Supplementary Material (ESI) for Organic & Biomolecular Chemistry

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# A Highly Efficient One-Pot Reaction of 2-(*gem*-Dibromovinyl)phenols(thiophenols) with $K_4Fe(CN)_6$ to 2-Cyanobenzofurans(thiophenes)

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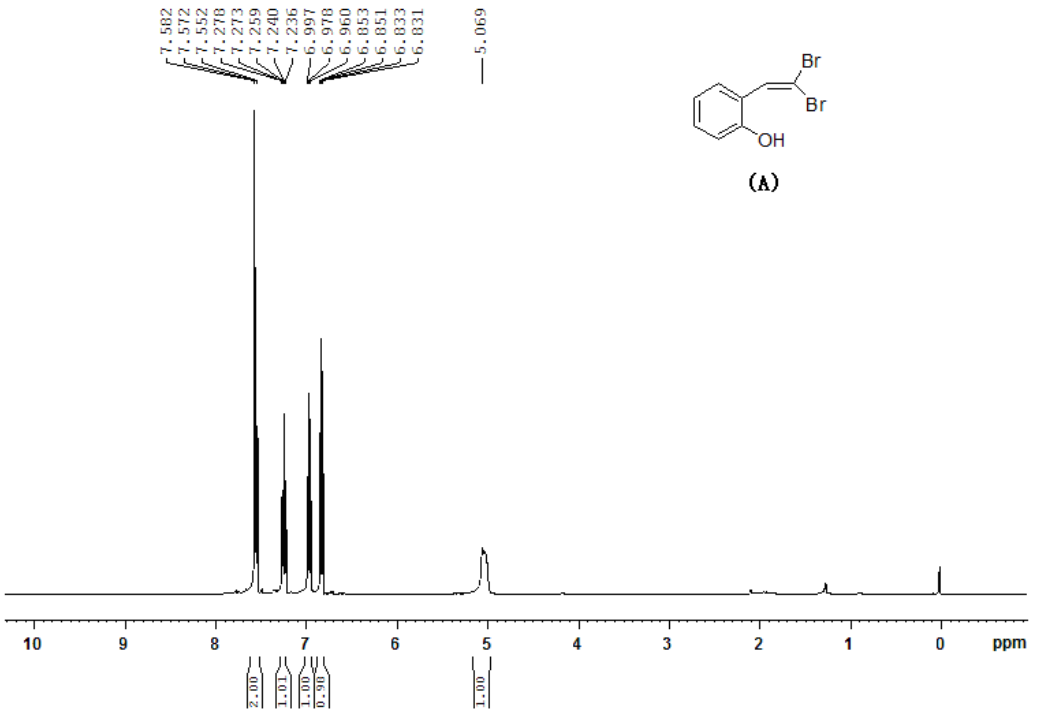
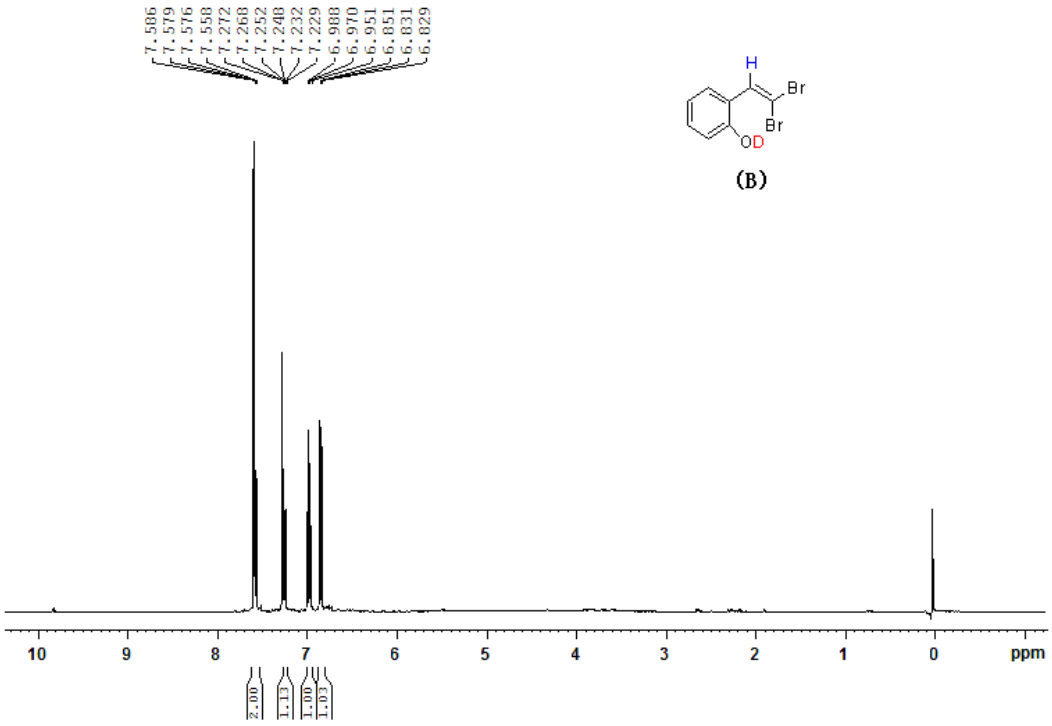
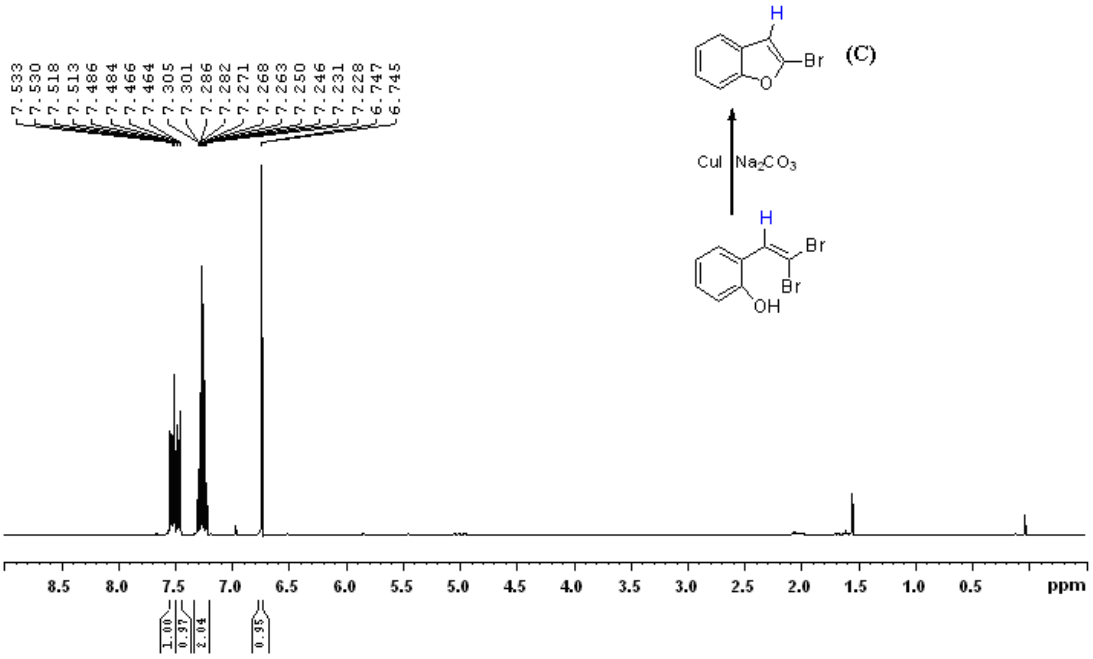
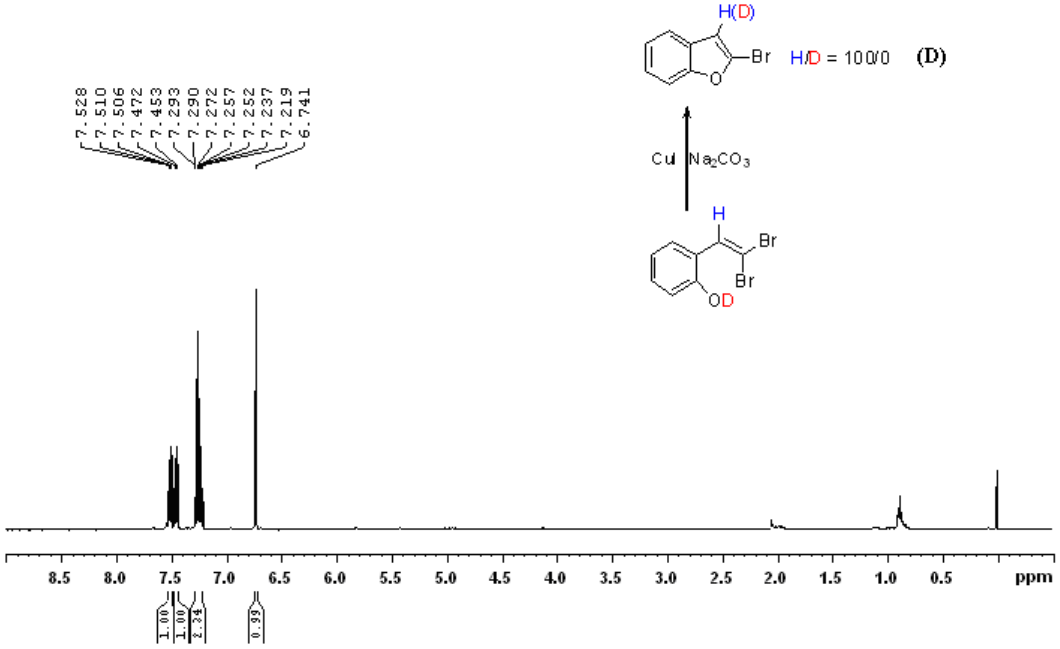
# 1. D-Labelled spectra of substrate and product

