

## ***Supporting Information***

# **Synthesis of 2-Selenyl(Sulfenyl)benzofurans via Cu-Catalyzed Tandem Reactions of 2-(*gem*-Dibromovinyl)phenols with Diorganyl Diselenides(Disulfides)**

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<sup>b</sup> *College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou, Jiangsu 215123 P.R. China*

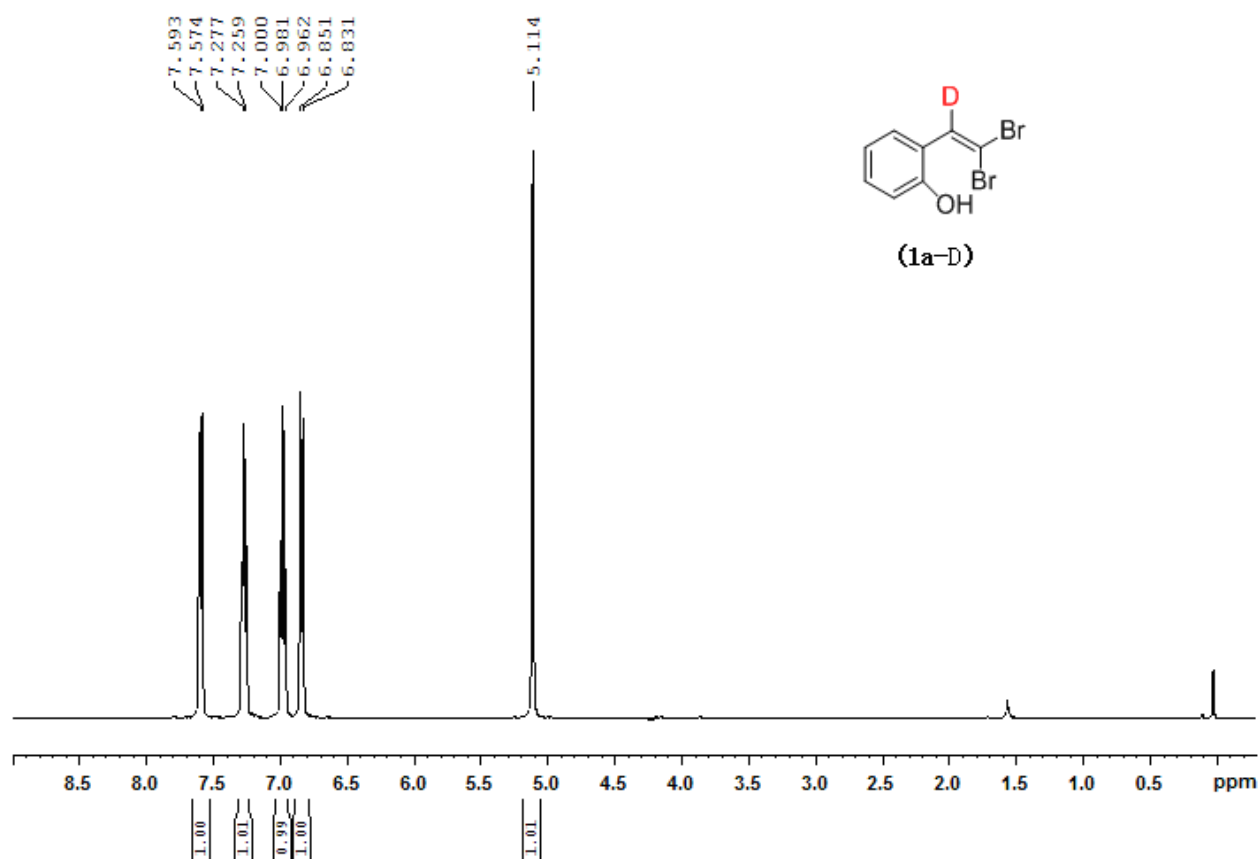
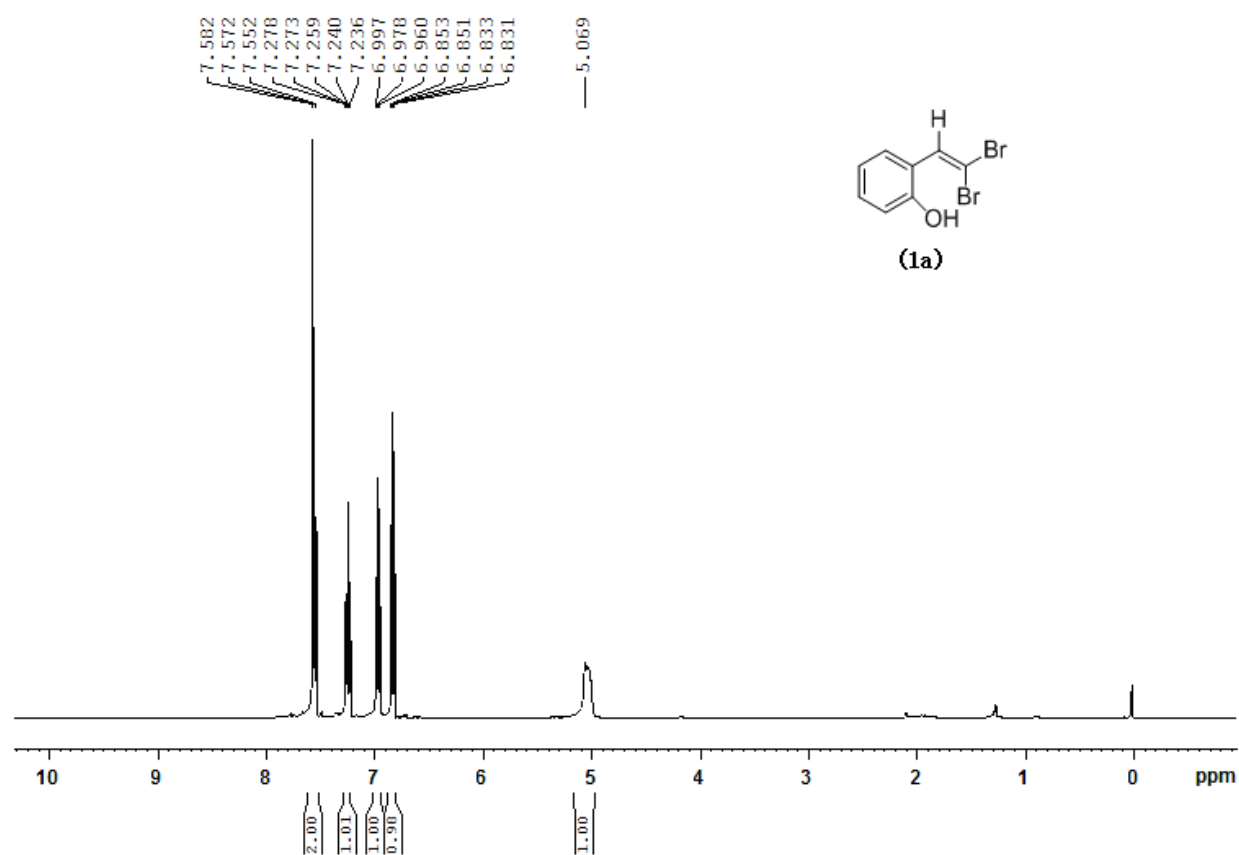
<sup>c</sup> *State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032 P.R. China*

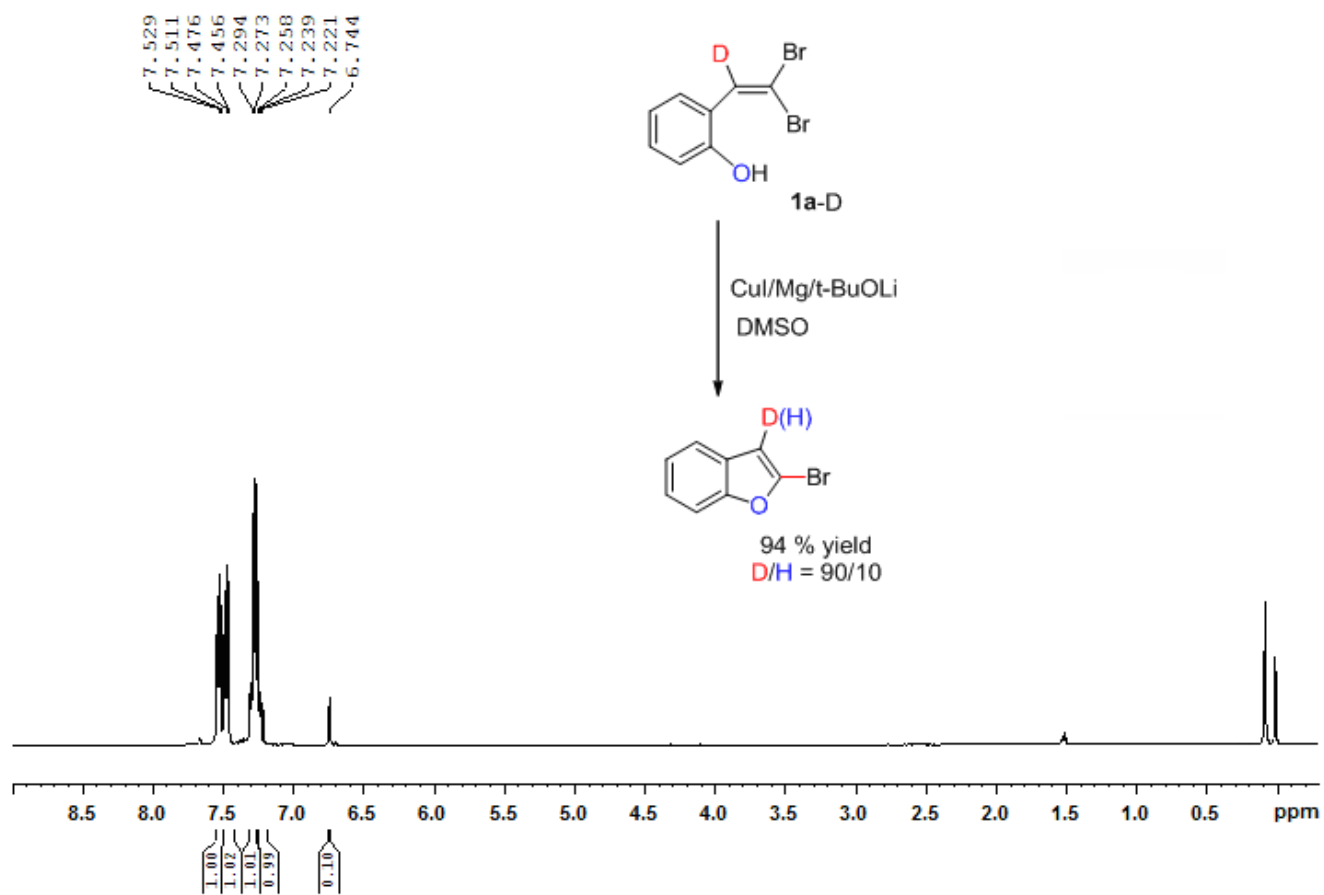
[leiwang@chnu.edu.cn](mailto:leiwang@chnu.edu.cn)

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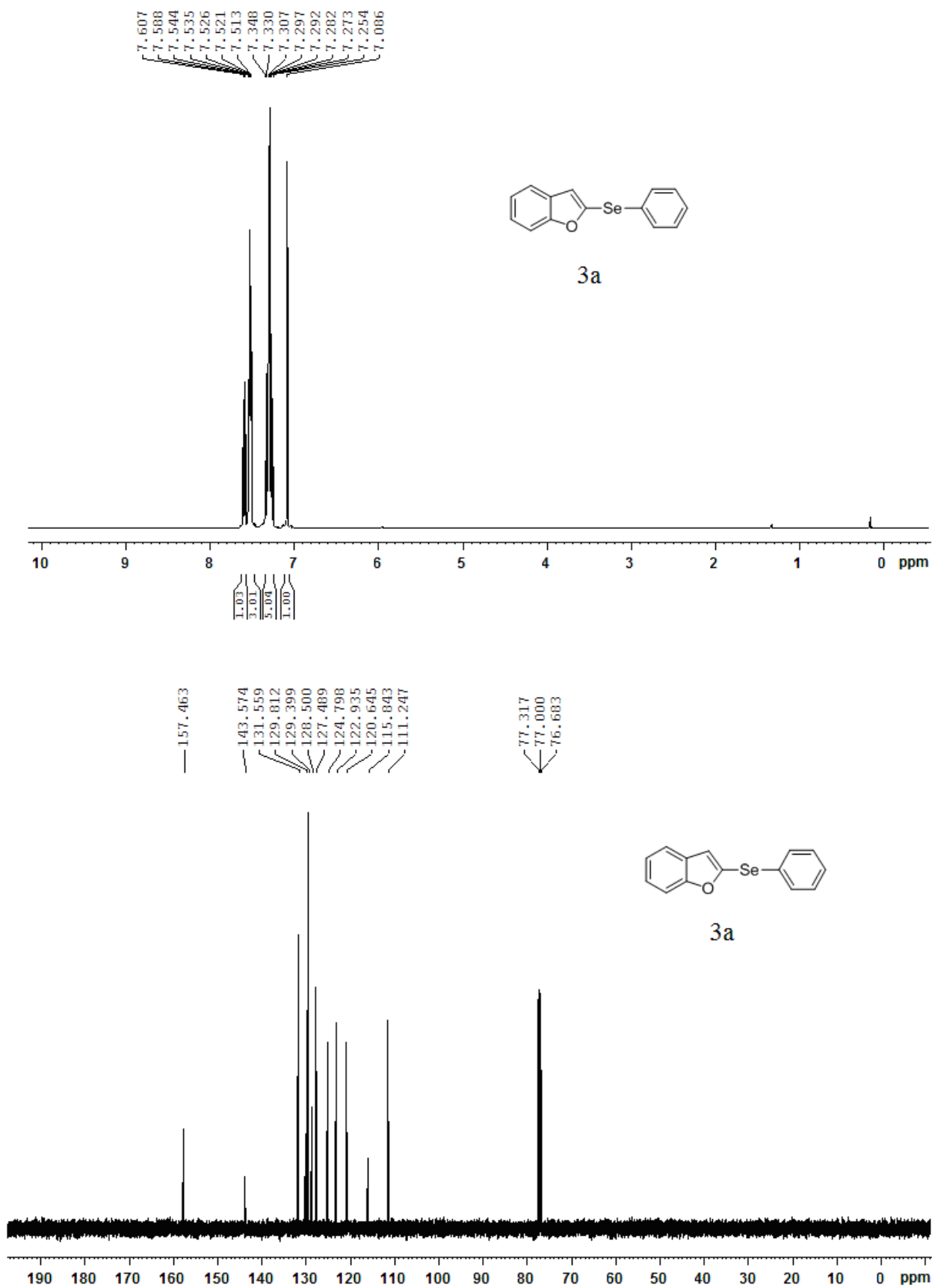
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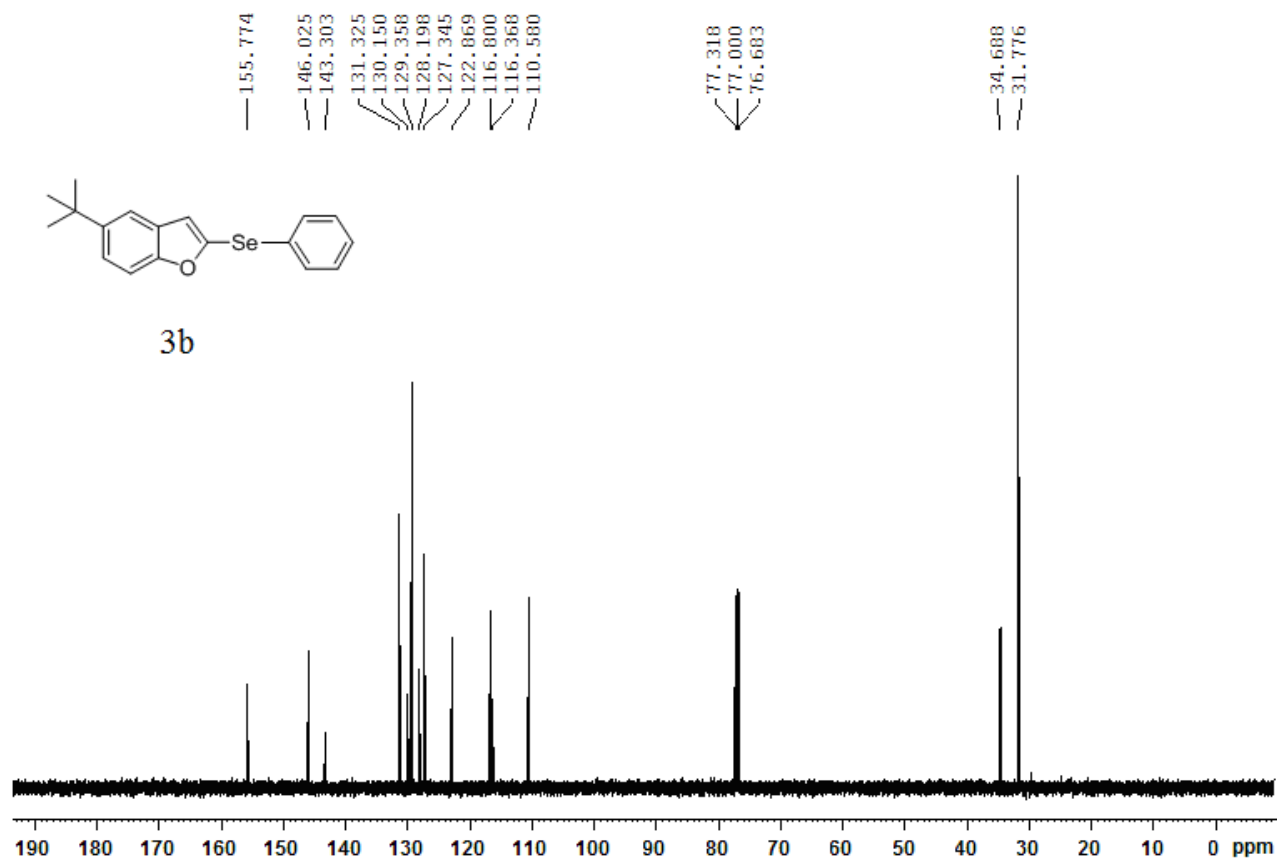
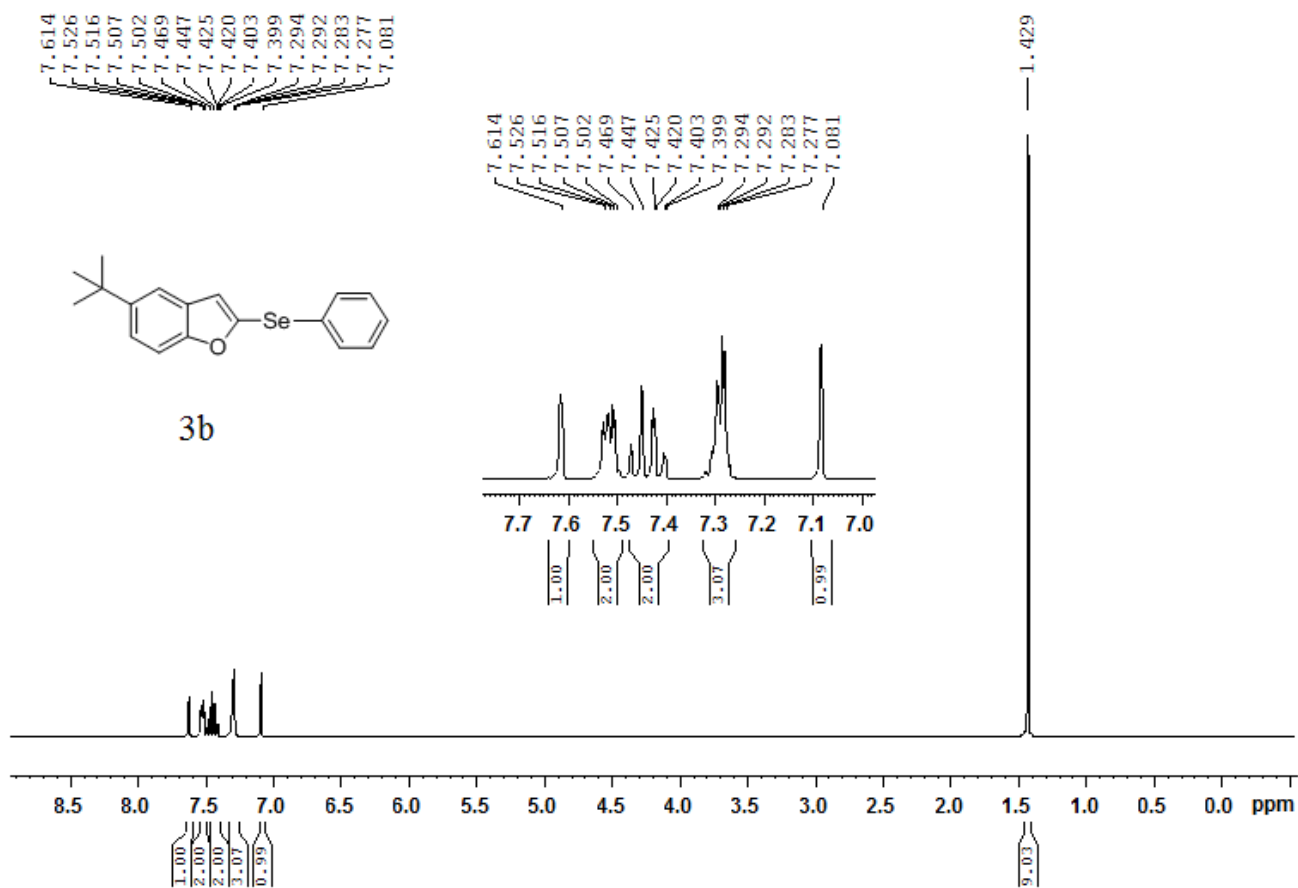
## 1. D-Labeled $^1\text{H}$ NMR spectra of substrate and product

