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Palladium-catalyzed direct *ortho*-acylation through an oxidative coupling of 2-arylbenzothiazoles with benzylic alcohols

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Abstract: An efficient protocol was developed for Pd-catalyzed direct C−H bond acylation by cross-dehydrogenative-coupling of arylbenzothiazoles and benzylic alcohols using *tert*-butyl hydroperoxide (TBHP) as the oxidant. The acylation reactions exhibit good reactivities and excellent regioselectivity.

Keywords: *ortho*-acylation; 2-arylbenzothiazoles; benzylic alcohols; *tert*-butyl hydroperoxide

Introduction

Transition-metal-catalyzed intermolecular cross-dehydrogenative-coupling (CDC) of inert C−H bonds has recently emerged as a powerful method for the construction of new

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C−C bonds and C-X (X = N, O, S, X) bonds.[1] The combination of transition-metal-catalysts and directing groups is very important to success in this context. Various transition metals such as Pd, Rh, Ru, Fe, Co, and Cu have been widely employed.[2] Recently, the direct C−H bond acylation of aromatic compounds containing various directing groups has been described. In 2009, Cheng firstly reported Pd-catalyzed oxidative sp^2 C–H acylation reactions of 2-arylpyridines from aldehydes.[3] Subsequently, other groups (such as Li, Ge, and Wang) also developed many 2-arylpyridine-directed sp^2 C–H acylation by different carbonyl sources.[4] In addition, Yu and Kim described separately the Pd-catalyzed direct C−H bond acylation using *O*-methyl oximes as a directing group.[5] Anilide was also employed as a directing group for direct C−H bond acylation with aldehydes.[6] Rh-catalyzed benzamide-directed oxidative acylation and Pd-catalyzed *ortho*-acylation of *N*-benzyltriflamides with aldehydes *via* sp^2 C–H bonds activation were described by Kim.[7] Cyclic enamides participated intermolecular C−H bond acylation reactions was reported by Duan.[8] Most recently, Wu and co-workers reported Pd-catalyzed *ortho*-acylation of 2-arylbenzoxazole in moderate to good yields using aldehydes as acyl source.[9a] Patel also developed an efficient protocol for the *ortho*-acylation of 2-arylbenzoxazoles and 2-arylbenzothiazoles with aldehydes *via* Pd(II)-catalyzed C-H activation/C-C bond formation.[9b] Decarboxylative cross-coupling reaction of benzoic acids with α-oxocarboxylic acids was reported by Ge group.[10]

In most cases, aldehyde was employed as carbonyl source in transition-metal-catalyzed C−H bond acylation reaction. In addition, α-oxocarboxylic acids,[4b,5b,8,11] benzylic alcohols,[4c,12] α-diketones,[4d] toluene derivatives,[13] and carboxylic acids[14] are also very useful carbonyl sources in the presence of transition-metal catalyst and oxidant.

As a privileged fragment, the benzothiazole core is a ubiquitous subunit in many natural products and pharmaceuticals with remarkable biological activities.[15] For example, compounds **I** or their salts (Figure 1) containing a benzothiazole core are useful for treatment of parkinsonism, hypertension, depression, etc.[16] Thus, it is highly desired to develop efficient and general synthetic methods for access to functionalized benzothiazoles in order to explore their potential applications. More recently, we has developed the Pd-catalyzed direct *ortho* sp^2 C−H arylation of 2-arylbenzothiazoles.[17] Inspired by the above-mentioned direct acylation protocols and our interest in 2-arylbenzothiazoles, herein we would like to report the acylation reaction of 2-arylbenzothiazoles and benzylic alcohols using *tert*-butyl hydroperoxide (TBHP) as the oxidant in the presence of catalytic palladium acetate *via* oxidative CDC reaction.

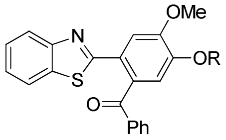
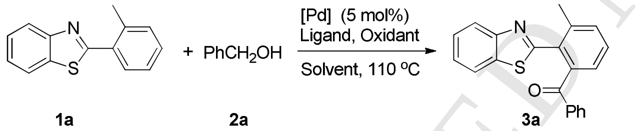


Figure 1 Compounds I

Results and discussions

We initially used 2-(*o*-tolyl)benzo[*d*]thiazole **1a** and phenylmethanol **2a** as model substrates to optimize the reaction conditions, and selected results are summarized in Table 1. To our delight, the combination of $Pd(OAc)_2$ and TBHP (65 wt.% aqueous solution) in PhCl solvent at 110 ^{o}C can catalyze the CDC reaction and provide the acylated product **3a** in 31% yield (Table 1, entry 1). A screening of catalysts demonstrated that other Pd catalysts, such as $PdCl_2$, $Pd_2(dba)_3$, $Pd(CH_3CN)_2Cl_2$, $Pd(PhCN)_2Cl_2$, and $Pd(PPh_3)_2Cl_2$ were inferior to $Pd(OAc)_2$ (Table 1, entries 1-6). Then, the use of other oxidants, such as *ditert*-butyl peroxide (DTBP), O_2, oxone, and $K_2S_2O_8$, was also ineffective in this transformation (Table 1, entries 7-10). Further optimization showed the coupling yield could be raised to 61% in the presence of 7.0 equiv of TBHP (Table 1, entries 11-13). Subsequently, the effects of several ligands were investigated, and the results showed that the presence of ligand affected the reaction to some extent. Among them, benzoquinone (BQ) increased the yield to 68%, some other generally used ligands, such as TMEDA, DMEDA, PPh_3, L-proline, DDQ, and 1,10-phen showed ineffective (Table 1, entries 14-20). The effect of solvents on this reaction was also examined. PhCl was found to be the best choice, and other solvents such as toluene, AcOH, DMAc, DMF, DMSO, NMP, and CH_3CN failed to yield better results (Table 1, entries 21-27).

Table 1. Optimization of the reaction conditions[a]



Entry	[Pd]	Solvent	Oxidant	Ligand	Yield (%)[b]
1	$Pd(OAc)_2$	PhCl	TBHP	-	31
2	$PdCl_2$	PhCl	TBHP	-	15
3	$Pd_2(dba)_3$	PhCl	TBHP	-	27
4	$PdCl_2(CH_3CN)_2$	PhCl	TBHP	-	24
5	$PdCl_2(PhCN)_2$	PhCl	TBHP	-	13
6	$PdCl_2(PPh_3)_2$	PhCl	TBHP	-	11
7	$Pd(OAc)_2$	PhCl	DTBP	-	18
8	$Pd(OAc)_2$	PhCl	O_2	-	-
9	$Pd(OAc)_2$	PhCl	Oxone	-	-
10	$Pd(OAc)_2$	PhCl	$K_2S_2O_8$	-	-
11[c]	$Pd(OAc)_2$	PhCl	TBHP	-	45
12[d]	$Pd(OAc)_2$	PhCl	TBHP	-	52
13[e]	$Pd(OAc)_2$	PhCl	TBHP	-	61
14[e]	$Pd(OAc)_2$	PhCl	TBHP	TMEDA	37
15[e]	$Pd(OAc)_2$	PhCl	TBHP	DMEDA	32
16[e]	$Pd(OAc)_2$	PhCl	TBHP	PPh_3	28
17[e]	$Pd(OAc)_2$	PhCl	TBHP	L-proline	42
18[e]	$Pd(OAc)_2$	PhCl	TBHP	BQ	68
19[e]	$Pd(OAc)_2$	PhCl	TBHP	DDQ	trace
20[e]	$Pd(OAc)_2$	PhCl	TBHP	1,10-phen	-
21[e]	$Pd(OAc)_2$	toluene	TBHP	BQ	50

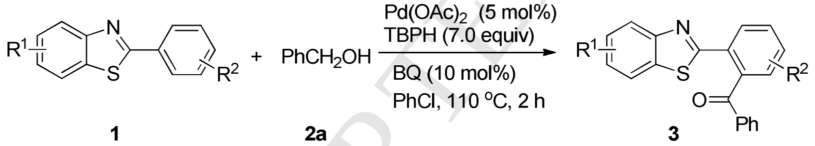
22[e]	$Pd(OAc)_2$	AcOH	TBHP	BQ	30
23[e]	$Pd(OAc)_2$	DMAc	TBHP	BQ	trace
24[e]	$Pd(OAc)_2$	DMF	TBHP	BQ	-
25[e]	$Pd(OAc)_2$	DMSO	TBHP	BQ	trace
26[e]	$Pd(OAc)_2$	NMP	TBHP	BQ	20
27[e]	$Pd(OAc)_2$	CH_3CN	TBHP	BQ	35

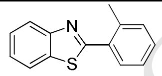
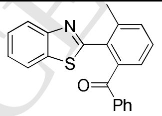
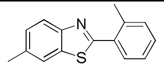
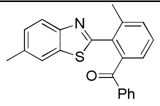
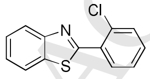
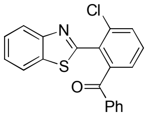
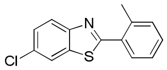
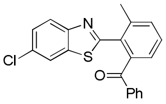
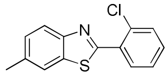
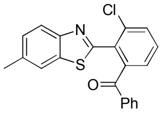
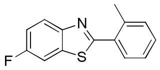
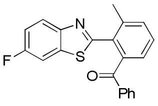
[a] Conditions: **1a** (0.2 mmol), **2a** (0.6 mmol), [Pd] catalyst (5 mol %), oxidant (3.0 equiv), ligand (10 mol%) 110 ^{o}C, 2 h; [b] Isolated yield based on **1a**; [c] 4.0 equiv of TBHP were used; [d] 6.0 equiv of TBHP were used; [e] 7.0 equiv of TBHP were used.

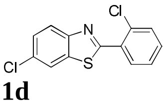
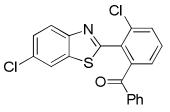
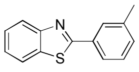
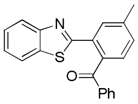
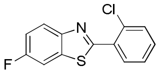
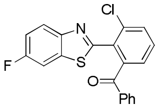
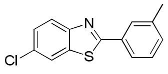
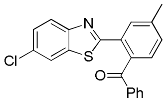
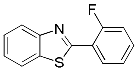
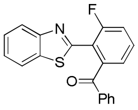
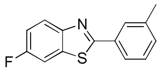
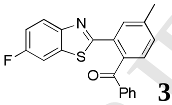
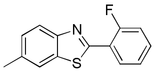
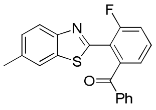
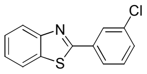
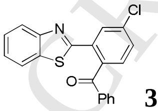
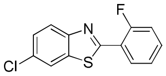
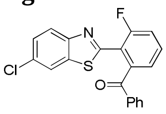
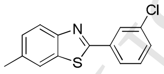
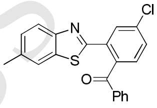
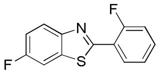
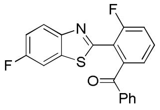
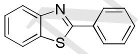
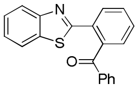
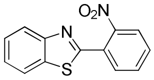
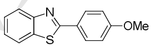
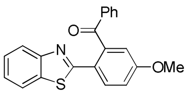
Under the optimized reaction conditions [$Pd(OAc)_2$ (5 mol%), TBHP (7.0 equiv), BQ (10 mol%), PhCl, 110 ^{o}C], the scope of the sp^2 C−H acylation reactions between the 2-arylbenzo[*d*]thiazoles **1** with phenylmethanol **2a** was investigated. The coupling of 2-arylbenzo[*d*]thiazoles **1b-1i** with middle electron-withdrawing groups (Cl, F) at the *ortho*-position of 2-phenyl ring underwent smoothly the CDC acylation reaction to afford the corresponding products **3b-3i** in good to excellent yields (Table 2, entries 2-9). For instance, 2-(2-chlorophenyl)benzo[*d*]thiazole **1b** reacted with phenylmethanol **2a** leading to the formation of acylation product **3b** in 95% yield (Table 2, entry 2). The reaction of 2-(2-fluorophenyl)benzo[*d*]thiazole **1f** under the standard conditions gave **3f** in 82% yield (Table 2, entry 6). Generally, the benzothiazole parts with electron-neutral substituents or electron-withdrawing groups were relatively more reactive than those with electron-donating ones, and afforded relatively higher yields (Table 2, entries 2, 4-6, 8 and 9 *vs* entries 3 and 7). Regrettably, 2-(2-nitrophenyl)benzo[d]thiazole **1j** containing strongly electron-withdrawing group (NO_2) reacted with phenylmethanol **2a** under the present reaction conditions no desired products was obtained. If the substituents at the benzothiazole parts and the *ortho*-position of 2-phenyl ring parts both were electron-donating groups, gave the acylation product in poor yield. For example, when 6-methyl-

2-(*o*-tolyl)benzo[*d*]thiazole **1k** was used as substrate, only a 22% yield was obtained (Table 2, entry 11). At the same time, substituted benzo[*d*]thiazole with a strong electron-donating methoxy group at the *ortho* position of the benzene ring showed poor reactivity. To those 2-arylbenzo[*d*]thiazoles **1n-1r** with electron-donating or -withdrawing group at the *meta*-position of 2-phenyl ring provided *ortho*-acylation products **3m-3q** exclusively at the less sterically hindered position in good yields (Table 2, entries 14-18). Fortunately, unsubstituted 2-phenylbenzo[*d*]thiazole **1s**, also reacted with phenylmethanol **2a** smoothly under standard reaction conditions and moderate isolated yield (62%) of the monoacylated product **3r** was obtained, and only trace amount of bis-acylated product was observed by TLC (Table 2, entry 19). On the other hand, *para*-position substituted 2-arylbenzo[*d*]thiazole **1t** afforded in moderate yield (67%) and an inferior selectivity with mono- and bis-acylated products in almost the same amount (Table 2, entry 20).

Table 2. Reaction of phenylmethanol with 2-arylbenzo[*d*]thiazoles[a]



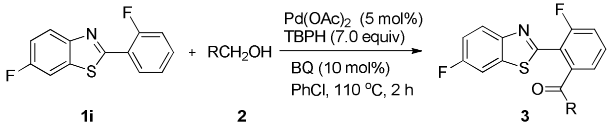
Entry	1	Product 3	Yield (%)[b]	Entry	1	Product 3	Yield (%)[b]
1	 **1a**	 **3a**	68	11	 **1k**	 **3j**	22
2	 **1b**	 **3b**	95	12	 **1l**	 **3k**	70
3	 **1c**	 **3c**	85	13	 **1m**	 **3l**	83

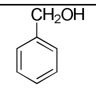
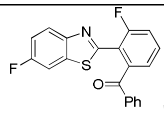
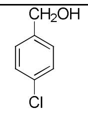
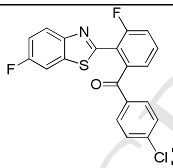
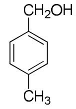
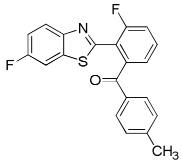
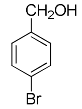
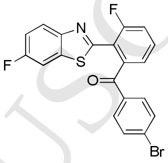
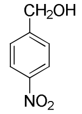
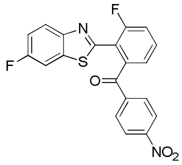
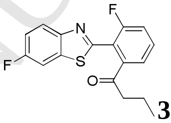
4	 **1d**	 **3d**	92	14	 **1n**	 **3m**	65
5	 **1e**	 **3e**	83	15	 **1o**	 **3n**	65
6	 **1f**	 **3f**	82	16	 **1p**	 **3o**	81
7	 **1g**	 **3g**	75	17	 **1q**	 **3p**	72
8	 **1h**	 **3h**	80	18	 **1r**	 **3q**	67
9	 **1i**	 **3i**	92	19	 **1s**	 **3r**	62
10	 **1j**	-	-	20	 **1t**	 **3s**	32[c]

[a] Conditions: 2-arylbenzo[*d*]thiazole **1** (0.2 mmol), phenylmethanol **2a** (0.6 mmol), Pd(OAc)$_2$ (5 mol%), TBHP (7.0 equiv), BQ (10 mol%), PhCl, 110 ^{o}C, 2h; [b] Isolated yield based on **1**; [c] With 35% yield of bis-acylated product.

The substituent effects of various primary alcohols on this reaction were then studied under the optimized reaction conditions (Table 3). It was noticed that benzylic alcohols bearing electron-donating groups (CH$_3$) (entry 2) and electron-withdrawing substituents (NO$_2$, Cl) at the aromatic ring (entries 3 and 4) provided good to high yields. However, the reaction yield decreased dramatically when 4-bromobenzyl alcohol **2e** was used as the substrate, and the desired product **3w** was achieved in 35% yield. Unfortunately, to aliphatic alcohol such as ^{n}BuOH **2f** the reaction could not occur under the recommended reaction conditions.

Table 3. Acylation of 2-arylbenzo[*d*]thiazole with primary alcohols[a]

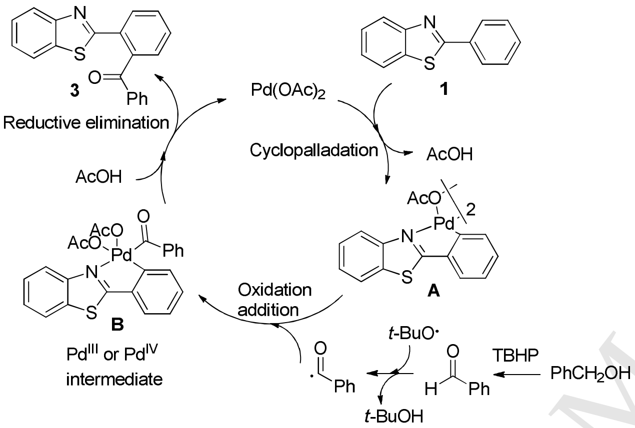


Entry	2	Product 3	Yield (%)[b]	Entry	2	Product 3	Yield (%)[b]
1	 **2a**	 **3i**	92	4	 **2d**	 **3v**	87
2	 **2b**	 **3t**	74	5	 **2e**	 **3w**	35
3	 **2c**	 **3u**	85	6	^{n}BuOH **2f**	 **3x**	-

[a] Conditions: 2-arylbenzo[*d*]thiazole **1i** (0.2 mmol), primary alcohols **2** (0.6 mmol), $Pd(OAc)_2$ (5 mol%), TBHP (7.0 equiv), BQ (10 mol%), PhCl, 110 °C, 2h; [b] Isolated yield based on **1i**.

To understand the reaction mechanism, we test some other experiments. First, using PhCHO as the alternative of $PhCH_2OH$, the desired coupling product **3a** was obtained in 70% yield under the standard conditions. Subsequently, 2.0 equiv. TEMPO as a radical-trapping reagent was used in our model reaction, and only trace of desired product **3a** was observed, suggesting that free radical intermediate was involved in the reaction.

Based on the previous research[5a,6-9,12,13] and our results[17], a plausible reaction pathway of the palladium-catalyzed *ortho*-acylation of 2-arylbenzo[*d*]thiazole with phenylmethanol through direct C−H bond activation was suggested in Scheme 1. First, sp^2 C−H bond activation of 2-arylbenzo[*d*]thiazole occurs in the presence of the palladium catalyst to form a five-membered palladacycle intermediate **A** (was observed by NMR). Second, the palladacycle **A** reacted with the acyl radical which was produced in situ from the oxidation of alcohol by TBHP to form either reactive Pd^{III} or Pd^{IV} intermediate **B**.[5a,6,12,13] Finally, the reductive elimination of intermediate **B** afforded coupling product **3** and regenerates Pd^{II} for the next catalytic cycle.



Scheme 1 Plausible mechanism for the Pd-catalyzed *ortho*-acylation reaction.

In summary, we have developed an efficient method for the synthesis of aromatic ketones via a Pd-catalyzed direct sp^2 C−H bond acylation of 2-arylbenzo[*d*]thiazoles. The cheap and readily available benzylic alcohols were used as acylation sources in the presence of TBHP. The reaction exhibited good functional group tolerance with good to excellent yield and high selectivity.

Experimental Section

General experimental procedures and characterizations: 2-Arylbenzo[*d*]thiazole (0.2 mmol), benzylic alcohol (0.6 mmol), Pd(OAc)$_2$ (0.01 mmol), TBHP (1.4 mmol, 196 μL, 65% aq), BQ (0.02 mmol), and PhCl (2.0 mL) were added in a 25 mL sealed tube with a

Teflon-lined cap. The mixture was heated at 110 °C for 2 h. After being cooled to room temperature, the volatiles were removed under reduced pressure, and the residue was purified by a flash column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to give the corresponding pure coupling product **3**.

(2-(benzo[d]thiazol-2-yl)-3-methylphenyl)(phenyl)methanone **3a**. Isolated as a yellow solid (68% yield, 44.7 mg), mp: 135-136 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.43 (s, 3H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.37-7.42 (m, 3H), 7.46-7.48 (m, 2H), 7.69 (d, *J* = 7.6 Hz, 2H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.5, 121.3, 123.4, 125.2, 126.0, 126.6, 128.0, 129.3, 129.9, 132.5, 132.7, 132.8, 136.2, 137.4, 138.2, 140.7, 152.9, 165.2, 197.3; IR (KBr) ν/cm^{-1}: 1735, 1458, 1087, 775; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{16}NOS$: 330.0953; found: 330.0950.

(2-(benzo[d]thiazol-2-yl)-3-chlorophenyl)(phenyl)methanone **3b**. Isolated as a yellow solid (95% yield, 66.3 mg), mp: 178-179 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (t, *J* = 7.6 Hz, 2H), 7.31-7.41 (m, 3H), 7.49-7.56 (m, 2H), 7.65 (d, *J* = 7.6 Hz, 2H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 121.3, 123.6, 125.6, 126.1, 127.5, 128.1, 129.4, 130.6, 131.8, 132.0, 132.9, 134.2, 136.3, 137.0, 142.9, 152.2, 162.1, 195.8; IR (KBr) ν/cm^{-1}: 1669, 1317, 758; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{20}H_{13}ClNOS$: 350.0406, found: 350.0400.

(3-chloro-2-(6-methylbenzo[d]thiazol-2-yl)phenyl)(phenyl)methanone **3c**. Isolated as a yellow solid (85% yield, 61.7 mg), mp: 134-135 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.43 (s, 3H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.25 (t, *J* = 7.2 Hz, 2H), 7.36 (t, *J* = 7.2 Hz, 1H), 7.47-7.52 (m, 2H), 7.57 (s, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.74 (d, *J* =

8.4 Hz, 1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 21.6, 120.9, 123.0, 127.4, 127.7, 128.1, 129.4, 130.5, 131.8, 131.9, 132.8, 134.1, 135.8, 136.5, 137.0, 142.9, 150.4, 160.9, 195.8; IR (KBr) ν/cm^{-1}: 1670, 1276, 707; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{21}H_{15}ClNOS$: 364.0563, found: 364.0568.

(3-chloro-2-(6-chlorobenzo[d]thiazol-2-yl)phenyl)(phenyl)methanone **3d**. Isolated as a yellow solid (92% yield, 70.5 mg), mp:147-148 °C; ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.26 (t, *J* = 7.6 Hz, 2H), 7.34 (d, *J* = 8.8 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.76 (t, *J* = 4.0 Hz, 2H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 120.9, 124.3, 127.0, 127.6, 128.2, 129.4, 130.9, 131.3, 131.6, 132.1, 133.0, 134.1, 136.9, 137.5, 142.9, 150.7, 162.7, 195.6; IR (KBr) ν/cm^{-1}: 1672, 1303, 826; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{20}H_{12}Cl_2NOS$: 384.0017, found: 384.0021.

(3-chloro-2-(6-fluorobenzo[d]thiazol-2-yl)phenyl)(phenyl)methanone **3e**. Isolated as a yellow solid (83% yield, 60.9 mg), mp: 152-153 °C; ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.13 (t, *J* = 8.8 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.46-7.51 (m, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.81 (dd, *J* = 4.8, 8.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 107.4 (d, $^2J_{C\text{-}F}$ = 27.0 Hz), 114.9 (d, $^2J_{C\text{-}F}$ = 25.0 Hz), 124.6 (d, $^3J_{C\text{-}F}$ = 10.0 Hz), 127.6, 128.2, 129.4, 130.8, 131.4, 132.0, 132.9, 134.1, 136.9, 137.3 (d, $^3J_{C\text{-}F}$ = 11.0 Hz), 142.9, 148.8, 160.6 (d, $^1J_{C\text{-}F}$ = 245.0 Hz), 195.7; IR (KBr) ν/cm^{-1}: 1667, 1321, 750; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{20}H_{12}ClFNOS$: 368.0312, found: 368.0310.

(2-(benzo[d]thiazol-2-yl)-3-fluorophenyl)(phenyl)methanone **3f**. Isolated as a yellow solid (82% yield, 54.6 mg), mp: 108-109 °C; ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25-7.40

(m, 8H), 7.53-7.59 (m, 1H), 7.73 (d, J = 8.4 Hz, 2H), 7.87 (dd, J = 4.0, 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 117.6 (d, $^2J_{C\text{-}F}$ = 23.0 Hz), 120.4 (d, $^3J_{C\text{-}F}$ = 13.0 Hz), 121.3, 123.4, 124.7, 125.5, 126.1, 128.2, 129.0, 131.7 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 132.6, 135.8, 137.6, 142.4, 152.0, 158.3, 160.1 (d, $^1J_{C\text{-}F}$ = 252.0 Hz), 196.0; IR (KBr) ν/cm^{-1}: 1668, 1299, 1273, 757; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{20}H_{13}FNOS$: 334.0702, found: 334.0700.

(3-fluoro-2-(6-methylbenzo[d]thiazol-2-yl)phenyl)(phenyl)methanone **3g**. Isolated as a yellow solid (75% yield, 52.0 mg), mp:131-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 7.15 (d, J = 8.4 Hz, 1H), 7.26 (t, J = 7.6 Hz, 2H), 7.34 (d, J = 6.8 Hz, 2H), 7.37 (t, J = 9.2 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.57 (s, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.71 (d, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.6, 117.6 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 120.5 (d, $^2J_{C\text{-}F}$ = 14.0 Hz), 120.9, 122.9, 124.7, 127.8, 128.2, 128.9, 131.5 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 132.6, 135.8, 136.0, 137.6, 142.3, 150.2, 157.1, 160.0 (d, $^1J_{C\text{-}F}$ = 253.0 Hz), 196.1; IR (KBr) ν/cm^{-1}: 1671, 1299, 745; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{15}FNOS$: 348.0858, found: 348.0859.

(2-(6-chlorobenzo[d]thiazol-2-yl)-3-fluorophenyl)(phenyl)methanone **3h**. Isolated as a yellow solid (80% yield, 58.7 mg), mp: 170-171 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.42 (m, 6H), 7.57-7.62 (m, 1H), 7.65 (d, J = 8.8 Hz, 1H), 7.71 (d, J = 7.6 Hz, 2H), 7.78 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 117.7 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 120.0 (d, $^2J_{C\text{-}F}$ = 13.0 Hz), 120.8, 124.1, 124.8, 127.0, 128.3, 128.9, 131.5, 132.0 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 132.7, 136.9 (d, $^3J_{C\text{-}F}$ = 6.0 Hz), 137.5, 142.3, 150.5, 158.8, 160.1 (d, $^1J_{C\text{-}F}$ = 253.0 Hz), 195.8; IR (KBr) ν/cm^{-1}: 1671, 1309, 722; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{20}H_{12}ClFNOS$: 368.0312, found: 368.0315.

(3-fluoro-2-(6-fluorobenzo[d]thiazol-2-yl)phenyl)(phenyl)methanone **3i**. Isolated as a colorless solid (92% yield, 64.6 mg), mp:124-125 °C; ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.08 (t, J = 8.8 Hz, 1H), 7.28 (t, J = 7.6 Hz, 2H), 7.34-7.41 (m, 3H), 7.47 (d, J = 8.0 Hz, 1H), 7.56-7.61 (m, 1H), 7.67-7.73 (m, 3H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 107.3 (d, $^2J_{C\text{-}F}$ = 27.0 Hz), 114.9 (d, $^2J_{C\text{-}F}$ = 25.0 Hz), 117.6 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 120.1 (d, $^3J_{C\text{-}F}$ = 13.0 Hz), 124.4 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 124.8, 128.3, 128.9, 131.8 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 132.7, 136.9, 137.5, 142.3, 148.6, 158.1, 160.0 (d, $^1J_{C\text{-}F}$ = 252.0 Hz), 160.6 (d, $^1J_{C\text{-}F}$ = 245.0 Hz), 195.9; IR (KBr) ν/cm^{-1}: 1665, 1279, 7788; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{20}H_{12}F_2NOS$: 352.0608, found: 352.0612.

(3-methyl-2-(6-methylbenzo[d]thiazol-2-yl)phenyl)(phenyl)methanone **3j**. Isolated as a brown solid (22% yield, 15.1 mg), mp: 70-71 °C; ^{1}H NMR (400 MHz, CDCl$_3$) δ 2.43 (s, 3H), 2.45 (s, 3H), 7.22 (d, J = 8.4 Hz, 1H), 7.28 (t, J = 7.6 Hz, 2H), 7.38-7.44 (m, 2H), 7.46-7.49 (m, 2H), 7.57 (s, 1H), 7.69 (d, J = 7.2 Hz, 2H), 7.80 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 20.5, 21.5, 121.0, 122.8, 126.5, 127.6, 128.0, 129.2, 129.9, 132.6, 132.7, 132.8, 135.3, 136.4, 137.4, 138.2, 140.7, 151.1, 164.0, 197.4; IR (KBr) ν/cm^{-1}: 1668, 1275, 774; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{22}H_{18}NOS$: 344.1109, found: 344.1111.

(2-(6-chlorobenzo[d]thiazol-2-yl)-3-methylphenyl)(phenyl)methanone ***3k***. Isolated as a White solid (70% yield, 50.8 mg); mp:122-123 °C; ^{1}H NMR (400 MHz, CDCl$_3$) δ 2.43 (s, 3H), 7.30 (t, J = 7.6 Hz, 2H), 7.37 (d, J = 8.8 Hz,1H), 7.39-7.44 (m, 2H), 7.49 (d, J = 3.6 Hz, 2H), 7.69 (d, J = 7.6 Hz, 2H), 7.76 (s, 1H), 7.83 (d, J = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 20.5, 120.9, 124.1, 126.8, 126.9, 128.1, 129.5, 129.9, 131.2, 132.1, 132.8, 132.9, 137.3, 137.4, 138.2, 140.6, 151.4, 165.8, 197.2; IR (KBr) ν/cm^{-1}: 1668,

1279, 719; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{21}H_{15}ClNOS$: 364.0563, found: 364.0568.

(2-(6-fluorobenzo[d]thiazol-2-yl)-3-methylphenyl)(phenyl)methanone ***3l***. Isolated as a yellow solid (83% yield, 57.6 mg), mp:132-133 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.43 (s, 3H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.38-7.48 (m, 5H), 6.68 (d, *J* = 7.6 Hz, 2H), 7.85 (dd, *J* = 4.8, 8.4 Hz,1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.5, 107.5 (d, $^2J_{C\text{-}F}$ = 26.0 Hz), 114.7 (d, $^2J_{C\text{-}F}$ = 25.0 Hz), 124.3 (d, $^3J_{C\text{-}F}$ = 10.0 Hz), 126.7, 128.1, 129.4, 129.9, 132.2, 132.8, 132.9, 137.2 (d, $^3J_{C\text{-}F}$ = 11.0 Hz), 137.4, 138.2, 140.6, 149.5, 160.4 (d, $^1J_{C\text{-}F}$ = 245.0 Hz), 165.0, 197.2; IR (KBr) ν/cm^{-1}: 1668, 1282, 849; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{21}H_{15}FNOS$: 348.0858, found: 348.0862.

(2-(benzo[d]thiazol-2-yl)-4-methylphenyl)(phenyl)methanone ***3m***. Isolated as a white solid (65% yield, 42.8 mg), mp: 129-130 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.52 (s, 3H), 7.25-7.30 (m, 3H), 7.32-7.39 (m, 2H), 7.41 (s, 7.41), 7.45 (d, *J* = 7.6 Hz, 1H), 7.73-7.81 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 121.4, 123.4, 125.2, 126.1, 128.2, 129.1, 129.3, 130.3, 131.0, 132.3, 132.6, 135.4, 137.0, 138.0, 140.6, 153.5, 165.6, 197.7; IR (KBr) ν/cm^{-1}: 1663, 1281, 732; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{21}H_{16}NOS$: 330.0953, found: 330.0949.

(2-(6-chlorobenzo[d]thiazol-2-yl)-4-methylphenyl)(phenyl)methanone ***3n***. Isolated as a yellow solid (65% yield, 47.2 mg), mp:125-126 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.52 (s, 3H), 7.25-7.32 (m, 3H), 7.35-7.46 (m, 3H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.69 (s, 1H), 7.71-7.76 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 121.0, 124.1, 127.0, 128.2, 129.2, 130.2, 131.1, 131.2 131.9, 132.7, 136.5, 137.0, 137.9, 140.8, 152.0, 166.1, 197.5;

IR (KBr) ν/cm^{-1}: 1683, 1292, 814; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{21}H_{15}ClNOS$: 364.0563, found: 364.0567.

(2-(6-fluorobenzo[d]thiazol-2-yl)-4-methylphenyl)(phenyl)methanone ***3o***. Isolated as a yellow solid (81% yield, 56.2 mg), mp:138-139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.51 (s, 3H), 7.08 (t, *J* = 8.8 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 2H), 7.35-7.46 (m, 4H), 7.68 (s, 1H), 7.70-7.75 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 107.6 (d, $^2J_{C\text{-}F}$ = 27.0 Hz), 114.8 (d, $^2J_{C\text{-}F}$ = 24.0 Hz), 124.3 (d, $^3J_{C\text{-}F}$ = 10.0 Hz), 128.2, 129.2, 129.3, 130.2, 131.0, 132.0, 132.6, 136.3 (d, $^3J_{C\text{-}F}$ = 12.0 Hz), 136.9, 137.9, 140.7, 150.1, 160.5 (d, $^1J_{C\text{-}F}$ = 244.0 Hz), 165.4, 197.6; IR (KBr) ν/cm^{-1}: 1663, 1280, 929, 733; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{21}H_{15}FNOS$: 348.0858, found: 348.0861.

(2-(benzo[d]thiazol-2-yl)-4-chlorophenyl)(phenyl)methanone ***3p***. Isolated as a white solid (72% yield, 50.2 mg), mp:134-135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25-7.34 (m, 3H), 7.35-7.41 (m, 2H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 7.6 Hz, 2H), 7.79 (t, *J* = 6.8 Hz, 2H), 7.93 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 121.5, 123.6, 125.7, 126.4, 128.3, 129.2, 129.5, 130.2, 130.3, 132.9, 133.9, 135.4, 136.2, 137.5, 138.0, 153.3, 163.7, 196.5; IR (KBr) ν/cm^{-1}: 1665, 1277, 778; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{20}H_{13}ClNOS$: 350.0406, found: 350.0411.

(4-chloro-2-(6-methylbenzo[d]thiazol-2-yl)phenyl)(phenyl)methanone ***3q***. Isolated as a yellow solid (67% yield, 48.6 mg), mp: 87-88 °C ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.41 (s, 3H), 7.17 (d, *J* = 8.4 Hz, 1H), 7.28 (t, *J* = 7.2 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.56 (s, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 7.6 Hz, 2H), 7.90 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.6, 121.2, 123.1, 128.0, 128.3, 129.2, 129.3, 130.1, 130.3, 132.9, 134.0, 135.6, 136.0, 136.2, 137.5, 137.9, 151.5,

162.5, 196.6; IR (KBr) ν/cm^{-1}: 1666, 1273, 738; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{15}ClNOS$: 364.0563, found: 364.0559.

*((2-(benzo[d]thiazol-2-yl)phenyl)(phenyl)methanone **3r**[9b]*. Isolated as a yellow solid (62% yield, 40.8 mg), mp: 109-110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.6 Hz, 3H), 7.34- 7.38 (m, 2H), 7.54 (d, *J* = 6.8 Hz, 1H), 7.60-7.64 (m, 2H), 7.77 (t, *J* = 7.6 Hz, 4H), 7.93 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 121.4, 123.4, 125.3, 126.2, 128.2, 128.9, 129.3, 129.6, 130.2, 130.3, 132.1, 132.7, 135.3, 137.8, 139.7, 153.5, 165.3, 197.7; IR (KBr) ν/cm^{-1}: 1666, 1256, 799; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{20}H_{14}NOS$: 316.0796, found: 316.0791.

(2-(benzo[d]thiazol-2-yl)-5-methoxyphenyl)(phenyl)methanone **3s** Isolated in 32% yield. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 3.81 (s, 3H), 6.94 (s, 1H), 7.03 (d, *J* = 8.8 Hz, 1H), 7.16-7.30 (m, 5H), 7.65 (t, *J* = 6.4 Hz, 2H), 7.69 (d, *J* = 7.6 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 55.6, 113.9, 115.8, 121.2, 123.1, 124.6, 124.9, 125.9, 128.2, 129.2, 131.1, 132.6, 135.1, 137.7, 141.3, 153.5, 161.2, 165.0, 197.2; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{21}H_{16}NO_2S$: 346.0902, found: 346.0897.

(2-(benzo[d]thiazol-2-yl)-5-methoxy-1,3-phenylene)bis(phenylmethanone) **3s'** Isolated in 35% yield. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 3.93 (s, 3H), 7.15 (t, *J* = 7.2 Hz, 2H), 7.20-7.26 (m, 7H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.66-7.73 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 56.0, 115.7, 121.0, 123.1, 123.4, 125.0, 125.9, 128.2, 129.5, 133.1, 136.3, 136.7, 142.6, 152.5, 160.4, 162.7, 196.6; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{28}H_{20}NO_3S$: 450.1164, found: 450.1173.

*(3-fluoro-2-(6-fluorobenzo[d]thiazol-2-yl)phenyl)(p-tolyl)methanone **3t***. Isolated as a yellow solid (74% yield, 54.0 mg), mp: 135-136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.29

(s, 3H), 7.07-7.11 (m, 3H), 7.31 (d, *J* = 7.2 Hz, 1H), 7.37 (t, *J* = 9.2 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.54-7.59 (m, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.70 (dd, *J* = 4.8, 8.8 Hz,1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 21.7, 107.3 (d, $^2J_{C\text{-}F}$ = 26.0 Hz), 114.9 (d, $^2J_{C\text{-}F}$ = 25.0 Hz), 117.5 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 120.0 (d, $^3J_{C\text{-}F}$ = 14.0 Hz), 124.5 (d, $^3J_{C\text{-}F}$ = 10.0 Hz), 124.6, 129.1, 129.3, 131.7 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 134.9, 136.9 (d, $^3J_{C\text{-}F}$ = 11.0 Hz), 142.5, 143.7, 148.7, 158.2, 160.1 (d, $^1J_{C\text{-}F}$ = 252.0 Hz), 160.6 (d, $^1J_{C\text{-}F}$ = 244.0 Hz), 195.7; IR (KBr) ν/cm^{-1}: 1661, 1279, 788; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{21}H_{14}F_2NOS$: 366.0764, found: 366.0771.

(4-chlorophenyl)(3-fluoro-2-(6-fluorobenzo[d]thiazol-2-yl)phenyl)methanone ***3u***. Isolated as a yellow solid (85% yield, 54.0 mg), mp: 107-108 °C; ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.10 (dt, *J* = 2.4, 8.8 Hz, 1H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 8.4 Hz, 1H), 7.49 (dd, *J* = 2.8, 8.0 Hz, 1H), 7.59 (dt, *J* = 5.2, 8.0 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.8 Hz, 1H)□^{13}C NMR (100 MHz, CDCl$_3$) δ 107.4 (d, $^2J_{C\text{-}F}$ = 27.0 Hz), 115.2 (d, $^2J_{C\text{-}F}$ = 25.0 Hz), 117.8 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 119.9 (d, $^3J_{C\text{-}F}$ = 14.0 Hz), 124.3 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 124.6, 128.7, 130.2, 131.9 (d, $^3J_{C\text{-}F}$ = 9.0 Hz), 136.0, 136.7, 139.0, 141.7, 148.5, 157.9, 158.8 (d, $^1J_{C\text{-}F}$ = 252.0 Hz), 159.4 (d, $^1J_{C\text{-}F}$ = 245.0 Hz), 194.7; IR (KBr) ν/cm^{-1}: 1670, 1275, 843; HRMS (ESI): *m/z* [M + H]$^+$ calcd for $C_{20}H_{11}ClF_2NOS$: 386.0218, found: 386.0225.

