Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Content

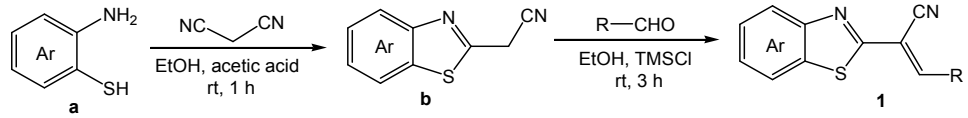
1. General information

The products were purified by column chromatography on silica gel (200-300 mesh). For thin-layer chromatography (TLC) analysis, silica gel plates (HSGF254) were used. Visualization of the developed TLC plates was performed with ultraviolet irradiation (254 nm) or staining potassium permanganate solution followed by heating using a heat gun. High resolution mass spectra on a Bruker Apex IV RTMS spectrometer. ^{1}H and ^{13}C NMR spectra were recorded on Bruker AVANCE-400 (400 MHz) spectrometer. Chemical shifts were reported in parts per million (ppm, δ), and the residual solvent peak was used as an internal reference: proton (chloroform δ 7.26 ppm), carbon (chloroform δ 77.0 ppm) or tetramethylsilane (TMS δ 0.00 ppm) was used as a reference. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), bs (broad singlet). Coupling constants were reported in Hertz (Hz). Melting points were determined on a SGW X-4 melting apparatus. Analytical HPLC was performed on a Thermo 3000 Series instrument using Daicel Chiralcel® columns as noted.

All reactions were carried out under argon atmosphere. All solvents were purified and dried according to standard methods prior to use. Racemic samples were prepared by using racemic BINAP as ligand.

2. General procedure for the preparation of substrates 1.

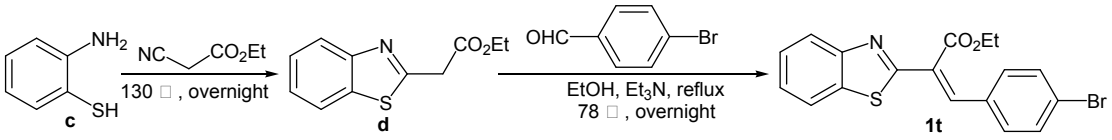
*Preparation of **1a-1s**, **1u** and **1v**.[1]*



Scheme S1. Preparation of substrates **1**

A solution of 2-aminothiophenol **a** (30 mmol), malononitrile (30 mmol) and acetic acid (30 mmol) in ethanol (50 mL) was stirred at room temperature for 1 h. The precipitate was filtered off and recrystallized from ethanol to afford benzothiazol-2-yl acetonitrile **b**. A solution of the corresponding aldehyde (5 mmol), benzothiazol-2-yl acetonitrile (5 mmol) and TMSCl (1.3 mL) in EtOH (10 mL) was stirred at room temperature for 3 h. Then, the mixture was poured into H_2O (20 mL), the precipitated solid was filtered and washed by *i*-PrOH to afford the product **1a-1s, 1u** and **1v**. All the substrates **1** were listed in **Figure S1**.

*Preparation of **1t**.*



Scheme S2. Preparation of substrates **1t**.

A mixture of 2-aminothiophenol **c** (20 mmol), ethyl cyanoacetate (20 mmol) was stirred at 130 ℃ for overnight. The residue was purified by flash column chromatography (5% EtOAc in petroleum ether, silica gel) to afford benzothiazol-2-yl acetic acid ethyl ester **d**. A solution of the corresponding aldehyde (5 mmol), benzothiazol-2-yl acetic acid ethyl ester **d** (5 mmol) and Et_3N (2.0 equiv) in EtOH (10 mL) was stirred at 78 ℃ for overnight and then concentrated in *vacuo*. The crude reaction mixture was purified by flash column chromatography (1.5% EtOAc in petroleum ether, silica gel) to afford the product **1t**.

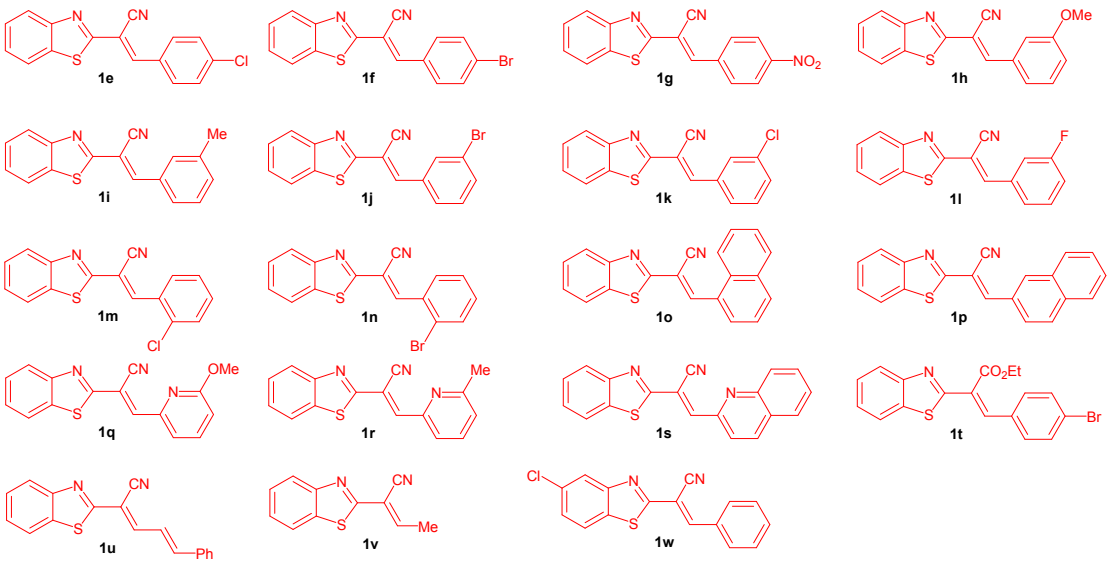


Figure S1. Structures of substrates **1**.

3. General procedure for the preparation of substrates 2.

Substrates **2** were synthesized from the 2-methylene-1,3-propanediol.[2]

Scheme S3. Preparation of substrates **2**.

To a solution of 2-methylene-1,3-propanediol (25 mmol) in anhydrous CH_2Cl_2 (25 mL) was added pyridine (50 mmol) at 0 °C and stirred for 10 minutes. To the mixture was added a solution of chloroformate (26 mmol) in anhydrous CH_2Cl_2 (25 mL) dropwise for 40 minutes. After stirring for 2 h, the reaction mixture was quenched with H_2O, extracted with CH_2Cl_2 and then concentrated in *vacuo*. The residue was purified by flash chromatography by silica gel (PE/EA = 5/1) to afford allyl carbonate **2** as a colorless oil. All the substrates **2** were listed in **Figure S2**.

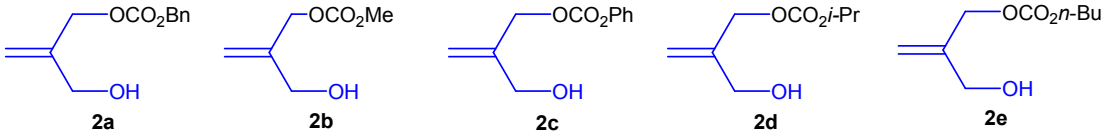


Figure S2. Structures of substrates **2**.

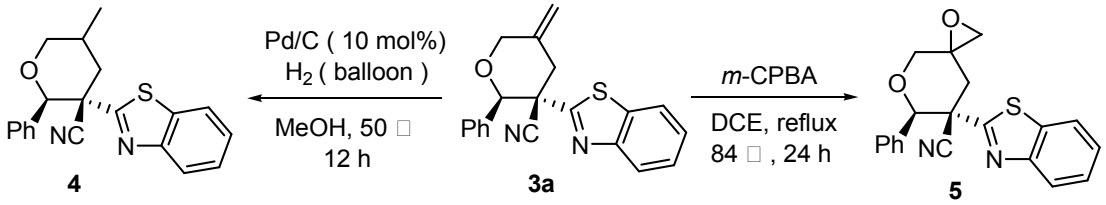
4. General procedure for the synthetic transformation of 3a

*Preparation of **4**.*

To a solution of **3a** (33 mg, 0.1 mmol) in EtOH (1 mL) was added Pd/C (23 mg) and the mixture was stirred at 50 ℃ under H_2 atmosphere (ballon) for 12 h. The conversion was monitored by TLC. The mixture was filtrated through a pad of Celite and the filtration was concentrated in *vacuo*, the residue was purified by column chromatography on silica gel to afford the product **4** in 90% yield (30.1 mg).

*Preparation of **5**.*

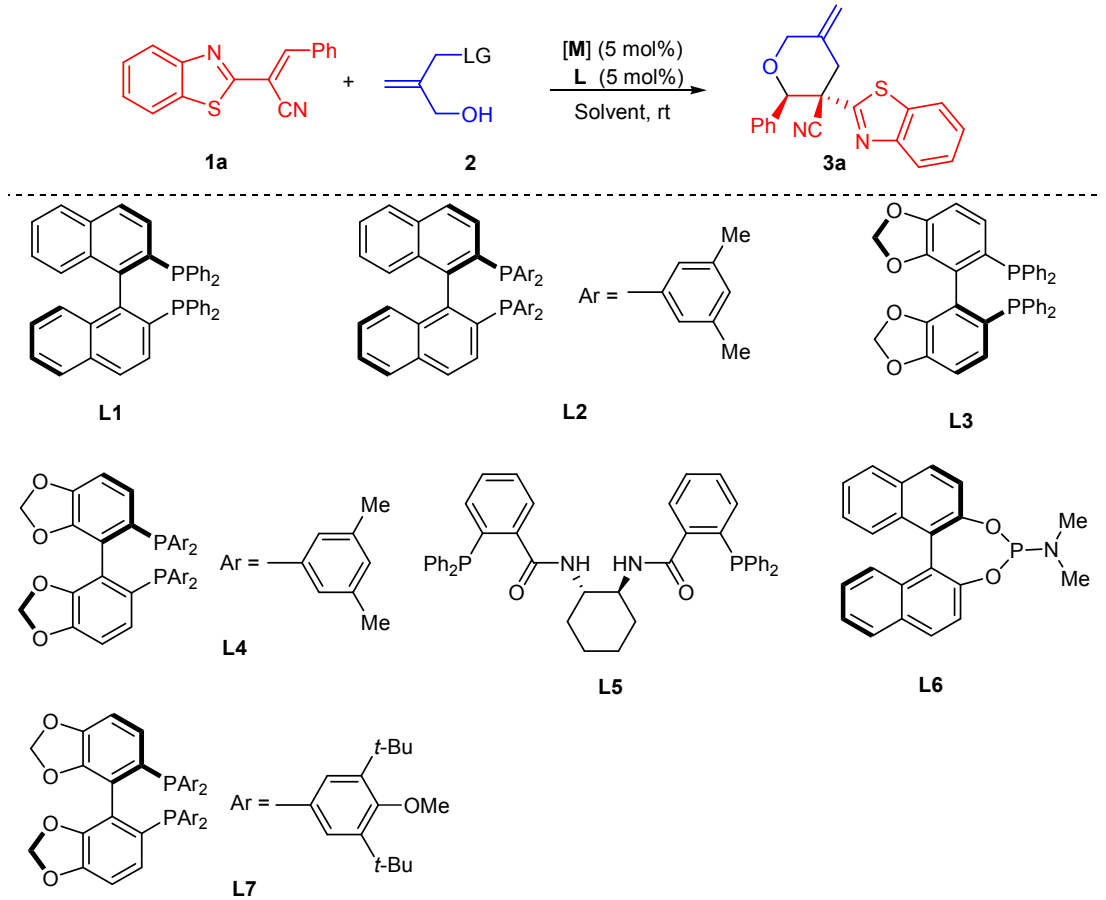
To a solution of **3a** (33 mg, 0.1 mmol) in DCE (1 mL) was added *m*-CPBA (0.18 mmol, 31 mg) in three pots and the mixture was stirred at 84 ℃ for 24 h. After the reaction was completed, the solid was filtrated through a pad of Celite and the filtration was concentrated in *vacuo*, the residue was purified by column chromatography on silica gel to afford the product **5** in 61% yield (21.3 mg).



Scheme S4. Synthetic transformation of 3a

5. Screening of asymmetric reaction Conditions.

Table S1. Optimization of the reaction conditions.[a]



Entry	LG	[M] (mol %)	L	Solvent	t (h)	dr (%)[c]	Yield (%)[b]	ee (%)[d]
1	OCO_2Bn	$Pd(OAc)_2$	**L1**	THF	15	>20:1	95	5
2	OCO_2Bn	$Pd_2(dba)_3$	**L1**	THF	24	-	NR	-
3	OCO_2Bn	$Pd(dba)_2$	**L1**	THF	24	-	NR	-
4	OCO_2Bn	$Pd_2(dba)_3{\cdot}CHCl_3$	**L1**	THF	24	-	NR	-
5	OCO_2Bn	$Pd(MeCN)_2Cl_2$	**L1**	THF	24	-	NR	-
6	OCO_2Bn	$[IrCl(cod)_2]_2$	**L1**	THF	24	-	NR	-

7	OCO_2Bn	$Pd(OAc)_2$	**L1**	Et_2O	12	>20:1	85	6
8	OCO_2Bn	$Pd(OAc)_2$	**L1**	1,4-Dioxane	24	-	NR	-
9	OCO_2Bn	$Pd(OAc)_2$	**L1**	Toluene	24	-	NR	-
10	OCO_2Bn	$Pd(OAc)_2$	**L1**	DCM	24	-	NR	
11	OCO_2Bn	$Pd(OAc)_2$	**L1**	MeCN	24	-	NR	
12	OCO_2Bn	$Pd(OAc)_2$	**L1**	TBME	12	>20:1	95	12
13	OCO_2Bn	$Pd(OAc)_2$	**L2**	TBME	20	>20:1	92	3
14	OCO_2Bn	$Pd(OAc)_2$	**L3**	TBME	20	-	NR	-
15	**OCO_2Bn**	**$Pd(OAc)_2$**	**L4**	TBME	**24**	**>20:1**	**95**	**37**
16	OCO_2Bn	$Pd(OAc)_2$	**L5**	TBME	24	-	NR	-
17	OCO_2Bn	$Pd(OAc)_2$	**L6**	TBME	24	-	NR	-
18	OCO_2Bn	$Pd(OAc)_2$	**L7**	TBME	24	-	NR	-
19	OCO_2Me	$Pd(OAc)_2$	**L4**	TBME	48	>20:1	96	34
20	OCO_2Ph	$Pd(OAc)_2$	**L4**	TBME	70	>20:1	98	33
21	OCO_2i-Pr	$Pd(OAc)_2$	**L4**	TBME	48	>20:1	99	34
22	OCO_2n-Bu	$Pd(OAc)_2$	**L4**	TBME	70	>20:1	95	33
23[e]	OCO_2Bn	$Pd(OAc)_2$	**L3**	TBME	24	-	NR	-
24[e]	OCO_2Bn	$Pd(OAc)_2$	**L5**	TBME	24	-	NR	-
25[e]	OCO_2Bn	$Pd(OAc)_2$	**L6**	TBME	24	-	NR	-
26[e]	OCO_2Bn	$Pd(OAc)_2$	**L7**	TBME	24	-	NR	-

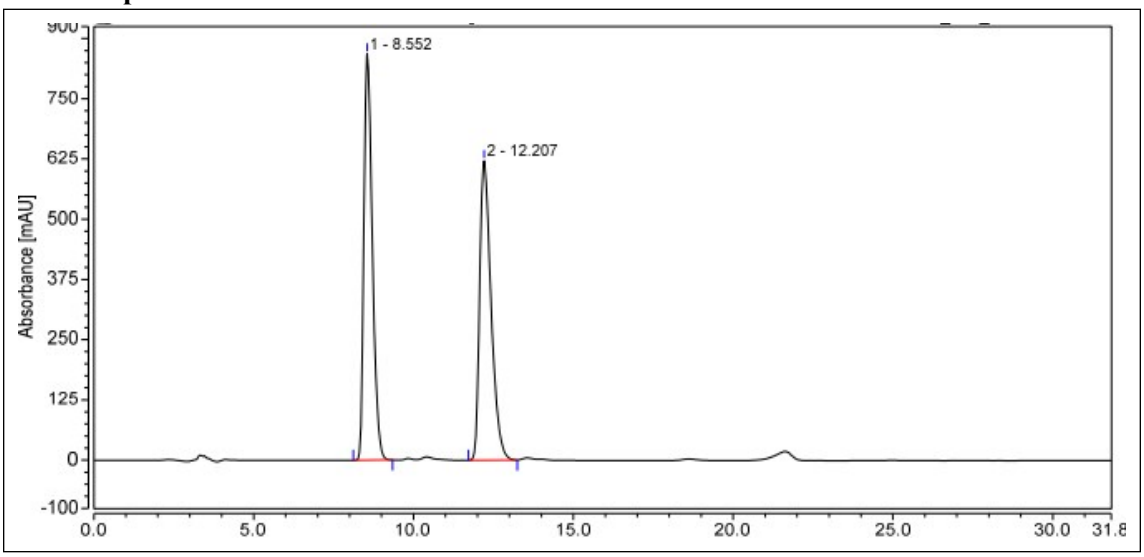
[a] General conditions: **1a** (0.1 mmol), **2a** (0.15 mmol), [Pd] (5 mol %), and **L** (5 mol %) in solvent (1.0 mL) at room temperature. [b] All yields refer to the isolated yields. [c] The dr values were determined by ^{1}H NMR spectroscopy. [d] Enantiomeric excess was determined by chiral HPLC. NR = No reaction. [e] 50 ℃.

HPLC acquisition parameters:

Chiral column: CHIRALCEL ® OD-H, Wave length: 254 nm,

Mobile phase: *n*-hexane:*i*-PrOH =5:95, Flow rate: 1.0 mL/min, Temperature: 30 ℃.

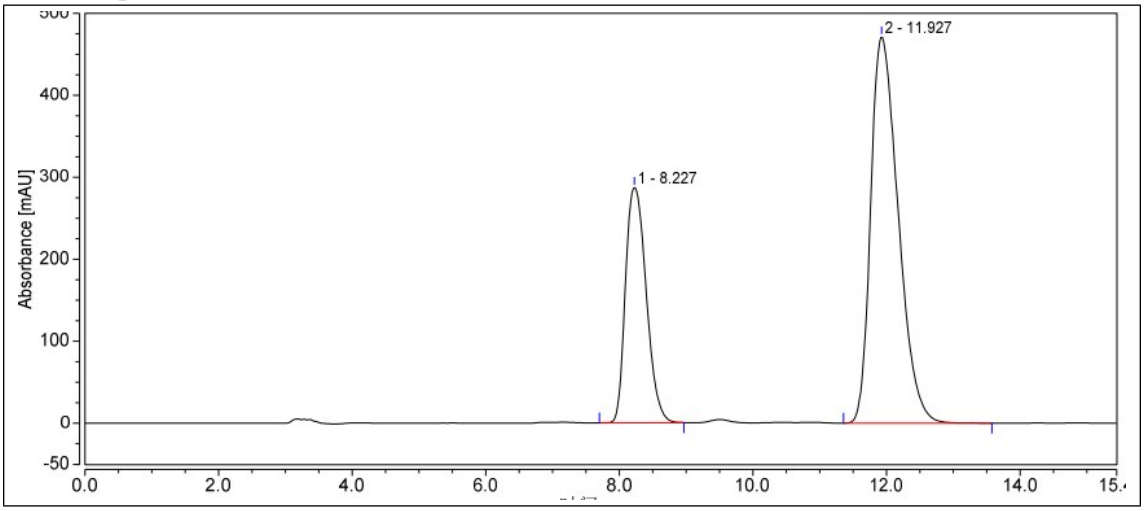
HPLC Spectra of racemic 3a



Peak	RetTime	Area	Height	Area	Height

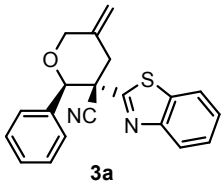
	(min)	(mAu*min)	(mAu)	(%)	(%)
1	8.552	258.716	842.896	50.13	57.55
2	12.207	257.398	621.718	49.87	42.45

HPLC Spectra of enantiomeric 3a



Peak	RetTime (min)	Area (mAu*min)	Height (mAu)	Area (%)	Height (%)
1	8.227	103.068	287.026	31.42	37.86
2	11.927	224.932	471.163	68.58	62.14

6. Analytical data



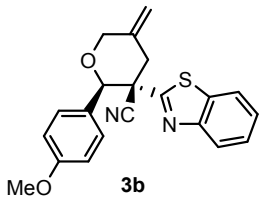
3a

The compound **3a** was prepared according to the general procedure. The product was obtained as a white solid (31.6 mg, 95% yield). Melting point 130-132 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.3, 0.9 Hz, 1H), 7.78 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.70 – 7.44 (m, 1H), 7.48 – 7.30 (m, 1H), 7.25 – 7.17 (m, 1H), 7.15 (d, *J* = 4.3 Hz, 4H), 5.34 – 5.26 (m, 1H), 5.24 – 5.17 (m, 1H), 5.09 (s, 1H), 4.62 (dd, *J* = 12.6, 1.9 Hz, 1H), 4.41 (d, *J* = 12.5 Hz, 1H), 3.68 (dd, *J* = 14.0, 1.6 Hz, 1H), 3.10 (dd, *J* = 14.0, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.94, 153.08, 137.00, 135.96, 134.56, 128.87, 128.12, 127.03, 126.62, 125.75, 123.26, 121.80, 118.34, 115.20, 84.76, 73.03, 53.25, 43.58.

HRMS (ESI) m/z Calcd for $C_{20}H_{16}N_2OS$, $[M+H]^+$: 333.1056; Found:333.1051.



