Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Synthesis of (*Z*)-3-Aryloxy-acrylonitriles, (*E*)-3-Aryloxy-acrylonitriles and 3-Cyanobenzofurans through the Sequential Reactions of Phenols with Propiolonitriles

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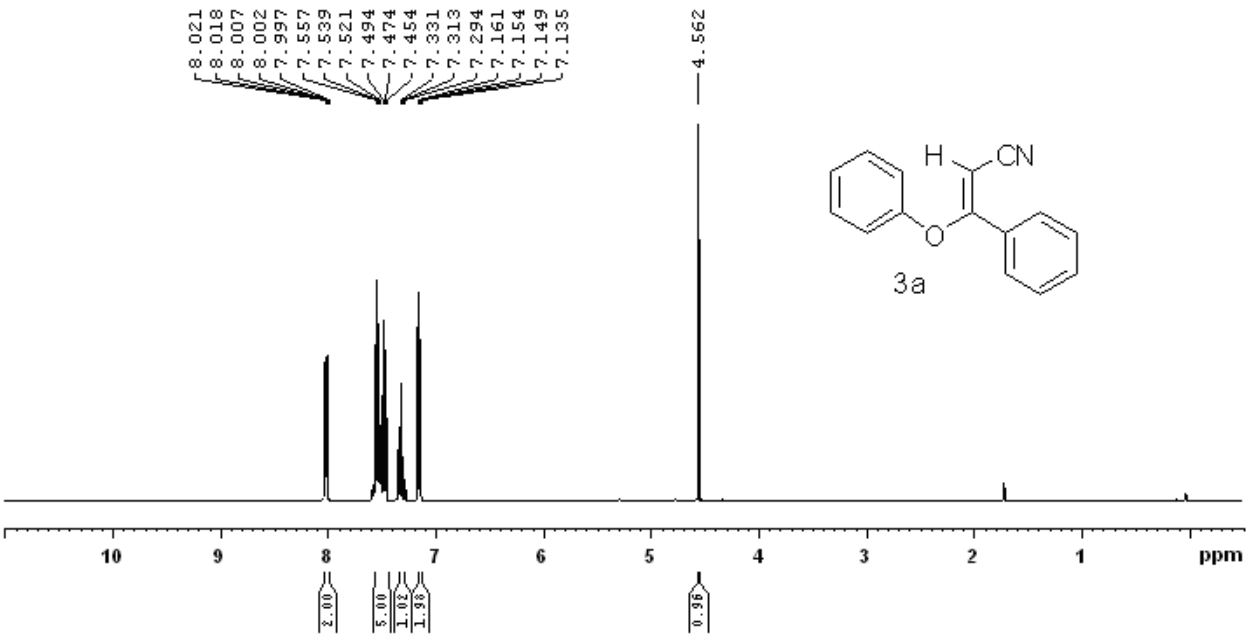

