Supplementary Material (ESI) for Organic & Biomolecular Chemistry This journal is (c) The Royal Society of Chemistry 2012

Synthesis of (Z)-3-Aryloxy-acrylonitriles, (E)-3-Aryloxy-acrylonitriles and 3-Cyanobenzofurans through the Sequential Reactions of Phenols with Propiolonitriles

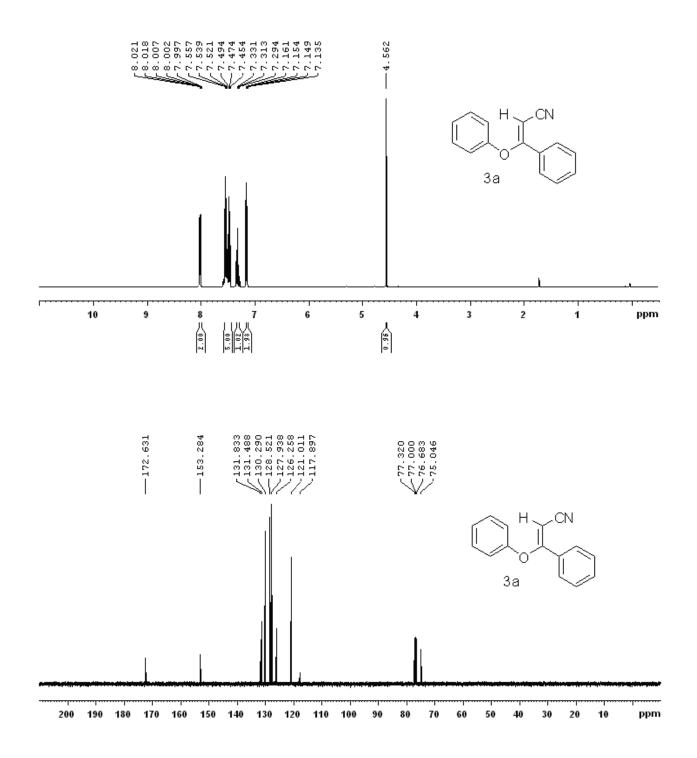
Wei Zhou,[†] Yicheng Zhang,[†] Pinhua Li,[†] and Lei Wang^{*†,‡}

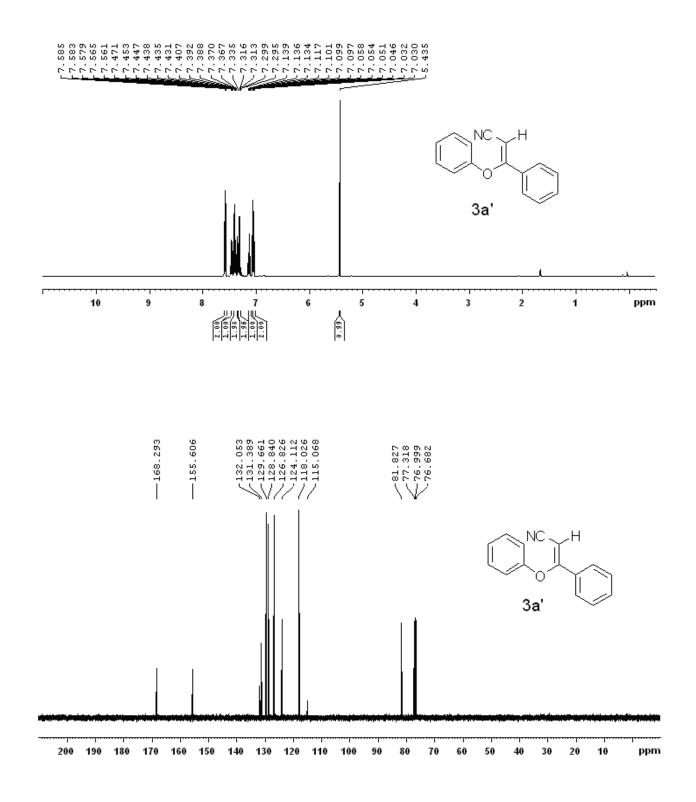
[†] Department of Chemistry, Huaibei Normal University, Huaibei, Anhui 235000, P. R. China [‡] State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry

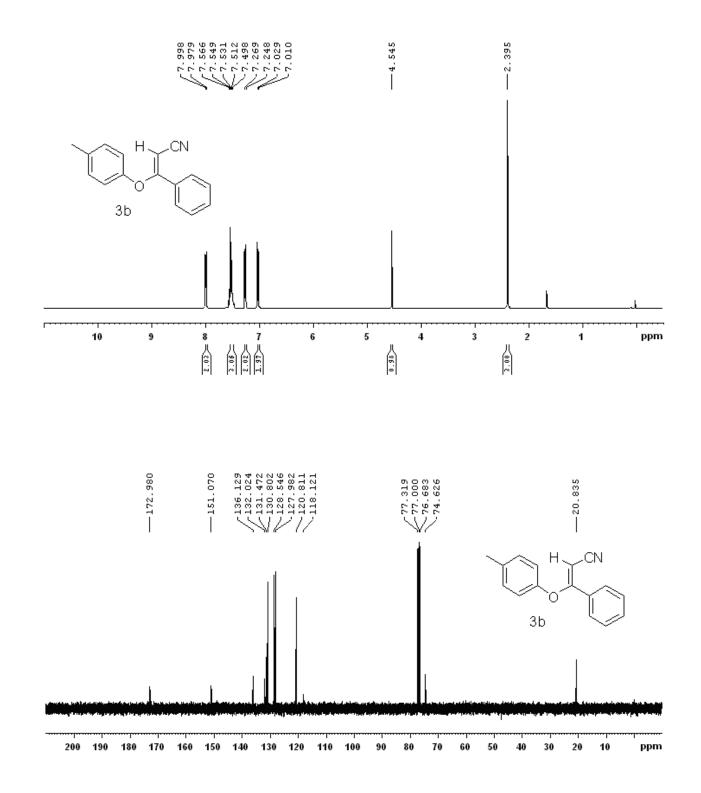
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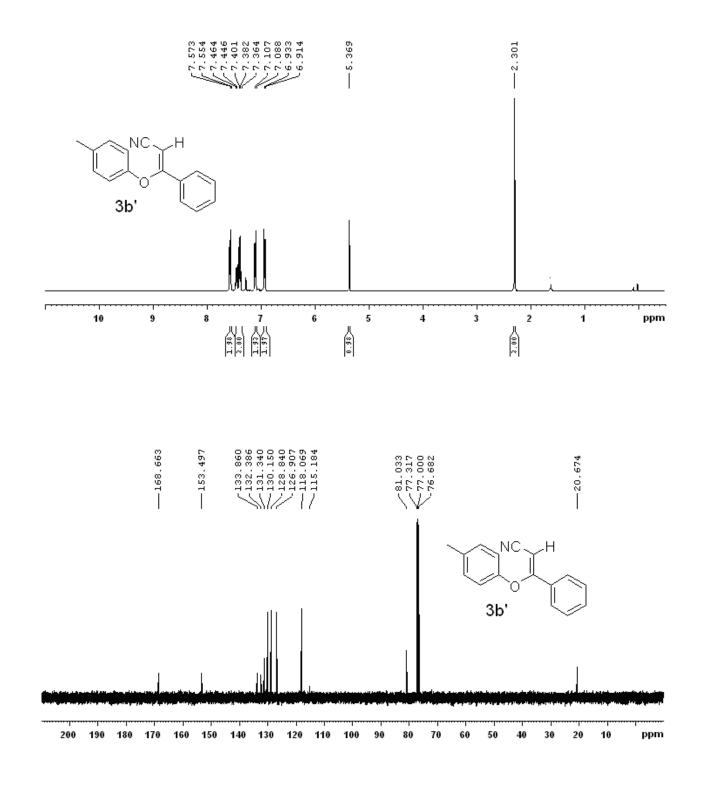
leiwang@chnu.edu.cn

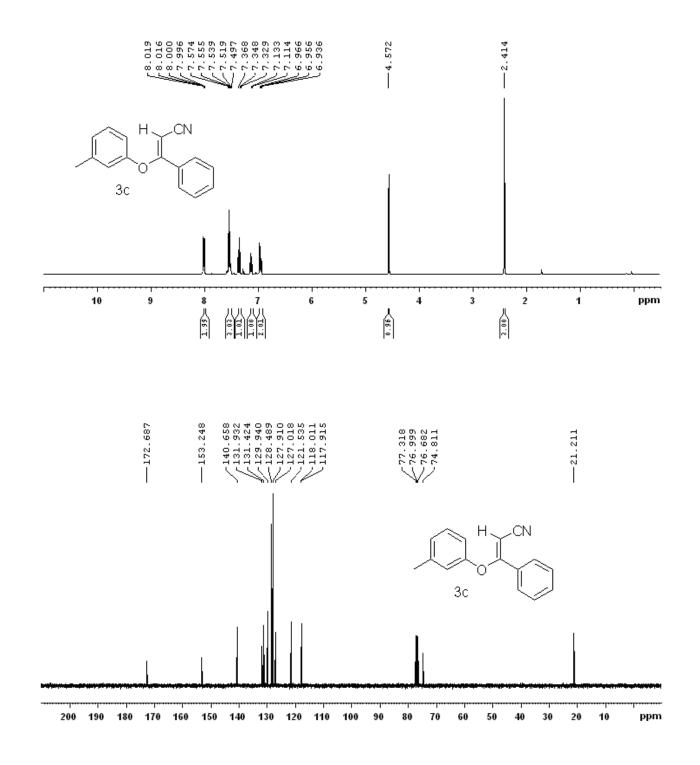
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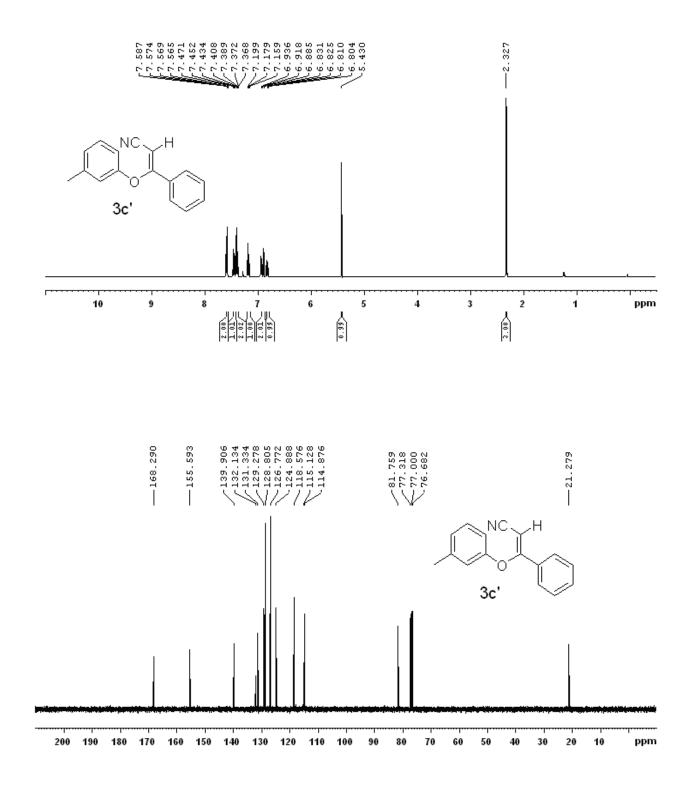


