-NMR- date/ 2019-1-hxxw-C/ 227.fid
2 标题	2019-1-hxxw-C.227.fid
3 Comment	13C
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
14 Number of Scans	40
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2019-10-10T22:36:00
21 Modification Date	2019-10-10T22:37:28
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536



# 4-(4-Ethylphenyl)-2-methyl-1-tosyl-1H-imidazole (3c)



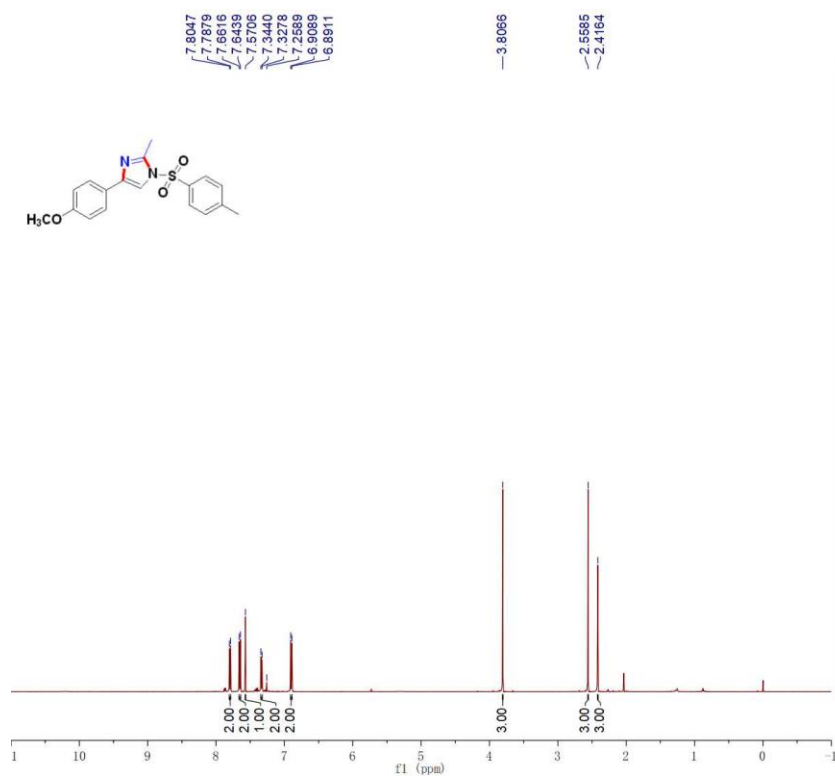
Parameters		
Parameter		Value
1 Data File Name	D:/体系2/核磁/H/4-乙基/	
2 标题	2020-1-sy-j-H.16.fid	
3 Comment	1H ztt	
4 Origin	Braker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	294.6	
11 Pulse Sequence	zg30	
12 Experiment	ID	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	30.7	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2019-12-30T11:00:05	
21 Modification Date	2019-12-30T11:00:06	
22 Class		
23 Spectrometer Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



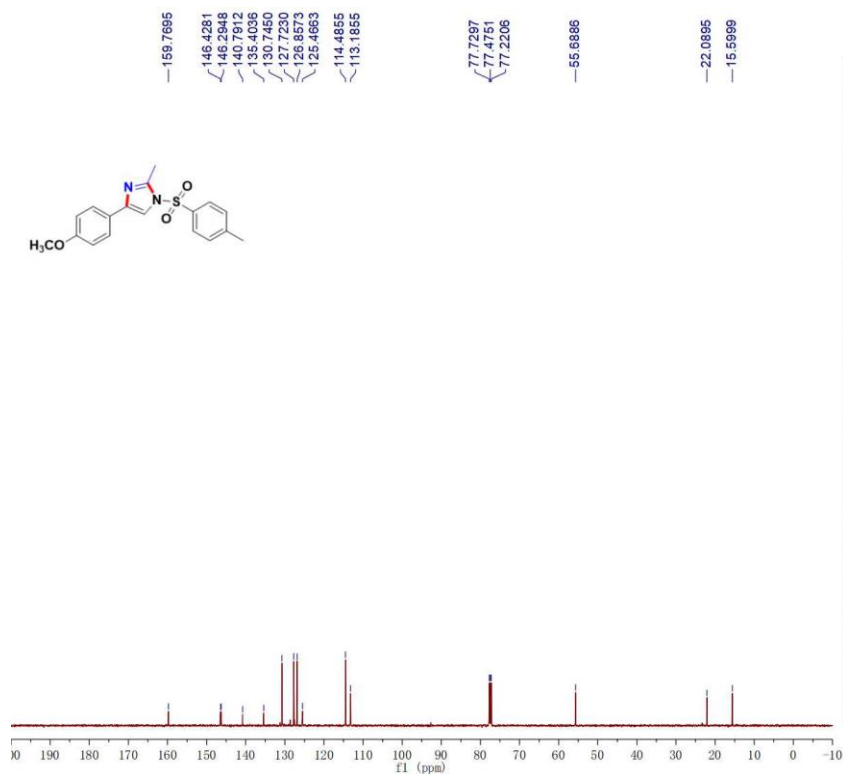
Parameters		
Parameter		Value
1 Data File Name	D:/核磁数据/ mmr/ mmr/	
2 标题	2020-1-sy-j-C-1.fid	
3 Comment	13C	
4 Origin	Braker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.3	
11 Pulse Sequence	zgpg30	
12 Experiment	ID	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	55	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation Frequency		
19 Acquisition Time	0.5505	
20 Acquisition Date	2019-12-30T11:31:59	
21 Modification Date	2019-12-30T11:32:02	
22 Class		
23 Spectrometer Frequency	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	



# 4-(4-Methoxyphenyl)-2-methyl-1-tosyl-1H-imidazole (3d)



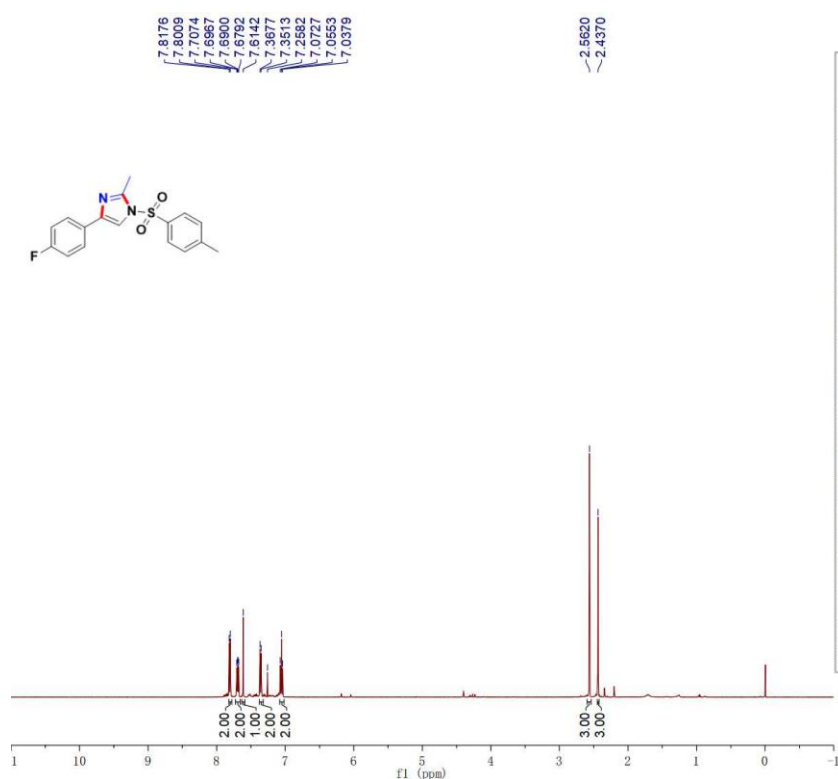
Parameters	
Parameter	Value
1 Data File Name	D:/ 体系2/ 核磁/ H/ 4-甲氧基/ fid
2 标题	2019-1-lxw-H.340.fid
3 Comment	1H
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
14 Number of Scans	2
15 Receiver Gain	30.7
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2019-12-10T12:42:00
21 Modification Date	2019-12-10T12:42:30
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1518.8
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



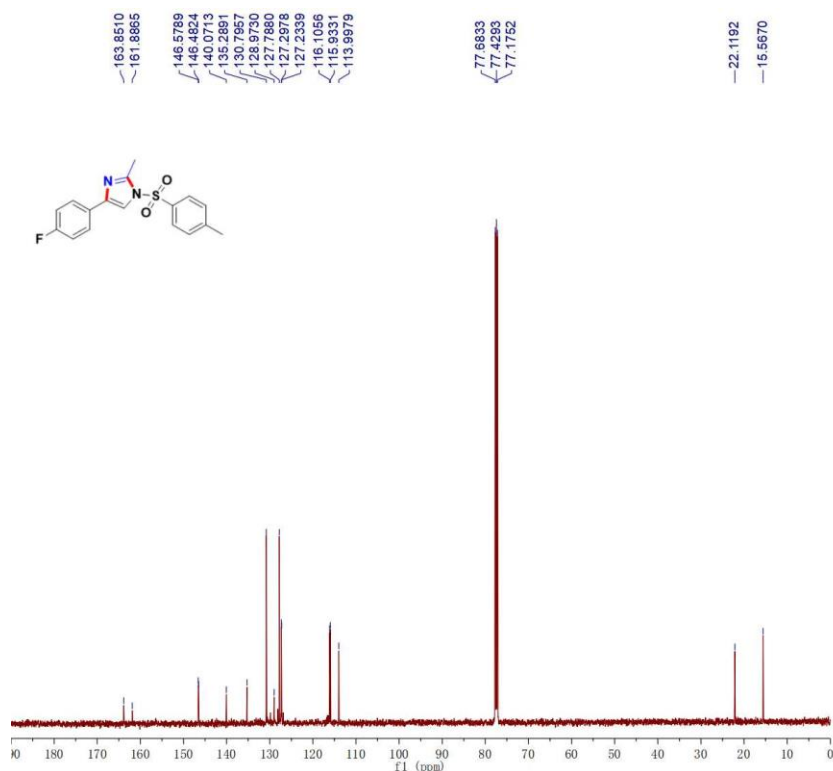
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 500M- NMR-date/ 2019-1-lxw-C/ 262.fid
2 标题	2019-1-lxw-C.262.fid
3 Comment	13C
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
14 Number of Scans	30
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2019-12-11T11:27:00
21 Modification Date	2019-12-11T11:28:54
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536



# 4-(4-Fluorophenyl)-2-methyl-1-tosyl-1H-imidazole (3e)



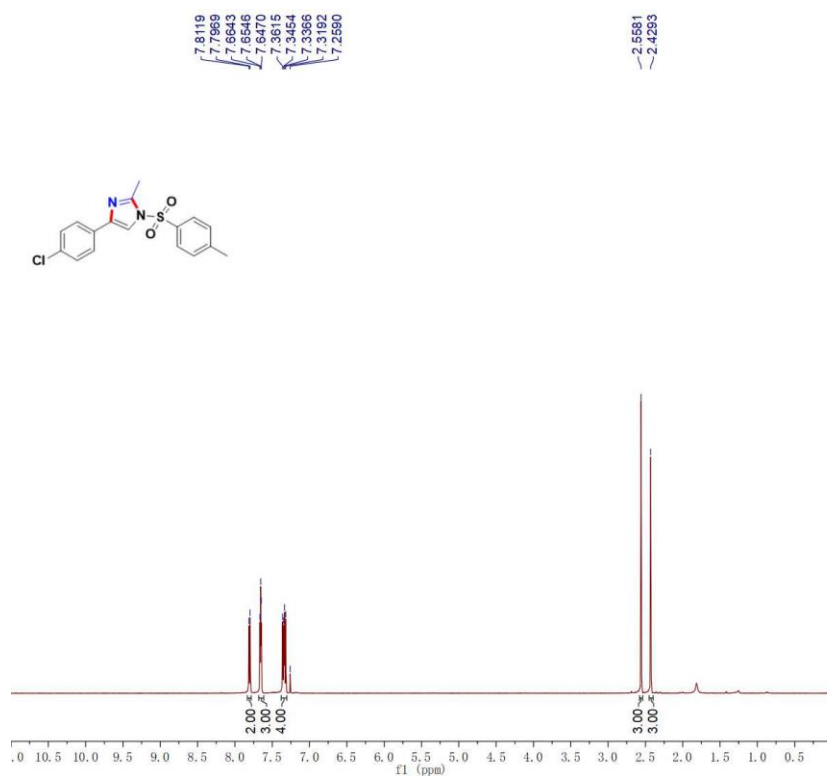
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 2020-1-hw-H/ 15/ fid	
2 标题	2020-1-hw-H.15.fid	
3 Comment	1H	
4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.7	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	87.0	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2019-12-26T11:01:59	
21 Modification Date	2019-12-26T11:02:00	
22 Class		
23 Spectrometer Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



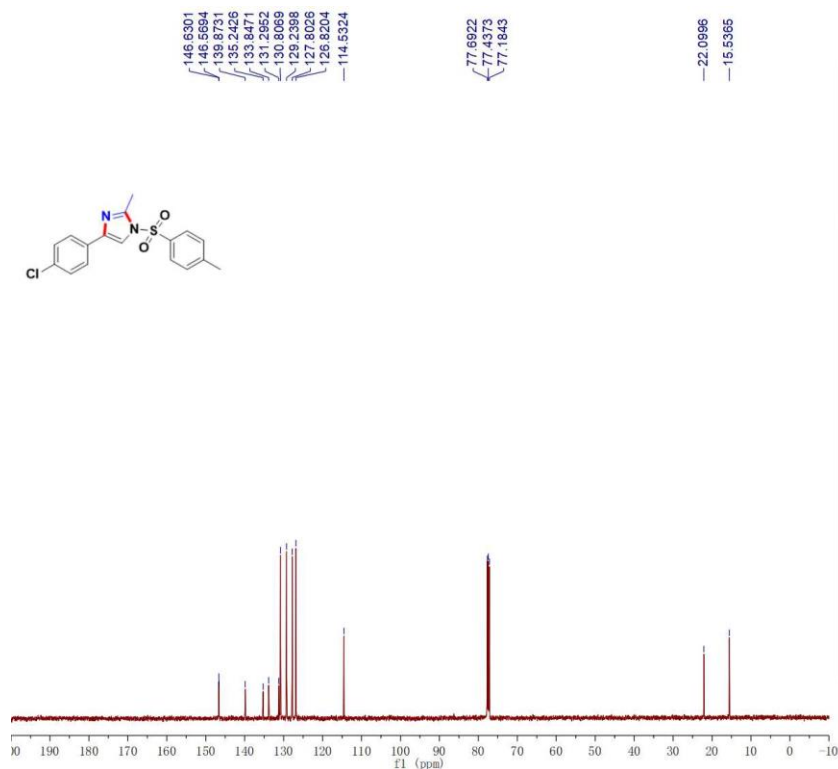
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 2020-1-hw-C/ 15/ fid	
2 标题	2020-1-hw-C.15.fid	
3 Comment	13C	
4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	296.0	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	180	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation Frequency		
19 Acquisition Time	0.5505	
20 Acquisition Date	2019-12-26T11:12:06	
21 Modification Date	2019-12-26T11:12:08	
22 Class		
23 Spectrometer Frequency	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	



# 4-(4-Chlorophenyl)-2-methyl-1-tosyl-1H-imidazole (3f)



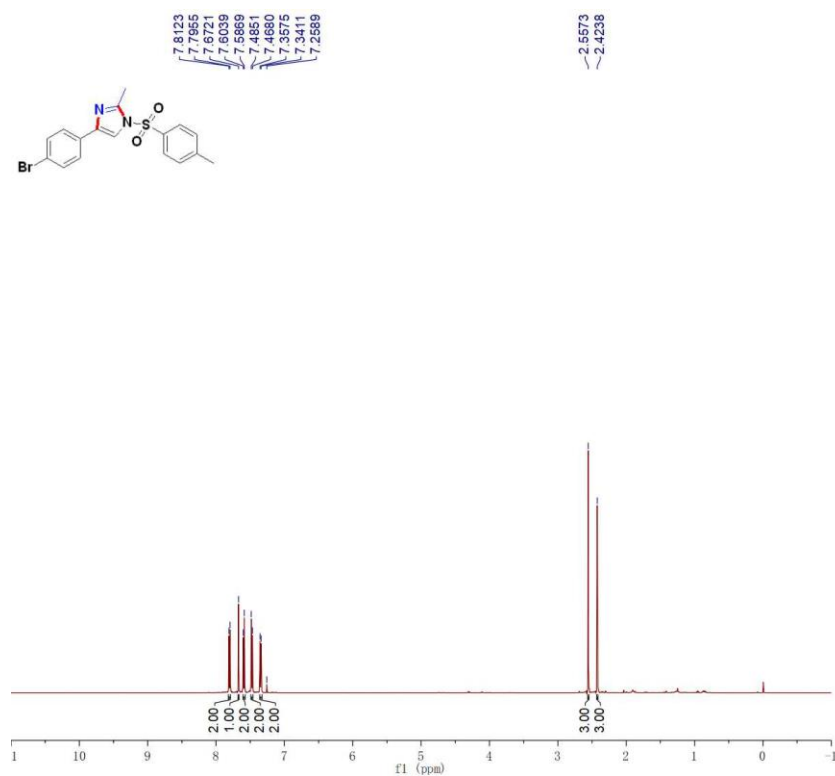
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy5-H-274.fid
2 标题	2020-1-sy5-H-274.fid
3 Comment	1H ztt
4 Origin	Brucker BioSpin GmbH
5 Owner	unusu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500SI BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	66.5
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2020-08-01T10:45:24
21 Modification Date	2020-08-01T10:45:26
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



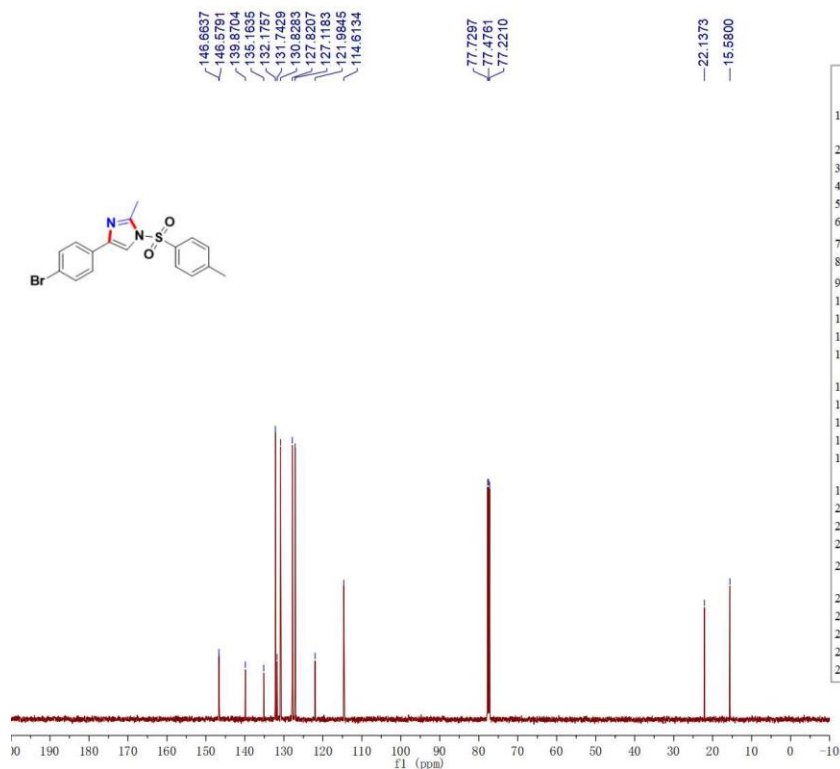
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy5-C-117.fid
2 标题	2020-1-sy5-C-117.fid
3 Comment	13C ztt
4 Origin	Brucker BioSpin GmbH
5 Owner	unusu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500SI BBF-H-D-05 Z SP)
14 Number of Scans	90
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2020-08-01T16:31:49
21 Modification Date	2020-08-01T16:31:52
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536



# 4-(4-Bromophenyl)-2-methyl-1-tosyl-1H-imidazole (3g)



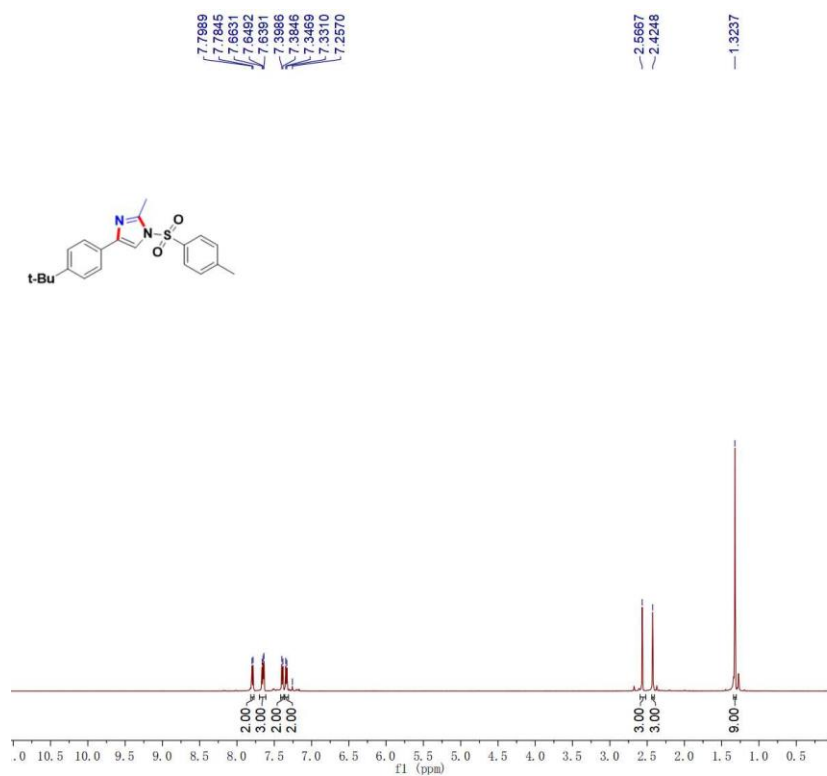
Parameters	
Parameter	Value
1 Data File Name	D:\核磁数据\nmr\ 2020-1-sy-j-H/ 17.fid
2 标题	2020-1-sy-j-H/ 17.fid
3 Comment	1H ztt
4 Origin	Braker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	48.1
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2019-12-30T11:03:18
21 Modification Date	2019-12-30T11:03:20
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



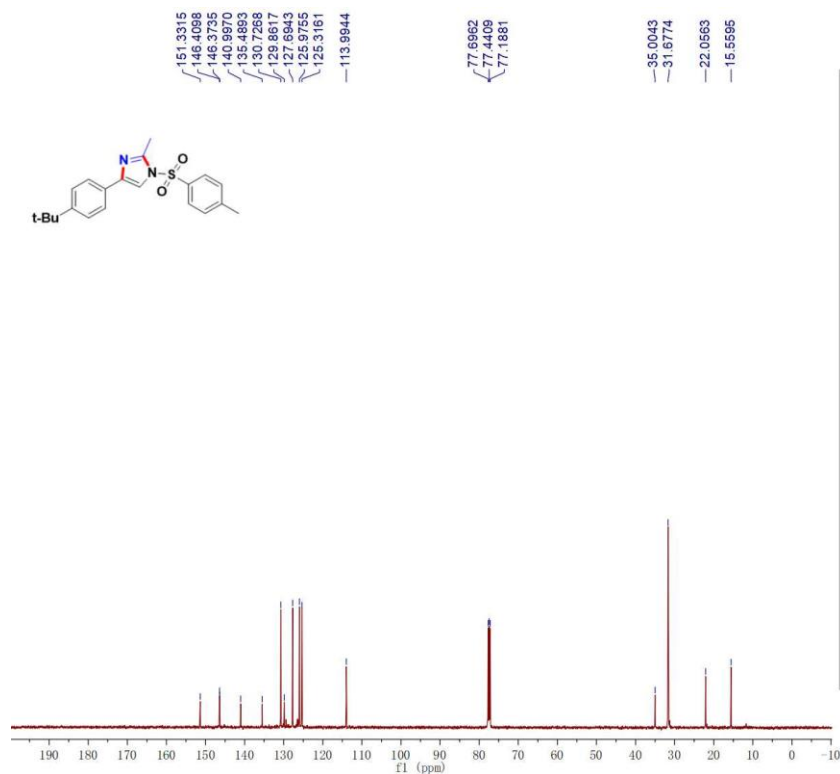
Parameters	
Parameter	Value
1 Data File Name	D:\核磁数据\ 2020-1-sy-j-C/ 2.fid
2 标题	2020-1-sy-j-C/ 2.fid
3 Comment	13C ztt
4 Origin	Braker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	60
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2019-12-30T11:38:07
21 Modification Date	2019-12-30T11:38:10
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536



