

# Supporting Information

## Design, Synthesis and Structure-Activity Relationship Studies of Nicotinamide Derivatives as Potent Antifungal Agents by Disrupting Cell Wall

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<sup>2</sup> School of Pharmacy, Naval Medical University, No.325 Guohe Road, Shanghai 200433, China

<sup>3</sup> School of Chinese Materia Medica, Shenyang Pharmaceutical University, Shenyang 110016, China

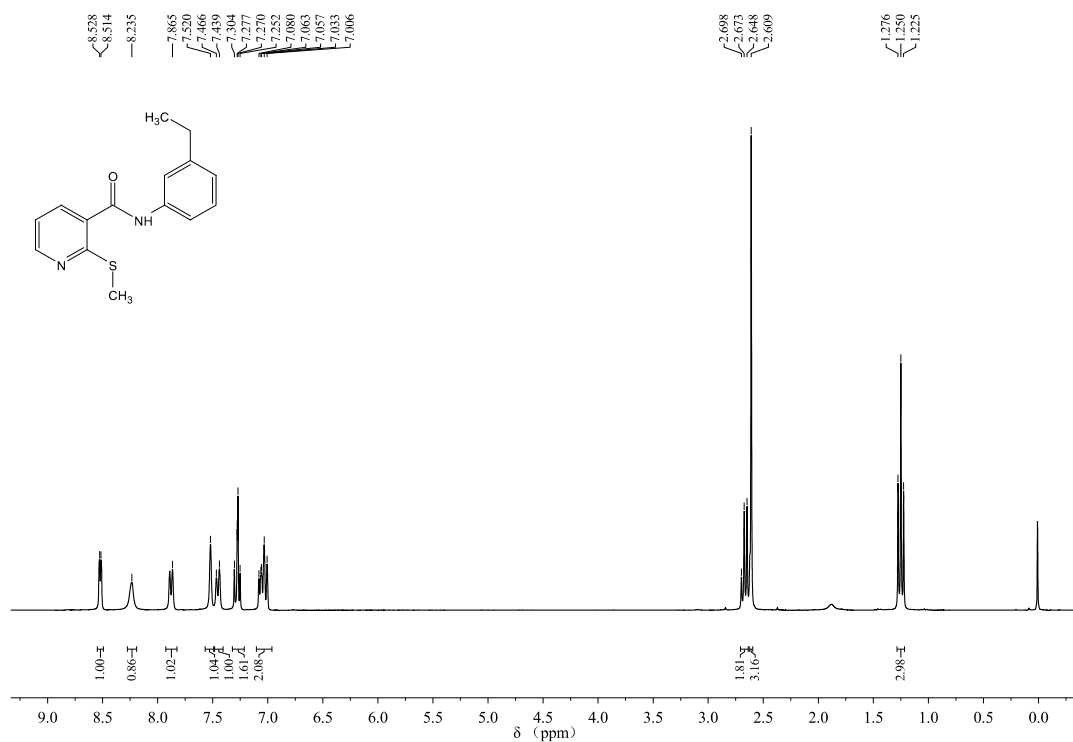
\* Correspondence: zdzhang\_yjhx@smmu.edu.cn (D.Z.); 13761571578@163.com (Y.J.); lvquanzhen2011@163.com (Q.L.)

† These authors contributed equally to this work.

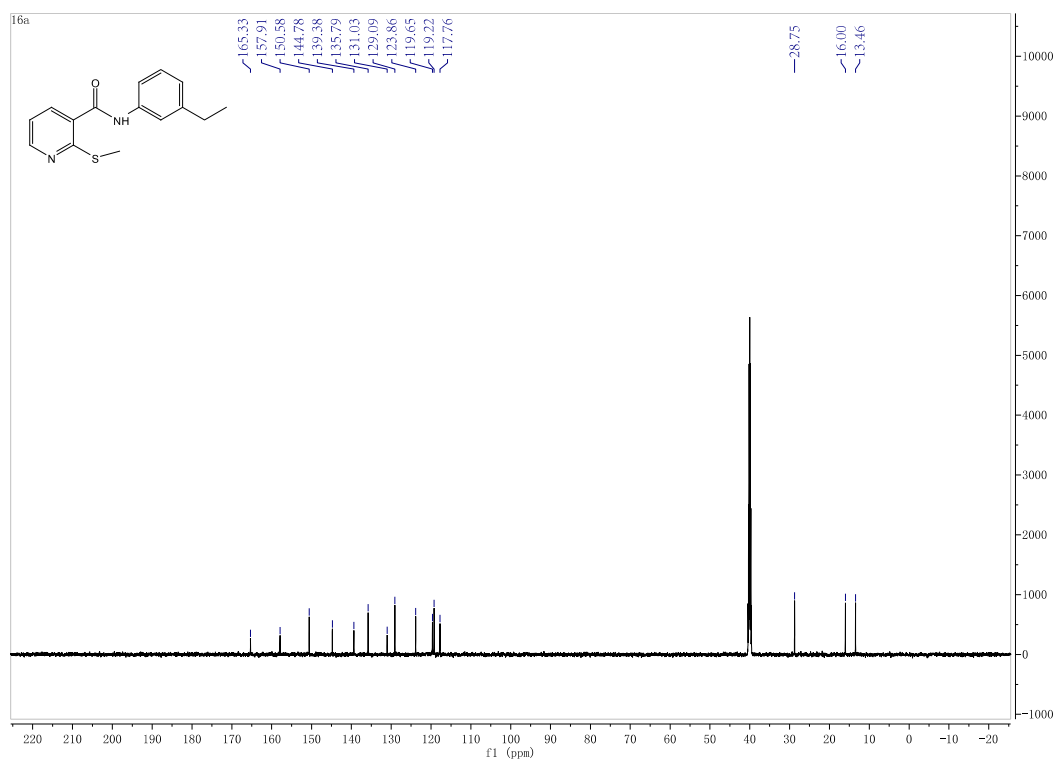
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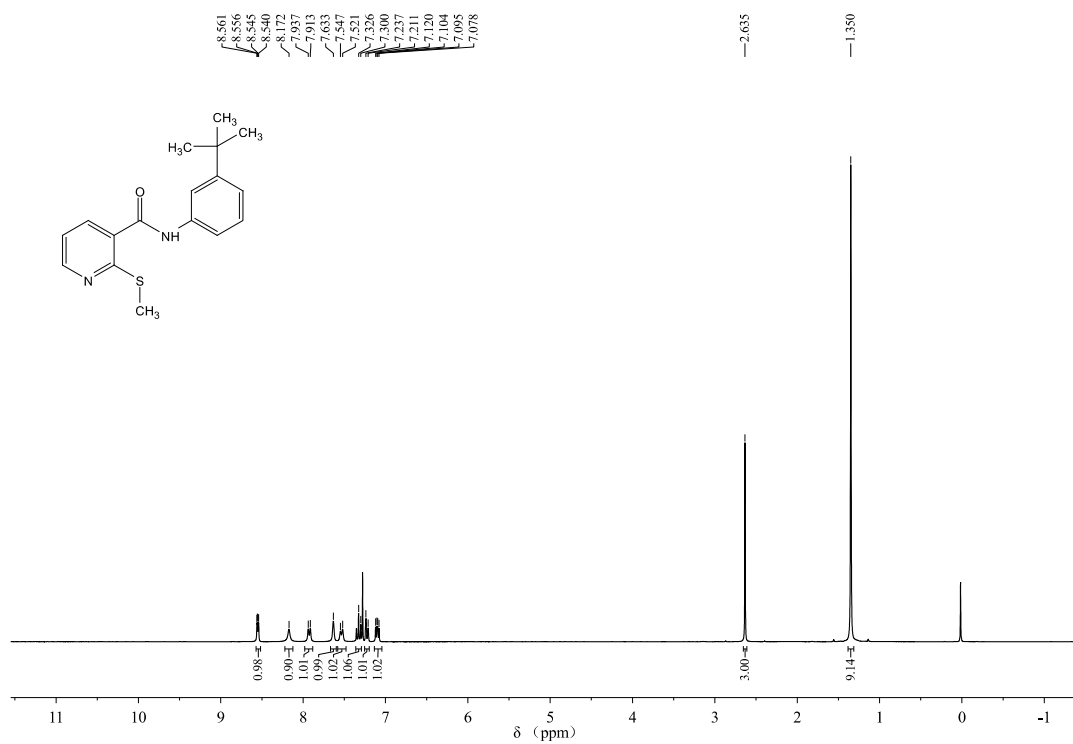
# NMR Spectra of Target Compounds