3b

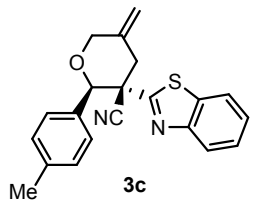
The compound **3b** was prepared according to the general procedure. The product was obtained as a white solid (28.3 mg, 78% yield). Melting point 65-67 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (dt, *J* = 8.2, 0.9 Hz, 1H), 7.79 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.53 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.41 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H), 7.15 – 6.92 (m, 2H), 6.82 – 6.55 (m, 2H), 5.27 (q, *J* = 1.4 Hz, 1H), 5.22 – 5.15 (m, 1H), 5.04 (s, 1H), 4.60 (dd, *J* = 12.6, 1.9 Hz, 1H), 4.39 (d, *J* = 12.5 Hz, 1H), 3.71 (s, 3H), 3.69 – 3.60 (m, 1H), 3.08 (dd, *J* = 14.0, 1.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.12, 159.84, 153.07, 137.11, 134.58, 128.27, 128.22, 126.58,

125.71, 123.24, 121.82, 118.52, 115.11, 113.49, 84.42, 73.09, 55.14, 53.42, 43.50.

HRMS (ESI) m/z Calcd for $C_{21}H_{18}N_2O_2S$, $[M+H]^+$: 363.1162; Found: 363.1160.



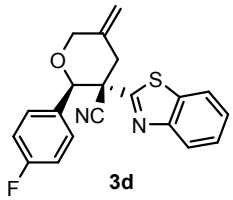
3c

The compound **3c** was prepared according to the general procedure. The product was obtained as a white solid (33.3 mg, 96% yield). Melting point 128-130 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.2, 0.9 Hz, 1H), 7.79 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.53 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.41 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H), 7.04 (d, *J* = 8.2 Hz, 2H), 6.95 (d, *J* = 8.0 Hz, 2H), 5.27 (t, *J* = 1.5 Hz, 1H), 5.23 – 5.14 (m, 1H), 5.06 (s, 1H), 4.60 (dd, *J* = 12.5, 1.8 Hz, 1H), 4.40 (d, *J* = 12.5 Hz, 1H), 3.66 (dd, *J* = 14.0, 1.6 Hz, 1H), 3.09 (dd, *J* = 13.9, 1.8 Hz, 1H), 2.23 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.08, 153.08, 138.61, 137.10, 134.57, 133.01, 128.80, 126.89, 126.58, 125.70, 123.25, 121.80, 118.47, 115.08, 84.63, 73.03, 53.32, 43.62, 21.18.

HRMS (ESI) m/z Calcd for $C_{21}H_{18}N_2OS$, $[M+H]^+$: 347.1213 ; Found: 347.1218.



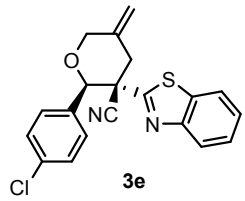
3d

The compound **3d** was prepared according to the general procedure. The product was obtained as a white solid (30.8 mg, 88% yield). Melting point 113-115 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.2 Hz, 1H), 7.89 – 7.70 (m, 1H), 7.54 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.43 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H), 7.19 – 7.04 (m, 2H), 6.93 – 6.65 (m, 2H), 5.28 (q, *J* = 1.4 Hz, 1H), 5.21 – 5.15 (m, 1H), 5.09 (s, 1H), 4.60 (dd, *J* = 12.6, 1.9 Hz, 1H), 4.40 (d, *J* = 12.6 Hz, 1H), 3.65 (dd, *J* = 14.0, 1.6 Hz, 1H), 3.09 (dd, *J* = 14.0, 1.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.74, 164.12, 161.66, 153.07, 136.79, 134.47, 131.92, 131.89, 128.89, 128.80, 126.72, 125.88, 123.28, 121.85, 118.20, 115.35, 115.21, 114.99, 84.00, 73.06, 53.29 , 43.51.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}FN_2OS$, $[M+H]^+$: 351.0962; Found: 351.0960.



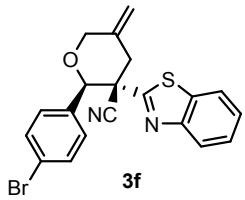
3e

The compound **3e** was prepared according to the general procedure. The product was obtained as a white solid (30.4 mg, 83% yield). Melting point 161-163 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.3, 0.9 Hz, 1H), 7.81 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.55 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.43 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.18 – 6.97 (m, 4H), 5.28 (p, *J* = 1.2 Hz, 1H), 5.23 – 5.16 (m, 1H), 5.10 (s, 1H), 4.60 (dd, *J* = 12.5, 1.8 Hz, 1H), 4.40 (d, *J* = 12.6 Hz, 1H), 3.79 – 3.59 (m, 1H), 3.09 (dd, *J* = 13.9, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.60, 153.07, 136.69, 134.77, 134.53, 134.45, 128.41, 128.32, 126.76, 125.92, 123.29, 121.90, 118.11, 115.40, 83.91, 73.00, 53.17, 43.57.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}ClN_2OS$, $[M+H]^+$: 367.0666; Found: 367.0662.



3f

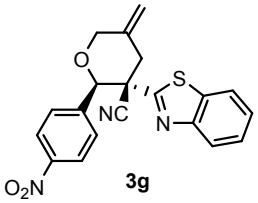
The compound **3f** was prepared according to the general procedure. The product was obtained as a white solid (39.1 mg, 95% yield). Melting point 182-184ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (dt, *J* = 8.3, 0.9 Hz, 1H), 7.94 – 7.72 (m, 1H), 7.55 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.43 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.30 – 7.26 (m, 2H), 7.09 – 6.86 (m, 2H), 5.28 (d, *J* = 1.7 Hz, 1H), 5.24 – 5.13 (m, 1H), 5.09 (s, 1H),

4.60 (dd, *J* = 12.6, 1.9 Hz, 1H), 4.39 (d, *J* = 12.5 Hz, 1H), 3.64 (dq, *J* = 14.0, 1.8 Hz, 1H), 3.09 (dd, *J* = 14.0, 1.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.57, 153.07, 136.68, 135.04, 134.45, 131.26, 128.71, 126.76, 125.93, 123.29, 123.07, 121.92, 118.08, 115.40, 83.93, 72.99, 53.11, 43.60.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}BrN_2OS$, $[M+H]^+$: 411.0161; Found: 411.0165.



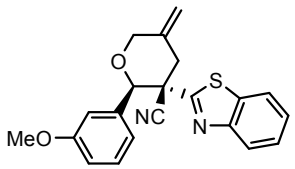
3g

The compound **3g** was prepared according to the general procedure. The product was obtained as a white solid (30.6 mg, 81% yield). Melting point 148-150 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (dt, *J* = 8.2, 0.9 Hz, 1H), 8.04 – 7.89 (m, 2H), 7.82 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.57 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.46 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.35 – 7.28 (m, 2H), 5.34 – 5.29 (m, 1H), 5.27 (s, 1H), 5.24 – 5.19 (m, 1H), 4.63 (dd, *J* = 12.6, 1.8 Hz, 1H), 4.43 (d, *J* = 12.6 Hz, 1H), 3.65 (dd, *J* = 14.0, 1.5 Hz, 1H), 3.12 (dd, *J* = 13.9, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.96, 153.07, 148.10, 142.86, 136.19, 134.29, 128.13, 127.00, 126.20, 123.36, 123.19, 121.98, 117.66, 115.80, 83.42, 72.94, 52.96, 43.69.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}N_3O_3S$, $[M+H]^+$: 378.0907; Found: 378.0905 .



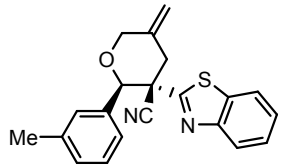
3h

The compound **3h** was prepared according to the general procedure. The product was obtained as a white solid (29.0 mg, 80% yield). Melting point 96-98 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.3, 0.9 Hz, 1H), 7.79 (ddd, *J* = 8.0, 1.2, 0.6 Hz, 1H), 7.53 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.41 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H), 7.01 (td, *J* = 7.8, 0.9 Hz, 1H), 6.75 (dt, *J* = 9.2, 1.4 Hz, 2H), 6.66 (dt, *J* = 7.6, 1.3 Hz, 1H), 5.36 – 5.25 (m, 1H), 5.20 (t, *J* = 1.4 Hz, 1H), 5.07 (s, 1H), 4.62 (dd, *J* = 12.5, 1.8 Hz, 1H), 4.41 (d, *J* = 12.4 Hz, 1H), 3.68 (dd, *J* = 14.0, 1.5 Hz, 1H), 3.51 (s, 3H), 3.10 (dd, *J* = 14.0, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.04, 159.23, 153.08, 137.30, 136.95, 134.59, 129.08, 126.63, 125.77, 123.18, 121.82, 119.33, 118.40, 115.75, 115.25, 111.30, 84.81, 73.03, 54.96, 53.22, 43.50.

HRMS (ESI) m/z Calcd for $C_{21}H_{18}N_2O_2S$, $[M+H]^+$: 363.1162 ; Found: 363.1158.



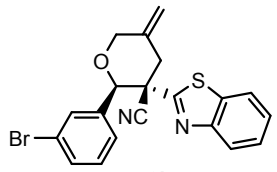
3i

The compound **3i** was prepared according to the general procedure. The product was obtained as a white solid (31.2 mg, 90% yield). Melting point 133-135 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.3, 0.9 Hz, 1H), 7.78 (dt, *J* = 8.1, 0.9 Hz, 1H), 7.53 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.49 – 7.36 (m, 1H), 7.06 (d, *J* = 1.9 Hz, 1H), 7.05 – 6.93 (m, 2H), 6.90 – 6.77 (m, 1H), 5.28 (d, *J* = 1.6 Hz, 1H), 5.24 – 5.12 (m, 1H), 5.05 (s, 1H), 4.61 (dd, *J* = 12.5, 1.8 Hz, 1H), 4.40 (d, *J* = 12.6 Hz, 1H), 3.68 (dq, *J* = 13.8, 1.8 Hz, 1H), 3.10 (dd, *J* = 14.0, 1.8 Hz, 1H), 2.16 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.02, 153.04, 137.86, 137.06, 135.82, 134.56, 129.59, 127.86, 127.56, 126.59, 125.72, 124.16, 123.22, 121.74, 118.37, 115.17, 84.88, 73.06, 53.23, 43.53, 21.29.

HRMS (ESI) m/z Calcd for $C_{21}H_{18}N_2OS$, $[M+H]^+$: 347.1213; Found: 347.1211.



3j

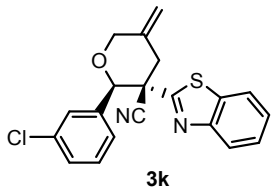
The compound **3j** was prepared according to the general procedure.

The product was obtained as a white solid (26.7 mg, 65% yield). Melting point 137-139 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.2 Hz, 1H), 7.81 (d, *J* = 8.1 Hz, 1H), 7.55 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.50 – 7.38 (m, 1H), 7.34 (d, *J* = 3.8 Hz, 2H), 7.05 – 6.91 (m, 2H), 5.29 (d, *J* = 1.7 Hz, 1H), 5.22 – 5.17 (m, 1H), 5.08 (s, 1H), 4.61 (dd, *J* = 12.6, 1.8 Hz, 1H), 4.39 (d, *J* = 12.6 Hz, 1H), 3.64 (dd, *J* = 14.0, 1.6 Hz, 1H), 3.10 (dd, *J* = 14.0, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.48, 153.05, 138.10, 136.60, 134.43, 131.95, 130.20, 129.56, 126.77, 125.94, 125.60, 123.30, 122.21, 121.85, 117.95, 115.50, 83.82, 73.00, 53.09, 43.56.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}BrN_2OS$, $[M+H]^+$: 411.0161; Found: 411.0163.



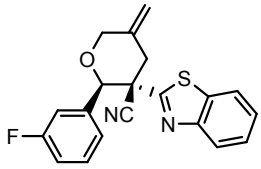
3k

The compound **3k** was prepared according to the general procedure. The product was obtained as a white solid (30.4 mg, 83% yield). Melting point 130-132 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.3, 0.9 Hz, 1H), 7.81 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.55 (ddd, *J* = 8.4, 7.3, 1.2 Hz, 1H), 7.43 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.23 – 7.13 (m, 2H), 7.04 (t, *J* = 7.8 Hz, 1H), 6.94 (dt, *J* = 7.9, 1.4 Hz, 1H), 5.29 (q, *J* = 1.5 Hz, 1H), 5.24 – 5.14 (m, 1H), 5.09 (s, 1H), 4.61 (dd, *J* = 12.6, 1.8 Hz, 1H), 4.40 (d, *J* = 12.6 Hz, 1H), 3.76 – 3.45 (m, 1H), 3.10 (dd, *J* = 13.9, 1.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.50, 153.05, 137.90, 136.62, 134.44, 134.12, 129.27, 129.03, 127.33, 126.76, 125.93, 125.18, 123.30, 121.83, 117.97, 115.45, 83.87, 72.99, 53.07, 43.61.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}ClN_2OS$, $[M+H]^+$: 367.0666; Found: 367.0661.



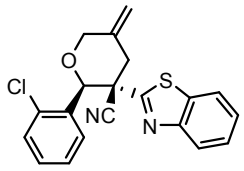
3l

The compound **3l** was prepared according to the general procedure. The product was obtained as a white solid (32.2 mg, 92% yield). Melting point 155-157 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.2, 0.8 Hz, 1H), 7.87 – 7.70 (m, 1H), 7.55 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.43 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H), 7.08 (td, *J* = 8.0, 5.8 Hz, 1H), 7.03 – 6.87 (m, 2H), 6.83 (dt, *J* = 7.8, 1.3 Hz, 1H), 5.29 (q, *J* = 1.5 Hz, 1H), 5.23 – 5.15 (m, 1H), 5.12 (s, 1H), 4.61 (dd, *J* = 12.6, 1.8 Hz, 1H), 4.40 (d, *J* = 12.5 Hz, 1H), 3.65 (dq, *J* = 14.0, 1.8 Hz, 1H), 3.10 (dd, *J* = 13.9, 1.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.57, 163.59, 161.14, 153.07, 138.41, 138.34, 136.65, 134.45, 129.62, 129.54, 126.76, 125.92, 123.30, 122.75, 122.72, 121.84, 118.05, 115.95, 115.74, 115.42, 114.41, 114.18, 83.90, 72.98, 53.07, 43.68.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}FN_2OS$, $[M+H]^+$: 351.0962; Found: 351.0966.



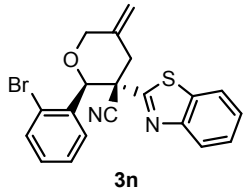
3m

The compound **3m** was prepared according to the general procedure. The product was obtained as a white solid (31.5 mg, 86% yield). Melting point 161-163 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.99 (m, 2H), 7.77 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.50 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.40 (tdd, *J* = 7.2, 3.6, 1.3 Hz, 2H), 7.23 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.07 (dd, *J* = 8.0, 1.3 Hz, 1H), 5.42 (s, 1H), 5.29 (d, *J* = 1.6 Hz, 1H), 5.26 – 5.19 (m, 1H), 4.59 (dd, *J* = 12.5, 1.8 Hz, 1H), 4.41 (d, *J* = 12.6 Hz, 1H), 3.94 (dq, *J* = 14.1, 1.8 Hz, 1H), 3.16 (dd, *J* = 14.1, 1.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.86, 152.65, 136.99, 135.55, 133.77, 133.72, 130.22, 129.43, 128.71, 127.24, 126.52, 125.77, 123.54, 121.62, 118.57, 115.36, 80.05, 73.18 , 52.49, 42.42.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}ClN_2OS$, $[M+H]^+$: 367.0666; Found: 367.0662.



3n

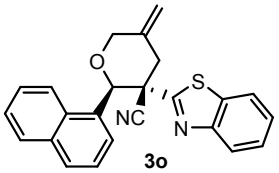
The compound **3n** was prepared according to the general procedure. The

product was obtained as a white solid (26.3 mg, 64% yield). Melting point 164-166 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 – 7.91 (m, 2H), 7.83 – 7.69 (m, 1H), 7.57 – 7.34 (m, 3H), 7.29 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.18 (td, *J* = 7.8, 1.7 Hz, 1H), 5.39 (s, 1H), 5.29 (d, *J* = 1.4 Hz, 1H), 5.25 – 5.18 (m, 1H), 4.59 (dd, *J* = 12.6, 1.8 Hz, 1H), 4.41 (d, *J* = 12.5 Hz, 1H), 3.94 (dd, *J* = 14.1, 1.6 Hz, 1H), 3.17 (dd, *J* = 14.1, 1.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.80, 152.59, 137.01, 135.77, 135.34, 132.11, 130.55, 129.76, 127.84, 126.51, 125.77, 124.38, 123.58, 121.62, 118.61, 115.38, 82.40, 73.21, 52.42, 42.43.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}BrN_2OS$, $[M+H]^+$: 411.0161; Found: 411.0164.



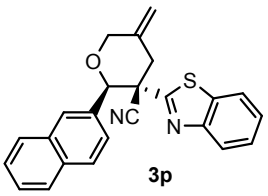
3o

The compound **3o** was prepared according to the general procedure. The product was obtained as a white solid (29.1 mg, 76% yield). Melting point 178-180 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 7.3, 1.2 Hz, 1H), 8.02 (dd, *J* = 8.6, 1.1 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.63 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.45 (dtd, *J* = 7.4, 2.9, 1.3 Hz, 3H), 7.26 – 7.20 (m, 1H), 7.07 (ddd, *J* = 8.0, 6.8, 1.0 Hz, 1H), 6.79 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 5.78 (s, 1H), 5.34 (q, *J* = 1.5 Hz, 1H), 5.29 – 5.21 (m, 1H), 4.69 (dd, *J* = 12.6, 1.8 Hz, 1H), 4.52 (d, *J* = 12.6 Hz, 1H), 4.16 – 3.93 (m, 1H), 3.20 (dd, *J* = 14.1, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.09, 152.64, 137.25, 135.14, 132.62, 131.99, 130.53, 129.50, 128.38, 126.34, 125.94, 125.46, 125.31, 124.96, 123.10, 121.80, 121.35, 118.78, 115.28, 112.73, 79.97, 73.48, 53.52, 42.99.

HRMS (ESI) m/z Calcd for $C_{24}H_{18}N_2OS$, $[M+H]^+$: 383.1213; Found: 383.1221.



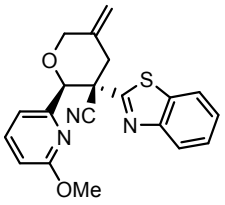
3p

The compound **3p** was prepared according to the general procedure. The product was obtained as a white solid (32.5 mg, 85% yield). Melting point 128-130 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.2 Hz, 1H), 7.79 – 7.69 (m, 3H), 7.68 – 7.60 (m, 1H), 7.61 – 7.49 (m, 2H), 7.48 – 7.32 (m, 3H), 7.16 (dd, *J* = 8.5, 1.7 Hz, 1H), 5.32 (d, *J* = 1.8 Hz, 1H), 5.28 (s, 1H), 5.24 (d, *J* = 1.9 Hz, 1H), 4.67 (dd, *J* = 12.6, 1.8 Hz, 1H), 4.47 (d, *J* = 12.5 Hz, 1H), 3.74 (dq, *J* = 14.0, 1.7 Hz, 1H), 3.14 (dd, *J* = 13.9, 1.9 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.93, 153.09, 137.02, 134.56, 133.50, 133.39, 132.80, 128.42, 127.71, 127.54, 126.73, 126.64, 126.37, 126.06, 125.76, 124.48, 123.24, 121.82, 118.38, 115.28, 84.81, 73.14, 53.38, 43.71.

HRMS (ESI) m/z Calcd for $C_{24}H_{18}N_2OS$, $[M+H]^+$: 383.1213; Found: 383.1212.



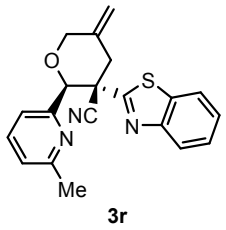
3q

The compound **3q** was prepared according to the general procedure. The product was obtained as a white solid (32.3 mg, 89% yield). Melting point 160-162 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.1 Hz, 1H), 7.86 – 7.68 (m, 1H), 7.65 – 7.45 (m, 2H), 7.45 – 7.34 (m, 1H), 7.16 (d, *J* = 7.3 Hz, 1H), 6.55 (d, *J* = 8.3 Hz, 1H), 5.27 (d, *J* = 1.8 Hz, 1H), 5.21 – 5.18 (m, 1H), 5.15 (s, 1H), 4.61 (dd, *J* = 12.5, 1.8 Hz, 1H), 4.42 (d, *J* = 12.5 Hz, 1H), 3.65 (dd, *J* = 13.9, 1.5 Hz, 1H), 3.14 (d, *J* = 1.8 Hz, 1H), 3.11 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.12, 162.58, 153.20, 152.70, 139.13, 136.85, 134.71, 126.50, 125.59, 123.17, 121.63, 118.47, 115.24, 115.10, 111.09, 84.76, 72.89, 52.69, 51.68, 43.89.

HRMS (ESI) m/z Calcd for $C_{20}H_{17}N_3O_2S$, $[M+H]^+$: 364.1114; Found: 364.1119.



