Stereospecific and Efficient Alkynylation at the More Hindered Carbon of Trisubstituted Epoxides

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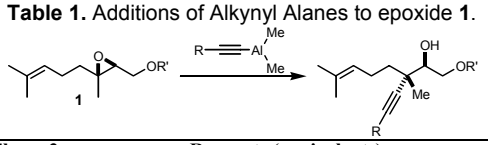
Optimization of Alane Additions

The normal reactivity manifold for alkyl and alkynyl alanes with *disubstituted* 2,3-epoxy alcohols is for C(3) addition, but their performance with *trisubstituted* geraniol epoxide **1**, an archetypal epoxide, was lackluster (Table 1). Temperature had no noticeable effect on yield (result not shown), and therefore the reactions reported in Table 1 were all carried out at 0 °C. Non-coordinative solvents gave similar yields (entries 6 and 7), and polar solvents, such as diethyl ether and THF, suppressed the reaction (entries 8 and 9), protecting the alcohol as its benzyl ether had no effect on yields (entry 10), pentyne and substrates with a simple ether functionality were even less effective reagents (entries 11 and 12). Epoxide activation with Me_3Al led to competitive methyl addition (entry 13). The most efficient results with alane additions were observed with activation with more Lewis-acidic BF_3•OEt_2 increased the yield to 44% while requiring only 1 equivalent of alane (entries 14 and 15).

Table 1. Additions of Alkynyl Alanes to epoxide **1**.



	Alkyne 2			Reagents (equivalents)					Isolated
Entry	R	eq	Sol.	^{n}BuLi	Me_2AlCl	BF_3[a]	Me_3Al	R'	Yield
1	Ph	2.2	CH_2Cl_2	2.1	2.0	–	–	H	38%
2	Ph	4.5	CH_2Cl_2	4.2	4.0	–	–	H	56%
3	Ph	4.5	CH_2Cl_2	4.2	2.0	–	–	H	33%
4	Ph	4.5	CH_2Cl_2	4.0	6.0	–	–	H	35%[b]
5	Ph	10	CH_2Cl_2	10	8.0	–	–	H	55%
6	Ph	4.5	Hexanes	4.2	4.0	–	–	H	54%
7	Ph	4.5	Toluene	4.2	4.0	–	–	H	55%
8	Ph	4.5	Et_2O	4.2	4.0	–	–	H	nr[c]
9	Ph	4.5	THF	4.2	4.0	–	–	H	nr
10	Ph	4.5	CH_2Cl_2	4.2	4.0	–	–	Bn	53%
11	^{n}Pr	4.5	CH_2Cl_2	4.2	4.0	–	–	H	32%
12	[d]	4.5	CH_2Cl_2	4.2	4.0	–	–	Bn	24%
13	Ph	1.2	CH_2Cl_2	1.2	1.1	–	1.0	Bn	33%[e]
14	Ph	4.5	CH_2Cl_2	4.2	4.0	2.0	–	Bn	54%
15	Ph	1.2	Et_2O	1.2	1.1	2.0	–	Bn	44%

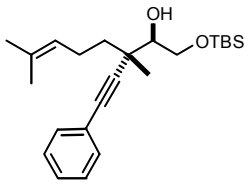
[a] BF_3•OEt_2. [b] plus 12% C(3) chloride addition. [c] no reaction. [d] R = $TBSOCH_2$. [e] plus 18% C(3) methyl addition.

Experimental section

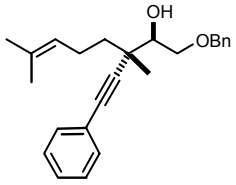
All reactions were run with stirring under an atmosphere of argon unless otherwise indicated. Flasks were oven or flamed-dried and allowed to cool in a desiccator prior to use.

Solvents and reagents were purified by standard methods.[1] Reaction progress was monitored by thin layer chromatography (TLC) using EM 250 Kieselgel 60 F254 silica gel plates. The plates were visualized by staining with CAM or potassium permanganate. HRMS (CI) was made with a VG analytical ZAB2-E instrument. Epoxides were prepared either according to Sharpless epoxidation[2] or by *m*-CPBA oxidation of known alkenes.[3-5]

Representative General Procedure:



1-(*tert*-Butyl-dimethyl-silanyloxy)-3,7-dimethyl-3-phenyl-ethynyl-oct-6-en-2-ol (8b). To a 0 °C solution of phenylacetylene (72 μL, 0.65 mmol) in Et_2O (3 mL) was added *n*-BuLi (27 μL, 0.65 mmol, 2.41 M solution in hexanes) dropwise followed by Me_3Al (31 μL, 0.62 mmol, 2.0 M solution in toluene) 30 min later. The resultant mixture was allowed to warm to room temperature and after 30 min geraniol epoxy ether **1b** (147 mg, 0.52 mmol) was added. The reaction mixture was cooled to –78 °C and BF_3•Et_2O (0.13 mL, 1.04 mmol) was added dropwise over ca. 2 min. When the reaction was complete (TLC, 1.5 h), dry MeOH (0.6 mL) was added at –78 °C, and after 15 min the resulting mixture was poured into 0 °C pH 10 $NaHCO_3$ / NaOH buffer (20 mL). The heterogeneous mixture was vigorously stirred for 10 min, the organic phase was separated, and the aqueous solution was extracted with EtOAc (3 x 20 mL). Concentration of the combined organic layers and purification of the residual oil by silica gel chromatography afforded a colorless oil (147 mg, 73%). R_f 0.33 (15% EtOAc/hexanes); IR (thin film) ν 3600-3250, 2959, 2881, 2850, 2333 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.38-7.35 (m, 2H), 7.28-7.24 (m, 3H), 5.16 (t, *J* = 7.2 Hz, 1H), 3.97 (dd, *J* = 3.3 Hz, 9.9 Hz, 1H), 374 (dd, *J* = 7.8 Hz, 7.8 Hz, 1H), 3.67-3.63 (m, 1H), 2.67 (d, *J* = 3.0 Hz, 1H), 2.27-2.15 (m, 2H), 1.67 (s, 3H), 1.63 (s, 3H), 1.72-1.59 (m, 1H), 1.54-1.44 (m, 1H), 1.25 (s, 3H), 0.90 (s, 9H), 0.09 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 131.7, 131.5, 128.2, 127.7, 124.3, 123.7, 93.5, 83.3, 75.4, 64.4, 38.8, 38.8, 25.9, 25.7, 23.5, 21.3, 18.3, 17.7, -5.30, -5.33; HRMS m/z calcd for $C_{24}H_{39}O_2Si$ $[M+H]^+$ 387.2719, found: 387.2715.



(2R,3S)-1-benzyloxy-3,7-dimethyl-3-phenylethynyl-oct-6-en-2-ol (8a). The title compound was prepared from phenylacetylene and **1a** according to the procedure used for **8b** (yellow oil, 142 mg, 76%). R_f 0.33 (15% EtOAc/ hexanes); IR (thin film) ν 3600-3200, 2970, 2914, 2853, 2330 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.35-7.25 (m, 10H), 5.16 (t, *J* = 6.9 Hz, 1H), 4.59 (s, 2H), 3.91 (dd, *J* = 2.7 Hz, 9.3 Hz, 1H), 3.85 (ddd, *J* = 8.1 Hz, 3.3 Hz, 3.3 Hz, 1H), 3.62 (dd, *J* = 8.7 Hz, 8.7 Hz, 1H), 2.52 (d, *J* = 3.3 Hz, 1H), 2.27-2.13 (m, 2H), 1.68 (s, 3H), 1.63 (s, 3H), 1.74-1.61 (m, 1H), 1.54-1.44 (m, 1H), 1.26 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.0, 131.8, 131.6, 128.5, 128.2, 127.8, 124.2, 123.5, 93.3, 83.4, 74.3, 73.4, 72.0, 38.8, 38.6, 25.7, 23.5, 21.3, 17.6; HRMS m/z calcd for $C_{25}H_{31}O_2$ $[M+H]^+$ 363.2324, found: 363.2323.

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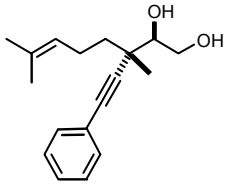
[1] Armarego, W. L. F.; Perrin, D. D. *Purification of Laboratory Chemicals*; 4th Ed.; Oxford: Butterworth Heinemann, 1996.

[2] See footnote 50 in: Gao, Y.; Hanson, R. M.; Klunder, J. M.; Ko, S. Y.; Masamune, H.; Sharpless, K. B. *J. Am. Chem. Soc.* **1987**, *109*, 5765-5780.

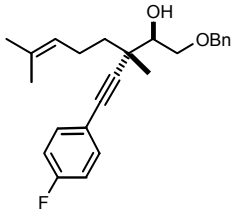
[3] Mori, K.; Hazra, B. G.; Pfeiffer, R. J.; Gupta A. K.; Lindgren, B, S. *Tetrahedron* **1987**, 43, 2249-2254.

[4] Meyers, A. I.; Collington, E. W. *Tetrahedron* **1971**, 27, 5979-5985.

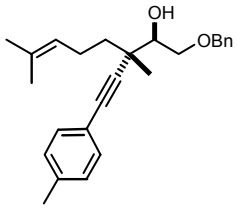
[5] Malnar, I.; Juric, S.; Vrcek, V.; Zjuranovic, Z.; Mihalic, Z.; Kronja, O. *J. Org. Chem.* **2002**, 67, 1490-1495.



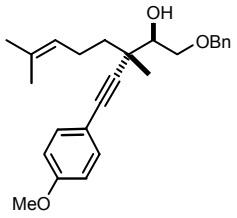
3,7-Dimethyl-3-phenylethynyl-oct-6-ene-1,2-diol (8c). The title compound was prepared from geraniol epoxide **1c** and 2.2 equivalents of phenylacetylene-aluminum ate complex according to the procedure used for **8b** (yellow oil, 86 mg, 61%). R_f 0.42 (40% EtOAc/ hexanes); IR (thin film) ν 3650-3050, 2971, 2940, 2874, 2334 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.39-7.34 (m, 2H), 7.29-7.25 (m, 3H), 5.14 (t, *J* = 7.1 Hz, 1H), 3.93 (d, *J* = 8.1 Hz, 1H), 3.74-3.62 (m, 2H), 2.39 (br, 1H), 2.22-2.16 (m, 3H), 1.68 (s, 3H), 1.62 (s, 3H), 1.49-1.08 (m, 2H), 1.29 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 132.0, 131.6, 128.2, 128.0, 124.0, 123.1, 92.6, 84.1, 76.8, 63.7, 39.4, 38.0, 25.7, 23.5, 22.0, 17.7; HRMS m/z calcd for $C_{18}H_{25}O_2$ $[M+H]^+$ 273.1855, found: 273.1859.



1-Benzyloxy-3-(4-fluoro-phenylethynyl)-3,7-dimethyl-oct-6-en-2-ol (9a). The title compound was prepared from 1-ethynyl-4-fluoro-benzene and **1a** according to the procedure used for **8b** (yellow oil, 132 mg, 67%). R_f 0.35 (15% EtOAc/hexanes); IR (thin film) ν 3600-3200, 2971, 2924, 2870, 2337 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.40-7.29 (m, 7H), 7.01 (dd, *J* = 9.0 Hz, 9.0 Hz, 2H), 5.21 (t, *J* = 7.2 Hz, 1H), 4.64 (s, 2H), 3.96-3.88 (m, 2H), 3.66 (t, *J* = 9.0 Hz, 1H), 2.54 (d, *J* = 3.0 Hz, 1H), 2.30-2.17 (m, 2H), 1.79-1.49 (m, 2H), 1.74 (s, 3H), 1.68 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.8, 160.5, 137.9, 133.4, 133.3, 131.8, 128.4, 127.7, 124.1, 119.6, 119.5, 115.5, 115.2, 92.9, 82.3, 74.3, 73.3, 71.9, 38.8, 38.5, 25.7, 23.5, 21.3, 17.6; HRMS m/z calcd for $C_{25}H_{29}FO_2$ $[M+H]^+$ 381.2230, found: 381.2240.

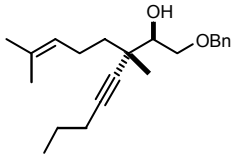


1-Benzyloxy-3,7-dimethyl-3-*p*-tolylethynyl-oct-6-en-2-ol (10a). The title compound was prepared from 1-ethynyl-4-methyl-benzene and **1a** according to the procedure used for **8b** (yellow oil, 144 mg, 74%). R_f 0.35 (15% EtOAc/hexanes); IR (thin film) ν 3600-3150, 2971, 2920, 2862, 2337 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.36-7.29 (m, 5H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 2H), 5.17 (t, *J* = 7.2 Hz, 1H), 4.59 (s, 2H), 3.92 (dd, *J* = 2.4 Hz, 9.3 Hz, 1H), 3.86 (ddd, *J* = 2.7 Hz, 2.7 Hz, 8.7 Hz, 1H), 3.62 (dd, *J* = 9.0 Hz, 9.0 Hz, 1H), 2.54 (d, *J* = 3.3 Hz, 1H), 2.33 (s, 3H), 2.27-2.16 (m, 2H), 1.75-1.66 (m, 1H), 1.69 (s, 3H), 1.64 (s, 3H), 1.54-1.44 (m, 1H), 1.26 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.0, 137.7, 131.7, 131.4, 128.9, 128.4, 127.7, 124.3, 120.4, 92.4, 83.4, 74.3, 73.3, 72.0, 38.8, 38.6, 25.7, 23.5, 21.4, 21.3, 17.6; HRMS m/z calcd for $C_{26}H_{33}O_2$ $[M+H]^+$ 377.2481, found: 381.2486.

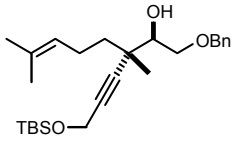


1-Benzyloxy–3-(4–methoxy-phenylethynyl)-3,7-dimethyl-oct-6-en-2-ol (11a). The title compound was prepared from 1-ethynyl-4-methoxy-benzene and **1a** according to the procedure used for **8b** (colorless oil, 156 mg, 77%). R_f 0.35 (15% EtOAc/hexanes); IR (thin film) ν 3600-3150, 2967, 2917, 2862, 2342 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.35-7.28 (m, 5H), 7.26 (d, *J* = 8.8 Hz, 2H), 6.80 (d, 8.8 Hz, 2H), 5.16 (tt, *J* = 1.2 Hz, 7.2 Hz, 1H), 4.59 (s, 2H), 3.91 (dd, *J* = 2.8 Hz, 9.2 Hz, 1H), 3.85 (ddd, *J* = 2.8 Hz, 2.8 Hz, 8.4 Hz, 1H), 3.79 (s, 3H), 3.62 (dd, *J* = 8.8 Hz, 9.2 Hz, 1H), 2.53 (d, *J* = 3.6 Hz, 1H), 2.26-2.16 (m, 2H), 1.73-1.60 (m, 1H), 1.69 (s, 3H), 1.63 (s, 3H), 1.52-1.45 (m, 1H), 1.26 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 138.0, 132.9, 131.7, 128.4, 127.7, 124.3, 115.7, 113.7, 91.6, 83.2, 74.4, 73.3, 72.0, 55.3,

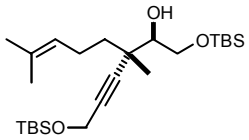
38.8, 38.6, 25.7, 23.5, 21.4, 17.6; HRMS m/z calcd for $C_{26}H_{33}O_3$ $[M+H]^+$ 393.2430, found: 393.2436.



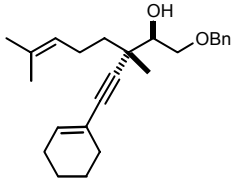
1-Benzyloxy-3,7-dimethyl-3-pent-1-ynyl-oct-6-en-2-ol (12a). The title compound was prepared from 1-pentyne and **1a** according to the procedure used for **8b** (colorless oil, 123 mg, 72%). R_f 0.33(15% EtOAc/hexanes); IR (thin film) ν 3700-3100, 2967, 2928, 2870, 2338 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.34-7.26 (m, 5H), 5.11 (t, *J* = 7.2 Hz, 1H), 4.56 (s, 2H), 3.82 (dd, *J* = 2.7 Hz, 9.6 Hz, 1H), 3.71 (ddd, *J* = 8.4 Hz, 3.0 Hz, 3.0 Hz, 1H), 3.52 (t, *J* = 8.4 Hz, 1H), 2.41 (d, *J* = 3.3 Hz, 1H), 2.10 (t, *J* = 6.9 Hz, 2H), 2.17-2.05 (m, 2H), 1.66 (s, 3H), 1.60 (s, 3H), 1.55-1.29 (m, 4H), 1.13 (s, 3H), 0.93 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.3, 131.8, 128.7, 128.0, 124.7, 83.9, 83.5, 74.9, 73.6, 72.3, 38.8, 38.6, 26.0, 23.7, 22.7, 22.1, 20.9, 17.8, 13.7; HRMS m/z calcd for $C_{22}H_{33}O_2$ $[M+H]^+$ 329.2481, found: 329.2479.



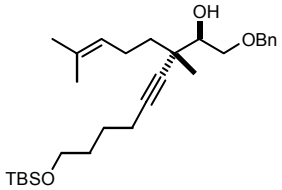
1-Benzyloxy-3-[3-(*tert*-butyl-dimethyl-silanyloxy)-prop-1-ynyl]-3,7-dimethyl-oct-6-en-2-ol (13a). The title compound was prepared from *tert*-butyl-dimethyl-prop-2-ynyloxy-silane and **1a** according to the procedure used for **8b** (colorless oil, 188 mg, 71%). R_f 0.33 (15% EtOAc/ hexanes); IR (thin film) ν 3600-3250, 2959, 2928, 2854, 2229 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.34-7.26 (m, 5H), 5.10 (tt, *J* = 1.5 Hz, 7.2 Hz, 1H), 4.55 (s, 2H), 4.28 (s, 2H), 3.82 (dd, *J* = 2.7 Hz, 9.3 Hz, 1H), 3.74 (ddd, *J* = 2.7 Hz, 2.7 Hz, 8.4 Hz, 1H), 3.53 (dd, *J* = 8.7 Hz, 8.7 Hz, 1H), 2.45 (d, *J* = 3.0 Hz, 1H), 2.17-2.05 (m, 2H), 1.66 (s, 3H), 1.59 (s, 3H), 1.61-1.52 (m, 1H), 1.43-1.33 (m, 1H), 1.16 (s, 3H), 0.89 (s, 9H), 0.09 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.0, 131.7, 128.4, 127.8, 127.7, 124.2, 88.3, 81.8, 74.2, 73.4, 71.9, 51.8, 38.3, 38.3, 25.8, 25.7, 23.3, 21.3, 18.2, 17.6, -5.1; HRMS m/z calcd for $C_{26}H_{43}O_3Si$ $[M-H]^+$ 431.2981, found: 431.2983.



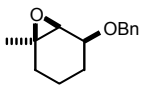
1-Benzyloxy-3-[3-(*tert*-butyl-dimethyl-silanyloxy)-prop-1-ynyl]-3,7-dimethyl-oct-6-en-2-ol (13b). The title compound was prepared from *tert*-butyl-dimethyl-prop-2-ynyloxy-silane and **1b** according to the procedure used for **8b** (colorless oil, 158 mg, 67%). R_f 0.33 (7% EtOAc/ hexanes); ^1H NMR (300 MHz, $CDCl_3$) δ 5.10 (tt, *J* = 1.5 Hz, 7.2 Hz, 1H), 4.29 (s, 2H), 3.88 (dd, *J* = 3.3 Hz, 9.6 Hz, 1H), 3.63 (dd, *J* = 7.8 Hz, 9.3 Hz, 1H), 3.53 (d, *J* = 8.1 Hz, 1H), 2.61 (d, *J* = 2.7 Hz, 1H), 2.17-2.03 (m, 2H), 1.66 (s, 3H), 1.60 (s, 3H), 1.62-1.52 (m, 1H), 1.44-1.33 (m, 1H), 1.14 (s, 3H), 0.88 (s, 18H), 0.09 (s, 6H), 0.06 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 131.6, 124.3, 88.3, 81.6, 75.2, 64.2, 51.8, 38.6, 38.1, 25.8, 25.7, 23.3, 21.2, 18.2, 17.6, -5.1, -5.3, -5.4;



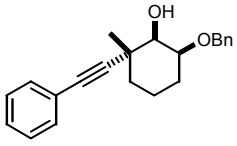
1-Benzyloxy-3-cyclohex-1-enylethynyl-3,7-dimethyl-oct-6-en-2-ol (14a). The title compound was prepared from ethynylcyclohexene and **1a** according to the procedure used for **8b** (yellow oil, 162 mg, 85%). R_f 0.33 (15% EtOAc/hexanes); IR (thin film) ν 3650-3150, 2975, 2928, 2854, 2722, 2338 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.34-7.26 (m, 5H), 5.96 (m, 1H), 5.13 (tt, *J* = 1.6 Hz, 7.2 Hz, 1H), 4.57 (s, 2H), 3.84 (dd, *J* = 2.4 Hz, 9.2 Hz, 1H), 3.76 (dd, *J* = 2.8 Hz, 8.8 Hz, 1H), 3.55 (dd, *J* = 9.2 Hz, 9.2 Hz, 1H), 2.20-2.04 (m, 6H), 1.68 (s, 3H), 1.62 (s, 3H), 1.56-1.54 (m, 5H), 1.45-1.37 (m, 1H), 1.19 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.0, 133.7, 131.6, 128.4, 127.7, 127.7, 124.3, 120.6, 90.2, 85.2, 74.4, 73.3, 72.0, 38.7, 38.6, 29.5, 25.7, 25.5, 23.5, 22.3, 21.5, 21.5, 17.6; HRMS m/z calcd for $C_{25}H_{35}O_2$ $[M+H]^+$ 367.2637, found: 367.2637.



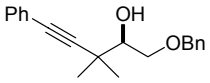
1-Benzyloxy-9-(*tert*-butyl-dimethyl-silanyloxy)-3-methyl-3-(4-methyl-pent-3-enyl)-non-4-yn-2-ol (15a). The title compound was prepared from *tert*-butyl-hex-5-ynyloxy-dimethyl-silane and **1a** according to the procedure used for **8b** (colorless oil, 199 mg, 81%). R_f 0.33 (15% EtOAc/ hexanes); IR (thin film) ν 3650-3150, 2951, 2920, 2858, 2334 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$) δ 7.37-7.25 (m, 5H), 5.11 (tt, *J* = 1.5 Hz, 7.2 Hz, 1H), 4.56 (s, 2H), 3.81 (dd, *J* = 2.4 Hz, 9.3 Hz, 1H), 3.71 (d, *J* = 8.7 Hz, 1H), 3.61-3.49 (m, 3H), 2.43 (d, *J* = 3.3 Hz, 1H), 2.16 (t, *J* = 6.9 Hz, 2H), 2.19-2.05 (m, 2H), 1.66 (s, 3H), 1.59 (s, 3H), 1.64-1.47 (m, 5H), 1.39-1.24 (m, 1H), 1.13 (s, 3H), 0.88 (s, 9H), 0.03 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 138.1, 131.5, 128.4, 127.7, 124.4, 83.6, 83.1, 74.6, 73.3, 72.0, 62.7, 38.6, 38.3, 31.9, 25.9, 25.7, 25.5, 23.4, 21.8, 18.5, 18.3, 17.6, -5.3; HRMS m/z calcd for $C_{29}H_{49}O_3Si$ $[M+H]^+$ 473.3451, found: 473.3456.



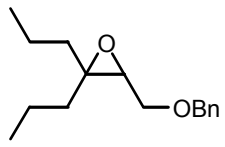
5-Benzyloxy-1-methyl-7-oxa-bicyclo[4.1.0]heptane. ^1H NMR (400 MHz, $CDCl_3$) δ 7.39-7.25 (m, 5H), 4.66 (s, 2H), 3.77 (ddd, *J* = 2.4 Hz, 5.6 Hz, 8.0 Hz, 1H), 3.12 (d, *J* = 2.0 Hz, 1H), 1.85-1.78 (m, 1H), 1.66-1.51 (m, 5H), 1.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 128.3, 127.7, 127.5, 74.2, 70.0, 60.3, 60.0, 28.4, 24.7, 24.0, 19.4.



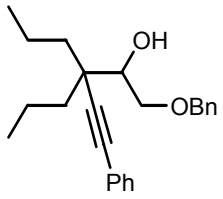
6-Benzyloxy-2-methyl-2-phenylethynyl-cyclohexanol. The title compound was prepared from phenylacetylene and 5-benzyloxy-1-methyl-7-oxa-bicyclo[4.1.0]heptane according to the procedure used for **8b** (colorless oil, 143 mg, 89%). R_f 0.33 (15% EtOAc/hexanes); IR (thin film) ν 3697-3250, 2937, 2863, 1945, 1454 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36-7.26 (m, 10H), 4.62 (d, *J* = 11.6 Hz, 1H), 4.58 (d, *J* = 12.0 Hz, 1H), 3.94-3.91 (m, 2H), 2.27 (br, 1H), 1.78-1.45 (m, 6H), 1.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 131.5, 128.4, 128.2, 127.79, 127.75, 127.7, 123.5, 94.0, 83.4, 76.9, 72.7, 70.1, 37.4, 31.6, 25.8, 24.9, 20.9; HRMS m/z calcd for $C_{22}H_{25}O_2$ $[M+H]^+$ 321.1846, found: 321.1855.



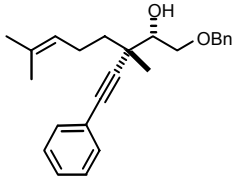
1-Benzyloxy-3,3-dimethyl-5-phenyl-pent-4-yn-2-ol. The title compound was prepared from phenylacetylene and 3-benzyloxymethyl-2,2-dimethyl-oxirane according to the procedure used for **8b** (yellow oil, 147 mg, 92%). R_f 0.30 (16% EtOAc/hexanes); IR (thin film) ν 3635-3219, 2975, 2932, 2870, 1076 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.37-7.26 (m, 10H), 4.60 (s, 2H), 3.88 (dd, *J* = 2.4 Hz, 9.2 Hz, 1H), 3.75 (dd, *J* = 2.8 Hz, 8.8 Hz, 1H), 3.63 (dd, *J* = 8.4 Hz, 9.2 Hz, 1H), 1.34 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.9, 131.6, 128.4, 128.1, 127.74, 127.72, 123.4, 94.2, 82.1, 76.0, 73.3, 71.8, 35.1, 26.4, 24.5; HRMS m/z calcd for $C_{20}H_{23}O_2$ $[M+H]^+$ 295.1698, found: 295.1686.



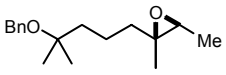
3-Benzyloxymethyl-2,2-dipropyl-oxirane. ^1H NMR (400 MHz, $CDCl_3$) δ 7.35-7.24 (m, 5H), 4.63 (d, *J* = 11.6 Hz, 1H), 4.51 (d, *J* = 12.0 Hz, 1H), 3.70 (dd, *J* = 4.4 Hz, 11.2 Hz, 1H), 3.54 (dd, *J* = 6.0 Hz, 10.8 Hz, 1H), 2.99 (dd, *J* = 4.8 Hz, 4.8 Hz, 1H), 1.64-1.56 (m, 1H), 1.53-1.33 (m, 7H), 0.93-0.89 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.9, 128.3, 127.7, 127.6, 73.1, 68.5, 62.6, 61.2, 37.0, 32.5, 18.5, 17.9, 14.3, 14.1.



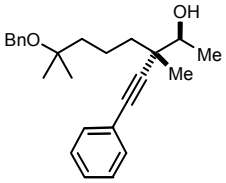
1-Benzyloxy-3-phenylethynyl-3-propyl-hexan-2-ol. The title compound was prepared from phenylacetylene and 3-benzyloxymethyl-2,2-dipropyl-oxirane according to the procedure used for **8b** (colorless oil, 91 mg, 50%). R_f 0.17 (8% EtOAc/hexanes); IR (thin film) ν 3597-3250, 2961, 2926, 2867, 1599, 1447 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35-7.25 (m, 10H), 4.61 (d, *J* = 11.6 Hz, 1H), 4.57 (d, *J* = 12.0 Hz, 1H), 3.92 (dd, *J* = 2.4 Hz, 8.8 Hz, 1H), 3.86 (dd, *J* = 2.4 Hz, 9.6 Hz, 1H), 3.64 (dd, *J* = 8.8 Hz, 8.8 Hz, 1H), 2.34 (br, 1H), 1.69-1.34 (m, 8H), 0.94 (t, *J* = 6.8 Hz, 3H), 0.92 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.0, 131.6, 128.5, 128.4, 128.1, 127.7, 127.6, 123.6, 92.8, 84.0, 73.32, 73.28, 71.9, 42.7, 37.2, 36.7, 17.8, 17.7, 14.7, 14.6; HRMS m/z calcd for $C_{24}H_{31}O_2$ $[M+H]^+$ 351.2324, found: 351.2324.



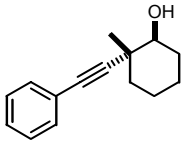
(2S,3S)-1-Benzyloxy-3,7-dimethyl-3-phenylethynyl-oct-6-en-2-ol. The title compound was prepared from phenylacetylene and nerol epoxide according to the procedure used for **8b** (yellow oil, 163 mg, 89%). R_f 0.33 (15% EtOAc/ hexanes); IR (thin film) ν 3700-3150, 2976, 2933, 2871, 2338 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35-7.25 (m, 10H), 5.15 (t, *J* = 7.2 Hz, 1H), 4.58 (s, 2H), 3.82 (dd, *J* = 9.6 Hz, 2.8 Hz, 1H), 3.77 (dd, *J* = 8.8 Hz, 2.4 Hz, 1H), 3.63 (dd, *J* = 8.0 Hz, 8.0 Hz, 1H), 2.25-2.10 (m, 2H), 1.67 (s, 3H), 1.62 (s, 3H), 1.73-1.51 (m, 2H), 1.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.0, 131.7, 131.6, 128.4, 128.1, 127.7, 124.2, 123.5, 93.1, 83.5, 75.8, 73.4, 71.6, 39.4, 37.1, 25.7, 23.5, 22.7, 17.6; HRMS m/z calcd for $C_{25}H_{31}O_2$ $[M+H]^+$ 363.2324, found: 363.2316.



2-(4-Benzyloxy-4-methyl-pentyl)2,3-dimethyl-oxirane. ^1H NMR (400 MHz, $CDCl_3$) δ 7.32-7.31 (m, 5H), 4.39 (s, 2H), 2.82 (q, *J* = 5.2 Hz, 1H), 1.61-1.39 (m, 6H), 1.26 (d, *J* = 5.6 Hz, 3H), 1.23 (s, 6H), 1.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 128.3, 127.3, 127.1, 75.1, 63.7, 60.8, 59.0, 40.5, 39.0, 25.64, 25.59, 19.6, 16.3, 14.1.

