Supplementary Material

Synthesis of 2-aroyl-(4 or 5)-aryl-1*H*-imidazoles and 2-hydroxy-3,6-diaryl-pyrazines via a cascade process

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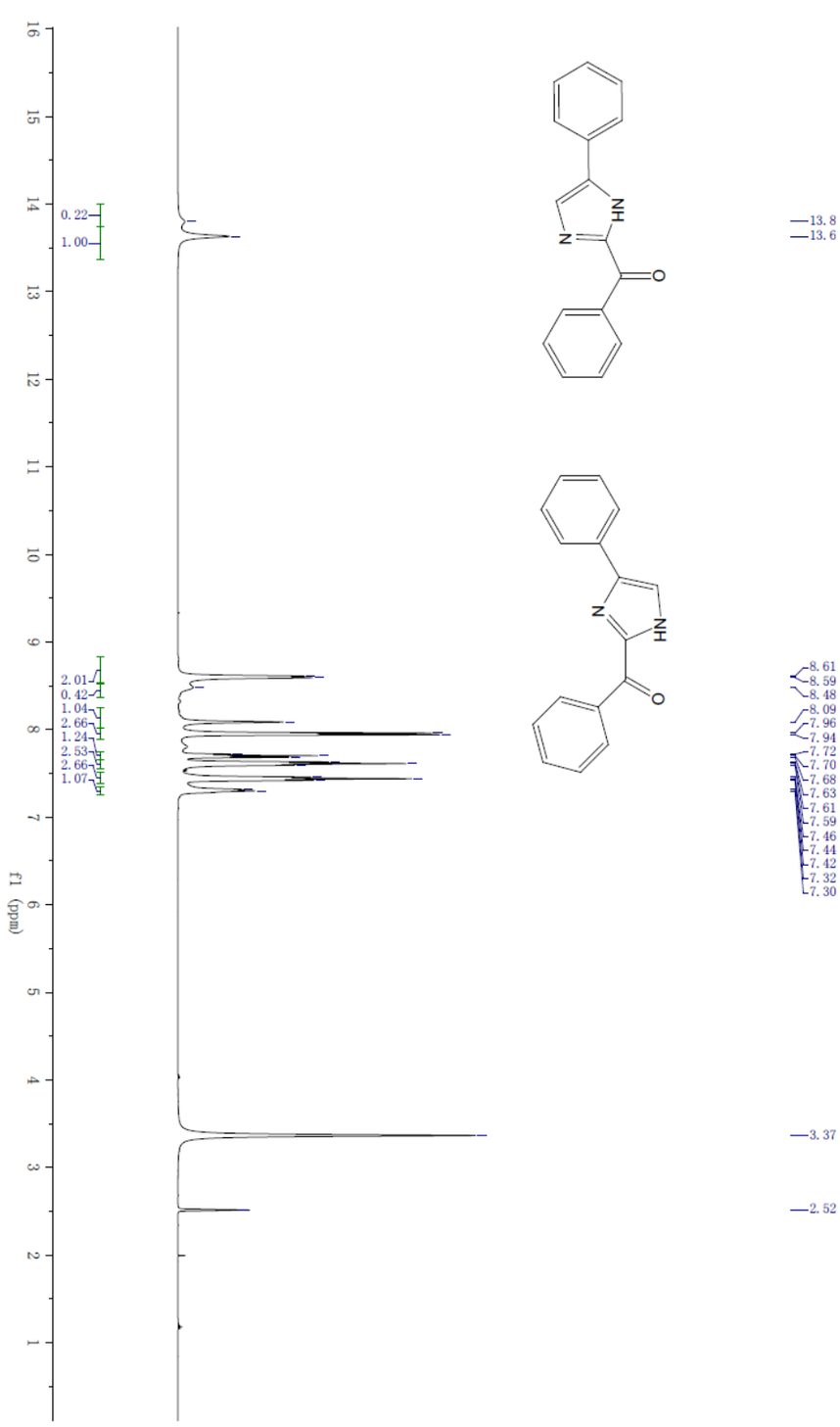

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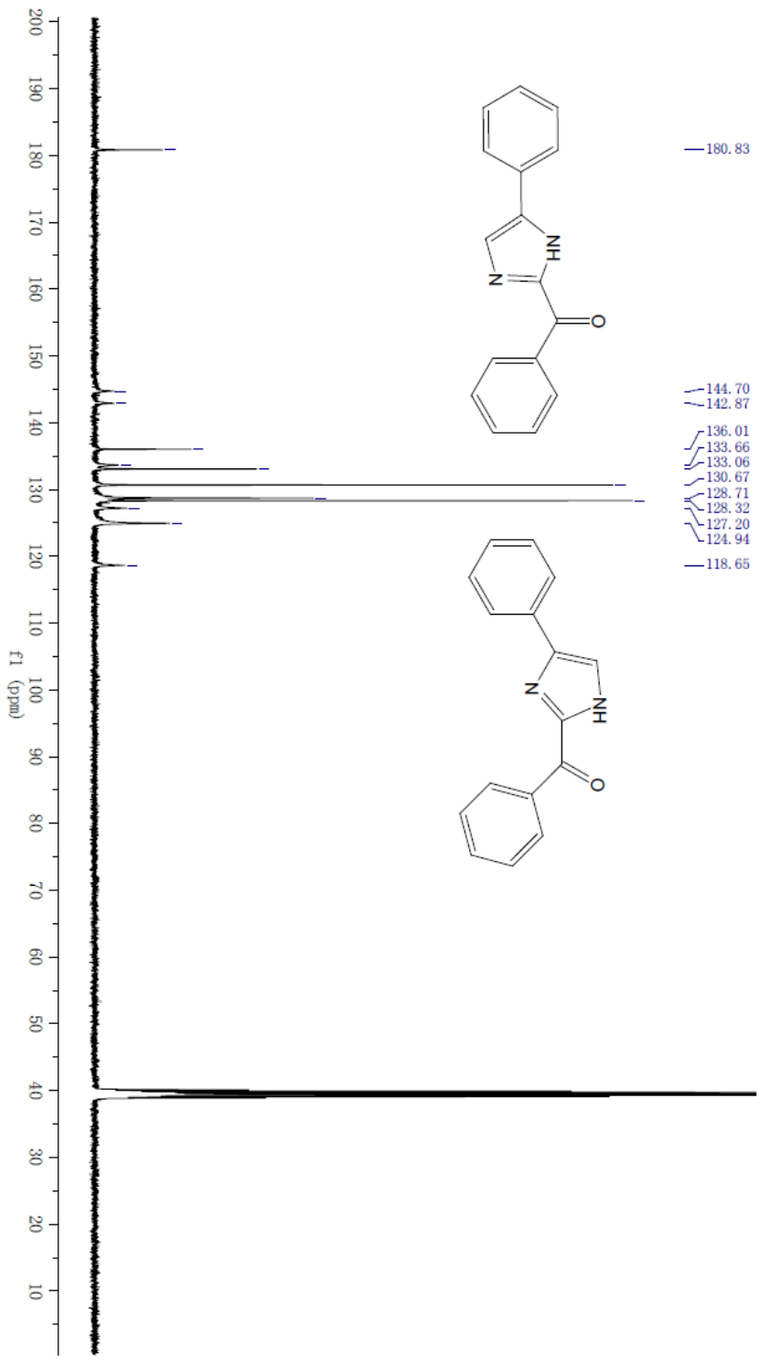
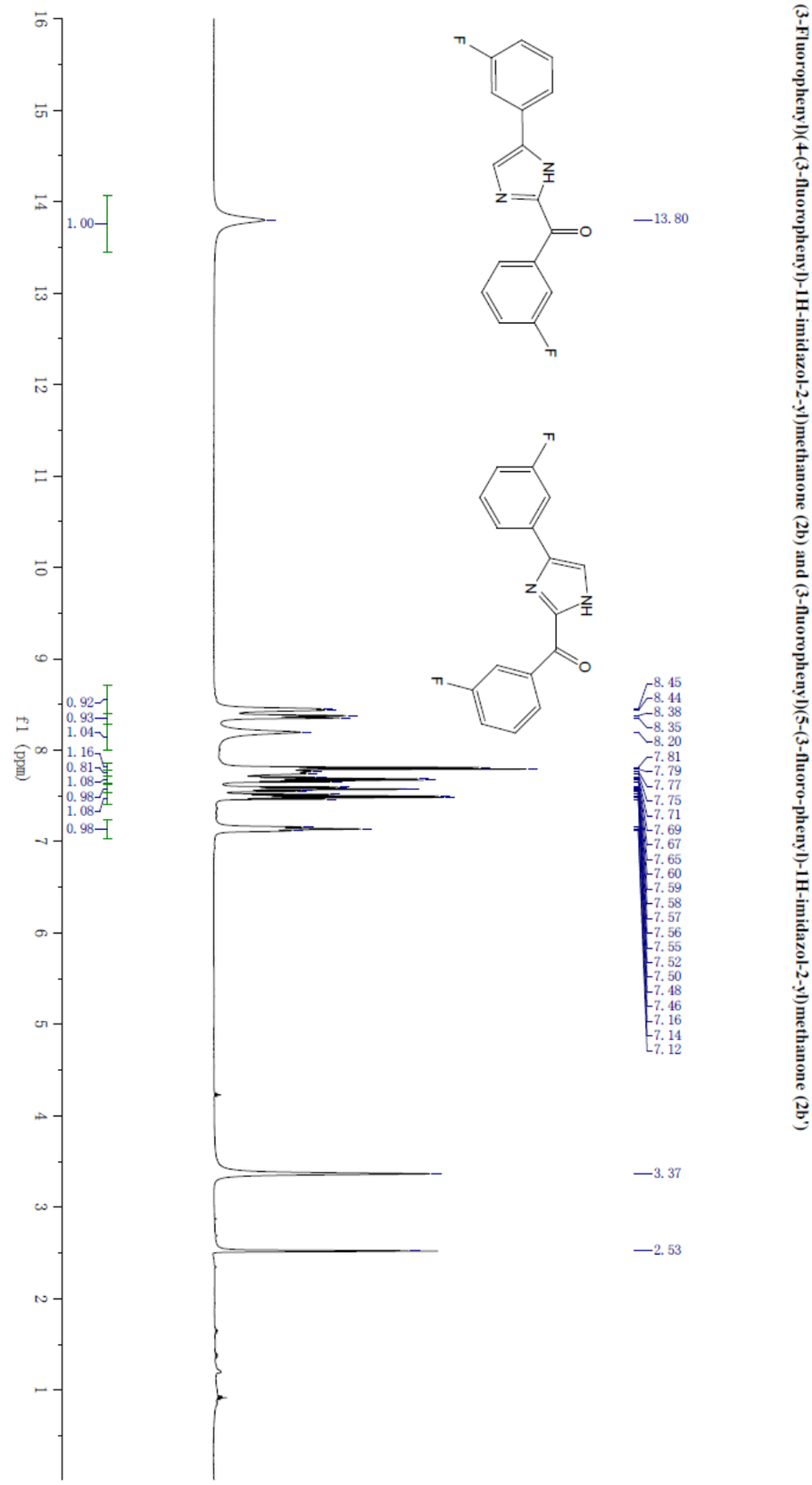
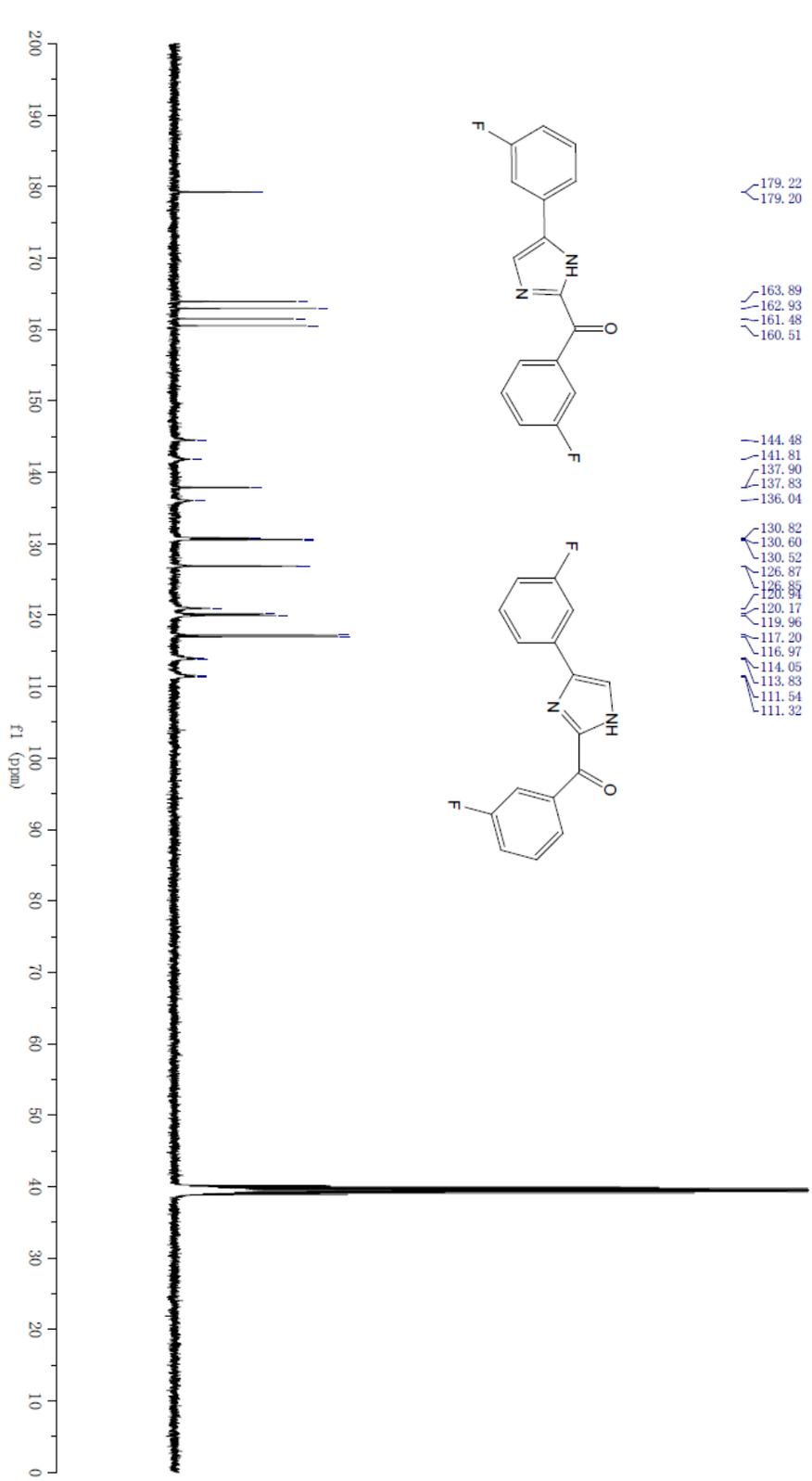
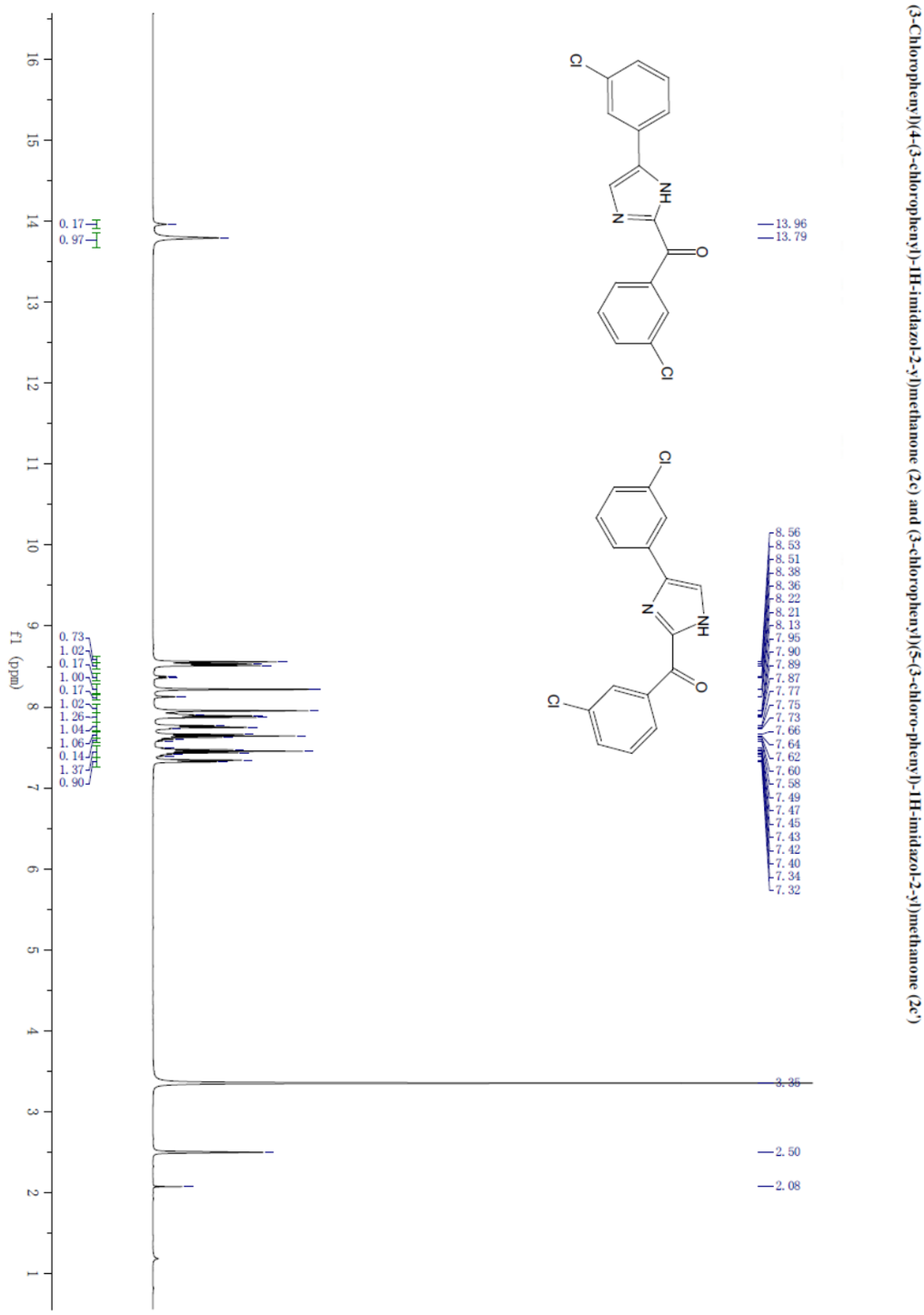
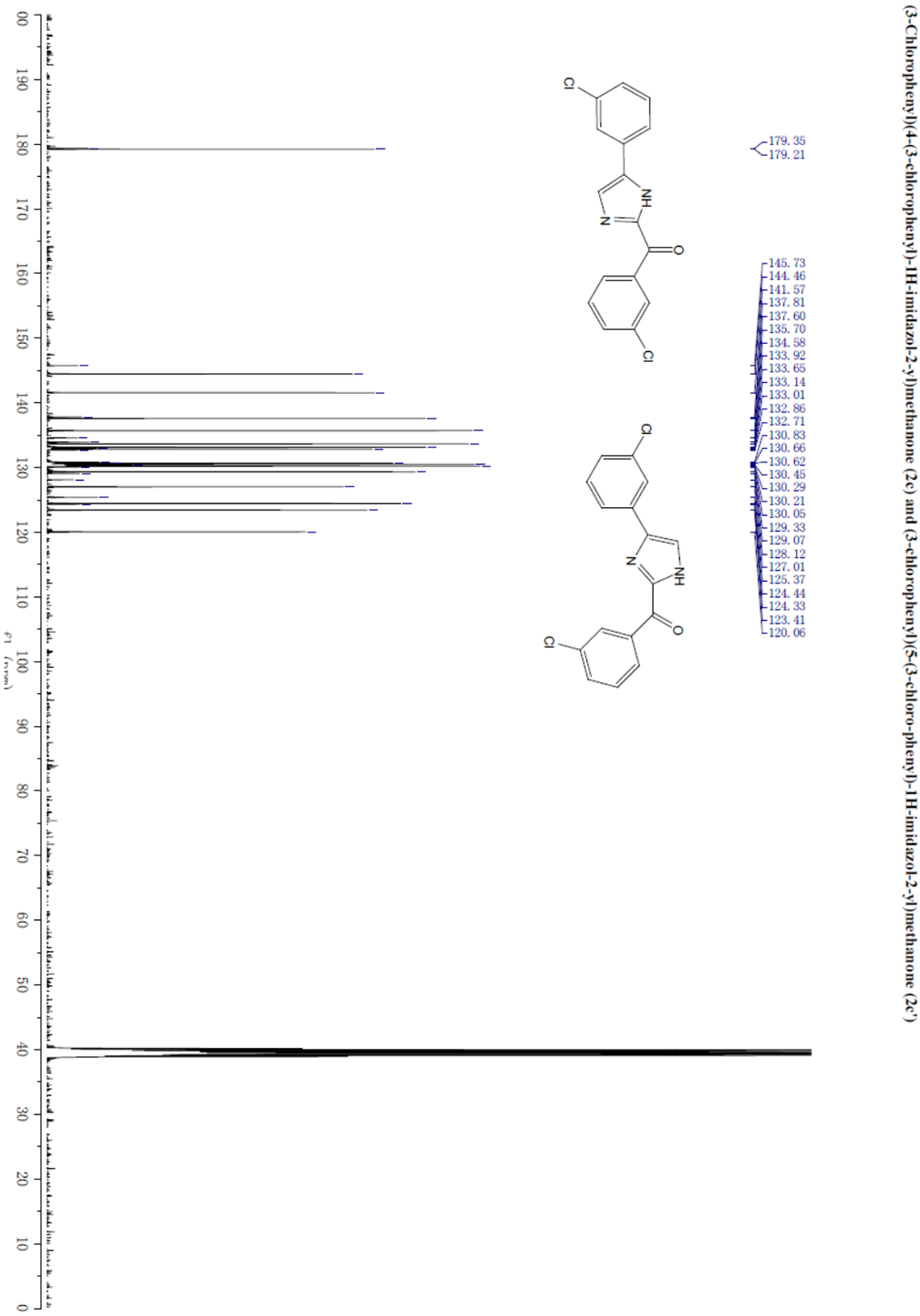
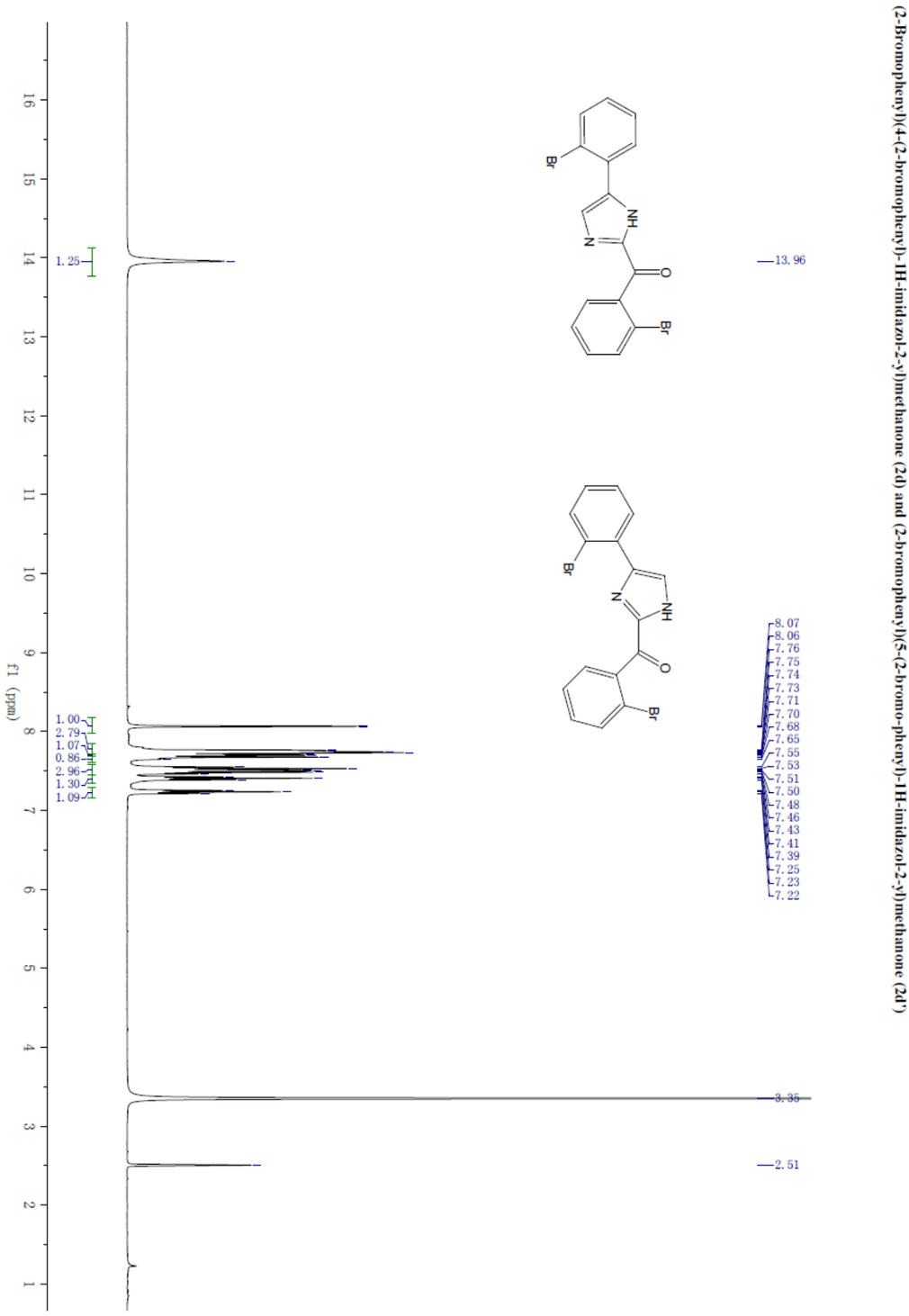