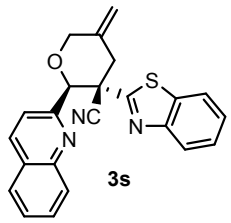
3r

The compound **3r** was prepared according to the general procedure. The product was obtained as a white solid (32.0 mg, 92% yield). Melting point 163-165 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.1 Hz, 1H), 7.81 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 1H), 7.49 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.43 – 7.35 (m, 2H), 6.95 (d, *J* = 7.6 Hz, 1H), 5.27 (d, *J* = 1.7 Hz, 1H), 5.23 – 5.19 (m, 1H), 5.18 (s, 1H), 4.62 (dd, *J* = 12.5, 1.8 Hz, 1H), 4.43 (d, *J* = 12.5 Hz, 1H), 3.68 (dq, *J* = 13.9, 1.8 Hz, 1H), 3.13 (dd, *J* = 13.9, 1.8 Hz, 1H), 1.98 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.09, 156.98, 154.54, 153.02, 136.91, 136.89, 134.76, 126.30, 125.48, 123.38, 123.00, 121.42, 118.90, 118.35, 115.23, 85.40, 72.95, 51.97, 43.47, 23.69.

HRMS (ESI) m/z Calcd for $C_{20}H_{17}N_3OS$, $[M+H]^+$: 348.1165; Found: 348.1166.



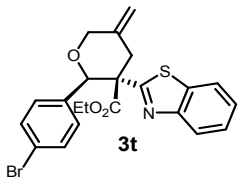
3s

The compound **3s** was prepared according to the general procedure. The product was obtained as a white solid (33.4 mg, 87% yield). Melting point 206-208 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.6 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.75 (dd, *J* = 11.1, 8.2 Hz, 3H), 7.47 (dddt, *J* = 1715.4, 11.2, 8.0, 3.4 Hz, 4H), 7.41 – 7.33 (m, 1H), 5.47 (s, 1H), 5.38 – 5.26 (m, 1H), 5.23 (d, *J* = 1.9 Hz, 1H), 4.68 (dd, *J* = 12.5, 1.8 Hz, 1H), 4.51 (d, *J* = 12.5 Hz, 1H), 3.71 (dt, *J* = 14.2, 2.0 Hz, 1H), 3.18 (dd, *J* = 13.9, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.49, 155.24, 153.04, 146.61, 136.86, 136.81, 134.80, 129.38, 129.24, 127.75, 127.41, 126.81, 126.30, 125.47, 123.31, 121.56, 119.55, 118.58, 115.32, 85.33, 73.04, 51.29, 43.98.

HRMS (ESI) m/z Calcd for $C_{23}H_{17}N_3OS$, $[M+H]^+$: 348.1165; Found: 384.1163.



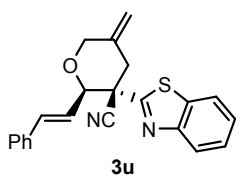
3t

The compound **3t** was prepared according to the general procedure. The product was obtained as a white solid (28.0 mg, 61% yield). Melting point 97-99 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.3, 0.9 Hz, 1H), 7.93 – 7.72 (m, 1H), 7.51 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.41 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H), 7.26 – 7.01 (m, 2H), 6.96 – 6.75 (m, 2H), 5.27 (s, 1H), 5.02 (d, *J* = 1.9 Hz, 1H), 4.96 (d, *J* = 2.0 Hz, 1H), 4.52 (d, *J* = 12.8 Hz, 1H), 4.40 (d, *J* = 12.7 Hz, 1H), 4.29 – 3.98 (m, 2H), 3.65 – 3.43 (m, 1H), 3.24 (d, *J* = 14.3 Hz, 1H), 1.20 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.05, 169.58, 152.16, 139.59, 136.98, 135.28, 130.38, 129.07, 126.13, 125.34, 123.13, 121.73, 121.50, 111.63, 84.44, 72.65, 61.62, 59.09, 42.37, 13.90.

HRMS (ESI) m/z Calcd for $C_{22}H_{20}BrNO_3S$, $[M+H]^+$: 458.0420; Found: 458.0421.



3u

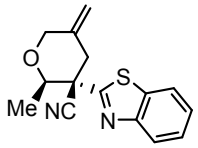
The compound **3u** was prepared according to the general procedure. The product was obtained as a brown solid (11.1 mg, 31% yield). Melting point 99-101 ºC.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.23 – 8.13 (m, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.54 – 7.47 (m, 1H), 7.40 – 7.14 (m, 5H), 6.58 (dd, *J* = 16.0, 1.2 Hz, 1H), 6.09 (dd, *J* = 15.9, 6.2 Hz, 1H), 5.23 (s, 1H), 5.17 (d, *J* = 1.9 Hz, 1H), 4.82 (dd, *J*

= 6.3, 1.2 Hz, 1H), 4.46 (d, *J* = 12.2 Hz, 1H), 4.38 (d, *J* = 12.4 Hz, 1H), 3.40 (s, 1H), 3.26 – 3.10 (m, 1H), .

^{13}C NMR (100 MHz, DMSO-d_6) δ 166.42, 152.79, 138.15, 135.89, 134.60, 134.53, 129.18, 128.79, 127.39, 126.99, 126.49, 123.76, 123.54, 123.14, 118.82, 114.96, 81.62, 71.63, 52.49, 42.85.

HRMS (ESI) m/z Calcd for $C_{22}H_{18}N_2OS$, $[M+H]^+$: 359.1213; Found:359.1210.



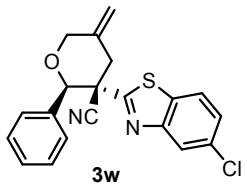
3v

The compound **3v** was prepared according to the general procedure. The product was obtained as a brown solid (7.1 mg, 26% yield). Melting point 99-101 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dt, *J* = 8.2, 1.0 Hz, 1H), 7.92 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.54 (ddd, *J* = 8.4, 7.2, 1.3 Hz, 1H), 7.45 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 5.18 (q, *J* = 1.4 Hz, 1H), 5.15 – 5.07 (m, 1H), 4.40 (dd, *J* = 12.4, 2.0 Hz, 1H), 4.28 – 4.13 (m, 2H), 3.29 (dq, *J* = 14.1, 1.9 Hz, 1H), 3.00 (dd, *J* = 13.9, 1.9 Hz, 1H), 1.29 (d, *J* = 6.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.20, 153.28, 137.14, 134.33, 126.75, 125.91, 123.41, 121.79, 118.32, 114.71, 77.85, 72.30, 52.40, 43.71, 17.64.

HRMS (ESI) m/z Calcd for $C_{15}H_{14}N_2OS$, $[M+H]^+$: 271.0900; Found: 271.0904.



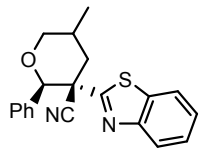
3w

The compound **3w** was prepared according to the general procedure. The product was obtained as a white solid (34.9 mg, 95% yield). Melting point 159-161 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 2.0 Hz, 1H), 7.68 (d, *J* = 8.6 Hz, 1H), 7.39 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.22 (d, *J* = 6.7 Hz, 1H), 7.19 – 7.07 (m, 4H), 5.29 (q, *J* = 1.4 Hz, 1H), 5.23 – 5.17 (m, 1H), 5.06 (s, 1H), 4.61 (dd, *J* = 12.6, 1.8 Hz, 1H), 4.41 (d, *J* = 12.6 Hz, 1H), 3.65 (dd, *J* = 13.9, 1.6 Hz, 1H), 3.09 (dd, *J* = 13.9, 1.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.01, 153.86, 136.77, 135.81, 132.78, 132.76, 128.97, 128.18, 126.97, 126.39, 123.15, 122.56, 118.16, 115.40, 84.81, 73.06, 53.38, 43.46.

HRMS (ESI) m/z Calcd for $C_{20}H_{15}ClN_2OS$, $[M+H]^+$: 367.0666; Found:367.0664.



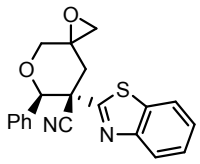
4

The compound **4** was prepared according to the general procedure. The product was obtained as a white solid (30.1 mg, 90% yield). Melting point 123-125 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dt, *J* = 8.2, 0.9 Hz, 1H), 7.90 – 7.70 (m, 1H), 7.54 (d, *J* = 1.2 Hz, 1H), 7.48 – 7.36 (m, 1H), 7.22 (dt, *J* = 5.3, 3.1 Hz, 1H), 7.20 – 7.11 (m, 4H), 5.02 (s, 1H), 4.44 – 3.73 (m, 2H), 3.10 (dd, *J* = 14.2, 5.5 Hz, 1H), 2.50 (d, *J* = 14.2 Hz, 1H), 2.22 (dd, *J* = 3.6, 1.9 Hz, 1H), 1.61 (d, *J* = 7.5 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.02, 153.19, 136.59, 134.59, 128.71, 128.03, 126.99, 126.58, 125.66, 123.23, 121.80, 120.67, 85.52, 74.17, 47.94, 41.06, 27.80, 18.26.

HRMS (ESI) m/z Calcd for $C_{20}H_{18}N_2OS$, $[M+H]^+$: 334.1213; Found: 335.1214.



5

The compound **5** was prepared according to the general procedure. The product was obtained as a white solid (21.3 mg, 61% yield). Melting point 168-170 ºC.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.2 Hz, 1H), 7.81 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.57 (ddd, *J* = 8.3, 7.1, 1.3 Hz, 1H), 7.45 (ddd, *J* = 8.2, 7.2, 1.2 Hz, 1H), 7.28 – 7.23 (m, 1H), 7.22 – 7.11 (m, 4H), 5.09 (s, 1H), 4.26 (dd, *J* = 11.6, 2.0 Hz, 1H), 3.83 (dd, *J* = 11.6, 2.2 Hz, 1H), 3.51 (dd, *J* = 13.4, 1.7 Hz, 1H), 3.14 (ddd, *J* = 15.3, 4.7, 1.8 Hz, 2H), 2.25 (dd, *J* =

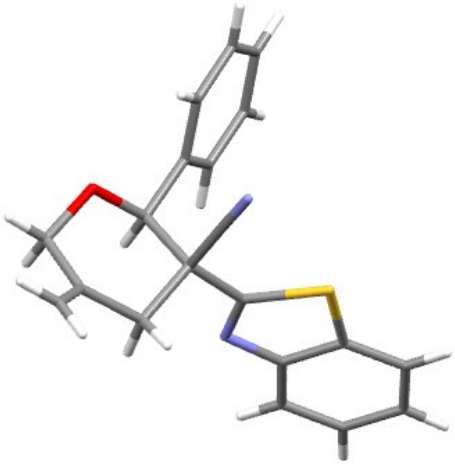
13.5, 2.2 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.82, 152.99, 135.17, 134.51, 129.12, 128.22, 127.00, 126.76, 125.95, 123.43, 121.83, 118.33, 84.87, 72.77, 55.79, 53.11, 52.45, 41.74.

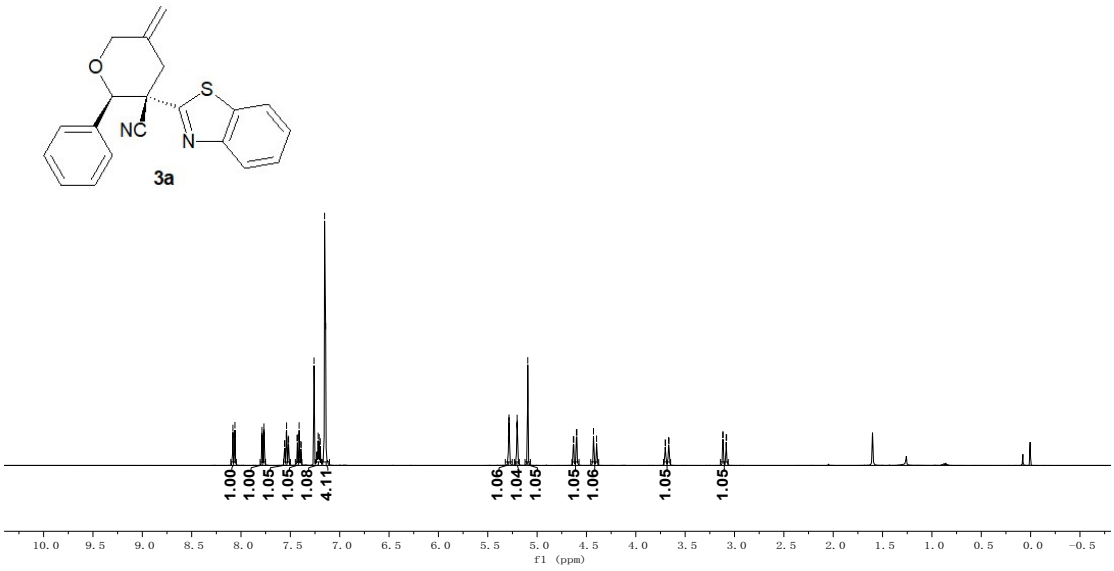
HRMS (ESI) m/z Calcd for $C_{20}H_{16}N_2O_2S$, $[M+H]^+$: 349.1005; Found: 349.1002.

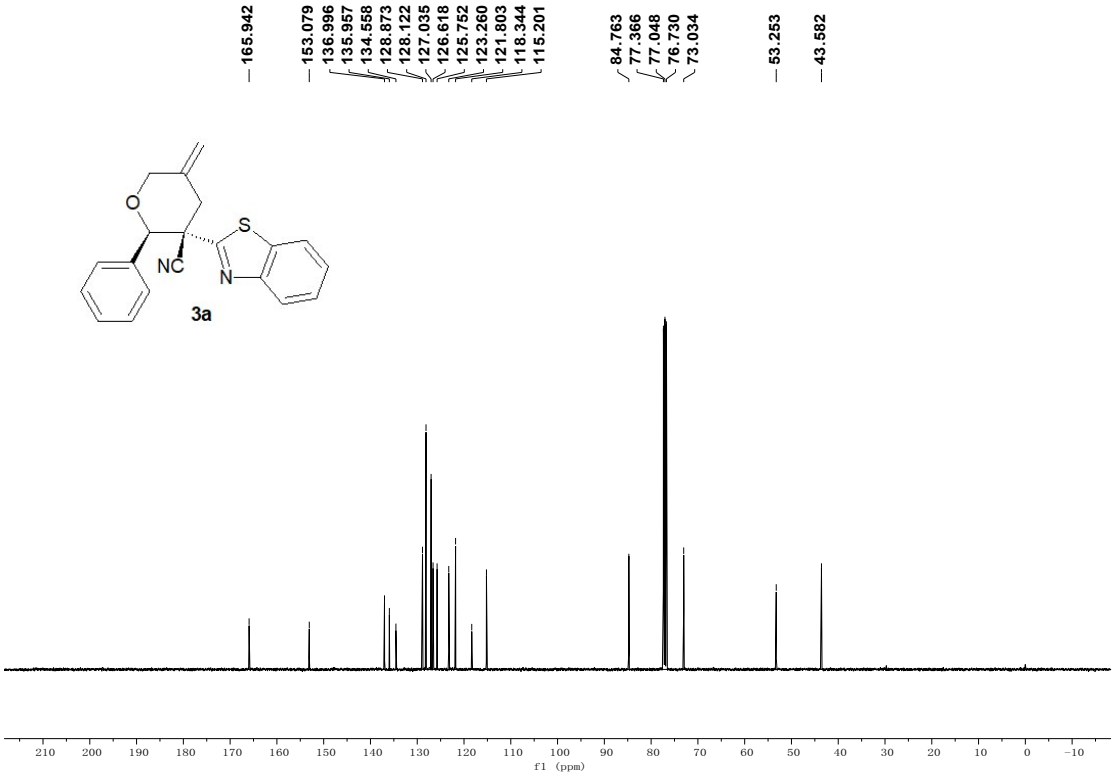
7. X-ray crystallographic analysis

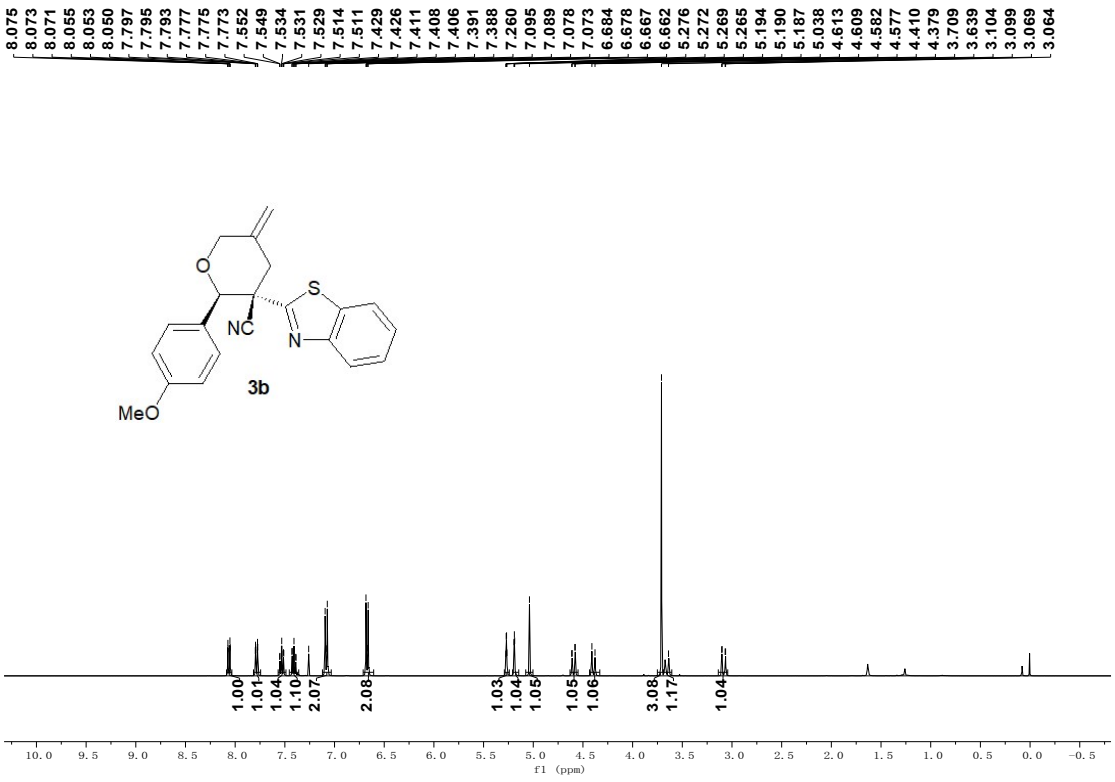
The structure of **3a** was assigned by X-ray crystallographic analysis:



8. NMR spectra



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N
MeO
3b
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1.10
2.07
2.08
1.03
1.04
1.05
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1.06
3.08
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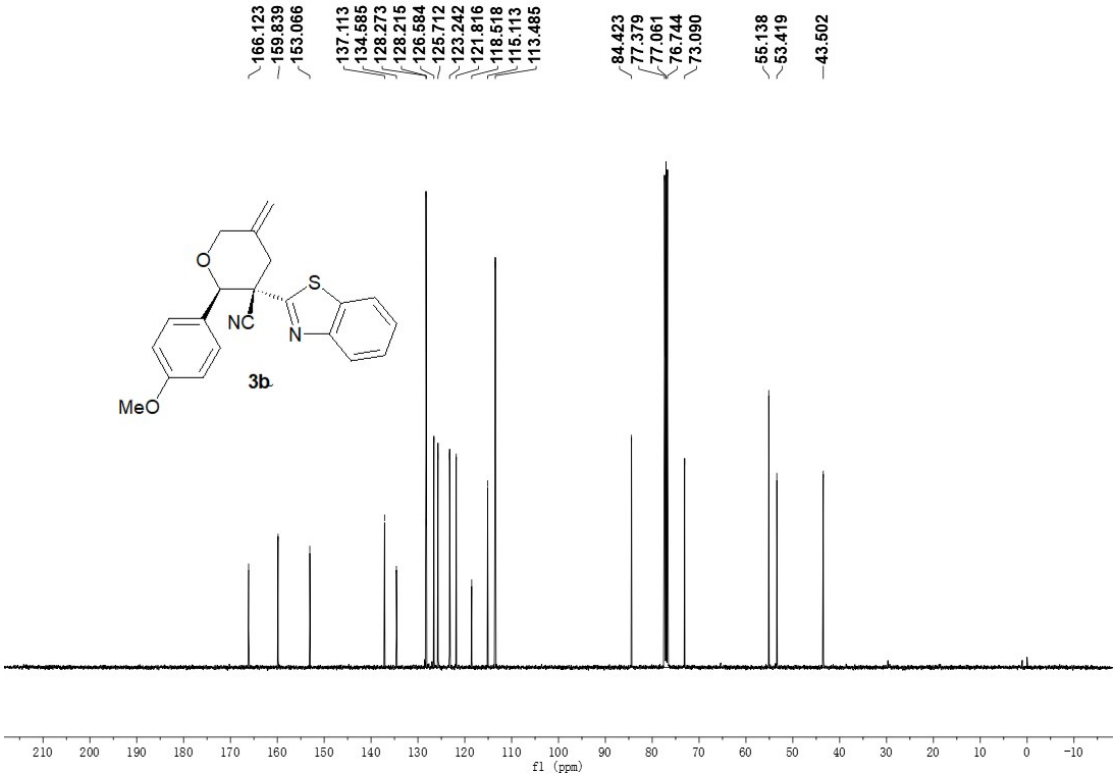
f1 (ppm)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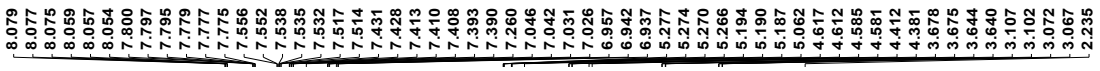
f1 (ppm)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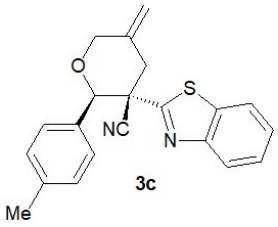
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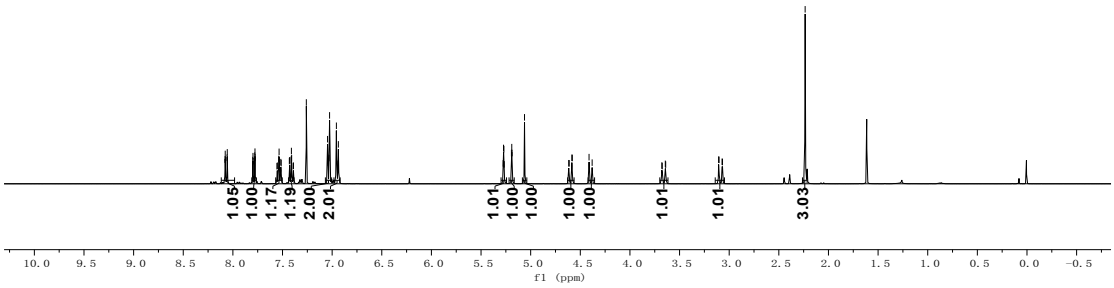
Me