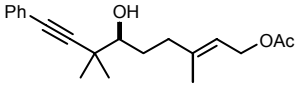


7-Benzyloxy-3,7-dimethyl-3-phenylethynyl-octan-2-ol. The title compound was prepared from phenylacetylene and 2-(4-benzyloxy-4-methyl-pentyl)-2,3-dimethyl-oxirane according to the procedure used for **8b** (yellow oil, 130 mg, 70%). R_f 0.16 (22% EtOAc/ hexanes); IR (thin film) ν 3650-3100, 2971, 2945, 1373, 1086 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.38-7.21 (m, 10H), 4.42 (s, 2H), 3.71 (q, *J* = 6.0 Hz, 1H), 1.85 (br, 1H), 1.76-1.58 (m, 5H), 1.44-1.36 (m, 1H), 1.30 (d, *J* = 6.4 Hz, 3H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 131.6, 128.20, 128.17, 127.7, 127.3, 127.0, 123.4, 93.5, 83.6, 75.2, 73.3, 63.6, 42.0, 40.8, 37.5, 25.79, 25.77, 21.9, 19.4, 18.2; HRMS m/z calcd for $C_{25}H_{33}O_2$ $[M+H]^+$ 365.2481, found: 365.2464.

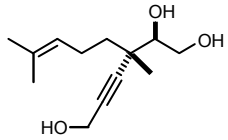


2-Methyl-2-phenylethynyl-cyclohexanol. The title compound was prepared from phenylacetylene and 1-methyl-7-oxa-bicyclo[4.1.0]heptane according to the procedure used for **8b** (colorless oil, 105 mg, 93%). R_f 0.20 (10% EtOAc/hexanes); IR (thin film) ν 3700-3050, 2941, 2856, 2217, 1602, 1050 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.40-7.37 (m, 2H), 7.28-7.25 (m, 3H), 3.76 (dd,

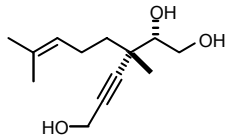
J = 7.2 Hz, 3.6 Hz, 1H), 2.03-1.97 (m, 1H), 1.86-1.69 (m, 2H), 1.70-1.41 (m, 6H), 1.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.6, 128.2, 127.7, 123.6, 95.9, 82.2, 74.3, 37.6, 35.0, 29.1, 21.7, 21.6; HRMS m/z calcd for $C_{15}H_{19}O$ $[M+H]^+$ 215.1429, found: 215.1436.



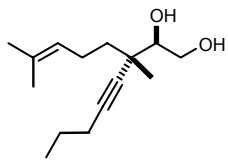
Acetic acid 6-hydroxy-3,7,7-trimethyl-9-phenyl-non-2-en-8-ynyl ester. The title compound was prepared from phenylacetylene and Acetic acid 5-(3,3-dimethyl-oxiranyl)-3-methyl-pent-2-enyl ester according to the procedure used for **8b** (yellow oil, 109 mg, 76%). R_f 0.24 (25% EtOAc/ hexanes); IR (thin film) ν 3650-3200, 2969, 2929, 1731, 1232 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.36 (m, 2H), 7.27-7.26 (m, 3H), 5.40 (dt, J = 0.8 Hz, 7.2 Hz, 1H), 4.58 (d, J = 7.2 Hz, 2H), 3.35 (d, J = 10.0 Hz, 1H), 2.39-2.32 (m, 1H), 2.19-2.09 (m, 1H), 2.03 (s, 3H), 1.89-1.81 (m, 1H), 1.76 (br, 1H), 1.71 (s, 3H), 1.58-1.49 (m, 1H), 1.29 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 142.1, 131.6, 128.2, 127.9, 123.3, 118.6, 94.5, 82.5, 77.6, 61.3, 37.8, 36.4, 29.9, 25.2, 25.0, 21.0, 16.5; HRMS m/z calcd for $C_{20}H_{27}O_3$ $[M+H]^+$ 315.1960, found: 315.1946.



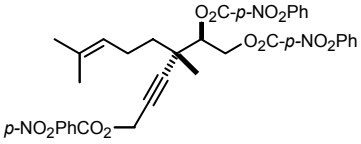
(2R,3S)-1-Methyl-3-(4-methyl-pent-3-enyl)-hex-4-yne-1,2,6-triol. The title compound was prepared from **13b** by TBAF de-protection (colorless oil, 79 mg, quantitative). R_f 0.3 (EtOAc); IR (thin film) ν 3650-3000, 2971, 2924, 2847, 2353, 1445 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.07 (t, J = 7.5 Hz, 1H), 4.20 (s, 2H), 3.84 (dd, J = 2.7 Hz, 11.1 Hz, 1H), 3.62 (dd, J = 8.7 Hz, 11.1 Hz, 1H), 3.49 (dd, J = 2.7 Hz, 9.0 Hz, 1H), 2.15-1.97 (m, 2H), 1.65 (s, 3H), 1.58 (s, 3H), 1.55-1.46 (m, 1H), 1.33-1.23 (m, 1H), 1.19 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 131.9, 123.9, 89.1, 81.5, 77.2, 63.5, 50.8, 38.9, 37.5, 25.6, 23.3, 22.2, 17.6; HRMS m/z calcd for $C_{13}H_{23}O_3$ $[M+H]^+$ 227.1647, found: 227.1641.



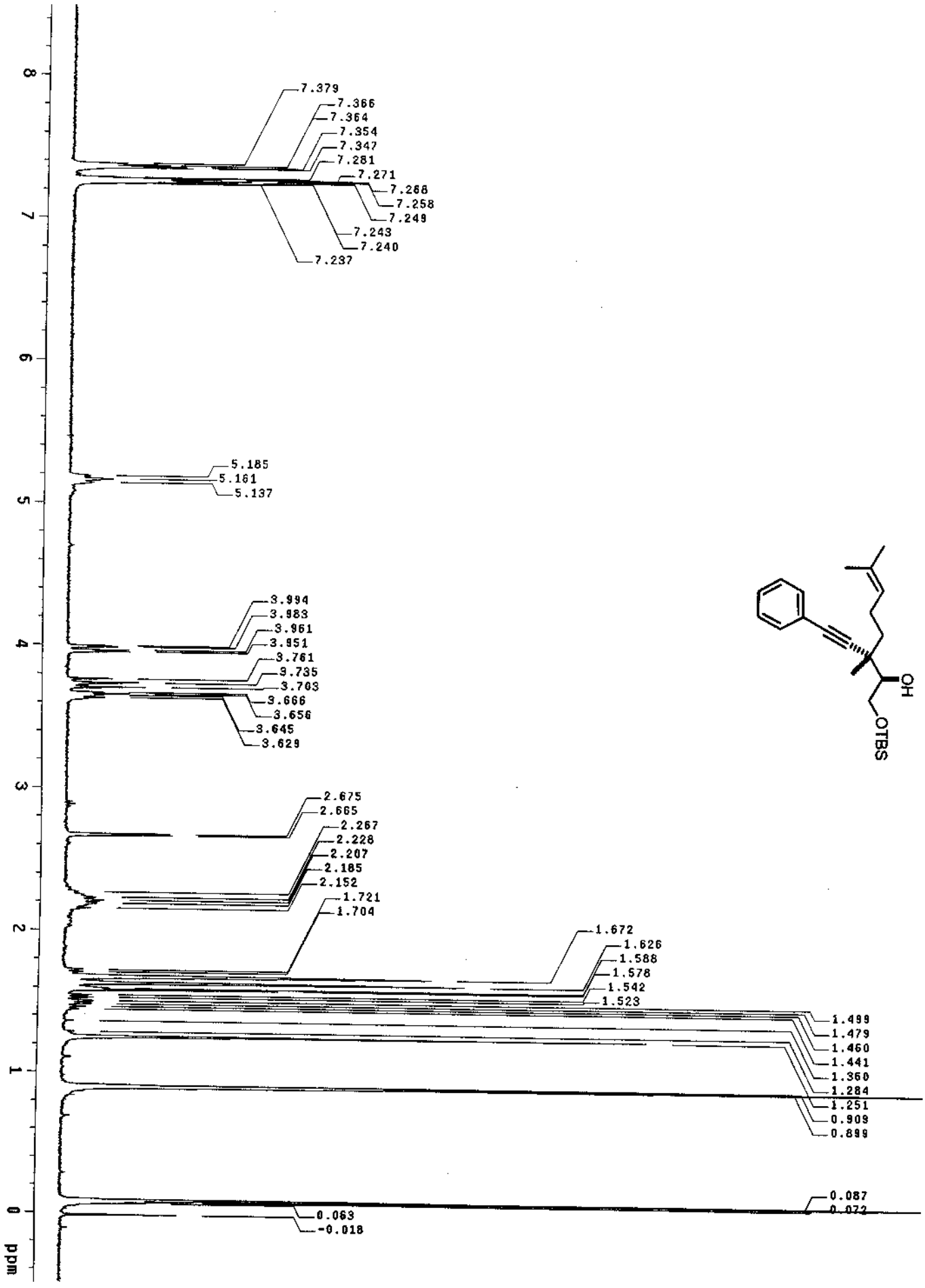
(2S,3S)-1-Methyl-3-(4-methyl-pent-3-enyl)-hex-4-yne-1,2,6-triol. The title compound was prepared from *tert*-butyl-dimethyl-prop-2-ynyloxy-silane and nerol epoxide and followed by TBAF de-protection (colorless oil, 75 mg, 64% over two steps). R_f 0.3 (EtOAc); IR (thin film) ν 3600-3000, 2971, 2924, 2854, 2361, 1449 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.09 (t, J = 6.8 Hz, 1H), 4.23 (s, 2H), 3.78 (d, J = 9.6 Hz, 1H), 3.67 (dd, J = 8.8 Hz, 8.8 Hz, 1H), 3.51 (dd, J = 2.8 Hz, 8.4 Hz, 1H), 2.81 (br, 3H), 2.13-2.02 (m, 2H), 1.66 (s, 3H), 1.68-1.61 (m, 1H) 1.59 (s, 3H), 1.45-1.37 (m, 1H), 1.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.8, 124.0, 89.1, 81.4, 77.2, 63.1, 50.6, 38.9, 37.9, 25.6, 23.1, 21.8, 17.6; HRMS m/z calcd for $C_{13}H_{23}O_3$ $[M+H]^+$ 227.1647, found: 227.1650.

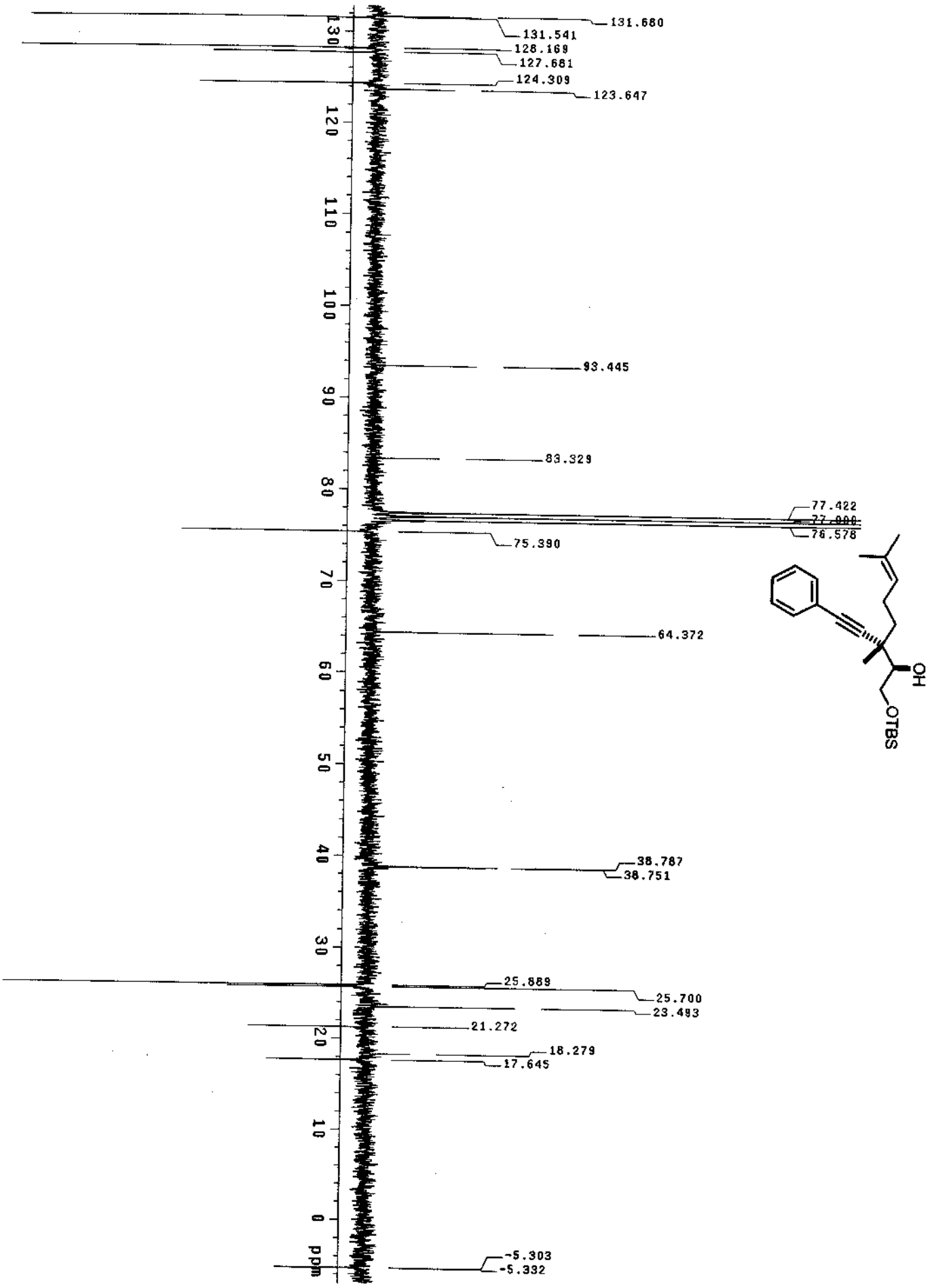


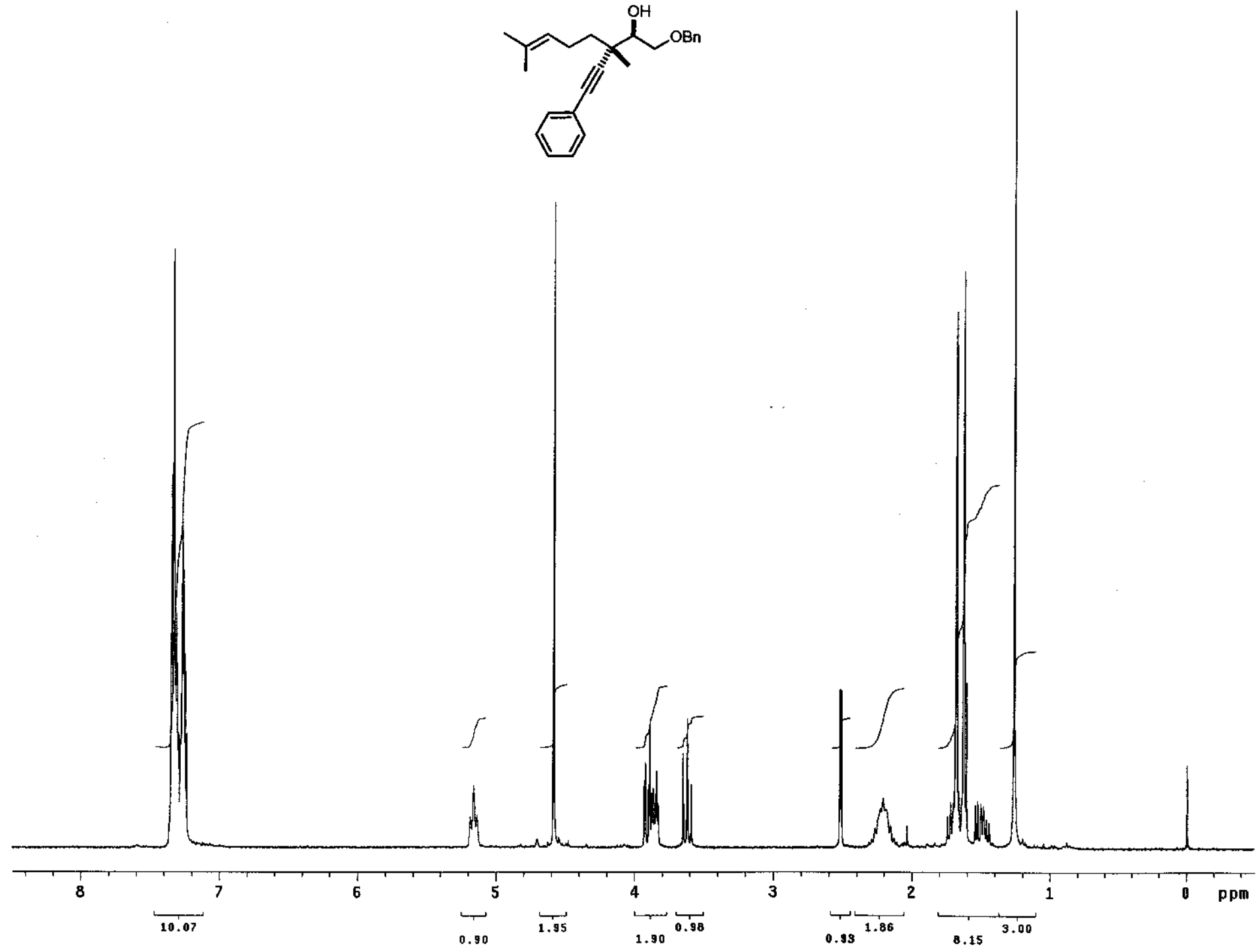
3,7-Dimethyl-3-pent-1-ynyl-oct-6-ene-1,2-diol. R_f 0.30 (40% EtoAc/hexanes); IR (thin film) ν 3697-3041, 2971, 2936, 2878, 2206 cm^{-1}; ^{1}H NMR (250 MHz, $CDCl_3$) δ 5.10 (t, J = 7.2 Hz, 1H), 3.82 (dd, J = 8.2 Hz, 8.2 Hz, 1H), 3.62 (dd, J = 8.6 Hz, 8.6 Hz, 1H), 3.51-3.41 (m, 1H), 2.28 (d, J = 6.2 Hz, 1H), 2.12 (t, J = 7.0 Hz, 2H), 2.20-2.03 (m, 3H), 1.66 (s, 3H), 1.59 (s, 3H), 1.55-1.47 (m, 3H), 1.44-1.22 (m, 1H), 1.17 (s, 3H), 0.94 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 131.8, 124.1, 84.2, 83.0, 76.9, 63.7, 39.0, 38.0, 25.7, 23.4, 22.6, 22.4, 20.6, 17.6, 13.4; HRMS m/z calcd for $C_{15}H_{26}O_2$ $[M-H]^+$ 237.1855, found: 237.1848.

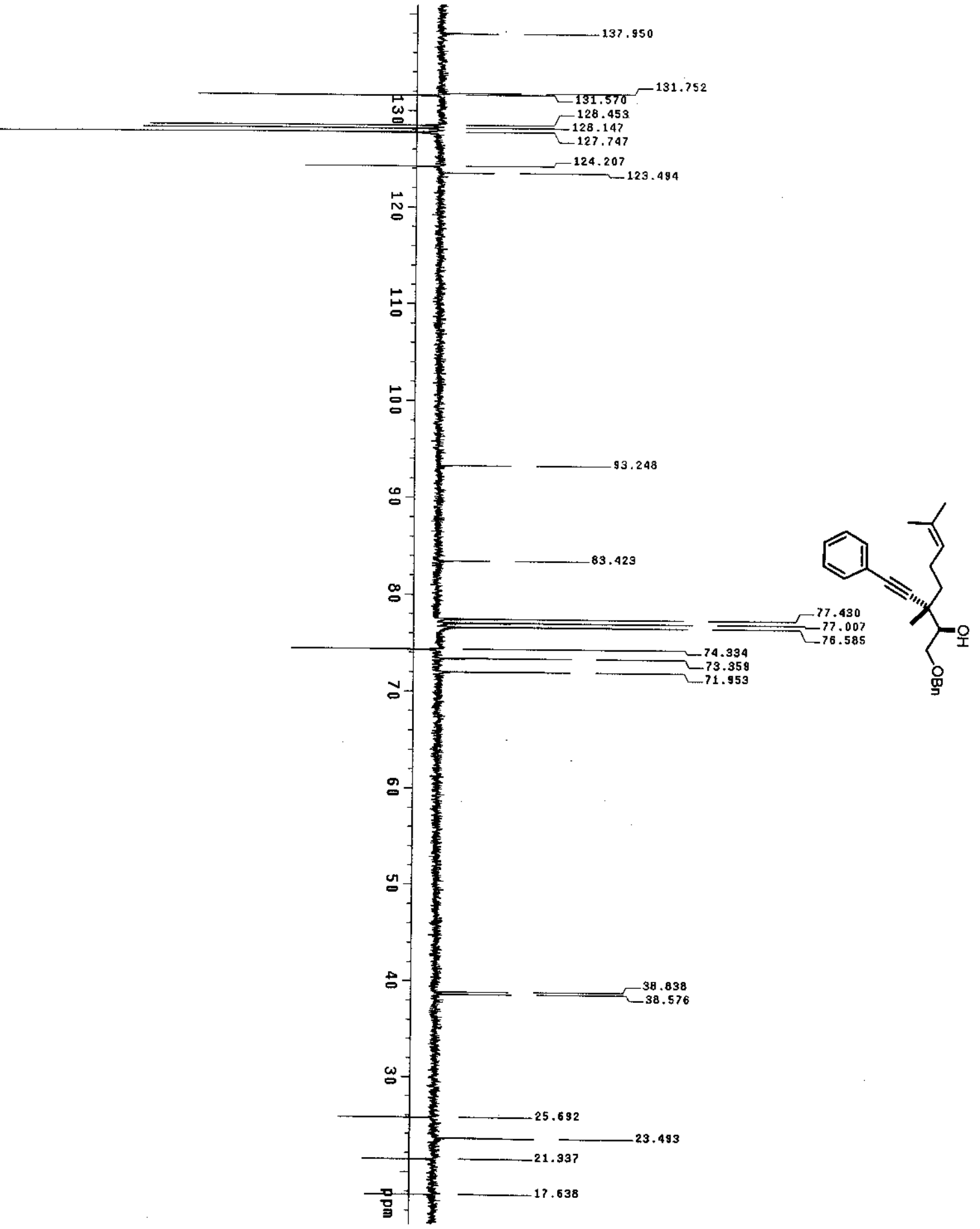


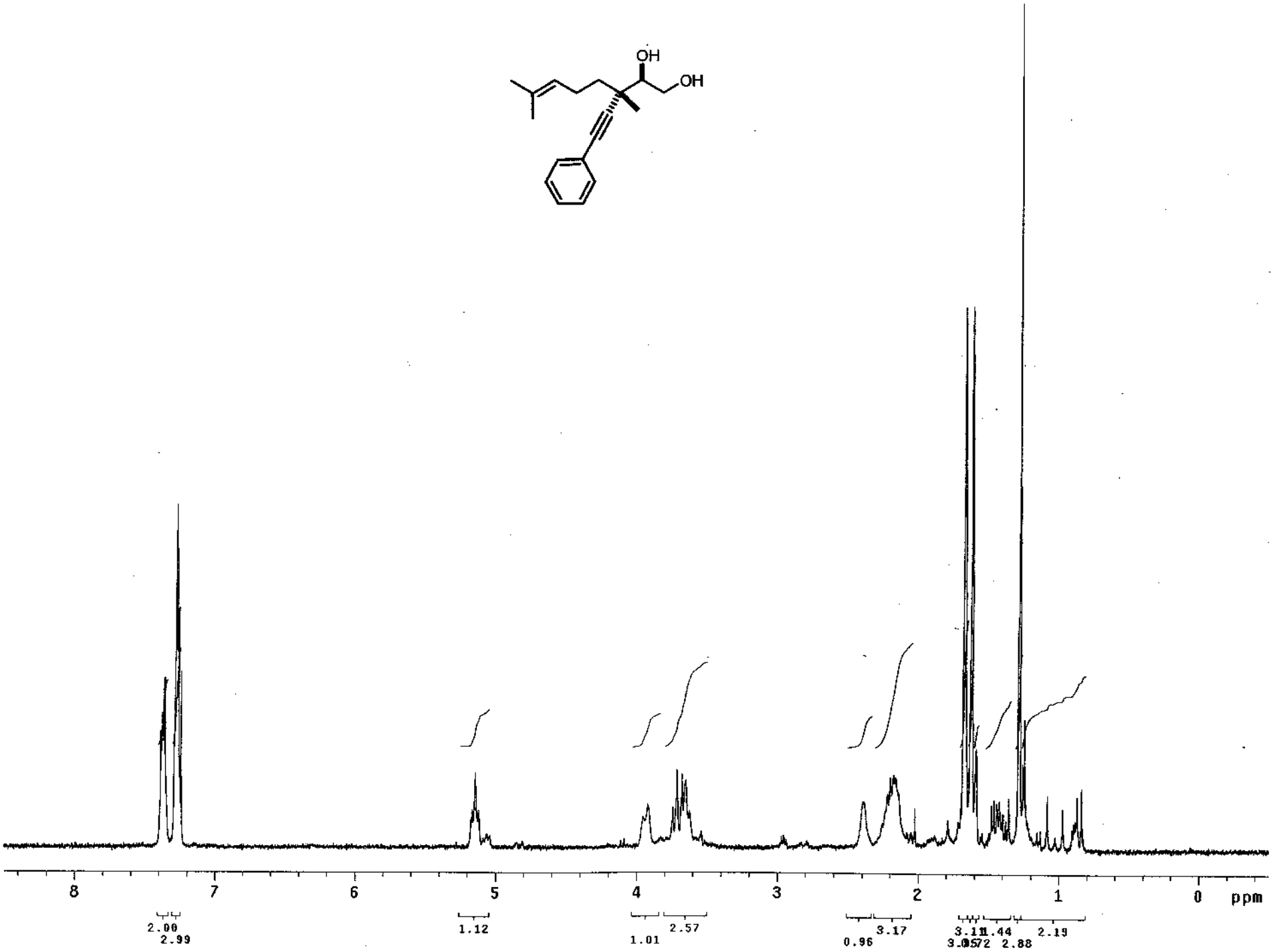
The title compound was prepared from (2S,3S)-1-Methyl-3-(4-methyl-pent-3-enyl)-hex-4-yne-1,2,6-triol and *p*-nitrobenzoyl chloride (white solid, 166 mg, 70%). R_f 0.3 (30% EtOAc/Hexanes); IR (thin film) ν 3116, 2969, 2926, 2860, 1731,1525,1268 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 8.30-8.05 (m, 12H), 5.62 (dd, *J* = 2.4 Hz, 9.2 Hz, 1H), 5.05 (t, *J* = 7.2 Hz, 1H), 4.99 (s, 2H), 4.95 (dd, *J* = 2.4 Hz, 12.0 Hz, 1H), 4.63 (dd, *J* = 8.8 Hz, 11.6 Hz, 1H), 2.27-2.11 (m, 2H), 1.63 (s, 3H), 1.54 (s, 3H), 1.67-1.46 (m, 2H), 1.40 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.3, 163.9, 150.8, 150.6, 134.8, 134.73, 134.70, 132.67, 130.9, 130.8, 130.7, 123.7, 123.6, 122.9, 89.1, 77.9, 75.8, 65.3, 53.6, 38.2, 25.6, 23.3, 22.1, 17.6; HRMS m/z calcd for $C_{34}H_{32}N_3O_{12}$ $[M+H]^+$ 674.1986, found: 674.1981.