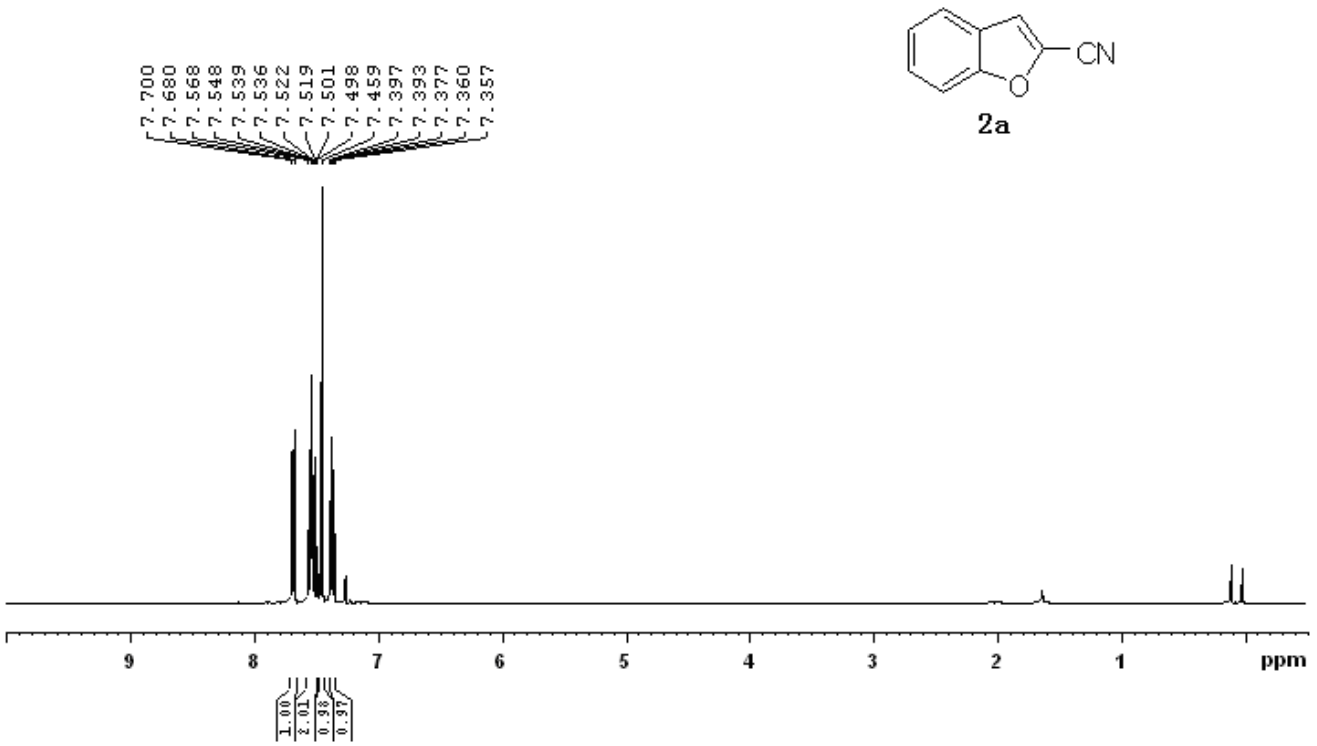


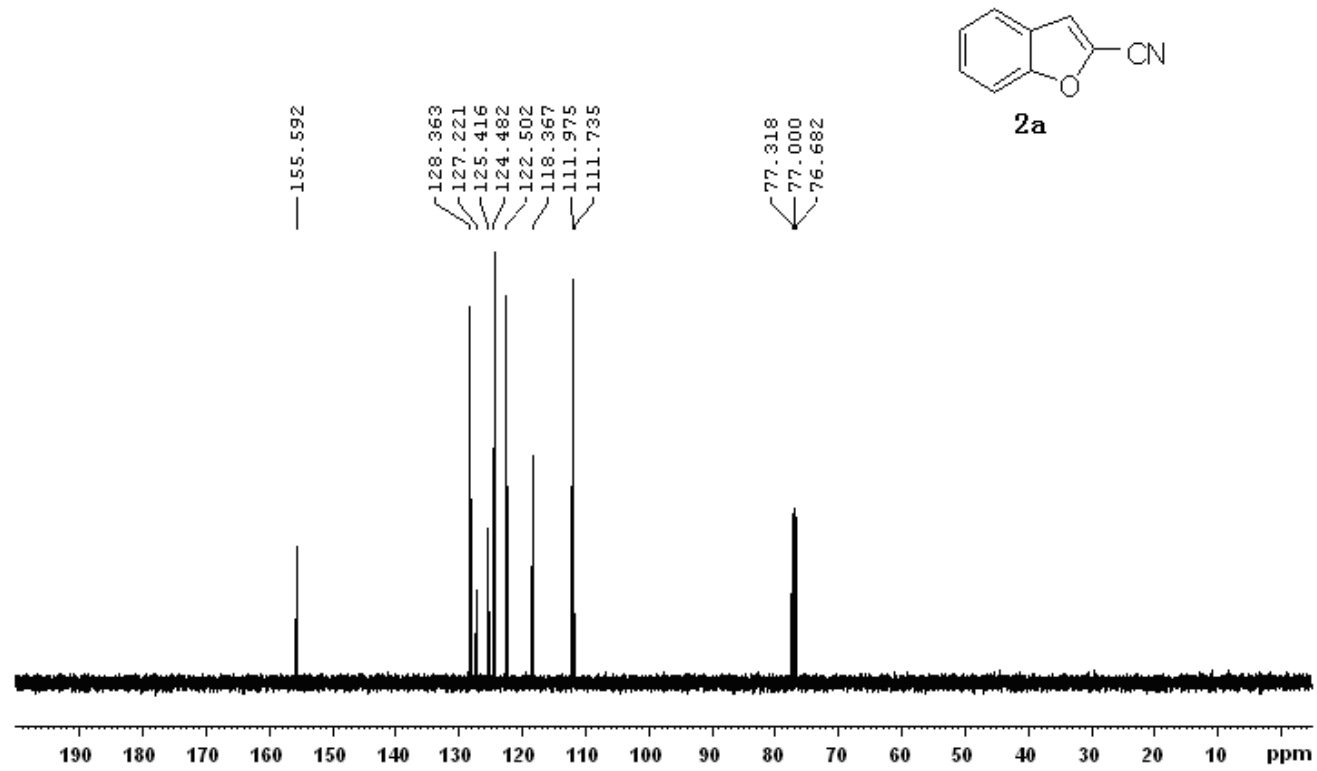



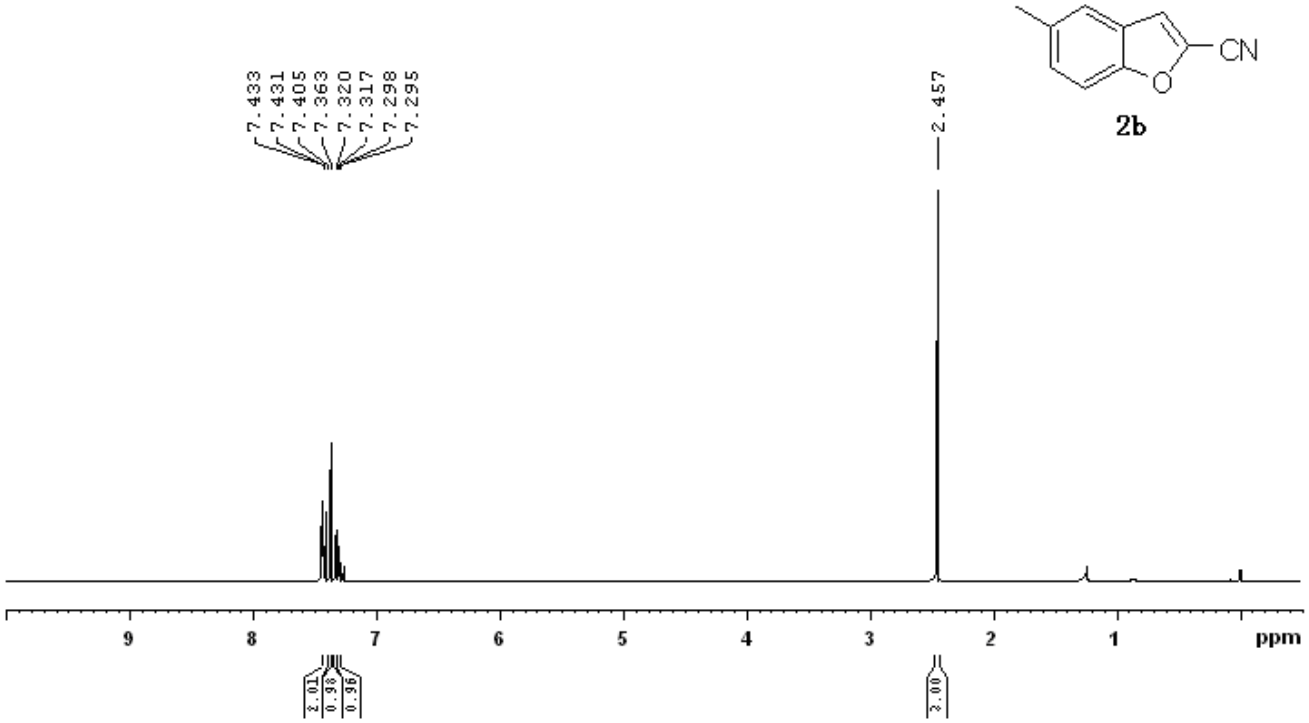


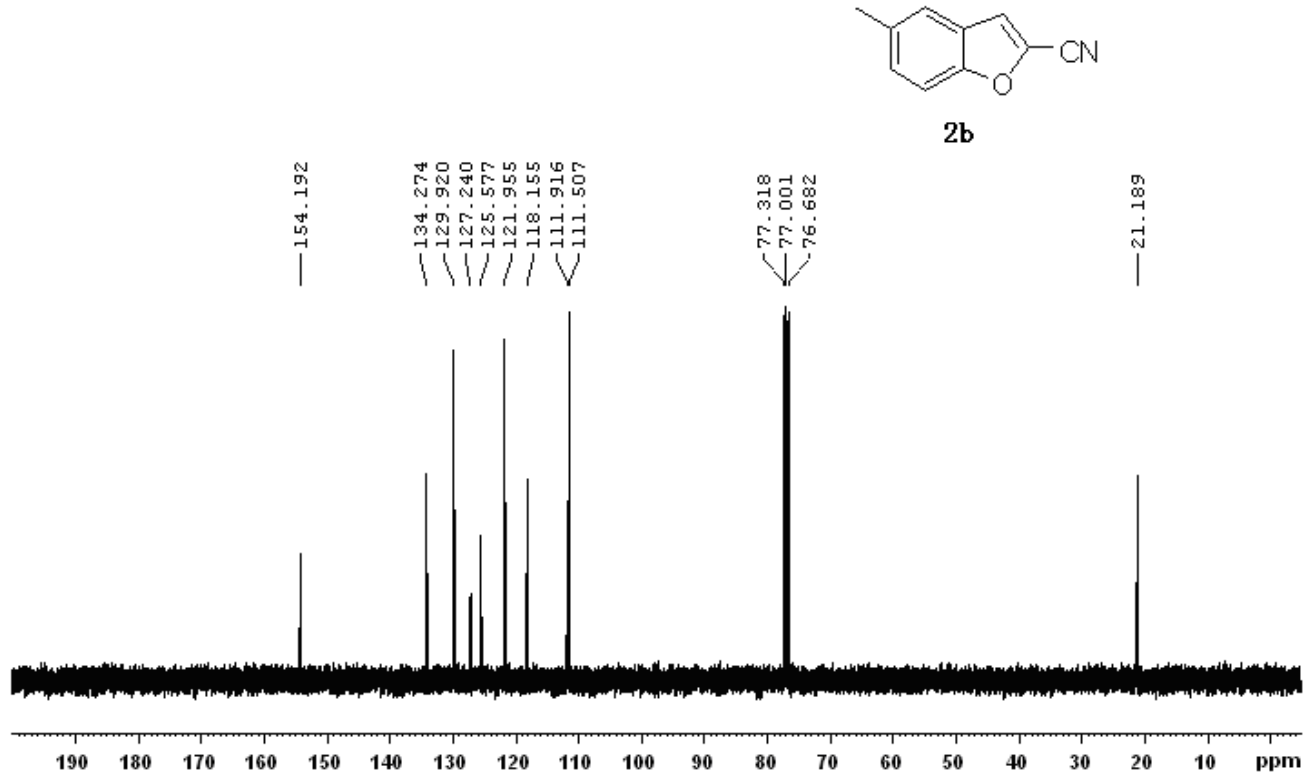



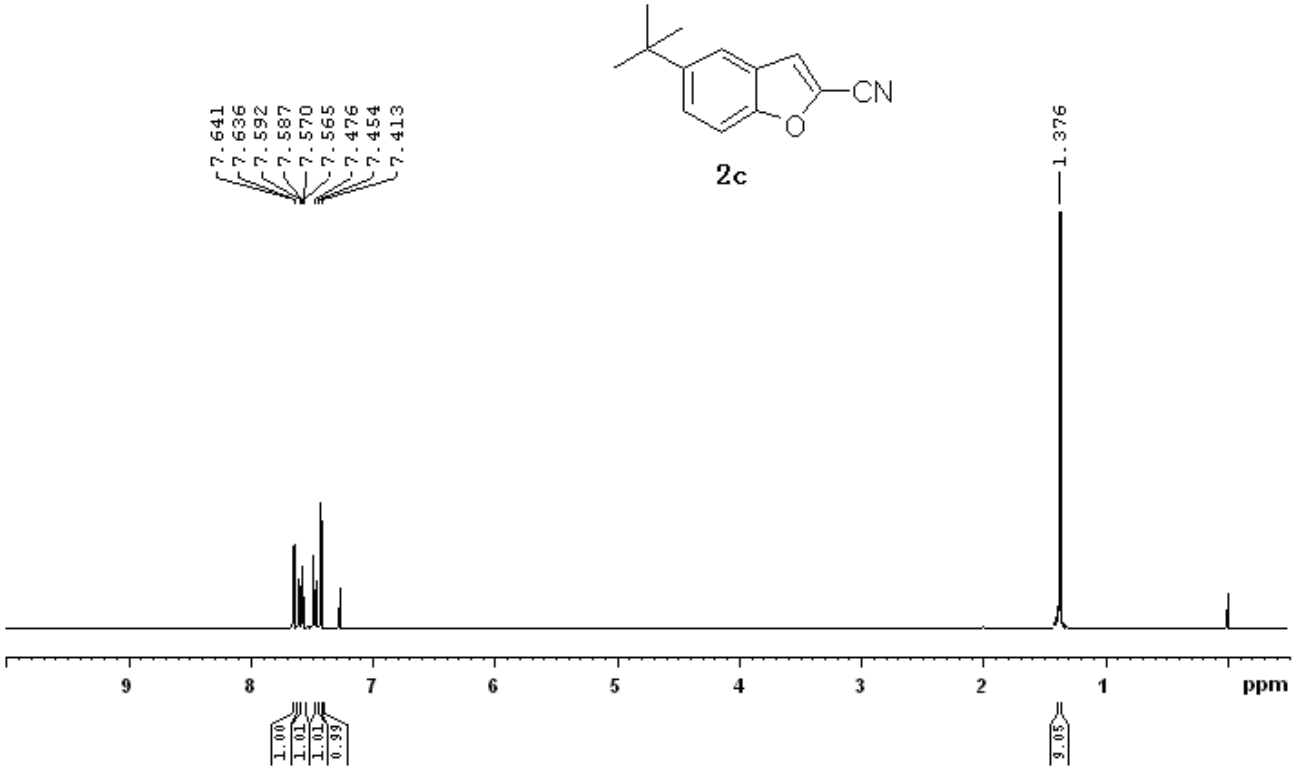
# 2. $^{1}H$, $^{13}C$ NMR and HRMS spectra of the products



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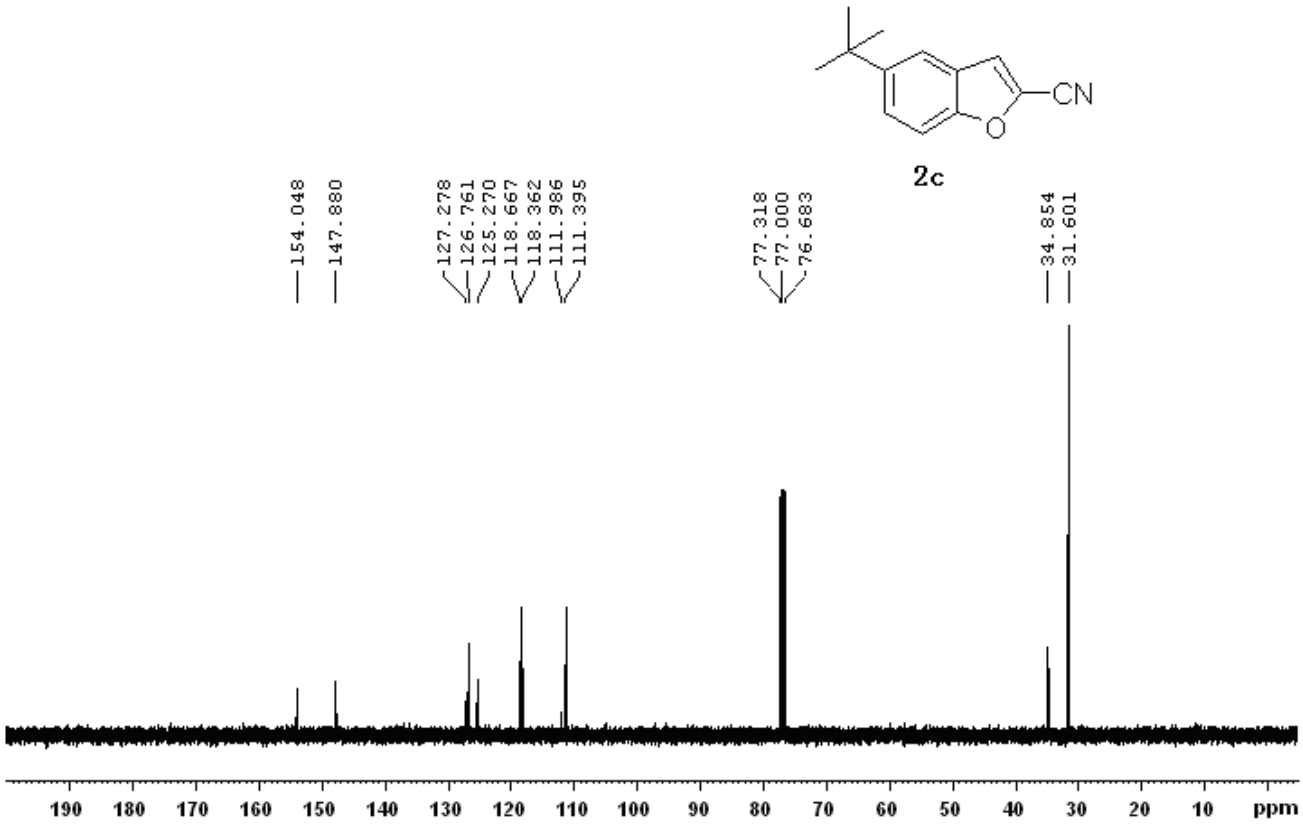
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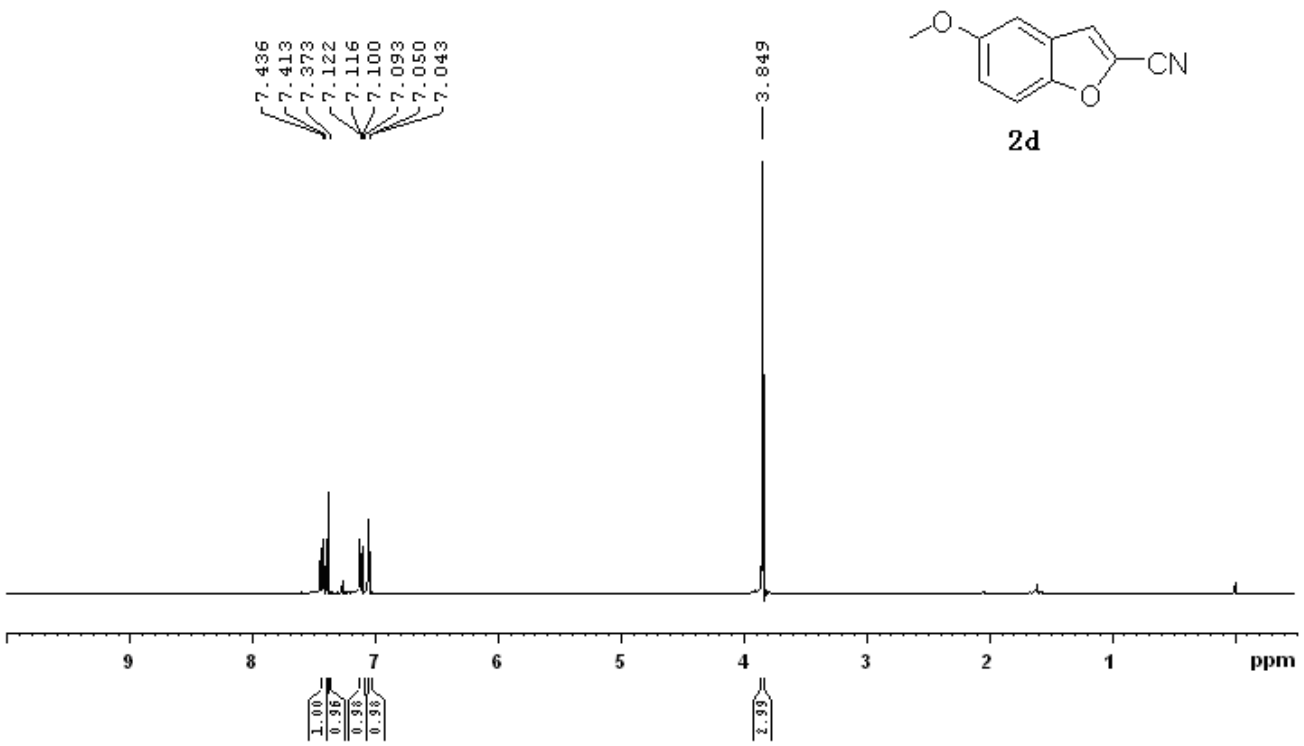


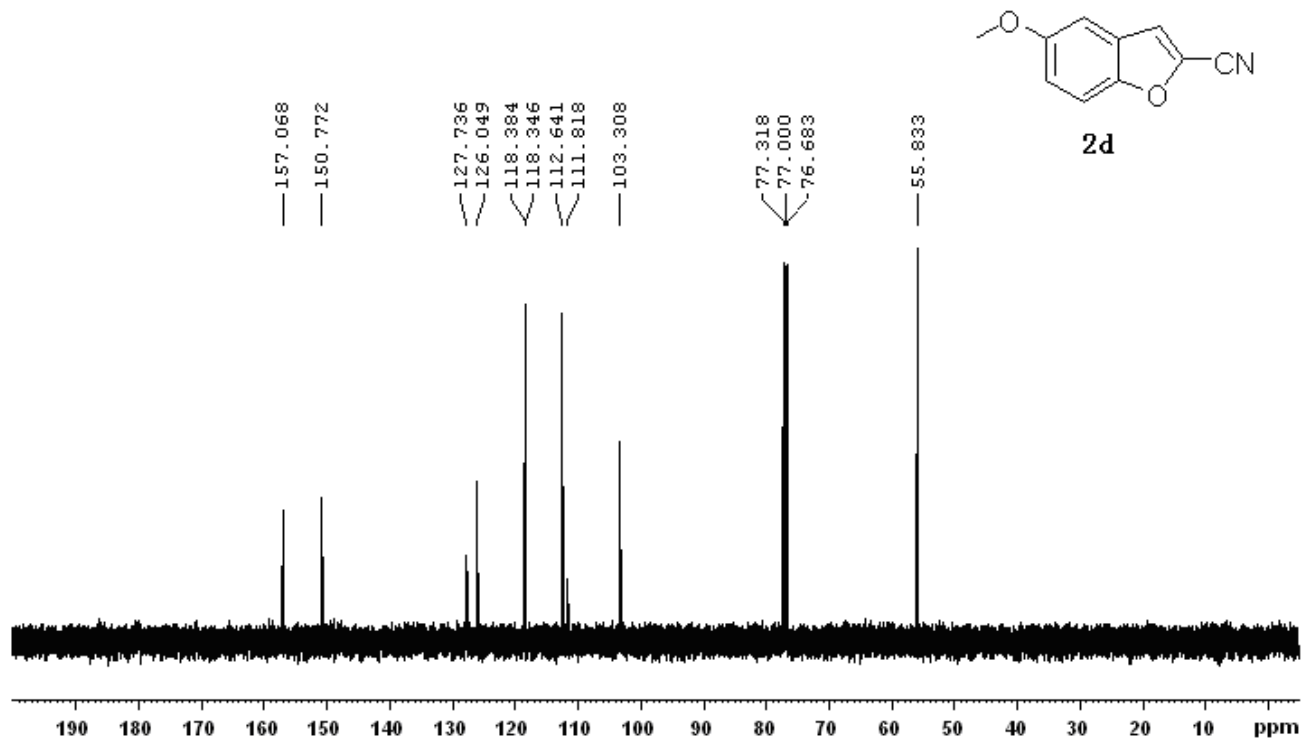

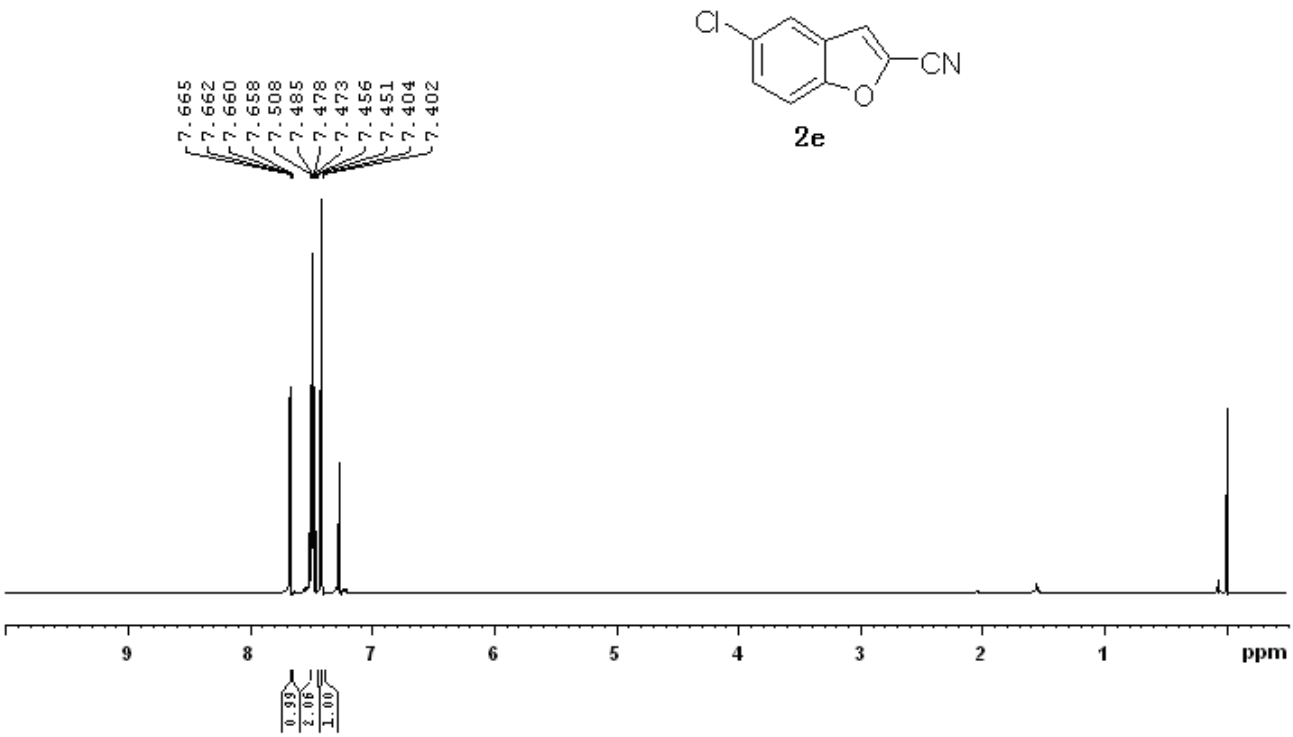
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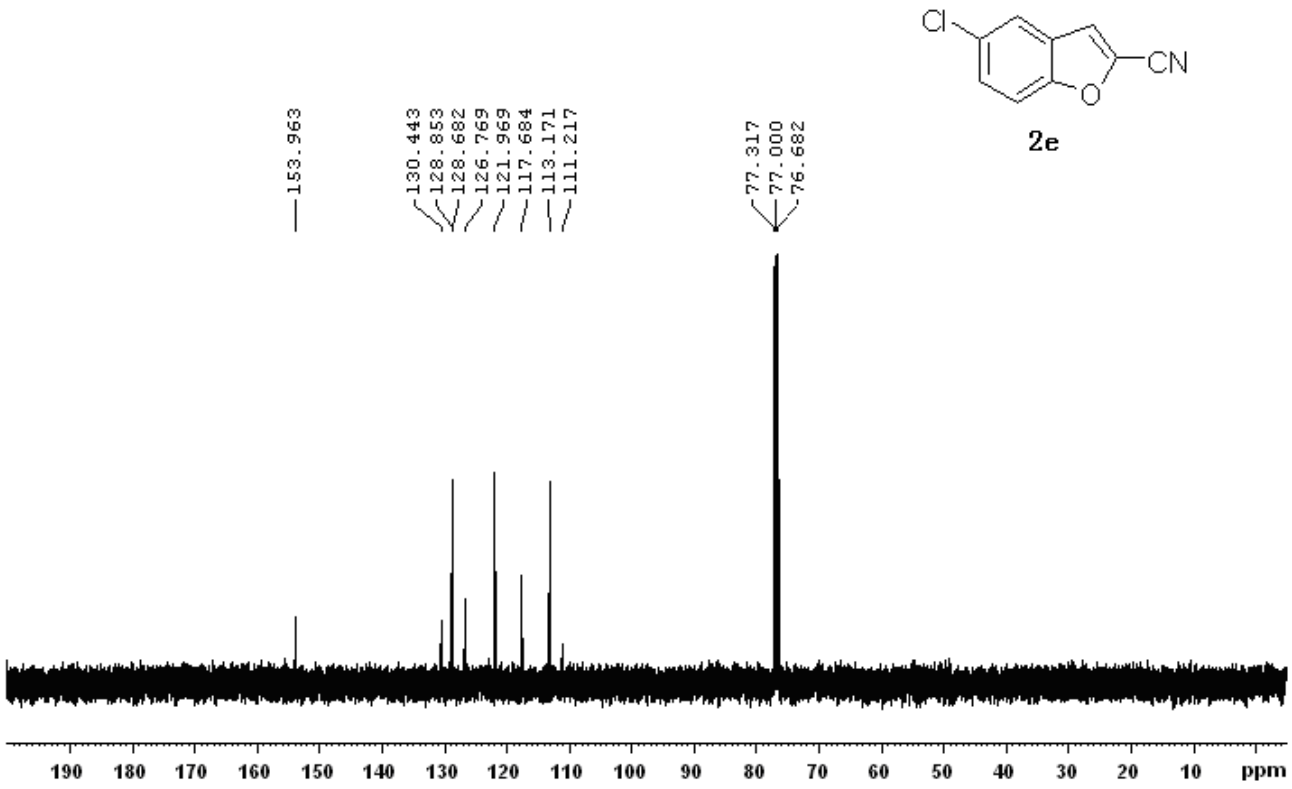
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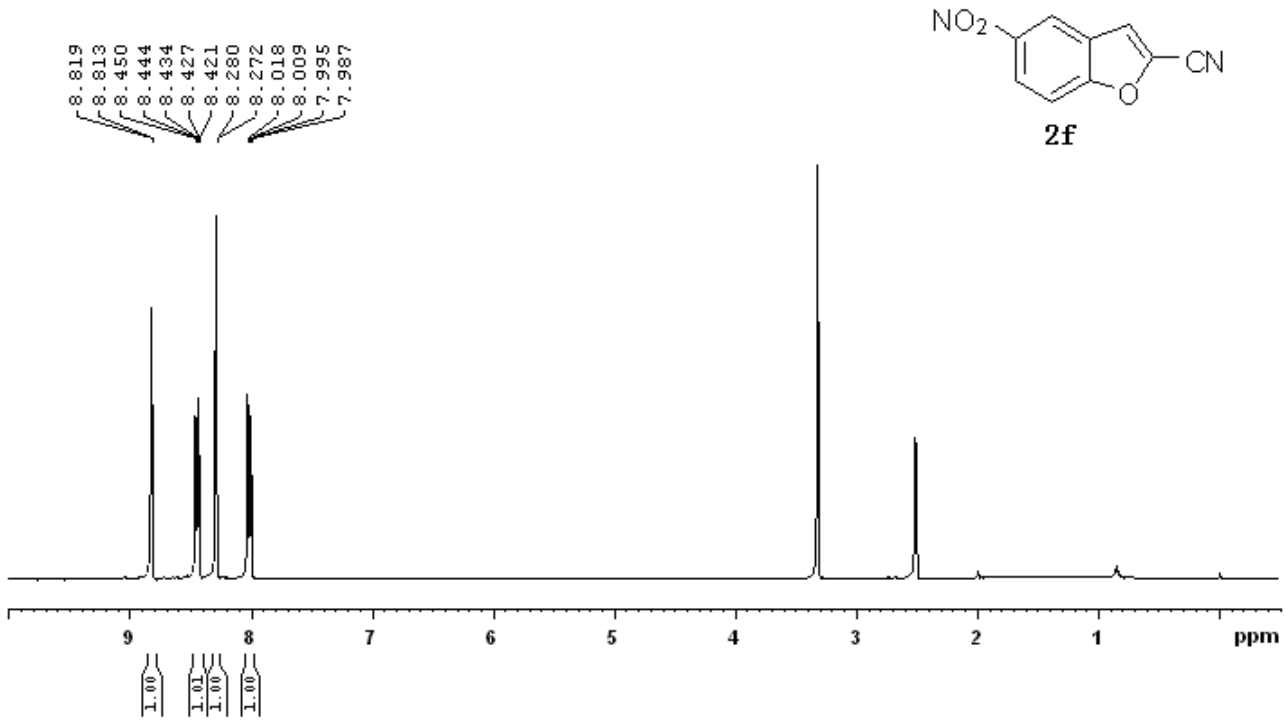


