

Supplementary information

Oxidative Coupling of Alkenes with Amides Using Peroxides: Selective Amide C(sp³)-H versus C(sp²)-H Functionalization

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(A) Typical experimental procedure

(a) Typical Experimental Procedure for the Synthesis of β -Amino Ketones (3):

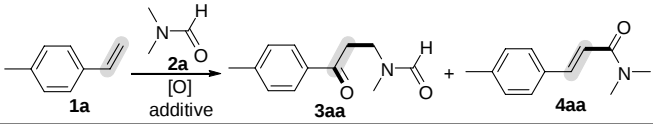
To a Schlenk tube were added alkenes **1** (0.4 mmol), amides **2** (4.0 mmol) TBHP (0.8 mmol, 5 M in decane), ^tBuOK (10 mol%), and CH₃CN (2 mL). Then the tube was charged with argon, and was stirred at 100 °C (oil bath temperature) for the indicated time until complete consumption of starting material as monitored by TLC and/or GC-MS analysis. After the reaction was finished, the reaction mixture was washed with brine. The aqueous phase was re-extracted with ethyl acetate. The combined organic extracts were dried over Na₂SO₄, concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **3**.

(b) Typical Experimental Procedure for the Synthesis of α,β -Unsaturated Amides (4):

To a Schlenk tube were added alkenes **1** (0.4 mmol), formylamides **2** (2 mL), FeCl₃ (30 mol%), DABCO (30 mol%) and DTBP (5 equiv). Then the tube was charged with argon, and was stirred at 110 °C (oil bath temperature) for 48 h until complete consumption of starting material as monitored by TLC and GC-MS analysis. After the reaction was finished, the reaction mixture was cooled to room temperature, diluted in diethyl ether, and washed with brine. The aqueous phase was re-extracted with diethyl ether. The combined organic extracts were dried over Na₂SO₄ and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **4**.

(c) Table S1. Screening Optimal Conditions

Table S1. Screening Optimal Conditions^a



Entry	[O] [equiv]	Base [mol%]	Solvent	T [°C]	Isolated yield [%]	
					3aa	4aa
1	TBHP (2)	—	DMF	110	0	0
2	TBHP (2)	^t BuOK (5)	DMF	110	26	0
3	TBHP (2)	^t BuOK (10)	DMF	110	70	0
4	TBHP (2)	^t BuOK (20)	DMF	110	69	0
5	TBHP (2)	NaOH (10)	DMF	110	40	0
6	TBHP (2)	K ₂ CO ₃ (10)	DMF	110	65	0
7	TBHP (2)	DBU (10)	DMF	110	46	0
8	TBHP (2)	DABCO (10)	DMF	110	19	0
9 ^b	TBHP (2)	^t BuOK (10)	DMF	110	66	0
10	TAHP (2)	^t BuOK (10)	DMF	110	61	0
11	CHP (2)	^t BuOK (10)	DMF	110	28	0
12	DTBP (2)	^t BuOK (10)	DMF	110	trace	0
13	BPO (2)	^t BuOK (10)	DMF	110	trace	0
14	—	^t BuOK (10)	DMF	110	0	0
15	TBHP (2)	^t BuOK (10)	DMF	80	10	0
16	TBHP (2)	^t BuOK (10)	DMF	120	69	0
17 ^c	TBHP (2)	^t BuOK (10)	MeCN	110	70	0
18 ^c	TBHP (2)	^t BuOK (10)	toluene	100	26	0
19 ^c	TBHP (2)	^t BuOK (10)	1,4-dioxane	100	16	0
20 ^d	TBHP (2)	^t BuOK (10)	DMF	110	8	5
21 ^d	TBHP (2)	DABCO (10)	DMF	110	trace	9
22 ^d	DTBP (2)	DABCO (10)	DMF	110	0	43
23 ^d	DTBP (5)	DABCO (30)	DMF	110	0	85
24 ^e	DTBP (5)	DABCO (30)	DMF	110	0	56
25 ^f	DTBP (5)	DABCO (30)	DMF	110	0	19
24 ^g	DTBP (5)	DABCO (30)	DMF	110	0	53
25 ^h	DTBP (5)	DABCO (30)	DMF	110	0	trace
26 ⁱ	DTBP (5)	DABCO (30)	DMF	110	0	18

^a Reaction conditions: **1a** (0.4 mmol), **2a**, [O] (2 equiv), base and solvent (2 mL) for 24 h. TBHP (5 M in decane). ^b TBHP (70% in water).

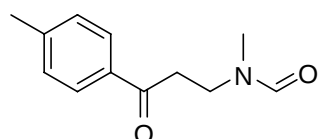
^c DMF (4 mmol) was added. ^d FeCl₃ (30 mol%) was added for 48 h. ^e

FeCl₂ (10 mol%) was added for 48 h. ^f FeCl₂ (60 mol%) was added for

48 h. ^g FeCl₂ (30 mol%) was added for 48 h. ^h Fe(Cp)₂ (30 mol%) was

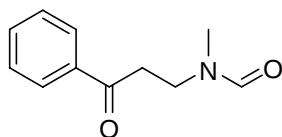
added for 48 h. ⁱ CuCl₂ (30 mol%) was added for 48 h.

(B) Analytical data



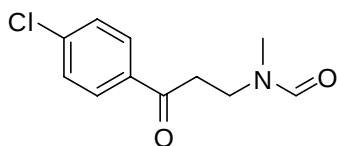
N-Methyl-N-(3-oxo-3-*p*-tolylpropyl)formamide (3aa):

Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 8.17 (s, 0.5H), 8.02 (s, 0.5H), 7.85 (t, $J = 8.4$ Hz, 2H), 7.26 (d, $J = 7.2$ Hz, 2H), 3.73 (s, 2H), 3.26 (t, $J = 6.4$ Hz, 1H), 3.20 (t, $J = 6.4$ Hz, 1H), 3.02 (s, 1.5H), 2.88 (s, 1.5H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 198.0, 196.8, 163.1, 162.8, 144.5, 144.2, 134.0, 133.8, 129.4, 129.3, 128.1, 128.0, 44.5, 40.5, 36.5, 36.0, 35.6, 21.6; IR (KBr, cm^{-1}): 1678, 1648; LRMS (EI, 70 eV) m/z (%): 205 (M^+ , 11), 177 (61), 119 (100); HRMS m/z (ESI) calcd for $\text{C}_{12}\text{H}_{16}\text{NO}_2$ ($[\text{M}+\text{H}]^+$) 206.1176, found 206.1184.



***N*-Methyl-*N*-(3-oxo-3-phenylpropyl)formamide (3ba):¹**

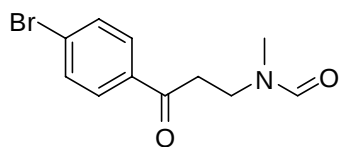
^1H NMR (400 MHz, CDCl_3) δ : 8.18 (s, 0.5H), 8.03 (s, 0.5H), 7.95 (t, $J = 8.4$ Hz, 2H), 7.59 (t, $J = 8.0$ Hz, 1H), 7.51-7.46 (m, 2H), 3.74 (t, $J = 6.4$ Hz, 2H), 3.30 (t, $J = 6.4$ Hz, 1H), 3.24 (t, $J = 6.4$ Hz, 1H), 3.04 (s, 1.5H), 2.89 (s, 1.5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 198.4, 197.2, 163.1, 162.8, 136.4, 136.3, 133.6, 133.4, 128.8, 128.7, 128.1, 127.9, 44.4, 40.5, 36.7, 36.2, 35.7.



***N*-(3-(4-Chlorophenyl)-3-oxopropyl)-*N*-methylformamide (3ca):**

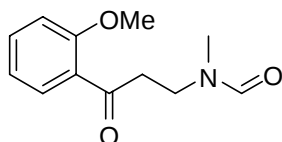
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 8.18 (s, 0.5H), 8.02 (s, 0.5H), 7.81 (t, $J = 8.0$ Hz, 2H), 7.62 (t, $J = 7.2$ Hz, 2H), 3.72 (t, $J = 5.6$ Hz, 2H), 3.26 (t, $J = 6.8$ Hz, 1H), 3.20 (t, $J = 6.4$ Hz, 1H), 3.04 (s, 1.5H), 2.83 (s, 1.5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 197.3, 196.1, 163.1, 162.8, 135.1, 135.0, 132.1, 132.0, 129.6, 129.4, 128.9, 128.6, 44.3, 40.5, 36.6, 36.1, 35.7; IR (KBr, cm^{-1}): 1672, 1643; LRMS (EI, 70 eV)

m/z (%): 227 ($M^+ + 2$, 2), 225 (M^+ , 7), 127 (26), 71 (100); HRMS m/z (ESI) calcd for $C_{11}H_{13}ClNO_2$ ($[M+H]^+$) 226.0629, found 226.0635.



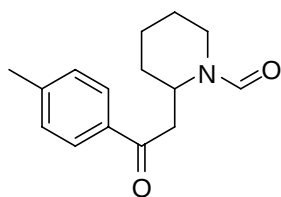
***N*-(3-(4-Bromophenyl)-3-oxopropyl)-*N*-methylformamide (3da):**

Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ : 8.18 (s, 0.5H), 8.02 (s, 0.5H), 7.81 (t, J = 8.4 Hz, 2H), 7.62 (t, J = 7.6 Hz, 2H), 3.72 (t, J = 5.6 Hz, 2H), 3.26 (t, J = 6.4 Hz, 1H), 3.20 (t, J = 6.4 Hz, 1H), 3.04 (s, 1.5H), 2.83 (s, 1.5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 197.3, 196.1, 163.1, 162.8, 135.1, 135.0, 132.1, 132.0, 129.6, 129.4, 128.9, 128.6, 44.3, 40.5, 36.6, 36.1, 35.7; IR (KBr, cm^{-1}): 1674, 1650; LRMS (EI, 70 eV) m/z (%): 271 ($M^+ + 2$, 3), 269 (M^+ , 3), 183 (35), 86 (100); HRMS m/z (ESI) calcd for $C_{11}H_{13}BrNO_2$ ($[M+H]^+$) 270.0124, found 270.0132.



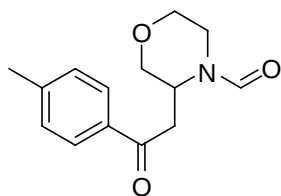
***N*-(3-(2-Methoxyphenyl)-3-oxopropyl)-*N*-methylformamide (3ea):**

Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ : 8.13 (s, 0.6H), 8.01 (s, 0.4H), 7.71 (d, J = 4.0 Hz, 1H), 7.52-7.46 (m, 1H), 7.04-6.96 (m, 2H), 3.93 (s, 3H), 3.91-3.65 (m, 2H), 3.29-3.23 (m, 2H), 3.01 (s, 1H), 2.87 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 200.2, 199.2, 163.1, 162.7, 158.7, 134.2, 133.9, 130.4, 130.3, 127.5, 127.2, 120.8, 120.6, 111.5, 55.5, 55.4, 44.8, 42.1, 41.3, 40.2, 35.4; IR (KBr, cm^{-1}): 1671, 1642; LRMS (EI, 70 eV) m/z (%): 221 (M^+ , 4), 162 (38), 135 (100); HRMS m/z (ESI) calcd for $C_{12}H_{16}NO_3$ ($[M+H]^+$) 222.1125, found 222.1136.



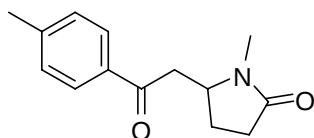
2-(2-Oxo-2-*p*-Tolylethyl)piperidine-1-carbaldehyde (3ab):

Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 8.14 (s, 0.4H), 8.00 (s, 0.6H), 7.90 (d, $J = 7.6$ Hz, 0.4H), 7.84 (d, $J = 7.6$ Hz, 0.6H), 7.27 (d, $J = 5.6$ Hz, 2H), 7.18-7.09 (m, 1H), 3.48-3.39 (m, 2H), 3.31-3.25 (m, 2H), 3.18-3.12 (m, 1H), 2.42 (s, 2H), 2.34 (s, 1H), 1.79-1.68 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ : 197.2, 196.6, 161.5, 160.7, 144.3, 144.0, 134.0, 133.9, 129.3, 129.2, 128.3, 128.0, 50.1, 46.7, 40.5, 26.4, 24.9, 24.6, 21.5; IR (KBr, cm^{-1}): 1679, 1652; LRMS (EI, 70 eV) m/z (%): 245 (M^+ , 21), 217 (41), 126 (100); HRMS m/z (ESI) calcd for $\text{C}_{15}\text{H}_{20}\text{NO}_2$ ($[\text{M}+\text{H}]^+$) 246.1494, found 246.1498.



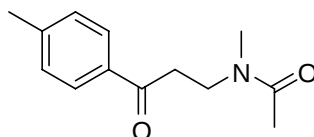
3-(2-Oxo-2-*p*-Tolylethyl)morpholine-4-carbaldehyde (3ac):

Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 8.22 (s, 0.5H), 8.03 (s, 0.5H), 7.84 (d, $J = 7.6$ Hz, 2H), 7.27 (d, $J = 6.8$ Hz, 2H), 4.29-4.14 (m, 1H), 3.98-3.87 (m, 2H), 3.70-3.38 (m, 5H), 3.10-2.97 (m, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 196.8, 196.5, 161.6, 161.1, 144.6, 144.2, 134.1, 133.9, 129.4, 129.3, 128.1, 128.0, 70.5, 66.7, 50.2, 50.0, 37.9, 36.9, 36.6, 21.6; IR (KBr, cm^{-1}): 1680, 1647; LRMS (EI, 70 eV) m/z (%): 247 (M^+ , 3), 119 (100), 113 (35); HRMS m/z (ESI) calcd for $\text{C}_{14}\text{H}_{18}\text{NO}_3$ ($[\text{M}+\text{H}]^+$) 248.1287, found 248.1295.



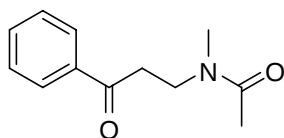
1-Methyl-5-(2-oxo-2-*p*-tolylethyl)pyrrolidin-2-one (3ad):

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.85 (d, $J = 4.0$ Hz, 2H), 7.28 (t, $J = 9.6$ Hz, 2H), 4.17 (s, 1H), 3.41-3.36 (m, 1H), 3.04 (t, $J = 8.4$ Hz, 1H), 2.82 (s, 3H), 2.43 (s, 3H), 2.41-2.35 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ : 197.9, 196.9, 175.1, 174.8, 144.4, 144.0, 133.9, 133.8, 129.3, 129.1, 128.0, 127.9, 56.2, 41.8, 29.5, 27.8, 24.8, 21.4; IR (KBr, cm^{-1}): 1679, 1642; LRMS (EI, 70 eV) m/z (%): 231 (M^+ , 12), 146 (13), 112 (100); HRMS m/z (ESI) calcd for $\text{C}_{14}\text{H}_{18}\text{NO}_2$ ($[\text{M}+\text{H}]^+$) 232.1332, found 232.1341.



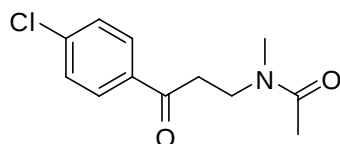
***N*-Methyl-*N*-(3-oxo-3-*p*-tolylpropyl)acetamide (3ae):**

Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.85 (t, $J = 7.2$ Hz, 2H), 7.26 (t, $J = 9.2$ Hz, 2H), 3.77-3.71 (m, 2H), 3.24 (t, $J = 6.4$ Hz, 2H), 3.06 (s, 2H), 2.94 (s, 1H), 2.39 (s, 3H), 2.15 (s, 1H), 2.05 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ : 198.2, 197.0, 170.5, 170.2, 144.1, 143.7, 133.8, 133.5, 129.1, 128.9, 127.8, 127.7, 45.5, 43.9, 37.0, 36.3, 36.2, 32.7, 21.5, 21.2 (2), 20.9; IR (KBr, cm^{-1}): 1675, 1645; LRMS (EI, 70 eV) m/z (%): 219 (M^+ , 21), 119 (100), 100 (62); HRMS m/z (ESI) calcd for $\text{C}_{13}\text{H}_{18}\text{NO}_2$ ($[\text{M}+\text{H}]^+$) 220.1332, found 220.1342.



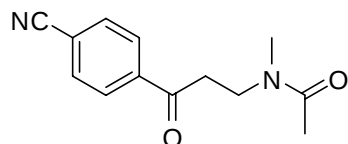
***N*-Methyl-*N*-(3-oxo-3-phenylpropyl)acetamide (3be):²**

¹H NMR (400 MHz, CDCl₃) δ: 7.97 (t, *J* = 8.8 Hz, 2H), 7.57 (t, *J* = 9.2 Hz, 1H), 7.52-7.45 (m, 2H), 3.78-3.73 (m, 2H), 3.31-3.26 (m, 2H), 3.08 (s, 2H), 2.95 (s, 1H), 2.16 (s, 1H), 2.07 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ: 199.1, 197.6, 170.9, 136.6, 136.3, 133.6, 133.3, 128.8, 128.6, 128.1, 127.9, 45.8, 44.3, 37.6, 36.8, 33.2, 21.9, 21.2.



***N*-(3-(4-Chlorophenyl)-3-oxopropyl)-*N*-methylacetamide (3ce):**

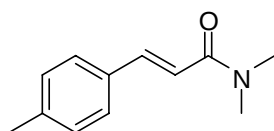
Colorless oil; ¹H NMR (400 MHz, CDCl₃) δ: 7.91 (t, *J* = 8.8 Hz, 2H), 7.45 (t, *J* = 10.0 Hz, 2H), 3.77-3.71 (m, 2H), 3.28-3.23 (m, 2H), 3.09 (s, 2.2H), 2.95 (s, 0.8H), 2.16 (s, 0.8H), 2.07 (s, 2.2H); ¹³C NMR (100 MHz, CDCl₃) δ: 197.8, 196.3, 170.9, 170.5, 140.1, 139.7, 134.8, 134.5, 129.5, 129.3, 129.1, 128.9, 45.6, 44.3, 37.5, 36.7, 33.2, 21.9, 21.2; IR (KBr, cm⁻¹): 1673, 1647; LRMS (EI, 70 eV) *m/z* (%): 241 (M⁺+2, 5), 239 (M⁺, 15), 196 (62), 58 (100); HRMS *m/z* (ESI) calcd for C₁₂H₁₅ClNO₂ ([M+H]⁺) 240.0785, found 240.0791.



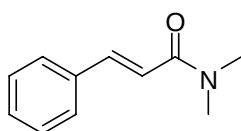
***N*-(3-(4-Cyanophenyl)-3-oxopropyl)-*N*-methylacetamide (3ge):**

Colorless oil; ¹H NMR (400 MHz, CDCl₃) δ: 8.07 (t, *J* = 8.4 Hz, 2H), 7.82-7.74 (m, 2H), 3.82-3.72 (m, 2H), 3.33-3.28 (m, 2H), 3.11 (s, 2.5H), 2.95 (s, 0.5H), 2.17 (s,

0.5H), 2.08 (s, 2.5H); ^{13}C NMR (100 MHz, CDCl_3) δ : 197.6, 171.0, 139.4, 132.7, 132.5, 128.5, 128.3, 117.8, 116.5, 45.4, 44.2, 37.6, 37.1, 21.9; IR (KBr, cm^{-1}): 1671, 1640; LRMS (EI, 70 eV) m/z (%): 230 (M^+ , 3), 134 (100), 109 (73); HRMS m/z (ESI) calcd for $\text{C}_{13}\text{H}_{15}\text{N}_2\text{O}_2$ ($[\text{M}+\text{H}]^+$) 231.1128, found 231.1139.