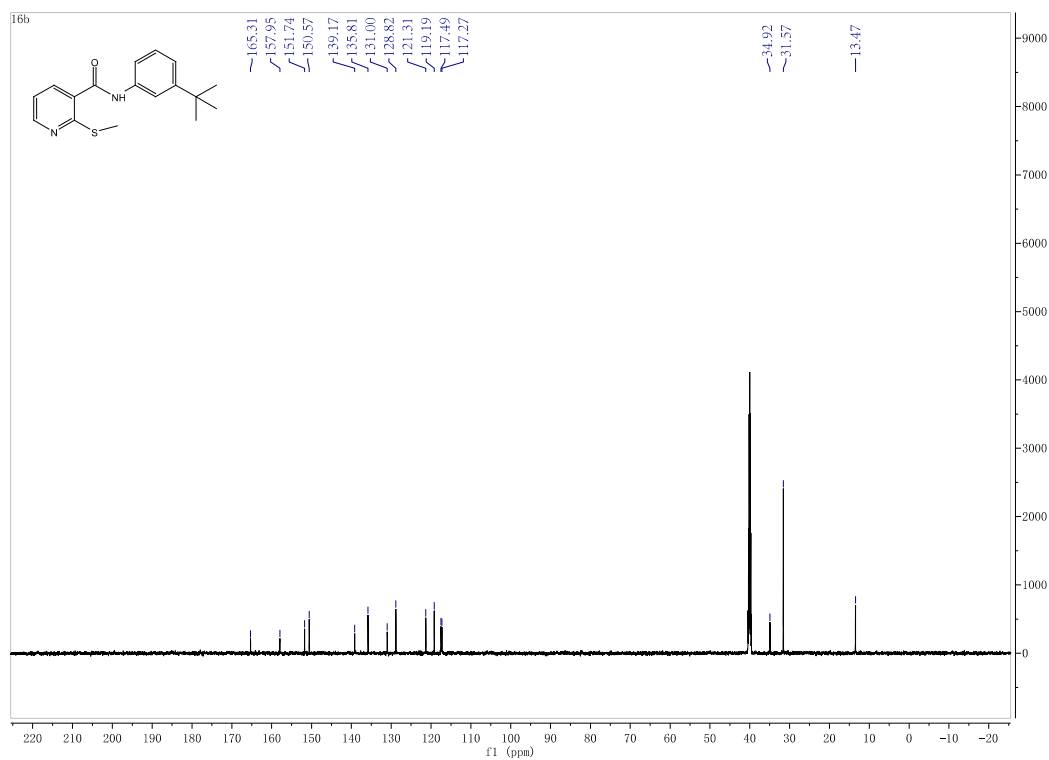
<sup>1</sup>H NMR spectra of 16a



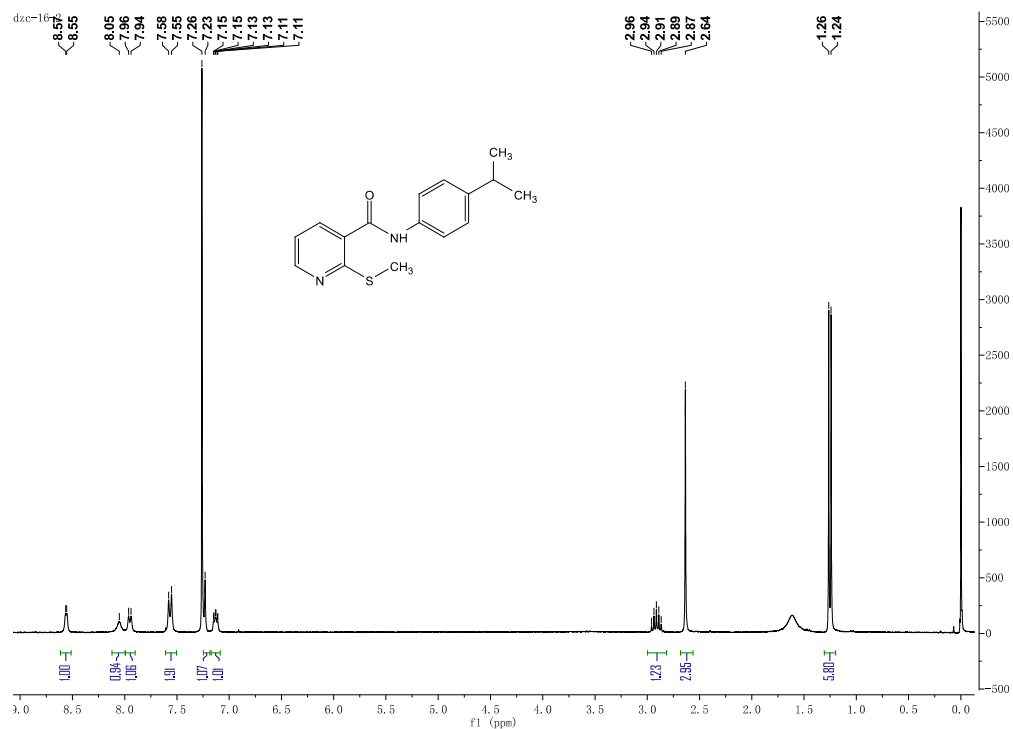
<sup>13</sup>C NMR spectra of 16a



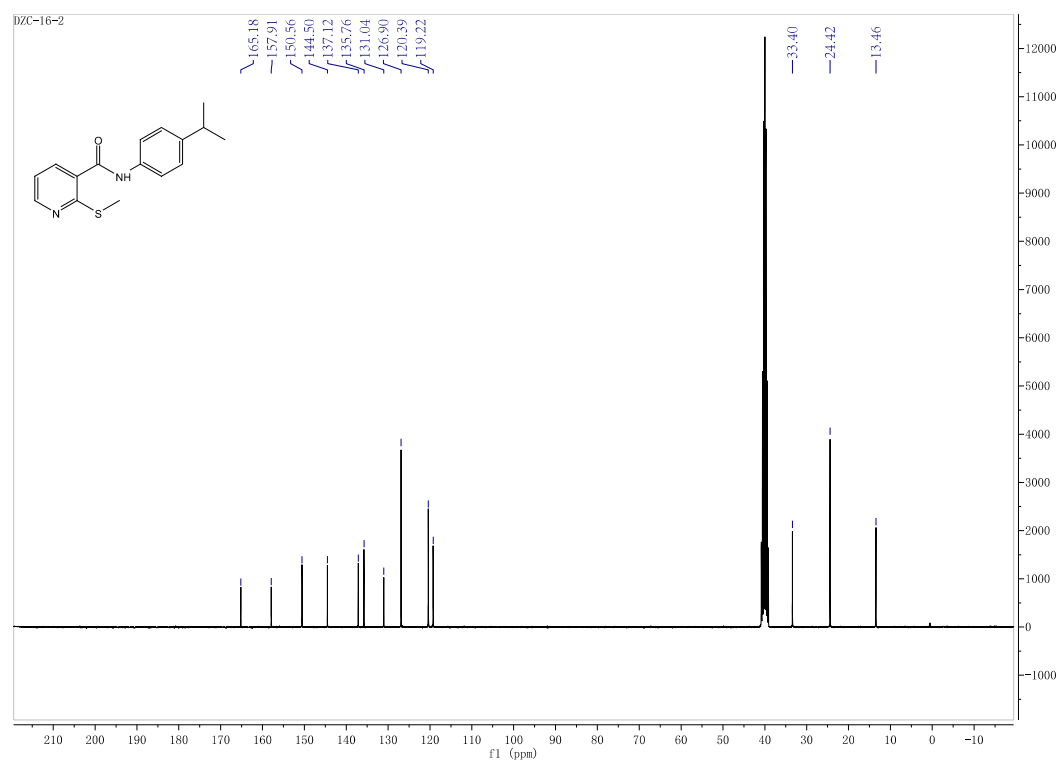
**<sup>1</sup>H NMR spectra of 16b**



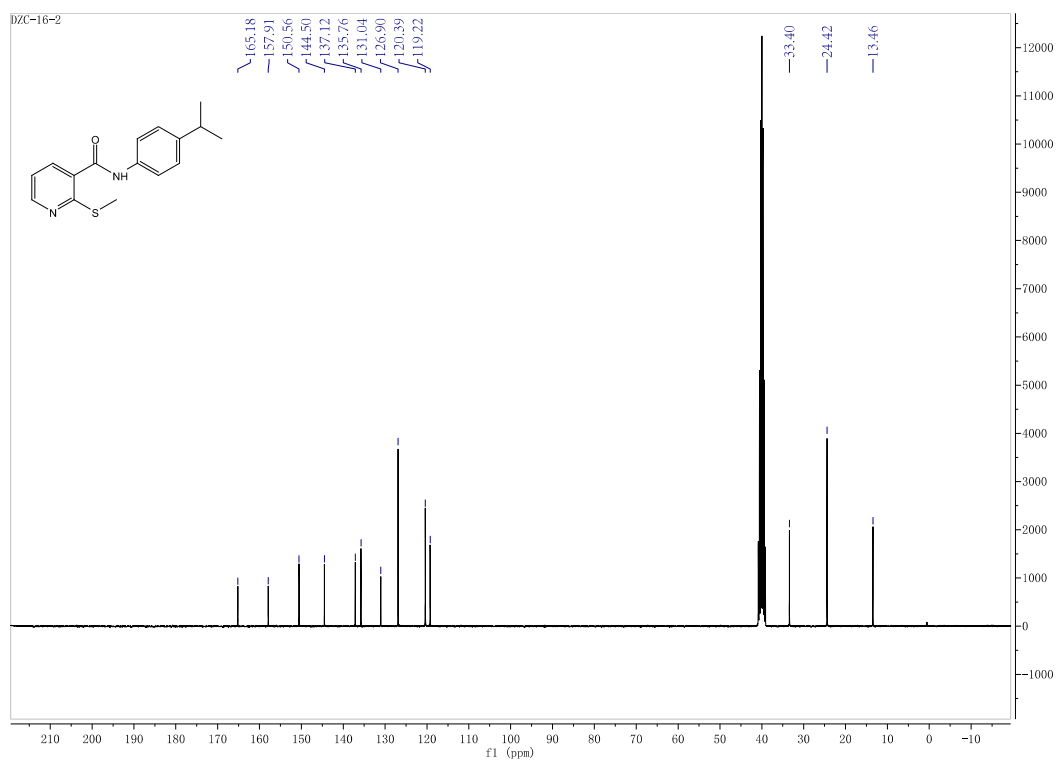
**<sup>13</sup>C NMR spectra of 16b**



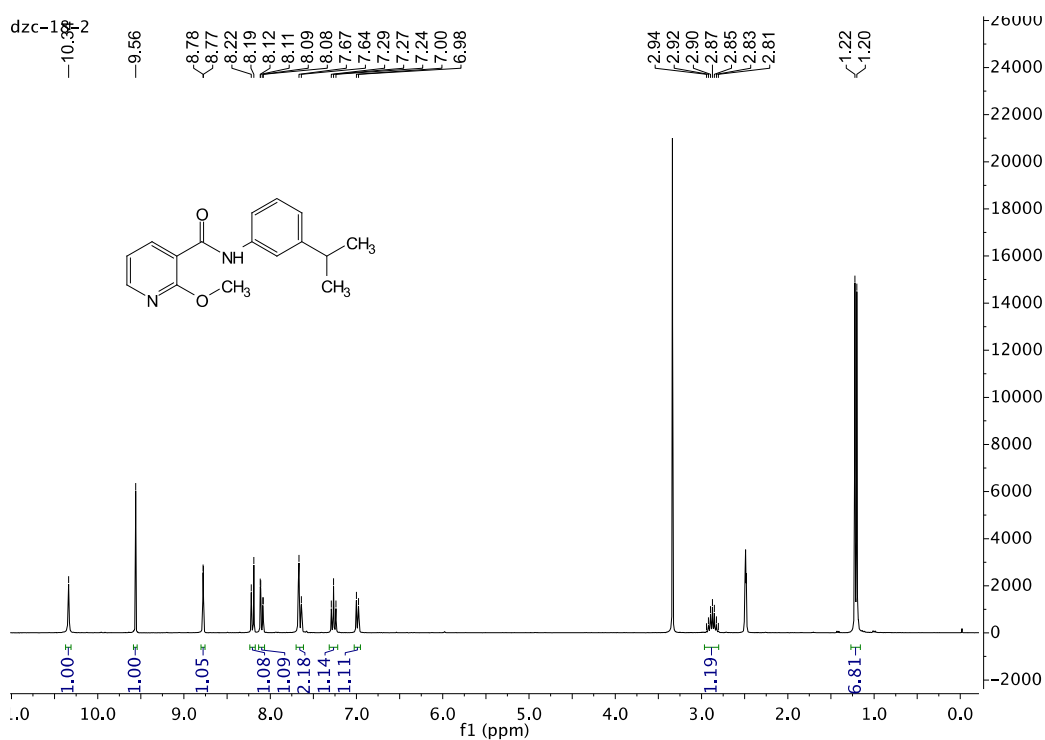
**<sup>1</sup>H NMR spectra of 16c**



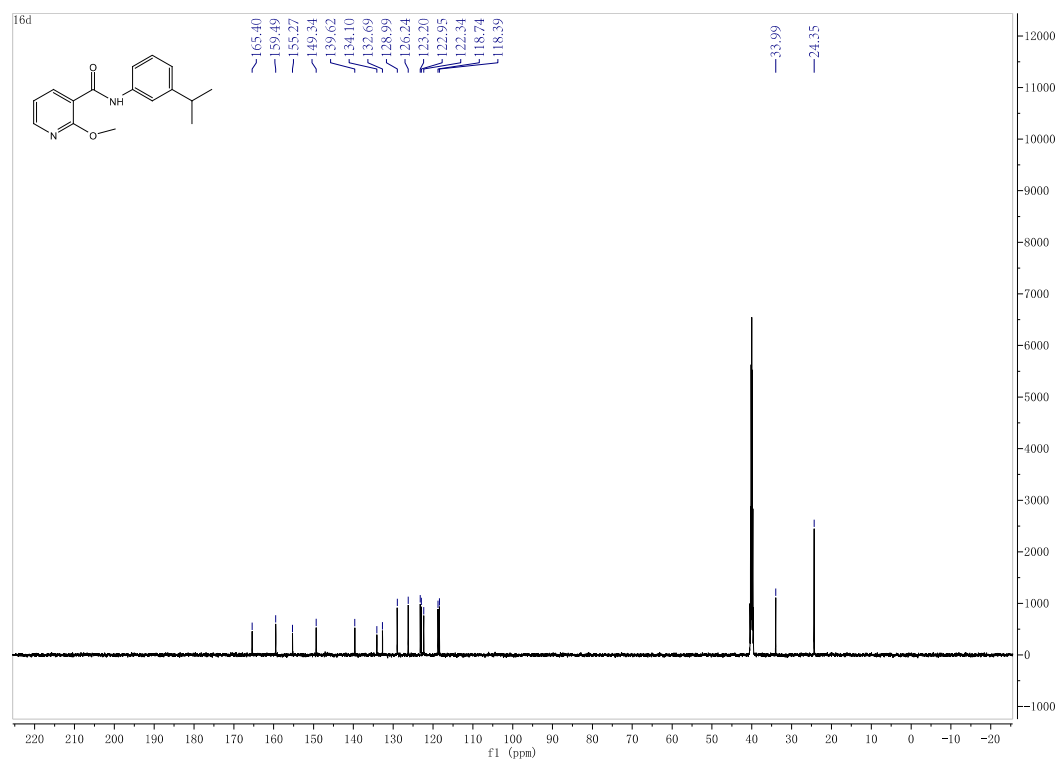
**<sup>13</sup>C NMR spectra of 16c**



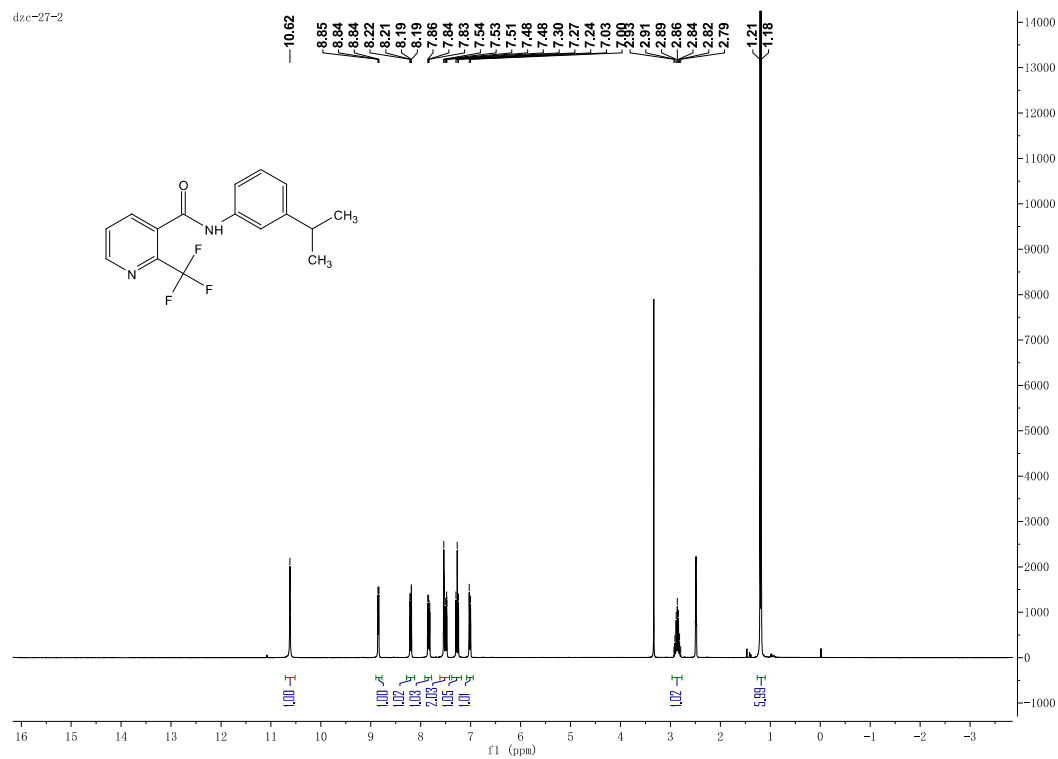
**<sup>13</sup>C NMR spectra of 16c**



**<sup>1</sup>H NMR spectra of 16d**

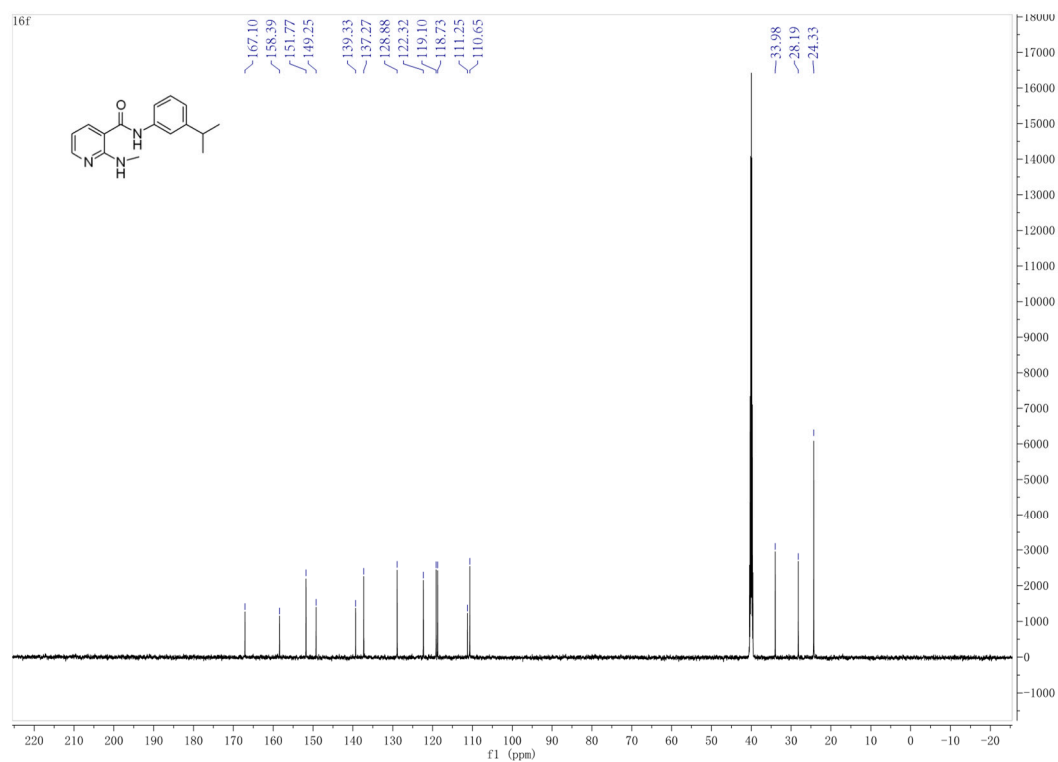


### <sup>13</sup>C NMR spectra of 16d

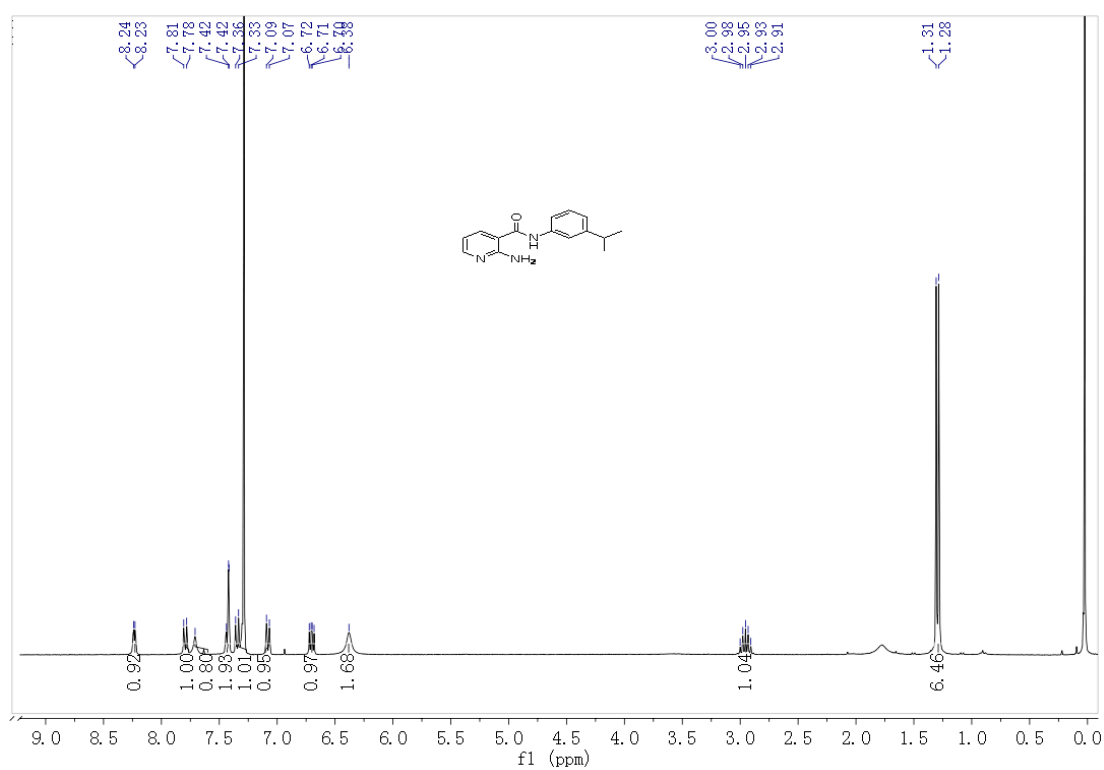


### <sup>1</sup>H NMR spectra of 16e



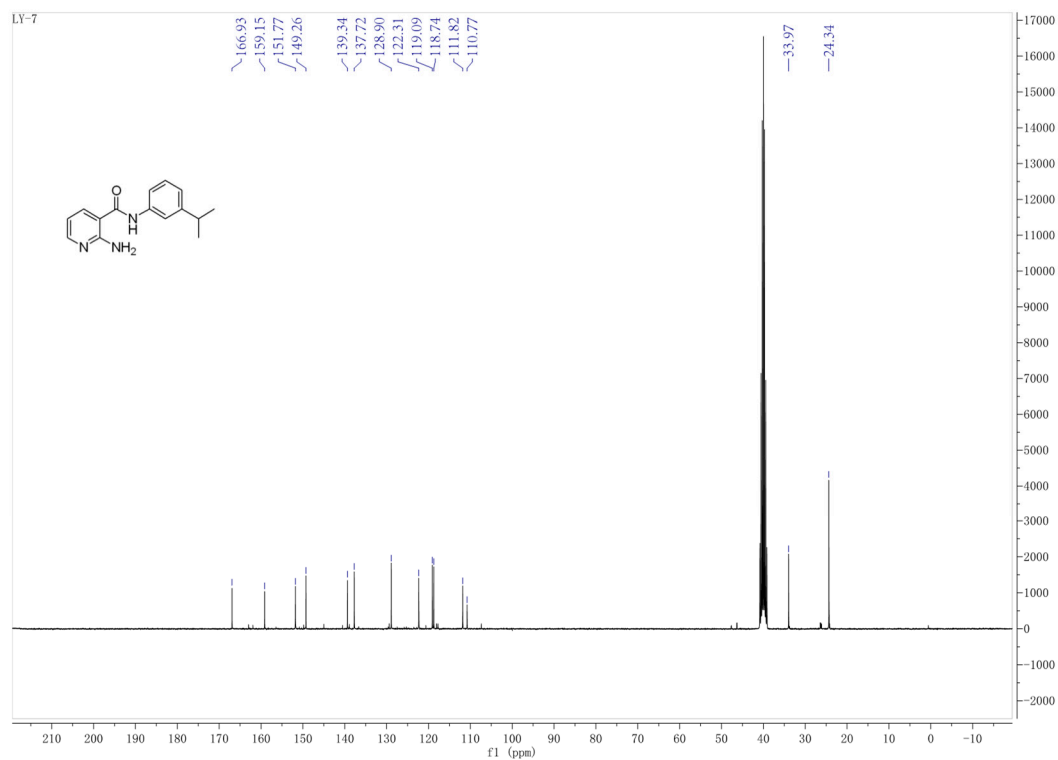


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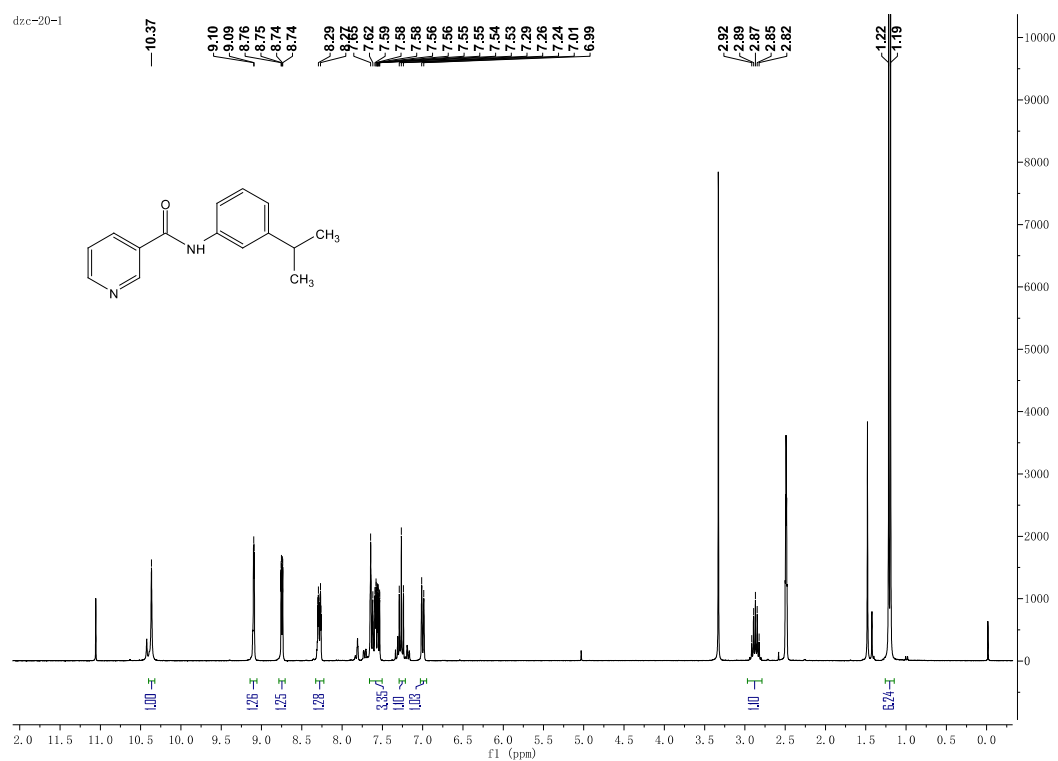


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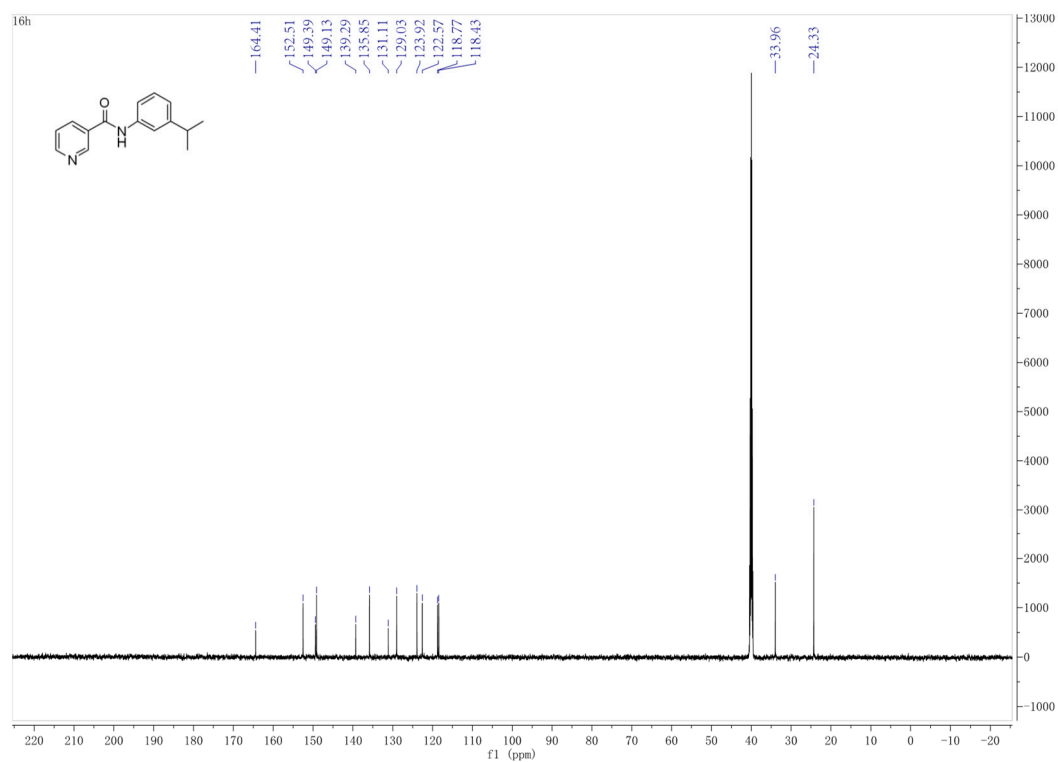




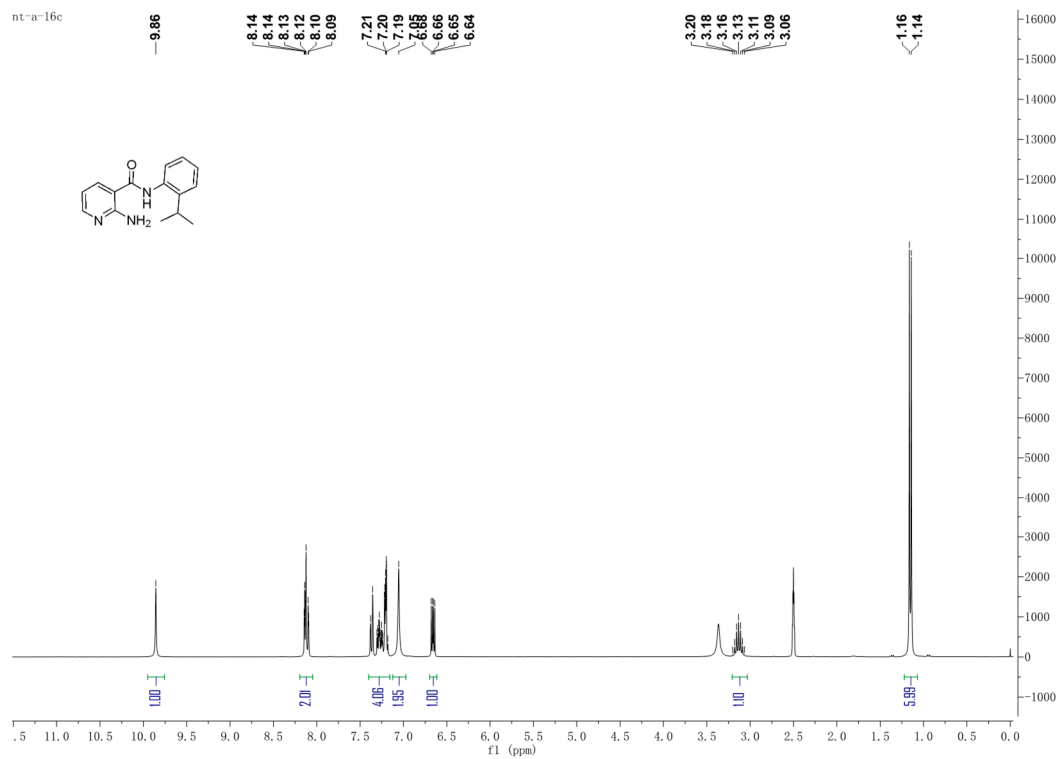
**$^{13}\text{C}$  NMR spectra of 16g**



**$^1\text{H}$  NMR spectra of 16h**

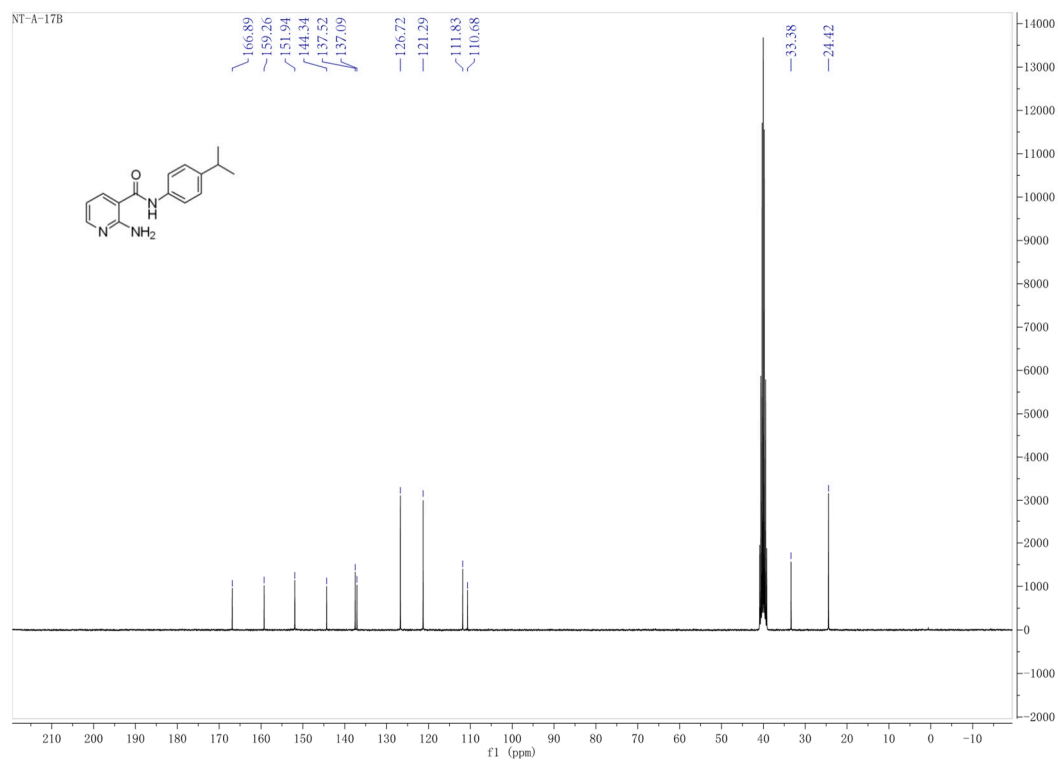


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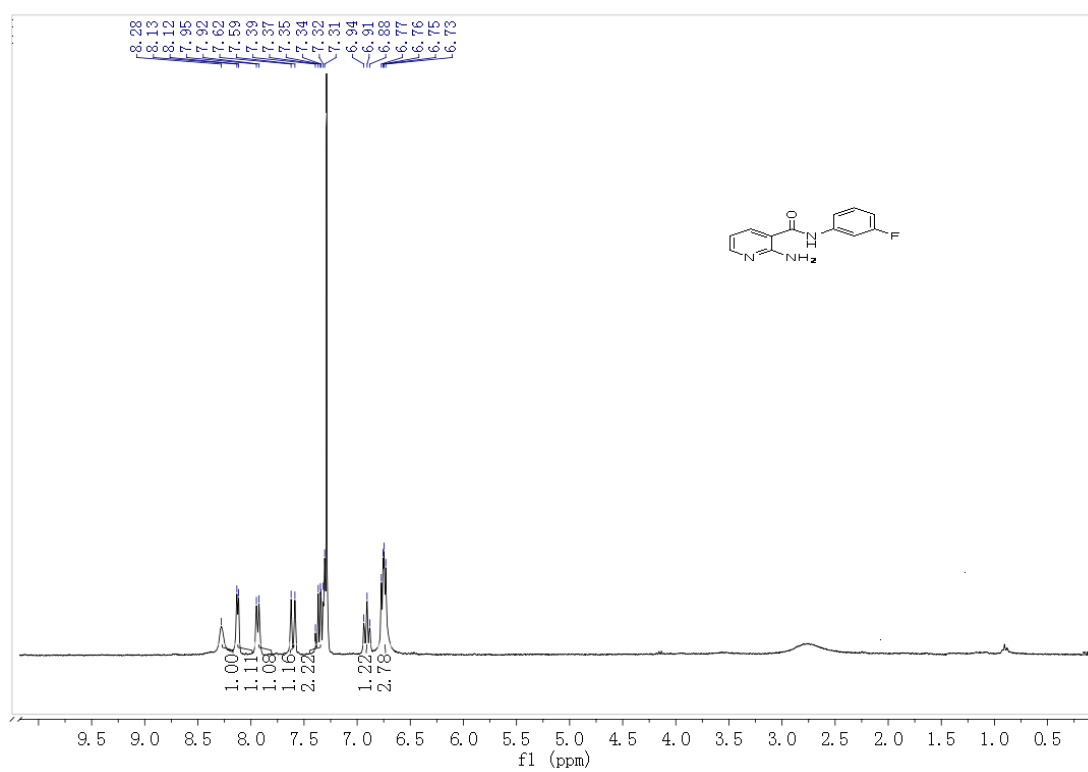


