Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Transition-metal free cyano 1,3 migration of unsaturated cyanohydrins

Jing Tao, Ting-Ting Yang, Qing-Hua Li*, and Tang-Lin Liu*

School of Chemistry and Chemical Engineering, Southwest University. Chongqing 400715, China.

E-mail: liuschop@swu.edu.cn, liqinghua@swu.edu.cn

I General information

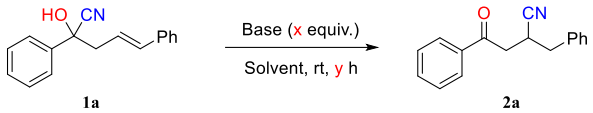
All reactions were maintained under a nitrogen atmosphere unless otherwise stated. Commercially available reagents were used without further purification. Solvents including: Toluene, TBME, *p*-xylene, *o*-xylene and THF were dried with sodium and degassed via liquid nitrogen. Other dried solvents were directly used from purchased. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 14A04336 (600 MHz) spectrometer. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: proton (chloroform δ 7.26), carbon (chloroform δ 77.0) or tetramethylsilane (TMS δ 0.00) was used as a reference. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, dd =doublet of doublets, m = multiplet), coupling constants (Hz) and integration. Coupling constants were reported in Hertz (Hz). High resolution mass spectra (HRMS) were recorded on a Bruker 19A01643 Q-TOF LC/MS with Electron Spray Ionization (ESI) resource. For thin layer chromatography (TLC), and compounds were visualized with a UV light at 254 nm. Further visualization was achieved by staining with 2,4-dinitrophenylhydrazine, or potassium permanganate solution followed by heating using a heat gun. The starting material unsaturated cyanohydrins were prepared by the addition of TMSCN to ketones according to the reported procedures.[1,2]

II General Procedure for preparation of product from unsaturated cyanohydrins and the transformation of functional groups of product 2a

Condition a: To a vial equipped with a dried stir bar was added unsaturated cyanohydrins (0.1 mmol), DBU (20 mol%) and *o*-xylene (1 mL) in the glovebox. The reaction mixture was taken outside the glovebox and allowed to stir at room temperature for 20 hours. The crude reaction mixture was concentrated under reduced pressure and directly purified by silica gel chromatography to give pure products.

Condition b: To a vial equipped with a dried stir bar was added unsaturated cyanohydrins (0.1 mmol), DBU (40 mol%) and *o*-xylene (1 mL) in the glovebox. The reaction mixture was taken outside the glovebox and allowed to stir at 65 ^{o}C for 20 hours. The crude reaction mixture was concentrated under reduced pressure and directly purified by silica gel chromatography to give pure products.

Table S1. Table Condition Screening for cyano 1,3-migration[a]



1a 2a

entry	temp. (^{o}C)	Base	x	Solvent	Yield (%)[b]
1	120	DBU	1	Toluene	53
2	100	DBU	1	Toluene	60
3	80	DBU	1	Toluene	60
4	60	DBU	1	Toluene	66
5	40	DBU	1	Toluene	62
6	rt	DBU	1	Toluene	60
7	rt	DBU	0.4	Toluene	66
8	rt	DBU	0.2	Toluene	69
9	rt	DBU	0.1	Toluene	24
10	rt	DBU	0.20	DCE	36
12	rt	DBU	0.20	TBME	61
13	rt	DBU	0.20	Hexane	56
14	rt	DBU	0.20	*p*-Xylene	71
16	rt	DBU	0.20	*o*-Xylene	81
17	rt	DBU	0.20	DMF	41
18	rt	DBU	0.20	THF	36
19	rt	DMAP	0.20	*o*-Xylene	0
20	rt	DABCO	0.20	*o*-Xylene	0
21	120	NaOH	1	Toluene	0
22	120	KOH	1	Toluene	0
23	120	LiOH	1	Toluene	0
24	120	KOt-Bu	1	Toluene	0
25	rt	TEA	0.20	*o*-Xylene	trace
26	rt	TMG	0.20	*o*-Xylene	trace

[a] The reaction was carried out with 0.1 mmol of 1a and 20 mol% base in 1 mL of solvent at room temperature for 18 h. [b] Isolated yield. DBU = 1,8-Diazabicyclo [5.4.0] undec-7-ene, DMAP = 4-Dim-ethylaminopyridine, DABCO = 1,4-Diazabicyclo[2.2.2]octane, TEA = Triethylamine, TMG= 1,1,3,3-Tetramethylguanidine.

The Scale-up reaction c: To a vial equipped with a dried stir bar was added unsaturated cyanohydrins (3.6 mmol), DBU (20 mol%) and *o*-xylene (36 mL) in the glovebox. The reaction mixture was taken outside the glovebox and allowed to stir at room temperature for 20 hours. The crude reaction mixture was concentrated under reduced pressure and directly purified by silica gel chromatography to give pure products.

The general procedure of synthetic transformations of the product

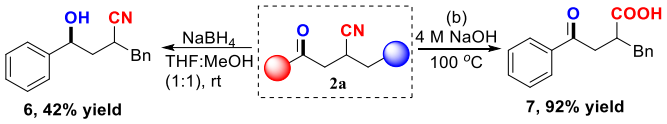
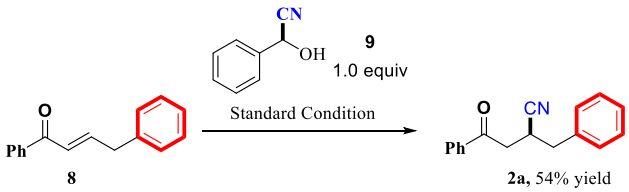


Figure S1 the transformation of functional groups of product **2a.**

the general procedure synthesis of 6[3]**:** A 25 mL round bottle flask equipped with a dried stir bar was added **2a** (1 mmol, 250 mg, 1.0 equiv.) and the mixed solvents of THF and CH_3OH (2 mL, 1:1). After **2a** was complete solvent, $NaBH_4$ (2 mmol, 76 mg) was added at 0 °C. The reaction temperature was allowed to stirring at room temperature. One hour later, the reaction was quenched by saturated NH_4Cl aqueous. The aqueous was extracted with EA (5 mL×2). The organic layer was combined and dried with Na_2SO_4. Then concentrated under reduced pressure and directly purified by silica gel chromatography to give pure products **5o** in 42% yields.

the general procedure synthesis of 7[4]**:** A 25 ml round bottle flask equipped with a dried stir bar was added **2a** (1 mmol, 250 mg, 1.0 equiv.), and 5 mL of 4 M NaOH (aq)was added at room temperature. Then, the reaction mixture was refluxed at 100 °C for 4 hours. After the reaction finished, the mixture was cooled to room temperatuer, and acidify with HCl until the pH = 1~2. The productof **5p** was precipitated out, filtered and dried, to give white powder with a yield of 92% yield without further purification.

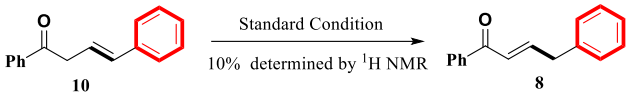
III The mechanism study



The mechanism study of experiment **A**

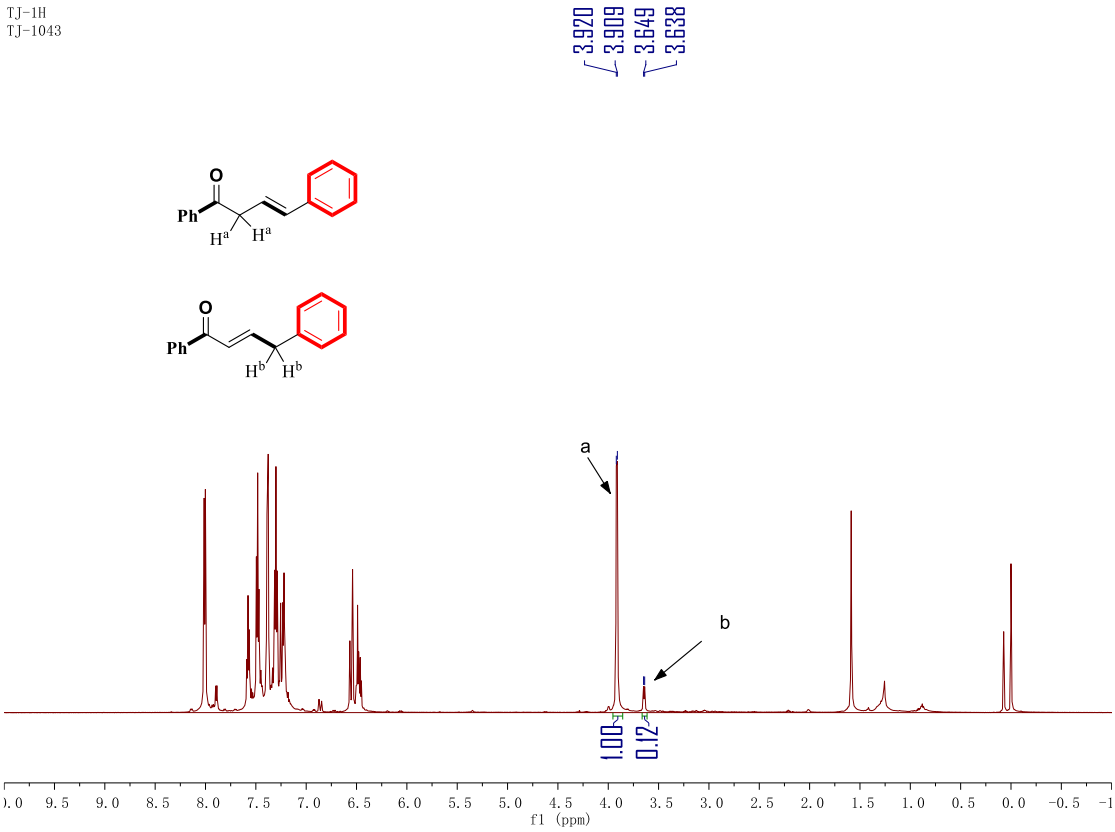
Experimental **A**: To a vial equipped with a dried stir bar was added α,β-unsaturated ketone (**8**, 0.1 mmol), benzaldehyde cyanohydrin (**9**, 0.1 mmol), DBU (3.2 μL), anhydrous *o*-xylene (1 mL) in the glovebox. After then, the reaction mixture was allowed to stir at room temperature for 20 hours. The products of **2a**

was isolated with 54% yields, which shows that α,β-unsaturated ketone **8** was an intermediate for the cyano migration.

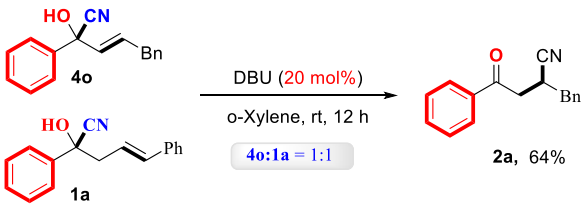


The mechanism study of experiment **B**

Then experiment **B**: To a vial equipped with a dried stir bar was added β,γ-Unsaturated ketone **10**, DBU (3.2 μL), anhydrous *o*-xylene (1 mL) in the glovebox. After then, the reaction mixture was allowed to stir at room temperature for 20 hours. The crude reaction mixture was concentrated under reduced pressure, and quick filtrate through a short silicagel column. Then the crude products were analysis via ^{1}H NMR, which shown 10% conversion of β,γ-Unsaturated ketone **10** transformation into α,β-Unsaturated ketone **8**. It is consistent with our hypothesis, and further illustrated α,β-unsaturated ketone **8** was an intermediate in this catalytic system.



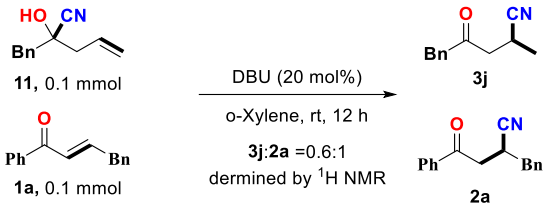
The ^{1}H NMR of experiment **B**



The mechanism study of experiment **C**

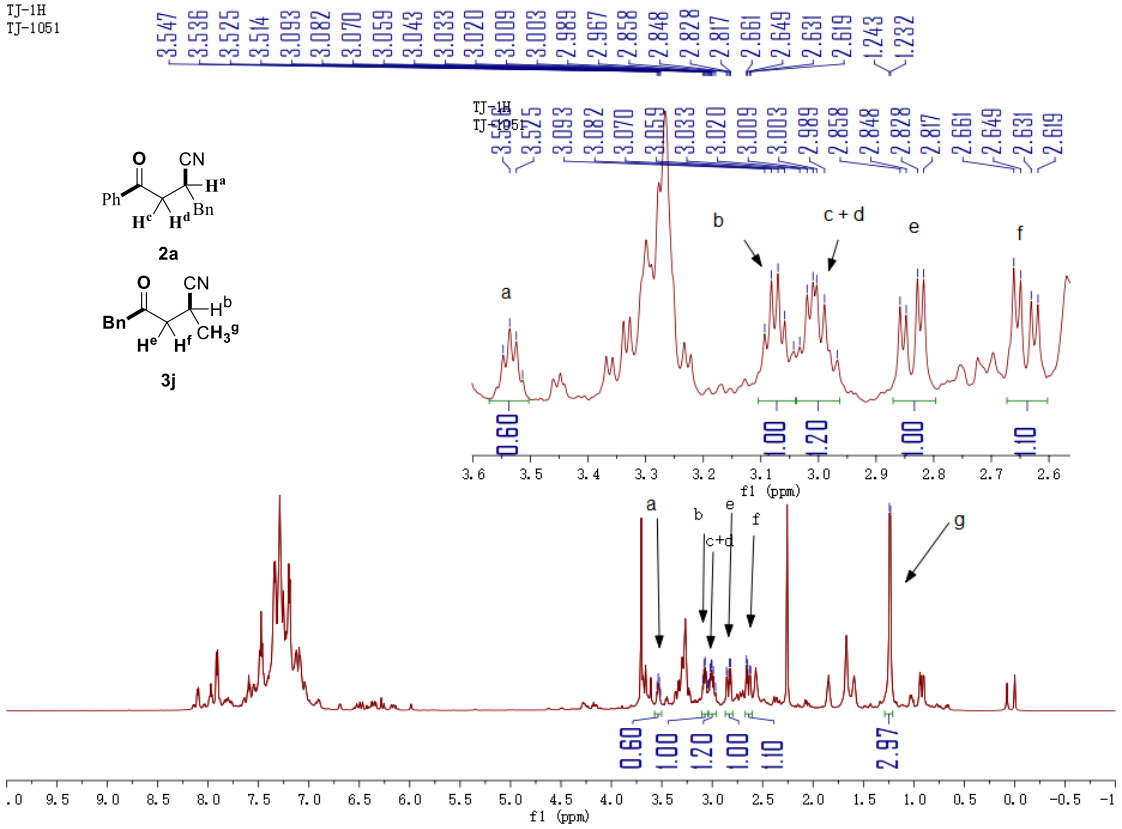
Experimental **C**: To a vial equipped with a dried stir bar was added α,β-unsaturated cyanohydrin (**4o**, 0.1

mmol), β,γ-unsaturated cyanohydrin (**1a**, 0.1 mmol), DBU (3.2 μL), anhydrous *o*-xylene (1 mL) in the glovebox. After then, the reaction mixture was allowed to stir at room temperature for 20 hours. The total yield of **2a** was obtained in 64%. And the result of this experimental show that DBU played a role as base involved in the reaction, which lead the total yield reduced.



The mechanism study of experiment **D**

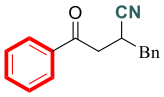
Experimental **D**: To a vial equipped with a dried stir bar was added β,γ-unsaturated cyanohydrin (**11**, 0.1 mmol), β,γ-unsaturated cyanohydrin (**1a**, 0.1 mmol), DBU (3.2 μL), anhydrous *o*-xylene (1 mL) in the glovebox. After then, the reaction mixture was allowed to stir at room temperature for 20 hours. The crude reaction mixture was concentrated under reduced pressure, and analysis via ^{1}H NMR. The corresponding products **3j** and **2a** with the ratio of 0.6:1 were observed in the spectrum, which was demonstrate that the CN^- was free state.



The ^{1}H NMR of experiment **D**

IV Characterization of products

2-Benzyl-4-oxo-4-phenylbutanenitrile (2a)[5]



The title compound 2a was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 81% yield.

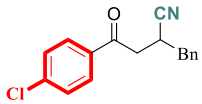
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.8 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.35-7.32 (m, 2H), 7.22-7.25 (m, 3H), 3.56-3.52 (m, 1H), 3.35 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 3.25 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 3.04-3.97 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.2, 136.4, 135.9, 133.8, 129.1, 128.8, 128.0, 127.4, 121.3, 39.7, 37.5, 28.2.

HRMS(ESI) m/z: $C_{17}H_{16}NO$, $[M+H]^+$, Calcd: 250.1265, Found: 250.1226.

IR (KBr, cm^{-1}) 2964, 2926, 2245, 1685, 1596, 1450, 1265, 1218, 1076, 1002, 986, 747, 700, 685, 580, 486.

2-Benzyl-4-(4-chlorophenyl)-4-oxobutanenitrile (2b)



The title compound 2b was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 81% yield.

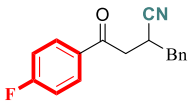
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.8 Hz, 2H), 7.46 (d, *J* = 7.8 Hz, 2H), 7.35 (t, *J* = 7.2 Hz, 2H), 7.31-7.24 (m, 3H), 3.55-3.50 (m, 1H), 3.32 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.20 (dd, *J* = 17.2 Hz, 6.6 Hz, 1H), 3.06-2.95 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.0, 140.4, 136.2, 134.2, 129.4, 129.2, 129.1, 128.9, 127.5, 121.2, 39.7, 37.5, 28.1.

HRMS(ESI) m/z: $C_{17}H_{14}ClNNaO$, $[M+Na]^+$, Calcd: 306.0656, Found: 306.0655.

IR (KBr, cm^{-1}) 2924, 2241, 1687, 1587, 1453, 1399, 1264, 1216, 1093, 1033, 827, 748, 699, 576.

2-Benzyl-4-(4-fluorophenyl)-4-oxobutanenitrile (2c)



The title compound **2c** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 86% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95-7.93 (m, 2H), 7.34 (t, *J* = 7.2 Hz, 2H), 7.30-7.25 (m, 3H), 7.16-7.13 (m, 2H), 3.54-3.52 (m, 1H), 3.32 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.20 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.05-2.98 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 193.6, 166.1 (d, *J* = 256.3 Hz), 136.2, 132.4, 130.7 (d, *J* = 9.5 Hz), 129.1,

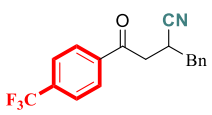
128.8, 127.5, 121.2, 116.1 (d, J = 22.0 Hz), 115.9, 39.6, 37.5, 28.1.

^{19}F NMR (376 MHz, CDCl3) δ -103.53.

HRMS(ESI) m/z: $C_{17}H_{15}FNO$, $[M+H]^+$, Calcd: 268.1132, Found: 268.1131.

IR (KBr, cm^{-1}) 2925, 2245, 1686, 1579, 1505, 1237, 1222, 1156, 834, 635, 485.

2-Benzyl-4-oxo-4-(4-(trifluoromethyl)phenyl)butanenitrile (2d)



The title compound **2d** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 76% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 (d, J =7.8 Hz, 2H), 7.75 (d, J = 8.4 Hz, 2H), 7.35 (t, J = 7.2 Hz, 2H), 7.32-7.24 (m, 3H), 3.56-3.52 (m, 1H), 3.37 (dd, J = 18.0 Hz, 6.6 Hz, 1H), 3.25 (dd, J = 18.0 Hz, 6.6 Hz, 1H), 3.03 (d, J= 7.2 Hz, 2H).

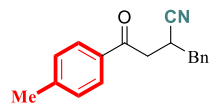
^{13}C NMR (151 MHz, $CDCl_3$) δ 194.3, 138.5, 136.1,135.2 (q, J =32.9 Hz), 129.1, 128.9, 128.3, 127.6, 125.9 (q, J = 3.7 Hz), 123.4 (q, J = 272.8 Hz), 121.0, 40.0, 37.4, 28.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.24.

HRMS(ESI) m/z: $C_{18}H_{15}F_3NO$, $[M+H]^+$, Calcd: 318.1100, Found: 318.1099.

IR (KBr, cm^{-1}) 2959, 2247, 1692, 1330, 1109, 845, 832, 742, 701.

2-Benzyl-4-oxo-4-(p-tolyl)butanenitrile (2e)



The title compound **2e** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 76% yield.

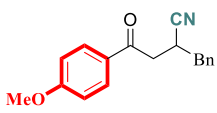
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, J = 6.6 Hz, 2H), 7.35-7.32 (m, 2H), 7.29-7.25 (m, 5H), 3.56-3.51 (m, 1H), 3.32 (dd, J = 18.0 Hz, 6.6 Hz, 1H), 3.22 (dd, J = 18.0 Hz, 6.6 Hz, 1H), 3.04-2.95 (m, 2H), 2.42 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.8, 144.8, 136.4, 133.5, 129.5, 129.2, 128.8, 128.1, 127.4, 121.4, 39.6, 37.5, 28.2, 21.6.

HRMS(ESI) m/z: $C_{18}H_{18}NO$, $[M+H]^+$, Calcd: 264.1383, Found: 264.1381.

IR (KBr, cm^{-1}) 2928, 2240, 1679, 1378,1323, 1266, 1181, 1106, 816, 700.

2-Benzyl-4-(4-methoxyphenyl)-4-oxobutanenitrile (2f)



The title compound **2f** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 57% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (d, J = 9.0 Hz, 2H), 7.33 (d, J = 7.2 Hz, 2H), 7.28-7.25 (m, 3H), 6.95 (d, J = 9.0 Hz, 2H), 3.88 (s, 3H), 3.56-3.52 (m, 1H), 3.30 (dd, J = 17.4 Hz, 6.6 Hz, 1H), 3.20 (dd, J = 18.0

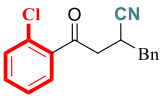
Hz, 7.2 Hz, 1H), 3.03 (dd, *J* = 13.2 Hz, 6.0 Hz, 1H), 2.97 (dd, *J* = 13.8 Hz, 8.4 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 193.6, 164.1, 136.5, 130.3, 129.2, 129.0, 128.8, 127.4, 121.5, 114.0, 55.5, 39.3, 37.5, 28.3.

HRMS(ESI) m/z: $C_{18}H_{18}NO_2$, $[M+H]^+$, Calcd: 280.1332, Found: 280.1328.

IR (KBr, cm^{-1}) 2862, 2242, 1684, 1592, 1453, 1431, 1267, 1043, 787, 766, 622.

2-Benzyl-4-(2-chlorophenyl)-4-oxobutanenitrile (2g)



The title compound **2g** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 86% yield.

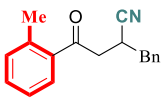
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 4.2 Hz, 2H), 7.36-7.33 (m, 3H), 7.30-7.27 (m, 3H), 3.53-3.47 (m, 1H), 3.37 (dd, *J* = 18.0 Hz, 7.2 Hz, 1H), 3.27 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 3.05-2.98 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 198.1, 137.7, 136.2, 132.6, 131.3, 130.8, 129.4, 129.1, 128.8, 127.5, 127.1, 121.0, 44.0, 37.5, 28.5.

HRMS(ESI) m/z: $C_{17}H_{15}ClNO$, $[M+H]^+$, Calcd: 284.0837, Found: 284.0835.

IR (KBr, cm^{-1}) 2928, 2242, 1700, 1589, 1433, 1213,1162, 755, 701.

2-Benzyl-4-oxo-4-(o-tolyl)butanenitrile (2h)



The title compound **2h** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 88% yield.

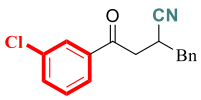
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 7.3 Hz, 1H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.22-7.17 (m, 5H), 3.46-3.42 (m, 1H), 3.21 (dd, *J* = 17.4 Hz, 6.6 Hz, 1H), 3.09 (dd, *J* = 17.4 Hz, 6.6 Hz, 1H), 2.93-2.91 (m, 2H), 2.45 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 198.5, 138.9, 136.3, 136.3, 132.3, 132.1, 129.1, 128.8, 128.5, 127.4, 125.8, 121.4, 42.3, 37.6, 28.3, 21.4.

HRMS(ESI) m/z: $C_{18}H_{18}NO$, $[M+H]^+$, Calcd: 264.1383, Found: 264.1382.

IR (KBr, cm^{-1}) 2926, 2242, 1686, 1409, 1271, 976,757, 702.

2-Benzyl-4-(3-chlorophenyl)-4-oxobutanenitrile (2i)



The title compound **2i** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 70% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.43 (t, *J*

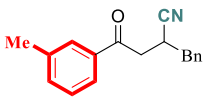
= 7.9 Hz, 1H), 7.36 (t, *J* = 7.2 Hz, 2H), 7.29 (m, 3H), 3.55-3.50 (m, 1H), 3.35-3.31 (dd, *J* = 18.0 Hz, 6.6 Hz,1H), 3.21 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.02 (d, *J* = 7.2 Hz, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.0, 137.4, 136.1, 135.2, 133.7, 130.1, 129.1, 128.9, 128.1, 127.5, 126.0, 121.1, 39.8, 37.5, 28.1.

HRMS(ESI) m/z: $C_{17}H_{15}ClNO$, $[M+H]^+$, Calcd: 284.0837, Found: 284.0836.

IR (KBr, cm^{-1}) 2861, 2219, 1646, 1372, 1160, 1105, 1078, 759, 697.

2-Benzyl-4-oxo-4-(m-tolyl)butanenitrile (2j)



The title compound **2j** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 85% yield.

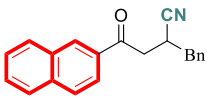
^{1}HNMR (600 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.8 Hz, 2H), 7.35-7.32 (m, 2H), 7.28-7.25 (m, 5H), 3.55-3.52 (m, 1H), 3.32 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 3.22 (dd, *J* = 18.0 Hz, 7.2 Hz, 1H), 3.02 (dd, *J* = 13.8 Hz, 6.0 Hz, 1H), 2.97 (dd, *J* = 13.2 Hz, 7.8 Hz, 1H), 2.42 (s, 3H);

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.8, 144.8, 136.5, 133.5, 129.5, 129.2, 128.8, 128.1, 127.4, 121.5, 39.6, 37.6, 28.2, 21.7.

HRMS(ESI) m/z: $C_{18}H_{18}ClNO$, $[M+H]^+$, Calcd: 264.1383, Found: 264.1382.

IR (KBr, cm^{-1}) 2862, 2241, 1683, 1450, 1270, 1203, 1183, 786, 689.

2-Benzyl-4-(naphthalen-2-yl)-4-oxobutanenitrile (2k)



The title compound **2k** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 87% yield.

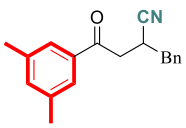
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (s, 1H), 8.97-7.94 (m, 2H), 7.91-7.87 (m, 2H), 7.63-7.62 (m, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.36-7.33 (m, 2H), 7.31-7.29 (m, 3H), 3.62-3.58 (m, 1H), 3.48 (dd, *J* = 17.2 Hz, 6.0 Hz, 1H), 3.39 (dd, *J* = 17.2 Hz, 6.6 Hz, 1H), 3.08-3.00 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.1, 136.4, 135.9, 133.2, 132.4, 129.9, 129.6, 129.2, 128.9, 128.8, 128.8, 127.8, 127.5, 127.0, 123.4, 121.4, 39.8, 37.5, 28.3.

HRMS(ESI) m/z: $C_{21}H_{18}NO$, $[M+H]^+$, Calcd: 300.1383, Found: 300.1381.

IR (KBr, cm^{-1}) 2924, 2244, 1677, 1451, 1275, 1263, 1184, 1122, 889, 766, 699, 494.

2-Benzyl-4-(3,5-dimethylphenyl)-4-oxobutanenitrile (2l)



The title compound **2l** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 77% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.52 (s, 2H), 7.35-7.33 (m, 2H), 7.29-7.27 (m, 3H), 7.23 (s, 1H), 3.56-3.51 (m, 1H), 3.33 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.23 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 3.30-2.94 (m, 2H), 2.37 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.6, 138.5, 136.5, 136.0, 135.4, 129.2, 128.8, 127.4, 125.8, 121.4, 39.8, 37.5, 28.2, 21.2.

HRMS(ESI) m/z: $C_{19}H_{20}NO$, $[M+H]^+$, Calcd: 278.1539, Found: 278.1539.

IR (KBr, cm^{-1}) 2921, 2241, 1682. 1646, 1603, 1449, 1358, 1301, 1206, 1185, 1159, 852, 754, 689.

2-Benzyl-4-oxopentanenitrile (2m)[6]

The title compound **2m** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 8:1) resulting in a yellow oil in 78% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 (t, *J* = 6.6 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.24 (d, *J* = 6.6 Hz, 2H), 3.3-3.28 (m, 1H), 2.91 (d, *J* = 6.6 Hz, 2H), 2.81 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 2.68 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 2.17 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 203.5, 136.2, 129.1, 128.8, 127.5, 121.1, 44.2, 37.3, 29.9, 27.7.

HRMS(ESI) m/z: $C_{12}H_{13}NO$, [M], Calcd: 188.1070, Found: 188.1070.

IR (KBr, cm^{-1}) 3063, 2927, 2241, 1718, 1496, 1366, 1180, 1162, 747, 702.

2-Benzyl-5-methyl-4-oxohexanenitrile (2n)

The title compound **2n** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a yellow oil in 62% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.34 (t, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 2H), 3.35-3.31 (m, 1H), 2.91 (d, *J* = 7.2 Hz, 2H), 2.77 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 2.63 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 2.32-2.24 (m, 2H), 2.14 (m, 1H), 0.92 (t, *J* = 5.4 Hz, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 205.7, 136.3, 129.1, 128.8, 127.4, 121.2, 51.8, 44.0, 37.4, 27.7, 24.6, 22.4, 22.4.

HRMS(ESI) m/z: $C_{15}H_{19}NNaO$, $[M+Na]^+$ Calcd: 252.1359, Found: 252.1357.

2957, 2243, 1708, 1403, 1371, 1095, 1079, 960, 749, 710, 584.