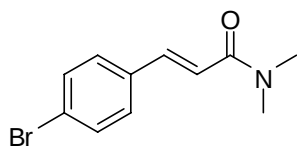


(E)-N,N-Dimethyl-3-p-tolylacrylamide (4aa): White solid; mp 99-102 °C; ^1H NMR (500 MHz) δ : 7.57 (d, J = 8.0 Hz, 2H), 7.41 (d, J = 15.5 Hz, 1H), 7.20 (d, J = 8.0 Hz, 2H), 7.12 (d, J = 15.0 Hz, 1H), 3.14(s, 3H), 2.92 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (125 MHz) δ : 166.3, 141.5, 139.8, 132.9, 129.9, 128.5, 117.9, 37.4, 35.9, 21.5; IR (KBr, cm^{-1}): 3060, 1654, 1601, 1397; LRMS (EI, 70 eV) m/z (%): 189 (M^+ , 40), 188(16), 115 (40), 145 (100); HRMS (EI) for $\text{C}_{12}\text{H}_{16}\text{NO}$ (M^++H): calcd. 190.1226, found. 190.1225.



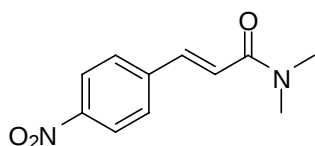
(E)-N,N-Dimethylcinnamamide (4ba):

White solid; mp 86-89 °C; ^1H NMR (500 MHz) δ : 7.65 (d, J = 15.5 Hz, 1H), 7.50 (d, J = 7.5 Hz, 2H), 7.35-7.31 (m, 3H), 6.66 (d, J = 15.5 Hz, 1H), 3.09(s, 6H); ^{13}C NMR (125 MHz) δ : 166.6, 142.3, 135.2, 129.4, 128.6, 127.6, 117.3, 36.5; IR (KBr, cm^{-1}): 3076, 1732, 1654, 1563; LRMS (EI, 70 eV) m/z (%): 175 (M^+ , 41), 174(20), 131 (100), 103 (70); HRMS (EI) for $\text{C}_{11}\text{H}_{14}\text{NO}$ (M^++H): calcd. 176.1070, found. 176.1078.



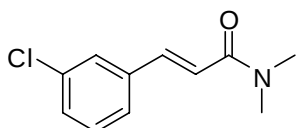
(E)-3-(4-Bromophenyl)-N,N-dimethylacrylamide (4ca):

White solid; mp 120-125 °C; ^1H NMR (500 MHz) δ : 7.66 (d, J = 8.0 Hz, 2H), 7.58 (d, J = 8.5 Hz, 2H), 7.41 (d, J = 15.5 Hz, 1H), 7.23 (d, J = 15.5 Hz, 1H), 3.14 (s, 3H), 2.92 (s, 3H); ^{13}C NMR (125 MHz) δ : 165.9, 140.2, 135.0, 132.4, 130.6, 123.2, 120.0, 37.4, 35.9; IR (KBr, cm^{-1}): 3064, 1654, 1393, 1262; LRMS (EI, 70 eV) m/z (%): 255 ($\text{M}^+ + 2$, 35), 253 (M^+ , 36), 102 (100), 209 (65); HRMS (EI) for $\text{C}_{11}\text{H}_{13}^{79}\text{BrNO}$ ($\text{M}^+ + \text{H}$): calcd. 254.0175, found. 254.0173.



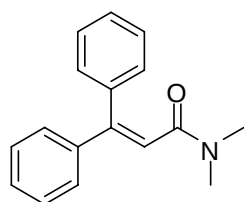
(E)-N,N-Dimethyl-3-(4-nitrophenyl)acrylamide (4ha):

Yellow solid; mp 148-153 °C; ^1H NMR (500 MHz) δ : 8.22 (d, J = 8.0 Hz, 2H), 7.98 (d, J = 8.0 Hz, 2H), 7.53 (d, J = 15.5 Hz, 1H), 7.41 (d, J = 15.5 Hz, 1H), 3.17 (s, 3H), 2.94 (s, 3H); ^{13}C NMR (125 MHz) δ : 165.5, 148.0, 142.3, 138.8, 129.5, 124.3, 123.7, 37.4, 35.9; IR (KBr, cm^{-1}): 3062, 1654, 1397, 1143; LRMS (EI, 70 eV) m/z (%): 220 (M^+ , 26), 219 (15), 118 (41), 146 (100); HRMS (EI) for $\text{C}_{11}\text{H}_{13}\text{N}_2\text{O}_3$ ($\text{M}^+ + \text{H}$): calcd. 221.0921, found. 221.0919.



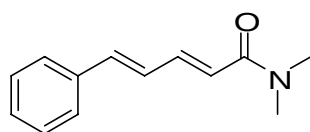
(E)-3-(3-Chlorophenyl)-N,N-dimethylacrylamide (4ia):

White solid; mp 70-75 °C; ^1H NMR (500 MHz) δ : 7.85 (s, 1H), 7.63 (t, J = 8.5 Hz, 1H), 7.43-7.40 (m, 3H), 7.27 (d, J = 15.5 Hz, 1H), 3.15 (s, 3H), 2.92 (s, 3H); ^{13}C NMR (125 MHz) δ : 165.9, 139.9, 138.0, 134.2, 131.1, 129.7, 120.9, 37.5, 35.9; IR (KBr, cm^{-1}): 3060, 1654, 1397, 1143; LRMS (EI, 70 eV) m/z (%): 211 ($\text{M}^+ + 2$, 13), 209 (M^+ , 40), 165 (100), 102 (43); HRMS (EI) for $\text{C}_{11}\text{H}_{13}\text{ClNO}$ ($\text{M}^+ + \text{H}$): calcd. 210.0680, found. 210.0684.



N,N-Dimethyl-3,3-diphenylacrylamide (4ja):

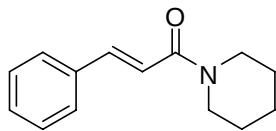
White solid; mp 63-68 °C; ^1H NMR (500 MHz) δ : 7.26-7.18 (m, 10H), 6.28 (s, 1H), 2.72 (s, 6H); ^{13}C NMR (125 MHz) δ : 168.5, 147.5, 141.1, 138.9, 129.3, 128.5, 128.3, 128.3, 128.1, 121.2, 31.2, 27.9; IR (KBr, cm^{-1}): 3060, 1663, 1436, 1115; LRMS (EI, 70 eV) m/z (%): 251 (M^+ , 25), 178 (65), 105 (29), 207 (100); HRMS (EI) for $\text{C}_{17}\text{H}_{18}\text{NO}$ ($\text{M}^+ + \text{H}$): calcd. 252.1383, found. 252.1392.



(2E,4E)-N,N-Dimethyl-5-phenylpenta-2,4-dienamide (4ka):

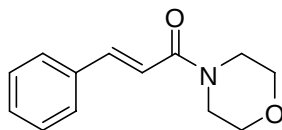
White solid; ^1H NMR (500 MHz) δ : 7.77-7.71 (m, 1H), 7.47 (d, J = 7.0 Hz, 2H), 7.31-7.22 (m, 3H), 6.71 (d, J = 15.5 Hz, 1H), 6.56 (t, J = 22.5 Hz, 1H), 6.03 (d, J = 11.5 Hz, 1H), 3.05 (s, 6H); ^{13}C NMR (125 MHz) δ : 162.8, 139.3, 138.5, 136.6, 128.5, 128.3, 127.2, 125.3, 119.7, 32.9, LRMS (EI, 70 eV) m/z (%): 201 (M^+ , 60), 157 (100),

128 (87), 115 (14); HRMS (EI) for $C_{13}H_{16}NO$ ($M^+ + H$): calcd. 202.1227, found. 202.1235.



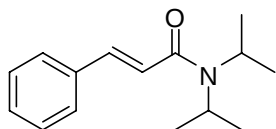
(E)-3-phenyl-1-(piperidin-1-yl)prop-2-en-1-one (4bb):

White solid; mp 113-119 °C; 1H NMR (500 MHz) δ : 7.63 (d, $J = 15.5$ Hz, 1H), 7.51 (d, $J = 7.0$ Hz, 2H), 7.37-7.31 (m, 3H), 6.89 (d, $J = 15.5$ Hz, 1H), 3.62 (s, 4H), 1.68 (d, $J = 5.0$ Hz, 2H), 1.61 (d, $J = 4.0$ Hz, 4H); ^{13}C NMR (125 MHz) δ : 165.3, 142.1, 135.4, 129.3, 128.7, 127.6, 117.7, 49.3, 47.0, 43.3, 33.6, 25.4, 24.8, 24.6; IR (KBr, cm^{-1}): 3060, 1646, 1432, 1256; LRMS (EI, 70 eV) m/z (%): 215 (M^+ , 57), 103 (67), 131 (100), 77 (38); HRMS (EI) for $C_{14}H_{18}NO$ ($M^+ + H$): calcd. 216.1383, found. 216.1382.



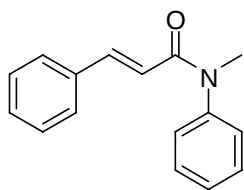
(E)-1-Morpholino-3-phenylprop-2-en-1-one (4bc):

White solid; mp 141-143 °C; 1H NMR (500 MHz) δ : 7.69 (d, $J = 15.5$ Hz, 1H), 7.51 (t, $J = 8.0$ Hz, 2H), 7.38-7.34 (m, 3H), 6.84 (d, $J = 17.5$ Hz, 1H), 3.71 (s, 8H); ^{13}C NMR (125 MHz) δ : 165.5, 143.1, 135.0, 129.7, 128.7, 127.7, 116.4, 66.8; IR (KBr, cm^{-1}): 3080, 1650, 1429, 1115; LRMS (EI, 70 eV) m/z (%): 217 (M^+ , 23), 131 (100), 103 (45), 77 (25), 56 (10); HRMS (EI) for $C_{13}H_{16}NO_2$ ($M^+ + H$): calcd. 218.1176, found. 218.1177.

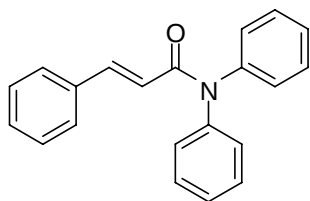


(E)-N,N-Diisopropylcinnamamide (4bg):

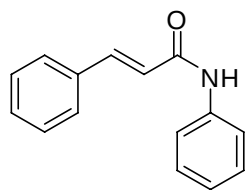
White solid; mp 72-76 °C; ^1H NMR (500 MHz) δ : 7.61 (d, J = 15.5 Hz, 1H), 7.50 (d, J = 2.5 Hz, 2H), 7.37-7.31 (m, 3H), 6.82 (d, J = 15.5 Hz, 1H), 4.03 (d, J = 15.0 Hz, 2H), 1.36 (s, 12H); ^{13}C NMR (125 MHz) δ : 166.2, 141.0, 135.6, 129.2, 128.7, 127.5, 120.4, 48.1, 45.9, 21.6, 20.6; IR (KBr, cm^{-1}): 3060, 1652, 1489, 1238; LRMS (EI, 70 eV) m/z (%): 231 (M^+ , 14), 103 (30), 131 (100), 86 (20); HRMS (EI) for $\text{C}_{15}\text{H}_{22}\text{NO}$ ($\text{M}^+ + \text{H}$): calcd. 232.1696, found. 232.1690.



(E)-N-Methyl-N-phenylcinnamamide (4bh): White solid; mp 78-81 °C; ^1H NMR (500 MHz) δ : 7.69 (d, J = 16.0 Hz, 1H), 7.86 (t, J = 15.5 Hz, 2H), 7.37 (t, J = 14.5 Hz, 1H), 7.31-7.26 (m, 5H), 7.23 (d, J = 8.0 Hz, 2H), 6.37 (d, J = 15.5 Hz, 1H), 3.42 (s, 3H); ^{13}C NMR (125 MHz) δ : 166.1, 143.6, 141.7, 135.1, 129.6, 129.5, 128.6, 127.8, 127.5, 127.2, 118.6, 37.5; IR (KBr, cm^{-1}): 3060, 1658, 1495, 1123; LRMS (EI, 70 eV) m/z (%): 237 (M^+ , 16), 107 (64), 131 (100); HRMS (EI) for $\text{C}_{16}\text{H}_{16}\text{NO}$ ($\text{M}^+ + \text{H}$): calcd. 238.1226, found. 238.1224.



(E)-N,N-Diphenylcinnamamide (4bi): White solid; mp 153-158 °C; ^1H NMR (500 MHz) δ : 7.78 (d, J = 15.5 Hz, 1H), 7.40-7.26 (m, 15H), 6.49 (d, J = 15.5 Hz, 1H); ^{13}C NMR (125 MHz) δ : 166.1, 142.7, 142.6, 135.0, 129.7, 129.3, 128.7, 127.9, 119.7; IR (KBr, cm^{-1}): 3075, 1662, 1489, 1258; LRMS (EI, 70 eV) m/z (%): 299 (M^+ , 18), 169 (84), 131 (100), 103 (49), 77 (24); HRMS (EI) for $\text{C}_{21}\text{H}_{18}\text{NO}$ ($\text{M}^+\text{+H}$): calcd. 300.1383, found. 300.1399.



(E)-N-Methyl-N-phenylcinnamamide (4bj):

White solid; mp 148-151 °C; ^1H NMR (500 MHz) δ : 7.83 (brs, 1H), 7.76 (t, J = 15.0 Hz, 1H), 7.64 (s, 2H), 7.48 (s, 2H), 7.34 (t, J = 6.5 Hz, 5H), 7.12 (s, 1H), 6.61 (d, J = 15.5 Hz, 1H); ^{13}C NMR (125 MHz) δ : 164.2, 142.3, 138.1, 134.5, 129.9, 129.0, 128.8, 128.0, 124.4, 120.8, 120.0; IR (KBr, cm^{-1}): 3023, 1662, 1597, 1544; LRMS (EI, 70 eV) m/z (%): 223 (M^+ , 21), 131 (100), 103 (47), 77 (28); HRMS (EI) for $\text{C}_{15}\text{H}_{14}\text{NO}$ ($\text{M}^+\text{+H}$): calcd. 224.1070, found. 224.1066.

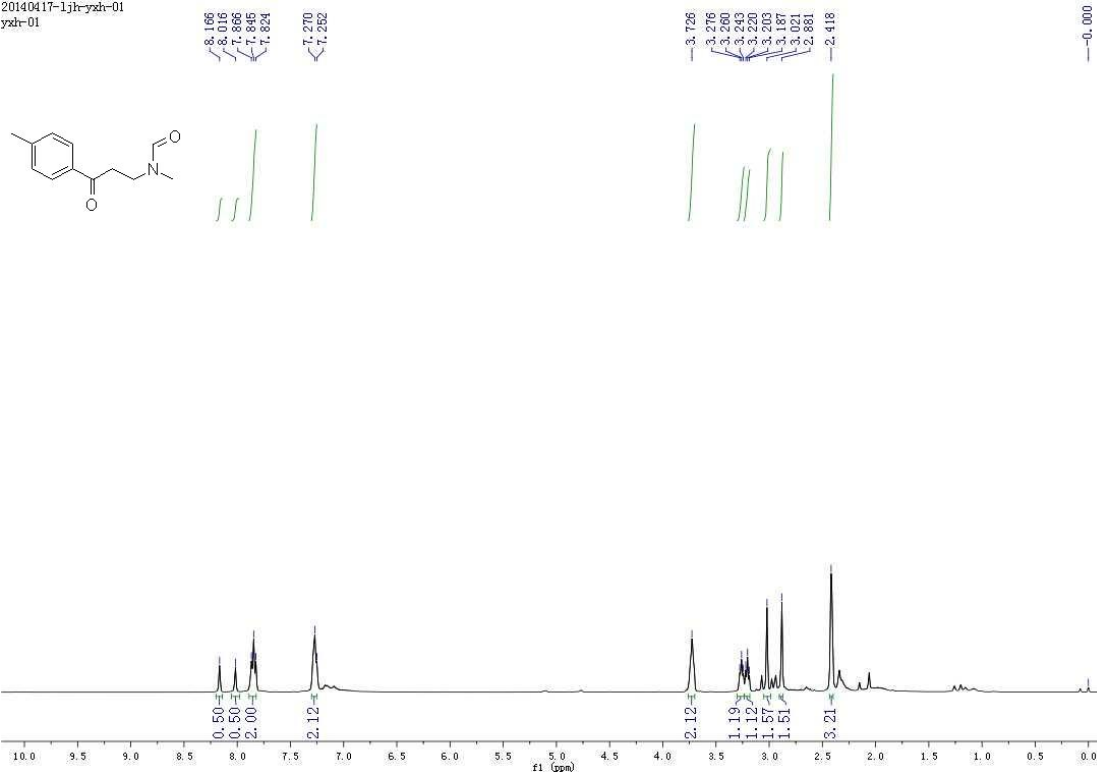
(C) References

- (1) A. T. Soldatenkov, A. V. Temesgen and I. A. Bekro, *Chemistry of Heterocyclic Compounds*, 2001, **37**, 1216.
- (2) I. Kiyoshi, T. Yoshiyasu and S. Minoru, *Chem. Pharm. Bull.* 1981, **29**, 1156.