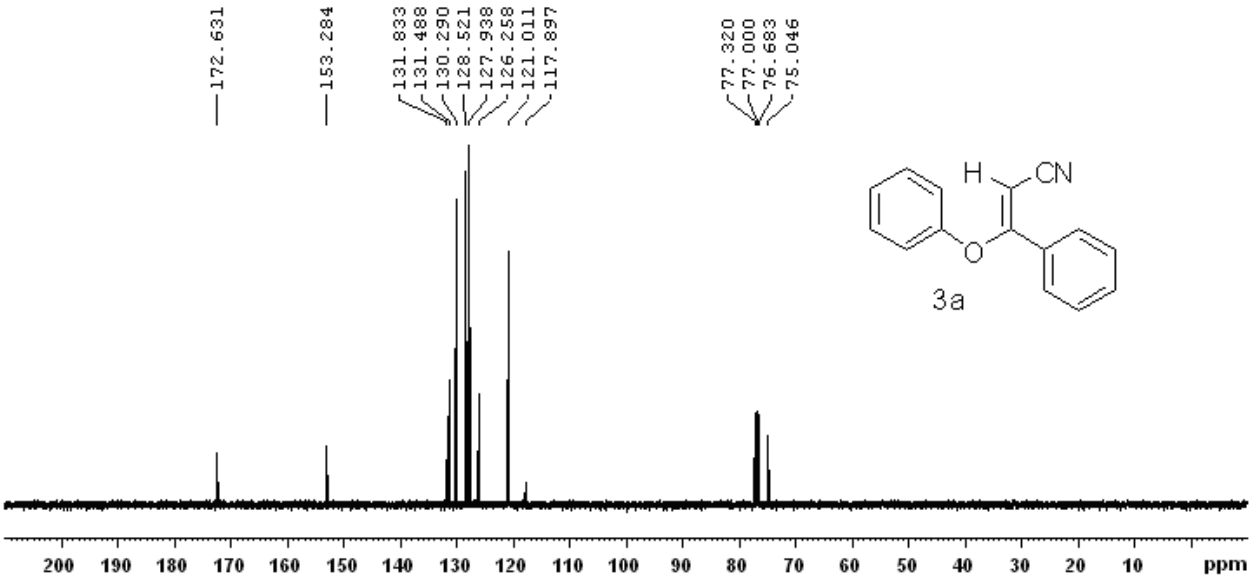

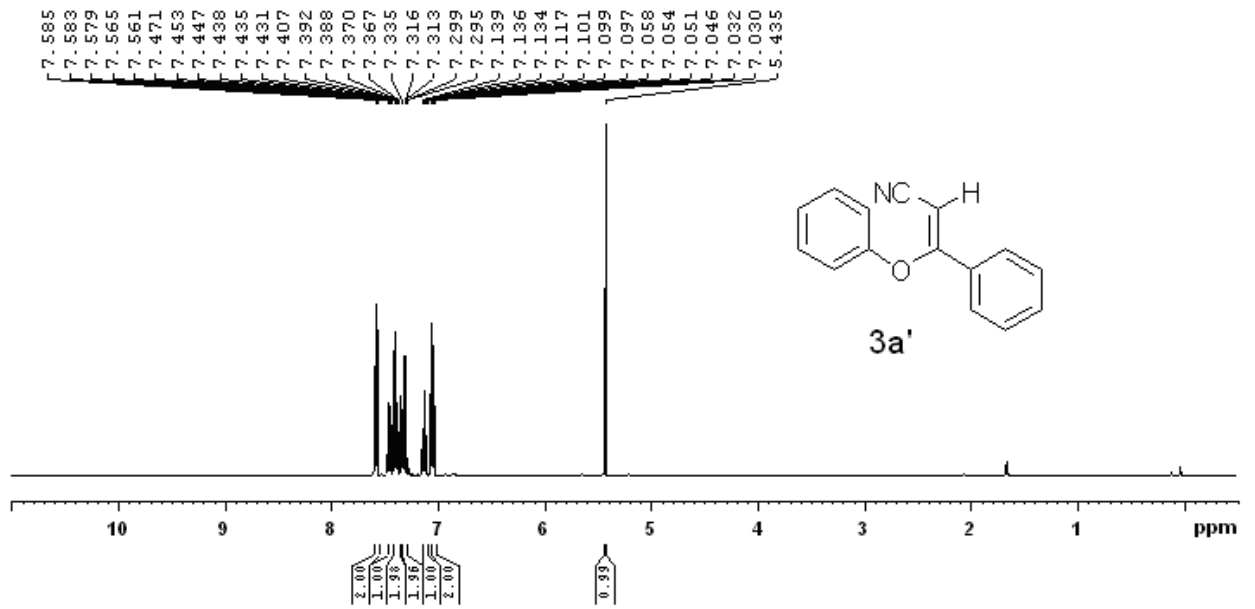

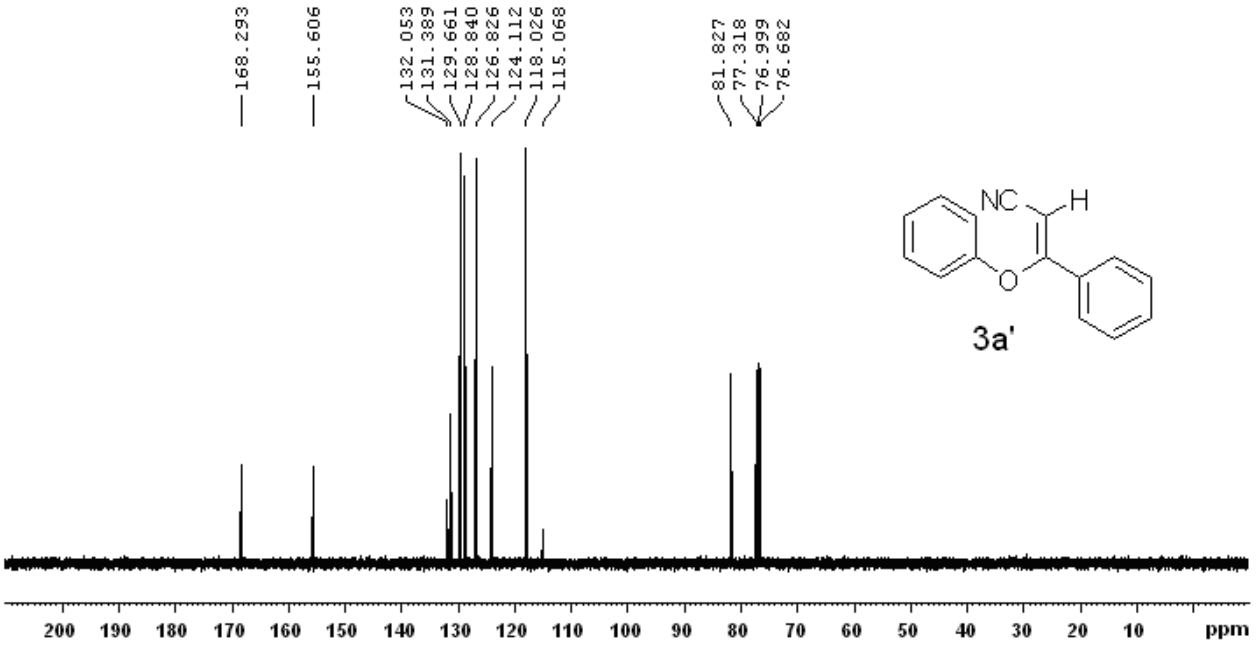

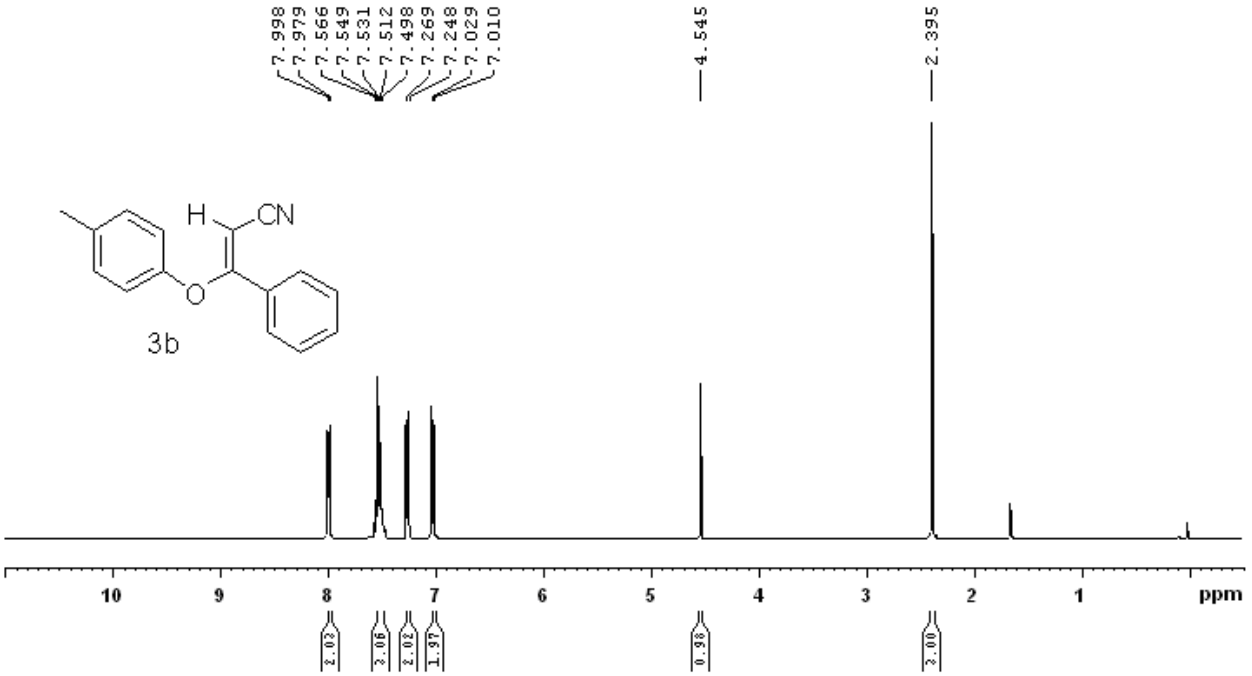

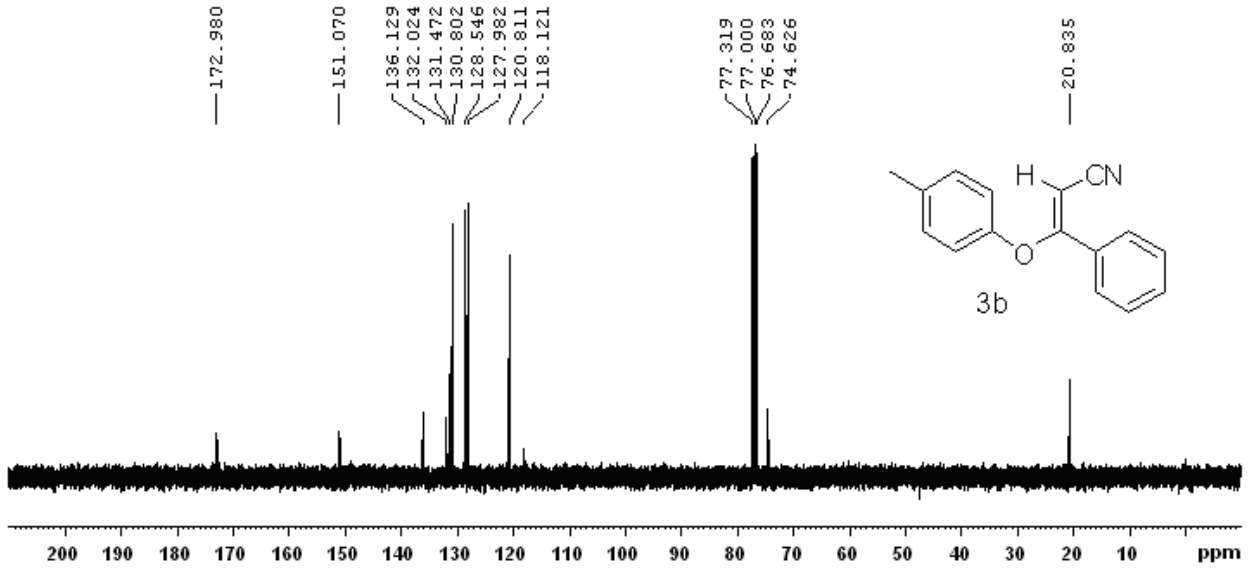

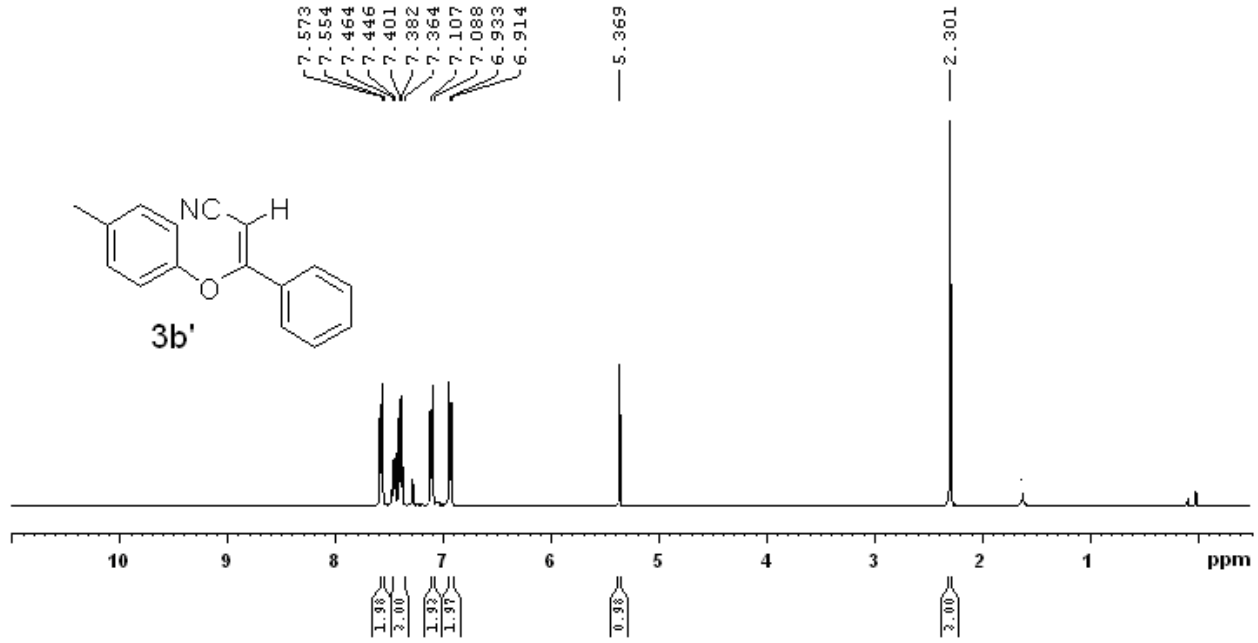

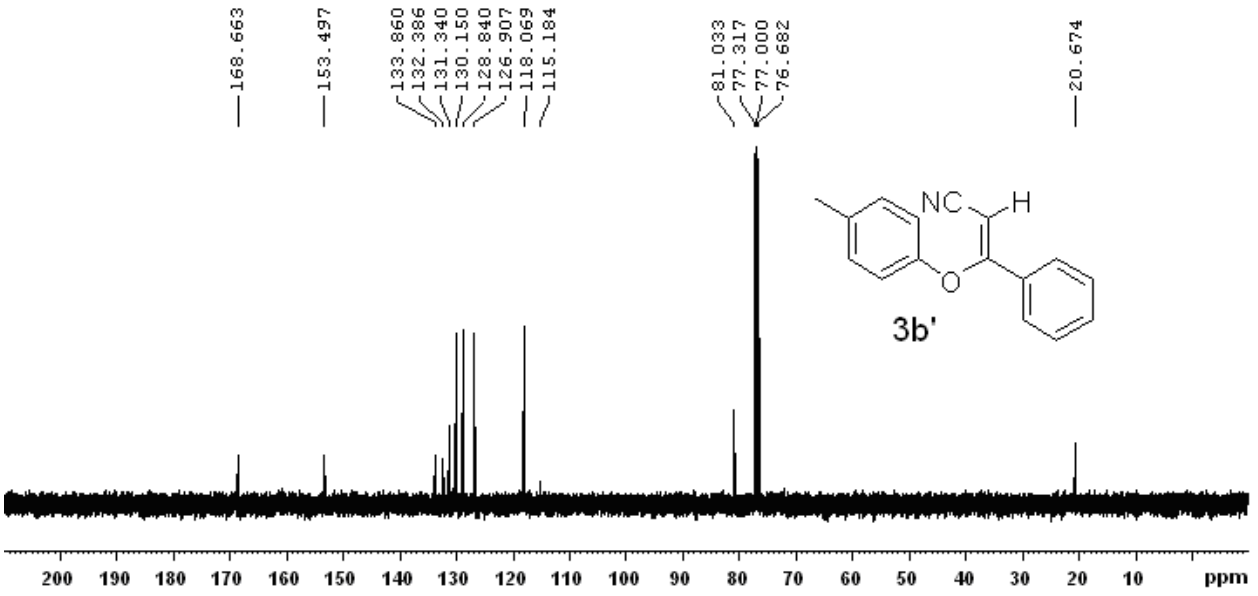

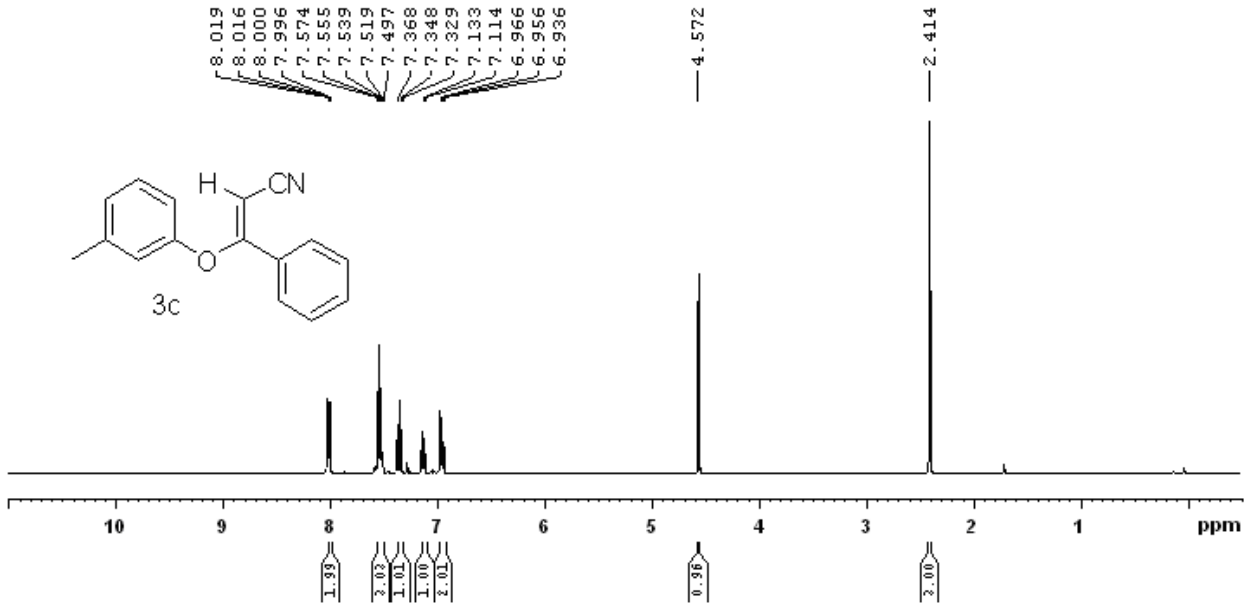

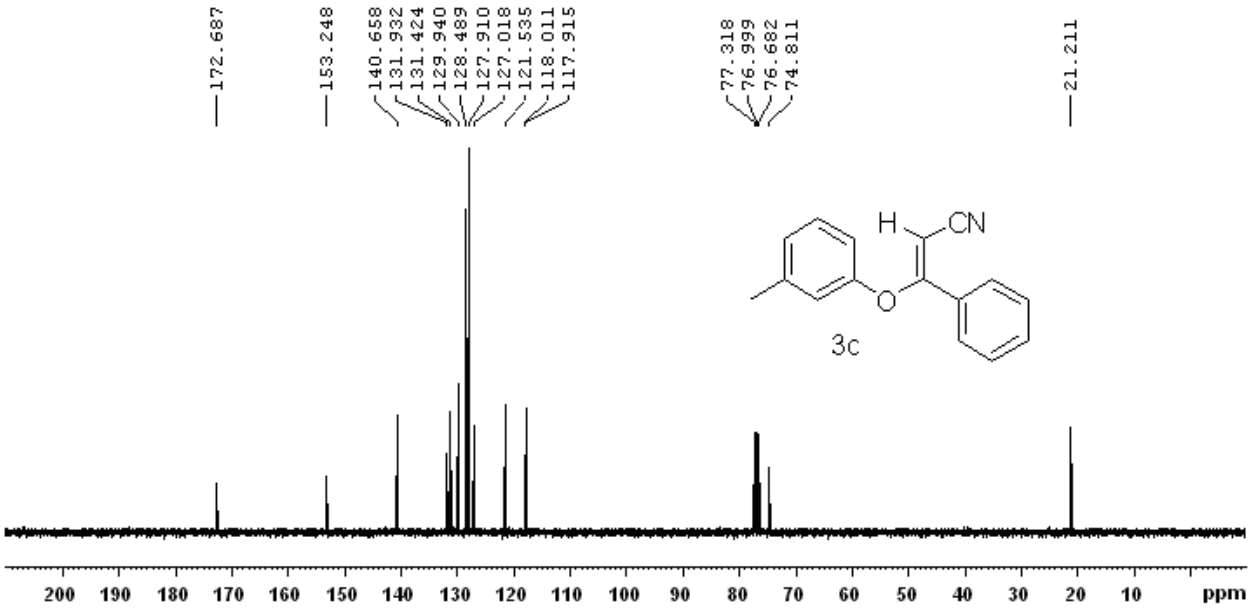

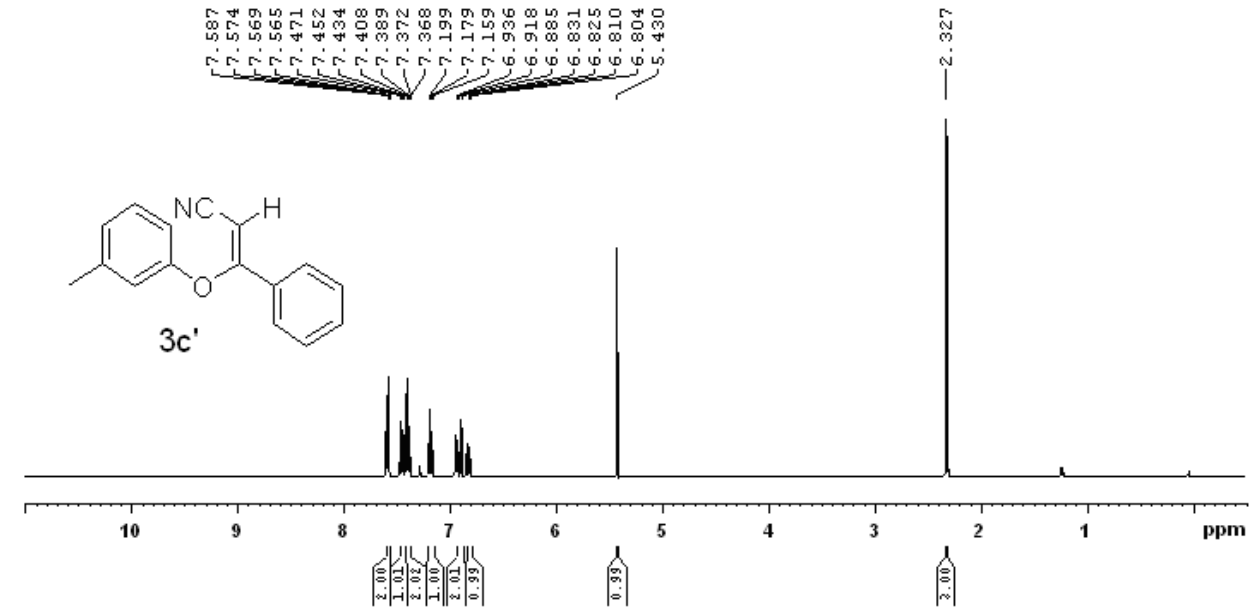

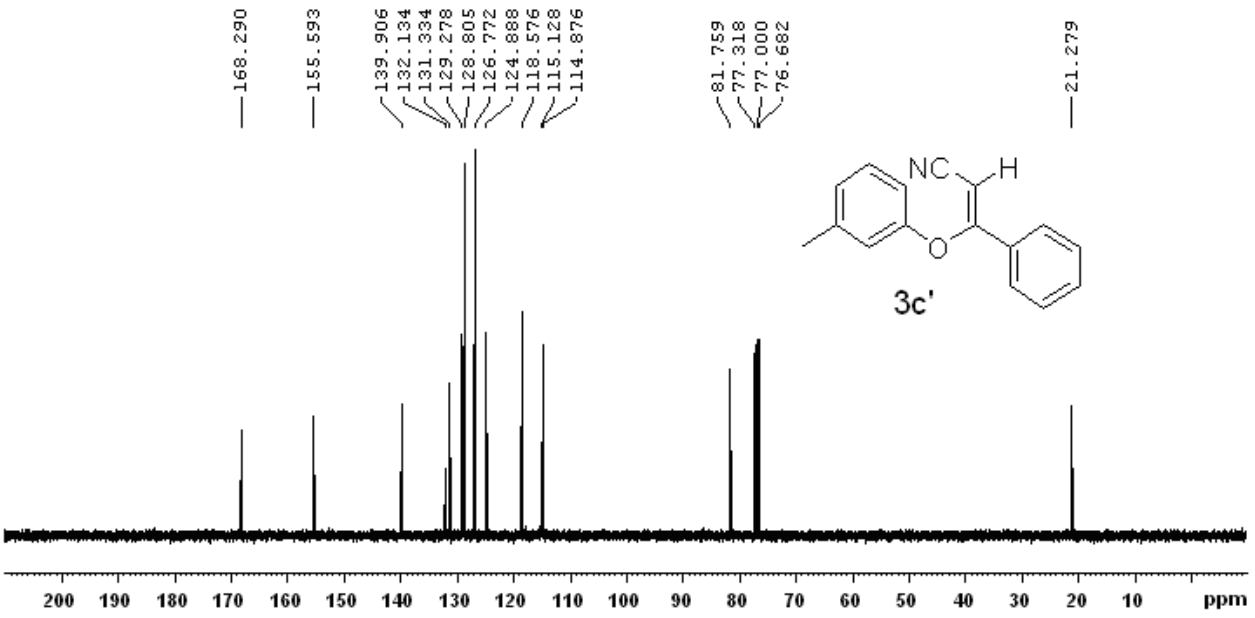

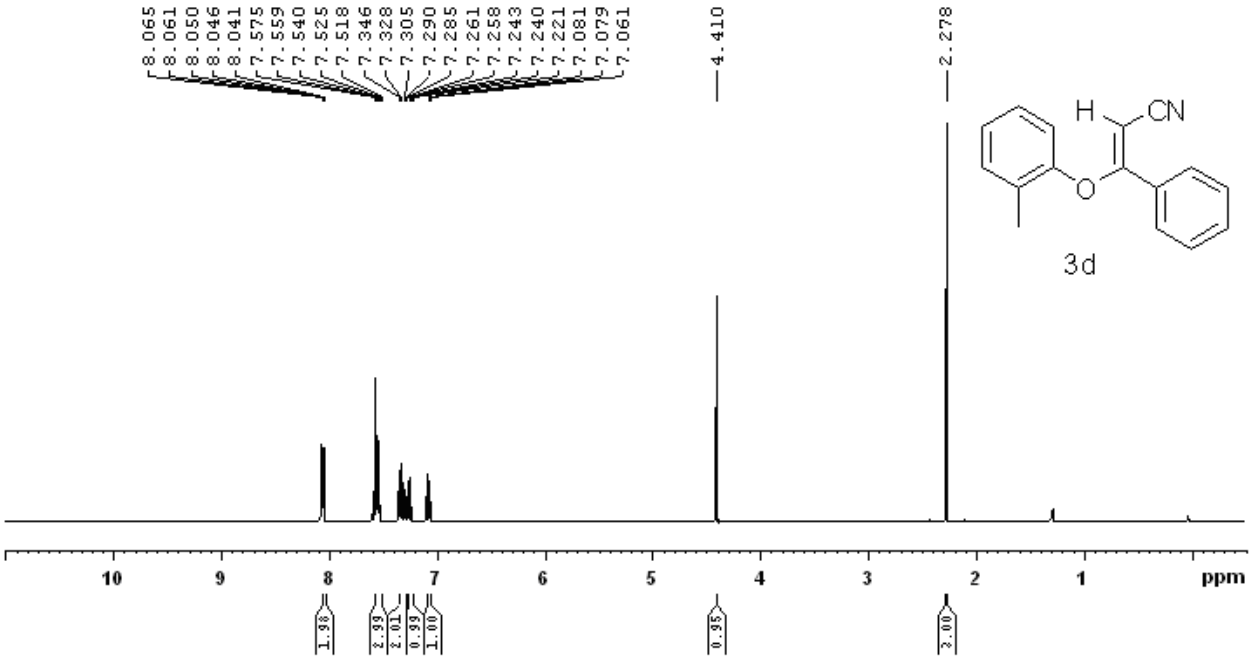

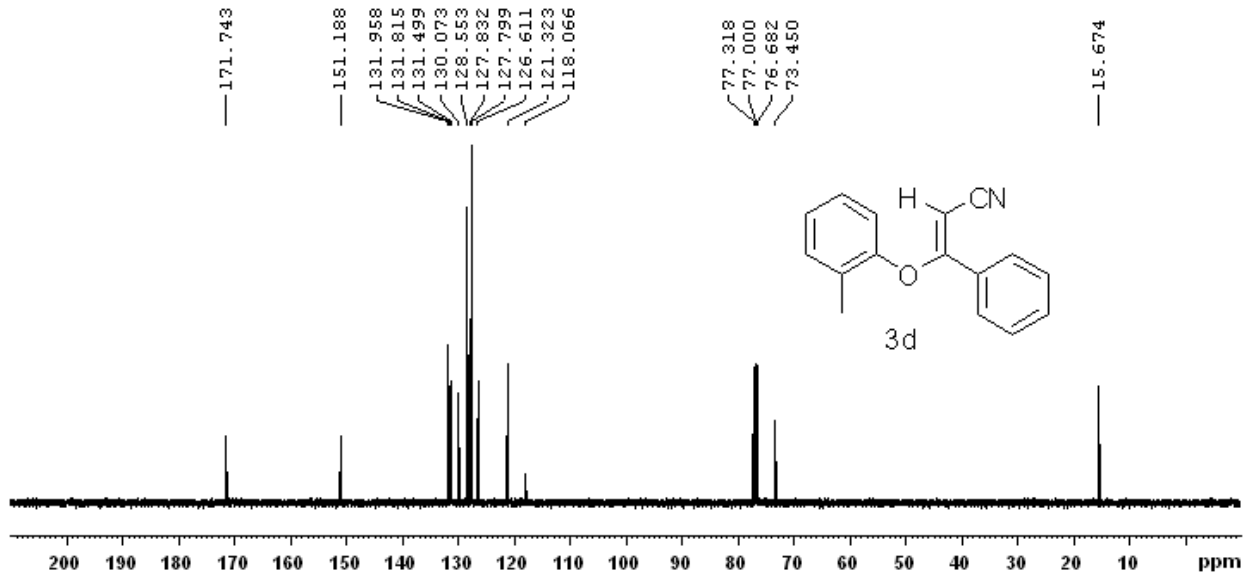

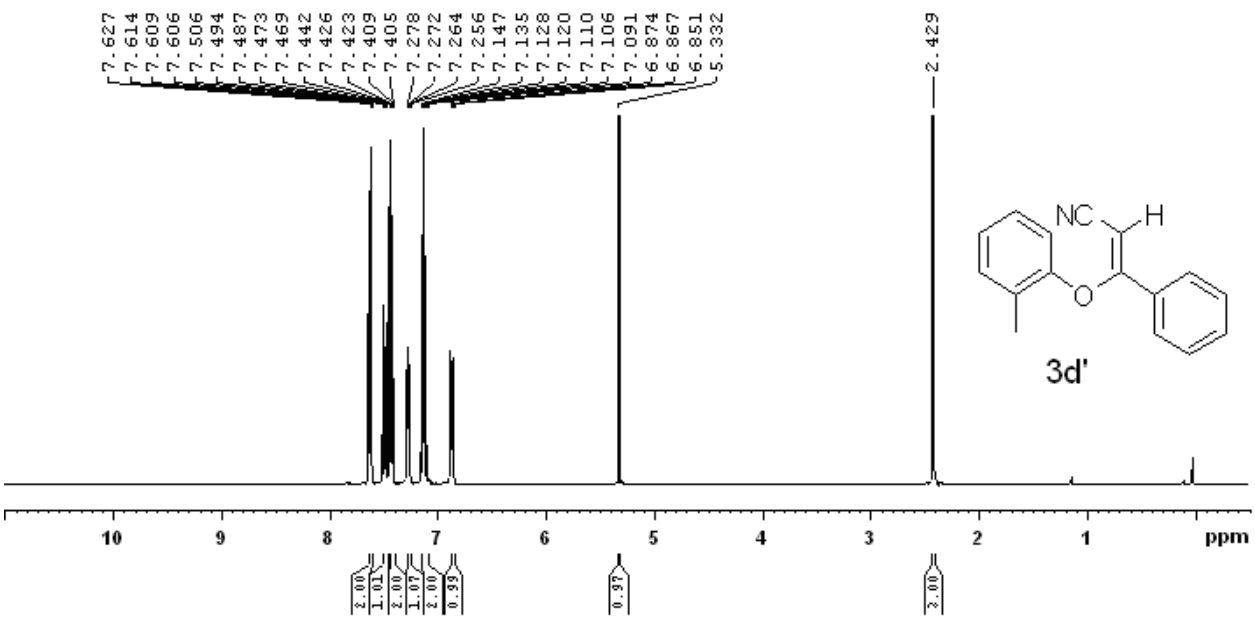

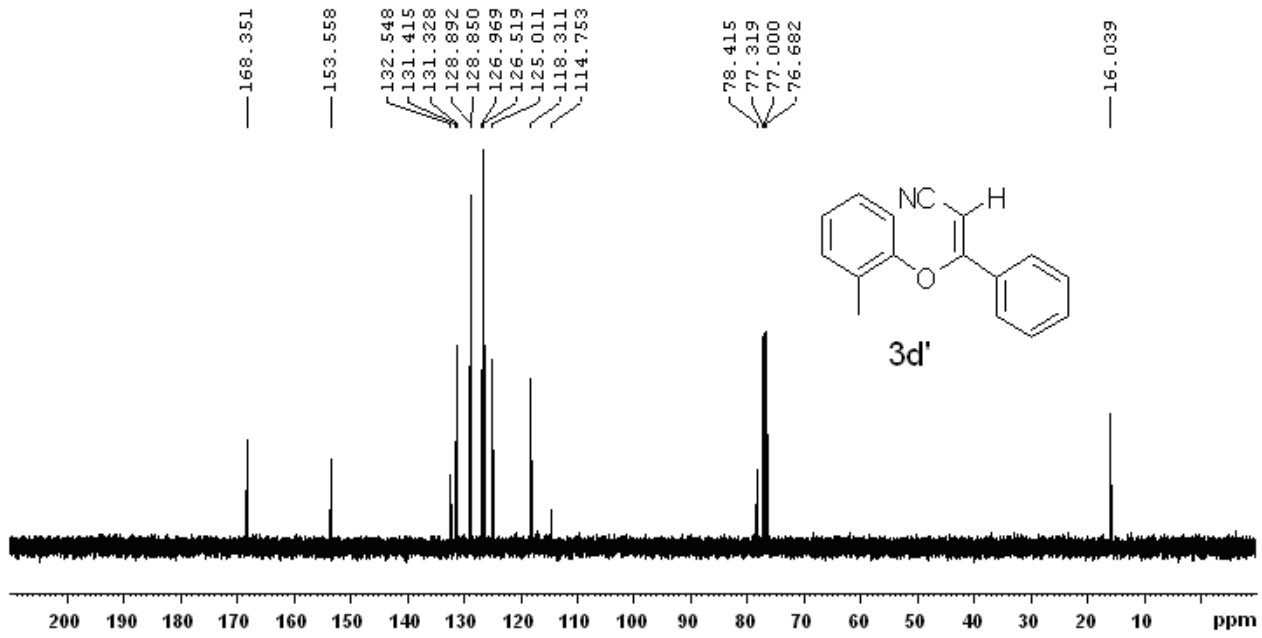

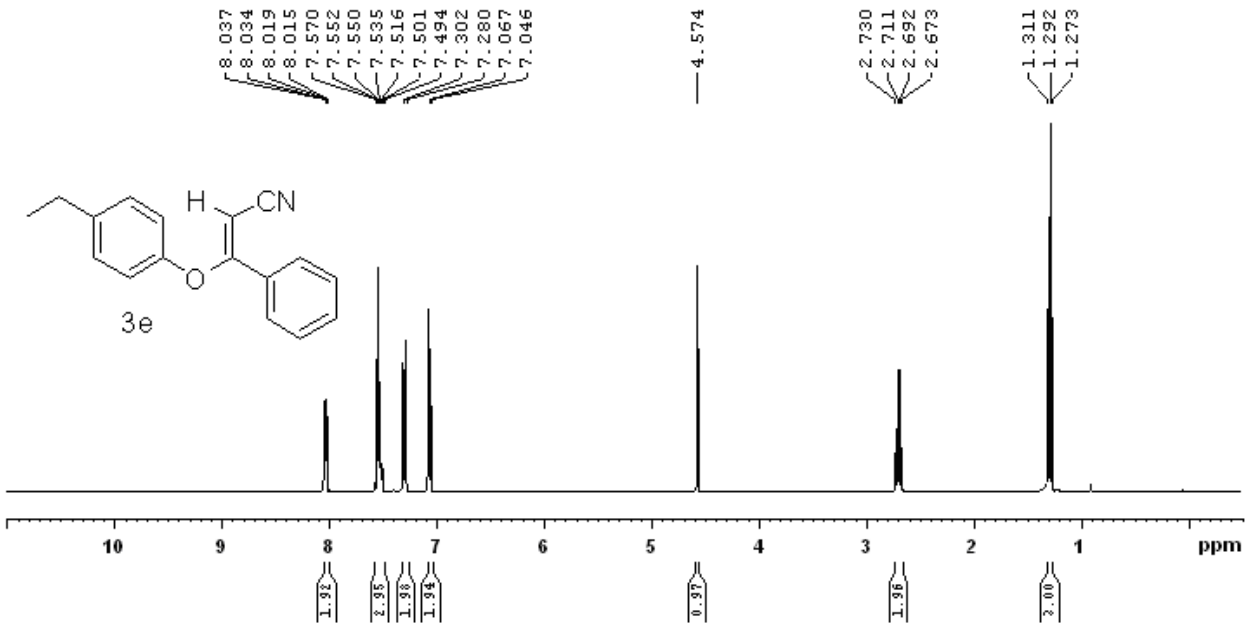

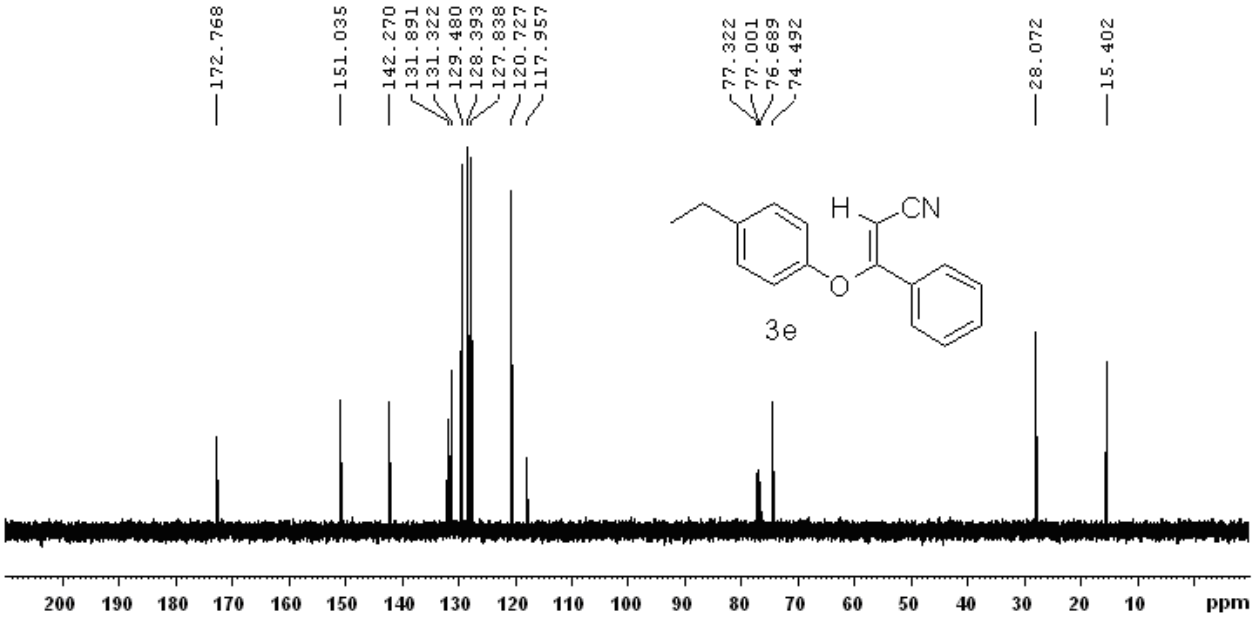

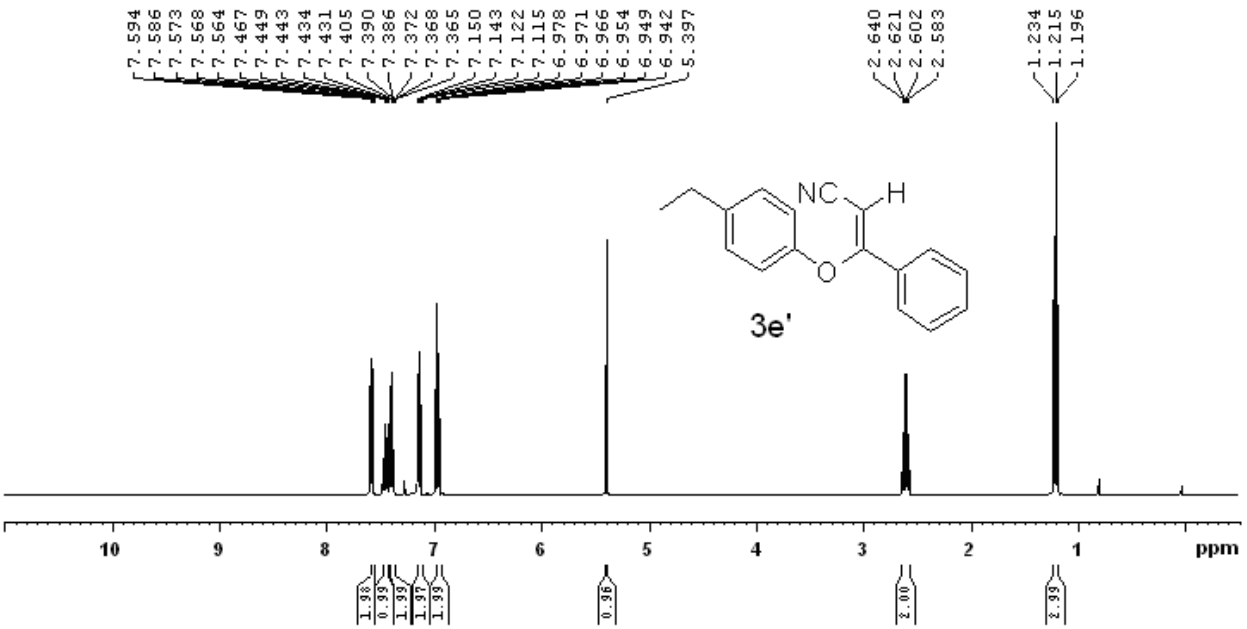

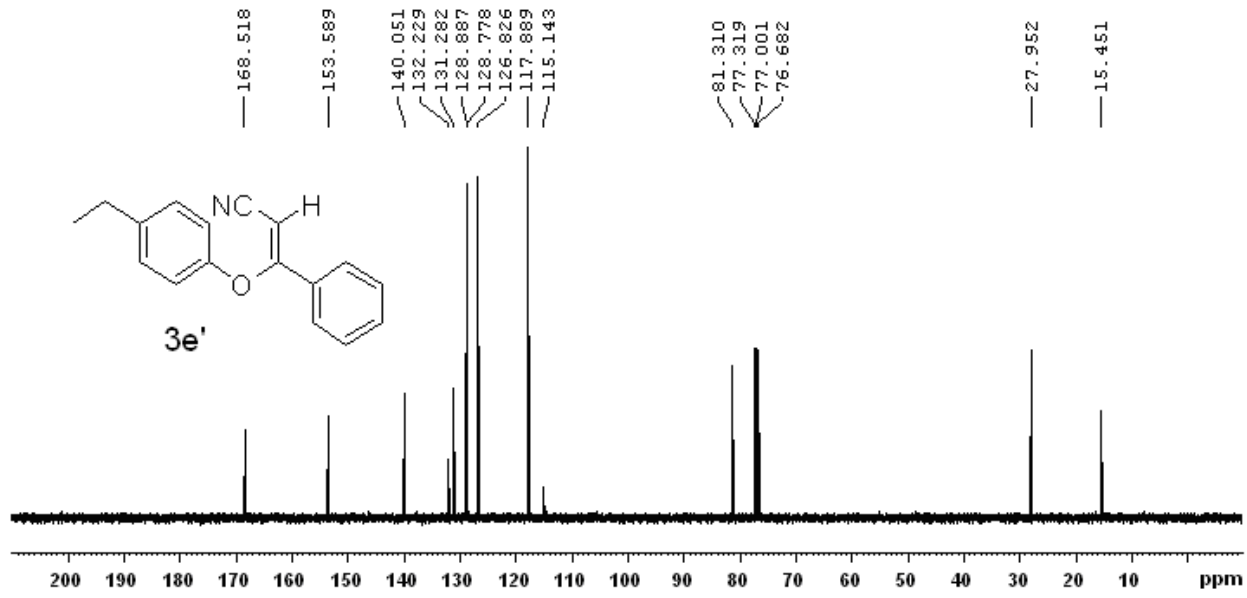

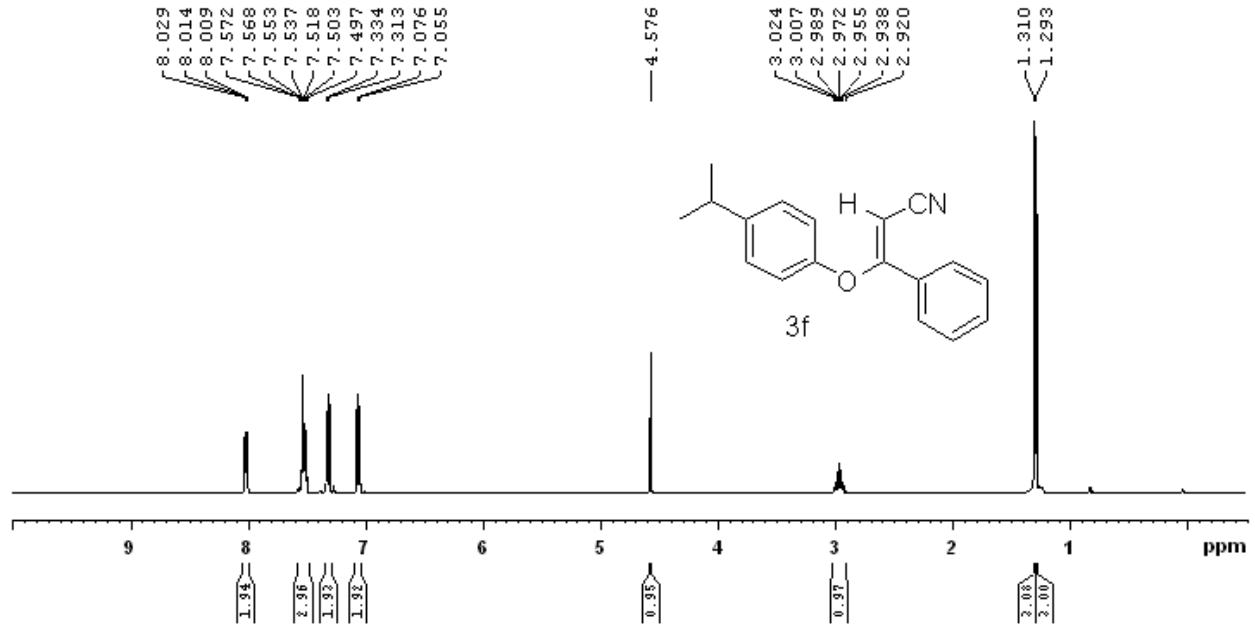
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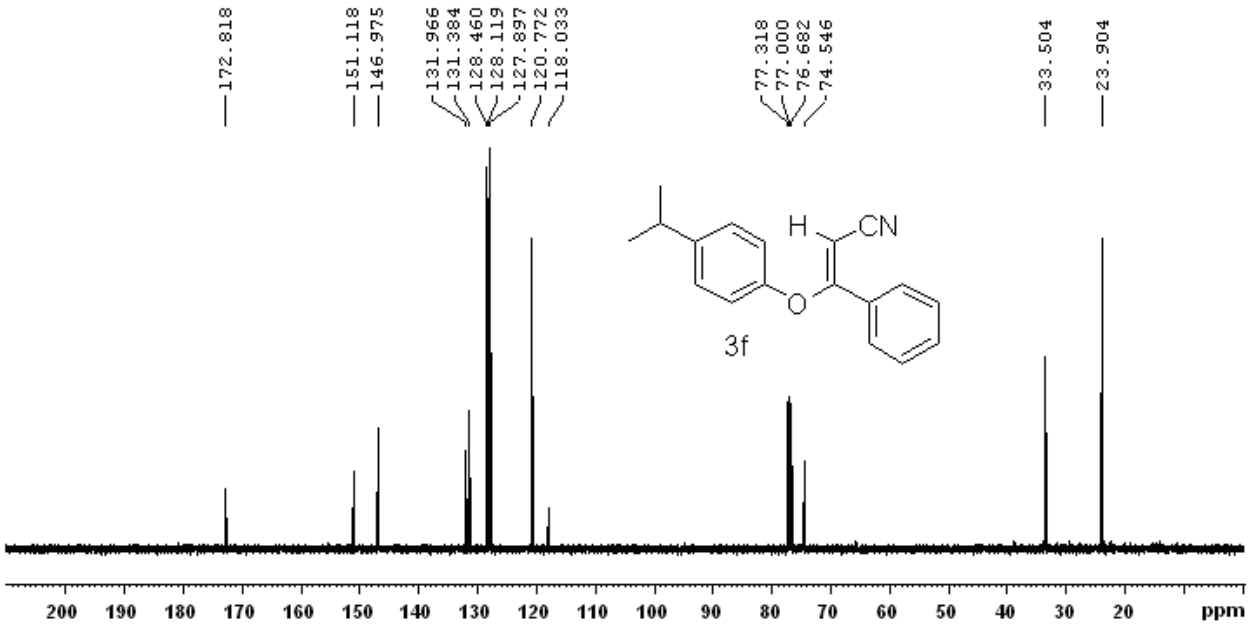
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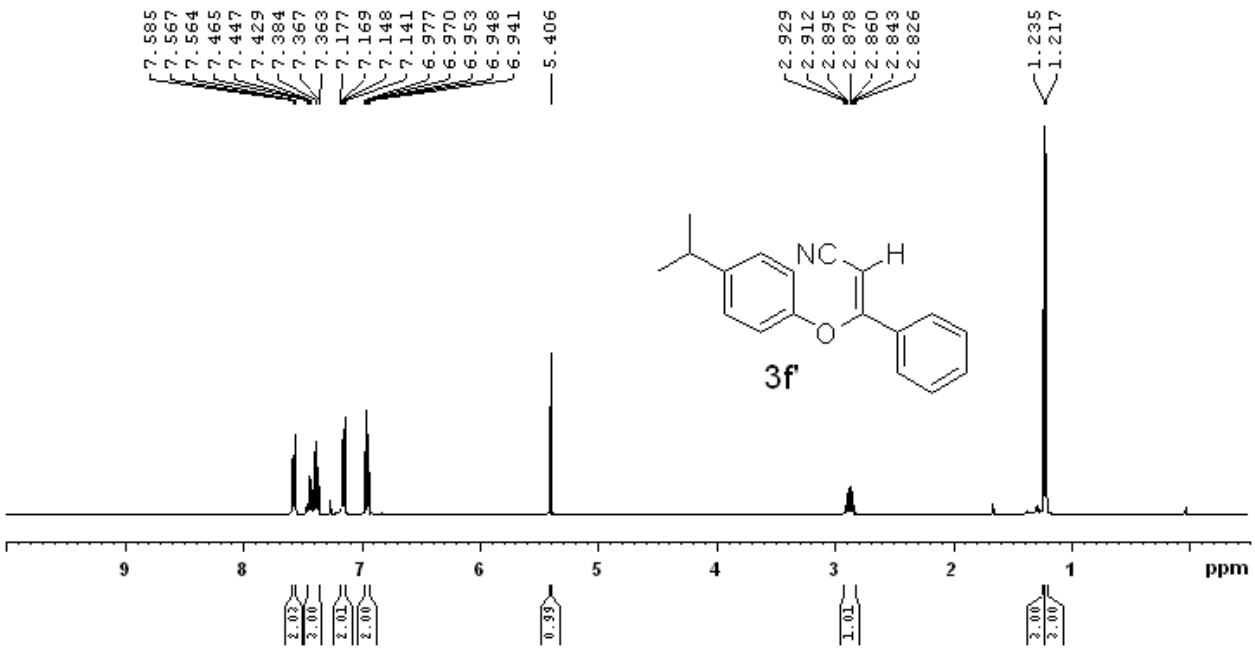
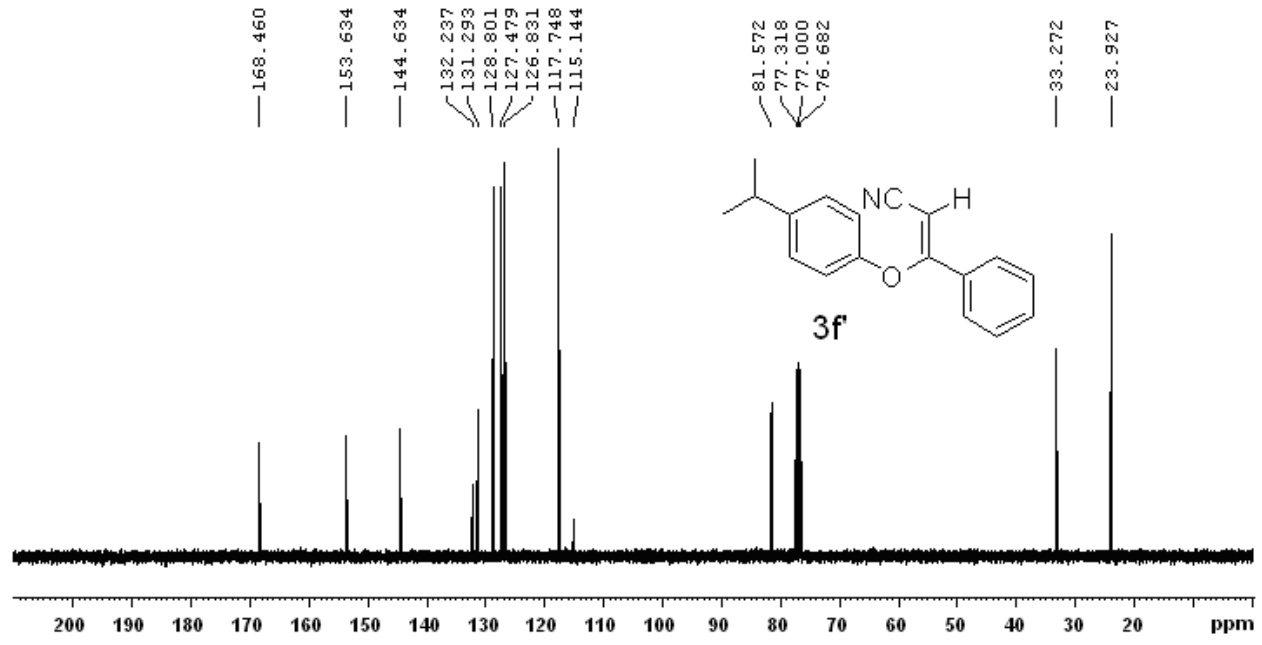
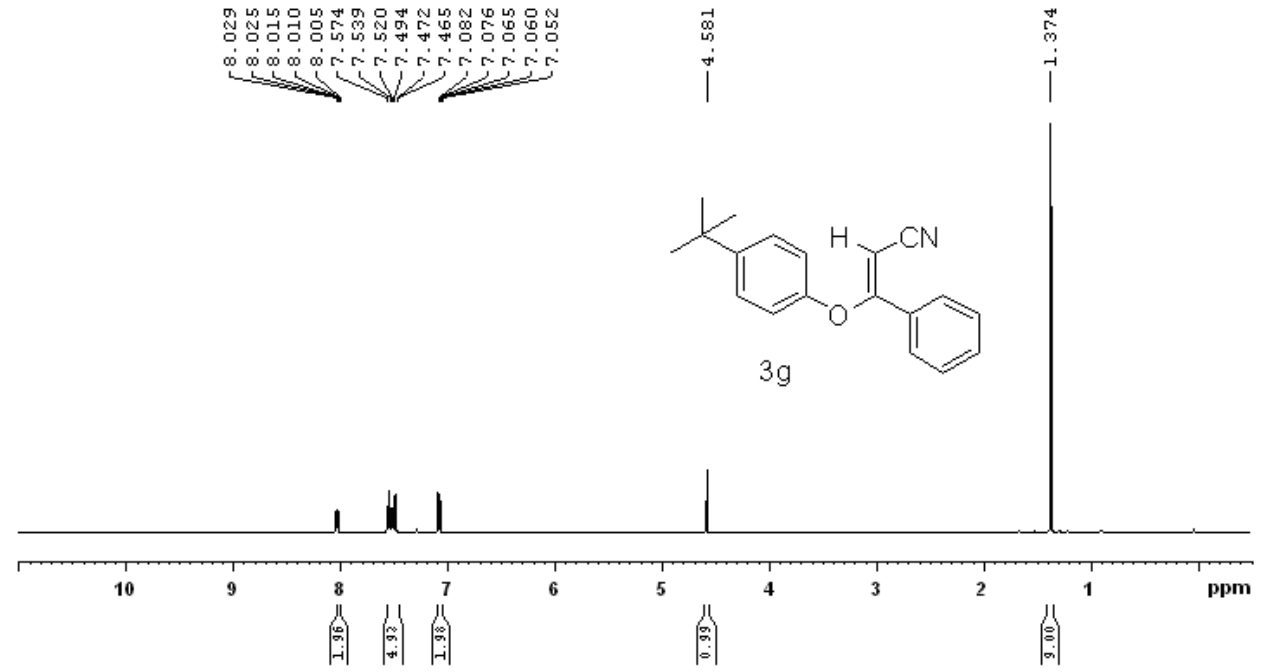
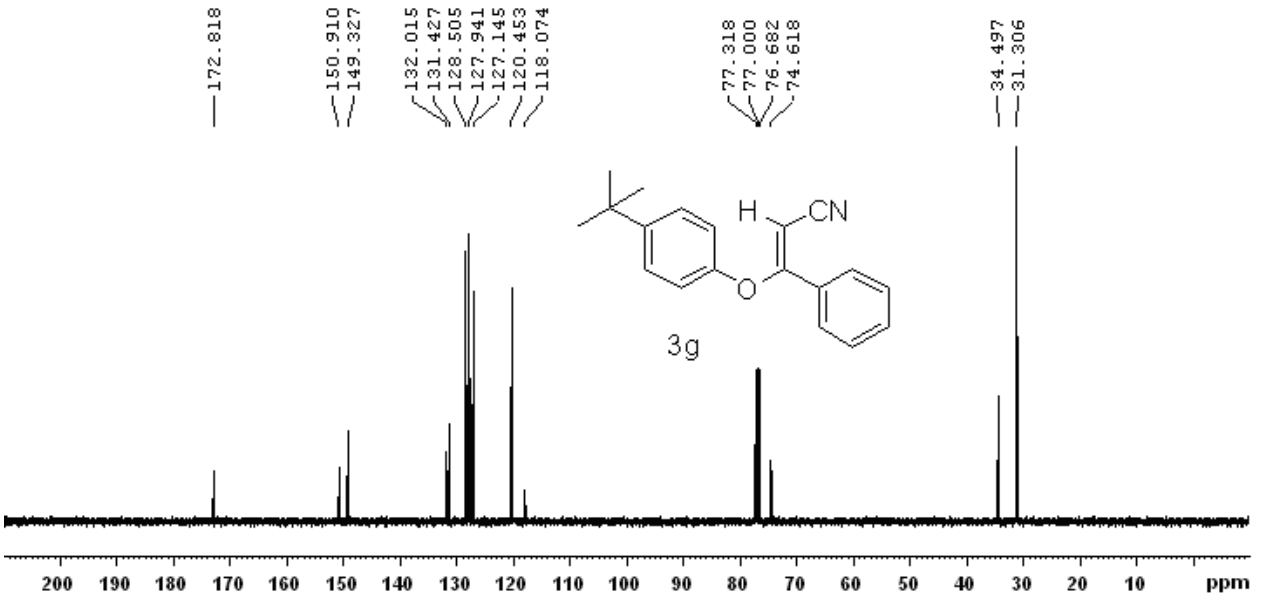
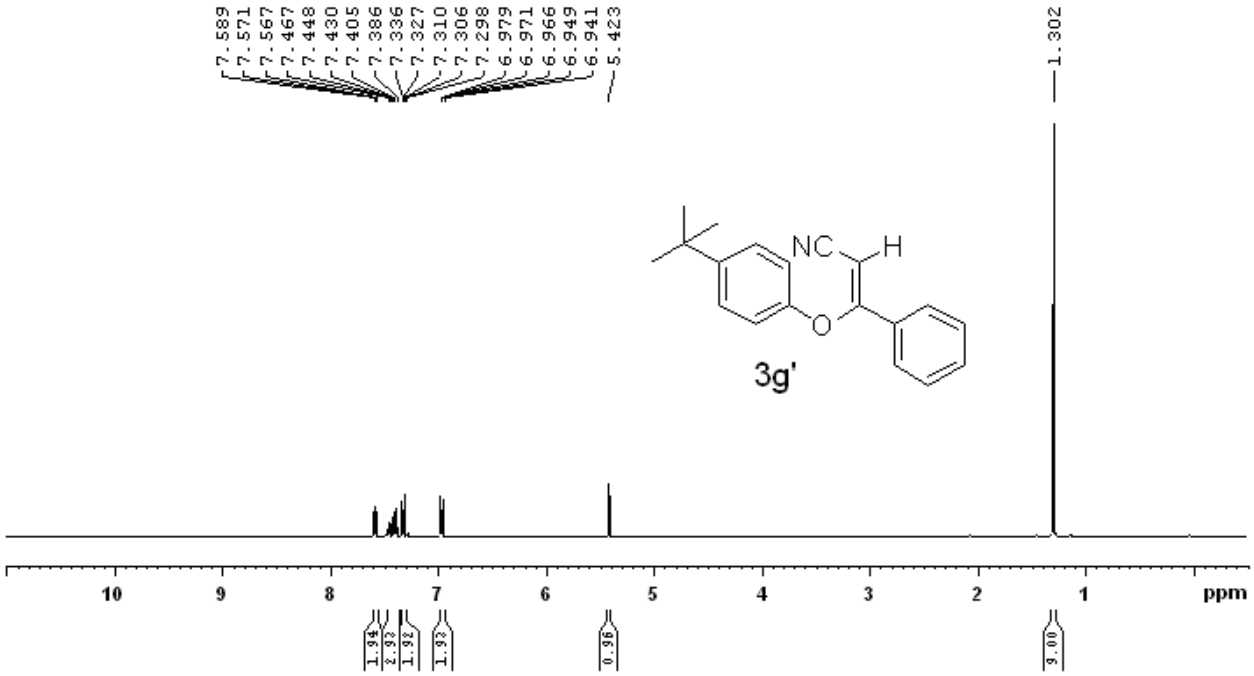
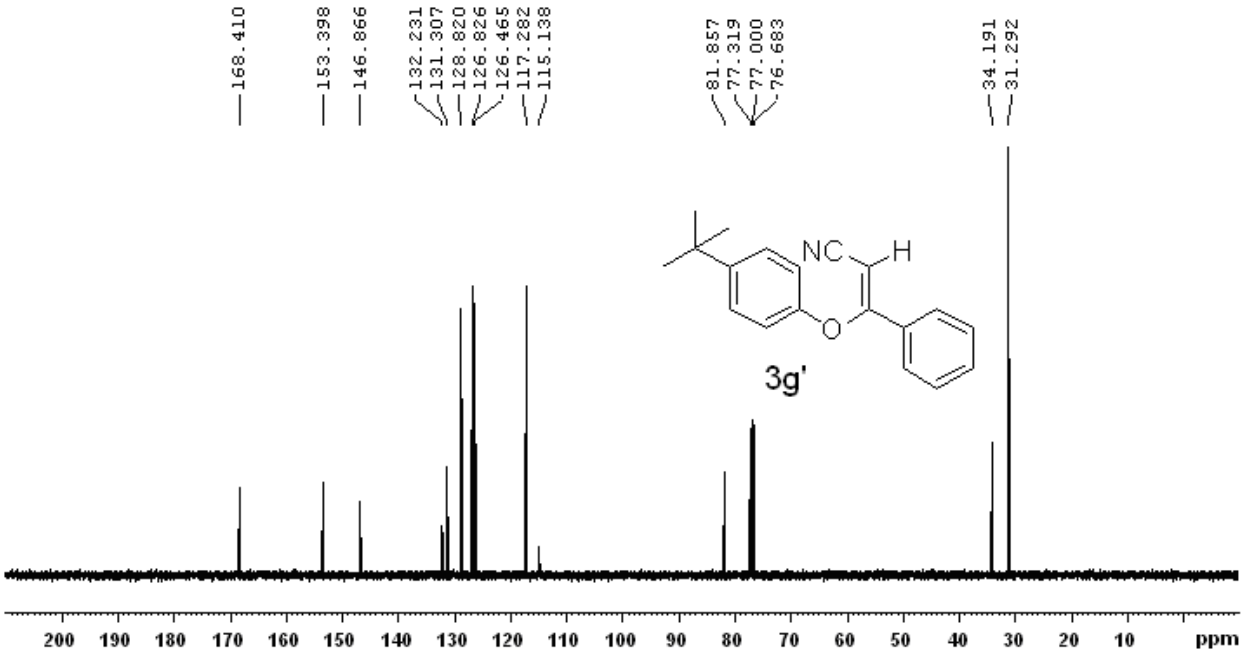