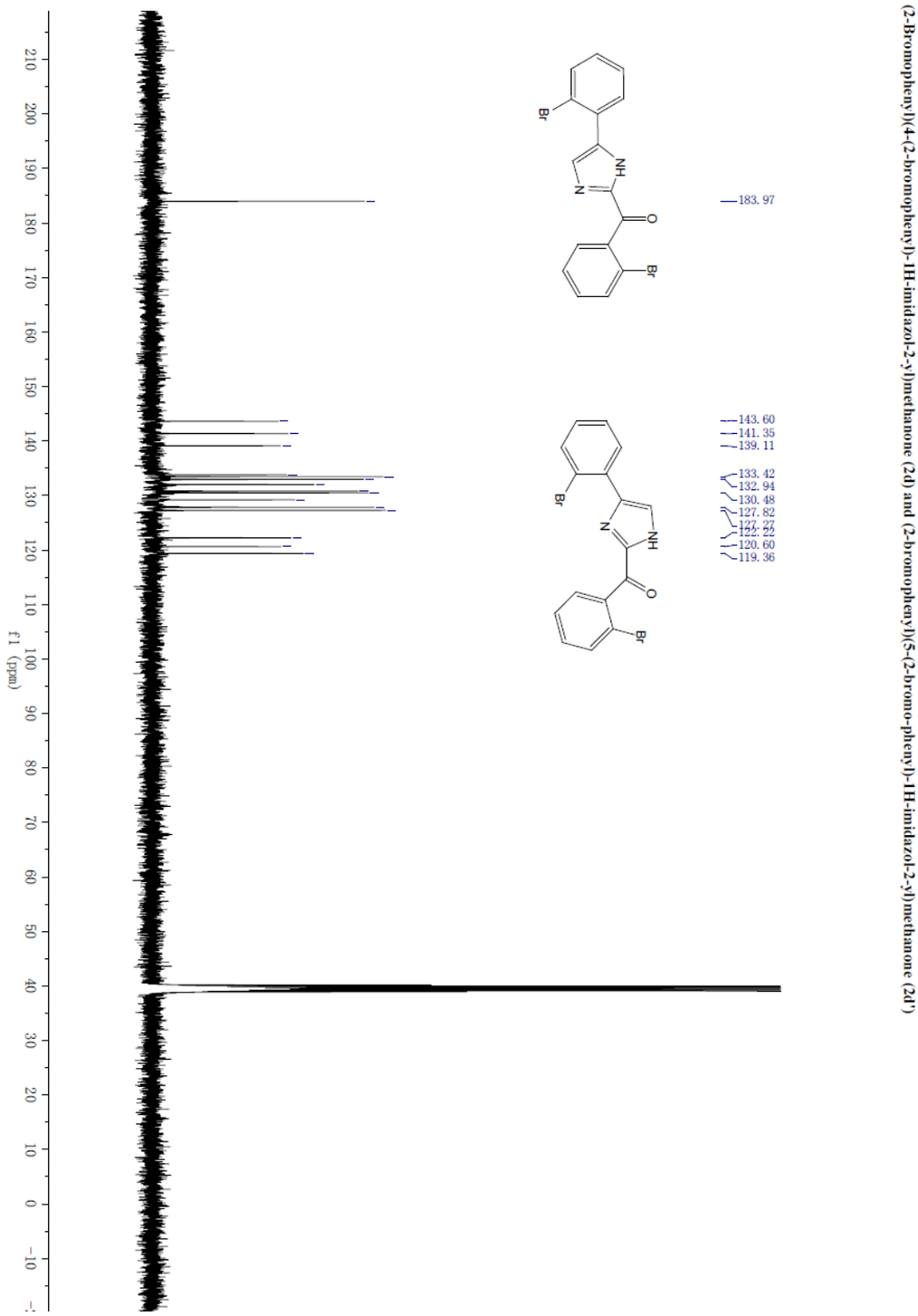


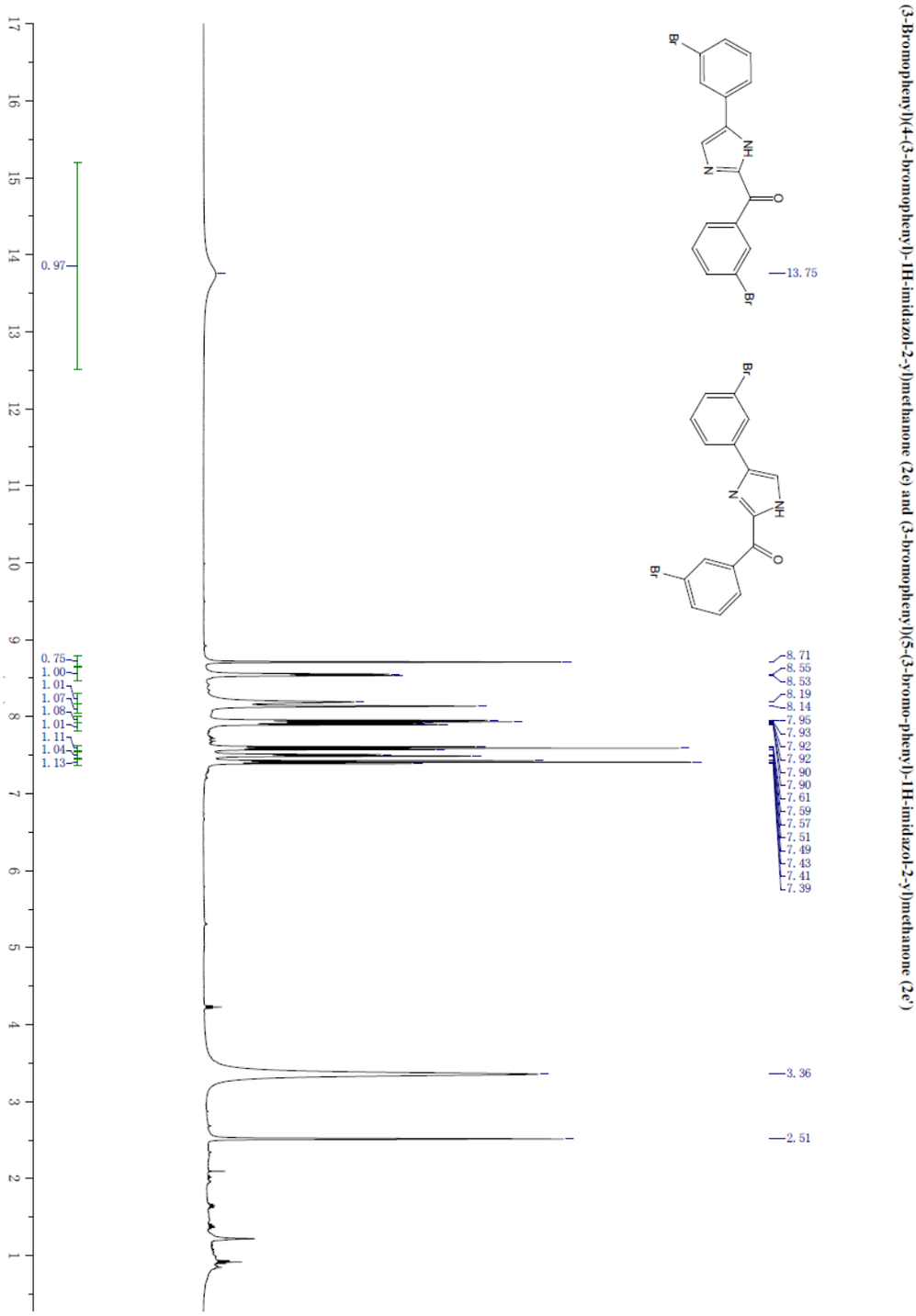


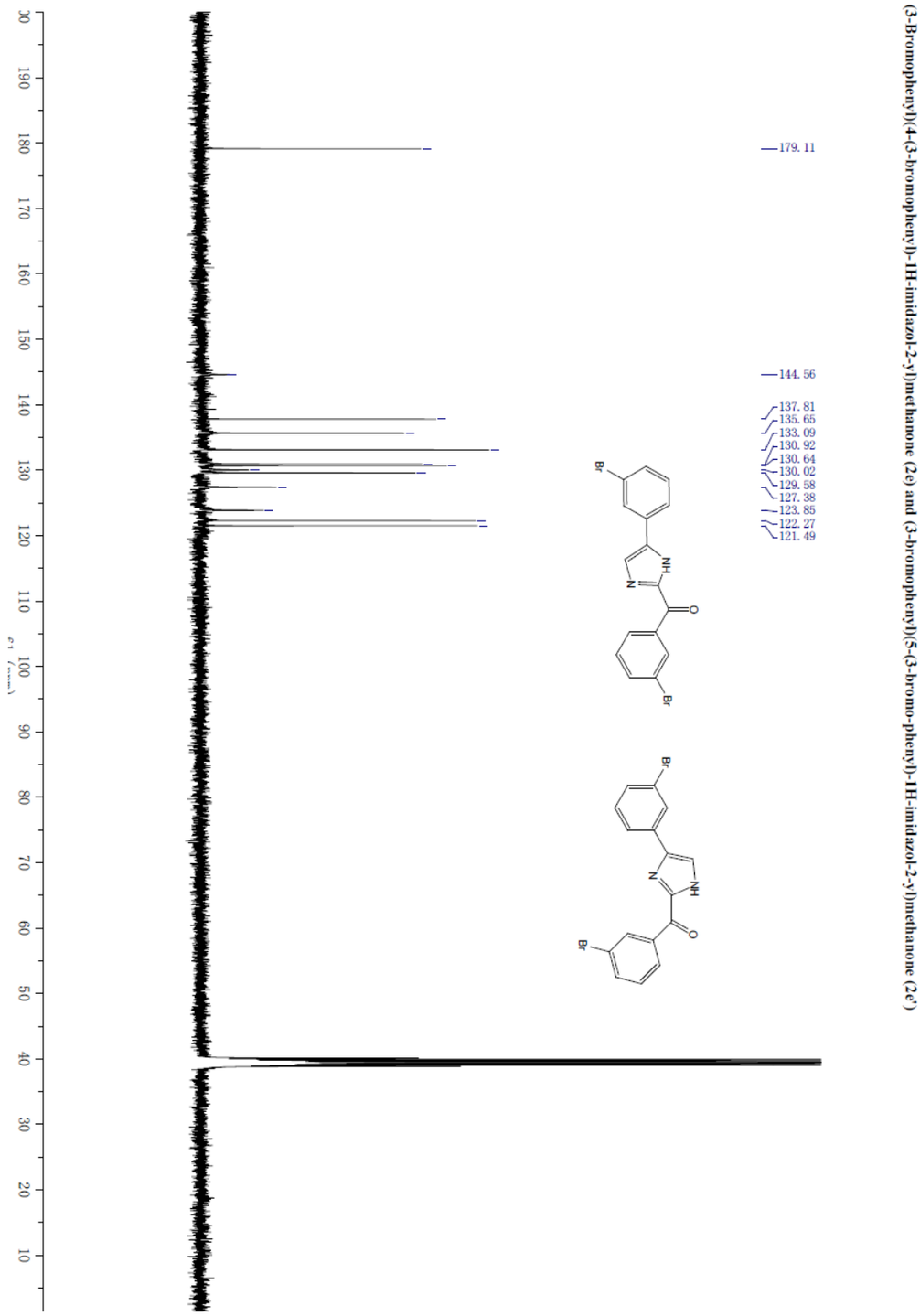


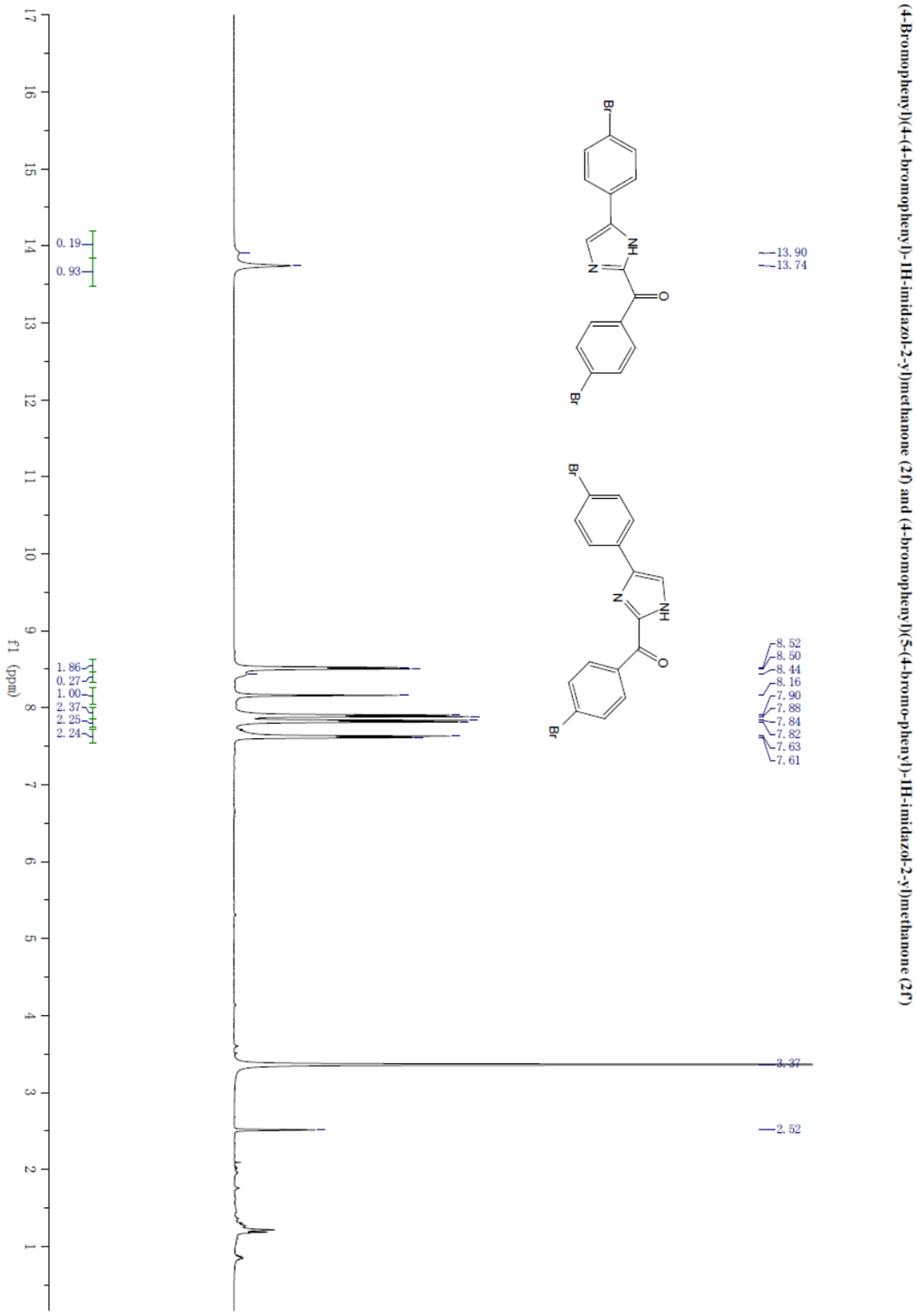


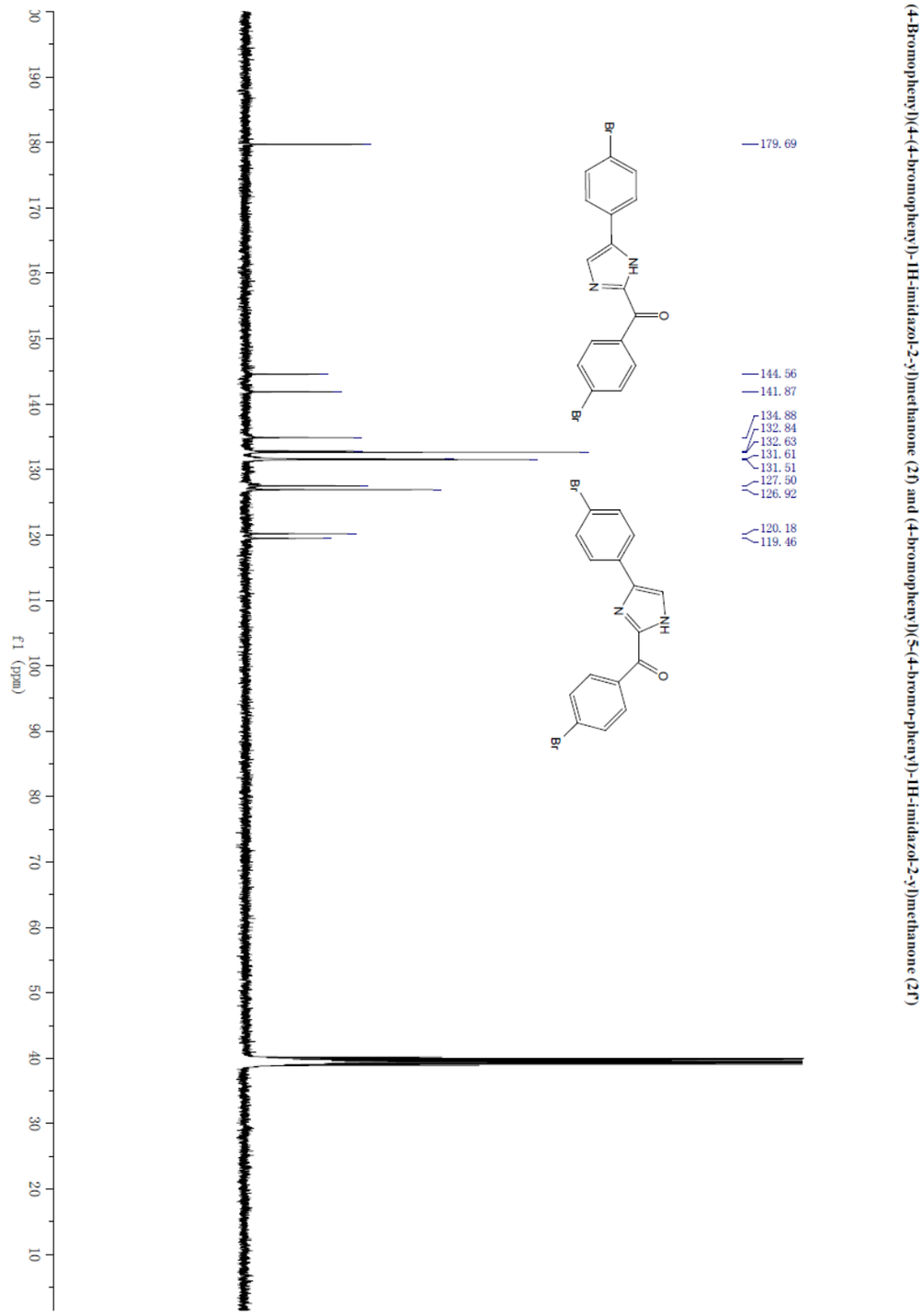




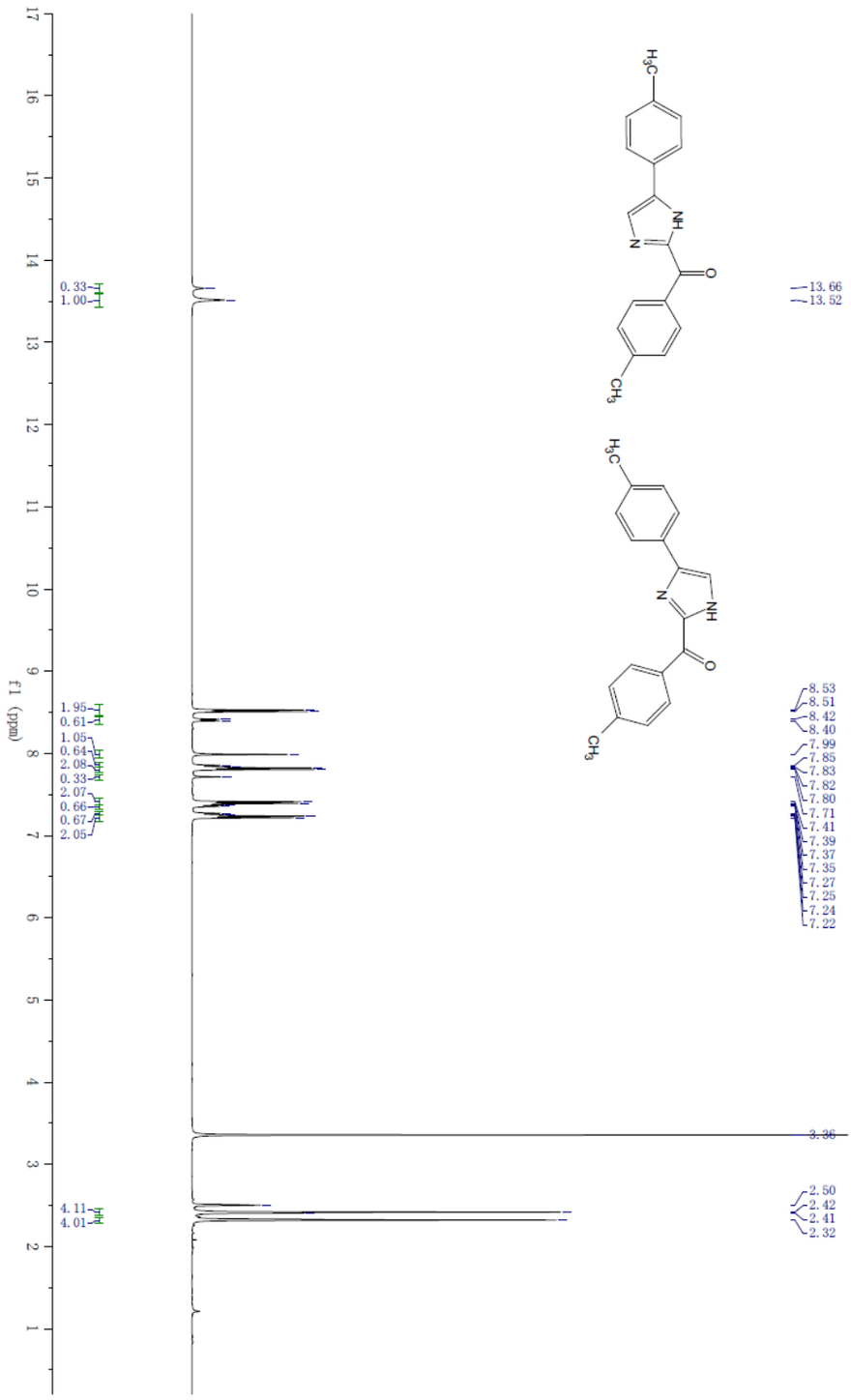




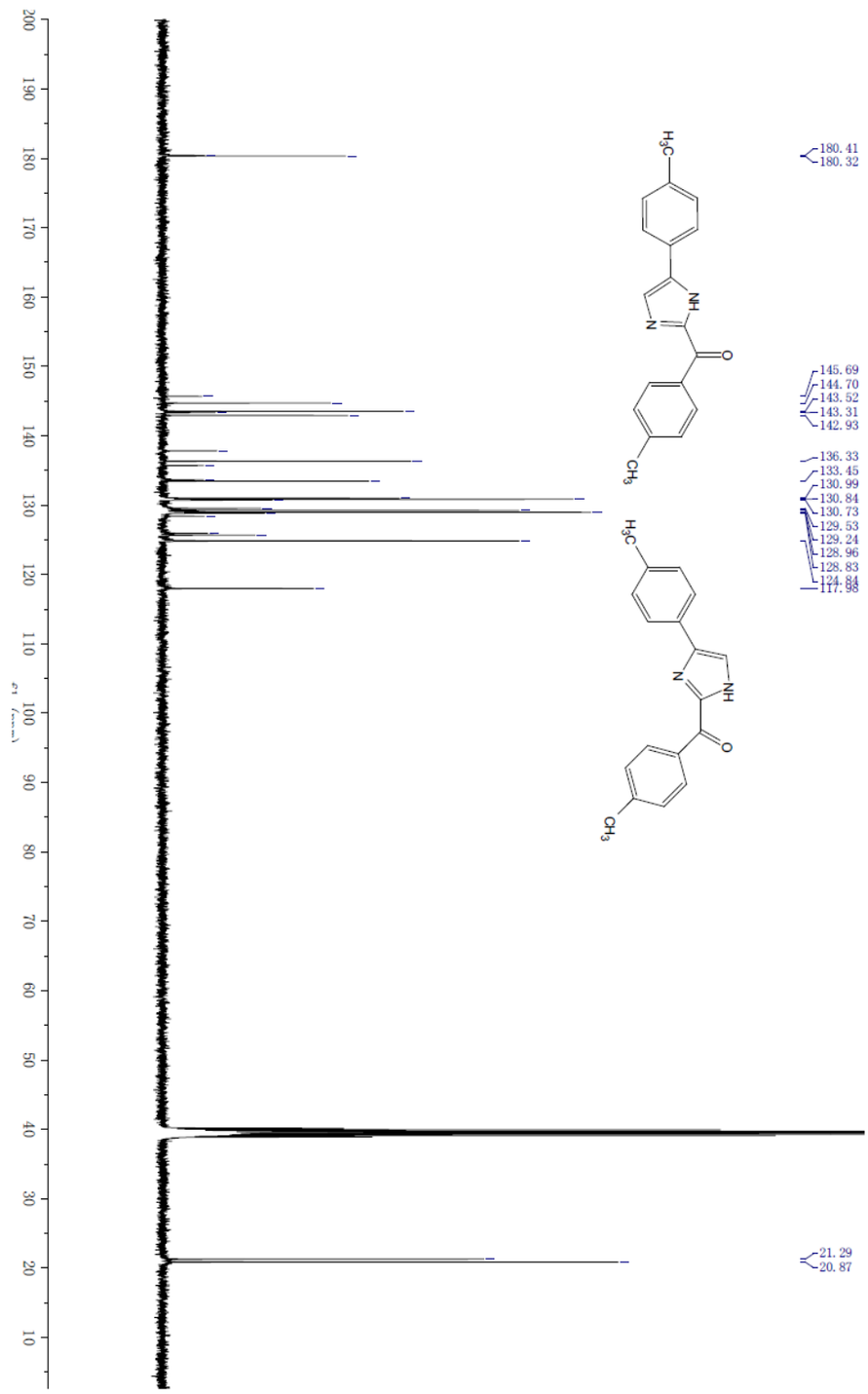


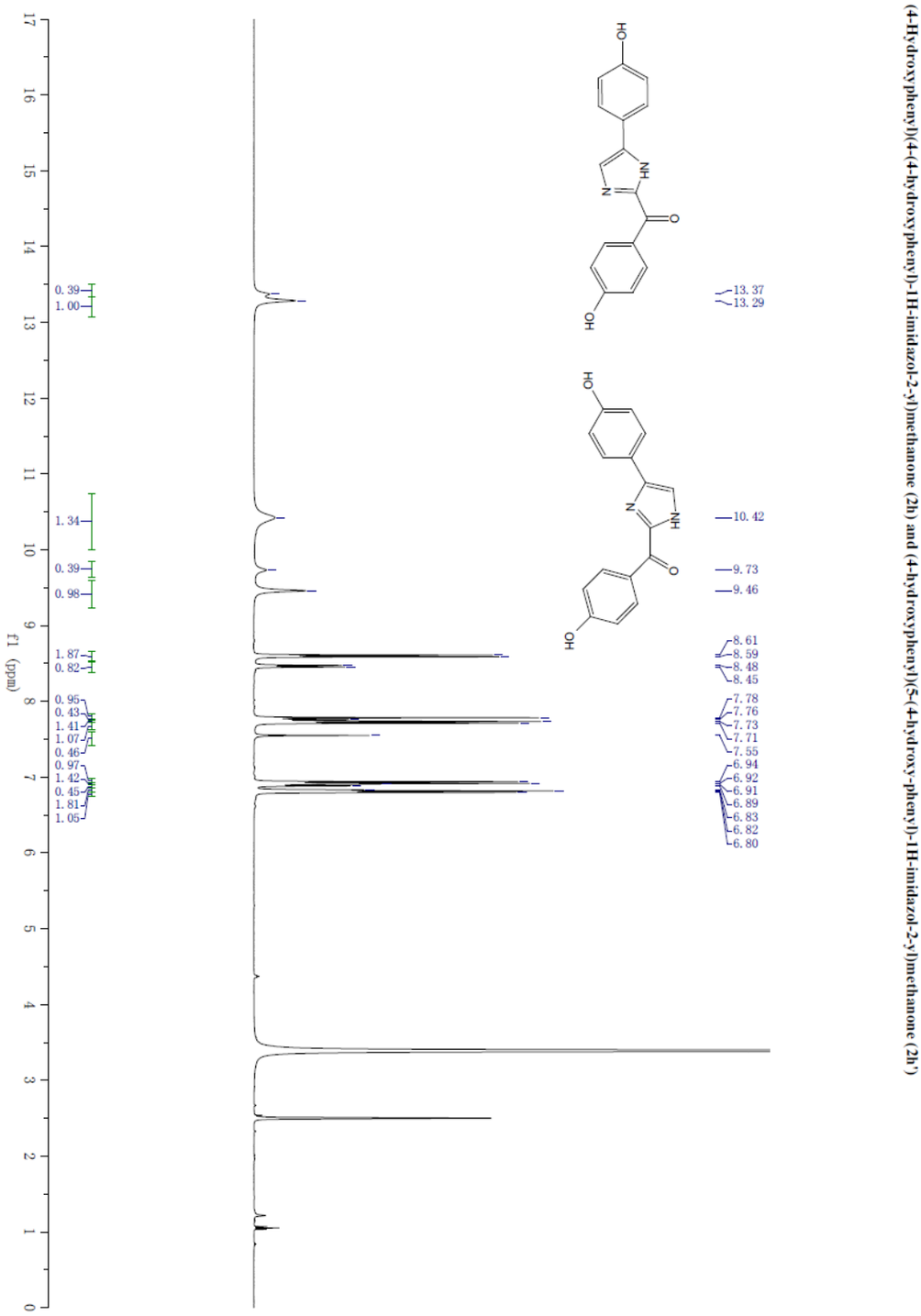


p-Tolyl(4-(p-tolyl)-1H-imidazol-2-yl)methanone (2g) and p-tolyl(5-(p-tolyl)-1H-imidazol-2-yl)methanone (2g')

