Electronic Supplementary Material (ESI) for Chemical Communications

Ruthenium-Catalyzed Annulation of Alkynes with Amides via Formyl Translocation

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Supporting Information

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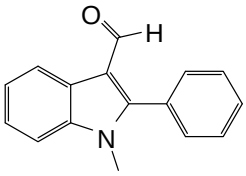
(A) Typical Experimental Procedure

Typical procedure for the [Ru(II)Cl_2(*p*-cym)]$_2$-catalyzed Annulation of Alkynes with Amides via Formyl Translocation:

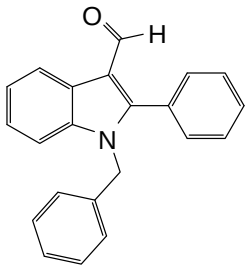
To a Schlenk tube were added *N*-methyl-*N*-(2-(phenylethynyl)phenyl) formamide **1** (0.2 mmol), [Ru(II)Cl_2($C_{10}H_{14}$)]$_2$ (3 mol %), and DCE (1.5 mL). The tube was charged with argon, and was stirred under reflux (about 87 ^oC) for the indicated time until complete consumption of starting material 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 Na_2SO_4 and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired product **2**.

(B) Analytical data of 2-9



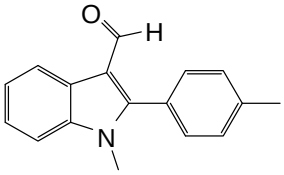
1-Methyl-2-phenyl-1*H*-indole-3-carbaldehyde (2a):[1]

White solid, mp 119.6-120.1 ^oC (uncorrected); ^1H NMR (500 MHz, $CDCl_3$). δ: 9.67 (s, 1H), 8.33 (d, *J* = 8.5 Hz, 1H), 7.46-7.45 (m, 3H), 7.38-7.36 (m, 2H), 7.29-7.25 (m, 3H), 3.55 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.5, 151.4, 137.3, 130.8, 129.8, 128.6, 128.5, 125.1, 123.9, 123.2, 122.1, 115.7, 109.7, 30.9; IR (KBr, cm^{-1}): 1644; LRMS (EI 70 ev) *m*/z (%): 235 (M^+, 74), 234 (100), 204 (11).



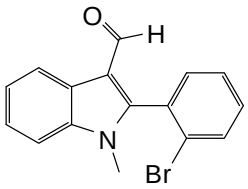
1-Benzyl-2-phenyl-1*H*-indole-3-carbaldehyde (2b):[2]

Pale yellow solid, mp 173.8-174.7 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.77 (s, 1H), 8.47 (d, *J* = 8.0 Hz, 1H), 7.51-7.41 (m, 5H), 7.36-7.33 (m, 1H), 7.33-7.22 (m, 5H), 6.98-6.96 (m, 2H), 5.29 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.8, 151.6, 136.8, 136.4, 130.7, 129.9, 128.9, 128.6, 128.4, 127.7, 125.9, 125.4, 124.2, 123.4, 122.2, 116.1, 110.7, 47.7; IR (KBr, cm^{-1}): 1644; LRMS (EI 70 ev) *m*/z (%): 311 (M^+, 32), 310 (15), 91 (63), 40 (100).



1-Methyl-2-*p*-tolyl-1*H*-indole-3-carbaldehyde (2d):[3]

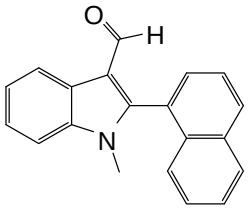
White solid, mp 154.2-155.1 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$). δ: 9.73 (s, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 7.39-7.25 (m, 7H), 3.65 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.6, 151.7, 140.0, 137.3, 130.7, 129.3, 125.5, 125.2, 123.9, 123.2, 122.1, 115.6, 109.7, 30.9, 21.4; IR (KBr, cm^{-1}): 1639; LRMS (EI 70 ev) *m*/z (%): 249 (M^+, 85), 248 (100), 204 (17).



2-(2-Bromophenyl)-1-methyl-1*H*-indole-3-carbaldehyde (2e):

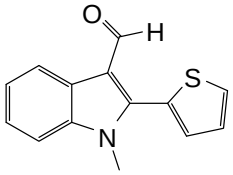
White solid, mp 195.7-196.5 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$). δ:

9.60 (s, 1H), 8.42 (d, *J* = 9.0 Hz, 1H), 7.78-7.77 (m, 1H), 7.51-7.48 (m, 1H), 7.45-7.36 (m, 5H), 3.59 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 185.7, 149.5, 137.2, 133.1, 133.0, 131.6, 130.4, 127.4, 125.0, 124.9, 124.1, 123.3, 122.3, 115.9, 109.8, 30.7; IR (KBr, cm^{-1}): 1644; LRMS (EI 70 ev) *m*/z (%): 315 (M^++2, 5), 313 (M^+, 5), 234 (100), 219 (28), 204 (45), 102 (24), 32 (54); HRMS *m/z* (EI) calcd for $C_{16}H_{12}BrNO$ (M^+) 313.0102, found 313.0105.



1-Methyl-2-(naphthalen-1-yl)-1*H*-indole-3-carbaldehyde (2f):

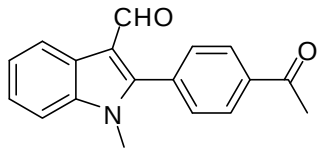
White solid, mp 161.4-162.5 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.45 (s, 1H), 8.39 (d, *J* = 9.0 Hz, 1H), 7.98（d, *J* = 8.5 Hz, 1H）， 7.90（d, *J* = 3.0 Hz, 1H）, 7.56-7.46 (m, 3H), 7.41-7.33 (m, 5H), 3.41 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.1, 150.7, 137.5, 133.4, 132.7, 130.7, 130.1, 128.6, 127.6, 126.7, 125.9, 125.2 (2C), 125.0, 124.2, 123.5, 122.3, 116.8, 109.8, 31.0; IR (KBr, cm^{-1}): 1665; LRMS (EI 70 ev) *m*/z (%): 285 (M^+, 42), 284 (53), 135 (27), 44 (29), 40 (100); HRMS *m/z* (EI) calcd for $C_{20}H_{15}NO$ (M^+) 285.1154, found 285.1152.



1-Methyl-2-(thiophen-2-yl)-1*H*-indole-3-carbaldehyde (2g):

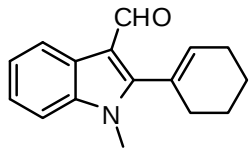
White solid, mp 106.5-107.4 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.79 (s, 1H), 8.34 (d, *J* = 9.5 Hz, 1H), 7.57-7.56 (m, 1H). 7.31-7.28 (m, 3H), 7.26 （d, *J* = 4.0 Hz, 1H）, 7.23-7.17 (m, 1H), 3.68 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.3, 143.9, 137.6, 131.8, 129.7, 127.9, 127.7, 125.0, 124.5, 123.5, 122.2, 116.8,

109.9, 31.1; IR (KBr, cm^{-1}): 1646; LRMS (EI 70 ev) *m*/z (%): 241 (M^+, 4), 240 (18), 44 (21), 40 (100); HRMS *m/z* (EI) calcd for $C_{14}H_{11}NOS$ (M^+) 241.0561, found 241.0558.



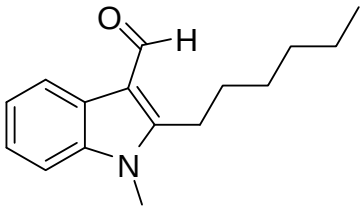
2-(4-Acetylphenyl)-1-methyl-1*H*-indole-3-carbaldehyde (2h):

White solid, mp 186.5-187.4 °C (uncorrected); ^1H NMR (500 MHz, $CDCl_3$) δ: 9.68 (s, 1H), 8.37 (d, *J* = 8.0 Hz, 1H), 8.08 (d, *J* = 7.5 Hz, 2H). 7.56 (d, *J* = 7.5 Hz, 2H), 7.38-7.31 (m, 3H), 3.64 (s, 3H), 2.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 197.2, 186.0, 171.1, 138.0, 137.6, 133.3, 131.3, 128.5, 125.2, 124.5, 123.6, 122.4, 116.2, 109.8, 31.1, 26.7; IR (KBr, cm^{-1}): 1646, 1652; LRMS (EI 70 ev) *m*/z (%): 278 (22), 277 (M^+, 100), 204 (17), 44 (12), 40 (39); HRMS *m/z* (EI) calcd for $C_{18}H_{15}NO_2$ (M^+) 277.1103, found 277.1101.



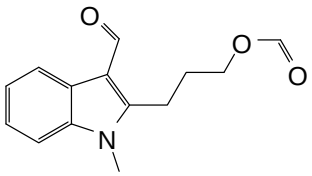
2-Cyclohexenyl-1-methyl-1*H*-indole-3-carbaldehyde (2i):[4]

White solid, mp 94.1-96.6 °C (uncorrected); ^1H NMR (500 MHz, $CDCl_3$) δ: 9.87 (s, 1H), 8.33 (d, *J* = 8.0 Hz, 1H), 7.31-7.25 (m, 3H), 6.03-6.02 (m, 1H), 3.66 (s, 3H), 2.32-2.27 (m, 4H), 1.86-1.84 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.0, 154.7, 137.0, 135.5, 126.9, 125.0, 123.5, 122.8, 121.9, 114.4, 109.4, 30.5, 30.2, 25.4, 22.4, 21.6; IR (KBr, cm^{-1}): 1643; LRMS (EI 70 ev) *m*/z (%): 239 (M^+, 100), 238 (57), 222 (31), 210 (52).



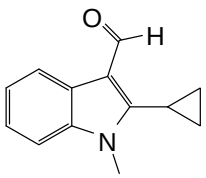
2-Hexyl-1-methyl-1*H*-indole-3-carbaldehyde (2j):

Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.99 (s, 1H), 8.19 (d, *J* = 8.0 Hz, 1H), 7.22-7.20 (m, 3H), 3.62 (s, 3H), 2.96 (t, *J* = 7.5 Hz, 2H), 1.61-1.55 (m, 2H), 1.36-1.33 (m, 2H), 1.25-1.22 (m, 4H), 0.81 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 183.7, 152.8, 137.1, 125.5, 123.2, 123.0, 121.1, 113.7. 109.4, 31.4, 30.0, 29.8, 29.0, 24.4, 22.4, 14.0; IR (KBr, cm^{-1}): 1652; LRMS (EI 70 ev) *m*/z (%): 243 (M^+, 89), 214 (24), 186 (100), 158 (45), 144 (99), 115 (34); HRMS *m/z* (EI) calcd for $C_{16}H_{21}NO$ (M^+) 243.1623, found 243.1620.



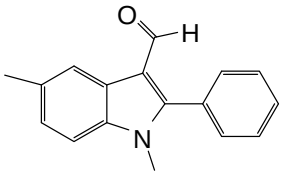
3-(3-Formyl-1-methyl-1*H*-indol-2-yl)propyl formate (2k):

Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 10.05 (s, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 8.03 (s, 1H), 7.27-7.22 (m, 3H), 4.18 (t, *J* = 6.0 Hz, 2H), 3.67 (s, 3H), 3.14 (t, *J* = 8.0 Hz, 2H), 2.01-1.95 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 184.0, 160.8, 149.8, 137.0, 125.8, 123.4, 123.0, 120.5, 113.9, 109.5, 62.5, 29.7, 28.6, 21.1; IR (KBr, cm^{-1}): 1645; LRMS (EI 70 ev) *m*/z (%): 245 (M^+, 14), 217 (47), 186 (57), 173 (50), 144 (63), 43 (54), 40 (100); HRMS *m/z* (EI) calcd for $C_{14}H_{15}NO_3$ (M^+) 245.1052, found 245.1050.



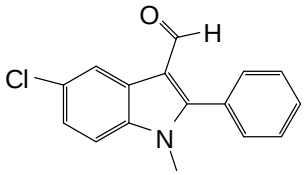
2-Cyclopropyl-1-methyl-1*H*-indole-3-carbaldehyde (2l):

White solid, mp 135.1-135.9 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 10.35 (s, 1H), 8.31 (d, *J* = 9.5 Hz, 1H), 7.28-7.24 (m, 3H), 3.79 (s, 3H), 1.95-1.90 (m, 1H), 1.25-1.20 (m, 2H), 0.90-0.86 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 185.4, 151.6, 136.6, 124.9, 123.3, 122.8, 121.8, 115.2, 109.1, 30.4, 6.3, 5.8; IR (KBr, cm^{-1}): 1642; LRMS (EI 70 ev) *m*/z (%): 199 (M^+, 86), 184 (100), 167 (26), 128 (24), 42 (22); HRMS *m/z* (EI) calcd for $C_{13}H_{13}NO$ (M^+) 199.0997, found 199.0995.



1,5-Dimethyl-2-phenyl-1*H*-indole-3-carbaldehyde (2m):

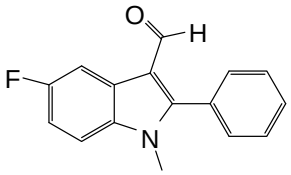
White solid, mp 107.9-108.3 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.69 (s, 1H), 8.25 (s, 1H), 7.55-7.53 (m, 3H), 7.47-7.45 (m, 2H), 7.28-7.25 (m, 1H), 7.20-7.18 (m, 1H), 3.63 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.8, 151.4, 135.7, 133.0, 129.7, 128.7, 128.6, 125.4, 125.3, 121.8, 115.3, 109.4, 30.9, 21.4; IR (KBr, cm^{-1}): 1645; LRMS (EI 70 ev) *m*/z (%): 249 (M^+, 73), 248 (100), 204 (12); HRMS *m/z* (EI) calcd for $C_{17}H_{15}NO$ (M^+) 249.1154, found 249.1151.



5-Chloro-1-methyl-2-phenyl-1*H*-indole-3-carbaldehyde (2n):

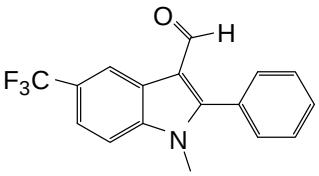
White solid, mp 166.8-167.7 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.78 (s, 1H), 8.30 (d, *J* = 8.5 Hz, 1H), 7.57-7.53 (m, 3H), 7.48-7.46 (m, 2H), 7.35 (s, 1H), 7.29-7.26 (m, 1H), 3.61 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.3, 151.8, 137.8, 130.8, 130.0, 129.7, 128.7, 128.0, 123.6 (2C), 122.9, 115.5, 109.9, 31.0; IR

(KBr, cm^{-1}): 1642; LRMS (EI 70 ev) *m*/z (%): 271 (M^++2, 9), 269 (M^+, 27), 268 (33), 40 (100); HRMS *m/z* (EI) calcd for $C_{16}H_{12}ClNO$ (M^+) 269.0607, found 269.0605.



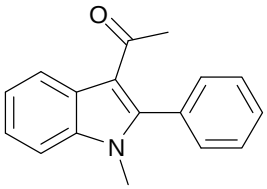
5-Fluoro-1-methyl-2-phenyl-1*H*-indole-3-carbaldehyde (2o):

White solid, mp 168.5-168.9 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$). δ: 9.57 (s, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 7.49-7.47 (m, 3H), 7.40-7.38 (m, 2H), 7.24-7.02 (m, 1H), 7.00-6.99 (m, 1H), 3.59 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.1, 160.0 (d, *J* = 237.6 Hz, 1C), 152.6, 133.8, 130.7, 130.1, 128.7, 128.1, 125.7 (d, *J* = 10.9 Hz, 1C), 115.5 (d, *J* = 4.5 Hz, 1C), 112.2 (d, *J* = 26.1 Hz, 1C), 110.7 (d, *J* = 9.5 Hz, 1C), 107.6 (d, *J* = 24.5 Hz, 1C), 31.2; IR (KBr, cm^{-1}): 1646; LRMS (EI 70 ev) *m*/z (%): 253 (M^+, 80), 252 (100), 222 (13); HRMS *m/z* (EI) calcd for $C_{16}H_{12}FNO$ (M^+) 253.0903, found 253.0900.



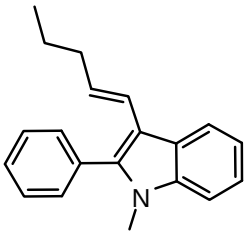
1-Methyl-2-phenyl-5-(trifluoromethyl)-1*H*-indole-3-carbaldehyde (2p):

White solid, mp 184.2-185.6 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.64 (s, 1H), 8.64 (s, 1H), 7.51-7.49 (m, 4H), 7.42-7.36 (m, 3H), 3.63 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.4, 152.9, 138.7, 130.8, 130.3, 128.9, 127.9 (2C), 124.9 (q, *J* = 270.4 Hz, 1C), 124.7, 120.8 (d, *J* = 3.5 Hz, 1C), 119.9 (d, *J* = 4.0 Hz, 1C), 115.9, 110.2, 31.3; IR (KBr, cm^{-1}): 1638; LRMS (EI 70 ev) *m*/z (%): 303 (M^+, 26), 302 (43), 40 (100); HRMS *m/z* (EI) calcd for $C_{17}H_{12}F_3NO$ (M^+) 303.0871, found 303.0875.



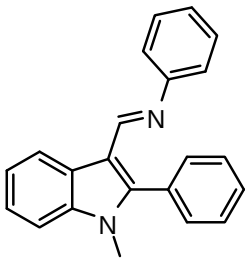
1-(1-Methyl-2-phenyl-1*H*-indol-3-yl)ethanone (2q)[1]

White solid, mp 102.1-102.9 °C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$). δ: 8.42 (d, *J* = 9.0 Hz, 1H), 7.49-7.48 (m, 3H), 7.36-7.34 (m, 2H), 7.30-7.18 (m, 3H), 3.44 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 194.7, 146.6, 136.6, 132.1, 130.2, 129.7, 128.9, 126.6, 123.4, 122.9, 122.8, 115.9, 109.5, 30.9, 30.0; IR (KBr, cm^{-1}): 1641; LRMS (EI 70 ev) *m*/z (%): 249 (M^+, 43), 235 (18), 234 (100), 204 (13), 40 (10).



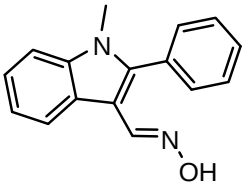
(*E*/*Z*)-1-Methyl-3-(pent-1-enyl)-2-phenyl-1*H*-indole (3):

Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.88 (s, 1H), 7.44-7.41 (m, 2H), 7.38-7.27 (m, 3H), 7.22-7.18 (m, 1H), 7.14-7.11 (m, 3H), 6.30-6.27 (m, 1H), 6.15-6.12 (m, 1H), 3.51 (s, 3H), 2.07-2.04 (m, 2H), 1.40-1.36 (m, 2), 0.85 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 171.2, 138.8, 137.7, 131.8, 131.1, 128.6, 128.3, 125.8, 122.9, 122.1, 120.5, 120.1, 112.0, 109.5, 36.1, 30.9, 23.1, 14.2; IR (KBr, cm^{-1}): 1469, 1704; LRMS (EI 70 ev) *m*/z (%): 276 (10), 275 (M^+, 38), 247 (15), 246 (73), 40 (100); HRMS *m/z* (EI) calcd for $C_{20}H_{21}N$ (M^+) 275.1674, found 275.1670.



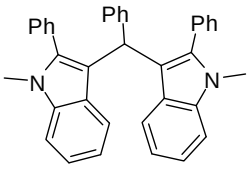
(*E/Z*)-*N*-((1-Methyl-2-phenyl-1*H*-indol-3-yl)methylene)aniline (4):

White solid; mp 109.8-110.9 ^{o}C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.73 (d, *J* = 3.5 Hz, 1H), 8.378 (s, 1H), 7.54-7.49 (m, 3H), 7.47-7.45 (m, 2H), 7.40-7.34 (m, 3H), 7.31 (t, *J* = 8.5 Hz. 2H), 7.15-7.10 (m, 3H), 3.66 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 155.7, 153.9, 146.8, 137.7, 130.9, 129.8, 129.2, 128.9, 128.6, 125.1, 124.3, 123.5, 123.1, 122.1, 120.9, 113.1, 109.4, 31.0; IR (KBr, cm^{-1}): 1690, 1572; LRMS (EI 70 ev) *m*/z (%): 311 (7), 310 (M^+, 41), 309 (100), 218 (9), 40 (82); HRMS *m/z* (EI) calcd for $C_{22}H_{18}N_2$ (M^+) 310.1470, found 310.1465.



(*E/Z*)-1-Methyl-2-phenyl-1*H*-indole-3-carbaldehyde oxime (5):

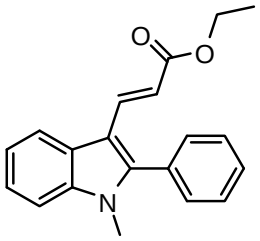
White solid; mp 105.2-106.5 ^{o}C (uncorrected); ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.19 (d, *J* = 7.5 Hz, 1H), 8.14 (s, 1H), 7.52-7.49 (m, 3H), 7.41-7.32 (m, 5H), 7.29-7.25 (m, 1H), 3.63 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 147.2, 143.6, 137.7, 130.8, 123.0, 129.1, 128.6, 124.8, 123.2, 122.4, 121.5, 109.5, 107.0, 31.0; IR (KBr, cm^{-1}): 1626; LRMS (EI 70 ev) *m*/z (%): 251 (2), 250 (M^+, 100), 234 (92), 178 (34), 152 (10.2), 89 (16.3); HRMS *m/z* (EI) calcd for $C_{16}H_{14}N_2O$ (M^+) 250.1106, found 250.1103.



3,3'-(Phenylmethylene)bis(1-methyl-2-phenyl-1*H*-indole) (6):[5]

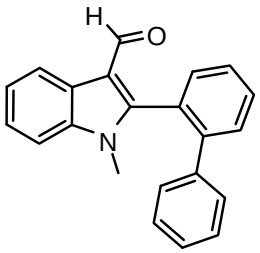
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.26-7.11 (m, 15H), 6.91-6.89 (m, 2H), 6.83-6.80 (m, 6H), 5.69 (s, 1H), 3.41 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 145.2,

138.6, 137.1, 131.9, 130.4, 129.1, 127.9, 127.7, 127.6, 127.5, 125.6, 121.3, 118.9, 115.3, 108.9, 40.3, 30.6; IR (KBr, cm^{-1}): 3048, 1467, 735; LRMS (EI 70 ev) *m*/z (%): 503 (43), 502 (M^+, 100), 425 (93), 218 (47), 212 (20), 40 (18).



(*E/Z*)-Ethyl 3-(1-methyl-2-phenyl-1*H*-indol-3-yl)acrylate (7):

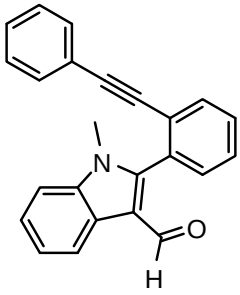
White solid; mp 104.1-104.9 ^oC (uncorrected); ^1H NMR (500 MHz, $CDCl_3$) δ: 8.01(d, *J* = 4.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.54-7.50 (m, 3H), 7.42-7.37 (m, 3H), 7.36-7.33 (m, 1H), 7.32-7.24 (m, 2H), 6.48 (d, *J* = 8.0 Hz, 1H), 4.22-4.18 (m, 2H), 3.62 (s, 3H), 1.29 (t, *J* = 3.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 168.5, 145.3, 138.8, 137.9, 130.9, 130.0, 129.2, 128.6, 125.0, 123.0, 121.7, 120.7, 112.9, 110.4, 110.0, 59.9, 31.1, 14.4; IR (KBr, cm^{-1}): 1613; LRMS (EI 70 ev) *m*/z (%): 306 (15), 305 (M^+, 64), 233 (20), 232 (100), 217 (64), 40 (45); HRMS *m/z* (EI) calcd for $C_{20}H_{19}NO_2$ (M^+) 305.1416, found 305.1412.



2-(Biphenyl-2-yl)-1-methyl-1*H*-indole-3-carbaldehyde (8):

Yellow solid; mp 102.7-103.4 ^oC (uncorrected); ^1H NMR (500 MHz, $CDCl_3$) δ: 9.74 (s, 1H), 8.32 (d, *J* = 7.5 Hz, 1H), 7.58-7.54 (m, 2H), 7.44 (d, *J* = 4.0 Hz, 2H), 7.27-7.18 (m, 2H), 7.11-7.10 (m, 6H), 3. 06 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.4, 151.4, 142.9, 139.8, 137.0, 133.2, 130.7, 130.5, 128.6, 128.5, 127.6, 127.3,

126.9, 125.2, 123.8, 123.3, 122.1, 116.3, 109.6, 30.6; IR (KBr, cm^{-1}): 1659; LRMS (EI 70 ev) *m*/z (%): 312 (23), 311 (M^+, 93), 310 (25), 267 (49), 234 (28), 40 (29); HRMS *m/z* (EI) calcd for $C_{22}H_{17}NO$ (M^+) 311.1310, found 311.1308.



1-Methyl-2-(2-(phenylethynyl)phenyl)-1*H*-indole-3-carbaldehyde (9):

Red oil; ^1H NMR (500 MHz, $CDCl_3$) δ: 9.64 (s, 1H), 8.40-8.38 (m, 1H), 7.67-7.65 (m, 1H), 7.50-7.47 (m, 1H), 7.43-7.42 (m, 2H), 7.35-7.30 (m, 3H), 7.18-7.13 (m, 1H), 7.10-7.07 (m, 2H), 6.98-6.96 (m, 2H), 3.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 186.3, 150.0, 137.4, 132.3, 131.8, 131.5, 131.3, 130.0, 128.7, 128.3, 128.2, 125.2, 125.1, 124.0, 123.3, 122.3, 122.2, 116.1, 109.7, 94.1, 87.0, 31.0; IR (KBr, cm^{-1}): 1659; LRMS (EI 70 ev) *m*/z (%): 335 (M^+, 2), 307 (7), 44 (16), 40 (100); HRMS *m/z* (EI) calcd for $C_{24}H_{17}NO$ (M^+) 335.1310, found 335.1306.