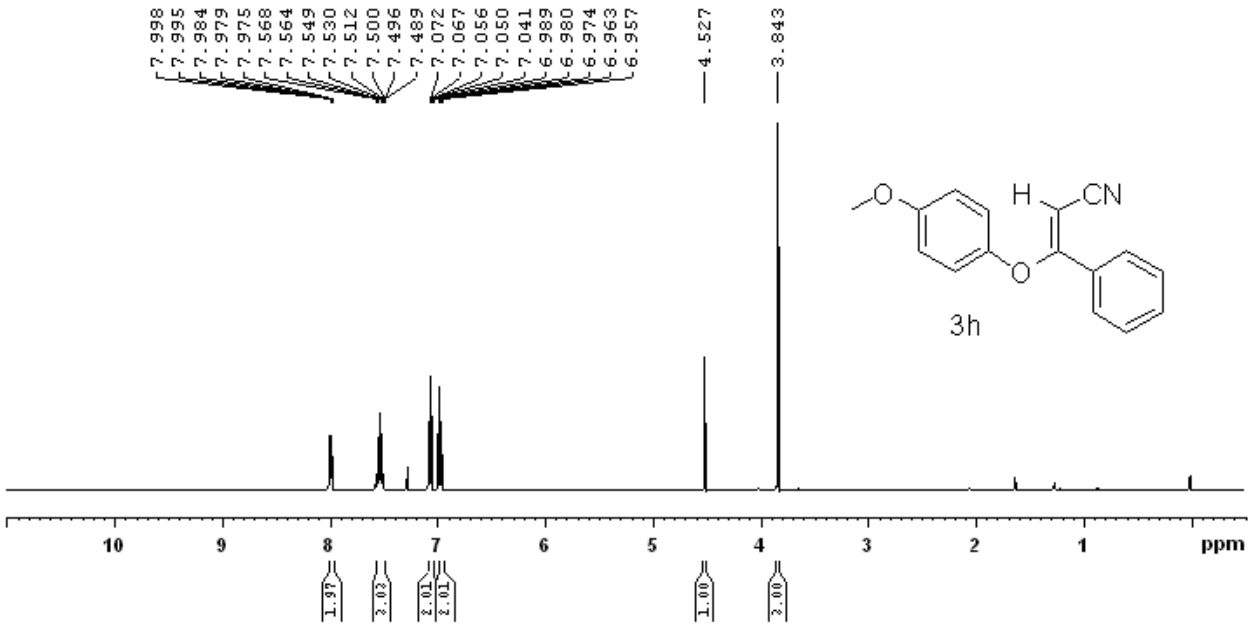


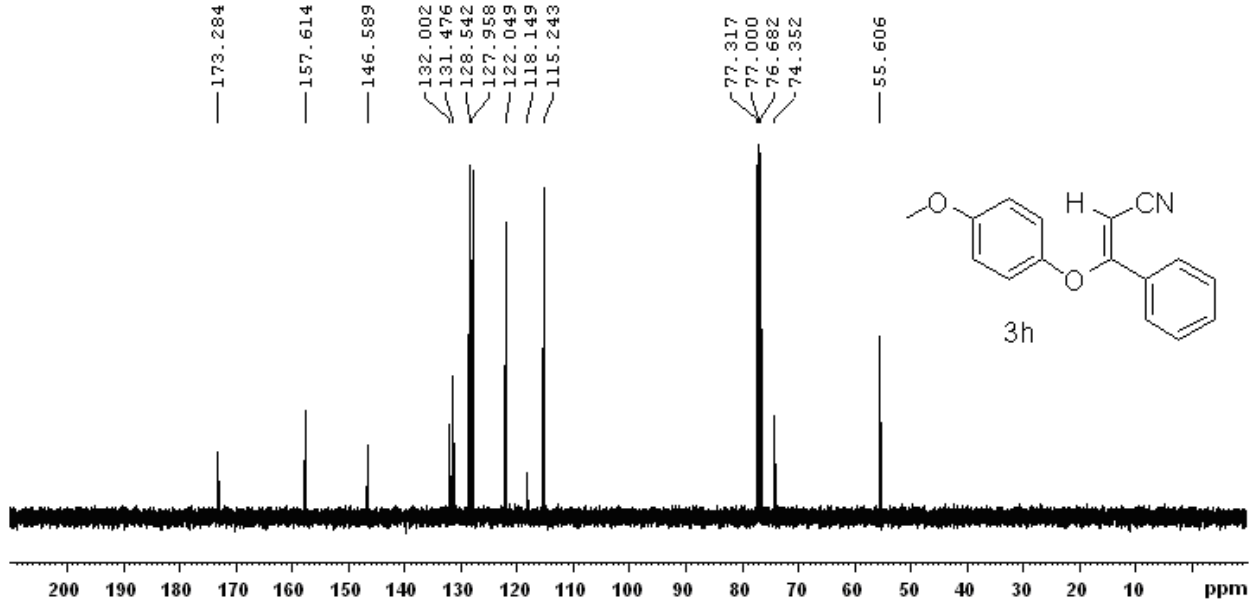


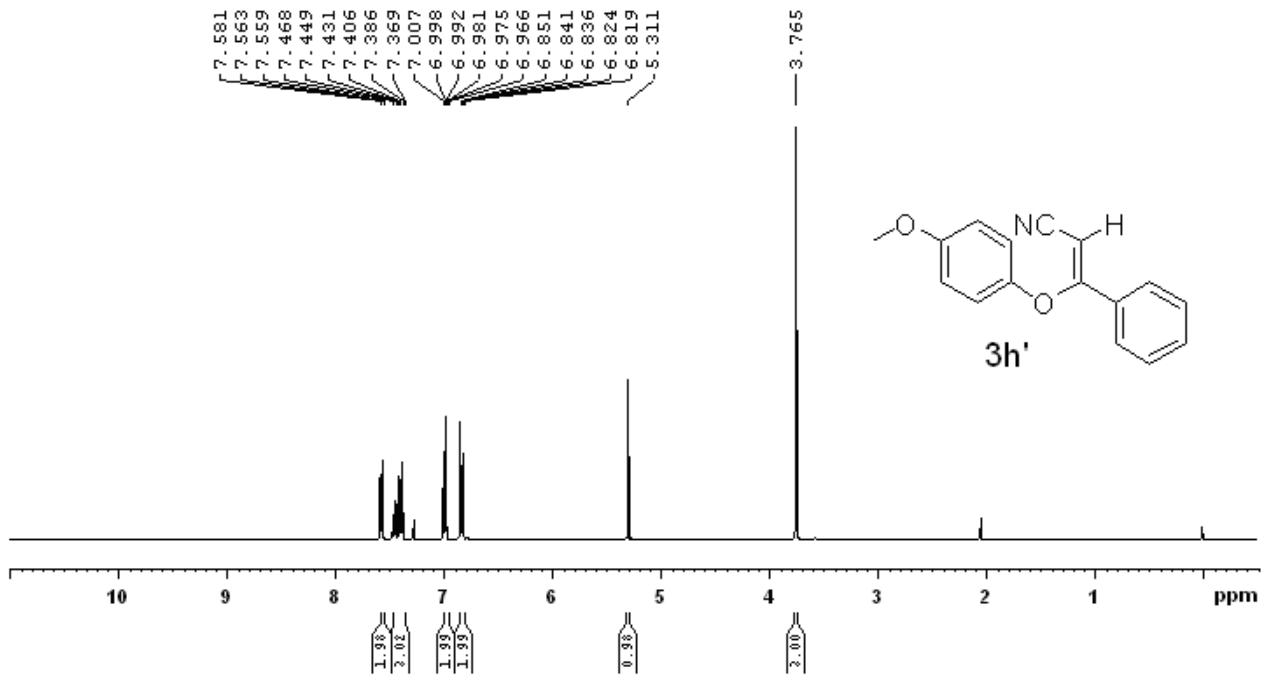


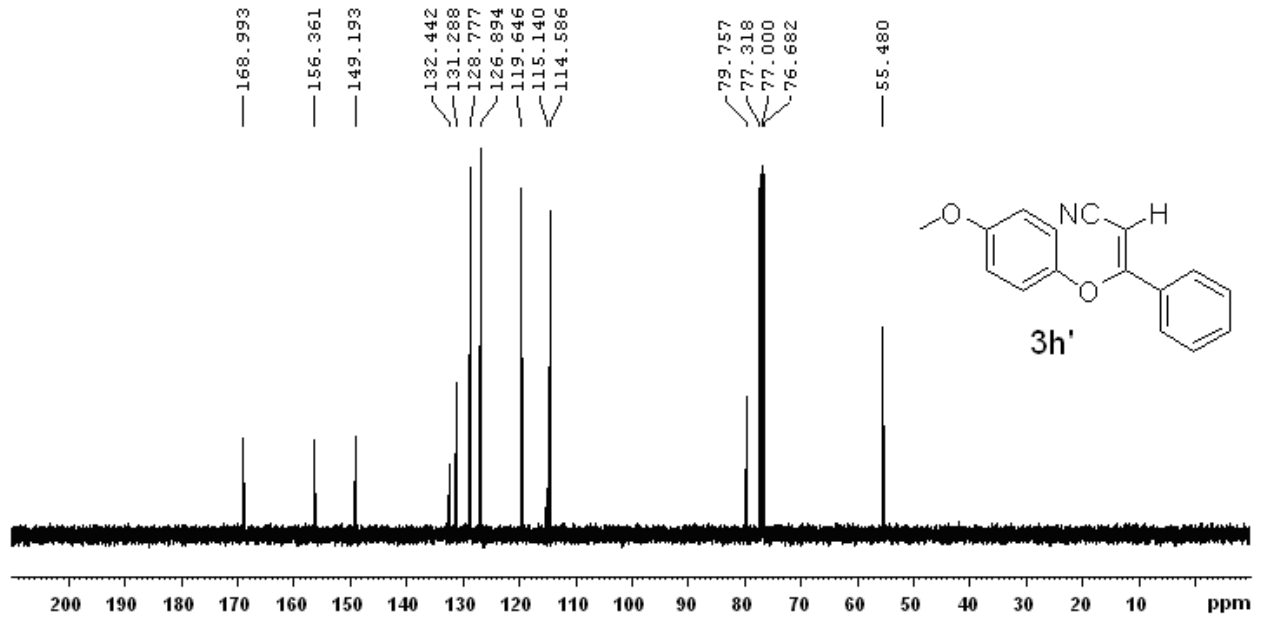


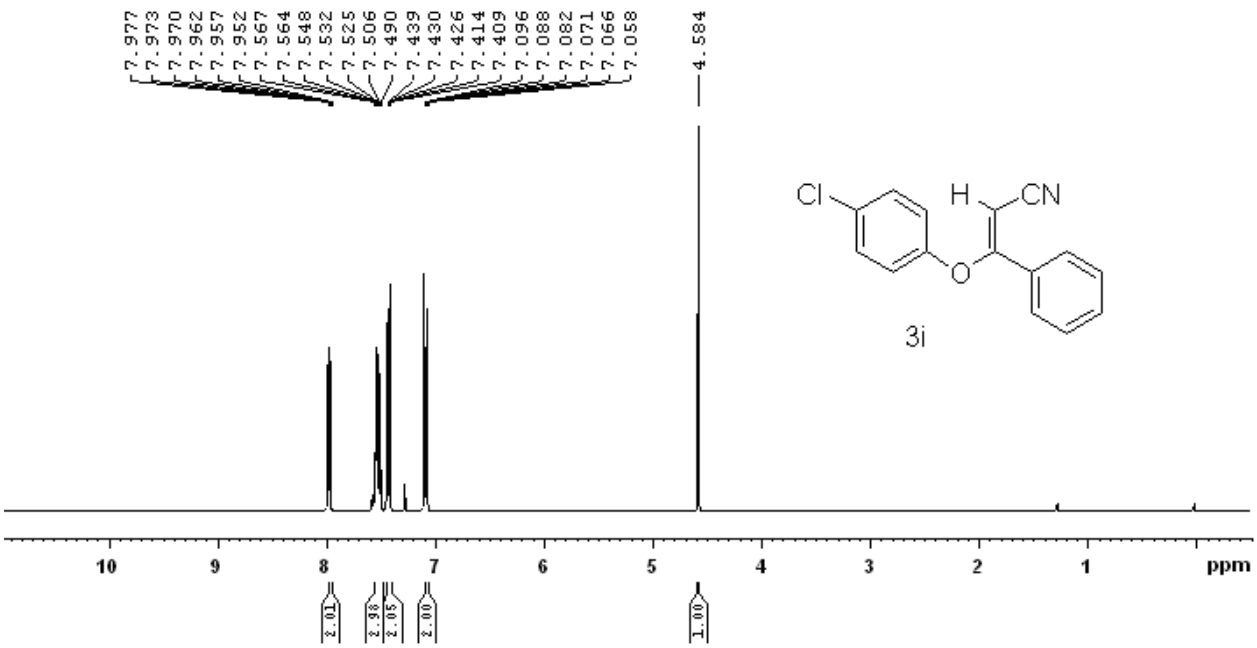


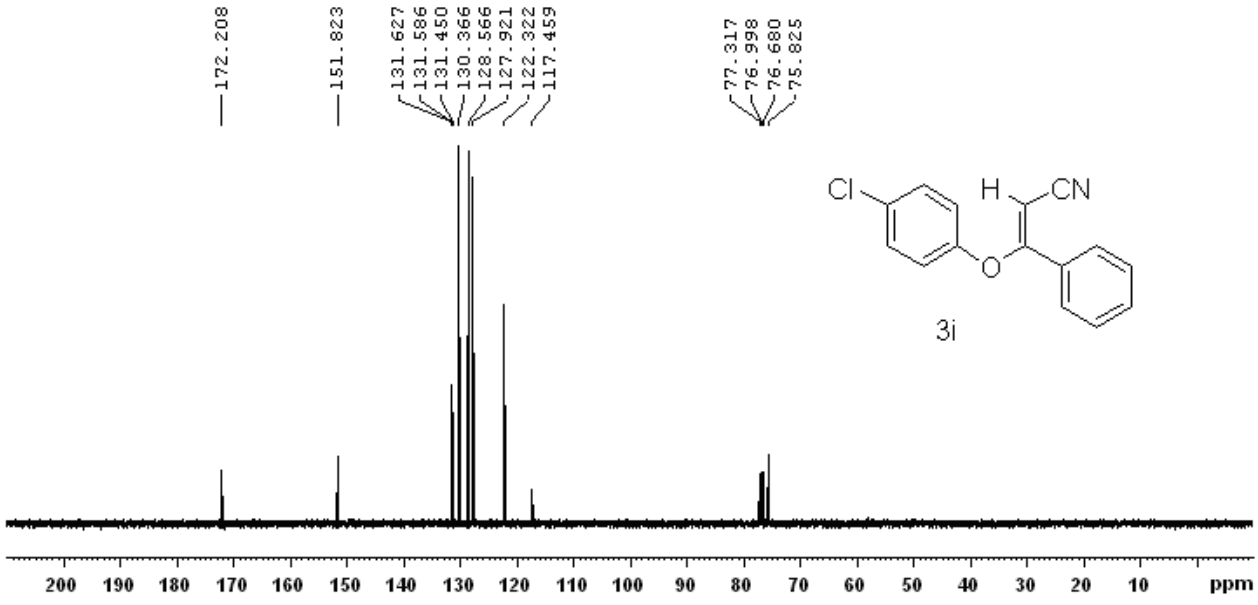


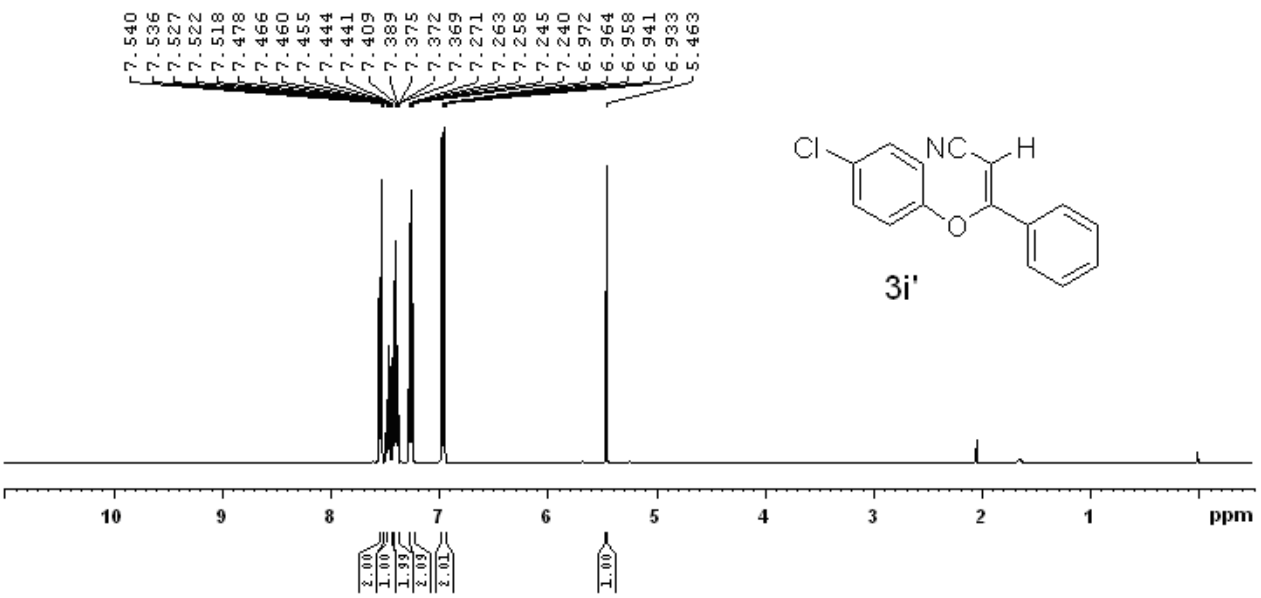


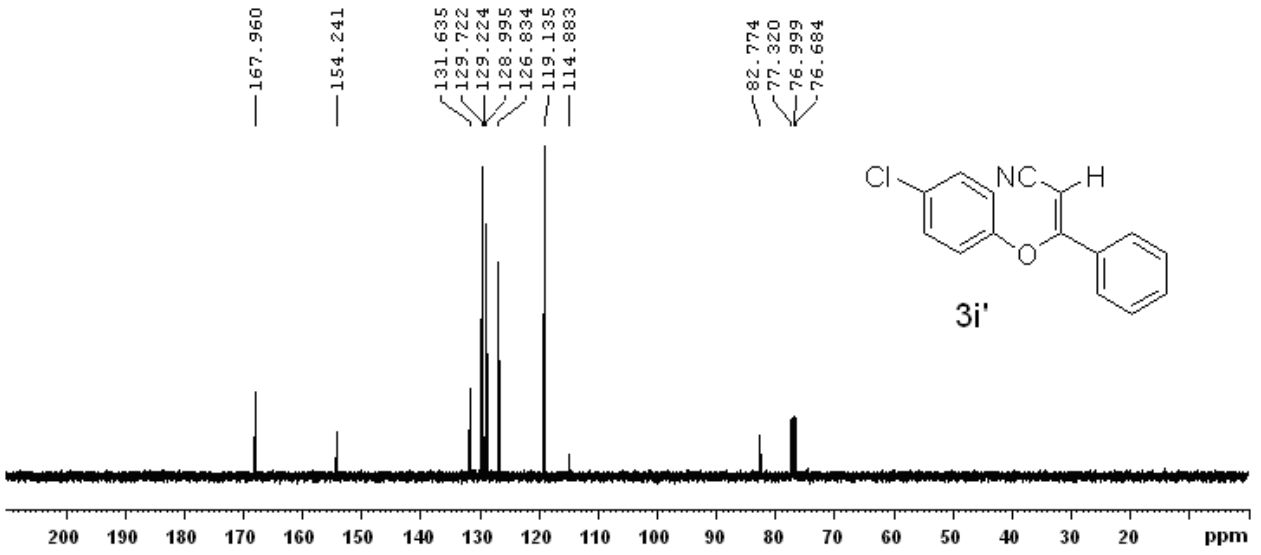


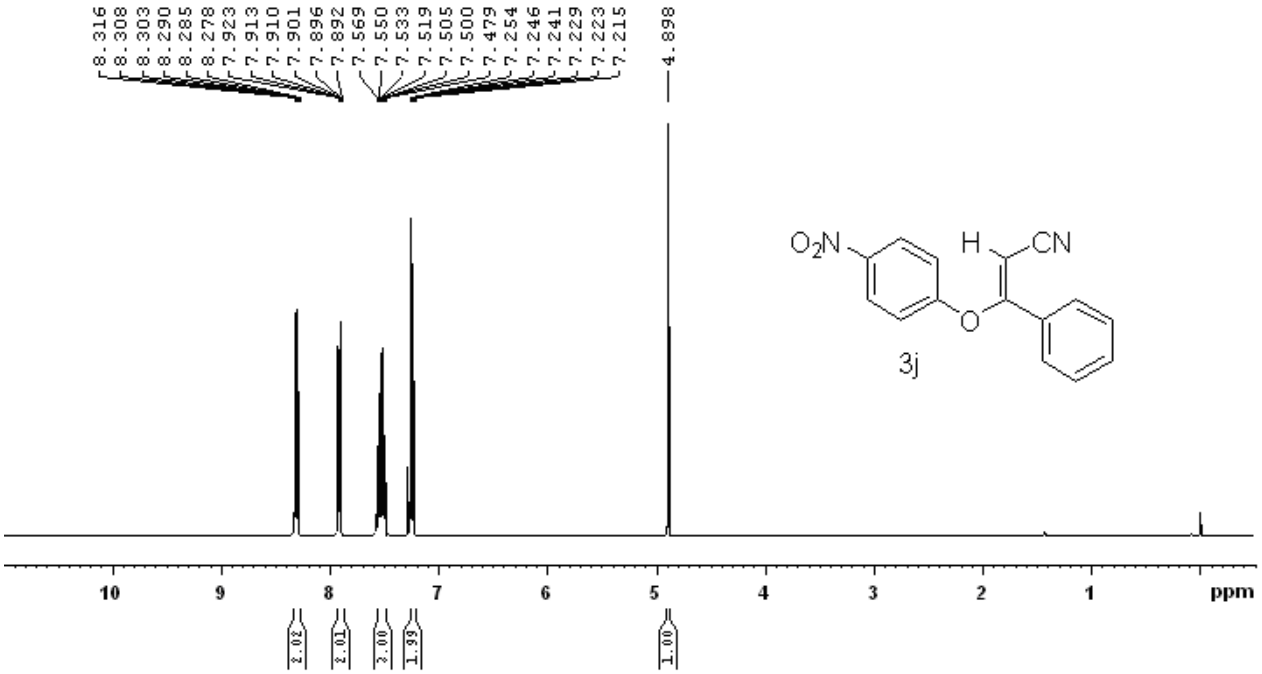


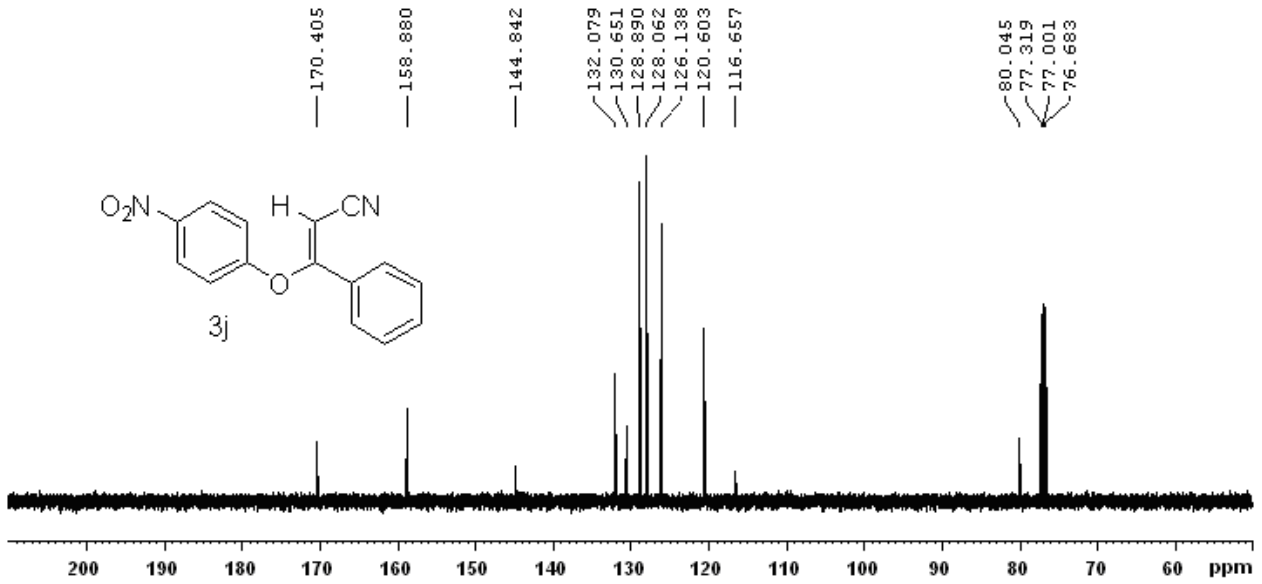


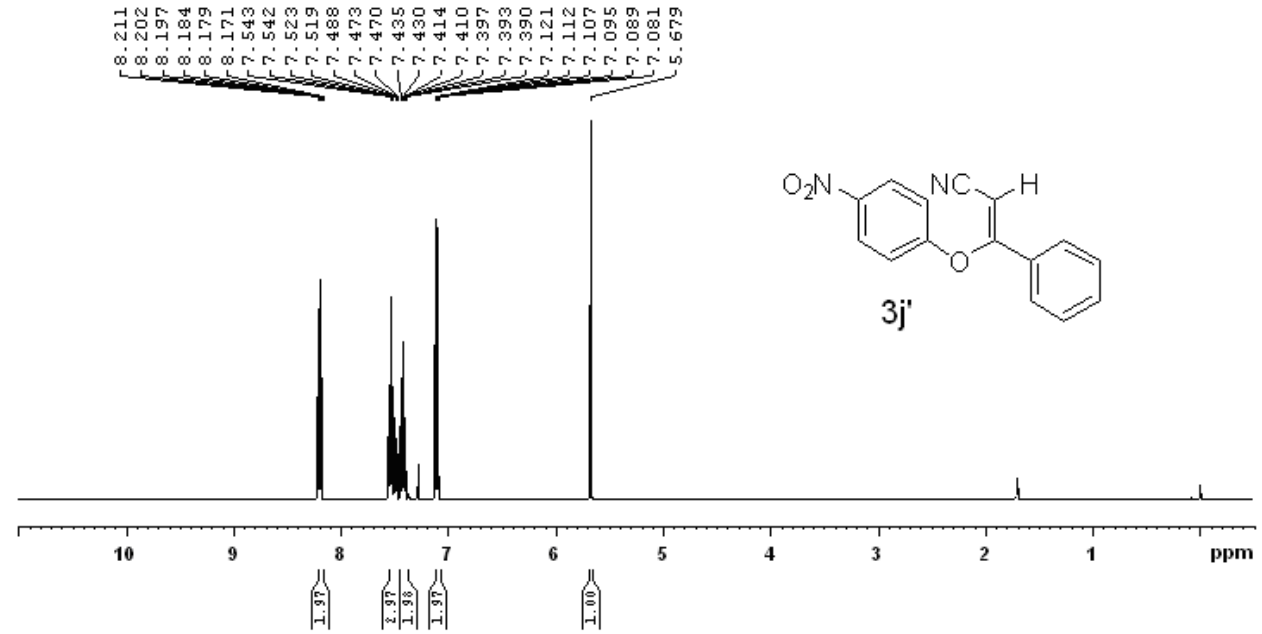


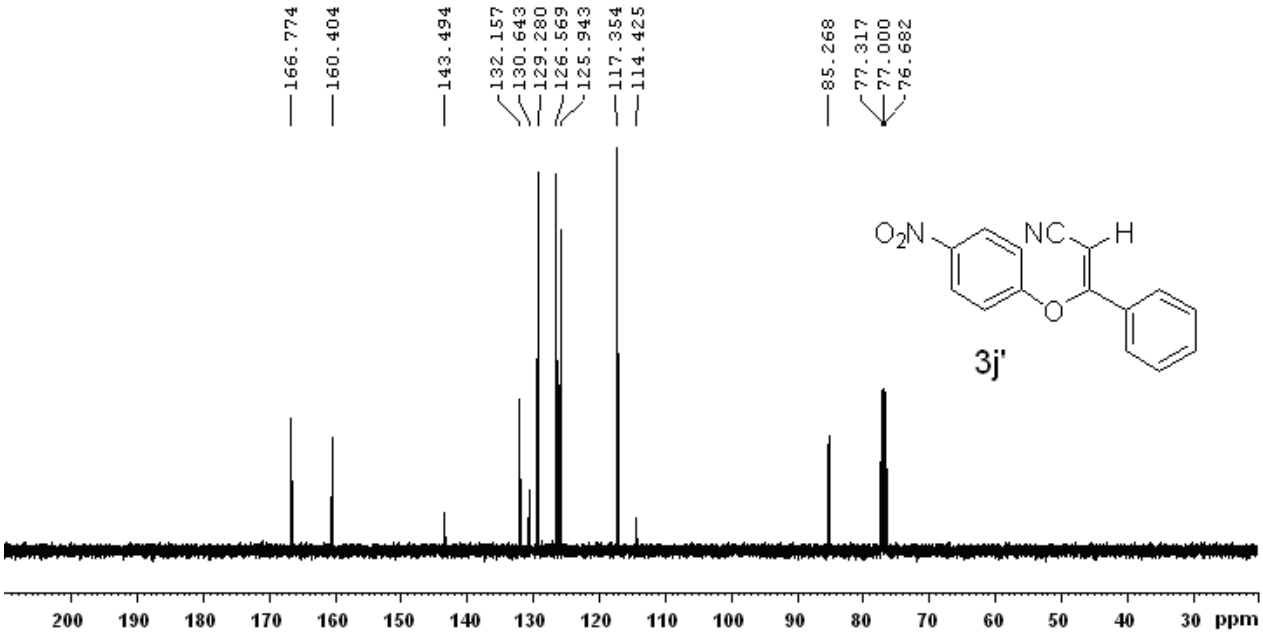


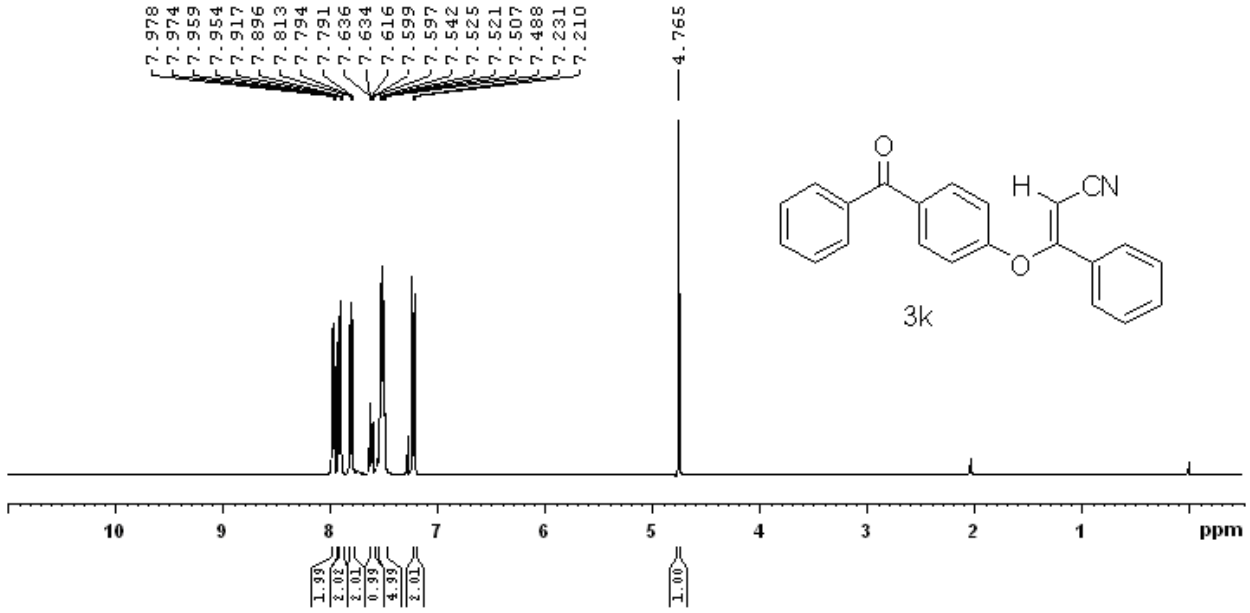


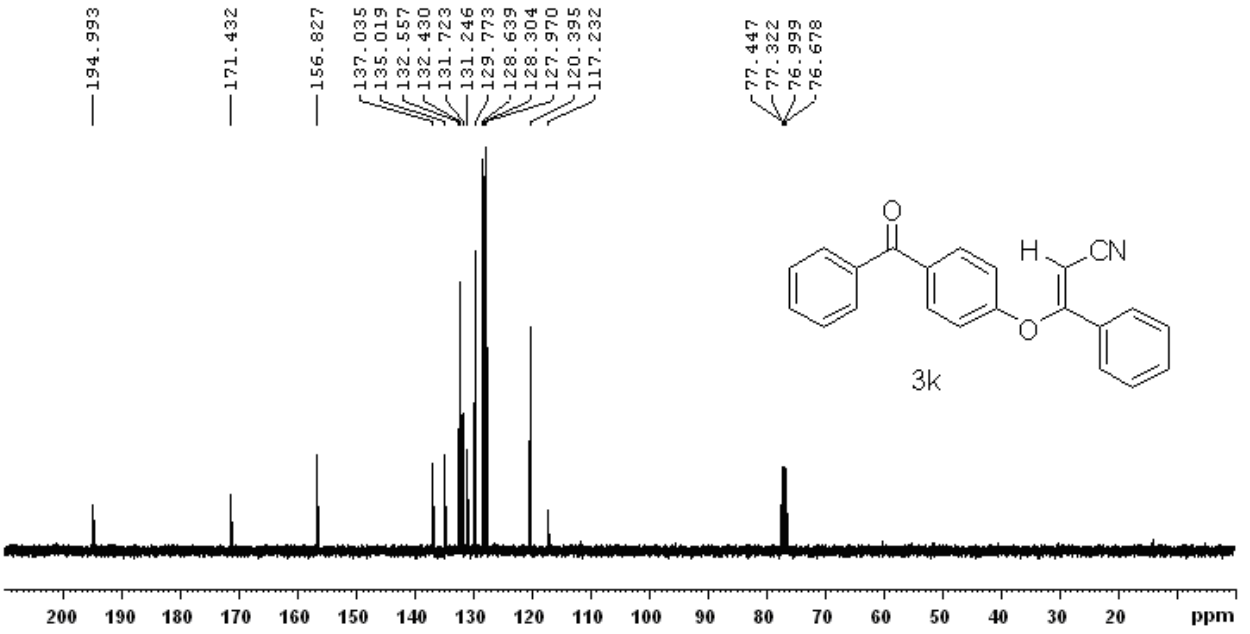


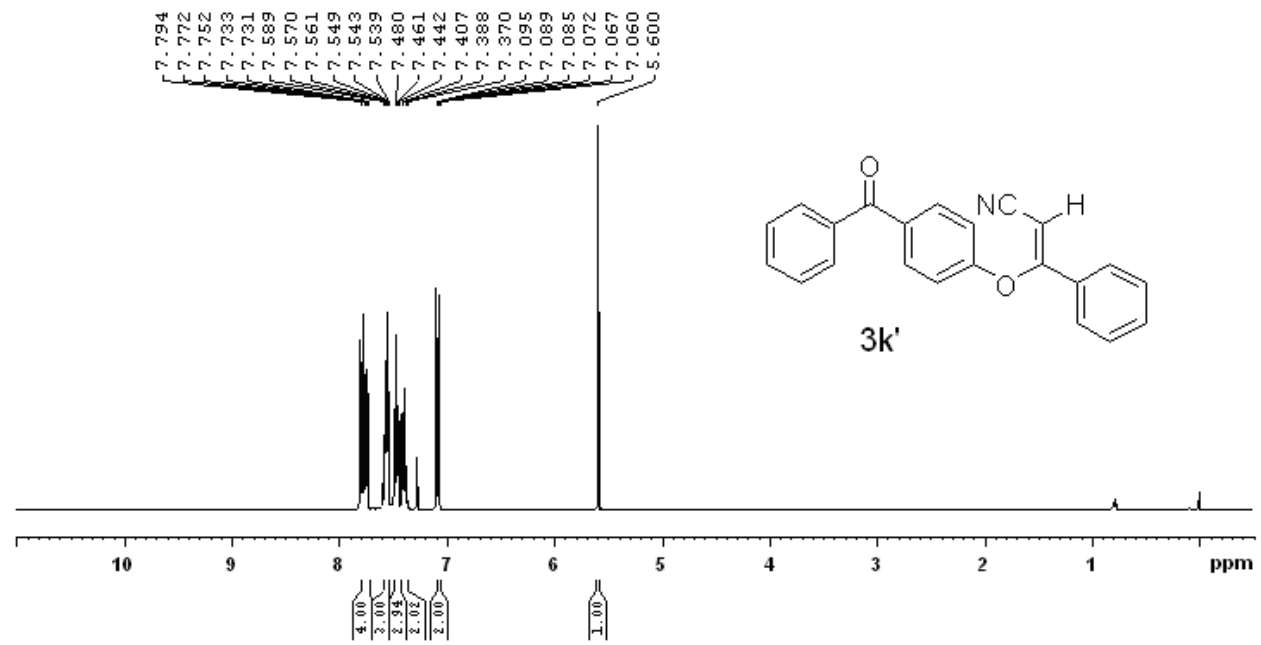


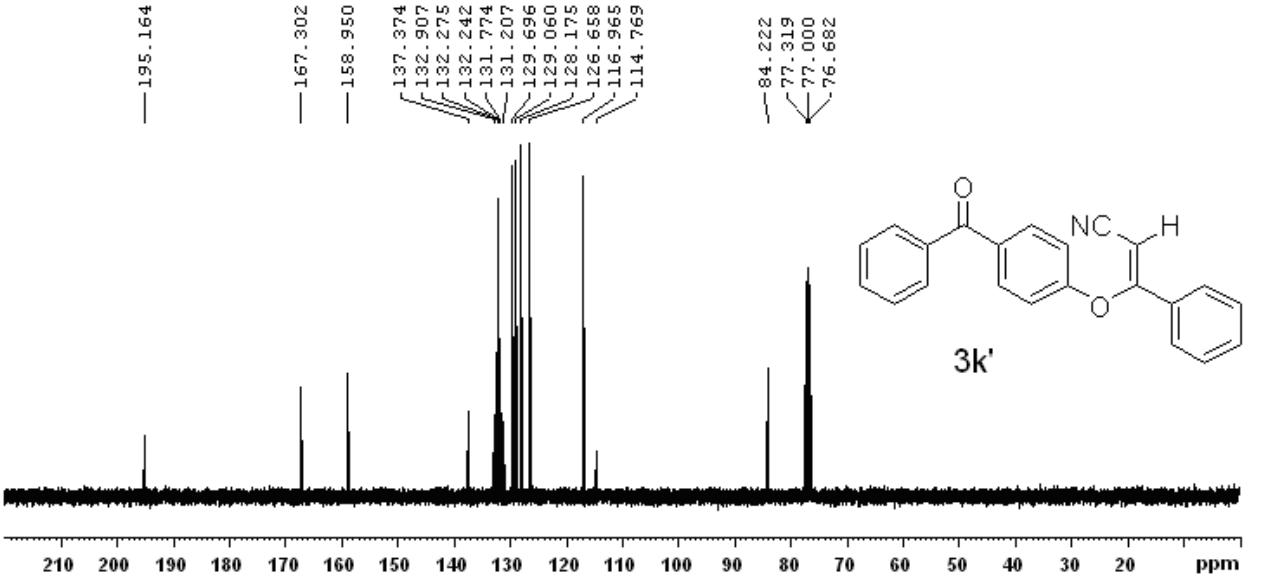


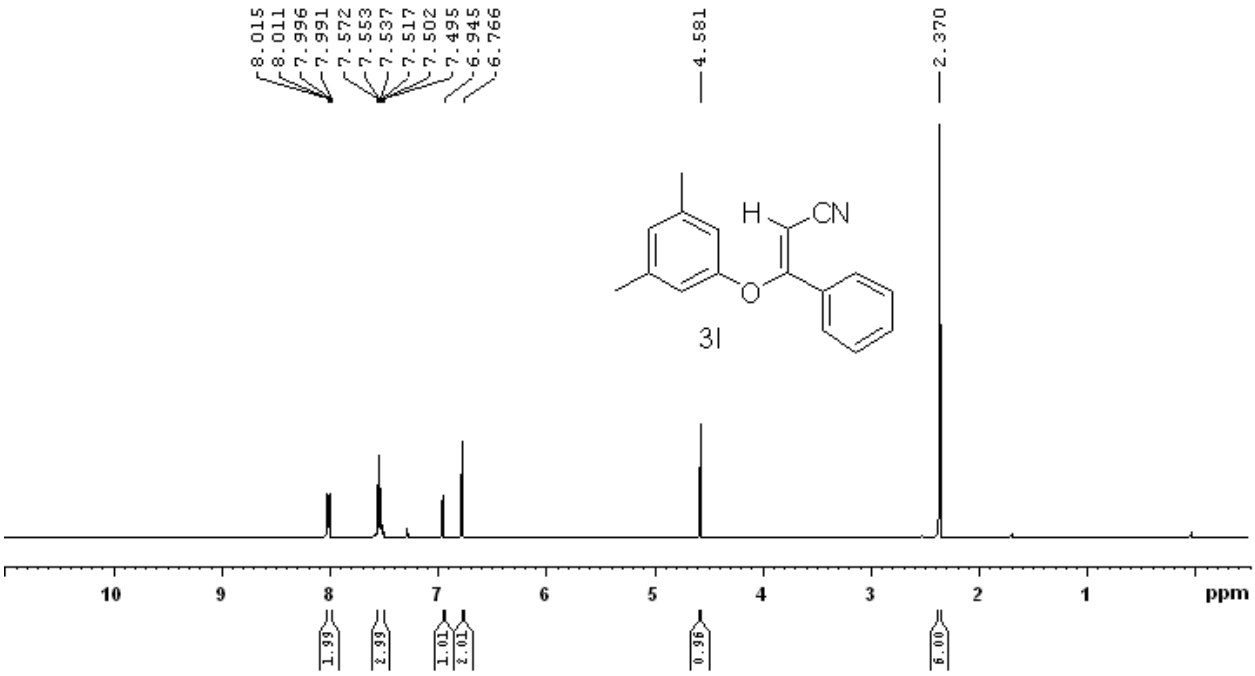


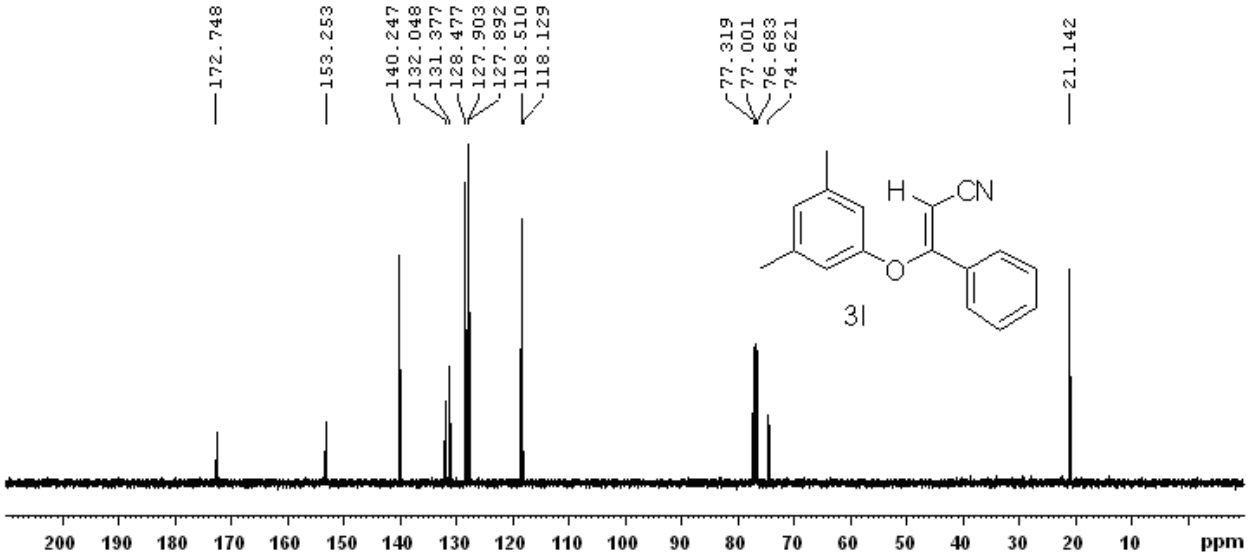


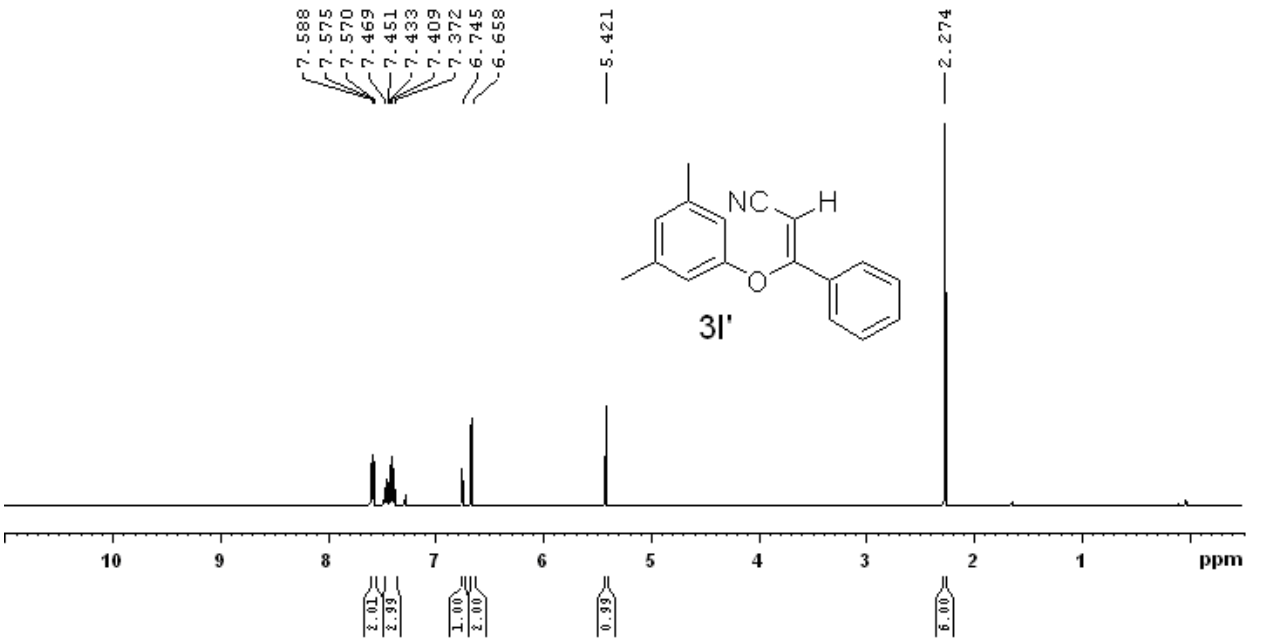