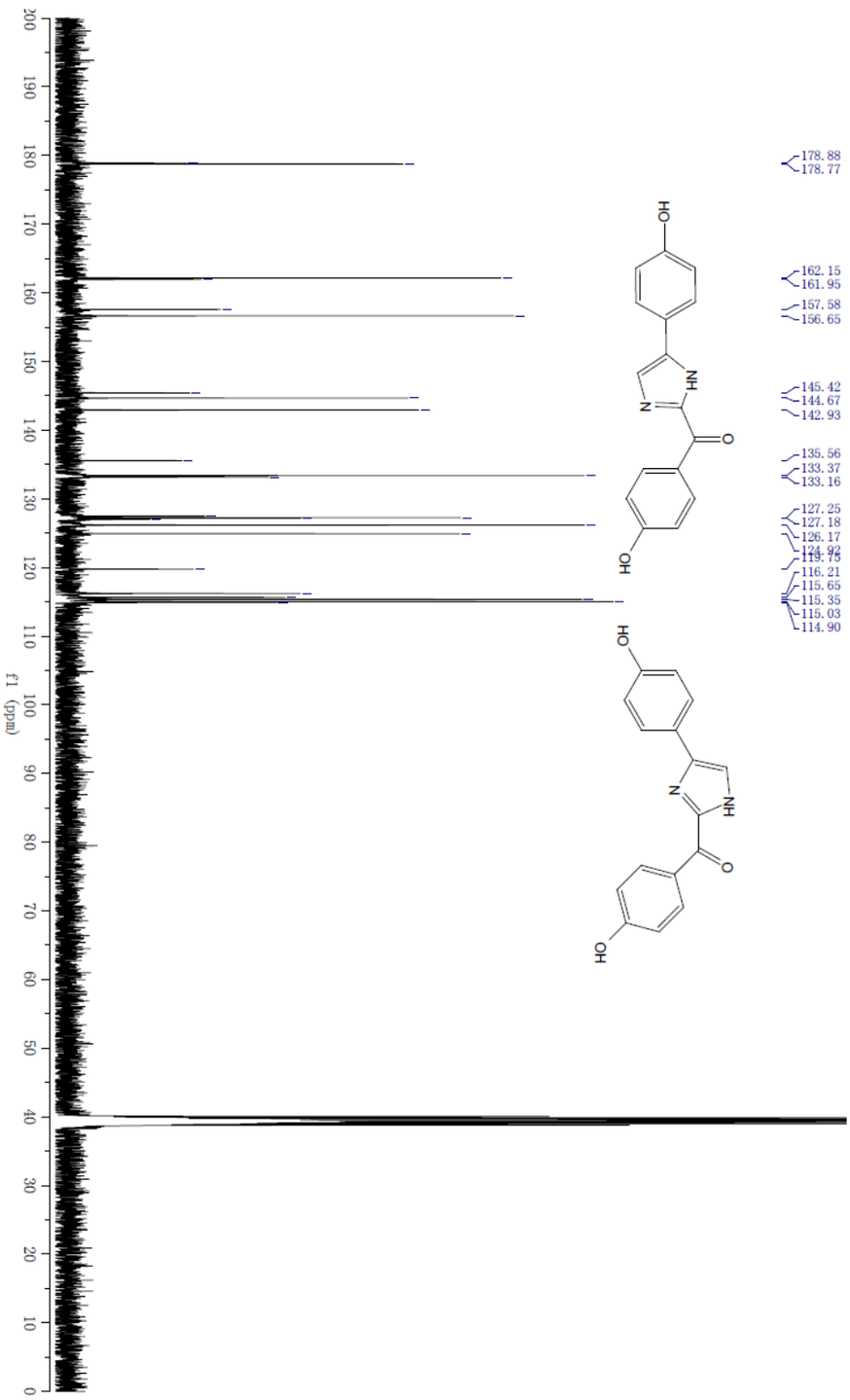


p-Tolyl(4-(p-tolyl)-1H-imidazol-2-yl)methanone (2g) and p-tolyl(5-(p-tolyl)-1H-imidazol-2-yl)methanone (2g')

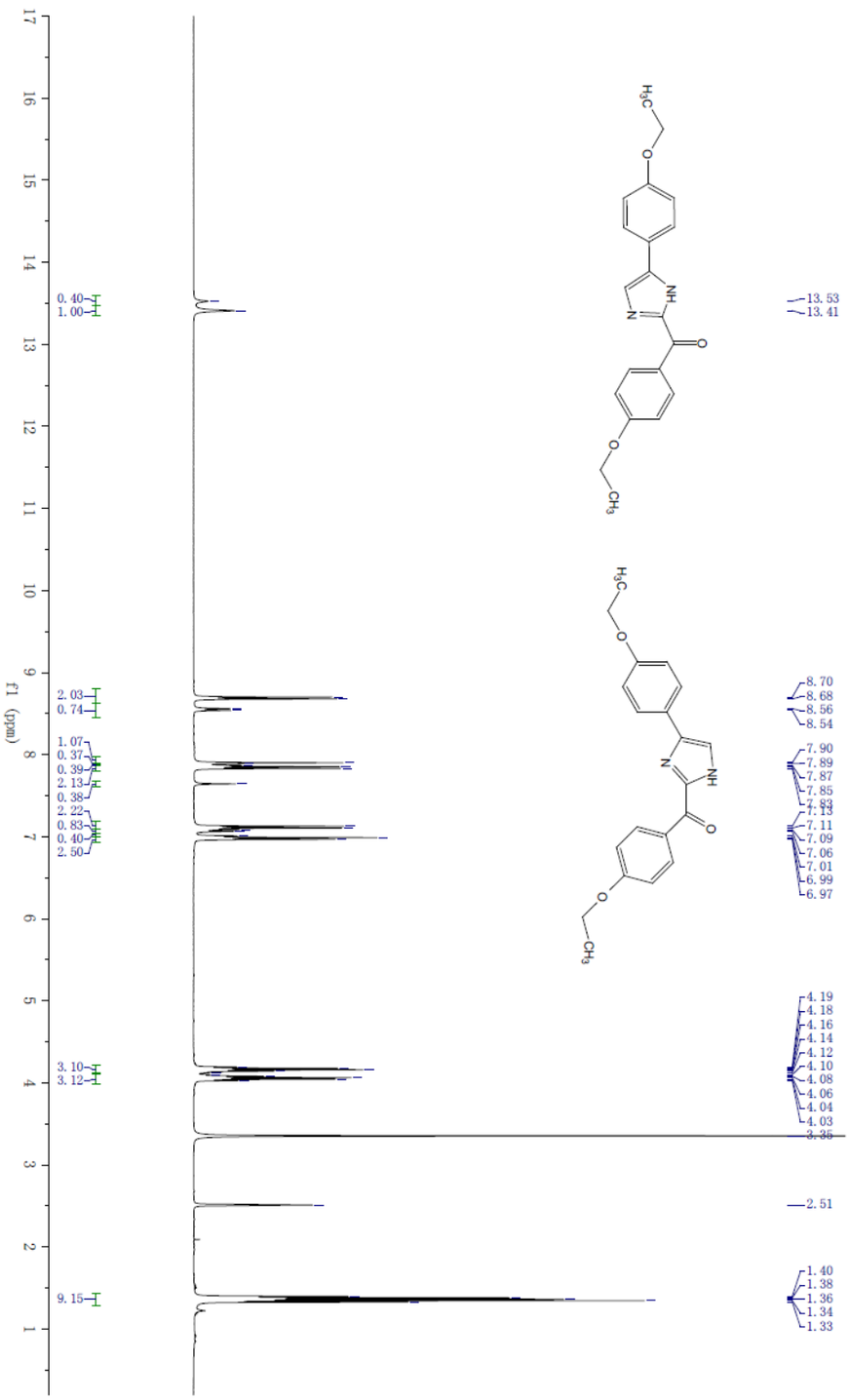


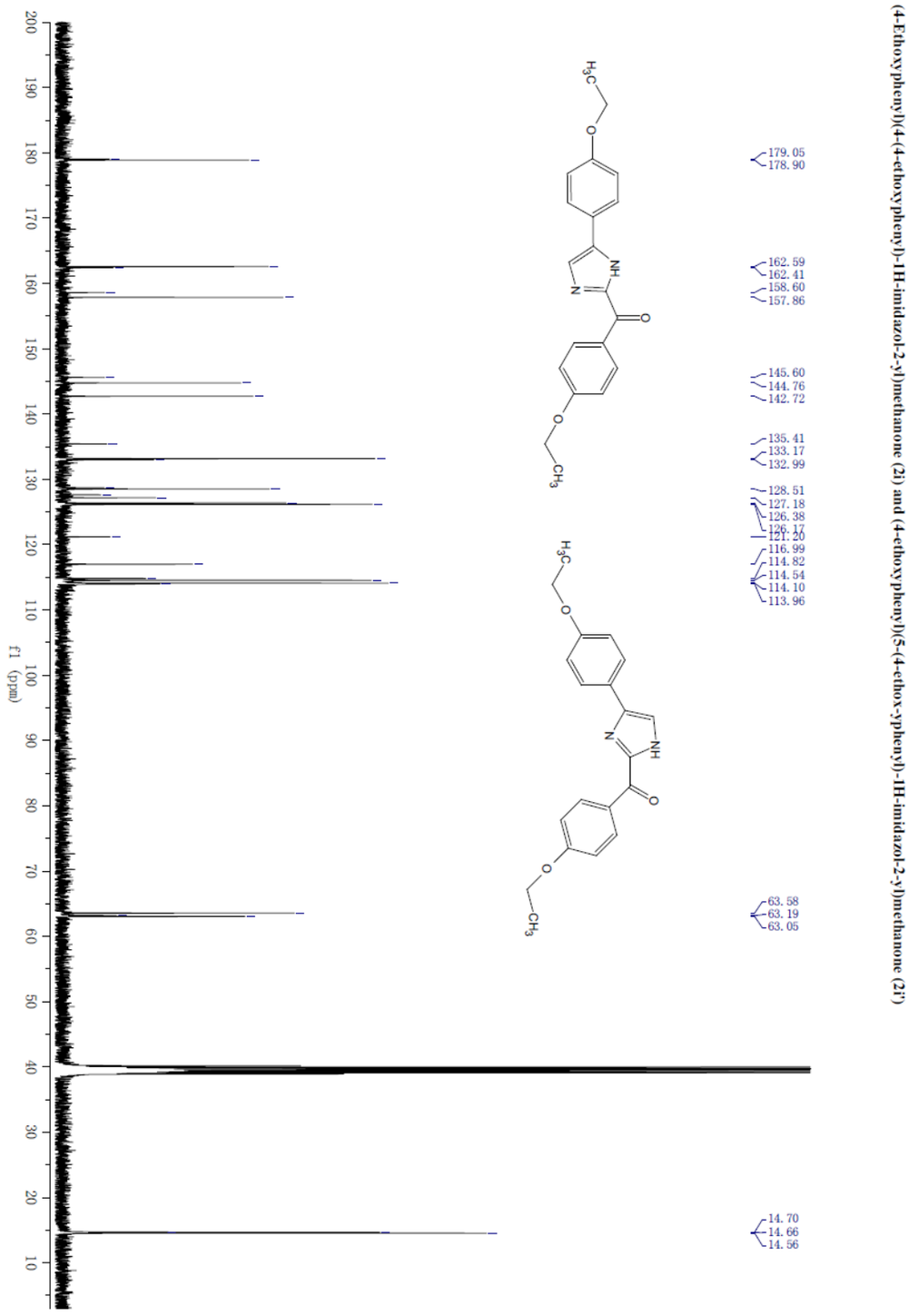


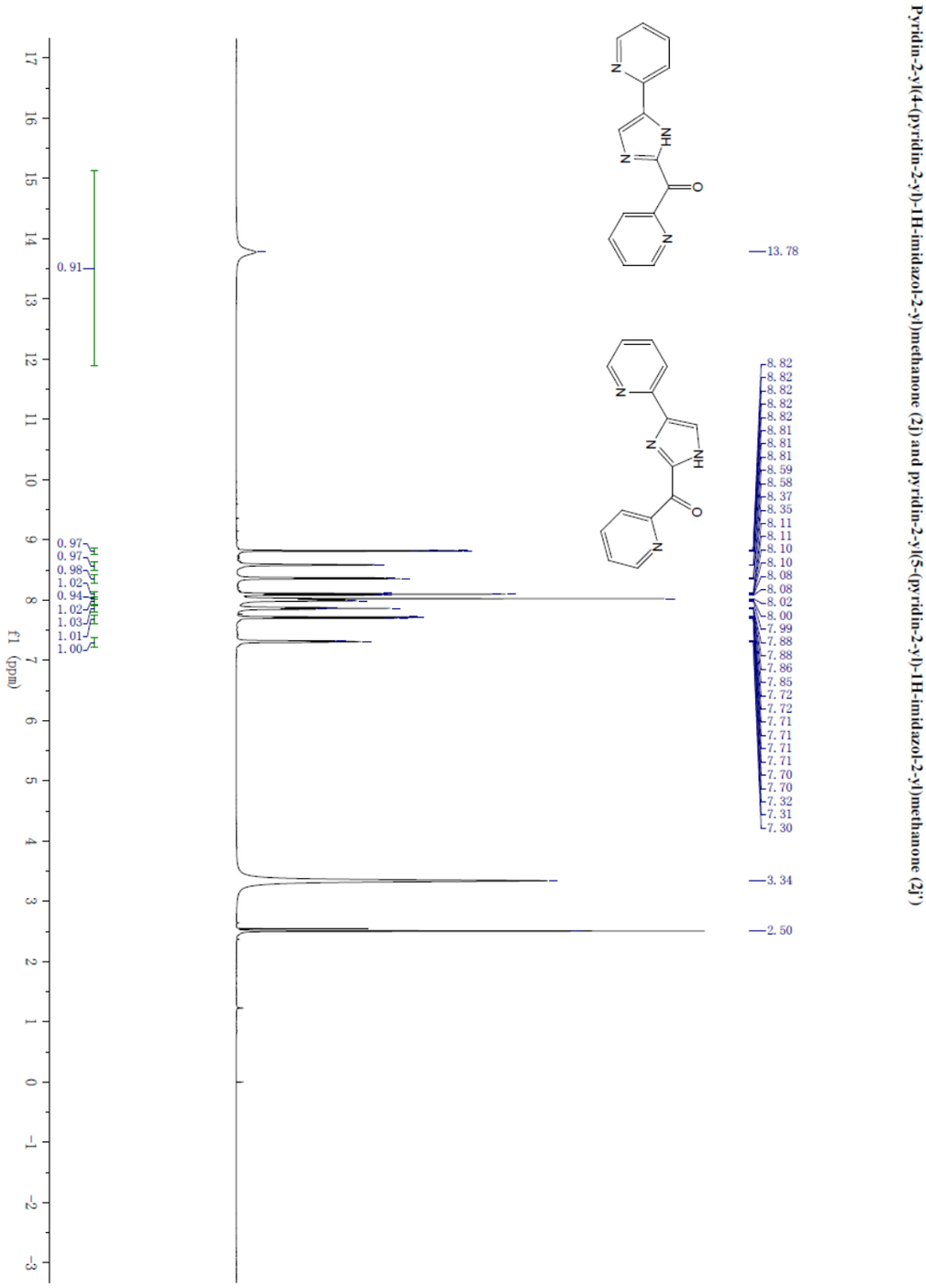
(4-Hydroxyphenyl)(4-(4-hydroxyphenyl)-1H-imidazol-2-yl)methanone (2h) and (4-hydroxyphenyl)(5-(4-hydroxy-phenyl)-1H-imidazol-2-yl)methanone (2h')



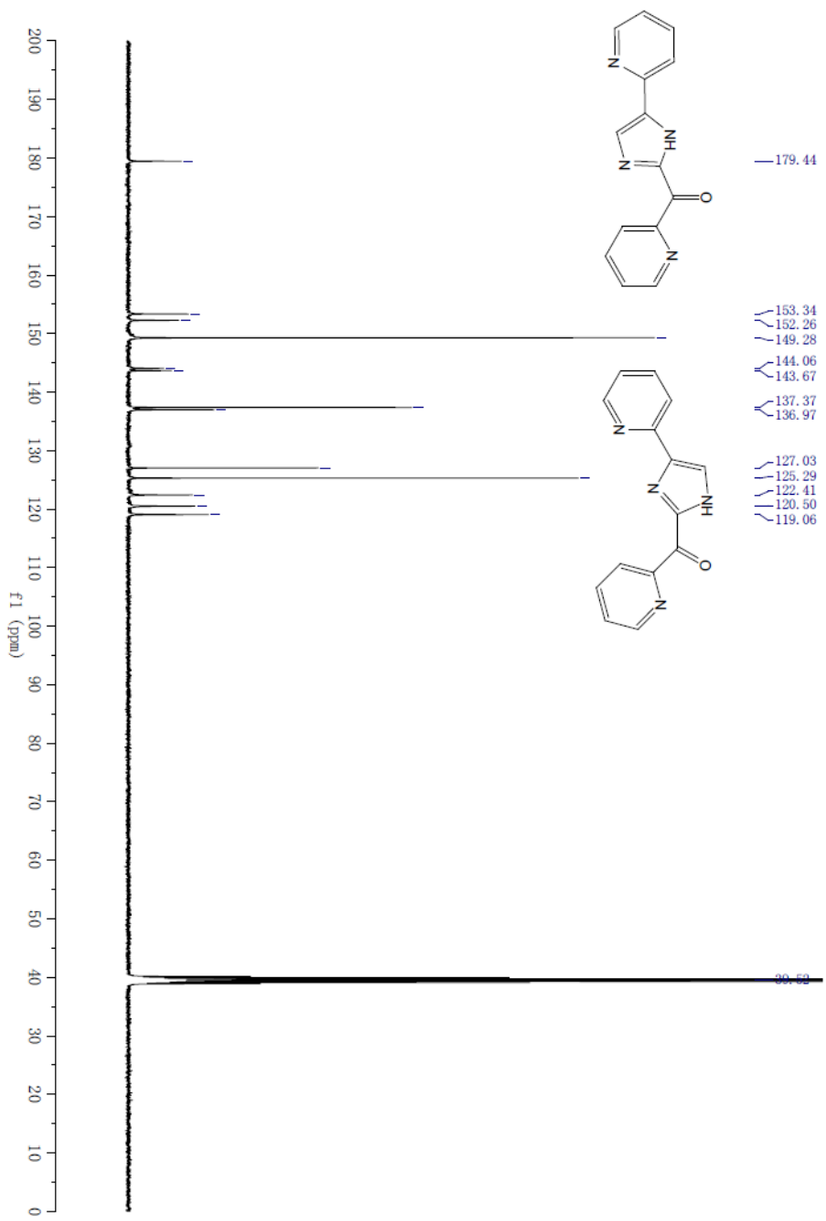
(4-Hydroxyphenyl)(4-(4-hydroxyphenyl)-1H-imidazol-2-yl)methanone (2h) and (4-hydroxyphenyl)(5-(4-hydroxy-phenyl)-1H-imidazol-2-yl)methanone (2h')

