

Oxidative 1,2-Difunctionalization of Activated Alkenes with Benzylic C(sp³)-H Bonds and Aryl C(sp²)-H Bonds

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(A) Typical experimental procedure

(a) Typical Procedures for the Synthesis of Substrates 1:

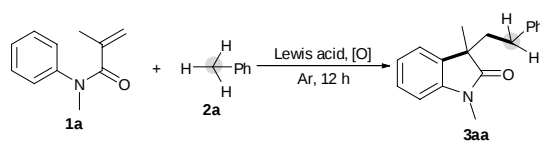
Substrates **1** were synthesized according to the literatures.¹

(b) Typical Experimental Procedure for the Organomediated Oxidative 1,2-Difunctionalization of Activated Alkenes:

To a Schlenk tube were added *N*-arylacrylamide **1** (0.5 mmol), arylmethane **2** (7.5 mmol), IrCl₃ (3 mol%), and DTBP (2 equiv). Then the tube was charged with argon, and was stirred at 120 °C 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 = 10 : 1) to afford the desired product.

(c) Table S1: Screening the optimal conditions

Table S1 Screening Optimal Conditions^a



Entry	Lewis acid (mol%)	[O]	Solvent	Isolated Yield (%)
1	—	DTBP	neat	53
2	—	TBHP	neat	47
3	—	BPO	neat	22
4	—	PhI(OAc) ₂	neat	42
5	FeCl ₃ (10)	DTBP	neat	68
6	Fe(acac) ₃ (10)	DTBP	neat	62
7	CuCl ₂ (10)	DTBP	neat	63
8	ZnCl ₂ (10)	DTBP	neat	65
9	InBr ₃ (10)	DTBP	neat	67
10	CoCl ₂ (10)	DTBP	neat	64
11	PdCl ₂ (10)	DTBP	neat	81
12	RuCl ₃ (10)	DTBP	neat	78
13	RhCl ₃ (10)	DTBP	neat	79

14	IrCl ₃ (10)	DTBP	neat	85
15 ^b	IrCl ₃ (10)	DTBP	neat	80
16 ^c	IrCl ₃ (10)	DTBP	neat	8
17 ^d	IrCl ₃ (3)	DTBP	neat	83
18 ^d	IrCl ₃ (3)	DCP	neat	81
19 ^{d,e}	IrCl ₃ (3)	DTBP	DMSO	79
20 ^{d,e}	IrCl ₃ (3)	DTBP	NMP	trace
21 ^{d,f}	IrCl ₃ (3)	DTBP	neat	75
22 ^{d,g}	IrCl ₃ (3)	DTBP	neat	86

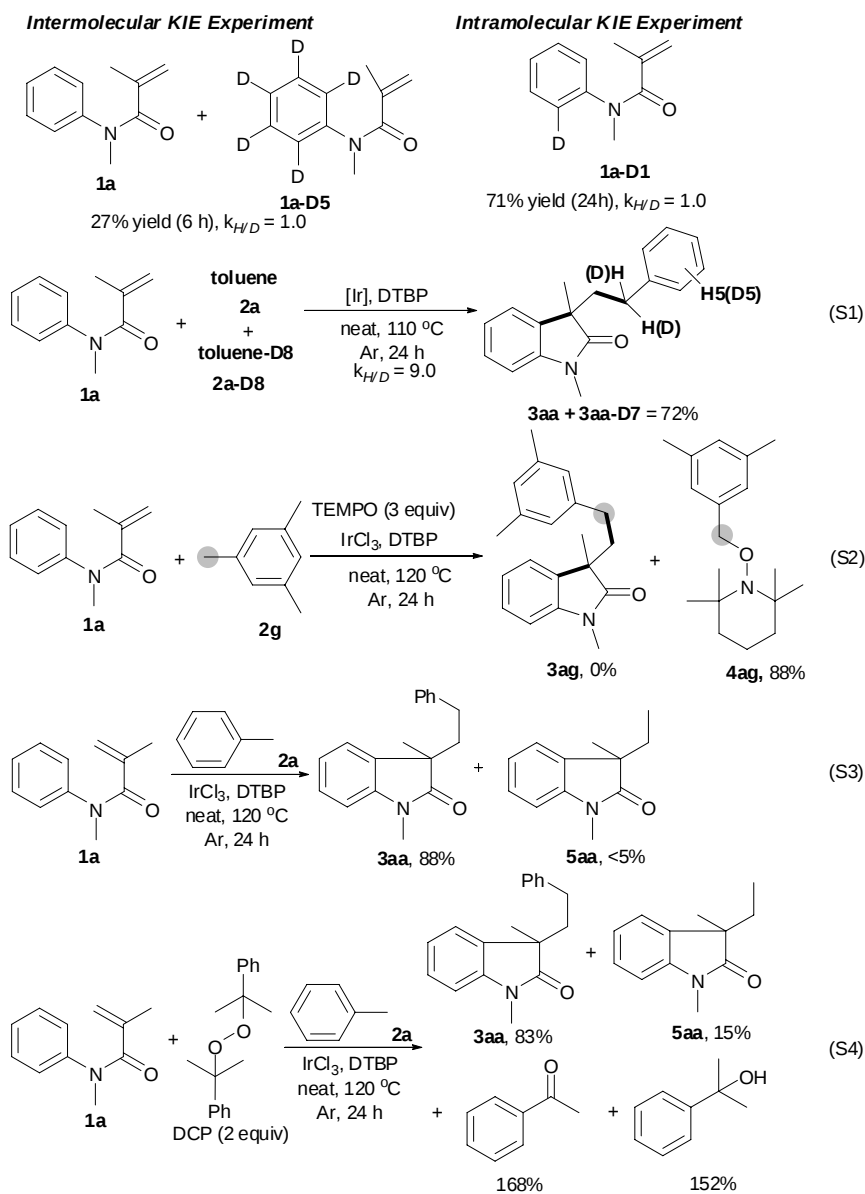
^a Reaction conditions: **1a** (0.5 mmol), **2a** (7.5 mmol), Lewis acid and [O] (1.0 mmol) at 120 °C under argon atmosphere for 12 h.

^b At 130 °C. ^c At 90 °C. ^d For 24 h. ^e **2a** (5 mmol) in solvent (anhydrous, 0.5 mL). ^f DTBP (0.6 mmol). ^g **1a** (10 mmol) and **2a** (15 equiv) for 48 h.

(d) The control experiments

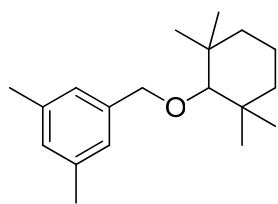
As shown in Scheme S1, some control experiments were carried out to understand the mechanism. The results demonstrated that no kinetic isotope effect ($k_H/k_D = 1.0$) in either intramolecular or intermolecular experiments was discovered, implying that the iron-catalyzed oxidative difunctionalization proceeds via either the SEAr mechanism or the free radical mechanism ((a) W. D. Jones, *Acc. Chem. Res.* 2003, **36**, 140; (b) A. Pinto, L. Neuville, P. Retailleau and J. Zhu, *Org. Lett.* 2006, **8**, 4927; (c) W. D. Jones and F. J. Feher, *J. Am. Chem. Soc.* 1986, **108**, 4814; (d) X. Chen, X.-S. Hao, C. E. Goodhue and J.-Q. Yu, *J. Am. Chem. Soc.* 2006, **128**, 6790.). The deuterated experiment between toluene and toluene-D₈ ($k_H/k_D = 9.0$) supports that benzyl C-H bond cleavage is the rate-limiting step (Eq S1). Notably, two radical inhibitors, TEMPO (Eq 3) and 2,6-di-*tert*-butylphenol, were added to the difunctionalization reaction: a stoichiometric amount of radical inhibitor (2 equiv) results in no conversion of amide **1a**; however, mesitylene (**2g**) was transferred by TEMPO into 1-(3,5-dimethylbenzyloxy)-2,2,6,6-tetramethylpiperidine (**6ag**) in 88% yield (Eq S2). The results suggest that a mesitylene radical is yielded and the current reaction includes a radical process.

The data of the reaction between **1a** and **2a** in-situ determined by GC-MS analysis showed that a DCP could be converted into a methyl group, a ketone and an alcohol (Eqs S3 and S4).



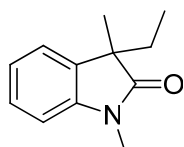
Scheme S1. Control Experiments.

1,3-Dimethyl-5-(((2,2,6,6-tetramethylcyclohexyl)oxy)methyl)benzene (4aa):



^1H NMR (400 MHz, CDCl_3) δ : 6.98 (s, 2H), 6.88 (s, 1H), 4.75 (s, 2H), 2.32 (s, 6H), 1.61-1.49 (m, 4H), 1.36-1.08 (m, 14H); ^{13}C NMR (100 MHz, CDCl_3) δ : 131.3, 131.0, 122.5, 118.8, 72.1, 53.3, 33.1, 26.5, 14.9, 13.8, 10.5.

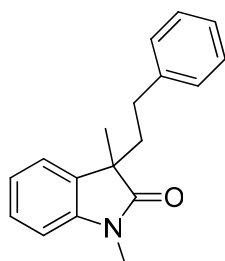
3-Ethyl-1,3-dimethylindolin-2-one (5aa):



Yellow oil; ^1H NMR (500 MHz, CDCl_3) δ : 7.26 (t, $J = 7.5$ Hz, 1H), 7.17 (d, $J = 7.5$ Hz, 1H), 7.07 (t, $J = 7.5$ Hz, 1H), 6.84 (d, $J = 8.0$ Hz, 1H), 3.22 (s, 3H), 1.97-1.89 (m, 1H), 1.81-1.74 (m, 1H), 1.35 (s, 3H), 0.59 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 180.7, 143.4, 133.9, 127.6, 122.5, 122.4, 107.8, 48.9, 31.4, 26.0, 23.3, 8.8; IR (KBr, cm^{-1}): 1722, 1461; LRMS (EI, 70 eV) m/z (%): 189 (M^+ , 21), 161 (100); HRMS m/z (ESI) calcd for $\text{C}_{12}\text{H}_{16}\text{NO}$ ($[\text{M}+\text{H}]^+$) 190.1308, found 190.1312.

(B) Analytical data

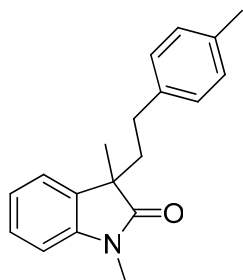
1,3-Dimethyl-3-phenethylindolin-2-one (3aa):



Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.30 (t, $J = 7.6$ Hz, 1H), 7.25-7.19 (m, 3H), 7.15-7.09 (m, 2H), 7.03 (d, $J = 7.6$ Hz, 2H), 6.87 (d, $J = 7.6$ Hz, 1H), 3.21 (s, 3H), 2.33-2.23 (m, 2H), 2.15-1.97 (m, 2H), 1.39 (s, 3H); ^{13}C NMR (100

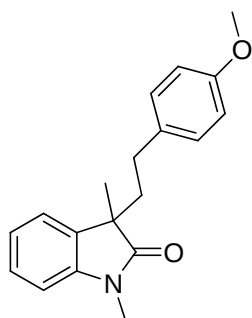
MHz, CDCl₃) δ : 180.3, 143.3, 141.3, 133.6, 128.2 (2C), 127.8, 125.8, 122.6, 122.4, 108.0, 48.3, 40.2, 30.9, 26.1, 23.9; IR (KBr, cm⁻¹): 1711, 1668, 1432; LRMS (EI, 70 eV) m/z (%): 265 (M⁺, 3), 161 (100); HRMS m/z (ESI) calcd for C₁₈H₂₀NO ([M+H]⁺) 266.1539, found 266.1543.

1,3-Dimethyl-3-(4-methylphenethyl)indolin-2-one (3ab):



Yellow oil; ¹H NMR (400 MHz, CDCl₃) δ : 7.29 (t, J = 7.6 Hz, 1H), 7.23 (d, J = 9.2 Hz, 1H), 7.10 (t, J = 7.2 Hz, 1H), 7.01 (d, J = 8.0 Hz, 2H), 6.91 (d, J = 8.0 Hz, 2H), 6.86 (d, J = 7.6 Hz, 1H), 3.20 (s, 3H), 2.29-2.20 (m, 2H), 2.24 (s, 3H), 2.10-1.95 (m, 2H), 1.38 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ : 180.4, 143.3, 138.2, 135.2, 133.7, 128.9, 128.1, 127.7, 122.5, 122.4, 108.0, 48.4, 40.4, 30.4, 26.1, 23.9, 20.9; IR (KBr, cm⁻¹): 1716, 1684, 1481; LRMS (EI, 70 eV) m/z (%): 279 (M⁺, 1), 161 (100); HRMS m/z (ESI) calcd for C₁₉H₂₂NO ([M+H]⁺) 280.1696, found 280.1702.

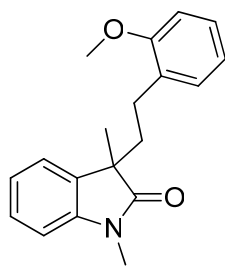
3-(4-Methoxyphenethyl)-1,3-dimethylindolin-2-one (3ac):



Yellow oil; ¹H NMR (400 MHz, CDCl₃) δ : 7.30-7.22 (m, 2H), 7.11 (t, J = 6.0 Hz, 1H), 6.94 (d, J = 6.8 Hz, 2H), 6.86 (d, J = 6.0 Hz, 1H), 6.75 (d, J = 6.8 Hz, 2H), 3.75 (s, 3H), 3.21 (s, 3H), 2.26-2.20 (m, 2H), 2.09-1.95 (m, 2H), 1.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ : 180.3, 157.8, 143.4, 133.8, 133.5, 129.1, 127.8,

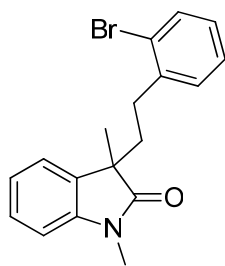
122.5 (2C), 113.7, 107.9, 55.2, 48.3, 40.5, 30.0, 26.1, 23.9; IR (KBr, cm^{-1}): 1723, 1668, 1413; LRMS (EI, 70 eV) m/z (%): 295 (M^+ , 3), 161 (100); HRMS m/z (ESI) calcd for $\text{C}_{19}\text{H}_{22}\text{NO}_2$ ($[\text{M}+\text{H}]^+$) 296.1645, found 296.1654.

3-(2-Methoxyphenethyl)-1,3-dimethylindolin-2-one (3ad):



Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.29-7.22 (m, 2H), 7.12-7.07 (m, 2H), 6.91 (d, $J = 7.6$ Hz, 1H), 6.84 (d, $J = 7.6$ Hz, 1H), 6.79-6.73 (m, 2H), 3.74 (s, 3H), 3.20 (s, 3H), 2.36-2.16 (m, 3H), 2.07-1.97 (m, 1H), 1.38 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 180.5, 157.4, 143.5, 134.0, 129.9, 129.7, 127.6, 127.1, 122.7, 122.3, 120.2, 110.1, 107.8, 55.1, 48.4, 38.1, 26.1, 25.6, 24.0; IR (KBr, cm^{-1}): 1716, 1614, 1471; LRMS (EI, 70 eV) m/z (%): 295 (M^+ , 1), 161 (100); HRMS m/z (ESI) calcd for $\text{C}_{19}\text{H}_{22}\text{NO}_2$ ($[\text{M}+\text{H}]^+$) 296.1645, found 296.1654.

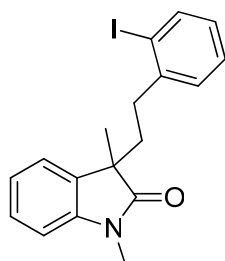
3-(2-Bromophenethyl)-1,3-dimethylindolin-2-one (3ae):



Yellow oil; ^1H NMR (500 MHz, CDCl_3) δ : 7.44 (d, $J = 8.0$ Hz, 1H), 7.30 (d, $J = 8.0$ Hz, 2H), 7.17-7.07 (m, 3H), 7.00 (t, $J = 7.0$ Hz, 1H), 6.88 (d, $J = 7.0$ Hz, 1H), 3.25 (s, 3H), 2.41-2.28 (m, 2H), 2.20-2.13 (m, 1H), 2.08-2.02 (m, 1H), 1.40 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 180.2, 143.3, 140.7, 133.4, 132.6, 130.4, 127.8, 127.6, 127.4, 124.1, 122.7, 122.5, 107.9, 48.3, 38.3, 31.5, 26.2, 23.8; IR (KBr,

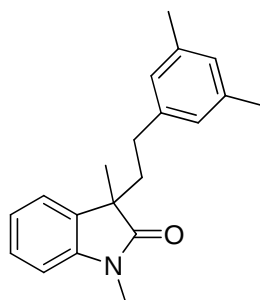
cm^{-1}): 1719, 1623, 1422; LRMS (EI, 70 eV) m/z (%): 345 ($M^+ + 2$, 2), 343 (M^+ , 2), 161 (100); HRMS m/z (ESI) calcd for $\text{C}_{18}\text{H}_{19}\text{BrNO}$ ($[M+H]^+$) 344.0652, found 344.0658.

3-(2-Iodophenethyl)-1,3-dimethylindolin-2-one (3af):



Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.72 (d, $J = 8.0$ Hz, 1H), 7.34-7.26 (m, 2H), 7.20 (t, $J = 7.2$ Hz, 1H), 7.11-7.08 (m, 2H), 6.88 (d, $J = 7.6$ Hz, 1H), 6.82 (t, $J = 7.2$ Hz, 1H), 3.23 (s, 3H), 2.44-2.36 (m, 1H), 2.30-2.27 (m, 1H), 2.15-1.99 (m, 2H), 1.41 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 180.2, 144.0, 143.2, 139.3, 133.3, 129.5, 128.3, 127.9, 127.8, 123.0, 122.5, 107.9, 100.0, 48.2, 38.6, 36.0, 26.2, 23.7; IR (KBr, cm^{-1}): 1708, 1633, 1413; LRMS (EI, 70 eV) m/z (%): 391 (M^+ , 3), 161 (100); HRMS m/z (ESI) calcd for $\text{C}_{18}\text{H}_{19}\text{INO}$ ($[M+H]^+$) 392.0513, found 392.0519.

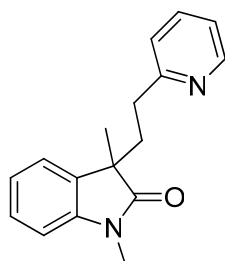
3-(3,5-Dimethylphenethyl)-1,3-dimethylindolin-2-one (3ag):



Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.29 (t, $J = 7.6$ Hz, 1H), 7.23 (d, $J = 7.2$ Hz, 1H), 7.10 (d, $J = 7.6$ Hz, 1H), 6.86 (d, $J = 7.6$ Hz, 1H), 6.77 (s, 1H), 6.66 (s, 2H), 3.22 (s, 3H), 2.29-2.17 (m, 2H), 2.23 (s, 6H), 2.08-1.95 (m, 2H), 1.39 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 180.4, 143.3, 141.3, 137.6, 133.7, 127.7, 127.4, 126.1, 122.5, 122.4, 107.9, 48.4, 40.4, 30.7, 26.1, 23.9, 21.1; IR (KBr, cm^{-1}):

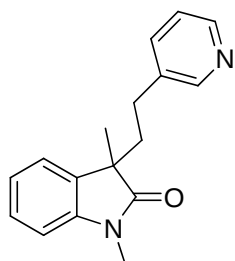
1703, 1621, 1406; LRMS (EI, 70 eV) m/z (%): 293 (M^+ , 8), 161 (100); HRMS m/z (ESI) calcd for $C_{20}H_{24}NO$ ($[M+H]^+$) 294.1832, found 294.1828.

1,3-Dimethyl-3-(2-(pyridin-2-yl)ethyl)indolin-2-one (3ah):



Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ : 8.45 (d, $J = 4.8$ Hz, 1H), 7.51 (t, $J = 7.6$ Hz, 1H), 7.29-7.20 (m, 2H), 7.09-7.04 (m, 2H), 7.00 (d, $J = 7.6$ Hz, 1H), 6.86 (d, $J = 7.6$ Hz, 1H), 3.24 (s, 3H), 2.53-2.19 (m, 4H), 1.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 180.3, 160.9, 148.9, 143.1, 136.3, 133.5, 127.8, 122.7 (2C), 121.1, 107.9, 48.2, 37.8, 33.2, 26.1, 23.8; IR (KBr, cm^{-1}): 1716, 1618, 1431; LRMS (EI, 70 eV) m/z (%): 266 (M^+ , 12), 161 (100); HRMS m/z (ESI) calcd for $C_{17}H_{19}N_2O$ ($[M+H]^+$) 267.1492, found 267.1498.

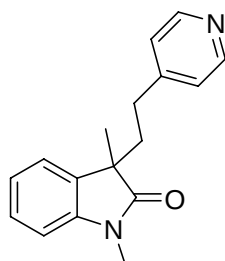
1,3-Dimethyl-3-(2-(pyridin-3-yl)ethyl)indolin-2-one (3ai):



Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ : 8.38 (d, $J = 4.0$ Hz, 1H), 8.21 (s, 1H), 7.38 (t, $J = 7.6$ Hz, 1H), 7.32 (t, $J = 7.6$ Hz, 1H), 7.23 (t, $J = 7.2$ Hz, 1H), 7.16-7.10 (m, 2H), 6.88 (d, $J = 7.6$ Hz, 1H), 3.20 (s, 3H), 2.34-2.26 (m, 2H), 2.25-2.10 (m, 1H), 2.09-1.99 (m, 1H), 1.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 180.1, 149.7, 147.5, 143.3, 136.5, 135.8, 133.3, 128.1, 123.2, 122.8, 122.5, 108.2, 48.3, 39.6, 28.3, 26.2, 24.1; IR (KBr, cm^{-1}): 1721, 1632, 1431; LRMS (EI, 70 eV) m/z (%): 266

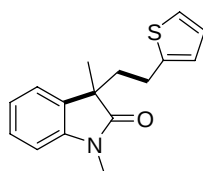
(M^+ , 4), 161 (100); HRMS m/z (ESI) calcd for $C_{17}H_{19}N_2O$ ($[M+H]^+$) 267.1492, found 267.1496.

1,3-Dimethyl-3-(2-(pyridin-4-yl)ethyl)indolin-2-one (3aj):



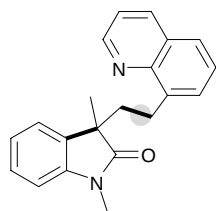
Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ : 8.41 (d, $J = 5.6$ Hz, 2H), 7.34-7.28 (m, 1H), 7.22 (d, $J = 6.8$ Hz, 1H), 7.12 (t, $J = 3.6$ Hz, 1H), 6.96 (d, $J = 6.0$ Hz, 2H), 6.89 (d, $J = 7.6$ Hz, 1H), 3.22 (s, 3H), 2.33-2.24 (m, 2H), 2.17-1.98 (m, 2H), 1.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 180.0, 150.2, 149.5, 143.2, 133.1, 128.0, 123.7, 122.7, 122.4, 108.1, 48.2, 38.7, 30.3, 26.1, 23.9; IR (KBr, cm^{-1}): 1723, 1646, 1406; LRMS (EI, 70 eV) m/z (%): 266 (M^+ , 17), 161 (100); HRMS m/z (ESI) calcd for $C_{17}H_{19}N_2O$ ($[M+H]^+$) 267.1492, found 267.1480.

1,3-Dimethyl-3-(2-(thiophen-2-yl)ethyl)indolin-2-one (3ak):



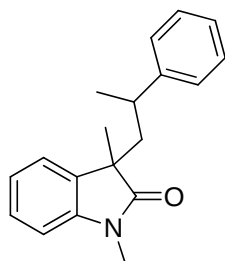
Brown oil; 1H NMR (500 MHz, $CDCl_3$) δ : 7.29 (d, $J = 7.5$ Hz, 1H), 7.21 (d, $J = 7.0$ Hz, 1H), 7.09 (t, $J = 7.5$ Hz, 1H), 7.04 (t, $J = 5.0$ Hz, 1H), 6.87-6.82 (m, 2H), 6.64 (d, $J = 3.5$ Hz, 1H), 3.21 (s, 3H), 2.57-2.49 (m, 1H), 2.40-2.30 (m, 2H), 2.14-2.07 (m, 1H), 1.41 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ : 180.0, 144.1, 143.3, 133.4, 127.9, 126.5, 124.0, 123.0, 122.6, 122.5, 108.0, 48.1, 40.1, 26.1, 25.0, 23.8; IR (KBr, cm^{-1}): 1731, 1651, 1422, 896; LRMS (EI, 70 eV) m/z (%): 271 (M^+ , 2), 161 (100); HRMS m/z (ESI) calcd for $C_{16}H_{18}NOS$ ($[M+H]^+$) 272.1111, found 272.1116.

1,3-Dimethyl-3-(2-(quinolin-8-yl)ethyl)indolin-2-one (3al):



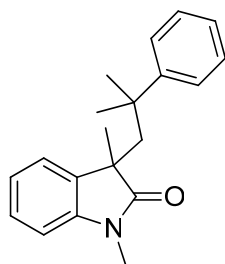
Brown oil; ^1H NMR (500 MHz, CDCl_3) δ : 8.86 (d, $J = 4.0$ Hz, 1H), 8.04 (d, $J = 8.0$ Hz, 1H), 7.57 (d, $J = 4.5$ Hz, 1H), 7.35-7.23 (m, 5H), 7.06 (t, $J = 7.5$ Hz, 1H), 6.82 (d, $J = 7.5$ Hz, 1H), 3.21 (s, 3H), 3.00-2.94 (m, 2H), 2.44-2.38 (m, 1H), 2.32-2.26 (m, 1H), 1.41 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 180.6, 149.1, 146.6, 143.3, 140.3, 136.0, 133.9, 128.6, 128.1, 127.6, 126.0 (2C), 122.8, 122.3, 120.7, 107.8, 48.5, 38.7, 26.8, 26.1, 24.1; IR (KBr, cm^{-1}): 1703, 1632, 1418, 982; LRMS (EI, 70 eV) m/z (%): 316 (M^+ , 1), 156 (100); HRMS m/z (ESI) calcd for $\text{C}_{21}\text{H}_{21}\text{N}_2\text{O}$ ($[\text{M}+\text{H}]^+$) 317.1656, found 317.1648.

1,3-Dimethyl-3-(2-phenylpropyl)indolin-2-one (3am):



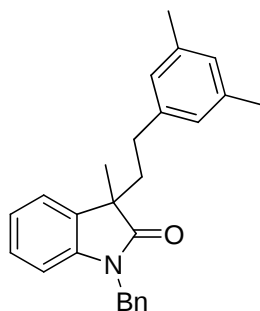
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.14 (t, $J = 7.6$ Hz, 1H), 7.08-7.00 (m, 3H), 6.93-6.85 (m, 4H), 6.72 (d, $J = 8.0$ Hz, 1H), 3.21 (s, 3H), 2.42-2.37 (m, 1H), 2.33-2.28 (m, 1H), 2.20-2.15 (m, 1H), 1.30 (s, 3H), 1.04 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 180.7, 147.3, 143.0, 133.4, 128.0, 127.4, 126.6, 125.7, 122.9, 122.3, 107.8, 48.2, 46.1, 37.2, 26.1, 26.0, 22.7; IR (KBr, cm^{-1}): 1709, 1665, 1412; LRMS (EI, 70 eV) m/z (%): 279 (M^+ , 6), 161 (100); HRMS m/z (ESI) calcd for $\text{C}_{19}\text{H}_{22}\text{NO}$ ($[\text{M}+\text{H}]^+$) 280.1696, found 280.1694.

1,3-Dimethyl-3-(2-methyl-2-phenylpropyl)indolin-2-one (3an):



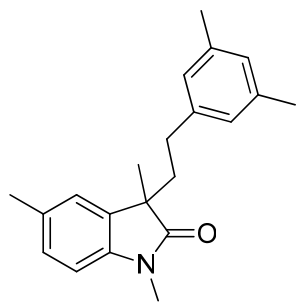
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.13-7.02 (m, 4H), 6.97 (d, $J = 7.6$ Hz, 2H), 6.72-6.63 (m, 3H), 2.99 (s, 3H), 2.54 (d, $J = 14.4$ Hz, 1H), 2.29 (d, $J = 14.4$ Hz, 1H), 1.23 (s, 3H), 1.10 (s, 3H), 1.05 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 180.4, 148.2, 142.5, 132.7, 127.4, 126.9, 125.9, 125.3, 123.9, 121.7, 107.5, 51.5, 47.4, 37.8, 31.0, 28.3, 28.1, 26.0; IR (KBr, cm^{-1}): 1721, 1653, 1401; LRMS (EI, 70 eV) m/z (%): 293 (M^+ , 5), 161 (100); HRMS m/z (ESI) calcd for $\text{C}_{20}\text{H}_{24}\text{NO}$ ($[\text{M}+\text{H}]^+$) 294.1781, found 294.1798.

1-Benzyl-3-(3,5-dimethylphenethyl)-3-methylindolin-2-one (3bg):



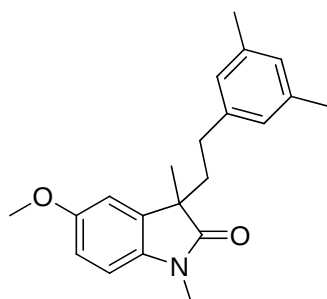
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.30-7.21 (m, 6H), 7.18 (d, $J = 7.6$ Hz, 1H), 7.13 (t, $J = 7.6$ Hz, 1H), 7.07-6.68 (m, 4H), 4.99 (d, $J = 16.0$ Hz, 1H), 4.87 (d, $J = 16.0$ Hz, 1H), 2.34-2.20 (m, 2H), 2.23 (s, 6H), 2.09-2.00 (m, 2H), 1.44 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 180.4, 142.5, 141.4, 137.7, 133.8, 128.7, 127.6, 127.5 (2C), 127.2, 126.2, 126.1, 122.5 (2C), 109.0, 48.4, 43.6, 40.5, 30.9, 24.2, 21.1; IR (KBr, cm^{-1}): 1703, 1621, 1406; LRMS (EI, 70 eV) m/z (%): 369 (M^+ , 1), 237 (100); HRMS m/z (ESI) calcd for $\text{C}_{26}\text{H}_{28}\text{NO}$ ($[\text{M}+\text{H}]^+$) 370.2165, found 370.2166.

3-(3,5-Dimethylphenethyl)-1,3,5-trimethylindolin-2-one (3eg):



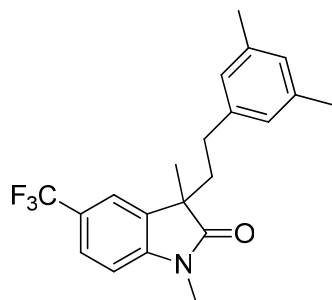
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.08 (d, J = 6.0 Hz, 1H), 7.03 (s, 1H), 6.75 (t, J = 6.4 Hz, 2H), 6.67 (s, 2H), 3.20 (s, 3H), 2.37 (s, 3H), 2.27-2.19 (m, 2H), 2.20 (s, 6H), 2.08-1.94 (m, 2H), 1.37 (s, 3H); ^{13}C NMR (100MHz, CDCl_3) δ : 180.3, 141.4, 140.9, 137.6, 133.7, 132.0, 127.4, 126.1, 123.3, 107.6, 48.4, 40.4, 30.7, 26.9, 23.9, 21.1 (2C); IR (KBr, cm^{-1}): 1711, 1655, 1432; LRMS (EI, 70 eV) m/z (%): 307 (M^+ , 5), 175 (100); HRMS m/z (ESI) calcd for $\text{C}_{21}\text{H}_{26}\text{NO}$ ($[\text{M}+\text{H}]^+$) 308.2009, found 308.2008.

3-(3,5-Dimethylphenethyl)-5-methoxy-1,3-dimethylindolin-2-one (3fg):



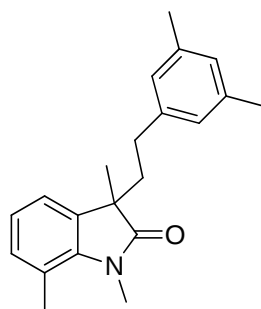
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 6.83-6.79 (m, 2H), 6.75 (d, J = 8.4 Hz, 2H), 6.65 (s, 2H), 3.82 (s, 3H), 3.19 (s, 3H), 2.29-2.19 (m, 2H), 2.20 (s, 6H), 2.08-1.92 (m, 2H), 1.37 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 180.0, 156.2, 141.3, 137.6, 137.0, 135.3, 127.4, 126.1, 111.7, 110.3, 108.1, 55.8, 48.9, 40.5, 30.8, 26.2, 24.0, 21.1; IR (KBr, cm^{-1}): 1708, 1621, 1493; LRMS (EI, 70 eV) m/z (%): 323 (M^+ , 12), 191 (100); HRMS m/z (ESI) calcd for $\text{C}_{21}\text{H}_{26}\text{NO}_2$ ($[\text{M}+\text{H}]^+$) 324.1965, found 324.1968.

3-(3,5-Dimethylphenethyl)-1,3-dimethyl-5-(trifluoromethyl)indolin-2-one (3gg):



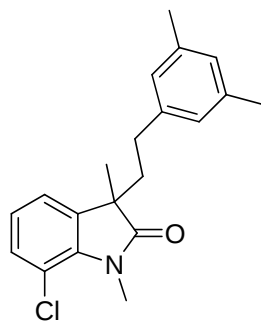
Yellow oil; ^1H NMR (500 MHz, CDCl_3) δ : 7.56 (d, $J = 8.0$ Hz, 1H), 7.41 (s, 1H), 6.91 (d, $J = 8.0$ Hz, 1H), 6.77 (s, 1H), 6.62 (s, 2H), 3.24 (s, 3H), 2.32-2.18 (m, 2H), 2.22 (s, 6H), 2.09-2.00 (m, 2H), 1.41 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 180.2, 146.3, 140.6, 137.7, 134.3, 127.6, 126.0, 125.6 (d, $J = 12.8$ Hz, 1C), 124.1 (q, $J = 186.6$ Hz, 1C), 119.5 (d, $J = 3.5$ Hz, 1C), 107.6, 48.4, 40.0, 30.7, 26.3, 23.9, 21.1; IR (KBr, cm^{-1}): 1716, 1624, 1416; LRMS (EI, 70 eV) m/z (%): 361 (M^+ , 1), 229 (100); HRMS m/z (ESI) calcd for $\text{C}_{21}\text{H}_{23}\text{F}_3\text{NO}$ ($[\text{M}+\text{H}]^+$) 362.1730, found 362.1726.