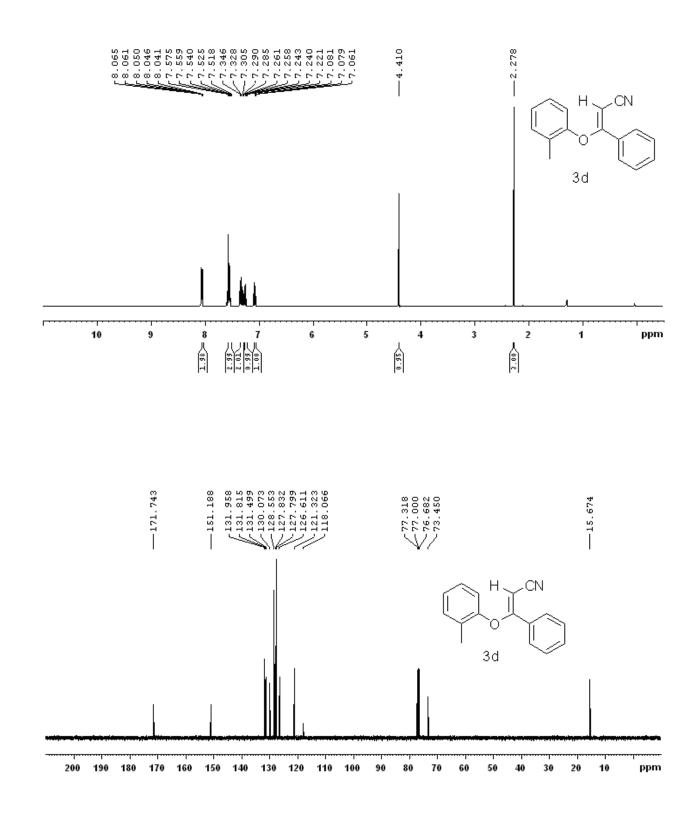


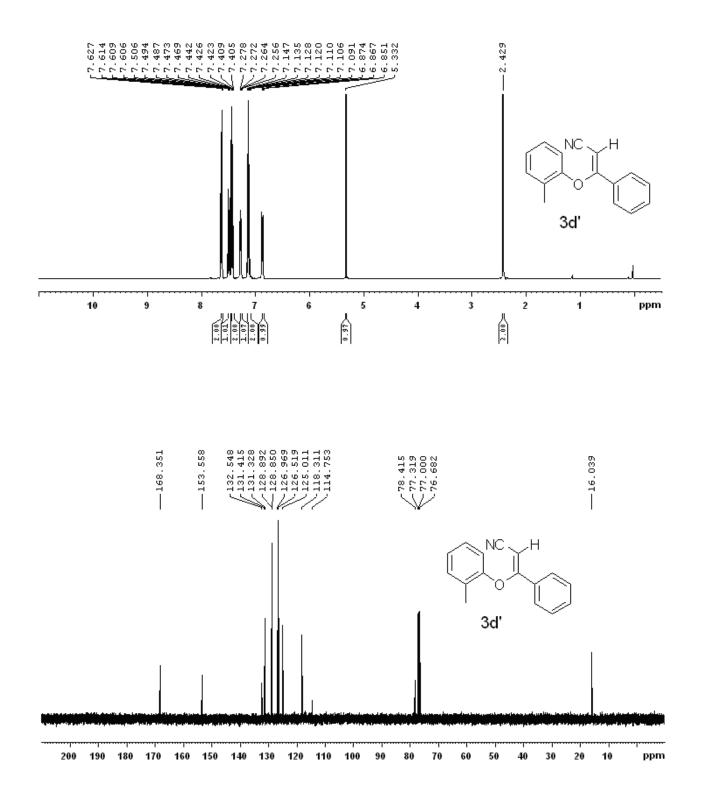


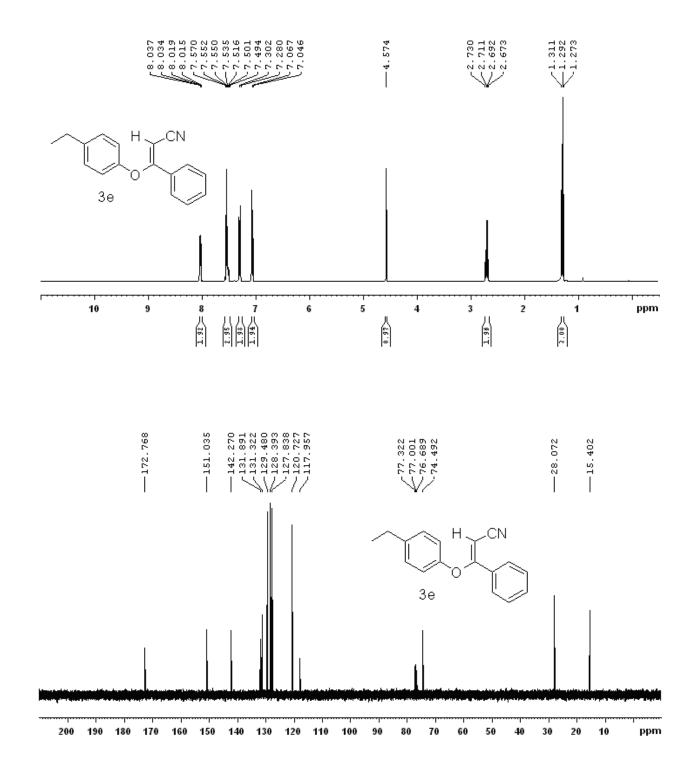


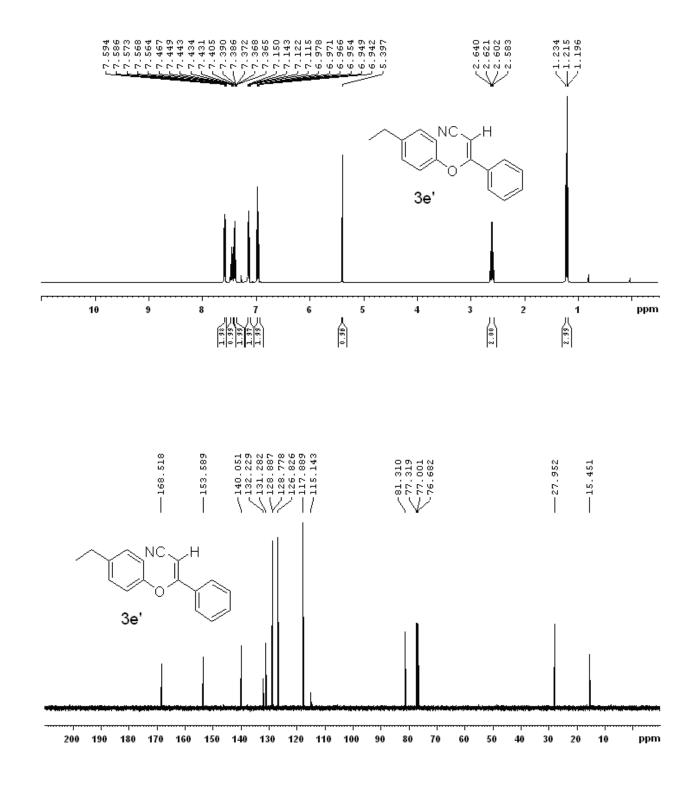


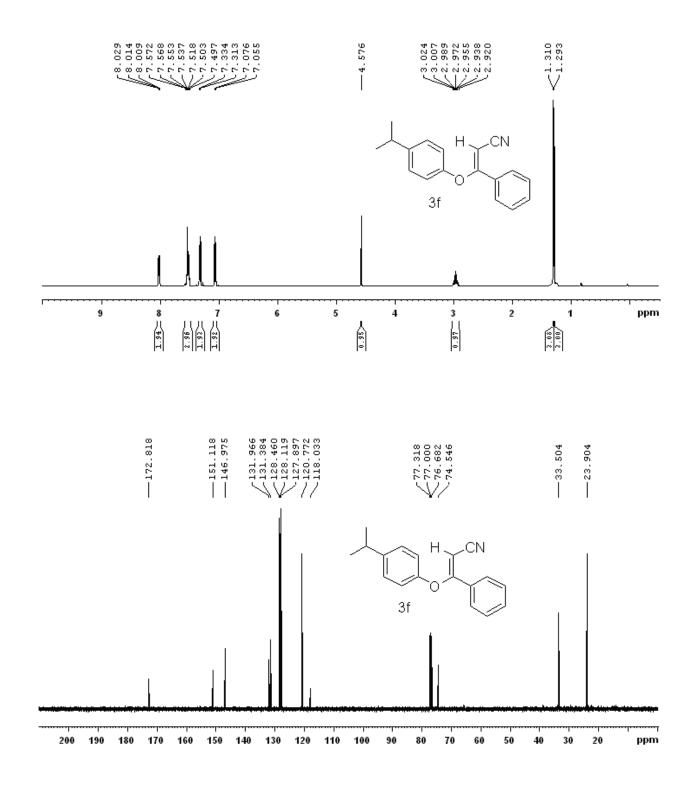


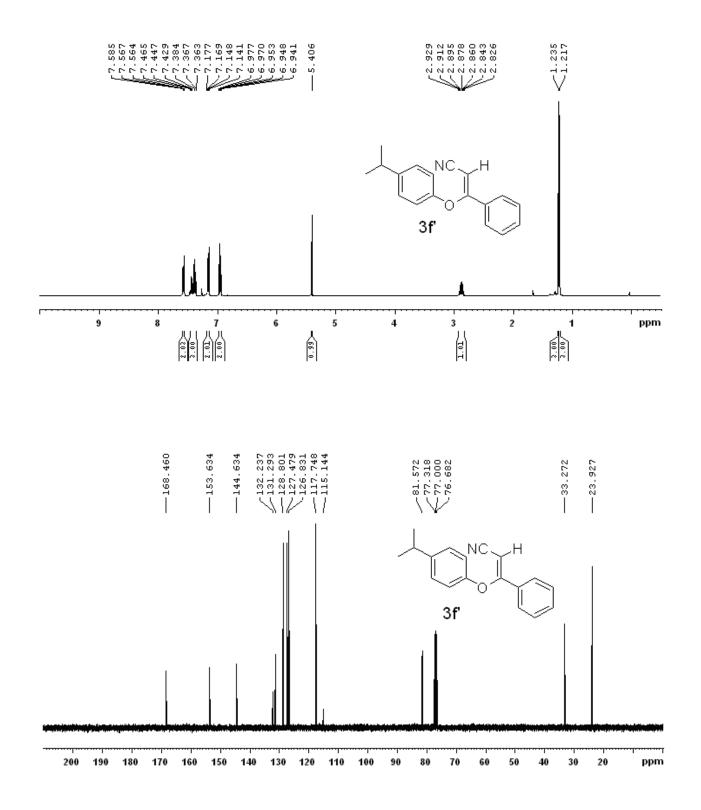


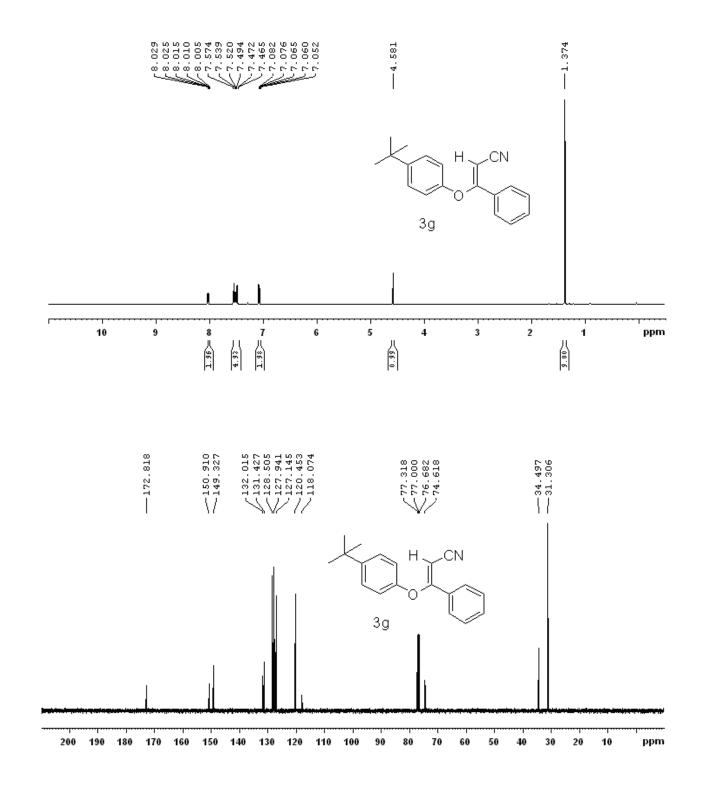


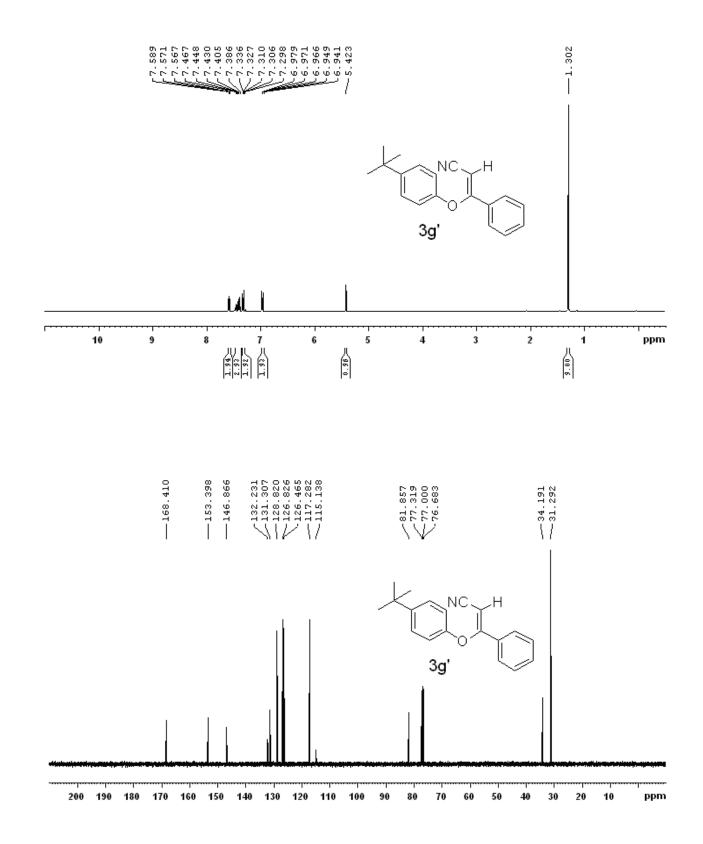


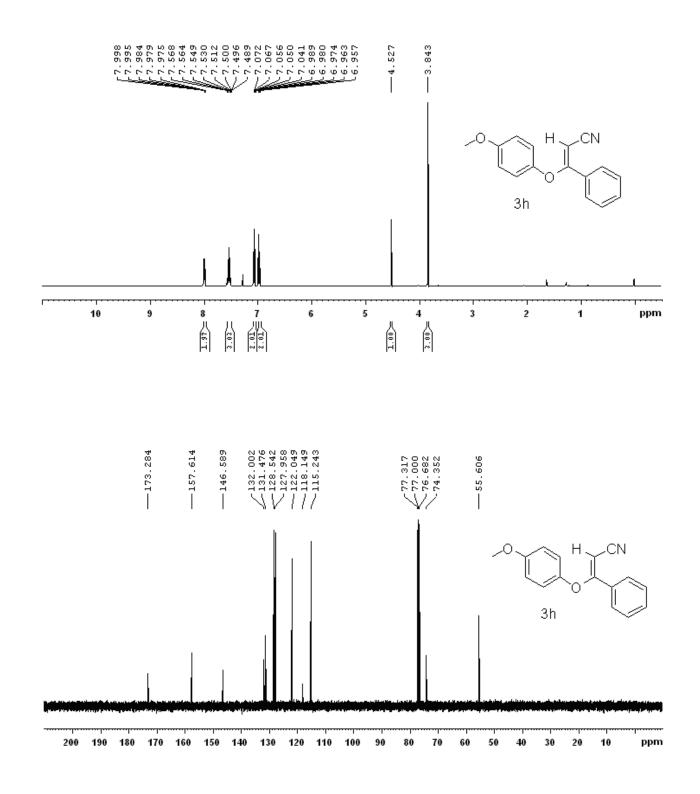


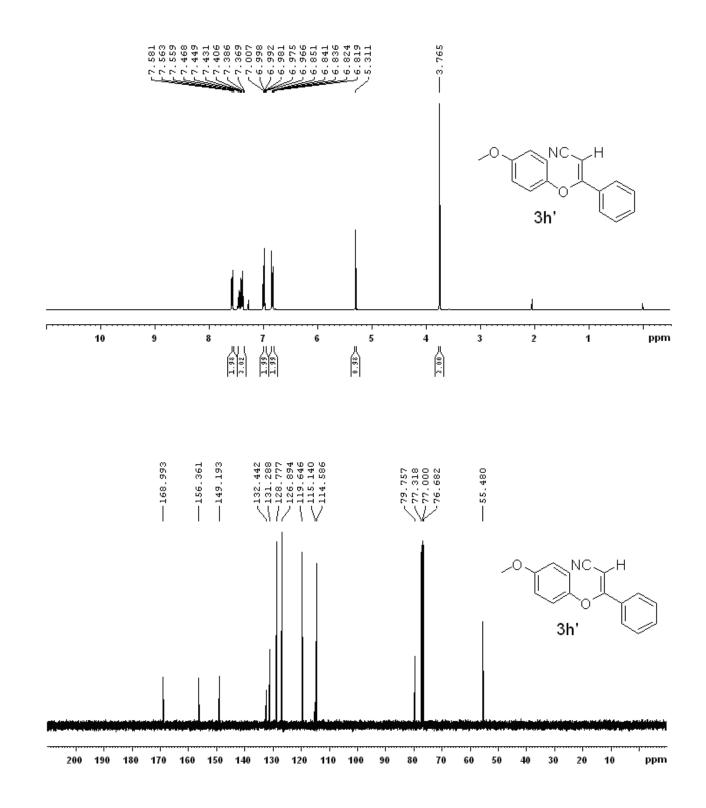


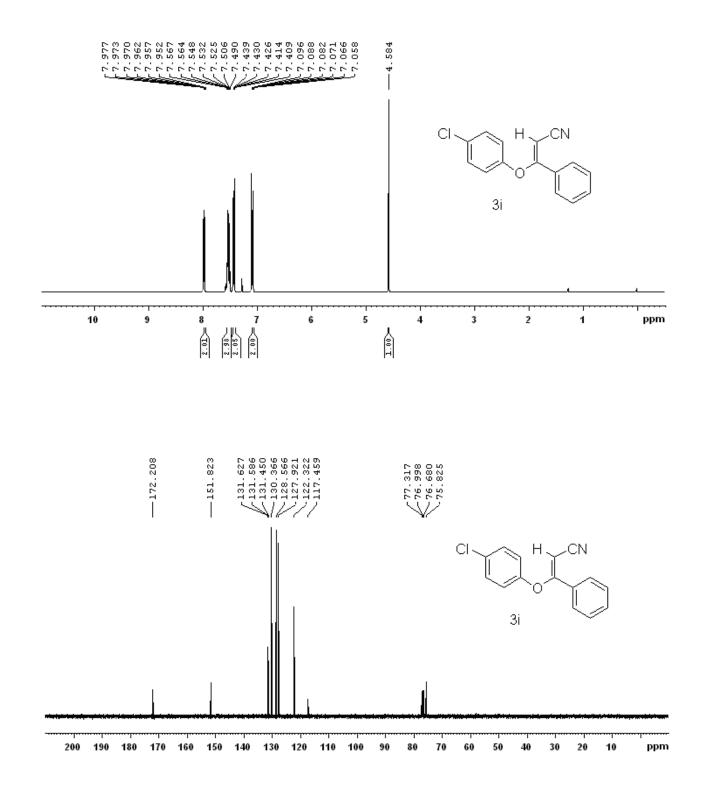


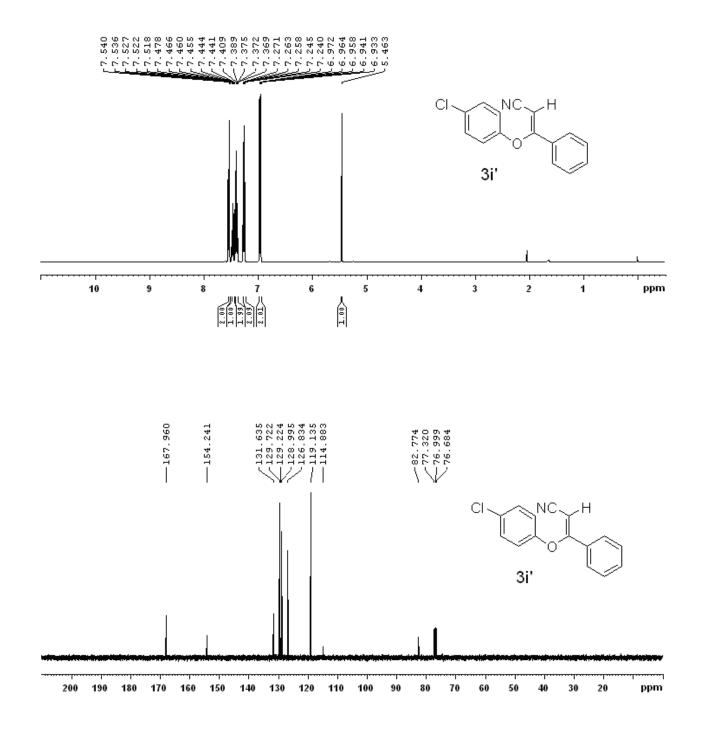


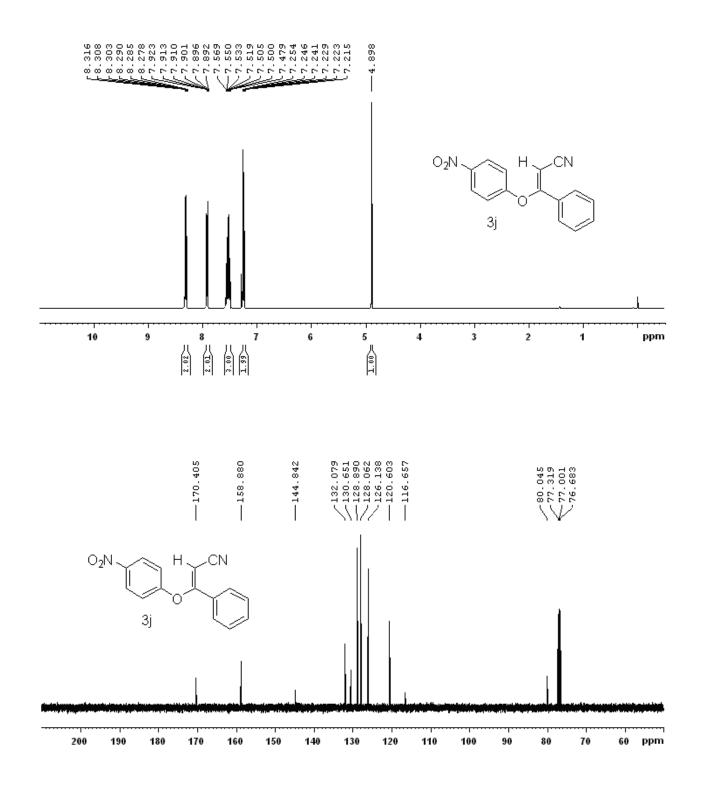


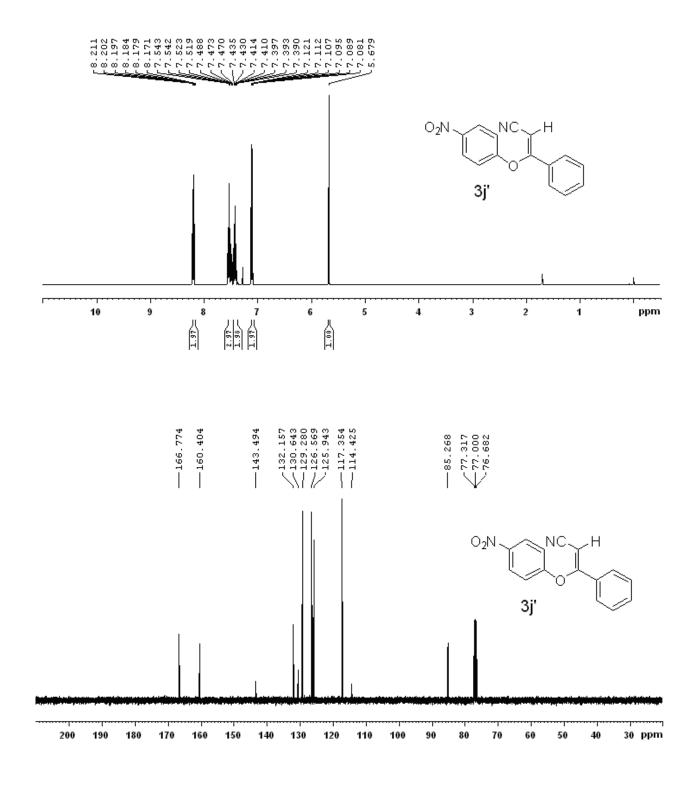


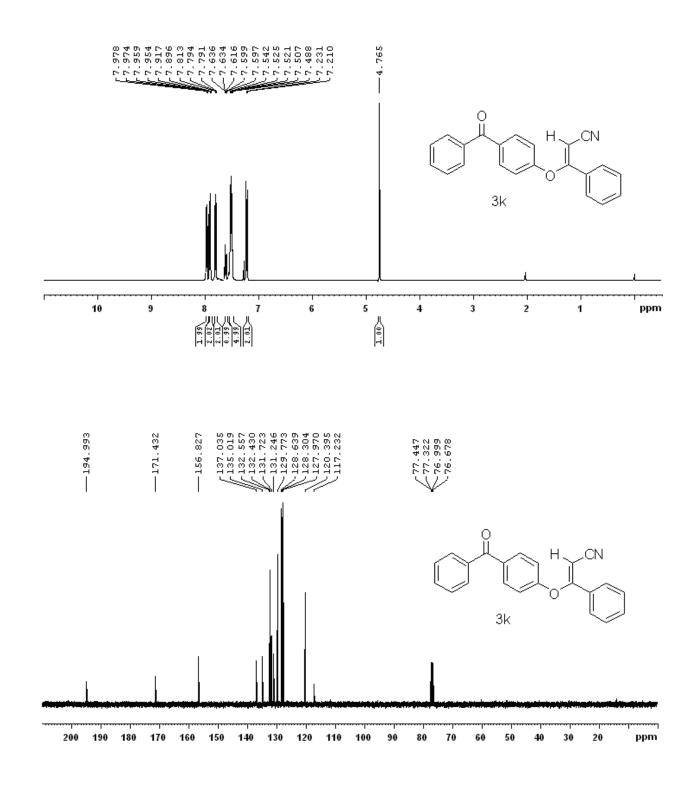


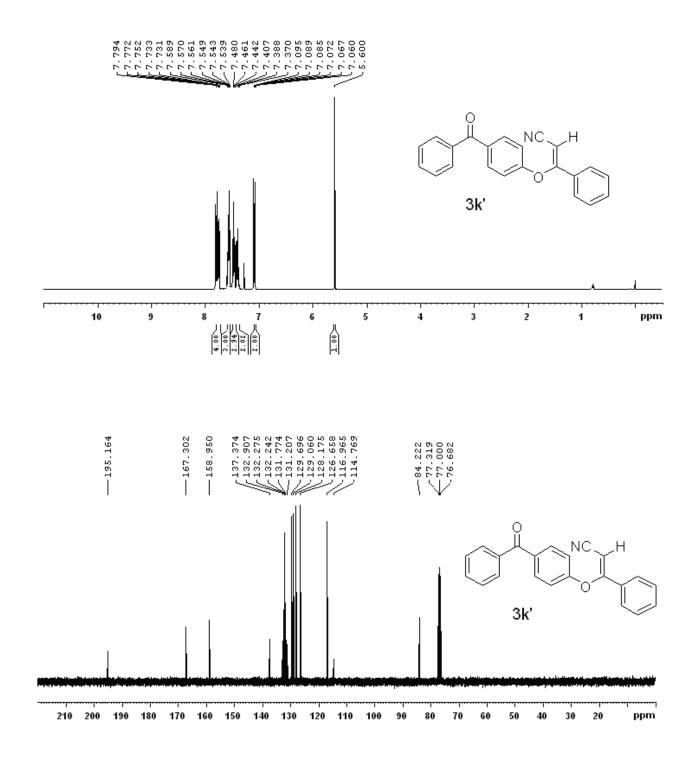


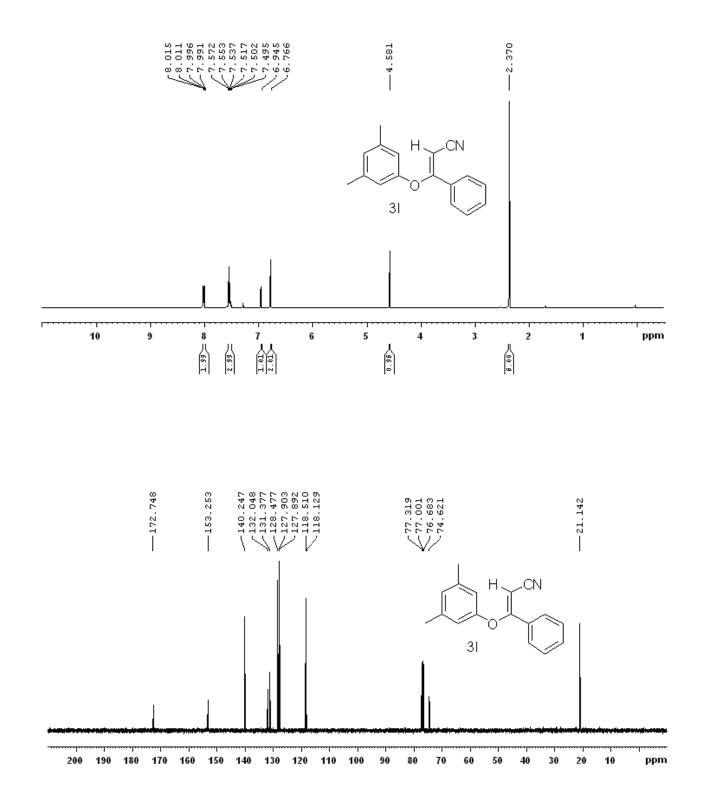


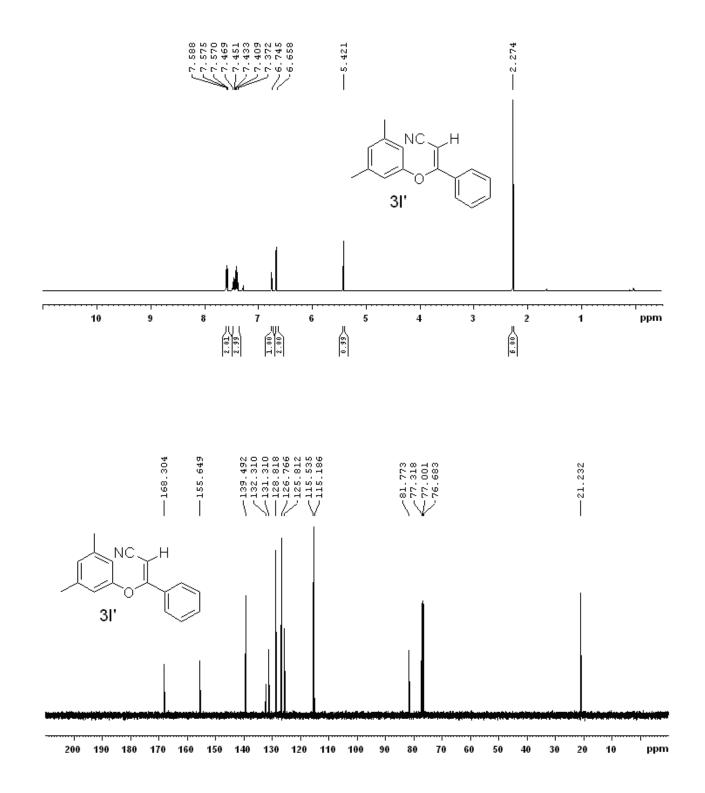