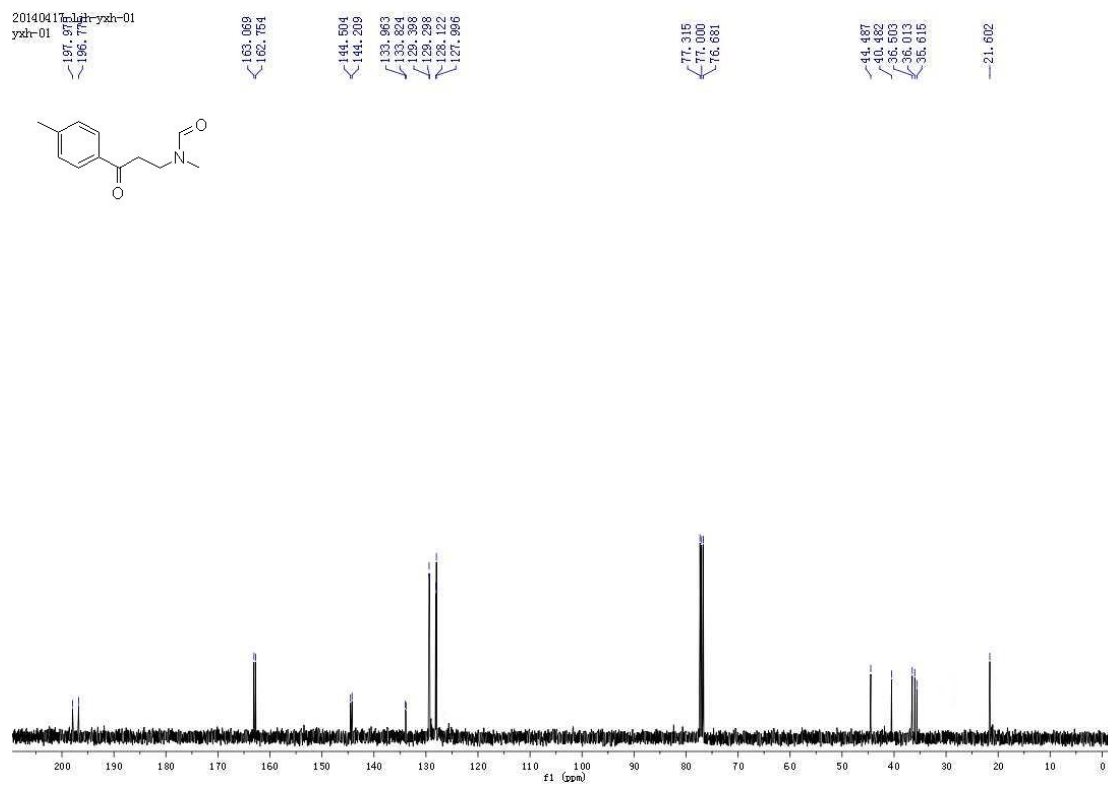
(D) Spectra

N-Methyl-*N*-(3-oxo-3-*p*-tolylpropyl)formamide (**3aa**)

20140417-1jht-yzh-01
yzh-01

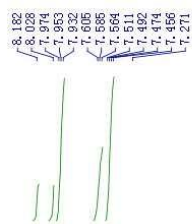
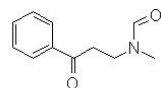


20140417-1jht-yzh-01
yzh-01

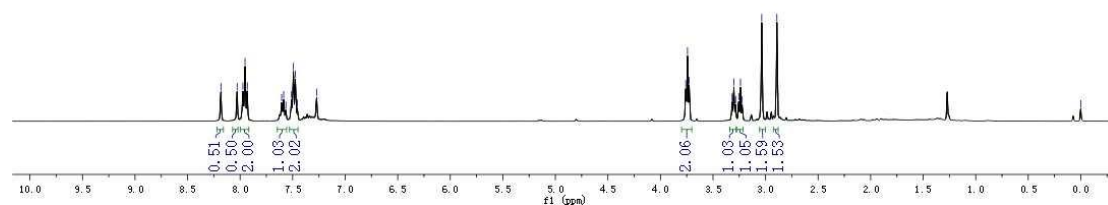


N-Methyl-*N*-(3-oxo-3-phenylpropyl)formamide (**3ba**)

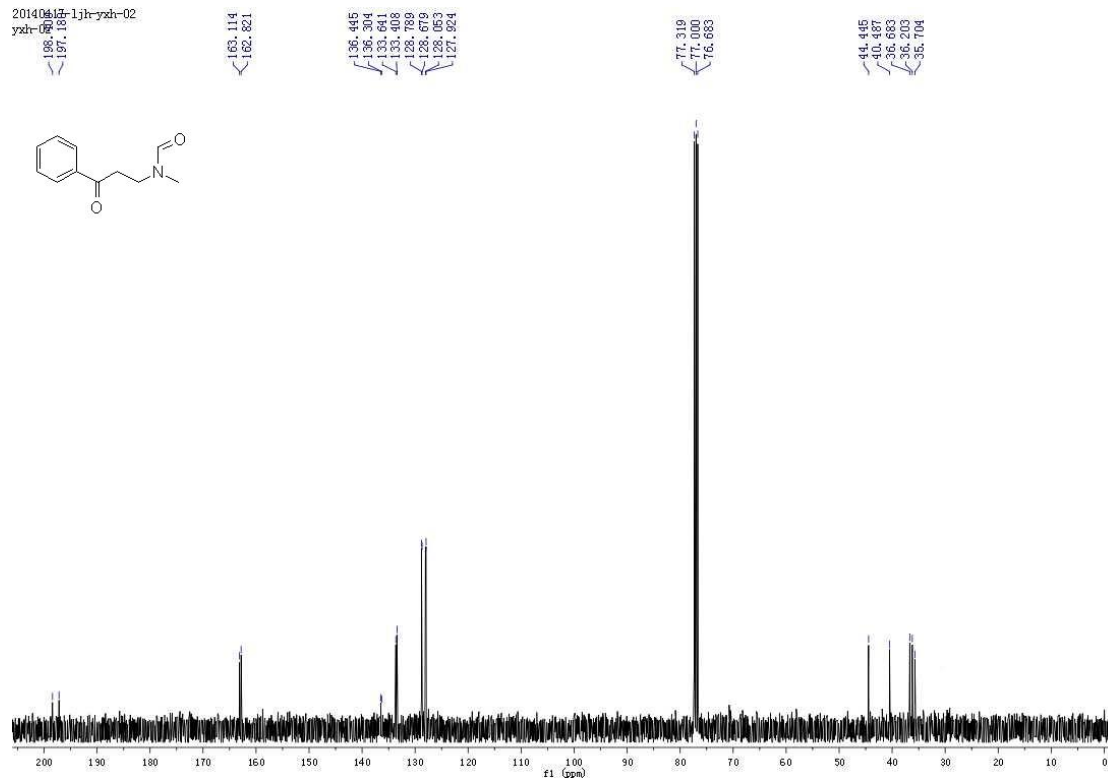
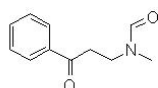
20140417-1jh-yzh-02
yzh-02



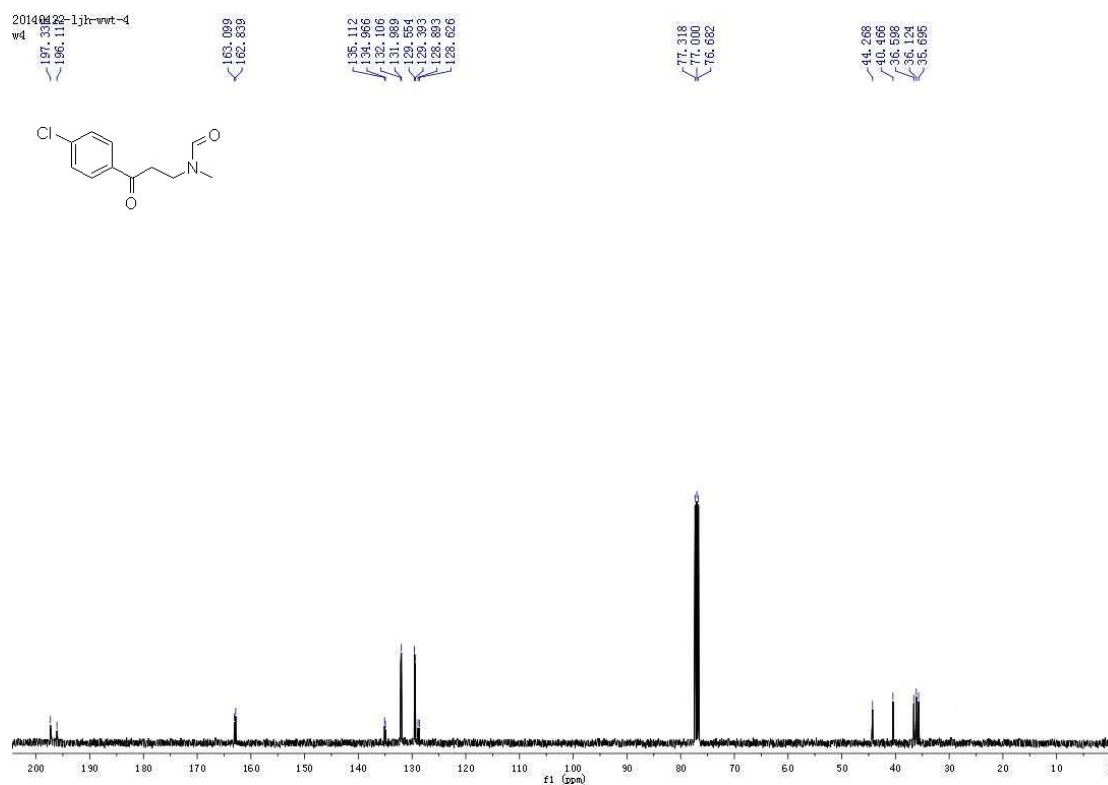
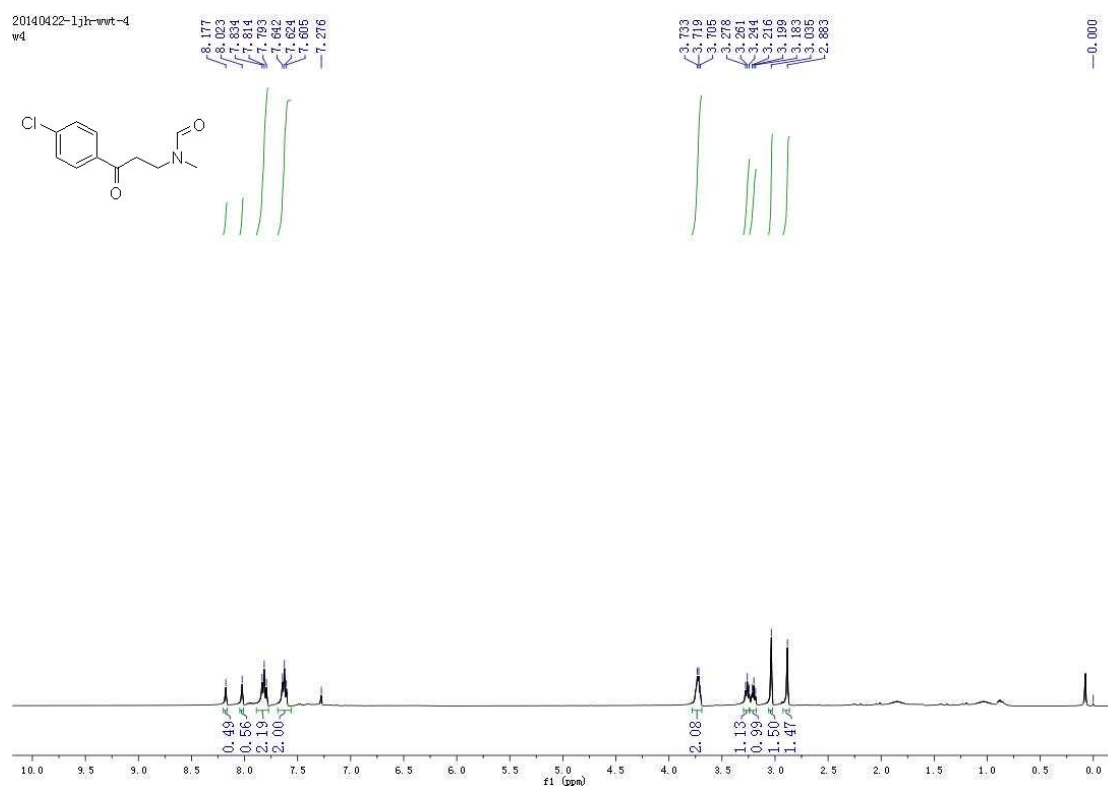
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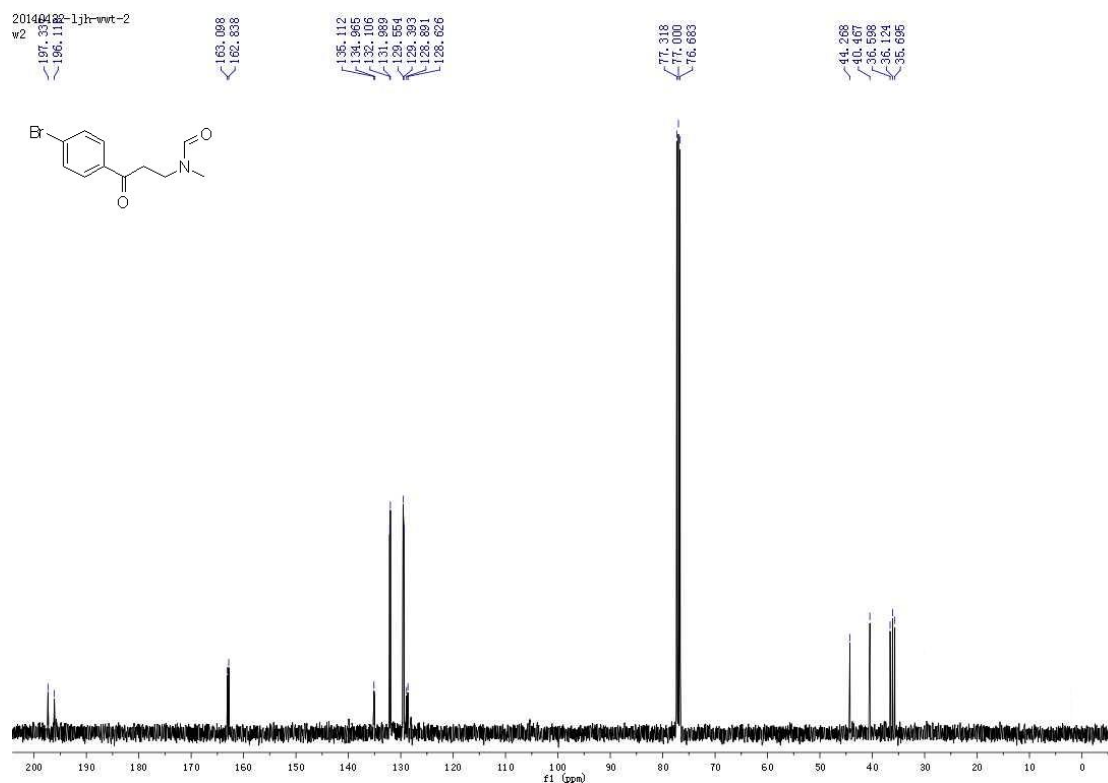
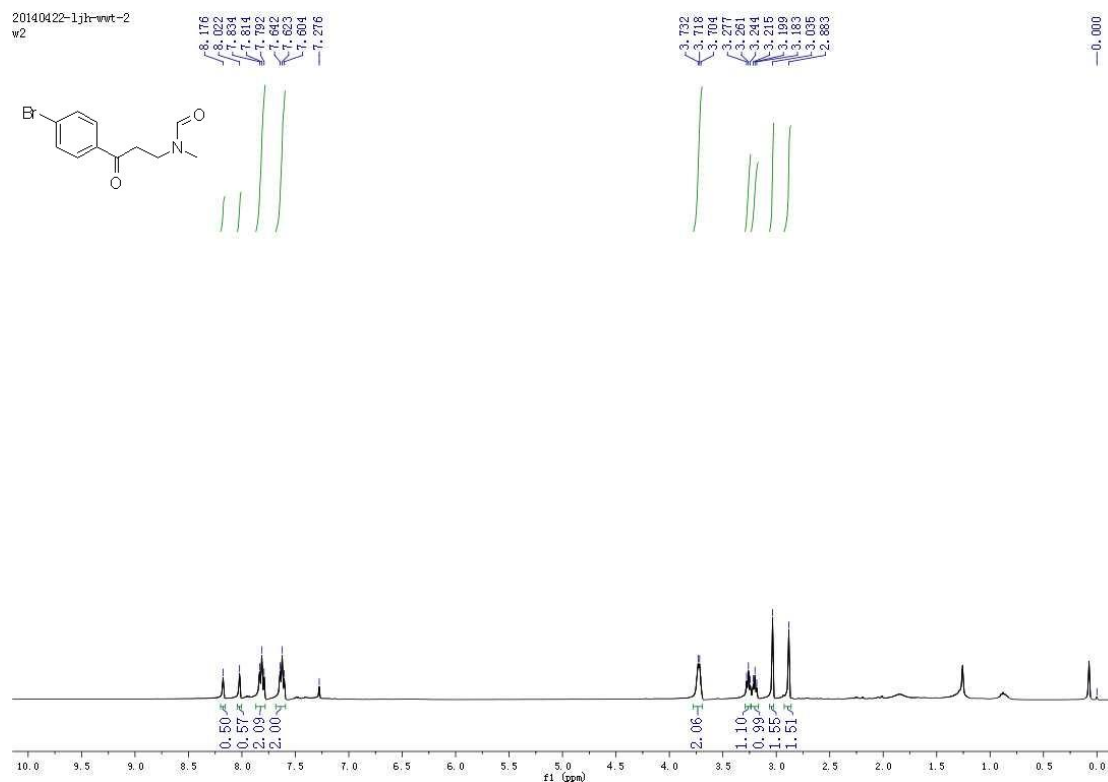
20140417-1jh-yzh-02
yzh-02



N-(3-(4-Chlorophenyl)-3-oxopropyl)-*N*-methylformamide (**3ca**)

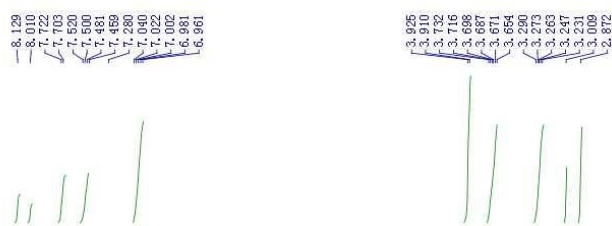
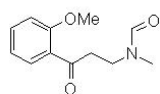


N-(3-(4-Bromophenyl)-3-oxopropyl)-*N*-methylformamide (**3da**)



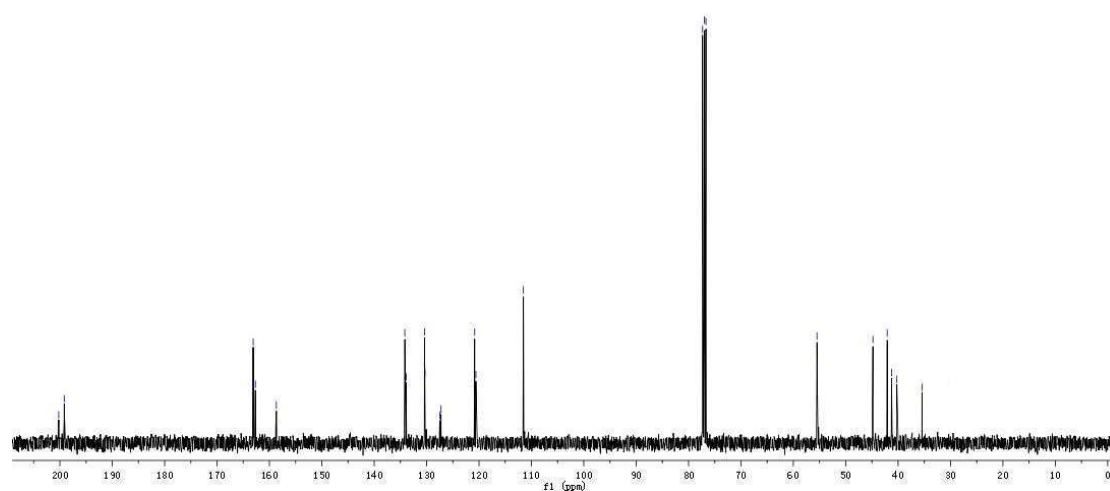
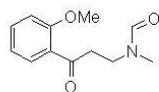
N-(3-(2-Methoxyphenyl)-3-oxopropyl)-*N*-methylformamide (**3ea**)