IR (KBr, cm^{-1}) 2957, 2243, 1708, 1403, 1371, 1095, 1079, 960, 749, 710, 584.

2-Benzyl-5,5-dimethyl-4-oxohexanenitrile (2o)

The title compound **2o** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30

in hexane: ethyl acetate = 15:1) resulting in a yellow oil in 58% yield.

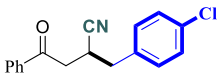
^{1}H NMR (600 MHz, CDCl3) δ 7.34 (t, *J* = 7.2 Hz, 2H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.26 (d, *J* = 9.0 Hz, 2H), 3.37-3.32 (m, 1H), 2.93-2.88 (m, 3H), 2.74 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 1.15 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 211.2, 136.4, 129.0, 128.8, 127.4, 121.4, 44.0, 38.2, 37.4, 28.1, 26.2.

HRMS(ESI) m/z: $C_{15}H_{19}NNaO$, $[M+Na]^+$, Calcd: 252.1359, Found: 252.1357.

IR (KBr, cm^{-1}) 2976, 2241, 1701, 1477, 1455, 1365, 1099, 1000, 879, 771, 738, 703.484.

2-(4-Chlorobenzyl)-4-oxo-4-phenylbutanenitrile (2p)



The title compound **2p** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 87% yield.

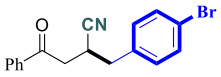
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.2 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.24 (t, *J* = 12.6 Hz, 2H), 3.54-3.50 (m, 1H), 3.37 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.26 (dd, *J* = 18.0 Hz, 7.2 Hz, 1H), 3.02 (dd, *J* = 13.8 Hz, 5.4 Hz, 1H), 2.93 (dd, *J* = 13.8 Hz, 8.4 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.0, 135.8, 134.8, 133.9, 133.5, 130.5, 129.0, 128.8, 128.0, 121.1, 39.7, 36.8, 28.2.

HRMS(ESI) m/z: $C_{17}H_{15}ClNO$, $[M+H]^+$, Calcd: 284.0837; Found: 284.0834.

IR (KBr, cm^{-1}) 2931, 2246, 1686, 1588, 1362, 1092, 829, 699, 699, 577, 484.

2-(4-Bromobenzyl)-4-oxo-4-phenylbutanenitrile (2q)



The title compound **2q** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 80% yield.

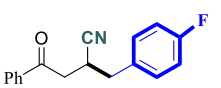
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.8 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.50-7.46 (m, 4H), 7.17 (d, *J* = 7.8 Hz, 2H), 3.563-3.51 (m, 1H), 3.36 (dd, *J* = 18.0 Hz, 5.0 Hz, 1H), 3.25 (dd, *J* = 18.0 Hz, 7.2 Hz, 1H), 3.00 (dd, *J* = 13.8 Hz, 5.4 Hz, 1H), 2.92 (dd, *J* = 13.2 Hz, 8.4 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.0, 135.8, 135.4, 133.9, 132.0, 130.9, 128.9, 128.0, 121.5, 121.1, 39.7, 36.9, 28.1.

HRMS(ESI) m/z: $C_{17}H_{15}BrNO$, $[M+H]^+$, Calcd: 328.0332, Found: 328.0329.

IR (KBr, cm^{-1}) 2933, 2246, 1683, 1594, 1487, 1217, 1180, 1042, 987, 821, 751, 686, 642, 500.

2-(4-Fluorobenzyl)-4-oxo-4-phenylbutanenitrile (2r)



The title compound **2r** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 75% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.2 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.26 (t, *J* = 6.6 Hz, 2H), 7.03 (t, *J* = 9.0 Hz, 2H), 3.54-3.49 (m, 1H), 3.37 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 3.26 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.02 (dd, *J* = 14.4 Hz, 6.0 Hz, 1H), 2.94 (dd, *J* = 13.2 Hz, 8.4 Hz, 1H).

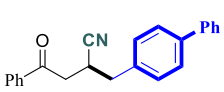
^{13}C NMR (151 MHz, $CDCl_3$) δ 195.1, 161.4 (d, *J* = 246.2 Hz), 135.8, 133.9, 132.1, 130.7 (d, *J* = 8.0 Hz), 128.8, 128.0, 121.2, 115.7 (d, *J* = 21.1 Hz), 39.7, 36.7, 28.4.

^{19}F NMR (376 MHz, $CDCl_3$) δ -114.96.

HRMS(ESI) m/z: $C_{17}H_{15}FNO$, $[M+H]^+$, Calcd: 268.1132, Found: 268.1130.

IR (KBr, cm^{-1}) 2967, 2245, 1684, 1598, 1508, 1448, 1266, 1222, 1157, 1096, 1037, 1034, 837, 749, 687, 550, 524.

2-([1,1'-Biphenyl]-4-ylmethyl)-4-oxo-4-phenylbutanenitrile (2s)



The title compound **2s** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10 :1) resulting in a yellow solid in 82% yield.

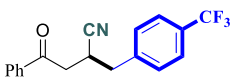
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.4 Hz, 2H), 7.61-7.56 (m, 5H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.43 (t, *J* = 7.2 Hz, 2H), 7.35 (t, *J* = 7.8 Hz, 3H), 3.60-3.56 (m, 1H), 3.38 (dd, *J* = 18.0 Hz, 6.4 Hz, 1H), 3.29 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.09-3.01 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.2, 140.6, 140.4, 135.9, 135.3, 133.8, 129.6, 128.8, 128.7, 128.0, 127.5, 127.3, 127.0, 121.4, 39.8, 37.2, 28.2.

HRMS(ESI) m/z: $[M+H]^+$ Calcd. for $C_{23}H_{17}NO$ 326.1539; Found 326.1539.

IR (KBr, cm^{-1}) 2925, 2241, 1680, 1646, 1595, 1485, 1477, 1261, 1213, 1107, 1074, 799, 691.

4-Oxo-4-phenyl-2-(4-(trifluoromethyl)benzyl)butanenitrile (2t)



The title compound **2t** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 75% yield.

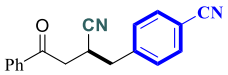
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.8 Hz, 2H), 7.63-7.60 (m, 3H), 7.50 (t, *J* = 7.8 Hz, 2H), 7.43 (d, *J* = 7.8 Hz, 2H), 3.59-3.55 (m, 1H), 3.40 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 3.29 (dd, *J* = 18.0 Hz, 7.8 Hz, 1H), 3.11 (dd, *J* = 13.8 Hz, 6.6 Hz, 1H), 3.01 (dd, *J* = 13.8 Hz, 8.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.9, 140.4, 135.7, 134.0, 129.9 (q, *J* = 32.4 Hz), 128.9, 128.0, 125.8 (q, *J* = 3.6Hz), 122.043 (q, *J* = 272.2 Hz), 120.9, 39.8, 37.3, 28.0.

HRMS(ESI) m/z: $C_{18}H_{15}F_3NO$, $[M+H]^+$, Calcd: 318.1100; Found: 318.1099.

IR (KBr, cm^{-1}) 2933, 2246, 1682, 1648, 1327, 1170, 1124, 850, 831, 687, 644, 571.

4-(2-Cyano-4-oxo-4-phenylbutyl)benzonitrile (2u)



The title compound **2u** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white crystal in 79% yield.

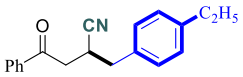
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.8 Hz, 2H), 7.66-7.62 (m, 3H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.44 (d, *J* = 7.8 Hz, 2H), 3.59-3.54 (m, 1H), 3.42 (dd, *J* = 18.0 Hz, 5.4 Hz, 1H), 3.30 (dd, *J* = 18.0 Hz, 7.8 Hz, 1H), 3.12 (dd, *J* = 13.8 Hz, 4.9 Hz, 1H), 3.00-2.97 (dd, *J* = 13.8 Hz, 8.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.7, 141.9, 135.7, 134.1, 132.6, 130.0, 128.9, 128.0, 120.6, 118.4, 111.7, 39.8, 37.5, 28.0.

HRMS(ESI) m/z: $C_{18}H_{15}N_2O$, $[M+H]^+$, Calcd: 275.1179, Found: 275.1178.

IR (KBr, cm^{-1}) 2870, 2243, 1679, 1593, 1447, 1357, 1214, 936, 848, 828, 758, 690, 597, 575.

2-(4-Ethylbenzyl)-4-oxo-4-phenylbutanenitrile (2v)



The title compound **2v** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 76% yield.

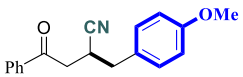
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.2 Hz, 2H), 7.83 (t, *J* = 7.2 Hz, 1H), 7.59 7.48 (t, *J* = 7.8 Hz, 2H), 7.45 (q, *J* = 7.8 Hz, 4H), 3.40 (dd, *J* = 17.4 Hz, 6.6 Hz, 1H), 3.54-3.50 (m, 1H), 3.35 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.25 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.01-2.94 (m, 2H), 2.63 (q, *J* = 7.5 Hz, 2H), 1.23 (t, *J* = 7.5 Hz, 3H)**.**

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.3, 143.4, 135.9, 133.8, 133.5, 129.1, 128.8, 128.3, 128.0, 121.5, 39.7, 37.1, 28.4, 28.2, 15.4.

HRMS(ESI) m/z: $C_{19}H_{20}NO$, $[M+H]^+$, Calcd: 278.1539, Found: 278.1536.

IR (KBr, cm^{-1}) 2924, 2235, 1680, 1452, 1376, 1179, 1109, 833, 696.

2-(4-Methoxyphenyl)-4-oxo-4-phenylbutanenitrile (2w)



The title compound **2w** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 79% yield.

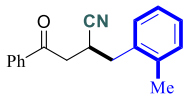
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (t, *J* = 7.2 Hz, 2H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.5 Hz, 2H), 3.80 (s, 3H), 3.51-3.49 (m, 1H), 3.34 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.25 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 2.99-2.91 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.3, 159.0, 135.9, 133.8, 130.2, 128.8, 128.3, 128.0, 121.5, 114.2, 55.2, 39.6, 36.7, 28.4.

HRMS(ESI) m/z: $C_{18}H_{18}NO_2$, $[M+H]^+$, Calcd: 280.1332, Found: 280.1331.

IR (KBr, cm^{-1}) 2945, 2212, 1678, 1587, 1359, 1276, 1250, 1185,1165, 815.

2-(2-Methylbenzyl)-4-oxo-4-phenylbutanenitrile (2x)



The title compound **2x** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 88% yield.

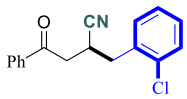
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.2 Hz, 2H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.22 (d, *J* = 41.3 Hz, 4H), 3.54-3.49 (m, 1H), 3.43 (dd, *J* = 17.8 Hz, 6.6 Hz, 1H), 3.31 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.05-2.98 (m, 2H), 2.40 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.2, 136.4, 135.9, 134.8, 133.8, 130.8, 130.0, 128.8, 128.0, 127.5, 126.3, 121.4, 40.3, 35.1, 27.3, 19.3.

HRMS(ESI) m/z: $C_{18}H_{17}NO$, $[M+H]^+$, Calcd: 264.1383, Found: 264.1382.

IR (KBr, cm^{-1}) 2924, 2235, 1680, 1452, 1376, 1179, 1109, 833, 696.

2-(2-Chlorobenzyl)-4-oxo-4-phenylbutanenitrile (2y)



The title compound **2y** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 68% yield.

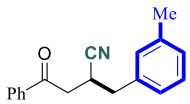
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.8 Hz, 2H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.40-7.38 (m, 2H), 7.27-7.23 (m, 2H), 3.68-3.63 (m, 1H), 3.44 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 3.30 (dd, *J* =18.0 Hz, 6.0 Hz, 1H), 3.22-3.13 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.0, 135.8, 134.2, 133.8, 131.6, 129.9, 129.0, 128.8, 128.0, 127.2, 121.0, 40.1, 35.2, 26.9.

HRMS(ESI) m/z: $C_{17}H_{15}ClNO$, $[M+H]^+$, Calcd: 284.0837, Found: 284.0834.

IR (KBr, cm^{-1}) 2984, 2244, 1737, 1689, 1475, 1448, 1372, 1244, 1047, 754, 689.

2-(3-Methylbenzyl)-4-oxo-4-phenylbutanenitrile (2z)



The title compound **2z** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 86% yield.

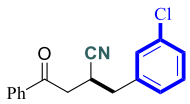
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92-7.90 (m, 2H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 2H), 7.22 (t, *J* = 7.8 Hz, 1H), 7.09-7.06 (m, 3H), 3.55-3.51(m, 1H), 3.35 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.24 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.01-2.92 (m, 2H), 2.33 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.3, 138.5, 136.3, 135.9, 133.8, 129.9, 128.8, 128.7, 128.2, 128.0, 126.2, 121.4, 39.8, 37.5, 28.1, 21.3.

HRMS(ESI) m/z: $C_{18}H_{18}NO$, $[M+H]^+$, Calcd: 264.1383, Found: 264.1382.

IR (KBr, cm^{-1}) 2986, 2240, 1740, 1685, 1473, 1444, 1370, 1248, 1049, 756, 670.

2-(3-Chlorobenzyl)-4-oxo-4-phenylbutanenitrile (2aa)



The title compound **2aa** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 84% yield.

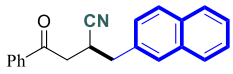
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.8 Hz, 2H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 2H), 7.28-7.26 (m, 3H), 7.20-7.19 (m, 1H), 3.56-3.52 (m, 1H), 3.38 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.27 (dd, *J* = 18.0 Hz, 7.2 Hz, 1H), 3.02 (dd, *J* = 13.8 Hz, 5.4 Hz, 1H), 2.94 (dd, *J* = 13.8 Hz, 8.4 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.0, 137.4, 136.1, 135.2, 133.7, 130.1, 129.1, 128.9, 128.1, 127.5, 126.0, 121.1, 39.8, 37.5, 28.1.

HRMS(ESI) m/z: $C_{17}H_{15}ClNO$, $[M+H]^+$, Calcd: 284.0837, Found: 284.0835.

IR (KBr, cm^{-1}) 2927, 2241, 1685, 1647, 1597, 1448, 1180, 999, 982, 755, 693.

2-(Naphthalen-2-ylmethyl)-4-oxo-4-phenylbutanenitrile (2ab)



The title compound **2ab** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a white solid in 93% yield.

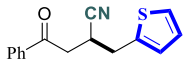
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.8 Hz, 2H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.80-7.77 (m, 1H), 7.72 (s, 1H), 7.58 (t, *J* = 7.2 Hz, 1H), 7.48-7.44 (m, 4H), 7.41 (d, *J* = 7.8 Hz, 1H), 3.66-3.61 (m, 1H), 3.37 (dd, *J* = 17.4 Hz, 6.6 Hz, 1H), 3.23 (dd, *J* = 18.0 Hz, 7.2 Hz, 1H), 3.20-3.12 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.3, 135.9, 133.8, 133.8, 133.5, 132.7, 128.8, 128.6, 128.0, 128.0, 127.7, 127.7, 127.0, 126.3, 126.0, 121.4, 39.8, 37.7, 28.1.

HRMS(ESI) m/z: $C_{21}H_{18}NO$, $[M+H]^+$, Calcd: 300.1383, Found: 300.1382.

IR (KBr, cm^{-1}) 2923, 2243, 1685, 1363, 1215, 747, 688, 477.

4-Oxo-4-phenyl-2-(thiophen-2-ylmethyl)butanenitrile (2ac)



The title compound **2ac** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.30 in hexane: ethyl acetate = 10:1) resulting in a yellow oil white solid in 80% yield.

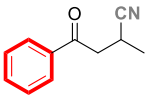
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.20 (d, *J* = 7.2 Hz, 2H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.22 (dd, *J* = 4.8 Hz, 1.8 Hz, 1H), 6.98-6.97 (m, 2H), 3.57 (m, 1H), 3.37 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 3.32-3.28 (m, 1H), 3.27 (d, *J* = 6.6 Hz, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.0, 137.8, 135.8, 133.8, 128.8, 128.0, 127.3, 127.0, 125.0, 121.1, 39.4, 31.5, 28.4.

HRMS(ESI) m/z: $C_{15}H_{14}NOS$, $[M+H]^+$, Calcd: 256.0791, Found: 256.0788.

IR (KBr, cm^{-1}) 2857, 2153, 1684, 1477, 1362, 1216, 1182, 756, 694.

2-Methyl-4-oxo-4-phenylbutanenitrile (3a)[7]



The title compound **3a** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a yellow oil in 96% yield.

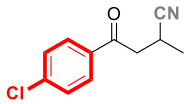
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96-7.84 (d, *J* = 7.2 Hz 2H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 2H), 3.42 (dd, *J* = 17.4 Hz, 6.0 Hz, 1H), 3.38-3.32 (m, 1H), 3.22 (dd, *J* = 17.4 Hz, 7.2 Hz, 1H), 1.43 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.1, 135.9, 133.8, 128.8, 128.0, 122.5, 42.2, 20.5, 17.9.

HRMS(ESI) m/z: $C_{11}H_{12}NO$, $[M+H]^+$, Calcd: 174.0913, Found: 174.0914.

IR (KBr, cm^{-1}) 2937, 2241, 1685, 1646, 1407, 1362, 1217, 754, 691.

4-(4-Chlorophenyl)-2-methyl-4-oxobutanenitrile (3b)[7]



The title compound **3b** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a colorless oil in 96% yield.

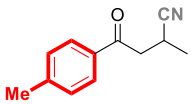
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 3.39 (dd, *J* = 17.4 Hz, 6.6 Hz, 1H), 3.33 (dd, *J* = 13.8 Hz, 7.2 Hz, 1H), 3.18 (dd, *J* = 17.4 Hz, 6.6 Hz, 1H), 1.43 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 193.9, 140.4, 134.2, 129.4, 129.1, 122.3, 42.2, 20.5, 17.8.

HRMS(ESI) m/z: $C_{11}H_{11}ClNO$, $[M+H]^+$, Calcd: 208.0524, Found: 208.0523.

IR (KBr, cm^{-1}) 3039, 2981, 2243, 1685, 1402, 1217, 1087, 822, 593, 523, 459.

2-Methyl-4-oxo-4-(p-tolyl)butanenitrile (3c)[7]



The title compound **3c** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a colorless oil in 92% yield.

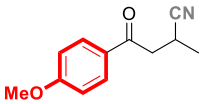
^{1}H NMR (600 MHz, CDCl3) δ 7.85 (d, *J* =7.8 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 2H), 3.40-3.31 (m, 2H), 3.19 (dd, *J* = 16.8 Hz, 6.6 Hz, 1H), 2.43 (s, 3H), 1.42 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.7, 144.7, 133.5, 129.5, 128.1, 122.6, 42.1, 21.6, 20.5, 17.9.

HRMS(ESI) m/z: $C_{12}H_{14}NO$, $[M+H]^+$, Calcd: 188.1070, Found: 188.1068.

IR (KBr, cm^{-1}) 2921, 2241, 1684, 1603, 1455, 1357, 1277, 1203, 999, 816.

4-(4-Methoxyphenyl)-2-methyl-4-oxobutanenitrile (3d)[7]



The title compound **3d** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a white crystal colorless oil in 83% yield.

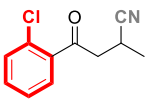
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.4 Hz, 2H), 6.96 (d, *J* = 8.4 Hz, 2H), 3.88 (s, 3H), 3.37-3.32 (m, 2H), 3.18-3.14 (m, 1H), 1.42 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 193.6, 164.0, 130.3, 129.1, 122.7, 114.0, 55.5, 41.8, 20.6, 17.9.

HRMS(ESI) m/z: $C_{12}H_{14}NO_2$, $[M+H]^+$, Calcd: 204.1019, Found: 204.1016.

IR (KBr, cm^{-1}) 2939, 2049, 1677, 1601, 1512, 1263, 1174, 1028, 835, 610, 586.

4-(2-Chlorophenyl)-2-methyl-4-oxobutanenitrile (3e)[8]



The title compound **3e** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a colorless oil in 93% yield.

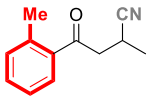
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.44 (t, *J* = 4.8 Hz, 2H), 7.37-7.35 (m, 1H), 3.40 (dd, *J* = 17.4 Hz, 6.0 Hz, 1H), 3.35-3.30 (m, 2H), 3.25 (dd, *J* = 18.0 Hz, 7.2 Hz, 1H), 1.43 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 198.1, 137.9, 132.5, 131.2, 130.8, 129.3, 127.2, 122.1, 46.4, 20.8, 17.7.

HRMS(ESI) m/z: $C_{11}H_{11}ClNO$, $[M+H]^+$, Calcd: 208.0524, Found: 208.0519.

IR (KBr, cm^{-1}) 2937, 2233, 1688, 1603, 1455, 1357, 1277, 1203, 980, 746.

2-Methyl-4-oxo-4-(*o*-tolyl)butanenitrile (3f)



The title compound **3f** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a colorless oil in 95% yield.

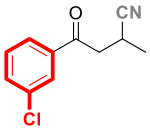
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (t, *J* = 8.4 Hz, 2H), 7.43-7.36 (m, 2H), 3.41-3.31 (m, 2H), 3.21 (dd, *J* = 17.2 Hz, 6.6 Hz, 1H), 2.42 (s, 3H), 1.42 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.3, 138.7, 136.0, 134.5, 128.7, 128.5, 125.2, 122.6, 42.3, 21.3, 20.5, 17.9.

HRMS(ESI) m/z: $C_{12}H_{13}NNaO$, $[M+H]^+$, Calcd: 210.0889, Found: 210.0887.

IR (KBr, cm^{-1}) 2939, 2249, 1683, 1512, 1363, 1174, 1028, 835, 740.

4-(3-Chlorophenyl)-2-methyl-4-oxobutanenitrile (3g)[8]



The title compound **3g** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a colorless oil in 87% yield.

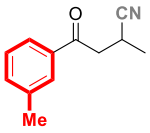
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.8 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 2H), 3.40 (dd, *J* = 17.2 Hz, 6.0 Hz, 1H), 3.36-3.03 (m, 1H), 3.19 (dd, *J* = 17.2 Hz, 6.6 Hz, 1H), 1.44 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 193.9, 137.4, 135.2, 133.7, 130.1, 128.1, 126.0, 122.3, 42.4, 20.5, 17.8.

HRMS(ESI) m/z: $C_{11}H_{11}ClNO$, $[M+H]^+$, Calcd: 208.0524, Found: 208.0523.

IR (KBr, cm^{-1}) 2923, 2242, 1685, 1603, 1587, 1484, 1359, 1276, 1250, 1185,1165, 785, 690.

2-Methyl-4-oxo-4-(m-tolyl)butanenitrile (3h)



The title compound **3h** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a colorless oil in 92% yield.

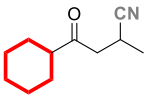
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.30-7.26 (m, 2H), 3.36-3.31 (m, 2H), 3.14 (dd, *J* = 16.2 Hz, 6.6 Hz, 1H), 2.53 (s, 3H), 1.42 (d, *J* = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 198.6, 138.9, 136.3, 132.3, 132.1, 128.5, 125.8, 122.5, 44.7, 21.4, 20.7, 17.8.

HRMS(ESI) m/z: $C_{12}H_{13}NNaO$, $[M+H]^+$, Calcd:210.0889, Found: 210.0887.

IR (KBr, cm^{-1}) 2940, 2051, 1679, 1600, 1514, 1260, 1175, 1028, 610.

4-Cyclohexyl-2-methyl-4-oxobutanenitrile (3i)



The title compound **3i** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (15:1) (Rf = 0.30 in hexane: ethyl acetate = 15:1) resulting in a colorless oil in 89% yield.

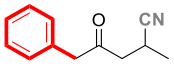
^{1}H NMR (600 MHz, $CDCl_3$) **^{1}H NMR** (600 MHz, $CDCl_3$) δ 3.16-3.12 (m, 1H), 2.87 (dd, *J* = 17.9 Hz, 6.4 Hz, 1H), 2.66 (dd, *J* = 17.9 Hz, 7.2 Hz, 1H), 2.35-2.31 (m, 1H), 1.85-1.78 (m, 4H), 1.71-1.65 (m, 2H), 1.37-1.27 (m, 7H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 209.0, 122.5, 50.7, 43.9, 28.2, 28.1, 25.7, 25.4, 25.4, 20.1, 17.7.

HRMS(ESI) m/z: $C_{11}H_{17}NNaO$, $[M+H]^+$, Calcd: 202.1202, Found: 202.1200.

IR (KBr, cm^{-1}) 2931, 2856, 2241, 1709, 1451, 1290, 1286, 1148, 1002, 699.

2-Methyl-4-oxo-5-phenylpentanenitrile (3j)[6]



The title compound **3j** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (20:1) (Rf = 0.20 in hexane: ethyl acetate = 20:1) resulting in a colorless oil in 76% yield.

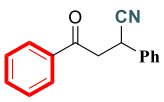
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.20 (t, *J* = 7.2 Hz, 2H), 7.30 (t, *J* = 7.2 Hz, 1H), 7.20 (d, *J* = 7.2 Hz, 2H), 3.71 (s, 2H), 3.11-3.06 (m, 1H), 2.85 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 2.65 (dd, *J* = 18.0 Hz, 7.2 Hz, 1H), 1.25 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 203.5, 133.1, 129.3, 129.0, 127.4, 122.2, 50.1, 44.9, 20.2, 17.5.

HRMS(ESI) m/z: $C_{12}H_{14}NO$, $[M+H]^+$, Calcd: 188.1070, Found: 188.1066.

IR (KBr, cm^{-1}) 2939, 2241, 1719, 1496, 1455, 1322, 1090,1039, 749, 702.

4-Oxo-2,4-diphenylbutanenitrile (5a)[5]



The title compound **5a** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a white solid in 75% yield.

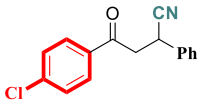
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 7.8 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.48-7.43 (m, 4H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.34 (t, *J* = 7.2 Hz, 1H), 4.57 (t, *J* = 6.6 Hz, 1H), 3.73 (dd, *J* = 17.4 Hz, 7.8 Hz, 1H), 3.51 (dd, ***J*** = 18.0 Hz, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.6, 135.7, 135.3, 133.8, 129.2, 128.8, 128.3, 128.1, 127.4, 120.5, 44.5, 31.9.

HRMS(ESI) m/z: $C_{16}H_{14}NO$, $[M+H]^+$, Calcd: 236.1070, Found: 236.1067.

IR (KBr, cm^{-1}) 2916, 2238, 1681, 1594, 1408, 1357, 1307, 1208, 1033, 760, 693, 617.

4-(4-Chlorophenyl)-4-oxo-2-phenylbutanenitrile (5b)[5]



The title compound **5b** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a white solid in 78% yield.

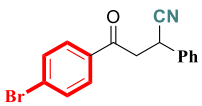
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 9.0 Hz, 2H), 7.45-7.38 (m, 6H), 7.34 (t, *J* = 7.2 Hz, 1H), 4.55 (dd, *J* = 8.4 Hz, 6.6 Hz, 1H), 3.69 (dd, *J* = 18.0 Hz, 7.8 Hz, 1H), 3.46 (dd, *J* = 17.2 Hz, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 193.4, 140.5, 135.1, 134.0, 129.4, 129.3, 129.1, 128.4, 127.4, 120.3, 44.4, 31.9.

HRMS(ESI) m/z: $C_{17}H_{16}NO$, $[M+H]^+$, Calcd: 252.1383, Found: 252.1383.

IR (KBr, cm^{-1}) 2927, 2241, 1678, 1587,1400, 1219, 1184,1901, 993, 829, 754, 601, 532, 455.

4-(4-Bromophenyl)-4-oxo-2-phenylbutanenitrile (5c)[5]



The title compound **5c** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a white solid in 73% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, *J* =9.0 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 7.43-7.38 (m, 4H), 7.34

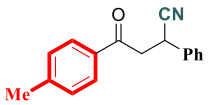
(t, J = 7.2 Hz, 1H), 4.55-4.53 (m, 1H), 3.68 (dd, J = 17.2 Hz, 7.8 Hz, 1H), 3.46 (dd, J = 17.2 Hz, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 193.6, 135.1, 134.5, 132.2, 129.5, 129.3, 128.4, 127.4,120.3, 44.4, 31.9.

HRMS(ESI) m/z: $C_{16}H_{13}BrNO$, $[M+H]^+$, Calcd: 314.0175, Found: 314.0173.

IR (KBr, cm^{-1}) 2926, 2247, 1685, 1593, 1446, 1348, 1211, 981, 840, 761, 690, 611.

4-Oxo-2-phenyl-4-(p-tolyl)butanenitrile (5d)[5]



The title compound **5d** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 82% yield.

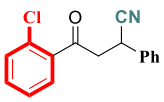
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 7.2 Hz, 2H), 7.38 (t, J = 7.5 Hz, 2H), 7.33 (t, J = 7.5 Hz, 1H), 7.25 (d, J = 3 Hz, 2H), 4.56 (dd, J = 7.8 Hz, 6.6 Hz, 1H), 3.69 (dd, J = 18.0 Hz, 7.8 Hz, 1H), 3.47 (dd, J = 17.2 Hz, 6.0 Hz, 1H), 2.41 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.2, 144.8, 135.4, 133.3, 129.5, 129.2, 128.3, 128.2, 127.5, 120.6, 44.4, 31.9, 21.6.

HRMS(ESI) m/z: $C_{17}H_{16}NO$, $[M+H]^+$, Calcd: 250.1226, Found: 250.1227.

IR (KBr, cm^{-1}) 2924, 2243, 1678, 1454, 1259, 1205, 1182, 810, 700.

4-(2-Chlorophenyl)-4-oxo-2-phenylbutanenitrile (5e)[5]



The title compound **5e** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a white solid in 75% yield.

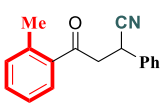
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 (d, J = 7.8 Hz, 1H), 7.41-7.37 (m, 6H), 7.35-7.32 (m, 2H), 4.54 (t, J = 7.2 Hz, 1H), 3.71 (dd, J = 18.0 Hz, 7.8 Hz, 1H), 3.54 (dd, J = 18.0 Hz, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 197.5, 137.6, 134.8, 132.6, 131.3, 130.7, 129.5, 129.2, 128.4, 127.5, 127.1, 120.2, 48.3, 32.2.