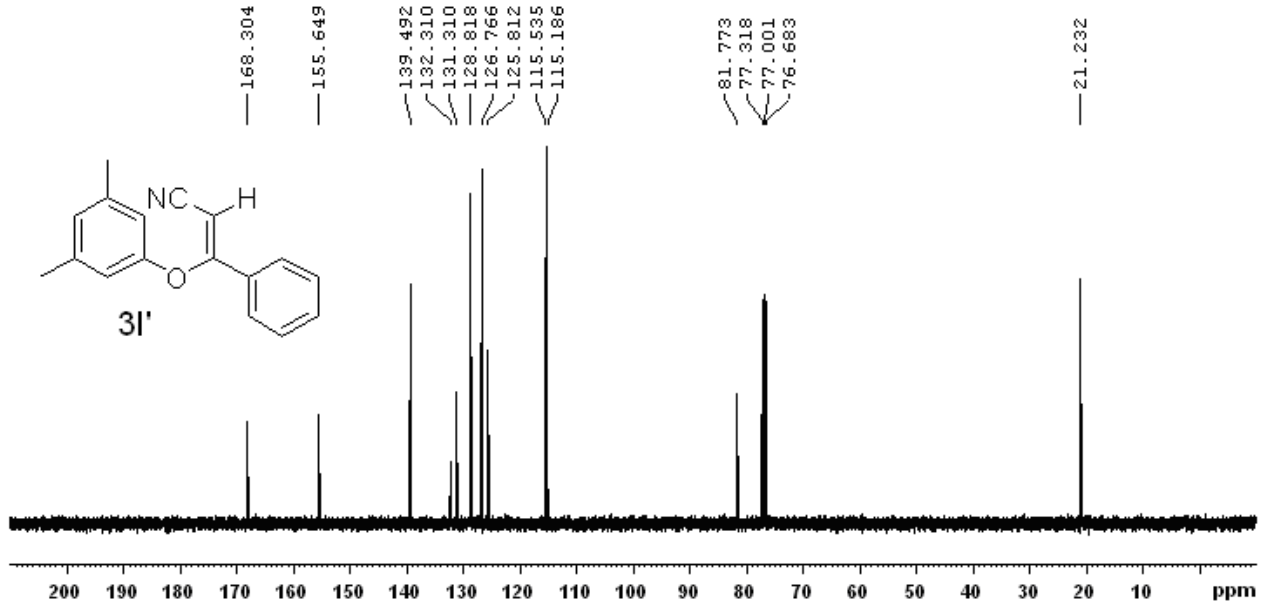


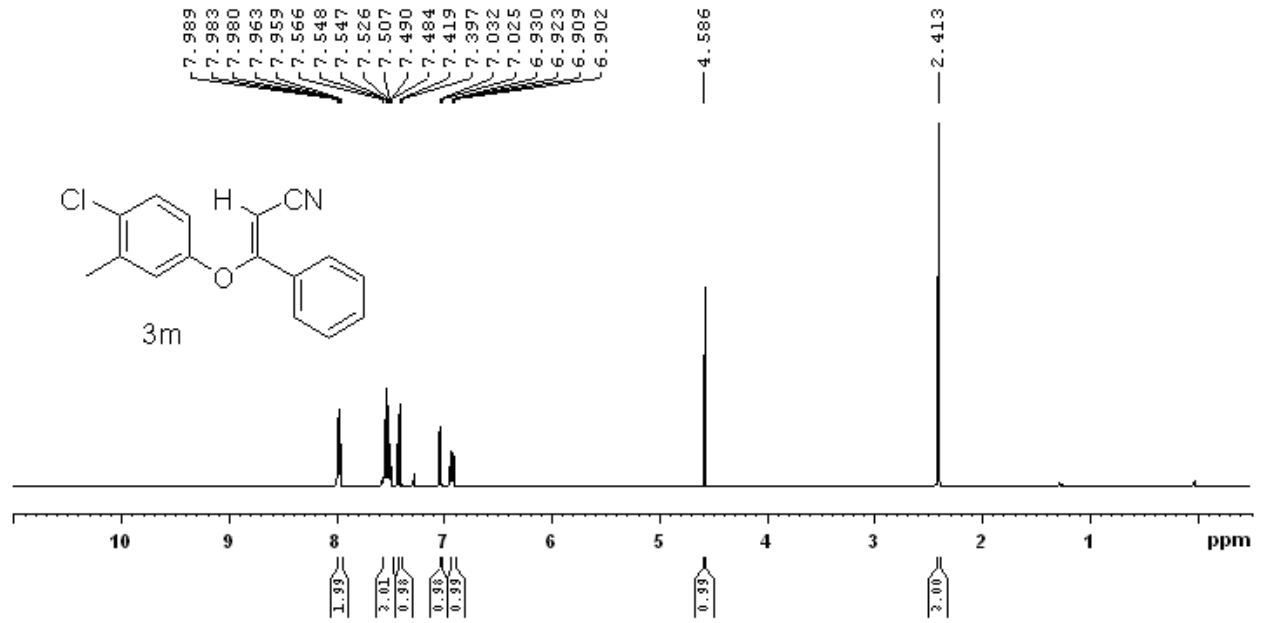


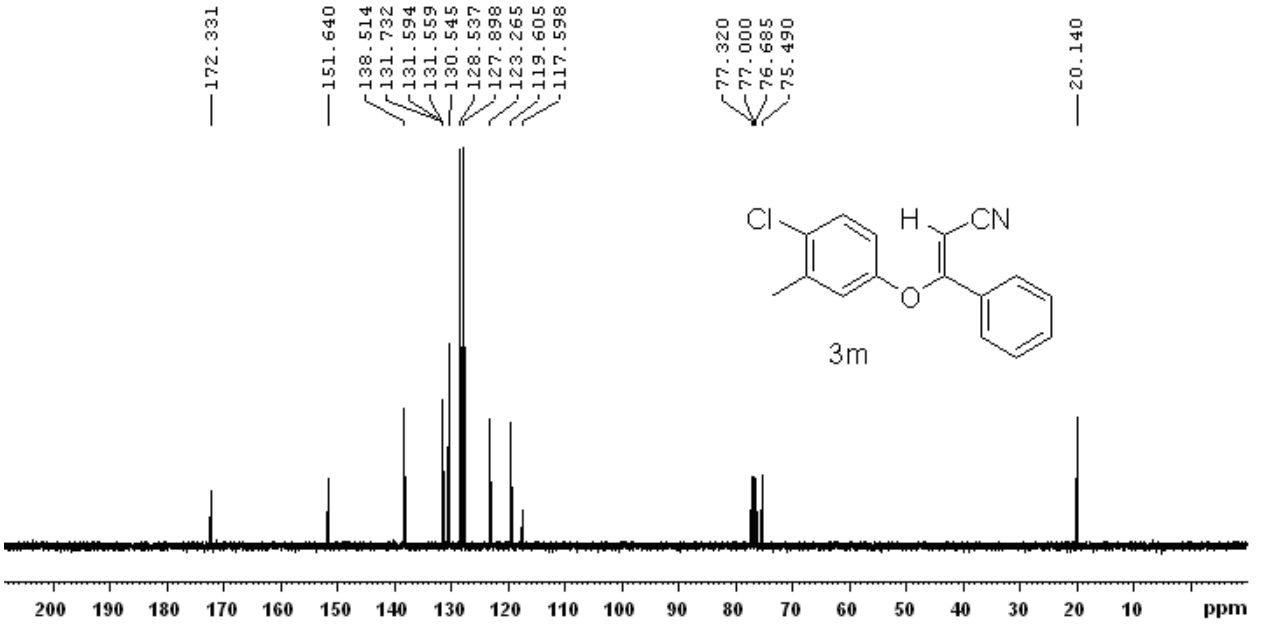


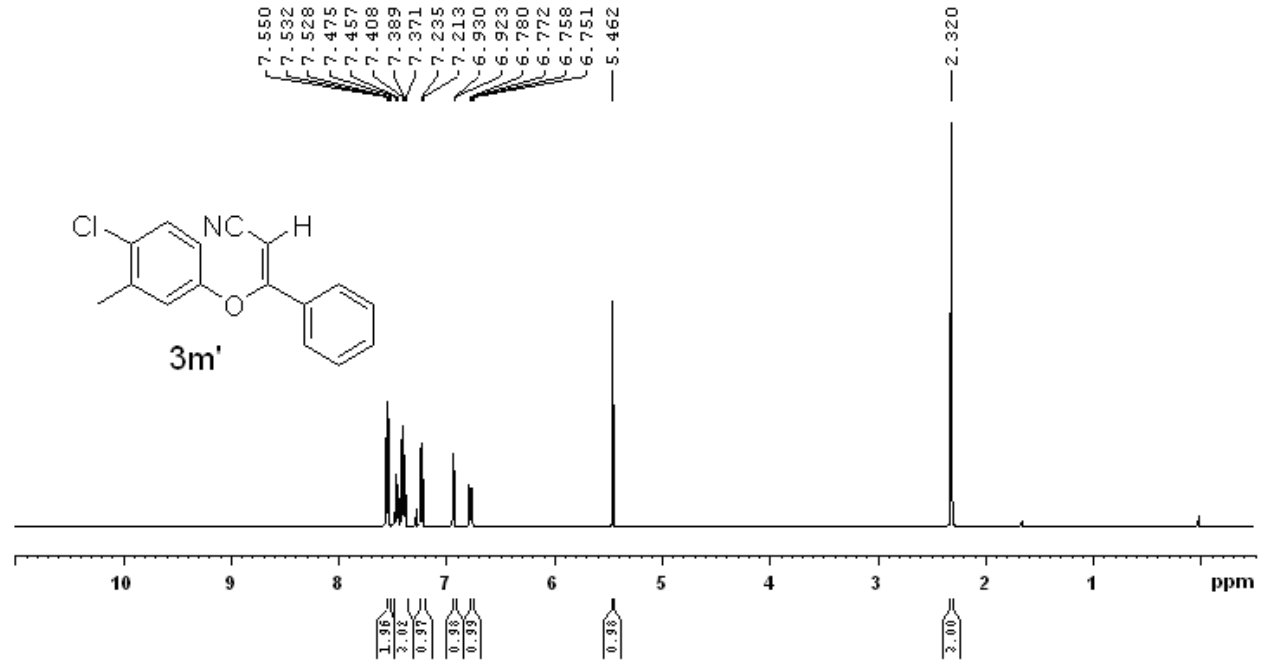


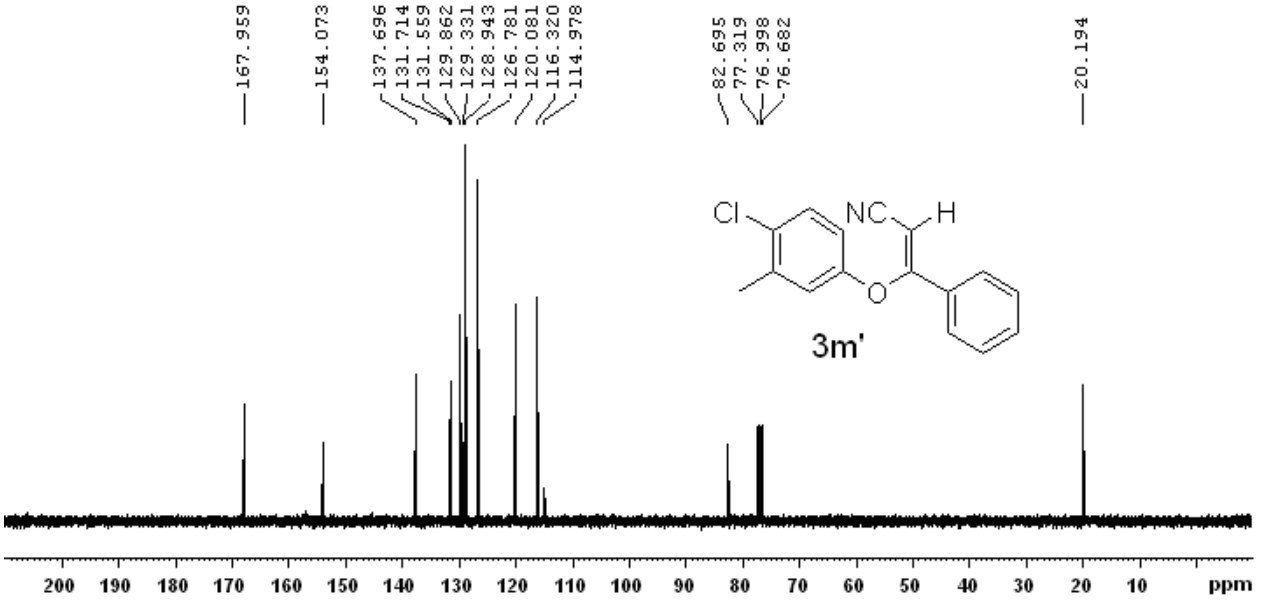


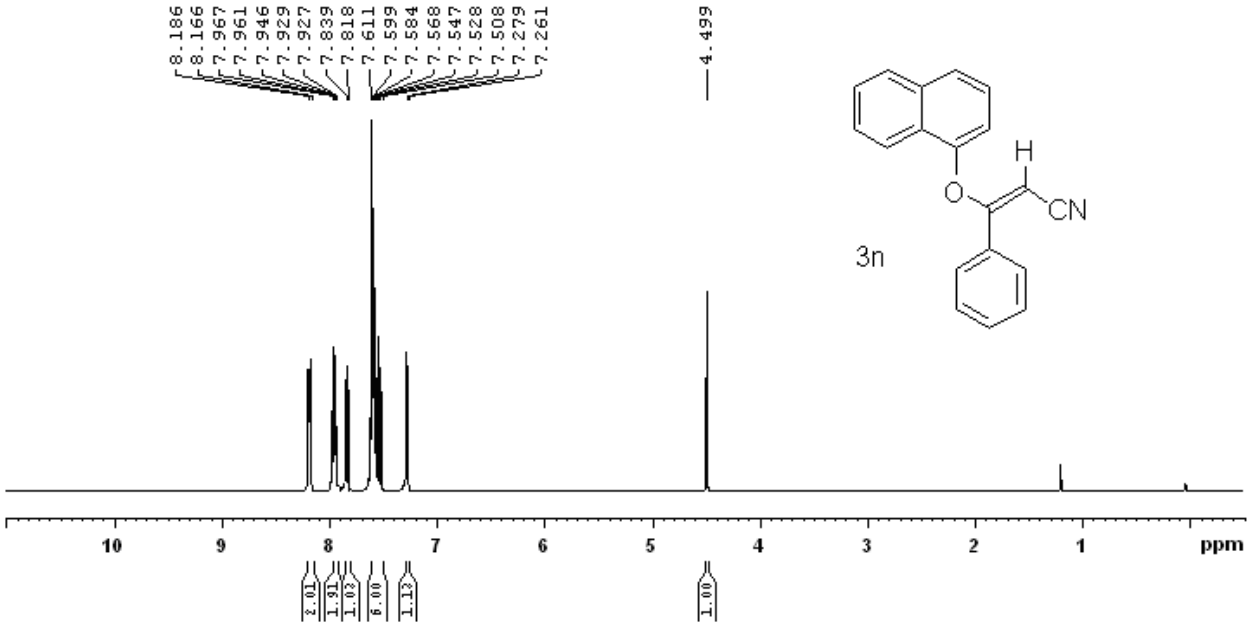


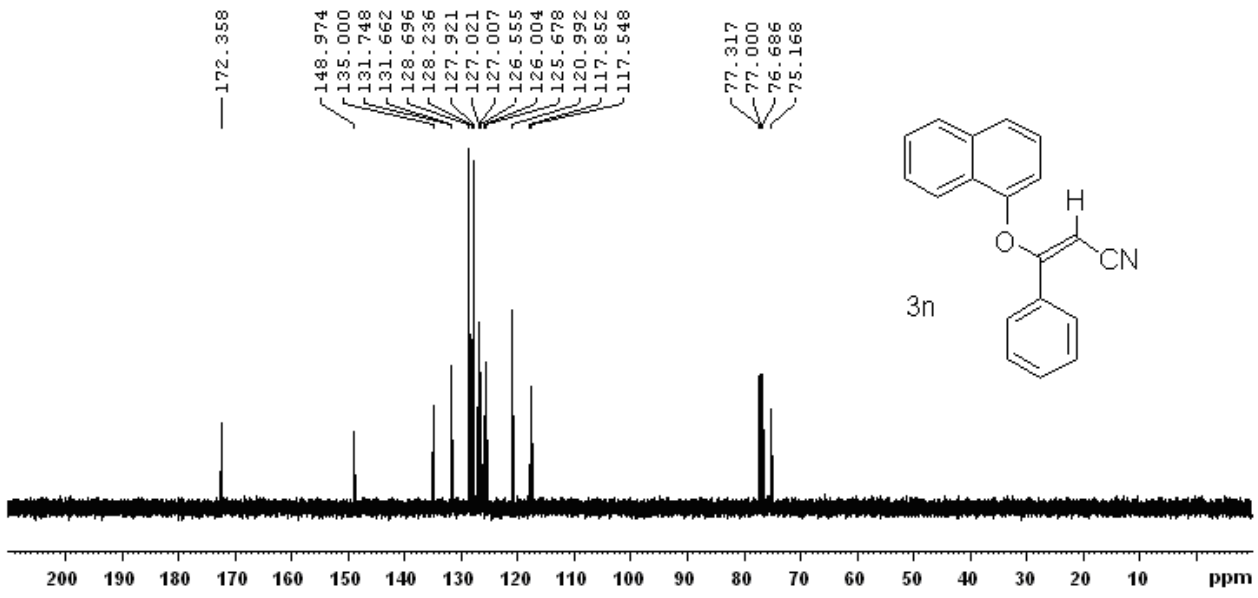


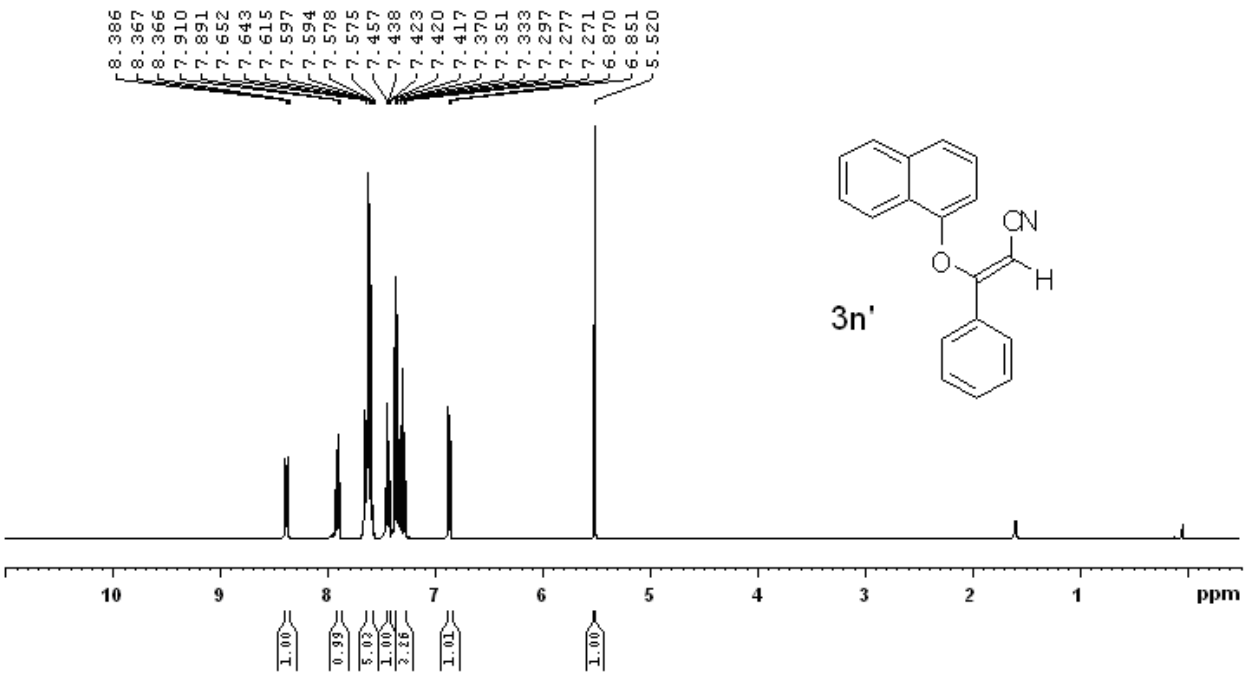


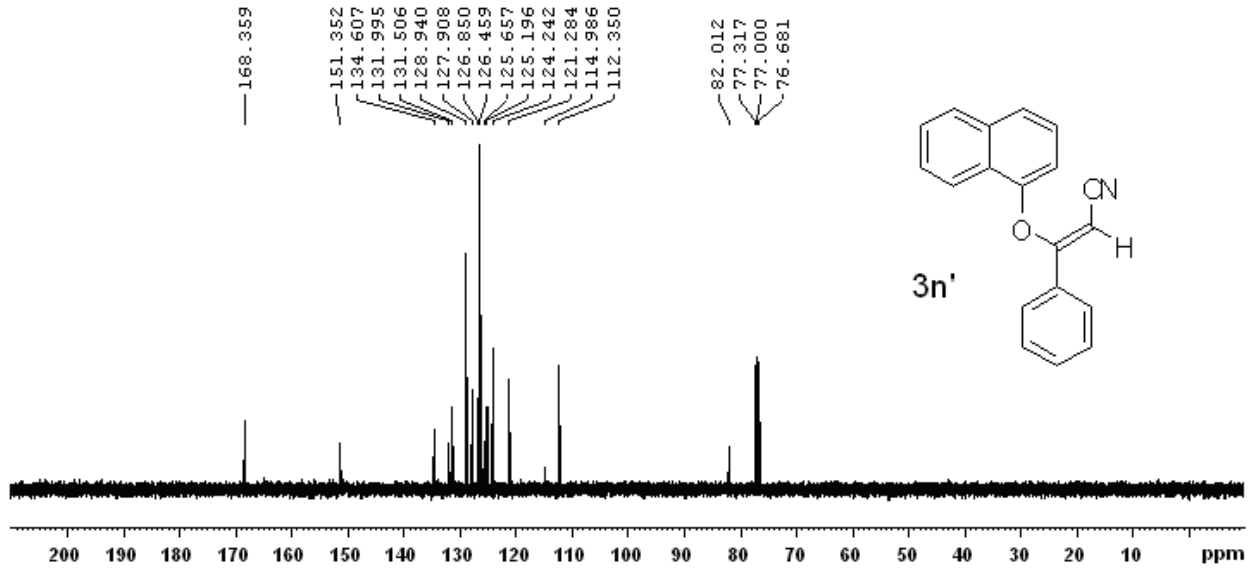


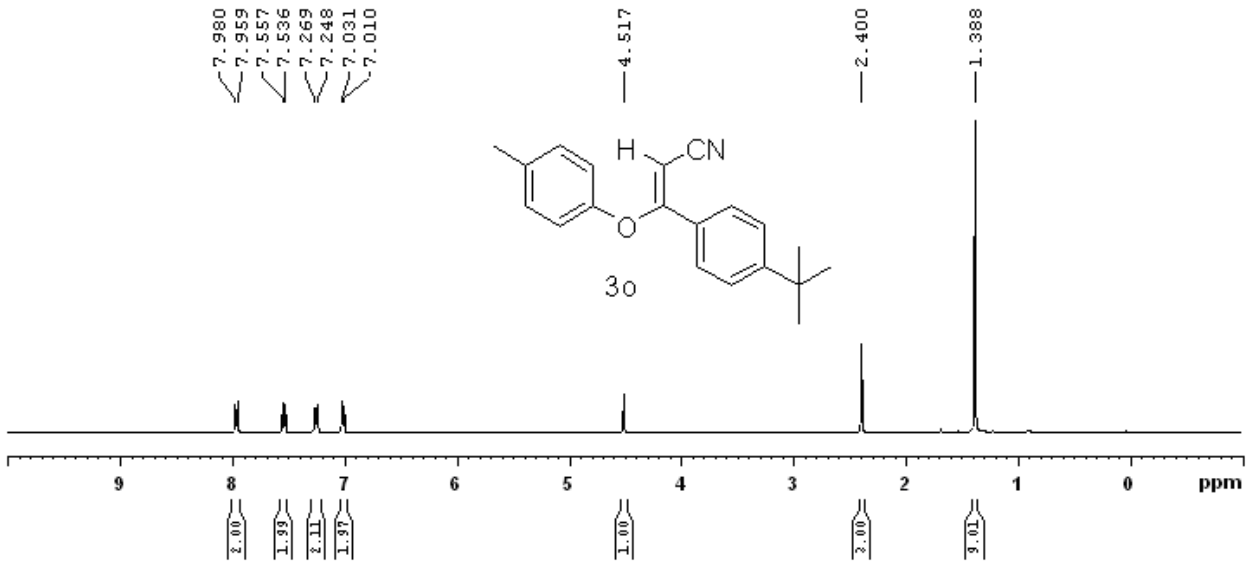


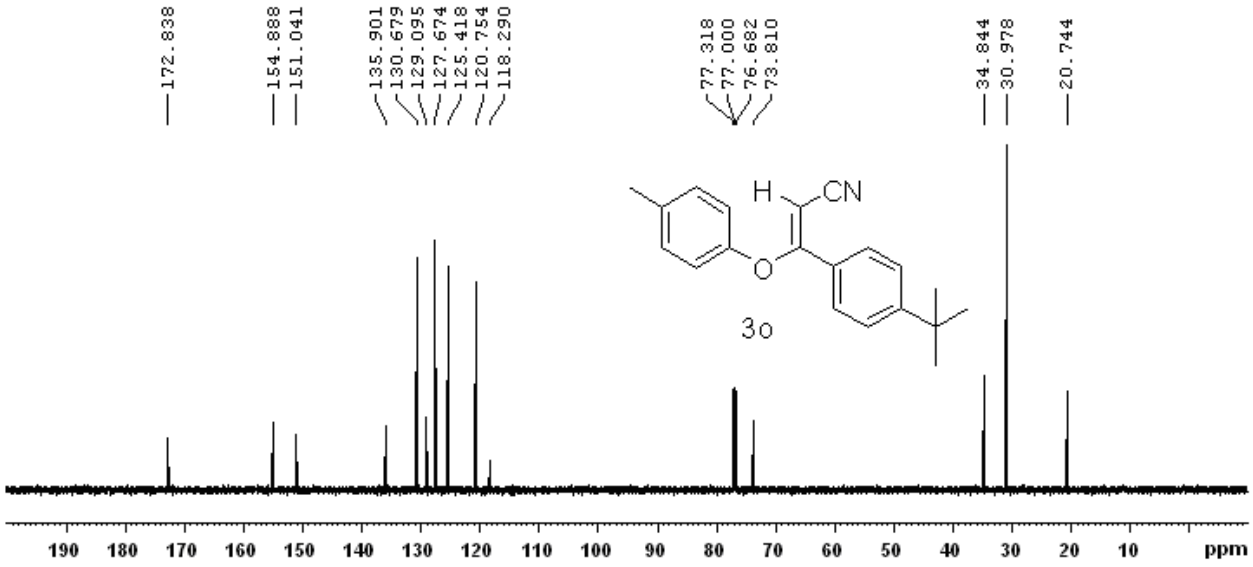


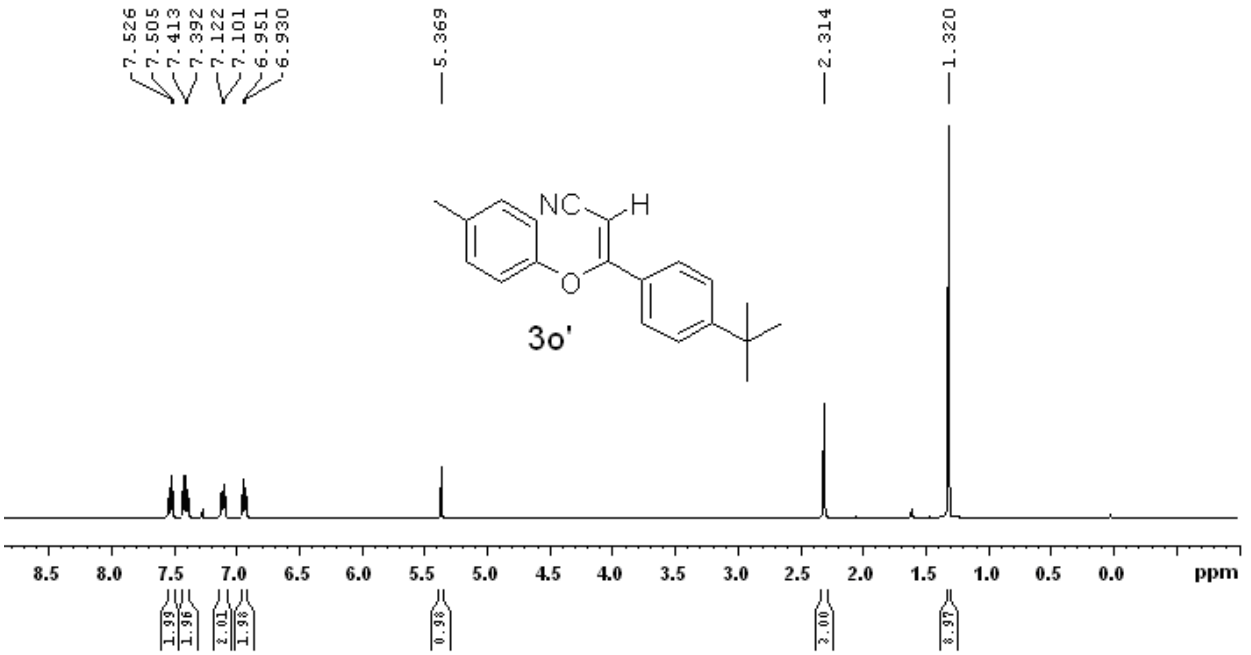


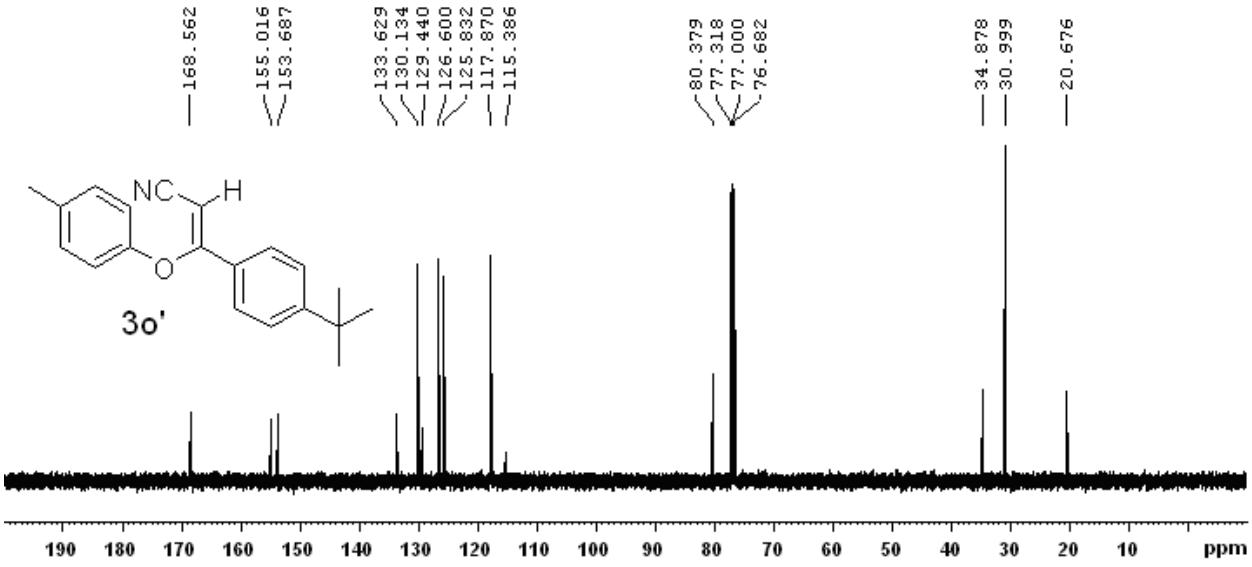


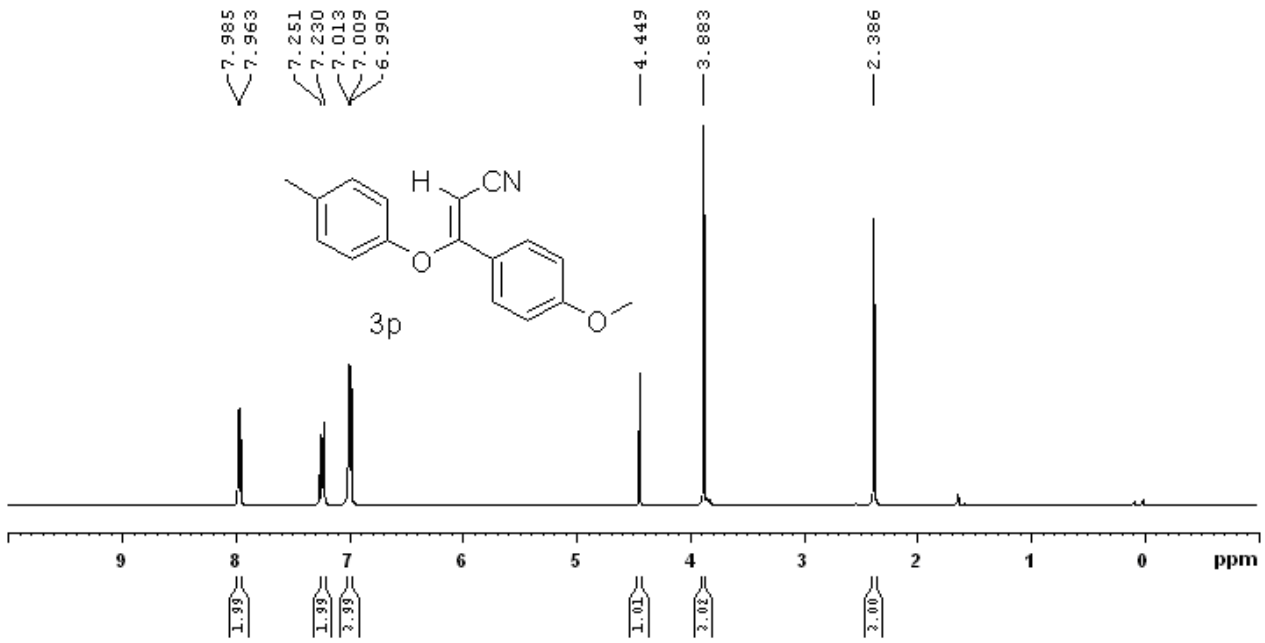


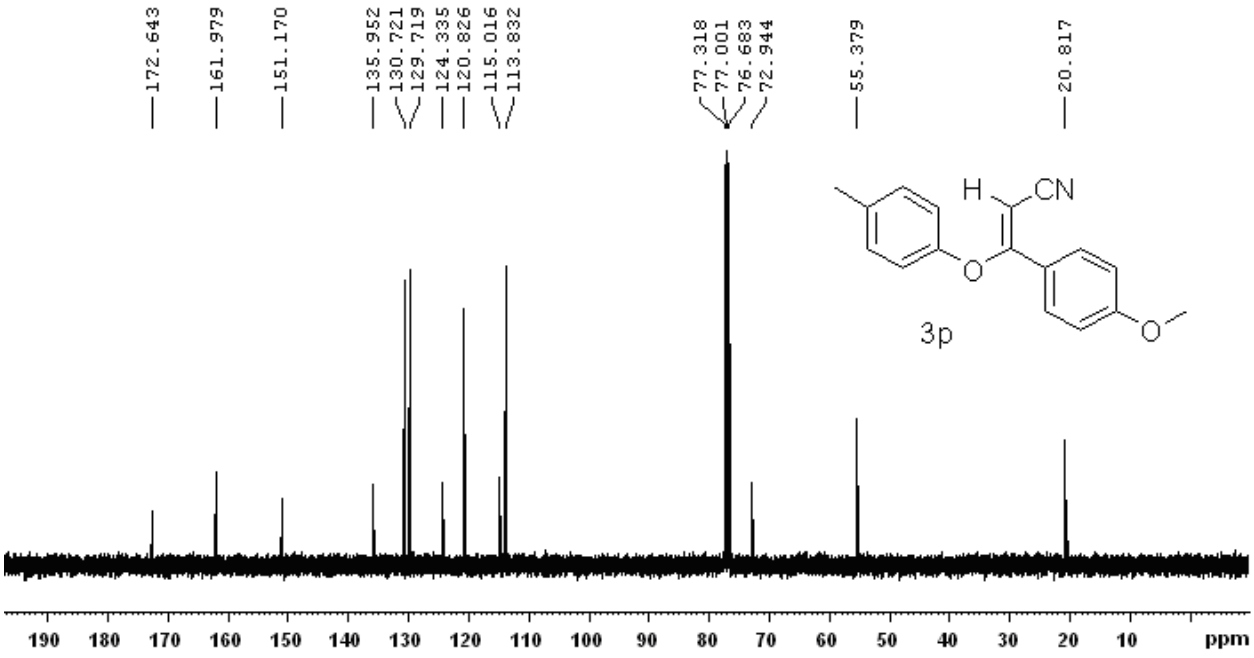


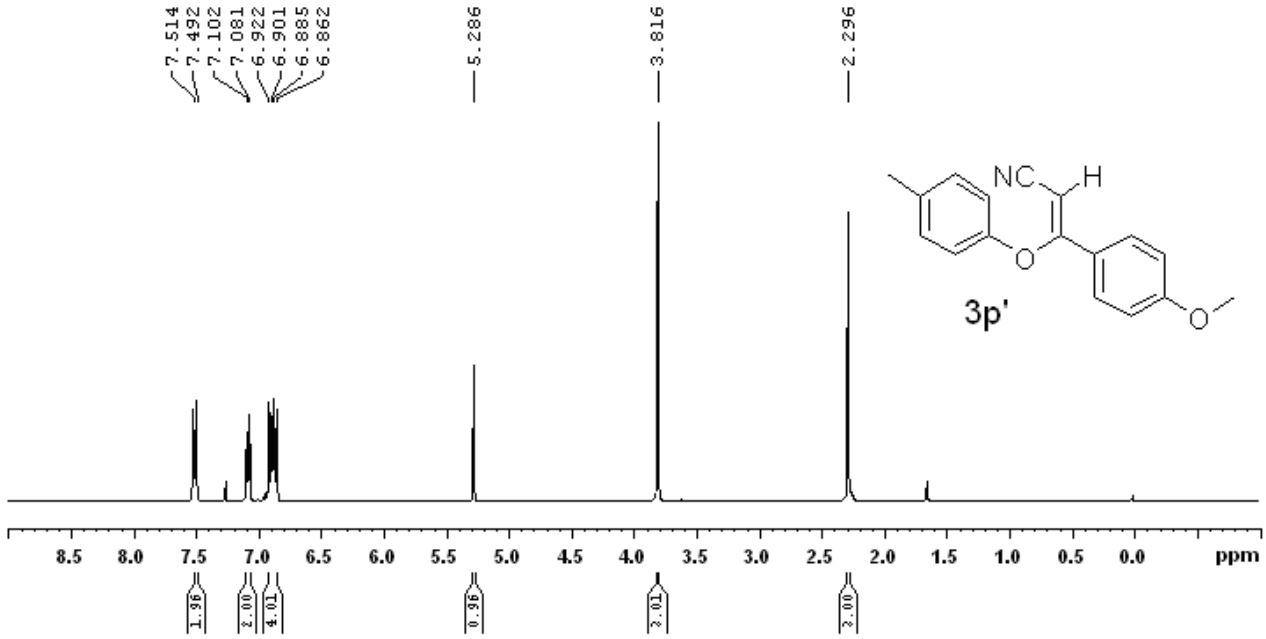


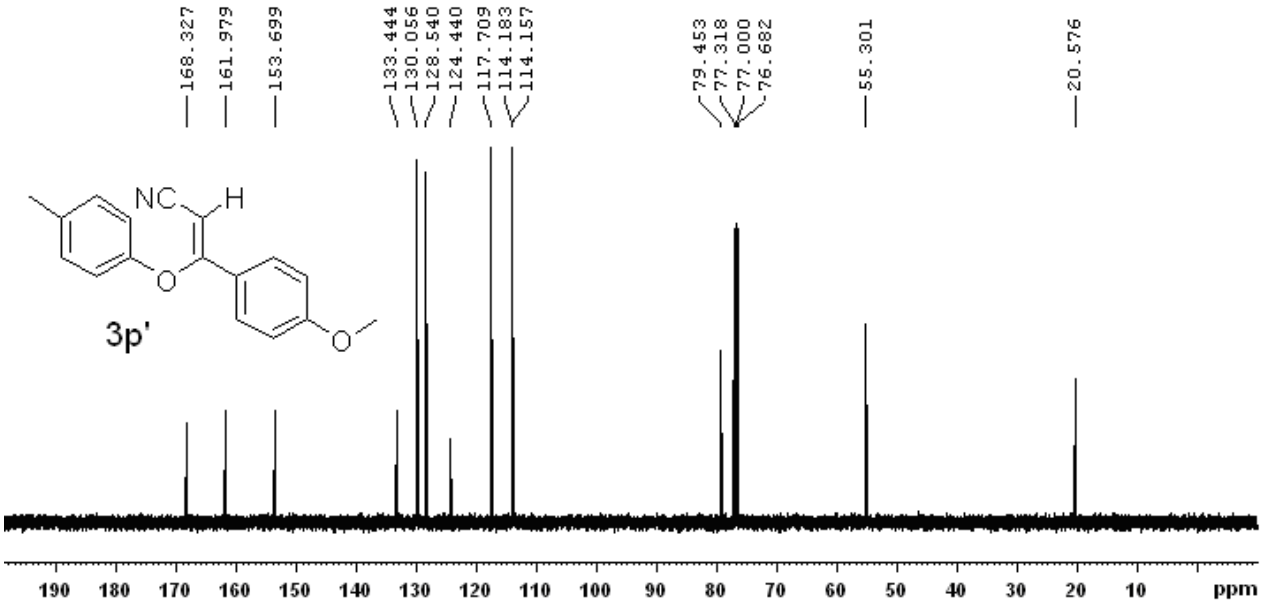


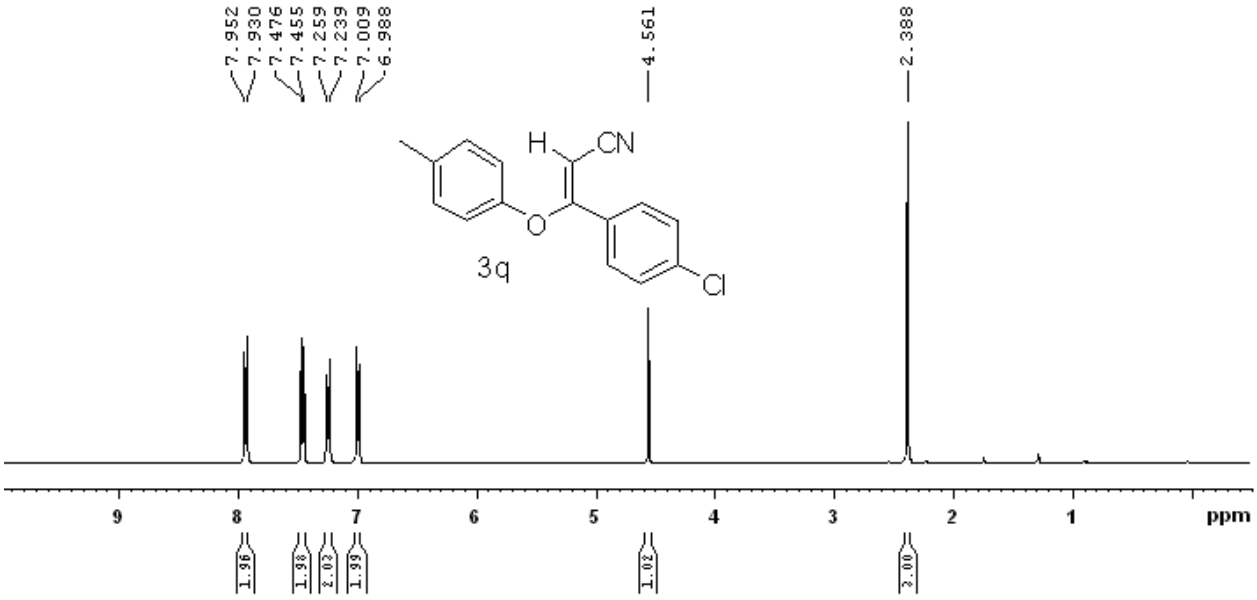


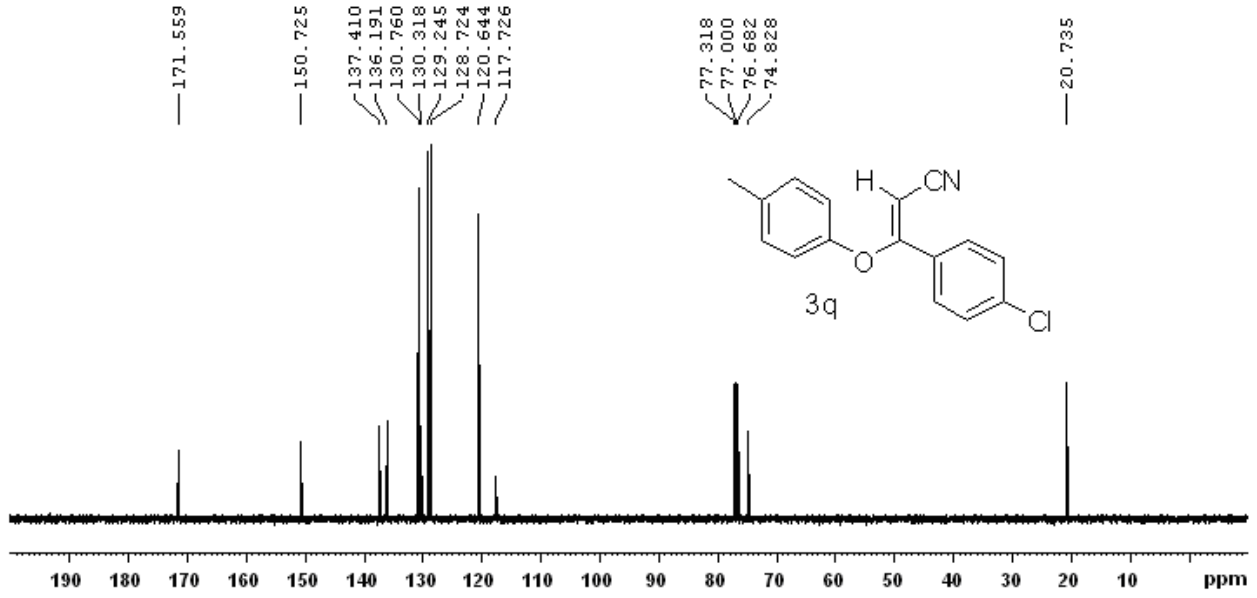


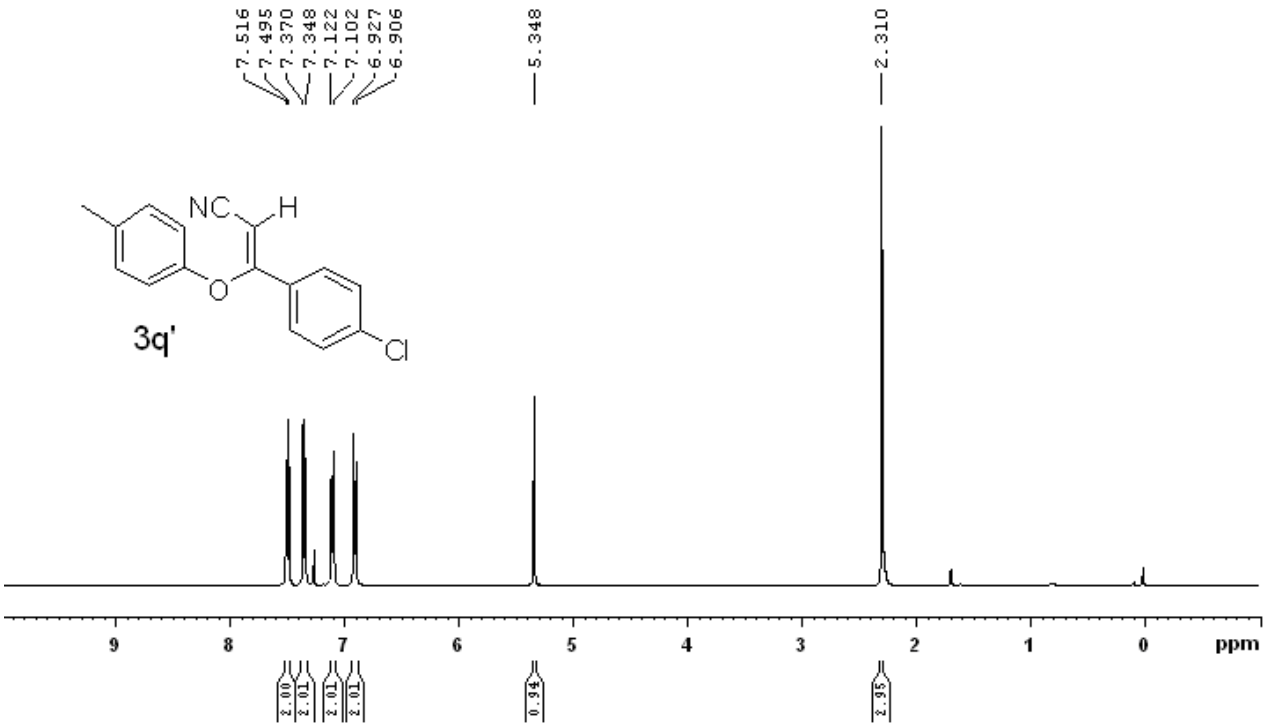