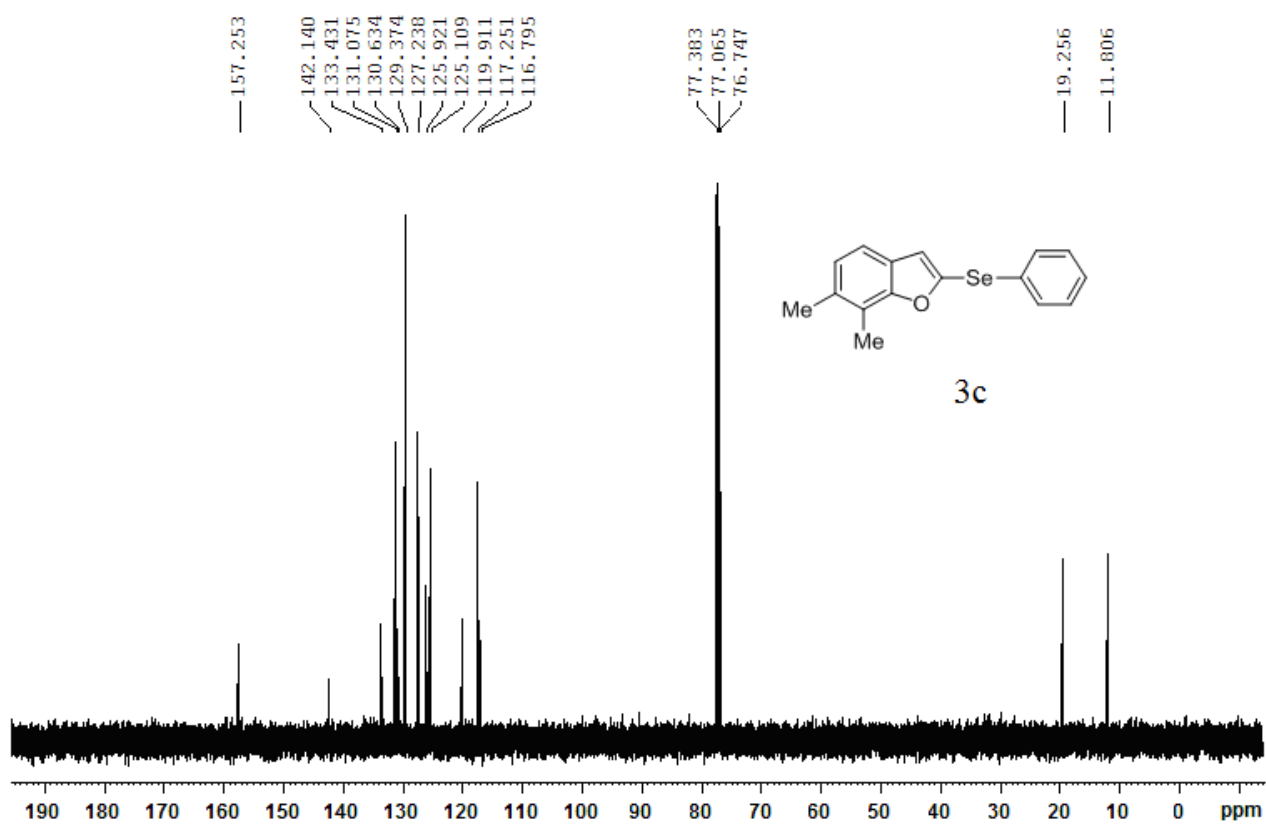
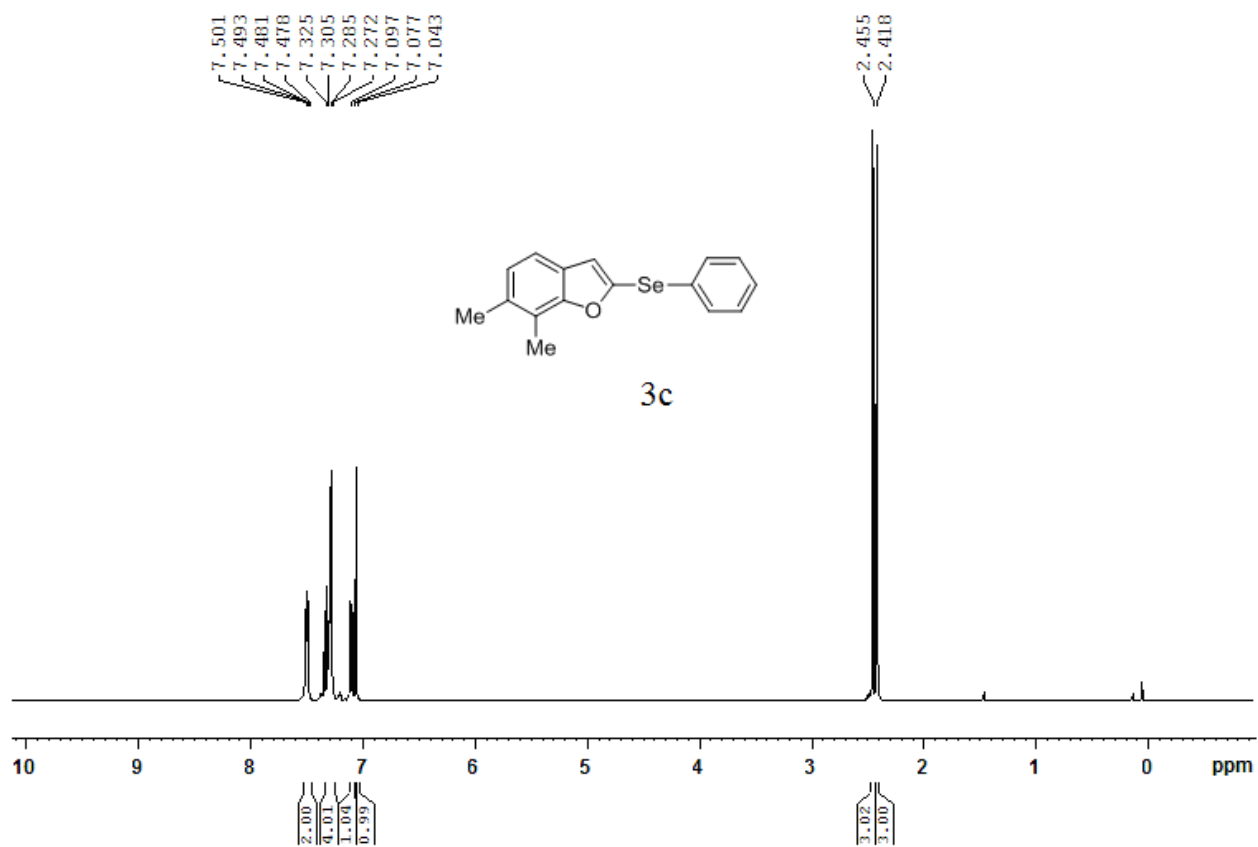


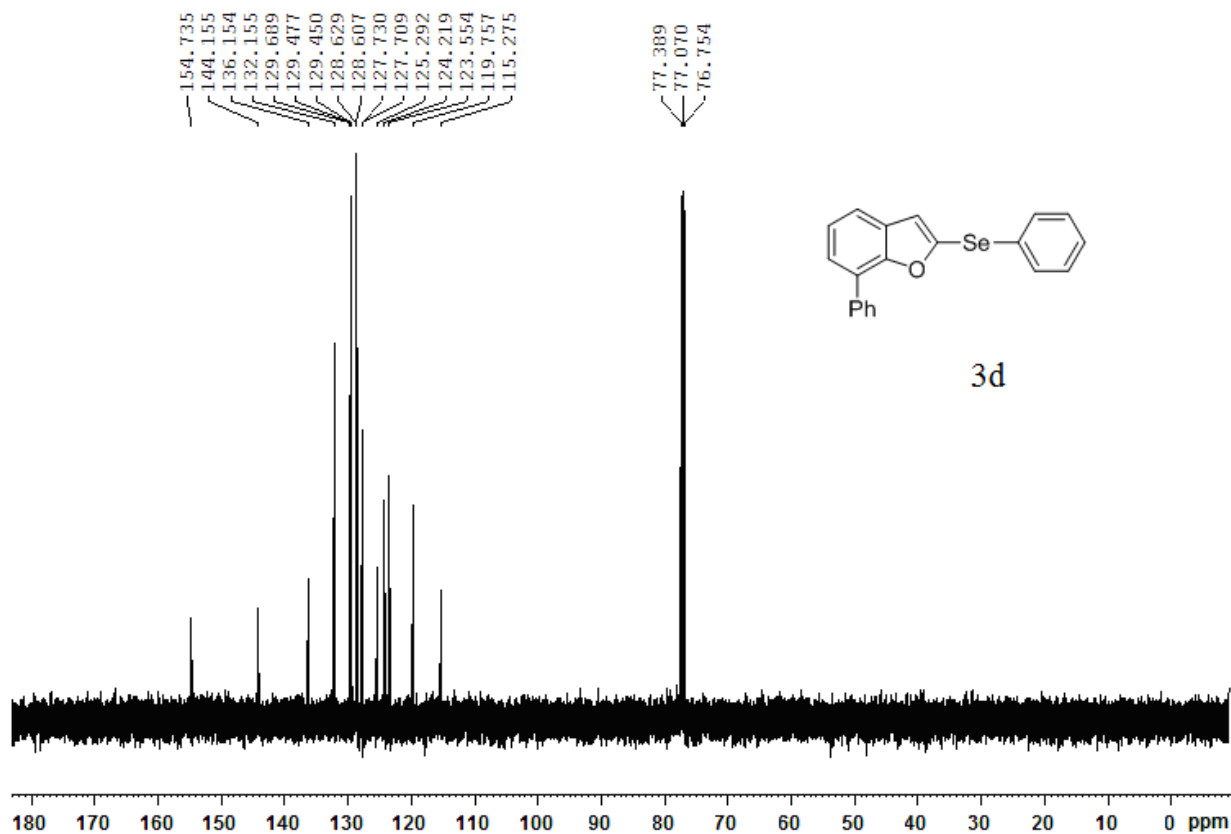
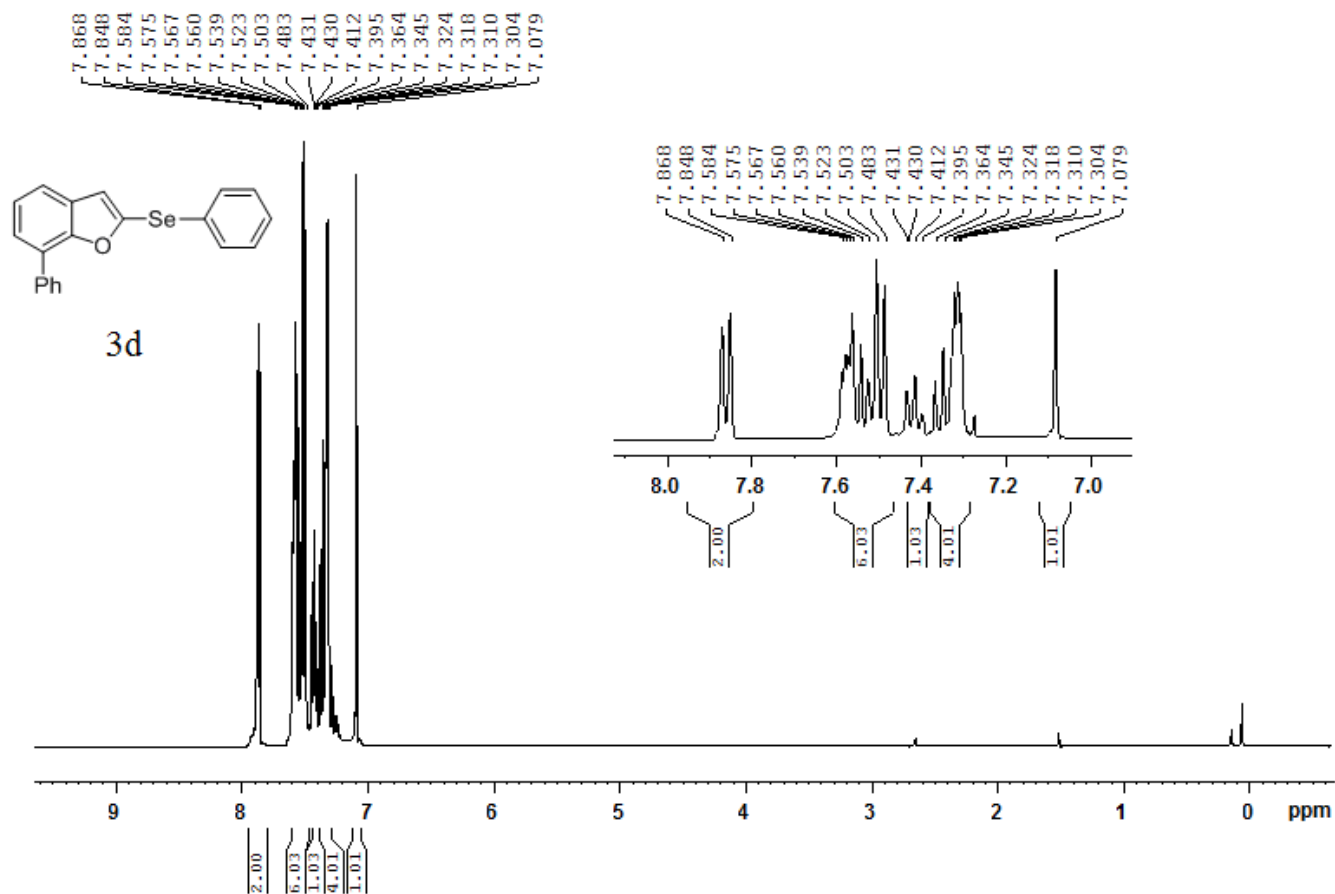


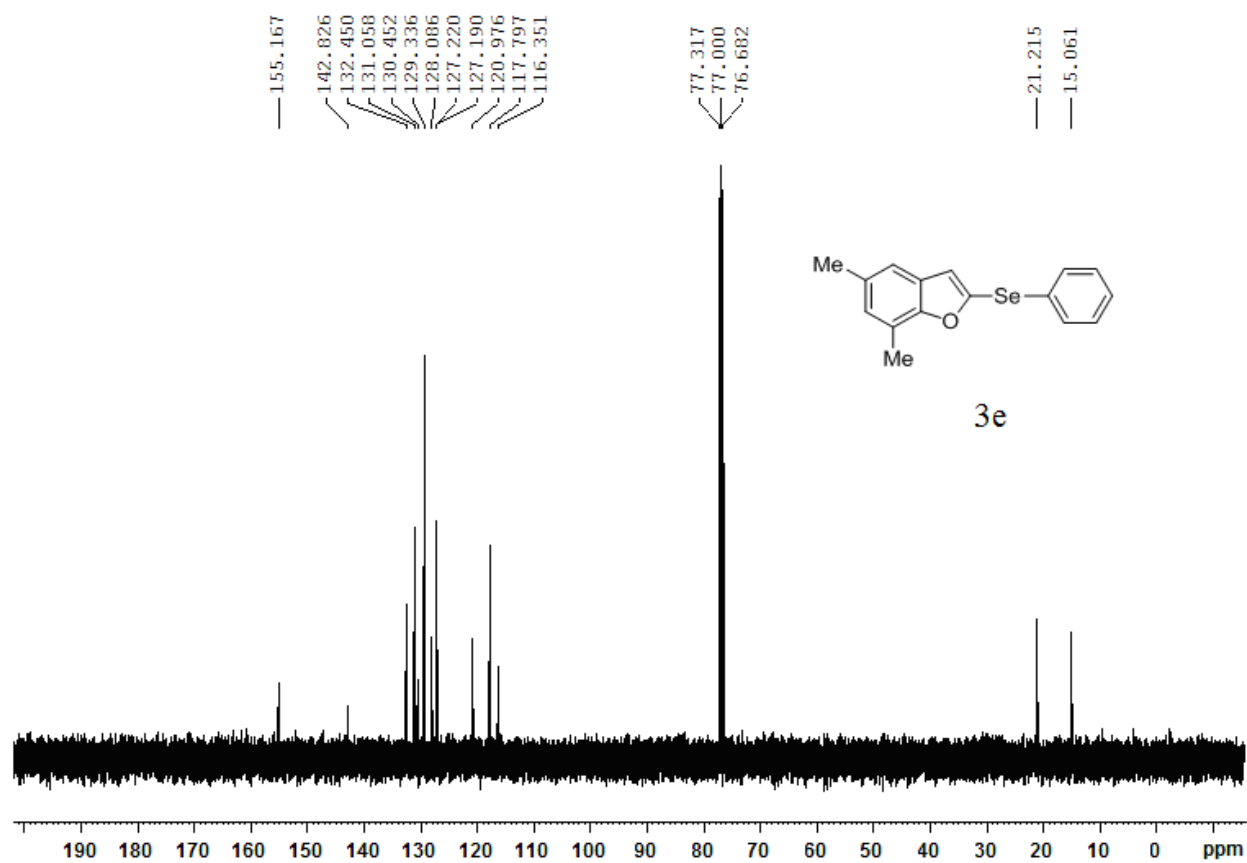
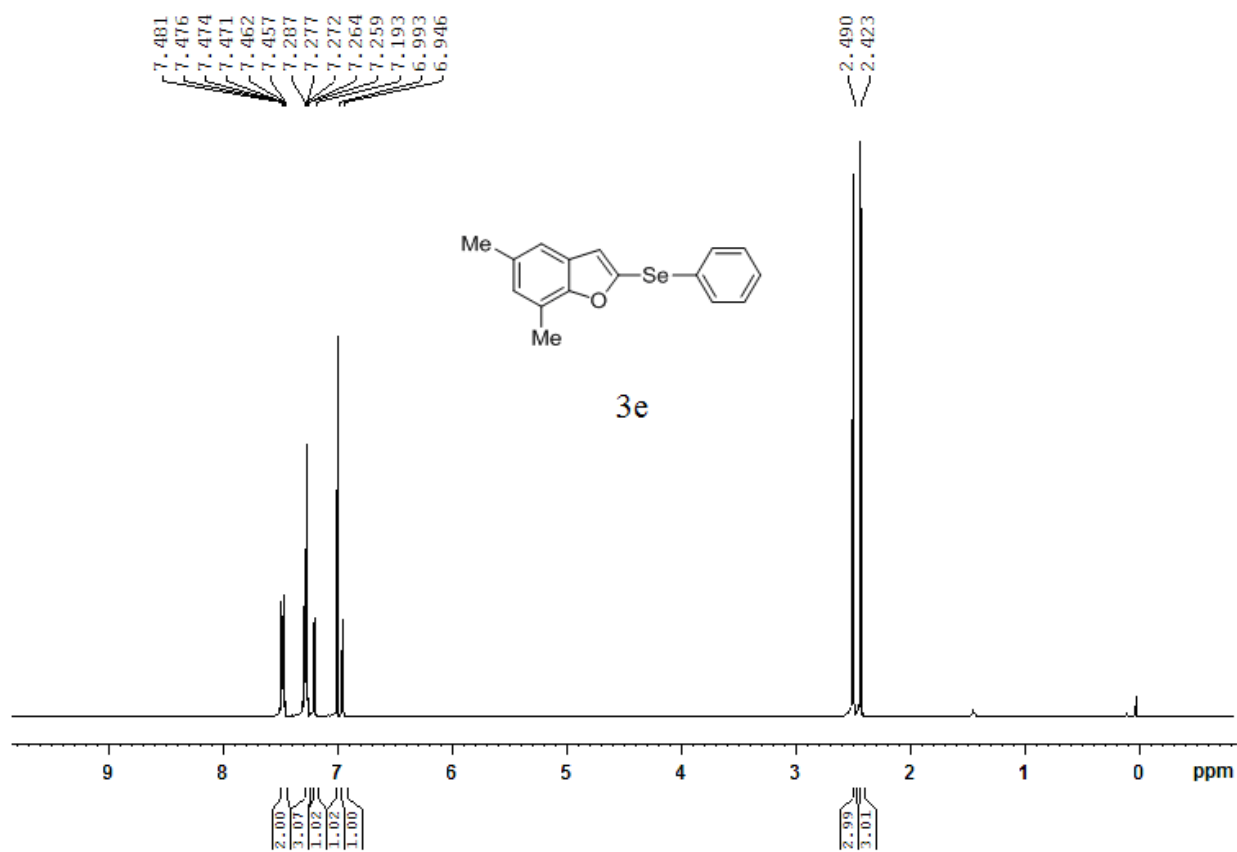
## 2. $^1\text{H}$ , $^{13}\text{C}$ NMR and HRMS spectra



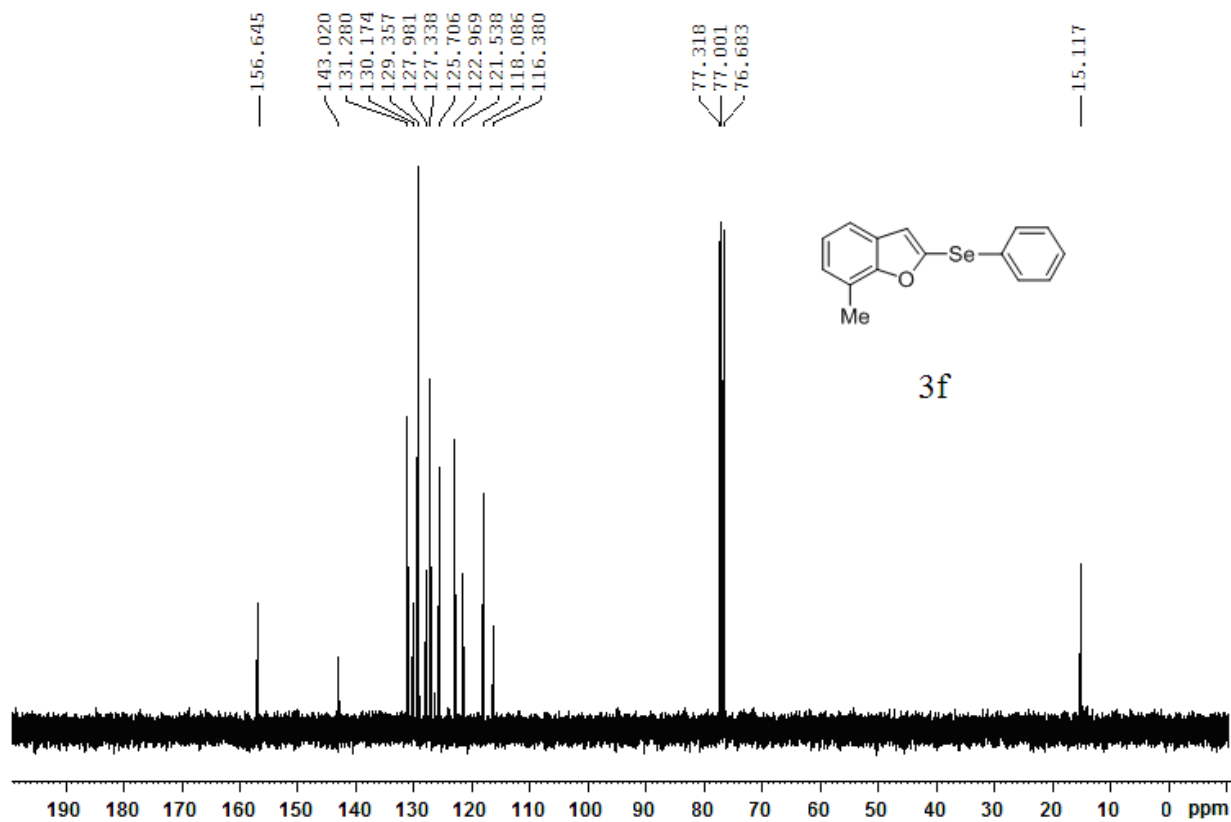
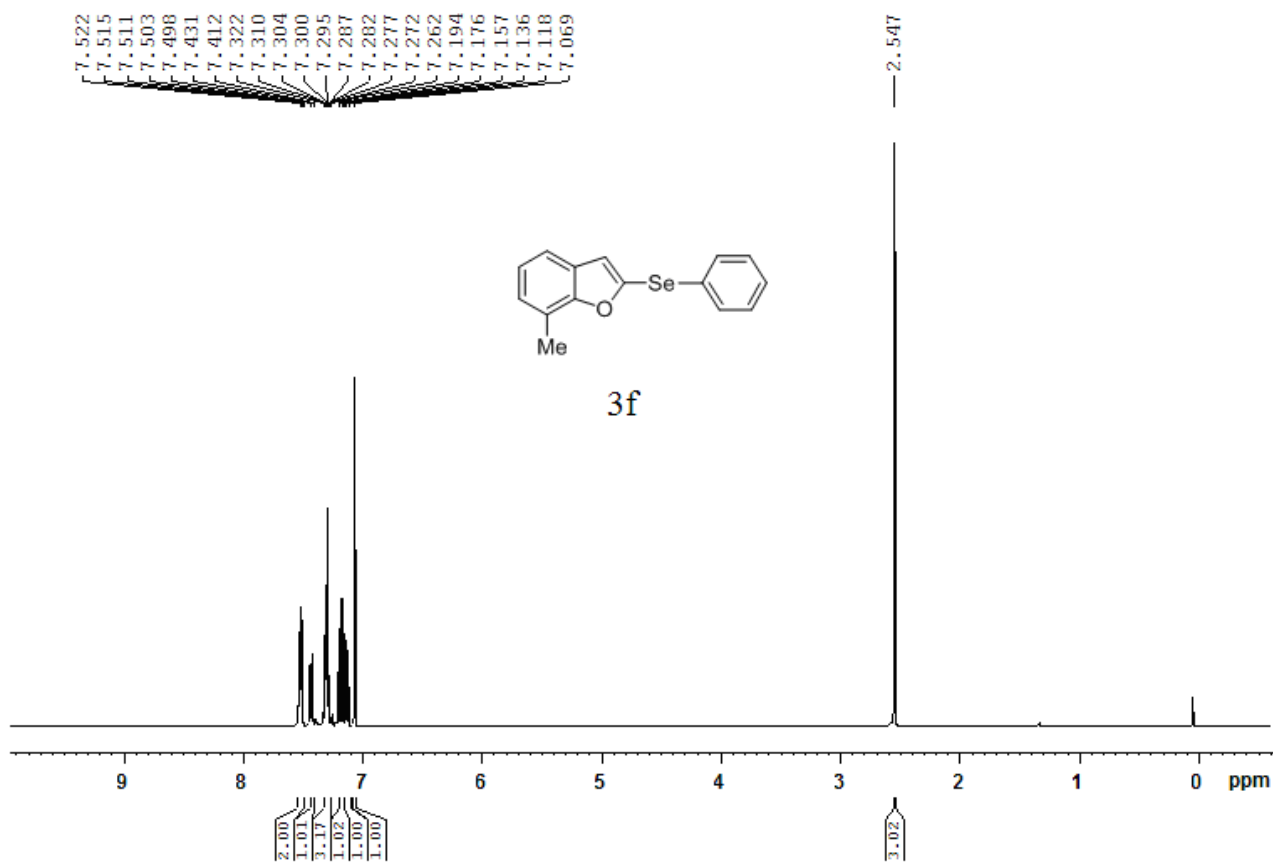