HRMS(ESI) m/z: $C_{16}H_{13}ClNO$, $[M+H]^+$, Calcd: 270.0680, Found: 270.0680.

IR (KBr, cm^{-1}) 3078, 2927, 2245, 1701, 1587, 1443, 1361, 1435, 1361, 1203, 1072, 756, 696.

4-Oxo-2-phenyl-4-(*o*-tolyl)butanenitrile (5f)[5]



The title compound **5f** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 70% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, J = 7.8 Hz, 1H), 7.42-7.37 m, 5H), 7.34 (t, J = 7.1 Hz, 1H), 7.27-7.24 (m, 2H), 4.56-4.53 (m, 1H), 3.65 (dd, J = 17.4 Hz, 7.8 Hz, 1H), 3.45 (dd, J = 17.4 Hz, 6.6 Hz, 1H),

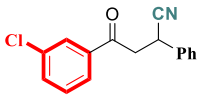
2.50 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 197.9, 139.1, 136.1, 135.2, 132.3, 132.1, 129.2, 128.5, 128.3, 127.5, 125.8, 120.6, 46.8, 32.2, 21.4.

HRMS(ESI) m/z: $C_{17}H_{16}ClNO$, $[M+H]^+$, Calcd: 250.1226, Found: 250.1226.

IR (KBr, cm^{-1}) 2929, 2241, 1678, 1598, 1454, 1217, 979, 758, 700, 601.

4-(3-Chlorophenyl)-4-oxo-2-phenylbutanenitrile (5g)[5]



The title compound **5g** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a white solid in 72% yield.

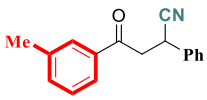
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.42-7.34 (m, 5H), 7.34 (t, *J* = 6.0 Hz, 1H), 4.54 (t, *J* = 6.0 Hz, 1H), 3.70 (dd, *J* = 18.0 Hz, 7.8 Hz, 1H), 3.48 (dd, *J* = 18.0 Hz, 5.4 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 193.4, 137.2, 135.2, 135.0, 133.8, 130.1, 129.3, 128.5, 128.2, 127.4, 126.1, 120.3, 44.6, 31.8.

HRMS(ESI) m/z: $C_{16}H_{13}ClNO$, $[M+H]^+$, Calcd: 270.0680, Found: 270.0677.

IR (KBr, cm^{-1}) 3089, 2489, 2240, 1688, 1569, 1542, 1217, 1140, 1027, 917, 787, 716, 696, 623, 454.

4-Oxo-2-phenyl-4-(*m*-tolyl)butanenitrile (5h)[5]



The title compound **5h** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 72% yield.

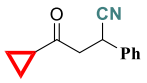
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35-7.70 (m, 2H), 7.43 (d, *J* = 7.2 Hz, 2H), 7.40-7.37 (m, 3H), 7.35-7.32 (m, 2H), 4.57 (dd, *J* = 7.6 Hz, 6.3 Hz, 1H), 3.71 (dd, *J* = 17.9 Hz, 7.9 Hz, 1H), 3.49 (dd, *J* = 17.8 Hz, 6.0 Hz, 1H), 2.40 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.7, 138.7, 135.8, 135.4, 134.6, 129.2, 128.6, 128.6, 128.3, 127.4, 125.3, 120.6, 44.5, 31.9, 21.2.

HRMS(ESI) m/z: $C_{17}H_{16}NO$, $[M+H]^+$, Calcd: 250.1226, Found: 250.1224.

IR (KBr, cm^{-1}) 2918, 2241, 1683, 1454, 1261, 1186, 999, 790, 690.

4-Cyclopropyl-4-oxo-2-phenylbutanenitrile (5i)[5]



The title compound **5i** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a colorless oil in 58% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39-7.32 (m, 5H), 4.38-4.35 (m, 1H), 3.31 (dd, *J* = 17.2 Hz, 7.8 Hz, 1H),

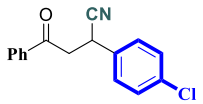
3.09 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H), 1.90-1.86 (m, 1H), 1.12-1.10(m, 1H), 1.06-1.05 (m, 1H), 0.98-0.89 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 205.2, 135.2, 129.2, 128.3, 127.3, 120.4, 48.4, 31.7, 20.7, 11.3, 11.3.

HRMS(ESI) m/z: $C_{13}H_{14}NO$, $[M+H]^+$, Calcd: 250.1270, Found: 200.1067.

IR (KBr, cm^{-1}) 2918, 2245, 1701, 1452, 1396, 1170, 1195, 1018, 698.

2-(4-Chlorophenyl)-4-oxo-4-phenylbutanenitrile (5j)[5]



The title compound **5j** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a yellow oil in 65% yield.

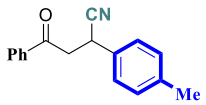
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.8 Hz, 2H), 7.61 (t, *J* = 6.9 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 2H), 7.49-7.36 (m, 4H), 4.57 (t, *J* = 6.9 Hz, 1H), 3.71 (dd, *J* = 17.2 Hz, 6.6 Hz, 1H), 3.51 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.3, 135.6, 134.4, 134.0, 133.8, 129.4, 128.8, 128.0, 128.0, 120.2, 44.2, 31.3.

HRMS(ESI) m/z: $C_{16}H_{13}ClNO$, $[M+H]^+$, Calcd: 270.0680, Found: 270.0676.

IR (KBr, cm^{-1}) 2933, 2243, 1679, 1489, 1406, 1220, 1095, 817, 750, 688, 597.

4-Oxo-4-phenyl-2-(*p*-tolyl)butanenitrile (5k)[5]



The title compound **5k** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a white solid in 80% yield.

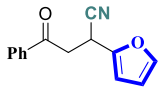
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.2 Hz, 2H), 7.59 (t, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.19 (d, *J* = 7.8 Hz, 2H), 4.54-4.52 (m, 1H), 3.70 (dd, *J* = 17.2 Hz, 7.8 Hz, 1H), 3.49 (dd, *J* = 18.0 Hz, 6.0 Hz, 1H), 2.35 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.7, 138.2, 133.8, 132.2, 129.9, 128.8, 128.0, 127.3, 120.7, 44.5, 31.5, 21.0.

HRMS(ESI) m/z: $C_{17}H_{16}NO$, $[M+H]^+$, Calcd: 250.1226, Found: 250.1224.

IR (KBr, cm^{-1}) 2916, 2239, 1674, 1593, 1448, 1350, 1205, 1110, 999, 821, 761, 690, 597.

2-(Furan-2-yl)-4-oxo-4-phenylbutanenitrile (5l)[5]



The title compound **5l** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a white solid in 67% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 2H),

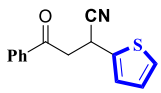
7.39 (s, 1H), 6.38 (d, *J* = 16.8 Hz, 2H), 4.69 (t, *J* = 6.6 Hz, 1H), 3.69 (d, *J* = 6.0 Hz, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.2, 146.9, 143.1, 135.6, 133.9, 128.8, 128.1, 118.3, 110.8, 108.2, 40.7, 26.0.

HRMS(ESI) m/z: $C_{14}H_{12}NO_2$, $[M+H]^+$, Calcd: 242.0633, Found: 242.0640.

IR (KBr, cm^{-1}) 2916, 2239, 1674, 1593,1448, 1350, 1205, 1110, 999, 821, 761, 690, 597.

4-Oxo-4-phenyl-2-(thiophen-2-yl)butanenitrile (5m)[5]



The title compound **5m** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a white solid in 69% yield.

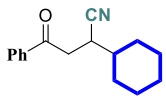
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.8 Hz, 2H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.27 (t, *J* = 6.0 Hz, 1H), 7.17 (d, *J* = 3.0 Hz, 1H), 6.89 (t, *J* = 4.2 Hz, 1H), 4.87 (t, *J* = 6.6 Hz, 1H), 3.77 (dd, *J* = 18.0 Hz, 7.2 Hz, 1H), 3.64 (dd, *J* = 18.0 Hz, 6.6 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 194.2, 137.0, 135.6, 134.0, 128.8, 128.1, 127.1, 126.7, 125.9, 119.7, 44.6, 27.2.

HRMS(ESI) m/z: $C_{14}H_{11}NOSK$, $[M+K]^+$, Calcd: 241.0561, Found: 264.0419.

IR (KBr, cm^{-1}) 2920, 2247, 1685, 1359, 1448, 1217, 1149, 761, 690.

2-Cyclohexyl-4-oxo-4-phenylbutanenitrile (5n)[5]



The title compound **5n** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (10:1) (Rf = 0.40 in hexane: ethyl acetate = 10:1) resulting in a colorless oil in 79% yield.

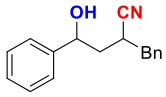
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.2 Hz, 2H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 3.40-3.35 (m, 1H), 3.27-3.22 (m, 2H), 1.89-1.88 (m, 1H), 1.81-1.79 (m, 3H), 1.70-1.68 (m, 1H), 1.29-1.18 (m, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.5, 136.0, 133.7, 128.8, 128.0, 120.9, 38.9, 38.4, 32.5, 31.4, 29.1, 25.9, 25.8, 25.8.

HRMS(ESI) m/z: $C_{16}H_{20}NO$, $[M+H]^+$, Calcd: 242.1539, Found: 242.1538.

IR (KBr, cm^{-1}) 2924, 2235, 1681, 1593, 1448, 1361, 1219, 767, 688, 599.

2-benzyl-4-hydroxy-4-phenylbutanenitrile (6)



The title compound **6** was prepared according to the general procedure as described, silica gel flash column chromatography was performed hexanes and ethyl acetate (8:1) (Rf = 0.30 in hexane: ethyl acetate = 5:1) resulting in a colorless crystal in 42% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.23 (m, 10H), 4.96 (d, *J* = 8.0 Hz, 1H), 3.33-3.26 (m, 1H), 2.92 (d,

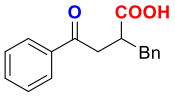
J = 8.0 Hz, 2H), 2.06 (s, 1H), 2.00-1.84 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 136.7, 129.0, 128.7, 128.0, 127.2, 125.5, 121.5, 71.7, 41.2, 38.51, 30.80.

HRMS(ESI) m/z: $C_{17}H_{18}NO$, $[M+H]^+$, Calcd: 252.1383, Found: 252.1383.

IR (KBr, cm^{-1}) 2912, 2234, 1595, 1444, 1352, 1205, 1110, 821, 761, 595.

2-benzyl-4-oxo-4-phenylbutanoic acid (7)[9]



The title compound **7** was prepared according to the general procedure as described, without further purification resulting in a white crystal in 92% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (t, *J* = 8.0 Hz, 2H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 2H), 7.30 (t, *J* = 8.0 Hz, 2H), 7.23 (t, *J* = 8.0 Hz, 3H), 3.43-3.35 (m, 2H), 3.21 (dd, *J* = 16.0, 4.0 Hz, 1H), 3.07-2.99 (m, 1H), 2.88 (dd, *J* = 16 Hz, 8.0 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 198.0, 143.6, 136.7, 129.0, 128.7, 128.0, 127.2, 125.5, 121.5, 71.7, 41.2, 38.5, 30.8.

HRMS(ESI) m/z: $C_{17}H_{18}NO$, $[M+H]^+$, Calcd: 269.1172, Found: 269.1171.

IR (KBr, cm^{-1}) 3125, 2920, 1678, 1592, 1448, 1350, 1205, 1115, 993, 821, 756, 695, 599.

V References

[1] Aramini, A.; Sablone, M. R.; Bianchini, G.; Amore, A.; Fan ỉ M.; Perrone, P.; Dolce, A.; Allegretti, M., Facile one-pot preparation of 2-arylpropionic and arylacetic acids from cyanohydrins by treatment with aqueous HI. *Tetrahedron.* **2009**, *65*, 2015-2021.

[2] Hudlicky, J. R.; Werner, L.; Semak, V.; Simionescu, R.; Hudlicky, T., Dauben–Michno oxidative transposition of allylic cyanohydrins-Enantiomeric switch of (–)-carvone to (+)-carvone. *Can. J. Chem.* **2011**, *89*, 535-543.

[3] Wu, Z.; Li, T.; Ding, Y.; Hu, A., Synthesis of Chiral Porous Organic Polymers Through Nucleophilic Substitution for Chiral Separation. *ACS Appl. Polym. Mater.* **2020,** *2*, 5414-5422.

[4] Sartillo-Piscil, J. R.-I. S. C.-G. L. Q. F., Concise and Environmentally Friendly Asymmetric Total Synthesis of the Putative Structure of a Biologically Active 3-Hydroxy-2-piperidone Alkaloid. *Synthesis.* **2018,** *50*, 2878-2886.

[5] Li, Z. F.; Li, Q.; Ren, L. Q.; Li, Q. H.; Peng, Y. G.; Liu, T. L., Cyano-borrowing reaction: nickel-catalyzed direct conversion of cyanohydrins and aldehydes/ketones to beta-cyano ketone. *Chem. Sci.* **2019**, *10*, 5787-5792.

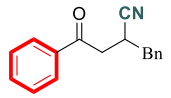
[6] Anders, E.; Stankowiak, A.; Riemer, R., Synthesen mit N-Trimethylsilylheteroarylium-Salzen: Umsetzungen mit Aldehyden, Ketonen und Carbonsäuren, Reaktivitätsvergleich mit analogen N-Acylheteroarylium-Salzen. *Synthesis.* **1987**, *1987*, 929-931.

[7] Provencher, B. A.; Bartelson, K. J.; Liu, Y.; Foxman, B. M.; Deng, L., Structural Study-Guided Development of Versatile Phase-Transfer Catalysts for Asymmetric Conjugate Additions of Cyanide. *Angew. Chem., Int. Ed.* **2011**, *50*, 10565-10569.

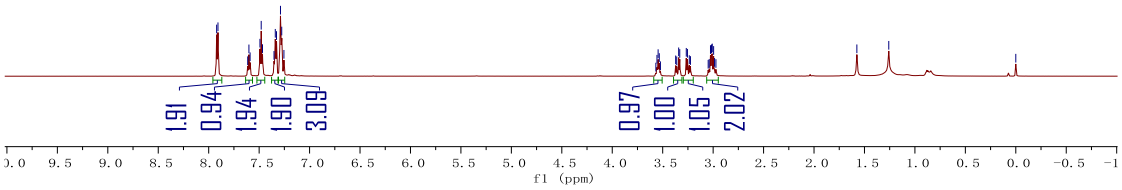
[8] Kurono, N.; Nii, N.; Sakaguchi, Y.; Uemura, M.; Ohkuma, T., Asymmetric Hydrocyanation of α,β-Unsaturated Ketones into β-Cyano Ketones with the [Ru(phgly)$_2$(binap)]/C_6H_5OLi Catalyst System. *Angew. Chem., Int. Ed.* **2011**, *50*, 5541-5544.

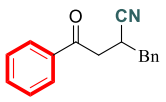
[9] Nashed, N. T.; Kaiser, E. T., Carboxypeptidase A catalyzed .alpha.,.beta.-elimination reactions: rapid catalysis of .alpha.,.beta.-elimination of hydrogen chloride from .beta.-chloro ketone substrates. *J. Am. Chem. Soc.* **1986,** *108*, 2710-2715.

VI NMR spectra of the products

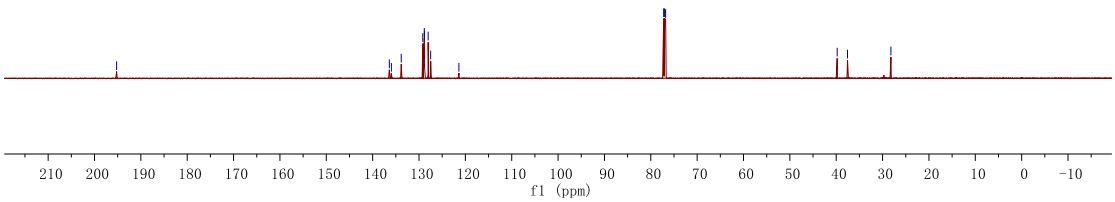


2a

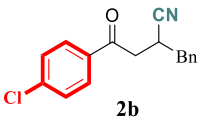




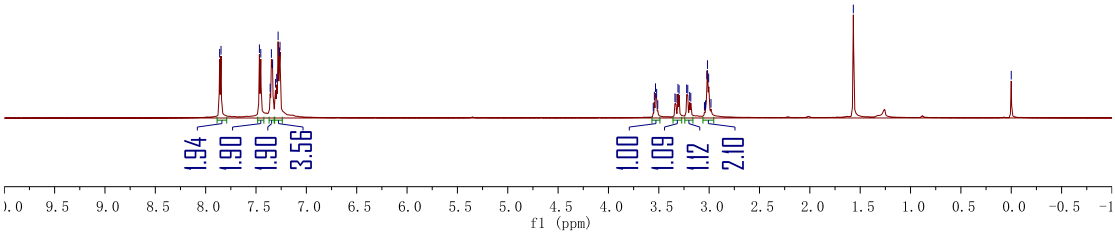
2a



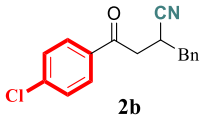

TJ-1H
TJ-958
7.861
7.848
7.466
7.453
7.359
7.347
7.335
7.306
7.294
7.281
7.267
7.262
3.544
3.533
3.521
3.340
3.310
3.299
3.223
3.212
3.194
3.182
3.023
3.017
3.005
1.568
0.000


O
CN
Bn
Cl

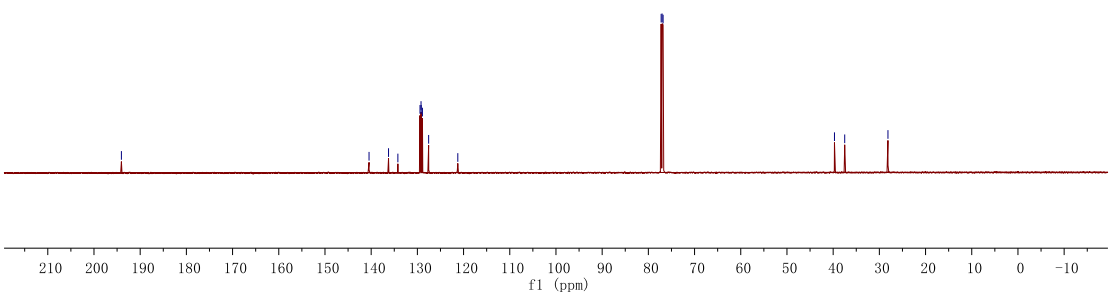
2b


1.94
1.90
1.90
3.56
1.00
1.09
1.12
2.10
f1 (ppm)

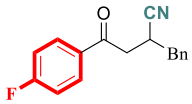

TJ-13C
TJ-958
194.065
140.461
136.242
134.221
129.427
129.207
129.174
128.906
127.560
121.247
77.234
77.022
76.811
39.716
37.500
28.139


O
CN
Bn
Cl

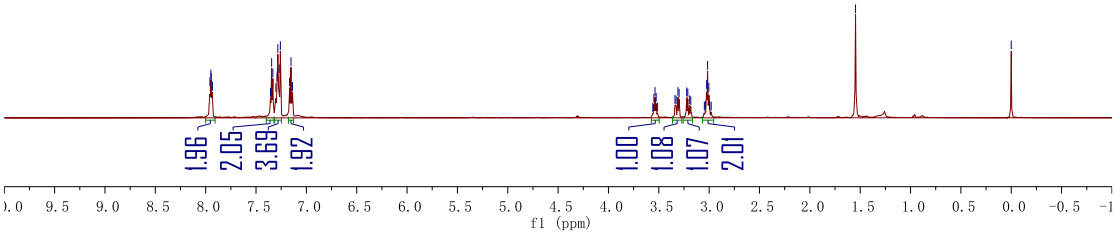
2b


f1 (ppm)

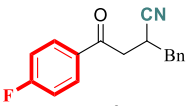

TJ-1H
TJ-881
7.957
7.948
7.945
7.936
7.934
7.356
7.345
7.332
7.303
7.290
7.283
7.270
7.258
7.166
7.153
7.140
7.138
3.549
3.538
3.526
3.339
3.328
3.310
3.299
3.223
3.212
3.194
3.182
3.037
3.025
3.016
3.003
2.994
2.980
1.546
-0.000


O
CN
Bn
F

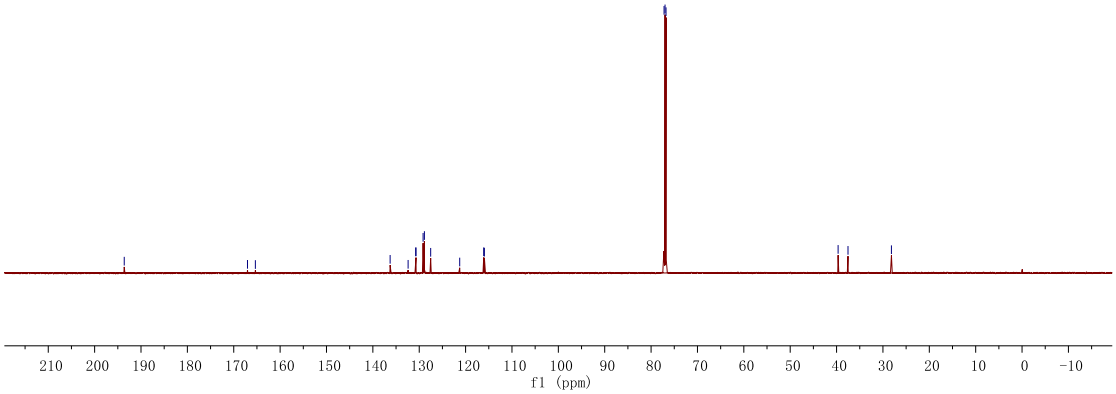
2c


1.96
2.05
3.69
1.92
1.00
1.08
1.07
2.01
f1 (ppm)


TJ-13C
TJ-881
193.615
167.035
165.337
136.277
132.399
130.759
130.696
129.166
128.883
127.533
121.270
116.098
115.952
77.202
76.990
76.779
39.668
37.535
28.170

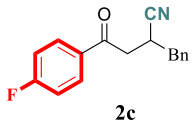

O
CN
Bn
F

2c

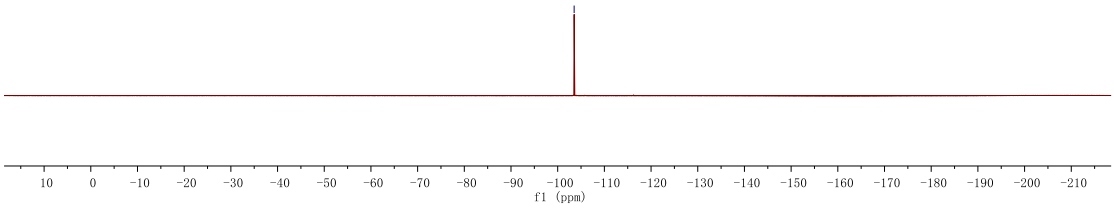

f1 (ppm)

TJ-881

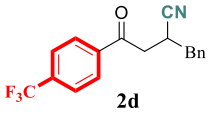
-103.525



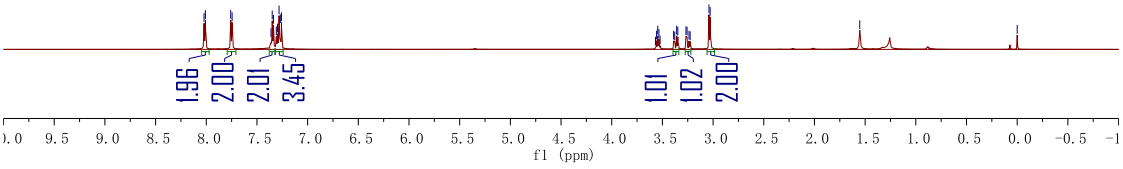
2c



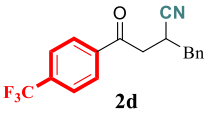

TJ-1H
TJ-922
8.022
8.009
7.759
7.745
7.361
7.349
7.337
7.309
7.297
7.282
7.270
7.258
3.557
3.546
3.534
3.389
3.378
3.359
3.348
3.268
3.257
3.238
3.227
3.041
3.029
1.553
0.000


O
CN
Bn
F3C

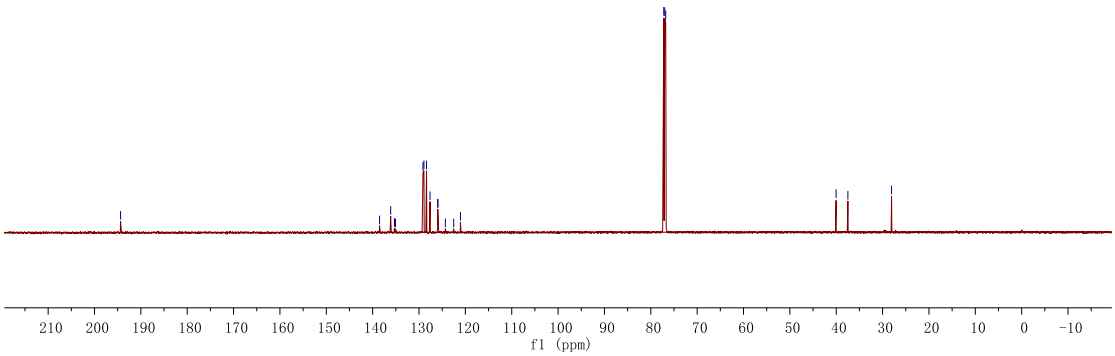
2d


1.96
2.00
2.01
3.45
1.01
1.02
2.00
f1 (ppm)

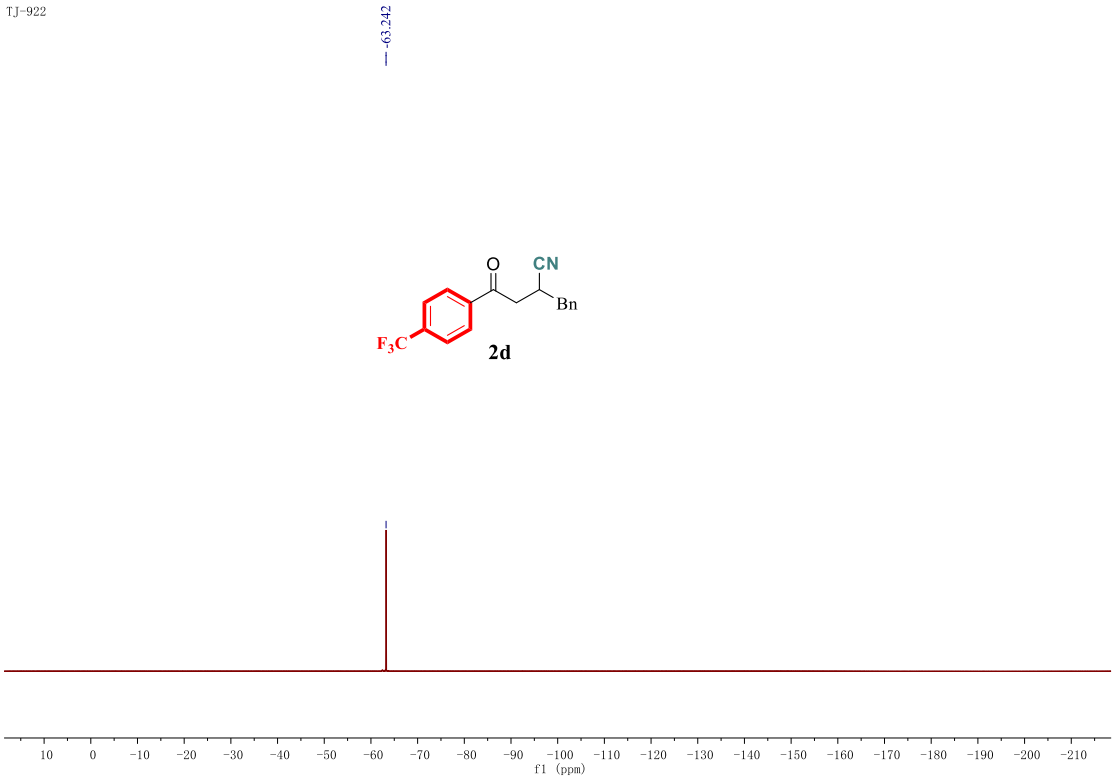

TJ-13C
TJ-922
194.375
138.506
136.110
135.295
135.077
129.147
128.938
128.380
127.618
125.952
125.927
124.321
122.514
121.059
77.204
76.992
76.780
40.031
37.481
28.071


O
CN
Bn
F3C

2d

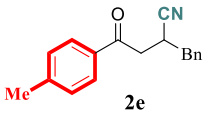

f1 (ppm)

TJ-922

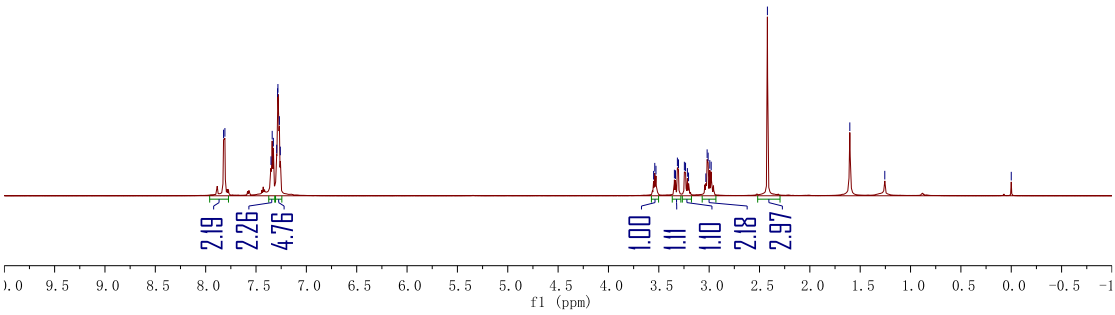

-63.242
O
CN
Bn
F3C
2d
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

TJ-1H
TJ-880

7.822 7.809 7.351 7.339 7.328 7.295 7.286 7.282 7.268 7.259 3.540 3.528 3.345 3.334 3.315 3.305 3.246 3.234 3.216 3.020 3.010 2.993 2.980 2.424 1.603 1.256 0.000