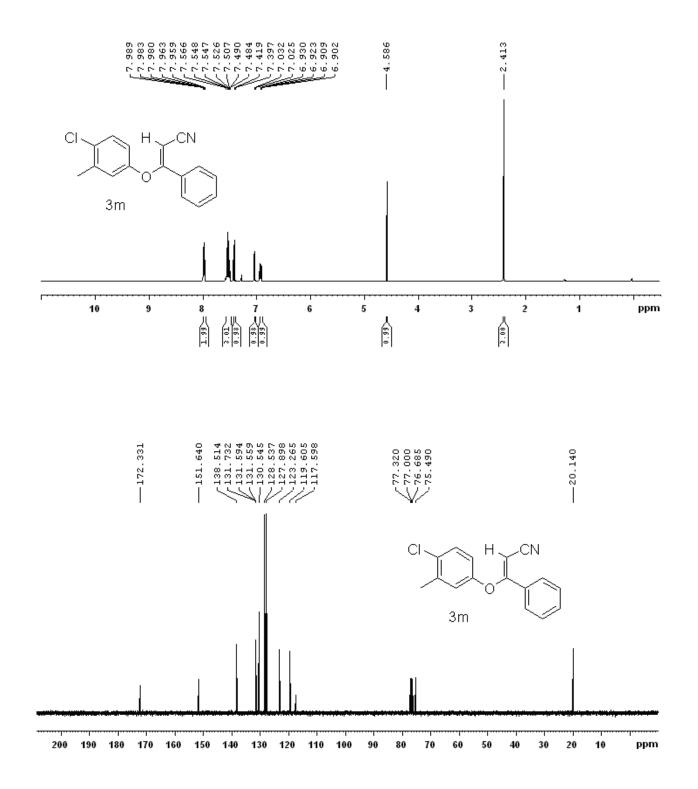


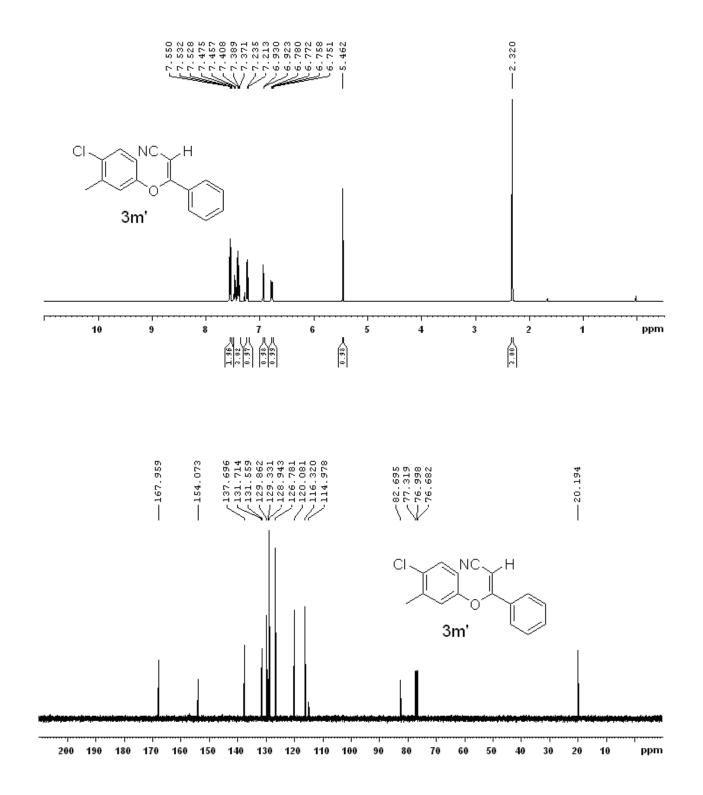


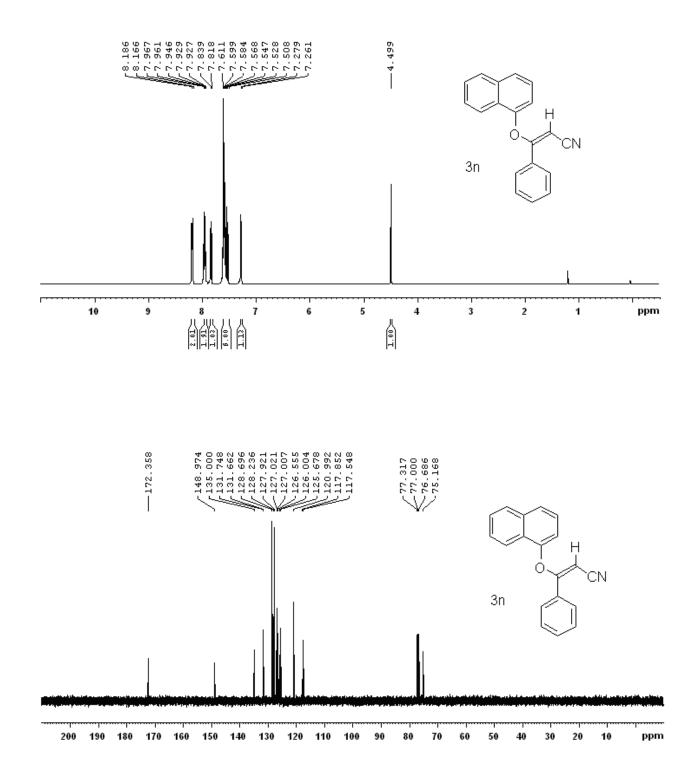


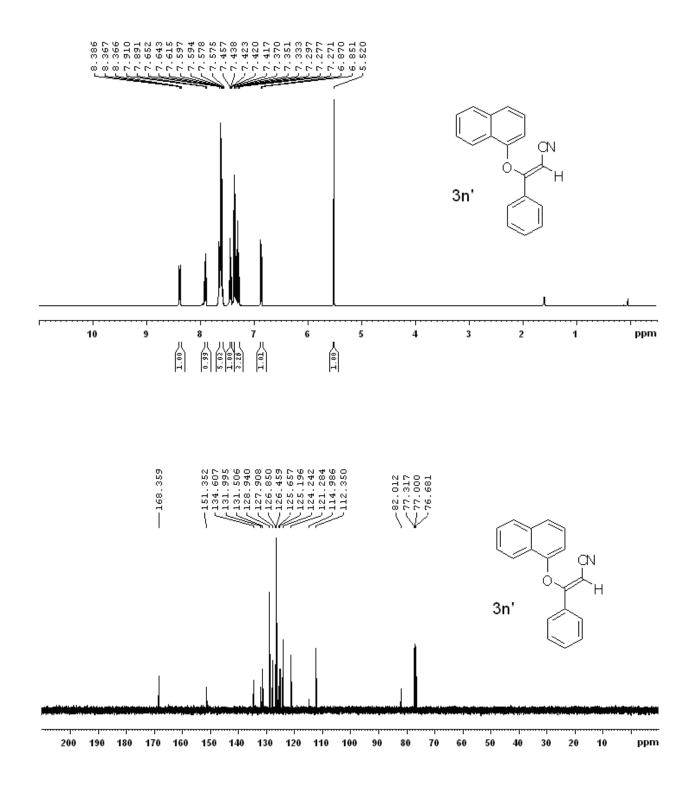


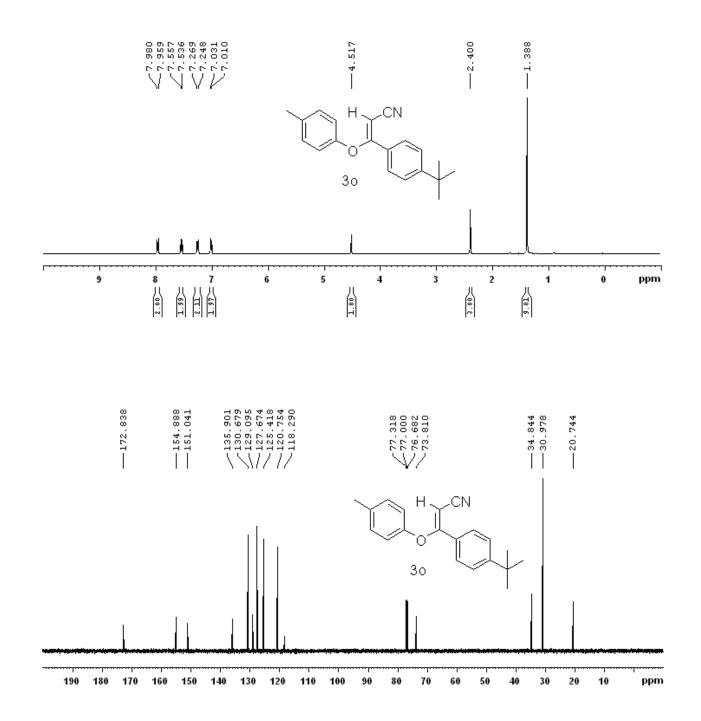




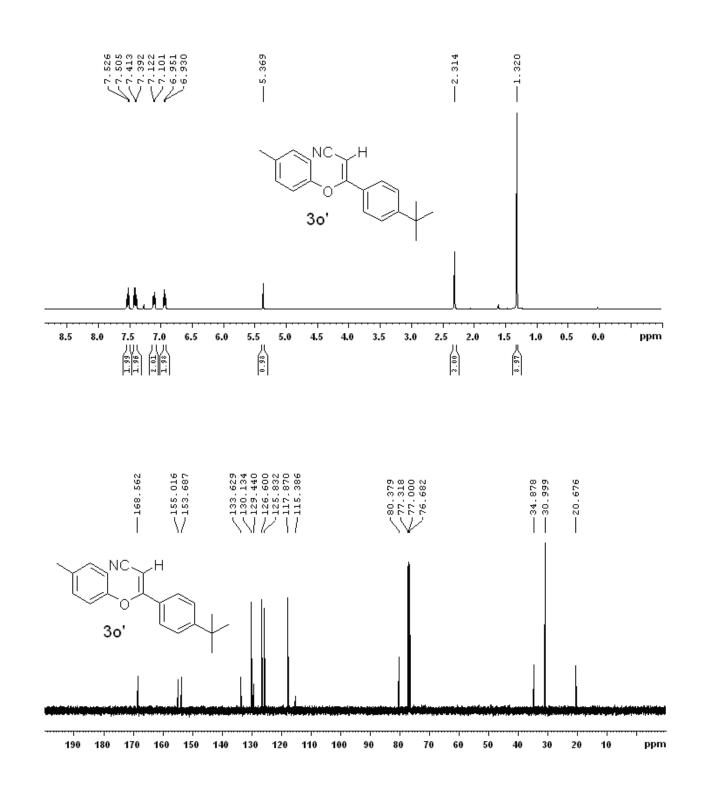


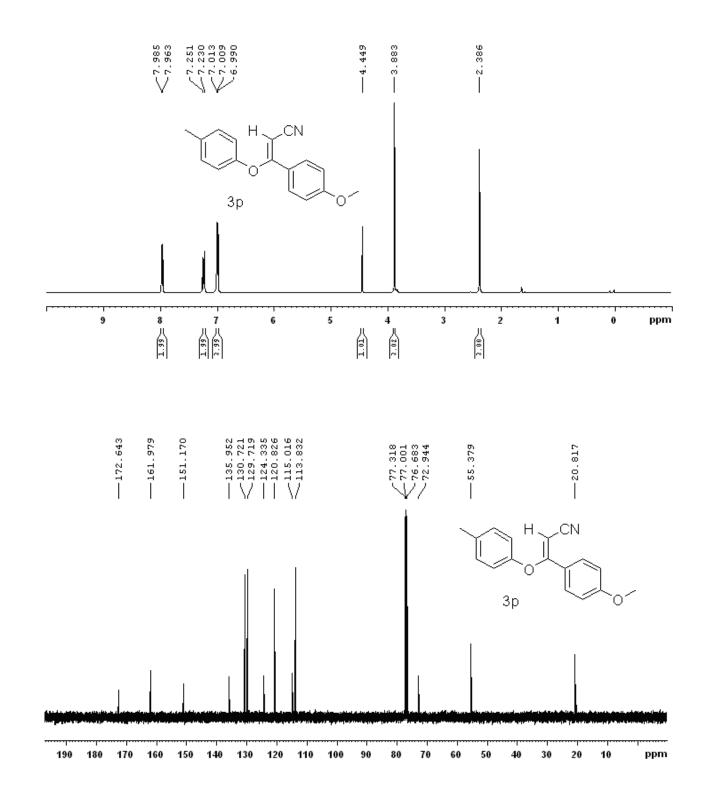




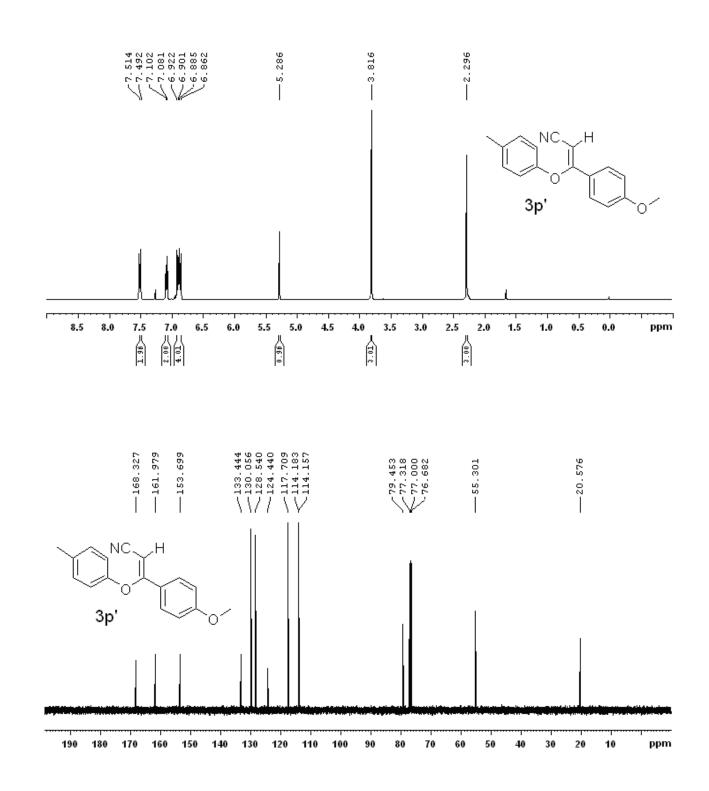


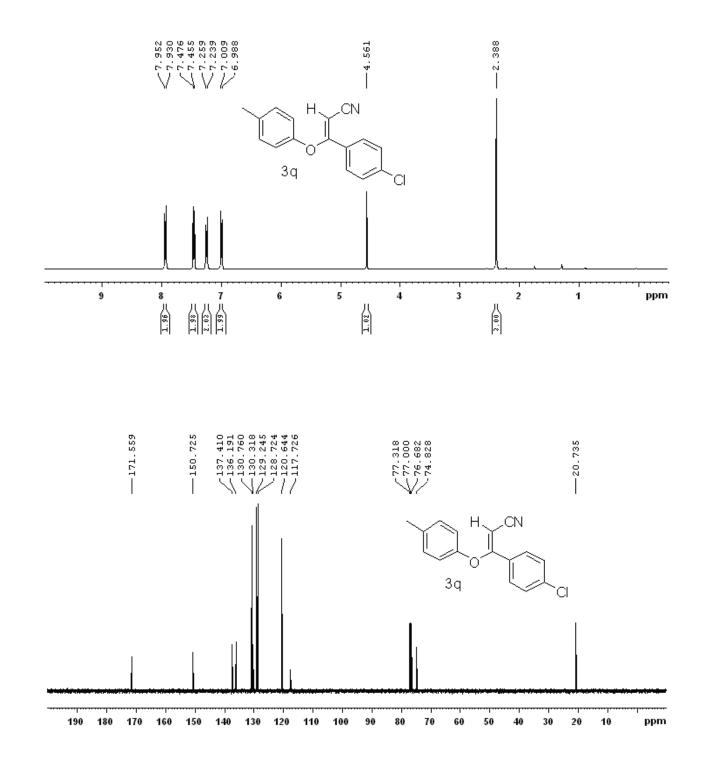
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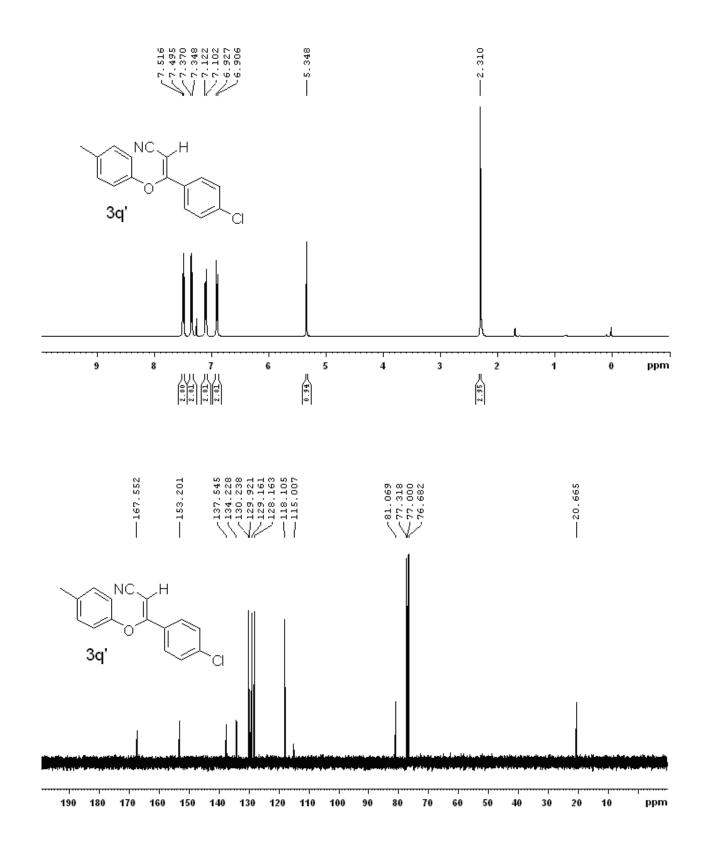


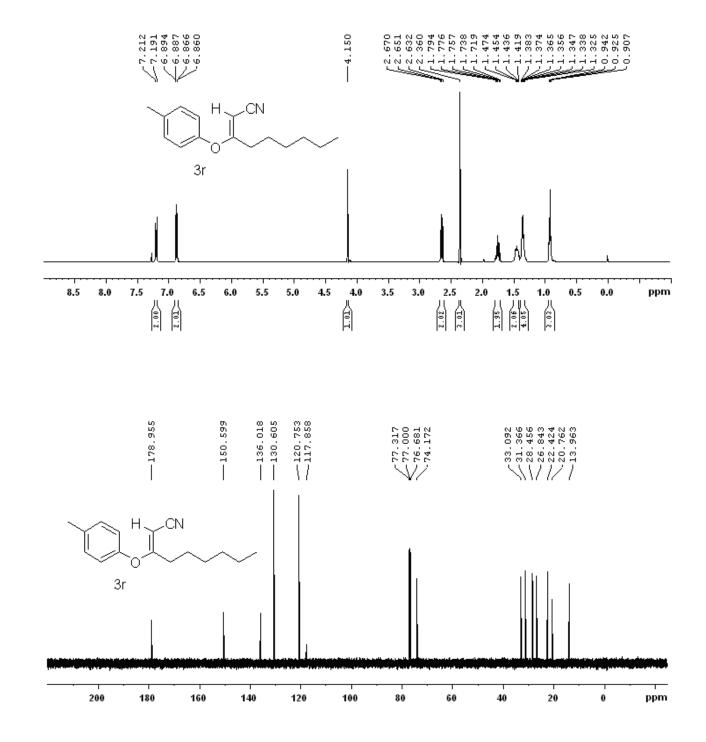


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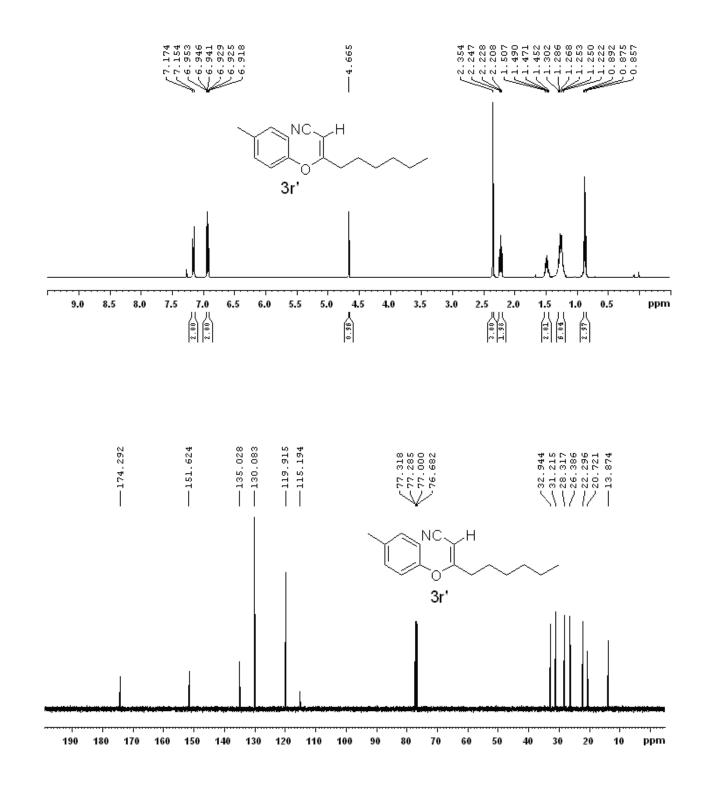




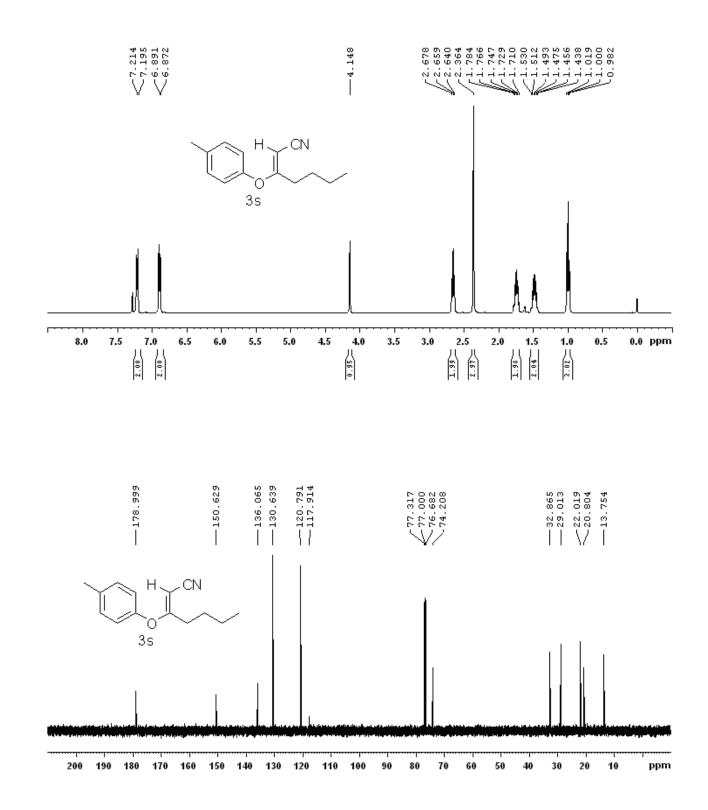




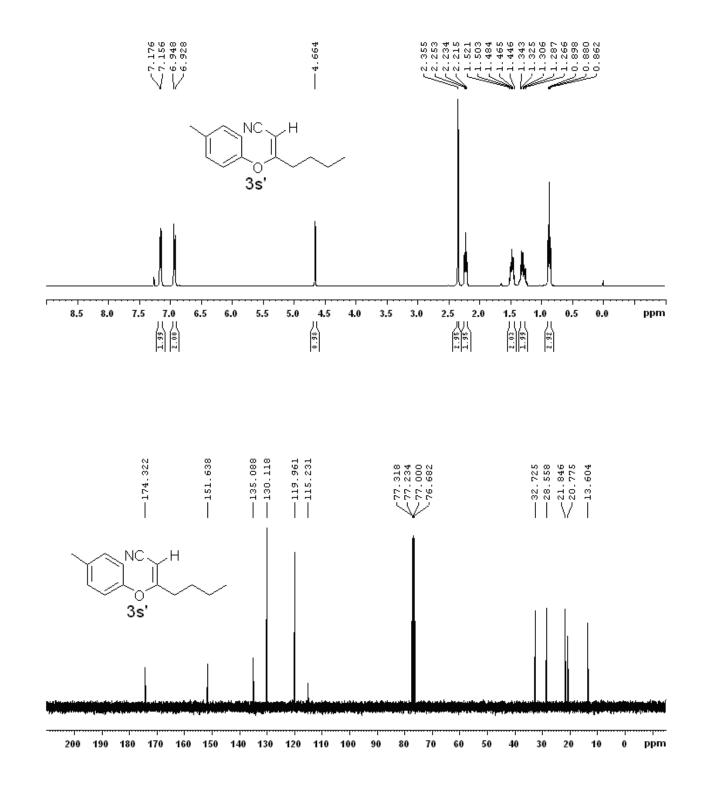
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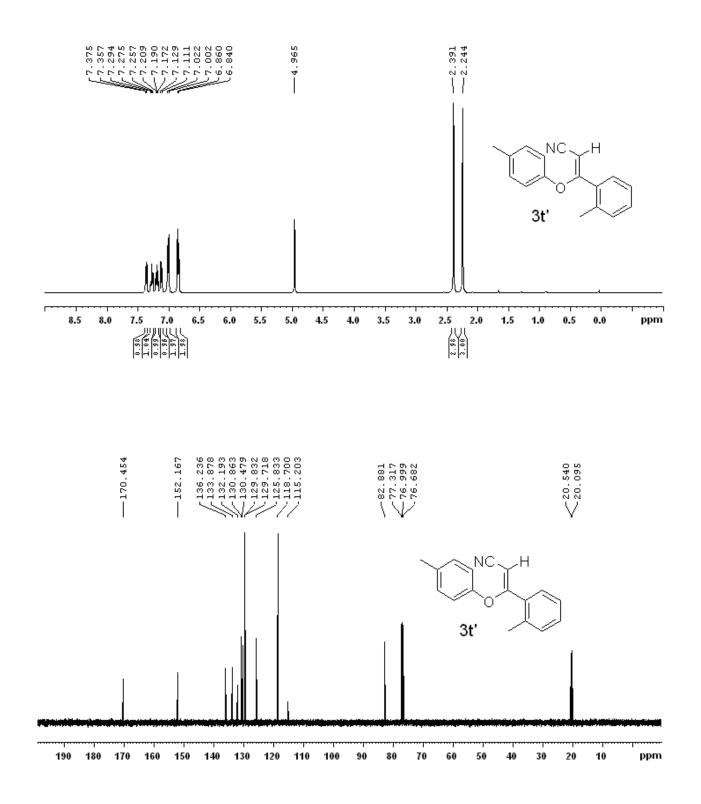