# 4-(4-(*tert*-Butyl)phenyl)-2-methyl-1-tosyl-1*H*-imidazole (3h)



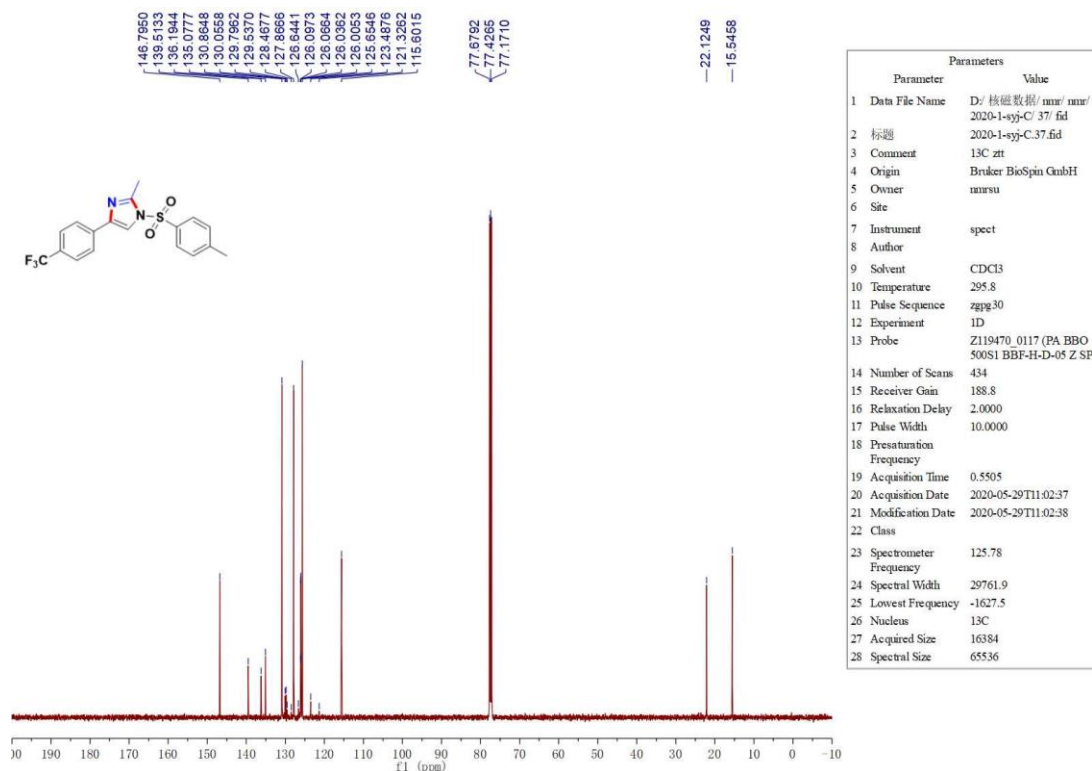
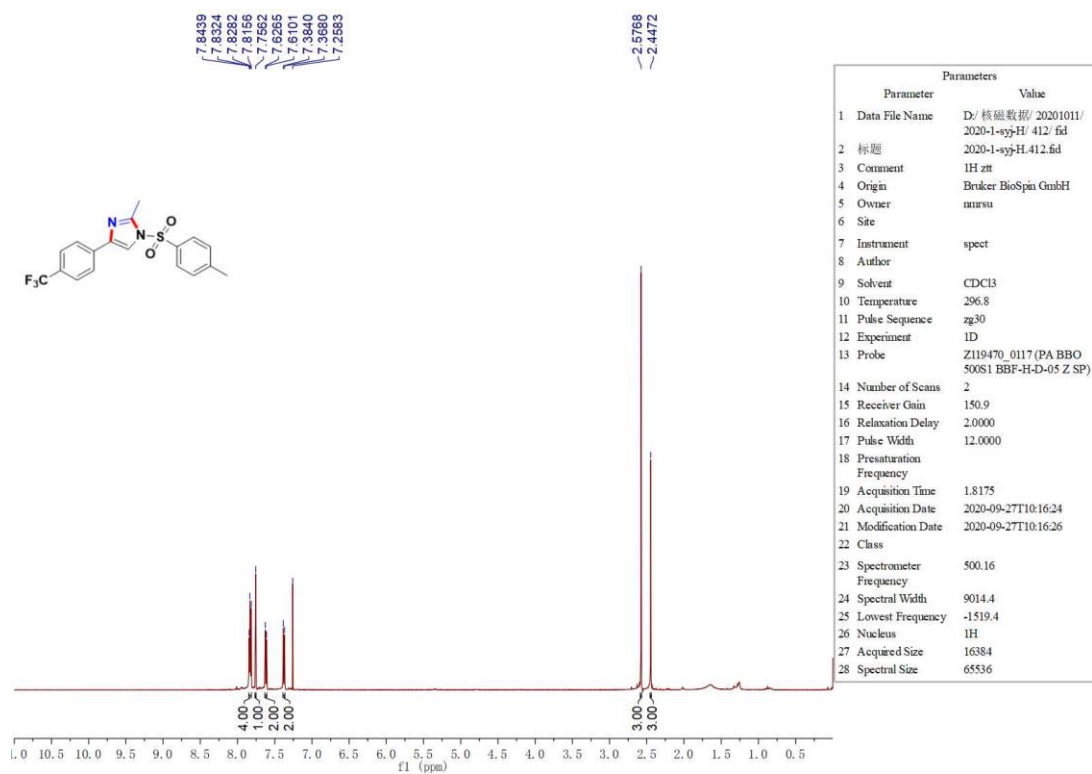
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-H/ 284.fid
2 标题	2020-1-sy-H.284.fid
3 Comment	1H ztt
4 Origin	Brüker BioSpin GmbH
5 Owner	nmusu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	301.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500SI BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	38.5
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2020-08-03T19:54:48
21 Modification Date	2020-08-03T19:54:50
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-C/ 128.fid
2 标题	2020-1-sy-C.128.fid
3 Comment	13C ztt
4 Origin	Brüker BioSpin GmbH
5 Owner	nmusu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	303.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500SI BBF-H-D-05 Z SP)
14 Number of Scans	189
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2020-08-05T20:51:46
21 Modification Date	2020-08-05T20:51:48
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536



## 2-Methyl-1-tosyl-4-(4-(trifluoromethyl)phenyl)-1H-imidazole (3i)



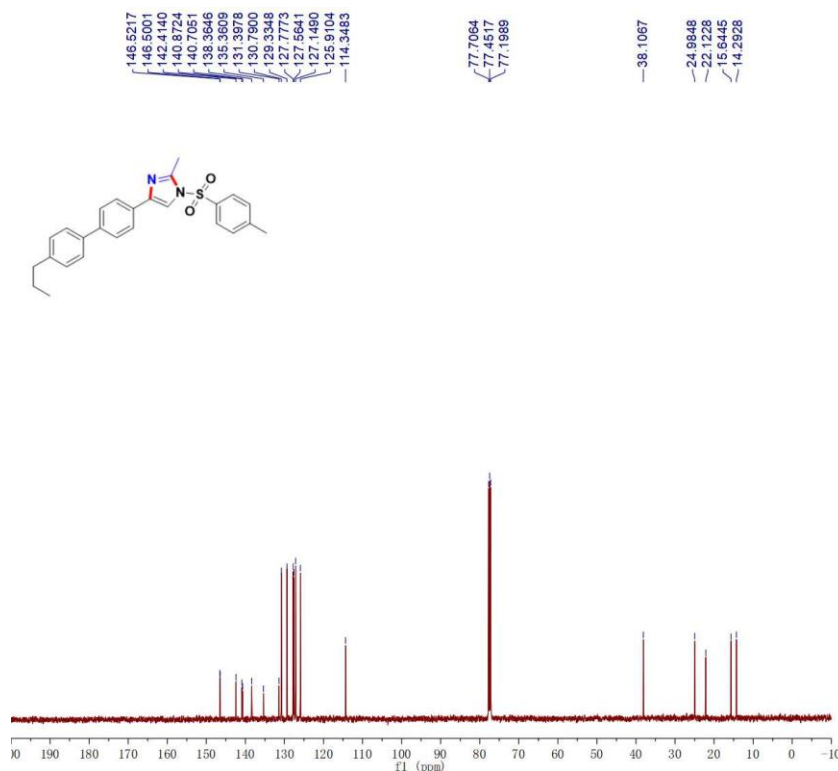


Chemical structure of compound 10: CCCC1=CC=C(C=C1)-c2ccc(cc2)/C=N/C(S(=O)(=O)c3ccc(cc3))C

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of compound 10. The x-axis represents the chemical shift in ppm, ranging from 1 to 11. The spectrum shows several peaks with corresponding integration values:

- Aromatic region (7.2-7.8 ppm):
  - 7.8313 (1.00)
  - 7.8144 (1.00)
  - 7.8043 (2.00)
  - 7.7872 (2.00)
  - 7.7132 (2.00)
  - 7.6332 (2.00)
  - 7.6060 (2.00)
  - 7.5844 (2.00)
  - 7.5393 (2.00)
  - 7.3864 (2.00)
  - 7.3505 (2.00)
  - 7.2635 (2.00)
  - 7.2468 (2.00)
- Aliphatic region (0.9-2.7 ppm):
  - 2.6457 (2.00)
  - 2.6308 (3.00)
  - 2.6151 (3.00)
  - 2.5930 (2.00)
  - 2.4358 (2.00)
  - 2.1189 (2.00)
  - 1.7189 (2.00)
  - 1.7039 (2.00)
  - 1.6889 (2.00)
  - 1.6737 (2.00)
  - 1.6587 (3.00)
  - 1.6441 (3.00)
  - 0.9898 (3.00)
  - 0.9752 (3.00)
  - 0.9605 (3.00)

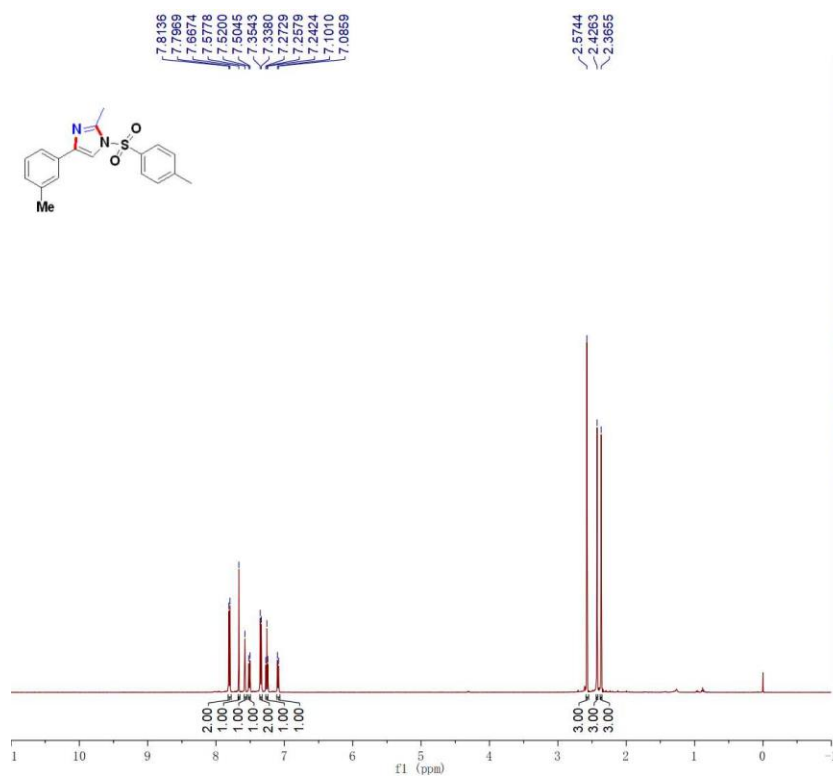
	Parameters	Value
1	Data File Name	D:/核磁数据/nmr/nmr/
2	标题	2020-1-sy-H.112.fid
3	Comment	1H ztt
4	Origin	2020-1-sy-H.112.fid
5	Owner	bruker BioSpin GmbH
6	Site	nmr5
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	2
15	Receiver Gain	385.1
16	Relaxation Delay	2.0000
17	Pulse Width	12.0000
18	Pretsaturation Frequency	
19	Acquisition Time	1.8175
20	Acquisition Date	2020-06-01T10:28:16
21	Modification Date	2020-06-01T10:28:18
22	Class	
23	Spectrometer Frequency	500.16
24	Spectral Width	9014.4
25	Lowest Frequency	-1519.4
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	65536



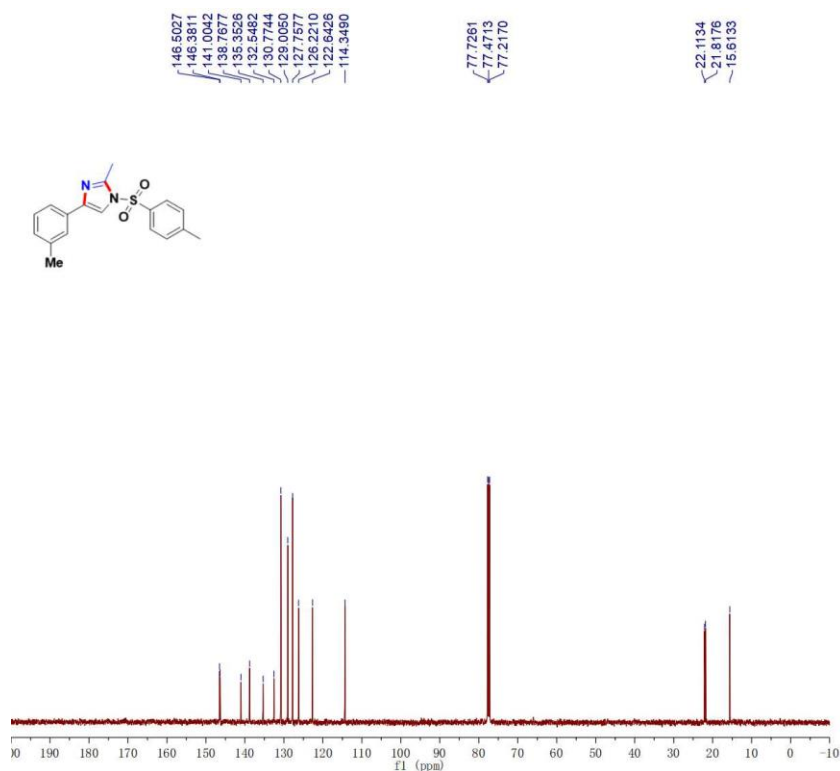
	Parameters	
	Parameter	Value
1	Data File Name	D:/ 核磁数据/ mmr/ mmr/ 2020-1-vy-C/ 40.fid
2	标题	2020-1-vy-C_40.fid
3	Comment	13C ztt
4	Origin	Braker BioSpin GmbH
5	Owner	mmru
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.8
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	13T19470_0117 (PA BBO 500S1 BBF-H-D-05 Z SE
14	Number of Scans	71
15	Receiver Gain	188.8
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Prestaturation Frequency	
19	Acquisition Time	0.5505
20	Acquisition Date	2020-06-01 T10:33:47
21	Modification Date	2020-06-01 T10:33:50
22	Class	
23	Spectrometer Frequency	125.78
24	Spectral Width	29761.9
25	Lowest Frequency	-1627.5
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536



## 2-Methyl-4-(*m*-tolyl)-1-tosyl-1H-imidazole (3k)



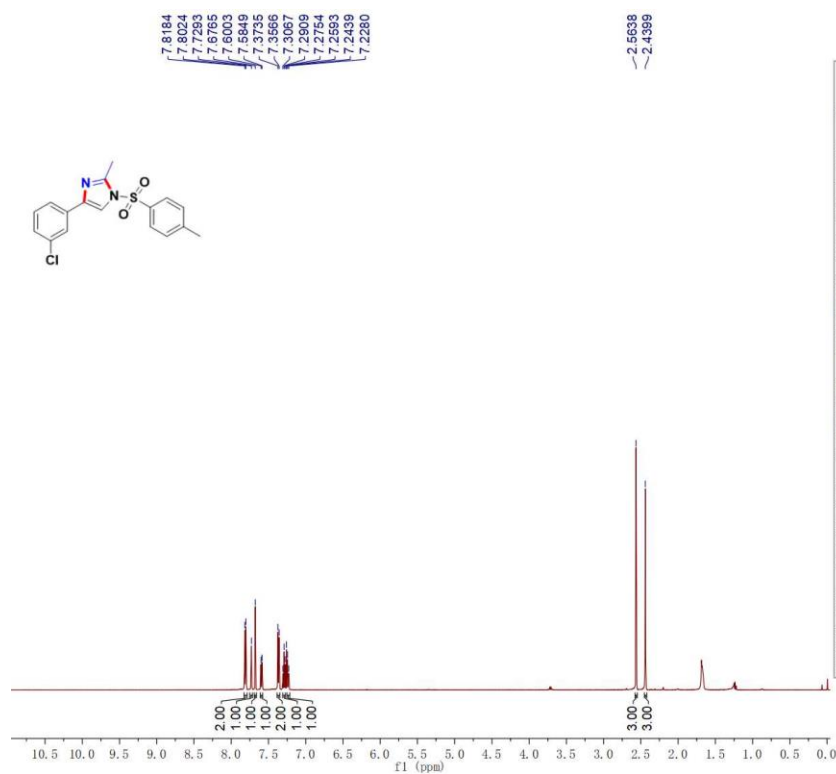
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-svj-H/ 18/ fid	
2 标题	2020-1-svj-H.18.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	294.6	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	48.1	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2019-12-30T11:06:28	
21 Modification Date	2019-12-30T11:06:30	
22 Class		
23 Spectrometer Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



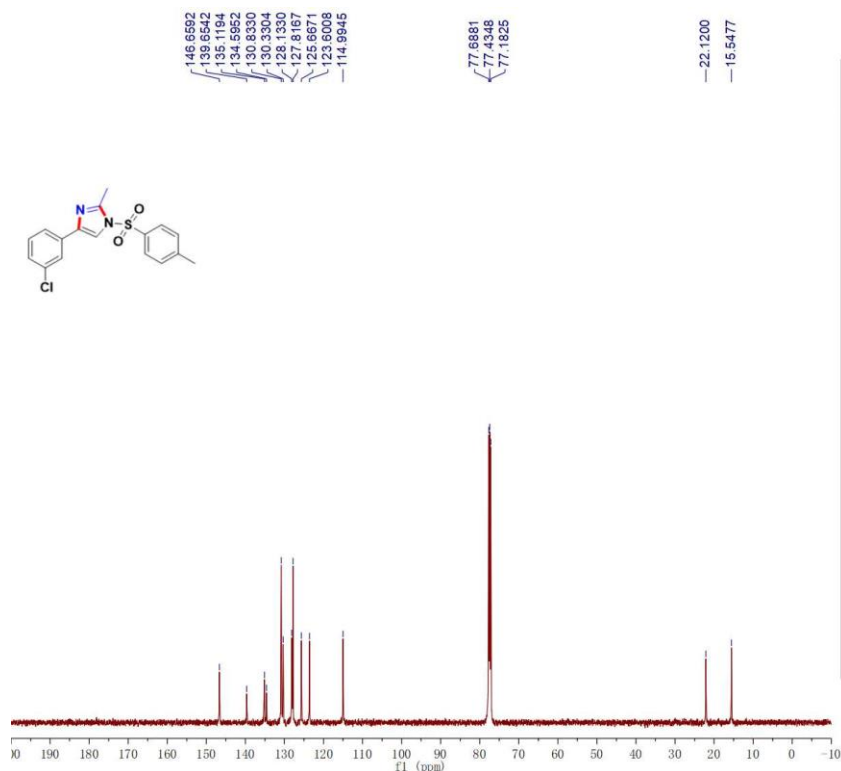
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-svj-C/ 3/ fid	
2 标题	2020-1-svj-C.3.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.4	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	60	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation Frequency		
19 Acquisition Time	0.5505	
20 Acquisition Date	2019-12-30T11:43:02	
21 Modification Date	2019-12-30T11:43:04	
22 Class		
23 Spectrometer Frequency	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	



# 4-(3-Chlorophenyl)-2-methyl-1-tosyl-1H-imidazole (3l)



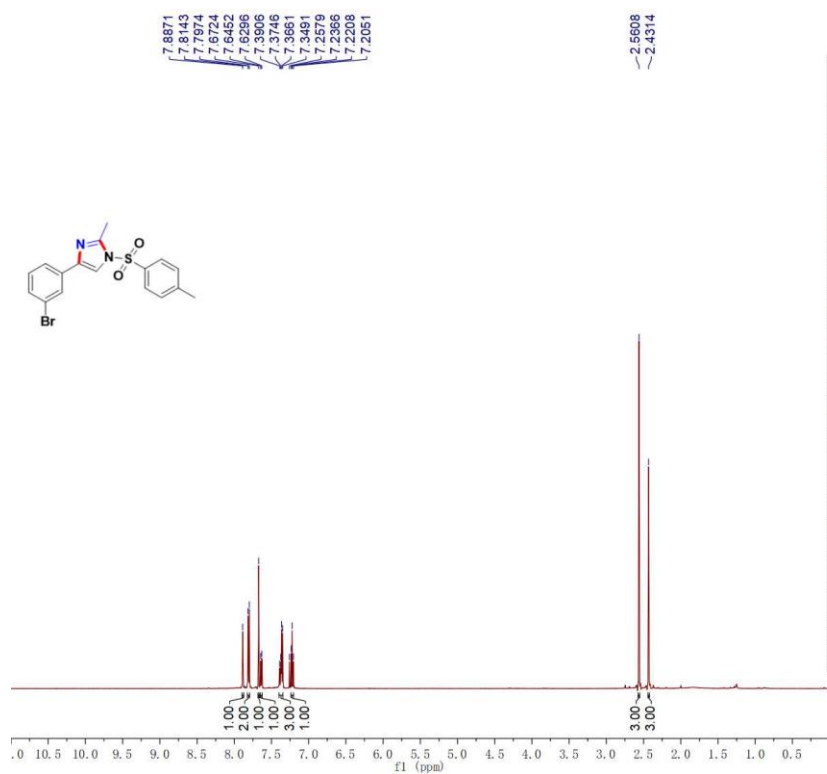
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-H/ 251/ f1d
2 标题	2020-1-sy-H-251.f1d
3 Comment	1H ztt
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	108.7
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2020-07-19T21:15:02
21 Modification Date	2020-07-19T21:15:04
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



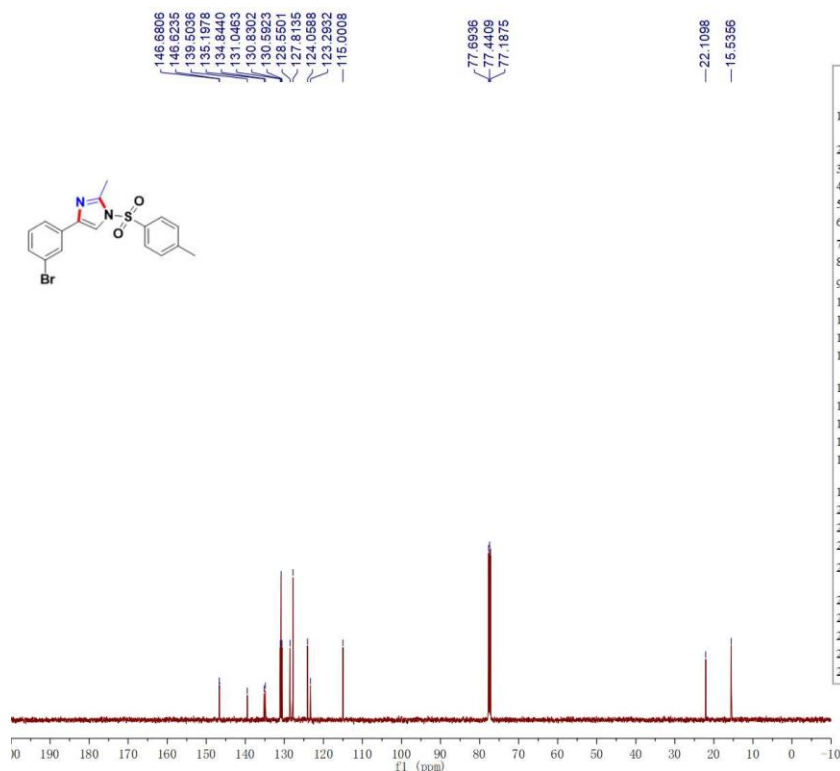
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-C/ 97/ f1d
2 标题	2020-1-sy-C-97.f1d
3 Comment	13C ztt
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	2000
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2020-07-17T13:43:42
21 Modification Date	2020-07-17T13:43:44
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536



