

Supporting Information

Substituent-controllable regioselective annulation of β -enaminones with *N*-sulfonyl triazoles for modular access to imidazoles and pyrroles

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1. X-ray crystallographic data of compound 3a

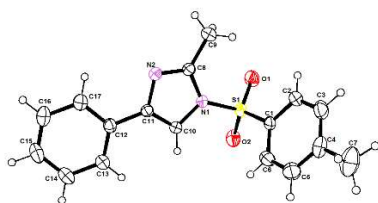


Figure S1. ORTEP drawing of compound **3a** (30% probability for the thermal ellipsoid).

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 ₁₇ H ₁₆ N ₂ O ₂ S
Formula weight	312.38
Temperature	298.15 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	$a = 12.6175(5)$ Å $\alpha = 90^\circ$. $b = 12.5587(5)$ Å $\beta = 99.2860(10)$. $c = 10.4154(4)$ Å $\gamma = 90^\circ$.
Volume	$1628.79(11)$ Å ³
Z	4
Density (calculated)	1.274 g/cm ³
μ	0.207 mm ⁻¹
F(000)	656.0
Crystal size	$0.21 \times 0.2 \times 0.19$ mm ³
2 θ range for data collection	5.722 to 55.072°
Index ranges	$-16 \leq h \leq 16$, $-16 \leq k \leq 16$, $-13 \leq l \leq 13$
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 ²	1.088
Final R indices [I>2sigma(I)]	$R_1 = 0.0429$, $wR_2 = 0.1112$
Final R indices (all data)	$R_1 = 0.0511$, $wR_2 = 0.1204$
Largest diff. peak and hole	0.21 and -0.43 eÅ ⁻³

1. X-ray crystallographic data of compound 5a

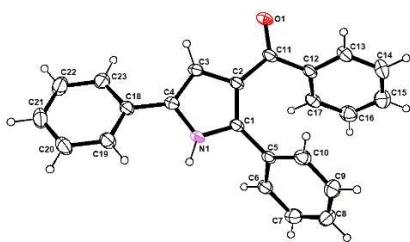


Figure S2. ORTEP drawing of compound **5a** (30% probability for the thermal

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.

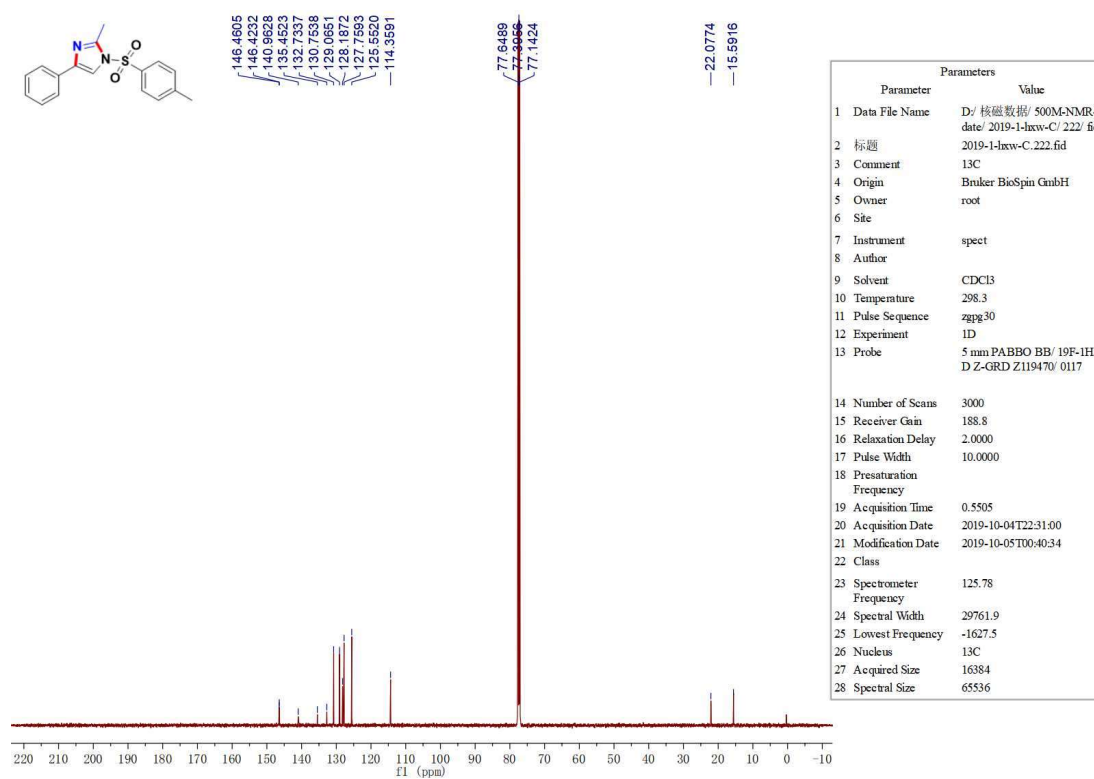
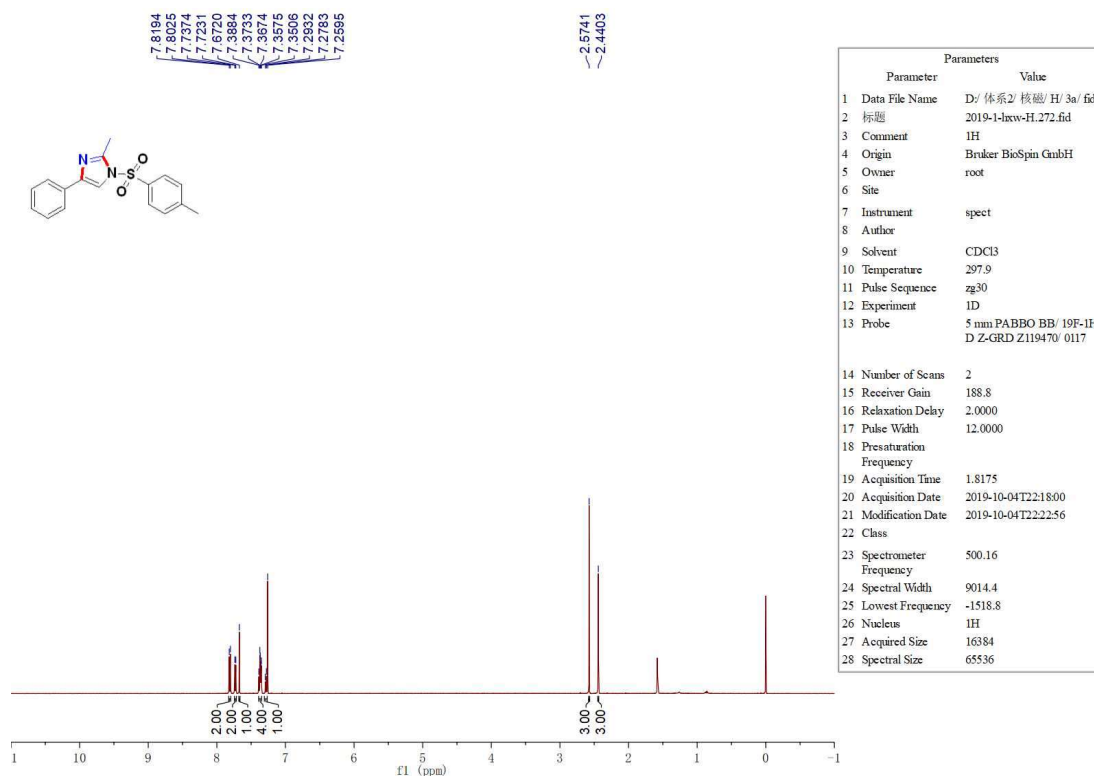
ellipsoid).

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

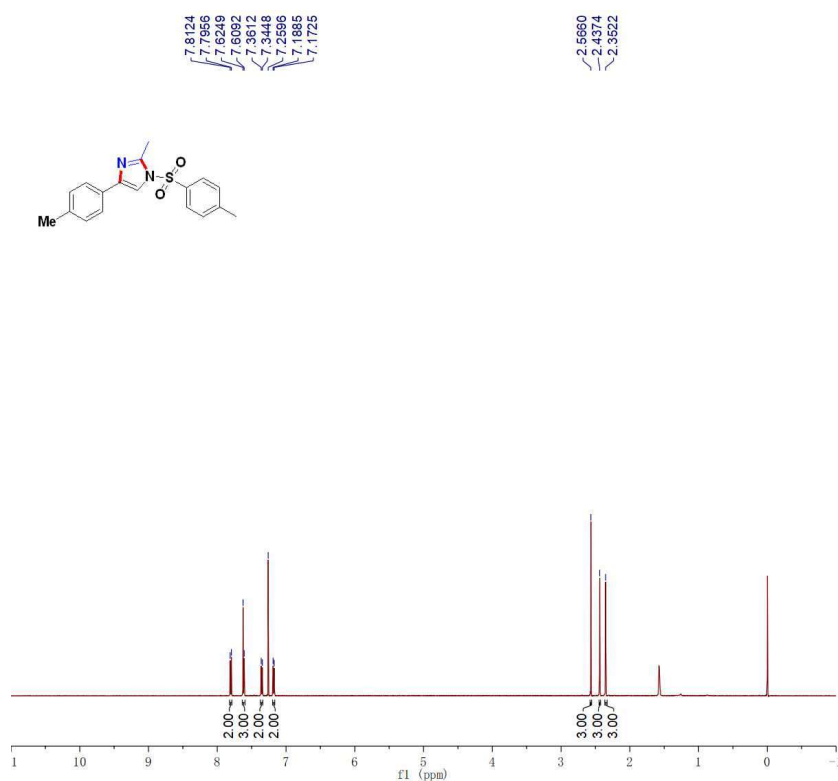
CCDC number	2260880
Identification code	mo_20200109b_0m_a
Empirical formula	C ₂₃ H ₁₇ N O
Formula weight	323.38
Temperature	298.15 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.9209(10) Å α = 113.914(4)°. b = 13.3600(16) Å β = 91.364(4)°. c = 14.6495(16) Å γ = 102.145(5)°.
Volume	1722.3(3) Å ³
Z	4
Density (calculated)	1.247 g/cm ³
μ	0.076 mm ⁻¹
F(000)	680.0
Crystal size	0.23 × 0.21 × 0.2 mm ³
2 θ 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 ²	1.046
Final R indices [I > 2sigma(I)]	R ₁ = 0.0547, wR ₂ = 0.1552
Final R indices (all data)	R ₁ = 0.0784, wR ₂ = 0.1779
Largest diff. peak and hole	0.26 and -0.29 eÅ ⁻³

3. NMR spectra for all compounds

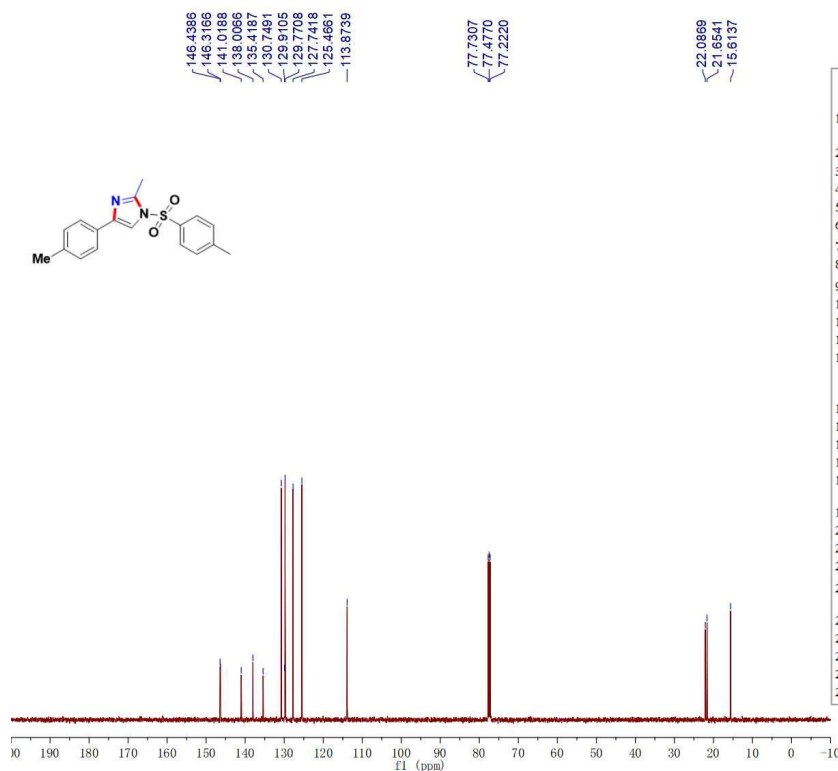
2-Methyl-4-phenyl-1-tosyl-1H-imidazole (3a)



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



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3 Comment	1H
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl ₃
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



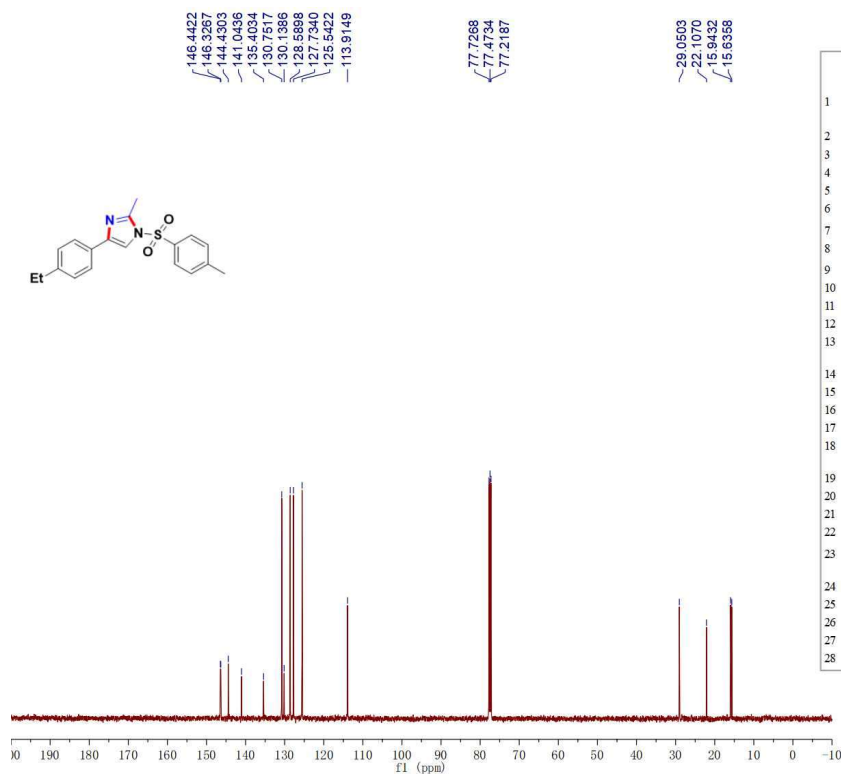
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3 Comment	13C
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl ₃
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
14 Number of Scans	40
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

Chemical Structure: CCc1ccc(cc1)/C=N/N(S(=O)(=O)c2ccccc2)C=C

¹H NMR Data (CDCl₃):

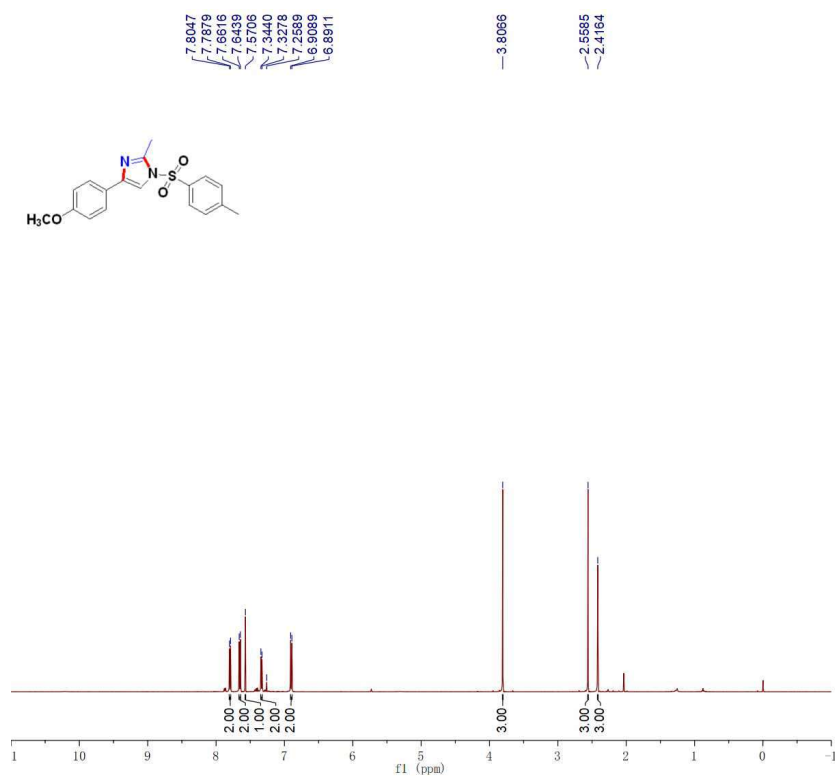
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~7.7	d	3.00
~7.4	m	2.00
~7.3	m	2.00
~2.6	s	3.00
~1.2	t	3.00

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3	Comment	1H ztt
4	Owner	Bruker BioSpin GmbH
5	Origin	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCB
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	30.7
16	Relaxation Delay	2.0000
17	Pulse Width	12.0000
18	Prestaturation 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

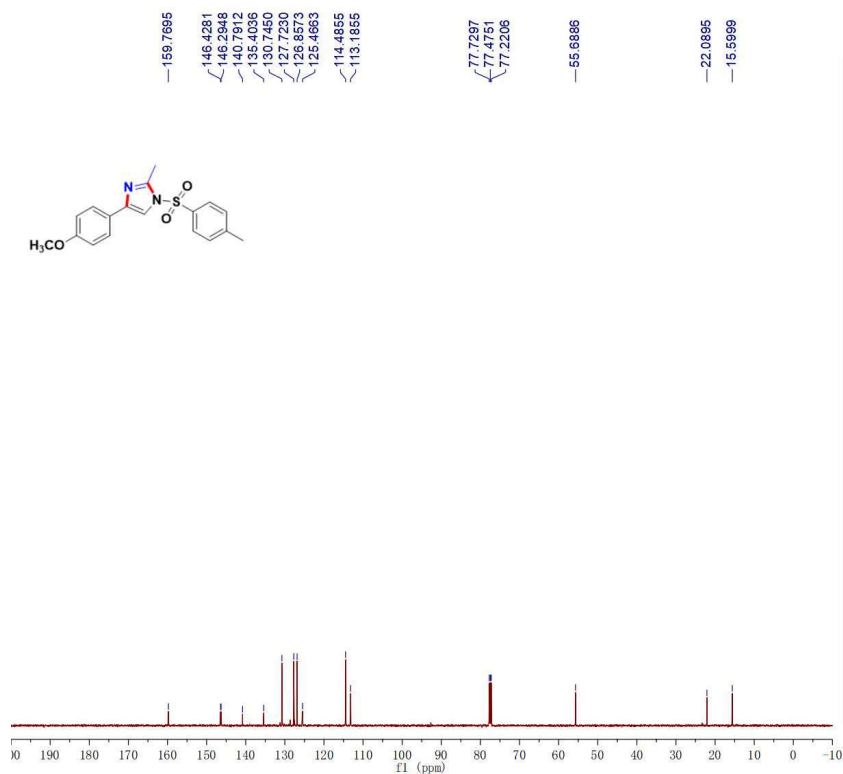


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5	Owner	root
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	UI19470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	55
15	Receiver Gain	188.8
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Prestaturation 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)

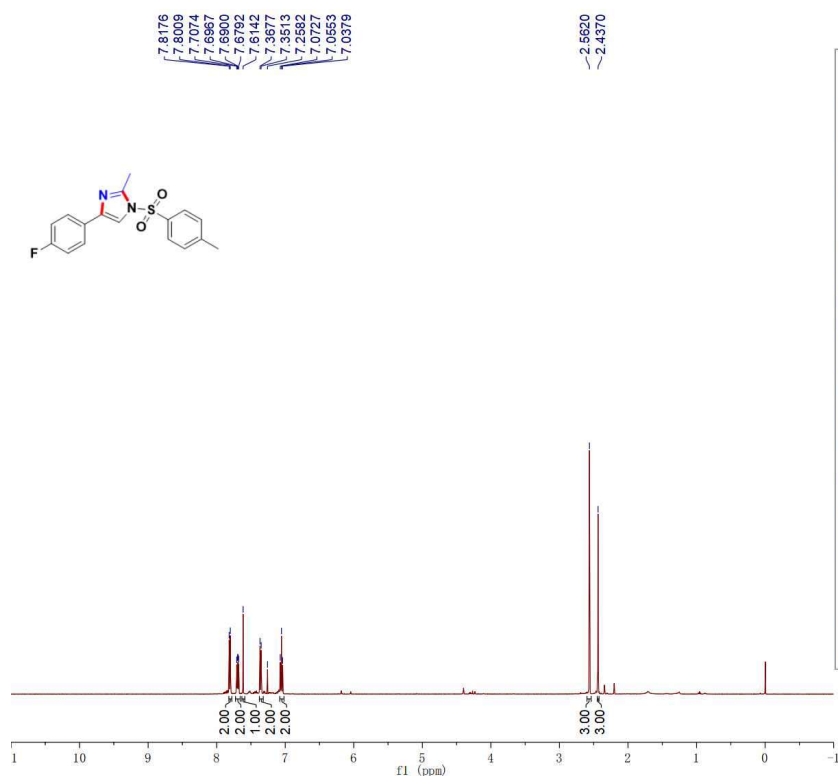


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3 Comment	1H	
4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl ₃	
10 Temperature	295.9	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117	
14 Number of 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	

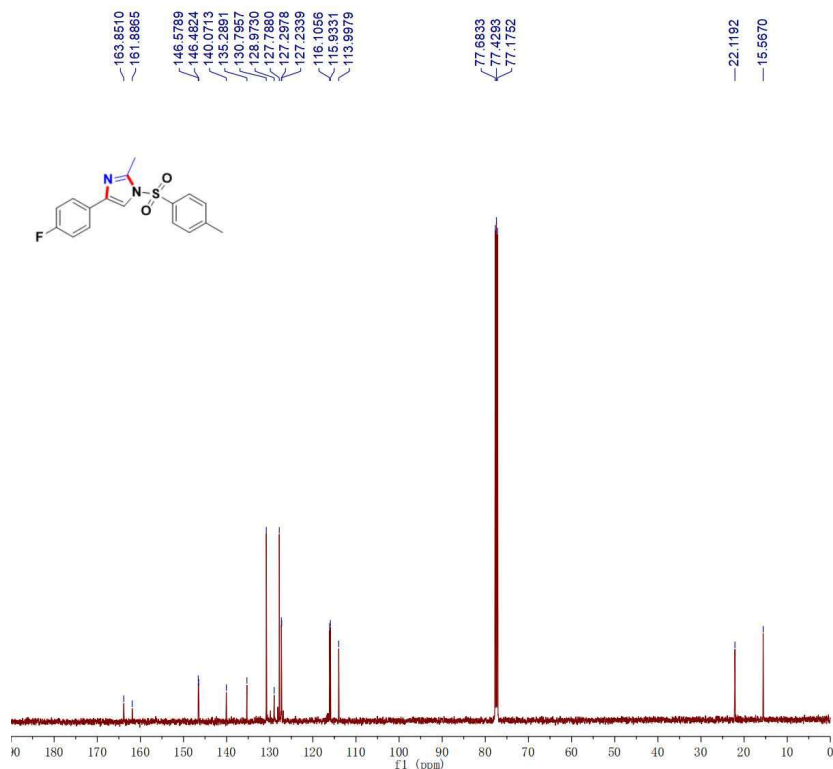


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5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl ₃	
10 Temperature	296.3	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117	
14 Number of Scans	30	
15 Receiver Gain	188.8	
16 Relaxation 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)

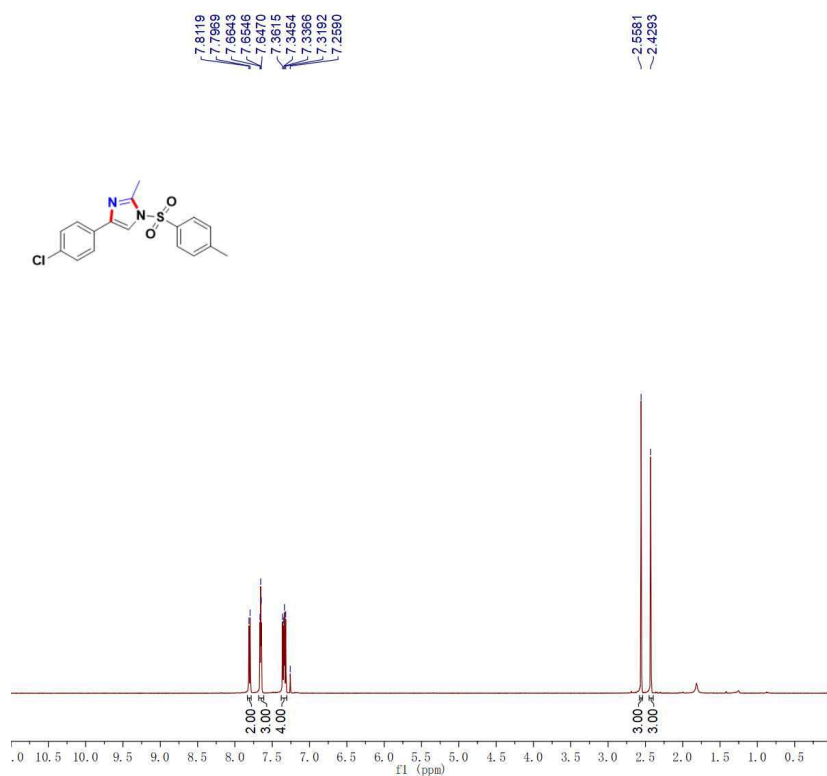


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4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
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7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.7	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 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	