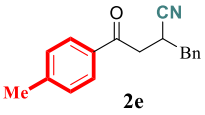


2e

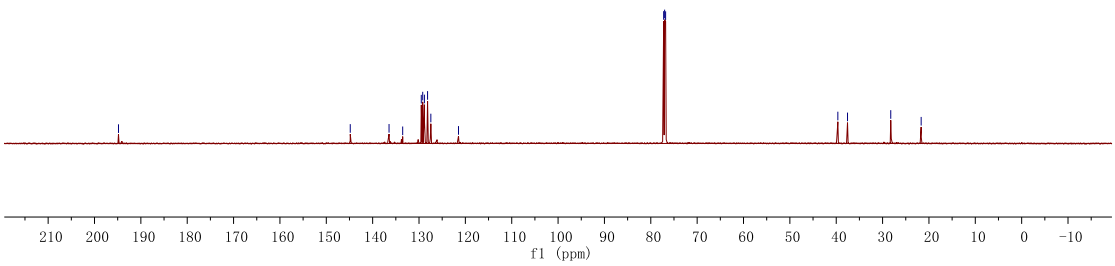


TJ-13C
TJ-880

194.825 144.831 136.465 133.521 129.508 129.200 128.834 128.153 127.448 121.482 77.227 77.016 76.804 39.650 37.565 28.238 21.679

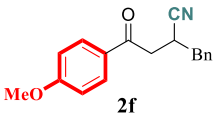


2e

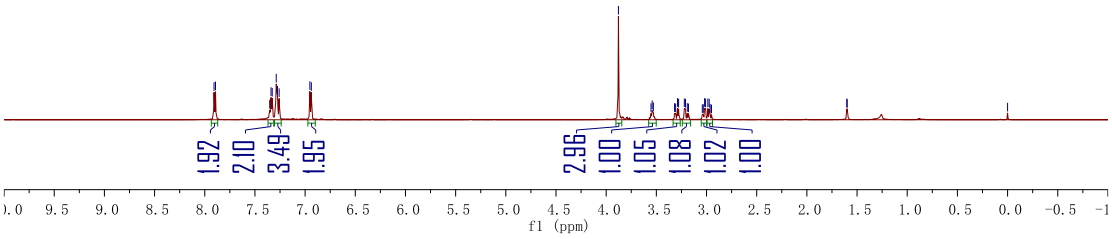


TJ-1H
TJ-968-D

7.908 7.893 7.352 7.340 7.328 7.288 7.275 7.259 6.953 6.938 3.878 3.542 3.530 3.318 3.289 3.278 3.221 3.210 3.192 3.019 3.009 2.987 2.973 1.602 1.599 0.000

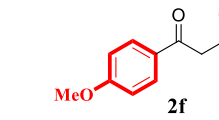


2f

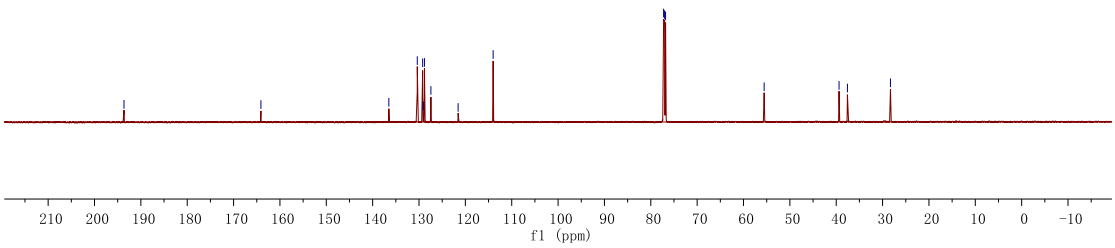


TJ-13C
TJ-968-D

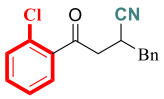
193.641 164.102 136.509 130.375 129.213 129.052 128.825 127.434 121.563 114.010 77.236 77.025 76.813 55.546 39.391 37.581 28.299



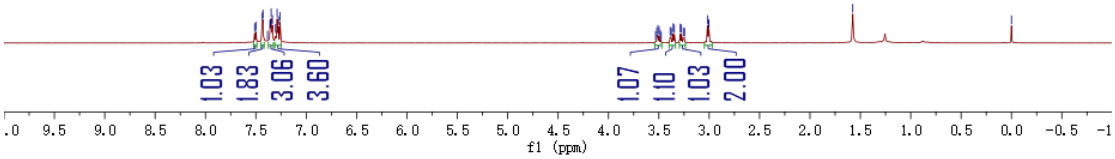
2f



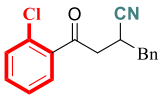

TJ-1H
TJ-930
7.512
7.499
7.436
7.429
7.384
7.360
7.353
7.348
7.336
7.304
7.289
7.276
7.259
3.521
3.510
3.497
3.388
3.358
3.346
3.287
3.276
3.257
3.018
3.007
3.004
1.575
0.000


Cl
O
CN
Bn

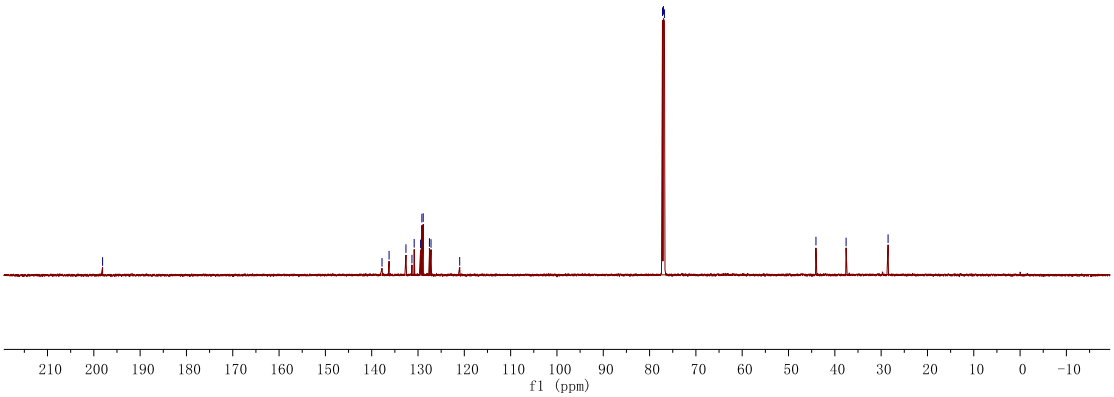
2g


1.03
1.83
3.06
3.60
1.07
1.10
1.03
2.00
f1 (ppm)


TJ-13C
TJ-930
198.108
137.774
136.249
132.604
131.308
130.828
129.444
129.166
128.879
127.538
127.192
120.998
77.217
77.005
76.793
44.075
37.572
28.502


Cl
O
CN
Bn

2g

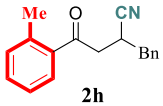

f1 (ppm)

TJ-1H
TJ-923

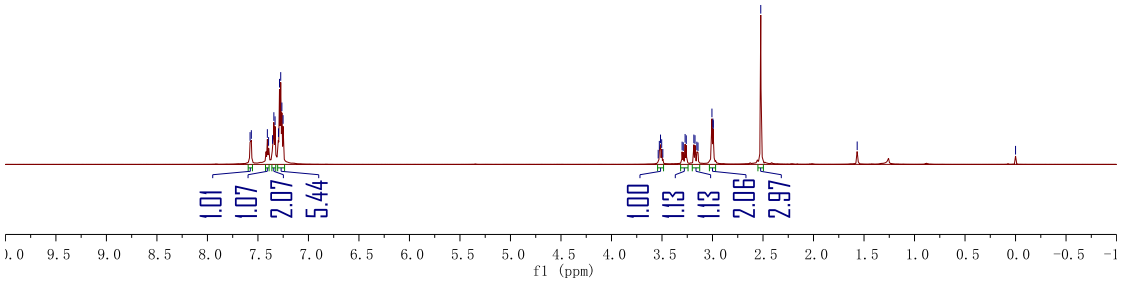
7.578 7.565 7.407 7.395 7.355 7.342 7.331 7.297 7.286 7.274 7.263 7.251

3.526 3.515 3.503 3.301 3.271 3.260 3.184 3.173 3.006 2.995 2.992 2.522 1.568

0.000



2h



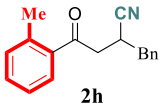
TJ-13C
TJ-923

198.590

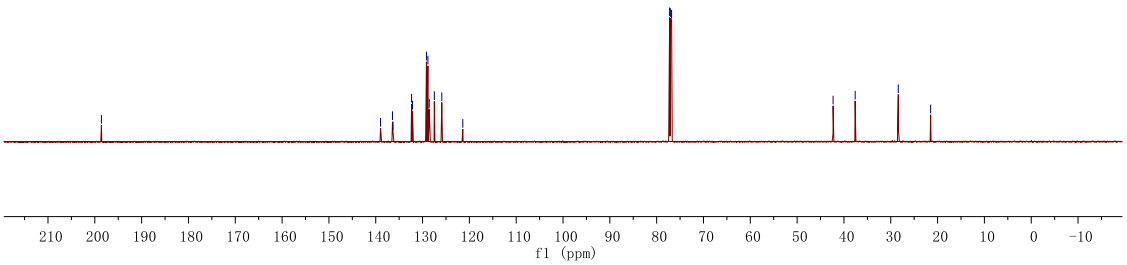
138.972 136.425 136.317 132.344 132.145 129.167 128.863 128.570 127.487 125.890 121.405

77.234 77.023 76.811

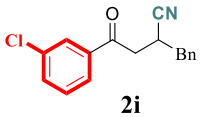
42.317 37.604 28.394 21.481



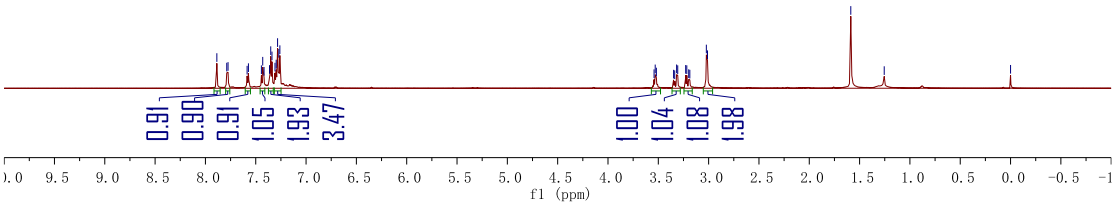
2h



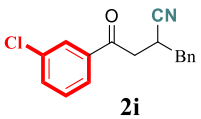

7.788
7.775
7.586
7.573
7.444
7.431
7.363
7.351
7.339
7.309
7.297
7.283
7.270
7.260
3.542
3.531
3.519
3.348
3.318
3.307
3.228
3.217
3.198
3.187
3.023
1.588
1.255
0.000


O
CN
Cl
Bn

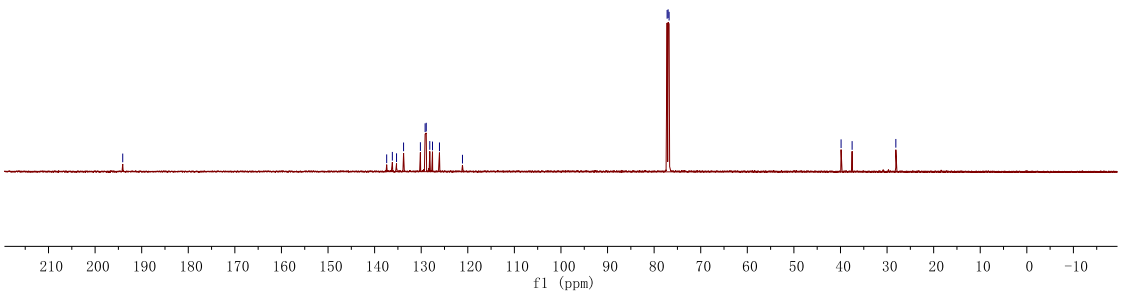
2i


0.91
0.90
0.91
1.05
1.93
3.47
1.00
1.04
1.08
1.98
f1 (ppm)

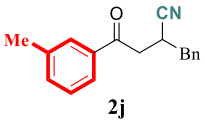

TJ-13C
TJ-878
194.069
137.412
136.191
135.294
133.785
130.174
129.159
128.916
128.161
127.574
126.079
121.142
77.214
77.002
76.790
39.872
37.502
28.117


O
CN
Cl
Bn

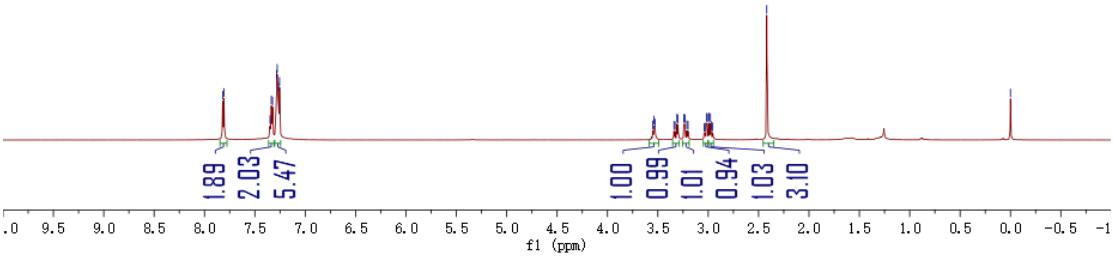
2i


f1 (ppm)

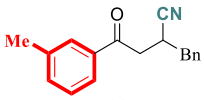
TJ-1H
TJ-879



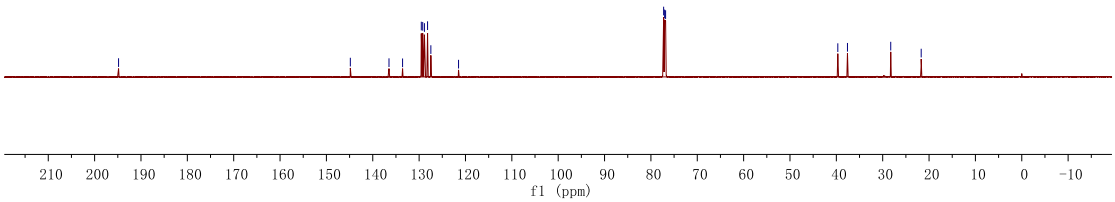
2j



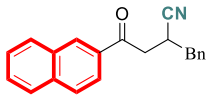
TJ-13C
TJ-879



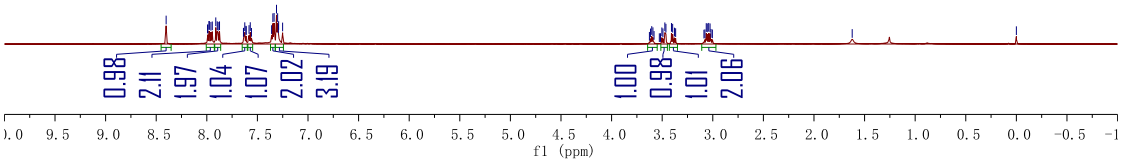
2j



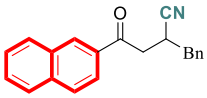

8.427
7.963
7.990
7.978
7.976
7.959
7.946
7.911
7.897
7.888
7.874
7.625
7.613
7.612
7.583
7.571
7.360
7.347
7.335
7.311
7.300
7.294
7.290
7.251
3.603
3.591
3.503
3.474
3.463
3.408
3.397
3.065
3.055
3.040
3.027
-0.000


O
CN
Bn

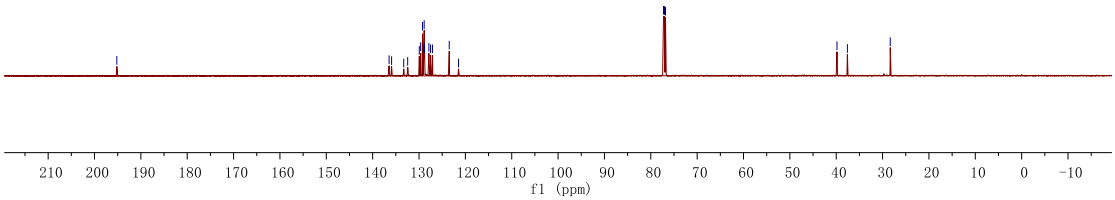
2k


0.98
2.11
1.97
1.04
1.07
2.02
3.19
1.00
0.98
1.01
2.06
f1 (ppm)


TJ-13C
TJ-924
195.188
136.454
135.913
133.294
132.442
129.941
129.647
129.239
128.935
128.883
128.801
127.869
127.503
127.084
123.477
121.477
77.254
77.043
76.831
39.835
37.591
28.344


O
CN
Bn

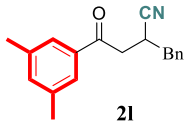
2k


f1 (ppm)

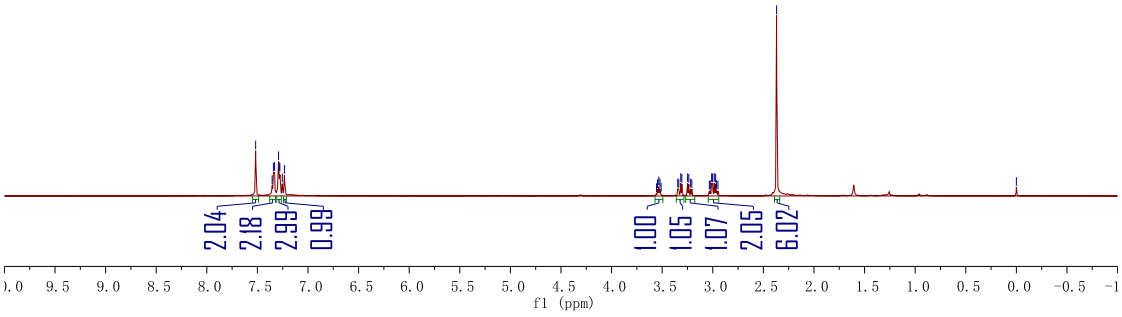
TJ-1H
TJ-962

7.517 7.354 7.342 7.330 7.291 7.286 7.278 7.254 7.233

3.546 3.534 3.522 3.346 3.336 3.316 3.306 3.249 3.237 3.219 3.207 3.024 3.011 3.001 2.985 2.972 2.963 2.949 2.369 1.000



2l



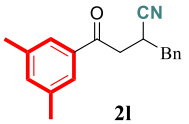
TJ-13C
TJ-962

195.614

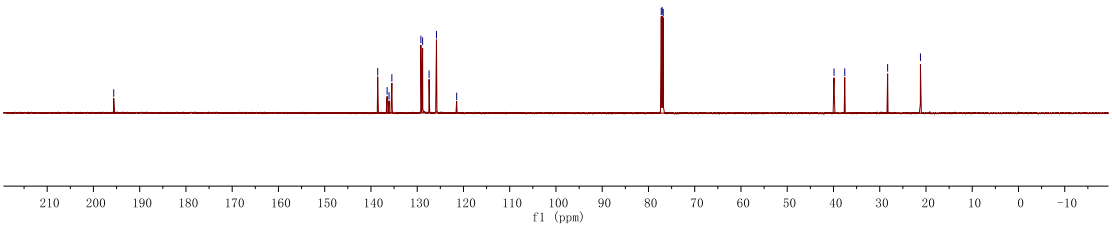
138.542 136.506 136.091 135.480 129.207 128.831 127.436 125.835 121.467

77.238 77.026 76.815

39.881 37.566 28.292 21.196



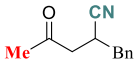
2l



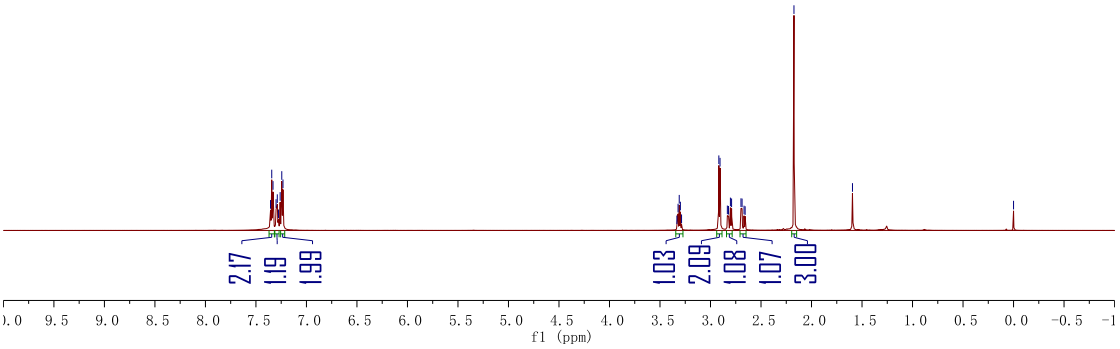
TJ-1H
TJ-989

7.355 7.344 7.331 7.301 7.289 7.276 7.260 7.244 7.232

3.333 3.321 3.310 3.298 3.286 2.917 2.906 2.833 2.822 2.803 2.791 2.698 2.687 2.668 2.657 2.174 1.594 0.000



2m



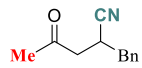
TJ-13C
TJ-989

203.553

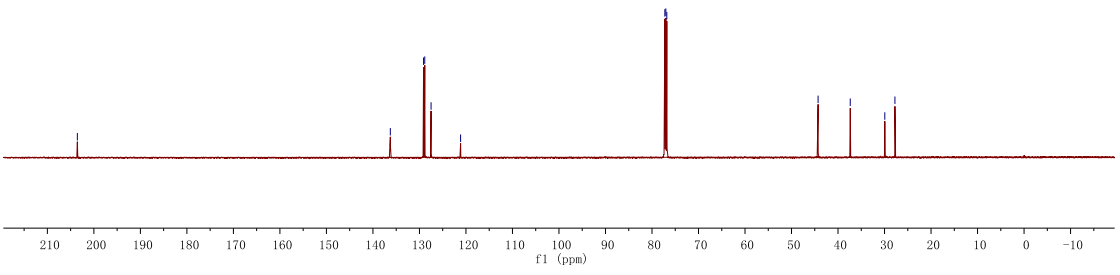
136.260 129.116 128.855 127.501 121.152

77.235 77.023 76.811

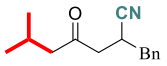
44.288 37.369 29.942 27.765



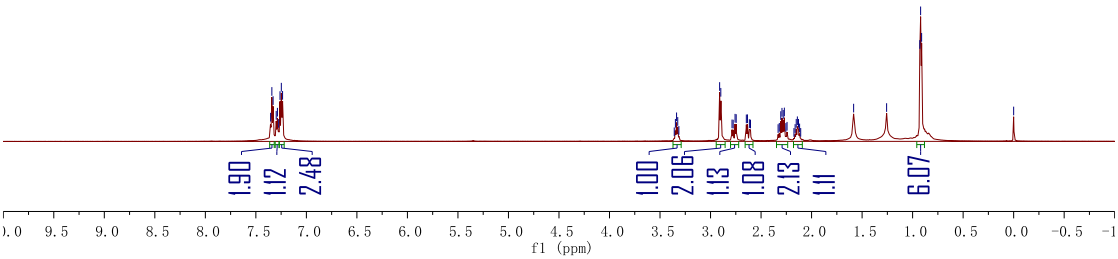
2m



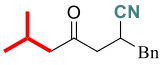

7.342
7.330
7.299
7.287
7.274
7.261
7.248
7.236
3.348
3.336
3.325
2.910
2.898
2.787
2.776
2.757
2.746
2.646
2.635
2.616
2.605
2.305
2.293
2.281
2.269
2.243
2.152
2.141
2.130
1.584
1.257
0.929
0.921
0.911
0.000


O
CN
Bn

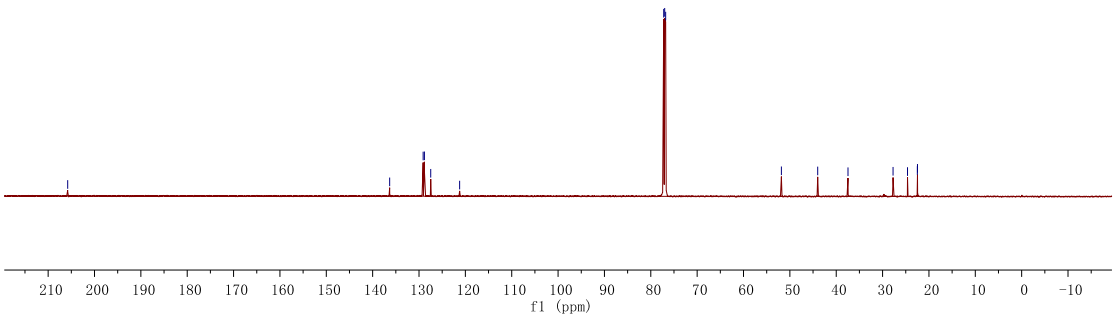
2n

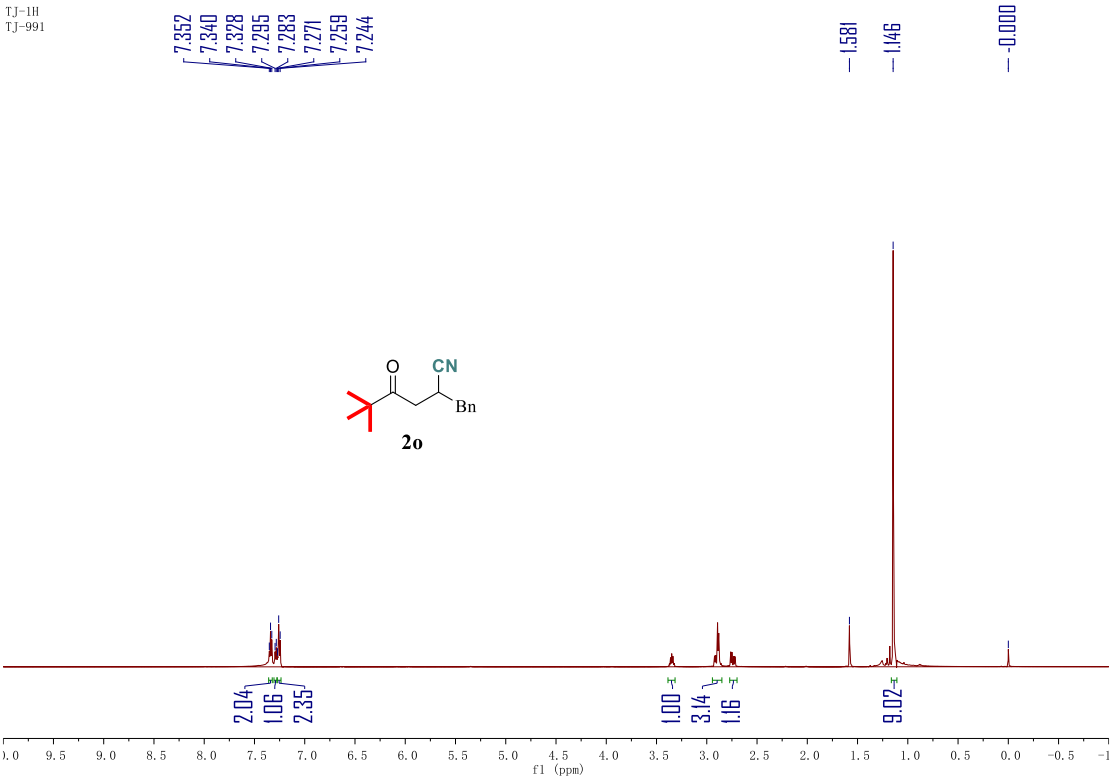

1.90
1.12
2.48
1.00
2.06
1.13
1.08
2.13
1.11
6.07
f1 (ppm)

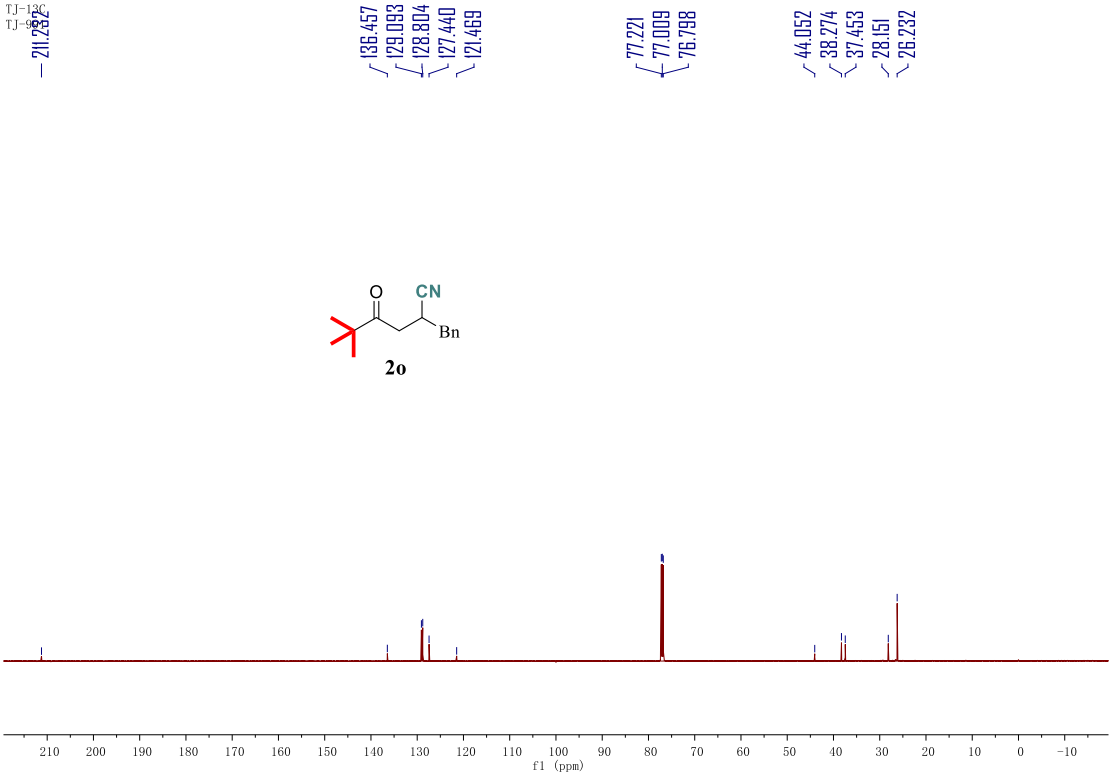

205.784
136.329
129.108
128.833
127.472
121.235
77.215
77.004
76.792
51.828
43.996
37.461
27.741
24.621
22.498
22.472


O
CN
Bn

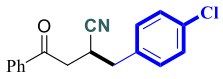
2n


f1 (ppm)