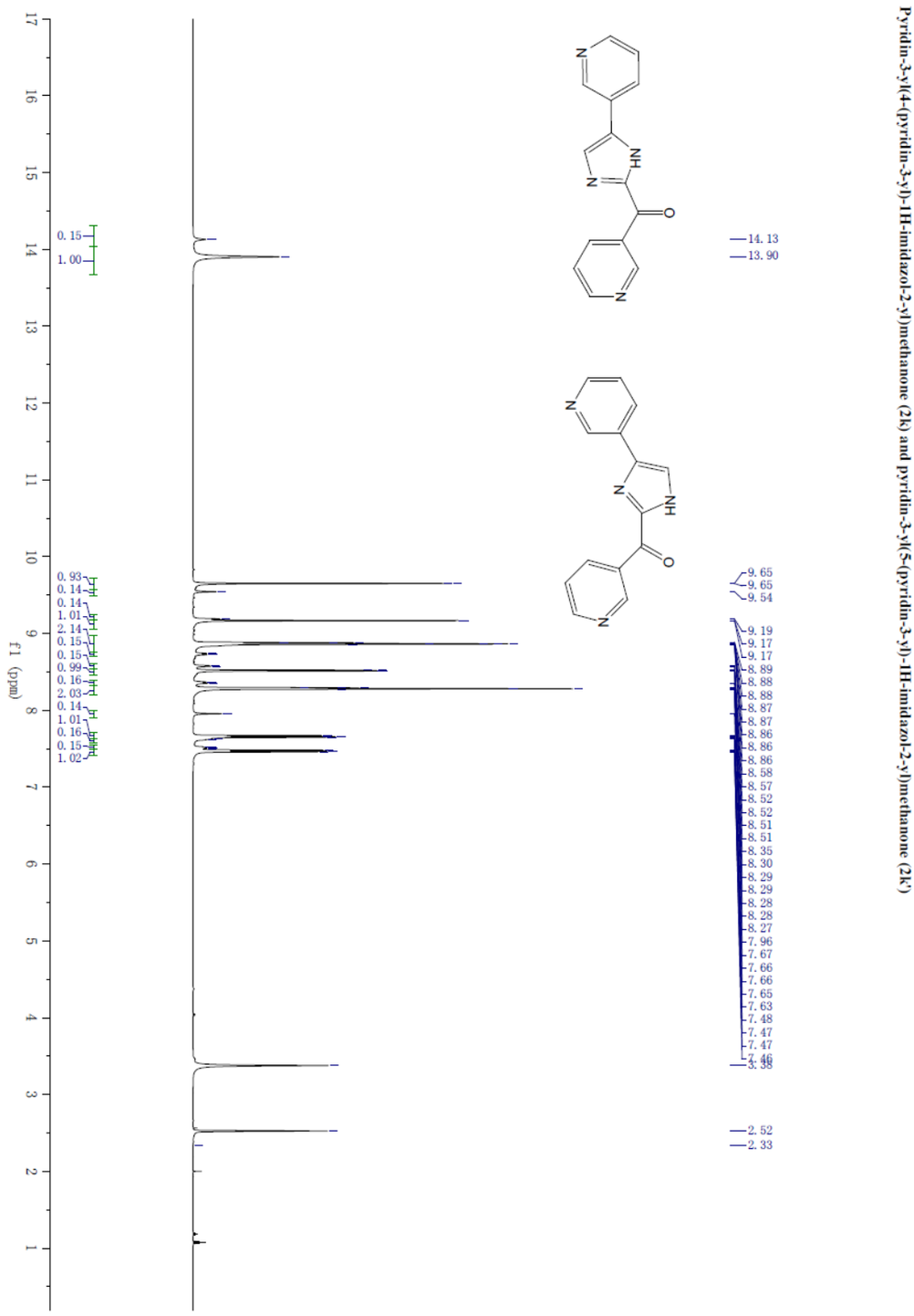


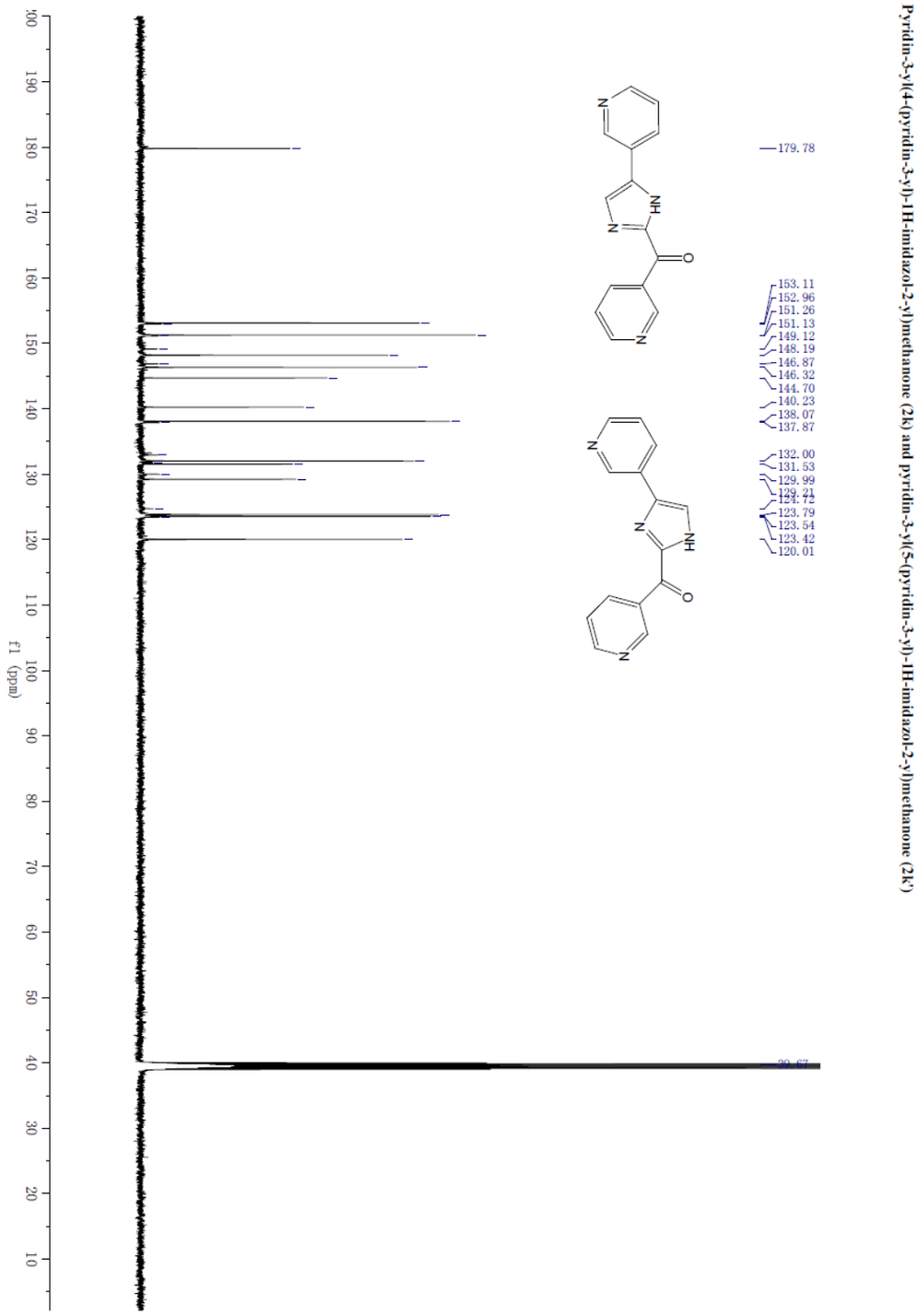


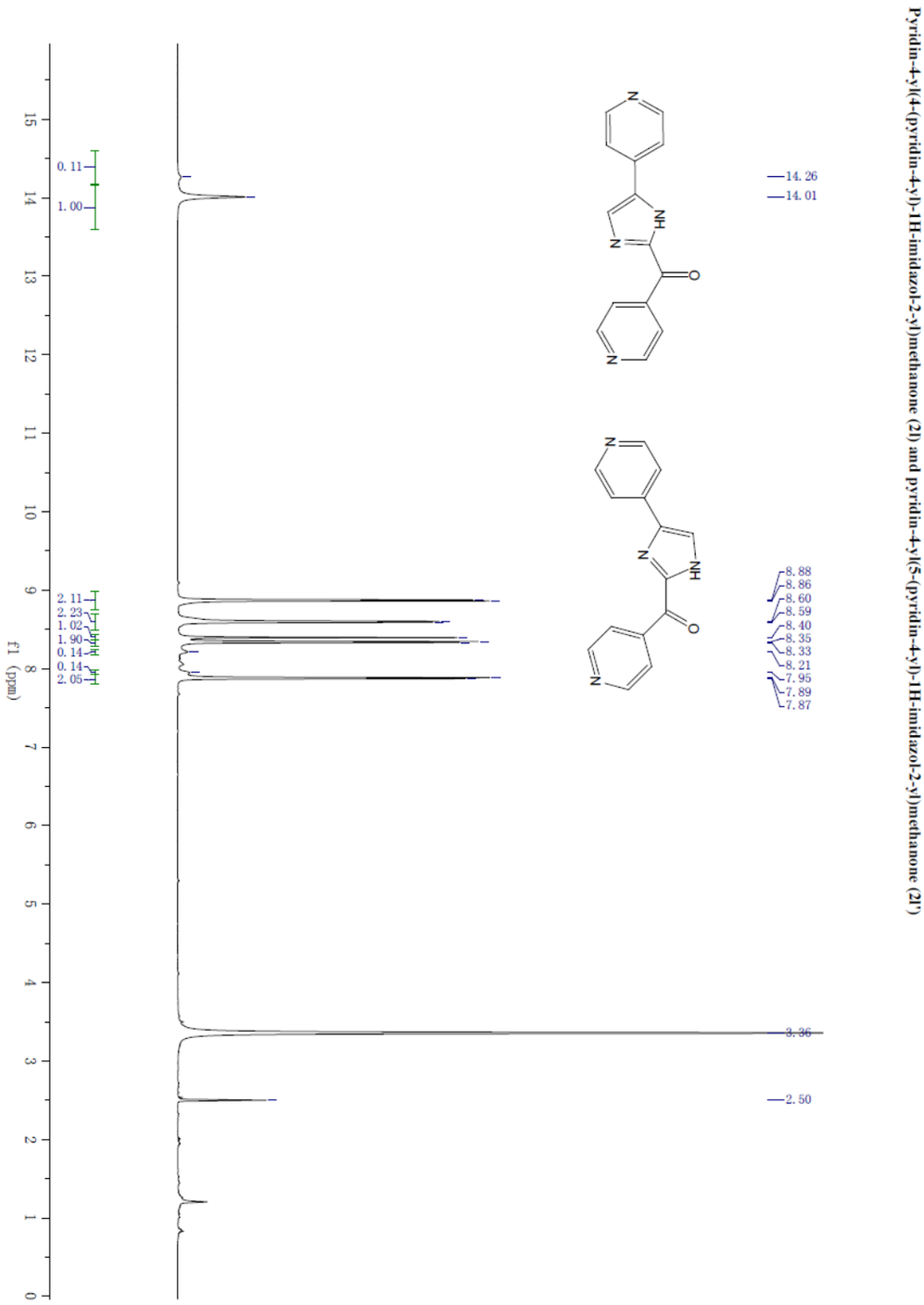


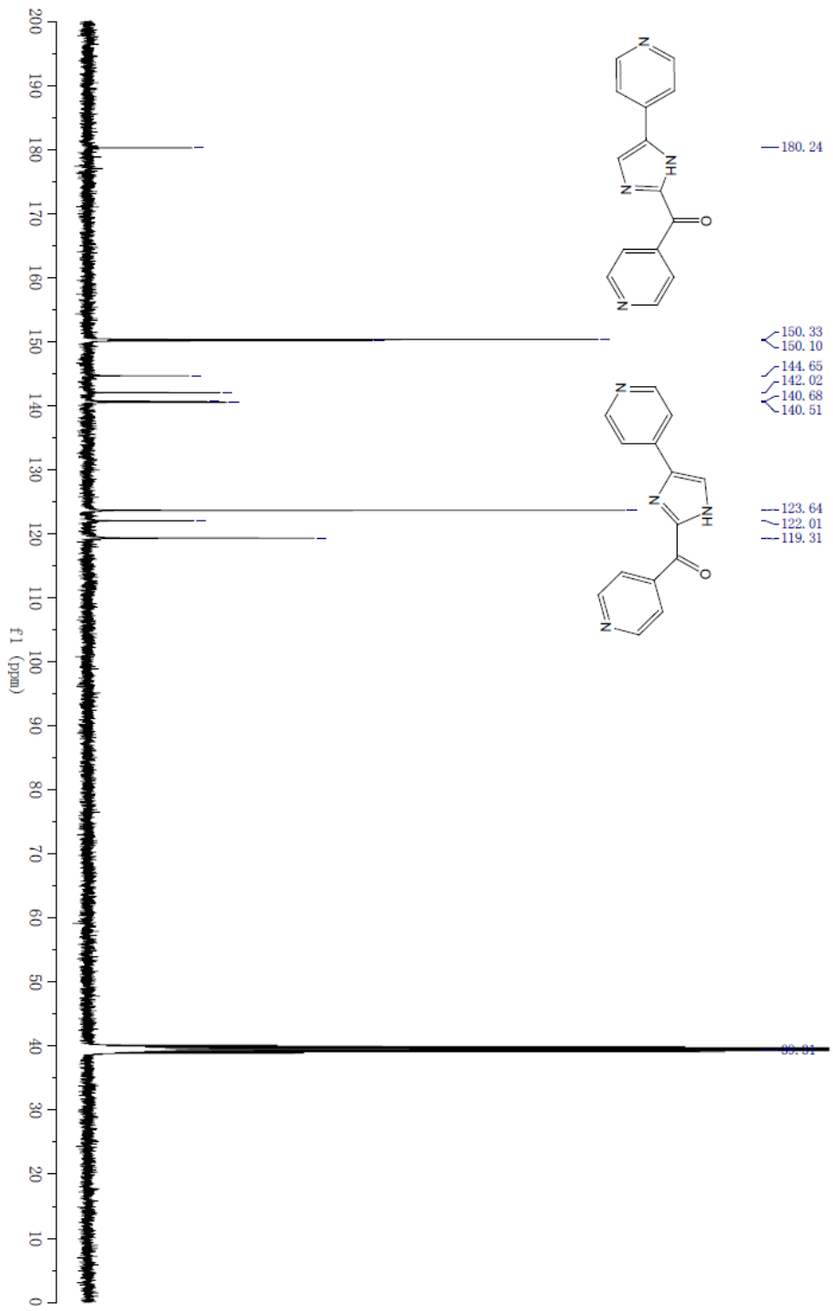
Pyridin-2-yl(4-(pyridin-2-yl)-1H-imidazol-2-yl)methanone (2j) and pyridin-2-yl(5-(pyridin-2-yl)-1H-imidazol-2-yl)methanone (2j')



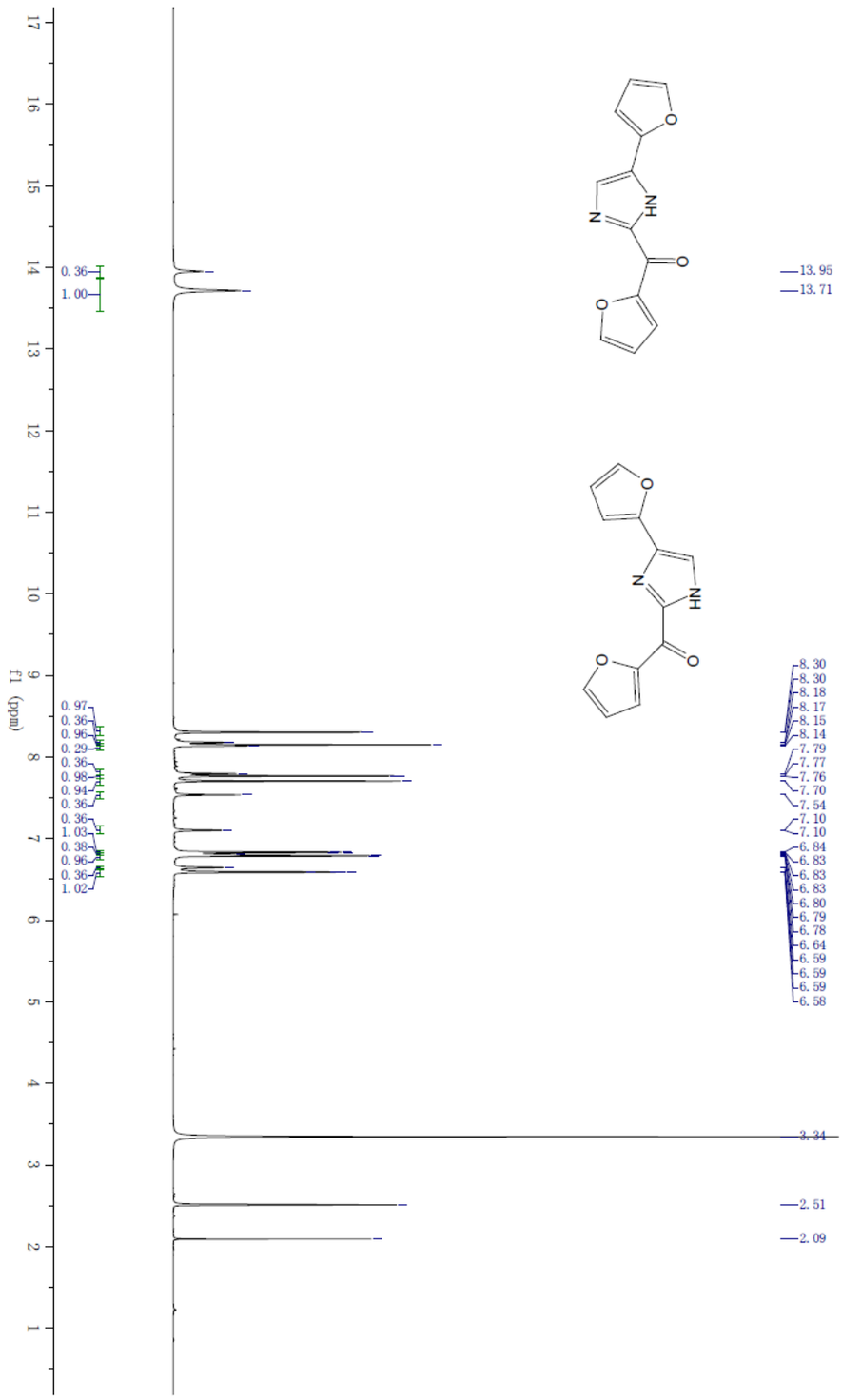




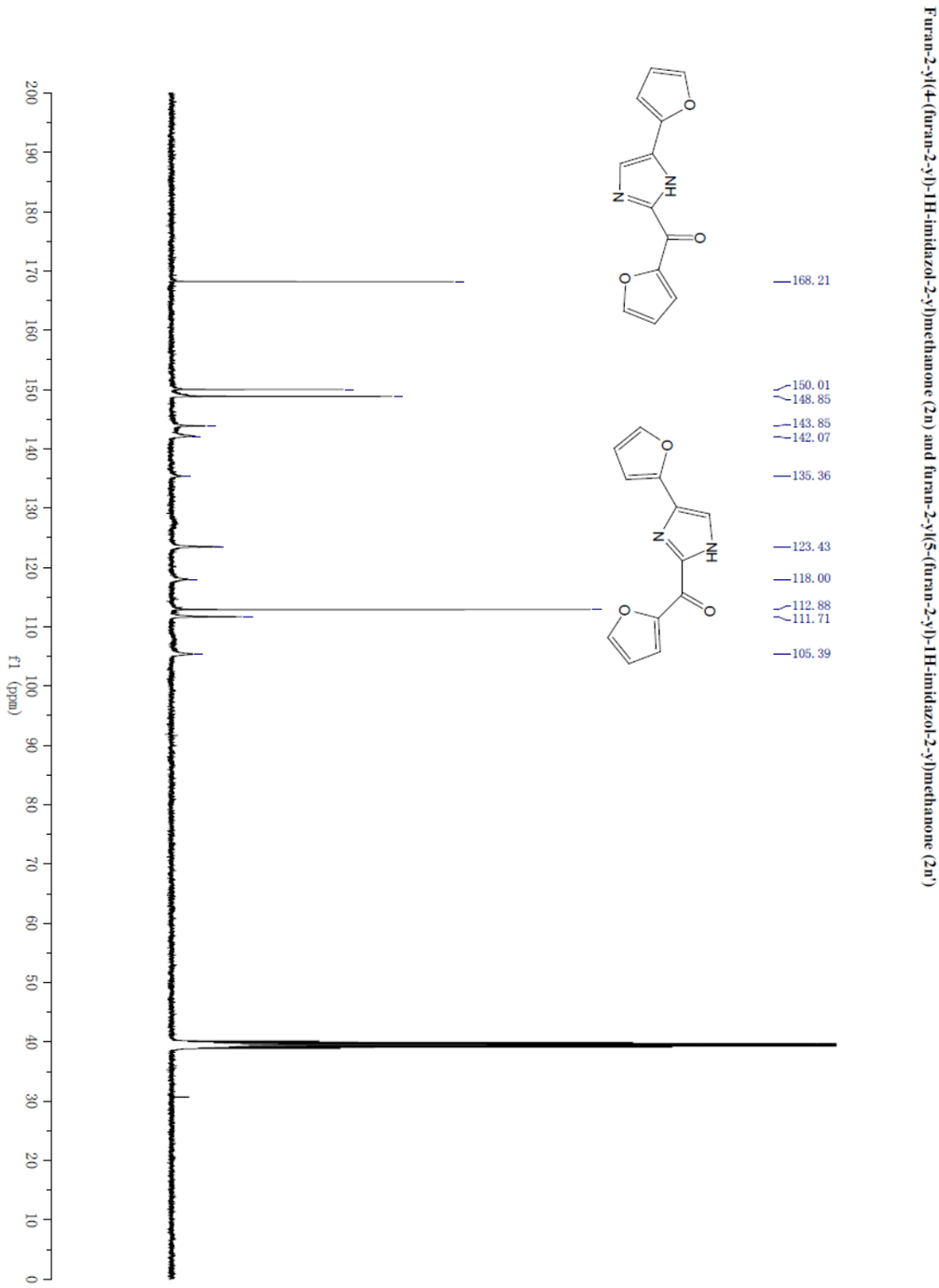


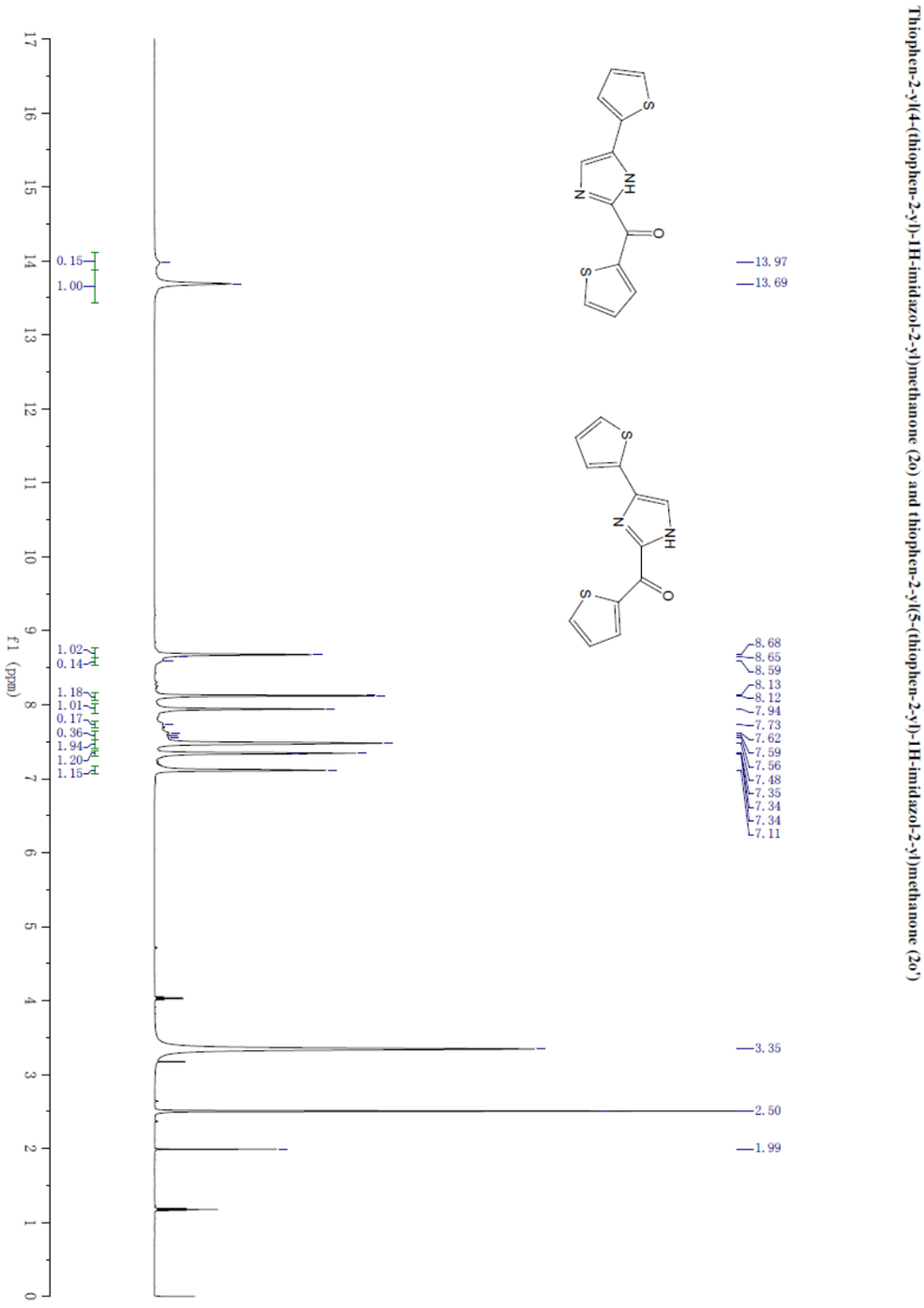


Pyridin-4-yl(4-(pyridin-4-yl)-1H-imidazol-2-yl)methanone (2l) and pyridin-4-yl(5-(pyridin-4-yl)-1H-imidazol-2-yl)methanone (2l')

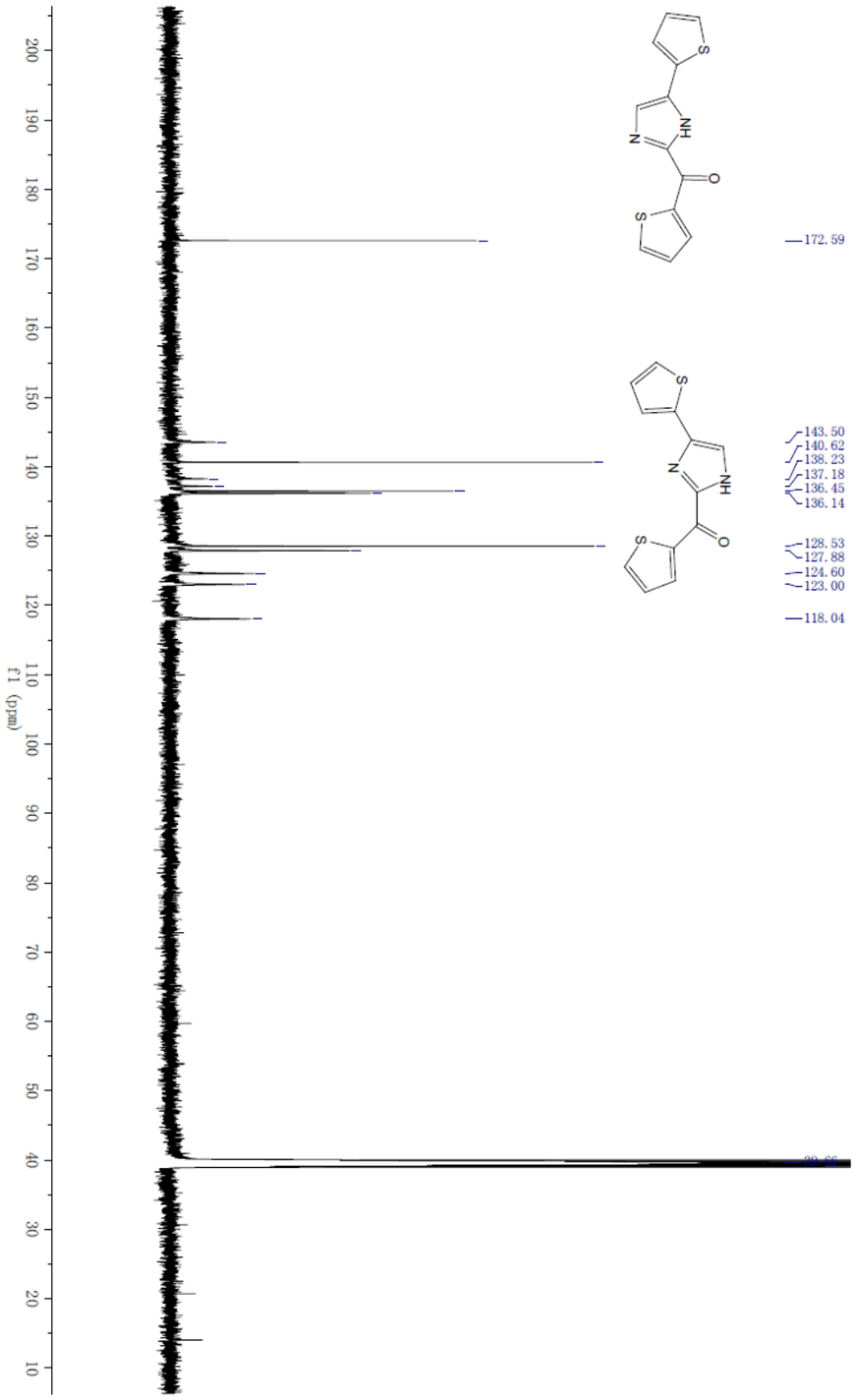


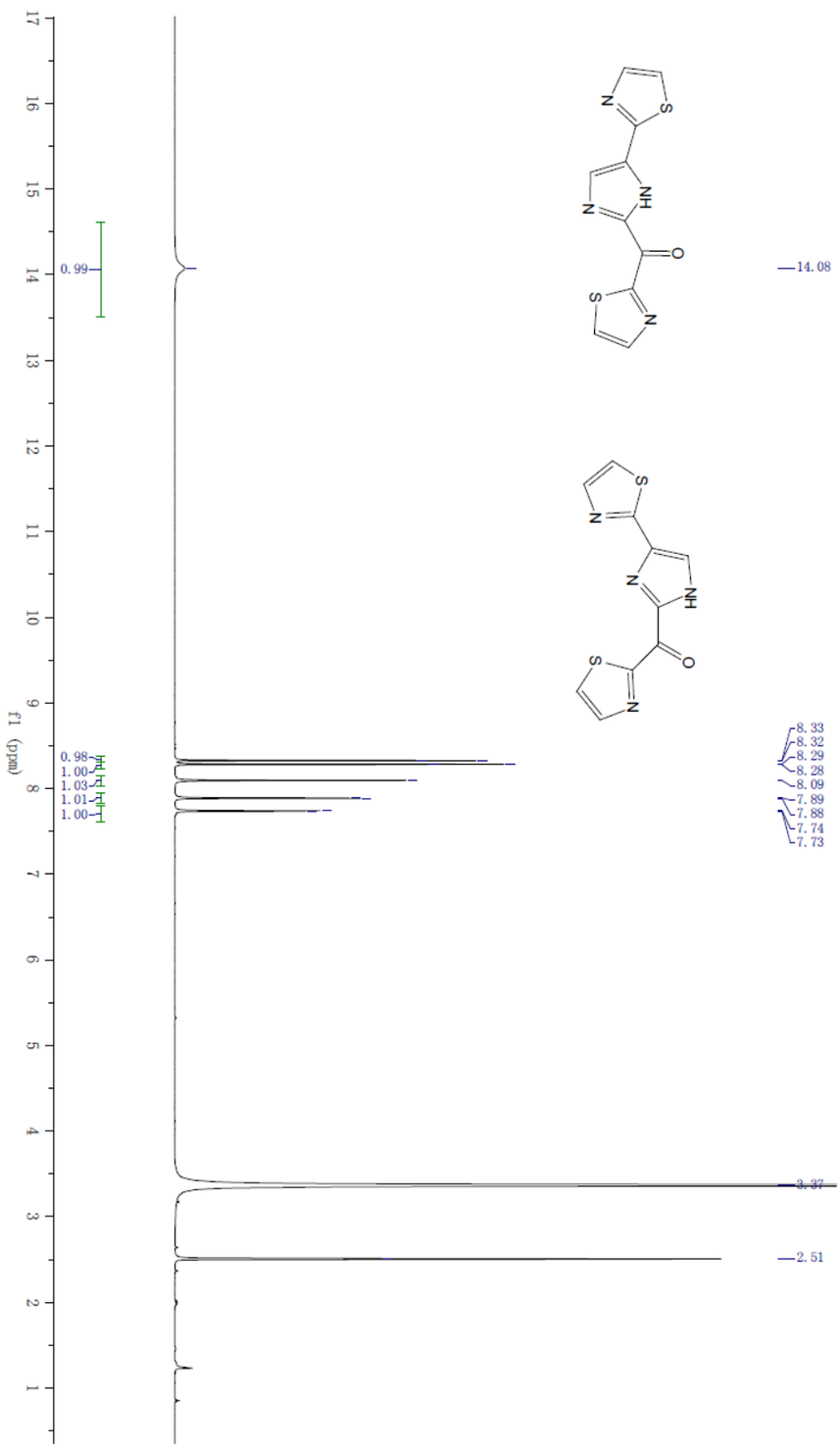
Furan-2-yl(4-(furan-2-yl)-1H-imidazol-2-yl)methanone (2n) and furan-2-yl(5-(furan-2-yl)-1H-imidazol-2-yl)methanone (2n')