3-(3,5-Dimethylphenethyl)-1,3,7-trimethylindolin-2-one (3hg):



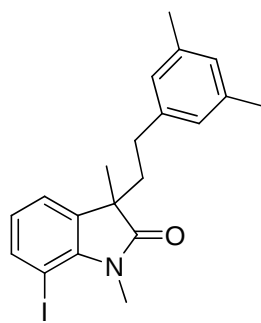
Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.05 (d, $J = 6.4$ Hz, 1H), 7.02-6.96 (m, 2H), 6.77 (s, 1H), 6.66 (s, 2H), 3.50 (s, 3H), 2.60 (s, 3H), 2.27-2.13 (m, 2H), 2.22 (s, 6H), 2.09-1.90 (m, 2H), 1.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 181.1, 141.3, 141.0, 137.6, 134.3, 131.4, 127.4 (2C), 126.1 (2C), 122.4, 120.3, 119.5, 47.7, 40.7, 30.7, 29.4, 24.3, 21.1, 19.0; IR (KBr, cm^{-1}): 1715, 1662, 1413; LRMS (EI, 70 eV) m/z (%): 307 (M^+ , 4), 175 (100); HRMS m/z (ESI) calcd for $\text{C}_{20}\text{H}_{26}\text{NO}$ ($[\text{M}+\text{H}]^+$) 308.2009, found 308.2008.

7-Chloro-3-(3,5-dimethylphenethyl)-1,3-dimethylindolin-2-one (3ig):



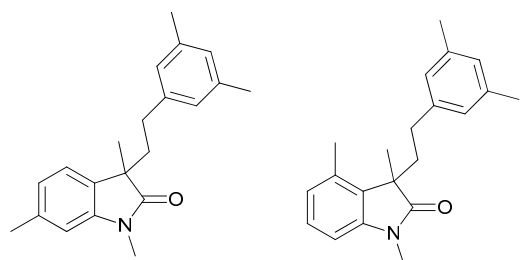
Yellow oil; ^1H NMR (500 MHz, CDCl_3) δ : 7.20 (d, $J = 8.0$ Hz, 1H), 7.08 (d, $J = 7.0$ Hz, 1H), 6.99 (d, $J = 7.5$ Hz, 1H), 6.77 (s, 1H), 6.64 (s, 2H), 3.57 (s, 3H), 2.30-2.18 (m, 2H), 2.25 (s, 6H), 2.07-1.92 (m, 2H), 1.37 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 180.5, 140.8, 139.2, 137.7, 136.5, 130.0, 127.5, 126.1, 123.3, 120.9, 115.4, 48.1, 40.5, 30.7, 29.4, 24.3, 21.1; IR (KBr, cm^{-1}): 1716, 1635, 1423; LRMS (EI, 70 eV) m/z (%): 327 (M^+ , 1), 197 (32), 195 (100); HRMS m/z (ESI) calcd for $\text{C}_{20}\text{H}_{23}\text{ClNO}$ ($[\text{M}+\text{H}]^+$) 328.1463, found 328.1461.

3-(3,5-Dimethylphenethyl)-7-iodo-1,3-dimethylindolin-2-one (3jg):



Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.67 (d, $J = 7.6$ Hz, 1H), 7.14 (d, $J = 7.2$ Hz, 1H), 6.78 (t, $J = 7.6$ Hz, 2H), 6.63 (s, 2H), 3.58 (s, 3H), 2.30-2.14 (m, 2H), 2.23 (s, 6H), 2.07-1.91 (m, 2H), 1.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 180.9, 143.6, 140.8, 140.3, 137.7, 136.8, 127.5, 126.1 (2C), 124.2, 122.2, 71.6, 47.9, 40.4, 30.7, 29.9, 24.3, 21.2; IR (KBr, cm^{-1}): 1716 1489, 1460; LRMS (EI, 70 eV) m/z (%): 419 (M^+ , 1), 287 (100); HRMS m/z (ESI) calcd for $\text{C}_{20}\text{H}_{23}\text{INO}$ ($[\text{M}+\text{H}]^+$) 420.0826, found 420.0833.

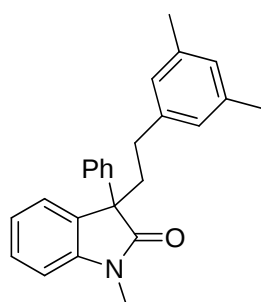
3-(3,5-Dimethylphenethyl)-1,3,6-trimethylindolin-2-one (3kg) and 3-(3,5-Dimethylphenethyl)-1,3,4-trimethylindolin-2-one (3kg')



3kg : 3kg' = 2:1

^1H NMR (400 MHz, CDCl_3) δ : 7.22-7.16 (m, 1H), 7.09 (d, $J = 7.6$ Hz, 0.5H), 6.90 (d, $J = 7.2$ Hz, 0.5H), 6.86-6.82 (m, 1H), 6.76 (s, 1.5H), 6.70-6.62 (m, 4.5H), 3.19 (s, 1.5H), 3.18 (s, 3H), 2.39 (s, 1.5H), 2.35 (s, 3H), 2.34-2.17 (m, 12H), 2.14-1.91 (m, 3H), 1.45 (s, 1.5H), 1.35 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ : 180.6, 180.3, 143.5, 143.3(2C), 141.1, 137.6, 137.5, 137.4, 134.0, 130.6, 130.0, 127.5, 127.3, 126.0 (2C), 124.9, 122.9, 122.1, 108.8, 105.6, 49.3, 48.1, 40.4, 38.2, 30.7, 31.2, 26.0, 25.9, 23.9, 22.3, 21.0, 20.9, 18.1, 14.1.

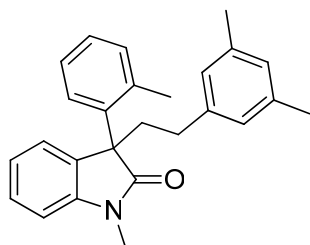
3-(3,5-Dimethylphenethyl)-1-methyl-3-phenylindolin-2-one (3lg):



Yellow oil; ^1H NMR (500 MHz, CDCl_3) δ : 7.38-7.34 (m, 3H), 7.30-7.26 (m, 3H), 7.23-7.20 (m, 1H), 7.17-7.14 (m, 1H), 6.92 (d, $J = 8.0$ Hz, 1H), 6.79 (s, 1H), 6.70 (s, 2H), 3.22 (s, 3H), 2.71 (d, $J = 4.0$ Hz, 1H), 2.47-2.41 (m, 1H), 2.37-2.31 (m, 1H), 2.24 (s, 6H), 2.15-2.10 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ : 178.3, 143.9, 141.1, 140.0, 137.7, 131.9, 128.5, 128.2, 127.5, 127.2, 126.8, 126.1, 124.7, 122.7, 108.3, 56.6, 39.8, 30.8, 26.3, 21.1; IR (KBr, cm^{-1}): 1716, 1681, 1422;

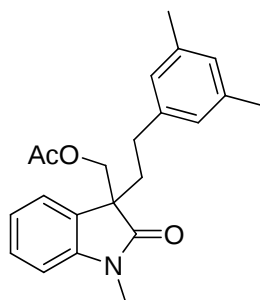
LRMS (EI, 70 eV) m/z (%): 355 (M^+ , 1), 223 (100); HRMS m/z (ESI) calcd for $C_{25}H_{26}NO$ ($[M+H]^+$) 356.2016, found 356.2019.

3-(3,5-Dimethylphenethyl)-1-methyl-3-(*o*-tolyl)indolin-2-one (3mg):



Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ : 7.66 (d, J = 8.0 Hz, 1H), 7.31 (t, J = 7.2 Hz, 1H), 7.24 (t, J = 6.4 Hz, 1H), 7.16 (t, J = 7.6 Hz, 1H), 7.06-7.01 (m, 2H), 6.90 (t, J = 7.6 Hz, 2H), 6.81 (s, 1H), 6.71 (s, 2H), 3.34 (s, 3H), 2.77-2.66 (m, 1H), 2.49-2.29 (m, 2H), 2.25 (s, 6H), 2.04-1.94 (m, 1H), 1.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 178.7, 144.0, 141.3, 138.1, 137.8, 136.9, 132.8, 132.0, 128.0, 127.6, 127.4, 127.3, 126.2, 125.9, 123.2, 123.1, 107.7, 55.9, 40.5, 29.4, 26.2, 21.2, 19.3; IR (KBr, cm^{-1}): 1709, 1665, 1412; LRMS (EI, 70 eV) m/z (%): 369 (M^+ , 2), 147 (100); HRMS m/z (ESI) calcd for $C_{26}H_{28}NO$ ($[M+H]^+$) 370.2165, found 370.2166.

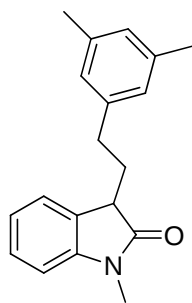
(3-(3,5-Dimethylphenethyl)-1-methyl-2-oxoindolin-3-yl)methyl acetate (3ng):



Yellow oil; 1H NMR (400 MHz, $CDCl_3$) δ : 7.32 (t, J = 7.6 Hz, 1H), 7.26 (d, J = 8.8 Hz, 1H), 7.10 (t, J = 7.2 Hz, 1H), 6.86 (d, J = 7.6 Hz, 1H), 6.77 (s, 1H), 6.63 (s, 2H), 4.53 (d, J = 10.8 Hz, 1H), 4.18 (d, J = 10.8 Hz, 1H), 3.22 (s, 3H), 2.28-2.21 (m, 2H), 2.22 (s, 6H), 2.10-2.05 (m, 2H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 177.2, 170.2, 144.2, 140.7, 137.7, 129.3, 128.4, 127.6, 126.1, 123.3, 122.6,

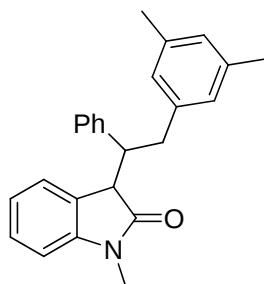
107.9, 67.3, 52.5, 35.4, 29.9, 26.1, 21.1, 20.5; IR (KBr, cm^{-1}): 1712, 1617, 1408;
LRMS (EI, 70 eV) m/z (%): 351 (M^+ , 1), 159 (100); HRMS m/z (ESI) calcd for $\text{C}_{22}\text{H}_{26}\text{NO}_3$ ($[\text{M}+\text{H}]^+$) 352.1907, found 352.1902.

3-(3,5-Dimethylphenethyl)-1-methylindolin-2-one (3og):



Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.30 (t, $J = 8.0$ Hz, 2H), 7.08 (t, $J = 8.0$ Hz, 1H), 6.85-6.80 (m, 4H), 3.49 (t, $J = 6.4$ Hz, 1H), 3.21 (s, 3H), 2.69-2.52 (m, 2H), 2.29-2.20 (m, 2H), 2.26 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ : 177.7, 144.4, 141.2, 137.8, 129.0, 127.9, 127.6, 126.3, 123.8, 122.3, 107.9, 45.0, 32.4, 31.8, 26.1, 21.2; IR (KBr, cm^{-1}): 1706, 1681, 1415; LRMS (EI, 70 eV) m/z (%): 279 (M^+ , 2), 147 (100); HRMS m/z (ESI) calcd for $\text{C}_{19}\text{H}_{22}\text{NO}$ ($[\text{M}+\text{H}]^+$) 280.1696, found 280.1698.

3-(2-(3,5-Dimethylphenyl)-1-phenylethyl)-1-methylindolin-2-one (3pg):



Yellow oil; ^1H NMR (400 MHz, CDCl_3) δ : 7.37-7.34 (m, 1H), 7.18 (t, $J = 6.0$ Hz, 2H), 7.14-7.10 (m, 4H), 6.87 (d, $J = 6.0$ Hz, 3H), 6.76 (s, 2H), 3.88 (d, $J = 2.0$ Hz, 1H), 3.39 (s, 3H), 3.22-3.19 (m, 1H), 3.02-2.98 (m, 1H), 2.48-2.43 (m, 1H), 2.30 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ : 171.2, 141.8, 140.0, 138.3, 138.0, 129.9, 128.6, 128.2, 128.0, 127.3, 127.0, 126.7, 126.3, 123.4, 114.7, 50.5, 44.4,

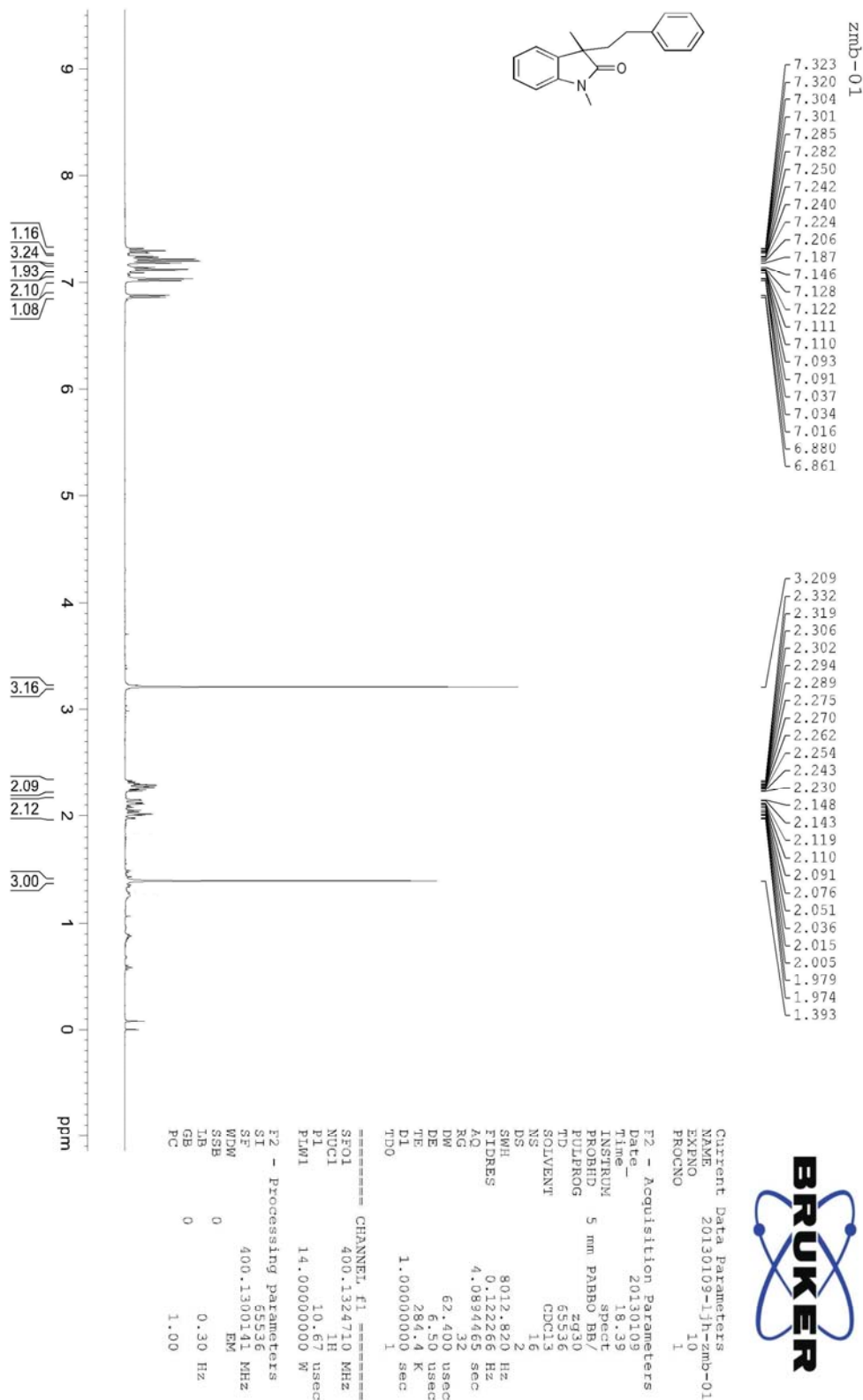
36.0, 29.6, 21.3; IR (KBr, cm^{-1}): 1719, 1665, 1403; LRMS (EI, 70 eV) m/z (%): 355 (M^+ , 3), 236 (100); HRMS m/z (ESI) calcd for $\text{C}_{25}\text{H}_{26}\text{NO}$ ($[\text{M}+\text{H}]^+$) 356.2009, found 356.2006.

(C) Reference

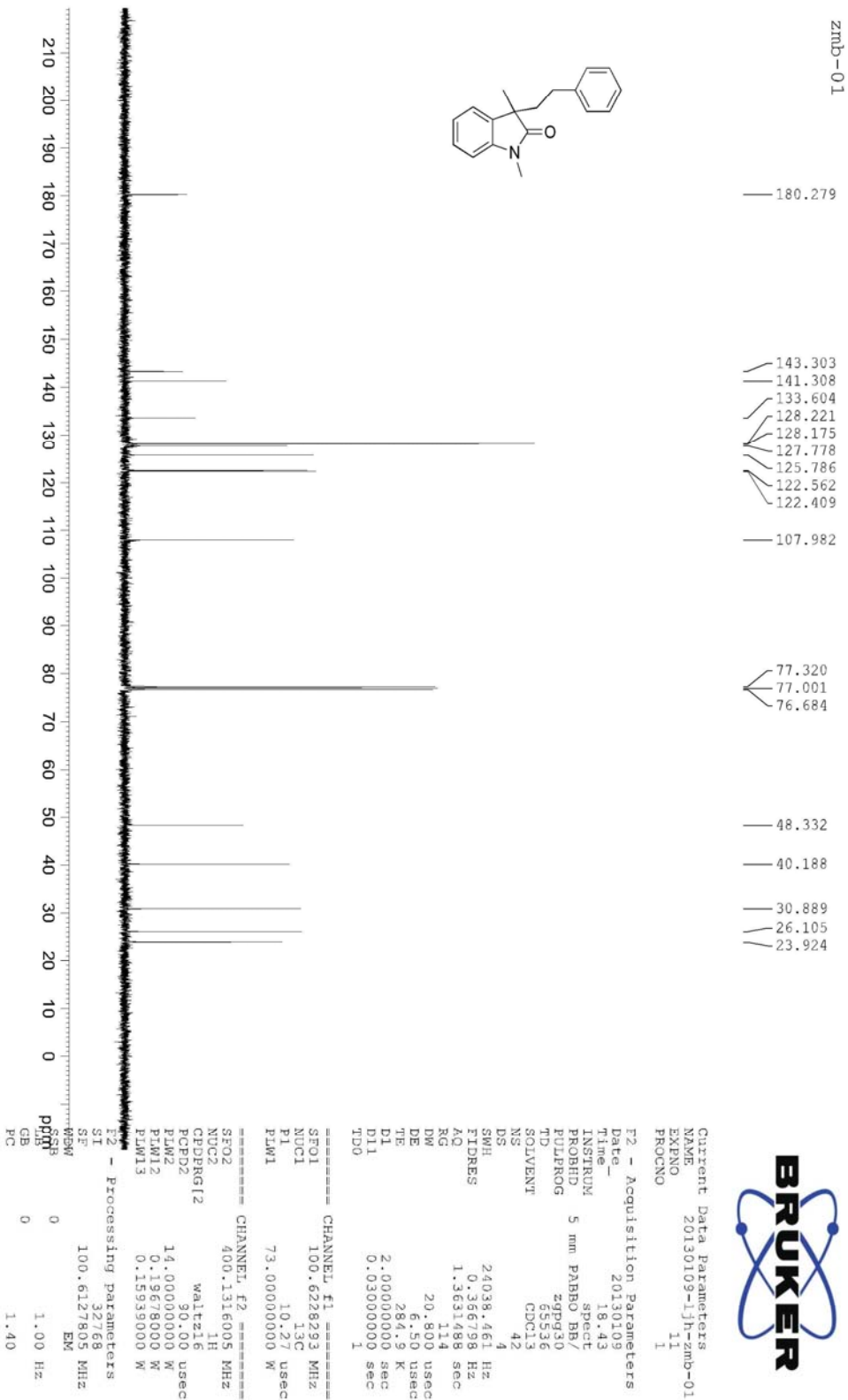
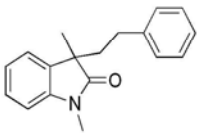
- [1] a) T. Wu, X. Mu, Y.-L. Guo, G.-S. Liu, *Angew. Chem. Int. Ed.* **2011**, *50*, 12578;
b) H. Wei, T. Piou, J. Dufour, L. Neuville, J. Zhu, *Org. Lett.*, **2011**, *13*, 2244; c)
X. Mu, T. Wu, H.-Y. Wang, Y.-L. Guo, G.-S. Liu, *J. Am. Chem. Soc.* **2012**, *134*,
878.
- [S2] T. Nishio, K. Iseki, N. Araki, T. Miyazaki, *Helv. Chim. Acta.* **2005**, *88*, 35.
- [S3] A. Pinto, Y. Jia, L. Neuville, J. Zhu, *Chem. Eur. J.* **2007**, *13*, 961.

(D) Spectra

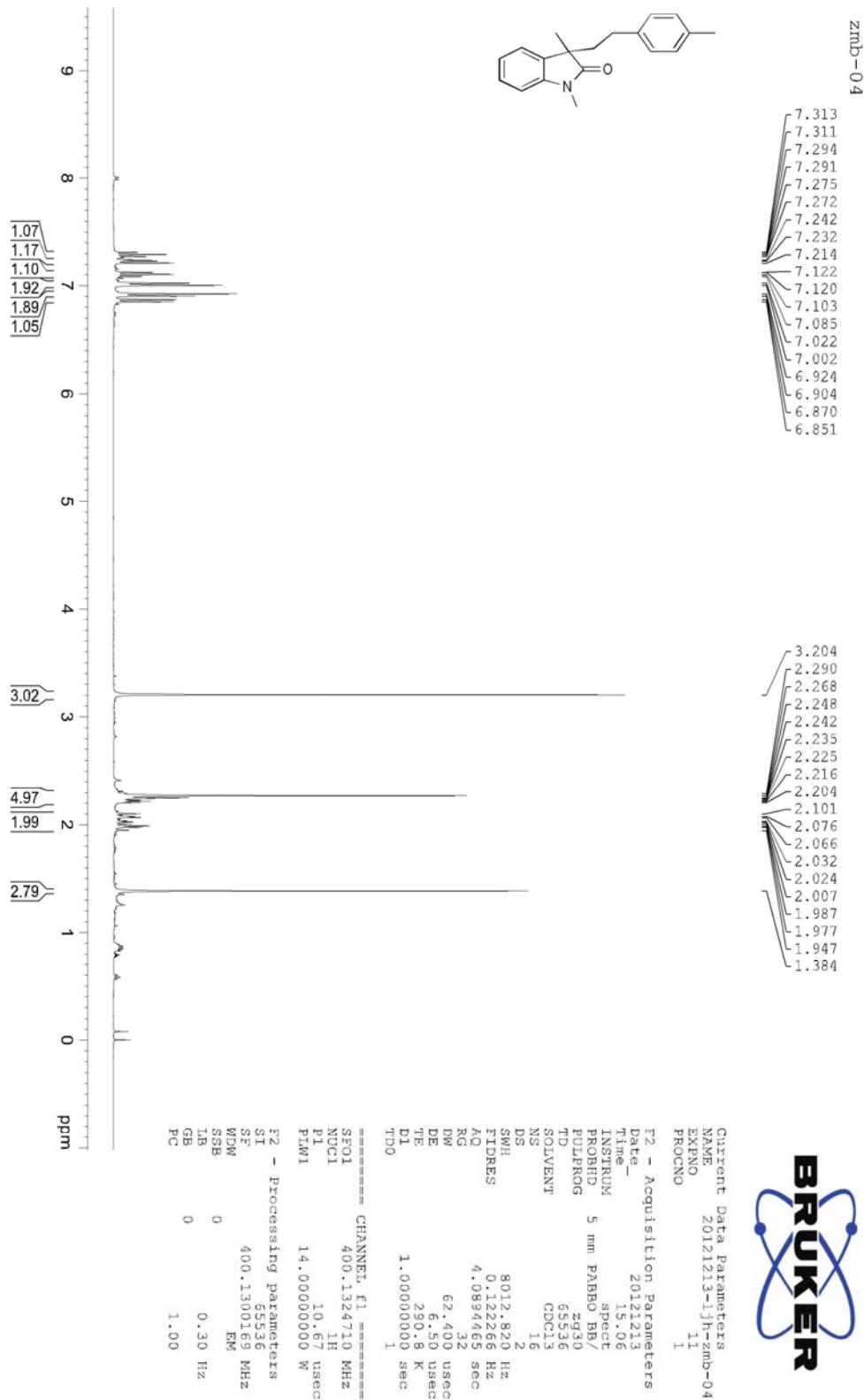
1,3-Dimethyl-3-phenethylindolin-2-one (3aa)



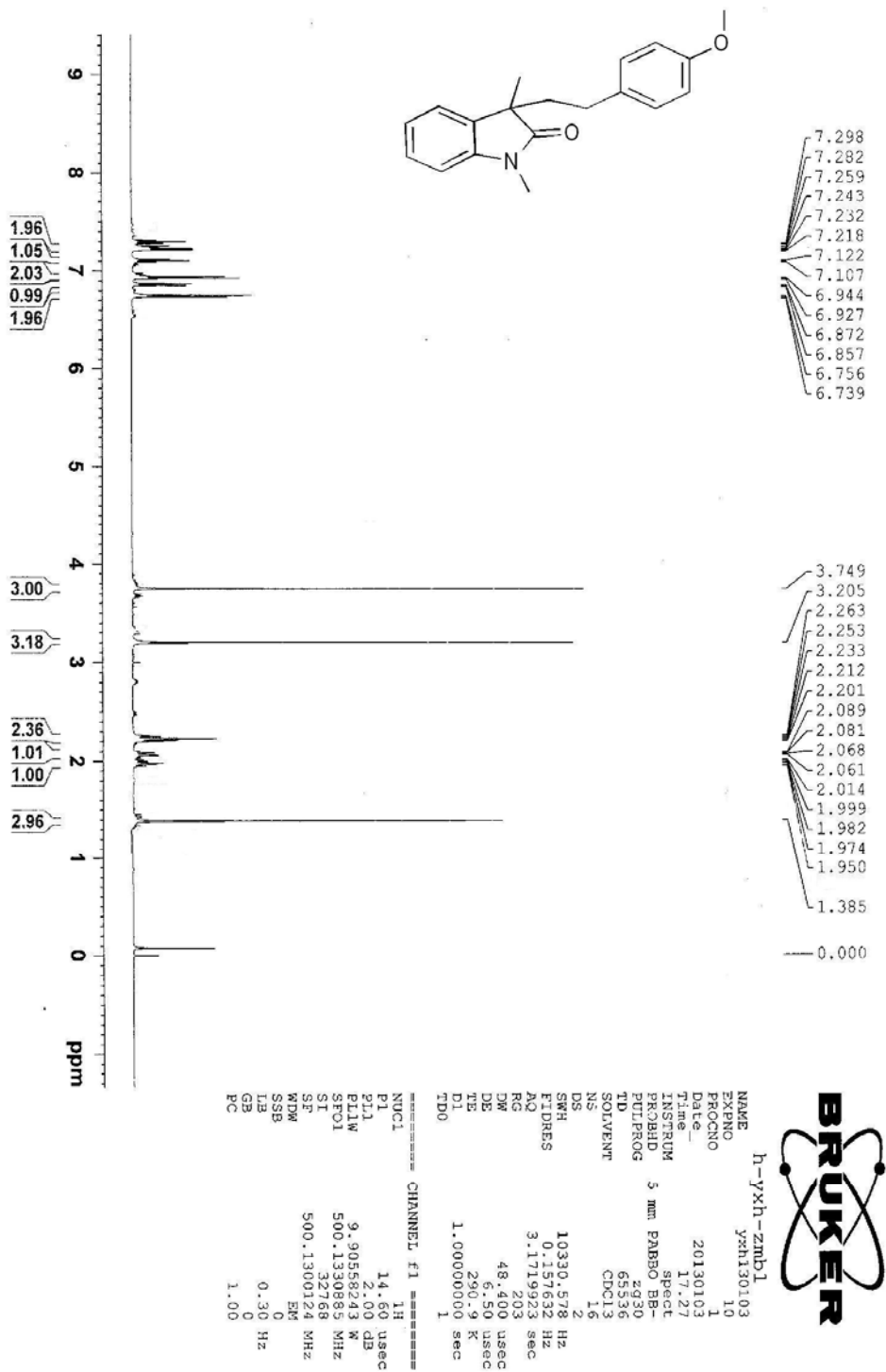
1,3-Dimethyl-3-phenethylindolin-2-one (3aa)



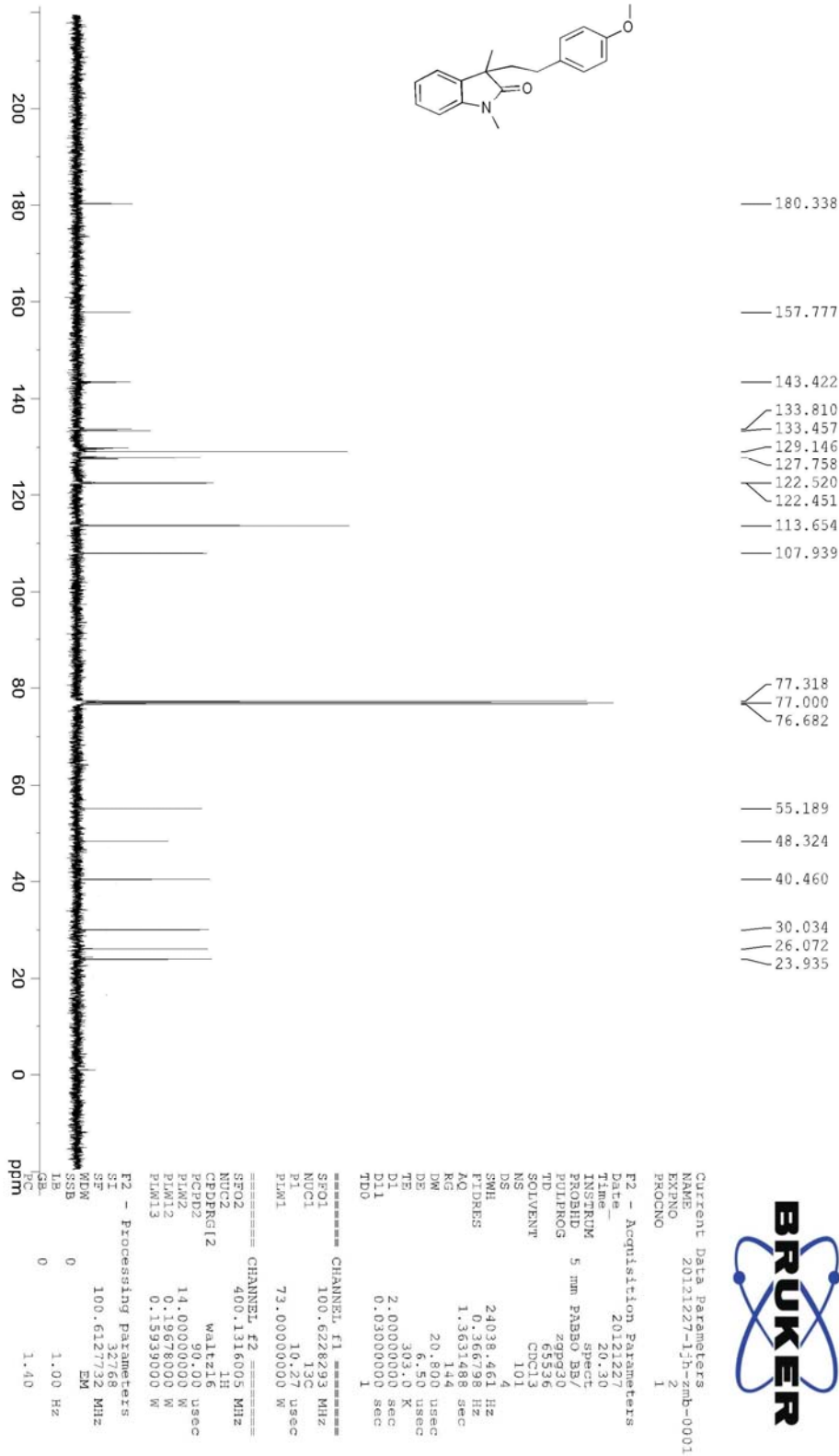
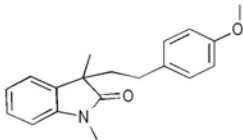
1,3-Dimethyl-3-(4-methylphenethyl)indolin-2-one (3ab)