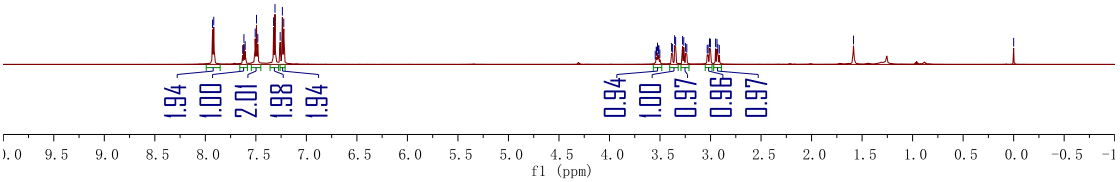

TJ-1H
TJ-991
7.352
7.340
7.328
7.295
7.283
7.271
7.259
7.244
1.581
1.146
0.000
O
CN
Bn
2o
2.04
1.06
2.35
1.00
3.14
1.16
9.02
f1 (ppm)


TJ-13C
211.292
136.457
129.093
128.804
127.440
121.469
77.221
77.009
76.798
44.052
38.274
37.453
28.151
26.232
O
CN
Bn
2o
f1 (ppm)

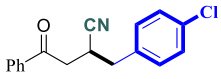

7.929
7.917
7.630
7.618
7.606
7.507
7.494
7.481
7.325
7.311
7.259
7.238
7.224
3.537
3.535
3.525
3.514
3.512
3.385
3.375
3.356
3.345
3.277
3.265
3.247
3.235
3.033
3.024
3.010
3.001
2.950
2.936
2.927
2.913
1.585
0.000


O
CN
Cl
Ph

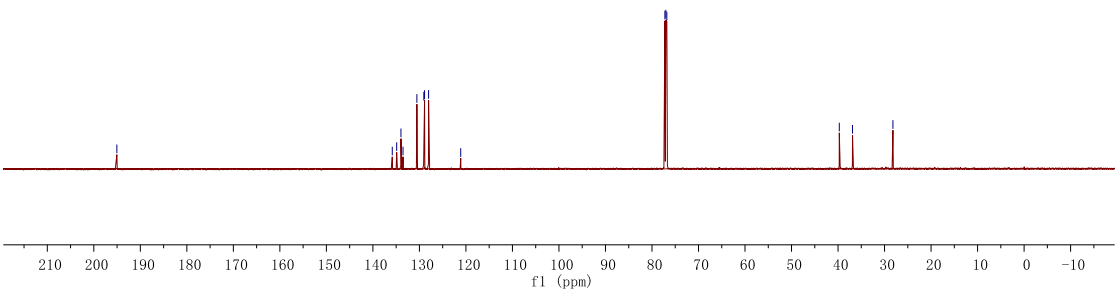
2p


1.94
1.00
2.01
1.98
1.94
0.94
1.00
0.97
0.96
0.97
f1 (ppm)

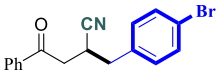

TJ-13C
TJ-985
195.045
135.833
134.883
133.967
133.523
130.541
129.046
128.895
128.026
121.119
77.227
77.015
76.803
39.729
36.888
28.198


O
CN
Cl
Ph

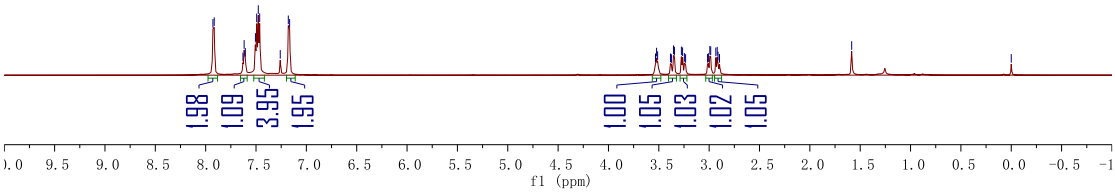
2p


f1 (ppm)

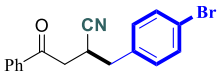

TJ-1H
TJ-993
7.928
7.915
7.630
7.618
7.606
7.506
7.493
7.477
7.464
7.259
7.179
7.166
3.522
3.512
3.354
3.345
3.276
3.264
3.246
3.007
2.993
2.985
2.934
2.920
2.912
1.585
0.000


O
CN
Ph
Br

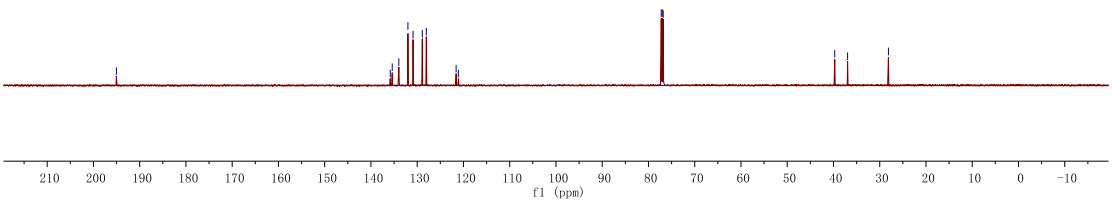
2q


1.98
1.09
3.95
1.95
1.00
1.05
1.03
1.02
1.05
f1 (ppm)

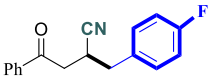

TJ-13C
TJ-993
195.042
135.824
135.401
133.974
132.010
130.899
128.898
128.030
121.588
121.105
77.238
77.027
76.815
39.728
36.948
28.120


O
CN
Ph
Br

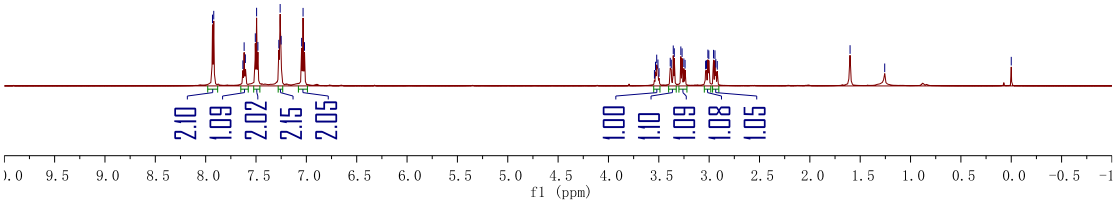
2q


f1 (ppm)

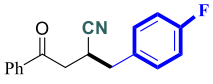

7.952
7.920
7.630
7.618
7.606
7.507
7.494
7.481
7.273
7.260
7.251
7.047
7.033
7.018
3.533
3.521
3.509
3.386
3.376
3.356
3.346
3.281
3.269
3.251
3.239
3.036
3.026
3.012
3.003
2.956
2.942
2.934
2.919
1.601
1.257
-0.000


O
CN
F
Ph

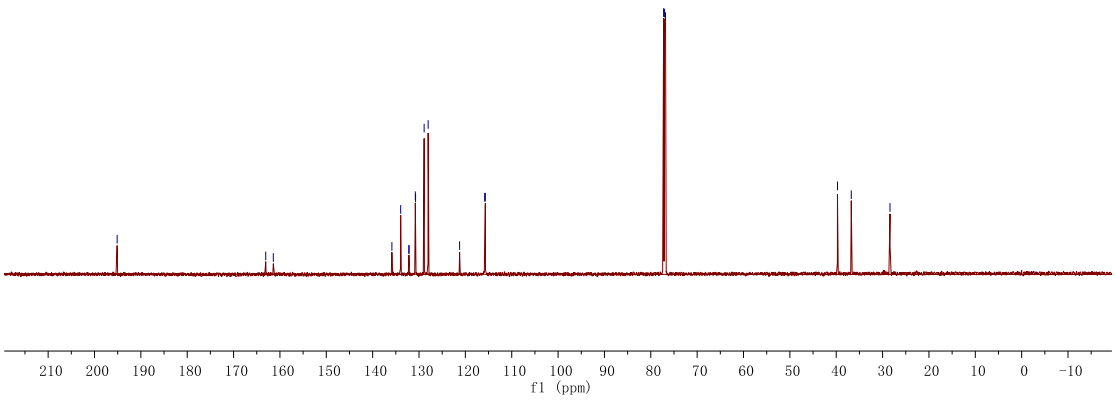
2r


2.10
1.09
2.02
2.15
2.05
1.00
1.10
1.09
1.08
1.05
f1 (ppm)


TJ-13C
TJ-968
195.118
163.061
161.430
135.848
133.955
132.183
130.795
130.742
128.893
128.029
121.243
115.835
115.693
77.241
77.029
76.818
39.733
36.756
28.397

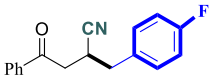

O
CN
F
Ph

2r

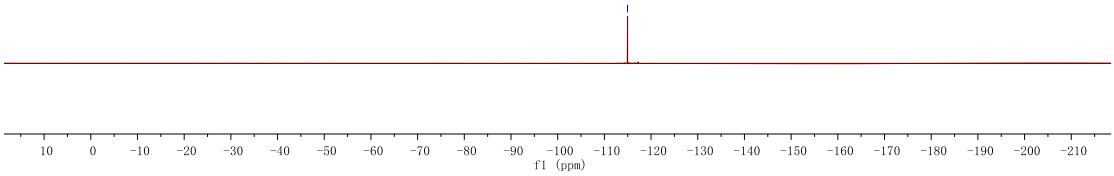

f1 (ppm)

TJ-936

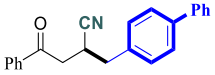
-114.965



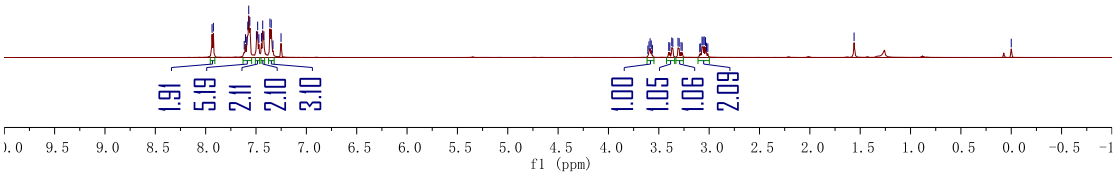
2r

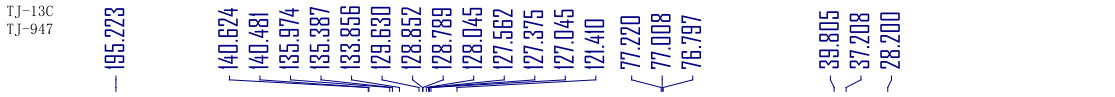


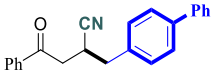

TJ-1H
TJ-947
7.957
7.953
7.923
7.617
7.605
7.592
7.582
7.572
7.561
7.496
7.484
7.471
7.446
7.434
7.421
7.362
7.349
7.332
7.252
3.598
3.586
3.575
3.401
3.390
3.371
3.361
3.309
3.298
3.279
3.268
3.070
3.061
3.049
3.036
3.027
1.561
-0.000


O
CN
Ph
Ph

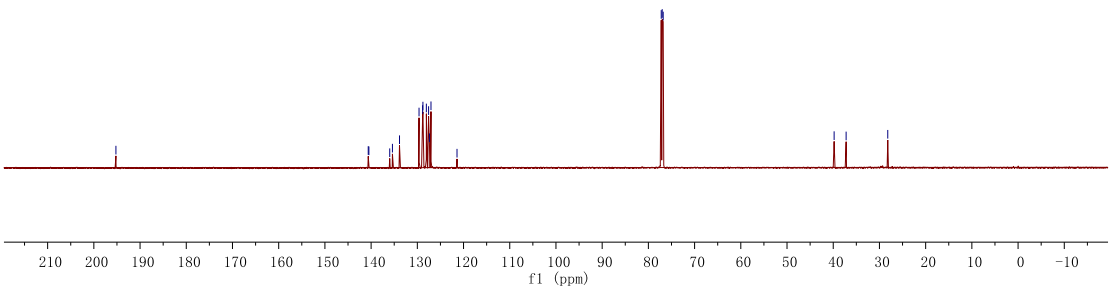
2s


1.91
5.19
2.11
2.10
3.10
1.00
1.05
1.06
2.09
f1 (ppm)

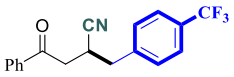

TJ-13C
TJ-947
195.223
140.624
140.481
135.974
135.387
133.856
129.630
128.852
128.789
128.045
127.562
127.375
127.045
121.410
77.220
77.008
76.797
39.805
37.208
28.200


O
CN
Ph
Ph

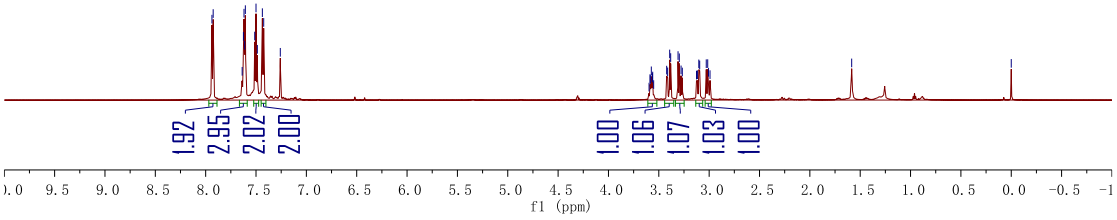
2s


f1 (ppm)

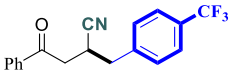

7.938
7.925
7.637
7.625
7.619
7.613
7.606
7.513
7.500
7.487
7.437
7.424
7.259
3.587
3.574
3.565
3.563
3.561
3.422
3.412
3.392
3.382
3.309
3.296
3.279
3.266
3.126
3.117
3.103
3.094
3.029
3.014
3.006
2.991
1.585
0.000


O
CN
Ph
CF3

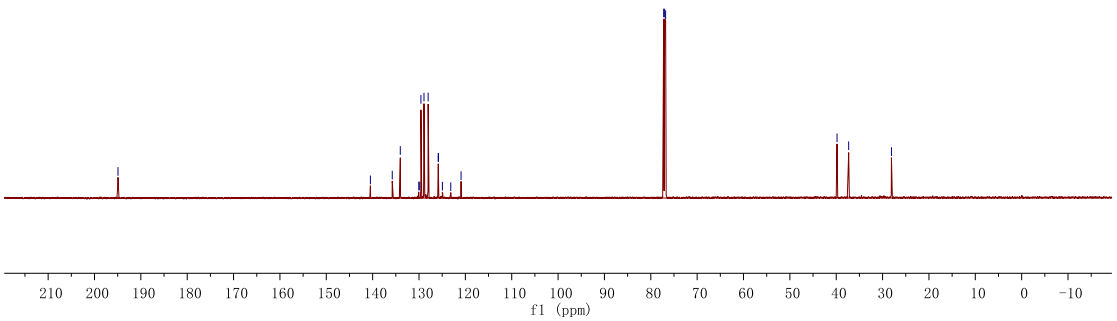
2t


1.92
2.95
2.02
2.00
1.00
1.06
1.07
1.03
1.00
f1 (ppm)

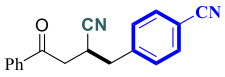

TJ-13C
TJ-987
194.932
140.485
135.770
134.037
130.057
129.842
129.585
128.923
128.029
125.844
125.819
124.952
123.149
120.928
77.223
77.011
76.800
39.826
37.315
28.086


O
CN
Ph
CF3

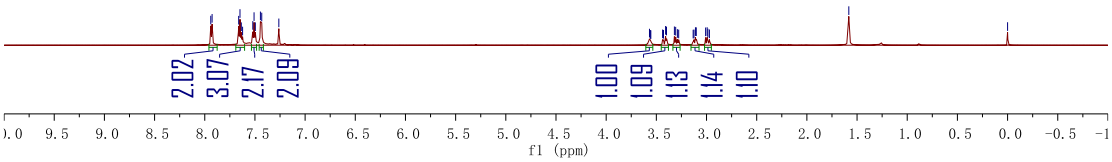
2t


f1 (ppm)

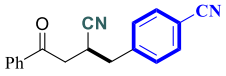

TJ-1H
TJ-929
7.940
7.927
7.662
7.649
7.636
7.623
7.521
7.509
7.496
7.445
7.432
7.262
3.568
3.438
3.408
3.399
3.320
3.307
3.290
3.110
3.102
3.009
2.994
2.986
2.971
1.582
0.000


O
CN
CN
Ph

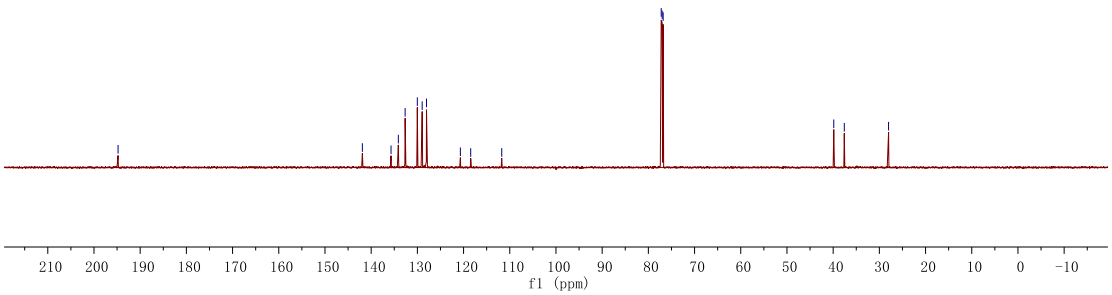
2u


2.02
3.07
2.17
2.09
1.00
1.09
1.13
1.14
1.10
f1 (ppm)

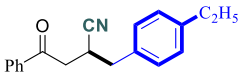

TJ-13C
TJ-929
194.787
141.907
135.700
134.122
132.649
130.014
128.960
128.025
120.692
118.455
111.739
77.221
77.010
76.798
39.869
37.590
28.005


O
CN
CN
Ph

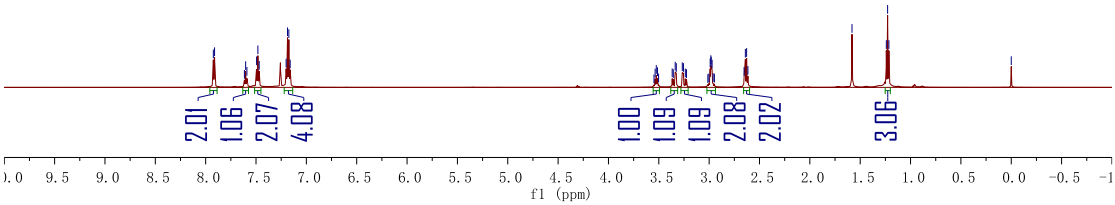
2u


f1 (ppm)

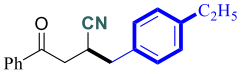

TJ-1H
7.974
7.972
7.615
7.603
7.591
7.494
7.481
7.468
7.201
7.187
7.174
7.161
3.537
3.525
3.513
3.367
3.356
3.337
3.326
3.267
3.255
3.237
3.225
2.990
2.983
2.980
2.971
2.653
2.640
2.628
2.615
1.582
1.241
1.228
1.215
-0.000


O
CN
Ph
C_2H_5

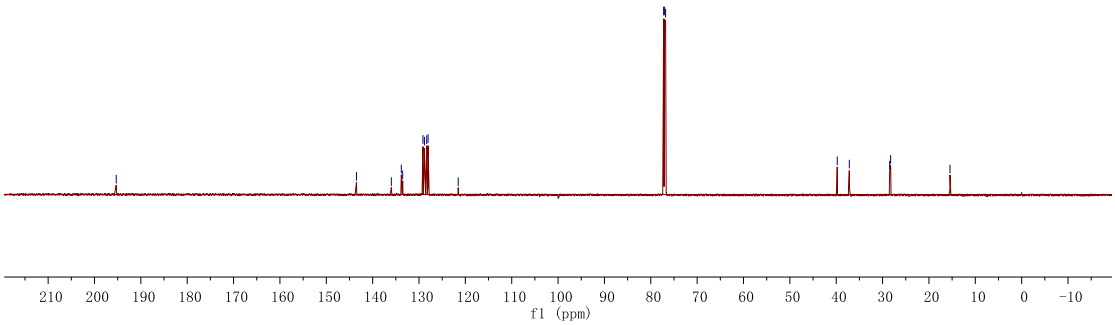
2v


2.01
1.06
2.07
4.08
1.00
1.09
1.09
2.08
2.02
3.06
f1 (ppm)

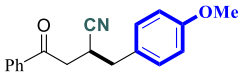

TJ-13C
TJ-948
195.313
143.494
135.969
133.817
133.520
129.148
128.827
128.334
128.039
121.539
77.232
77.020
76.809
39.779
37.180
28.477
28.261
15.457


O
CN
Ph
C_2H_5

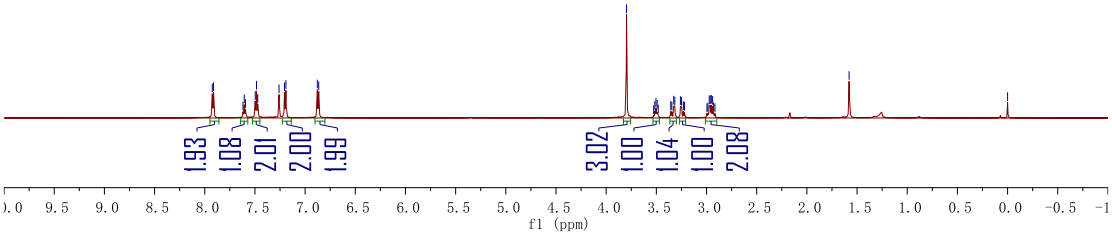
2v


f1 (ppm)

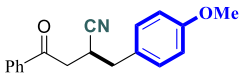

7.619
7.607
7.594
7.497
7.485
7.472
7.260
7.205
7.191
6.878
6.864
3.797
3.515
3.504
3.492
3.481
3.357
3.346
3.327
3.316
3.260
3.249
3.231
3.219
2.996
2.986
2.973
2.963
2.952
2.939
2.929
2.916
1.579
0.000


O
CN
OMe
Ph

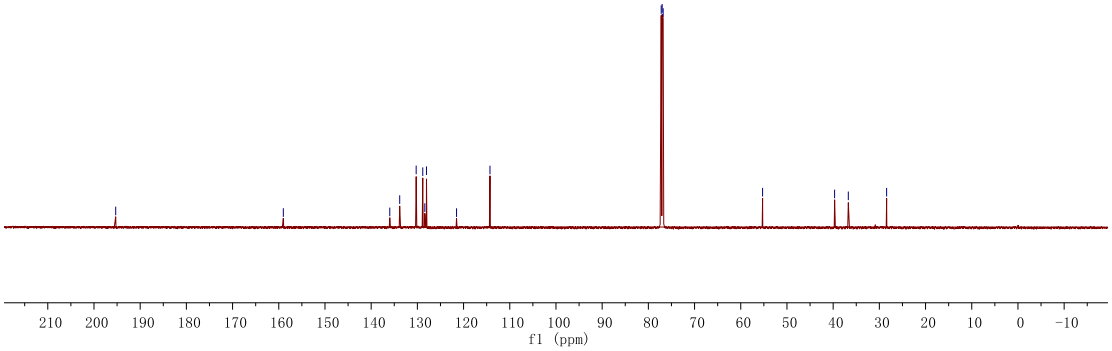
2w


1.93
1.08
2.01
2.00
1.99
3.02
1.00
1.04
1.00
2.08
f1 (ppm)


TJ-13C
TJ-1032
195.299
159.014
135.971
133.822
130.259
128.832
128.391
128.028
121.519
114.285
77.219
77.008
76.796
55.274
39.683
36.721
28.425

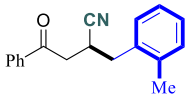

O
CN
OMe
Ph

2w

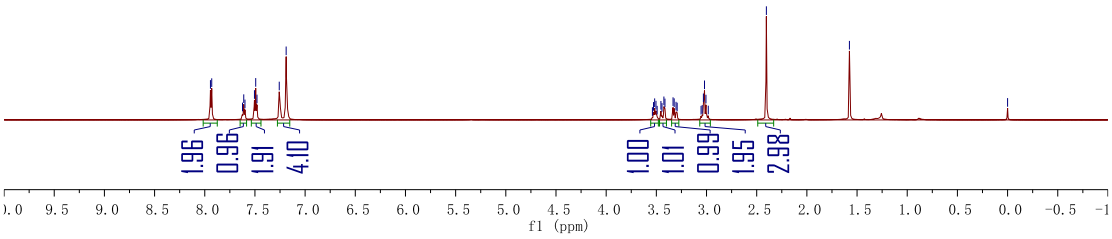

f1 (ppm)

TJ-1H
TJ-927

7.943 7.931 7.624 7.611 7.599 7.505 7.492 7.480 7.258 7.189 3.528 3.517 3.504 3.454 3.425 3.414 3.334 3.322 3.304 3.293 3.031 3.020 3.006 2.404 1.576 0.000

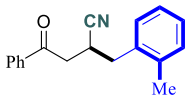


2x

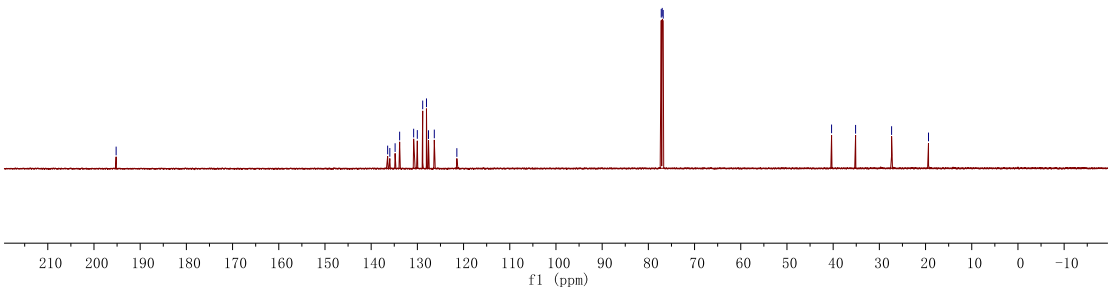


TJ-13C
TJ-927

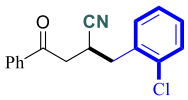
195.205 136.433 135.963 134.819 133.839 130.805 130.012 128.846 128.030 127.589 126.335 121.454 77.213 77.002 76.790 40.344 35.144 27.348 19.363



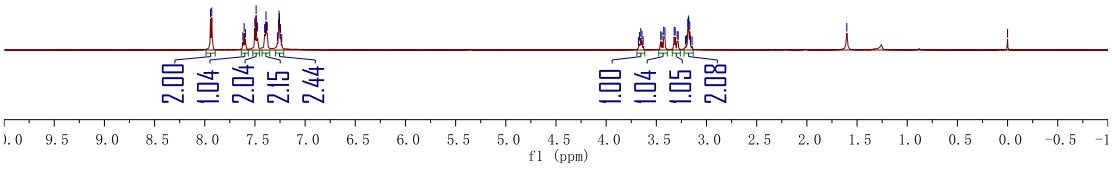
2x



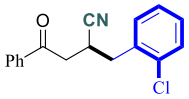

7.963
7.960
7.620
7.607
7.595
7.501
7.488
7.476
7.402
7.399
7.390
7.382
7.379
7.276
7.264
7.260
7.255
7.245
7.233
3.667
3.655
3.644
3.456
3.444
3.426
3.414
3.322
3.312
3.293
3.283
3.187
3.181
3.176
3.167
1.602
0.000


O
CN
Ph
Cl

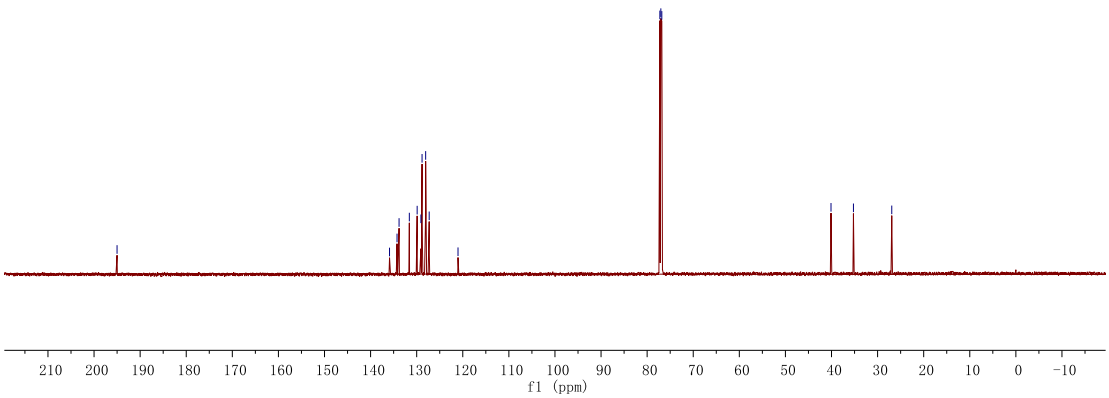
2y

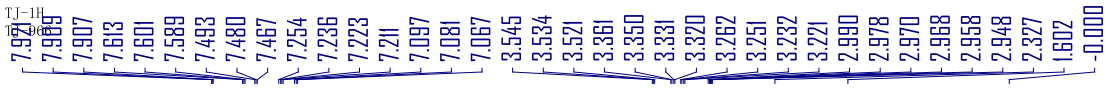

2.00
1.04
2.04
2.15
2.44
1.00
1.04
1.05
2.08
f1 (ppm)

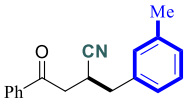

TJ-13C
TJ-984
195.010
135.893
134.265
133.824
131.595
129.899
129.082
128.836
128.052
127.286
121.034
77.238
77.027
76.815
40.109
35.239
26.925