**$^1\text{H}$  NMR spectra of 16i**

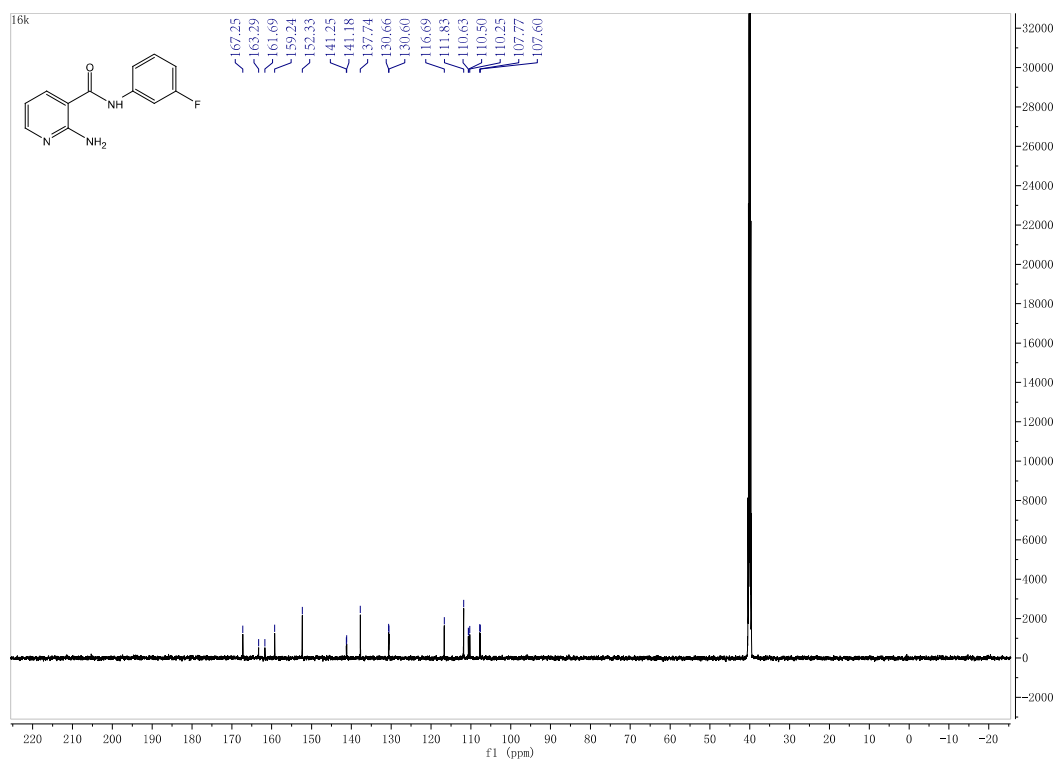




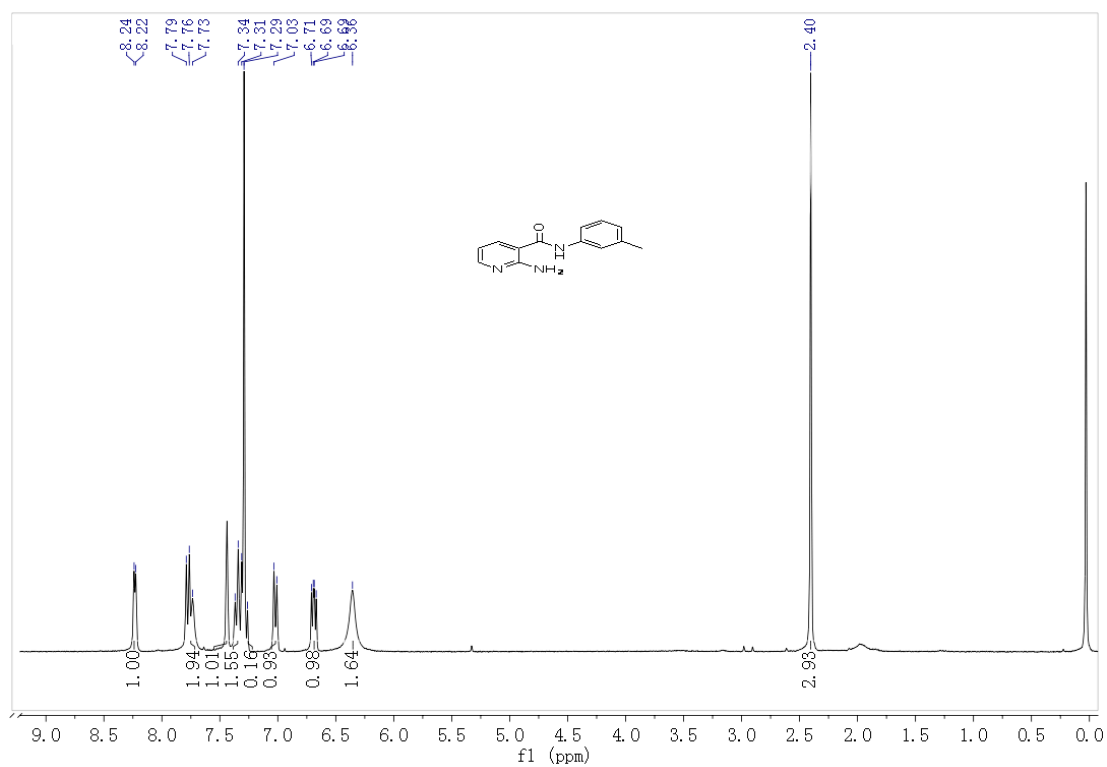
### <sup>13</sup>C NMR spectra of 16j



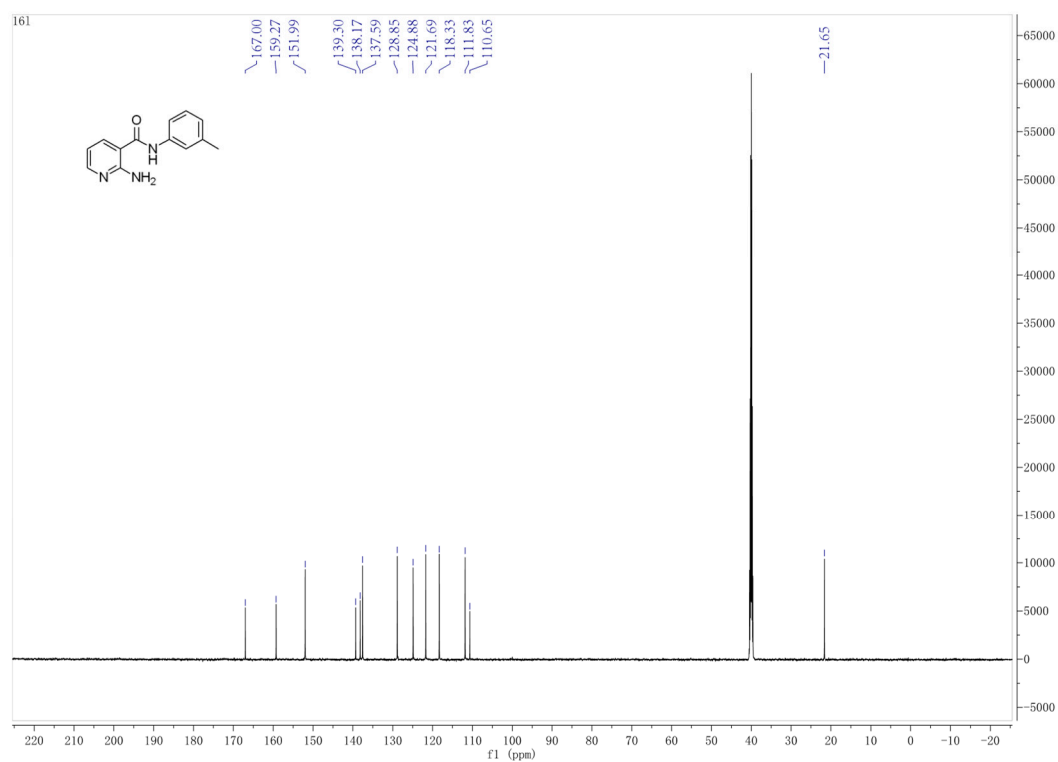
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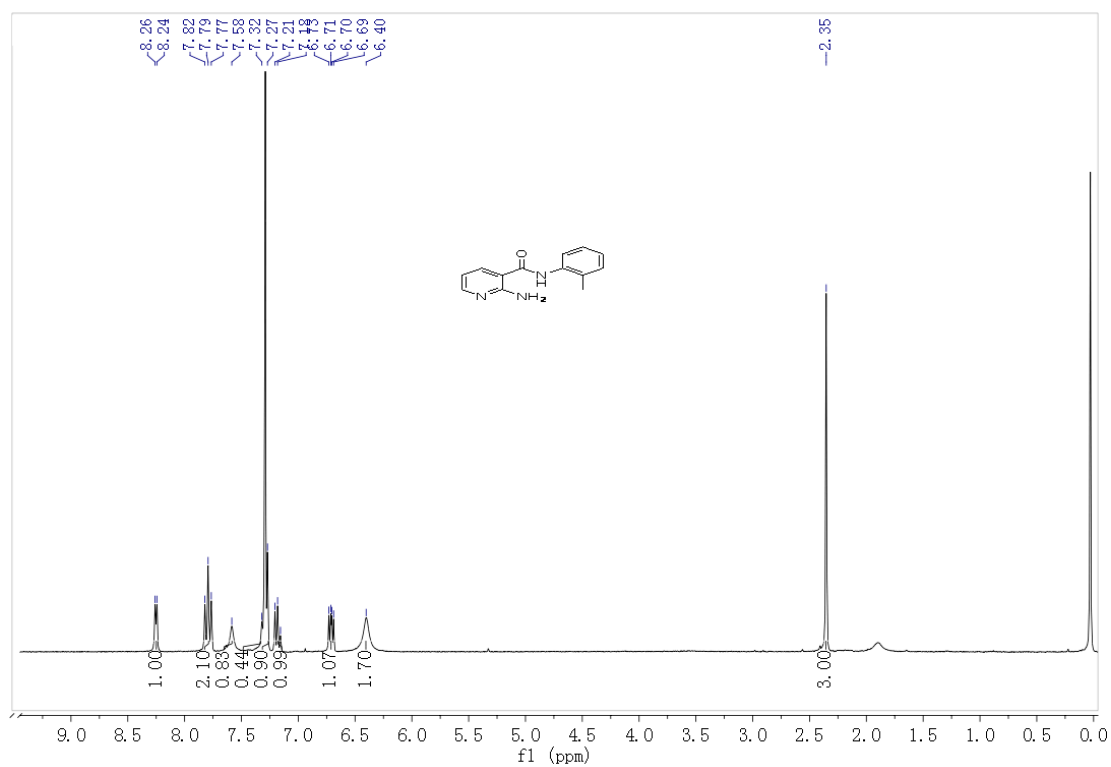
**$^{13}\text{C}$  NMR spectra of 16k**



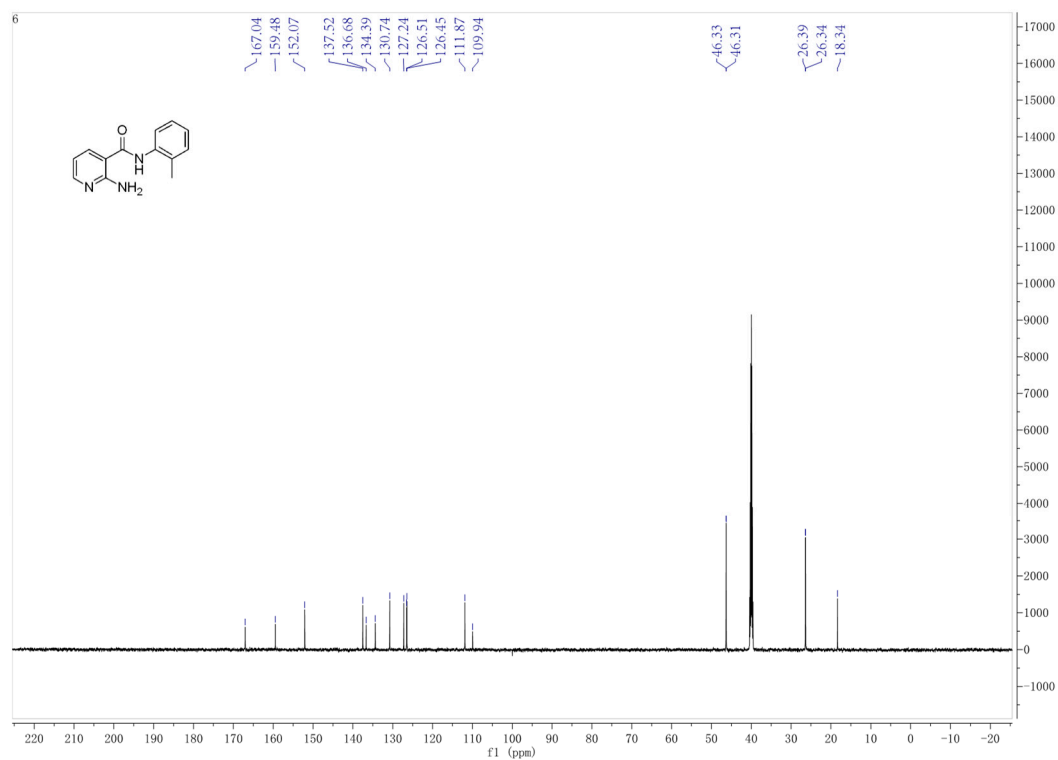
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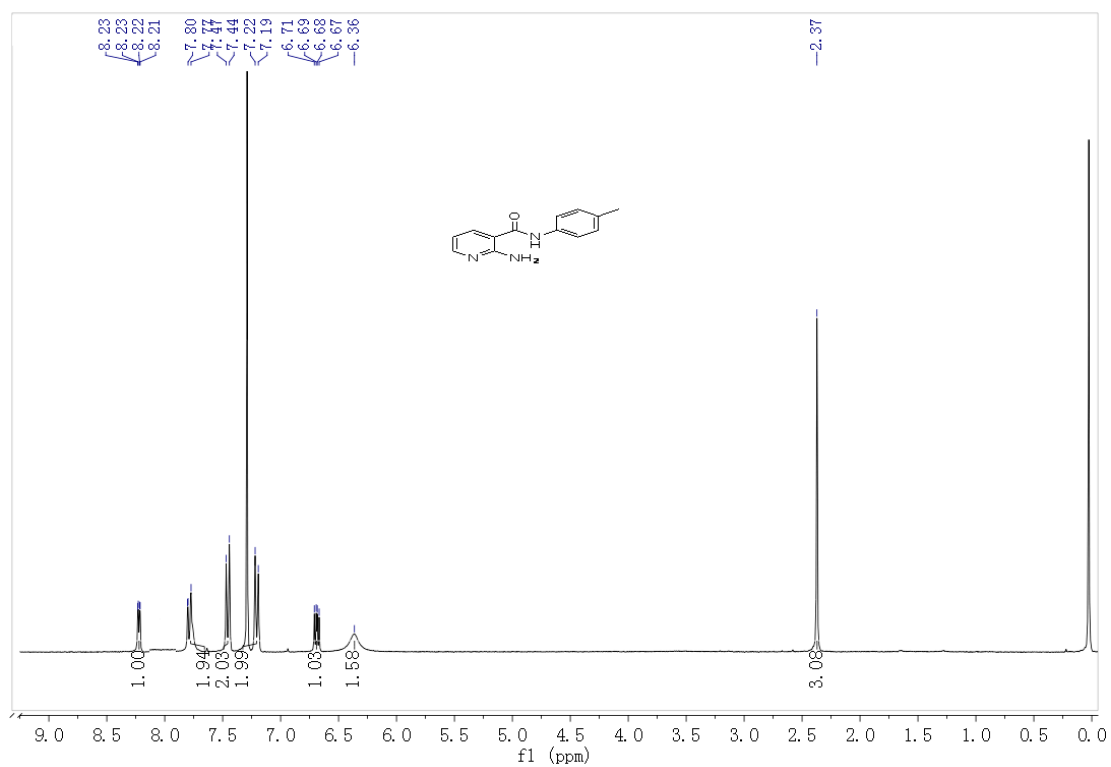
**$^{13}\text{C}$  NMR spectra of 16l**



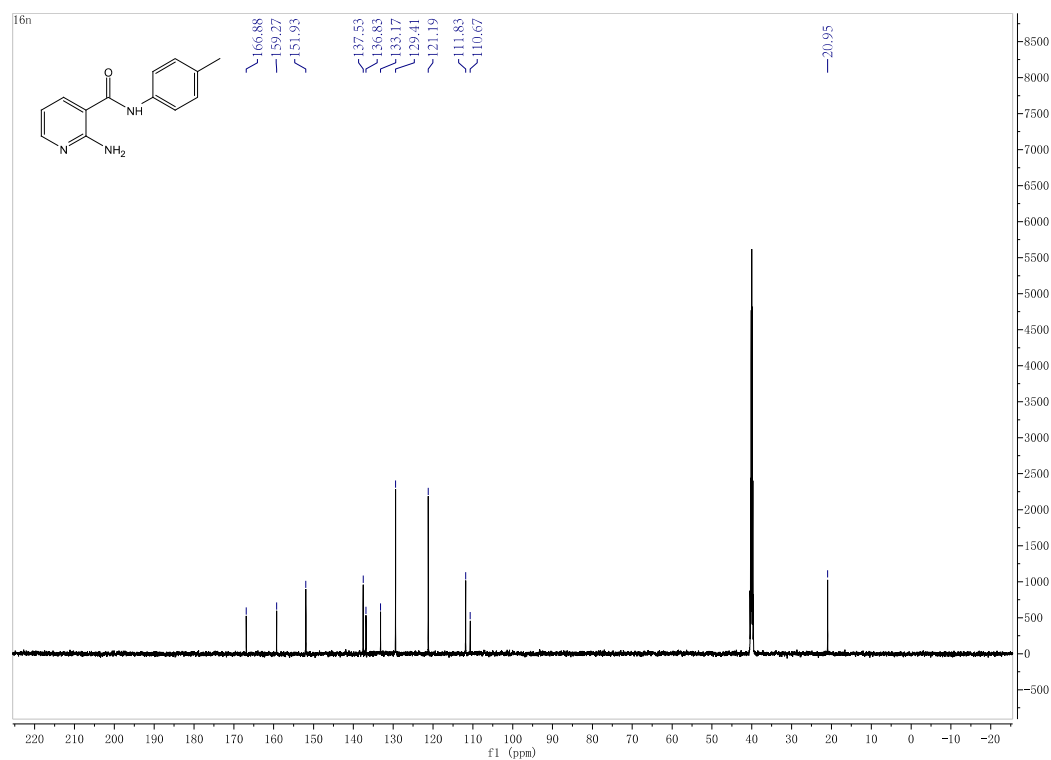
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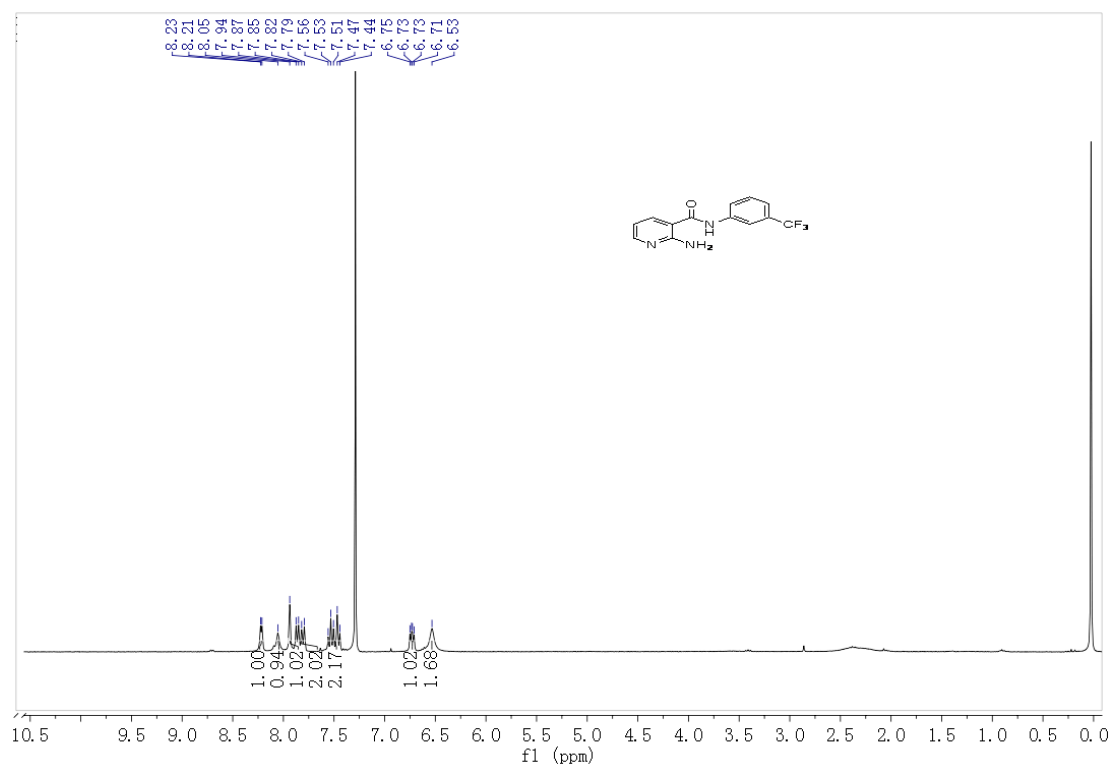
**$^{13}\text{C}$  NMR spectra of 16m**