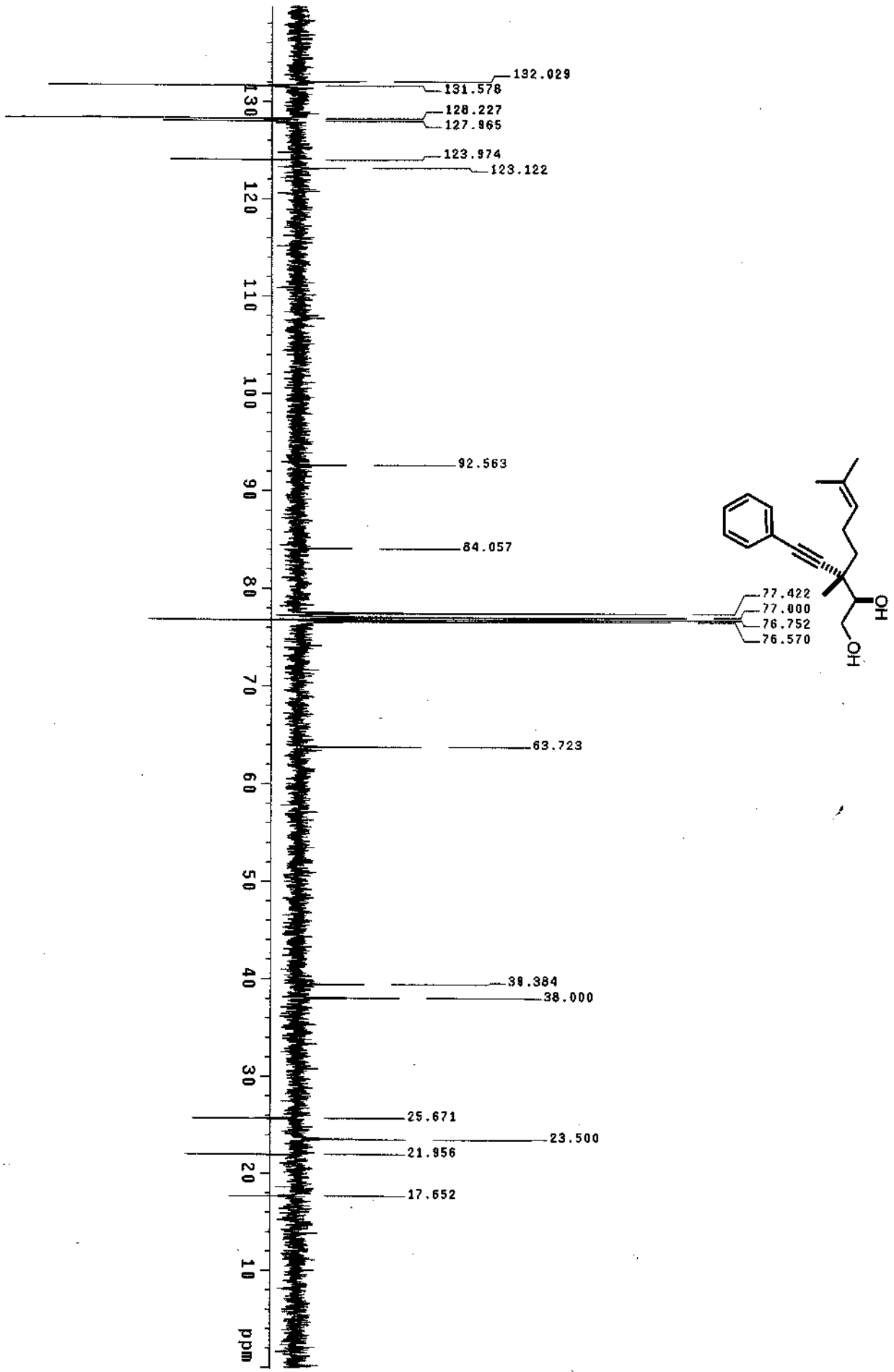

7.379
7.366
7.364
7.354
7.347
7.281
7.271
7.268
7.258
7.249
7.243
7.240
7.237
5.185
5.161
5.137
3.994
3.983
3.961
3.951
3.761
3.735
3.703
3.666
3.656
3.645
3.629
2.675
2.665
2.267
2.228
2.207
2.185
2.152
1.721
1.704
1.672
1.626
1.588
1.578
1.542
1.523
1.499
1.479
1.460
1.441
1.360
1.284
1.251
0.909
0.899
0.087
0.072
0.063
-0.018
OH
OTBS
ppm

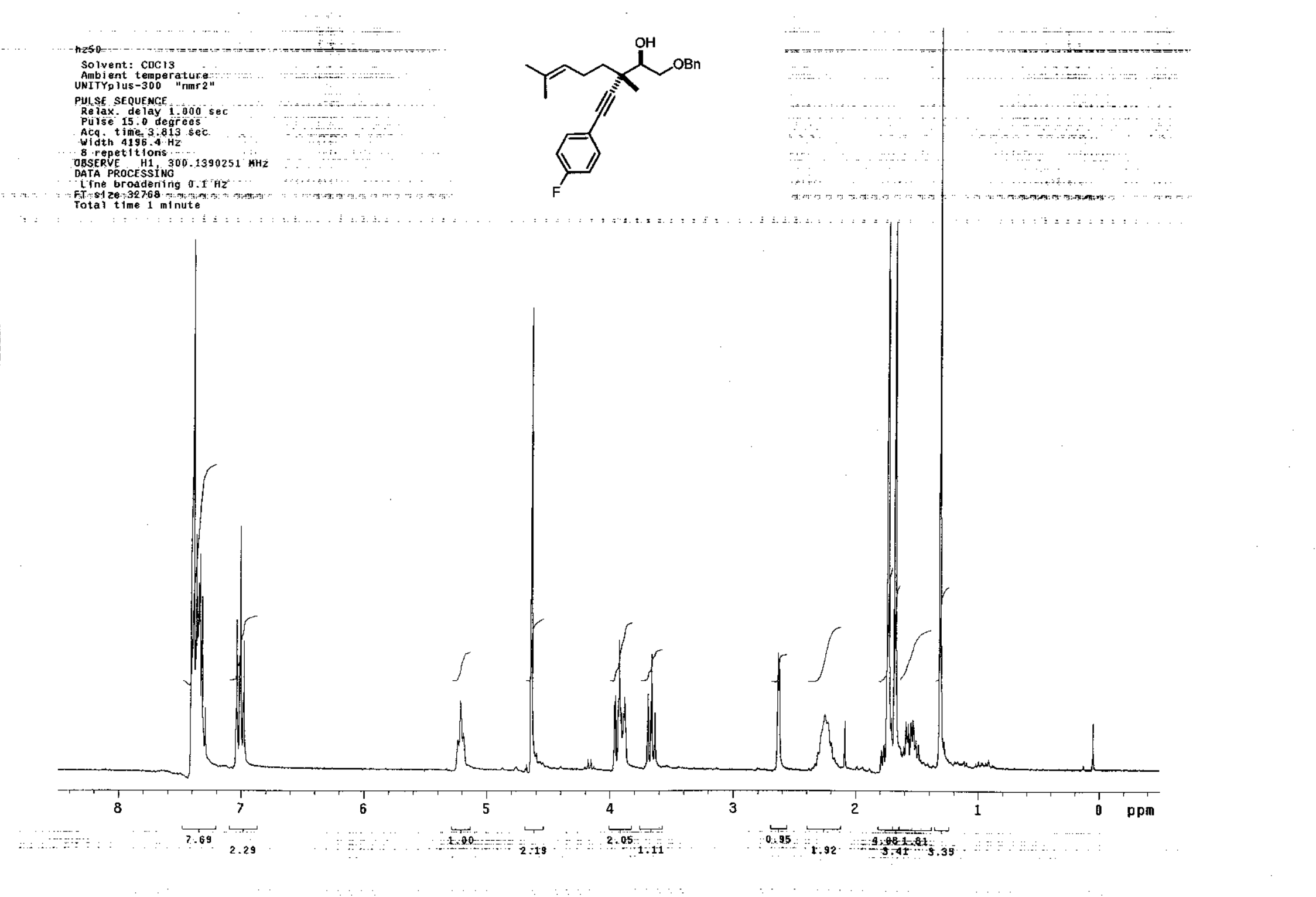

131.680
131.541
128.169
127.681
124.309
123.647
93.445
83.329
77.422
77.000
76.578
75.390
64.372
38.787
38.751
25.889
25.700
23.493
21.272
18.279
17.645
-5.303
-5.332
OH
OTBS
ppm

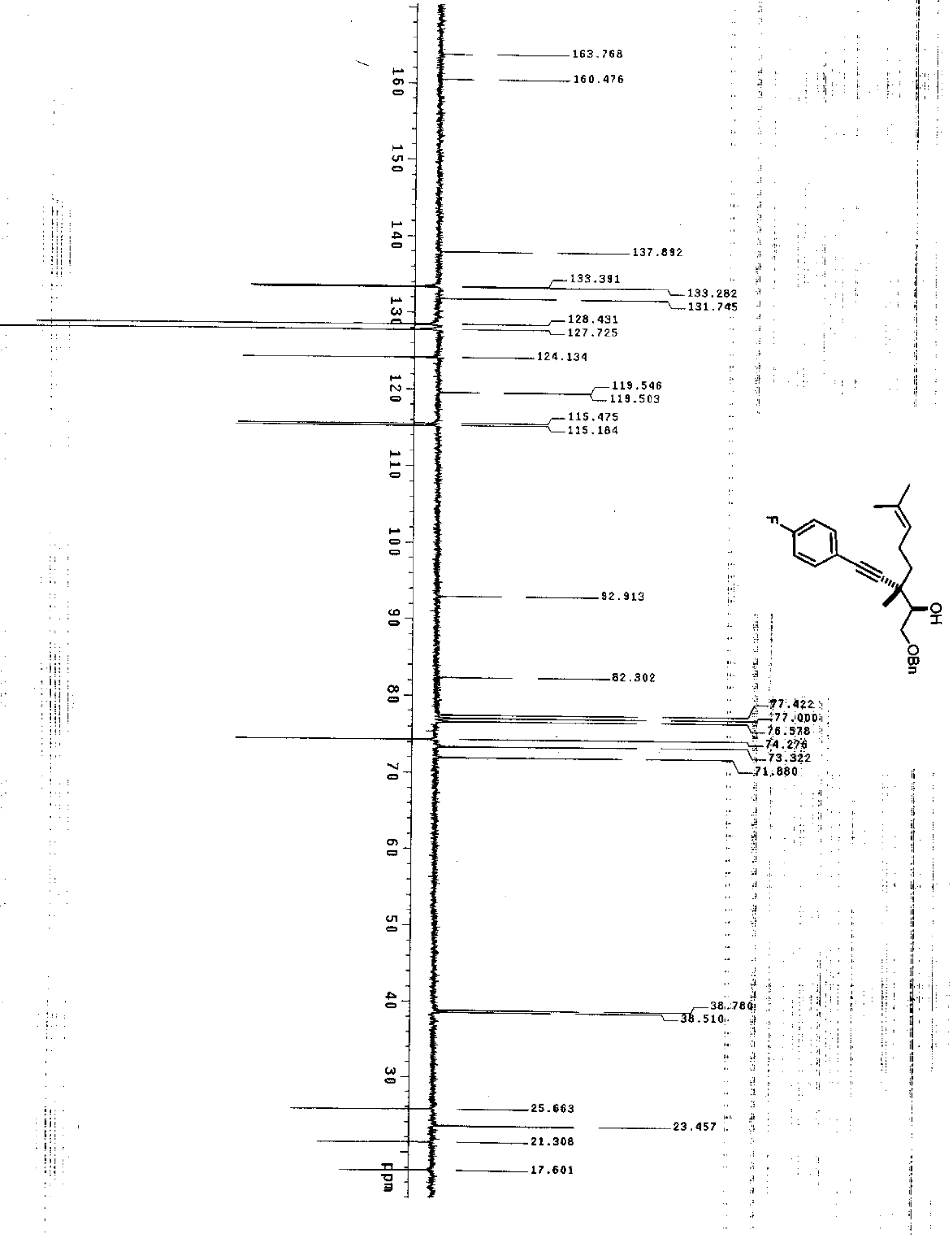

OH
OBn
8
7
6
5
4
3
2
1
0
ppm
10.07
0.90
1.95
1.90
0.98
0.93
1.86
8.15
3.00


137.950
131.752
131.570
128.453
128.147
127.747
124.207
123.494
93.248
83.423
77.430
77.007
76.585
74.334
73.359
71.953
38.638
38.576
25.692
23.493
21.337
17.638
ppm
OH
OBn

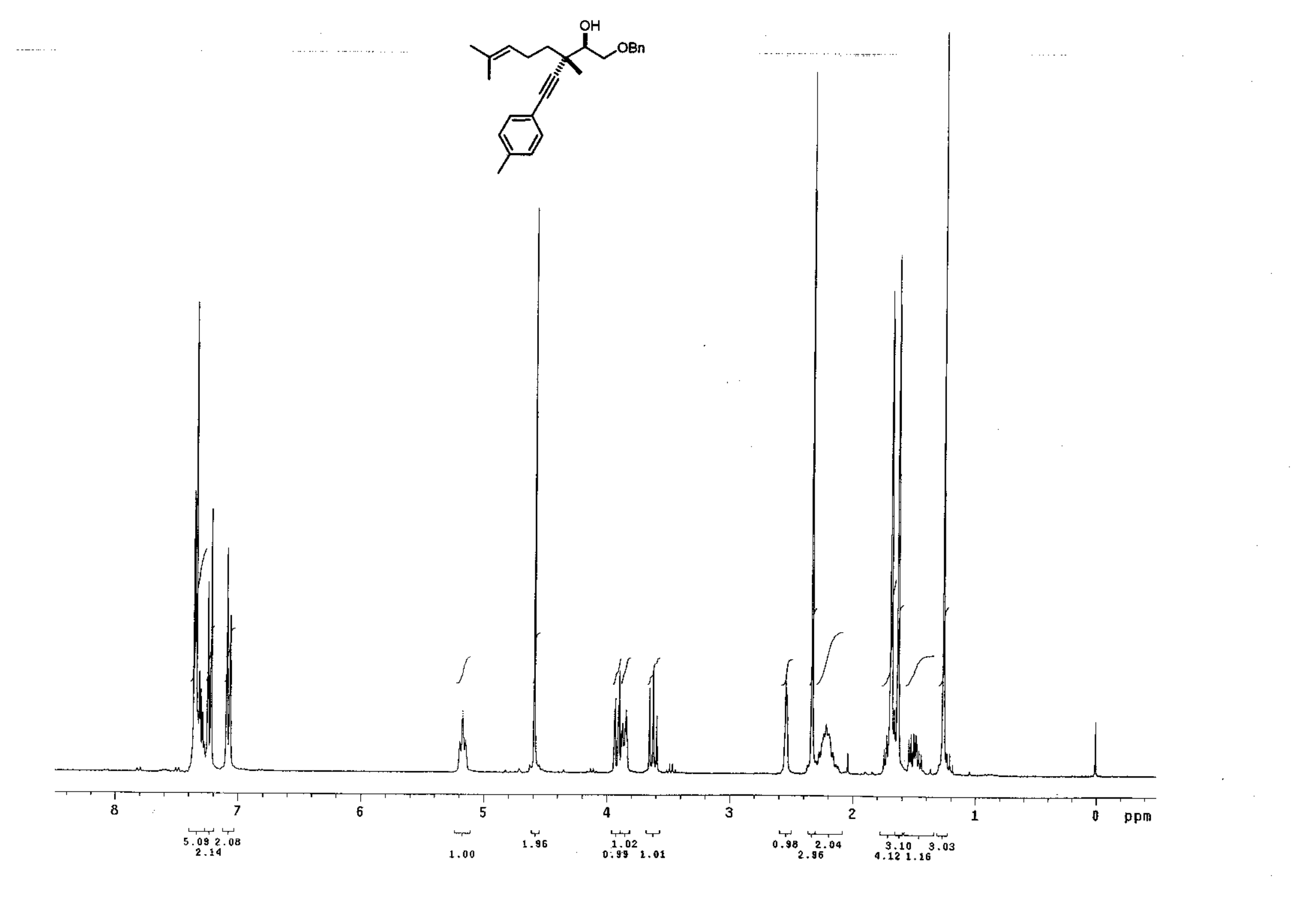

OH
OH
8
7
6
5
4
3
2
1
0
ppm
2.00
2.99
1.12
1.01
2.57
0.96
3.17
3.11
1.44
2.19
3.05
72
2.88

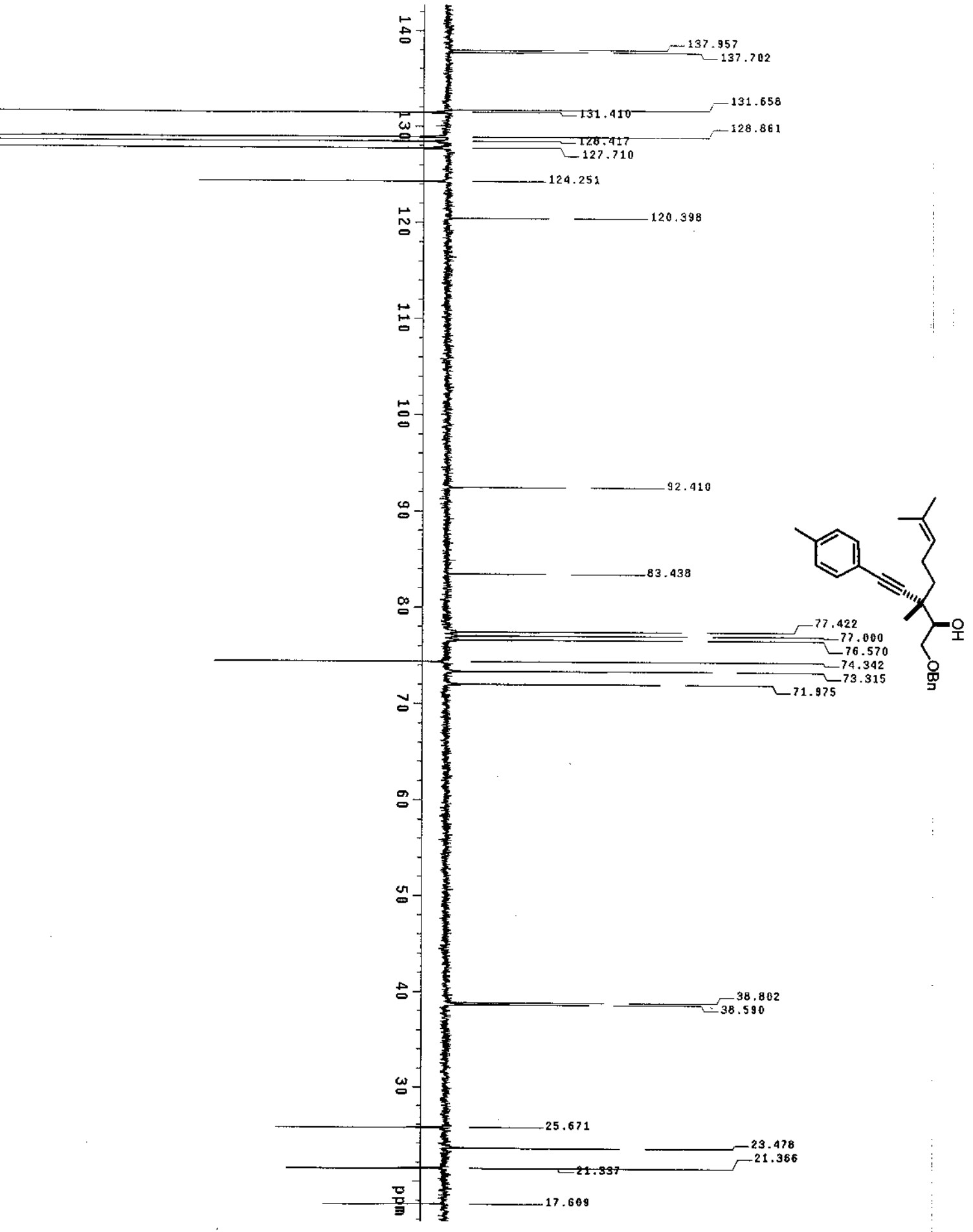

132.029
131.578
128.227
127.965
123.974
123.122
92.563
84.057
77.422
77.000
76.752
76.570
63.723
39.384
38.000
25.671
23.500
21.956
17.652
OH
OH
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

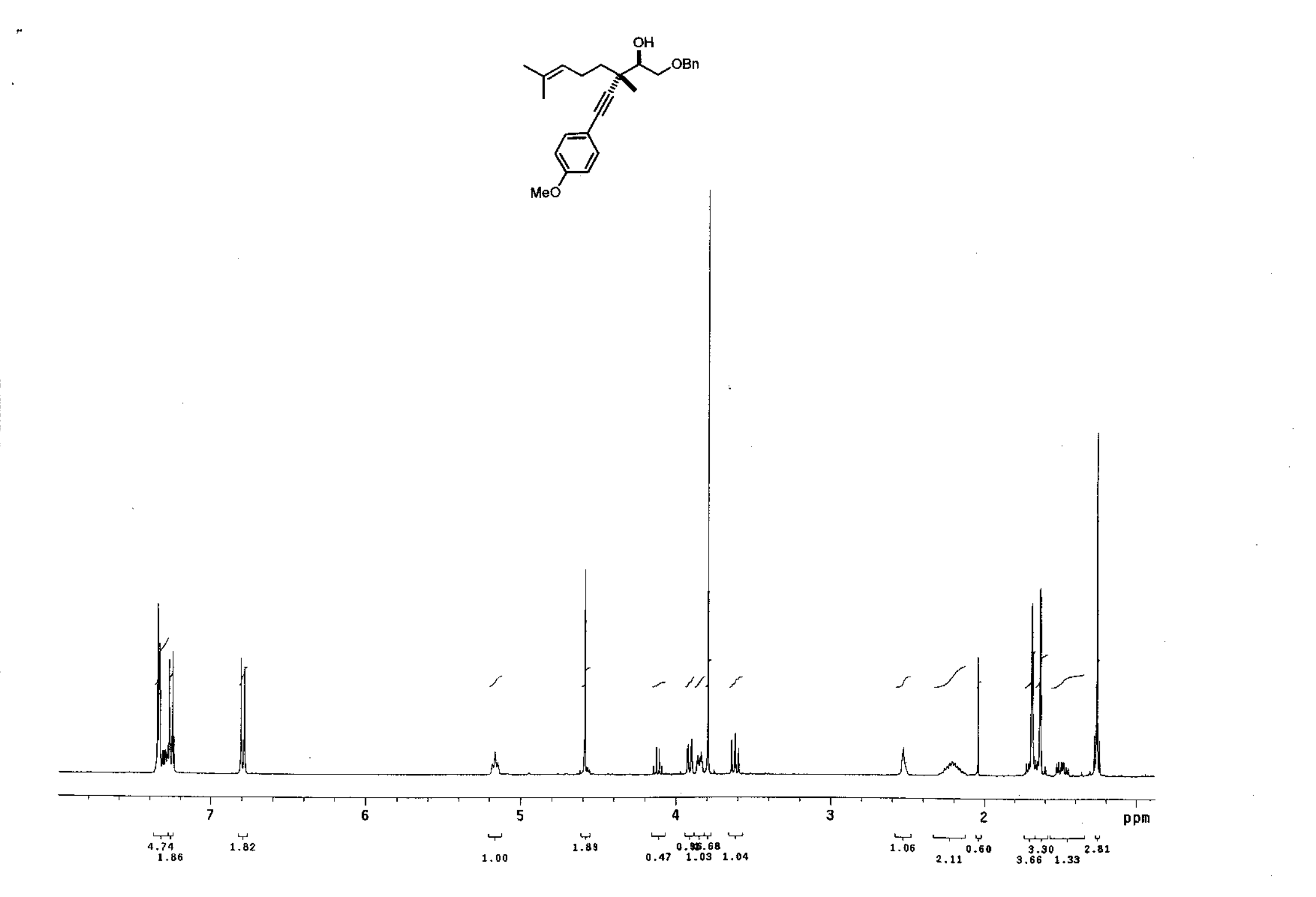

hz50
Solvent: CDCl3
Ambient temperature
UNITYplus-300 "nmr2"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 15.0 degrees
Acq. time 3.813 sec
Width 4196.4 Hz
8 repetitions
OBSERVE H1, 300.1390251 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute
OH
OBn
F
8
7
6
5
4
3
2
1
0
ppm
7.69
2.29
1.00
2.19
2.05
1.11
0.95
1.92
4.08
1.61
3.41
3.39

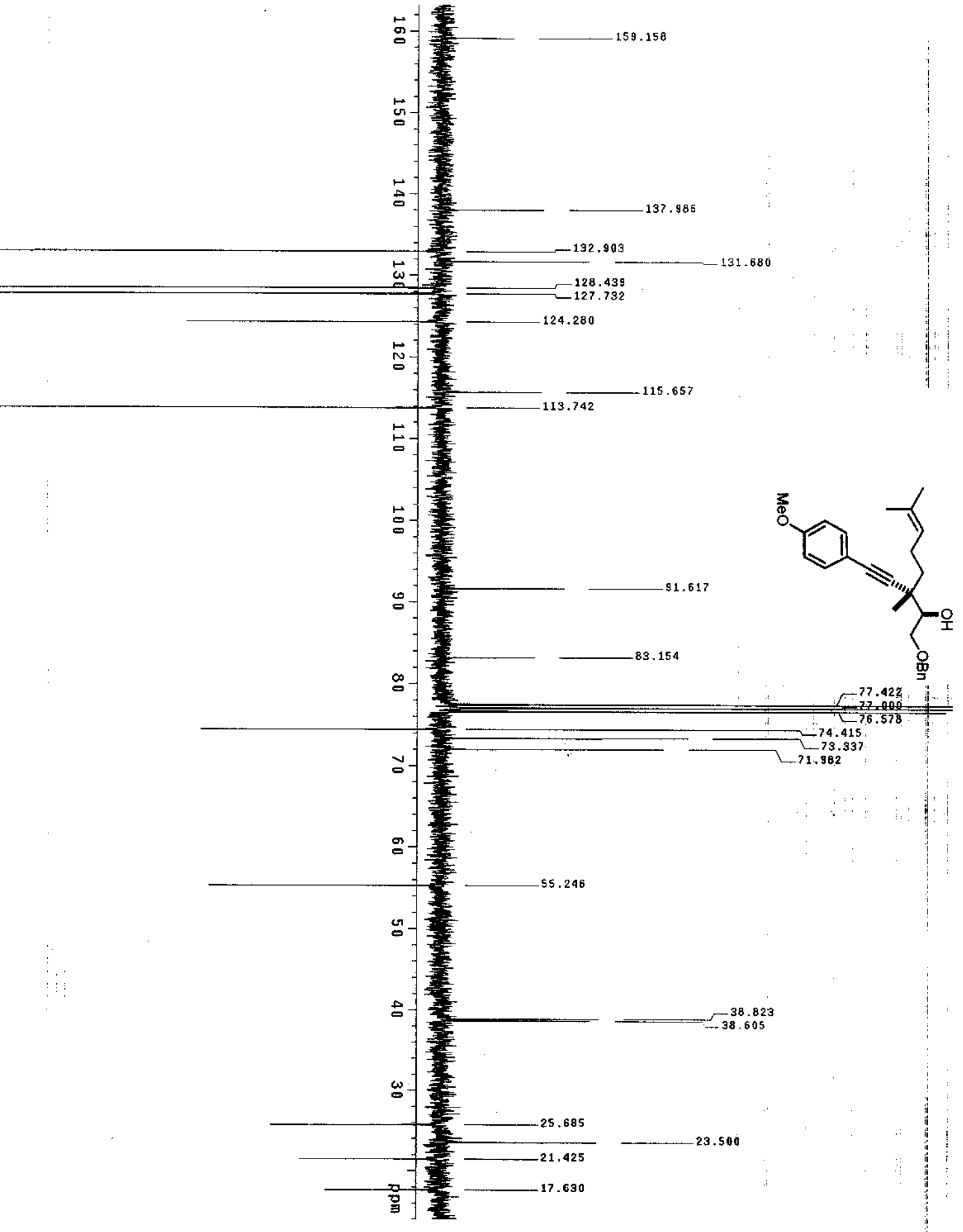


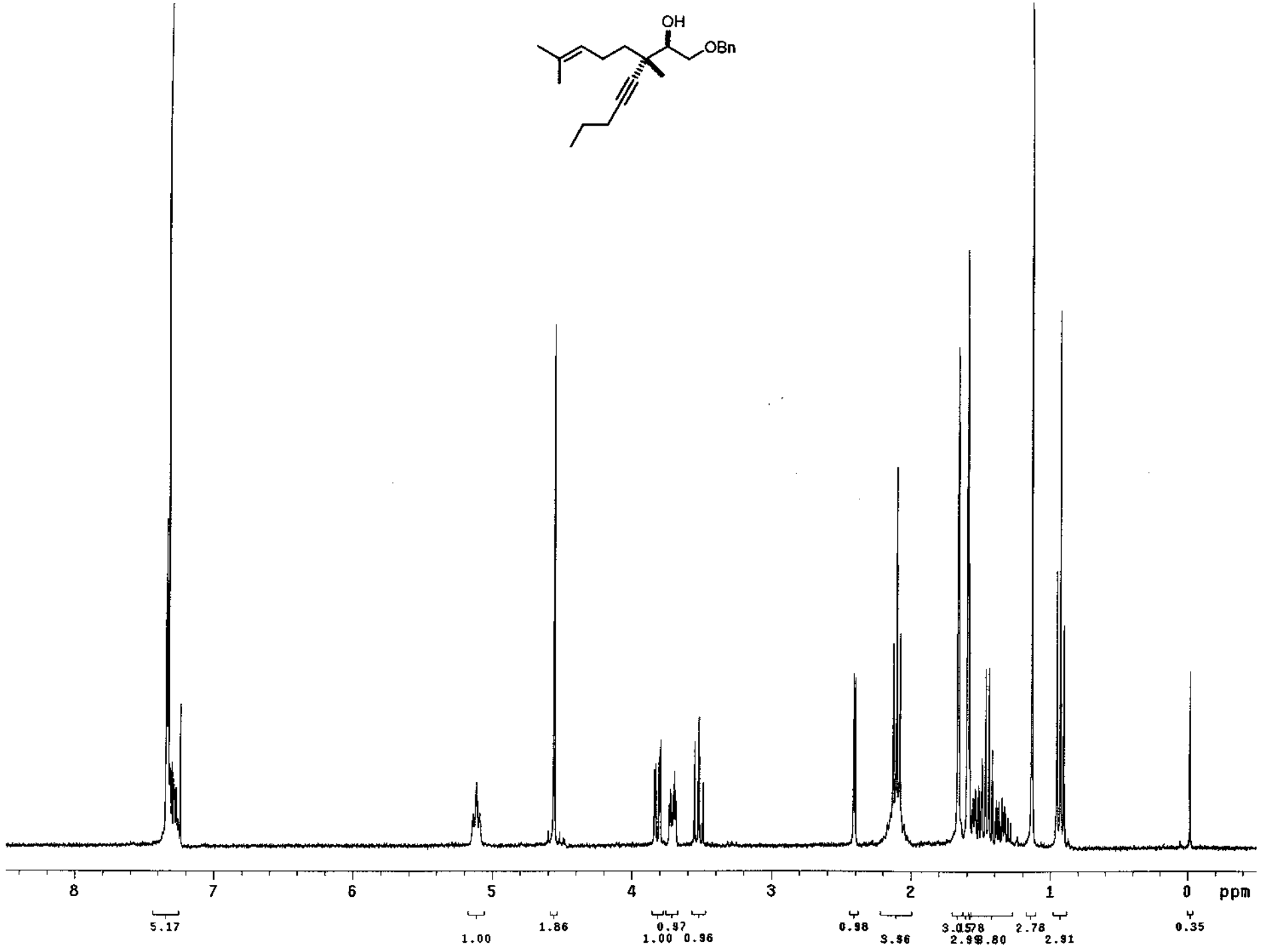
163.768
160.476
137.892
133.391
133.282
131.745
128.431
127.725
124.134
119.546
119.503
115.475
115.184
92.913
82.302
77.422
77.000
76.578
74.276
73.322
71.880
38.780
38.510
25.663
23.457
21.308
17.601
ppm
F
OH
OBn