(3-fluoro-2-(6-fluorobenzo[d]thiazol-2-yl)phenyl)(4-nitrophenyl)methanone ***3v***. Isolated as a yellow solid (87% yield, 68.9 mg), mp: 143-144 °C; ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.11 (dt, *J* = 1.6, 7.2 Hz, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.44-7.50 (m, 2H), 7.60-7.66 (m, 2H), 7.86 (d, *J* = 8.4 Hz, 2H), 8.12 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 107.6 (d, $^2J_{C\text{-}F}$ = 26.0 Hz), 115.4 (d, $^2J_{C\text{-}F}$ = 25.0 Hz), 118.4 (d, $^2J_{C\text{-}F}$ = 22.0 Hz), 119.8 (d,

$^3J_{C-F}$ = 13.0 Hz), 123.6, 124.1 (d, $^3J_{C-F}$ = 10.0 Hz), 124.8, 129.3, 132.3 (d, $^3J_{C-F}$ = 9.0 Hz), 136.7, 140.7, 142.6, 148.0, 149.7, 157.6, 158.8 (d, $^1J_{C-F}$ = 253.0 Hz), 159.5 (d, $^1J_{C-F}$ = 246.0 Hz), 194.0; IR (KBr) ν/cm^{-1}: 1673, 1255, 797; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{20}H_{11}F_2N_2O_3S$: 397.0458, found: 397.0465.

(4-bromophenyl)(3-fluoro-2-(6-fluorobenzo[d]thiazol-2-yl)phenyl)methanone ***3w***. Isolated as a yellow solid (35% yield, 30.0 mg), mp: 124-125 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.12 (dt, *J* = 2.4, 8.8 Hz, 1H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.38-7.41 (m, 1H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.51 (dd, *J* = 2.4, 8.0 Hz, 1H), 7.57-7.63 (m, 3H), 7.68 (dd, *J* = 4.8, 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 107.5 (d, $^2J_{C-F}$ = 27.0 Hz), 115.2 (d, $^2J_{C-F}$ = 25.0 Hz), 117.8 (d, $^2J_{C-F}$ = 22.0 Hz), 119.9 (d, $^3J_{C-F}$ = 14.0 Hz), 124.3 (d, $^3J_{C-F}$ = 10.0 Hz), 124.6, 127.8, 130.3, 131.6, 131.9 (d, $^3J_{C-F}$ = 9.0 Hz), 136.4, 136.7, 141.6, 148.5, 157.8, 160.0 (d, $^1J_{C-F}$ = 254.0 Hz), 161.7 (d, $^1J_{C-F}$ = 245.0 Hz), 194.9; IR (KBr) ν/cm^{-1}: 1671, 1275, 795; HRMS (ESI): *m/z* $[M + H]^+$ calcd for $C_{20}H_{11}BrF_2NOS$: 429.9713, found: 429.9708.

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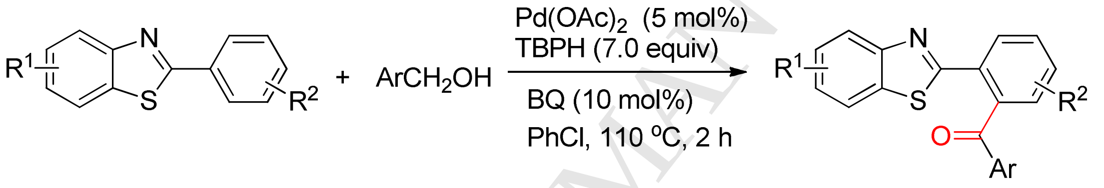
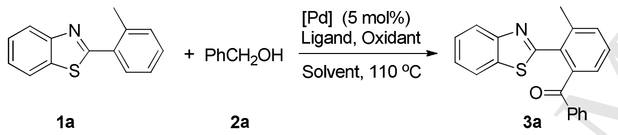


23 examples, up to 95% yield

Table 1. Optimization of the reaction conditions[a]



Entry	[Pd]	Solvent	Oxidant	Ligand	Yield (%)[b]
1	$Pd(OAc)_2$	PhCl	TBHP	-	31
2	$PdCl_2$	PhCl	TBHP	-	15
3	$Pd_2(dba)_3$	PhCl	TBHP	-	27
4	$PdCl_2(CH_3CN)_2$	PhCl	TBHP	-	24
5	$PdCl_2(PhCN)_2$	PhCl	TBHP	-	13
6	$PdCl_2(PPh_3)_2$	PhCl	TBHP	-	11
7	$Pd(OAc)_2$	PhCl	DTBP	-	18
8	$Pd(OAc)_2$	PhCl	O_2	-	-
9	$Pd(OAc)_2$	PhCl	Oxone	-	-
10	$Pd(OAc)_2$	PhCl	$K_2S_2O_8$	-	-
11[c]	$Pd(OAc)_2$	PhCl	TBHP	-	45
12[d]	$Pd(OAc)_2$	PhCl	TBHP	-	52
13[e]	$Pd(OAc)_2$	PhCl	TBHP	-	61
14[e]	$Pd(OAc)_2$	PhCl	TBHP	TMEDA	37
15[e]	$Pd(OAc)_2$	PhCl	TBHP	DMEDA	32
16[e]	$Pd(OAc)_2$	PhCl	TBHP	PPh_3	28
17[e]	$Pd(OAc)_2$	PhCl	TBHP	L-proline	42
18[e]	$Pd(OAc)_2$	PhCl	TBHP	BQ	68
19[e]	$Pd(OAc)_2$	PhCl	TBHP	DDQ	trace
20[e]	$Pd(OAc)_2$	PhCl	TBHP	1,10-phen	-
21[e]	$Pd(OAc)_2$	toluene	TBHP	BQ	50
22[e]	$Pd(OAc)_2$	AcOH	TBHP	BQ	30
23[e]	$Pd(OAc)_2$	DMAc	TBHP	BQ	trace
24[e]	$Pd(OAc)_2$	DMF	TBHP	BQ	-
25[e]	$Pd(OAc)_2$	DMSO	TBHP	BQ	trace

26[e]	Pd(OAc)$_2$	NMP	TBHP	BQ	20
27[e]	Pd(OAc)$_2$	CH$_3$CN	TBHP	BQ	35

[a] Conditions: **1a** (0.2 mmol), **2a** (0.6 mmol), [Pd] catalyst (5 mol %), oxidant (3.0 equiv), ligand (10 mol%) 110 °C, 2 h.

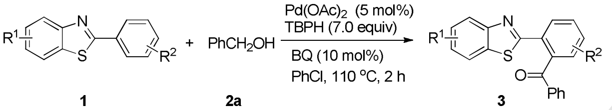
[b] Isolated yield based on **1a**.

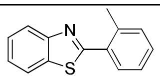
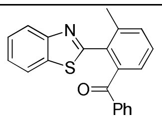
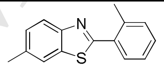
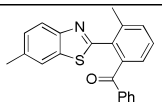
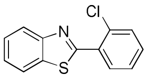
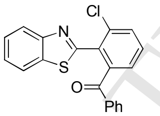
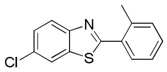
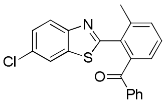
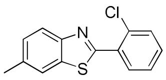
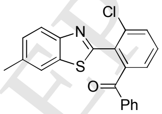
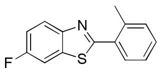
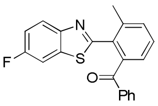
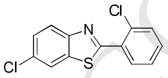
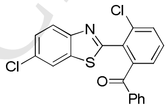
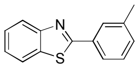
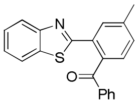
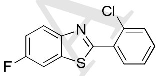
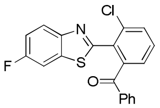
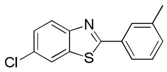
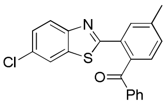
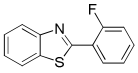
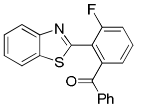
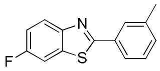
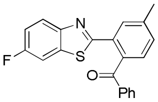
[c] 4.0 equiv of TBHP were used.

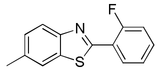
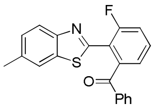
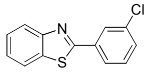
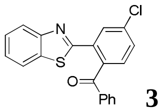
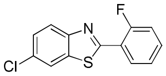
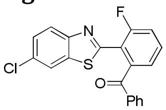
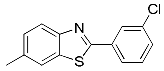
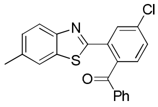
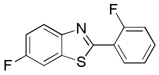
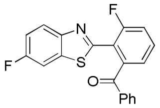
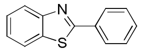
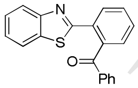
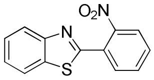
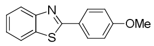
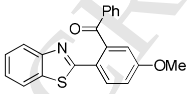
[d] 6.0 equiv of TBHP were used.

[e] 7.0 equiv of TBHP were used.

Table 2. Reaction of phenylmethanol with 2-arylbenzo[*d*]thiazoles[a]



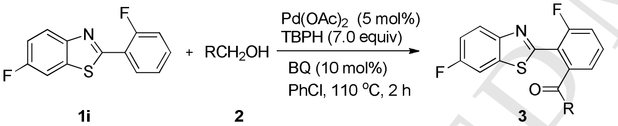
Entry	**1**	Product **3**	Yield (%)[b]	Entry	**1**	Product **3**	Yield (%)[b]
1	 **1a**	 **3a**	68	11	 **1k**	 **3j**	22
2	 **1b**	 **3b**	95	12	 **1l**	 **3k**	70
3	 **1c**	 **3c**	85	13	 **1m**	 **3l**	83
4	 **1d**	 **3d**	92	14	 **1n**	 **3m**	65
5	 **1e**	 **3e**	83	15	 **1o**	 **3n**	65
6	 **1f**	 **3f**	82	16	 **1p**	 **3o**	81

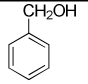
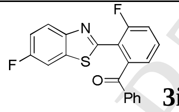
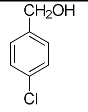
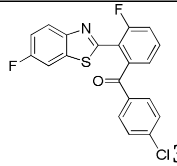
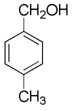
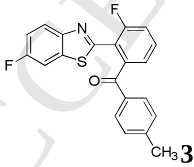
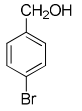
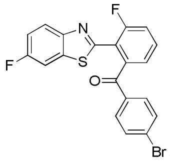
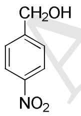
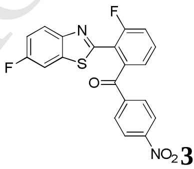
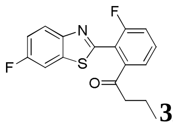
7	 **1g**	 **3g**	75	17	 **1q**	 **3p**	72
8	 **1h**	 **3h**	80	18	 **1r**	 **3q**	67
9	 **1i**	 **3i**	92	19	 **1s**	 **3r**	62
10	 **1j**	-	-	20	 **1t**	 **3s**	32[c]

[a] Conditions: 2-arylbenzo[*d*]thiazole **1** (0.2 mmol), phenylmethanol **2a** (0.6 mmol), $Pd(OAc)_2$ (5 mol%), TBHP (7.0 equiv), BQ (10 mol%), PhCl, 110 °C, 2h.

[b] Isolated yield based on **1**. [c] With 35% yield of bis-acylated product.

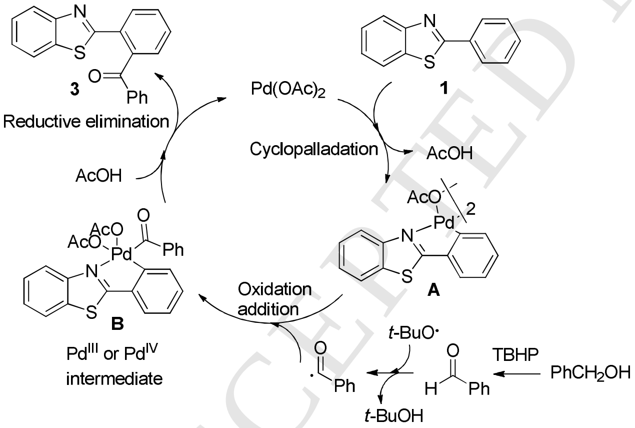
Table 3. Acylation of 2-arylbenzo[*d*]thiazole with primary alcohols[a]



Entry	2	Product 3	Yield (%)[b]	Entry	2	Product 3	Yield (%)[b]
1	 **2a**	 **3i**	92	4	 **2d**	 **3v**	87
2	 **2b**	 **3t**	74	5	 **2e**	 **3w**	35
3	 **2c**	 **3u**	85	6	^{n}BuOH **2f**	 **3x**	-

[a] Conditions: 2-arylbenzo[*d*]thiazole **1i** (0.2 mmol), primary alcohols **2** (0.6 mmol), $Pd(OAc)_2$ (5 mol%), TBHP (7.0 equiv), BQ (10 mol%), PhCl, 110 °C, 2h.

[b] Isolated yield based on **1i**.



Scheme 1 Plausible mechanism for the Pd-catalyzed *ortho*-acylation reaction.

Palladium-catalyzed direct *ortho*-acylation through an oxidative coupling of 2-arylbenzothiazoles with benzylic alcohols

Qiuping Ding,[*] Huafang Ji, Changqing Ye, Jiajia Wang, Junyan Wang, Liyun Zhou and Yiyuan Peng*

Key Laboratory of Functional Small Organic Molecules, Ministry of Education and College of Chemistry & Chemical Engineering, Jiangxi Normal University, Nanchang, Jiangxi 330022, China

Supporting Information

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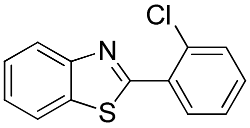
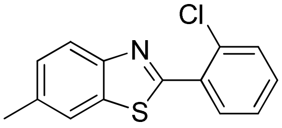
[*] Corresponding author: Tel.: +86 791 88120380; fax: +86 791 88120380; E-mail: dqpjxnu@gmail.com; yiyuanpeng@yahoo.com



2-(2-chlorophenyl)benzo[*d*]thiazole (**1b**) mp: 86-87 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.27-7.34 (m, 3H), 7.41-7.46 (m, 2H), 7.83 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 8.17 (dd, *J* = 2.4, 7.2 Hz, 1H);

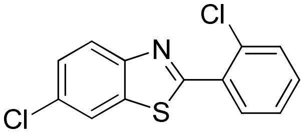
^{13}C NMR (100 MHz, CDCl$_3$) δ 121.4, 123.5, 125.5, 126.3, 127.1, 130.8, 131.1, 131.8, 132.3, 132.7, 136.2, 152.6, 164.1;



2-(2-chlorophenyl)-6-methylbenzo[*d*]thiazole (**1c**) mp: 101-102 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 2.45 (s, 3H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.30-7.35 (m, 2H), 7.46 (d, *J* = 6.4 Hz, 1H), 7.65 (s, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 6.4 Hz, 1H);

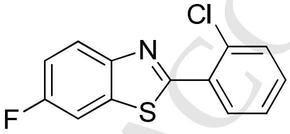
^{13}C NMR (100 MHz, CDCl$_3$) δ 21.6, 121.0, 123.0, 127.1, 128.0, 130.8, 130.9, 131.7, 132.4, 132.6, 135.6, 136.4, 150.7, 163.0;



6-chloro-2-(2-chlorophenyl)benzo[*d*]thiazole (**1d**) mp: 136-137 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.36-7.42 (m, 2H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.50-7.54 (m, 1H), 7.90 (s, 1H), 8.02 (d, *J* = 8.8 Hz, 1H), 8.20-8.24 (m, 1H);

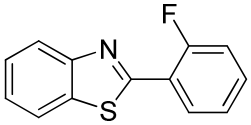
^{13}C NMR (100 MHz, CDCl$_3$) δ 120.9, 124.2, 127.2, 130.9, 131.4, 131.7, 131.8, 132.7, 137.3, 151.0, 164.6;



2-(2-chlorophenyl)-6-fluorobenzo[*d*]thiazole (**1e**) mp: 127-128 °C;

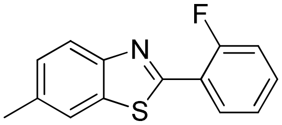
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.22 (t, *J* = 8.8 Hz, 1H), 7.35-7.37 (m, 2H), 7.46-7.52 (m,1H), 7.57 (d, *J* = 8.0 Hz, 1H), 8.01-8.05 (m, 1H), 8.17-8.21 (m, 1H);

^{13}C NMR (100 MHz, CDCl$_3$) δ 107.4 (d, $^{2}J_{C\text{-}F}$ = 26.5 Hz), 115.1 (d, $^{2}J_{C\text{-}F}$ = 24.7 Hz), 124.5 (d, $^{3}J_{C\text{-}F}$ = 9.3 Hz), 127.1, 130.8, 131.2, 131.6, 131.9, 132.6, 137.1 (d, $^{3}J_{C\text{-}F}$ = 11.1 Hz), 149.1, 160.6 (d, $^{1}J_{C\text{-}F}$ = 244.8 Hz), 163.8;



2-(2-fluorophenyl)benzo[*d*]thiazole (**1f**) mp: 97-98 °C;

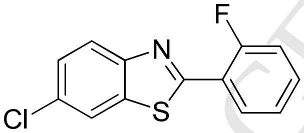
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.19 (t, J = 9.6 Hz, 1H), 7.26 (t, J = 7.6 Hz, 1H), 7.35-7.44 (m, 2H), 7.48 (t, J = 7.6 Hz, 1H), 7.89 (d, J = 7.6 Hz, 1H), 8.11 (d, J = 8.0 Hz, 1H), 8.39 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 116.4 (d, $^{2}J_{C\text{-}F}$ = 21.8 Hz), 121.4, 121.5, 123.3, 124.7, 125.3, 126.3, 129.8, 132.1 (d, $^{3}J_{C\text{-}F}$ = 6.8 Hz), 135.8 (d, $^{3}J_{C\text{-}F}$ = 6.8 Hz), 152.6, 160.6 (d, $^{1}J_{C\text{-}F}$ = 252.0 Hz), 161.0;



2-(2-fluorophenyl)-6-methylbenzo[*d*]thiazole (**1g**) mp: 111-112 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 2.46 (s, 3H), 7.15-7.29 (m, 3H), 7.37-7.42 (m, 1H), 7.65 (s, 1H), 7.97 (d, J = 8.4 Hz, 1H), 8.37 (dt, J = 1.6, 8.0 Hz, 1H);

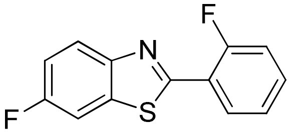
^{13}C NMR (100 MHz, CDCl$_3$) δ 21.6, 116.3 (d, $^{2}J_{C\text{-}F}$ = 21.9 Hz), 121.1, 121.6 (d, $^{3}J_{C\text{-}F}$ = 11.0 Hz), 122.8, 124.6, 128.0, 129.7, 131.9 (d, $^{3}J_{C\text{-}F}$ = 8.7 Hz), 135.5, 136.0 (d, $^{3}J_{C\text{-}F}$ = 7.8 Hz), 150.7, 160.0, 160.5 (d, $^{1}J_{C\text{-}F}$ = 251.8 Hz);



6-chloro-2-(2-fluorophenyl)benzo[*d*]thiazole (**1h**) mp: 149-149 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.22 (t, J = 9.2 Hz, 1H), 7.30 (t, J = 6.8 Hz, 1H), 7.45 (d, J = 8.0 Hz, 2H), 7.88 (s, 1H), 7.99 (d, J = 8.0 Hz, 1H), 8.35-8.43 (m, 1H);

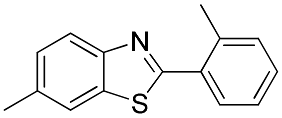
^{13}C NMR (100 MHz, CDCl$_3$) δ 116.4 (d, $^{2}J_{C\text{-}F}$ = 21.8 Hz), 121.0, 121.1, 124.0, 124.7, 127.2, 129.7, 131.2, 132.4 (d, $^{3}J_{C\text{-}F}$ = 8.7 Hz), 136.9 (d, $^{3}J_{C\text{-}F}$ = 8.4 Hz), 151.1, 160.6 (d, $^{1}J_{C\text{-}F}$ = 252.1 Hz), 161.5 (d, $^{3}J_{C\text{-}F}$ = 5.9 Hz);



6-fluoro-2-(2-fluorophenyl)benzo[*d*]thiazole (**1i**) mp: 124-125 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.19-7.31 (m, 3H), 7.43-7.46 (m, 1H), 7.59 (dd, J = 2.4, 8.0 Hz, 1H), 8.03 (dd, J = 4.8, 9.2 Hz, 1H), 8.36 (dt, J = 1.6, 8.0 Hz, 1H);

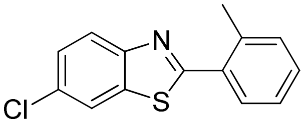
^{13}C NMR (100 MHz, CDCl$_3$) δ 107.5 (d, $^2J_{\text{C-F}}$ = 26.5 Hz), 115.1 (d, $^2J_{\text{C-F}}$ = 24.7 Hz), 116.4 (d, $^2J_{\text{C-F}}$ = 21.8 Hz), 121.2 (d, $^3J_{\text{C-F}}$ = 11.2 Hz), 124.3 (d, $^3J_{\text{C-F}}$ = 9.4 Hz), 124.7, 129.6, 132.2 (d, $^3J_{\text{C-F}}$ = 8.7 Hz), 136.7 (d, $^3J_{\text{C-F}}$ = 8.5 Hz), 136.8 (d, $^3J_{\text{C-F}}$ = 8.4 Hz), 149.2, 160.4 (d, $^1J_{\text{C-F}}$ = 251.9 Hz), 160.5 (d, $^3J_{\text{C-F}}$ = 244.3 Hz), 160.8;



6-methyl-2-(*o*-tolyl)benzo[*d*]thiazole (**1k**) mp: 97-98 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 2.56 (s, 3H), 2.71 (s, 3H), 7.39-7.44 (m, 2H), 7.50-7.53 (m, 2H), 7.80 (s, 1H), 8.01 (d, J = 7.6 Hz, 1H), 8.51 (d, J = 8.4 Hz, 1H);

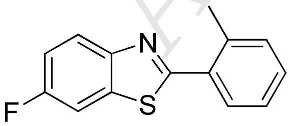
^{13}C NMR (100 MHz, CDCl$_3$) δ 21.6, 21.8, 120.8, 121.5, 127.0, 127.9, 130.2, 131.2, 132.1, 132.4, 132.6, 137.7, 138.2, 143.5, 169.6;



6-chloro-2-(*o*-tolyl)benzo[*d*]thiazole (**1l**) mp: 94-95 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 2.64 (s, 3H), 7.28-7.36 (m, 3H), 7.43 (dd, J = 2.0, 8.8 Hz, 1H), 7.72 (d, J = 7.6 Hz, 1H), 7.85 (d, J = 6.0 Hz,1H), 7.97 (d, J = 8.8 Hz, 1H);

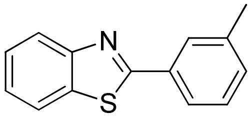
^{13}C NMR (100 MHz, CDCl$_3$) δ 21.5, 121.0, 124.1, 126.2, 127.0, 130.3, 130.5, 131.0, 131.7, 132.6, 136.7, 137.4, 152.4, 168.5;



6-fluoro-2-(*o*-tolyl)benzo[*d*]thiazole (**1m**) mp: 64-65 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 2.63 (s, 3H), 7.19 (dt, J = 2.4, 8.8 Hz, 1H), 7.25-7.33 (m, 3H), 7.52 (dd, J = 2.4, 8.0 Hz, 1H), 7.69 (d, J = 7.6 Hz, 1H), 8.00 (dd, J = 4.8, 9.2 Hz, 1H);

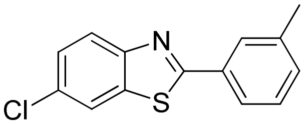
^{13}C NMR (100 MHz, CDCl$_3$) δ 21.5, 107.6 (d, $^2J_{C\text{-}F}$ = 26.6 Hz), 114.8 (d, $^2J_{C\text{-}F}$ = 24.6 Hz), 124.3 (d, $^3J_{C\text{-}F}$ = 9.3 Hz), 126.2, 130.1, 130.5, 131.7, 132.8, 136.5 (d, $^3J_{C\text{-}F}$ = 11.1 Hz), 137.3, 150.5, 160.5 (d, $^1J_{C\text{-}F}$ = 244.1 Hz), 167.7;



2-(m-tolyl)benzo[d]thiazole (**1n**) mp: 72-73 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 2.36 (s, 3H), 7.20 (d, J = 8.0 Hz, 1H), 7.28 (t, J = 7.6 Hz, 2H), 7.39-7.43 (m, 1H), 7.75-7.81 (m, 2H), 7.88 (s, 1H), 8.04 (d, J = 7.6 Hz, 1H);

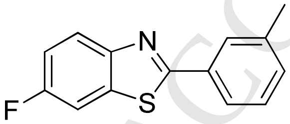
^{13}C NMR (100 MHz, CDCl$_3$) δ 21.4, 121.6, 123.2, 124.9, 125.1, 126.3, 128.0, 128.9, 131.8, 133.6, 135.1, 138.8, 154.2, 168.3;



6-chloro-2-(m-tolyl)benzo[d]thiazole (**1o**) mp: 136-137 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 2.42 (s, 3H), 7.27 (d, J = 7.2 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 7.40 (d, J = 8.4 Hz, 1H), 7.78 (d, J = 7.6 Hz, 1H), 7.79 (s, 1H), 7.86 (s,1H), 7.92 (d, J = 7.6 Hz, 1H);

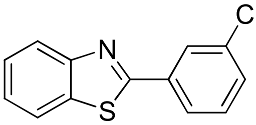
^{13}C NMR (100 MHz, CDCl$_3$) δ 21.4, 121.2, 123.8, 124.8, 127.1, 128.0, 128.9, 130.9, 132.0, 133.1, 136.2, 138.9, 152.7, 168.8;



6-fluoro-2-(m-tolyl)benzo[d]thiazole (**1p**) mp: 82-83 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 2.36 (s, 3H), 7.11-7.15 (m, 1H), 7.20 (d, J = 6.4 Hz, 1H), 7.27 (t, J = 6.0 Hz, 1H), 7.42 (d, J = 7.6 Hz, 1H), 7.72 (d, J = 6.0 Hz, 1H), 7.79 (s, 1H), 7.91-7.94 (m, 1H);

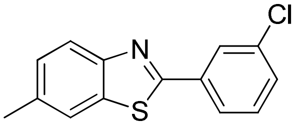
^{13}C NMR (100 MHz, CDCl$_3$) δ 21.3, 107.8 (d, $^{2}J_{\text{C-F}}$ = 26.6 Hz), 114.8 (d, $^{2}J_{\text{C-F}}$ = 24.5 Hz), 124.0 (d, $^{3}J_{\text{C-F}}$ = 9.3 Hz), 124.7, 127.8, 128.9, 131.8, 133.2, 136.0 (d, $^{3}J_{\text{C-F}}$ = 11.1 Hz), 138.8, 150.7, 160.4 (d, $^{1}J_{\text{C-F}}$ = 244.2 Hz), 167.9;



2-(3-chlorophenyl)benzo[*d*]thiazole (**1q**) mp: 111-112 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.25-7.34 (m, 3H), 7.43 (t, *J* = 5.6 Hz, 1H), 7.75-7.80 (m, 2H), 8.01 (d, *J* = 8.8 Hz, 2H);

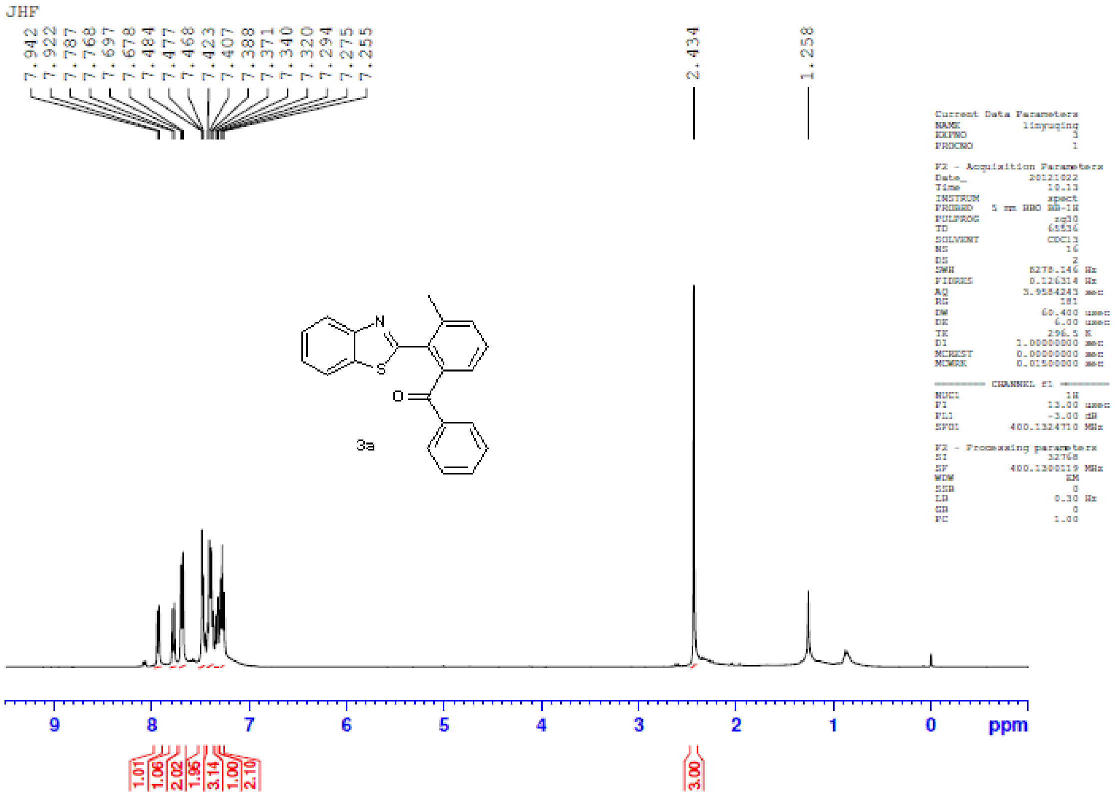
^{13}C NMR (100 MHz, CDCl$_3$) δ 121.7, 123.5, 125.5, 125.6, 126.5, 127.3, 130.2, 130.8, 135.0, 135.1, 135.2, 154.0, 166.1;



2-(3-chlorophenyl)-6-methylbenzo[*d*]thiazole (**1r**) mp: 120-121 °C;

^{1}H NMR (400 MHz, CDCl$_3$) δ 2.40 (s, 3H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 6.8 Hz, 1H), 7.52 (s, 1H), 7.79 (d, *J* = 6.8 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 8.01 (s, 1H);

^{13}C NMR (100 MHz, CDCl$_3$) δ 21.6, 121.4, 122.9, 125.5, 127.2, 128.1, 130.1, 130.5, 135.1, 135.2, 135.4, 135.7, 152.1, 165.1;



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PROCNO                    1

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TE                    296.5 K
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MCREST           0.00000000 sec
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PL1                   -3.00 dB
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F2 - Processing parameters
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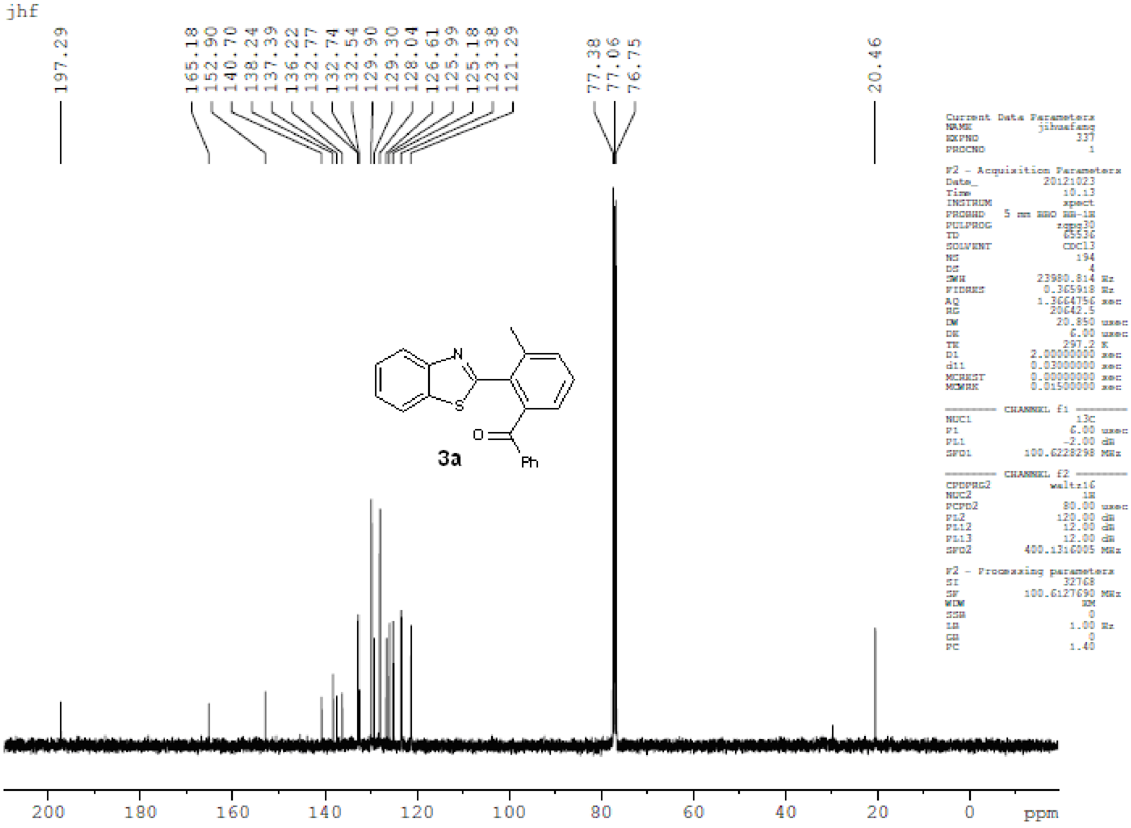

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PROCNO                     1

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DS                         4
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TE                     297.2 K
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PL1                    -2.00 dB
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NUC2                      1H
PCPD2                  80.00 usec
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PL12                   12.00 dB
PL13                   12.00 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
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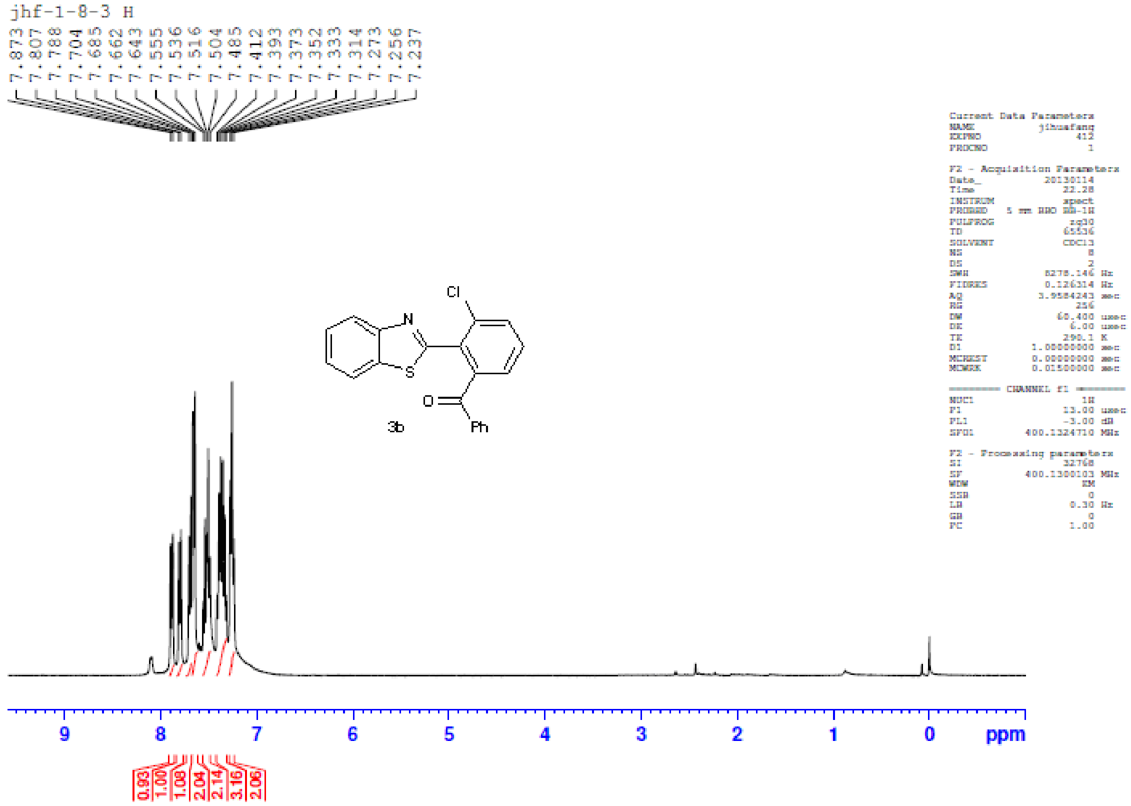

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FIDRES          0.126314 Hz
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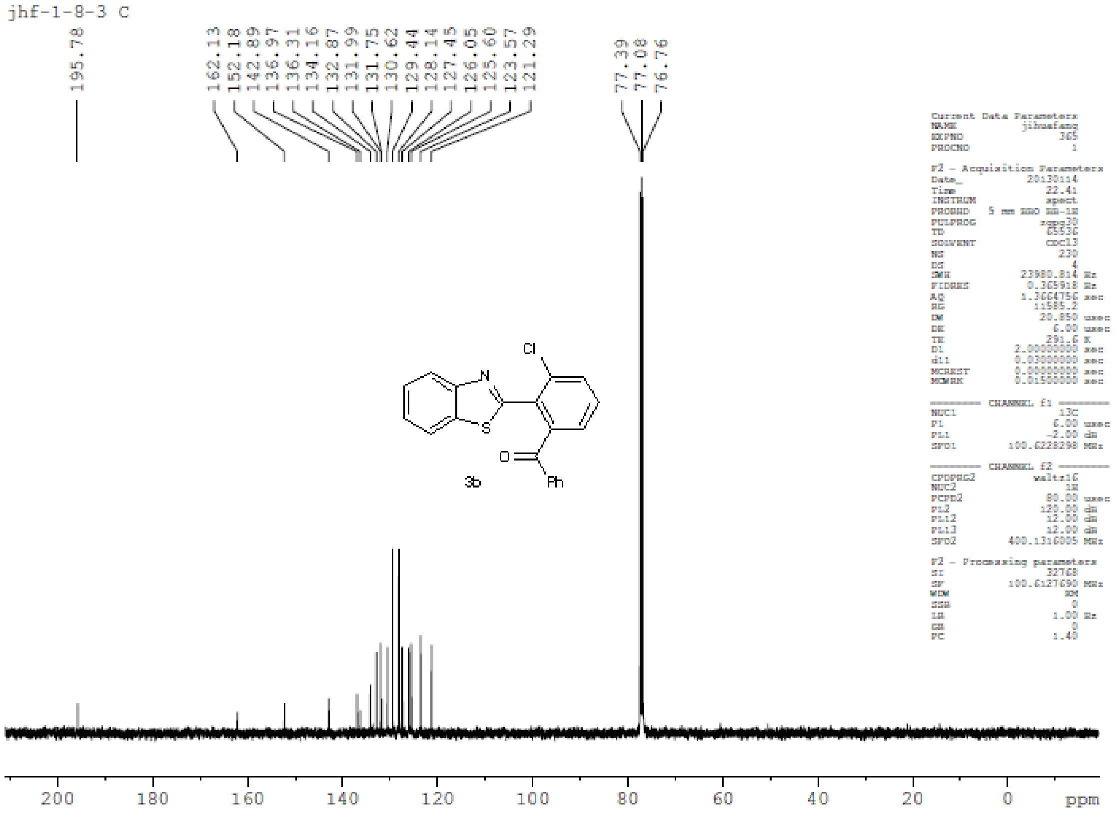