**$^1\text{H}$  NMR spectra of 16n**

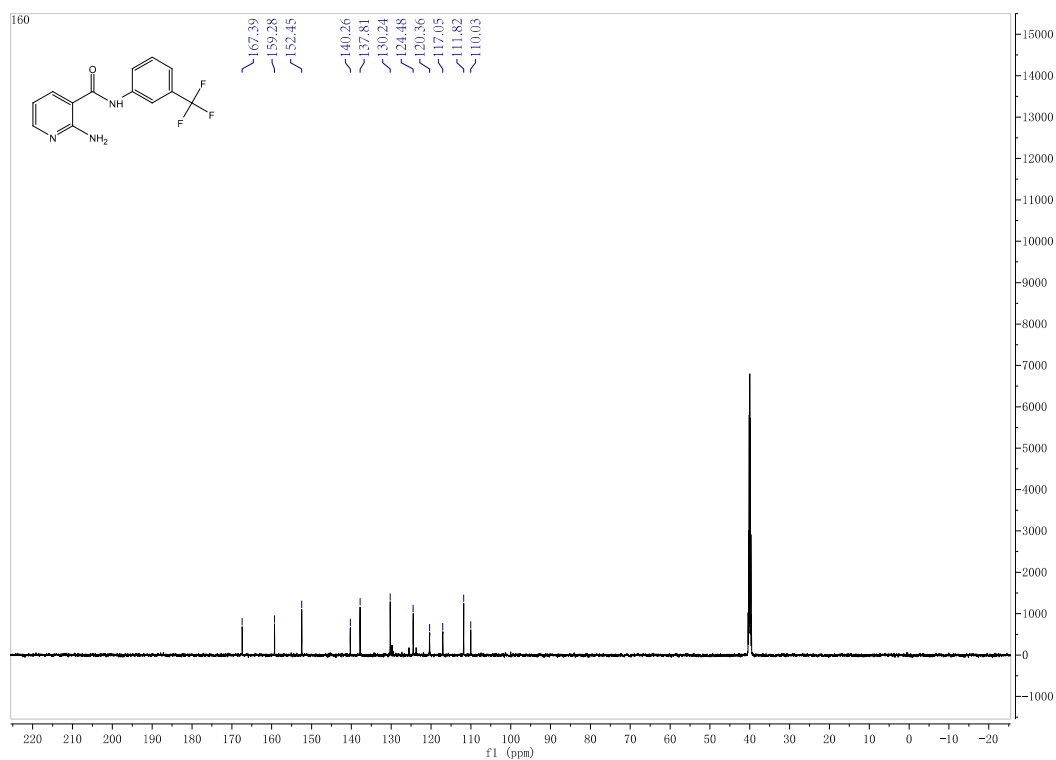


**<sup>13</sup>C NMR spectra of 16n**

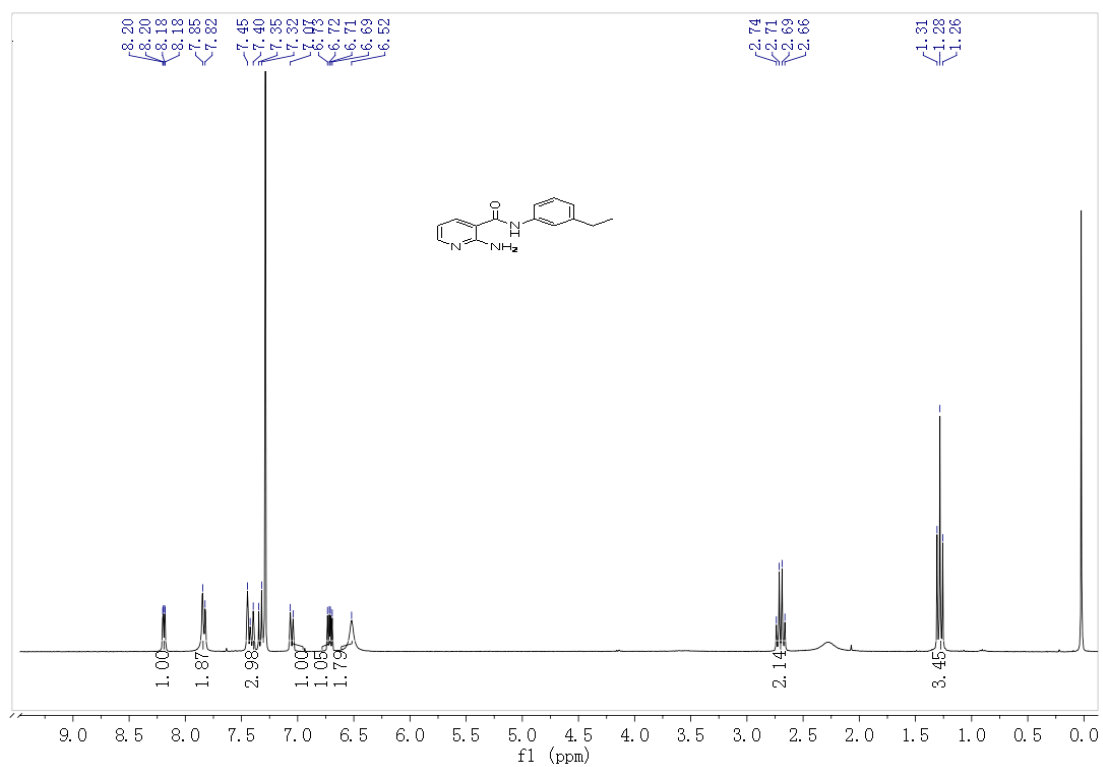


**<sup>1</sup>H NMR spectra of 16o**

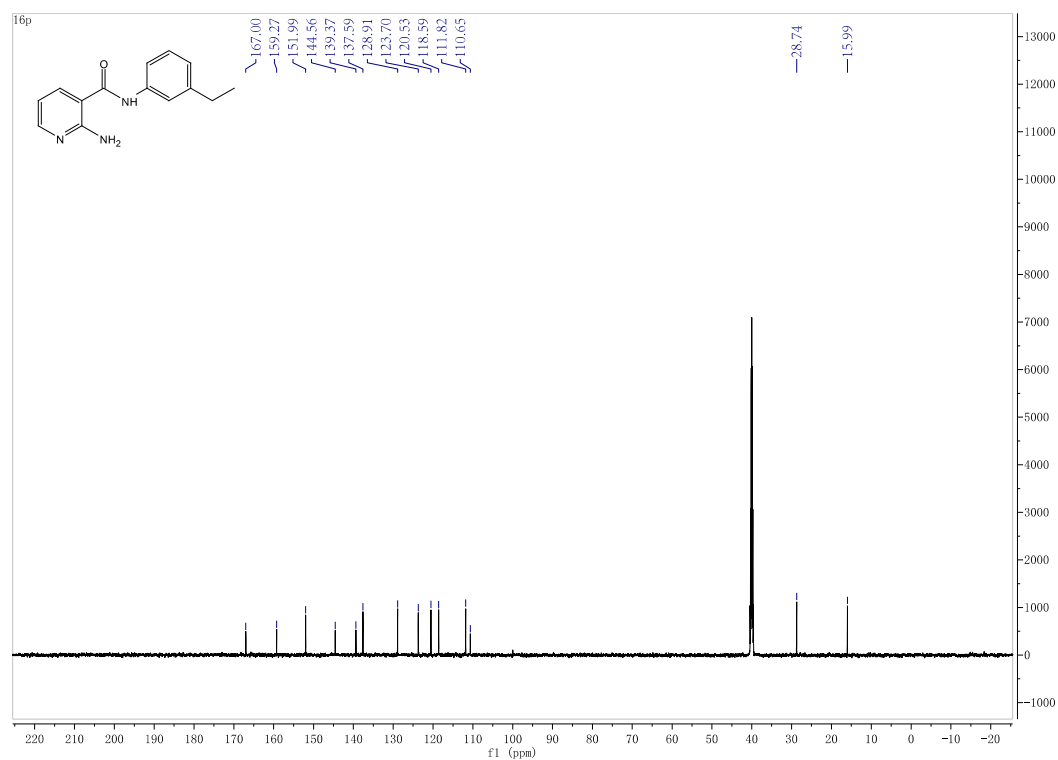




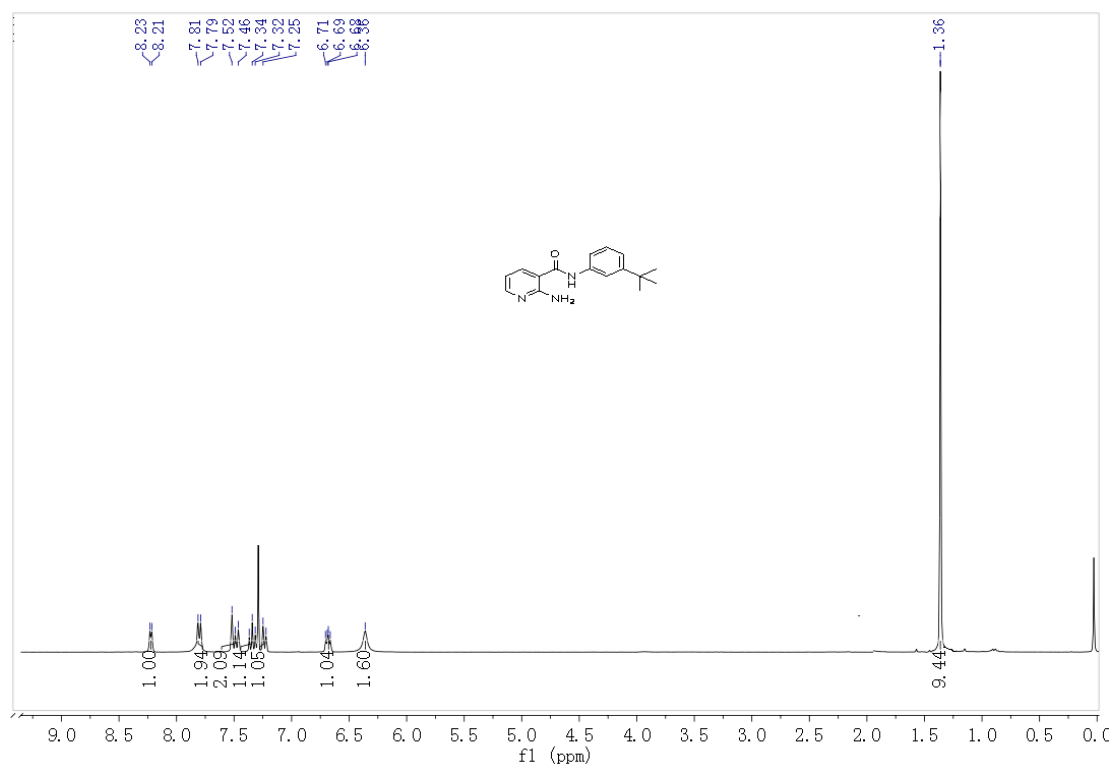
**<sup>13</sup>C NMR spectra of 16o**



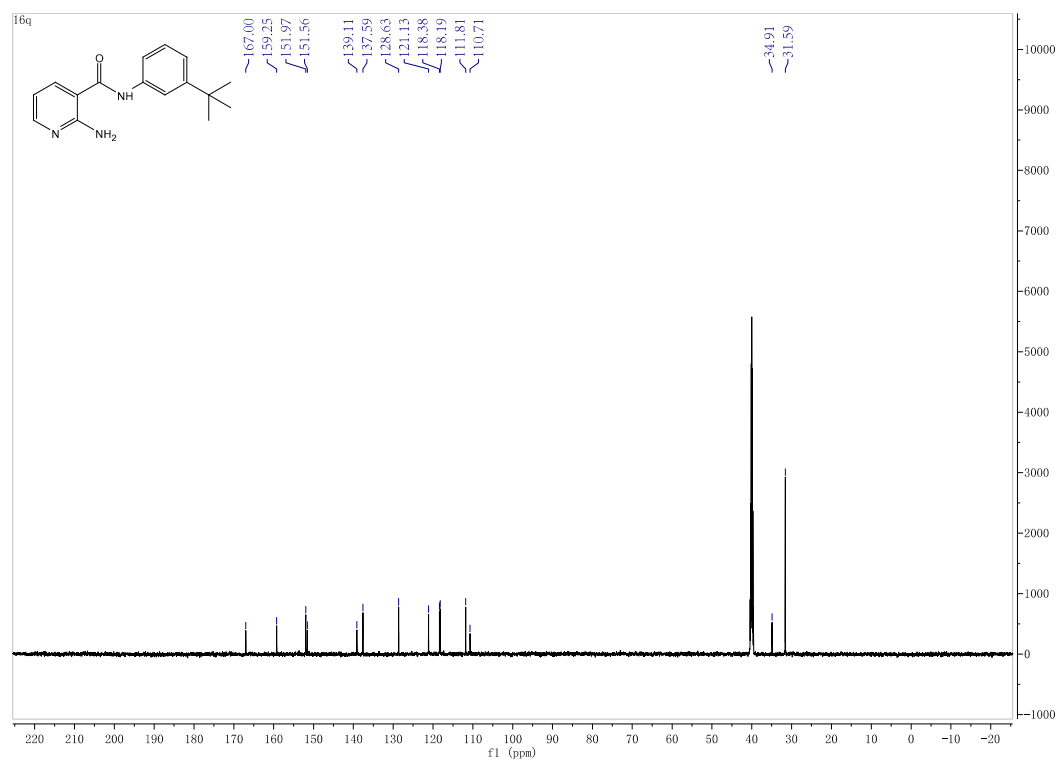
**<sup>1</sup>H NMR spectra of 16p**



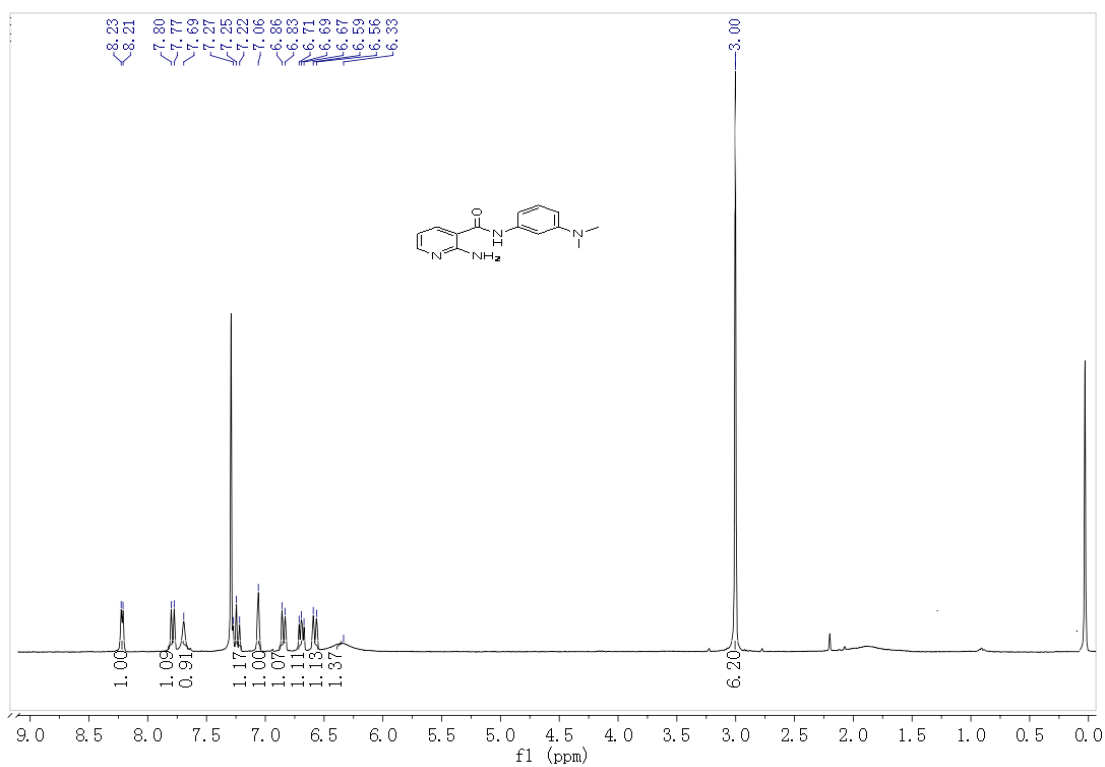
**<sup>13</sup>C NMR spectra of 16p**



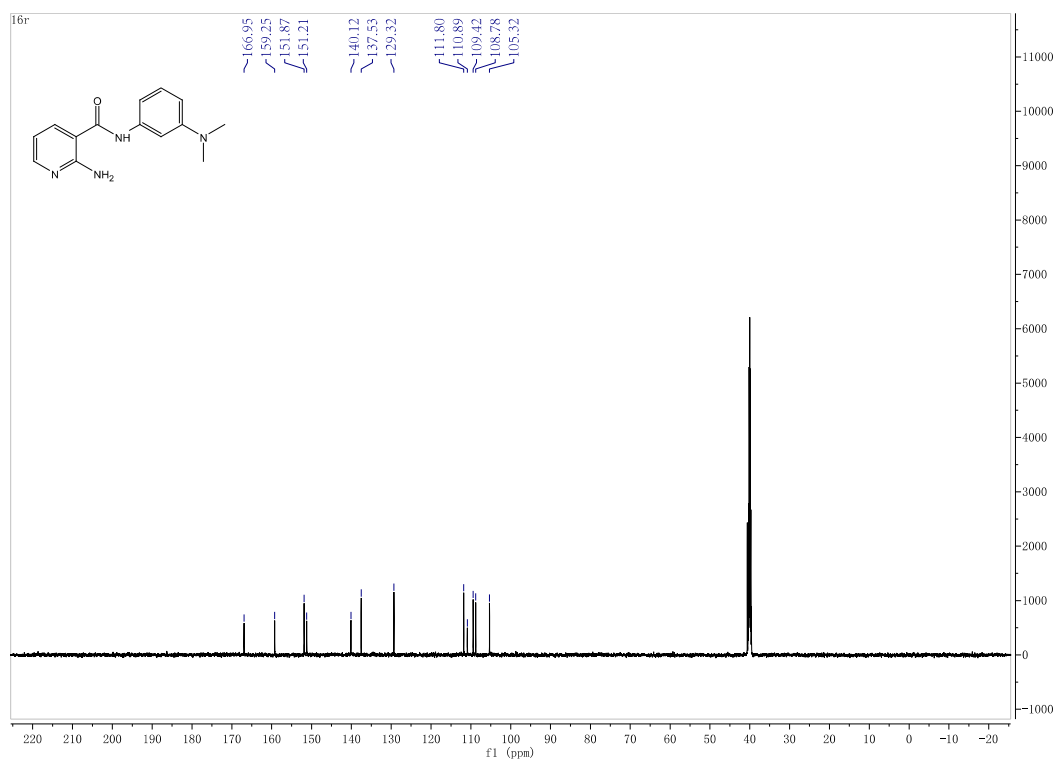
**<sup>1</sup>H NMR spectra of 16q**



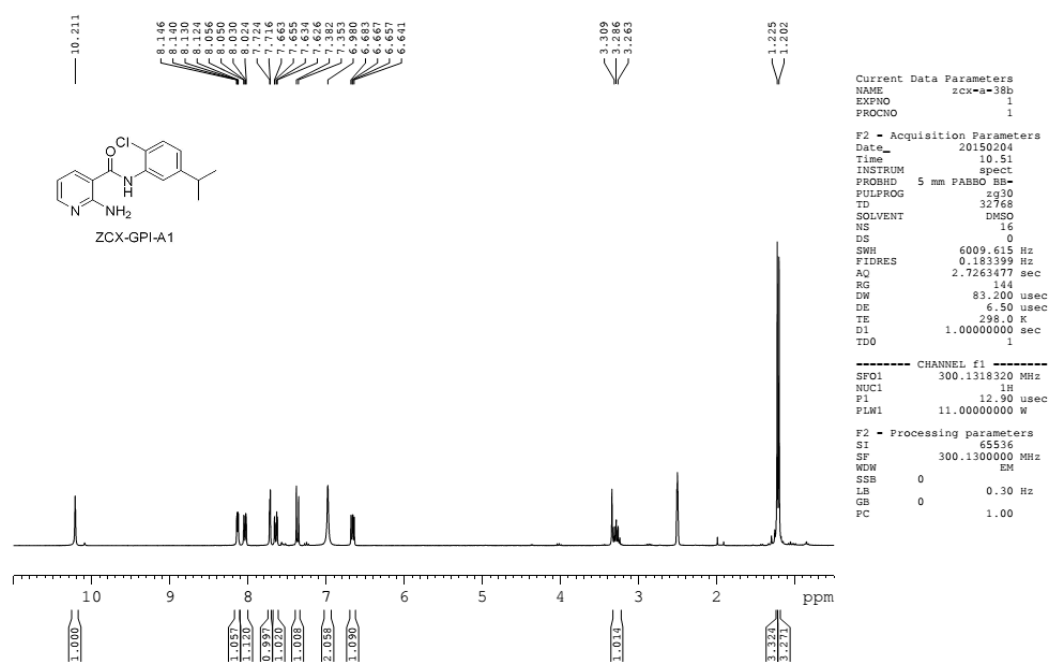
**<sup>13</sup>C NMR spectra of 16q**



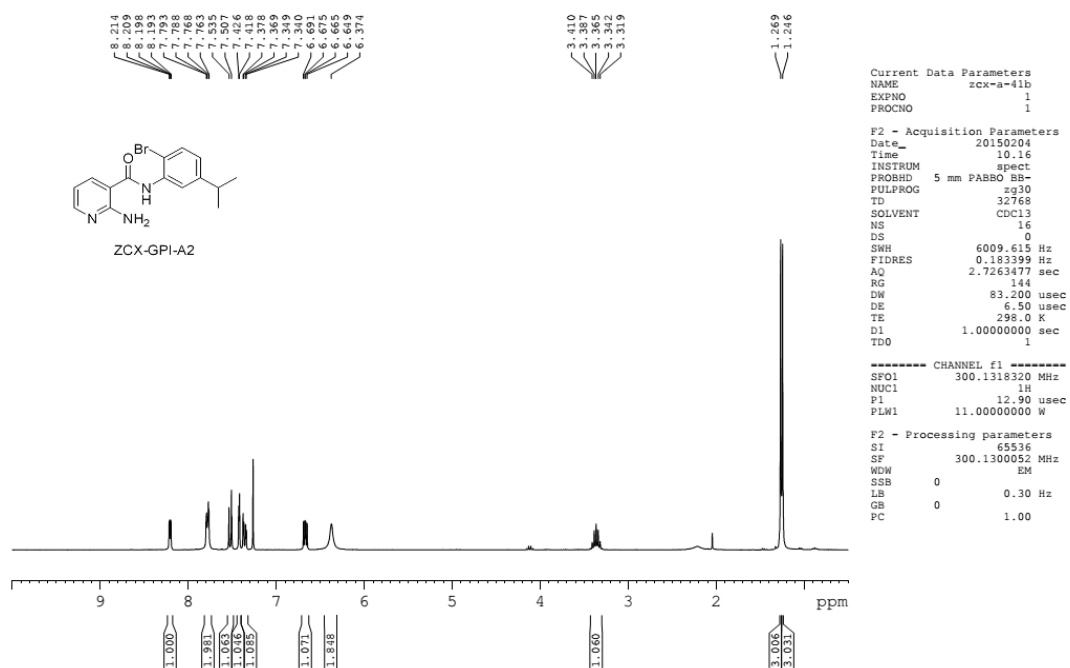
**<sup>1</sup>H NMR spectra of 16r**



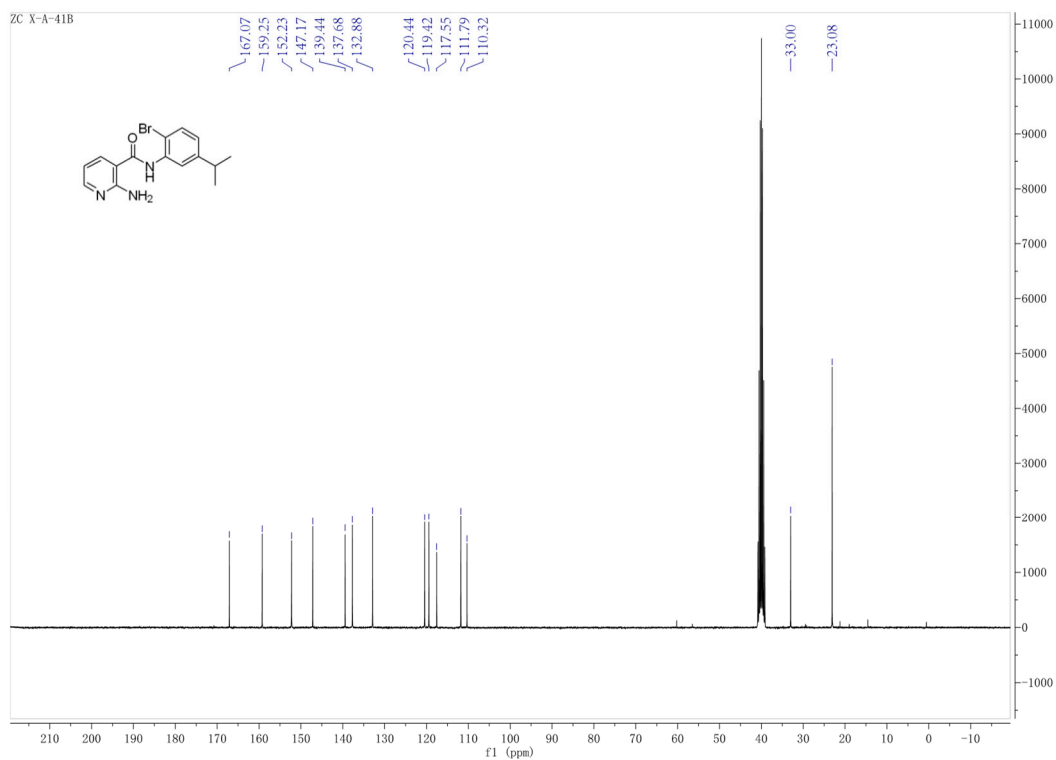