3c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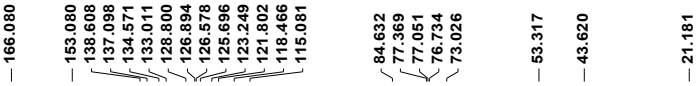
f1 (ppm)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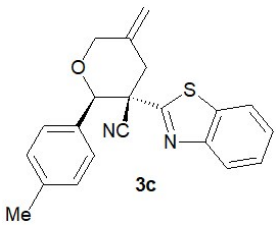
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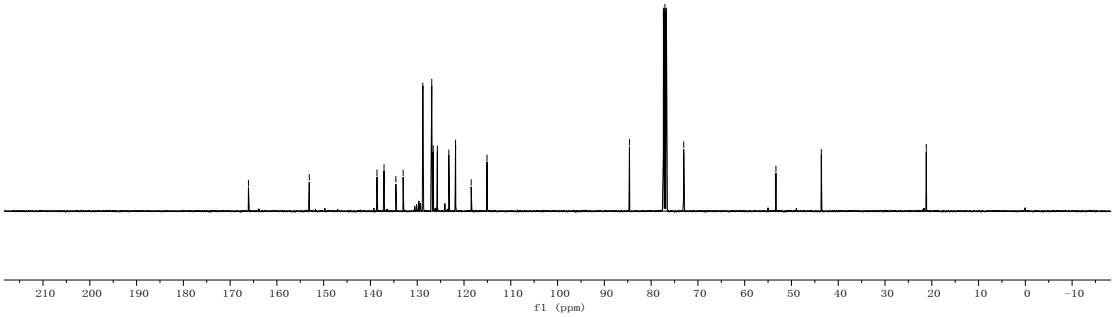
NC
N
Me

3c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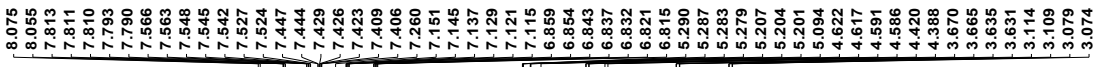
f1 (ppm)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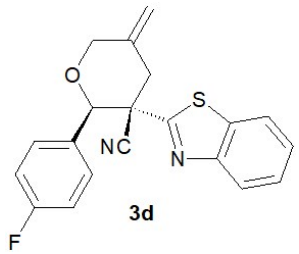
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NC
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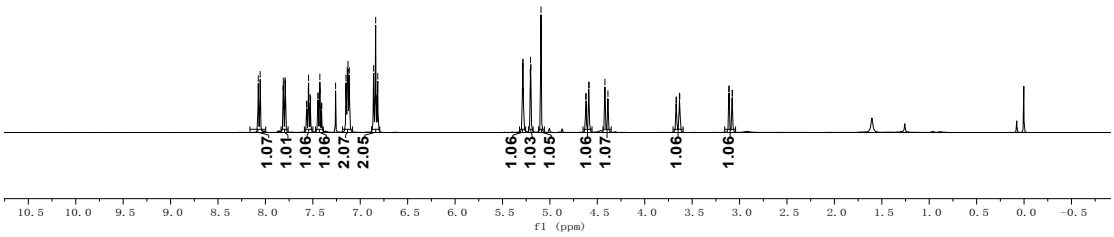
F

3d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f1 (ppm)


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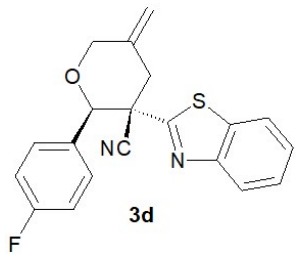
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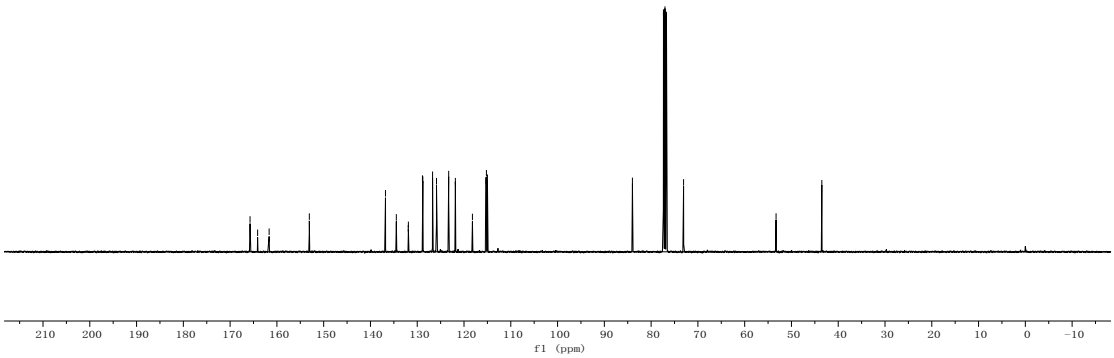
S
NC
N
F

3d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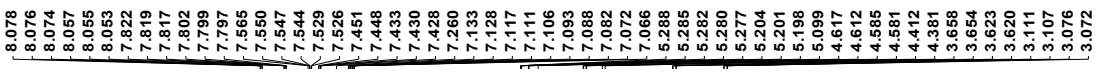
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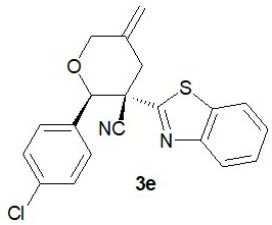
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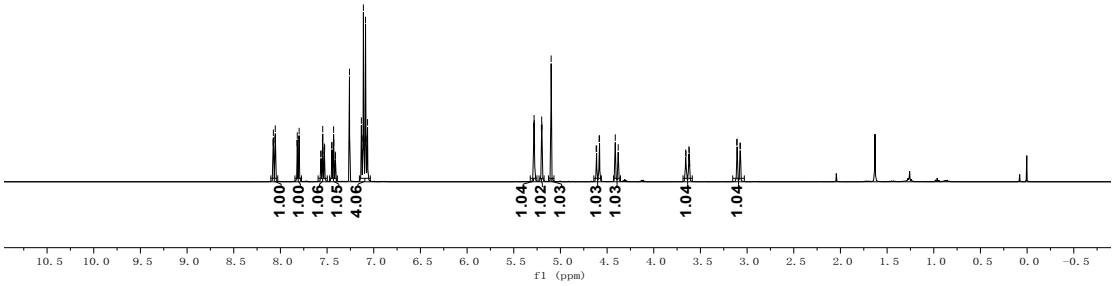
S
NC
N
Cl

3e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f1 (ppm)


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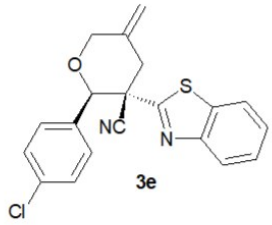
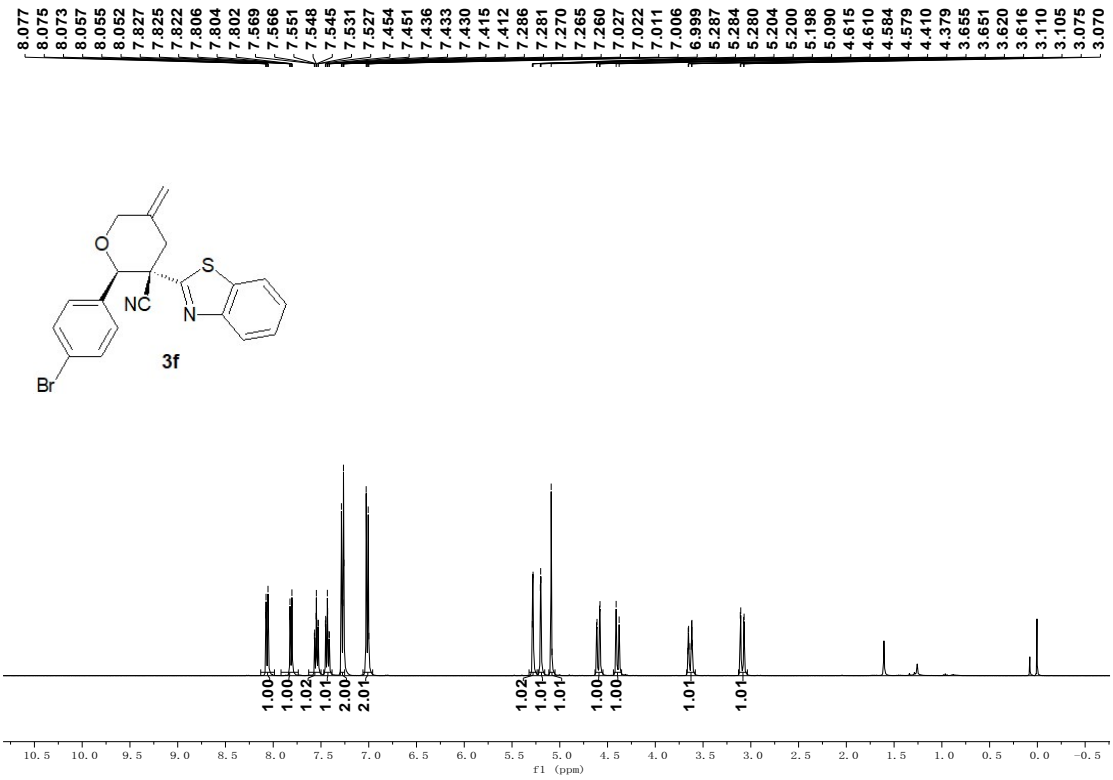