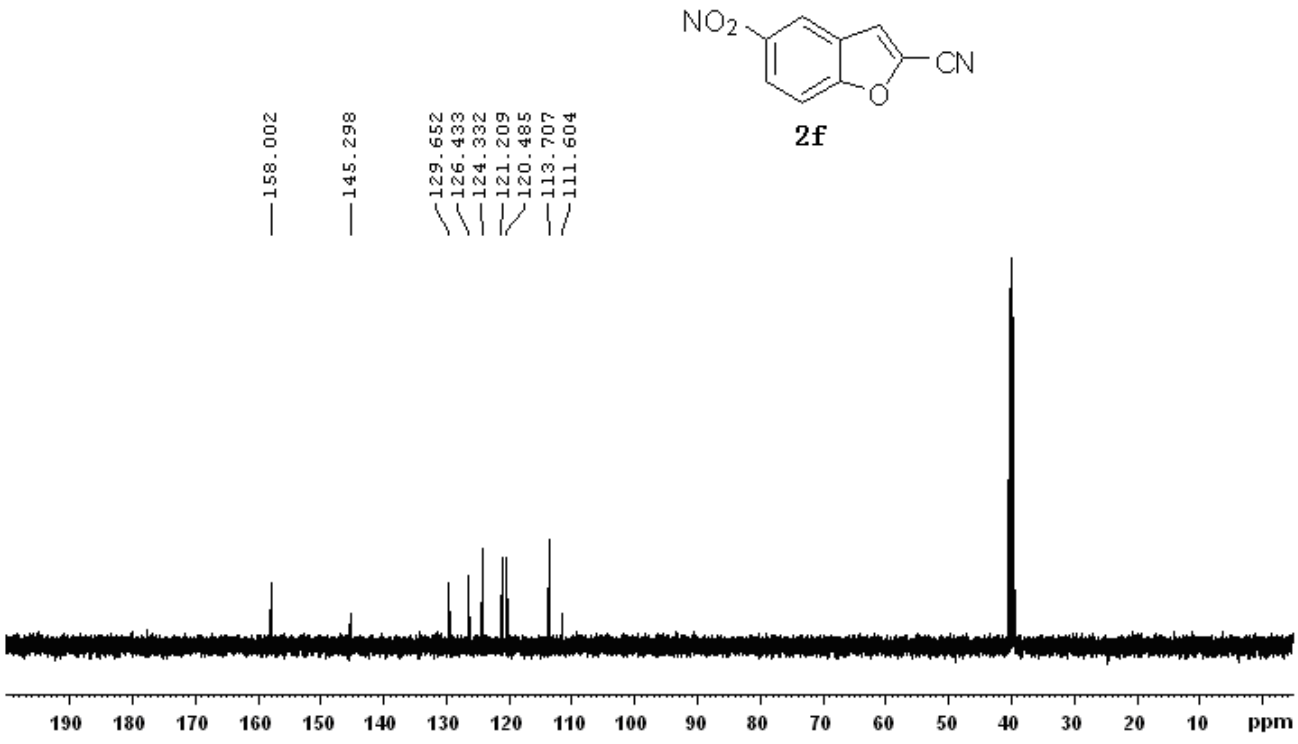

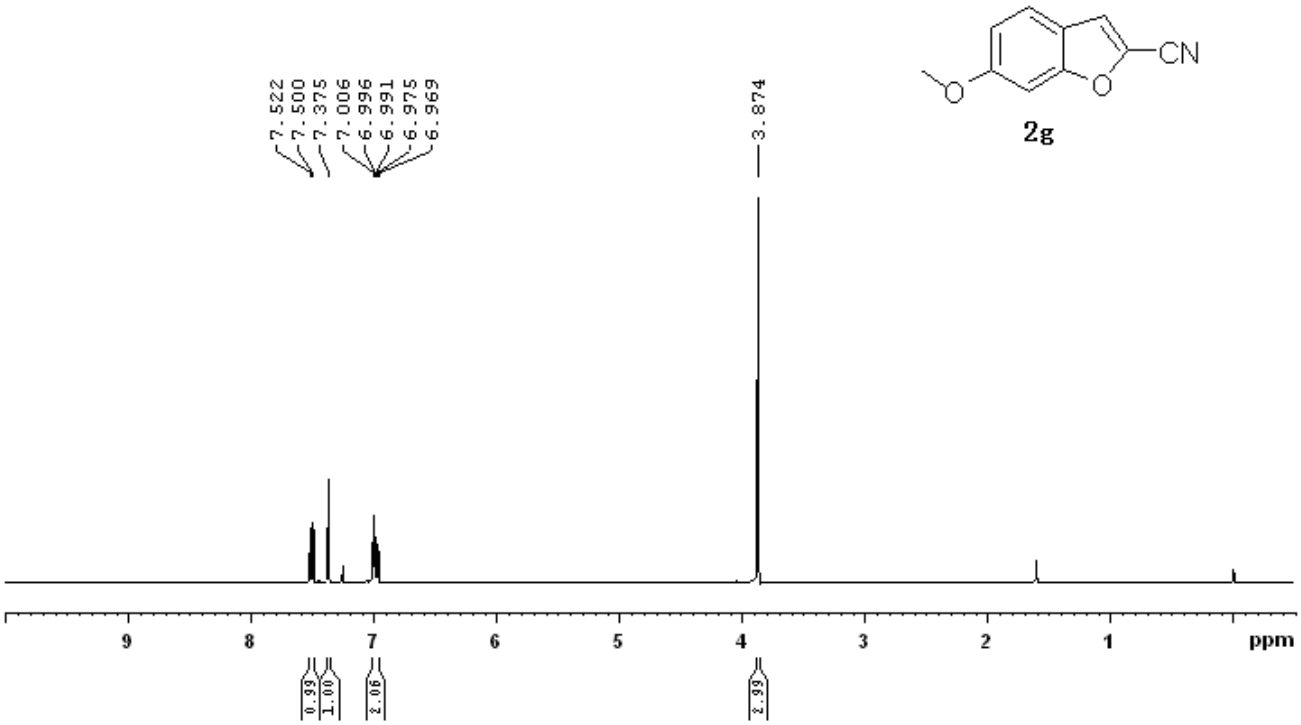


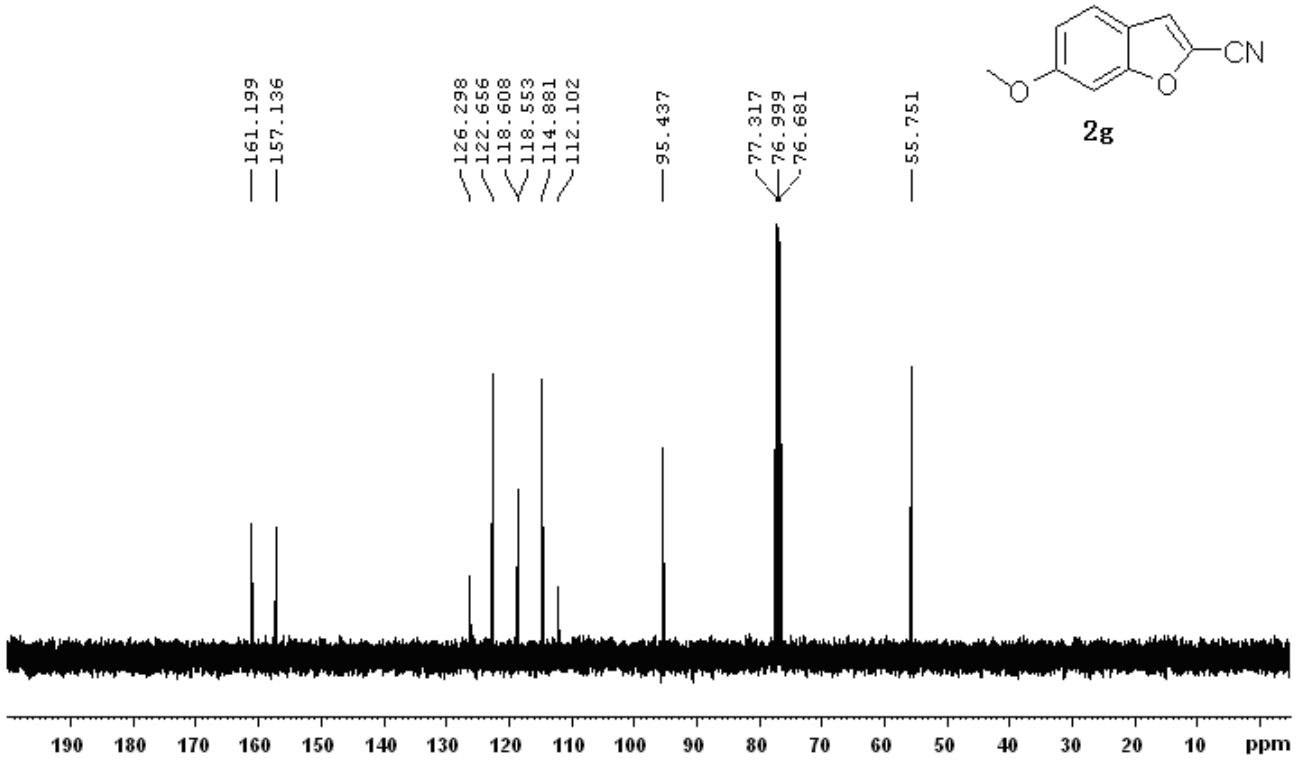

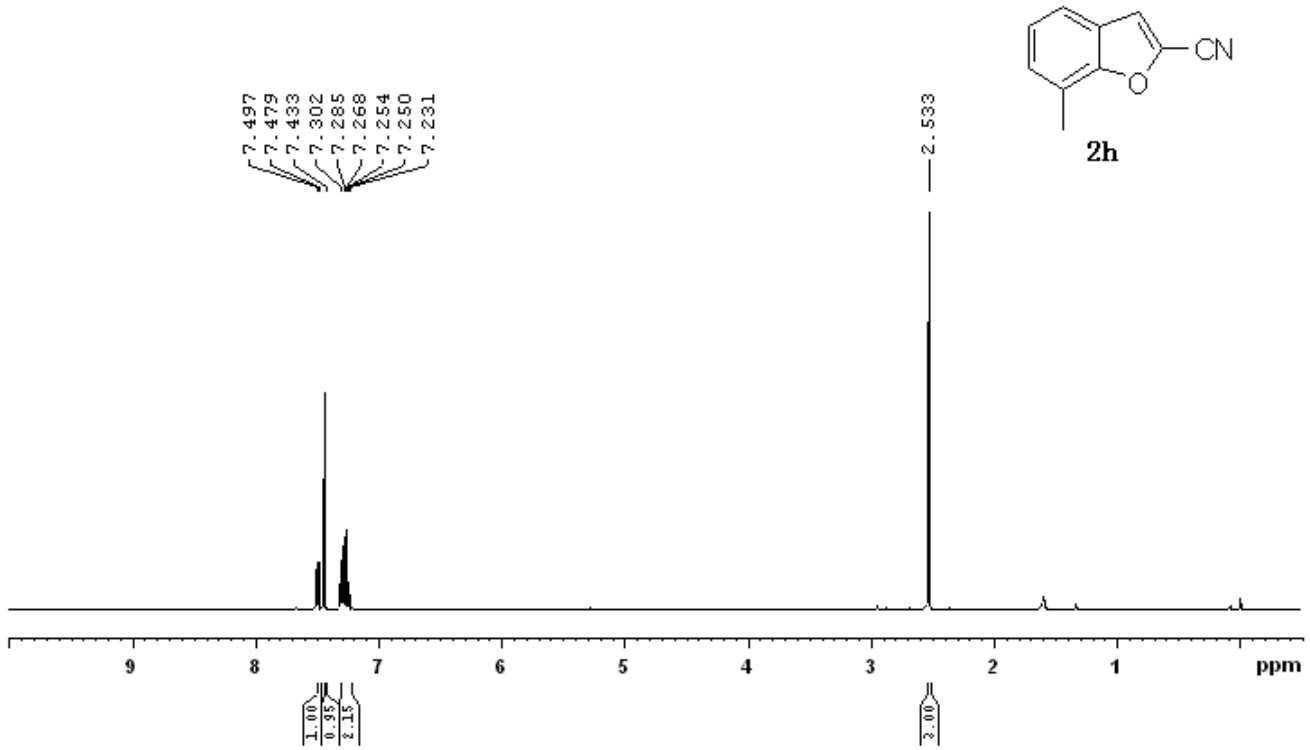
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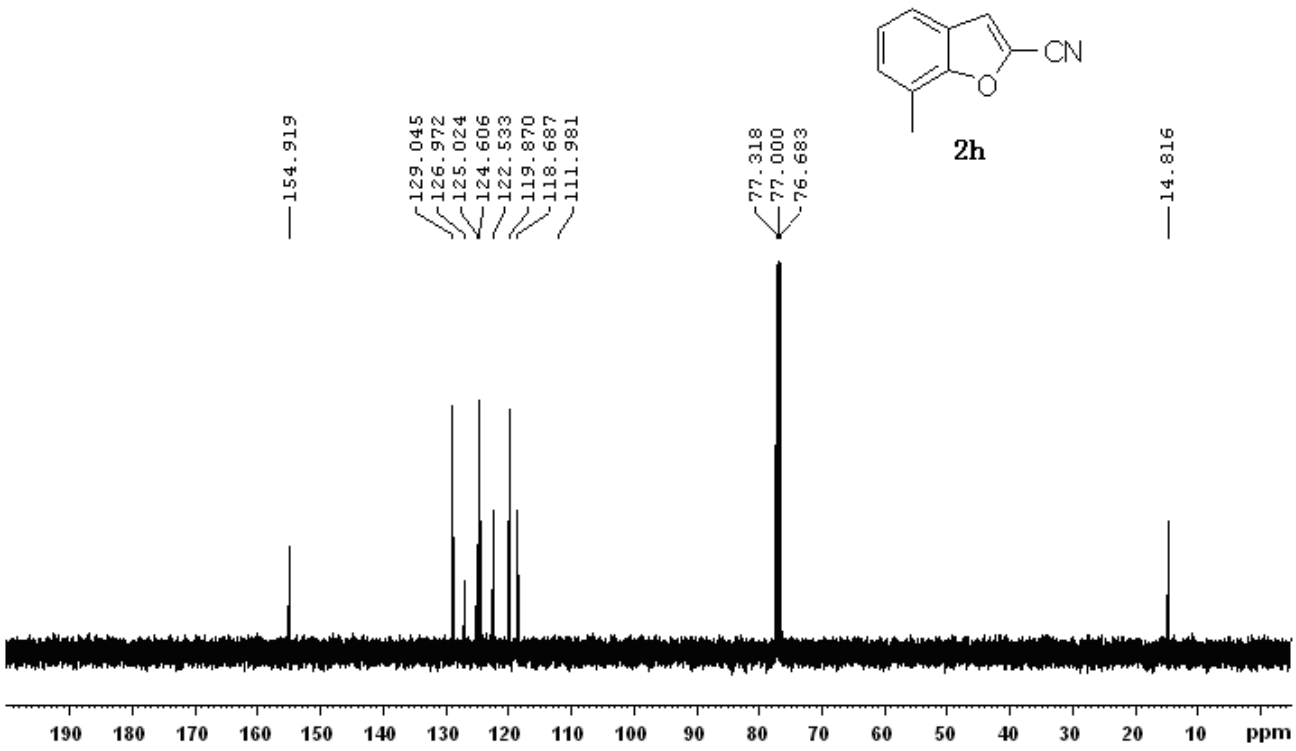
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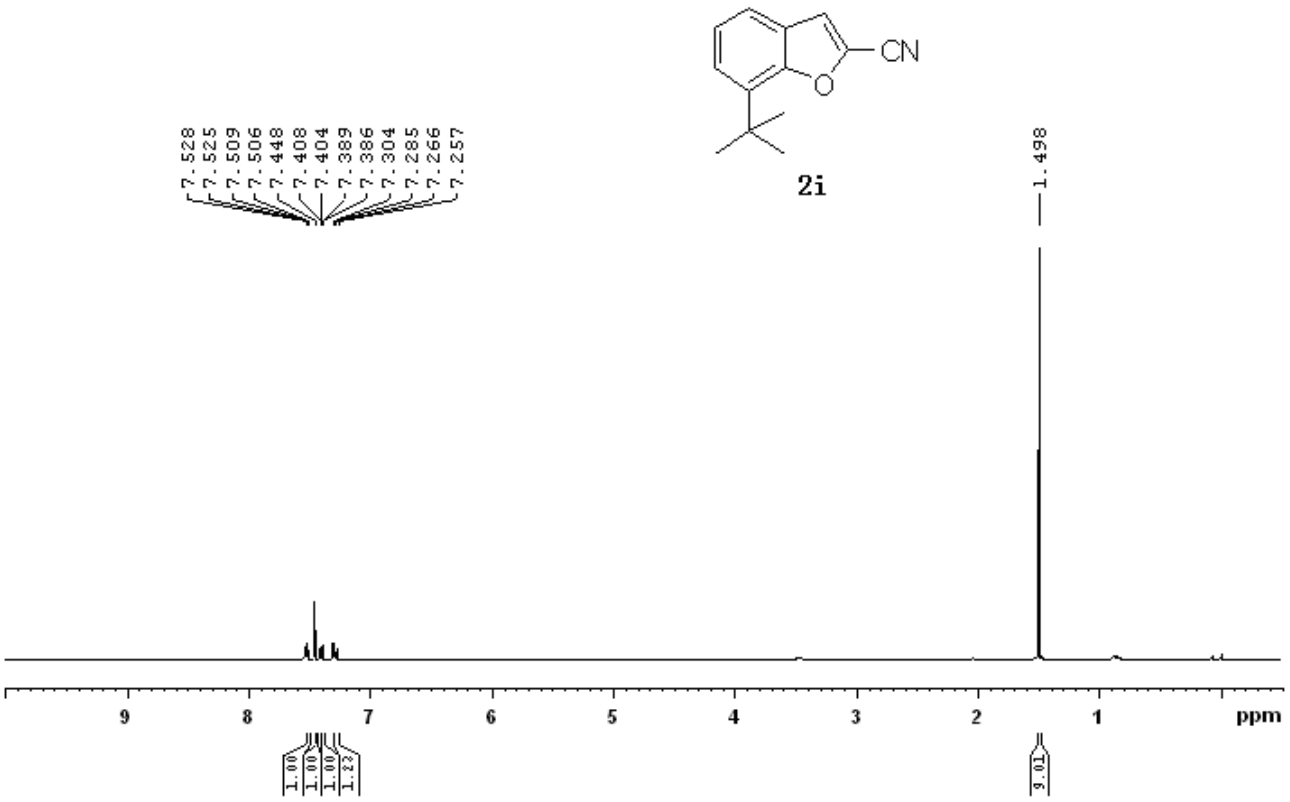