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AQ             1.3664756 sec
RG               11585.2
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MCWRK         0.01500000 sec

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PL1                -2.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
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PCPD2              80.00 usec
PL2               120.00 dB
PL12               12.00 dB
PL13               12.00 dB
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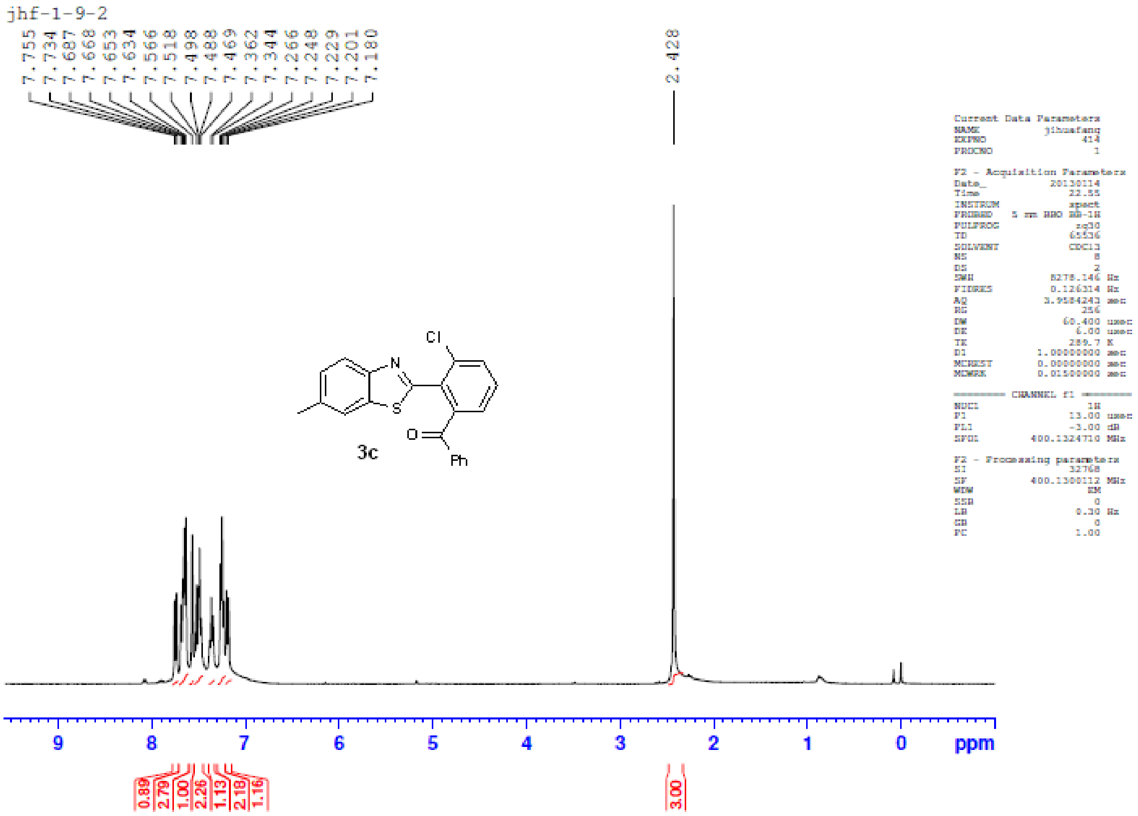
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Cl
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S
O
Ph
3c
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TE 289.7 K
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F2 - Processing parameters
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SF 400.1300112 MHz
WDW EM
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LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
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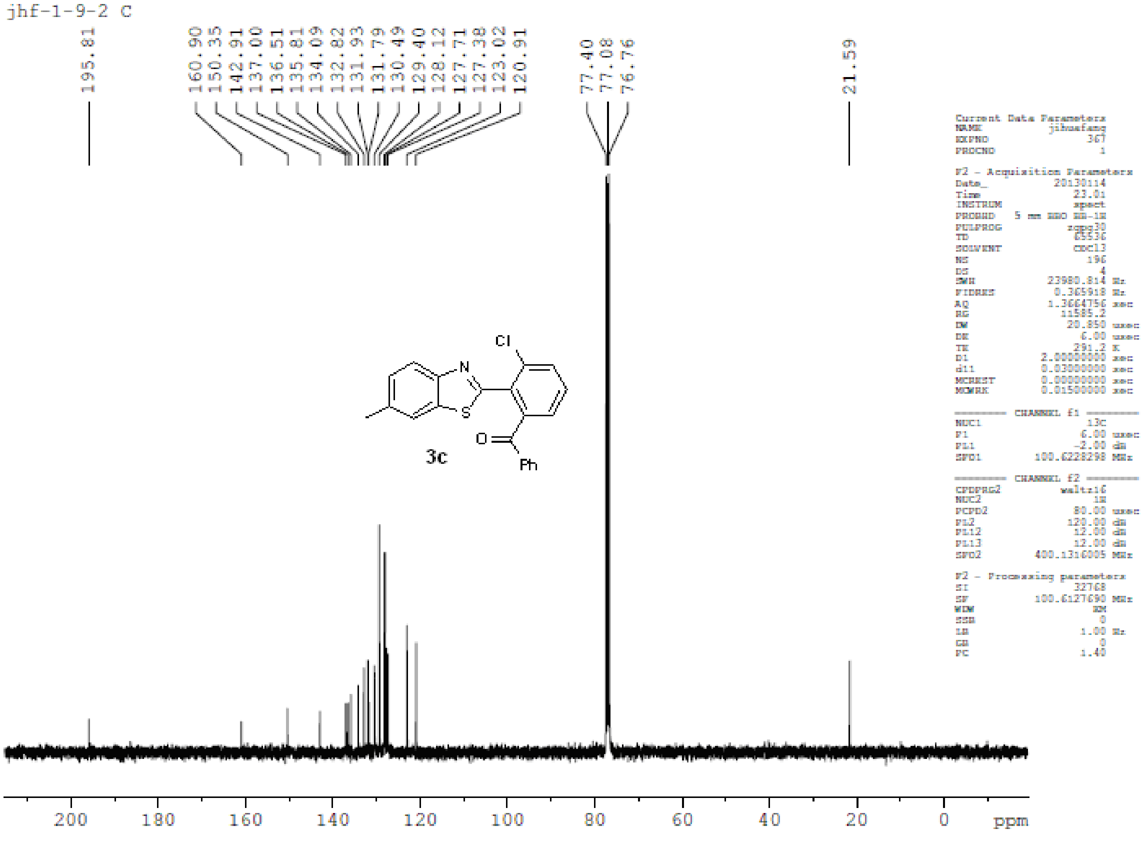
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S
O
Ph
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FIDRES 0.365918 Hz
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DW 20.850 usec
DE 6.00 usec
TE 291.2 K
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MCREST 0.00000000 sec
MCWRK 0.01500000 sec
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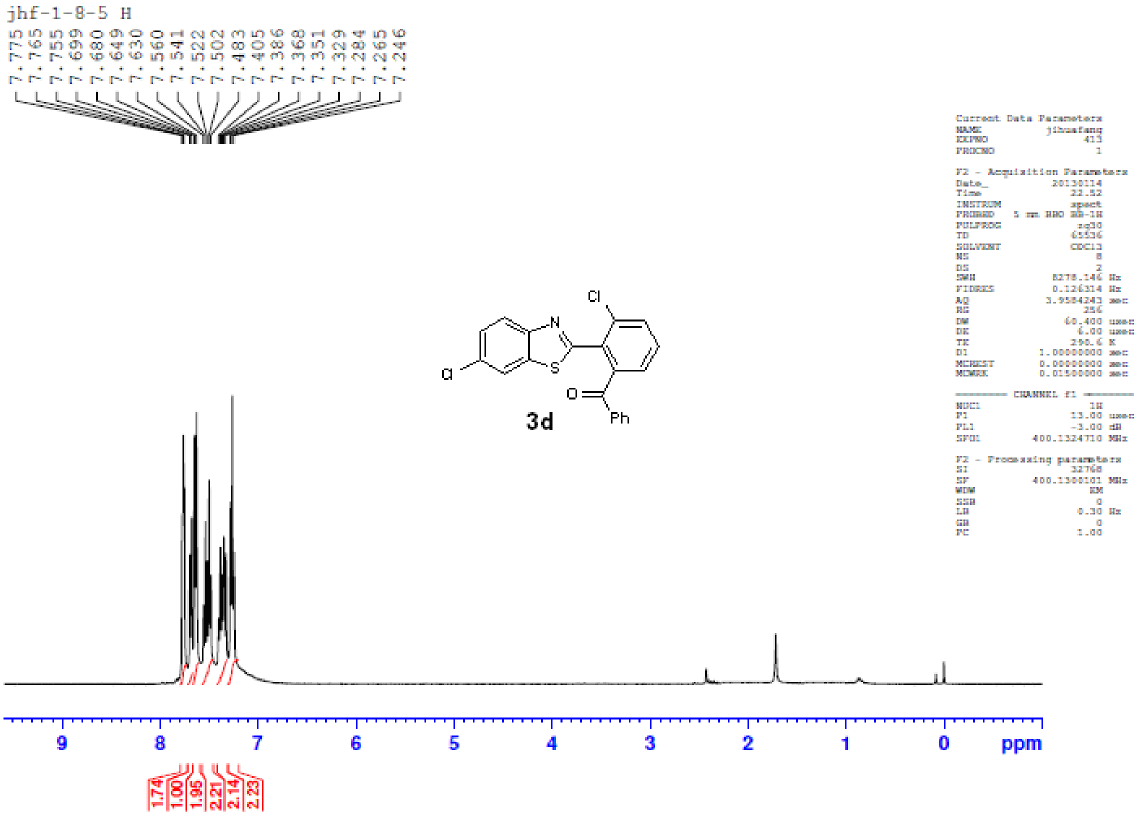
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PROCNO 1
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FIDRES 0.126314 Hz
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TE 290.6 K
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MCREST 0.00000000 sec
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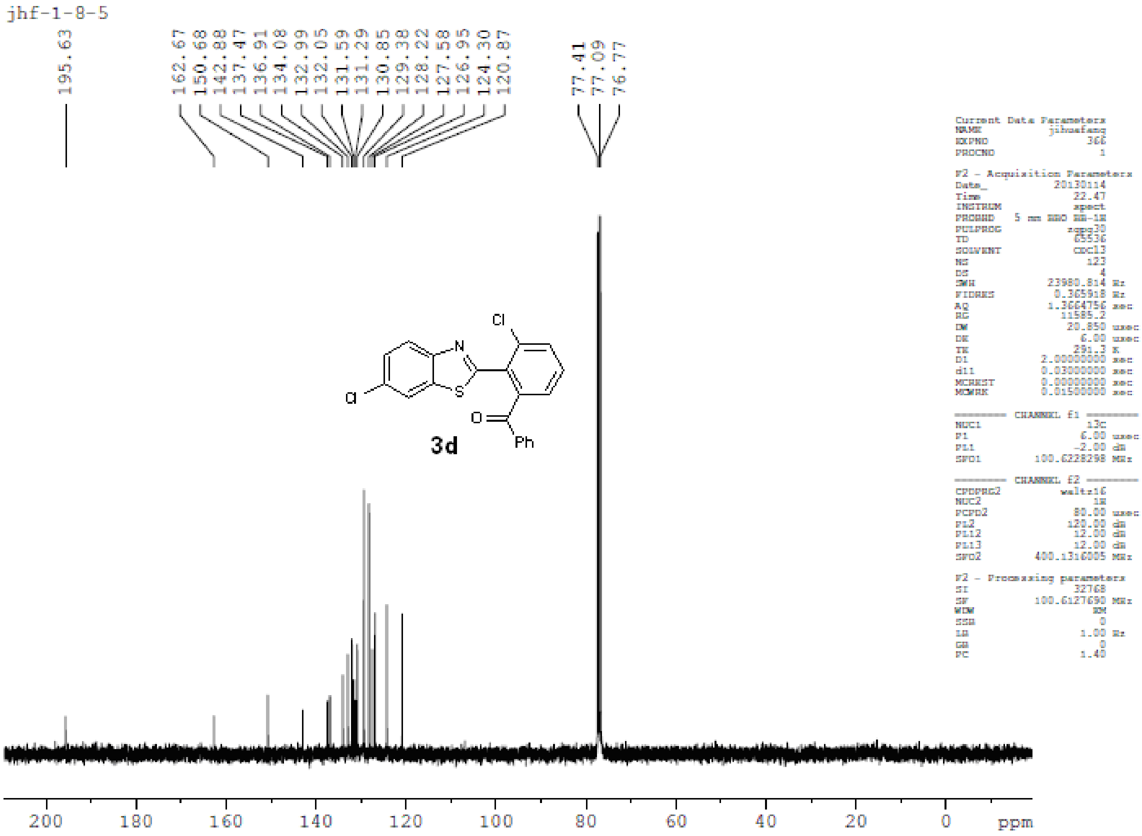
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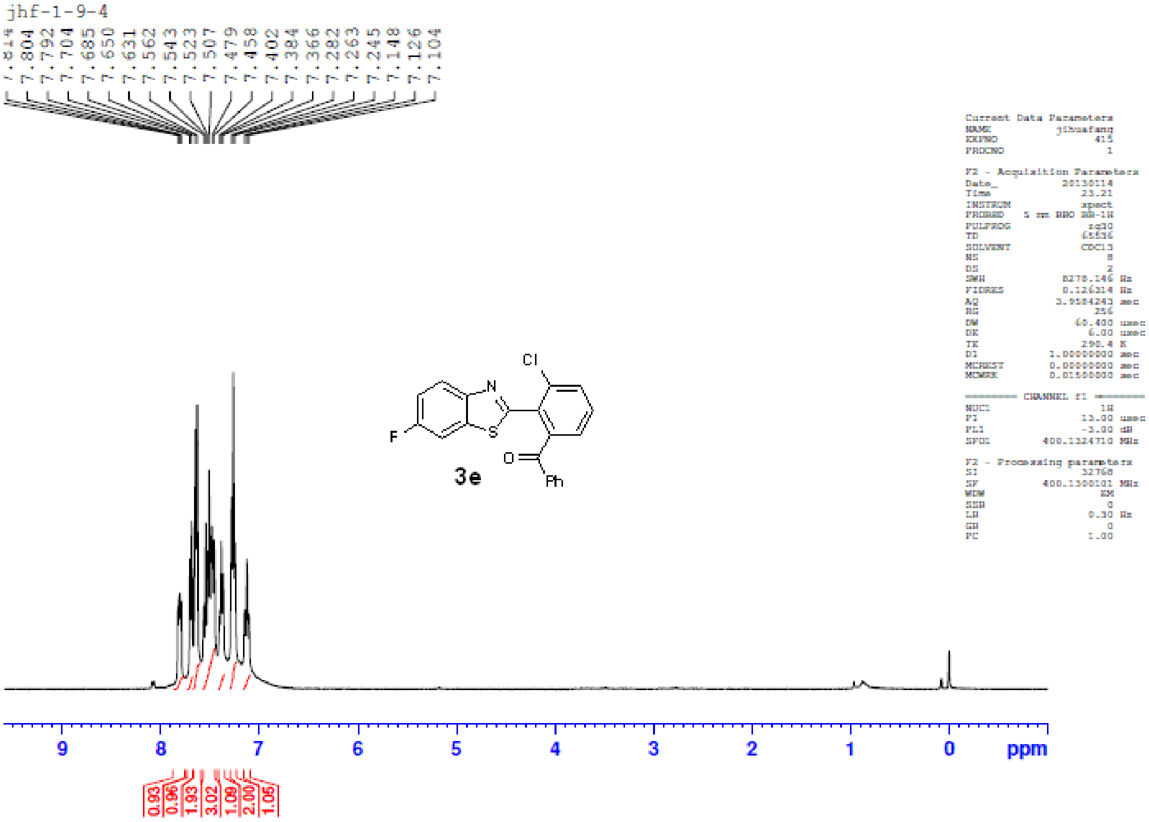
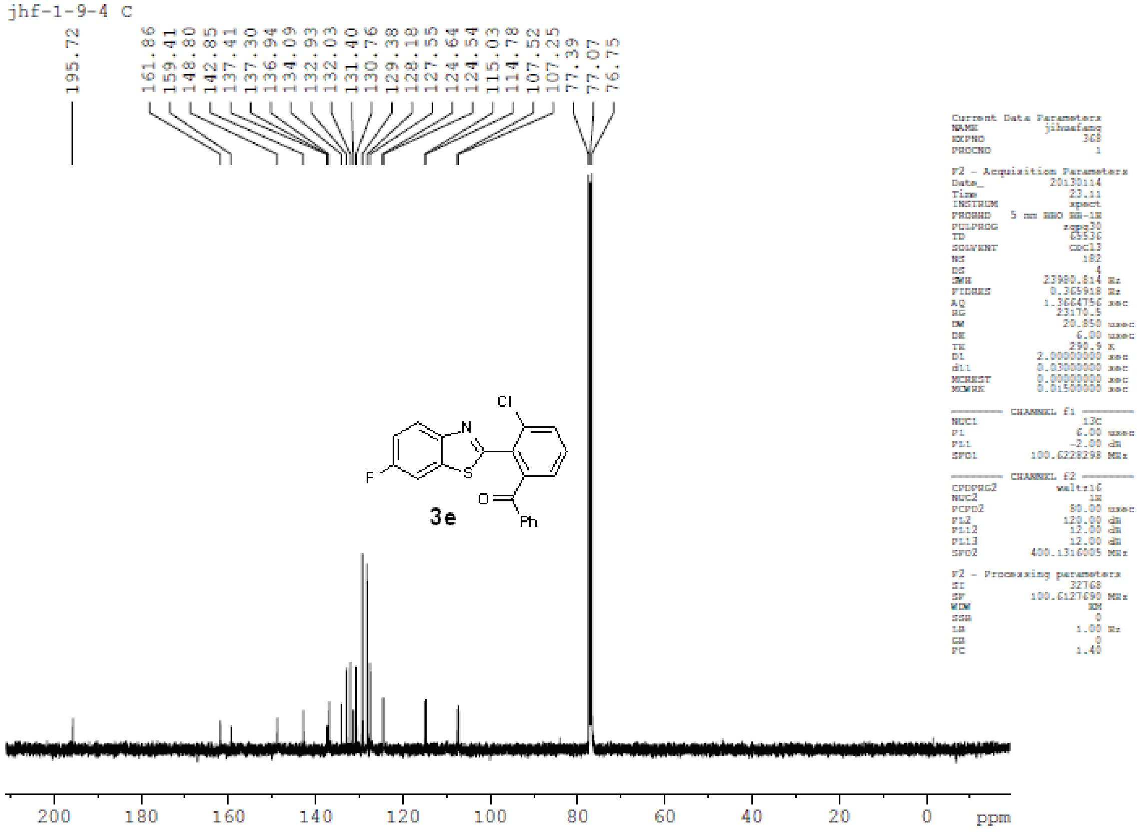
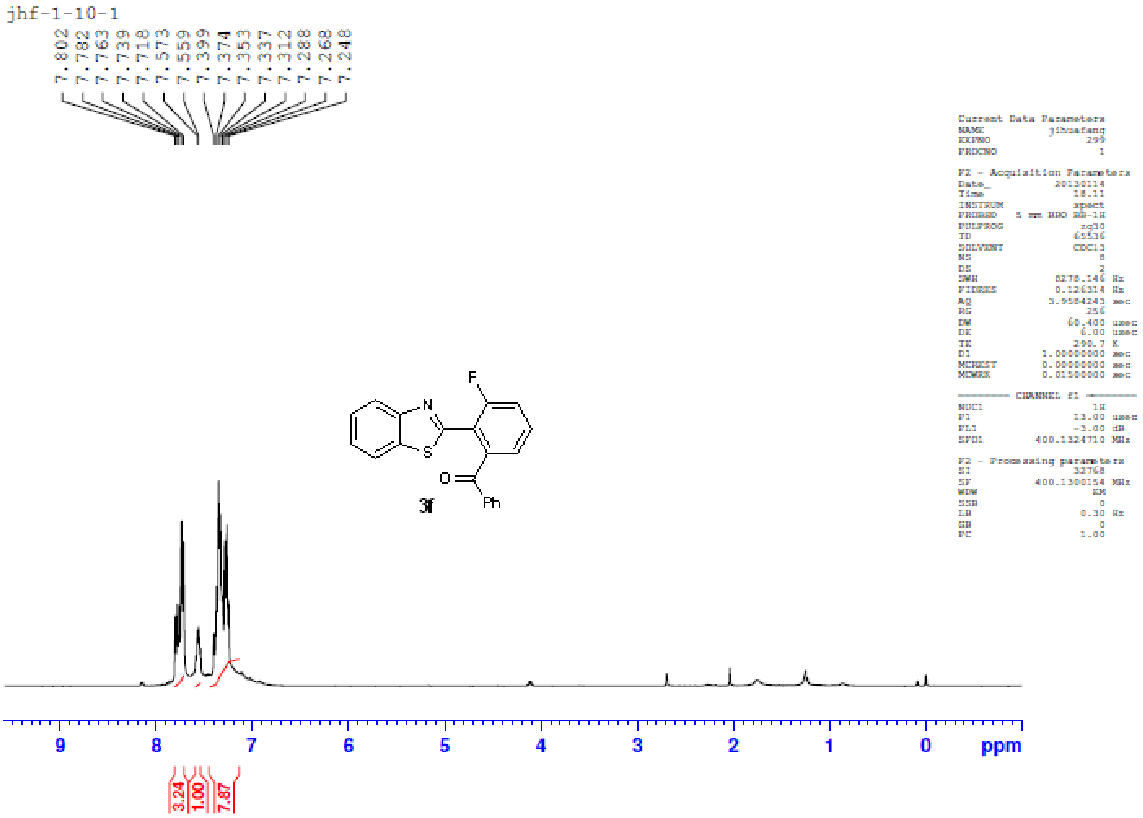
131.59
131.29
130.85
129.38
128.22
127.58
126.95
124.30
120.87
77.41
77.09
76.77
Cl
N
S
Cl
O
Ph
3d
Current Data Parameters
NAME jihuafang
EXPNO 366
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 22.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 123
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 291.3 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm



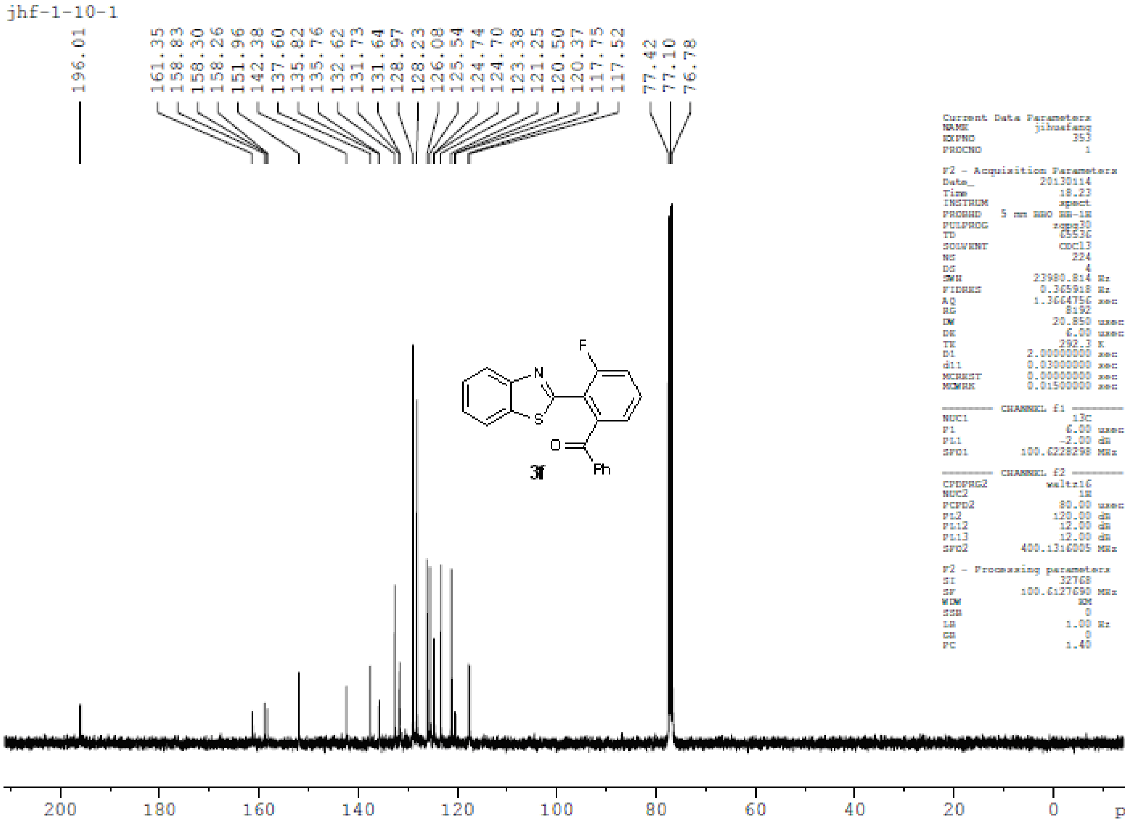
```
Current Data Parameters
NAME             jihuafang
EXPNO                  415
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130114
Time                 23.21
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ              3.9584243 sec
RG                     256
DW                  60.400 usec
DE                    6.00 usec
TE                   290.4 K
D1              1.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   13.00 usec
PL1                  -3.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                   32768
SF             400.1300101 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



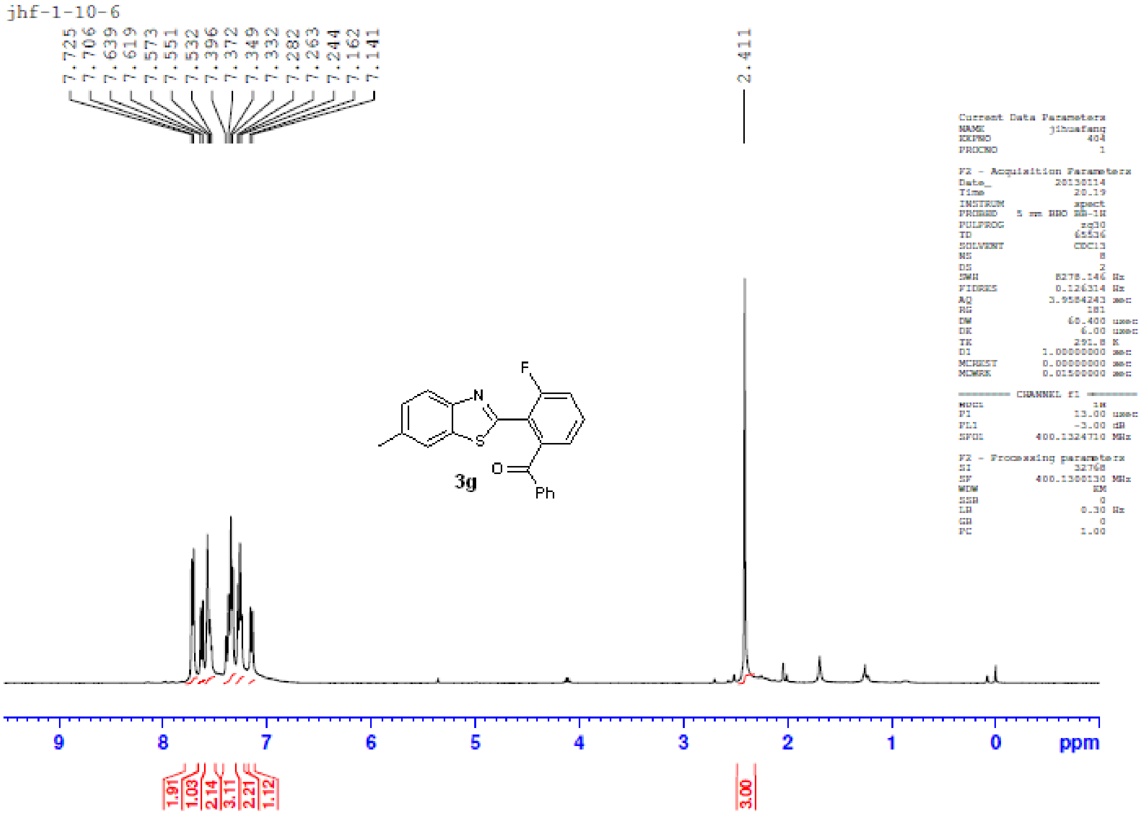
```
Current Data Parameters
NAME             jihuafang
EXPNO                  368
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130114
Time                 23.11
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     182
DS                       4
SWH             23980.814 Hz
FIDRES           0.365918 Hz
AQ              1.3664756 sec
RG                 23170.5
DW                  20.850 usec
DE                    6.00 usec
TE                   290.9 K
D1              2.00000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                    6.00 usec
PL1                  -2.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                 120.00 dB
PL12                 12.00 dB
PL13                 12.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF             100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

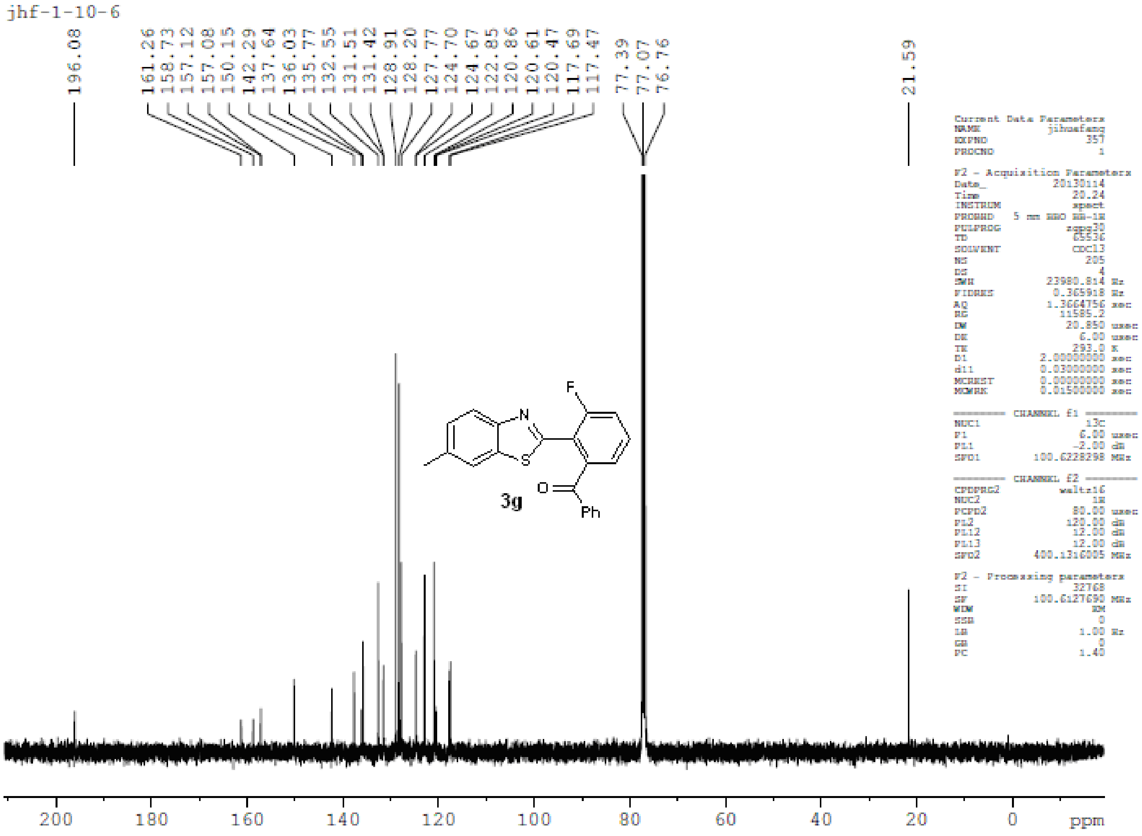


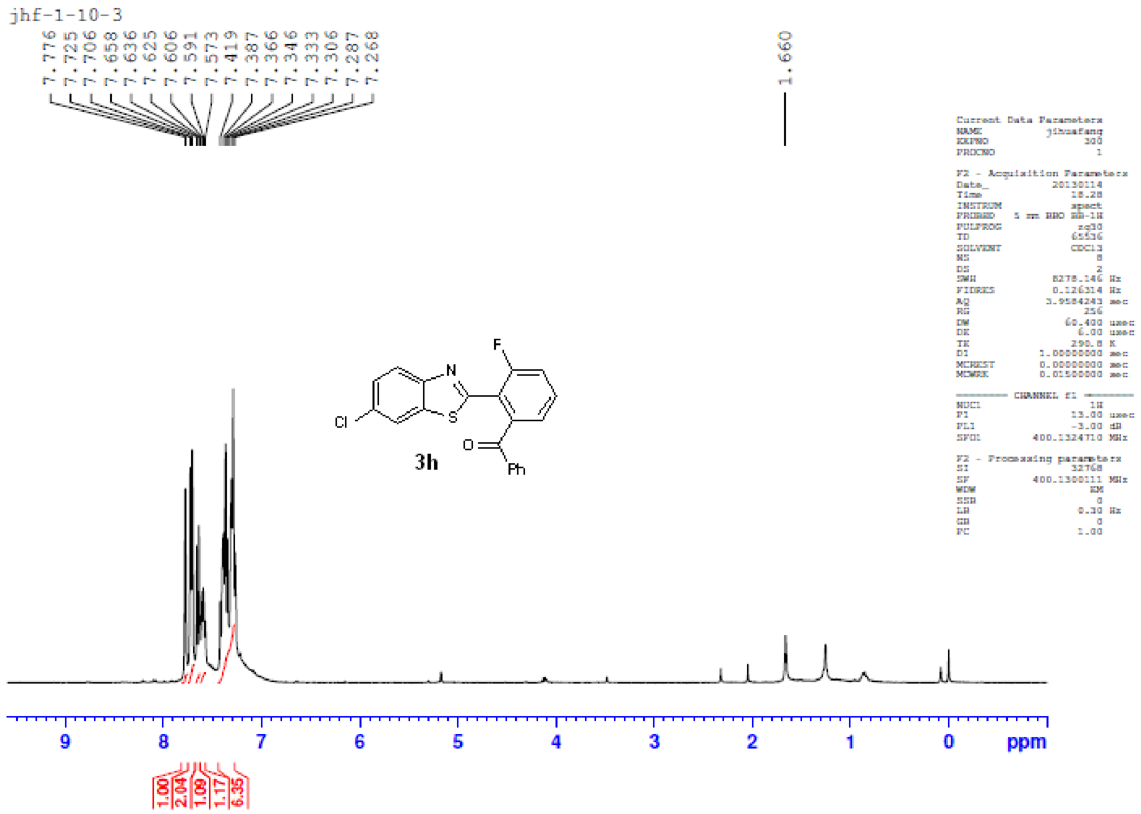
```
Current Data Parameters
NAME             jihuafang
EXPNO                  299
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130114
Time                 18.11
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8278.146 Hz
FIDRES            0.126314 Hz
AQ               3.9584243 sec
RG                     256
DW                  60.400 usec
DE                    6.00 usec
TE                   290.7 K
D1              1.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   13.00 usec
PL1                  -3.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                   32768
SF             400.1300154 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

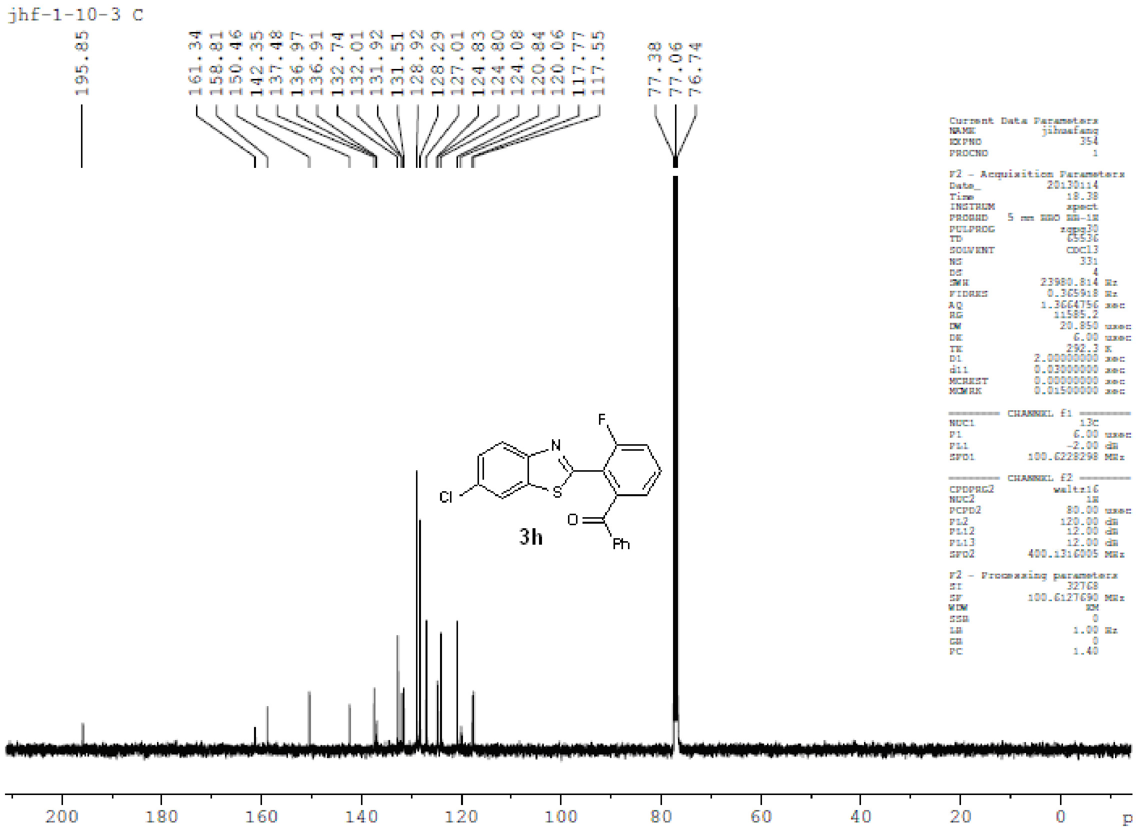


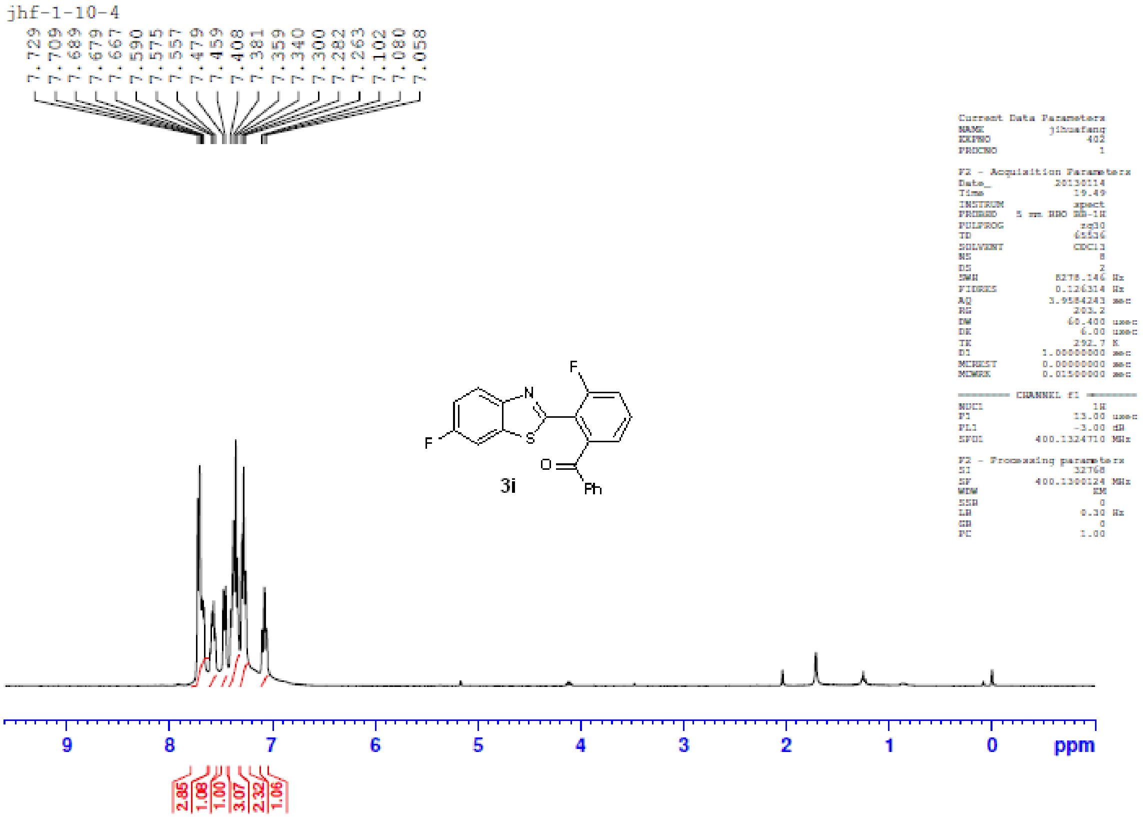
```
Current Data Parameters
NAME             jihuafang
EXPNO                  353
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130114
Time                 18.23
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     224
DS                       4
SWH              23980.814 Hz
FIDRES            0.365918 Hz
AQ               1.3664756 sec
RG                    8192
DW                  20.850 usec
DE                    6.00 usec
TE                   292.3 K
D1              2.00000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                    6.00 usec
PL1                  -2.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                 120.00 dB
PL12                 12.00 dB
PL13                 12.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF             100.6127690 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