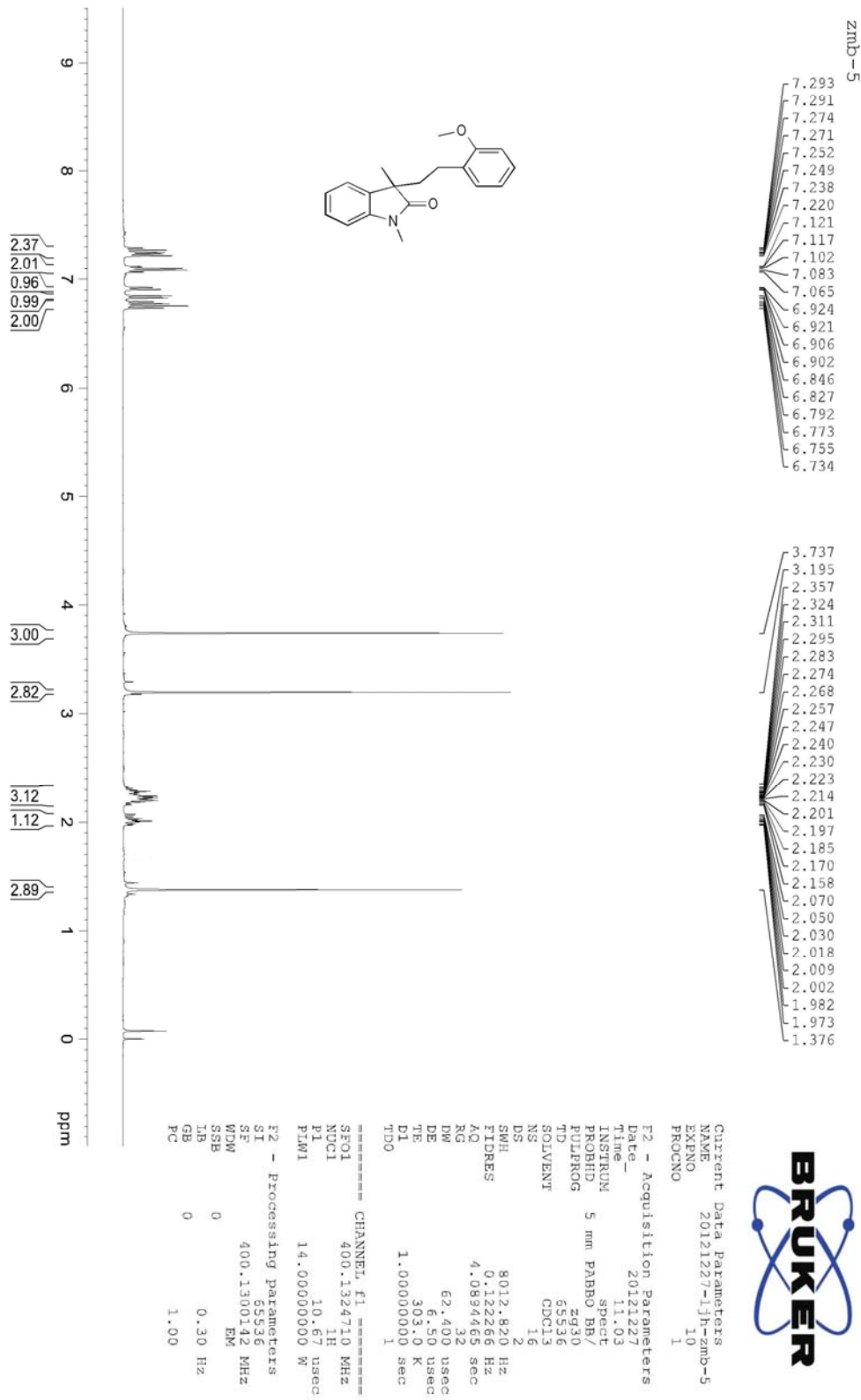
3-(4-Methoxyphenethyl)-1,3-dimethylindolin-2-one (3ac)



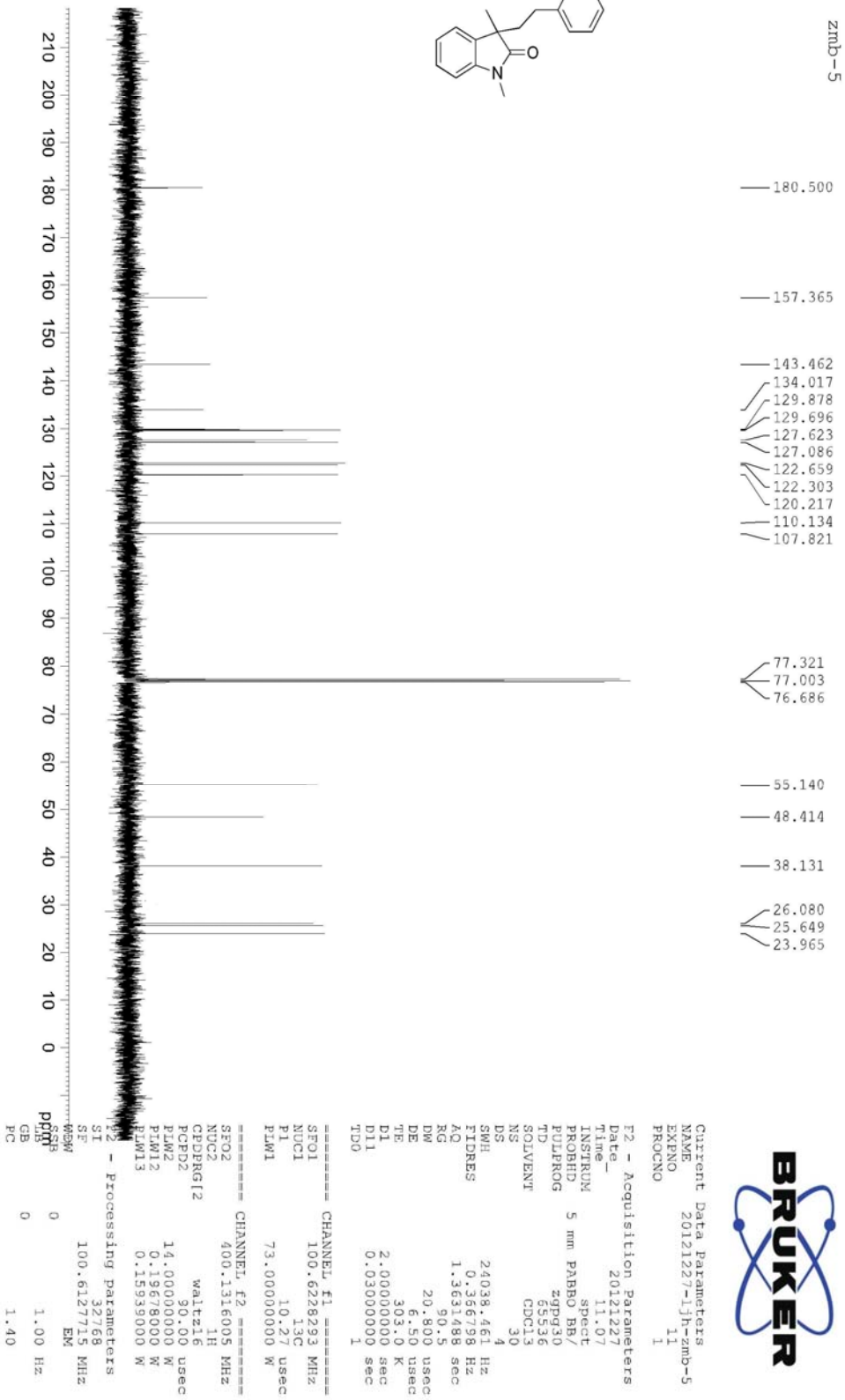
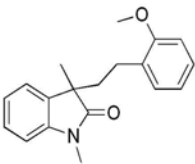
3-(4-Methoxyphenethyl)-1,3-dimethylindolin-2-one (3ac)



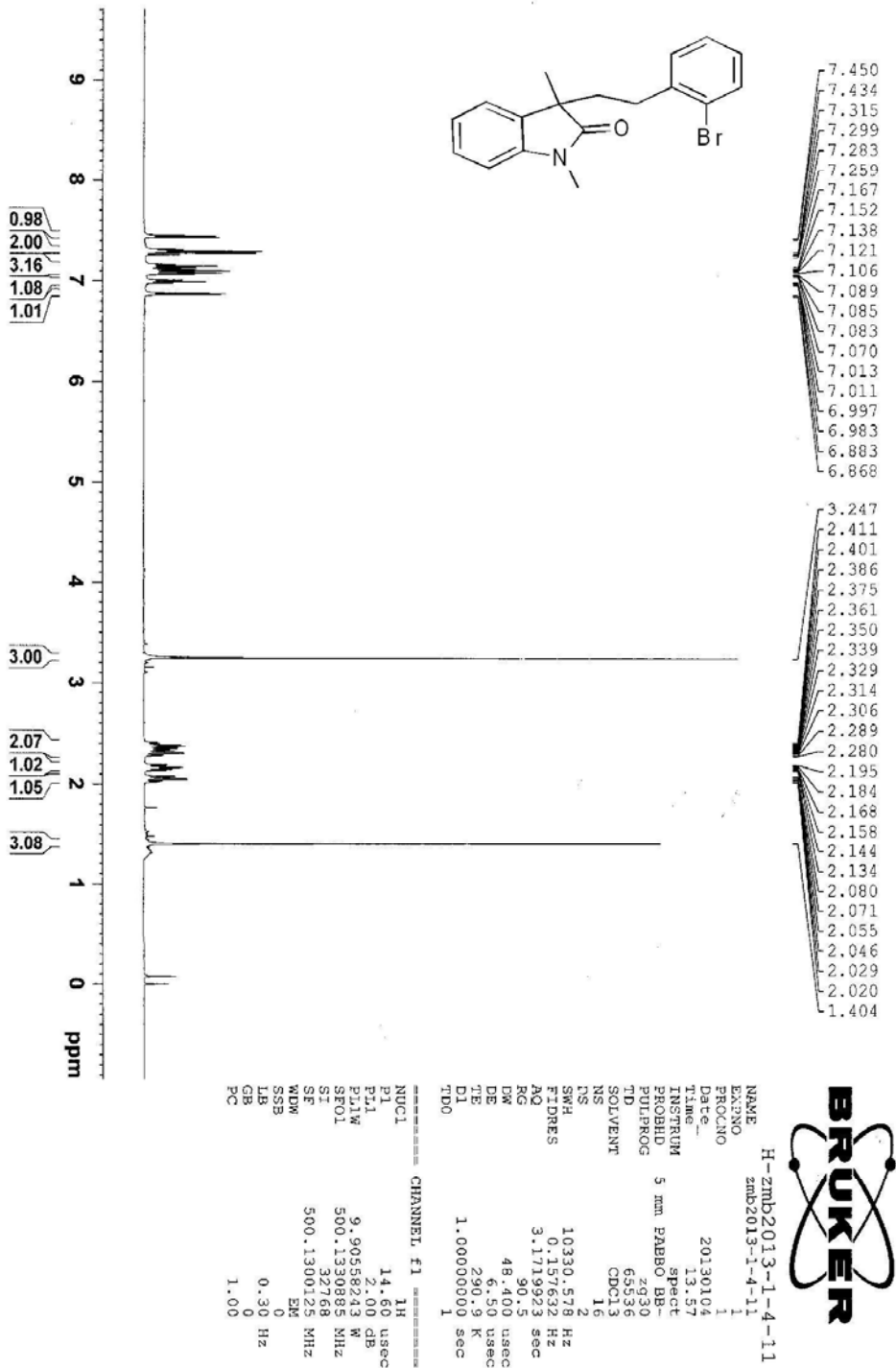
3-(2-Methoxyphenethyl)-1,3-dimethylindolin-2-one (3ad)



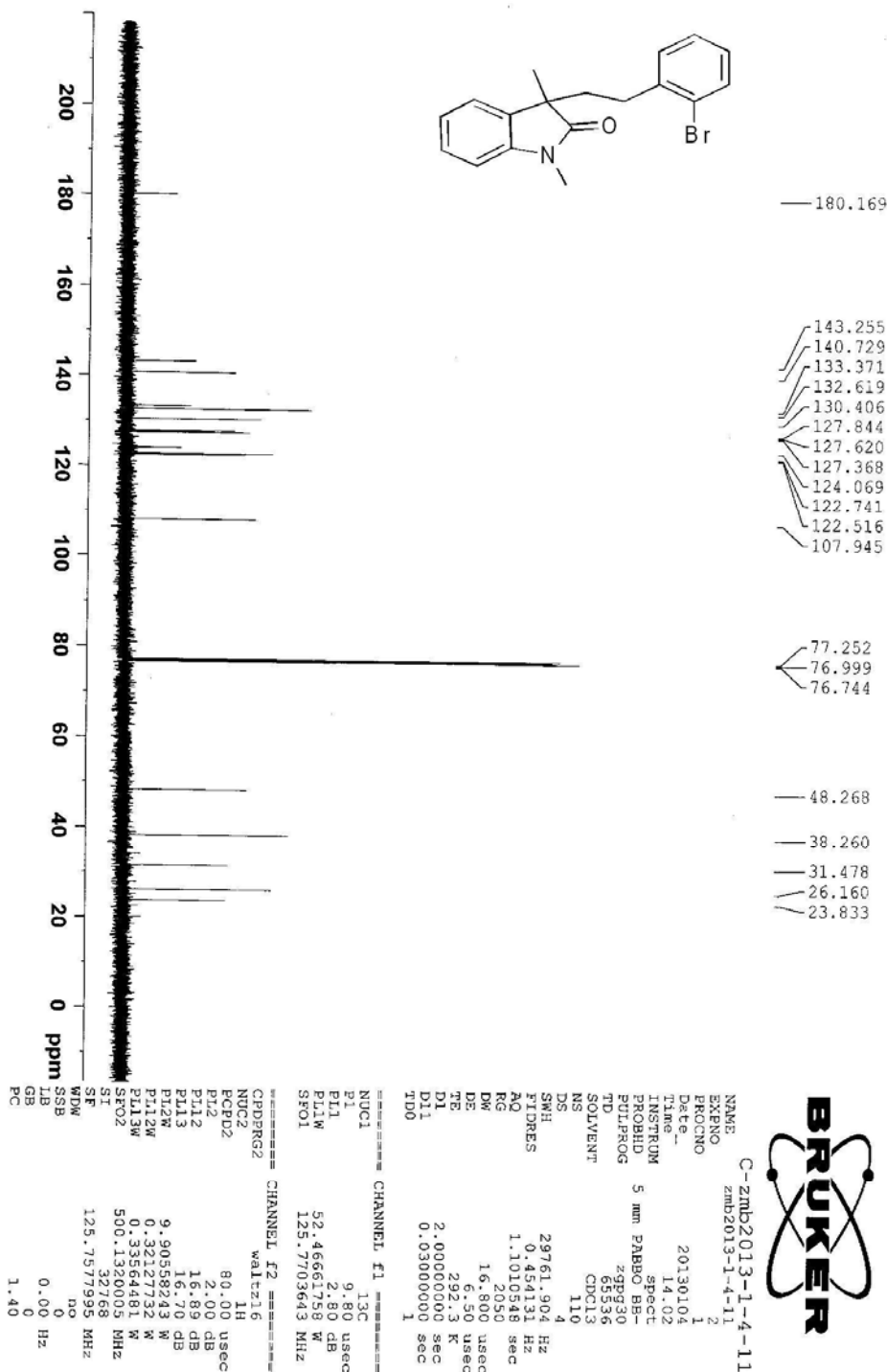
3-(2-Methoxyphenethyl)-1,3-dimethylindolin-2-one (3ad)



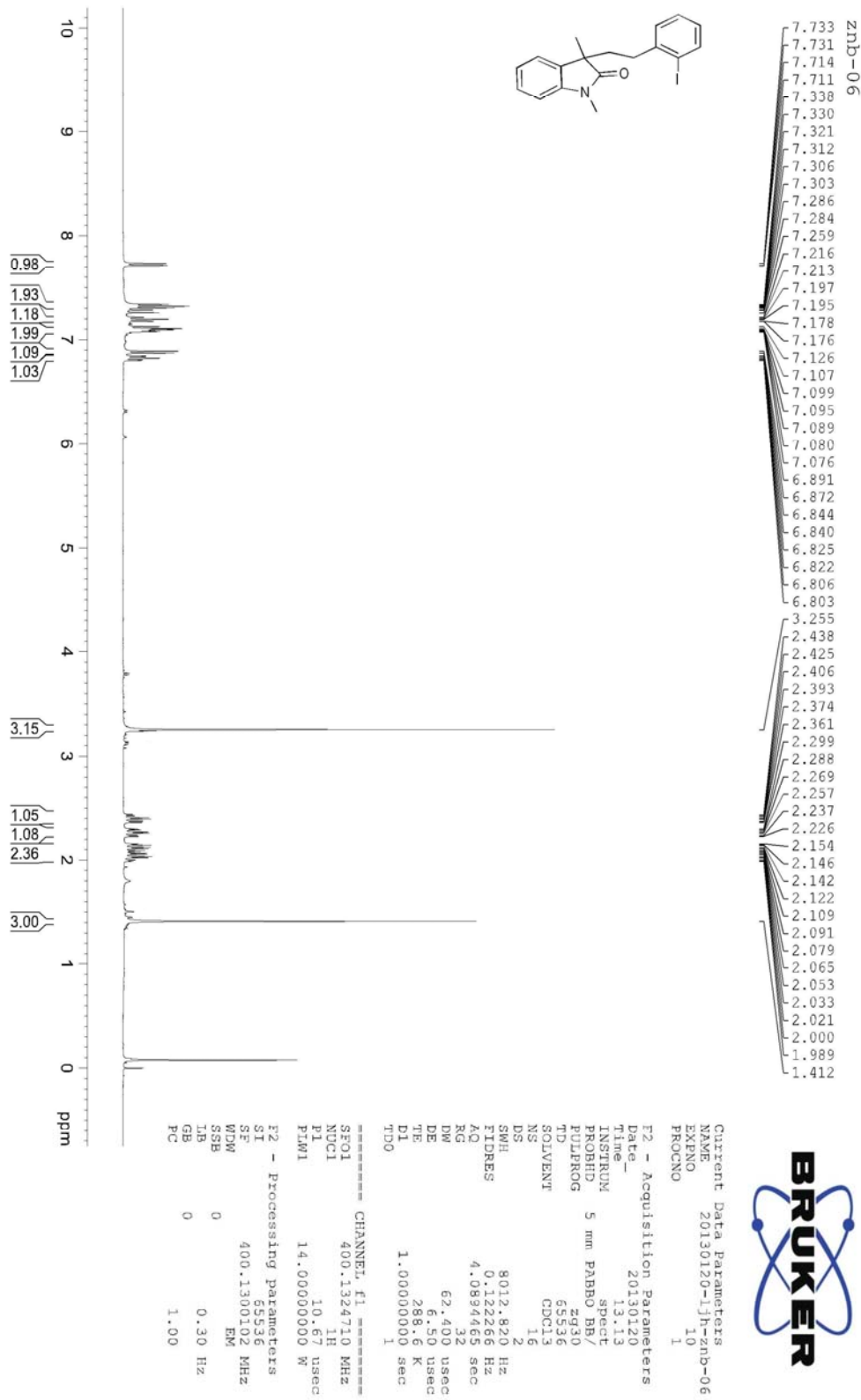
3-(2-Bromophenethyl)-1,3-dimethylindolin-2-one (3ae)



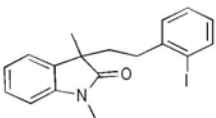
3-(2-Bromophenethyl)-1,3-dimethylindolin-2-one (3ae)



3-(2-Iodophenethyl)-1,3-dimethylindolin-2-one (3af)



3-(2-Iodophenethyl)-1,3-dimethylindolin-2-one (3af)



znb-06



Current Data Parameters
NAME 20130120-1jn-znb-06
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130120
Time 13.20

INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 85
DS 4

SWH 24038.461 Hz
FIDRES 0.366798 Hz
RG 1.363148 sec
RG 128

DW 20.800 usec
DE 6.50 usec
TE 289.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

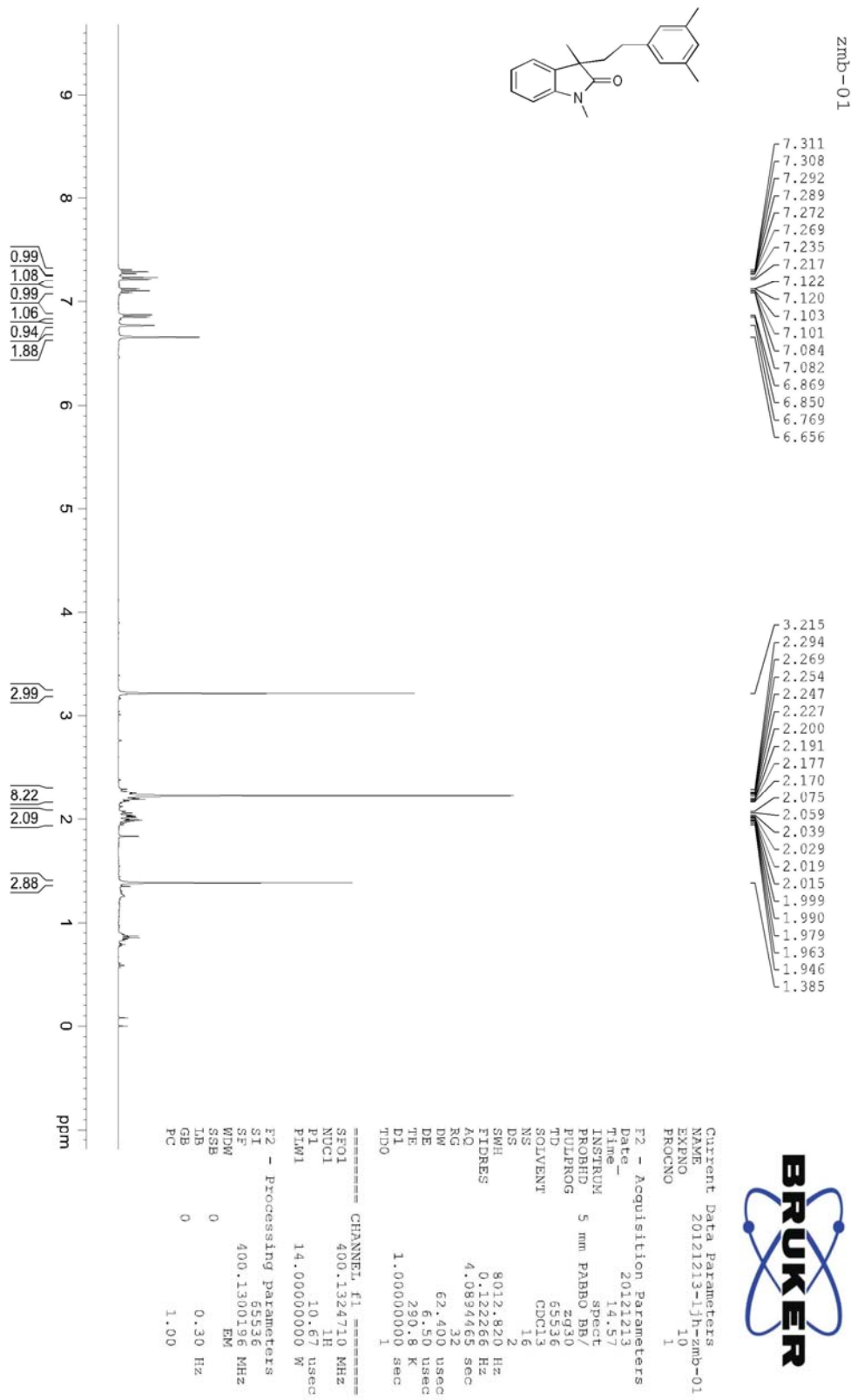
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
PLM1 73.0000000 W

CHANNEL f2
SFO2 400.1516005 MHz
NUC2 1H
P2 12.00 usec
PLM2 14.0000000 W

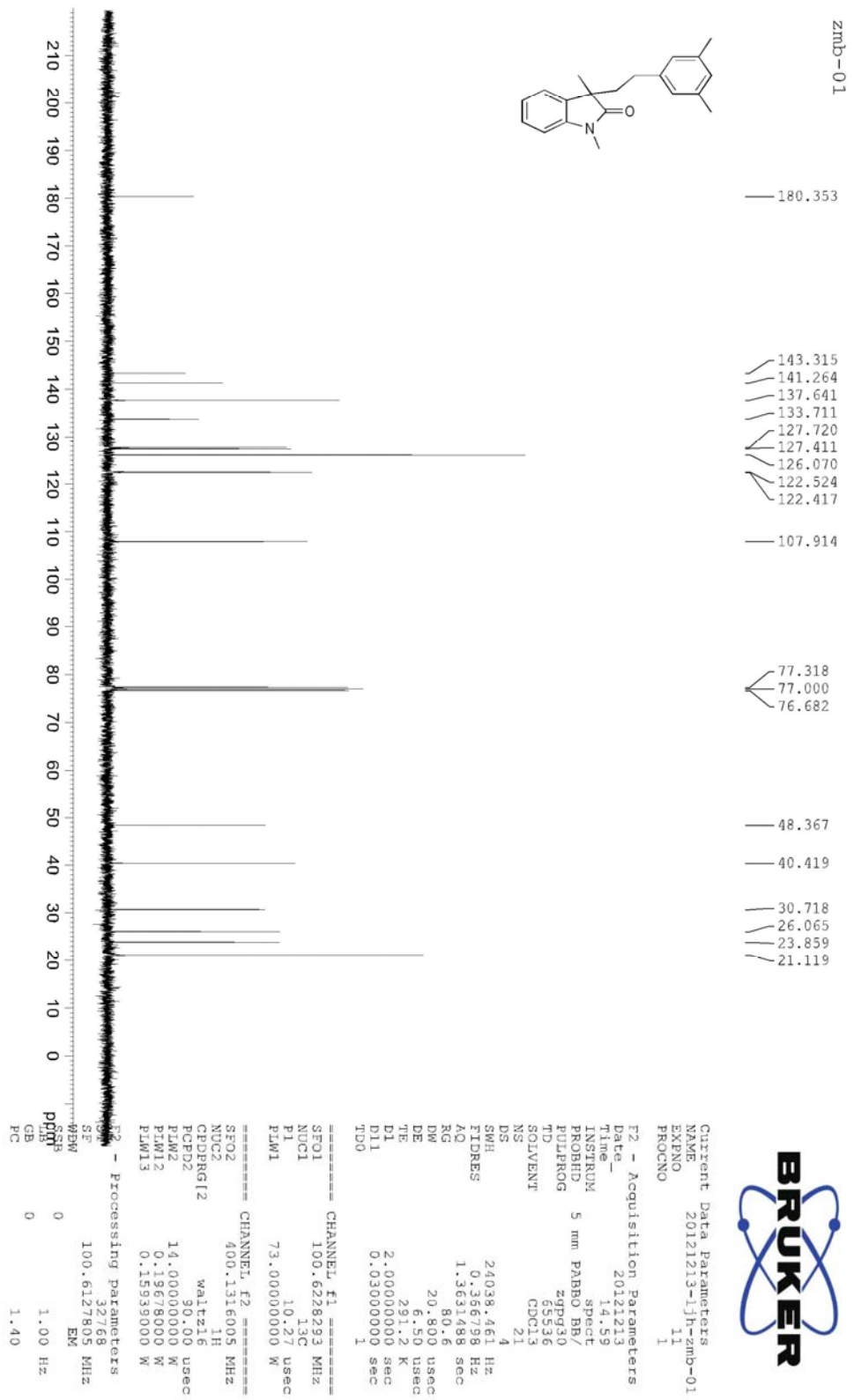
PCPD2 90.00 usec
PLM2 0.1967800 W
PLM13 0.1593900 W

SI 32768
SF 100.6127783 MHz
WDW EM
GB 0
PC 1.40

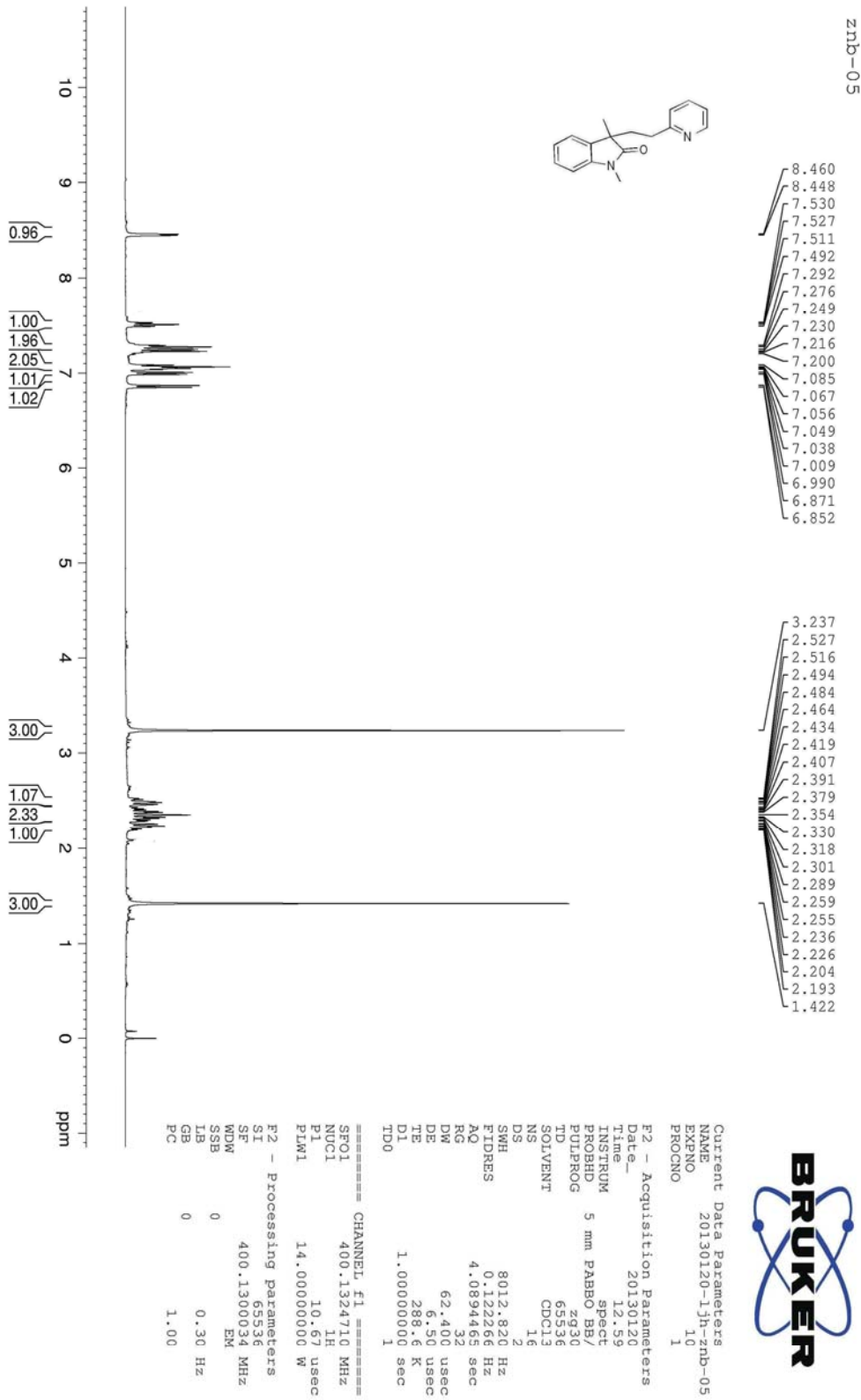
3-(3,5-Dimethylphenethyl)-1,3-dimethylindolin-2-one (3ag)



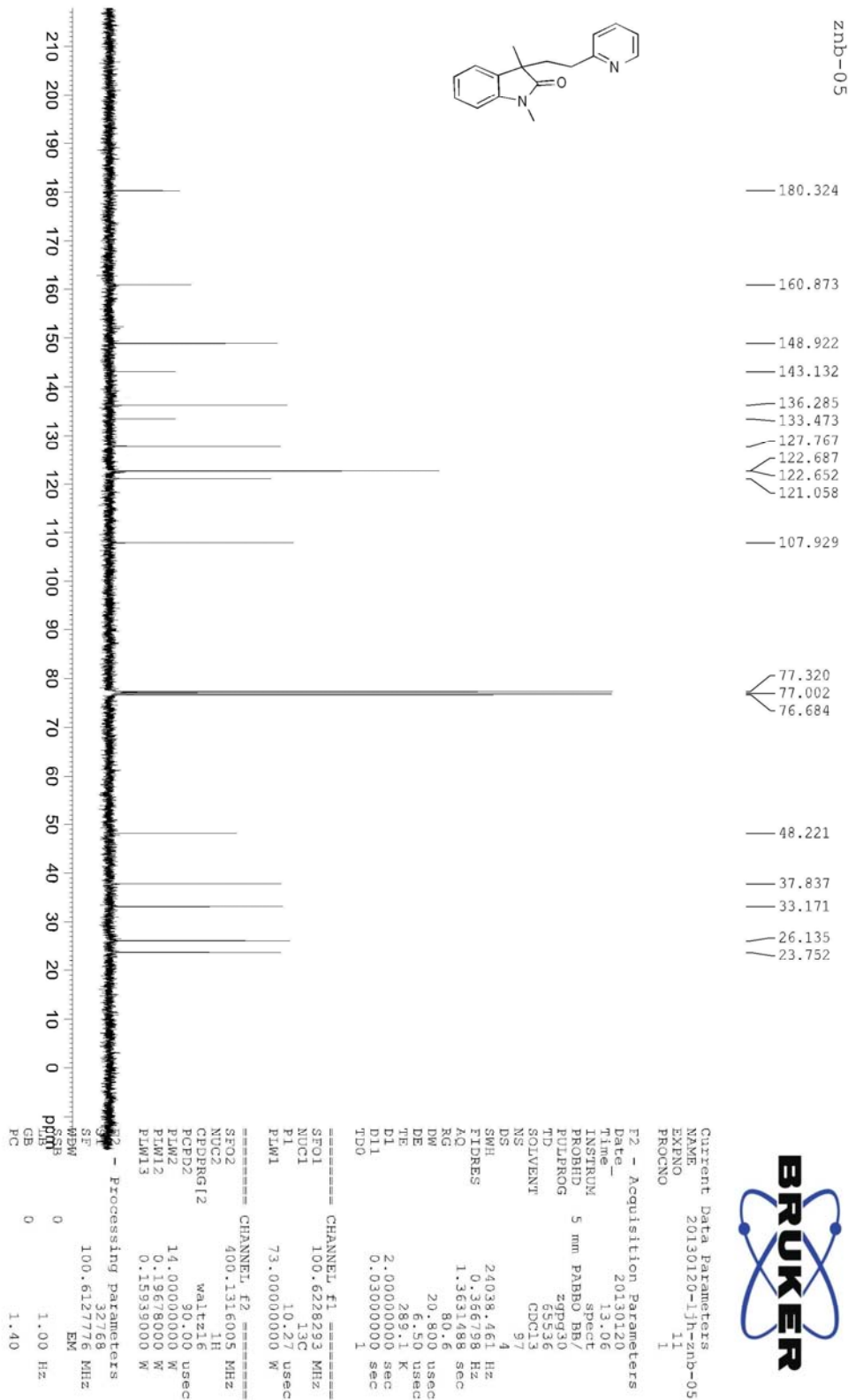
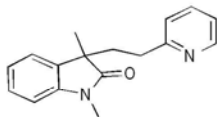
3-(3,5-Dimethylphenethyl)-1,3-dimethylindolin-2-one (3ag)