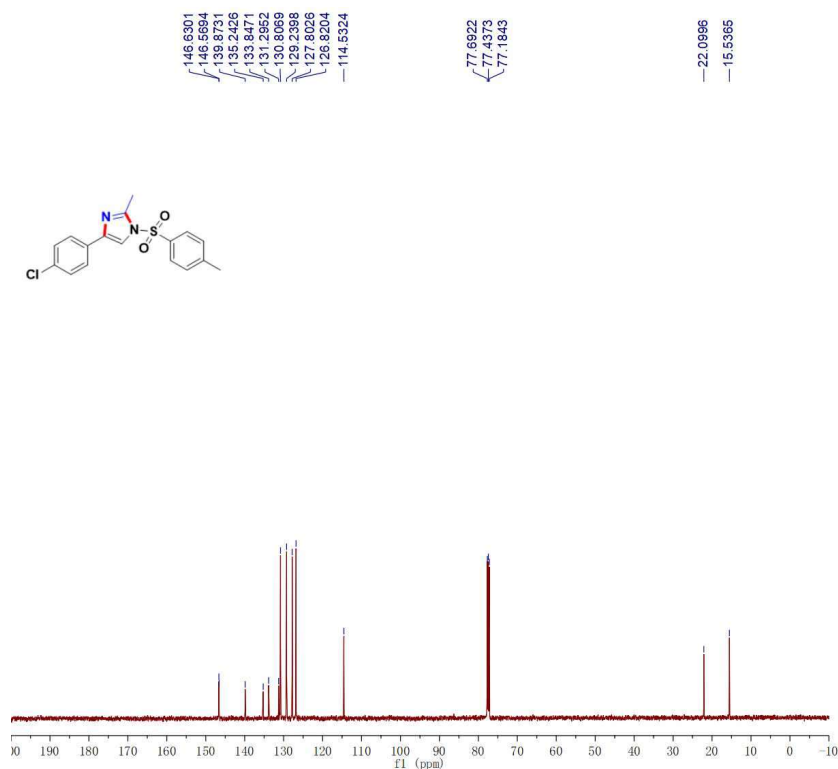


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4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	296.0	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	180	
15 Receiver Gain	188.8	
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17 Pulse Width	10.0000	
18 Presaturation Frequency		
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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)

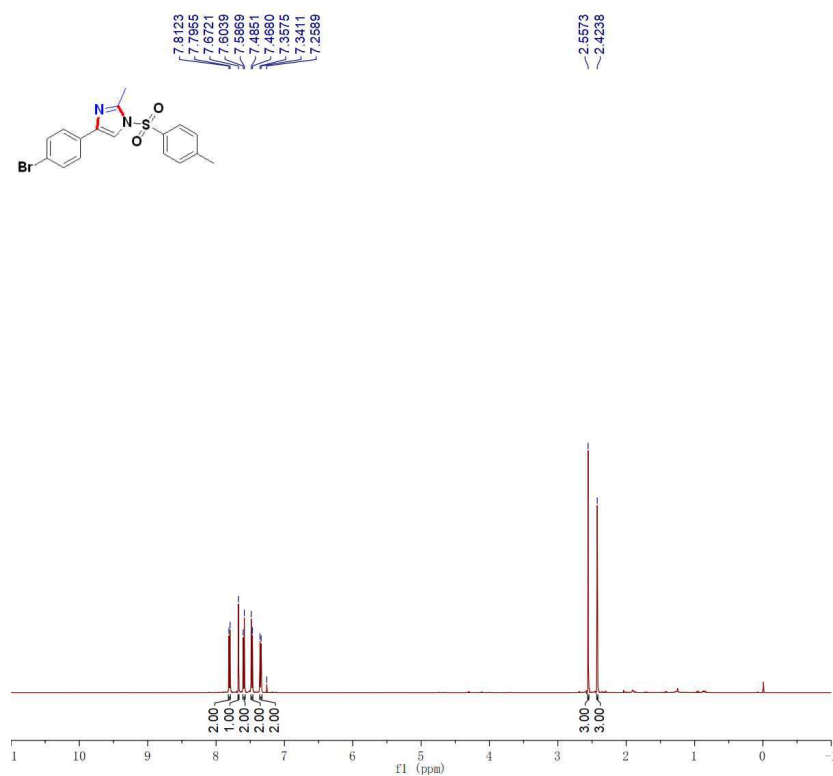


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5 Owner	nmusu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500SI BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	66.5
16 Relaxation Delay	2.0000
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	
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25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536

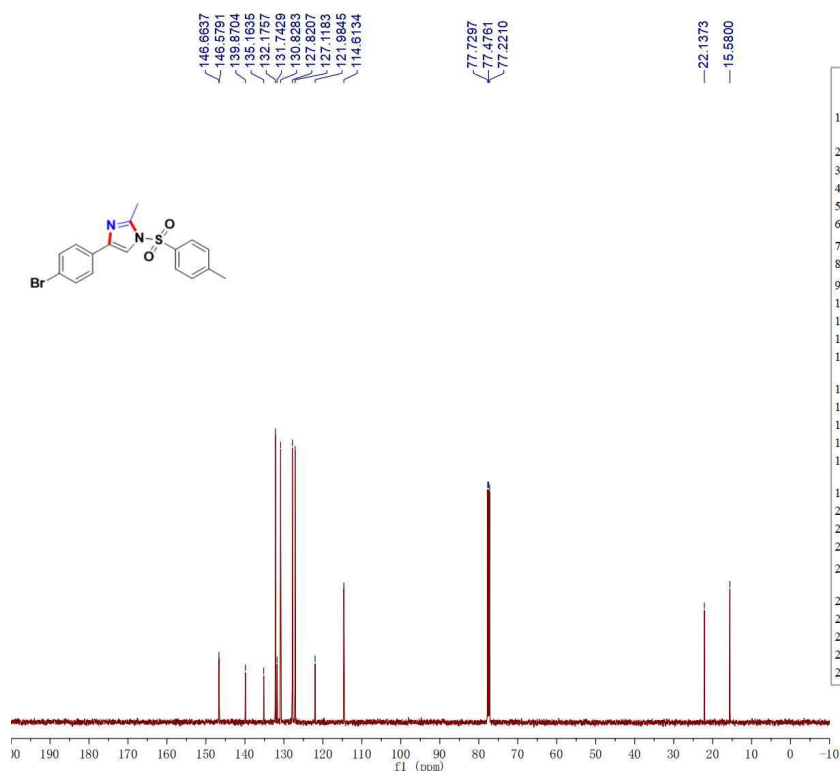


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5 Owner	nmusu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500SI BBF-H-D-05 Z SP)
14 Number of Scans	90
15 Receiver Gain	188.8
16 Relaxation Delay	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)

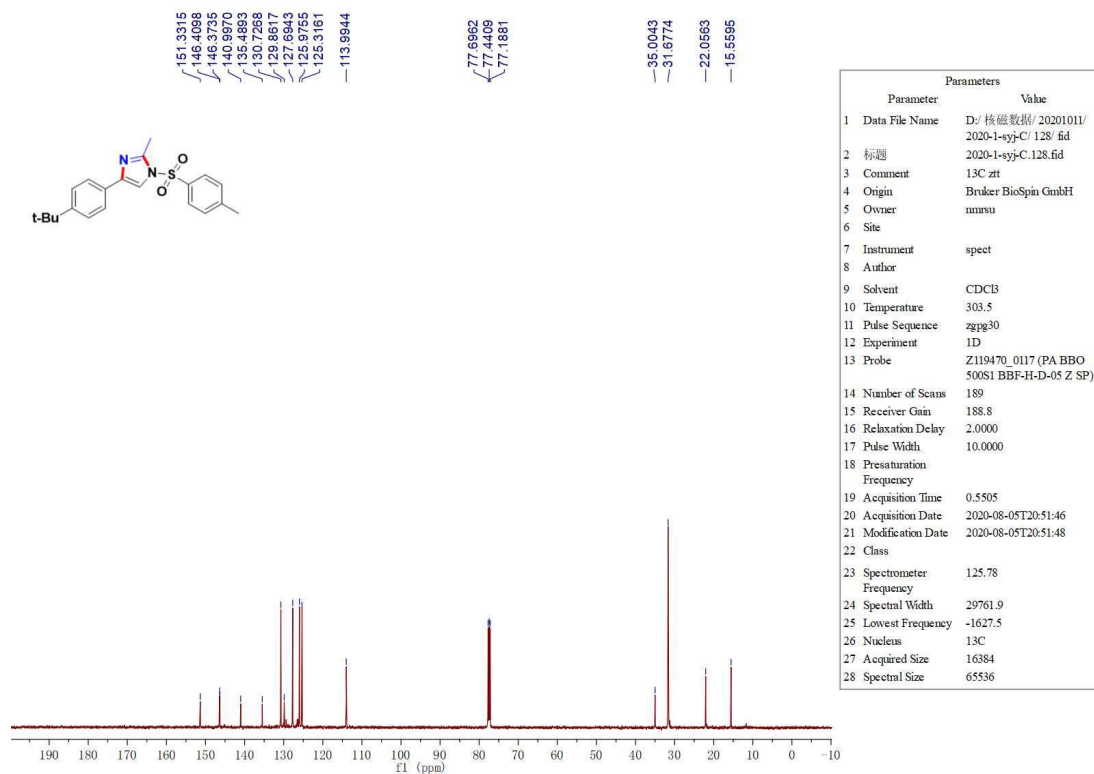
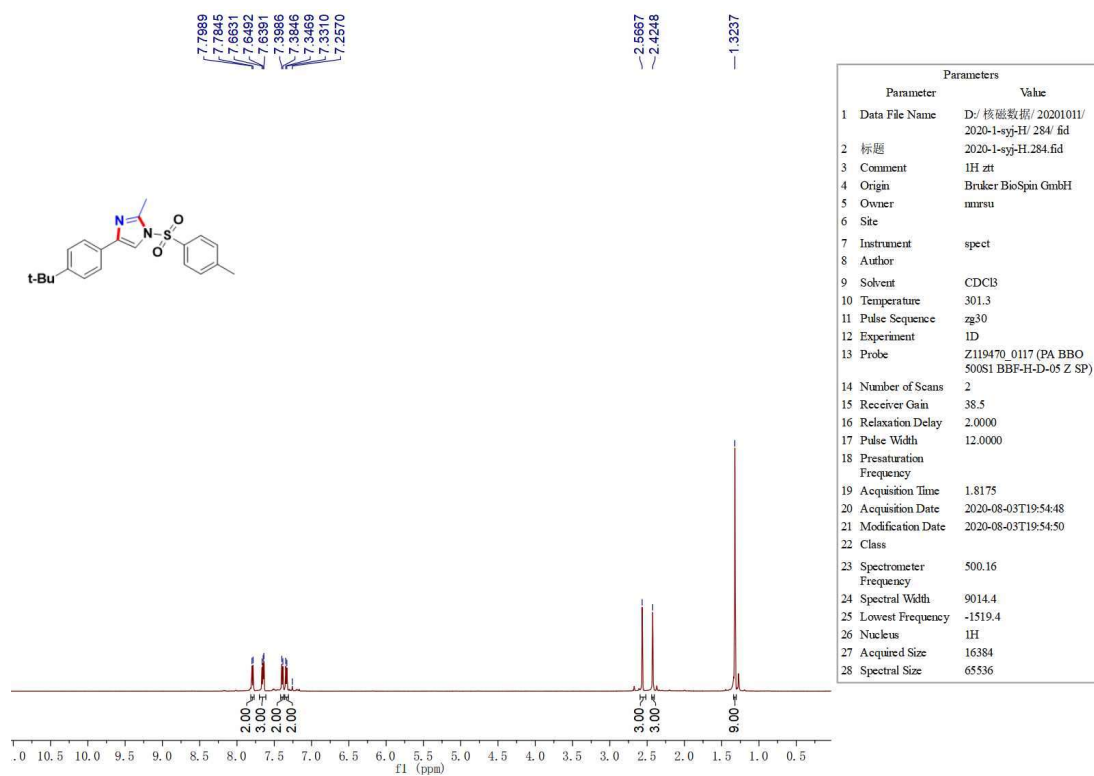


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5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	48.1
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
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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

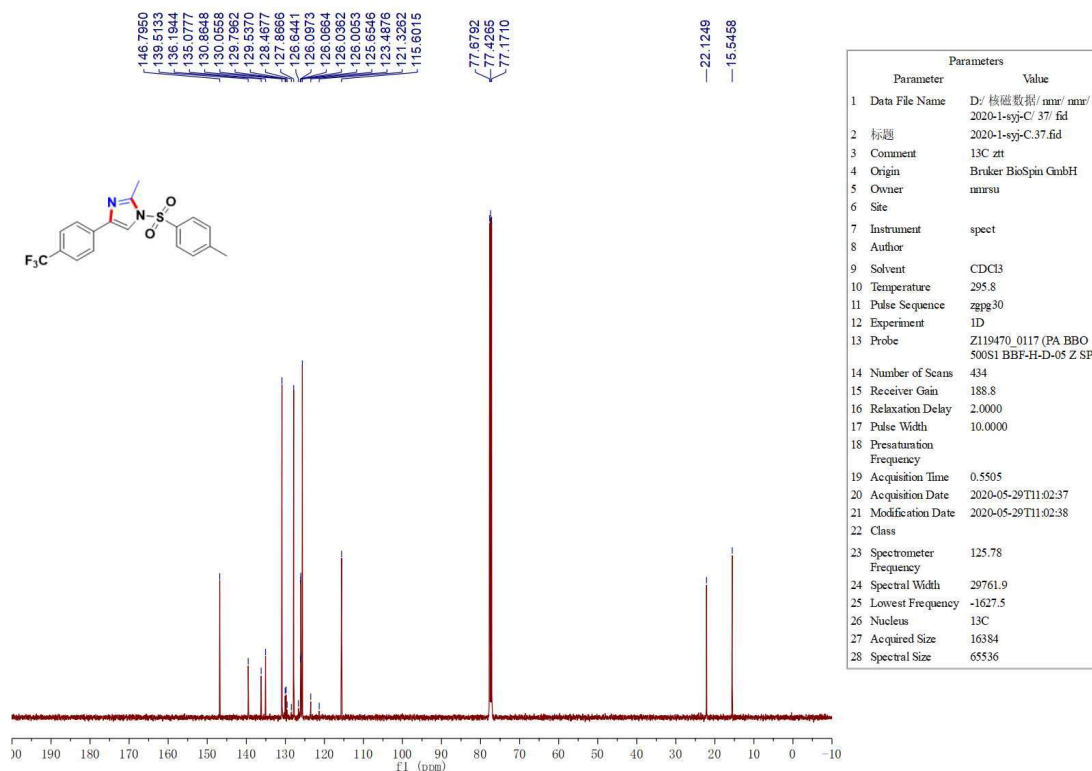
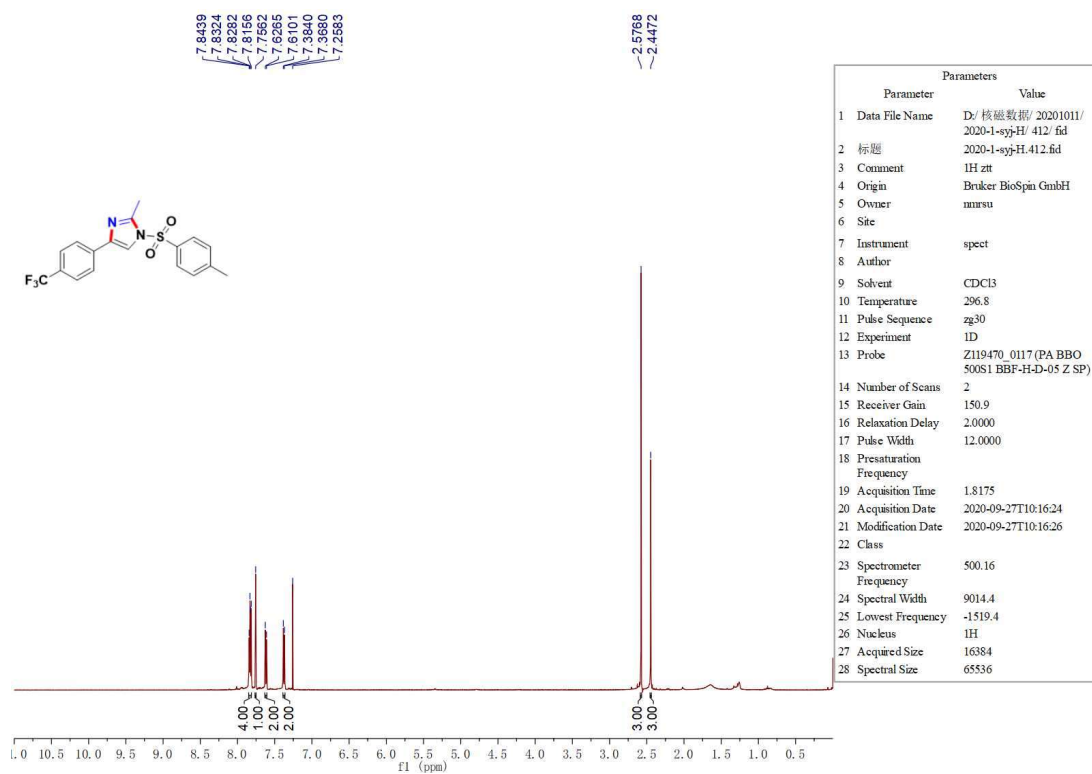


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5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	60
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
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	
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24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536

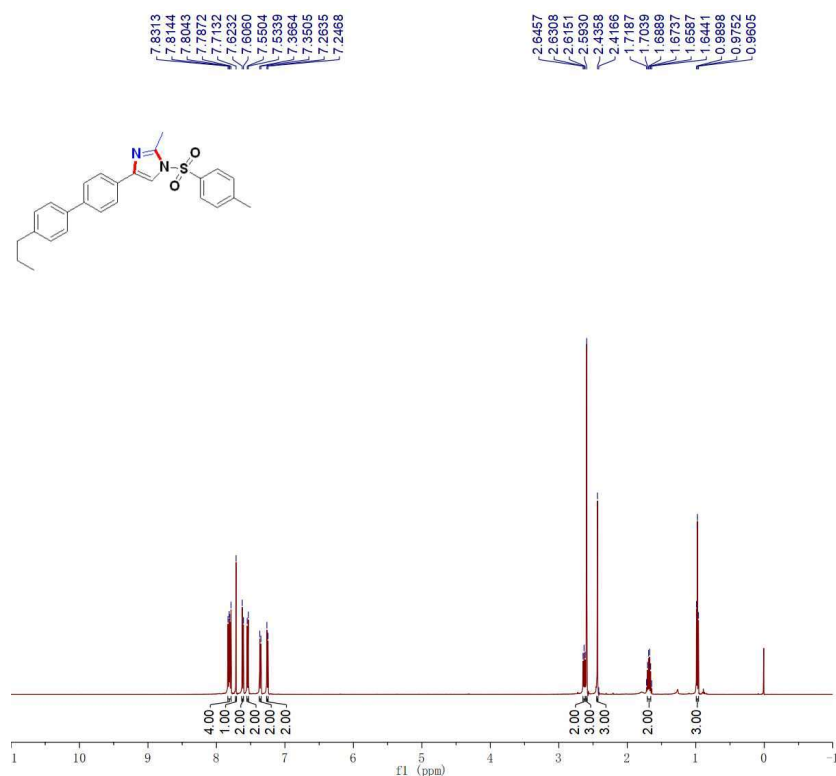
4-(4-(*tert*-Butyl)phenyl)-2-methyl-1H-imidazole (3h)



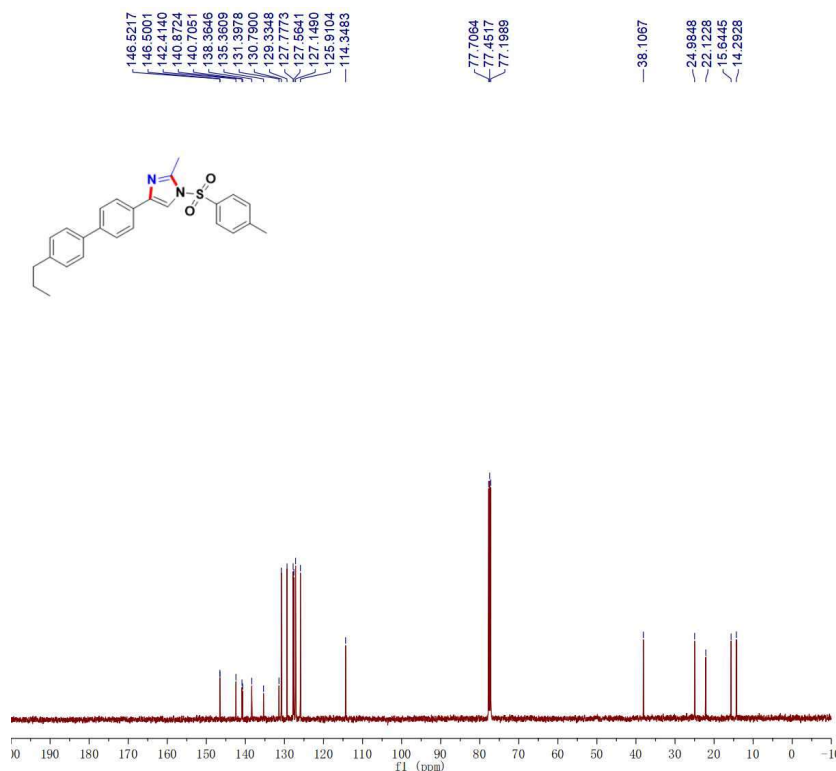
2-Methyl-1-tosyl-4-(4-(trifluoromethyl)phenyl)-1*H*-imidazole (3i)



2-Methyl-4-(4'-propyl-[1, 1'-biphenyl]-4-yl)-1-tosyl-1*H*-imidazole (3j)

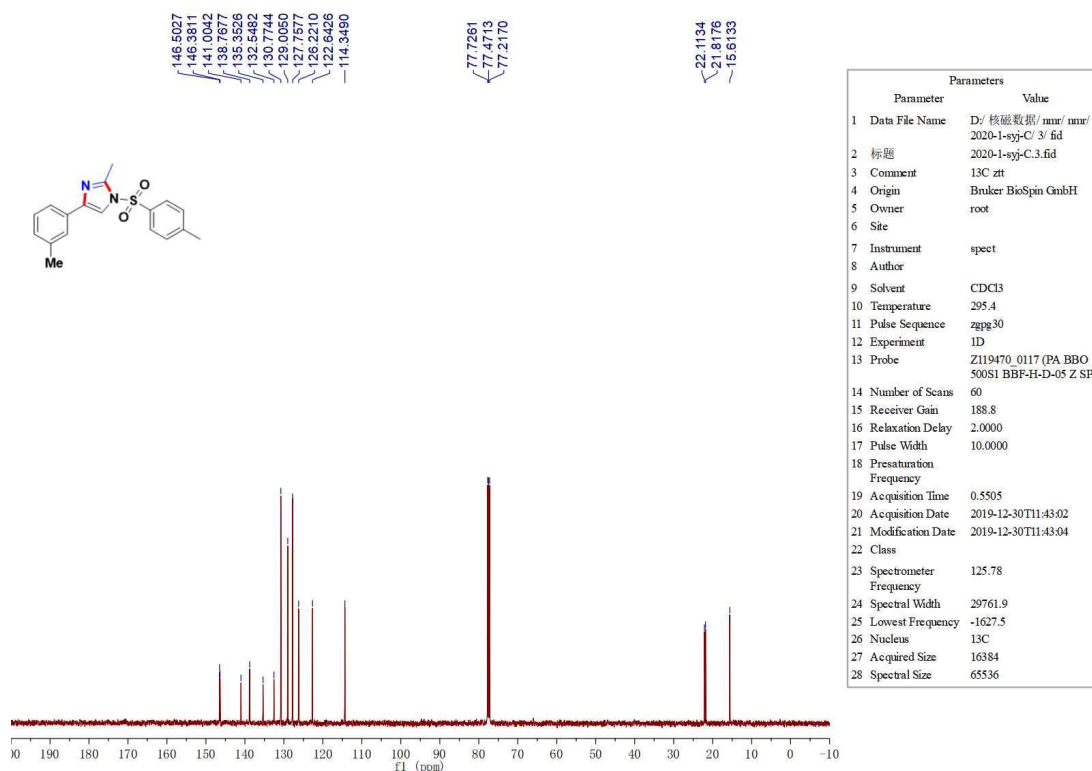
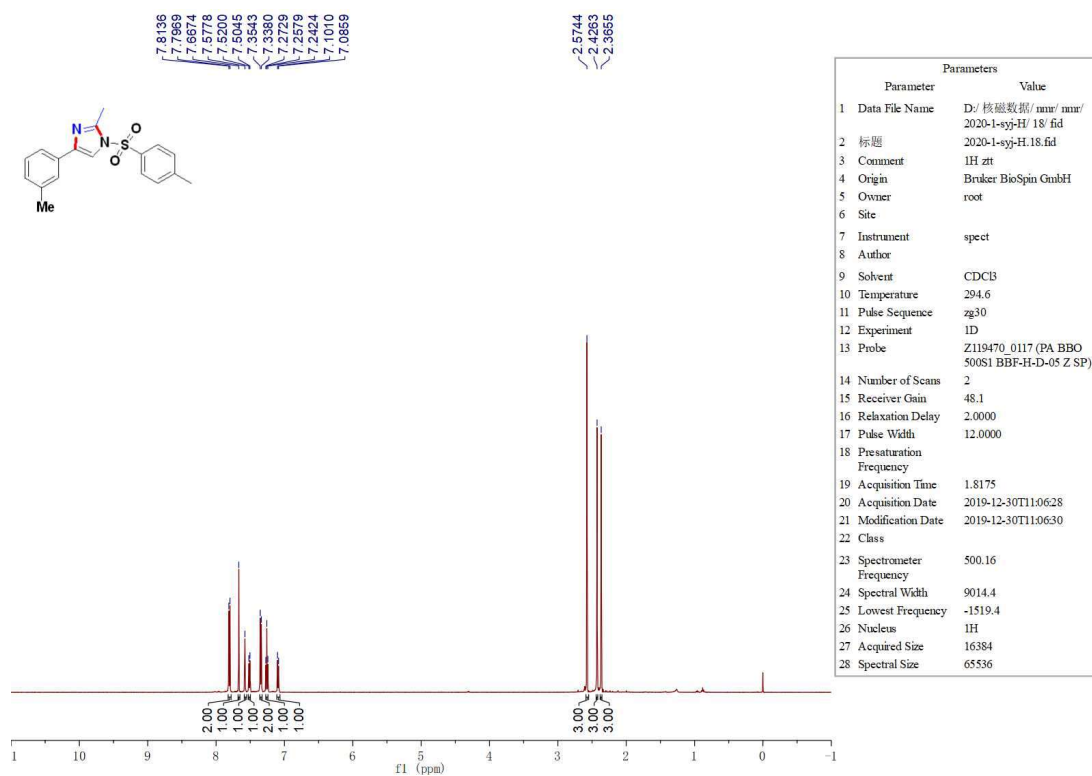