# 4-(3-Bromophenyl)-2-methyl-1-tosyl-1H-imidazole (3m)



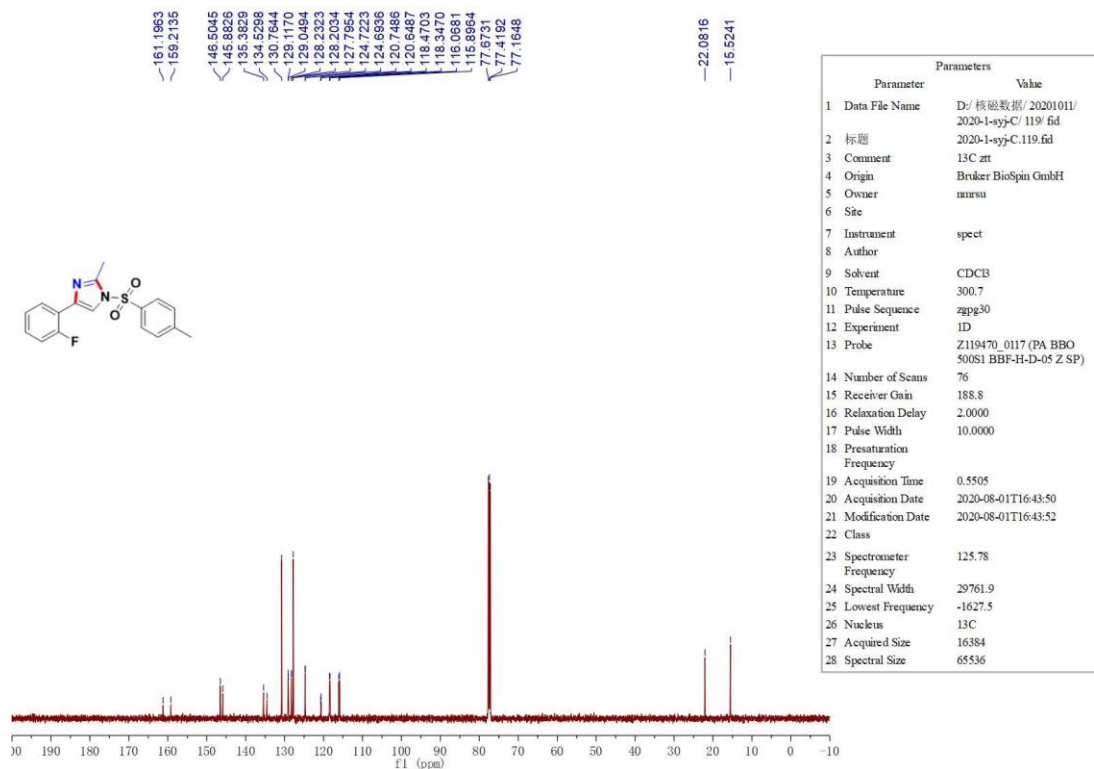
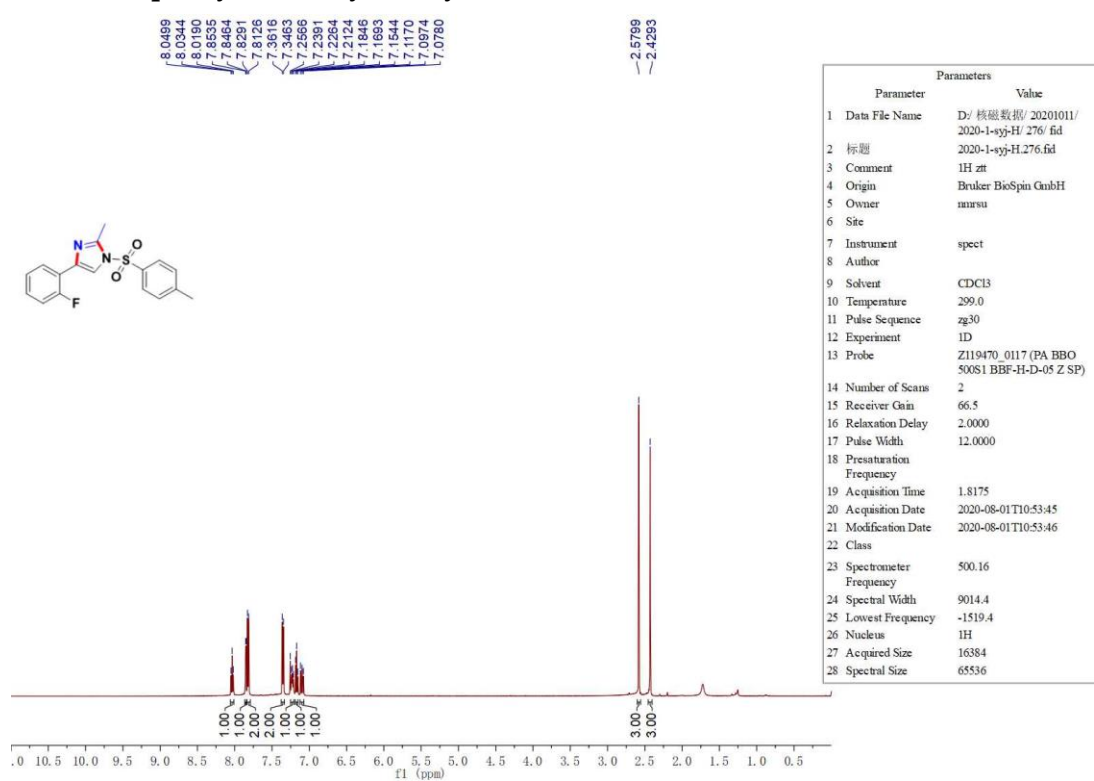
Parameters		
Parameter	Value	
1 Data File Name	D:\ 核磁数据\ 20201011\ 2020-1-yyj-H\ 275.fid	
2 标题	2020-1-yyj-H.275.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	299.0	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500SI BBR-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	66.5	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2020-08-01T10:49:13	
21 Modification Date	2020-08-01T10:49:14	
22 Class		
23 Spectrometer Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



Parameters		
Parameter	Value	
1 Data File Name	D:\ 核磁数据\ 20201011\ 2020-1-yyj-C\ 118.fid	
2 标题	2020-1-yyj-C.118.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	300.6	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500SI BBR-H-D-05 Z SP)	
14 Number of Scans	60	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation Frequency		
19 Acquisition Time	0.5505	
20 Acquisition Date	2020-08-01T16:37:30	
21 Modification Date	2020-08-01T16:37:32	
22 Class		
23 Spectrometer Frequency	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	

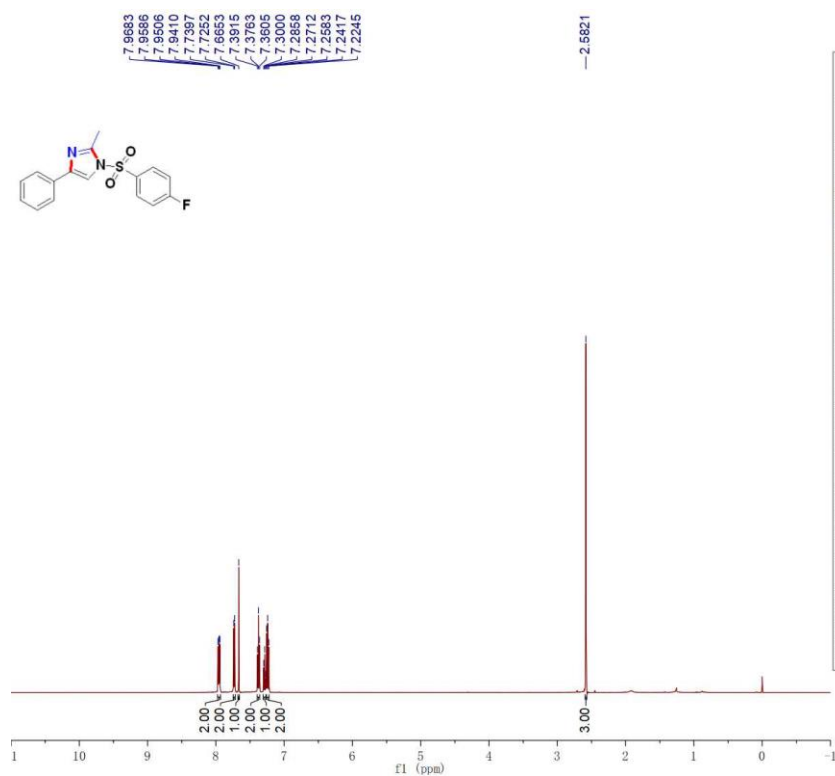


# 4-(2-Fluorophenyl)-2-methyl-1-tosyl-1H-imidazole (3n)

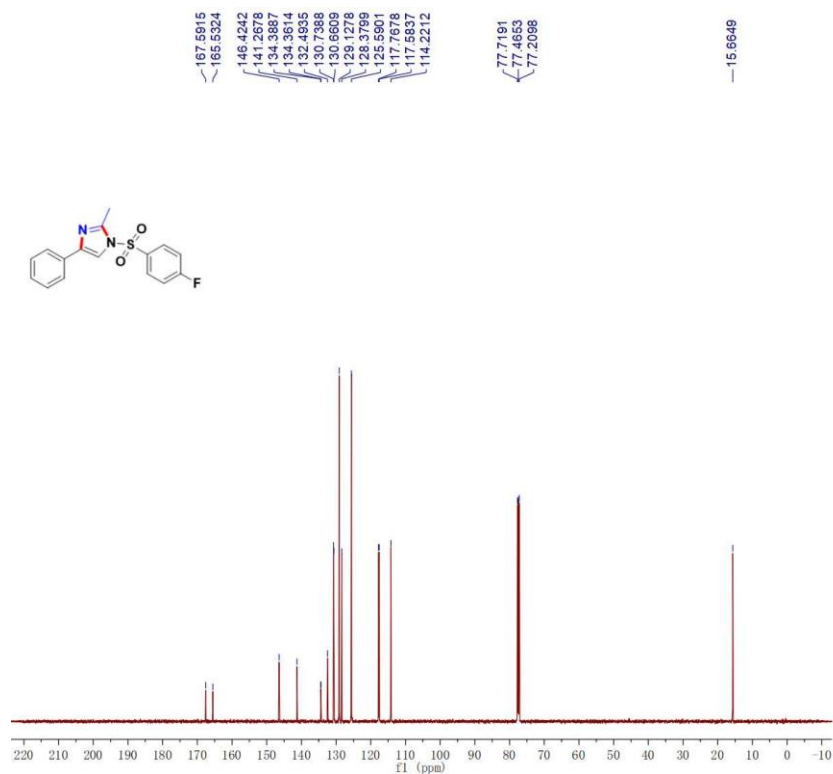




# 1-((4-Fluorophenyl)sulfonyl)-2-methyl-4-phenyl-1H-imidazole (3o)



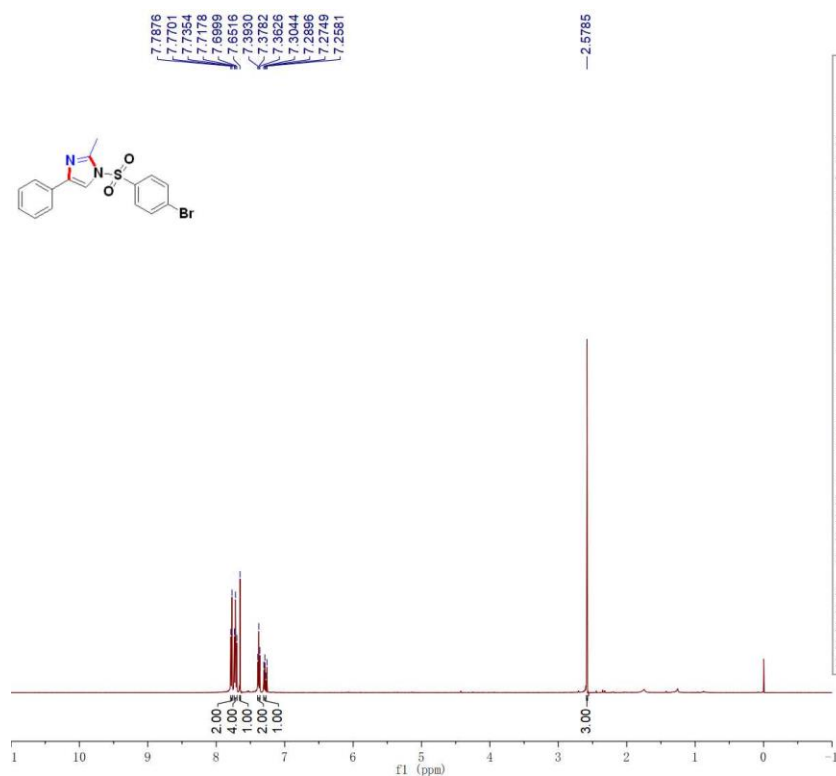
Parameters		
Parameter	Value	
1 Data File Name	D:\核磁数据\nmr\nmr\2020-1-yyj-H\114.fid	
2 标题	2020-1-yyj-H.114.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.7	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470.0117 (PA BBO 500S1 BBR-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	59.2	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation	Frequency	
19 Acquisition Time	1.8175	
20 Acquisition Date	2020-06-01T10:45:16	
21 Modification Date	2020-06-01T10:45:18	
22 Class		
23 Spectrometer	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



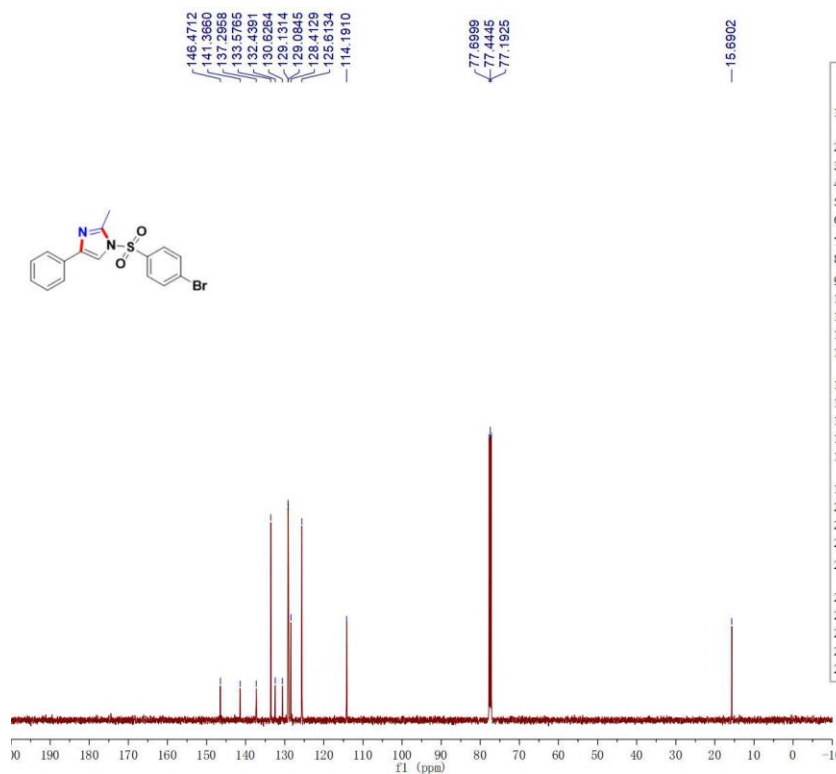
Parameters		
Parameter	Value	
1 Data File Name	D:\核磁数据\nmr\nmr\2020-1-yyj-C\42.fid	
2 标题	2020-1-yyj-C.42.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.6	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470.0117 (PA BBO 500S1 BBR-H-D-05 Z SP)	
14 Number of Scans	294	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation	Frequency	
19 Acquisition Time	0.5505	
20 Acquisition Date	2020-06-01T11:00:15	
21 Modification Date	2020-06-01T11:00:18	
22 Class		
23 Spectrometer	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	



# 1-((4-Bromophenyl)sulfonyl)-2-methyl-4-phenyl-1H-imidazole (3p)



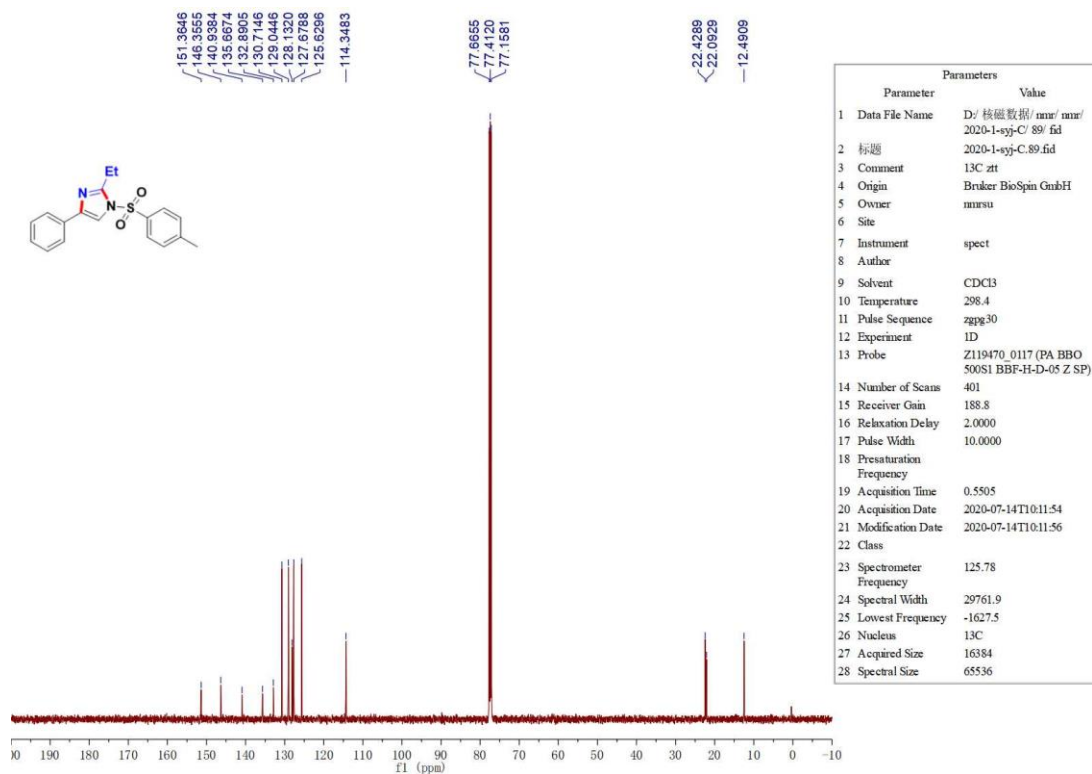
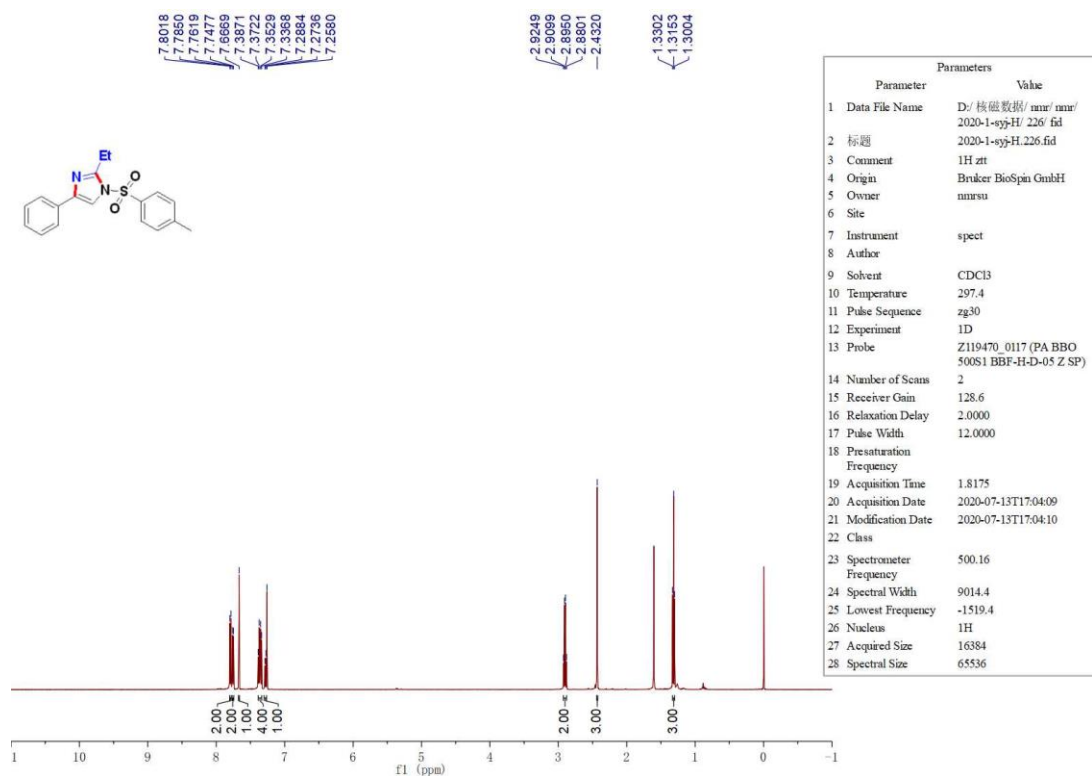
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-yyj-H/ 113/ fid	
2 标题	2020-1-yyj-H.113.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.6	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	87.0	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2020-06-01T10:36:18	
21 Modification Date	2020-06-01T10:36:20	
22 Class		
23 Spectrometer	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-yyj-C/ 41/ fid	
2 标题	2020-1-yyj-C.41.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.7	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	100	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation Frequency		
19 Acquisition Time	0.5505	
20 Acquisition Date	2020-06-01T10:42:46	
21 Modification Date	2020-06-01T10:42:48	
22 Class		
23 Spectrometer	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	