**<sup>13</sup>C NMR spectra of 16r**



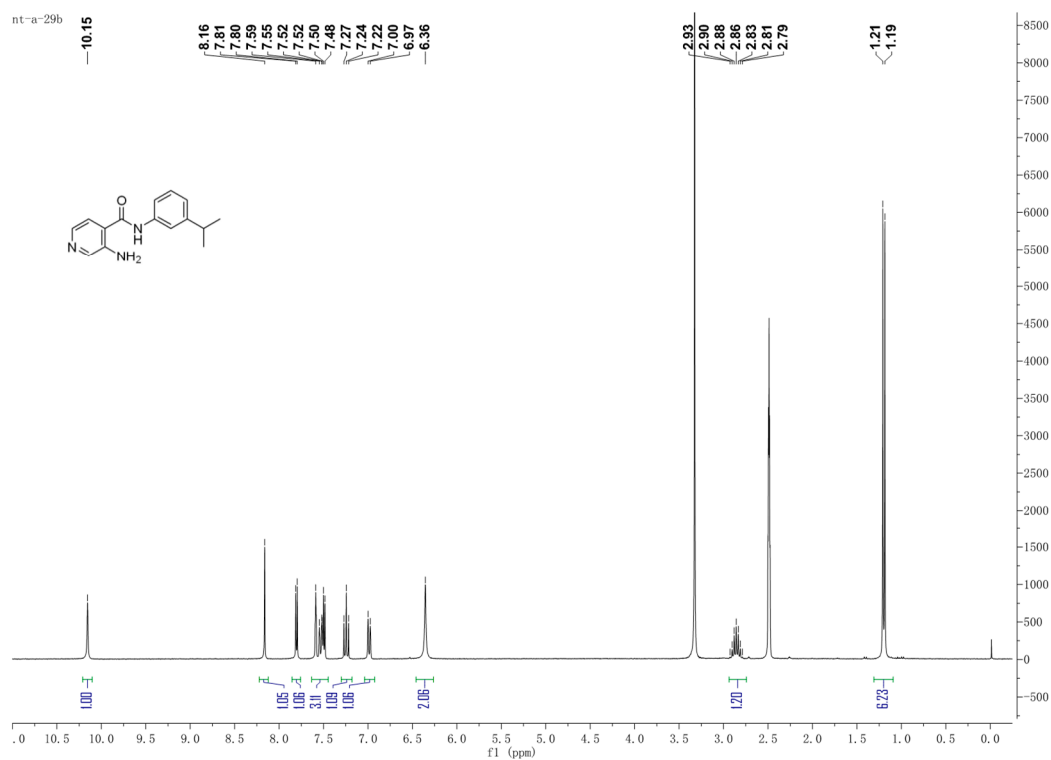
**<sup>1</sup>H NMR spectra of 16s**



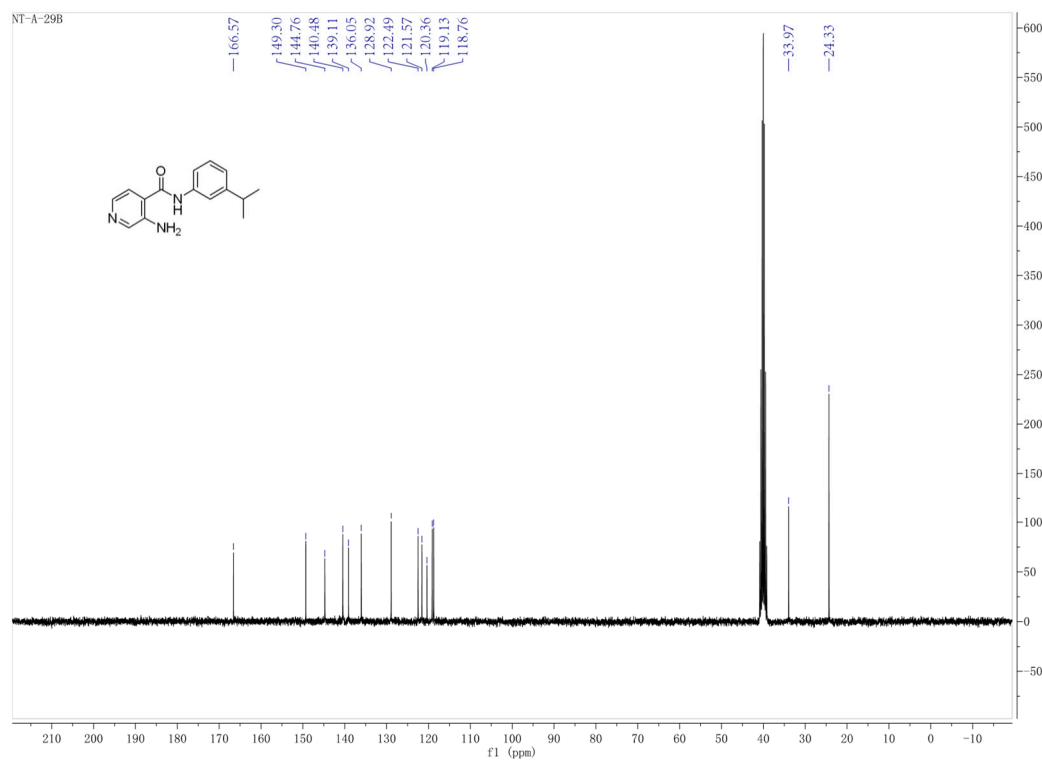
$^1\text{H}$  NMR spectra of 16t



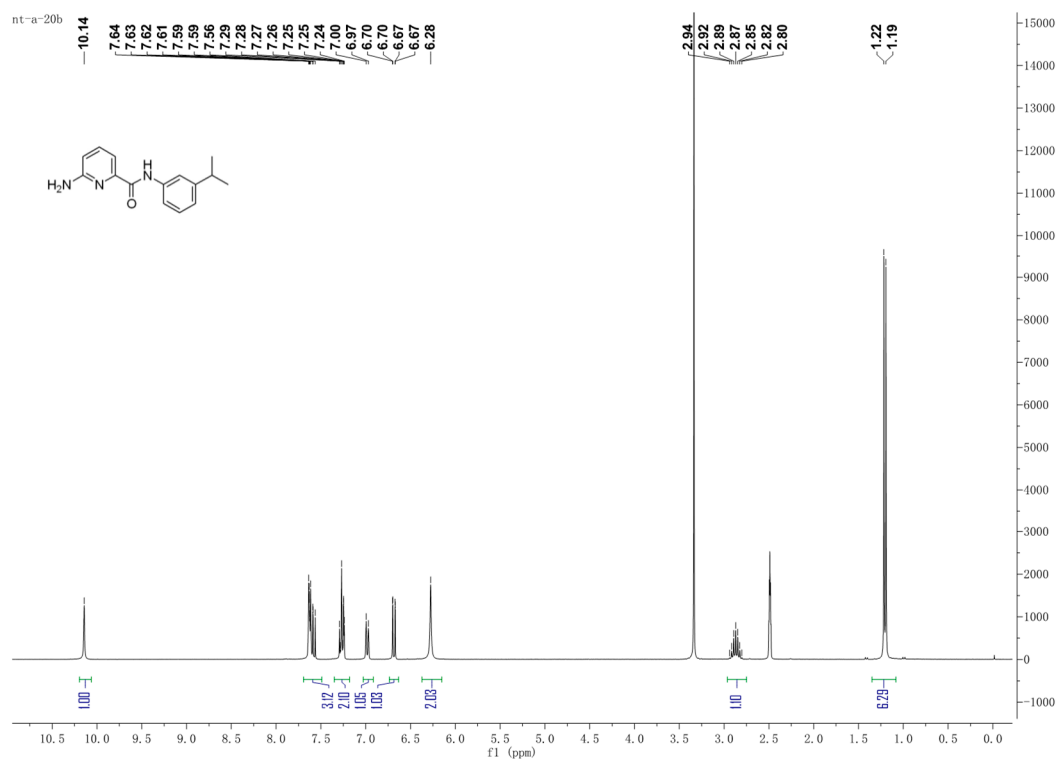
$^{13}\text{C}$  NMR spectra of 16t



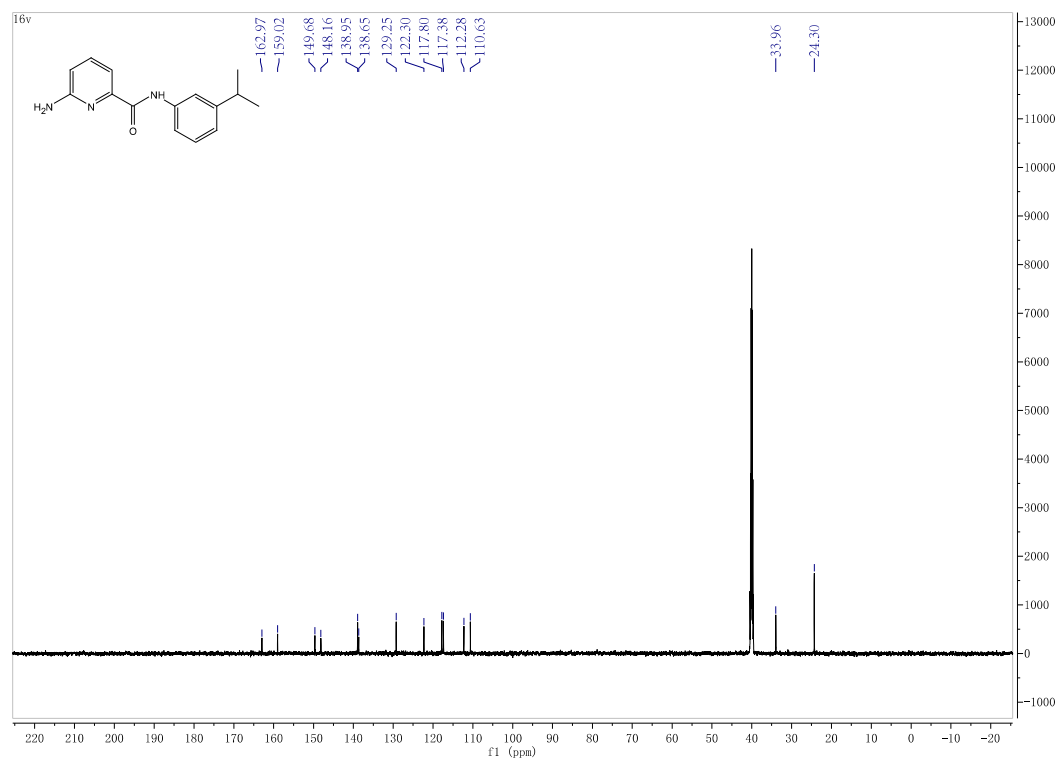
**<sup>1</sup>H NMR spectra of 16u**



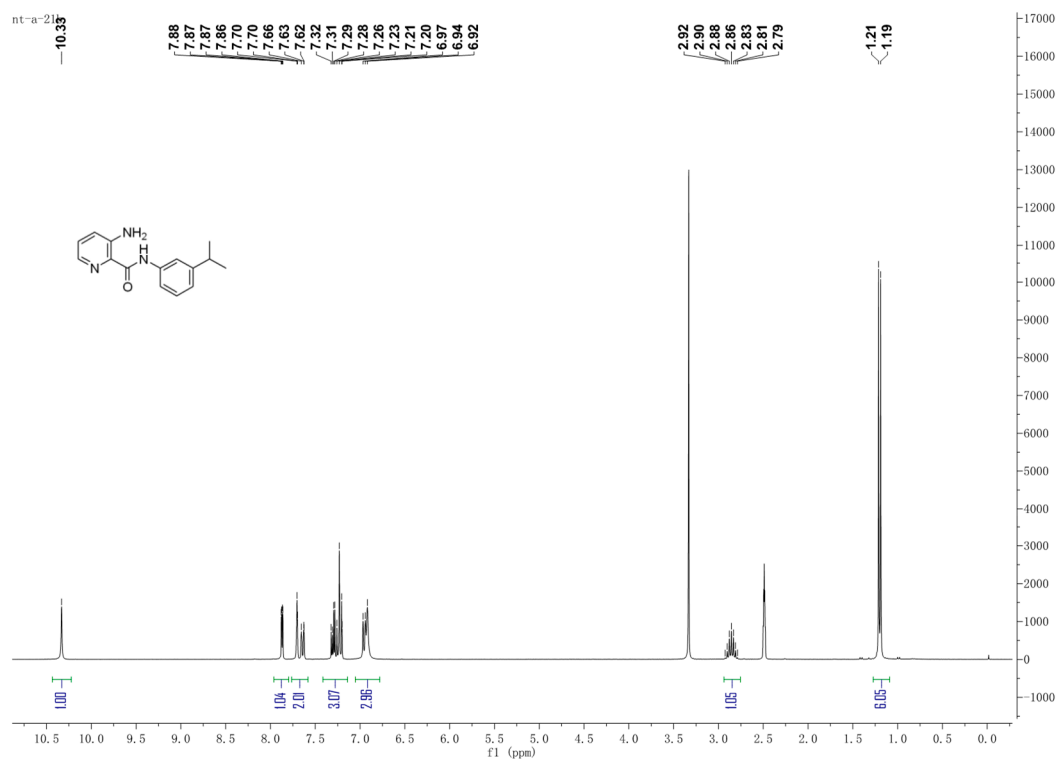
**<sup>13</sup>C NMR spectra of 16u**



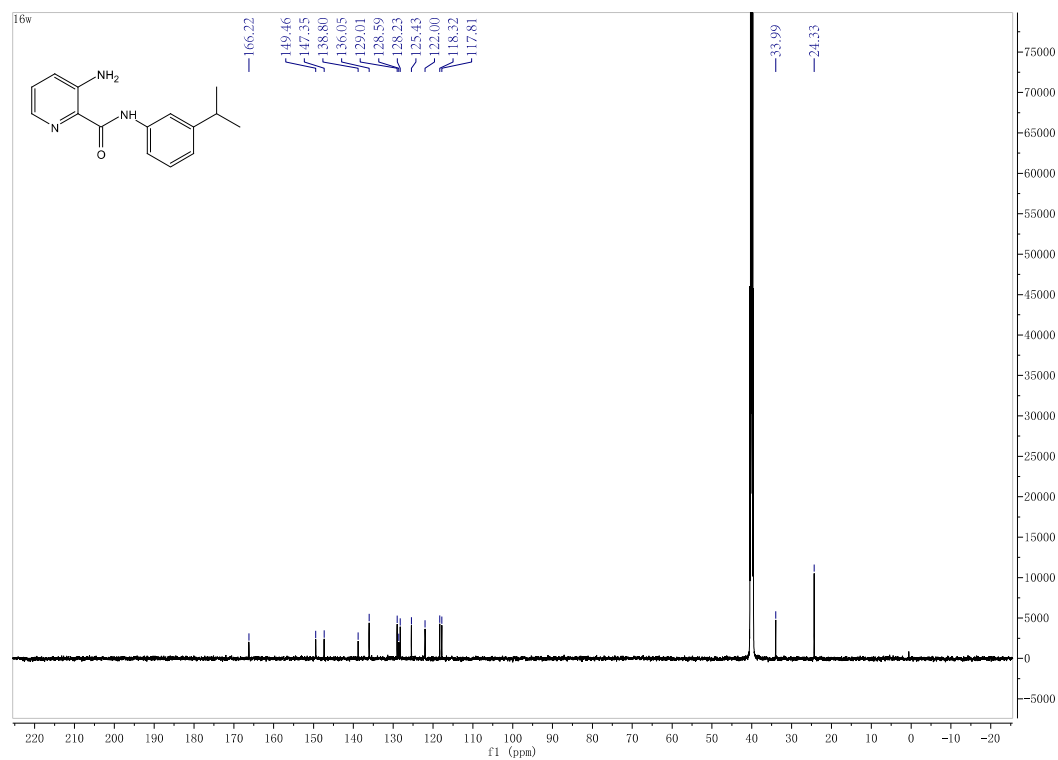
**<sup>1</sup>H NMR spectra of 16v**



**<sup>13</sup>C NMR spectra of 16v**

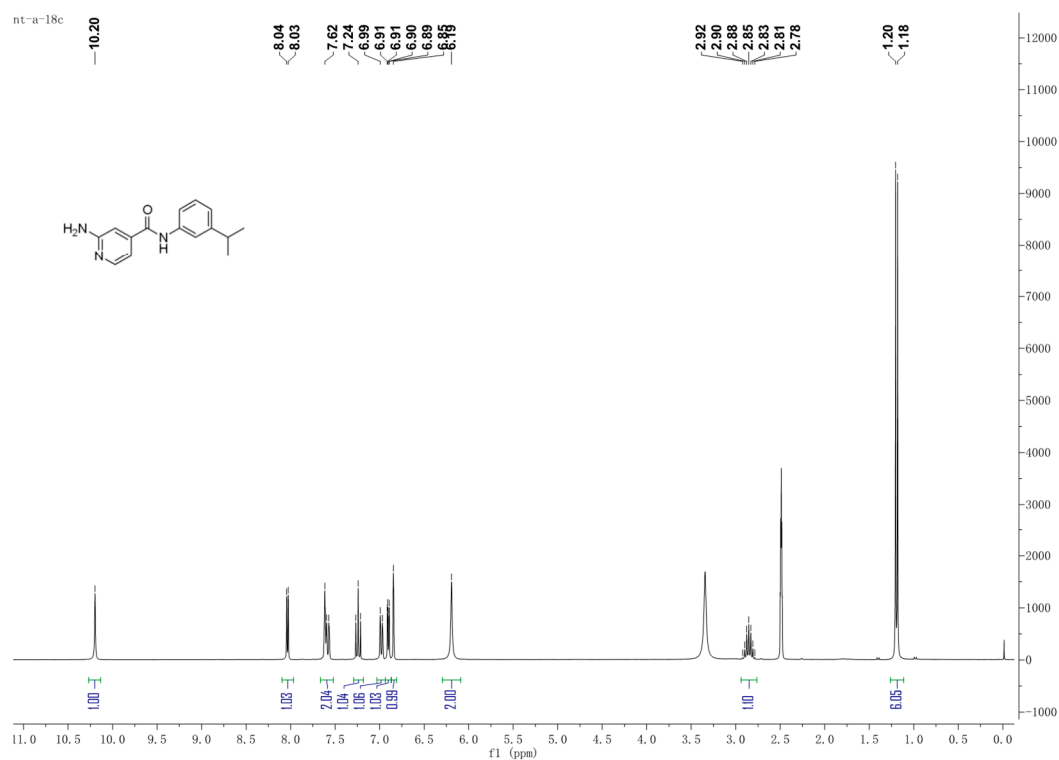


<sup>1</sup>H NMR spectra of 16w

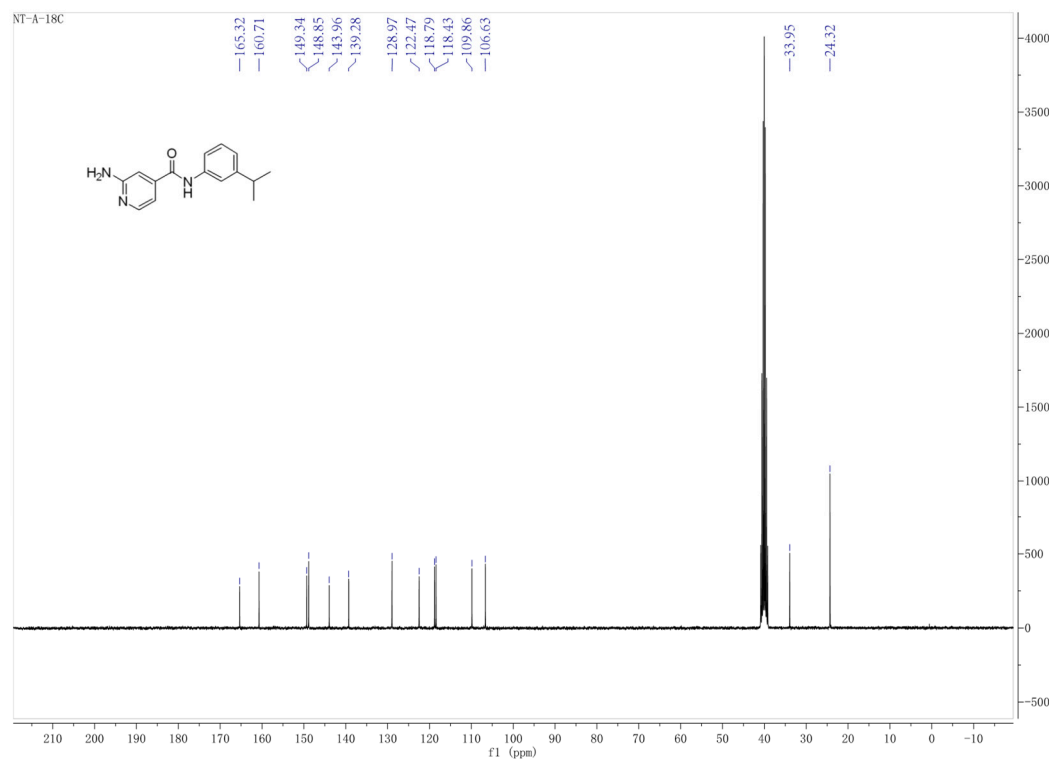


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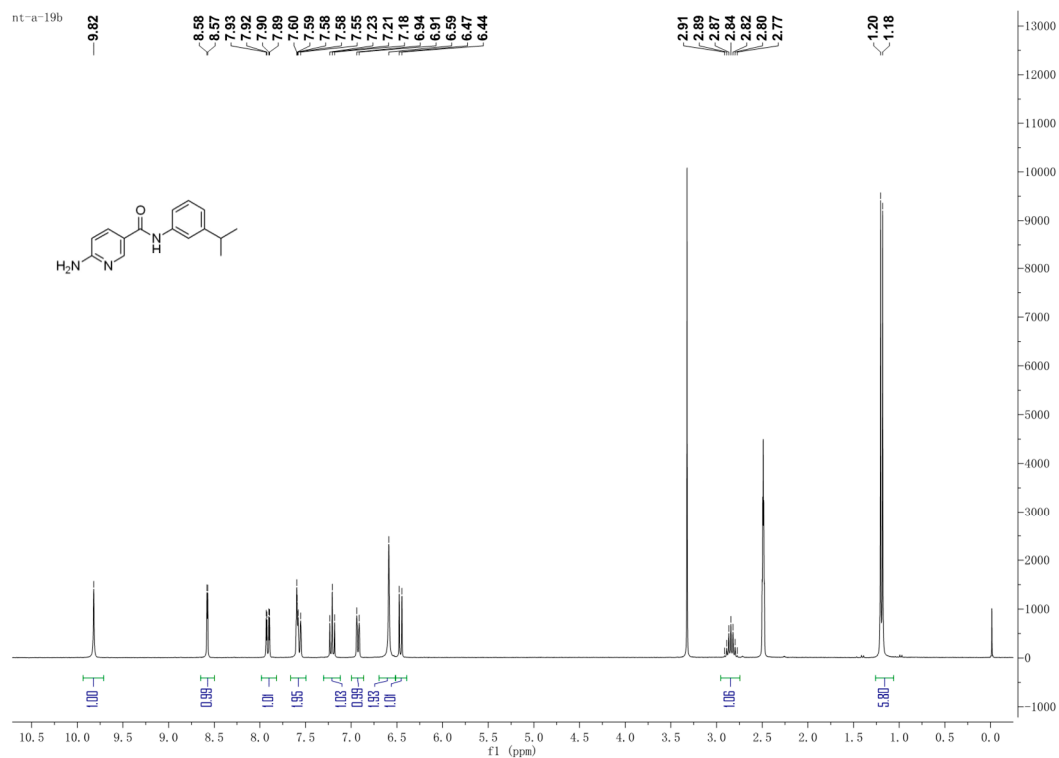