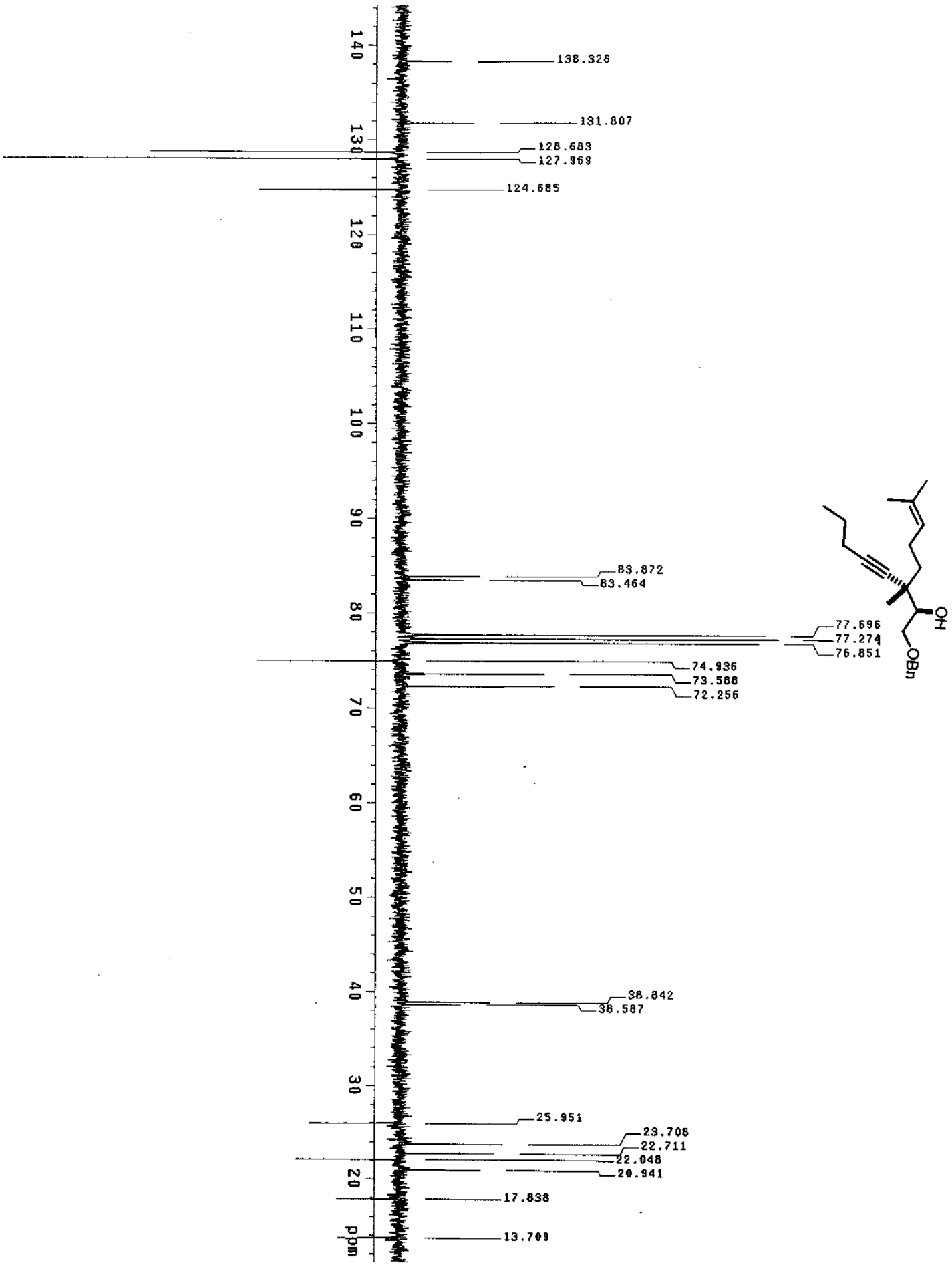

OH
OBn
8
7
6
5
4
3
2
1
0
ppm
5.09 2.08
2.14
1.00
1.96
1.02
0.99 1.01
0.98 2.04
2.96
3.10 3.03
4.12 1.16

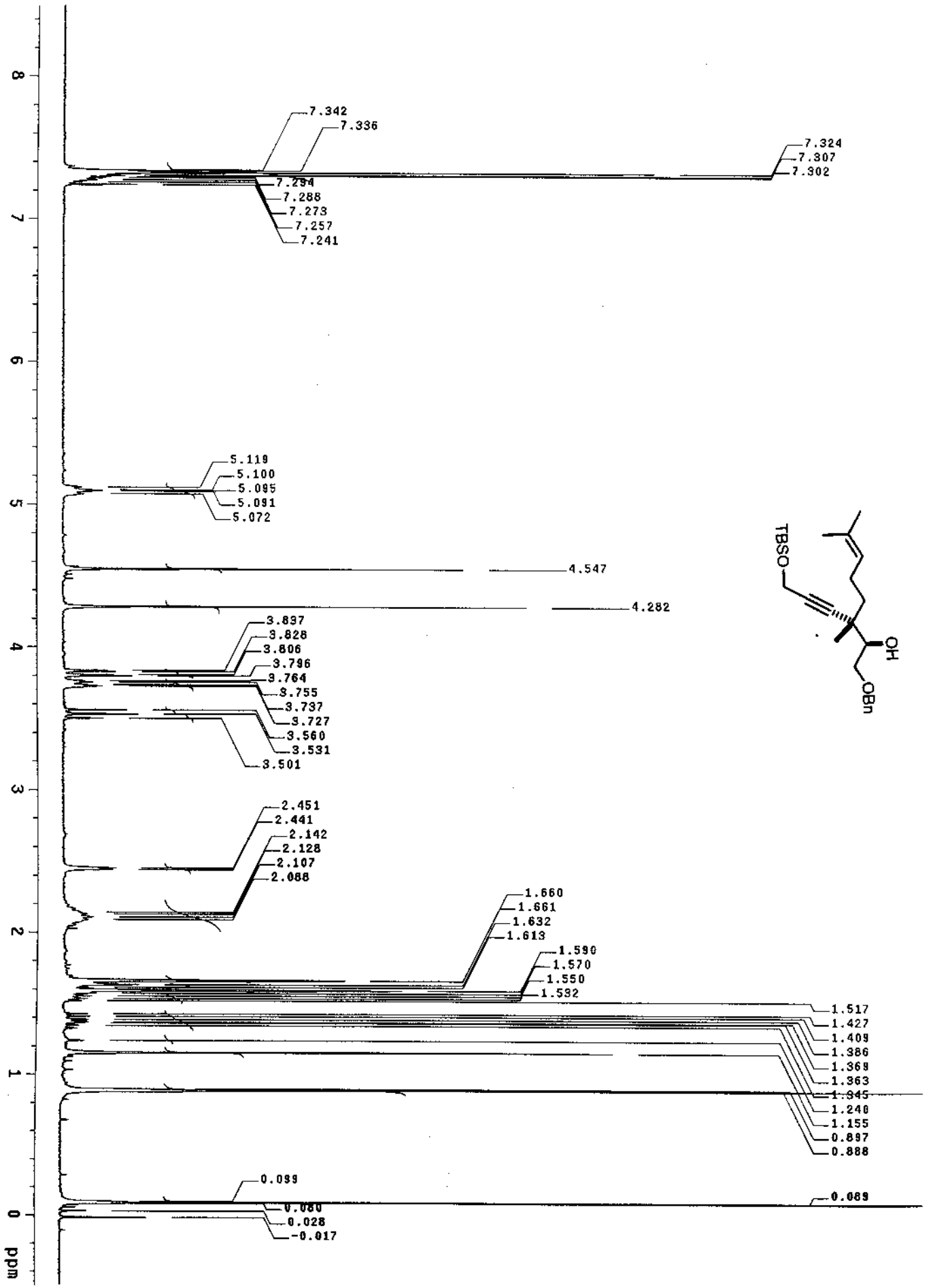

137.957
137.702
131.658
131.410
128.861
128.417
127.710
124.251
120.398
92.410
83.438
77.422
77.000
76.570
74.342
73.315
71.975
38.802
38.590
25.671
23.478
21.366
21.337
17.609
OH
OBn
ppm

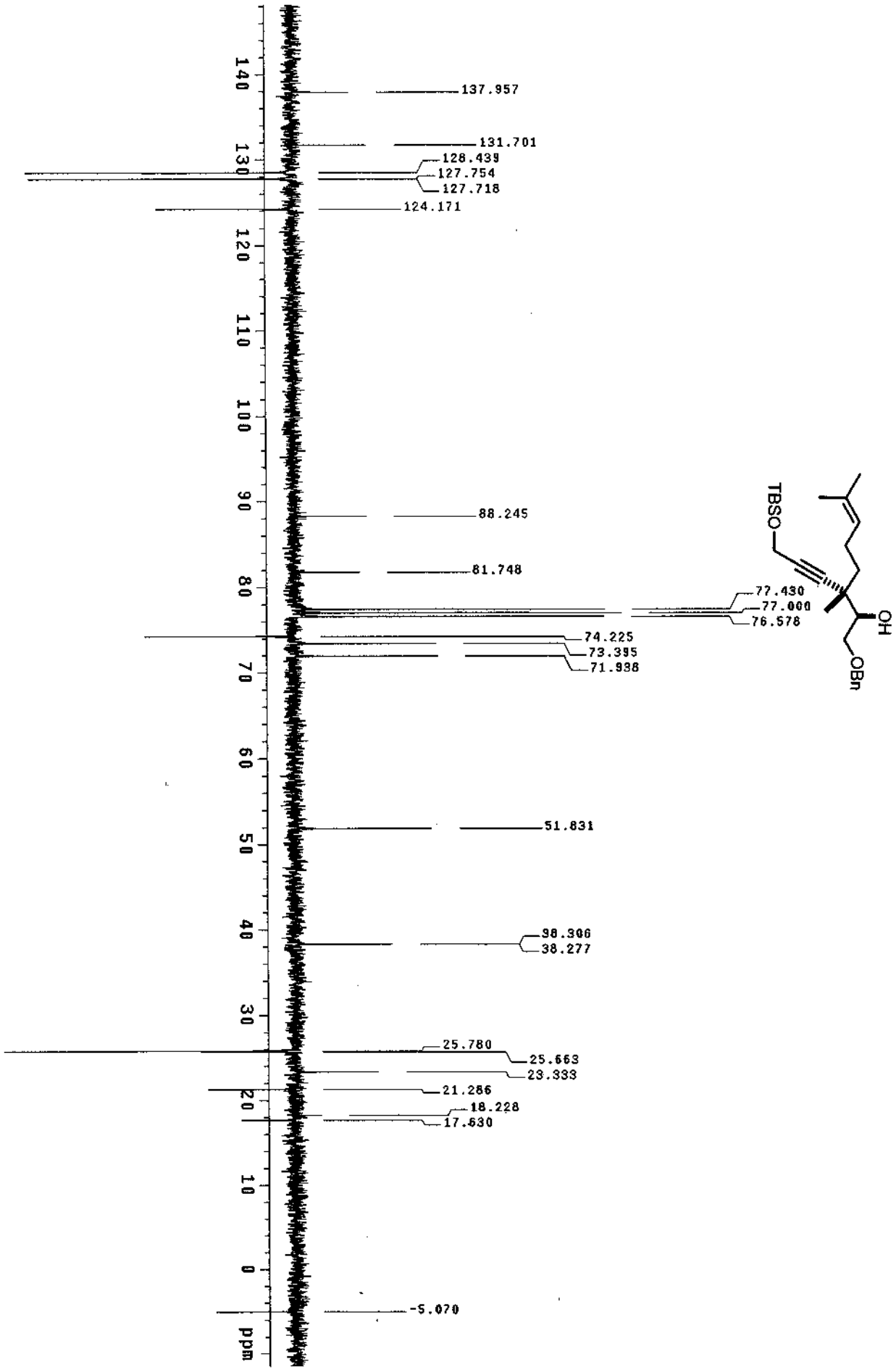

OH
OBn
MeO
7
6
5
4
3
2
ppm
4.74
1.86
1.82
1.00
1.89
0.47
1.03
1.04
1.06
2.11
0.60
3.66
1.33
2.81


159.158
137.986
132.903
131.680
128.439
127.732
124.280
115.657
113.742
91.617
83.154
77.422
77.000
76.578
74.415
73.337
71.982
55.246
38.823
38.605
25.685
23.500
21.425
17.630
ppm
MeO
OH
OBn


OH
OBn
8
7
6
5
4
3
2
1
0
ppm
5.17
1.00
1.86
0.97
1.00
0.96
0.98
3.96
2.78
2.91
0.35


138.326
131.807
128.683
127.969
124.685
83.872
83.464
77.696
77.274
76.851
74.936
73.588
72.256
38.842
38.587
25.951
23.708
22.711
22.048
20.941
17.838
13.709
ppm
OH
OBn

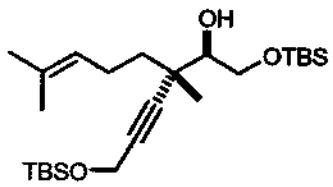

7.342
7.336
7.324
7.307
7.302
7.294
7.288
7.273
7.257
7.241
5.119
5.100
5.095
5.091
5.072
4.547
4.282
3.837
3.828
3.806
3.796
3.764
3.755
3.737
3.727
3.560
3.531
3.501
2.451
2.441
2.142
2.128
2.107
2.088
1.660
1.661
1.632
1.613
1.590
1.570
1.550
1.532
1.517
1.427
1.409
1.386
1.368
1.363
1.345
1.240
1.155
0.897
0.888
0.099
0.089
0.060
0.028
-0.017
TBSO
OH
OBn
8
7
6
5
4
3
2
1
0
ppm

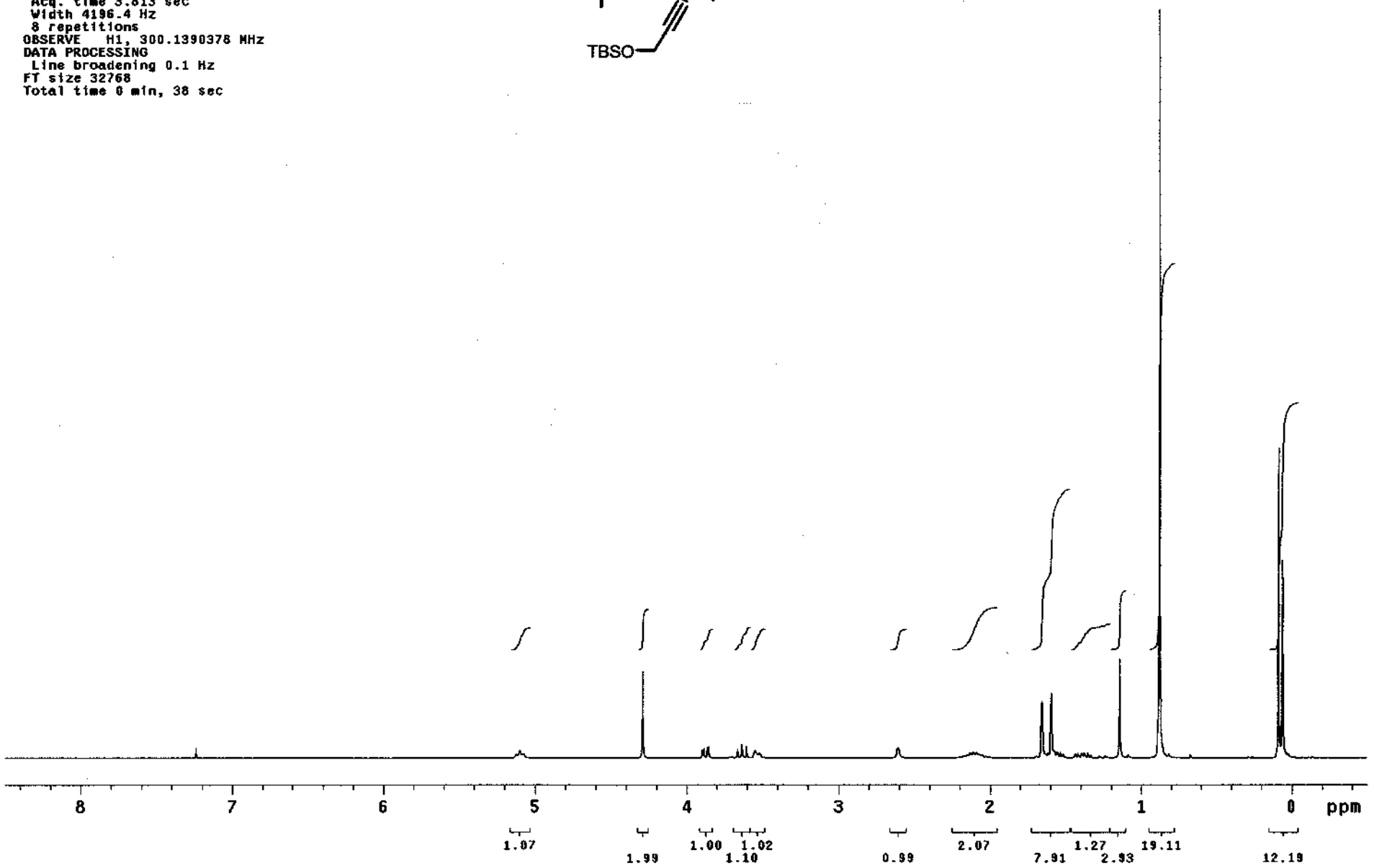

137.957
131.701
128.439
127.754
127.718
124.171
88.245
81.748
77.430
77.000
76.578
74.225
73.395
71.938
51.831
38.306
38.277
25.780
25.663
23.333
21.286
18.228
17.630
-5.070
ppm
TBSO
OH
OBn

hz-3-107

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
UNITYplus-300 "nmr2"

Relax. delay 1.000 sec
Pulse 15.0 degrees
Acq. time 3.813 sec
Width 4196.4 Hz
8 repetitions
OBSERVE H1, 300.1390378 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 38 sec



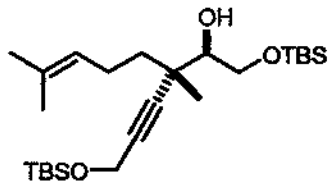


hz-3-107c; 300 Mhz NMR

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
UNITYplus-300 "nmr2"

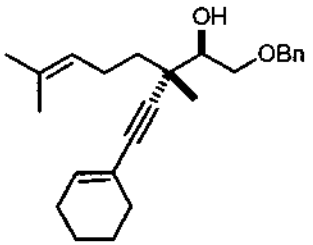
Relax. delay 2.000 sec
Pulse 36.0 degrees
Acq. time 1.777 sec
Width 18009.9 Hz
576 repetitions
OBSERVE C13, 75.4700194 MHz
DECOUPLE H1, 300.1409259 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
Single precision data
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 4 min, 38 sec

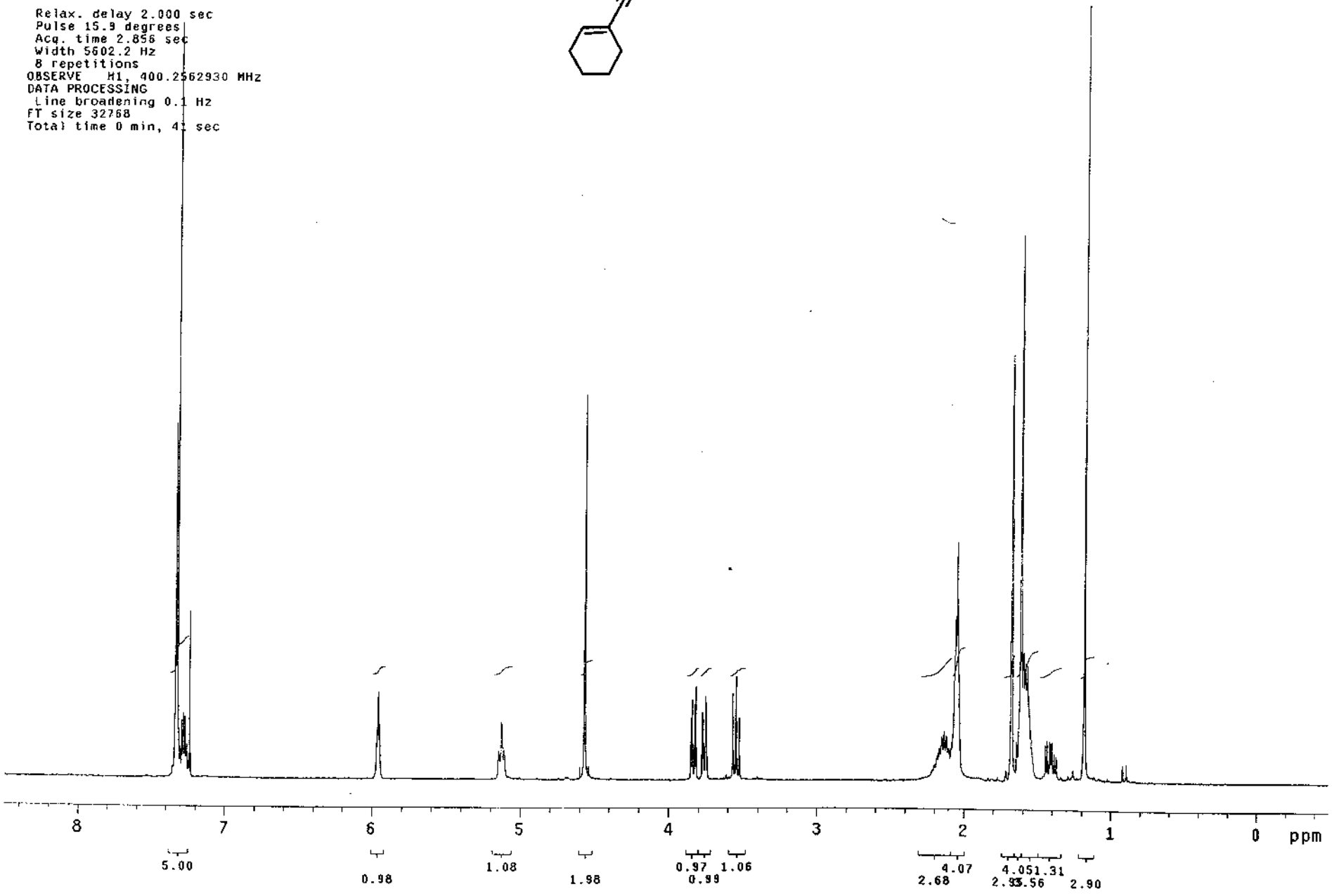


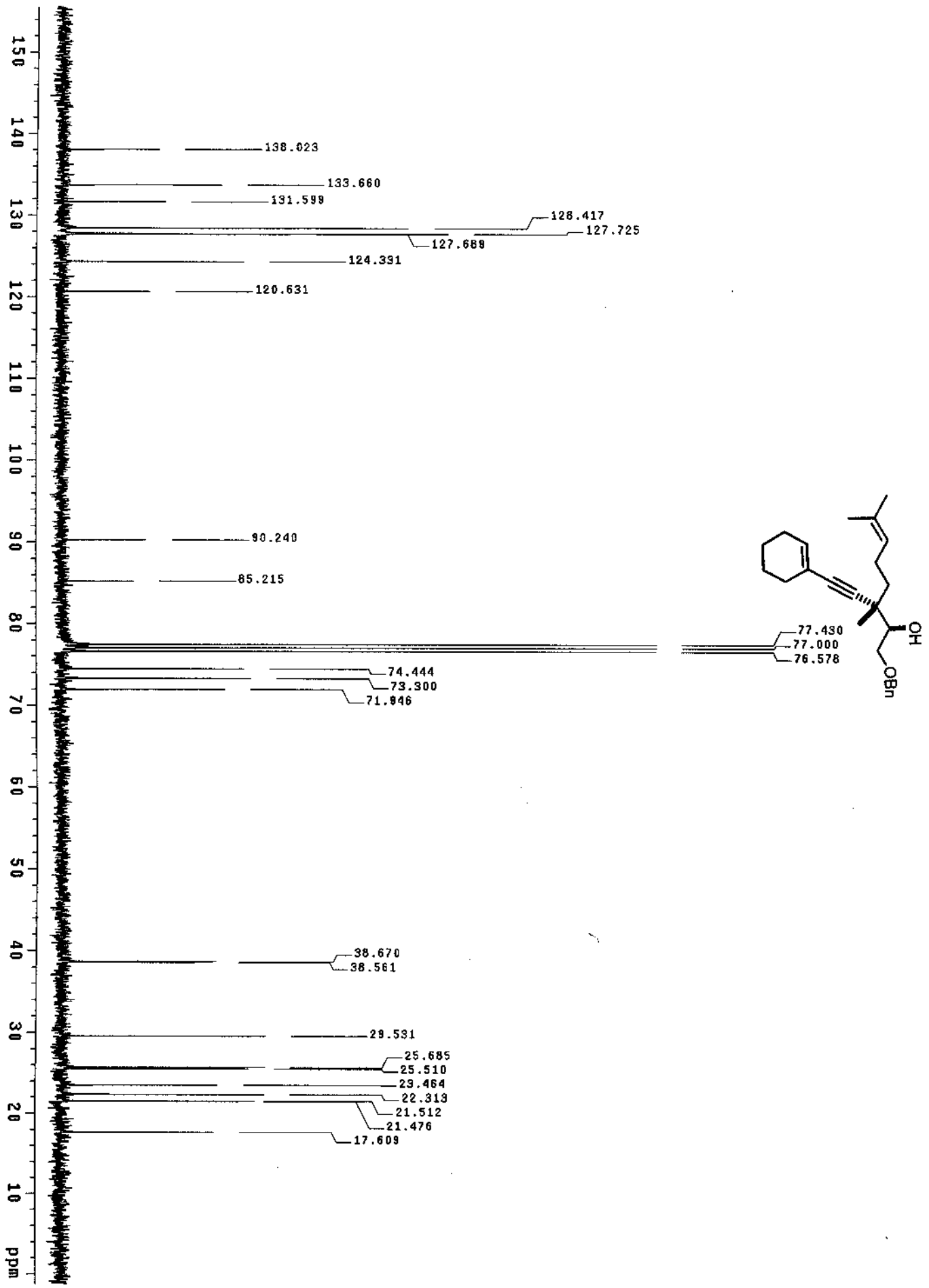
hz-3-27

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

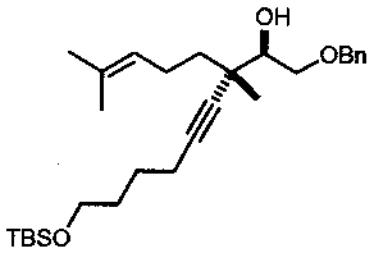
Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2562930 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 41 sec

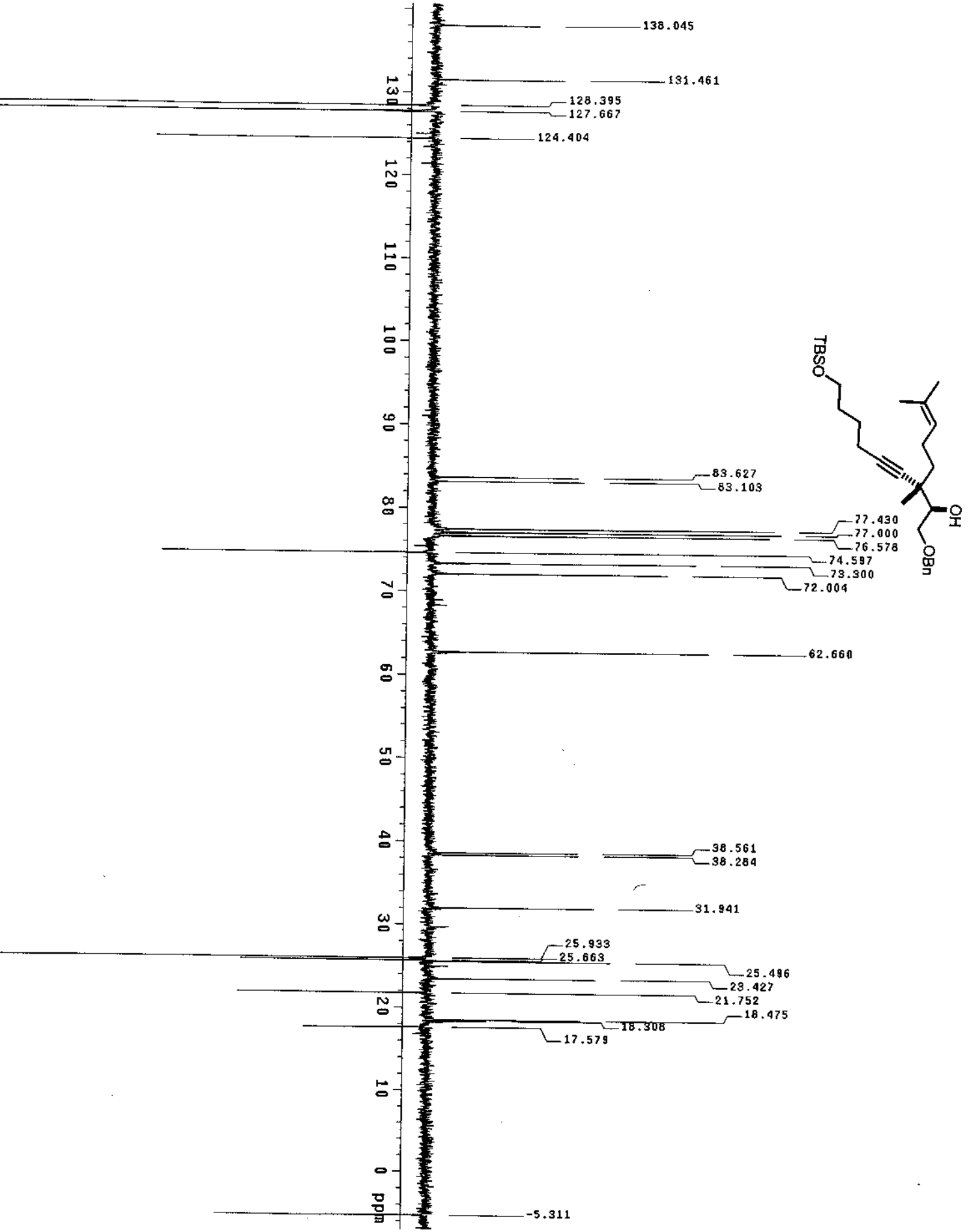





150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm
138.023
133.660
131.599
128.417
127.725
127.689
124.331
120.631
90.240
85.215
77.430
77.000
76.578
74.444
73.300
71.946
38.670
38.561
29.531
25.685
25.510
23.464
22.313
21.512
21.476
17.609
OH
OBn

hz33
Solvent: CDCl3
Ambient temperature
UNITYplus-300 "nmr2"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 15.0 degrees
Acq. time 3.813 sec
Width 4196.4 Hz
8 repetitions
OBSERVE H1, 300.1390403 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 1 minute