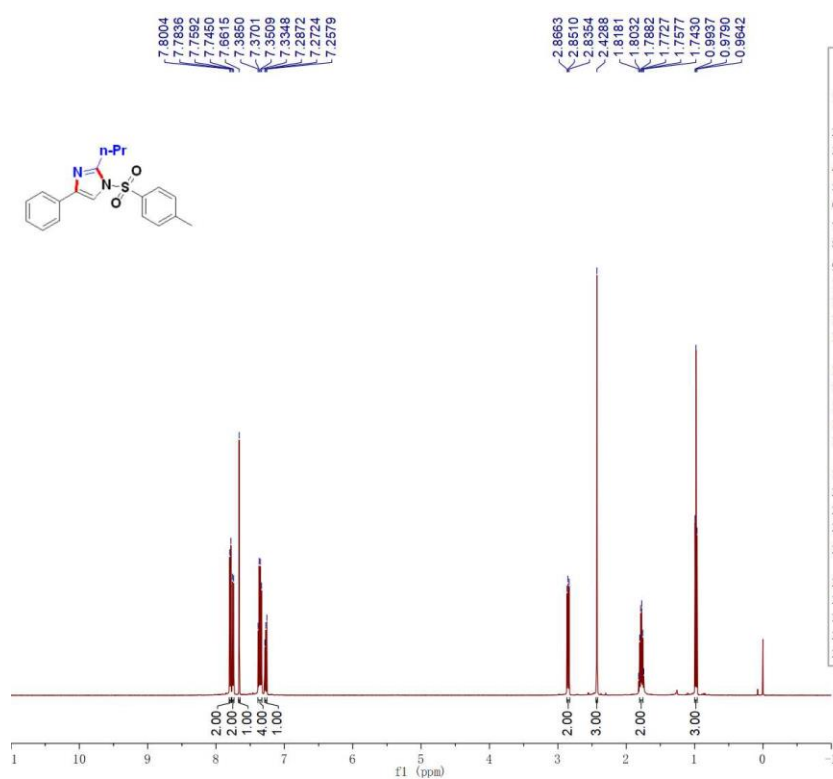


## 2-Ethyl-4-phenyl-1-tosyl-1H-imidazole (3q)

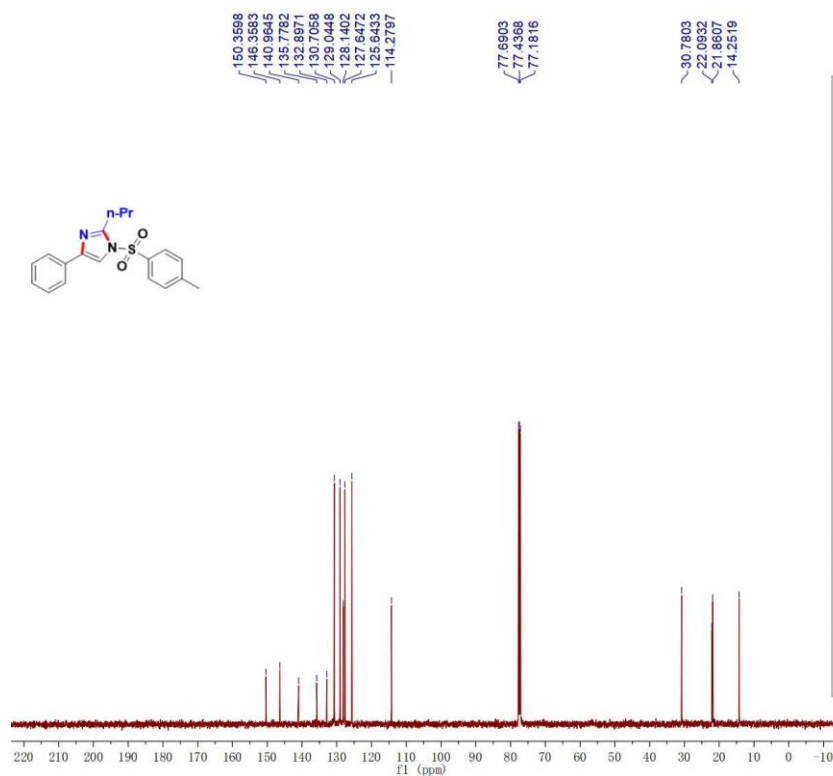




# 4-Phenyl-2-propyl-1-tosyl-1H-imidazole (3r)



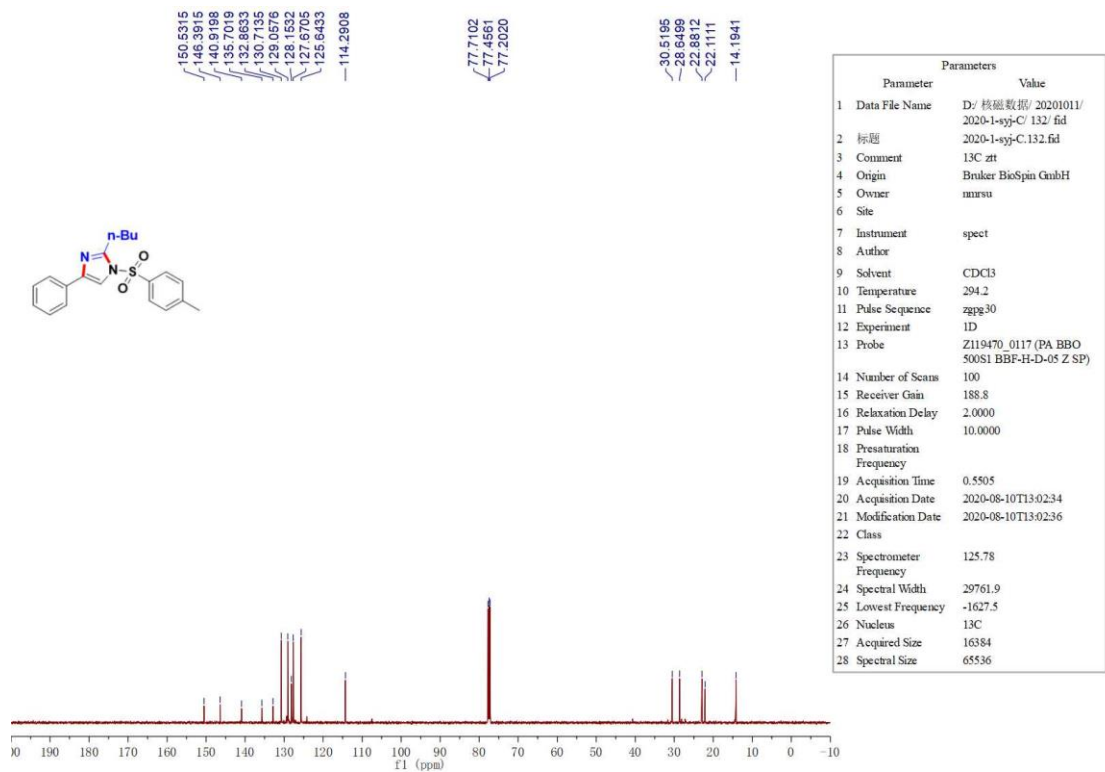
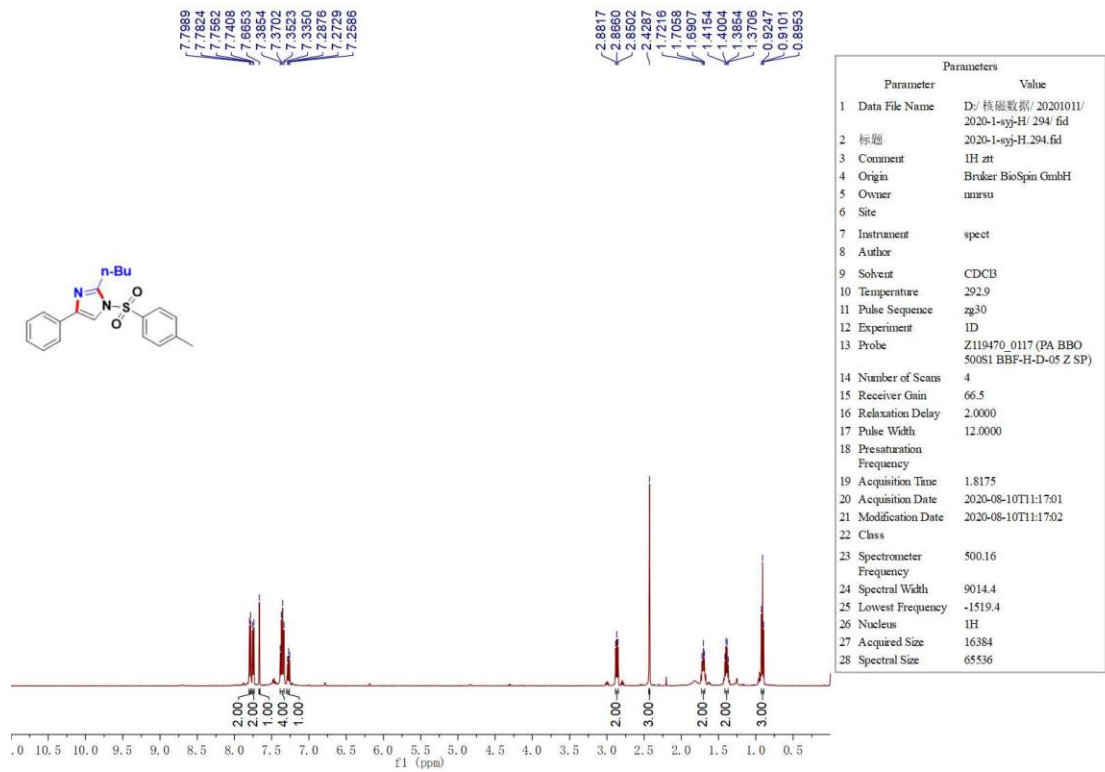
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-syy-H/ 224/ fid	
2 标题	2020-1-syy-H.224.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	297.4	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	66.5	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation	Frequency	
19 Acquisition Time	1.8175	
20 Acquisition Date	2020-07-13T16:48:36	
21 Modification Date	2020-07-13T16:48:38	
22 Class		
23 Spectrometer	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-syy-C/ 87/ fid	
2 标题	2020-1-syy-C.87.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	297.9	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	100	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation	Frequency	
19 Acquisition Time	0.5505	
20 Acquisition Date	2020-07-14T09:18:30	
21 Modification Date	2020-07-14T09:18:32	
22 Class		
23 Spectrometer	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	

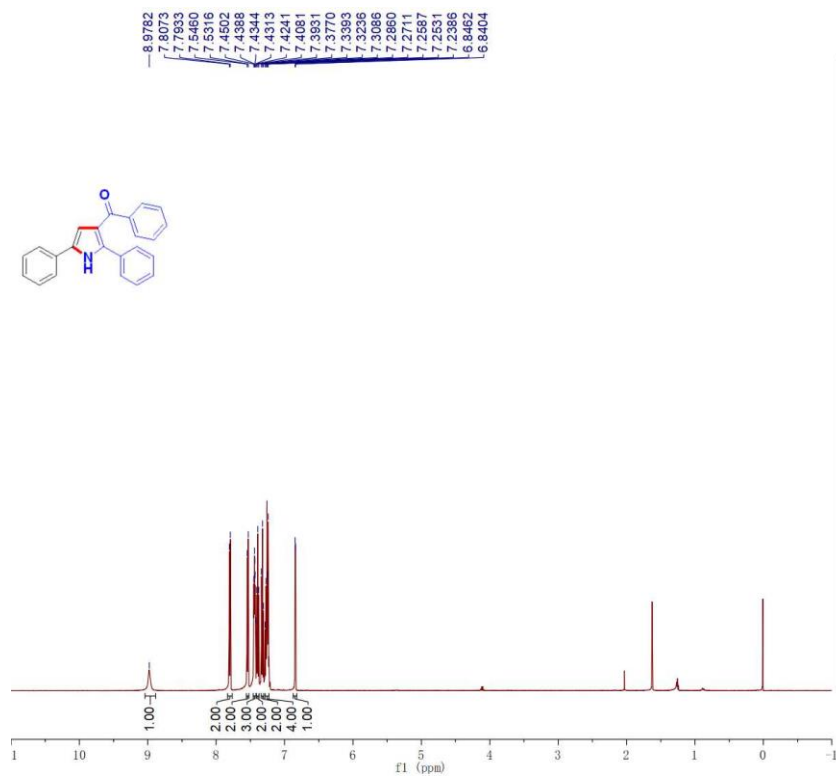


2-Butyl-4-phenyl-1-tosyl-1H-imidazole (3s)

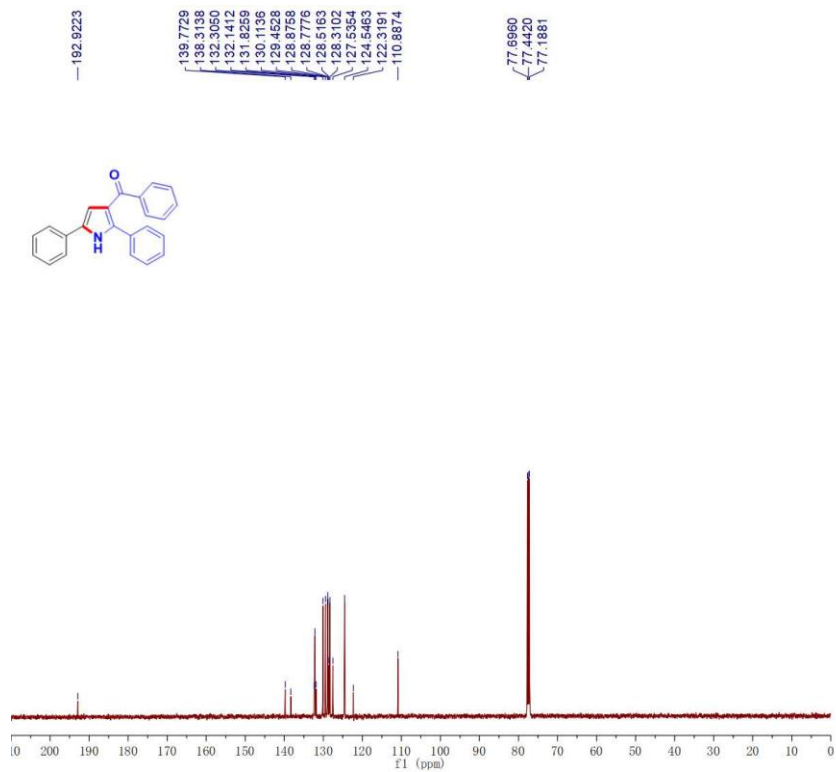




(2,5-Diphenyl-1H-pyrrol-3-yl)(phenyl)methanone (5a)



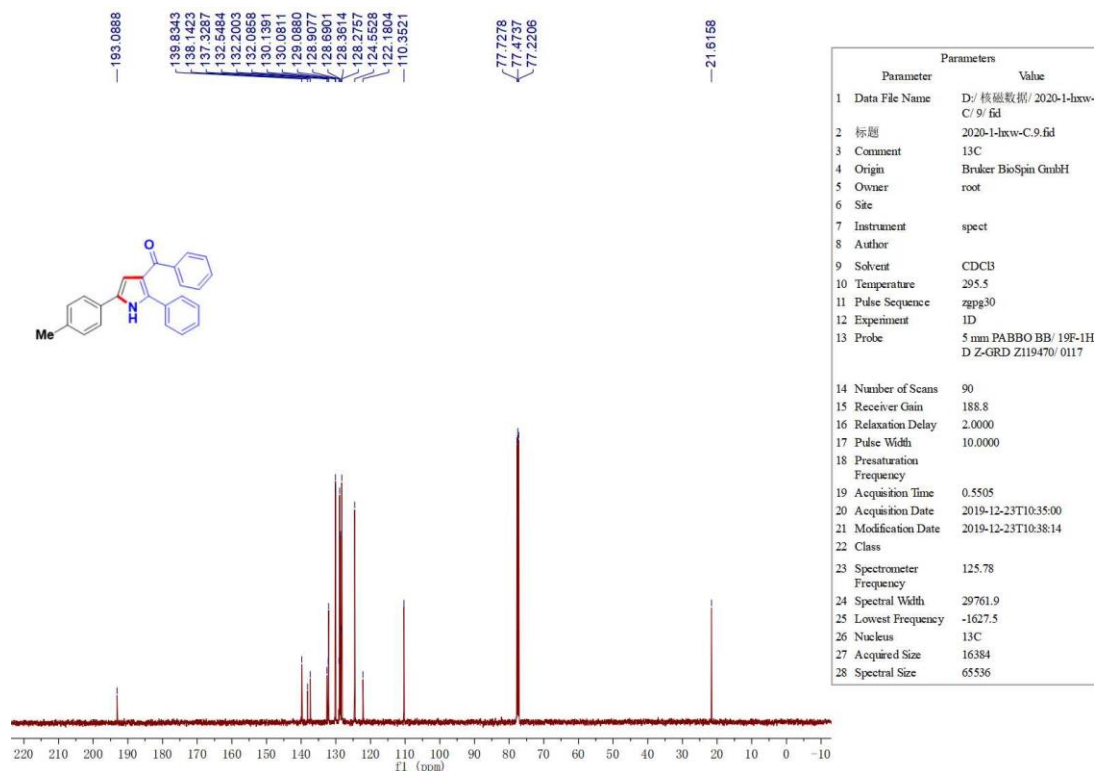
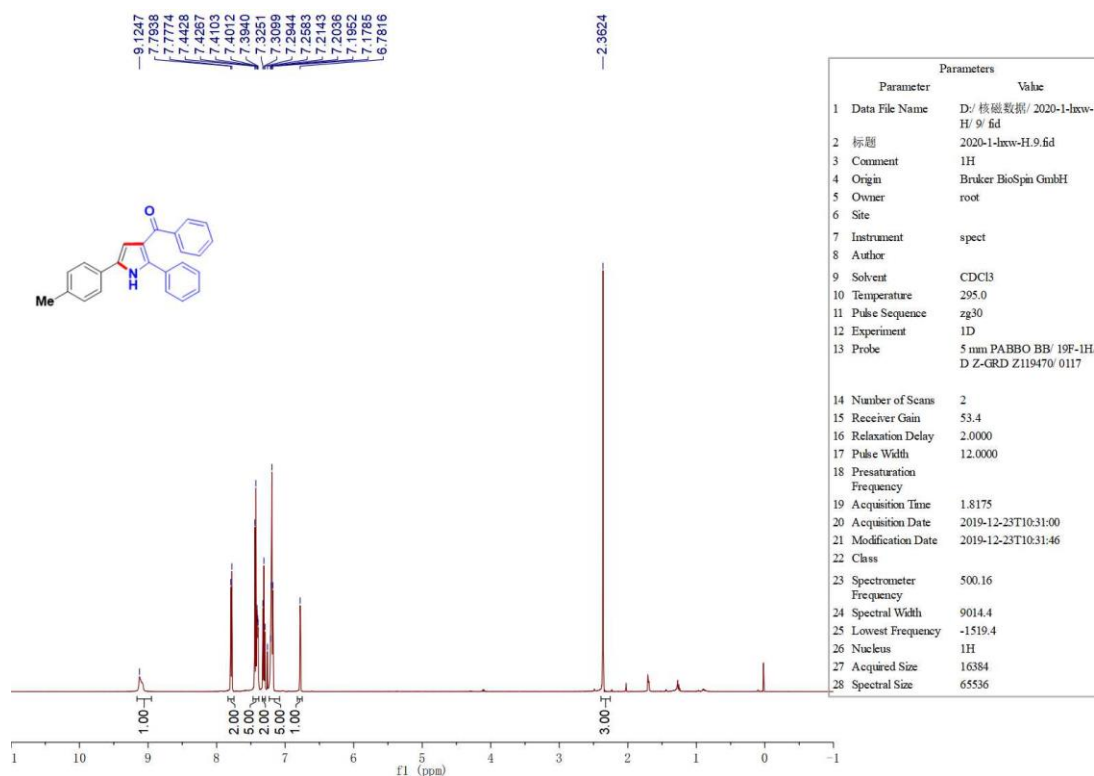
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 500M- NMR-date/ 2019-1-lxw-H/ 332.fid	
2 标题	2019-1-lxw-H.332.fid	
3 Comment	1H	
4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.2	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	76.5	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2019-11-29T11:27:38	
21 Modification Date	2019-11-29T11:27:40	
22 Class		
23 Spectrometer Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1518.8	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 500M- NMR-date/ 2019-1-lxw-C/ 255.fid	
2 标题	2019-1-lxw-C.255.fid	
3 Comment	13C	
4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.2	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	151	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation Frequency		
19 Acquisition Time	0.5505	
20 Acquisition Date	2019-11-29T11:37:06	
21 Modification Date	2019-11-29T11:37:08	
22 Class		
23 Spectrometer Frequency	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	

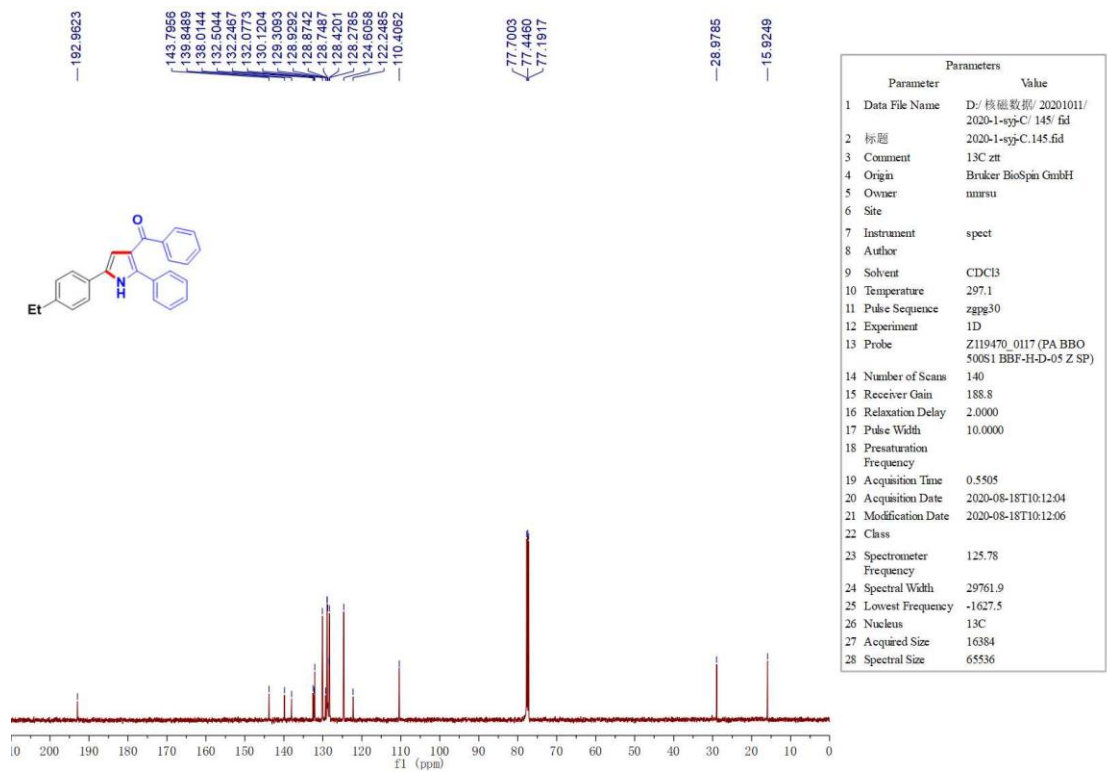
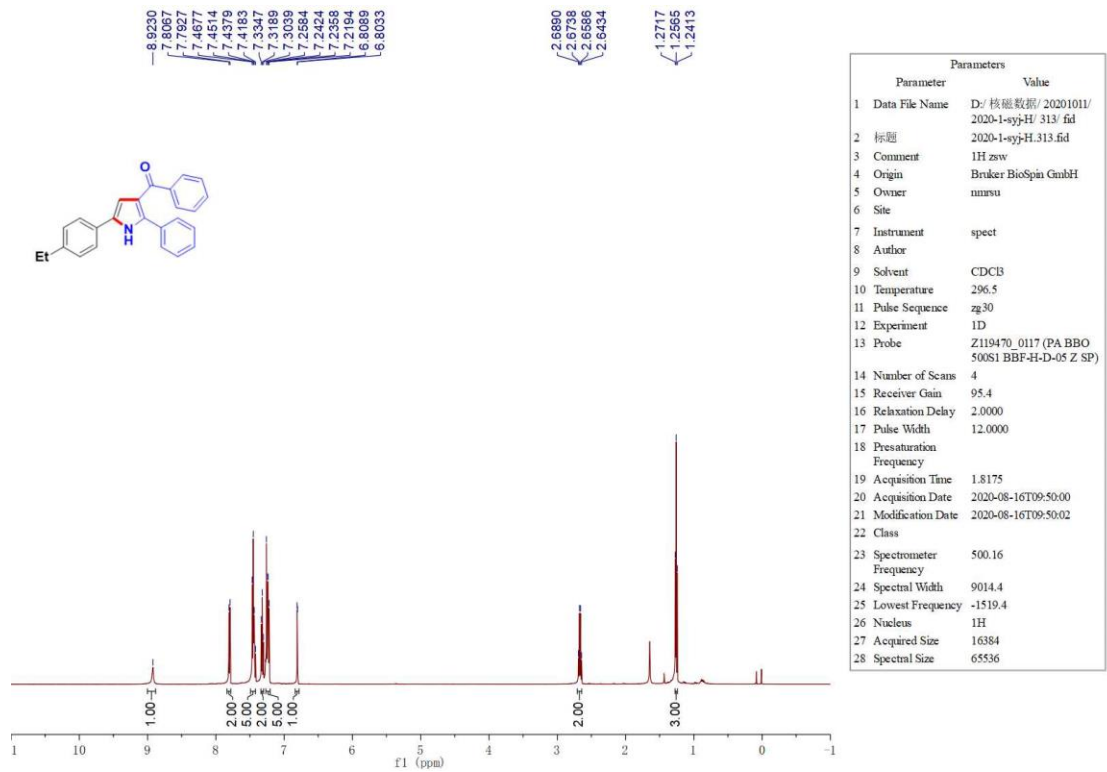


# Phenyl(2-phenyl-5-(*p*-tolyl)-1*H*-pyrrol-3-yl)methanone (5b)



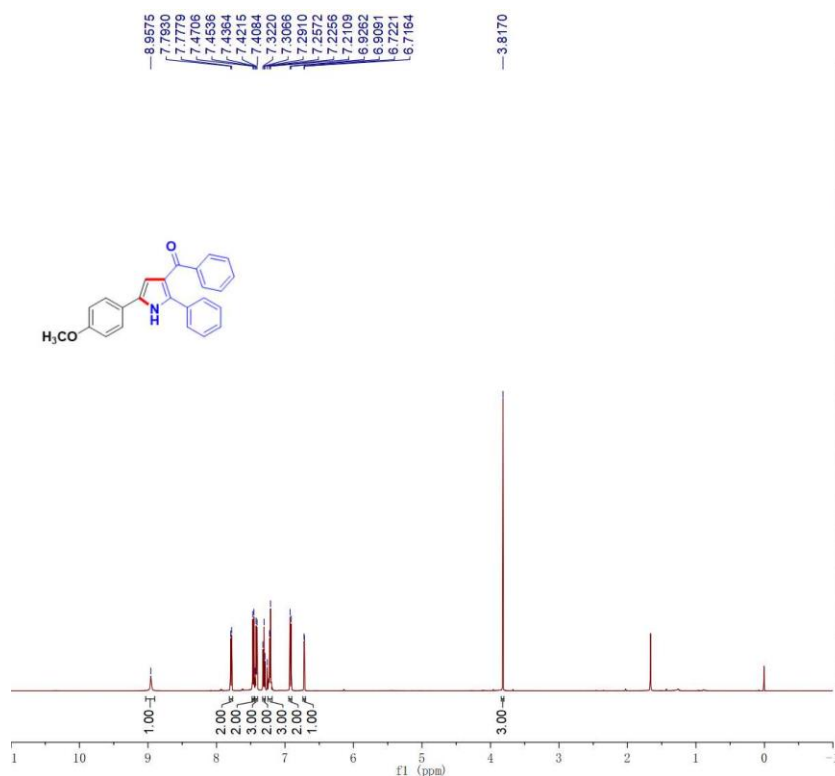


(5-(4-Ethylphenyl)-2-phenyl-1*H*-pyrrol-3-yl)(phenyl)methanone (5c)