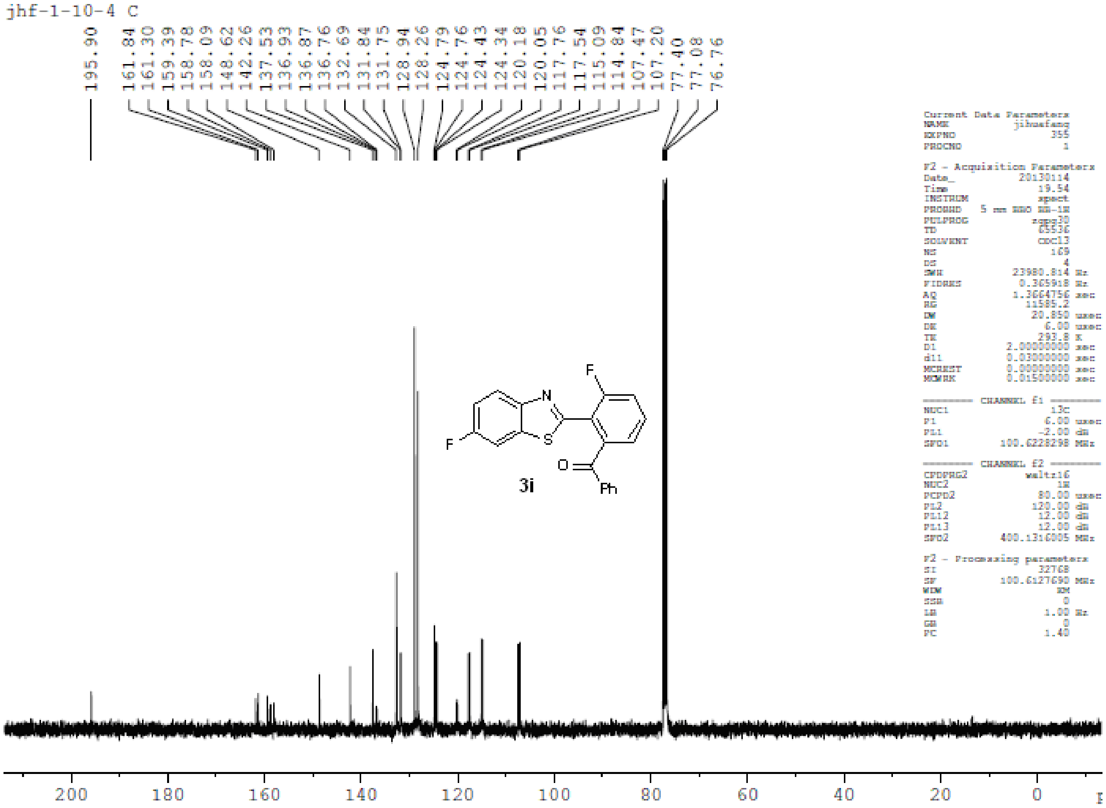

jhf-1-10-6
7.725
7.706
7.639
7.619
7.573
7.551
7.532
7.396
7.372
7.349
7.332
7.282
7.263
7.244
7.162
7.141
2.411
F
N
S
O
Ph
3g
Current Data Parameters
NAME jihuafang
EXPNO 404
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 20.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.00 usec
TE 291.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.91
1.03
2.14
3.11
2.21
1.12
3.00

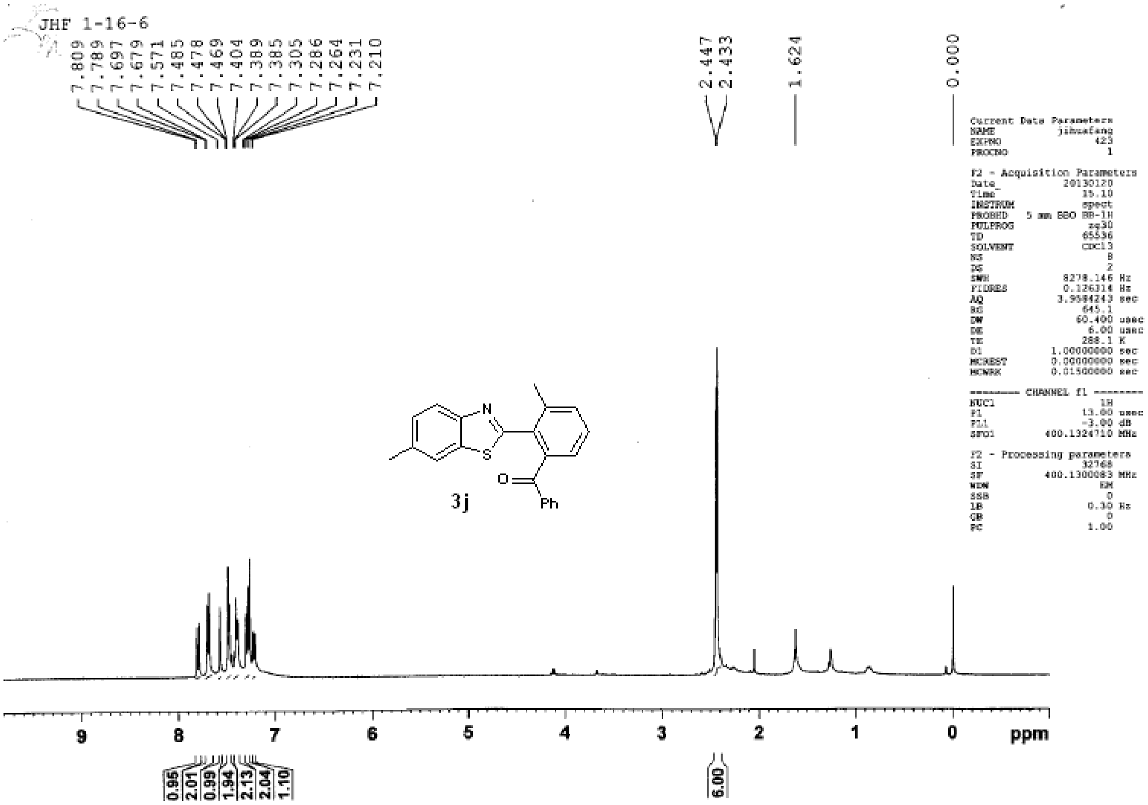

jhf-1-10-6
196.08
161.26
158.73
157.12
157.08
150.15
142.29
137.64
136.03
135.77
132.55
131.51
131.42
128.91
128.20
127.77
124.70
124.67
122.85
120.86
120.61
120.47
117.69
117.47
77.39
77.07
76.76
21.59
F
N
S
O
Ph
3g
Current Data Parameters
NAME jihuafang
EXPNO 357
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 20.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 205
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 293.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm


jhf-1-10-3
7.776
7.725
7.706
7.658
7.636
7.625
7.606
7.591
7.573
7.419
7.387
7.366
7.346
7.333
7.306
7.287
7.268
1.660
F
N
S
Cl
O
Ph
3h
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.04
1.09
1.17
6.35
Current Data Parameters

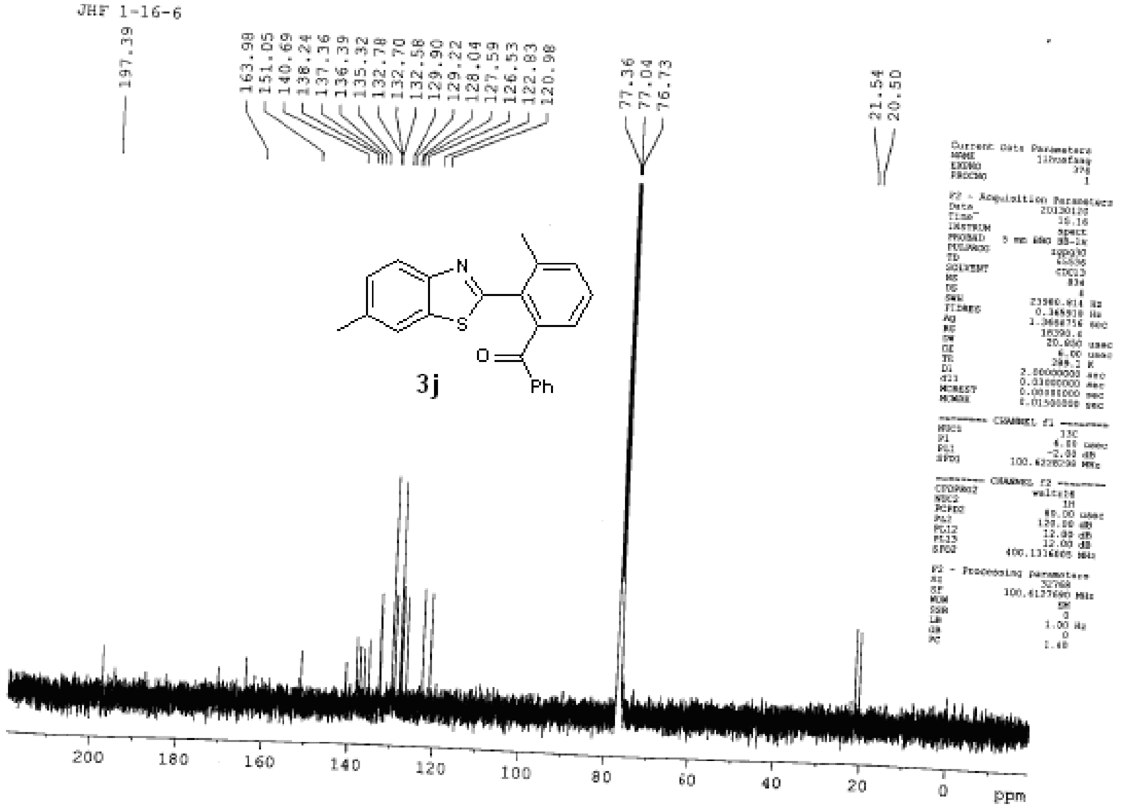

jhf-1-10-3 C
195.85
161.34
158.81
150.46
142.35
137.48
136.97
136.91
132.74
132.01
131.92
131.51
128.92
128.29
127.01
124.83
124.80
124.08
120.84
120.06
117.77
117.55
77.38
77.06
76.74
F
N
S
Cl
O
Ph
3h
200
180
160
140
120
100
80
60
40
20
0
p
Current Data Parameters

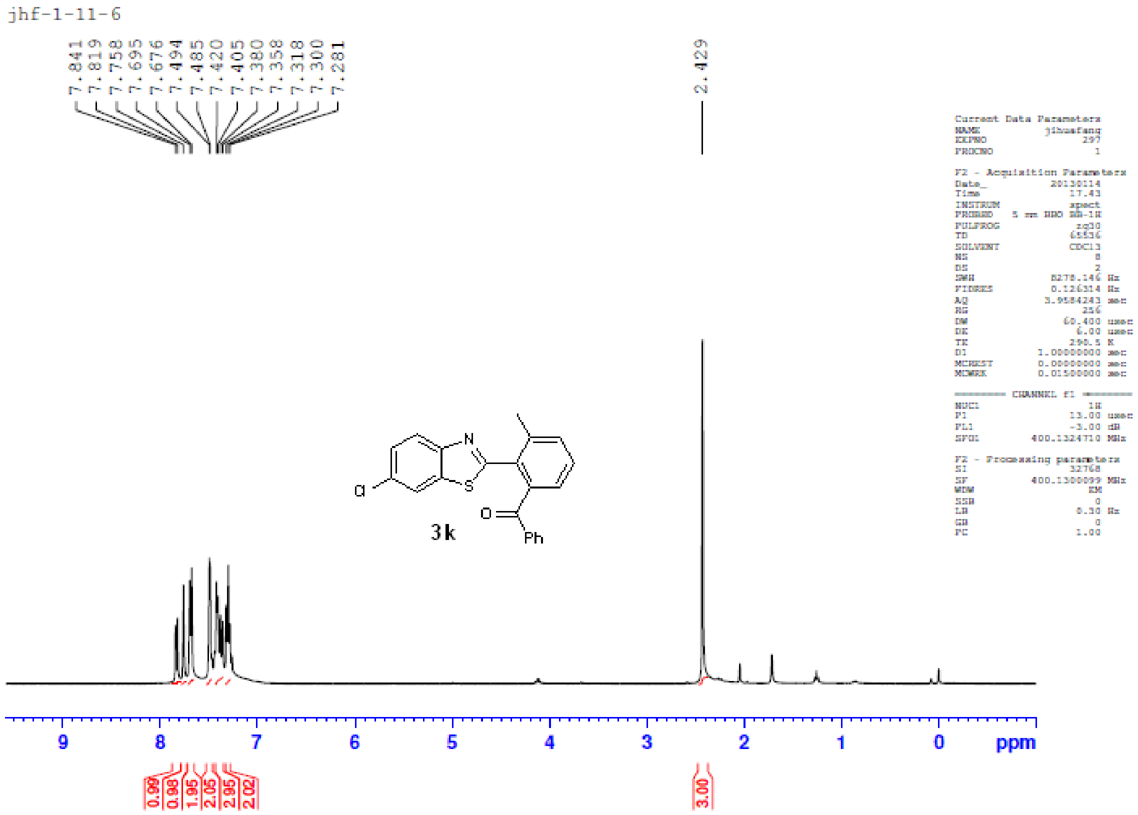

jhf-1-10-4
7.729
7.709
7.689
7.679
7.667
7.590
7.575
7.557
7.479
7.459
7.408
7.381
7.359
7.340
7.300
7.282
7.263
7.102
7.080
7.058
Current Data Parameters
NAME jihuafang
EXPNO 402
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 19.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 203.2
DW 60.400 usec
DE 6.00 usec
TE 292.7 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300124 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
F
N
S
F
O
Ph
3i
9
8
7
6
5
4
3
2
1
0
ppm
2.85
1.08
1.00
3.07
2.32
1.06

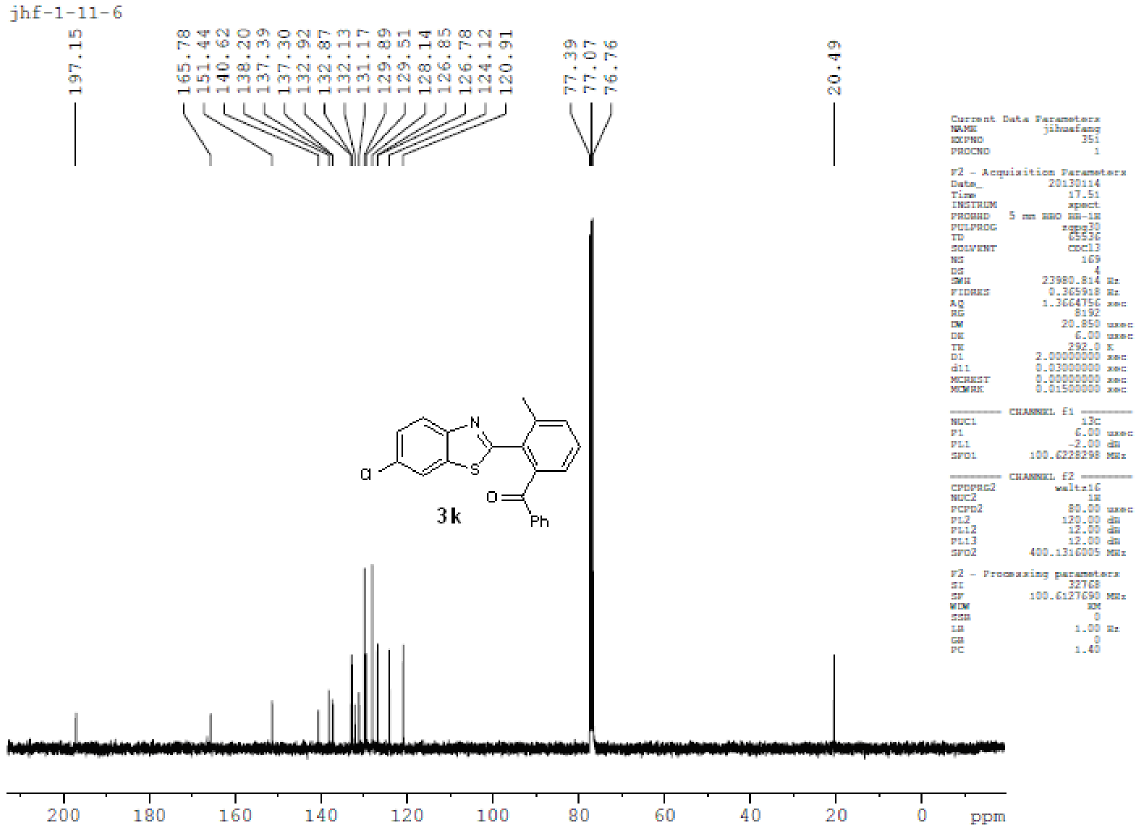

jhf-1-10-4 C
195.90
161.84
161.30
159.39
158.78
158.09
148.62
142.26
137.53
136.93
136.87
136.76
132.69
131.84
131.75
128.94
128.26
124.79
124.76
124.43
124.34
120.18
120.05
117.76
117.54
115.09
114.84
107.47
107.20
77.40
77.08
76.76
Current Data Parameters
NAME jihuafang
EXPNO 355
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 19.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 169
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 293.8 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
F
N
S
F
O
Ph
3i
200
180
160
140
120
100
80
60
40
20
0

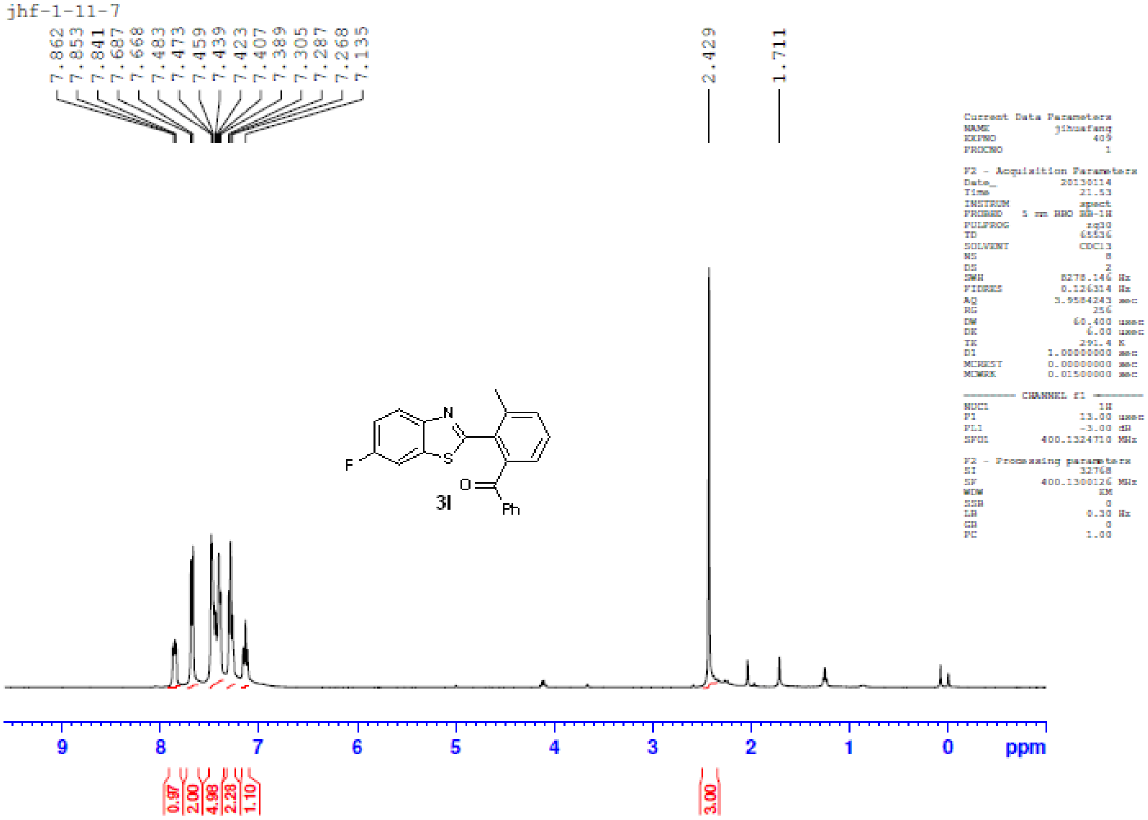


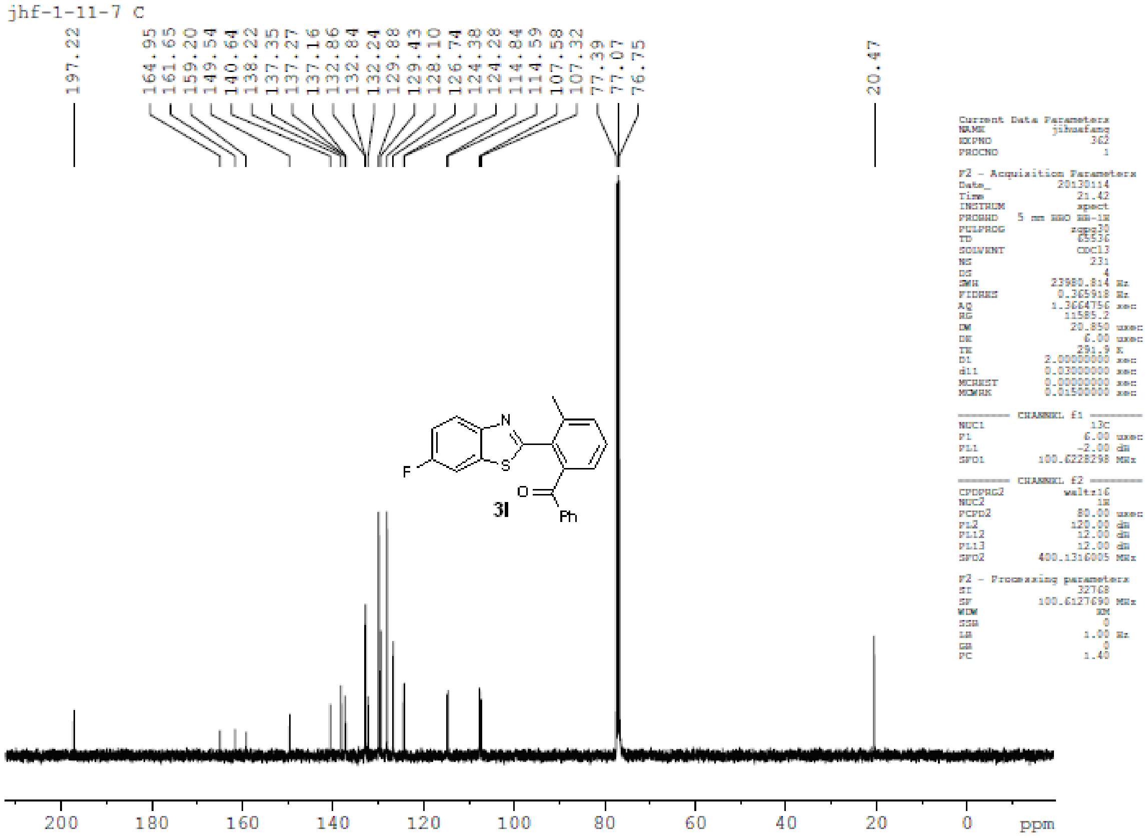
```
Current Data Parameters
NAME             jihuafang
EXPNO                  423
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130120
Time                 15.10
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8278.146 Hz
FIDRES            0.126314 Hz
AQ               3.9584243 sec
RG                   645.1
DW                  60.400 usec
DE                    6.00 usec
TE                   288.1 K
D1              1.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   13.00 usec
PL1                  -3.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                   32768
SF             400.1300083 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

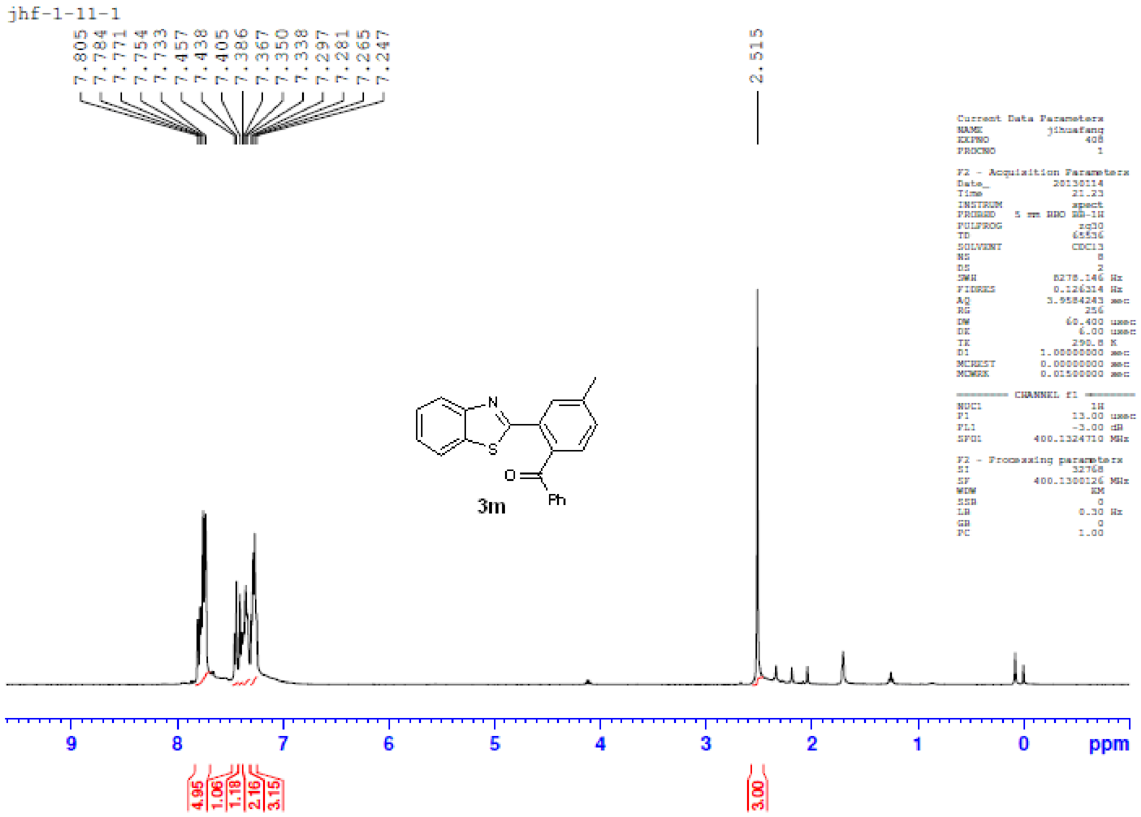


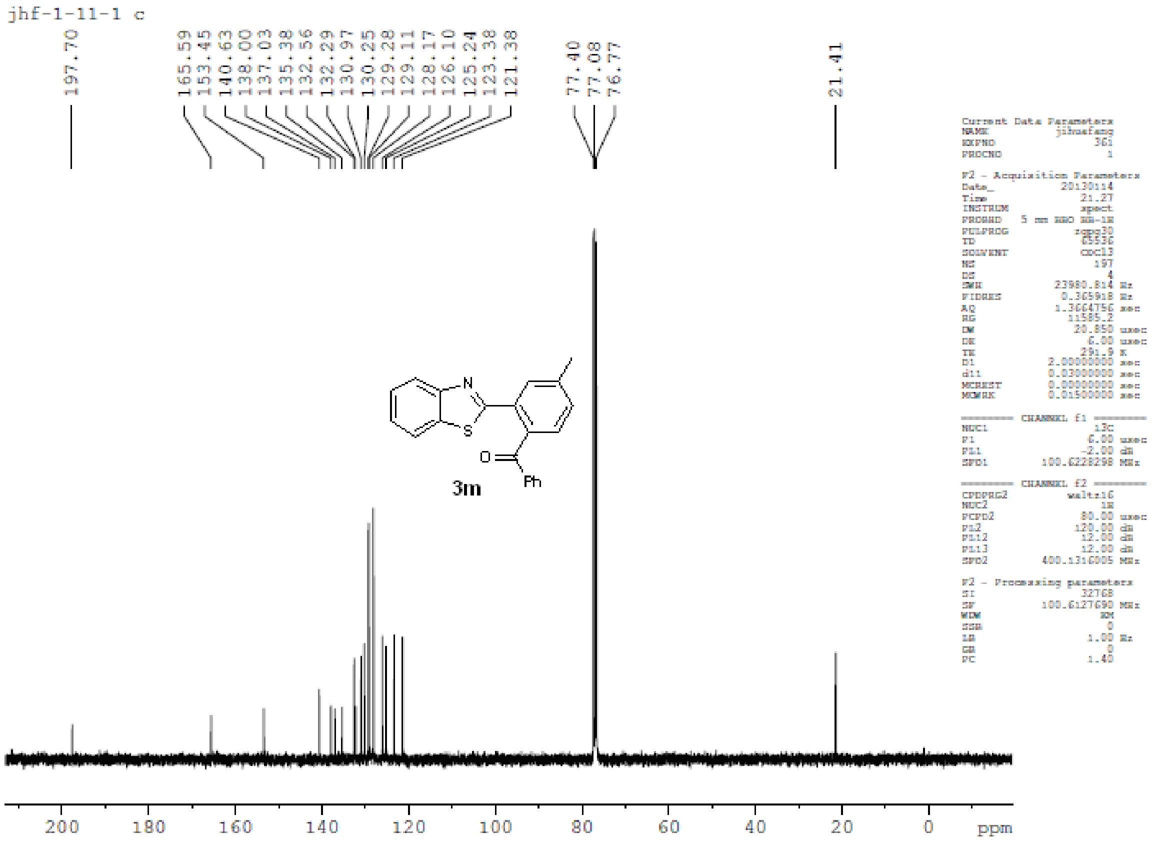

jhf-1-11-6
7.841
7.819
7.758
7.695
7.676
7.494
7.485
7.420
7.405
7.380
7.358
7.318
7.300
7.281
2.429
Current Data Parameters
NAME jihuafang
EXPNO 297
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 17.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 298.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
S
Cl
O
Ph
3k
9
8
7
6
5
4
3
2
1
0
ppm
0.99
0.98
1.95
2.05
2.95
2.02
3.00

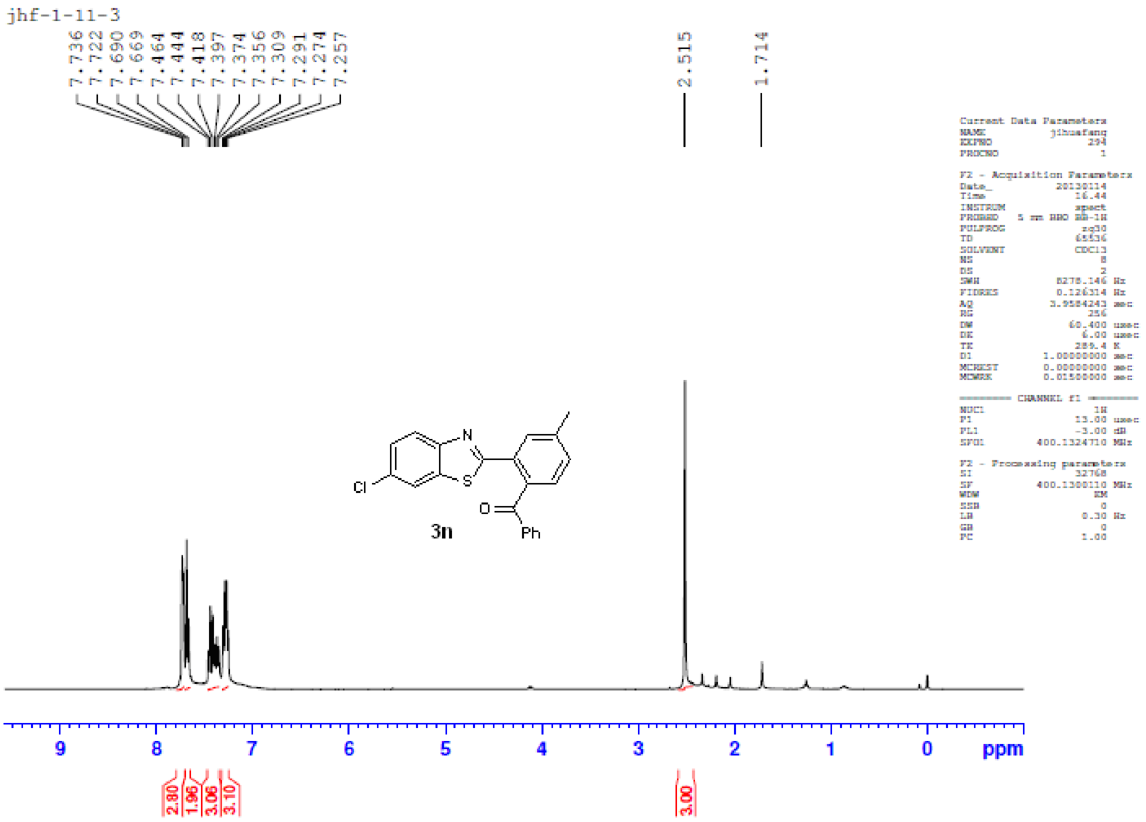

jhf-1-11-6
197.15
165.78
151.44
140.62
138.20
137.39
137.30
132.92
132.87
132.13
131.17
129.89
129.51
128.14
126.85
126.78
124.12
120.91
77.39
77.07
76.76
20.49
Current Data Parameters
NAME jihuafang
EXPNO 351
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 17.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 169
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 292.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
S
Cl
O
Ph
3k
200
180
160
140
120
100
80
60
40
20
0
ppm


jhf-1-11-7
7.862
7.853
7.841
7.687
7.668
7.483
7.473
7.459
7.439
7.423
7.407
7.389
7.305
7.287
7.268
7.135
2.429
1.711
Current Data Parameters
NAME jihuafang
EXPNO 409
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 21.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 291.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
S
F
O
Ph
3l
9
8
7
6
5
4
3
2
1
0
ppm
0.97
2.00
4.98
2.28
1.10
3.00

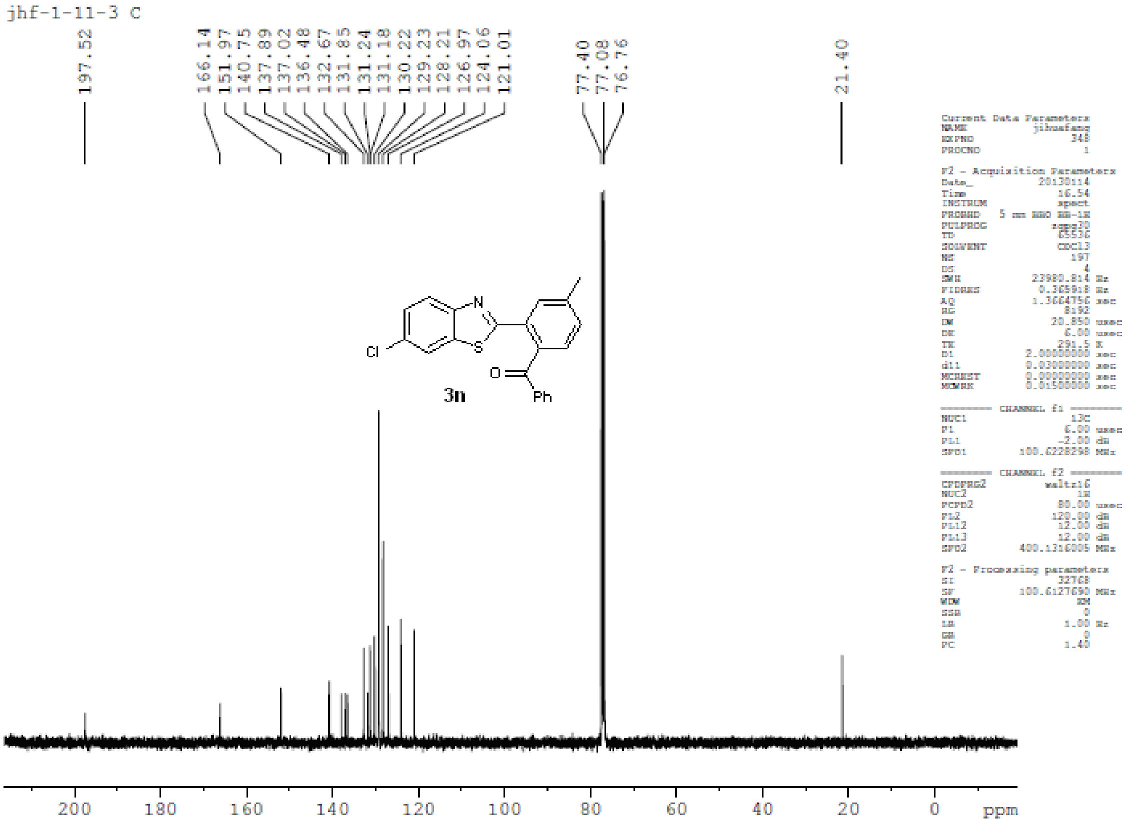

jhf-1-11-7 C
197.22
164.95
161.65
159.20
149.54
140.64
138.22
137.35
137.27
137.16
132.86
132.84
132.24
129.88
129.43
128.10
126.74
124.38
124.28
114.84
114.59
107.58
107.32
77.39
77.07
76.75
20.47
Current Data Parameters
NAME jihuafang
EXPNO 362
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 21.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 231
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 291.9 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
S
F
O
Ph
3l
200
180
160
140
120
100
80
60
40
20
0
ppm


jhf-1-11-1
7.805
7.784
7.771
7.754
7.733
7.457
7.438
7.405
7.386
7.367
7.350
7.338
7.297
7.281
7.265
7.247
2.515
N
S
O
Ph
3m
4.95
1.06
1.18
2.16
3.15
3.00
9
8
7
6
5
4
3
2
1
0
ppm
Current Data Parameters
NAME jihuafang
EXPNO 408
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 21.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 290.8 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

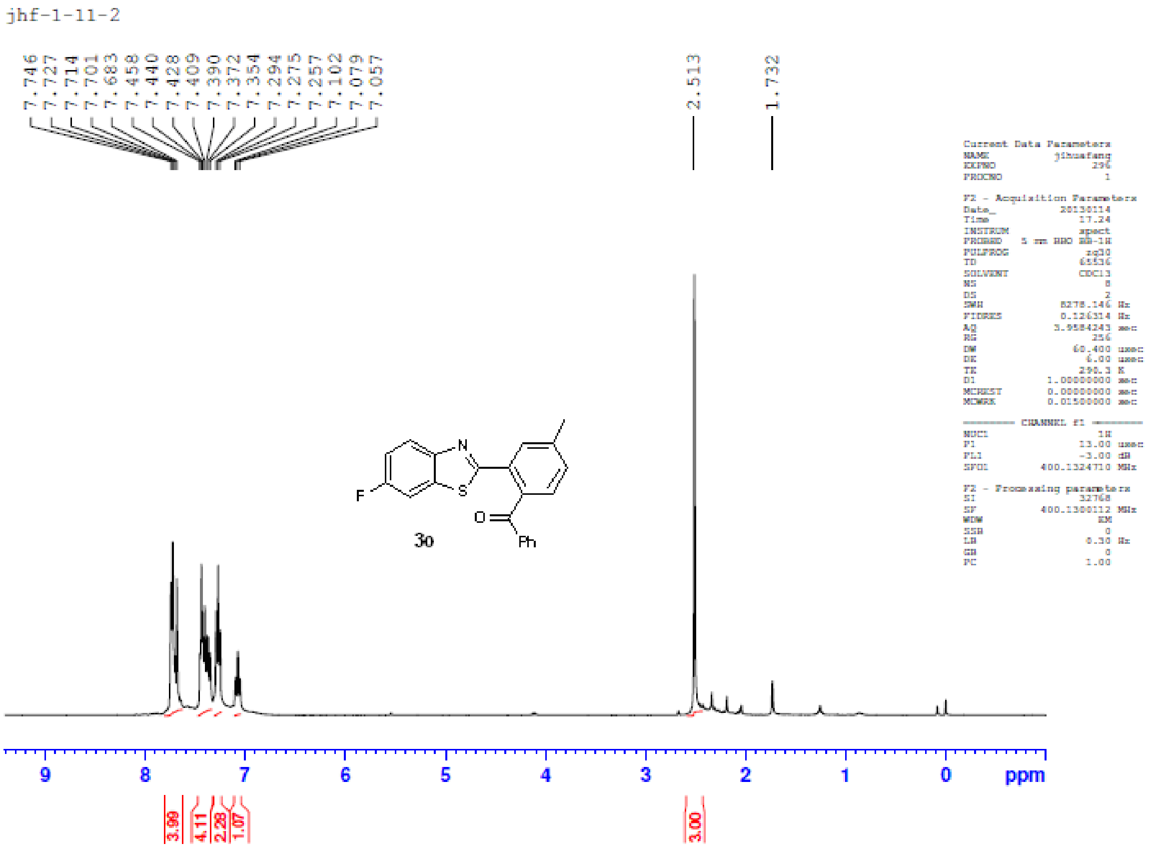

jhf-1-11-1 c
197.70
165.59
153.45
140.63
138.00
137.03
135.38
132.56
132.29
130.97
130.25
129.28
129.11
128.17
126.10
125.24
123.38
121.38
77.40
77.08
76.77
21.41
N
S
O
Ph
3m
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME jihuafang
EXPNO 361
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 21.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 197
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 11585.2
DW 20.850 usec
DE 6.00 usec
TE 291.9 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

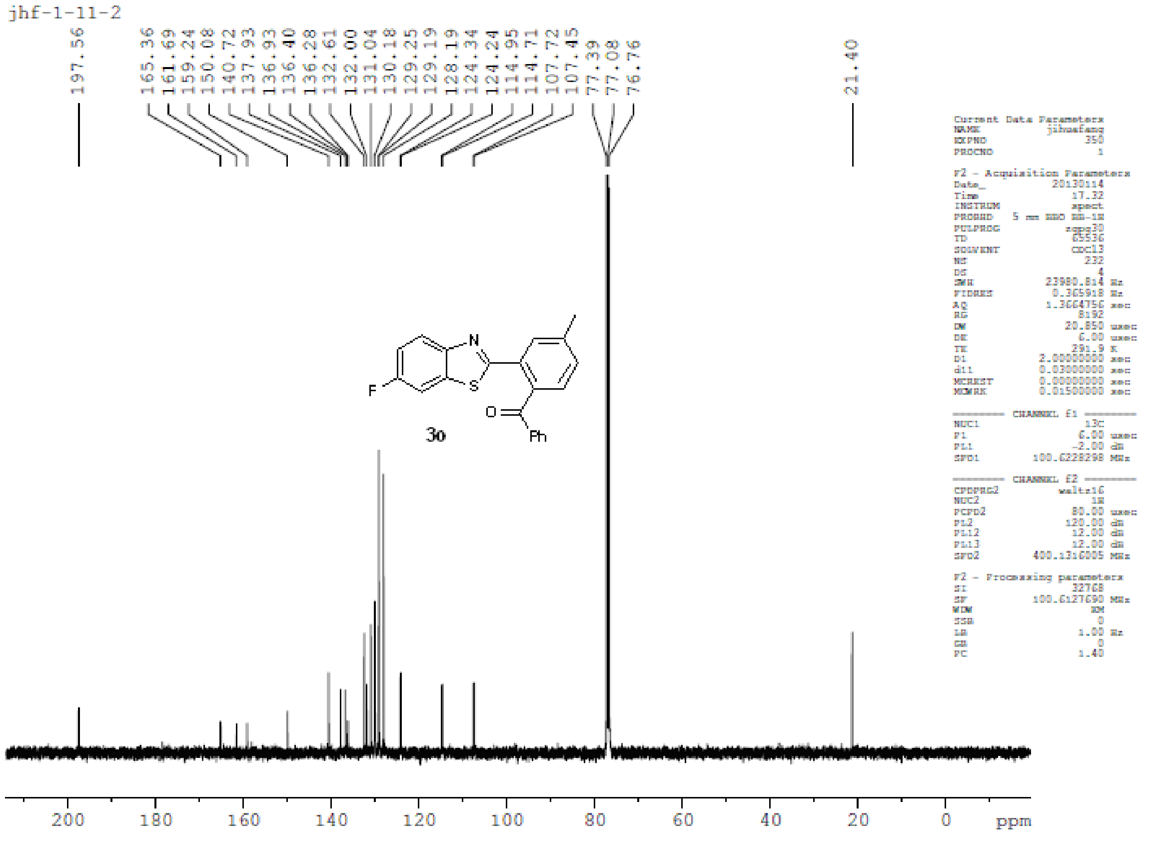


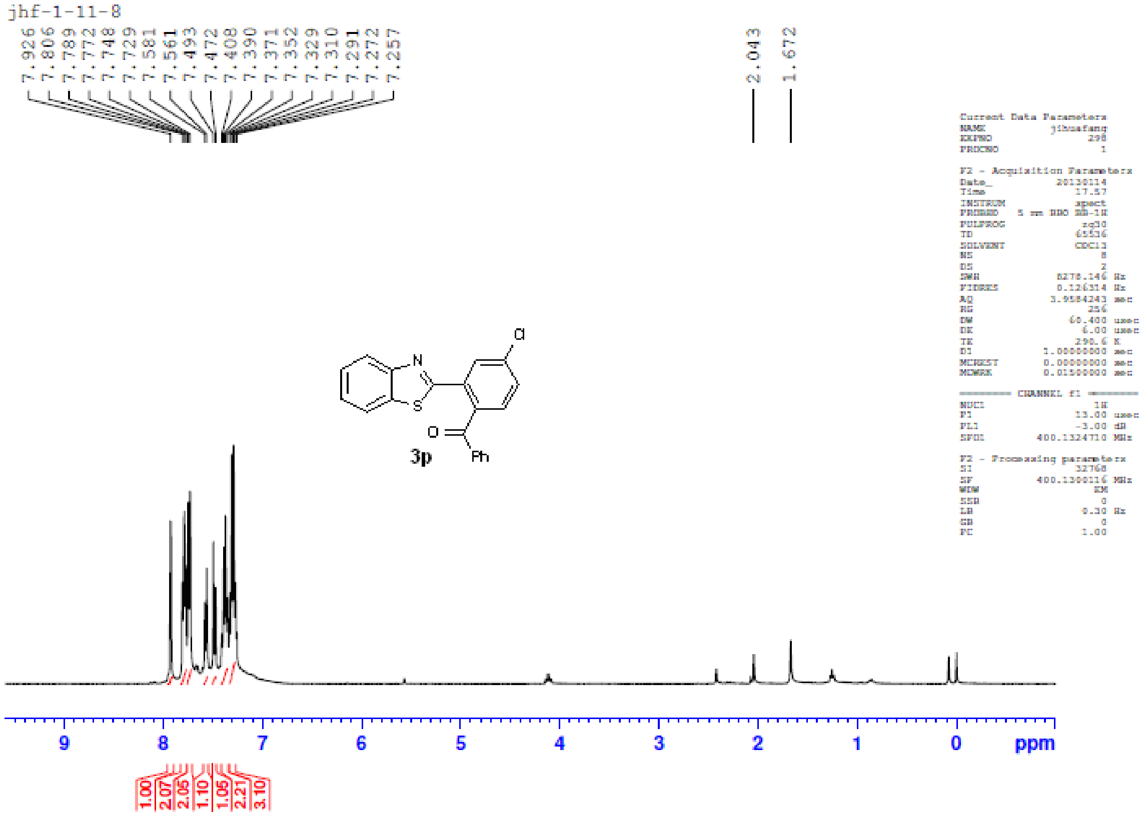
```
Current Data Parameters
NAME             jihuafang
EXPNO                  294
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130114
Time                 16.44
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ            3.9584243 sec
RG                     256
DW              60.400 usec
DE                6.00 usec
TE               289.4 K
D1          1.00000000 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1               13.00 usec
PL1              -3.00 dB
SFO1       400.1324710 MHz