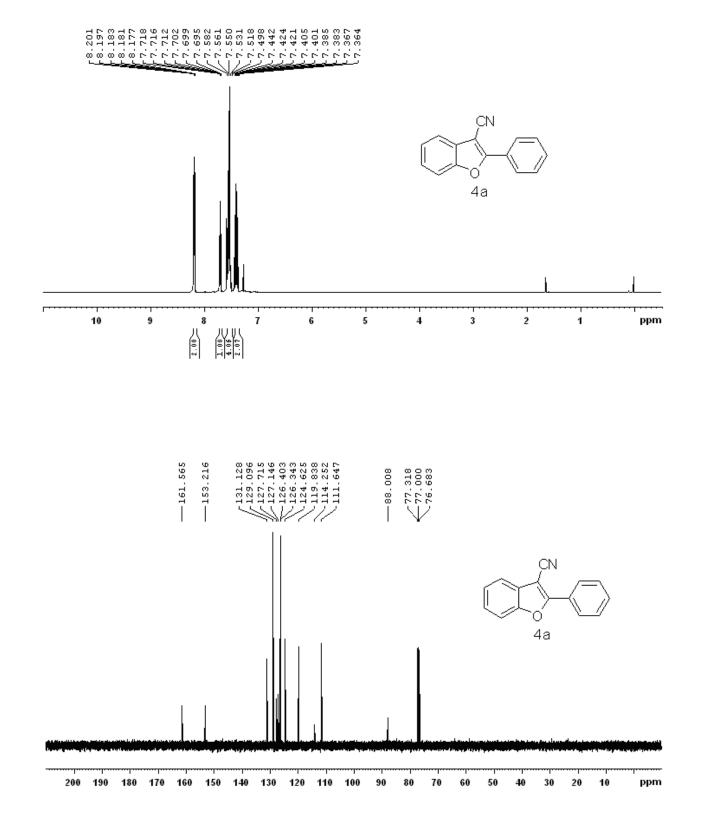
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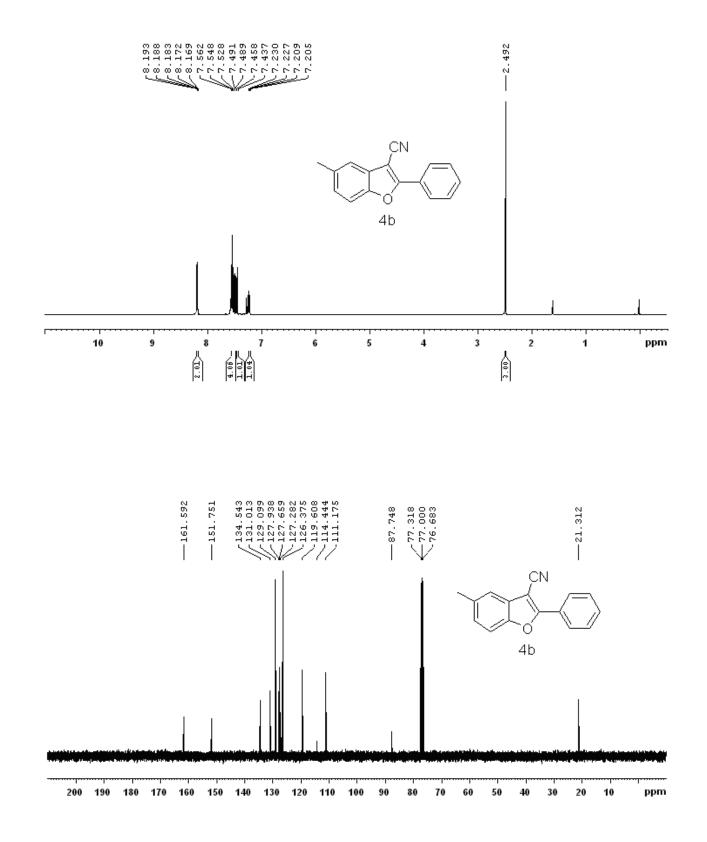


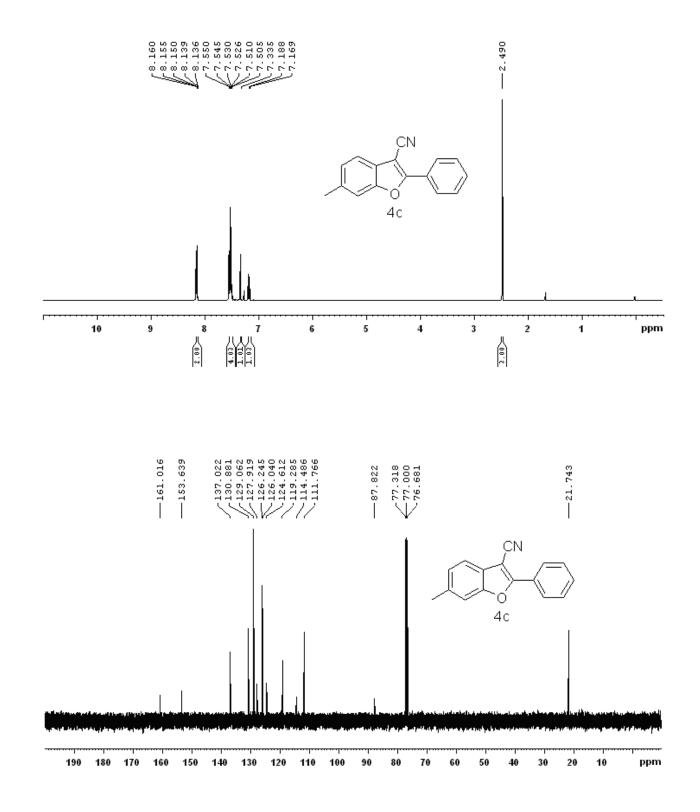
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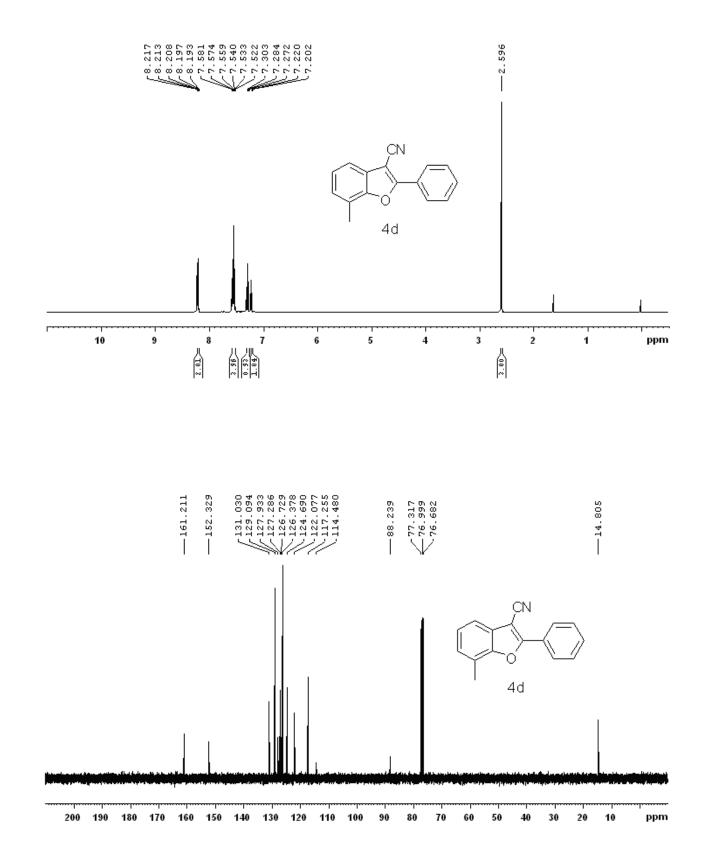