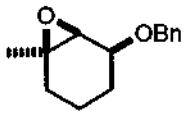


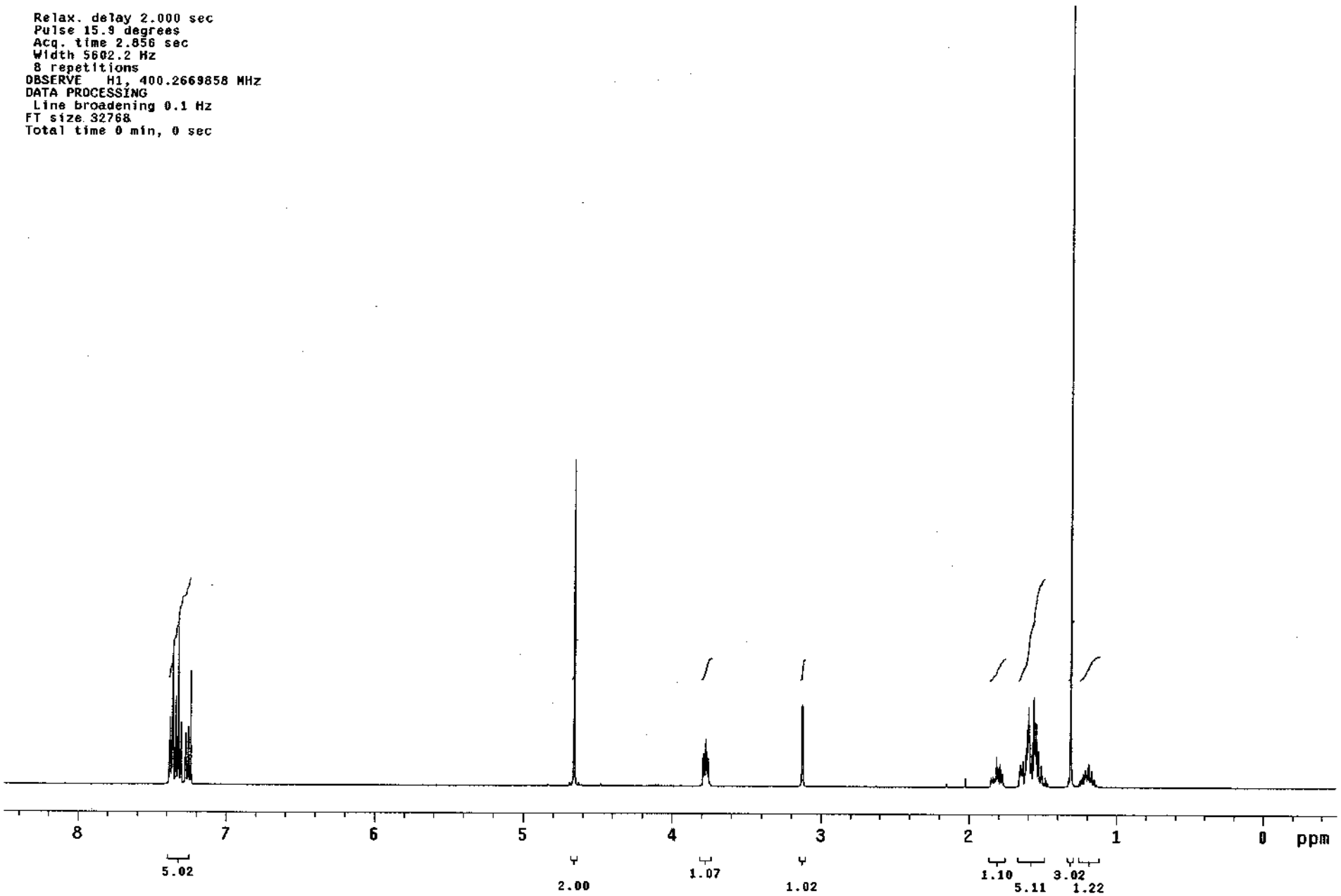

138.045
131.461
128.395
127.667
124.404
83.627
83.103
77.430
77.000
76.578
74.597
73.300
72.004
62.660
38.561
38.284
31.941
25.933
25.663
25.496
23.427
21.752
18.475
18.308
17.579
-5.311
ppm
TBSO
OH
OBn

hz-5-19

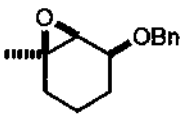
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

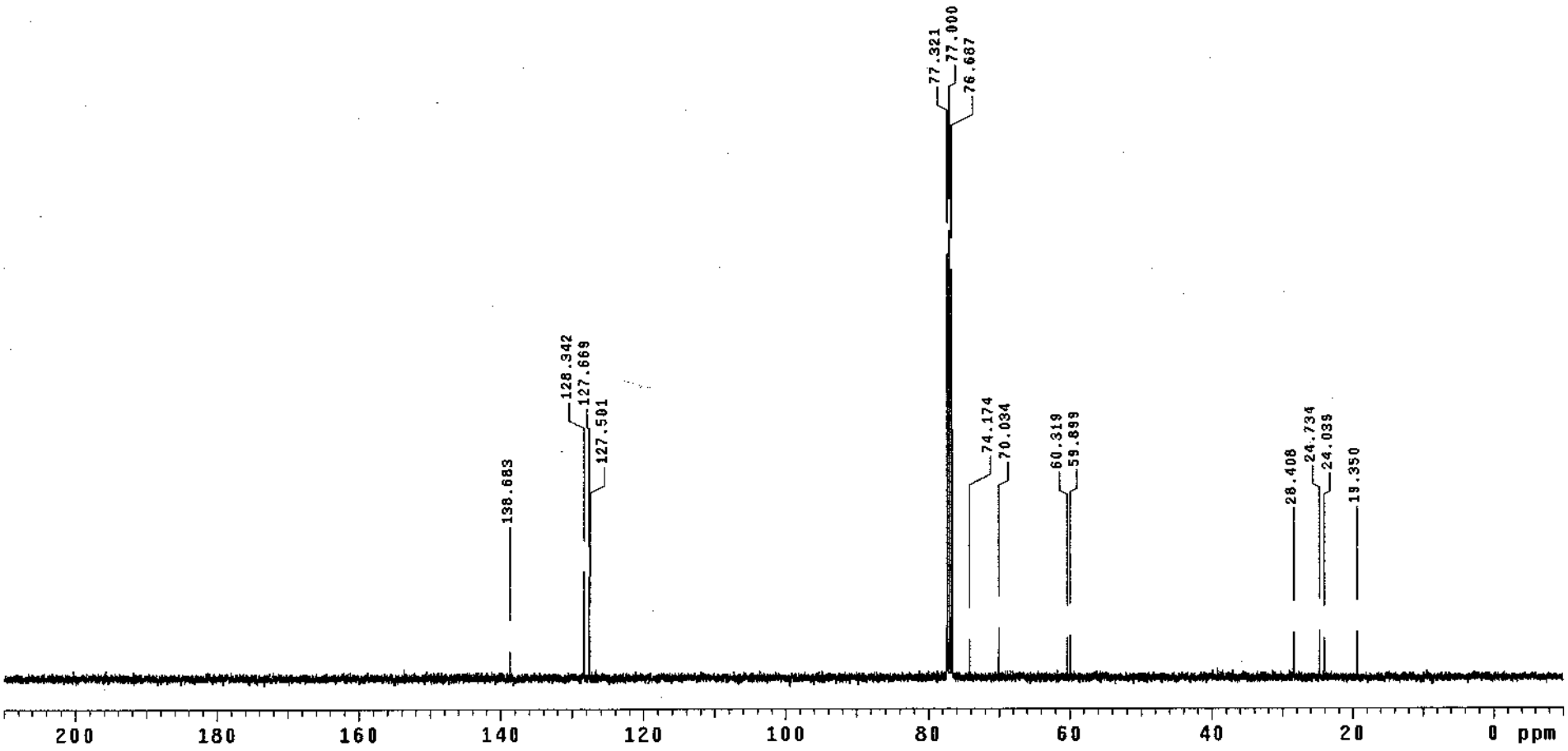
Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669858 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 0 sec





INDEX	FREQUENCY	PPM	HEIGHT
1	13958.084	138.683	4.2
2	12917.226	128.342	17.1
3	12849.578	127.669	16.2
4	12832.666	127.501	6.8
5	7782.122	77.321	67.8
6	7749.835	77.000	71.6
7	7718.318	76.687	65.4
8	7465.406	74.174	6.1
9	7048.755	70.034	7.9
10	6070.933	60.319	6.4
11	6028.653	59.899	6.8
12	2859.187	28.408	7.2
13	2489.428	24.734	7.5
14	2419.474	24.039	6.4
15	1947.475	19.350	7.3

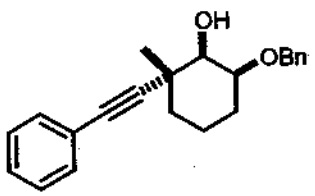




hz-5-20

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

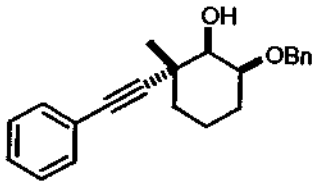
Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669851 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 0 sec

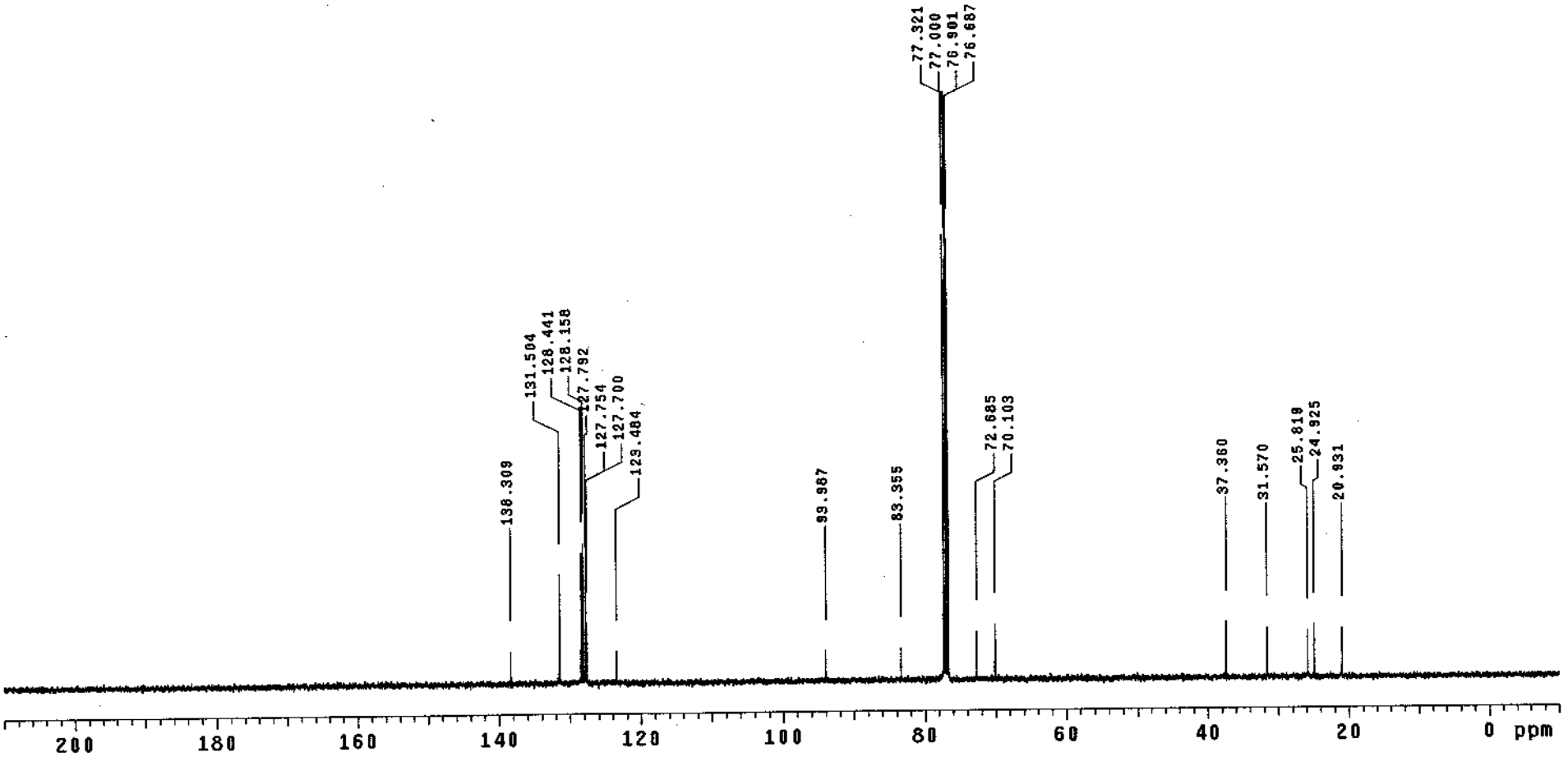


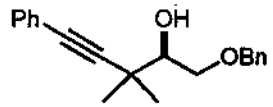
13C OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

Relax. delay 2.000 sec
Pulse 23.9 degrees
Acq. time 1.280 sec
Width 25188.9 Hz
622 repetitions
OBSERVE C13, 100.6472141 MHz
DECOUPLE H1, 400.2689955 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 47 sec



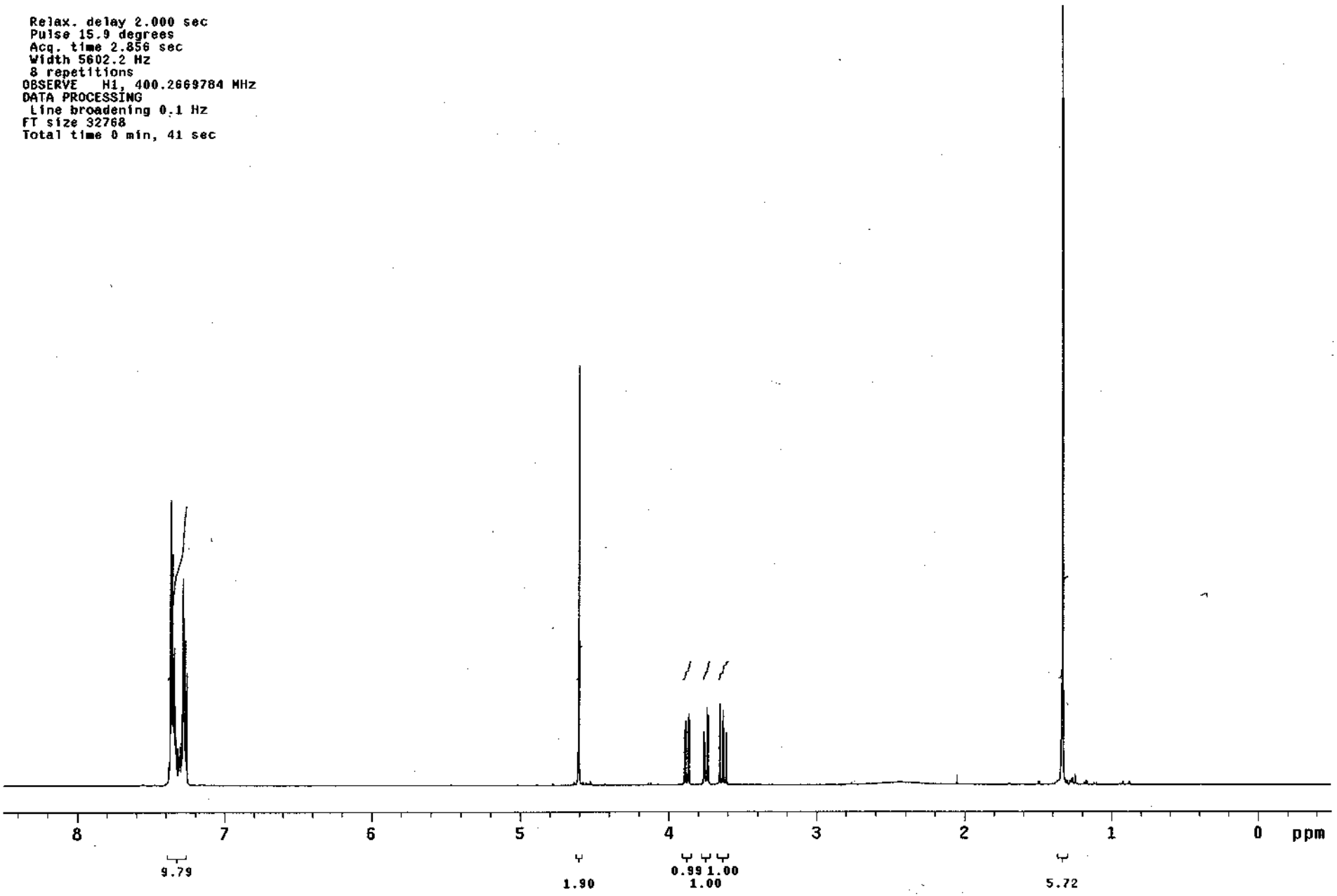




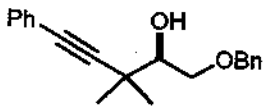
hz-5-53

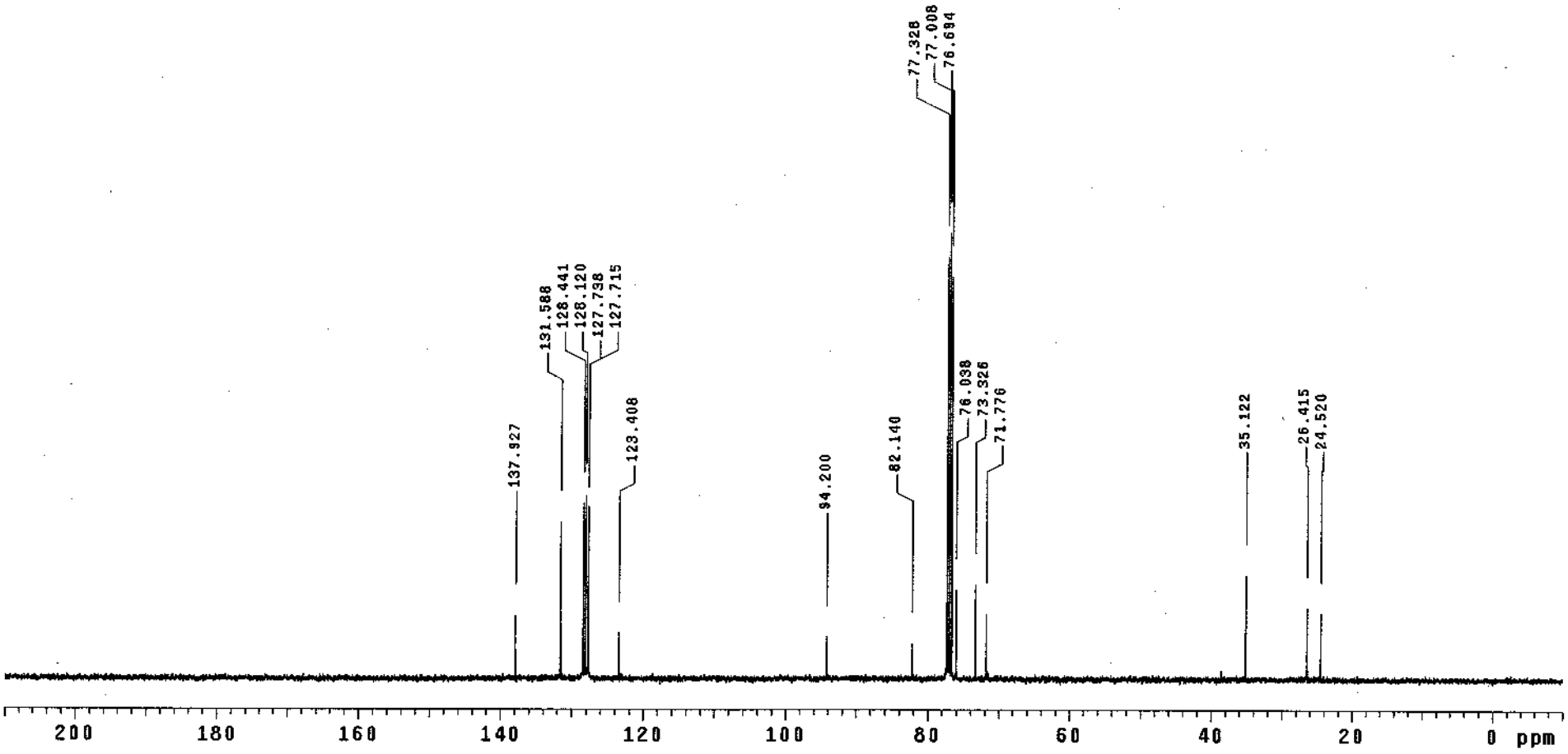
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669784 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 41 sec



INDEX	FREQUENCY	PPM	HEIGHT
1	13881.980	137.927	10.2
2	13243.936	131.588	25.2
3	12927.220	128.441	28.2
4	12894.933	128.120	29.5
5	12856.497	127.738	25.8
6	12854.191	127.715	27.7
7	12420.628	123.408	7.3
8	9481.011	94.200	6.7
9	8267.190	82.140	5.7
10	7782.891	77.328	67.8
11	7750.604	77.008	71.6
12	7719.086	76.694	64.6
13	7652.976	76.038	14.3
14	7380.077	73.326	15.1
15	7224.025	71.776	10.4
16	3534.899	35.122	16.6
17	2658.549	26.415	11.4
18	2467.904	24.520	10.6

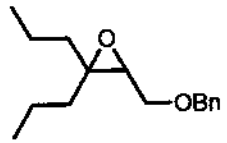


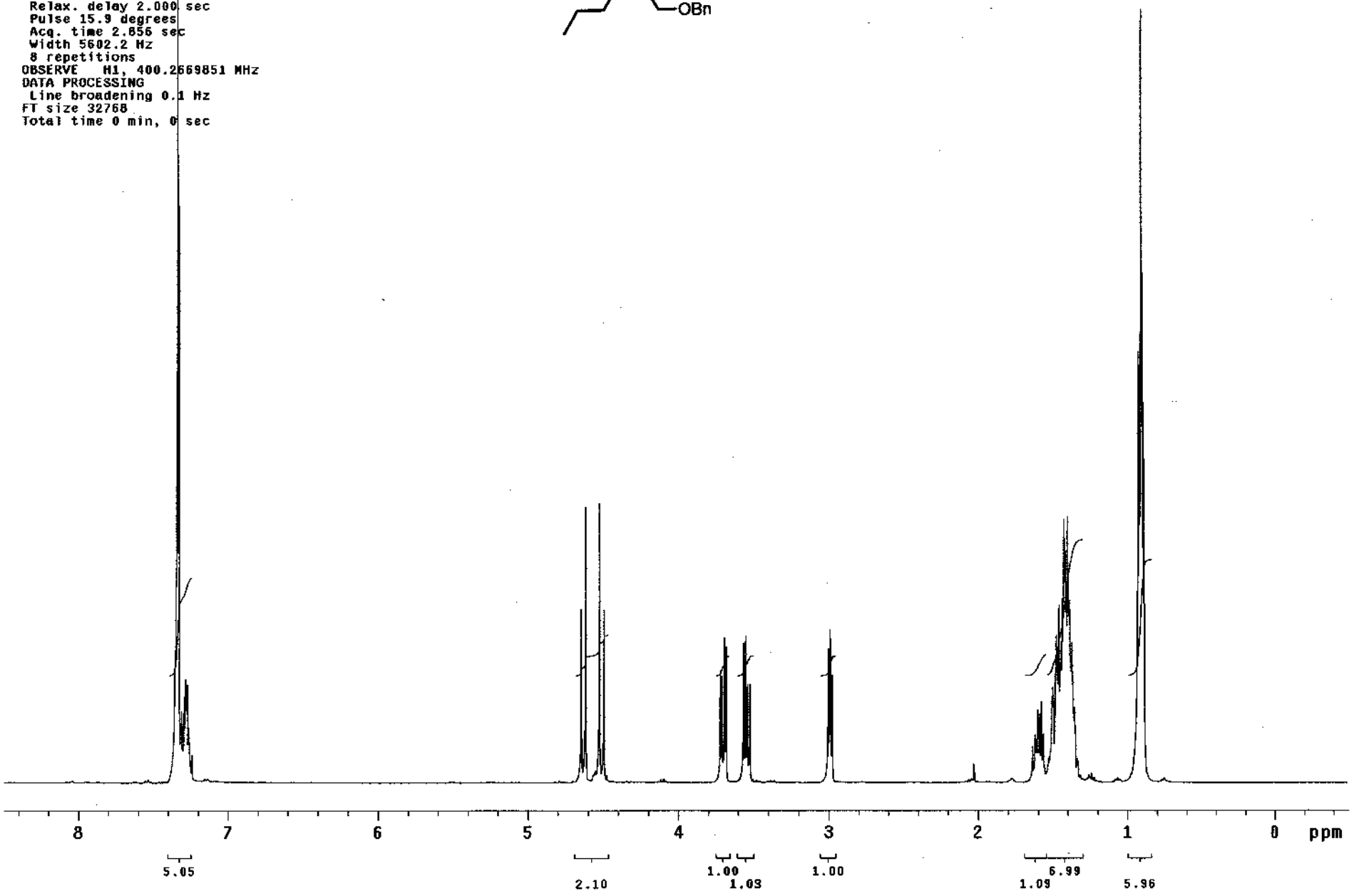


hz-4-60

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669851 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 0 sec

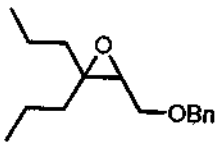


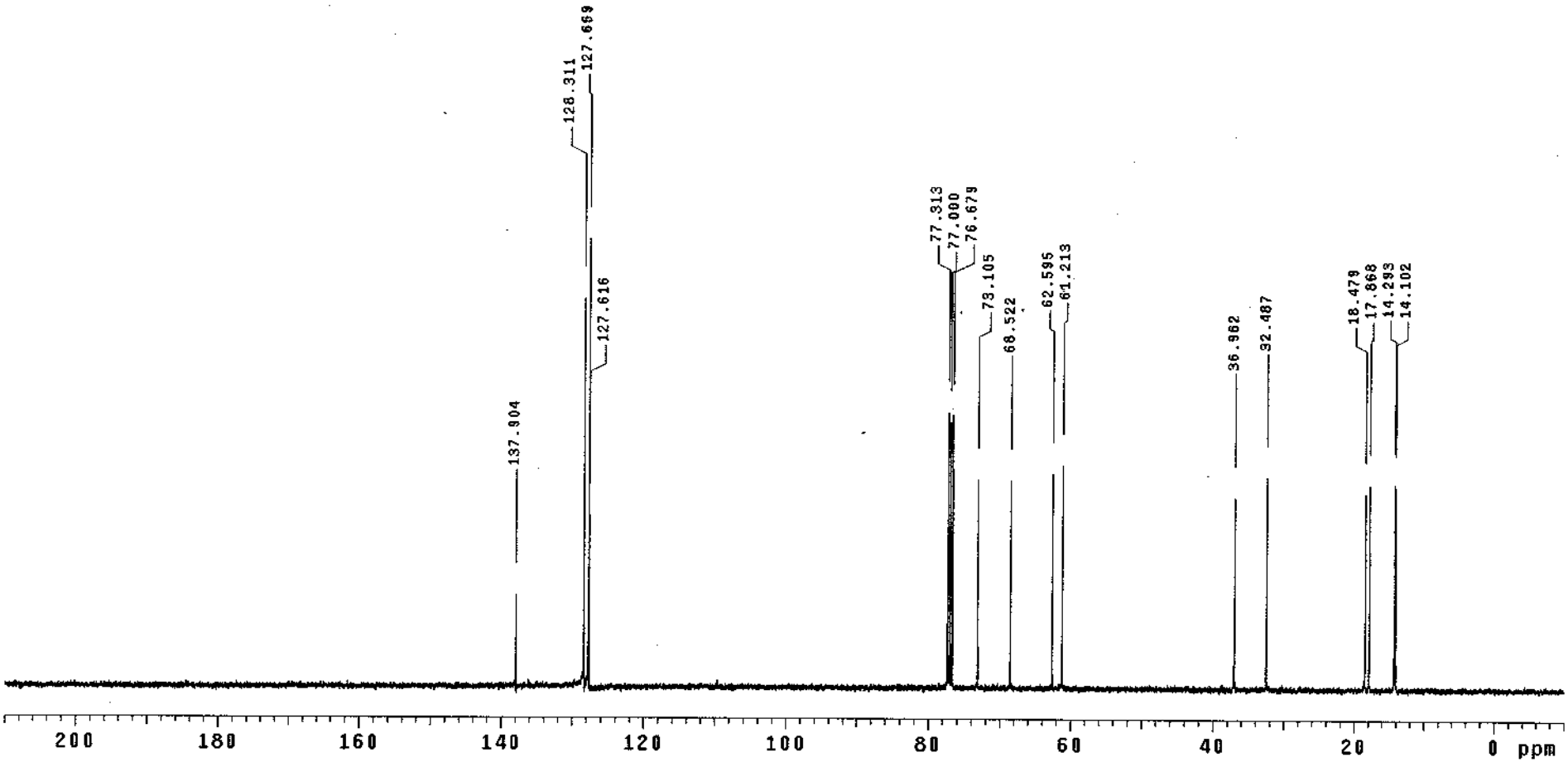


hz-4-60c

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

Relax. delay 2.000 sec
Pulse 23.3 degrees
Acq. time 1.280 sec
Width 25188.9 Hz
336 repetitions
OBSERVE C13, 100.6472218 MHz
DECOUPLE H1, 400.2689955 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 47 sec

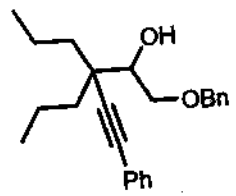




hz-4-63-2

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

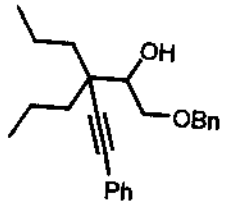
Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669855 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 0 sec