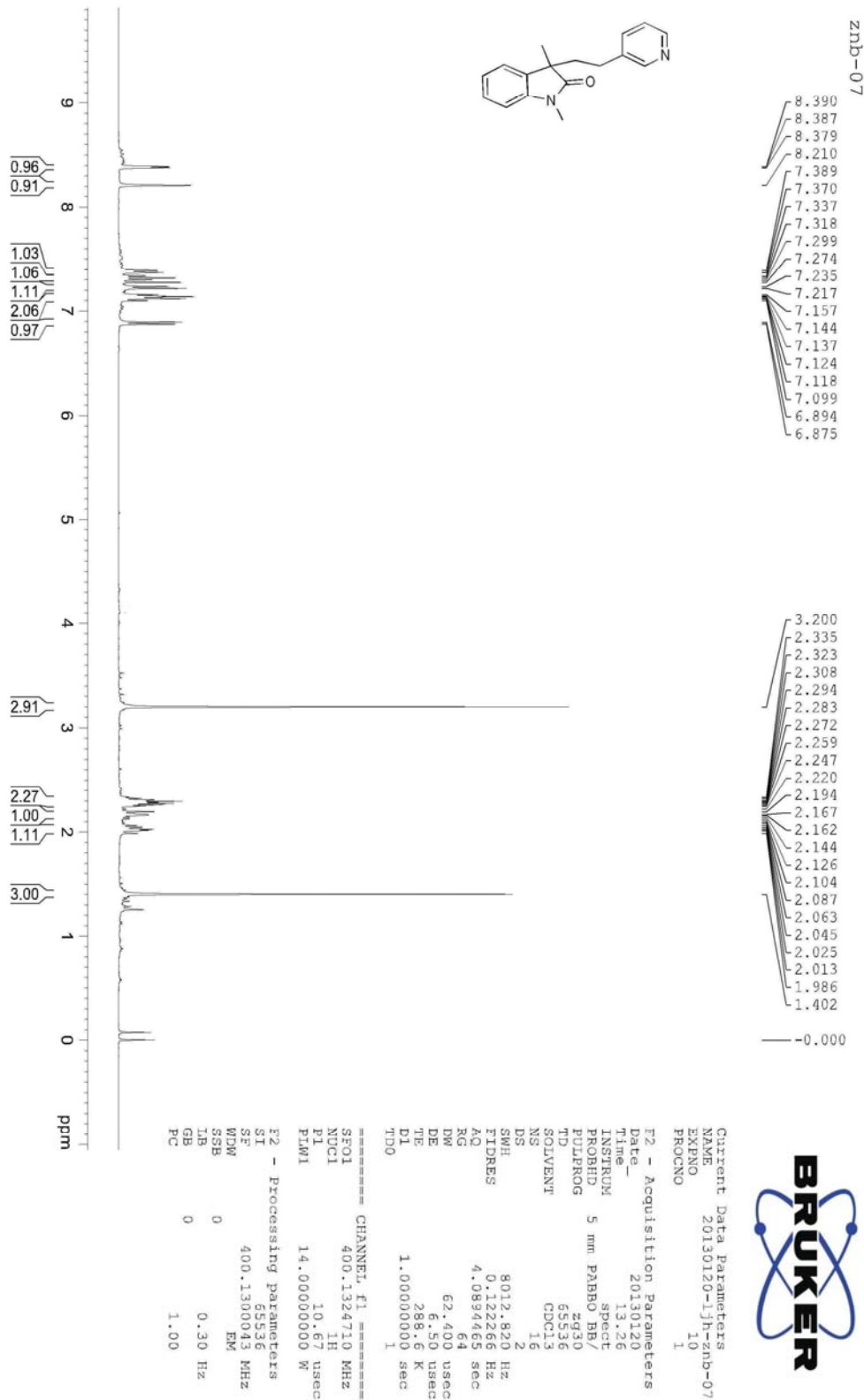
1,3-Dimethyl-3-(2-(pyridin-2-yl)ethyl)indolin-2-one (3ah)



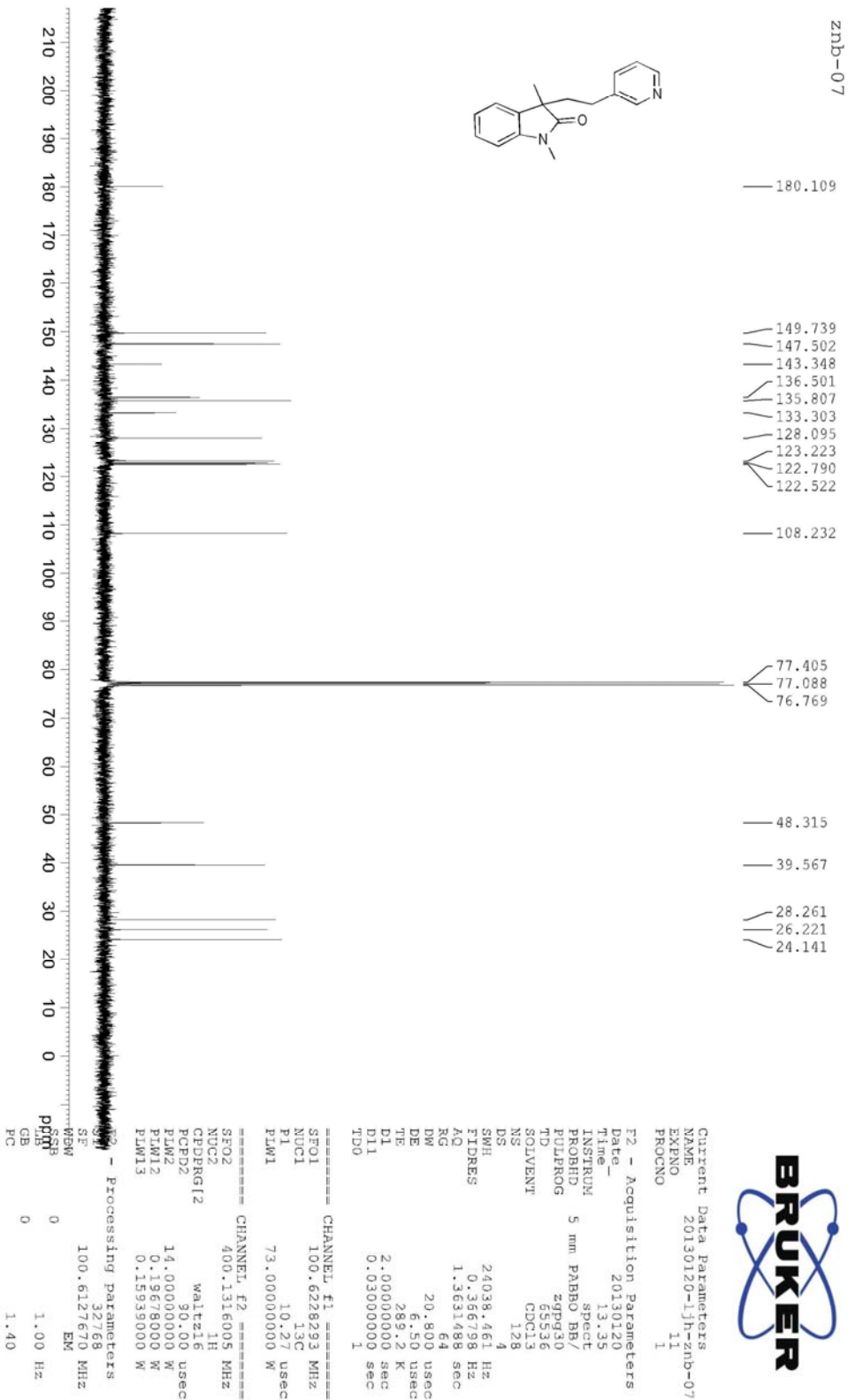
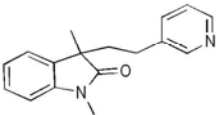
1,3-Dimethyl-3-(2-(pyridin-2-yl)ethyl)indolin-2-one (3ah)



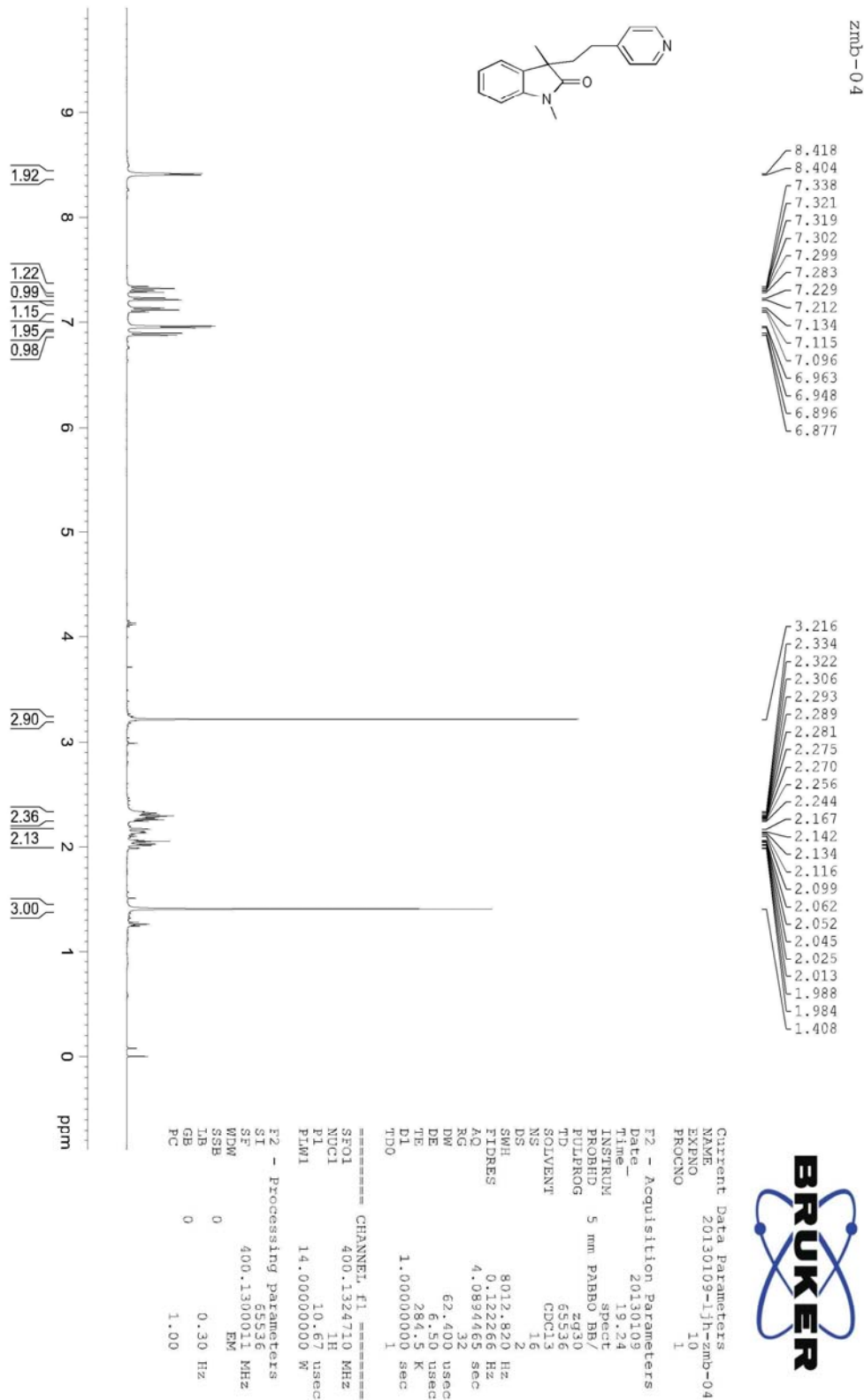
1,3-Dimethyl-3-(2-(pyridin-3-yl)ethyl)indolin-2-one (3ai)



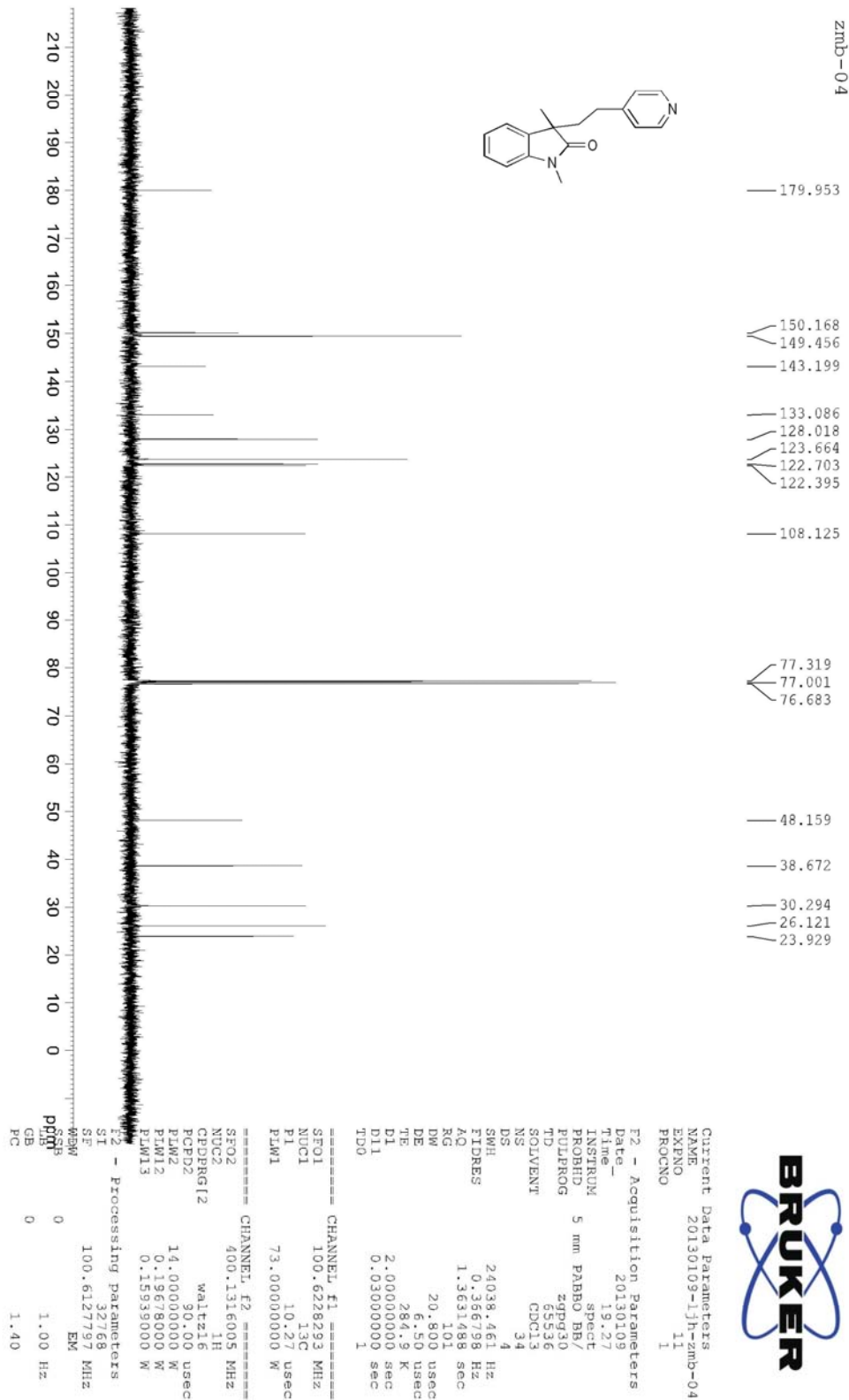
1,3-Dimethyl-3-(2-(pyridin-3-yl)ethyl)indolin-2-one (3ai)



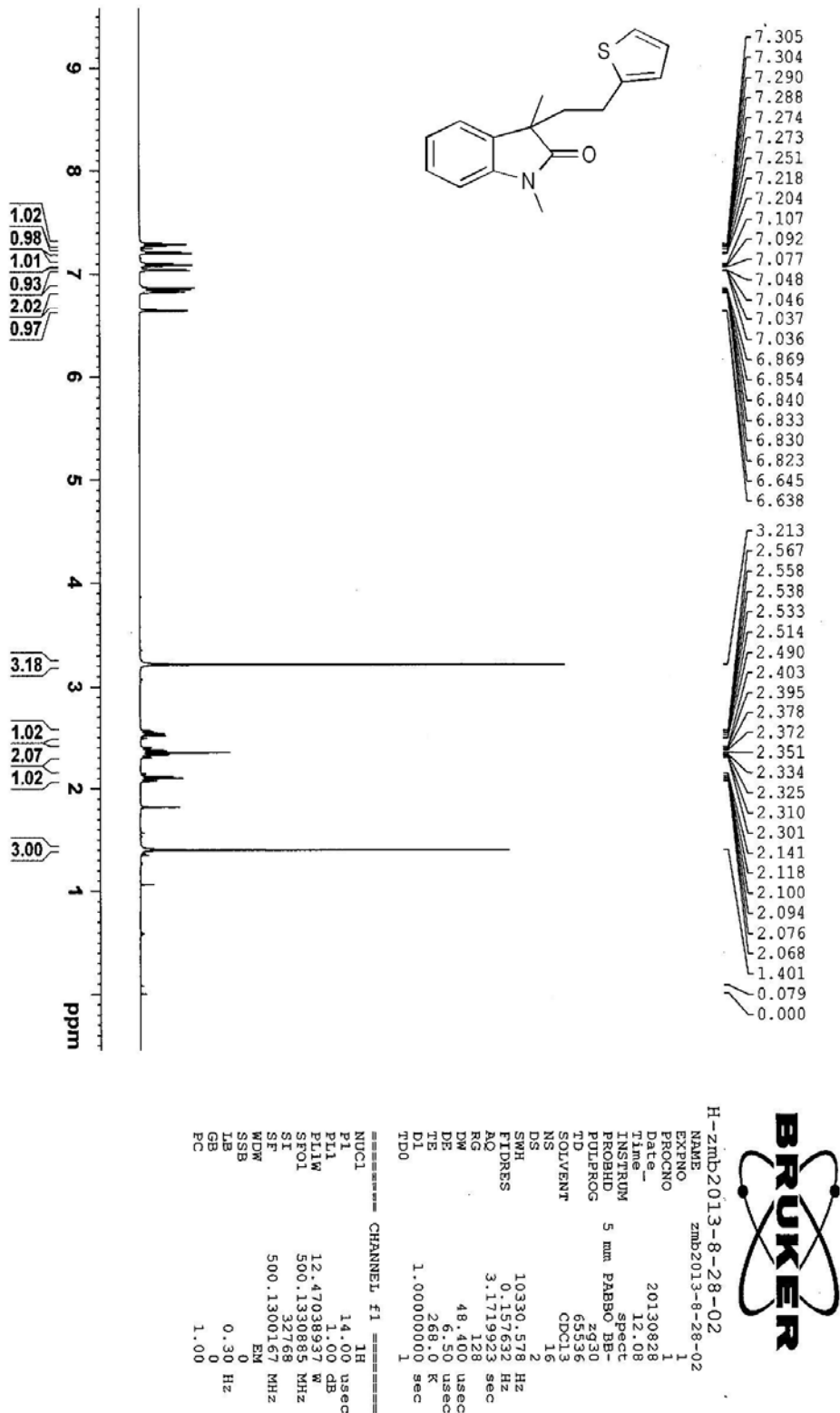
1,3-Dimethyl-3-(2-(pyridin-4-yl)ethyl)indolin-2-one (3aj)



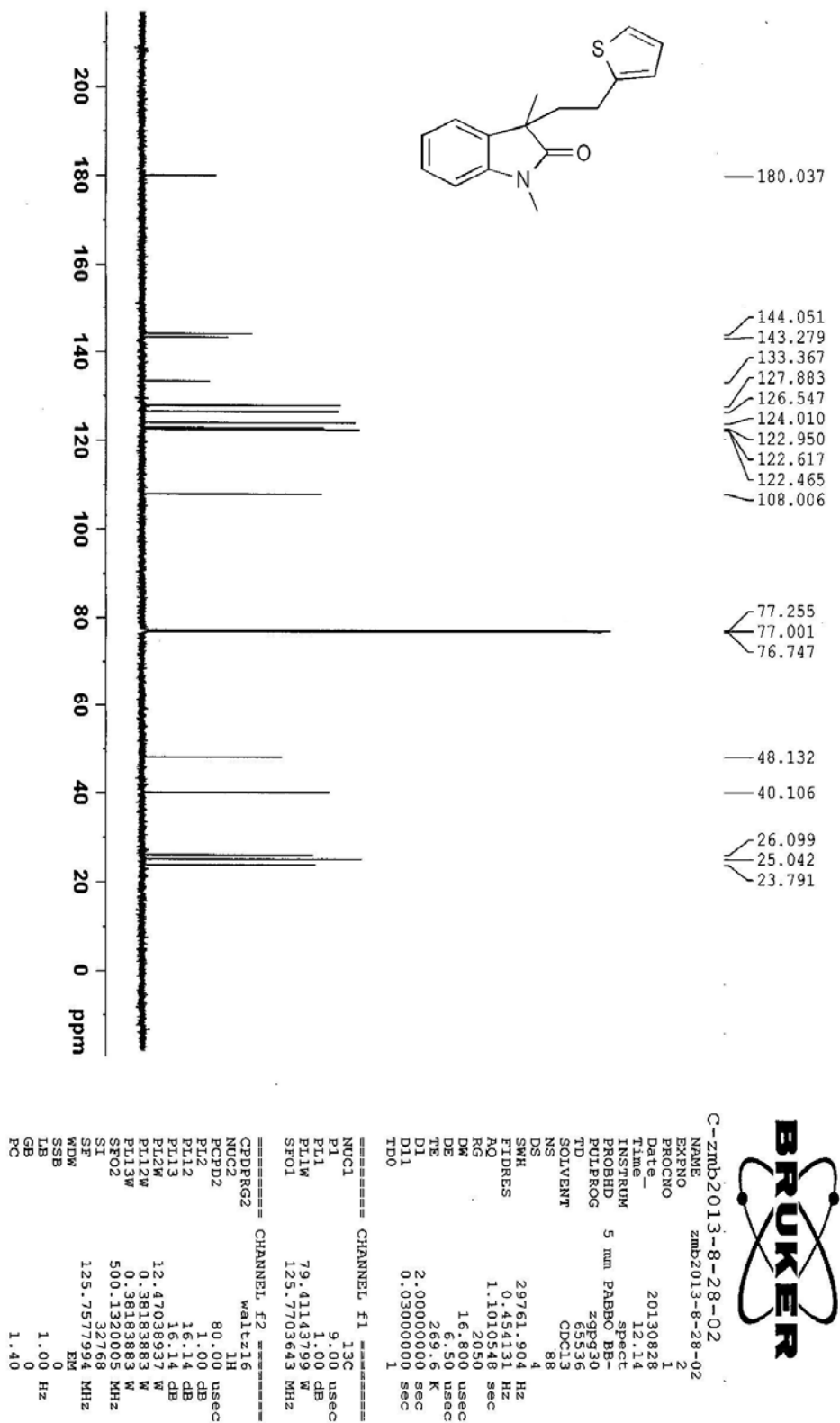
1,3-Dimethyl-3-(2-(pyridin-4-yl)ethyl)indolin-2-one (3aj)



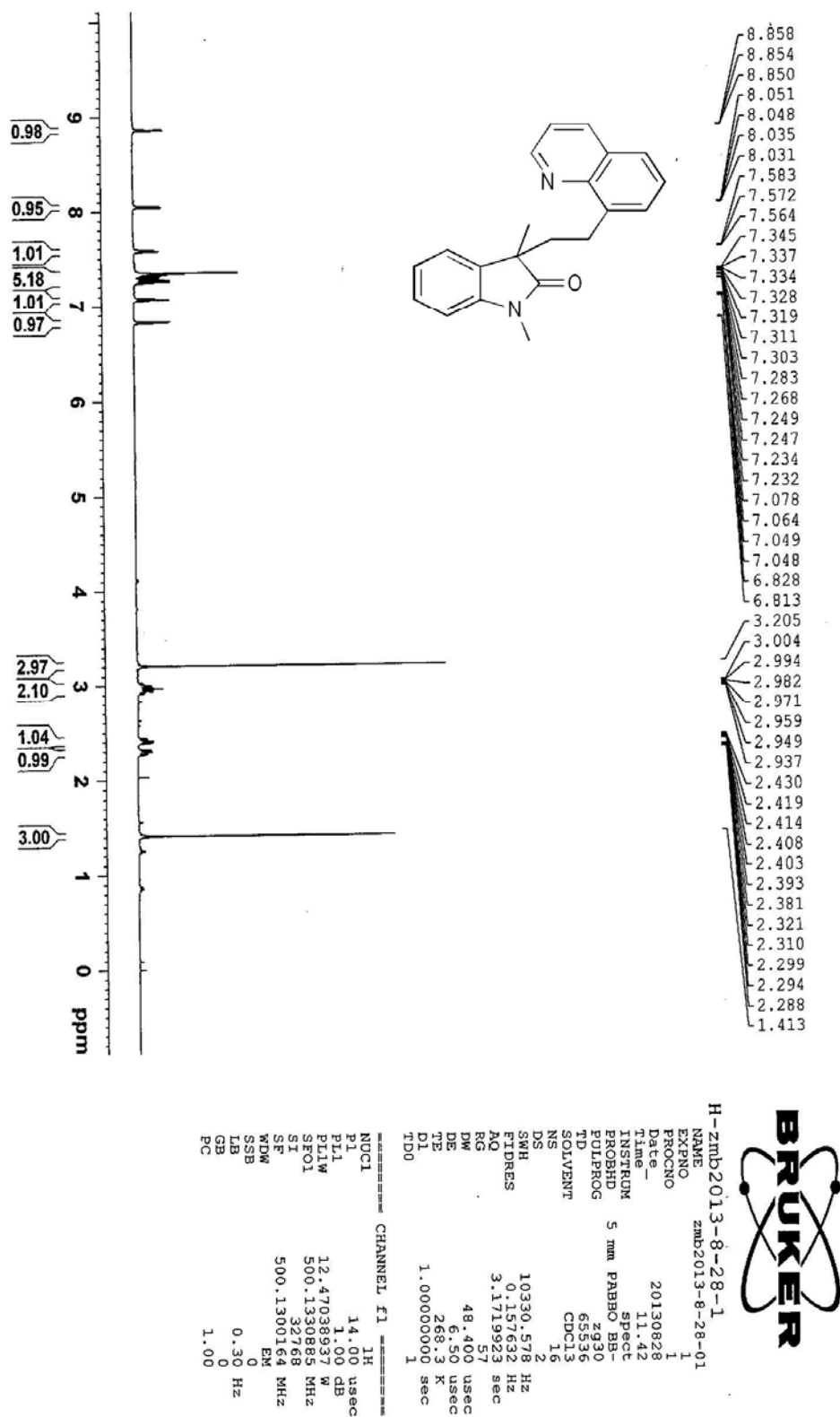
1,3-Dimethyl-3-(2-(thiophen-2-yl)ethyl)indolin-2-one (3ak):



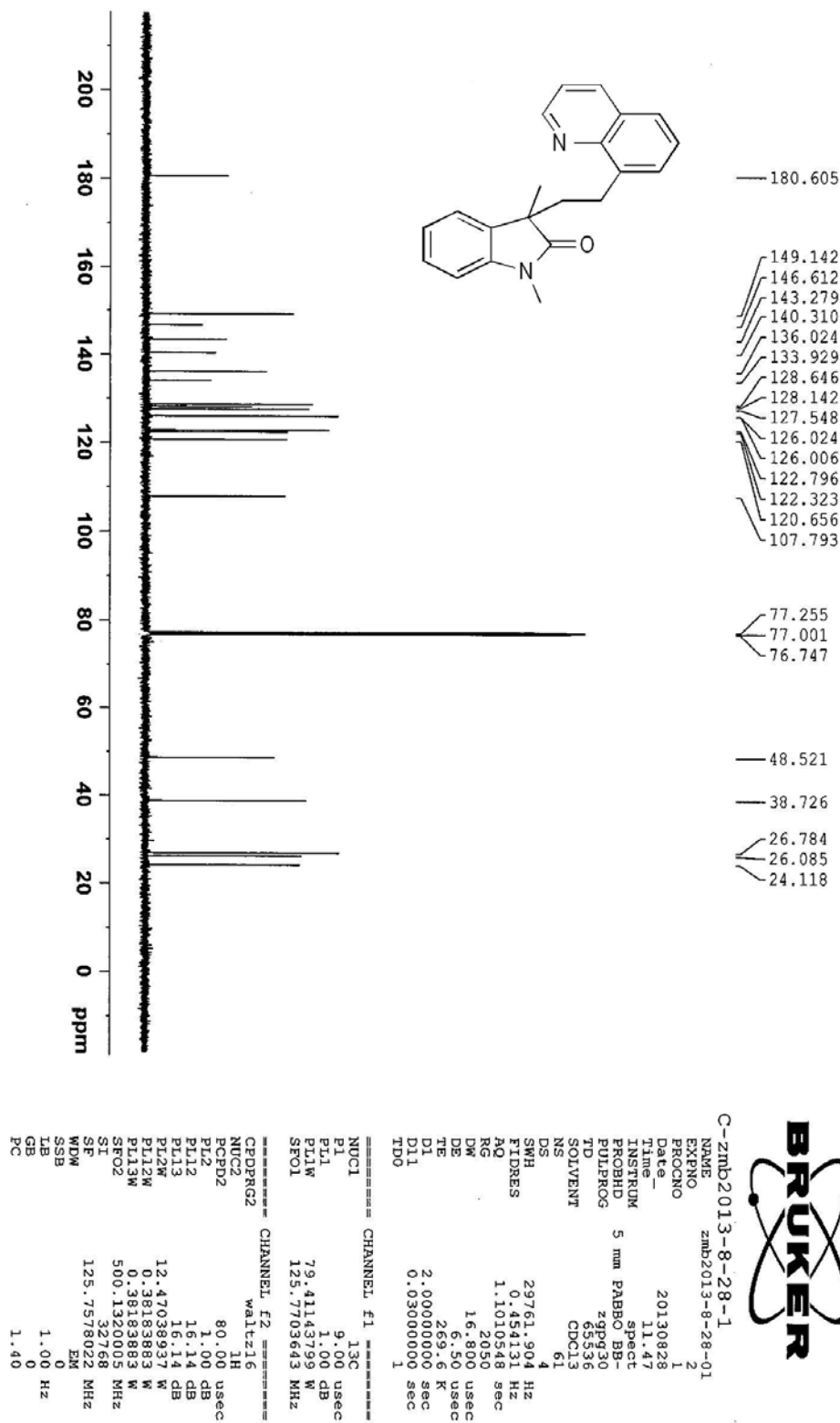
1,3-Dimethyl-3-(2-(thiophen-2-yl)ethyl)indolin-2-one (3ak):



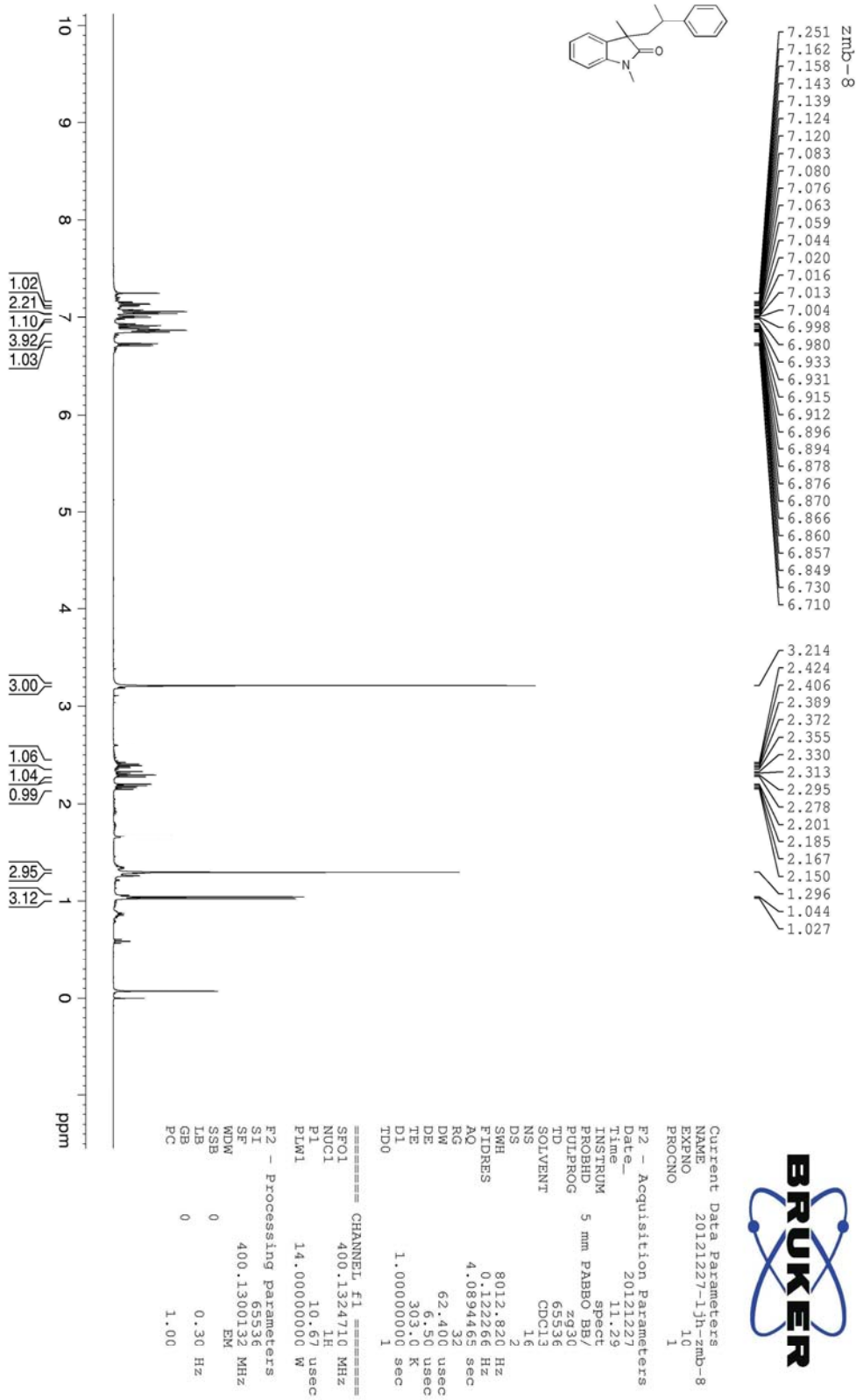
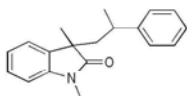
1,3-Dimethyl-3-(2-(quinolin-8-yl)ethyl)indolin-2-one (3al):