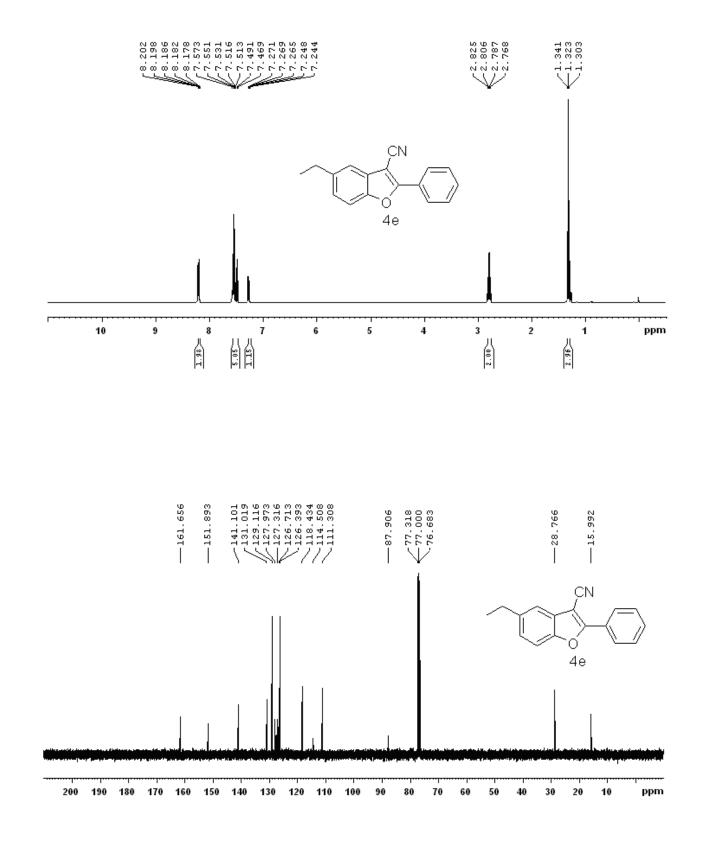


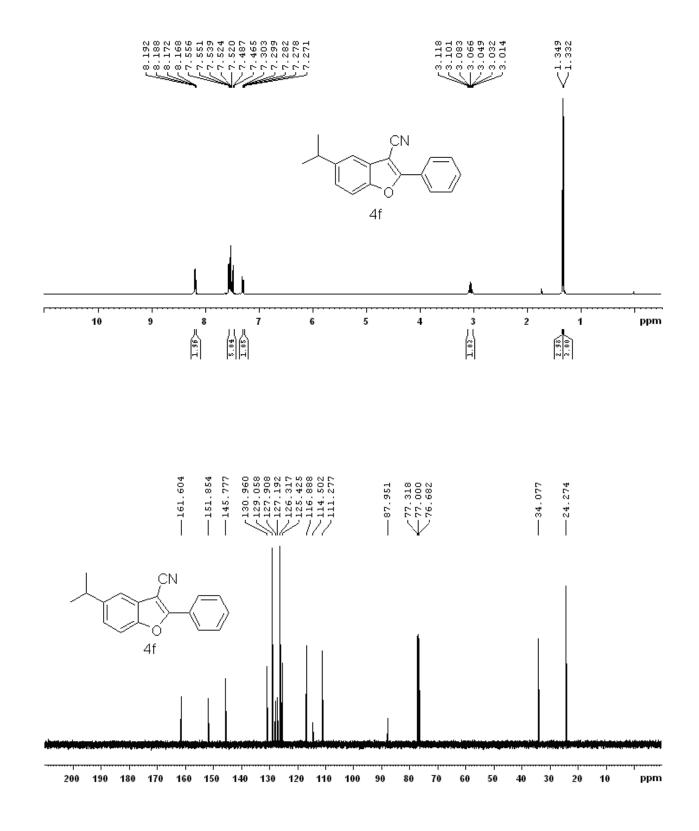


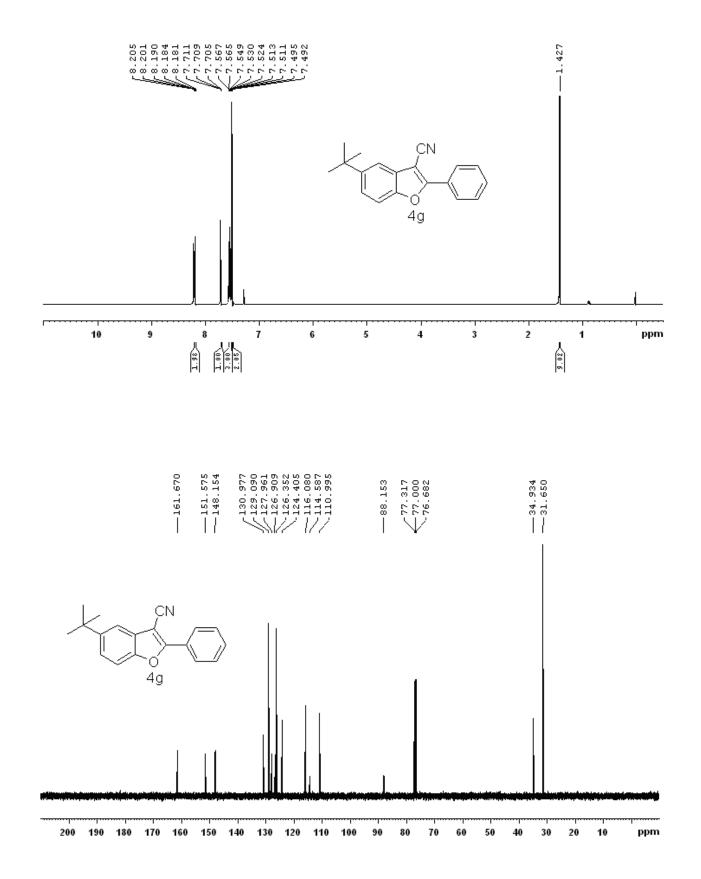


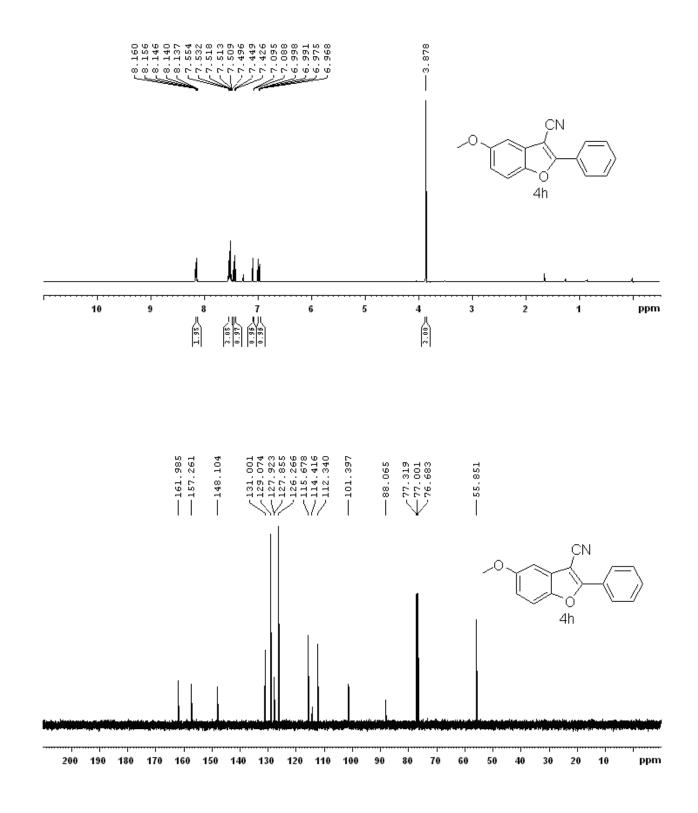


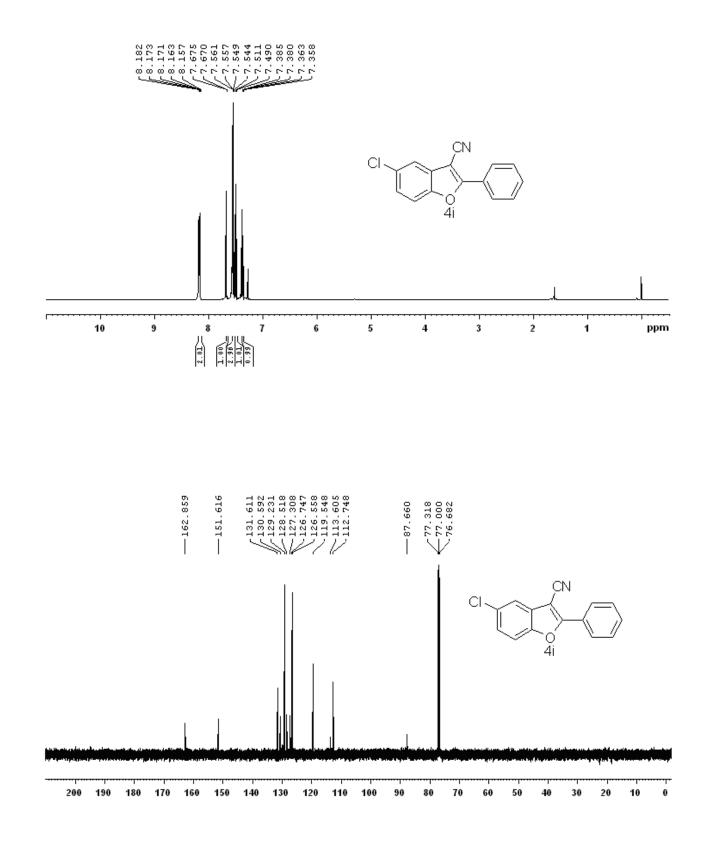


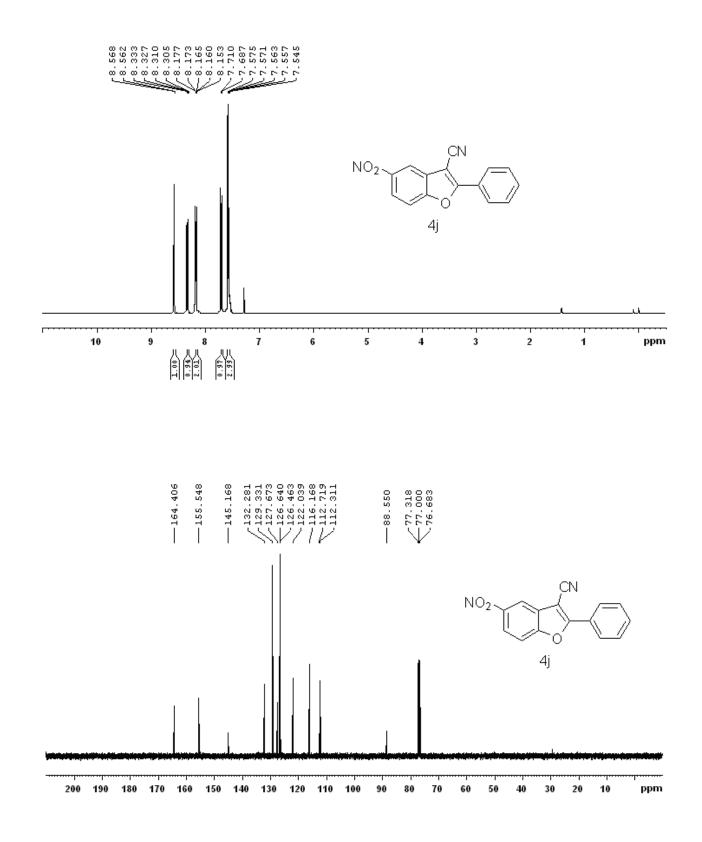


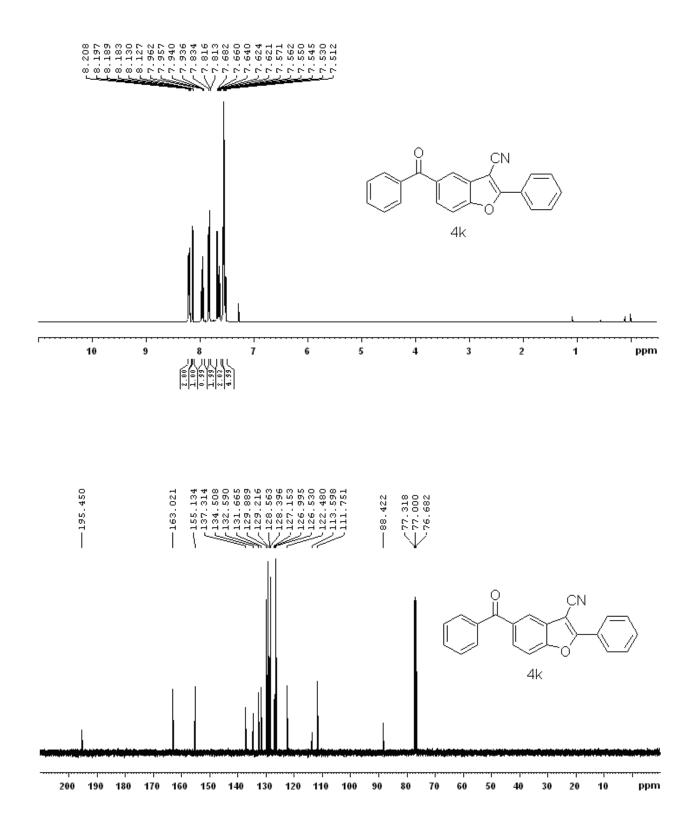


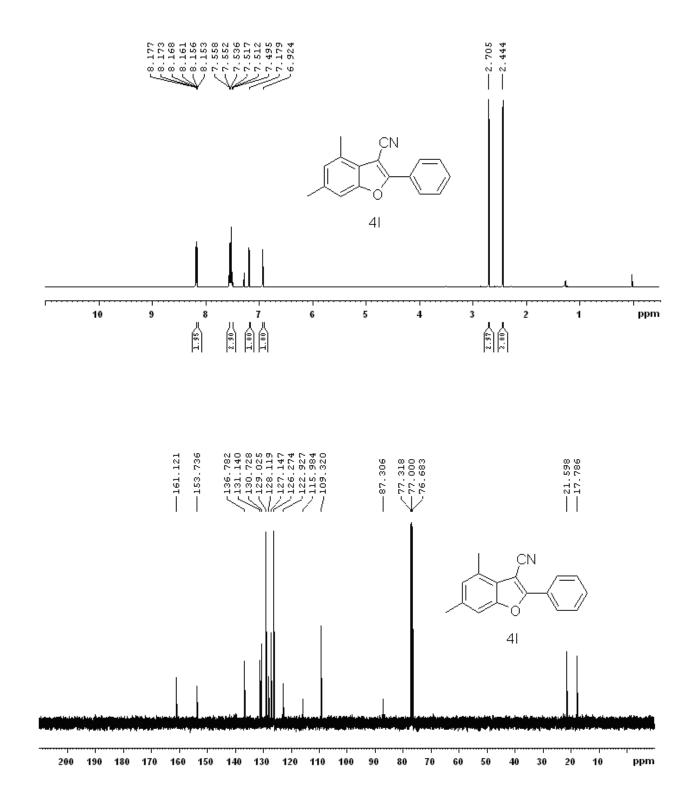


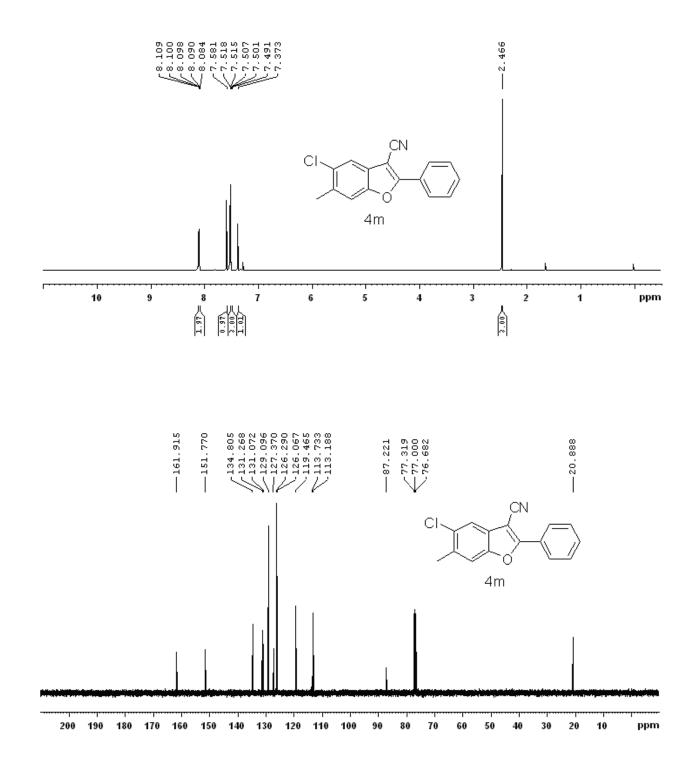


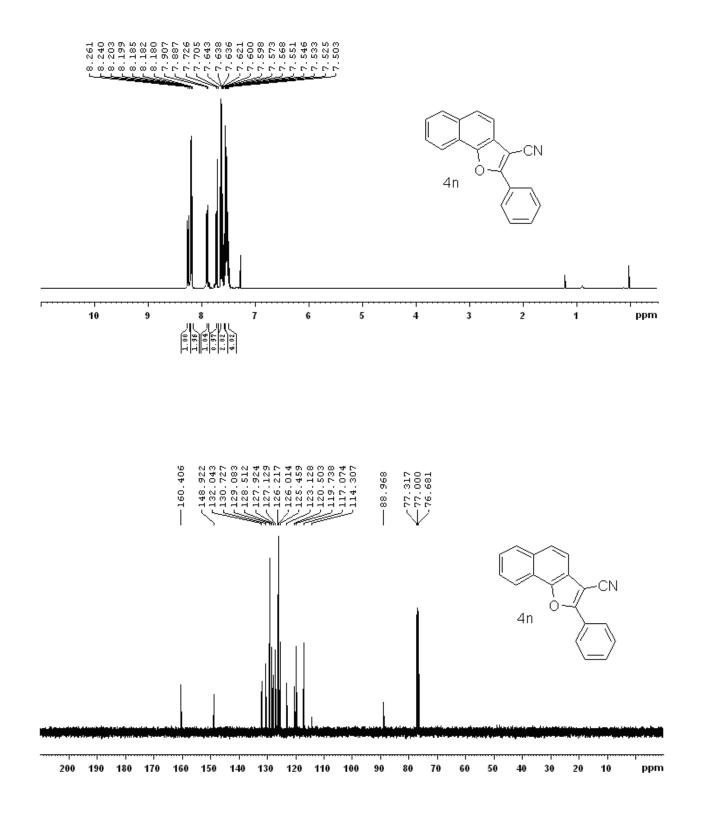


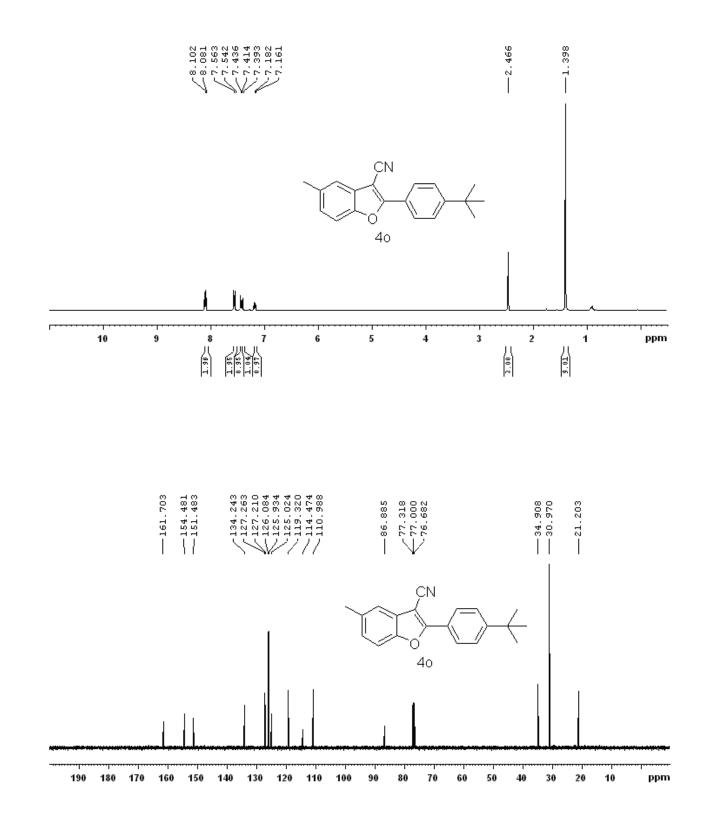


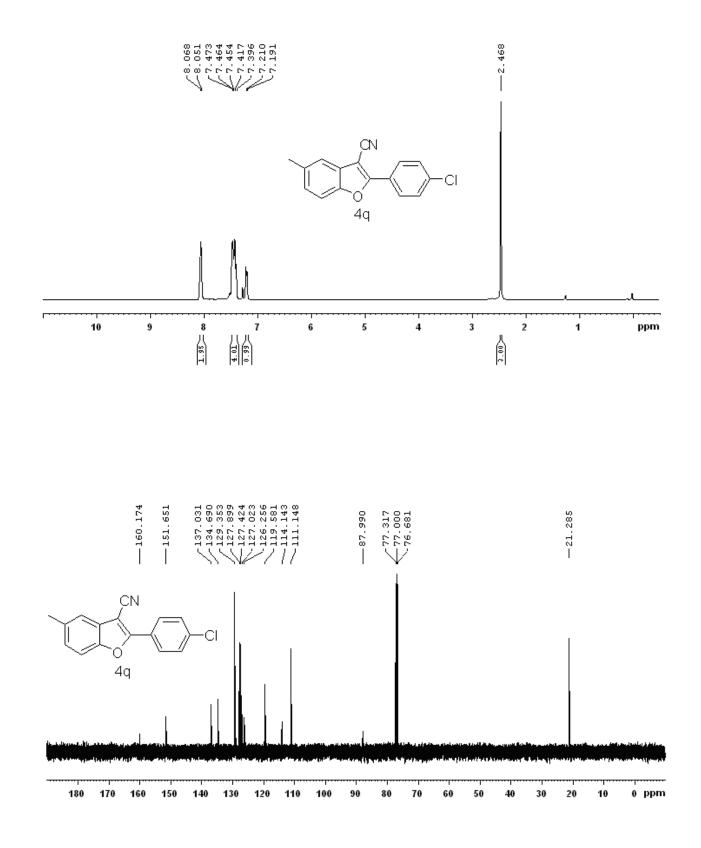




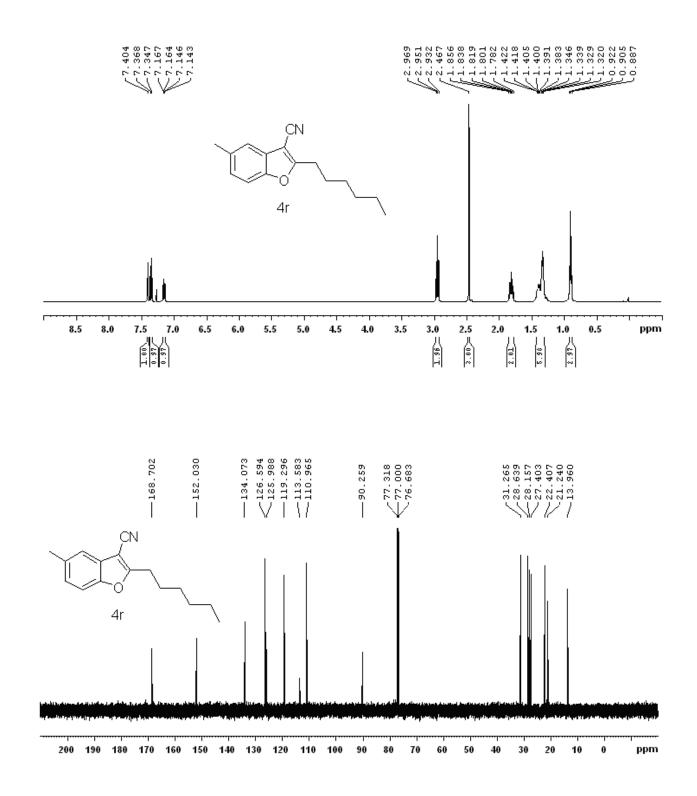


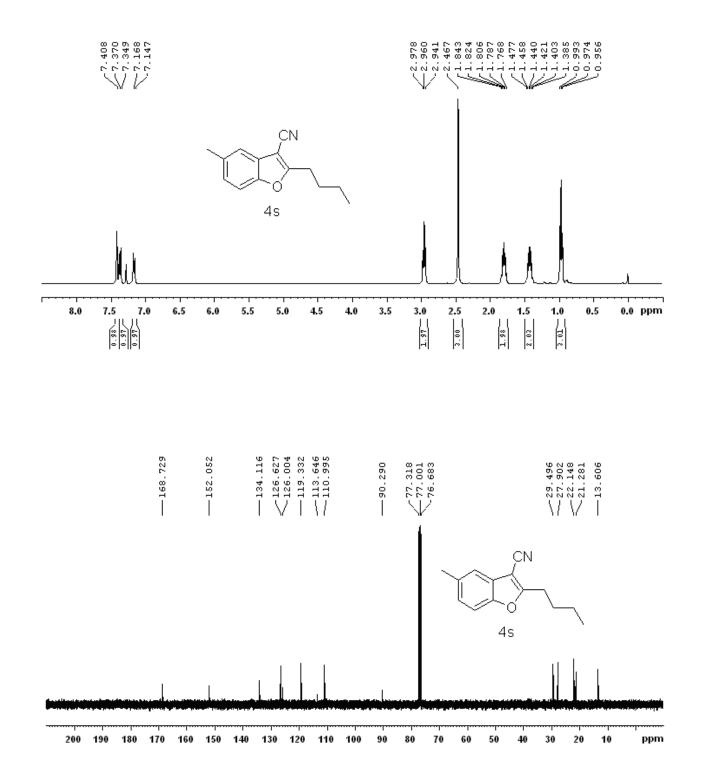






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Instrument: W Card Serial Sample Seria Operator: L Date: 2011/1 Elemental Co Single Mass						anghai Institute of Organic Chemi: ninese Academic of Sciences igh Resolution MS Data Report
Card Serial Sample Seria Operator: L Date: 2011/1 Elemental Co	Number: GCT-P	T Premier	Ionisa	tion Mode: EI+		Electron Energy: 70eV
Monoisotopic 295 formula(Elements Use Minimum: Maximum: Mass	iction: Off ↓ Mass, Odd and e) evaluated wi	Even Electro th 3 result:		ts (all res	ults (up to 1 Br: 0-1 + 1-FIT 12.1	000) for each mass)+' ' Formula+' C15 H11 N O +'
	221.0841 221.0834 221.0848	-0.1 0.6 -0.8	-0.5 2.7 -3.6	2.0 1.5	494.2 522.7	C7 H15 N3 O3 S+ C9 H17 O4 S+
(NC H 3a']	Sh Ci	nanghai Mass Spectrometry Center nanghai Institute of Organic Chemi hinese Academic of Sciences
					H	igh Resolution MS Data Report

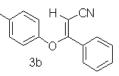
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Tolerance = 5.0 PPn / PPL. Min _____ Element prediction: Off 4 Monoisotopic Mass, Odd and Even Electron Ions4 295 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)4 The Predict O-60 H: O-80 N: O-4 O: O-6 S: O-1 Br: O-1 4 Minimum: -1.54 Maximum: 2.0 5.0 50.0↔ Mass Calc. Mass mDa PPMDBE i-FIT Formula⇔

C15 H11 N O e C9 H17 O4 S e C7 H15 N3 O3 S e 0.9 331.9 221.0842 221.0841 0.1 0.5 11.0 221.0848 -0.6 -2.7 1.5 0.8 3.6 221.0834 2.0 319.4

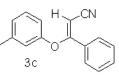




Instrument	Waters Micromass G	CT Premier	Ionia	ation Mode: EI+		Electron Energy: 70eV
Card Seria		C1 Fremer P-T11-12-0S09		auon moue. EF		EACCHOIL EAICE SY. 706 V
		F-111-12-030: 8SF-D28-S7⊬	910+			
Operator:		551 220 51				
Date: 2011						
	Composition Repo	rt⊌				
	s Analysis √	2.0.				
Tolerance		BE: min = -1	$.5, \max = 50$).0√		
	ediction: Off 4					
-	ic Mass, Odd and	Even Electr	on Ions⊬			
				nits (all resul	lts (up to 1	.000) for each mass)√
			0-4 0: 0-		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 4
	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 🗸
4						
24 A # # # #)	Ĭ	3b'		Sh Cł	anghai Mass Spectrometry Center anghai Institute of Organic Chemistry ninese Academic of Sciences gh Resolution MS Data Report
Instrument:	Waters Micromass G0	CT Premier	Ionis	ation Mode: EI+		Electron Energy: 70eV
Card Seria Sample Ser Operator: Date: 2011,	l Number: GCT-F ial Number: HB Li* /12/15*)-T11-12-0SO9 SF-D28-S8↔				
	Composition Repor	ct⊬				
	s Analysis ≁					
Tolerance :		BE: min = -1	.5, max = 50	.04		
El anna a t						
	ediction: Off +	Free Fleet	- Tened			
Monoisotop	ediction: Off 4 ic Mass, Odd and				1	
Monoisotop 325 formula	ediction: Off 4 ic Mass, Odd and a (e) evaluated 1	with 3 result	ts within li	•		1000) for each mass)+'
Monoisotop 325 formul: Elements U:	ediction: Off 4 ic Mass, Odd and a (e) evaluated w	with 3 result		6 S: O-1	lts (up to Br: 0-1 ↔	1000) for each mass)+ ^j
Monoisotop 325 formul: Elements U: Minimum:	ediction: Off 4 ic Mass, Odd and a (e) evaluated 1	with 3 resul (: 0-80 N:	ts within lin 0-4 O: O-	6 S: O−1 -1.5+ ^j		1000) for each mass)+ ^j
Monoisotop 325 formul: Elements U: Minimum: Maximum:	ediction: Off 4 ic Mass, Odd and a (e) evaluated a sed: C: O-60 H	with 3 resul; : 0-80 N: 2.0	ts within lin 0-4 0: 0- 5.0	6 S: O−1 −1.5⊬ 50.0⊬	Br: 0-1 ↔	
Nonoisotop 325 formul: Elements U: Minimum: Maximum: Mass	ediction: Off 4 ic Mass, Odd and a (e) evaluated 1 sed: C: O-60 H Calc. Mass	with 3 resul 1: 0-80 N: 2.0 mDa	ts within lin 0-4 O: O- 5.0 PPM	6 S: O−1 -1.5↔ 50.0↔ DBE	Br: O-1 ↔ i-FIT	Formula*'
Monoisotop 325 formul: Elements U: Minimum: Maximum:	ediction: Off 4 ic Mass, Odd and a (e) evaluated w sed: C: 0-60 H Calc. Mass 235.1004	with 3 resul 1: 0-80 N: 2.0 mDa -0.3	ts within lin 0-4 O: 0- 5.0 PPM -1.3	6 S: 0-1 -1.5↔ 50.0↔ DBE 1.5	Br: 0-1 ↔ i-FIT 2773044.8	Formula C10 H19 O4 S ب
Monoisotop 325 formul: Elements U: Minimum: Maximum: Mass	ediction: Off 4 ic Mass, Odd and a (e) evaluated m sed: C: 0-60 H Calc. Mass 235.1004 235.0997	with 3 resul : 0-80 N: 2.0 mDa -0.3 0.4	ts within lin 0-4 O: 0- 5.0 PPM -1.3 1.7	6 S: 0-1 -1.5+ 50.0+ DBE 1.5 11.0	Br: 0-1 ↔ i-FIT 2773044.8 2773015.3	Formula C10 H19 O4 S ඒ C16 H13 N O ඒ
Nonoisotop 325 formul: Elements U: Minimum: Maximum: Mass	ediction: Off 4 ic Mass, Odd and a (e) evaluated w sed: C: 0-60 H Calc. Mass 235.1004	with 3 resul 1: 0-80 N: 2.0 mDa -0.3	ts within lin 0-4 O: 0- 5.0 PPM -1.3	6 S: 0-1 -1.5↔ 50.0↔ DBE 1.5	Br: 0-1 ↔ i-FIT 2773044.8	Formula C10 H19 O4 S ඒ C16 H13 N O ඒ

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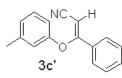




Instrument: Waters Micromass GCT Premier	Ionisation Mode: EI	+ Ele	ctron Energy: 70eV							
Card Serial Number: GCT-P-T11-12-0S091	.6+ ^J									
Sample Serial Number: HBSF-D28-S5⊬										
Operator: Li ⁴										
Date: 2011/12/15↔	Date: 2011/12/15+									
Elemental Composition Report+										
Single Mass Analysis 🗸										
Tolerance = 5.0 PPM / DBE: min = -1.5	5, max = 50.0⊬									
Element prediction: Off 4										
Monoisotopic Mass, Odd and Even Electron	n Ions+′									
325 formula(e) evaluated with 3 results	within limits (all re	sults (up to 100	D) for each mass)⊬							
Elements Used:C: 0-60 H: 0-80 N: 0-	-4 O: O-6 S: O-1	Br: 0-1 ↔								
Minimum:	-1.5↩									
Maximum: 2.0	5.0 50.04									
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 🗸							



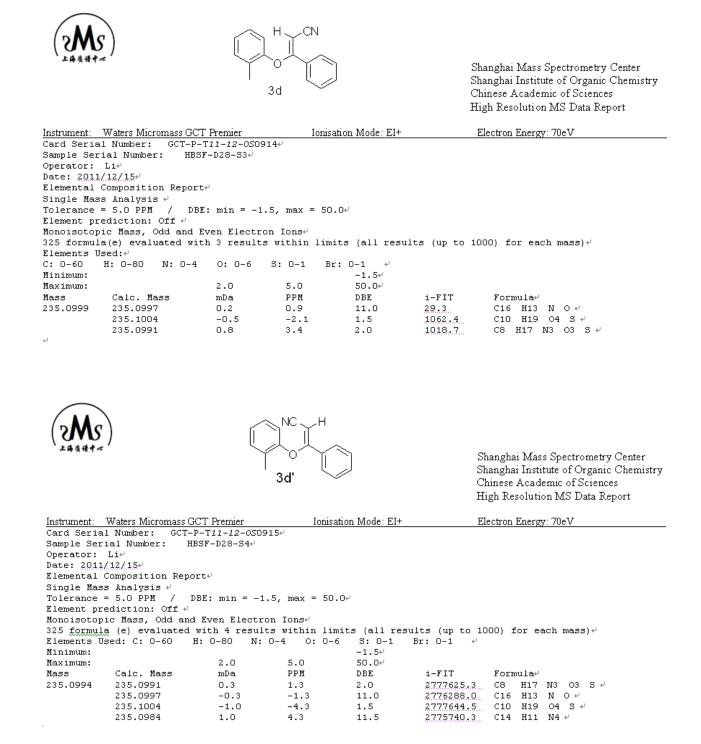
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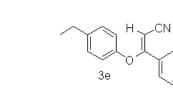


Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report

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	: = 50.04							
Element prediction: Off +								
Monoisotopic Mass, Odd and Even Electron Ions	له							
325 formula(e) evaluated with 3 results with:	n limits (all results (up to 1000) for each mass)↓							
Elements Used: C: 0-60 H: 0-80 N: 0-4	O: O-6 S: O-1 Br: O-1 ↔							
Minimum:	-1.5*							
Maximum: 2.0 5.0	50.0↔							
Mass Calc. Mass mDa PPH	DBE i-FIT Formula+							
235.0999 235.0997 0.2 0.9	11.0 <u>2.9</u> C16 H13 N O 4							
235.1004 -0.5 -2.	1 1.5 <u>161.9</u> C10 H19 O4 S↓							
235.0991 0.8 3.4	2.0 <u>153.9</u> C8 H17 N3 O3 S 4							

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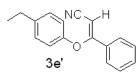




Instrument:	Waters Micromass GCT	Premier	Ionisatio	n Mode: EI+	E	lectron Energy: 70eV					
Card Seria	l Number: GCT-P-'	F11-12-0S0962	له								
Sample Ser	ial Number: HBSI	7-LiD21-S1↔									
Operator:	Li↩										
Date: 2011	Date: 2011/12/26+										
Elemental	Composition Report	له									
Single Mas	s Analysis 🗸										
Tolerance	= 5.0 PPM / DBE	: min = -1.5 ,	max = 50.04	J							
Element prediction: Off 4											
Monoisotop	ic Mass, Odd and E	ven Electron	Ions⊬								
386 formul	a(e) evaluated wit	h 4 results w	vithin limits	s (all result	s (up to 100	DO) for each mass)≁					
Elements U	sed:C: 0-60 H: (0-80 N: 0-4	0: 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 ↔					
له											

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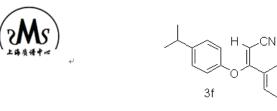




Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report

Instrument:	Waters Micromass	GCT Premier	Ionisat	ion Mode: EI+	- E	lectron Energy: 70eV
Card Seria	1 Number: GC	Г-Р-Т11-12-ОS0	1963₽			
Sample Ser	ial Number:	HBSF-LiD21-S2	ب			
Operator:	Li≁					
Date: 2011	/12/26+					
Elemental	Composition Re	port⊬				
Single Mas:	s Analysis 🗸					
Tolerance	= 5.0 PPM /	DBE: $min = -$	$1.5, \max = 50.$	04/		
Element pr	ediction: Off	t)				
Monoisotop	ic Mass, Odd a	nd Even Elect:	ron Ions⊬			
386 formula	a(e) evaluated	with 5 resul	ts within limi	ts (all res	ults (up to 10	00) for each mass)≁
Elements U	sed: C: 0-60	H: 0-80 N:	0-4 0:0-6	S: 0-1	Cl: O−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 +