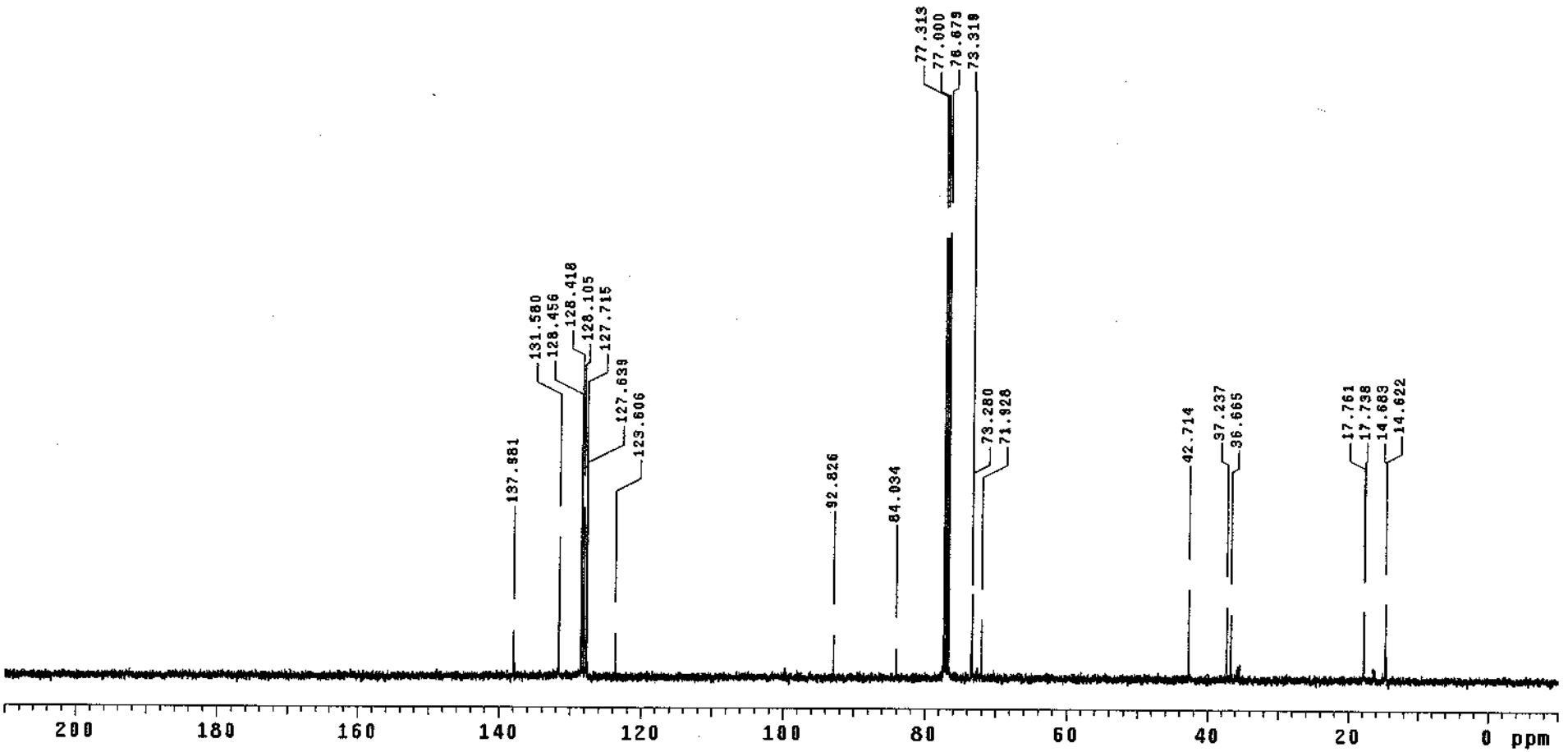


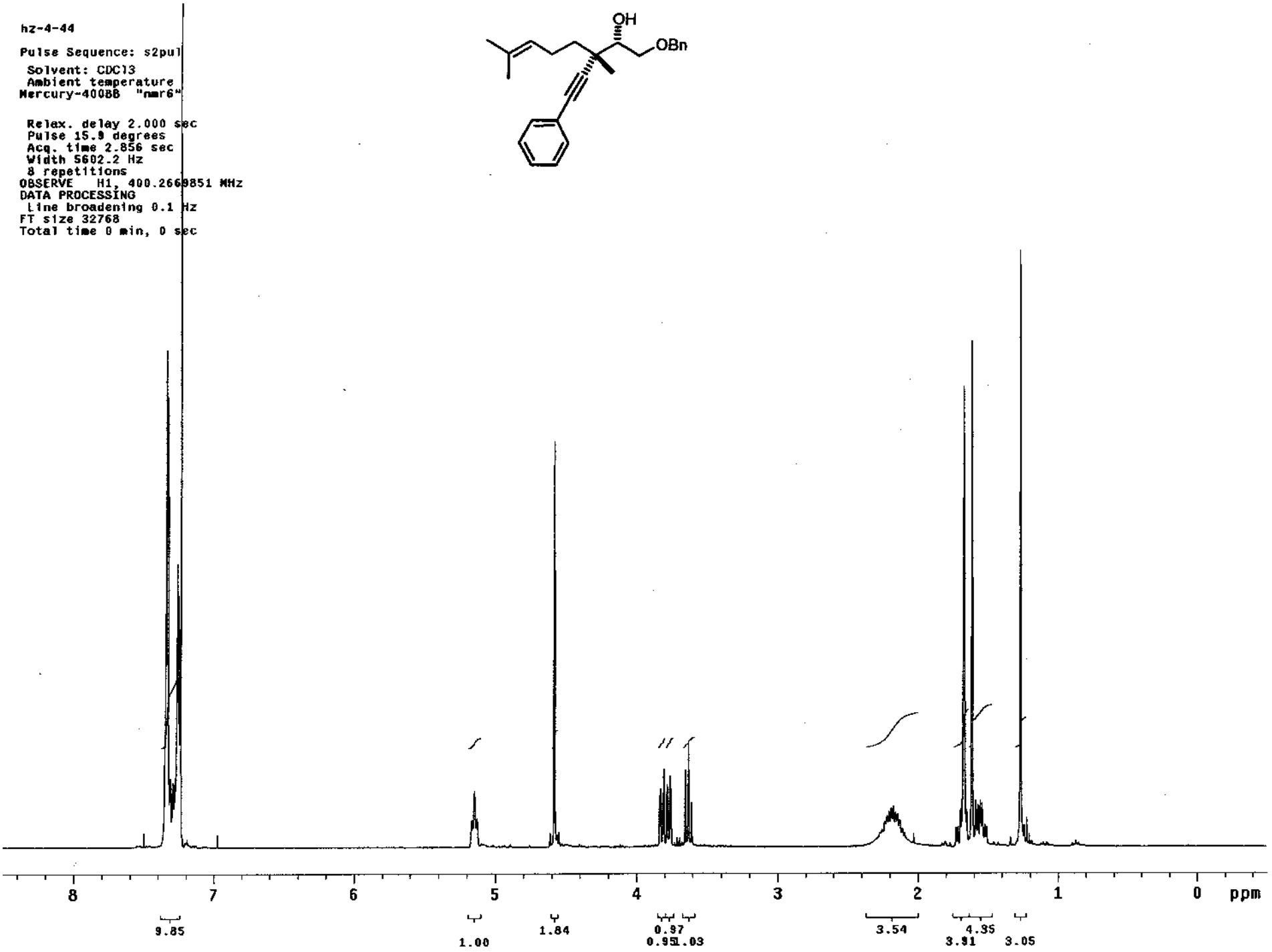
hz-4-63-2c

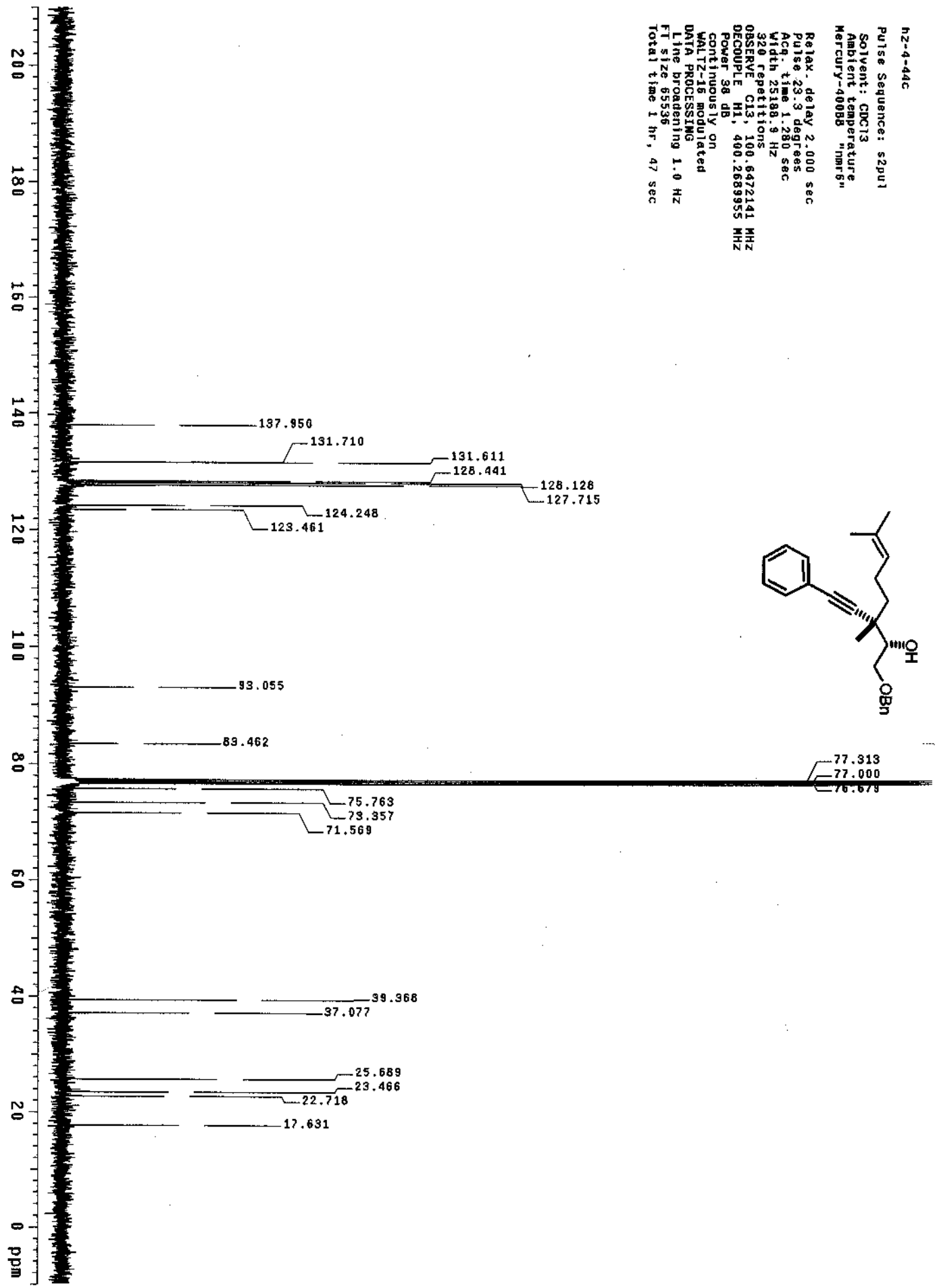
Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
Mercury-400BB "nmr6"

 Relax. delay 2.000 sec
 Pulse 23.3 degrees
 Acq. time 1.280 sec
 Width 25188.9 Hz
 272 repetitions
OBSERVE C13, 100.6472164 MHz
DECOUPLE H1, 400.2689955 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 47 sec





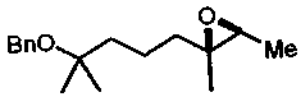

hz-4-44
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"
Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669851 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 0 sec
OH
OBn
8
7
6
5
4
3
2
1
0
ppm
9.85
1.00
1.84
0.87
0.95
1.03
3.54
4.35
3.91
3.05

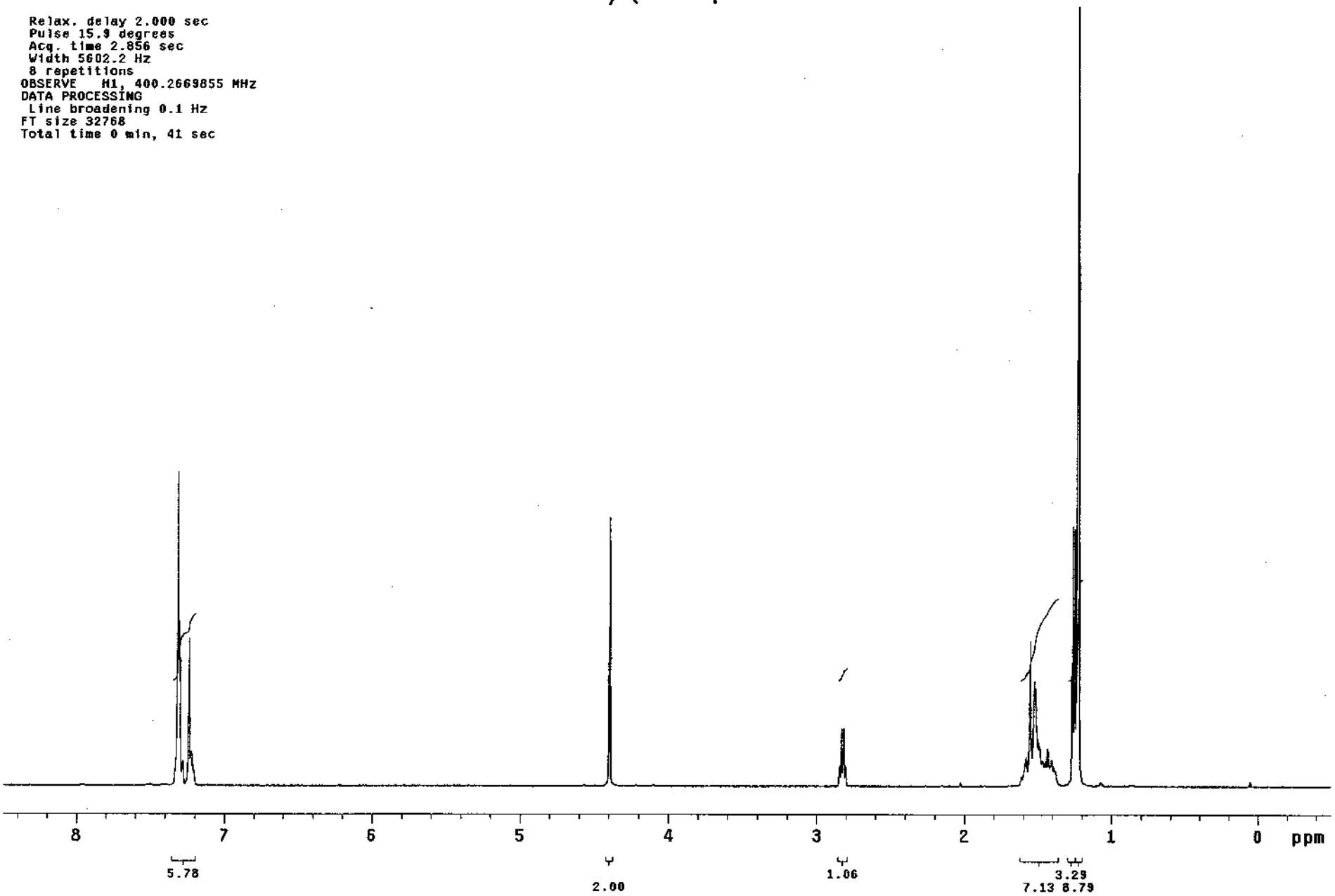

hz-4-44c
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmrf6"
Relax. delay 2.000 sec
Pulse 23.3 degrees
Acq. time 1.280 sec
Width 25188.9 Hz
320 repetitions
OBSERVE C13, 100.6472141 MHz
DECOUPLE H1, 400.2689955 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 47 sec
137.950
131.710
131.611
128.441
128.128
127.715
124.248
123.461
93.055
89.462
77.313
77.000
76.679
75.763
73.357
71.569
39.368
37.077
25.689
23.466
22.718
17.631
OH
OBn
200
180
160
140
120
100
80
60
40
20
0 ppm

hz-5-27

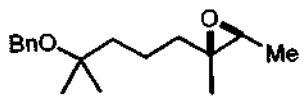
Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
Mercury-400BB "nmr6"

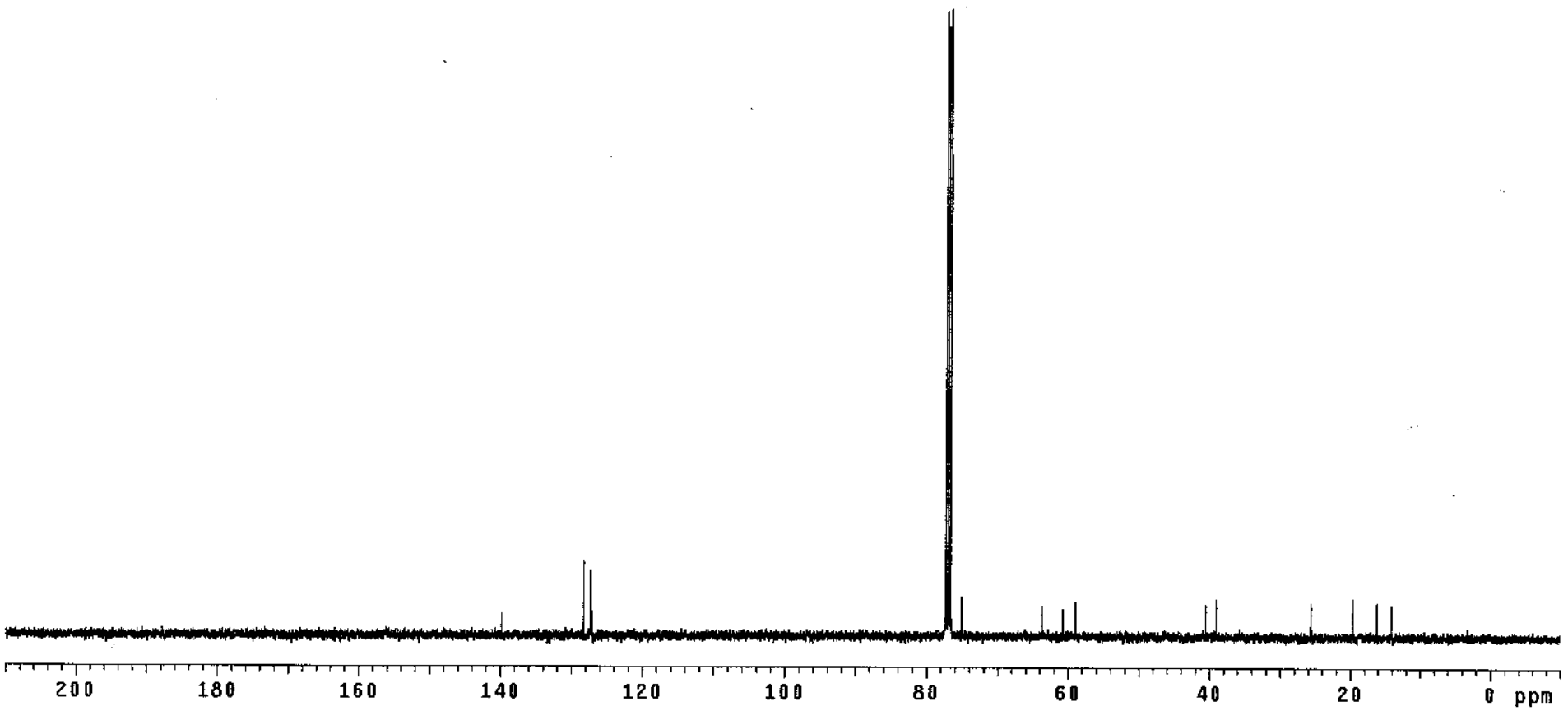
 Relax. delay 2.000 sec
 Pulse 15.9 degrees
 Acq. time 2.856 sec
 Width 5602.2 Hz
 8 repetitions
OBSERVE H1, 400.2669855 MHz
DATA PROCESSING
 Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 41 sec





INDEX	FREQUENCY	PPM	HEIGHT
1	14073.394	139.829	3.5
2	12908.770	128.258	12.0
3	12808.836	127.265	10.3
4	12790.386	127.081	3.9
5	7781.353	77.313	99.9
6	7749.835	77.000	97.5
7	7717.549	76.679	100.2
8	7556.885	75.083	6.8
9	6406.098	63.649	5.0
10	6113.982	60.747	4.5
11	5937.174	58.990	5.7
12	4079.927	40.537	5.2
13	3928.487	39.032	6.0
14	2580.138	25.635	5.1
15	2575.526	25.590	5.3
16	1974.380	19.617	6.1
17	1635.371	16.249	5.4
18	1420.127	14.110	5.0

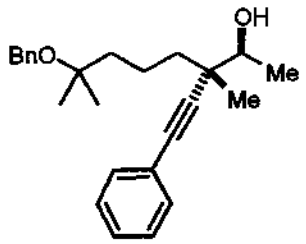




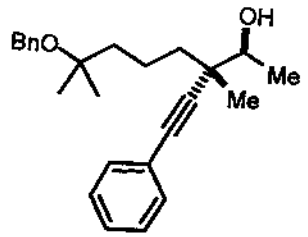
hz-5-28

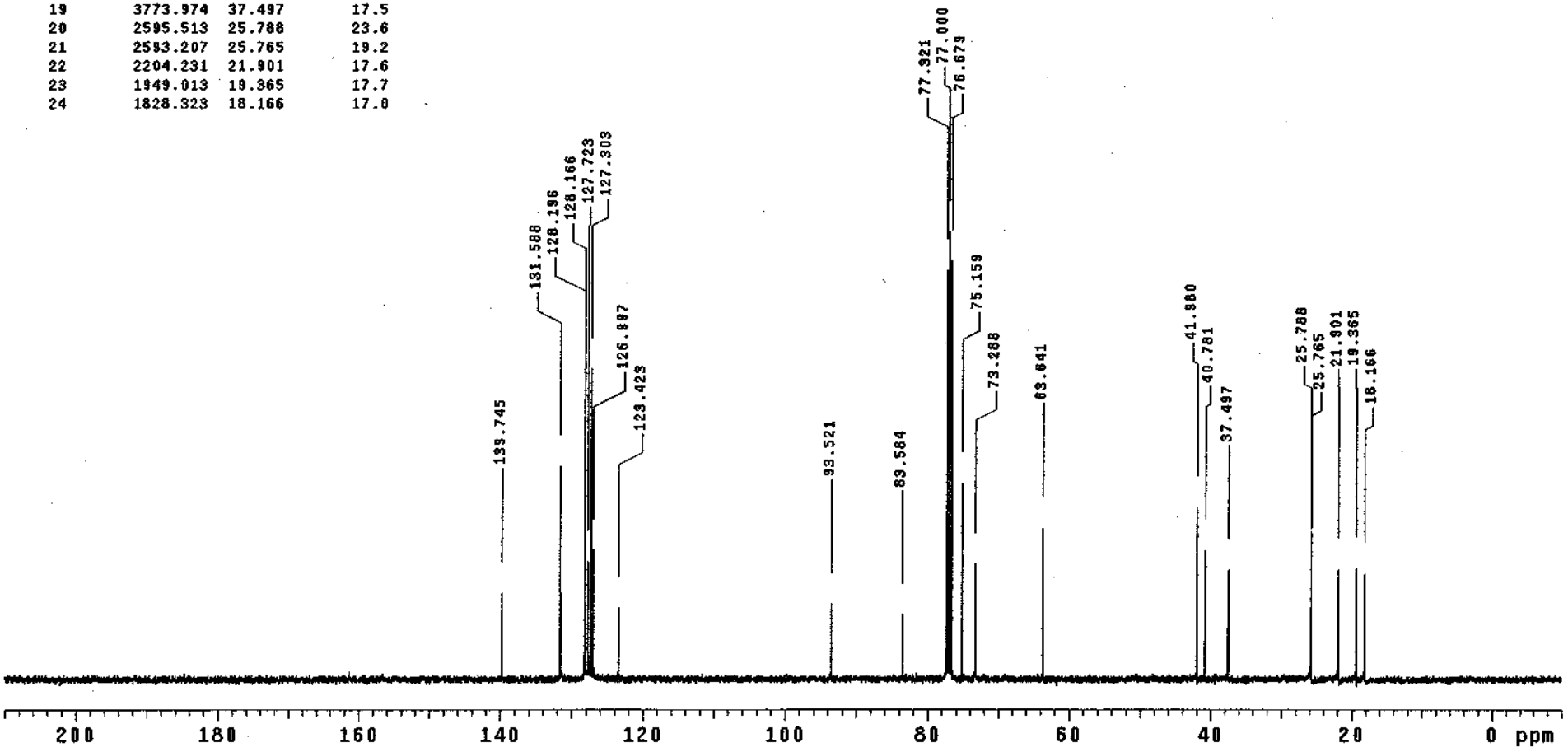
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669855 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 0 sec



INDEX	FREQUENCY	PPM	HEIGHT
1	14064.938	139.745	13.8
2	13243.936	131.588	34.0
3	12902.621	128.196	39.1
4	12899.546	128.166	46.0
5	12854.960	127.723	18.9
6	12812.680	127.303	49.7
7	12781.931	126.997	20.7
8	12422.166	123.423	11.5
9	9412.595	93.521	12.0
10	8412.480	83.584	10.3
11	7782.122	77.321	65.4
12	7749.896	77.000	71.6
13	7717.549	76.679	66.8
14	7564.572	75.159	31.4
15	7376.234	73.288	18.4
16	6405.330	63.641	24.2
17	4225.217	41.980	27.5
18	4104.527	40.781	20.6
19	3773.974	37.497	17.5
20	2595.513	25.788	23.6
21	2593.207	25.765	19.2
22	2204.231	21.901	17.6
23	1949.013	19.365	17.7
24	1828.323	18.166	17.0

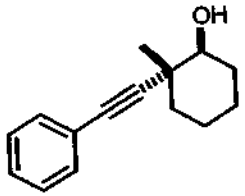




hz-5-4

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

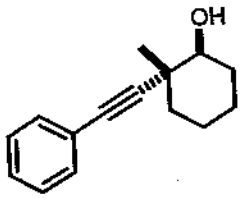
Relax. delay 2.000 sec
Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2669861 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 0 sec



13C OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
Mercury-400BB "nmr6"

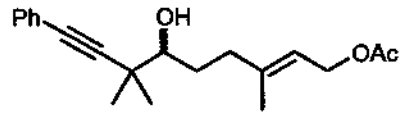
Relax. delay 2.000 sec
Pulse 23.3 degrees
Acq. time 1.280 sec
Width 25188.9 Hz
972 repetitions
OBSERVE C13, 100.6472126 MHz
DECOUPLE H1, 400.2689955 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1 hr, 47 sec



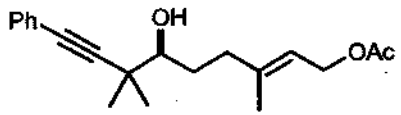
hz-5-43

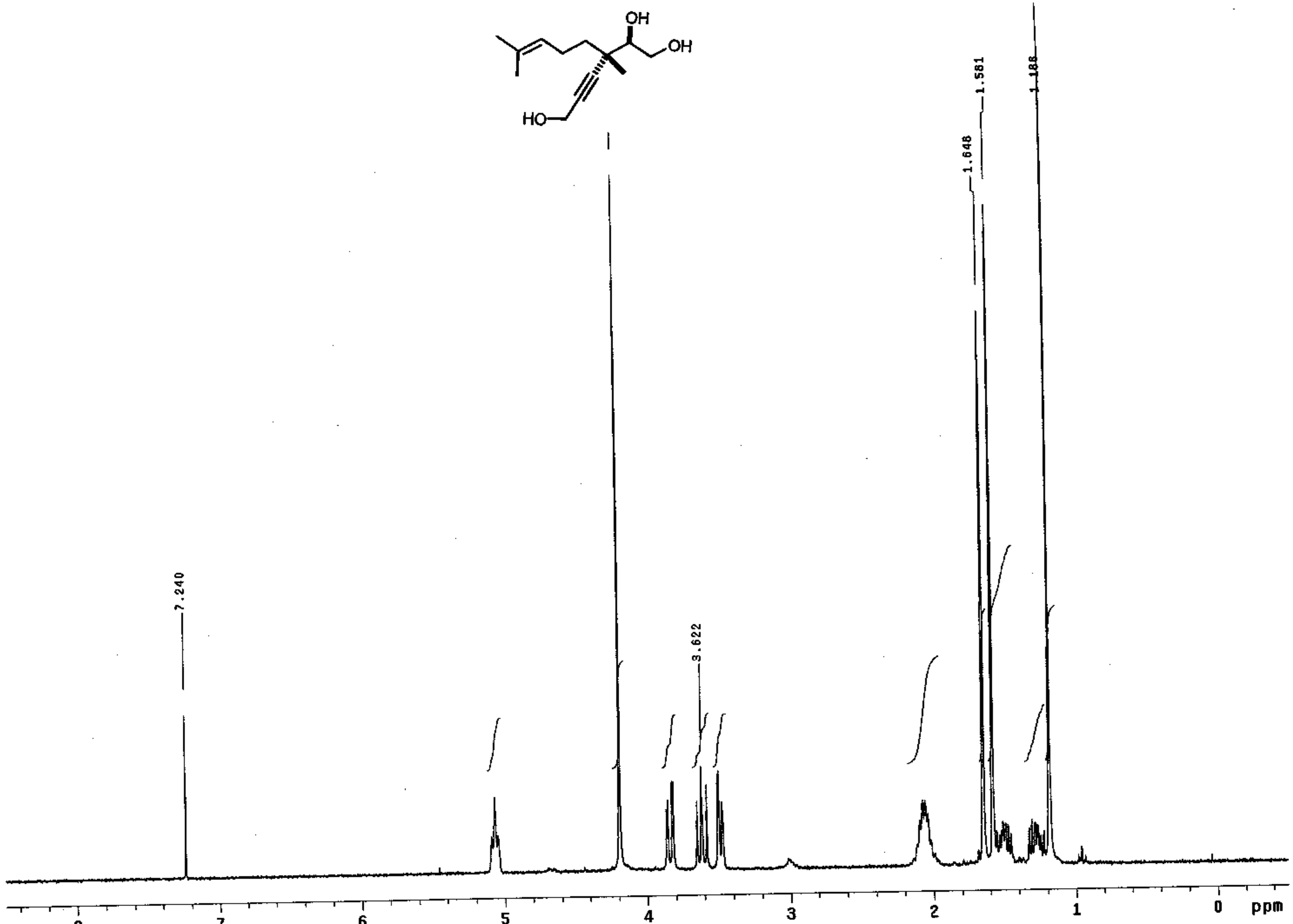
Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
Mercury-400BB "nmr6"

 Relax. delay 2.000 sec
 Pulse 15.9 degrees
 Acq. time 2.856 sec
 Width 5602.2 Hz
 8 repetitions
OBSERVE H1, 400.2669855 MHz
DATA PROCESSING
 Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 41 sec