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5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl ₃	
10 Temperature	295.5	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	2	
15 Receiver Gain	38.5	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation 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	

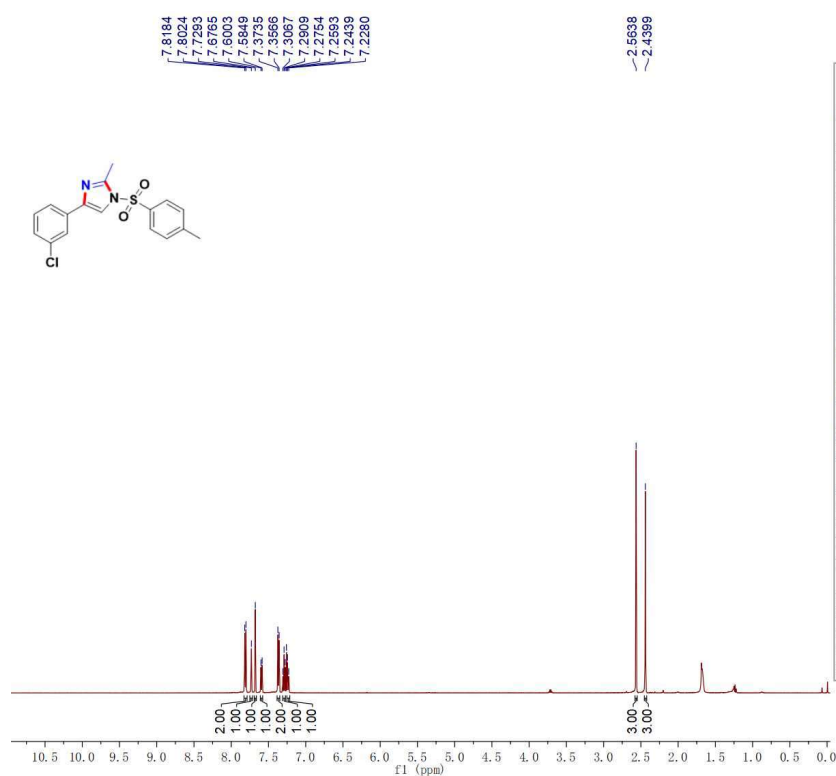


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/	
2 标题	2020-1-syy-C/ 40/ fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl ₃	
10 Temperature	295.8	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	71	
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	2020-06-01T10:33:47	
21 Modification Date	2020-06-01T10:33:50	
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	

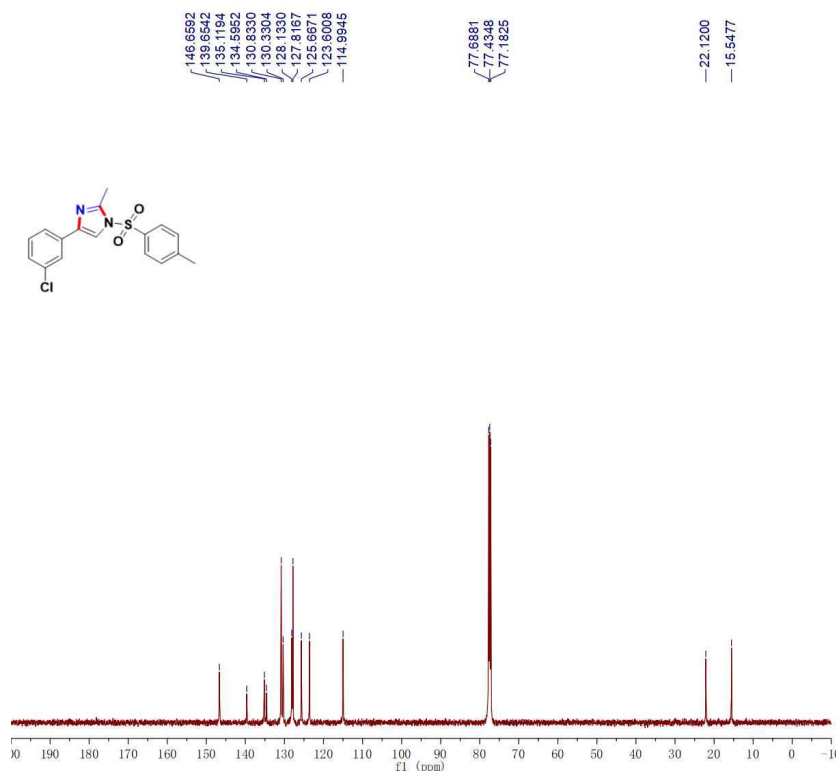
2-Methyl-4-(*m*-tolyl)-1-tosyl-1*H*-imidazole (3k)



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

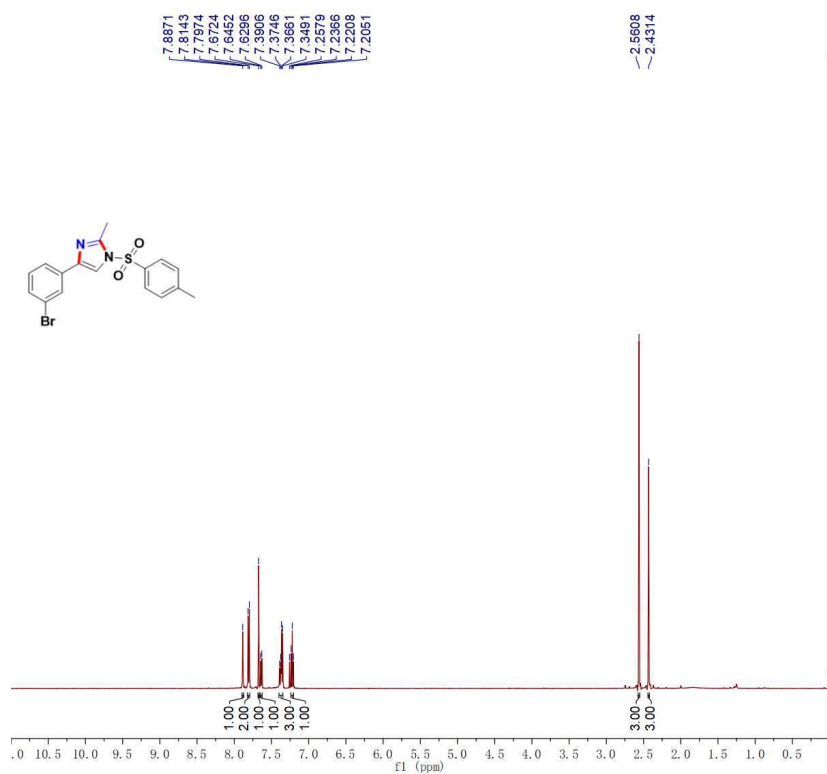


Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-H/ 251/ fid
2 标题	2020-1-sy-H-251.fid
3 Comment	1H ztt
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (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

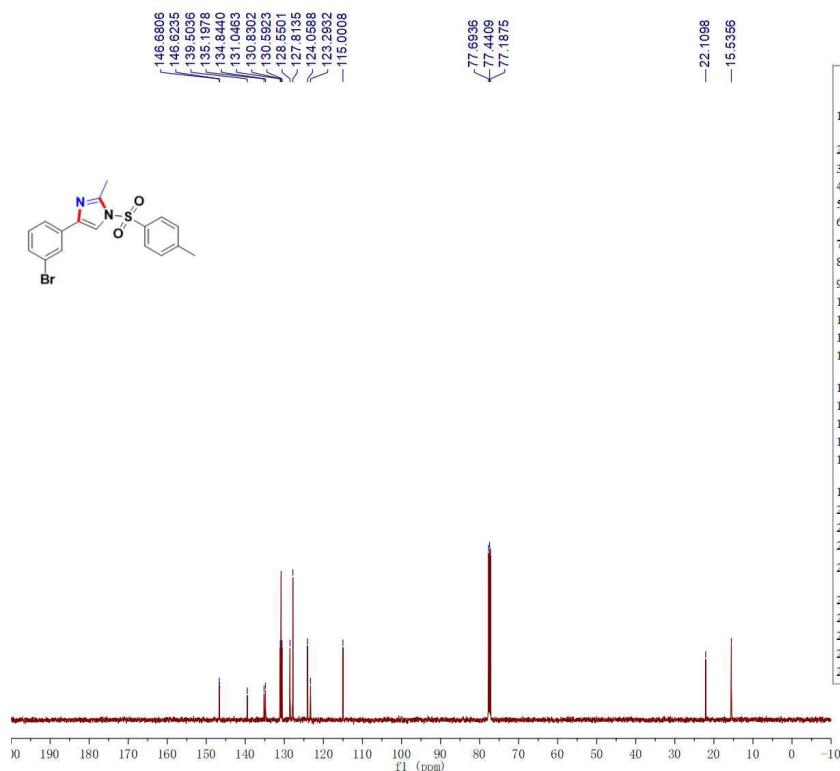


Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-C/ 97/ fid
2 标题	2020-1-sy-C-97.fid
3 Comment	13C ztt
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (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)

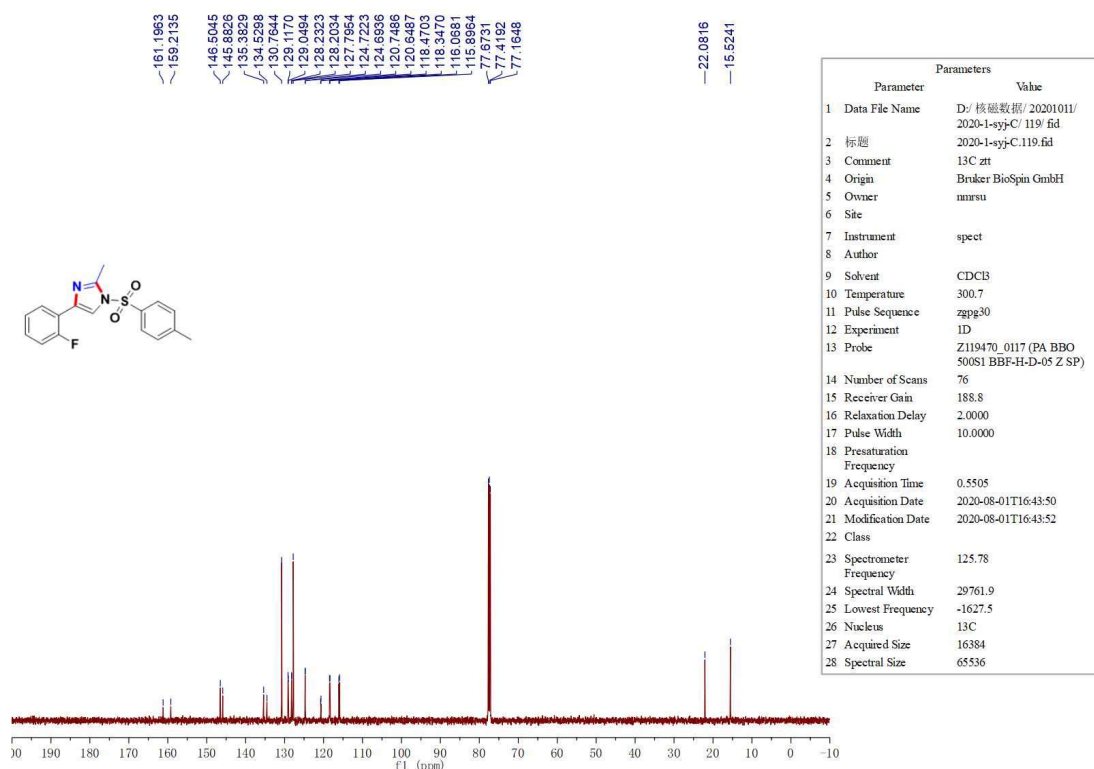
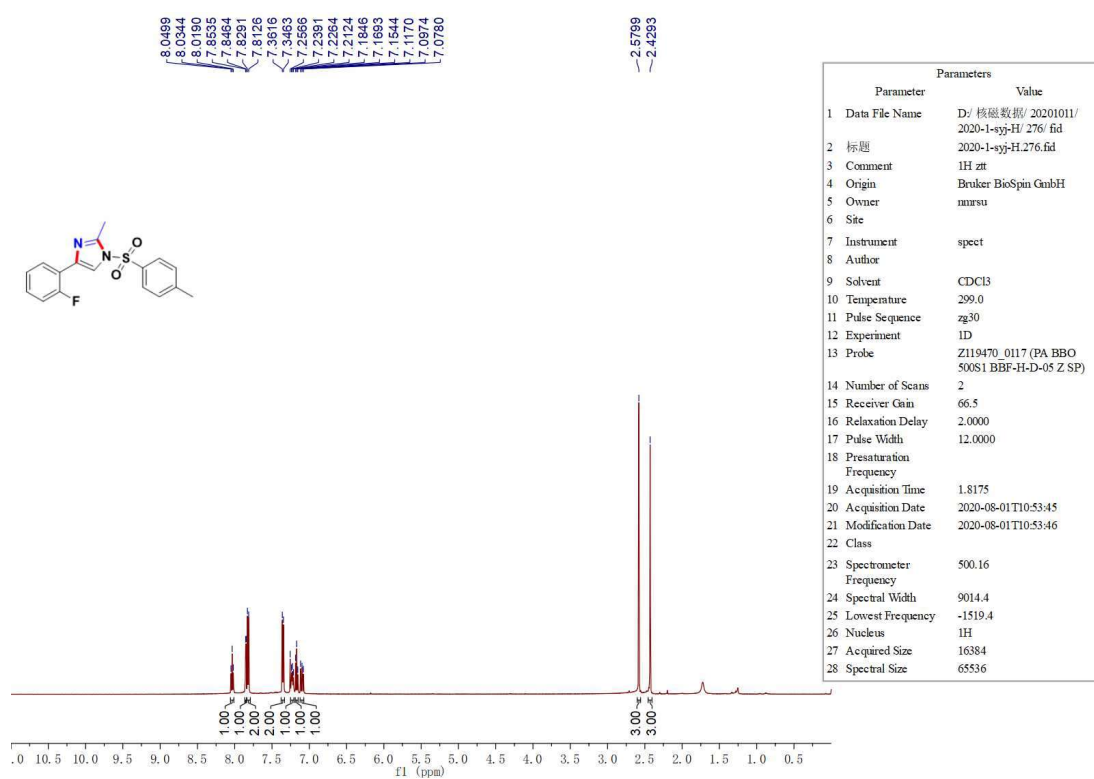


Parameters	
Parameter	Value
1 Data File Name	D:\核磁数据\20201011\2020-1-sy-H-275.fid
2 标题	2020-1-sy-H-275.fid
3 Comment	1H ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl ₃
10 Temperature	299.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBR-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	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	¹ H
27 Acquired Size	16384
28 Spectral Size	65536

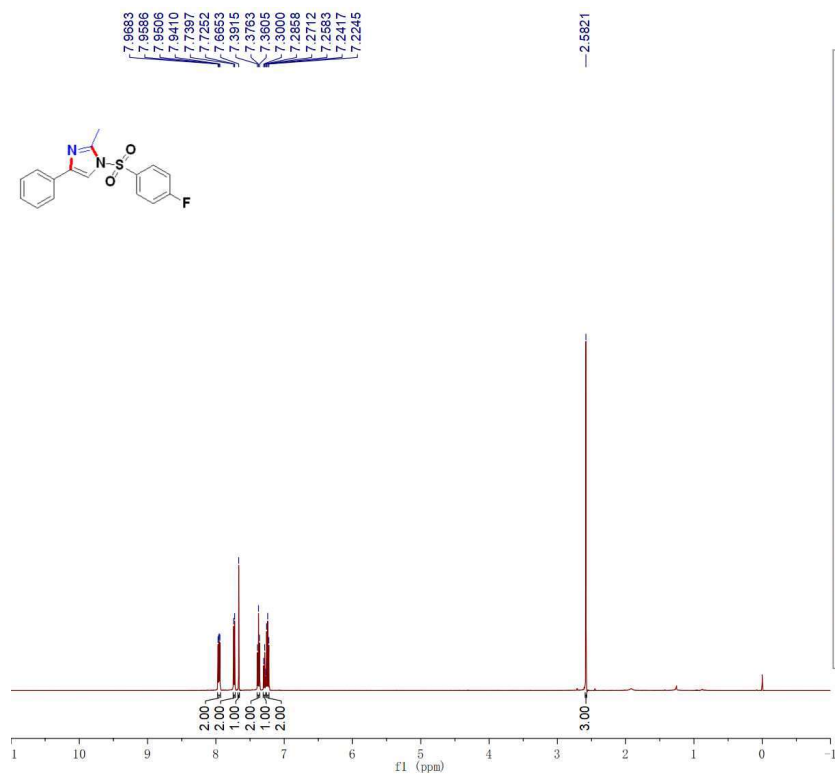


Parameters	
Parameter	Value
1 Data File Name	D:\核磁数据\20201011\2020-1-sy-C-118.fid
2 标题	2020-1-sy-C-118.fid
3 Comment	13C ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl ₃
10 Temperature	300.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBR-H-D-05 Z SP)
14 Number of Scans	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	¹³ C
27 Acquired Size	16384
28 Spectral Size	65536

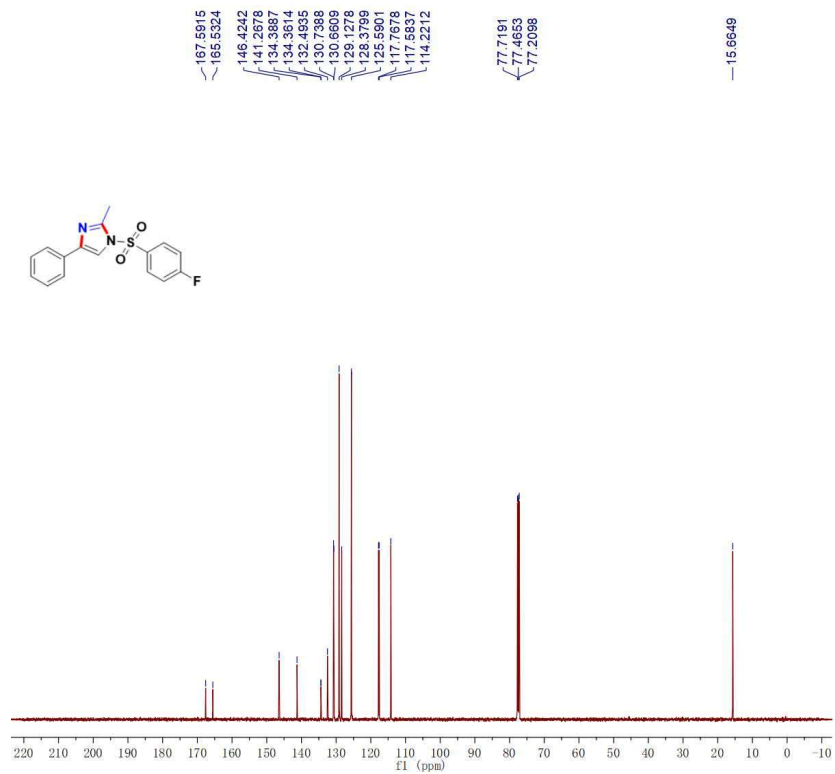
4-(2-Fluorophenyl)-2-methyl-1-tosyl-1H-imidazole (3n)



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

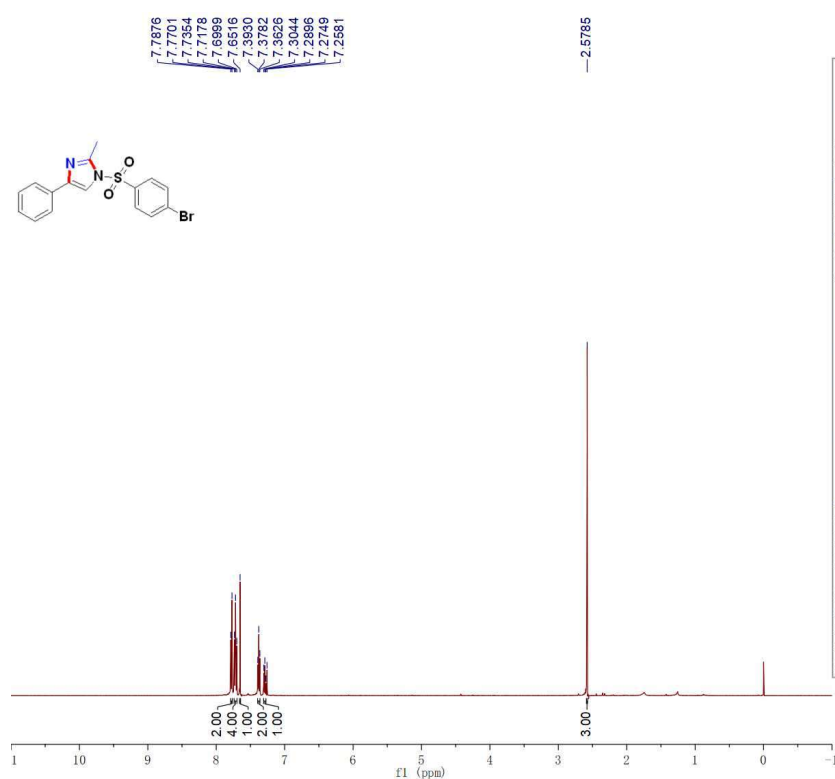


Parameters		
Parameter	Value	
1 Data File Name	D:\ 核磁数据\ nmr\ nmr\ 2020-1-syy-H\ 114.fid	
2 标题	2020-1-syy-H.114.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.7	
11 Pulse Sequence	zg30	
12 Experiment	1D	
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 Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	

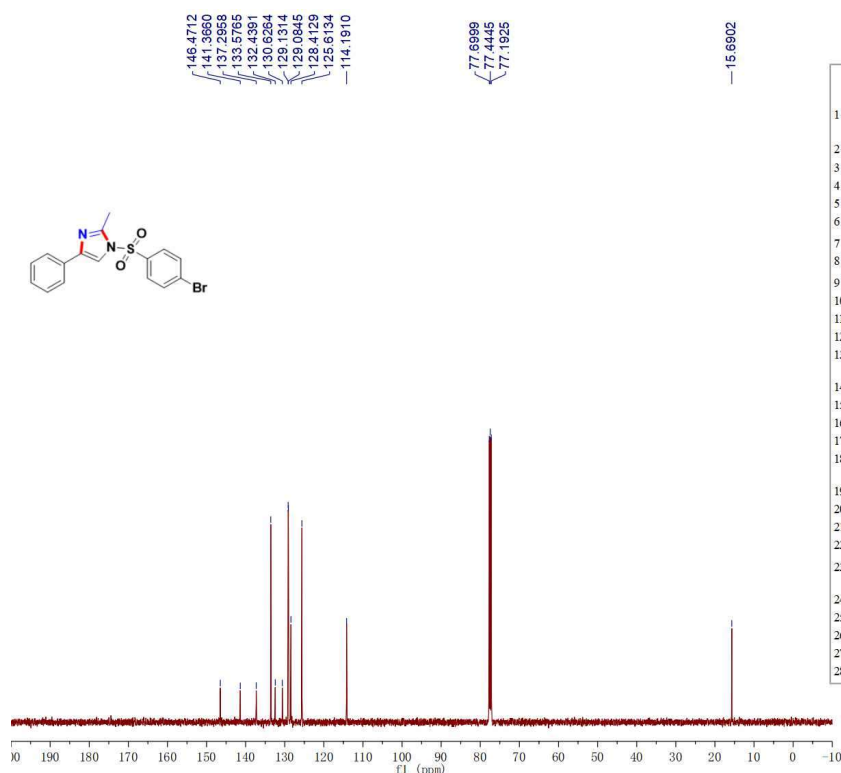


Parameters		
Parameter	Value	
1 Data File Name	D:\ 核磁数据\ nmr\ nmr\ 2020-1-syy-C\ 42.fid	
2 标题	2020-1-syy-C.42.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.6	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
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 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-((4-Bromophenyl)sulfonyl)-2-methyl-4-phenyl-1H-imidazole (3p)