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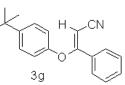


Instrument:	Waters Micromass G	CT Premier	Ionisa	ation Mode: EI+		Electron Energy: 70eV
Card Seri	al Number: GCT-3	P-T <i>11-12-0S</i> 096	54+ ^j			
Sample Se	rial Number: H	3SF-LiD21-S3≁				
Operator:	Li≁					
Date: <u>201</u>	1/12/26+					
Elemental	Composition Repo	rt+′				
Single Ma	ss Analysis 🗸					
Tolerance	= 5.0 PPM / D	BE: min = -1 .	5, max = 50	.O⊷		
Element p	rediction: Off 🗸					
Monoisoto	pic Mass, Odd and	Even Electro:	n Ions⊬			
414 formu	la(e) evaluated w	ith 5 results	within lim:	its (all res	ults (up to	1000) for each mass)√
Elements	Used: C: 0-60 1	H: 0-80 N: 0	0-4 0:0-	6 S: O-1	Cl: 0-1	به
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 4
	263.1315	-0.8	-3.0	6.5	7713.5	C15 H2O N2 C1 ↔
	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 🗸
ц.						
(M	(\mathbf{s})		NC H			Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report
	Waters Micromass (sation Mode: EI	+	Electron Energy: 70eV
		P-T11-12-0S09				
-		BSF-LiD21-S4↔				
Operator						
	11/12/26+					
	l Composition Rep	ort⇔				
-	ass Analysis 🗸					
		DBE: min = -1	$.5, \max = 50$	0.0√		
Element p	prediction: Off 4					
Monoisoto	opic Mass, Odd an	d Even Electro	on Ions⊬			

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:				-1.54		
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 H2O 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 🗸
له						

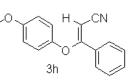




	Waters Micromass			n Mode: EI+	Electron Energy: 70eV
		T−P−T11 <i>−12−0S</i> 0968(μ L		
-	rial Number:	HBSF-LiD21-S7↔			
Operator:					
Date: <u>201</u>					
Elemental	Composition Re	port↓			
	ss Analysis 🗸				
Tolerance	= 5.0 PPM /	DBE: $\min = -1.5$,	max = 50.0⊬		
Element p	rediction: Off	La Contra			
		nd Even Electron			
434 formu	la(e) evaluated	. with 4 results w	ithin limits	(all result	ts (up to 1000) for each mass)≁
Elements	Used: C: 0-60	H: 0-80 N: 0-	4 0:0-6	S: 0-1 (Cl: O-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 C1 +
	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 +
له					
لد					
2.444	\mathbf{S}	3	g'		Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report
	Waters Micromas			n Mode: EI+	Electron Energy: 70eV
Card Seri	al Number: GC	T-P-T11-12-0S0969	le)		
Sample Se	rial Number:	HBSF-LiD21-S8↔			
Operator:	Li↔				
Date: 201					
	. Composition Re	eport⇔			
	ss Analysis 🗸				
	e = 5.0 PPM /	DBE: min = -1.5	, max = 50.0*	J	
	rediction: Off				
		and Even Electron			
					ts (up to 1000) for each mass)≁
	Used: C: 0-60	H: 0-80 N: 0-	-4 0: 0-6		Cl: 0-1 + ^J
Minimum:				-1.5↩	
Maximum:		2.0	5.0	50.0⊬	
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT Formula ^{↓J}
277.1469	277.1467	0.2	0.7	11.0	<u>2775578.3</u> C19 H19 N O ↔
	277.1472	-0.3	-1.1	6.5	<u>2776511.5</u> C16 H22 N2 C1 +
	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 ↔



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

Instrument:	Waters Micromass G	CT Premier	Ionisati	on Mode: EI+		Electron Energy: 70eV
		P-T11-12-0S097				
		BSF-LiD21-S9≁				
Operator:						
Date: 201:						
	Composition Repo	rt+				
	s Analysis 4					
		BE: min = -1 .	5. max = 50.0	له		
	ediction: Off +		-,			
-	oic Mass, Odd and	Even Electro	n Tons⊬			
-				s (all resul	lts (un to	1000) for each mass)√
		H: 0-80 N: 0		S: 0-1	Cl: 0-1	4
Minimum:				-1.5₽		
Maximum:		2.0	5.0	50.04		
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 C1 4
201.0919	251.0946	0.3	1.2	11.0	1.1	C16 H13 N O2 +
	251.0948	-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 S4
له	201.0940	0.9	3.0	2.0	310.0	CO III/ NO OF 5+
(MS (MS)	~~~_(3h'			Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistr Chinese Academic of Sciences High Resolution MS Data Report
nstrument:	Waters Micromass G(CT Premier	Ionisatio	n Mode: EI+		Electron Energy: 70eV
		-T11-12-0S097:				
		SF-LiD21-S10⊬				
perator:						
ate: 2011						
	Composition Repor	st⊬				
	s Analysis √					
	= 5.0 PPM / D	BE: min = -1.5	, max = 50.0↔			
	ediction: Off +					
	ic Mass, Odd and	Even Electron	Ions⊬			
-	,			(all result	ts (up to 1	1000) for each mass)√
		: 0-80 N: 0			Cl: 0-1 +	μ
finimum:				-1.5₽		
Maximum:		2.0	5.0	50.0⊬		
-	Calc. Mass	m Die	PPM	DDE		$\mathbf{E} = m m m 1 = 1$
Mass	cale. Mass	mDa	PPM	DBE	i-FIT	Formula#

 Maximum:
 2.0
 5.0
 500

 Mass
 Calc. Mass
 mDa
 PPM
 DBE
 i-FIT
 Formulae

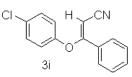
 251.0948
 251.0946
 0.2
 0.8
 11.0
 2773024.5
 C16
 H13
 N 02 e'

 251.0951
 -0.3
 -1.2
 6.5
 2773025.3
 C13
 H16
 N2
 0 C1 e'

 251.0953
 -0.5
 -2.0
 1.5
 2773027.0
 C10
 H19
 05
 5 e'

 251.0940
 0.8
 3.2
 2.0
 2773025.5
 C8
 H17
 N3<04</td>
 5 e'

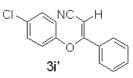




T	777	dott Barria	T	- Made TI		E1
	Waters Micromass			on Mode: EI+	-	Electron Energy: 70eV
		-P-T11-12-0S09				
•		HBSF-LiD21-S13	J			
Operator:	Li≁					
Date: 2011	/12/26+					
Elemental	Composition Rep	ort+				
Single Mas	s Analysis 🗸					
Tolerance	= 5.0 PPM /	DBE: min = -1 .	$5, \max = 50.0$)⊷		
Element pr	ediction: Off 🗸					
Monoisotop	ic Mass, Odd an	d Even Electro	n Ions⊷			
402 formul	a(e) evaluated	with 5 results	within limit	s (all res	ults (up to 1	000) for each mass)√
Elements U	sed: C: 0-60	H: 0-80 N:	0-4 0: 0-6	S: 0-1	C1: 0-1 +	
Minimum:				-1.54		
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 C1 ↔
	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 C1 4
	255.0444	0.8	3.1	2.0	50.3	C7 H14 N3 O3 S C1 4
	255.0440	1.2	4.7	6.5	307.1	C10 H11 N2 O4 S 4



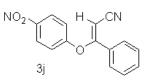
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Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report

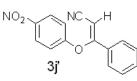
Instrument:	Waters Micromass GCT	Premier	Ionisatio	n Mode: EI+	E	ectron Energy: 70eV				
Card Seria	l Number: GCT-P-T	11-12-050975	له							
Sample Ser:	ial Number: HBSF	-LiD21-S14↔								
Operator:	Li⊷									
Date: 2011/12/26+										
Elemental Composition Report+										
Single Mass	Single Mass Analysis 4									
Tolerance :	= 5.0 PPM / DBE	min = -1.5,	max = 50.0*	J						
Element pre	ediction: Off √									
Monoisotopic Mass, Odd and Even Electron Ions4										
402 formula	a(e) evaluated with	n 6 results w	vithin limits	s (all result	ts (up to 100)0) for each mass)√				
Elements Us	sed: C: 0-60 H:	0-80 N: O-	4 0:0-6	S: 0-1 C	Cl: O−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 C1 🗸				





Instrument: Waters Micromass	GCT Premier	Ionisatio	n Mode: EI+	El	ectron Energy: 70eV			
Card Serial Number: GC	Г-Р-Т11 <i>-12-0S</i> 0978«	h						
Sample Serial Number:	HBSF-LiD21-S17₽							
Operator: Li↩								
Date: 2011/12/26+								
Elemental Composition Report4								
Single Mass Analysis 🗸								
Tolerance = 5.0 PPM /	DBE: $\min = -1.5$,	max = 50.0*	J					
Element prediction: Off	ų							
Monoisotopic Mass, Odd a	nd Even Electron	Ions⊬						
420 formula(e) evaluated	with 4 results w	ithin limits	s (all resul	ts (up to 100.	0) for each mass)√			
Elements Used: C: 0-60	H: 0-80 N: 0-4	4 0: 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 4			
266.0696	-0.4	-1.5	7.5	2773077.0	C12 H13 N3 O2 C1 🗸			
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 🗸			
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Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report

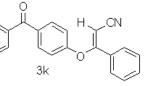
Instrument:	Waters Micromass	GCT Premier	Ionisatio	n Mode: EI+	El	ectron Energy: 70eV	
Card Seria	1 Number: GC	T-P-T11-12-0S097	94				
Sample Ser	ial Number:	HBSF-LiD21-S18↔					
Operator:	Li↔						
Date: <u>2011</u>	/12/26+						
Elemental Composition Report+							
Single Mas:	s Analysis 🗸						
Tolerance	= 5.0 PPM /	DBE: min = -1.5	5, max = 50.0+	J.			
Element pr	ediction: Off	ل ا					
Monoisotop	ic Mass, Odd a	nd Even Electron	lons⊬				
420 formula	a(e) evaluated	with 4 results	within limits	all resu	ilts (up to 100	10) for each mass)√	
Elements U	sed: C: 0-60	H: 0-80 N: 0	-4 0: 0-6	S: 0-1	Cl: O−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 C1 🗸	
	266.0698	-0.9	-3.4	2.5	2773316.8	C9 H16 N O6 S ↔	
4							

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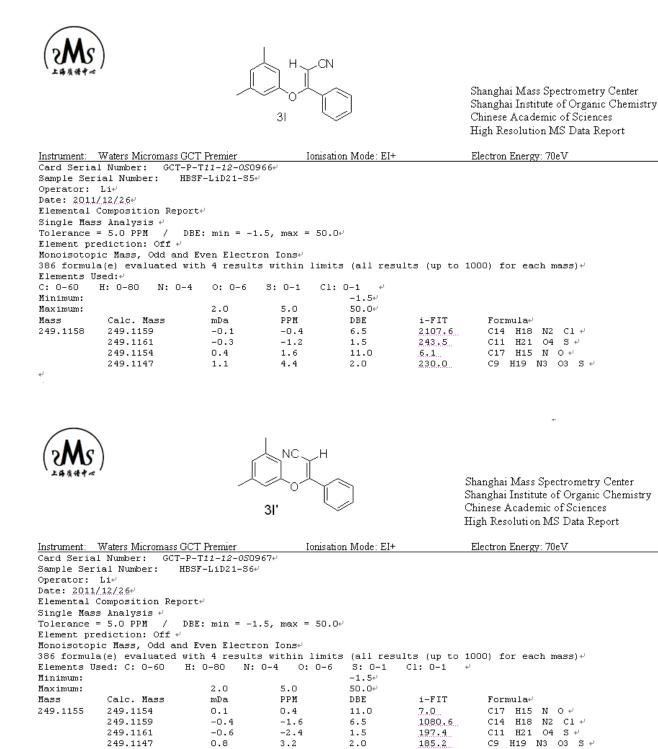


Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report

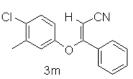
Instrument:	Waters Micromass	GCT Premier	Ionisati	on Mode: EI+	J	Electron Ener	:gy: 70eV	
Card Seris	al Number: GCT	Γ-Ρ-Τ <i>11-12-0S</i> Ο9	l804					
Sample Ser	ial Number:	HBSF-LiD21-S19	له ال					
Operator:	Li↩							
Date: 2011	/12/26+							
Elemental	Composition Re	port⊬						
-	s Analysis 🗸							
Tolerance			.5, max = 50.C)+ ^j				
-	ediction: Off							
)ic Mass, Odd a							
	la(e) evaluated)00) for ea	ach mass)√	
	Jsed: C: 0-60	H: 0-80 N:	0-4 0: 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	له	
325.1104	325.1103	0.1	0.3	16.0	6.1		5 N 02 +	
	325.1101	0.3	0.9	2.5	791.0	C11 H22	2 N4 O3 S C1 🖉	
	325.1108	-0.4	-1.2	11.5	735.2	C19 H18	B N2 O C1 ↔	
	325.1110	-0.6	-1.8	6.5	86.0	C16 H21	1 O5 S ↔	
	325.1096	0.8	2.5	7.0	79.2	C14 H19	9 N3 O4 S 🗸	
	325.1115	-1.1	-3.4	2.0	790.3	C13 H24		
	325.1089	1.5	4.6	16.5	2.4	C20 H13	3 N4 O ↔	
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$\langle \cdot \cdot \rangle$								
$(\mathbf{n} \mathbf{A} \mathbf{a})$		0						
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上满唐语中心			~_NC ∕ H					
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		~	ν Ο ή		Shangł	hai Mass Spo	ectrometry Center	
		3k'	լ				of Organic Chemistry	
				~			of Sciences	
					High K	lesolution M	IS Data Report	

Instrument:	Waters Micromass GCT	Premier	Ionisatio	n Mode: EI+	El	ectron Eners	y: 70eV	
Card Seria	1 Number: GCT-P-7	[<i>11–12–0S</i> 0981	له					
Sample Ser	ial Number: HBSF	'-LiD21-S20↔						
Operator:	Li≁							
Date: 2011/12/26+								
Elemental Composition Report+								
Single Mas:	s Analysis 🗸							
Tolerance :	= 5.0 PPM / DBE	: min = -1.5 ,	max = 50.0*	J				
	ediction: Off 🗸							
-	ic Mass, Odd and E							
	a(e) evaluated wit					10) for ea	ich mass)√	
Elements U	sed: C: O-60 H:	0-80 N: 0-	4 0:0-6		;l: 0−1 + ^J			
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		
	325.1103	0.3	0.9	16.0	2773040.0	C22 H15		
	325.1110	-0.4	-1.2	6.5	2773083.3	C16 H21		
	325.1101	0.5	1.5	2.5	2773156.3	C11 H22	N4 O3 S C1 🖉	
	325.1115	-0.9	-2.8	2.0	2773156.3	C13 H24		
	325.1096	1.0	3.1	7.0	2773079.5	C14 H19	N3 O4 S 🗸	

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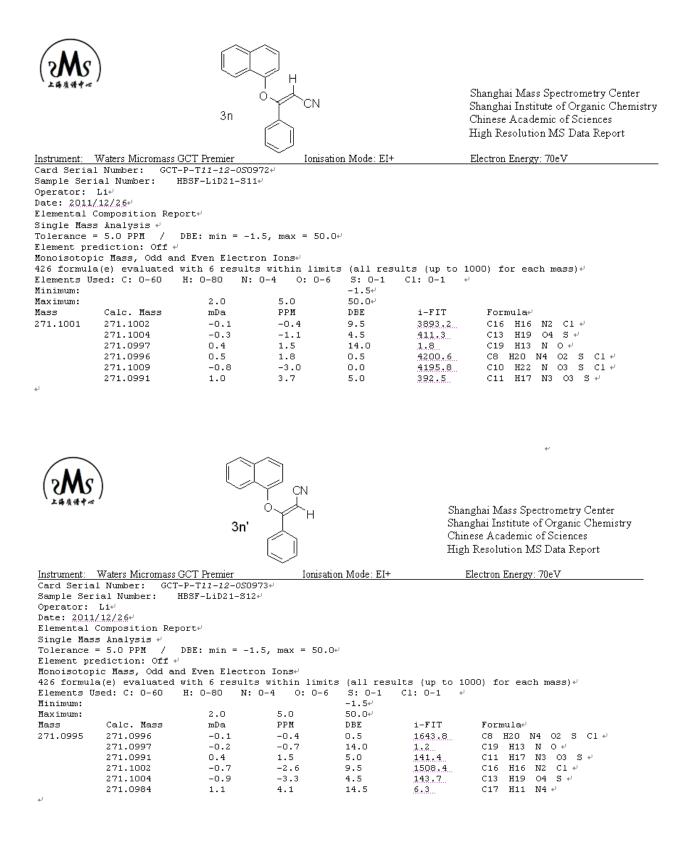


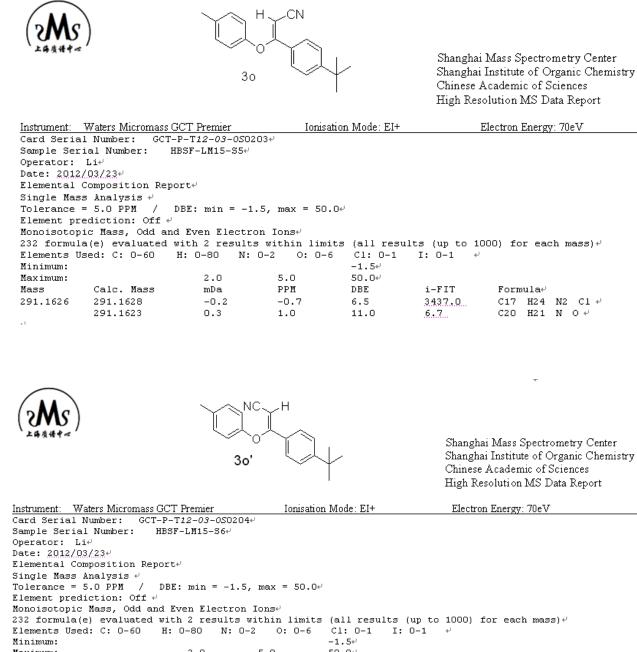




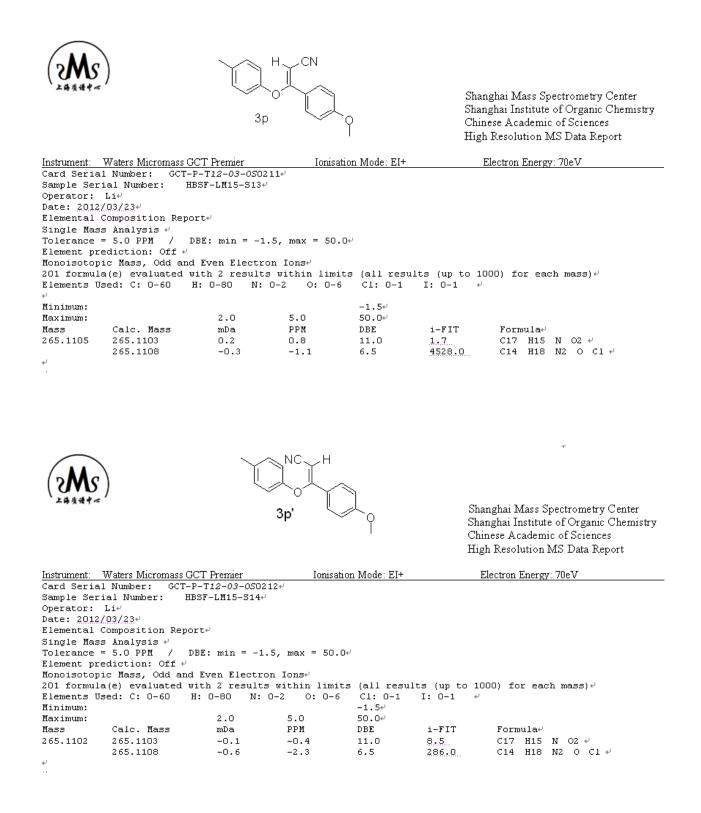
Instrument:	Waters Micromass	GCT Premier	Ionisatio	n Mode: El-	÷	Electron Energy: 70eV			
Card Seria	1 Number: GCT	-P-T11-12-0S097	76⊷						
Sample Ser	Sample Serial Number: HBSF-LiD21-S15+								
Operator:	Operator: Li+								
Date: 2011	/12/26+								
Elemental Composition Report#									
Single Mas	Single Mass Analysis +								
Tolerance		DBE: min = -1 .	5, max = 50.0*	J					
	ediction: Off +		,						
Monoisotop	ic Mass, Odd ar	d Even Electro	n Ions⊬						
				s (all res	sults (up to	1000) for each mass)≁			
	sed: C: 0-60	H: 0-80 N: 0		S: 0-1	Cl: 0-1	پ			
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 C1 🗸			
	269.0607	0.5	1.9	11.0	32.4	C16 H12 N O C1 +			
	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 C1 +			
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上海质谱中心	,	<u>ب</u> لا	~ ~ ~						
		/~/		<u>م</u>		Shanghai Mass Spectrometry Center			
						Shanghai Institute of Organic Chemistry			
		3n	n' 📈	~		Chinese Academic of Sciences			
						High Resolution MS Data Report			
						Then resolution has Data Report			

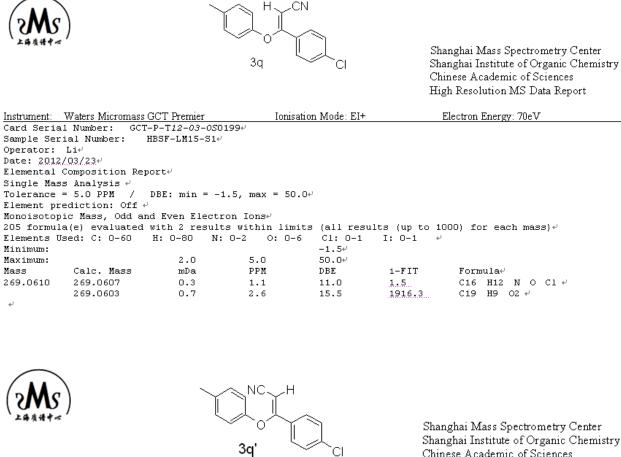
Instrument:	Waters Micromass GCT	Γ Premier	Ionisatio	n Mode: EI+	E	lectron Energy: 70eV			
Card Seria	1 Number: GCT-P-	T11-12-0S0977	lei I						
Sample Ser	ial Number: HBS	F-LiD21-S16↔							
Operator:	Li≁								
Date: 2011/12/26+									
Elemental Composition Report+									
Single Mass Analysis 🗸									
Tolerance	= 5.0 PPM / DBB	$C: \min = -1.5$, max = 50.04	J					
Element pr	ediction: Off 4								
-	ic Mass, Odd and E								
						00) for each mass)≁			
	sed: C: 0-60 H:	0-80 N: 0-	-4 0:0-6		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 C1+			
	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 +			
4J									