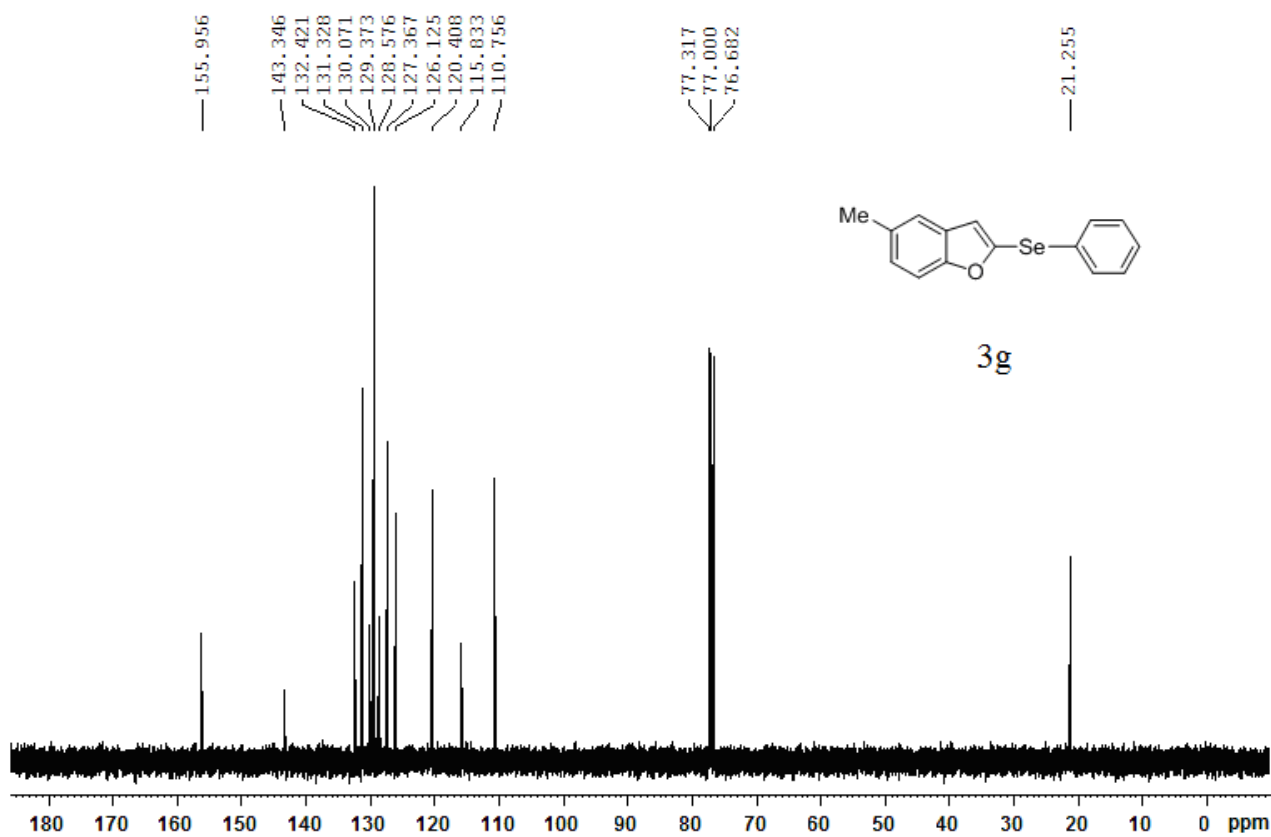
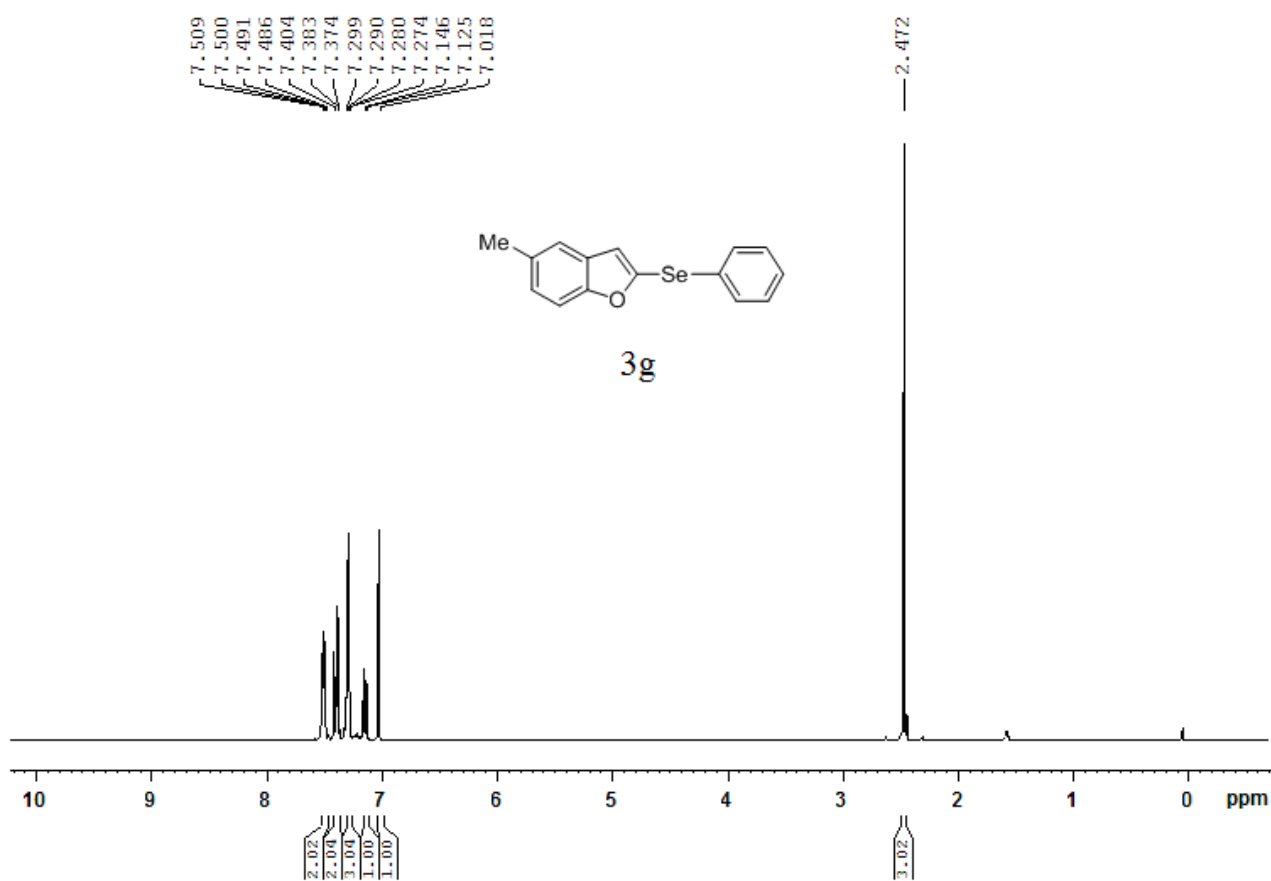


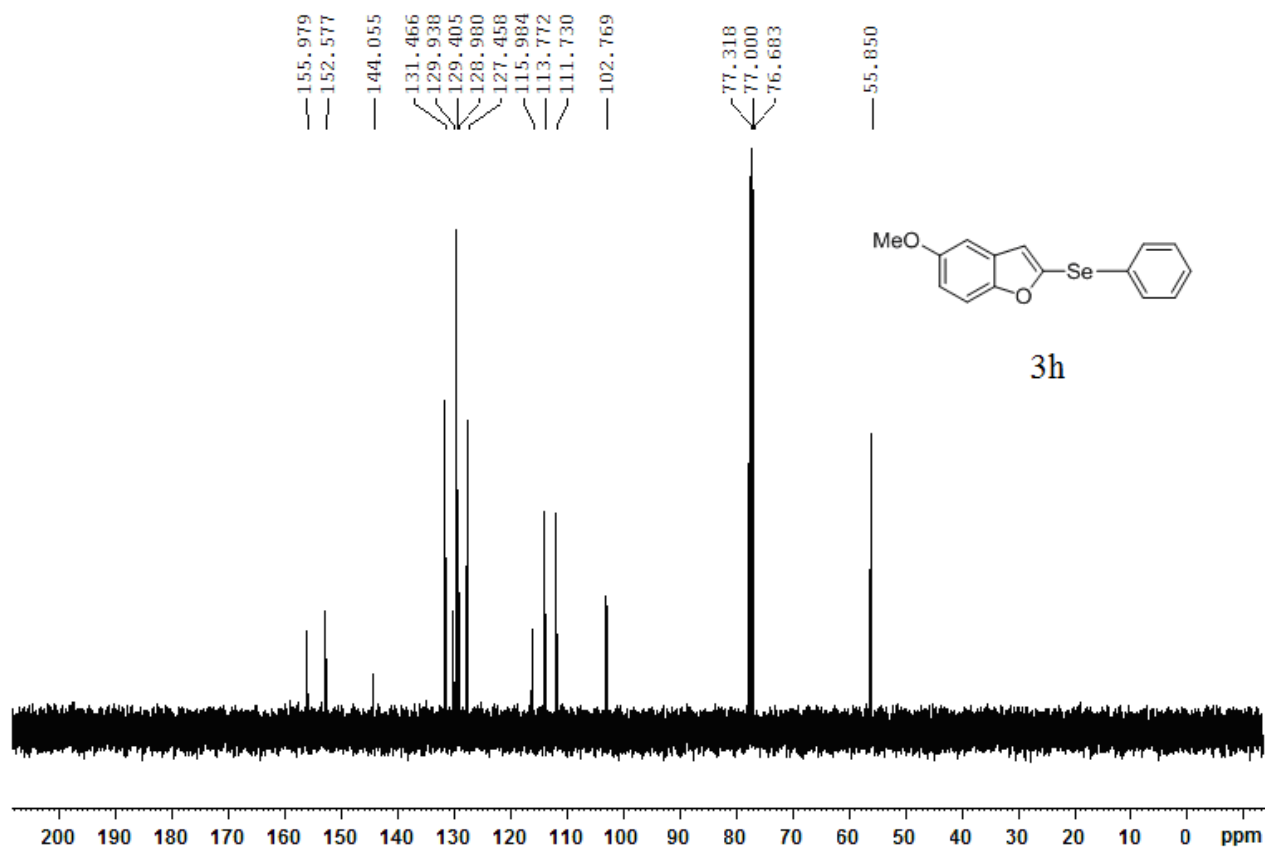
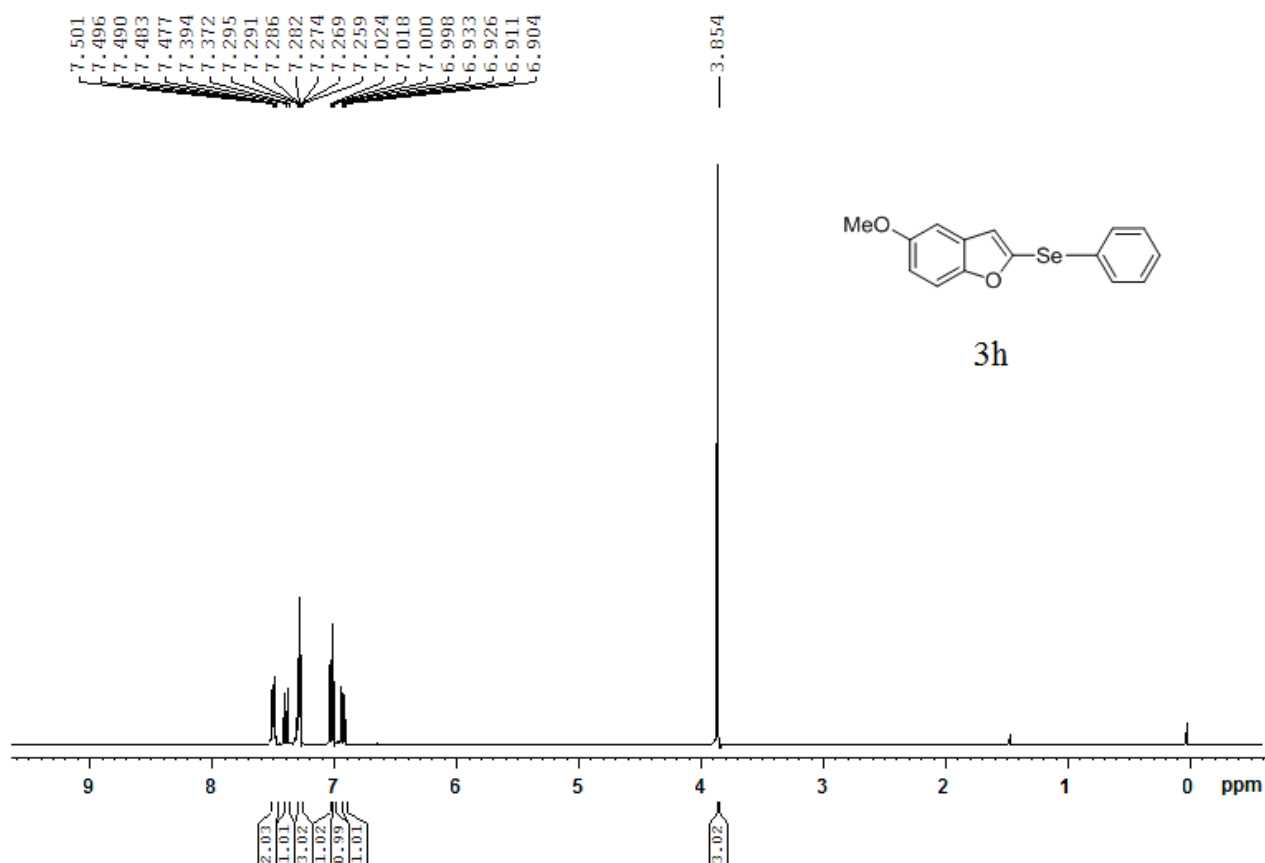


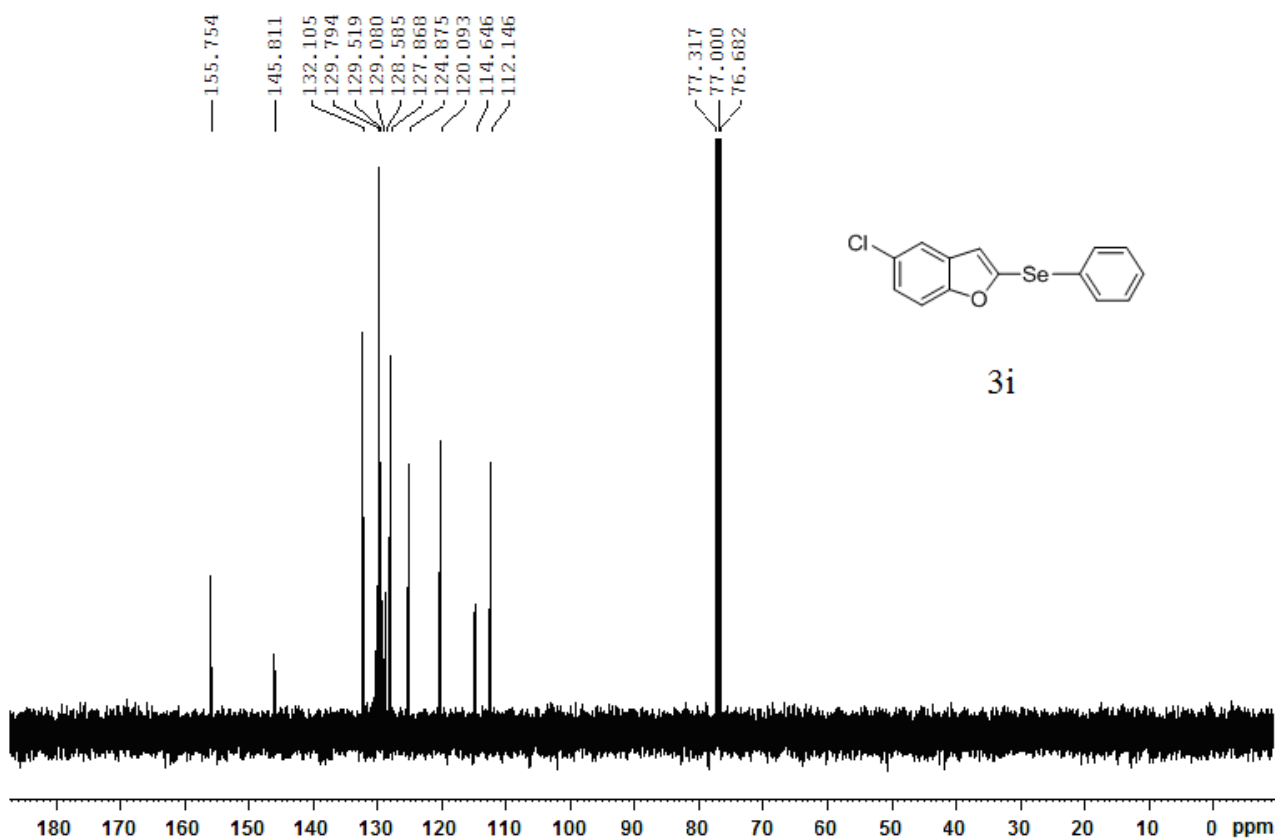
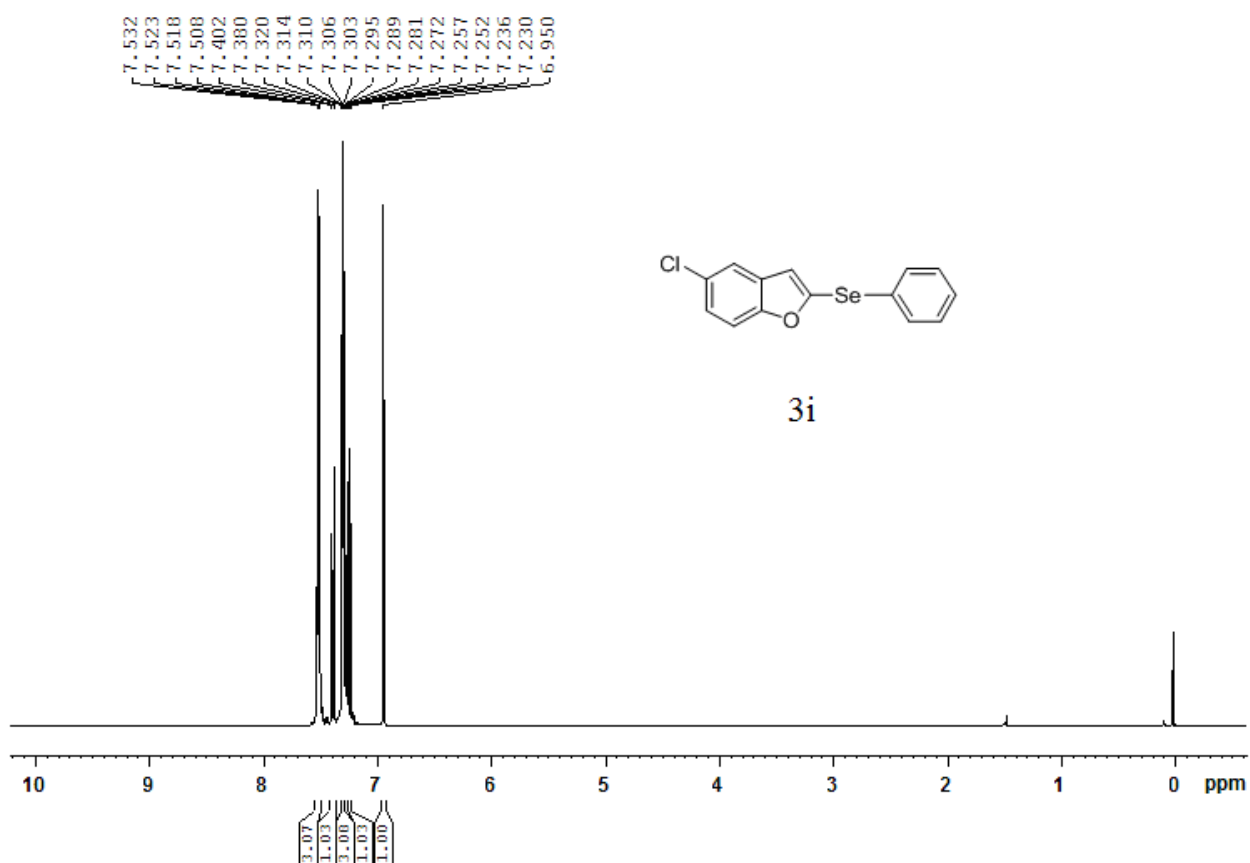