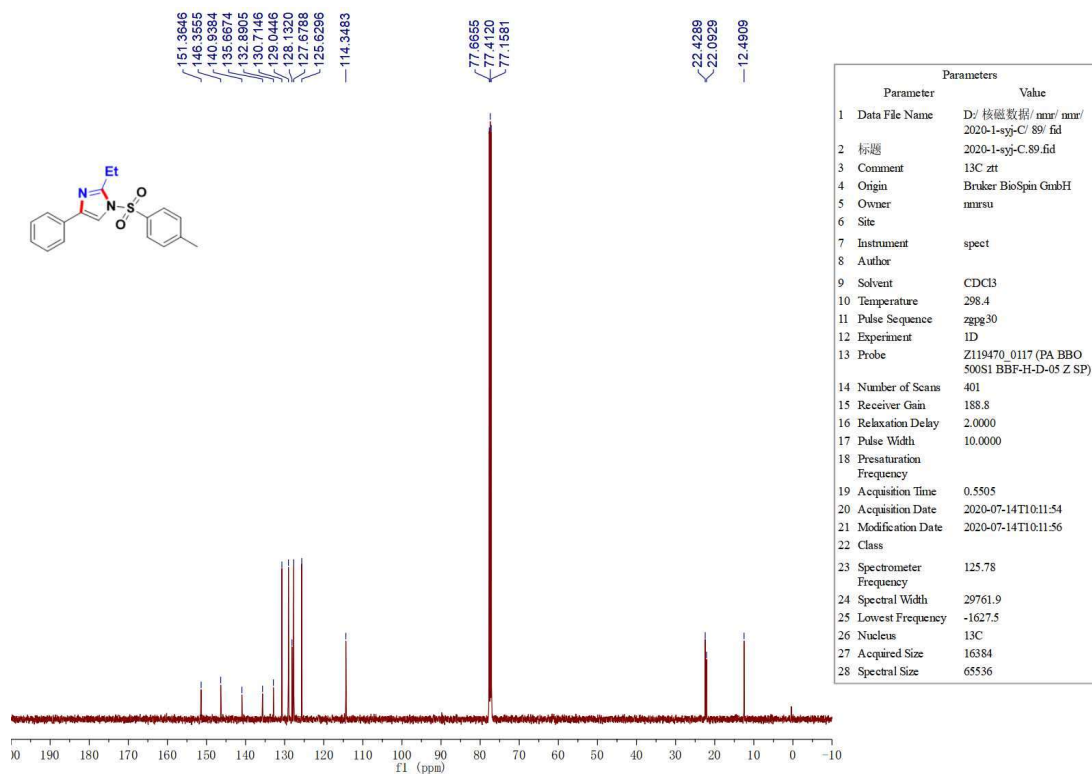
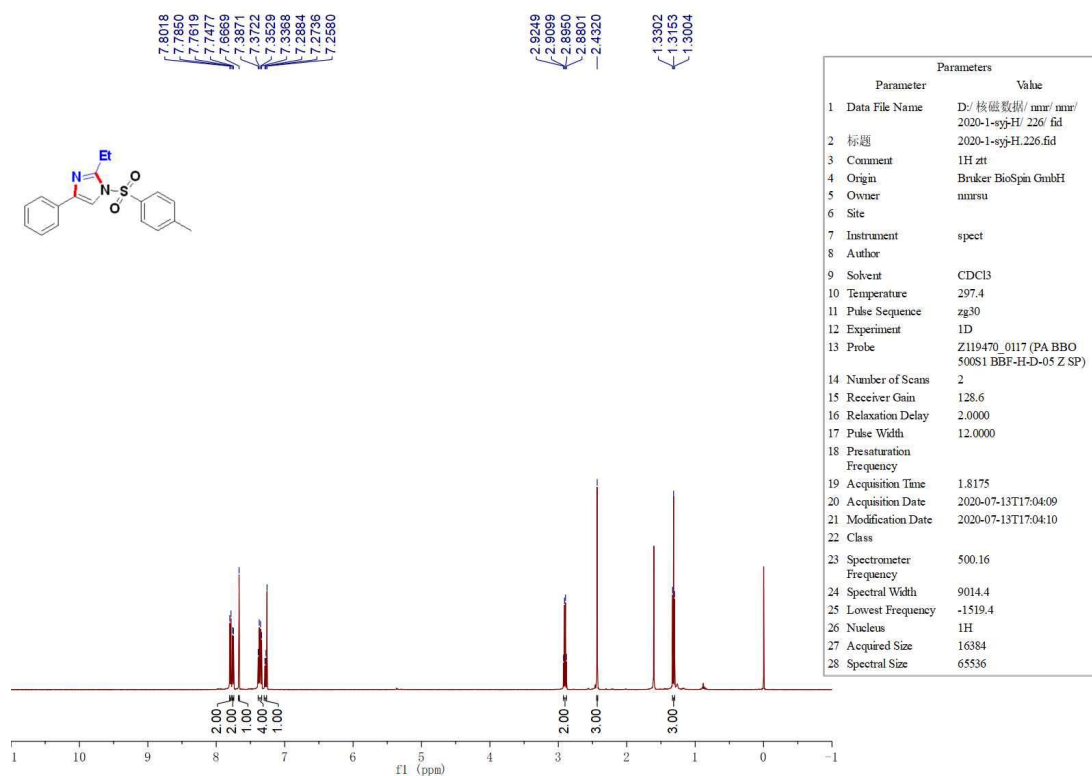


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-sy-H-113/ fid	
2 标题	2020-1-sy-H-113.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.6	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 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	

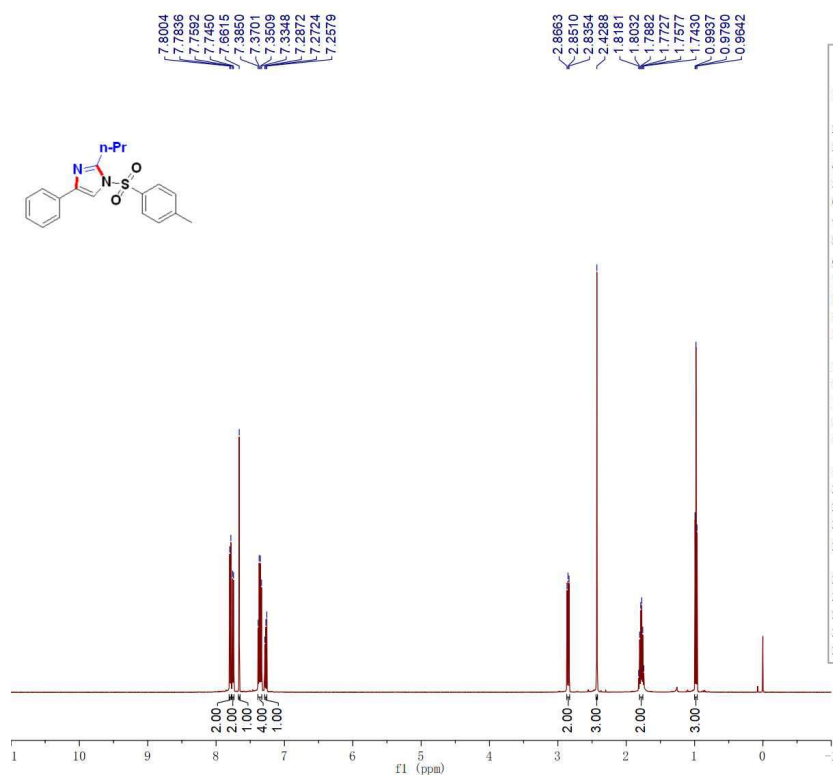


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-sy-C/ 41/ fid	
2 标题	2020-1-sy-C-41.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.7	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
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	

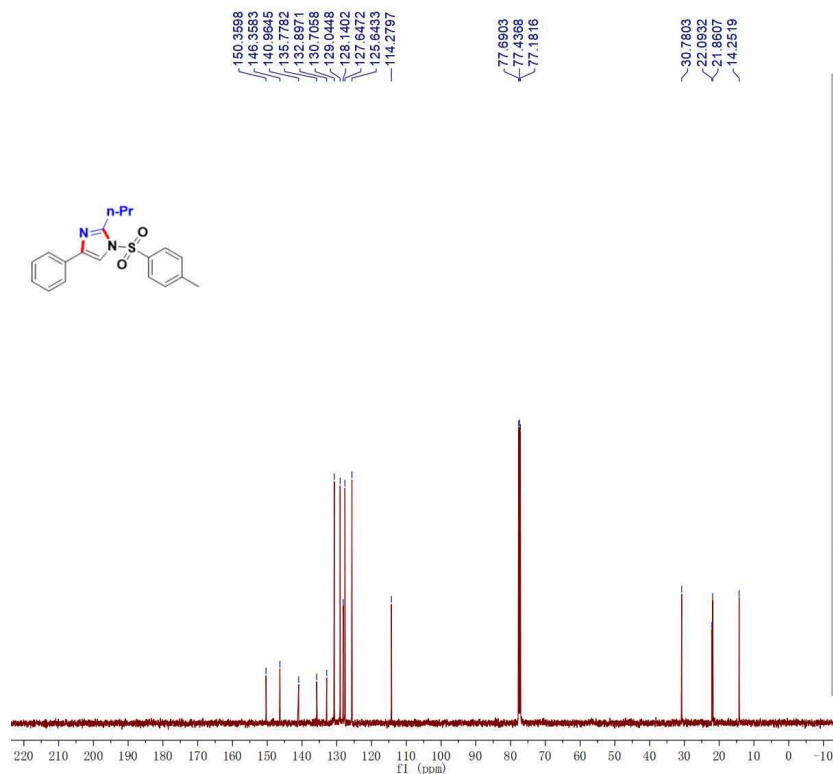
2-Ethyl-4-phenyl-1-tosyl-1H-imidazole (3q)



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

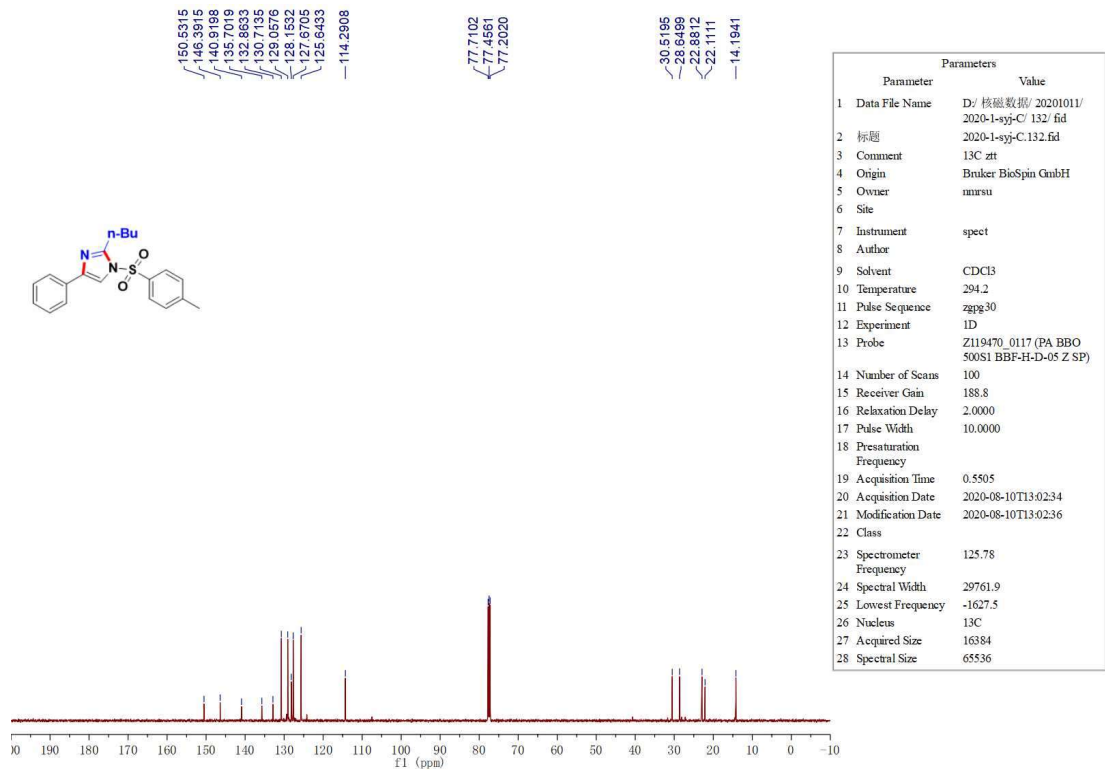
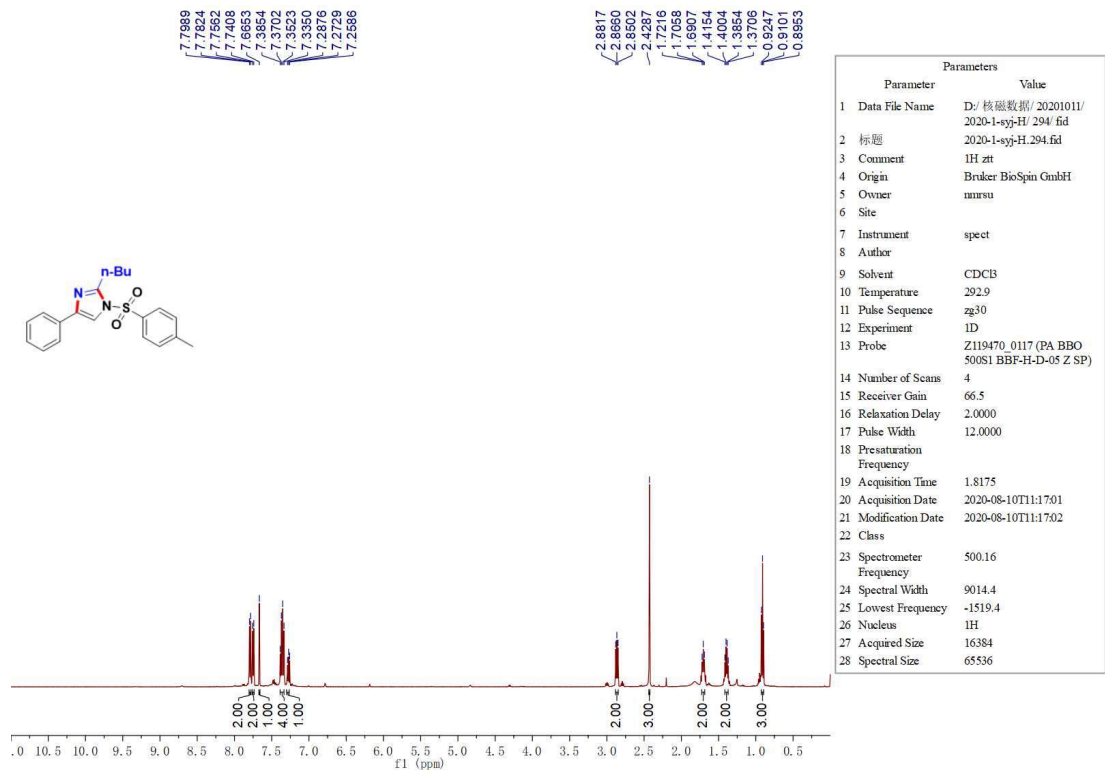


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-sy-H/ 224/ fid	
2 标题	2020-1-sy-H.224.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	297.4	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 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 Frequency	500.16	
24 Spectral Width	9014.4	
25 Lowest Frequency	-1519.4	
26 Nucleus	1H	
27 Acquired Size	16384	
28 Spectral Size	65536	

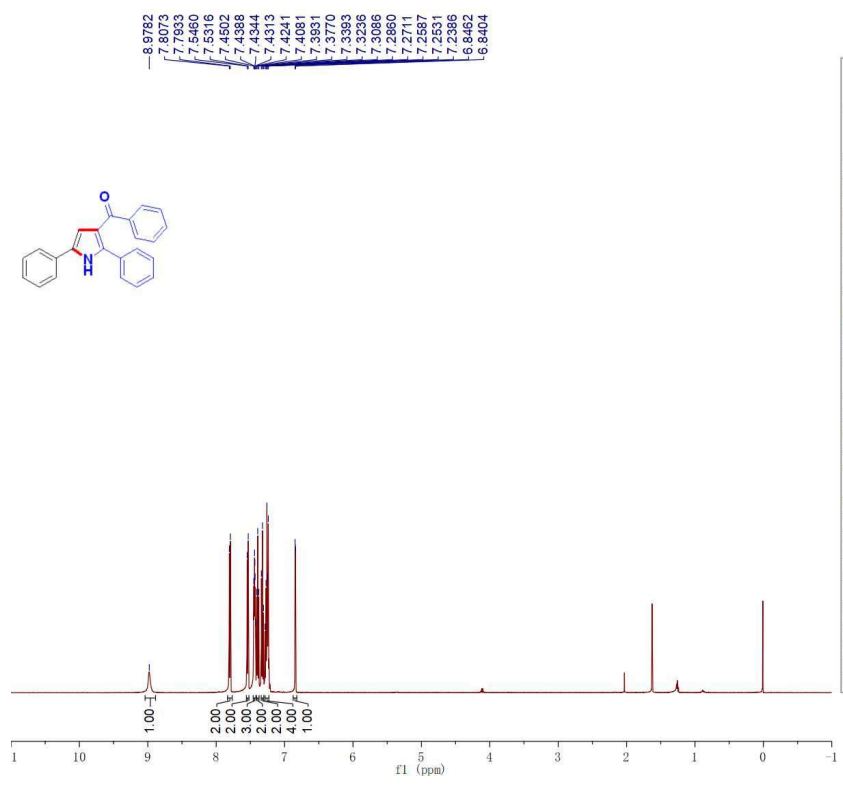


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/ 2020-1-sy-C/ 87/ fid	
2 标题	2020-1-sy-C.87.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	297.9	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
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 Frequency	125.78	
24 Spectral Width	29761.9	
25 Lowest Frequency	-1627.5	
26 Nucleus	13C	
27 Acquired Size	16384	
28 Spectral Size	65536	

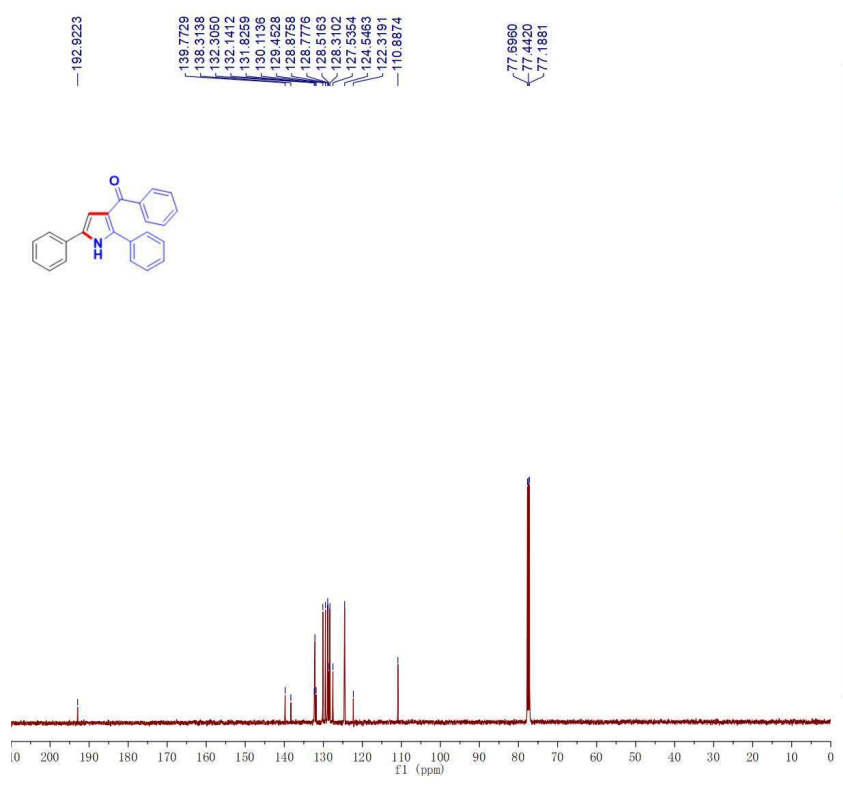
2-Butyl-4-phenyl-1-tosyl-1H-imidazole (3s)



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

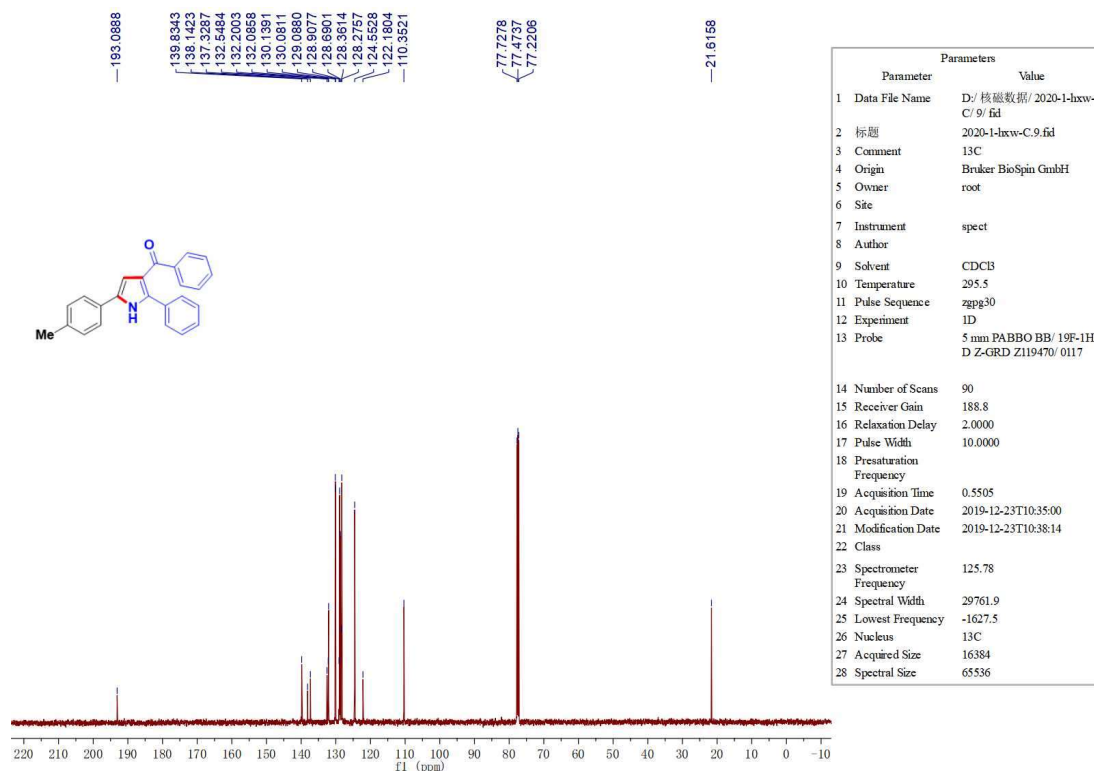
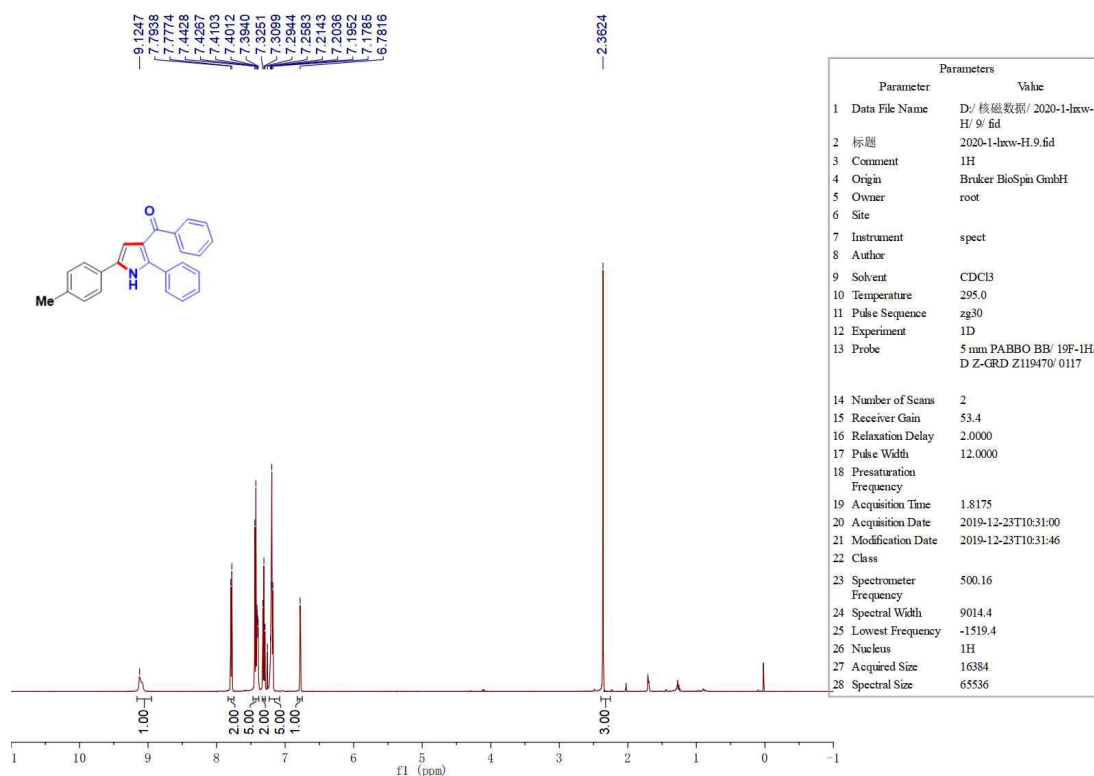


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 500M- NMR-date/ 2019-1-lxw-H/ 332.fid	
2 标题	2019-1-lxw-H.332.fid	
3 Comment	1H	
4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.2	
11 Pulse Sequence	zg30	
12 Experiment	1D	
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	

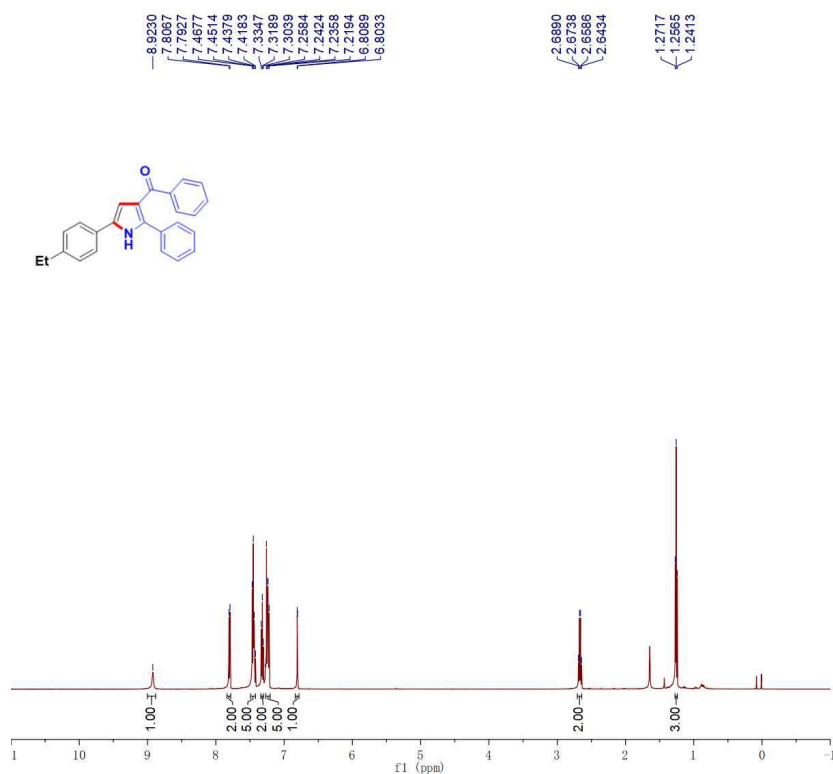


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 500M- NMR-date/ 2019-1-lxw-C/ 255.fid	
2 标题	2019-1-lxw-C.255.fid	
3 Comment	13C	
4 Origin	Bruker BioSpin GmbH	
5 Owner	root	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	295.2	
11 Pulse Sequence	zgpg30	
12 Experiment	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	