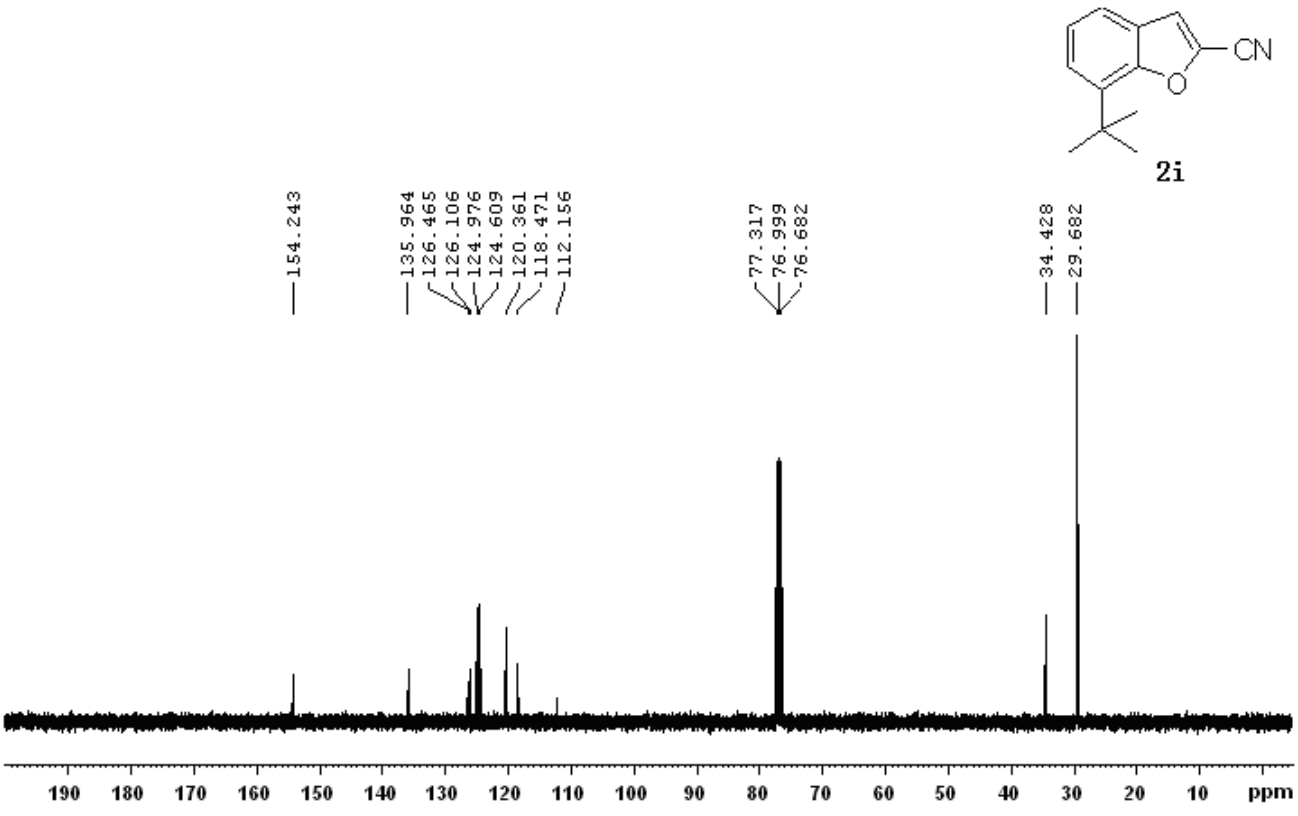

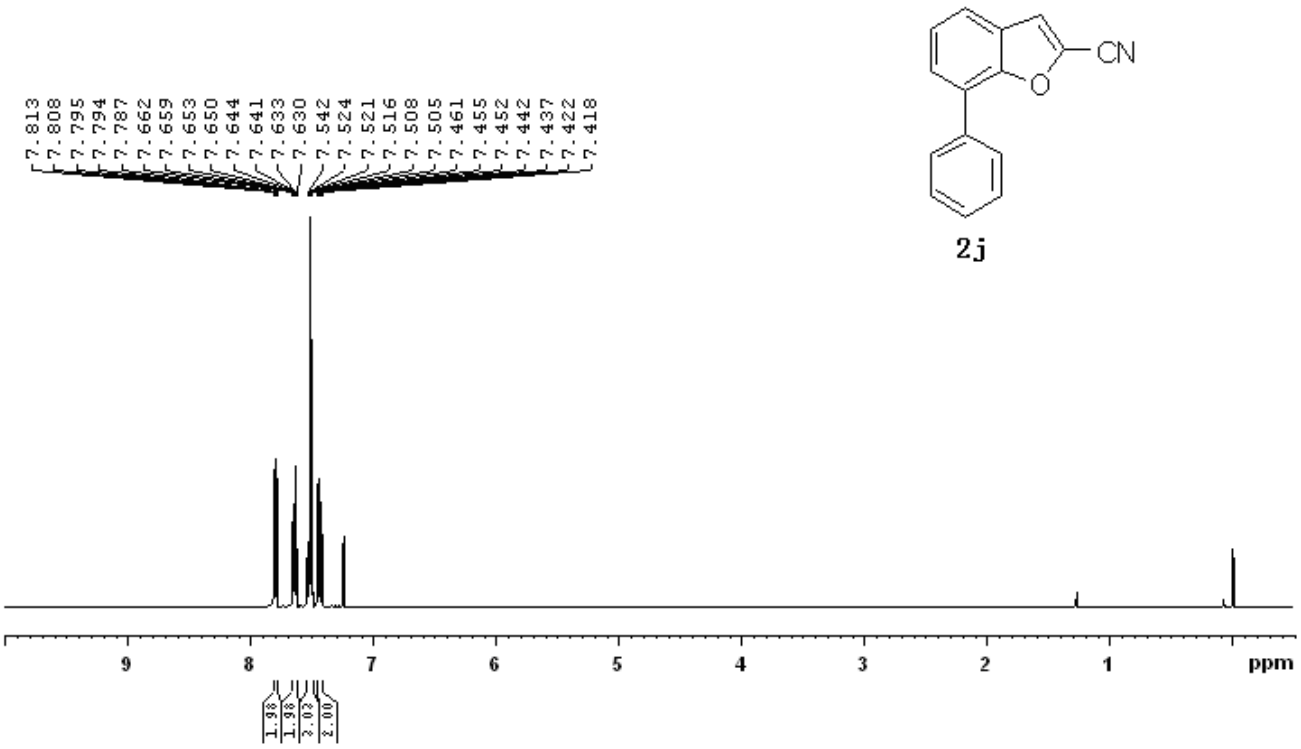


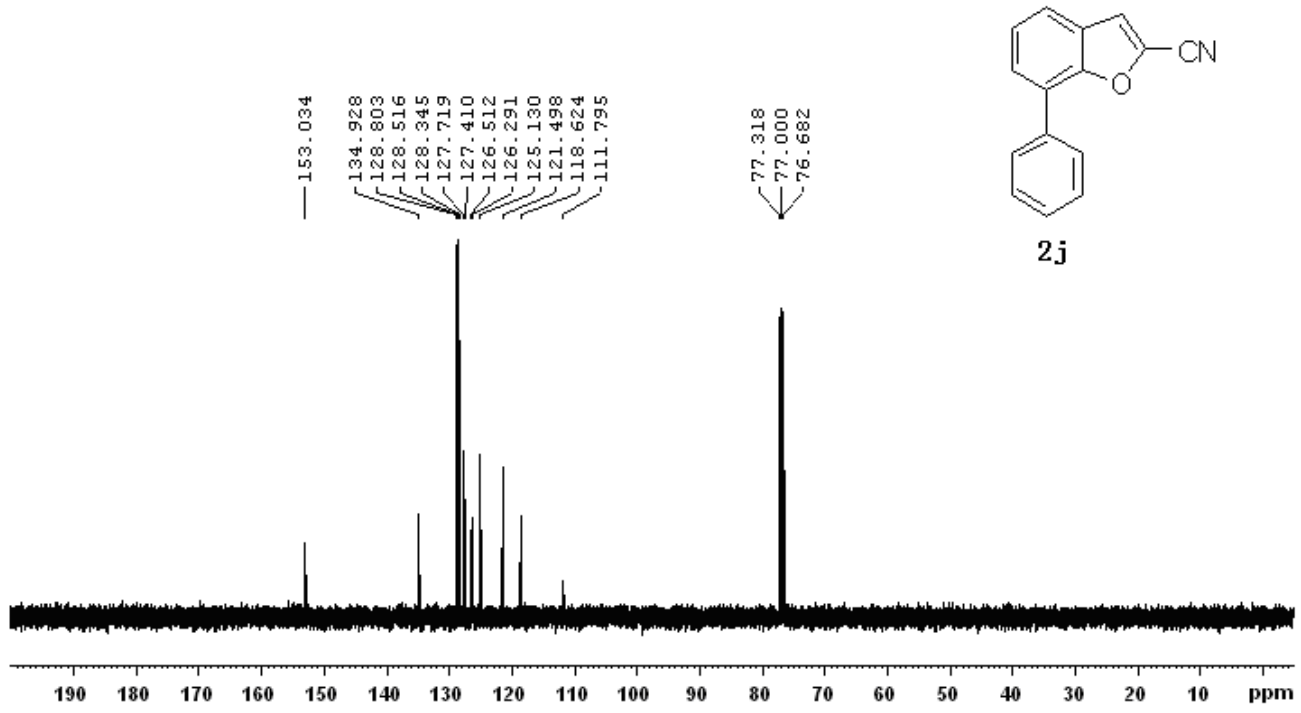

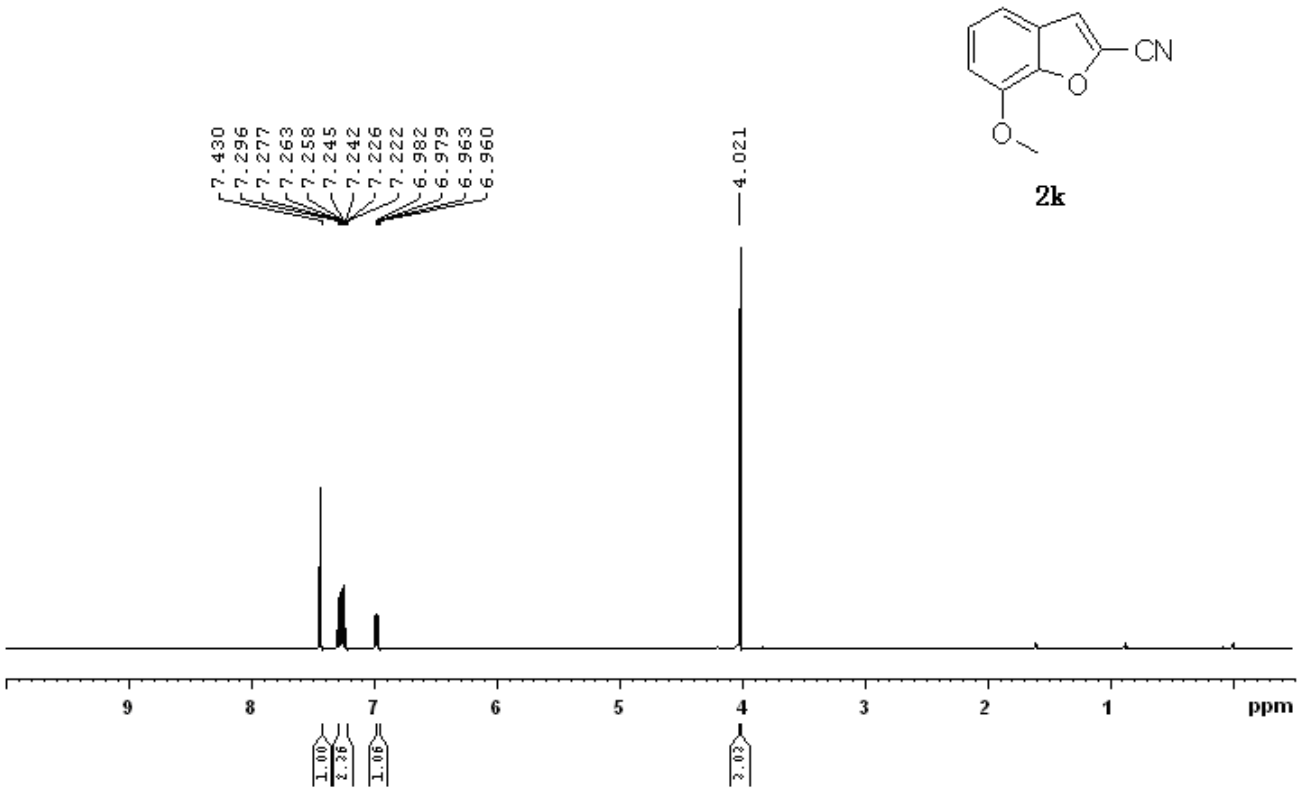


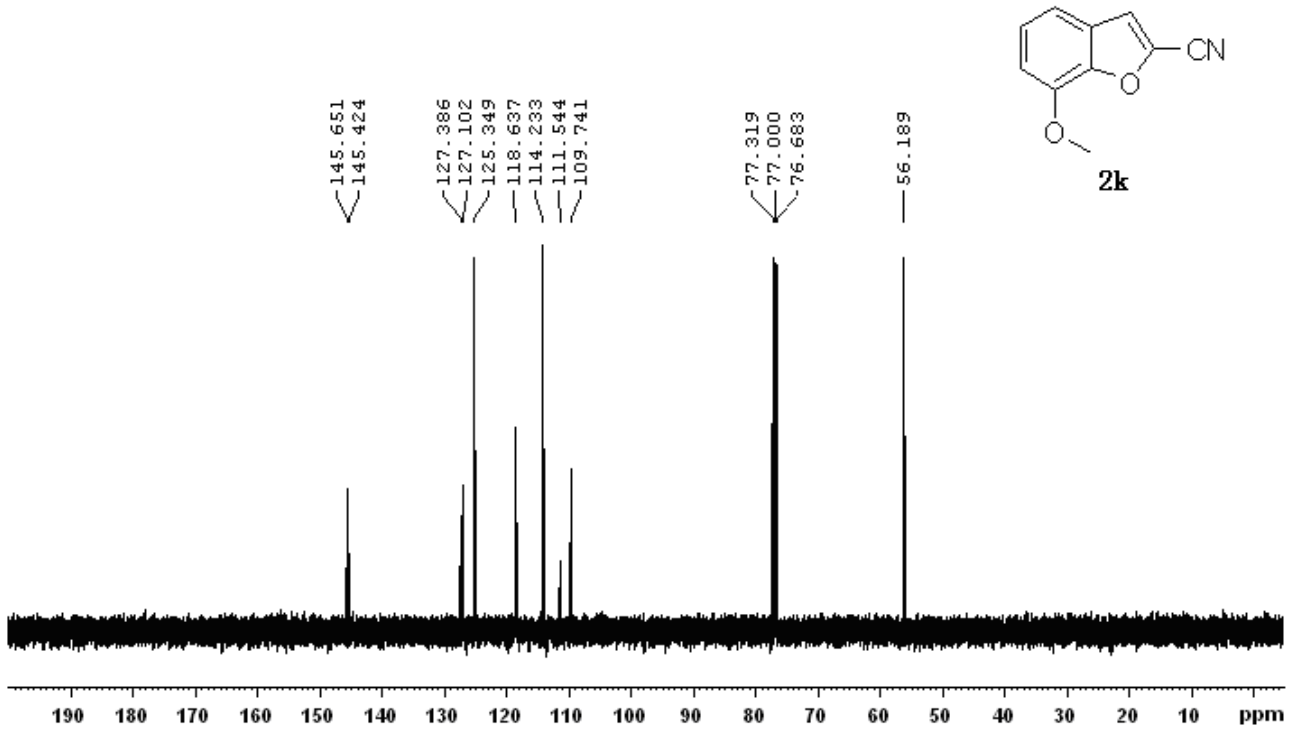

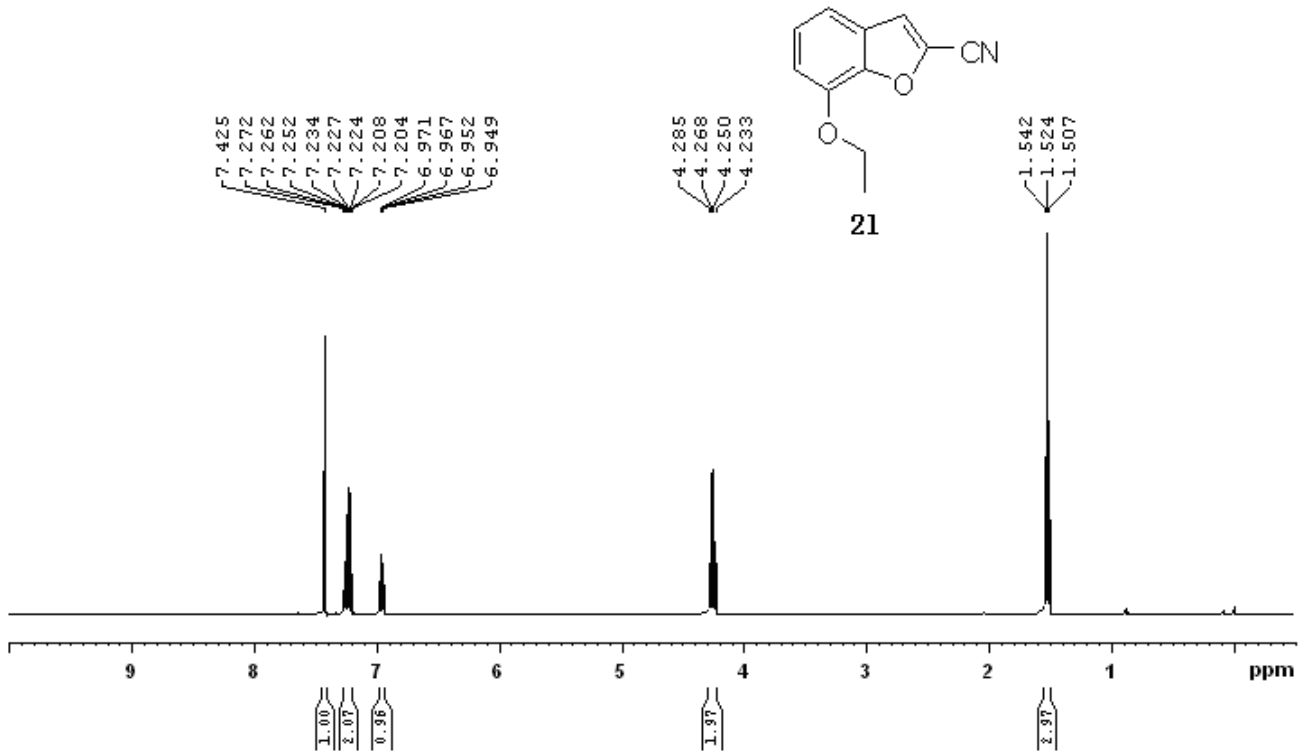


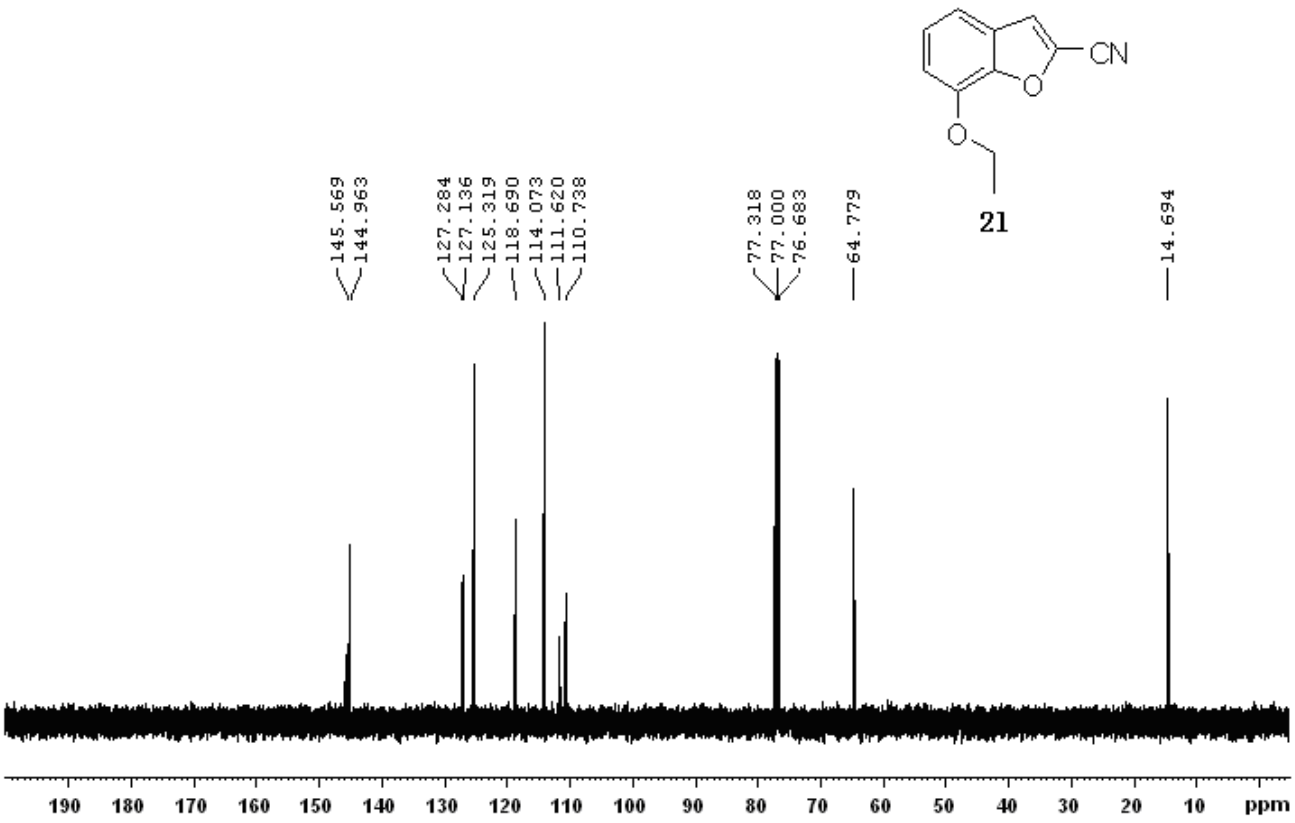

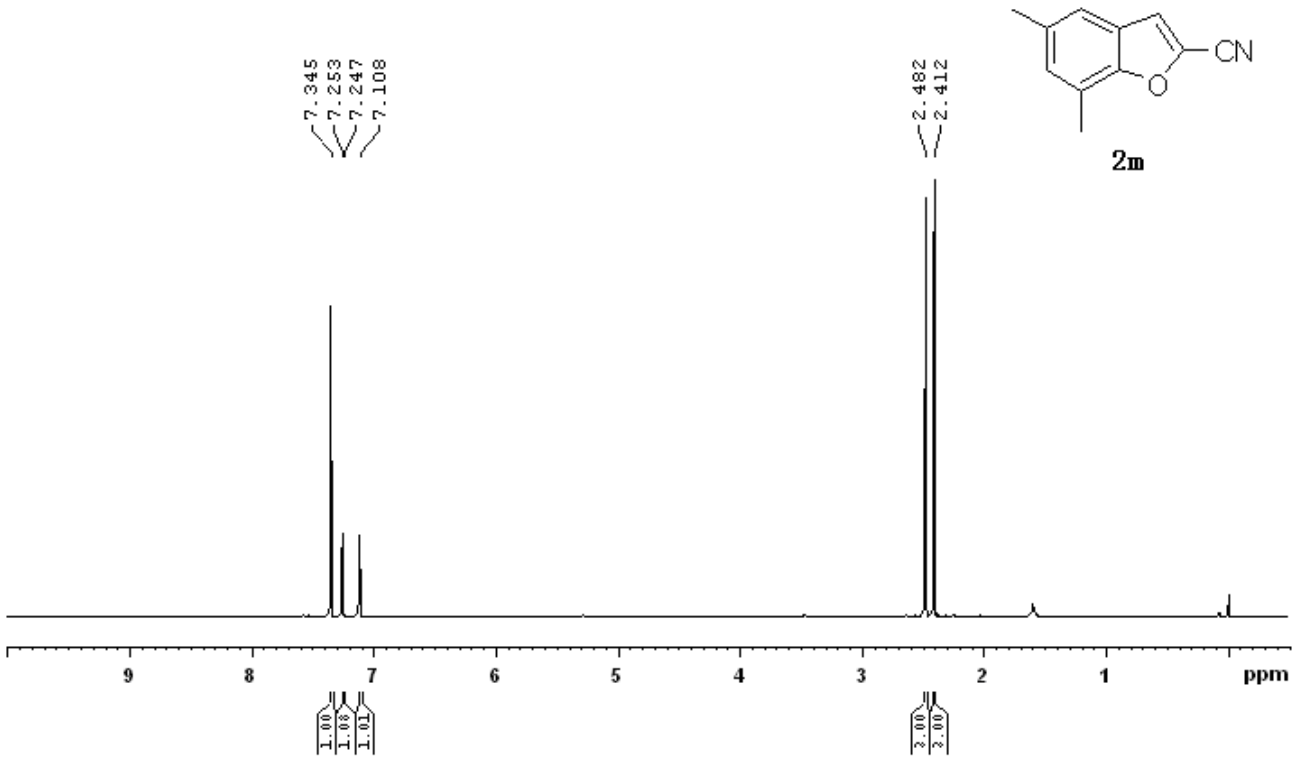


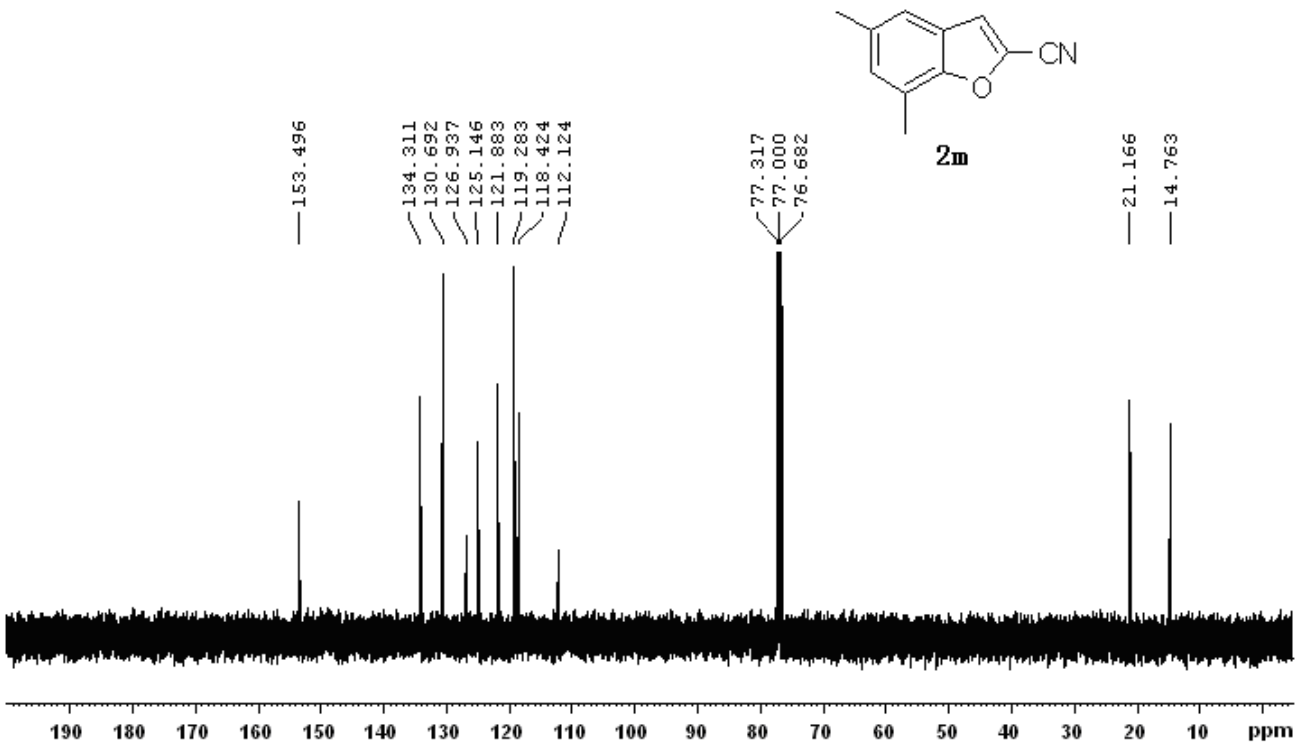

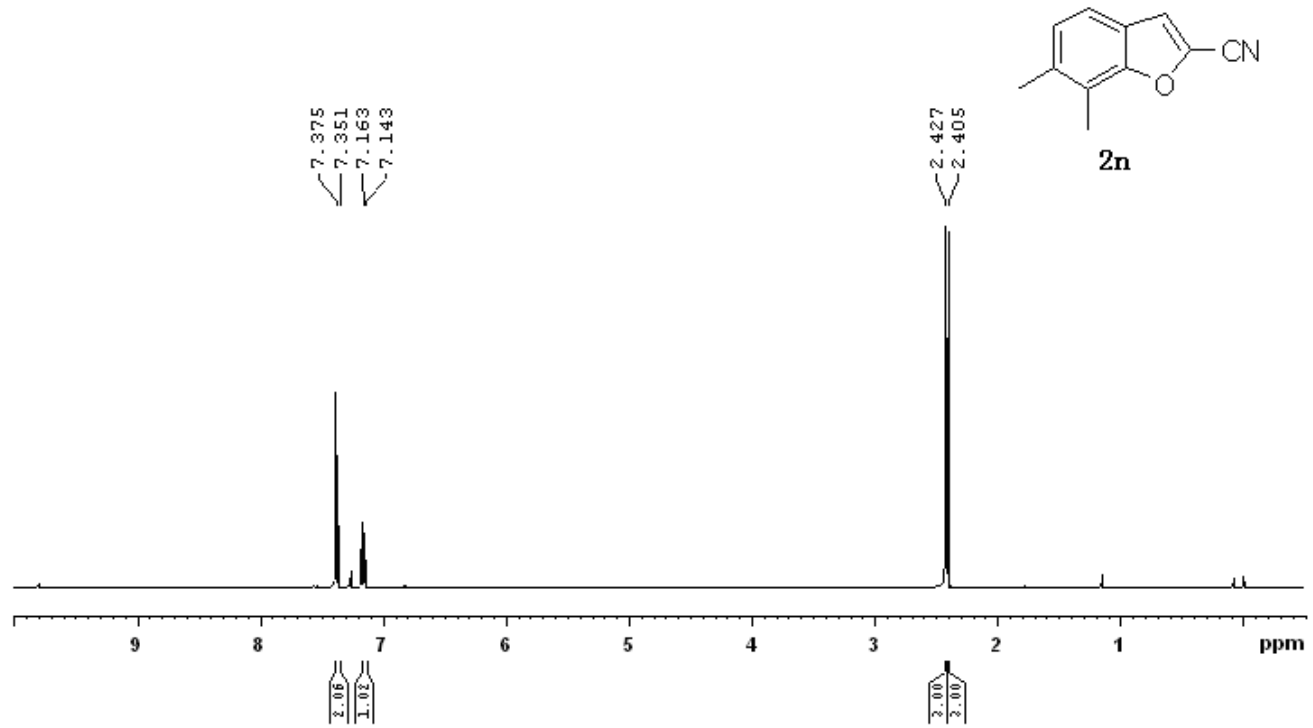