O
CN
Ph
Cl

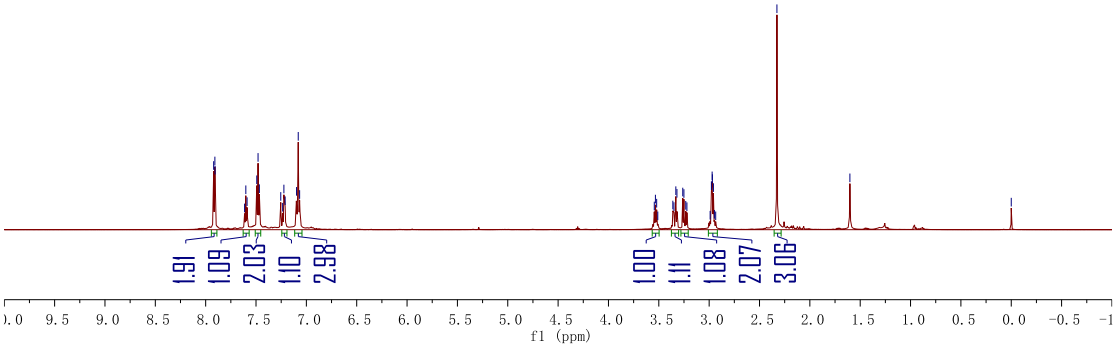
2y


f1 (ppm)

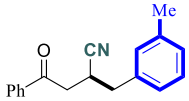

TJ-1H
7.954
7.950
7.907
7.613
7.601
7.589
7.493
7.480
7.467
7.254
7.236
7.223
7.211
7.097
7.081
7.067
3.545
3.534
3.521
3.361
3.350
3.331
3.320
3.262
3.251
3.232
3.221
2.990
2.978
2.970
2.968
2.958
2.948
2.327
1.602
-0.000


Me
O
CN
Ph

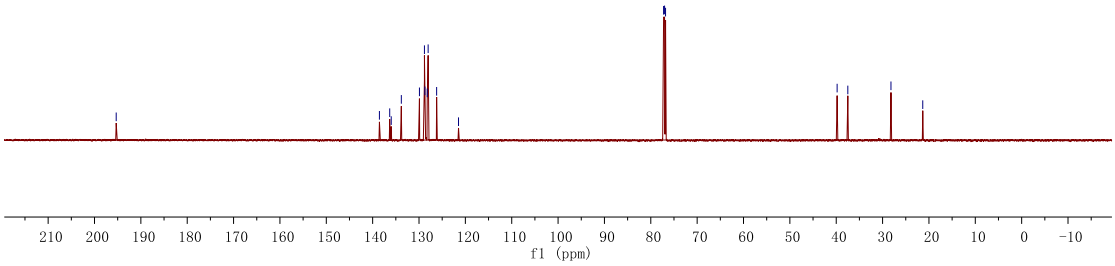
2z


1.91
1.09
2.03
1.10
2.98
1.00
1.11
1.08
2.07
3.06
f1 (ppm)

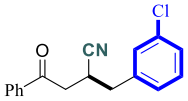

TJ-13C
TJ-966
195.319
138.540
136.320
135.994
133.815
129.905
128.828
128.727
128.226
128.031
126.196
121.476
77.240
77.028
76.816
39.806
37.499
28.192
21.333


Me
O
CN
Ph

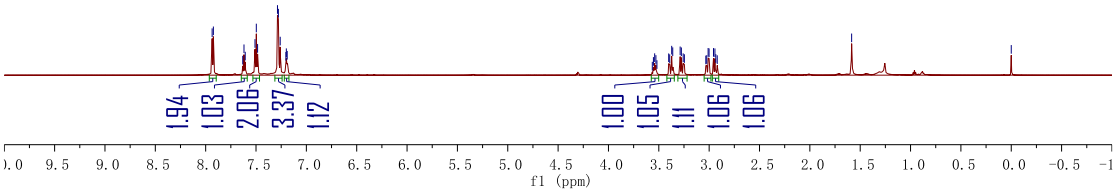
2z


f1 (ppm)

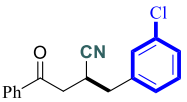

TJ-1H
TJ-983
7.956
7.953
7.923
7.632
7.619
7.607
7.510
7.497
7.484
7.287
7.278
7.260
7.203
7.199
7.190
3.553
3.541
3.529
3.519
3.402
3.392
3.372
3.362
3.288
3.276
3.258
3.246
3.033
3.024
3.010
3.001
2.957
2.943
2.934
2.920
1.585
-0.000


Cl
CN
O
Ph

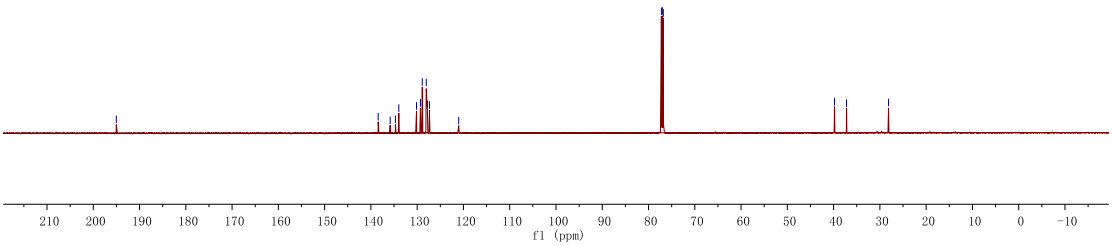
2aa


1.94
1.03
2.06
3.37
1.12
1.00
1.05
1.11
1.06
1.06
f1 (ppm)

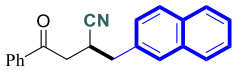

TJ-13C
TJ-983
195.021
138.426
135.832
134.700
133.966
130.141
129.289
128.898
128.040
127.792
127.348
121.023
77.226
77.015
76.803
39.814
37.211
28.128


Cl
CN
O
Ph

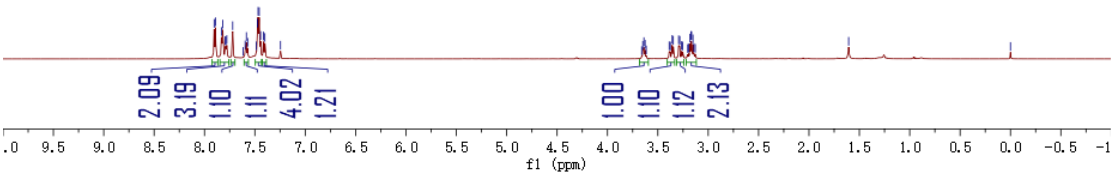
2aa


f1 (ppm)

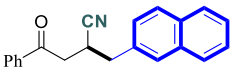

TJ-1H
TJ-949
7.951
7.851
7.832
7.818
7.793
7.789
7.778
7.720
7.596
7.584
7.572
7.485
7.473
7.468
7.457
7.443
7.414
7.401
7.245
3.650
3.638
3.627
3.387
3.377
3.358
3.347
3.294
3.282
3.264
3.253
3.180
3.170
3.165
3.152
1.606
0.000


O
CN
Ph

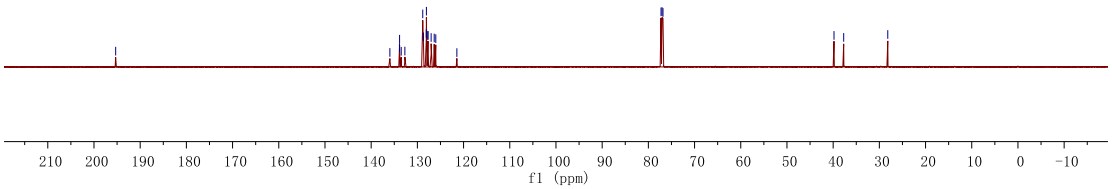
2ab


2.09
3.19
1.10
1.11
4.02
1.21
1.00
1.10
1.12
2.13
f1 (ppm)

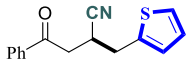

TJ-13C
TJ-949
195.305
135.951
133.879
133.850
133.497
132.703
128.835
128.686
128.074
128.044
127.737
127.706
127.021
126.358
126.015
121.450
77.257
77.045
76.833
39.818
37.719
28.177


O
CN
Ph

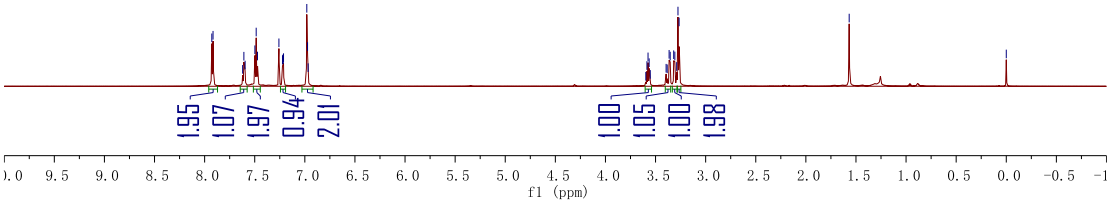
2ab


f1 (ppm)

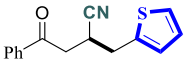

TJ-1H
TJ-982
7.928
7.916
7.608
7.596
7.498
7.485
7.473
7.259
7.223
7.220
7.215
7.213
6.980
6.973
6.967
3.586
3.575
3.564
3.395
3.365
3.354
3.319
3.308
3.289
3.276
3.265
1.568
0.000


O
CN
S
Ph

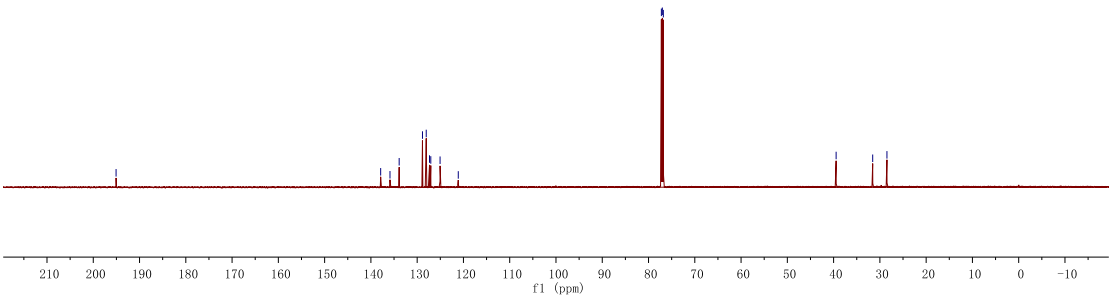
2ac


1.95
1.07
1.97
0.94
2.01
1.00
1.05
1.00
1.98
f1 (ppm)

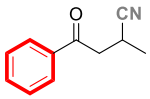

TJ-13C
TJ-982
195.071
137.888
135.876
133.891
128.853
128.041
127.332
127.055
125.049
121.116
77.224
77.012
76.801
39.458
31.554
28.475


O
CN
S
Ph

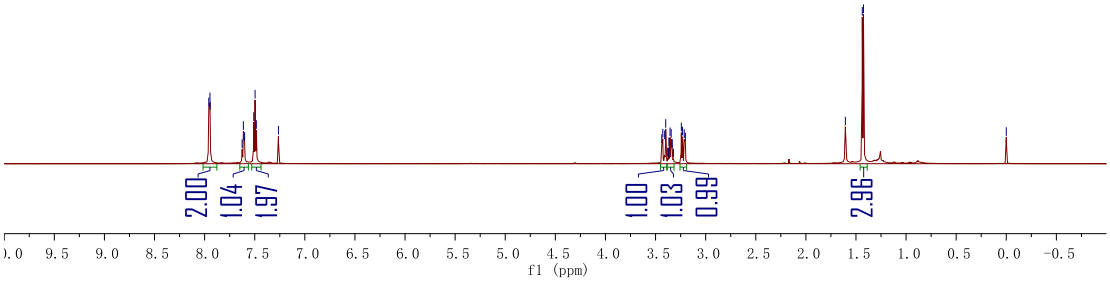
2ac


f1 (ppm)

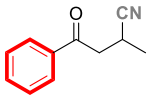

TJ-1H
TJ-921
7.959
7.947
7.945
7.626
7.613
7.601
7.510
7.497
7.484
7.263
3.438
3.428
3.409
3.399
3.378
3.367
3.355
3.344
3.333
3.243
3.231
3.214
1.437
1.425
0.000


O
CN

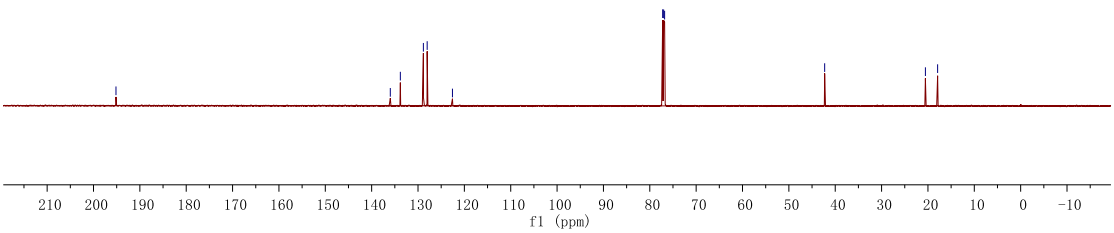
3a


2.00
1.04
1.97
1.00
1.03
0.99
2.96
f1 (ppm)


TJ-13C
TJ-921
195.152
135.974
133.810
128.843
128.023
122.569
77.225
77.014
76.802
42.279
20.547
17.911

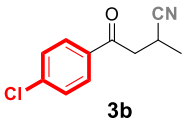

O
CN

3a

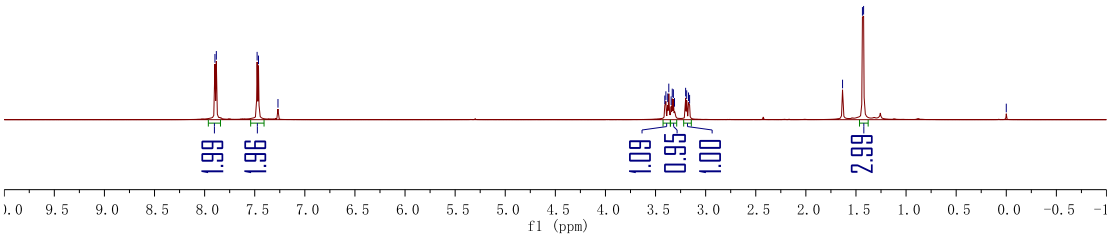

f1 (ppm)

TJ-1H
TJ-945

7.897
7.883
7.476
7.462
7.268
3.408
3.397
3.379
3.368
3.345
3.333
3.322
3.311
3.200
3.189
3.171
3.160
1.634
1.435
1.424
0.000

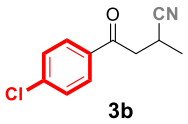


3b

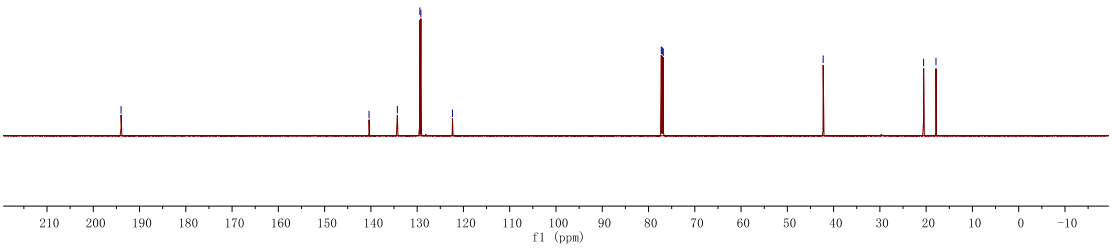


TJ-13C
TJ-945

193.990
140.400
134.282
129.418
129.193
122.375
77.237
77.025
76.814
42.258
20.546
17.874

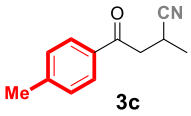


3b

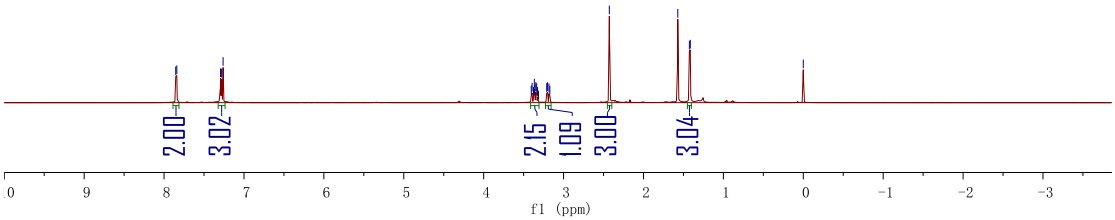


TJ-1H
TJ-959

7.854
7.841
7.293
7.280
7.261
3.404
3.394
3.376
3.366
3.359
3.348
3.337
3.211
3.200
3.183
3.172
2.427
2.411
1.425
1.414
0.000

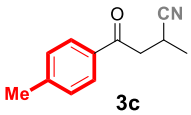


3c

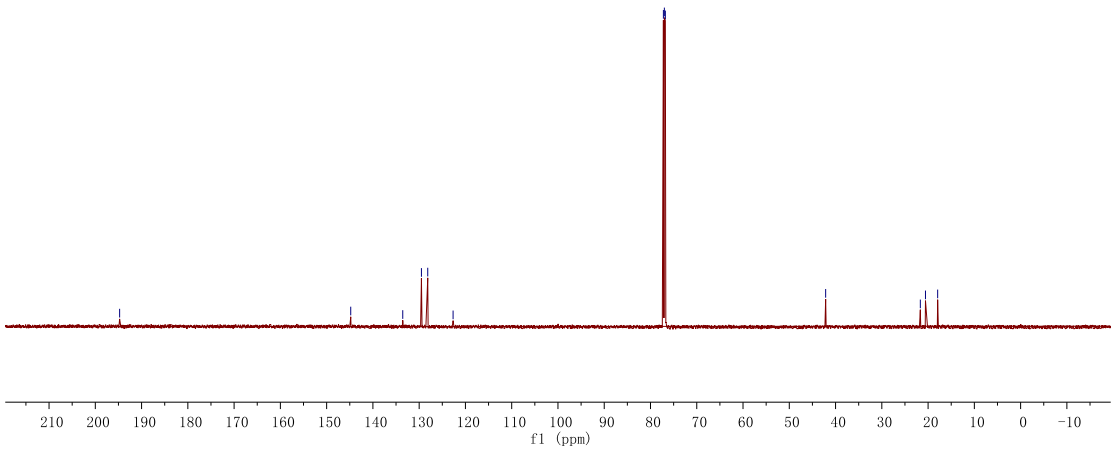


TJ-13C
TJ-959

194.744
144.791
133.548
129.511
128.148
122.667
77.213
77.002
76.790
42.139
21.675
20.563
17.929

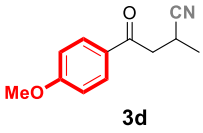


3c

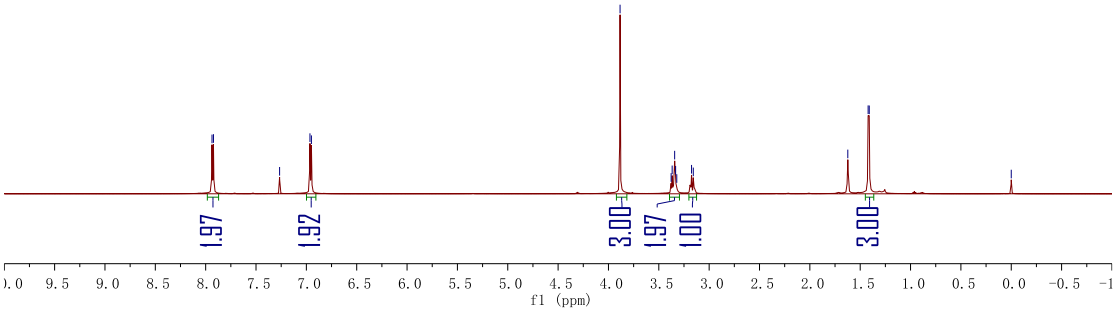


TJ-1H
TJ-951

7.937
7.923
7.266
6.964
6.950
3.885
3.378
3.367
3.343
3.333
3.322
3.175
3.158
1.623
1.421
1.410
0.000

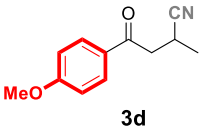


3d

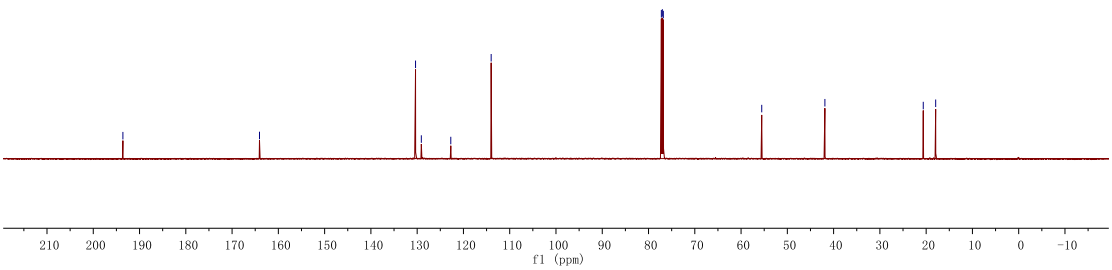


TJ-13C
TJ-951

193.597
164.075
130.352
129.103
122.734
114.008
77.226
77.015
76.803
55.535
41.885
20.625
17.941



3d

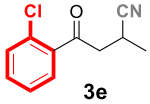


TJ-1H
TJ-944-1

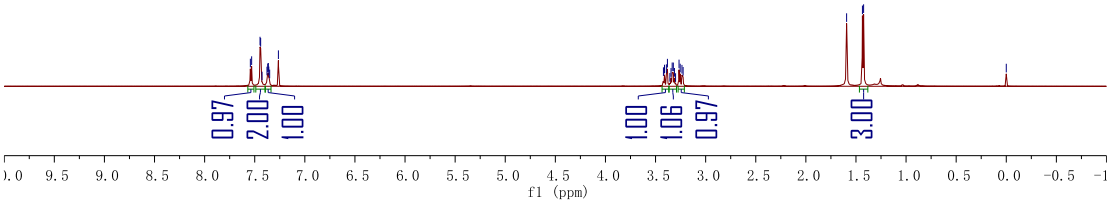
7.544 7.531 7.447 7.441 7.427 7.378 7.370 7.364 7.359 7.351 7.264

3.421 3.411 3.392 3.381 3.345 3.334 3.323 3.311 3.266 3.254 3.236 3.225 1.593 1.435 1.424

0.000



3e



TJ-13C
TJ-944-1

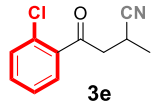
198.174

137.921 132.559 131.240 130.798 129.341 127.218 122.148

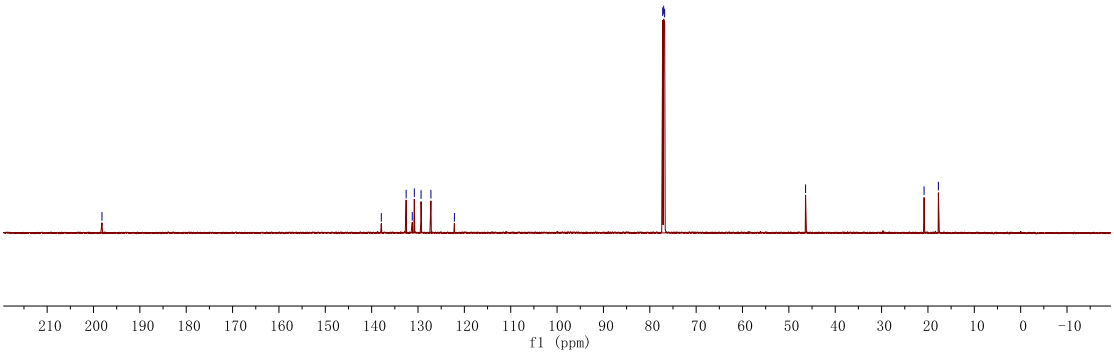
77.218 77.006 76.794

46.400

20.834 17.744

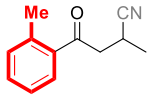


3e

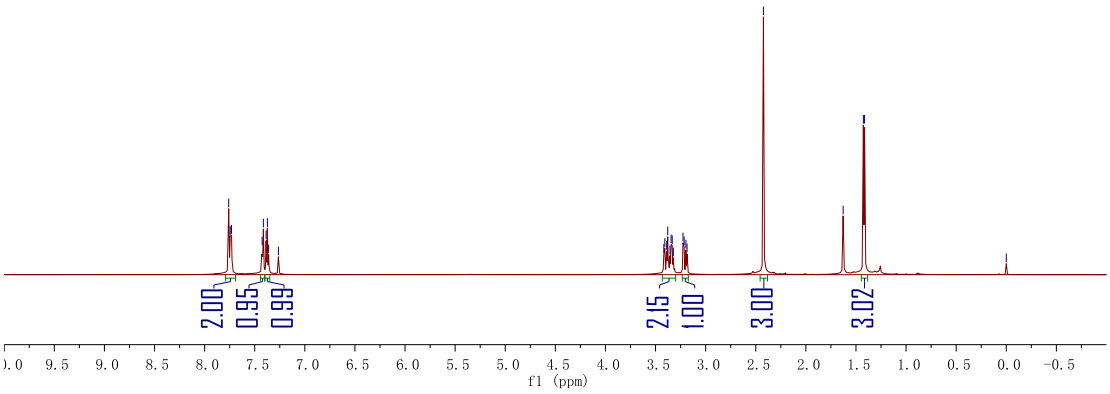


TJ-1H
TJ-943

7.760
7.745
7.732
7.428
7.414
7.386
7.374
7.361
7.264
3.418
3.407
3.389
3.379
3.356
3.345
3.334
3.226
3.215
3.197
3.186
2.424
1.628
1.426
1.415
0.000

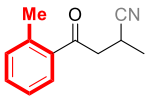


3f

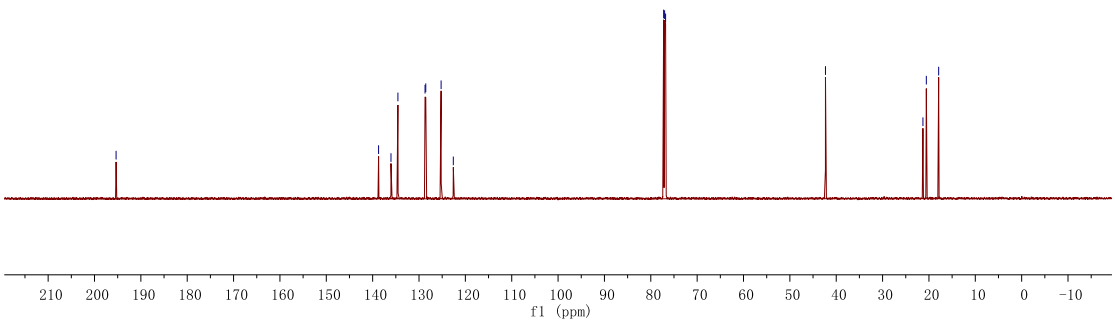


TJ-13C
TJ-943

195.344
138.722
136.044
134.551
128.696
128.542
125.233
122.599
77.230
77.018
76.807
42.320
21.297
20.562
17.901



3f



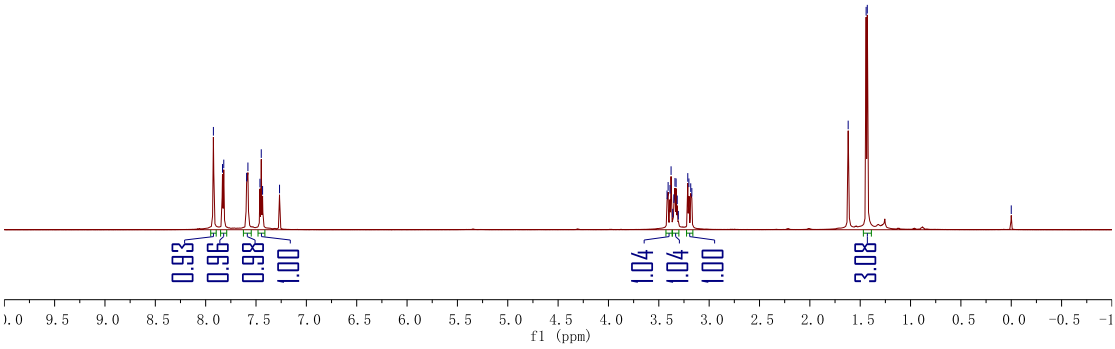
TJ-1H
TJ-952

7.923 7.833 7.820 7.594 7.580 7.461 7.448 7.435 7.266

3.418 3.407 3.389 3.378 3.362 3.351 3.339 3.328 3.317 3.212 3.201 3.183 3.172 1.619 1.441 1.430

0.000

3g



TJ-13C
TJ-952

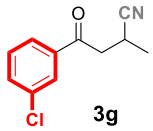
193.983

137.434 135.293 133.751 130.192 128.167 126.080 122.295

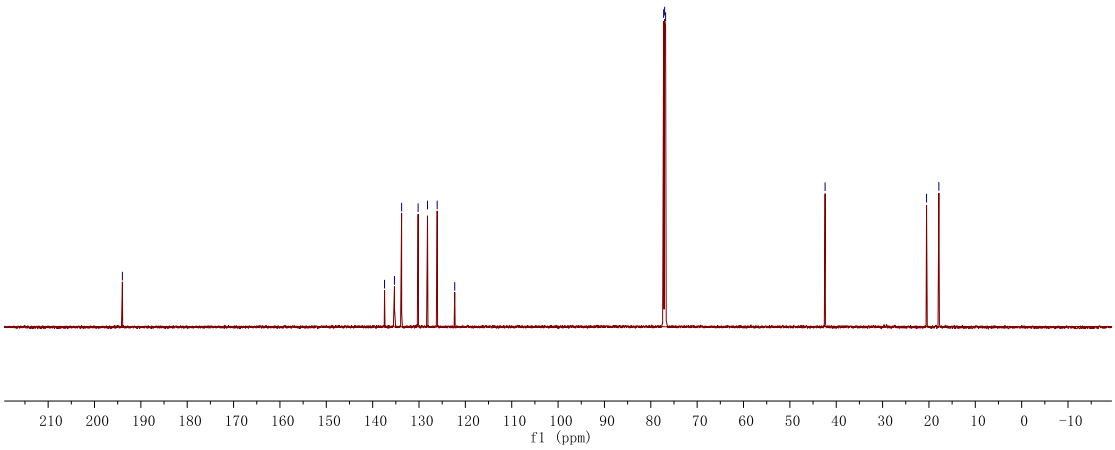
77.229 77.017 76.806

42.400

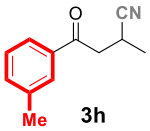
20.515 17.862



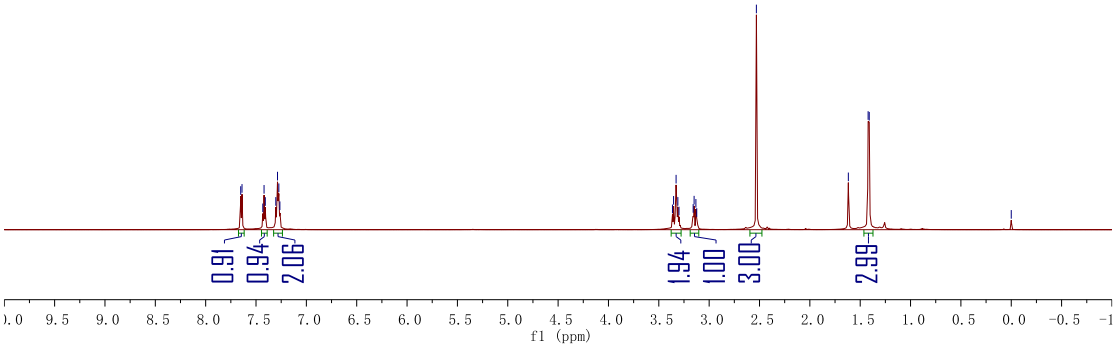
3g



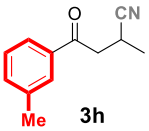

TJ-1H
TJ-942
7.652
7.639
7.433
7.420
7.408
7.304
7.287
7.273
7.263
3.364
3.353
3.328
3.311
3.300
3.159
3.149
3.132
3.123
2.531
1.618
1.421
1.410
0.000