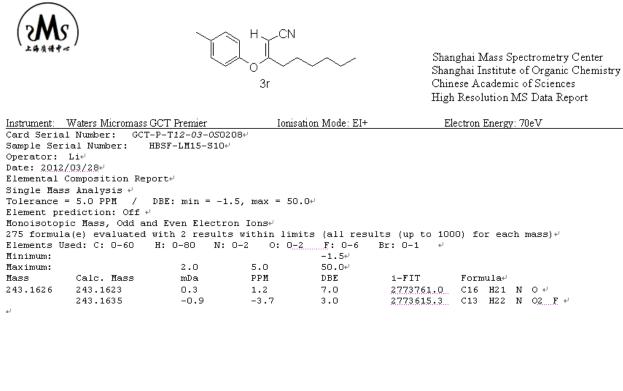
Maximum:		2.0	5.0	50.04		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula+
291.1622	291.1623	-0.1	-0.3	11.0	12.5	C2O H21 N O 🗸
	291.1628	-0.6	-2.1	6.5	958.2	C17 H24 N2 Cl 🗸



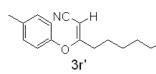


Instrument:	Waters Micromass	GCT Premier	Ionisation	n Mode: EI+	El	ectron Energy: 70eV		
Card Serial	. Number: GCT	-P-T12-03-0S0200₽						
Sample Seri	al Number: 1	HBSF-LM15-S2≁						
Operator:	Li≁							
Date: 2012/03/23+								
Elemental C	composition Rep	ort₽						
Single Mass	; Analysis 🗸							
Tolerance =	Tolerance = 5.0 PPM / DBE: min = -1.5 , max = 50.0^{+1}							
Element pre	diction: Off +							
Monoisotopi	c Mass, Odd an	d Even Electron I	lons⊬					
205 formula	(e) evaluated	with 2 results wi	thin limits	(all result	s (up to 100)O) for each mass)≁		
Elements Us	ed: C: 0-60	H: 0-80 N: 0-2	0: 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 +		

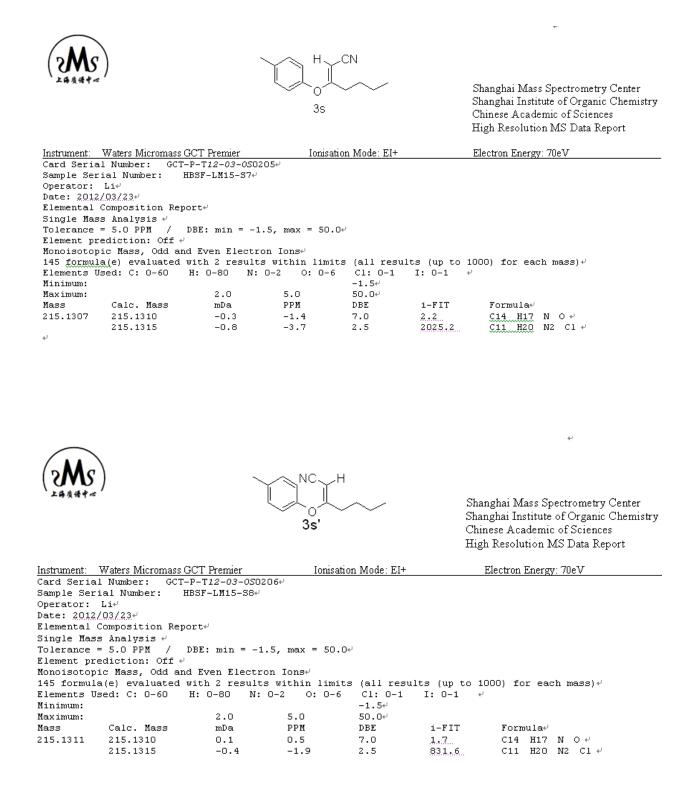
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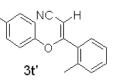




Instrument:	Waters Micromass GCT	Premier	Ionisatio	n Mode: EI+	E	lectron Energy: 70eV			
Card Serial	l Number: GCT-P-'	Г <i>12-03-05</i> 0209	Ψ.						
Sample Seri	ial Number: HBSH	7-LM15-S114							
Operator:	Li≁								
Date: 2012/	/03/28⊷								
Elemental (Composition Report	له ا							
Single Mass	Single Mass Analysis ↔								
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0^{+1}									
Element pre	ediction: Off 4								
Monoisotopi	ic Mass, Odd and E	ven Electron	Ions⊷						
275 formula	a(e) evaluated wit	h 2 results τ	Jithin limits	s (all result	ts (up to 10))) for each mass)⊬			
Elements Us	sed: C: 0-60 H:	0-80 N: 0-	2 0: 0-2	F: 0-6 H	3r: 0−1 +				
Minimum:				-1.5*					
Maximum:		2.0	5.0	50.04					
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 O <u>2 F</u> +			
4									

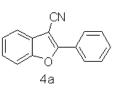






Instrument:	Waters Micromass GCT	Γ Premier	Ionisatio	on Mode: EI+	E	ectron Energy: 70eV
Card Seria	1 Number: GCT-P-	T <i>12-03-0S</i> 021	3≁			
Sample Ser	ial Number: HBS	F-LM15-S15⊬				
Operator:	Li≁					
Date: <u>2012</u>	/03/28+					
Elemental	Composition Report	لهز				
Single Mas:	s Analysis 🗸					
Tolerance	= 5.0 PPM / DBH	$: \min = -1.3$	5, max = 50.0	ų		
Element pr	ediction: Off 4					
Monoisotop	ic Mass, Odd and H	ven Electron	n Ions+'			
285 formula	a(e) evaluated wit	h 3 results	within limit:	s (all result	s (up to 100)0) for each mass)≁
Elements U	sed: C: 0-60 H:	0-80 N: C	-2 0: 0 <u>-2</u>	F: 0-6 B	r: 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 +
له						



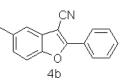


Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report

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Instrument:	Waters Micromass GCT	Premier	Ionisatio:	n Mode: EI+	El	ectron Energy: 70eV			
Card Serial	Number: GCT-P-7	Γ11-12-0S0920+	ų						
Sample Seri	al Number: HBSH	'-D28-S9⊬							
Operator:	Li↩								
Date: 2011/	12/15+								
Elemental C	Elemental Composition Report4								
Single Mass	: Analysis +								
Tolerance =	5.0 PPM / DBE	: min = -1.5 ,	max = 50.0⊬						
Element pre	diction: Off 4								
Monoisotopi	c Mass, Odd and E	ven Electron	Ions⊬						
297 formula	(e) evaluated wit	h 3 results w	ithin limits	(all result	s (up to 100	0) for each mass)√			
Elements Us	ed: C: O-60 H:	0-80 N: 0-4	4 0:0-6	S: 0-1 B	r: 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	С15 Н9 № О+/			
	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≁			
4									



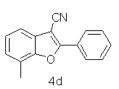


Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report

Instrument	Waters Micromass (CT Bromier	Ionic	ation Mode: EI+		Electron Energy: 70eV
Card Seria		-P-T11-12-0S09				Exection Energy. /oe v
			923₩			
•		IBSF-D28-S12≁				
Operator:						
Date: <u>2011</u>	/12/15+					
Elemental	Composition Rep	ort⊬				
Single Mas	s Analysis 🗸					
Tolerance		DBE: min = -1	$.5. \max = 50$.04		
	ediction: Off +					
	ic Mass, Odd an	d Even Electr	on Tonse			
				mite (all reev	ilte (un to	1000) for each mass)↔
			0-4 0: 0-		Br: 0-1 ↔	
	isea: L: U-60	H: U-80 N:	0-4 0:0-		BT: U−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 🗸
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(M 2 # § # † ~)	Ĺ		\supset	Sha	inghai Institute of Organic Chemistry
(M 2.46644~)	Í	CN CN 4c	\supset	Sha Chi	nghai Institute of Organic Chemistry nese Academic of Sciences
(M +######)	Ĺ			Sha Chi	inghai Institute of Organic Chemistry
(M +# § # † ~)	<u> </u>			Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
) Waters Micromass G		4c Ionisa	tion Mode: EI+	Sha Chi Hig	nghai Institute of Organic Chemistry nese Academic of Sciences
Card Seria	l Number: GCT-	P-T11-12-0S09	4c Ionisa	tion Mode: EI+	Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Seria: Sample Ser:	l Number: GCT- ial Number: H		4c Ionisa	tion Mode: EI+	Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Seria	l Number: GCT- ial Number: H	P-T11-12-0S09	4c Ionisa	tion Mode: EI+	Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Seria: Sample Ser:	l Number: GCT- ial Number: H Li≁	P-T11-12-0S09	4c Ionisa	tion Mode: EI+	Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Seria: Sample Ser: Operator: Date: <u>2011</u> /	l Number: GCT- ial Number: H Li¢ /12/15¢	P-T <i>11-12-OS</i> O9 BSF-D28-S11≁	4c Ionisa	tion Mode: EI+	Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (l Number: GCT- ial Number: H Li ⁴ /12/15 ⁴ Composition Repo	P-T <i>11-12-OS</i> O9 BSF-D28-S11≁	4c Ionisa	tion Mode: EI+	Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Seria Sample Ser: Operator: Date: 2011, Elemental (Single Mass	l Number: GCT- ial Number: H Li ⁴ / <u>12/15</u> ⁴ Composition Repo s Analysis 4	P-T11-12-0509 BSF-D28-S11+ ^J PTt+ ^J	4c Ionisa		Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance =	l Number: GCT- ial Number: H Li+ /12/15+ Composition Repo s Analysis + = 5.0 PPM / I	P-T <i>11-12-OS</i> O9 BSF-D28-S11≁	4c Ionisa		Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pre	l Number: GCT- ial Number: H Li ⁴ (12/15 ⁴⁾ Composition Repo s Analysis ⁴⁾ = 5.0 PPM / I ediction: Off ⁴⁾	P-T11-12-0509 BSF-D28-S11+ ¹ ort+ ¹)BE: min = -1.	4c Ionisa 22+'		Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pro Monoisotop:	l Number: GCT- ial Number: H Li+ (12/15+ Composition Repo s Analysis + = 5.0 PPM / I ediction: Off + ic Mass, Odd and	P-T11-12-0509 BSF-D28-S114 ort4 DBE: min = -1. L Even Electro	$\frac{1}{4c}$ Ionisa 224 ³ .5, max = 50. on Ions ⁴³	0+1	Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences ih Resolution MS Data Report Electron Energy: 70eV
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pre Monoisotop: 317 formula	l Number: GCT- ial Number: H Li $^{\downarrow}$ (12/15 $^{\downarrow}$ Composition Repo s Analysis $^{\downarrow}$ = 5.0 PPM / I ediction: Off $^{\downarrow}$ ic Mass, Odd and a(e) evaluated w	P-T11-12-0509 BSF-D28-S114 OBE: min = -1. L Even Electro rith 3 results	$\frac{1}{4c}$ $\frac{1}{22e^{4}}$ $\frac{1}{25e^{4}}$ $\frac{1}{25e^{4}}$ $\frac{1}{21e^{4}}$ $\frac{1}{21e^{4}}$	0≁ ts (all resul	Sha Chi Hig I ts (up to 10	inghai Institute of Organic Chemistry inese Academic of Sciences in Resolution MS Data Report
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pro Monoisotop: 317 formula Elements Us	l Number: GCT- ial Number: H Li+ /12/15+ Composition Repo s Analysis + = 5.0 PPM / I ediction: Off + ic Mass, Odd and a(e) evaluated w	P-T11-12-0509 BSF-D28-S114 OBE: min = -1. L Even Electro rith 3 results	$\frac{1}{4c}$ Ionisa 224 ³ .5, max = 50. on Ions ⁴³	0+ ² ts (all resul 5 S: 0-1 1	Sha Chi Hig	inghai Institute of Organic Chemistry inese Academic of Sciences ih Resolution MS Data Report Electron Energy: 70eV
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pre Monoisotop: 317 formula Elements Us Minimum:	l Number: GCT- ial Number: H Li $^{\downarrow}$ (12/15 $^{\downarrow}$ Composition Repo s Analysis $^{\downarrow}$ = 5.0 PPM / I ediction: Off $^{\downarrow}$ ic Mass, Odd and a(e) evaluated w	P-T11-12-0509 BSF-D28-S114 DEE: min = -1. L Even Electro rith 3 results H: 0-80 N:	$4c$ $4c$ $10nisa$ $22^{4'}$ $5, max = 50.$ $5 m Ions^{4}$ $8 within limi 0-4 0: 0-6$	04 ts (all resul 5 S: 0-1) -1.54	Sha Chi Hig I ts (up to 10	inghai Institute of Organic Chemistry inese Academic of Sciences ih Resolution MS Data Report Electron Energy: 70eV
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pro 317 formula Elements Us	l Number: GCT- ial Number: H Li $^{\downarrow}$ (12/15 $^{\downarrow}$ Composition Repo s Analysis $^{\downarrow}$ = 5.0 PPM / I ediction: Off $^{\downarrow}$ ic Mass, Odd and a(e) evaluated w	P-T11-12-0509 BSF-D28-S114 OBE: min = -1. L Even Electro rith 3 results	$\frac{1}{4c}$ $\frac{1}{22e^{4}}$ $\frac{1}{25e^{4}}$ $\frac{1}{25e^{4}}$ $\frac{1}{21e^{4}}$ $\frac{1}{21e^{4}}$	0+ ² ts (all resul 5 S: 0-1 1	Sha Chi Hig I ts (up to 10	inghai Institute of Organic Chemistry inese Academic of Sciences ih Resolution MS Data Report Electron Energy: 70eV
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pre Monoisotop: 317 formula Elements Us Minimum:	l Number: GCT- ial Number: H Li $^{\downarrow}$ (12/15 $^{\downarrow}$ Composition Repo s Analysis $^{\downarrow}$ = 5.0 PPM / I ediction: Off $^{\downarrow}$ ic Mass, Odd and a(e) evaluated w	P-T11-12-0509 BSF-D28-S114 OBE: min = -1. L Even Electro with 3 results H: 0-80 N:	$4c$ $4c$ $10nisa$ $22^{4'}$ $5, max = 50.$ $5 m Ions^{4}$ $8 within limi 0-4 0: 0-6$	04 ts (all resul 5 S: 0-1) -1.54	Sha Chi Hig I ts (up to 10	inghai Institute of Organic Chemistry inese Academic of Sciences ih Resolution MS Data Report Electron Energy: 70eV
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pra Monoisotop: 317 formula Elements Us Minimum: Maximum: Mass	l Number: GCT- ial Number: H Li+ /12/15+ Composition Repo s Analysis + = 5.0 PPM / I ediction: Off + ic Mass, Odd and a(e) evaluated t sed: C: 0-60	P-T11-12-0509 BSF-D28-S11+ OBE: min = -1. LEven Electro with 3 results H: 0-80 N: 2.0 mDa	$4c$ $4c$ $1onisa$ 22^{*} $5, max = 50.$	0+' ts (all resul 5 S: 0-1) -1.5+' 50.0+' DBE	Sha Chi Hig I ts (up to 10 Br: 0-1 + i-FIT	inghai Institute of Organic Chemistry inese Academic of Sciences th Resolution MS Data Report Electron Energy: 70eV 100) for each mass)+' Formula+'
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pre Monoisotop: 317 formula Elements Us Minimum: Maximum:	l Number: GCT- ial Number: H Li* (12/15* Composition Repo s Analysis * = 5.0 PPM / I ediction: Off * ic Mass, Odd and a(e) evaluated w sed: C: 0-60 Calc. Mass 233.0841	P-T11-12-0509 BSF-D28-S114 DEE: min = -1. BEE: min = -1. BE: D-80 N: 2.0 mDa 0.1	4c $4c$ $1onisa$ $22*$ $5, max = 50.$	0+ ¹ ts (all resul 5 S: 0-1) -1.5 ⁺¹ 50.0 ⁺¹ DBE 12.0	Sha Chi Hig ts (up to 10 Br: 0-1 + i-FIT 8.0	nghai Institute of Organic Chemistry inese Academic of Sciences th Resolution MS Data Report Electron Energy: 70eV 000) for each mass)+ Formula+ C16 H11 N 0+
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pra Monoisotop: 317 formula Elements Us Minimum: Maximum: Mass	<pre>1 Number: GCT- ial Number: H Li+ /12/15+ Composition Repo s Analysis + = 5.0 PPM / I ediction: Off + ic Mass, Odd and a(e) evaluated w sed: C: 0-60 f Calc. Mass 233.0841 233.0848</pre>	P-T11-12-0509 BSF-D28-S114 DEE: min = -1. DEE: min = -1. DEE: Description ith 3 results H: 0-80 N: 2.0 mDa 0.1 -0.6	1000000000000000000000000000000000000	0+' ts (all resul 5 S: 0-1) -1.5+' 50.0+' DBE 12.0 2.5	Sha Chi Hig ts (up to 10 Br: 0-1 + 1-FIT 8.0 596.9.	inghai Institute of Organic Chemistry inese Academic of Sciences th Resolution MS Data Report Electron Energy: 70eV 2000) for each mass)+' Formula+' C16 H11 N O+' C10 H17 O4 S+'
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pre Monoisotop: 317 formule Elements Us Minimum: Maximum: Mass 233.0842	l Number: GCT- ial Number: H Li* (12/15* Composition Repo s Analysis * = 5.0 PPM / I ediction: Off * ic Mass, Odd and a(e) evaluated w sed: C: 0-60 Calc. Mass 233.0841	P-T11-12-0509 BSF-D28-S114 DEE: min = -1. BEE: min = -1. BE: D-80 N: 2.0 mDa 0.1	4c $4c$ $1onisa$ $22*$ $5, max = 50.$	0+ ¹ ts (all resul 5 S: 0-1) -1.5 ⁺¹ 50.0 ⁺¹ DBE 12.0	Sha Chi Hig ts (up to 10 Br: 0-1 + i-FIT 8.0	nghai Institute of Organic Chemistry inese Academic of Sciences th Resolution MS Data Report Electron Energy: 70eV 000) for each mass)+ Formula+ C16 H11 N 0+
Card Serial Sample Ser: Operator: Date: 2011/ Elemental (Single Mass Tolerance = Element pra Monoisotop: 317 formula Elements Us Minimum: Maximum: Mass	<pre>1 Number: GCT- ial Number: H Li+ /12/15+ Composition Repo s Analysis + = 5.0 PPM / I ediction: Off + ic Mass, Odd and a(e) evaluated w sed: C: 0-60 f Calc. Mass 233.0841 233.0848</pre>	P-T11-12-0509 BSF-D28-S114 DEE: min = -1. DEE: min = -1. DEE: Description ith 3 results H: 0-80 N: 2.0 mDa 0.1 -0.6	1000000000000000000000000000000000000	0+' ts (all resul 5 S: 0-1) -1.5+' 50.0+' DBE 12.0 2.5	Sha Chi Hig ts (up to 10 Br: 0-1 + 1-FIT 8.0 596.9.	inghai Institute of Organic Chemistry inese Academic of Sciences th Resolution MS Data Report Electron Energy: 70eV 2000) for each mass)+' Formula+' C16 H11 N O+' C10 H17 O4 S+'

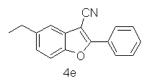
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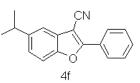
Instancest	Waters Micromass	CCT Branier	Ioniactic	n Mode: EI+	F	Jactron Energy 70-37				
				n moue. Er-	L	lectron Energy: 70eV				
		F-P-T11-12-0S092	14							
-	Sample Serial Number: HBSF-D28-S10+									
Operator: Li+										
Date: 2011/12/15+										
Elemental	Composition Re	port⊬								
Single Mas	s Analysis 🗸									
Tolerance	= 5.0 PPM /	DBE: min = -1 .	5, max = 50.0 +	J						
Element pr	ediction: Off	μ.								
Monoisotop	ic Mass, Odd a	nd Even Electro	n Ions⊬							
317 formul	a(e) evaluated	with 3 results	within limits	: (all resu	ults (up to 10	00) for each mass)⊬				
Elements U	sed: C: 0-60	H: 0-80 N: 0	D-4 O: O-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 4				
له										





Instrument:	Waters Micromass GC	T Premier	Ionisatio	n Mode: EI+	El	ectron Energy: 70eV	
Card Serial	Number: GCT-P-	-T11-12-0S0924+	J				
Sample Seri	al Number: HBS	SF-D28-S13≁					
Operator:	Li↓						
Date: <u>2011/</u>	12/15+						
Elemental Composition Report+							
Single Mass	8 Analysis 🗸						
Tolerance =	• 5.0 PPM / DB	$E: \min = -1.5,$	max = 50.0⊬				
Element pre	diction: Off 🖉						
Monoisotopi	c Mass, Odd and	Even Electron	Ions⊬				
346 formula	a(e) evaluated wi	th 3 results w	ithin limits	(all result	ts (up to 100)O) for each mass)⊬	
Elements Us	sed: C: 0-60 H:	: 0-80 N: 0-4	4 0:0-6	S: 0-1 E	8r: 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 🗸	
<u>ل</u> ه							