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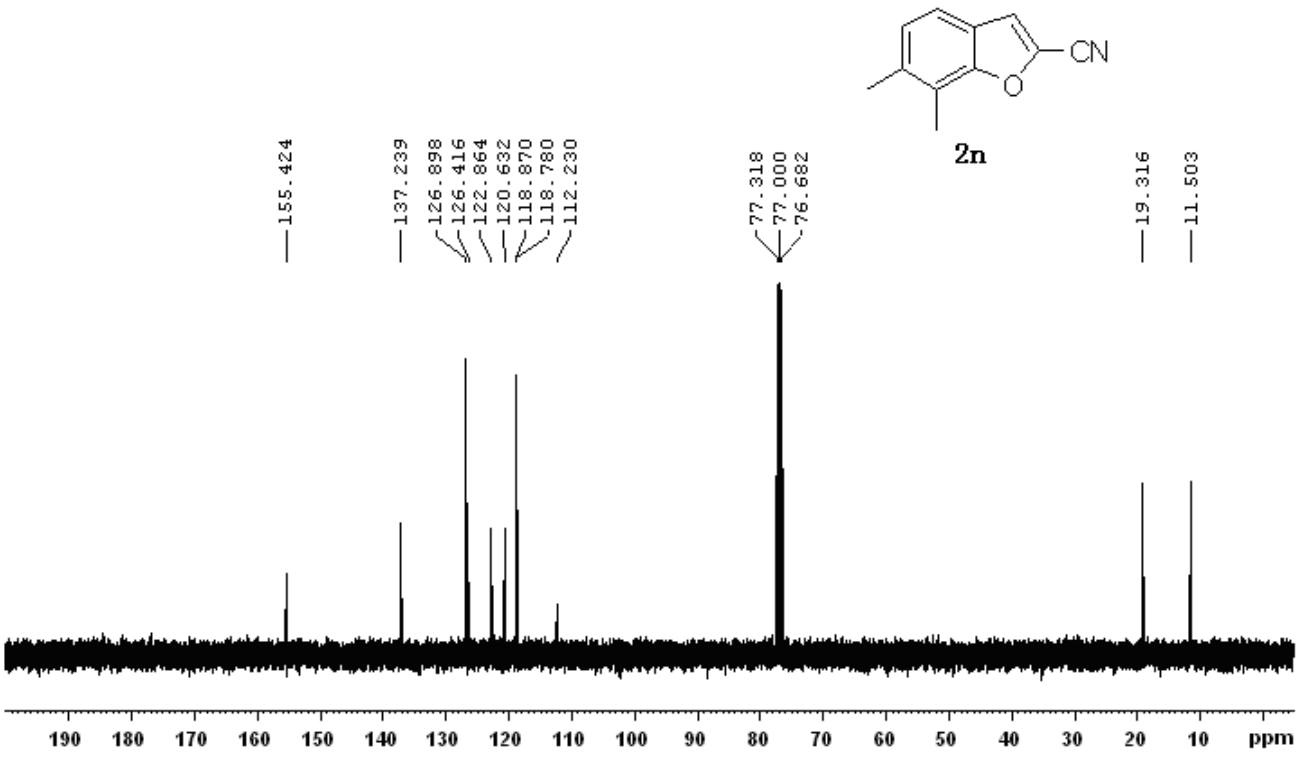
2.00
2.00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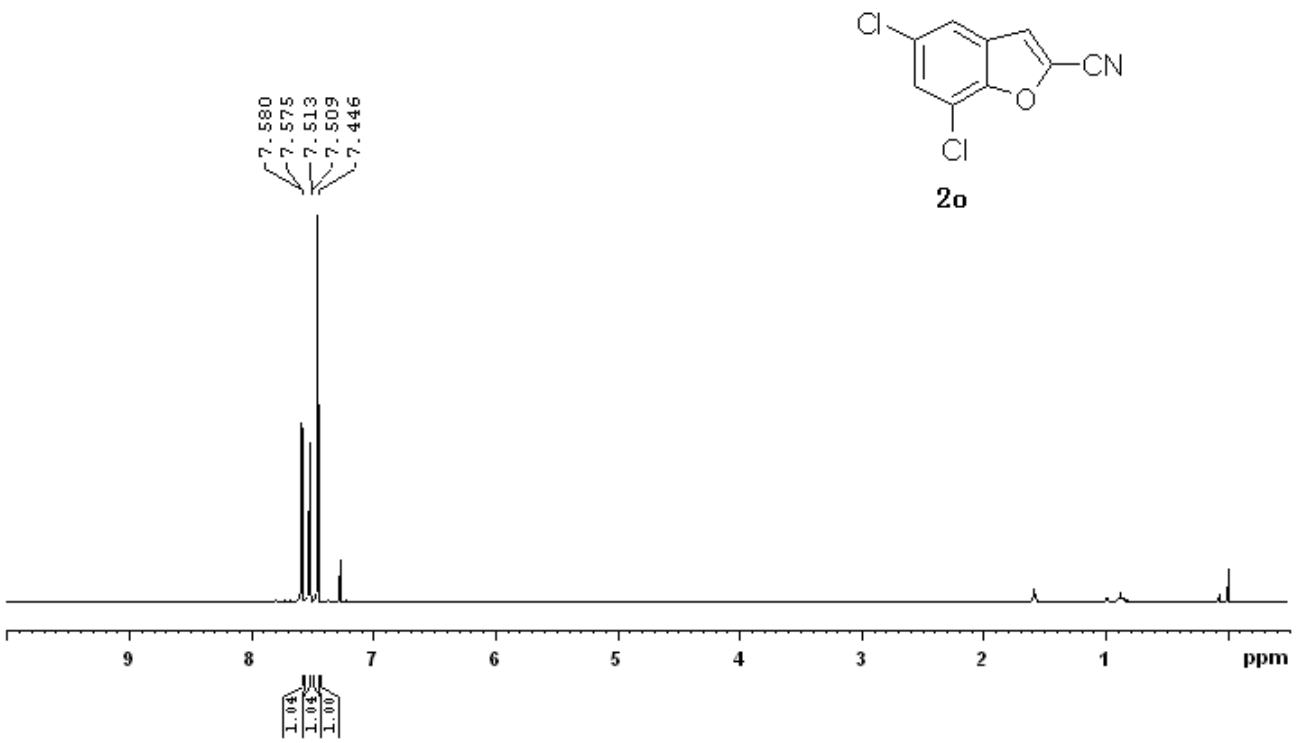
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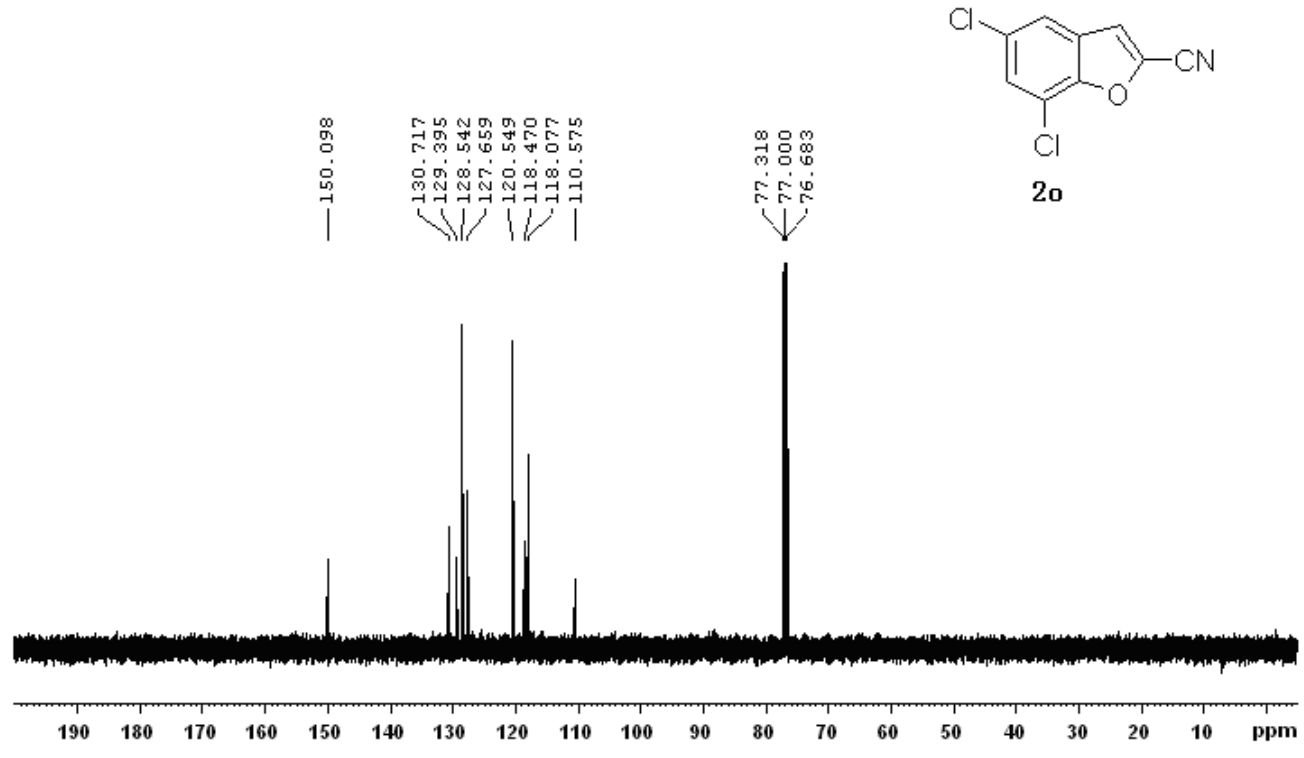
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O
Cl
2o
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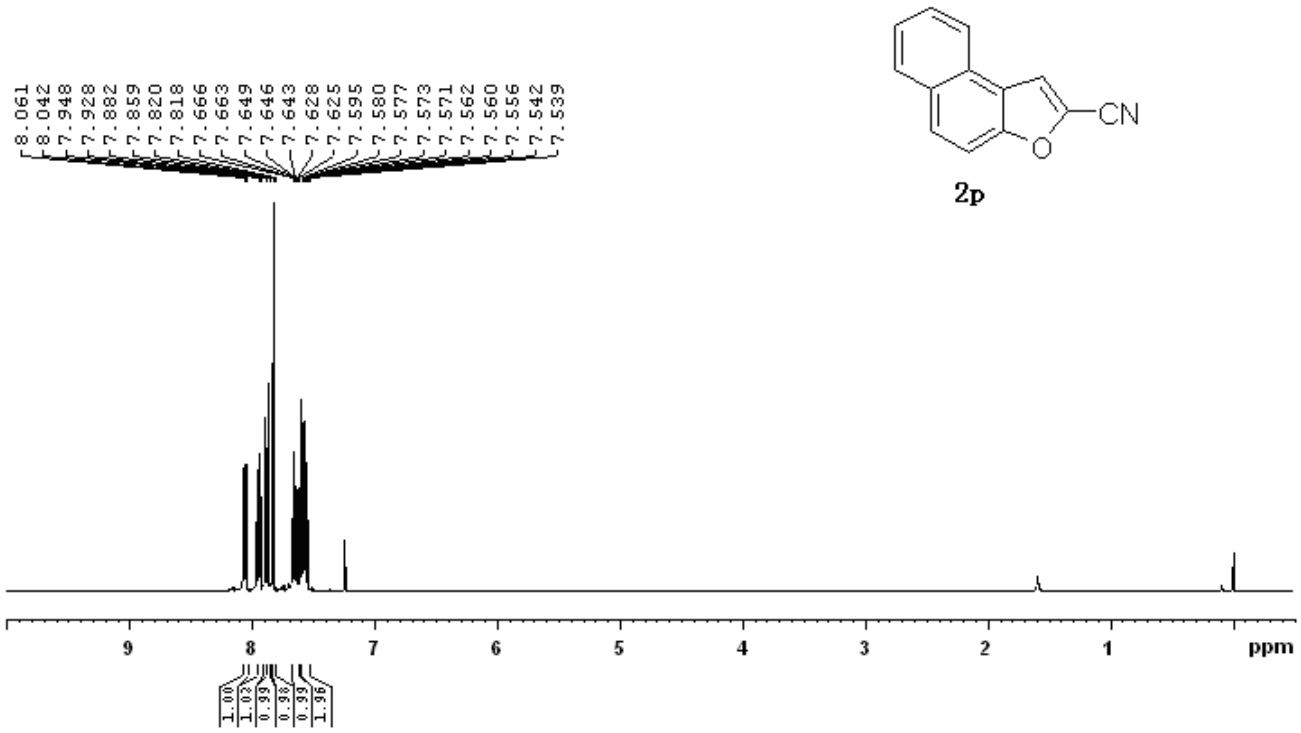


