Supporting Information

Synthesis of 3,3-Disubstituted Oxindoles by Palladium-Catalyzed Tandem Reaction of 2-(Alkynyl)aryl Isocyanates with Benzylic Alcohols

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General Methods. All reactions were carried out with standard Schlenk techniques under an argon atmosphere. Infrared spectra were recorded on a Shimadzu FTIR-8100 spectrometer or a Shimadzu FTIR-8400 spectrophotometer. ^{1}H and ^{13}C NMR spectra were recorded on a Varian Gemini 2000 (^{1}H at 300.07 MHz and ^{13}C at 75.46 MHz) spectrometer or a Varian Mercury-vx400 (^{1}H at 400.44 MHz and ^{13}C at 100.69 MHz) spectrometer. NMR data were obtained in $CDCl_3$. Proton chemical shifts were referenced to the residual proton signal of the solvent at 7.26 ppm ($CHCl_3$). Carbon chemical shifts were referenced to the carbon signal of the solvent at 77.0 ppm ($CDCl_3$). High-resolution mass spectra were recorded on a JEOL JMS-SX102A spectrometer. Optical rotations were measured on a JASCO P-1020 polarimeter with a sodium lamp. HPLC analysis was performed by a Waters alliance 2695 system. GC analysis was carried out using a Shimadzu GC-2010 gas chromatograph. Gel permeation chromatography (GPC) was carried out with a Japan Analytical Industry LC-908. Flash column chromatography was performed with silica gel 60N (Kanto). Preparative thin-layer chromatography (PTLC) was performed on silica gel plates with PF254 indicator (Merck).

Materials. THF, 1,4-dioxane, toluene, and DME were distilled from sodium/benzophenone ketyl. All benzylic or allylic alcohols **2** and **5** were purchased, and purified by distillation, recrystallization or flash column chromatography prior to use. CpPd(π-allyl) was prepared according to the literature method.[1] 2-(Alkynyl)anilines were prepared by Sonogashira reaction of the corresponding 2-iodoaniline derivatives with alkyne.[2] 2-(Alkynyl)aryl isocyanates were synthesized from the corresponding 2-(alkynyl)aniline according to the reported procedure.[3] The analytical data of compounds **1a**,[4] **1b**,[4] **1c**,[5] and **1d**[4] have been already reported. **3aa** and **3dc** were synthesized according to the reported procedure.[6]

Typical procedure for Pd(0)-Catalyzed Cyclization/[1,3] Rearrangement Reaction of 1a with Benzyl Alcohol (2a) (Table 1, entry 6). To an oven-dried flask equipped with a stirrer bar was added CpPd(π-allyl) (2.1 mg, 10 μmol, 5 mol % Pd) and dppf (5.5 mg, 10 μmol, 5 mol %). The flask was sealed with a rubber septum, evacuated and refilled with argon three times. Then, a solution of benzyl alcohol **2a** (61.8 μL, 0.6 mmol, 3.0 equiv) and substrate **1a** (39.8 mg, 0.20 mmol, 1.0 equiv) in dry toluene (2.0 mL) was added *via* syringe. After being heated at 80 °C for 12 h, the reaction mixture was cooled to room temperature. The resulting mixture was passed through a pad of Florisil® and eluted with ethyl acetate. The filtrate was concentrated under reduced pressure. The residue was purified by gel permeation chromatography (GPC, $CHCl_3$) to give product **4aa** (42.4 mg, 0.138 mmol, 69%).

4aa: Purified by GPC ($CHCl_3$): IR (KBr): 3250, 1717, 1678, 1474, 1339 cm^{-1}; ^{1}H NMR (300 MHz): δ = 0.78 (t, *J* = 7.2 Hz, 3H), 1.06–1.23 (m, 2H), 1.38–1.55 (m, 2H), 2.18 (ddd, *J* = 17.7, 8.1, 6.9 Hz, 1H), 2.50 (ddd, *J* = 17.7, 7.8, 6.3 Hz, 1H), 3.44 (d, *J* = 13.8 Hz, 1H), 3.52 (d, *J* = 13.2 Hz, 1H), 6.70 (d, *J* = 7.8 Hz, 1H), 6.83–6.88 (m, 2H), 6.98–7.11 (m, 4H), 7.17–7.25 (m, 2H), 7.46 (br s, 1H); ^{13}C NMR (75 MHz): δ = 13.7, 21.9, 25.4, 38.8, 38.9, 68.4, 110.0, 122.8, 124.5, 126.5, 127.5, 127.6, 129.1, 129.8, 135.0, 141.4, 176.9, 202.7; HRMS (EI^+): Calcd for $C_{20}H_{21}NO_2$, M^+ 307.1572. Found m/z 307.1569.

4ab: Purified by GPC ($CHCl_3$): IR (KBr): 3200, 1717, 1698, 1472, 1339 cm^{-1}; ^{1}H NMR (400 MHz): δ = 0.78 (t, *J* = 7.2 Hz, 3H), 1.06–1.24 (m, 2H), 1.42–1.59 (m, 2H), 2.11–2.21 (m, 1H), 2.43–2.54 (m, 1H), 4.00 (d, *J* = 14.4 Hz, 1H), 4.05 (d, *J* = 14.4 Hz, 1H), 6.61 (d, *J* = 8.0 Hz, 1H), 6.93 (td, *J* = 7.6, 0.8 Hz, 1H), 7.04 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.08–7.14 (m, 2H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.30–7.38 (m, 2H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.65–7.70 (m, 1H), 7.76 (br s, 1H), 8.06 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (75 MHz): δ = 13.6, 21.8, 25.4, 33.7, 38.7, 68.2, 110.2, 122.5, 124.3, 124.6, 124.8, 125.06, 125.09, 127.3, 127.5, 127.8, 128.1, 129.0, 131.7, 132.3, 133.4, 141.5, 177.4, 202.9; HRMS (EI^+): Calcd for $C_{24}H_{23}NO_2$, M^+ 357.1729. Found m/z 357.1726.

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4ac: Purified by GPC ($CHCl_3$): IR (KBr): 3310, 1717, 1684, 1472, 1389 cm^{-1}; ^1H NMR (400 MHz): δ = 0.78 (t, *J* = 7.2 Hz, 3H), 1.07–1.22 (m, 2H), 1.39–1.57 (m, 2H), 2.18 (s, 3H), 2.18 (ddd, *J* = 17.6, 8.0, 6.4 Hz, 1H), 2.51 (ddd, *J* = 18.0, 8.4, 6.4 Hz, 1H), 3.40 (d, *J* = 13.2 Hz, 1H), 3.47 (d, *J* = 14.0 Hz, 1H), 6.69–6.76 (m, 3H), 6.82 (d, *J* = 8.0 Hz, 2H), 7.07 (td, *J* = 7.6, 0.8, 1H), 7.18–7.25 (m, 2H), 7.36 (br s, 1H); ^{13}C NMR (100 MHz): δ = 13.7, 20.9, 21.9, 25.4, 38.4, 38.9, 68.4, 110.1, 122.8, 124.5, 127.7, 128.4, 129.1, 129.7, 131.9, 136.0, 141.5, 177.0, 202.9; HRMS (EI^+): Calcd for $C_{21}H_{23}NO_2$, M^+ 321.1729. Found m/z 321.1727.

4ad: Purified by GPC ($CHCl_3$): IR (KBr): 3240, 1717, 1678, 1472, 1340 cm^{-1}; ^1H NMR (300 MHz): δ = 0.77 (t, *J* = 7.5 Hz, 3H), 1.06–1.20 (m, 2H), 1.36–1.57 (m, 2H), 2.09 (s, 3H), 2.17 (ddd, *J* = 17.7, 7.8, 6.6 Hz, 1H), 2.48 (ddd, *J* = 17.4, 7.8, 6.3 Hz, 1H), 3.39 (d, *J* = 13.2 Hz, 1H), 3.48 (d, *J* = 13.5 Hz, 1H), 6.60–6.68 (m, 2H), 6.74 (d, *J* = 8.1 Hz, 1H), 6.82–6.90 (m, 2H), 7.04–7.11 (m, 1H), 7.18–7.25 (m, 2H), 8.06 (br s, 1H); ^{13}C NMR (100 MHz): δ = 13.7, 21.1, 21.8, 25.4, 38.7, 38.8, 68.4, 110.1, 122.7, 124.5, 126.8, 127.3, 127.5, 127.6, 129.1, 130.7, 134.9, 137.1, 141.5, 177.1, 202.9; HRMS (EI^+): Calcd for $C_{21}H_{23}NO_2$, M^+ 321.1729. Found m/z 321.1730.

4ae: Purified by GPC ($CHCl_3$): IR (KBr): 3250, 1717, 1678, 1472, 1339 cm^{-1}; ^1H NMR (300 MHz): δ = 0.76 (t, *J* = 7.2 Hz, 3H), 1.06–1.10 (m, 2H), 1.39–1.57 (m, 2H), 2.08–2.22 (m, 1H), 2.13 (s, 3H), 2.38–2.49 (m, 1H), 3.51 (d, *J* = 14.1 Hz, 1H), 3.62 (d, *J* = 14.4 Hz, 1H), 6.77–6.85 (m, 3H), 6.92–6.97 (m, 2H), 6.99–7.10 (m, 2H), 7.24 (td, *J* = 7.2, 1.8 Hz, 1H), 8.73 (br s, 1H); ^{13}C NMR (75 MHz): δ =13.7, 20.0, 21.9, 25.5, 34.5, 38.8, 68.0, 110.0, 122.7, 124.8, 125.2, 126.6, 127.8, 129.2, 129.8, 130.2, 133.8, 137.2, 141.5, 177.1, 202.9; HRMS (EI^+): Calcd for $C_{21}H_{23}NO_2$, M^+ 321.1729. Found m/z 321.1729.

4af: Purified by GPC ($CHCl_3$): IR (KBr): 3247, 1711, 1676, 1514, 1472, 1250 cm^{-1}; ^1H NMR (300 MHz): δ = 0.78 (t, *J* = 7.2 Hz, 3H), 1.08–1.22 (m, 2H), 1.41–1.56 (m, 2H), 2.18 (ddd, *J* = 17.7, 8.1, 6.9 Hz, 1H), 2.51 (ddd, *J* = 17.7, 7.8, 6.3 Hz, 1H), 3.38 (d, *J* = 13.5 Hz, 1H), 3.45 (d, *J* = 13.2 Hz, 1H), 3.67 (s, 3H), 6.52–6.58 (m, 2H), 6.70 (d, *J* = 7.8 Hz, 1H), 6.73–6.79 (m, 2H), 7.07 (td, *J* = 7.8, 1.2 Hz, 1H), 7.17–7.22 (m, 2H), 7.35 (br s, 1H); ^{13}C NMR (100 MHz): δ = 13.7, 21.8, 25.3, 38.0, 38.9, 54.9, 68.5, 110.1, 113.0, 122.8, 124.5, 126.9, 127.7, 129.1, 130.8, 141.5, 158.2, 177.1, 203.0; HRMS (EI^+): Calcd for $C_{21}H_{23}NO_3$, M^+ 337.1678. Found m/z 337.1682.

4ag: Purified by GPC ($CHCl_3$): IR (KBr): 3380, 3200, 1719, 1682, 1522, 1347 cm^{-1}; ^1H NMR (300 MHz): δ = 0.77 (t, *J* = 7.2 Hz, 3H), 1.04–1.23 (m, 2H), 1.39–1.57 (m, 2H), 2.09–2.22 (m, 1H), 2.46 (ddd, *J* = 17.7, 7.5, 6.3 Hz, 1H), 3.54 (d, *J* = 13.5 Hz, 1H), 3.59 (d, *J* = 13.5 Hz, 1H), 6.75 (d, *J* = 8.4 Hz, 1H), 7.00–7.06 (m, 2H), 7.11 (td, J =7.5, 1.2 Hz, 1H), 7.21–7.29 (m, 2H), 7.73 (br s, 1H), 7.85–7.91 (m, 2H); ^{13}C NMR (75 MHz): δ = 13.7, 21.9, 25.4, 38.4, 38.8, 67.8, 110.2, 122.9, 123.3, 124.4, 126.6, 129.7, 130.8, 141.0, 143.1, 146.9, 175.4, 201.9; HRMS (EI^+): Calcd for $C_{20}H_{20}N_2O_4$, M^+ 352.1423. Found m/z 352.1426.

4ah: Purified by flash column chromatography (CH_2Cl_2/acetone = 1/1): IR (KBr): 1723, 1707, 1617, 1472, 1327 cm^{-1}; ^1H NMR (400 MHz): δ = 0.77 (t, *J* = 7.6 Hz, 3H), 1.06–1.22 (m, 2H), 1.38–1.57 (m, 2H), 2.12–2.23 (m, 1H), 2.48 (ddd, *J* = 17.6, 7.6, 6.4 Hz, 1H), 3.45 (d, *J* = 14.0 Hz, 1H), 3.50 (d, *J* = 13.6 Hz, 1H), 6.72 (d, *J* = 7.2 Hz, 1H), 6.96 (dd, *J* = 7.6, 4.8 Hz, 1H), 7.08 (t, *J* =7.6 Hz, 1H), 7.18–7.25 (m, 3H), 8.11 (s, 1H), 8.29 (d, *J* = 4.0 Hz, 1H), 8.42 (br s, 1H); ^{13}C NMR (100 MHz): δ = 13.7, 21.9, 25.4, 35.9, 38.8, 67.9, 110.3, 122.7, 123.0, 124.3, 126.8, 129.5, 131.0, 137.5, 141.7, 147.7, 150.5, 176.2, 202.5; HRMS (EI^+): Calcd for $C_{19}H_{20}N_2O_2$, M^+ 308.1525. Found m/z 308.1526.

4bd: Purified by GPC ($CHCl_3$): IR (KBr): 3279, 1724, 1689, 1670, 1617, 1469 cm^{-1}; ^1H NMR (400 MHz): δ = 2.11 (s, 3H), 3.55 (d, *J* = 13.2 Hz, 1H), 3.63 (d, *J* = 13.2 Hz, 1H), 6.58–6.62 (m, 2H), 6.71 (d, *J* = 8.0 Hz, 1H), 6.86–6.93 (m, 2 H), 7.06 (td, *J* = 7.6, 0.8 Hz, 1H), 7.19–7.28 (m, 4H), 7.36–7.44 (m, 2H), 7.48–7.53 (m, 2H); ^{13}C NMR (100 MHz): δ = 21.1, 41.5, 66.3, 110.3, 123.0, 124.4, 127.1, 127.38, 127.40, 128.0, 128.4, 129.2, 129.3, 130.9, 132.7, 134.3, 136.5, 137.0, 140.9, 177.0, 194.7; HRMS (EI^+): Calcd for $C_{23}H_{19}NO_2$, M^+ 341.1416. Found m/z 341.1409.
$[\alpha]_D^{26.8}$ = +64.9 (c = 1.01, $CHCl_3$, 38% ee); HPLC (Daicel Chiralcel OD-H, hexane/*i*-PrOH = 90:10, flow rate = 0.6 mL/min, λ = 254 nm): t_1 = 13.0 min (major), t_2 = 15.9 min (minor).

4bf: Purified by GPC ($CHCl_3$): IR (KBr): 3150, 1707, 1678, 1512, 1472, 1248 cm^{-1}; ^1H NMR (400 MHz): δ = 3.54 (d, *J* = 13.2 Hz, 1H), 3.61 (d, *J* = 13.6 Hz, 1H), 3.66 (s, 3H), 6.52–6.57 (m, 2H), 6.69–6.74 (m, 3H), 7.05 (td, *J* = 8.0, 1.2 Hz, 1H), 7.19–7.25 (m, 4H), 7.38–7.43 (m, 1H), 7.48–7.51 (m, 2H), 7.71 (br s, 1H); ^{13}C NMR (100 MHz): δ = 40.8, 54.9, 66.4, 110.5, 113.0, 123.0, 124.2, 126.3, 127.9, 128.4, 129.1, 129.3, 131.1, 132.7, 136.4, 140.9, 158.3, 177.4, 194.8; HRMS (EI^+): Calcd for $C_{23}H_{19}NO_3$, M^+ 357.1365. Found m/z 357.1369.

4ca: Purified by reprecipitation from CH_2Cl_2/hexane: IR (KBr): 3119, 1706, 1668, 1614, 1471, 1237 cm^{-1}; ^1H NMR (400 MHz): δ = 3.59 (d, *J* = 13.2 Hz, 1H), 3.64 (d, *J* = 13.2 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 6.83 (d, *J* = 7.2 Hz, 2H), 7.02 (t, *J* = 7.2 Hz, 2H), 7.04–7.11 (m, 2H), 7.14 (dd, *J* = 4.8, 2.4 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 2H), 7.31 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.53 (br s, 1H), 7.57 (dd, *J* = 2.4, 0.8 Hz, 1H); ^{13}C NMR (100 MHz): δ = 40.9, 66.5, 110.0, 123.2, 124.8, 125.8, 126.7, 127.6, 127.7, 129.3, 129.4, 130.2, 132.2, 134.5, 139.5, 140.9, 176.0, 187.5; HRMS (EI^+): Calcd for $C_{20}H_{15}NO_2S$, M^+ 333.0823. Found m/z 333.0825.

Typical procedure for Pd(0)-Catalyzed Cyclization/[1,3] Rearrangement Reaction of 1a with Allyl Alcohol (5a) (Table 3, entry 1). To an oven-dried flask equipped with a stirrer bar was added CpPd(π-allyl) (2.1 mg, 10 μmol, 5 mol % Pd) and dppf (5.5 mg, 10 μmol, 5 mol %). The flask was sealed with a rubber septum, evacuated and refilled with argon three times. Then, a solution of allyl alcohol (**5a**, 136 μL, 2.0 mmol, 10 equiv) and substrate **1a** (39.8 mg, 0.20 mmol, 1.0 equiv) in dry toluene (2.0 mL) was added *via* syringe. After being heated at 40 °C for 10 min, the reaction mixture was cooled to room temperature. The resulting mixture was passed through a pad of Florisil® and eluted with ethyl acetate. The filtrate was concentrated under reduced pressure. The residue was purified by gel permeation chromatography (GPC, $CHCl_3$) to give product **6aa** (30.2 mg, 0.117 mmol, 59%).

6aa: Purified by GPC ($CHCl_3$): IR (KBr): 3280, 1717, 1698, 1663, 1472, 1399 cm^{-1}; ^1H NMR (400 MHz): δ = 0.76 (t, *J* = 7.2 Hz, 3H), 1.06–1.21 (m, 2H), 1.36–1.54 (m, 2H), 2.19 (ddd, *J* = 17.6, 8.0, 6.8 Hz, 1H), 2.47 (ddd, *J* = 17.6, 8.0, 6.4 Hz, 1H), 2.87 (dd, *J* = 14.0, 8.0 Hz, 1H), 2.98 (dd, *J* = 14.0, 6.8 Hz, 1H), 4.88–4.94 (m, 1H), 5.00–5.07 (m, 1H), 5.30–5.42 (m, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 7.07 (td, *J* = 7.6, 1.2 Hz, 1H), 7.14 (d, *J* = 7.6 Hz, 1H), 7.28 (td, *J* = 7.6, 1.2 Hz, 1H), 8.05 (br s, 1H); ^{13}C NMR (75 MHz): δ = 13.7, 21.9, 25.4, 37.5, 38.7, 66.9, 110.2, 119.4, 123.1, 124.2, 127.7, 129.1, 131.4, 141.5, 177.2, 202.6; HRMS (EI^+): Calcd for $C_{16}H_{19}NO_2$, M^+ 257.1416. Found m/z 257.1416.

6ab: Purified by GPC ($CHCl_3$): IR (KBr): 3210, 1717, 1674, 1619, 1472 cm^{-1}; ^1H NMR (400 MHz): δ = 0.75 (t, *J* = 7.2 Hz, 3H), 1.03–1.21 (m, 2H), 1.34 (s, 3H), 1.35–1.53 (m, 2H), 2.17 (ddd, *J* = 17.6, 8.0, 6.8 Hz, 1H), 2.46 (ddd, *J* = 17.6, 8.0, 6.0 Hz, 1H), 2.95 (d, *J* = 14.4 Hz, 1H), 3.00 (d, *J* = 14.0 Hz, 1H), 4.56–4.61 (m, 2H), 6.96 (d, *J* = 8.0 Hz, 1H), 7.06 (td, *J* = 7.6, 0.8 Hz, 1H), 7.11–7.16 (m, 1H), 7.28 (td, *J* = 7.6, 1.6 Hz, 1H), 8.88 (br s, 1H); ^{13}C NMR (75 MHz): δ = 13.7, 21.9, 23.7, 25.4, 38.3, 40.2, 67.2, 110.3, 115.0, 122.9, 124.5, 128.0, 129.1, 140.1, 141.6, 177.8, 202.5; HRMS (EI^+): Calcd for $C_{17}H_{21}NO_2$, M^+ 271.1572. Found m/z 271.1577.

6ac: Purified by GPC ($CHCl_3$): IR (KBr): 3210, 1717, 1676, 1472, 1339 cm^{-1}; ^1H NMR (300 MHz): δ = 0.76 (t, *J* = 7.2 Hz, 3H), 1.05–1.20 (m, 2H), 1.34–1.56 (m, 2H), 2.11–2.25 (m, 1H), 2.45 (ddd, *J* = 17.7, 8.1, 6.3 Hz, 1H), 2.92–3.03 (m, 1H), 3.14 (ddd, *J* = 13.5, 6.3, 1.2 Hz, 1H), 5.70–5.82 (m, 1H), 6.36 (d, *J* = 15.6 Hz, 1H), 6.92 (d, *J* = 7.5 Hz, 1H), 7.05-7.23 (m, 7H), 7.28 (td, *J* = 7.8, 1.2 Hz, 1H), 8.32 (br s, 1H); ^{13}C NMR (75 MHz): δ = 13.7, 21.9, 25.4, 36.8, 38.7, 66.9, 110.2, 122.9, 123.1, 124.3, 126.1, 127.2, 127.7, 128.3, 129.2, 134.3, 136.9, 141.3, 176.9, 202.6; HRMS (EI^+): Calcd for $C_{22}H_{23}NO_2$, M^+ 333.1729. Found m/z 333.1728.

6ad: Purified by GPC ($CHCl_3$): IR (KBr): 3263, 1717, 1692, 1,474 cm^{-1}; ^1H NMR (400 MHz): δ = 0.76 (t, *J* = 7.2 Hz, 3H), 1.04–1.22 (m, 2H), 1.36–1.55 (m, 2H), 1.50 (s, 3H), 1.51 (s, 3H), 2.20 (ddd, *J* = 17.6, 76, 6.4 Hz, 1H), 2.47 (ddd, *J* = 18.0, 8.0, 6.4 Hz, 1H), 2.84–2.90 (m, 1H), 2.90–2.96 (m, 1H), 4.67–4.74 (m, 1H), 6.94 (d, *J* = 8.0 Hz, 1H), 7.05 (td, *J* = 7.6, 1.2 Hz, 1H), 7.11–7.17 (m, 1H), 7.27 (td, *J* = 7.6, 1.2 Hz, 1H), 8.63 (br s, 1H); ^{13}C NMR (75 MHz): δ = 13.7, 18.0, 21.9, 25.4, 25.8, 32.0, 38.7, 67.0, 110.1, 116.6, 122.9, 124.1, 128.2, 128.9, 135.9, 141.5, 177.8, 203.1; HRMS (EI^+): Calcd for $C_{18}H_{23}NO_2$, M^+ 285.1729. Found m/z 285.1732.

6bd: Purified by GPC ($CHCl_3$): IR (KBr): 3276, 1723, 1686, 1667, 1468, 1233 cm^{-1}; ^1H NMR (400 MHz): δ = 1.46 (s, 3H), 1.52 (s, 3H), 3.00 (dd, *J* = 14.0, 8.4 Hz, 1H), 3.09 (dd, *J* = 14.0, 6.8 Hz, 1H), 4.78-4.85 (m, 1H), 6.94 (d, *J* = 7.6 Hz, 1H), 6.99 (t, *J* = 7.2 Hz, 1H), 7.09 (d, *J* = 6.8 Hz, 1H), 7.20–7.30 (m, 3H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.47–7.52 (m, 2H), 8.99 (br s, 1H); ^{13}C NMR (100 MHz): δ = 17.9, 25.9, 34.6, 65.1, 110.6, 116.3, 123.0, 124.0, 128.0, 128.1, 128.4, 129.0, 129.9, 132.7, 136.5, 141.0, 178.4, 194.8; HRMS (EI^+): Calcd for $C_{20}H_{19}NO_2$, M^+ 305.1416. Found m/z 305.1415.

6ae: Purified by GPC ($CHCl_3$): IR (KBr): 3290, 1717, 1655, 1472 cm^{-1}; ^1H NMR (300 MHz): δ = 0.67 (t, *J* = 7.5 Hz, 3H), 0.76 (t, *J* = 6.9 Hz, 3H), 1.06–1.21 (m, 4H), 1.24–1.57 (m, 2H), 1.70–1.80 (m, 2H), 2.20 (ddd, *J* = 18.0, 7.8, 6.9 Hz, 1H), 2.47 (ddd, *J* = 17.7, 7.5, 6.9 Hz, 1H), 2.80 (dd, *J* = 13.8, 7.8 Hz, 1H), 2.92 (dd, *J* = 13.8, 6.9 Hz, 1H), 4.80–5.02(m, 1H), 5.40 (dt, *J* = 15.0, 6.9 Hz, 1H), 6.92–6.97 (m, 1H), 7.06 (td, *J* = 7.8, 0.9 Hz, 1H), 7.12–7.17 (m, 1H), 7.27 (td, *J* = 7.5, 1.2 Hz, 1H), 8.67 (br s, 1H); ^{13}C NMR (100 MHz): δ = 13.3, 13.7, 21.9, 22.3, 25.4, 34.4, 36.5, 38.7, 67.2, 110.1, 122.5, 122.9, 124.3, 128.1, 128.9, 135.7, 141.5, 177.6, 203.0; HRMS (EI^+): Calcd for $C_{19}H_{25}NO_2$, M^+ 299.1885. Found m/z 299.1883.