（C）Reference

(1) Bursavich, M. G.; Brooijmans, N.; Feldberg, L.; Hollander, I.; Kim, S.; Lombardi, S.; Park, K.; Mallon, R.; Gilbert. A. M. *Bioorg. Med. Chem. Lett.* **2010**, *20*, 2586.

(2) Zahran, M. A. H.; Ibrahim. A. M. *J. Chem. Sci.* **2009**, *121*, 455.

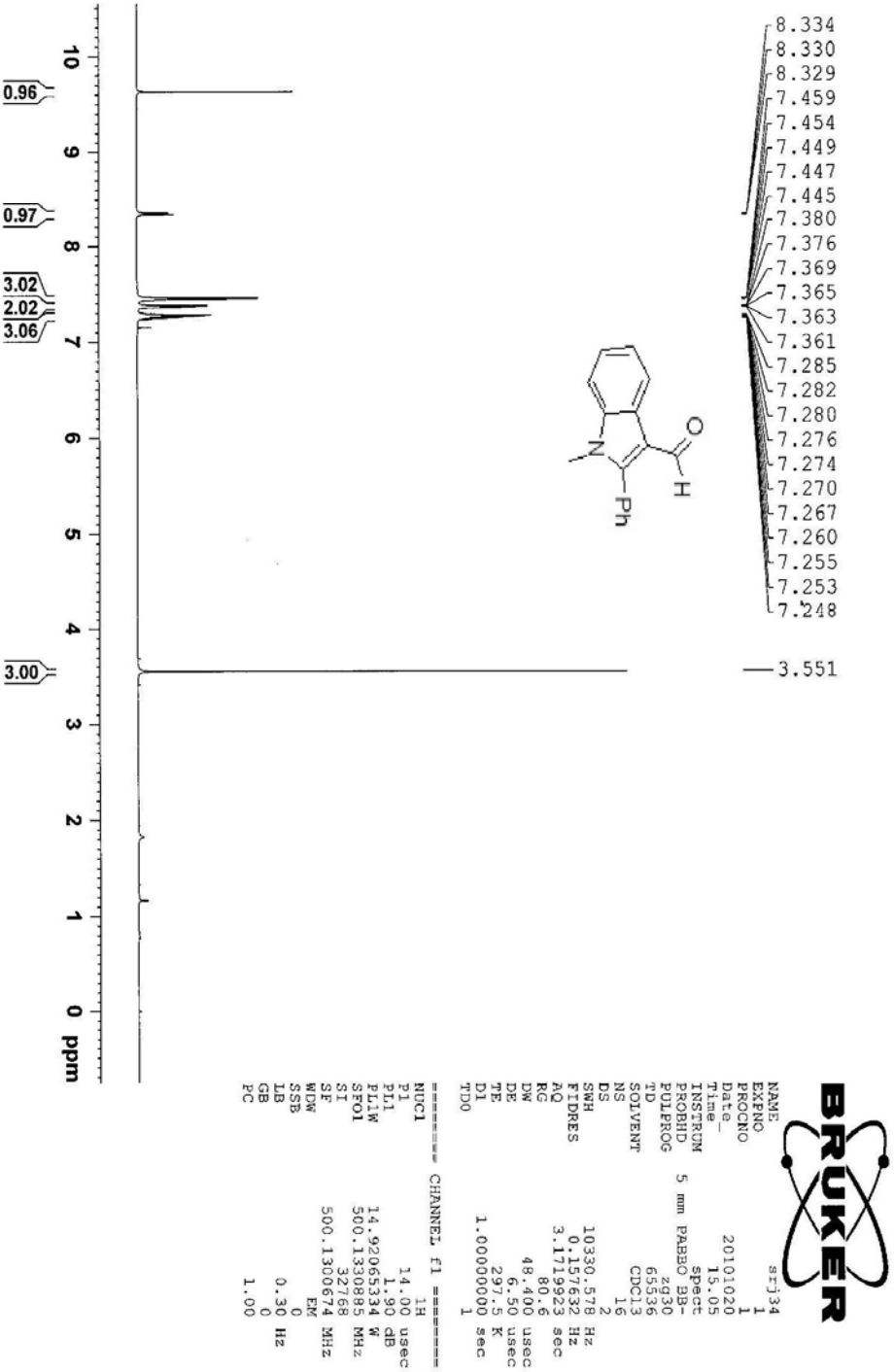
(3) Cortés, E.; Martínez, R.; Gómez, M. B. G. *J. Heterocycl. Chem.* **1991**, *28*, 1413.

(4) Rohbogner, C. J.; Wunderlich, S. H.; Clososki, G. C.; Knochel, P. *Eur. J. Org. Chem.* **2009**, 1781.

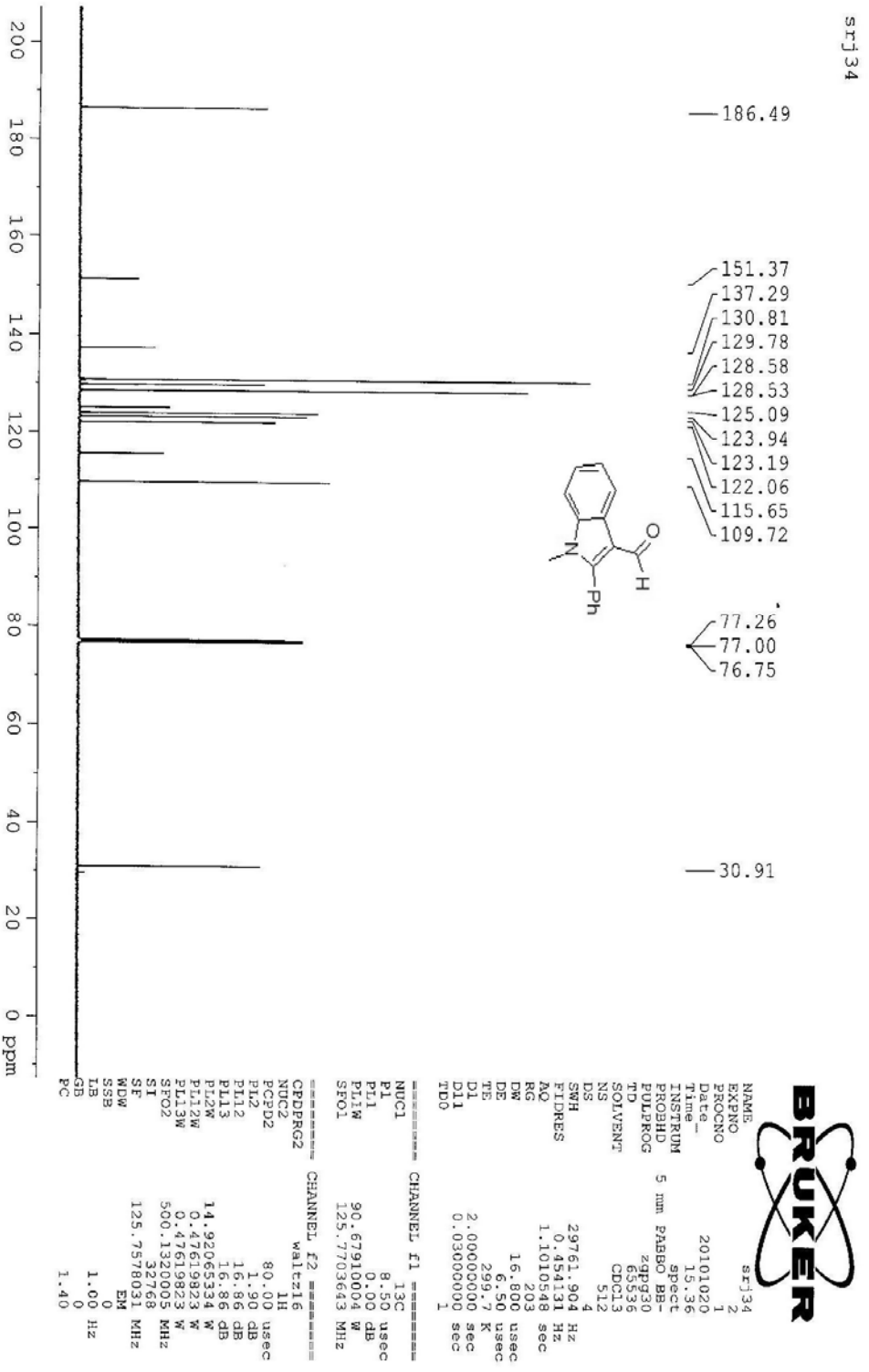
(5) (a) Blume, R. C.; Lindwall, H. G. *J. Org. Chem.* **1945**, *10*, 255. (b) Berti, C.; Greci, L.; Marchetti, L. *J. Heterocycl. Chem.* **1978**, *15*, 433.

(D) Spectra

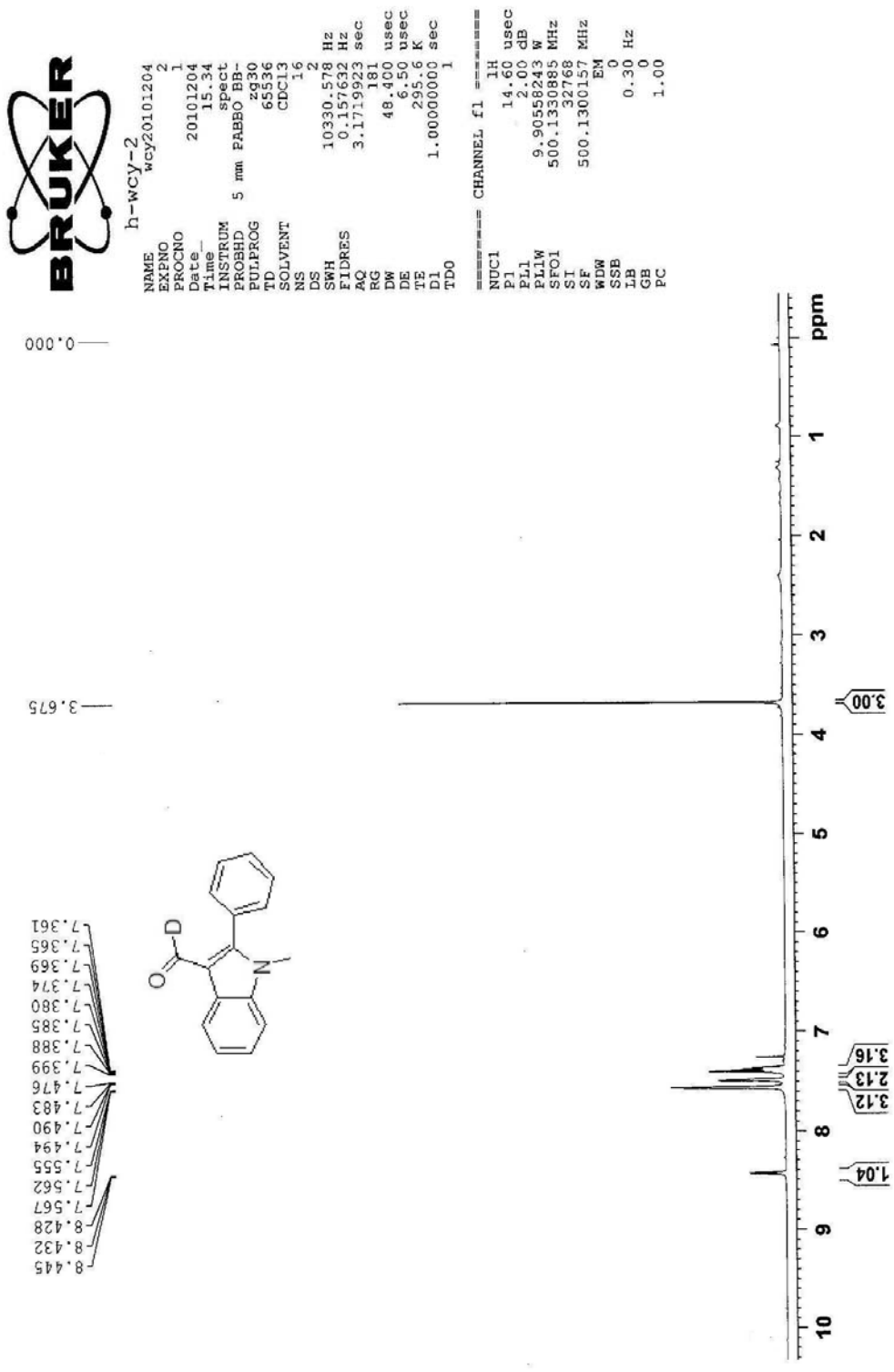
1-Methyl-2-phenyl-1*H*-indole-3-carbaldehyde (2a)



1-Methyl-2-phenyl-1*H*-indole-3-carbaldehyde (2a)



2a-D1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TE 295.6 K
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TD0 1
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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N
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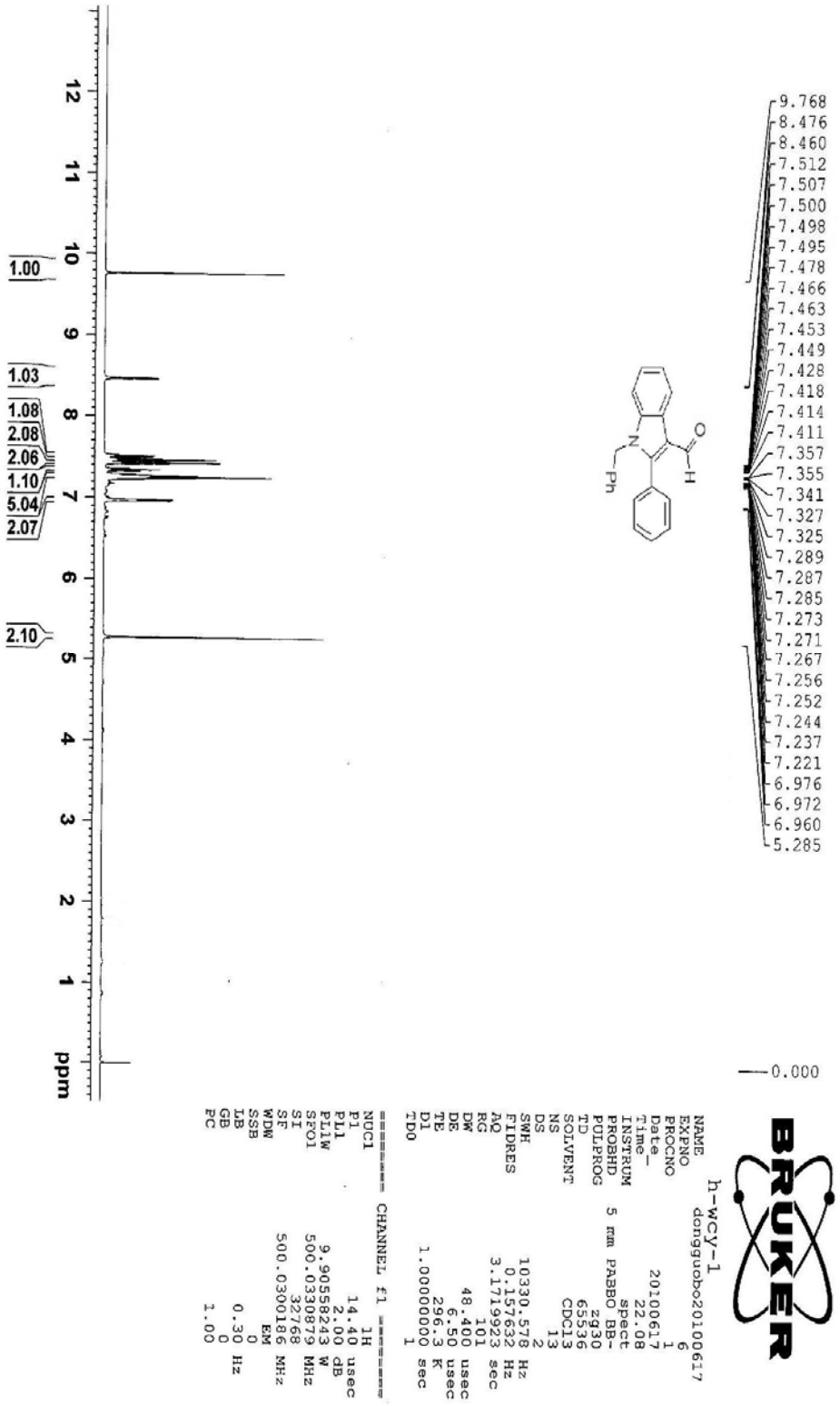
1-Benzyl-2-phenyl-1*H*-indole-3-carbaldehyde (2b)



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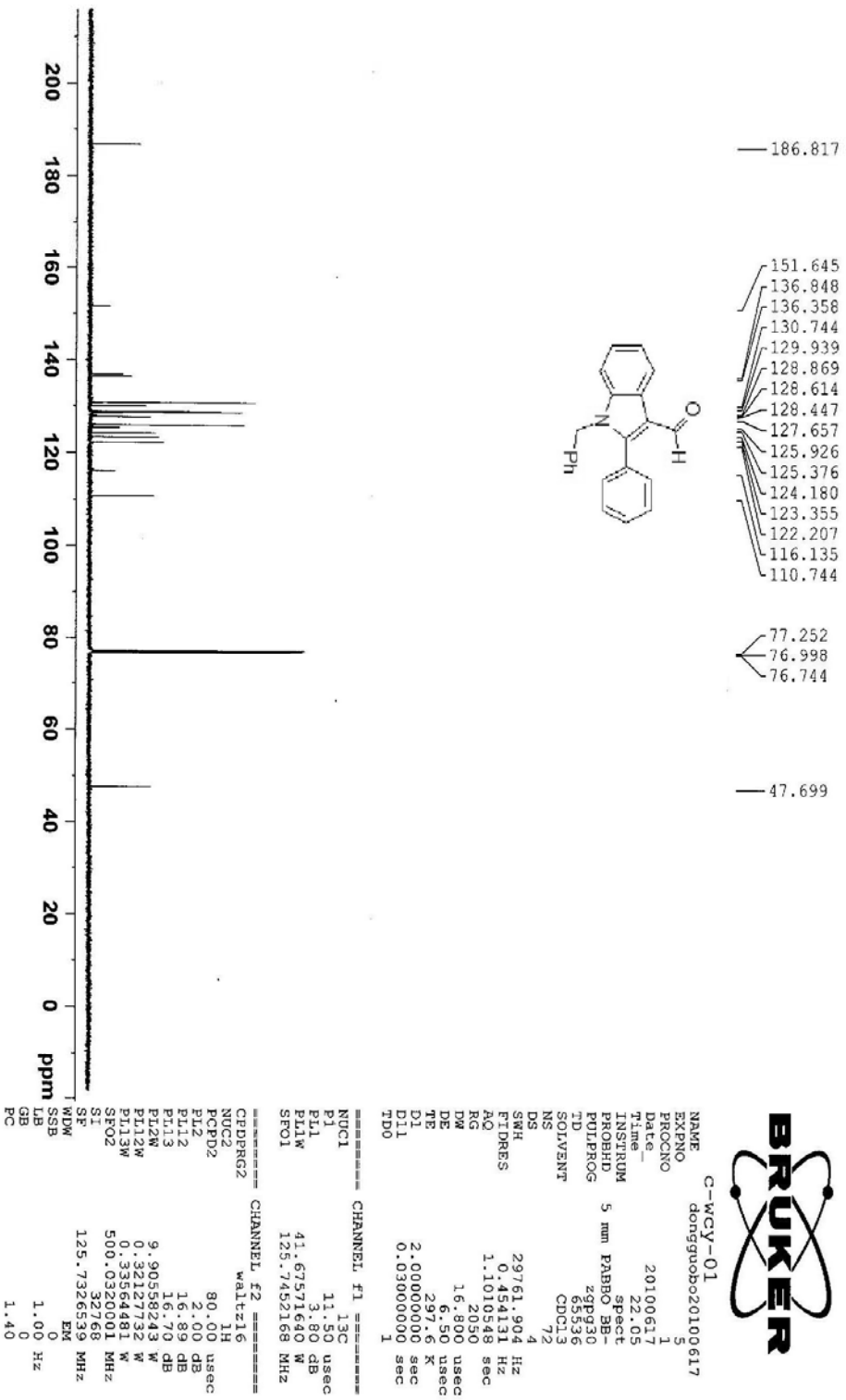

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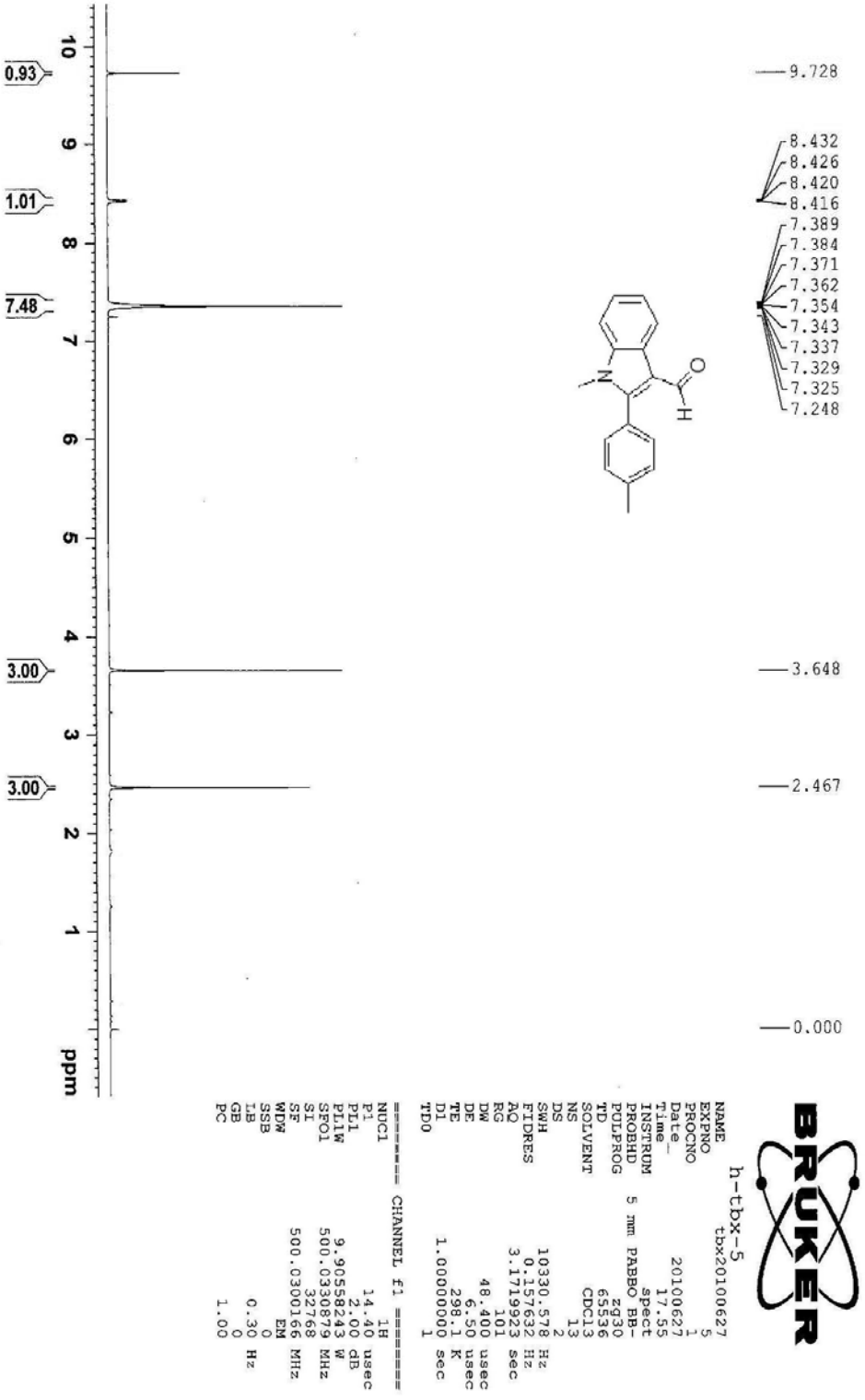