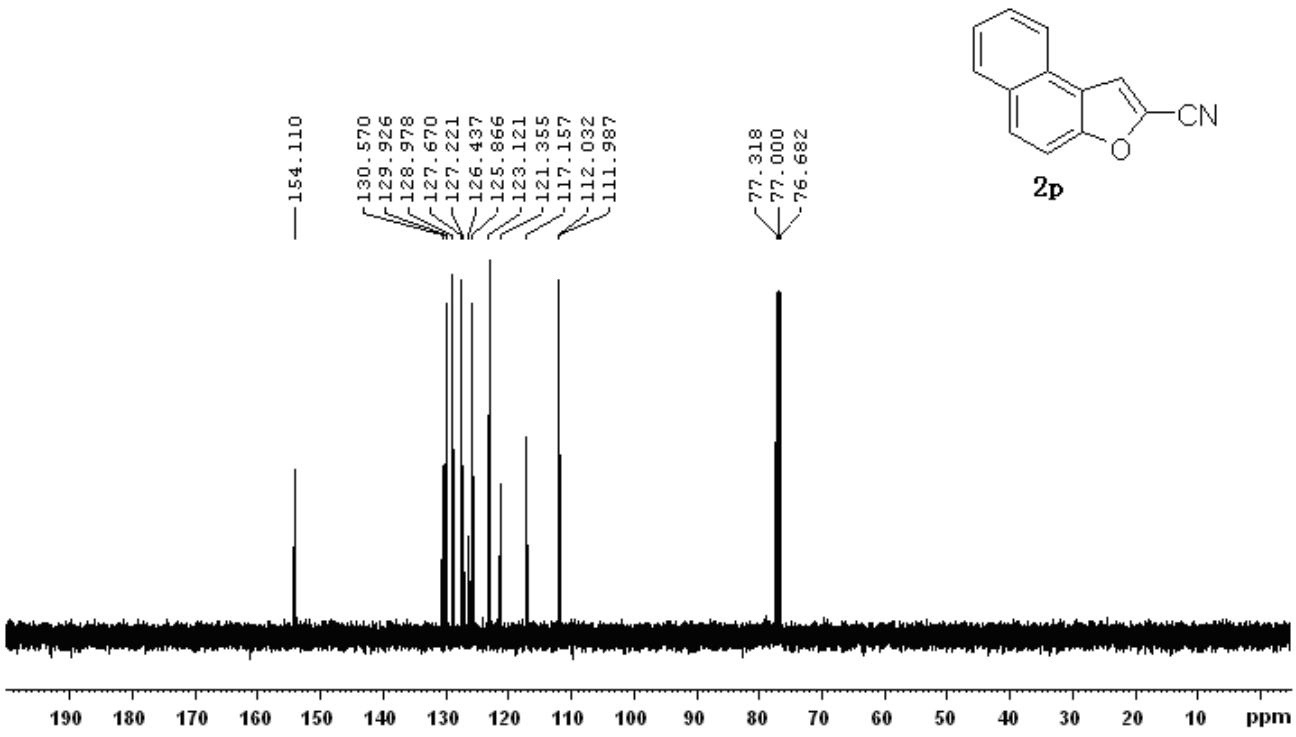

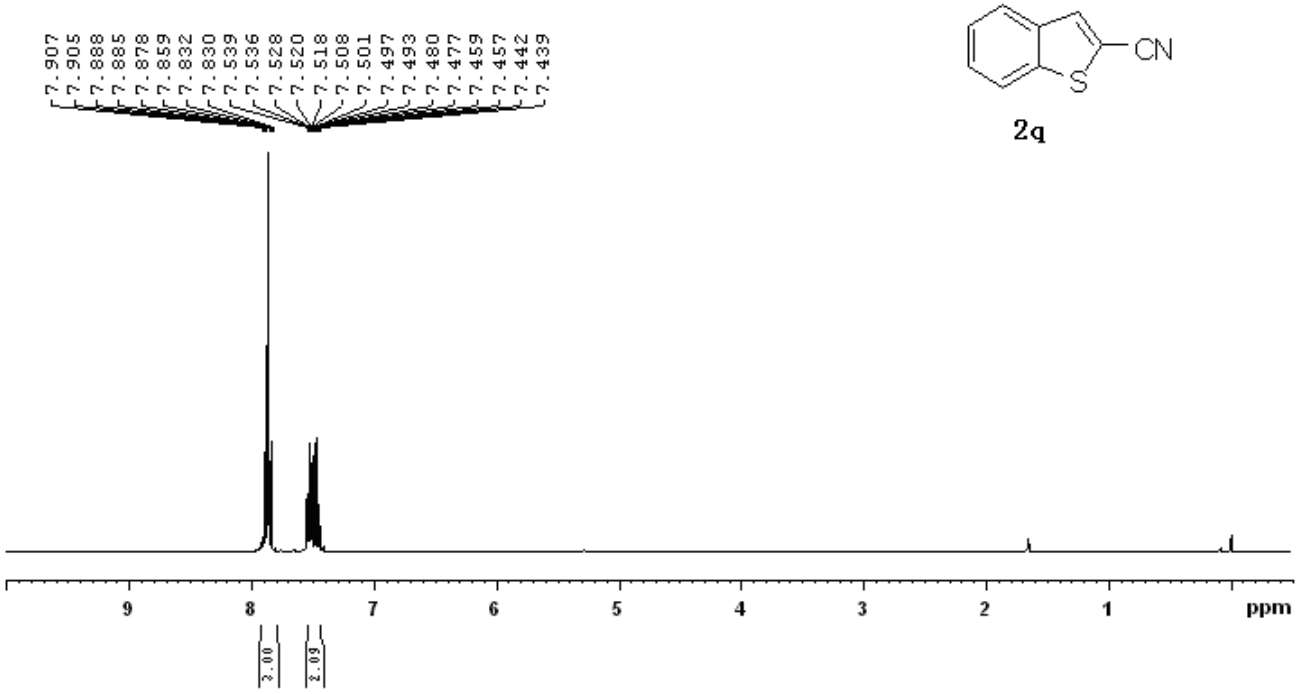


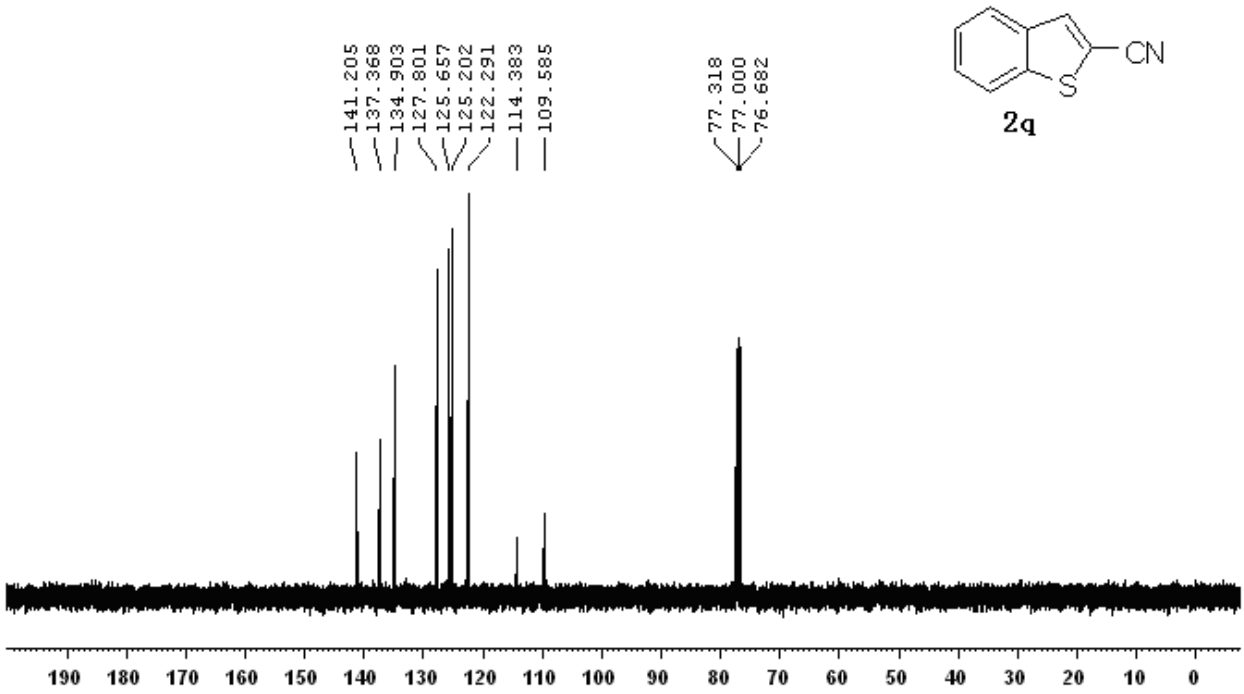

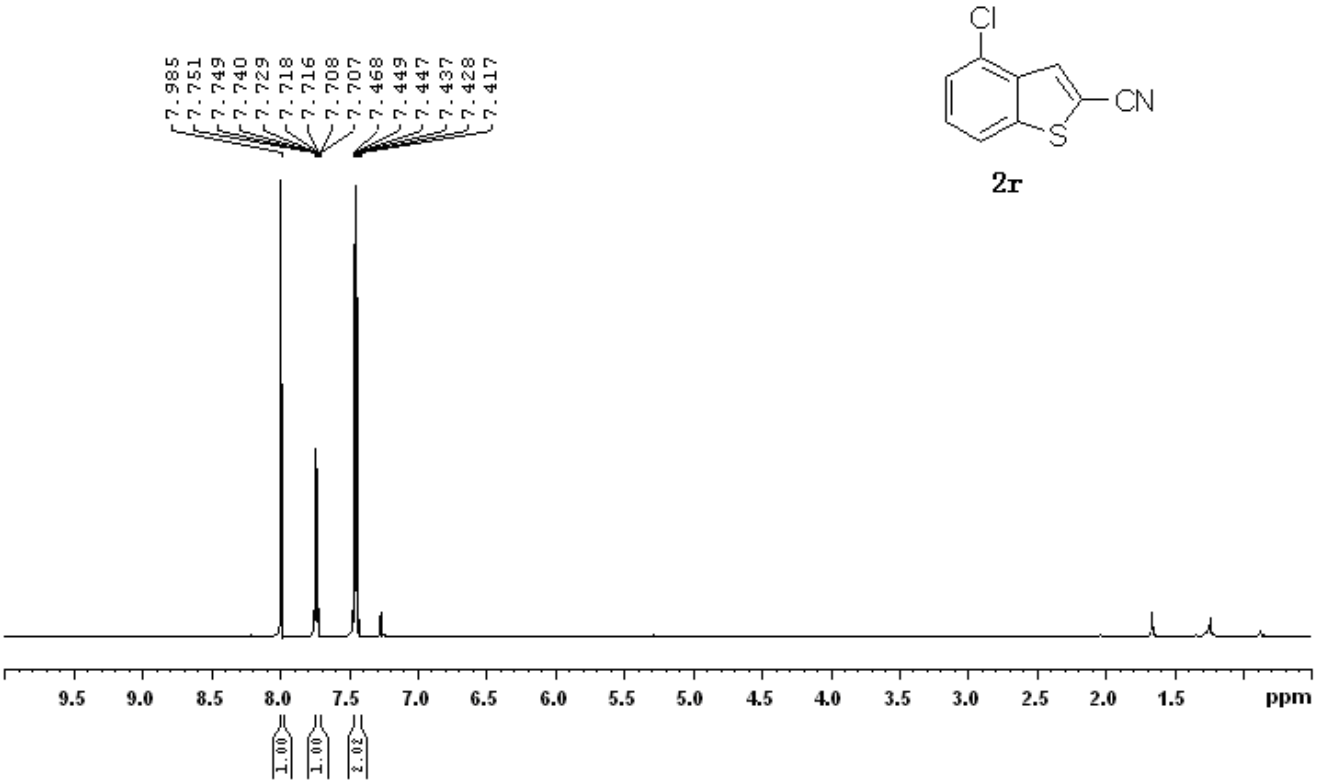


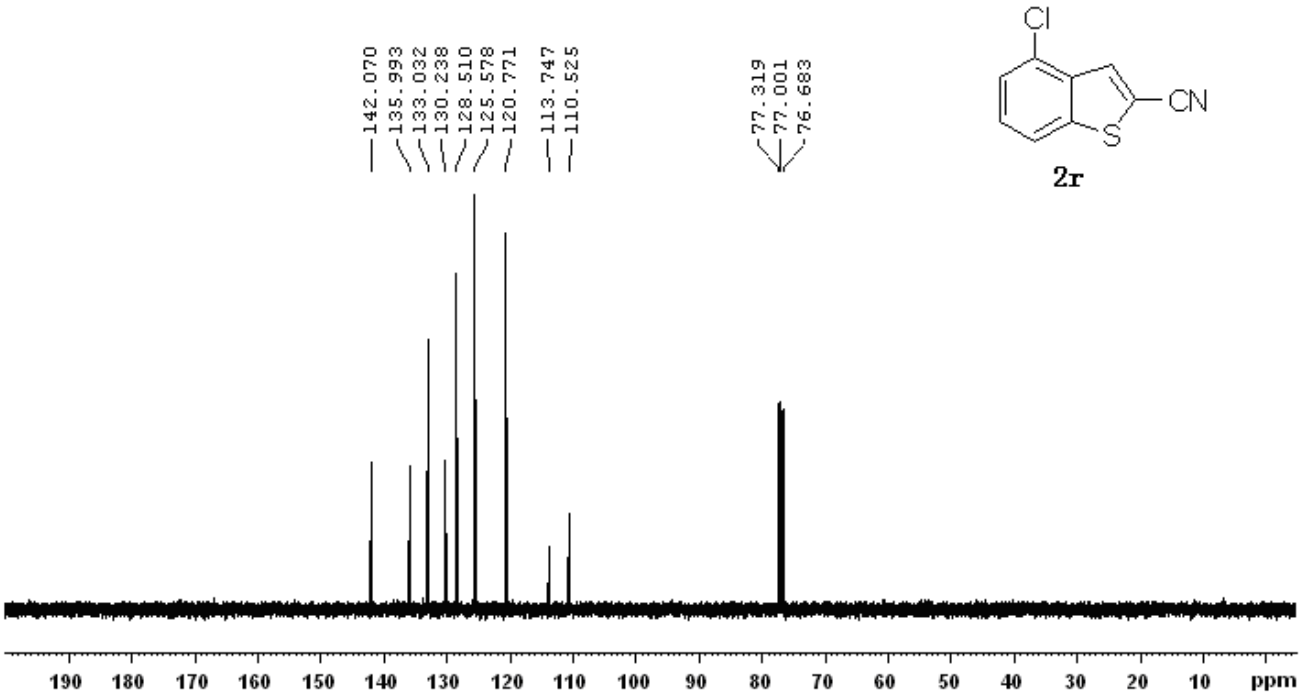

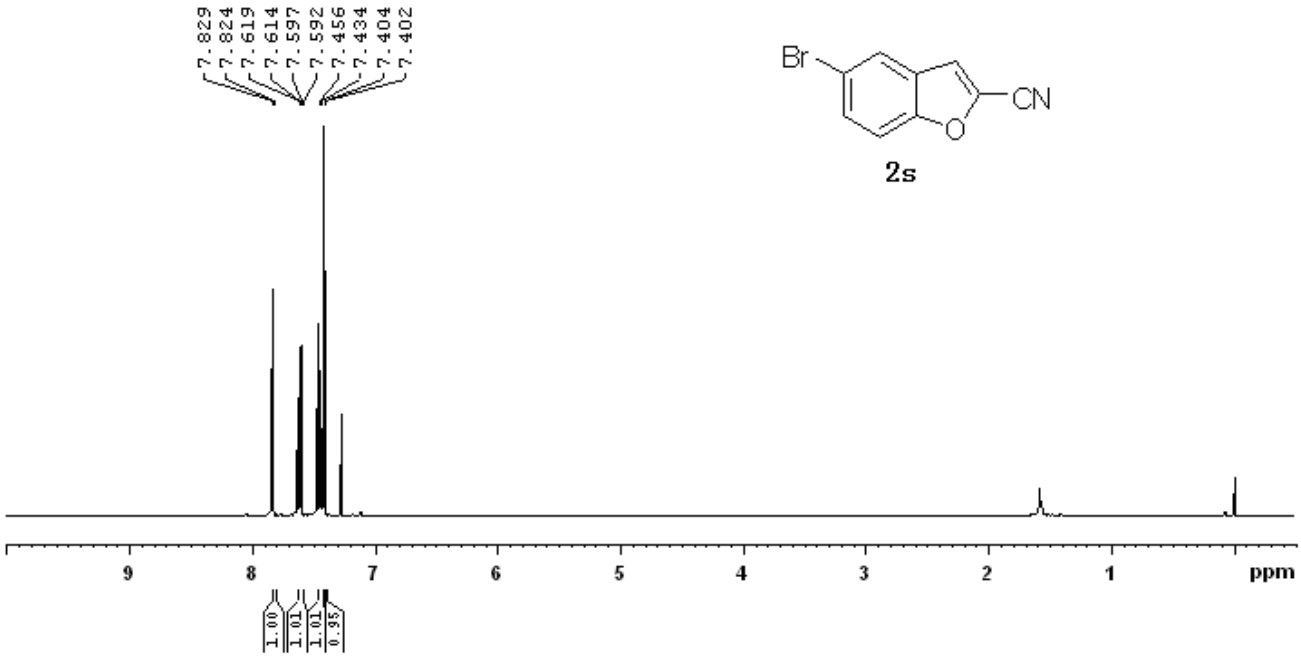
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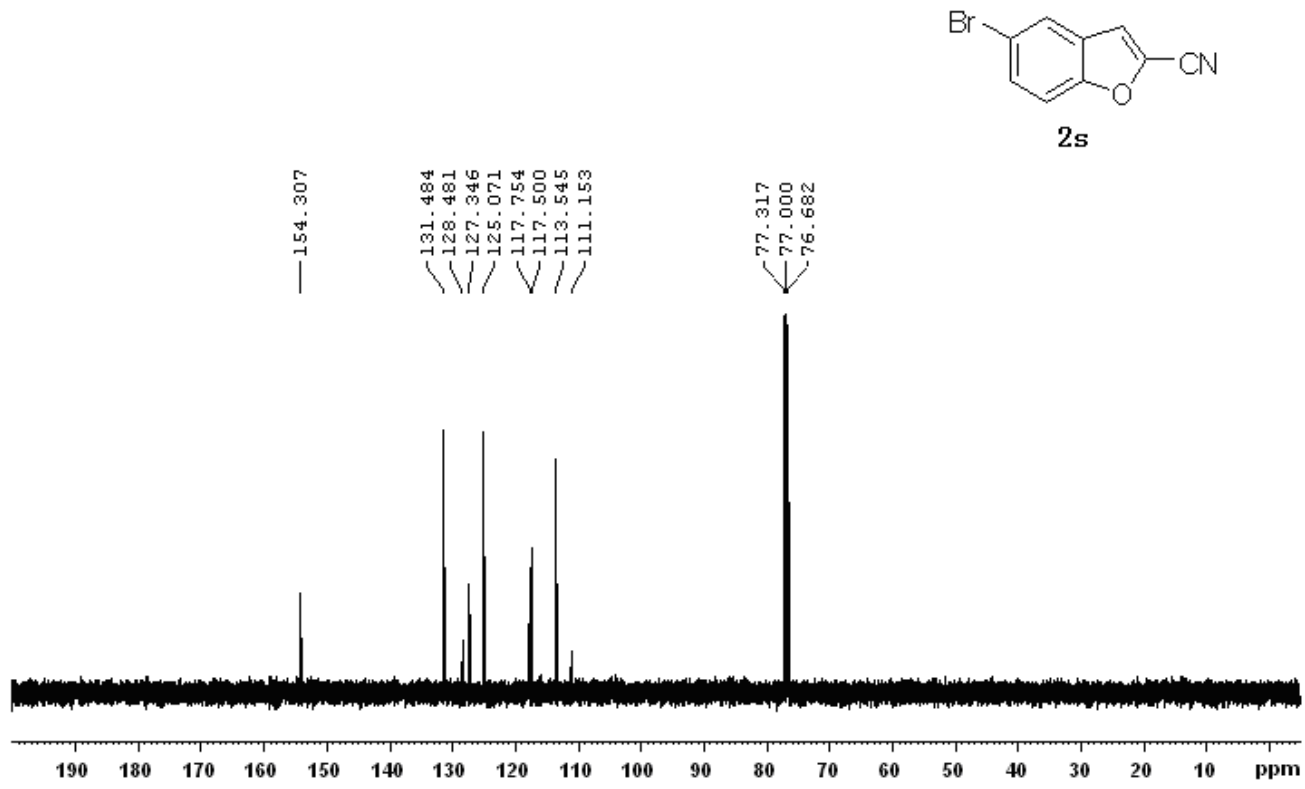
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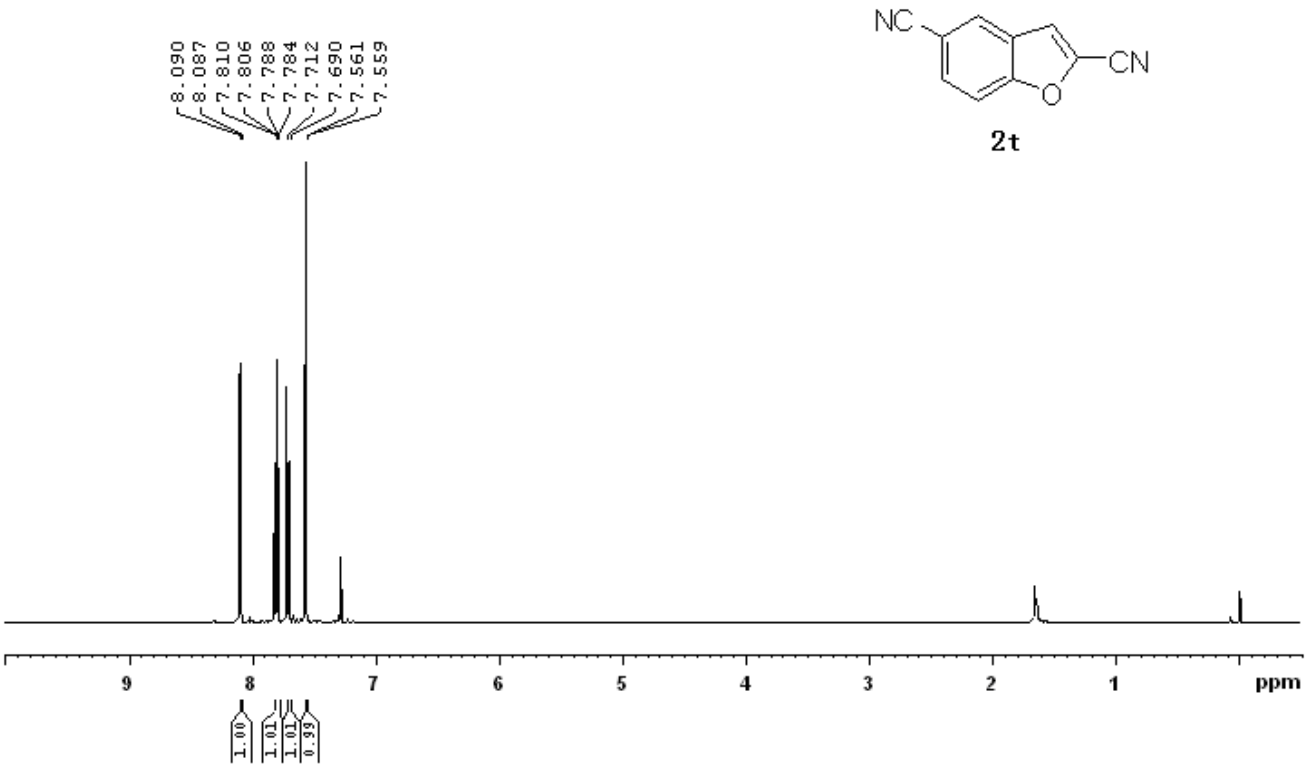