6af: Purified by GPC ($CHCl_3$): IR (KBr): 3300, 1717, 1698, 1670, 1472, 1339 cm^{-1}; ^1H NMR (300 MHz): δ = 0.73 (t, *J* = 7.2 Hz, 1H), 0.76 (t, *J* = 7.2 Hz, 1H), 1.04-1.23 (m, 2H), 1.34-1.56 (m, 2H), 1.68-1.74 (m, 2H), 2.20 (ddd, *J* = 17.7, 7.5, 6.6 Hz, 1H), 2.46 (ddd, *J* = 17.7, 7.8, 6.6 Hz, 1H), 2.78 (dd, *J* = 13.5, 7.8 Hz, 1H), 2.92 (dd, *J* = 13.8, 6.9 Hz, 1H), 4.89-5.09 (m, 1H), 5.38-5.50 (m, 1H), 6.92-6.98 (m, 1H), 7.02-7.09 (m, 1H), 7.10-7.17 (m, 1H), 7.27 (td, *J* = 7.8, 1.5 Hz, 1H), 8.82 (br s, 1H); ^{13}C NMR: δ = 13.7, 21.9, 25.3, 25.4, 36.5, 38.8, 67.2, 110.0, 121.3, 122.9, 124.3, 128.1, 128.9, 137.5, 141.5, 177.4, 203.0; HRMS (EI^+): Calcd for $C_{18}H_{23}NO_2$, M^+ 285.1729. Found m/z 285.1728.

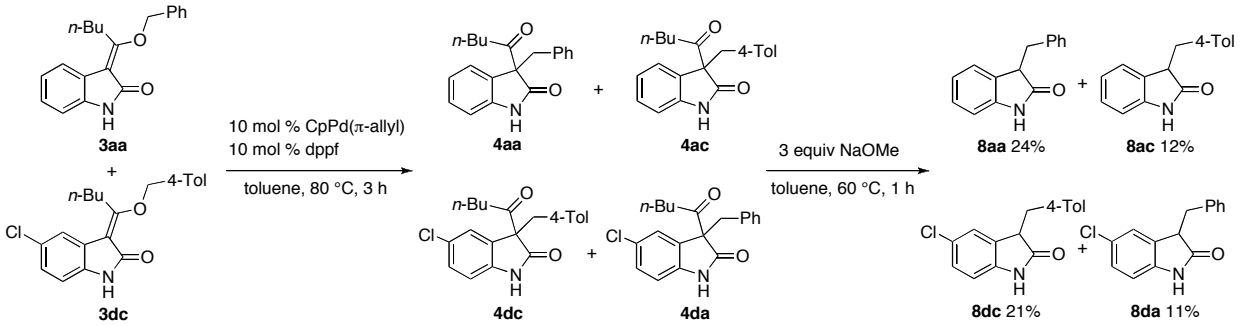
Typical procedure for Pd(0)-Catalyzed Cyclization/ [1,3] Rearrangement/Allylation Reaction of 1a with Allyl Alcohol (5a) (Table 4). To an oven-dried flask equipped with a stirrer bar was added CpPd(π-allyl) (2.1 mg, 10 μmol, 5 mol % Pd) and dppf (5.5 mg, 10 μmol, 5 mol %). The flask was sealed with a rubber septum, evacuated and refilled with argon three times. Then, a solution of allyl alcohol (**5a**, 272 μL, 4.0 mmol, 20 equiv) and substrate **1a** (39.8 mg, 0.20 mmol, 1.0 equiv) in dry toluene (2.0 mL) was added *via* syringe. After being heated at 40 °C for 12 h, the reaction mixture was cooled to room temperature. The resulting mixture was passed through a pad of Florisil® and eluted with ethyl acetate. The filtrate was concentrated under reduced pressure. The residue was purified by gel permeation chromatography (GPC, $CHCl_3$) to give product **7aa** (42.2 mg, 0.142 mmol, 71%).

7aa: Purified by GPC ($CHCl_3$): IR (neat): 1725, 1609, 1487, 1466, 1356 cm^{-1}; ^1H NMR (300 MHz): δ = 0.75 (t, *J* = 7.5 Hz, 3H), 1.02–1.22 (m, 2H), 1.32–1.53 (m, 2H), 2.09 (ddd, *J* = 17.7, 7.2, 6.9 Hz, 1H), 2.40 (ddd, *J* = 17.7, 7.8, 6.3 Hz, 1H), 2.82–2.92 (m, 1H), 2.94–3.03 (m, 1H), 4.30–4.48 (m, 2H), 4.84–4.92 (m, 1H), 4.96–5.04 (m, 1H), 5.20–5.37 (m, 3H), 5.75–5.89 (m, 1H), 6.87 (d, *J* = 7.8 Hz, 1H), 7.07 (td, *J* = 7.5, 1.2 Hz, 1H), 7.14–7.18 (m, 1H), 7.30 (td, *J* = 7.8, 1.2 Hz, 1H); ^{13}C NMR (100 MHz): δ = 13.6, 21.9, 25.3, 37.5, 38.6, 42.5, 66.1, 109.3, 117.9, 119.4, 123.0, 123.9, 127.0, 128.9, 131.0, 131.5, 143.4, 174.3, 202.8; HRMS (EI^+): Calcd for $C_{19}H_{23}NO_2$, M^+ 297.1729. Found m/z 297.1729.

7ab: Purified by GPC ($CHCl_3$): IR (neat): 1728, 1609, 1487, 1466, 1354 cm^{-1}; ^1H NMR (400 MHz): δ = 0.75 (t, *J* = 7.2 Hz, 3H), 1.03-1.21 (m, 2H), 1.30-1.33 (m, 3H), 1.35-1.52 (m, 2H), 1.74-1.77 (m, 3H), 2.08 (ddd, *J* = 17.6, 8.0, 6.4 Hz, 1H), 2.43 (ddd, *J* = 17.6, 8.0, 6.0 Hz, 1H), 2.97 (s, 2H), 4.24 (d, *J* =16.4 Hz, 1H), 4.34 (d, *J* = 16.0 Hz, 1H), 4.53-4.57 (m, 1H), 4.57-4.61 (m, 1H), 4.88-4.93 (m, 1H), 4.93-4.97 (m, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 7.06 (td, *J* = 7.6, 0.8 Hz, 1H), 7.15-7.19 (m, 1H), 7.28 (td, *J* = 8.0, 1.6 Hz, 1H); ^{13}C NMR (100 MHz): δ = 13.6, 20.0, 21.8, 24.0, 25.3, 38.4, 40.2, 46.2, 66.4, 109.5, 112.8, 115.3, 122.7, 124.2, 127.3, 129.0, 138.9, 140.0, 143.9, 174.7, 202.8; HRMS (EI^+): Calcd for $C_{21}H_{27}NO_2$, M^+ 325.2042. Found m/z 325.2043.

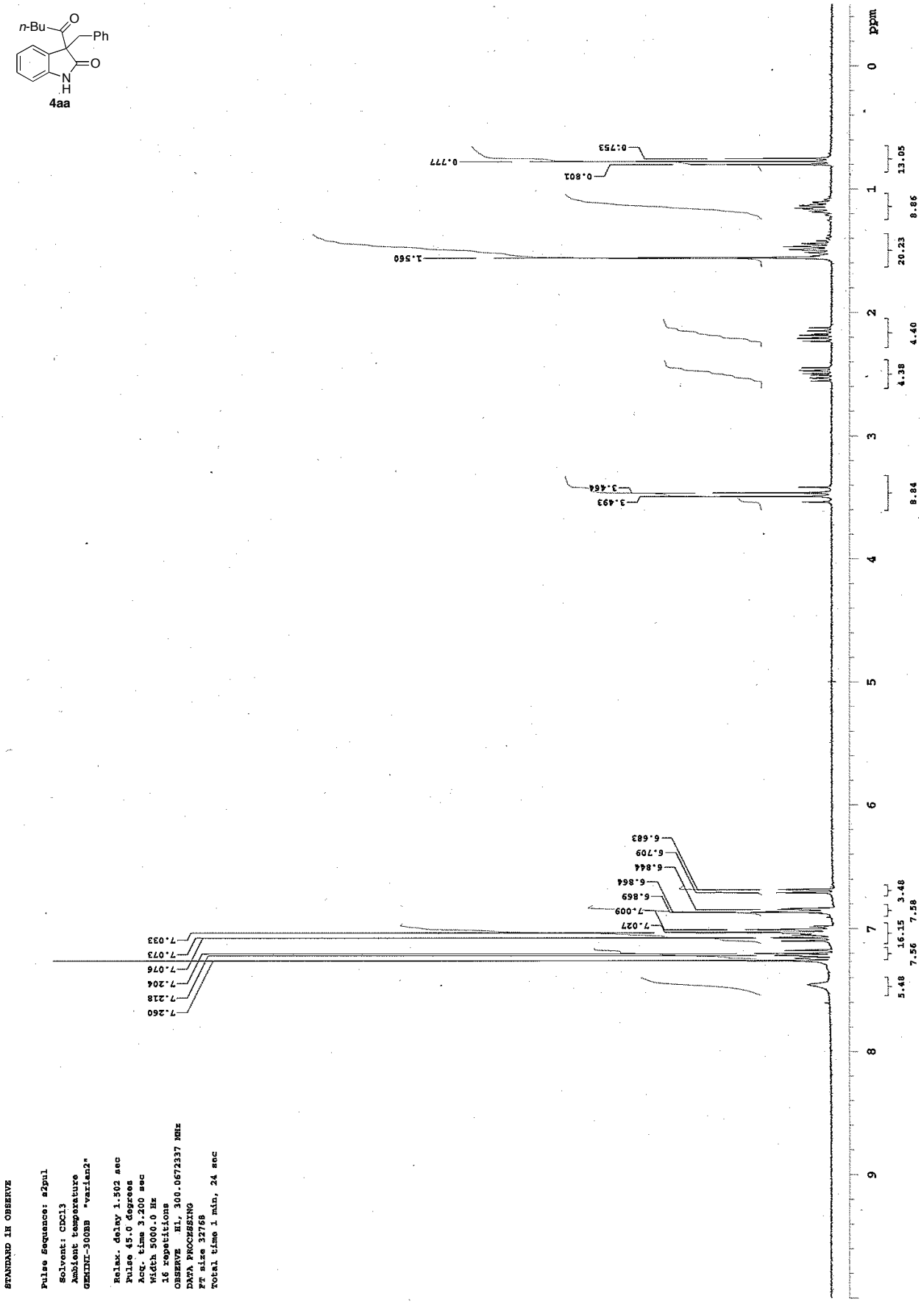
7ac: Purified by PTLC (hexane/ethyl acetate = 10:1): IR (neat): 1715, 1609, 1485, 1466, 1354 cm^{-1}; ^1H NMR (300 MHz): δ = 0.77 (t, *J* = 7.2 Hz, 3H), 1.07–1.22 (m, 2H), 1.38–1.56 (m, 2H), 2.14 (ddd, *J* = 17.7, 8.1, 7.2 Hz, 1H), 2.45 (ddd, *J* = 17.7, 7.8, 6.3 Hz, 1H), 3.04 (ddd, *J* = 13.8, 8.7, 0.9 Hz, 1H), 3.18 (ddd, *J* = 13.8, 6.3, 1.5 Hz, 1H), 4.34 (ddd, *J* = 15.9, 7.2, 1.5 Hz, 1H), 4.72 (ddd, *J* = 16.2, 5.4, 1.8 Hz, 1H), 5.69 (ddd, *J* = 15.3, 8.4, 6.3 Hz, 1H), 5.95 (ddd, *J* = 12.0, 6.9, 5.1 Hz, 1H), 6.38 (d, *J* = 15.9 Hz, 1H), 6.56 (d, *J* = 15.9 Hz, 1H), 6.91 (d, *J* = 7.5 Hz, 1H), 7.00–7.32 (m, 13H); ^{13}C NMR (75 MHz): δ = 13.7, 21.9, 25.3, 36.8, 38.7, 42.2, 66.4, 109.4, 122.3, 122.8, 123.0, 123.9, 126.0, 126.3, 127.0, 127.2, 127.7, 128.40, 128.45, 129.1, 133.5, 134.3, 135.7, 136.8, 143.3, 174.3, 202.8; HRMS (EI^+): Calcd for $C_{31}H_{31}NO_2$, M^+ 449.2355. Found m/z 449.2360.

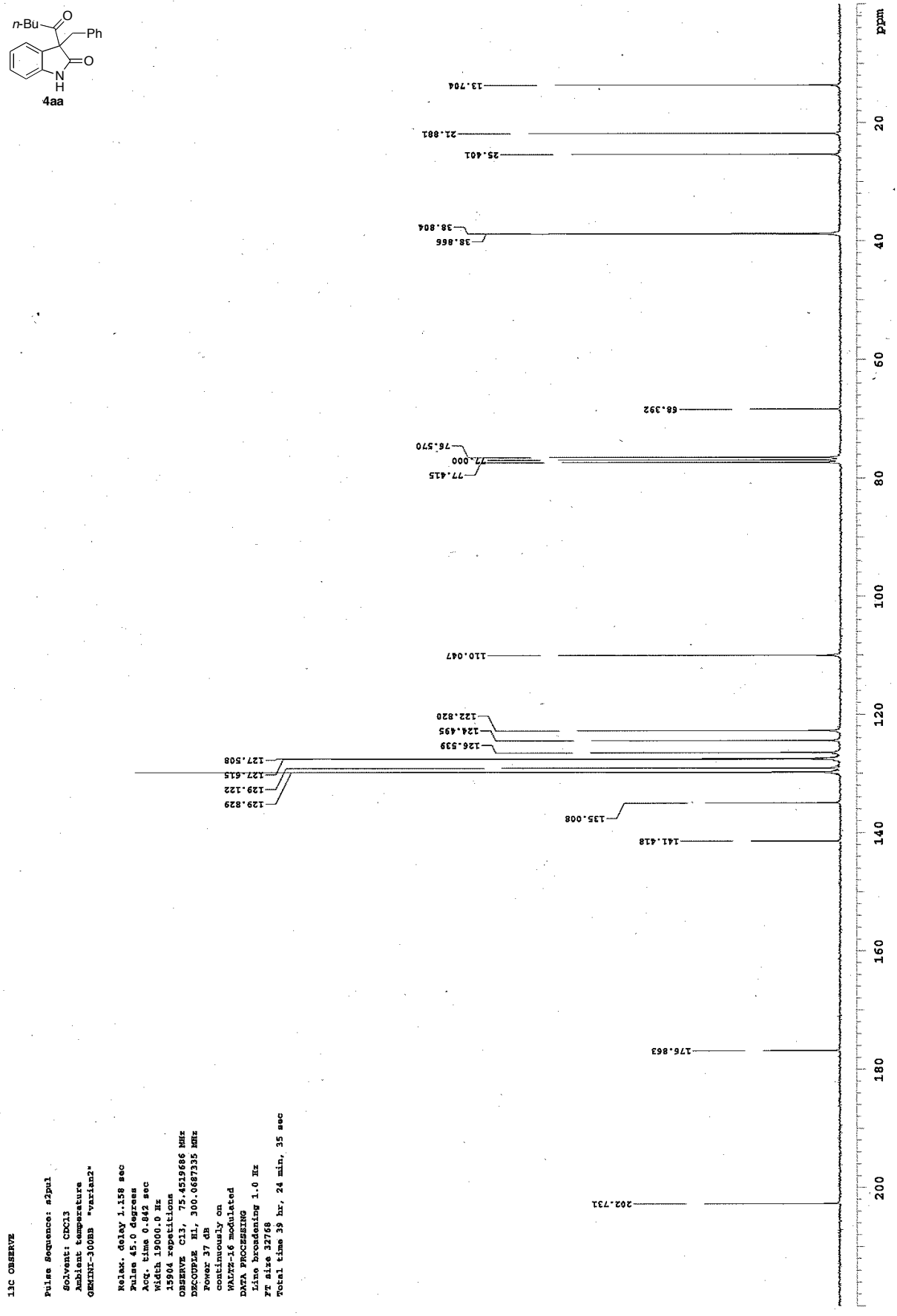
Cross-over Experiment on the Reaction with 3aa and 3dc.

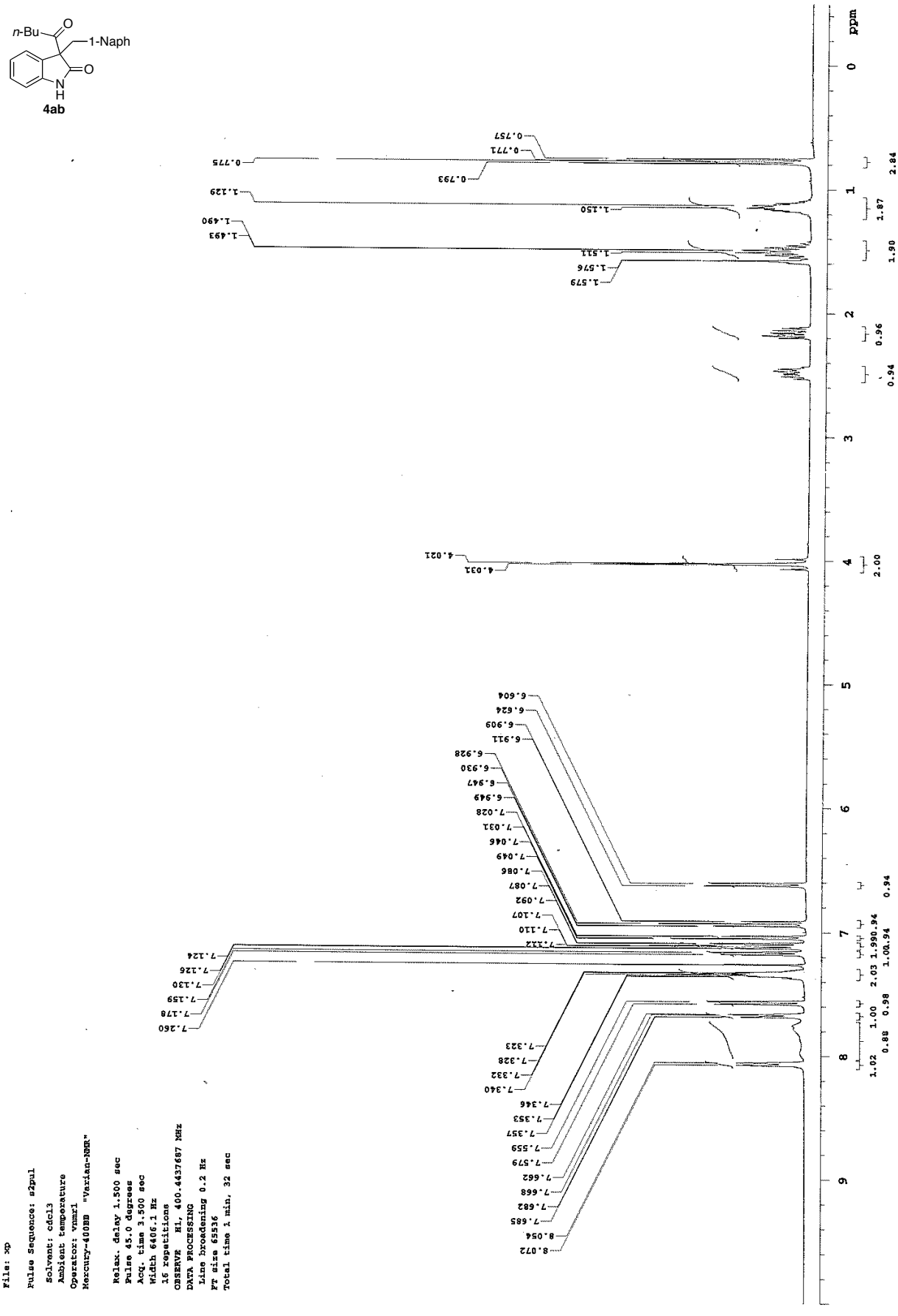


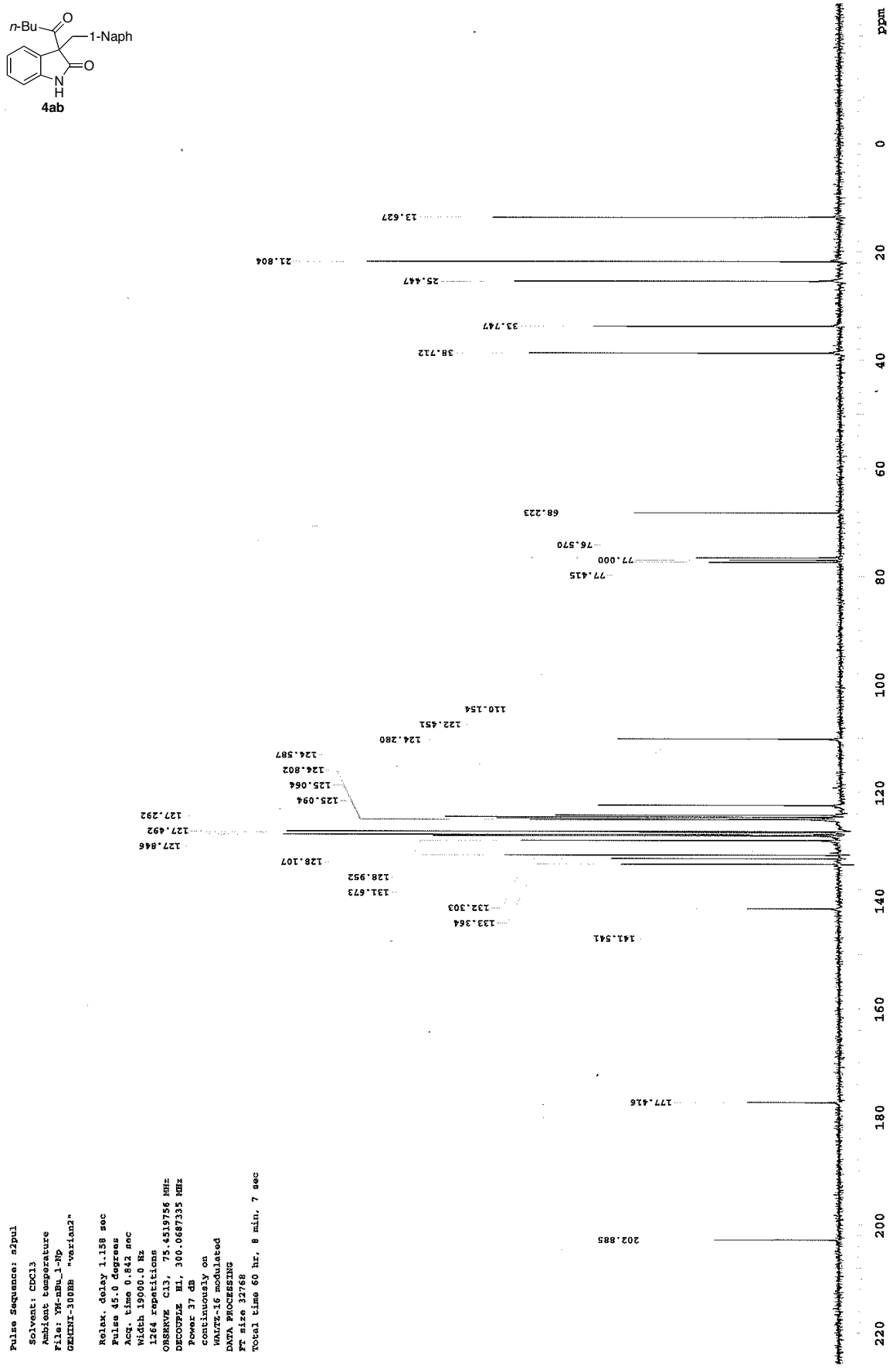
To an oven-dried flask equipped with a stirrer bar was added CpPd(π-allyl) (2.1 mg, 10 μmol, 10 mol % Pd), dppf (5.5 mg, 10 μmol, 10 mol %), **3aa** (30.7 mg, 0.10 mmol, 1.0 equiv), and **3dc** (35.6 mg, 0.10 mmol, 1.0 equiv). The flask was sealed with a rubber septum, evacuated and refilled with argon three times. Then, dry toluene (4.0 mL) was added *via* syringe. After being heated at 80 °C for 3 h, the reaction mixture was cooled to room temperature. The resulting mixture was passed through a pad of Florisil® and eluted with ethyl acetate. The filtrate was concentrated under reduced pressure to give a crude mixture of **4aa**, **4ac**, **4da** and **4dc**.

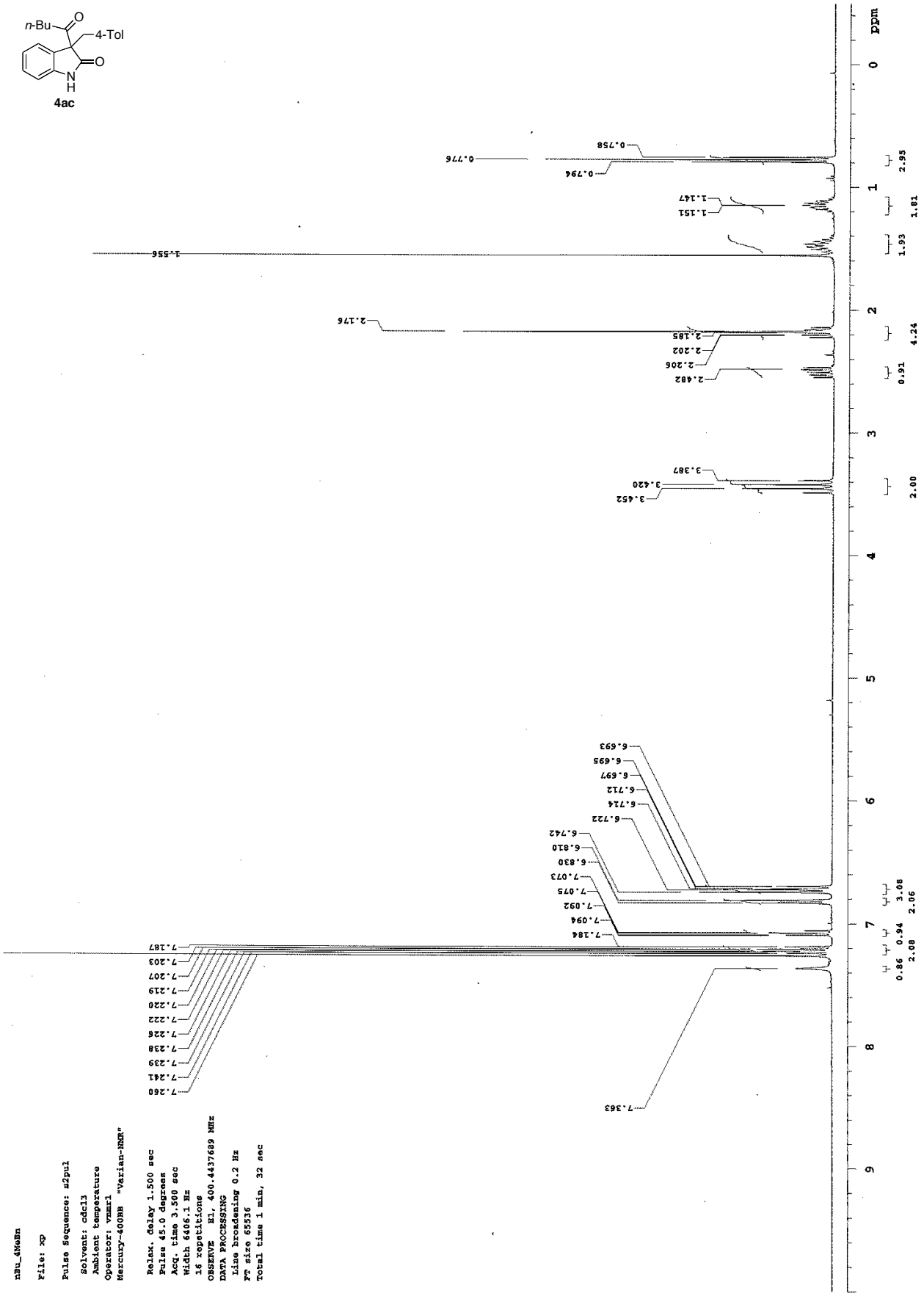
Without further purification, the mixture was treated with sodium methoxide (32.4 mg, 0.60 mmol, 6.0 equiv) in dry toluene (4.0 mL). After being stirred at 60 °C for 1 h, the reaction mixture was cooled to room temperature. The resulting mixture was quenched with addition of water. The aqueous layer was extracted with Et_2O. The combined organic extracts were dried over $MgSO_4$ and concentrated under reduced pressure to give hydrolytic products **8aa**, **8ac**, **8da** and **8dc**. The yield was determined by GC analysis using *n*-nonadecane as an internal standard (GC conditions: Agilent Technologies DB-1, 15 m × 0.32 mm, Injection 250 °C; detector temperature 290 °C; oven temperature: 80 °C for 5 min, increase by 20 °C/min to 280 °C, and keep the temperature for 5 min, R_t **8aa** 12.5 min, **8ac** 13.0 min, **8da** 13.5 min, **8dc** 14.0 min).