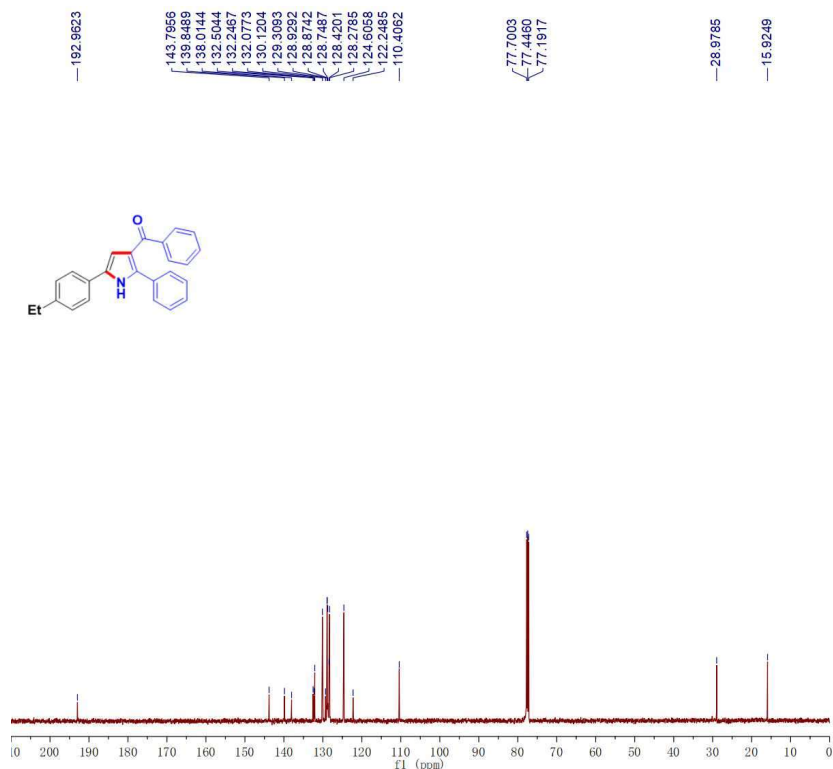
Phenyl(2-phenyl-5-(*p*-tolyl)-1*H*-pyrrol-3-yl)methanone (5b)



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

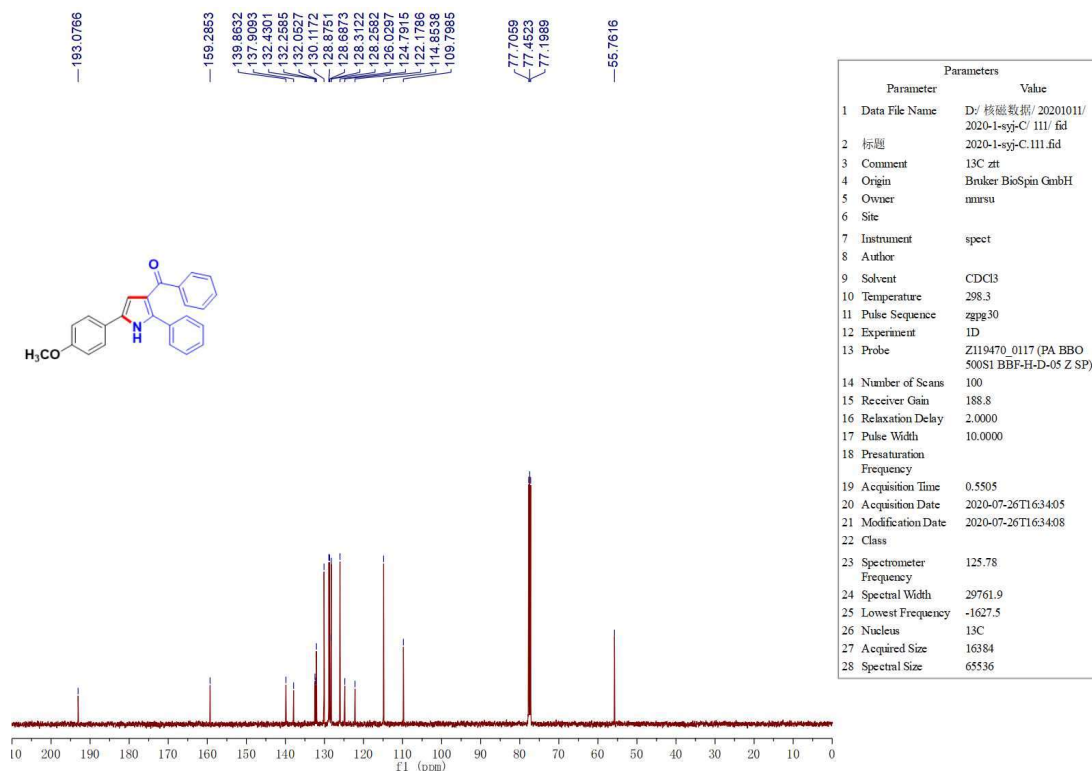
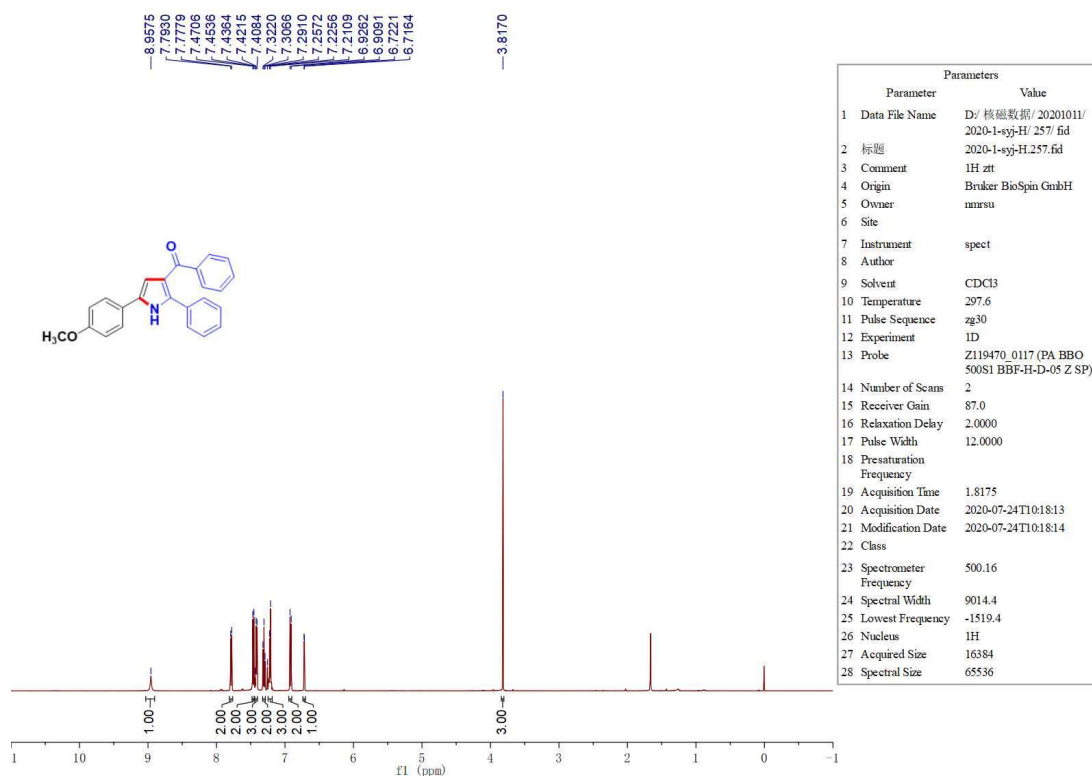


Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-yyj-H/ 313/ fid
2 标题	2020-1-yyj-H-313.fid
3 Comment	1H zsw
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	95.4
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2020-08-16T09:50:00
21 Modification Date	2020-08-16T09:50:02
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

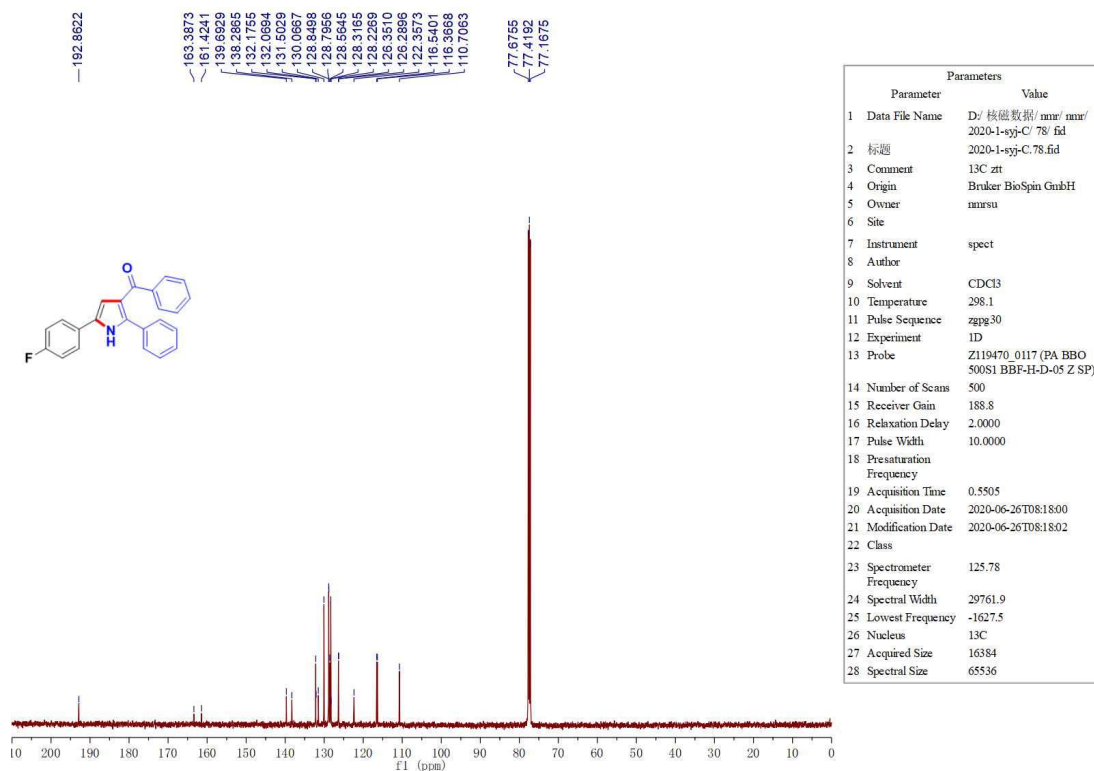
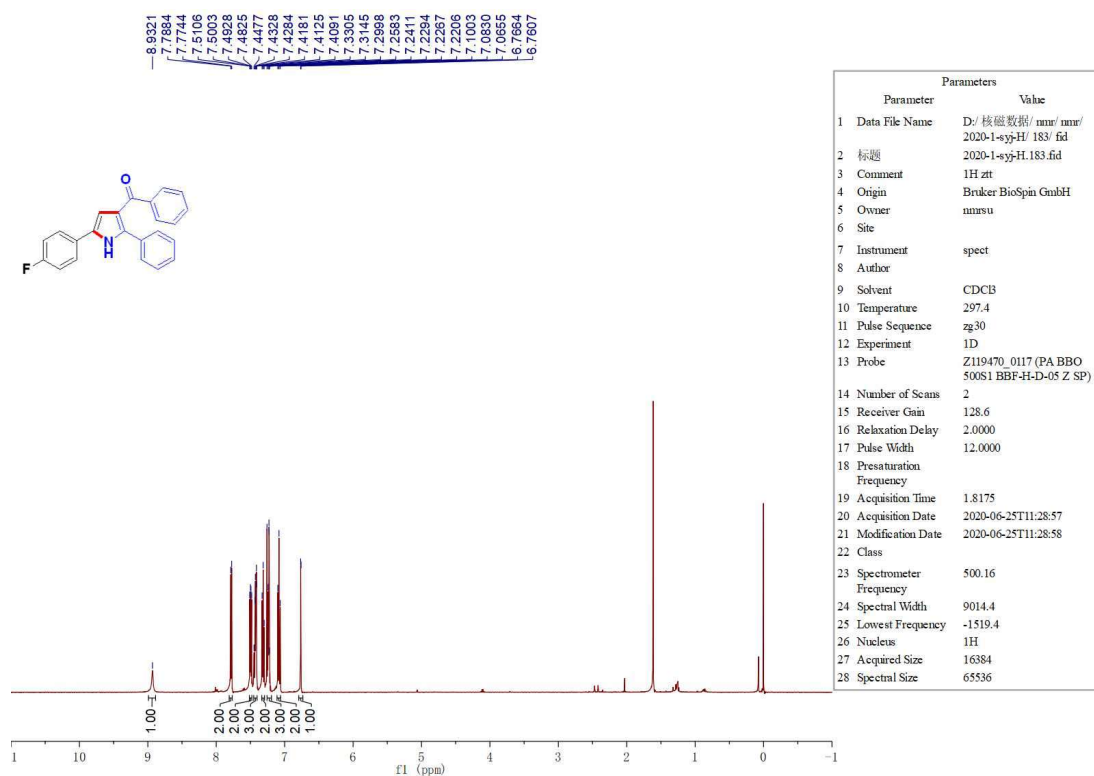


Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-yyj-C/ 145/ fid
2 标题	2020-1-yyj-C-145.fid
3 Comment	13C ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	140
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	2020-08-18T10:12:04
21 Modification Date	2020-08-18T10:12:06
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

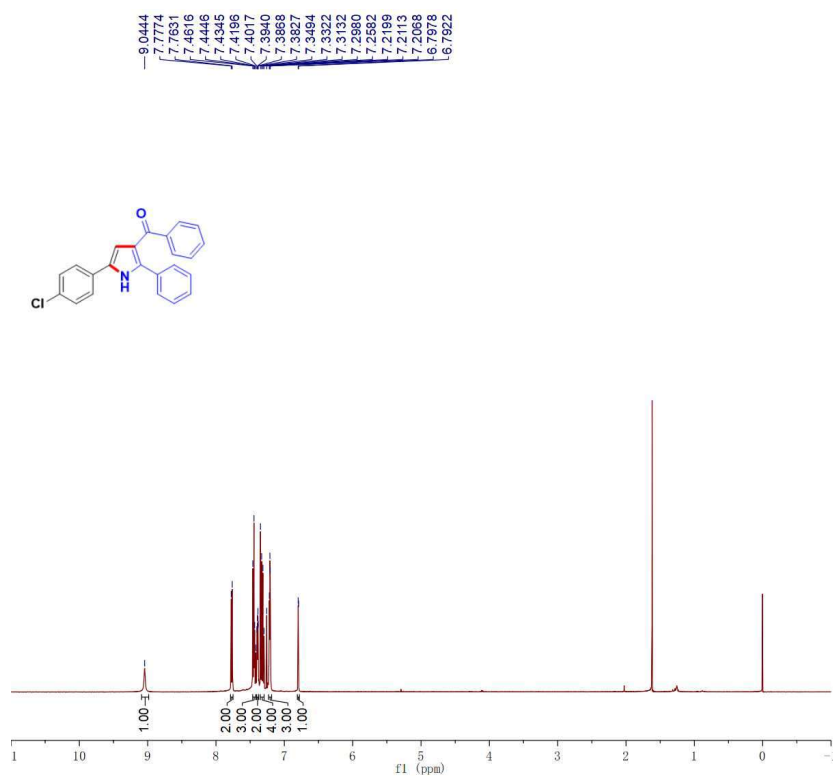
(5-(4-Methoxyphenyl)-2-phenyl-1*H*-pyrrol-3-yl)(phenyl)methanone (5d)



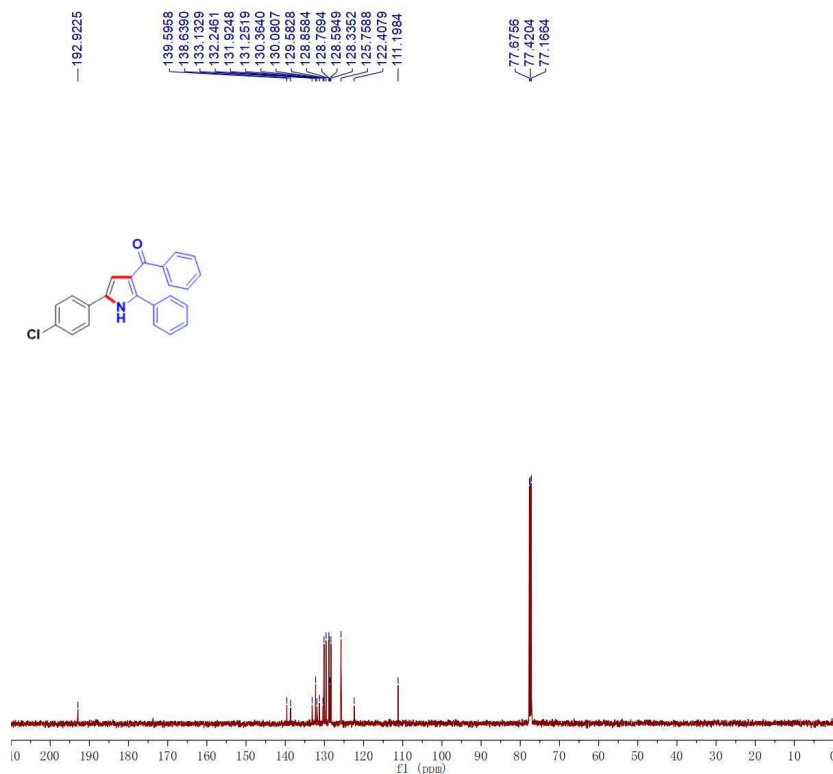
(5-(4-Fluorophenyl)-2-phenyl-1H-pyrrol-3-yl)(phenyl)methanone (5e)



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



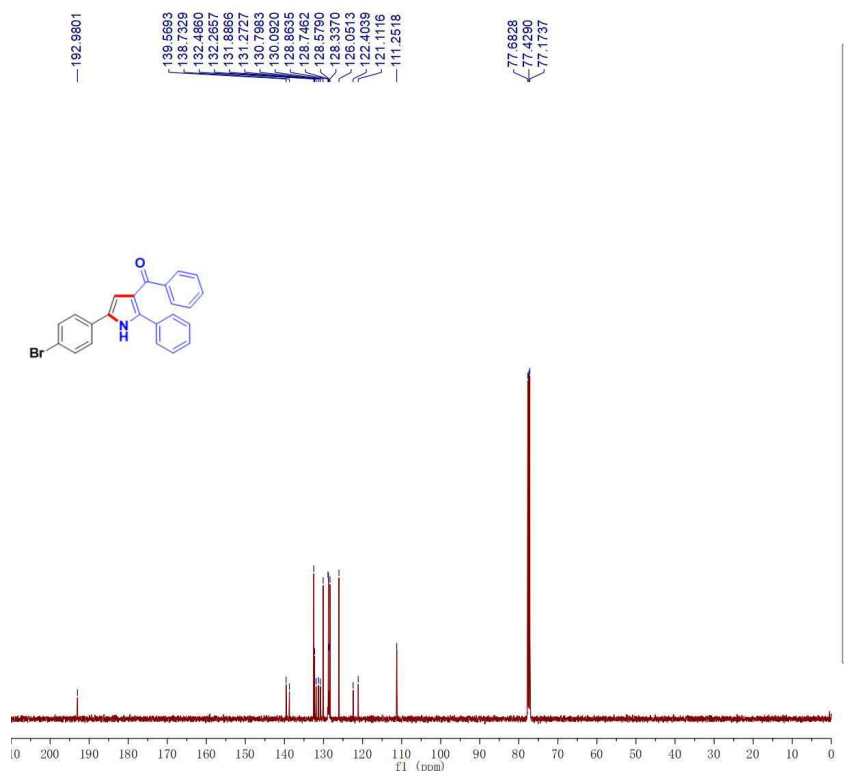
Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy3-H/ 267.fid
2 标题	2020-1-sy3-H.267.fid
3 Comment	1H ztt
4 Origin	Braker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	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	Braker 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

Chemical structure of 4-bromo-1-(4-phenyl-1H-indol-3-yl)-1H-pyrrole-2-carbonylbenzene is shown. The ¹H NMR spectrum (CDCl₃) displays peaks in the aromatic region (6.8-8.8 ppm) and a reference peak at 0 ppm. Integration values are provided below the peaks.

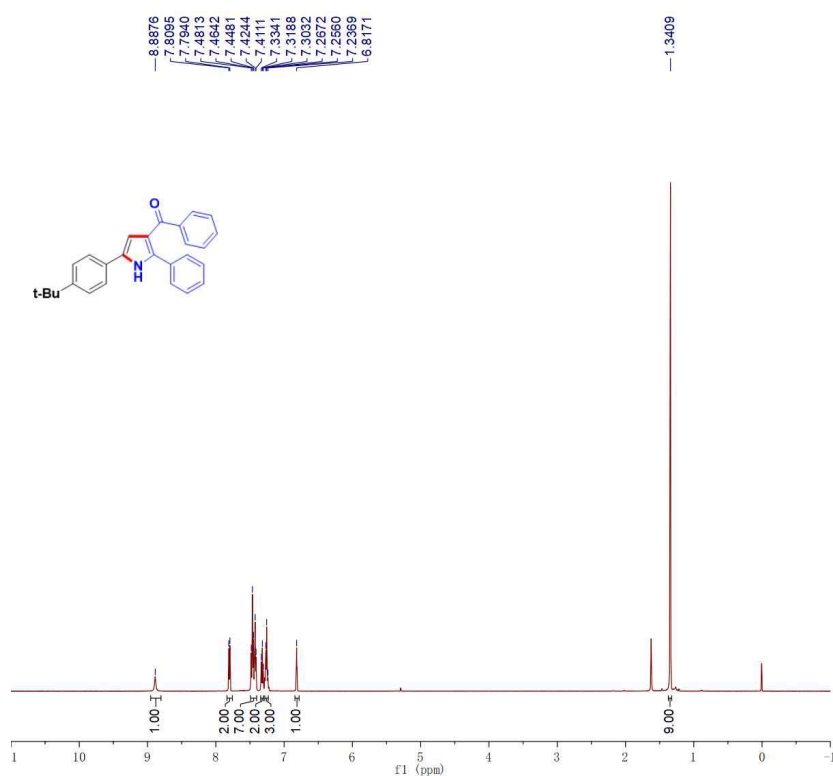
Chemical Shift (ppm)	Integration
~8.8	1.00
~7.8	2.00
~7.6	2.00
~7.5	3.00
~7.4	2.00
~7.3	2.00
~7.2	2.00
~7.1	3.00
~7.0	2.00
~6.9	1.00
0	-



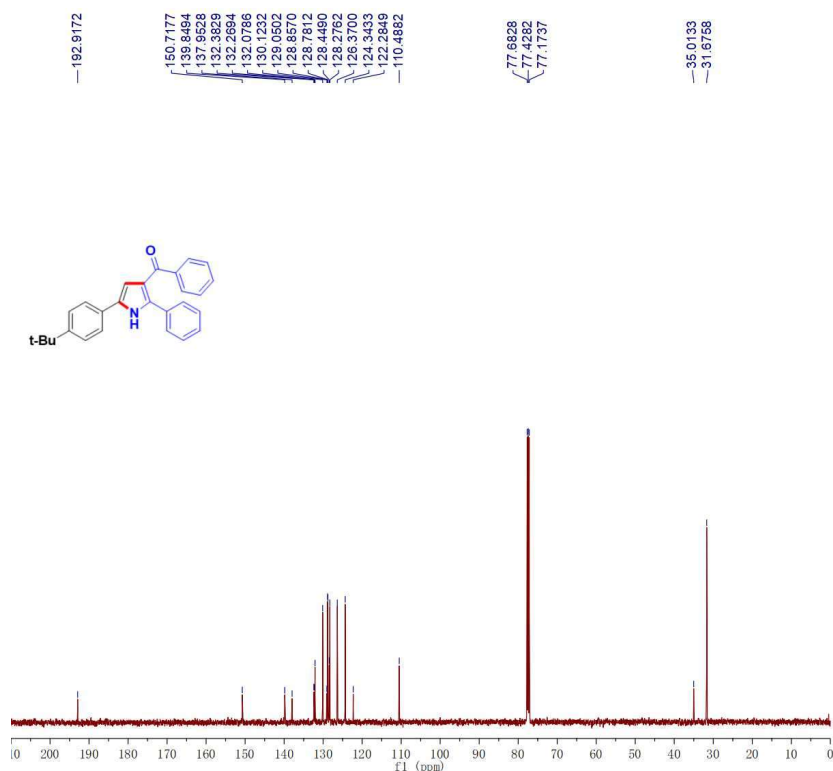
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	Parameter	Value
1	Data File Name	D:/核磁数据/nmr/nmr/2020-1-yy-H/127.fid
2	标题	2020-1-yy-H.127.fid
3	Comment	1H ztt
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDC13
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14	Number of Scans	2
15	Receiver Gain	188.8
16	Relaxation Delay	2.0000
17	Pulse Width	12.0000
18	Prestaturation Frequency	
19	Acquisition Time	1.8175
20	Acquisition Date	2020-06-04T12:55:35
21	Modification Date	2020-06-04T12:55:36
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		
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1	Data File Name	D:\核磁数据\mmr\mmr\2020-1-xyj-C\51.fid
2	标题	2020-1-xyj-C.51.fid
3	Comment	13C ztt
4	Origin	Braker BioSpin GmbH
5	Owner	mmrnu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP
14	Number of Scans	201
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	2020-06-05T12:23:03
21	Modification Date	2020-06-05T12:23:06
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

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



Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 20201011/	
2 标题	2020-1-sy-H-268.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin CnubH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl ₃	
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	87.0	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2020-07-26T11:42:58	
21 Modification Date	2020-07-26T11:43:00	
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/ 20201011/	
2 标题	2020-1-sy-C-112.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin CnubH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl ₃	
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	123	
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	2020-07-26T16:42:14	
21 Modification Date	2020-07-26T16:42:16	
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	

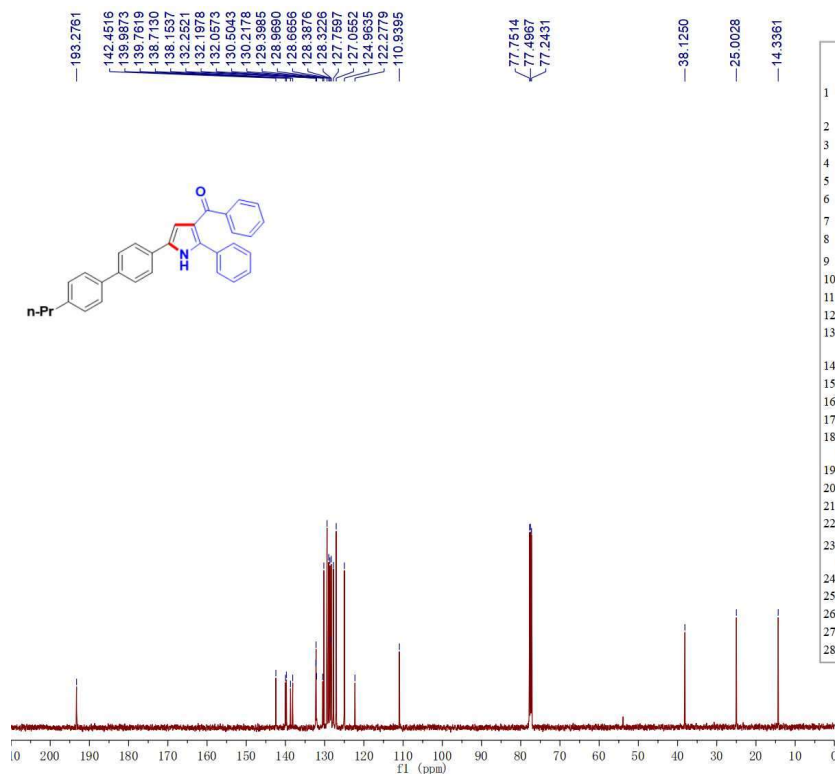
Chemical structure of compound 10: CCCC1=CC=C(C=C1)-c2ccc(cc2)-c3c[nH]c4c3C(=O)c5ccccc54

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift (f1) in ppm, ranging from 0 to 11. The y-axis represents the intensity. The spectrum shows several peaks, with integration values provided below the peaks: 1.00, 4.00, 2.00, 2.00, 2.00, 2.00, 3.00, 2.00, and 3.00. A list of peak chemical shifts (f1) is provided on the right side of the spectrum.