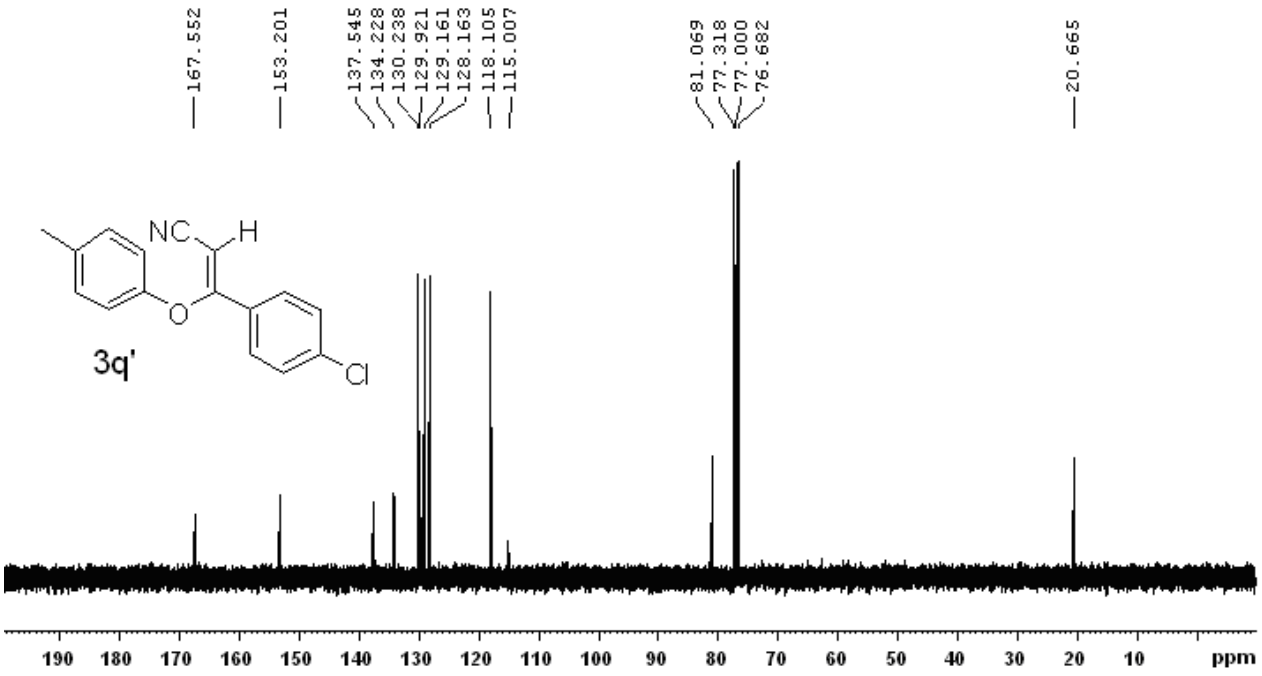


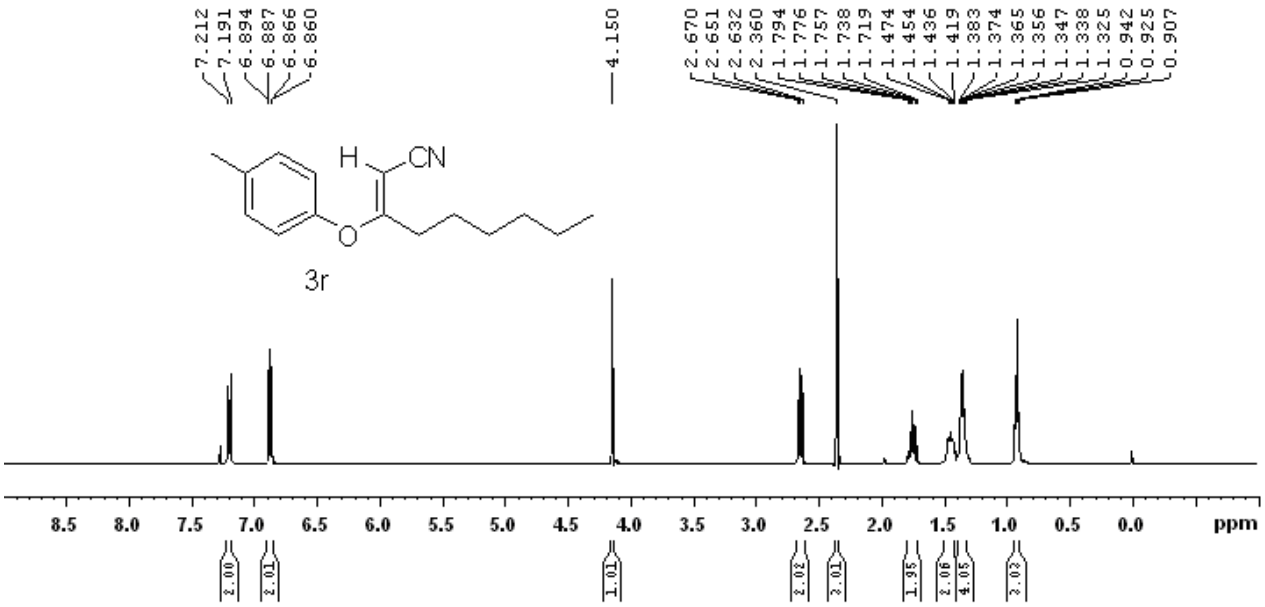


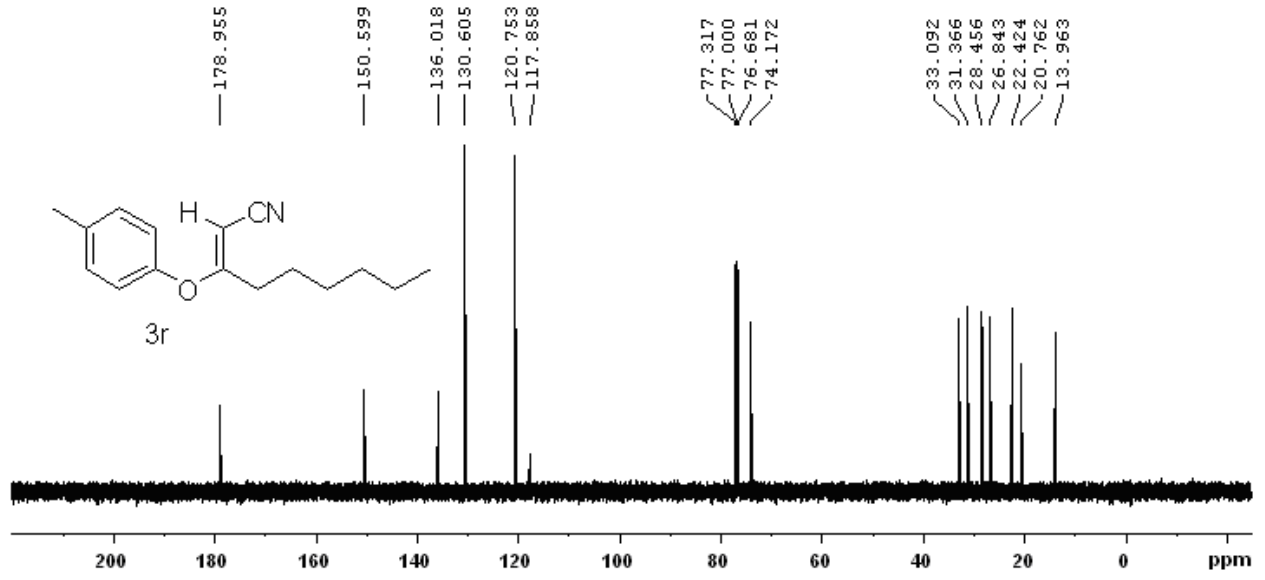


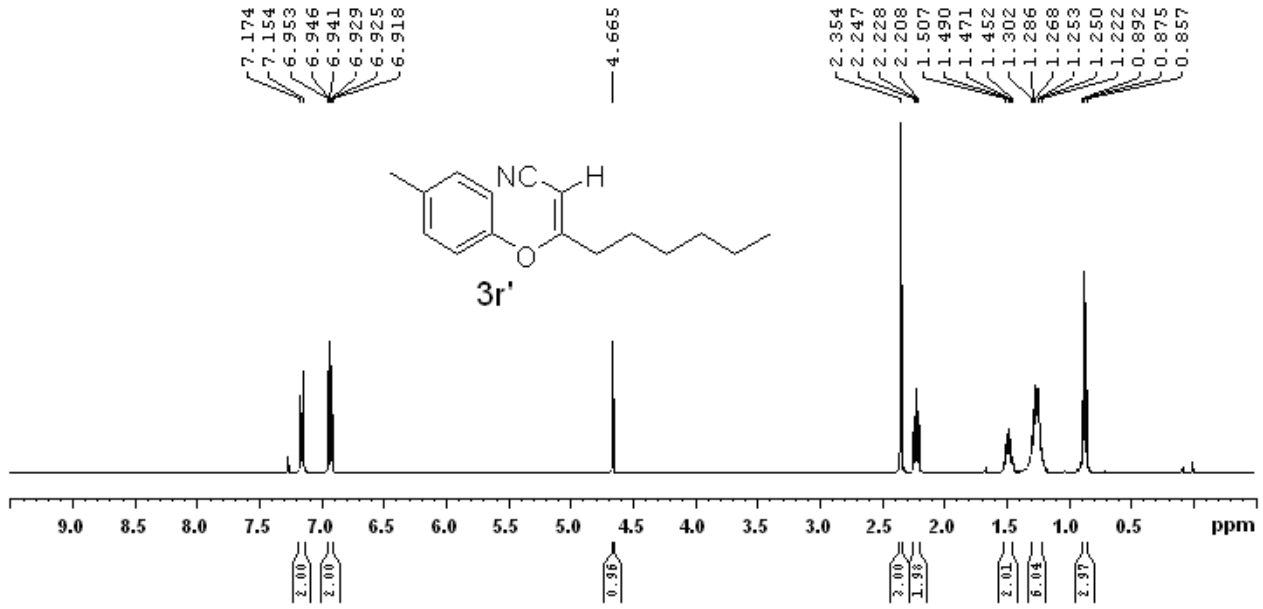


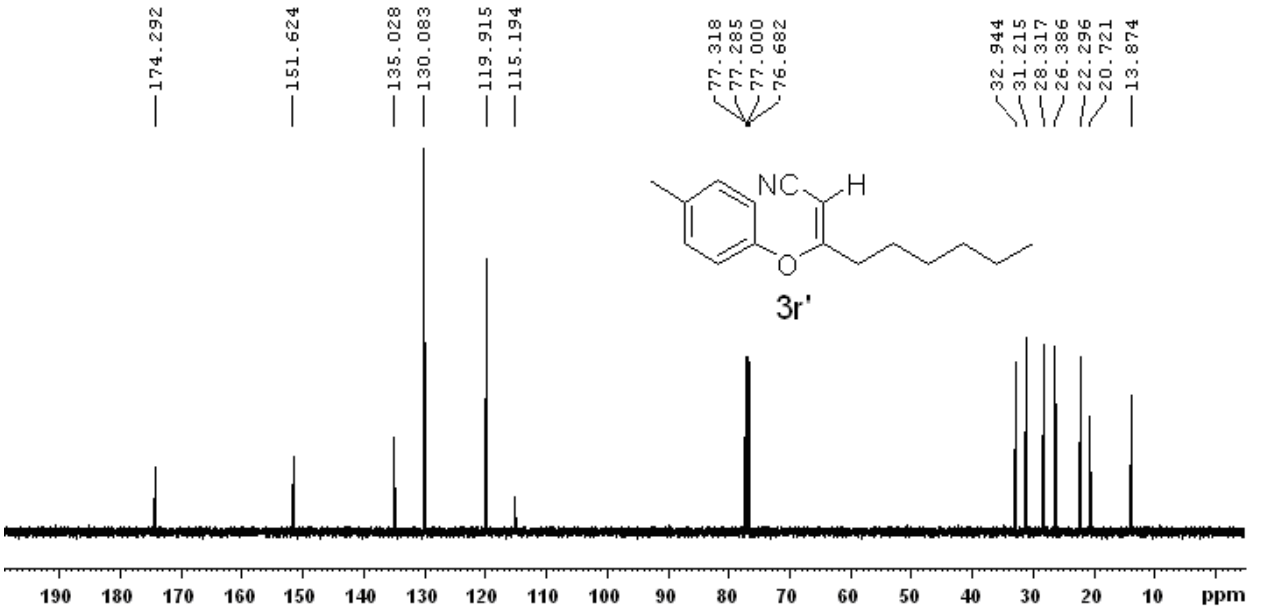


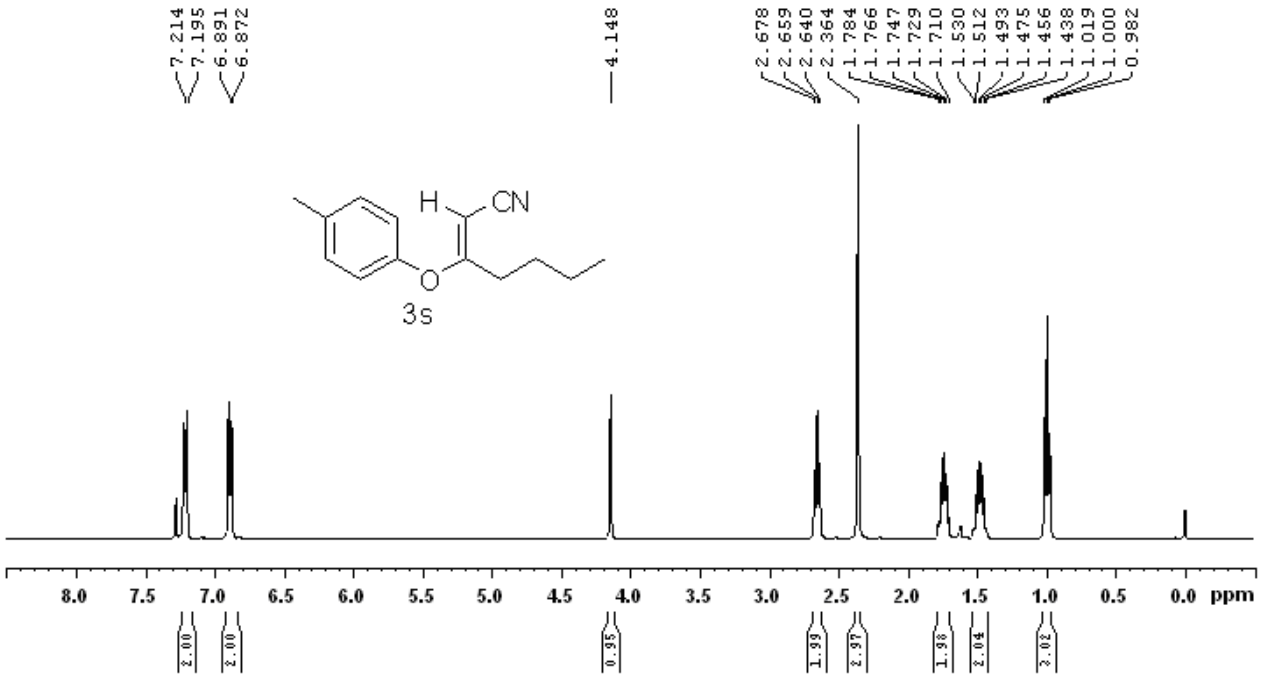


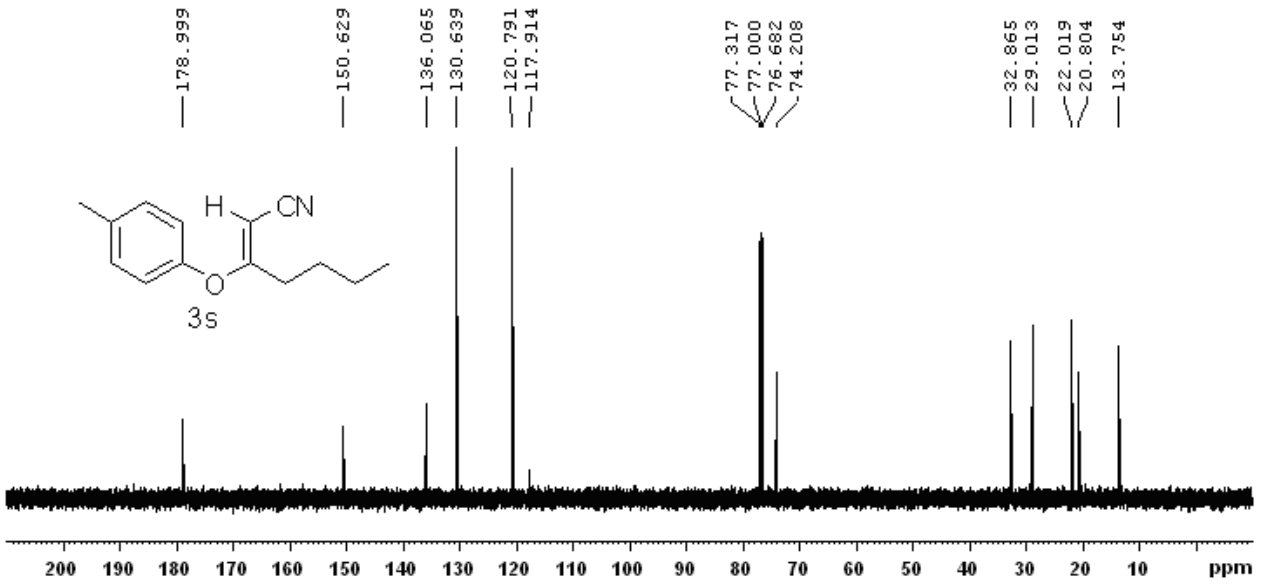


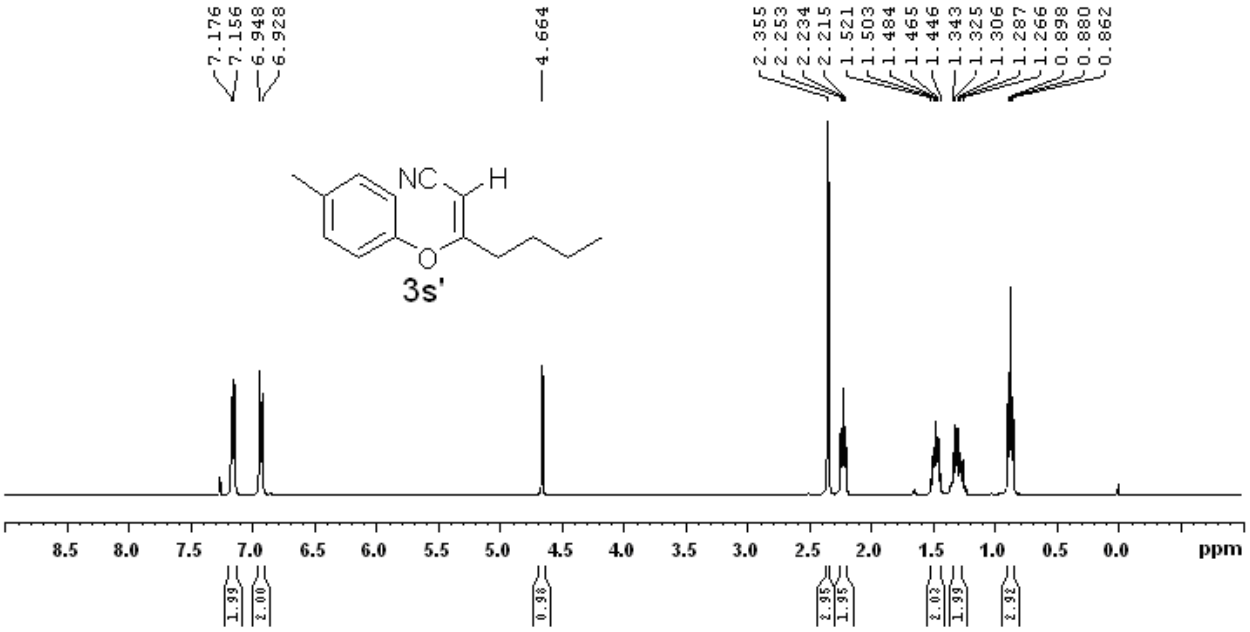


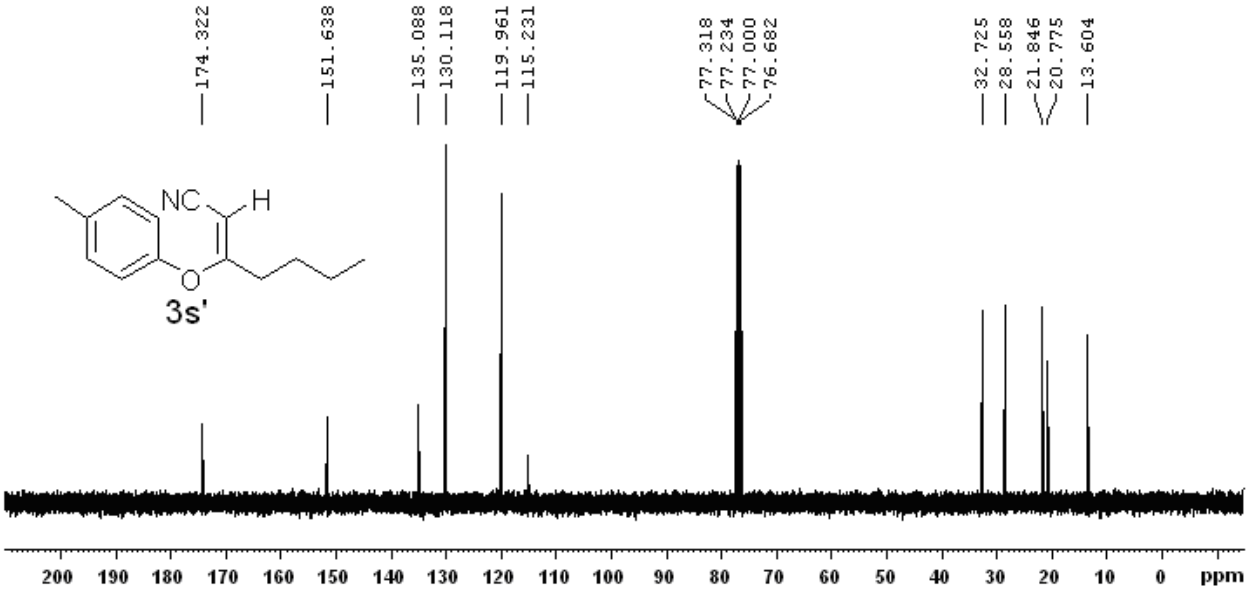


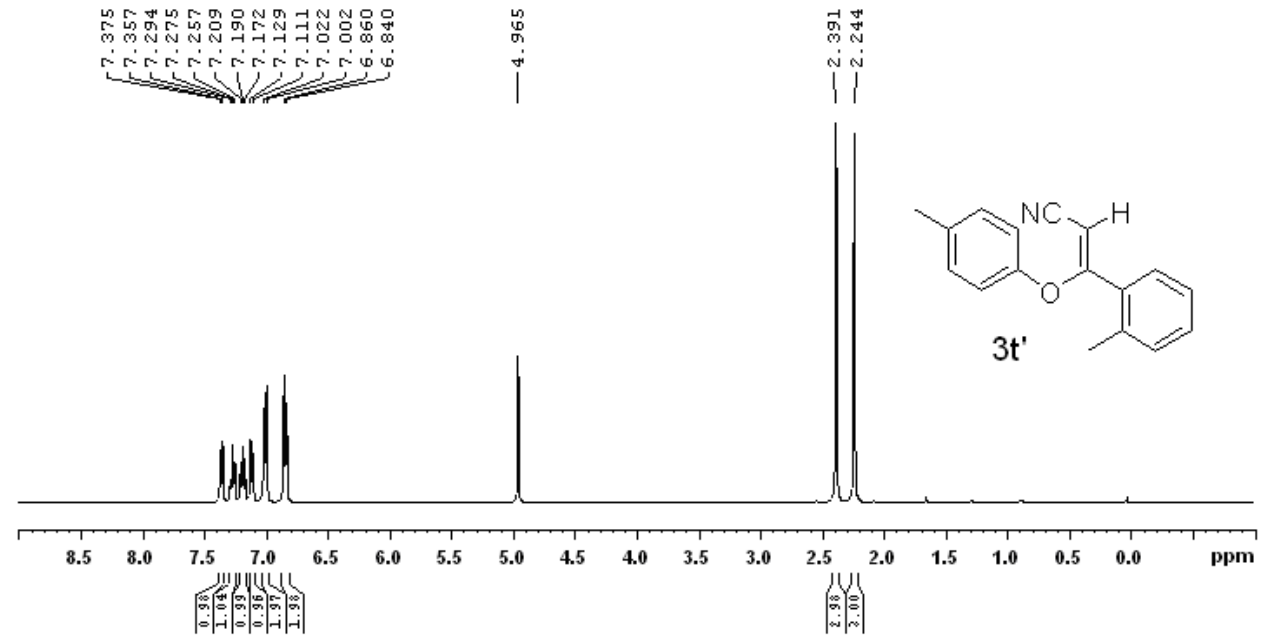


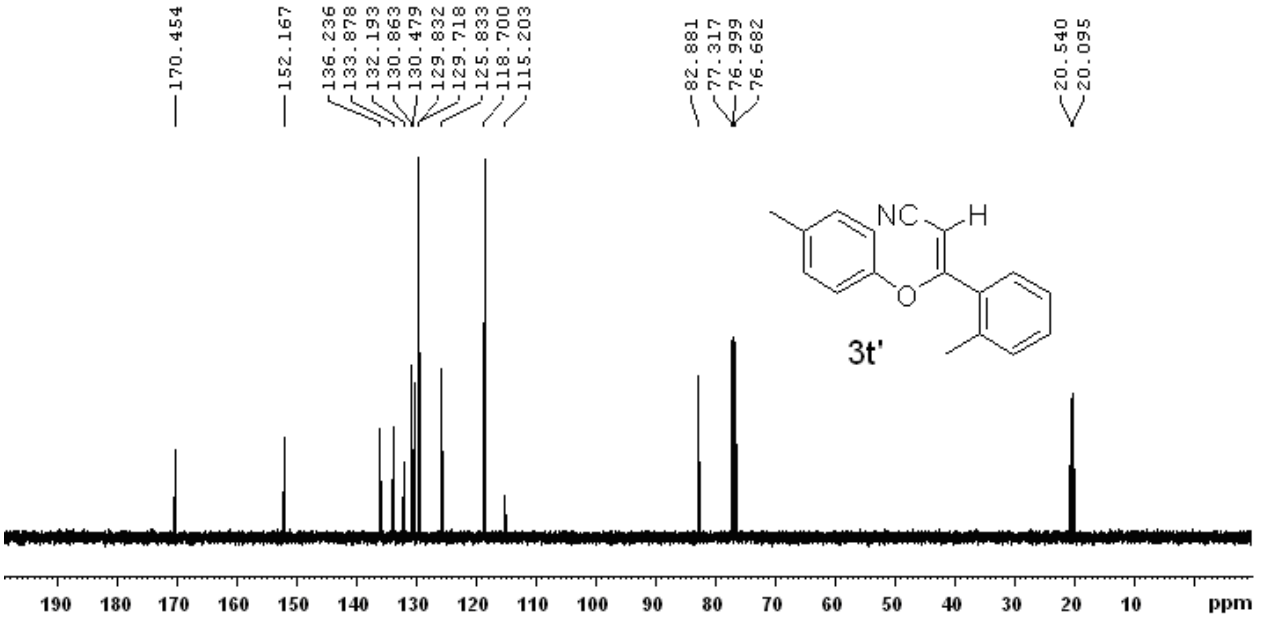


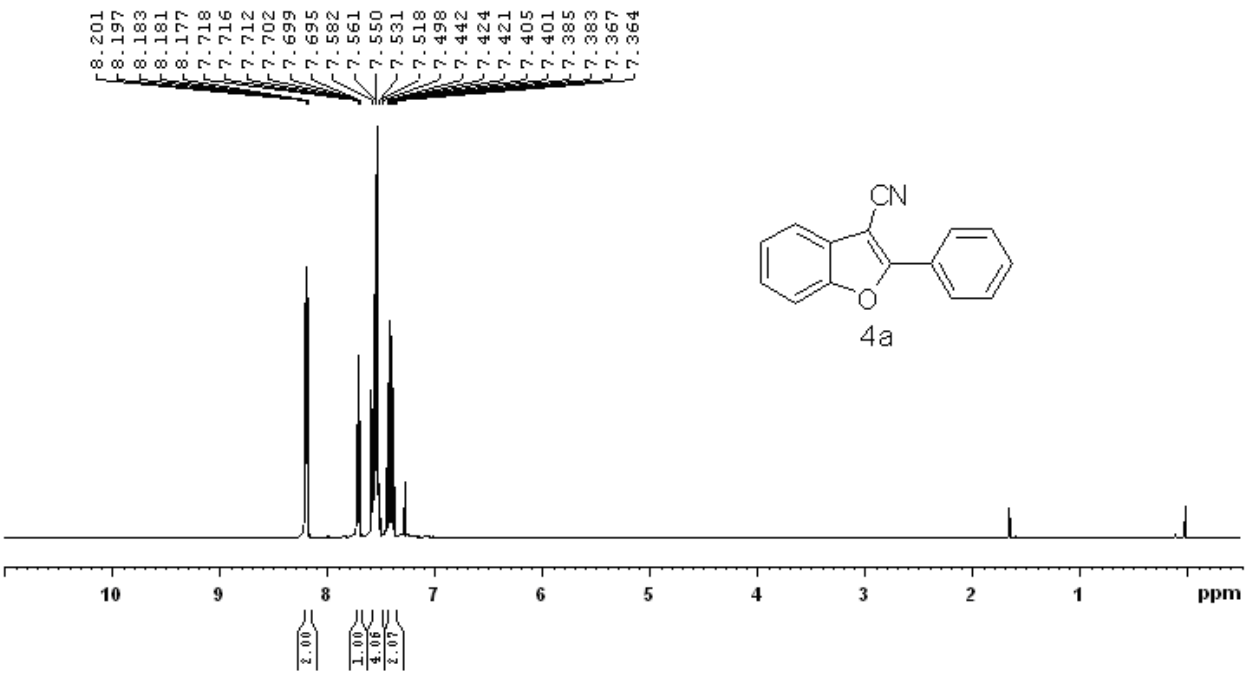


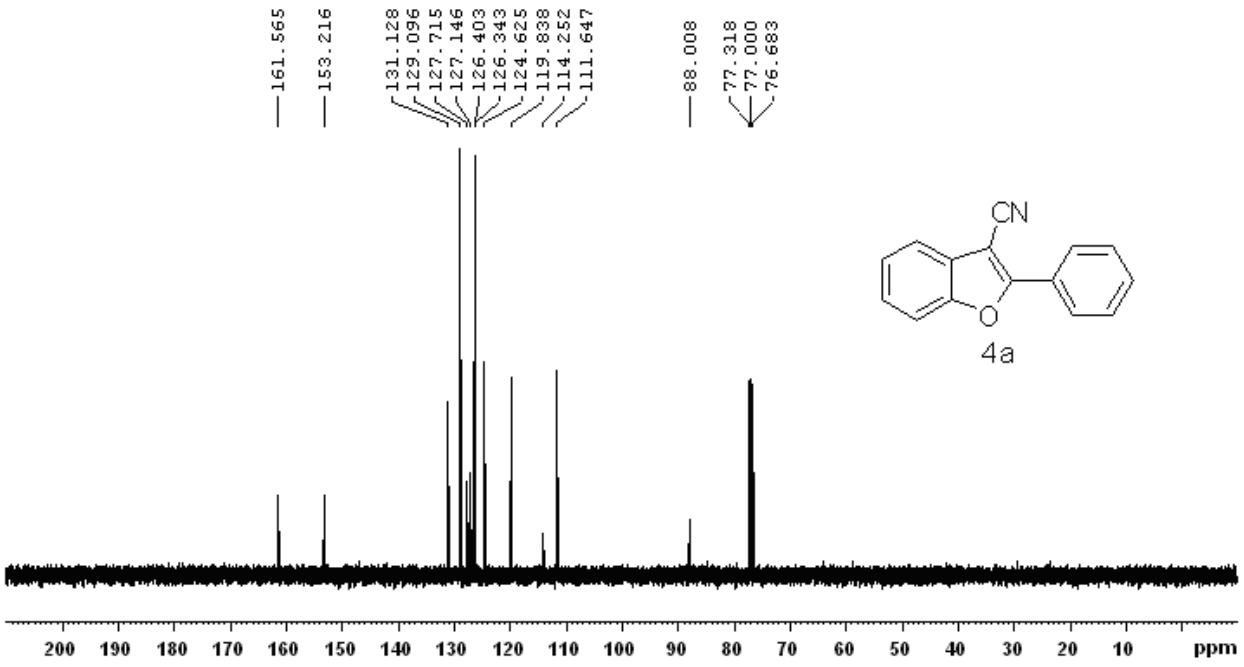


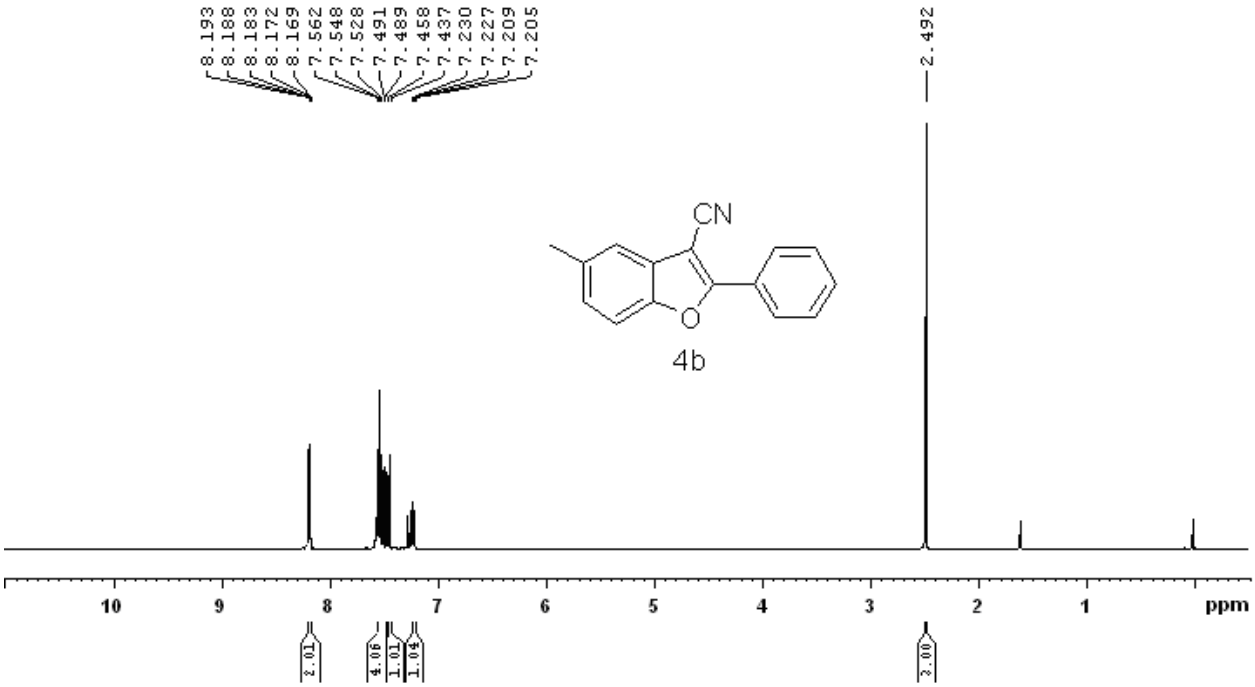


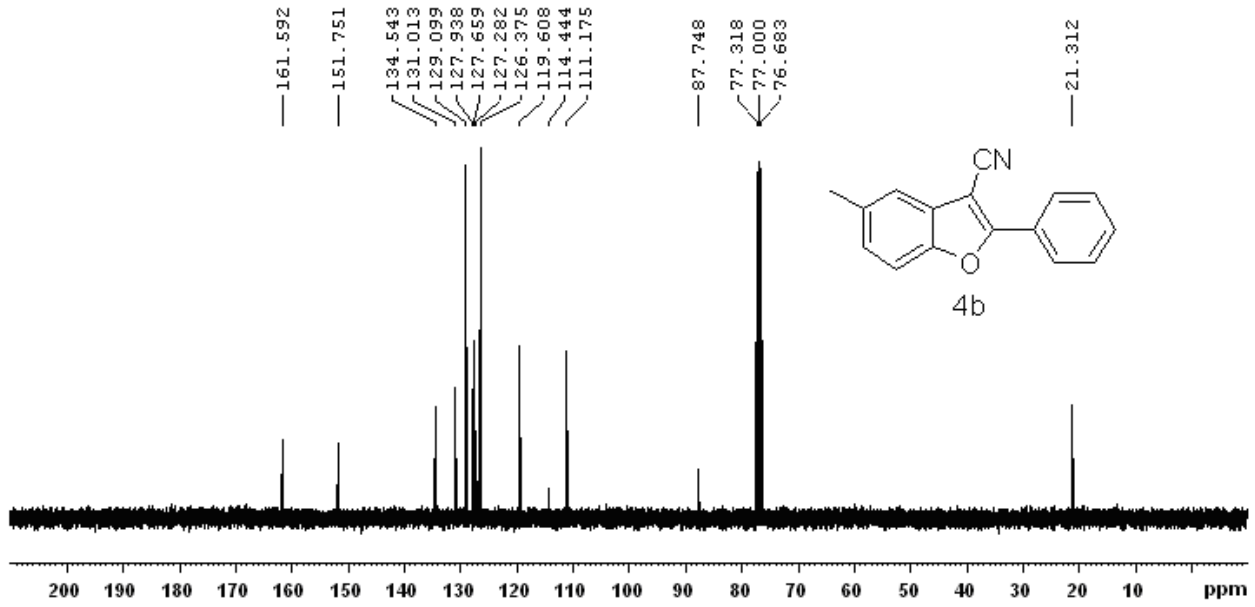


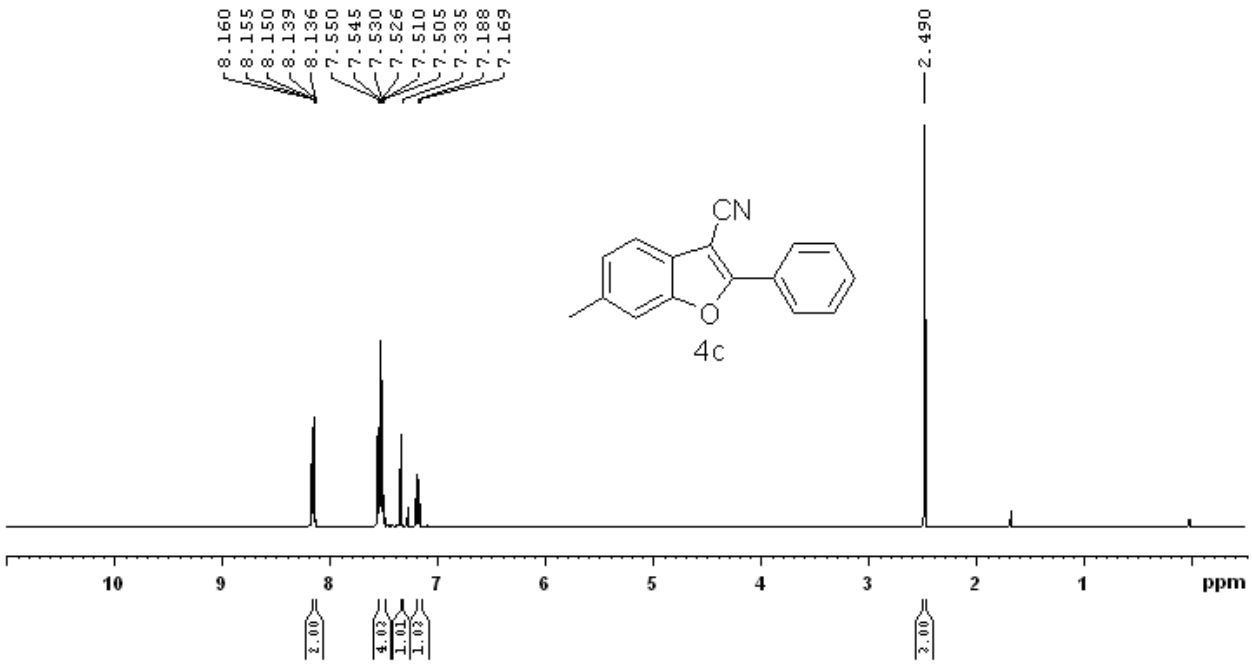


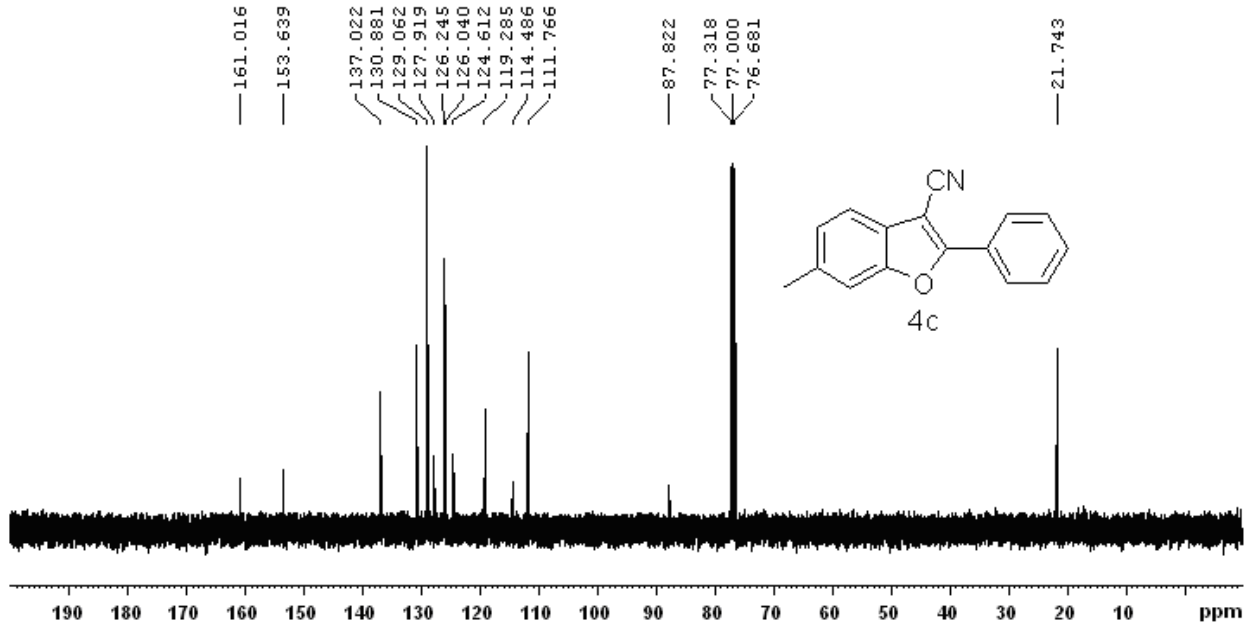


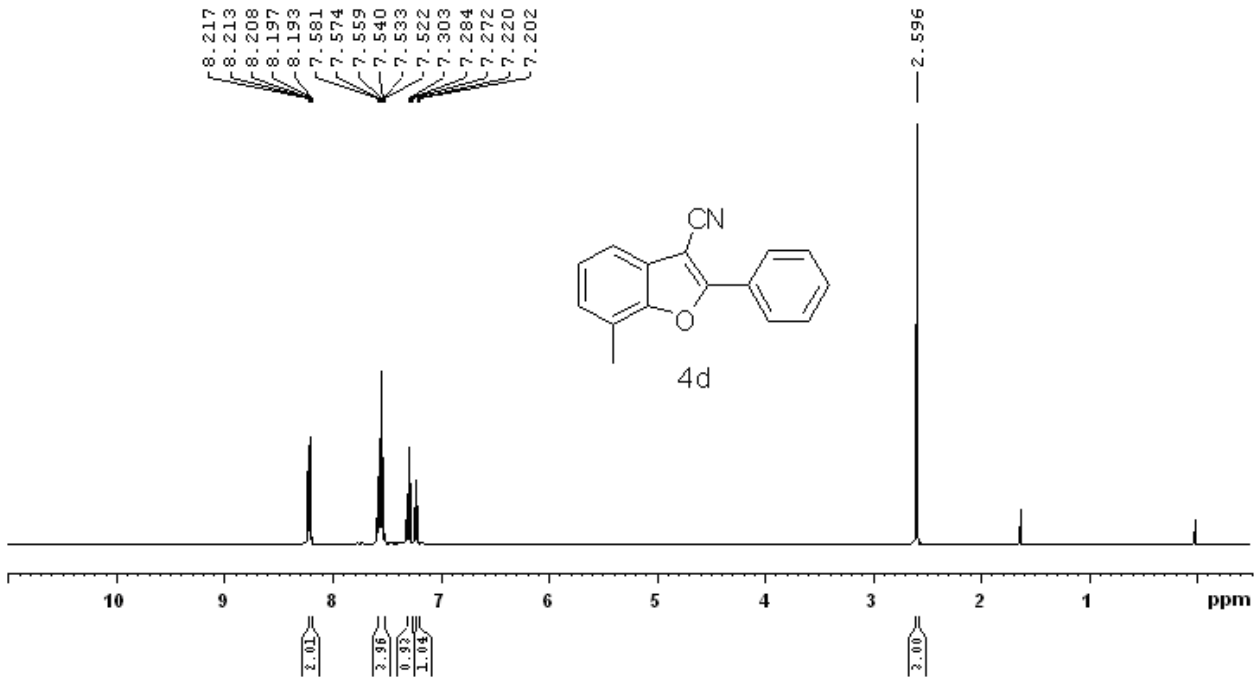


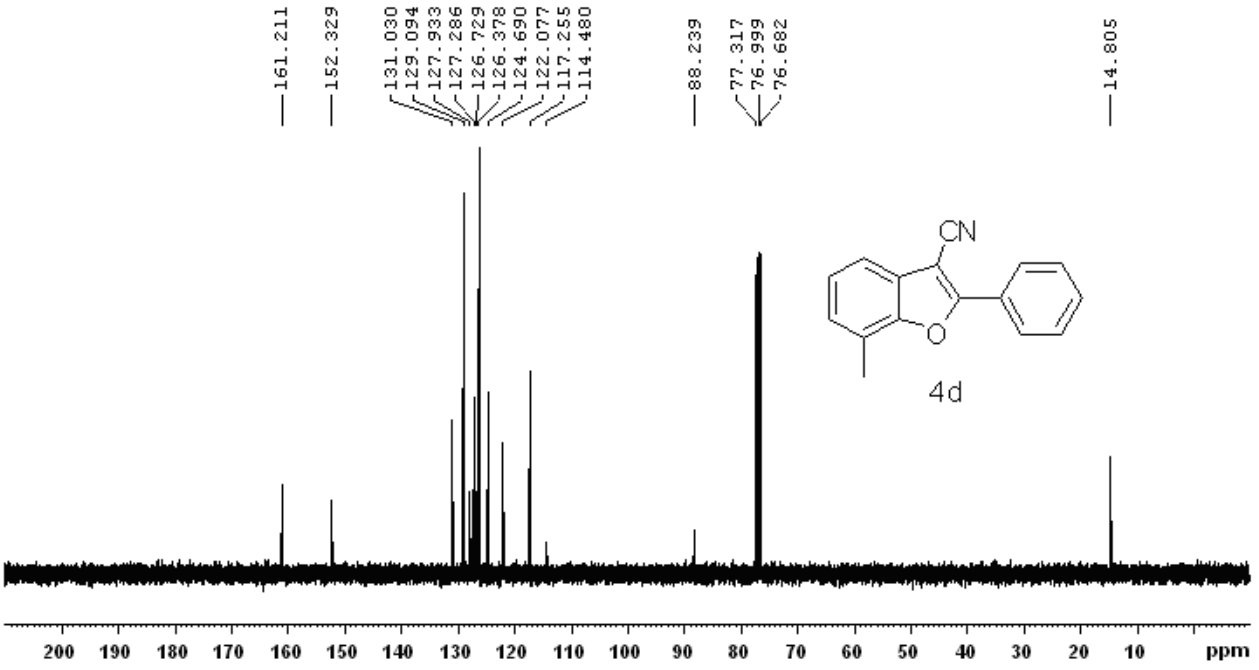