O
S
NC
N
Cl

3e

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)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S
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Br
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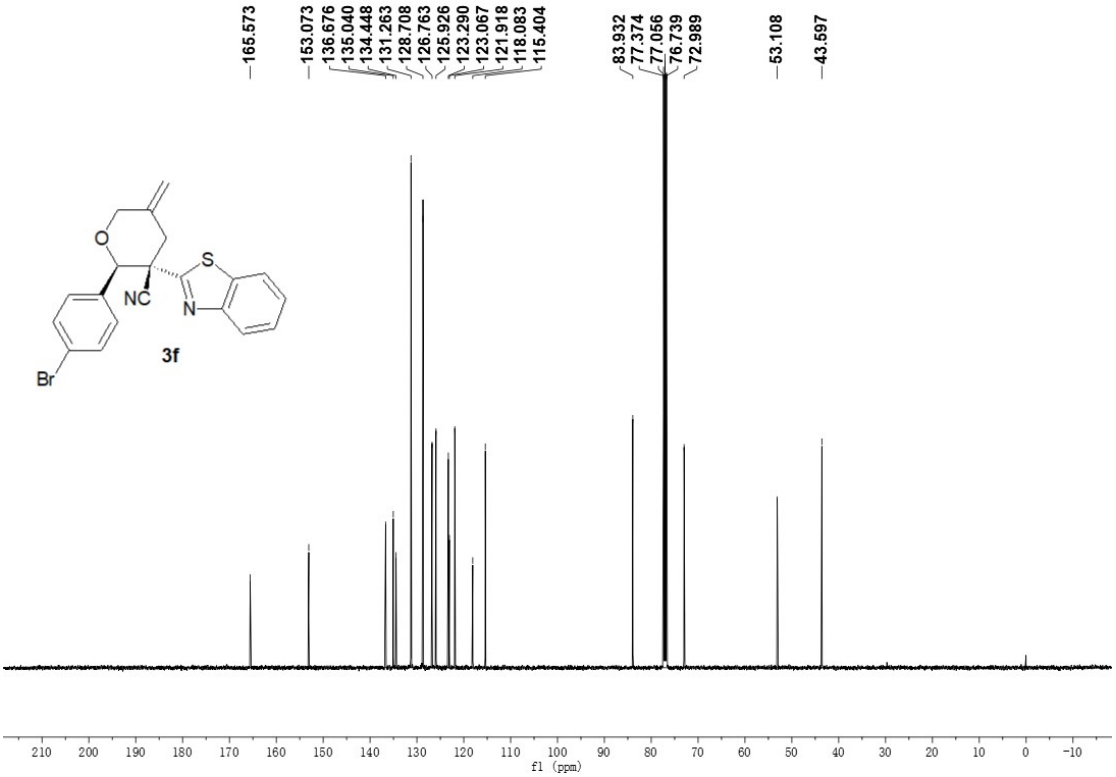
2.01
1.02
1.01
1.01
1.00
1.00
1.01
1.01
f1 (ppm)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118.083
115.404
83.932
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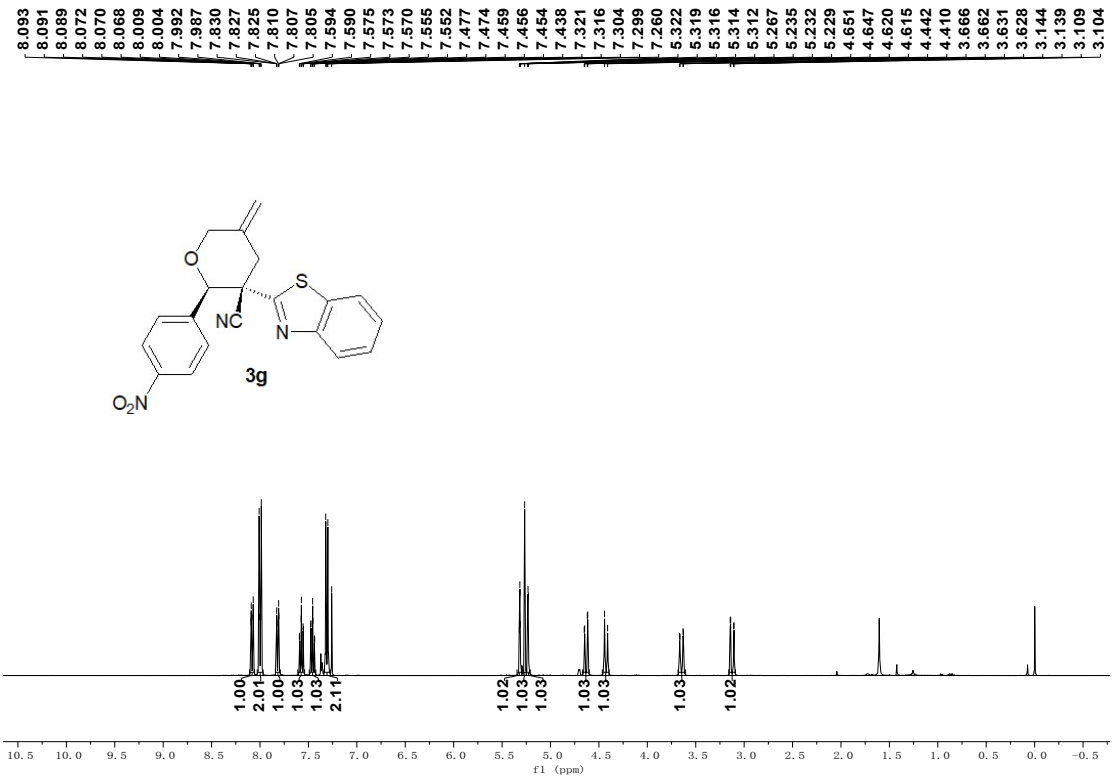
76.739
72.989
53.108
43.597
O
S
NC
N
Br
3f
f1 (ppm)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8.004
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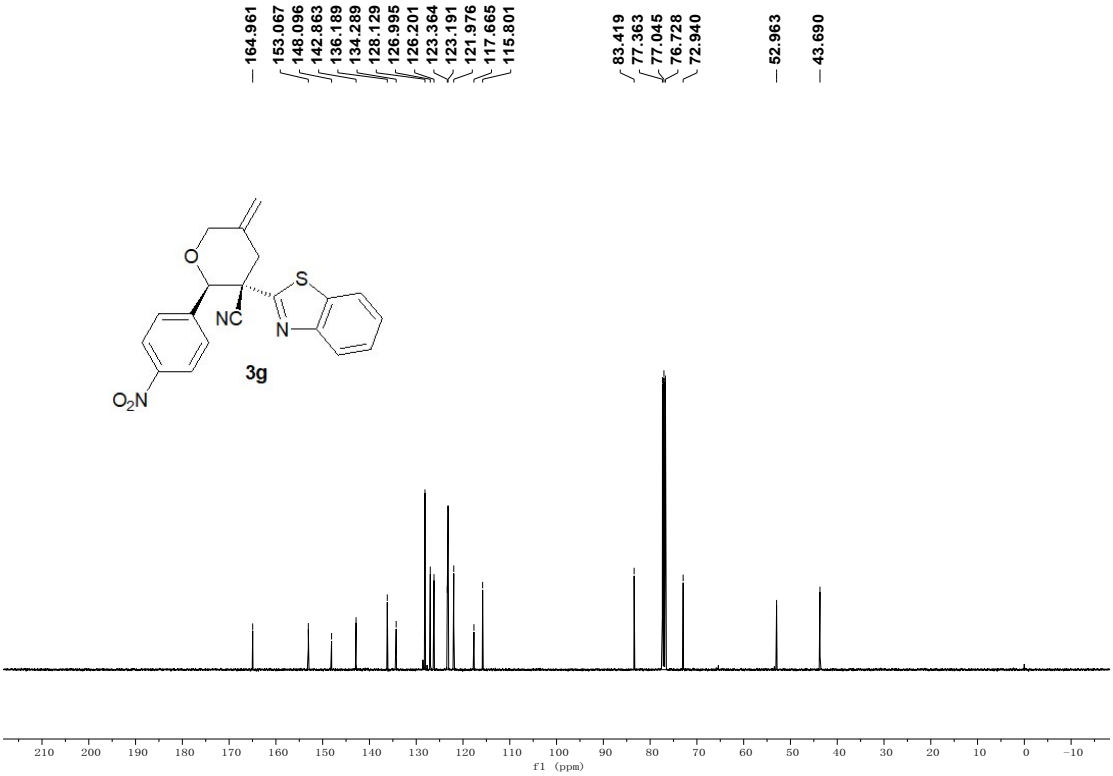
7.825
7.810
7.807
7.805
7.594
7.590
7.575
7.573
7.570
7.555
7.552
7.477
7.474
7.459
7.456
7.454
7.438
7.321
7.316
7.304
7.299
7.260
5.322
5.319
5.316
5.314
5.312
5.267
5.235
5.232
5.229
4.651
4.647
4.620
4.615
4.442
4.410
3.666
3.662
3.631
3.628
3.144
3.139
3.109
3.104
O
S
NC
N
3g
O2N
1.00
2.01
1.00
1.03
1.03
2.11
1.02
1.03
1.03
1.03
1.03
1.02
f1 (ppm)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123.191
121.976
117.665
115.801
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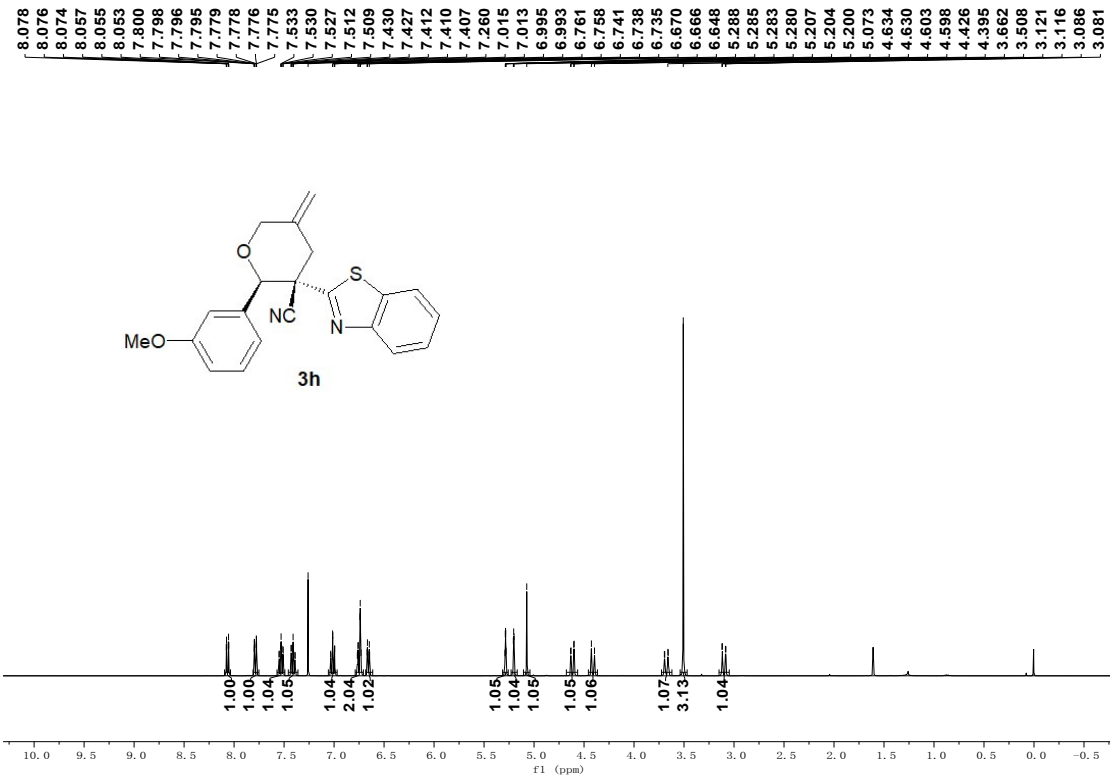
76.728
72.940
52.963
43.690
O
S
NC
N
3g
O2N
f1 (ppm)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7.776
7.775
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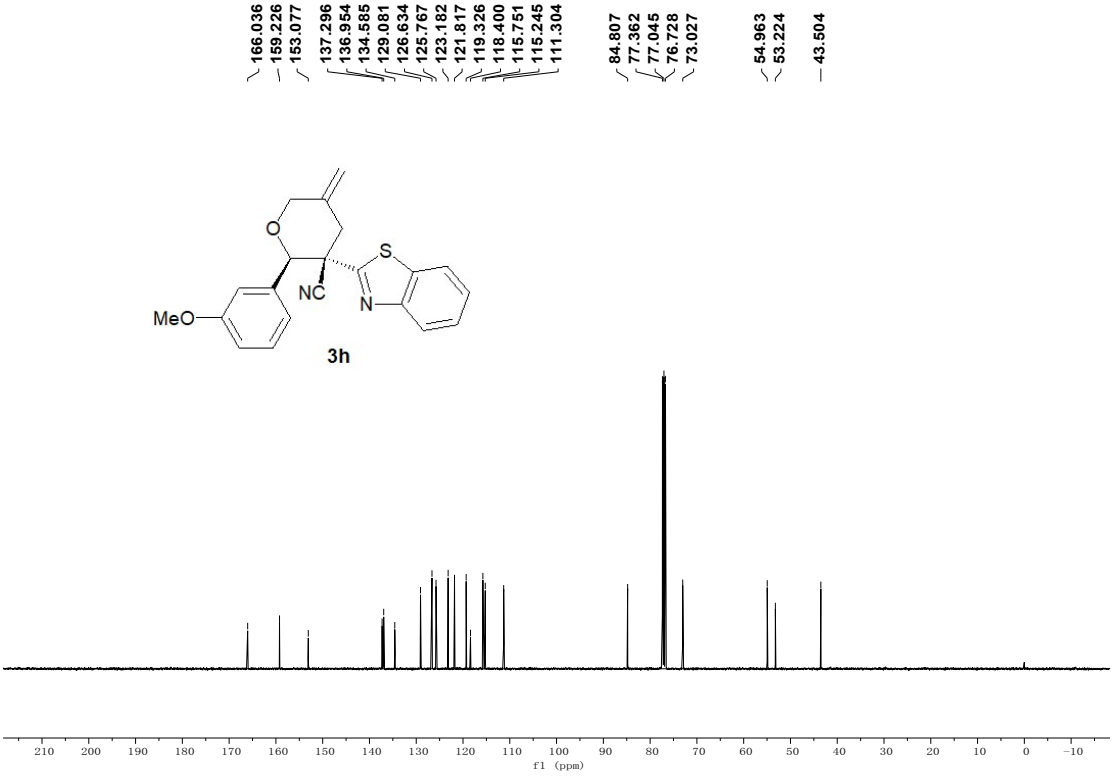
7.530
7.527
7.512
7.509
7.430
7.427
7.412
7.410
7.407
7.260
7.015
7.013
6.995
6.993
6.761
6.758
6.741
6.738
6.735
6.670
6.666
6.648
5.288
5.285
5.283
5.280
5.207
5.204
5.200
5.073
4.634
4.630
4.603
4.598
4.426
4.395
3.662
3.508
3.121
3.116
3.086
3.081
O
S
NC
N
MeO
3h
1.00
1.00
1.04
1.05
1.04
2.04
1.02
1.05
1.04
1.05
1.05
1.06
1.07
3.13
1.04
f1 (ppm)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123.182
121.817
119.326
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115.245
111.304
84.807
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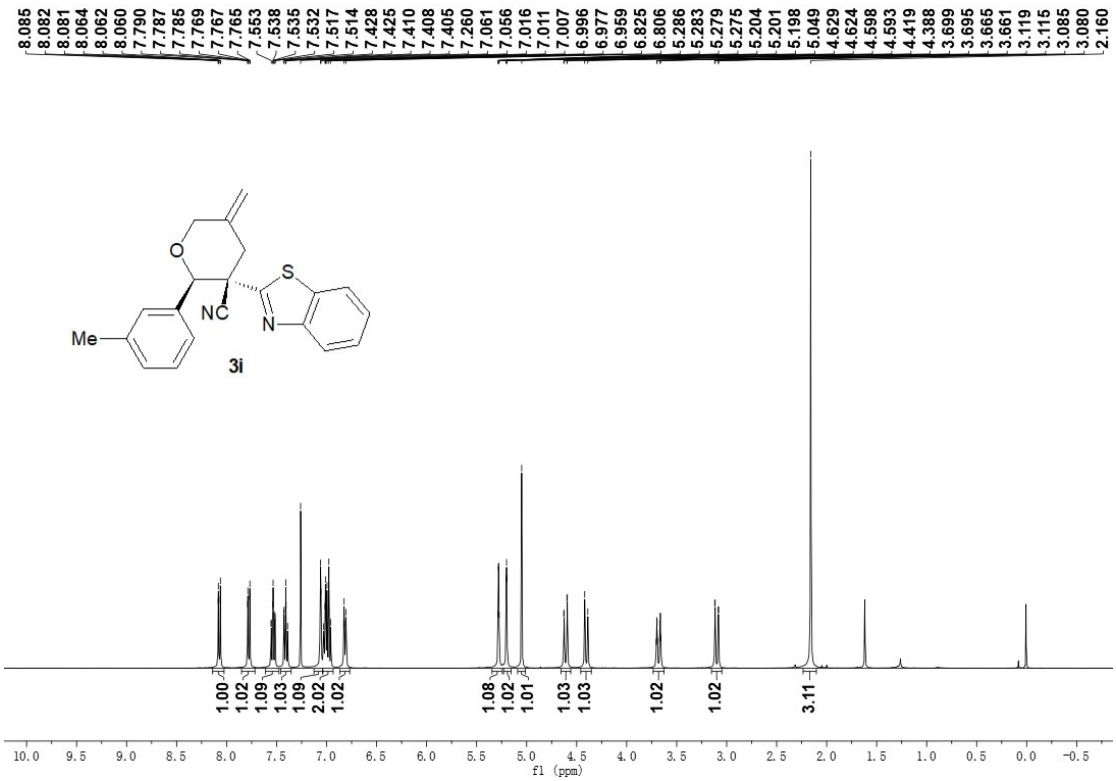
77.045
76.728
73.027
54.963
53.224
43.504
O
S
NC
N
MeO
3h
f1 (ppm)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8.081
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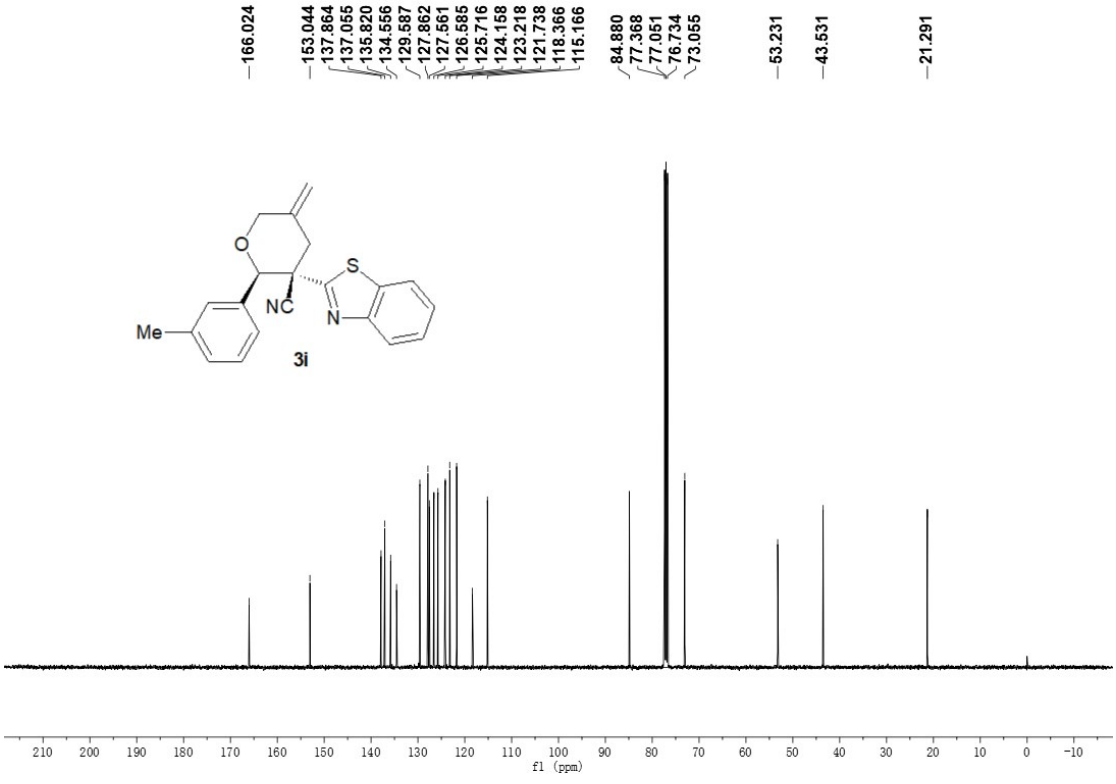
8.062
8.060
7.790
7.787
7.785
7.769
7.767
7.765
7.553
7.538
7.535
7.532
7.517
7.514
7.428
7.425
7.410
7.408
7.405
7.260
7.061
7.056
7.016
7.011
7.007
6.996
6.977
6.959
6.825
6.806
5.286
5.283
5.279
5.275
5.204
5.201
5.198
5.049
4.629
4.624
4.598
4.593
4.419
4.388
3.699
3.695
3.665
3.661
3.119
3.115
3.085
3.080
2.160
O
S
NC
N
Me
3i
1.00
1.02
1.09
1.03
1.09
2.02
1.02
1.08
1.02
1.01
1.03
1.03
1.02
1.02
3.11
f1 (ppm)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129.587
127.862
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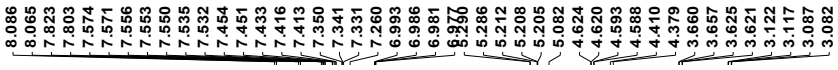
125.716
124.158
123.218
121.738
118.366
115.166
84.880
77.368
77.051
76.734
73.055
53.231
43.531
21.291
O
S
NC
N
Me
3i
f1 (ppm)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7.553
7.550
7.535
7.532
7.454
7.451
7.433
7.416
7.413
7.350
7.341
7.331
7.260
6.993
6.986
6.981
5.286
5.212
5.208
5.205
5.082
4.624
4.620
4.593
4.588
4.410
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3.657
3.625
3.621
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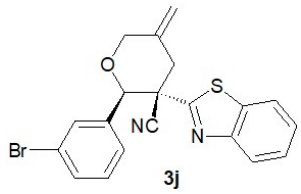
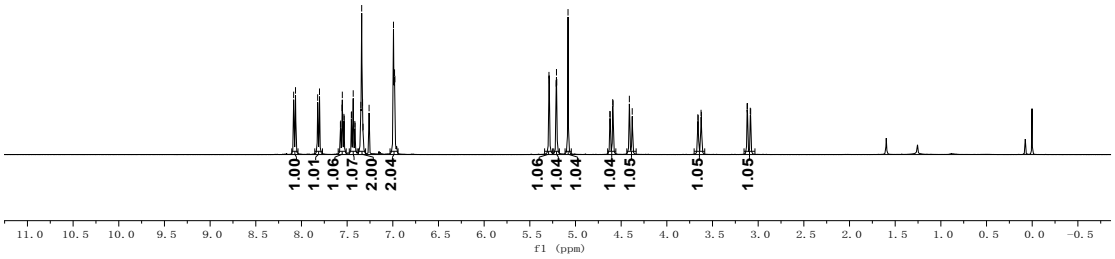
3.117
3.087
3.082


O
S
NC
N
Br

3j


1.00
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1.06
1.07
2.00
2.04
1.06
1.04
1.04
1.04
1.05
1.05
1.05
11.0 10.5 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)


165.480
153.050
138.102
136.600
134.433
131.950
130.202
129.564
126.774
125.941
125.601
123.297
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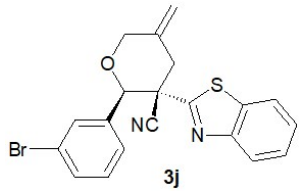
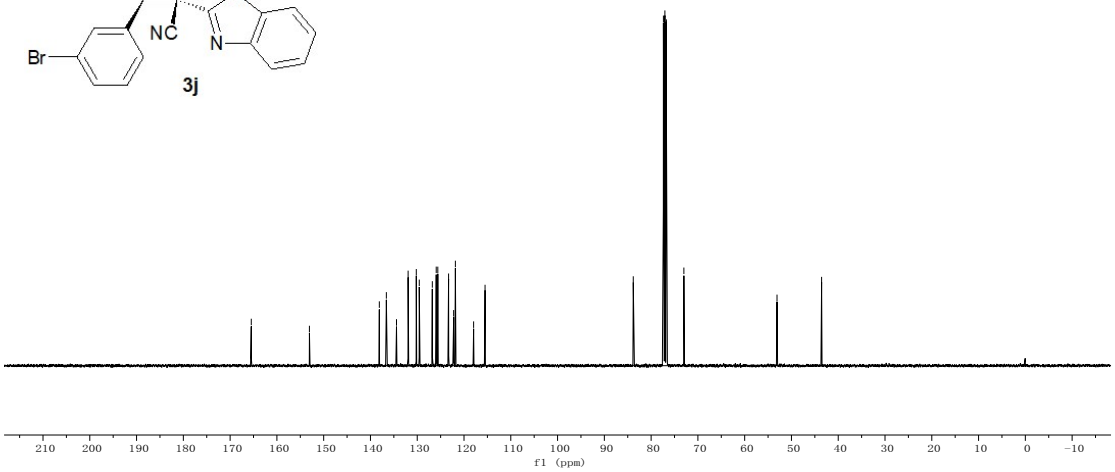
117.946
115.501
83.818
77.374
77.057
76.739
72.998
53.087
43.555


O
S
NC
N
Br

3j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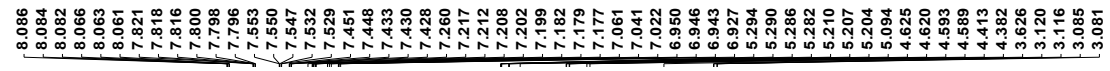
f1 (ppm)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8.082
8.066
8.063
8.061
7.821
7.818
7.816
7.800
7.798
7.796
7.553
7.550
7.547
7.532
7.529
7.451
7.448
7.433
7.430
7.428
7.260
7.217
7.212
7.208
7.202
7.199
7.182
7.179
7.177
7.061
7.041
7.022
6.950
6.946
6.943
6.927
5.294
5.290
5.286
5.282
5.210
5.207
5.204
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4.620
4.593
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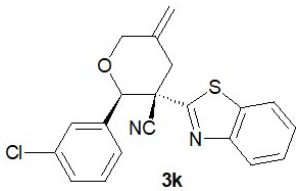
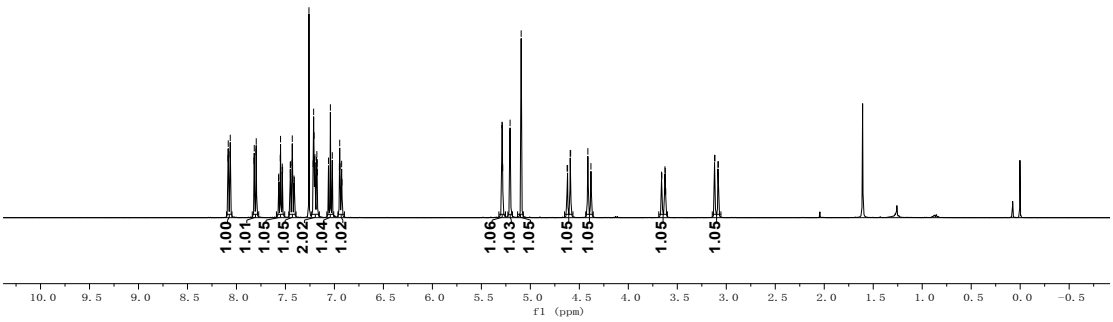
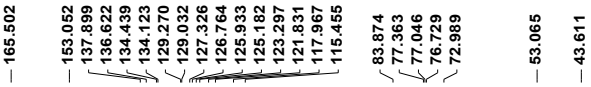
4.382
3.626
3.120
3.116
3.085
3.081


O
S
NC
N
Cl

3k


1.00
1.01
1.05
1.05
2.02
1.04
1.02
1.06
1.03
1.05
1.05
1.05
1.05
1.05
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)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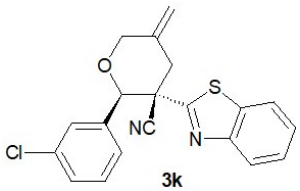
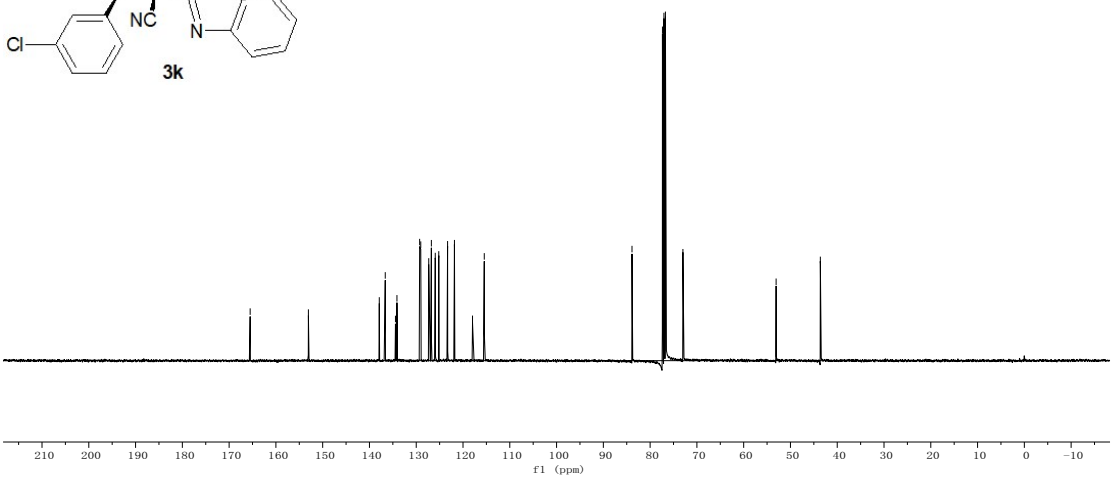
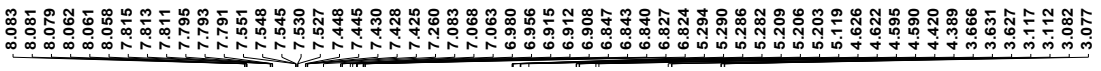
136.622
134.439
134.123
129.270
129.032
127.326
126.764
125.933
125.182
123.297
121.831
117.967
115.455
83.874
77.363
77.046
76.729
72.989
53.065
43.611


O
S
NC
N
Cl

3k


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)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8.058
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7.548
7.545
7.530
7.527
7.448
7.445
7.430
7.428
7.425
7.260
7.083
7.068
7.063
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6.956
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6.847
6.843
6.840
6.827
6.824
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5.290
5.286
5.282
5.209
5.206
5.203
5.119
4.626
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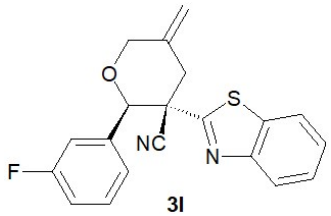
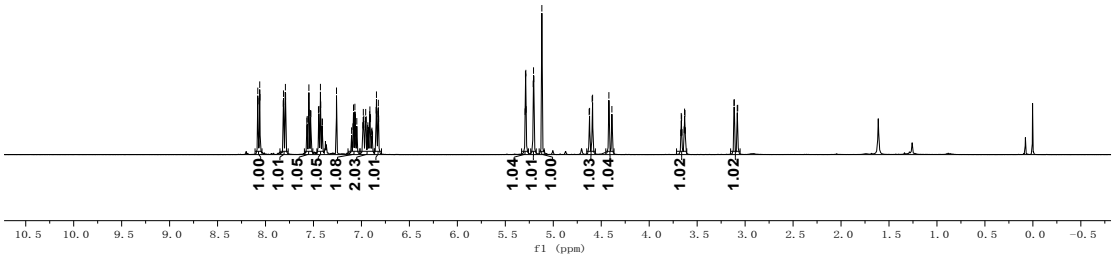
3.631
3.627
3.117
3.112
3.082
3.077