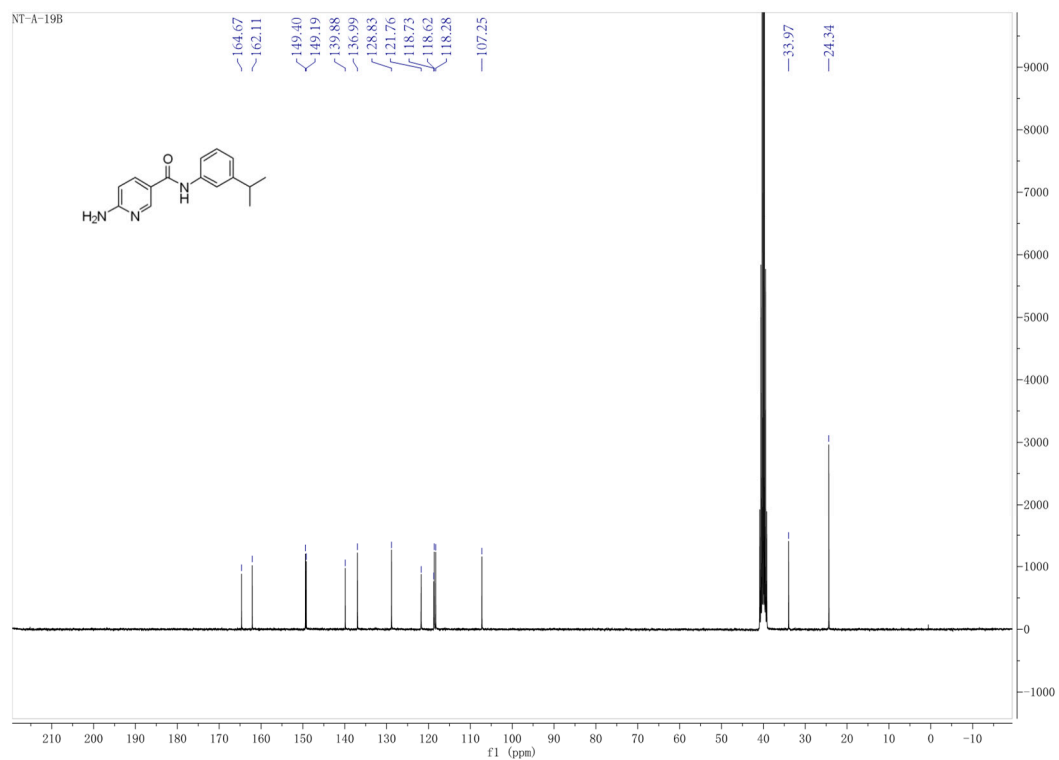
**<sup>1</sup>H NMR spectra of 16x**



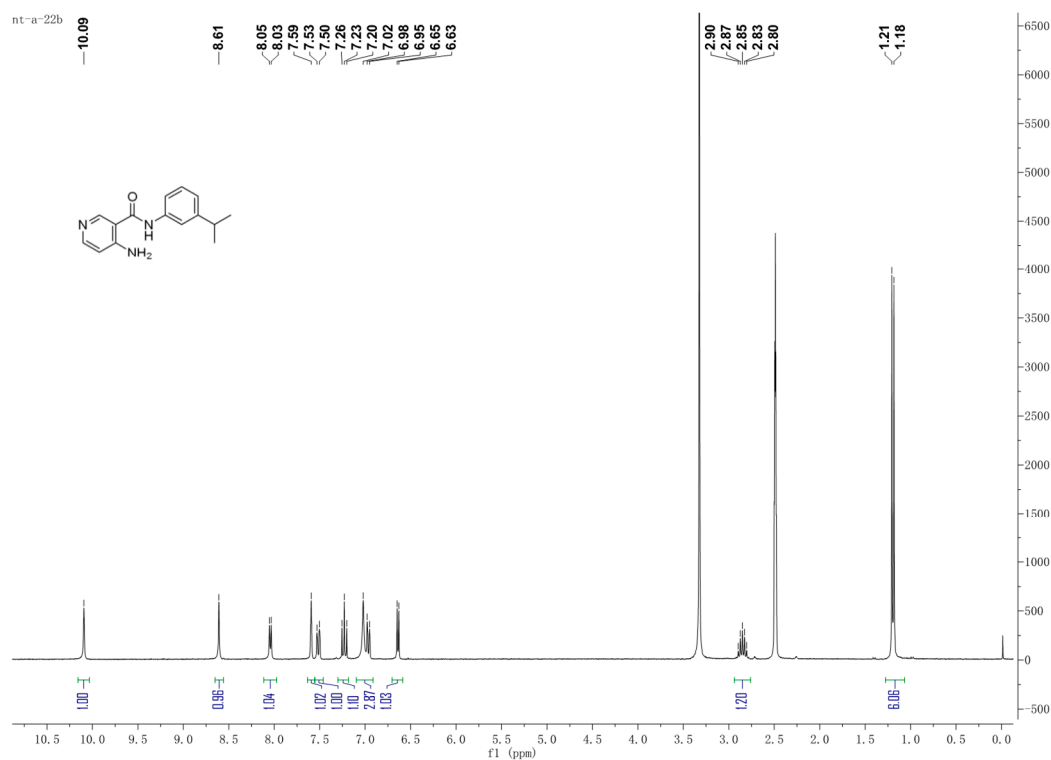
**<sup>13</sup>C NMR spectra of 16x**



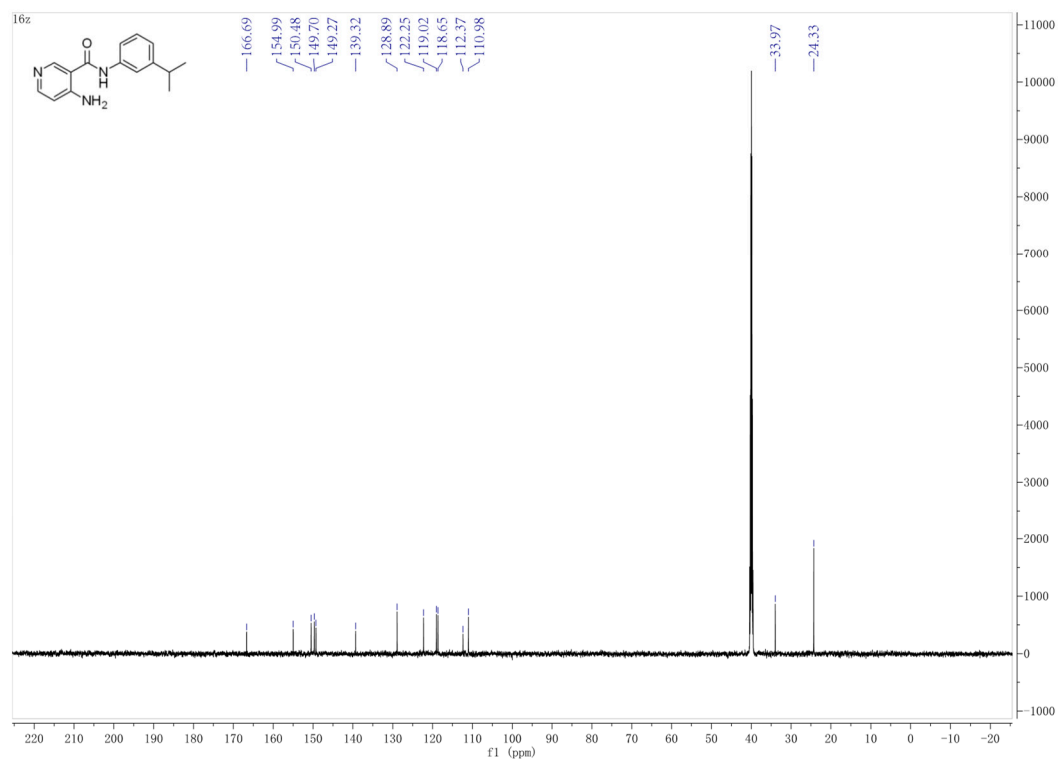
**<sup>1</sup>H NMR spectra of 16y**



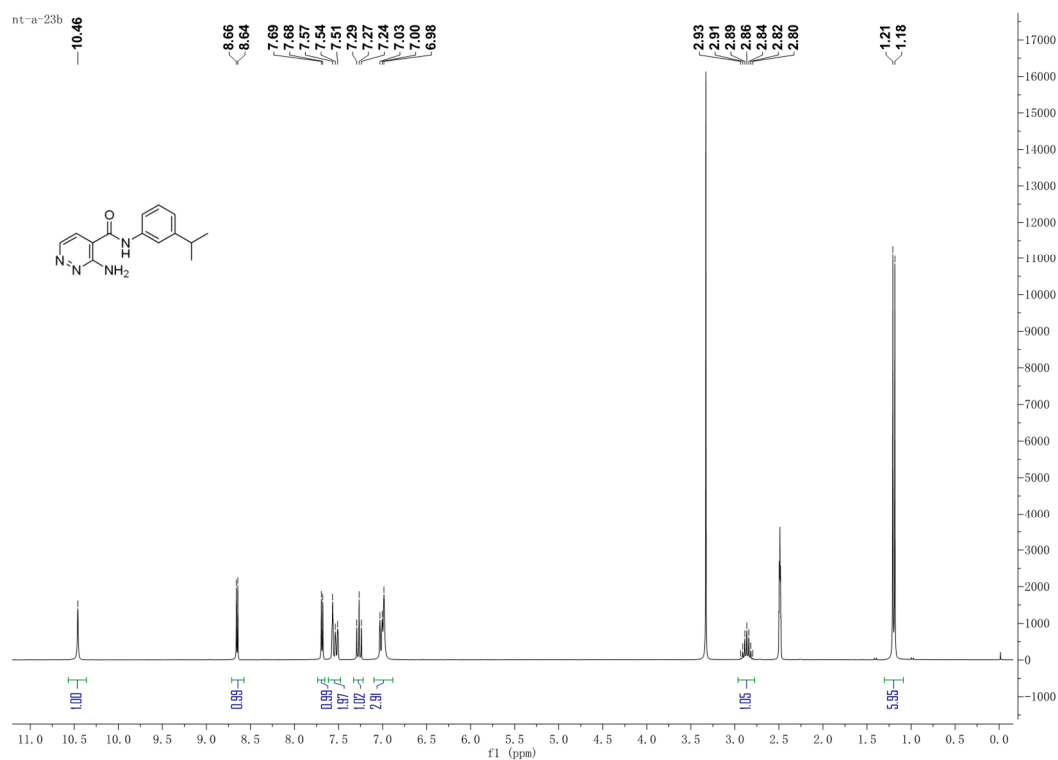
**<sup>13</sup>C NMR spectra of 16y**



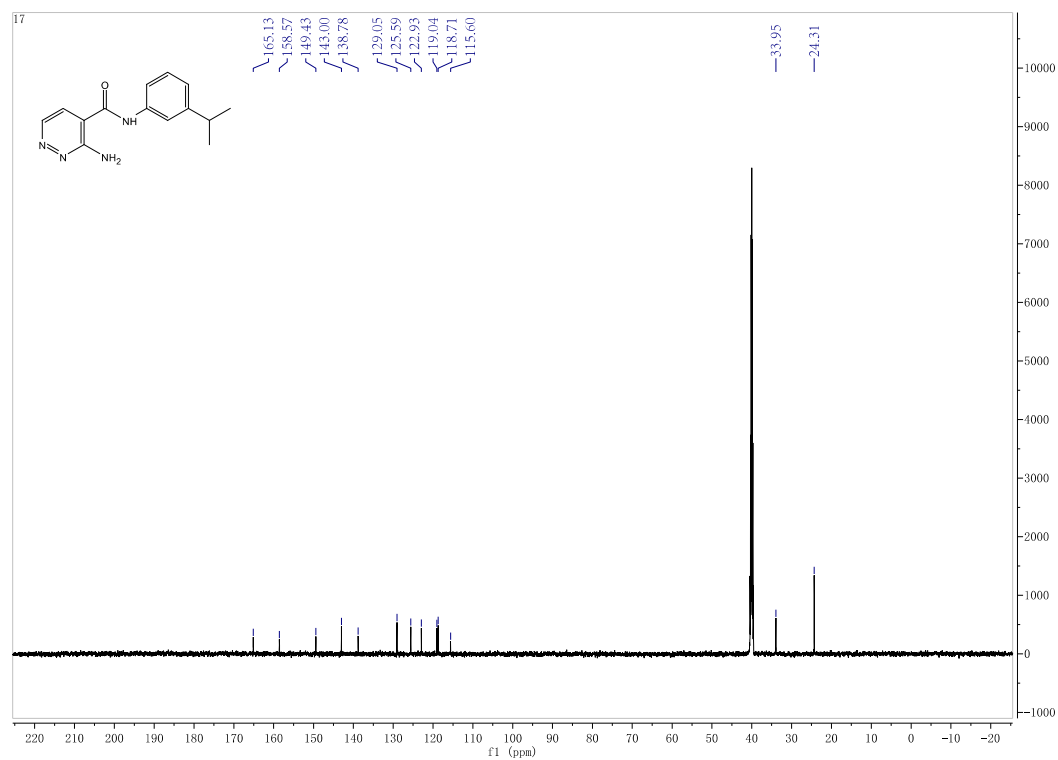
**<sup>1</sup>H NMR spectra of 16z**



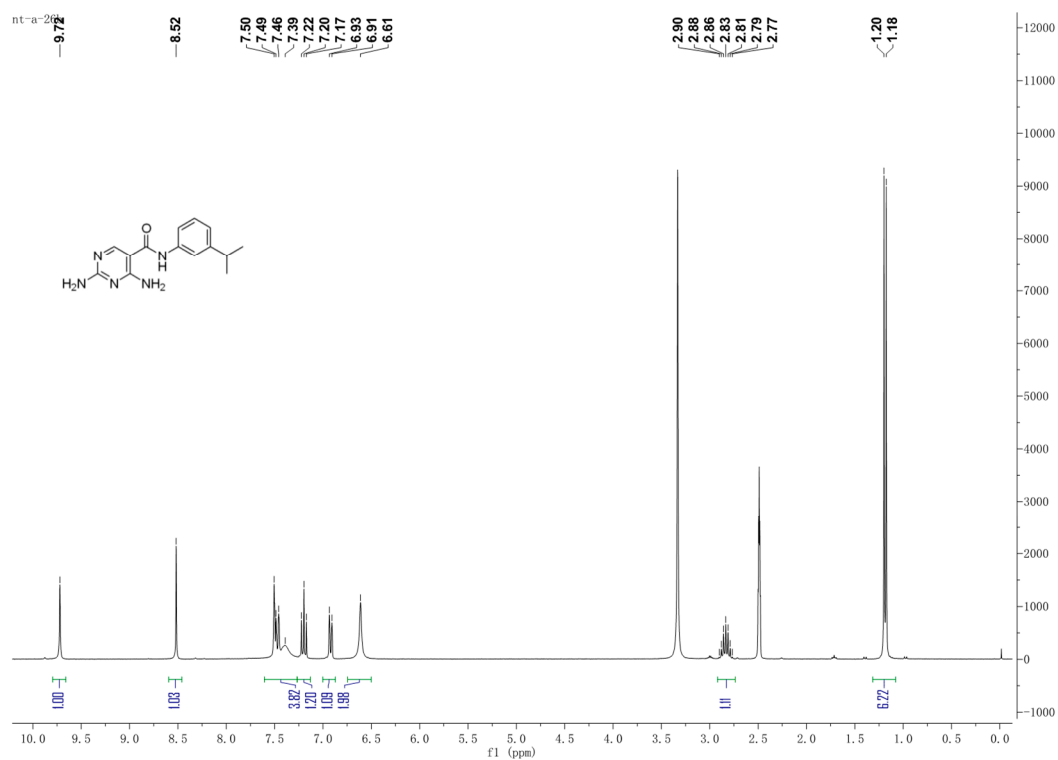
**<sup>13</sup>C NMR spectra of 16z**



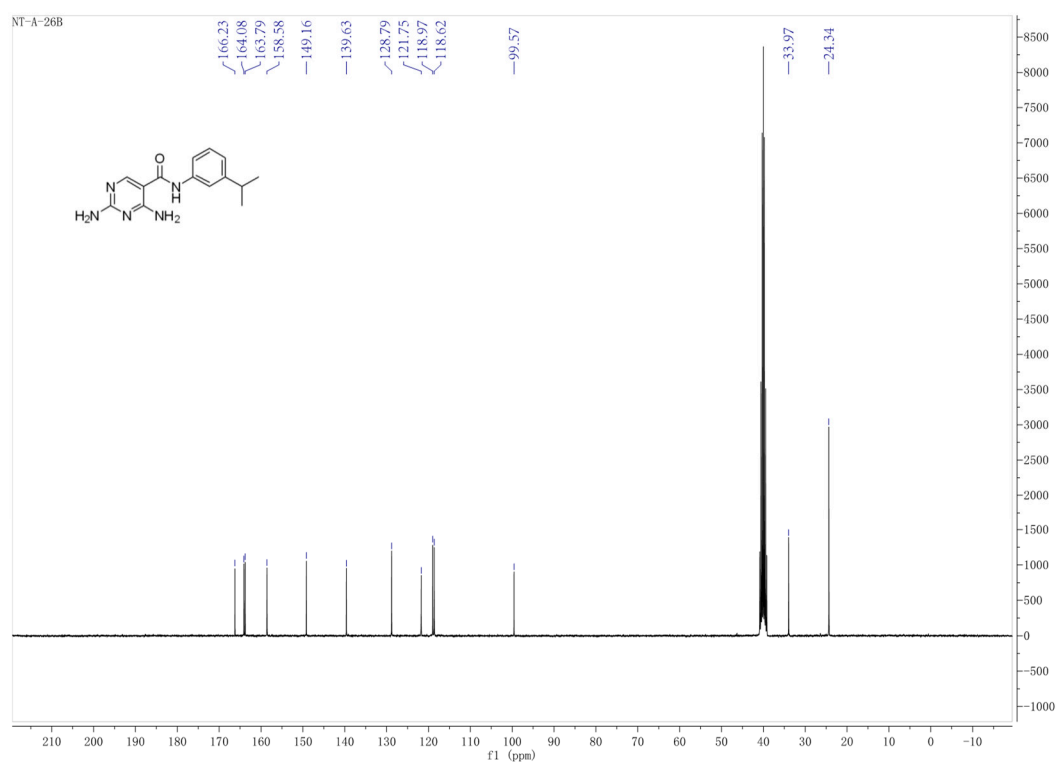
**<sup>1</sup>H NMR spectra of 17**



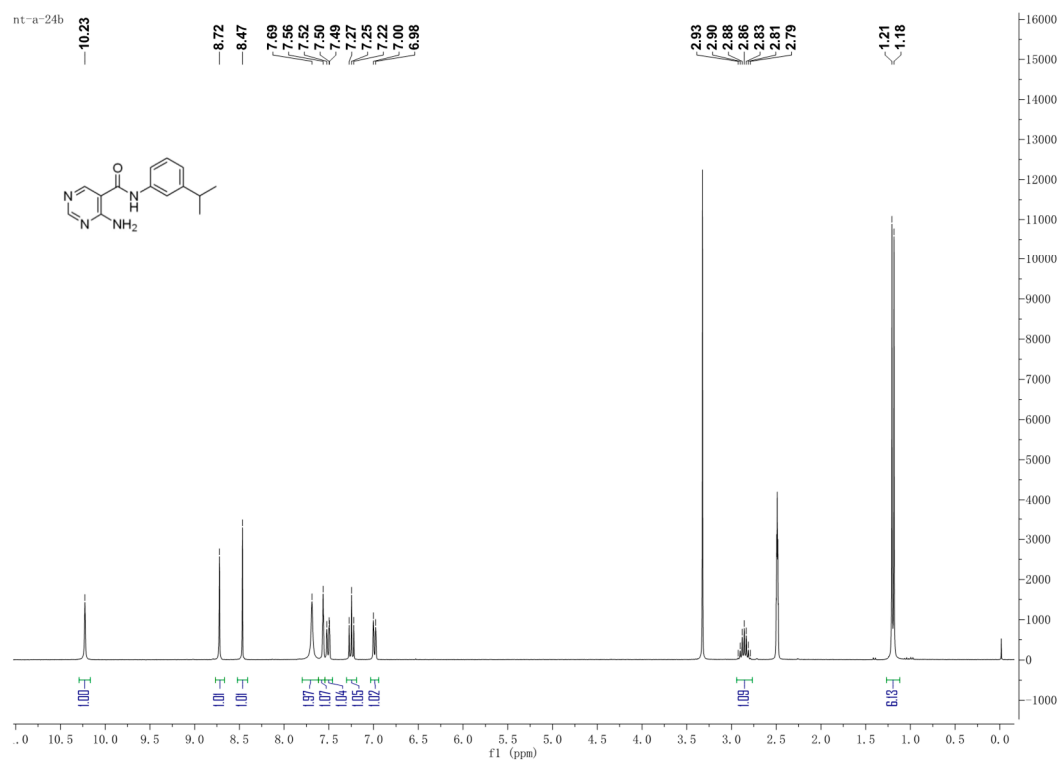
**<sup>13</sup>C NMR spectra of 17**



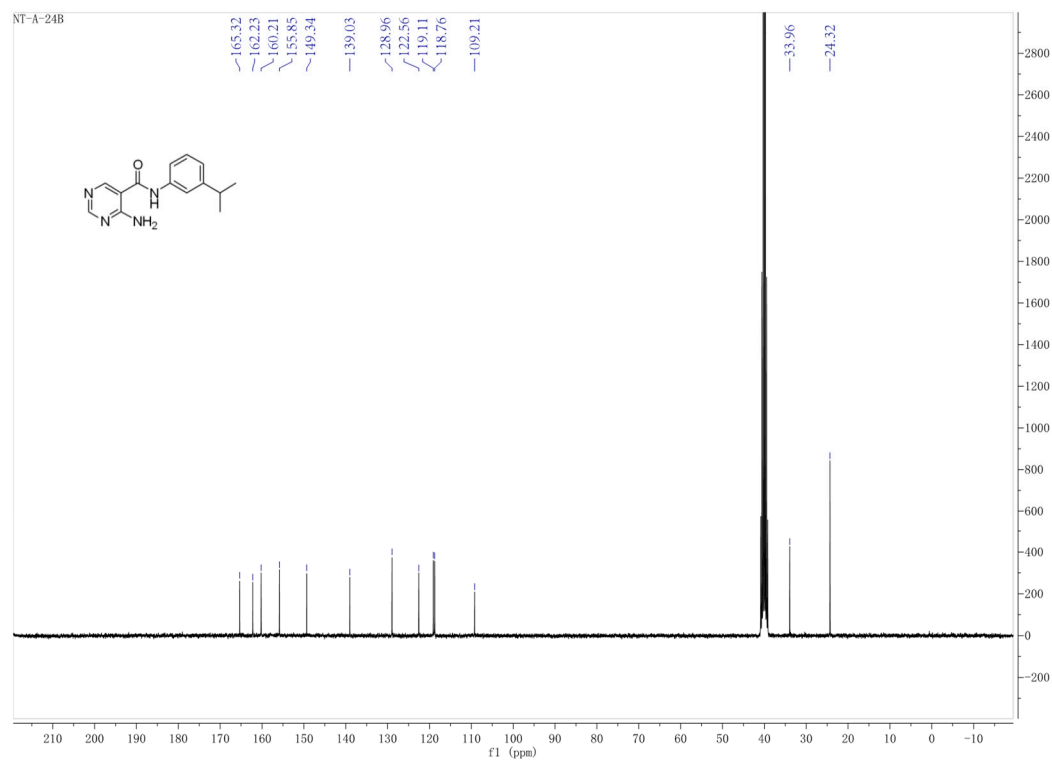
**<sup>1</sup>H NMR spectra of 18a**



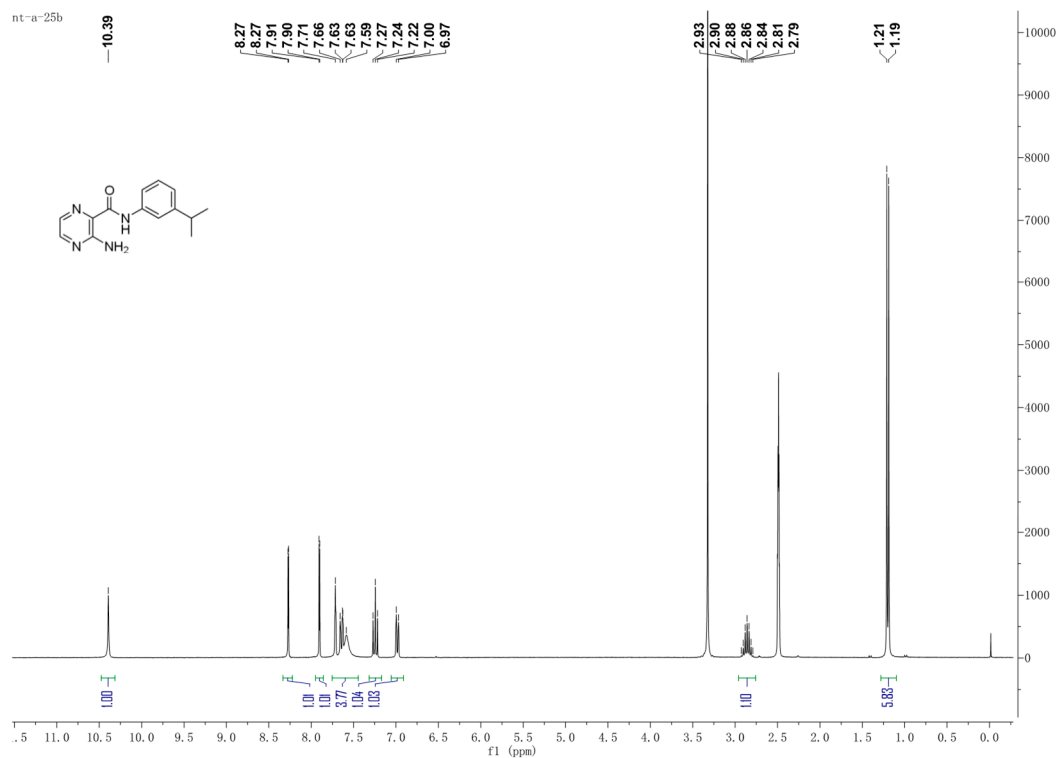
**<sup>13</sup>C NMR spectra of 18a**



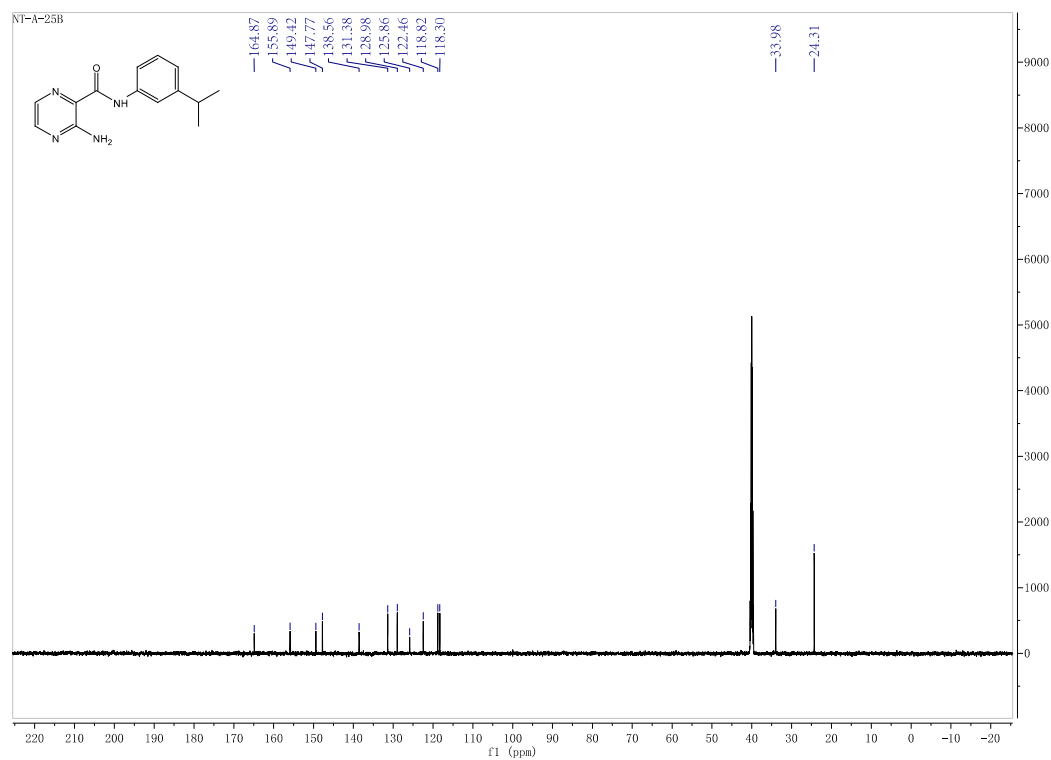
**<sup>1</sup>H NMR spectra of 18b**



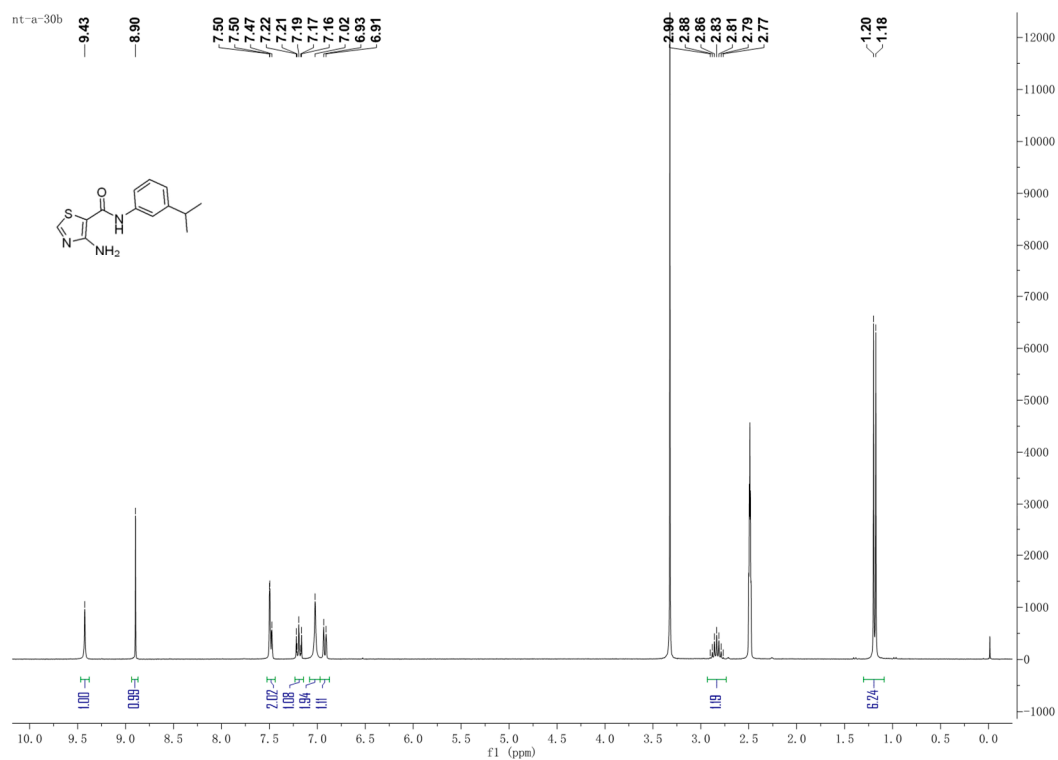
**<sup>13</sup>C NMR spectra of 18b**



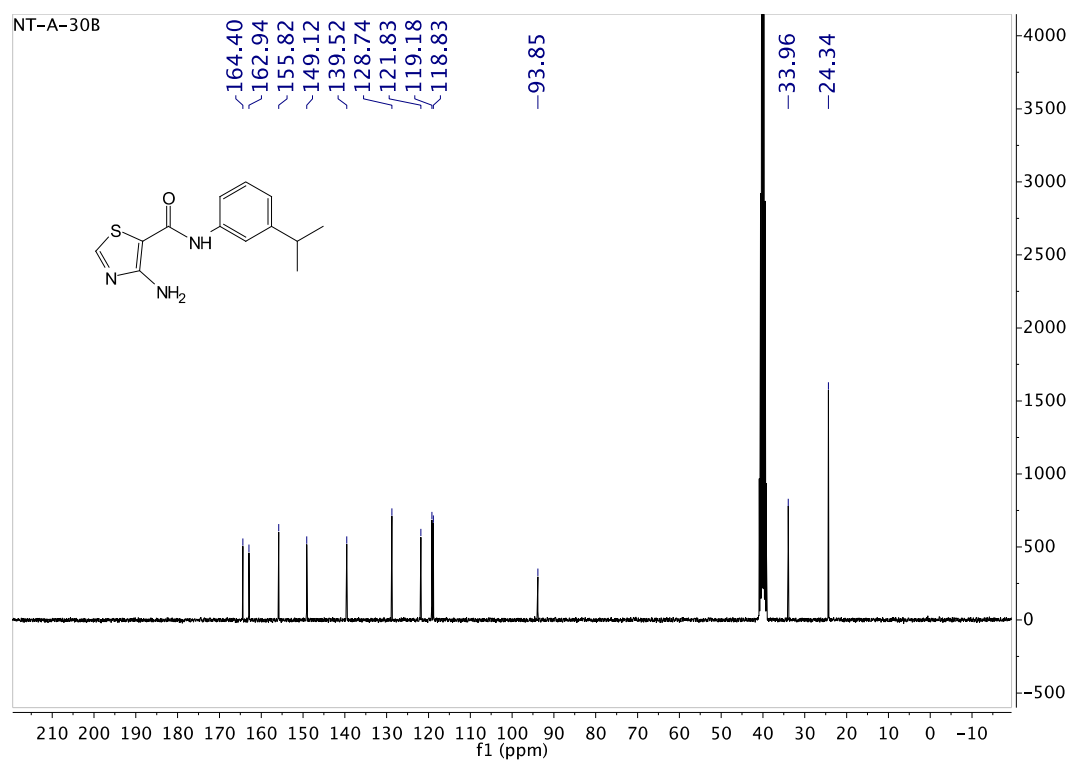
**<sup>1</sup>H NMR spectra of 19**



**<sup>13</sup>C NMR spectra of 19**

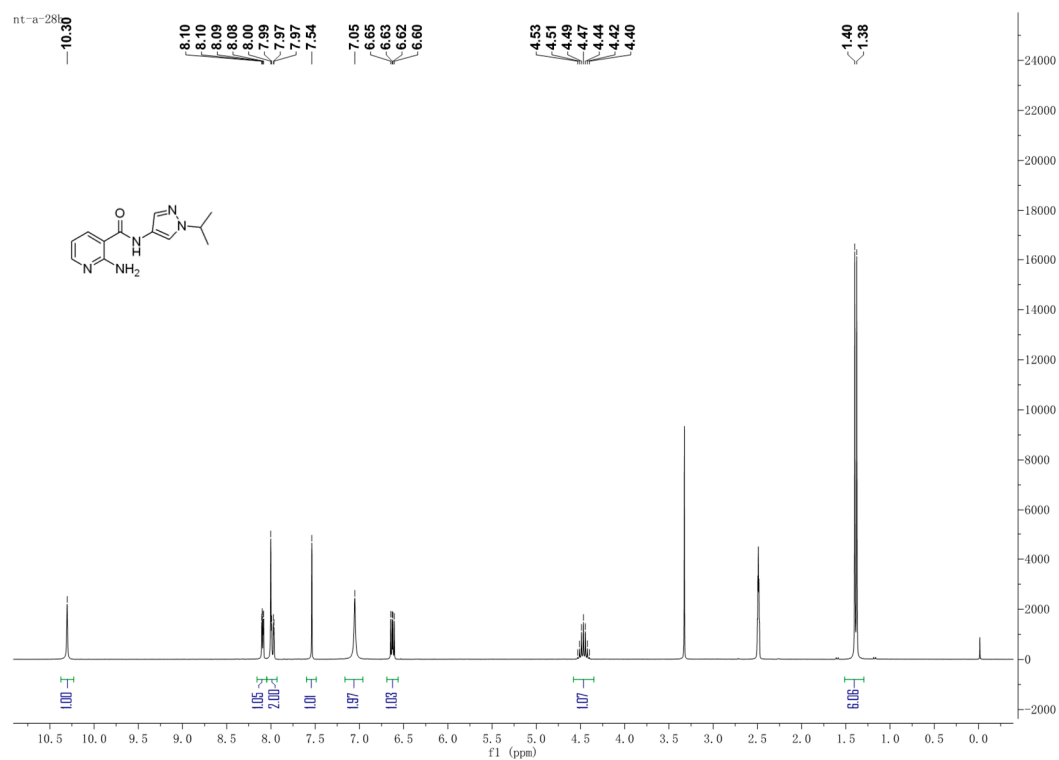


**<sup>1</sup>H NMR spectra of 20**

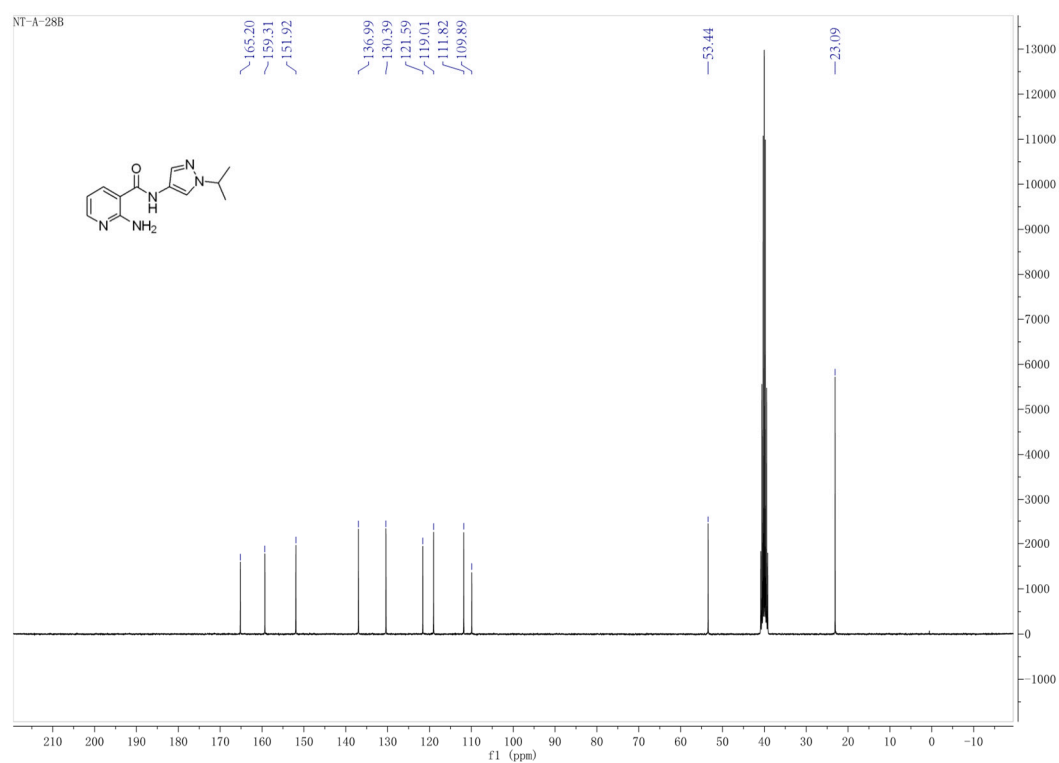


**<sup>13</sup>C NMR spectra of 20**

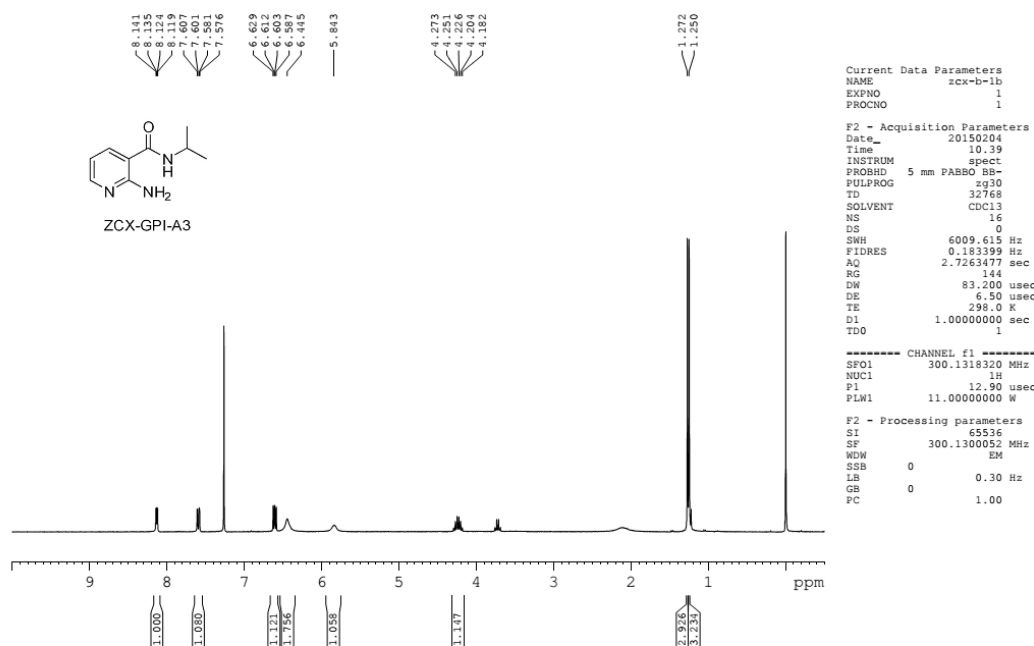




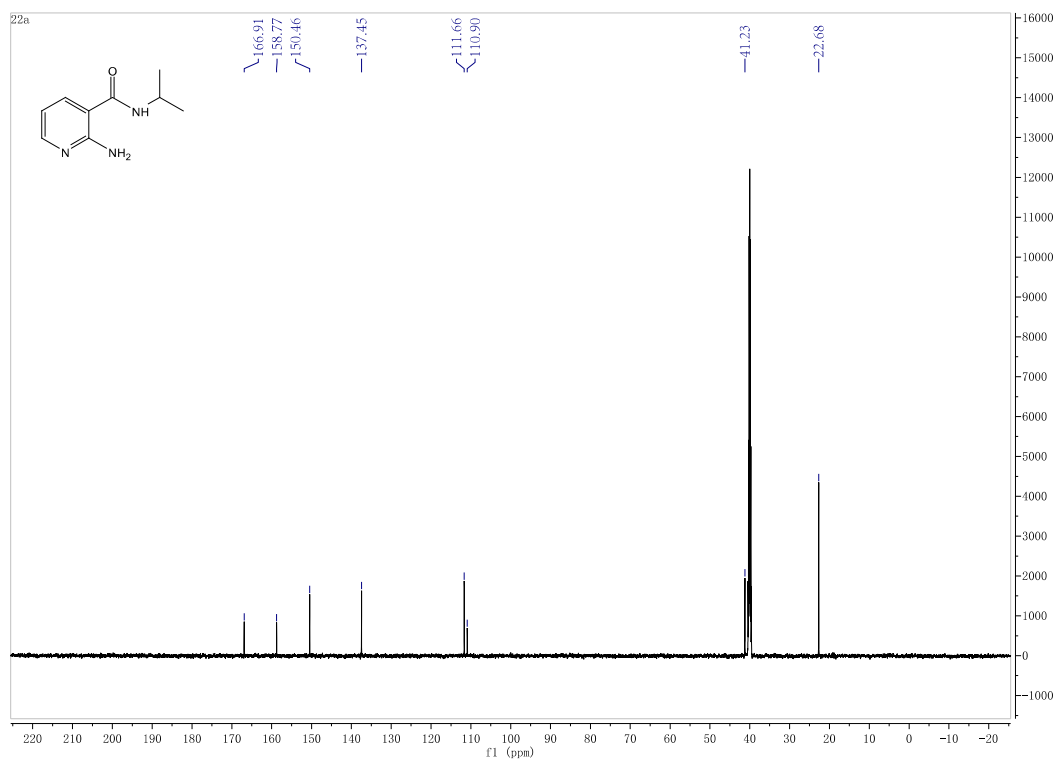
**<sup>1</sup>H NMR spectra of 21**



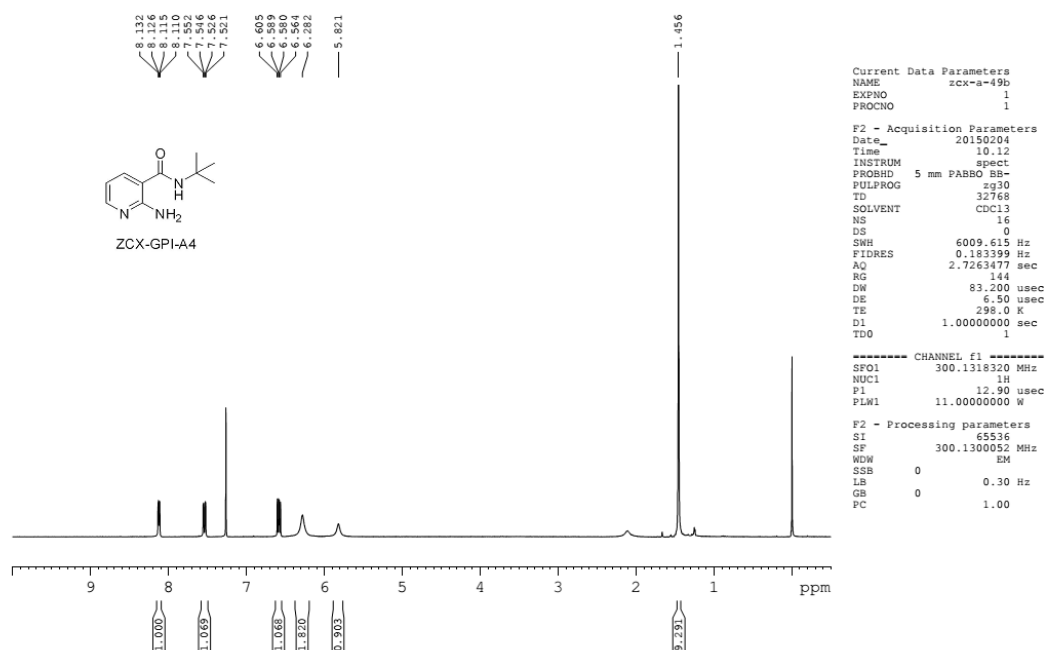
**<sup>13</sup>C NMR spectra of 21**



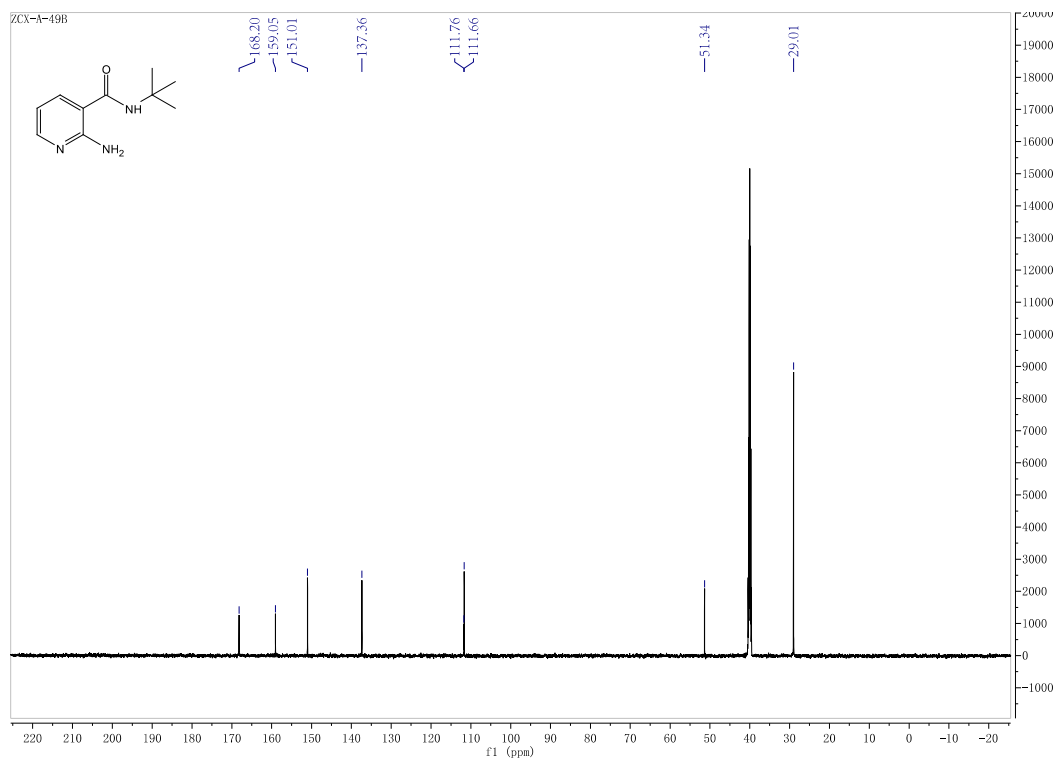
**<sup>1</sup>H NMR spectra of 22a**



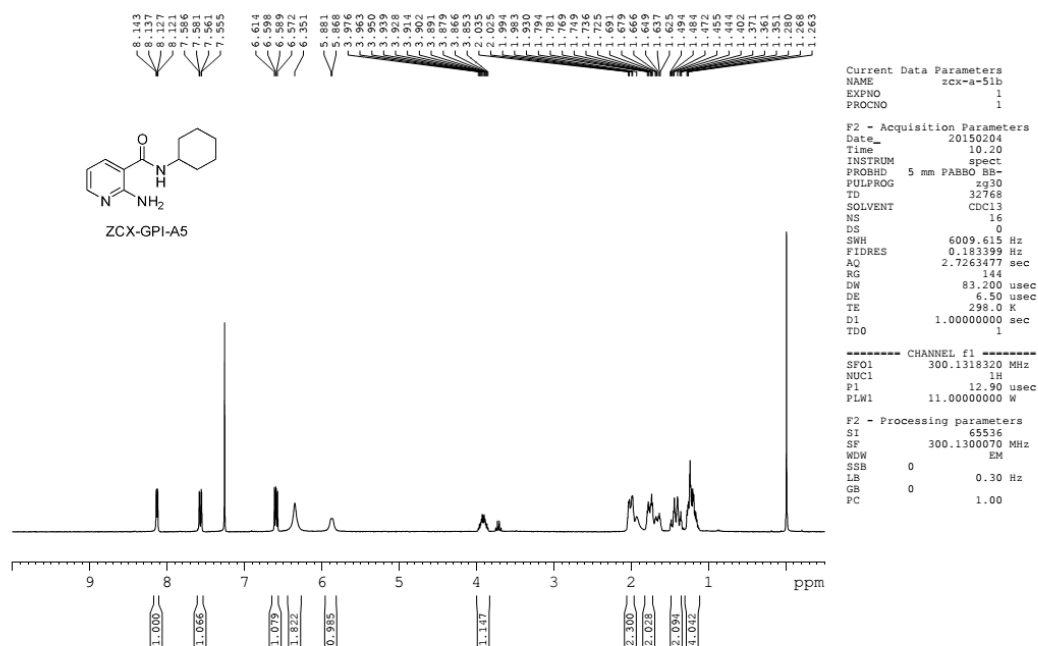
**<sup>13</sup>C NMR spectra of 22a**



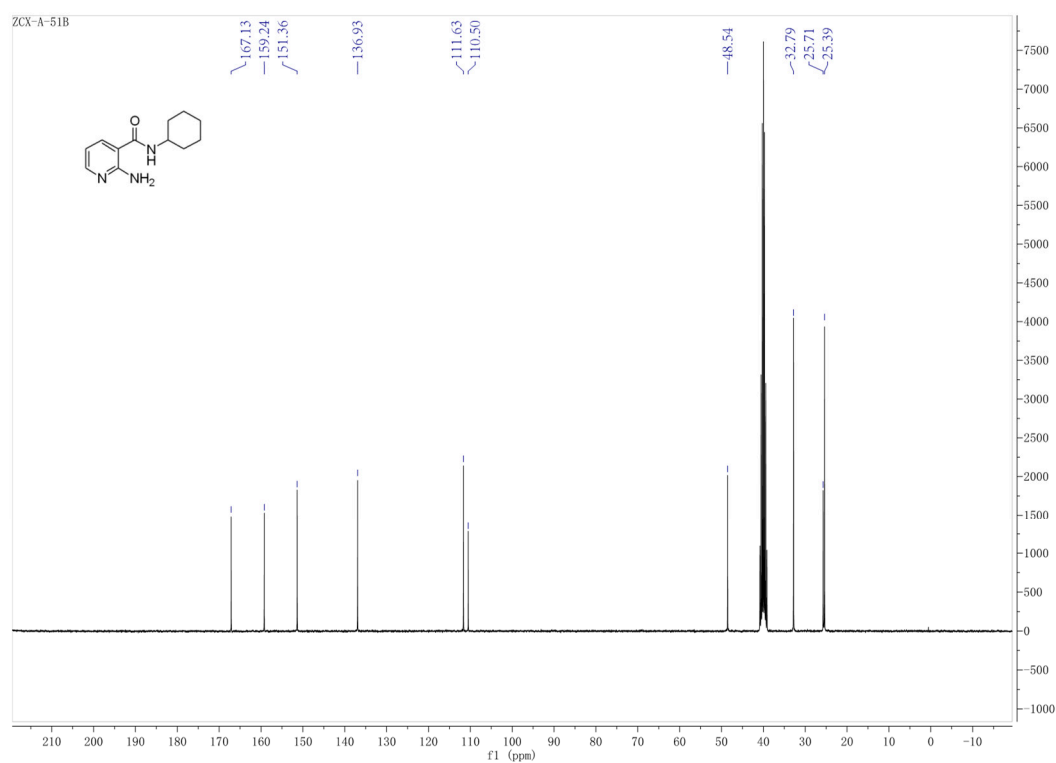
### <sup>1</sup>H NMR spectra of 22b



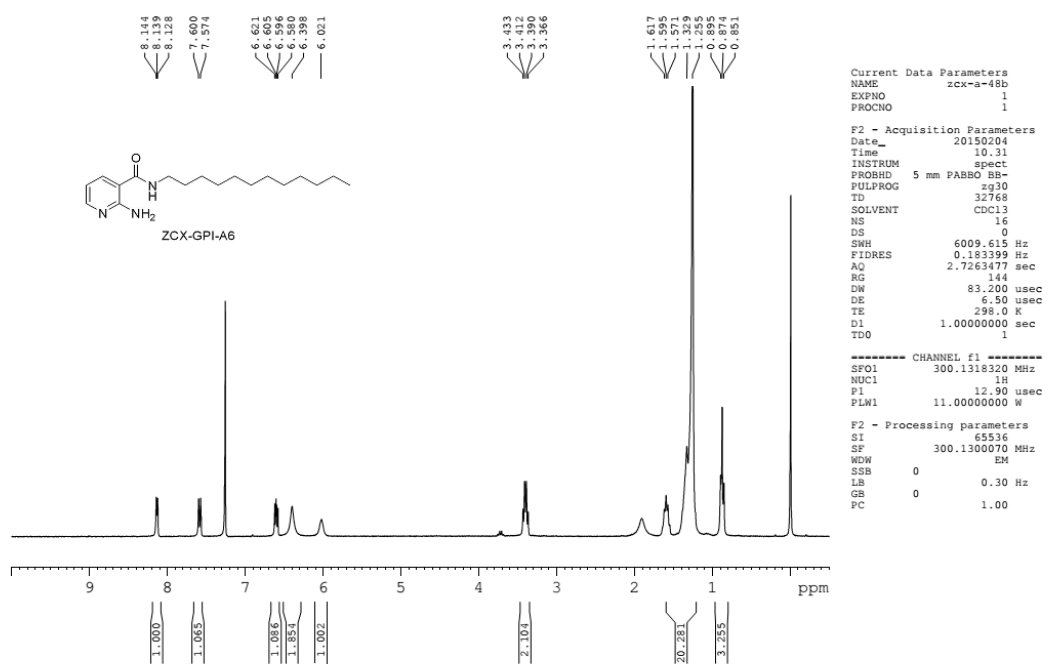
### <sup>13</sup>C NMR spectra of 22b



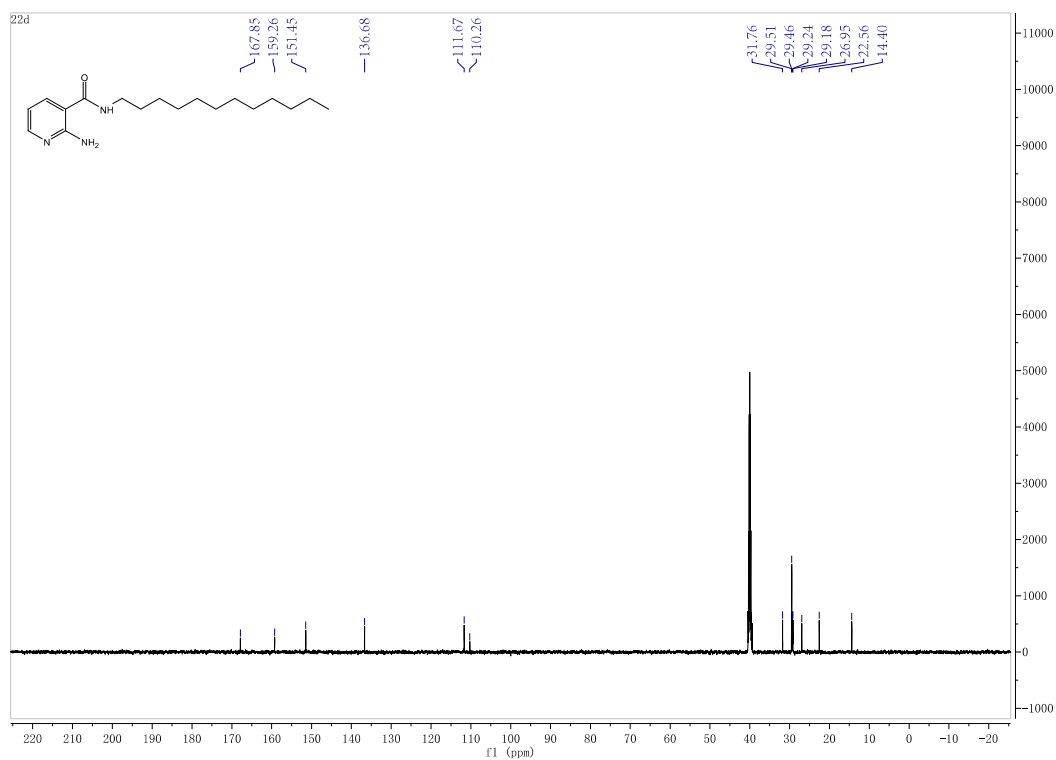
**<sup>1</sup>H NMR spectra of 22c**



**<sup>13</sup>C NMR spectra of 22c**



**$^1\text{H}$  NMR spectra of 22d**



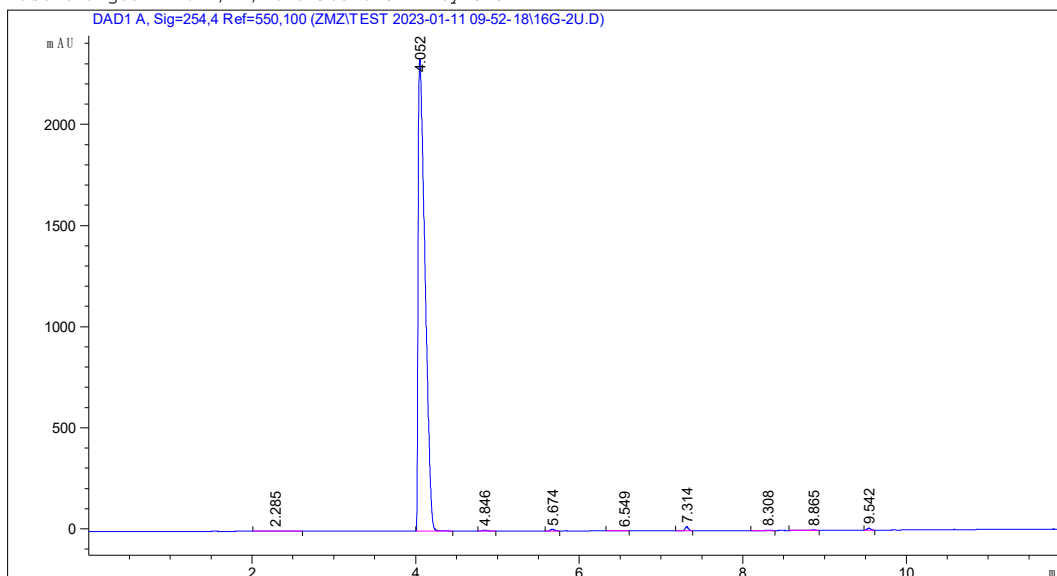
**$^{13}\text{C}$  NMR spectra of 22d**

# HPLC Spectra of Representative Compounds

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Acq. Instrument : 12601c                     Location  : Vial 41
Injection Date  : 1/11/2023 11:43:21 AM      Inj       :    1
                                           Inj Volume: 5.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 2.000 µl