20140423-1jh-wvt-01
w1



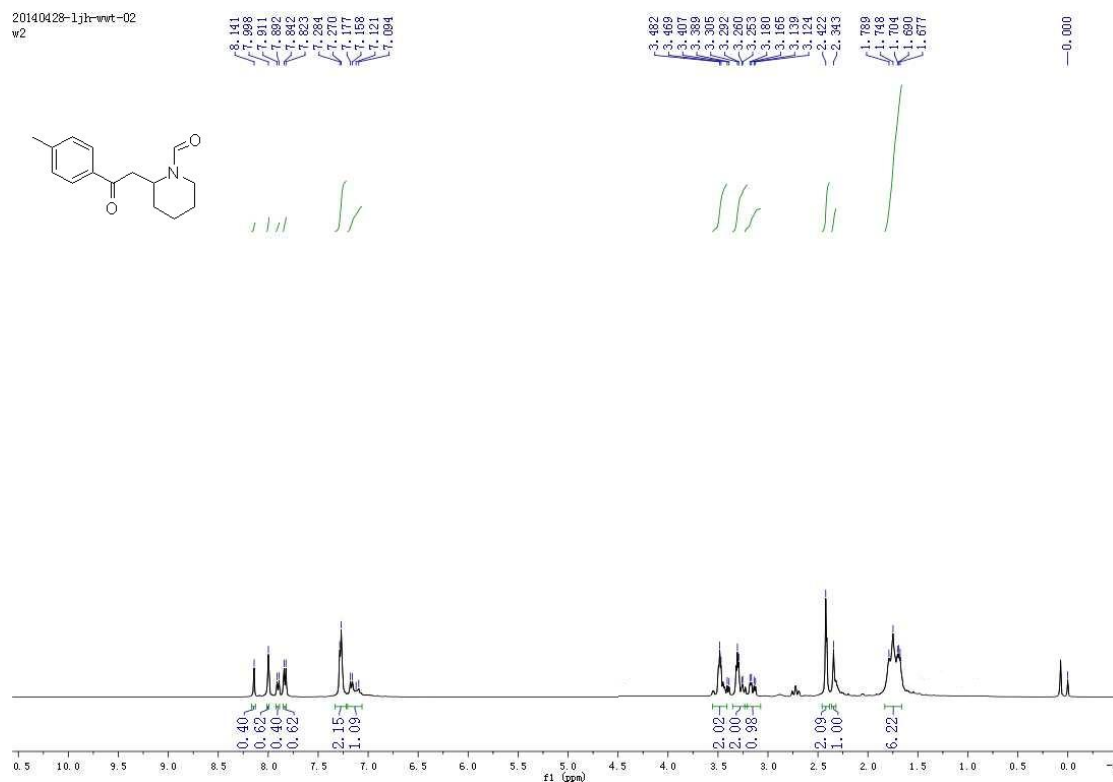
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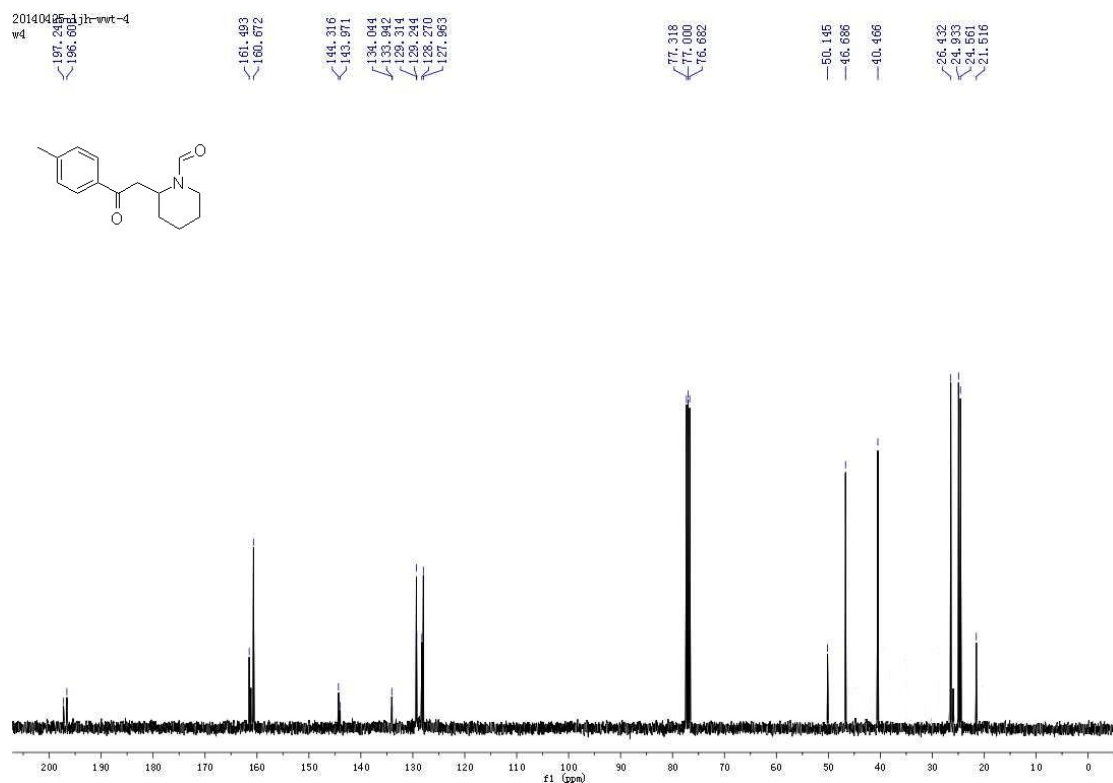


2-(2-oxo-2-*p*-Tolylethyl)piperidine-1-carbaldehyde (**3ab**)

20140428-1jh-wvt-02
w2

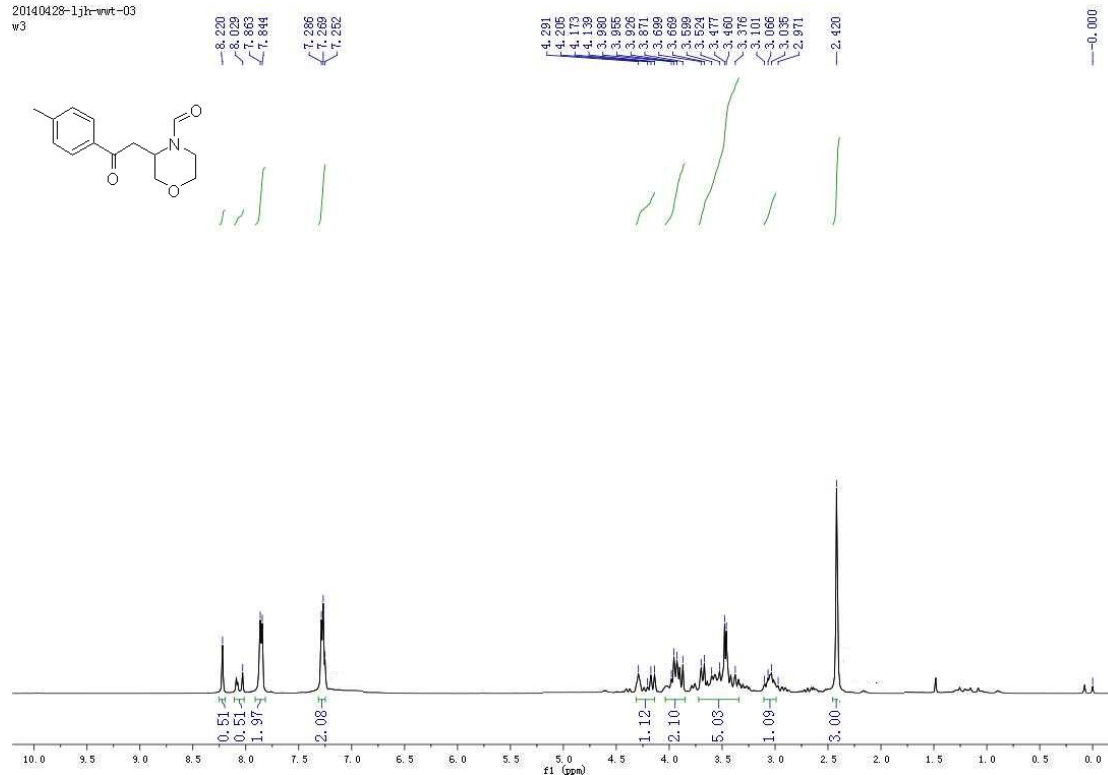


20140428-1jh-wvt-4
w4

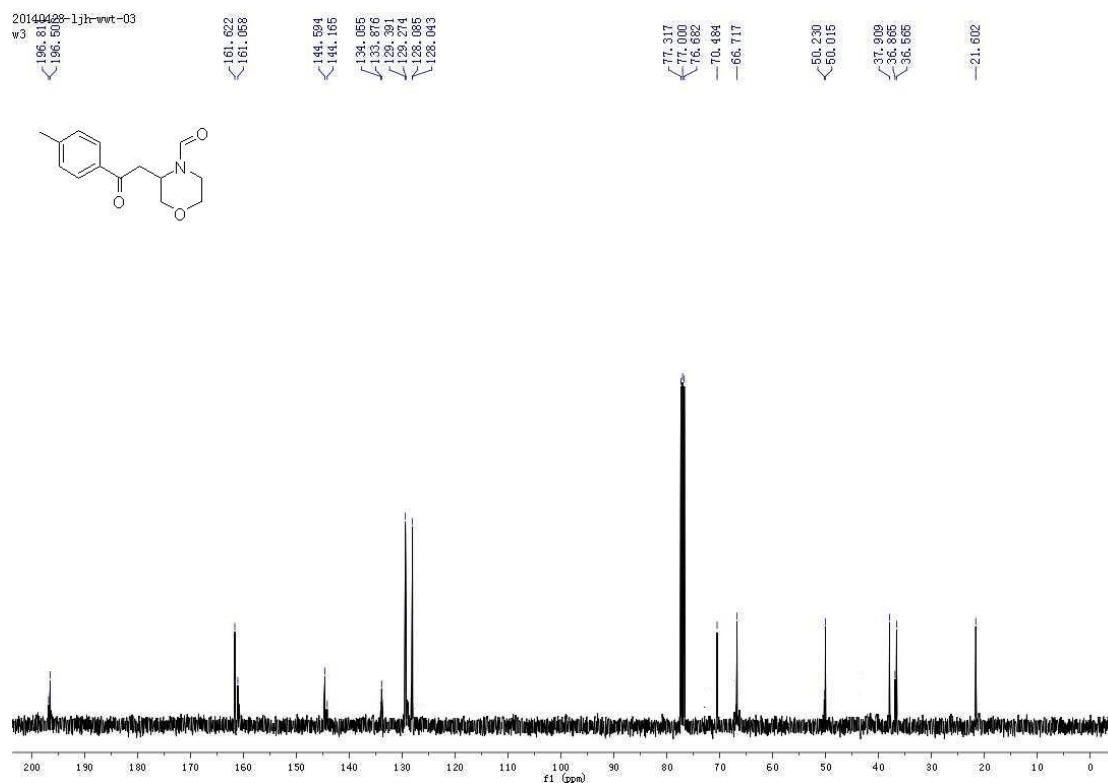


3-(2-oxo-2-*p*-Tolyylethyl)morpholine-4-carbaldehyde (**3ac**)

20140428-1jh-wwt-03
w3

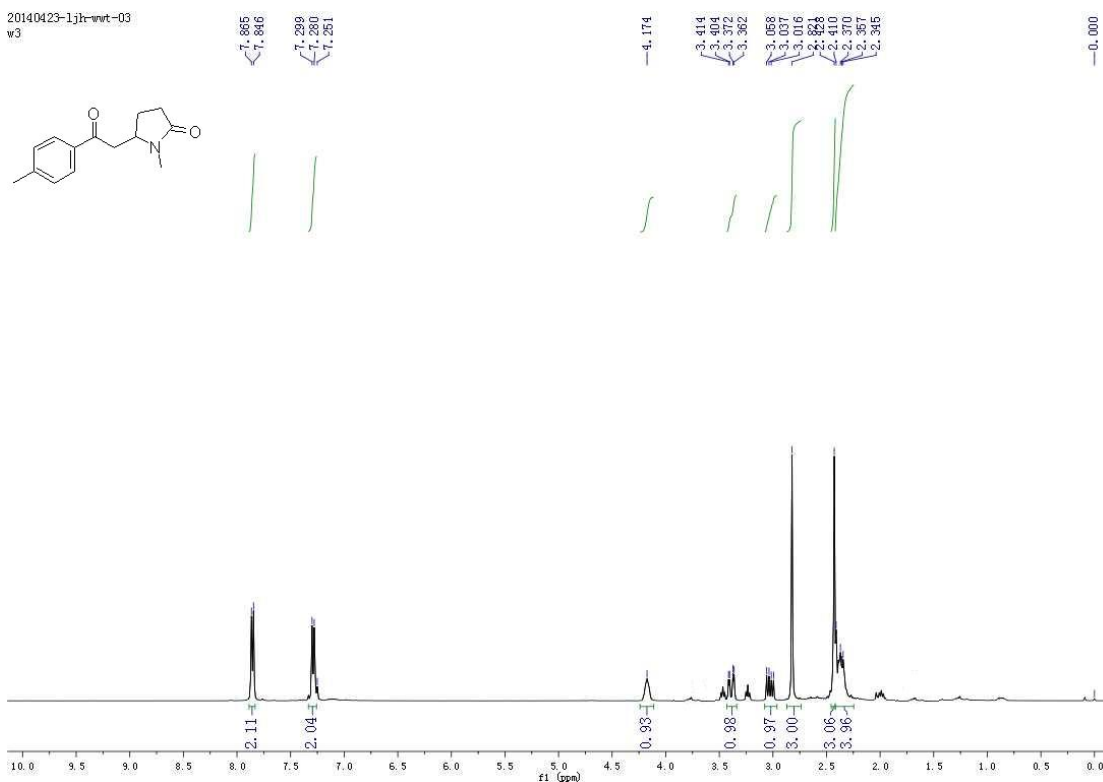


20140428-1jh-wwt-03
v3

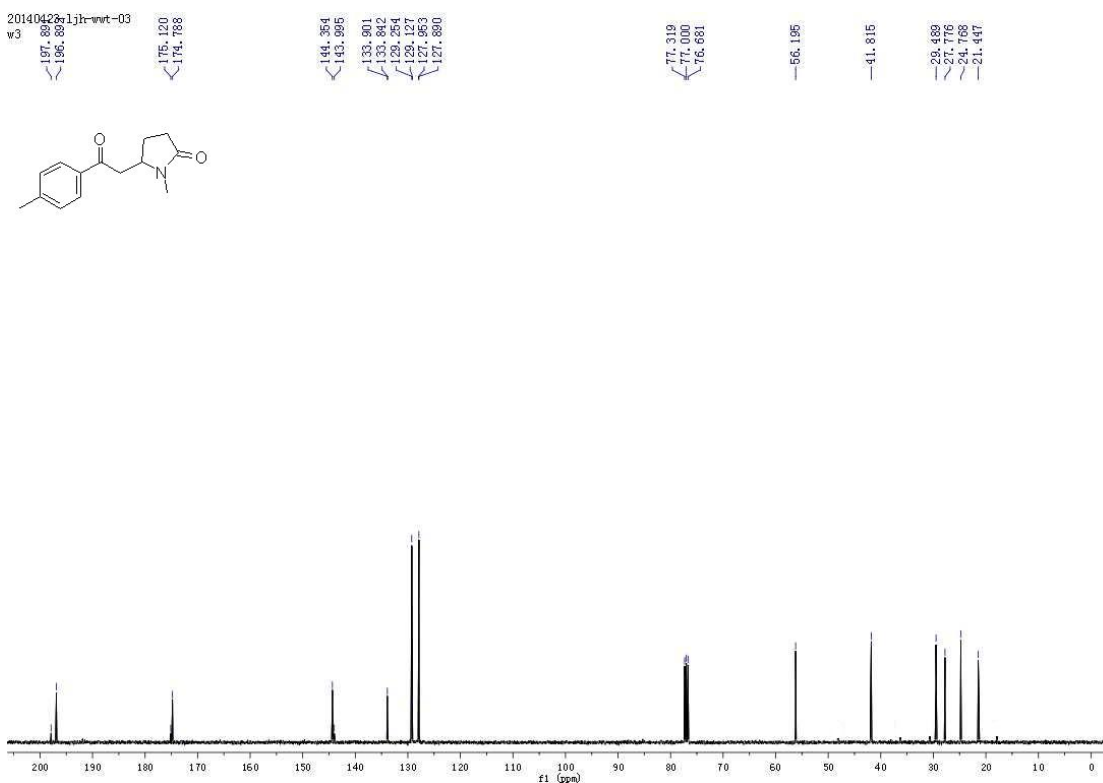


1-Methyl-5-(2-oxo-2-*p*-tolylethyl)pyrrolidin-2-one (3ad)

20140423-1jh-wwt-03
w3

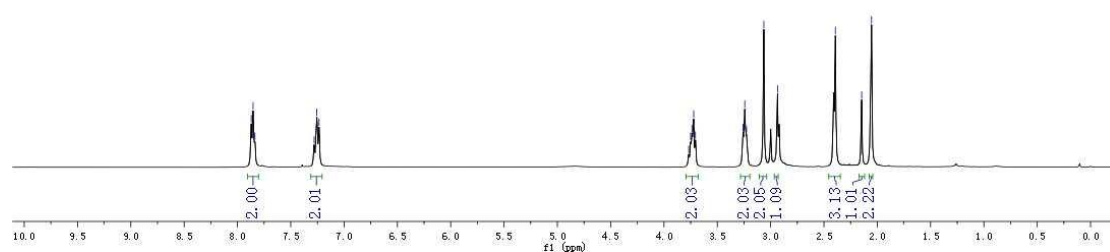
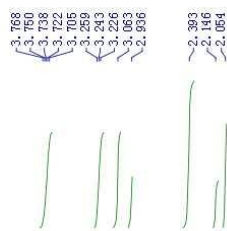
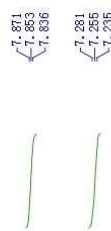
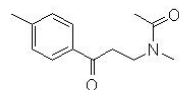