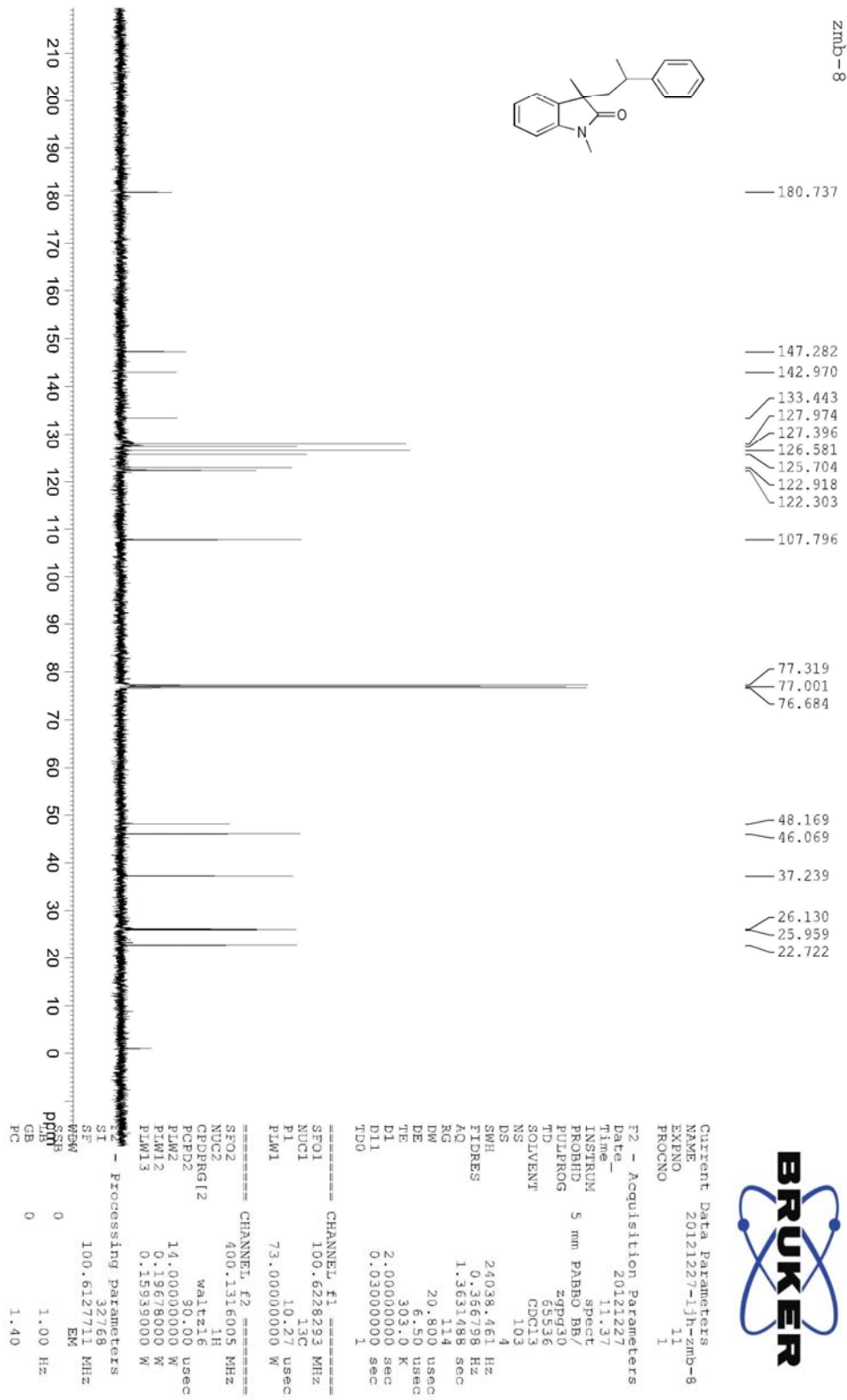
1,3-Dimethyl-3-(2-(quinolin-8-yl)ethyl)indolin-2-one (3al):



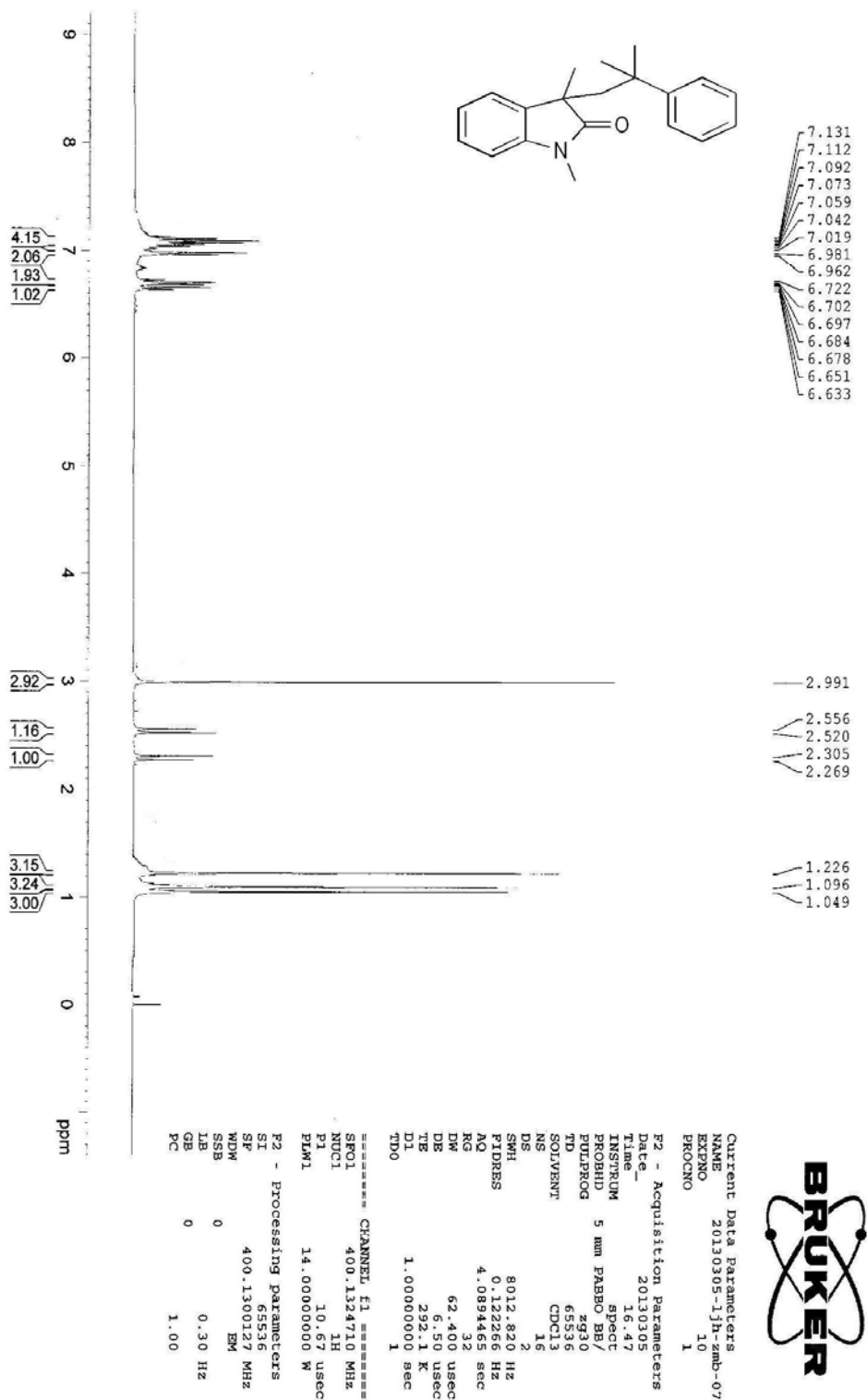
1,3-Dimethyl-3-(2-phenylpropyl)indolin-2-one (3am)



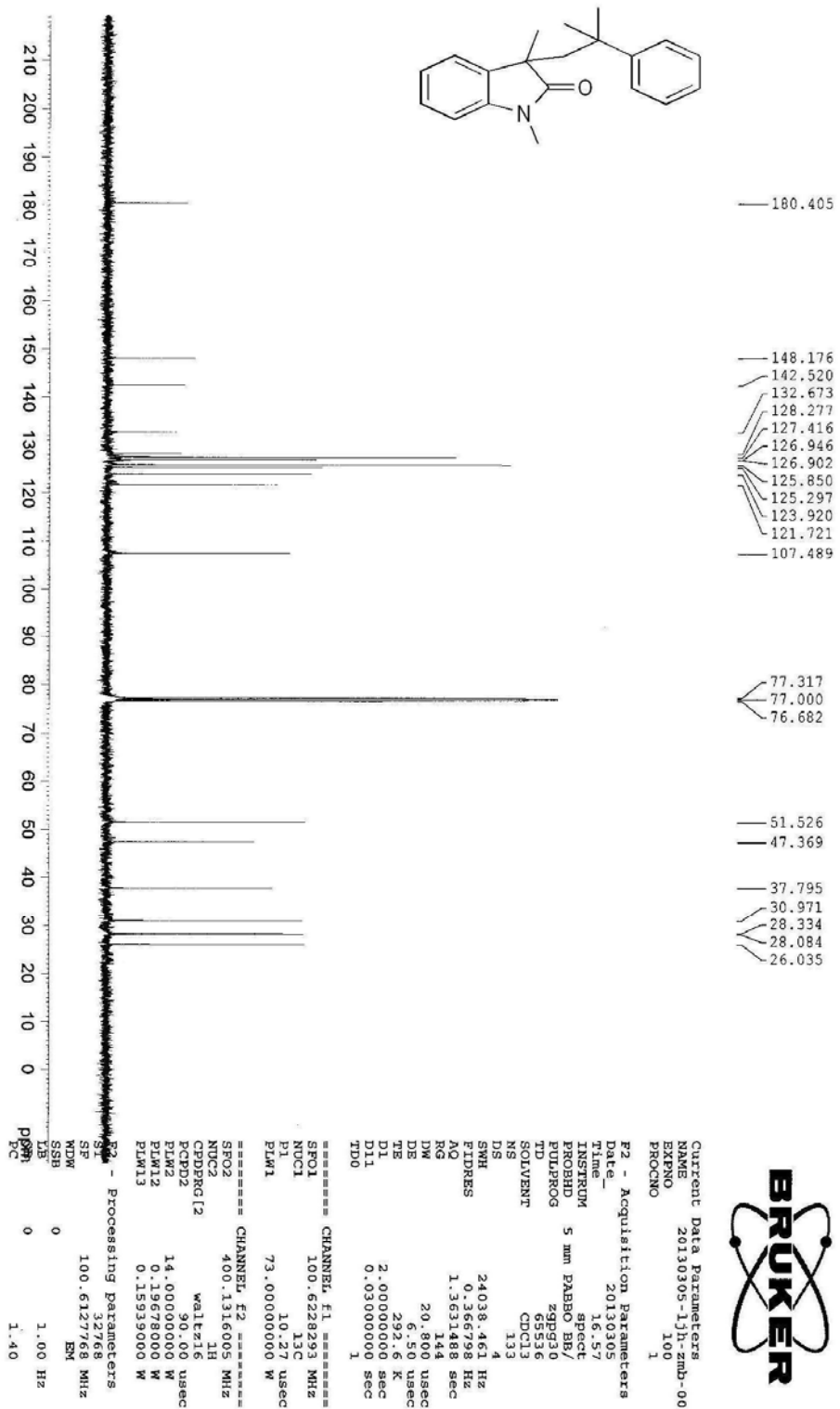
1,3-Dimethyl-3-(2-phenylpropyl)indolin-2-one (3am)



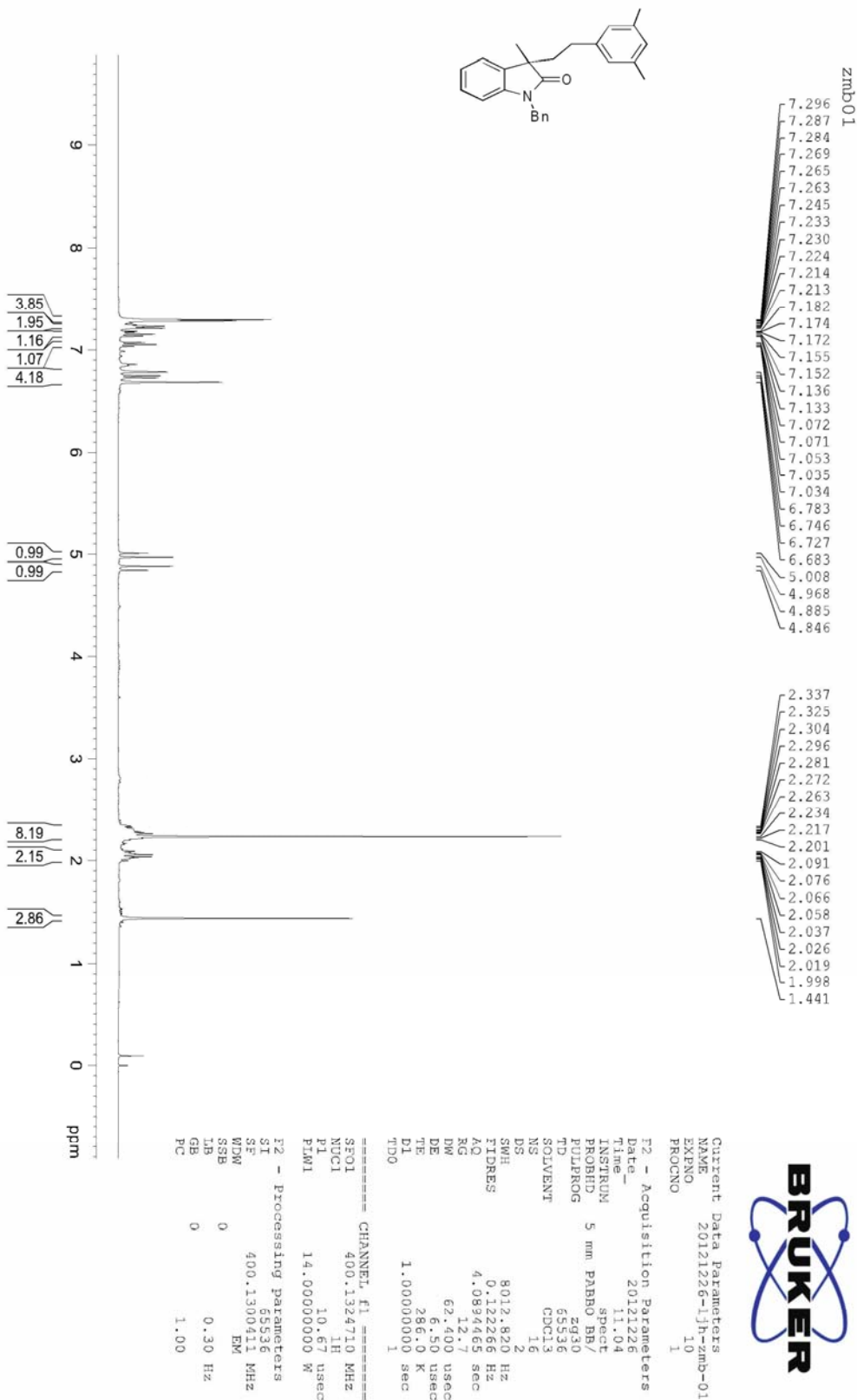
1,3-Dimethyl-3-(2-methyl-2-phenylpropyl)indolin-2-one (3an)



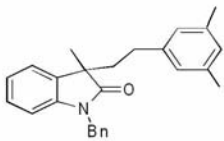
1,3-Dimethyl-3-(2-methyl-2-phenylpropyl)indolin-2-one (3an)



1-Benzyl-3-(3,5-dimethylphenethyl)-3-methylindolin-2-one (3bg)

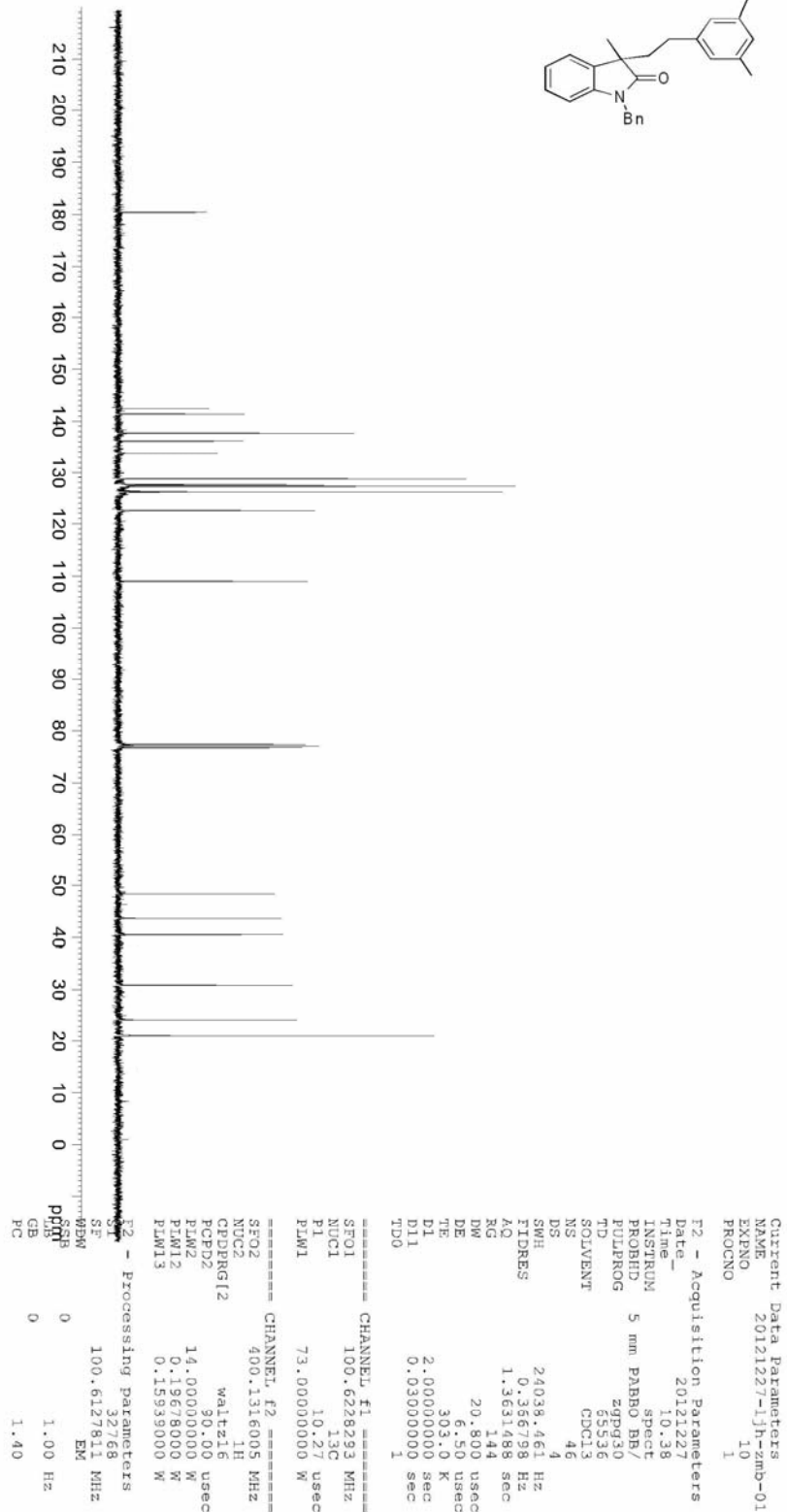


1-Benzyl-3-(3,5-dimethylphenethyl)-3-methylindolin-2-one (3bg)

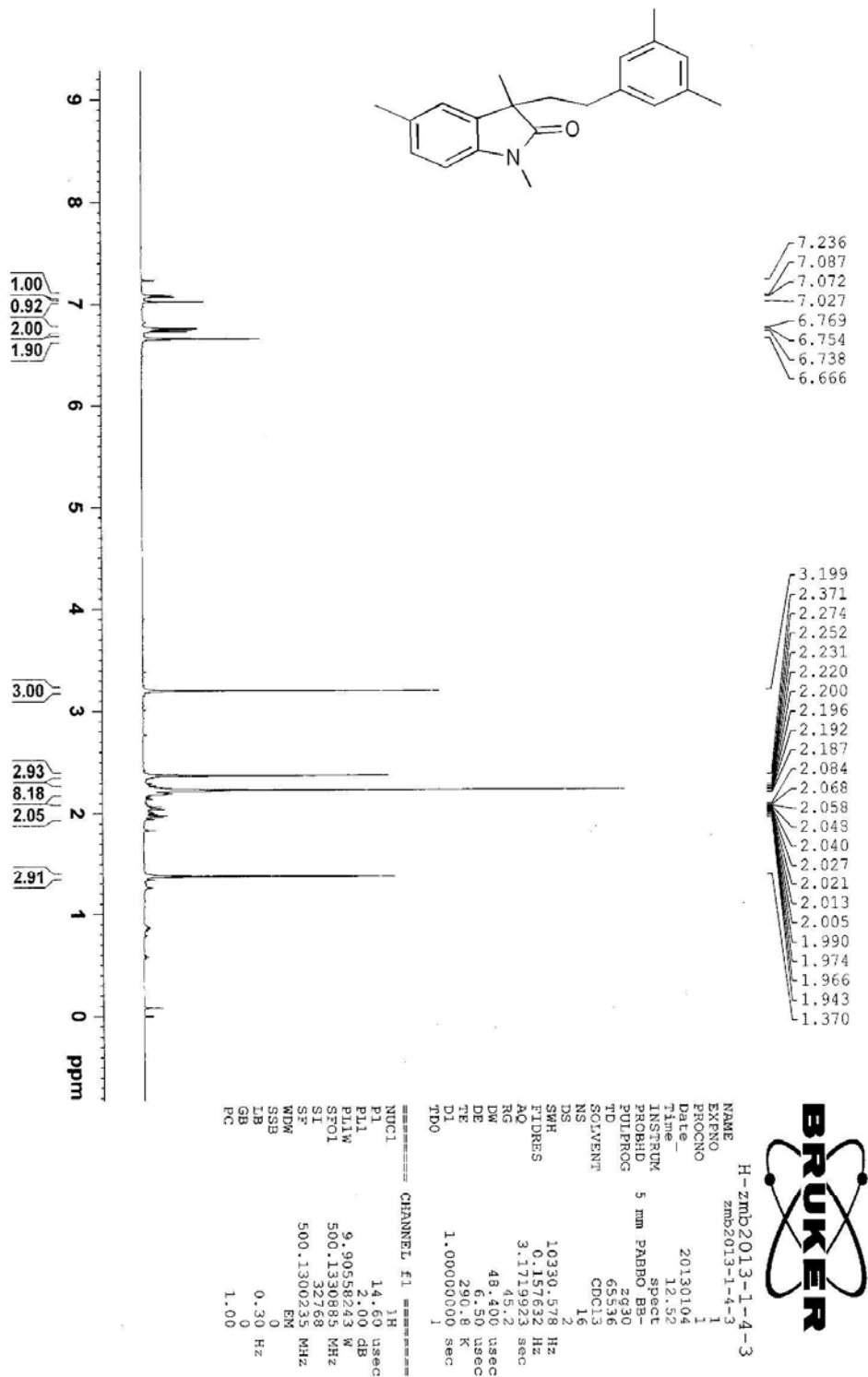


zmb-01

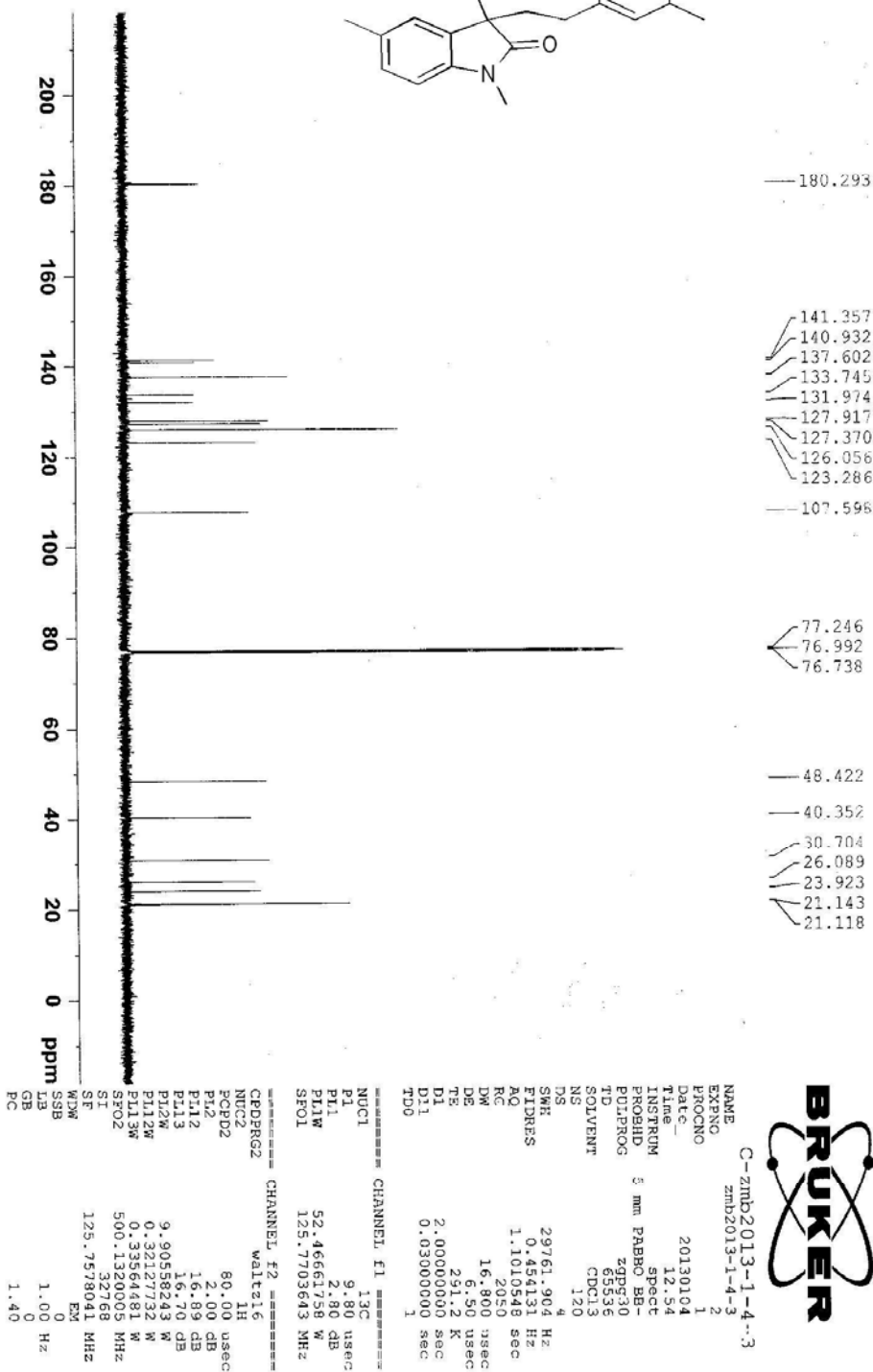
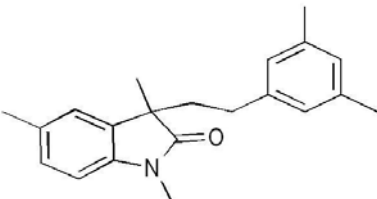
- 180.412
- 142.476
- 141.383
- 137.687
- 136.126
- 133.780
- 128.701
- 127.637
- 127.492
- 127.459
- 127.232
- 126.174
- 126.095
- 122.535
- 122.505
- 109.003
- 77.320
- 77.002
- 76.683
- 48.375
- 43.643
- 40.539
- 30.877
- 24.190
- 21.107



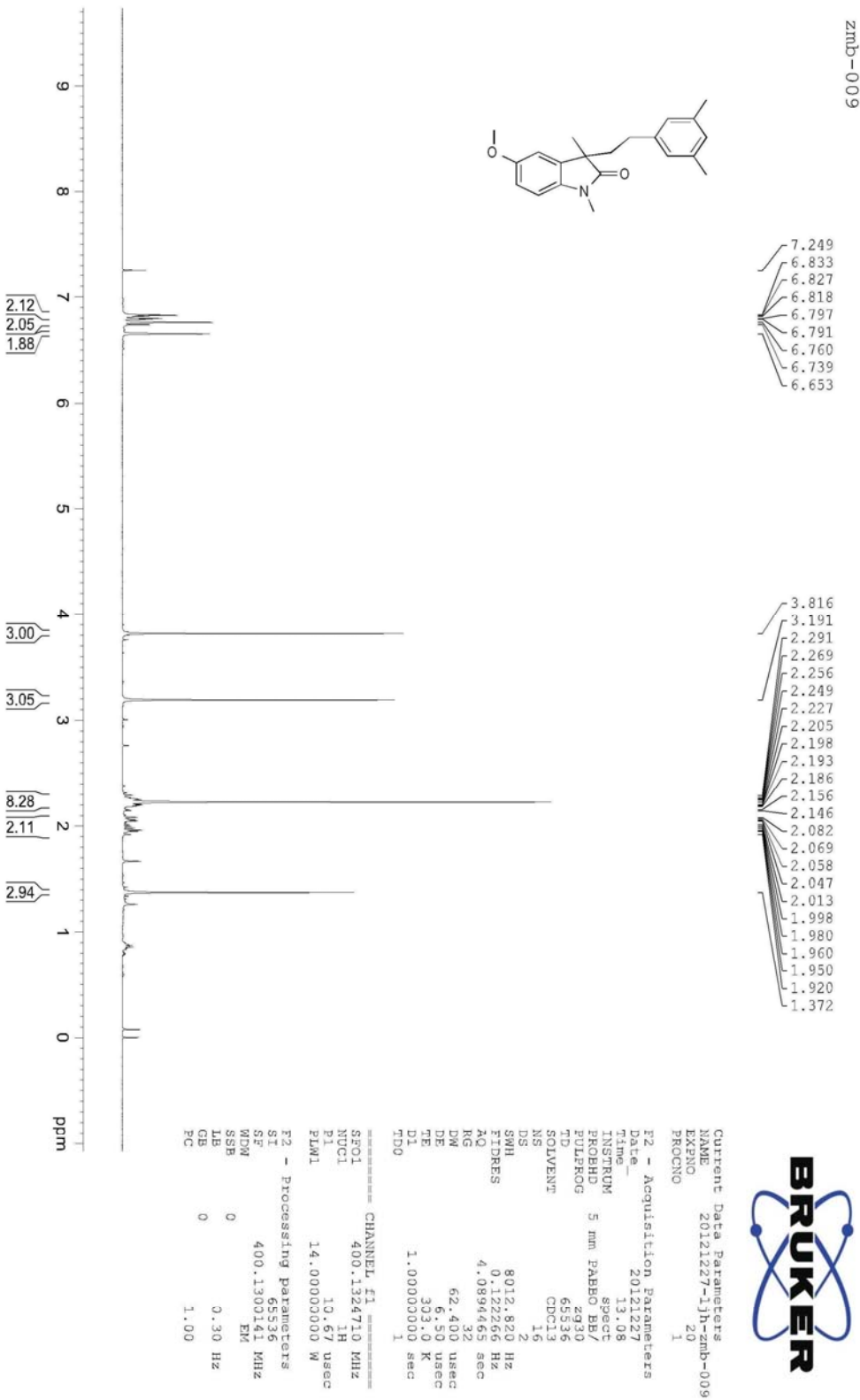
3-(3,5-Dimethylphenethyl)-1,3,5-trimethylindolin-2-one (3eg)