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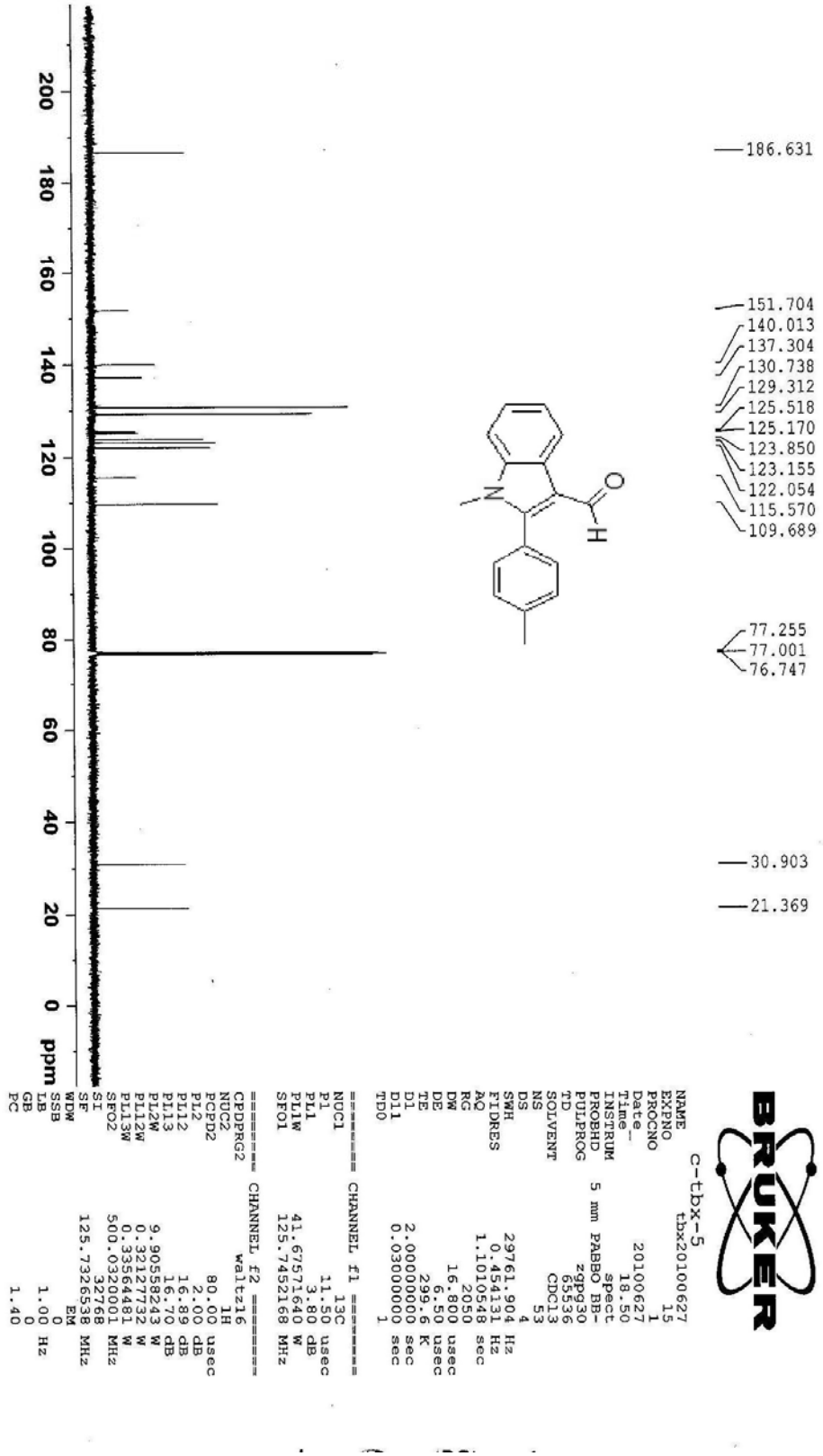
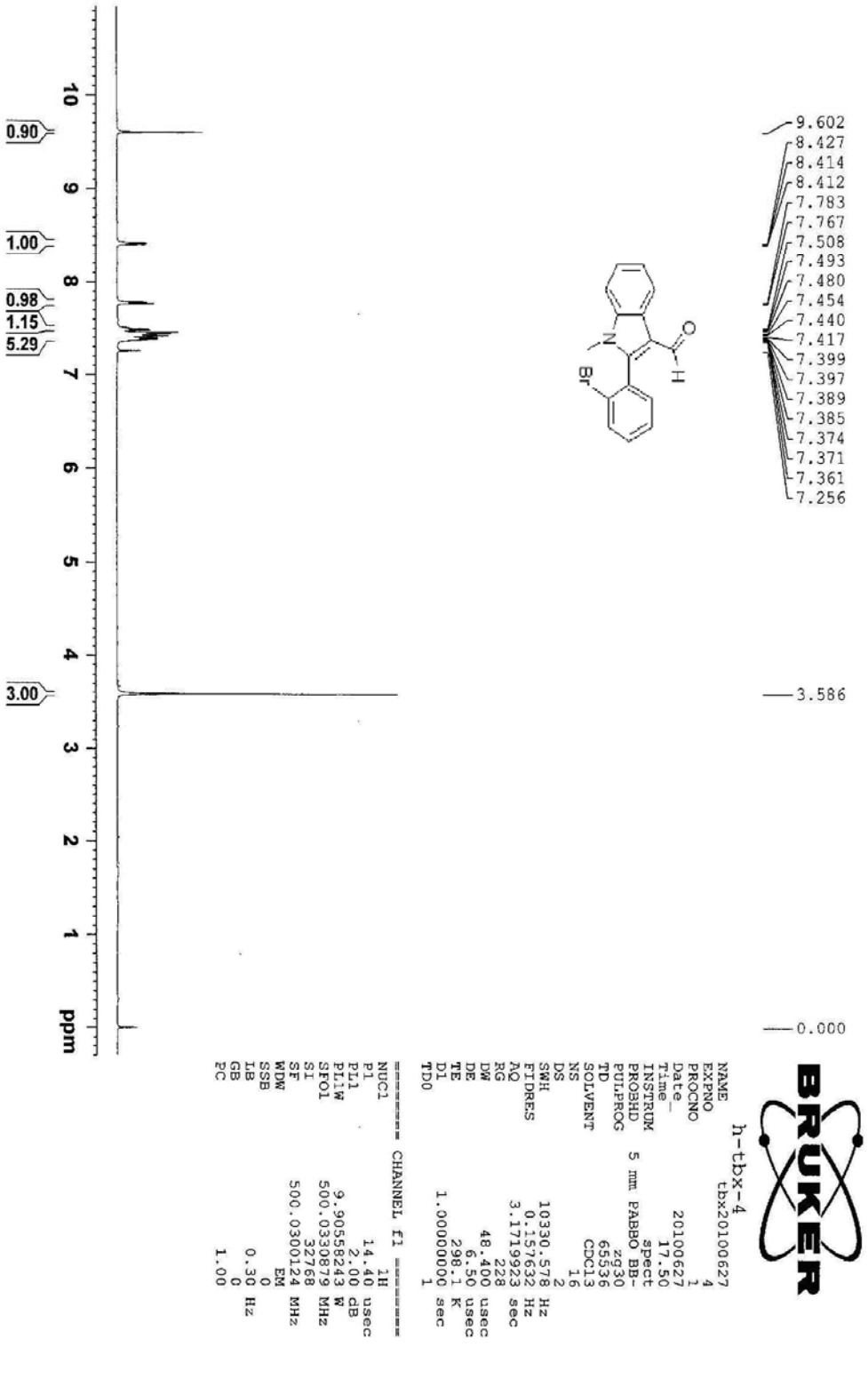


2-(2-Bromophenyl)-1-methyl-1*H*-indole-3-carbaldehyde (2e)



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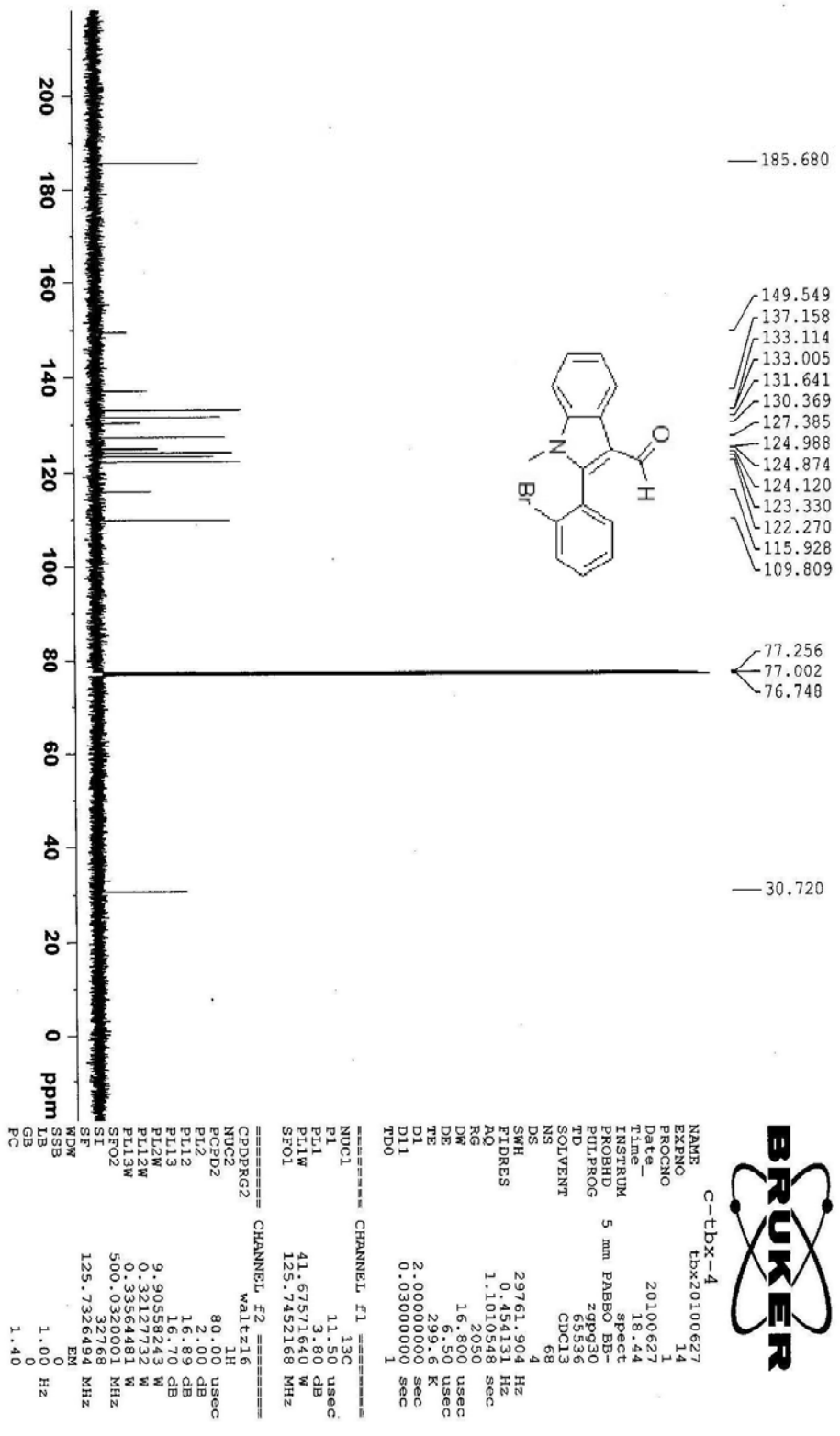
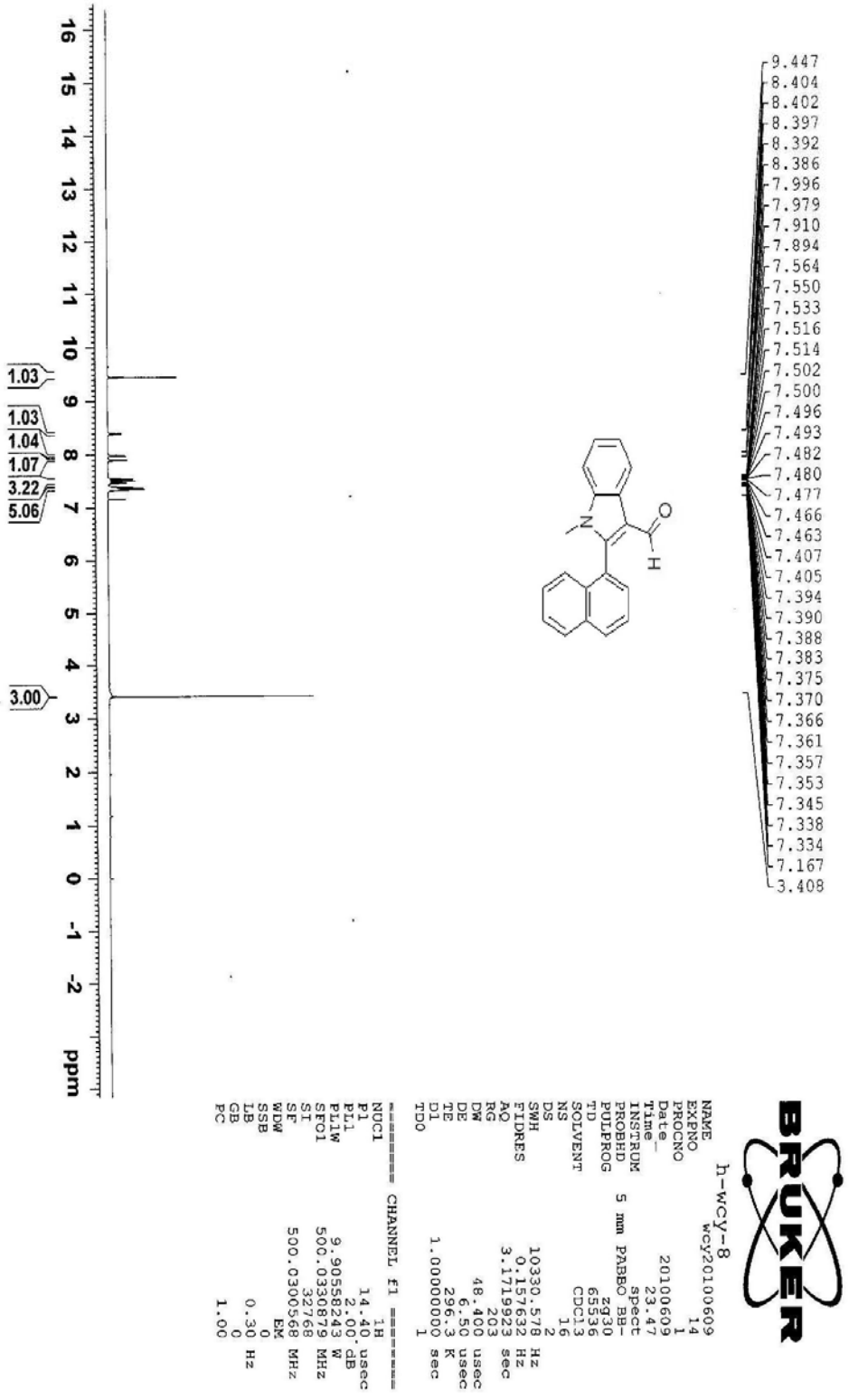


1-Methyl-2-(naphthalen-1-yl)-1*H*-indole-3-carbaldehyde (2f)



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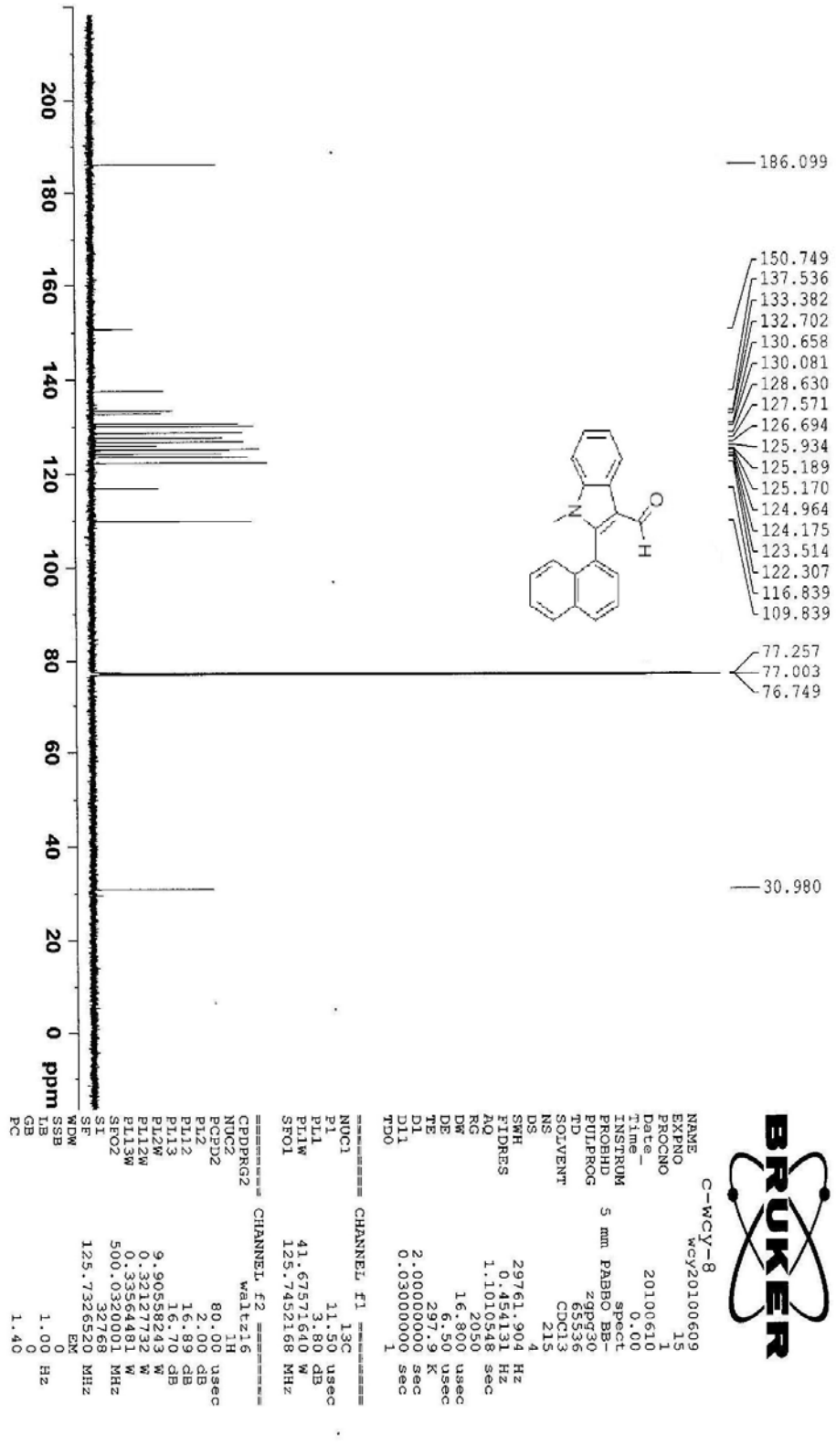

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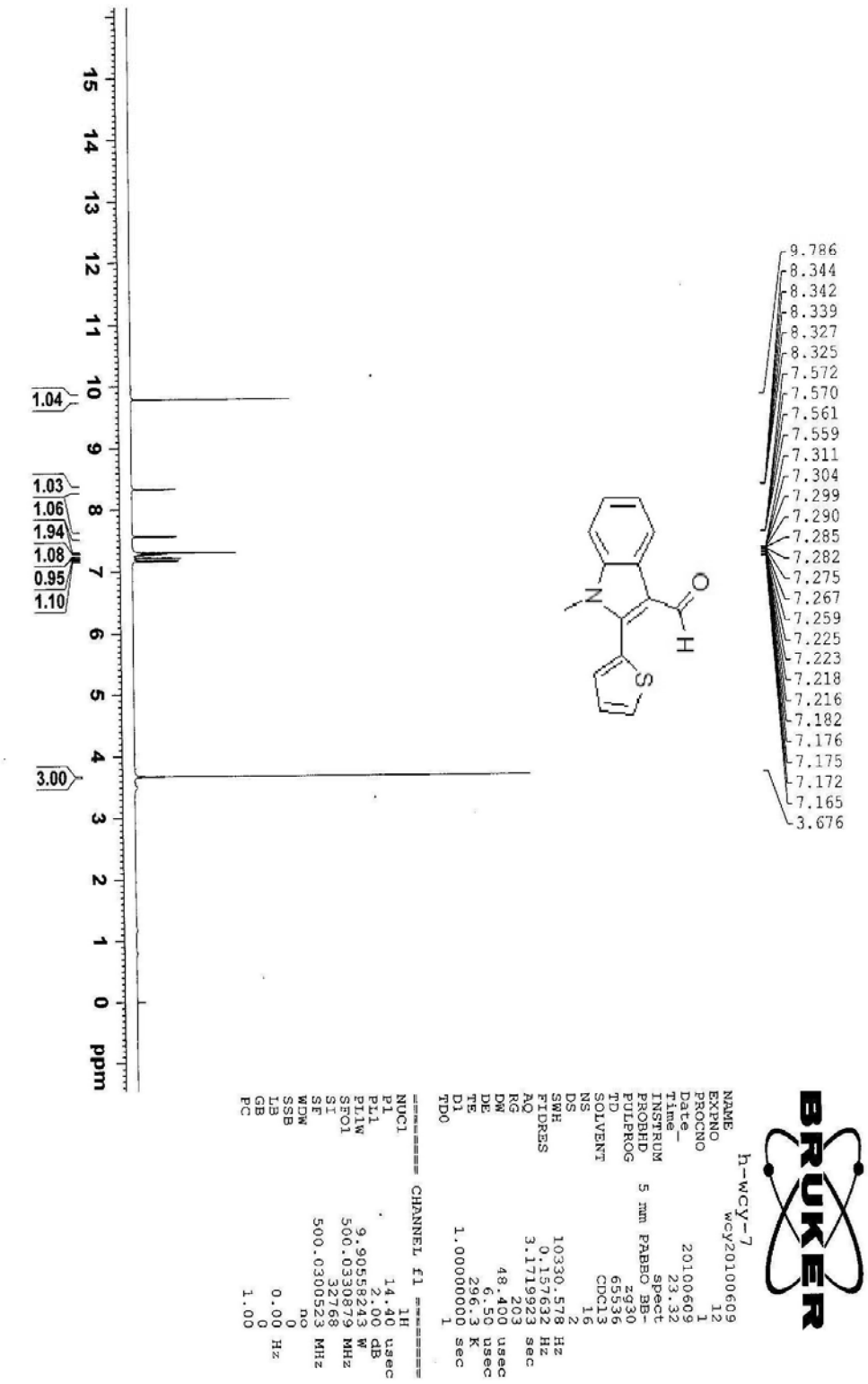