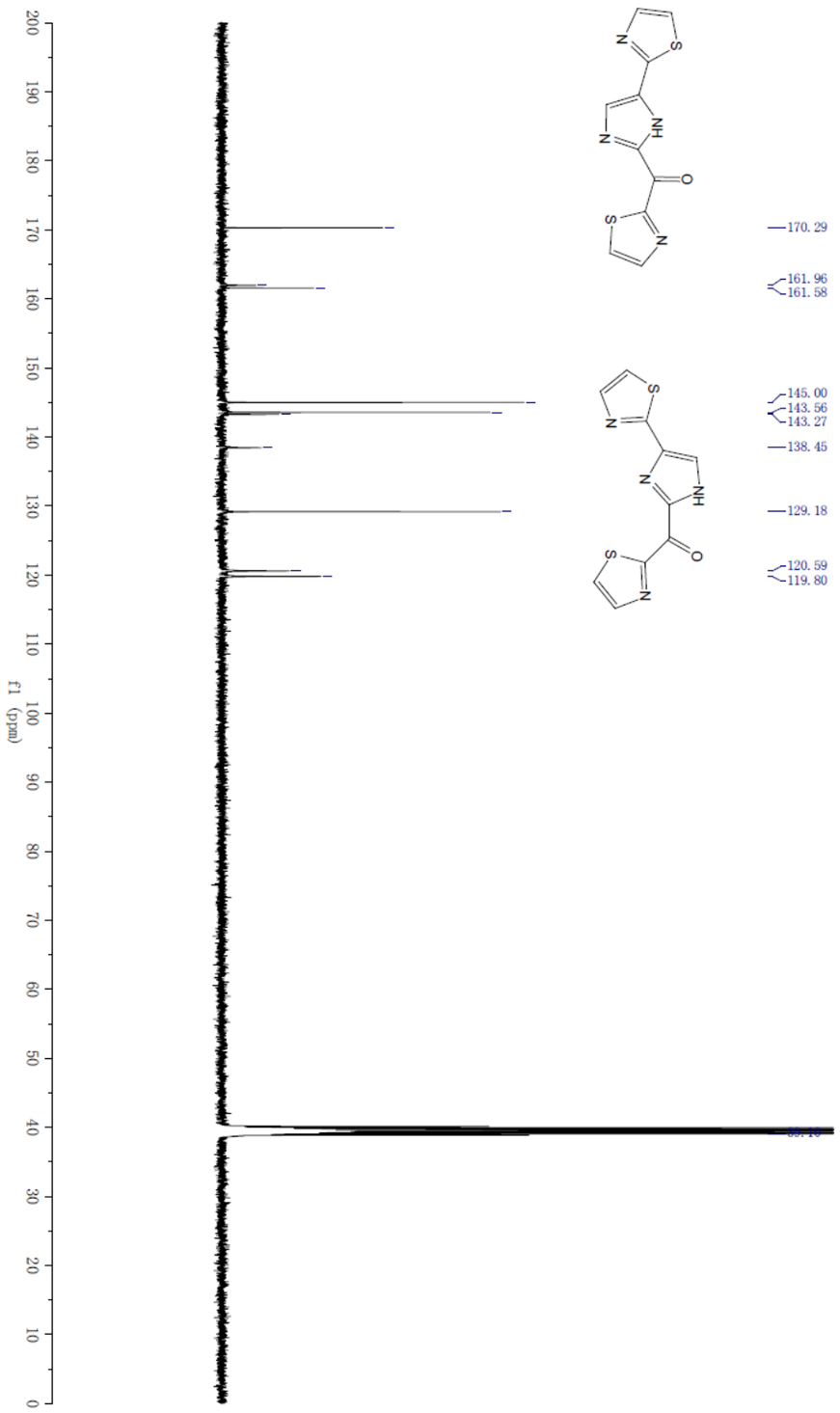


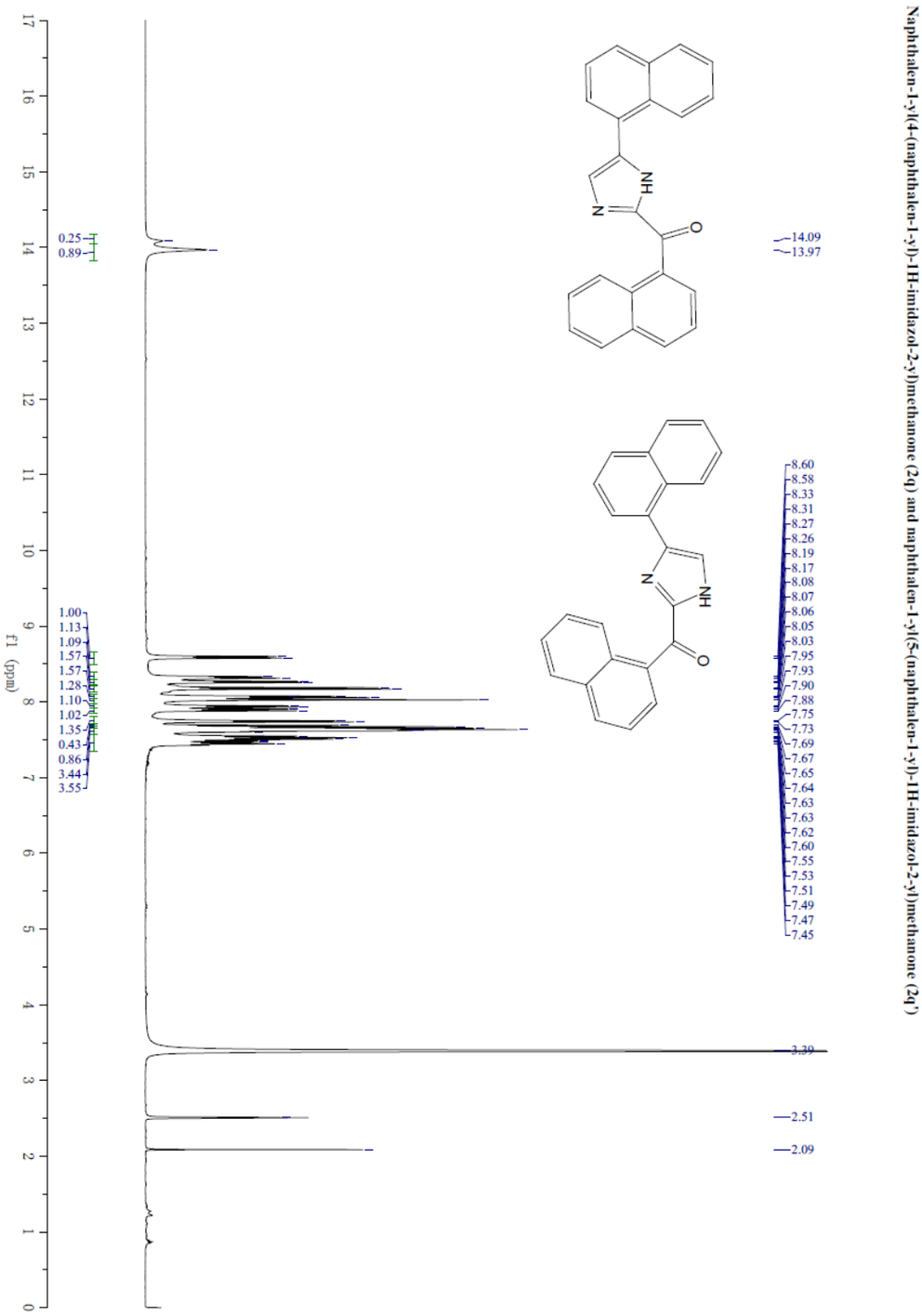
Thiophen-2-yl(4-(thiophen-2-yl)-1H-imidazol-2-yl)methanone (2o) and thiophen-2-yl(5-(thiophen-2-yl)-1H-imidazol-2-yl)methanone (2o')

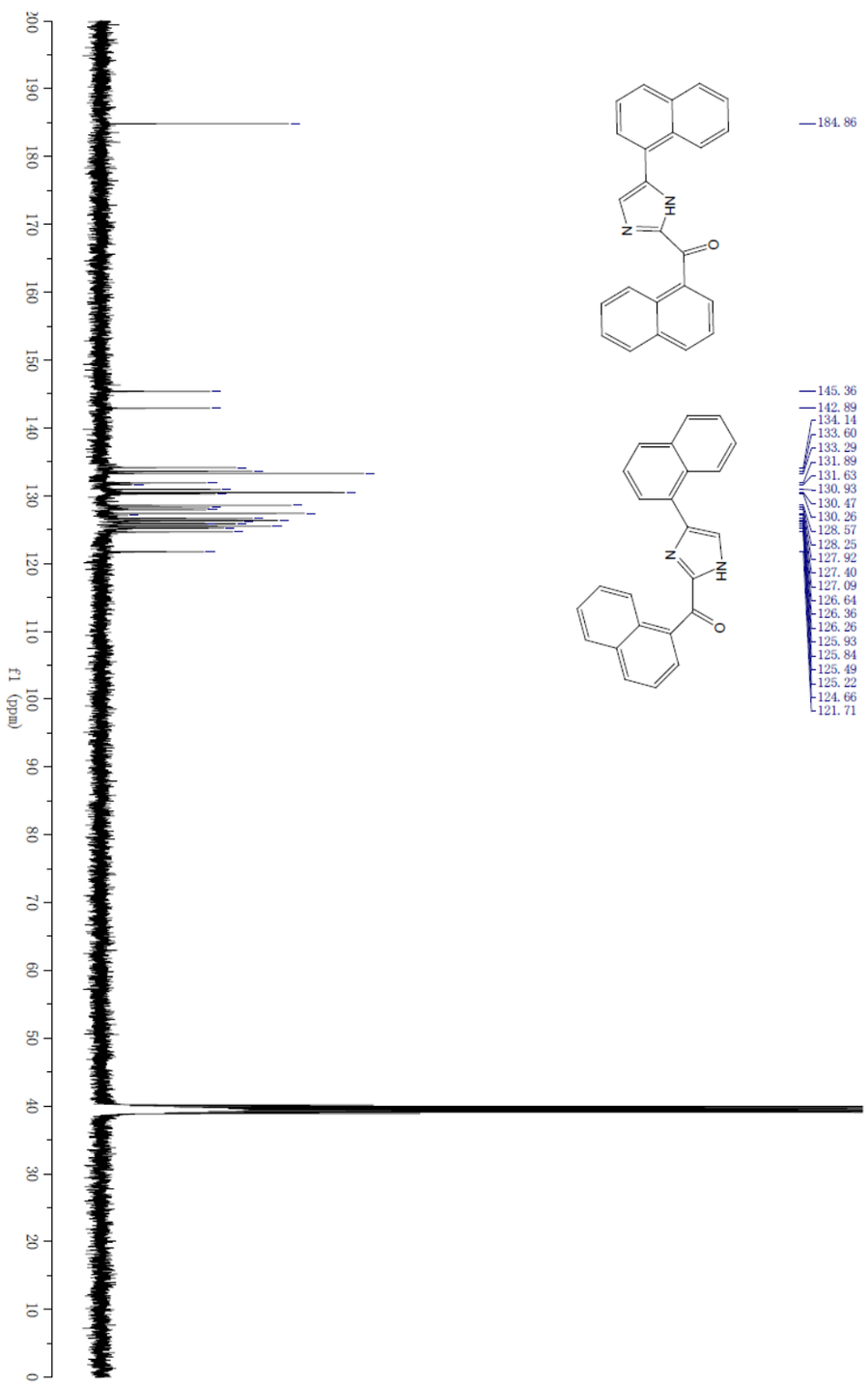


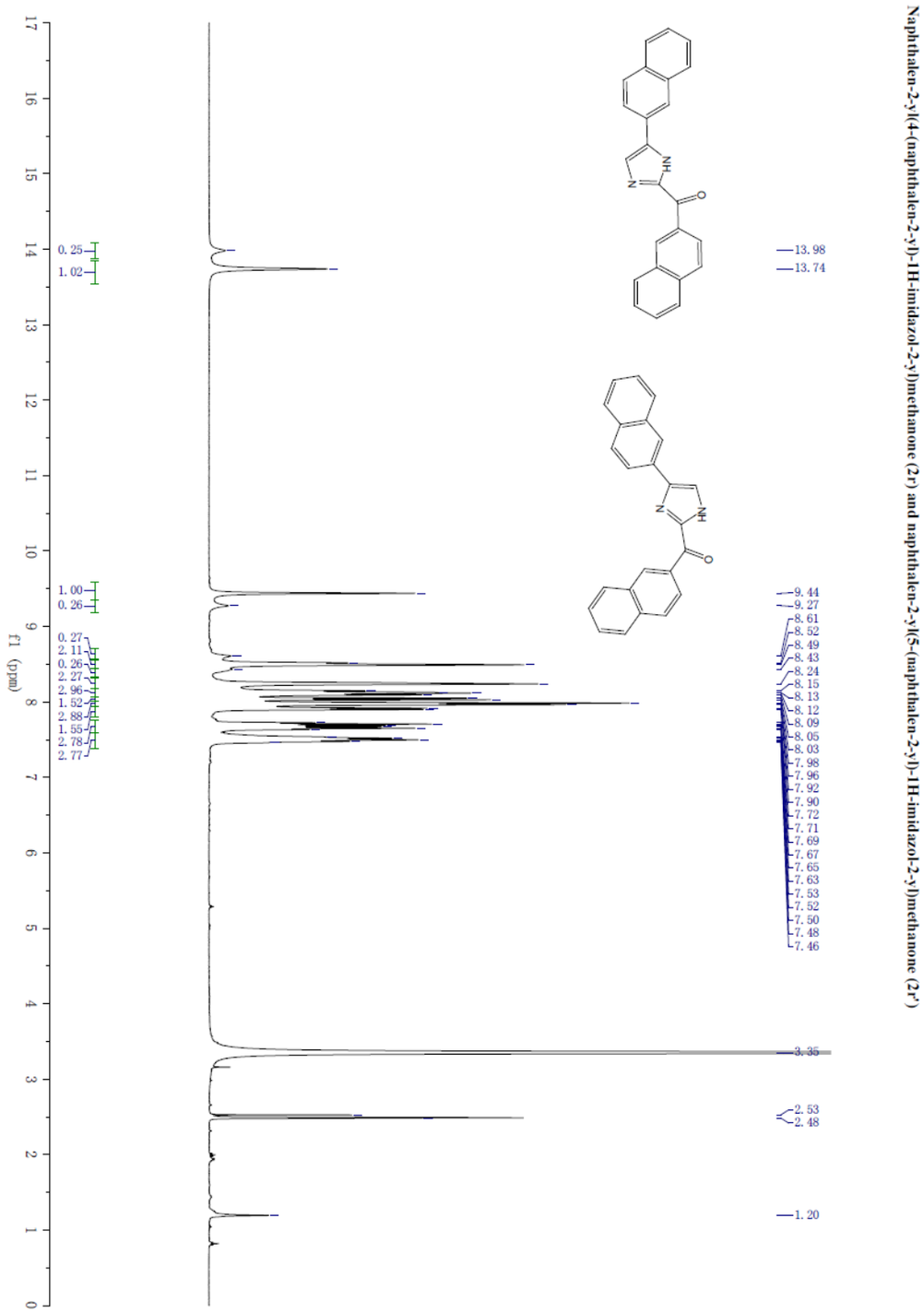


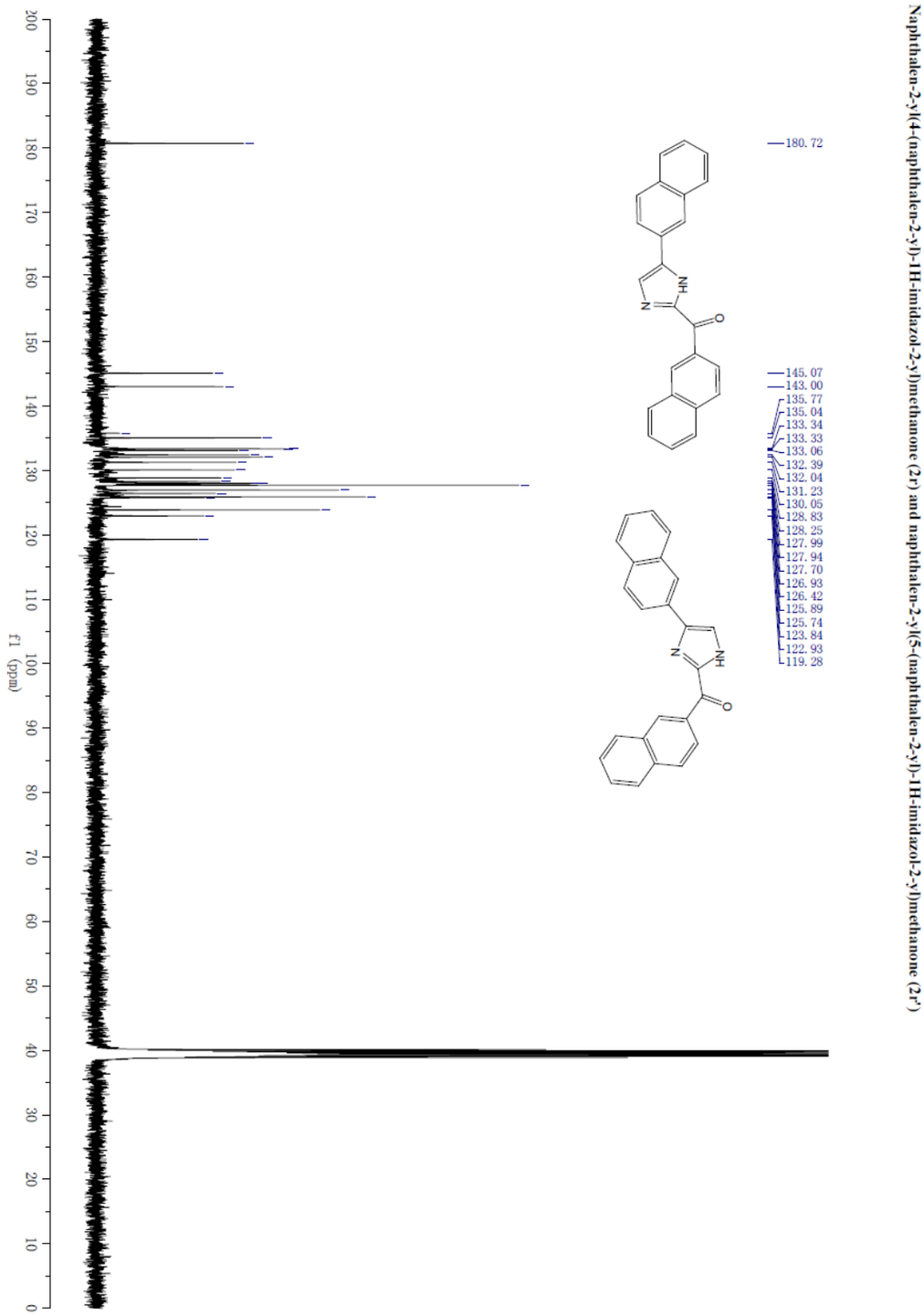
Thiazol-2-yl(4-(thiazol-2-yl)-1H-imidazol-2-yl)methanone (2p) and thiazol-2-yl(5-(thiazol-2-yl)-1H-imidazol-2-yl)methanone (2p')