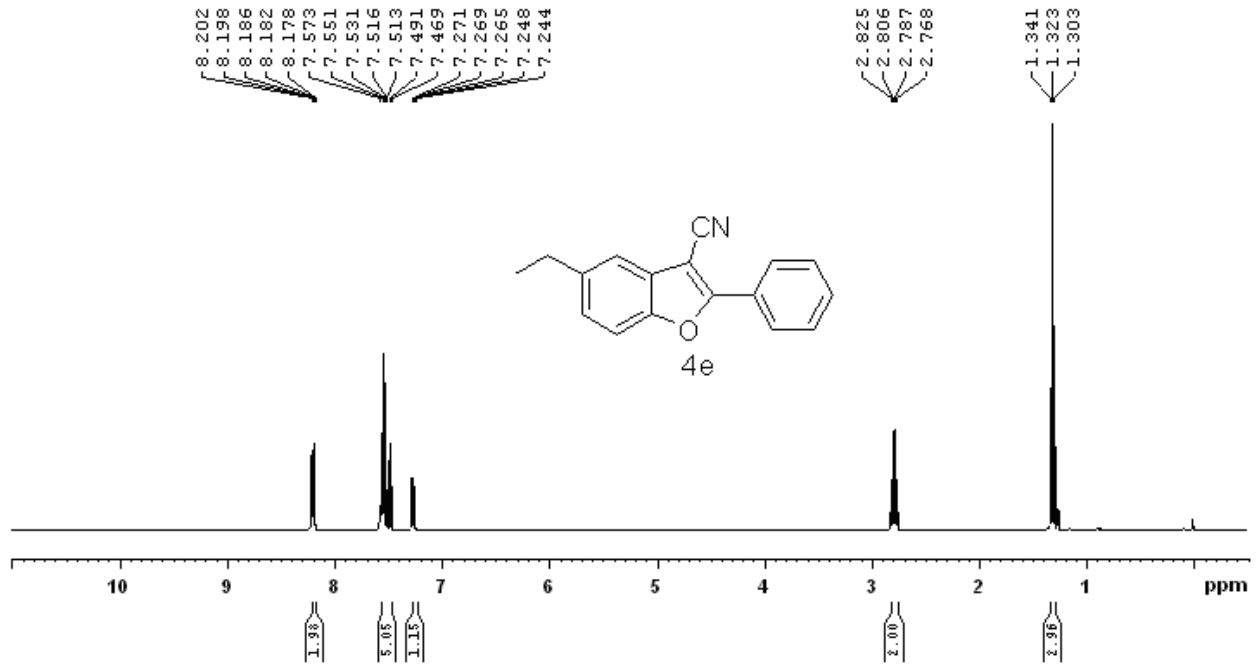


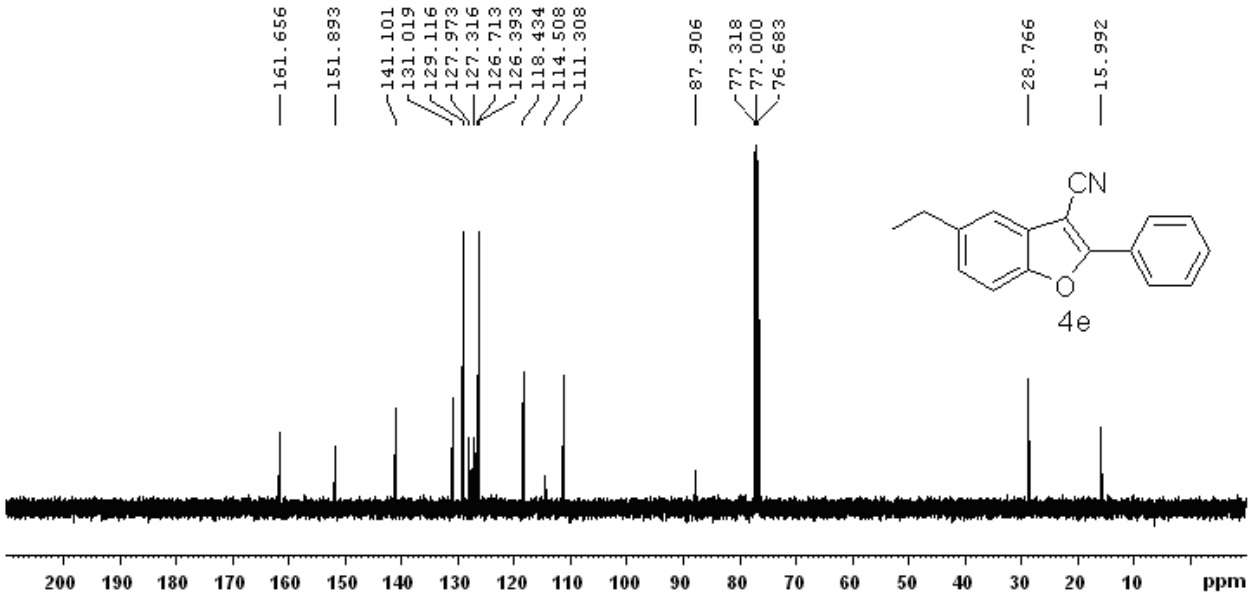


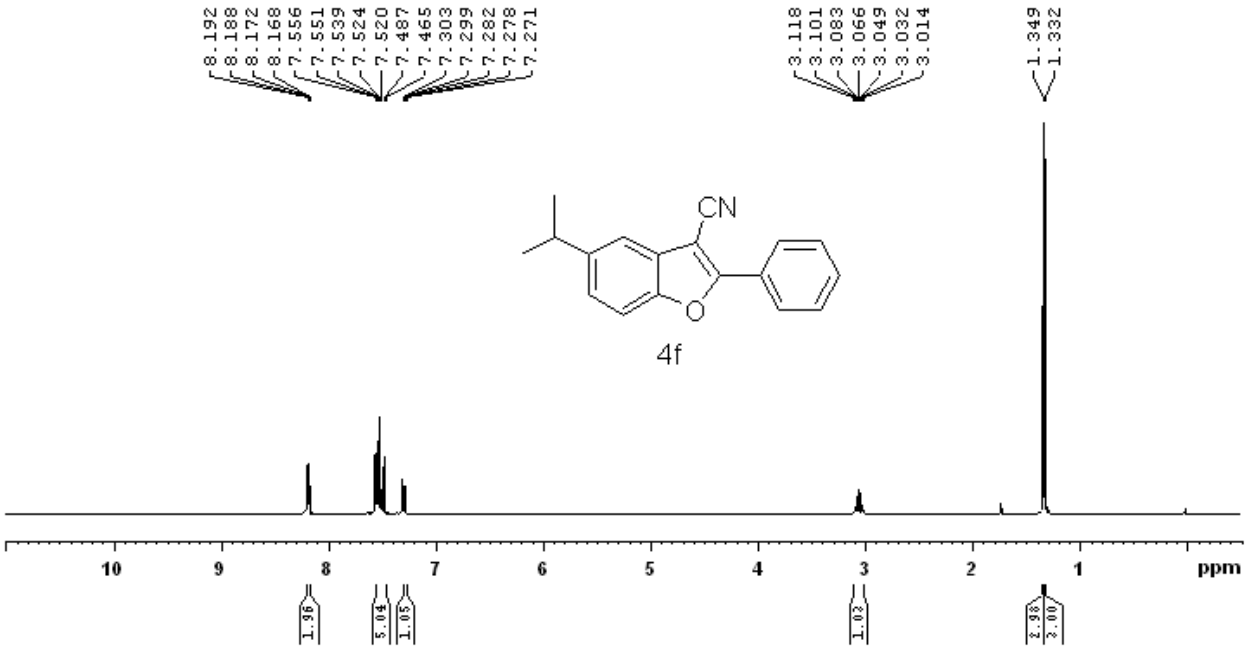


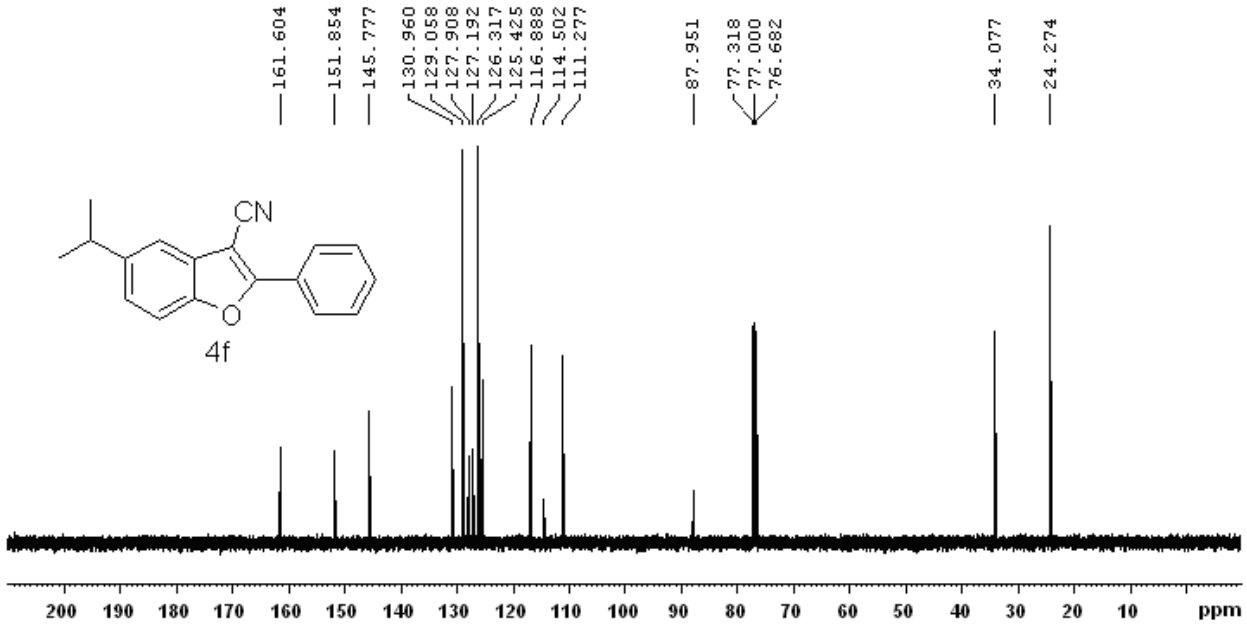


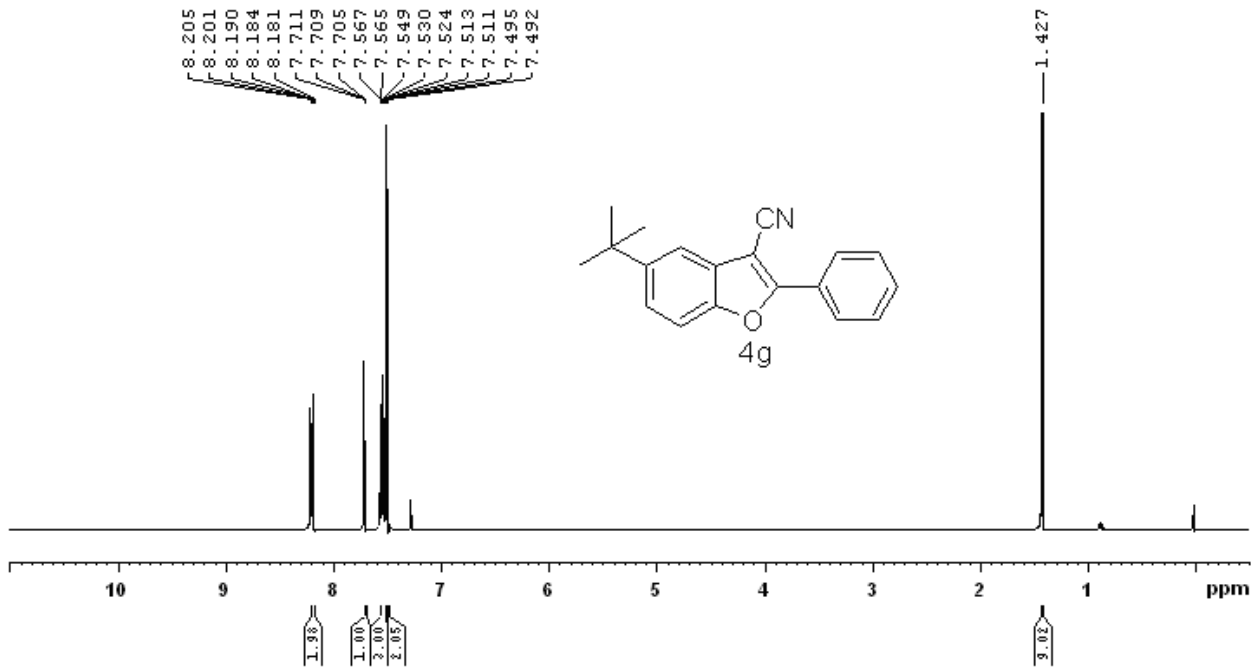


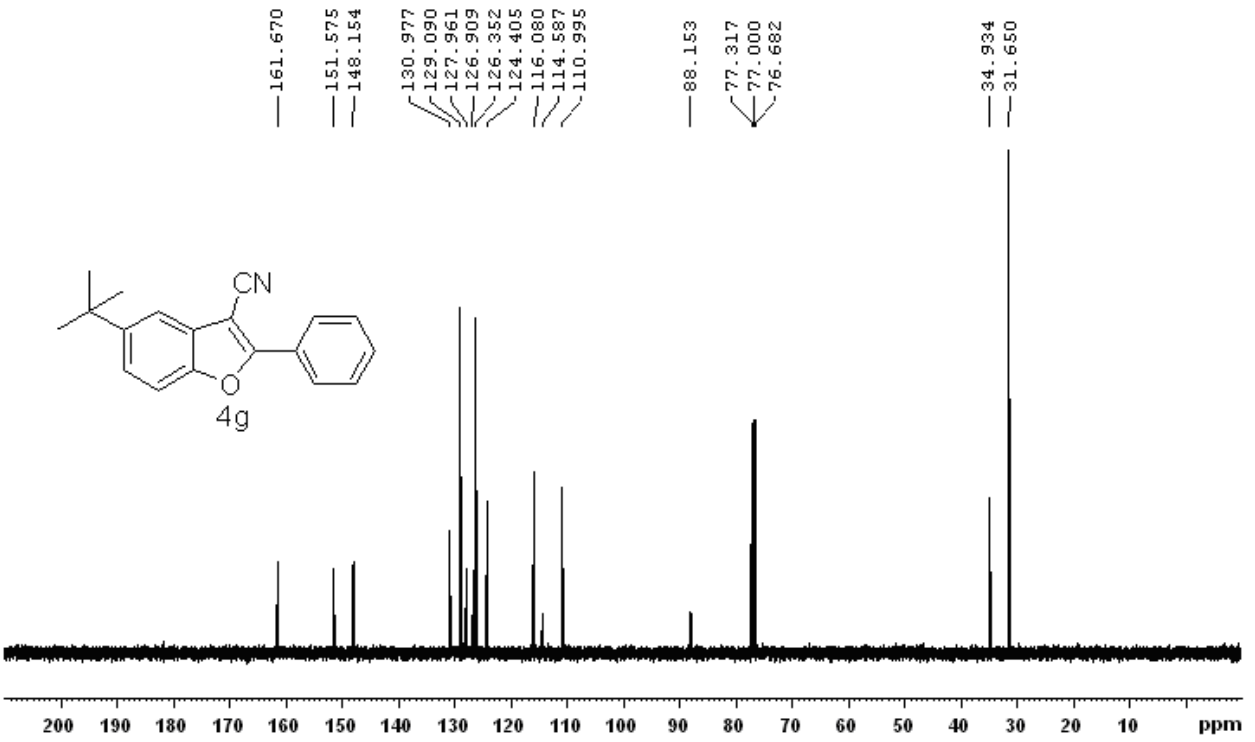


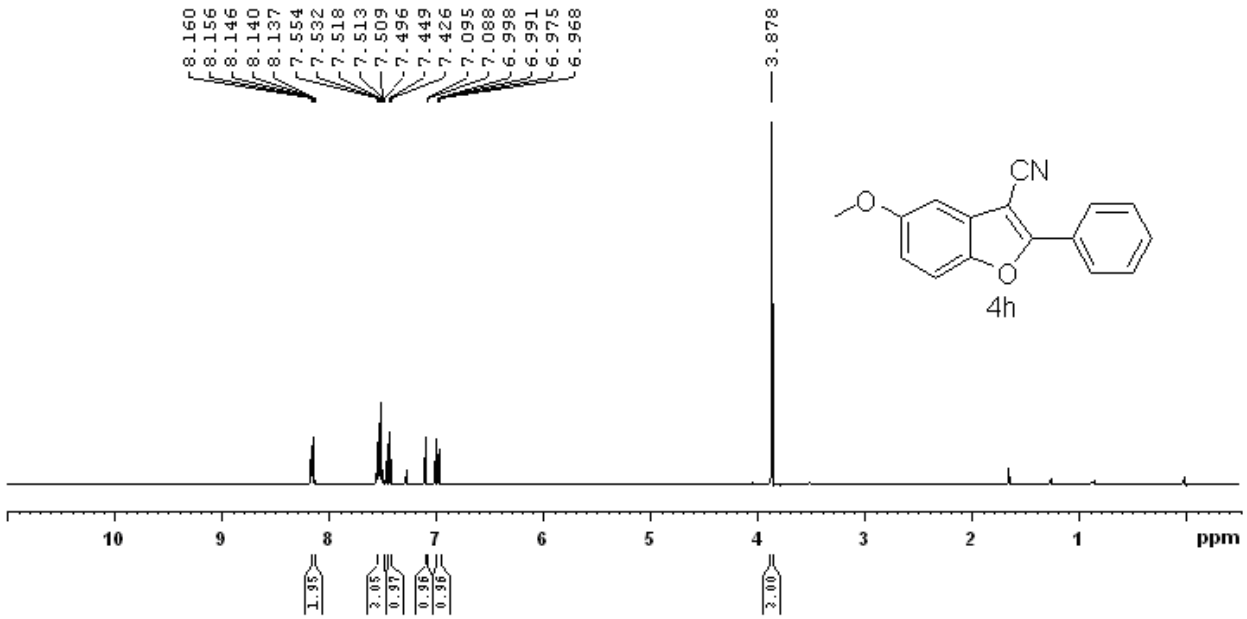


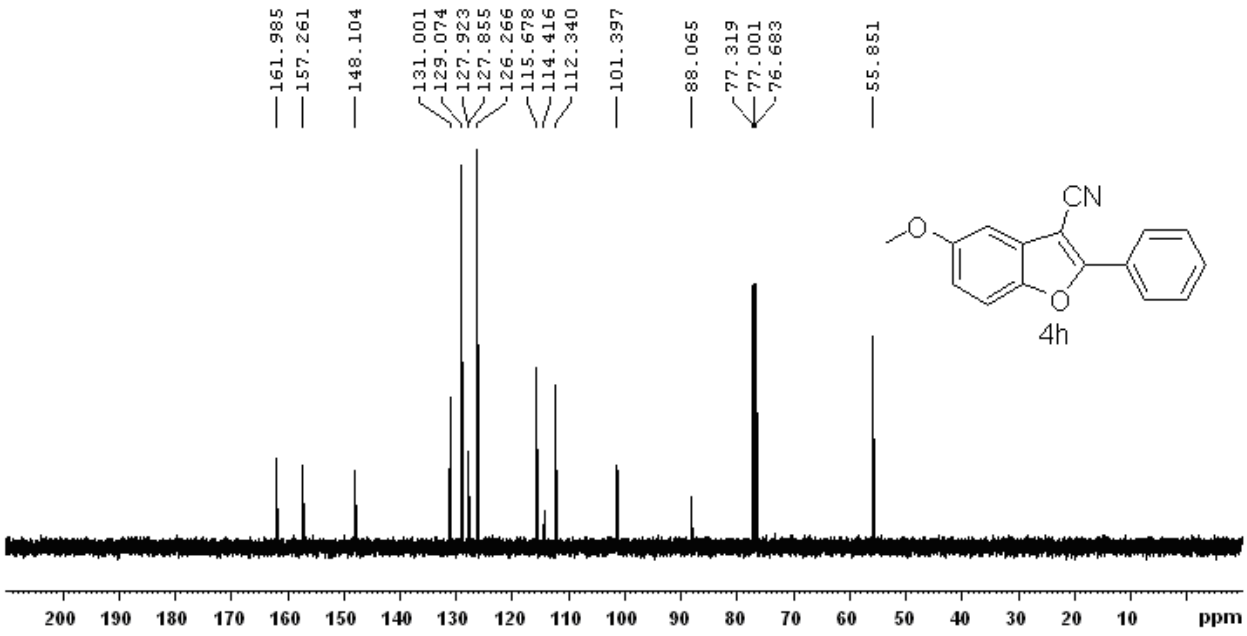


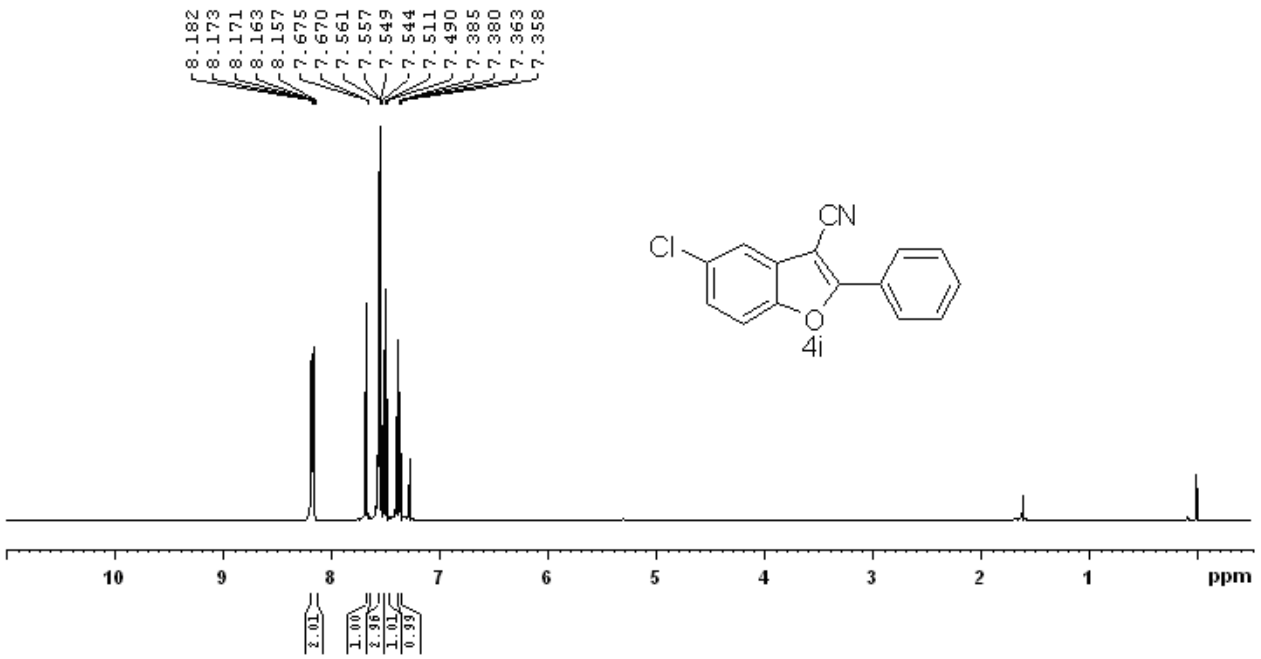


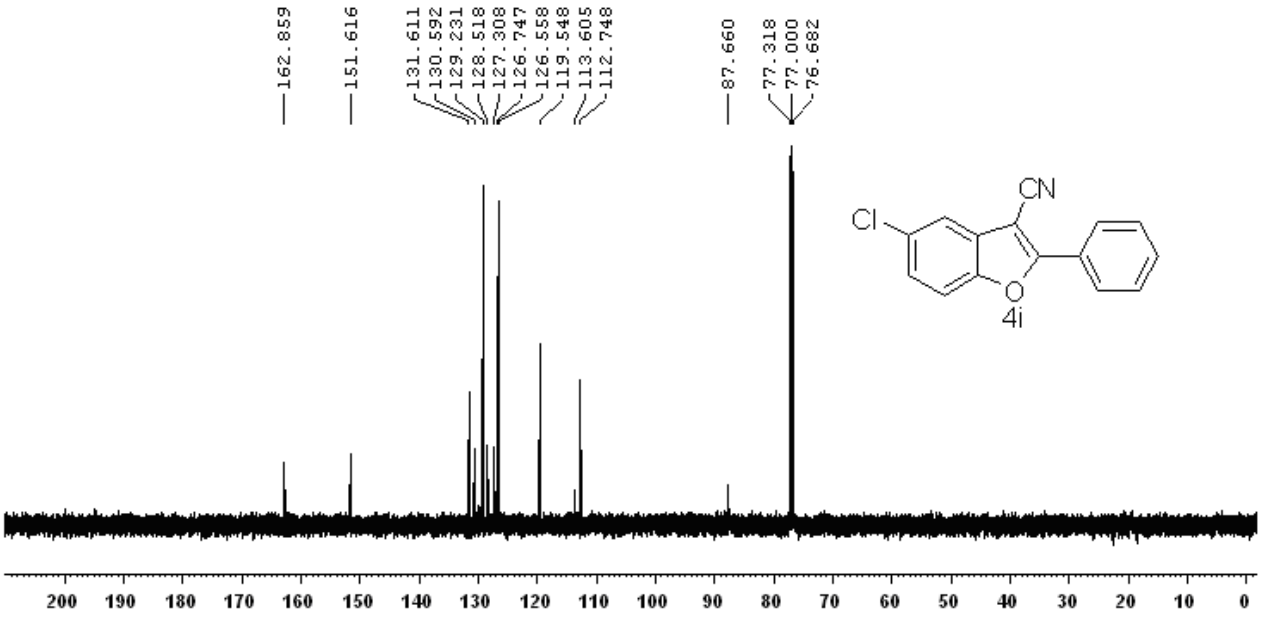


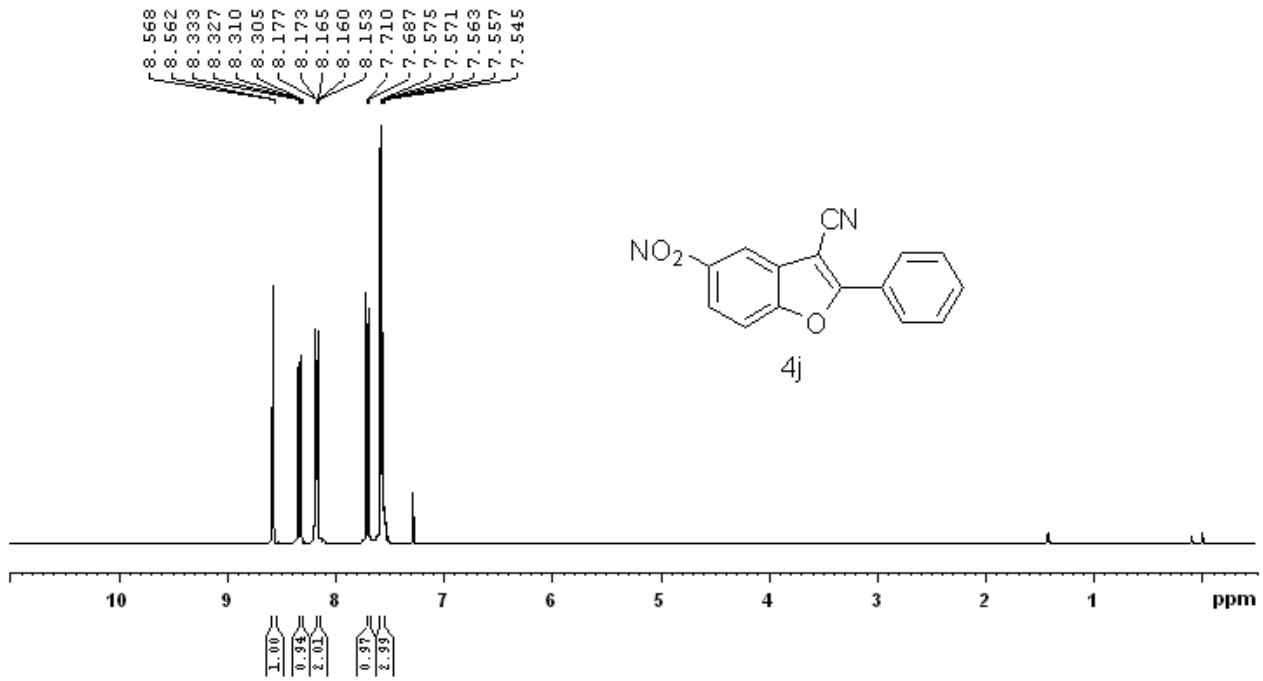


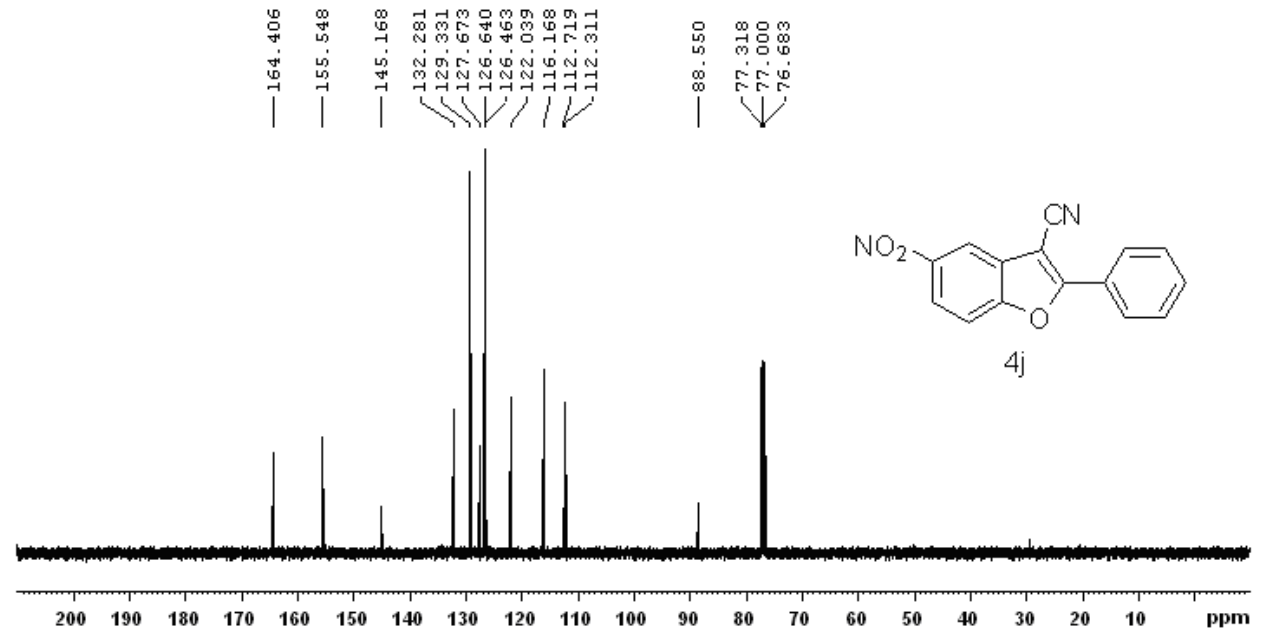


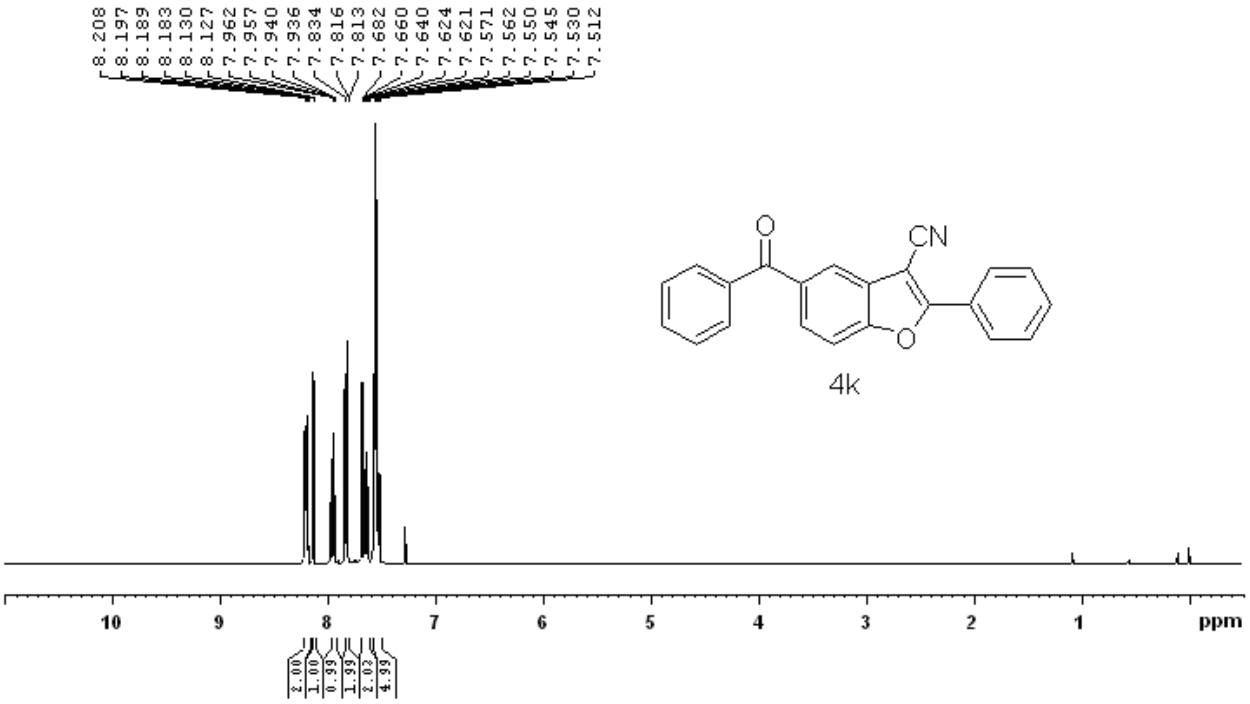


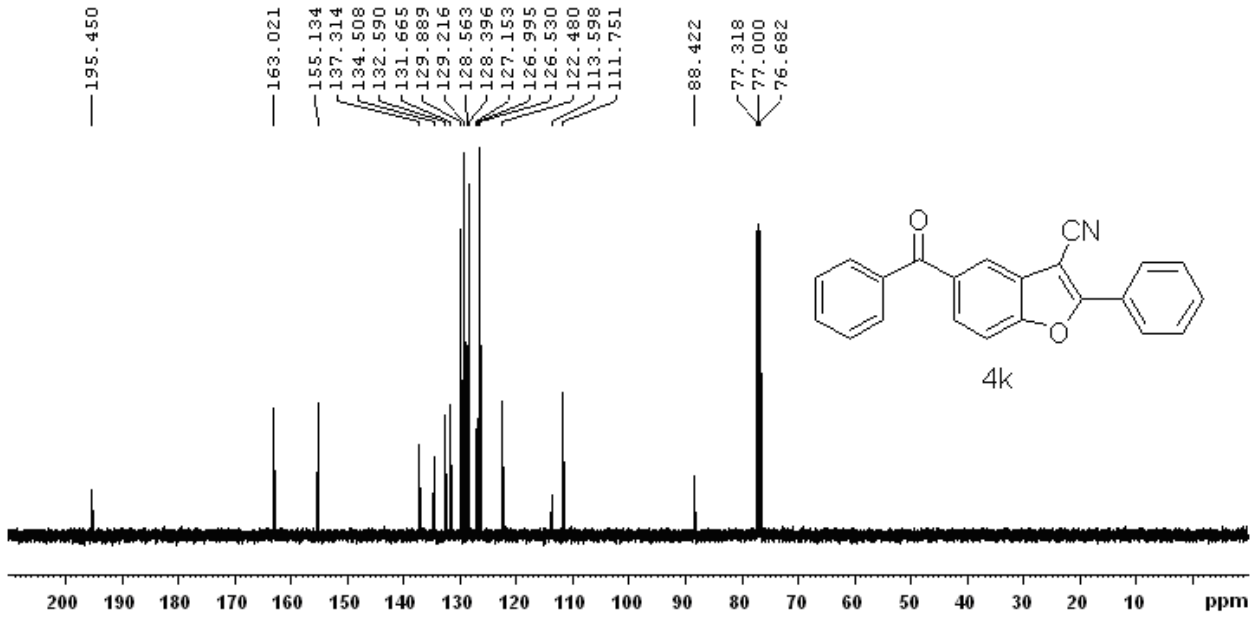


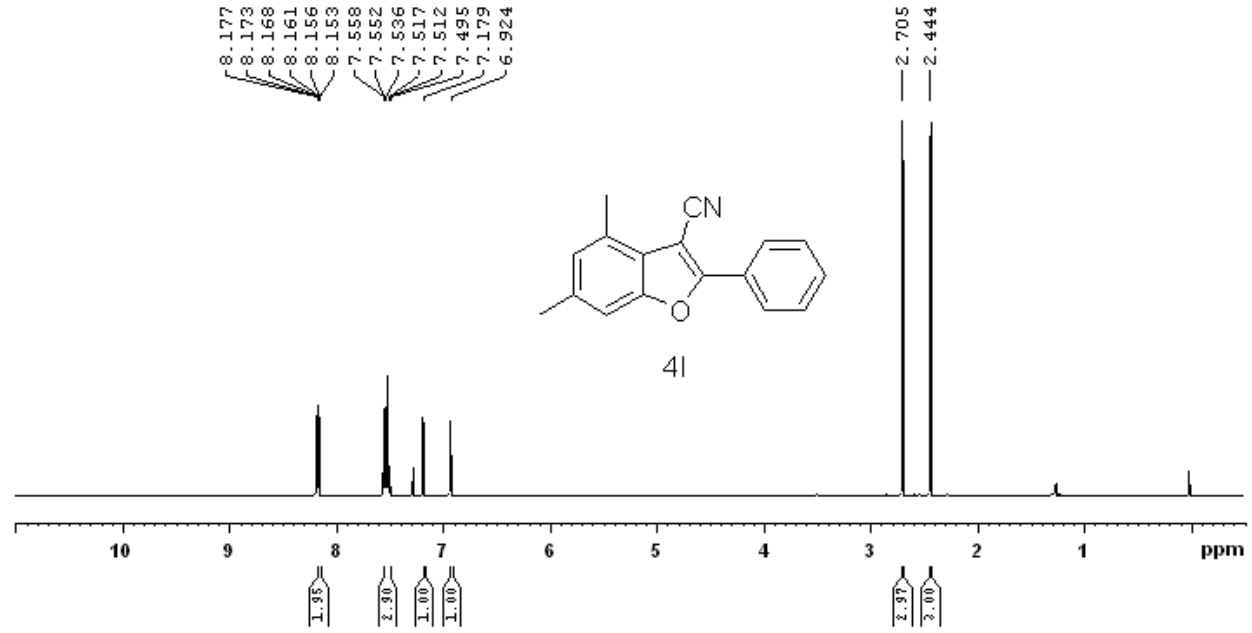


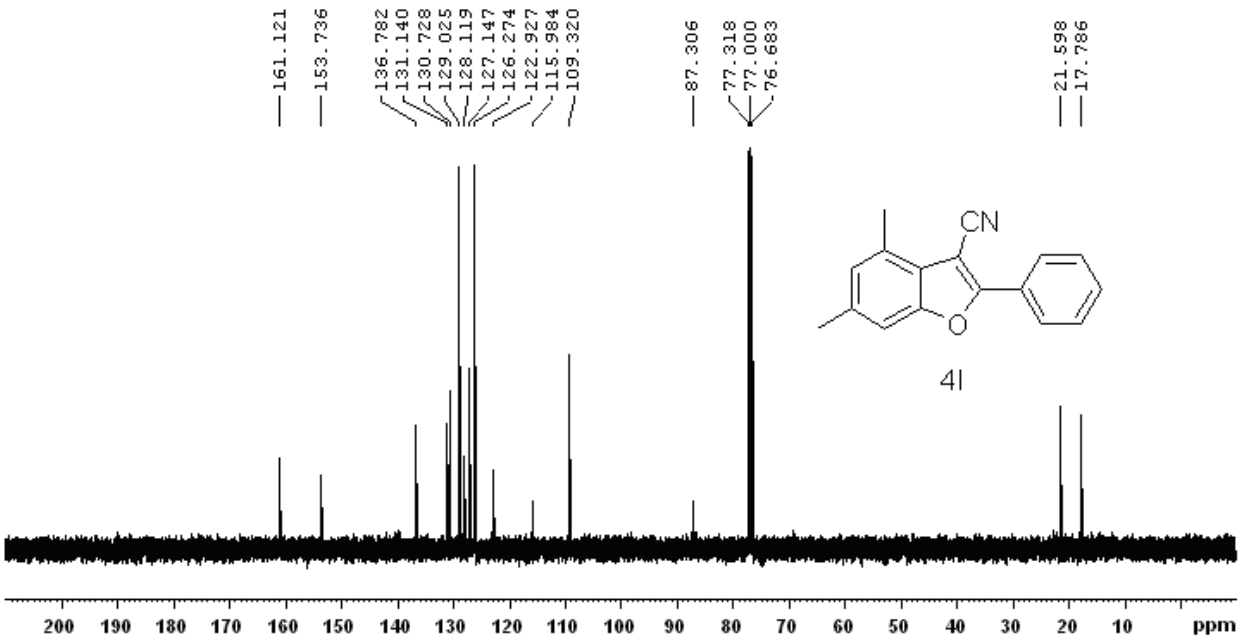


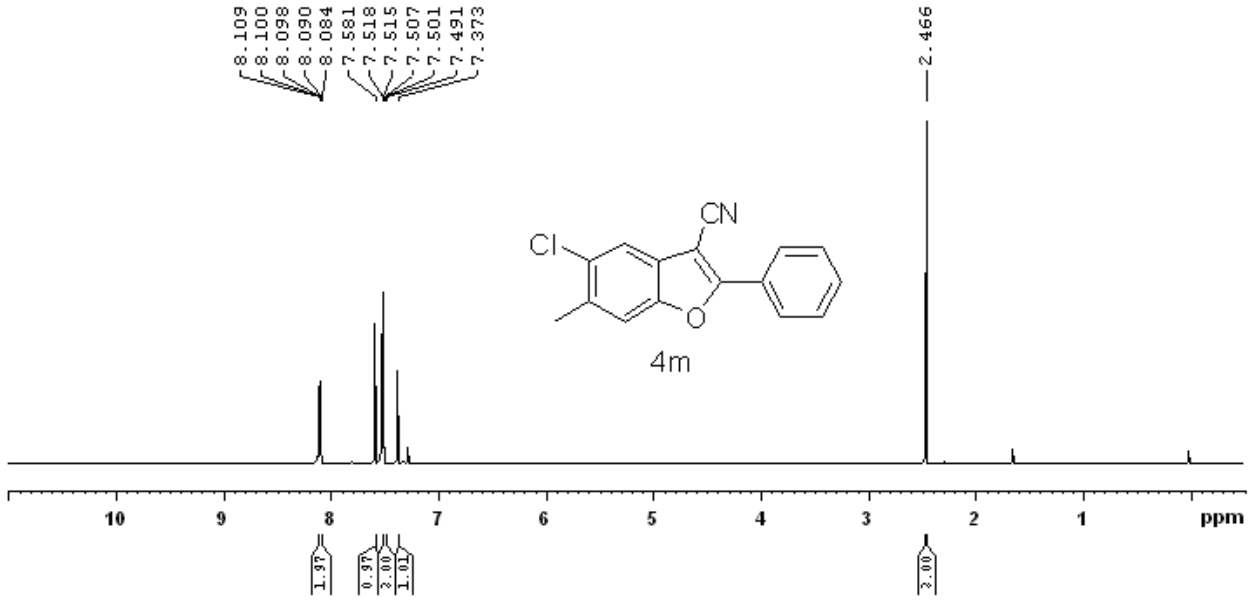


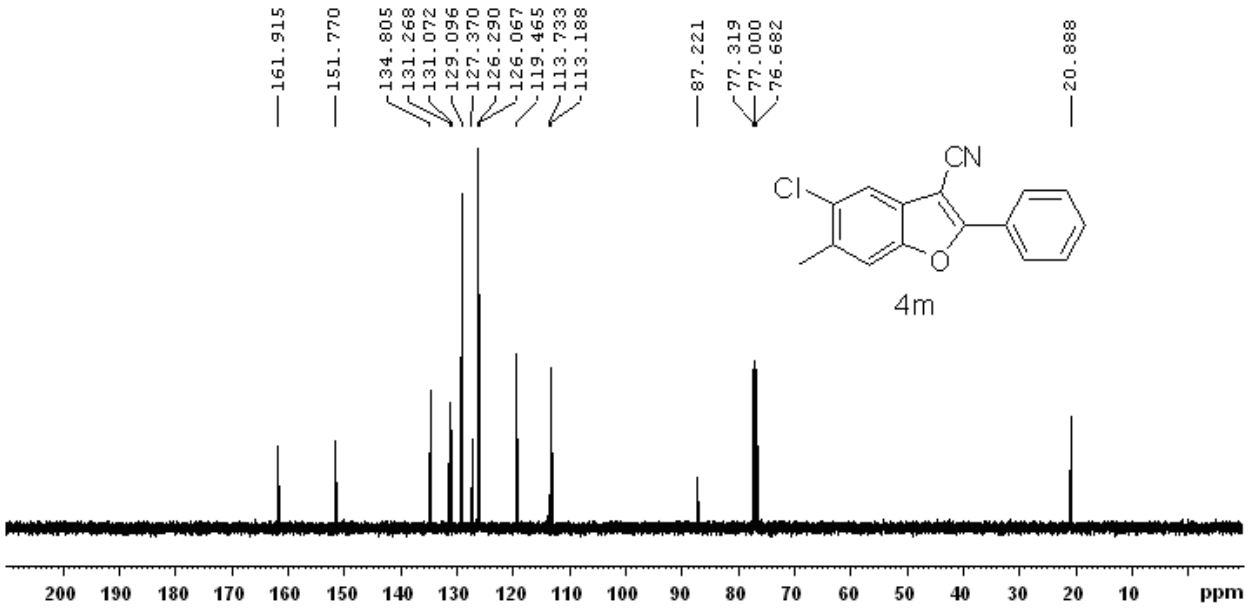


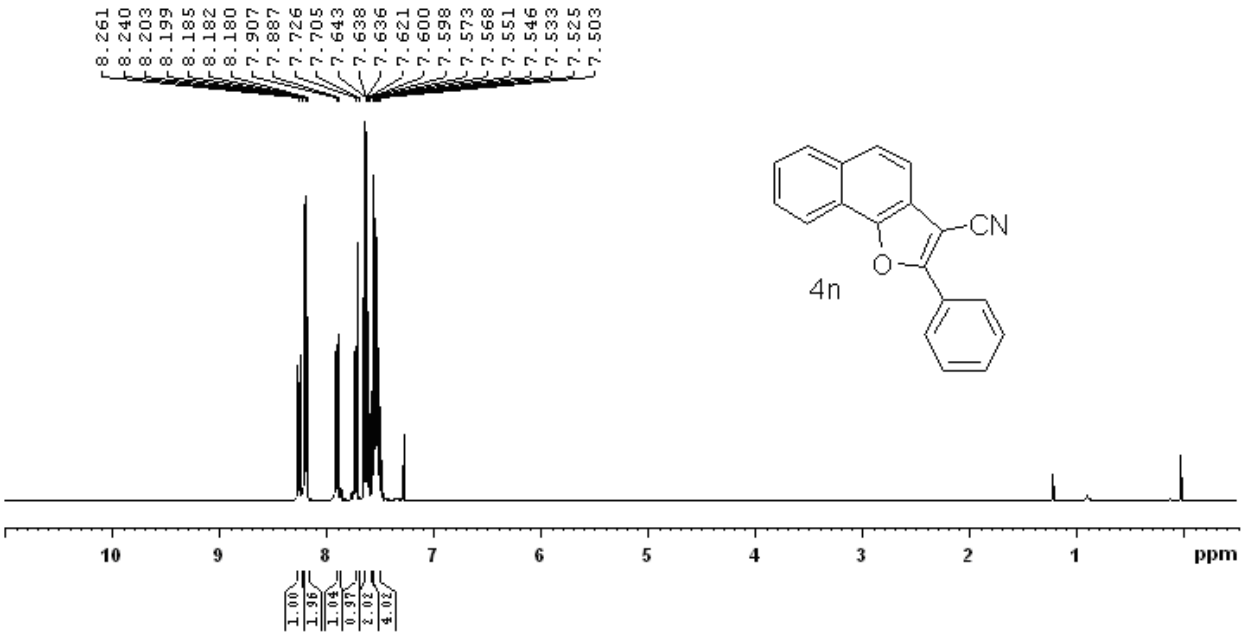


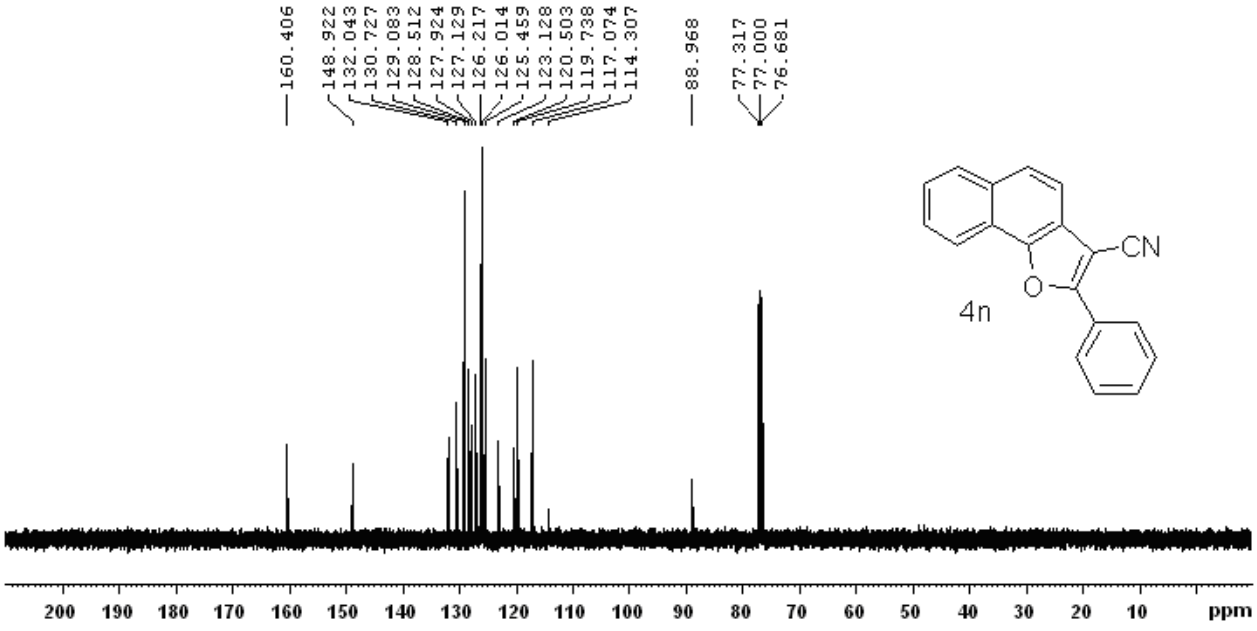