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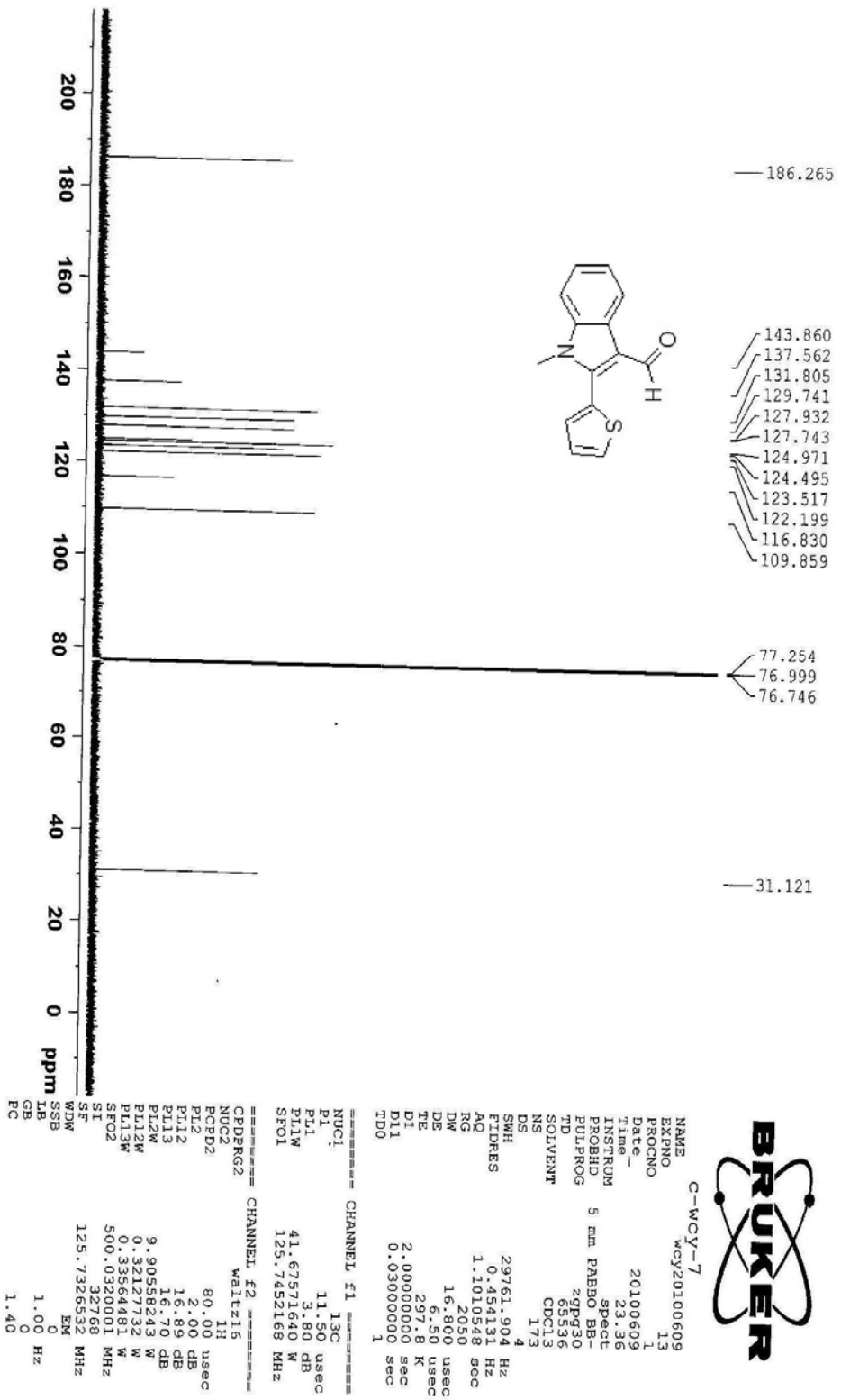
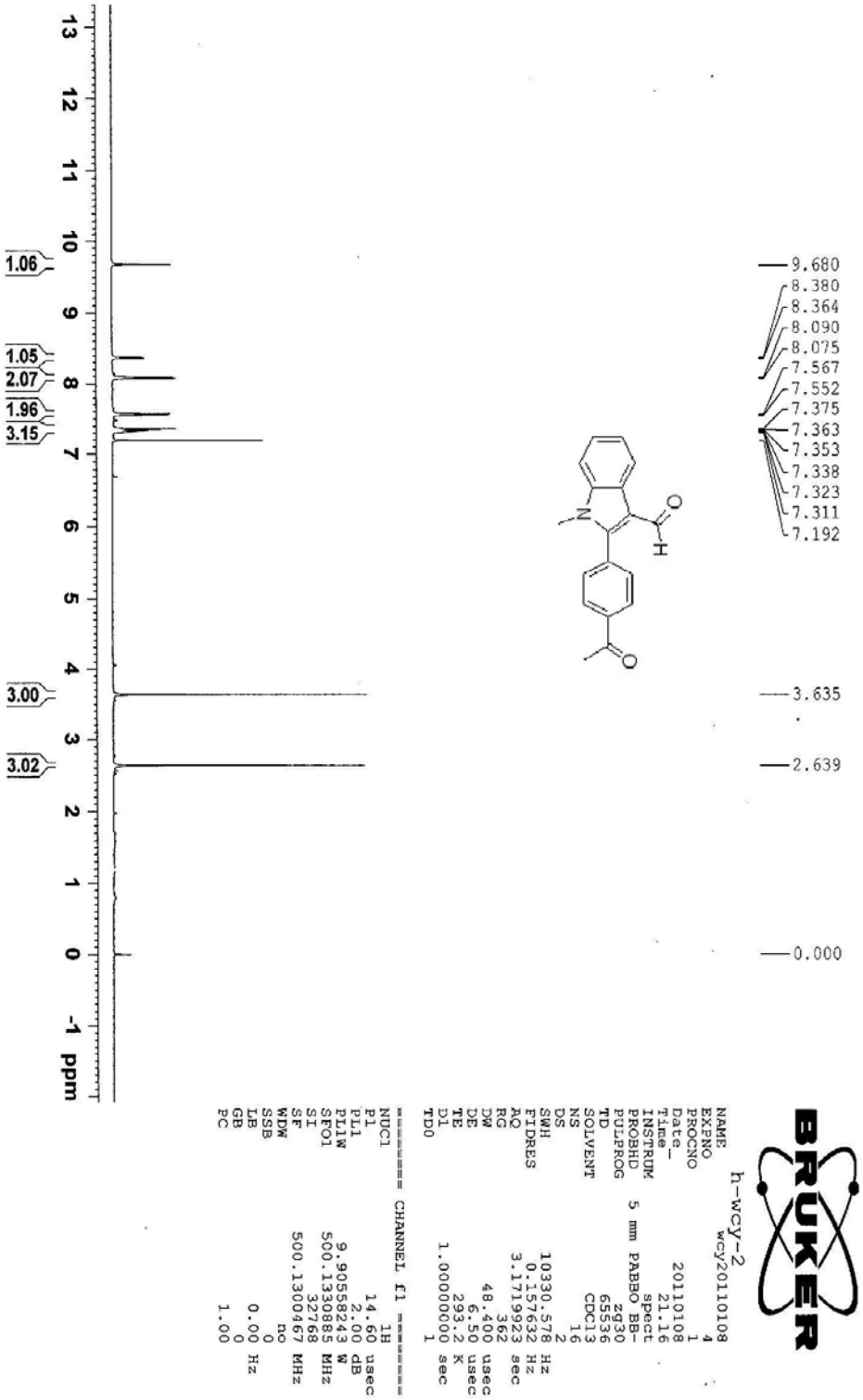
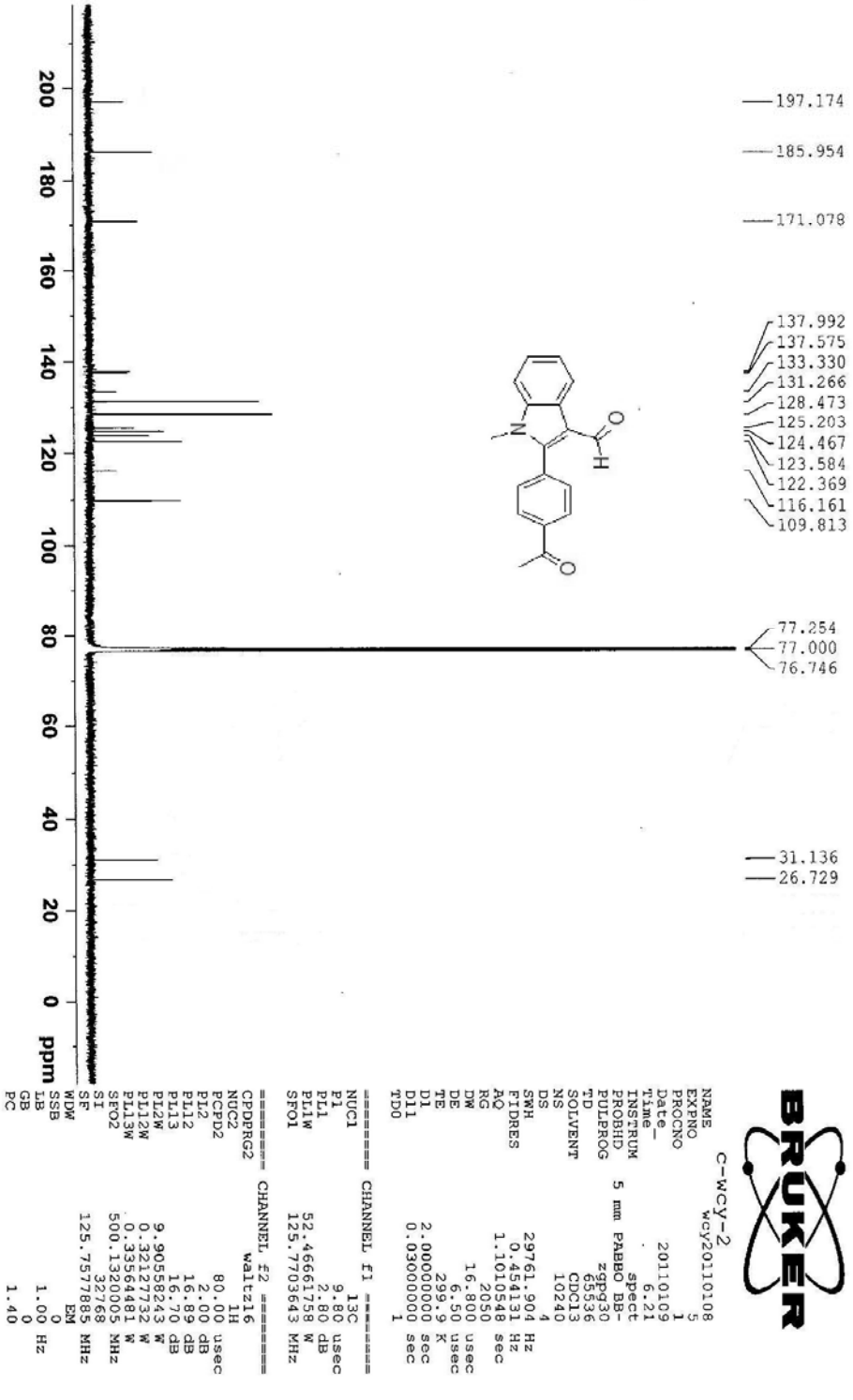


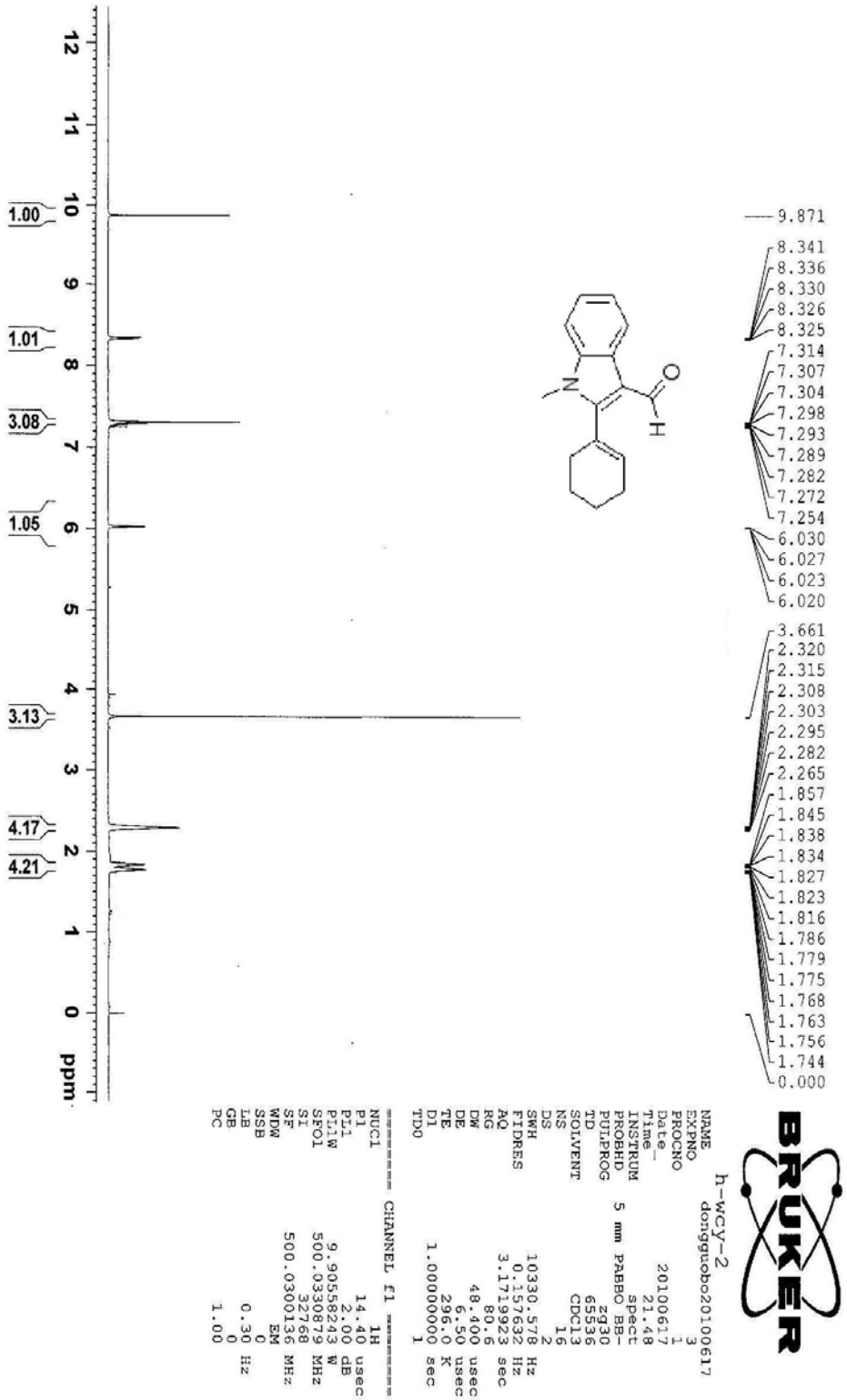
2-(4-Acetylphenyl)-1-methyl-1*H*-indole-3-carbaldehyde (2h)



2-(4-Acetylphenyl)-1-methyl-1*H*-indole-3-carbaldehyde (2h)



2-Cyclohexenyl-1-methyl-1*H*-indole-3-carbaldehyde (2i)



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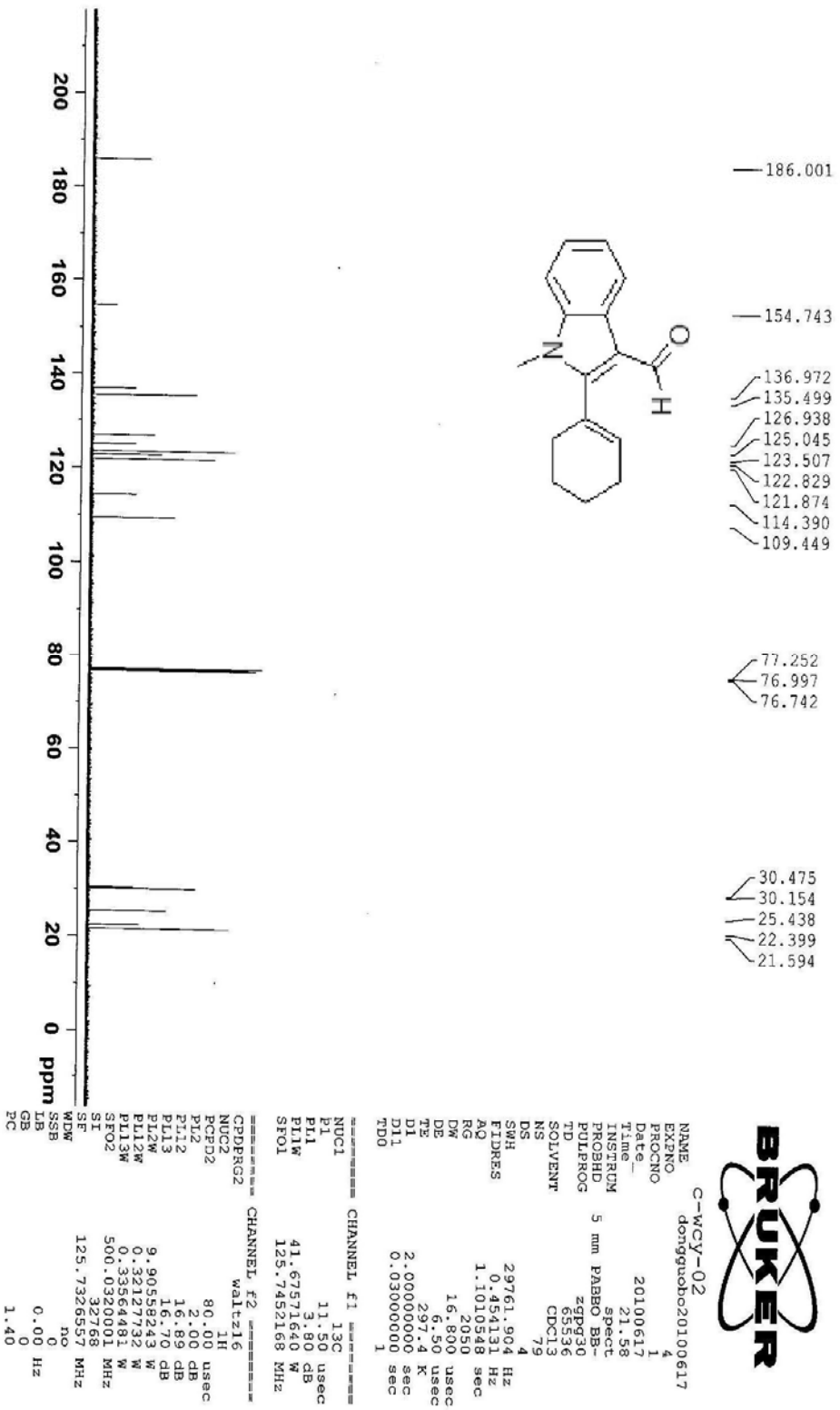

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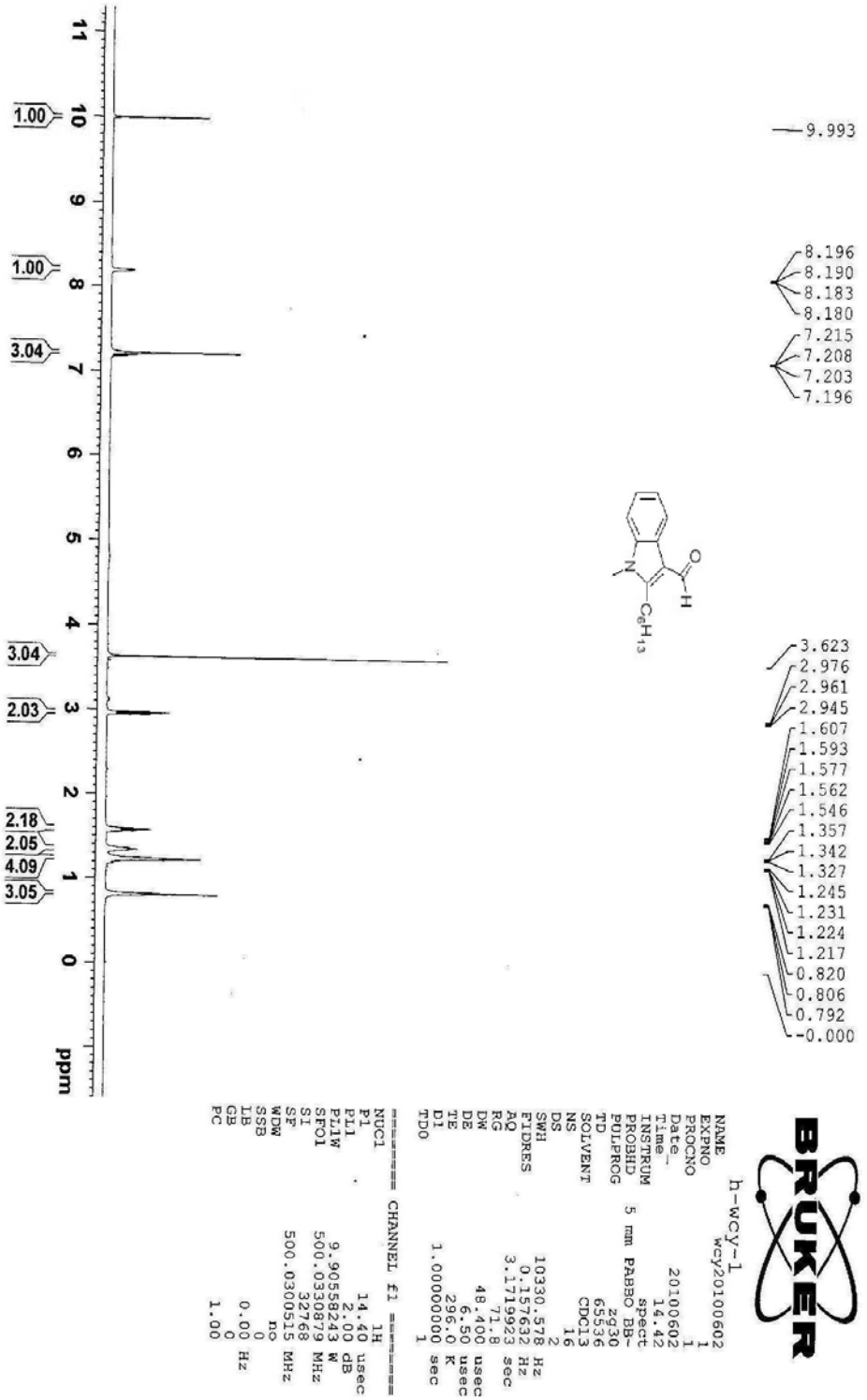

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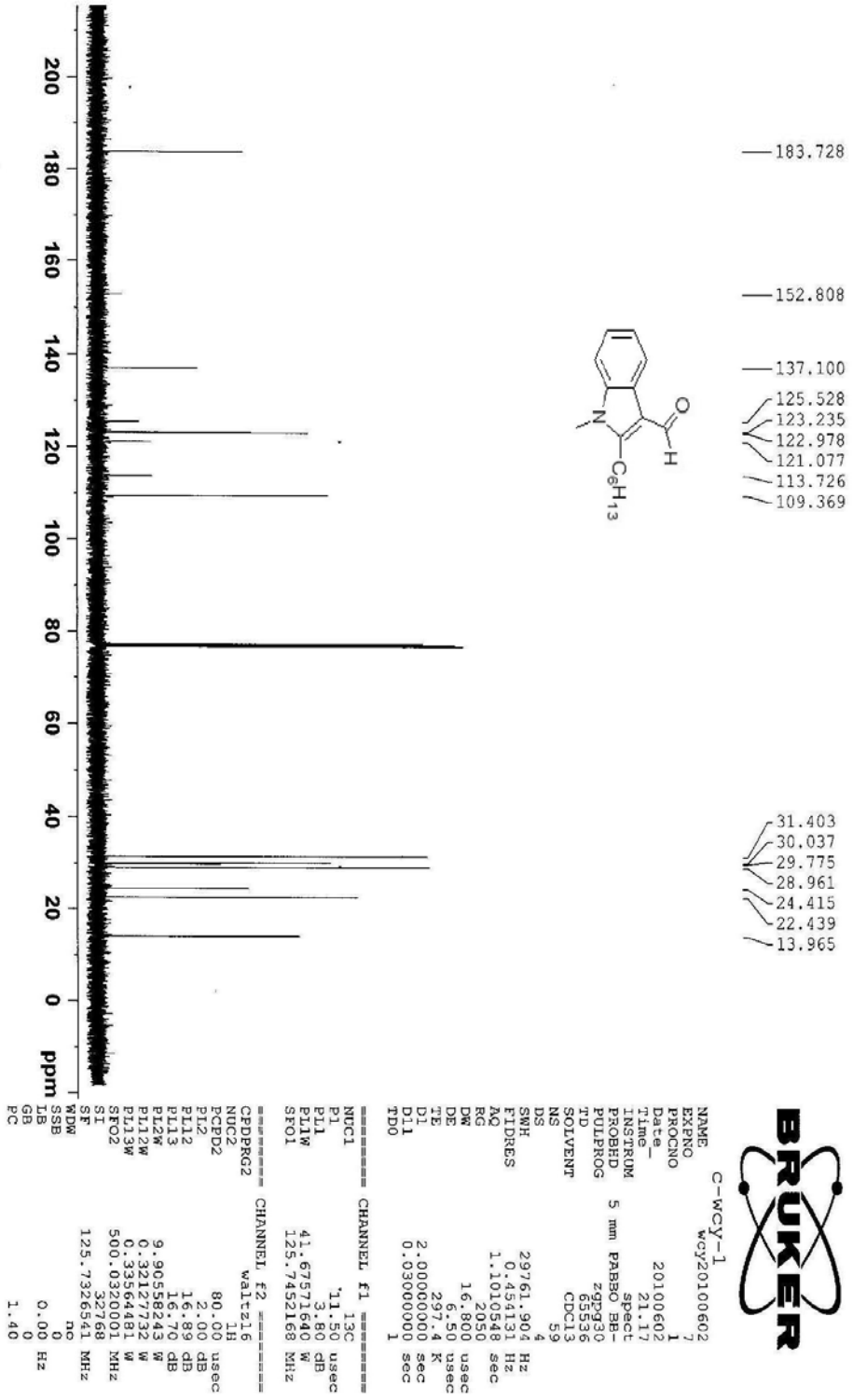
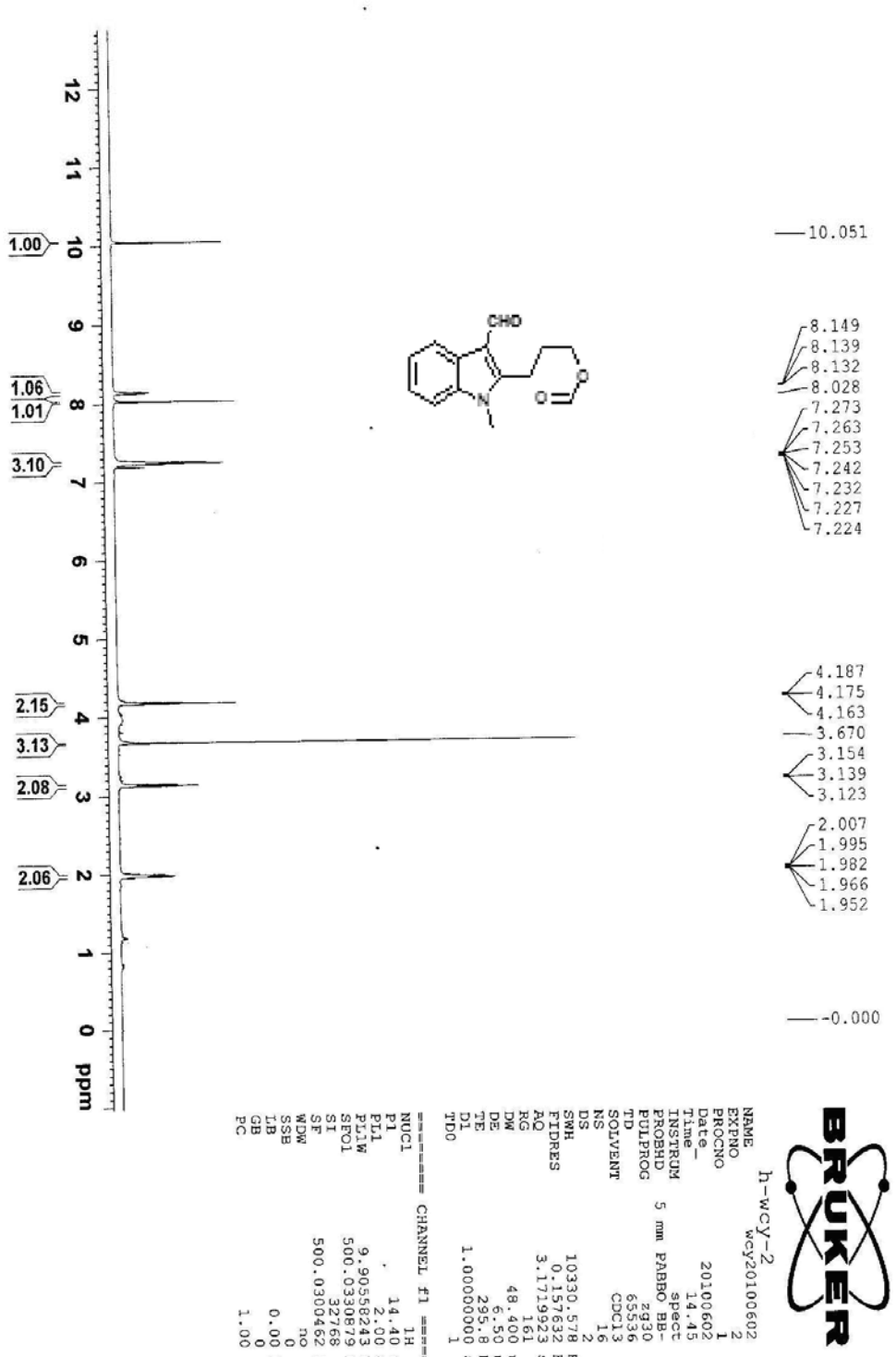
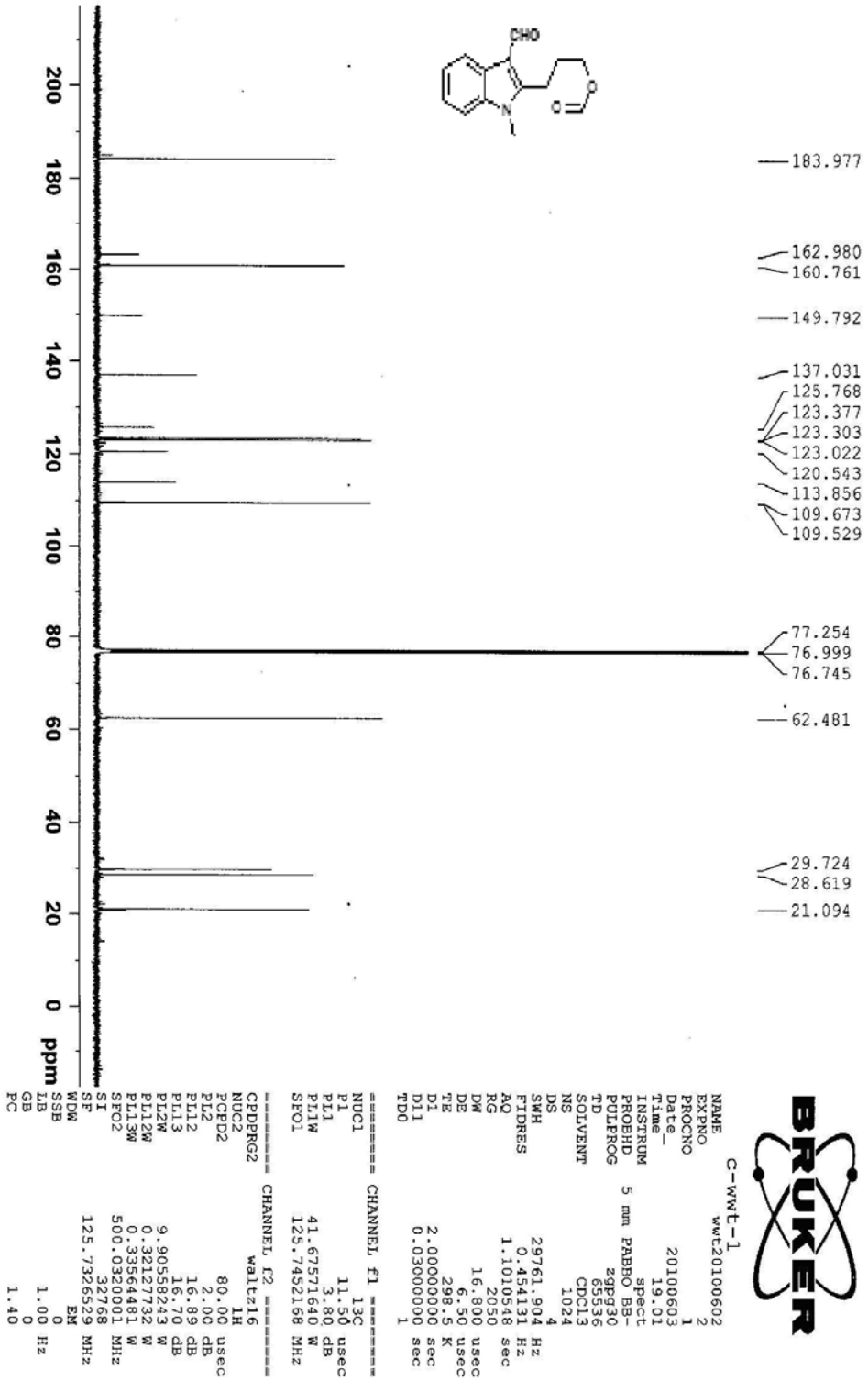