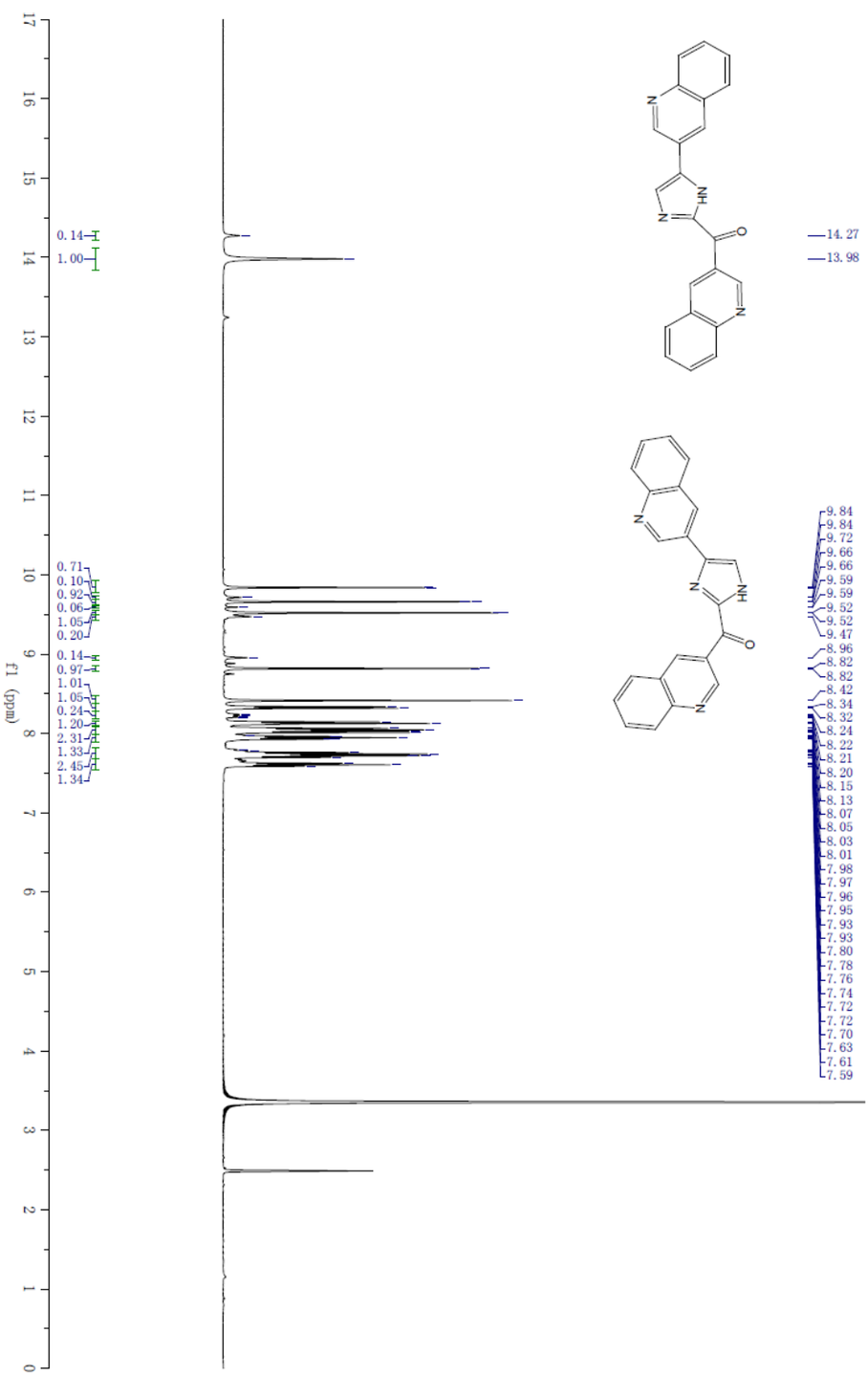


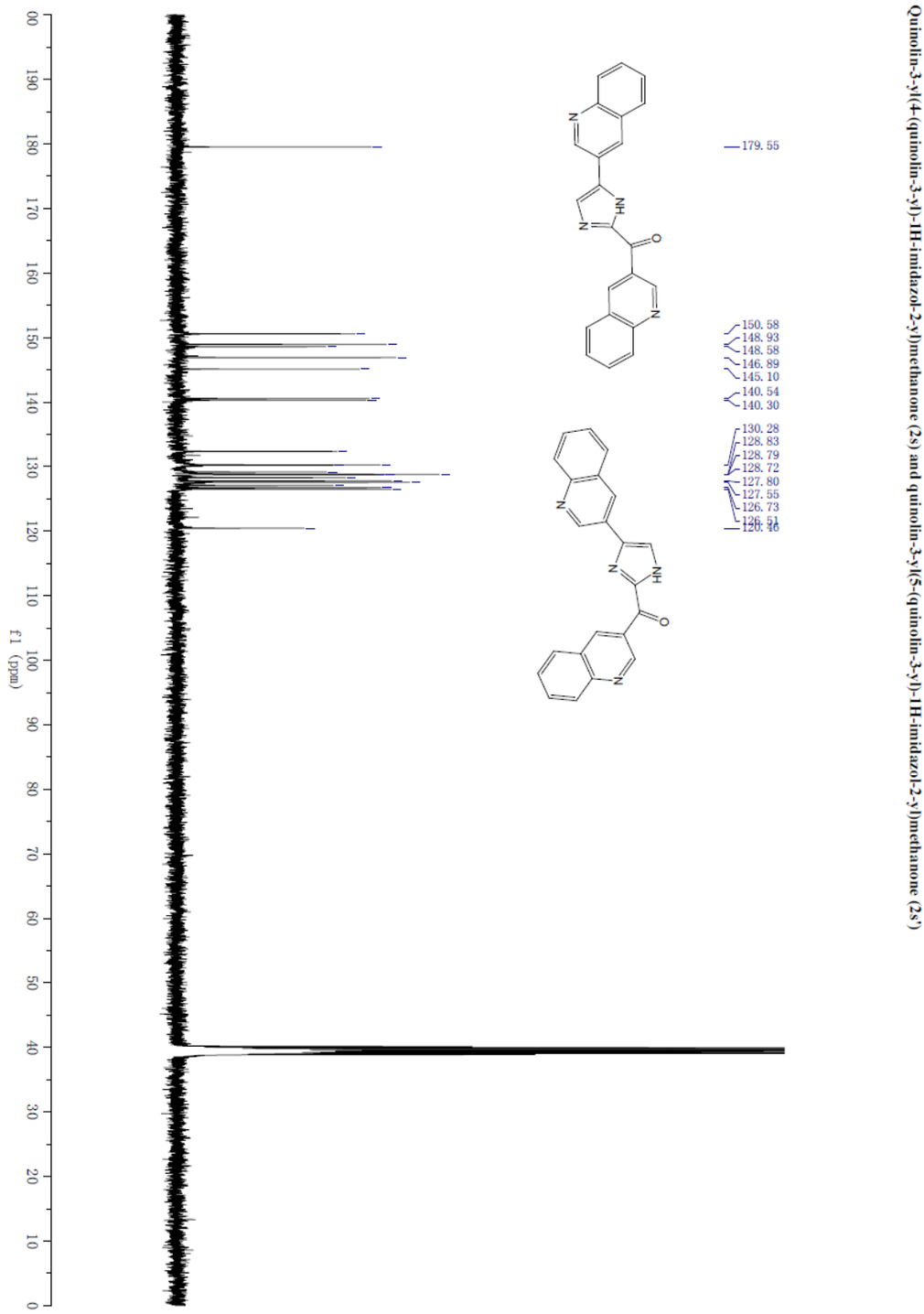


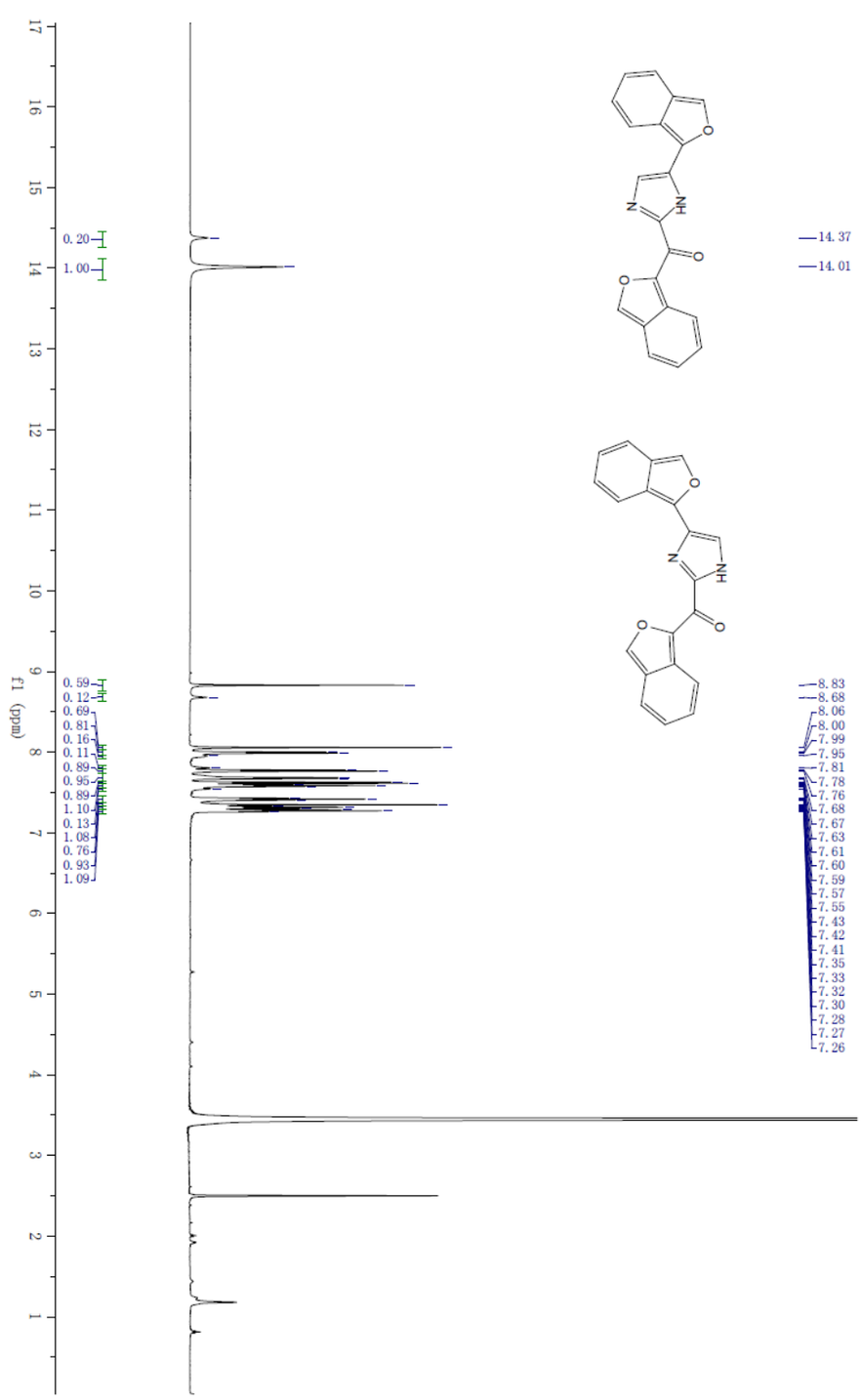




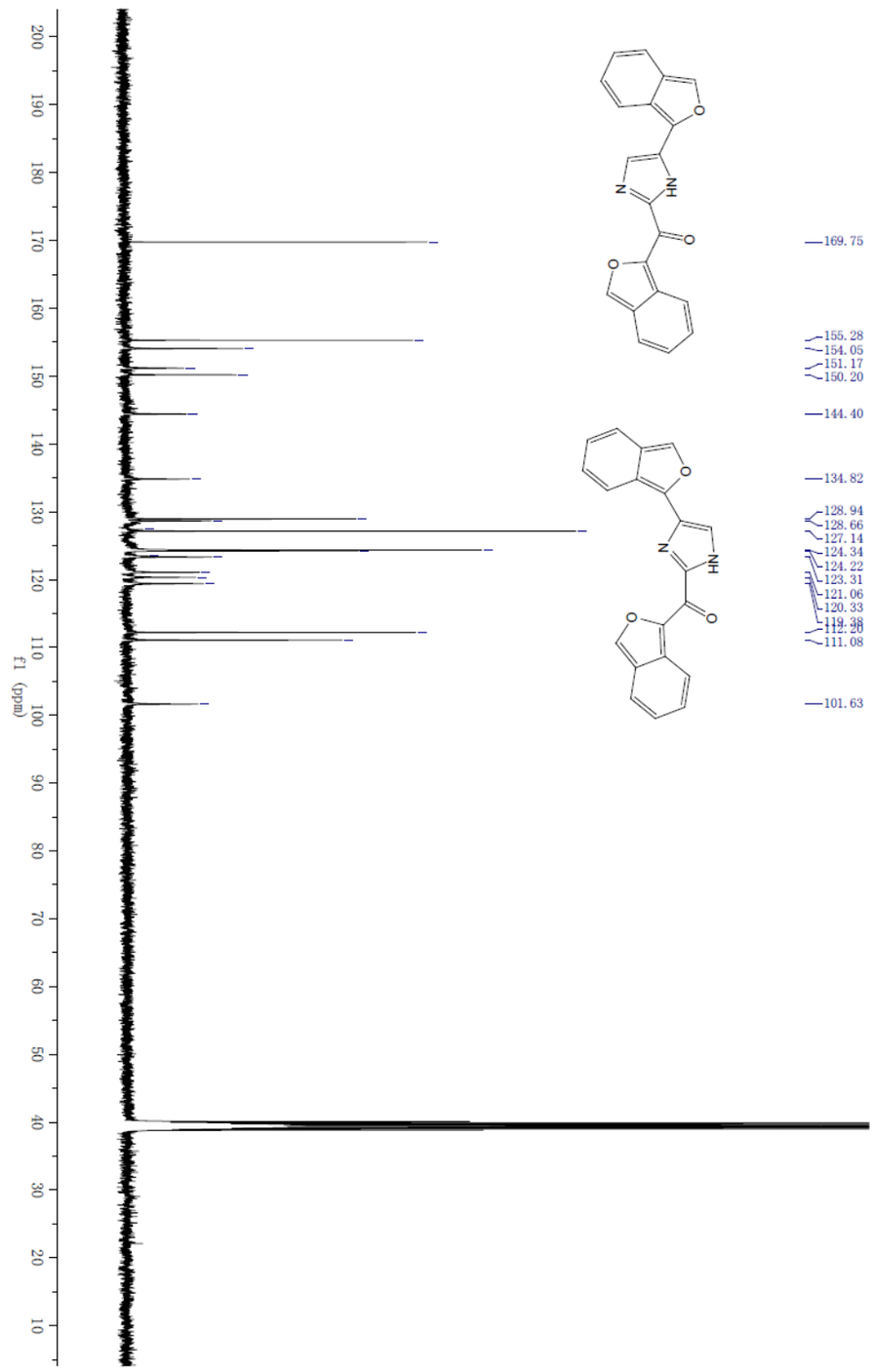




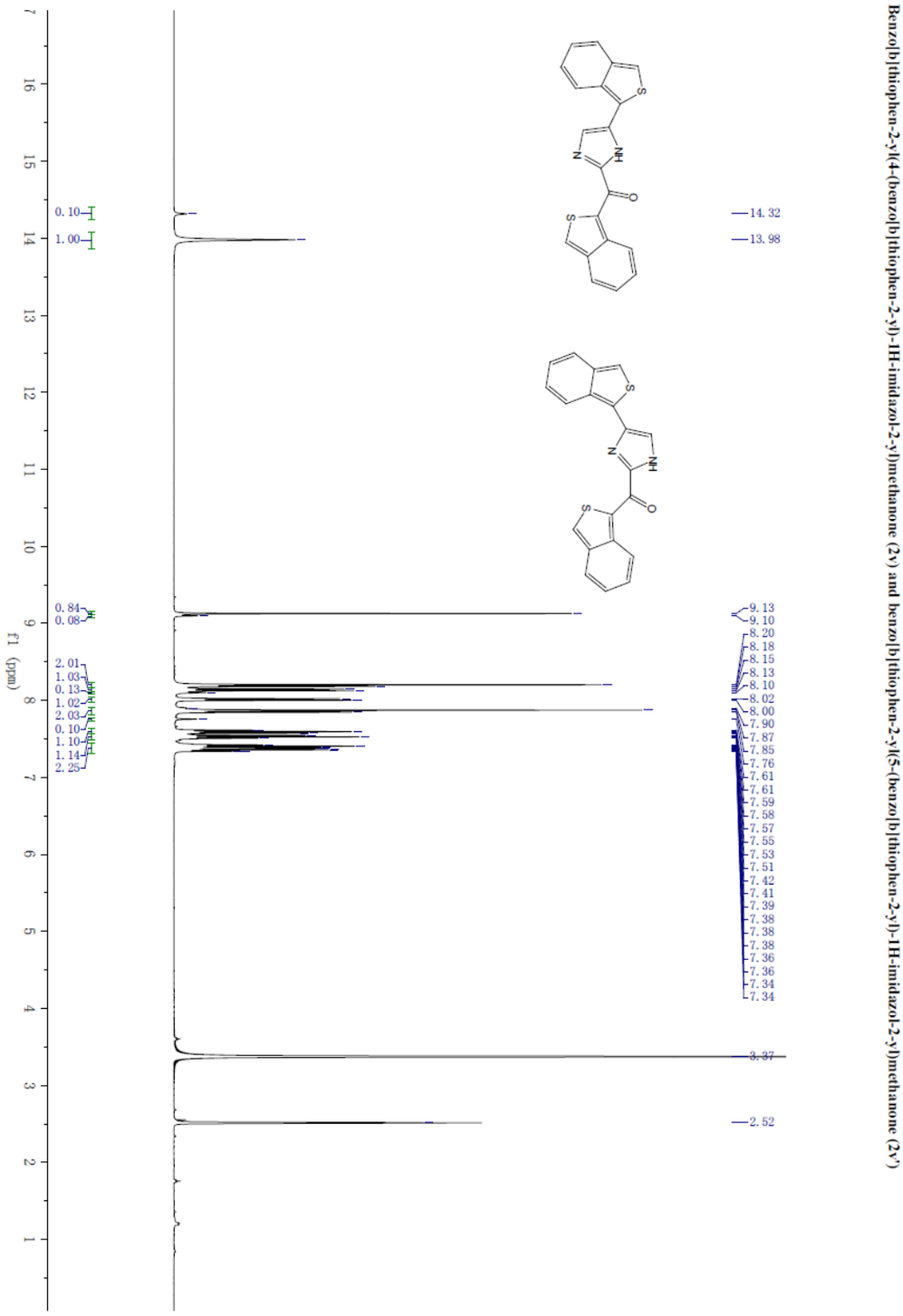


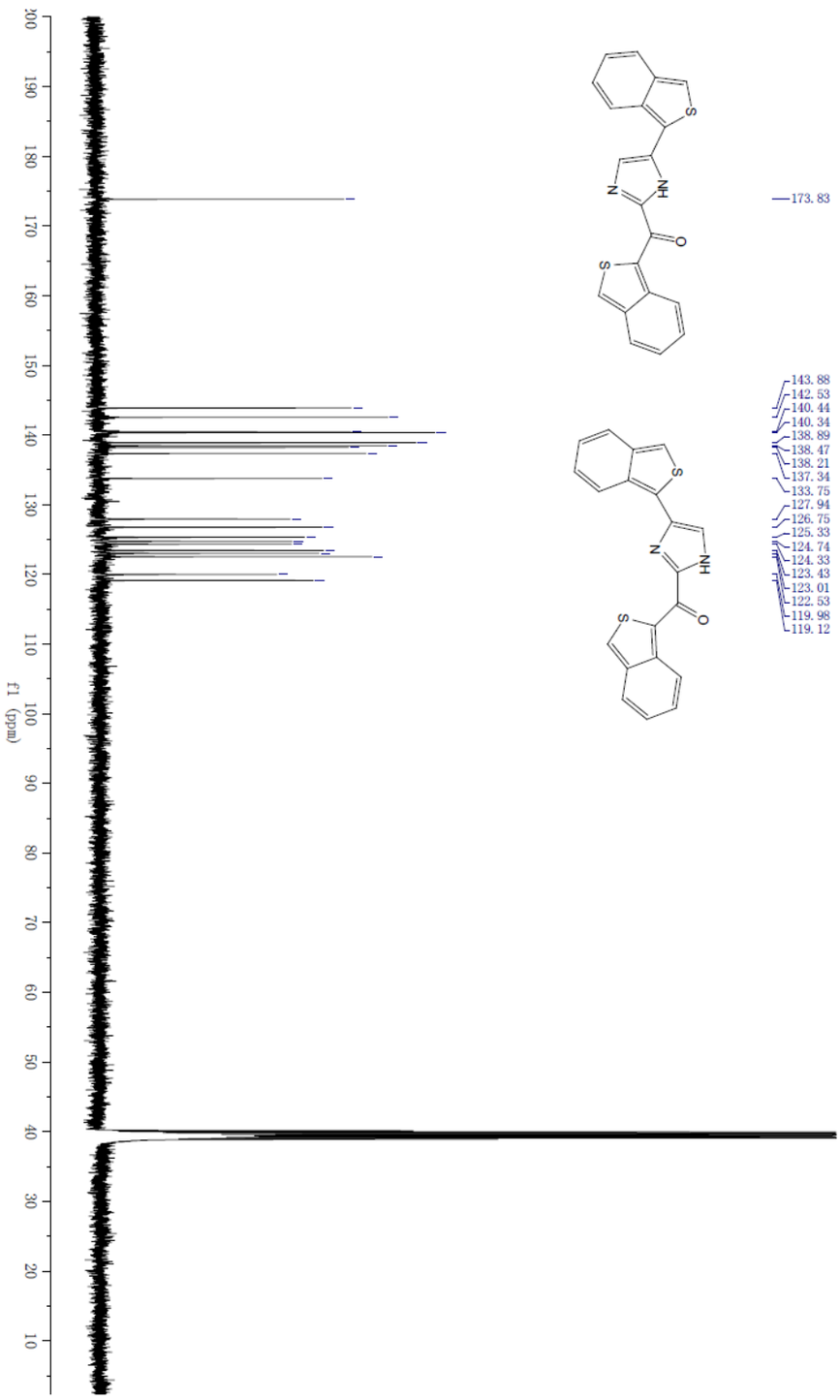


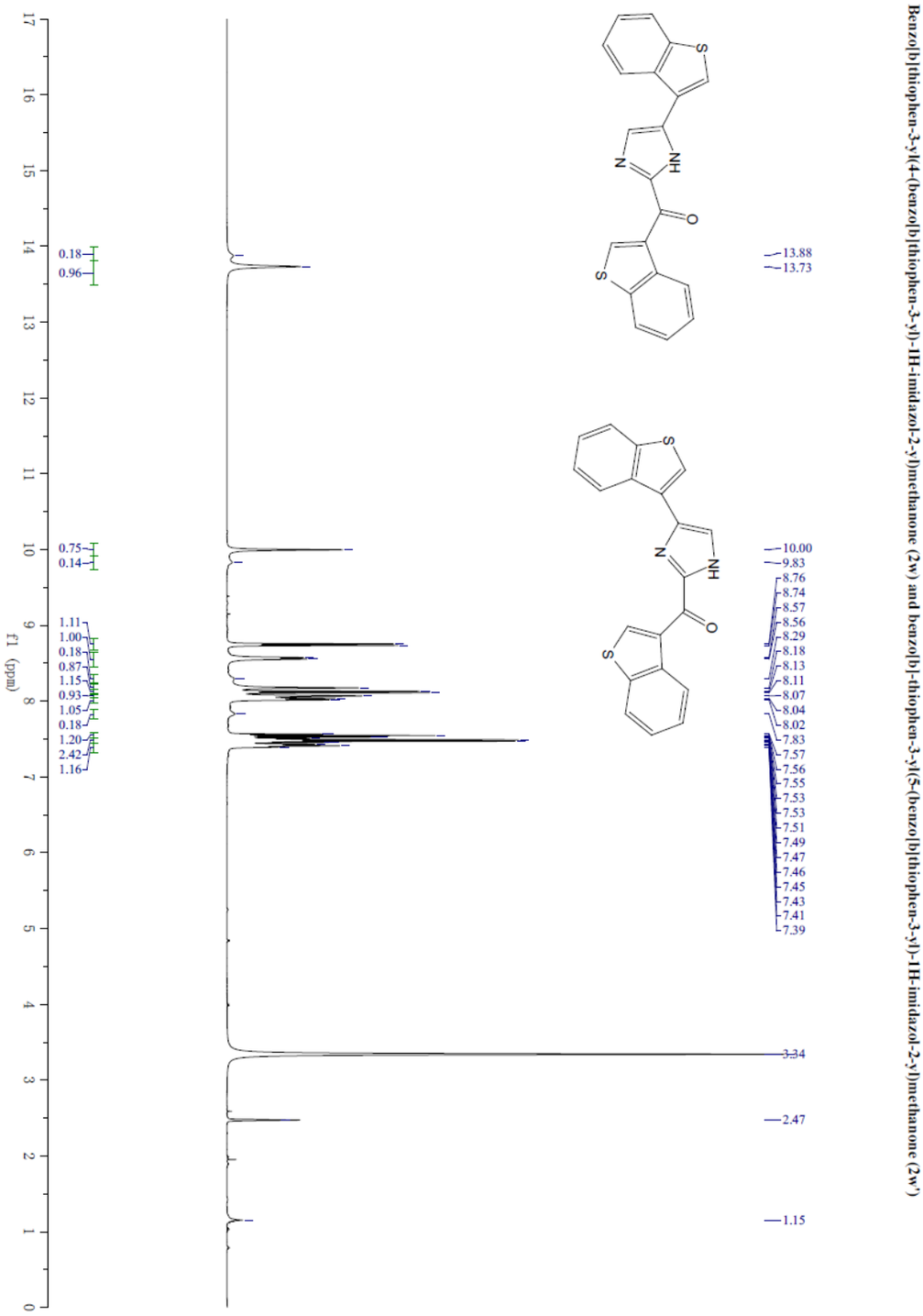
Isobenzofuran-1-yl(4-(isobenzofuran-1-yl)-1H-imidazol-2-yl)methanone (2u) and isobenzofuran-1-yl(5-(isobenzofuran-1-yl)-1H-imidazol-2-yl)methanone (2u')

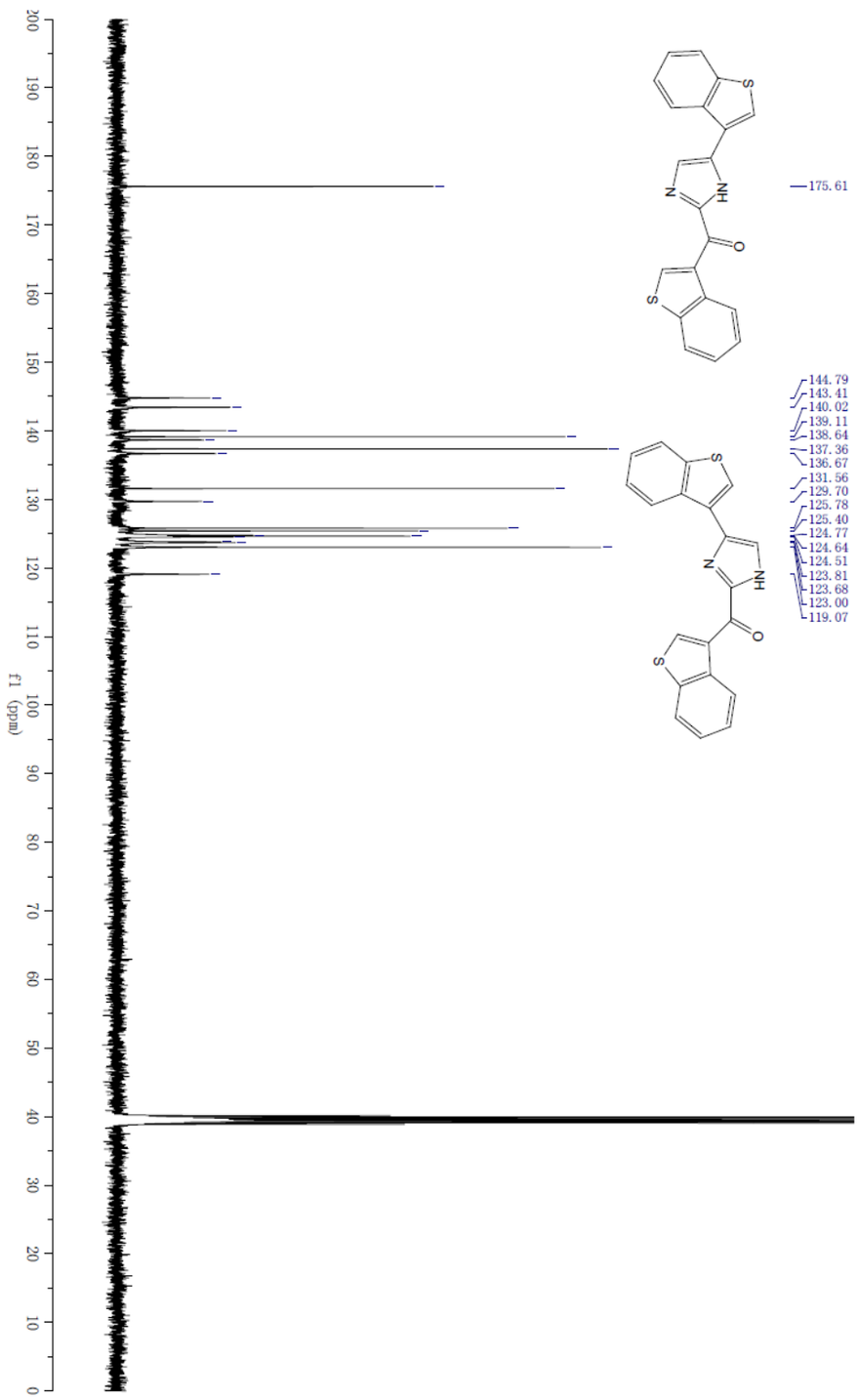


Isobenzofuran-1-yl(4-(isobenzofuran-1-yl)-1H-imidazol-2-yl)methanone (2u) and isobenzofuran-1-yl(5-(isobenzofuran-1-yl)-1H-imidazol-2-yl)methanone (2u')