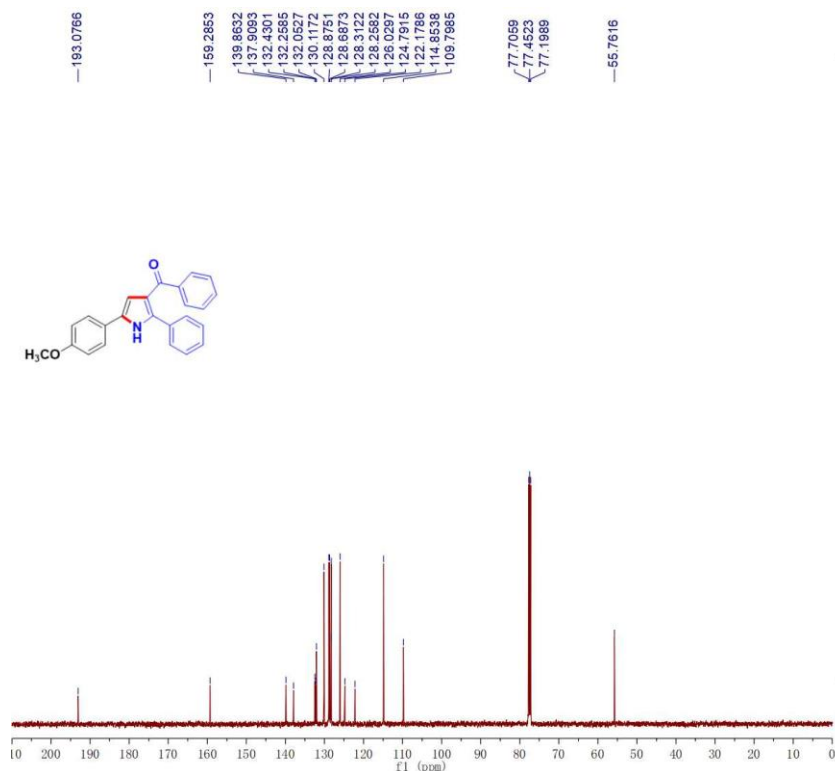




# (5-(4-Methoxyphenyl)-2-phenyl-1H-pyrrol-3-yl)(phenyl)methanone (5d)



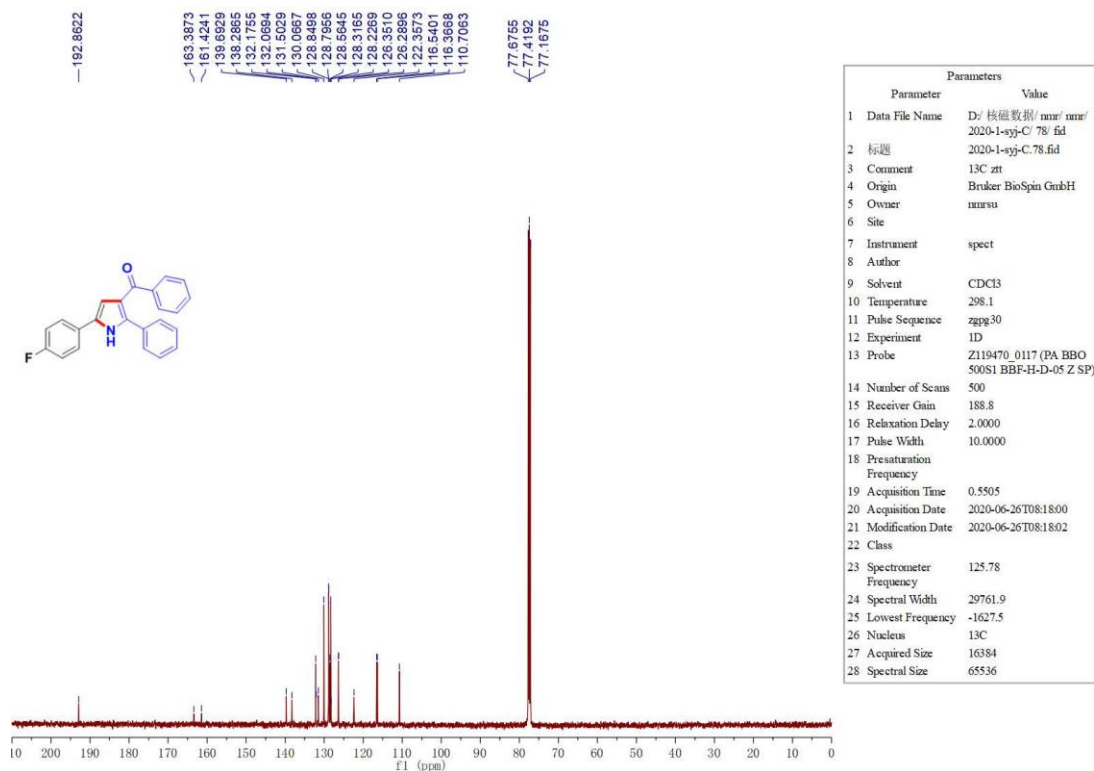
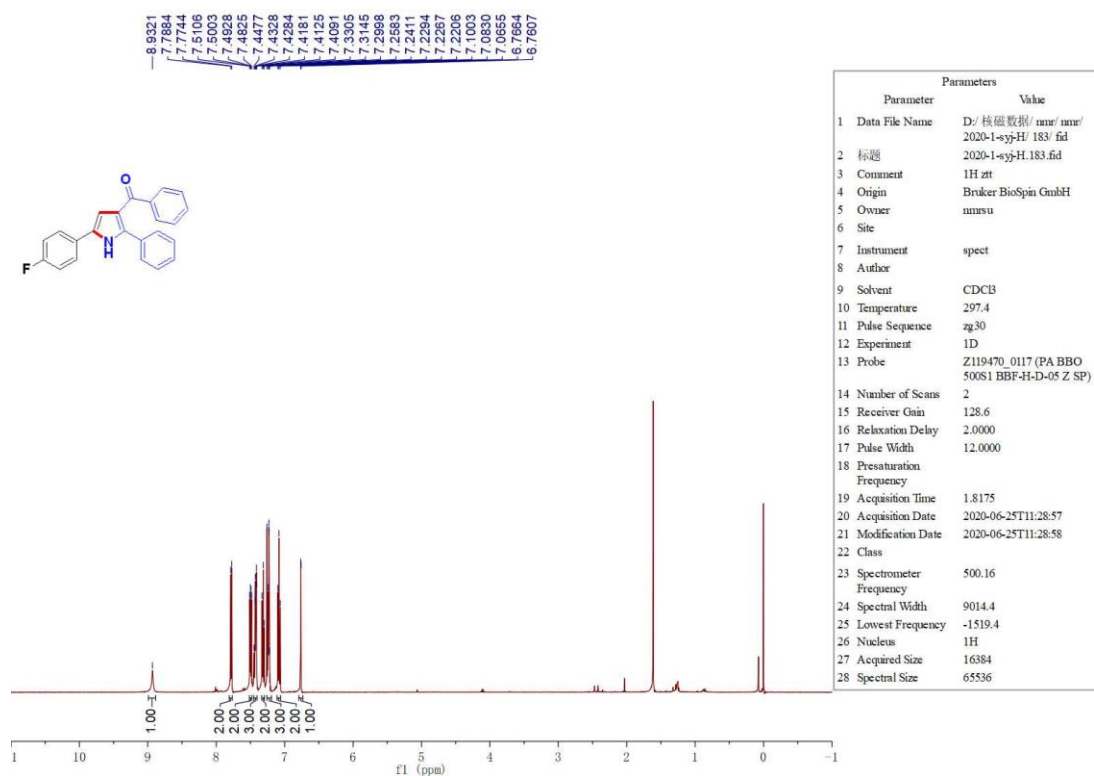
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-H- 257.fid	
2 标题	2020-1-sy-H-257.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nnusu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl <sub>3</sub>	
10 Temperature	297.6	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500SI BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	87.0	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2020-07-24T10:18:13	
21 Modification Date	2020-07-24T10:18:14	
22 Class		
23 Spectrometer Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-C/ 111.fid	
2 标题	2020-1-sy-C-111.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nnusu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl <sub>3</sub>	
10 Temperature	298.3	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500SI BBF-H-D-05 Z SP)	
14 Number of Scans	100	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation Frequency		
19 Acquisition Time	0.5505	
20 Acquisition Date	2020-07-26T16:34:05	
21 Modification Date	2020-07-26T16:34:08	
22 Class		
23 Spectrometer Frequency	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	

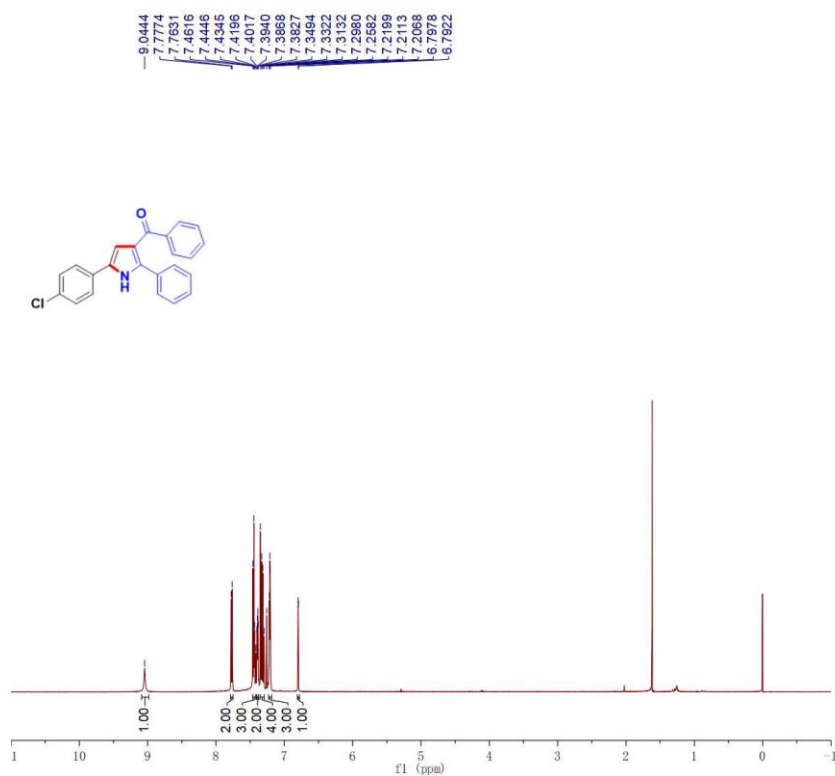


# (5-(4-Fluorophenyl)-2-phenyl-1H-pyrrol-3-yl)(phenyl)methanone (5e)

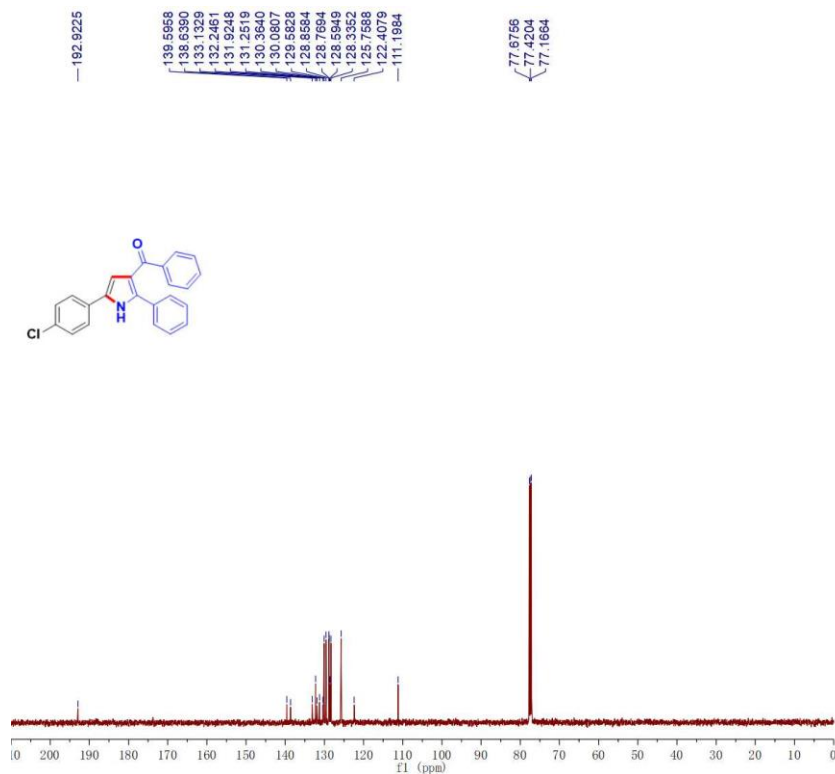




# (5-(4-Chlorophenyl)-2-phenyl-1H-pyrrol-3-yl)(phenyl)methanone (5f)



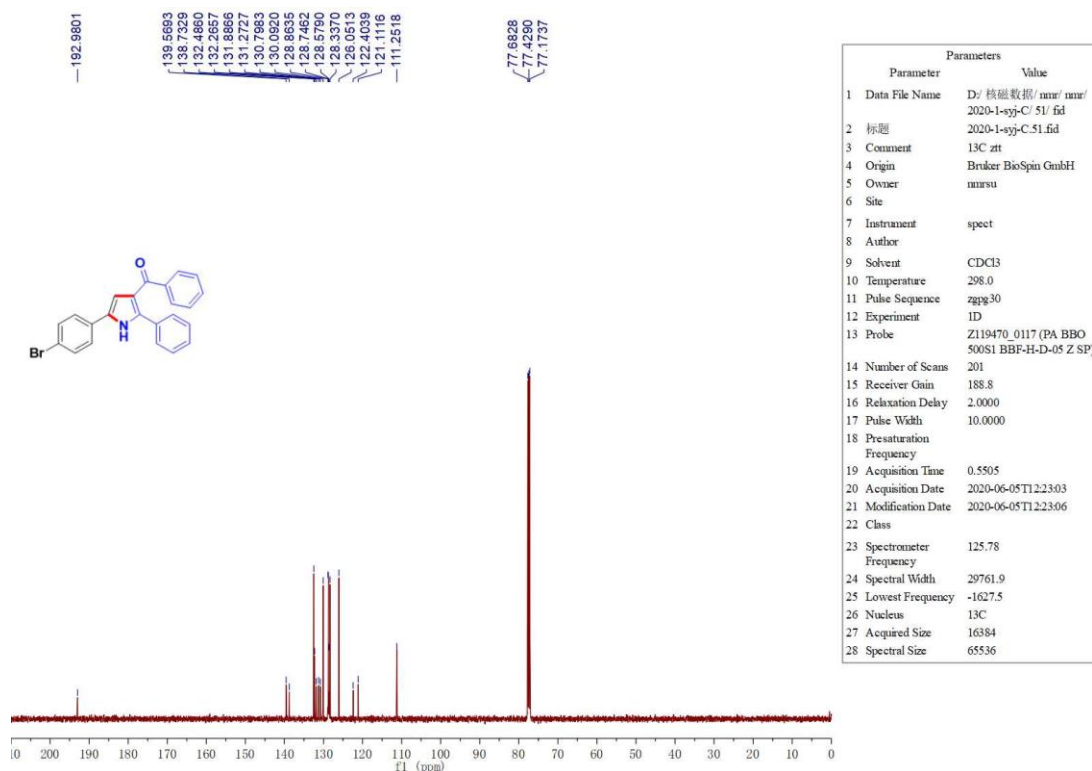
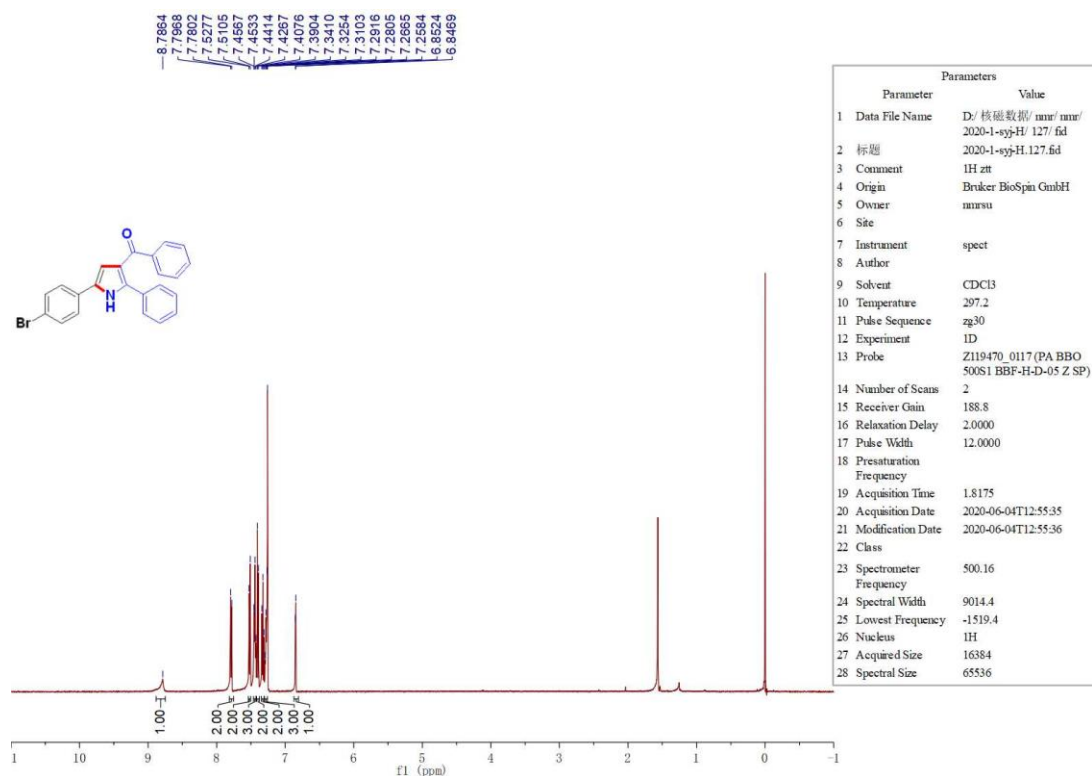
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy3-H/ 267.fid	
2 标题	2020-1-sy3-H.267.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	297.4	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	114.1	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2020-07-26T11:37:31	
21 Modification Date	2020-07-26T11:37:32	
22 Class		
23 Spectrometer Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy3-C/ 114.fid	
2 标题	2020-1-sy3-C.114.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	298.3	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	83	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation Frequency		
19 Acquisition Time	0.5505	
20 Acquisition Date	2020-07-26T16:59:52	
21 Modification Date	2020-07-26T16:59:54	
22 Class		
23 Spectrometer Frequency	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	

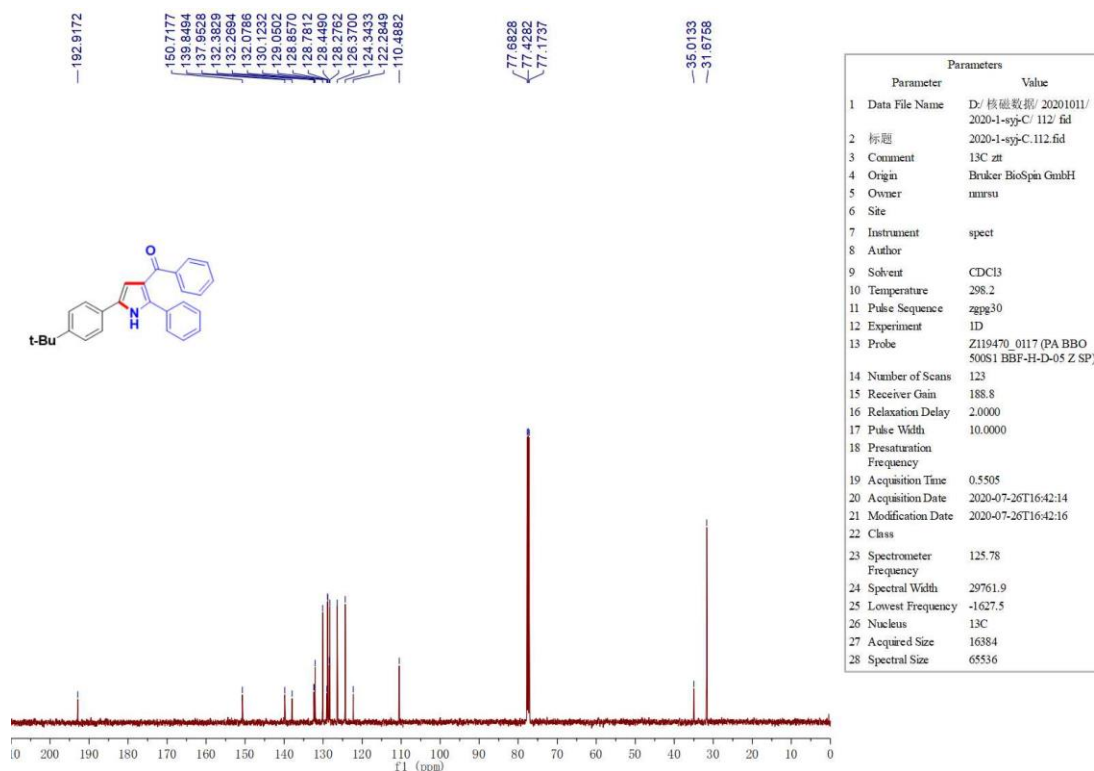
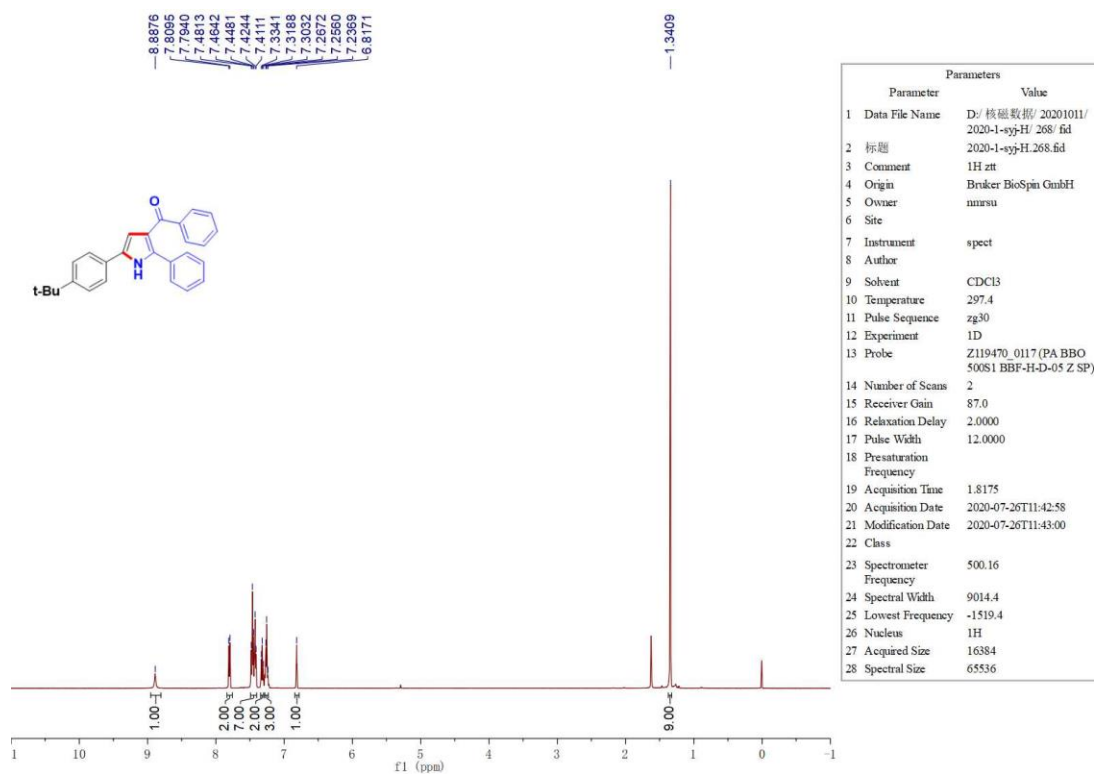


# (5-(4-Bromophenyl)-2-phenyl-1H-pyrrol-3-yl)(phenyl)methanone (5g)





(5-(4-(*tert*-Butyl)phenyl)-2-phenyl-1*H*-pyrrol-3-yl)(phenyl)methanone (**5h**)



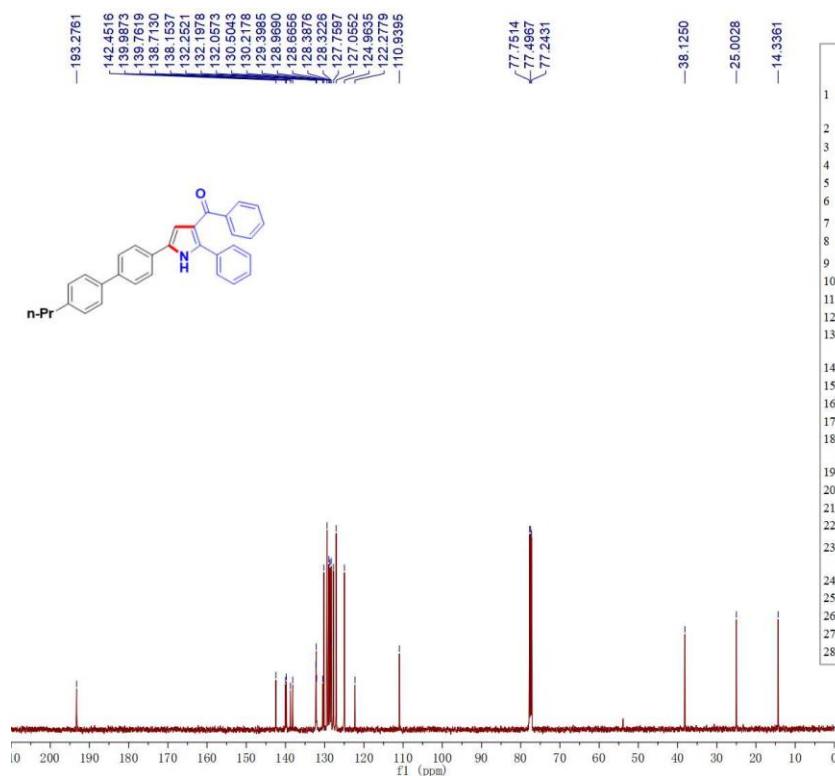


Chemical structure of compound 10: CCCC1=CC=C(C=C1)-C2=CC=C(C=C2)-c3c[nH]c4c3C(=O)c5ccccc54

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of compound 10. The x-axis is labeled f1 (ppm). The spectrum shows peaks from 0 to 10 ppm. Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
9.4257	1.00
7.8075	2.00
7.7932	2.00
7.6885	2.00
7.5319	2.00
7.5158	2.00
7.4571	2.00
7.4421	2.00
7.4274	2.00
7.4019	2.00
7.3978	2.00
7.3568	2.00
7.3351	2.00
7.3194	2.00
7.3044	2.00
7.2525	2.00
7.2465	2.00
7.1795	2.00
7.1730	2.00
7.1681	2.00
6.8560	3.00
6.8504	3.00
2.6556	2.00
2.6407	2.00
2.6250	2.00
1.7323	2.00
1.7176	2.00
1.7024	2.00
1.6873	2.00
1.6724	2.00
1.6577	2.00
1.0066	3.00
0.9950	3.00
0.9803	3.00

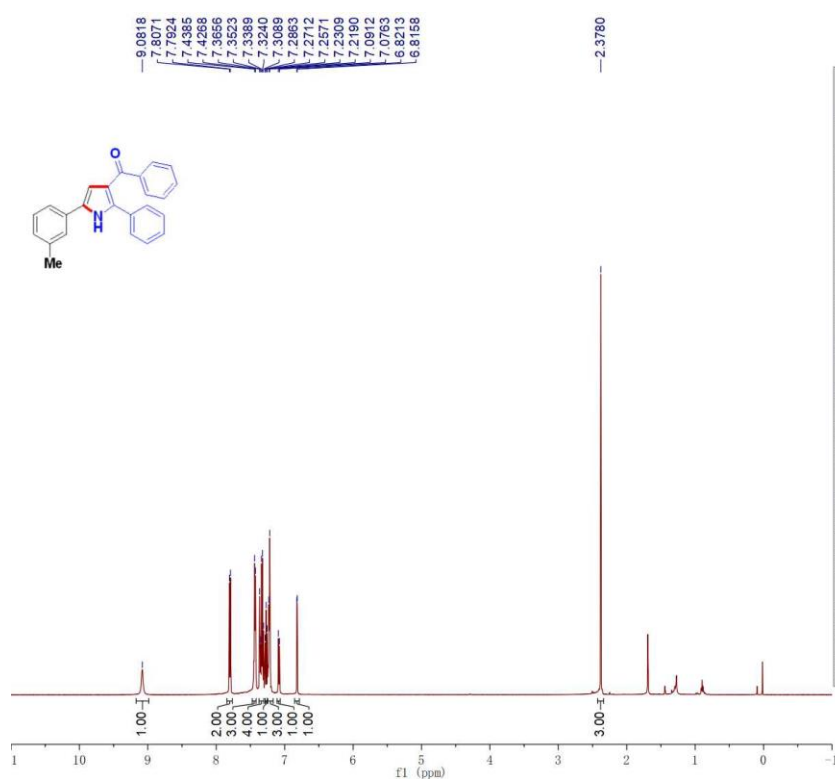
Parameters		
	Parameter	Value
1	Data File Name	D:\核磁数据\20201011\2020-1-xyj-H_314.fid
2	标题	2020-1-xyj-H_314.fid
3	Comment	1H ztt
4	Origin	Broker BioSpin GmbH
5	Owner	nmru
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.5
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	4
15	Receiver Gain	27.1
16	Relaxation Delay	2.0000
17	Pulse Width	12.0000
18	Pretsaturation Frequency	
19	Acquisition Time	1.8175
20	Acquisition Date	2020-08-16T09:54:42
21	Modification Date	2020-08-16T09:54:44
22	Class	
23	Spectrometer Frequency	500.16
24	Spectral Width	9014.4
25	Lowest Frequency	-1519.4
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	65536