Peak chemical shifts (f1) in ppm:

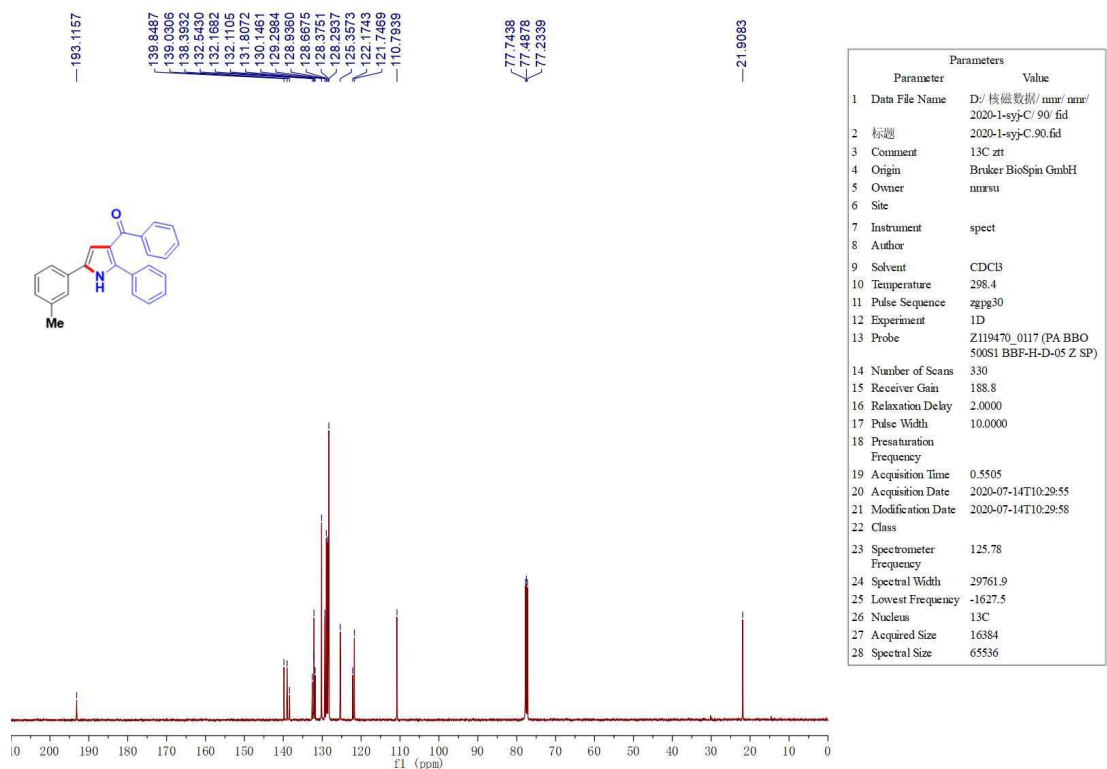
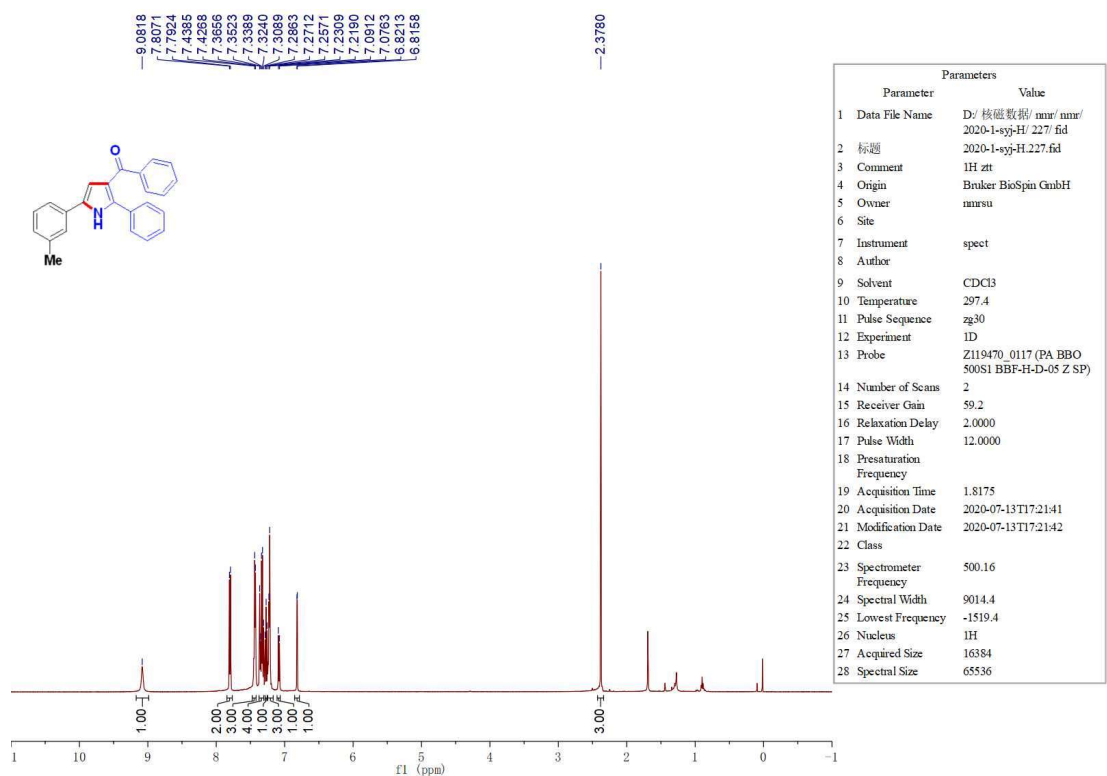
- 9.4257
- 7.8075
- 7.7932
- 7.6885
- 7.5319
- 7.5158
- 7.4421
- 7.4274
- 7.4019
- 7.3976
- 7.3858
- 7.3351
- 7.3194
- 7.3044
- 7.2625
- 7.2465
- 7.1785
- 7.1730
- 7.1681
- 6.8560
- 6.8504
- 2.6556
- 2.6407
- 2.6250
- 1.7323
- 1.7176
- 1.7024
- 1.6873
- 1.6724
- 1.6577
- 1.0096
- 0.9850
- 0.9803

Parameters		
	Parameter	Value
1	Data File Name	D:/ 核磁数据/ 20201011/
2	标题	2020-1-syjh-H314.fid
3	Comment	1H ztt
4	Origin	Broker BioSpin GmbH
5	Owner	mursu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCI3
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	207.1
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



	Parameters	
	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 ztt
4	Origin	Braker BioSpin GmbH
5	Owner	nursu
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	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

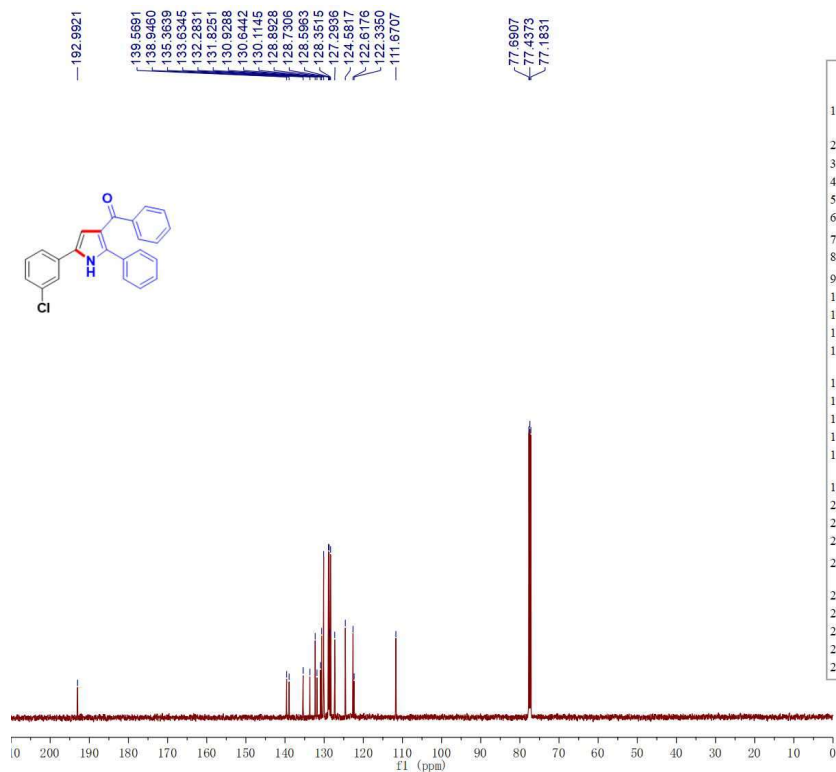
Phenyl(2-phenyl-5-(*m*-tolyl)-1*H*-pyrrol-3-yl)methanone (5j)



Chemical structure: O=C1C=C(c2ccc(Cl)cc2)Nc3ccccc31

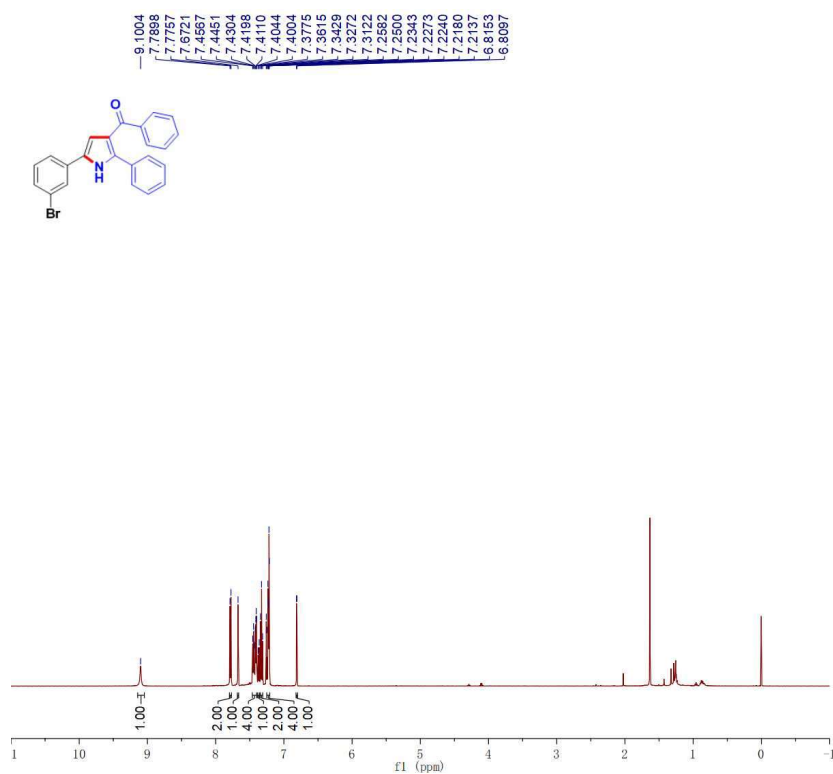
¹H NMR spectrum (CDCl₃) showing peaks from 6.7 to 8.2 ppm. Integration values are provided below the peaks: 1.00, 2.00, 1.00, 1.00, 3.00, 3.00, 4.00, and 1.00.

Parameters		Value
Parameter		
1	Data File Name	D:/ 核磁数据/ mmr/ mmr/ 2020-1-syyj-H/ 228.fid
2	标题	2020-1-syyj-H.228.fid
3	Comment	1H ztt
4	Origin	Broker BioSpin GmbH
5	Owner	mmru
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCB
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	95.4
16	Relaxation Delay	2.0000
17	Pulse Width	12.0000
18	Preturbation Frequency	
19	Acquisition Time	1.8175
20	Acquisition Date	2020-07-13T17:26:47
21	Modification Date	2020-07-13T17:26:48
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	6536

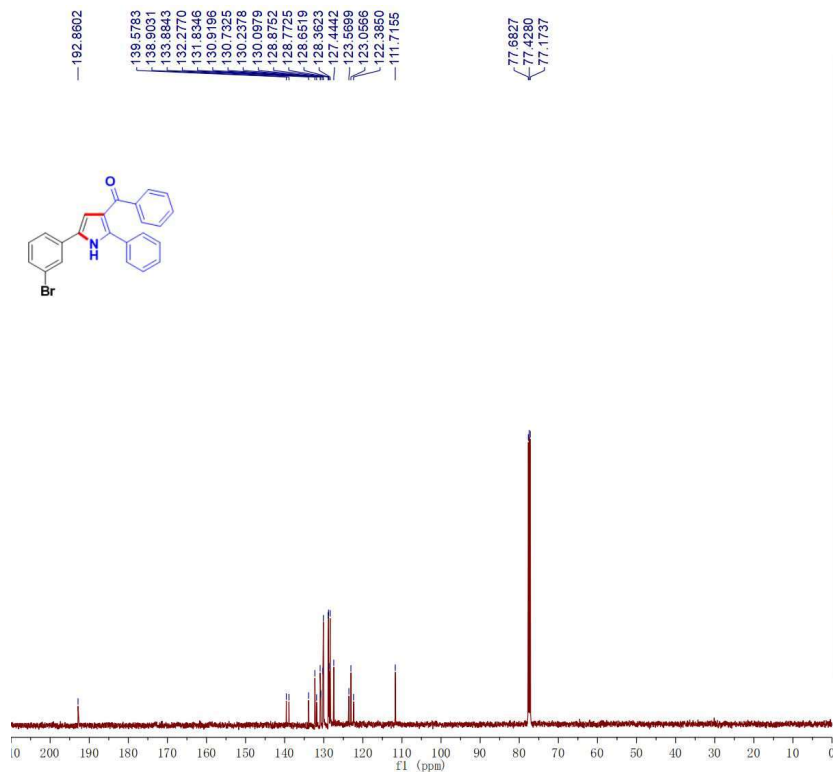


	Parameters	Value
1	Data File Name	D\ 核磁数据\ nmr\ nmr\ 2020-1-syJ-C\ 91\ fid
2	标题	2020-1-syJ-C.91.fid
3	Comment	13C att
4	Origin	Broker BioSpin GrubH
5	Owner	nmru
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z119470_0117 (PA BBO 500SI BBF-H-D-05 Z SP)
14	Number of Scans	140
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	2020-07-14T10:40:25
21	Modification Date	2020-07-14T10:40:28
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

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

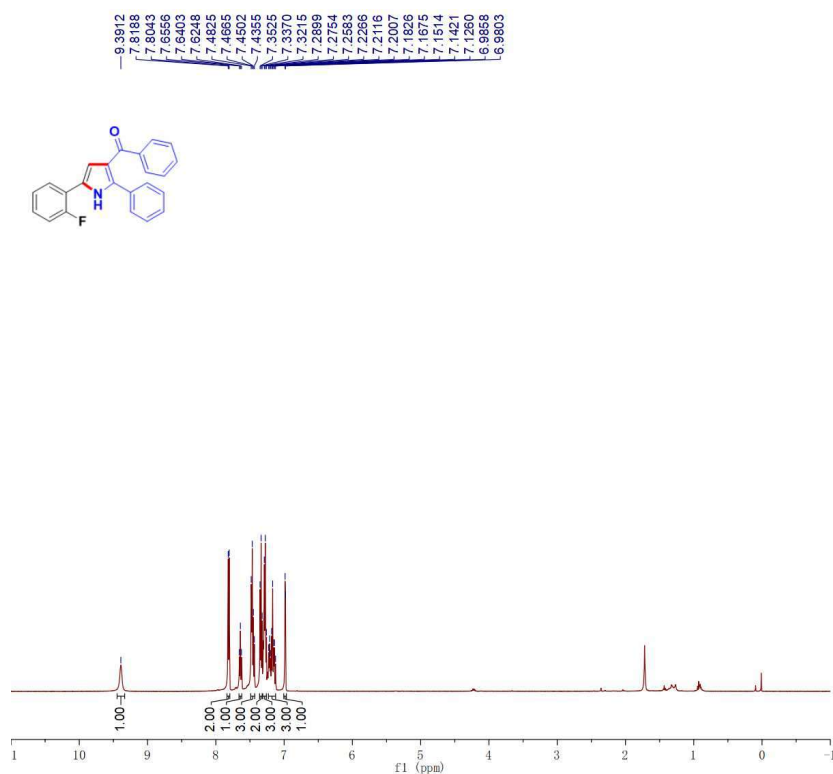


Parameters	
Parameter	Value
1 Data File Name	D:\核磁数据\20201011\2020-1-sy-H-266.fid
2 标题	2020-1-sy-H-266.fid
3 Comment	1H ztt
4 Origin	Braker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500SI 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

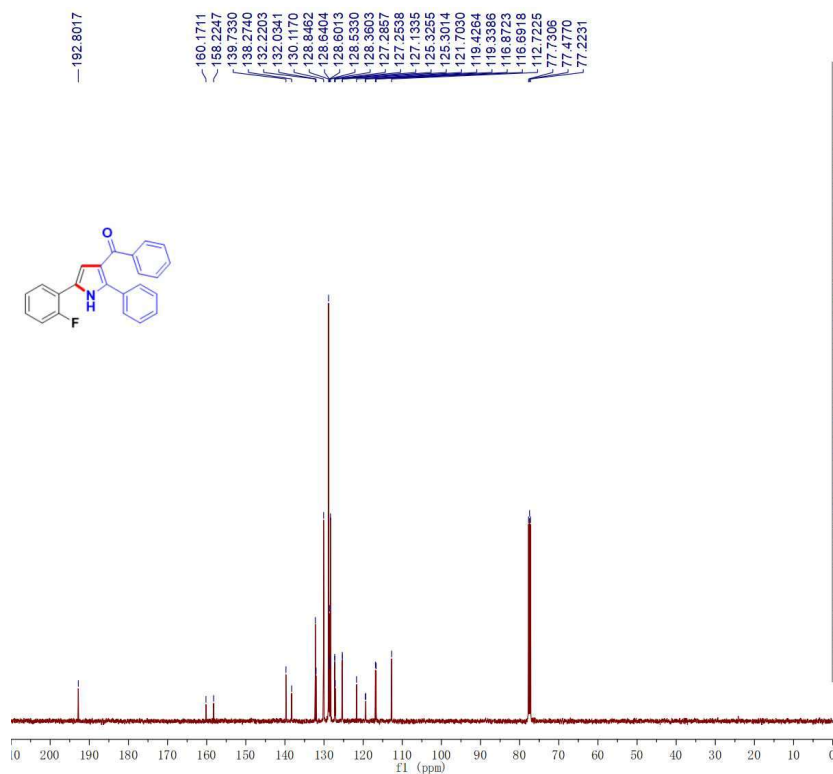


Parameters	
Parameter	Value
1 Data File Name	D:\核磁数据\20201011\2020-1-sy-C-113.fid
2 标题	2020-1-sy-C-113.fid
3 Comment	13C ztt
4 Origin	Braker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500SI 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)

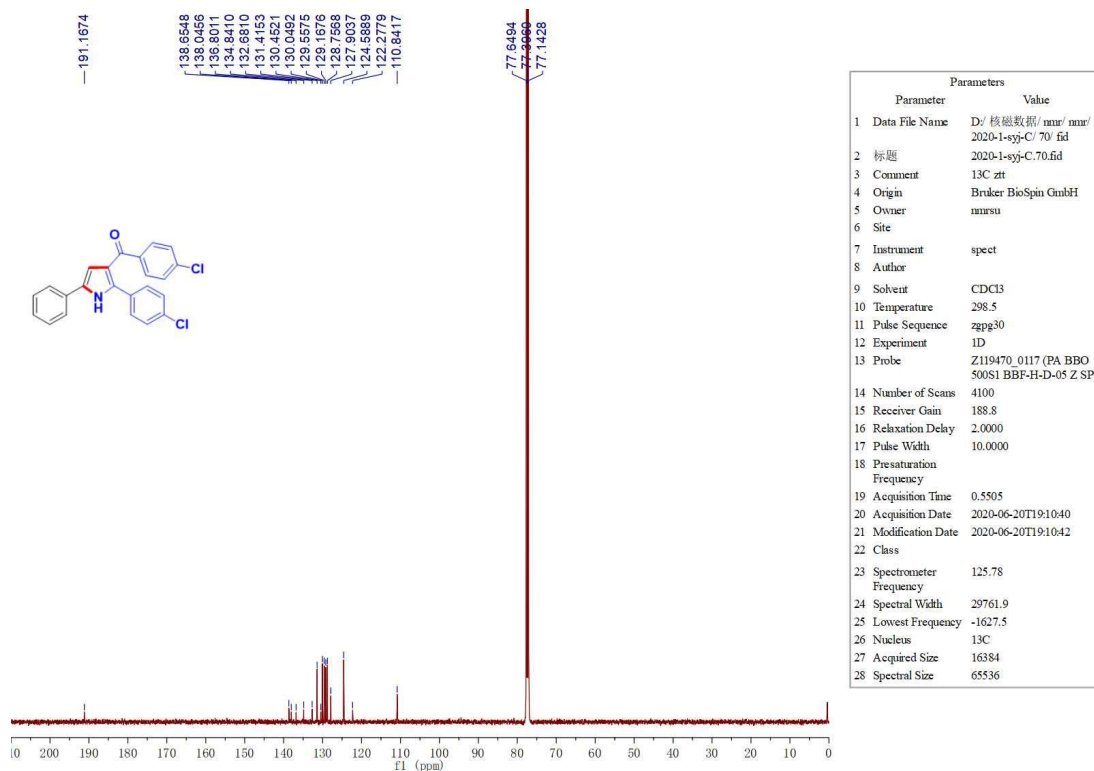
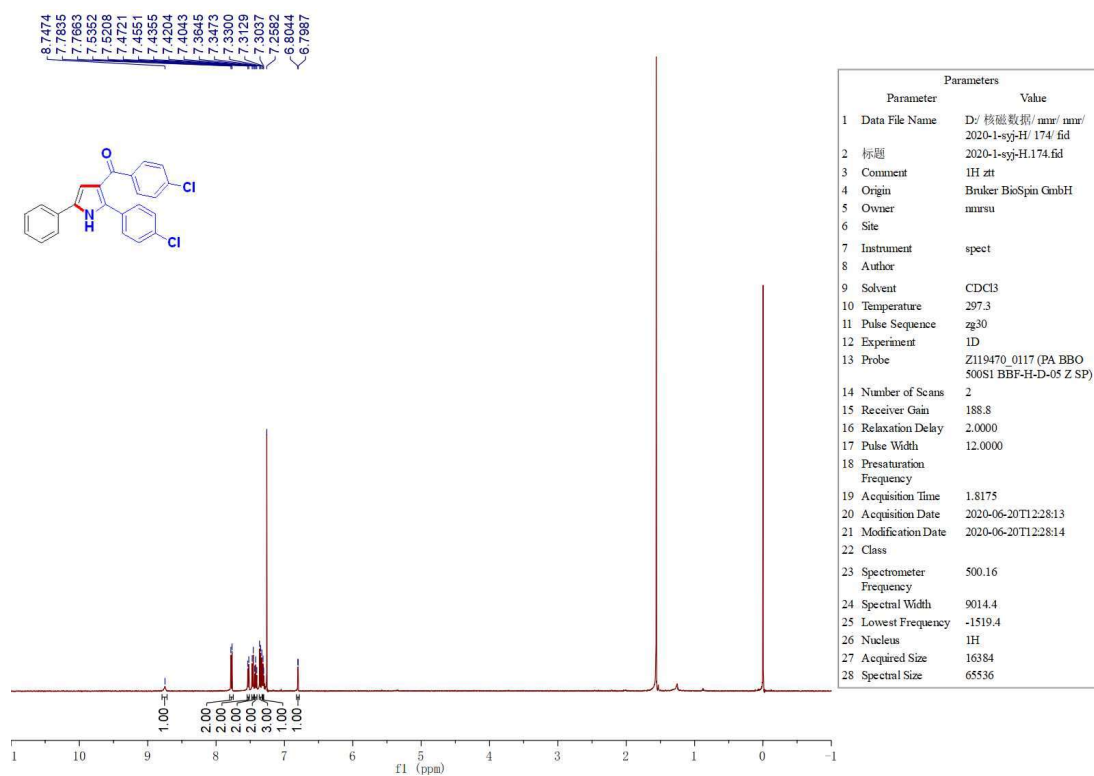


Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-syf-H/ 292.fid
2 标题	2020-1-syf-H-292.fid
3 Comment	1H zt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	292.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (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

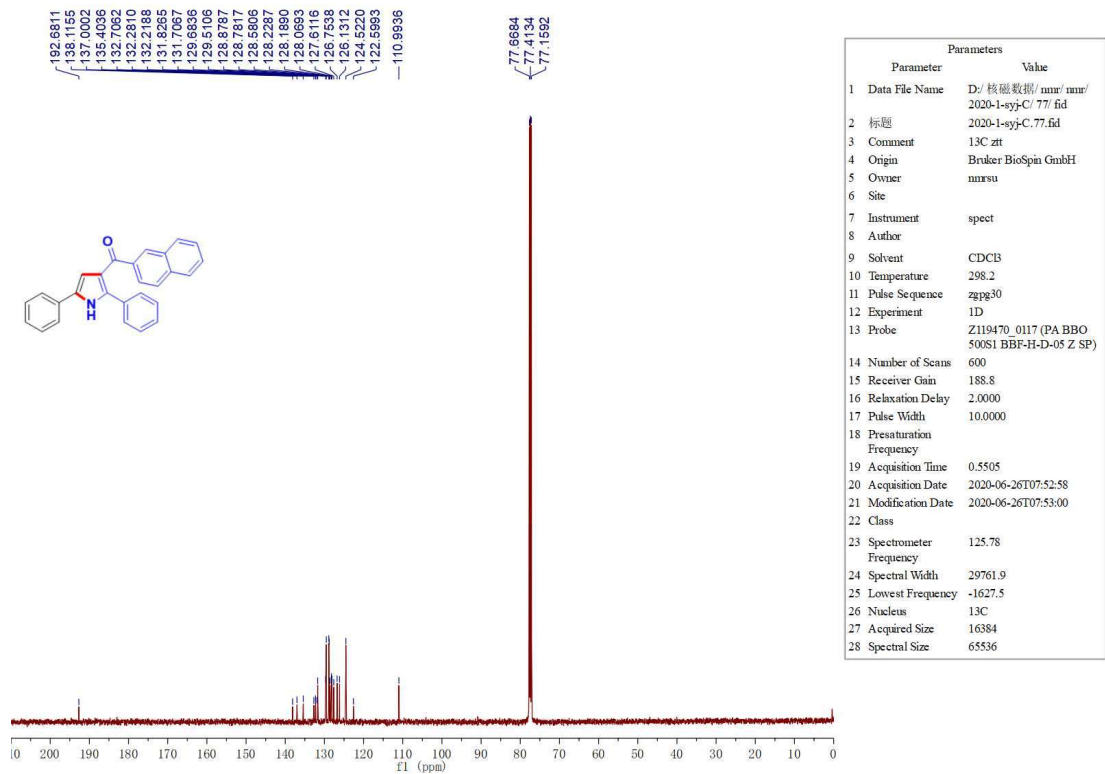
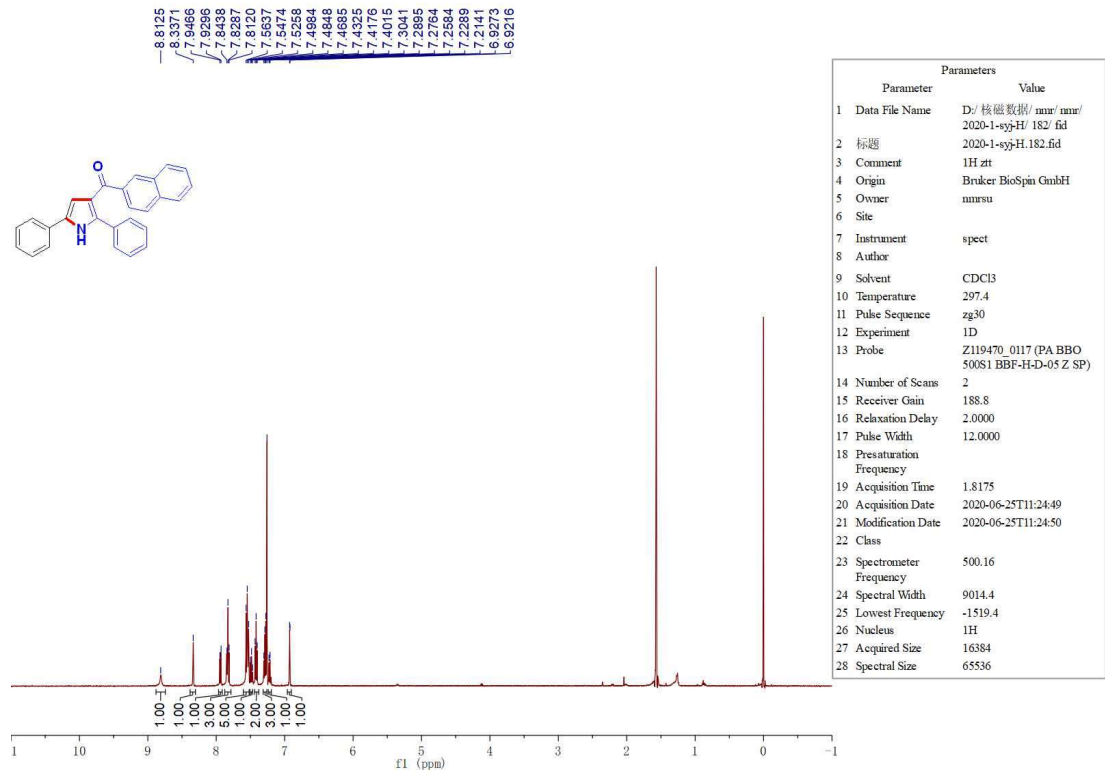


Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-syf-C/ 130.fid
2 标题	2020-1-syf-C-130.fid
3 Comment	13C zt
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z119470_0117 (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

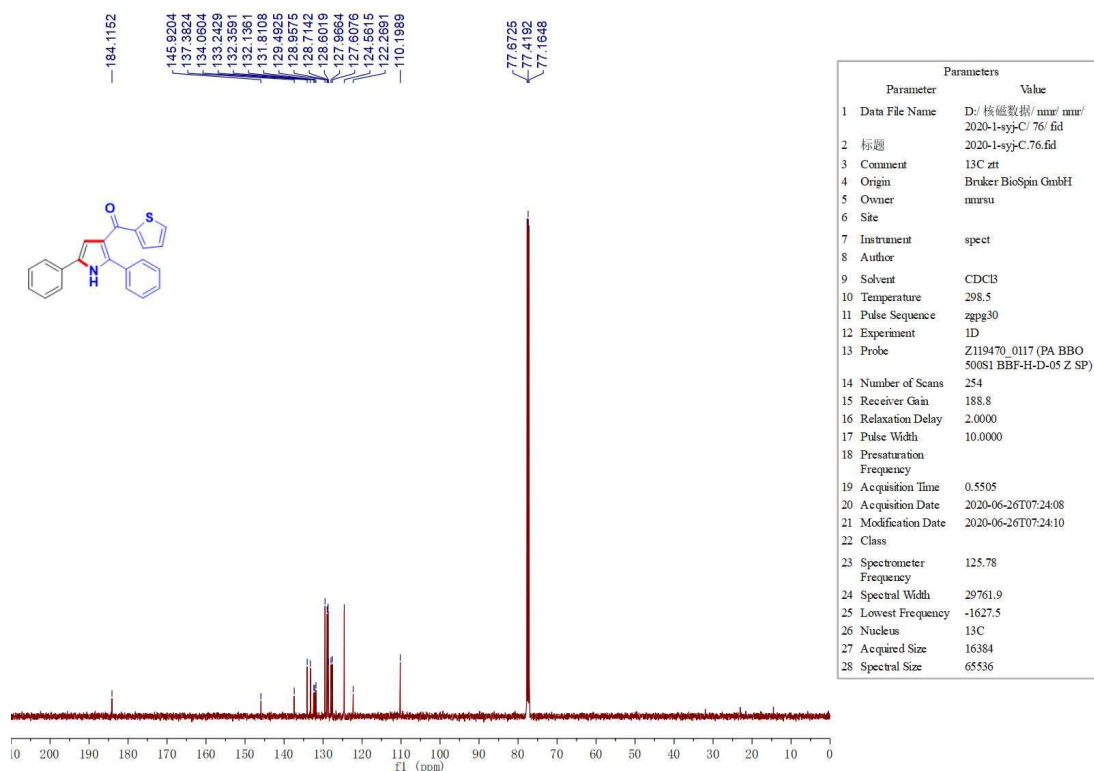
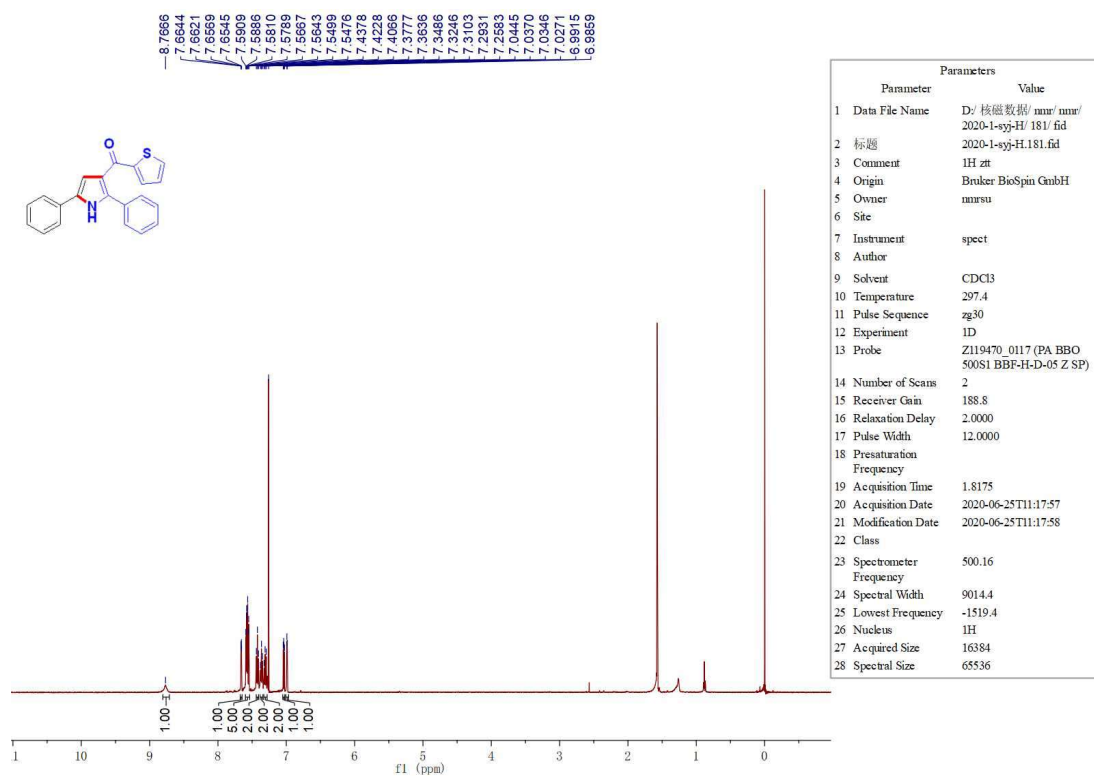
(4-Chlorophenyl)(2-(4-chlorophenyl)-5-phenyl-1*H*-pyrrol-3-yl) methanone (5n)



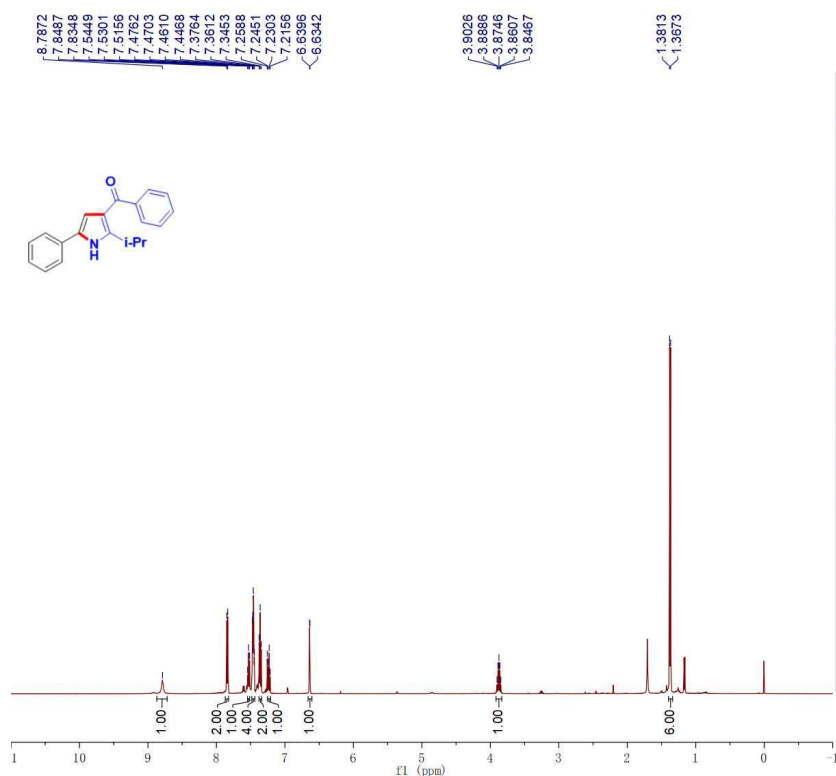
(2,5-Diphenyl-1*H*-pyrrol-3-yl) (naphthalen-2-yl) methanone (5o)



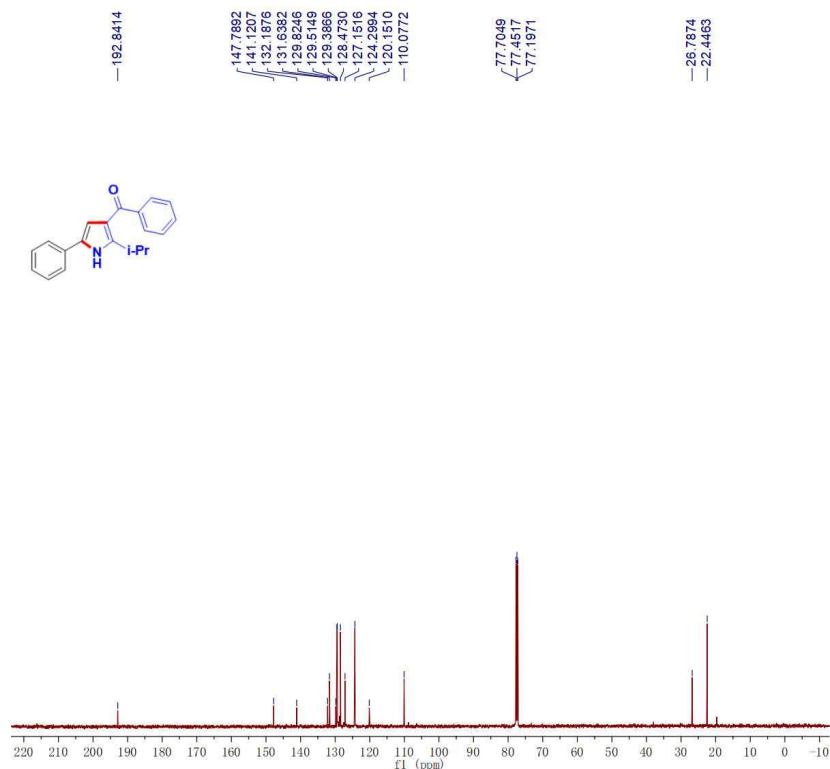
(2,5-Diphenyl-1*H*-pyrrol-3-yl) (thiophen-2-yl) methanone (5p)



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

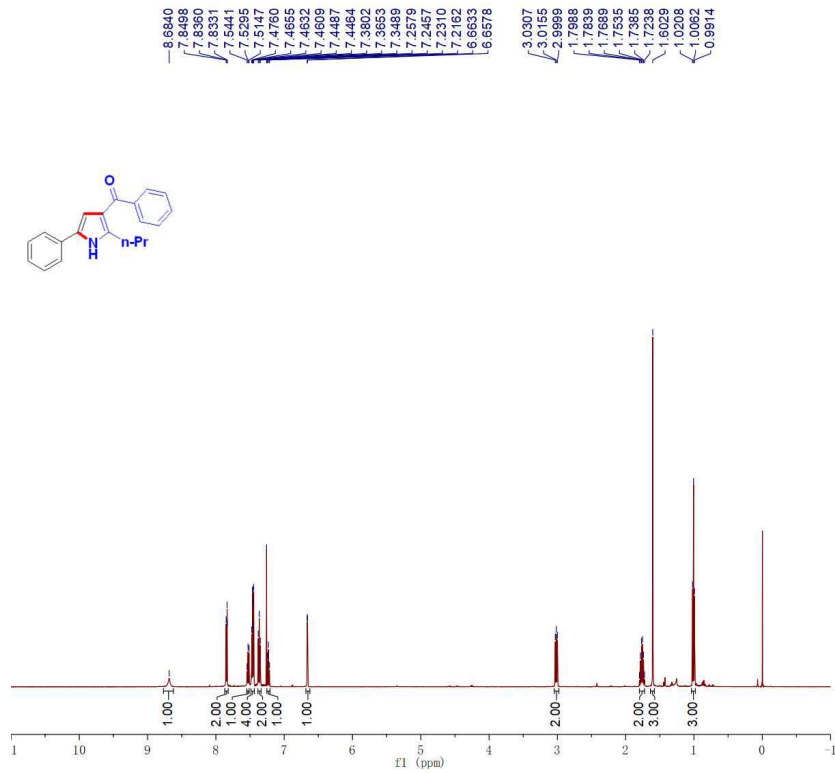


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-H/ 295/ f1d	
2 标题	2020-1-sy-H.295.f1d	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	292.9	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	4	
15 Receiver Gain	66.5	
16 Relaxation Delay	2.0000	
17 Pulse Width	12.0000	
18 Presaturation Frequency		
19 Acquisition Time	1.8175	
20 Acquisition Date	2020-08-10T11:24:54	
21 Modification Date	2020-08-10T11:24:56	
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	

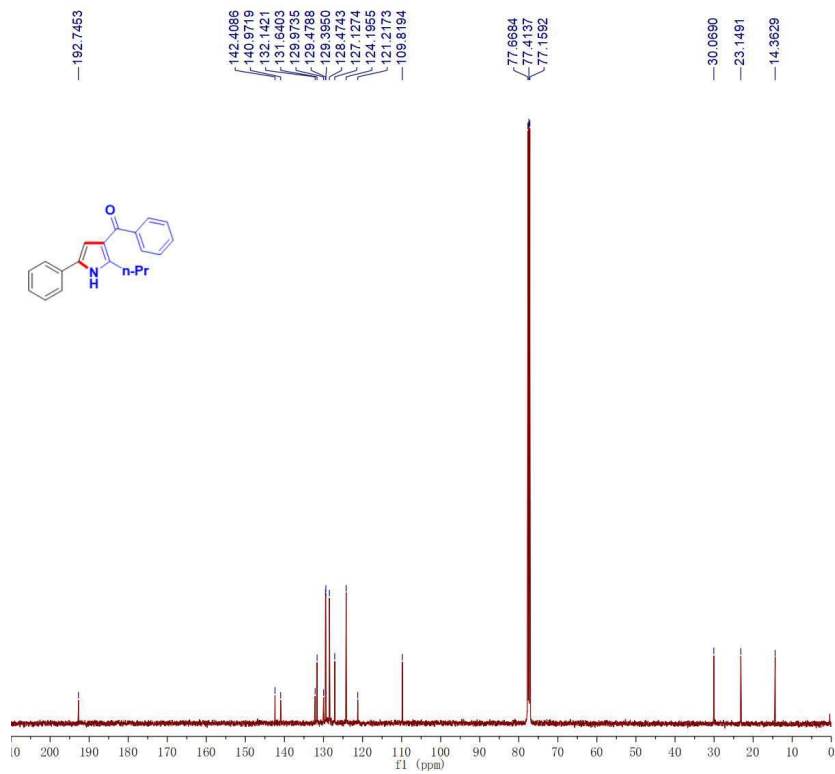


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-C/ 133/ f1d	
2 标题	2020-1-sy-C.133.f1d	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	294.0	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)	
14 Number of Scans	120	
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	2020-08-10T13:09:58	
21 Modification Date	2020-08-10T13:10:00	
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(5-phenyl-2-propyl-1*H*-pyrrol-3-yl) methanone (5r)

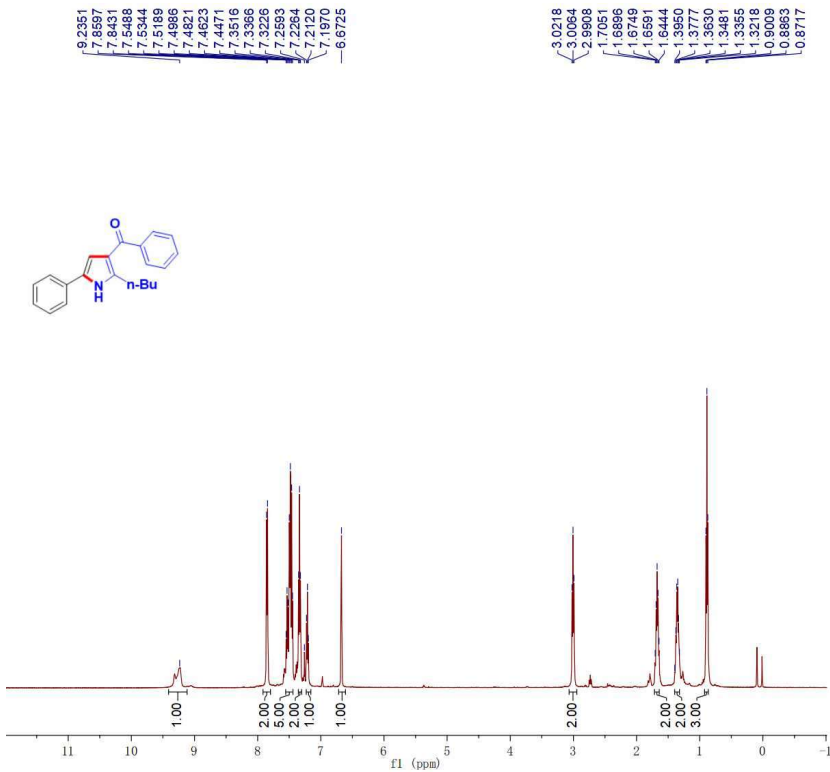


Parameters		
Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/	
2 标题	2020-1-sy-H-225.fid	
3 Comment	1H ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	297.4	
11 Pulse Sequence	zg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500SI 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 Presaturation 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	

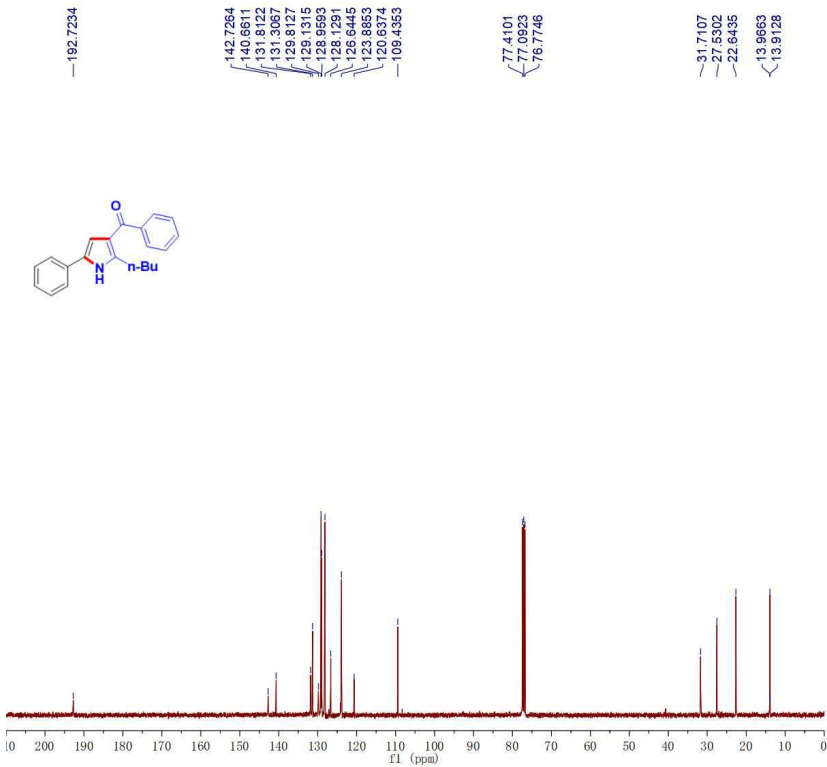


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Parameter	Value	
1 Data File Name	D:/ 核磁数据/ nmr/ nmr/	
2 标题	2020-1-sy-C-88.fid	
3 Comment	13C ztt	
4 Origin	Bruker BioSpin GmbH	
5 Owner	nmrsu	
6 Site		
7 Instrument	spect	
8 Author		
9 Solvent	CDCl3	
10 Temperature	298.3	
11 Pulse Sequence	zgpg30	
12 Experiment	1D	
13 Probe	Z119470_0117 (PA BBO 500SI 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	65536	