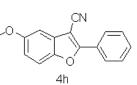


THE PLOTICITY.	Waters Micromass C	CT Premier	Ionis	ation Mode: EI+	Electron Energy: 70eV
Card Seria	al Number: GCT-	P-T11-12-0S0	925₽		
Sample Ser	rial Number: H	BSF-D28-S14≁			
Operator:	Li∜				
Date: 201	1/12/15+				
	Composition Repo	ort≁			
	ss Analysis √				
		DBE: min = -1	.5. max = 50	1.04	
	rediction: Off 4				
-	pic Mass, Odd and	N Even Electr	on Toned		
				wite (all rea	ults (up to 1000) for each mass)+
			0-4 0: 0-		Br: 0-1 4
Minimum:	usea: t: 0-60	n: 0-00 N:	0-4 0:0-	-o 5:0-1 -1.5⊬	br: U-1 +
Maximum:		2.0	5.0	50.04	
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	<u>2783190.0</u> C10 H19 N3 O3 S 4
	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 🗸
4					
)	K	CN 4g		Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report
	Waters Micromass GC			ion Mode: EI+	Electron Energy: 70eV
Card Serial	Number: GCT-P-	-T11-12-0S092		ion Mode: EI+	Electron Energy: 70eV
Card Serial Sample Seri	Number: GCT-P- al Number: HBS			ion Mode: EI+	Electron Energy: 70eV
Card Serial Sample Seri Operator: J	Number: GCT-P- al Number: HBS Li ⁴¹	-T11-12-0S092		ion Mode: EI+	Electron Energy: 70eV
Card Serial Sample Seri Operator: J Date: <u>2011/</u>	Number: GCT-P- al Number: HBS Lit 12/15	-T <i>11−12−0S</i> 092 F−D28−S15↔		ion Mode: EI+	Electron Energy: 70eV
Card Serial Sample Seri Operator: J Date: <u>2011/</u>	Number: GCT-P- al Number: HBS Li ⁴¹	-T <i>11−12−0S</i> 092 F−D28−S15↔		ion Mode: EI+	Electron Energy: 70eV
Card Serial Sample Seri Operator: J Date: <u>2011/</u>	Number: GCT-P- al Number: HBS Li ^{4/} 12/15 ^{4/} omposition Report	-T <i>11−12−0S</i> 092 F−D28−S15↔		ion Mode: EI+	Electron Energy: 70eV
Card Serial Sample Seri Operator: 1 Date: 2011/ Elemental C	Number: GCT-P- al Number: HBS Li+ 12/15+ omposition Report Analysis +	-T <i>11−12−0S</i> 092 F−D28−S15↔	641		Electron Energy: 70eV
Card Serial Sample Seri Operator: 1 Date: <u>2011/</u> Elemental C Single Mass Tolerance =	Number: GCT-P- al Number: HBS Li+ 12/15+ omposition Report Analysis +	-T <i>11−12−0S</i> 092 ;F−D28−S15+ ^J t+ ^J	641		Electron Energy: 70eV
Card Serial Sample Seri Operator: 1 Date: 2011/ Elemental C Single Mass Tolerance = Element pre	Number: GCT-P- al Number: HBS L1+ ⁰ 12/15+ ⁰ omposition Report Analysis + ⁰ 5.0 PPM / DB:	T <i>ii-12-0S</i> 092 F-D28-S15* ¹ t* ¹ E: min = -1.5	64 ¹ 5, max = 50.1		Electron Energy: 70eV
Card Serial Sample Seri Operator: 1 Date: 2011/ Elemental C Single Mass Tolerance = Element pre Monoisotopi	Number: GCT-P- al Number: HBS Li ⁴ 12/15 ⁴ omposition Report Analysis ⁴ 5.0 PPM / DB diction: Off ⁴ c Mass, Odd and D	T <i>11-12-0S</i> 092 F-D28-S15+ ¹ t+ ¹ E: min = -1.5 Even Electron	64) 5, max = 50.1 n Ions4	J+1	Electron Energy: 70eV
Card Serial Sample Seri Operator: D Date: 2011/ Elemental C Single Mass Tolerance = Element pre Monoisotopi 396 formula	Number: GCT-P- al Number: HBS Li ⁴⁷ 12/15 ⁴⁷ omposition Report Analysis ⁴⁷ 5.0 PPM / DB diction: Off ⁴⁷ c Mass, Odd and D (e) evaluated with	T <i>11-12-0S</i> 092 F-D28-S15+ ¹ t+ ¹ E: min = -1.5 Even Electron	64) 5, max = 50.1 n Ions4) Within limit	یہ: s (all result)	
Card Serial Sample Seri Operator: D Date: 2011/ Elemental C Single Mass Tolerance = Element pre Monoisotopi 396 formula	Number: GCT-P- al Number: HBS Li ⁴⁷ 12/15 ⁴⁷ omposition Report Analysis ⁴⁷ 5.0 PPM / DB diction: Off ⁴⁷ c Mass, Odd and D (e) evaluated with	T11-12-0S092 F-D28-S15+ E: min = -1.3 Even Electroi th 4 results	64 ⁾ 5, max = 50.1 n Ions4) within limi1	یہ: s (all result)	:s (up to 1000) for each mass)산
Card Serial Sample Seri Operator: 1 Date: 2011/ Elemental C Single Mass Tolerance = Element pre Monoisotopi 396 formula Elements Us	Number: GCT-P- al Number: HBS Li ⁴⁷ 12/15 ⁴⁷ omposition Report Analysis ⁴⁷ 5.0 PPM / DB diction: Off ⁴⁷ c Mass, Odd and D (e) evaluated with	T11-12-0S092 F-D28-S15+ E: min = -1.3 Even Electroi th 4 results	64 ⁾ 5, max = 50.1 n Ions4) within limi1	0↔ cs (all result S: 0-1 F	:s (up to 1000) for each mass)산
Card Serial Sample Seri Operator: 1 Date: 2011// Elemental C Single Mass Tolerance = Element pre Monoisotopi 396 formula Elements Us Minimum:	Number: GCT-P- al Number: HBS Li ⁴⁷ 12/15 ⁴⁷ omposition Report Analysis ⁴⁷ 5.0 PPM / DB diction: Off ⁴⁷ c Mass, Odd and D (e) evaluated with	T11-12-05092 FF-D28-515+ t+ E: min = -1.1 Even Electron th 4 results 0-80 N: C	64 ⁰ 5, max = 50.1 n Ions4 within limit 1-4 O: 0-6	ეყ :s (all result S: 0-1 E -1.54	:s (up to 1000) for each mass)산
Card Serial Sample Seri Operator: J Date: 2011// Elemental C Single Mass Tolerance = Element pre Monoisotopi 396 formula Elements Us Minimum:	Number: GCT-P- al Number: HBS L1+ mposition Report Analysis + 5.0 PPM / DB diction: Off + c Mass, Odd and D (e) evaluated wit ed: C: 0-60 H:	T11-12-05092 FF-D28-515+ t+ E: min = -1.3 Even Electron th 4 results 0-80 N: C 2.0	64 ⁰ 5, max = 50.1 n Ions4 ⁰ within limit 0-4 O: 0-6 5.0	D+ cs (all result S: O-1 F -1.5+ 50.0+	is (up to 1000) for each mass)+' br: 0-1 +' i-FIT Formula+'
Card Serial Sample Seri Operator: J Date: 2011// Elemental C Single Mass Tolerance = Element pre Monoisotopi 396 formula Elements Us Minimum: Maximum: Mass	Number: GCT-P- al Number: HBS Lit Momposition Report Analysis + 5.0 PPM / DB diction: Off + c Mass, Odd and D (e) evaluated wit ed: C: 0-60 H: Calc. Mass 275.1304	T11-12-05092 F-D28-515*' E: min = -1.3 Even Electron th 4 results 0-80 N: C 2.0 mDa 0.3	6+ ⁰ 5, max = 50.1 n Ions+ ⁰ within limin D-4 O: O-6 5.0 PPM	0+' S: 0-1 E -1.5+' 50.0+' DBE 3.0	is (up to 1000) for each mass)+' br: 0-1 +' i-FIT Formula+' <u>2781439.3</u> C11 H21 N3 O3 5 +'
Card Serial Sample Seri Operator: J Date: 2011// Elemental C Single Mass Tolerance = Element pre Monoisotopi 396 formula Elements Us Minimum: Maximum: Mass	Number: GCT-P- al Number: HBS Lit ⁴ omposition Report Analysis t ⁴ 5.0 PPM / DB diction: Off t ⁴ c Mass, Odd and D (e) evaluated wi ed: C: 0-60 H: Calc. Mass 275.1304 275.1310	T11-12-05092 F-D28-S15+ E: min = -1.1 Even Electron th 4 results 0-80 N: C 2.0 mDa 0.3 -0.3	64 ⁰ 5, max = 50.1 n Ions4 within limi1 0-4 0: 0-6 5.0 PPM 1.1 -1.1	0ب s (all result s: 0-1 F -1.5ب 50.0ب DBE 3.0 12.0	:s (up to 1000) for each mass)+ br: 0-1 + i-FIT Formula+ 2781439.3. C11 H21 N3 O3 S+ 2780515.5. C19 H17 N O+
Card Serial Sample Seri Operator: J Date: 2011// Elemental C Single Mass Tolerance = Element pre Monoisotopi 396 formula Elements Us Minimum: Maximum: Mass	Number: GCT-P- al Number: HBS Lit Momposition Report Analysis + 5.0 PPM / DB diction: Off + c Mass, Odd and D (e) evaluated wit ed: C: 0-60 H: Calc. Mass 275.1304	T11-12-05092 F-D28-515*' E: min = -1.3 Even Electron th 4 results 0-80 N: C 2.0 mDa 0.3	64 5, max = 50.1 n Ions4 within limin)-4 O: 0-6 5.0 PPM 1.1	0+' S: 0-1 E -1.5+' 50.0+' DBE 3.0	is (up to 1000) for each mass)+' br: 0-1 +' i-FIT Formula+' <u>2781439.3</u> C11 H21 N3 O3 5 +'

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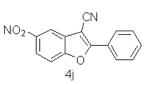
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Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report

		an i	• · · · ·		
	Waters Micromass G			on Mode: EI+	Electron Energy: 70eV
Card Seria		P-T11-12-0S09	2.74		
-		BSF-D28-S16↔			
Operator:					
Date: 2011		art al			
	Composition Repo	L C**			
-	s Analysis ↔ = 5.0 PPM / I	BF. min - 1	5 may - 50 0	J	
	= 5.0 PPM / I ediction: Off +	-1 = -1	.5, max = 50.04	F	
	ic Mass, Odd and	Figen Flectro	n Tonst		
				s (all resul	lts (up to 1000) for each mass)≁
			0-4 0: 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+ ^J
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 4
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上海质谱中心	, /	$\sim \sim \sim$	Y /-/		
		Į		}	Shanghai Mass Spectrometry Center
		\sim	~~o` ``		Shanghai Institute of Organic Chemistry
			4i		Chinese Academic of Sciences
					High Resolution MS Data Report
					THEIL RESOLUTION MID TARA REPORT
Instrument	Waters Micromass G	CT Premier	Ionisation	n Mode: EI+	Electron Energy: 70eV
Card Seria		P-T11-12-0S09		11110000.151	Incomon Intelay. root
		. 111 12 0805. 8SF-D28-S17⊬			
Operator:					
Date: 2011					
	Composition Repo	rt⊬			
	s Analysis √				
	= 5.0 PPM / D	BE: min = -1 .	5, max = 50.0₽		
	ediction: Off 4				
	ic Mass, Odd and				
					ts (up to 1000) for each mass)⊬
	/sed: C: O-60 H	H: 0-80 N:	0-4 0:0-6		Cl: 0-1 +
Minimum:				-1.5↔	
Maximum:		2.0	5.0	50.04	
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 C1 4
	253.0288	0.4	1.6	3.0	663.3 C7 H12 N3 O3 S C1 +
	253.0301	-0.9	-3.6	2.5	499.1 C9 H14 O4 S C1 +
	253.0283	0.9	3.6	7.5	4625.2 C10 H9 N2 O4 S -
ت	253.0281	1.1	4.3	12.5	26.8 C13 H6 N4 C1 +

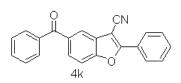




Shanghai Mass Spectrometry Center Shanghai Institute of Organic Chemistry Chinese Academic of Sciences High Resolution MS Data Report

Instrument:	Waters Micromass GO	T Premier	Ionisatio	n Mode: EI+	El	ectron Energy: 70eV		
Card Seria	1 Number: GCT-P	-T11-12-0S092	94					
Sample Ser	ial Number: HB	SF-D28-S18⊬						
Operator:	Li≁							
Date: 2011/12/15+								
Elemental	Composition Repor	t⊬						
Single Mas	s Analysis 🗸							
Tolerance	= 5.0 PPM / DH	BE: min = -1 .	5, max = 50.04	h				
Element pr	ediction: Off 🖉							
Monoisotop	ic Mass, Odd and	Even Electro:	n Ions⊬					
416 formul	a(e) evaluated wi	th 5 results.	within limits	s (all resul	lts (up to 100)O) for each mass)≁		
Elements U	sed: C: 0-60 H	:0-80 N:0	0-4 0:0-6	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 C1≁		
	264.0528	1.0	3.8	4.0	2776282.3	C7 H12 N4 O5 S 🗸		
4								

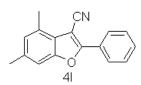




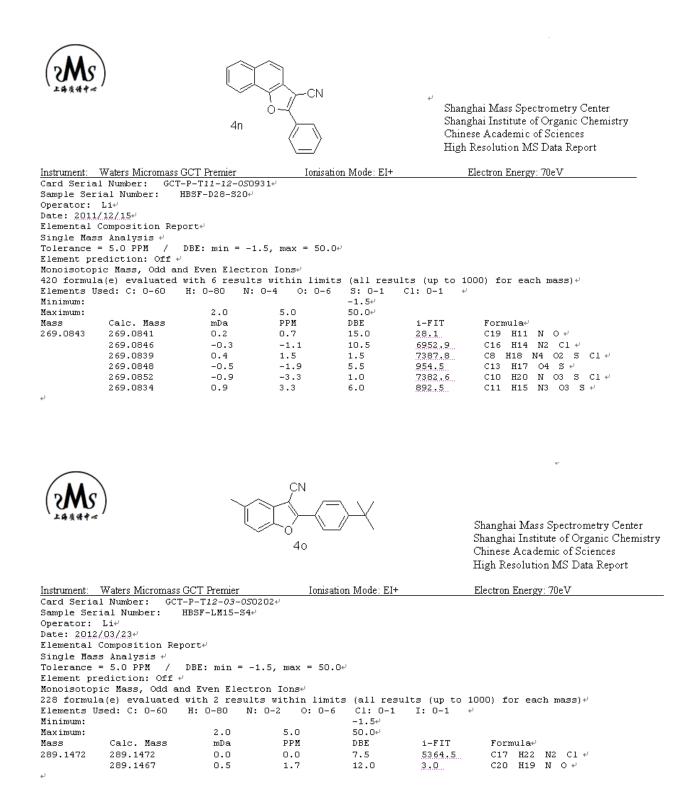
Instrument:	Waters Micromass GCT	Premier	Ionisation	Mode: EI+	Ele	ectron Energy: 70eV			
Card Seria	l Number: GCT-P-'	Γ11−12−0S0930⊬							
Sample Ser	ial Number: HBSH	/-D28-S19⊬							
Operator:	Li₽								
Date: 2011/12/15+									
Elemental Composition Report+									
Single Mass Analysis +									
Tolerance :	= 5.0 PPM / DBE	: min = -1.5 , mag	x = 50.0↔						
Element pro	ediction: Off 🗸								
-	ic Mass, Odd and E								
						0) for each mass)√			
	sed: C: O-60 H:	0-80 N: 0-4	0: 0-6		l: 0−1 +)				
Minimum:				-1.5↔					
Maximum:		2.0 5.0		50.0≁					
Mass	Calc. Mass	mDa PPI		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	3	12.5	2775069.0	C19 H16 N2 O C1 +			
	323.0946	0.6 1.9	9	17.0	2774555.8	C22 H13 N O2 +			
	323.0958	-0.6 -1	.9	3.0	2775071.3	C13 H22 N O4 S C1+			
	323.0945	0.7 2.3	2	3.5	2775071.0	C11 H2O N4 O3 S C1+			
	323.0940	1.2 3.1	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 ↔			
له									

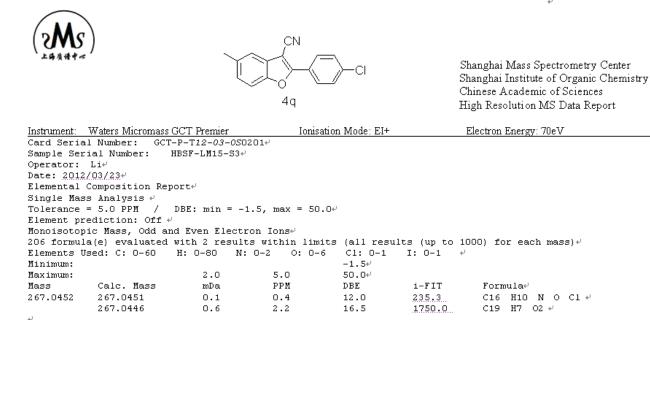


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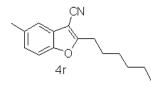


Card Serial Number: GCT-P-T <i>11-12-OS</i> O9334 Sample Serial Number: HBSF-D28-S224 Operator: Li4 Date: <u>2011/12/15</u> 4	zy: 70eV							
Operator: Li+'								
•								
Date: 2011/12/154								
Elemental Composition Report#								
Single Mass Analysis +								
Tolerance = 5.0 PPM / DBE: min = -1.5 , max = 50.0^{+1}								
Element prediction: Off 4								
Monoisotopic Mass, Odd and Even Electron Ions4								
346 formula(e) evaluated with 3 results within limits (all results (up to 1000) for ea Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Br: 0-1 +	ach mass)+							
Minimum: -1.5^{4}								
Maximum: 2.0 5.0 50.04								
Mass Calc. Mass mDa PPM DBE i-FIT Formula:	J							
	04 S √							
247.1001 247.1004 -0.3 -1.2 2.3 1044.5 C11 h19 247.0997 0.4 1.6 12.0 12.3 C17 H13								
247.0991 1.0 4.0 3.0 <u>994.5</u> C9 H17								
247.0391 1.0 4.0 5.0 <u>223.02.</u> C9 III	M3 03 9 4							
T.								
Shanghai Mass Spect	rometry Center							
Shanghai Institute of	Organic Chemistry							
4m Chinese Academic of	Sciences							
High Resolution MS	Data Report							
	D dud 100p 010							
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70	eV							
Card Serial Number: GCT-P-T11-12-0S0932+								
Sample Serial Number: HBSF-D28-S214								
	Operator: Li+							
Operator: Liv								
Operator: Li4 Date: <u>2011/12/15</u> 4								
Operator: Liゼ Date: <u>2011/12/15</u> ゼ Elemental Composition Reportゼ								
Operator: Liゼ Date: <u>2011/12/15</u> ゼ Elemental Composition Reportゼ Single Mass Analysis ゼ								
Operator: Liゼ Date: <u>2011/12/15</u> ゼ Elemental Composition Reportゼ Single Mass Analysis ゼ Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0ゼ								
Operator: Li ⁴ Date: <u>2011/12/15</u> ⁴⁷ Elemental Composition Report ⁴⁷ Single Mass Analysis ⁴⁷ Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 ⁴⁷ Element prediction: Off ⁴⁷								
Operator: Li ⁴ Date: 2011/12/15 ⁴⁷ Elemental Composition Report ⁴⁷ Single Mass Analysis ⁴⁷ Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 ⁴⁷ Element prediction: Off ⁴⁷ Monoisotopic Mass, Odd and Even Electron Ions ⁴⁷	a33) با							
Operator: Li ⁴ Date: <u>2011/12/15</u> ⁴⁷ Elemental Composition Report ⁴⁷ Single Mass Analysis ⁴⁷ Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 ⁴⁷ Element prediction: Off ⁴⁷	ass)+							
Operator: Li ⁴⁷ Date: 2011/12/15 ⁴⁷ Elemental Composition Report ⁴⁷ Single Mass Analysis ⁴⁷ Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 ⁴⁷ Element prediction: Off ⁴⁷ Monoisotopic Mass, Odd and Even Electron Ions ⁴⁷ 422 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each m	ass)+ ^j							
Operator: Li ⁴⁷ Date: 2011/12/15 ⁴⁷ Elemental Composition Report ⁴⁷ Single Mass Analysis ⁴⁷ Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 ⁴⁷ Element prediction: Off ⁴⁷ Monoisotopic Mass, Odd and Even Electron Ions ⁴⁷ 422 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each m Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 ⁴⁷	ass)+ ^J							
Operator: Li ⁴ Date: 2011/12/15 ⁴⁷ Elemental Composition Report ⁴⁷ Single Mass Analysis ⁴⁷ Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 ⁴⁷ Element prediction: Off ⁴⁷ Monoisotopic Mass, Odd and Even Electron Ions ⁴⁷ 422 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each m Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 ⁴⁷ Minimum: -1.5 ⁴⁷ Maximum: 2.0 5.0 50.0 ⁴⁷ Mass Calc. Mass mDa PPM DBE i-FIT	ass)+ ^j							
Operator: Li ^{4/} Date: 2011/12/15 ^{4/} Elemental Composition Report ^{4/} Single Mass Analysis ^{4/} Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 ^{4/} Element prediction: Off ^{4/} Monoisotopic Mass, Odd and Even Electron Ions ^{4/} 422 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each m Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 e/ Minimum: -1.5 ^{4/} Maximum: 2.0 5.0 50.0 ^{4/} Mass Calc. Mass mDa PPM DBE i-FIT Formula ^{4/} 267.0452 267.0451 0.1 0.4 12.0 74.7 Cl6 H10 N								
Operator: Li ⁴ Date: 2011/12/15 ⁴⁷ Elemental Composition Report ⁴⁷ Single Mass Analysis ⁴⁷ Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 ⁴⁷ Element prediction: Off ⁴⁷ Monoisotopic Mass, Odd and Even Electron Ions ⁴⁷ 422 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each m Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 e ⁴ Minimum: -1.5 ⁴⁷ Maximum: 2.0 5.0 50.0 ⁴⁷ Mass Calc. Mass mDa PPM DBE i-FIT Formula ⁴⁷ 267.0452 267.0451 0.1 0.4 12.0 74.7. Cl6 H10 N 267.0446 0.6 2.2 16.5 2385.0. Cl9 H7 02 4	0 C1 ↔							
Operator: Li ^{4/} Date: 2011/12/15 ^{4/} 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 m Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 */ Minimum: -1.5*/ Mass Calc. Mass mDa PPM DBE i-FIT Formula*/ 267.0452 267.0451 0.1 0.4 12.0 74.7 Cl6 H10 N 267.0458 -0.6 2.2 16.5 2385.0 Cl9 H7 02 *	0 C1 원 S C1 원							
Operator: Li ^{4/} Date: 2011/12/15 ^{4/} Elemental Composition Report ^{4/} Single Mass Analysis ^{4/} Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0 ^{4/} Element prediction: Off ^{4/} Monoisotopic Mass, Odd and Even Electron Ions ^{4/} 422 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each m Elements Used: C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 e/ Minimum: -1.5 ^{4/} Mass Calc. Mass mDa PPM DBE i-FIT Formula ^{4/} 267.0452 267.0451 0.1 0.4 12.0 74.7. Cl6 H10 N 267.0458 -0.6 -2.2 2.5 509.2. Cl0 H16 O4	0 C1 & S C1 & 03 S C1 &							





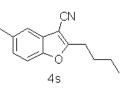




Ψ

Instrument:	Waters Micromass GCT	Premier	Ionisation I	/Iode: EI+	Electron Ene	rgy: 70eV	
Card Seria	l Number: GCT-P-7	[12-03-0S0210↔					
Sample Serial Number: HBSF-LM15-S12+'							
Operator:	Li≁						
Date: 2012,	/03/28+						
Elemental (Composition Report	ų					
Single Mass	s Analysis 🗸						
Tolerance = 5.0 PPM / DBE: min = -1.5 , max = 50.0^{4}							
Element prediction: Off 4							
Monoisotopic Mass, Odd and Even Electron Ions+							
274 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass) $^{ m el}$							
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 5	0.04			
Mass	Calc. Mass	mDa Pl	PM D	BE i-FI	Γ Formula	24 ^J	
241.1471	241.1467		.7 ε	.0 1.9	C16 H1	9 N O 4	
	241.1478	-0.7 -2	2.9 4	.0 15.4	C13 H2	O N O2 F ↔	
4							





Instrument: Waters Micromass GCT Premier	Ionisation Mode: EI+	Electron Energy: 70eV				
Card Serial Number: GCT-P-T12-03-0.	S0207₽					
Sample Serial Number: HBSF-LM15-S9	Ы ^J					
Operator: Li≁						
Date: 2012/03/23+						
Elemental Composition Report+						
Single Mass Analysis 🗸						
Tolerance = 5.0 PPM / DBE: min = -1.5 , max = 50.0^{4}						
Element prediction: Off 4						
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: O-2 O: O-6 Cl: O-1]	I: 0-1 +				
Minimum:	-1.54					
Maximum: 2.0	5.0 50.04					
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	<u>2773245.3</u> C11 H18 N2 C1 4				