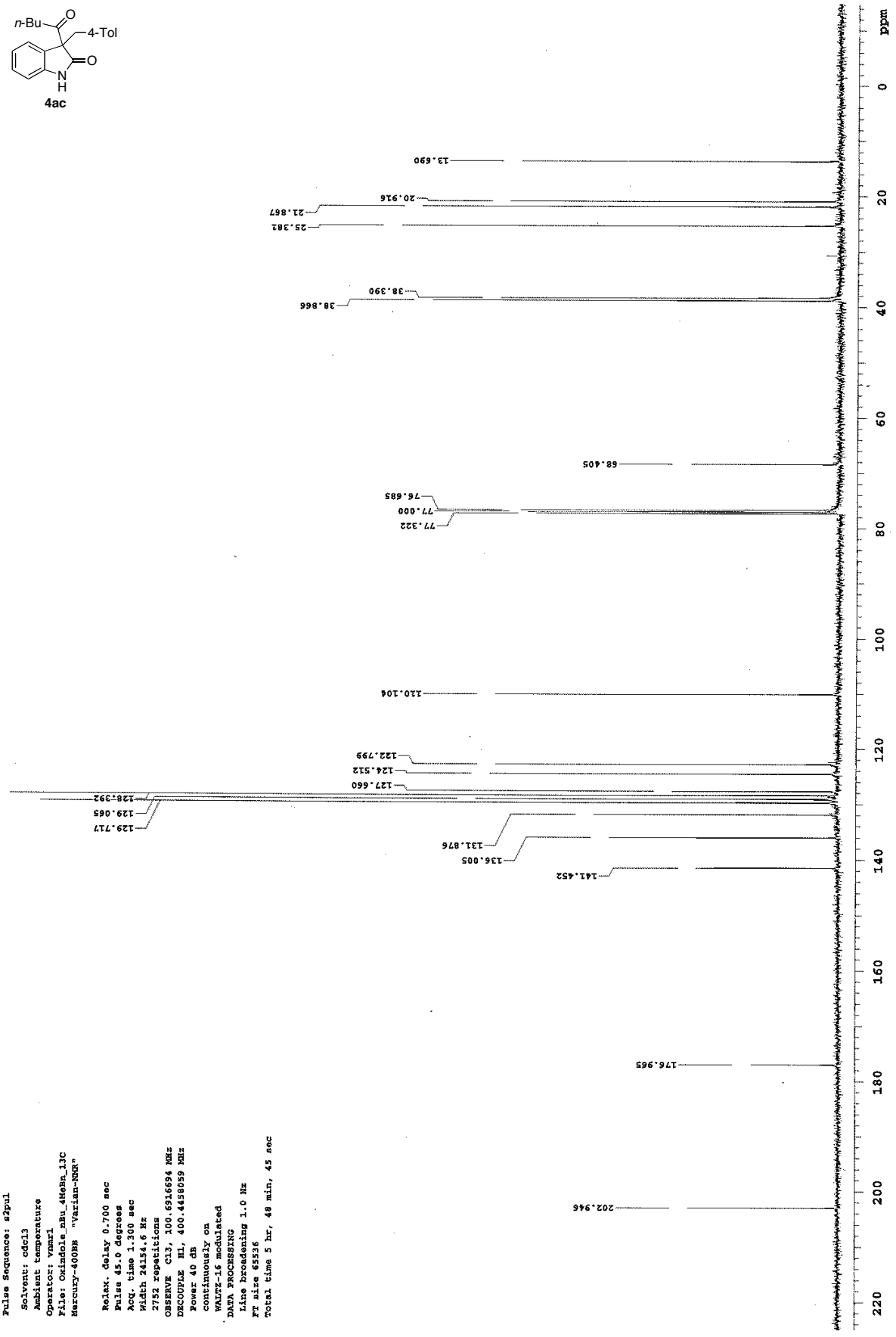

n-Bu
Ph
O
O
N
H
4aa
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.502 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 5000.0 Hz
16 repetitions
OBSERVE H1, 300.0672337 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 24 sec
7.260
7.218
7.204
7.076
7.073
7.033
7.027
7.009
6.869
6.864
6.844
6.709
6.683
3.493
3.464
1.560
0.802
0.777
0.753
ppm
0
1
2
3
4
5
6
7
8
9
5.48
16.15
3.48
7.56
7.58
8.84
4.38
4.40
20.23
8.86
13.05

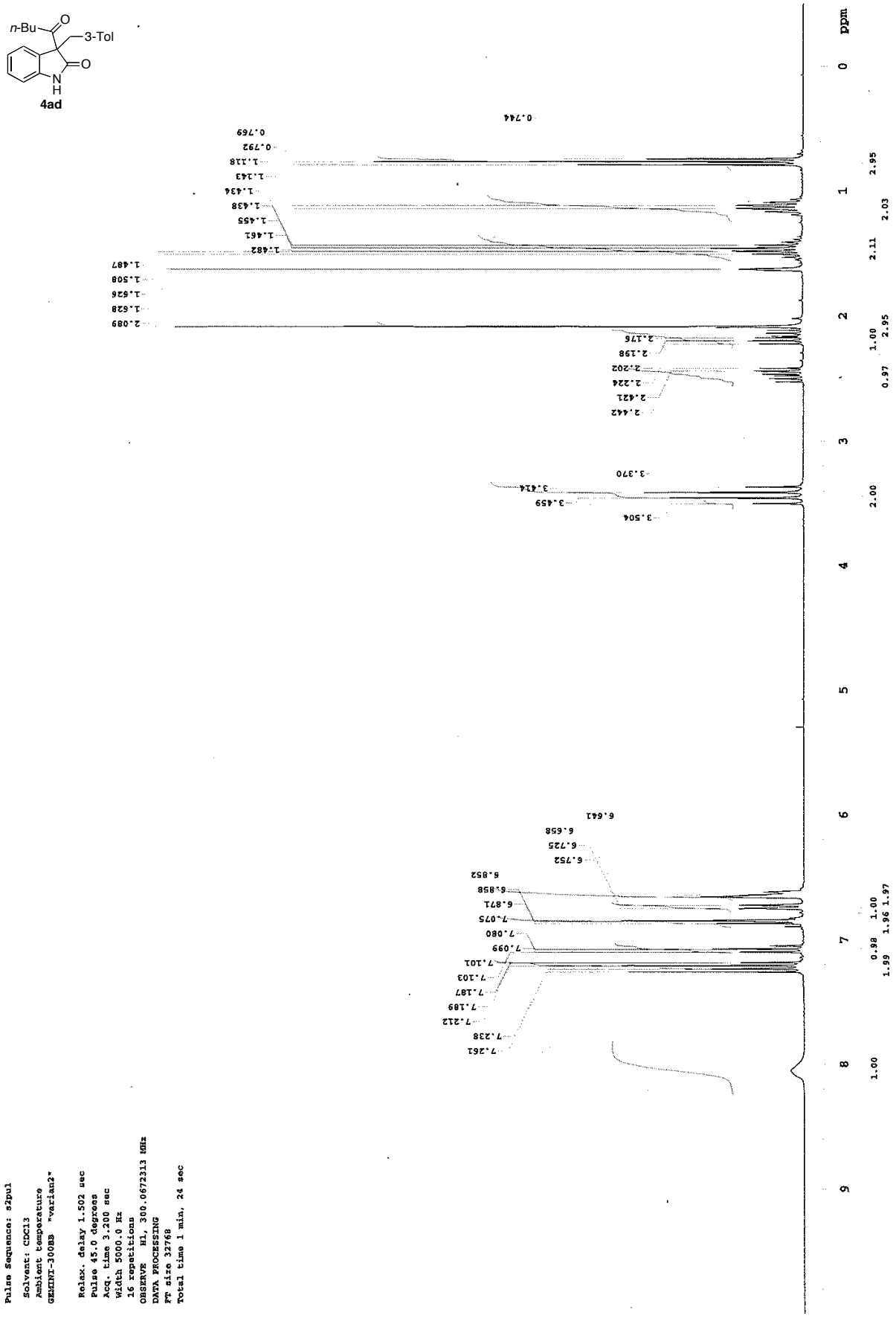

n-Bu
Ph
O
O
N
H
4aa
13.704
21.881
25.401
38.804
38.866
58.392
76.570
77.000
77.415
110.047
122.820
124.495
126.539
127.508
127.615
129.122
129.829
135.008
141.418
176.863
202.731
ppm
20
40
60
80
100
120
140
160
180
200
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.158 sec
Pulse 45.0 degrees
Acq. time 0.842 sec
Width 19000.0 Hz
15904 repetitions
OBSERVE C13, 75.4519686 MHz
DECOUPLE H1, 300.0687335 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 39 hr, 24 min, 35 sec

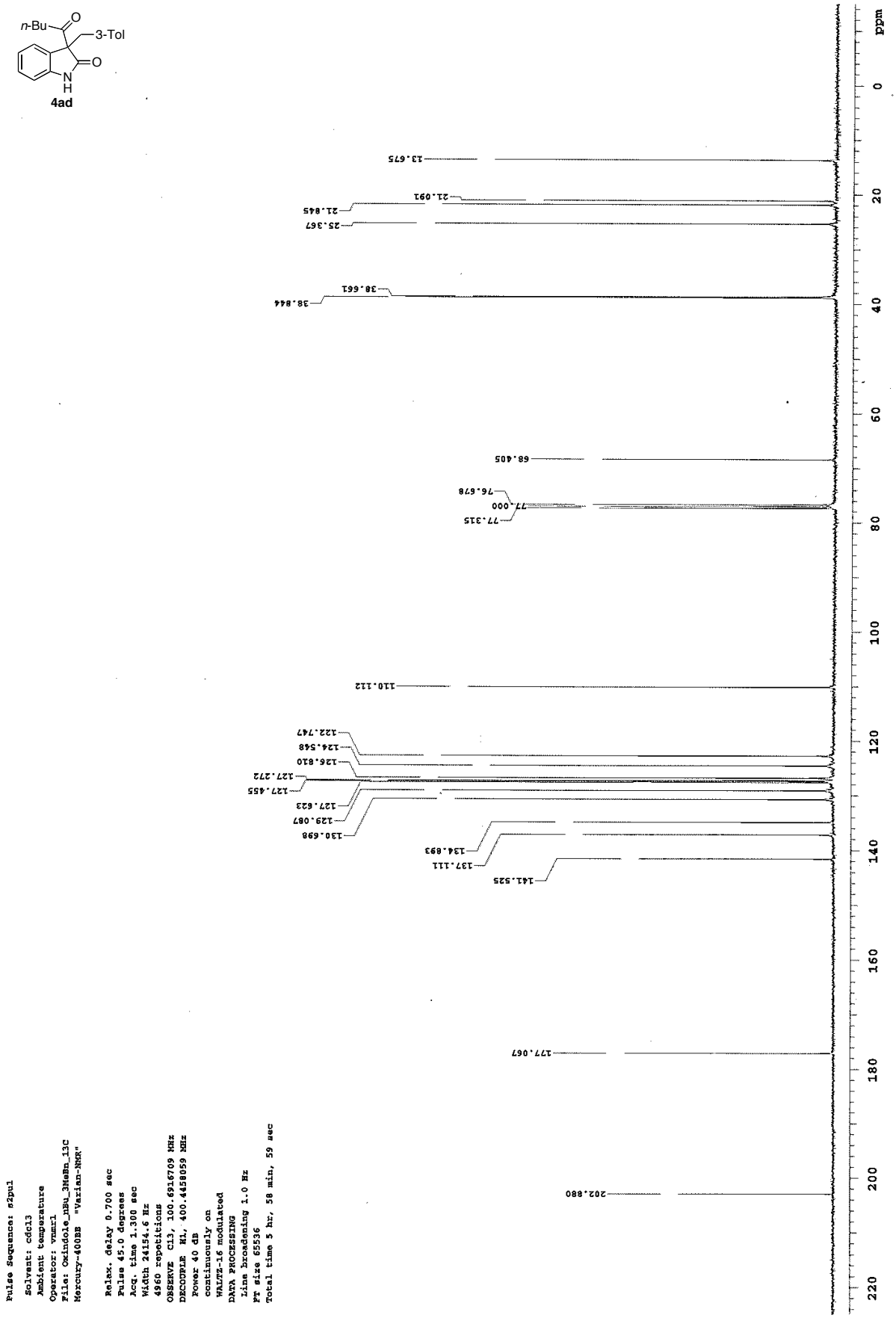

n-Bu
1-Naph
O
O
N
H
4ab
File: xp
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmrl
Mercury-400BB "Varian-NMR"
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437687 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec
ppm

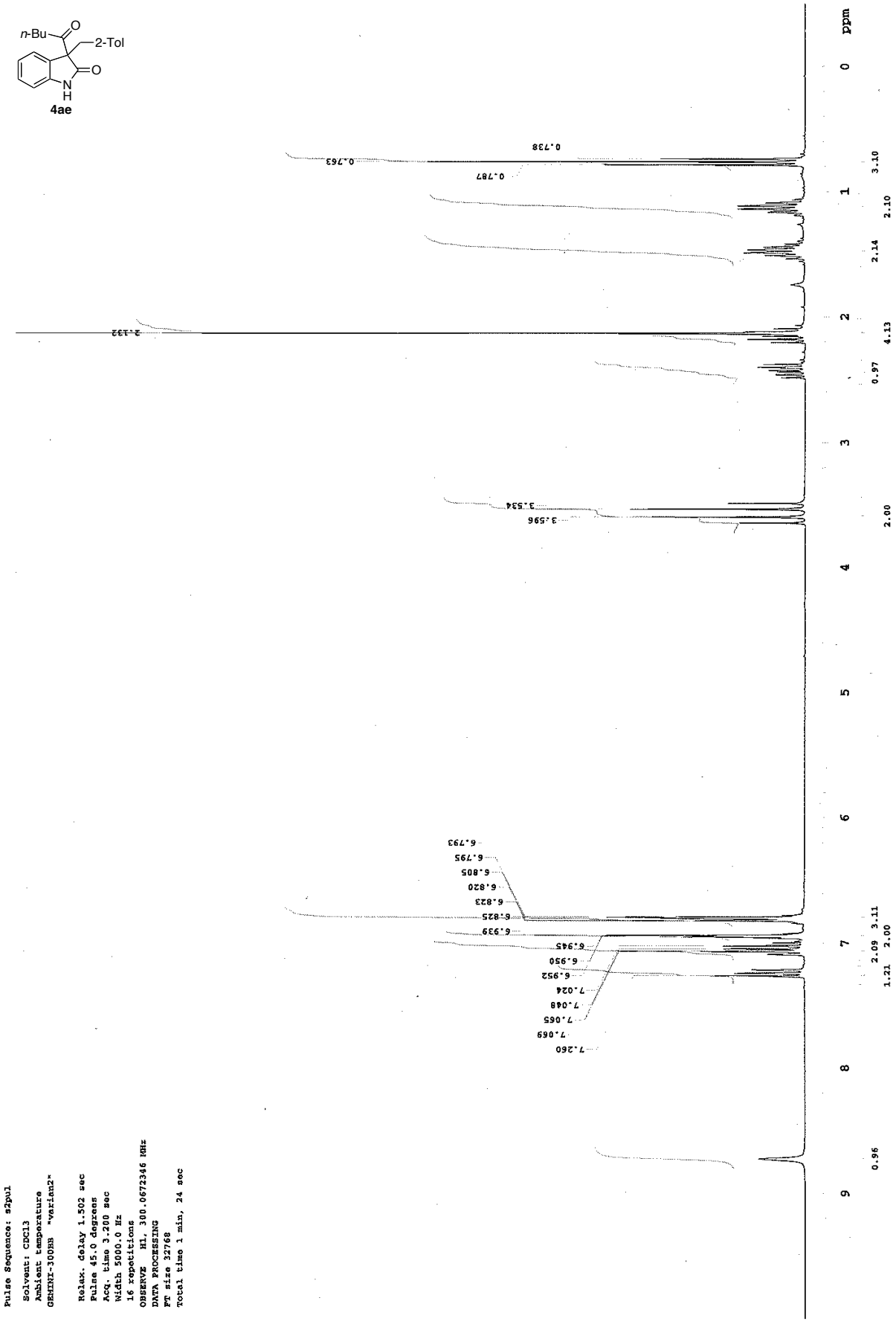

n-Bu
1-Naph
O
O
N
H
4ab
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: YM-nBu_1-Np
GEMINI-300BB "varian2"
Relax. delay 1.158 sec
Pulse 45.0 degrees
Acq. time 0.842 sec
Width 19000.0 Hz
1264 repetitions
OBSERVE C13, 75.4519756 MHz
DECOUPLE H1, 300.0687335 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
FT size 32768
Total time 60 hr, 8 min, 7 sec
13.627
21.804
25.447
33.747
38.712
68.223
76.570
77.000
77.415
110.154
122.451
124.280
124.587
124.802
125.064
125.094
127.292
127.492
127.846
128.107
128.952
131.673
132.303
133.364
141.541
177.416
202.885
ppm
0
20
40
60
80
100
120
140
160
180
200
220

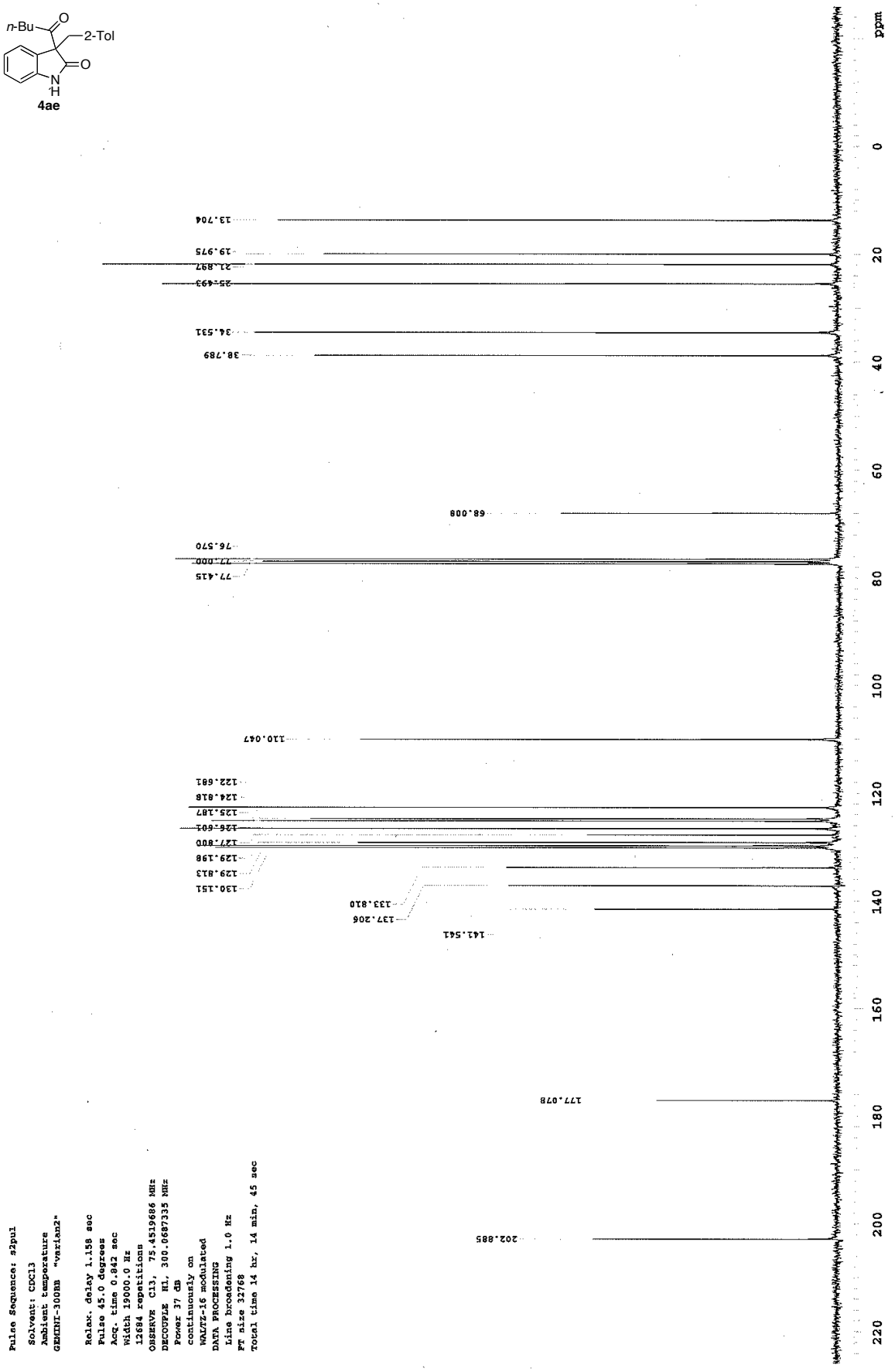

n-Bu
4-Tol
O
O
N
H
4ac
nBu_4MeBn
File: xp
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
Mercury-400BB "Varian-NMR"
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437689 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec
ppm

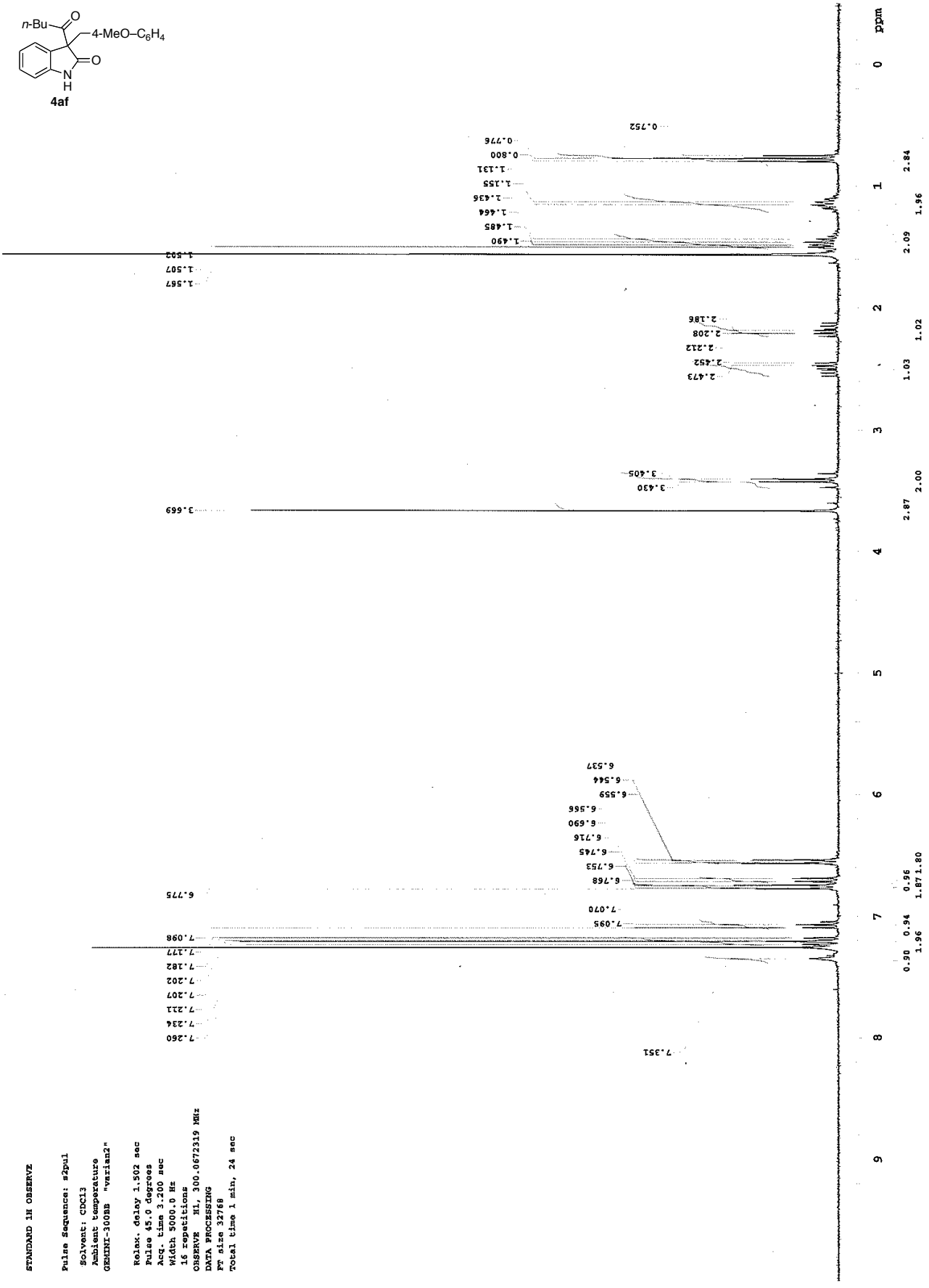

n-Bu
4-Tol
O
O
N
H
4ac
13.690
20.946
21.867
25.381
38.390
38.866
68.405
76.685
77.000
77.322
110.104
122.799
124.512
127.660
128.392
129.065
129.717
131.876
136.005
141.452
176.965
202.946
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
File: Oxindole_nBu_4Me3n_13C
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
2752 repetitions
OBSERVE C13, 100.6316694 MHz
DECOUPLE H1, 400.4458059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 5 hr, 48 min, 45 sec