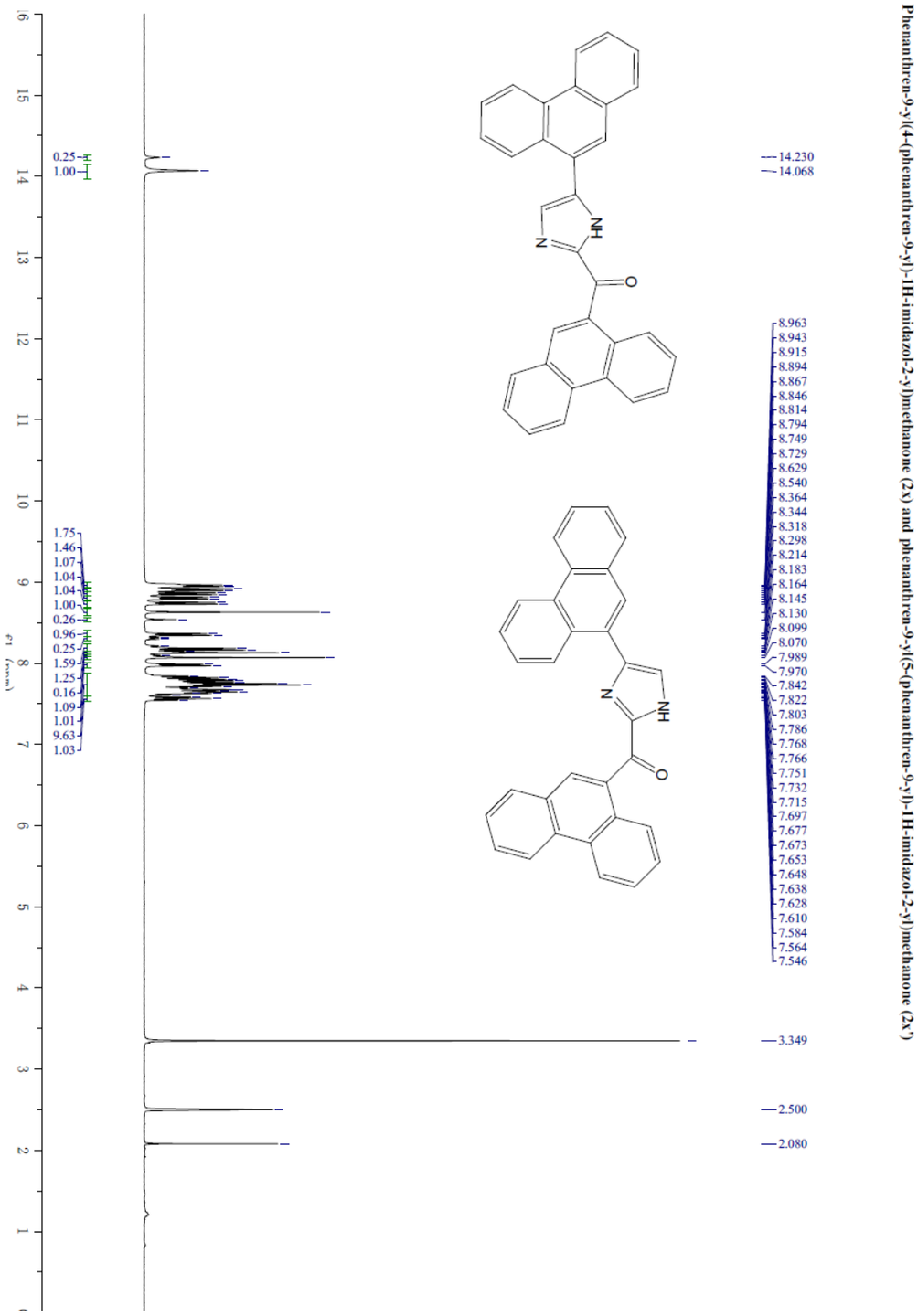


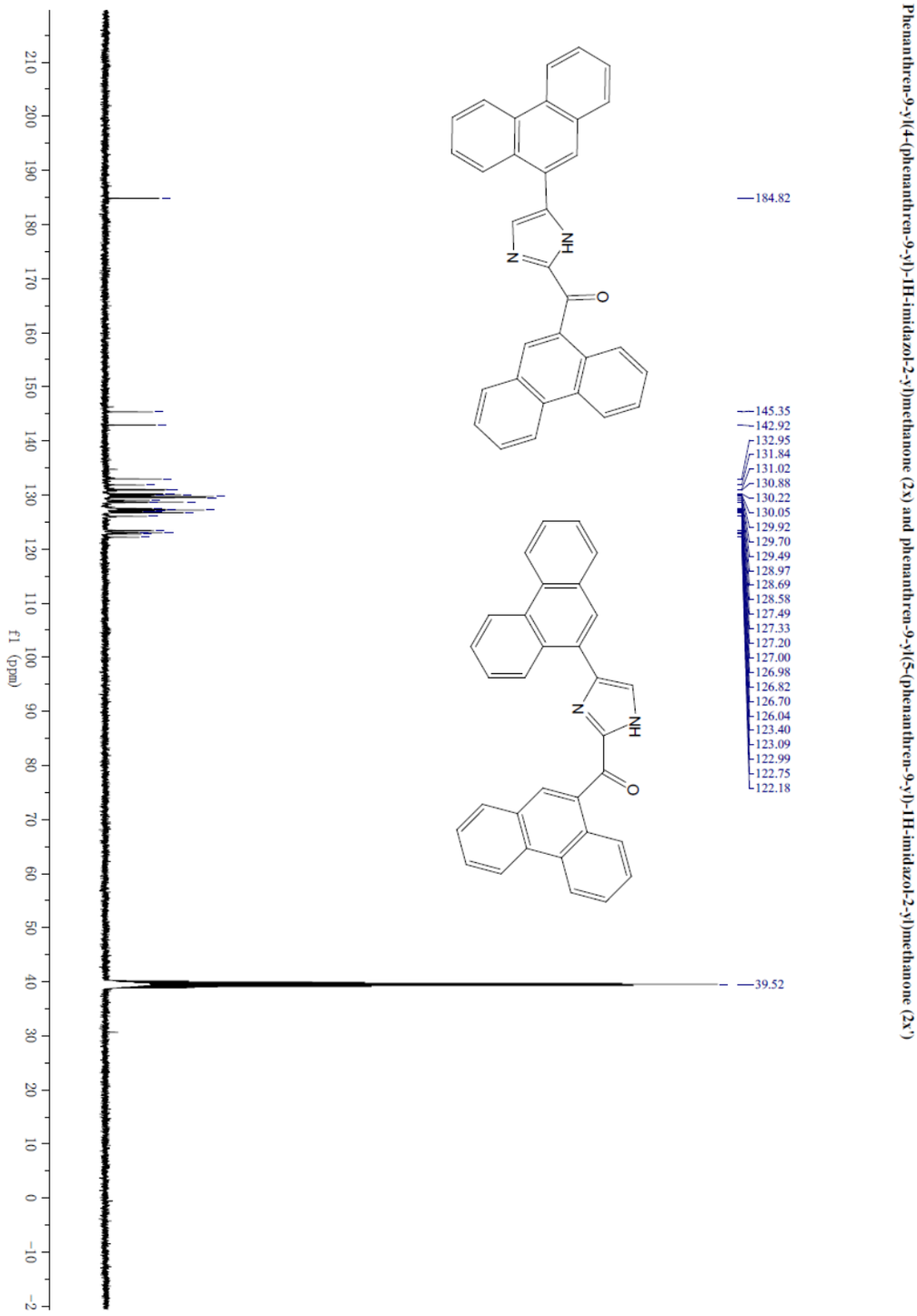




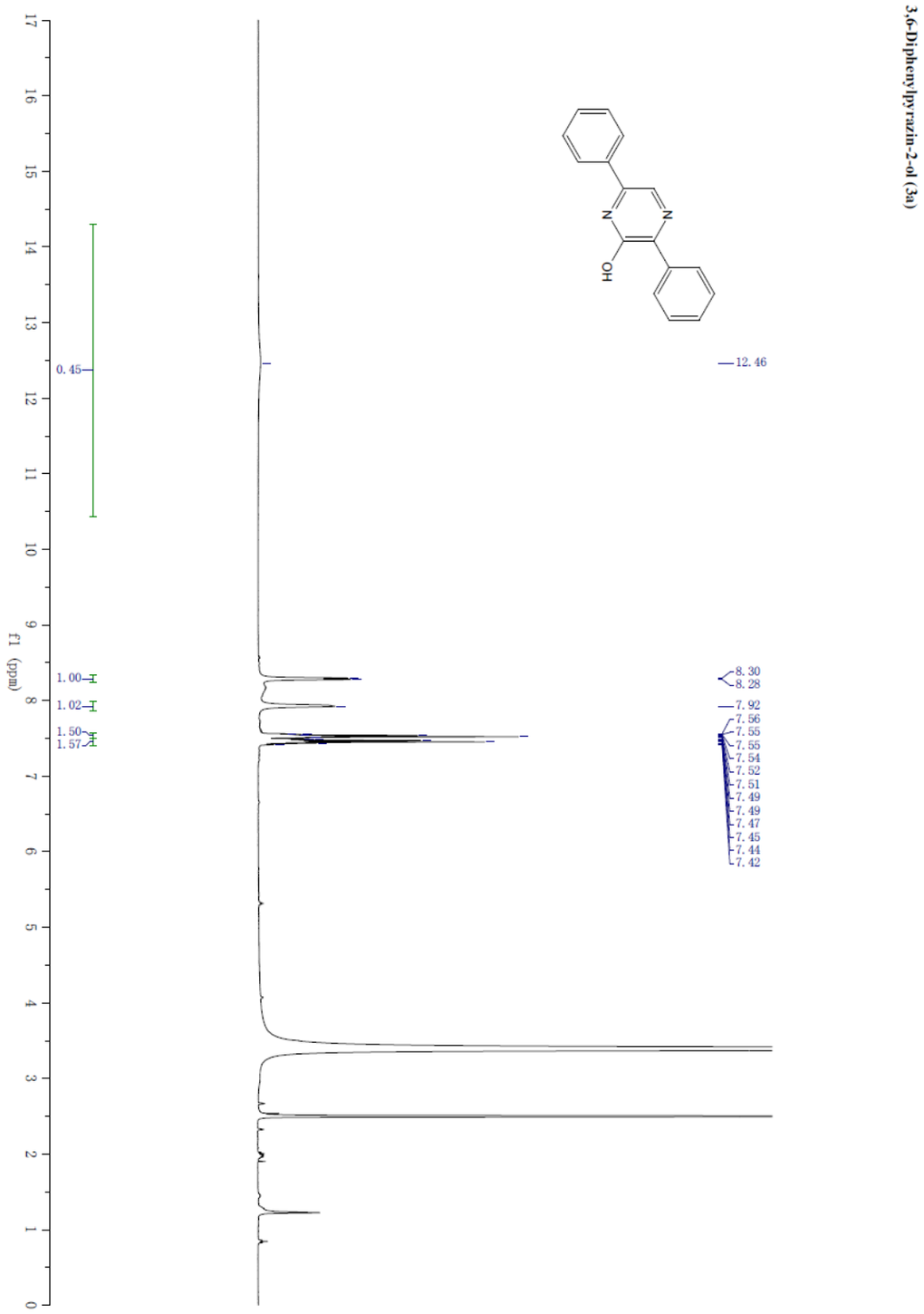


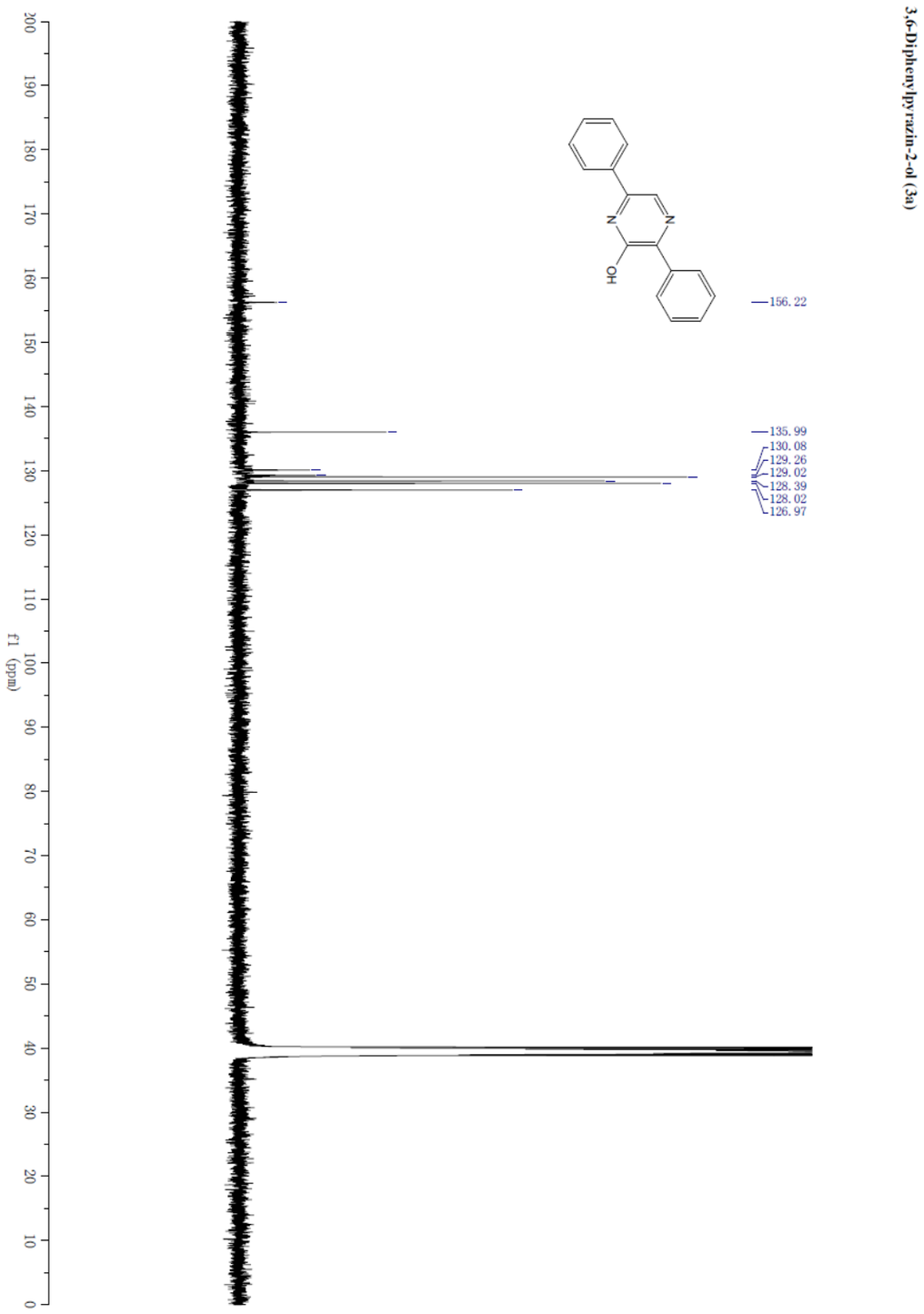
Benzo[b]thiophen-3-yl(4-(benzo[b]thiophen-3-yl)-1H-imidazol-2-yl)methanone (2w) and benzo[b]-thiophen-3-yl(5-(benzo[b]thiophen-3-yl)-1H-imidazol-2-yl)methanone (2w')

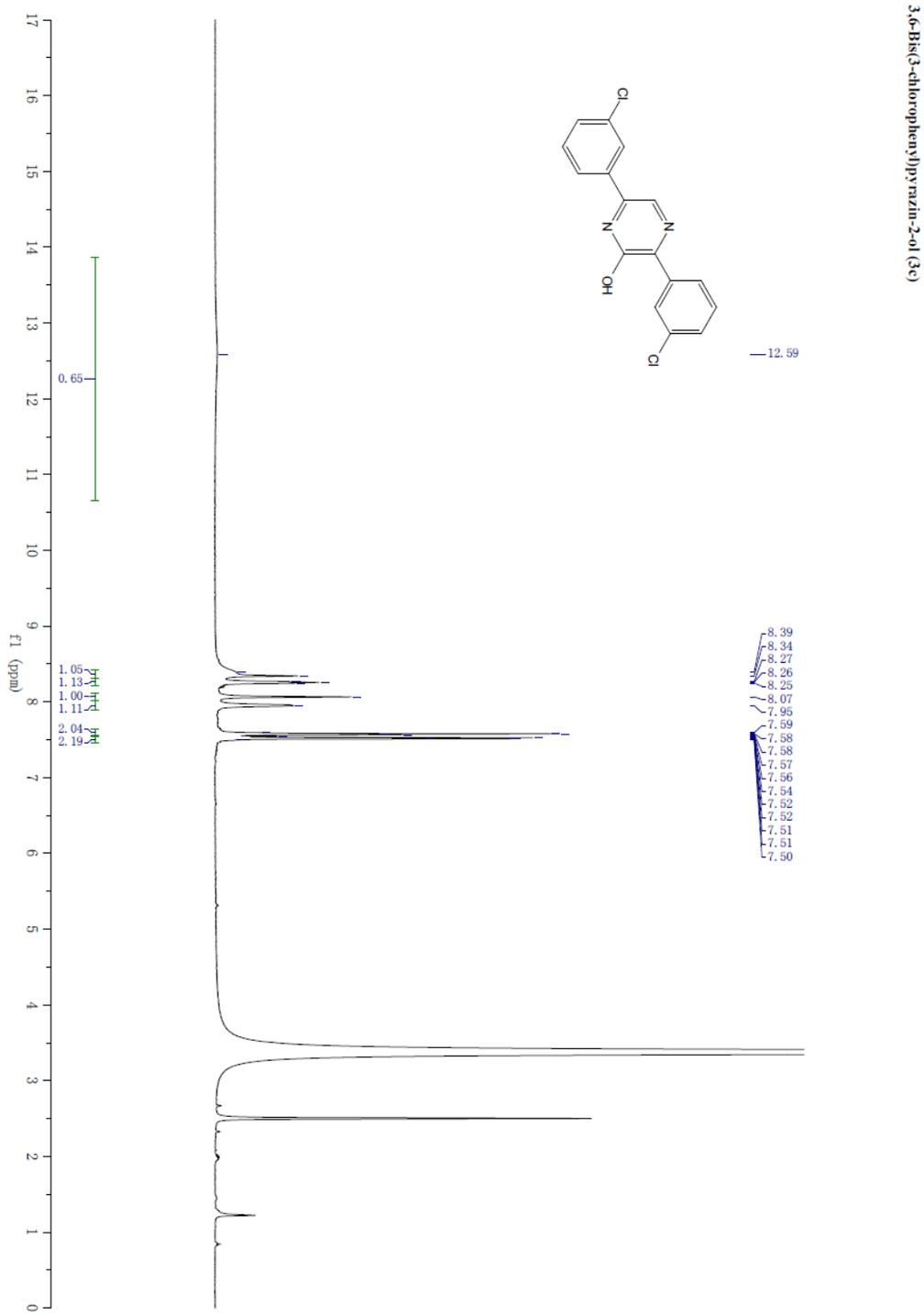


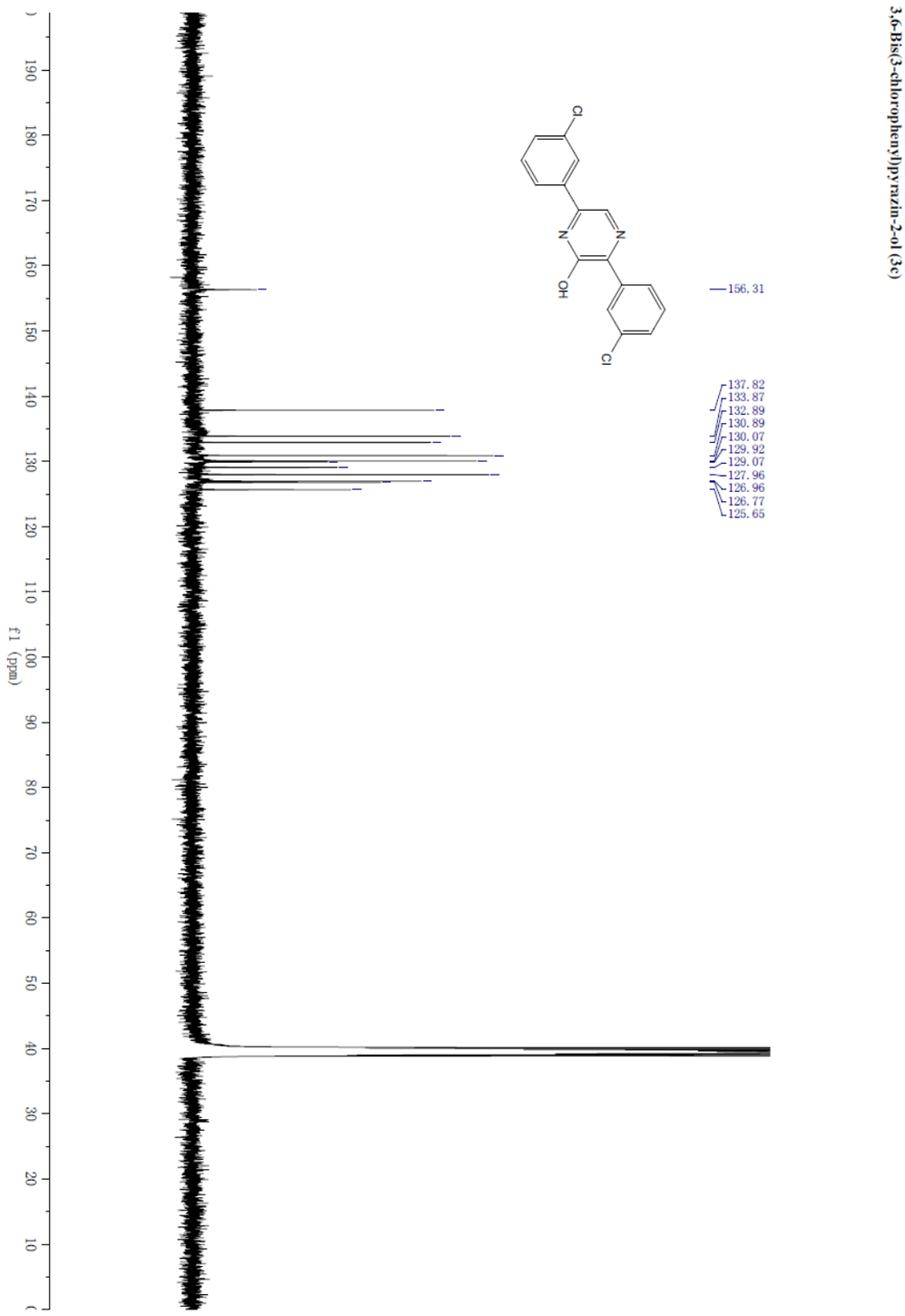


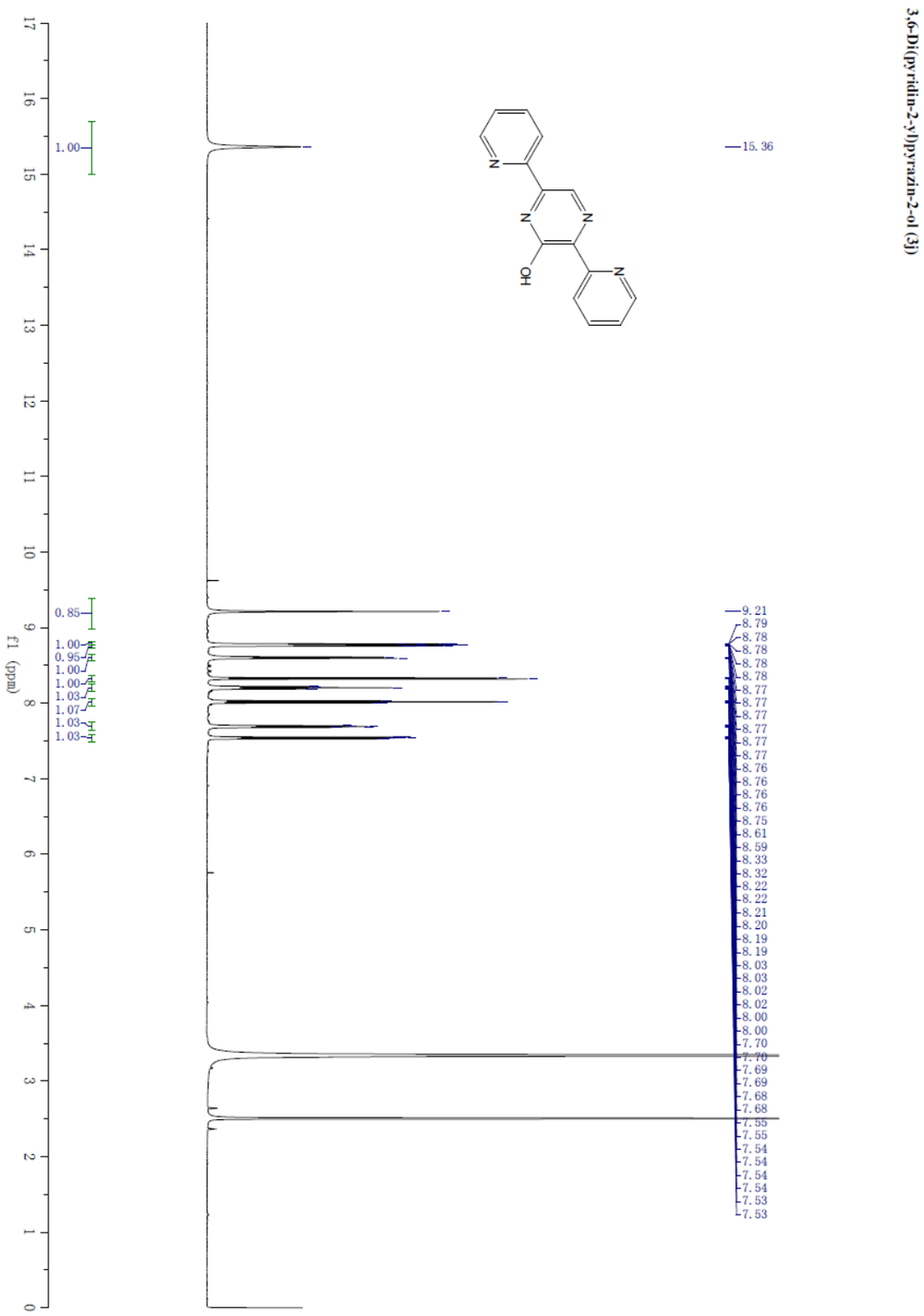
Phenanthren-9-yl(4-(phenanthren-9-yl)-1H-imidazol-2-yl)methanone (2x) and phenanthren-9-yl(5-(phenanthren-9-yl)-1H-imidazol-2-yl)methanone (2x')