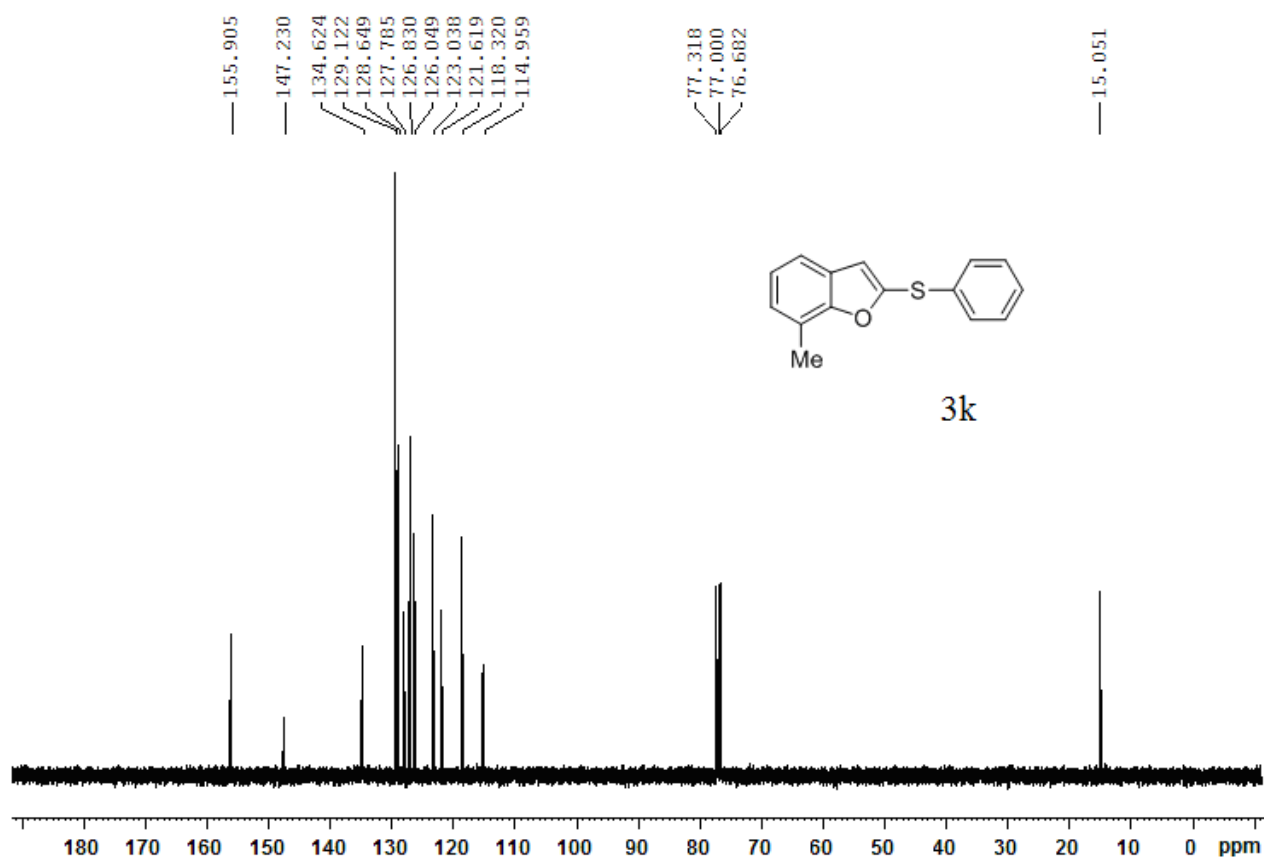
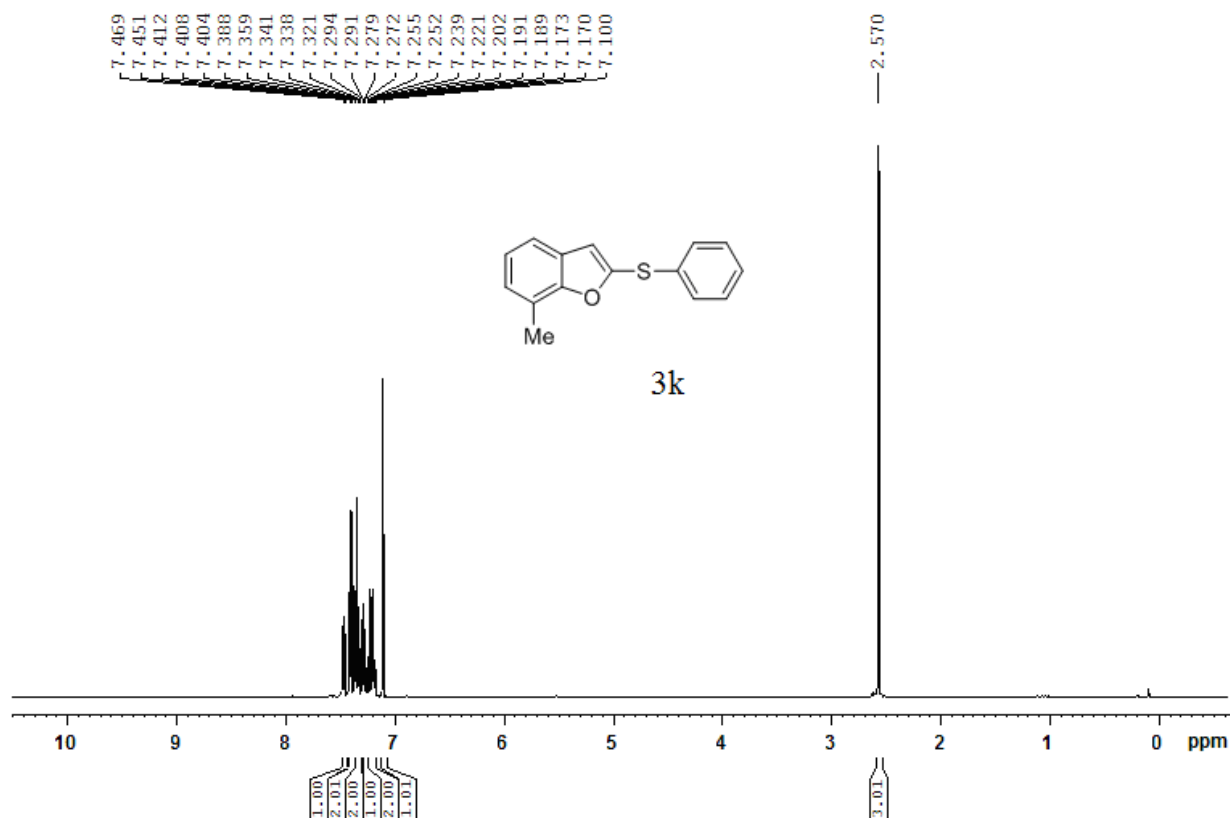


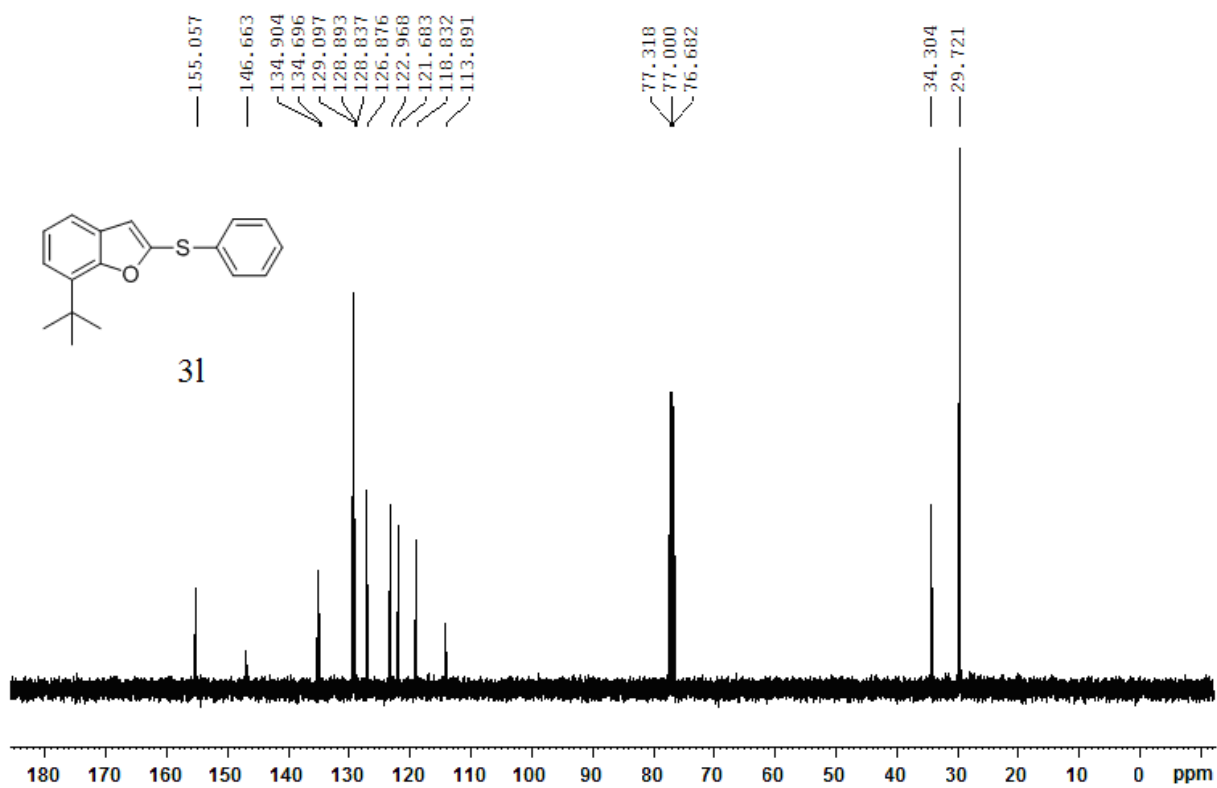
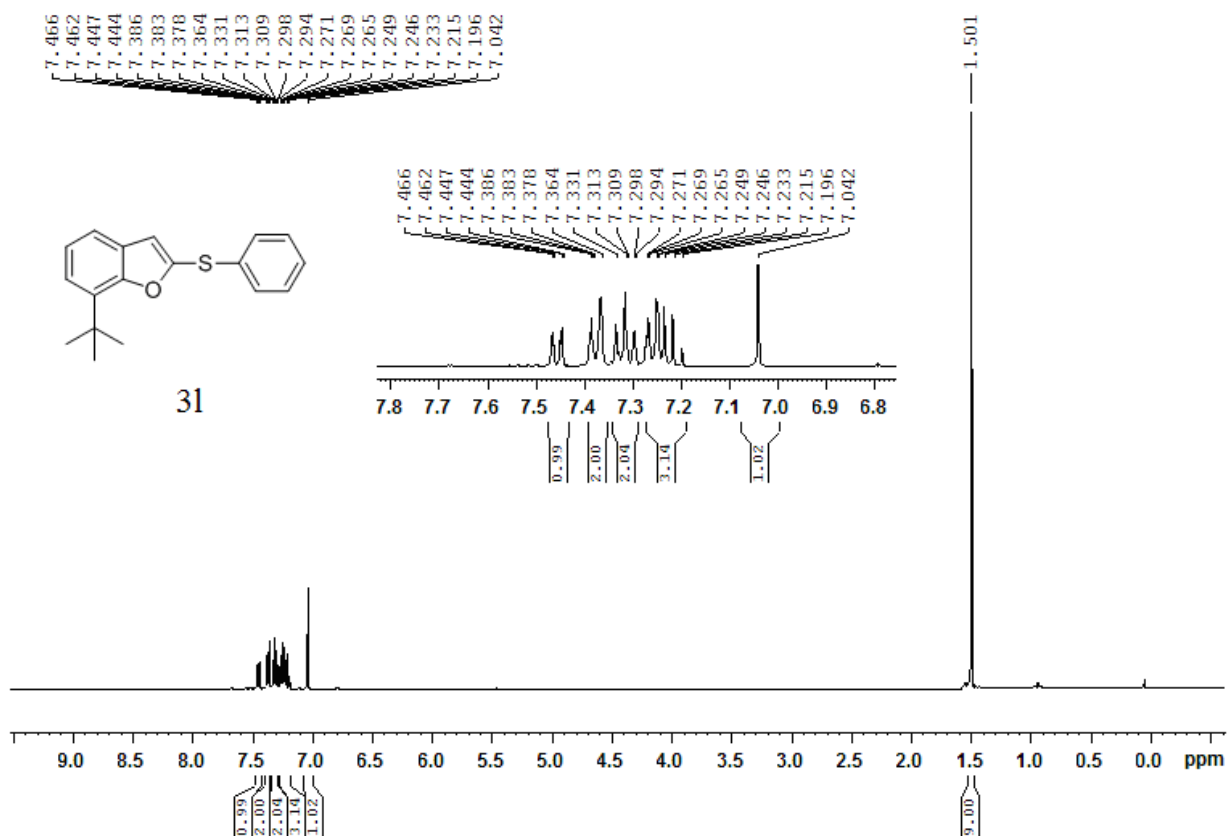


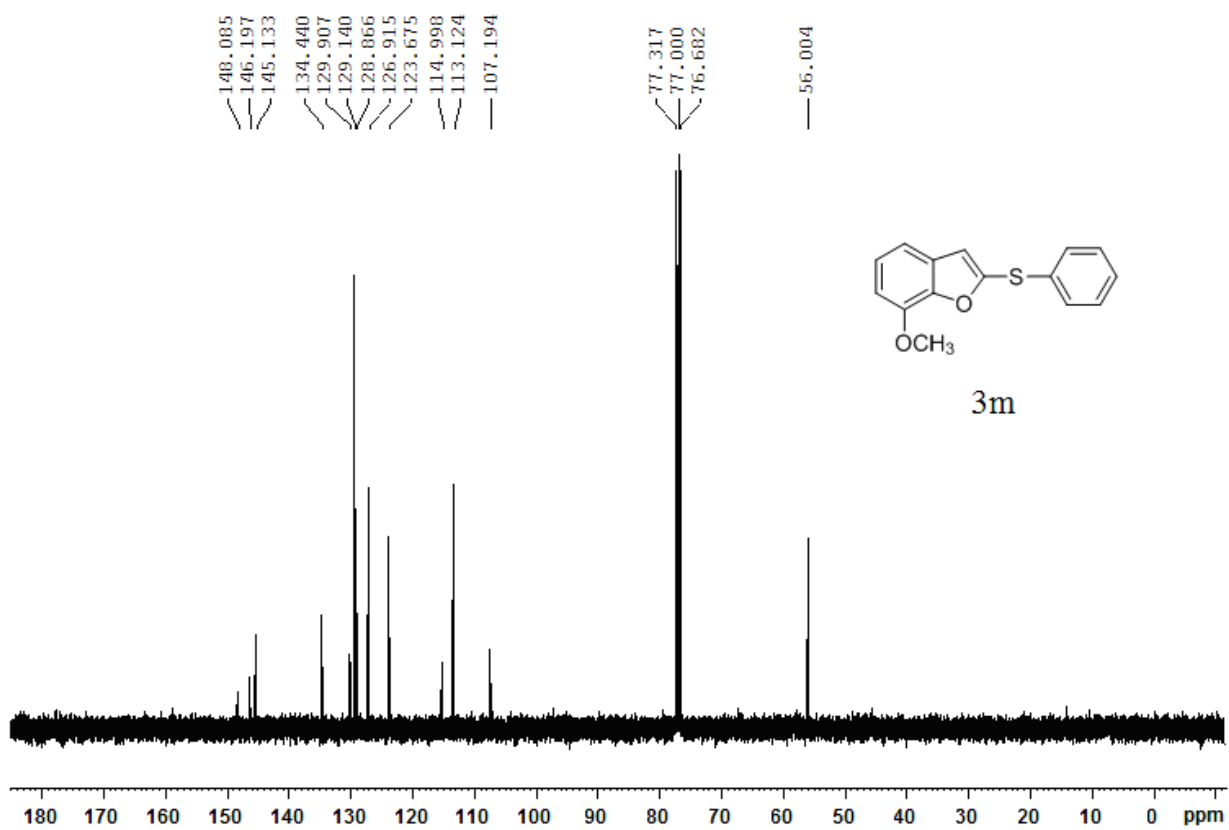
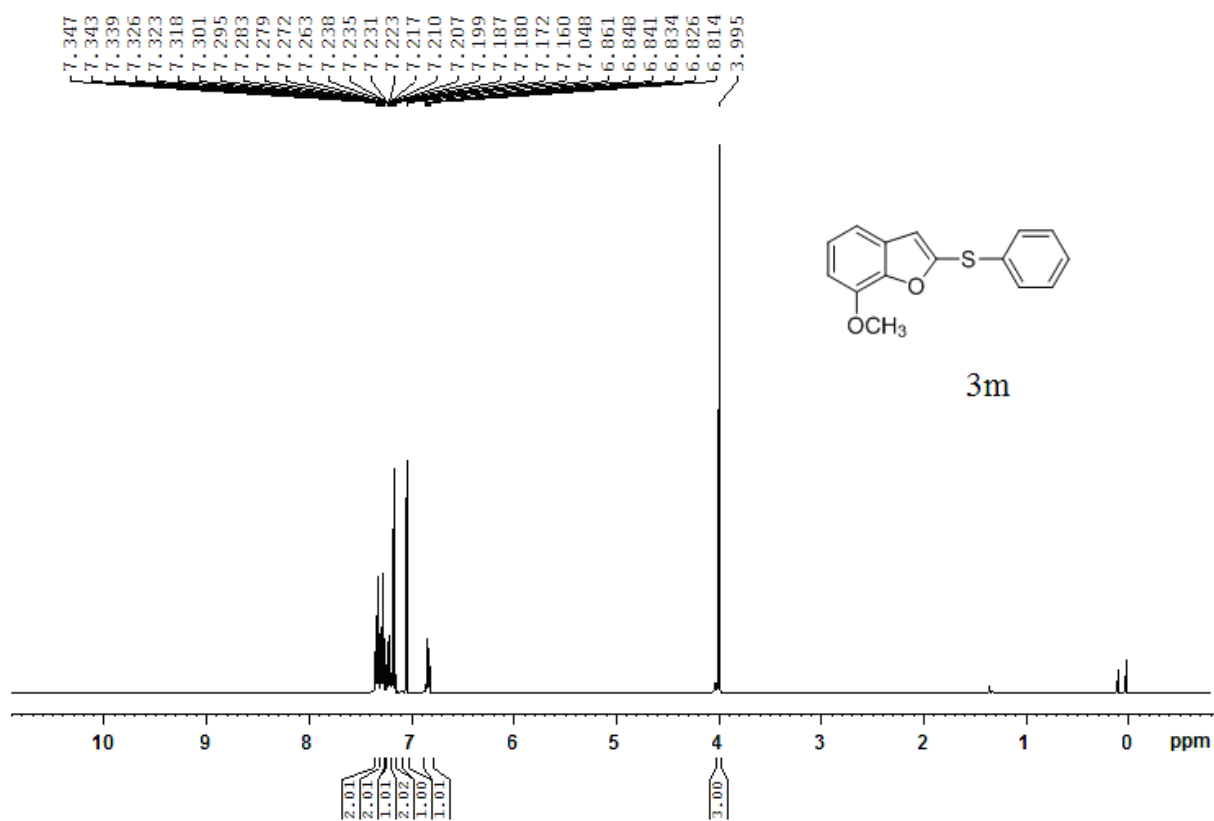




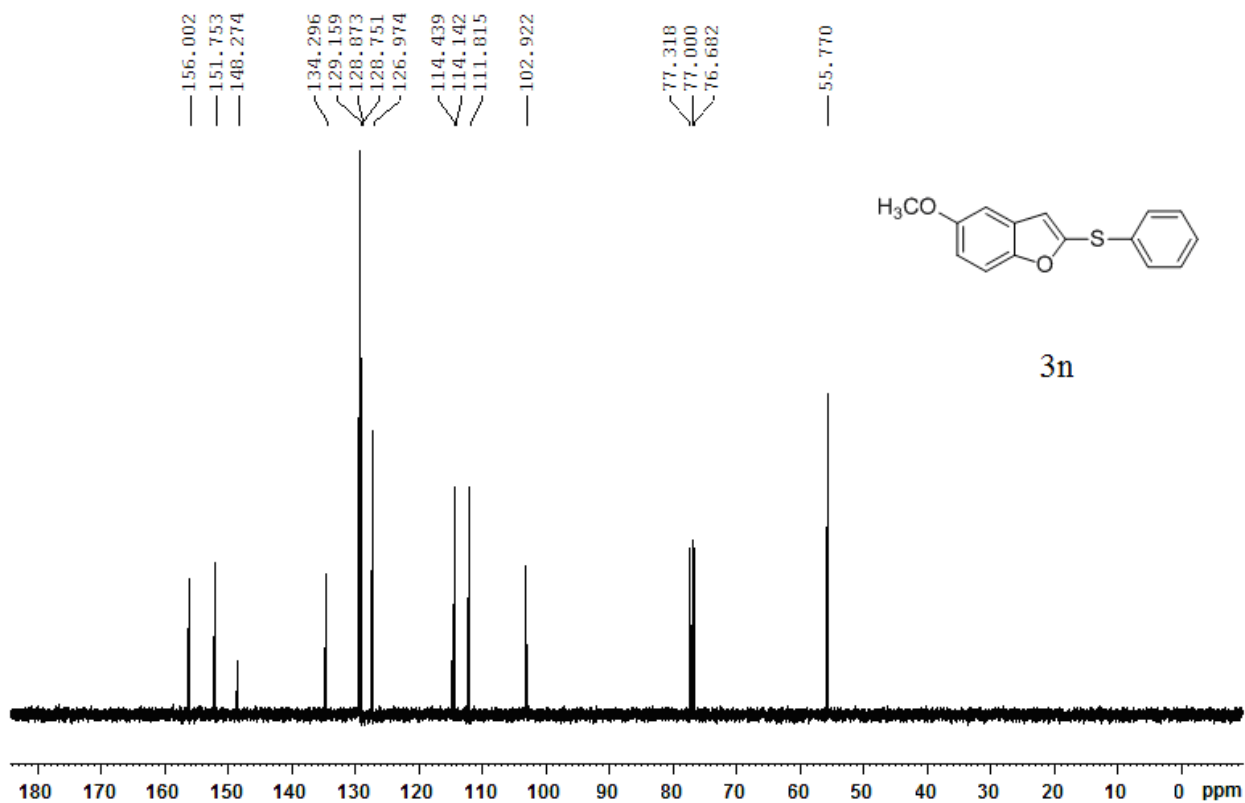
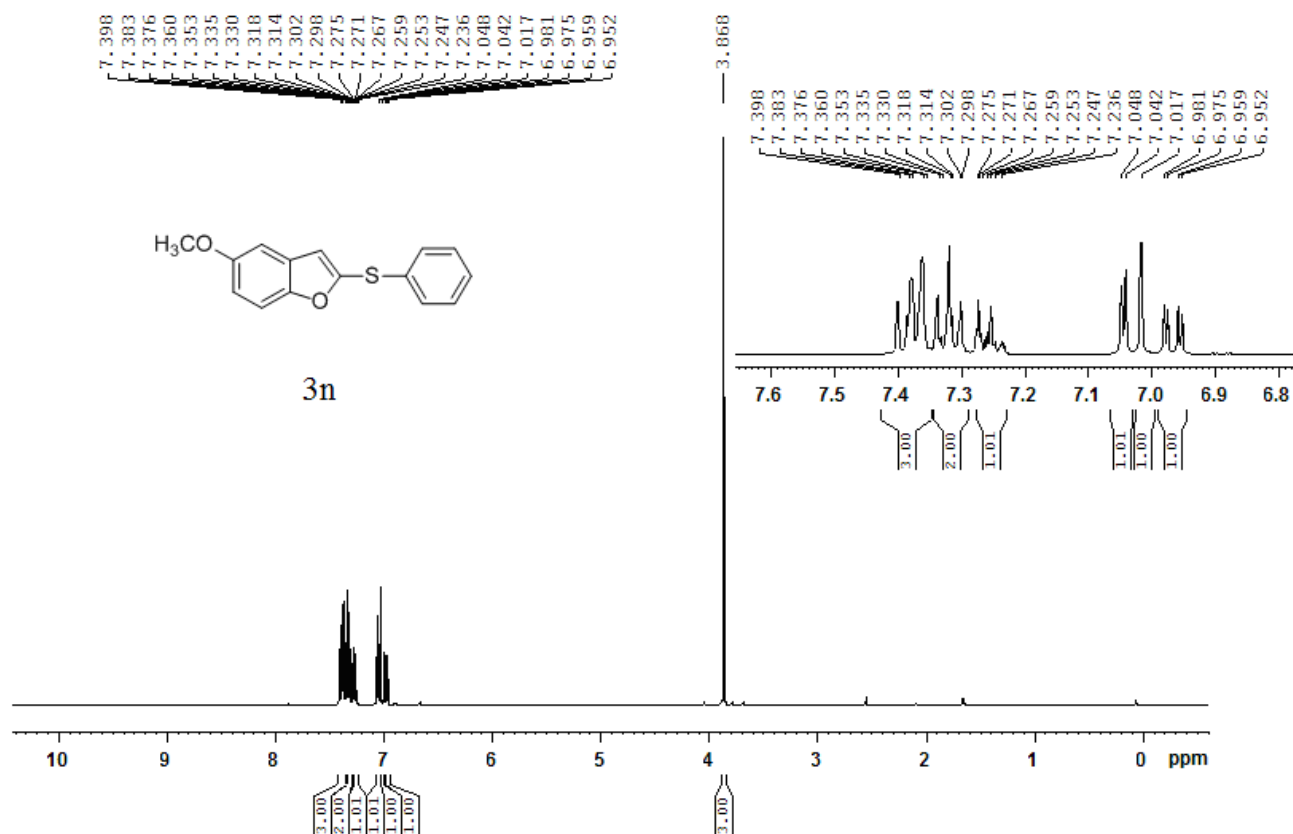