Method          : C:\CHEM32\1\DATA\ZMZ\TEST 2023-01-11 09-52-18\TEST NTJH.M (Sequence Method)
Last changed    : 1/11/2023 9:52:18 AM by SYSTEM
=====
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## Area Percent Report

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Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
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Signal 1: DAD1 A, Sig=254,4 Ref=550,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.285	BB	0.1964	31.20372	1.89748	0.2260
2	4.052	BB	0.0910	1.36156e4	2334.45874	98.6292
3	4.846	BB	0.0629	16.27699	3.96648	0.1179
4	5.674	BV	0.0497	28.58175	8.85165	0.2070
5	6.549	BV	0.0664	7.33513	1.54507	0.0531
6	7.314	BV	0.0414	55.62617	20.65764	0.4029
7	8.308	BB	0.0623	8.81839	1.98709	0.0639
8	8.865	BB	0.0692	13.28968	2.68589	0.0963
9	9.542	BB	0.0439	28.09934	9.96804	0.2035

## HPLC spectra of 16g

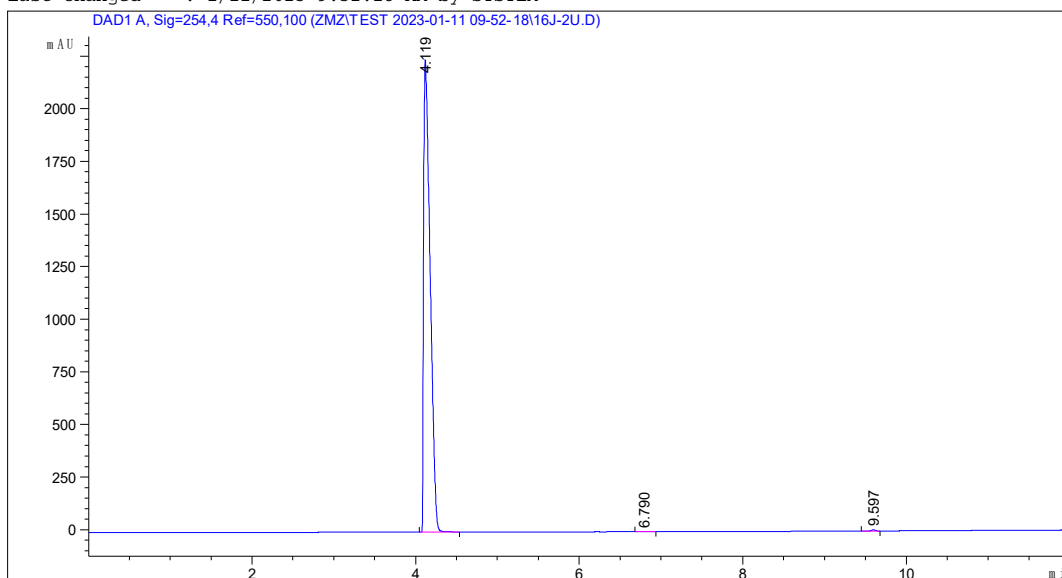
Sample Name: 16j-2u

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Injection Date  : 1/11/2023 12:24:45 PM      Inj       :    1
                                           Inj Volume: 5.000 µl

Different Inj Volume from Sample Entry! Actual Inj Volume : 2.000 µl
Acq. Method     : C:\CHEM32\1\DATA\ZMZ\TEST 2023-01-11 09-52-18\TEST NTJH.M
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                          Area Percent Report
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Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

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Signal 1: DAD1 A, Sig=254,4 Ref=550,100

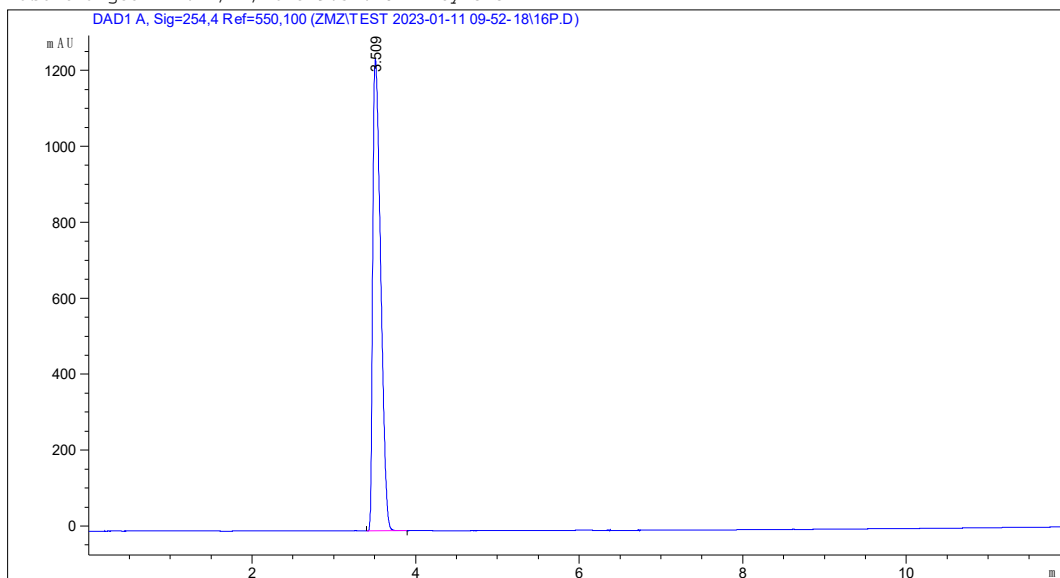
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.119	BV	0.0841	1.23168e4	2243.02368	99.8032
2	6.790	BB	0.0612	5.75675	1.27470	0.0466
3	9.597	BV	0.0453	18.52760	6.20405	0.1501

```
Totals :                      1.23410e4  2250.50243
```

**HPLC spectra of 16j**

Sample Name: 16p

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    6
Acq. Instrument : 12601c                     Location  : Vial 45
Injection Date  : 1/11/2023 11:02:04 AM      Inj       :    1
                                           Inj Volume: 5.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 2.000 µl
Method         : C:\CHEM32\1\DATA\ZMZ\TEST 2023-01-11 09-52-18\TEST NTJH.M (Sequence Method)
Last changed    : 1/11/2023 9:52:18 AM by SYSTEM
=====
```



```
=====