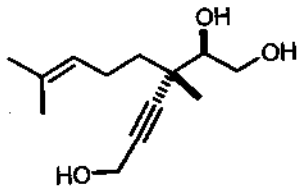


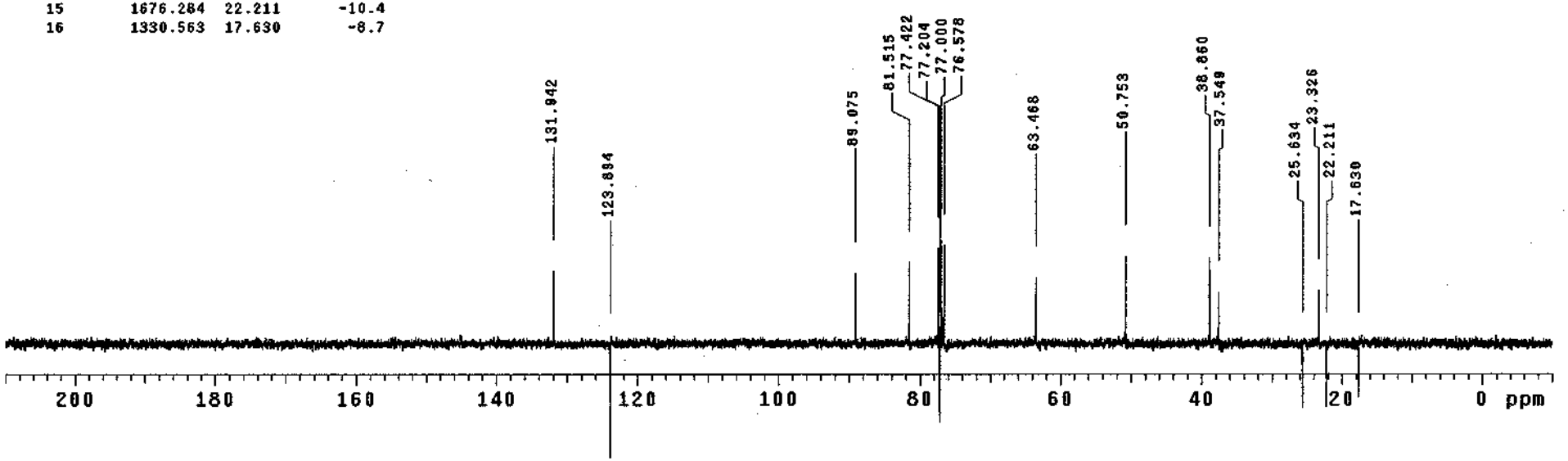
INDEX	FREQUENCY	PPM	HEIGHT
1	17223.642	171.129	8.7
2	14304.781	142.128	12.5
3	13245.473	131.603	27.7
4	12903.389	128.204	30.7
5	12868.028	127.853	13.2
6	12409.866	123.301	7.0
7	11934.792	118.560	14.2
8	9507.148	94.460	6.4
9	8305.626	82.522	6.2
10	7813.640	77.634	13.2
11	7782.122	77.321	121.5
12	7749.835	77.000	130.2
13	7717.549	76.679	122.0
14	6173.174	61.335	15.2
15	3800.110	37.757	13.2
16	3667.120	36.435	14.9
17	3006.014	29.867	13.7
18	2534.783	25.185	10.4
19	2518.640	25.024	10.3
20	2117.364	21.037	12.2
21	1659.971	16.493	12.5

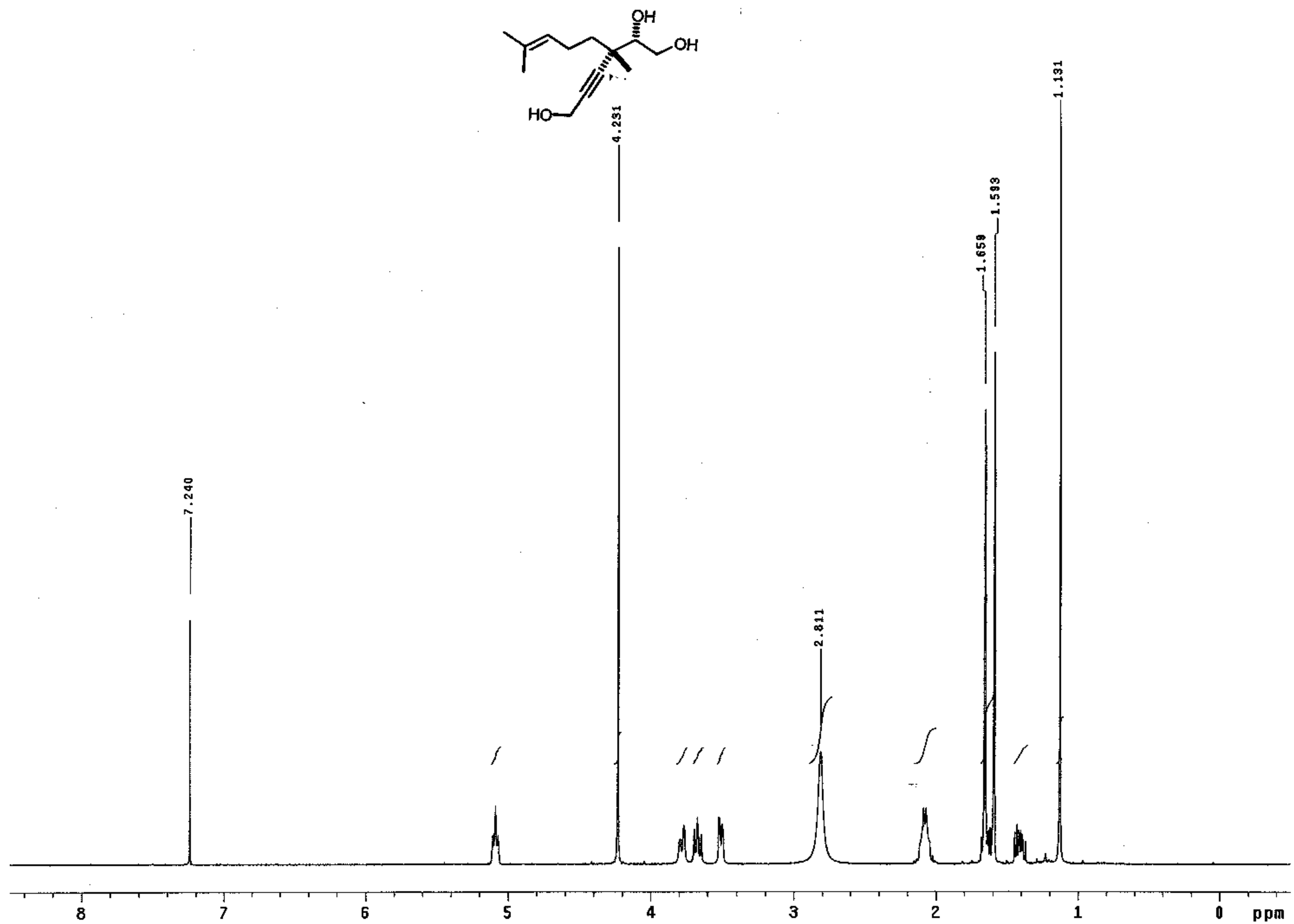



OH
OH
HO
7.240
3.622
1.648
1.581
1.188
8
7
6
5
4
3
2
1
0
ppm

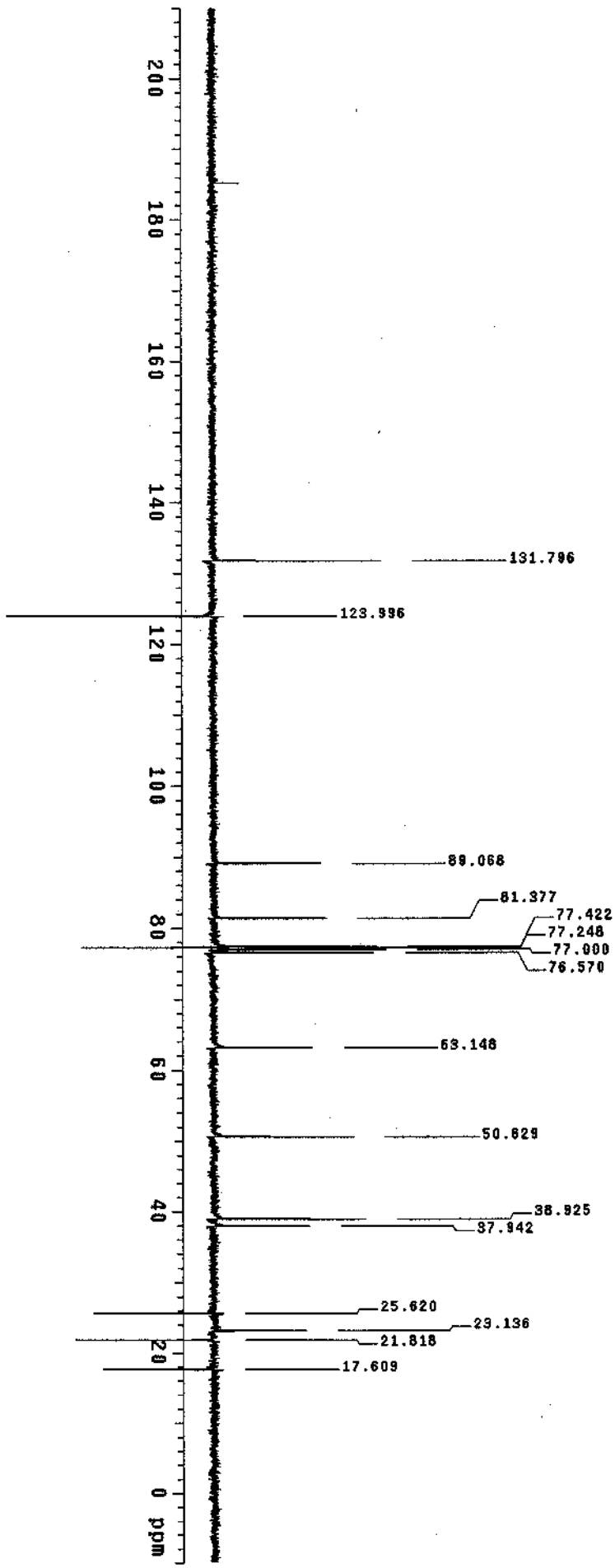
INDEX	FREQUENCY	PPM	HEIGHT
1	9957.642	131.942	11.8
2	9350.294	123.894	-18.6
3	6722.487	89.075	11.4
4	6151.966	81.515	13.2
5	5843.071	77.422	15.4
6	5826.581	77.204	-12.7
7	5811.192	77.000	16.8
8	5779.313	76.578	15.9
9	4789.969	63.468	10.6
10	3830.305	50.753	14.2
11	2932.751	38.860	13.9
12	2833.816	37.549	8.3
13	1934.613	25.634	-10.4
14	1760.378	23.326	8.6
15	1676.284	22.211	-10.4
16	1330.563	17.630	-8.7

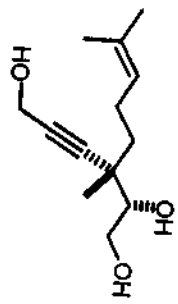


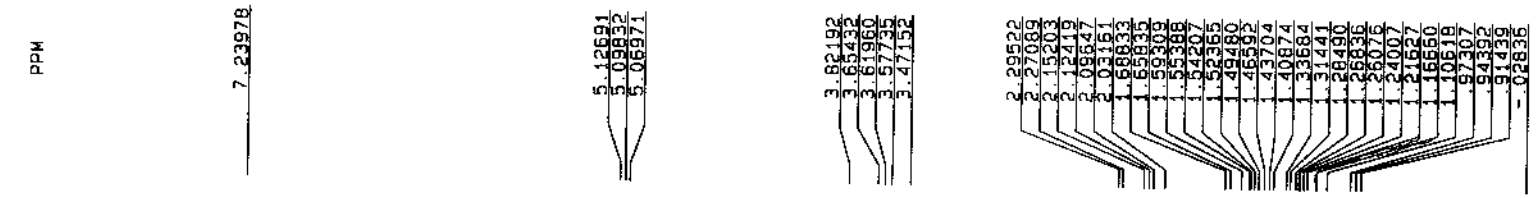


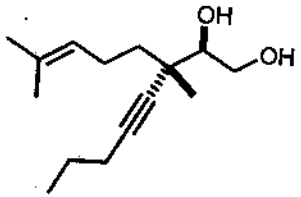


OH
OH
HO
7.240
4.231
2.811
1.659
1.593
1.131
8
7
6
5
4
3
2
1
0
ppm


200
180
160
140
120
100
80
60
40
20
0 ppm
131.796
123.996
89.068
81.377
77.422
77.248
77.000
76.570
68.148
50.829
38.925
37.942
25.620
23.136
21.818
17.609


HO
OH
OH

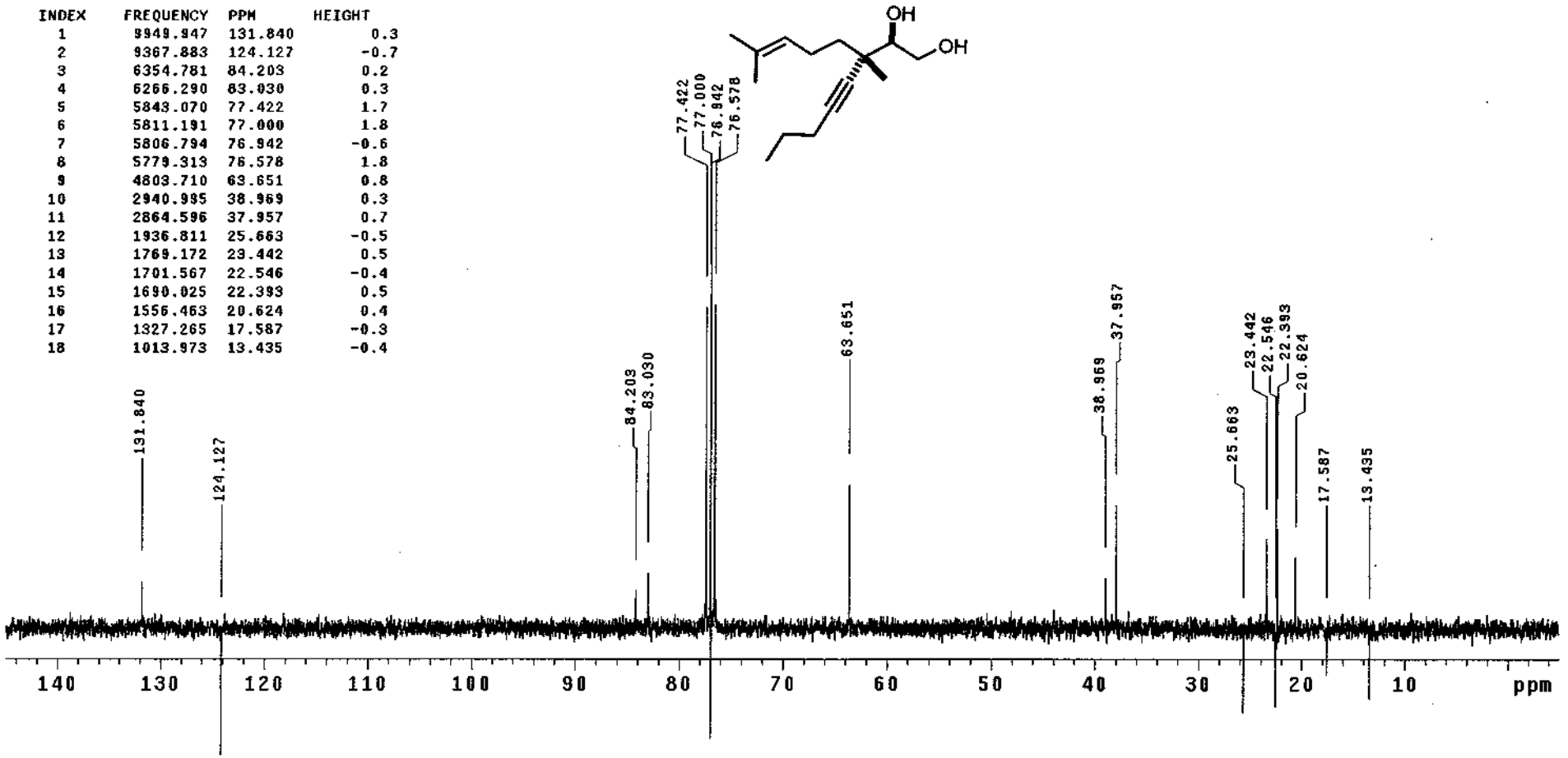


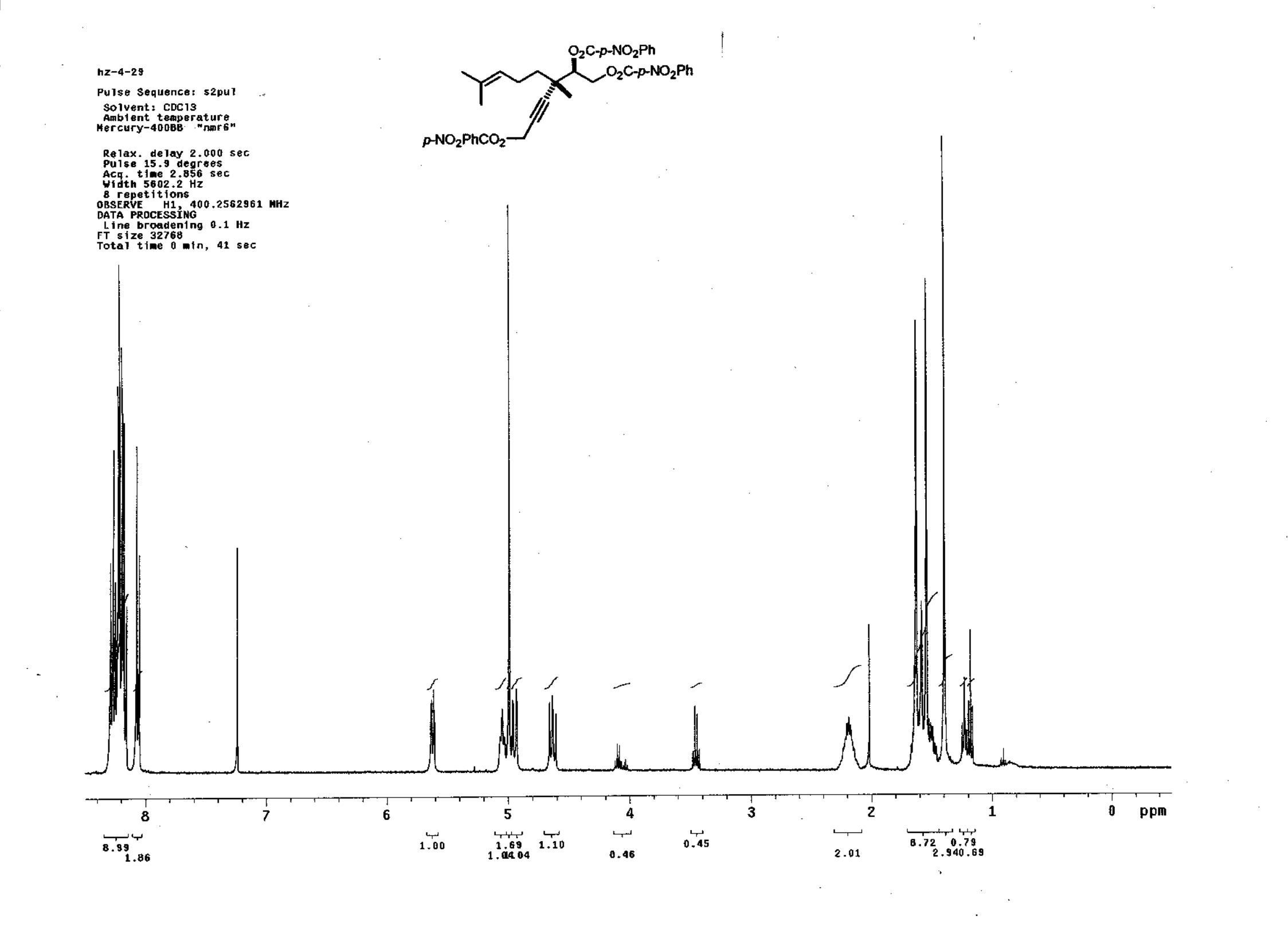


DATE 15-6-2

SF	250.133
SY	100.0
O1	4112.988
SI	16384
TD	16384
SW	3496.503
HZ/PT	.427
PW	2.0
RD	1.000
AQ	2.343
RG	20
NS	16
TE	297
FW	4400
O2	1000.000
DP	63L PO
LB	.100
GB	.100
CX	21.00
CY	13.00
F1	8.501P
F2	-.498P
HZ/CM	107.193
PPM/CM	.429
SR	2859.03

INDEX	FREQUENCY	PPM	HEIGHT
1	9949.947	131.840	0.3
2	9367.883	124.127	-0.7
3	6354.781	84.203	0.2
4	6266.290	83.030	0.3
5	5843.070	77.422	1.7
6	5811.191	77.000	1.8
7	5806.794	76.942	-0.6
8	5779.313	76.578	1.8
9	4803.710	63.651	0.8
10	2940.995	38.969	0.3
11	2864.596	37.957	0.7
12	1936.811	25.663	-0.5
13	1769.172	23.442	0.5
14	1701.567	22.546	-0.4
15	1690.025	22.393	0.5
16	1556.463	20.624	0.4
17	1327.265	17.587	-0.3
18	1013.973	13.435	-0.4

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Pulse 15.9 degrees
Acq. time 2.856 sec
Width 5602.2 Hz
8 repetitions
OBSERVE H1, 400.2562961 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min, 41 sec
O2C-p-NO2Ph
O2C-p-NO2Ph
p-NO2PhCO2
8
7
6
5
4
3
2
1
0
ppm
8.99
1.86
1.00
1.69
1.04
1.10
0.46
0.45
2.01
6.72
0.79
2.94
0.69

hz-4-29c

Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
UNITYplus-300 "nmr2"

 Relax. delay 2.000 sec
 Pulse 36.0 degrees
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 Width 18009.9 Hz
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OBSERVE C13, 75.4700216 MHz
DECOUPLE H1, 300.1409259 MHz
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 WALTZ-16 modulated
Single precision data
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FT size 65536
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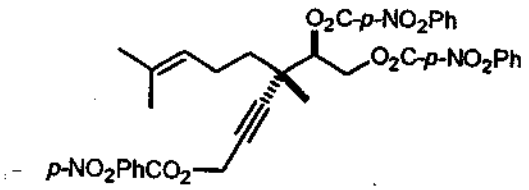
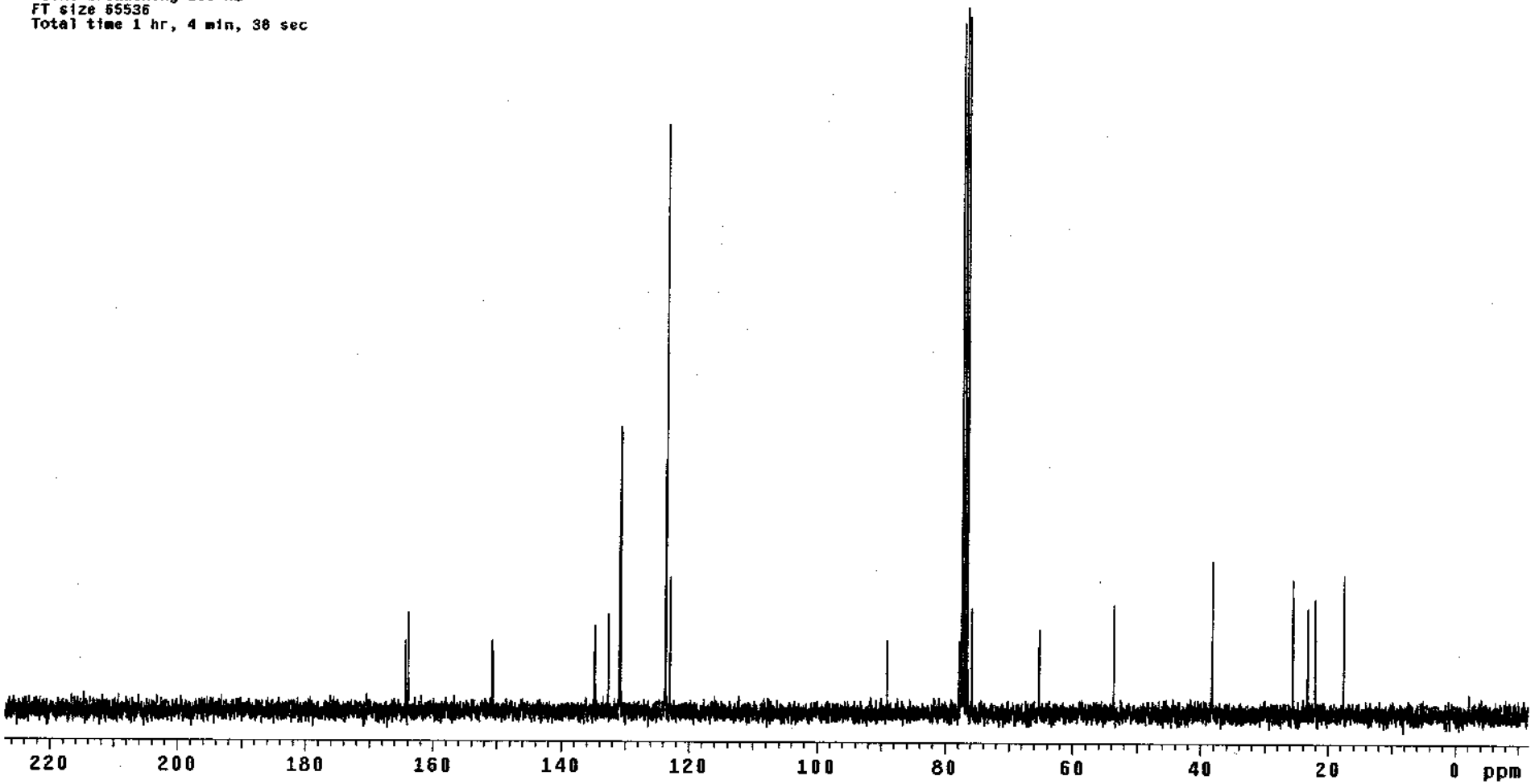
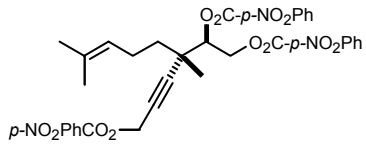




Crystallographic Material for



In this experimental section, compound **1** stands for the structure shown above.

Table 1. Crystallographic Data for **1**.

Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($Å^2$) for the non-hydrogen atoms of **1**.

Table 3. Bond Lengths (Å) and Angles (^{o}) for the non-hydrogen atoms of **1**.

Table 4. Anisotropic thermal parameters for the non-hydrogen atoms of **1**.

Table 5. Fractional coordinates and isotropic thermal parameters ($Å^2$) for the hydrogen atoms of **1**.

Table 6. Torsion Angles (^{o}) for the non-hydrogen atoms of **1**.

Table 7. Observed and calculated structure factor amplitudes for **1**. Values for Fo, Fc and σ(Fo) have been multiplied by 10.

Figure 1. View of **1** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. Most hydrogen atoms have been removed for clarity. The minor component of the disordered p-nitrobenzoate is not shown.

Figure 2. View of **1** showing a partial atom labeling scheme. Atoms from the minor component of the disordered p-nitrobenzoate have labels appended by an A. The site occupancy factor for the minor component refined to 44(2)%.

Figure 3. Unit cell packing diagram for **1**. The view is approximately down the **a** axis.

X-ray Experimental for $C_{34}H_{31}N_3O_{12}$: Crystals grew as very thin, colorless lathes by slow diffusion of EtOAc into a Et_2O solution. The data crystal was a long lathe that had approximate dimensions; 0.60 x 0.06 x 0.02 mm. The data were collected on a Nonius Kappa CCD diffractometer using a graphite monochromator with MoKα radiation (λ = 0.71073Å). A total of 212 frames of data were collected using ω-scans with a scan range of 1.5° and a counting time of 258 seconds per frame. The data were collected at 153 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in Table 1. Data reduction were performed using DENZO-SMN.[1] The structure was solved by direct methods using SIR92[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-97.[3] The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms).

One of the p-nitrobenzoate groups was found to be disordered by rotation about the C-ester O bond connecting the affected group to the remainder of the molecule (Figure 2). The disorder was modeled by first idealizing the phenyl ring of two components and restraining the acetate groups to have the same geometry. The site occupancy factors for one orientation was assigned a value of x, while the second orientation had a site occupancy of 1-x. A common isotropic displacement parameter was refined for the two groups. In this way, the site occupancy factor for the minor component was determined to be 44(2)%. In subsequent refinement, the site occupancies for the two groups were fixed and individual isotropic and eventually anisotropic displacement parameters were refined. In the final refinement model, the anisotropic displacement parameters were refined while being restrained to be approximately isotropic.

The crystals were very thin and diffracted very poorly. The disordered group contributed to the poor diffraction quality of the crystals. X-ray quality crystals were very difficult to come by despite several attempts to grow superior crystals. The high value of the internal R (Rint = 0.37) was due in large measure to the poor scattering power of the crystal. Of the 4139 unique reflections, only 1208 reflections had $I>2(\sigma(I))$.
The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.02*P)^2]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.226, with R(F) equal to 0.131 and a goodness of fit, S, = 1.17. Definitions used for calculating R(F), $R_w(F^2)$ and the goodness of fit, S, are given below.[4] The data were corrected for secondary extinction effects. The correction takes the form: $F_{corr} = kF_c/[1 + (1.3(6)x10^{-6})* F_c^2 \lambda^3/(\sin 2\theta)]^{0.25}$ where k is the overall scale factor. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[5] All figures were generated using SHELXTL/PC.[6] Tables of positional and thermal parameters, bond lengths and angles, torsion angles, figures and lists of observed and calculated structure factors are located in tables 1 through 7.

Table 1. Crystal data and structure refinement for 1.