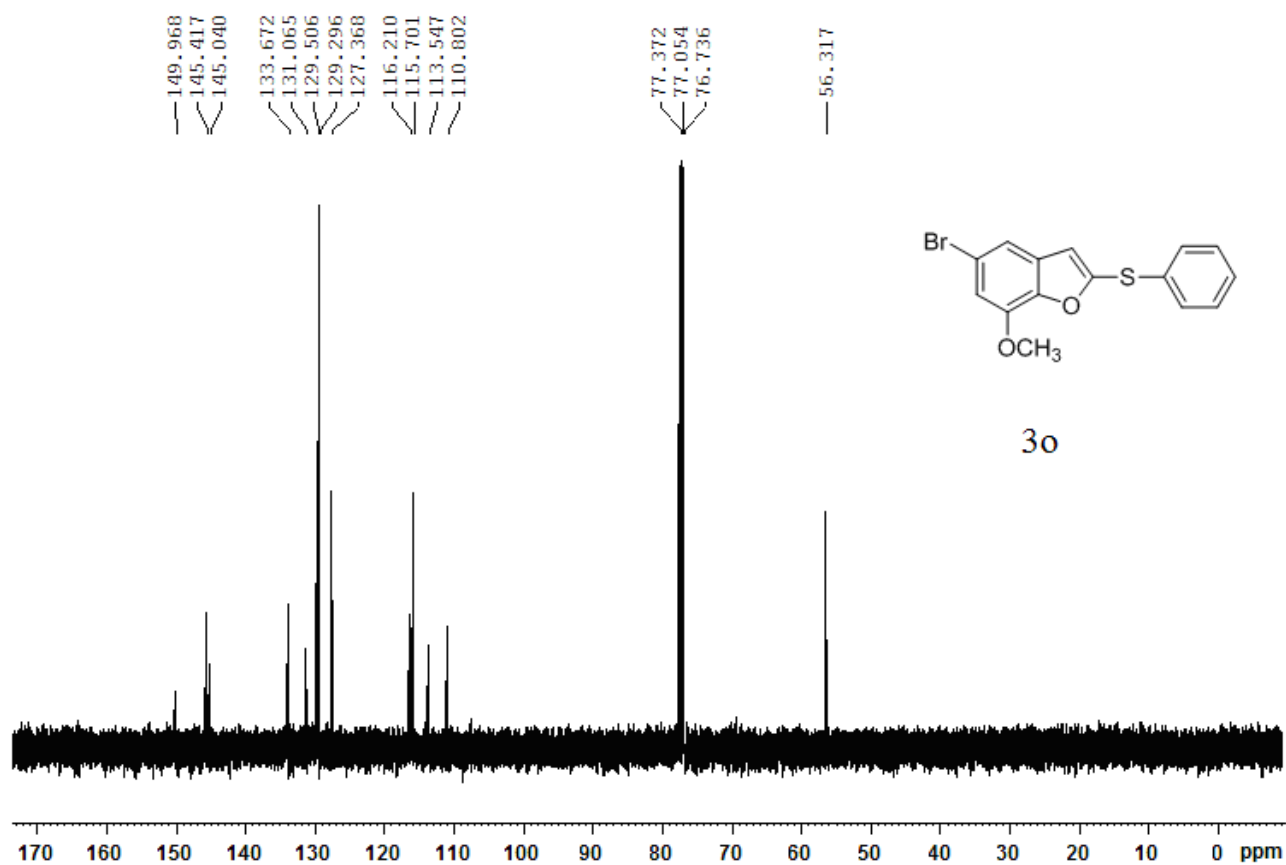
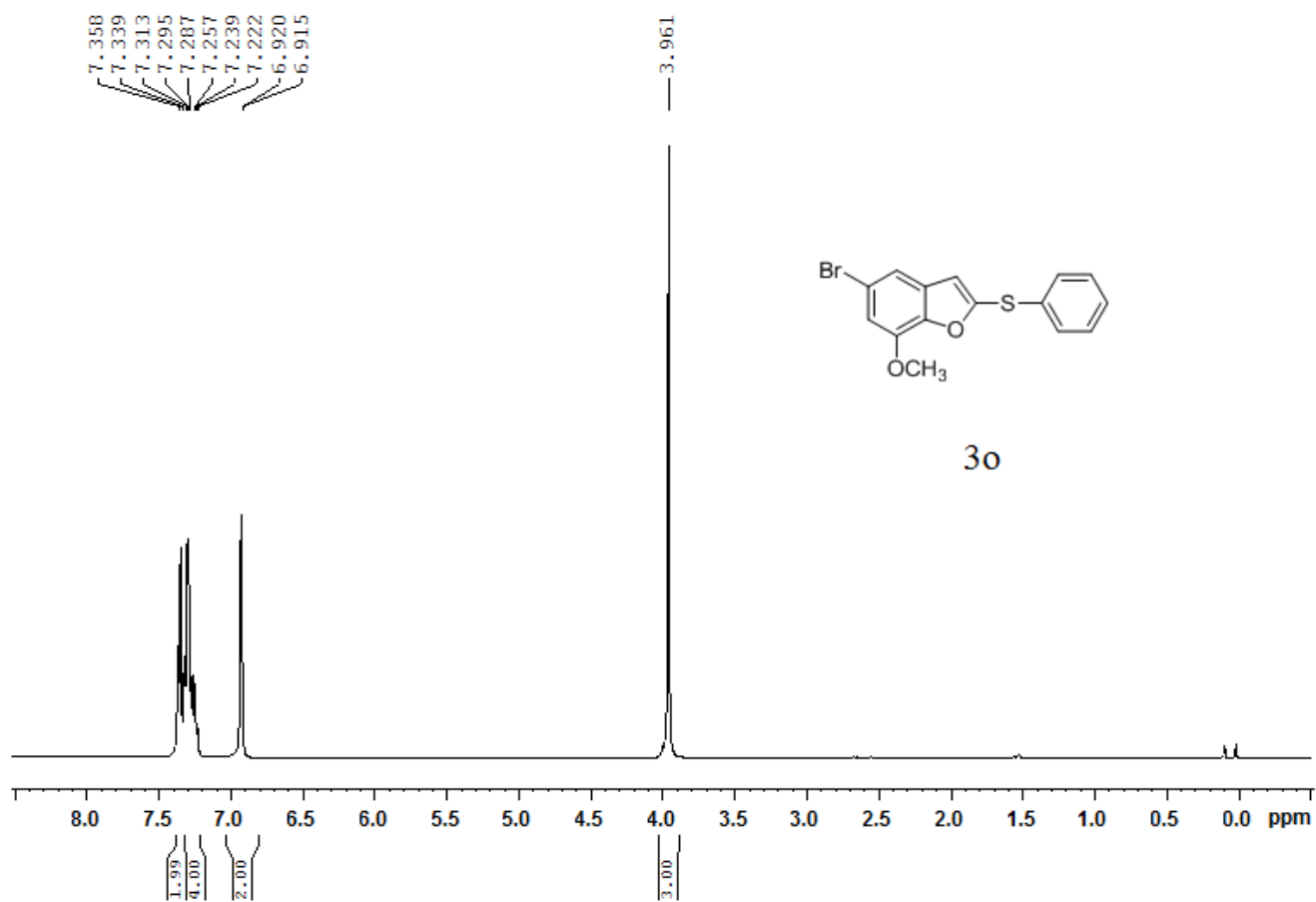


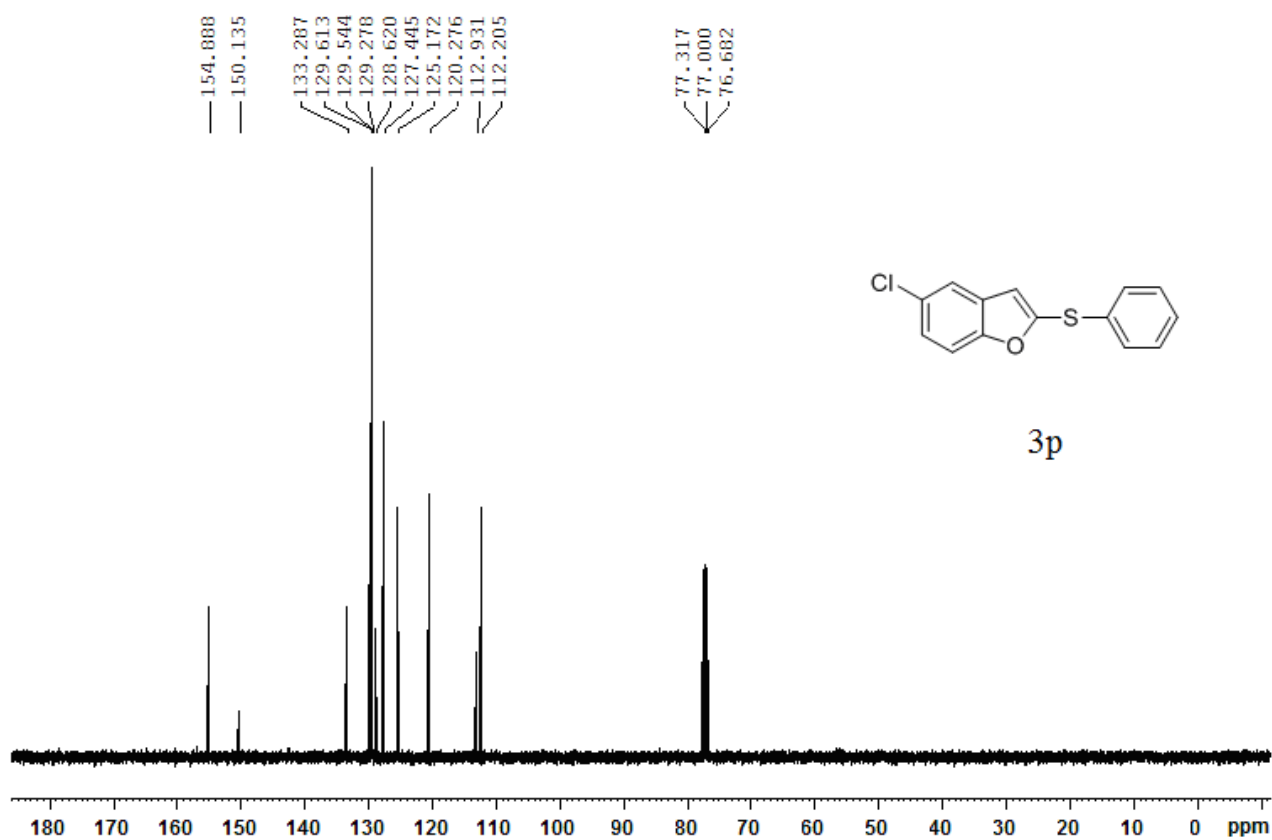
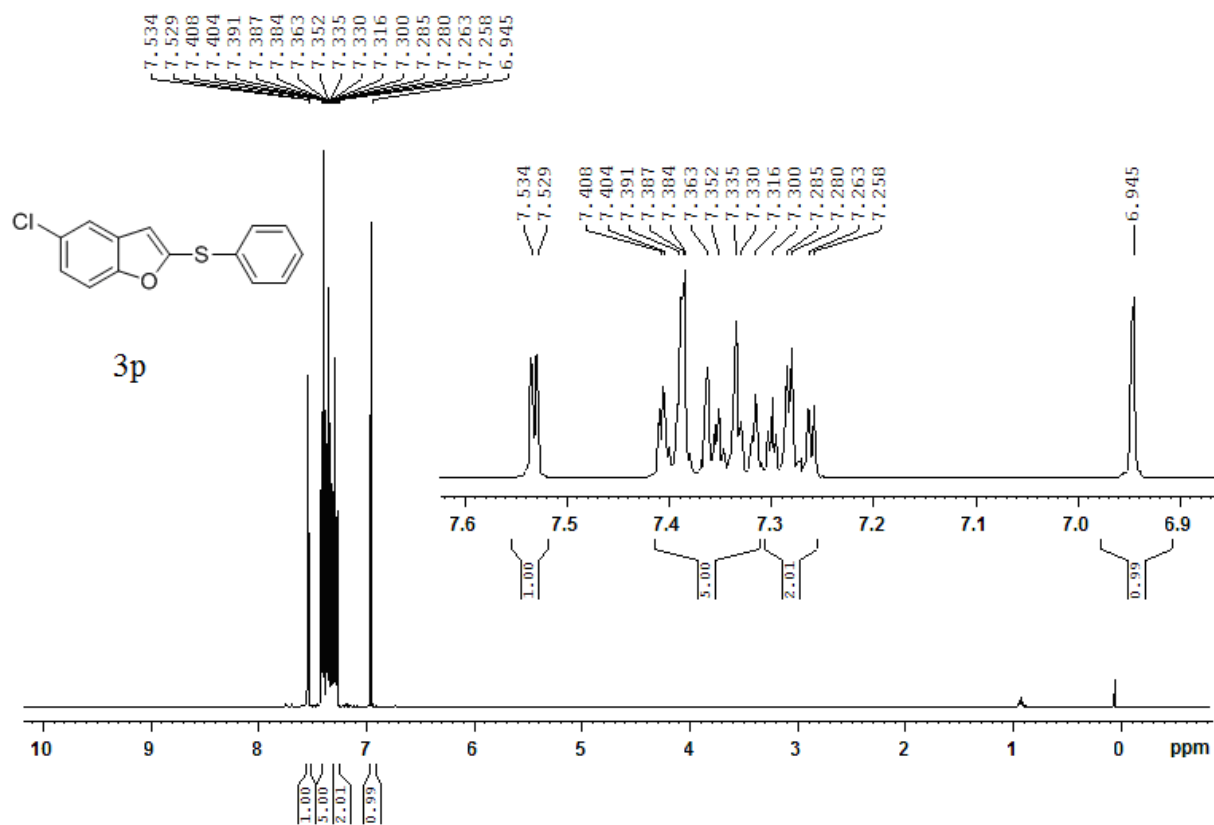


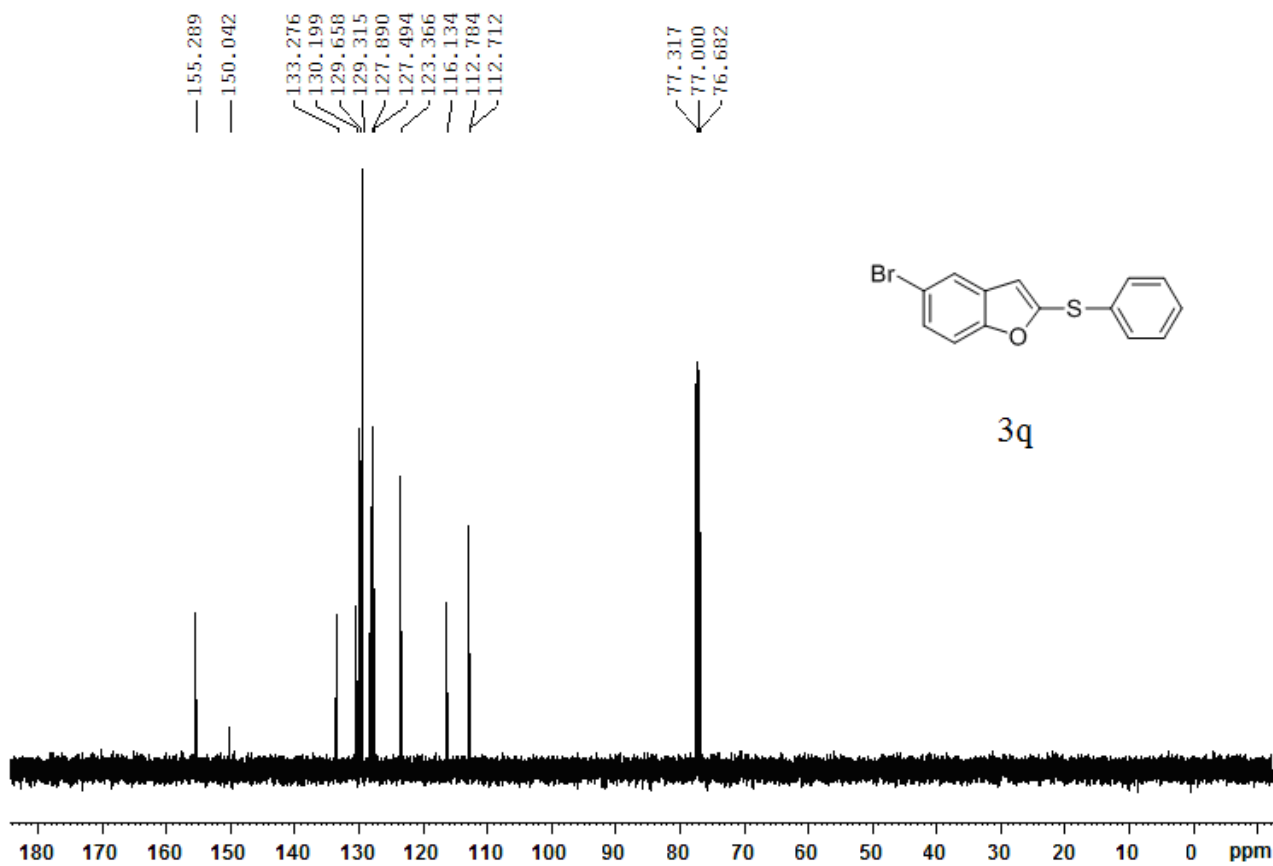
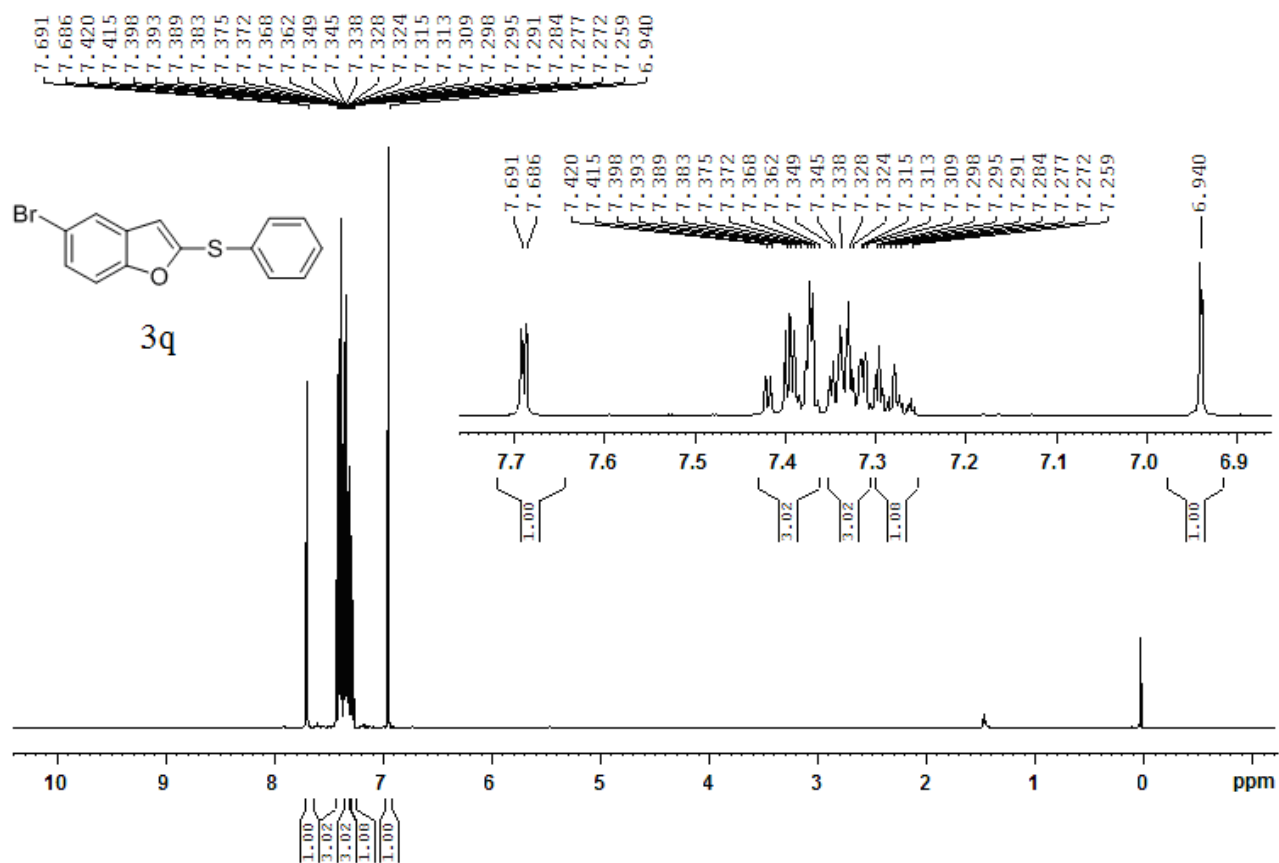