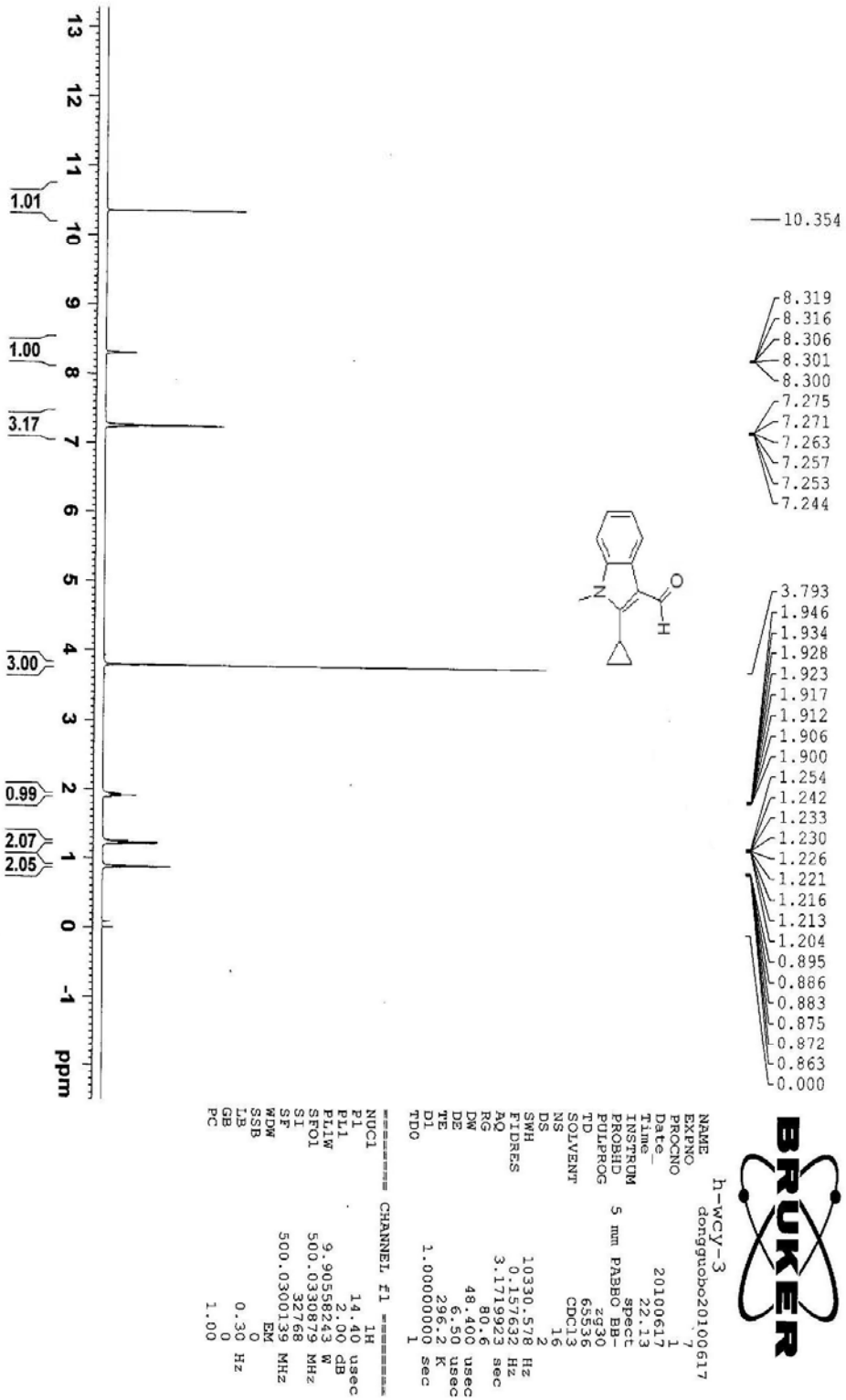
3-(3-Formyl-1-methyl-1*H*-indol-2-yl)propyl formate (2k)



3-(3-Formyl-1-methyl-1*H*-indol-2-yl)propyl formate (2k)



2-Cyclopropyl-1-methyl-1*H*-indole-3-carbaldehyde (2l)



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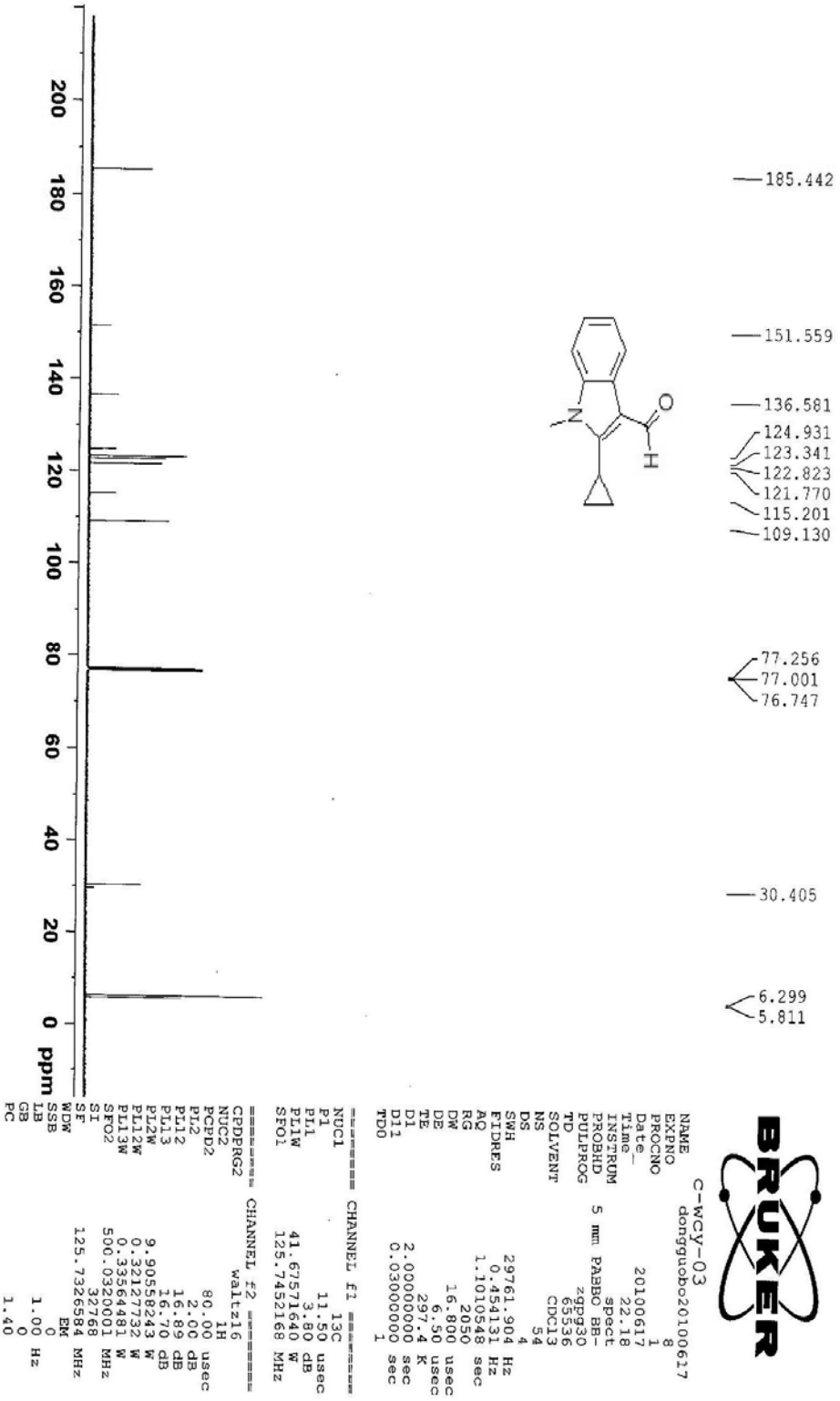

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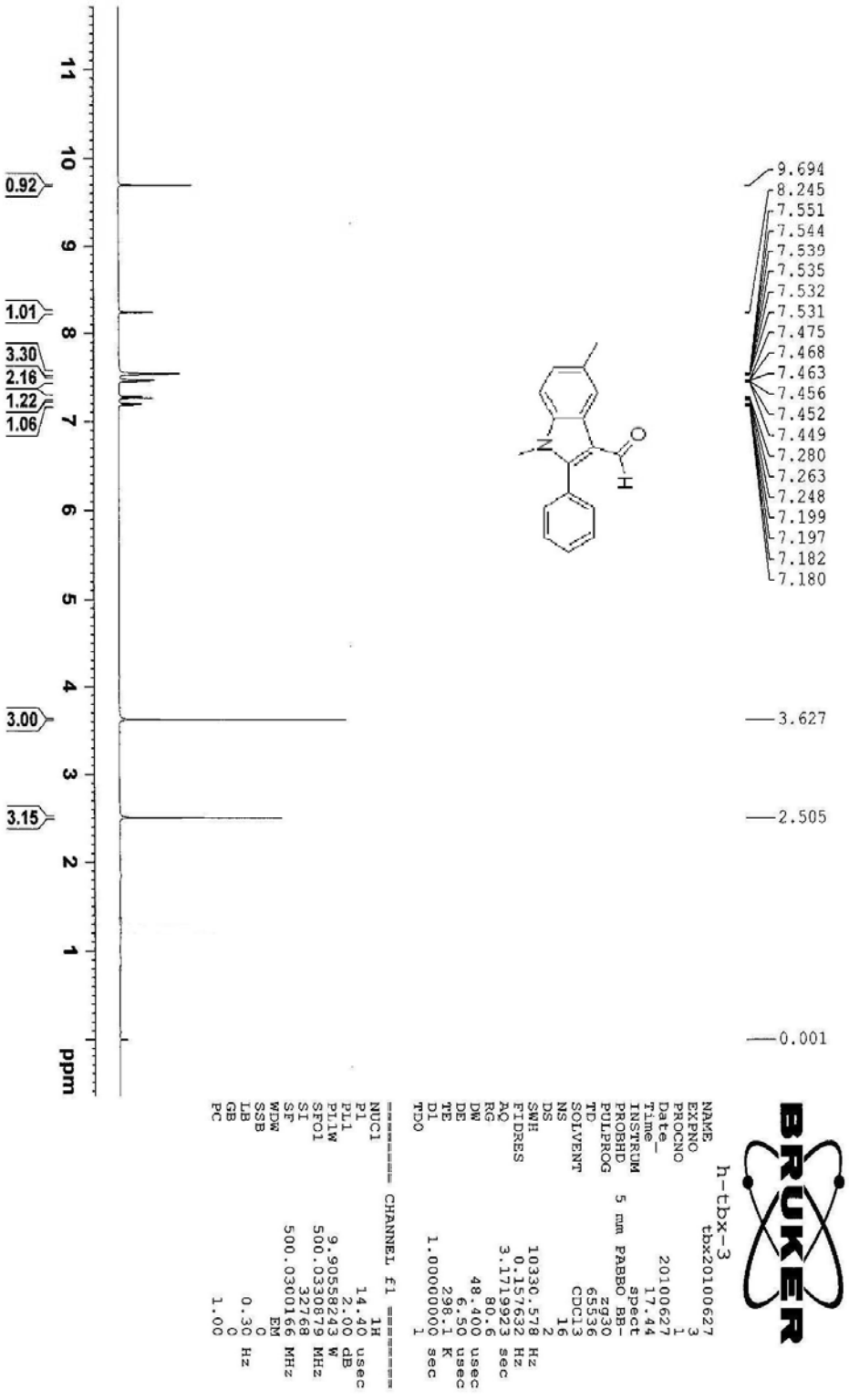
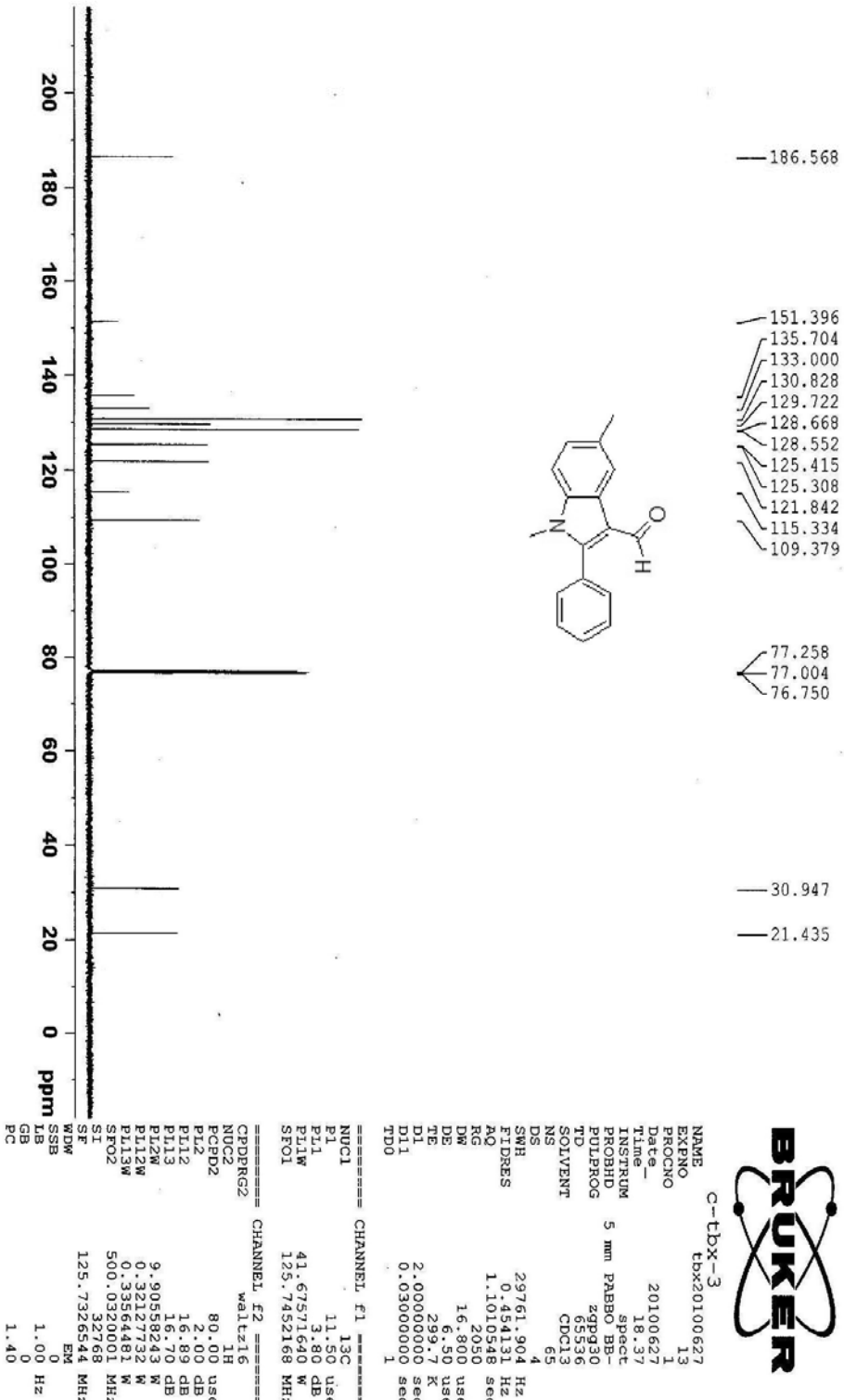
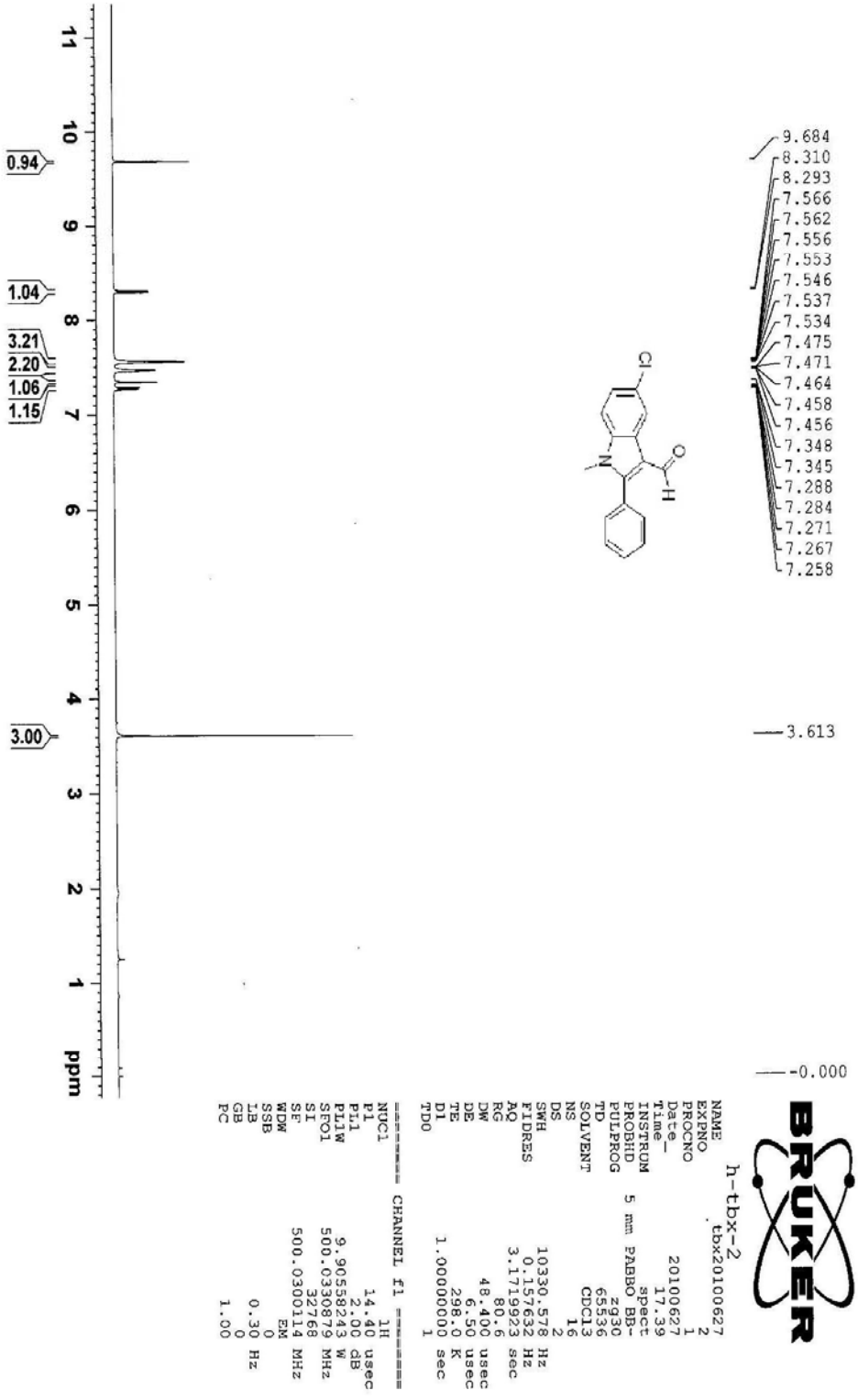