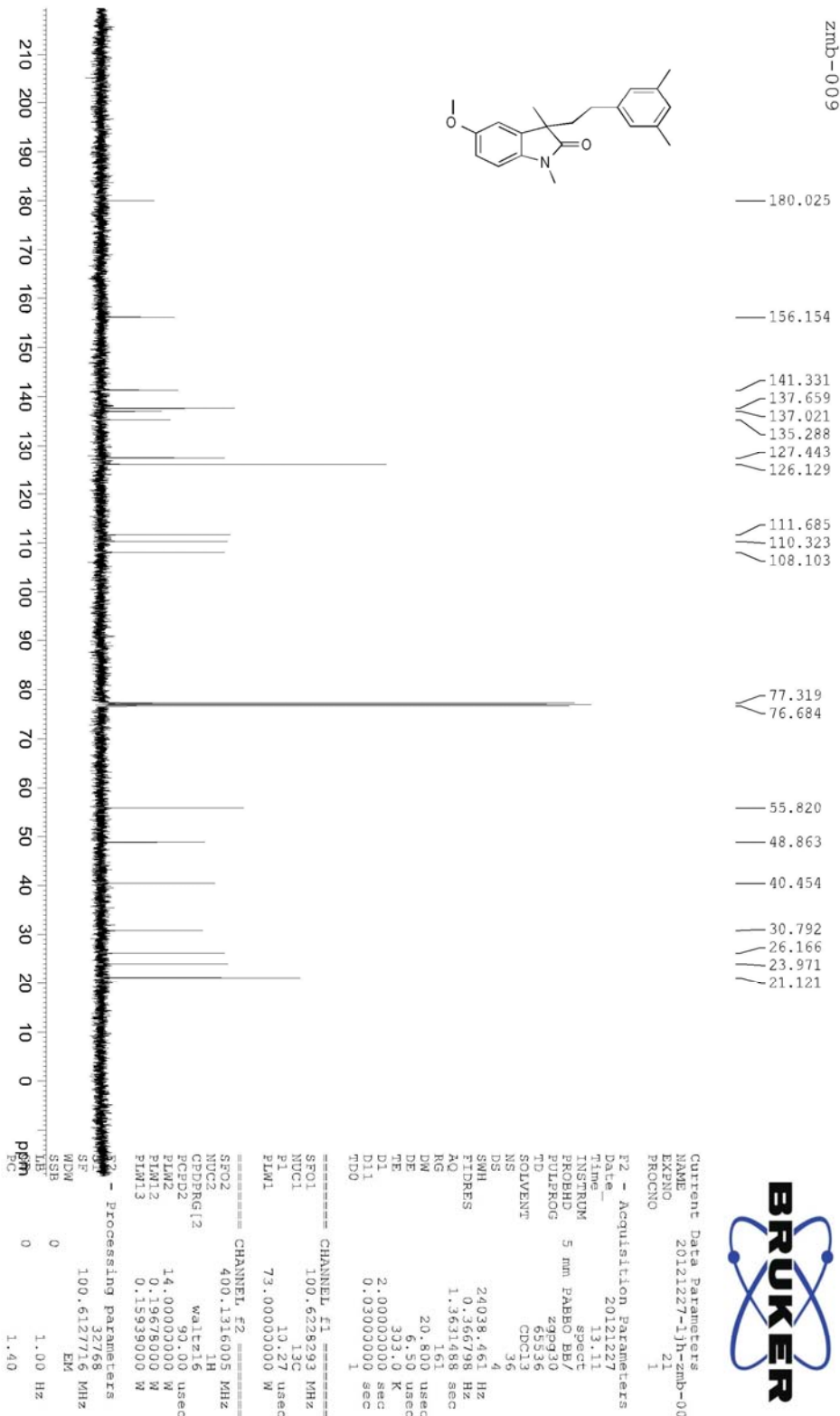
3-(3,5-Dimethylphenethyl)-1,3,5-trimethylindolin-2-one (3eg)



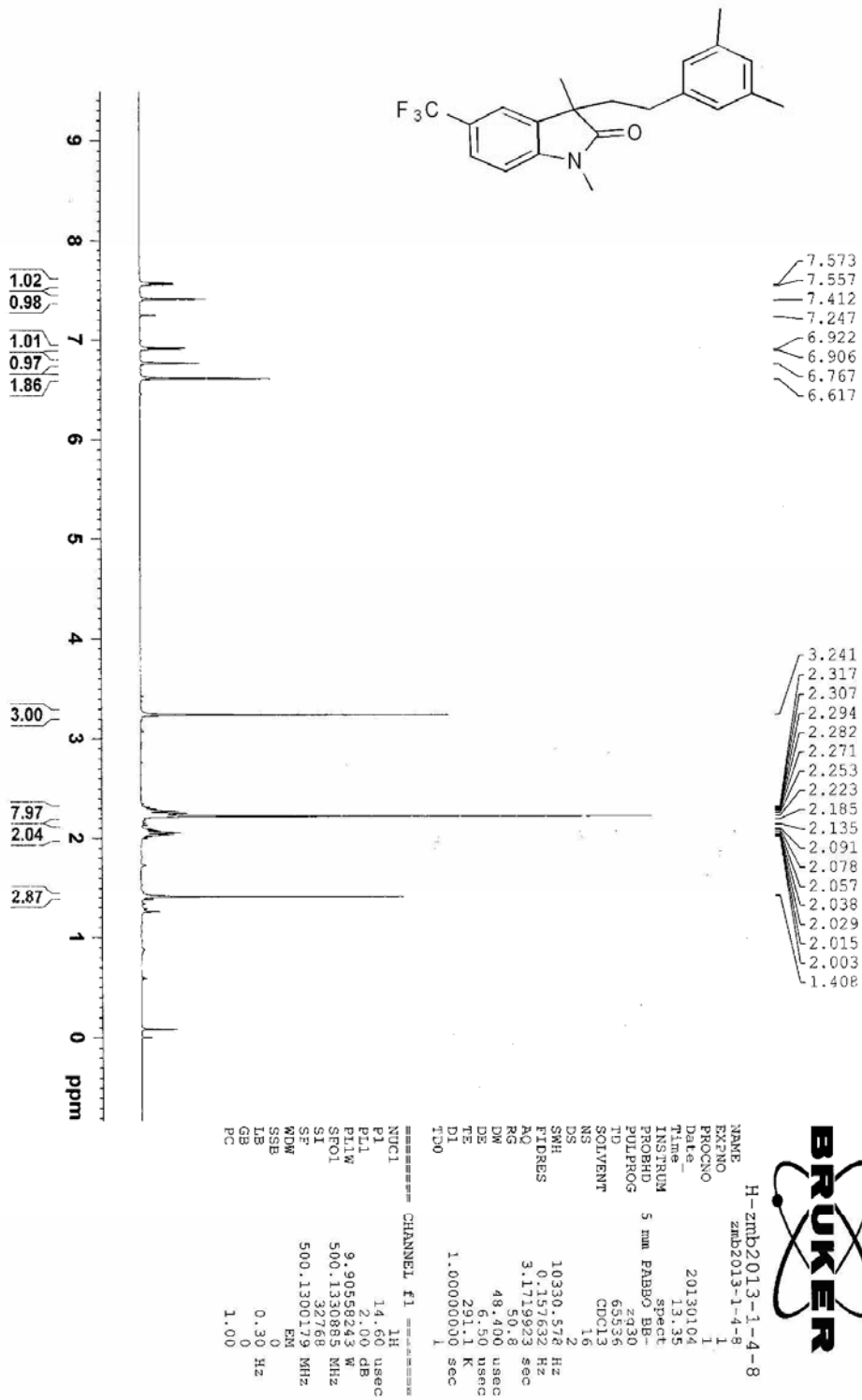
3-(3,5-Dimethylphenethyl)-5-methoxy-1,3-dimethylindolin-2-one (3fg)



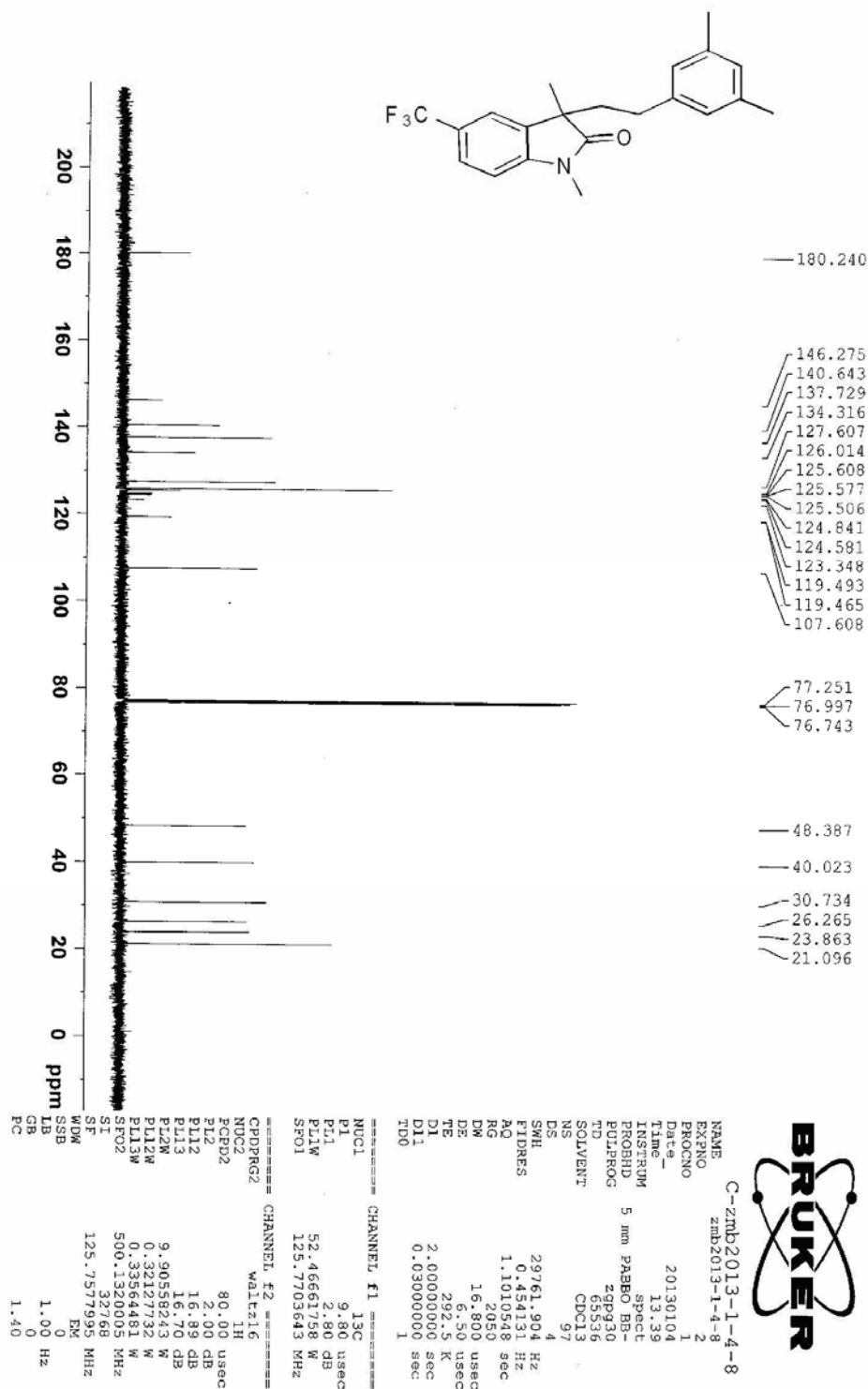
3-(3,5-Dimethylphenethyl)-5-methoxy-1,3-dimethylindolin-2-one (3fg)



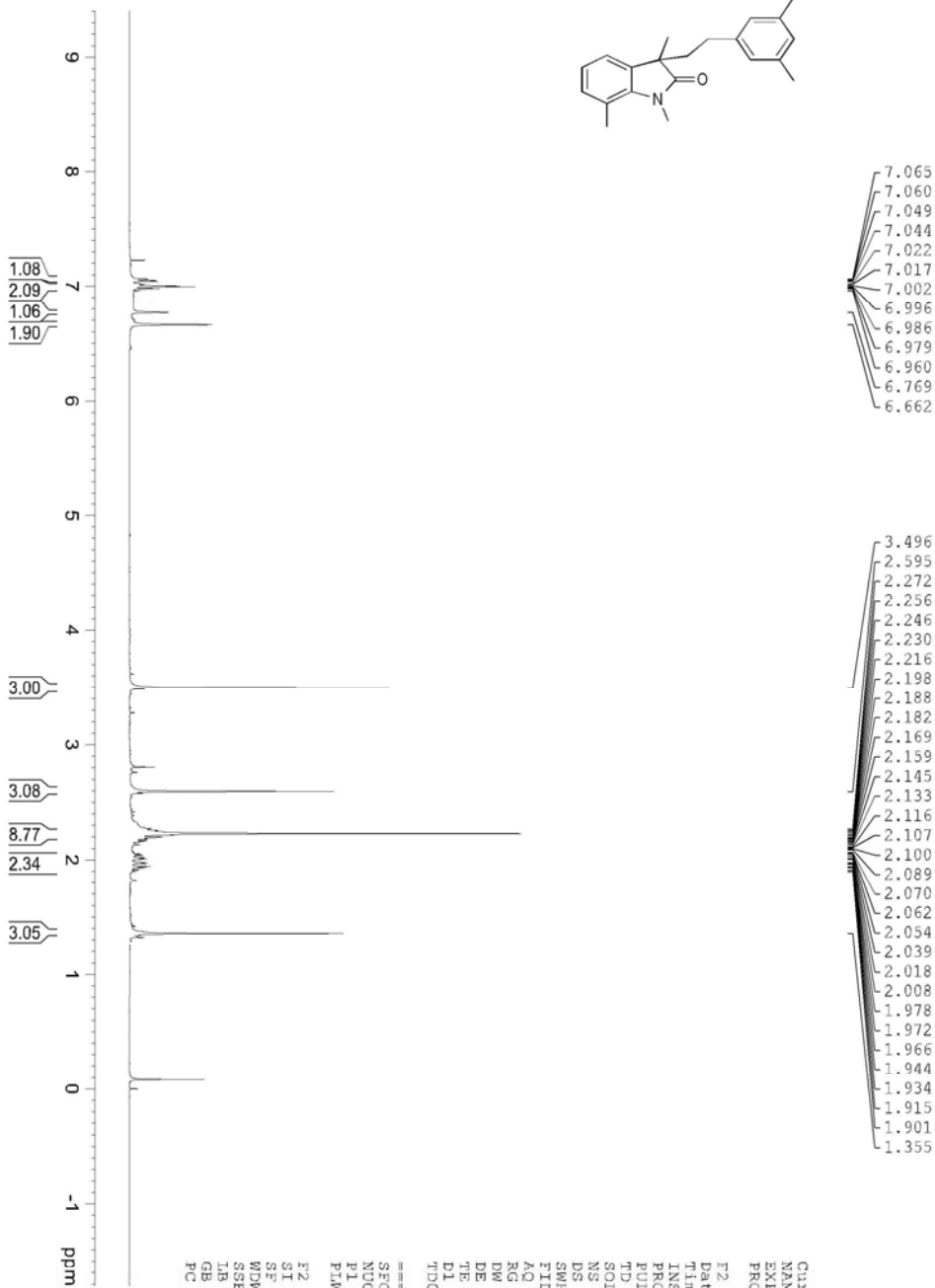
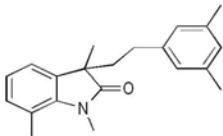
3-(3,5-Dimethylphenethyl)-1,3-dimethyl-5-(trifluoromethyl)indolin-2-one (3gg)



3-(3,5-Dimethylphenethyl)-1,3-dimethyl-5-(trifluoromethyl)indolin-2-one (3gg)



3-(3,5-Dimethylphenethyl)-1,3,7-trimethylindolin-2-one (3hg)



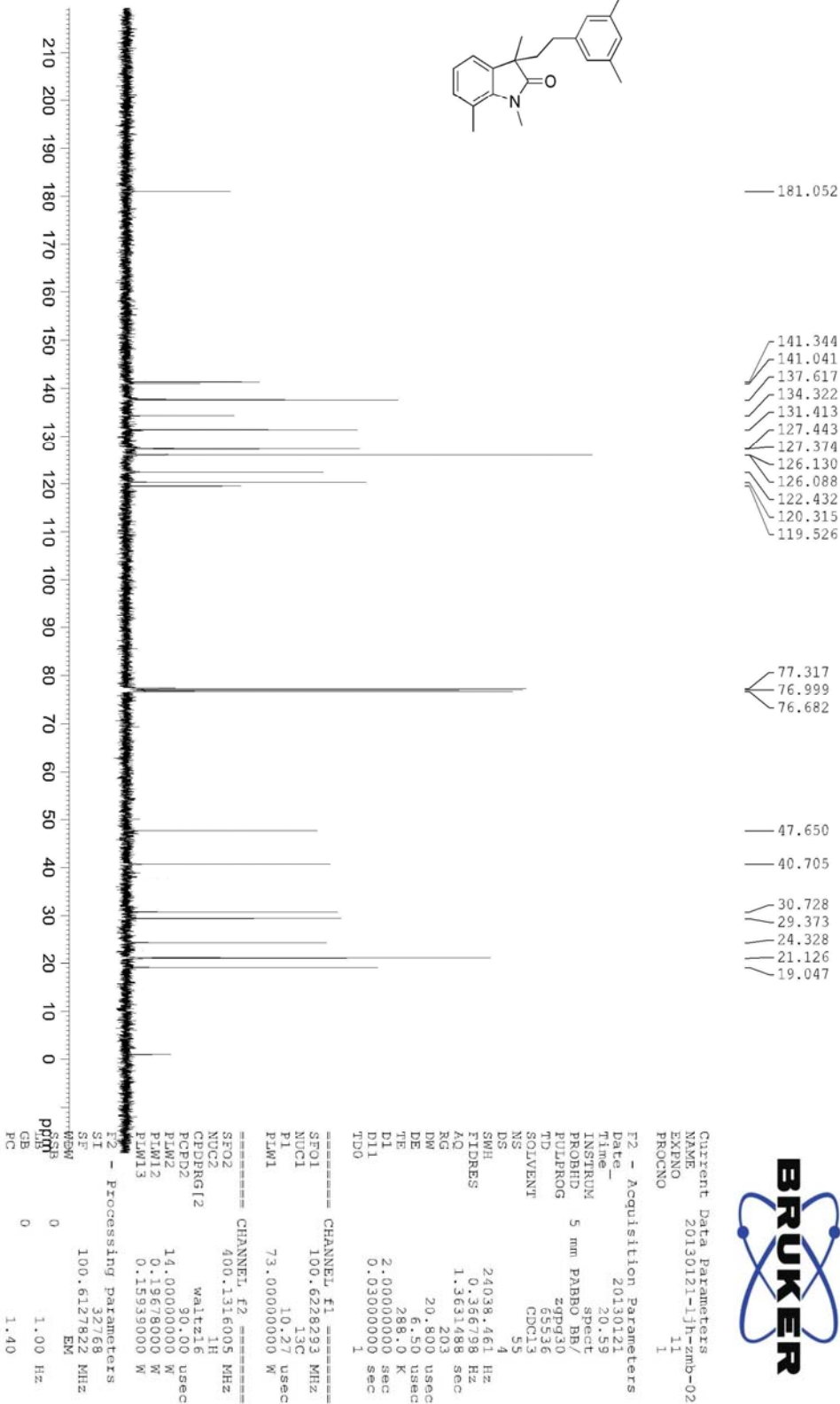
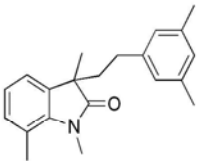
Current Data Parameters
NAME 20130121-1jh-zmb-02
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130121
Time 20.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
RG 4.089465 sec
AQ 18
DW 62.400 usec
DE 6.50 usec
TE 287.6 K
D1 1.00000000 sec
TD0 1

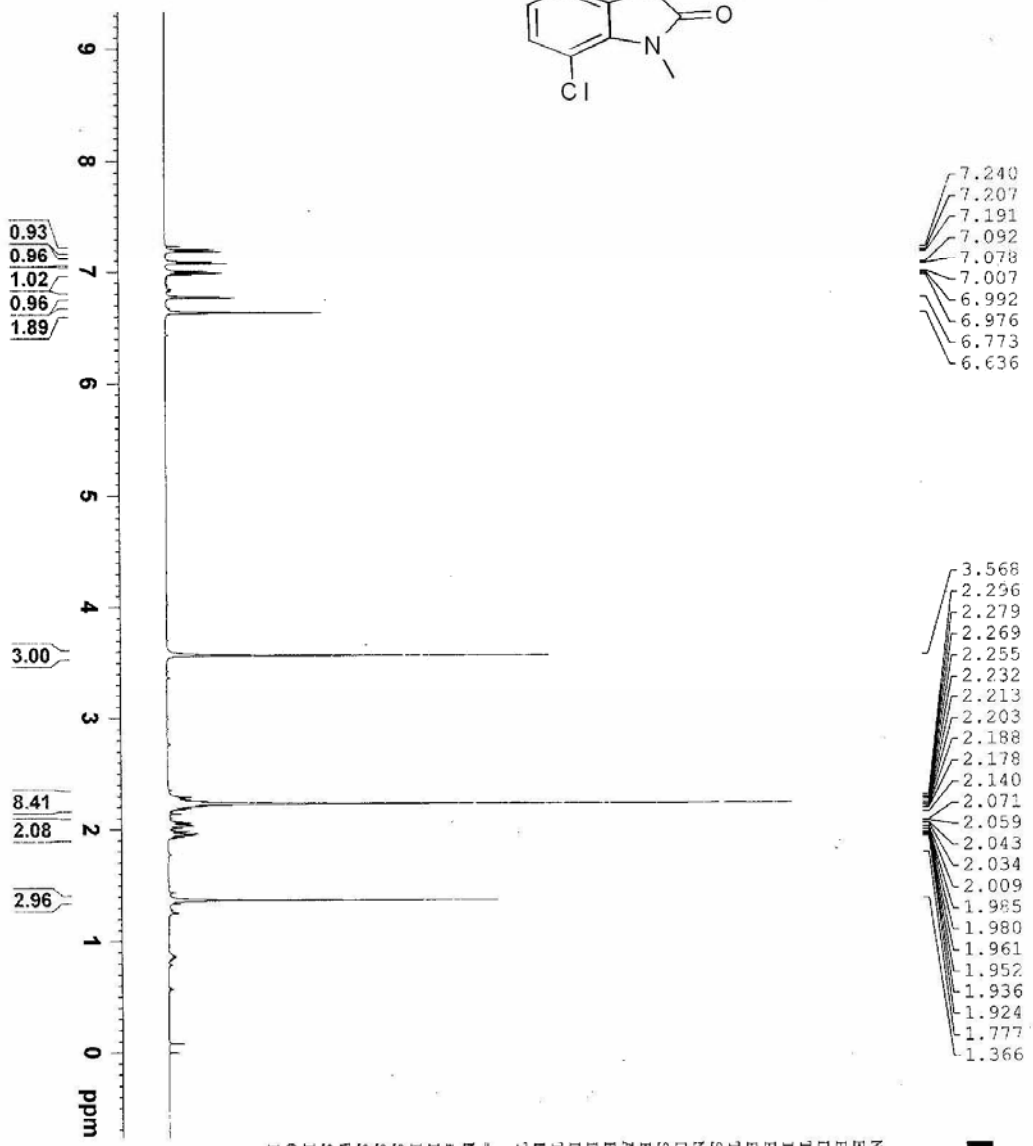
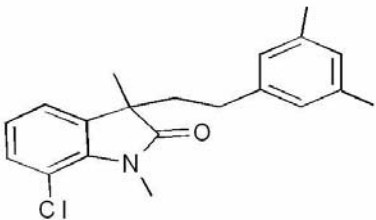
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 10.67 usec
PLM1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300232 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3-(3,5-Dimethylphenethyl)-1,3,7-trimethylindolin-2-one (3hg)



7-Chloro-3-(3,5-dimethylphenethyl)-1,3-dimethylindolin-2-one (3ig)

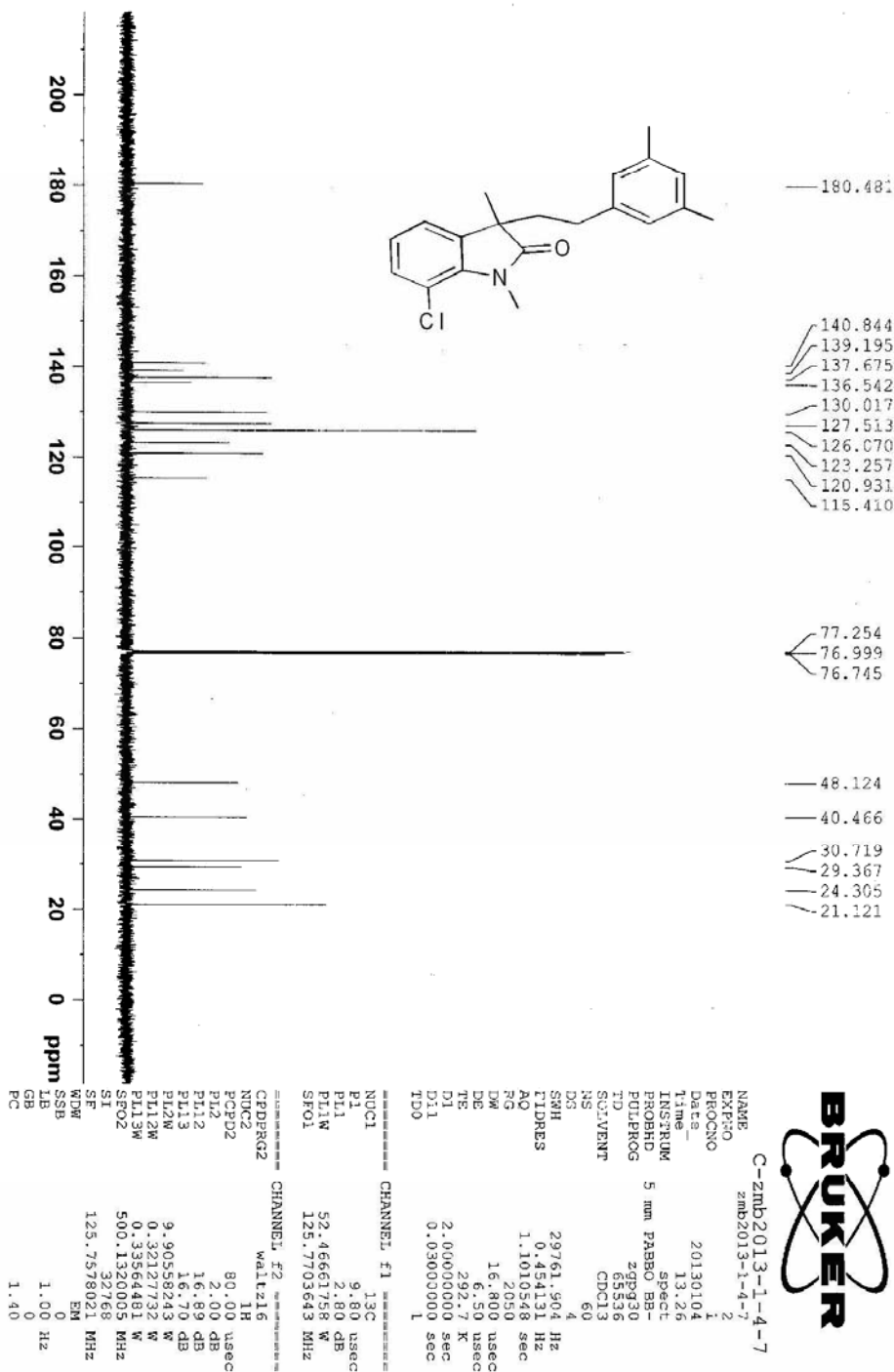


NAME H-zmb2013-1-4-7
EXPNO 1
PROCNO 1
Date_ 20130104
Time 13.07
INSTRUM spect
PROBHD 5 mm PABBO BBO
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719823 sec
RG 45.2
DW 48.400 usec
DE 6.50 usec
TE 291.0 K
D1 1.00000000 sec
TDO 1

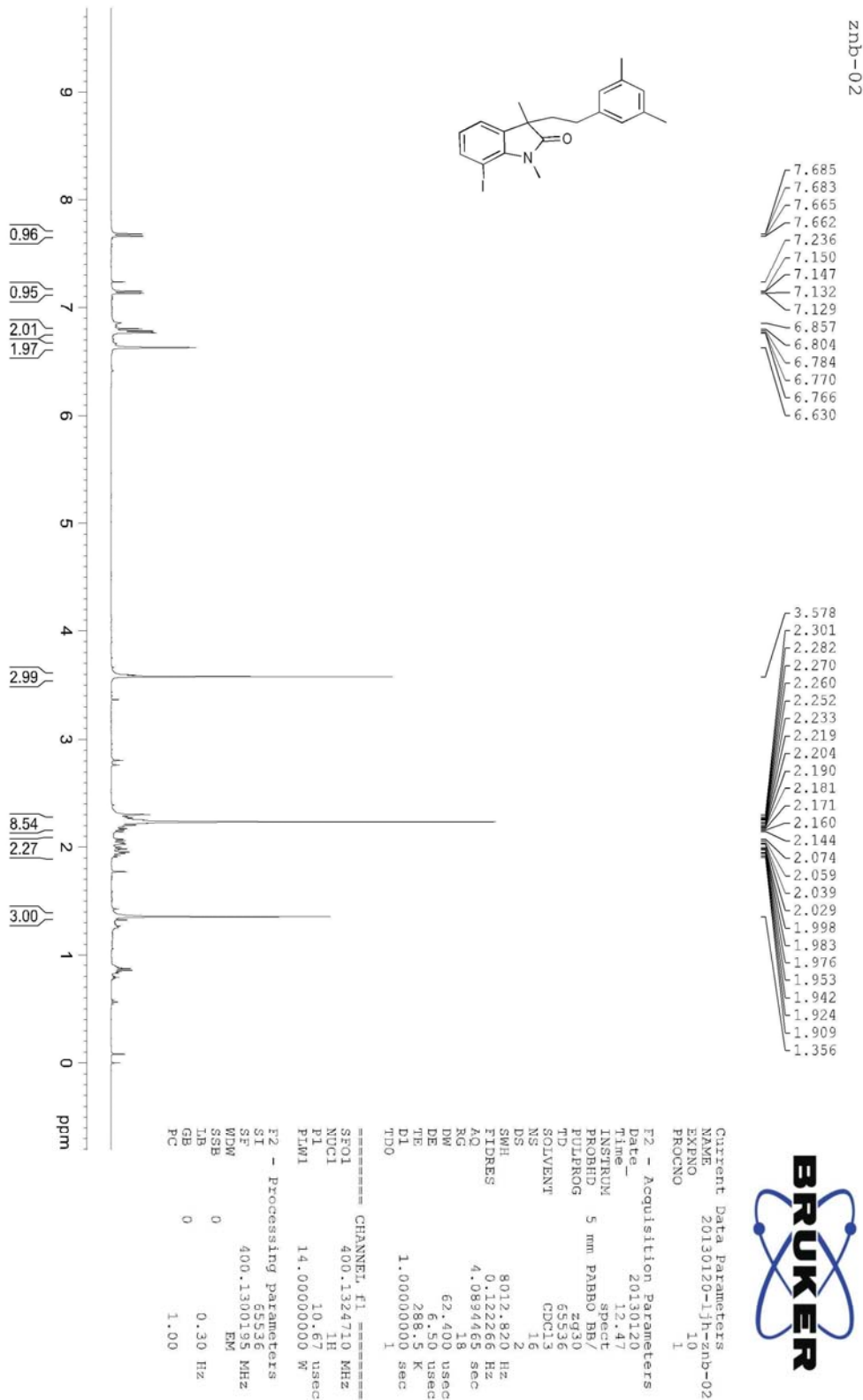
===== CHANNEL f1 =====
NUC1 1H
P1 14.60 usec
PL1 2.00 dB
PL1W 9.90558243 W
SFO1 500.130885 MHz
SI 32768
SF 500.1300211 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



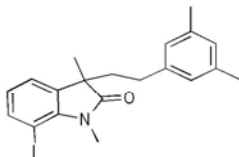
7-Chloro-3-(3,5-dimethylphenethyl)-1,3-dimethylindolin-2-one (3ig)



3-(3,5-Dimethylphenethyl)-7-iodo-1,3-dimethylindolin-2-one (3jg)



3-(3,5-Dimethylphenethyl)-7-iodo-1,3-dimethylindolin-2-one (3jg)



znb-02



Current Data Parameters
NAME 20130120-1jg-znb-02
EXPNO 1
PROCNO 1

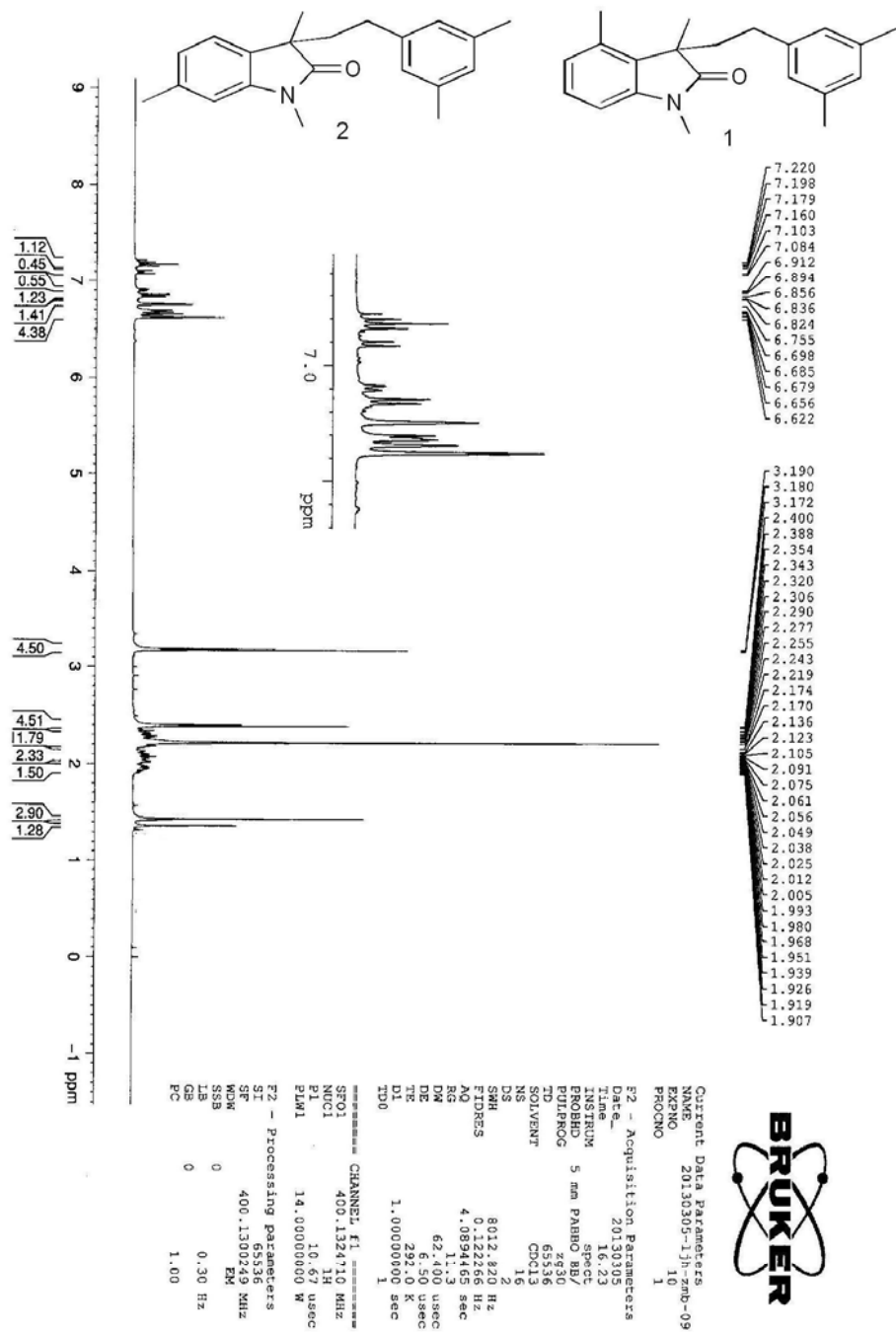
F2 - Acquisition Parameters
Date_ 20130120
Time 12.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 50
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
RG 1.363148 sec
AQ 80.6
RG 20.800 usec
DE 6.50 usec
TE 289.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 10.27 usec
PLM1 73.0000000 W