O
CN
Me

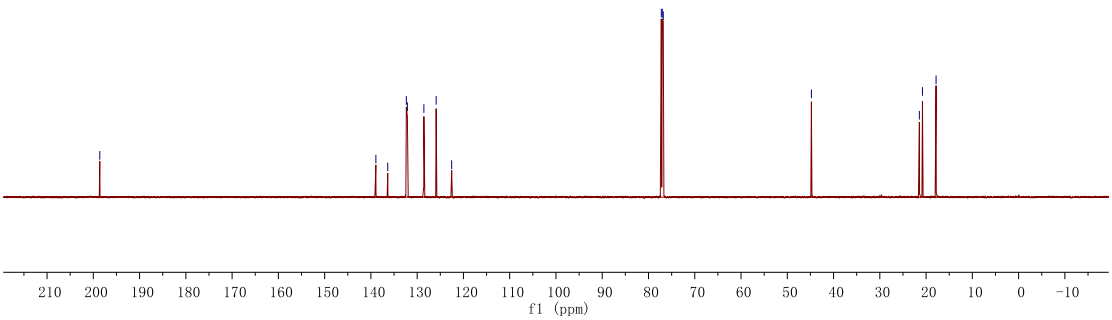
3h


0.91
0.94
2.06
1.94
1.00
3.00
2.99
f1 (ppm)

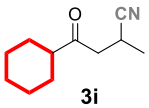

TJ-13C
TJ-942
198.603
138.928
136.363
132.340
132.115
128.550
125.895
122.546
77.230
77.019
76.807
44.786
21.450
20.781
17.840


O
CN
Me

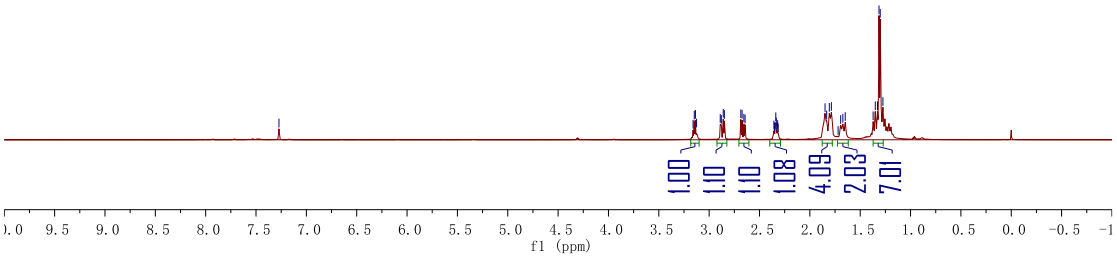
3h


f1 (ppm)

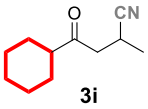

TJ-1H
TJ-950
7.272
3.148
3.136
3.125
2.890
2.879
2.860
2.849
2.685
2.673
2.655
2.643
2.338
2.333
1.849
1.833
1.807
1.786
1.694
1.672
1.649
1.372
1.350
1.328
1.313
1.301


O
CN

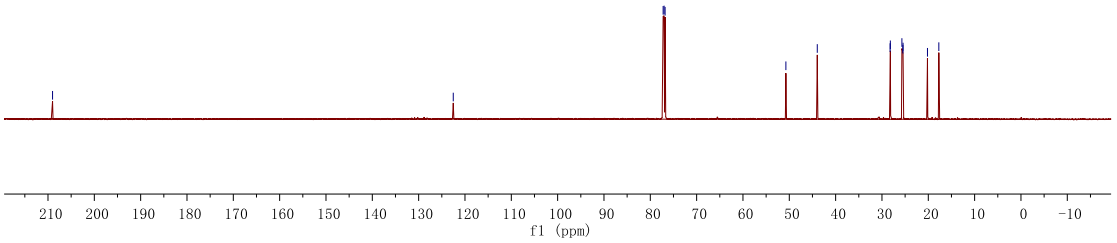
3i


1.00
1.10
1.10
1.08
4.09
2.03
7.01
f1 (ppm)


209.815
122.527
77.231
77.019
76.807
50.736
43.961
28.240
28.190
25.697
25.486
25.449
20.177
17.727

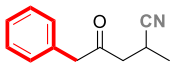

O
CN

3i

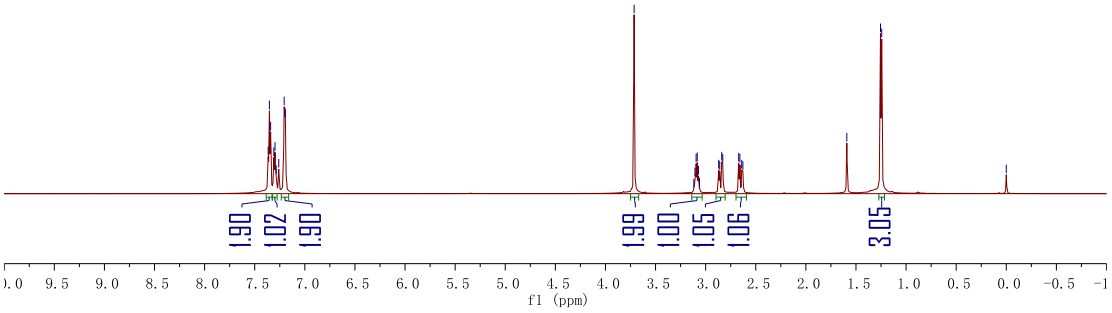

f1 (ppm)

TJ-1H
TJ-994

7.366 7.354 7.341 7.310 7.298 7.286 7.260 7.206 7.194 3.714 3.107 3.095 3.084 3.072 2.870 2.860 2.840 2.829 2.671 2.659 2.640 2.628 1.591 1.255 1.243 0.000

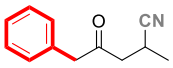


3j

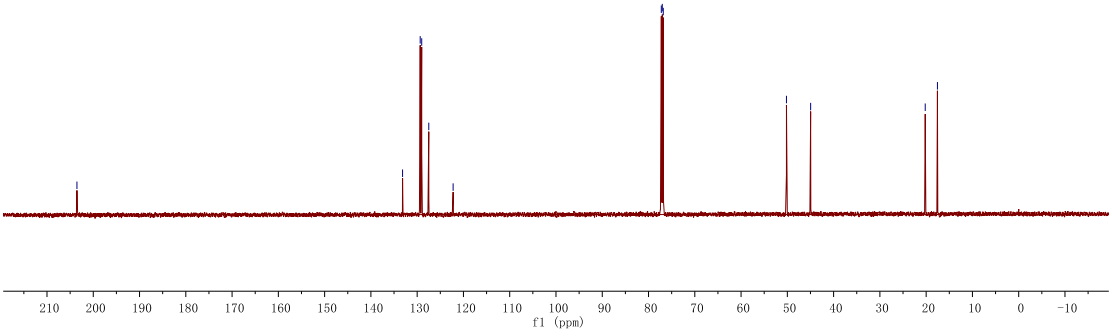


TJ-13C
TJ-994

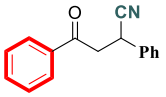
203.528 133.157 129.343 129.018 127.490 122.230 77.239 77.027 76.815 50.190 44.963 20.201 17.562



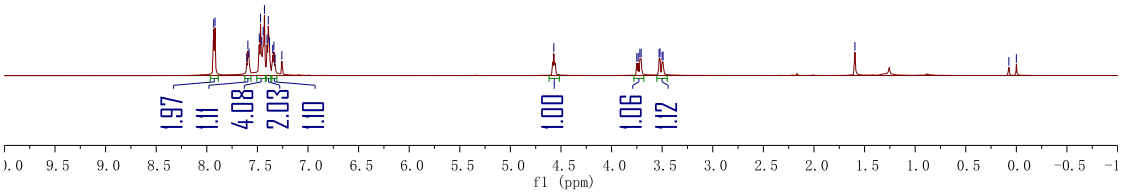
3j



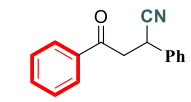

7.606
7.594
7.582
7.481
7.469
7.456
7.443
7.431
7.405
7.392
7.380
7.349
7.337
7.325
7.258
4.571
3.750
3.737
3.721
3.708
3.531
3.521
3.501
3.491
1.595
0.074
0.000


O
CN
Ph

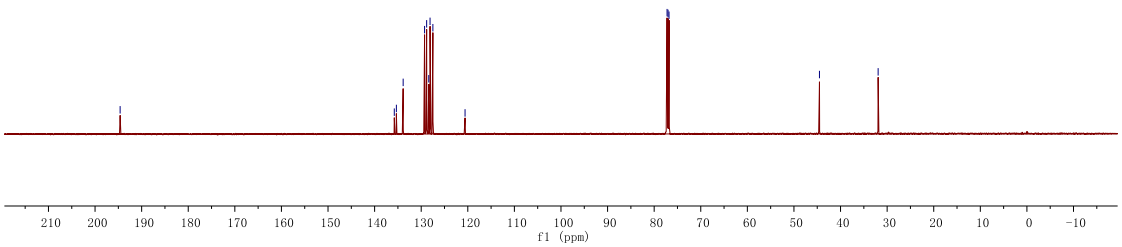
5a


1.97
1.11
4.08
2.03
1.10
1.00
1.06
1.12
f1 (ppm)

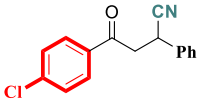

TJ-13C
TJ-995
194.619
135.776
135.329
133.873
129.277
128.833
128.379
128.099
127.494
120.588
77.234
77.023
76.811
44.523
31.932


O
CN
Ph

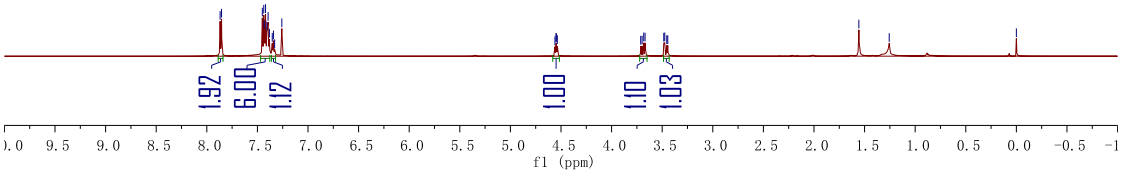
5a


f1 (ppm)

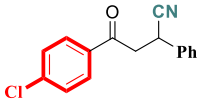

TJ-1H
TJ-1000
7.869
7.854
7.451
7.437
7.432
7.420
7.407
7.394
7.381
7.353
7.341
7.330
7.259
4.560
4.549
4.546
4.536
3.699
3.682
3.669
3.484
3.474
3.455
3.445
1.556
1.257
0.000


O
CN
Ph
Cl

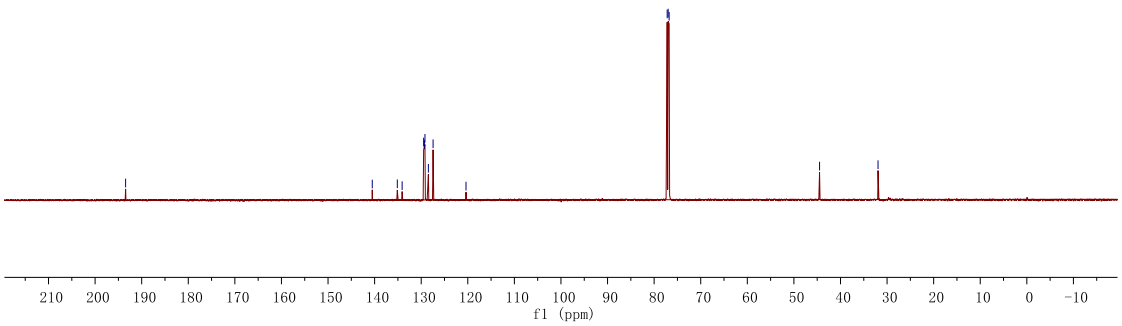
5b


1.92
6.00
1.12
1.00
1.10
1.03
f1 (ppm)

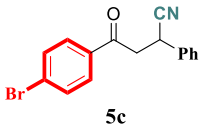

TJ-13C
TJ-1000
193.450
140.507
135.127
134.093
129.476
129.316
129.194
128.461
127.450
120.383
77.202
76.991
76.779
44.493
31.939


O
CN
Ph
Cl

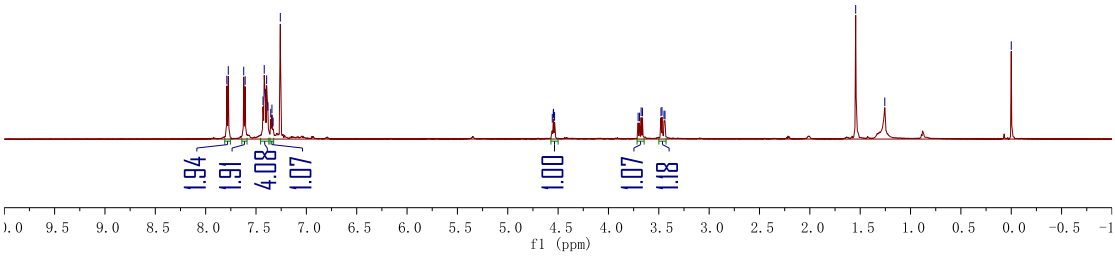
5b


f1 (ppm)

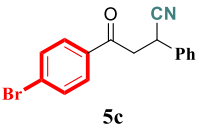

TJ-1H
TJ-1014
7.790
7.775
7.622
7.608
7.430
7.418
7.407
7.394
7.382
7.354
7.342
7.330
7.259
4.558
4.548
4.545
4.535
3.692
3.676
3.662
3.478
3.468
3.449
3.439
1.545
1.256
0.000


O
CN
Ph
Br

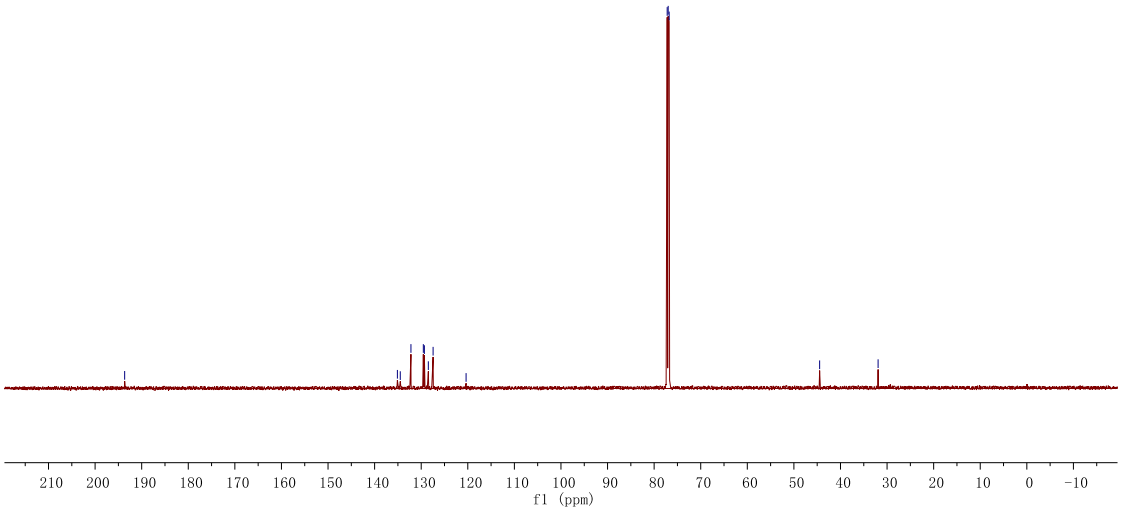
5c


1.94
1.91
4.08
1.07
1.00
1.07
1.18
f1 (ppm)

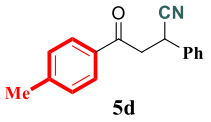

TJ-13C
TJ-1014
193.655
135.110
134.490
132.203
129.543
129.320
128.469
127.448
120.365
77.198
76.987
76.775
44.475
31.924


O
CN
Ph
Br

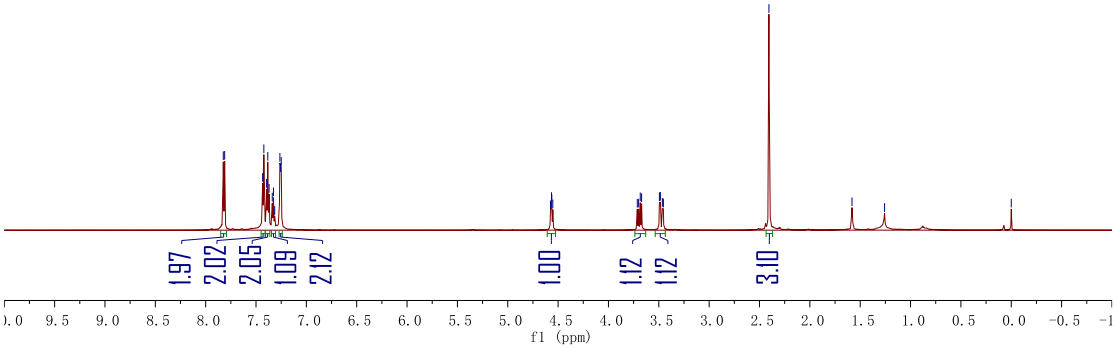
5c


f1 (ppm)

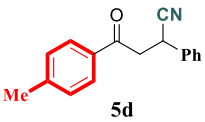

TJ-1H
TJ-101
7.825
7.811
7.434
7.422
7.395
7.383
7.370
7.339
7.327
7.314
7.263
7.255
7.250
4.576
4.565
4.563
4.552
3.684
3.671
3.494
3.484
3.465
2.406
1.581
1.258
0.000


O
CN
Ph
Me

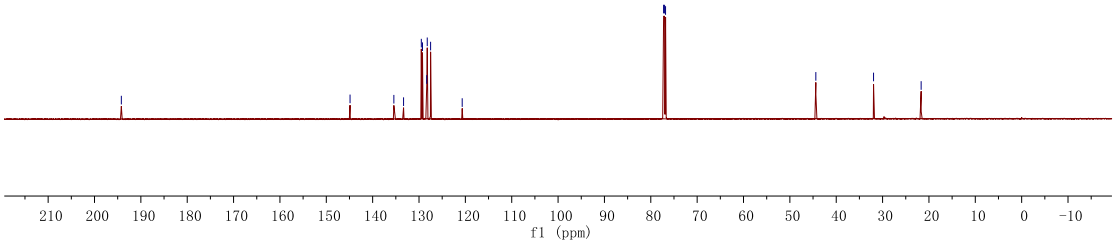
5d


1.97
2.02
2.05
1.09
2.12
1.00
1.12
1.12
3.10
f1 (ppm)


TJ-13C
TJ1017
194.212
144.877
135.426
133.333
129.503
129.252
128.332
128.224
127.498
120.681
77.239
77.027
76.816
44.398
31.948
21.682

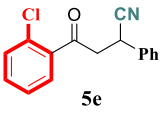

O
CN
Ph
Me

5d

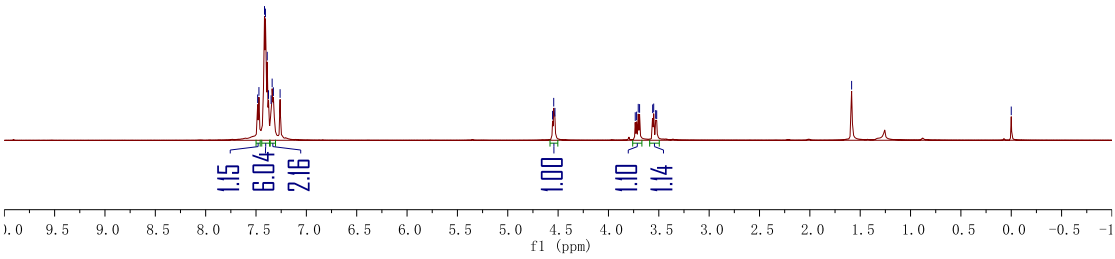

f1 (ppm)

TJ-1H
TJ-1022

7.484 7.471 7.416 7.406 7.389 7.376 7.350 7.340 7.327 7.261 4.555 4.544 4.531 3.721 3.704 3.691 3.561 3.551 3.531 3.521 1.585 -0.000

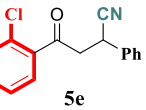


5e

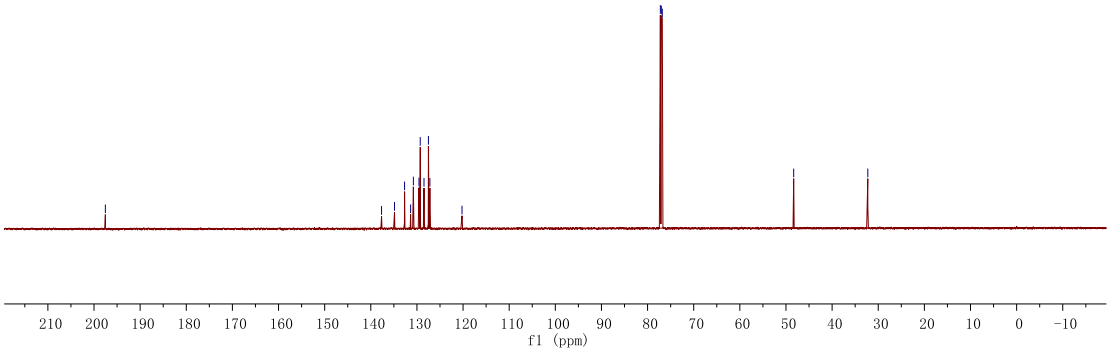


TJ-13C
TJ-1022

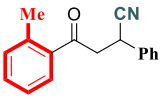
197.540 137.669 134.861 132.677 131.371 130.771 129.550 129.281 128.466 127.510 127.193 120.227 77.233 77.021 76.810 48.332 32.264



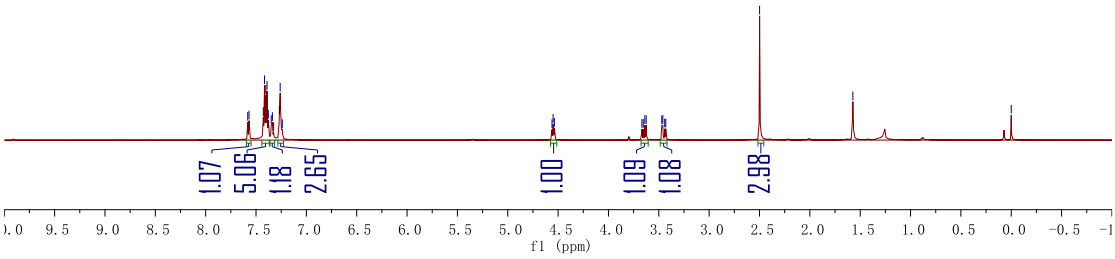
5e



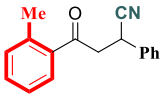

TJ-1H
TJ-997
7.582
7.569
7.427
7.415
7.403
7.391
7.378
7.349
7.337
7.325
7.268
7.260
7.239
4.561
4.550
4.537
3.639
3.625
3.470
2.499
1.573
0.000


Me
O
CN
Ph

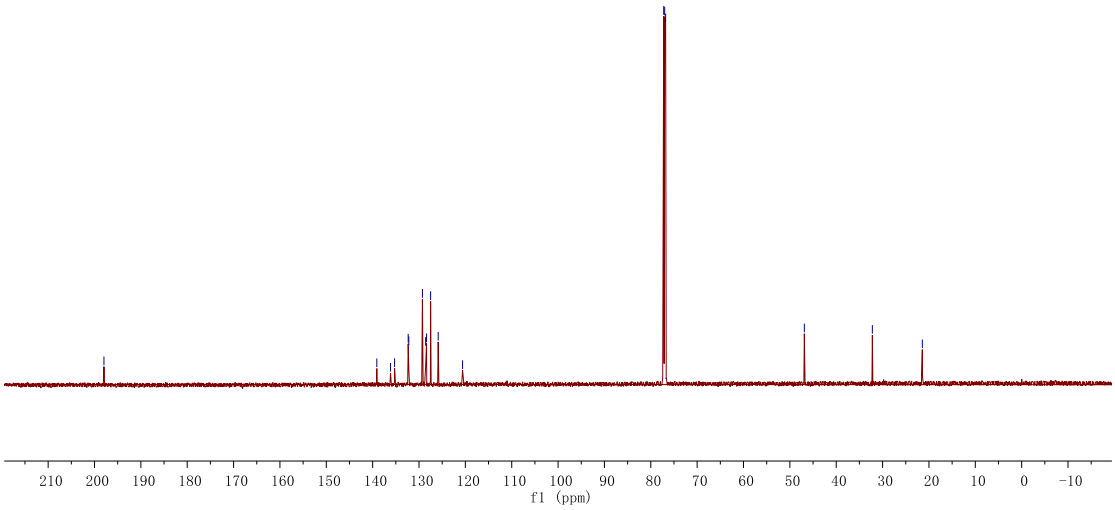
5f


1.07
5.06
1.18
2.65
1.00
1.09
1.08
2.98
f1 (ppm)

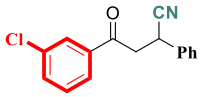

TJ-13C
TJ-997
197.962
139.103
136.144
135.268
132.334
132.195
129.262
128.566
128.375
127.495
125.860
120.604
77.219
77.008
76.796
46.877
32.206
21.427


Me
O
CN
Ph

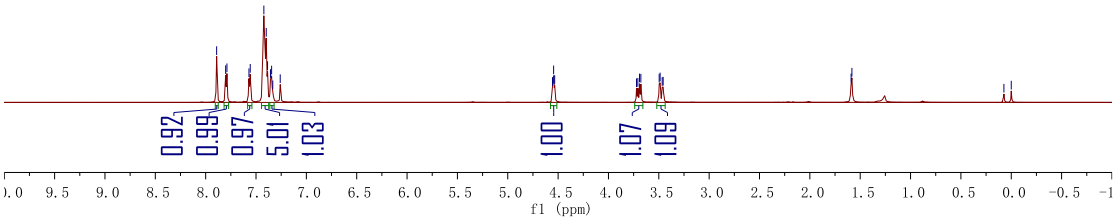
5f


f1 (ppm)

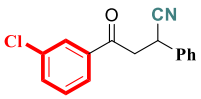

TJ-1H
TJ-999
7.891
7.802
7.789
7.570
7.557
7.422
7.398
7.386
7.356
7.345
7.334
7.260
4.555
4.545
4.534
3.708
3.691
3.678
3.496
3.487
3.466
3.457
1.590
1.582
0.073
0.000


O
CN
Cl
Ph

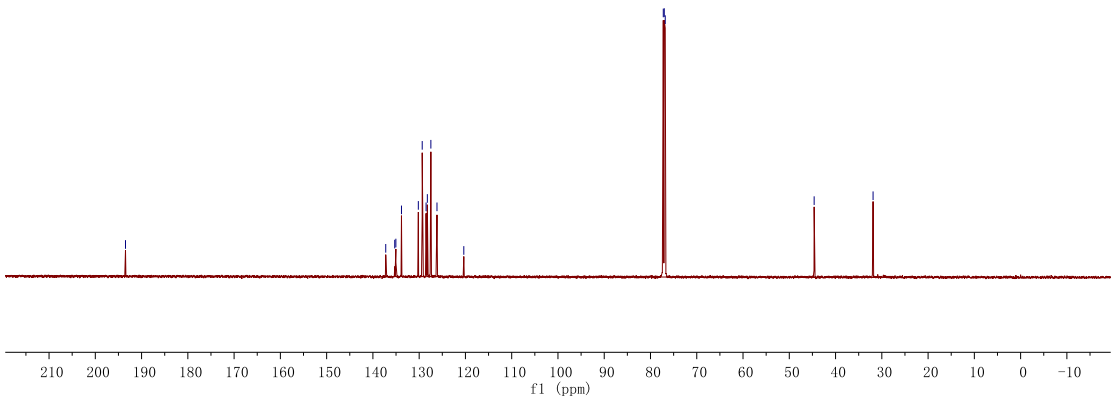
5g


0.92
0.99
0.97
5.01
1.03
1.00
1.07
1.09
f1 (ppm)

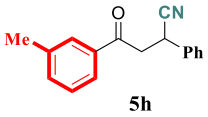

TJ-13C
TJ-999
193.476
137.224
135.281
135.035
133.824
130.182
129.342
128.503
128.234
127.471
126.151
120.353
77.236
77.025
76.813
44.626
31.892