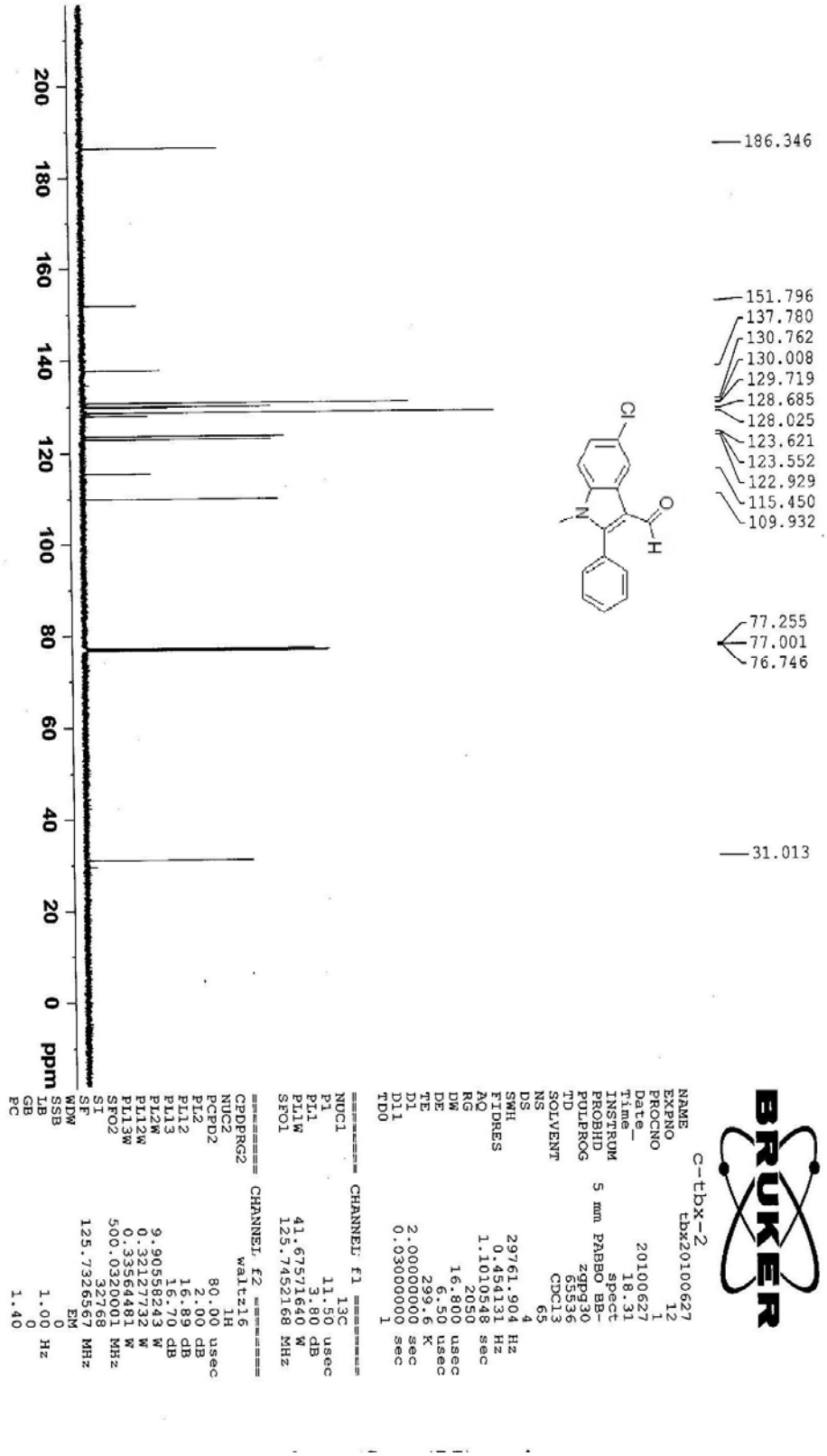
1,5-Dimethyl-2-phenyl-1*H*-indole-3-carbaldehyde (2m)



5-Chloro-1-methyl-2-phenyl-1*H*-indole-3-carbaldehyde (2n)



5-Chloro-1-methyl-2-phenyl-1*H*-indole-3-carbaldehyde (2n)



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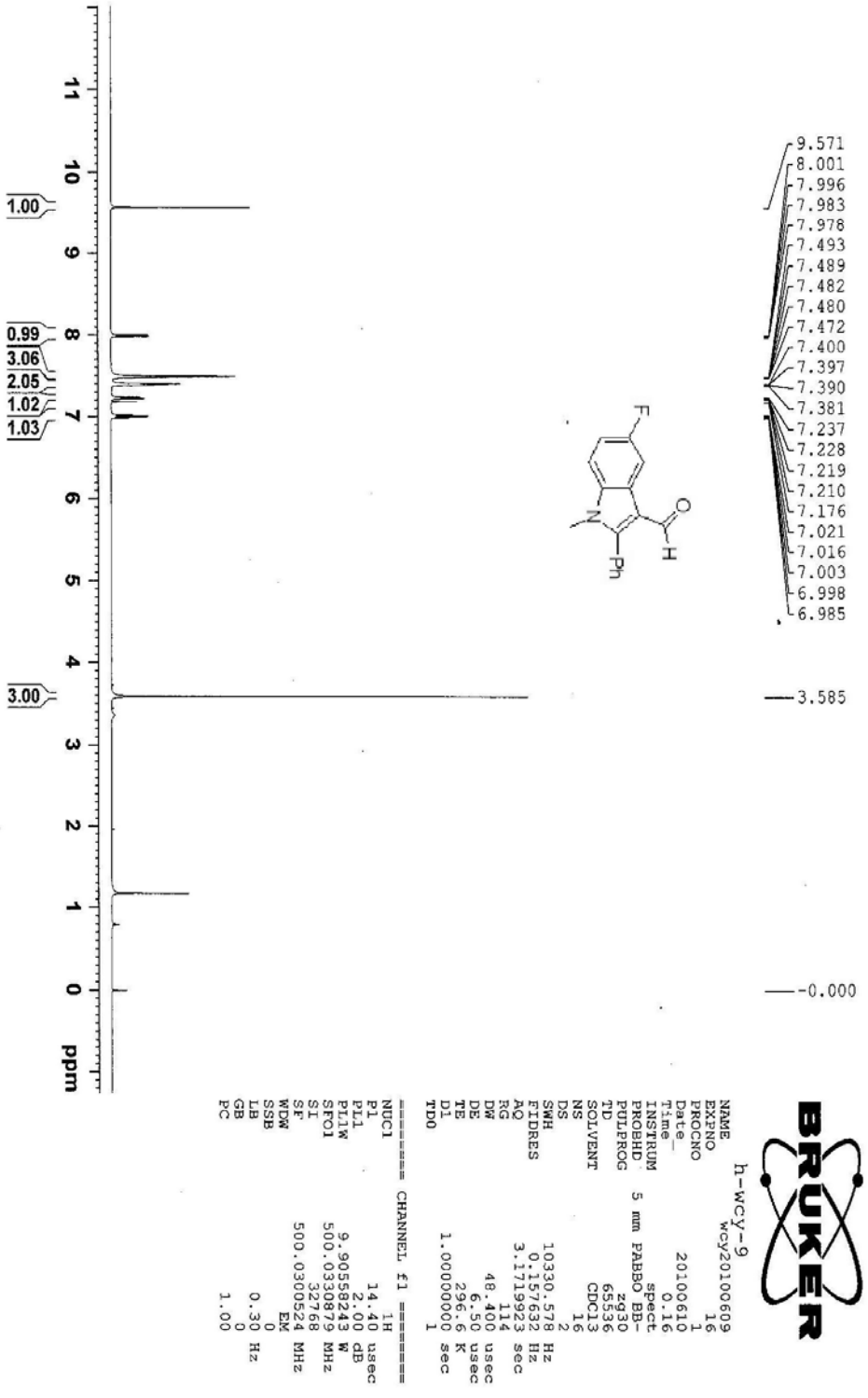
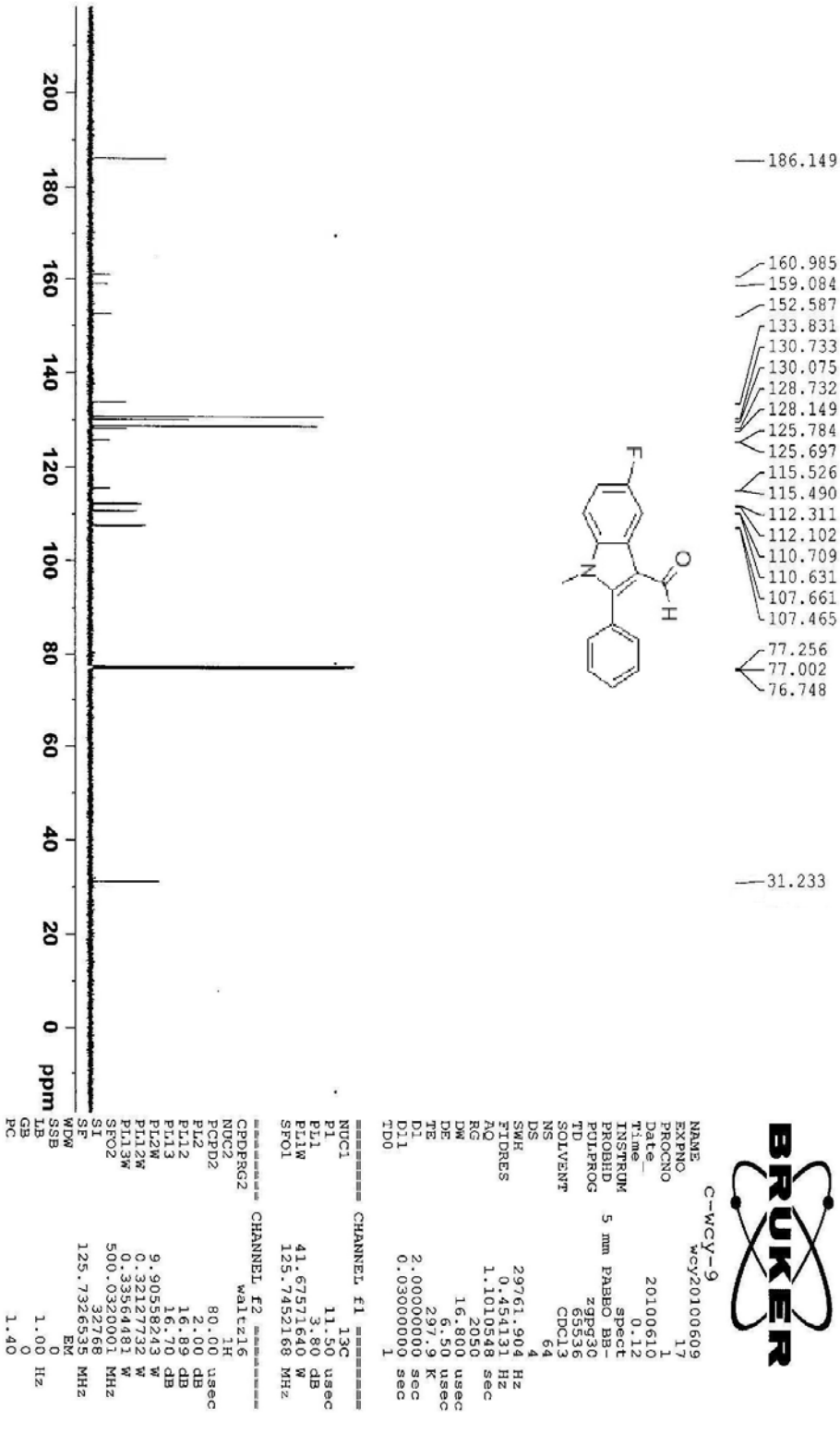
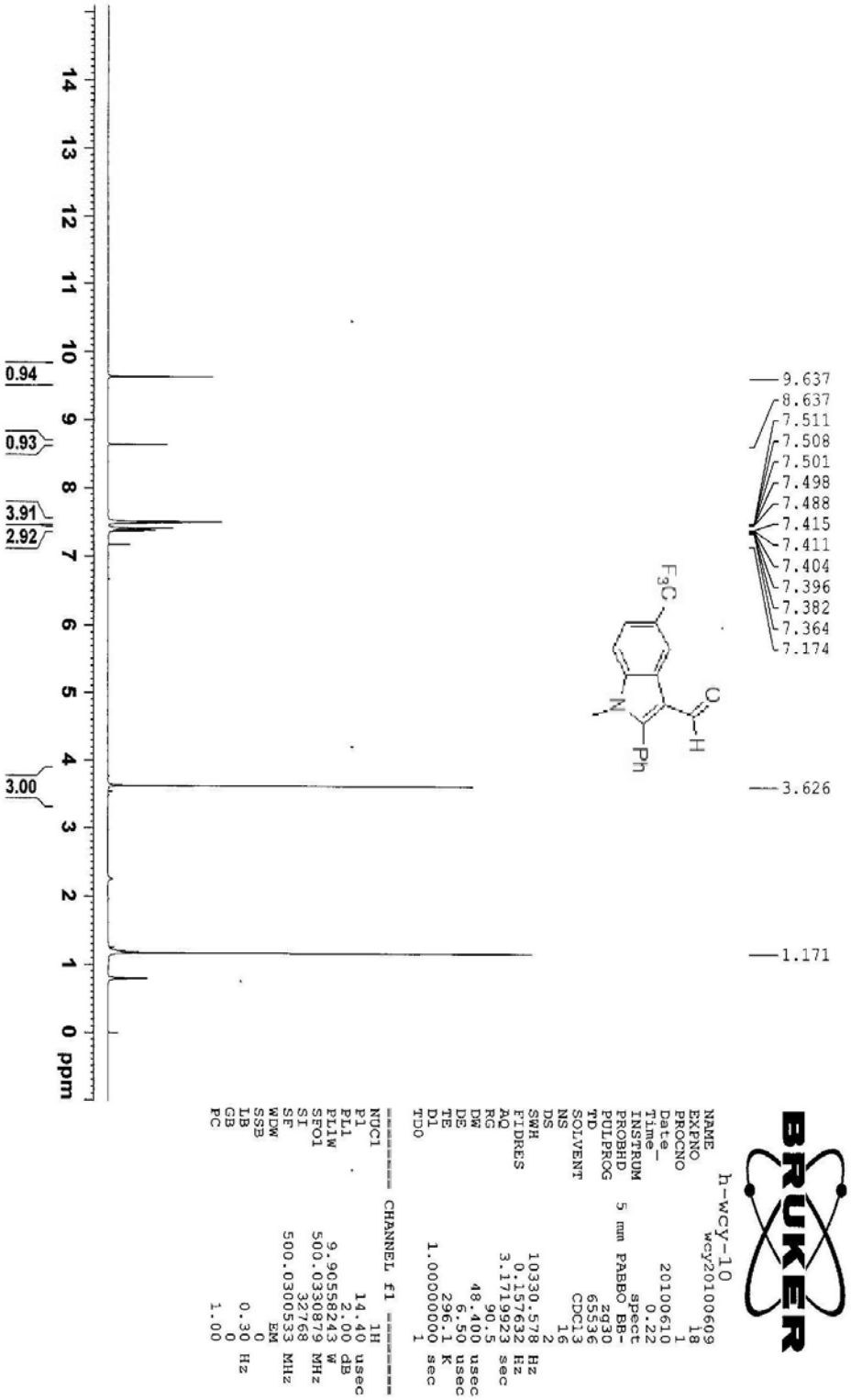


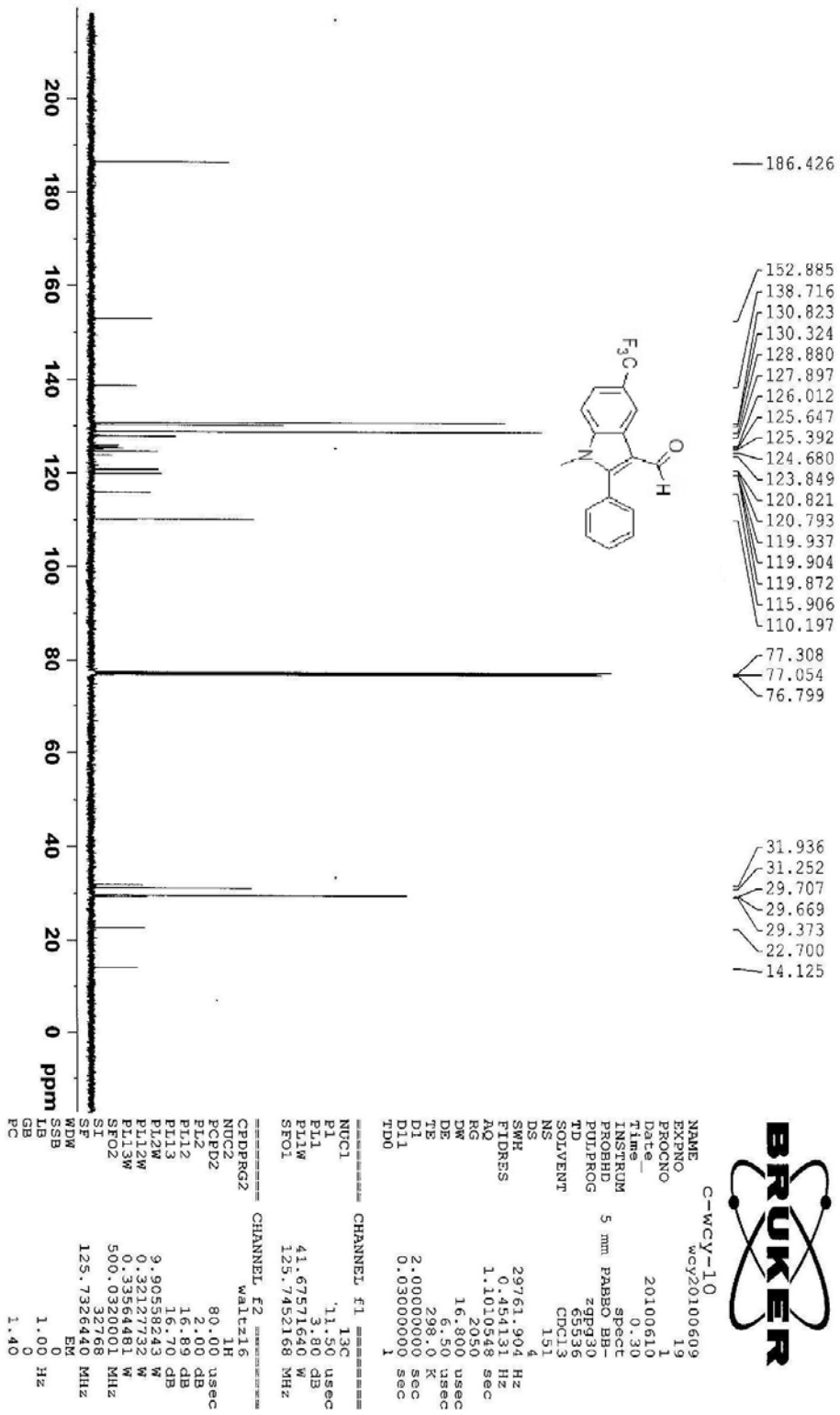
5-Fluoro-1-methyl-2-phenyl-1*H*-indole-3-carbaldehyde (2o)



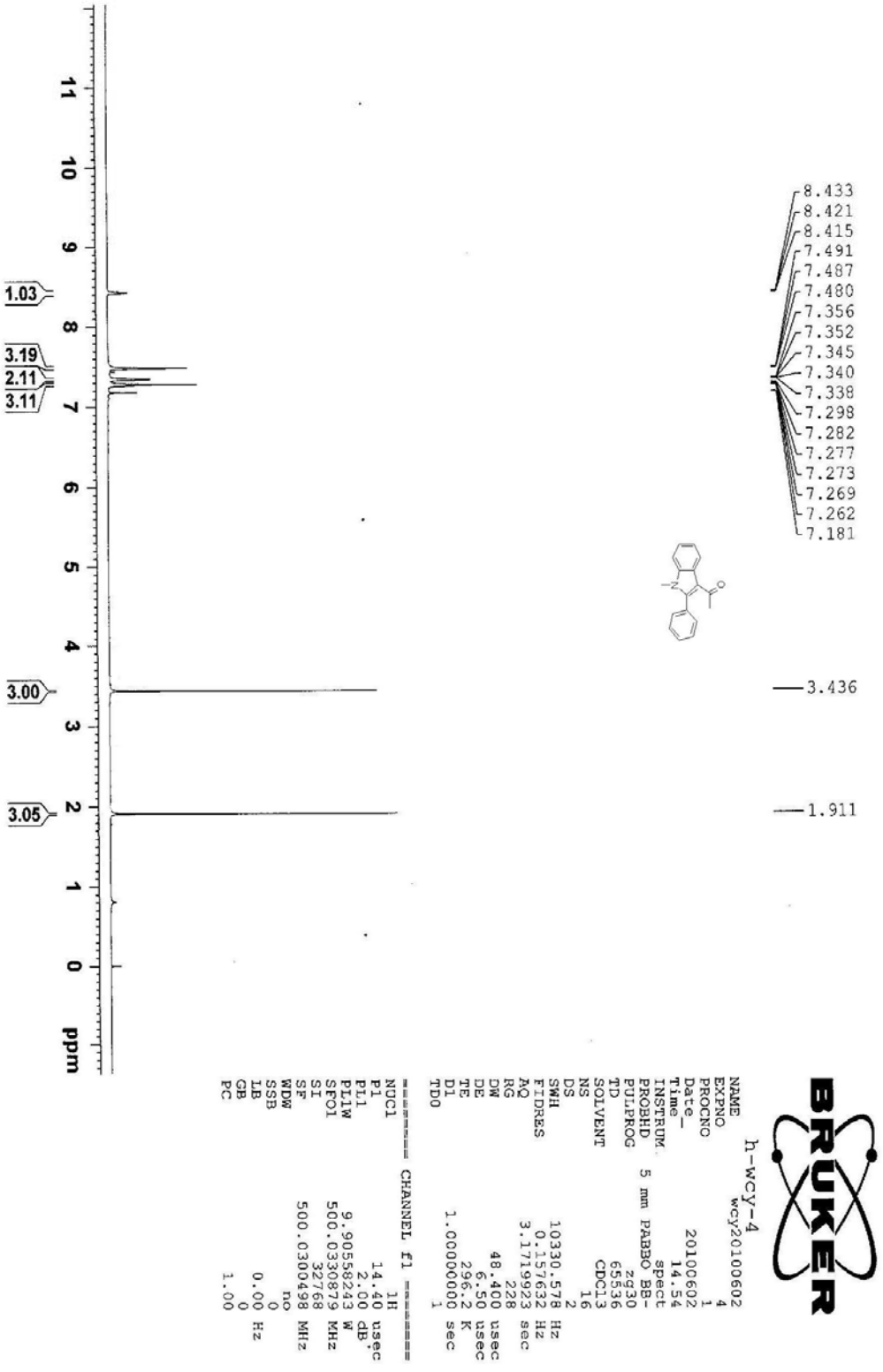
1-Methyl-2-phenyl-5-(trifluoromethyl)-1*H*-indole-3-carbaldehyde (2p)



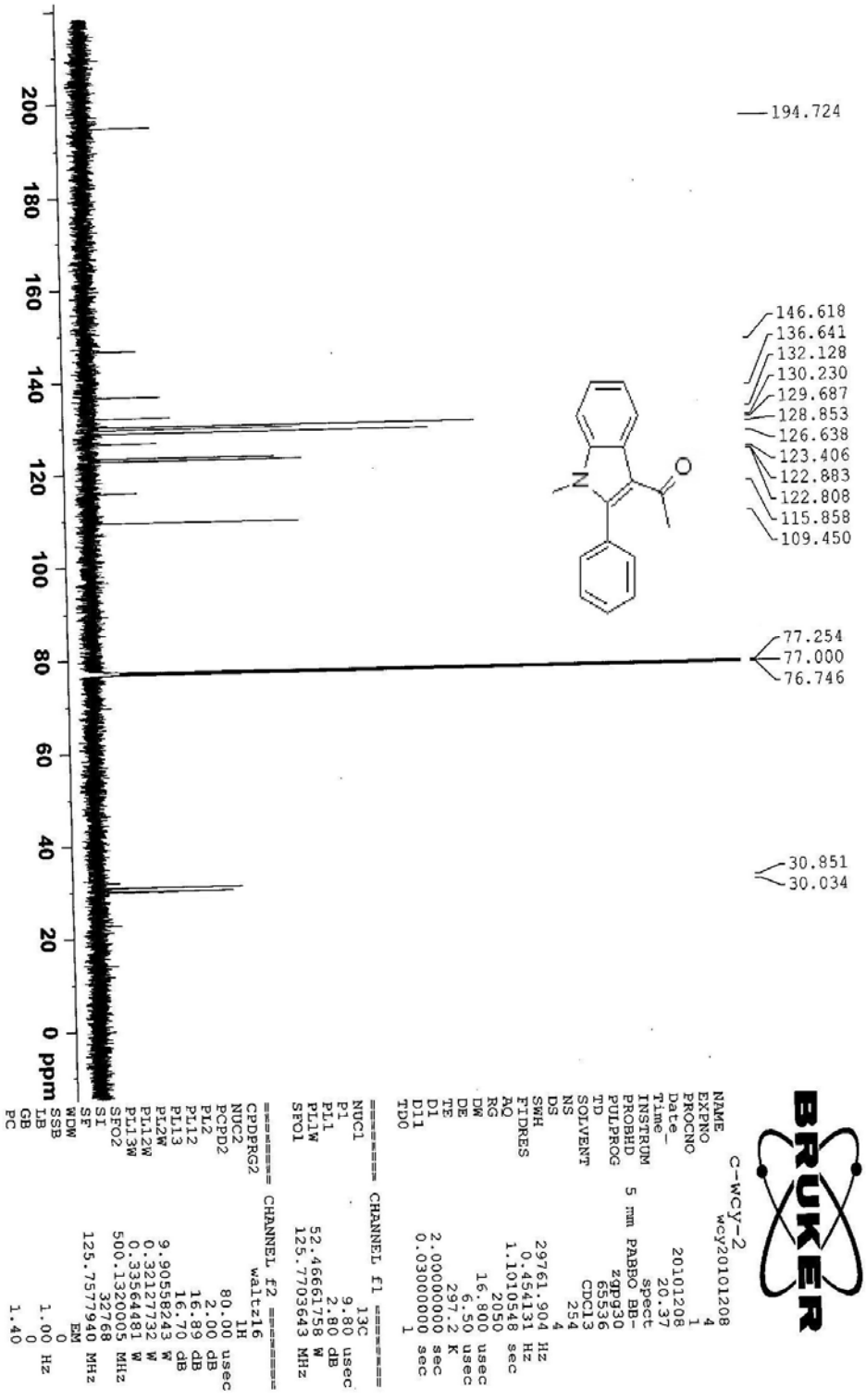
1-Methyl-2-phenyl-5-(trifluoromethyl)-1*H*-indole-3-carbaldehyde (2p)