20140423-1jh-wwt-03
w3

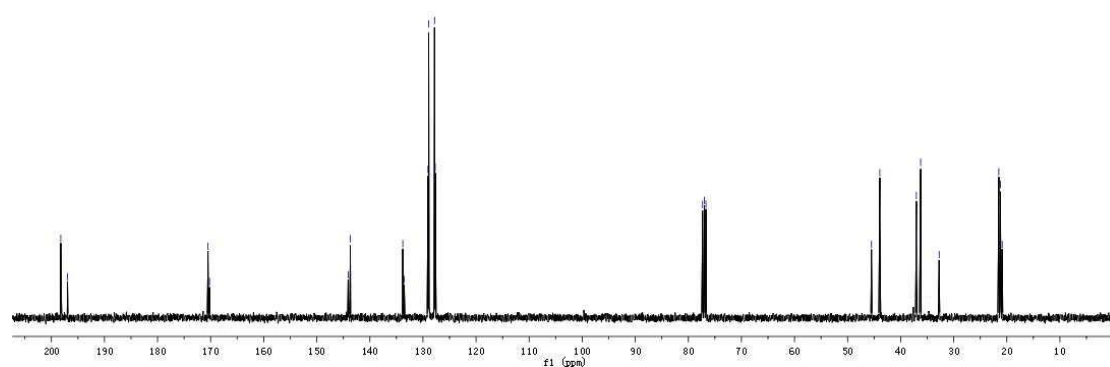
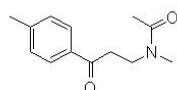


N-Methyl-N-(3-oxo-3-*p*-tolylpropyl)acetamide (3ae)

20140423-1jh-wvt-02
w2

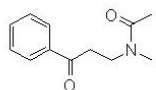


20140423-1jh-wvt-02
w2



N-Methyl-*N*-(3-oxo-3-phenylpropyl)acetamide (**3be**)

20140425-1jh-wvt-2
w2

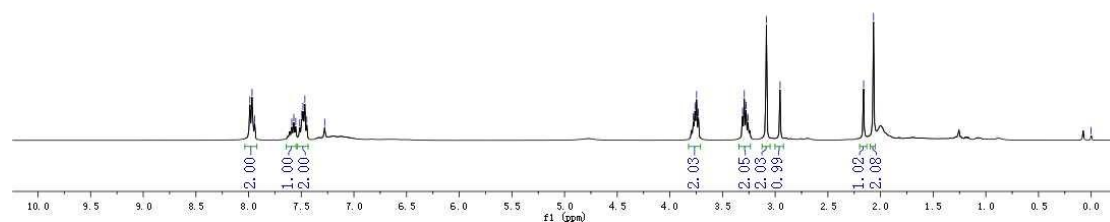


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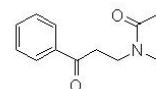
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20140425-1jh-wvt-2
w2



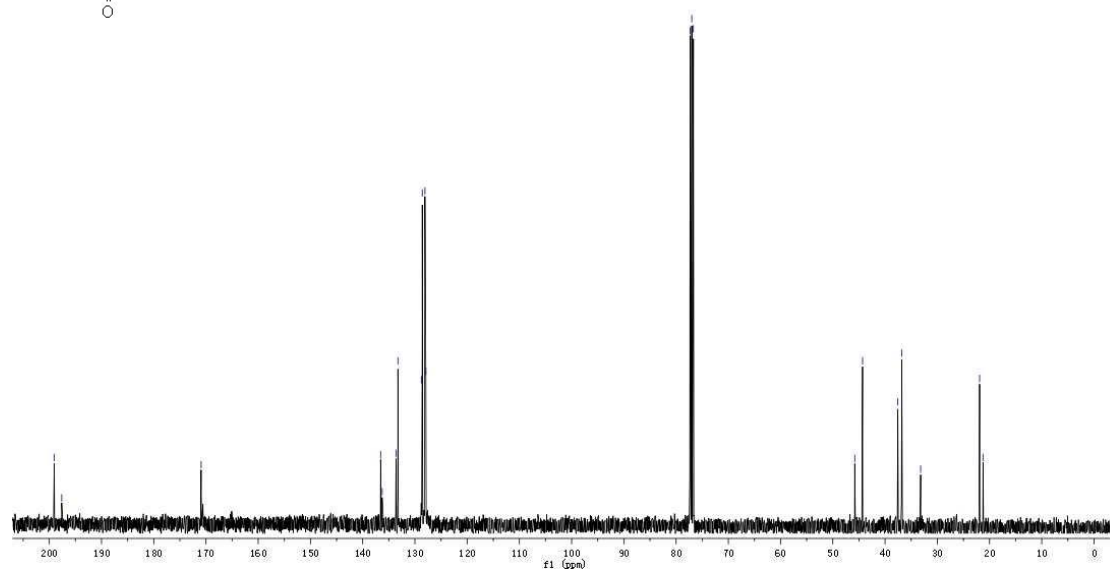
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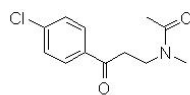
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N-(3-(4-Chlorophenyl)-3-oxopropyl)-N-methylacetamide (3ce)

20140425-1jh-wvt-1
w1

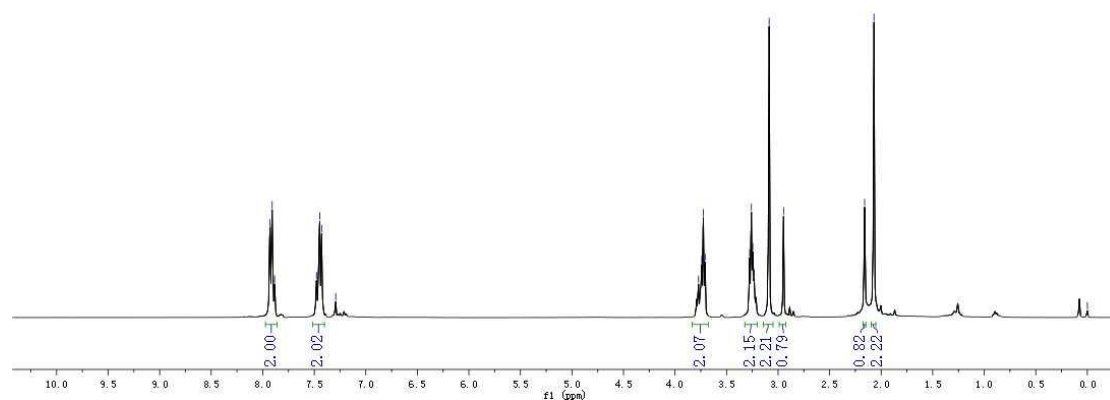


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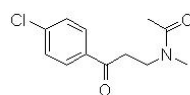
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20140425-1jh-wvt-1
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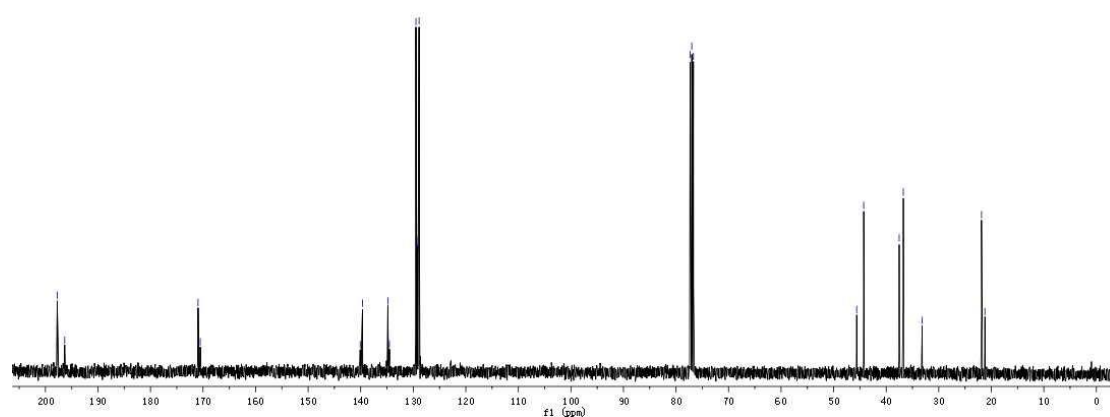
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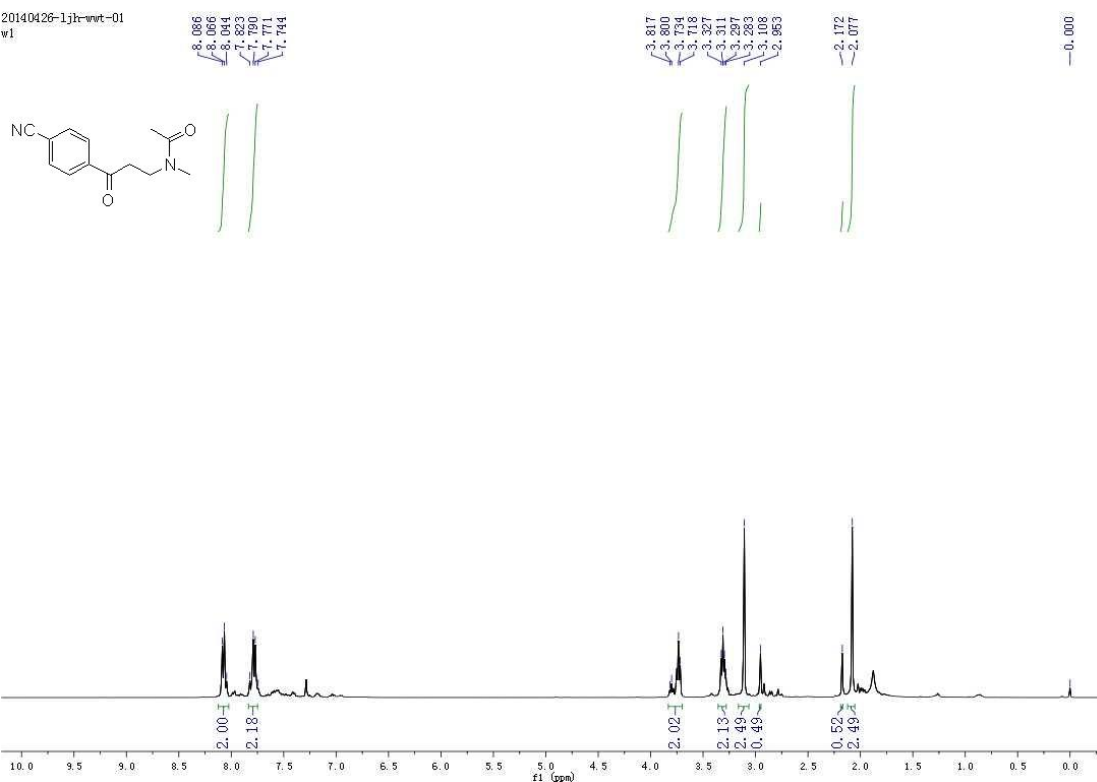
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21.858
21.223

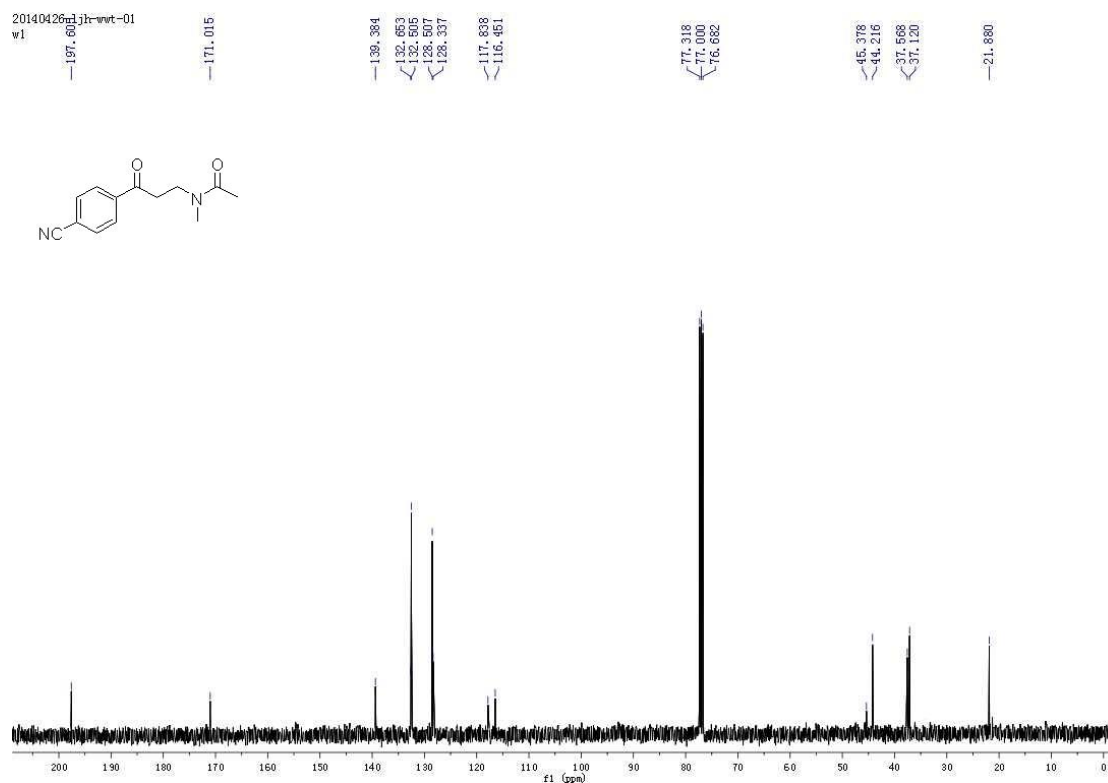


N-(3-(4-Cyanophenyl)-3-oxopropyl)-*N*-methylacetamide (**3ge**)

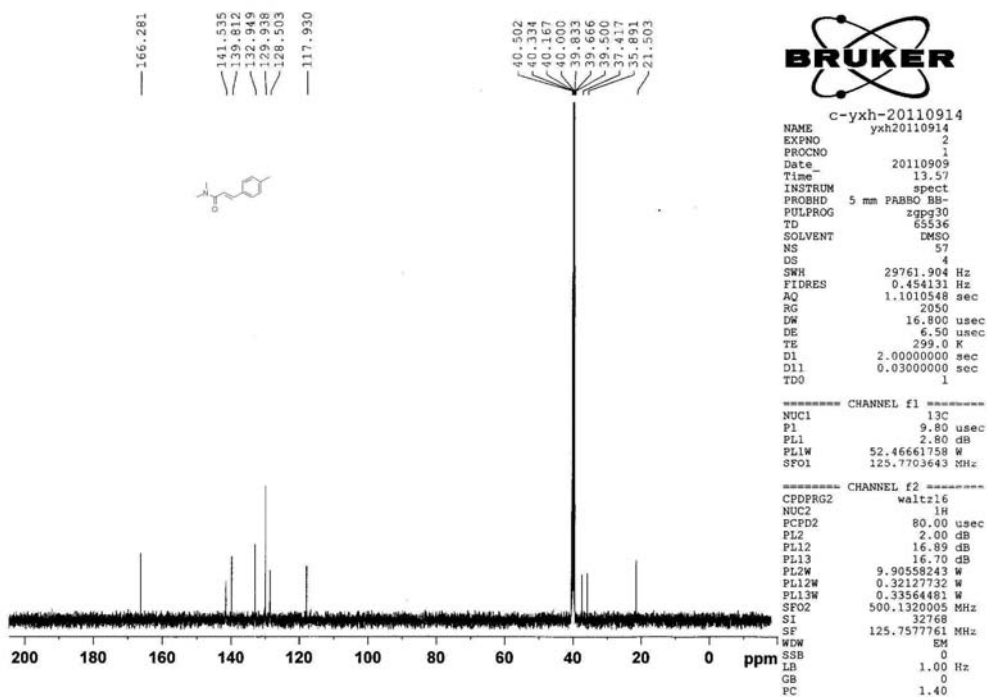
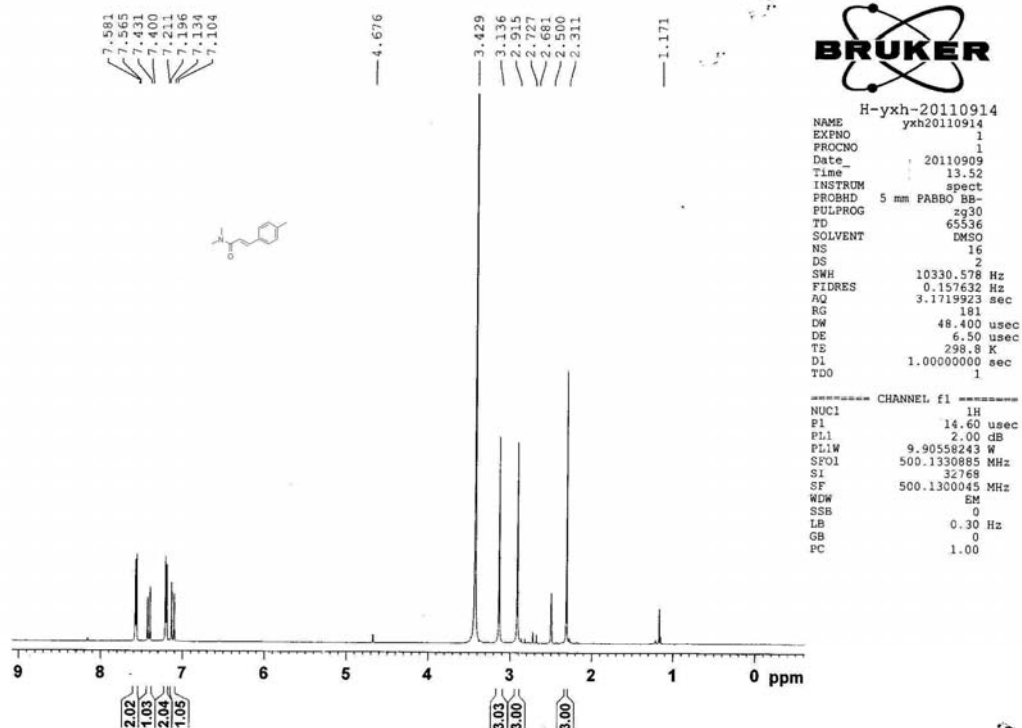
20140426-1jh-wvt-01
w1