F2 - Processing parameters
SI                   32768
SF         400.1300110 MHz
WDW                     EM
SSB                      0
LB                0.30 Hz
GB                       0
PC                    1.00
```



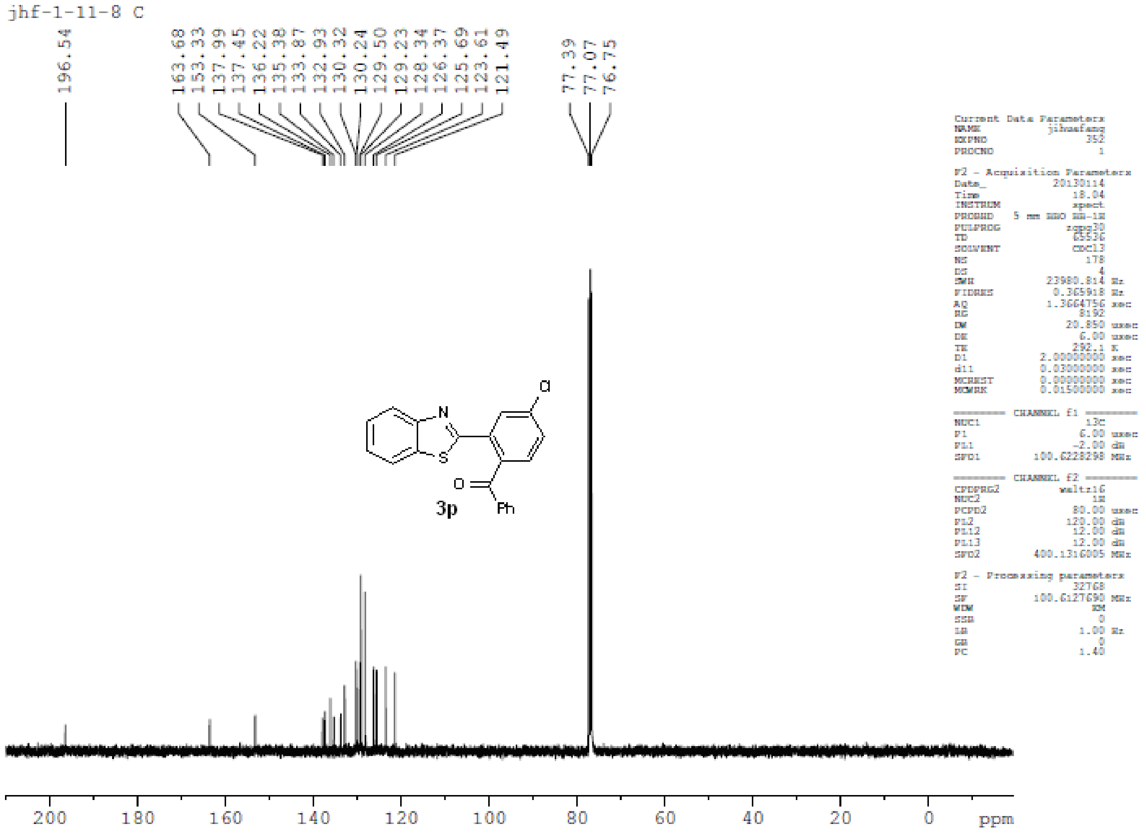
```
Current Data Parameters
NAME             jihuafang
EXPNO                  348
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130114
Time                 16.54
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     197
DS                       4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                    8192
DW              20.850 usec
DE                6.00 usec
TE               291.5 K
D1          2.00000000 sec
d11         0.03000000 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                6.00 usec
PL1              -2.00 dB
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2            80.00 usec
PL2             120.00 dB
PL12             12.00 dB
PL13             12.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF         100.6127690 MHz
WDW                     EM
SSB                      0
LB                1.00 Hz
GB                       0
PC                    1.40
```


jhf-1-11-2
7.746
7.727
7.714
7.701
7.683
7.458
7.440
7.428
7.409
7.390
7.372
7.354
7.294
7.275
7.257
7.102
7.079
7.057
2.513
1.732
F
N
S
O
Ph
3o
Current Data Parameters
NAME jihuafang
EXPNO 296
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 17.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 290.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
3.99
4.11
2.28
1.07
3.00

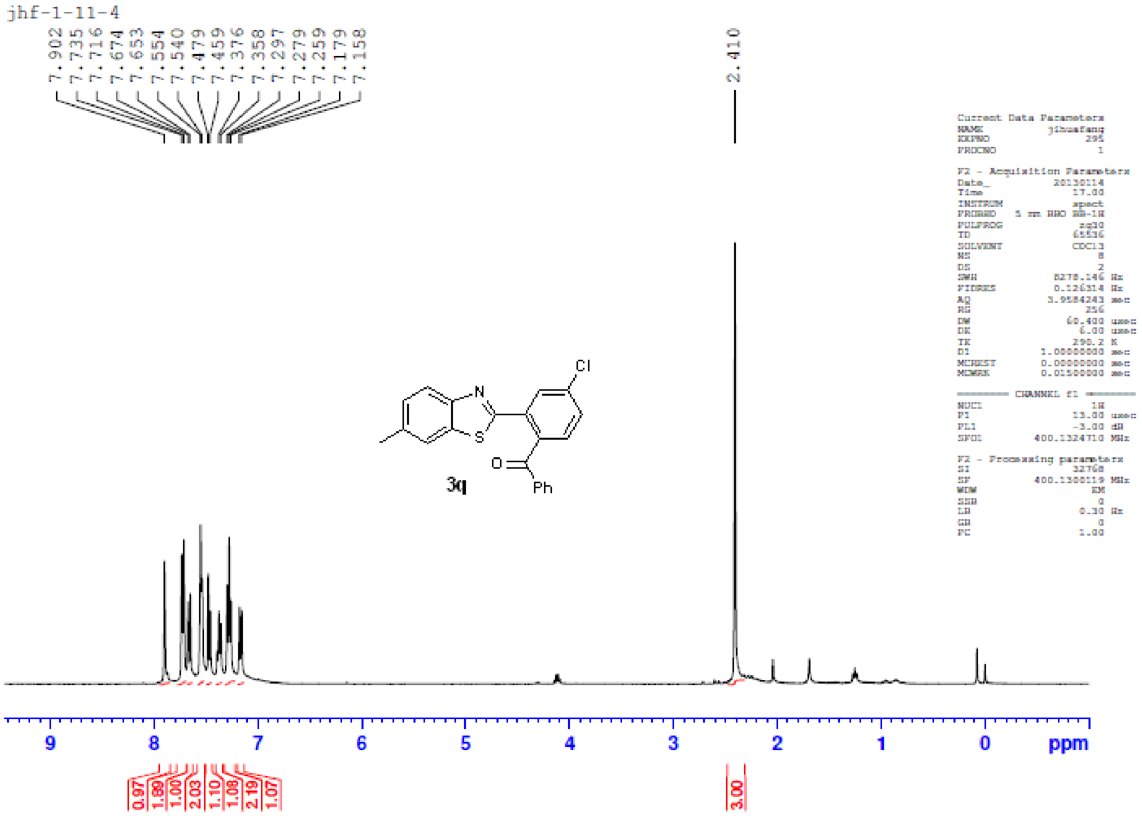

jhf-1-11-2
197.56
165.36
161.69
159.24
150.08
140.72
137.93
136.93
136.40
136.28
132.61
132.00
131.04
130.18
129.25
129.19
128.19
124.34
124.24
114.95
114.71
107.72
107.45
77.39
77.08
76.76
21.40
F
N
S
O
Ph
3o
Current Data Parameters
NAME jihuafang
EXPNO 350
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 17.32
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 232
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 291.9 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

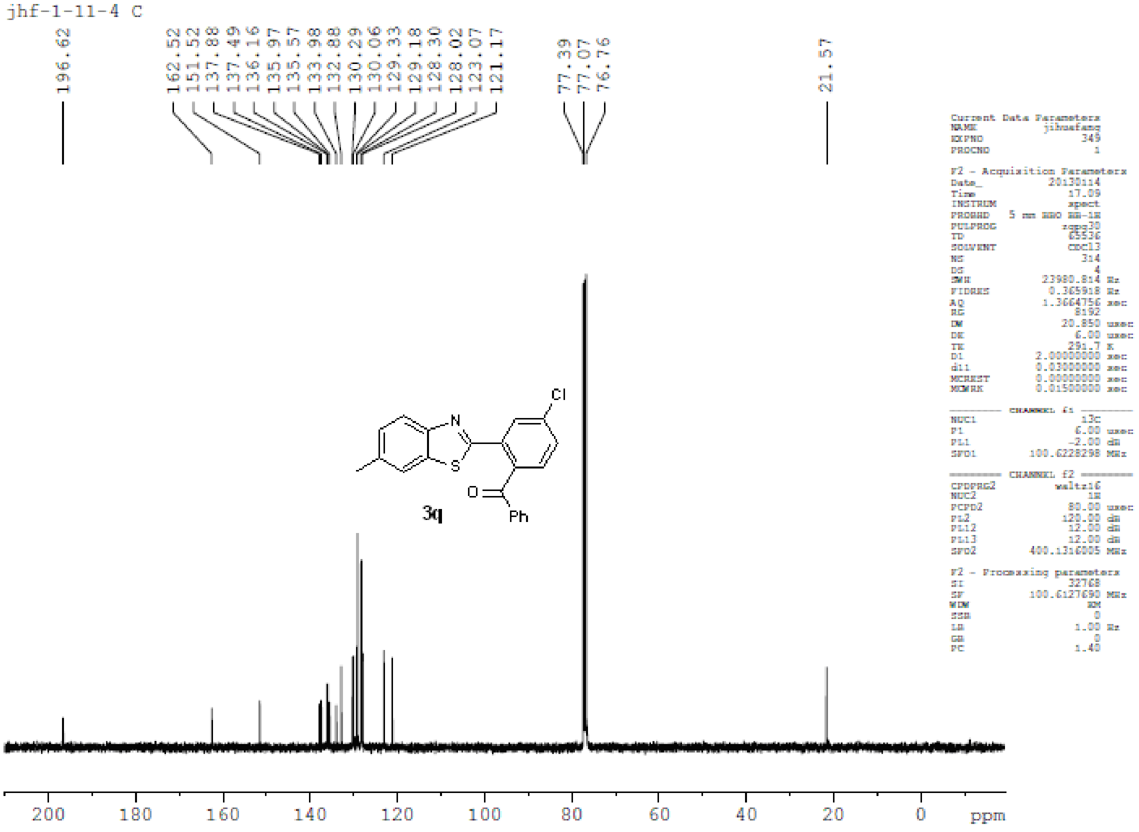


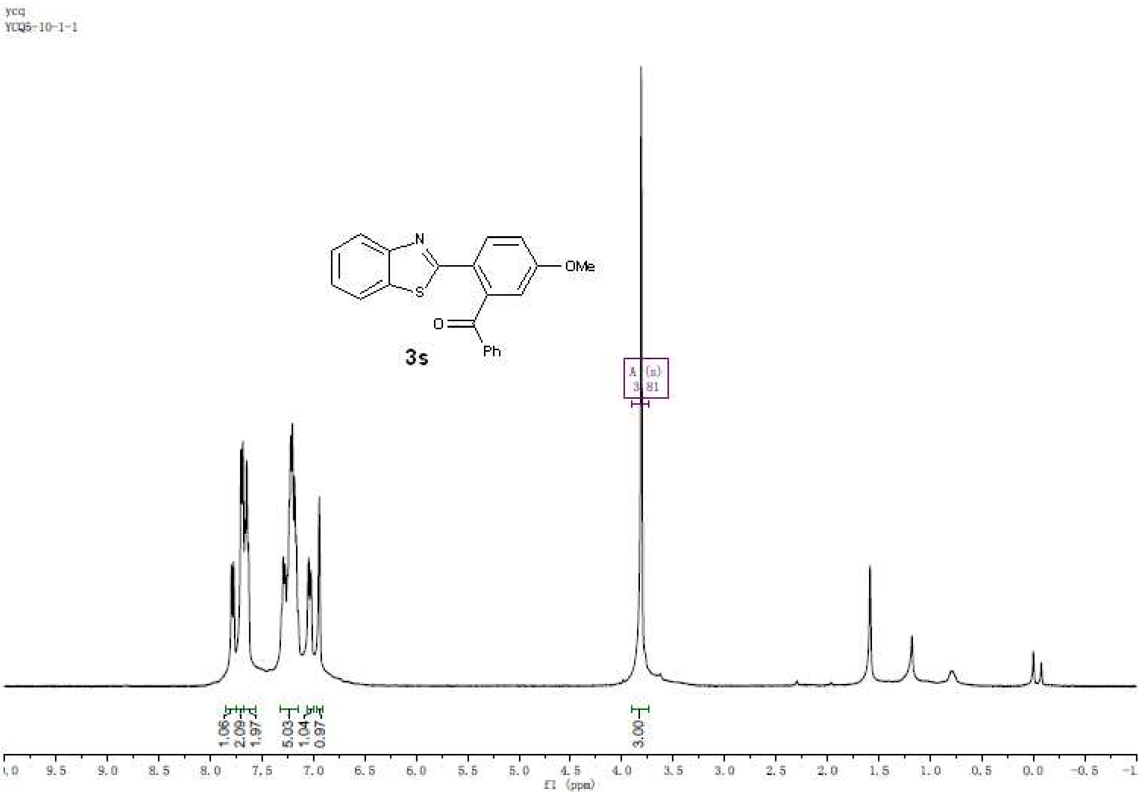
```
Current Data Parameters
NAME              jihuafang
EXPNO                   298
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130114
Time                  17.57
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8278.146 Hz
FIDRES             0.126314 Hz
AQ                3.9584243 sec
RG                      256
DW                   60.400 usec
DE                     6.00 usec
TE                    290.6 K
D1               1.00000000 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    13.00 usec
PL1                   -3.00 dB
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF              400.1300116 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

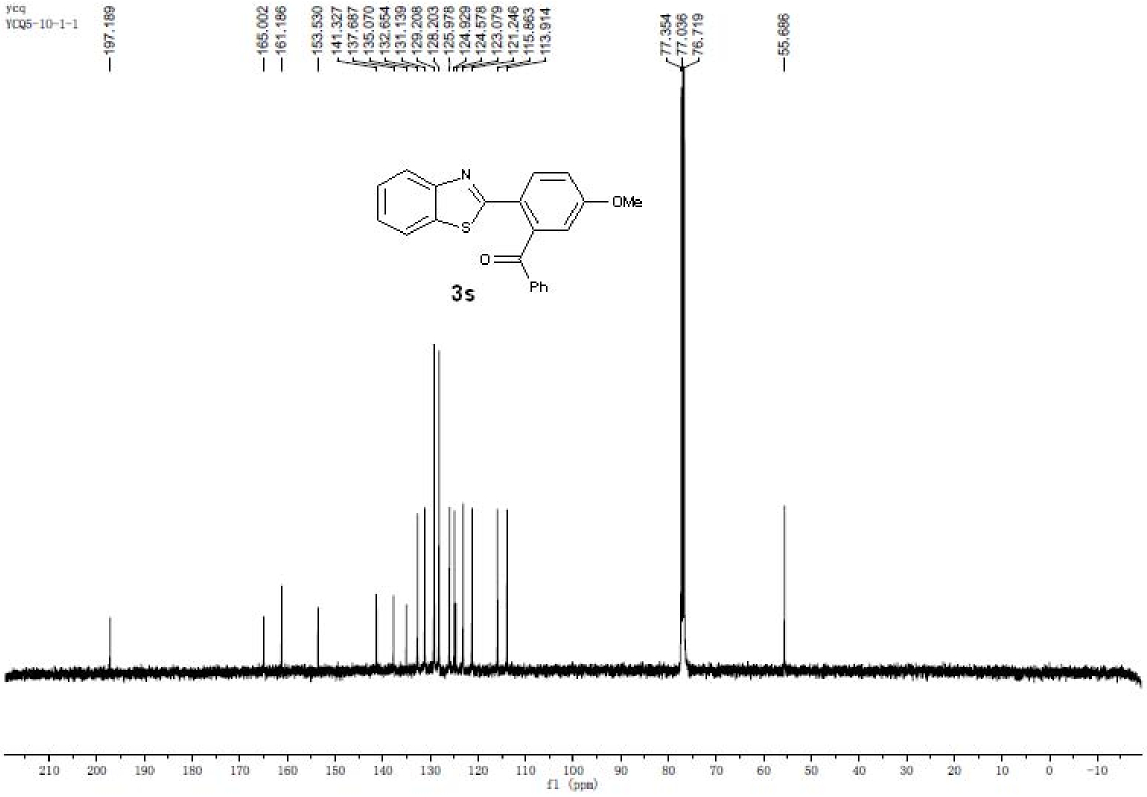


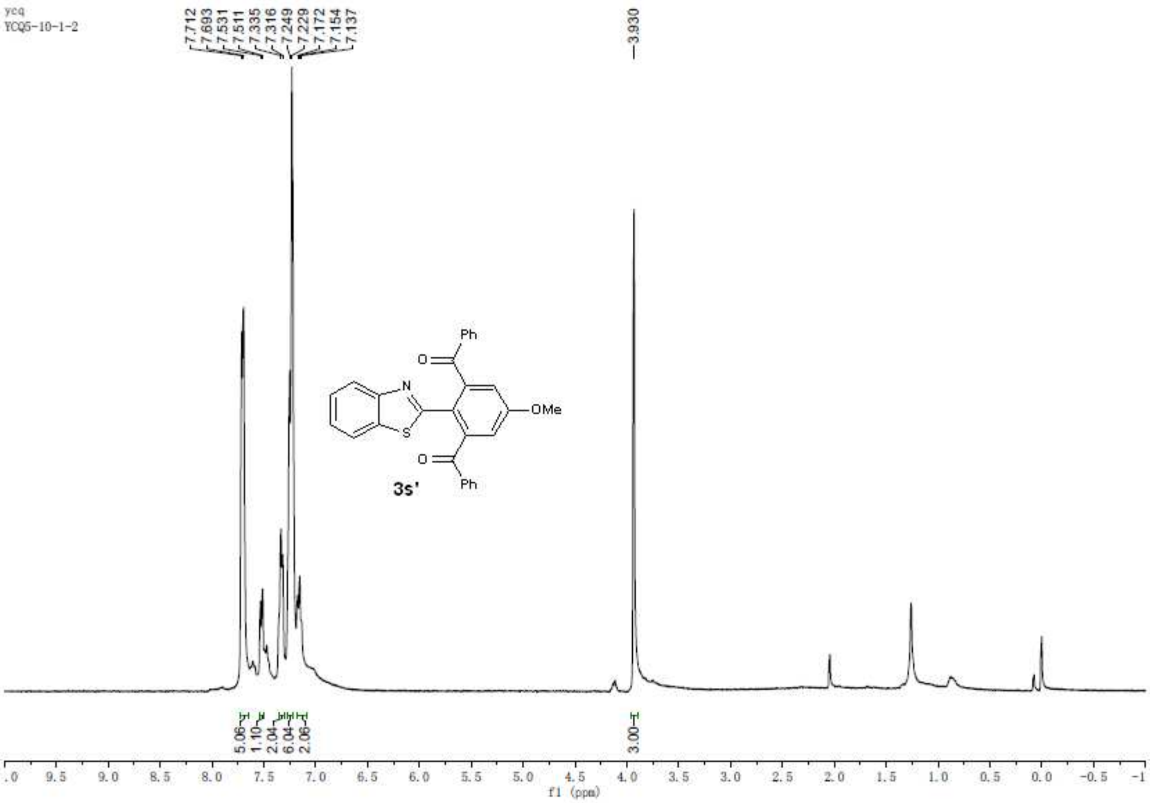
```
Current Data Parameters
NAME              jihuafang
EXPNO                   352
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130114
Time                  18.04
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      178
DS                        4
SWH               23980.814 Hz
FIDRES             0.365918 Hz
AQ                1.3664756 sec
RG                     8192
DW                   20.850 usec
DE                     6.00 usec
TE                    292.1 K
D1               2.00000000 sec
d11              0.03000000 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                     6.00 usec
PL1                   -2.00 dB
SFO1            100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                  120.00 dB
PL12                  12.00 dB
PL13                  12.00 dB
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF              100.6127690 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

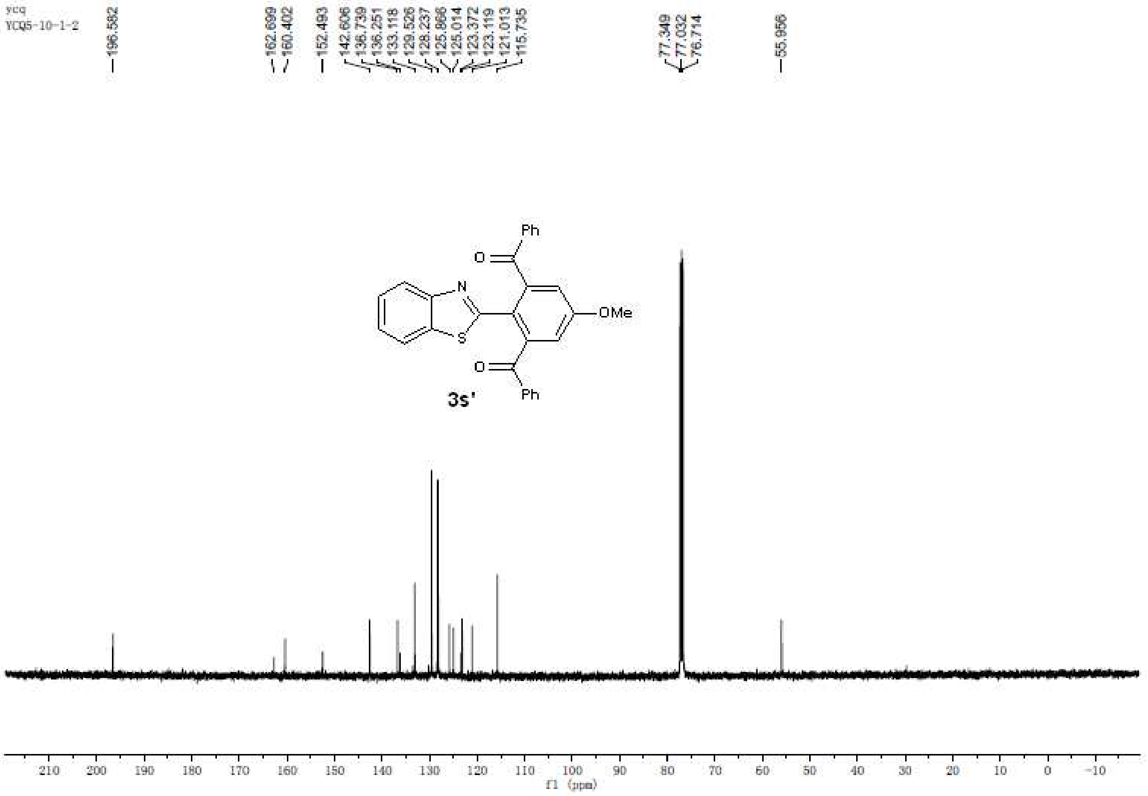

jhf-1-11-4
7.902
7.735
7.716
7.674
7.653
7.554
7.540
7.479
7.459
7.376
7.358
7.297
7.279
7.259
7.179
7.158
2.410
N
S
Cl
O
Ph
3q
Current Data Parameters
NAME jihuafang
EXPNO 295
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 17.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 290.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300119 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
0.97
1.89
1.00
2.03
1.10
1.08
2.19
1.07
3.00

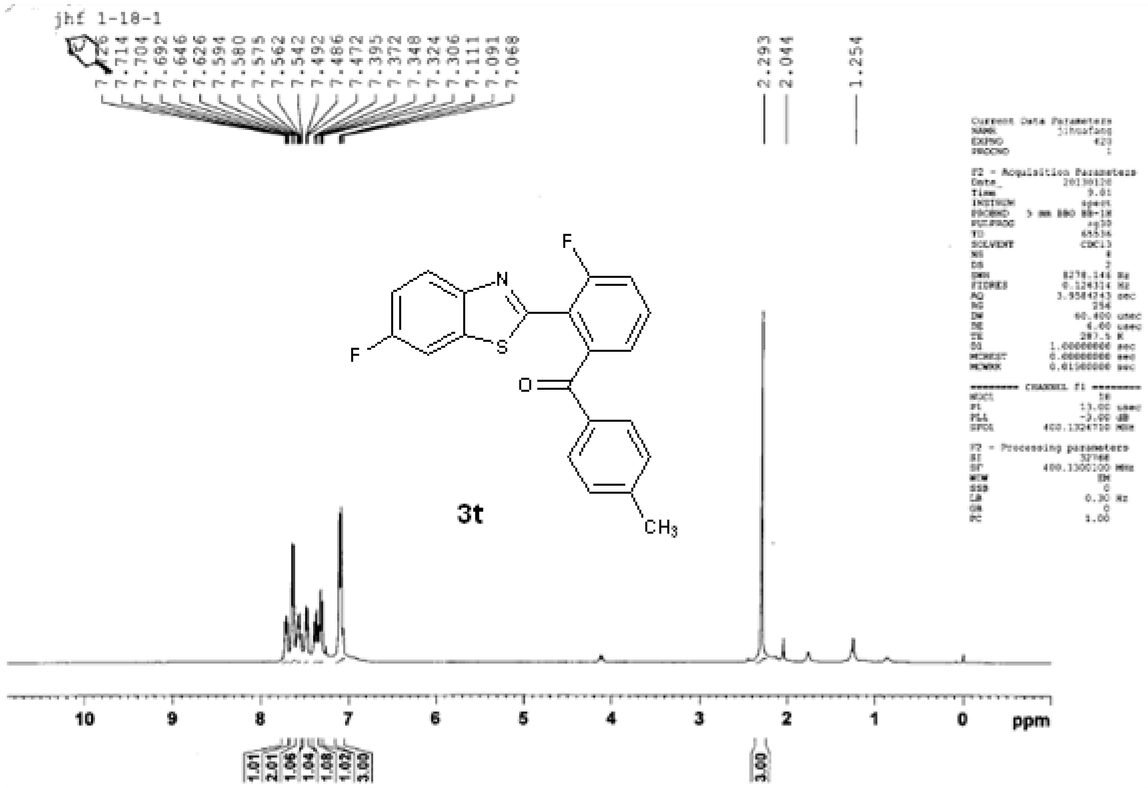

jhf-1-11-4 C
196.62
162.52
151.52
137.88
137.49
136.16
135.97
135.57
133.98
132.88
130.29
130.06
129.33
129.18
128.30
128.02
123.07
121.17
77.39
77.07
76.76
21.57
N
S
Cl
O
Ph
3q
Current Data Parameters
NAME jihuafang
EXPNO 349
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130114
Time 17.09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 314
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 291.7 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.00 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

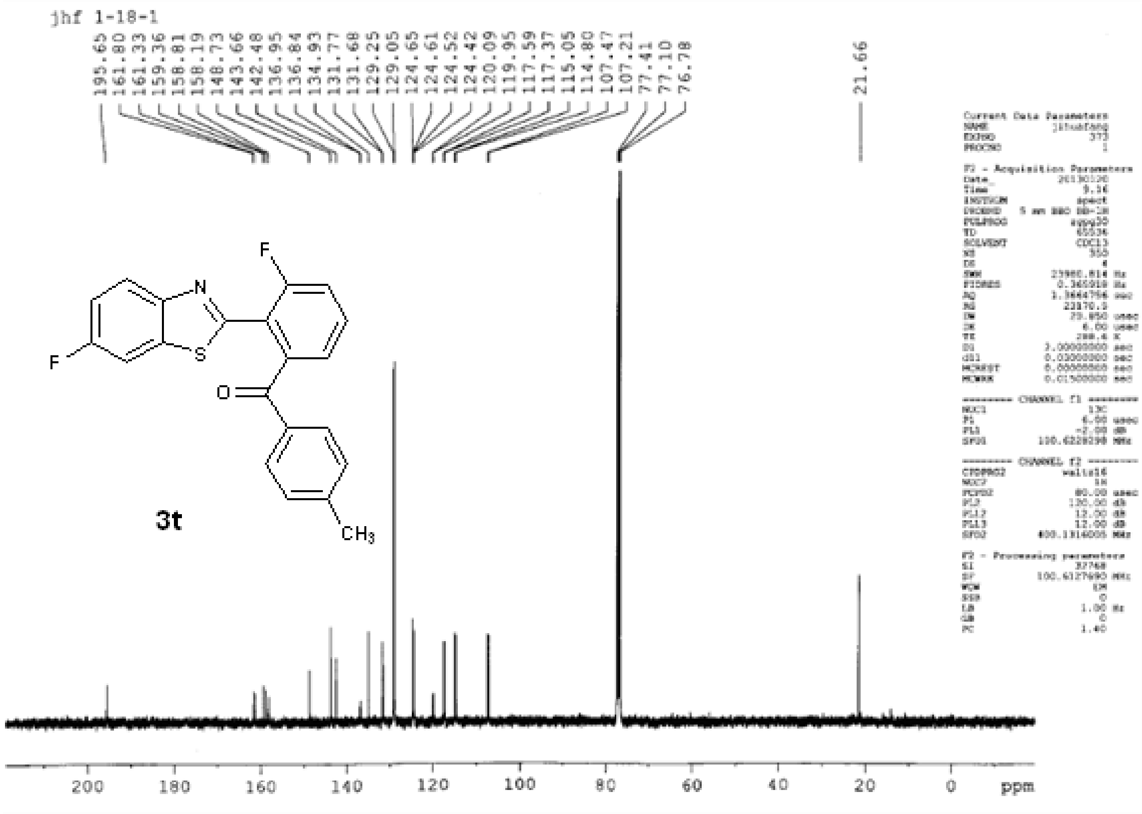

ycq
YCQ5-10-1-1
N
S
OMe
O
Ph
3s
A (s)
3.81
1.06
2.09
1.97
5.03
1.04
0.97
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

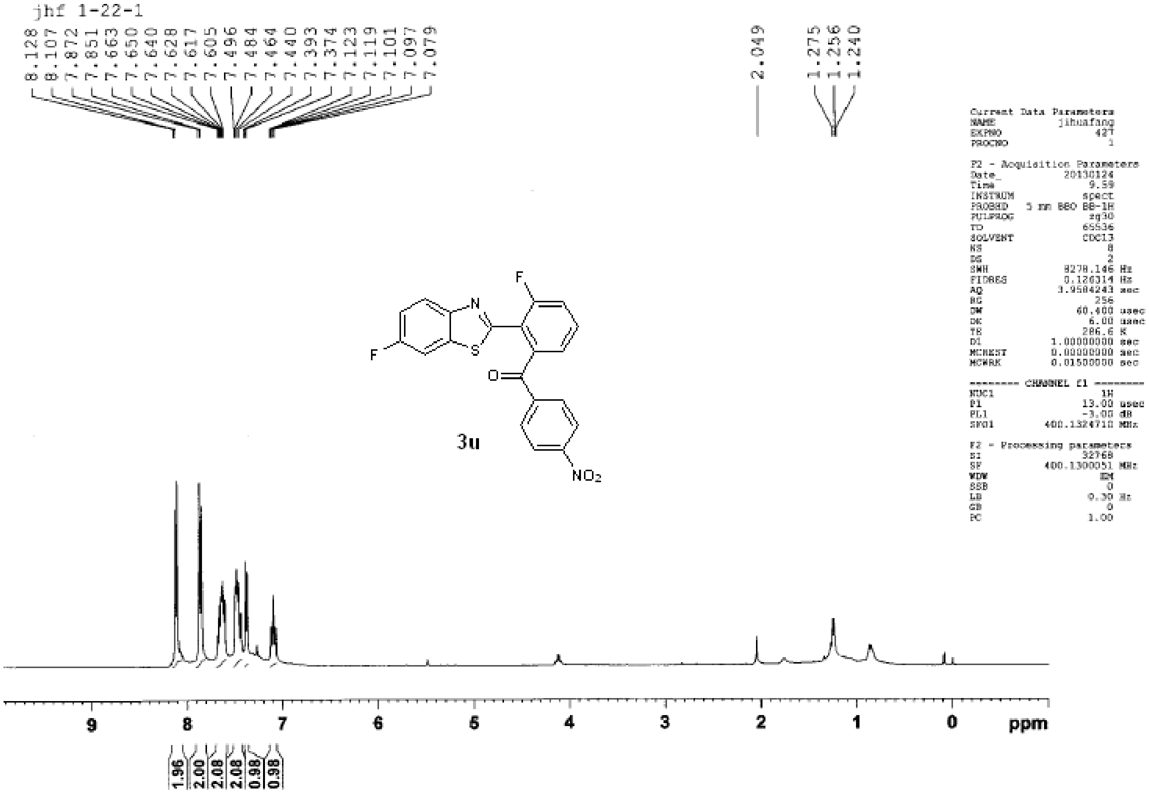

ycq
YCQ5-10-1-1
197.189
165.002
161.186
153.530
141.327
137.687
135.070
132.654
131.139
129.208
128.203
125.978
124.929
124.578
123.079
121.246
115.863
113.914
77.354
77.036
76.719
55.686
N
S
OMe
O
Ph
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


ycq
YCQ5-10-1-2
7.712
7.693
7.531
7.511
7.335
7.316
7.249
7.229
7.172
7.154
7.137
3.930
Ph
O
N
S
OMe
O
Ph
3s'
5.06
1.10
2.04
6.04
2.06
3.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1
f1 (ppm)

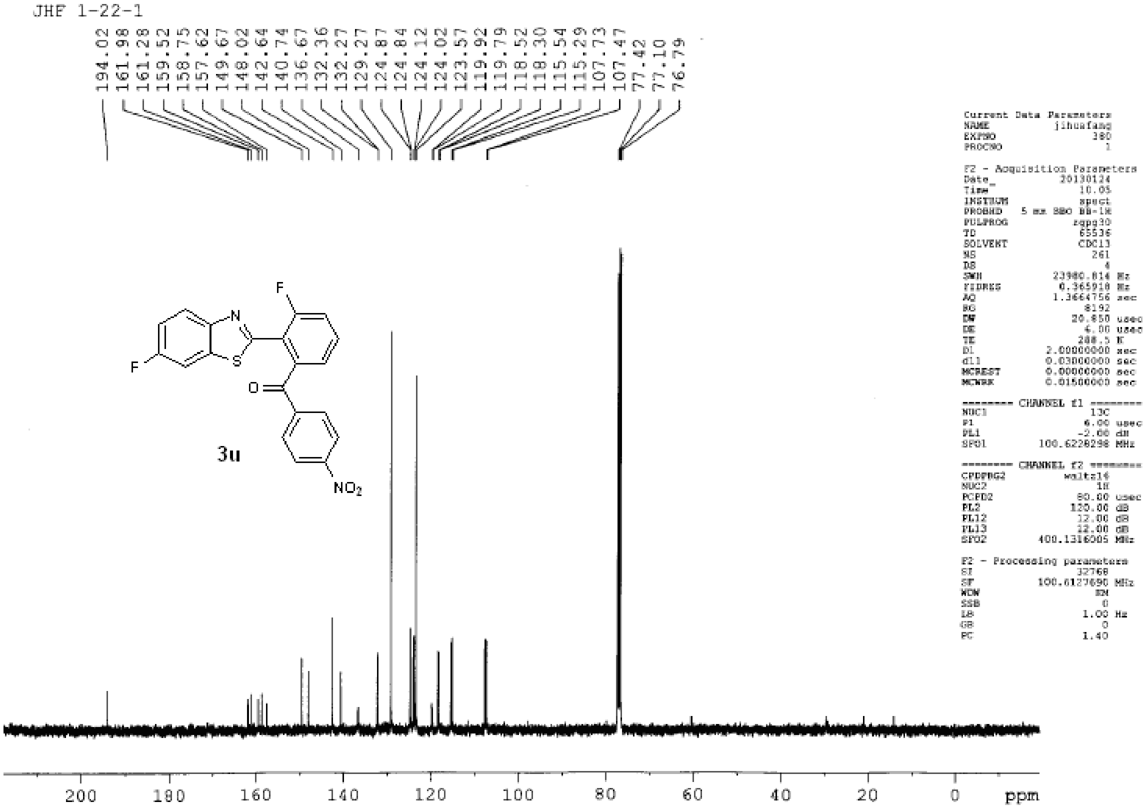

ycq
YCQ5-10-1-2
196.582
162.699
160.402
152.493
142.606
136.739
136.251
133.118
129.526
128.237
125.868
125.014
123.372
123.119
121.013
115.735
77.349
77.032
76.714
55.956
Ph
O
N
S
OMe
O
Ph
3s'
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


jhf 1-18-1
7.726
7.714
7.704
7.692
7.646
7.626
7.594
7.580
7.575
7.562
7.542
7.492
7.486
7.472
7.395
7.372
7.348
7.324
7.306
7.111
7.091
7.068
2.293
2.044
1.254
F
N
S
F
O
CH3
3t
Current Data Parameters
F2 - Acquisition Parameters
CHANNEL f1
F2 - Processing parameters
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
2.01
1.06
1.04
1.04
1.08
1.02
3.00
3.00

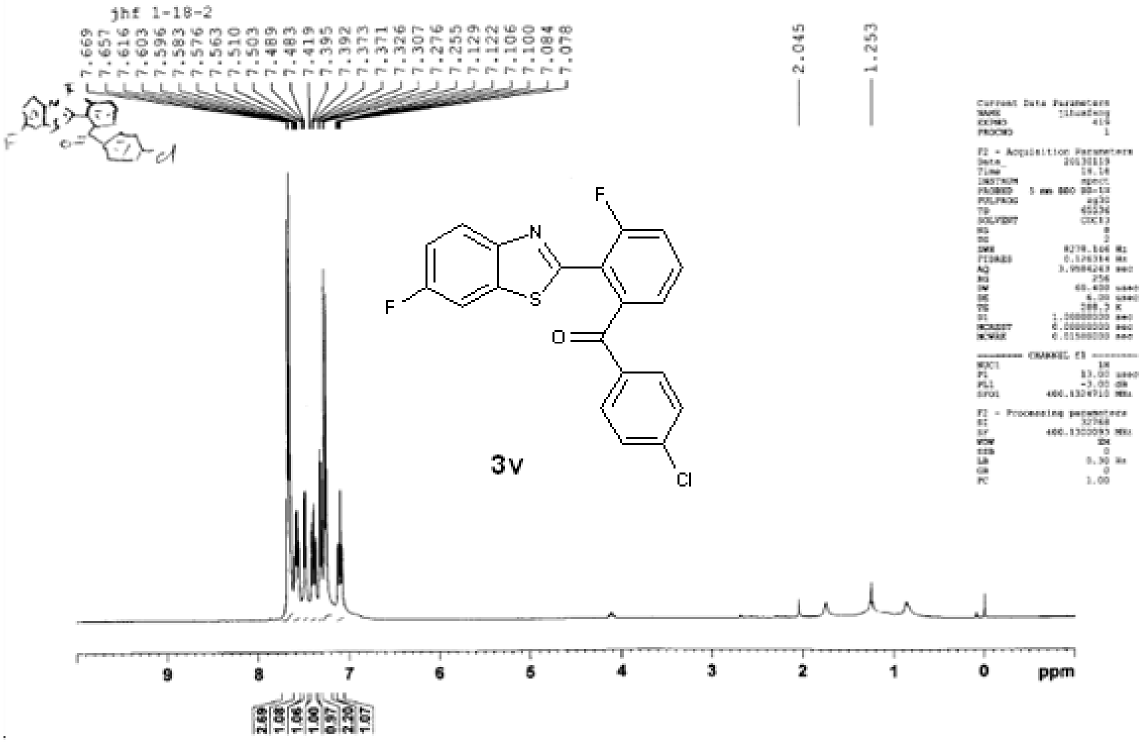

jhf 1-18-1
195.65
161.80
161.33
159.36
158.81
158.19
148.73
143.66
142.48
136.95
136.84
134.93
131.77
131.68
129.25
129.05
124.65
124.61
124.52
124.42
120.09
119.95
117.59
117.37
115.05
114.80
107.47
107.21
77.41
77.10
76.78
21.66
F
N
S
F
O
CH3
3t
Current Data Parameters
F2 - Acquisition Parameters
CHANNEL f1
CHANNEL f2
F2 - Processing parameters
200
180
160
140
120
100
80
60
40
20
0
ppm

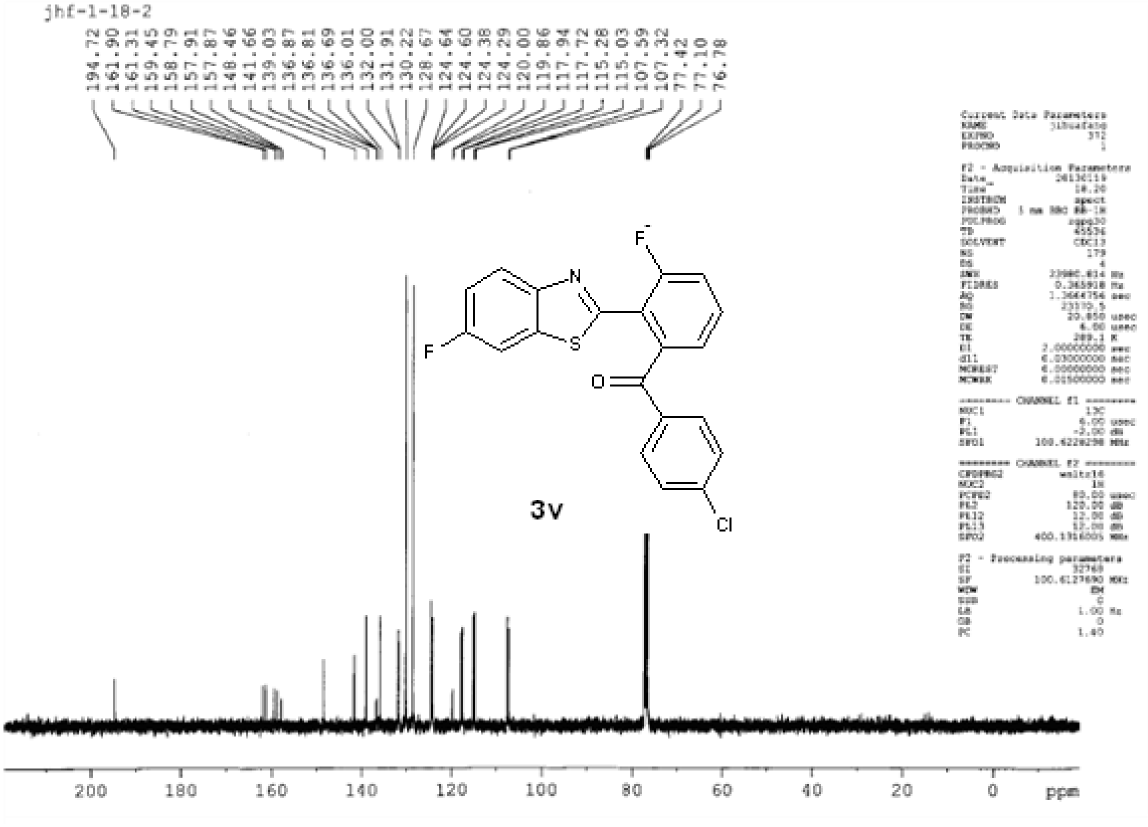


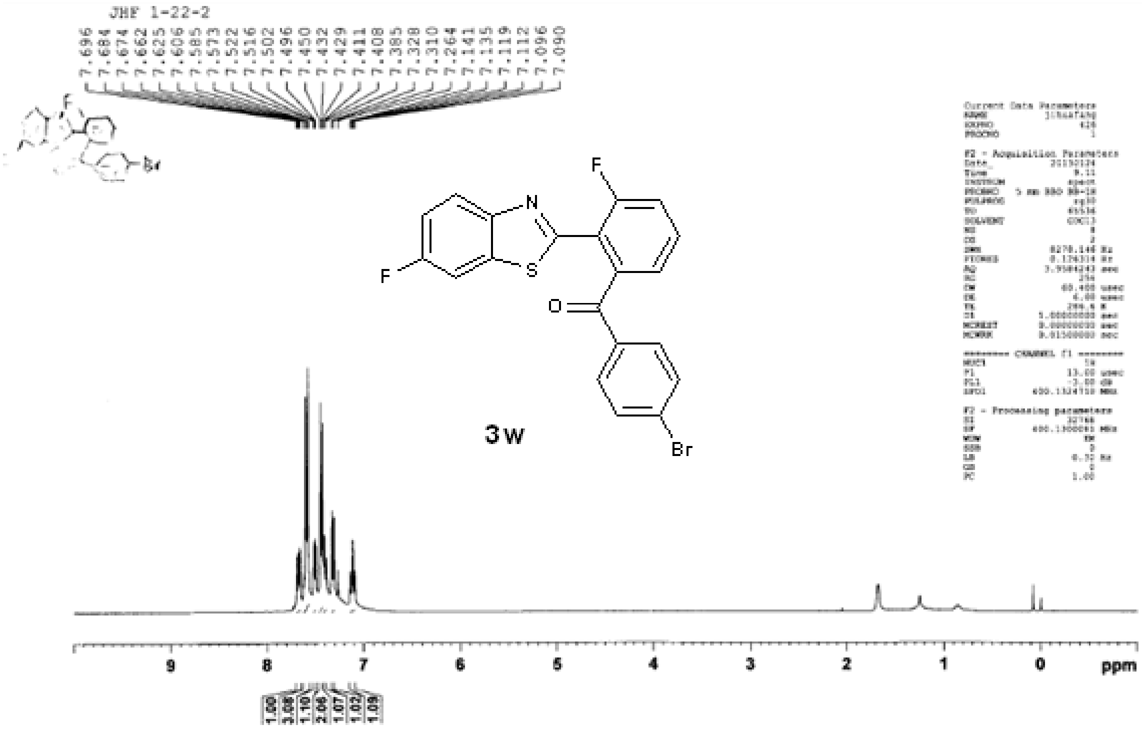
```
Current Data Parameters
NAME          jihuafang
EXPNO               427
PROCNO                1