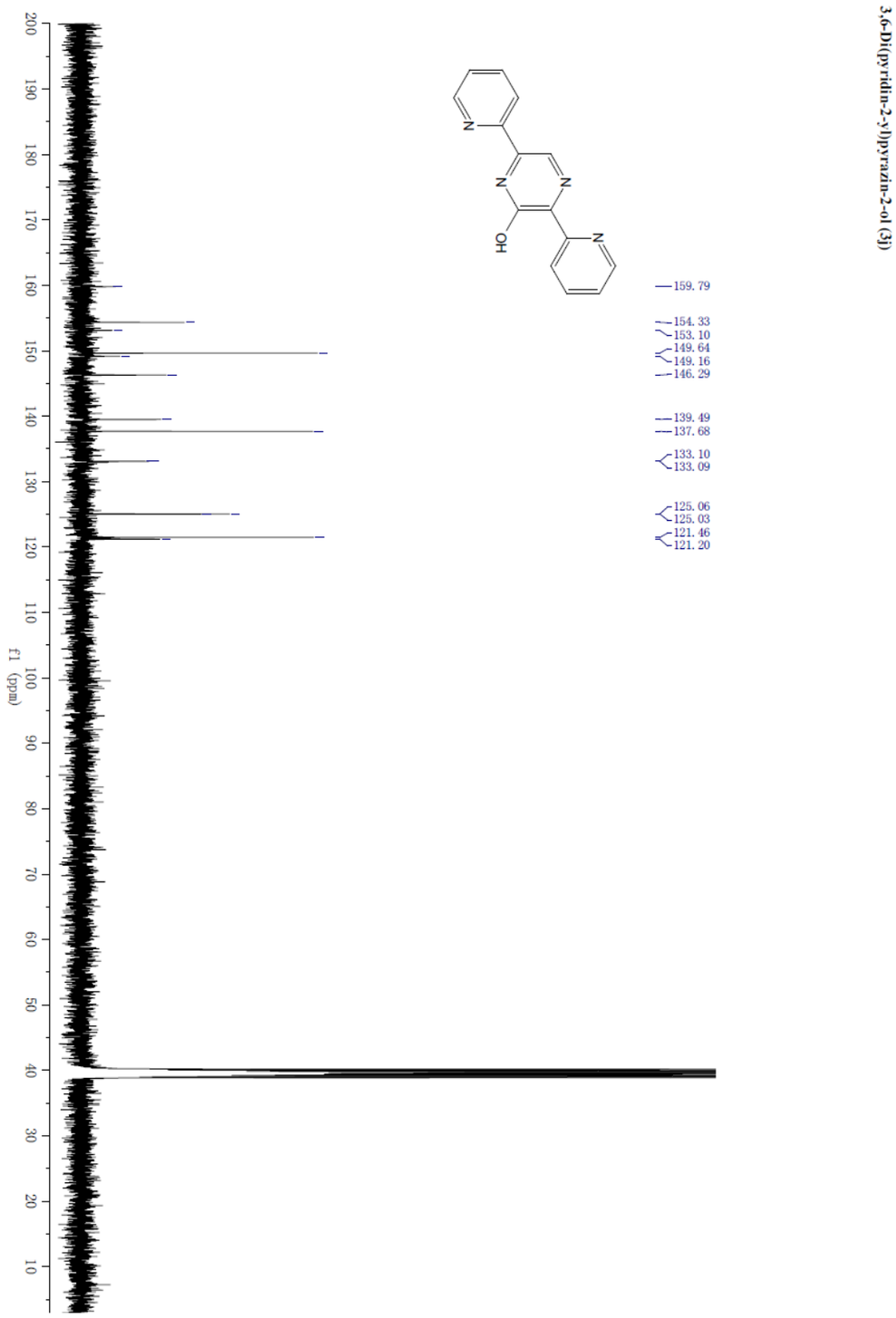


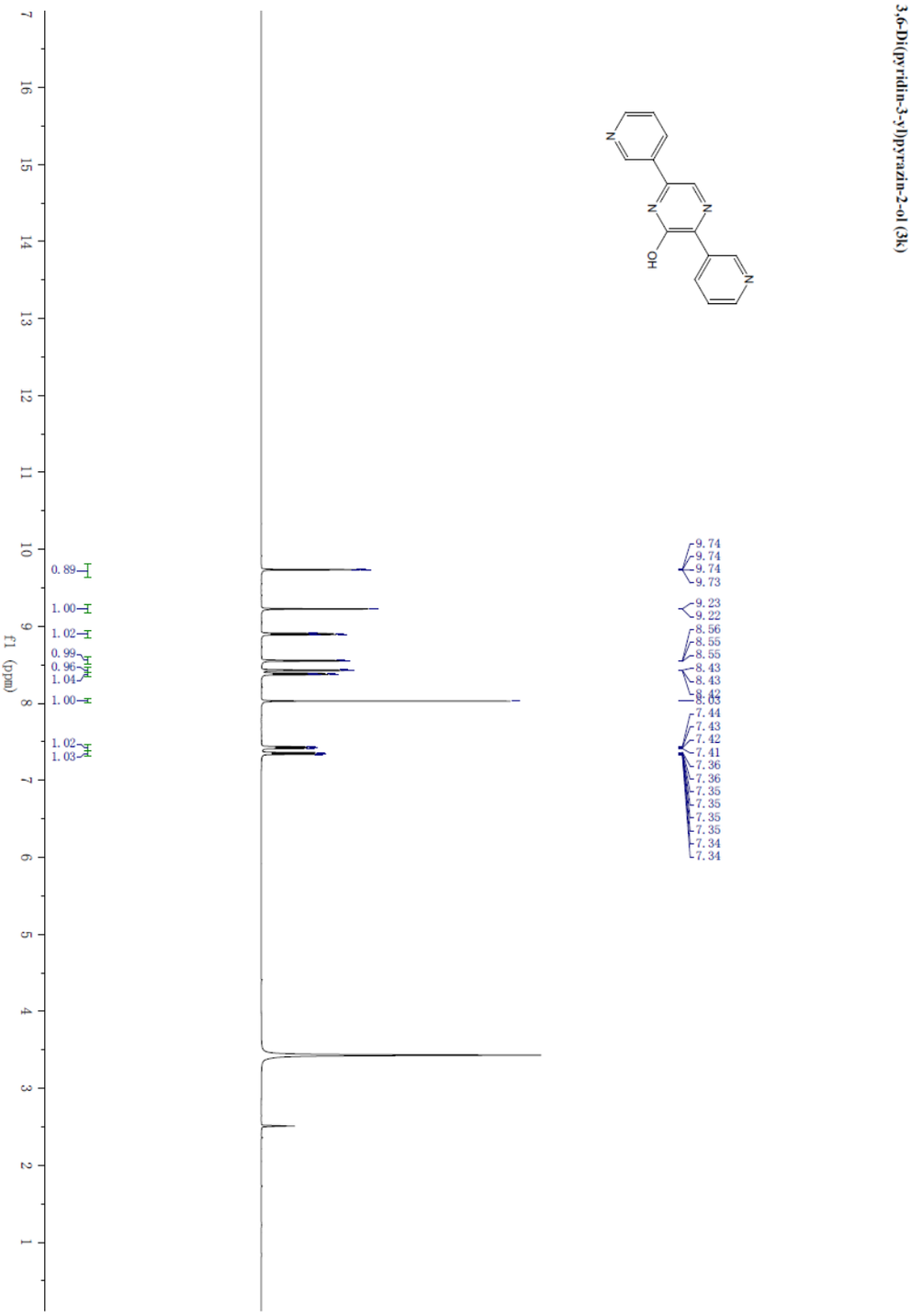


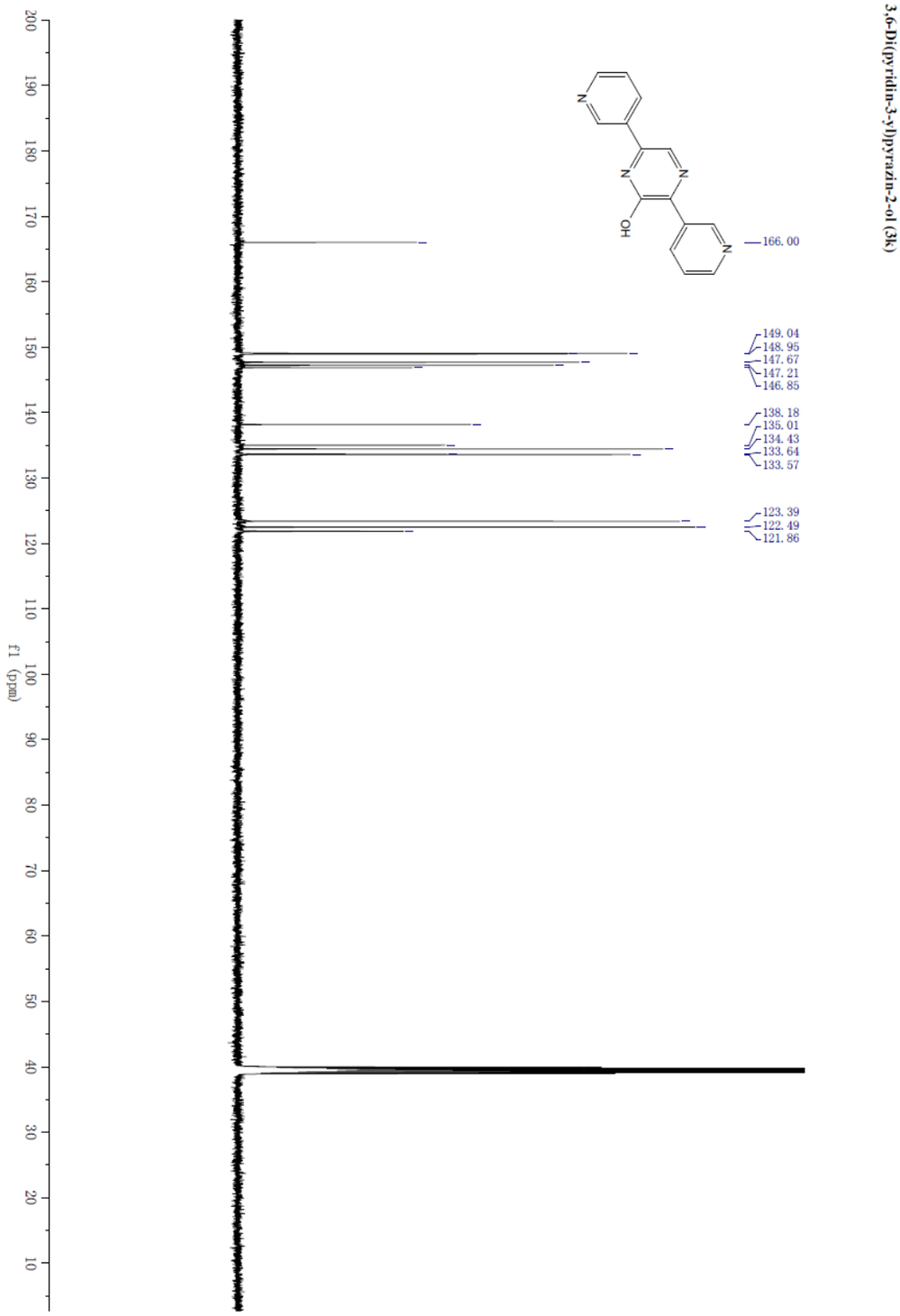


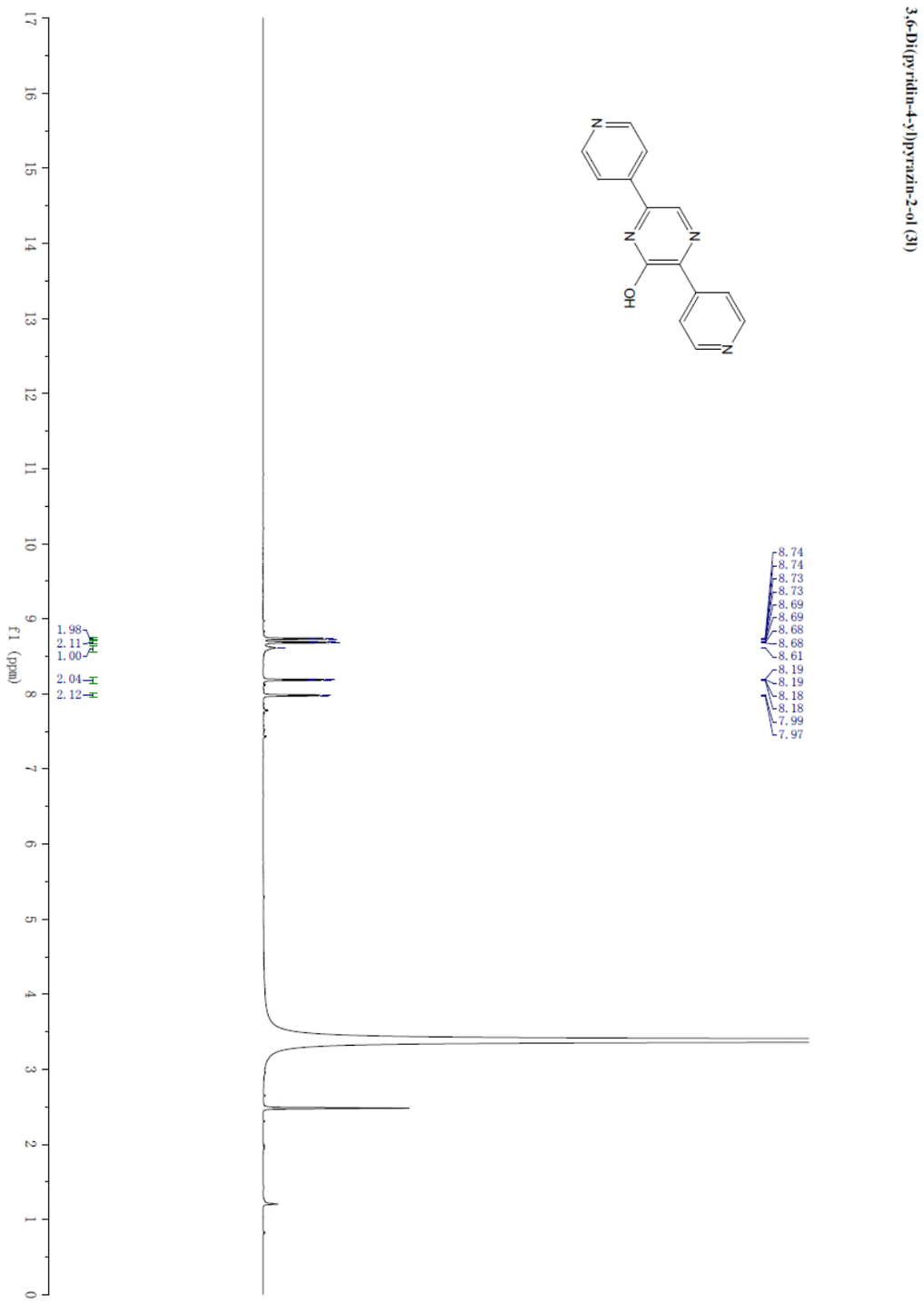


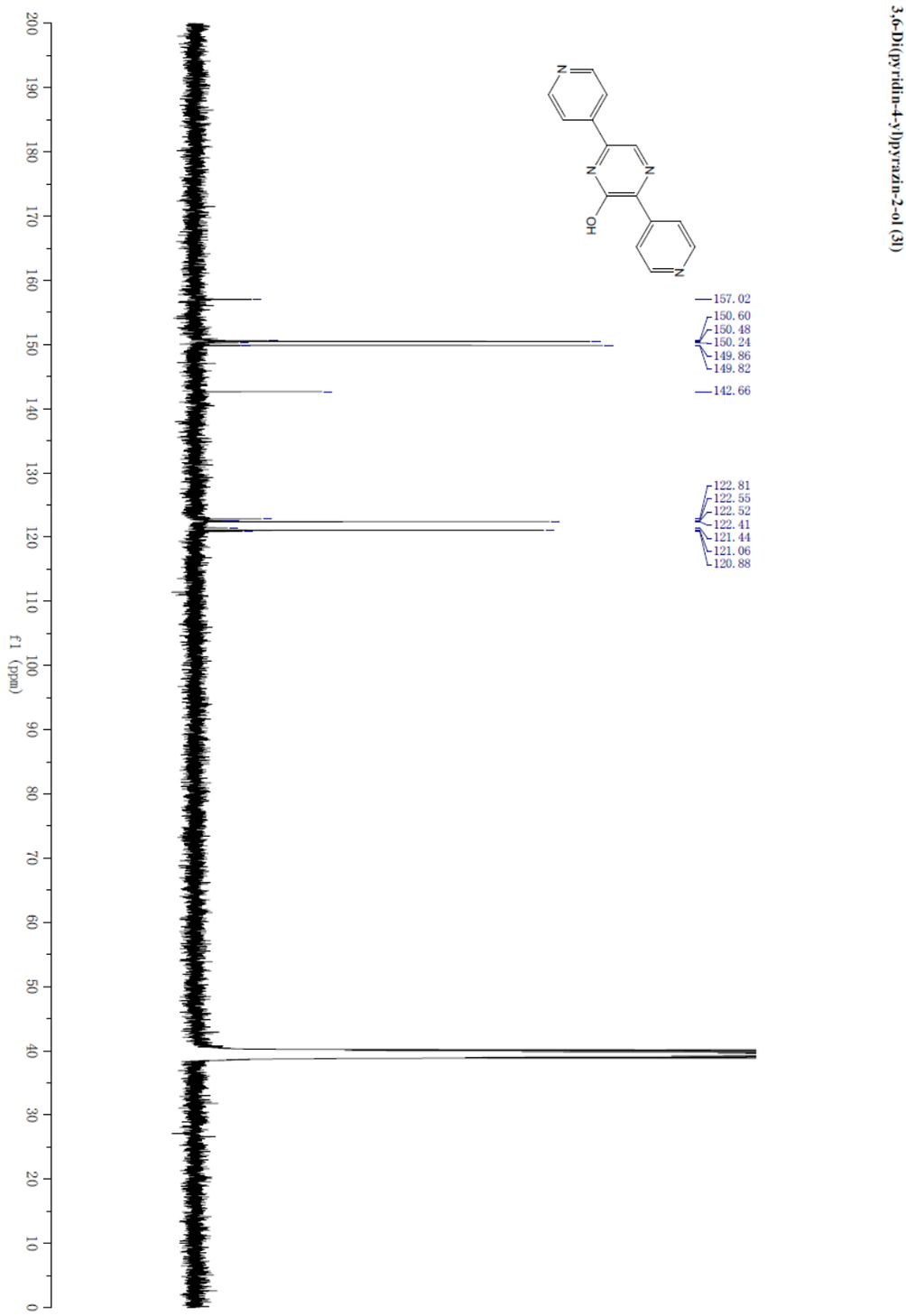


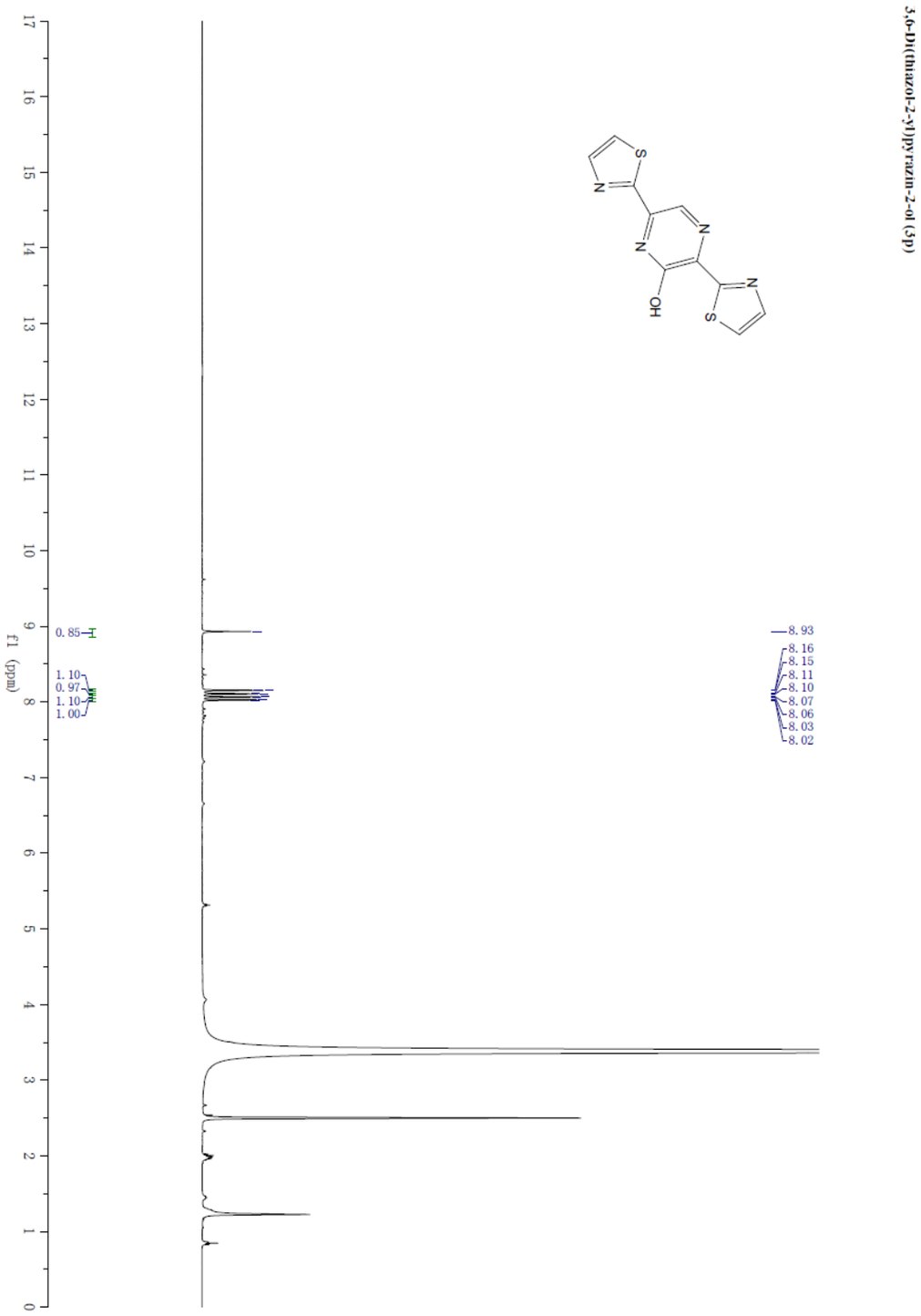


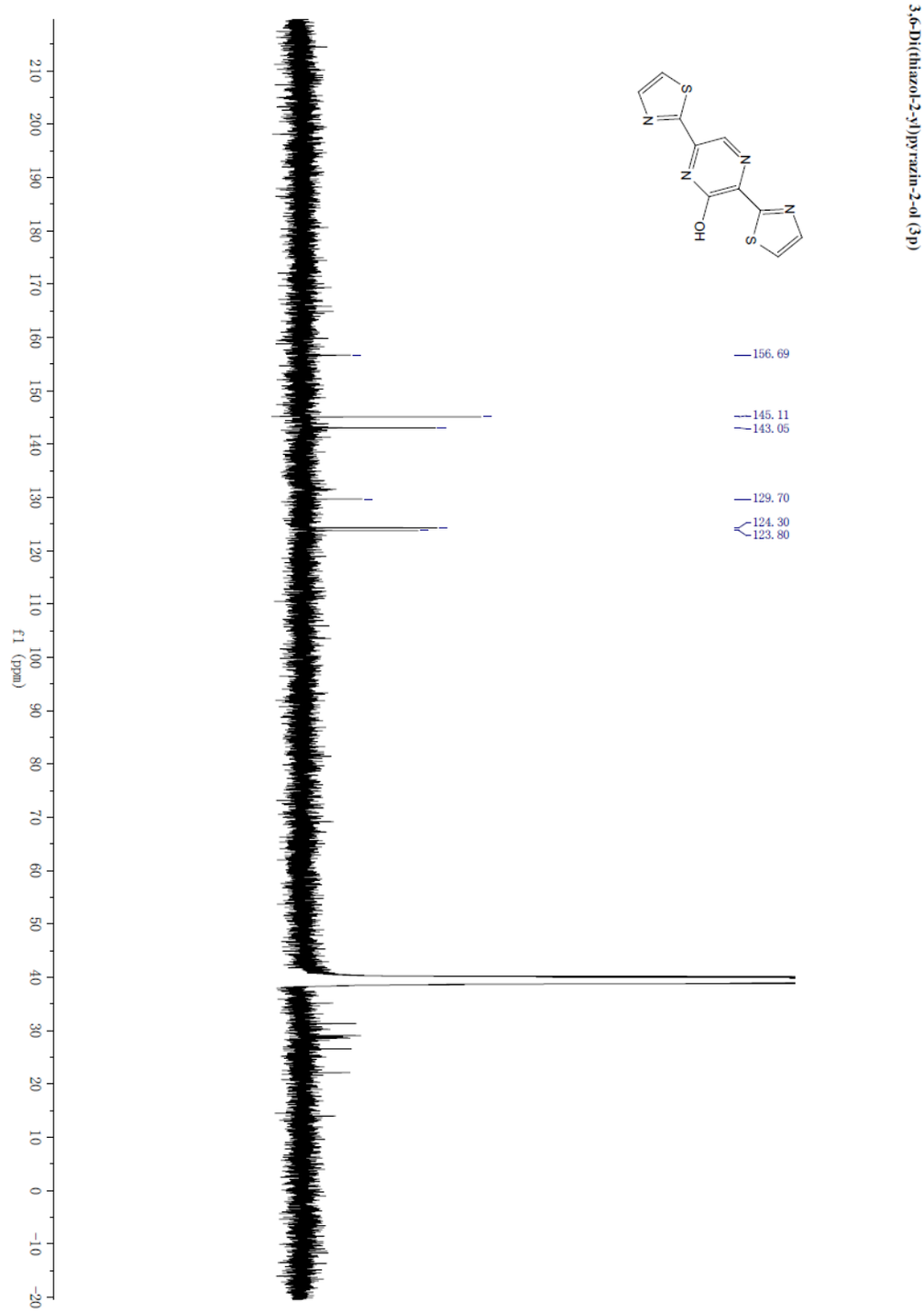












Note for NMR spectra: The NMR signals of some compounds (like **3p**) are very weak. The reason is that their solubility in DMSO-*d6* is extremely low, and even lower in other deuterated reagents. The signals of deuterated solvent DMSO-*d6* at δ 2.45-2.55 (ppm) in respective ^{1}H-NMR spectrum and at δ 39.4-39.6 (ppm) for DMSO-*d6* in respective ^{13}C-NMR spectrum were observed. The signals of water (DMSO-*d6* absorbs water easily) around δ 3.33 (ppm) in respective ^{1}H-NMR spectrum were observed. The signals of residual acetone around 2.09 (ppm) in ^{1}H-NMR spectrum and around 30.6 (ppm) in ^{13}C-NMR spectrum were observed in some compounds like **2n** and **2n'**.

Single-crystal data for compounds **2j** (CCDC 920522), **2k** (CCDC 873930) and **3p** (CCDC 920523) have been deposited in the Cambridge Crystallographic Data Centre. These data can be obtained free of charge via http://www.ccdc.ac.ck./data_request/cif.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2j

```
Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:            a=7.264(3)     b=8.306(3)          c=21.005(7)
                 alpha=90       beta=97.327(4)      gamma=90
Temperature:     133 K
```

	Calculated	Reported
Volume	1257.0(8)	1256.9(7)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C14 H10 N4 O, H2 O	?
Sum formula	C14 H12 N4 O2	C14 H12 N4 O2
Mr	268.28	268.28
Dx,g cm-3	1.418	1.418
Z	4	4
Mu (mm-1)	0.099	0.099
F000	560.0	560.0
F000'	560.23	
h,k,lmax	9,11,28	9,11,28
Nref	3381	3290
Tmin,Tmax	0.978,0.984	0.947,0.984
Tmin'	0.946	

```
Correction method= MULTI-SCANS

Data completeness= 0.973          Theta(max)= 29.140

R(reflections)= 0.0545( 3024)     wR2(reflections)= 0.1272( 3290)

S = 0.999                 Npar= 193
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as Multi-scans
```

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.973
```

Alert level G

```
ABSTY01_ALERT_1_G  Extra text has been found in the _exptl_absorpt_correction_type
            field, which should be only a single keyword. A literature
            citation should be included in the _exptl_absorpt_process_details
            field.
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2
              H2 O
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

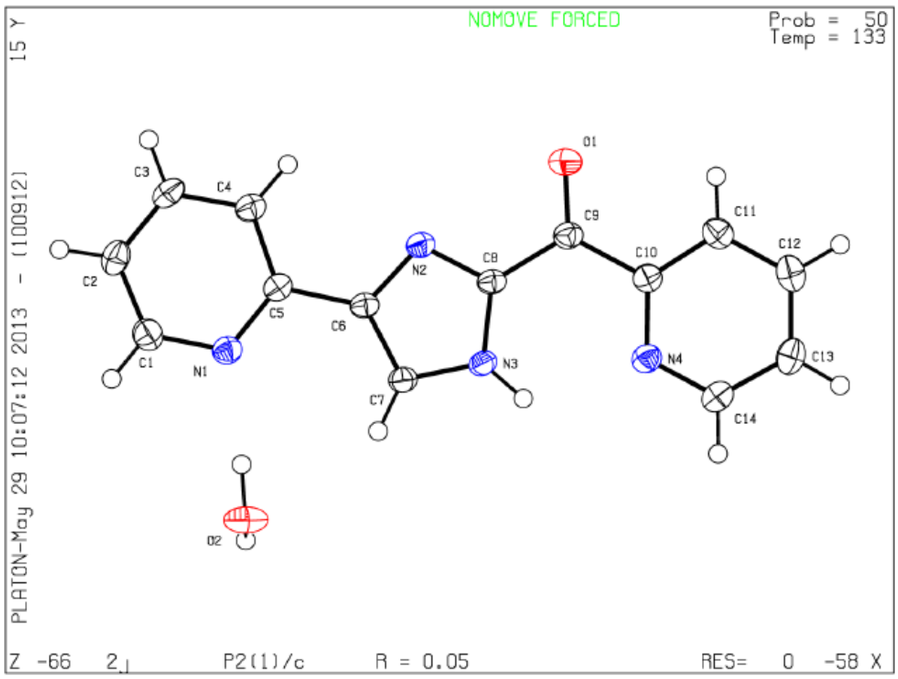
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 24/04/2013; check.def file version of 23/04/2013

Datablock 2j - ellipsoid plot



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 2k

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=4.417(3) b=25.392(14) c=10.491(6)
alpha=90 beta=101.058(8) gamma=90
Temperature: 153 K

	Calculated	Reported
Volume	1154.8(12)	1154.9(12)
Space group	C c	Cc
Hall group	C -2yc	?
Moiety formula	C14 H10 N4 O	?
Sum formula	C14 H10 N4 O	C14 H10 N4 O
Mr	250.26	250.26
Dx,g cm-3	1.439	1.439
Z	4	4
Mu (mm-1)	0.096	0.096
F000	520.0	520.0
F000'	520.19	
h,k,lmax	6,34,14	6,34,14
Nref	3123[1570]	2435
Tmin,Tmax	0.981,0.987	
Tmin'	0.951	

Correction method= Not given

Data completeness= 1.55/0.78 Theta(max)= 29.160

R(reflections)= 0.0353(2051) wR2(reflections)= 0.0840(2435)

S = 1.001 Npar= 176

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

STRVA01_ALERT_4_C Flack parameter is too small
From the CIF: _refine_ls_abs_structure_Flack -1.800
From the CIF: _refine_ls_abs_structure_Flack_su 1.400

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      1.400
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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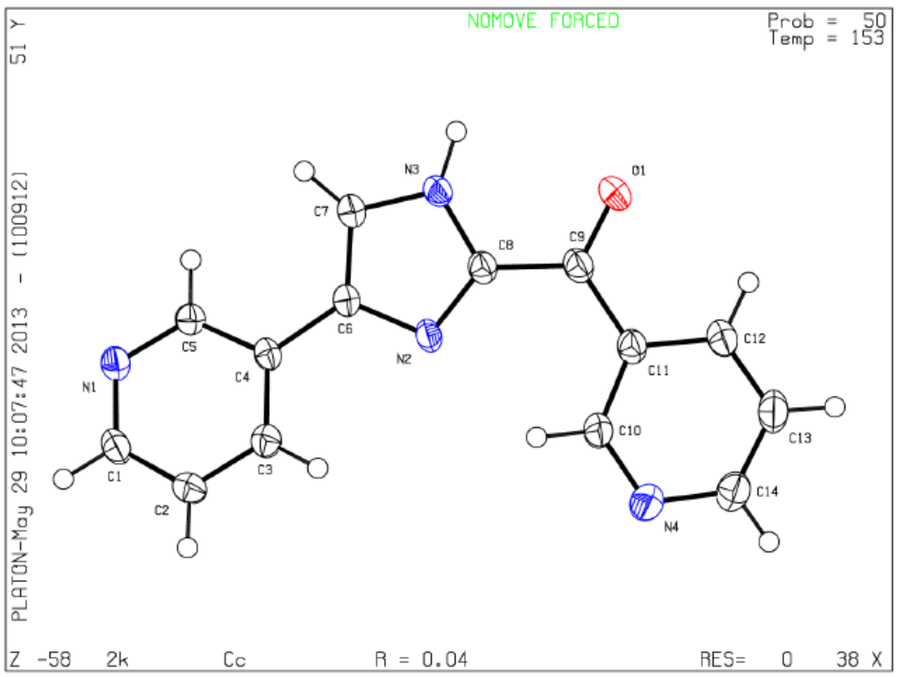
PLATON version of 24/04/2013; check.def file version of 23/04/2013

Datablock 2k - ellipsoid plot



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 3p

Bond precision: C-C = 0.0035 A Wavelength=0.71073

Cell: a=19.908(8) b=10.770(4) c=13.126(5)
alpha=90 beta=130.374(4) gamma=90
Temperature: 153 K

	Calculated	Reported
Volume	2144.1(14)	2144.1(14)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C10 H6 N4 O S2	?
Sum formula	C10 H6 N4 O S2	C10 H6 N4 O S2
Mr	262.33	262.31
Dx,g cm-3	1.625	1.625
Z	8	8
Mu (mm-1)	0.483	0.483
F000	1072.0	1072.0
F000'	1074.29	
h,k,lmax	27,14,17	27,14,17
Nref	2850	2847
Tmin,Tmax	0.966,0.976	0.796,0.974
Tmin'	0.785	

Correction method= MULTI-SCANS

Data completeness= 0.999 Theta(max)= 28.990

R(reflections)= 0.0474(2388) wR2(reflections)= 0.1267(2847)

S = 1.002 Npar= 172

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.
Absorption correction given as Multi-scans

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.01
```

Alert level G

```
ABSTY01_ALERT_1_G  Extra text has been found in the _exptl_absorpt_correction_type
            field, which should be only a single keyword. A literature
            citation should be included in the _exptl_absorpt_process_details
            field.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT301_ALERT_3_G Note: Main Residue  Disorder ...................        18 %
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          1
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......         5
```

```
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```

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PLATON version of 24/04/2013; check.def file version of 23/04/2013

Datablock 3p - ellipsoid plot