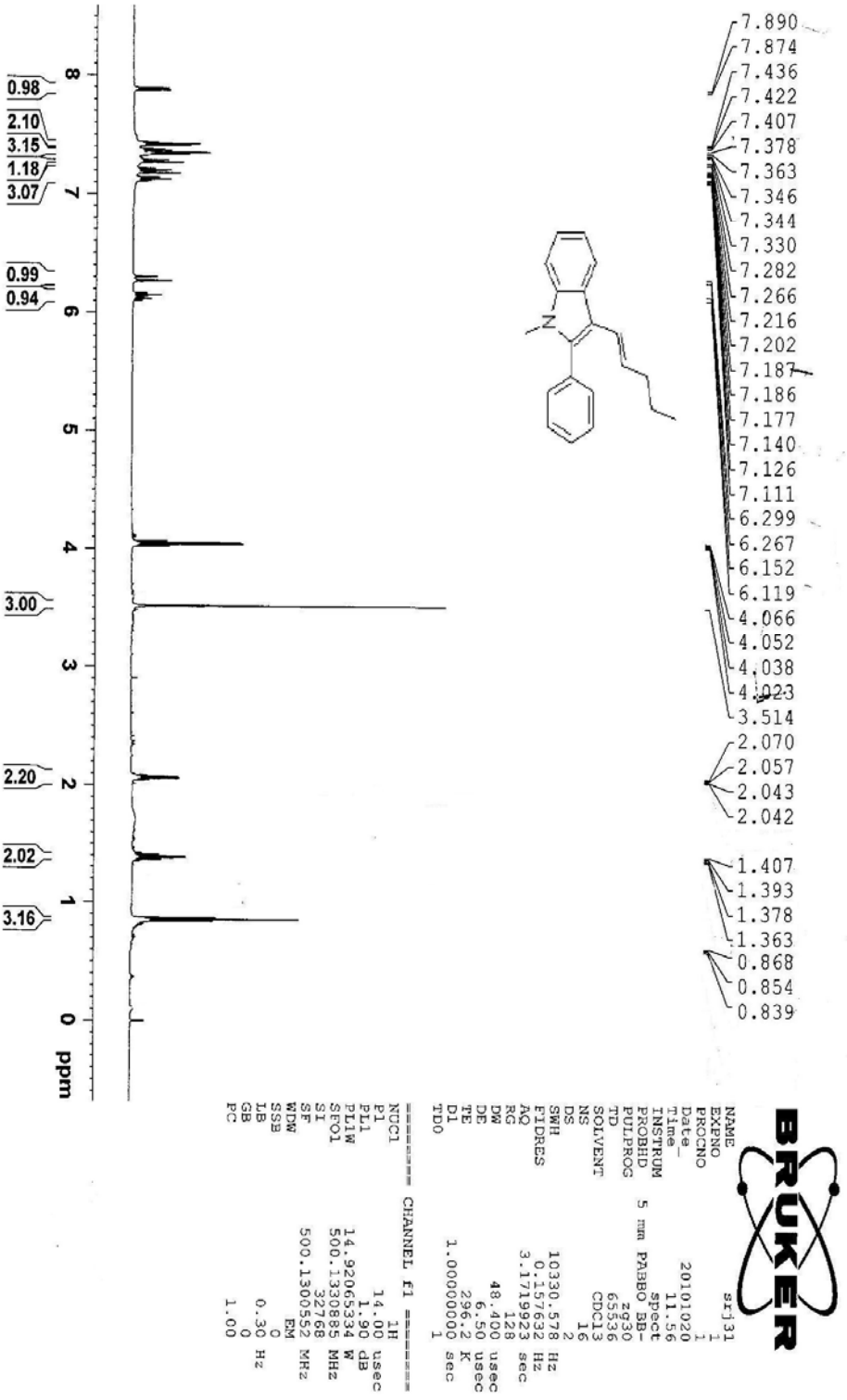
1-(1-methyl-2-phenyl-1*H*-indol-3-yl)ethanone (2q)



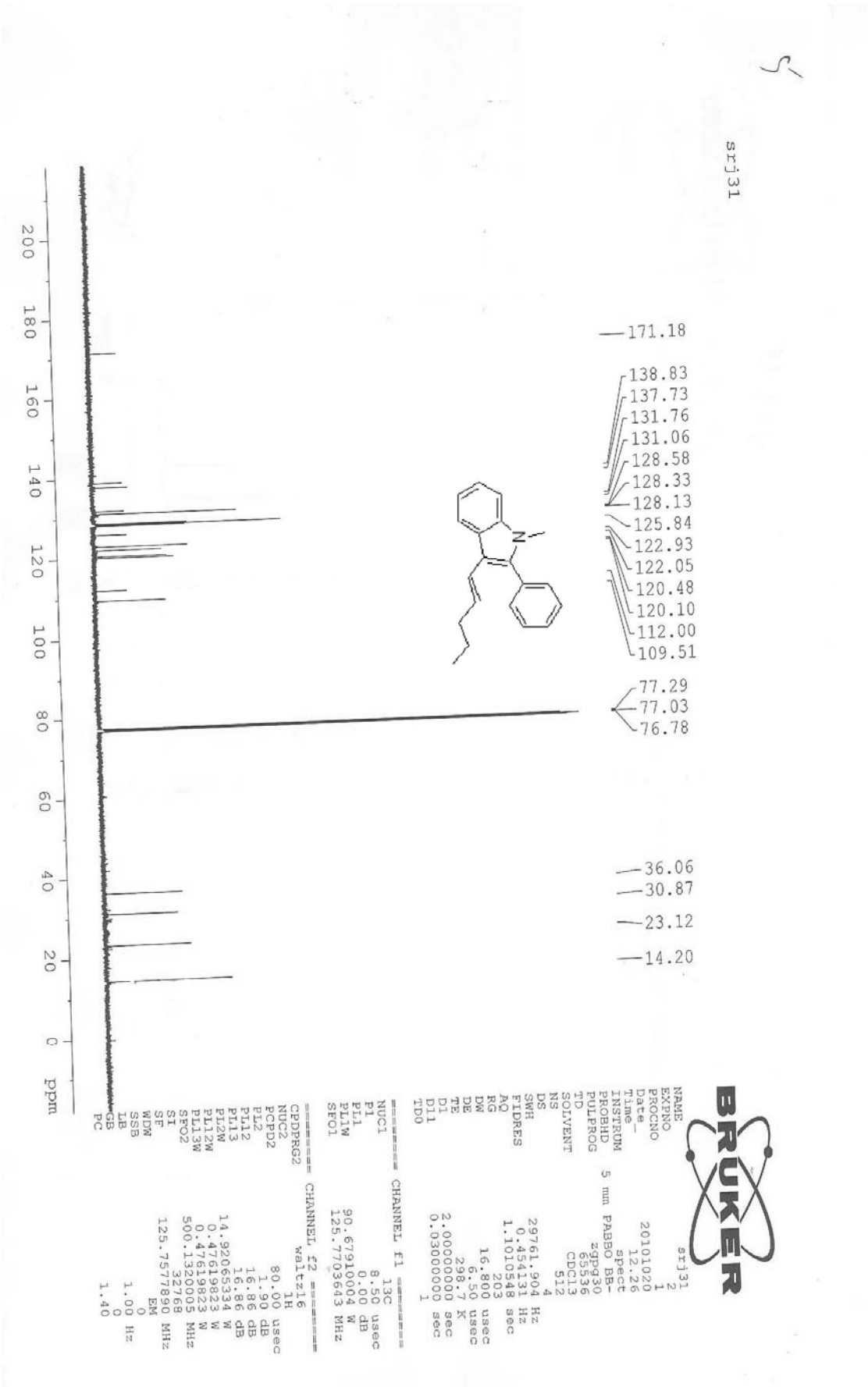
1-(1-methyl-2-phenyl-1*H*-indol-3-yl)ethanone (2q)



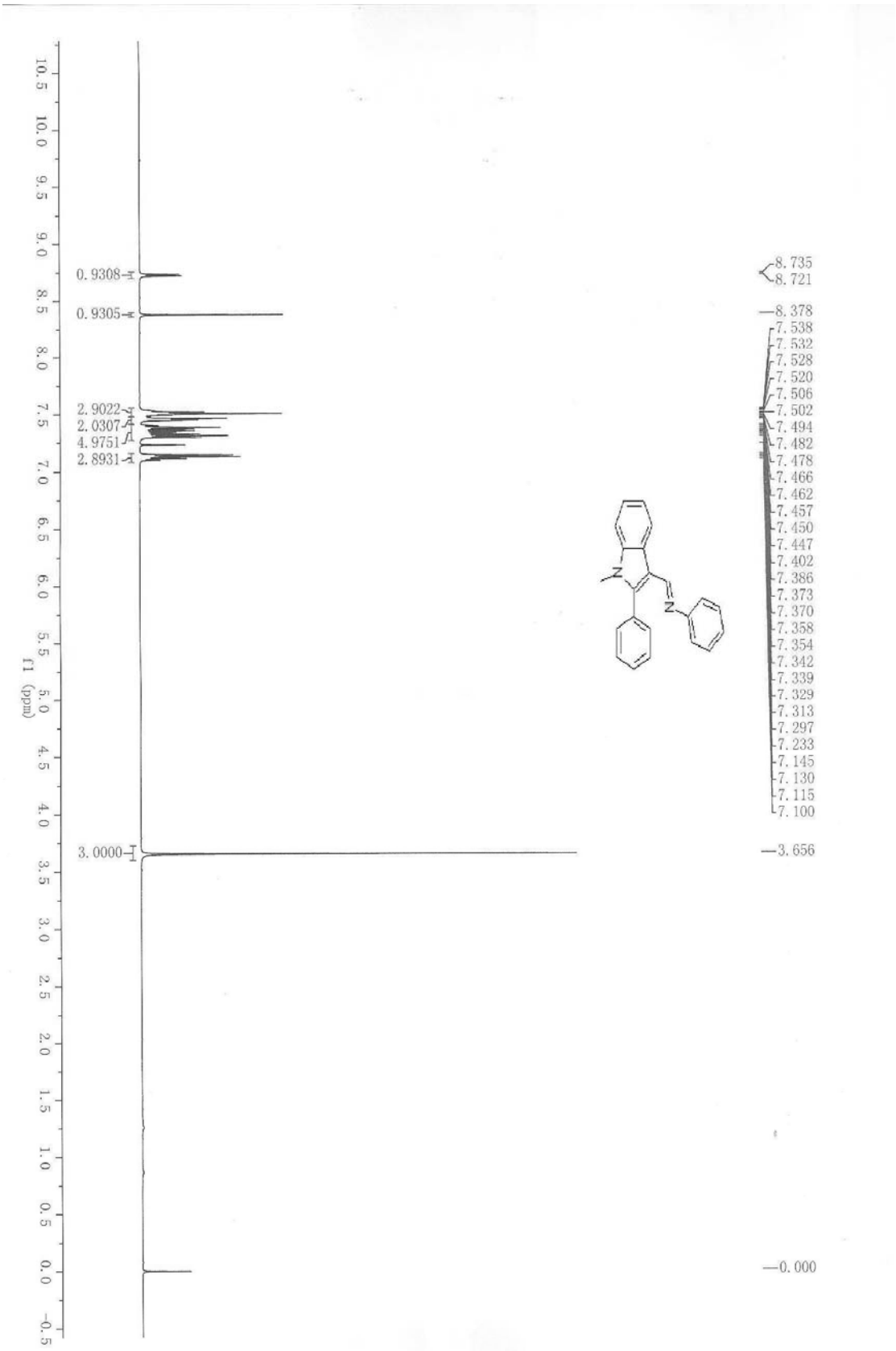
(*E*/*Z*)-1-Methyl-3-(pent-1-enyl)-2-phenyl-1*H*-indole (3)



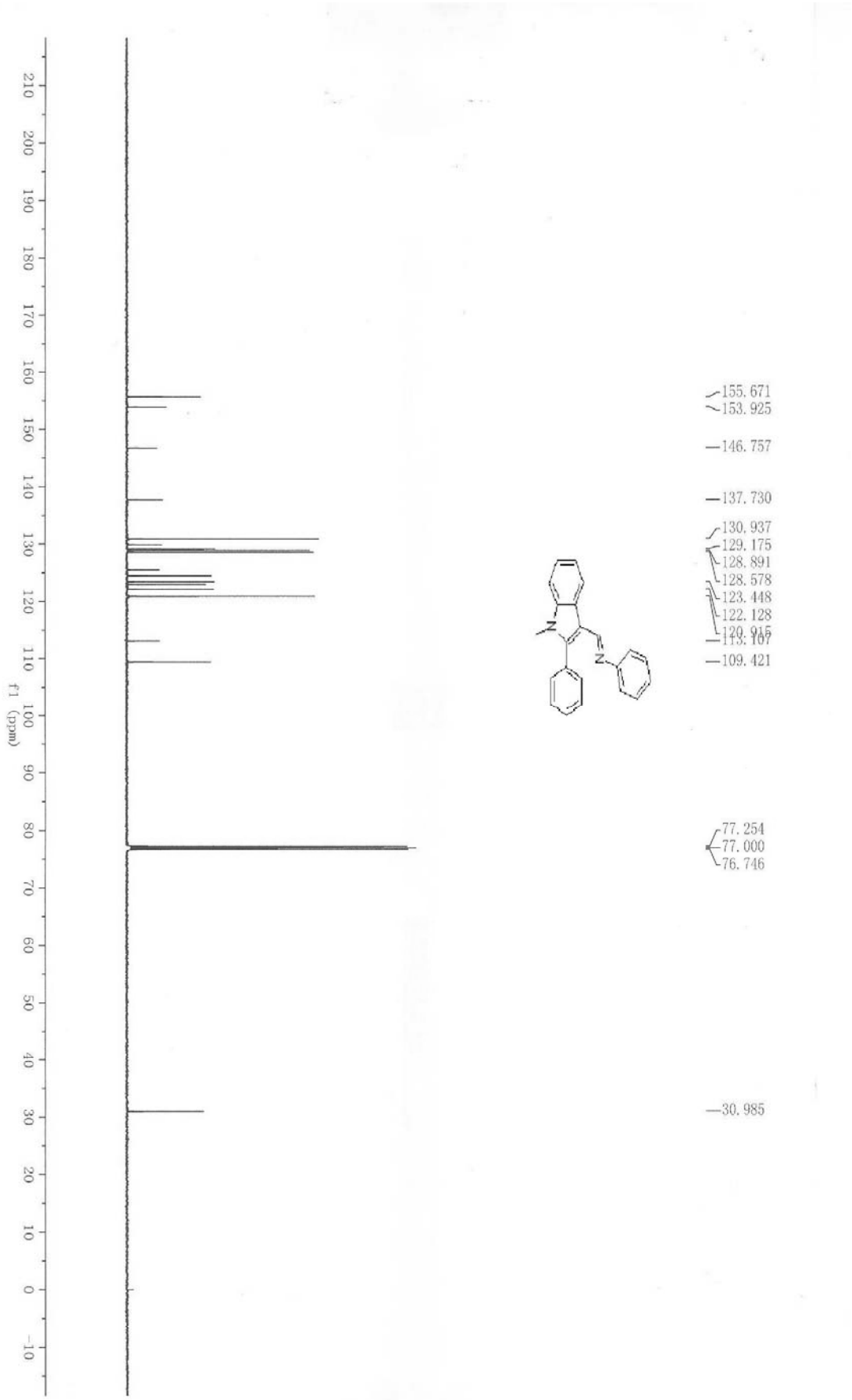
(*E*/*Z*)-1-Methyl-3-(pent-1-enyl)-2-phenyl-1*H*-indole (3)



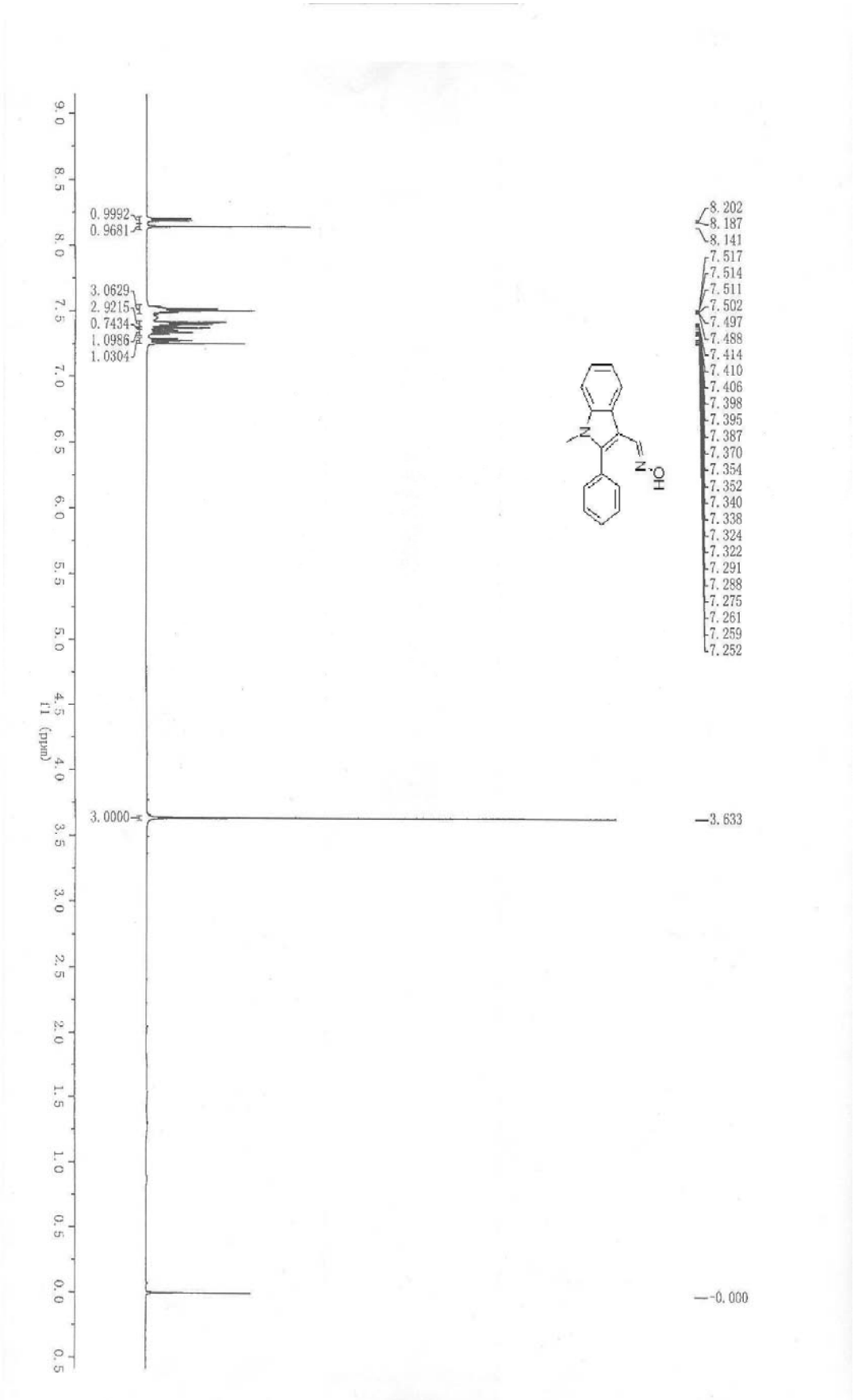
(*E*/*Z*)-*N*-((1-Methyl-2-phenyl-1*H*-indol-3-yl)methylene)aniline (4)



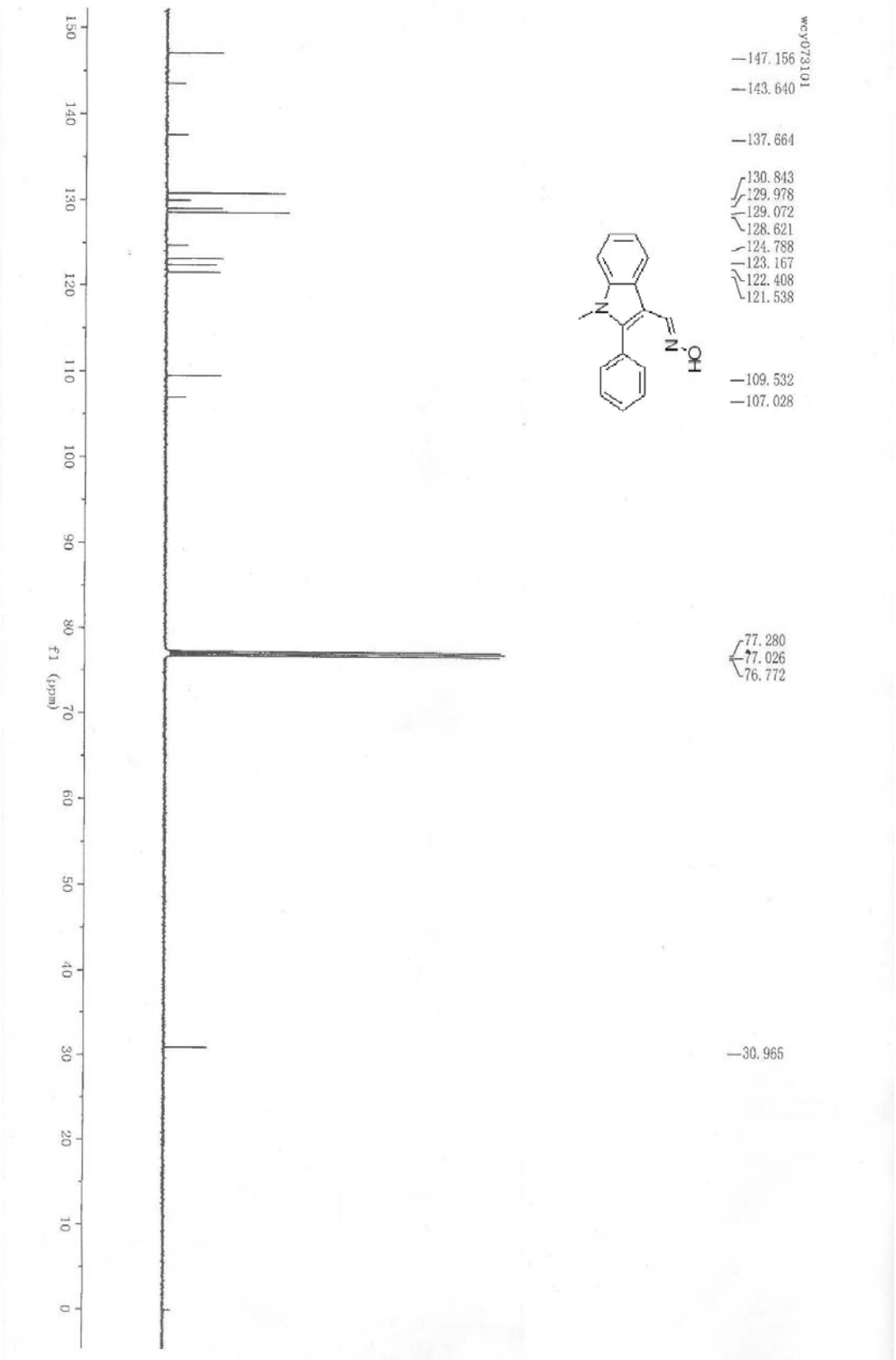
(*E*/*Z*)-*N*-((1-Methyl-2-phenyl-1*H*-indol-3-yl)methylene)aniline (4)



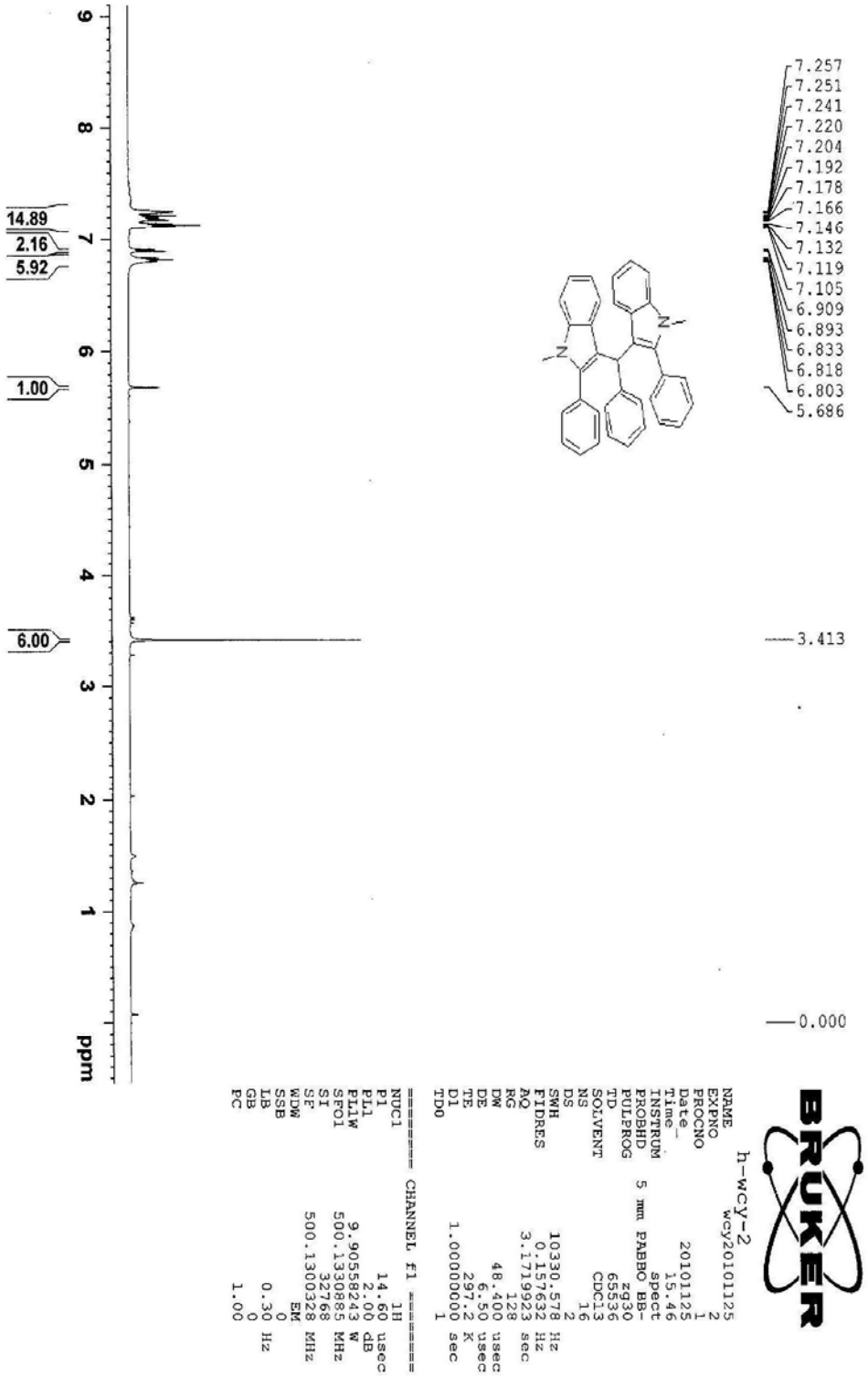
(*E*/*Z*)-1-Methyl-2-phenyl-1*H*-indole-3-carbaldehyde oxime (5)