F2 - Acquisition Parameters
Date_          20130124
Time               9.59
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ            3.9584243 sec
RG                  256
DW               60.400 usec
DE                 6.00 usec
TE                286.6 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                13.00 usec
PL1               -3.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300051 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

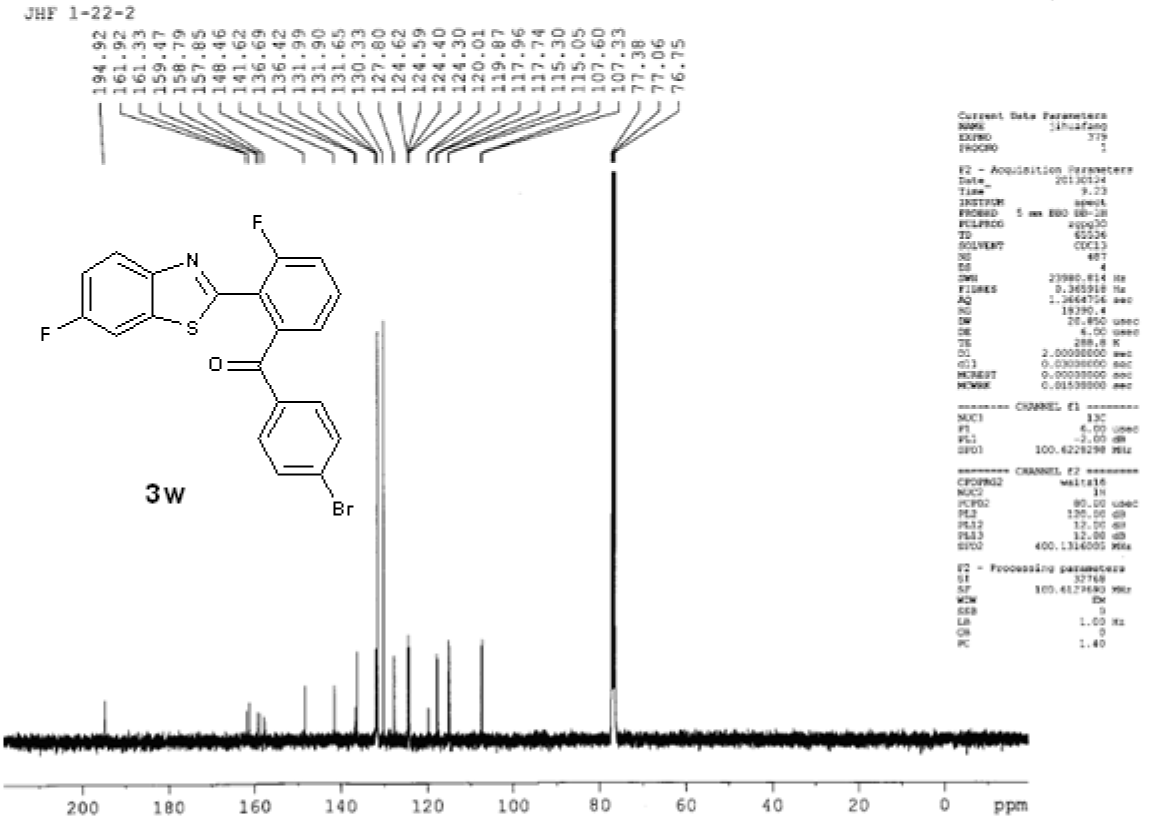


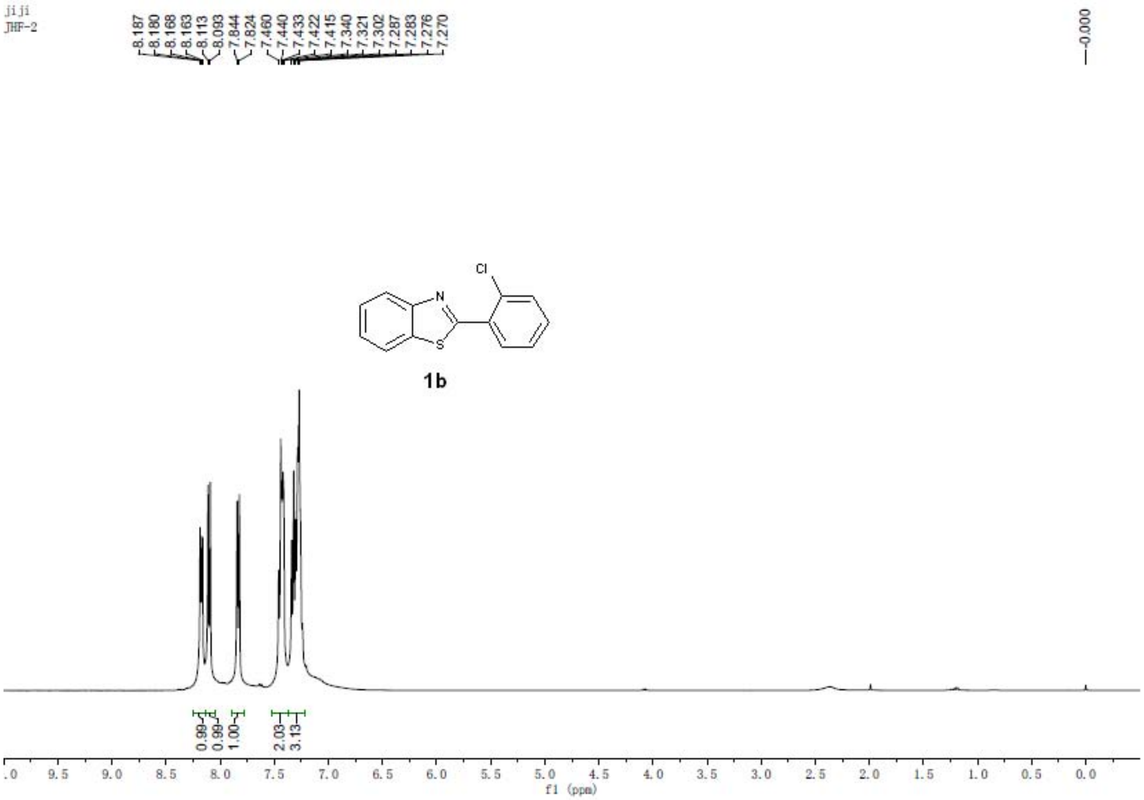
```
Current Data Parameters
NAME          jihuafang
EXPNO               380
PROCNO                1

F2 - Acquisition Parameters
Date_          20130124
Time              10.05
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  261
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                 8192
DW               20.850 usec
DE                 6.00 usec
TE                288.5 K
D1           2.00000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 6.00 usec
PL1               -2.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2              120.00 dB
PL12              12.00 dB
PL13              12.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

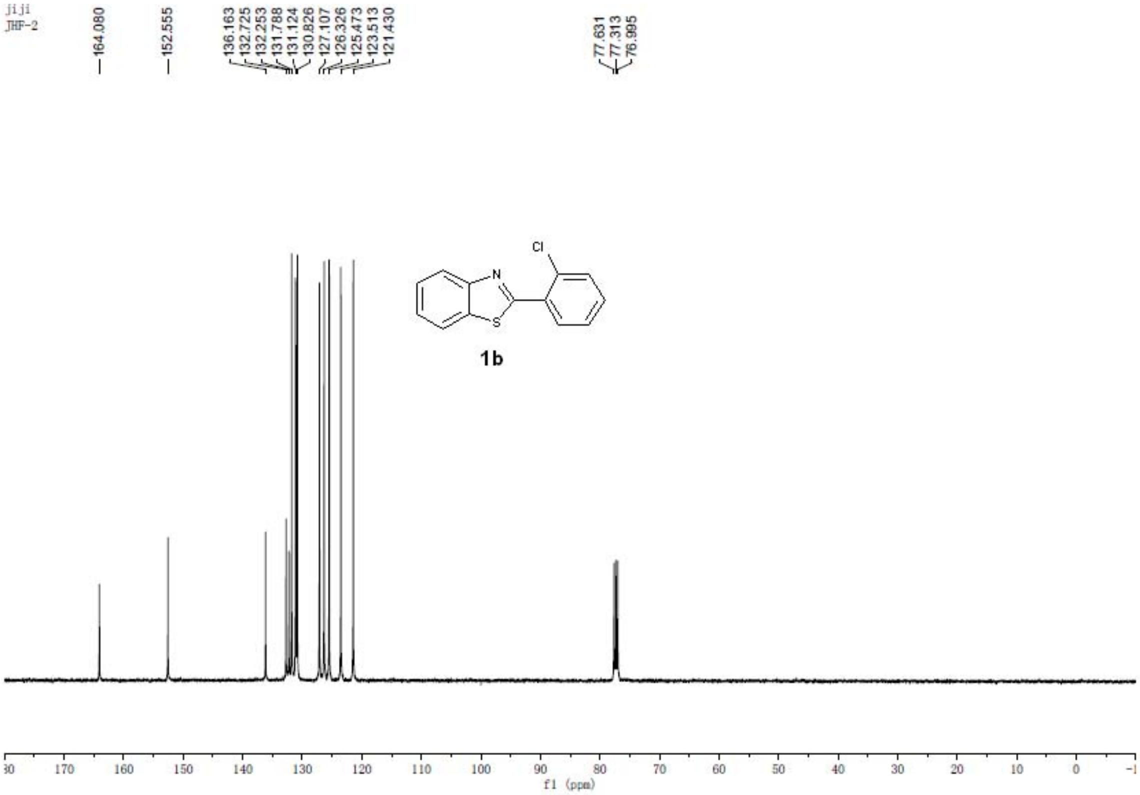

jhf 1-18-2
7.669
7.657
7.616
7.603
7.596
7.583
7.576
7.563
7.510
7.503
7.489
7.483
7.419
7.395
7.392
7.373
7.371
7.326
7.307
7.276
7.255
7.129
7.122
7.106
7.100
7.084
7.078
2.045
1.253
F
N
S
F
O
Cl
3v
9
8
7
6
5
4
3
2
1
0
ppm
2.69
1.08
1.06
1.00
0.97
2.30
1.07

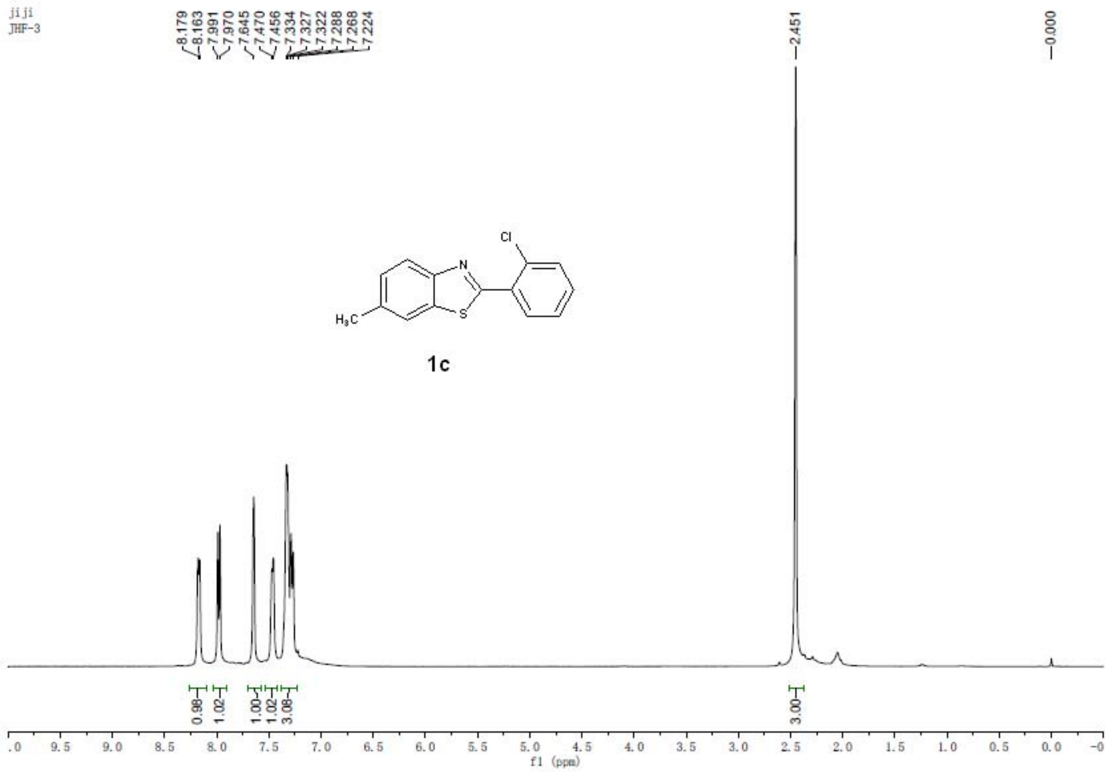

jhf-1-18-2
194.72
161.90
161.31
159.45
158.79
157.91
157.87
148.46
141.66
139.03
136.87
136.81
136.69
136.01
132.00
131.91
130.22
128.67
124.64
124.60
124.38
124.29
120.00
119.86
117.94
117.72
115.28
115.03
107.59
107.32
77.42
77.10
76.78
F
N
S
F
O
Cl
3v
200
180
160
140
120
100
80
60
40
20
0
ppm

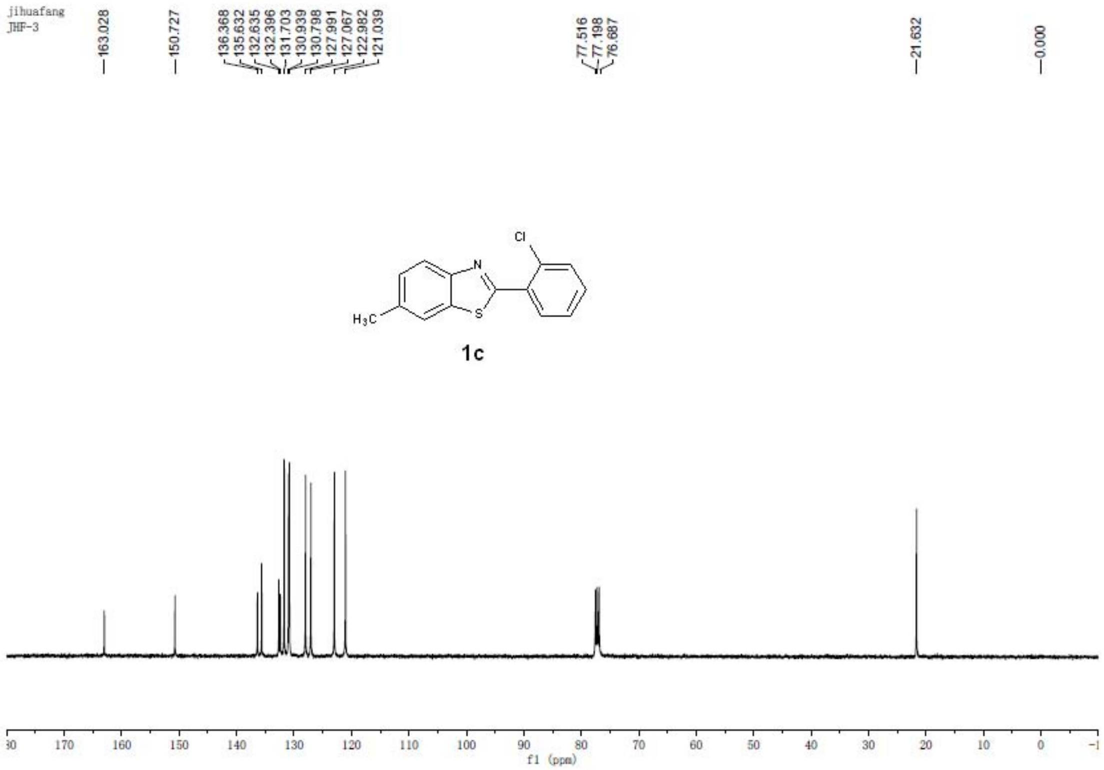

JHF 1-22-2
7.696
7.684
7.674
7.662
7.625
7.606
7.585
7.573
7.522
7.516
7.502
7.496
7.450
7.432
7.429
7.411
7.408
7.385
7.328
7.310
7.264
7.141
7.135
7.119
7.112
7.096
7.090
F
N
S
O
Br
3w
9
8
7
6
5
4
3
2
1
0
ppm
1.00
3.08
1.10
2.06
1.07
1.02
1.09

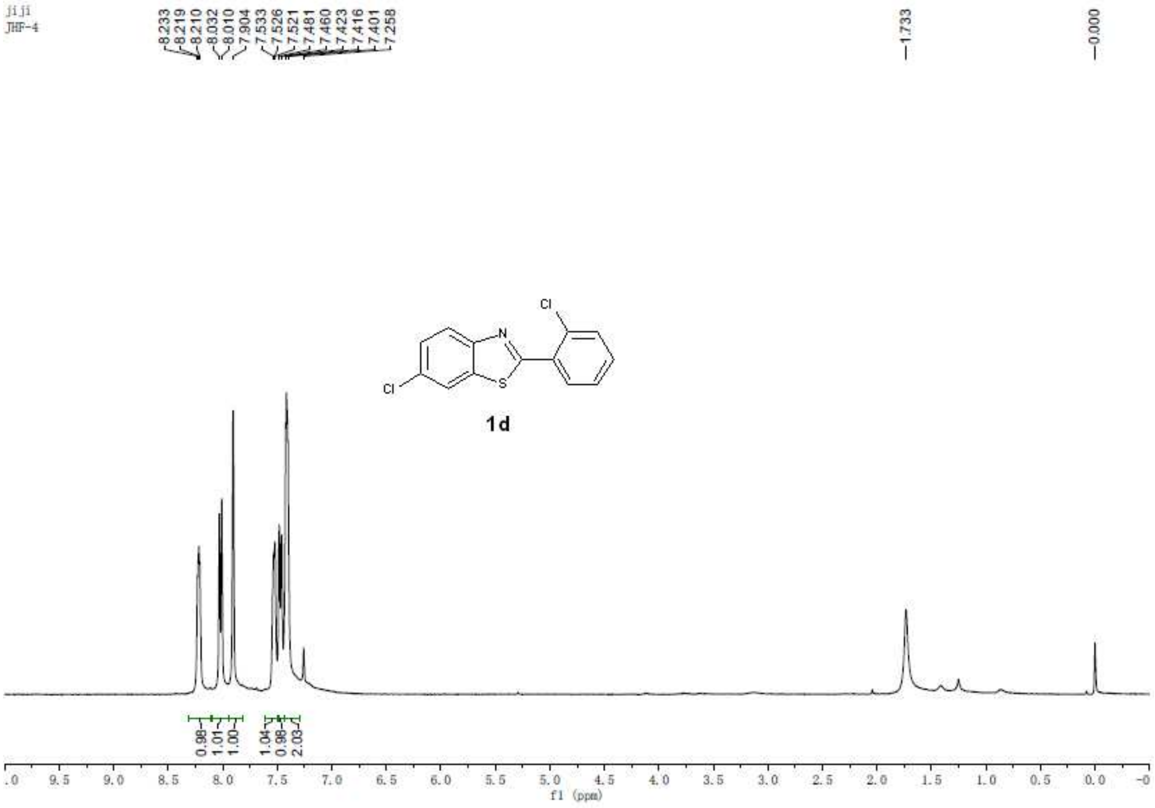

JHF 1-22-2
194.92
161.92
161.33
159.47
158.79
157.85
148.46
141.62
136.69
136.42
131.99
131.90
131.65
130.33
127.80
124.62
124.59
124.40
124.30
120.01
119.87
117.96
117.74
115.30
115.05
107.60
107.33
77.38
77.06
76.75
F
N
S
O
Br
3w
200
180
160
140
120
100
80
60
40
20
0
ppm

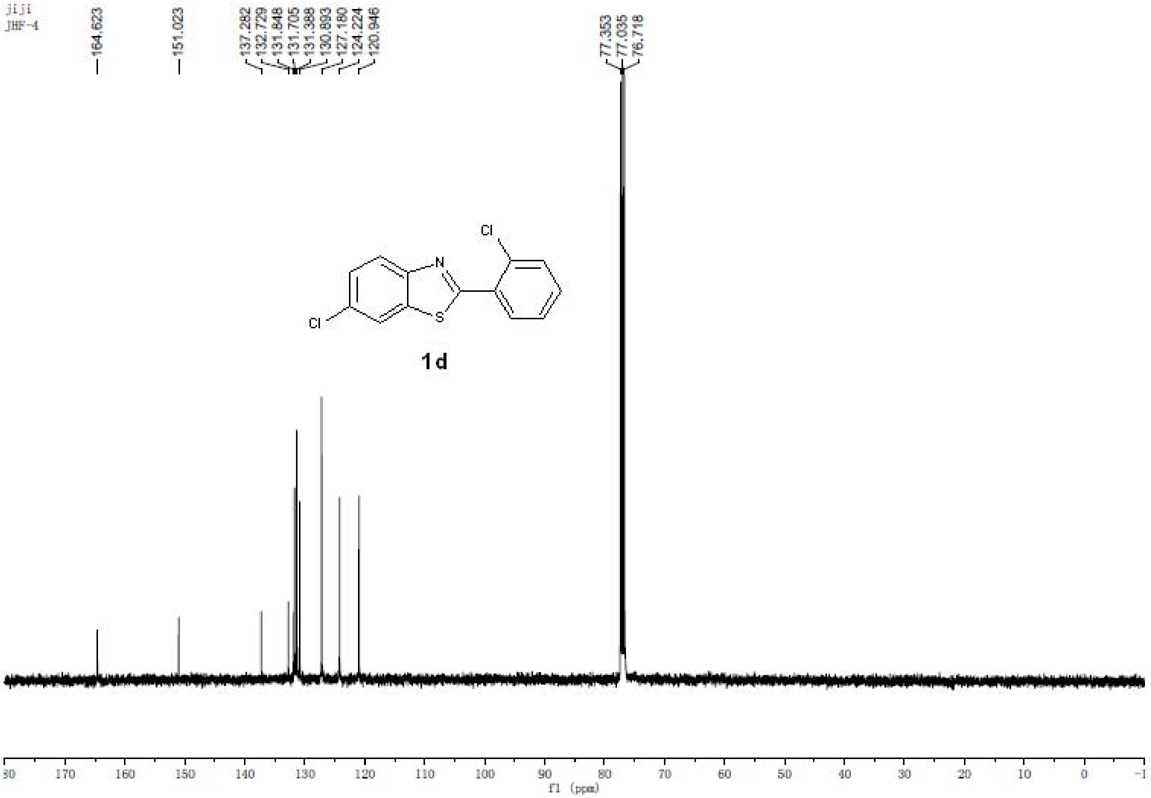

jiji
JHF-2
8.187
8.180
8.168
8.163
8.113
8.093
7.844
7.824
7.460
7.440
7.433
7.422
7.415
7.340
7.321
7.302
7.287
7.283
7.276
7.270
0.000
Cl
N
S
1b
0.99
0.99
1.00
2.03
3.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

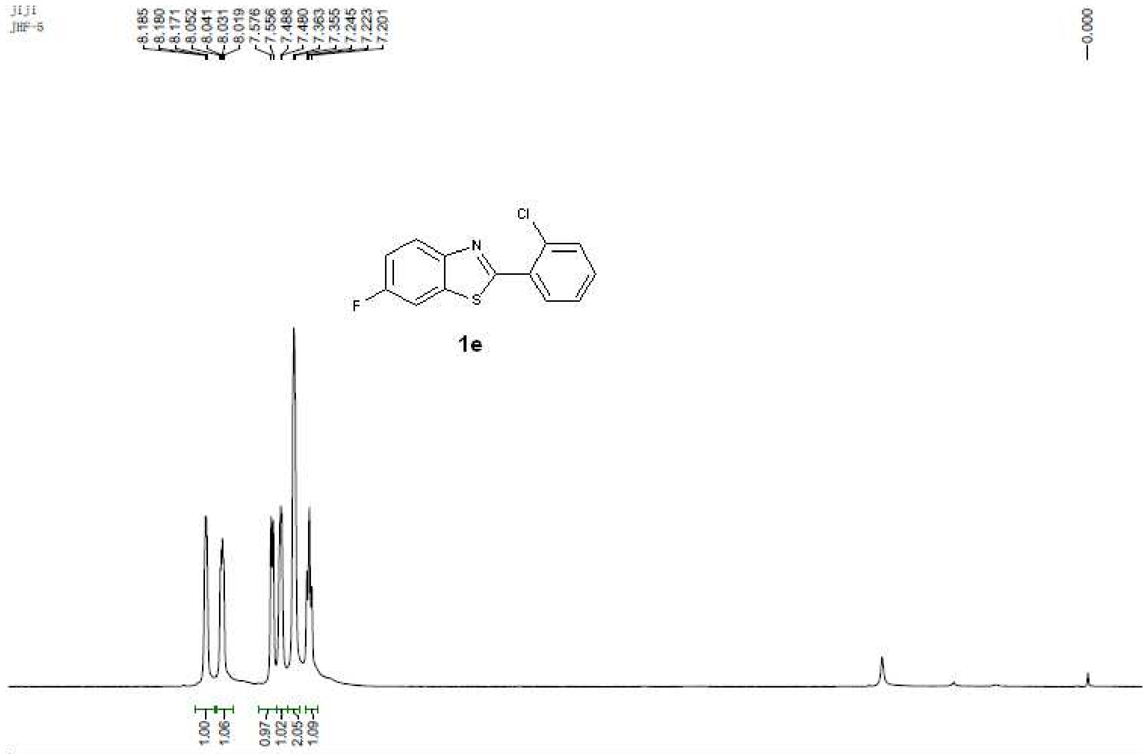

jiji
JHF-2
164.080
152.555
136.163
132.725
132.253
131.788
131.124
130.826
127.107
126.326
125.473
123.513
121.430
77.631
77.313
76.995
Cl
N
S
1b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

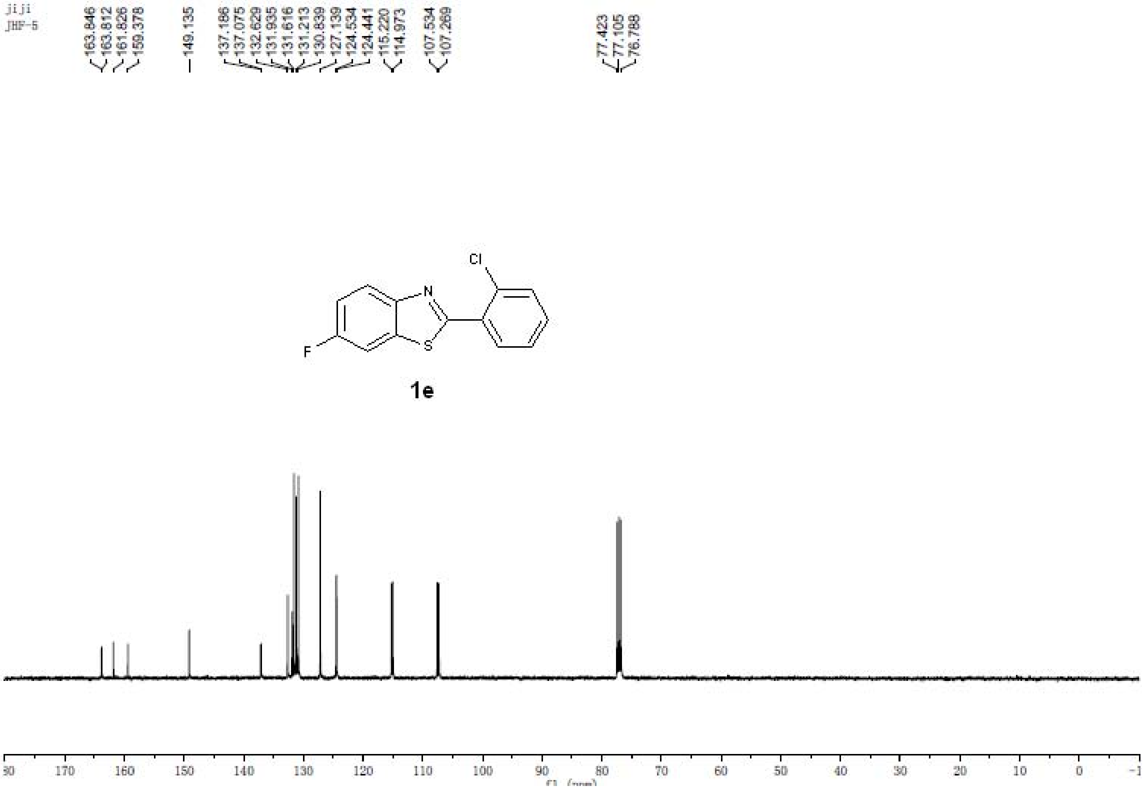

jiji
JHF-3
8.179
8.163
7.991
7.970
7.645
7.470
7.456
7.334
7.327
7.322
7.288
7.268
7.224
2.451
0.000
Cl
N
S
H3C
1c
0.98
1.02
1.00
1.02
3.08
3.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

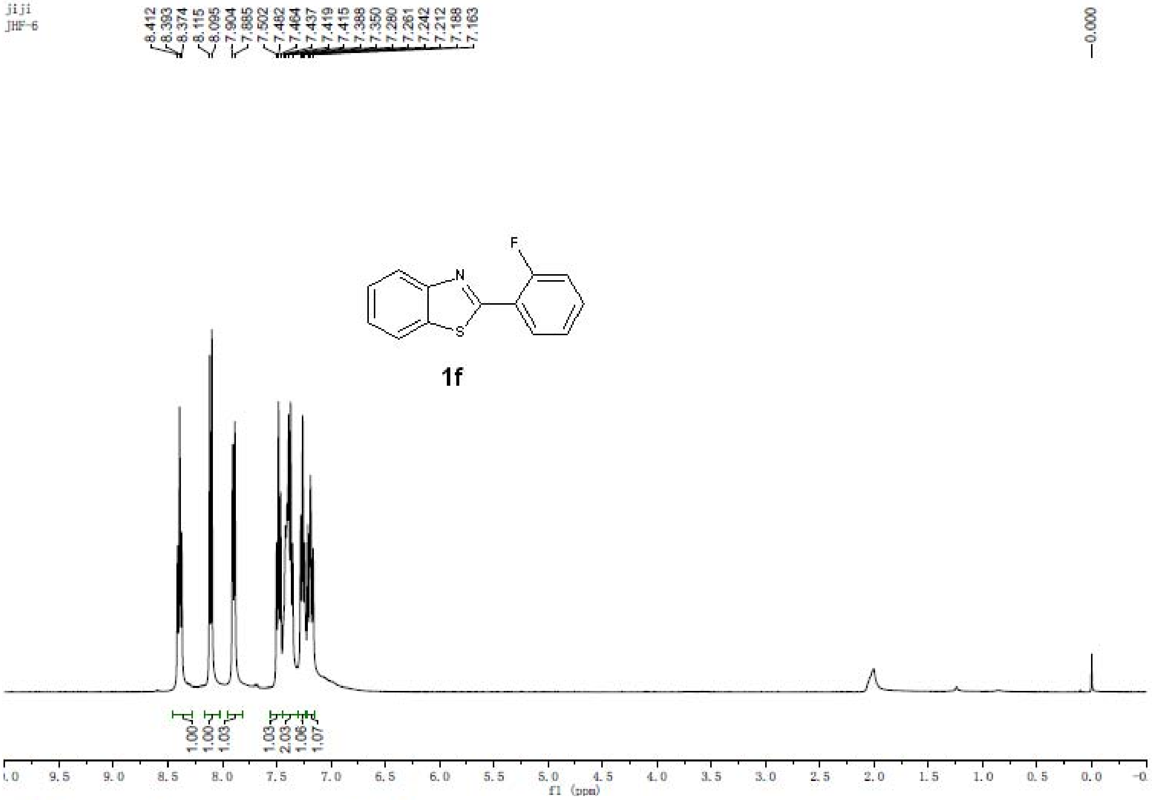

jihuafang
JHF-3
163.028
150.727
136.368
135.632
132.635
132.396
131.703
130.939
130.798
127.991
127.067
122.982
121.039
77.516
77.198
76.687
21.632
0.000
Cl
N
S
H3C
1c
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

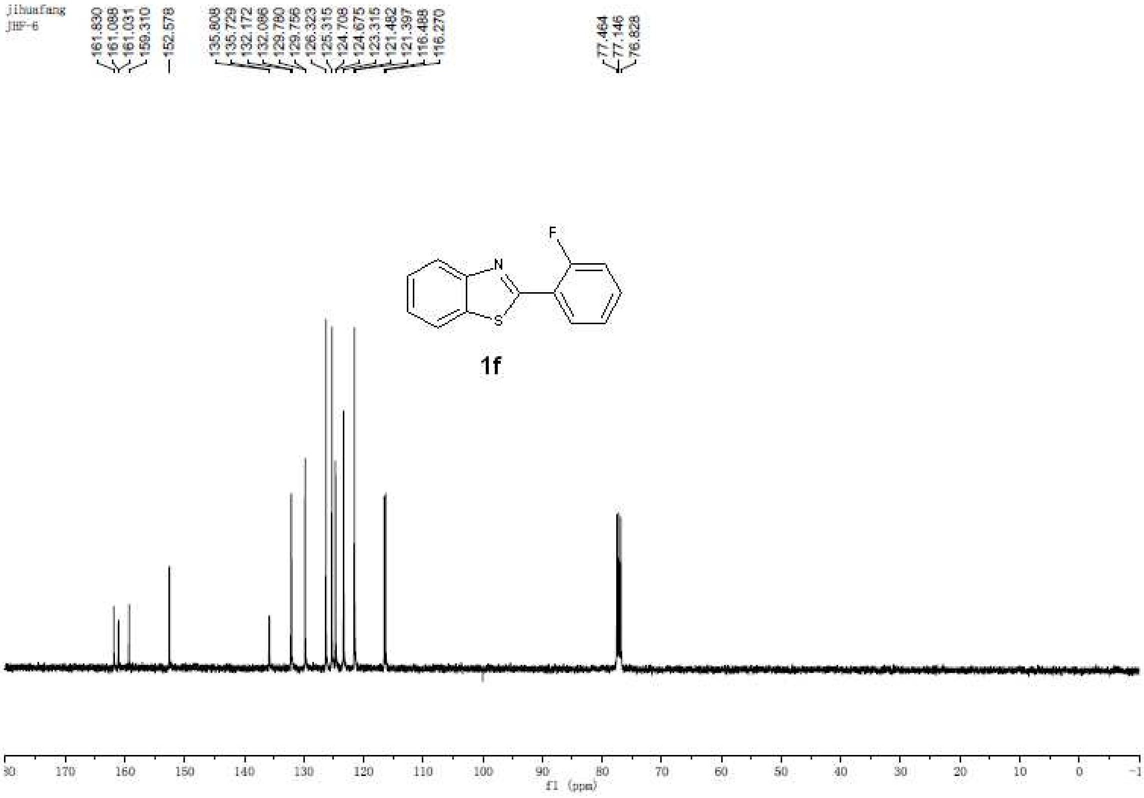

jiji
JHF-4
8.233
8.219
8.210
8.032
8.010
7.904