O
S
NC
N
F

3l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1.05
1.05
1.08
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1.01
1.04
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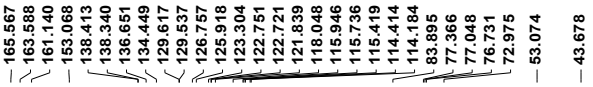
1.00
1.03
1.04
1.02
1.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.449
129.617
129.537
126.757
125.918
123.304
122.751
122.721
121.839
118.048
115.946
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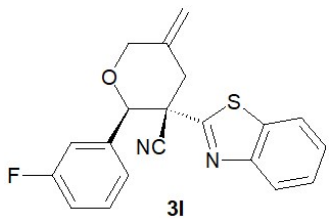
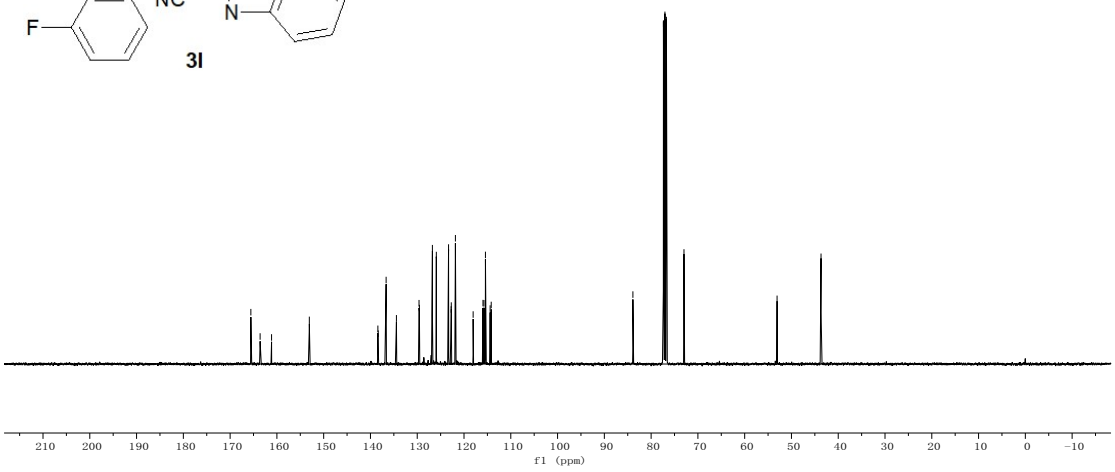
114.414
114.184
83.895
77.366
77.048
76.731
72.975
53.074
43.678


O
S
NC
N
F

3l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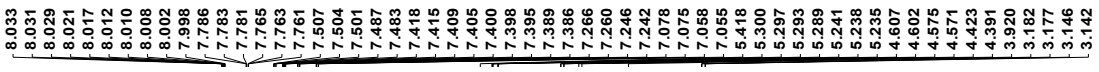
f1 (ppm)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8.010
8.008
8.002
7.998
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7.783
7.781
7.765
7.763
7.761
7.507
7.504
7.501
7.487
7.483
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7.415
7.409
7.405
7.400
7.398
7.395
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7.386
7.266
7.260
7.246
7.242
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7.075
7.058
7.055
5.418
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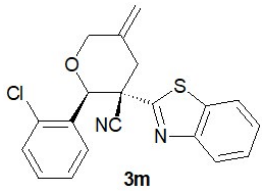
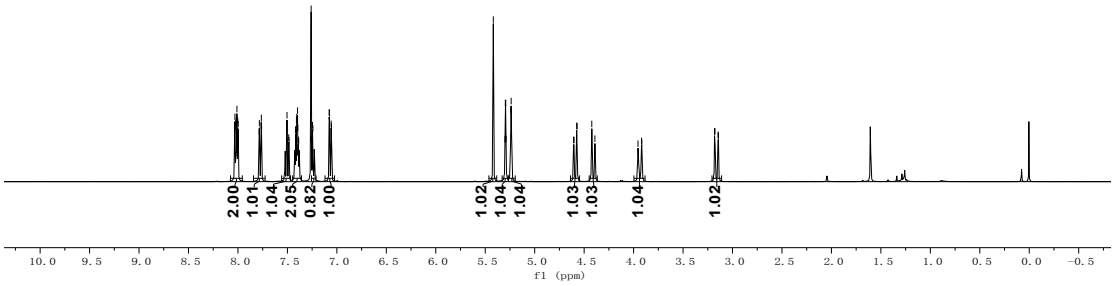
3.142


O
Cl
NC
S
N

3m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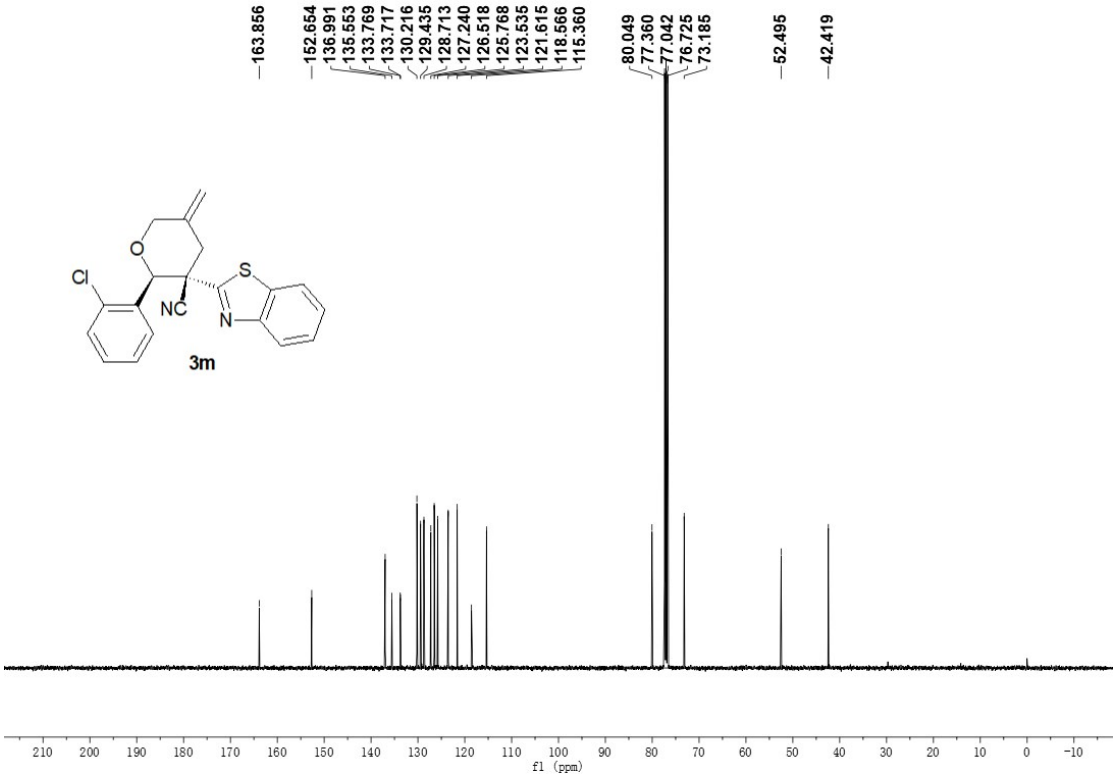
1.04
2.05
0.82
1.00
1.02
1.04
1.04
1.03
1.03
1.04
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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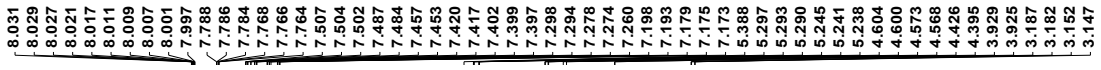
136.991
135.553
133.769
133.717
130.216
129.435
128.713
127.240
126.518
125.768
123.535
121.615
118.566
115.360
80.049
77.360
77.042
76.725
73.185
52.495
42.419
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

O
Cl
NC
S
N

3m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7.784
7.768
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7.764
7.507
7.504
7.502
7.487
7.484
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7.453
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7.294
7.278
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7.260
7.198
7.193
7.179
7.175
7.173
5.388
5.297
5.293
5.290
5.245
5.241
5.238
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3.925
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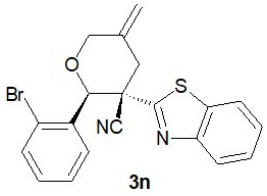
3.182
3.152
3.147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Br
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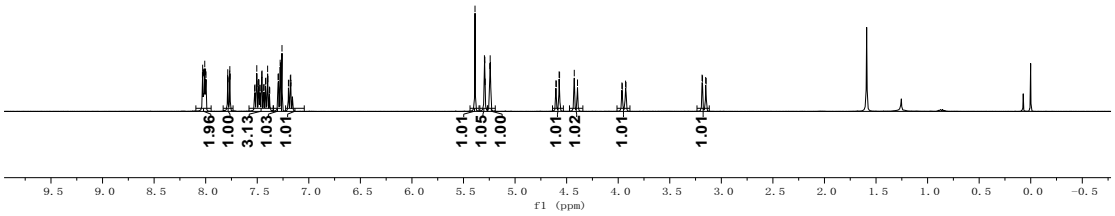
S
N

3n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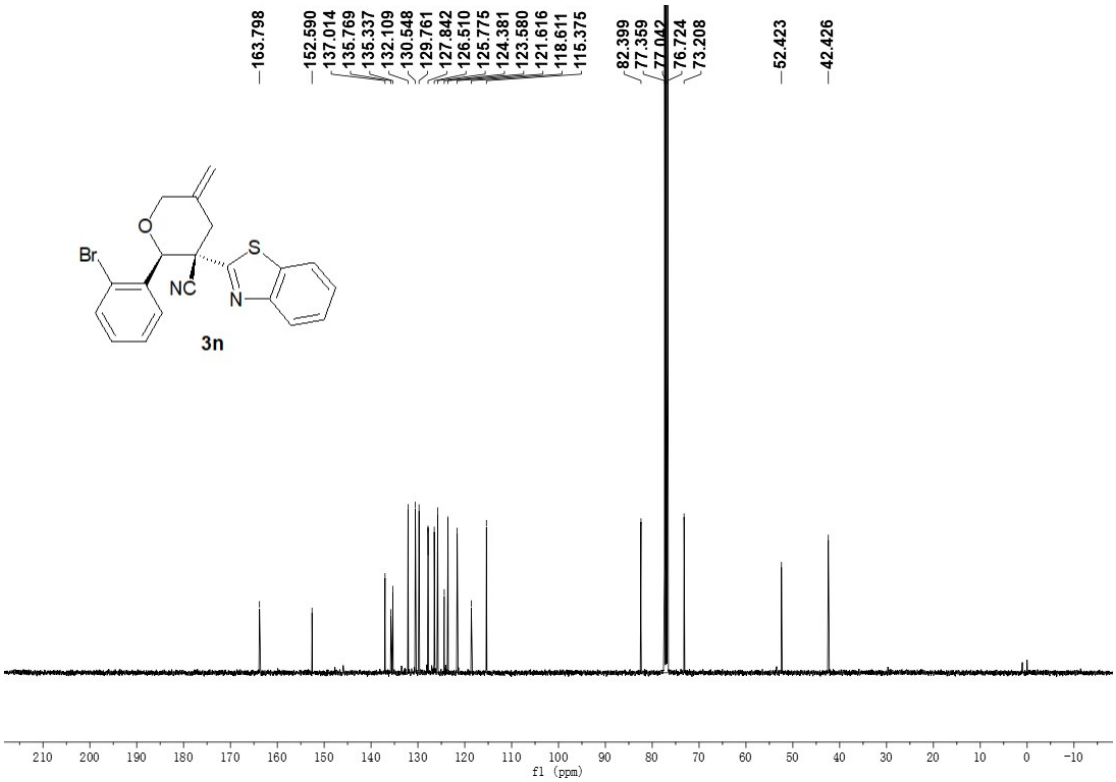
1.01
1.05
1.00
1.01
1.02
1.01
1.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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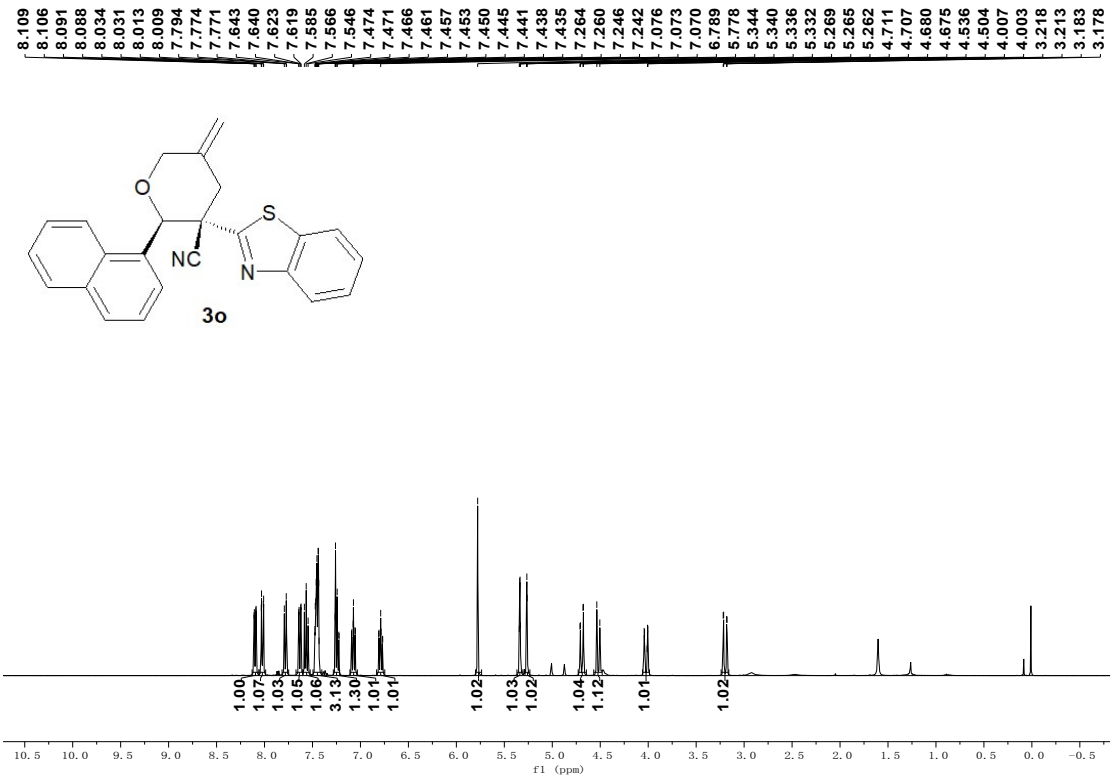
124.381
123.580
121.616
118.611
115.375
82.399
77.359
77.042
76.724
73.208
52.423
42.426
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