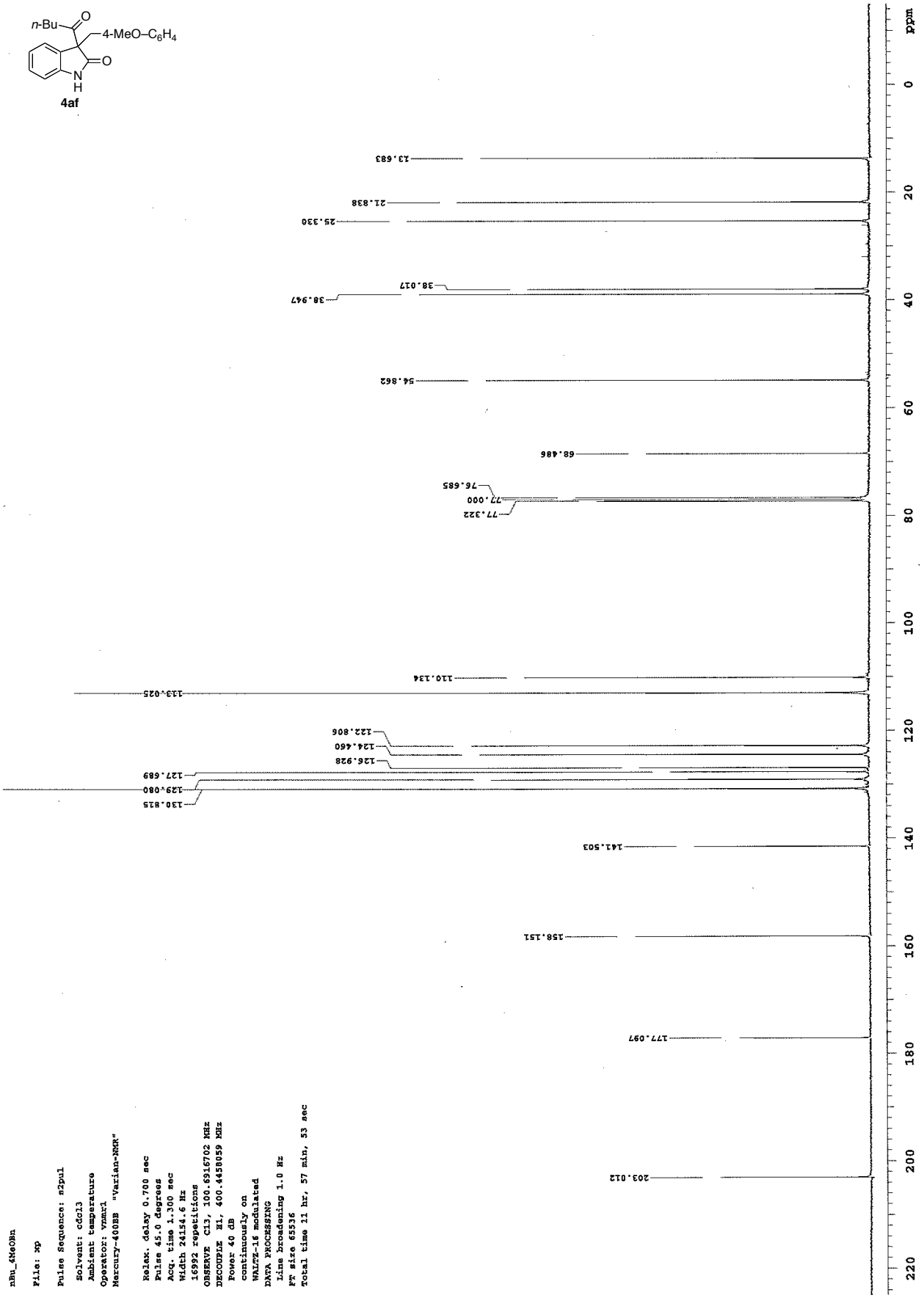

n-Bu
3-Tol
O
O
N
H
4ad
ppm
0.744
0.769
0.792
1.118
1.143
1.434
1.438
1.455
1.461
1.482
1.487
1.508
1.526
1.628
2.089
2.176
2.198
2.202
2.224
2.421
2.442
3.370
3.424
3.459
3.504
6.641
6.658
6.725
6.752
6.852
6.858
6.871
7.075
7.080
7.099
7.101
7.103
7.187
7.189
7.212
7.238
7.261
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.502 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 5000.0 Hz
16 repetitions
OBSERVE H1, 300.0672313 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 24 sec

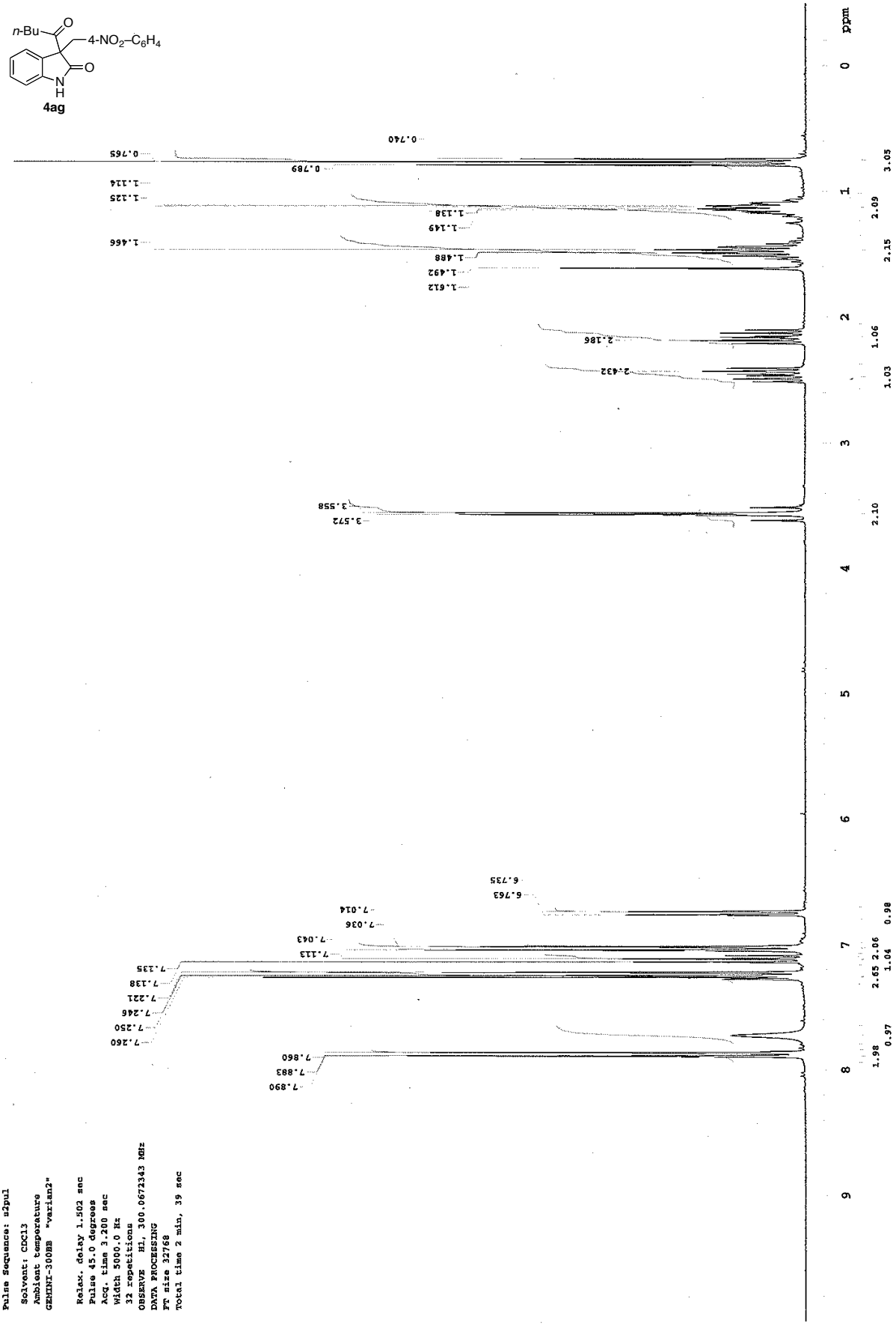

n-Bu
3-Tol
O
O
N
H
4ad
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmrl
File: Oxindole_nBu_3MeBn_13C
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
4960 repetitions
OBSERVE C13, 100.6916709 MHz
DECOUPLE H1, 400.4458059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 5 hr, 58 min, 59 sec
13.675
21.091
21.845
25.367
38.661
38.844
68.405
76.678
77.000
77.315
110.112
122.747
124.548
126.810
127.272
127.455
127.623
129.087
130.698
134.893
137.111
141.525
177.067
202.880
ppm
0
20
40
60
80
100
120
140
160
180
200
220

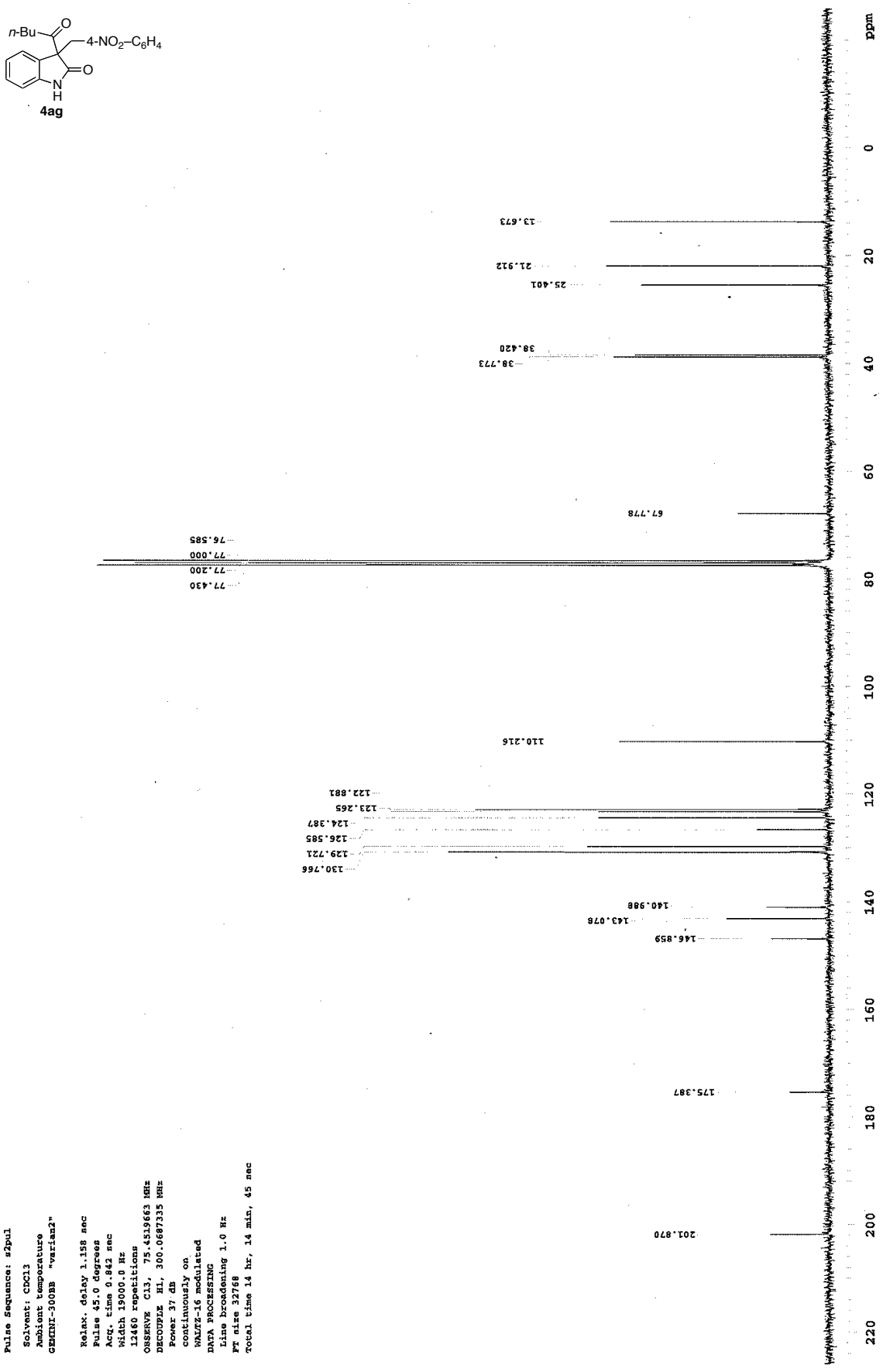

n-Bu
2-Tol
O
O
N
H
4ae
ppm
0.738
0.763
0.787
2.133
3.534
3.596
6.793
6.795
6.805
6.820
6.823
6.825
6.939
6.945
6.950
6.952
7.024
7.048
7.065
7.069
7.260
3.10
2.10
2.14
4.13
0.97
2.00
2.09
3.11
1.21
2.00
0.96
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.502 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 5000.0 Hz
16 repetitions
OBSERVE H1, 300.0672346 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 24 sec

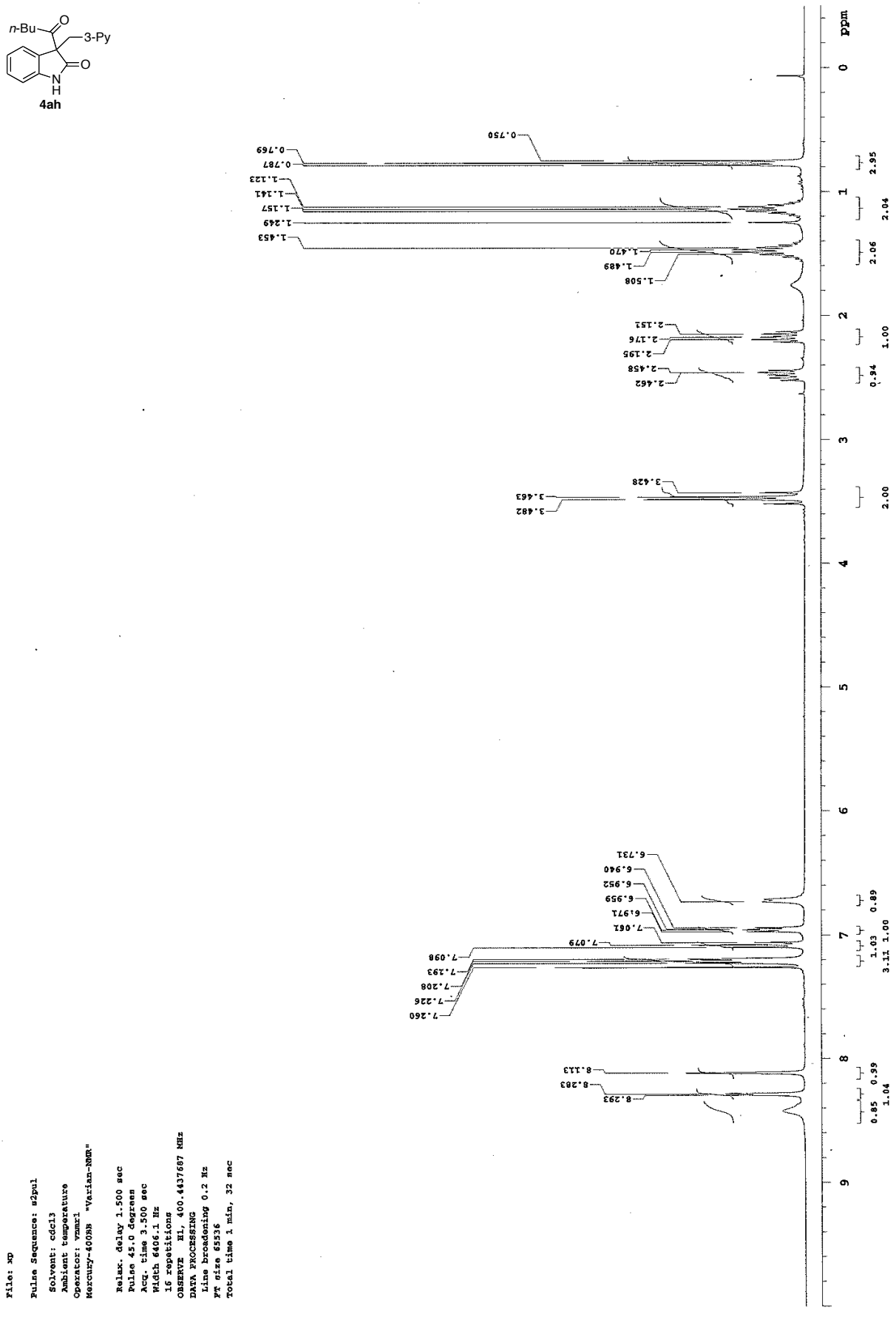

n-Bu
2-Tol
O
O
N
H
4ae
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.158 sec
Pulse 45.0 degrees
Acq. time 0.842 sec
Width 19000.0 Hz
12684 repetitions
OBSERVE C13, 75.4519686 MHz
DECOUPLE H1, 300.0687335 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 14 hr, 14 min, 45 sec
13.704
19.975
21.897
25.493
34.531
38.789
68.008
76.570
77.000
77.415
110.047
122.681
124.818
125.187
126.601
127.800
129.198
129.813
130.151
133.810
137.206
141.541
177.078
202.885
ppm
0
20
40
60
80
100
120
140
160
180
200
220

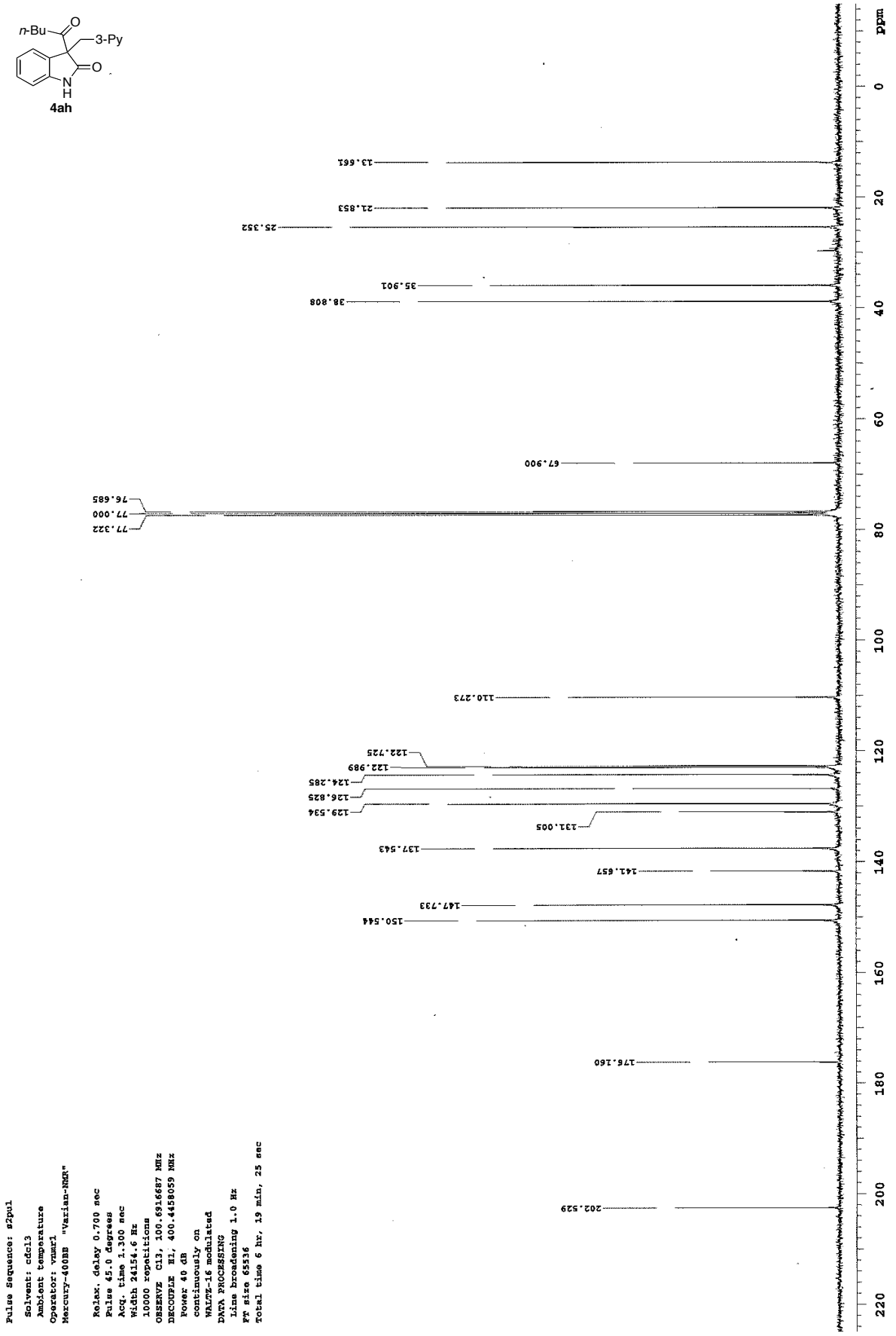

n-Bu
4-MeO–C6H4
O
O
N
H
4af
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.502 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 5000.0 Hz
16 repetitions
OBSERVE H1, 300.0672319 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 24 sec
ppm
0.752
0.776
0.800
1.131
1.155
1.436
1.464
1.485
1.490
1.502
1.507
1.567
2.186
2.208
2.212
2.452
2.473
3.405
3.430
3.669
6.537
6.544
6.559
6.566
6.690
6.716
6.745
6.753
6.768
6.775
7.070
7.095
7.098
7.177
7.182
7.202
7.207
7.211
7.234
7.260
7.351

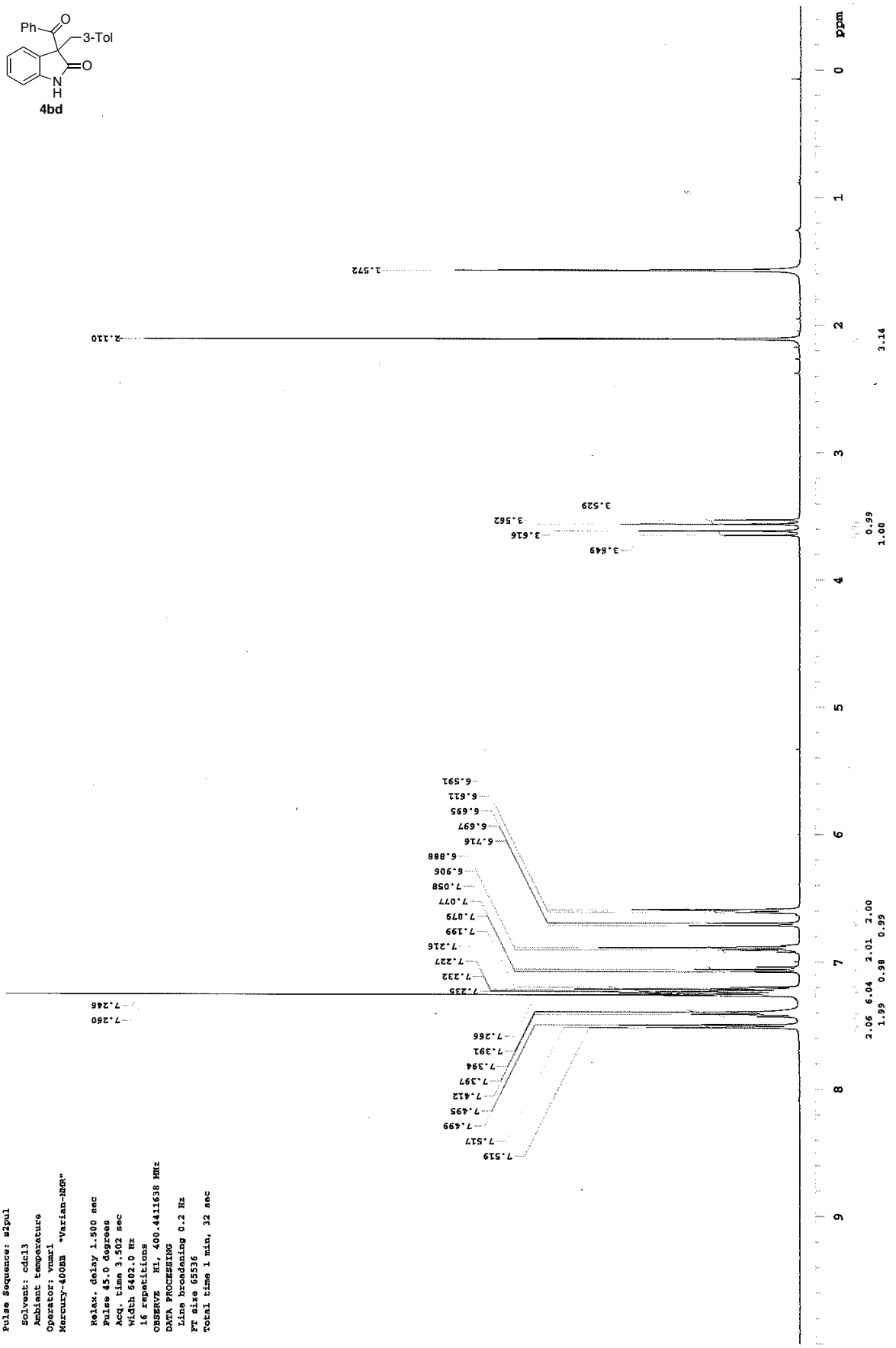

n-Bu
4-MeO–C6H4
O
O
N
H
4af
nBu_4MeOBn
File: xp
Pulse Sequence: n2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
16992 repetitions
OBSERVE C13, 100.6916702 MHz
DECOUPLE H1, 400.4450059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 11 hr, 57 min, 53 sec
13.683
21.838
25.330
38.017
38.947
54.862
68.486
76.685
77.000
77.322
110.134
113.025
122.806
124.460
126.928
127.689
129.080
130.815
141.503
158.151
177.097
203.012
ppm