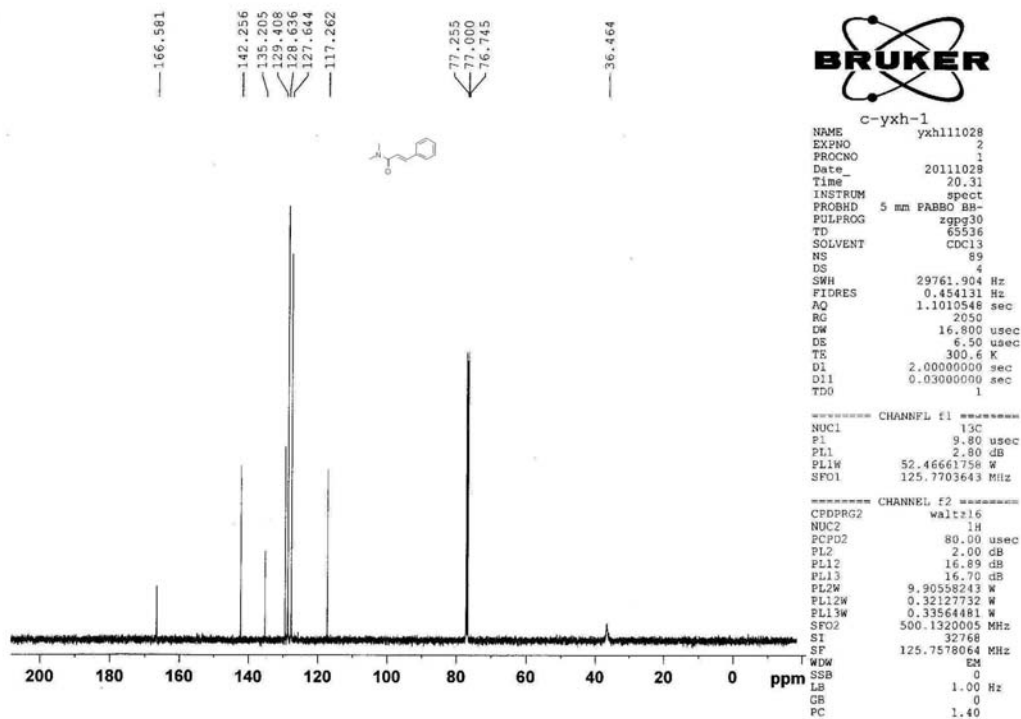
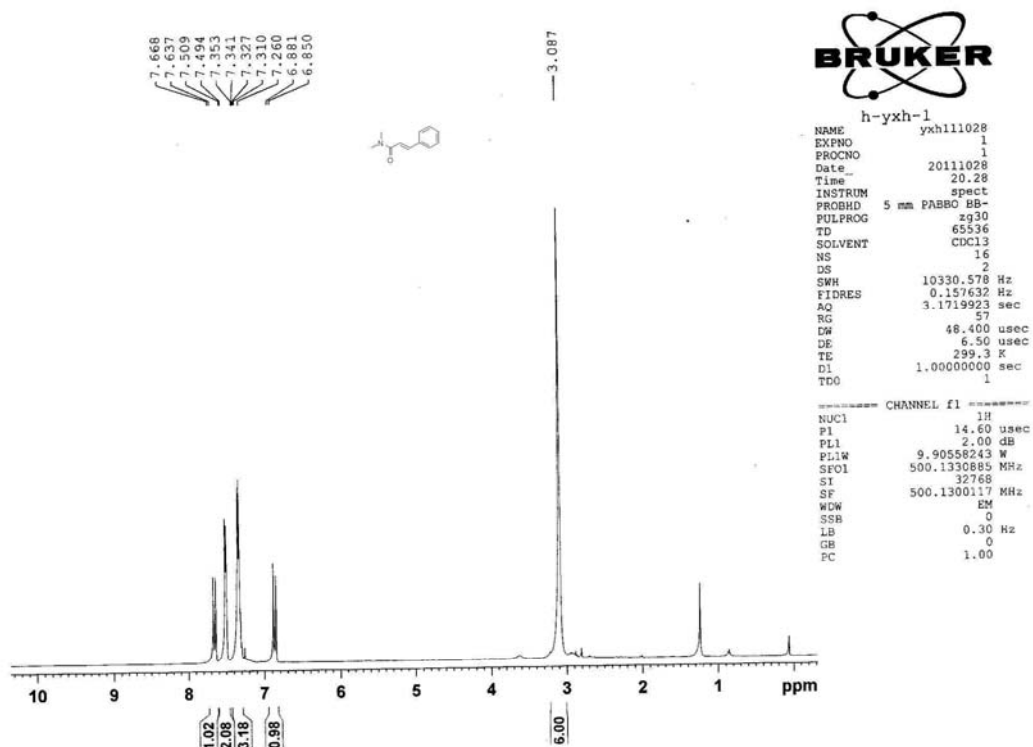
20140426-1jh-wvt-01
w1



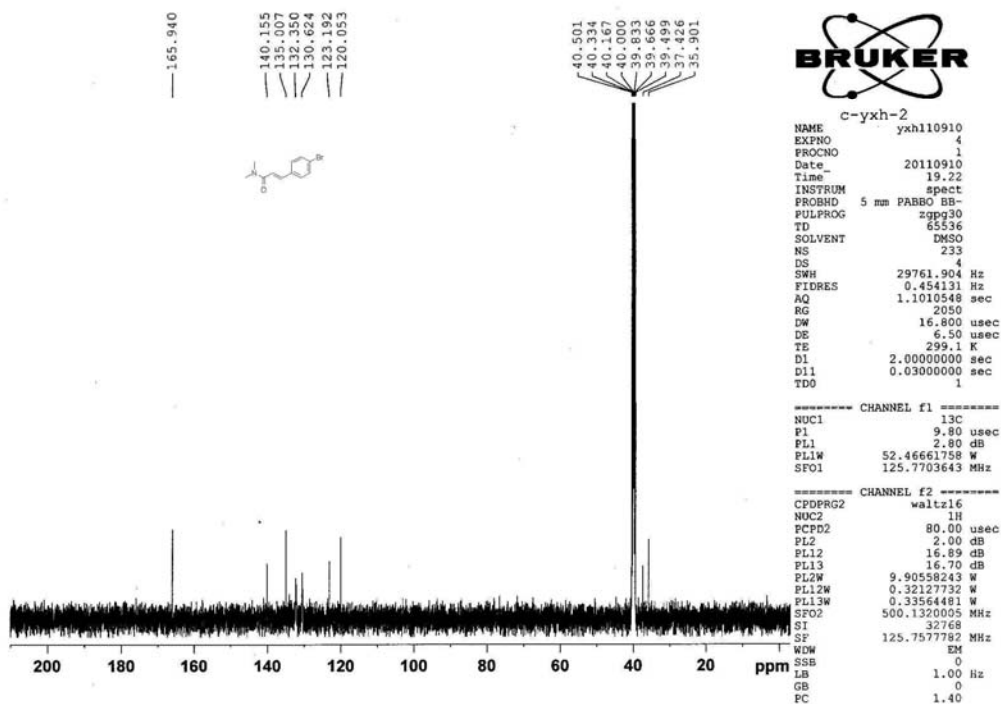
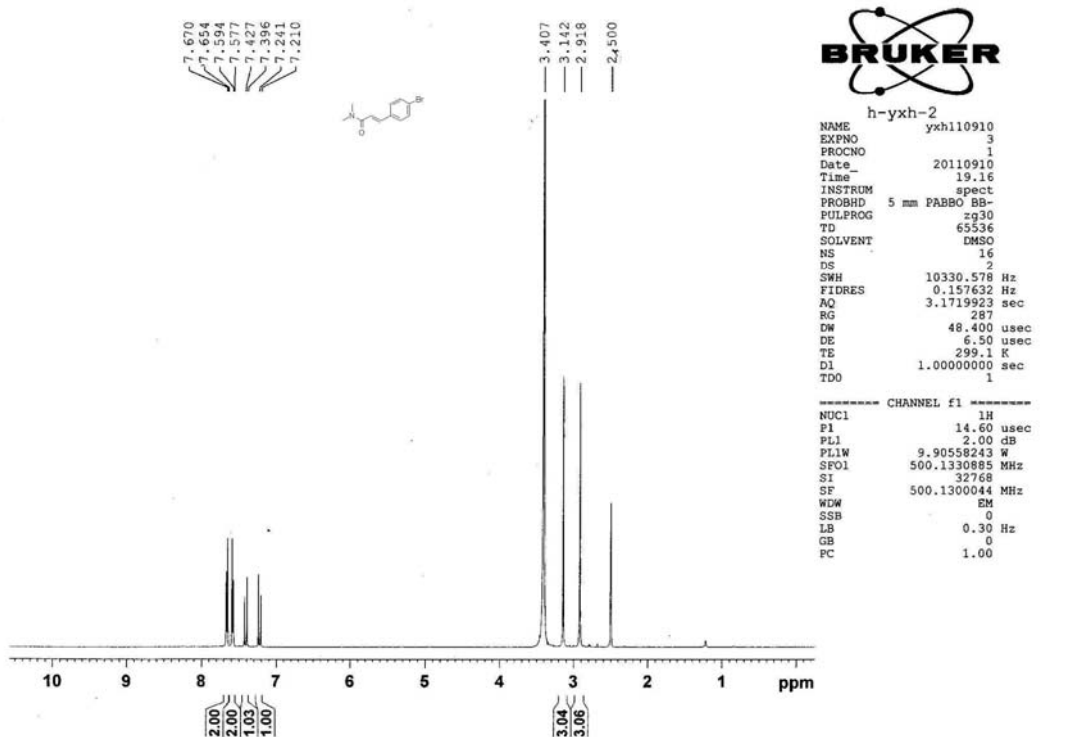
(E)-N,N-dimethyl-3-p-tolylacrylamide (4aa)



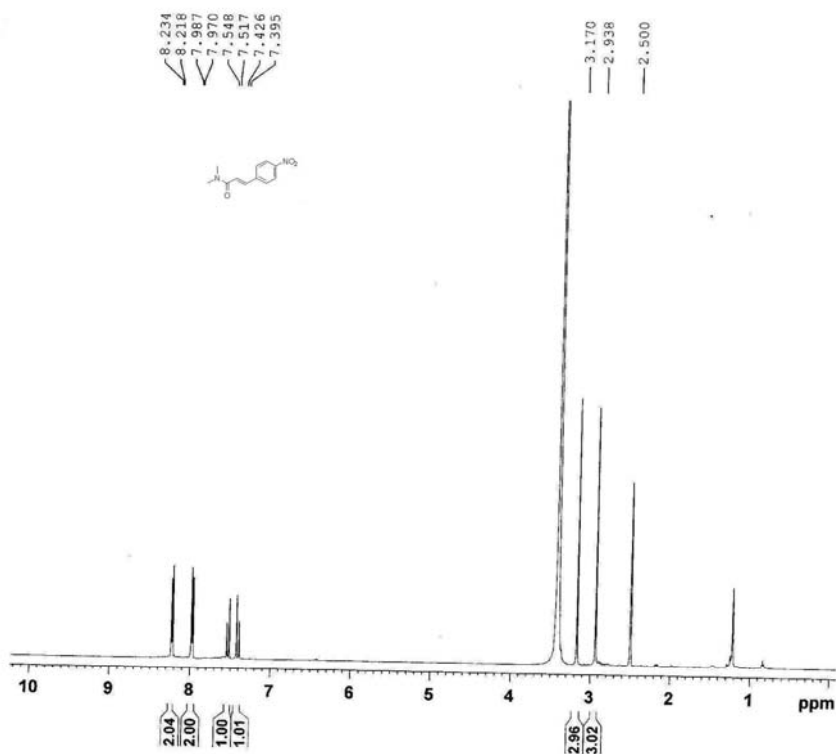
(E)-N,N-dimethylcinnamamide (4ba)



(E)-3-(4-bromophenyl)-N,N-dimethylacrylamide (4ca)

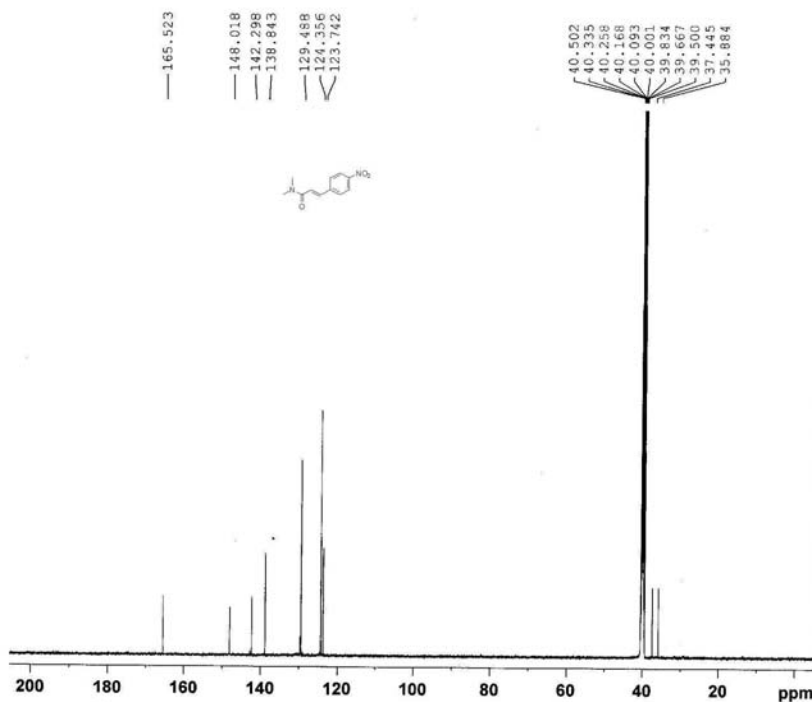


(E)-N,N-dimethyl-3-(4-nitrophenyl)acrylamide (4ha)



c-yxh-0915-1
 NAME yxh20110915
 EXPNO 2
 PROCNO 1
 Date 20110916
 Time 6.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719923 sec
 RG 128
 DW 48.400 usec
 DE 6.50 usec
 TE 299.8 K
 D1 1.00000000 sec
 TD0 1

CHANNEL f1
 NUC1 1H
 P1 14.60 usec
 PL1 2.00 dB
 PL1W 9.90558243 W
 SFO1 500.1330885 MHz
 SI 32768
 SF 500.1300048 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

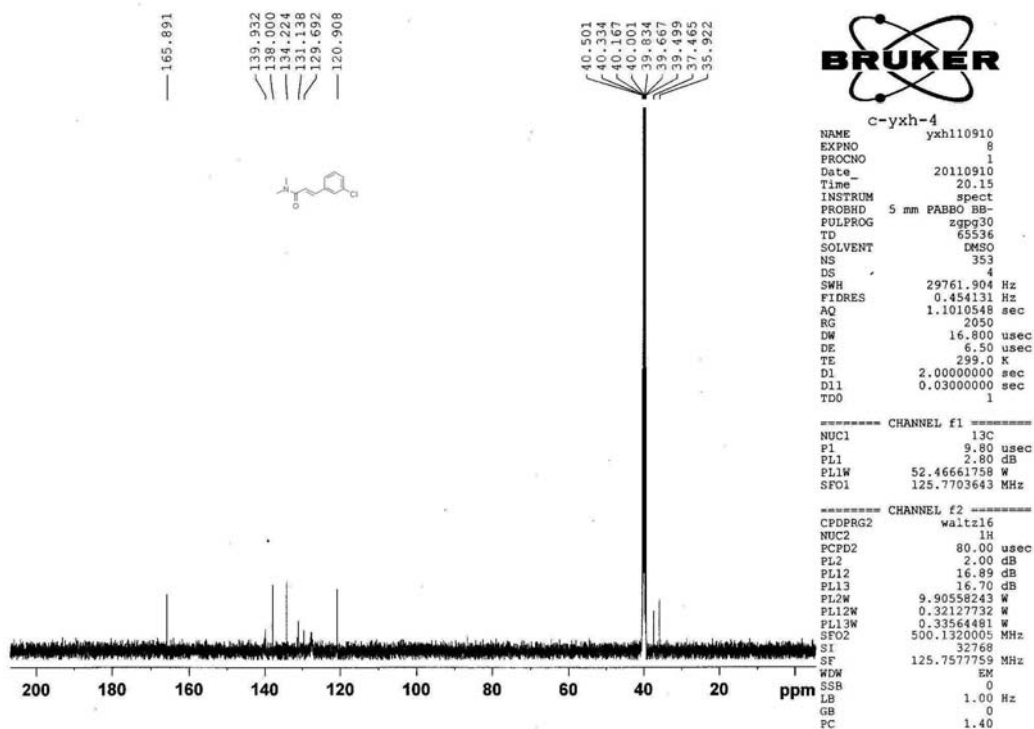
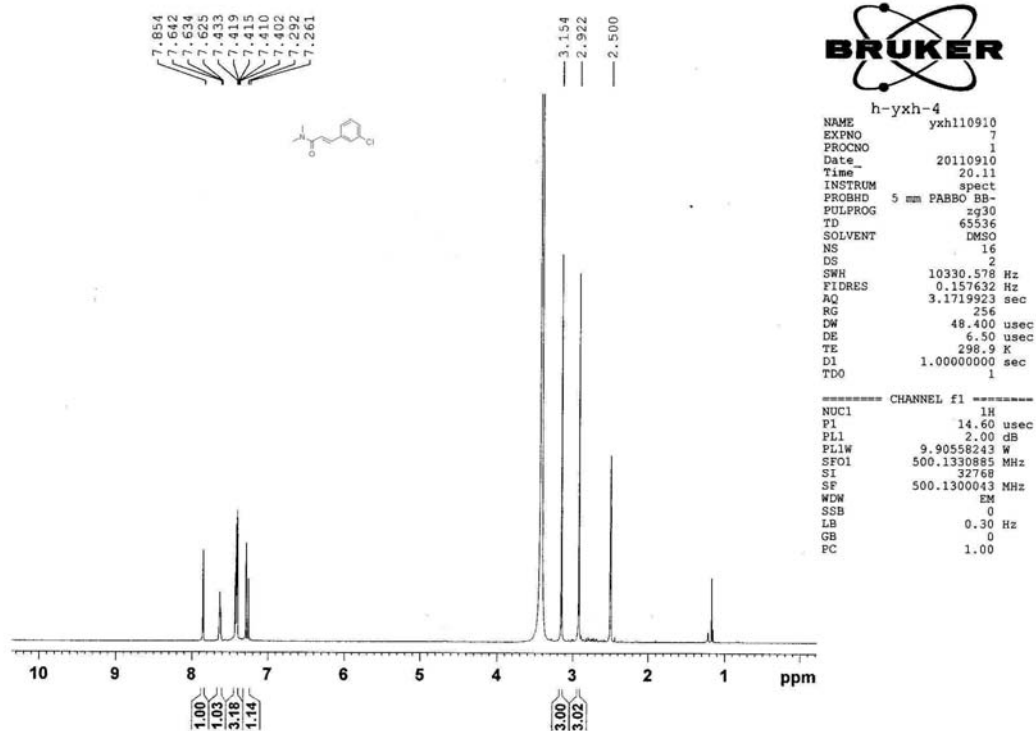


c-yxh-0915-1
 NAME yxh20110915
 EXPNO 1
 PROCNO 1
 Date 20110916
 Time 6.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 9249
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010548 sec
 RG 2050
 DW 16.800 usec
 DE 6.50 usec
 TE 302.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