7.533
7.526
7.521
7.481
7.460
7.423
7.416
7.401
7.258
1.733
0.000
Cl
N
S
Cl
1d
0.98
1.01
1.00
1.04
0.98
2.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

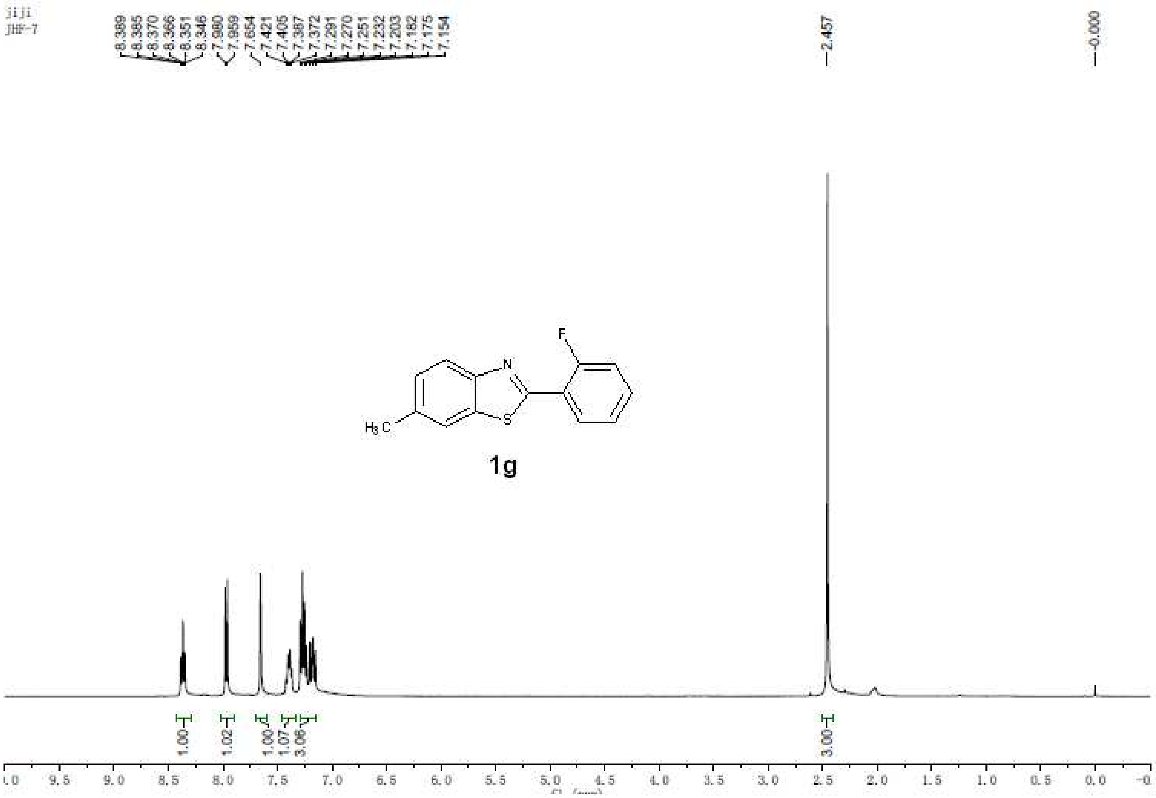

jiji
JHF-4
164.623
151.023
137.282
132.729
131.848
131.705
131.388
130.893
127.180
124.224
120.946
77.353
77.035
76.718
Cl
N
S
Cl
1d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


jiji
JHF-5
8.185
8.180
8.171
8.052
8.041
8.031
8.019
7.576
7.556
7.488
7.480
7.363
7.355
7.245
7.223
7.201
0.000
Cl
N
S
F
1e
1.00
1.06
0.97
1.02
2.05
1.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

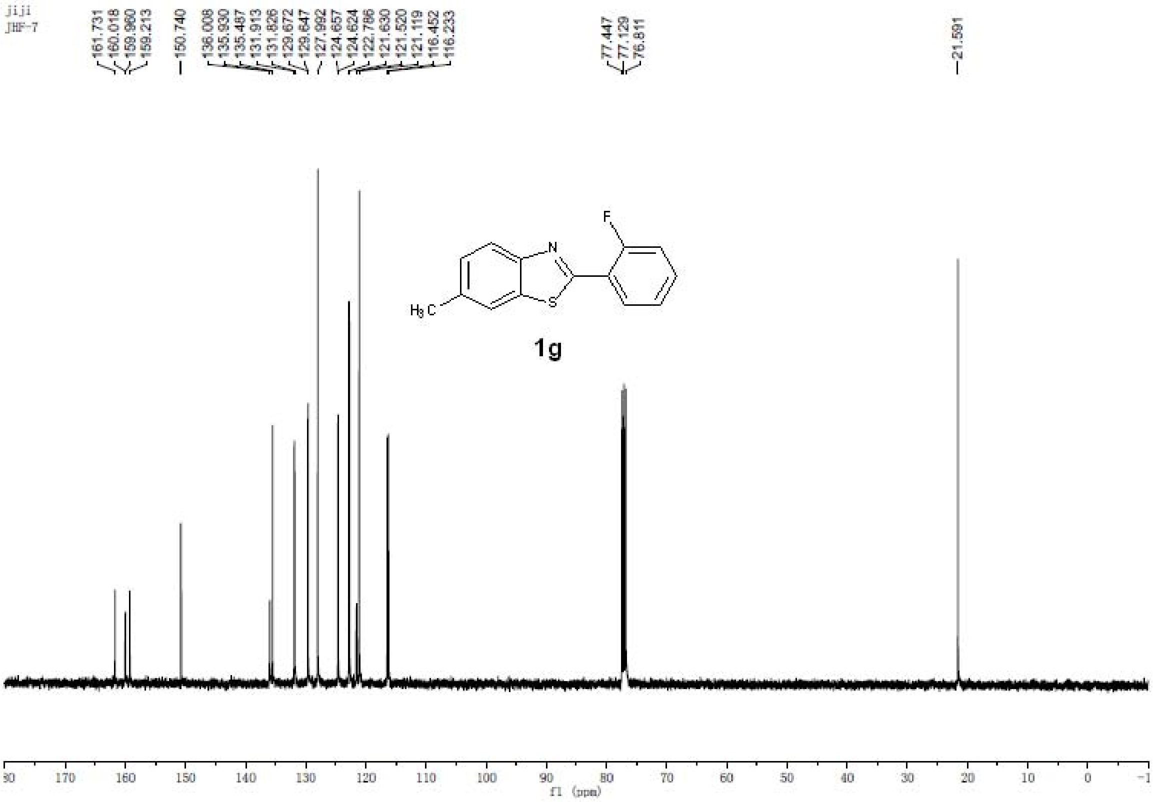

jiji
JHF-5
163.846
163.812
161.826
159.378
149.135
137.186
137.075
132.629
131.935
131.616
131.213
130.839
127.139
124.534
124.441
115.220
114.973
107.534
107.269
77.423
77.105
76.788
Cl
N
S
F
1e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


jiji
JHF-6
8.412
8.393
8.374
8.115
8.095
7.904
7.885
7.502
7.482
7.464
7.437
7.419
7.415
7.388
7.350
7.280
7.261
7.242
7.212
7.188
7.163
0.000
F
N
S
1f
1.00
1.00
1.03
1.03
2.03
1.06
1.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

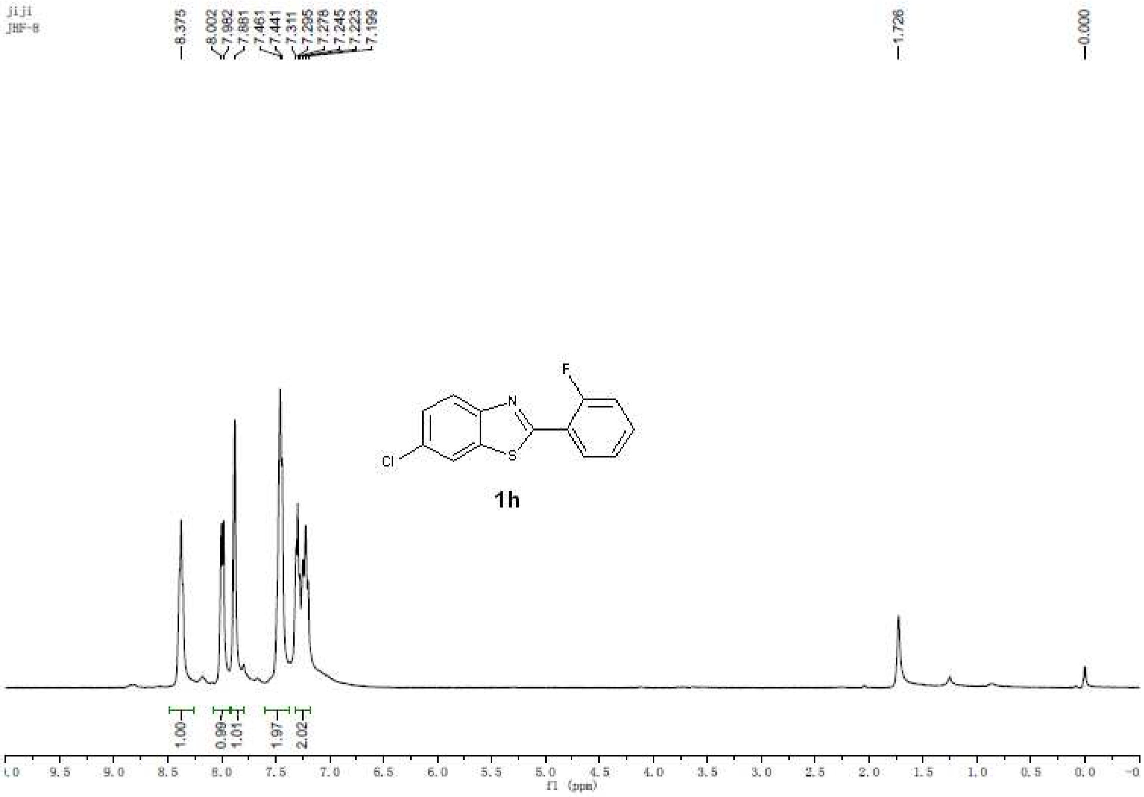

jihuafang
JHF-6
161.830
161.088
161.031
159.310
152.578
135.808
135.729
132.172
132.086
129.780
129.756
126.323
125.315
124.708
124.675
123.315
121.482
121.397
116.488
116.270
77.464
77.146
76.828
F
N
S
1f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

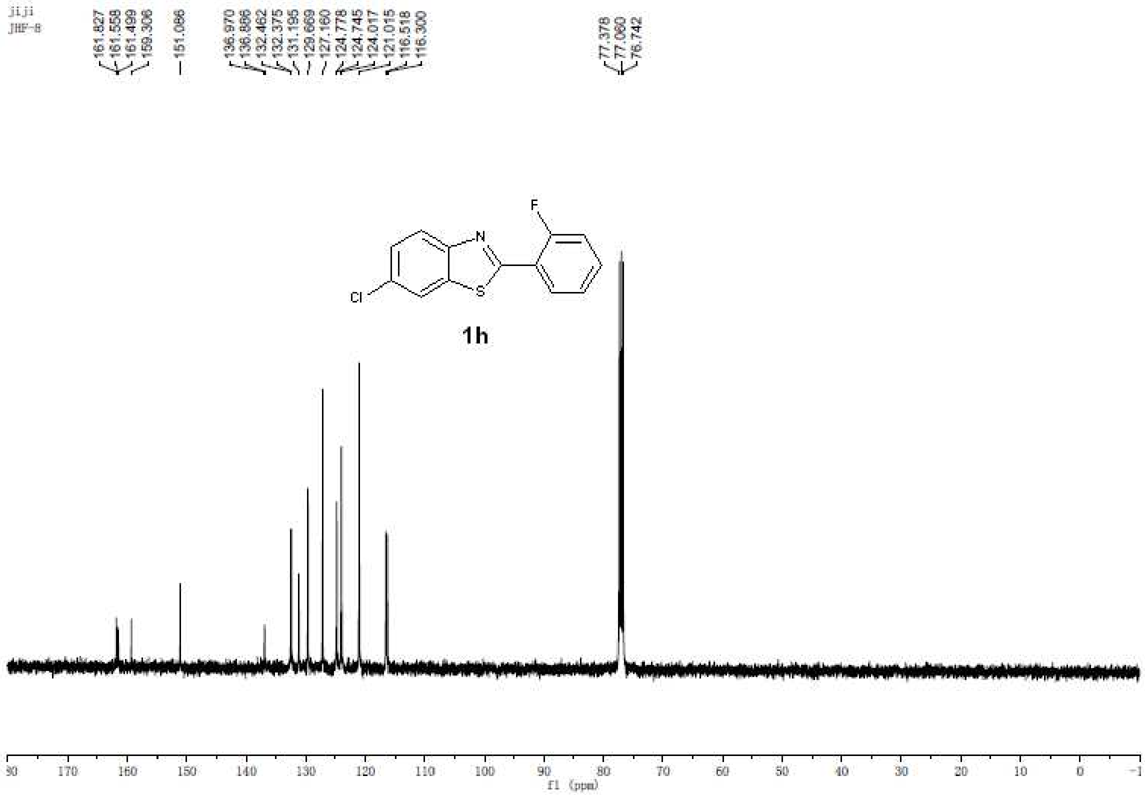

jiji
JHF-7
8.389
8.385
8.370
8.366
8.351
8.346
7.980
7.959
7.654
7.421
7.405
7.387
7.372
7.291
7.270
7.251
7.232
7.203
7.182
7.175
7.154
2.457
0.000
F
N
S
H3C
1.00
1.02
1.00
1.07
3.06
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

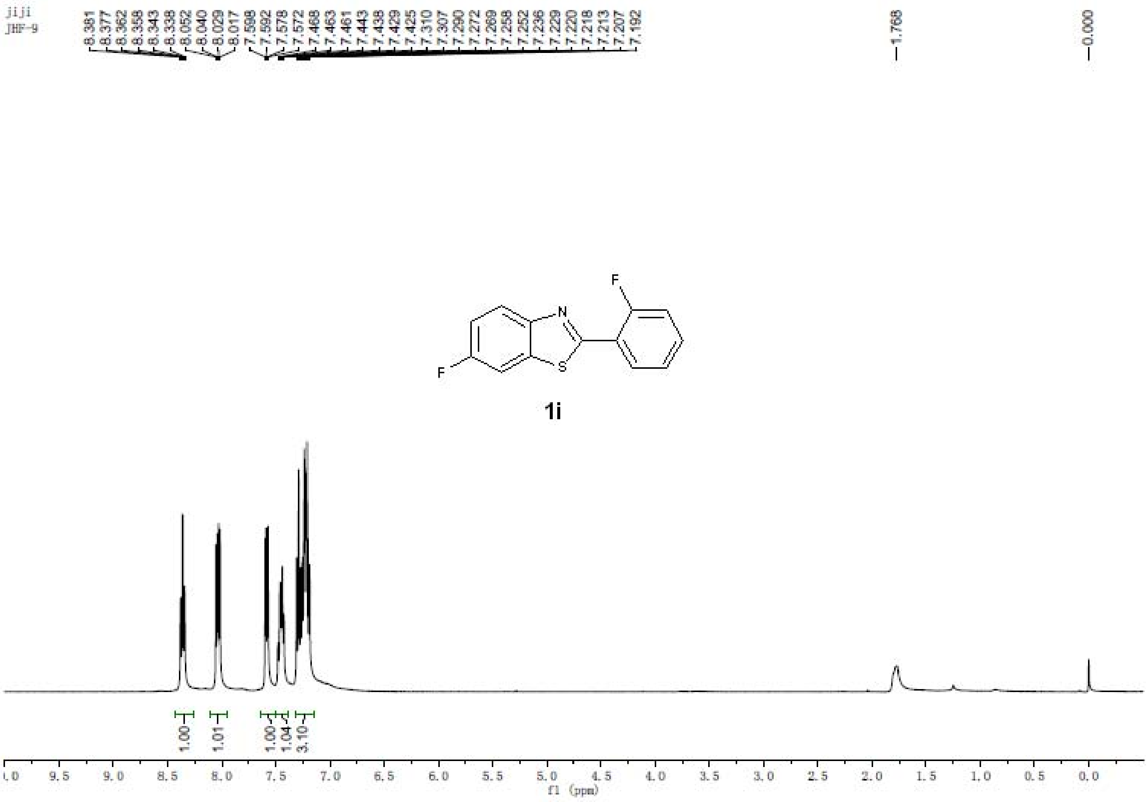
1g

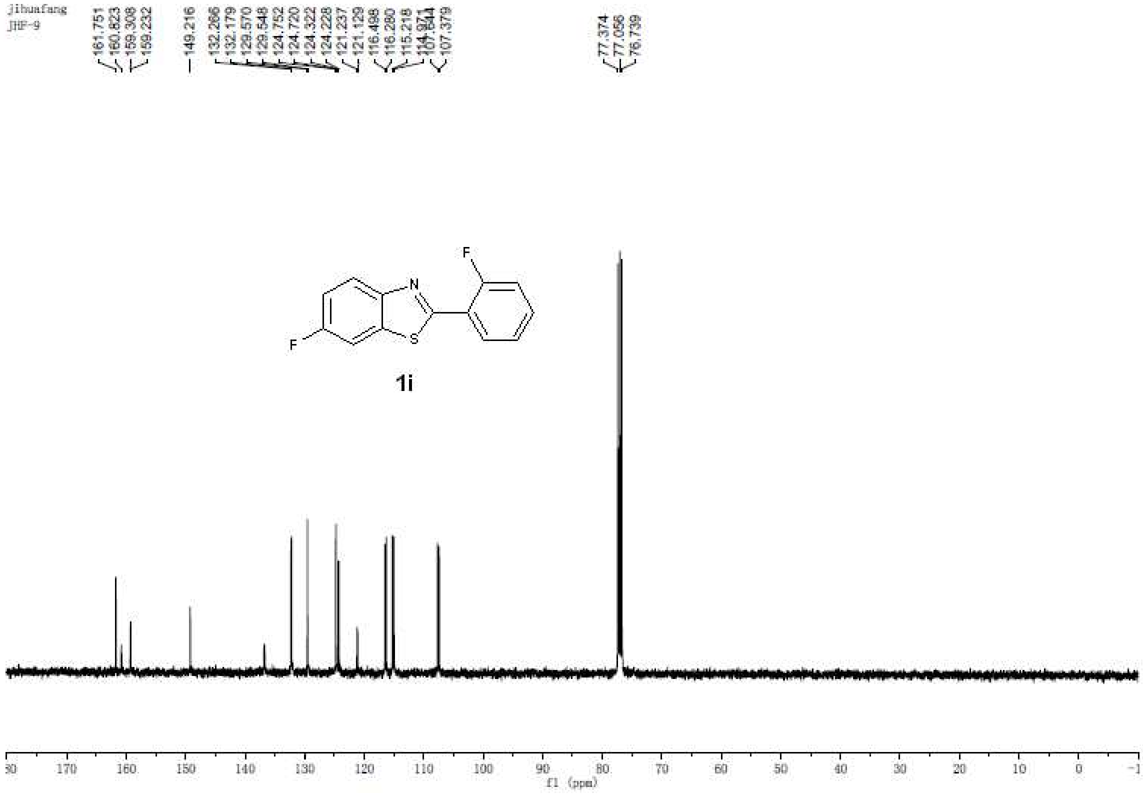

jiji
JHF-7
161.731
160.018
159.960
159.213
150.740
136.008
135.930
135.487
131.913
131.826
129.672
129.647
127.992
124.657
124.624
122.786
121.630
121.520
121.119
116.452
116.233
77.447
77.129
76.811
21.591
F
N
S
H3C
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

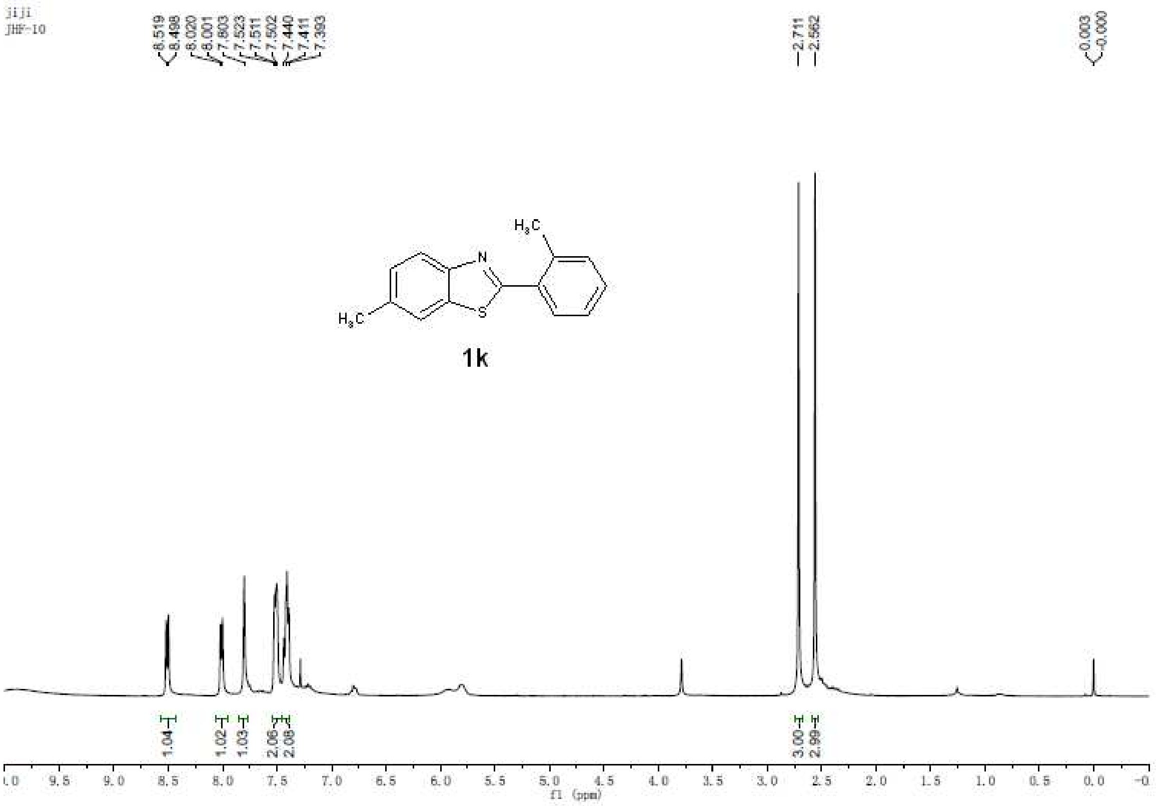
1g

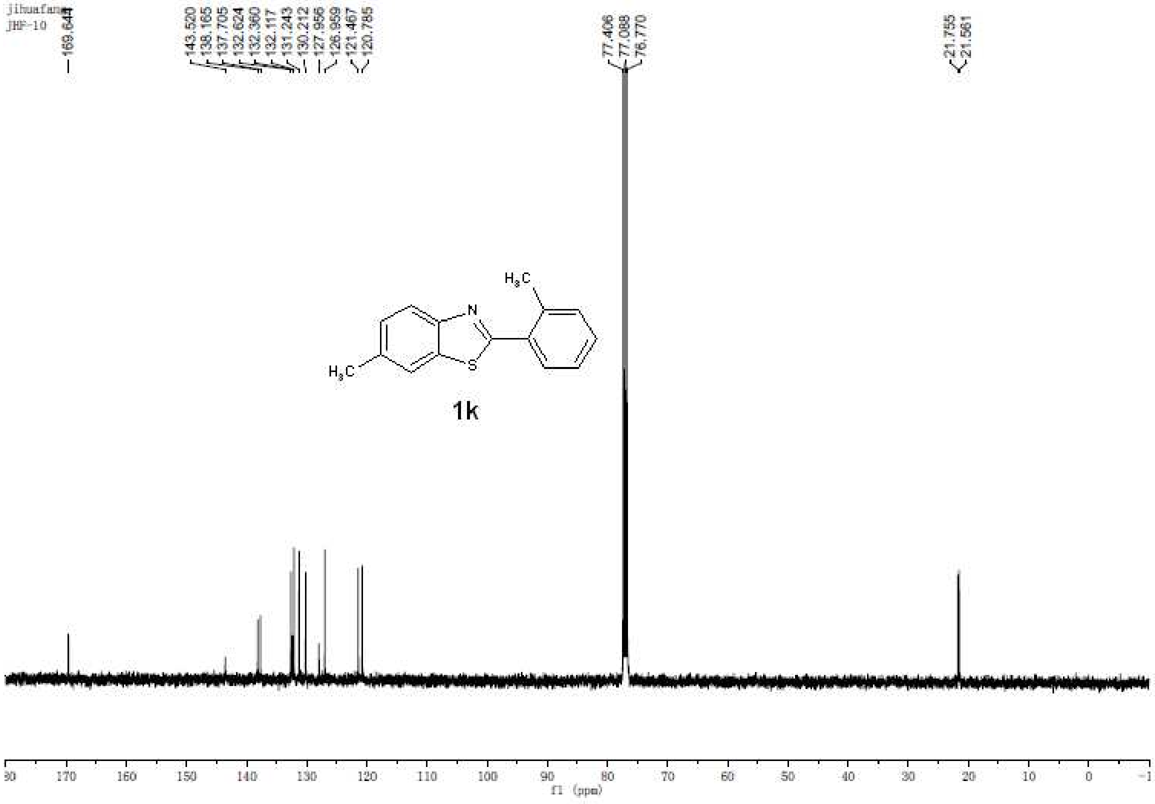

jiji
JHF-8
8.375
8.002
7.982
7.881
7.461
7.441
7.311
7.295
7.278
7.245
7.223
7.199
1.726
0.000
F
N
S
Cl
1h
1.00
0.99
1.01
1.97
2.02
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

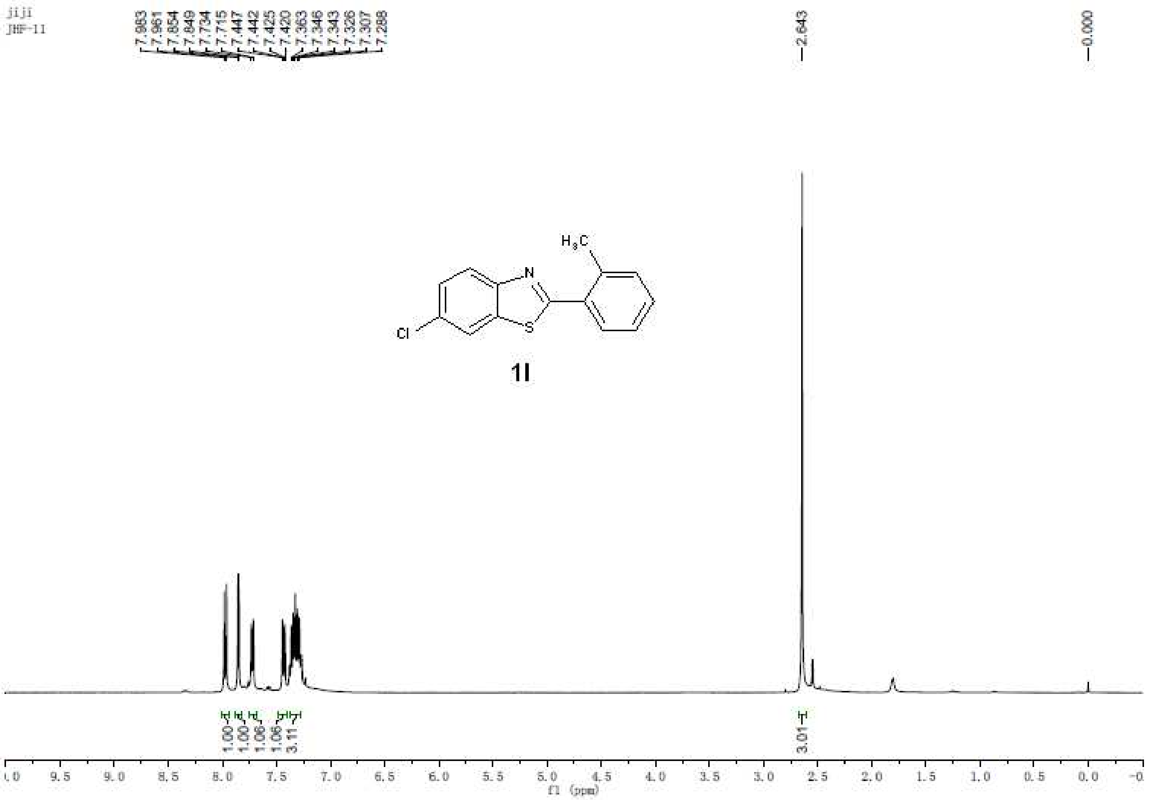

jiji
JHF-8
161.827
161.558
161.499
159.306
151.086
136.970
136.866
132.462
132.375
131.195
129.669
127.160
124.778
124.745
124.017
121.015
116.518
116.300
77.378
77.060
76.742
F
N
S
Cl
1h
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

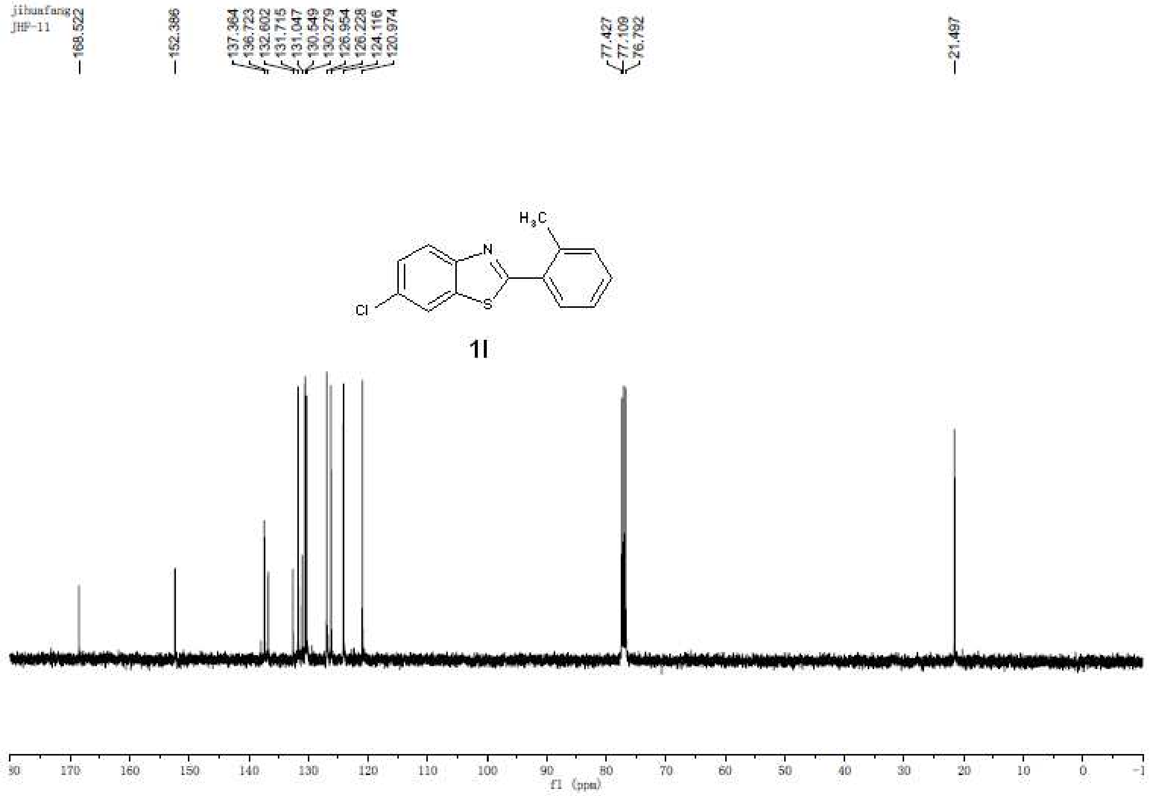

jiji
JHF-9
8.381
8.377
8.362
8.358
8.343
8.338
8.052
8.040
8.029
8.017
7.598
7.592
7.578
7.572
7.468
7.463
7.461
7.443
7.438
7.429
7.425
7.310
7.307
7.290
7.272
7.269
7.258
7.252
7.236
7.229
7.220
7.218
7.213
7.207
7.192
1.768
0.000
F
N
S
F
1i
1.00
1.01
1.00
1.04
3.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

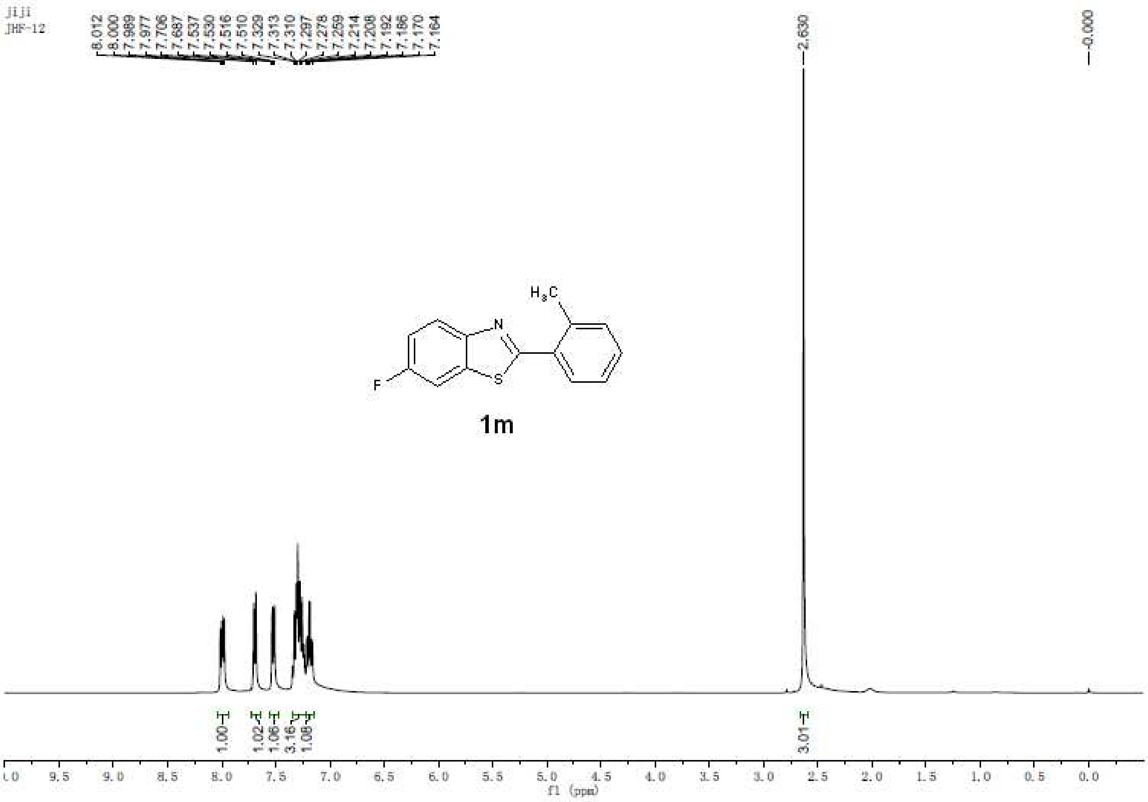

jihuafang
JHF-9
161.751
160.823
159.308
159.232
149.216
132.266
132.179
129.570
129.548
124.752
124.720
124.322
124.228
121.237
121.129
116.498
116.280
115.218
114.971
107.644
107.379
77.374
77.056
76.739
F
N
S
F
1i
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


jiji
JHF-10
8.519
8.498
8.020
8.001
7.803
7.523
7.511
7.502
7.440
7.411
7.393
2.711
2.562
0.003
-0.000
H3C
N
S
H3C
1k
1.04
1.02
1.03
2.06
2.08
3.00
2.99
f1 (ppm)

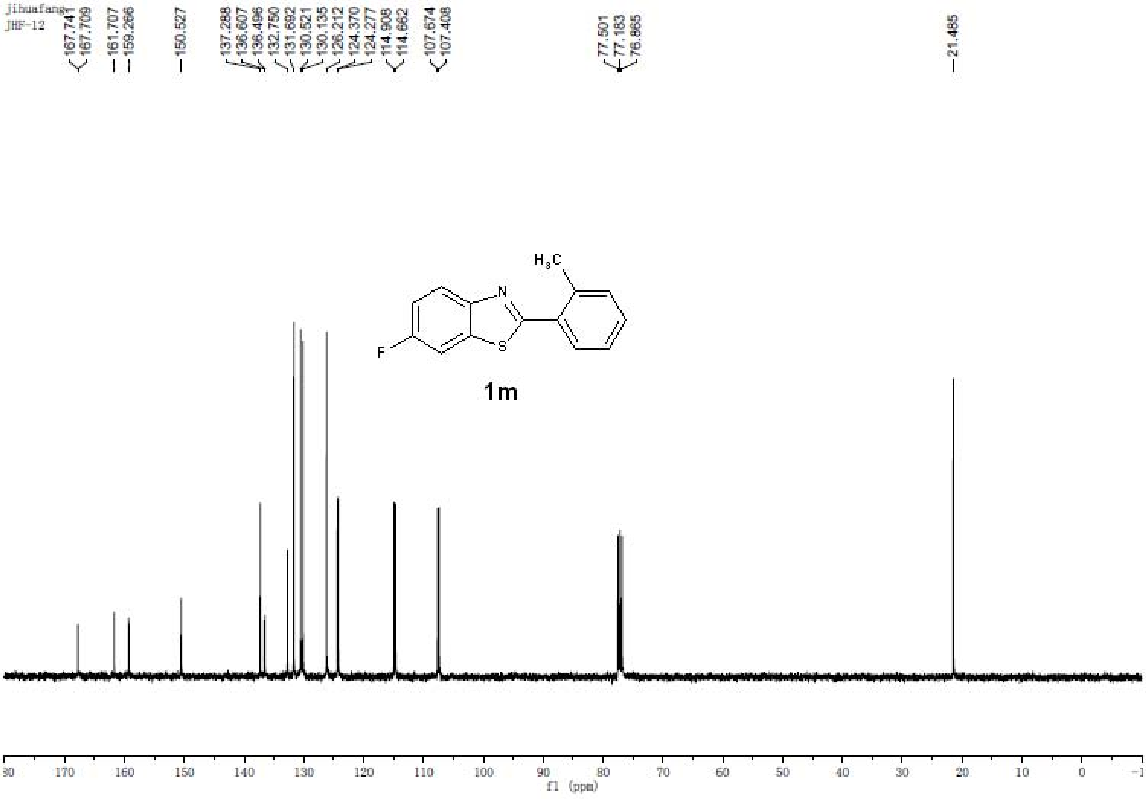

jihuafang
JHF-10
169.644
143.520
138.165
137.705
132.624
132.360
132.117