                        Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=254,4 Ref=550,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.509	BB	0.1074	8352.11426	1243.42444	100.0000

```
Totals :                      8352.11426 1243.42444
```

```
=====
*** End of Report ***
=====
```

## HPLC spectra of 16p

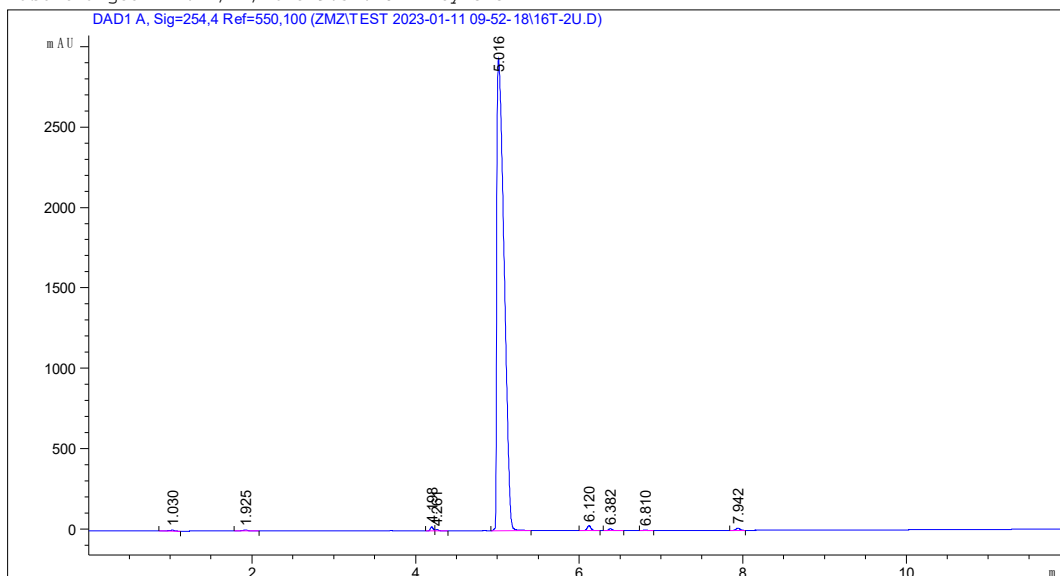


Sample Name: 16t-2u

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :   11
Acq. Instrument : 12601c                     Location  : Vial 43
Injection Date  : 1/11/2023 12:11:00 PM      Inj       :    1
                                           Inj Volume: 5.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 2.000 µl
Method         : C:\CHEM32\1\DATA\ZMZ\TEST 2023-01-11 09-52-18\TEST NTJH.M (Sequence Method)
Last changed    : 1/11/2023 9:52:18 AM by SYSTEM
=====

```



```

=====
                        Area Percent Report
=====

```

```

Sorted By           :      Signal
Multiplier          :      1.0000
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

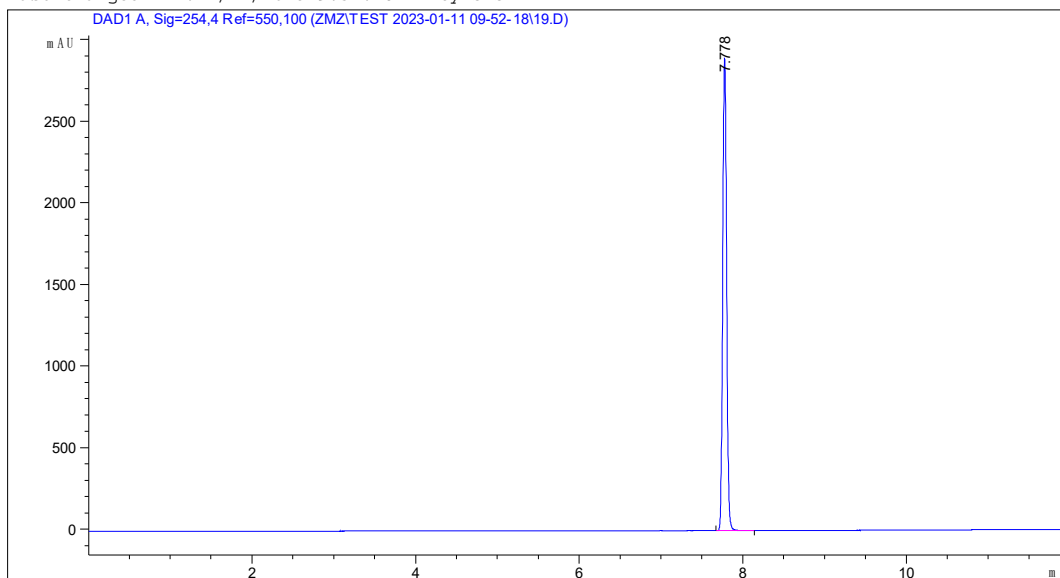
Signal 1: DAD1 A, Sig=254,4 Ref=550,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.030	BB	0.0534	29.00068	7.28464	0.1583
2	1.925	BB	0.0601	29.14332	6.85114	0.1591
3	4.198	BV	0.0347	55.14526	24.55021	0.3010
4	4.261	VB	0.0359	18.40388	7.68926	0.1005
5	5.016	BV	0.0966	1.80087e4	2935.12622	98.3058
6	6.120	BB	0.0468	91.93481	30.36506	0.5019
7	6.382	BB	0.0442	31.55243	10.92328	0.1722
8	6.810	BB	0.0458	12.31413	4.19324	0.0672
9	7.942	BB	0.0474	42.86133	14.12904	0.2340

## HPLC spectra of 16t

Data File C:\CHEM32\1\DATA\ZMZ\TEST 2023-01-11 09-52-18\19.D  
Sample Name: 19

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    7
Acq. Instrument : 12601c                     Location  : Vial 46
Injection Date  : 1/11/2023 11:15:49 AM      Inj       :    1
                                           Inj Volume: 5.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 2.000 µl
Method         : C:\CHEM32\1\DATA\ZMZ\TEST 2023-01-11 09-52-18\TEST NTJH.M (Sequence Method)
Last changed    : 1/11/2023 9:52:18 AM by SYSTEM
=====
```



```
=====
                          Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=254,4 Ref=550,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.778	BV	0.0524	9641.09277	2891.20068	100.0000

Totals :                      9641.09277 2891.20068

```
=====
*** End of Report ***
=====
```

## HPLC spectra of 19