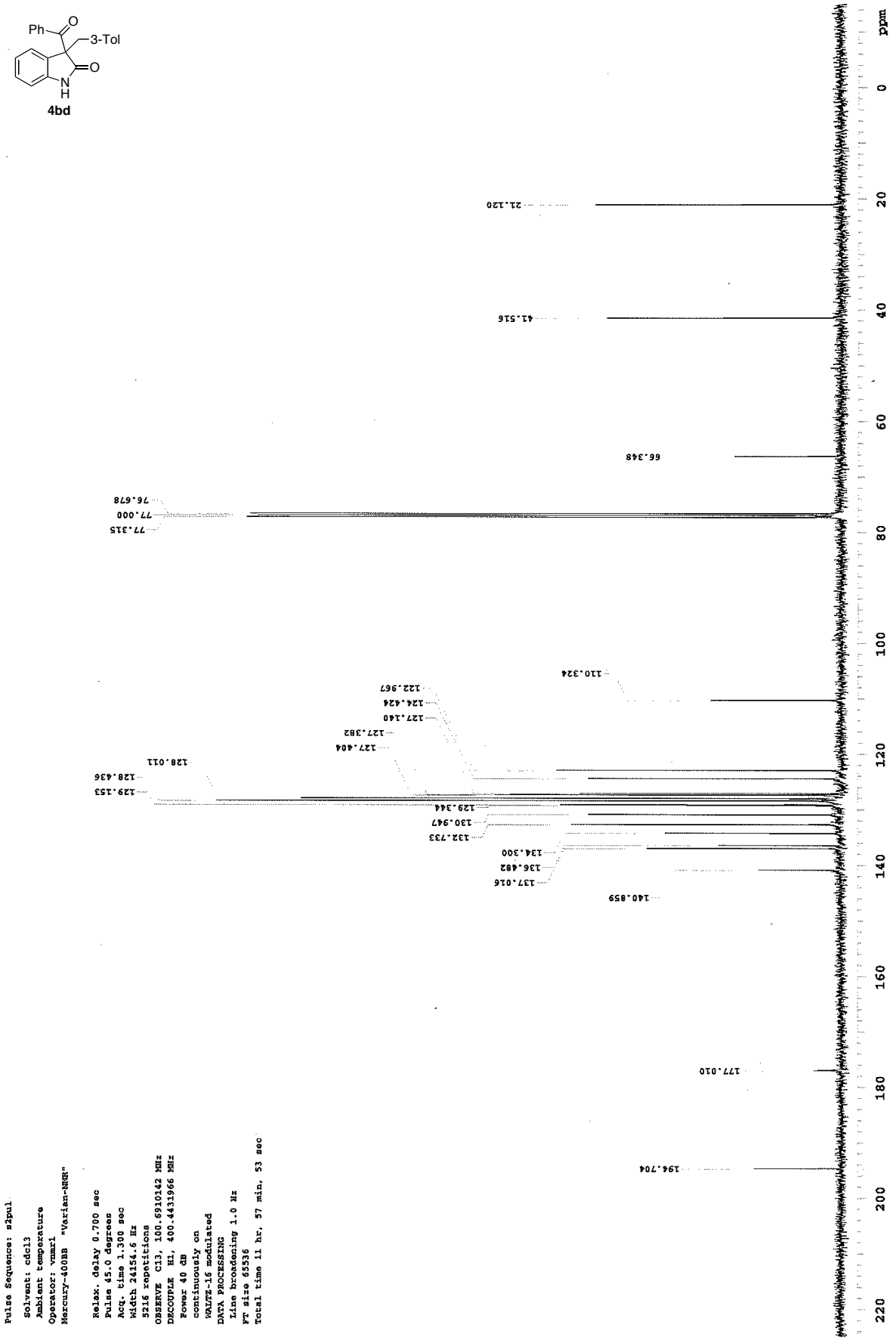

n-Bu
4-NO2–C6H4
4ag
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.502 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 5000.0 Hz
32 repetitions
OBSERVE H1, 300.0672343 MHz
DATA PROCESSING
FT size 32768
Total time 2 min, 39 sec
ppm

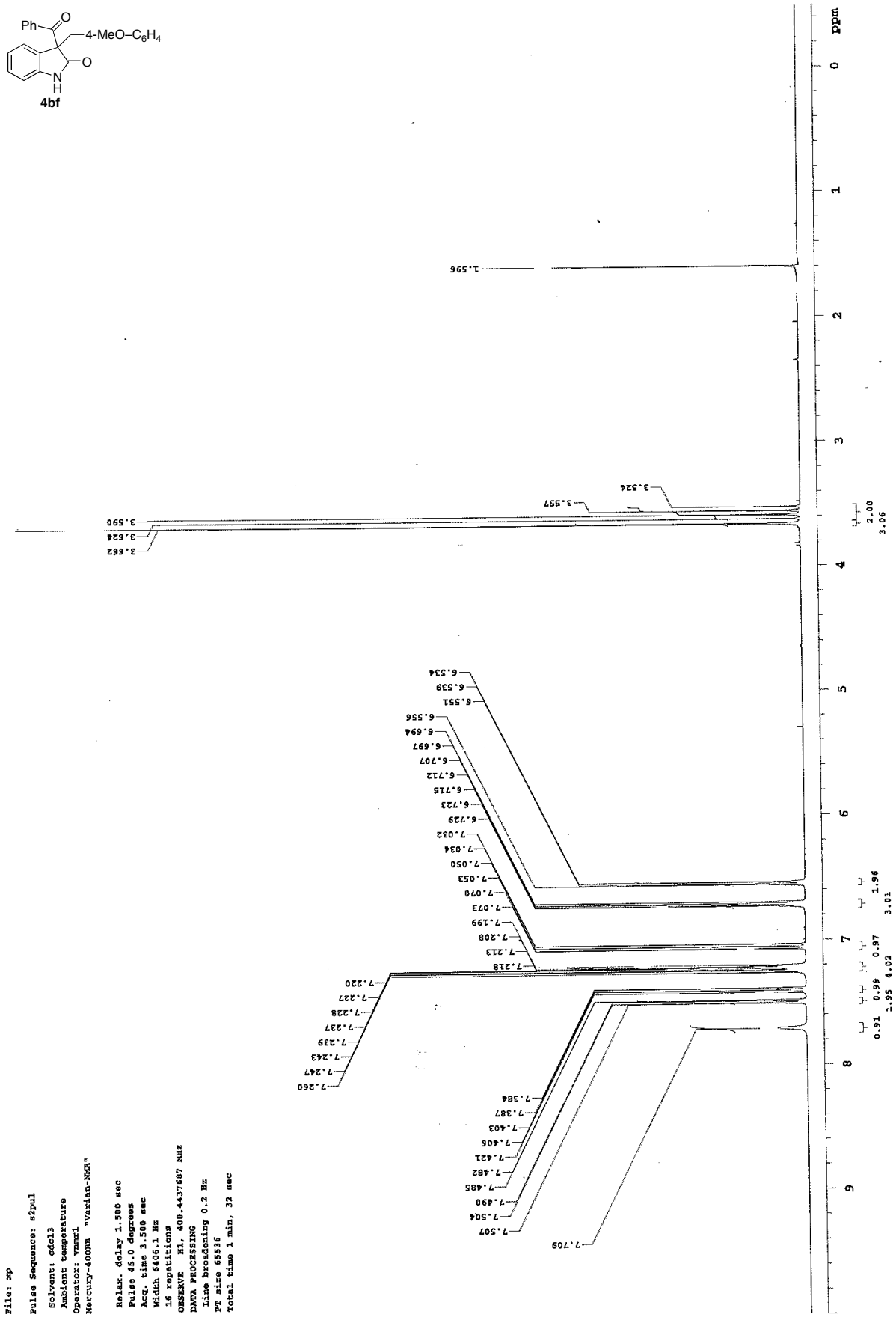

n-Bu
4-NO2–C6H4
O
O
N
H
4ag
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.158 sec
Pulse 45.0 degrees
Acq. time 0.842 sec
Width 19000.0 Hz
12460 repetitions
OBSERVE C13, 75.4519663 MHz
DECOUPLE H1, 300.0687335 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 14 hr, 14 min, 45 sec
13.673
21.912
25.401
38.420
38.773
67.778
76.585
77.000
77.200
77.430
110.216
122.881
123.265
124.387
126.585
129.721
130.766
140.988
143.078
146.859
175.387
201.870
ppm
0
20
40
60
80
100
120
140
160
180
200
220

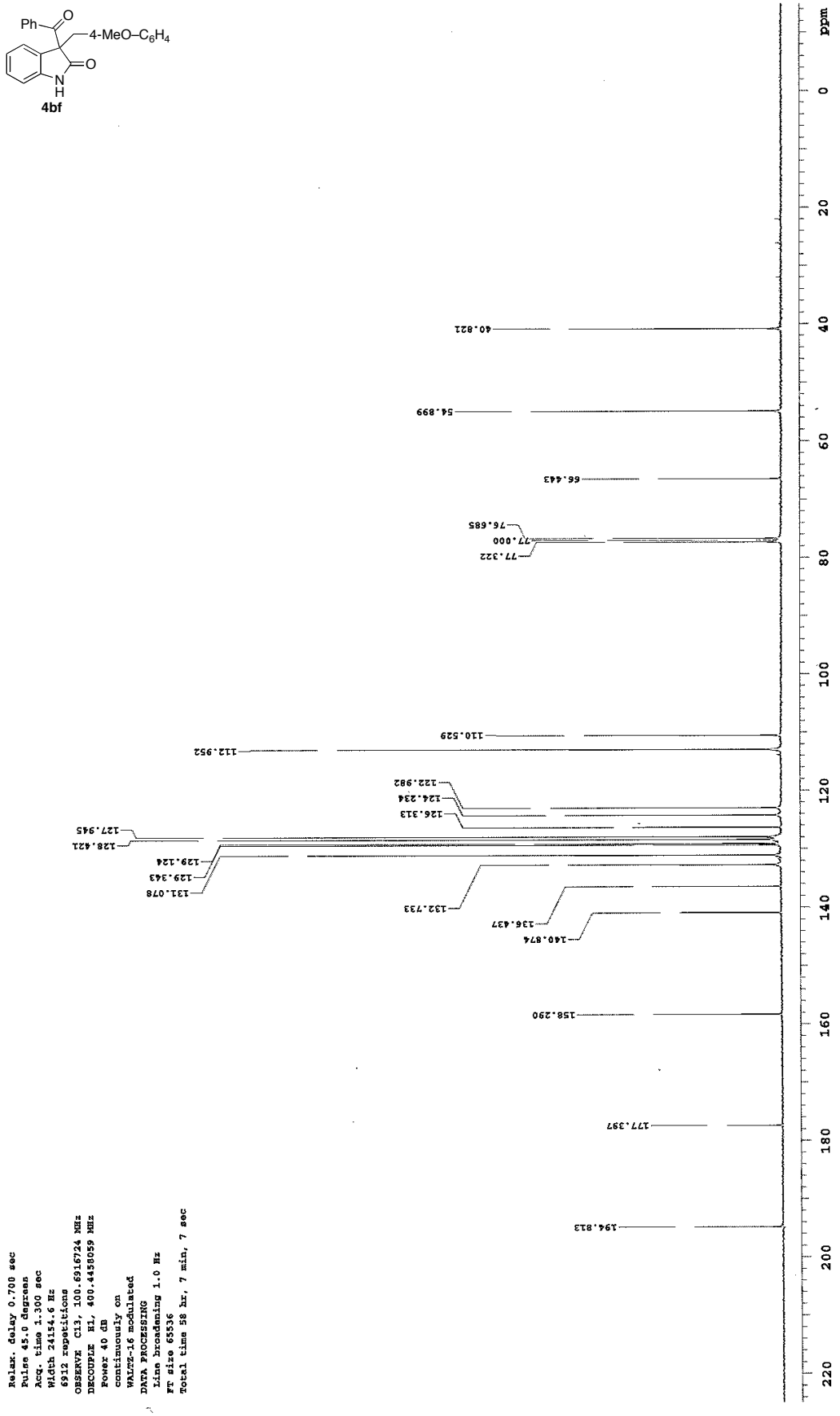

n-Bu
3-Py
O
O
N
H
4ah
File: xp
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
Mercury-400BB "Varian-NMR"
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437687 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec
0.750
0.769
0.787
1.123
1.141
1.157
1.249
1.453
1.470
1.489
1.508
2.151
2.176
2.195
2.458
2.462
3.428
3.463
3.482
6.731
6.940
6.952
6.959
6.971
7.061
7.079
7.098
7.193
7.208
7.226
7.260
8.113
8.283
8.293
ppm
0 1 2 3 4 5 6 7 8 9
2.95
2.04
2.06
1.00
0.94
2.00
0.89
1.03
3.11 1.00
0.99
0.85
1.04

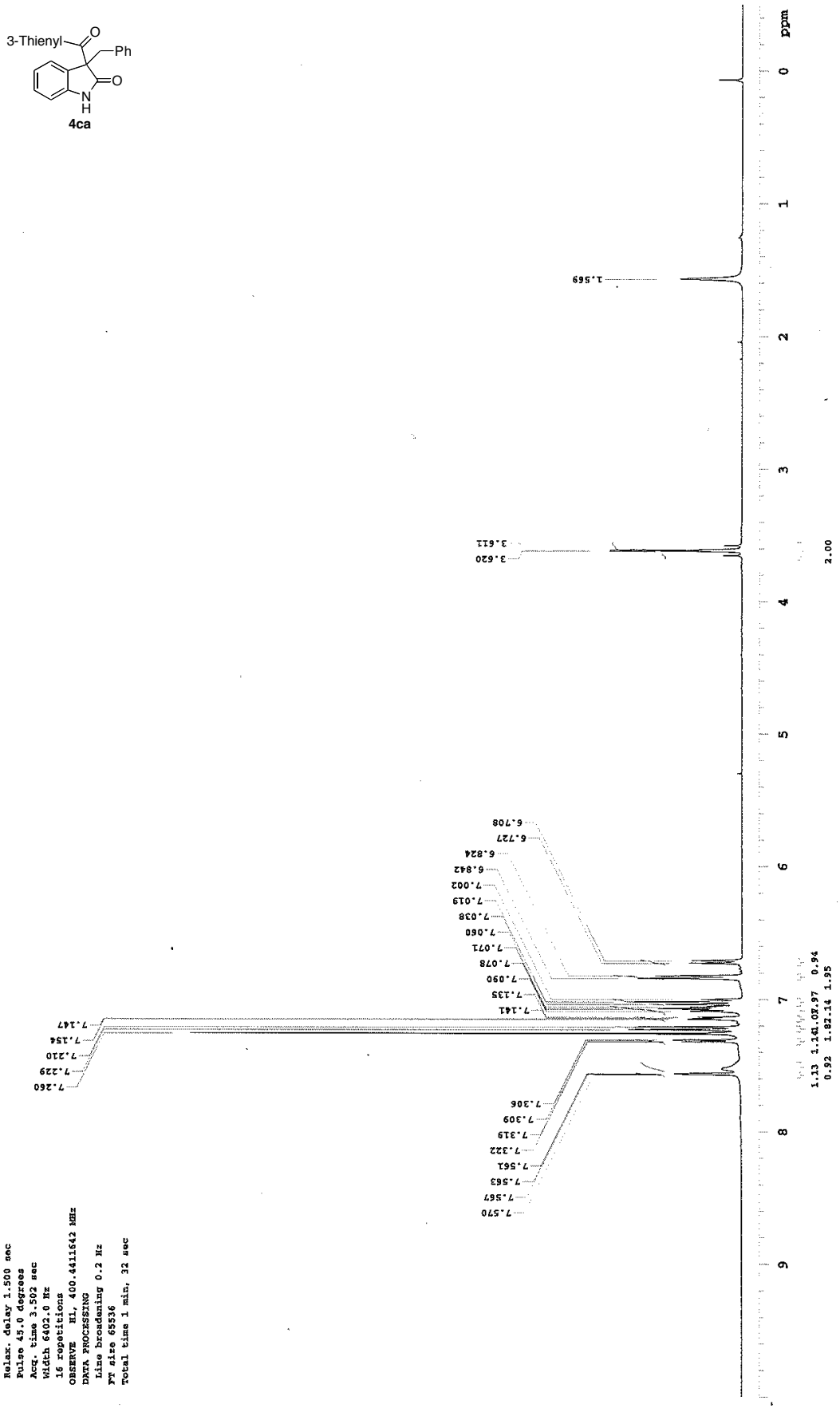

n-Bu
3-Py
O
O
N
H
4ah
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
10000 repetitions
OBSERVE C13, 100.6916687 MHz
DECOUPLE H1, 400.4458059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 6 hr, 19 min, 25 sec
13.661
21.853
25.352
35.901
38.808
67.900
76.685
77.000
77.322
110.273
122.725
122.989
124.285
126.825
129.534
131.005
137.543
141.857
147.733
150.544
176.160
202.529
ppm
0
20
40
60
80
100
120
140
160
180
200
220

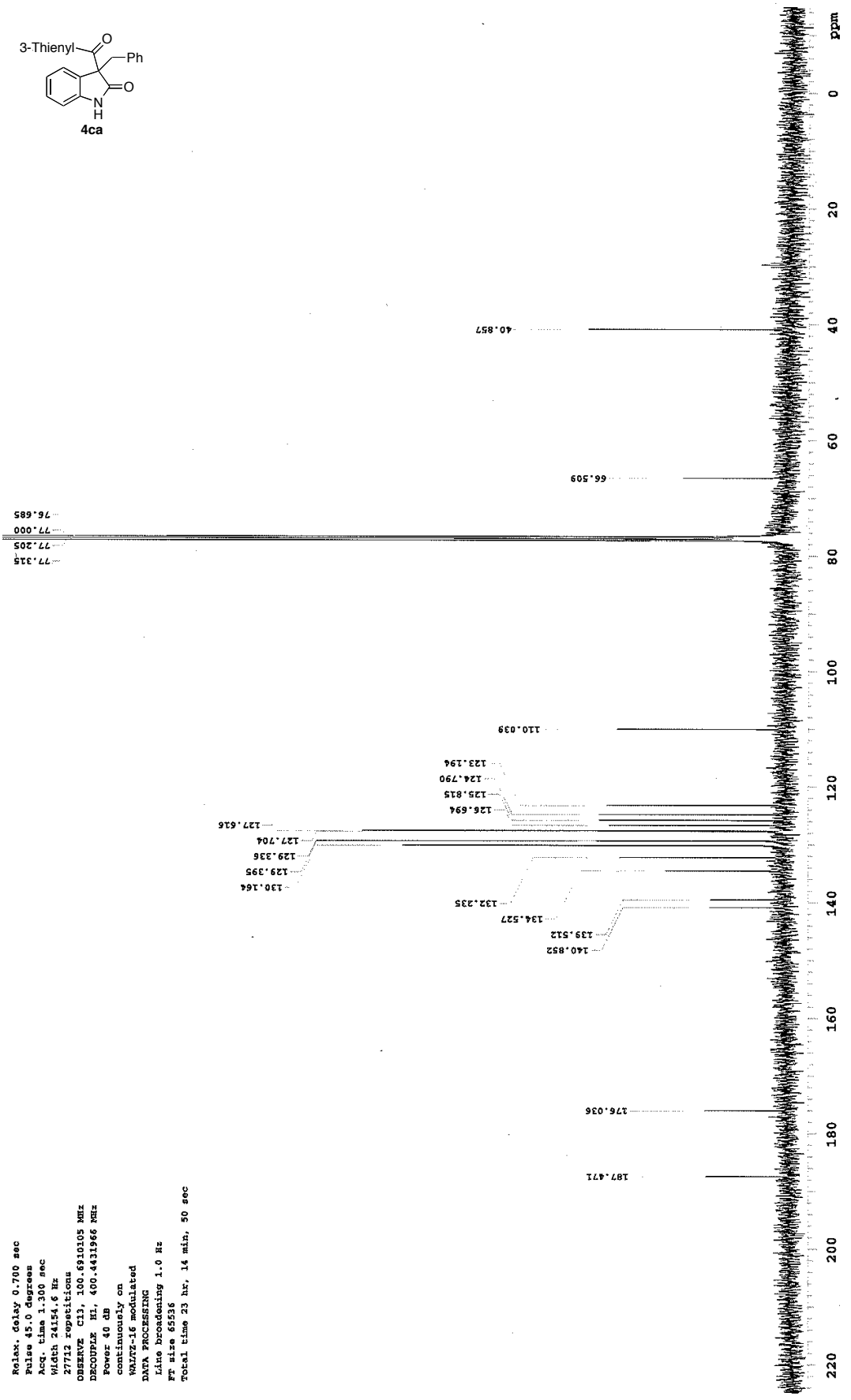

Ph
O
3-Tol
O
N
H
4bd
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmrl
Mercury-400BB "Varian-NMR"
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.502 sec
Width 6402.0 Hz
16 repetitions
OBSERVE H1, 400.4411638 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec
ppm
1.572
2.110
3.529
3.562
3.616
3.849
6.591
6.611
6.695
6.697
6.716
6.888
6.906
7.058
7.077
7.079
7.199
7.216
7.227
7.232
7.235
7.246
7.260
7.266
7.391
7.394
7.397
7.412
7.495
7.499
7.517
7.519
3.14
0.99
1.00
2.06
6.04
2.01
2.00
1.99
0.98
0.99

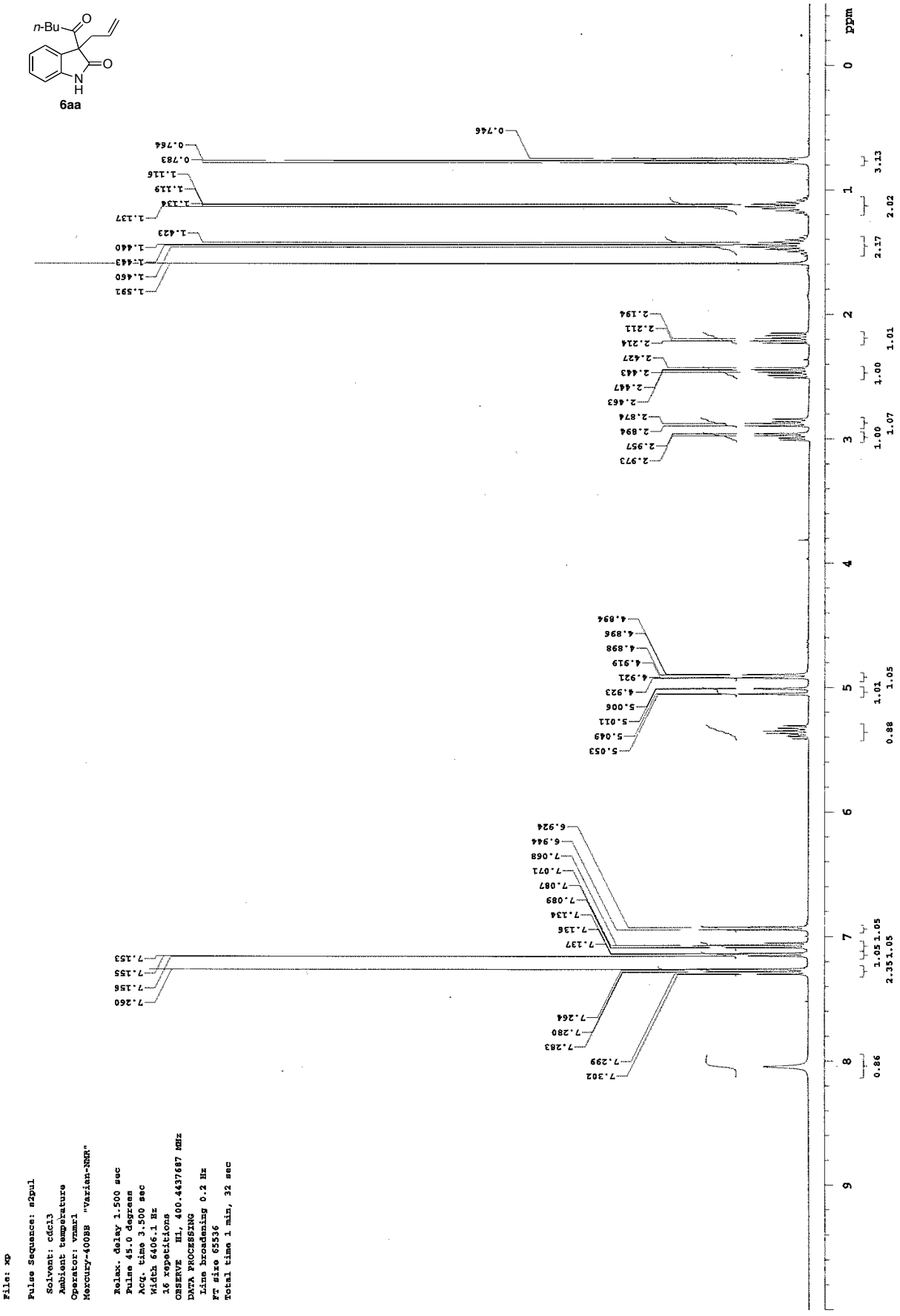

Ph
O
3-Tol
O
N
H
4bd
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
5216 repetitions
OBSERVE C13, 100.6910142 MHz
DECOUPLE H1, 400.4431966 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 11 hr, 57 min, 53 sec
21.120
41.516
66.348
76.678
77.000
77.315
110.324
122.967
124.424
127.140
127.382
127.404
128.011
128.436
129.153
129.344
130.947
132.733
134.300
136.482
137.016
140.859
177.010
194.704
ppm
0
20
40
60
80
100
120
140
160
180
200
220