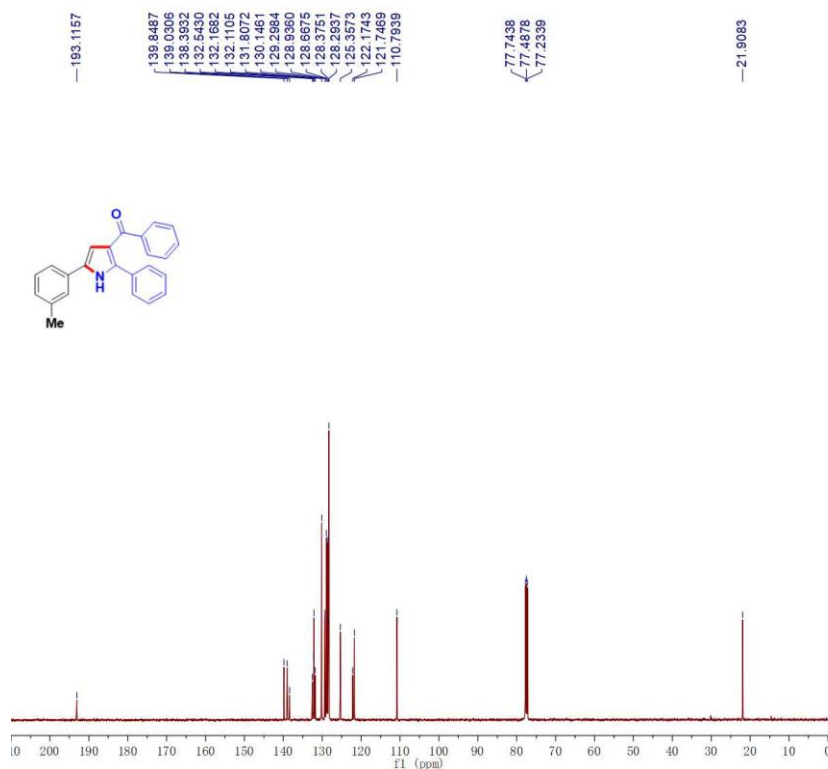
	Parameter	Value
1	Data File Name	D:\核磁数据\2020-yyj\HC\2020-1-yyj-C\358.fid
2	标题	2020-1-yyj-C.358.fid
3	Comment	13C att
4	Origin	Braker BioSpin GmbH
5	Owner	nmru
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl <sub>3</sub>
10	Temperature	295.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z119470_0117 (PA BBO 50181 BBF-H-D-05 Z SP)
14	Number of Scans	100
15	Receiver Gain	188.8
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Pretsaturation Frequency	
19	Acquisition Time	0.5505
20	Acquisition Date	2020-12-24T19:25:57
21	Modification Date	2020-12-24T19:26:00
22	Class	
23	Spectrometer Frequency	125.78
24	Spectral Width	29761.9
25	Lowest Frequency	-1627.5
26	Nucleus	13C
27	Acquired Size	16384
28	Spectral Size	65536



# Phenyl(2-phenyl-5-(*m*-tolyl)-1H-pyrrol-3-yl)methanone (5j)



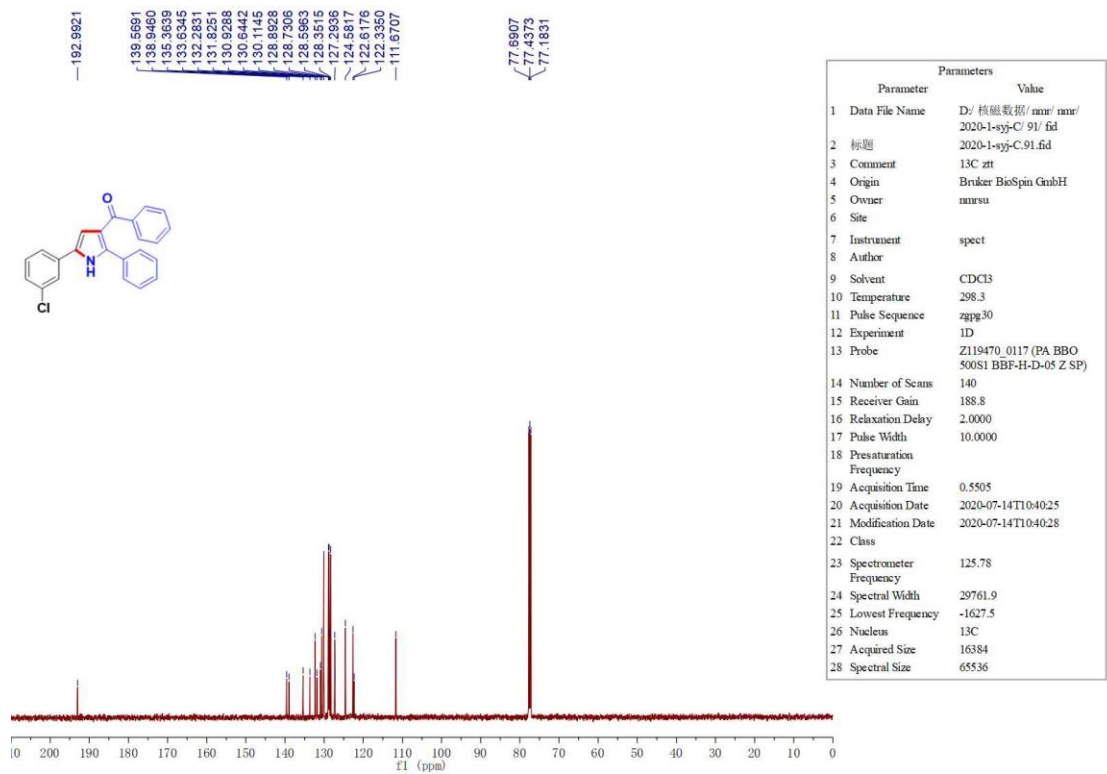
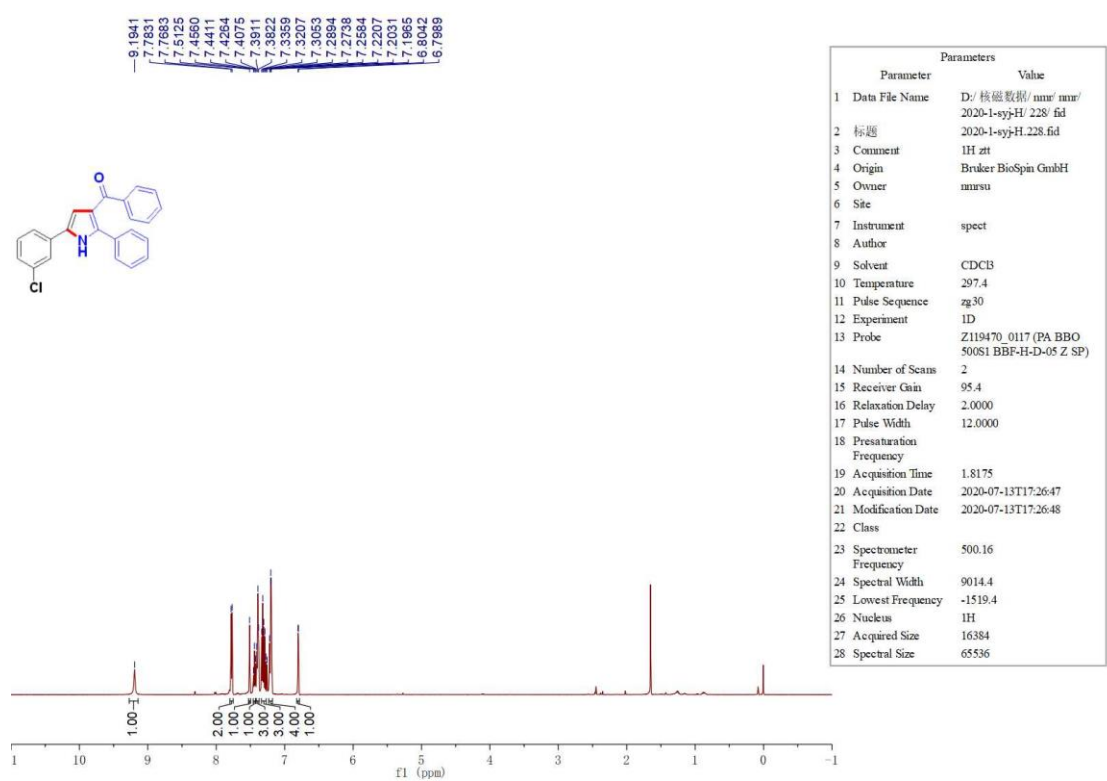
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-syy-H/ 227.fid
2 标题	2020-1-syy-H.227.fid
3 Comment	1H ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	59.2
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2020-07-13T17:21:41
21 Modification Date	2020-07-13T17:21:42
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-syy-C/ 90.fid
2 标题	2020-1-syy-C.90.fid
3 Comment	13C ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	330
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2020-07-14T10:29:55
21 Modification Date	2020-07-14T10:29:58
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536

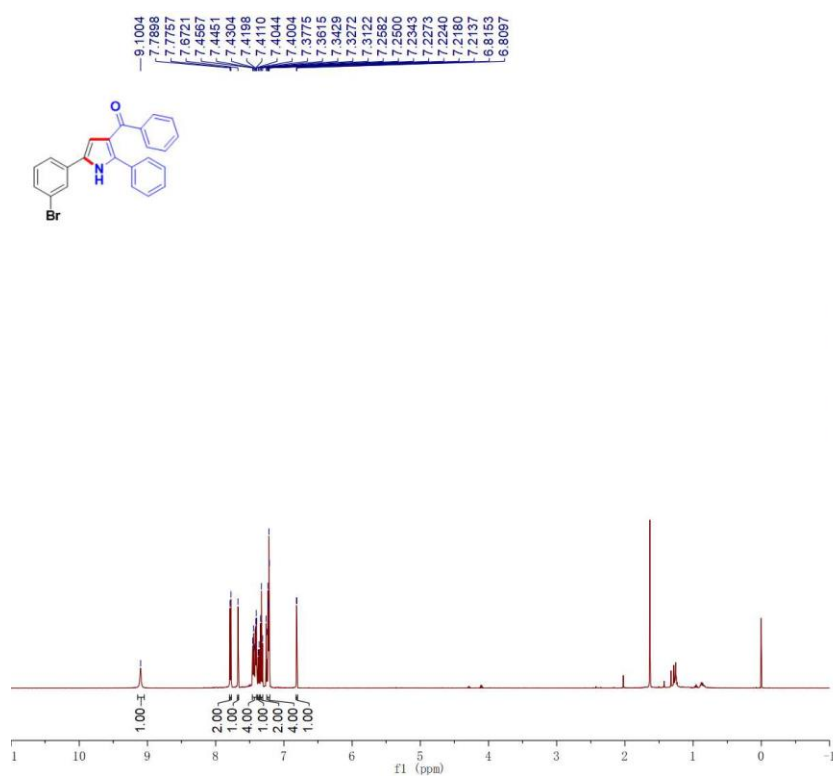


(5-(3-Chlorophenyl)-2-phenyl-1H-pyrrol-3-yl)(phenyl)methanone (5k)

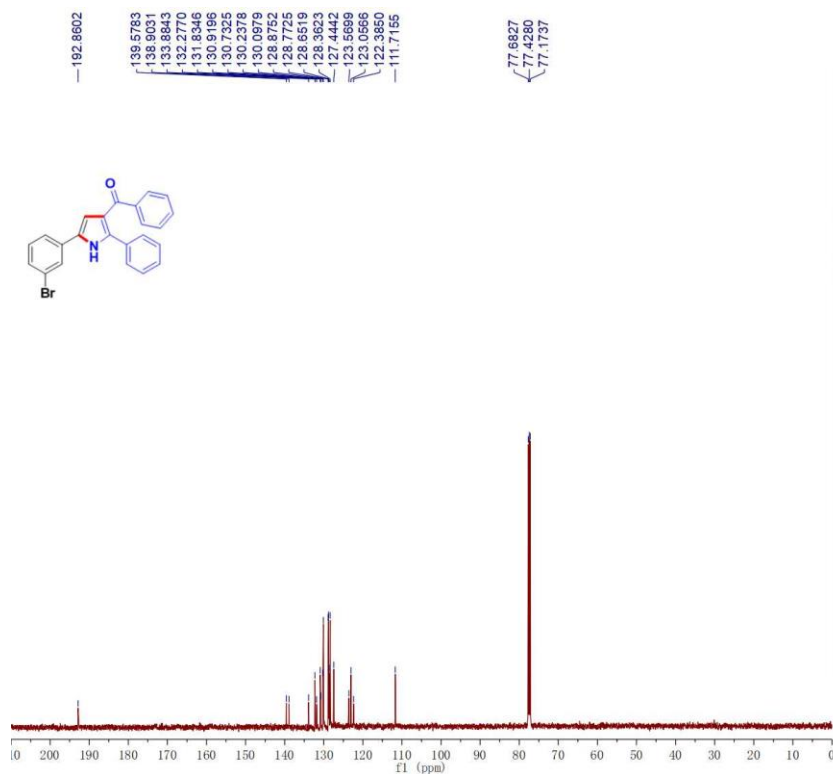




# (5-(3-Bromophenyl)-2-phenyl-1H-pyrrol-3-yl)(phenyl)methanone (51)



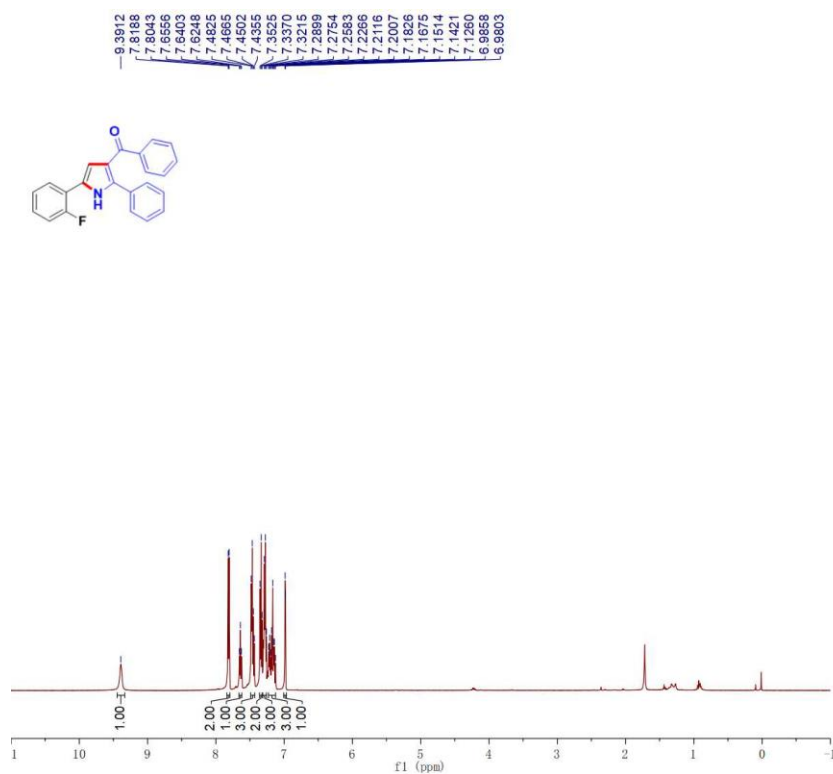
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-H- 266.fid	
2 标题	2020-1-sy-H-266.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nnrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	297.4	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	114.1	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2020-07-26T11:32:32	
21 Modification Date	2020-07-26T11:32:34	
22 Class		
23 Spectrometer Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	



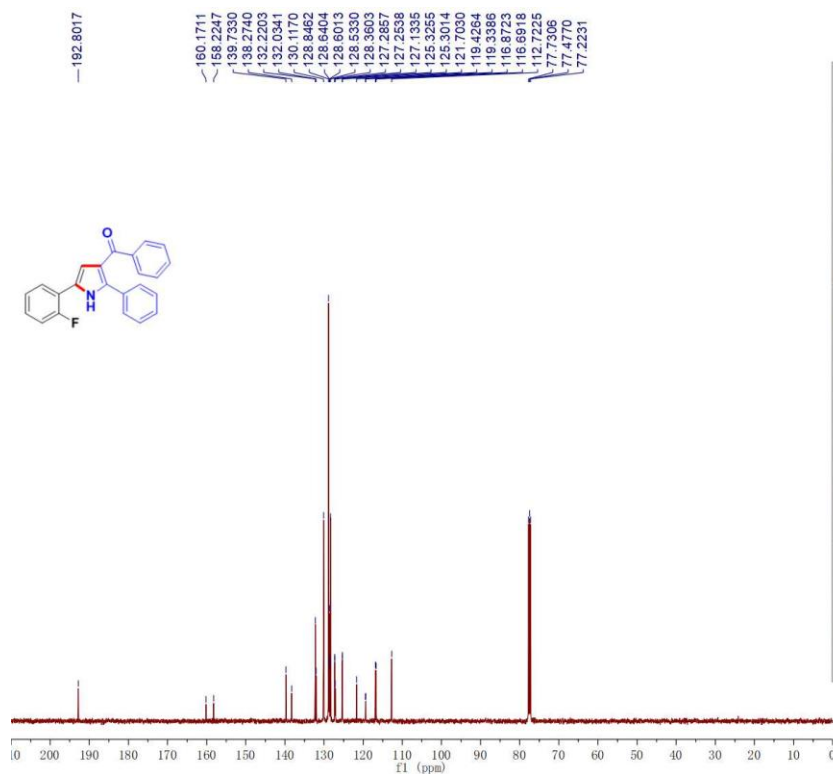
Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-C/ 113.fid	
2 标题	2020-1-sy-C-113.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nnrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	298.3	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	99	
15 Receiver Gain	188.8	
16 Relaxation Delay	2.0000	
17 Pulse Width	10.0000	
18 Presaturation Frequency		
19 Acquisition Time	0.5505	
20 Acquisition Date	2020-07-26T16:50:55	
21 Modification Date	2020-07-26T16:50:58	
22 Class		
23 Spectrometer Frequency	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	



# (5-(2-Fluorophenyl)-2-phenyl-1H-pyrrol-3-yl)(phenyl)methanone (5m)



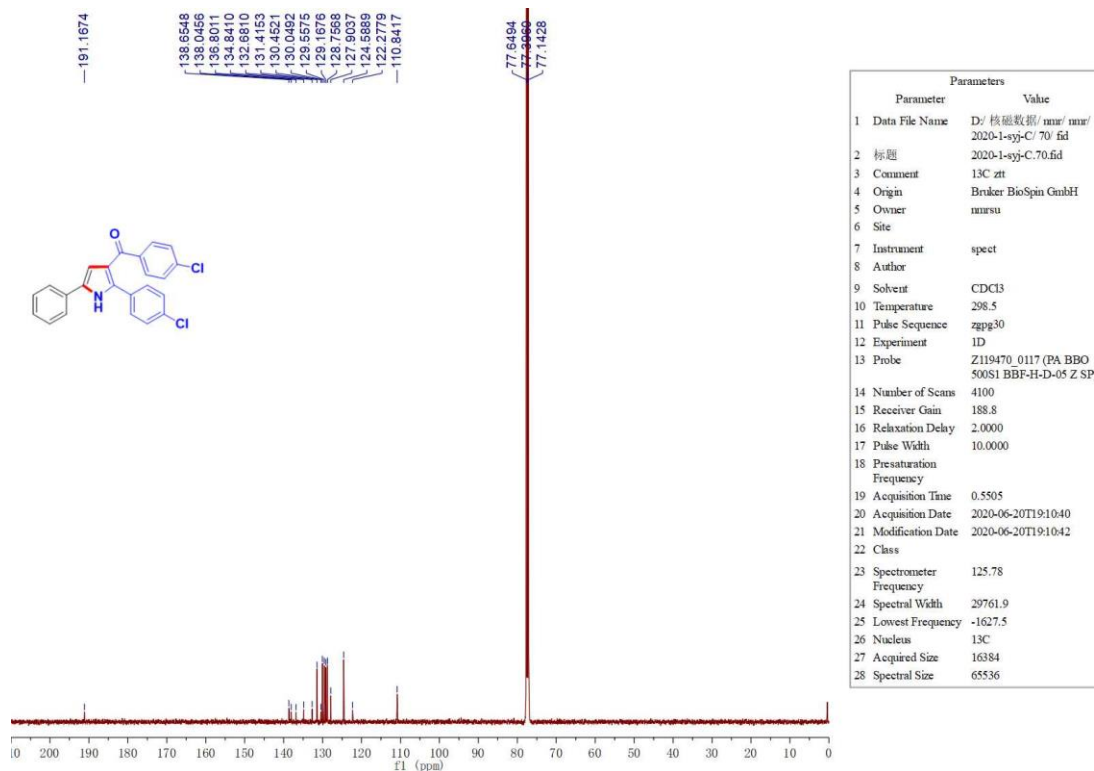
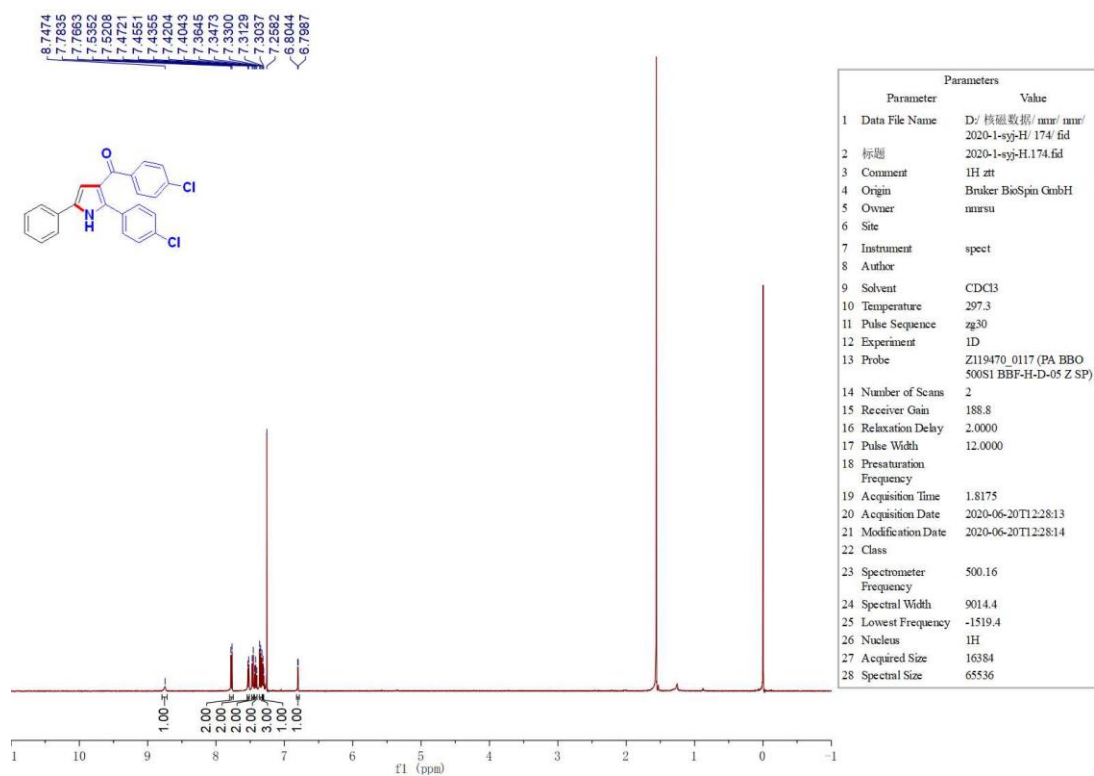
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-syy-H/ 292.fid
2 标题	2020-1-syy-H.292.fid
3 Comment	1H zt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmusu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	292.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470 0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	59.2
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2020-08-10T11:02:25
21 Modification Date	2020-08-10T11:02:26
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-syy-C/ 130.fid
2 标题	2020-1-syy-C.130.fid
3 Comment	13C zt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmusu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470 0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	100
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2020-08-10T12:41:04
21 Modification Date	2020-08-10T12:41:06
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536