O
Br
NC
S
N

3n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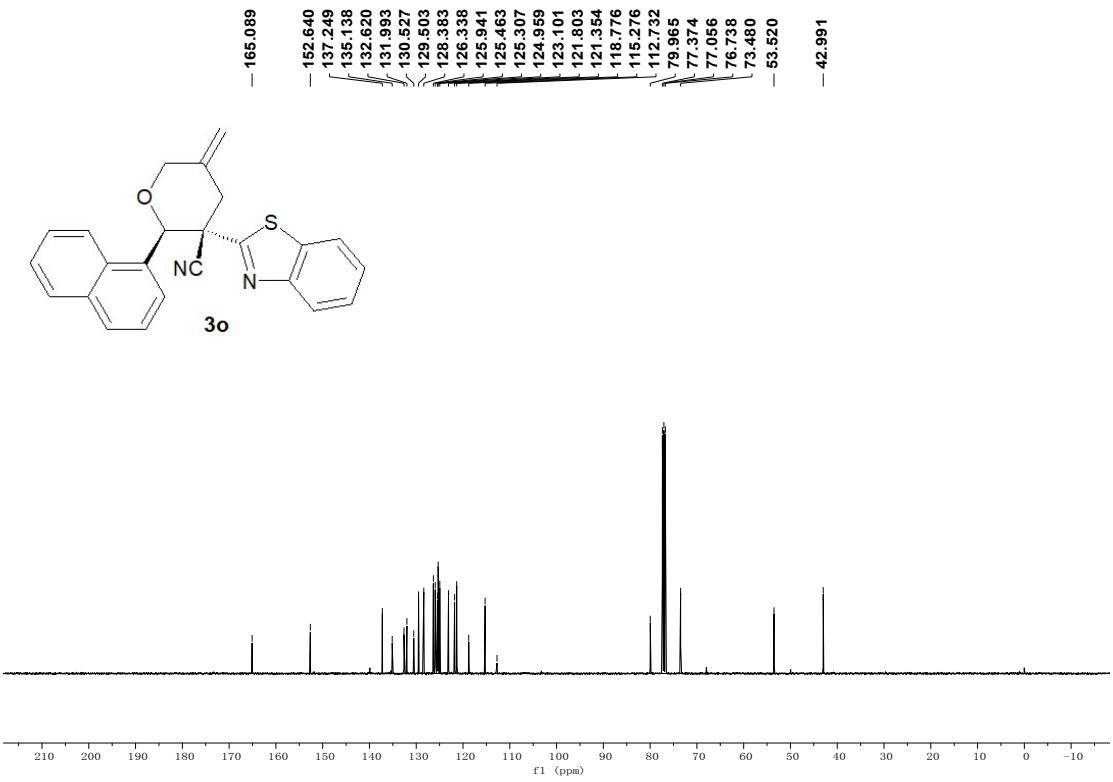
7.643
7.640
7.623
7.619
7.585
7.566
7.546
7.474
7.471
7.466
7.461
7.457
7.453
7.450
7.445
7.441
7.438
7.435
7.264
7.260
7.246
7.242
7.076
7.073
7.070
6.789
5.778
5.344
5.340
5.336
5.332
5.269
5.265
5.262
4.711
4.707
4.680
4.675
4.536
4.504
4.007
4.003
3.218
3.213
3.183
3.178
O
S
NC
N
3o
1.00
1.07
1.03
1.05
1.06
3.13
1.30
1.01
1.01
1.02
1.03
1.02
1.04
1.12
1.01
1.02
f1 (ppm)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125.307
124.959
123.101
121.803
121.354
118.776
115.276
112.732
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53.520
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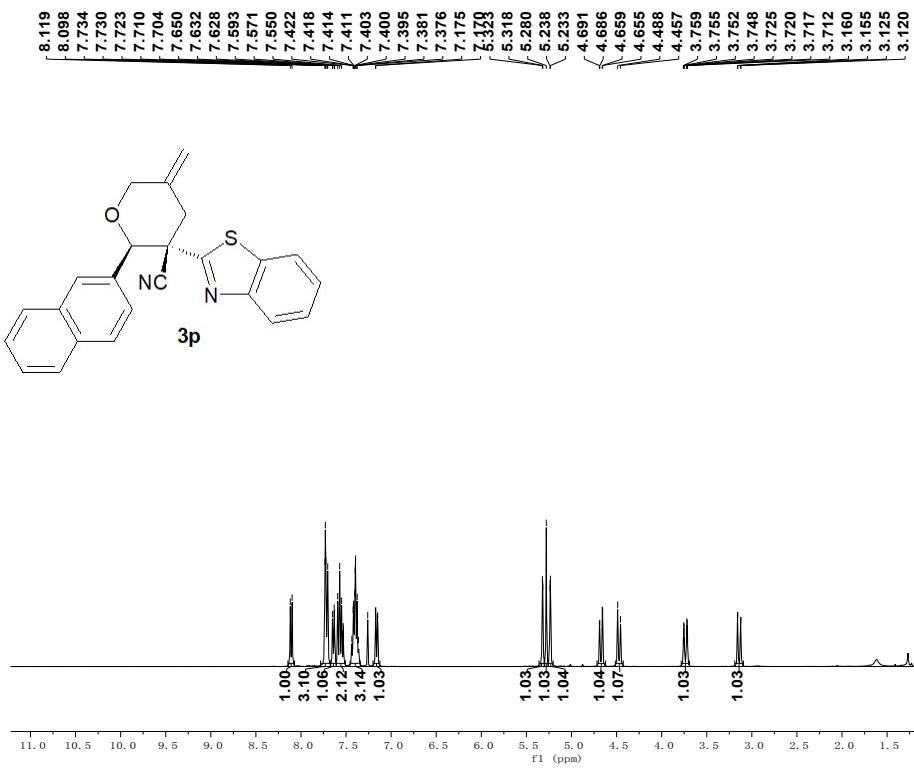
O
S
NC
N
3o
f1 (ppm)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7.550
7.422
7.418
7.414
7.411
7.403
7.400
7.395
7.381
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7.175
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5.280
5.238
5.233
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4.686
4.659
4.655
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4.457
3.759
3.755
3.752
3.748
3.725
3.720
3.717
3.712
3.160
3.155
3.125
3.120
O
S
NC
N
3p
1.00
3.10
1.06
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1.03
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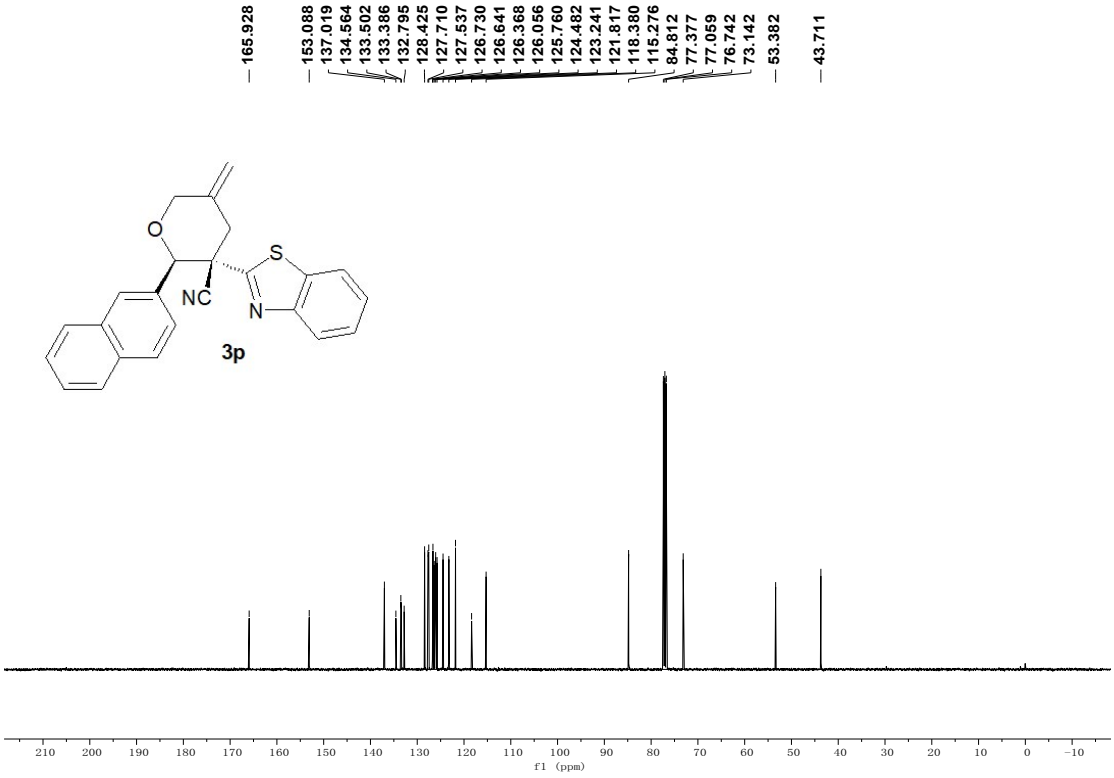
1.03
1.04
1.04
1.07
1.03
1.03
f1 (ppm)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132.795
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126.730
126.641
126.368
126.056
125.760
124.482
123.241
121.817
118.380
115.276
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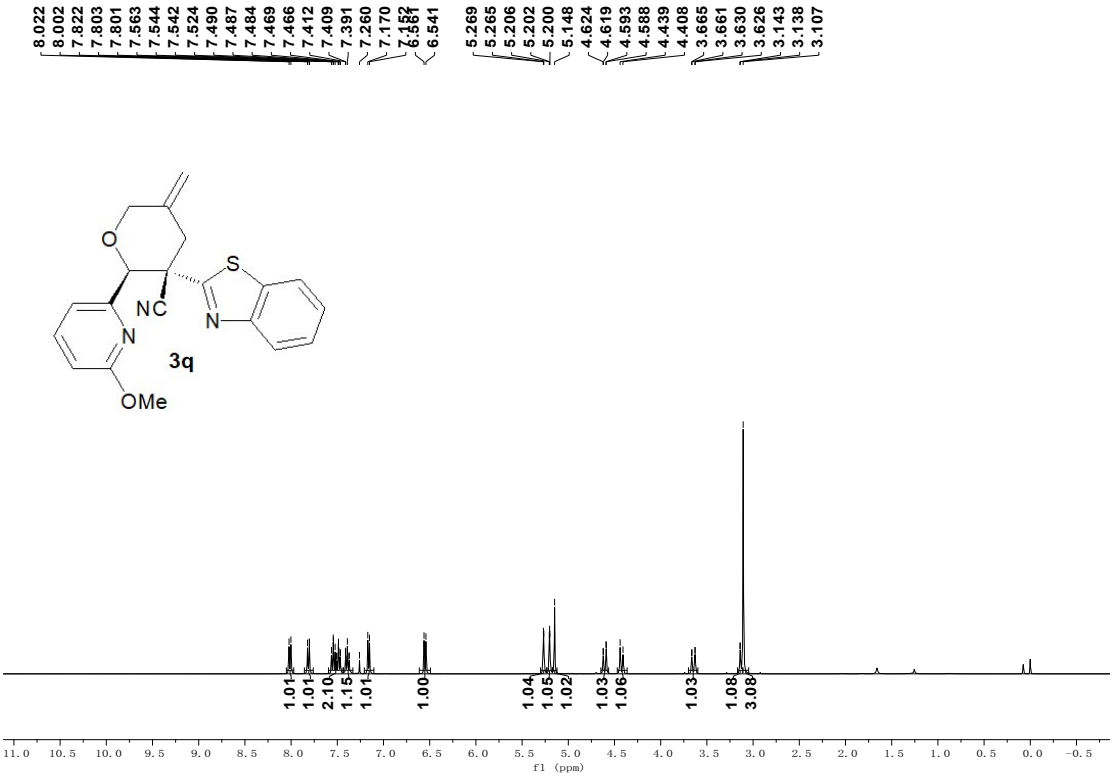
77.059
76.742
73.142
53.382
43.711
O
S
NC
N
3p
f1 (ppm)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7.544
7.542
7.524
7.490
7.487
7.484
7.469
7.466
7.412
7.409
7.391
7.260
7.170
7.152
6.581
6.541
5.269
5.265
5.206
5.202
5.200
5.148
4.624
4.619
4.593
4.588
4.439
4.408
3.665
3.661
3.630
3.626
3.143
3.138
3.107
O
S
NC
N
N
3q
OMe
1.01
1.01
2.10
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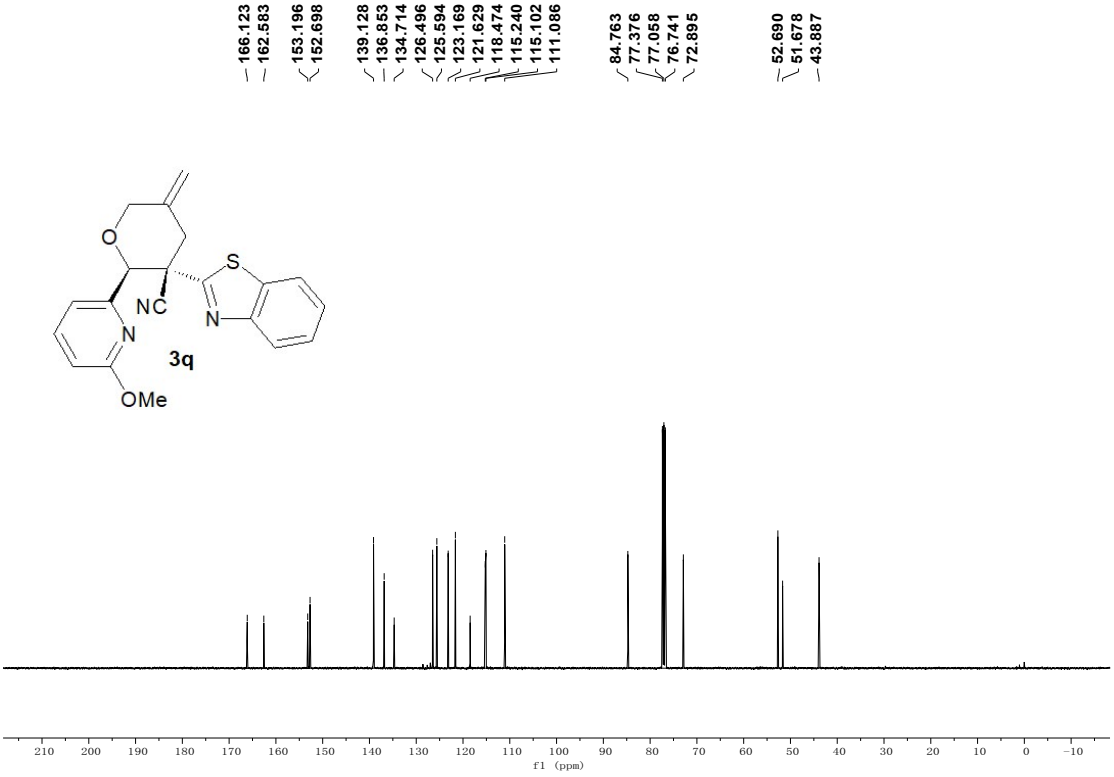
1.06
1.03
1.08
3.08
f1 (ppm)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115.240
115.102
111.086
84.763
77.376
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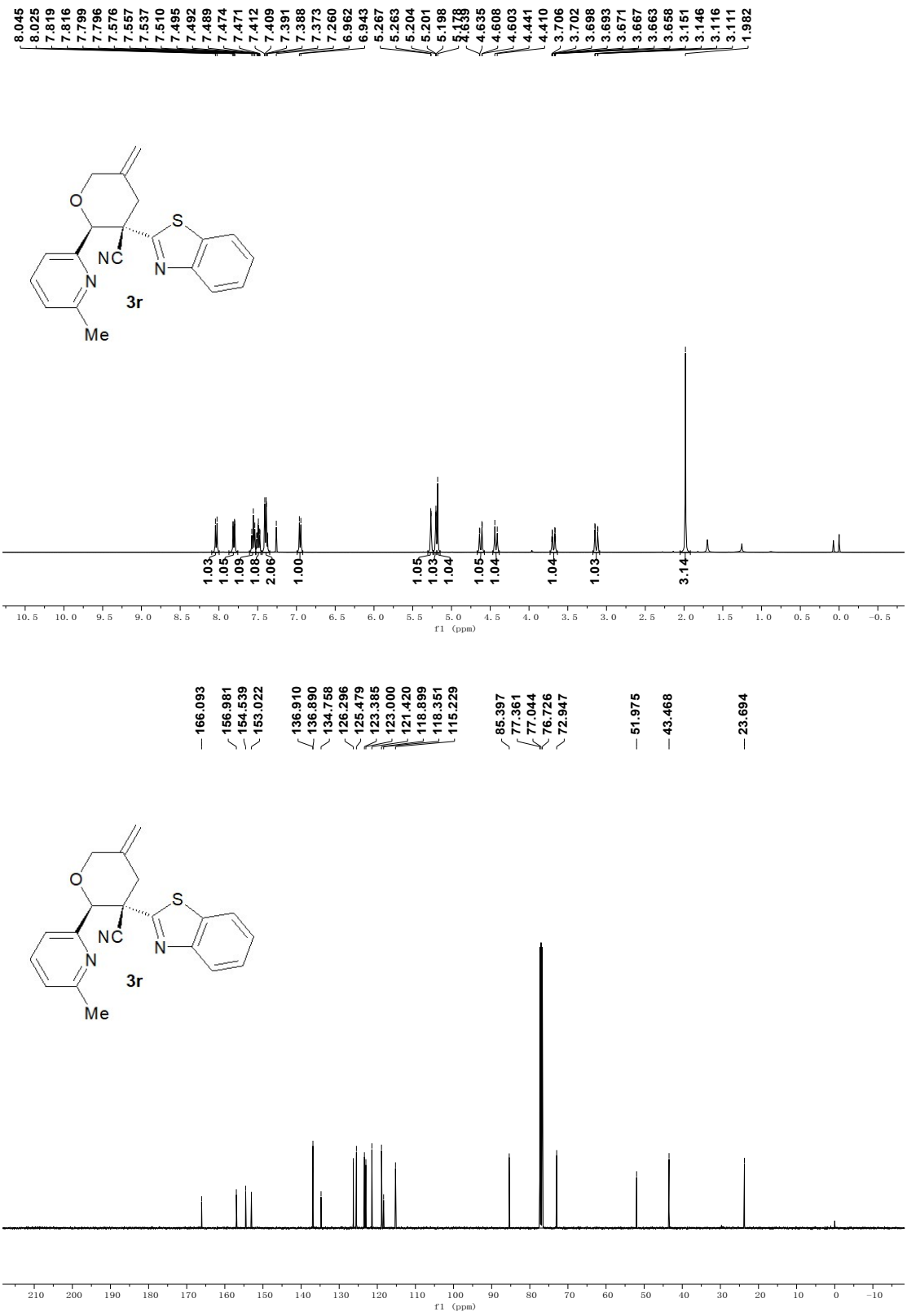
51.678
43.887
O
S
NC
N
N
3q
OMe
f1 (ppm)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7.796
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7.557
7.537
7.510
7.495
7.492
7.489
7.474
7.471
7.412
7.409
7.391
7.388
7.373
7.260
6.962
6.943
5.267
5.263
5.204
5.201
5.198
5.178
4.635
4.608
4.603
4.441
4.410
3.706
3.702
3.698
3.693
3.671
3.667
3.663
3.658
3.151
3.146
3.116
3.111
1.982
O
S
NC
N
N
3r
Me
1.03
1.05
1.09
1.08
2.06
1.00
1.05
1.03
1.04
1.05
1.04
1.04
1.03
3.14
f1 (ppm)
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154.539
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136.890
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123.000
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118.899
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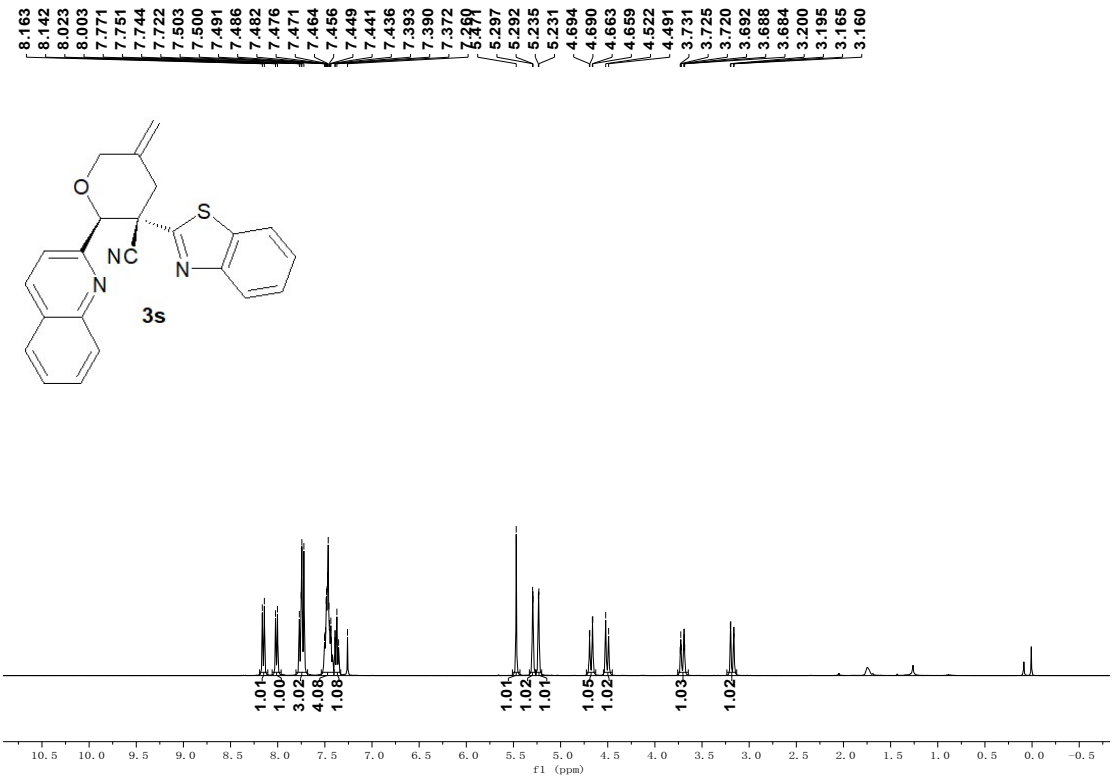
51.975
43.468
23.694
f1 (ppm)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7.722
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7.486
7.482
7.476
7.471
7.464
7.456
7.449
7.441
7.436
7.393
7.390
7.372
5.297
5.292
5.235
5.231
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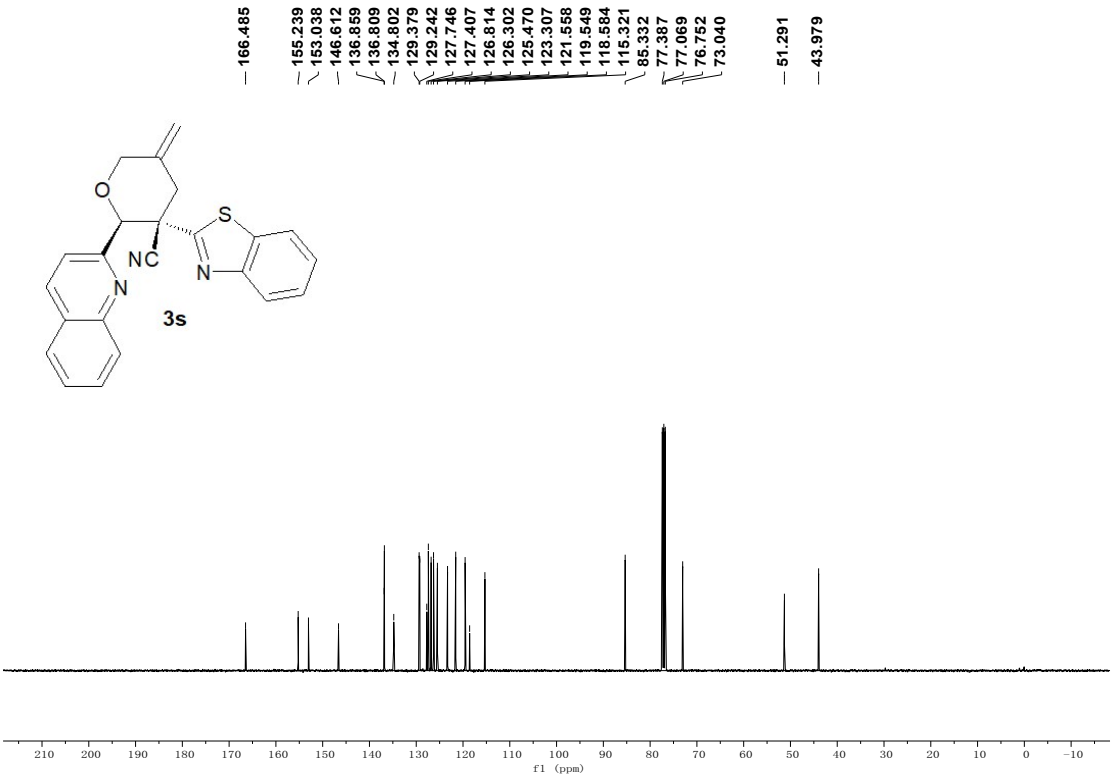
4.690
4.663
4.659
4.522
4.491
3.731
3.725
3.720
3.692
3.688
3.684
3.200
3.195
3.165
3.160
O
S
NC
N
N
3s
1.01
1.00
3.02
4.08
1.08
1.01
1.02
1.01
1.05
1.02
1.03
1.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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126.814
126.302
125.470
123.307
121.558
119.549
118.584
115.321
85.332
77.387
77.069
76.752
73.040
51.291
43.979
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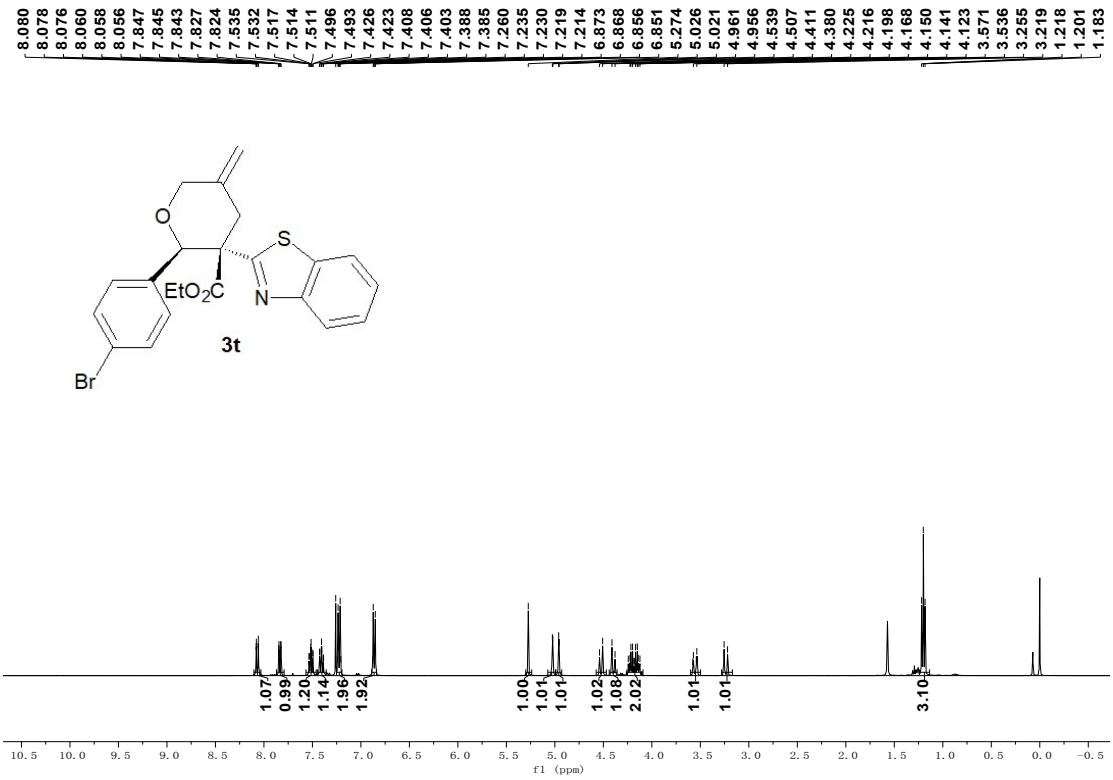
S
NC
N
N
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.517
7.514
7.511
7.496
7.493
7.426
7.423
7.408
7.406
7.403
7.388
7.385
7.260
7.235
7.230
7.219
7.214
6.873
6.868
6.856
6.851
5.274
5.026
5.021
4.961
4.956
4.539
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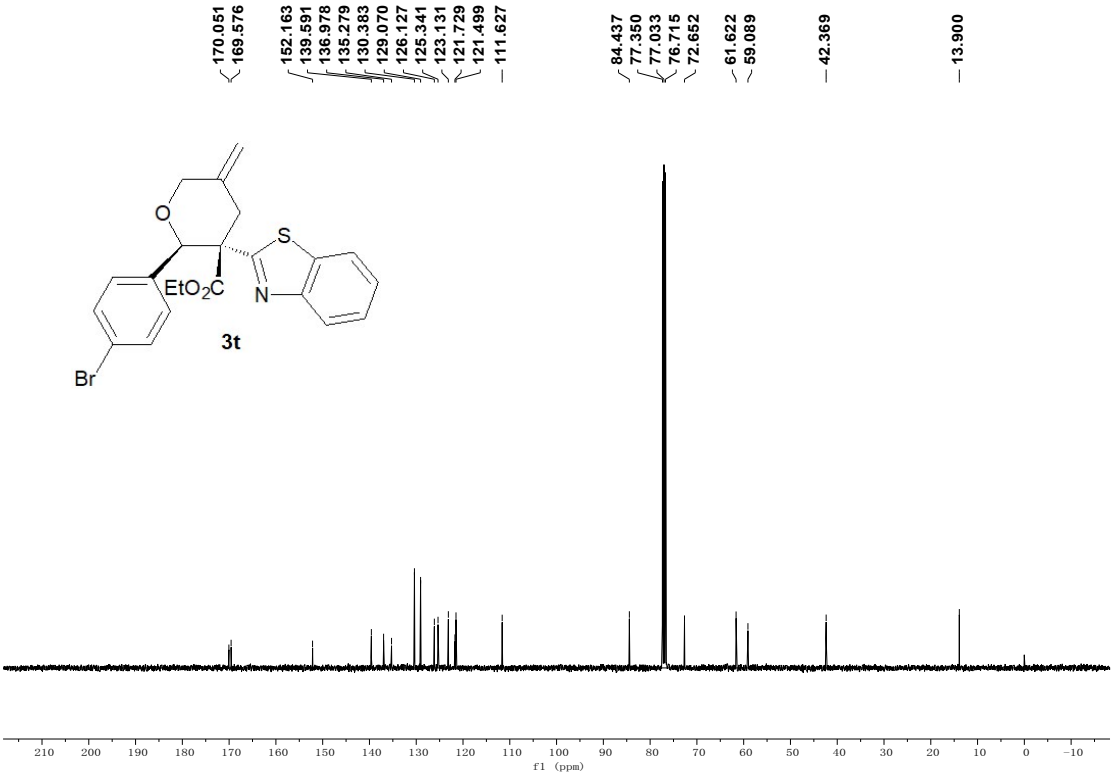
4.411
4.380
4.225
4.216
4.198
4.168
4.150
4.141
4.123
3.571
3.536
3.255
3.219
1.218
1.201
1.183
O
S
EtO2C
N
3t
Br
1.07
0.99
1.20
1.14
1.96
1.92
1.00
1.01
1.01
1.02
1.08
2.02
1.01
1.01
3.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.070
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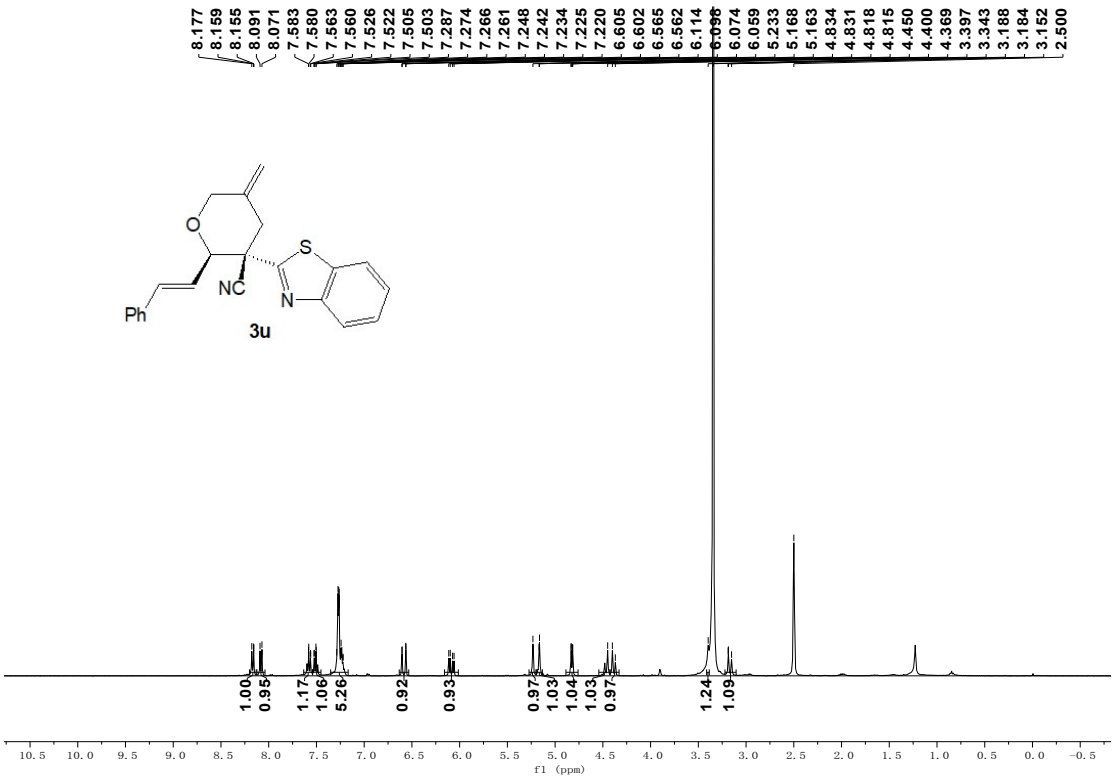
125.341
123.131
121.729
121.499
111.627
84.437
77.350
77.033
76.715
72.652
61.622
59.089
42.369
13.900
O
S
EtO2C
N
3t
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.560
7.526
7.522
7.505
7.503
7.287
7.274
7.266
7.261
7.248
7.242
7.234
7.225
7.220
6.605
6.602
6.565
6.562
6.114
6.098
6.074
6.059
5.233
5.168
5.163
4.834
4.831
4.818
4.815
4.450
4.400
4.369
3.397
3.343
3.188
3.184
3.152
2.500
O
S
NC
N
Ph
3u
1.00
0.95
1.17
1.06
5.26
0.92
0.93
0.97
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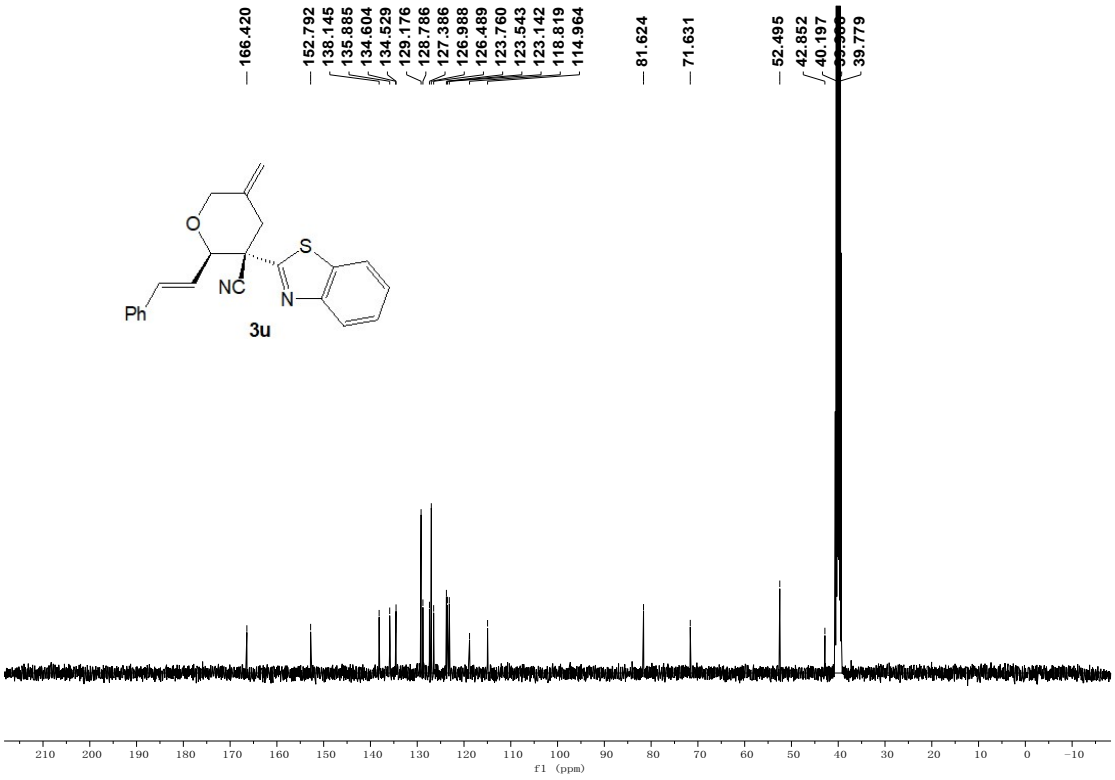
1.04
1.03
0.97
1.24
1.09
f1 (ppm)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128.786
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126.988
126.489
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123.543
123.142
118.819
114.964
81.624
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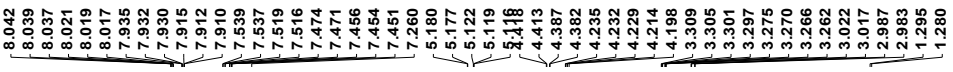
52.495
42.852
40.197
39.779
O
S
NC
N
Ph
3u
f1 (ppm)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7.539
7.537
7.519
7.516
7.474
7.471
7.456
7.454
7.451
7.260
5.180
5.177
5.122
5.119
4.413
4.387
4.382
4.235
4.232
4.229
4.214
4.198
3.309
3.305
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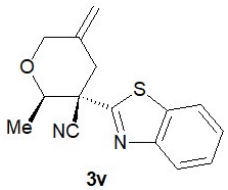
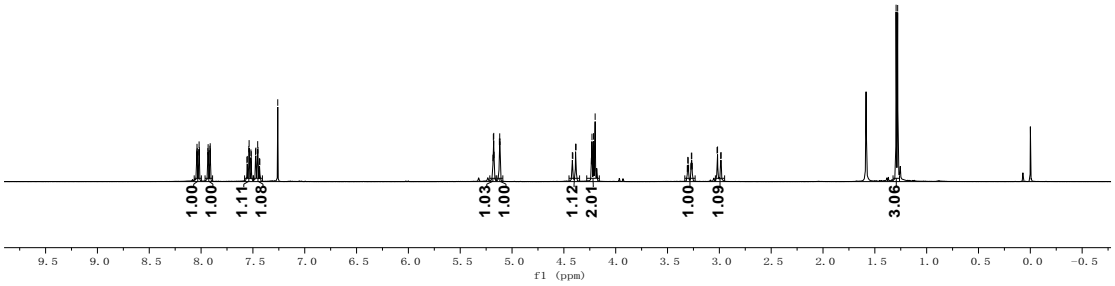
1.280