O
CN
Cl
Ph

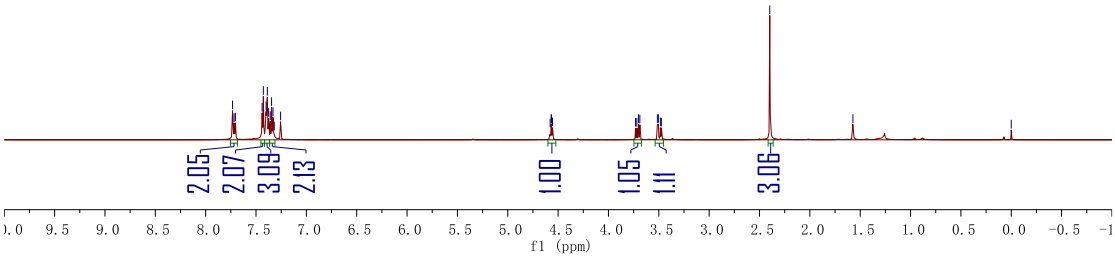
5g


f1 (ppm)

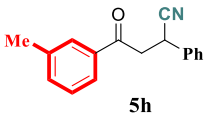

TJ-1H
TJ-1011
7.733
7.718
7.705
7.439
7.427
7.400
7.388
7.375
7.359
7.346
7.331
7.319
7.256
4.579
4.568
4.566
4.556
3.701
3.688
3.514
3.504
1.572
0.000


O
CN
Me
Ph

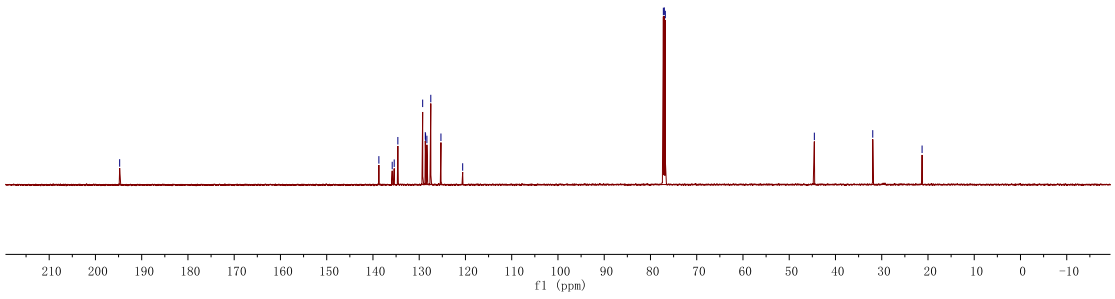
5h


2.05
2.07
3.09
2.13
1.00
1.05
1.11
3.06
f1 (ppm)

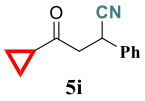

TJ-13C
TJ-1011
194.763
138.720
135.839
135.407
134.616
129.250
128.688
128.619
128.337
127.494
125.302
120.600
77.215
77.003
76.792
44.572
31.940
21.275


O
CN
Me
Ph

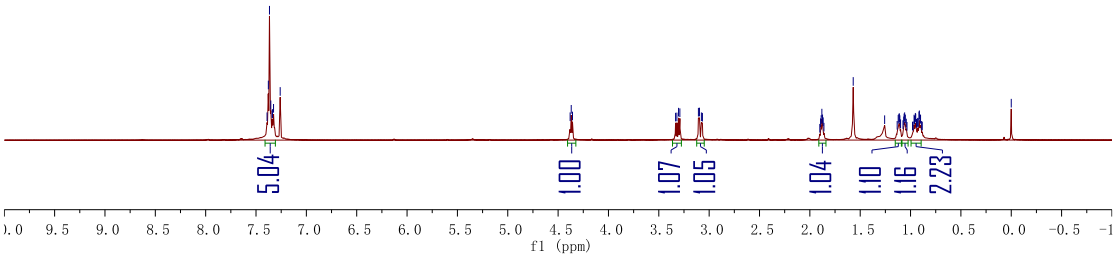
5h


f1 (ppm)

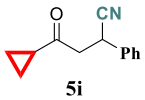

7.366
7.353
7.340
7.337
7.326
7.260
4.381
4.370
4.357
3.333
3.320
3.304
3.291
3.107
3.096
3.077
3.067
1.881
1.874
1.569
1.123
1.115
1.111
1.064
1.059
1.052
0.965
0.952
0.949
0.916
0.912
0.904
0.901
0.000


O
CN
Ph

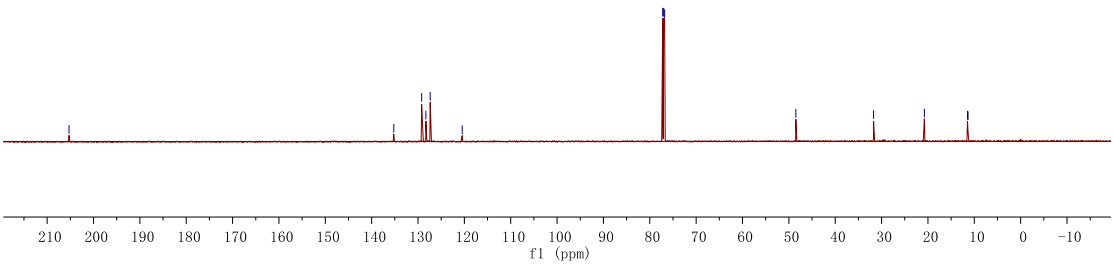
5i


5.04
1.00
1.07
1.05
1.04
1.10
1.16
2.23
f1 (ppm)

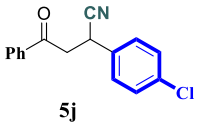

TJ-13C
TJ1021
205.288
135.230
129.210
128.303
127.371
120.464
77.219
77.008
76.796
48.491
31.726
20.771
11.462
11.351


O
CN
Ph

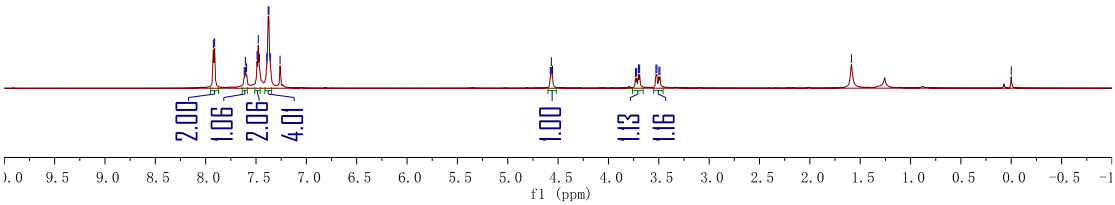
5i


f1 (ppm)

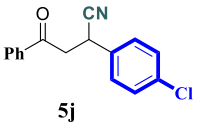

TJ-1H
TJ-1016
7.924
7.911
7.617
7.606
7.594
7.490
7.478
7.466
7.393
7.379
7.372
7.359
7.261
4.578
4.567
4.556
3.720
3.702
3.690
3.529
3.519
3.499
3.489
1.587
0.000


O
CN
Ph
Cl

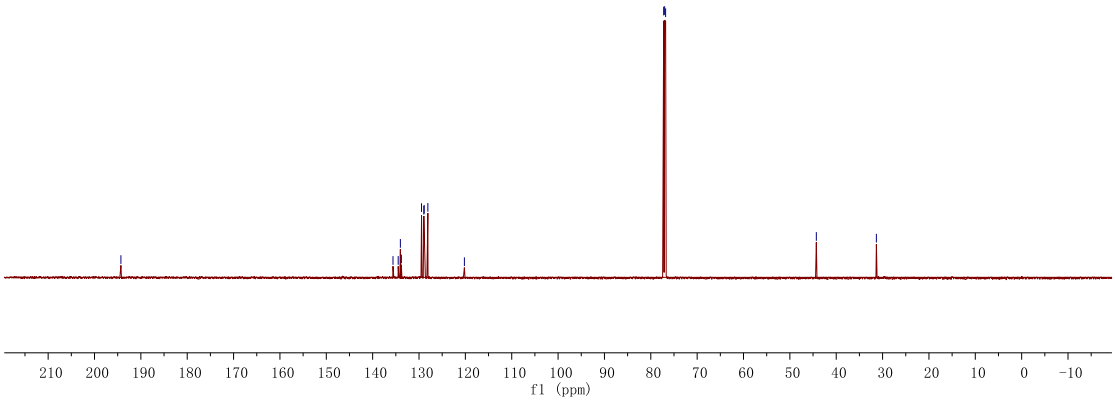
5j


2.00
1.06
2.06
4.01
1.00
1.13
1.16
f1 (ppm)

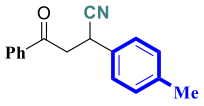

TJ-13C
TJ-1016
194.305
135.610
134.489
134.021
133.805
129.457
128.956
128.889
128.092
120.212
77.224
77.013
76.801
44.292
31.338


O
CN
Ph
Cl

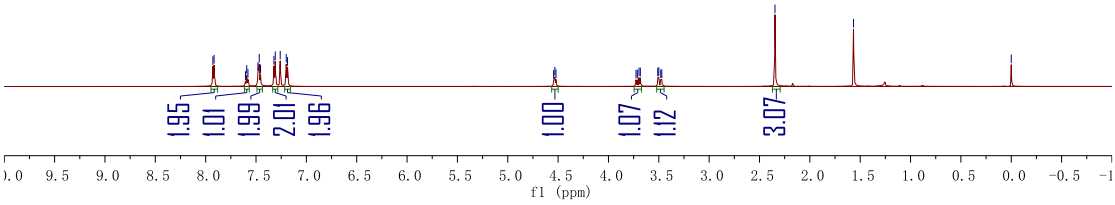
5j

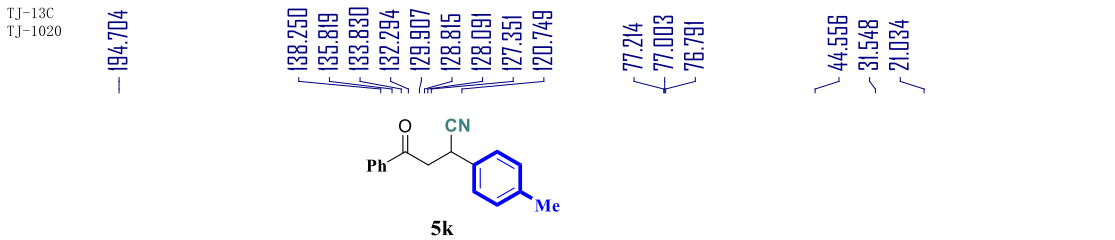

f1 (ppm)


TJ-1H
TJ-1020
7.928
7.916
7.605
7.592
7.580
7.481
7.468
7.455
7.322
7.309
7.260
7.200
7.187
4.545
4.532
4.521
3.697
3.684
3.510
3.500
3.480
2.346
1.566
0.000


O
CN
Ph
Me

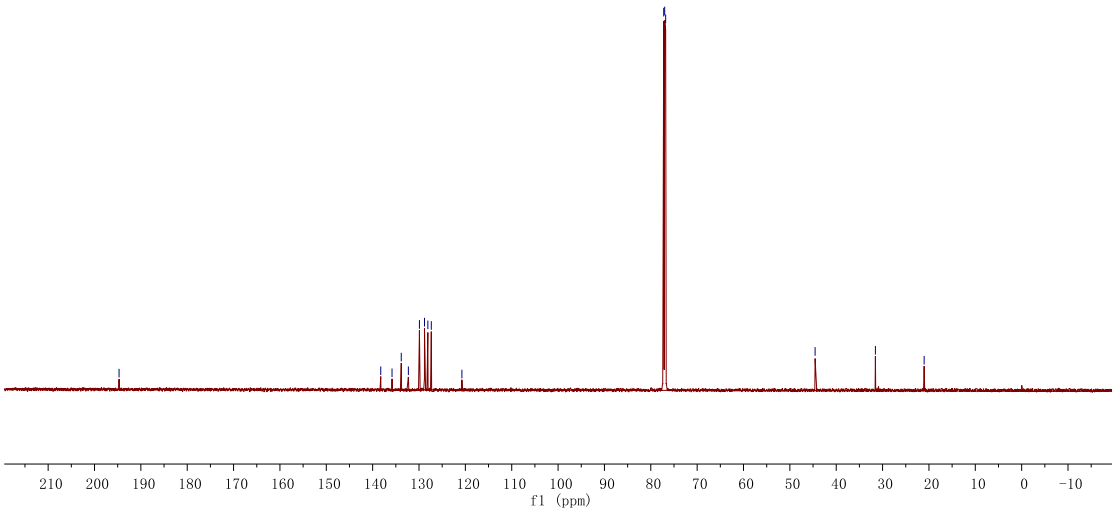
5k


1.95
1.01
1.99
2.01
1.96
1.00
1.07
1.12
3.07
f1 (ppm)

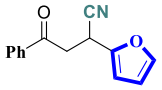

TJ-13C
TJ-1020
194.704
138.250
135.819
133.830
132.294
129.907
128.815
128.091
127.351
120.749
77.214
77.003
76.791
44.556
31.548
21.034

O
CN
Ph
Me

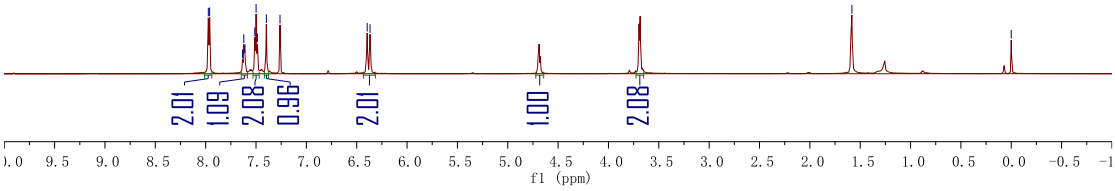
5k


f1 (ppm)

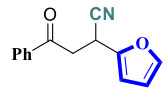

TJ-1H
7.964
7.960
7.633
7.621
7.609
7.512
7.499
7.487
7.397
7.262
6.396
6.368
1.583
0.000


O
CN
Ph
O

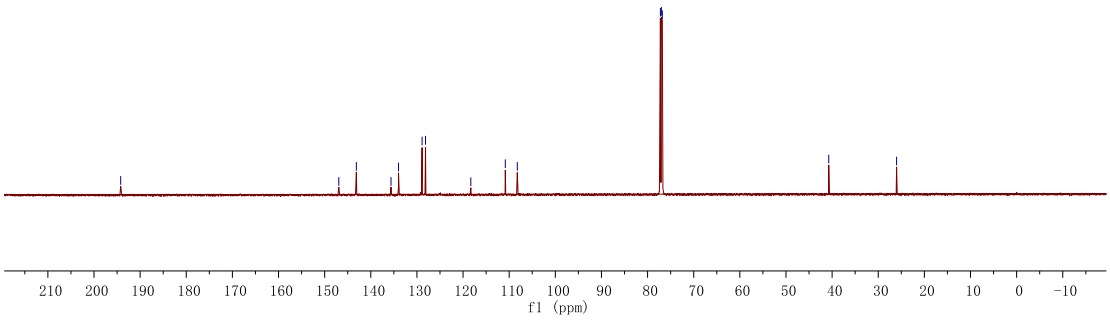
5l

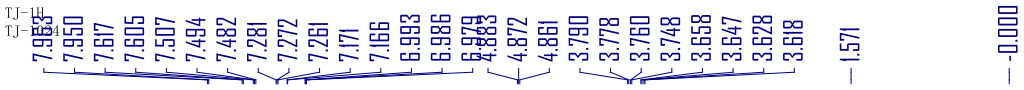

2.01
1.09
2.08
0.96
2.01
1.00
2.08
f1 (ppm)

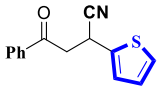

TJ-13C
TJ-1023
194.216
146.935
143.133
135.621
133.988
128.882
128.141
118.315
110.844
108.242
77.223
77.011
76.799
40.729
26.021


O
CN
Ph
O

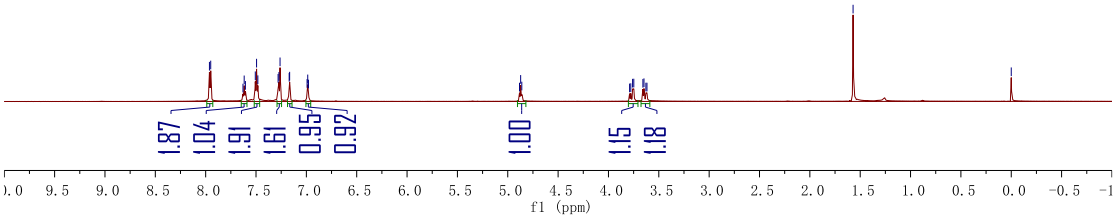
5l


f1 (ppm)

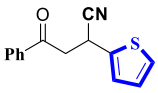

TJ-1H
TJ-1024
7.963
7.950
7.617
7.605
7.507
7.494
7.482
7.281
7.272
7.261
7.171
7.166
6.993
6.986
4.872
4.861
3.790
3.778
3.760
3.748
3.658
3.647
3.628
3.618
1.571
0.000


O
CN
Ph
S

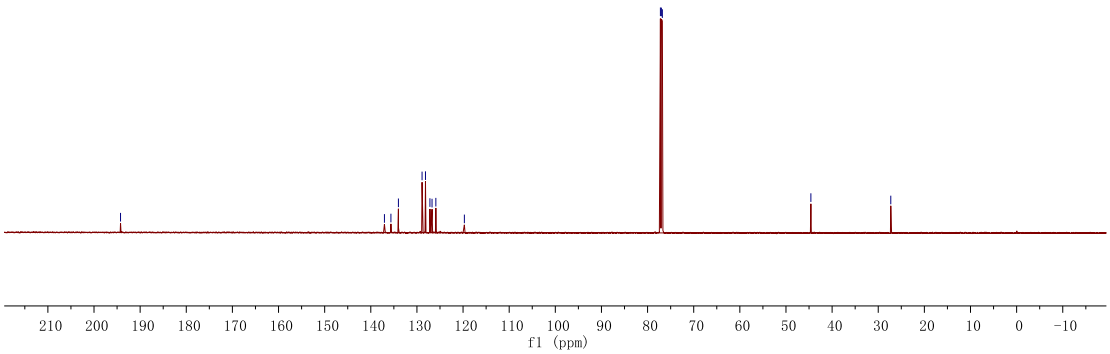
5m


1.87
1.04
1.91
1.61
0.95
0.92
1.00
1.15
1.18
f1 (ppm)

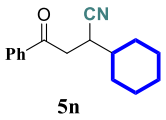

TJ-13C
TJ-1024
194.251
137.043
135.638
134.012
128.888
128.147
127.182
126.726
125.897
119.716
77.218
77.006
76.795
44.600
27.280


O
CN
Ph
S

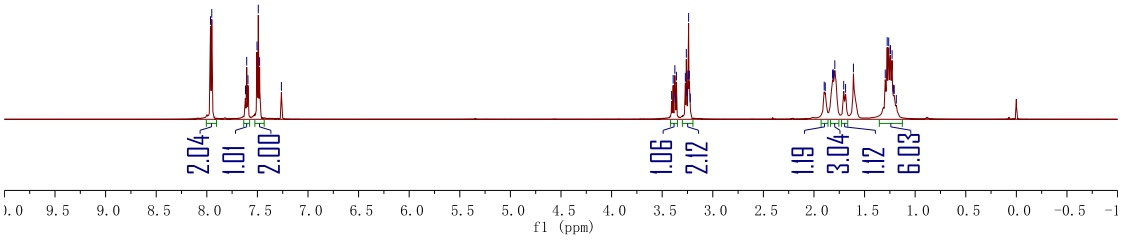
5m

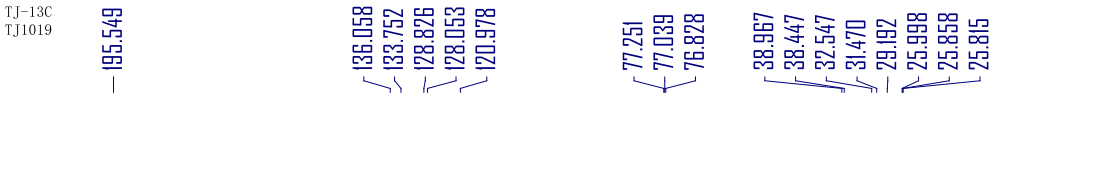

f1 (ppm)

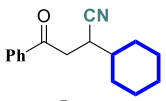

7.618
7.606
7.593
7.504
7.491
7.478
7.263
3.407
3.391
3.375
3.359
3.271
3.261
3.256
3.246
3.239
3.232
1.899
1.888
1.816
1.811
1.806
1.794
1.706
1.688
1.610
1.296
1.277
1.261
1.247
1.244
1.228
1.213
1.207


O
CN
Ph

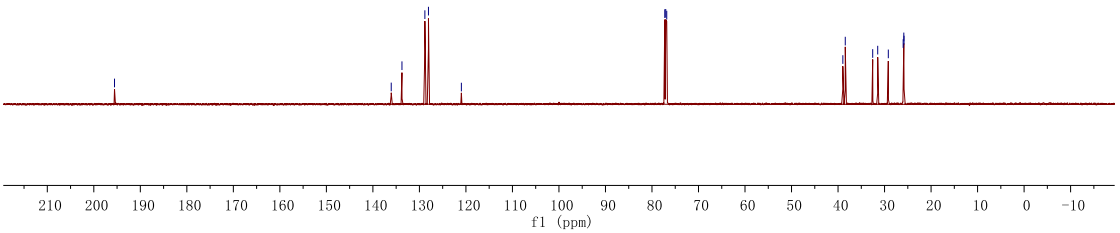
5n


2.04
1.01
2.00
1.06
2.12
1.19
3.04
1.12
6.03
f1 (ppm)

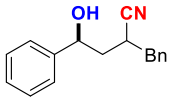

TJ-13C
TJ1019
195.549
136.058
133.752
128.826
128.053
120.978
77.251
77.039
76.828
38.967
38.447
32.547
31.470
29.192
25.998
25.858
25.815


O
CN
Ph

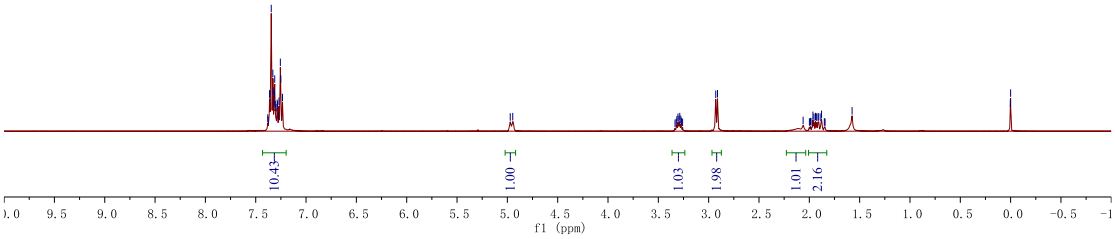
5n


f1 (ppm)

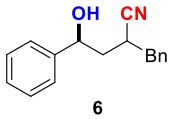
TJ-1060



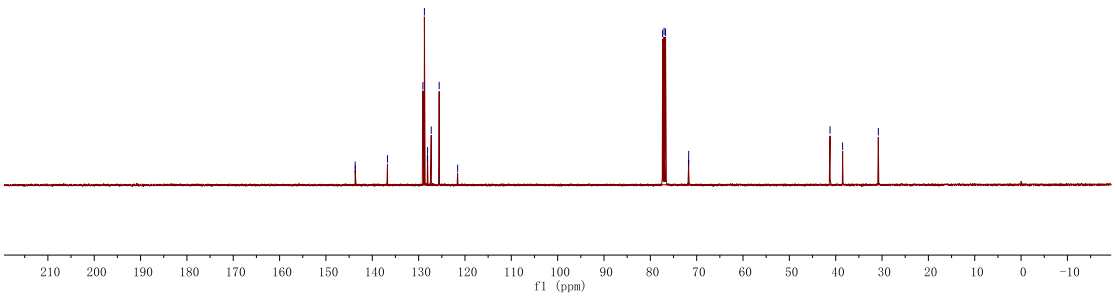
6

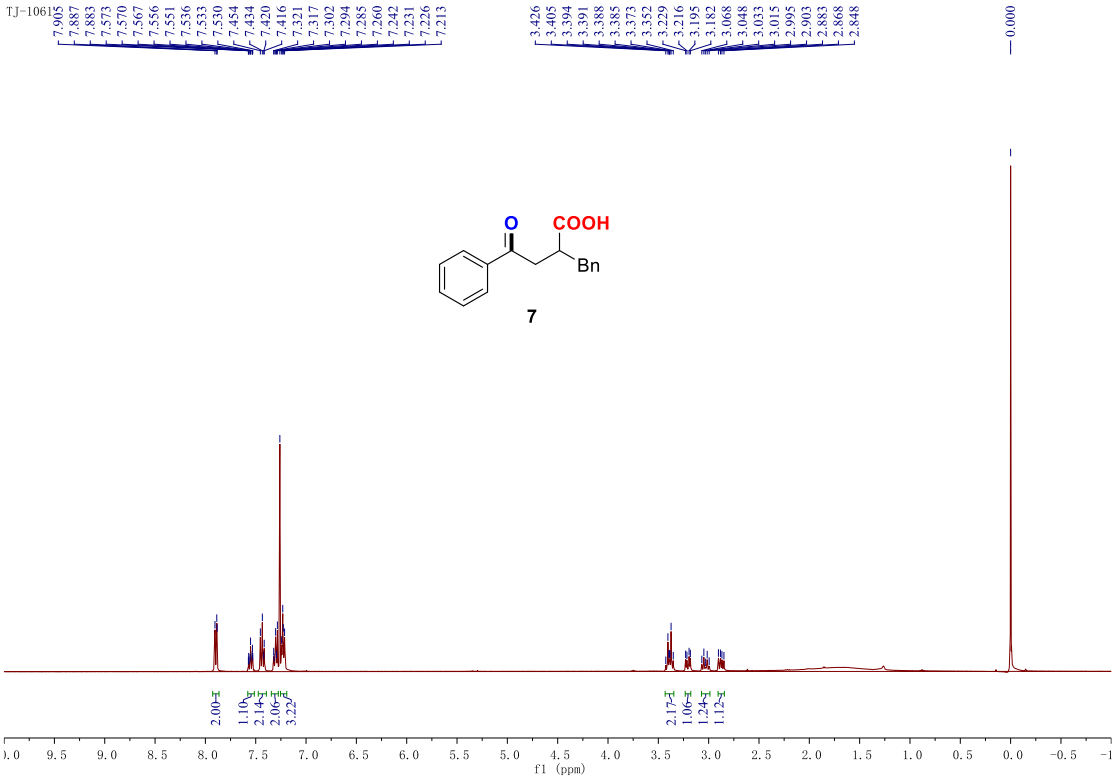


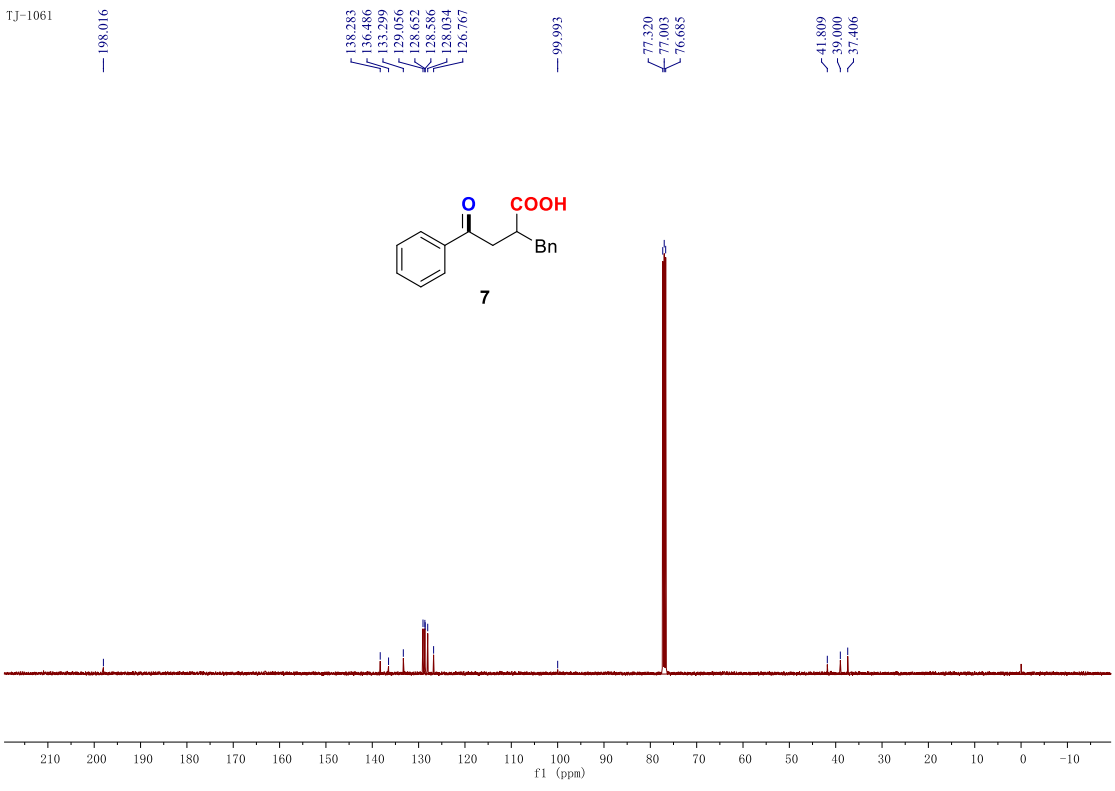
TJ-1060



6




TJ-1061
7.905
7.887
7.883
7.573
7.570
7.567
7.556
7.551
7.536
7.533
7.530
7.454
7.434
7.420
7.416
7.321
7.317
7.302
7.294
7.285
7.260
7.242
7.231
7.226
7.213
3.426
3.405
3.394
3.391
3.388
3.385
3.373
3.352
3.229
3.216
3.195
3.182
3.068
3.048
3.033
3.015
2.995
2.903
2.883
2.868
2.848
0.000
O
COOH
Bn
7
2.00
1.10
2.14
2.06
3.22
2.17
1.06
1.24
1.12
f1 (ppm)


TJ-1061
198.016
138.283
136.486
133.299
129.056
128.652
128.586
128.034
126.767
99.993
77.320
77.003
76.685
41.809
39.000
37.406
O
COOH
Bn
7
f1 (ppm)