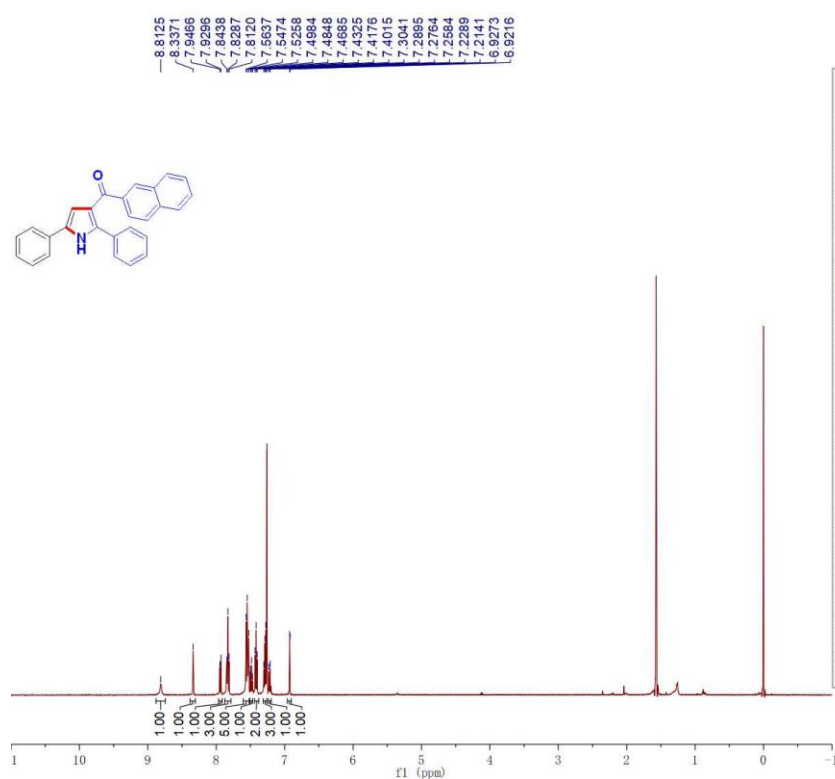


(4-Chlorophenyl)(2-(4-chlorophenyl)-5-phenyl-1H-pyrrol-3-yl) methanone (5n)

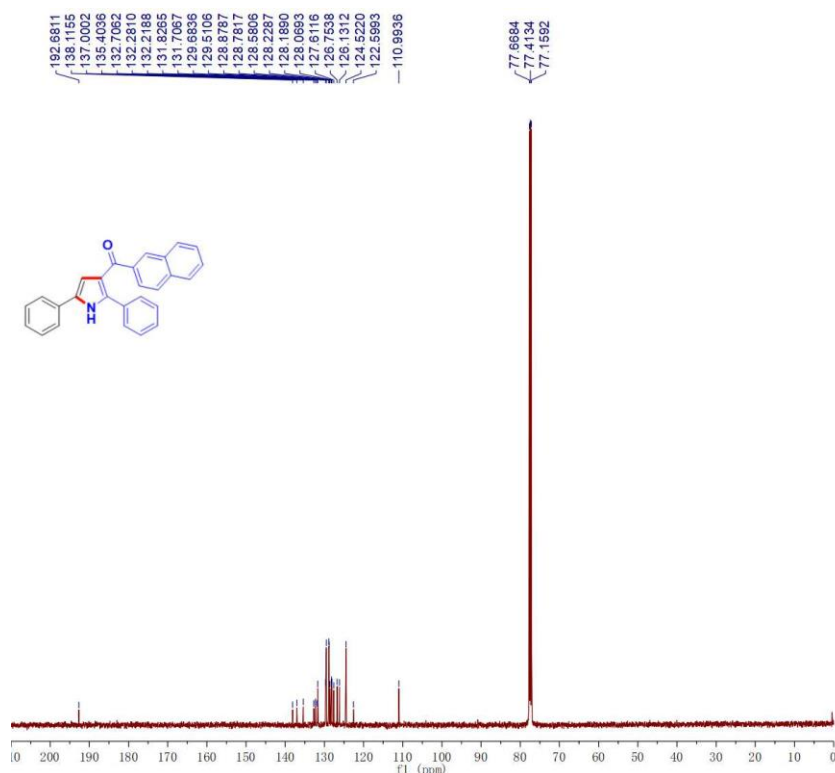




# (2,5-Diphenyl-1H-pyrrol-3-yl) (naphthalen-2-yl) methanone (5o)



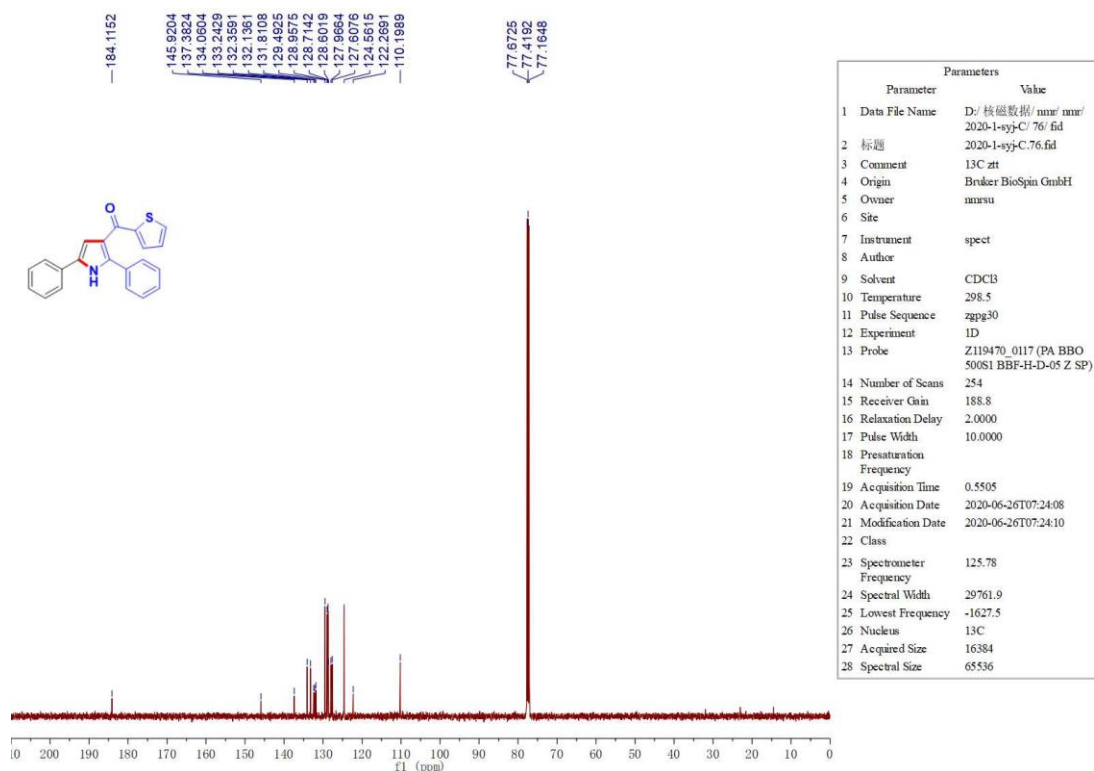
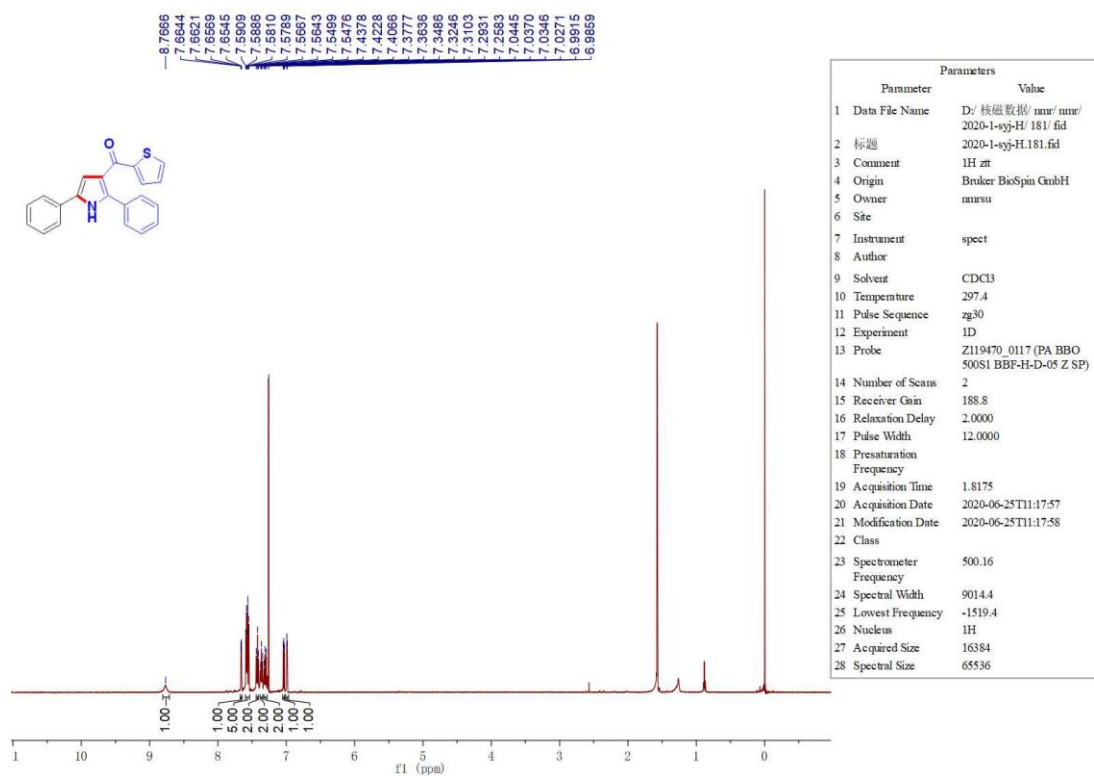
Parameters	
Parameter	Value
1 Data File Name	D:\核磁数据\nmr\182.fid
2 标题	2020-1-yyj-H.182.fid
3 Comment	1H ztt
4 Origin	Braker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2020-06-25T11:24:49
21 Modification Date	2020-06-25T11:24:50
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



Parameters	
Parameter	Value
1 Data File Name	D:\核磁数据\nmr\77.fid
2 标题	2020-1-yyj-C.77.fid
3 Comment	13C ztt
4 Origin	Braker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	600
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2020-06-26T07:52:58
21 Modification Date	2020-06-26T07:53:00
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536

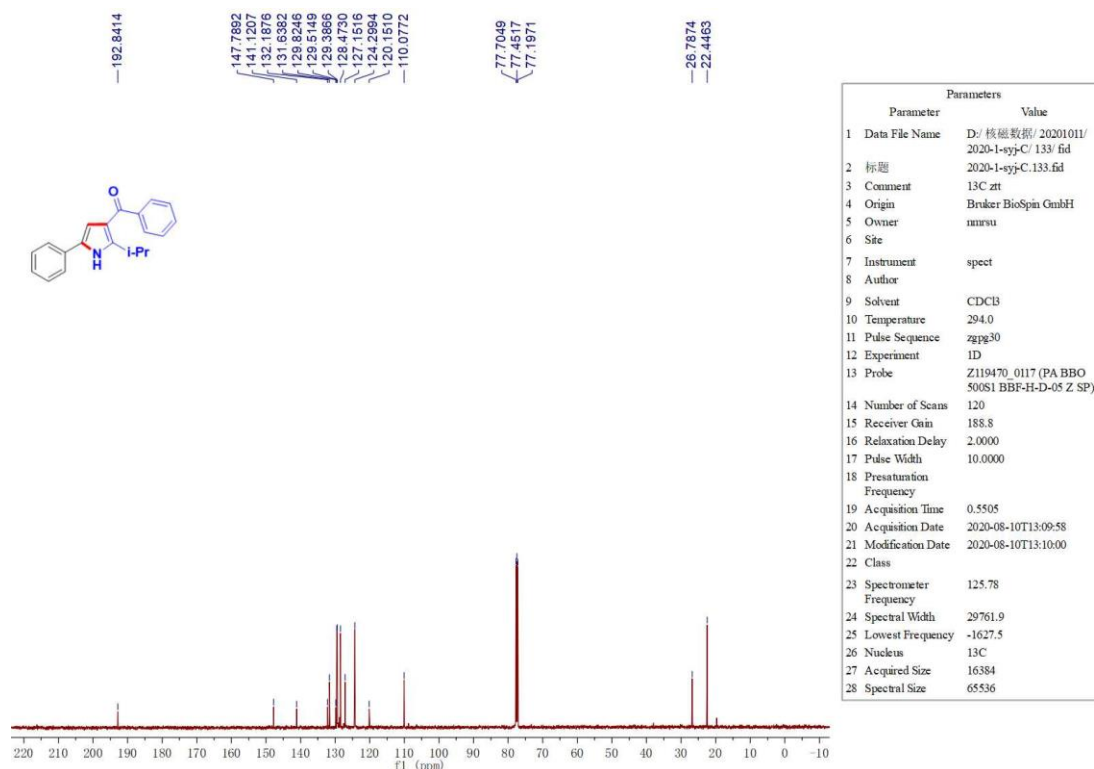
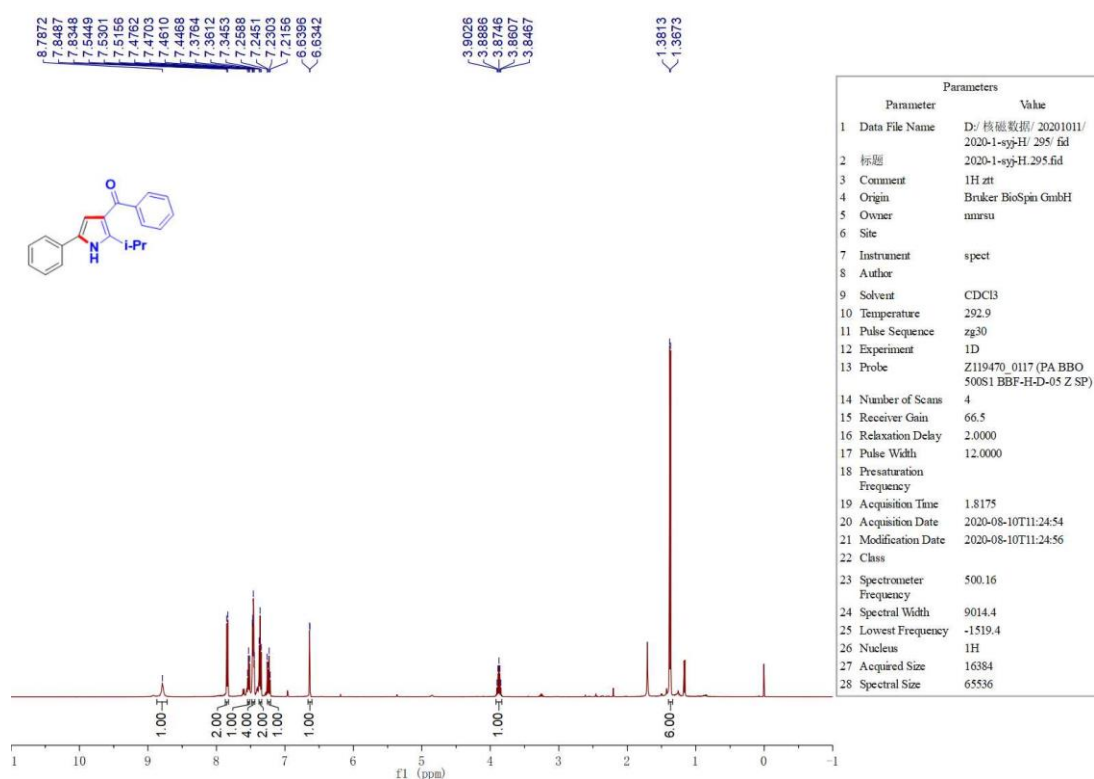


# (2,5-Diphenyl-1*H*-pyrrol-3-yl) (thiophen-2-yl) methanone (5p)





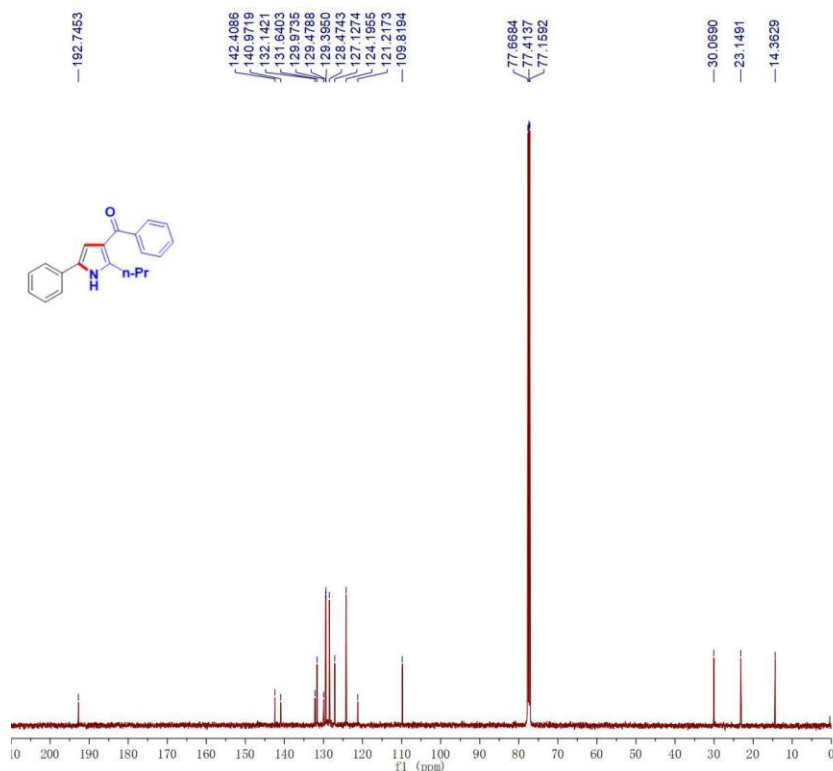
# (2-Isopropyl-5-phenyl-1H-pyrrol-3-yl) (phenyl)methanone (5q)





Chemical structure of **1-(4-phenyl-1H-imidazol-2-yl)propan-1-one** (SMILES: CCC(=O)c1c[nH]c2ccccc12) is shown. The <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) displays the following peaks (ppm): 8.6840, 7.8498, 7.8360, 7.8331, 7.5441, 7.5295, 7.5147, 7.4760, 7.4655, 7.4609, 7.4487, 7.4464, 7.3802, 7.3653, 7.3489, 7.2579, 7.2457, 7.2310, 7.2162, 6.6633, 6.6578, 3.0307, 3.0155, 2.9999, 1.7988, 1.7839, 1.7689, 1.7535, 1.7385, 1.7238, 1.6029, 1.0208, 1.0052, 0.9914. Integration values are provided below the baseline: 1.00, 2.00, 1.00, 4.00, 2.00, 1.00, 1.00, 1.00, 2.00, 3.00, 3.00, 3.00.

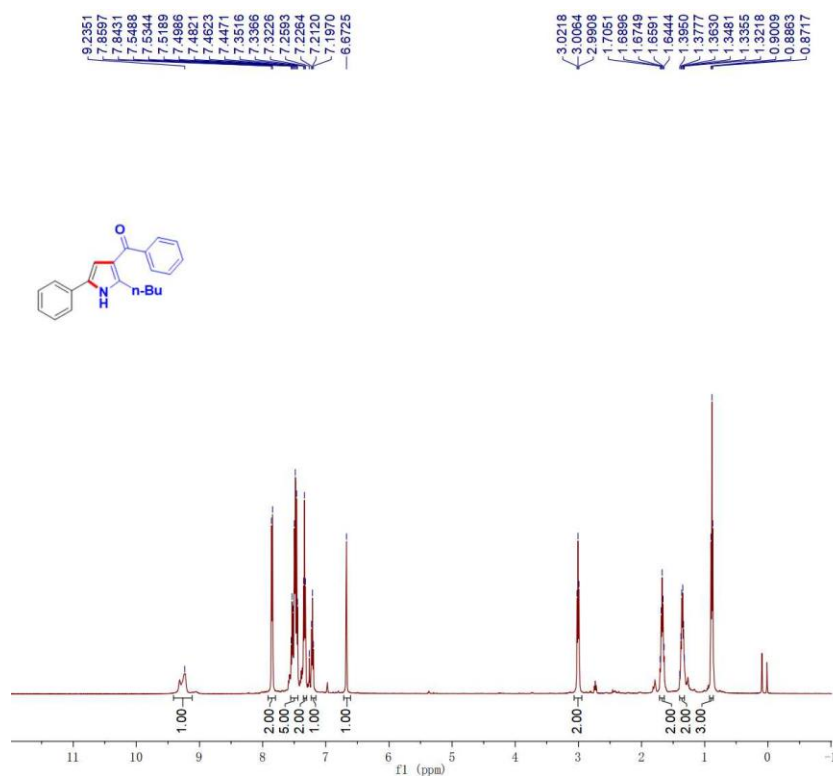
Parameters		
	Parameter	Value
1	Data File Name	D:/核磁数据/nmr/nmr/ 2020-1-syy-H/225.fid
2	标题	2020-1-syy-H.225.fid
3	Comment	1H ztt
4	Origin	Braker BioSpin GmbH
5	Owner	nmrnu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDC3
10	Temperature	297.4
11	Pulse Sequence	zg30
12	Experiment	1D40
13	Probe	500MHz_0117 (PA BBO Z101 BBF-H-D-05 Z SP
14	Number of Scans	2
15	Receiver Gain	128.6
16	Relaxation Delay	2.0000
17	Pulse Width	12.0000
18	Preset/Relaxation Frequency	
19	Acquisition Time	1.8175
20	Acquisition Date	2020-07-13T17:00:08
21	Modification Date	2020-07-13T17:00:10
22	Class	
23	Spectrometer Frequency	500.16
24	Spectral Width	9014.4
25	Lowest Frequency	-1519.4
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	65536



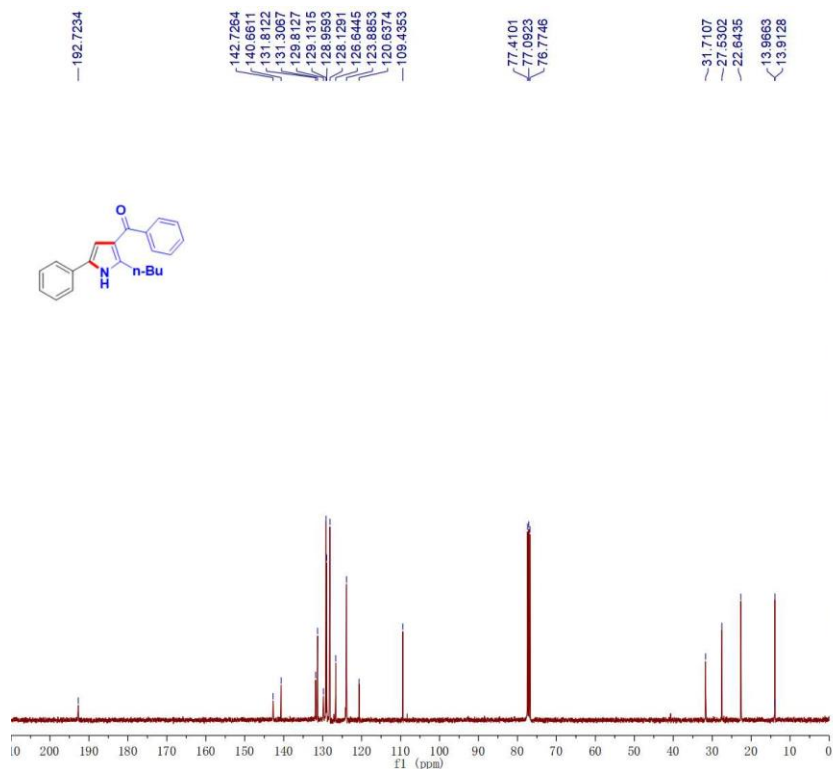
Parameters	
Parameter	Value
1 Data File Name	D:/核磁数据/nmr/nmr/
2 标题	2020-1-syy-C/88.fid
3 Comment	13C ztt
5 Owner	Braker BioSpin GmbH
6 Site	nmru
7 Instrument	spect
8 Author	
9 Solvent	CDC13
10 Temperature	298.3
11 Pulse Sequence	zgpg30
12 Experiment	1d
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP
14 Number of Scans	660
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2020-07-14T09:50:55
21 Modification Date	2020-07-14T09:50:58
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65336



# (2-Butyl-5-phenyl-1H-pyrrol-3-yl) (phenyl)methanone (5s)



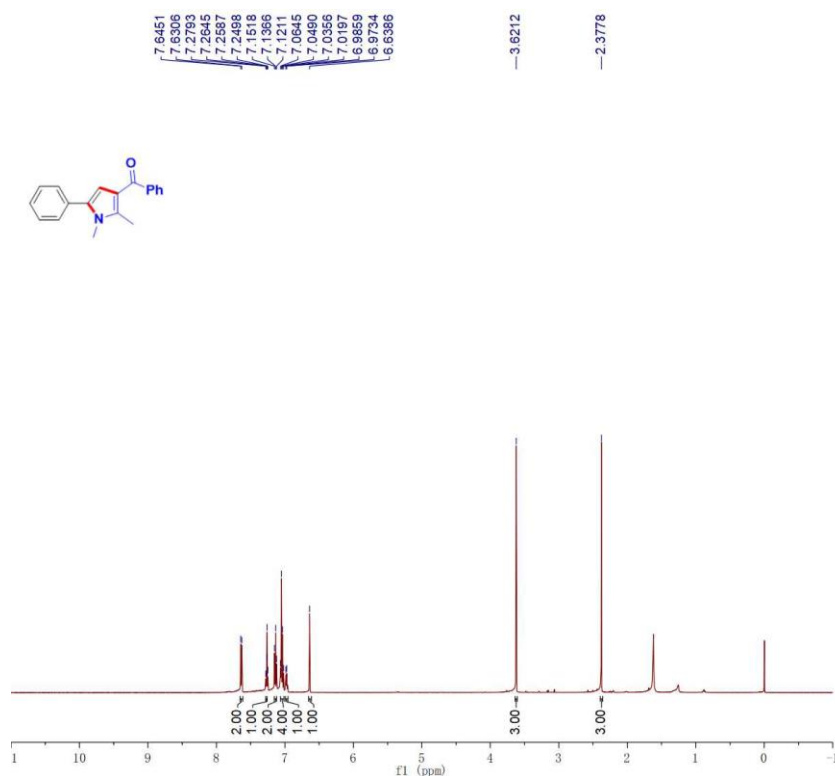
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 2021-syj-500/ 2021-1-syj-H/ 6/ fid
2 标题	2021-1-syj-H.6.fid
3 Comment	1H ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	nursu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	291.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	53.4
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2021-01-10T16:00:03
21 Modification Date	2021-01-10T16:00:04
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