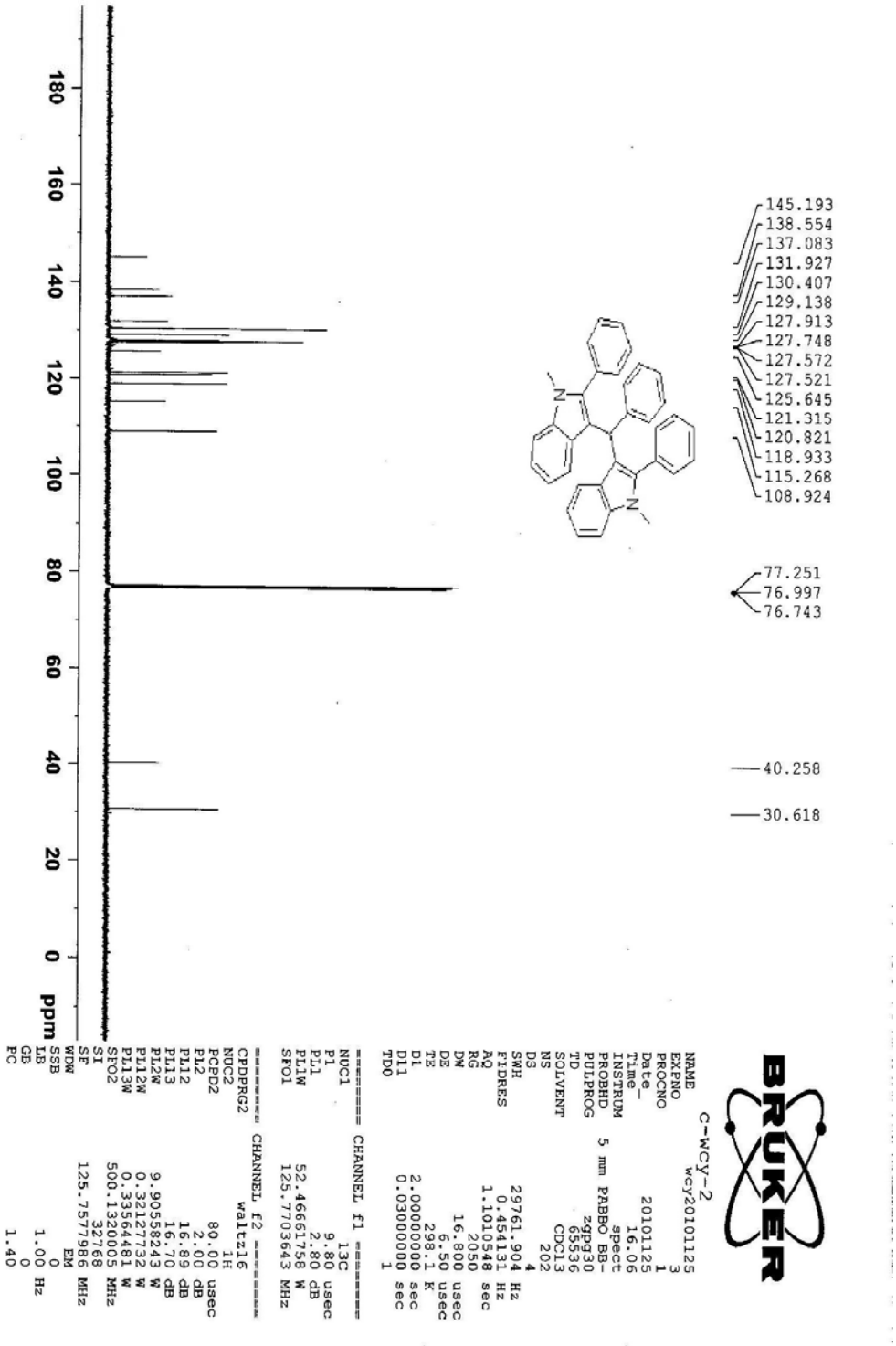
(*E*/*Z*)-1-Methyl-2-phenyl-1*H*-indole-3-carbaldehyde oxime (5)



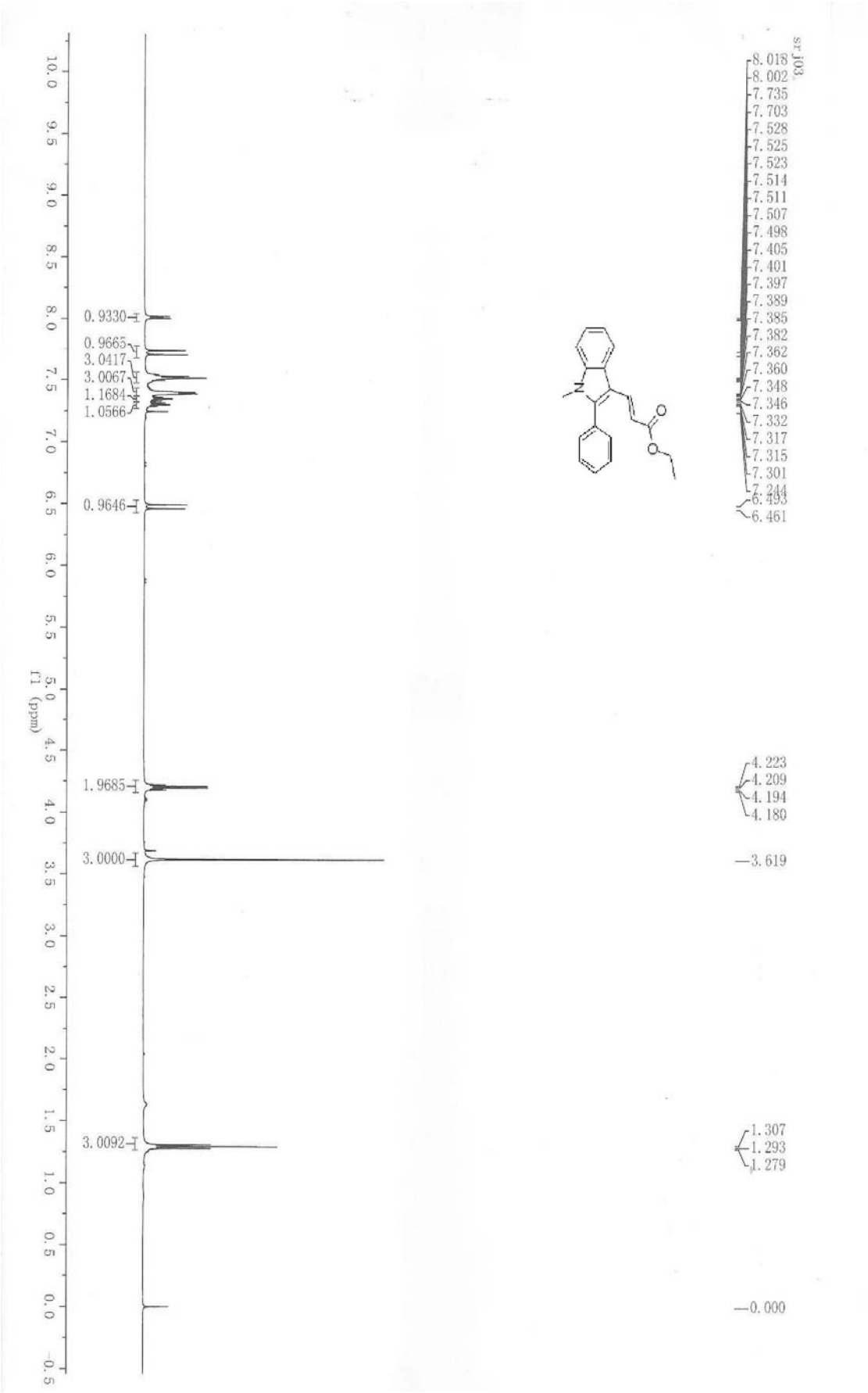
3,3'-(Phenylmethylene)bis(1-methyl-2-phenyl-1*H*-indole) (6)



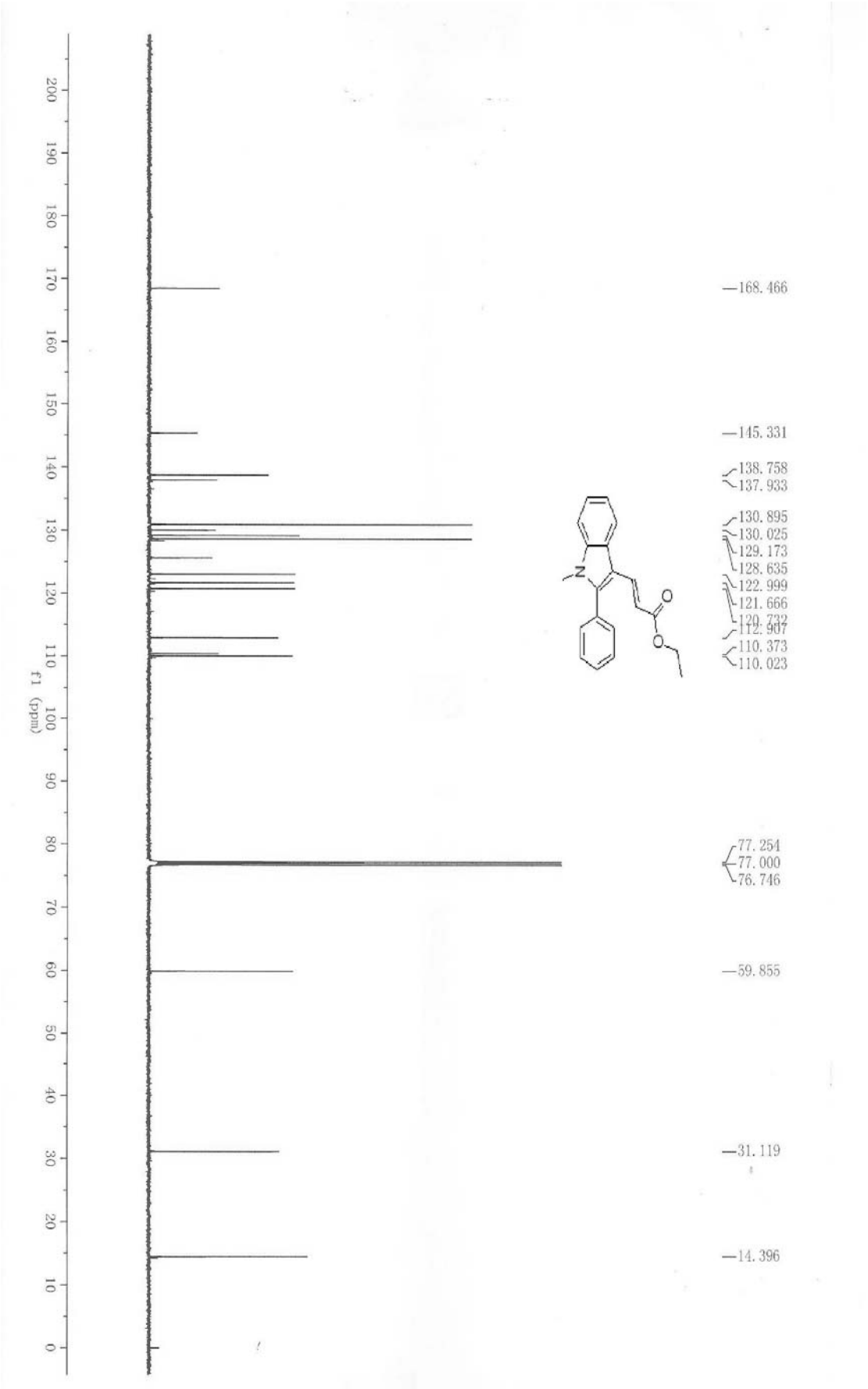
3,3'-(Phenylmethylene)bis(1-methyl-2-phenyl-1*H*-indole) (6)



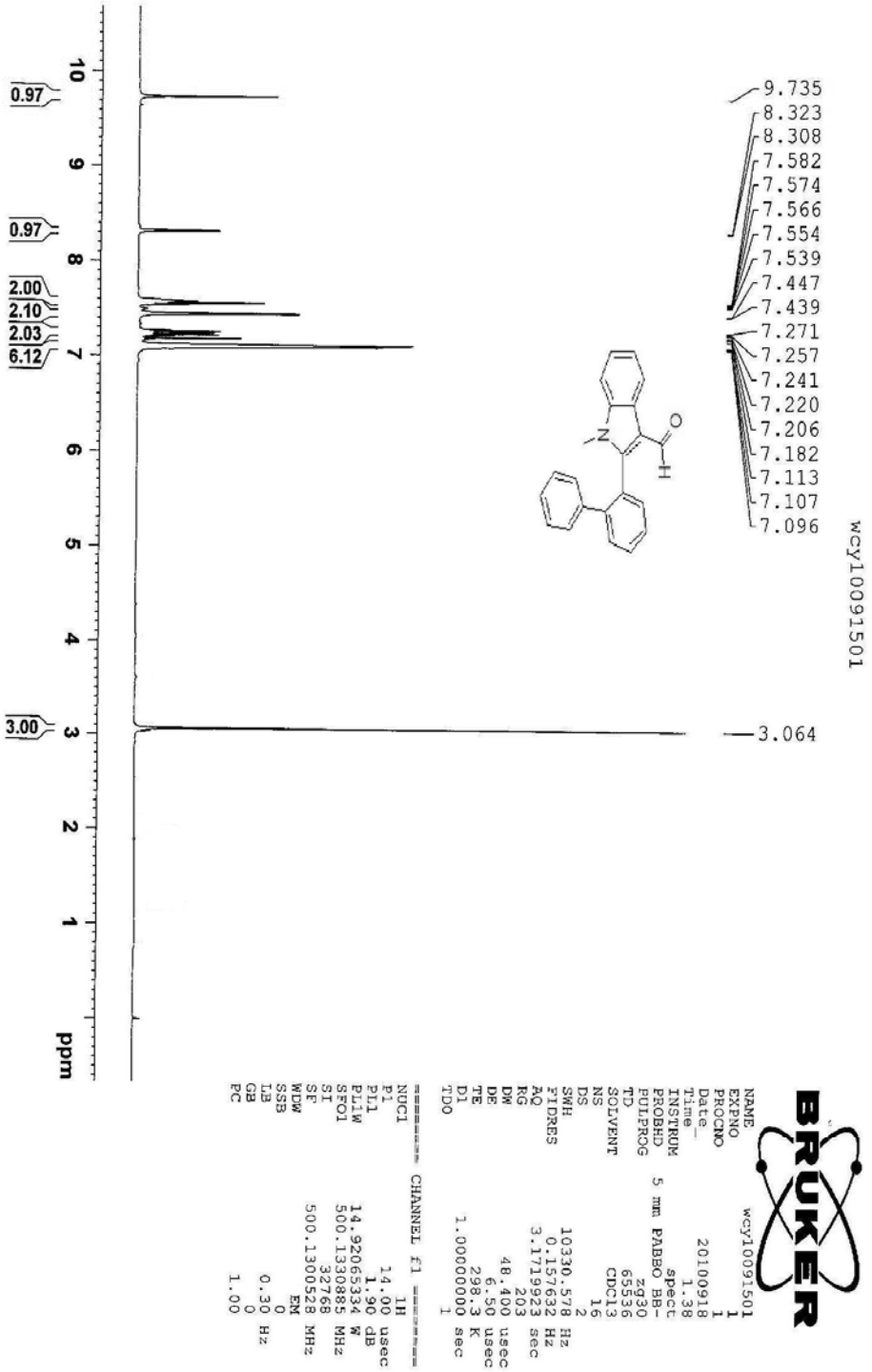
(*E*/*Z*)-Ethyl 3-(1-methyl-2-phenyl-1*H*-indol-3-yl)acrylate (7)



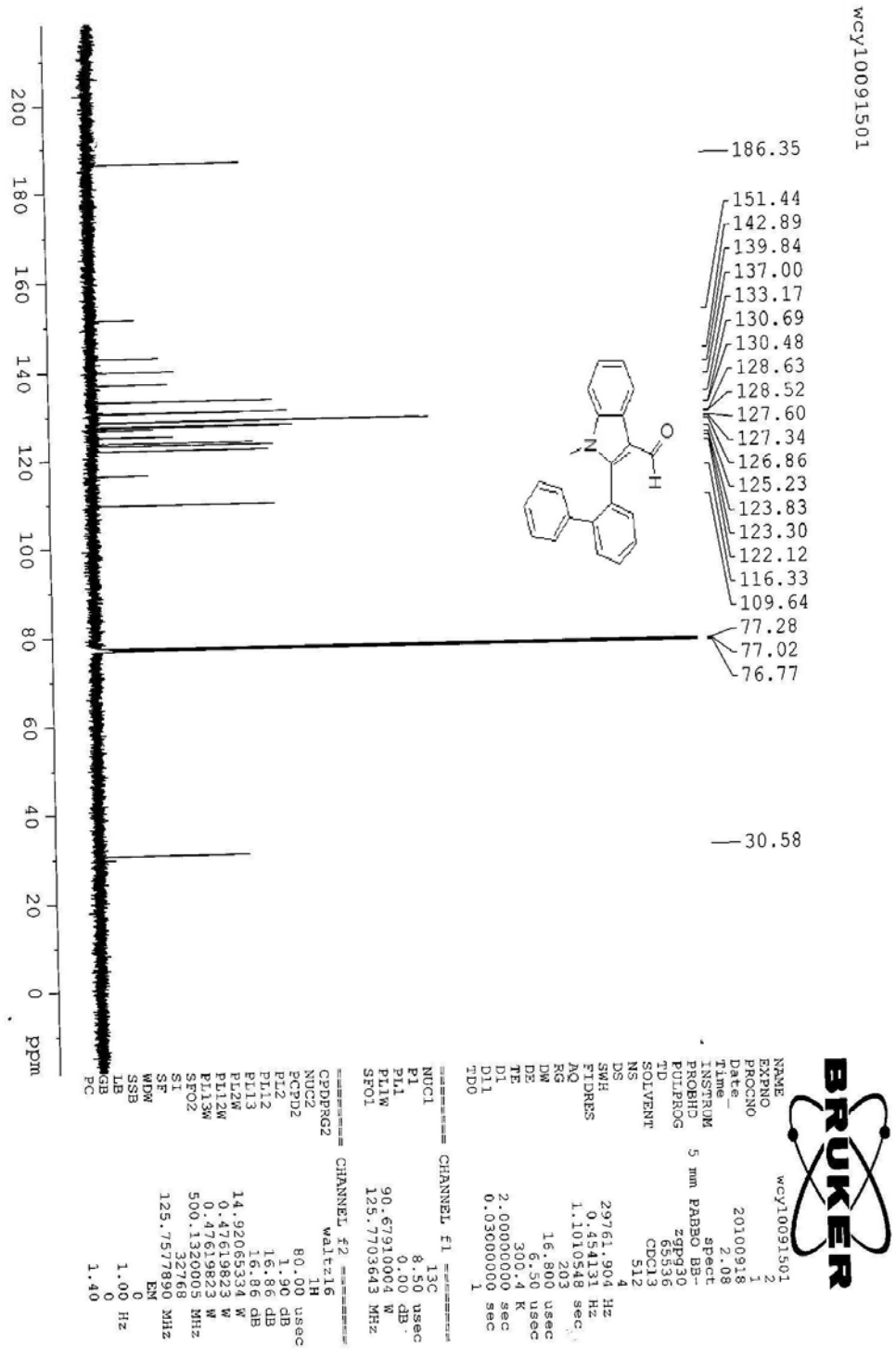
(*E*/*Z*)-Ethyl 3-(1-methyl-2-phenyl-1*H*-indol-3-yl)acrylate (7)



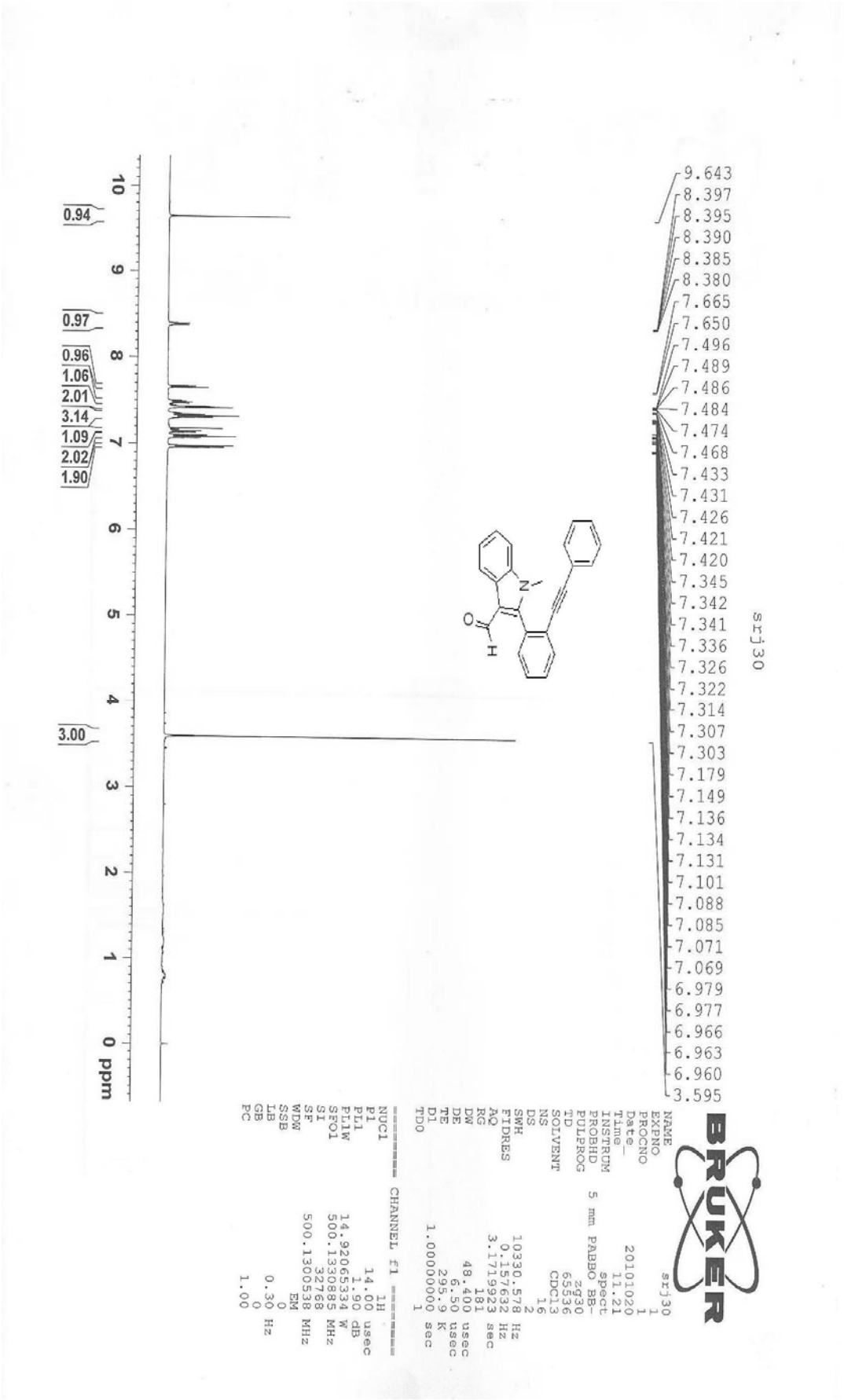
2-(Biphenyl-2-yl)-1-methyl-1*H*-indole-3-carbaldehyde (8)



2-(Biphenyl-2-yl)-1-methyl-1*H*-indole-3-carbaldehyde (8)



1-Methyl-2-(2-(phenylethynyl)phenyl)-1*H*-indole-3-carbaldehyde (9)



1-Methyl-2-(2-(phenylethynyl)phenyl)-1*H*-indole-3-carbaldehyde (9)