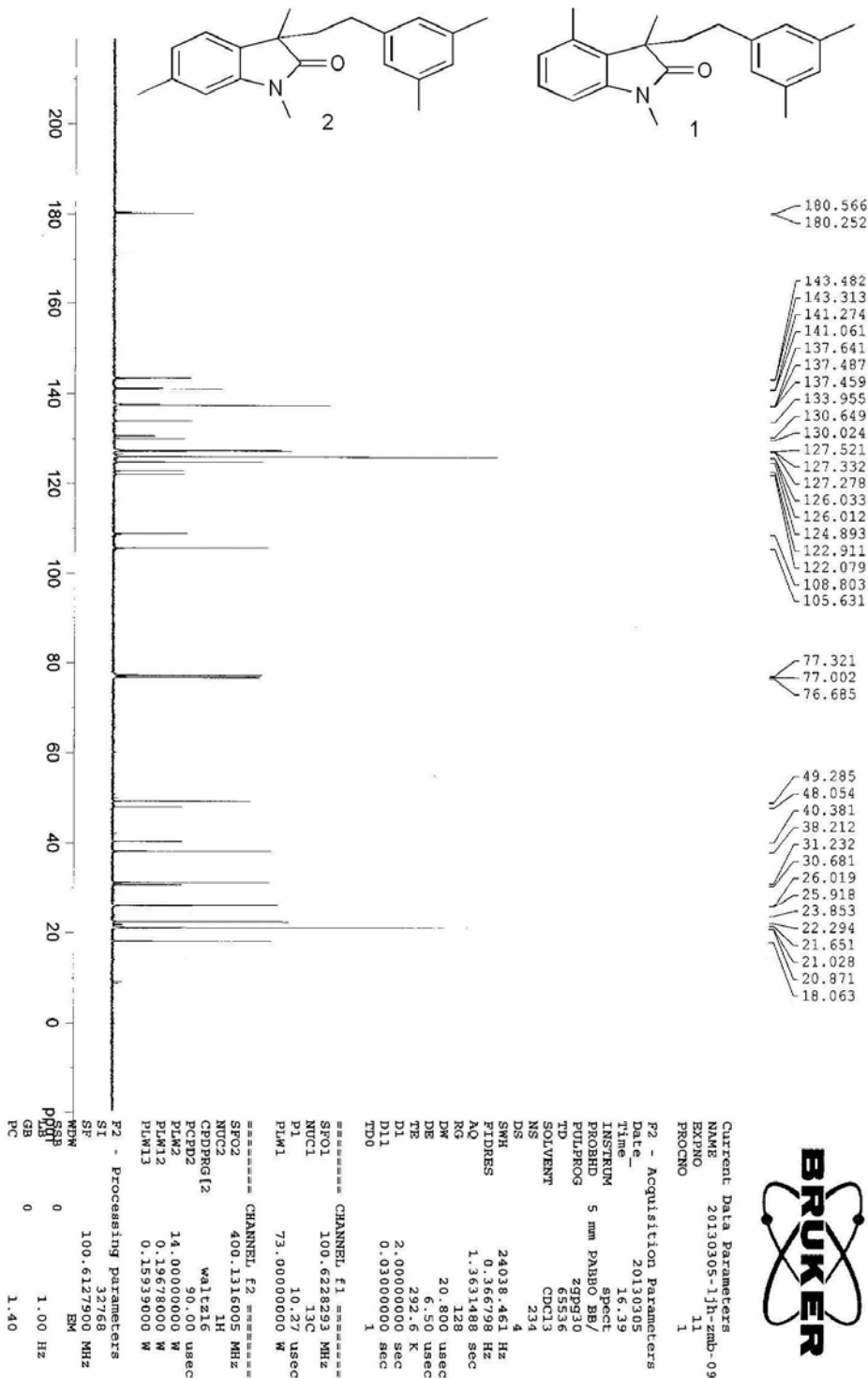
CHANNEL f2
SFO2 400.1516005 MHz
NUC2 1H
PCPD2 90.00 usec
PLM2 14.0000000 W
PLM12 0.19678000 W
PLM13 0.15939000 W

Processing Parameters
SI 32768
SF 100.6127819 MHz
WDW EM
SSB 0
GB 0
PC 1.40

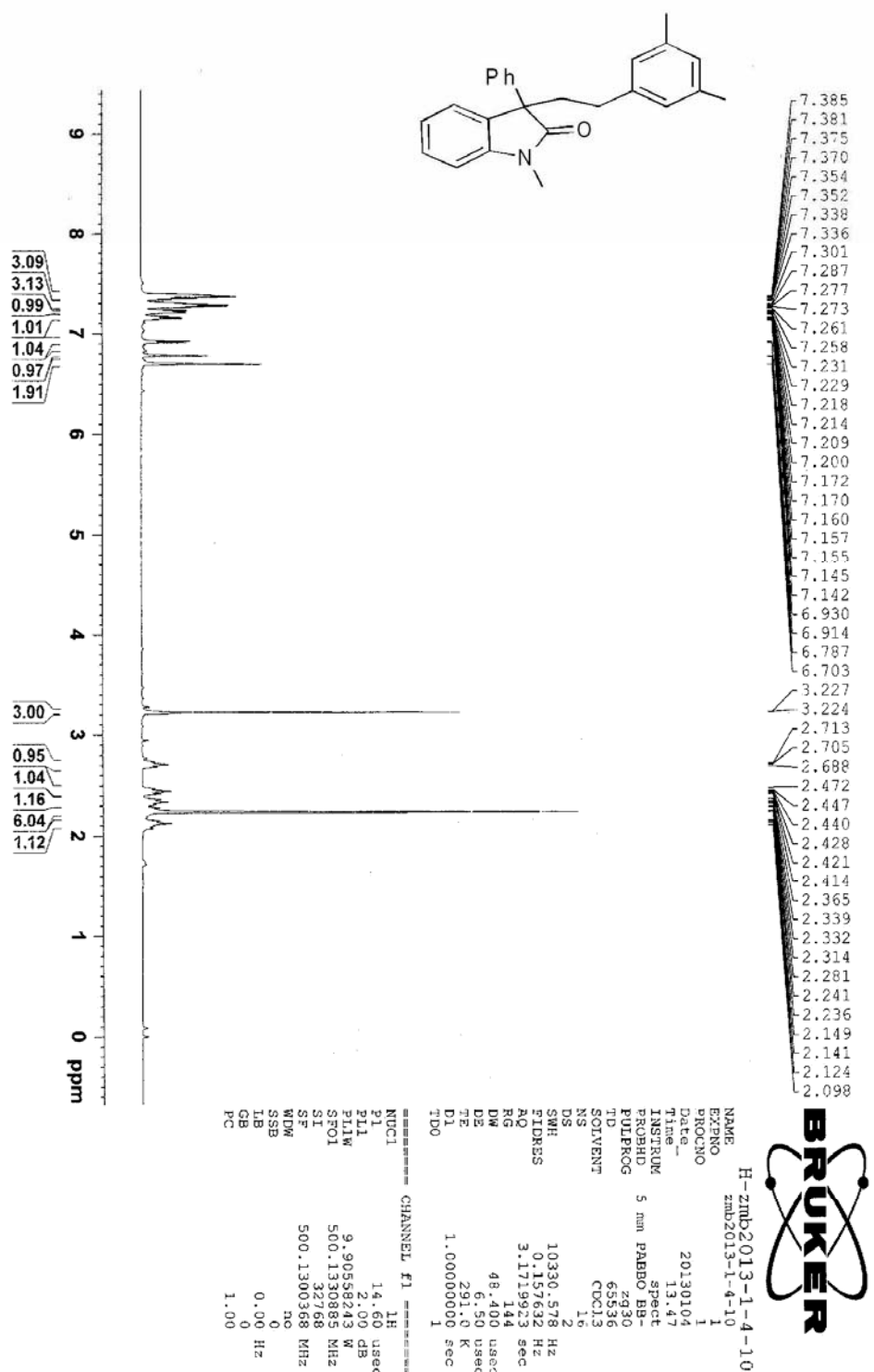
3-(3,5-Dimethylphenethyl)-1,3,6-trimethylindolin-2-one (3kg) and 3-(3,5-Dimethylphenethyl)-1,3,4-trimethylindolin-2-one (3kg')



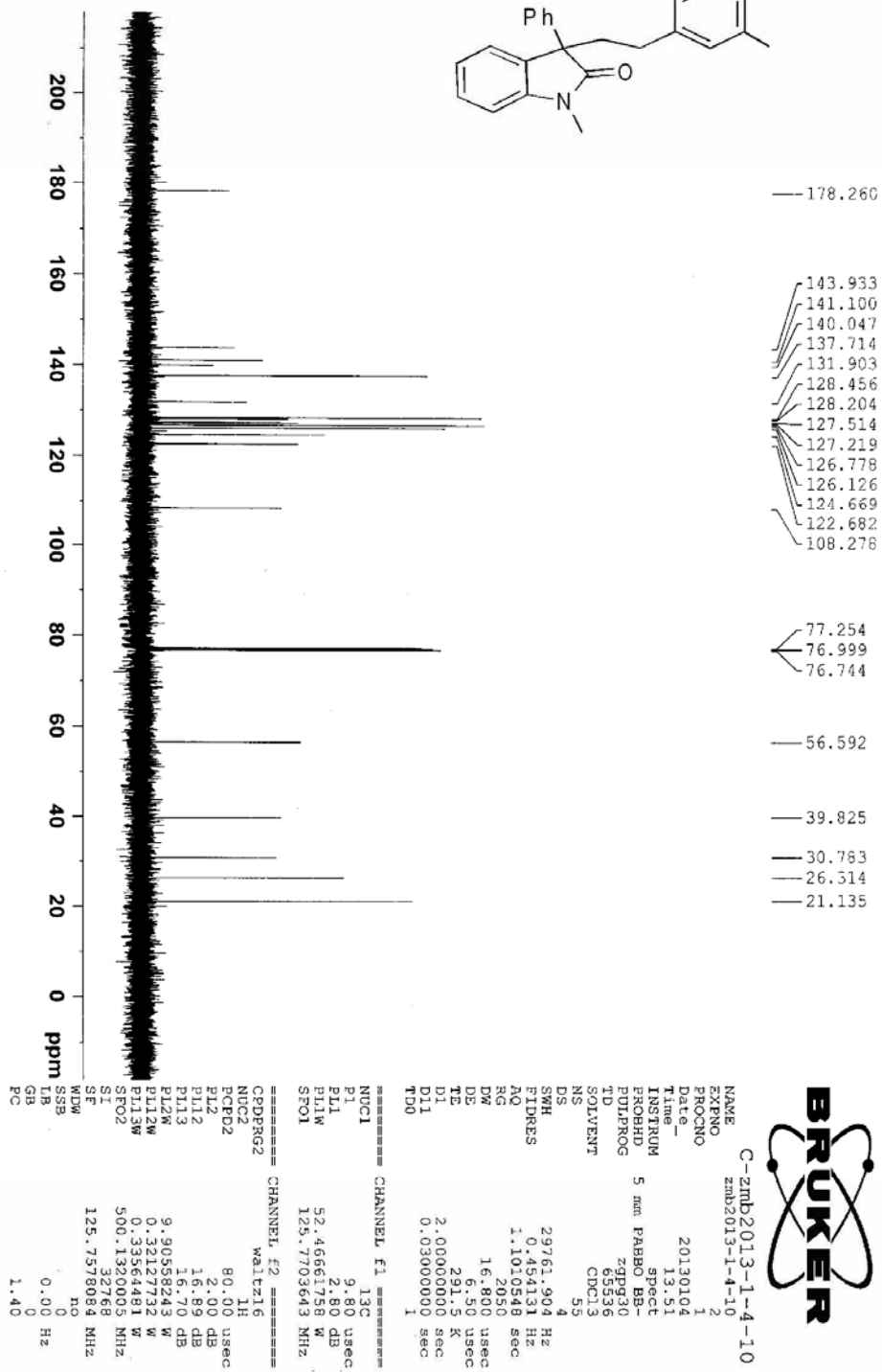
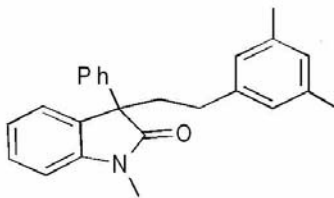
3-(3,5-Dimethylphenethyl)-1,3,6-trimethylindolin-2-one (3kg) and 3-(3,5-Dimethylphenethyl)-1,3,4-trimethylindolin-2-one (3kg')



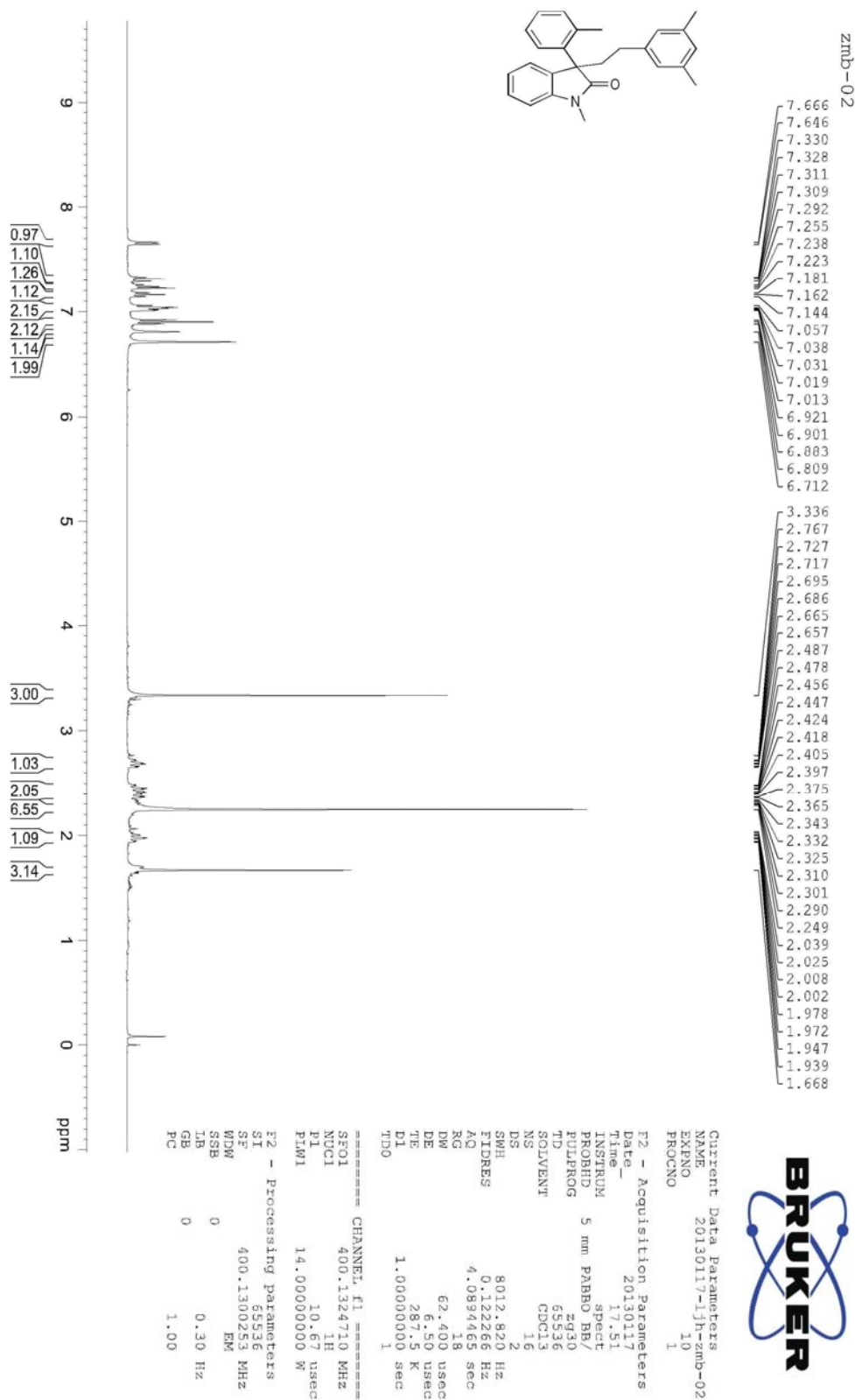
3-(3,5-Dimethylphenethyl)-1-methyl-3-phenylindolin-2-one (3lg)



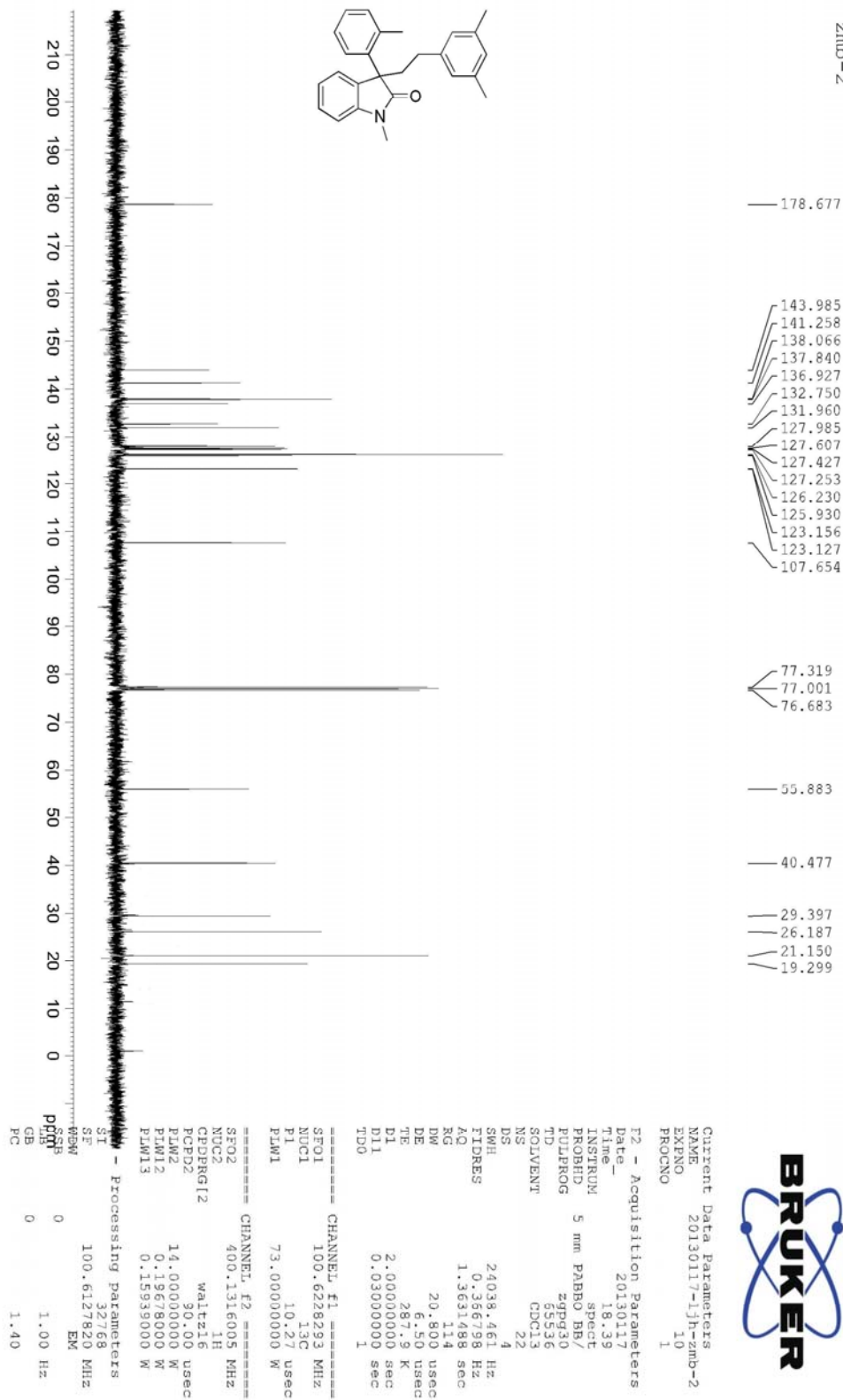
3-(3,5-Dimethylphenethyl)-1-methyl-3-phenylindolin-2-one (3lg)



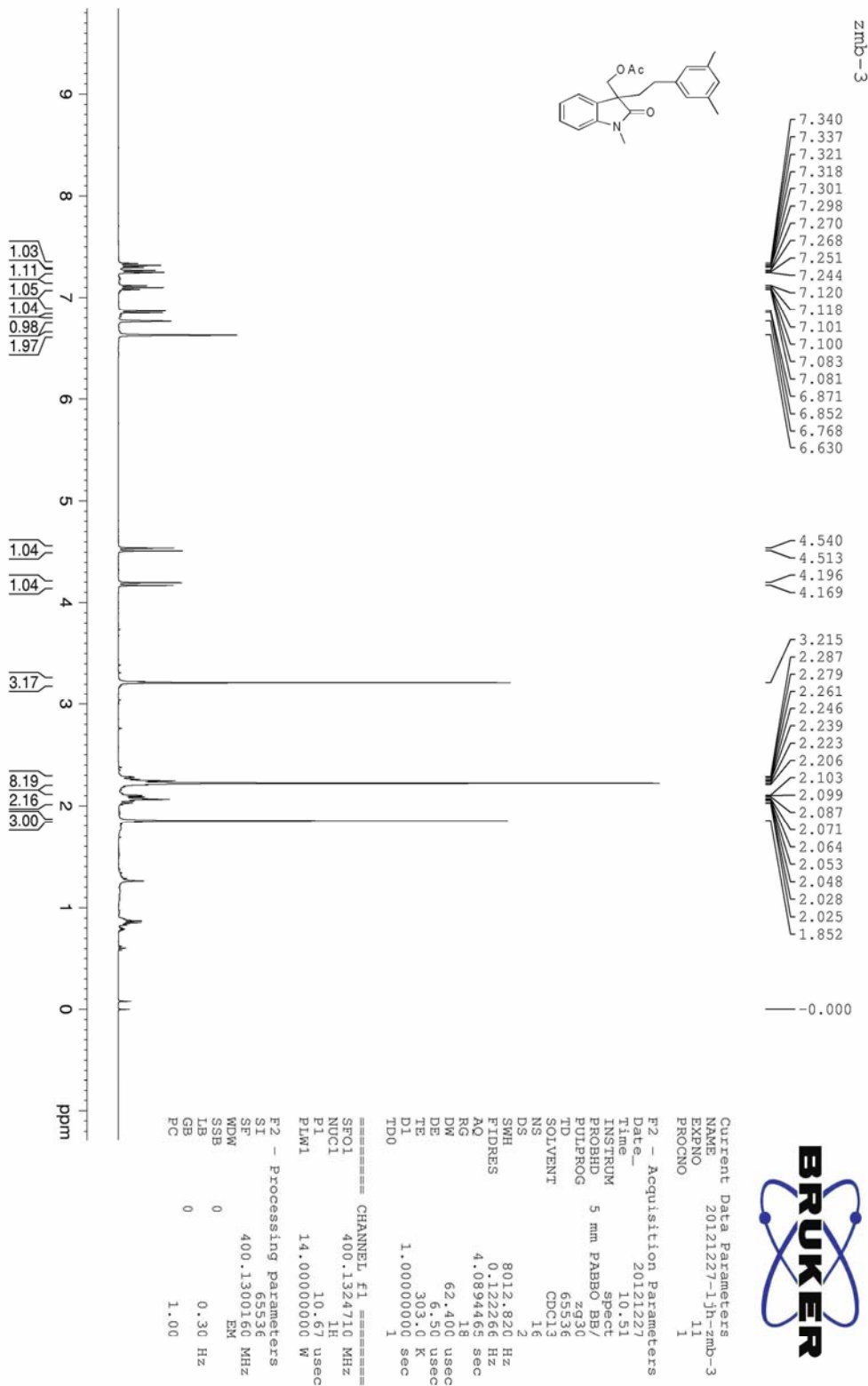
3-(3,5-Dimethylphenethyl)-1-methyl-3-(o-tolyl)indolin-2-one (3mg)



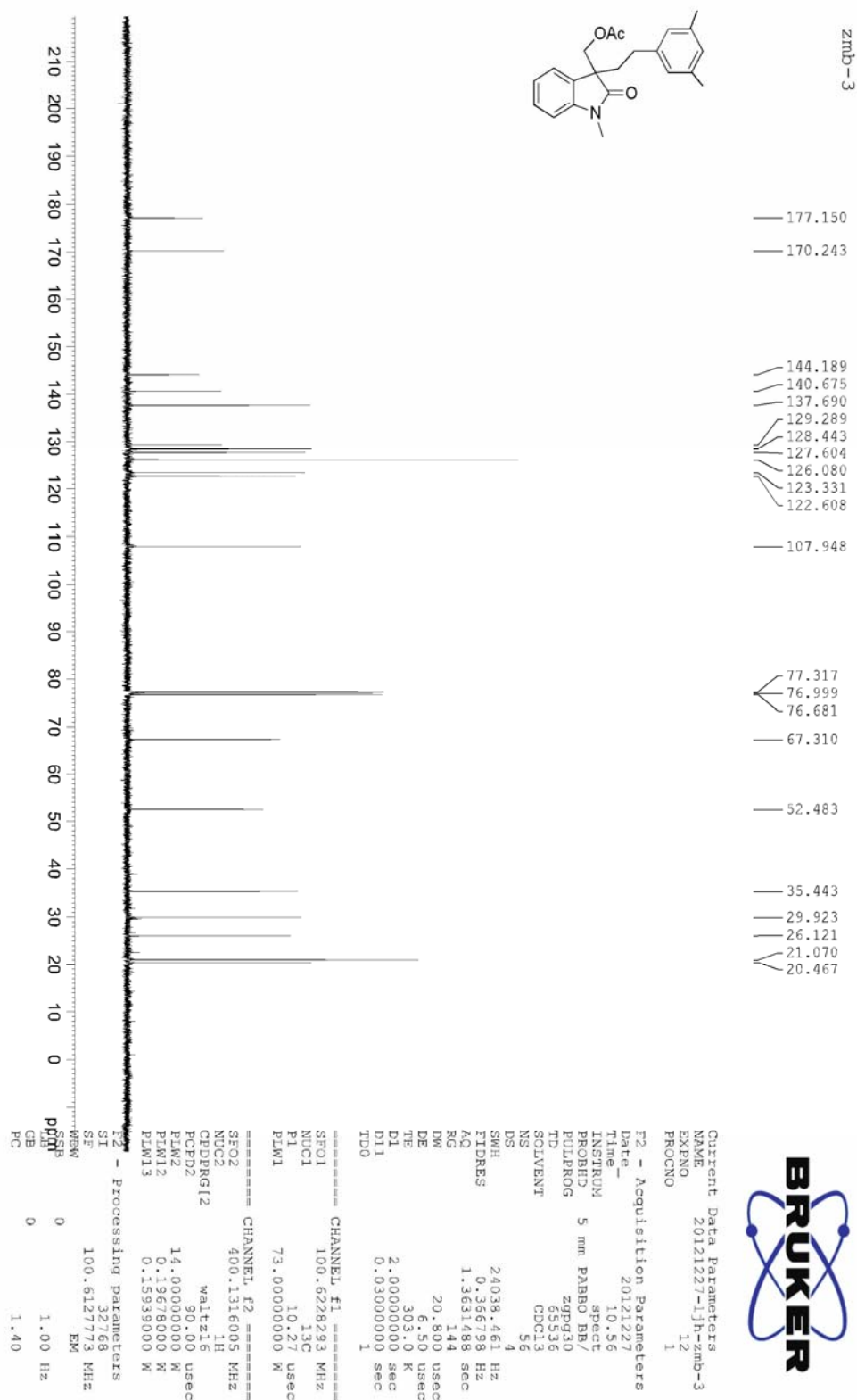
3-(3,5-Dimethylphenethyl)-1-methyl-3-(o-tolyl)indolin-2-one (3mg)



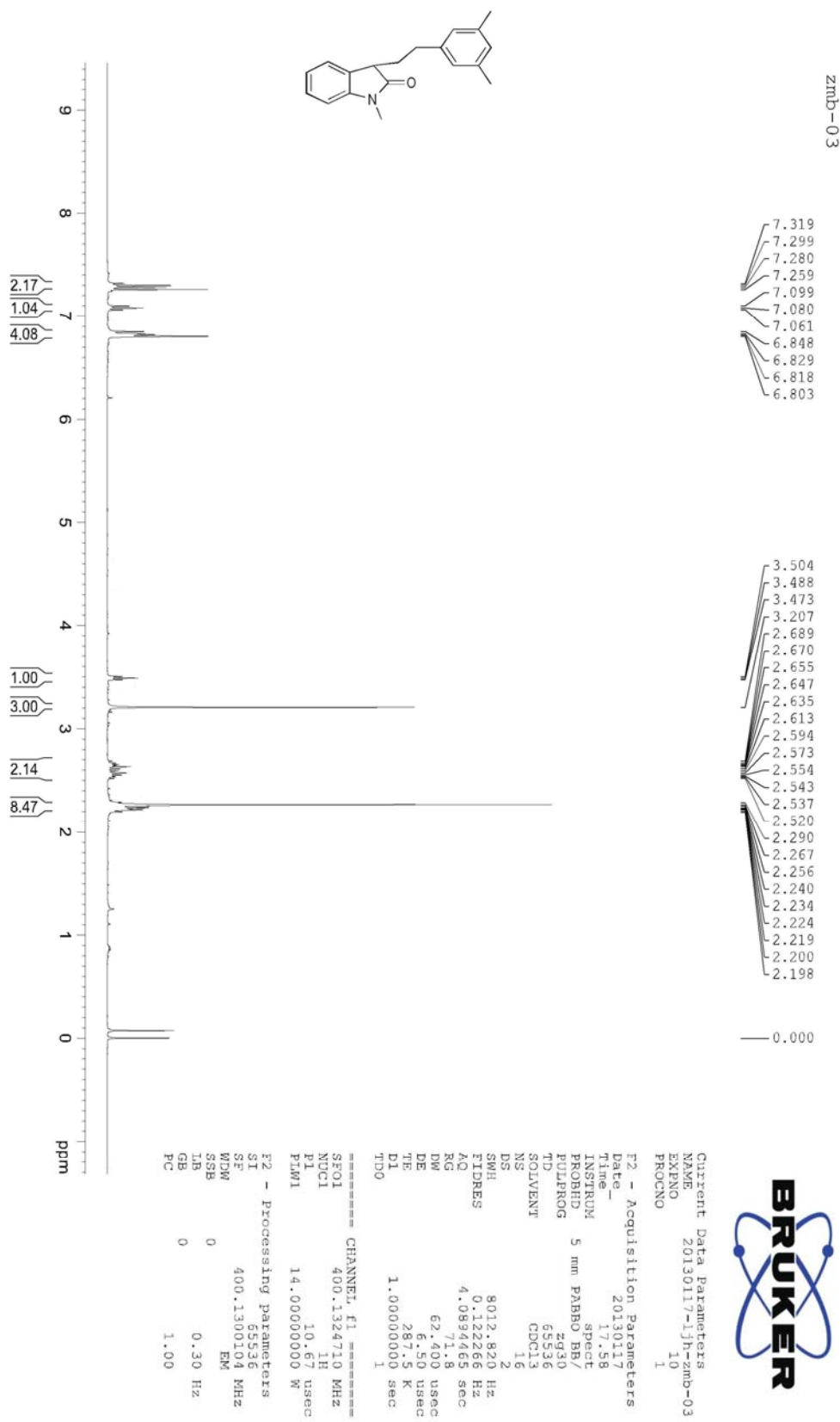
(3-(3,5-Dimethylphenethyl)-1-methyl-2-oxoindolin-3-yl)methyl acetate (3ng)