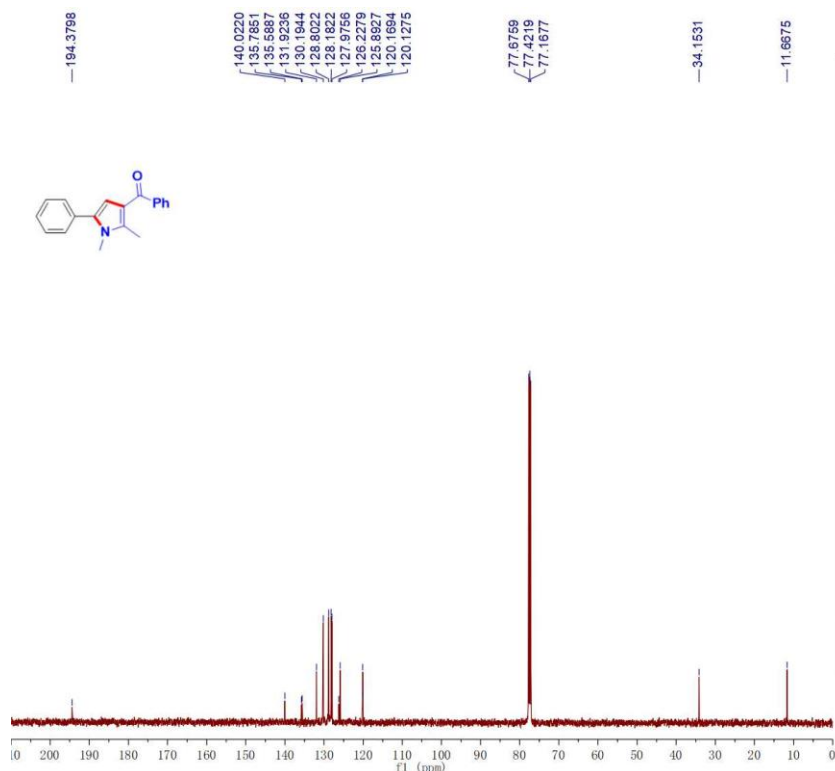
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 400/ 2021-1-syj-C/ 13/ fid
2 标题	2021-1-syj-C.13.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nursu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	191
15 Receiver Gain	48.1
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2021-01-17T14:08:08
21 Modification Date	2021-01-17T14:07:32
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536



# (1,2-Dimethyl-5-phenyl-1H-pyrrol-3-yl) (phenyl)methanone (7a)



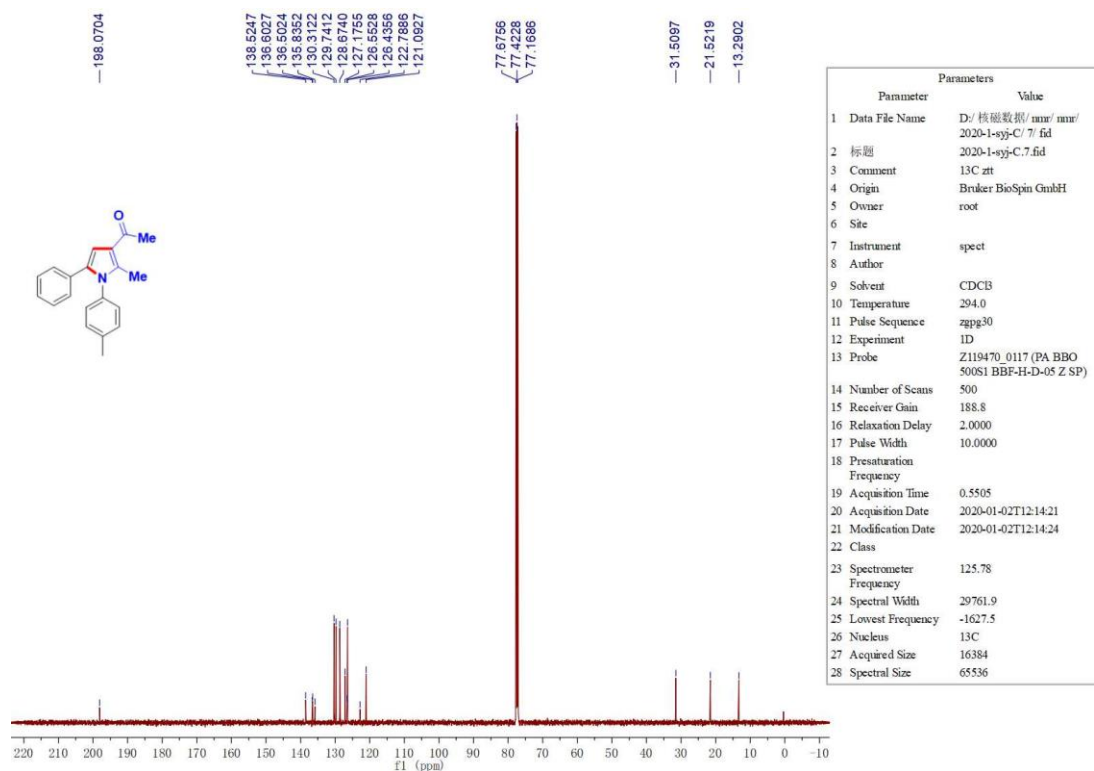
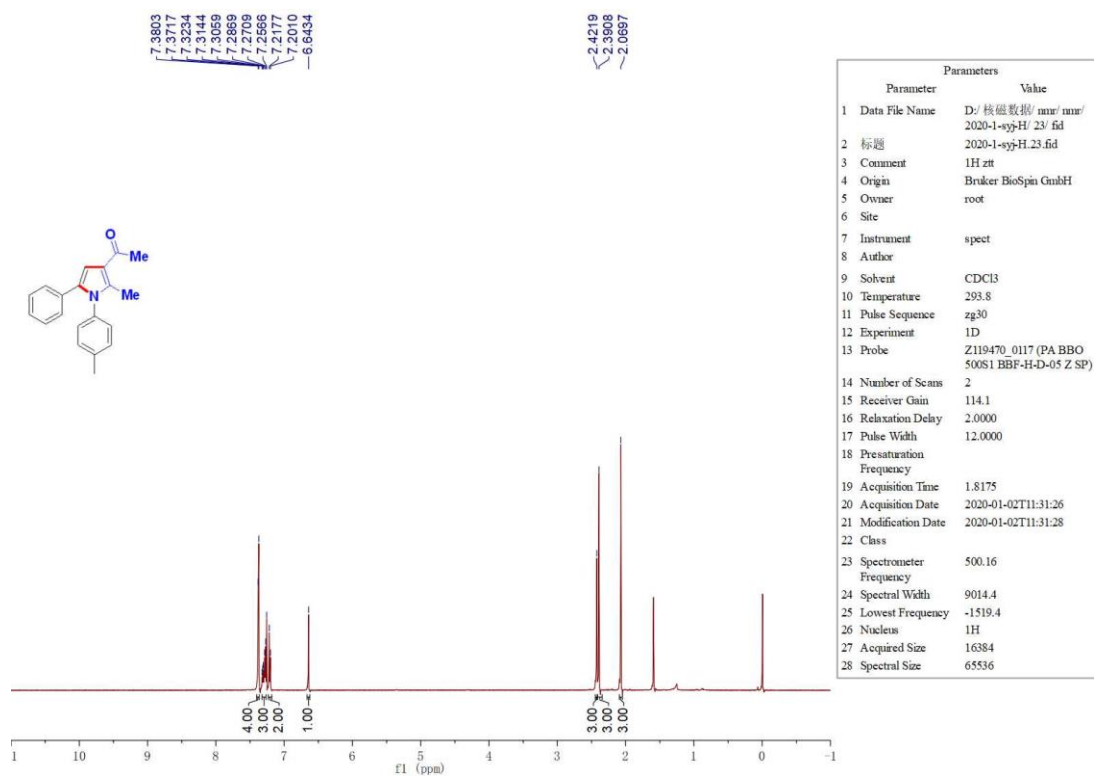
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/
2 标题	2020-1-sy-j-H/ 305/ fid
3 Comment	1H ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	114.1
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2020-08-14T11:19:29
21 Modification Date	2020-08-14T11:19:30
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536



Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/
2 标题	2020-1-sy-j-C/ 138/ fid
3 Comment	13C ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	208
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2020-08-16T17:48:08
21 Modification Date	2020-08-16T17:48:10
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536

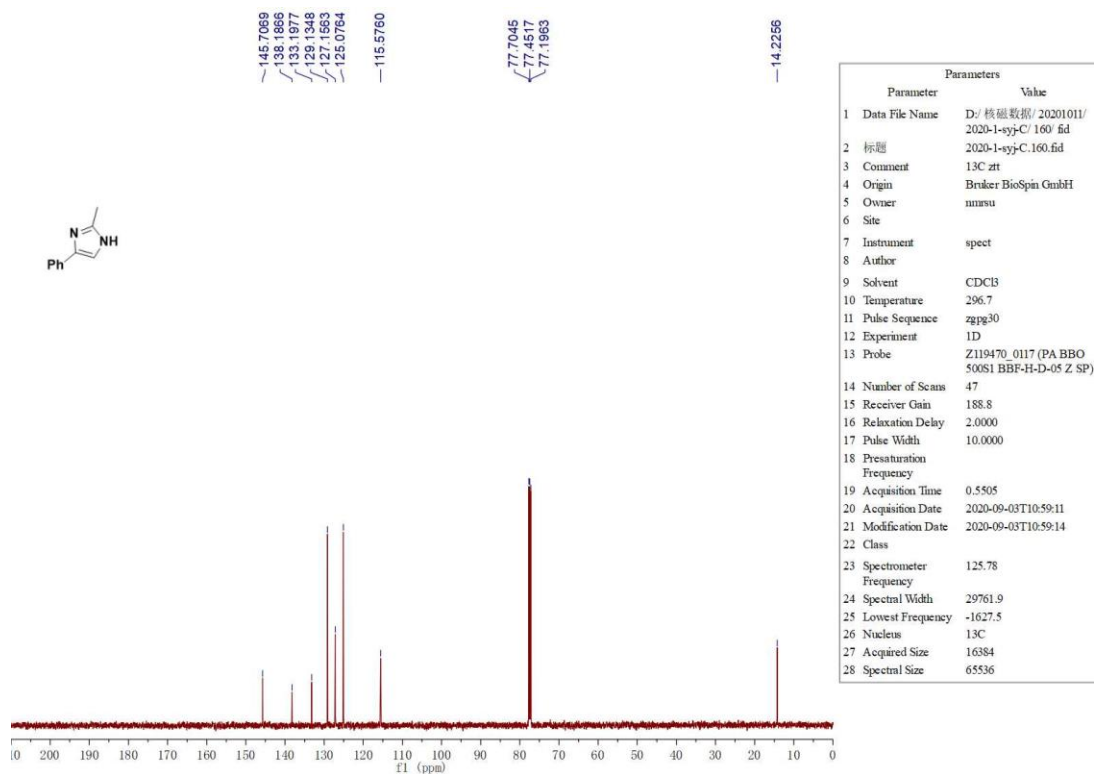
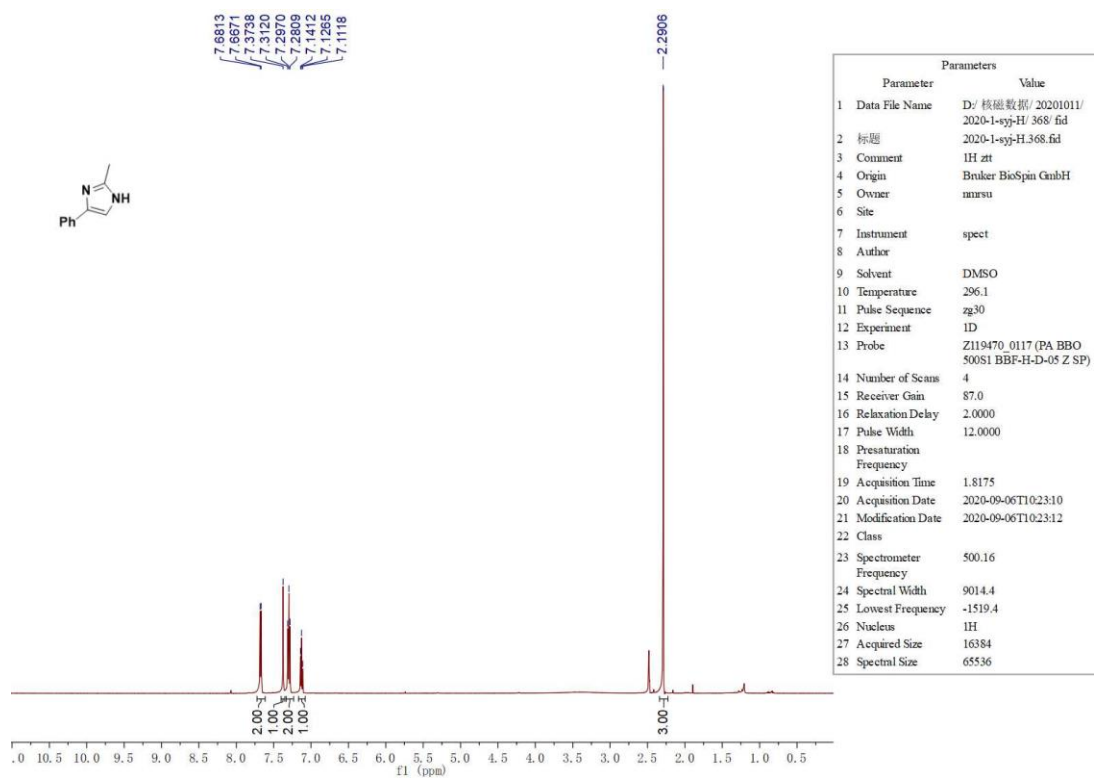


# 1-(2-Methyl-5-phenyl-1-(*p*-tolyl)-1*H*-pyrrol-3-yl) ethan-1-one (7b)



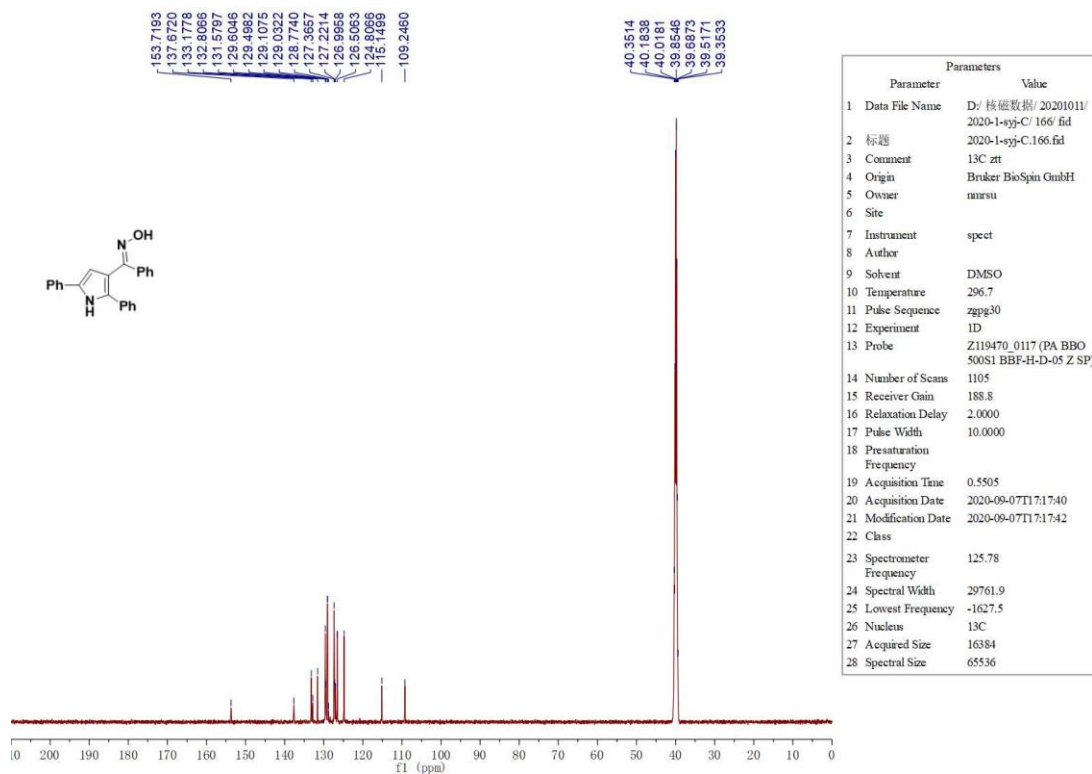
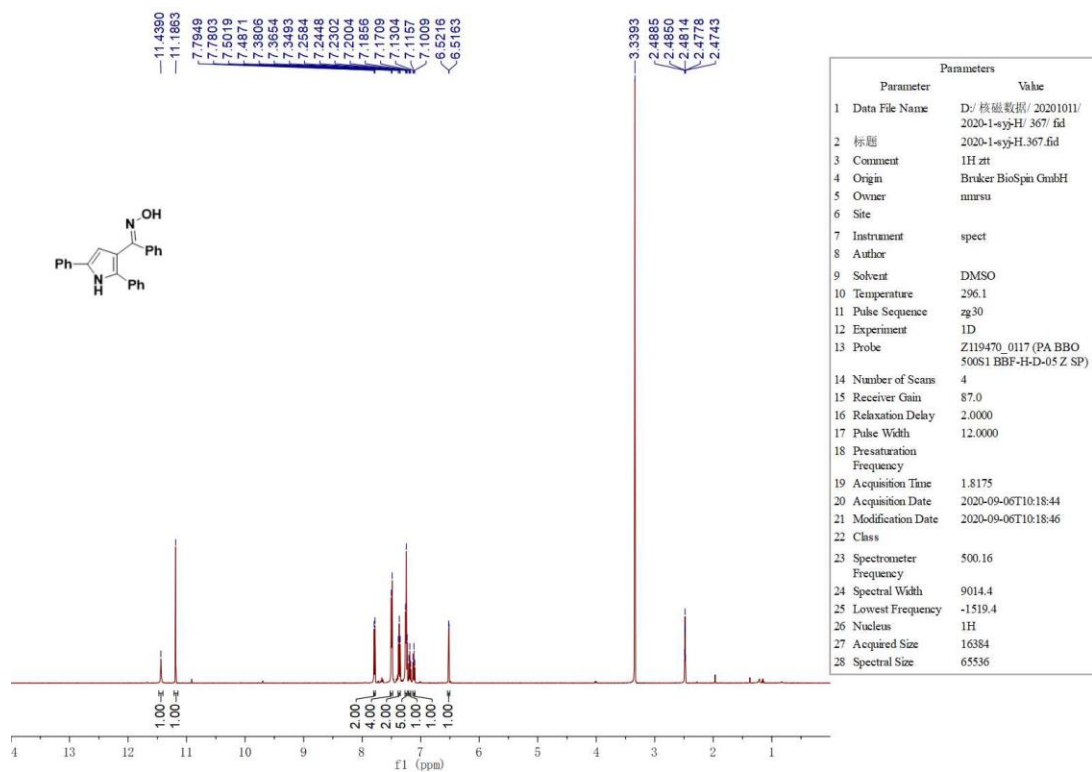


## 2-Methyl-4-phenyl-1H-imidazole (8)



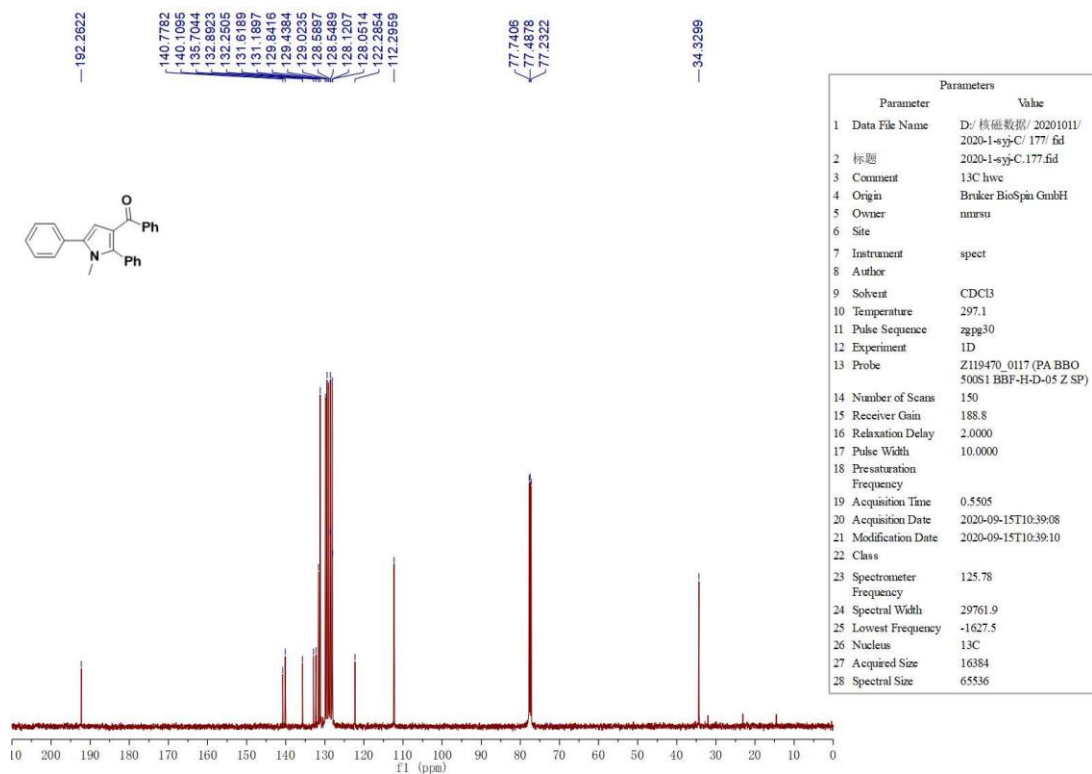
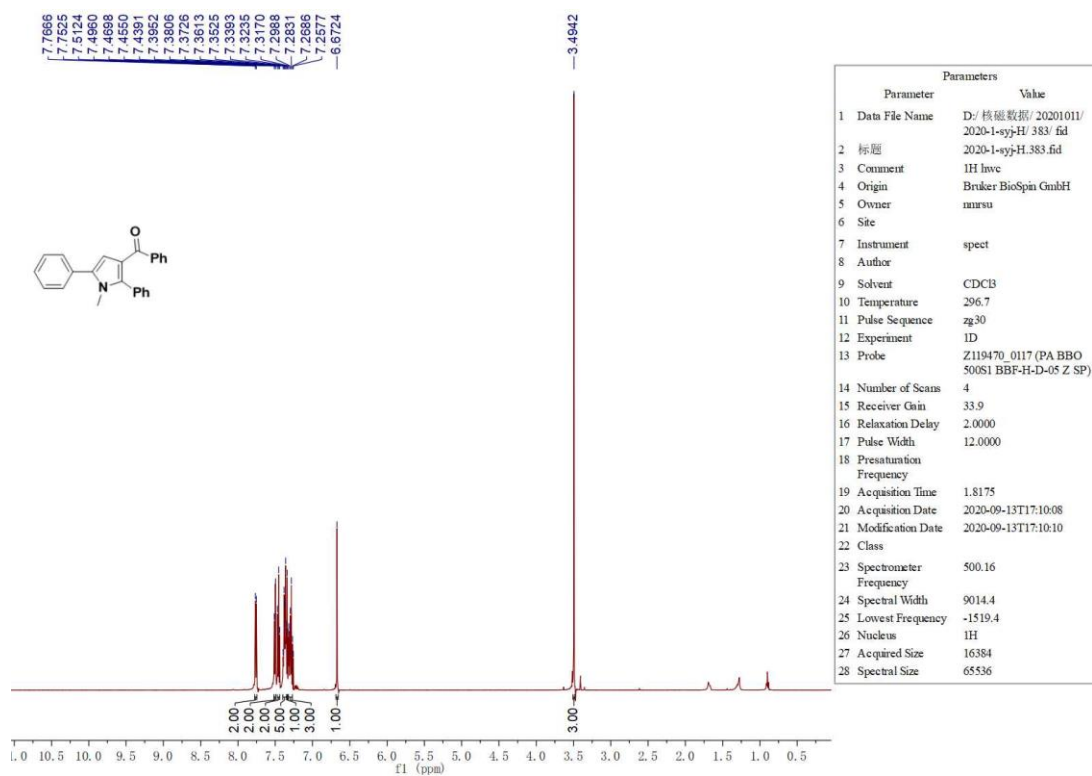


(E)-(2,5-Diphenyl-1H-pyrrol-3-yl) (phenyl)methanone oxime (9)





# (1-Methyl-2,5-diphenyl-1H-pyrrol-3-yl) (phenyl)methanone (10)





#### 4. GC-MS spectra for mechanistic investigations