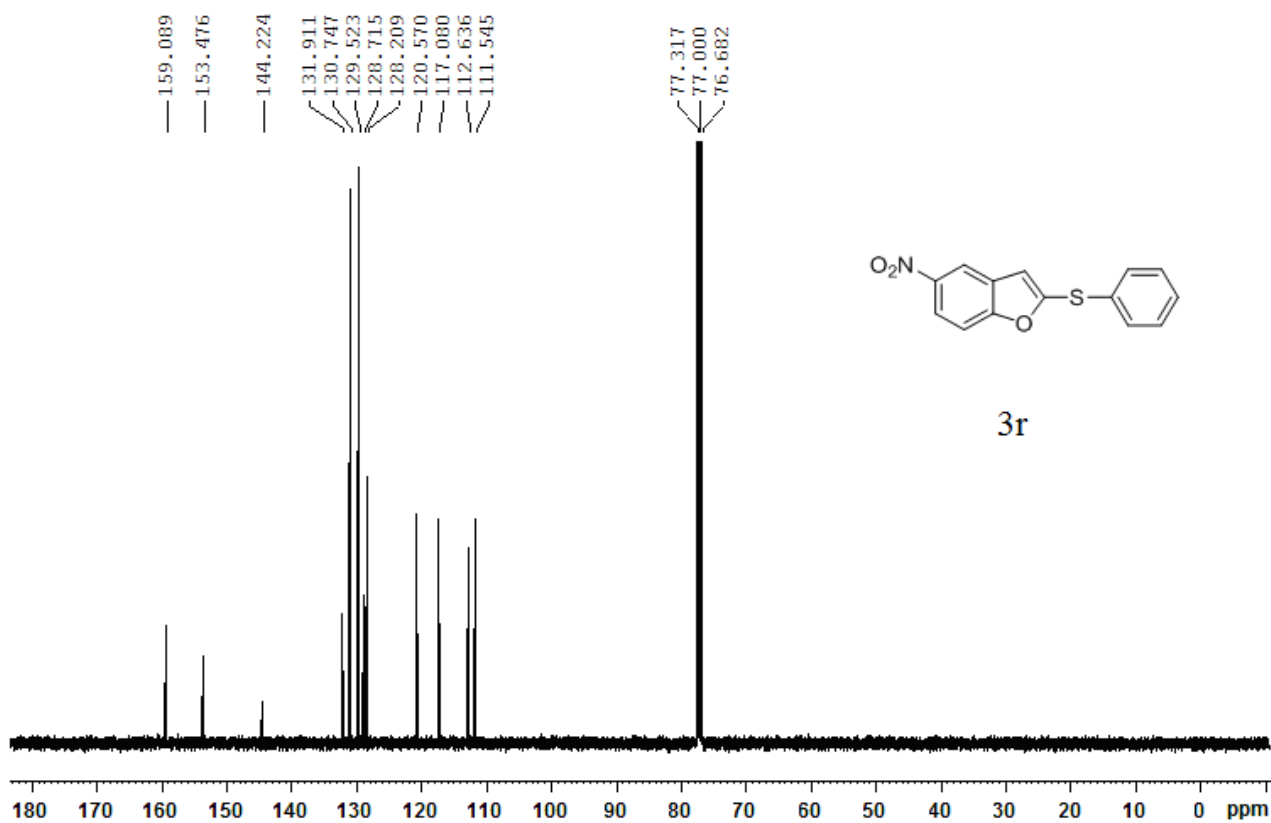
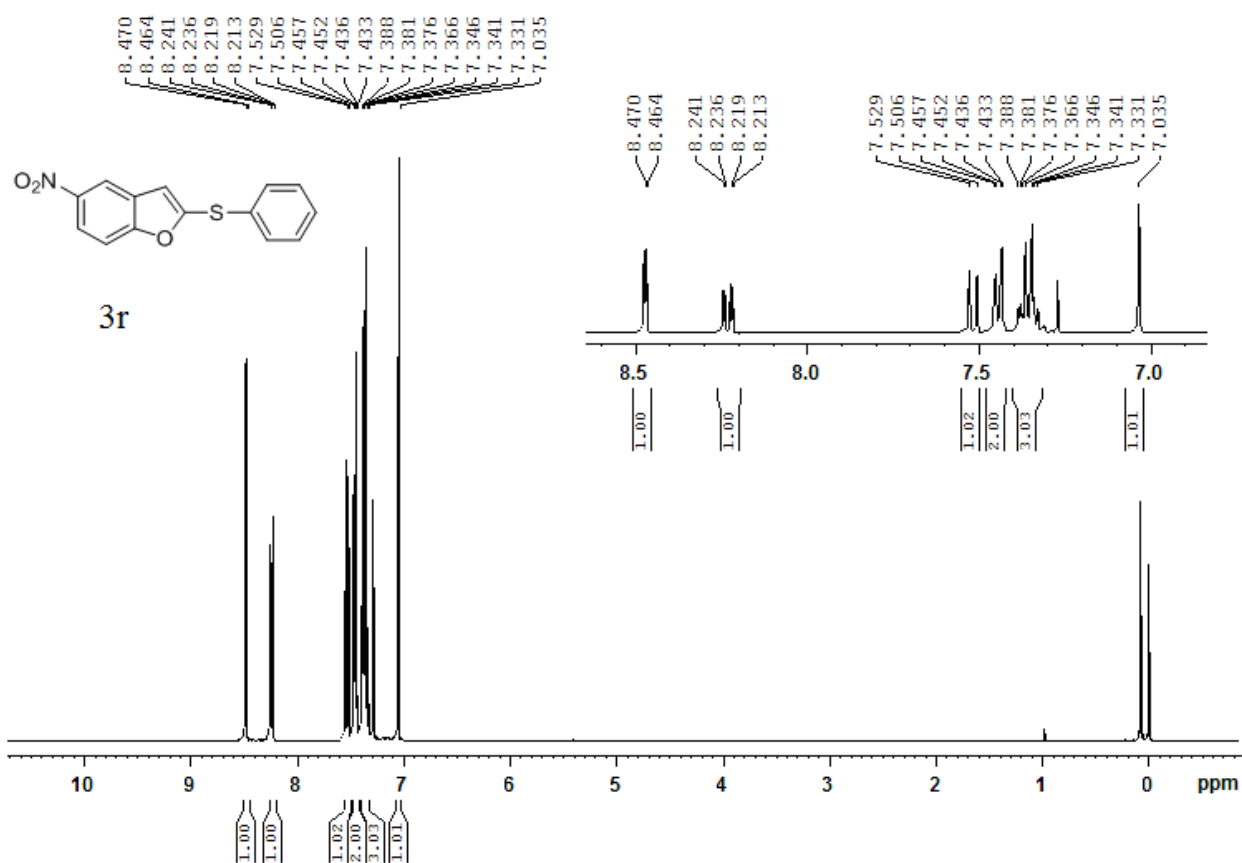


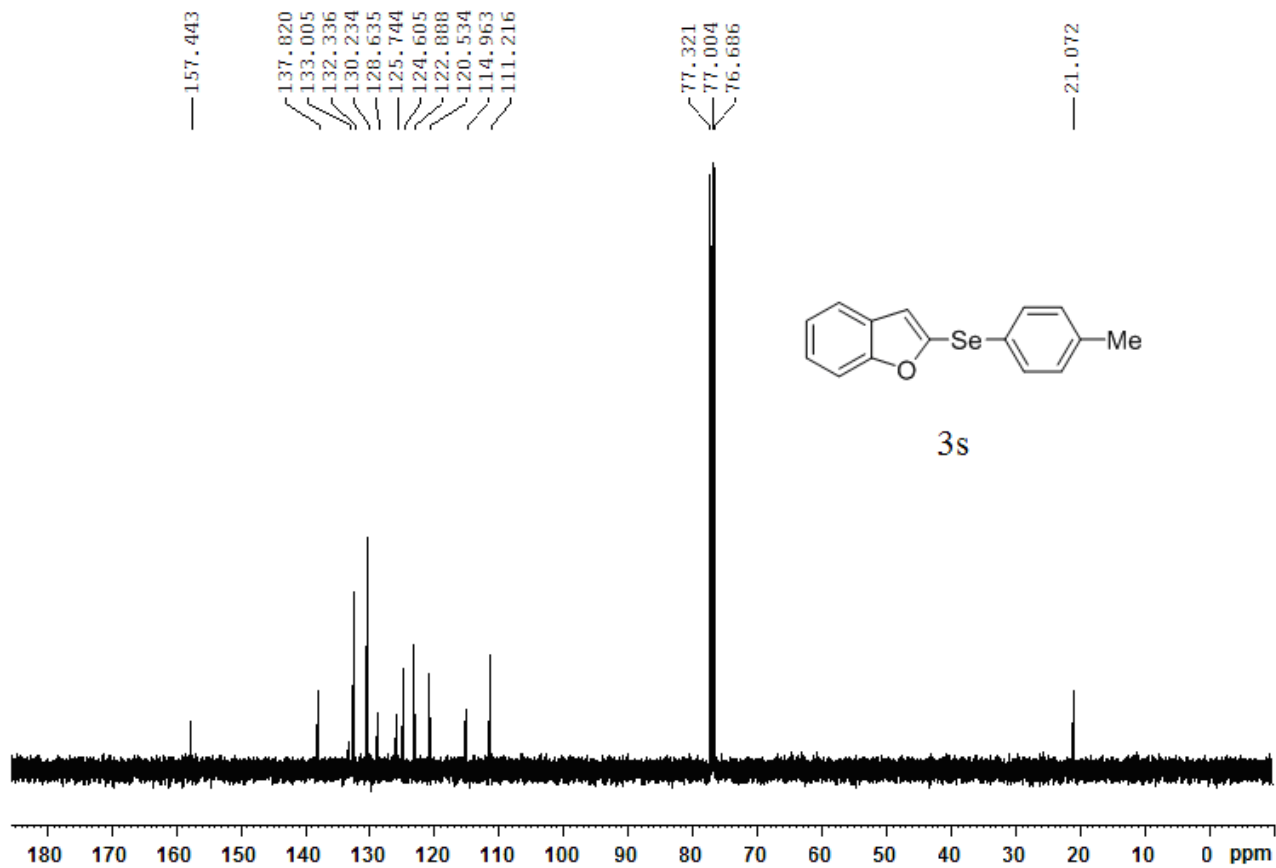
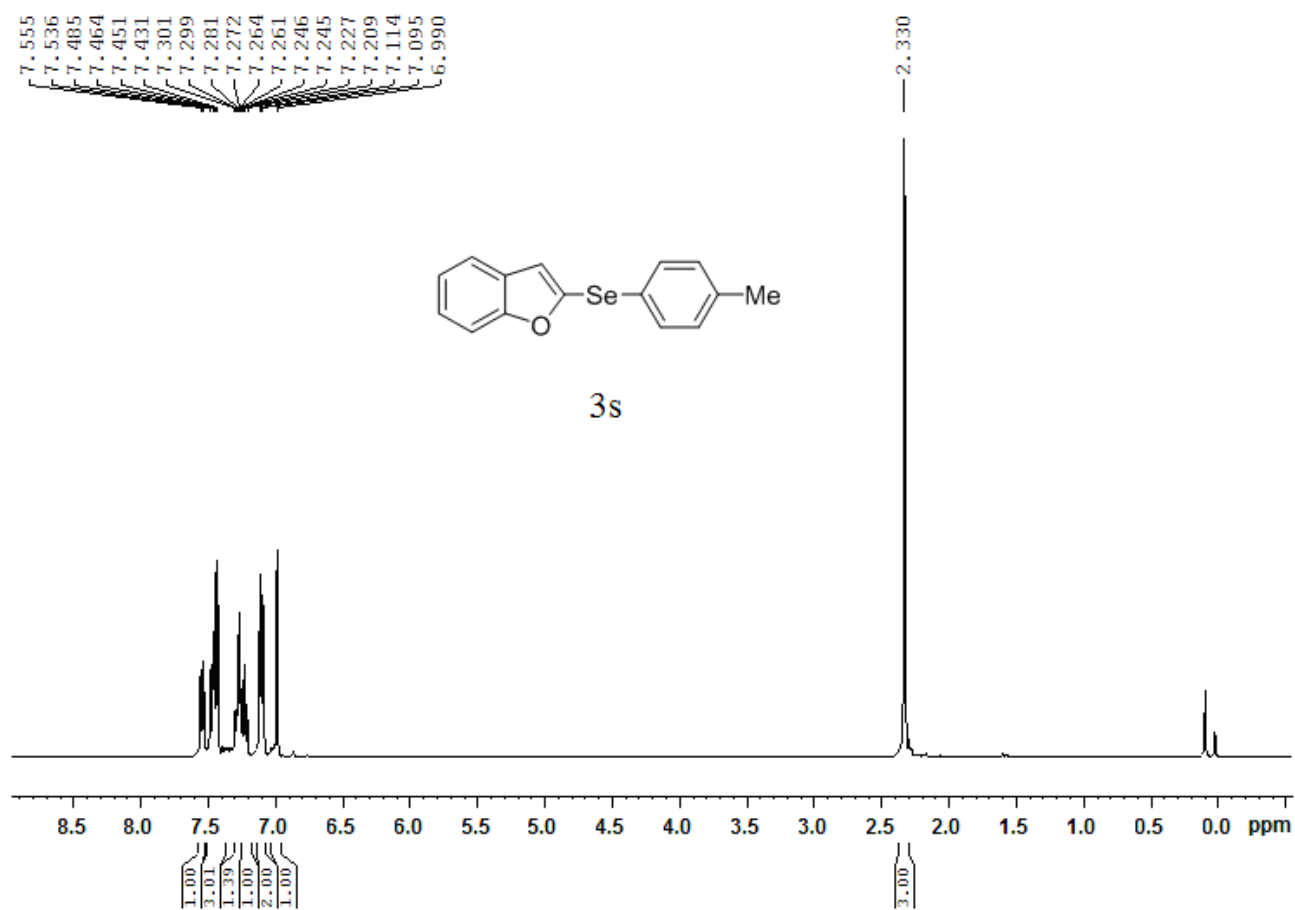


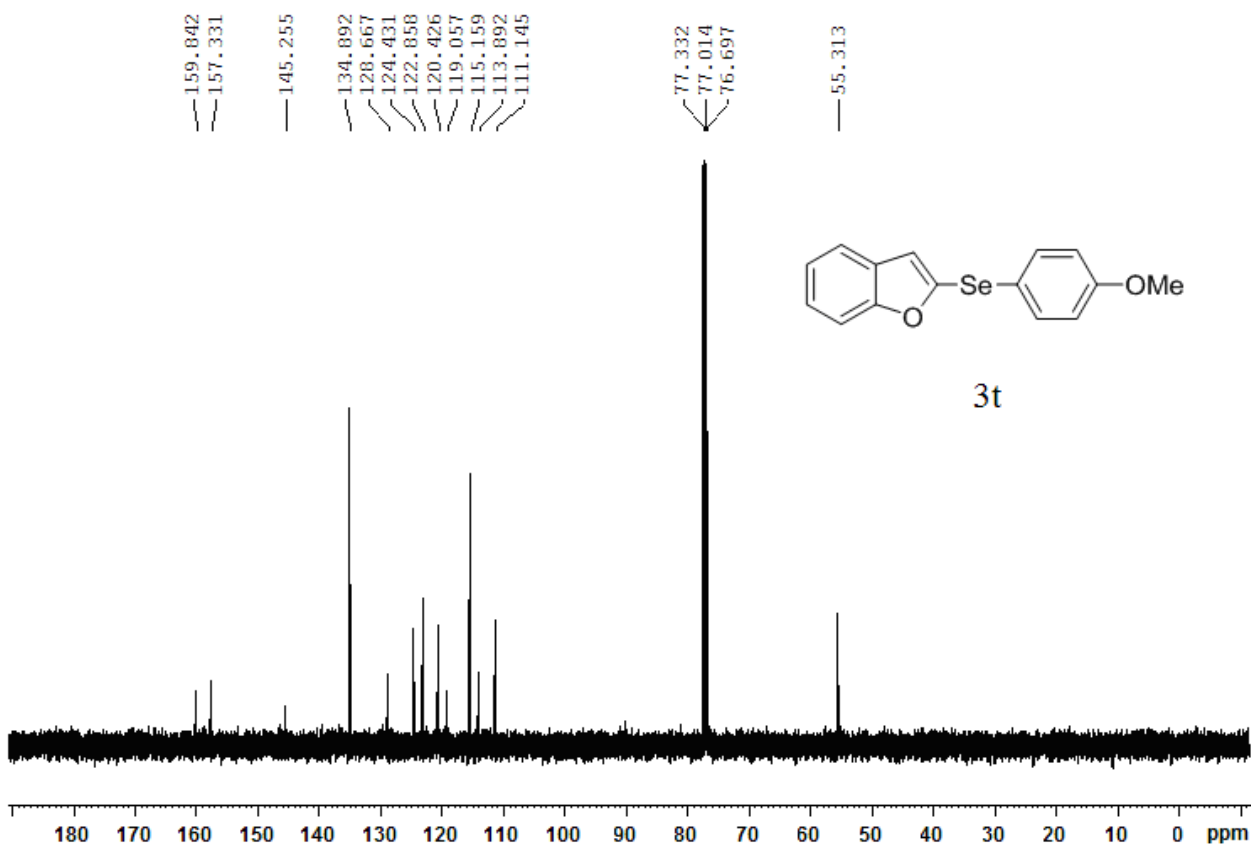
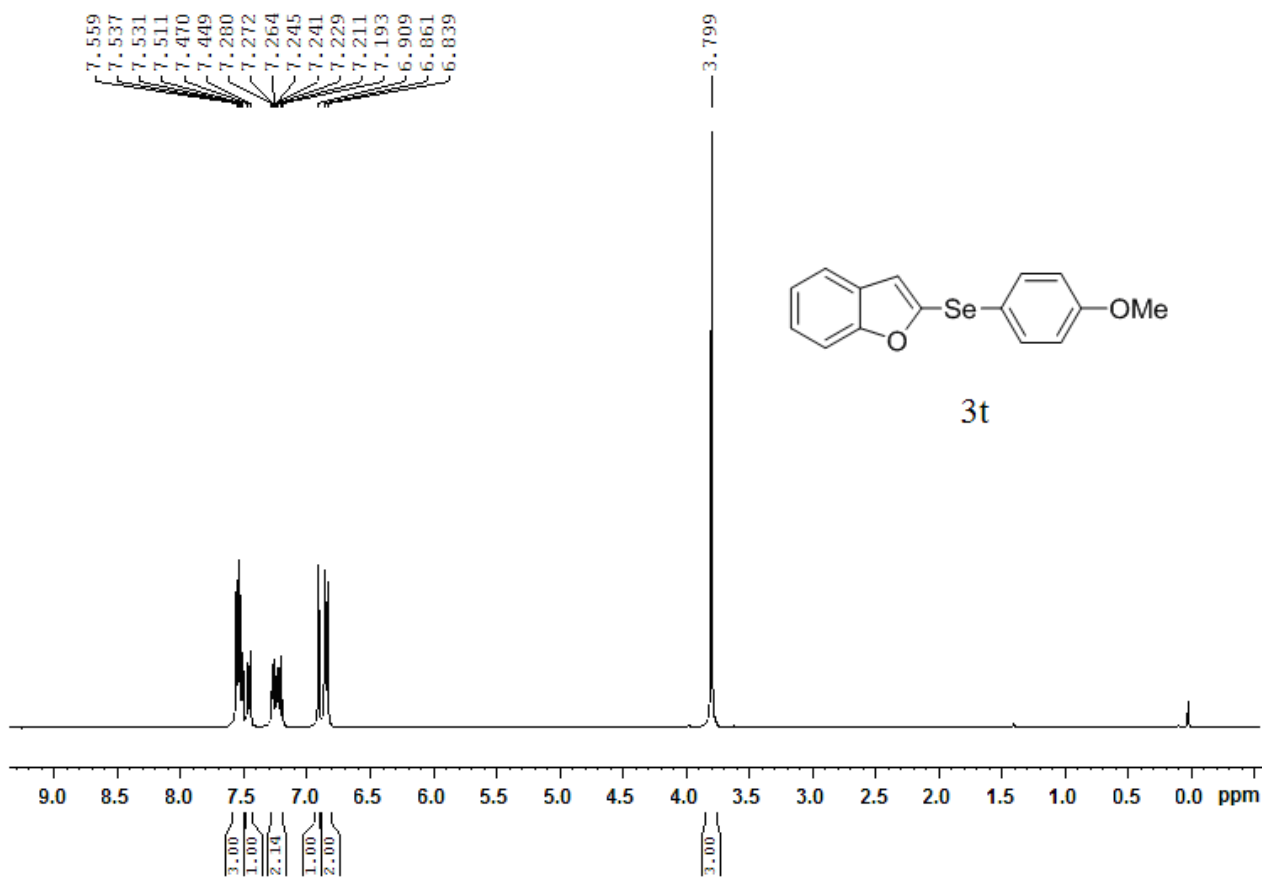