O
S
Me
NC
N

3v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1.00
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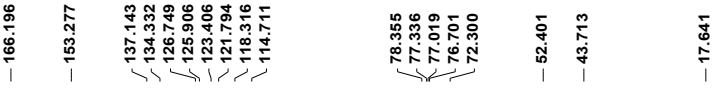
1.08
1.03
1.00
1.12
2.01
1.00
1.09
3.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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134.332
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125.906
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78.355
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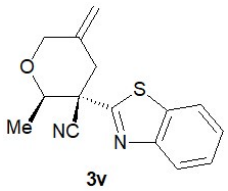
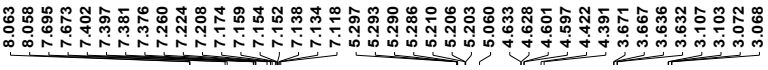
77.019
76.701
72.300
52.401
43.713
17.641


O
S
Me
NC
N

3v

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)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7.154
7.152
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5.210
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4.633
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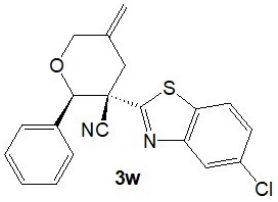
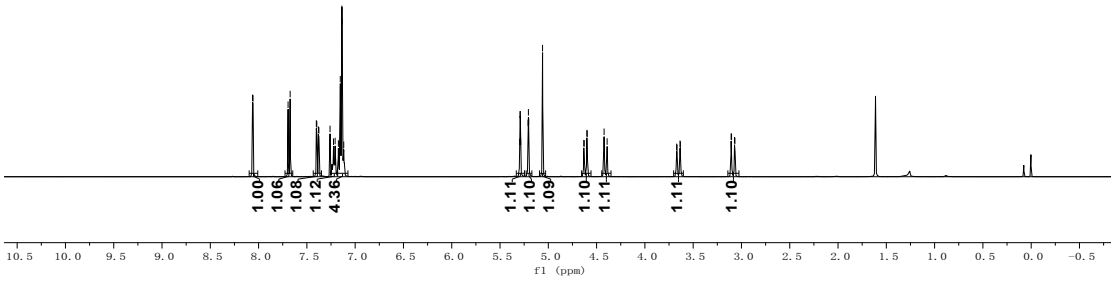
3.068


O
S
NC
N
Cl

3w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1.10
1.09
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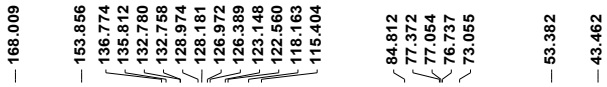
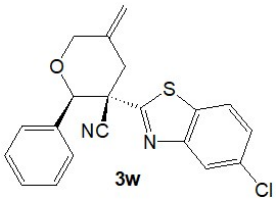
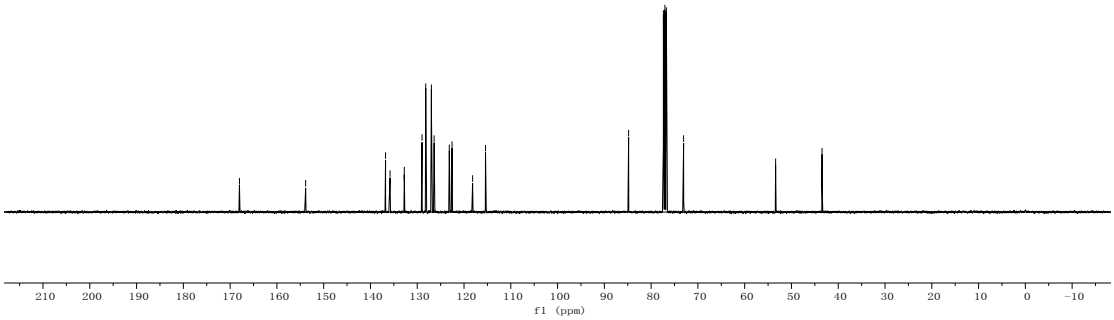
1.11
1.11
1.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

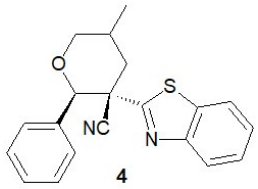

168.009
153.856
136.774
135.812
132.780
132.758
128.974
128.181
126.972
126.389
123.148
122.560
118.163
115.404
84.812
77.372
77.054
76.737
73.055
53.382
43.462


O
S
NC
N
Cl

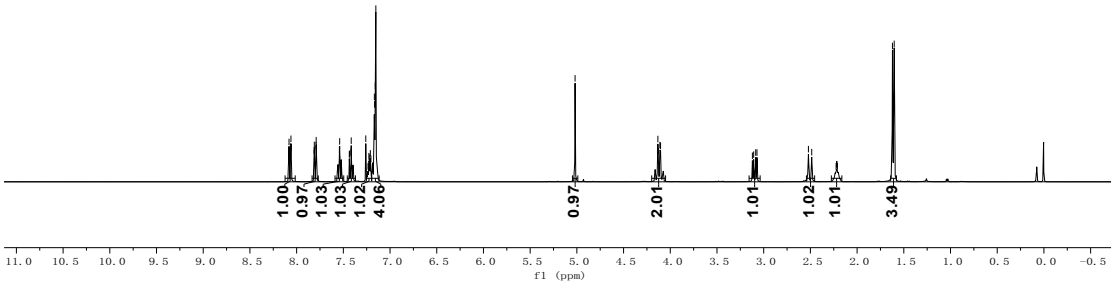
3w

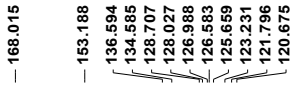

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

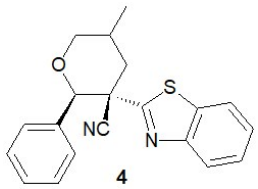

8.084
8.081
8.079
8.063
8.061
8.059
7.813
7.811
7.809
7.793
7.791
7.789
7.542
7.539
7.436
7.433
7.418
7.416
7.413
7.260
7.227
7.223
7.218
7.211
7.205
7.168
7.165
7.158
5.018
4.137
4.133
4.128
4.112
4.104
3.121
3.107
3.086
3.072
2.521
2.486
2.225
2.220
2.216
2.211
1.622
1.603


O
S
NC
N

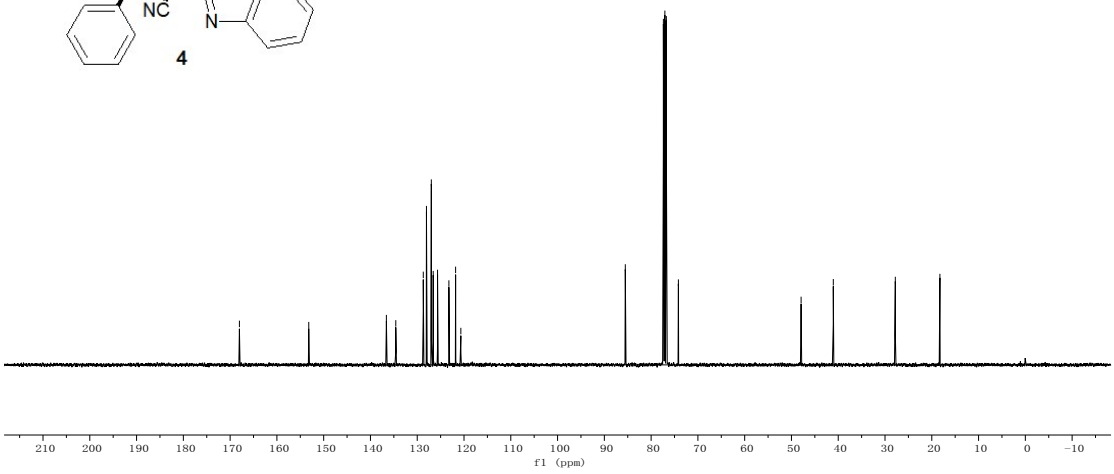
4

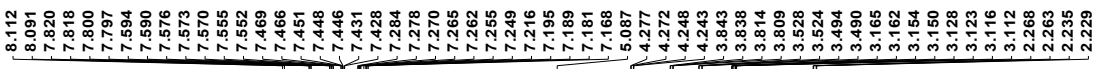

1.00
0.97
1.03
1.03
1.02
4.06
0.97
2.01
1.01
1.02
1.01
3.49
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

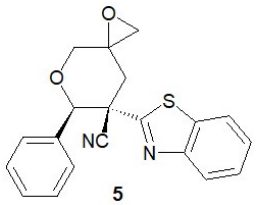

168.015
153.188
136.594
134.585
128.707
128.027
126.988
126.583
125.659
123.231
121.796
120.675
85.520
77.379
77.061
76.744
74.169
47.937
41.055
27.798
18.265


O
S
NC
N

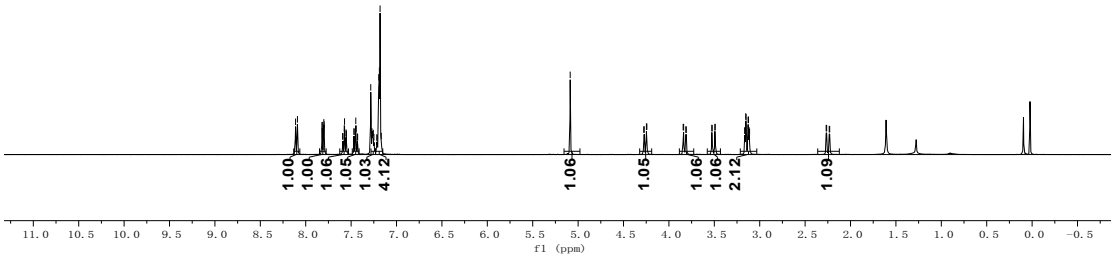
4


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)

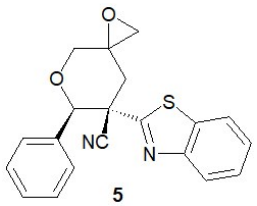

8.112
8.091
7.820
7.818
7.800
7.797
7.594
7.590
7.576
7.573
7.570
7.555
7.552
7.469
7.466
7.451
7.448
7.446
7.431
7.428
7.284
7.278
7.270
7.265
7.262
7.255
7.249
7.216
7.195
7.189
7.181
7.168
5.087
4.277
4.272
4.248
4.243
3.843
3.838
3.814
3.809
3.528
3.524
3.494
3.490
3.165
3.162
3.154
3.150
3.128
3.123
3.116
3.112
2.268
2.263
2.235
2.229


O
O
S
NC
N

5


1.00
1.00
1.06
1.05
1.03
4.12
1.06
1.05
1.06
1.06
2.12
1.09
11.0 10.5 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)


164.823
152.995
135.173
134.512
129.118
128.223
127.004
126.756
125.948
123.435
121.831
118.328
84.871
77.363
77.045
76.728
72.767
55.788
53.108
52.452
41.740


O
O
S
NC
N

5

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)

9. Reference

[1] K. Wang, C. Chen, X. Liu, D. Li, T. Peng, X. Liu, D. Yang, and L. Wang, *Org. Lett.*, **2018**, *20*, 5260-5263.

[2] Z. Yuan, R. Pan, H. Zhang, L. Liu, A. Lin, and H. Yao, *Adv. Synth. Catal.*, **2017**, *359*, 4244-4249.