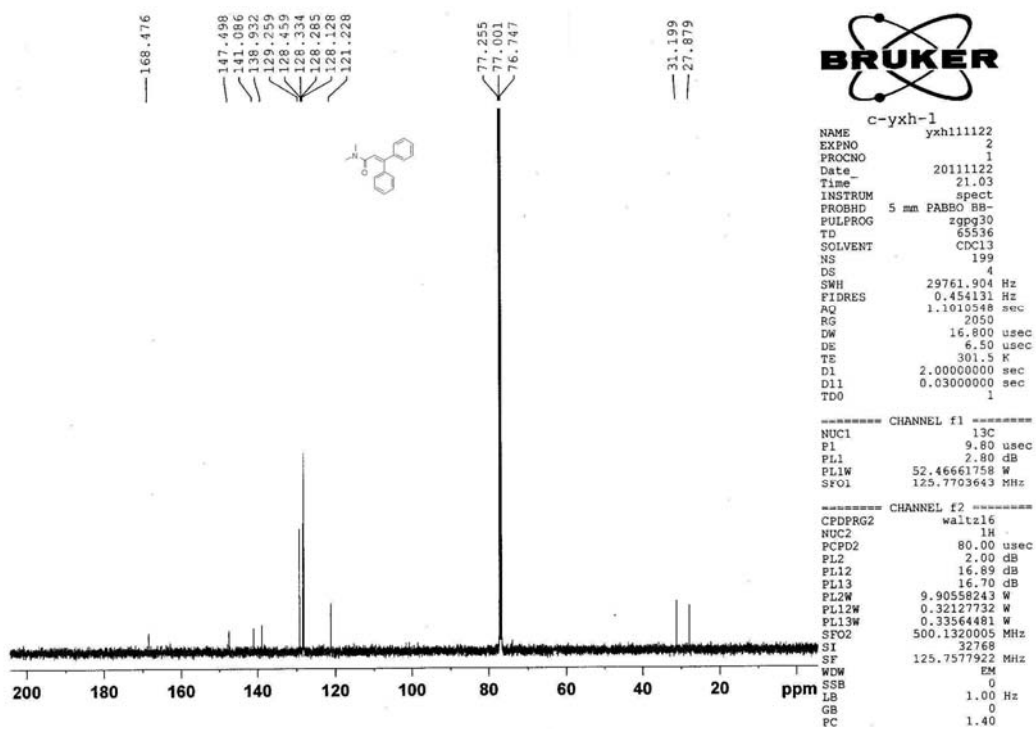
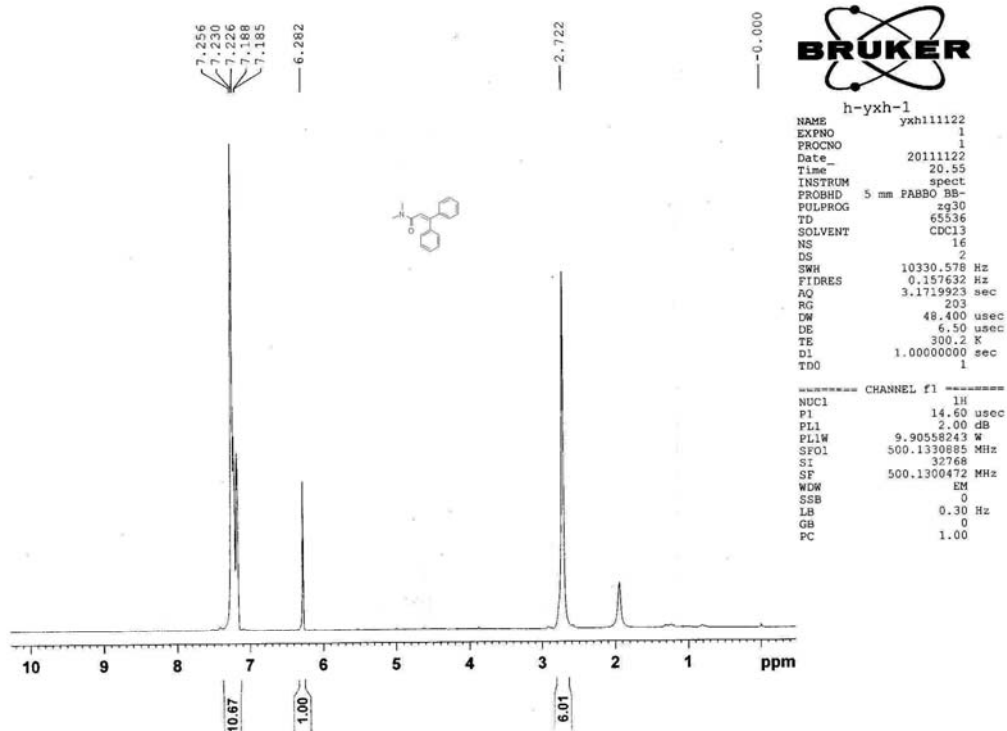
CHANNEL f1
 NUC1 13C
 P1 9.80 usec
 PL1 2.80 dB
 PL1W 52.46661758 W
 SFO1 125.7703643 MHz

CHANNEL f2
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 2.00 dB
 PL12 16.89 dB
 PL13 16.70 dB
 PL2W 9.90558243 W
 PL12W 0.32127732 W
 PL13W 0.33564481 W
 SFO2 500.1320005 MHz
 SI 32768
 SF 125.7577841 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

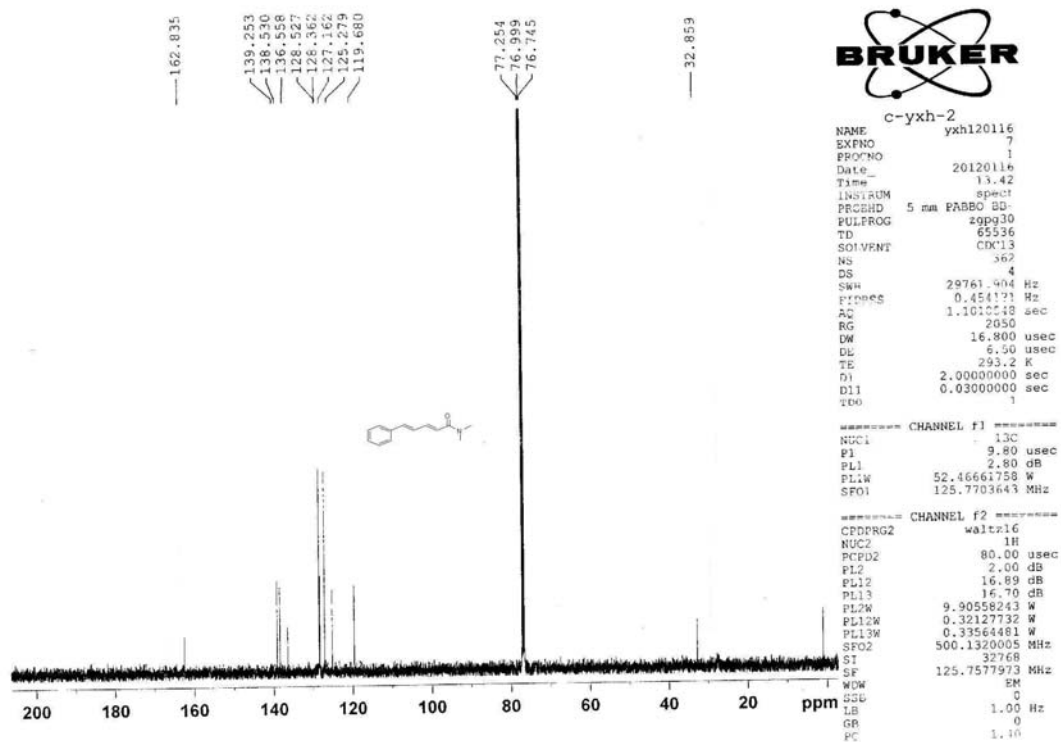
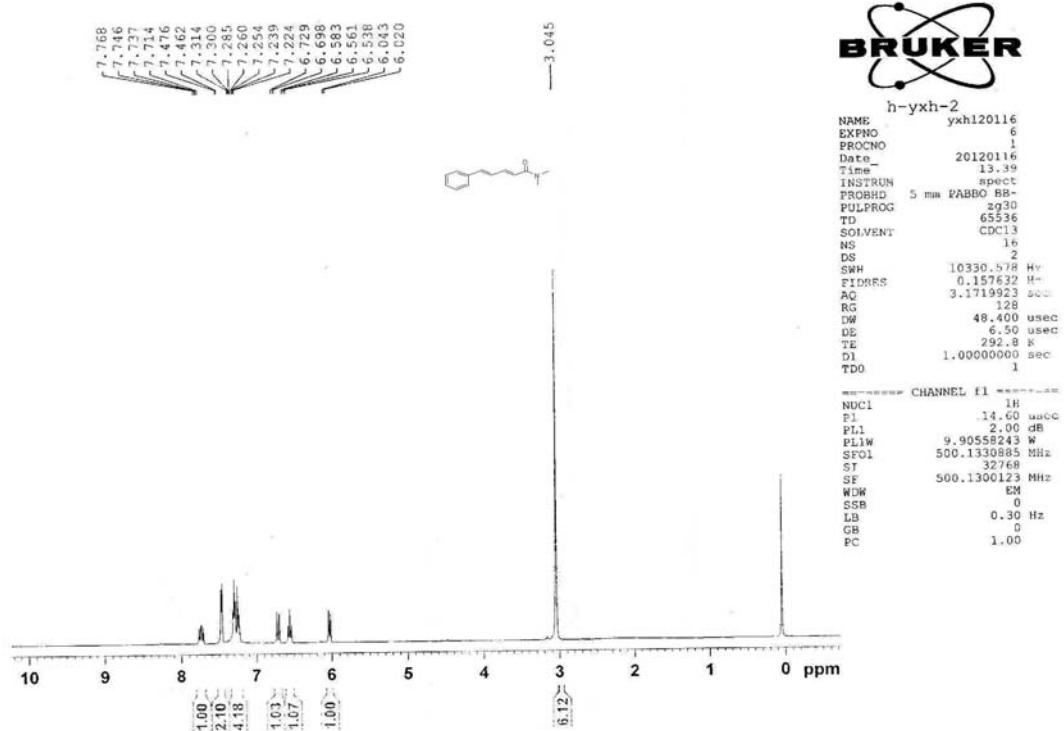
(E)-3-(3-chlorophenyl)-N,N-dimethylacrylamide (4ia)



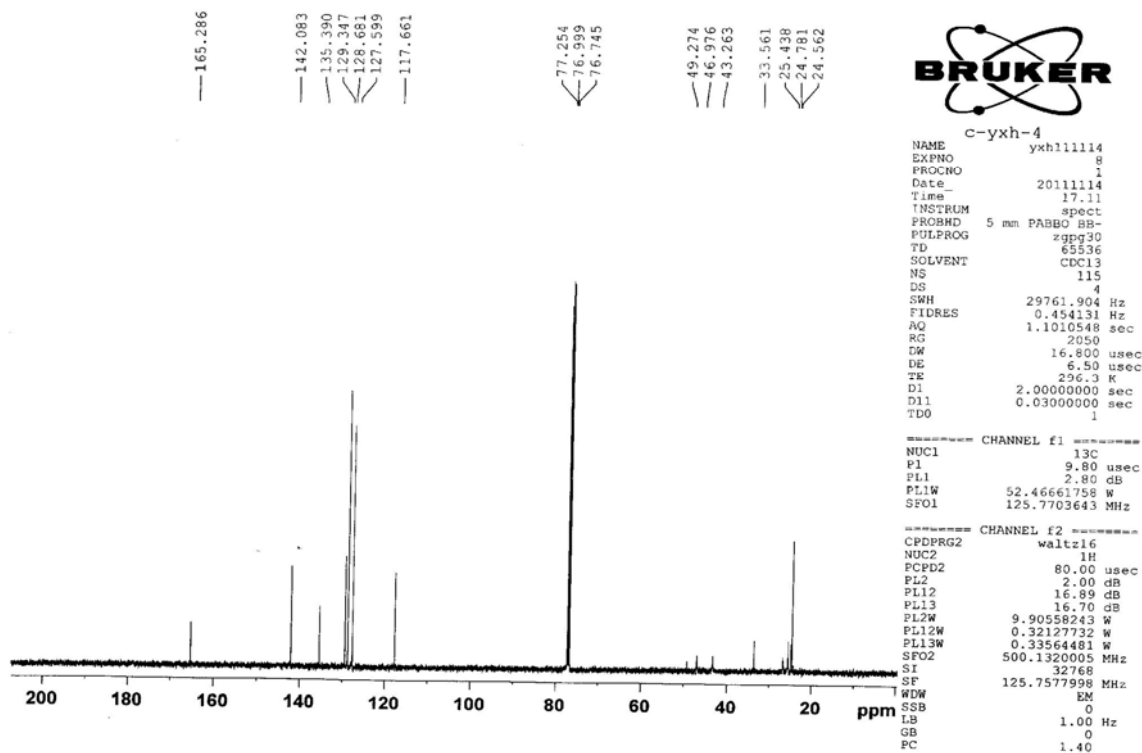
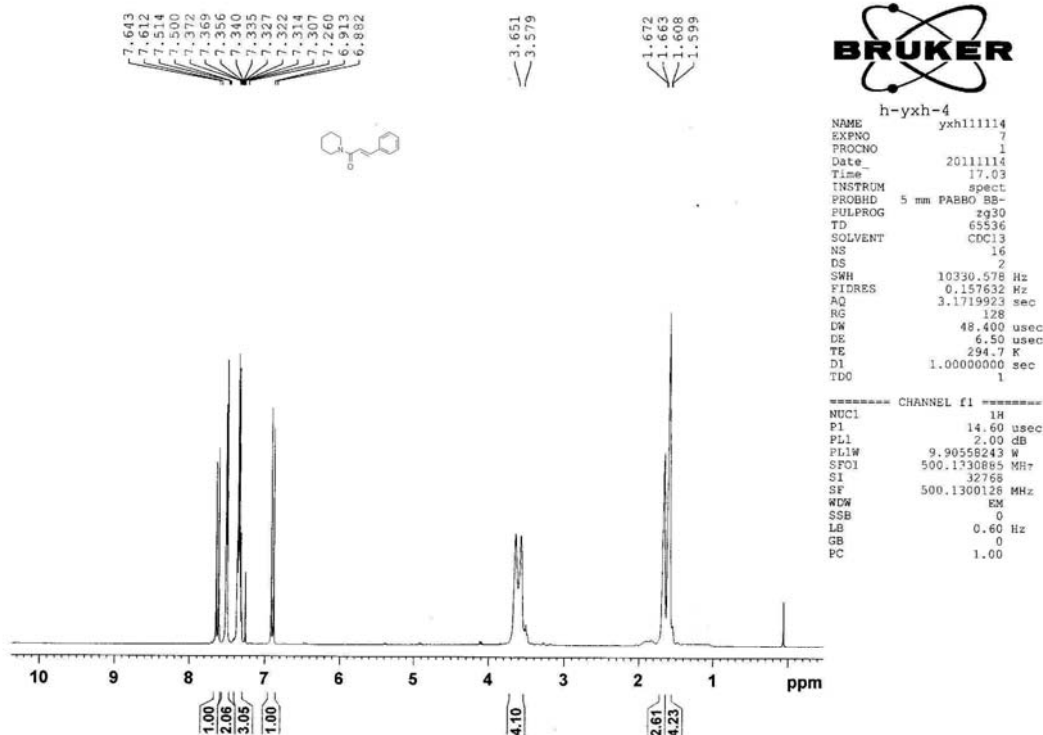
N,N-dimethyl-3,3-diphenylacrylamide (4ja)



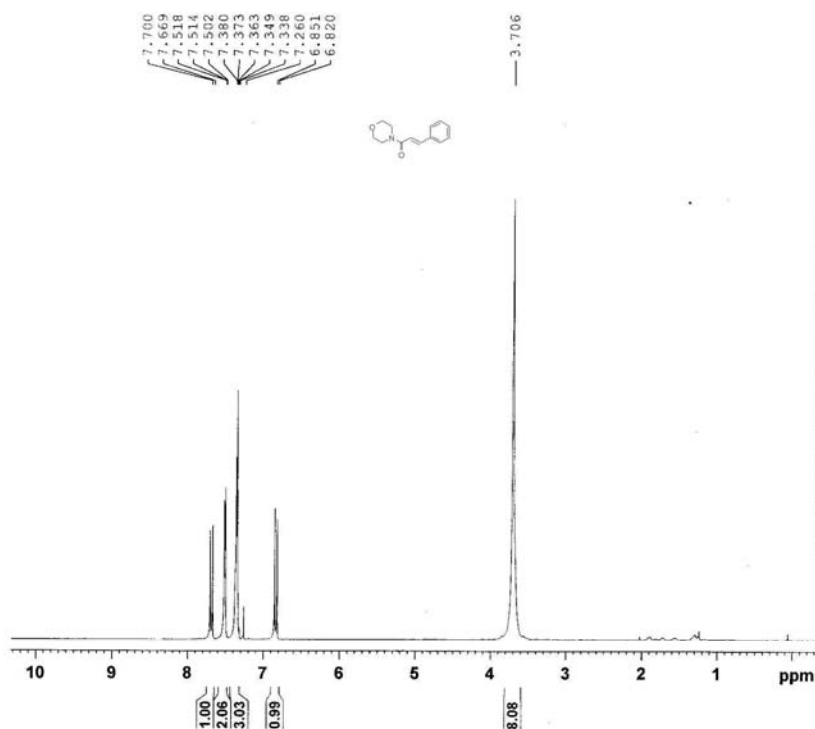
(2E,4E)-N,N-dimethyl-5-phenylpenta-2,4-dienamide(4ka)



(E)-3-phenyl-1-(piperidin-1-yl)prop-2-en-1-one (4bb)



(E)-1-morpholino-3-phenylprop-2-en-1-one (4bc)

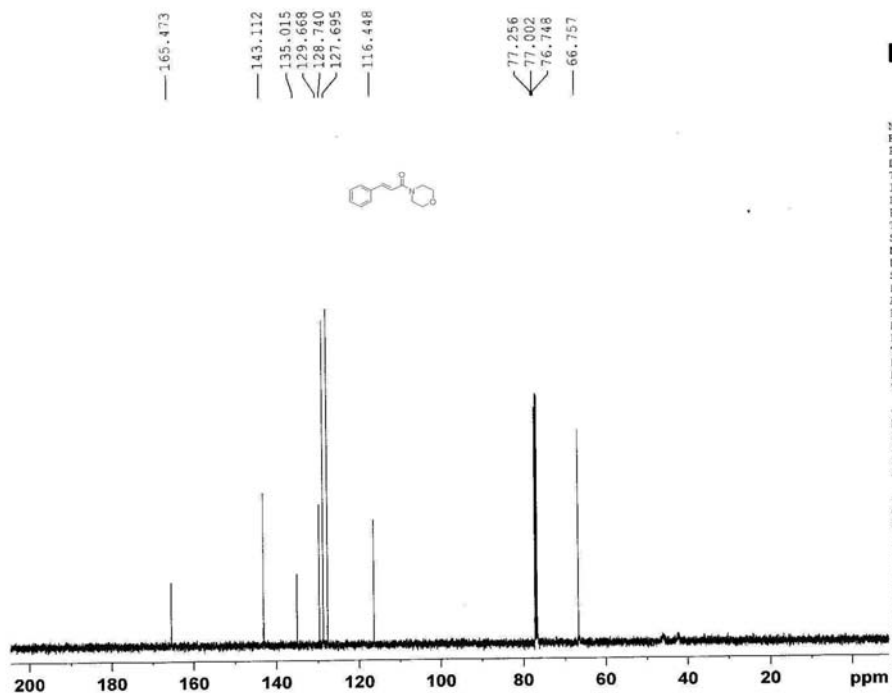


h-yxh-5

NAME	yxh111114
EXPNO	9
PROCNO	1
Date_	20111114
Time	17.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	128
DW	48.400 usec
DE	6.50 usec
TE	294.9 K
D1	1.00000000 sec
TDO	1

CHANNEL f1

NUC1	1H
P1	14.60 usec
PL1	2.00 dB
PL1W	9.90558243 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300123 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



c-yxh-5

NAME	yxh111114
EXPNO	10
PROCNO	1
Date_	20111114
Time	17.26
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	296.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TDO	1