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

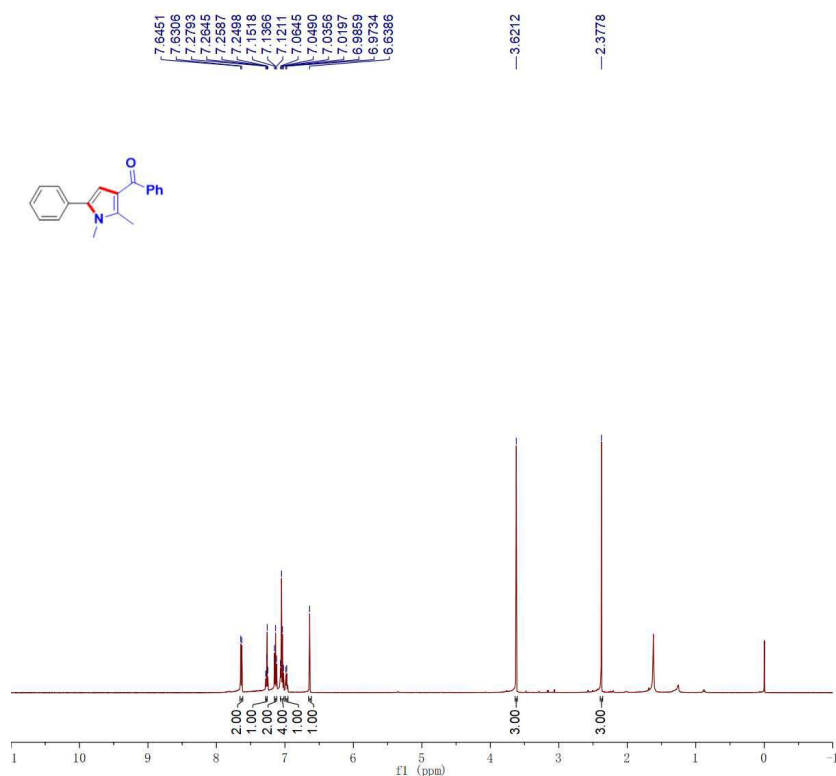


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Parameter	Value
1 Data File Name	D:/ 核磁数据/ 2021-syj-500/ 2021-1-syj-H/ 6/ fid
2 标题	2021-1-syj-H.6.fid
3 Comment	1H ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	nursu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	291.5
11 Pulse Sequence	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

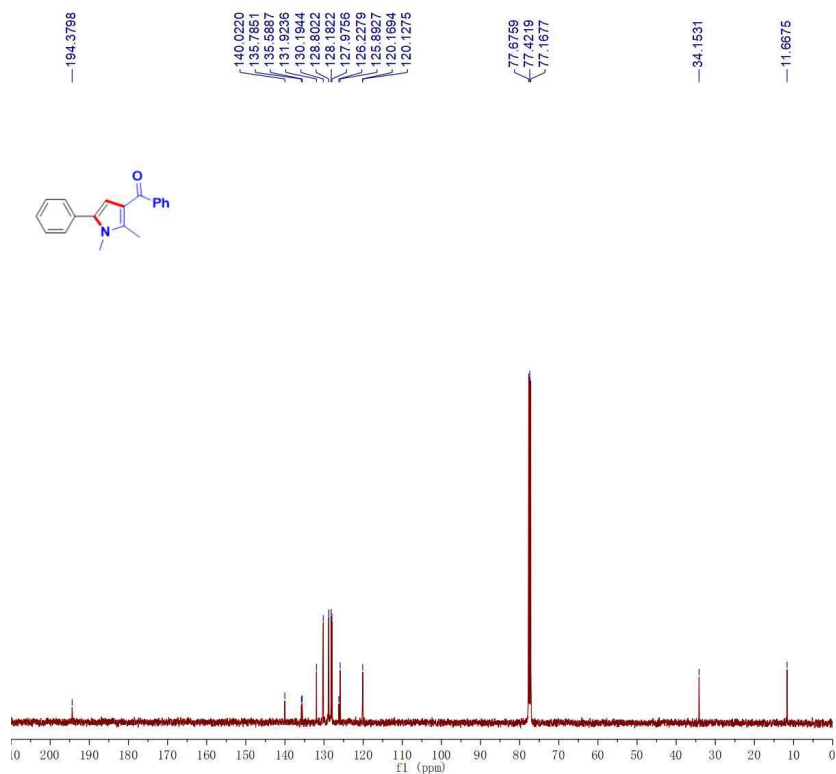


Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 400/ 2021-1-syj-C/ 13/ fid
2 标题	2021-1-syj-C.13.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nursu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI 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)

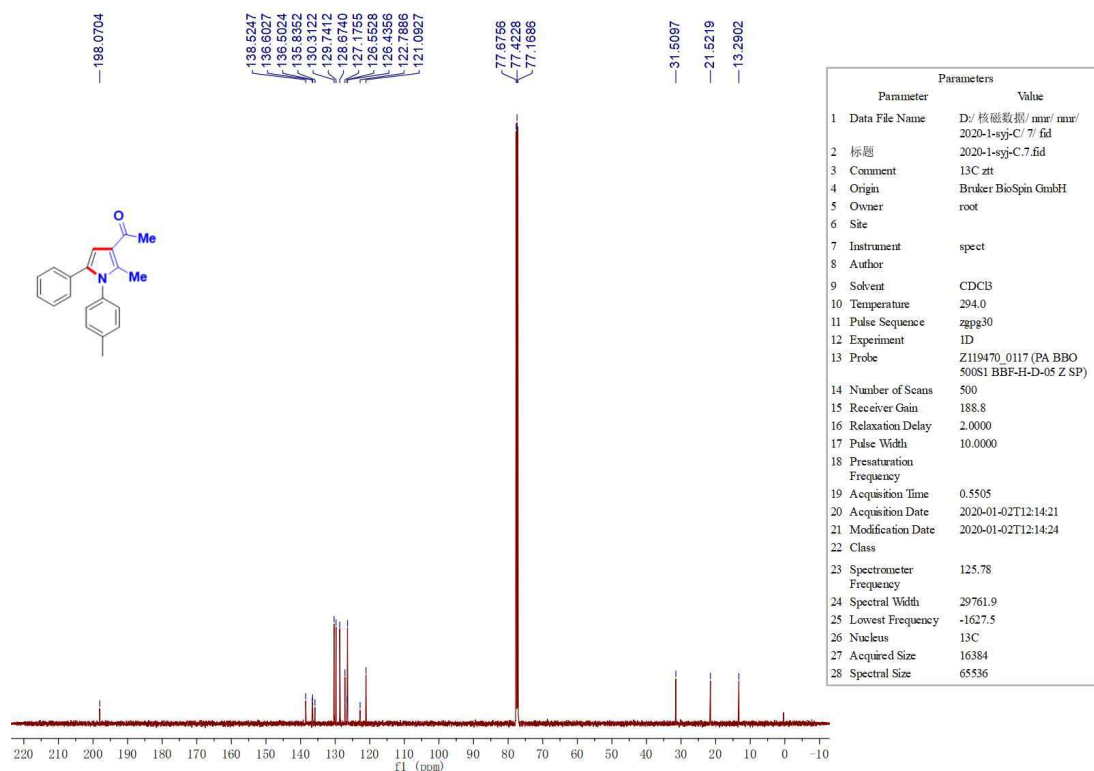
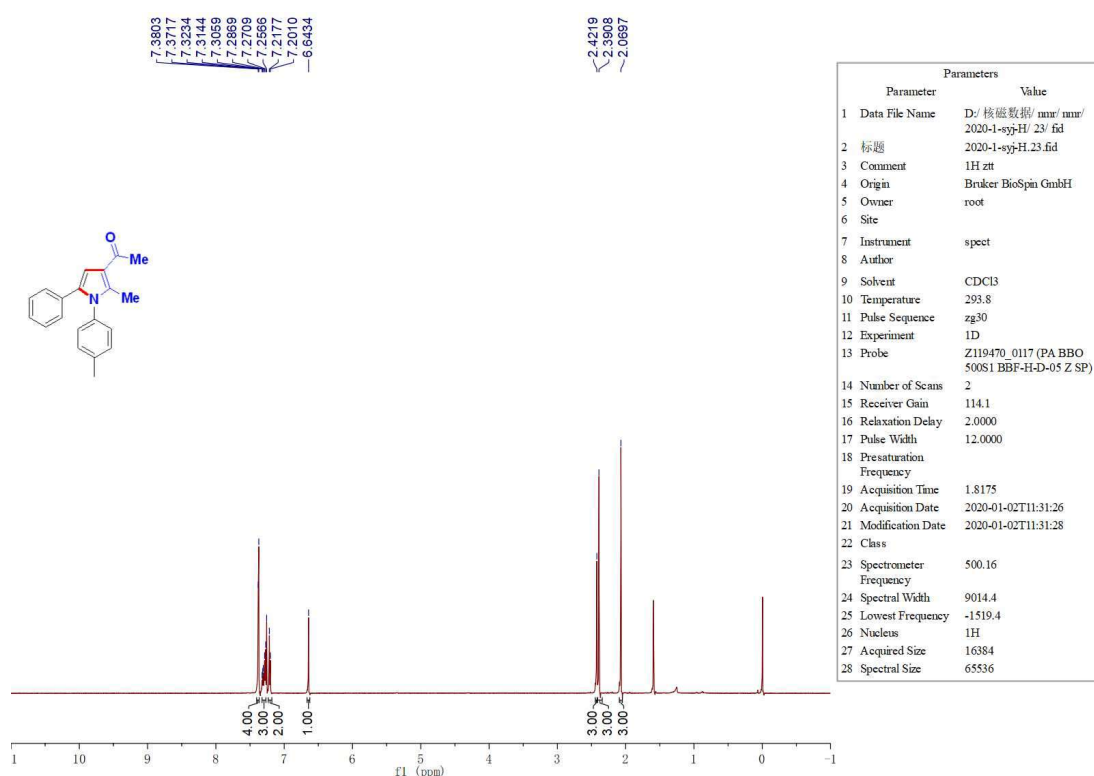


Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-j-H/ 305/ fid
2 标题	2020-1-sy-j-H-305.fid
3 Comment	1H ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	mrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (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

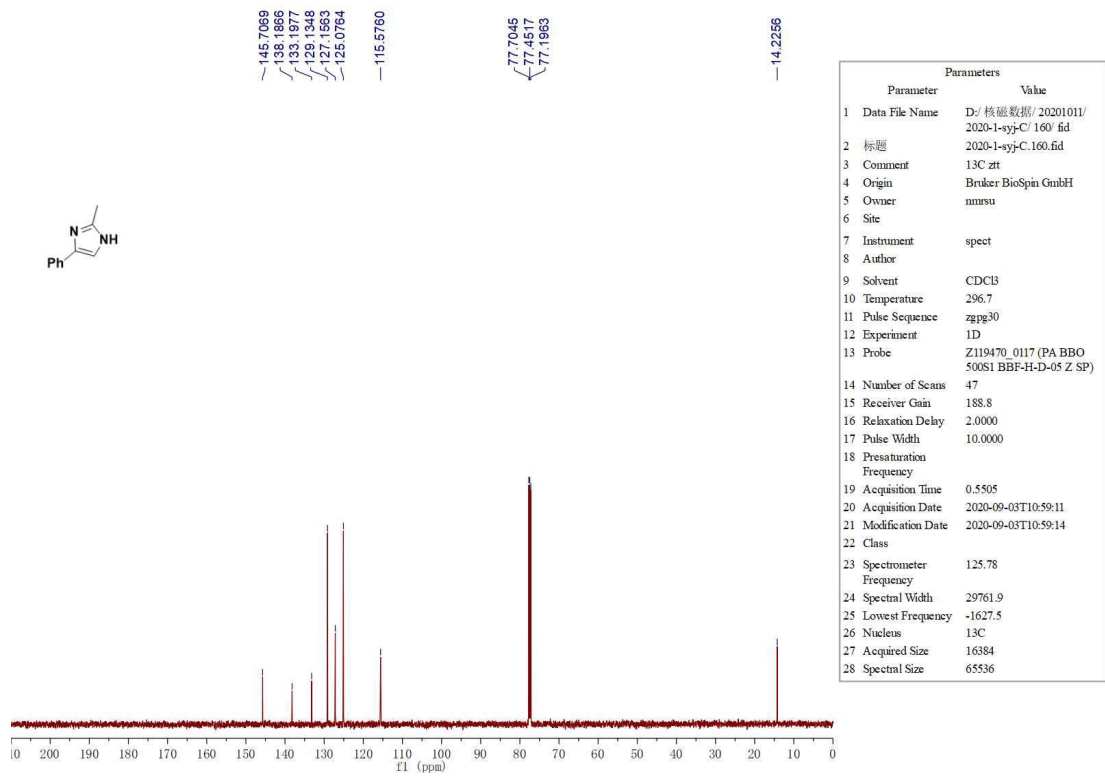
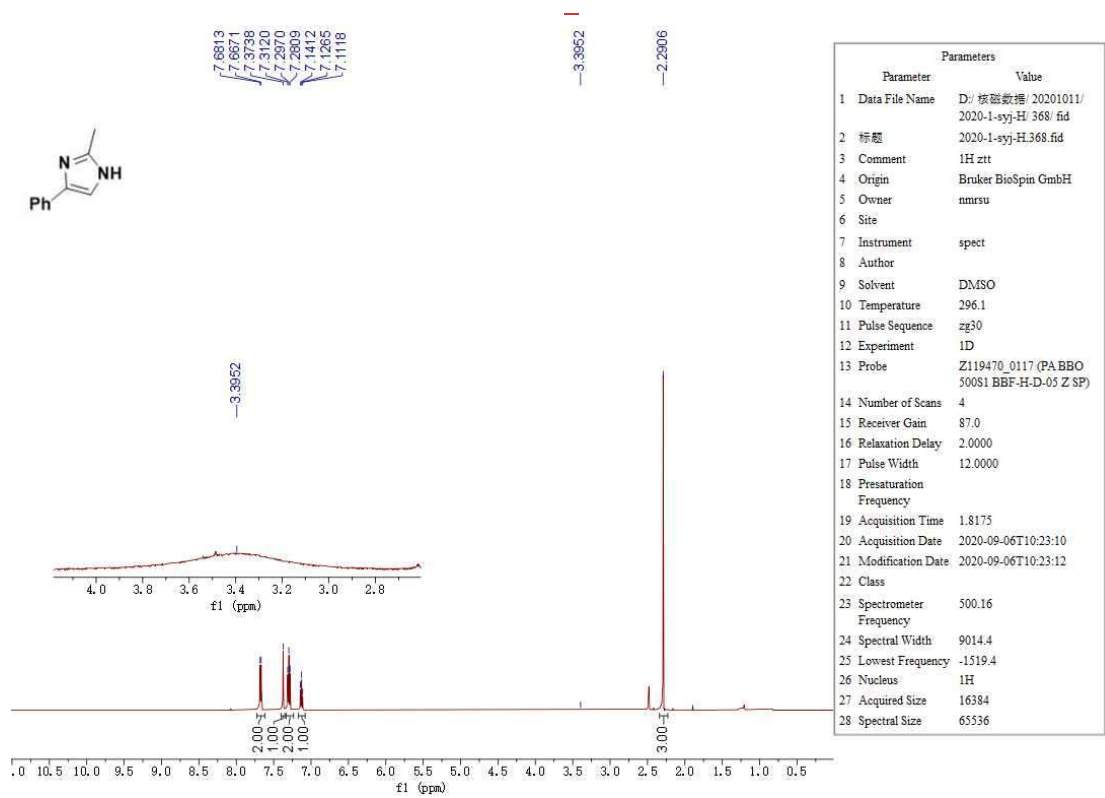


Parameters	
Parameter	Value
1 Data File Name	D:/ 核磁数据/ 20201011/ 2020-1-sy-j-C/ 138/ fid
2 标题	2020-1-sy-j-C-138.fid
3 Comment	13C ztt
4 Origin	Bruker BioSpin GmbH
5 Owner	mrsu
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	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

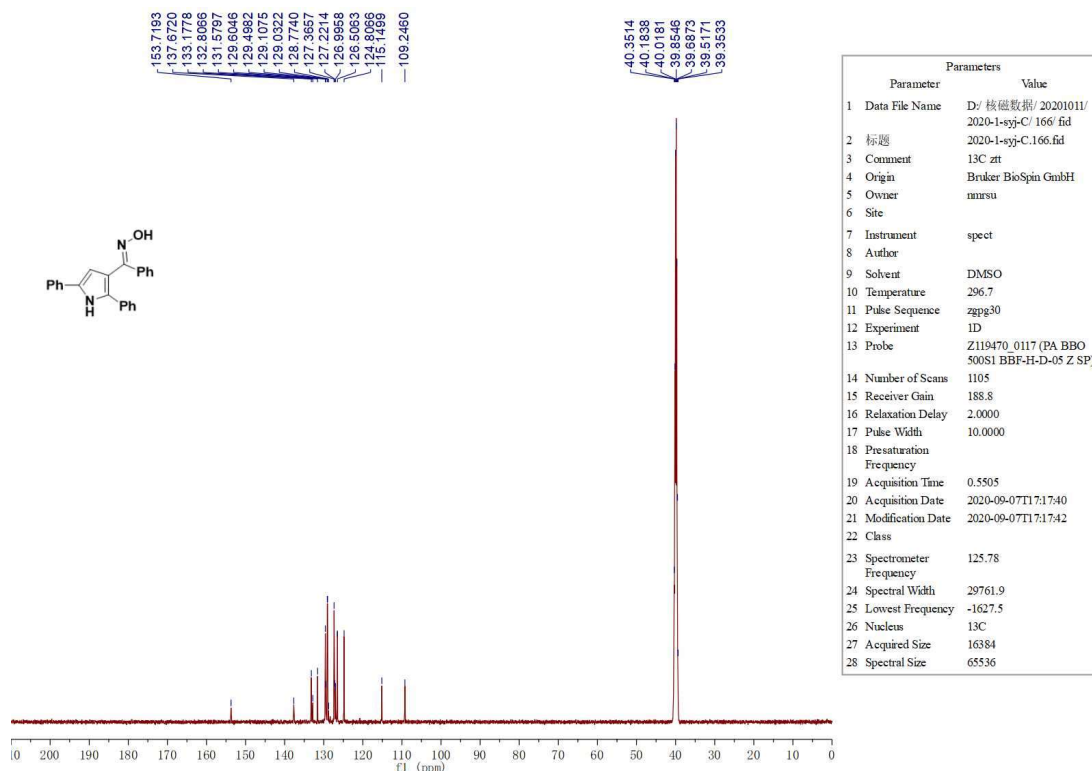
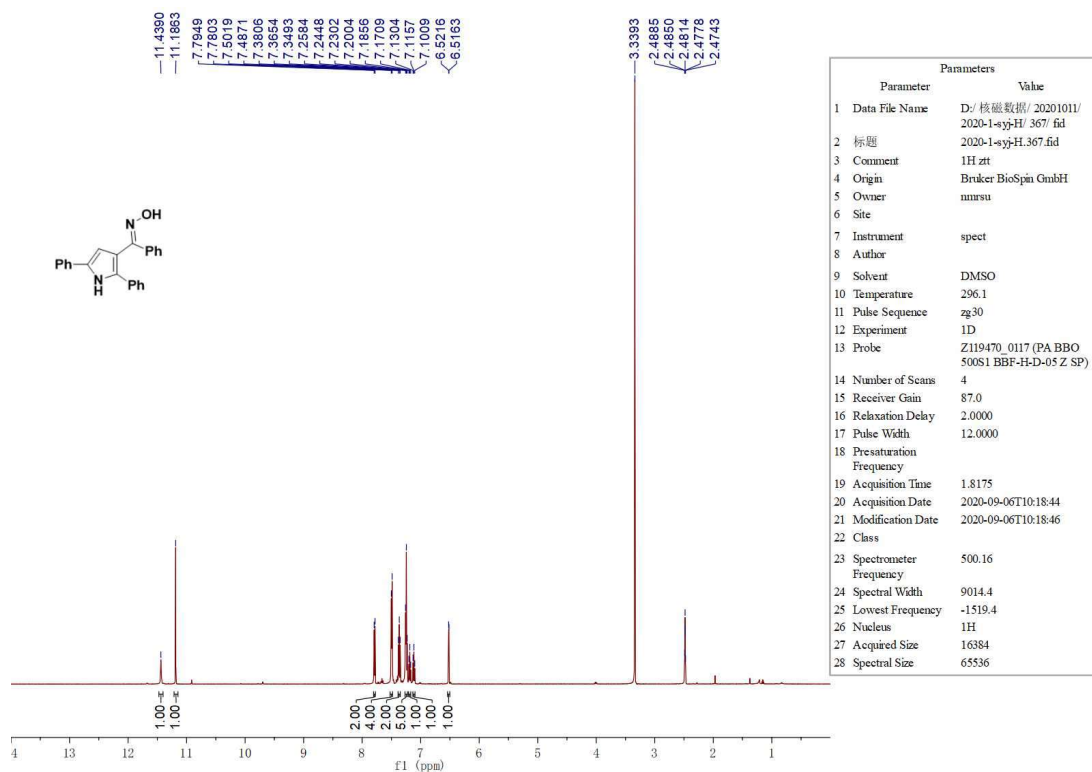
1-(2-Methyl-5-phenyl-1-(*p*-tolyl)-1*H*-pyrrol-3-yl) ethan-1-one (7b)



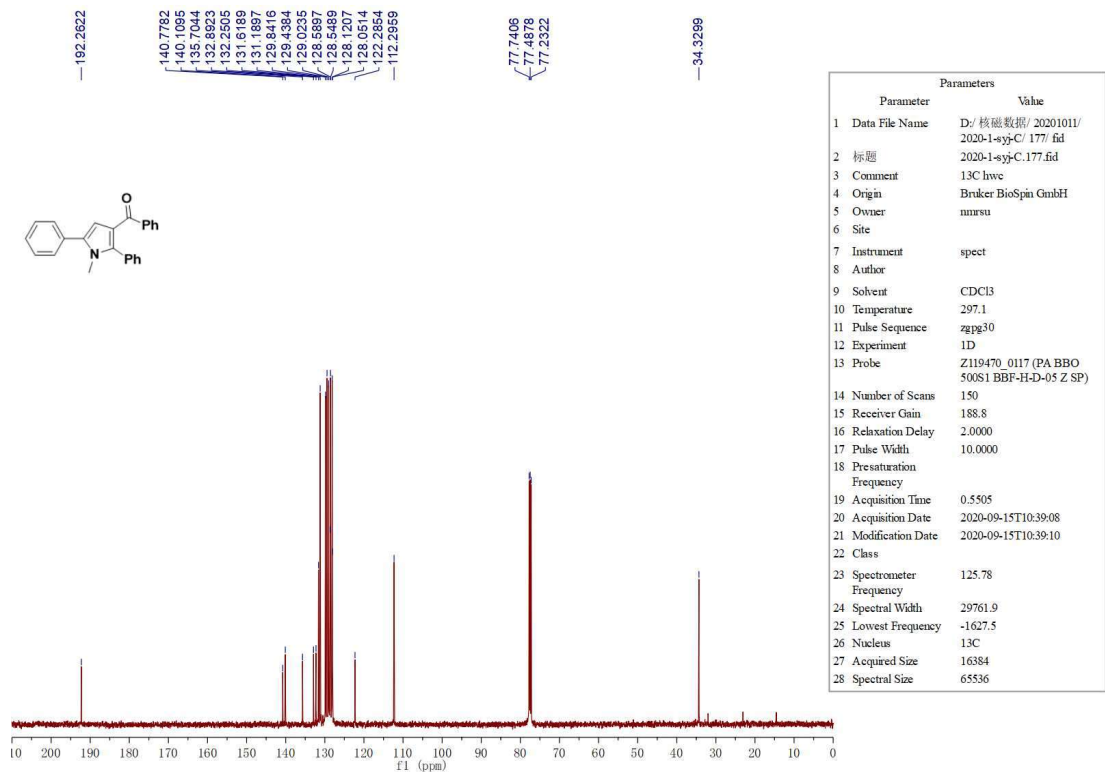
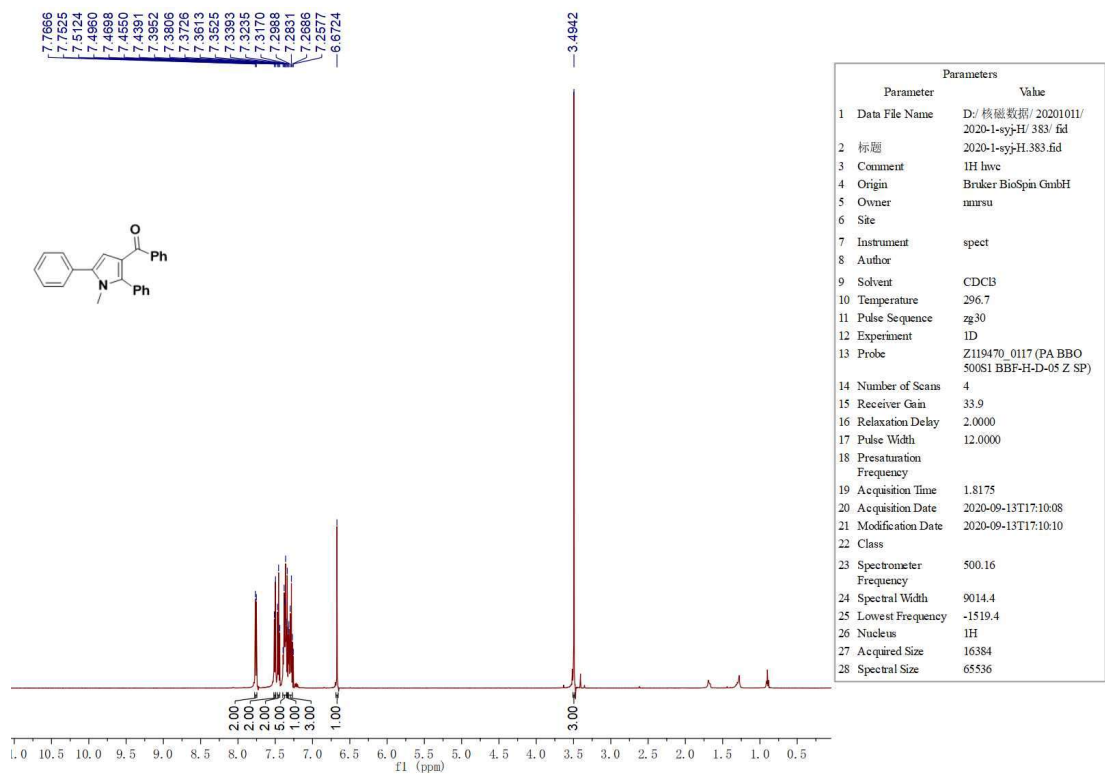
2-Methyl-4-phenyl-1H-imidazole (8)



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



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



4. GC-MS spectra for mechanistic investigations