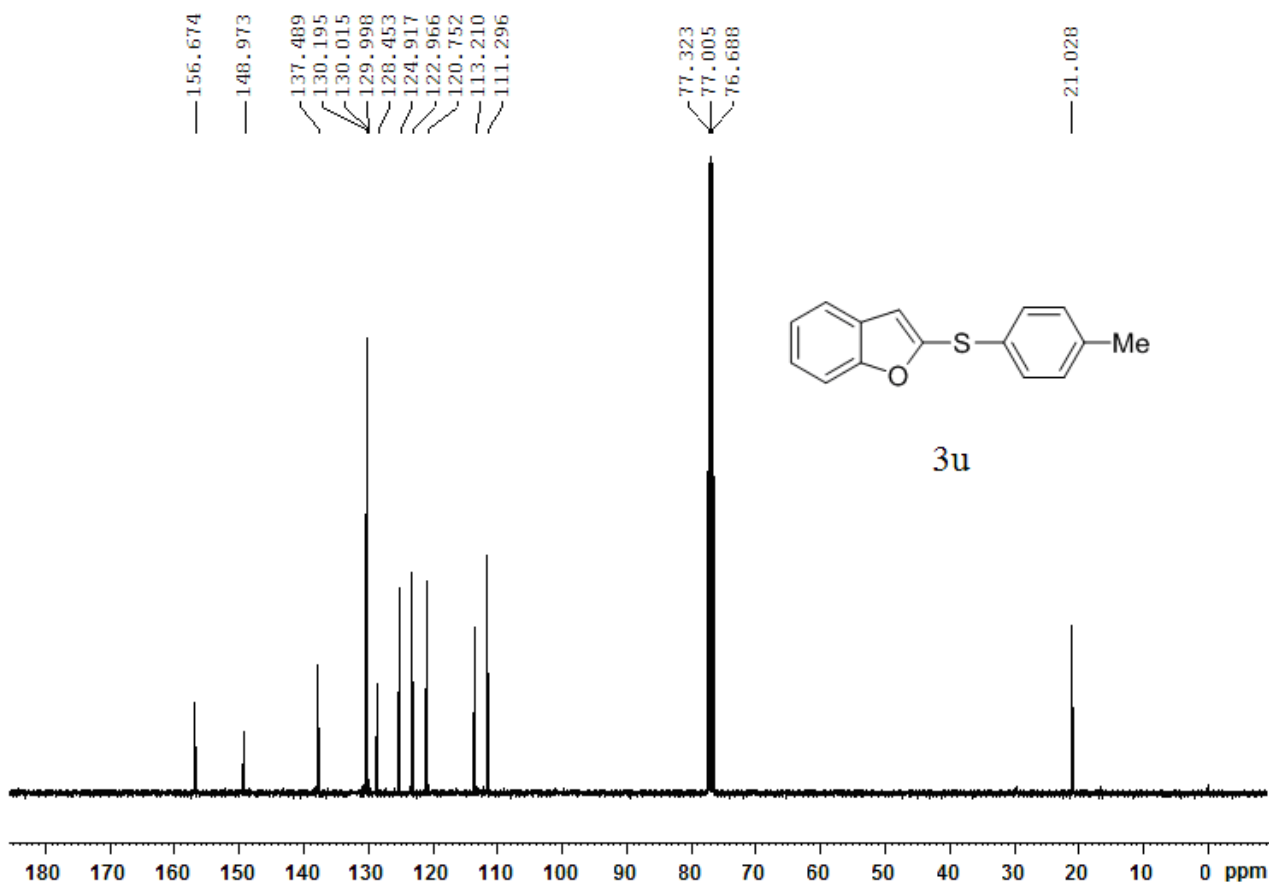
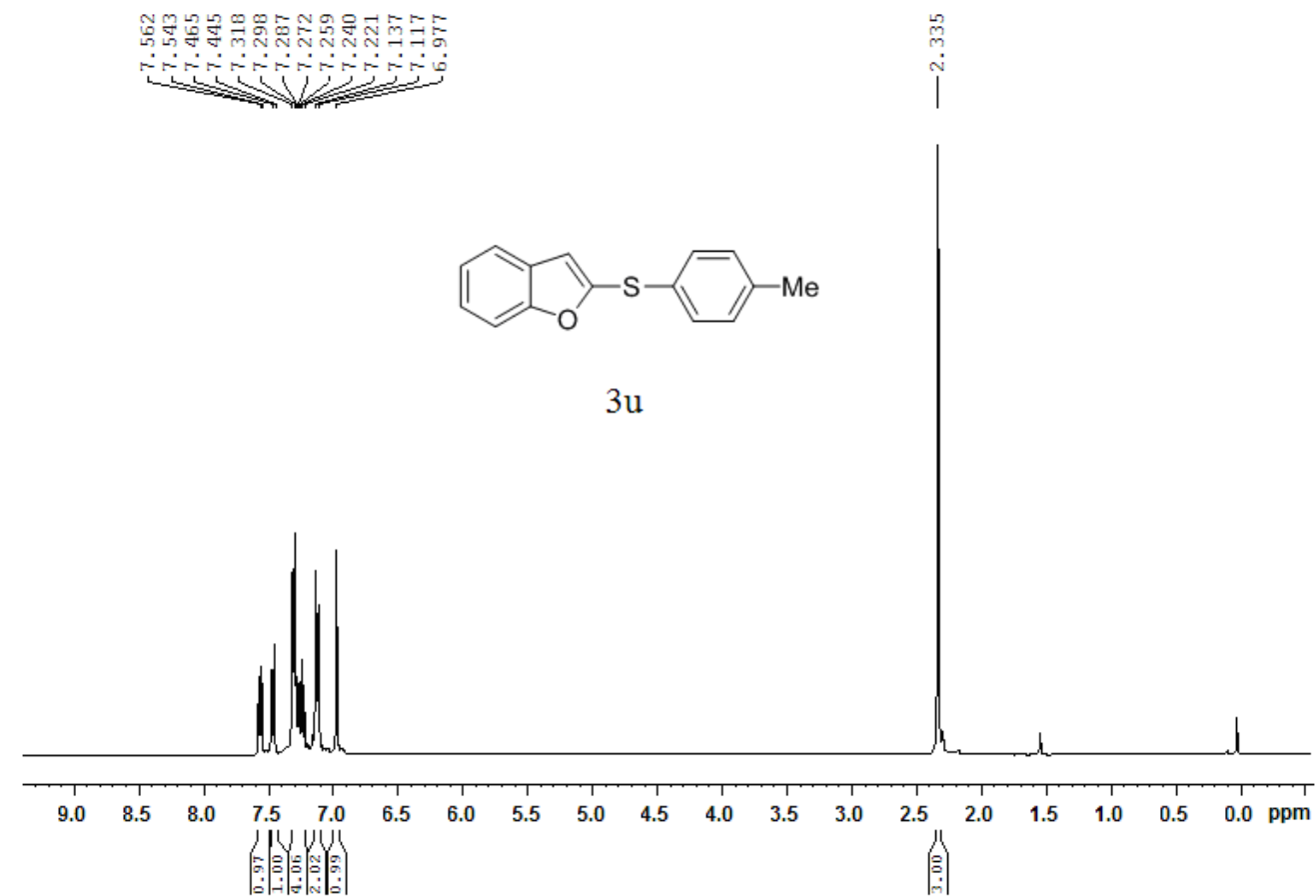




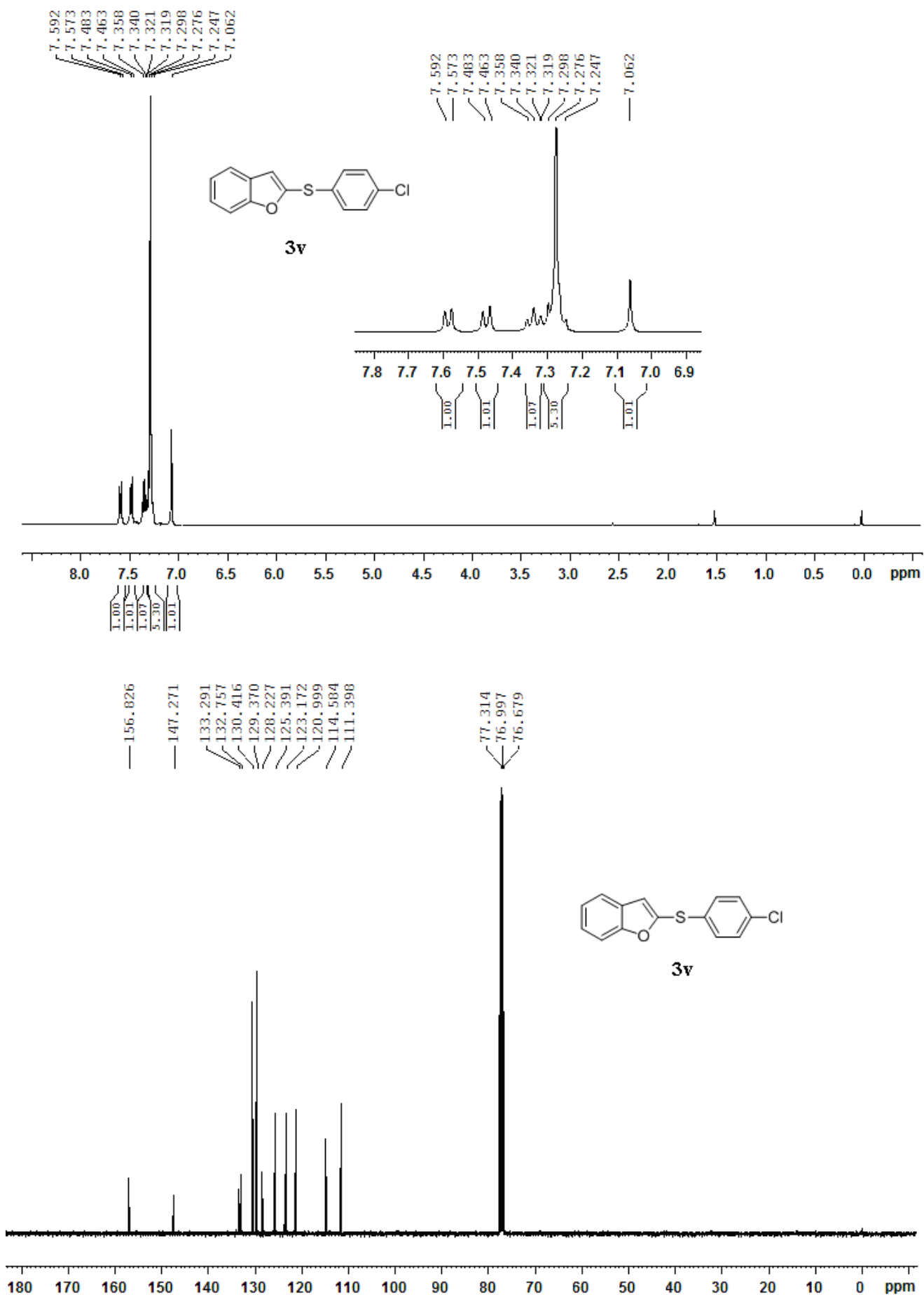


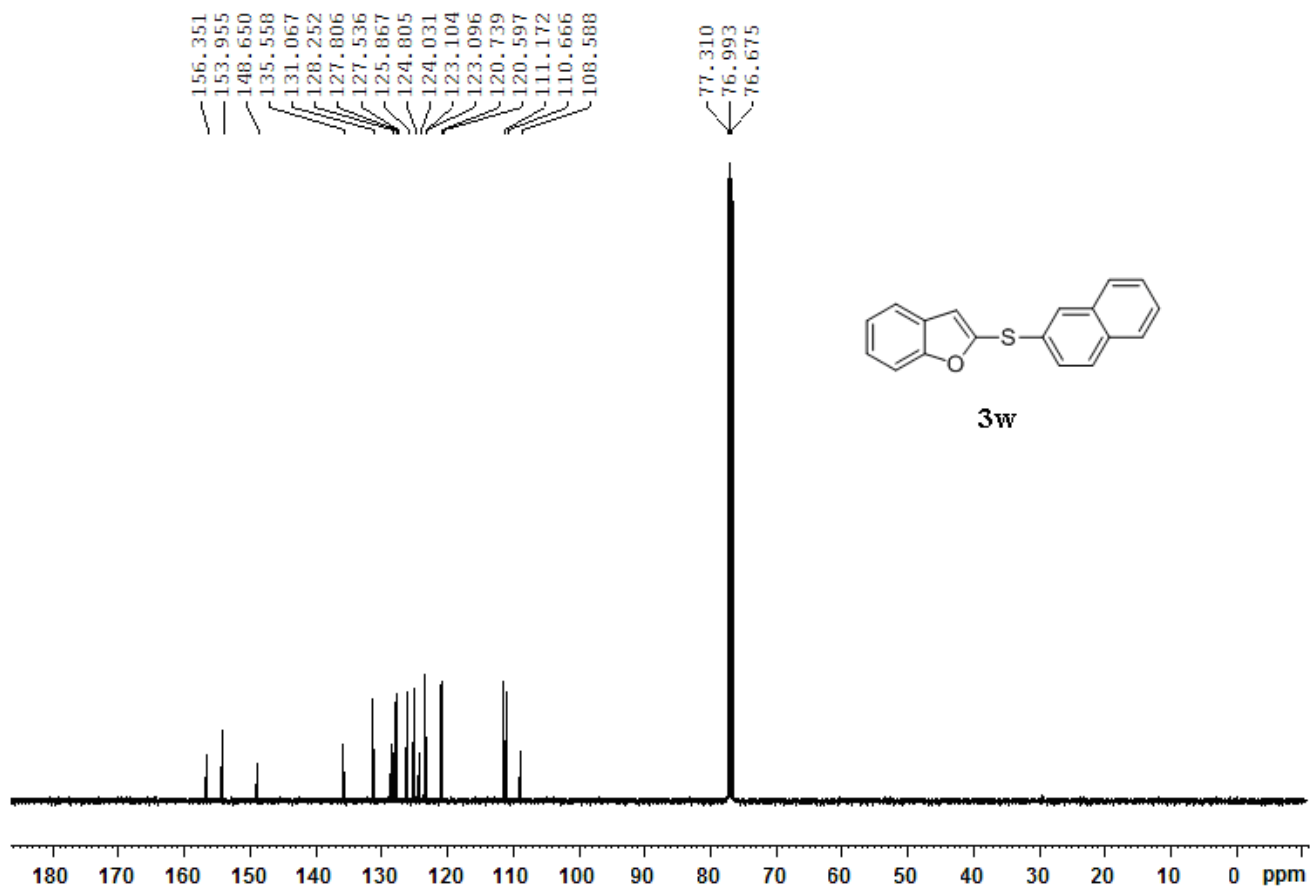
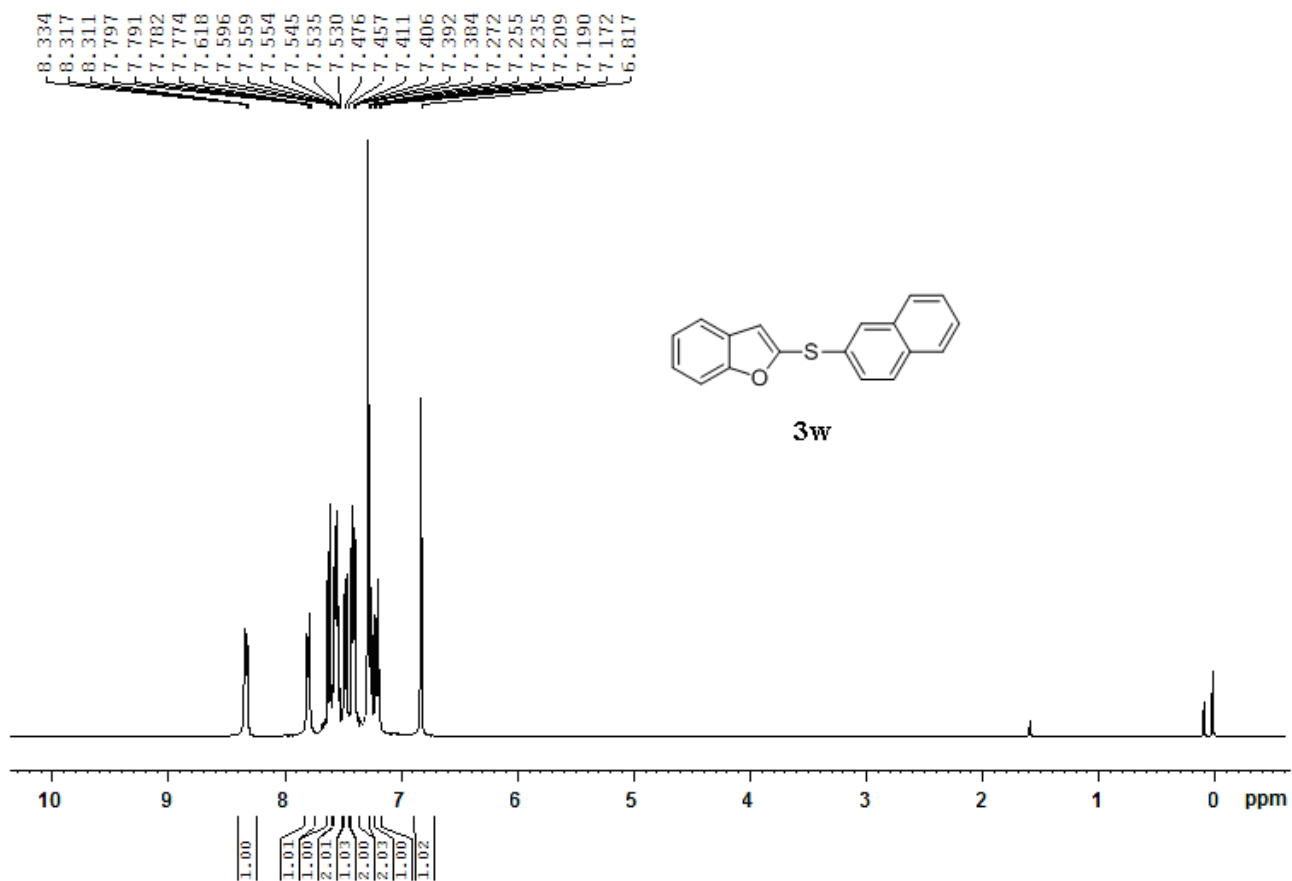


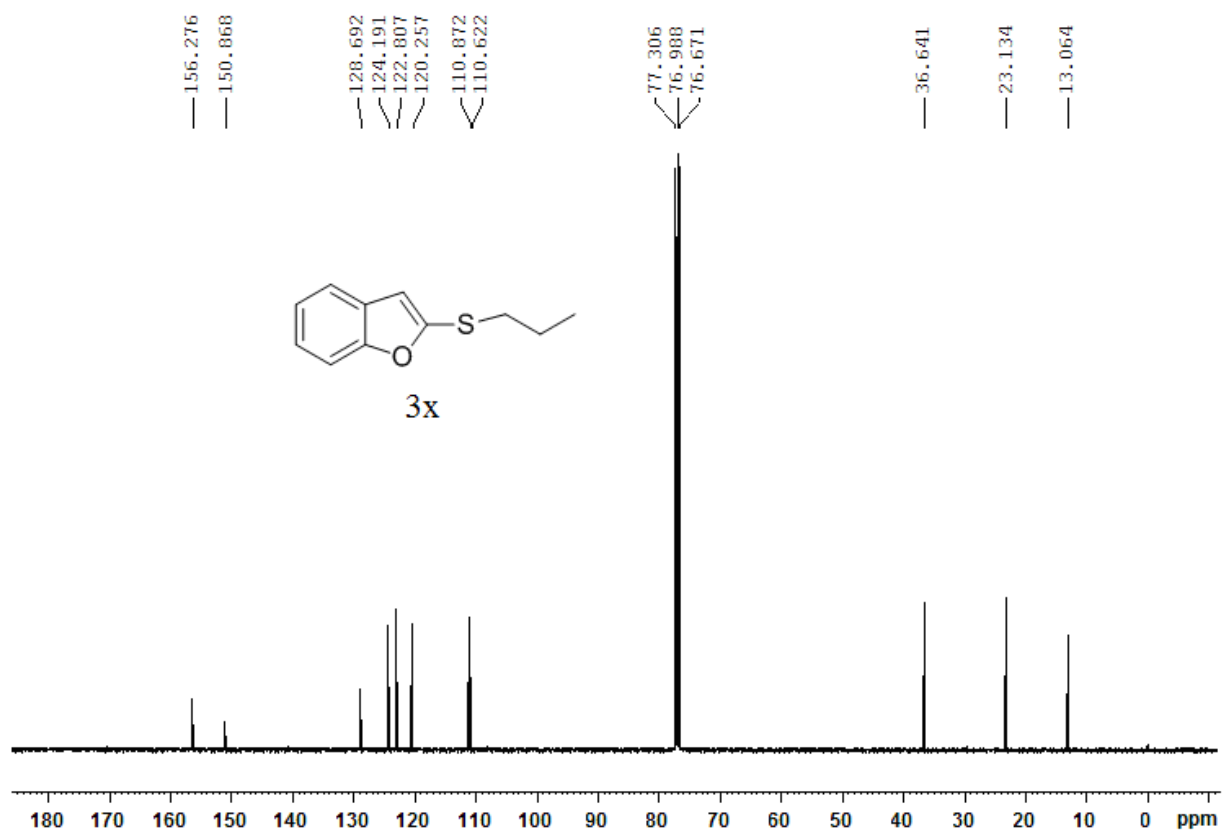
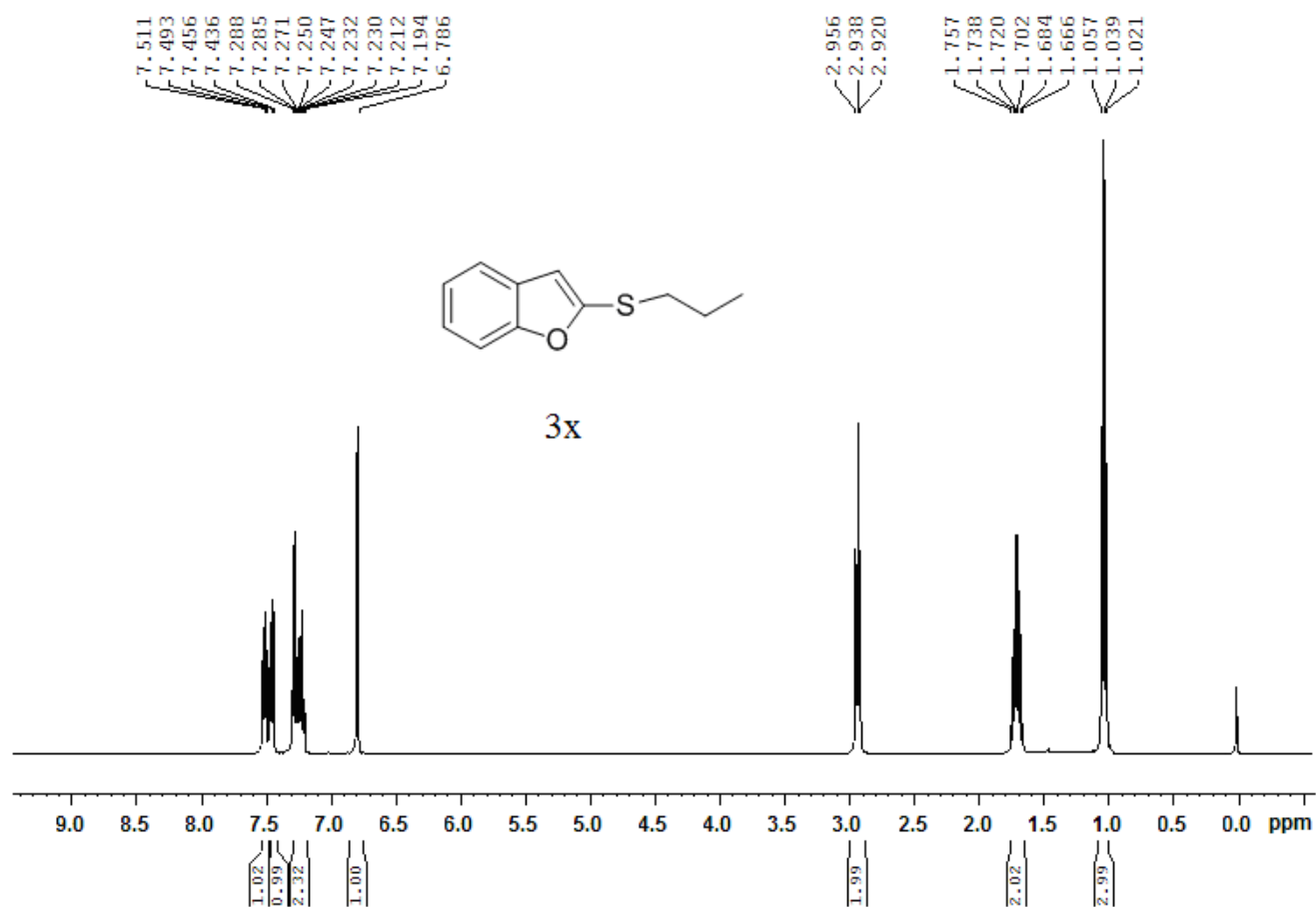












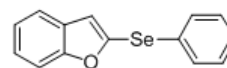
Shanghai Mass Spectrometry Center  
 Shanghai Institute of Organic Chemistry  
 Chinese Academic of Sciences  
 High Resolution MS Data Report



Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV  
 Card Serial Number: GCT-P-T11-03-OS0269

Sample Serial Number: HBSF-M35-S01

Operator: Li



3a

Date: 2011/04/01

Elemental Composition Report

Single Mass Analysis

Tolerance = 1.5 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

306 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-20 H: 0-80 N: 0-4 O: 0-4 F: 0-1 Se: 0-1

Minimum:

Maximum: 1.5 5.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
273.9900	273.9897	0.3	1.1	11.0	2.6	C14 H10 O Se
	273.9895	0.5	1.8	7.5	32.3	C9 H9 N3 O F Se
	273.9908	-0.8	-2.9	7.0	16.9	C11 H11 O2 F Se
	273.9889	1.1	4.0	16.5	475.8	C14 N3 O4

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

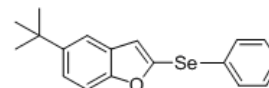


Instrument: Waters Micromass GCT Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-T11-11-OS0832

Sample Serial Number: HBSF-LiN9-213

Operator: Li



3b

Date: 2011/11/02

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions

387 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)

Minimum:

Maximum: 2.0 5.0 -1.5 50.0

Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
324.0579	324.0582	-0.3	-0.8	12.0	2	C19 H18 78Se
	324.0582	-0.3	-1.1	11.0	1	C18 H18 O 74Se
	324.0575	0.4	1.2	22.0	5	C25 H8 O
	324.0585	-0.6	-1.7	-1.5	4	C10 H29 O 77Se 82Se
	324.0589	-1.0	-3.0	1.0	3	C12 H28 74Se 78Se

Shanghai Mass Spectrometry Center<sup>†</sup>  
 Shanghai Institute of Organic Chemistry<sup>†</sup>  
 Chinese Academic of Sciences<sup>†</sup>  
 High Resolution MS Data Report



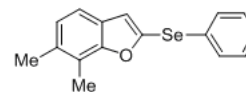
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-11-OS0848<sup>†</sup>

Sample Serial Number: HBSF-Li-N8-07<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/11/14<sup>†</sup>



3c

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Element prediction: Off <sup>†</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

898 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)<sup>†</sup>

Elements Used:<sup>†</sup>

C: 0-60 H: 0-80 N: 0-2 O: 0-2 74Se: 0-1 76Se: 0-1 77Se: 0-1 78Se: 0-1 80Se: 0-1 82Se: 0-1 <sup>†</sup>

Minimum: -1.5<sup>†</sup>

Maximum: 2.0 5.0 50.0<sup>†</sup>

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>†</sup>
296.0271	296.0272	-0.1	-0.3	-1.5	1332.4...	C8 H25 O 77Se 82Se <sup>†</sup>
	296.0269	0.2	0.7	11.0	22.7...	C16 H14 O 74Se <sup>†</sup>
	296.0269	0.2	0.7	12.0	718.0...	C17 H14 78Se <sup>†</sup>
	296.0273	-0.2	-0.7	9.0	1284.9...	C13 H14 N2 O 82Se <sup>†</sup>
	296.0276	-0.5	-1.7	1.0	620.8...	C10 H24 74Se 78Se <sup>†</sup>

Shanghai Mass Spectrometry Center<sup>†</sup>  
 Shanghai Institute of Organic Chemistry<sup>†</sup>  
 Chinese Academic of Sciences<sup>†</sup>  
 High Resolution MS Data Report



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

Card Serial Number: GCT-P-T11-11-OS0849<sup>†</sup>

Sample Serial Number: HBSF-Li-N8-08<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/11/14<sup>†</sup>

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Element prediction: Off <sup>†</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

870 formula(e) evaluated with 8 results within limits (all results (up to 1000) for each mass)<sup>†</sup>

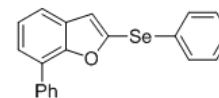
Elements Used:<sup>†</sup>

C: 0-60 H: 0-80 N: 0-1 O: 0-2 74Se: 0-1 76Se: 0-1 77Se: 0-1 78Se: 0-1 80Se: 0-1 82Se: 0-1 <sup>†</sup>

Minimum: -1.5<sup>†</sup>

Maximum: 2.0 5.0 50.0<sup>†</sup>

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>†</sup>
344.0264	344.0262	0.2	0.6	26.0	91.4...	C27 H4 O <sup>†</sup>
	344.0269	-0.5	-1.5	16.0	48.3...	C21 H14 78Se <sup>†</sup>
	344.0269	-0.5	-1.5	15.0	1.4...	C20 H14 O 74Se <sup>†</sup>
	344.0272	-0.8	-2.3	2.5	96.1...	C12 H25 O 77Se 82Se <sup>†</sup>
	344.0254	1.0	2.9	5.0	81.8...	C13 H23 N 74Se 77Se <sup>†</sup>
	344.0276	-1.2	-3.5	5.0	38.8...	C14 H24 74Se 78Se <sup>†</sup>
	344.0276	-1.2	-3.5	1.0	87.8...	C10 H25 N O2 76Se 77Se <sup>†</sup>
	344.0247	1.7	4.9	16.0	93.3...	C20 H13 N 77Se <sup>†</sup>



3d

Shanghai Mass Spectrometry Center<sup>†</sup>  
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Chinese Academic of Sciences<sup>†</sup>  
High Resolution MS Data Report<sup>†</sup>



Instrument: Waters Micromass GCT Premier

Ionisation Mode: EI+

Electron Energy: 70eV

Card Serial Number: GCT-P-T11-12-OS0872<sup>†</sup>

Sample Serial Number: HBSF-D11-CW-2<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/11/28<sup>†</sup>

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Element prediction: Off <sup>†</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

560 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)<sup>†</sup>

Elements Used:<sup>†</sup>

C: 0-60 H: 0-80 O: 0-6 74Se: 0-1 76Se: 0-1 77Se: 0-1 78Se: 0-1 80Se: 0-1 82Se: 0-1

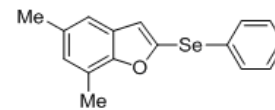
<sup>†</sup>

Minimum: -1.5<sup>†</sup>

Maximum: 2.0 5.0 50.0<sup>†</sup>

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>†</sup>
296.0267	296.0269	-0.2	-0.7	12.0	2773020.0	C17 H14 78Se <sup>†</sup>
	296.0269	-0.2	-0.7	11.0	2773012.8	C16 H14 O 74Se <sup>†</sup>
	296.0262	0.5	1.7	22.0	2773032.0	C23 H4 O <sup>†</sup>
	296.0272	-0.5	-1.7	-1.5	2773034.5	C8 H25 O 77Se 82Se <sup>†</sup>
	296.0276	-0.9	-3.0	1.0	2773024.5	C10 H24 74Se 78Se <sup>†</sup>

<sup>†</sup>



3e

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Shanghai Institute of Organic Chemistry<sup>†</sup>  
Chinese Academic of Sciences<sup>†</sup>  
High Resolution MS Data Report<sup>†</sup>



Instrument: Waters Micromass GCT Premier

Ionisation Mode: EI+

Electron Energy: 70eV

Card Serial Number: GCT-P-T11-12-OS0874<sup>†</sup>

Sample Serial Number: HBSF-D11-CW-4<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/11/28<sup>†</sup>

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Element prediction: Off <sup>†</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

498 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)<sup>†</sup>

Elements Used:<sup>†</sup>

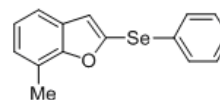
C: 0-60 H: 0-80 O: 0-6 74Se: 0-1 76Se: 0-1 77Se: 0-1 78Se: 0-1 80Se: 0-1 82Se: 0-1 <sup>†</sup>

<sup>†</sup>

Minimum: -1.5<sup>†</sup>

Maximum: 2.0 5.0 50.0<sup>†</sup>

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>†</sup>
282.0118	282.0119	-0.1	-0.4	1.0	2773050.8	C9 H22 74Se 78Se <sup>†</sup>
	282.0115	0.3	1.1	-1.5	2773063.5	C7 H23 O 77Se 82Se <sup>†</sup>
	282.0113	0.5	1.8	11.0	2773013.0	C15 H12 O 74Se <sup>†</sup>
	282.0112	0.6	2.1	12.0	2773032.0	C16 H12 78Se <sup>†</sup>
	282.0106	1.2	4.3	22.0	2773058.8	C22 H2 O <sup>†</sup>



3f

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Shanghai Institute of Organic Chemistry<sup>†</sup>  
Chinese Academic of Sciences<sup>†</sup>  
High Resolution MS Data Report<sup>†</sup>



Instrument: Waters Micromass GCT Ionisation Mode: EI<sup>+</sup> Electron Energy: 70eV<sup>†</sup>

Card Serial Number: GCT-T11-11-OS0833<sup>†</sup>

Sample Serial Number: HBSF-LiN9-214<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/11/02<sup>†</sup>

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

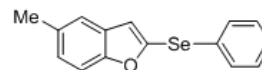
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%<sup>†</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

296 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)<sup>†</sup>

Minimum:				-1.5 <sup>†</sup>		
Maximum:		2.0	5.0	50.0 <sup>†</sup>		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula <sup>†</sup>
282.0109	282.0112	-0.3	-1.1	12.0	2...	C16 H12 78Se <sup>†</sup>
	282.0106	0.3	1.2	22.0	1...	C22 H2 O <sup>†</sup>
	282.0113	-0.4	-1.4	11.0	3...	C15 H12 O 74Se <sup>†</sup>
	282.0115	-0.6	-2.2	-1.5	4...	C7 H23 O 77Se 82Se <sup>†</sup>
	282.0119	-1.0	-3.7	1.0	5...	C9 H22 74Se 78Se <sup>†</sup>



3g

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Chinese Academic of Sciences<sup>†</sup>  
High Resolution MS Data Report<sup>†</sup>



Instrument: Waters Micromass GCT Premier Ionisation Mode: EI<sup>+</sup> Electron Energy: 70eV

Card Serial Number: GCT-P-T11-12-OS0873<sup>†</sup>

Sample Serial Number: HBSF-D11-CW-3<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/11/28<sup>†</sup>

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Element prediction: Off <sup>†</sup>

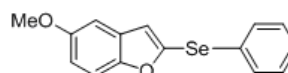
Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

571 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)<sup>†</sup>

Elements Used:<sup>†</sup>

C: 0-60 H: 0-80 O: 0-6 74Se: 0-1 76Se: 0-1 77Se: 0-1 78Se: 0-1 80Se: 0-1 82Se: 0-1

Minimum:									
Maximum:		2.0	5.0	50.0 <sup>†</sup>					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>†</sup>			
298.0061	298.0061	0.0	0.0	12.0	114.6...	C16 H12 O 78Se <sup>†</sup>			
	298.0062	-0.1	-0.3	11.0	3.9...	C15 H12 O2 74Se <sup>†</sup>			
	298.0064	-0.3	-1.0	-1.5	191.9...	C7 H23 O2 77Se 82Se <sup>†</sup>			
	298.0055	0.6	2.0	22.0	181.6...	C22 H2 O2 <sup>†</sup>			
	298.0068	-0.7	-2.3	1.0	146.3...	C9 H22 O 74Se 78Se <sup>†</sup>			



3h

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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-OS0878

Sample Serial Number: HBSF-D11-CW-8

Operator: Li

Date: 2011/11/28

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

1017 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)

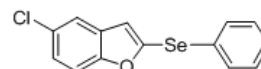
Elements Used:

C: 0-60 H: 0-80 O: 0-6 Cl: 0-1 74Se: 0-1 76Se: 0-1 77Se: 0-1 78Se: 0-1 80Se: 0-1 82Se: 0-1

Minimum:

Maximum: 2.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
301.9570	301.9569	0.1	0.3	1.5	2773127.0	C7 H17 O3 76Se 77Se
	301.9569	0.1	0.3	-1.5	2773128.3	C6 H20 O Cl 77Se 82Se
	301.9573	-0.3	-1.0	1.0	2773113.3	C8 H19 Cl 74Se 78Se
	301.9567	0.3	1.0	11.0	2773015.5	C14 H9 O Cl 74Se
	301.9566	0.4	1.3	12.0	2773090.5	C15 H9 Cl 78Se



3i

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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-OS0871

Sample Serial Number: HBSF-D11-CW-1

Operator: Li

Date: 2011/11/28

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

537 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

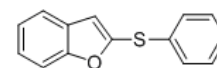
Elements Used:

C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 Br: 0-1

Minimum:

Maximum: 2.0 5.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
226.0454	226.0452	0.2	0.9	10.0	3.5	C14 H10 O S
	226.0457	-0.3	-1.3	5.5	7124.3	C11 H13 N S Cl
	226.0464	-1.0	-4.4	6.5	647.9	C8 H8 N3 O5



3j



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 High Resolution MS Data Report<sup>†</sup>



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

Card Serial Number: GCT-P-T11-12-OS0876<sup>†</sup>

Sample Serial Number: HBSF-D11-CW-6<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/11/28<sup>†</sup>

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Element prediction: Off <sup>†</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

373 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)<sup>†</sup>

Elements Used:<sup>†</sup>

C: 0-60 H: 0-80 N: 0-2 O: 0-6 S: 0-1 Cl: 0-1 Br: 0-1 <sup>†</sup>

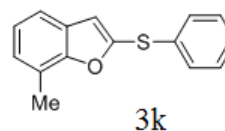
Minimum:

-1.5<sup>†</sup>

Maximum:

50.0<sup>†</sup>

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>†</sup>
240.0610	240.0609	0.1	0.4	10.0	3.6..	C15 H12 O S <sup>†</sup>
	240.0614	-0.4	-1.7	5.5	822.4..	C12 H15 N S Cl <sup>†</sup>
	240.0599	1.1	4.6	-0.5	1398.9..	C8 H19 N O2 Br <sup>†</sup>



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

Card Serial Number: GCT-P-T11-12-OS0937<sup>†</sup>

Sample Serial Number: HBSF-D28-S26<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/12/15<sup>†</sup>

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Element prediction: Off <sup>†</sup>

<sup>†</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

403 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)<sup>†</sup>

Elements Used:<sup>†</sup>

C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Br: 0-1 <sup>†</sup>

<sup>†</sup>

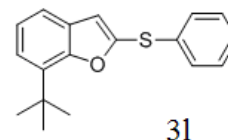
Minimum:

-1.5<sup>†</sup>

Maximum:

50.0<sup>†</sup>

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>†</sup>
282.1079	282.1078	0.1	0.4	10.0	50.2..	C18 H18 O S <sup>†</sup>
	282.1069	1.0	3.5	-0.5	13310.2..	C11 H25 N O2 Br <sup>†</sup>
	282.1090	-1.1	-3.9	6.5	404.5..	C12 H16 N3 O5 <sup>†</sup>
	282.1065	1.4	5.0	10.5	18.9..	C16 H16 N3 S <sup>†</sup>



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

Card Serial Number: GCT-P-T11-12-OS0938

Sample Serial Number: HBSF-D28-S27

Operator: Li

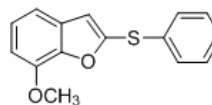
Date: 2011/12/15

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off



3m

Monoisotopic Mass, Odd and Even Electron Ions

359 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: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
256.0560	256.0558	0.2	0.8	10.0	9.3	C15 H12 O2 S
	256.0570	-1.0	-3.9	6.5	25.6	C9 H10 N3 O6
	256.0548	1.2	4.7	-0.5	722.6	C8 H19 N O3 Br

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

Card Serial Number: GCT-P-T11-12-OS0875

Sample Serial Number: HBSF-D11-CW-5

Operator: Li

Date: 2011/11/28

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

404 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)

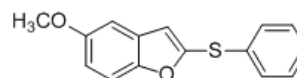
Elements Used:

C: 0-60 H: 0-80 N: 0-2 O: 0-6 S: 0-1 Cl: 0-1 Br: 0-1

Minimum: -1.5

Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
256.0554	256.0558	-0.4	-1.6	10.0	40.6	C15 H12 O2 S
	256.0548	0.6	2.3	-0.5	14143.4	C8 H19 N O3 Br
	256.0563	-0.9	-3.5	5.5	8267.1	C12 H15 N O S Cl



3n

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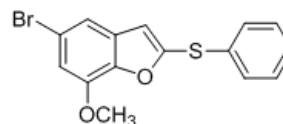
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T12-04-OS0317

Sample Serial Number: HBSF-LiA22-S17

Operator: Li

Date: 2012/04/25



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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 3 results within limits (all results (up to 1000) for each mass)  
Elements Used:

C: 0-60 H: 0-80 N: 0-1 O: 0-6 S: 0-1 Br: 0-3 I: 0-1

Minimum:		2.0	5.0	-1.5			
Maximum:				50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
333.9666	333.9667	-0.1	-0.3	-0.5	262.8	C8 H18 N Br I	
	333.9663	0.3	0.9	10.0	173.7	C15 H11 O2 S Br	
	333.9653	1.3	3.9	-0.5	246.5	C8 H18 N O3 Br2	

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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-OS0877

Sample Serial Number: HBSF-D11-CW-7

Operator: Li

Date: 2011/11/28

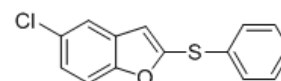
Elemental Composition Report

Single Mass Analysis  
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0  
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions  
414 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)  
Elements Used:

C: 0-60 H: 0-80 N: 0-2 O: 0-6 S: 0-1 Cl: 0-1 Br: 0-1

Minimum:		2.0	5.0	-1.5			
Maximum:				50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula	
260.0066	260.0063	0.3	1.2	10.0	81.5	C14 H9 O S Cl	
	260.0069	-0.3	-1.2	11.0	2337.0	C11 H4 N2 O6	
	260.0075	-0.9	-3.5	8.5	2361.6	C13 H11 N Br	



3p

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

Card Serial Number: GCT-P-T11-12-OS0936<sup>†</sup>

Sample Serial Number: HBSF-D28-S25<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/12/15<sup>†</sup>

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Element prediction: Off <sup>†</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

446 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mas:

Elements Used:<sup>†</sup>

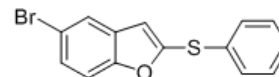
C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Br: 0-1 <sup>†</sup>

<sup>†</sup>

Minimum: -1.5<sup>†</sup>

Maximum: 50.0<sup>†</sup>

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>†</sup>
303.9554	303.9557	-0.3	-1.0	10.0	8.8...	C14 H9 O S Br <sup>†</sup>
	303.9544	1.0	3.3	10.5	3.5...	C12 H7 N3 S Br <sup>†</sup>
	303.9569	-1.5	-4.9	6.5	48.2...	C8 H7 N3 O5 Br <sup>†</sup>



3q

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

Card Serial Number: GCT-P-T11-12-OS0939<sup>†</sup>

Sample Serial Number: HBSF-D28-S28<sup>†</sup>

Operator: Li<sup>†</sup>

Date: 2011/12/15<sup>†</sup>

Elemental Composition Report<sup>†</sup>

Single Mass Analysis <sup>†</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>†</sup>

Element prediction: Off <sup>†</sup>

<sup>†</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>†</sup>

387 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)<sup>†</sup>

Elements Used:<sup>†</sup>

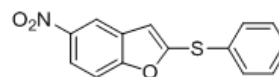
C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Br: 0-1 <sup>†</sup>

<sup>†</sup>

Minimum: -1.5<sup>†</sup>

Maximum: 50.0<sup>†</sup>

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>†</sup>
271.0304	271.0303	0.1	0.4	11.0	5546827.0...	C14 H9 N O3 S <sup>†</sup>
	271.0296	0.8	3.0	20.5	5546835.0...	C20 H3 N2 <sup>†</sup>
	271.0293	1.1	4.1	0.5	5546847.5...	C7 H16 N2 O4 Br <sup>†</sup>



3r



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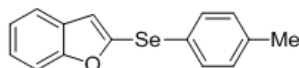
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T12-06-OS0576

Sample Serial Number: HBSF-LiJ9-S-38

Operator: Li

Date: 2012/06/26



3s

Elemental Composition Report

Single Mass Analysis

Tolerance = 2.0 mDa / DBE: min = -1.5, max = 50.0  
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

296 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-60 H: 0-80 O: 0-2 74Se: 0-1 76Se: 0-1 77Se: 0-1 78Se: 0-1 80Se: 0-1 82Se: 0-1

Minimum:						
Maximum:						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
282.0112	282.0112	0.0	0.0	12.0	221.8	C16 H12 78Se
	282.0113	-0.1	-0.4	11.0	5.6	C15 H12 O 74Se
	282.0115	-0.3	-1.1	-1.5	559.6	C7 H23 O 77Se 82Se
	282.0106	0.6	2.1	22.0	512.3	C22 H2 O
	282.0119	-0.7	-2.5	1.0	241.4	C9 H22 74Se 78Se

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Chinese Academic of Sciences  
High Resolution MS Data Report



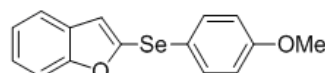
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T12-07-OS0652

Sample Serial Number: HBSF-LiJ03-S39

Operator: Li

Date: 2012/07/17



3t

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

626 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: 0-1 O: 0-2 74Se: 0-1 76Se: 0-1 77Se: 0-1 78Se: 0-1 80Se: 0-1 82Se: 0-1

Minimum:						
Maximum:						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
298.0059	298.0061	-0.2	-0.7	12.0	5546041.5	C16 H12 O 78Se
	298.0062	-0.3	-1.0	11.0	5546042.0	C15 H12 O2 74Se
	298.0055	0.4	1.3	22.0	5546033.5	C22 H2 O2
	298.0064	-0.5	-1.7	-1.5	5546042.0	C7 H23 O2 77Se 82Se
	298.0068	-0.9	-3.0	1.0	5546041.5	C9 H22 O 74Se 78Se
	298.0047	1.2	4.0	1.0	5546041.5	C8 H21 N O 74Se 77Se
	298.0046	1.3	4.4	2.0	5546041.0	C9 H21 N 77Se 78Se



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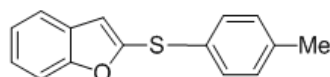
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T12-07-OS0653

Sample Serial Number: HBSF-LiJ03-S40

Operator: Li

Date: 2012/07/17



3u

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

203 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1

Minimum: -1.5

Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
240.0610	240.0609	0.1	0.4	10.0	1.6	C15 H12 O S
	240.0620	-1.0	-4.2	6.5	139.1	C9 H10 N3 O5

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

Card Serial Number: GCT-P-T12-07-OS0677

Sample Serial Number: HBSF-LiO13-S42

Operator: Li

Date: 2012/08/15

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

319 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

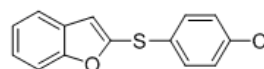
Elements Used:

C: 0-60 H: 0-80 N: 0-2 O: 0-4 S: 0-1 Cl: 0-1 Br: 0-1

Minimum: -1.5

Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
260.0067	260.0063	0.4	1.5	10.0	9.9	C14 H9 O S Cl
	260.0075	-0.8	-3.1	8.5	1679.4	C13 H11 N Br



3v

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

Card Serial Number: GCT-P-T12-07-0S0678<sup>+</sup>

Sample Serial Number: HBSF-LiO13-S43<sup>+</sup>

Operator: Li<sup>+</sup>

Date: 2012/08/15<sup>+</sup>

Elemental Composition Report<sup>+</sup>

Single Mass Analysis <sup>+</sup>

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0<sup>+</sup>

Element prediction: Off <sup>+</sup>

Monoisotopic Mass, Odd and Even Electron Ions<sup>+</sup>

345 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)<sup>+</sup>

Elements Used:<sup>+</sup>

C: 0-60 H: 0-80 N: 0-2 O: 0-4 S: 0-1 Cl: 0-1 Br: 0-1 <sup>+</sup>

Minimum:

Maximum: -1.5<sup>+</sup>

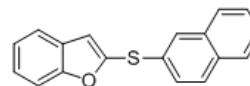
Mass Calc. Mass mDa PPM DBE i-FIT Formula<sup>+</sup>

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula <sup>+</sup>
276.0614	276.0614	0.0	0.0	8.5	5546025.0	C15 H15 N S Cl <sup>+</sup>
	276.0609	0.5	1.8	13.0	5546025.5	C18 H12 O S <sup>+</sup>

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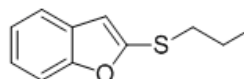
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T12-07-0S0654

Sample Serial Number: HBSF-LiJ03-S41

Operator: Li

Date: 2012/07/17



3x

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

163 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1

Minimum:

Maximum: -1.5

Mass Calc. Mass mDa PPM DBE i-FIT Formula

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
192.0611	192.0609	0.2	1.0	6.0	4.0	C11 H12 O S
	192.0620	-0.9	-4.7	2.5	2773014.5	C5 H10 N3 O5