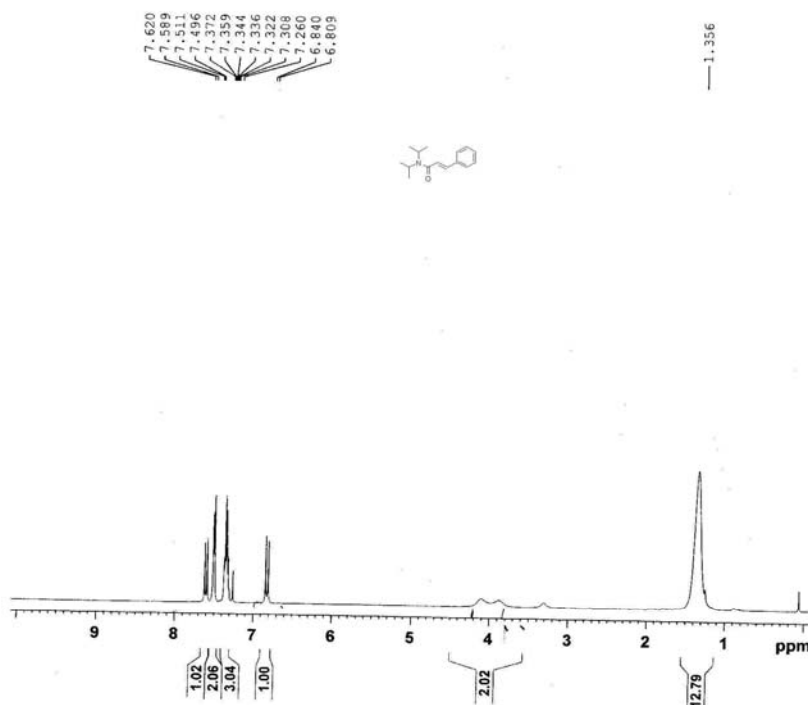
CHANNEL f1

NUC1	13C
P1	9.80 usec
PL1	2.80 dB
PL1W	52.46661758 W
SFO1	125.7703643 MHz

CHANNEL f2

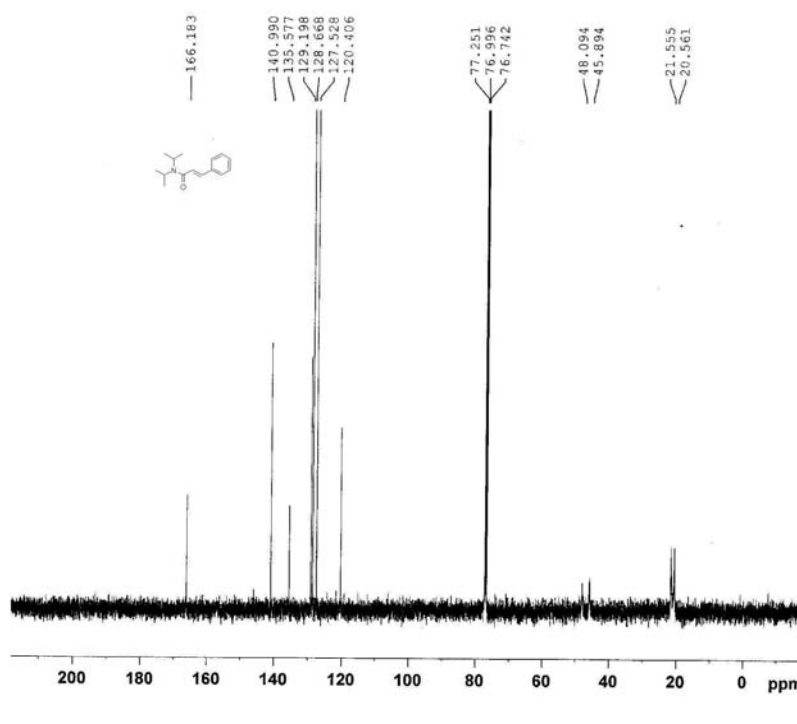
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	16.89 dB
PL13	16.70 dB
PL2W	9.90558243 W
PL12W	0.32127732 W
PL13W	0.33564481 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7578022 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

(E)-N,N-diisopropylcinnamamide(4bg)



h-yxh-3
NAME yxh111122
EXPNO 4
PROCNO 1
Date_ 20111122
Time 21.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 144
LW 48.400 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
TDO 1

CHANNEL f1
NUC1 1H
P1 14.60 usec
PL1 2.00 dB
PL1W 9.90558243 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

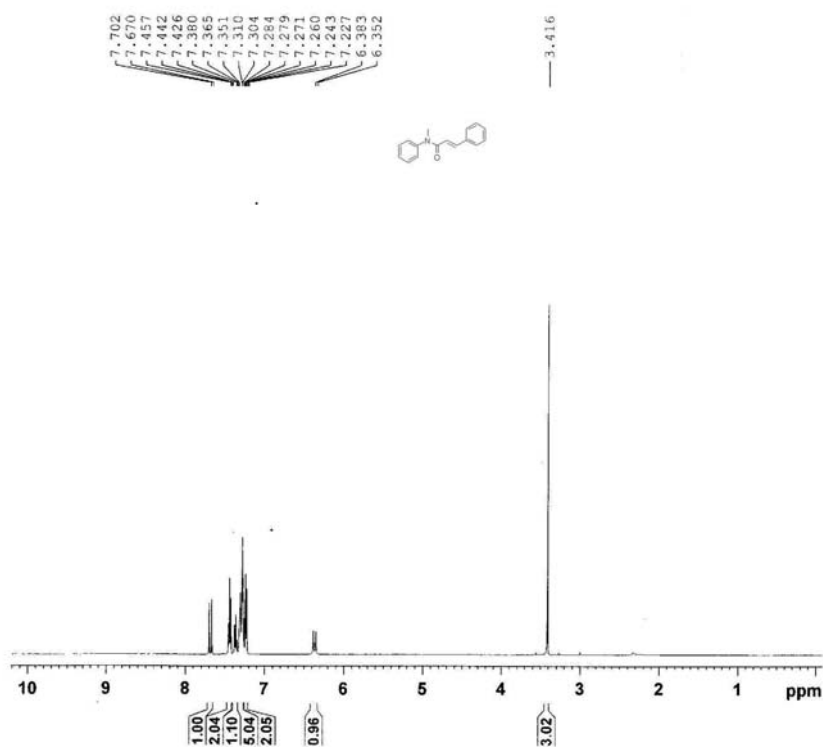


c-yxh-2
NAME yxh111114
EXPNO 4
PROCNO 1
Date_ 20111114
Time 16.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 125
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010546 sec
RG 2050
LW 16.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

CHANNEL f1
NUC1 13C
P1 9.80 usec
PL1 2.80 dB
PL1W 52.46661758 W
SFO1 125.7703643 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.89 dB
PL13 16.70 dB
PL2W 9.90558243 W
PL12W 0.32127732 W
PL13W 0.33564481 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577994 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

(E)-N-methyl-N-phenylcinnamamide(4bh)

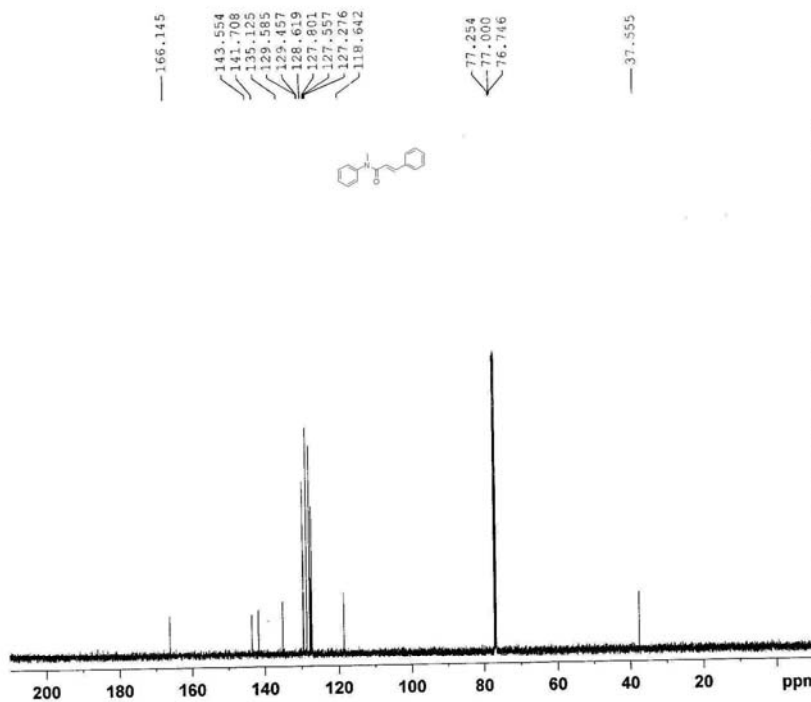


h-yxh-6

NAME	yxh111114
EXPNO	11
PROCNO	1
Date_	20111114
Time	17.33
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	362
DW	48.400 usec
DE	6.50 usec
TE	295.0 K
D1	1.00000000 sec
TDO	1

===== CHANNEL f1 =====

NUC1	1H
P1	14.60 usec
PL1	2.00 dB
PL1W	9.90558243 W
SFO1	500.1330885 MHz
SI	32768
SF	500.1300132 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



c-yxh-6

NAME	yxh111114
EXPNO	12
PROCNO	1
Date_	20111114
Time	17.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	62
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	295.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TDO	1

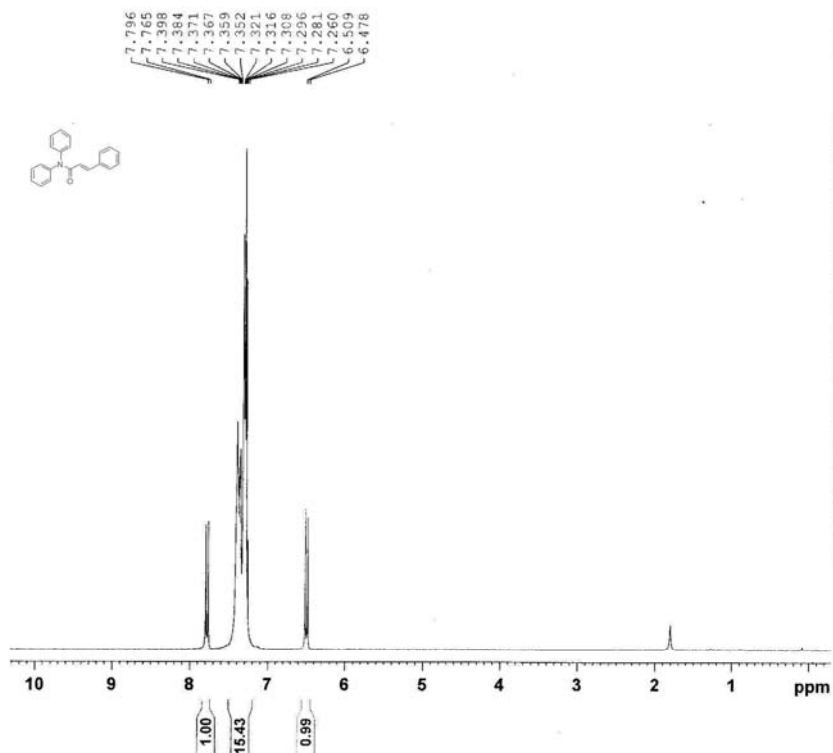
===== CHANNEL f1 =====

NUC1	13C
P1	9.80 usec
PL1	2.80 dB
PL1W	52.46661758 W
SFO1	125.7703643 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	16.89 dB
PL13	16.70 dB
PL2W	9.90558243 W
PL12W	0.32127732 W
PL13W	0.33564481 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577976 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

(E)-N,N-diphenylcinnamamide(4bi)

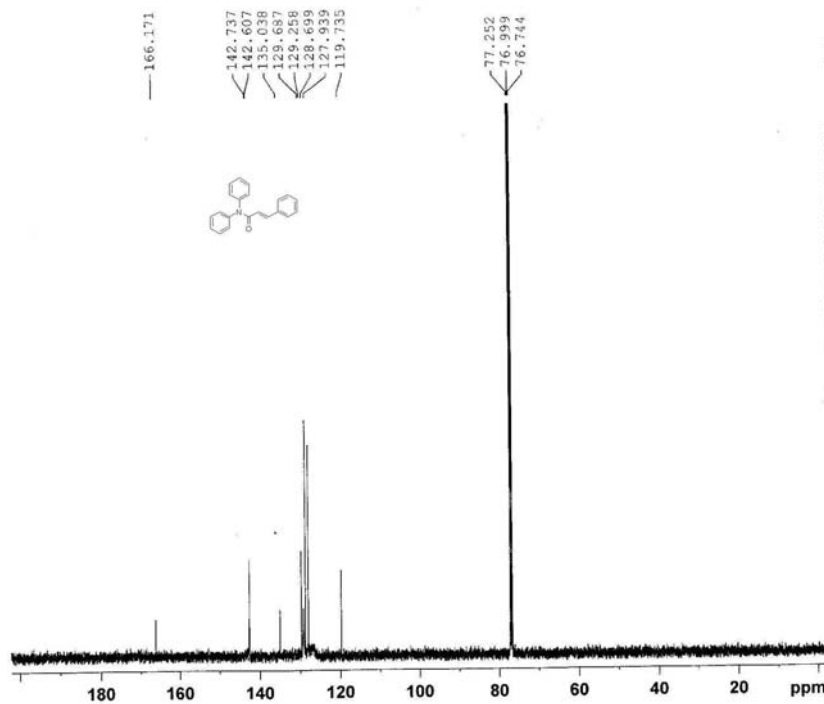


h-yxh-1

NAME yxh111125
EXPNO 2
PROCNO 1
Date_ 20111125
Time 21.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TDO 1

CHANNEL f1

NUC1 1H
P1 14.60 usec
PL1 2.00 dB
PL1W 9.90558243 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



c-yxh-1

NAME yxh111125
EXPNO 3
PROCNO 1
Date_ 20111125
Time 21.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 112
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

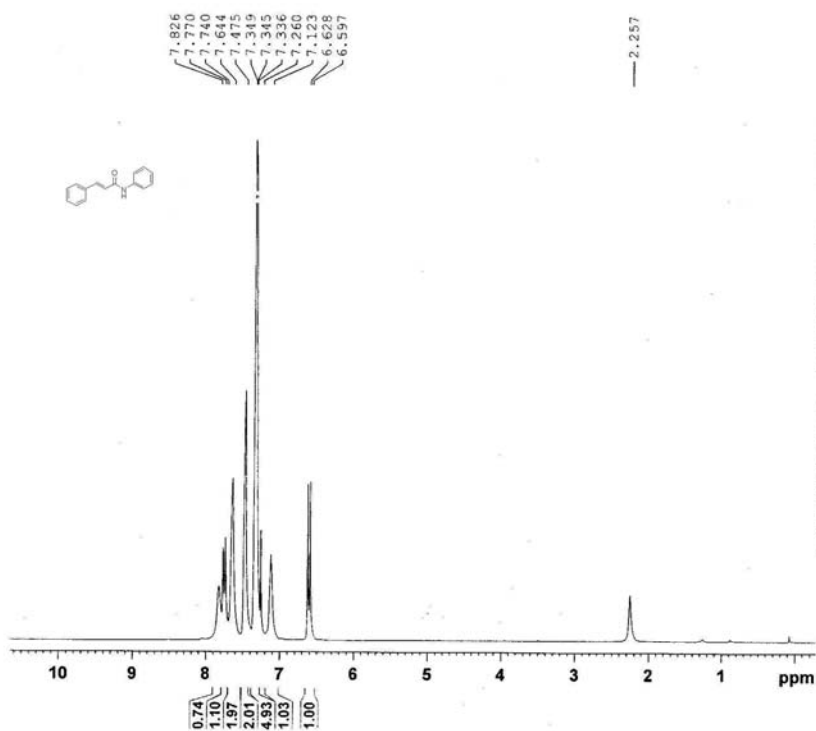
CHANNEL f1

NUC1 13C
P1 9.80 usec
PL1 2.80 dB
PL1W 52.46661758 W
SFO1 125.7703643 MHz

CHANNEL f2

CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.89 dB
PL13 16.70 dB
PL2W 9.90558243 W
PL12W 0.32127732 W
PL13W 0.33564481 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577977 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

(E)-N-phenylcinnamamide (4bj)

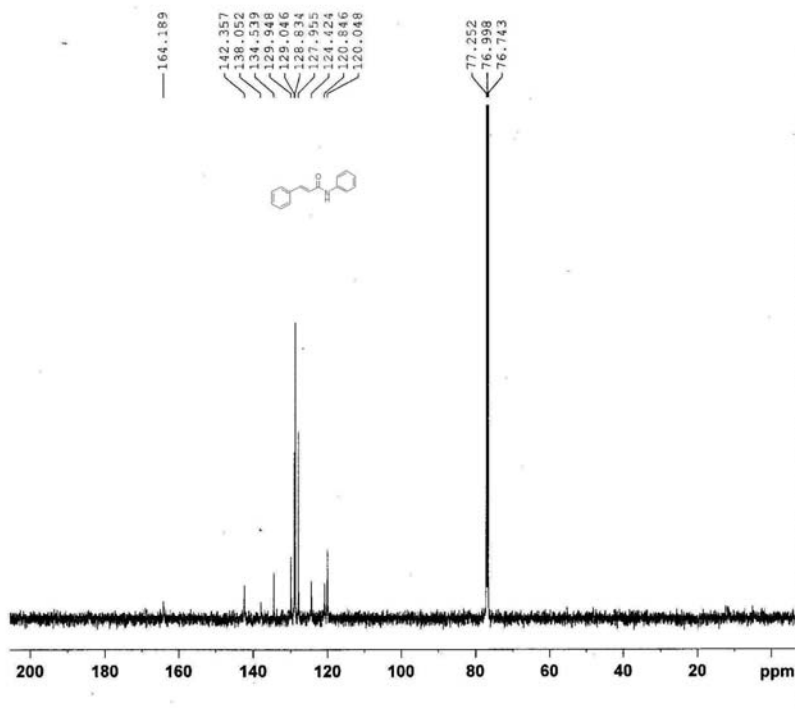


h-yxh-1

NAME	yxh111129
EXPNO	7
PROCNO	1
Date_	20111129
Time	19.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10330.578 Hz
FIDRES	0.157632 Hz
AQ	3.1719923 sec
RG	228
DW	48.400 usec
DE	6.50 usec
TE	296.6 K
D1	1.00000000 sec
TDO	1

===== CHANNEL f1 =====

NUC1	1H
P1	14.60 usec
PL1	2.00 dB
PL1W	9.90558243 W
SFO1	500.1330865 MHz
SI	32768
SF	500.1300136 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



c-yxh-1

NAME	yxh111129
EXPNO	8
PROCNO	1
Date_	20111129
Time	19.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	282
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	2050
DW	16.800 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TDO	1

===== CHANNEL f1 =====

NUC1	13C
P1	9.80 usec
PL1	2.80 dB
PL1W	52.46661758 W
SFO1	125.7703643 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	16.89 dB
PL13	16.70 dB
PL2W	9.90558243 W
PL12W	0.32127732 W
PL13W	0.33564481 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577949 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40