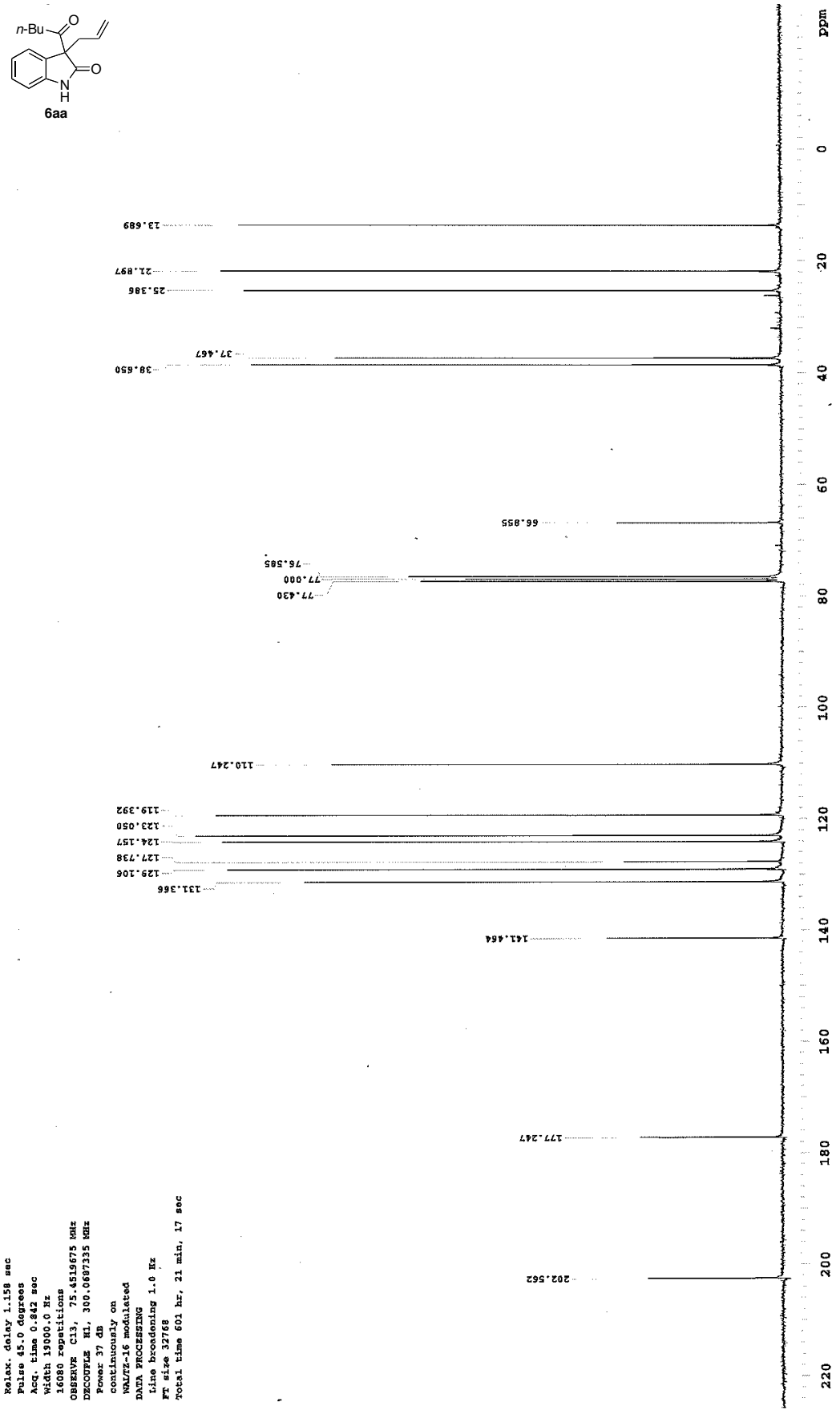

Ph
O
4-MeO–C6H4
O
N
H
4bf
ppm
1.596
3.524
3.557
3.590
3.624
3.662
6.534
6.539
6.551
6.556
6.694
6.697
6.707
6.712
6.715
6.723
6.729
7.032
7.034
7.050
7.053
7.070
7.073
7.199
7.208
7.213
7.218
7.220
7.227
7.228
7.237
7.239
7.243
7.247
7.260
7.384
7.387
7.403
7.406
7.421
7.482
7.485
7.490
7.504
7.507
7.709
2.00
3.06
1.96
3.01
0.97
4.02
0.99
1.95
0.91
File: xp
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmrl
Mercury-400BB "Varian-NMR"
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437687 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec

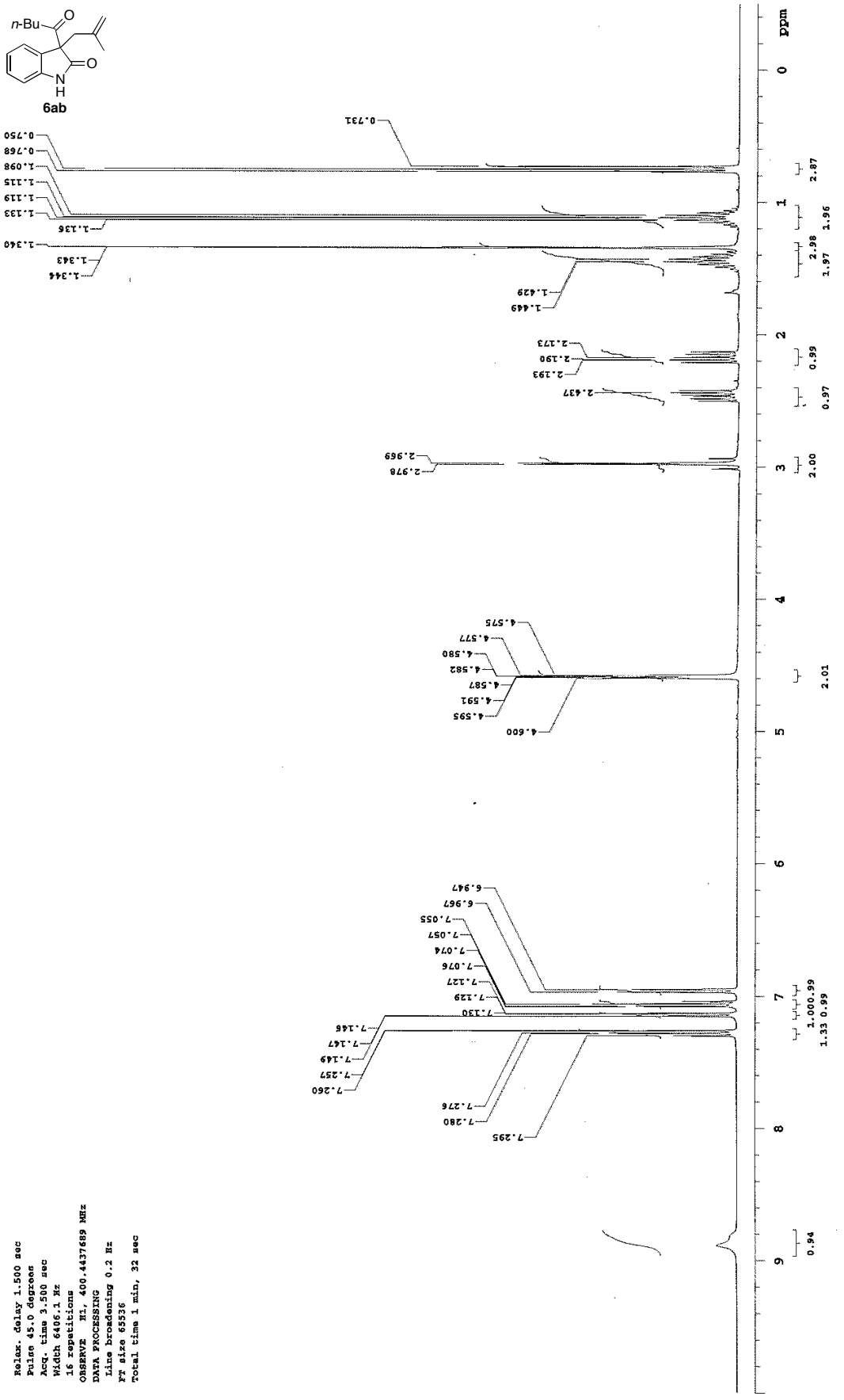

Ph
O
4-MeO–C6H4
O
N
H
4bf
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
6912 repetitions
OBSERVE C13, 100.6916724 MHz
DECOUPLE H1, 400.4458059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 58 hr, 7 min, 7 sec
40.821
54.899
66.443
76.685
77.000
77.322
110.529
112.952
122.982
124.234
126.313
127.945
128.421
129.124
129.343
131.078
132.733
136.437
140.874
158.290
177.397
194.813
ppm
0
20
40
60
80
100
120
140
160
180
200
220

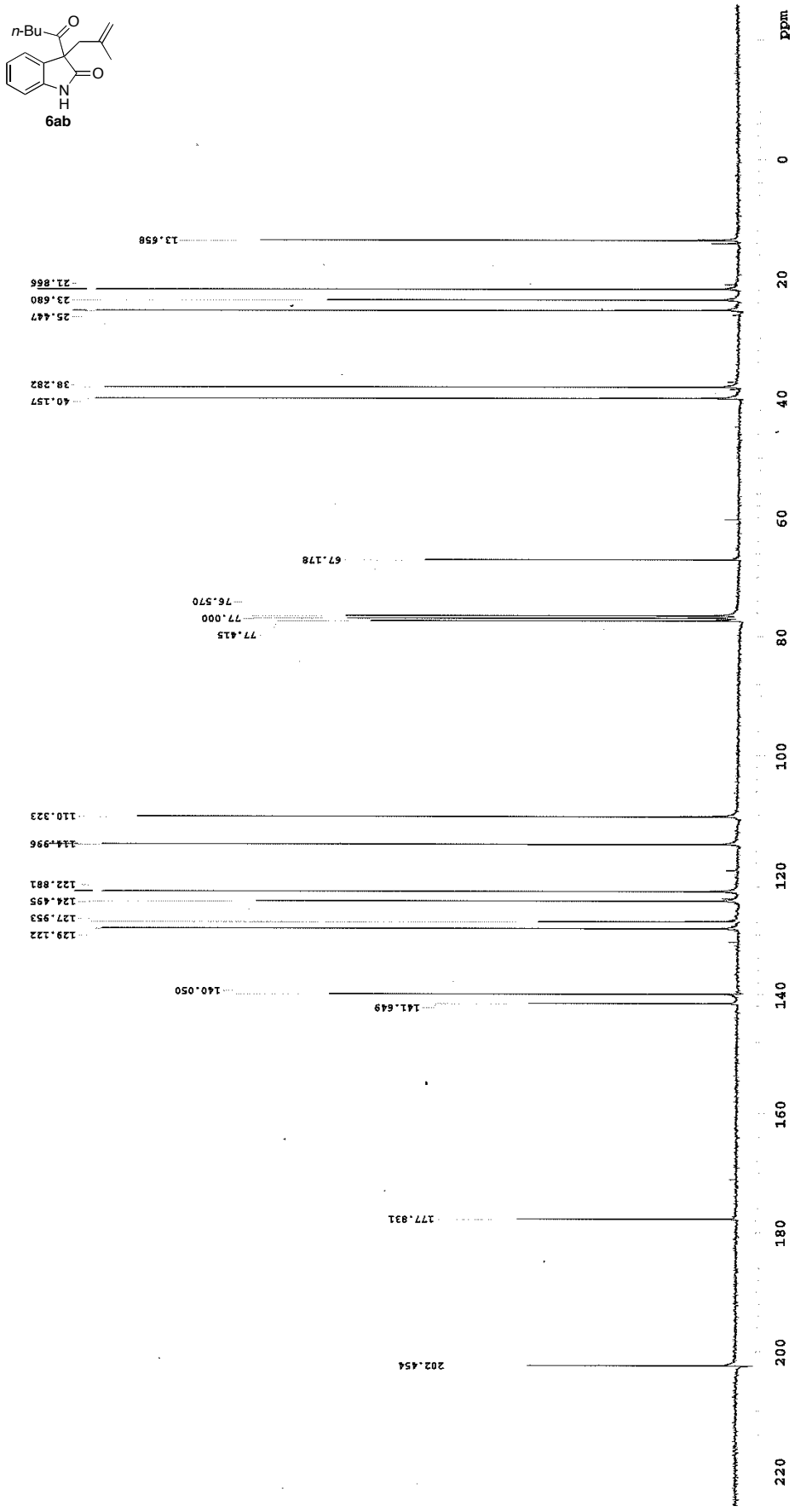

3-Thienyl
Ph
O
O
N
H
4ca
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.502 sec
Width 6402.0 Hz
16 repetitions
OBSERVE H1, 400.4411642 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec
1.569
3.611
3.620
6.708
6.727
6.824
6.842
7.002
7.019
7.038
7.060
7.071
7.078
7.090
7.135
7.141
7.147
7.154
7.210
7.229
7.260
7.306
7.309
7.319
7.322
7.561
7.563
7.567
7.570
2.00
1.13 1.14 1.07 0.97 0.94
0.92 1.82 1.14 1.95
ppm

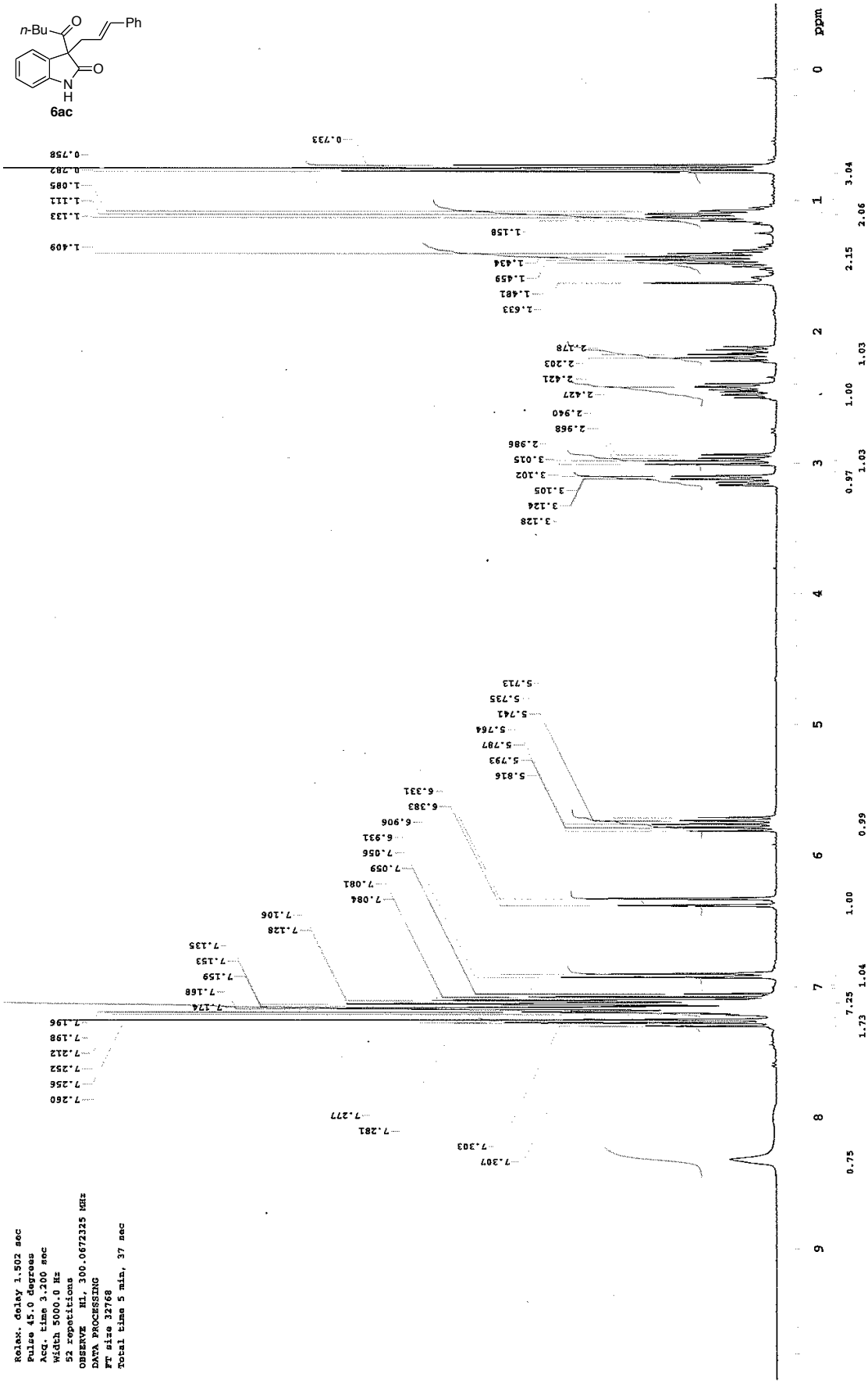

3-Thienyl
O
Ph
O
N
H
4ca
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
27712 repetitions
OBSERVE C13, 100.6910105 MHz
DECOUPLE H1, 400.4431966 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 23 hr, 14 min, 50 sec
187.471
176.036
140.852
139.512
134.527
132.335
130.164
129.395
129.336
127.704
127.616
126.694
125.815
124.790
123.194
110.039
77.315
77.205
77.000
76.685
66.509
40.857
ppm
0
20
40
60
80
100
120
140
160
180
200
220

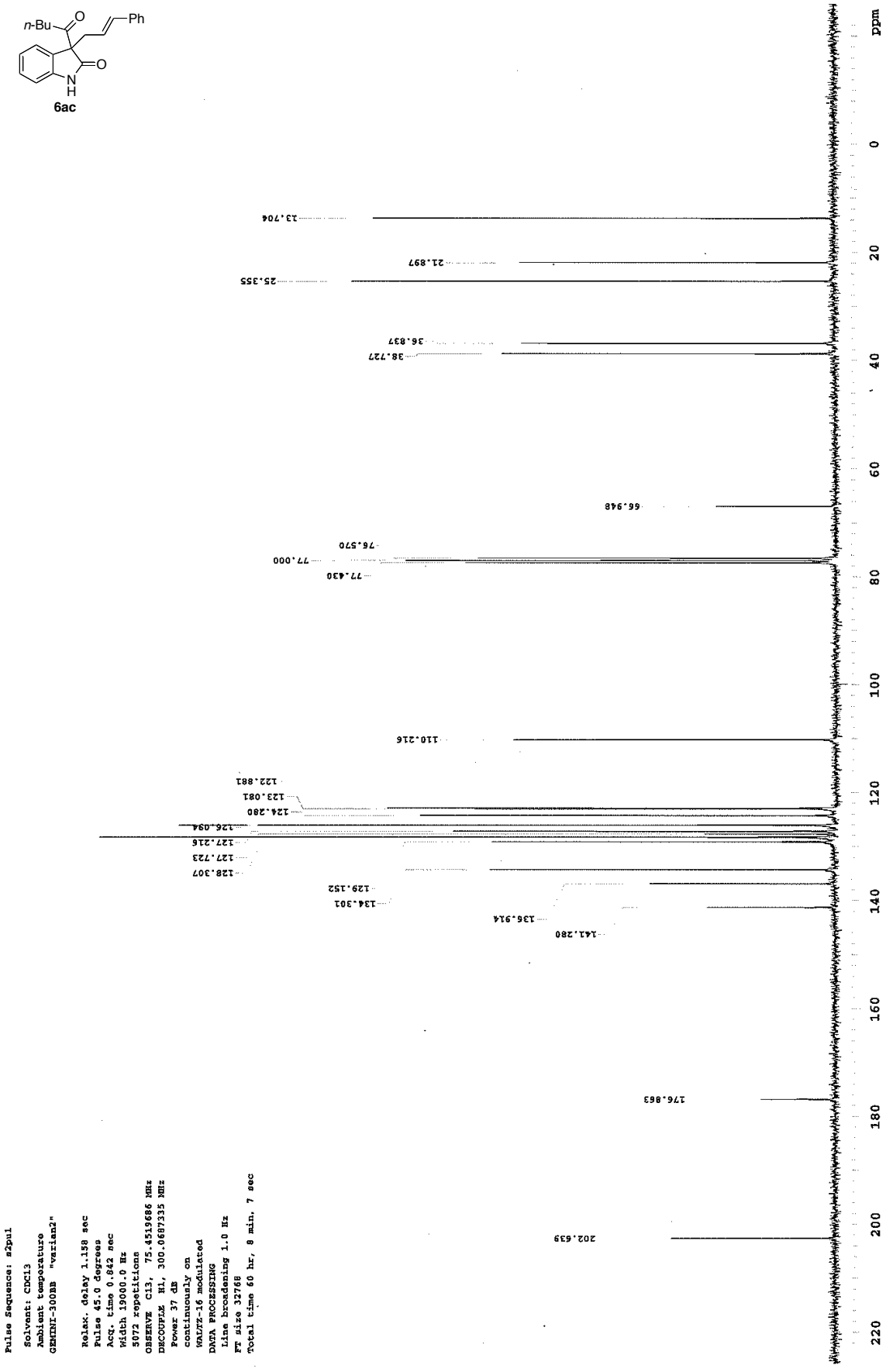

n-Bu
O
O
N
H
6aa
File: mp
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
Mercury-400BB "Varian-NMR"
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437687 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec
ppm

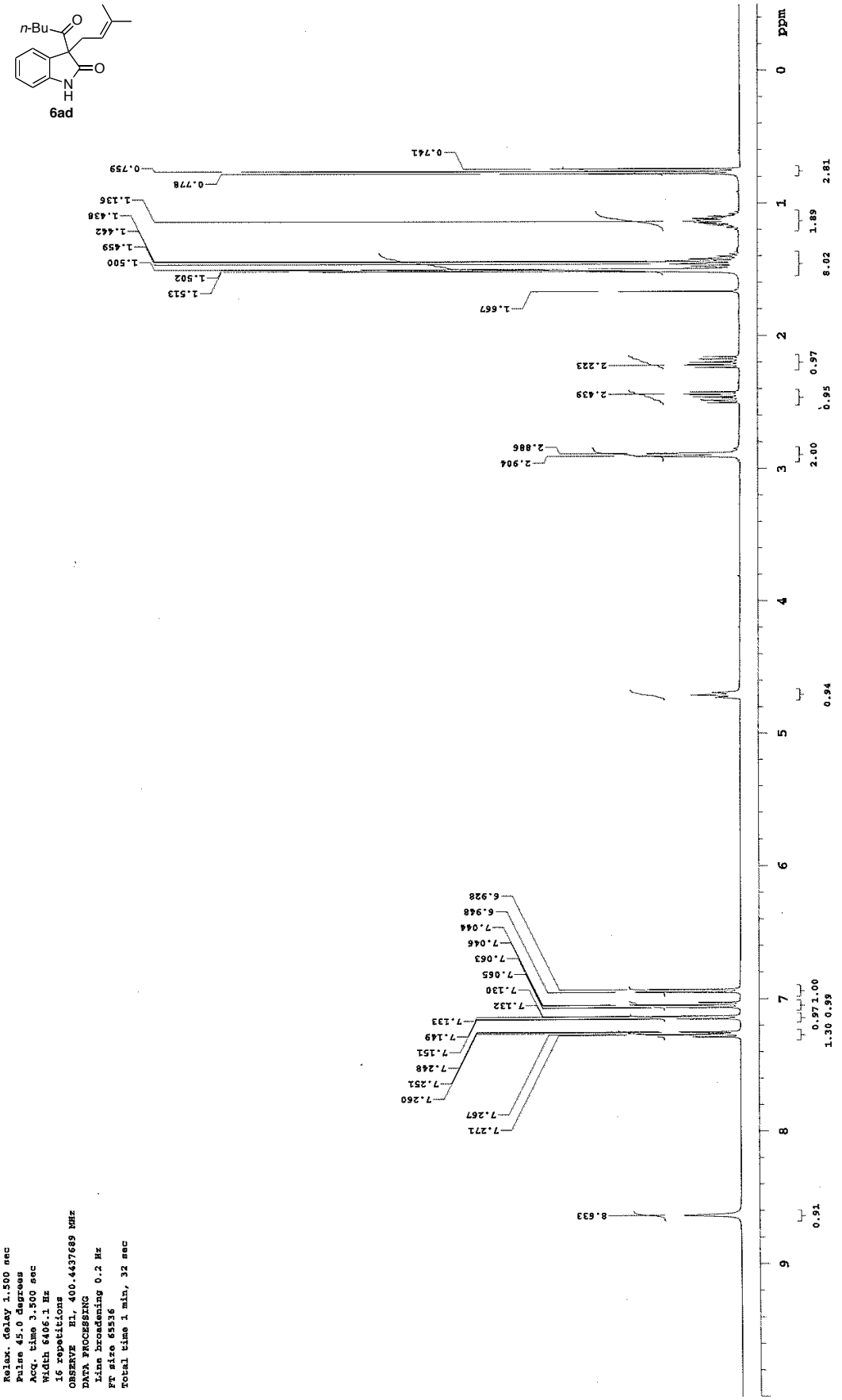

n-Bu
O
O
N
H
6aa
13.689
21.897
25.386
37.467
38.850
66.855
76.585
77.000
77.430
110.347
119.392
123.050
124.157
127.738
129.106
131.366
141.464
177.247
202.562
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Relax. delay 1.158 sec
Pulse 45.0 degrees
Acq. time 0.842 sec
Width 19000.0 Hz
16080 repetitions
OBSERVE C13, 75.4519675 MHz
DECOUPLE H1, 300.0687335 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 601 hr, 21 min, 17 sec

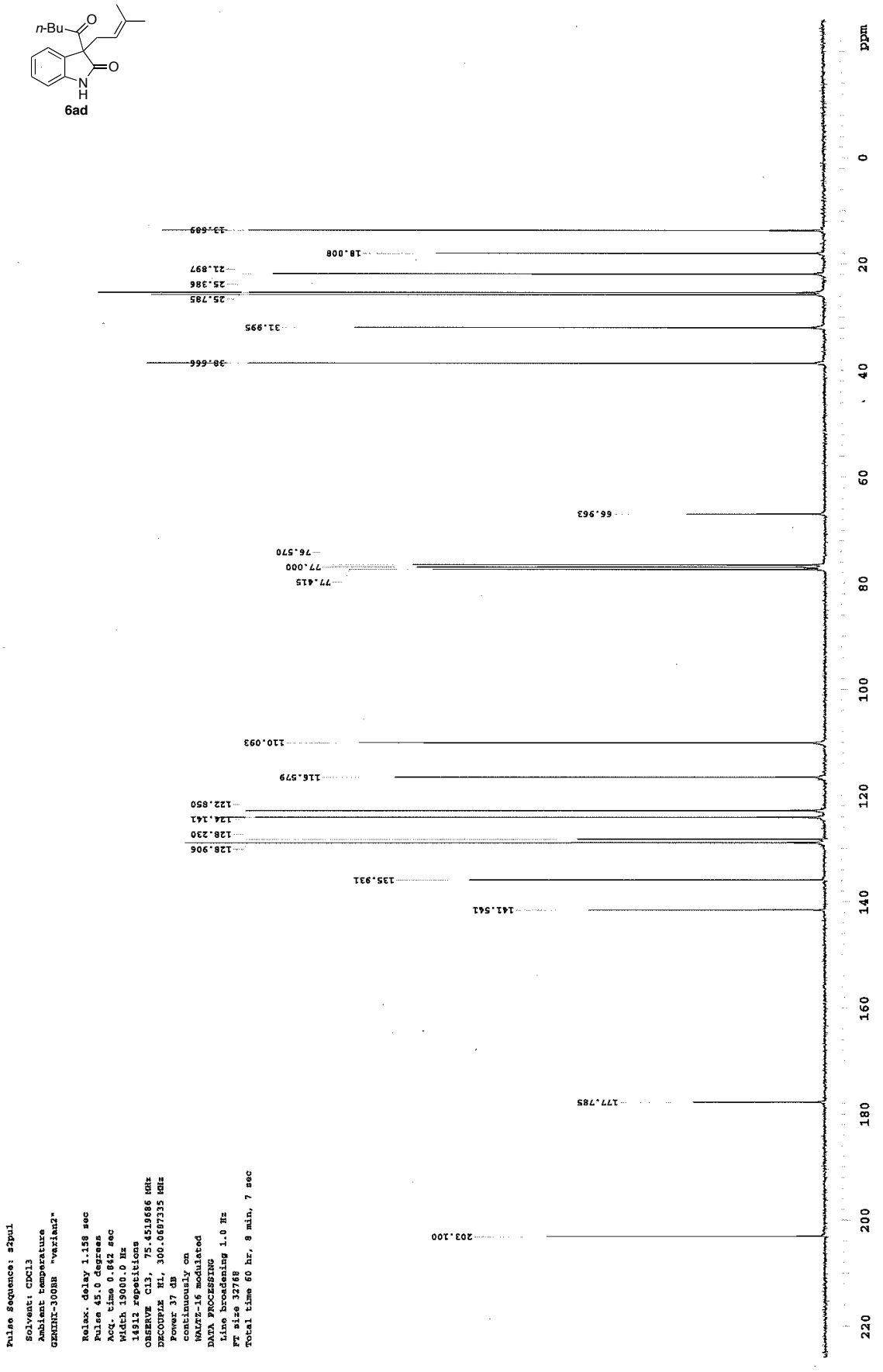

n-Bu
O
O
N
H
6ab
0.731
0.750
0.768
1.098
1.115
1.119
1.133
1.136
1.340
1.343
1.344
1.429
1.449
2.173
2.190
2.193
2.437
2.969
2.978
4.575
4.577
4.580
4.582
4.587
4.591
4.595
4.600
6.947
6.967
7.055
7.057
7.074
7.076
7.127
7.129
7.130
7.146
7.147
7.149
7.257
7.260
7.276
7.280
7.295
ppm
0 1 2 3 4 5 6 7 8 9
2.87 1.96 2.98 1.97 0.99 0.97 2.00 2.01 1.000.99 1.33 0.99 0.94
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437689 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec

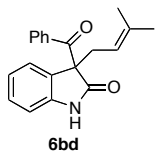

n-Bu
O
O
N
H
6ab
ppm
0
20
40
60
80
100
120
140
160
180
200
220
13.658
21.866
23.680
25.447
38.282
40.157
67.178
76.570
77.000
77.415
110.323
114.996
122.881
124.495
127.953
129.122
140.050
141.649
177.831
202.454


n-Bu
O
Ph
O
N
H
6ac
ppm
Relax. delay 1.502 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 5000.0 Hz
52 repetitions
OBSERVE H1, 300.0672325 MHz
DATA PROCESSING
FT size 32768
Total time 5 min, 37 sec

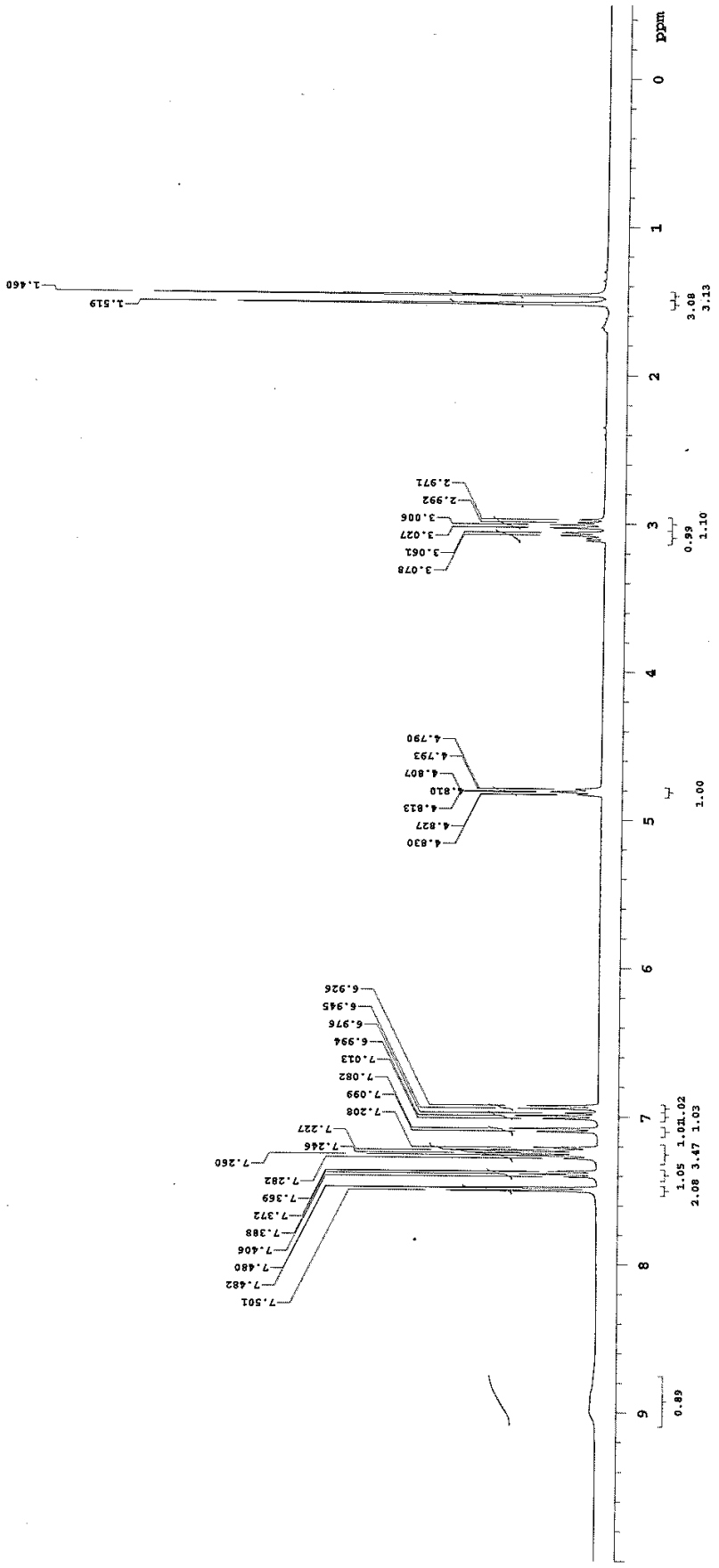

n-Bu
O
Ph
O
N
H
6ac
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "vzian2"
Relax. delay 1.158 sec
Pulse 45.0 degrees
Acq. time 0.842 sec
Width 19000.0 Hz
5072 repetitions
OBSERVE C13, 75.4519686 MHz
DECOUPLE H1, 300.0687335 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 60 hr, 8 min, 7 sec
202.639
176.863
141.280
136.914
134.301
129.152
128.307
127.723
127.216
126.094
124.280
123.081
122.881
110.216
77.430
77.000
76.570
66.948
38.727
36.837
25.355
21.897
13.704
ppm
0
20
40
60
80
100
120
140
160
180
200
220


n-Bu
O
O
N
H
6ad
0.741
0.759
0.778
1.136
1.438
1.442
1.459
1.500
1.502
1.513
1.667
2.223
2.439
2.886
2.904
6.928
6.948
7.044
7.046
7.063
7.065
7.130
7.132
7.133
7.149
7.151
7.248
7.251
7.260
7.267
7.271
8.633
ppm
0 1 2 3 4 5 6 7 8 9
2.81 1.89 8.02 0.97 0.95 2.00 0.94 0.97 1.00 1.30 0.99 0.91
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437689 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec

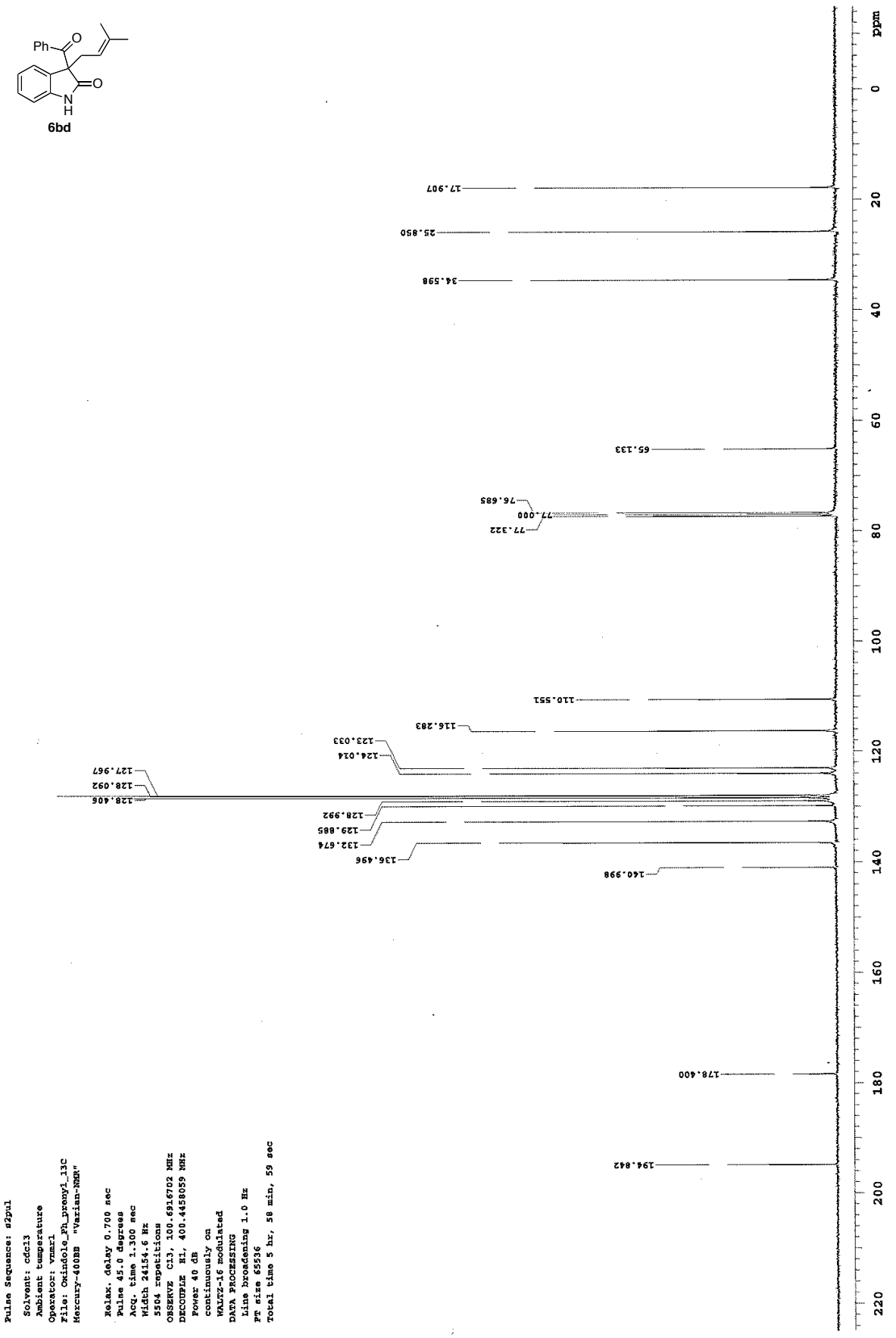

n-Bu
O
O
N
H
6ad
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.158 sec
Pulse 45.0 degrees
Acq. time 0.862 sec
Width 19000.0 Hz
14912 repetitions
OBSERVE C13, 75.4519686 MHz
DECOUPLE H1, 300.0607335 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
line broadening 1.0 Hz
FT size 32768
Total time 60 hr, 8 min, 7 sec
13.689
18.008
21.897
25.386
25.785
31.995
38.666
66.963
76.570
77.000
77.415
110.093
116.579
122.850
124.141
128.230
128.906
135.931
141.541
177.785
203.100
ppm
0
20
40
60
80
100
120
140
160
180
200
220

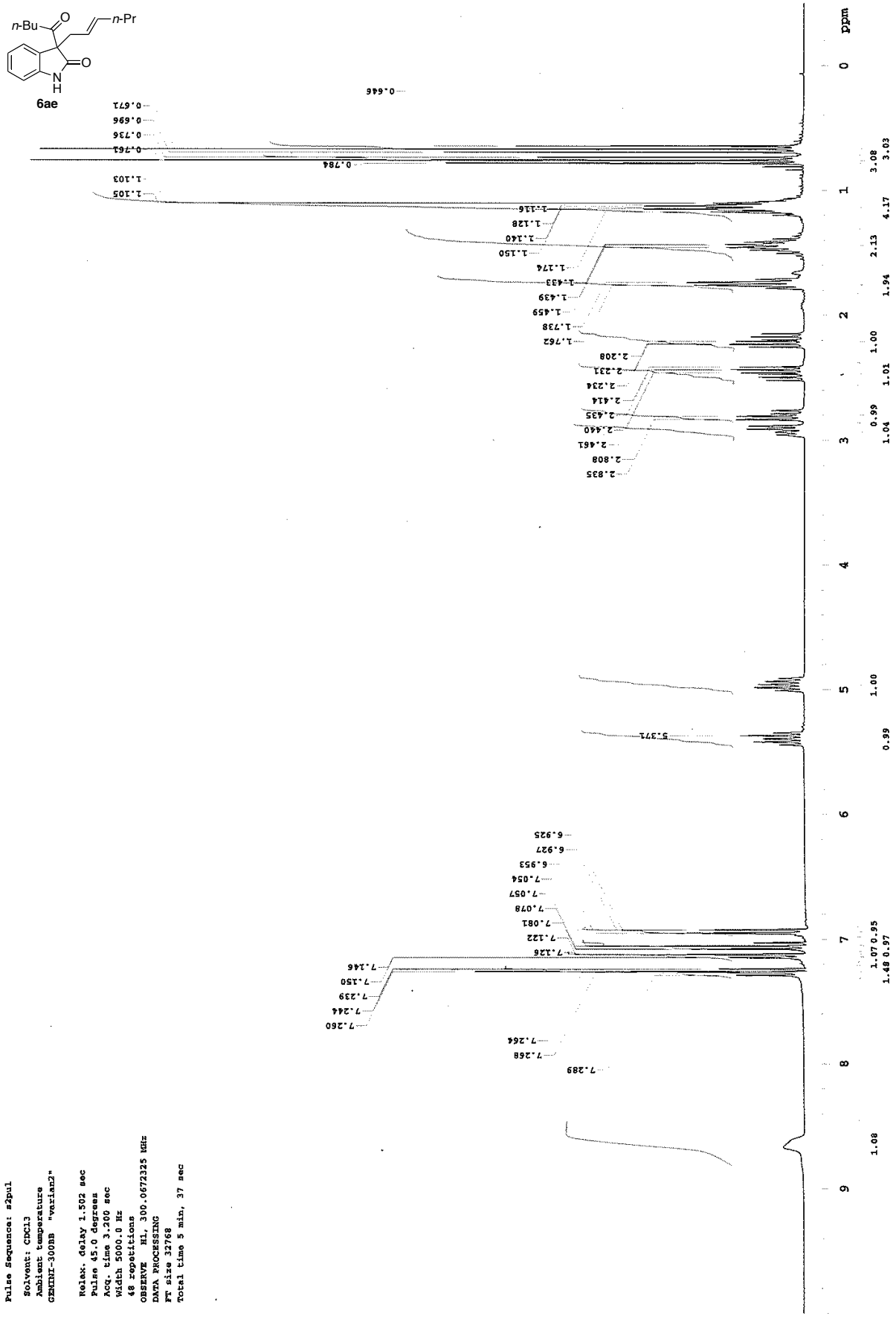


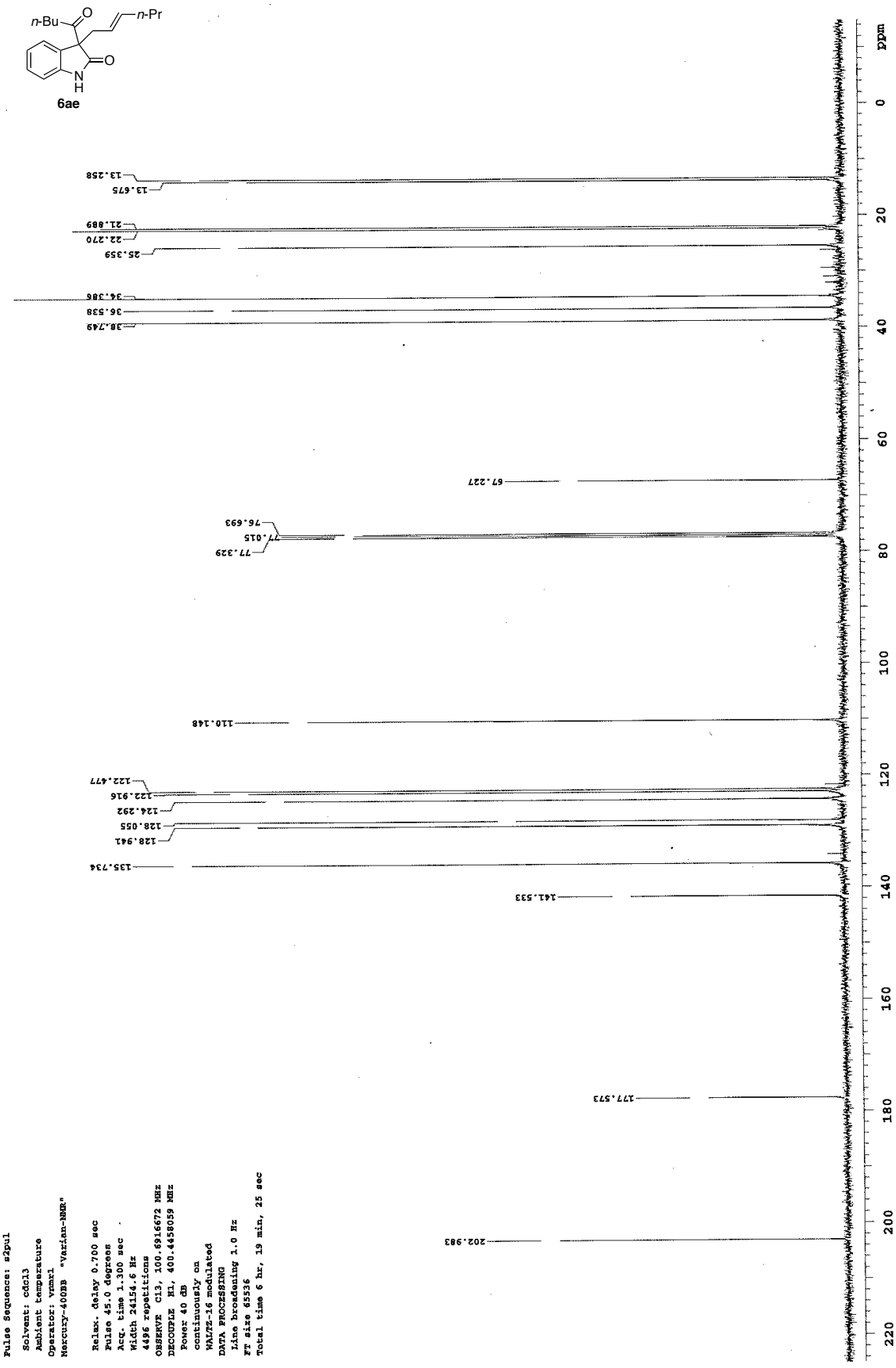
6bd

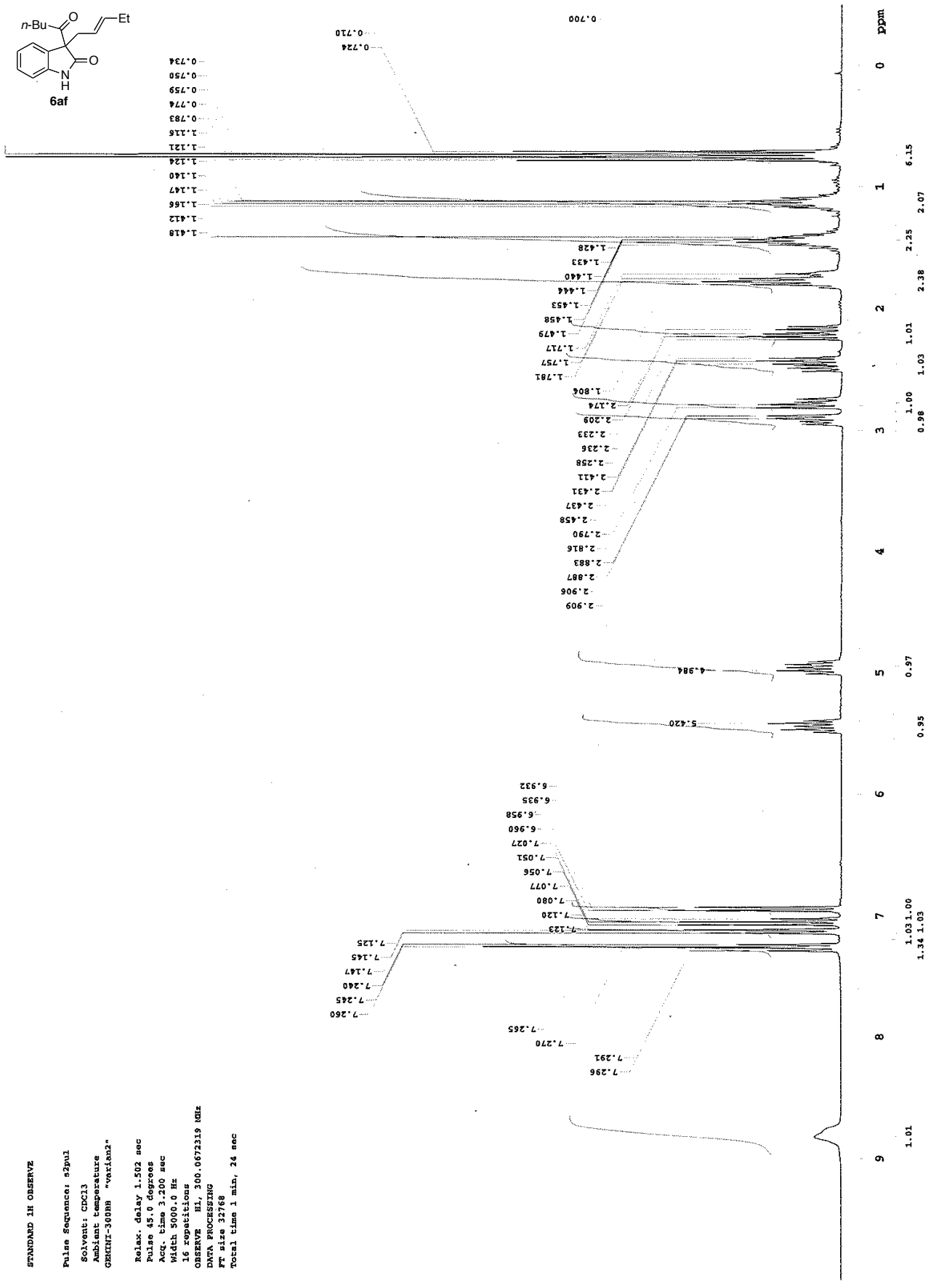


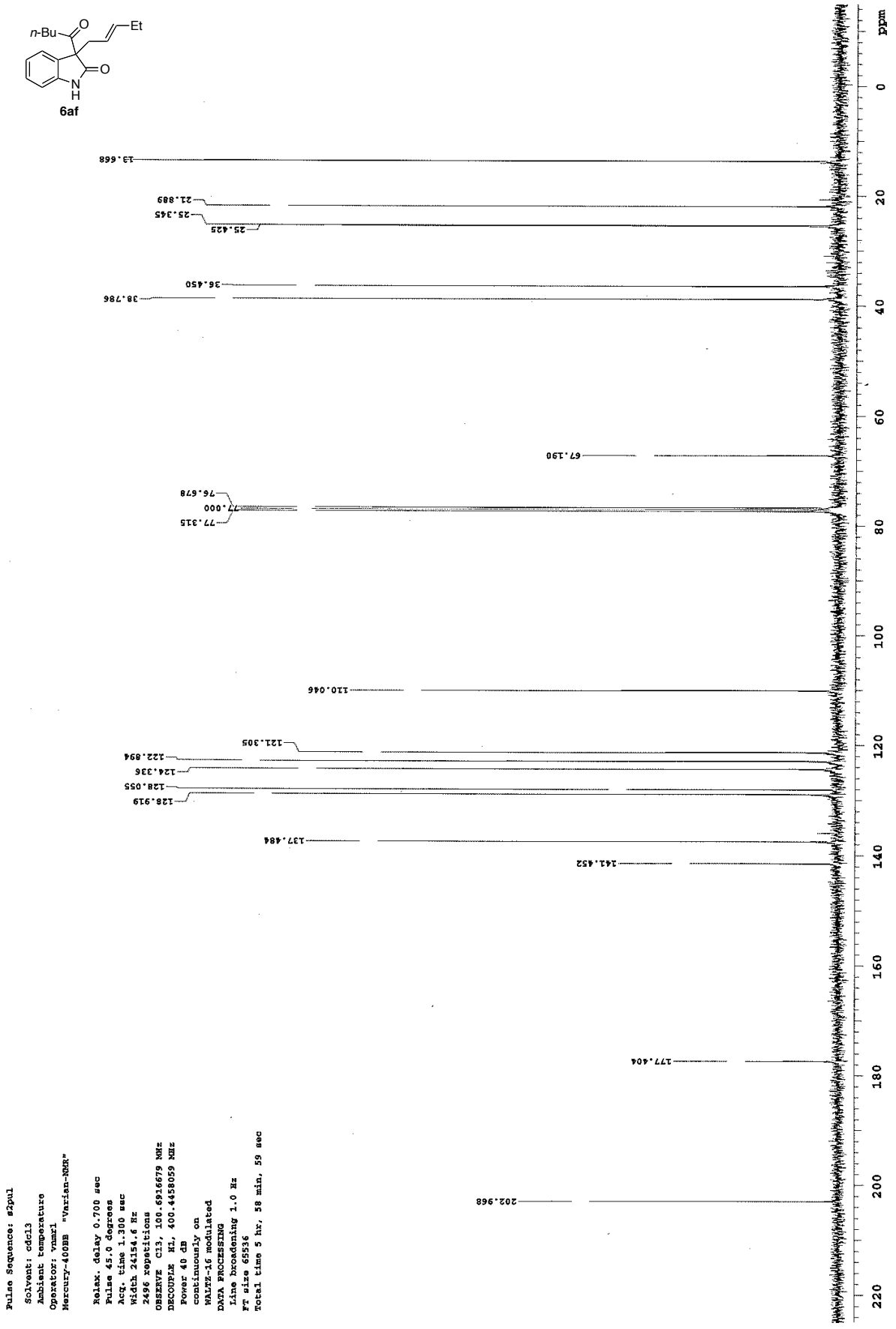
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437687 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec