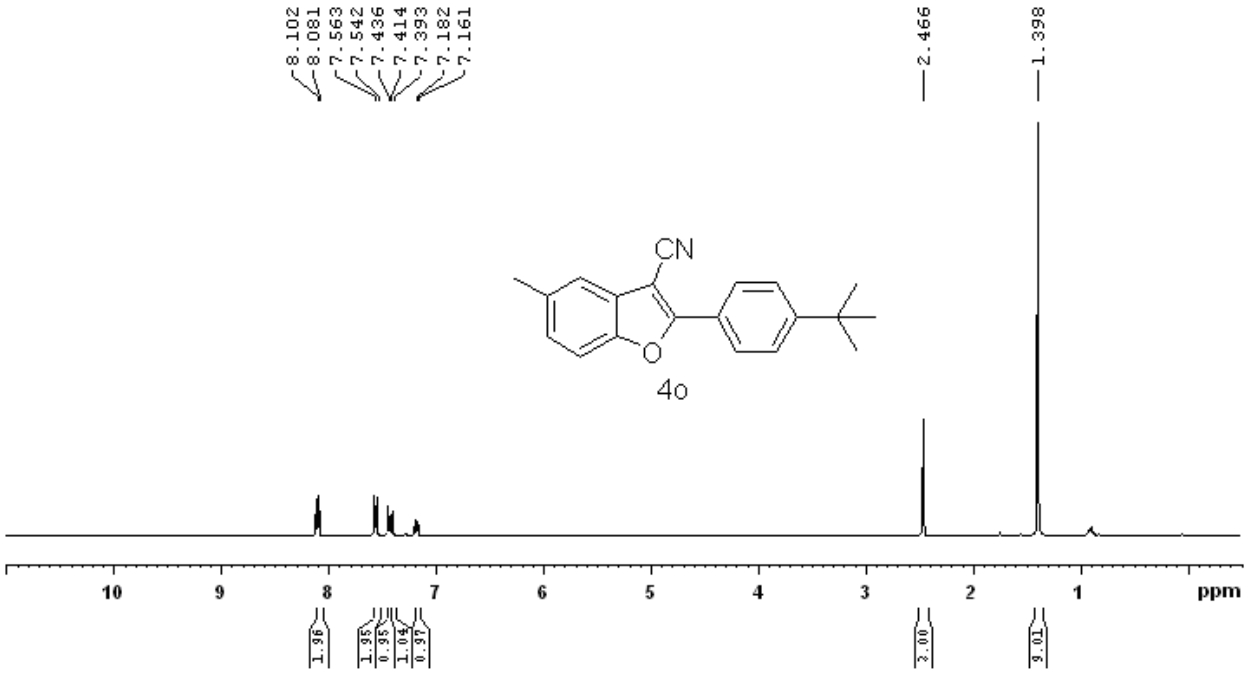


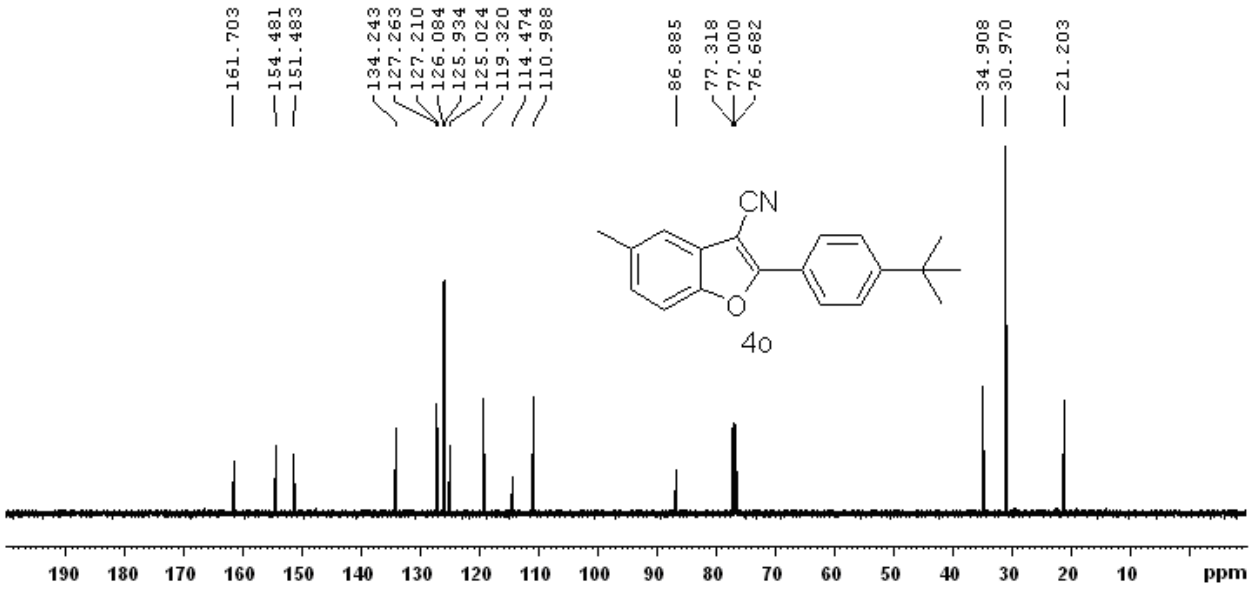


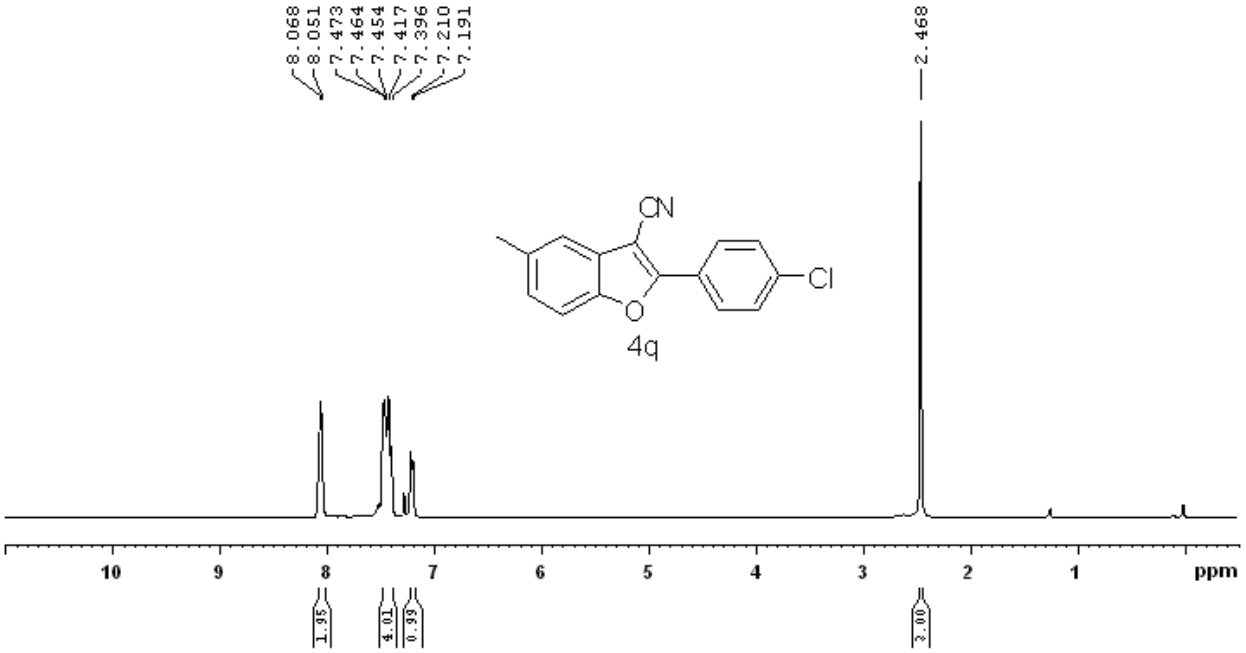


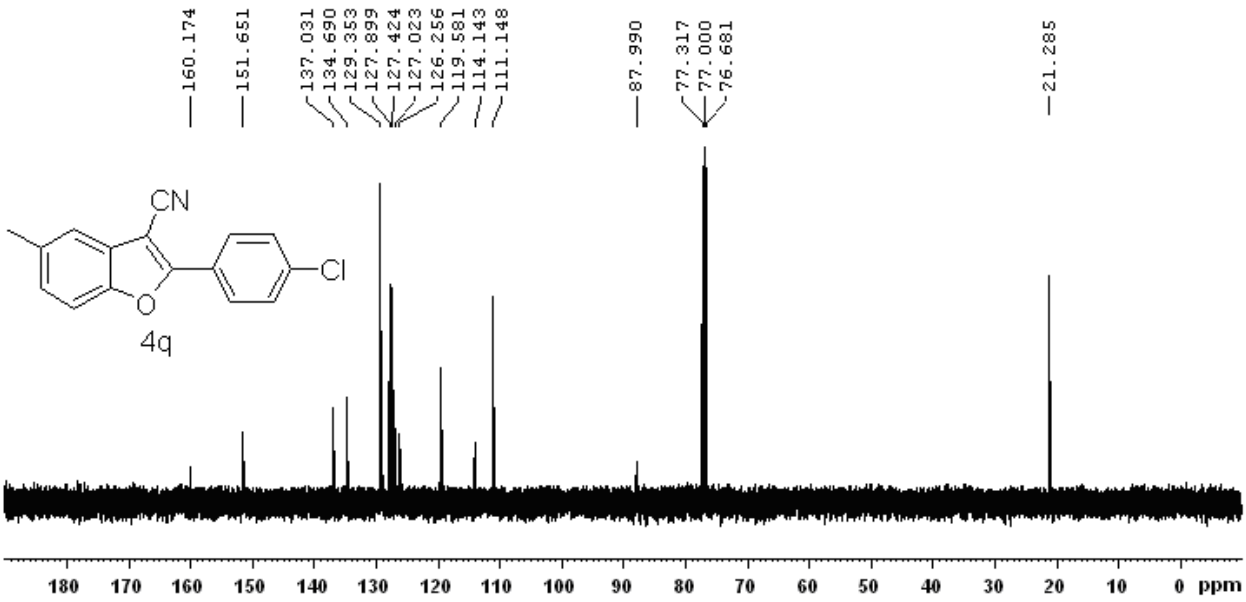


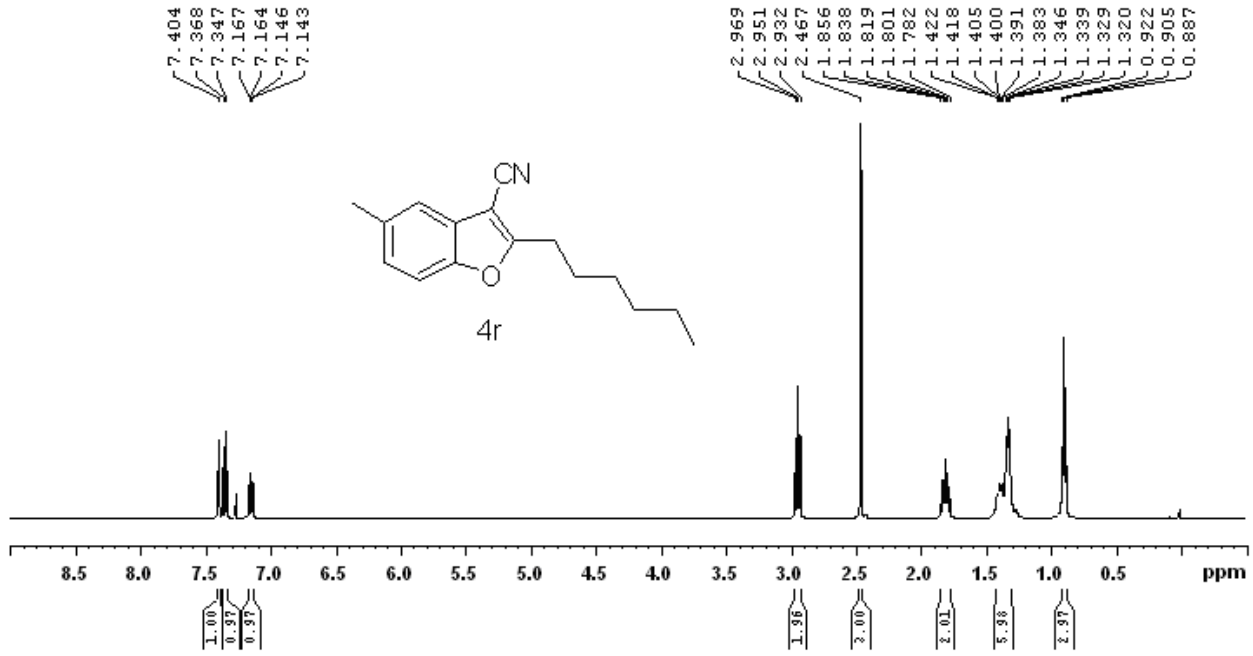


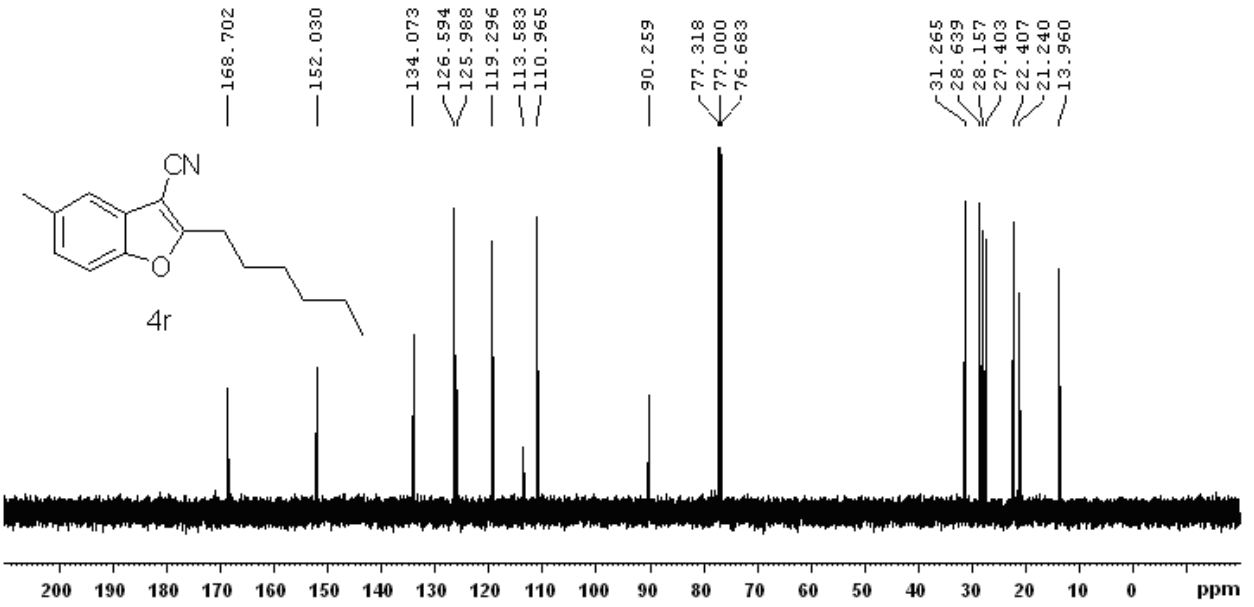


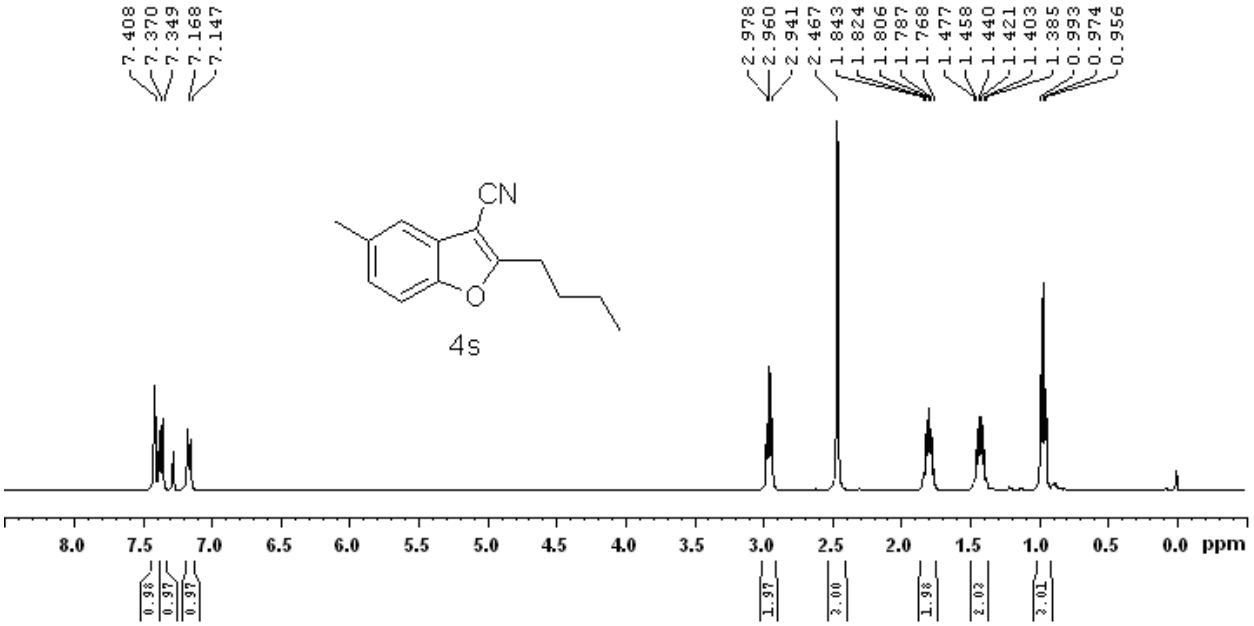


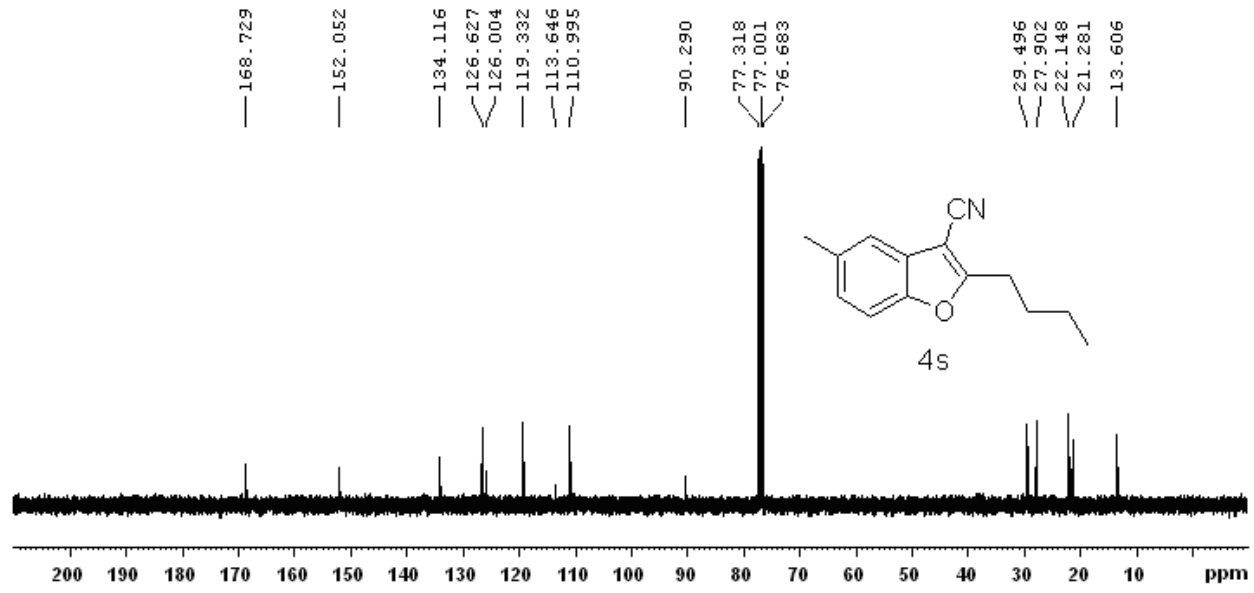


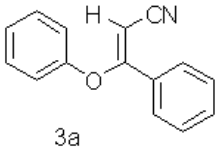












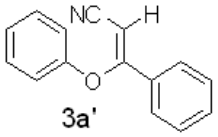
3a

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-T11-12-0S0912
Sample Serial Number: HBSF-D28-S1
Operator: Li
Date: 2011/12/15
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
295 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.0840	221.0841	-0.1	-0.5	11.0	12.1	C15 H11 N O
	221.0834	0.6	2.7	2.0	494.2	C7 H15 N3 O3 S
	221.0848	-0.8	-3.6	1.5	522.7	C9 H17 O4 S