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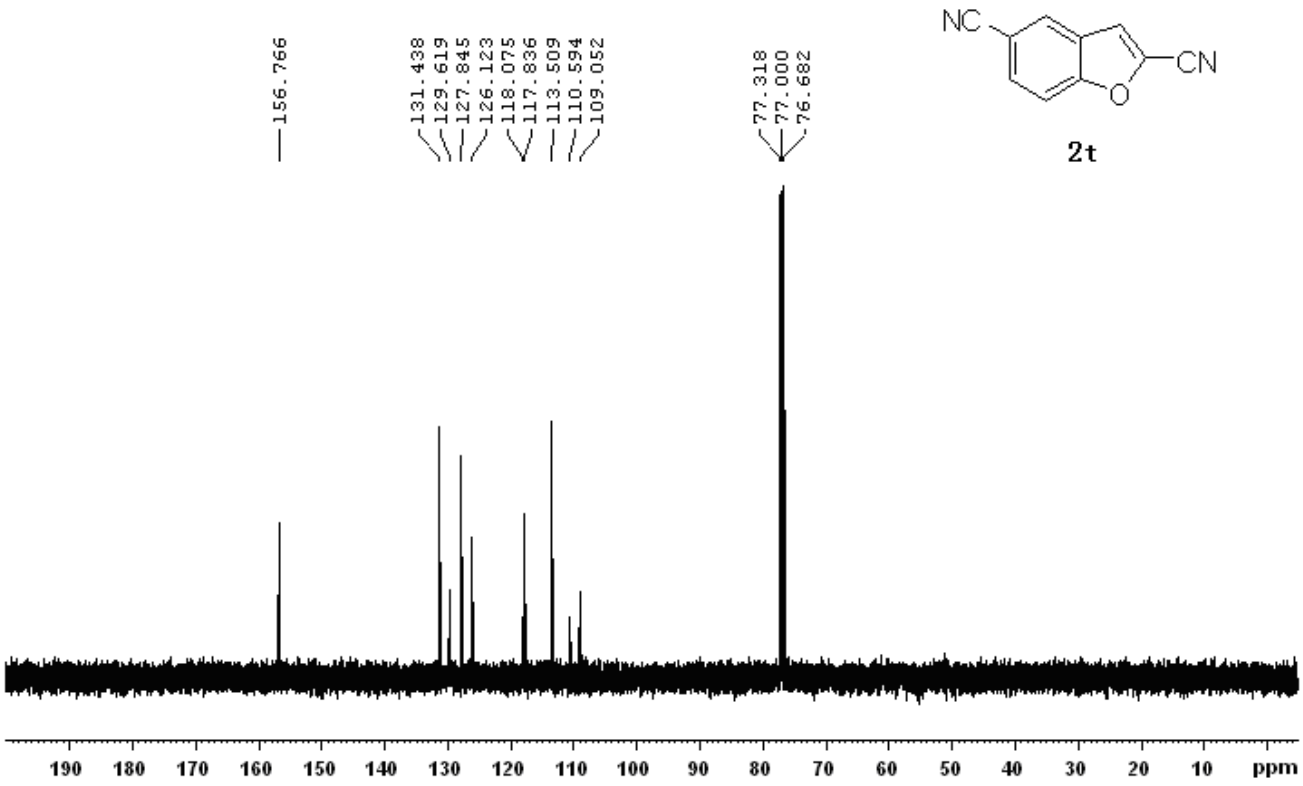
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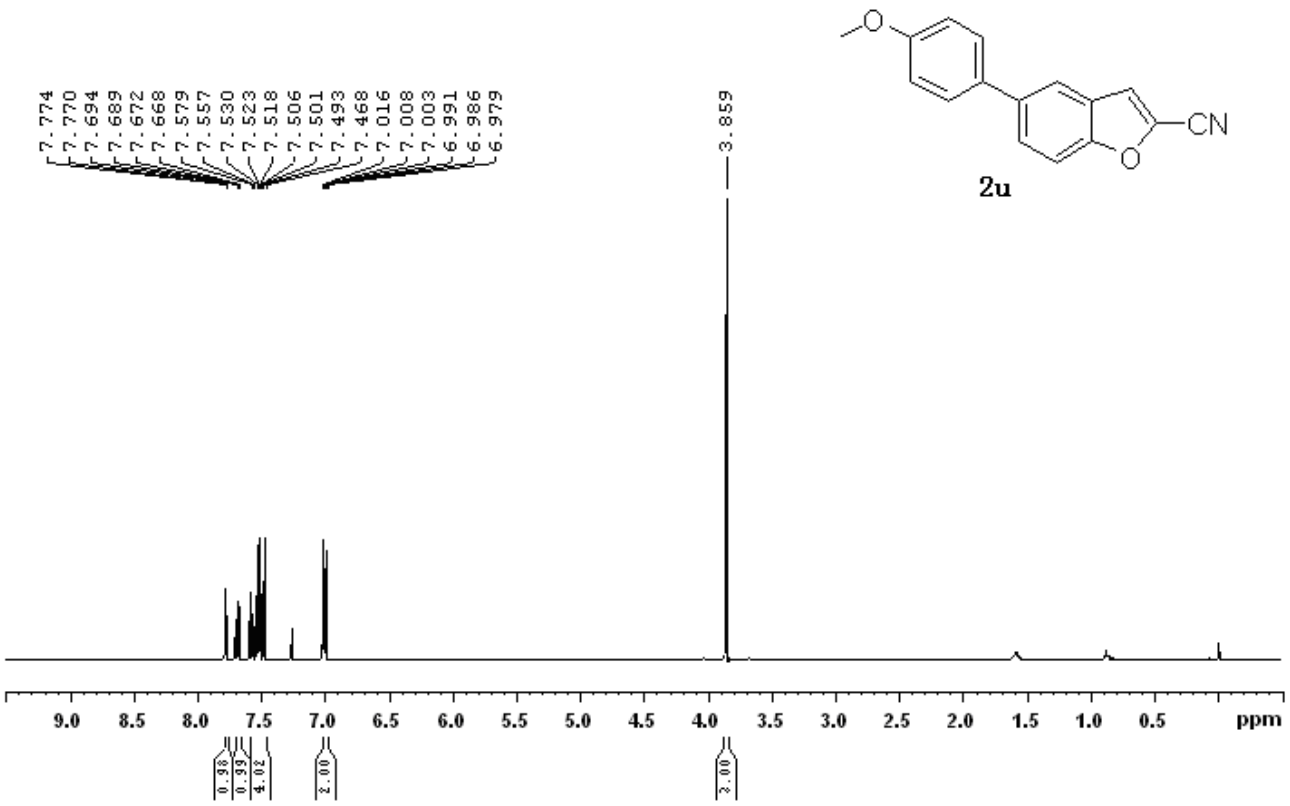
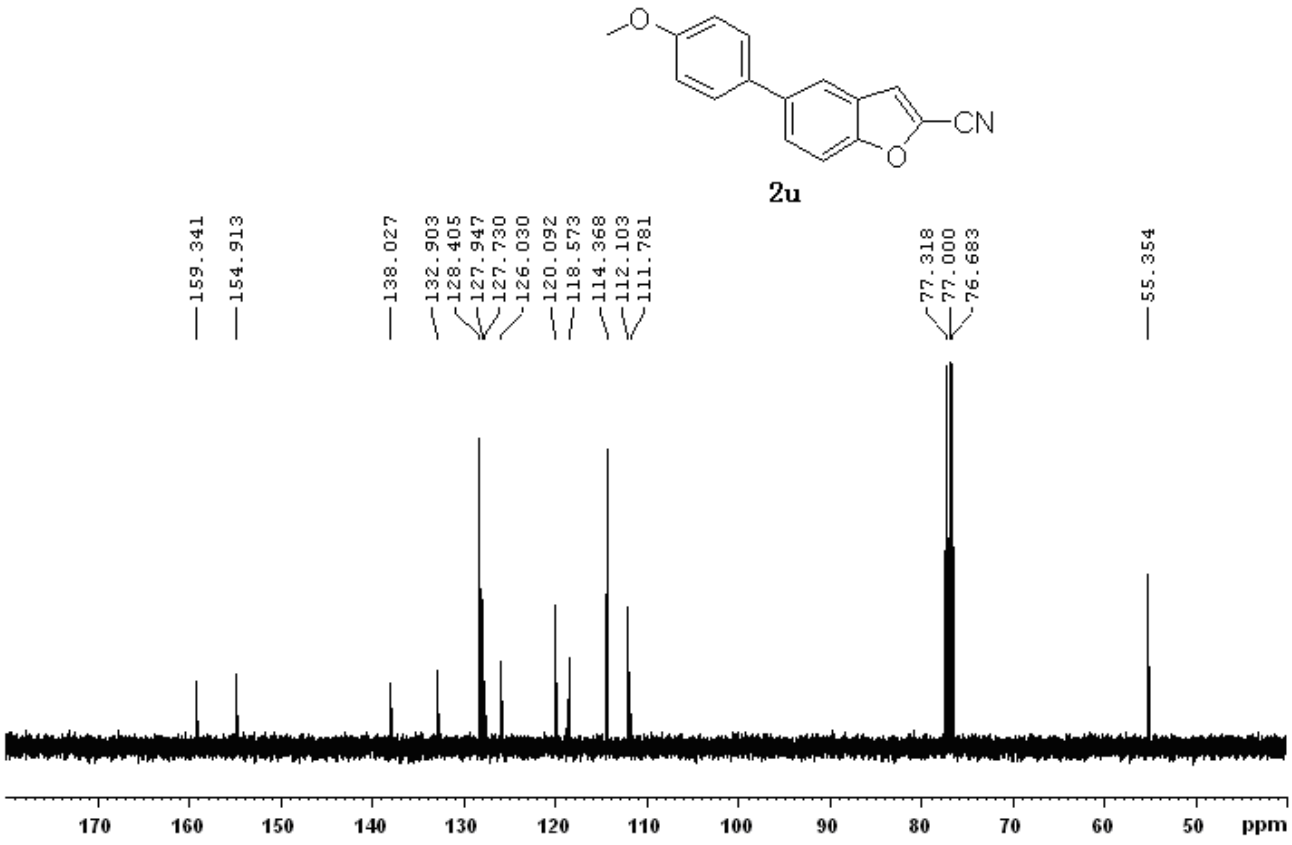
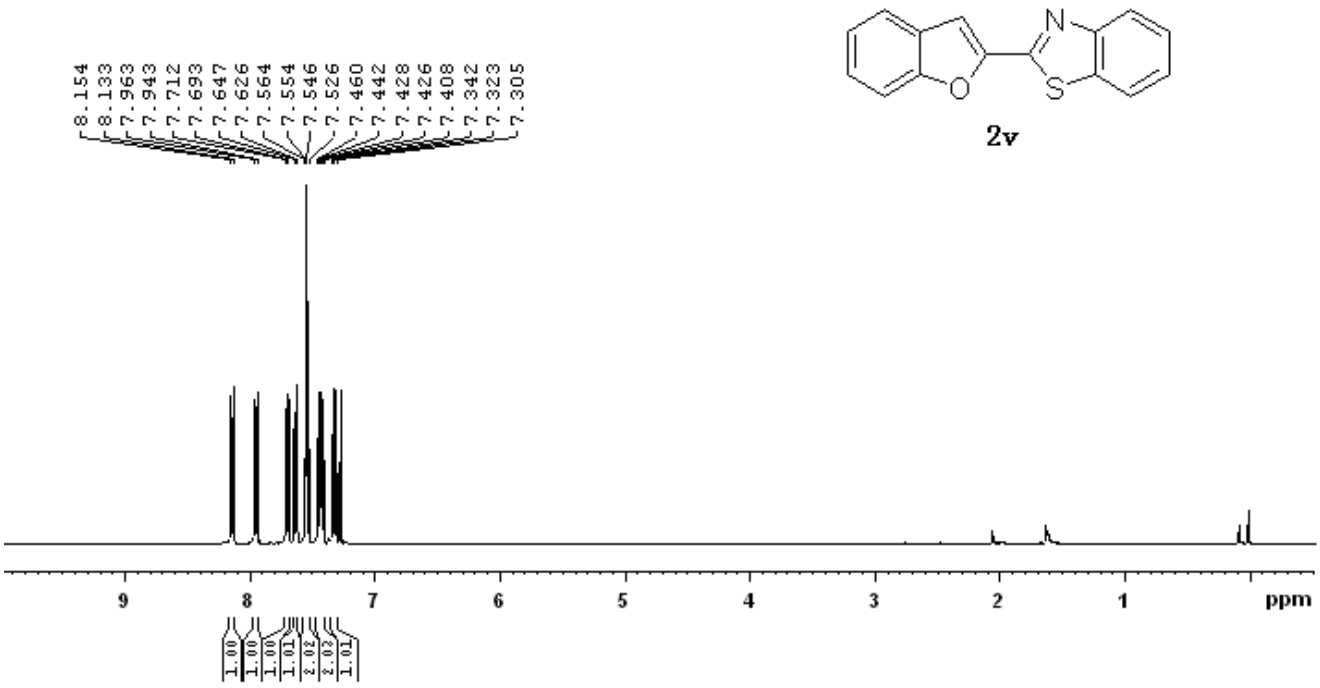
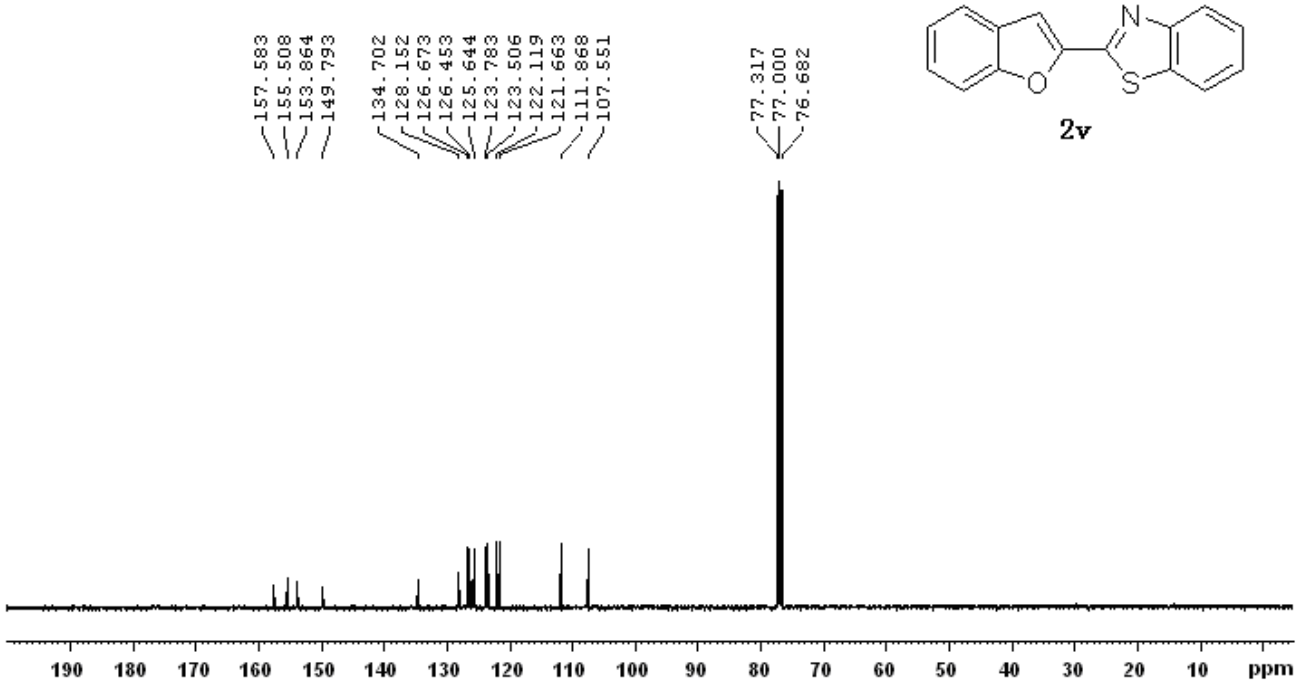
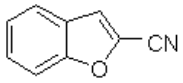