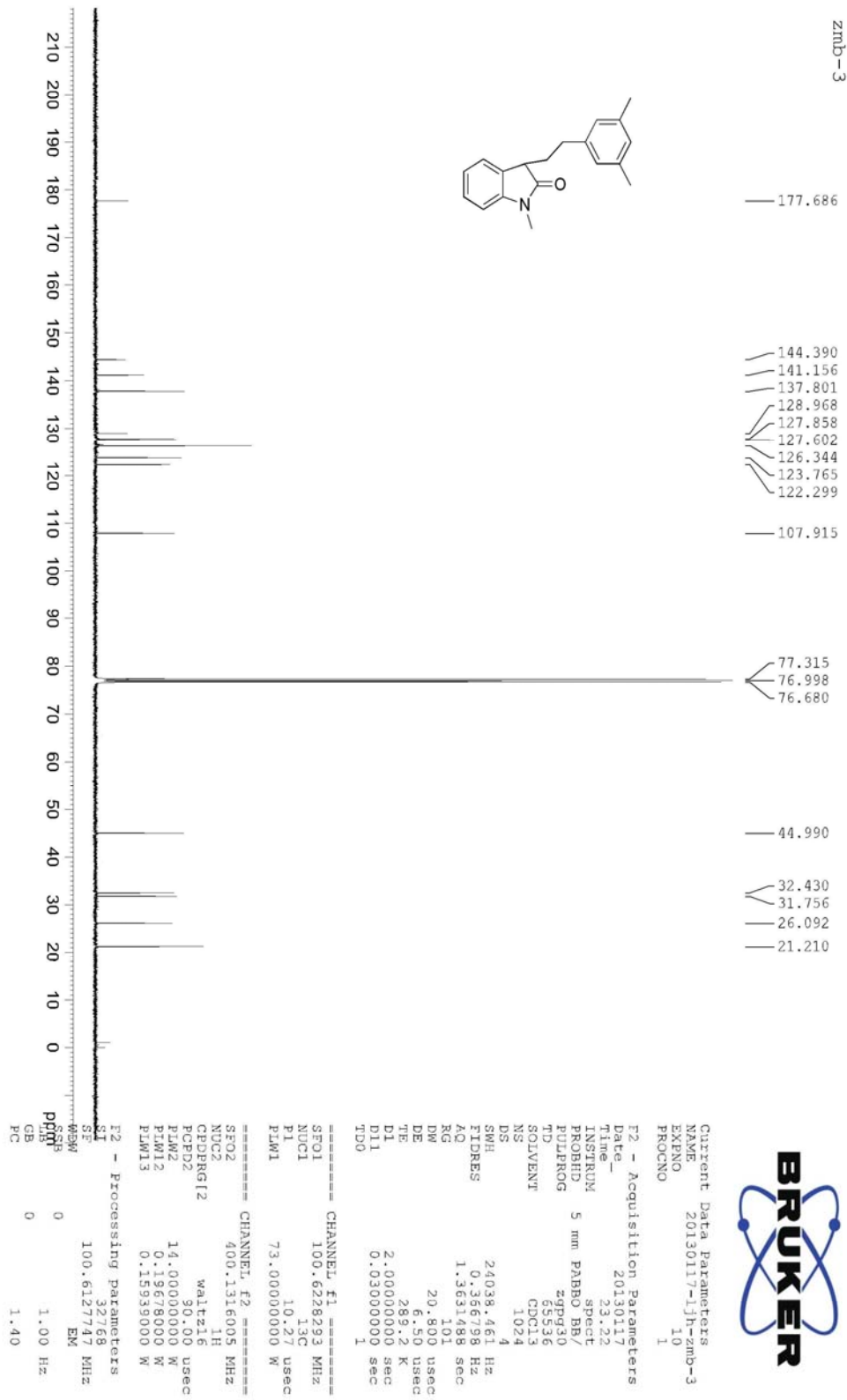
(3-(3,5-Dimethylphenethyl)-1-methyl-2-oxoindolin-3-yl)methyl acetate (3ng)



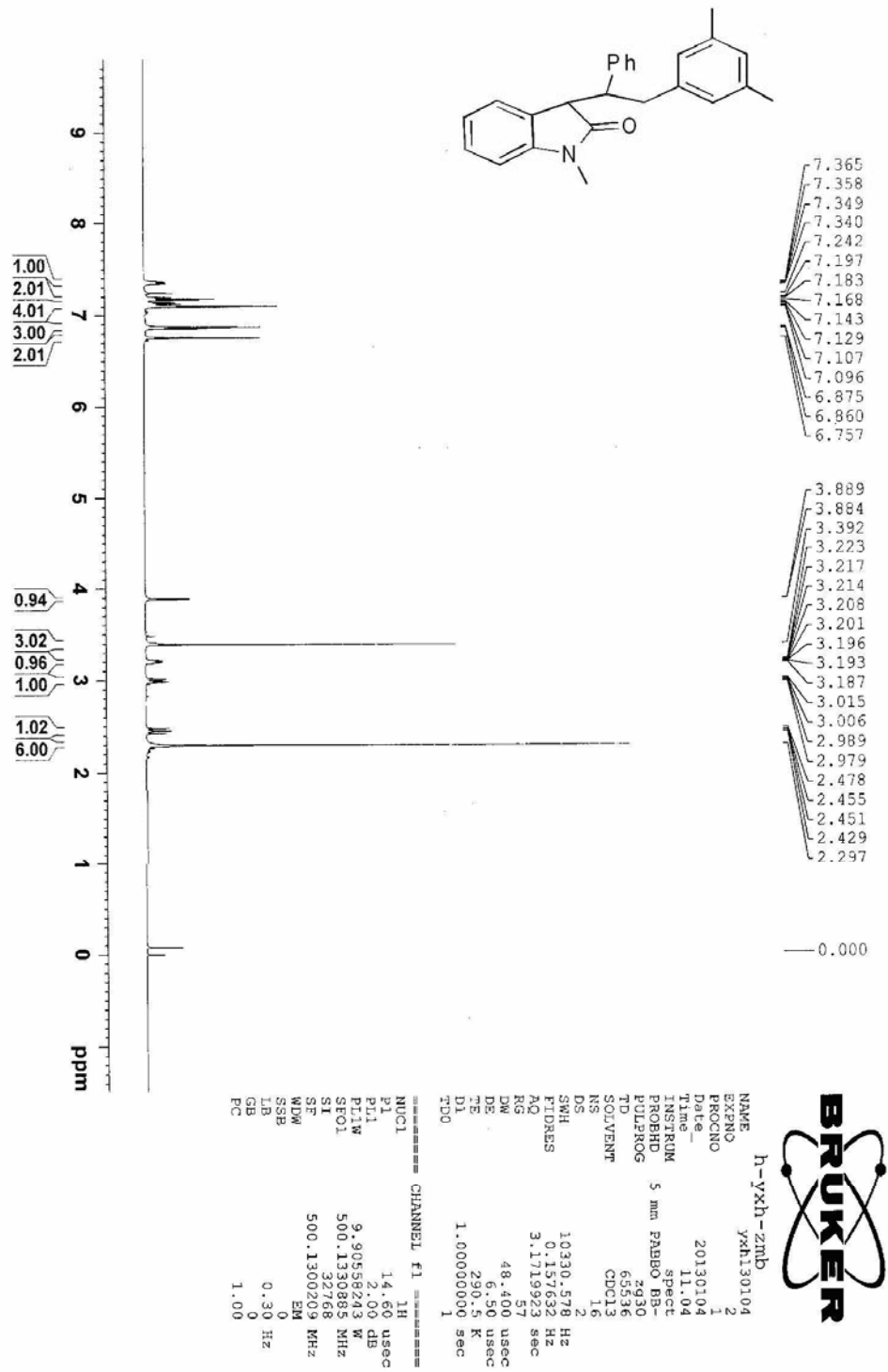
3-(3,5-Dimethylphenethyl)-1-methylindolin-2-one (3og)



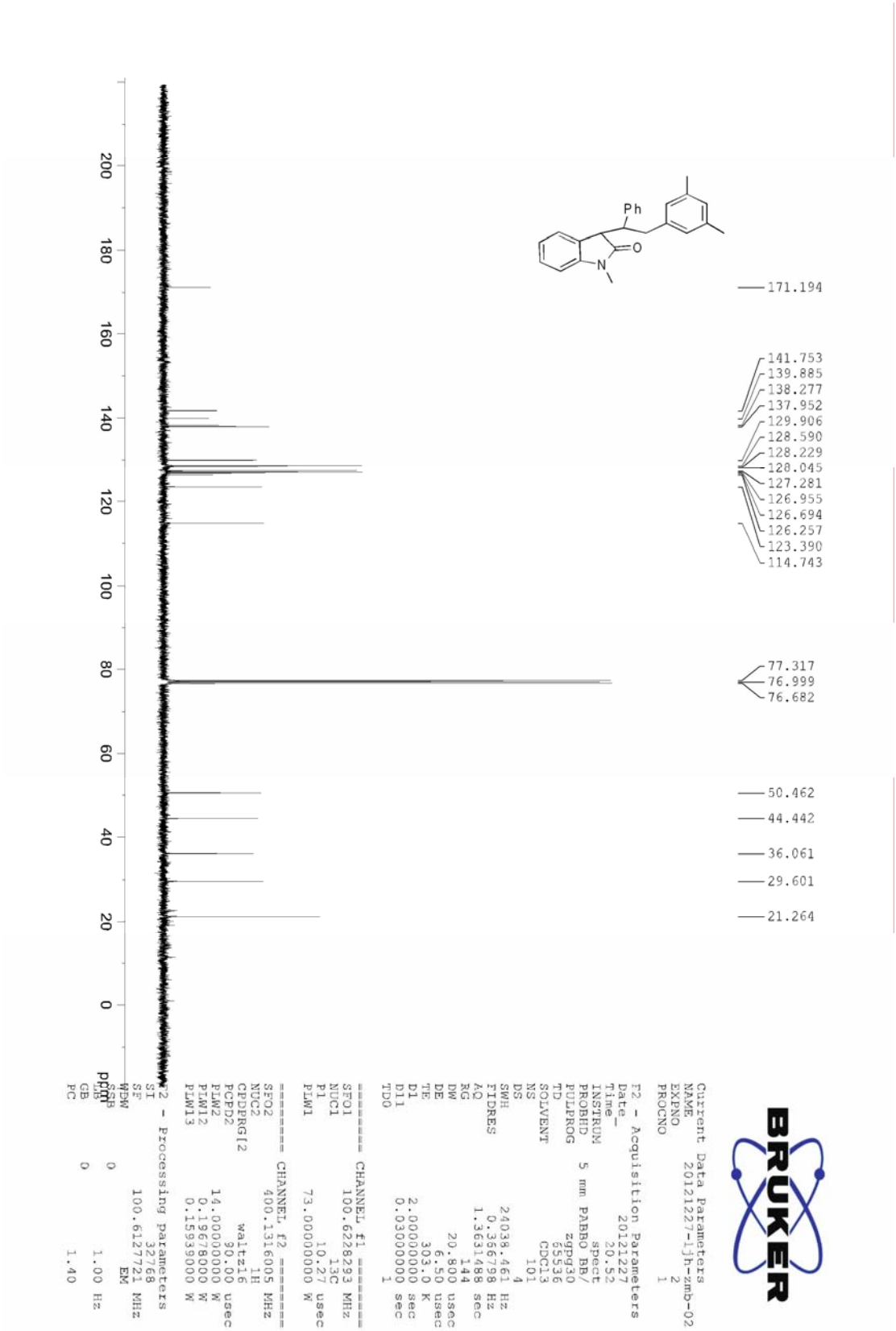
3-(3,5-Dimethylphenethyl)-1-methylindolin-2-one (3og)



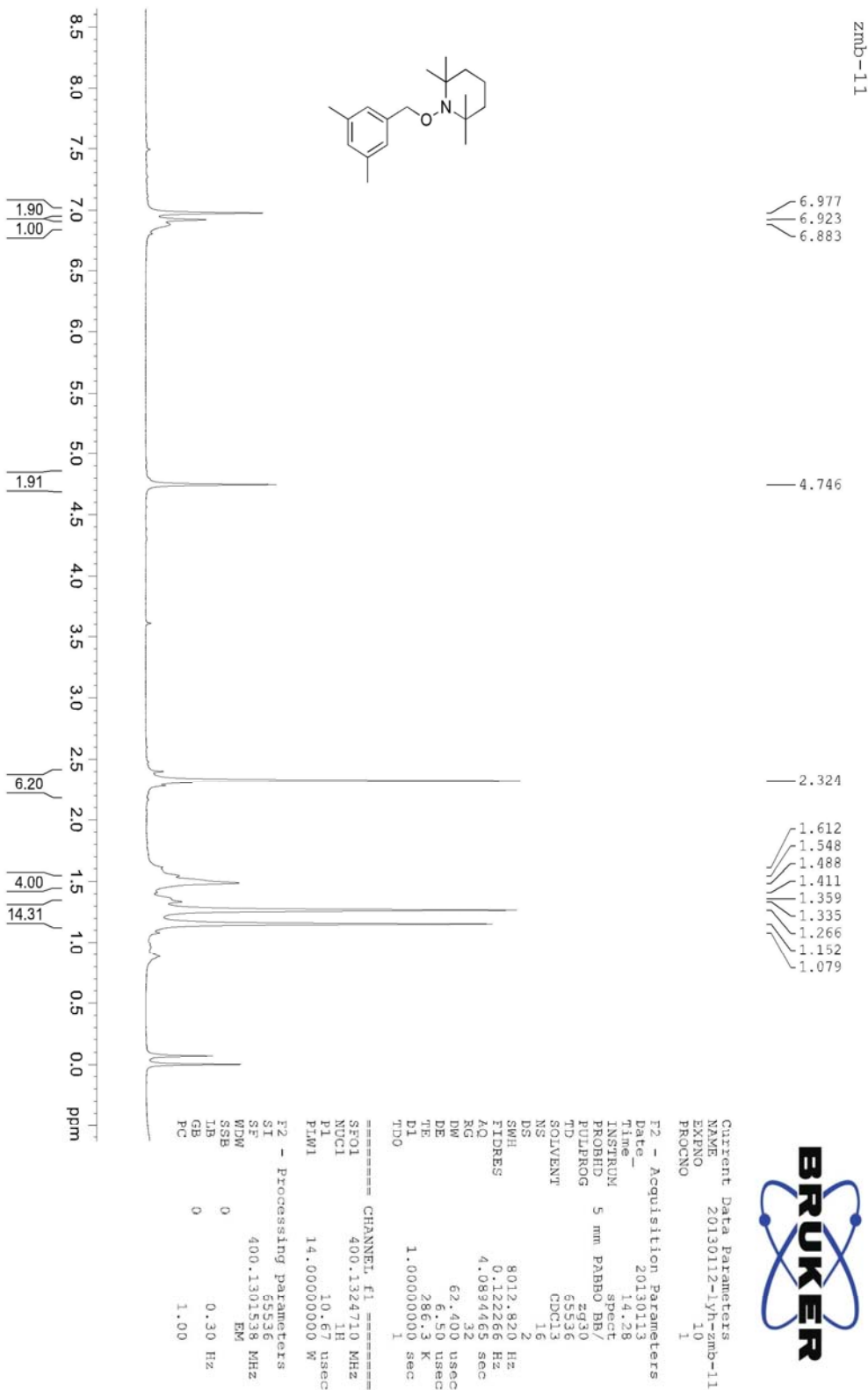
3-(2-(3,5-Dimethylphenyl)-1-phenylethyl)-1-methylindolin-2-one (3pg)



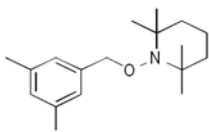
3-(2-(3,5-Dimethylphenyl)-1-phenylethyl)-1-methylindolin-2-one (3pg)



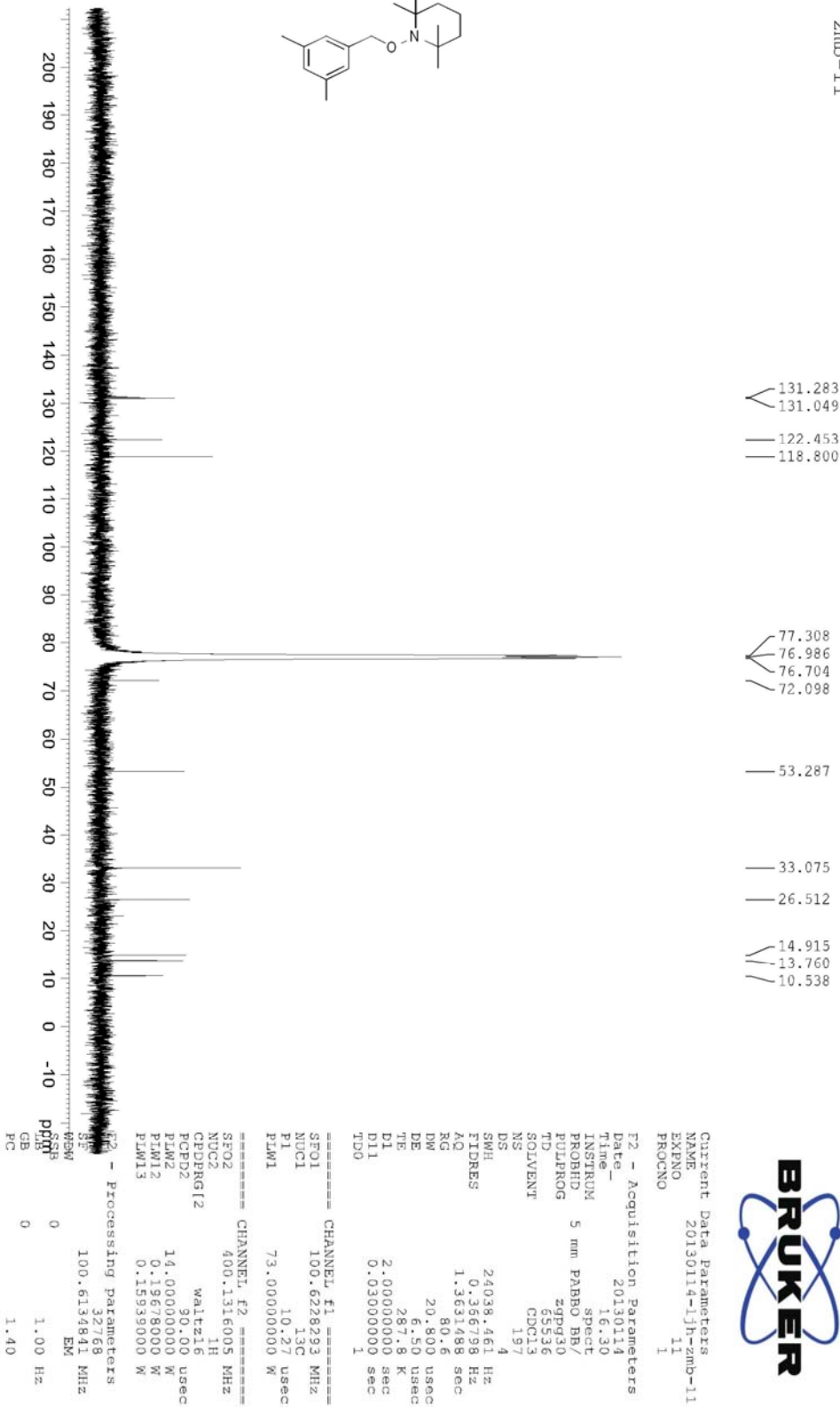
1-((3,5-Dimethylbenzyl)oxy)-2,2,6,6-tetramethylpiperidine (4ag)



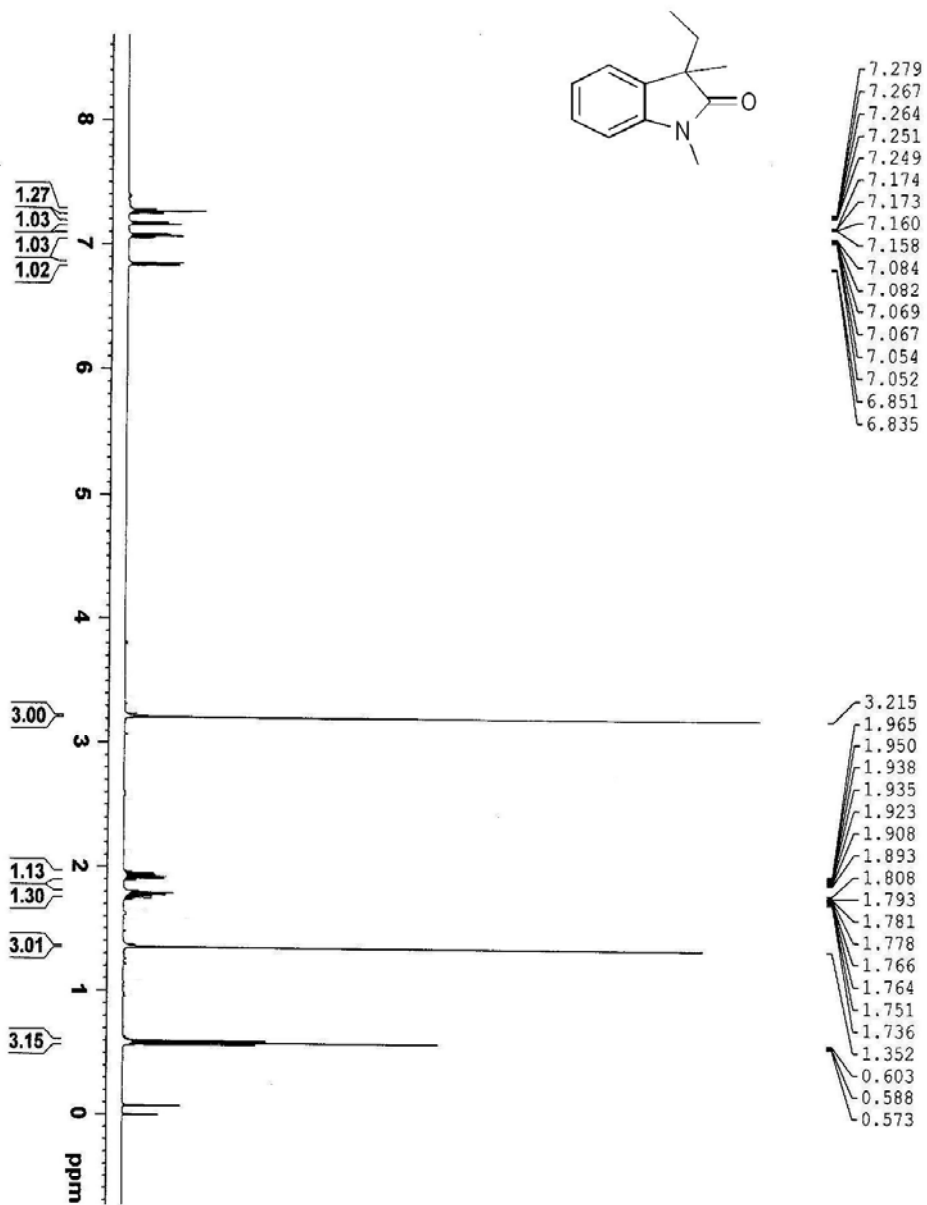
1-((3,5-Dimethylbenzyl)oxy)-2,2,6,6-tetramethylpiperidine (4ag)



zmb-11



3-Ethyl-1,3-dimethylindolin-2-one (5aa)

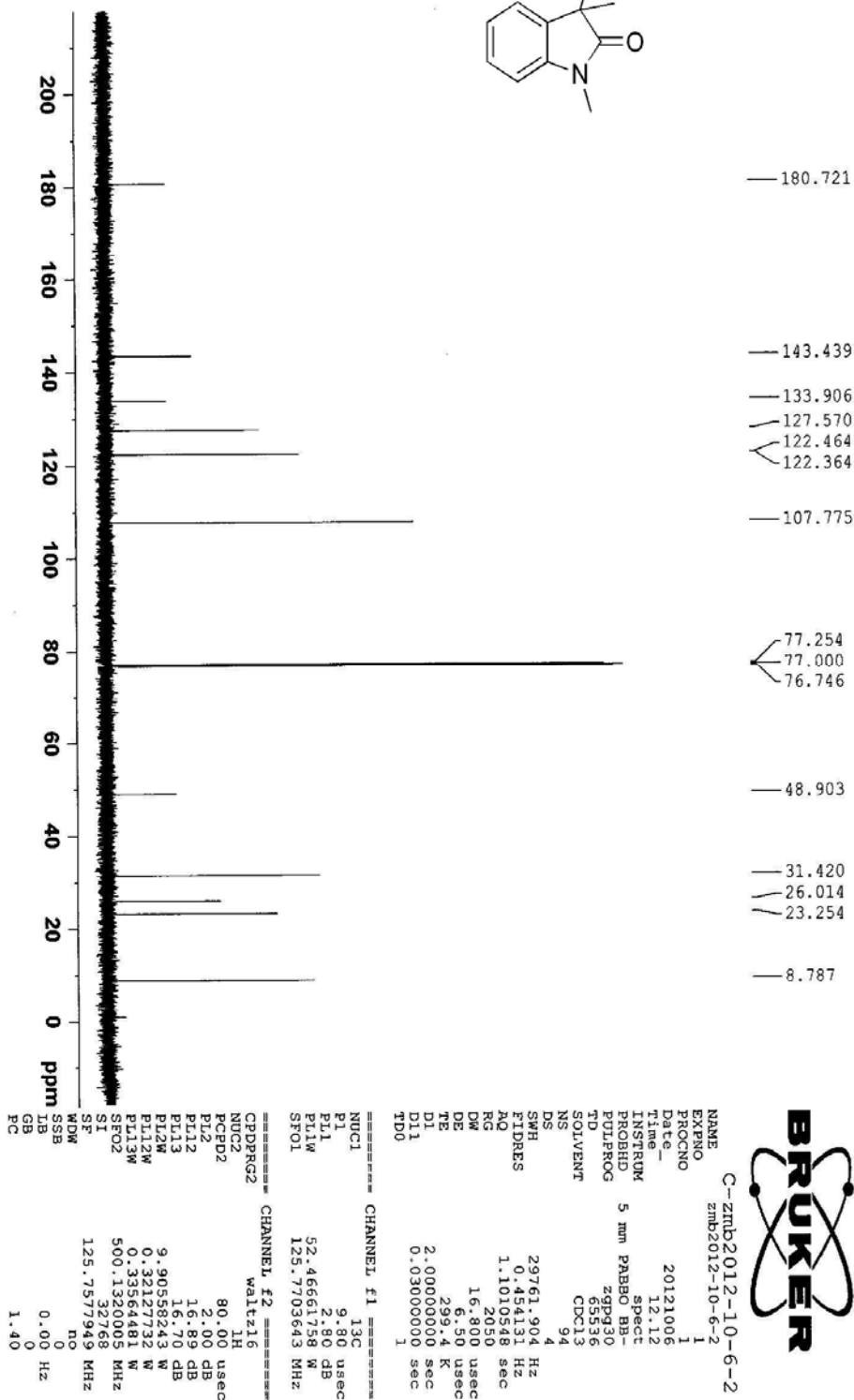
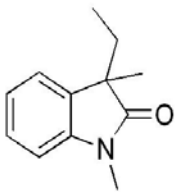


NAME H-zimb2012-10-6-2
EXPNO 2
PROCNO 1
Date_ 20121006
Time 12.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 144
DW 48.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
ID0 1

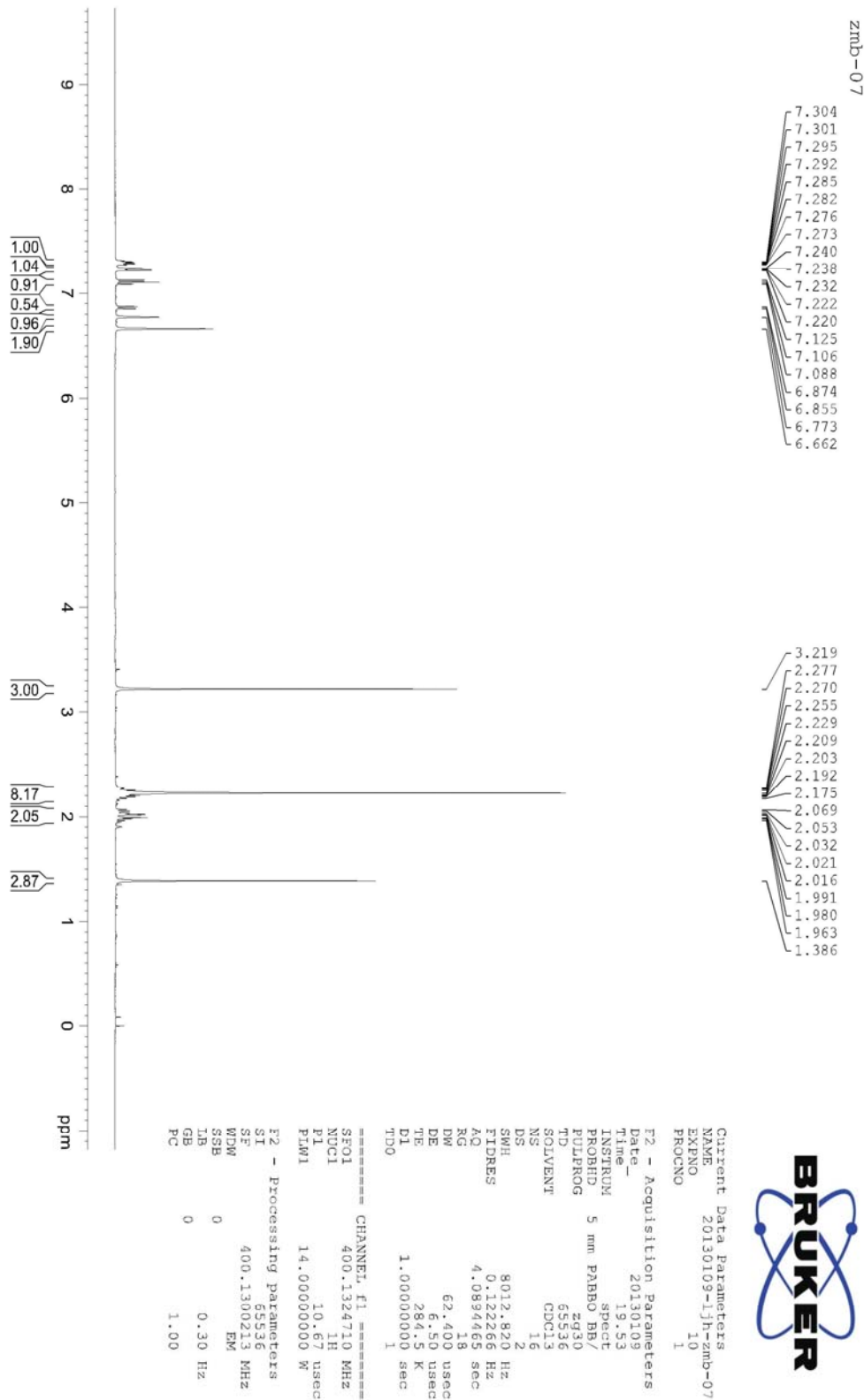
CHANNEL f1
NUC1 1H
P1 14.60 usec
PL1 2.00 dB
PL1W 9.90558243 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300088 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



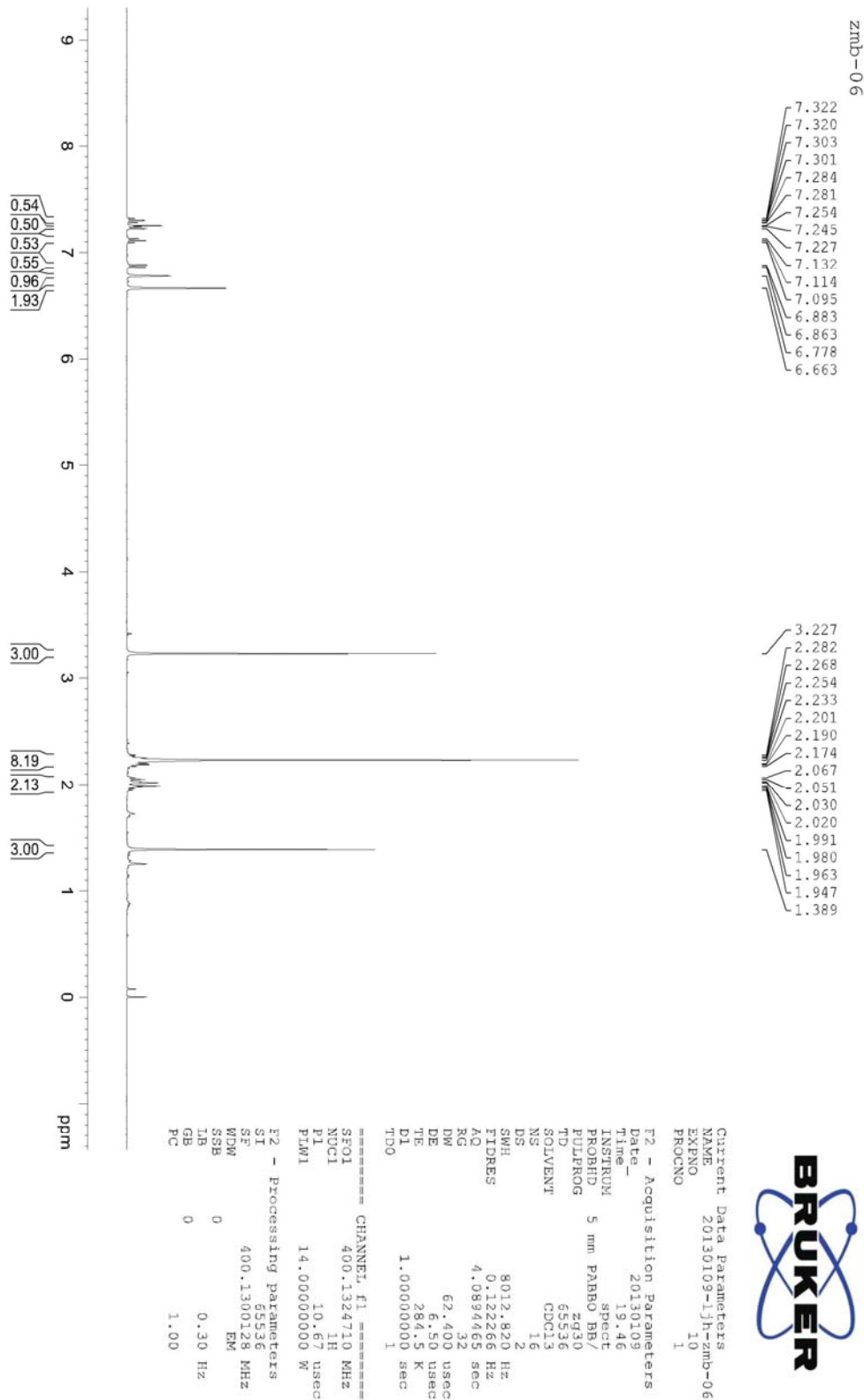
3-Ethyl-1,3-dimethylindolin-2-one (5aa)



3aa and 3aa-D1



3aa and 3aa-D5



3aa and 3aa-D8