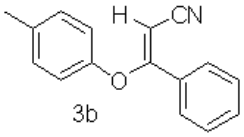
3a'

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-T11-12-0S0913
Sample Serial Number: HBSF-D28-S2
Operator: Li
Date: 2011/12/15
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
295 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
221.0842	221.0841	0.1	0.5	11.0	0.9	C15 H11 N O
	221.0848	-0.6	-2.7	1.5	331.9	C9 H17 O4 S
	221.0834	0.8	3.6	2.0	319.4	C7 H15 N3 O3 S

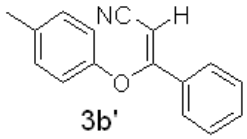


3b

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-T11-12-0S0918
Sample Serial Number:    HBSF-D28-S7
Operator:  Li
Date: 2011/12/15
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
325 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    Br: 0-1
Minimum:                                        -1.5
Maximum:                      2.0         5.0   50.0
Mass        Calc. Mass        mDa         PPM   DBE         i-FIT       Formula
235.0992    235.0991          0.1         0.4   2.0         737.5       C8  H17  N3  O3  S
            235.0997          -0.5        -2.1  11.0        85.0        C16  H13  N  O
            235.0984          0.8         3.4   11.5        45.0        C14  H11  N4
```

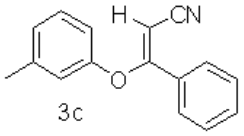


3b'

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-T11-12-0S0919
Sample Serial Number:    HBSF-D28-S8
Operator:  Li
Date: 2011/12/15
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
325 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    Br: 0-1
Minimum:                                        -1.5
Maximum:                      2.0         5.0   50.0
Mass        Calc. Mass        mDa         PPM   DBE         i-FIT       Formula
235.1001    235.1004          -0.3        -1.3  1.5         2773044.8   C10  H19  O4  S
            235.0997          0.4         1.7   11.0        2773015.3   C16  H13  N  O
            235.0991          1.0         4.3   2.0         2773042.8   C8  H17  N3  O3  S
```

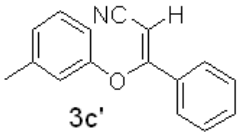


3c

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-T11-12-0S0916
Sample Serial Number:    HBSF-D28-S5
Operator:  Li
Date: 2011/12/15
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
325 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    Br: 0-1
Minimum:                                                -1.5
Maximum:                        2.0         5.0         50.0
Mass        Calc. Mass          mDa         PPM         DBE         i-FIT       Formula
235.0998    235.0997            0.1         0.4         11.0        31.4        C16  H13  N  O
            235.1004            -0.6        -2.6        1.5         333.5       C10  H19  O4  S
            235.0991            0.7         3.0         2.0         316.8       C8  H17  N3  O3  S
```

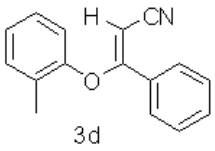


3c'

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-T11-12-0S0917
Sample Serial Number:    HBSF-D28-S6
Operator:  Li
Date: 2011/12/15
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
325 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    Br: 0-1
Minimum:                                                -1.5
Maximum:                        2.0         5.0         50.0
Mass        Calc. Mass          mDa         PPM         DBE         i-FIT       Formula
235.0999    235.0997            0.2         0.9         11.0        2.9         C16  H13  N  O
            235.1004            -0.5        -2.1        1.5         161.9       C10  H19  O4  S
            235.0991            0.8         3.4         2.0         153.9       C8  H17  N3  O3  S
```



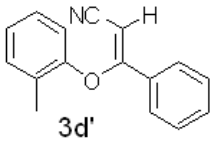
3d

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-T11-12-0S0914
Sample Serial Number: HBSF-D28-S3
Operator: Li
Date: 2011/12/15
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
325 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
235.0999	235.0997	0.2	0.9	11.0	29.3	C16 H13 N O
	235.1004	-0.5	-2.1	1.5	1062.4	C10 H19 O4 S
	235.0991	0.8	3.4	2.0	1018.7	C8 H17 N3 O3 S



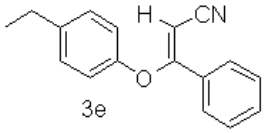
3d'

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-T11-12-0S0915
Sample Serial Number: HBSF-D28-S4
Operator: Li
Date: 2011/12/15
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
325 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
235.0994	235.0991	0.3	1.3	2.0	2777625.3	C8 H17 N3 O3 S
	235.0997	-0.3	-1.3	11.0	2776288.0	C16 H13 N O
	235.1004	-1.0	-4.3	1.5	2777644.5	C10 H19 O4 S
	235.0984	1.0	4.3	11.5	2775740.3	C14 H11 N4



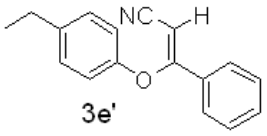
3e

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-T11-12-0S0962
Sample Serial Number: HBSF-LiD21-S1
Operator: Li
Date: 2011/12/26
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
386 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
249.1153	249.1154	-0.1	-0.4	11.0	6.7	C17 H15 N O
	249.1147	0.6	2.4	2.0	269.7	C9 H19 N3 O3 S
	249.1159	-0.6	-2.4	6.5	2310.1	C14 H18 N2 Cl
	249.1161	-0.8	-3.2	1.5	285.9	C11 H21 O4 S



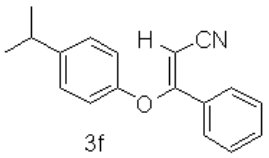
3e'

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-T11-12-0S0963
Sample Serial Number: HBSF-LiD21-S2
Operator: Li
Date: 2011/12/26
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
386 formula(e) evaluated with 5 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
249.1152	249.1154	-0.2	-0.8	11.0	10.1	C17 H15 N O
	249.1147	0.5	2.0	2.0	220.7	C9 H19 N3 O3 S
	249.1159	-0.7	-2.8	6.5	1147.1	C14 H18 N2 Cl
	249.1161	-0.9	-3.6	1.5	235.4	C11 H21 O4 S
	249.1140	1.2	4.8	11.5	3.6	C15 H13 N4



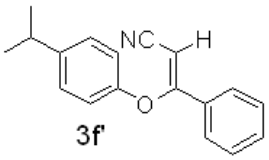
3f

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-T11-12-0S0964
Sample Serial Number: HBSF-LiD21-S3
Operator: Li
Date: 2011/12/26
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
414 formula(e) evaluated with 5 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
263.1307	263.1304	0.3	1.1	2.0	788.6	C10 H21 N3 O3 S
	263.1310	-0.3	-1.1	11.0	5.9	C18 H17 N O
	263.1315	-0.8	-3.0	6.5	7713.5	C15 H20 N2 Cl
	263.1317	-1.0	-3.8	1.5	823.2	C12 H23 O4 S
	263.1297	1.0	3.8	11.5	11.3	C16 H15 N4



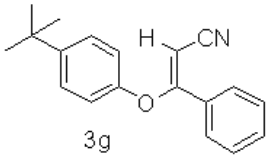
3f'

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-T11-12-0S0965
Sample Serial Number: HBSF-LiD21-S4
Operator: Li
Date: 2011/12/26
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
414 formula(e) evaluated with 5 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
263.1309	263.1310	-0.1	-0.4	11.0	5.1	C18 H17 N O
	263.1304	0.5	1.9	2.0	174.4	C10 H21 N3 O3 S
	263.1315	-0.6	-2.3	6.5	1125.6	C15 H20 N2 Cl
	263.1317	-0.8	-3.0	1.5	184.6	C12 H23 O4 S
	263.1297	1.2	4.6	11.5	2.6	C16 H15 N4



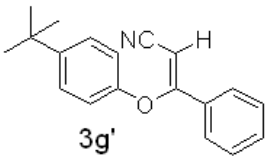
3g

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-T11-12-0S0968
Sample Serial Number: HBSF-LiD21-S7
Operator: Li
Date: 2011/12/26
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
434 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
277.1473	277.1474	-0.1	-0.4	1.5	2776115.8	C13 H25 O4 S
	277.1472	0.1	0.4	6.5	2776279.3	C16 H22 N2 Cl
	277.1467	0.6	2.2	11.0	2775363.0	C19 H19 N O
	277.1460	1.3	4.7	2.0	2776100.0	C11 H23 N3 O3 S



3g'

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

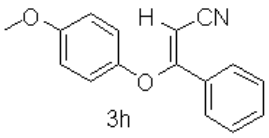
Card Serial Number: GCT-P-T11-12-0S0969

Sample Serial Number: HBSF-LiD21-S8

Operator: Li

Date: 2011/12/26
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
434 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
277.1469	277.1467	0.2	0.7	11.0	2775578.3	C19 H19 N O
	277.1472	-0.3	-1.1	6.5	2776511.5	C16 H22 N2 Cl
	277.1474	-0.5	-1.8	1.5	2776347.5	C13 H25 O4 S
	277.1460	0.9	3.2	2.0	2776332.3	C11 H23 N3 O3 S

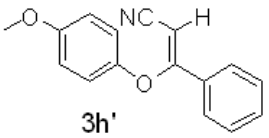


3h

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-T11-12-OS0970
Sample Serial Number:    HBSF-LiD21-S9
Operator:  Li
Date: 2011/12/26
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
394 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:                        2.0         5.0         50.0
Mass        Calc. Mass          mDa         PPM         DBE         i-FIT       Formula
251.0949    251.0951            -0.2        -0.8        6.5         3167.8      C13  H16  N2  O  Cl
            251.0946            0.3         1.2         11.0        1.1         C16  H13  N  O2
            251.0953            -0.4        -1.6        1.5         313.7       C10  H19  O5  S
            251.0940            0.9         3.6         2.0         310.6       C8  H17  N3  O4  S
```

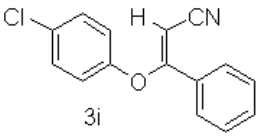


3h'

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-T11-12-OS0971
Sample Serial Number:    HBSF-LiD21-S10
Operator:  Li
Date: 2011/12/26
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
394 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:                        2.0         5.0         50.0
Mass        Calc. Mass          mDa         PPM         DBE         i-FIT       Formula
251.0948    251.0946            0.2         0.8         11.0        2773024.5   C16  H13  N  O2
            251.0951            -0.3        -1.2        6.5         2773065.3   C13  H16  N2  O  Cl
            251.0953            -0.5        -2.0        1.5         2773027.0   C10  H19  O5  S
            251.0940            0.8         3.2         2.0         2773025.5   C8  H17  N3  O4  S
```



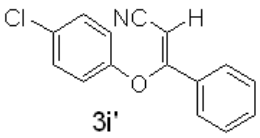
3i

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-T11-12-0S0974
Sample Serial Number: HBSF-LiD21-S13
Operator: Li
Date: 2011/12/26
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
402 formula(e) evaluated with 5 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
255.0452	255.0451	0.1	0.4	11.0	0.5	C15 H10 N O Cl
	255.0446	0.6	2.4	15.5	387.5	C18 H7 O2
	255.0458	-0.6	-2.4	1.5	38.0	C9 H16 O4 S Cl
	255.0444	0.8	3.1	2.0	50.3	C7 H14 N3 O3 S Cl
	255.0440	1.2	4.7	6.5	307.1	C10 H11 N2 O4 S



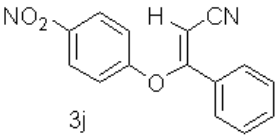
3i'

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-T11-12-0S0975
Sample Serial Number: HBSF-LiD21-S14
Operator: Li
Date: 2011/12/26
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
402 formula(e) evaluated with 6 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
255.0450	255.0451	-0.1	-0.4	11.0	0.3	C15 H10 N O Cl
	255.0446	0.4	1.6	15.5	227.5	C18 H7 O2
	255.0444	0.6	2.4	2.0	24.3	C7 H14 N3 O3 S Cl
	255.0458	-0.8	-3.1	1.5	17.8	C9 H16 O4 S Cl
	255.0440	1.0	3.9	6.5	175.9	C10 H11 N2 O4 S
	255.0437	1.3	5.1	11.5	1.1	C13 H8 N4 Cl

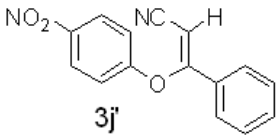


3j

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-T11-12-0S0978
Sample Serial Number:    HBSF-LiD21-S17
Operator:  Li
Date: 2011/12/26
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
420 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:                      2.0         5.0     50.0
Mass        Calc. Mass        mDa         PPM     DBE         i-FIT         Formula
266.0692    266.0691          0.1         0.4     12.0        2773019.5     C15  H10  N2  O3
            266.0696          -0.4        -1.5    7.5         2773077.0     C12  H13  N3  O2  Cl
            266.0698          -0.6        -2.3    2.5         2773030.8     C9  H16  N  O6  S
            266.0685          0.7         2.6     3.0         2773029.3     C7  H14  N4  O5  S
```

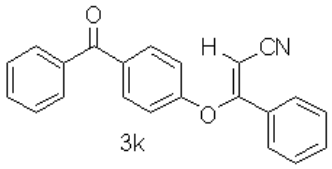


3j'

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-T11-12-0S0979
Sample Serial Number:    HBSF-LiD21-S18
Operator:  Li
Date: 2011/12/26
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
420 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:                      2.0         5.0     50.0
Mass        Calc. Mass        mDa         PPM     DBE         i-FIT         Formula
266.0689    266.0691          -0.2        -0.8    12.0        2773092.5     C15  H10  N2  O3
            266.0685          0.4         1.5     3.0         2773309.5     C7  H14  N4  O5  S
            266.0696          -0.7        -2.6    7.5         2773436.5     C12  H13  N3  O2  Cl
            266.0698          -0.9        -3.4    2.5         2773316.8     C9  H16  N  O6  S
```

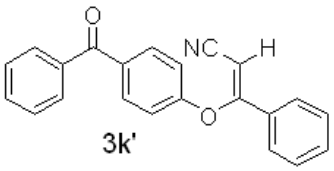


3k

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-T11-12-0S0980
Sample Serial Number:    HBSF-LiD21-S19
Operator:  Li
Date: 2011/12/26
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
514 formula(e) evaluated with 7 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:                          2.0          5.0        50.0
Mass        Calc. Mass        mDa          PPM          DBE          i-FIT        Formula
325.1104    325.1103          0.1          0.3          16.0         6.1          C22  H15  N  O2
            325.1101          0.3          0.9          2.5          791.0        C11  H22  N4  O3  S  Cl
            325.1108          -0.4         -1.2         11.5         735.2        C19  H18  N2  O  Cl
            325.1110          -0.6         -1.8         6.5          86.0         C16  H21  O5  S
            325.1096          0.8          2.5          7.0          79.2         C14  H19  N3  O4  S
            325.1115          -1.1         -3.4         2.0          790.3        C13  H24  N  O4  S  Cl
            325.1089          1.5          4.6          16.5         2.4          C20  H13  N4  O
```

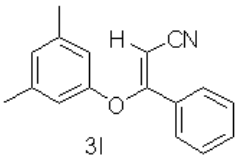


3k'

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-T11-12-0S0981
Sample Serial Number:    HBSF-LiD21-S20
Operator:  Li
Date: 2011/12/26
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
514 formula(e) evaluated with 6 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:                          2.0          5.0        50.0
Mass        Calc. Mass        mDa          PPM          DBE          i-FIT        Formula
325.1106    325.1108          -0.2         -0.6         11.5         2773154.0    C19  H18  N2  O  Cl
            325.1103          0.3          0.9          16.0         2773040.0    C22  H15  N  O2
            325.1110          -0.4         -1.2         6.5          2773083.3    C16  H21  O5  S
            325.1101          0.5          1.5          2.5          2773156.3    C11  H22  N4  O3  S  Cl
            325.1115          -0.9         -2.8         2.0          2773156.3    C13  H24  N  O4  S  Cl
            325.1096          1.0          3.1          7.0          2773079.5    C14  H19  N3  O4  S
```

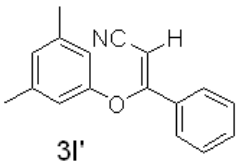


3l

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-T11-12-OS0966
Sample Serial Number:    HBSF-LiD21-S5
Operator:  Li
Date: 2011/12/26
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
386 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:                    2.0     5.0   50.0
Mass        Calc. Mass      mDa     PPM   DBE      i-FIT      Formula
249.1158    249.1159        -0.1    -0.4  6.5      2107.6     C14  H18  N2  Cl
            249.1161        -0.3    -1.2  1.5      243.5      C11  H21  O4  S
            249.1154        0.4     1.6   11.0     6.1        C17  H15  N  O
            249.1147        1.1     4.4   2.0      230.0      C9  H19  N3  O3  S
```

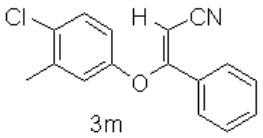


3l'

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-T11-12-OS0967
Sample Serial Number:    HBSF-LiD21-S6
Operator:  Li
Date: 2011/12/26
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
386 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:                    2.0     5.0   50.0
Mass        Calc. Mass      mDa     PPM   DBE      i-FIT      Formula
249.1155    249.1154        0.1     0.4   11.0     7.0        C17  H15  N  O
            249.1159        -0.4    -1.6  6.5      1080.6     C14  H18  N2  Cl
            249.1161        -0.6    -2.4  1.5      197.4      C11  H21  O4  S
            249.1147        0.8     3.2   2.0      185.2      C9  H19  N3  O3  S
```



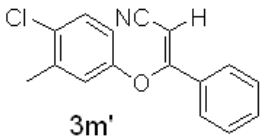
3m

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-T11-12-0S0976
Sample Serial Number: HBSF-LiD21-S15
Operator: Li
Date: 2011/12/26
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
420 formula(e) evaluated with 5 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
269.0612	269.0614	-0.2	-0.7	1.5	209.3	C10 H18 O4 S Cl
	269.0607	0.5	1.9	11.0	32.4	C16 H12 N O Cl
	269.0603	0.9	3.3	15.5	1092.3	C19 H9 O2
	269.0623	-1.1	-4.1	11.0	873.6	C14 H11 N3 O S
	269.0601	1.1	4.1	2.0	250.7	C8 H16 N3 O3 S Cl



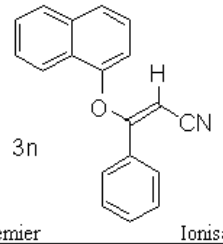
3m'

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-T11-12-0S0977
Sample Serial Number: HBSF-LiD21-S16
Operator: Li
Date: 2011/12/26
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
420 formula(e) evaluated with 6 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
269.0605	269.0603	0.2	0.7	15.5	169.8	C19 H9 O2
	269.0607	-0.2	-0.7	11.0	4.5	C16 H12 N O Cl
	269.0601	0.4	1.5	2.0	35.4	C8 H16 N3 O3 S Cl
	269.0614	-0.9	-3.3	1.5	29.4	C10 H18 O4 S Cl
	269.0596	0.9	3.3	6.5	146.7	C11 H13 N2 O4 S
	269.0594	1.1	4.1	11.5	7.2	C14 H10 N4 Cl



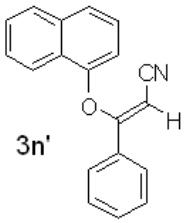
3n

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-T11-12-0S0972
Sample Serial Number: HBSF-LiD21-S11
Operator: Li
Date: 2011/12/26
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
426 formula(e) evaluated with 6 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
271.1001	271.1002	-0.1	-0.4	9.5	3893.2	C16 H16 N2 Cl
	271.1004	-0.3	-1.1	4.5	411.3	C13 H19 O4 S
	271.0997	0.4	1.5	14.0	1.8	C19 H13 N O
	271.0996	0.5	1.8	0.5	4200.6	C8 H20 N4 O2 S Cl
	271.1009	-0.8	-3.0	0.0	4195.8	C10 H22 N O3 S Cl
	271.0991	1.0	3.7	5.0	392.5	C11 H17 N3 O3 S



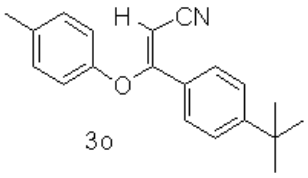
3n'

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-T11-12-0S0973
Sample Serial Number: HBSF-LiD21-S12
Operator: Li
Date: 2011/12/26
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
426 formula(e) evaluated with 6 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
271.0995	271.0996	-0.1	-0.4	0.5	1643.8	C8 H20 N4 O2 S Cl
	271.0997	-0.2	-0.7	14.0	1.2	C19 H13 N O
	271.0991	0.4	1.5	5.0	141.4	C11 H17 N3 O3 S
	271.1002	-0.7	-2.6	9.5	1508.4	C16 H16 N2 Cl
	271.1004	-0.9	-3.3	4.5	143.7	C13 H19 O4 S
	271.0984	1.1	4.1	14.5	6.3	C17 H11 N4



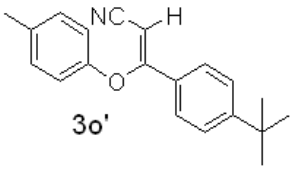
3o

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-T12-03-0S0203
Sample Serial Number: HBSF-LM15-S5
Operator: Li
Date: 2012/03/23
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
232 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: 0-2 O: 0-6 Cl: 0-1 I: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
291.1626	291.1628	-0.2	-0.7	6.5	3437.0	C17 H24 N2 Cl
	291.1623	0.3	1.0	11.0	6.7	C20 H21 N O



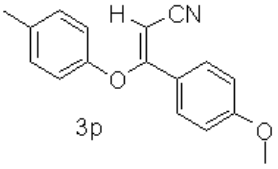
3o'

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-T12-03-0S0204
Sample Serial Number: HBSF-LM15-S6
Operator: Li
Date: 2012/03/23
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
232 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: 0-2 O: 0-6 Cl: 0-1 I: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
291.1622	291.1623	-0.1	-0.3	11.0	12.5	C20 H21 N O
	291.1628	-0.6	-2.1	6.5	958.2	C17 H24 N2 Cl



3p

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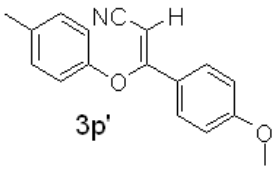
Chinese Academic of Sciences
High Resolution MS Data Report

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

```
Card Serial Number:   GCT-P-T12-03-0S0211
Sample Serial Number:    HBSF-LM15-S13
Operator:  Li
Date: 2012/03/23
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
201 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: 0-2    O: 0-6    Cl: 0-1    I: 0-1

Minimum:                                          -1.5
Maximum:                        2.0         5.0   50.0
Mass        Calc. Mass          mDa         PPM   DBE         i-FIT       Formula
265.1105    265.1103            0.2         0.8   11.0        1.7         C17  H15  N  O2
            265.1108            -0.3        -1.1  6.5         4528.0      C14  H18  N2  O  Cl
```



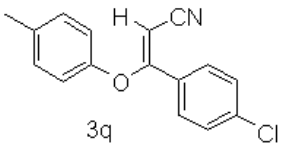
3p'

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-T12-03-0S0212
Sample Serial Number:    HBSF-LM15-S14
Operator:  Li
Date: 2012/03/23
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
201 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: 0-2    O: 0-6    Cl: 0-1    I: 0-1

Minimum:                                          -1.5
Maximum:                        2.0         5.0   50.0
Mass        Calc. Mass          mDa         PPM   DBE         i-FIT       Formula
265.1102    265.1103            -0.1        -0.4  11.0        8.5         C17  H15  N  O2
            265.1108            -0.6        -2.3  6.5         286.0       C14  H18  N2  O  Cl
```

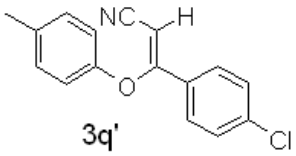


3q

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-T12-03-OS0199
Sample Serial Number:    HBSF-LM15-S1
Operator:  Li
Date: 2012/03/23
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
205 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: 0-2   O: 0-6   Cl: 0-1   I: 0-1
Minimum:                                    -1.5
Maximum:                      2.0      5.0  50.0
Mass        Calc. Mass        mDa      PPM   DBE        i-FIT       Formula
269.0610    269.0607          0.3      1.1   11.0       1.5         C16  H12  N  O  Cl
            269.0603          0.7      2.6   15.5       1916.3      C19  H9  O2
```

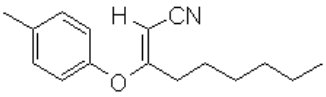


3q'

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-T12-03-OS0200
Sample Serial Number:    HBSF-LM15-S2
Operator:  Li
Date: 2012/03/23
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
205 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: 0-2   O: 0-6   Cl: 0-1   I: 0-1
Minimum:                                    -1.5
Maximum:                      2.0      5.0  50.0
Mass        Calc. Mass        mDa      PPM   DBE        i-FIT       Formula
269.0606    269.0607          -0.1     -0.4  11.0       0.6         C16  H12  N  O  Cl
            269.0603          0.3      1.1   15.5       172.6       C19  H9  O2
```

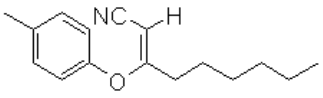


3r

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-T12-03-0S0208
Sample Serial Number:    HBSF-LM15-S10
Operator:  Li
Date: 2012/03/28
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
275 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: 0-2    O: 0-2    F: 0-6    Br: 0-1
Minimum:                                          -1.5
Maximum:                      2.0         5.0     50.0
Mass        Calc. Mass        mDa         PPM     DBE         i-FIT        Formula
243.1626    243.1623          0.3         1.2     7.0         2773761.0    C16  H21  N  O
            243.1635          -0.9        -3.7    3.0         2773615.3    C13  H22  N  O2  F
```

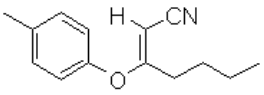


3r'

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-T12-03-0S0209
Sample Serial Number:    HBSF-LM15-S11
Operator:  Li
Date: 2012/03/28
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
275 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: 0-2    O: 0-2    F: 0-6    Br: 0-1
Minimum:                                          -1.5
Maximum:                      2.0         5.0     50.0
Mass        Calc. Mass        mDa         PPM     DBE         i-FIT        Formula
243.1624    243.1623          0.1         0.4     7.0         4.3          C16  H21  N  O
            243.1635          -1.1        -4.5    3.0         6.9          C13  H22  N  O2  F
```

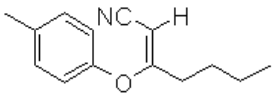


3s

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-T12-03-OS0205
Sample Serial Number:    HBSF-LM15-S7
Operator:  Li
Date: 2012/03/23
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
145 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: 0-2    O: 0-6    Cl: 0-1    I: 0-1
Minimum:                                          -1.5
Maximum:                        2.0         5.0         50.0
Mass        Calc. Mass          mDa         PPM         DBE         i-FIT       Formula
215.1307    215.1310            -0.3        -1.4        7.0         2.2         C14  H17  N  O
            215.1315            -0.8        -3.7        2.5         2025.2      C11  H20  N2  Cl
```

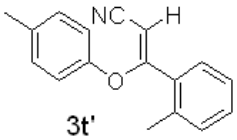


3s'

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-T12-03-OS0206
Sample Serial Number:    HBSF-LM15-S8
Operator:  Li
Date: 2012/03/23
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
145 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: 0-2    O: 0-6    Cl: 0-1    I: 0-1
Minimum:                                          -1.5
Maximum:                        2.0         5.0         50.0
Mass        Calc. Mass          mDa         PPM         DBE         i-FIT       Formula
215.1311    215.1310            0.1         0.5         7.0         1.7         C14  H17  N  O
            215.1315            -0.4        -1.9        2.5         831.6       C11  H20  N2  Cl
```



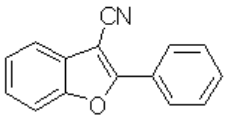
3t'

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-T12-03-0S0213
Sample Serial Number: HBSF-LM15-S15
Operator: Li
Date: 2012/03/28
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
285 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: 0-2 F: 0-6 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
249.1158	249.1154	0.4	1.6	11.0	0.3	C17 H15 N O
	249.1152	0.6	2.4	0.0	88.6	C9 H16 N O F5
	249.1165	-0.7	-2.8	7.0	10.1	C14 H16 N O2 F



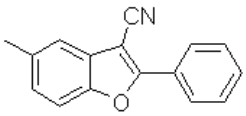
4a

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-T11-12-0S0920
Sample Serial Number: HBSF-D28-S9
Operator: Li
Date: 2011/12/15
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
297 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
219.0687	219.0684	0.3	1.4	12.0	8.8	C15 H9 N O
	219.0691	-0.4	-1.8	2.5	41.8	C9 H15 O4 S
	219.0678	0.9	4.1	3.0	45.3	C7 H13 N3 O3 S



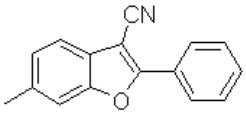
4b

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-T11-12-0S0923
Sample Serial Number: HBSF-D28-S12
Operator: Li
Date: 2011/12/15
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
317 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
233.0844	233.0841	0.3	1.3	12.0	31.3	C16 H11 N O
	233.0848	-0.4	-1.7	2.5	1305.0	C10 H17 O4 S
	233.0834	1.0	4.3	3.0	1302.1	C8 H15 N3 O3 S



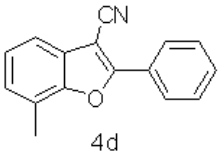
4c

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-T11-12-0S0922
Sample Serial Number: HBSF-D28-S11
Operator: Li
Date: 2011/12/15
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
317 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
233.0842	233.0841	0.1	0.4	12.0	8.0	C16 H11 N O
	233.0848	-0.6	-2.6	2.5	596.9	C10 H17 O4 S
	233.0834	0.8	3.4	3.0	567.9	C8 H15 N3 O3 S



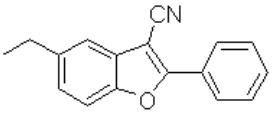
4d

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-T11-12-0S0921
Sample Serial Number: HBSF-D28-S10
Operator: Li
Date: 2011/12/15
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
317 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
233.0845	233.0848	-0.3	-1.3	2.5	2764.2	C10 H17 O4 S
	233.0841	0.4	1.7	12.0	42.5	C16 H11 N O
	233.0834	1.1	4.7	3.0	2626.9	C8 H15 N3 O3 S



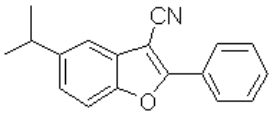
4e

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-T11-12-0S0924
Sample Serial Number: HBSF-D28-S13
Operator: Li
Date: 2011/12/15
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
346 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
247.0999	247.0997	0.2	0.8	12.0	19.7	C17 H13 N O
	247.1004	-0.5	-2.0	2.5	1960.0	C11 H19 O4 S
	247.0991	0.8	3.2	3.0	1866.9	C9 H17 N3 O3 S



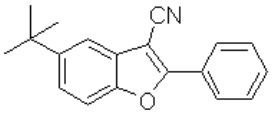
4f

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-T11-12-0S0925
Sample Serial Number: HBSF-D28-S14
Operator: Li
Date: 2011/12/15
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
367 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
261.1151	261.1154	-0.3	-1.1	12.0	2782052.8	C18 H15 N O
	261.1147	0.4	1.5	3.0	2783190.0	C10 H19 N3 O3 S
	261.1161	-1.0	-3.8	2.5	2783207.3	C12 H21 O4 S
	261.1140	1.1	4.2	12.5	2781507.5	C16 H13 N4



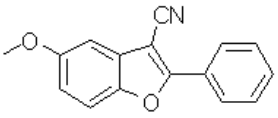
4g

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-T11-12-0S0926
Sample Serial Number: HBSF-D28-S15
Operator: Li
Date: 2011/12/15
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
396 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
275.1307	275.1304	0.3	1.1	3.0	2781439.3	C11 H21 N3 O3 S
	275.1310	-0.3	-1.1	12.0	2780515.5	C19 H17 N O
	275.1317	-1.0	-3.6	2.5	2781455.3	C13 H23 O4 S
	275.1297	1.0	3.6	12.5	2780103.5	C17 H15 N4



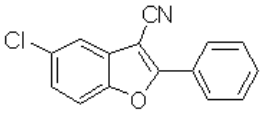
4h

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-T11-12-0S0927
Sample Serial Number: HBSF-D28-S16
Operator: Li
Date: 2011/12/15
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
347 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
249.0791	249.0790	0.1	0.4	12.0	2785364.5	C16 H11 N O2
	249.0797	-0.6	-2.4	2.5	4675.6	C10 H17 O5 S
	249.0783	0.8	3.2	3.0	4433.3	C8 H15 N3 O4 S



4i

Shanghai Mass Spectrometry Center
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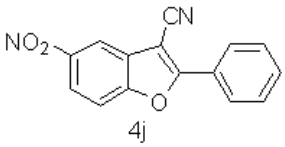
High Resolution MS Data Report

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

Card Serial Number: GCT-P-T11-12-0S0928
Sample Serial Number: HBSF-D28-S17
Operator: Li
Date: 2011/12/15
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
394 formula(e) evaluated with 6 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
253.0292	253.0290	0.2	0.8	16.5	6286.1	C18 H5 O2
	253.0294	-0.2	-0.8	12.0	36.1	C15 H8 N O Cl
	253.0288	0.4	1.6	3.0	663.3	C7 H12 N3 O3 S Cl
	253.0301	-0.9	-3.6	2.5	499.1	C9 H14 O4 S Cl
	253.0283	0.9	3.6	7.5	4625.2	C10 H9 N2 O4 S
	253.0281	1.1	4.3	12.5	26.8	C13 H6 N4 Cl



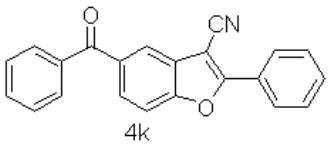
4j

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-T11-12-0S0929
Sample Serial Number: HBSF-D28-S18
Operator: Li
Date: 2011/12/15
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
416 formula(e) evaluated with 5 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
264.0538	264.0540	-0.2	-0.8	8.5	2776455.3	C12 H11 N3 O2 Cl
	264.0535	0.3	1.1	13.0	2775352.8	C15 H8 N2 O3
	264.0542	-0.4	-1.5	3.5	2776294.8	C9 H14 N O6 S
	264.0547	-0.9	-3.4	-1.0	2776457.3	C6 H17 N2 O5 S Cl
	264.0528	1.0	3.8	4.0	2776282.3	C7 H12 N4 O5 S



4k

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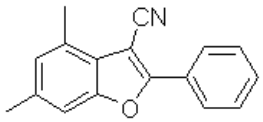
Chinese Academic of Sciences
High Resolution MS Data Report

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

Card Serial Number: GCT-P-T11-12-0S0930
Sample Serial Number: HBSF-D28-S19
Operator: Li
Date: 2011/12/15
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
514 formula(e) evaluated with 7 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
323.0952	323.0953	-0.1	-0.3	7.5	2774933.5	C16 H19 O5 S
	323.0951	0.1	0.3	12.5	2775069.0	C19 H16 N2 O Cl
	323.0946	0.6	1.9	17.0	2774555.8	C22 H13 N O2
	323.0958	-0.6	-1.9	3.0	2775071.3	C13 H22 N O4 S Cl
	323.0945	0.7	2.2	3.5	2775071.0	C11 H20 N4 O3 S Cl
	323.0940	1.2	3.7	8.0	2774920.0	C14 H17 N3 O4 S
	323.0967	-1.5	-4.6	12.5	2774915.8	C17 H15 N4 O S



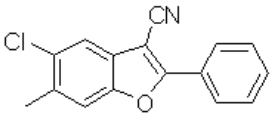
4l

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-T11-12-0S0933
Sample Serial Number: HBSF-D28-S22
Operator: Li
Date: 2011/12/15
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
346 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 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
247.1001	247.1004	-0.3	-1.2	2.5	1044.3	C11 H19 O4 S
	247.0997	0.4	1.6	12.0	12.3	C17 H13 N O
	247.0991	1.0	4.0	3.0	994.5	C9 H17 N3 O3 S



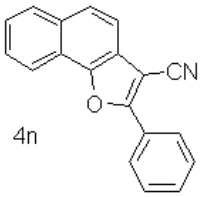
4m

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-T11-12-0S0932
Sample Serial Number: HBSF-D28-S21
Operator: Li
Date: 2011/12/15
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
422 formula(e) evaluated with 5 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
267.0452	267.0451	0.1	0.4	12.0	74.7	C16 H10 N O Cl
	267.0446	0.6	2.2	16.5	2385.0	C19 H7 O2
	267.0458	-0.6	-2.2	2.5	509.2	C10 H16 O4 S Cl
	267.0444	0.8	3.0	3.0	591.7	C8 H14 N3 O3 S Cl
	267.0440	1.2	4.5	7.5	1972.8	C11 H11 N2 O4 S



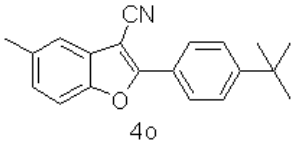
4n

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-T11-12-0S0931
Sample Serial Number: HBSF-D28-S20
Operator: Li
Date: 2011/12/15
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
420 formula(e) evaluated with 6 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:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
269.0843	269.0841	0.2	0.7	15.0	28.1	C19 H11 N O
	269.0846	-0.3	-1.1	10.5	6952.9	C16 H14 N2 Cl
	269.0839	0.4	1.5	1.5	7387.8	C8 H18 N4 O2 S Cl
	269.0848	-0.5	-1.9	5.5	954.5	C13 H17 O4 S
	269.0852	-0.9	-3.3	1.0	7382.6	C10 H20 N O3 S Cl
	269.0834	0.9	3.3	6.0	892.5	C11 H15 N3 O3 S



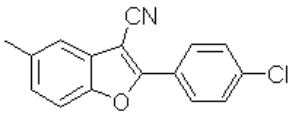
4o

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-T12-03-0S0202
Sample Serial Number: HBSF-LM15-S4
Operator: Li
Date: 2012/03/23
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
228 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: 0-2 O: 0-6 Cl: 0-1 I: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
289.1472	289.1472	0.0	0.0	7.5	5364.5	C17 H22 N2 Cl
	289.1467	0.5	1.7	12.0	3.0	C20 H19 N O



4q

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

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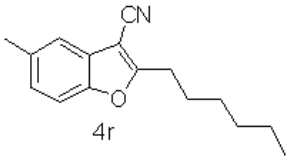
Card Serial Number:   GCT-P-T12-03-0S0201
Sample Serial Number:    HBSF-LM15-S3
Operator:  Li
Date: 2012/03/23
Elemental Composition Report
Single Mass Analysis
Tolerance = 5.0 PPM   /   DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Odd and Even Electron Ions
206 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used: C: 0-60    H: 0-80    N: 0-2    O: 0-6    Cl: 0-1    I: 0-1
Minimum:                                      -1.5
Maximum:                    2.0         5.0   50.0
Mass        Calc. Mass      mDa         PPM   DBE         i-FIT       Formula
267.0452    267.0451        0.1         0.4   12.0        235.3       C16  H10  N  O  Cl
            267.0446        0.6         2.2   16.5        1750.0      C19  H7  O2
```



4r

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

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Card Serial Number:   GCT-P-T12-03-0S0210
Sample Serial Number:    HBSF-LM15-S12
Operator:  Li
Date: 2012/03/28
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
274 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: 0-2    O: 0-2    F: 0-6    Br: 0-1
Minimum:                                      -1.5
Maximum:                    2.0         5.0   50.0
Mass        Calc. Mass      mDa         PPM   DBE         i-FIT       Formula
241.1471    241.1467        0.4         1.7   8.0         1.9         C16  H19  N  O
            241.1478        -0.7        -2.9  4.0         15.4        C13  H20  N  O2  F
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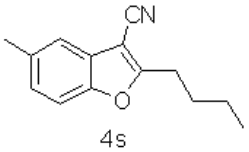

4s

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-T12-03-OS0207
Sample Serial Number: HBSF-LM15-S9
Operator: Li
Date: 2012/03/23
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
140 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: 0-2 O: 0-6 Cl: 0-1 I: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
213.1151	213.1154	-0.3	-1.4	8.0	2773035.0	C14 H15 N O
	213.1159	-0.8	-3.8	3.5	2773245.3	C11 H18 N2 Cl