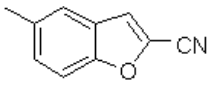

2a

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-05-0S0457
Sample Serial Number: HBSF-J08-Sample8
Operator: Li
Date: 2011/06/03
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
217 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 Br: 0-2 I: 0-2

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 143.0372 | 143.0371 | 0.1 | 0.7 | 8.0 | 15.0 | C9 H5 N O |
| | 143.0376 | -0.4 | -2.8 | 3.5 | 22522.6 | C6 H8 N2 Cl |
| | 143.0378 | -0.6 | -4.2 | -1.5 | 5097.6 | C3 H11 O4 S |



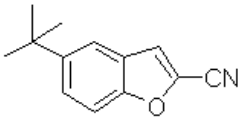

2b

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-07-0S0571
Sample Serial Number: HBSF-LJ12-S04
Operator: Li
Date: 2011/07/22
Elemental Composition Report
Single Mass Analysis
Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
161 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 Cl: 0-1 Br: 0-1 I: 0-2

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 157.0530 | 157.0528 | 0.2 | 1.3 | 8.0 | 2.9 | C10 H7 N O |
| | 157.0533 | -0.3 | -1.9 | 3.5 | 3631.9 | C7 H10 N2 Cl |

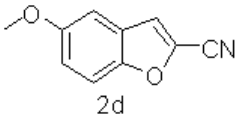



2c

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-07-OS0560
Sample Serial Number:    HBSF-WSH-J17-S16
Operator:  Li
Date: 2011/07/15
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
289 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60    H: 0-80    N: 0-4    O: 0-6    F: 0-1    Br: 0-1    I: 0-2
Minimum:                                          -1.5
Maximum:                        1.5         5.0   50.0
Mass        Calc. Mass          mDa         PPM   DBE         i-FIT         Formula
199.0995    199.0995            0.0         0.0   4.5         2783323.3     C8  H12  N4  O  F
            199.0997           -0.2        -1.0   8.0         2787109.8     C13  H13  N  O
```

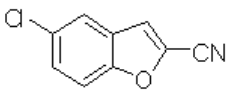



2d

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-07-OS0572
Sample Serial Number:    HBSF-LJ12-S05
Operator:  Li
Date: 2011/07/25
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
200 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:  C: 0-60    H: 0-80    N: 0-4    O: 0-6    Cl: 0-1    Br: 0-1    I: 0-2
Minimum:                                          -1.5
Maximum:                        1.5         5.0   50.0
Mass        Calc. Mass          mDa         PPM   DBE         i-FIT         Formula
173.0474    173.0477           -0.3        -1.7   8.0         9.6           C10  H7  N  O2
            173.0482           -0.8        -4.6   3.5         9514.1        C7  H10  N2  O  Cl
```



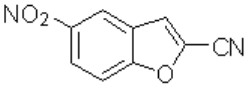

2e

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-05-0S0496
Sample Serial Number: HBSF-J19-S18
Operator: Li
Date: 2011/06/21
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
202 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 Cl: 0-1 Br: 0-1

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 176.9980 | 176.9981 | -0.1 | -0.6 | 8.0 | 8.1 | C9 H4 N O Cl |
| | 176.9977 | 0.3 | 1.7 | 12.5 | 2080.6 | C12 H O2 |



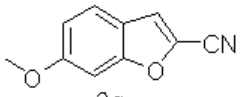

2f

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-05-0S0495
Sample Serial Number: HBSF-J19-S17
Operator: Li
Date: 2011/06/21
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
221 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 Cl: 0-1 Br: 0-1

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 188.0223 | 188.0222 | 0.1 | 0.5 | 9.0 | 13.9 | C9 H4 N2 O3 |
| | 188.0227 | -0.4 | -2.1 | 4.5 | 2354.9 | C6 H7 N3 O2 Cl |



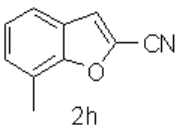

2g

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-07-OS0559
Sample Serial Number: HBSF-WSH-J17-S15
Operator: Li
Date: 2011/07/15
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
218 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 F: 0-1 Br: 0-1 I: 0-2

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 173.0475 | 173.0475 | 0.0 | 0.0 | 4.5 | 59.8 | C5 H6 N4 O2 F |
| | 173.0477 | -0.2 | -1.2 | 8.0 | 0.2 | C10 H7 N O2 |



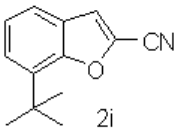

2h

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-07-OS0570
Sample Serial Number: HBSF-LJ12-S03
Operator: Li
Date: 2011/07/22
Elemental Composition Report
Single Mass Analysis
Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
105 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 Br: 0-1 I: 0-2

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 157.0525 | 157.0528 | -0.3 | -1.9 | 8.0 | 5.4 | C10 H7 N O |
| | 157.0514 | 1.1 | 7.0 | 8.5 | 59.6 | C8 H5 N4 |




2i

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

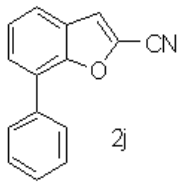
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-07-0S0560

Sample Serial Number:    HBSF-WSH-J17-S16

Operator:  Li

Date: 2011/07/15
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
289 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60    H: 0-80    N: 0-4    O: 0-6    F: 0-1    Br: 0-1    I: 0-2
Minimum:                                          -1.5
Maximum:                        1.5         5.0         50.0
Mass        Calc. Mass          mDa         PPM         DBE          i-FIT        Formula
199.0995    199.0995            0.0         0.0         4.5          2783323.3    C8   H12  N4  O  F
            199.0997           -0.2        -1.0         8.0          2787109.8    C13  H13  N   O
```

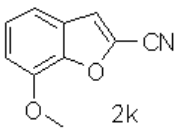



2j

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-07-0S0575
Sample Serial Number:    HBSF-LJ12-S08
Operator:  Li
Date: 2011/07/25
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
328 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:  C: 0-60    H: 0-80    N: 0-4    O: 0-6    Cl: 0-1    Br: 0-1    I: 0-2
Minimum:                                          -1.5
Maximum:                        1.5         5.0         50.0
Mass        Calc. Mass          mDa         PPM         DBE          i-FIT        Formula
219.0681    219.0684           -0.3        -1.4         12.0         2724432.0    C15  H9  N  O
            219.0689           -0.8        -3.7         7.5          2762153.3    C12  H12  N2  Cl
            219.0671            1.0         4.6         12.5         2765412.5    C13  H7  N4
```

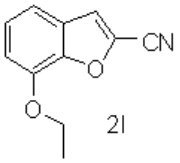



2k

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-05-OS0512
Sample Serial Number:    HBXF-HT7-S6
Operator:  Li
Date: 2011/06/29
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
247 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60    H: 0-80    N: 0-4    O: 0-6    S: 0-1    Cl: 0-1
Minimum:                                    -1.5
Maximum:                          1.5       5.0       50.0
Mass        Calc. Mass        mDa       PPM       DBE       i-FIT       Formula
173.0476    173.0477          -0.1      -0.6      8.0       6.0         C10  H7  N  O2
            173.0470          0.6       3.5       -1.0      2376.4      C2  H11  N3  O4  S
            173.0482          -0.6      -3.5      3.5       13455.6     C7  H10  N2  O  Cl
            173.0484          -0.8      -4.6      -1.5      2371.5      C4  H13  O5  S
```

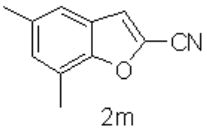



2l

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-05-OS0513
Sample Serial Number:    HBXF-HT7-S7
Operator:  Li Date: 2011/06/29
Elemental Composition Report Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
278 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
Elements Used:  C: 0-60    H: 0-80    N: 0-4    O: 0-6    S: 0-1    Cl: 0-1
Minimum:                                    -1.5
Maximum:                          1.5       5.0       50.0
Mass        Calc. Mass        mDa       PPM       DBE       i-FIT       Formula
187.0636    187.0638          -0.2      -1.1      3.5       2775588.5   C8  H12  N2  O  Cl
            187.0633          0.3       1.6       8.0       2773886.0   C11  H9  N  O2
            187.0640          -0.4      -2.1      -1.5      2775412.0   C5  H15  O5  S
            187.0627          0.9       4.8       -1.0      2775400.0   C3  H13  N3  O4  S
```



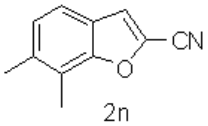

2m

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-07-OS0574
Sample Serial Number: HBSF-LJ12-S07
Operator: Li
Date: 2011/07/25
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
191 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 Cl: 0-1 Br: 0-1 I: 0-2

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 171.0686 | 171.0684 | 0.2 | 1.2 | 8.0 | 2797603.8 | C11 H9 N O |
| | 171.0689 | -0.3 | -1.8 | 3.5 | 2803425.0 | C8 H12 N2 Cl |



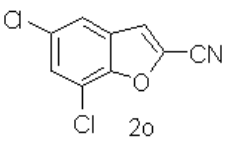

2n

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-07-OS0573
Sample Serial Number: HBSF-LJ12-S06
Operator: Li
Date: 2011/07/25
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
191 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 Cl: 0-1 Br: 0-1 I: 0-2

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 171.0680 | 171.0684 | -0.4 | -2.3 | 8.0 | 110.5 | C11 H9 N O |

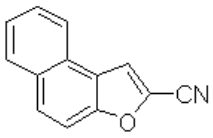



2o

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-05-OS0497
Sample Serial Number:    HBSF-J19-S19
Operator:  Li
Date: 2011/06/21
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
352 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60    H: 0-80    N: 0-4    O: 0-6    Cl: 0-2    Br: 0-1
Minimum:                                          -1.5
Maximum:                        1.5         5.0   50.0
Mass        Calc. Mass          mDa         PPM    DBE         i-FIT       Formula
210.9595    210.9593            0.2         0.9    2.0         329.7       C3  H6  N3  O3  Br
            210.9592            0.3         1.4    8.0         2.7         C9  H3  N  O  C12
            210.9587            0.8         3.8    12.5        324.5       C12  O2  Cl
```

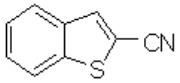



2p

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-07-OS0558
Sample Serial Number:    HBSF-WSH-J17-S14
Operator:  Li
Date: 2011/07/15
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
280 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60    H: 0-80    N: 0-4    O: 0-6    F: 0-1    Br: 0-1    I: 0-2
Minimum:                                          -1.5
Maximum:                        1.5         5.0   50.0
Mass        Calc. Mass          mDa         PPM    DBE         i-FIT       Formula
193.0529    193.0528            0.1         0.5    11.0        2783012.8   C13  H7  N  O
            193.0526            0.3         1.6    7.5         2779812.5   C8  H6  N4  O  F
```

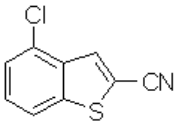



2q

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-08-OSO639
Sample Serial Number:    HBSF-A8-S3
Operator:  Li
Date: 2011/08/22
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
187 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60    H: 0-80    N: 0-6    O: 0-4    S: 0-1    Br: 0-1
Minimum:                                              -1.5
Maximum:                          1.5         5.0     50.0
Mass        Calc. Mass        mDa         PPM         DBE         i-FIT       Formula
159.0147    159.0143          0.4         2.5         8.0         1.8         C9  H5  N  S
            159.0154          -0.7        -4.4        4.5         551.6       C3  H3  N4  O4
```

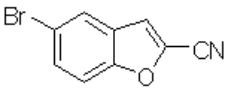



2r

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

```
Card Serial Number:   GCT-P-T11-08-OSO640
Sample Serial Number:    HBSF-A8-S4
Operator:  Li
Date: 2011/08/22
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
427 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60    H: 0-80    N: 0-6    O: 0-4    S: 0-1    Cl: 0-1    Br: 0-1
Minimum:                                              -1.5
Maximum:                          1.5         5.0     50.0
Mass        Calc. Mass        mDa         PPM         DBE         i-FIT       Formula
192.9756    192.9753          0.3         1.6         8.0         5.4         C9  H4  N  S  Cl
            192.9748          0.8         4.1         12.5        2712.3      C12  H  O  S
            192.9765          -0.9        -4.7        4.5         292.5       C3  H2  N4  O4  Cl
```



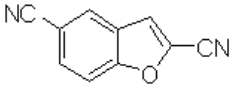

2s

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-08-0S0637
Sample Serial Number: HBSF-A8-S1
Operator: Li
Date: 2011/08/22
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
311 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60 H: 0-80 N: 0-6 O: 0-4 S: 0-1 Br: 0-1

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 220.9474 | 220.9476 | -0.2 | -0.9 | 8.0 | 3.0 | C9 H4 N O Br |
| | 220.9470 | 0.4 | 1.8 | -1.0 | 26.0 | C H8 N3 O3 S Br |
| | 220.9483 | -0.9 | -4.1 | -1.5 | 20.7 | C3 H10 O4 S Br |



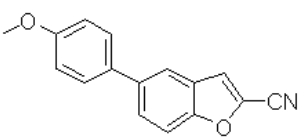

2t

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-08-0S0638
Sample Serial Number: HBSF-A8-S2
Operator: Li
Date: 2011/08/22
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
187 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60 H: 0-80 N: 0-6 O: 0-4 S: 0-1 Br: 0-1

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 1.5 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 168.0320 | 168.0317 | 0.3 | 1.8 | 1.0 | 2774561.8 | C2 H8 N4 O3 S |
| | 168.0324 | -0.4 | -2.4 | 10.0 | 2773286.8 | C10 H4 N2 O |




2u

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

Instrument: Waters Micromass GCT Premier  Ionisation Mode: EI+  Electron Energy: 70eV

Card Serial Number: GCT-P-T11-10-OS0796
Sample Serial Number: HBSF-Li012-S11
Operator: Li
Date: 2011/10/18
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
330 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60 H: 0-80 N: 0-2 O: 0-6 S: 0-1 Cl: 0-2

| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 2.0 | 5.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | i-FIT | Formula |
| 249.0788 | 249.0790 | -0.2 | -0.8 | 12.0 | 1.4 | C16 H11 N O2 |
| | 249.0795 | -0.7 | -2.8 | 7.5 | 4645.6 | C13 H14 N2 O Cl |
| | 249.0797 | -0.9 | -3.6 | 2.5 | 525.7 | C10 H17 O5 S |