131.243
130.212
127.956
126.959
121.467
120.785
77.406
77.088
76.770
21.755
21.561
H3C
N
S
H3C
1k
f1 (ppm)


jiji
JHF-11
7.983
7.961
7.854
7.849
7.734
7.715
7.447
7.442
7.425
7.420
7.363
7.346
7.343
7.326
7.307
7.288
2.643
0.000
H3C
N
S
Cl
1l
1.00
1.00
1.06
1.06
3.11
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

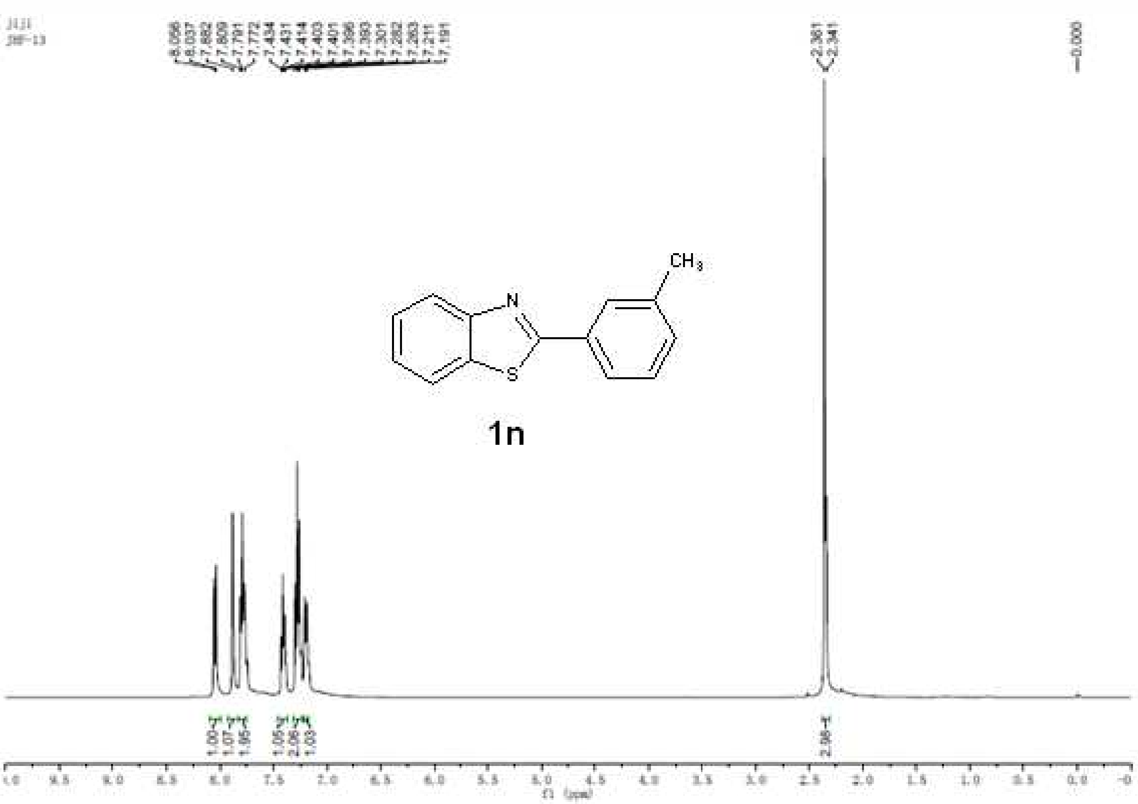

jihuafang
JHF-11
168.522
152.386
137.364
136.723
132.602
131.715
131.047
130.549
130.279
126.954
126.228
124.116
120.974
77.427
77.109
76.792
21.497
H3C
N
S
Cl
1l
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

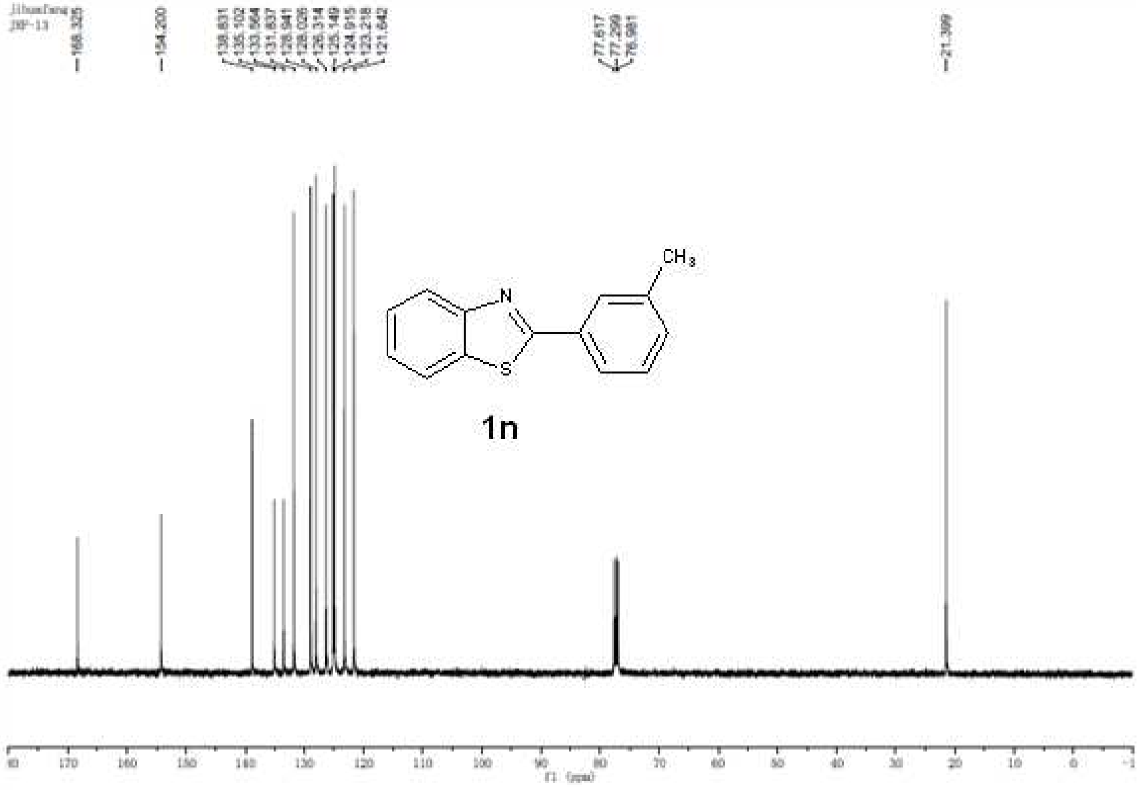

jiji
JHF-12
8.012
8.000
7.989
7.977
7.706
7.687
7.537
7.530
7.516
7.510
7.329
7.313
7.310
7.297
7.278
7.259
7.214
7.208
7.192
7.186
7.170
7.164
2.630
-0.000
H3C
N
S
F
1.00
1.02
1.06
3.16
1.08
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

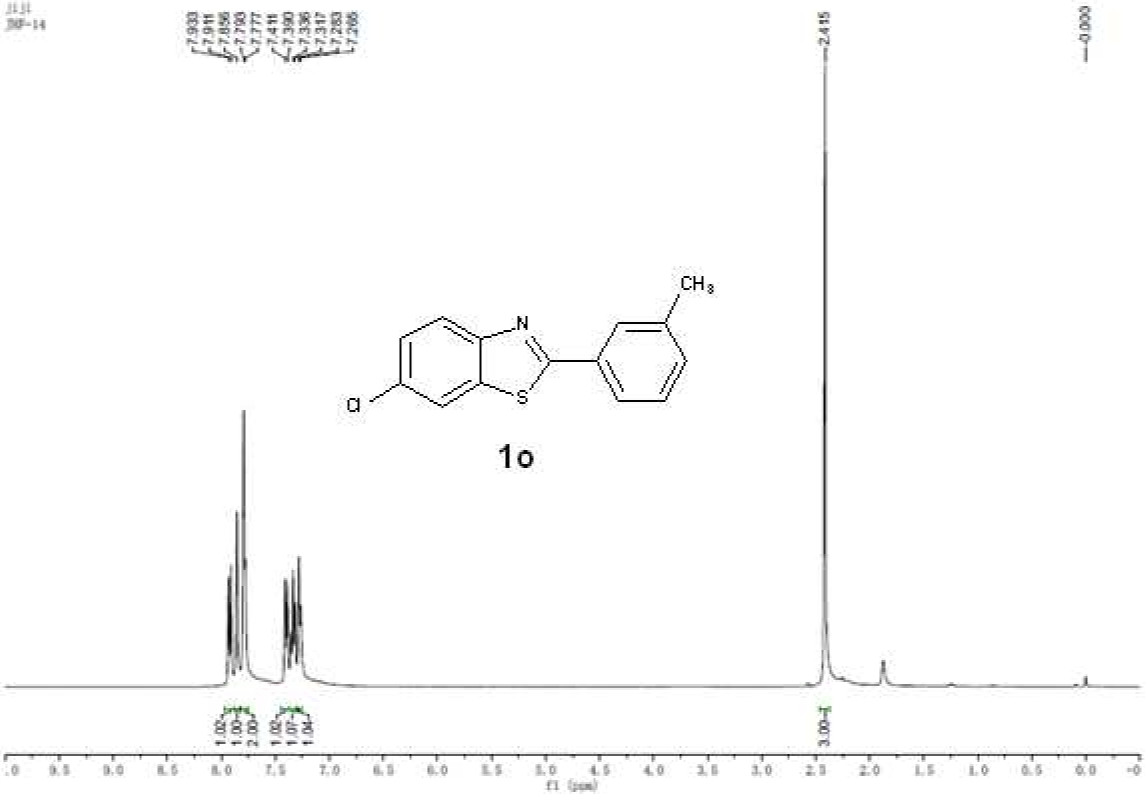
1m

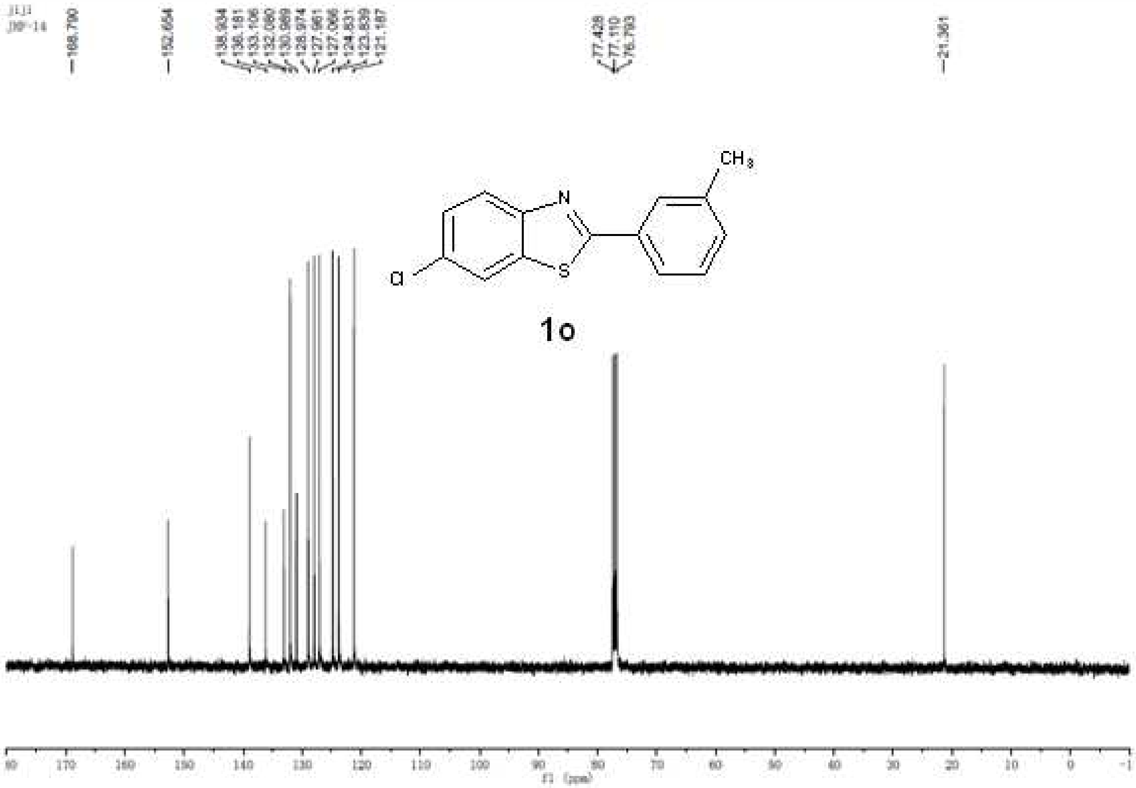

jihuafang
JHF-12
167.741
167.709
161.707
159.266
150.527
137.288
136.607
136.496
132.750
131.692
130.521
130.135
126.212
124.370
124.277
114.908
114.662
107.674
107.408
77.501
77.183
76.865
21.485
H3C
N
S
F
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

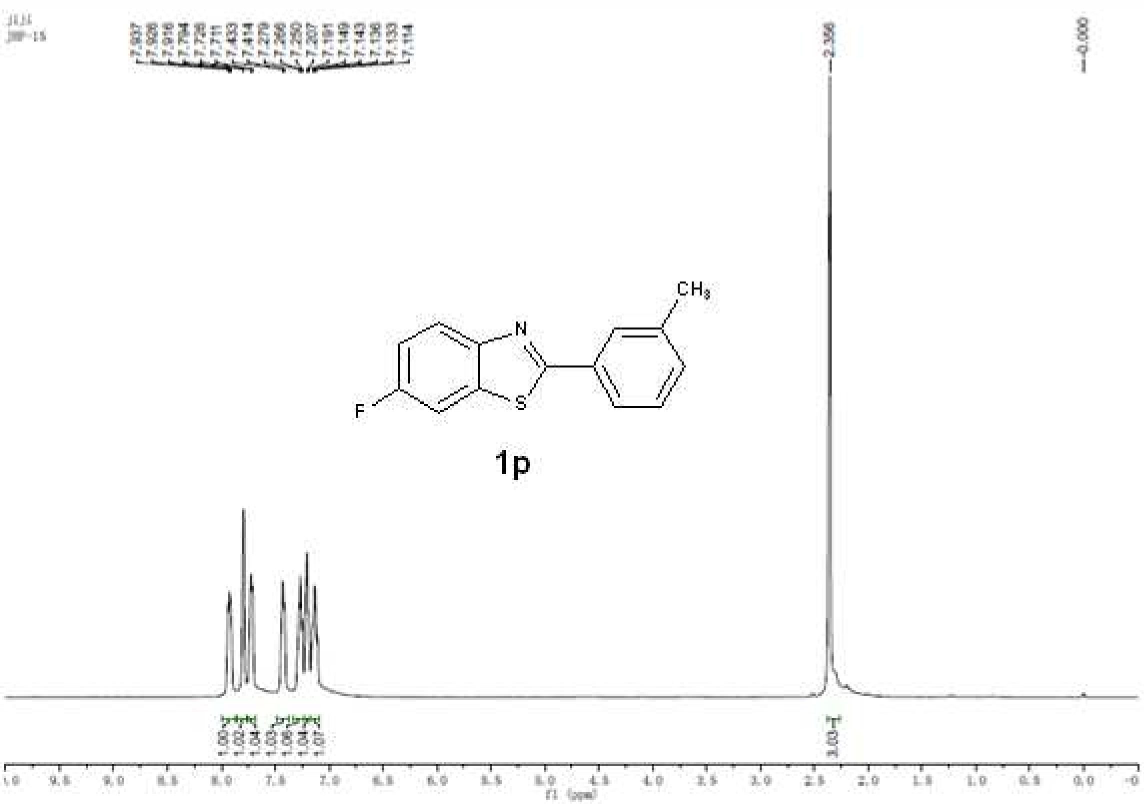
1m

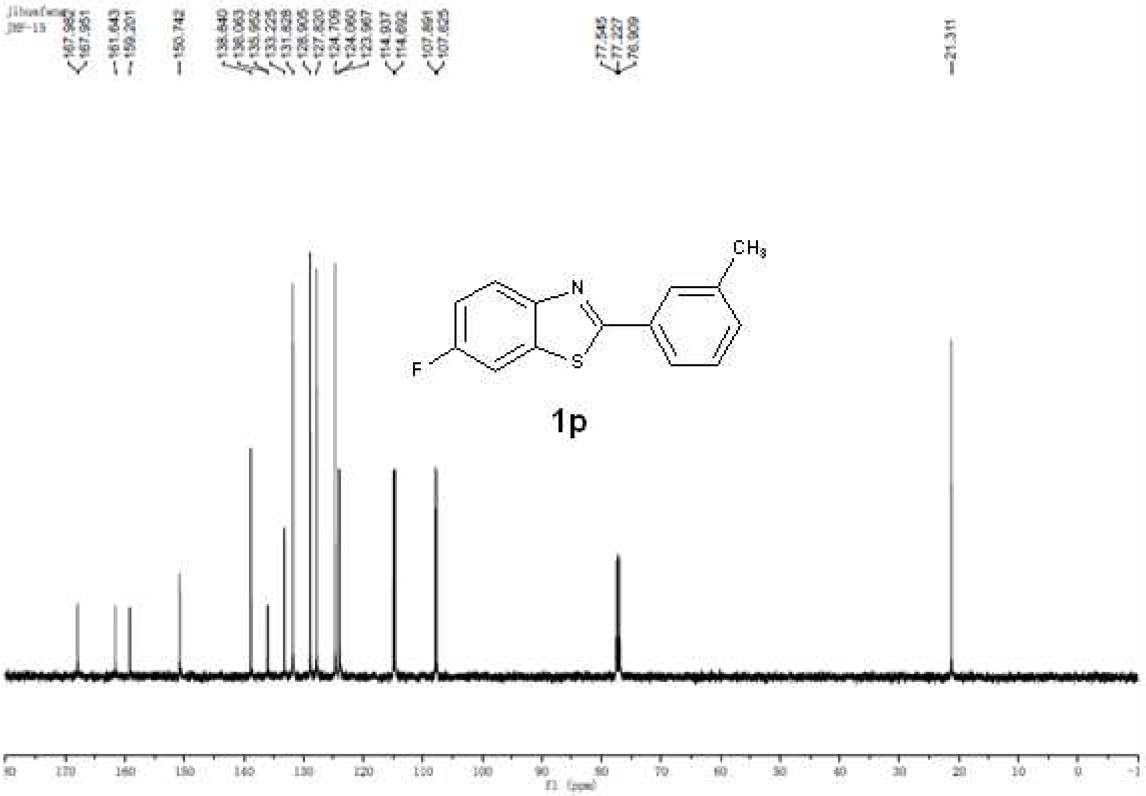

JJJJ
JHF-13
8.056
8.037
7.882
7.869
7.791
7.772
7.434
7.431
7.414
7.403
7.401
7.386
7.383
7.301
7.282
7.263
7.211
7.191
2.361
2.341
0.000
CH3
N
S
1n
1.00
1.07
1.95
1.05
2.06
1.03
2.98
f1 (ppm)

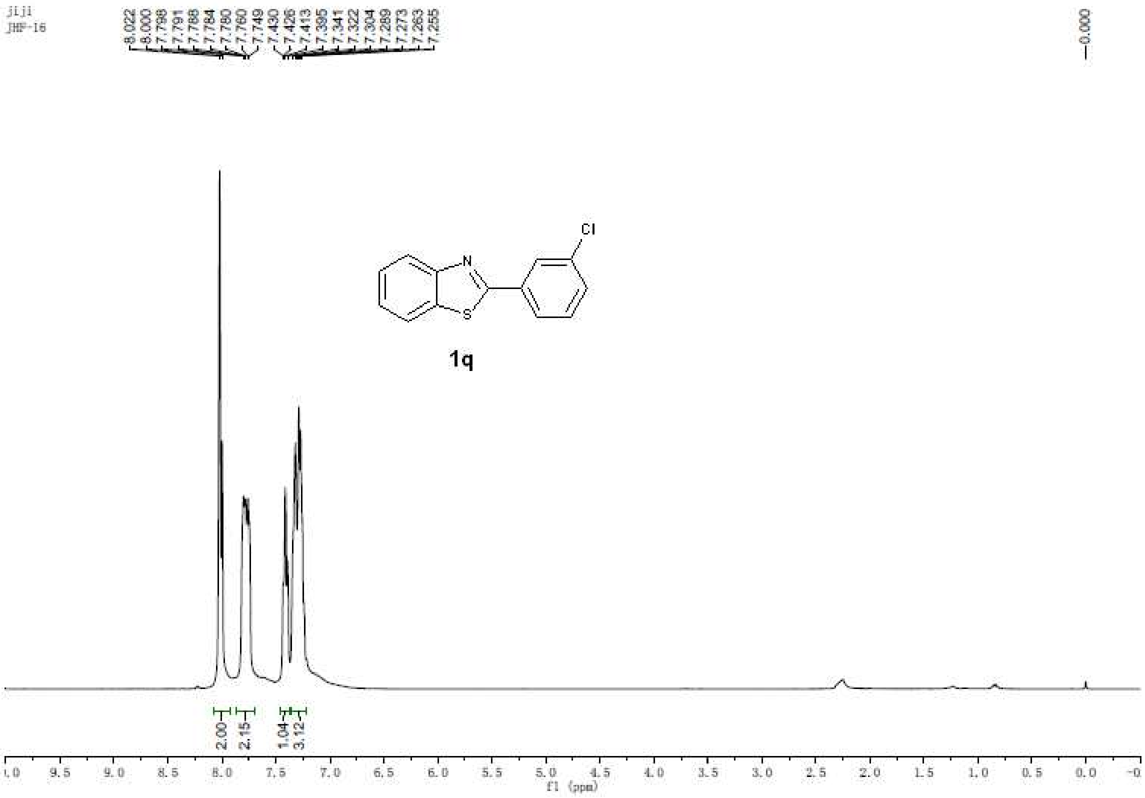

Jihuafang
JHF-13
168.325
154.200
138.831
135.102
133.564
131.637
128.941
128.026
126.314
125.149
124.915
123.218
121.642
77.617
77.299
76.981
21.399
CH3
N
S
1n
f1 (ppm)

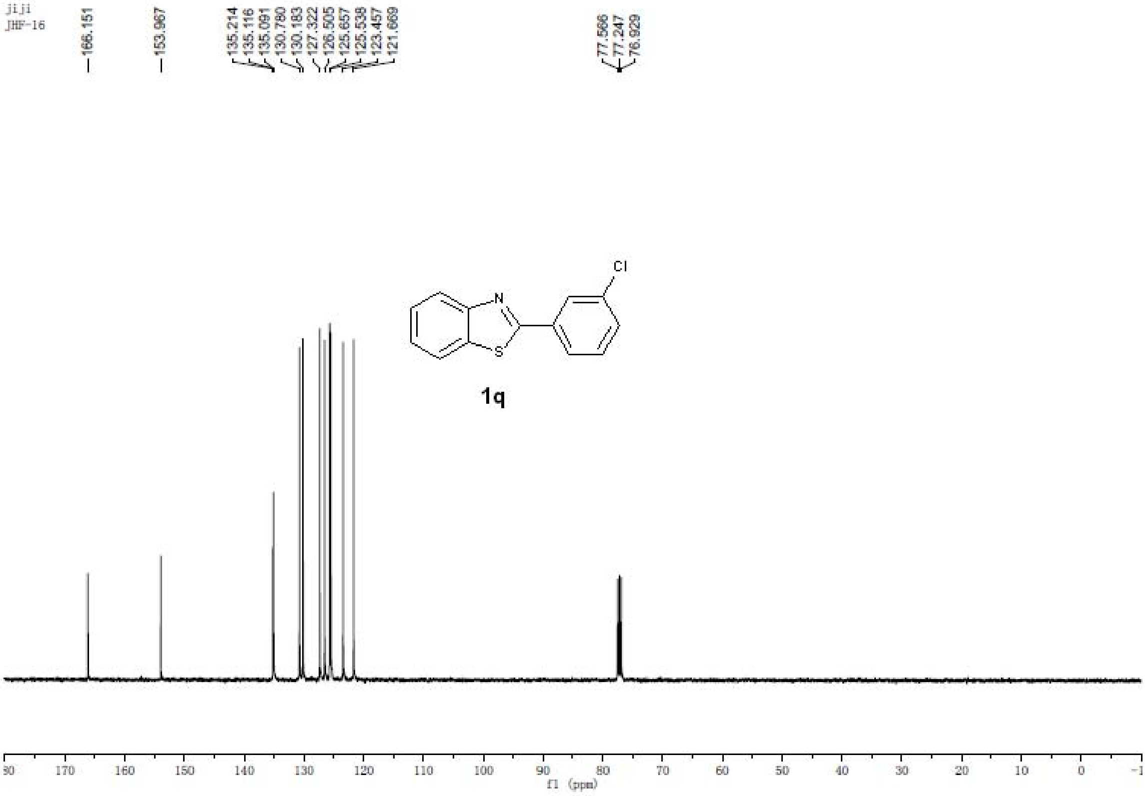

JJJ1
JMP-14
7.933
7.911
7.856
7.790
7.777
7.411
7.390
7.336
7.317
7.283
7.266
2.415
0.000
CH3
N
S
Cl
1o
1.02
1.00
2.00
1.02
1.07
1.04
3.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

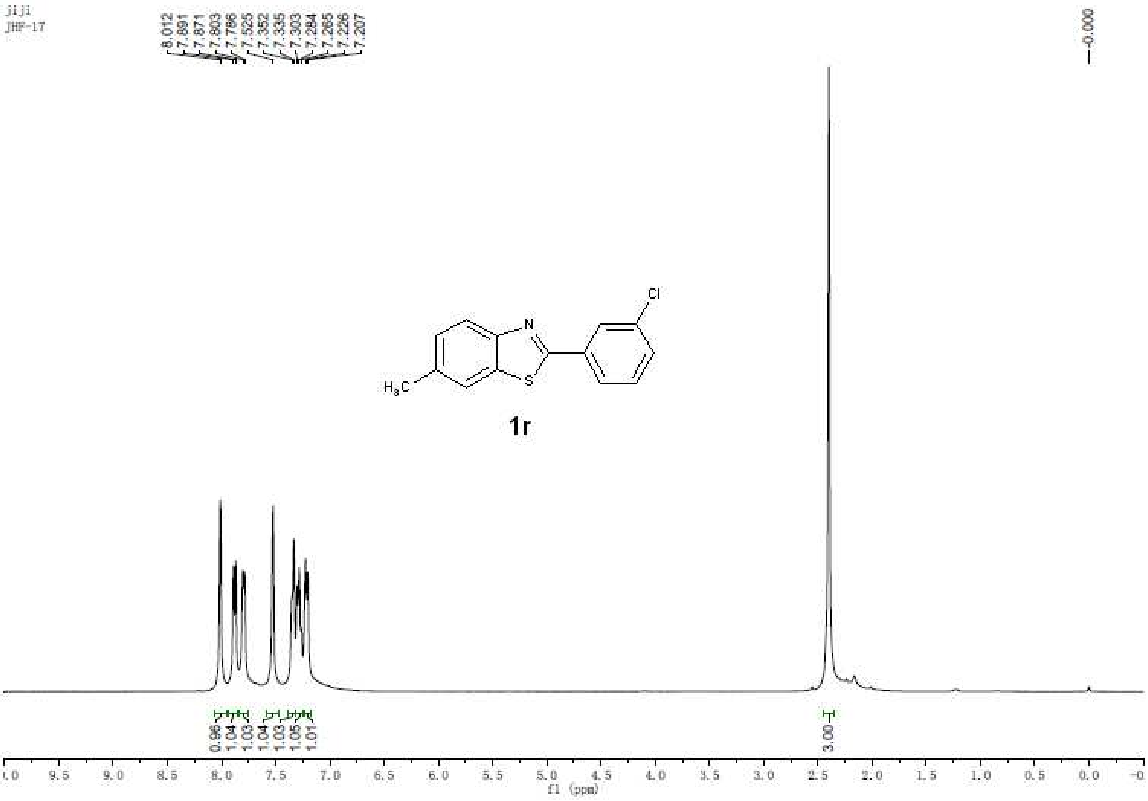

JJJ1
JMP-14
168.790
152.654
138.934
136.181
133.106
132.080
130.989
128.974
127.961
127.066
124.831
123.839
121.187
77.428
77.110
76.793
21.361
CH3
N
S
Cl
1o
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


jiji
JHP-15
7.937
7.926
7.916
7.794
7.726
7.711
7.433
7.414
7.279
7.266
7.250
7.207
7.191
7.149
7.143
7.136
7.133
7.114
2.356
0.000
CH3
N
S
F
1p
1.00
1.02
1.04
1.03
1.08
1.04
1.07
3.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

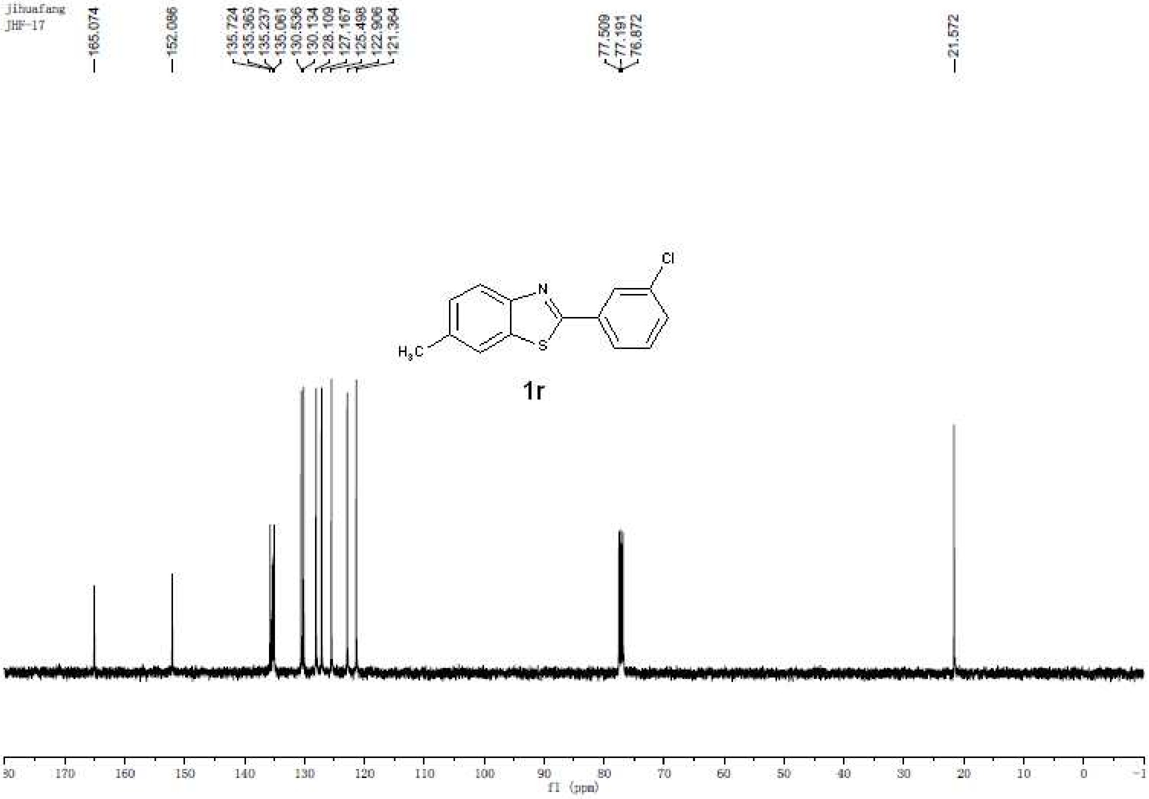

jihuafeng
JHP-15
167.982
167.951
161.643
159.201
150.742
138.840
136.063
135.962
133.225
131.828
128.905
127.820
124.709
124.060
123.967
114.937
114.692
107.891
107.625
77.545
77.227
76.909
21.311
CH3
N
S
F
1p
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


jiji
JHF-16
8.022
8.000
7.798
7.791
7.788
7.784
7.780
7.760
7.749
7.430
7.426
7.413
7.395
7.341
7.322
7.304
7.289
7.273
7.263
7.255
0.000
Cl
N
S
1q
2.00
2.15
1.04
3.12
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


jiji
JHF-16
166.151
153.967
135.214
135.116
135.091
130.780
130.183
127.322
126.505
125.657
125.538
123.457
121.669
77.566
77.247
76.929
Cl
N
S
1q
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


jiji
JHF-17
8.012
7.891
7.871
7.803
7.786
7.525
7.352
7.335
7.303
7.284
7.265
7.226
7.207
0.000
Cl
N
S
H3C
0.96
1.04
1.03
1.04
1.03
1.05
1.01
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

1r


jihuafang
JHF-17
165.074
152.086
135.724
135.363
135.237
135.061
130.536
130.134
128.109
127.167
125.496
122.906
121.364
77.509
77.191
76.872
21.572
Cl
N
S
H3C
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

1r