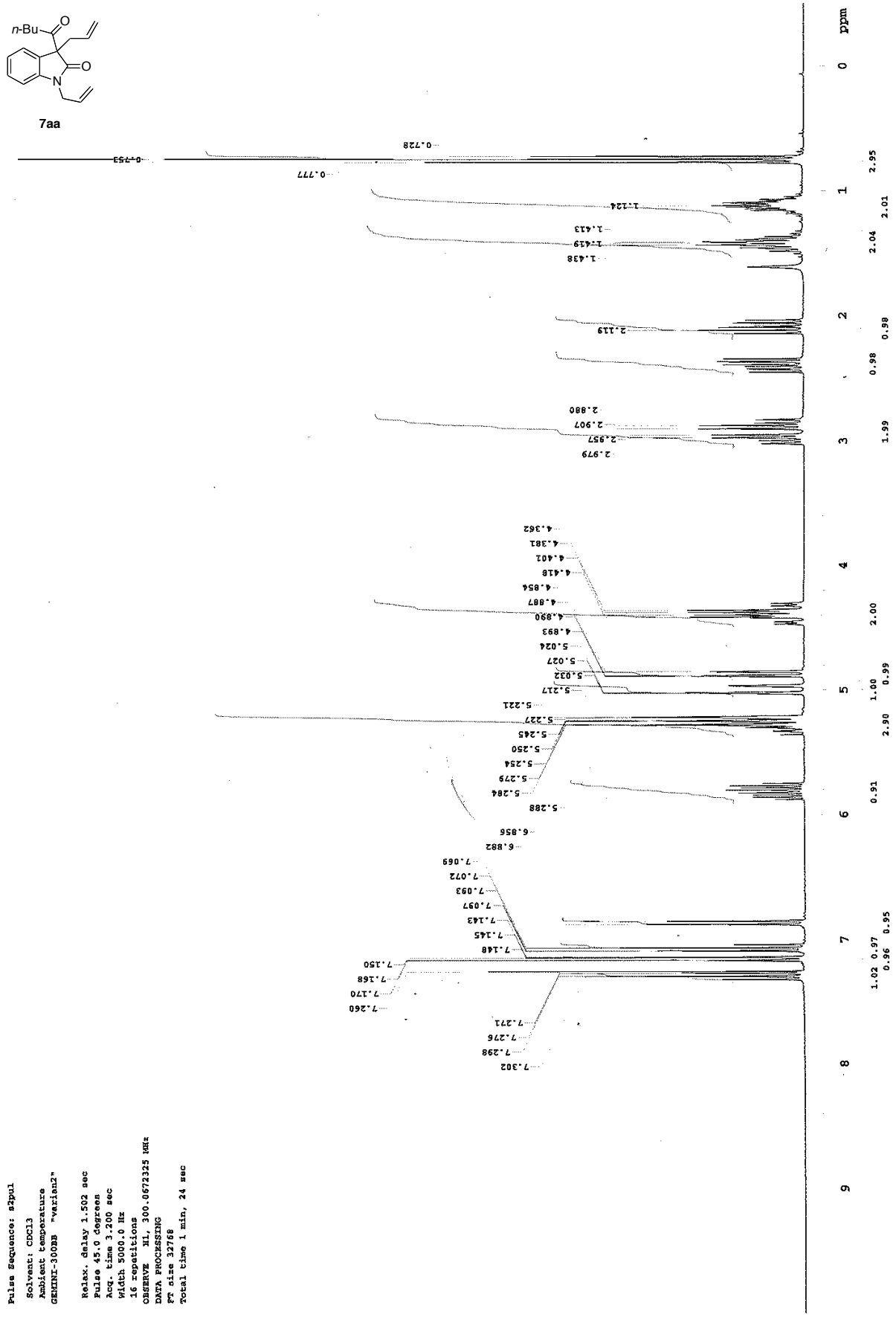

Ph
O
O
N
H
6bd
17.907
25.850
34.598
65.133
76.685
77.000
77.322
110.551
116.283
123.033
124.014
127.967
128.092
128.406
128.992
129.885
132.674
136.496
140.998
178.400
194.842
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmrl
File: Oxindole_Ph_prenyl_13C
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
5504 repetitions
OBSERVE C13, 100.6916702 MHz
DECOUPLE H1, 400.4458059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 5 hr, 58 min, 59 sec

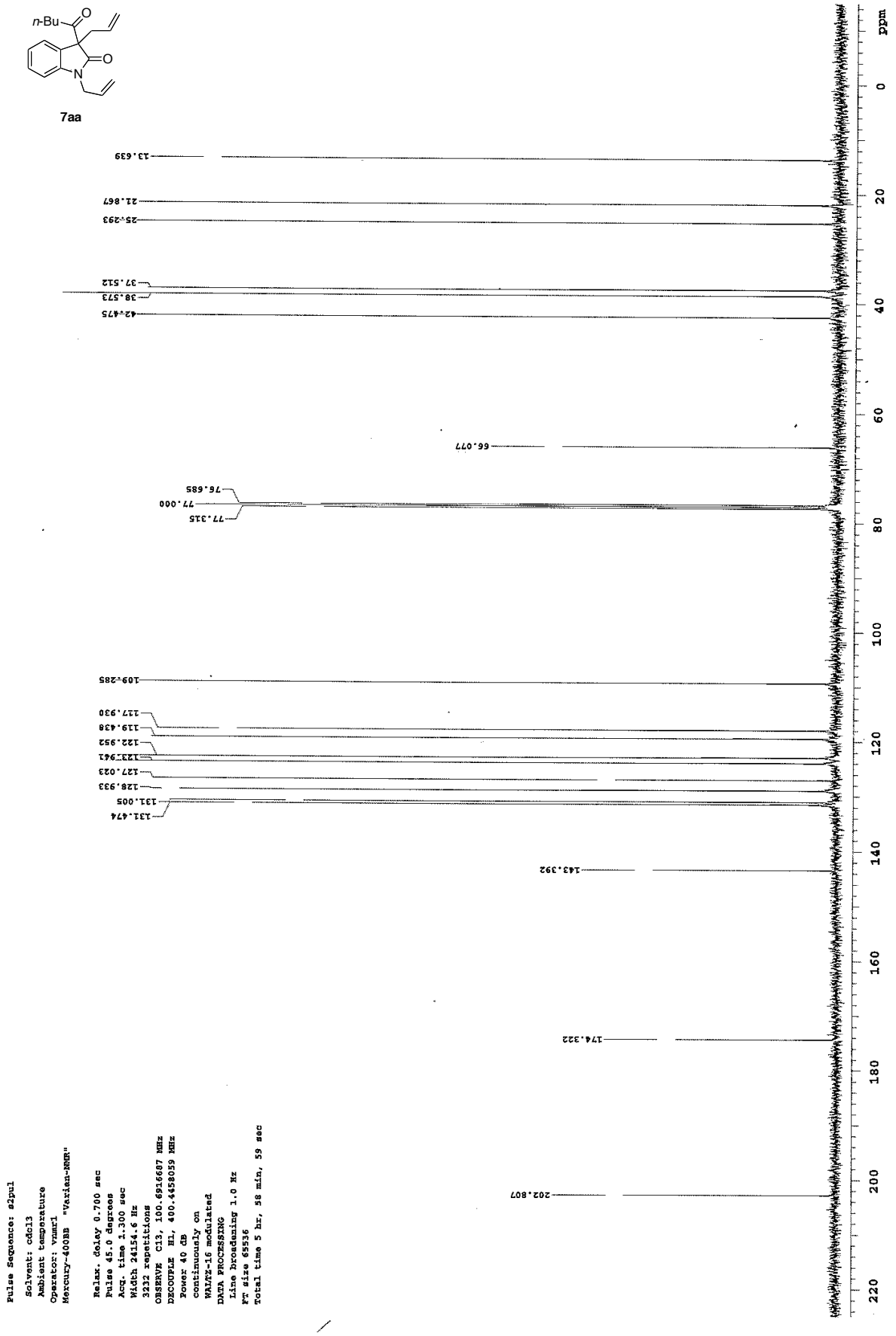

n-Bu
n-Pr
O
O
N
H
6ae
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.502 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 5000.0 Hz
48 repetitions
OBSERVE H1, 300.0672325 MHz
DATA PROCESSING
FT size 32768
Total time 5 min, 37 sec
ppm

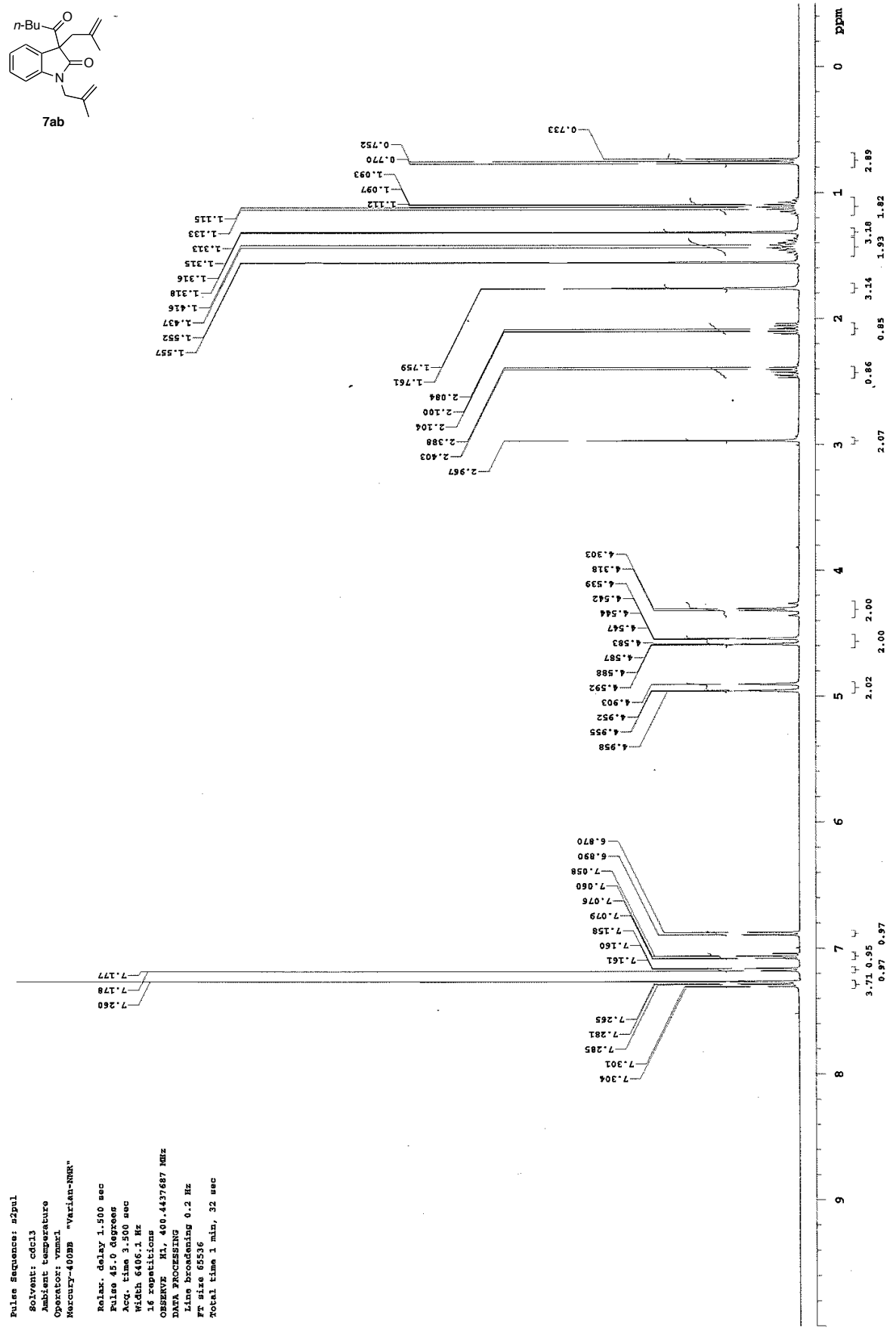

n-Bu
n-Pr
O
O
N
H
6ae
13.258
13.675
21.889
22.270
25.359
34.386
36.538
38.749
67.227
76.693
77.015
77.329
110.148
122.477
122.916
124.292
128.055
128.941
135.734
141.533
177.573
202.983
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmrl
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
4496 repetitions
OBSERVE C13, 100.6916672 MHz
DECOUPLE H1, 400.4458059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 6 hr, 19 min, 25 sec

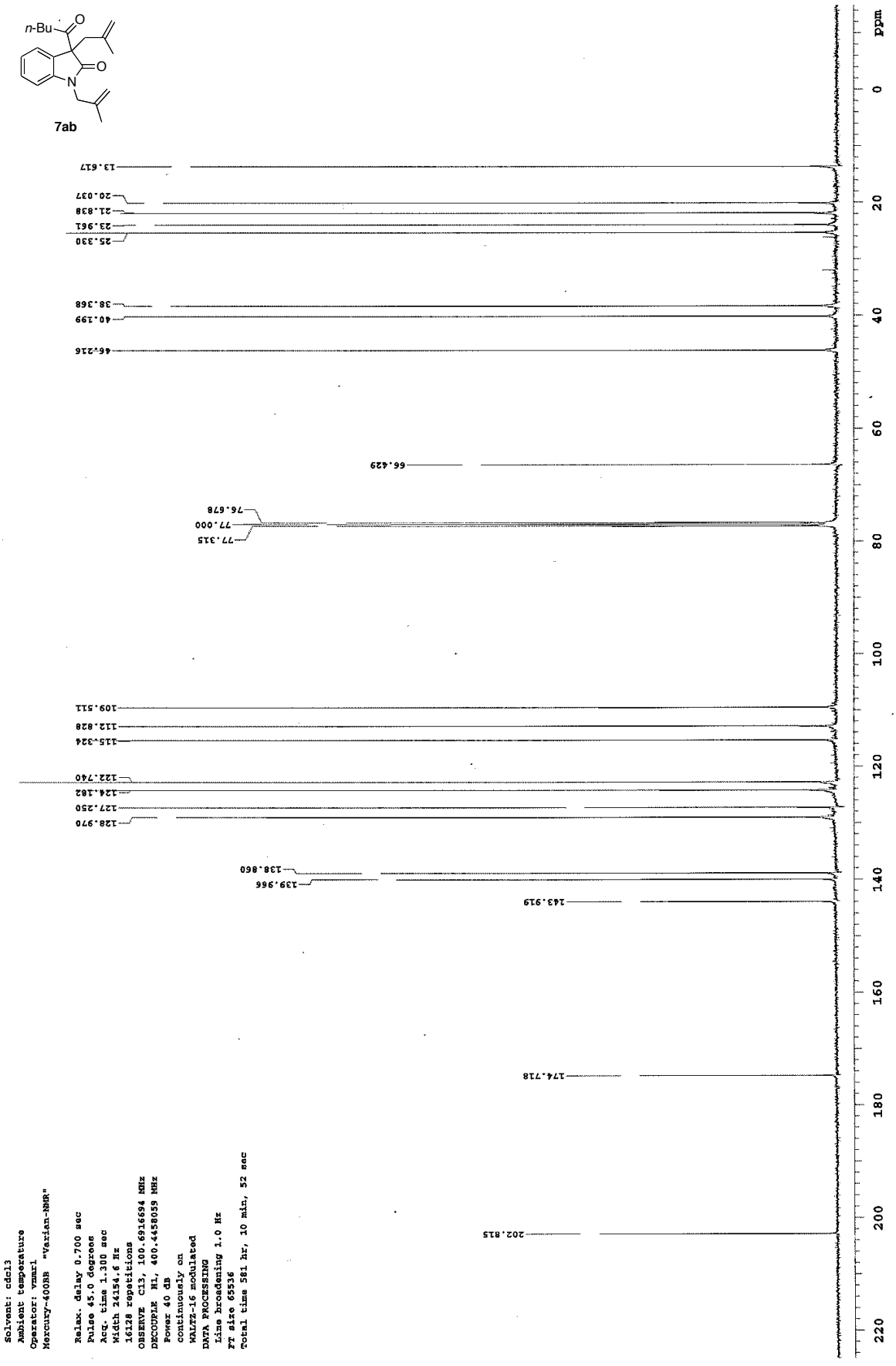

n-Bu
Et
O
O
N
H
6af
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.502 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 5000.0 Hz
16 repetitions
OBSERVE H1, 300.0672319 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 24 sec
ppm

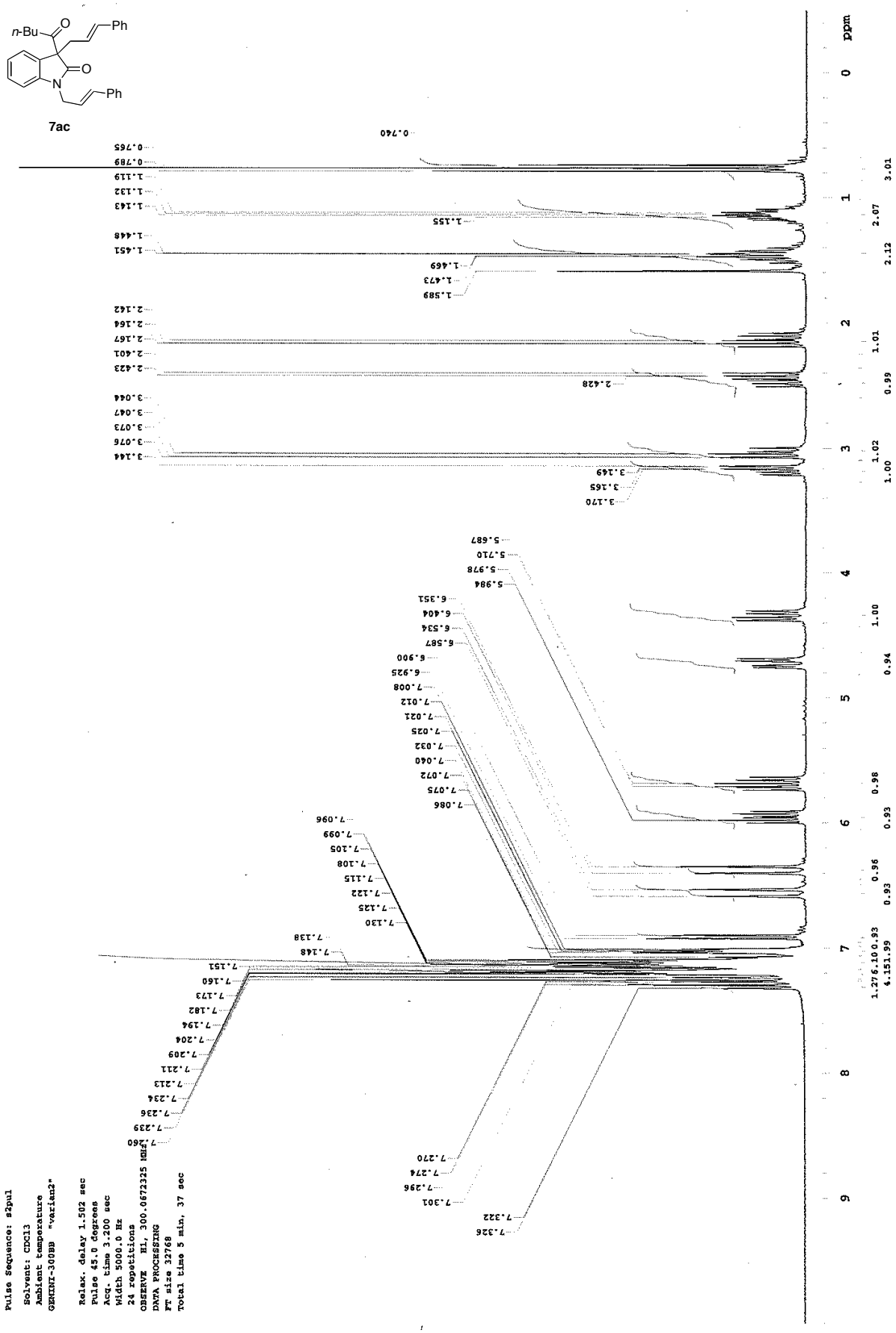

n-Bu
O
Et
O
N
H
6af
13.668
21.889
25.345
25.425
36.450
38.786
67.190
76.678
77.000
77.315
110.046
121.305
122.894
124.336
128.055
128.919
137.484
141.452
177.404
202.968
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
2496 repetitions
OBSERVE C13, 100.6916679 MHz
DECOUPLE H1, 400.4458059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 5 hr, 58 min, 59 sec

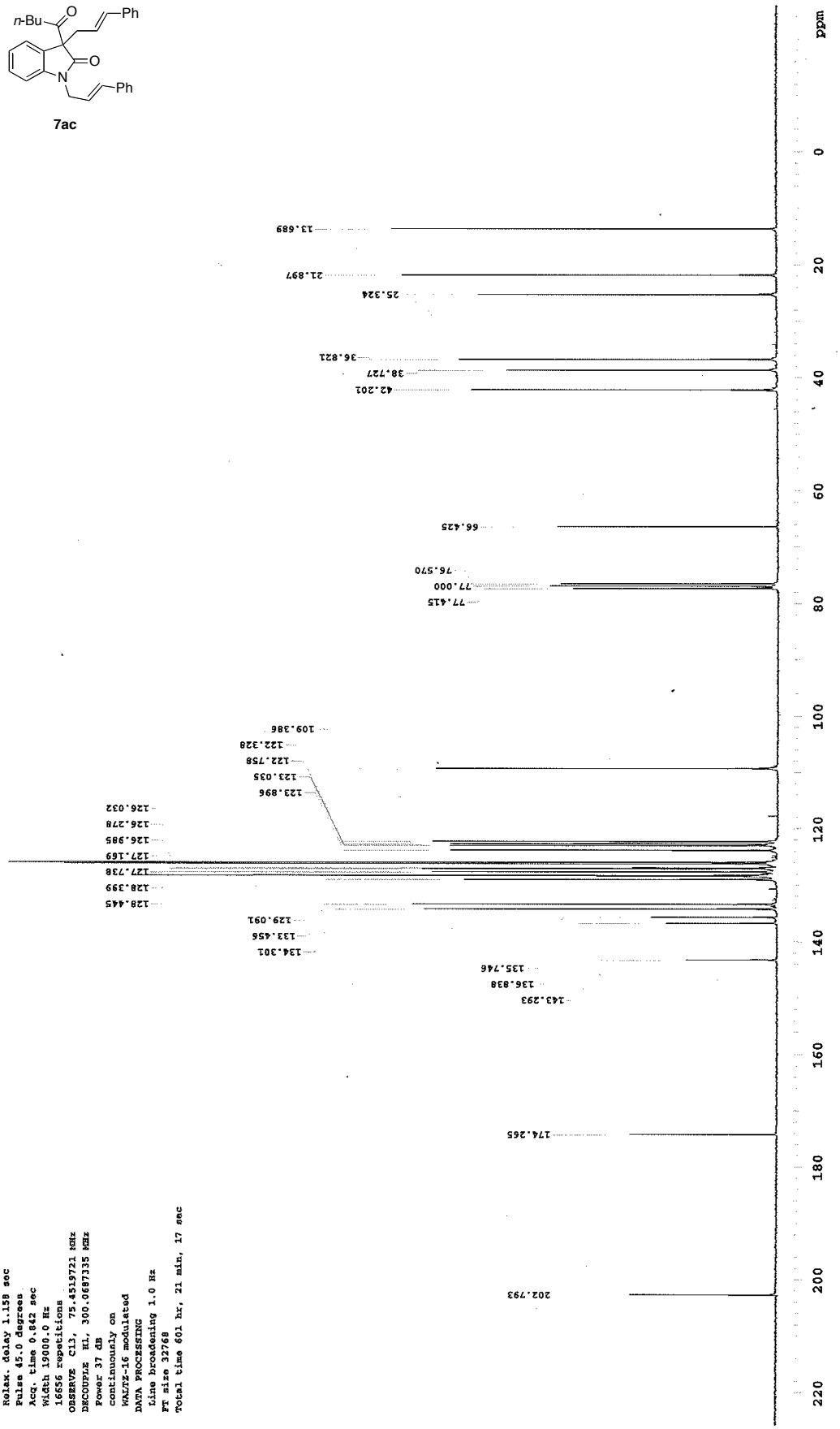

n-Bu
O
O
N
7aa
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.502 sec
Pulse 45.0 degree
Acq. time 3.200 sec
Width 5000.0 Hz
16 repetitions
OBSERVE H1, 300.0672325 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 24 sec
ppm


n-Bu
O
O
N
7aa
13.639
21.867
25.293
37.512
38.573
42.475
66.077
76.685
77.000
77.315
109.285
117.930
119.438
122.952
123.941
127.023
128.933
131.005
131.474
143.392
174.322
202.807
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
3232 repetitions
OBSERVE C13, 100.6916687 MHz
DECOUPLE H1, 400.4458059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line Broadening 1.0 Hz
FT size 65536
Total time 5 hr, 58 min, 59 sec


n-Bu
O
O
N
7ab
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
Mercury-400BB "Varian-NMR"
Relax. delay 1.500 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6406.1 Hz
16 repetitions
OBSERVE H1, 400.4437687 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min, 32 sec
ppm


n-Bu
O
O
N
7ab
13.617
20.037
21.838
23.961
25.330
38.368
40.199
46.216
66.429
76.678
77.000
77.315
109.511
112.828
115.334
122.740
124.182
127.250
128.970
138.860
139.966
143.919
174.718
202.815
ppm
0
20
40
60
80
100
120
140
160
180
200
220
Solvent: cdcl3
Ambient temperature
Operator: vnmrl
Mercury-400BB "Varian-NMR"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24154.6 Hz
16128 repetitions
OBSERVE C13, 100.6916694 MHz
DECOUPLE H1, 400.4458059 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 581 hr, 10 min, 52 sec


n-Bu
O
Ph
O
N
Ph
7ac
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
GEMINI-300BB "varian2"
Relax. delay 1.502 sec
Pulse 45.0 degrees
Acq. time 3.200 sec
Width 5000.0 Hz
24 repetitions
OBSERVE H1, 300.0672325 MHz
DATA PROCESSING
FT size 32768
Total time 5 min, 37 sec
ppm


n-Bu
O
Ph
O
N
Ph
7ac
ppm
0
20
40
60
80
100
120
140
160
180
200
220
13.689
21.897
25.324
36.821
38.727
42.201
66.425
76.570
77.000
77.415
109.386
122.328
122.758
123.035
123.896
126.032
126.278
126.985
127.169
127.738
128.399
128.445
129.091
133.456
134.301
135.746
136.838
143.293
174.265
202.793
Relax. delay 1.158 sec
Pulse 45.0 degrees
Acq. time 0.842 sec
Width 19000.0 Hz
16656 repetitions
OBSERVE C13, 75.4519721 MHz
DECOUPLE H1, 300.0687335 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 601 hr, 21 min, 17 sec