Empirical formula	C34 H31 N3 O12
Formula weight	673.62
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/c

Unit cell dimensions	a = 6.2704(5) Å	α= 90.000(5)°.
	b = 22.667(2) Å	β= 97.697(6)°.
	c = 22.866(3) Å	γ = 90.000(4)°.
Volume	3220.7(6) $Å^3$	
Z	4	
Density (calculated)	1.389 Mg/m^3	
Absorption coefficient	0.107 mm^{-1}	
F(000)	1408	
Crystal size	0.60 x 0.06 x 0.02 mm	
Theta range for data collection	3.24 to 22.50°.	
Index ranges	-6<=h<=6, -24<=k<=24, -24<=l<=23	
Reflections collected	12577	
Independent reflections	4139 [R(int) = 0.3700]	
Completeness to theta = 22.50°	98.2 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4139 / 414 / 512	
Goodness-of-fit on F^2	1.171	
Final R indices [I>2sigma(I)]	R1 = 0.1309, wR2 = 0.1684	
R indices (all data)	R1 = 0.3457, wR2 = 0.2264	
Extinction coefficient	$1.3(6)x10^{-6}$	
Largest diff. peak and hole	0.429 and -0.272 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O1	1189(11)	8096(3)	1304(3)	45(2)
O2	4232(13)	8161(4)	890(4)	59(3)
O3	-4260(17)	6947(5)	-1209(4)	92(4)
O4	-1632(15)	7186(4)	-1702(4)	94(4)
O5	3881(12)	7509(4)	2257(3)	50(2)
O6	3263(13)	7028(4)	3062(4)	72(3)
O7	12534(14)	5421(4)	2747(4)	77(3)
O8	12030(20)	5654(6)	1865(6)	160(5)
N1	-2560(20)	7182(5)	-1263(6)	69(4)
N2	11570(20)	5709(7)	2350(7)	103(5)
O9	5285(16)	9608(4)	3741(4)	79(3)
O10	5320(20)	10229(6)	4375(5)	51(4)
O10A	7550(20)	9560(8)	3193(6)	63(6)
C26	2690(20)	9515(6)	2861(6)	54(4)
C27	3670(20)	9917(5)	3352(5)	59(4)
C28A	7070(30)	9490(13)	3674(10)	62(10)
C29A	8560(30)	9276(10)	4199(6)	38(9)
C30A	8020(20)	9274(8)	4769(8)	41(9)
C31A	9440(30)	9043(9)	5231(6)	56(10)
C32A	11410(30)	8813(11)	5123(8)	40(14)
C33A	11950(30)	8815(12)	4553(10)	46(10)
C34A	10530(30)	9047(12)	4091(7)	70(11)
N3A	13000(30)	8507(15)	5536(9)	55(11)
O11A	14940(40)	8473(13)	5533(10)	90(7)
O12A	12240(40)	8435(18)	5995(12)	99(8)
C28	6130(30)	9822(10)	4181(9)	50(7)
C29	8010(20)	9477(8)	4475(7)	58(8)
C30	8320(30)	9512(7)	5088(7)	56(7)
C31	10100(30)	9243(9)	5407(6)	89(11)
C32	11570(30)	8940(10)	5114(9)	44(12)
C33	11260(30)	8905(10)	4502(9)	68(10)

C34	9480(30)	9174(9)	4182(6)	74(9)
N3	13300(30)	8683(10)	5525(10)	83(12)
O11	12880(40)	8433(16)	5968(10)	119(7)
O12	14620(30)	8473(9)	5238(8)	85(6)
C1	2727(18)	10950(5)	167(5)	57(4)
C2	5845(18)	10464(6)	795(5)	72(4)
C3	3500(20)	10470(6)	606(5)	49(4)
C4	2084(17)	10094(5)	786(5)	37(3)
C5	2609(18)	9608(6)	1229(5)	64(4)
C6	572(16)	9349(5)	1412(5)	44(3)
C7	698(19)	8911(6)	1935(5)	43(3)
C8	-1587(16)	8752(5)	2059(4)	50(4)
C9	2126(19)	8381(5)	1847(5)	44(4)
C10	2380(20)	8041(6)	844(5)	47(4)
C11	1010(20)	7822(5)	314(6)	43(3)
C12	1885(19)	7849(5)	-212(6)	51(4)
C13	680(20)	7648(5)	-733(6)	56(4)
C14	-1270(20)	7409(6)	-712(5)	47(4)
C15	-2234(19)	7365(6)	-210(5)	55(4)
C16	-1020(20)	7591(5)	314(5)	53(4)
C17	2214(18)	7927(5)	2340(5)	47(4)
C18	4370(20)	7082(6)	2670(5)	45(4)
C19	6180(20)	6734(6)	2543(6)	50(4)
C20	7123(19)	6789(6)	2052(5)	55(4)
C21	8910(20)	6437(6)	1968(6)	71(5)
C22	9580(20)	6050(6)	2404(6)	56(4)
C23	8780(20)	5995(6)	2927(6)	60(4)
C24	7020(20)	6333(6)	2979(6)	64(4)
C25	1810(20)	9243(5)	2445(6)	47(4)

Table 3. Bond lengths [Å] and angles [°] for 1.

O1-C10	1.376(11)	C33A-H33A	0.96
O1-C9	1.452(11)	C33A-H33	0.6934
O2-C10	1.182(12)	C34A-H34A	0.96
O3-N1	1.210(12)	N3A-O11A	1.2199
O4-N1	1.228(12)	N3A-O12A	1.2201
O5-C18	1.358(12)	C28-C29	1.50(2)
O5-C17	1.442(11)	C29-C30	1.3899
O6-C18	1.214(12)	C29-C34	1.3899
O7-N2	1.214(14)	C30-C31	1.3900
O8-N2	1.190(14)	C30-H30	0.96
N1-C14	1.496(14)	C31-C32	1.3899
N2-C22	1.485(16)	C31-H31	0.96
O9-C28	1.178(17)	C32-C33	1.3901
O9-C28A	1.182(18)	C32-N3	1.456(13)
O9-C27	1.436(12)	C33-C34	1.3899
O10-C28	1.171(18)	C33-H33	0.96
O10A-C28A	1.188(18)	C34-H34	0.96
C26-C25	1.204(15)	N3-O11	1.2200
C26-C27	1.510(16)	N3-O12	1.2201
C27-H27A	0.96	C1-C3	1.516(14)
C27-H27B	0.96	C1-H1A	0.96
C28A-C29A	1.50(2)	C1-H1B	0.96
C28A-H34	1.5619	C1-H1C	0.96
C29A-C30A	1.3899	C2-C3	1.475(13)
C29A-C34A	1.3900	C2-H2A	0.96
C29A-H34	1.1835	C2-H2B	0.96
C30A-C31A	1.3900	C2-H2C	0.96
C30A-H30A	0.96	C3-C4	1.336(14)
C31A-C32A	1.3901	C4-C5	1.502(14)
C31A-H31A	0.96	C4-H4	0.96
C31A-H31	1.4958	C5-C6	1.516(13)
C32A-C33A	1.3896	C5-H5A	0.96
C32A-N3A	1.455(13)	C5-H5B	0.96
C33A-C34A	1.3904	C6-C7	1.548(14)

C6-H6A	0.96	C14-C15	1.370(13)
C6-H6B	0.96	C15-C16	1.427(14)
C7-C25	1.483(16)	C15-H15	0.96
C7-C9	1.527(14)	C16-H16	0.96
C7-C8	1.540(13)	C17-H17A	0.96
C8-H8A	0.96	C17-H17B	0.96
C8-H8B	0.96	C18-C19	1.440(15)
C8-H8C	0.96	C19-C20	1.345(14)
C9-C17	1.522(13)	C19-C24	1.400(15)
C9-H9	0.96	C20-C21	1.409(14)
C10-C11	1.476(15)	C20-H20	0.96
C11-C16	1.376(14)	C21-C22	1.352(15)
C11-C12	1.390(13)	C21-H21	0.96
C12-C13	1.399(14)	C22-C23	1.363(14)
C12-H12	0.96	C23-C24	1.363(14)
C13-C14	1.342(14)	C23-H23	0.96
C13-H13	0.96	C24-H24	0.96

C10-O1-C9	119.6(9)	O9-C28A-C29A	118.0(19)
C18-O5-C17	118.6(9)	O10A-C28A-C29A	125.2(18)
O3-N1-O4	127.4(14)	C30A-C29A-C34A	120.0
O3-N1-C14	116.7(13)	C30A-C29A-C28A	123.1(15)
O4-N1-C14	115.1(13)	C34A-C29A-C28A	116.8(15)
O8-N2-O7	118.8(16)	C29A-C30A-C31A	120.0
O8-N2-C22	116.3(15)	C29A-C30A-H30A	120.0
O7-N2-C22	124.0(15)	C31A-C30A-H30A	120.0
C28-O9-C27	121.9(14)	C30A-C31A-C32A	120.0
C28A-O9-C27	129.2(14)	C30A-C31A-H31A	120.0
C25-C26-C27	173.4(15)	C32A-C31A-H31A	120.0
O9-C27-C26	110.3(10)	C33A-C32A-C31A	120.0
O9-C27-H27A	110.2	C33A-C32A-N3A	112.1(18)
C26-C27-H27A	109.3	C31A-C32A-N3A	127.6(18)
O9-C27-H27B	108.9	C32A-C33A-C34A	120.0
C26-C27-H27B	109.3	C32A-C33A-H33A	120.0
H27A-C27-H27B	108.8	C34A-C33A-H33A	120.0
O9-C28A-O10A	117(2)	C31-C32-C33	120.0

C31-C32-N3	111.7(17)	C5-C6-H6A	105.3
C33-C32-N3	128.3(17)	C7-C6-H6A	108.1
C34-C33-C32	120.0	C5-C6-H6B	106.7
C34-C33-H33	120.0	C7-C6-H6B	108.4
C32-C33-H33	120.0	H6A-C6-H6B	107.5
C33-C34-C29	120.0	C25-C7-C9	106.3(10)
C33-C34-H34	120.0	C25-C7-C8	108.9(10)
C29-C34-H34	120.0	C9-C7-C8	114.6(10)
O11-N3-O12	120.0	C25-C7-C6	104.6(10)
O11-N3-C32	120(2)	C9-C7-C6	111.9(9)
O12-N3-C32	108(2)	C8-C7-C6	109.9(10)
C3-C1-H1A	109.8	C7-C8-H8A	108.5
C3-C1-H1B	108.5	C7-C8-H8B	109.9
H1A-C1-H1B	109.5	H8A-C8-H8B	109.5
C3-C1-H1C	110.1	C7-C8-H8C	110.1
H1A-C1-H1C	109.5	H8A-C8-H8C	109.5
H1B-C1-H1C	109.5	H8B-C8-H8C	109.5
C3-C2-H2A	108.6	O1-C9-C17	107.6(9)
C3-C2-H2B	108.6	O1-C9-C7	106.6(9)
H2A-C2-H2B	109.5	C17-C9-C7	113.4(10)
C3-C2-H2C	111.3	O1-C9-H9	109.7
H2A-C2-H2C	109.5	C17-C9-H9	109.6
H2B-C2-H2C	109.5	C7-C9-H9	109.8
C4-C3-C2	125.5(12)	O2-C10-O1	122.6(12)
C4-C3-C1	119.6(12)	O2-C10-C11	127.5(12)
C2-C3-C1	114.8(11)	O1-C10-C11	109.9(11)
C3-C4-C5	125.5(11)	C16-C11-C12	119.4(13)
C3-C4-H4	118.9	C16-C11-C10	124.5(12)
C5-C4-H4	115.6	C12-C11-C10	116.1(12)
C4-C5-C6	110.7(10)	C11-C12-C13	119.4(12)
C4-C5-H5A	108.4	C11-C12-H12	118.1
C6-C5-H5A	107.9	C13-C12-H12	122.5
C4-C5-H5B	110.0	C14-C13-C12	119.4(13)
C6-C5-H5B	110.5	C14-C13-H13	119.0
H5A-C5-H5B	109.2	C12-C13-H13	121.6
C5-C6-C7	120.3(10)	C13-C14-C15	124.5(13)

C13-C14-N1	120.1(13)	C20-C19-C18	124.3(13)
C15-C14-N1	115.4(13)	C24-C19-C18	116.3(12)
C14-C15-C16	115.6(12)	C19-C20-C21	120.5(13)
C14-C15-H15	121.2	C19-C20-H20	118.9
C16-C15-H15	123.2	C21-C20-H20	120.6
C11-C16-C15	121.7(12)	C22-C21-C20	116.3(13)
C11-C16-H16	118.5	C22-C21-H21	120.7
C15-C16-H16	119.8	C20-C21-H21	123.0
O5-C17-C9	107.6(9)	C21-C22-C23	126.3(14)
O5-C17-H17A	111.0	C21-C22-N2	117.3(13)
C9-C17-H17A	111.2	C23-C22-N2	115.9(14)
O5-C17-H17B	109.7	C22-C23-C24	115.0(13)
C9-C17-H17B	108.2	C22-C23-H23	120.5
H17A-C17-H17B	109.1	C24-C23-H23	124.5
O6-C18-O5	119.2(12)	C23-C24-C19	122.4(13)
O6-C18-C19	129.6(12)	C23-C24-H24	119.1
O5-C18-C19	111.2(11)	C19-C24-H24	118.5
C20-C19-C24	119.3(13)	C26-C25-C7	179.4(15)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O1	36(5)	56(5)	42(5)	-13(4)	8(4)	-8(4)
O2	34(5)	72(6)	75(6)	-10(5)	15(4)	-10(5)
O3	86(7)	98(7)	84(6)	3(6)	-14(6)	-1(6)
O4	117(7)	98(7)	71(6)	-5(6)	31(6)	-8(6)
O5	48(5)	52(5)	49(5)	-5(5)	4(4)	13(5)
O6	71(6)	78(6)	73(6)	21(5)	32(5)	8(5)
O7	73(6)	79(6)	77(6)	8(5)	6(5)	3(5)
O8	164(9)	183(9)	145(9)	34(8)	58(7)	87(7)
N1	80(8)	56(7)	69(7)	-2(6)	-5(7)	5(6)
N2	110(9)	110(9)	93(9)	7(8)	22(8)	28(7)
O9	65(7)	68(6)	98(7)	8(6)	-7(6)	0(5)
O10	59(8)	45(8)	46(7)	-3(7)	0(6)	5(7)
O10A	62(9)	81(10)	50(9)	23(8)	20(8)	4(8)
C26	56(8)	48(8)	58(7)	3(6)	10(6)	5(6)
C27	67(8)	50(7)	53(7)	-2(6)	-10(6)	-3(7)
C28A	55(13)	67(13)	67(13)	-3(9)	19(10)	5(9)
C29A	37(11)	45(12)	35(12)	-13(9)	16(9)	-4(9)
C30A	28(12)	53(13)	43(11)	-9(9)	13(9)	2(9)
C31A	55(13)	55(13)	59(13)	0(9)	11(9)	-1(9)
C32A	45(17)	42(16)	35(17)	-3(9)	9(9)	-2(9)
C33A	43(13)	46(13)	48(13)	5(9)	6(9)	-3(9)
C34A	67(14)	67(14)	72(14)	5(9)	-1(9)	1(10)
N3A	55(13)	56(13)	56(13)	2(7)	14(7)	-3(7)
O11A	81(9)	102(9)	91(10)	-1(7)	20(7)	4(6)
O12A	98(10)	103(9)	97(9)	-1(6)	18(6)	-6(7)
C28	50(11)	50(11)	51(10)	-9(9)	12(9)	-3(9)
C29	57(11)	56(12)	63(11)	1(9)	17(9)	-10(9)
C30	46(11)	68(11)	55(11)	-2(9)	7(8)	-7(9)
C31	89(14)	85(14)	94(13)	-2(9)	13(9)	4(9)
C32	50(14)	48(14)	37(14)	5(8)	16(9)	0(9)
C33	65(12)	62(13)	78(13)	2(9)	13(9)	3(9)

C34	74(12)	72(13)	76(13)	-5(9)	4(9)	-8(9)
N3	86(14)	83(14)	83(14)	6(7)	23(7)	3(7)
O11	119(10)	119(9)	117(9)	-3(6)	6(6)	-2(7)
O12	76(8)	90(8)	91(9)	-9(7)	13(6)	6(6)
C1	57(7)	58(8)	58(7)	14(6)	6(6)	5(6)
C2	56(8)	80(8)	82(8)	1(7)	18(7)	-11(7)
C3	36(7)	60(7)	49(7)	5(6)	0(6)	11(6)
C4	26(7)	40(7)	46(7)	-2(6)	4(5)	16(6)
C5	57(8)	79(8)	58(7)	8(7)	12(6)	-7(7)
C6	38(7)	58(7)	39(6)	4(6)	16(5)	-3(6)
C7	41(7)	46(7)	42(7)	-5(6)	7(6)	-3(6)
C8	46(7)	62(7)	42(7)	1(6)	3(6)	-6(6)
C9	45(7)	49(7)	35(6)	6(6)	-1(6)	-3(6)
C10	40(7)	56(8)	49(7)	1(6)	20(7)	-2(6)
C11	36(7)	45(7)	47(7)	1(6)	7(6)	-1(6)
C12	42(7)	52(7)	62(7)	0(6)	23(6)	8(6)
C13	57(8)	54(8)	57(7)	-8(6)	11(7)	5(6)
C14	51(7)	50(7)	39(7)	-6(6)	-2(6)	8(6)
C15	51(7)	62(8)	51(7)	-2(6)	2(6)	-2(6)
C16	53(7)	50(7)	59(7)	-2(6)	21(6)	12(6)
C17	38(7)	53(7)	48(7)	-5(6)	4(6)	-1(6)
C18	55(8)	41(7)	38(7)	18(6)	3(6)	11(6)
C19	51(7)	52(7)	50(7)	-8(6)	16(6)	8(6)
C20	55(7)	57(8)	53(7)	9(6)	4(6)	7(6)
C21	71(8)	69(8)	74(8)	14(7)	16(7)	10(7)
C22	49(8)	60(8)	63(8)	3(7)	19(6)	0(6)
C23	63(8)	58(8)	57(7)	6(6)	4(6)	4(7)
C24	56(8)	65(8)	74(8)	4(7)	16(7)	1(7)
C25	40(7)	42(7)	58(7)	5(6)	4(6)	3(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U(eq)
H27A	4292	10254	3185	70
H27B	2566	10049	3574	70
H30A	6663	9433	4843	49
H31A	9066	9042	5624	67
H33A	13309	8657	4479	55
H34A	10906	9048	3698	84
H30	7310	9721	5290	67
H31	10320	9267	5830	107
H33	12270	8696	4299	81
H34	9260	9150	3759	89
H1A	1189	10932	74	86
H1B	3135	11326	342	86
H1C	3372	10902	-188	86
H2A	6178	10143	1067	108
H2B	6561	10404	454	108
H2C	6324	10828	984	108
H4	594	10130	627	45
H5A	3438	9773	1574	77
H5B	3439	9308	1068	77
H6A	-132	9154	1066	53
H6B	-317	9675	1493	53
H8A	-1471	8482	2385	75
H8B	-2324	9102	2158	75
H8C	-2379	8570	1718	75
H9	3556	8513	1809	53
H12	3282	8025	-205	61
H13	1234	7661	-1104	67
H15	-3647	7199	-221	66
H16	-1633	7590	678	63
H17A	2492	8112	2721	56

H17B	849	7729	2306	56
H20	6555	7071	1758	66
H21	9635	6466	1625	85
H23	9452	5734	3227	72
H24	6309	6291	3323	77

Table 6. Torsion angles [°] for 1.

C28-O9-C27-C26	-173.6(16)	C30-C31-C32-C33	0.0
C28A-O9-C27-C26	78(3)	C30-C31-C32-N3	-179(2)
C25-C26-C27-O9	-173(12)	C31-C32-C33-C34	0.0
C27-O9-C28A-O10A	-11(4)	N3-C32-C33-C34	179(3)
C27-O9-C28A-C29A	167.4(16)	C32-C33-C34-C29	0.0
O9-C28A-C29A-C30A	-7(4)	C30-C29-C34-C33	0.0
O10A-C28A-C29A-C30A	171(3)	C28-C29-C34-C33	175(2)
O9-C28A-C29A-C34A	169(2)	C31-C32-N3-O11	44(3)
O10A-C28A-C29A-C34A	-12(4)	C33-C32-N3-O11	-135(3)
C34A-C29A-C30A-C31A	0.0	C31-C32-N3-O12	-173.9(17)
C28A-C29A-C30A-C31A	177(2)	C33-C32-N3-O12	7(3)
C29A-C30A-C31A-C32A	0.0	C2-C3-C4-C5	2.1(19)
C30A-C31A-C32A-C33A	0.0	C1-C3-C4-C5	-178.3(11)
C30A-C31A-C32A-N3A	-174(3)	C3-C4-C5-C6	169.1(11)
C31A-C32A-C33A-C34A	0.0	C4-C5-C6-C7	-170.3(10)
N3A-C32A-C33A-C34A	175(3)	C5-C6-C7-C25	58.9(13)
C30A-C29A-C34A-C33A	0.0	C5-C6-C7-C9	-55.8(15)
C28A-C29A-C34A-C33A	-177(2)	C5-C6-C7-C8	175.6(10)
C32A-C33A-C34A-C29A	0.0	C10-O1-C9-C17	-117.8(11)
C33A-C32A-N3A-O11A	32(4)	C10-O1-C9-C7	120.2(11)
C31A-C32A-N3A-O11A	-153(3)	C25-C7-C9-O1	-173.0(9)
C33A-C32A-N3A-O12A	-168(3)	C8-C7-C9-O1	66.7(12)
C31A-C32A-N3A-O12A	6(4)	C6-C7-C9-O1	-59.3(12)
C28A-O9-C28-O10	150(3)	C25-C7-C9-C17	68.8(13)
C27-O9-C28-O10	18(3)	C8-C7-C9-C17	-51.5(14)
C28A-O9-C28-C29	-38(2)	C6-C7-C9-C17	-177.6(10)
C27-O9-C28-C29	-170.4(14)	C9-O1-C10-O2	8.1(18)
O10-C28-C29-C30	23(3)	C9-O1-C10-C11	-171.5(9)
O9-C28-C29-C30	-147.7(16)	O2-C10-C11-C16	167.9(13)
O10-C28-C29-C34	-152(2)	O1-C10-C11-C16	-12.6(17)
O9-C28-C29-C34	37(3)	O2-C10-C11-C12	-11(2)
C34-C29-C30-C31	0.0	O1-C10-C11-C12	168.3(10)
C28-C29-C30-C31	-175.6(18)	C16-C11-C12-C13	0.6(18)
C29-C30-C31-C32	0.0	C10-C11-C12-C13	179.8(11)

C11-C12-C13-C14	-2.7(18)
C12-C13-C14-C15	3(2)
C12-C13-C14-N1	-178.9(11)
O3-N1-C14-C13	176.6(13)
O4-N1-C14-C13	6.2(18)
O3-N1-C14-C15	-4.7(18)
O4-N1-C14-C15	-175.2(12)
C13-C14-C15-C16	0(2)
N1-C14-C15-C16	-178.9(10)
C12-C11-C16-C15	1.7(18)
C10-C11-C16-C15	-177.5(12)
C14-C15-C16-C11	-1.8(18)
C18-O5-C17-C9	175.4(10)
O1-C9-C17-O5	72.1(11)
C7-C9-C17-O5	-170.2(10)
C17-O5-C18-O6	7.1(18)
C17-O5-C18-C19	-175.5(10)
O6-C18-C19-C20	171.4(14)
O5-C18-C19-C20	-5.7(19)
O6-C18-C19-C24	-12(2)
O5-C18-C19-C24	171.4(11)
C24-C19-C20-C21	2(2)
C18-C19-C20-C21	178.9(12)
C19-C20-C21-C22	0(2)
C20-C21-C22-C23	-4(2)
C20-C21-C22-N2	-174.9(12)
O8-N2-C22-C21	-23(2)
O7-N2-C22-C21	167.8(15)
O8-N2-C22-C23	165.0(15)
O7-N2-C22-C23	-4(2)
C21-C22-C23-C24	6(2)
N2-C22-C23-C24	176.9(12)
C22-C23-C24-C19	-4(2)
C20-C19-C24-C23	0(2)
C18-C19-C24-C23	-177.1(12)

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5) $R_W(F^2) = \{\Sigma w(|F_O|^2 - |F_C|^2)^2/\Sigma w(|F_O|)^4\}^{1/2}$ where w is the weight given each reflection.
$R(F) = \Sigma(|F_O| - |F_C|)/\Sigma|F_O|\}$ for reflections with $F_O > 4(\sigma(F_O))$.
$S = [\Sigma w(|F_O|^2 - |F_C|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

6) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

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Table 7. Observed and calculated structure factors for 1 Page 1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	0	0	666	699	18	2	14	0	218	220	32	3	4	1	383	384	26	0	11	1	262	289	20	4	19	1	249	35	60
2	0	0	1478	1517	39	3	14	0	191	139	54	4	4	1	136	155	47	1	11	1	754	796	18	-3	20	1	0	95	1
3	0	0	630	605	26	4	14	0	0	67	1	5	4	1	21	106	21	2	11	1	563	482	44	-2	20	1	133	88	132
4	0	0	121	134	120	5	14	0	0	73	1	6	4	1	0	103	1	3	11	1	403	359	24	-1	20	1	0	143	1
5	0	0	77	48	76	1	15	0	113	20	72	-6	5	1	159	18	72	4	11	1	278	264	35	0	20	1	0	17	1
6	0	0	150	195	150	2	15	0	112	60	112	-5	5	1	59	14	59	5	11	1	0	11	1	1	20	1	0	24	1
1	1	0	675	688	10	3	15	0	120	48	77	-4	5	1	314	346	21	-5	12	1	130	60	88	2	20	1	135	130	134
2	1	0	251	214	23	4	15	0	0	35	1	-3	5	1	585	575	13	-4	12	1	151	159	127	3	20	1	197	45	118
3	1	0	175	184	79	5	15	0	131	88	130	-2	5	1	0	97	1	-3	12	1	142	126	53	-3	21	1	226	47	80
4	1	0	134	154	69	0	16	0	0	1	1	-1	5	1	1079	995	136	-2	12	1	608	590	31	-2	21	1	0	10	1
5	1	0	100	120	99	1	16	0	0	6	1	0	5	1	880	797	28	-1	12	1	0	94	1	-1	21	1	34	16	34
6	1	0	146	83	145	2	16	0	0	14	1	1	5	1	947	929	12	0	12	1	0	48	1	0	21	1	21	86	21
1	2	0	81	109	30	3	16	0	0	28	1	2	5	1	0	18	1	1	12	1	186	256	35	1	21	1	0	88	1
2	2	0	0	22	1	4	16	0	156	227	156	3	5	1	28	105	27	2	12	1	227	266	38	2	21	1	63	13	62
3	2	0	279	150	49	5	16	0	190	70	153	4	5	1	0	21	1	3	12	1	0	44	1	3	21	1	195	22	142
4	2	0	373	392	24	1	17	0	108	1	107	5	5	1	182	161	73	4	12	1	0	44	1	-2	22	1	119	45	118
5	2	0	146	55	57	2	17	0	201	153	40	6	5	1	187	41	145	5	12	1	0	9	1	-1	22	1	0	45	1
6	2	0	241	157	43	3	17	0	123	87	123	-6	6	1	78	3	77	-5	13	1	0	46	1	0	22	1	88	17	68
1	3	0	187	210	12	4	17	0	187	20	99	-5	6	1	190	134	79	-4	13	1	153	174	47	1	22	1	174	159	41
2	3	0	358	394	19	0	18	0	0	18	1	-4	6	1	442	383	30	-3	13	1	0	98	1	2	22	1	14	30	14
3	3	0	345	352	18	1	18	0	245	170	30	-3	6	1	121	158	120	-2	13	1	139	64	58	-2	23	1	66	129	65
4	3	0	103	99	102	2	18	0	72	94	71	-2	6	1	302	296	12	-1	13	1	0	38	1	-1	23	1	113	47	112
5	3	0	78	48	77	3	18	0	138	34	95	-1	6	1	1917	1732	56	0	13	1	248	281	32	0	23	1	0	70	1
6	3	0	0	37	1	4	18	0	335	8	335	0	6	1	958	870	45	1	13	1	194	223	90	1	23	1	26	63	26
0	4	0	540	577	70	1	19	0	72	95	71	1	6	1	2060	2052	31	2	13	1	375	353	31	2	23	1	90	74	90
1	4	0	844	849	16	2	19	0	265	206	64	2	6	1	0	55	1	3	13	1	174	131	38	-1	24	1	167	2	167

2	4	0	152	176	22	3	19	0	108	162	107	3	6	1	135	90	89	4	13	1	0	117	1	0	24	1	0	91	1
3	4	0	239	126	20	4	19	0	0	59	1	4	6	1	85	73	84	5	13	1	0	29	1	1	24	1	0	62	1
4	4	0	106	42	95	0	20	0	128	221	128	5	6	1	124	0	124	-5	14	1	250	148	147	-6	0	2	0	22	1
5	4	0	236	161	28	1	20	0	0	53	1	6	6	1	297	166	66	-4	14	1	148	132	75	-5	0	2	214	163	47
6	4	0	0	127	1	2	20	0	0	30	1	-6	7	1	0	32	1	-3	14	1	0	104	1	-4	0	2	341	288	32
1	5	0	323	29	45	3	20	0	0	69	1	-5	7	1	198	147	60	-2	14	1	135	160	43	-3	0	2	360	297	32
2	5	0	164	212	20	1	21	0	81	159	81	-4	7	1	176	87	35	-1	14	1	0	62	1	-2	0	2	853	832	19
3	5	0	261	201	26	2	21	0	103	100	102	-3	7	1	0	85	1	0	14	1	140	131	48	-1	0	2	2355	2323	49
4	5	0	228	168	36	3	21	0	196	3	196	-2	7	1	465	427	15	1	14	1	207	232	28	1	0	2	2040	2092	54
5	5	0	115	60	115	0	22	0	0	10	1	-1	7	1	1055	1017	37	2	14	1	0	62	1	2	0	2	356	358	24
6	5	0	0	22	1	1	22	0	67	32	67	0	7	1	607	611	46	3	14	1	160	125	51	3	0	2	343	344	66
1	6	0	2026	1927	63	2	22	0	0	73	1	1	7	1	299	319	12	4	14	1	0	12	1	4	0	2	233	277	61
2	6	0	126	95	45	1	23	0	224	195	47	2	7	1	84	18	83	5	14	1	49	72	48	5	0	2	336	255	49
3	6	0	169	165	45	2	23	0	0	10	1	3	7	1	56	149	55	-5	15	1	0	46	1	6	0	2	0	70	1
4	6	0	204	162	31	0	24	0	82	66	81	4	7	1	207	154	61	-4	15	1	45	56	44	-6	1	2	74	13	73
5	6	0	123	31	123	1	24	0	82	111	81	5	7	1	144	184	78	-3	15	1	262	244	43	-5	1	2	141	35	140
6	6	0	121	17	120	-6	1	1	0	29	1	6	7	1	160	77	159	-2	15	1	215	55	40	-4	1	2	194	83	65
1	7	0	821	827	25	-5	1	1	151	60	56	-6	8	1	114	75	114	-1	15	1	15	15	14	-3	1	2	276	269	19
2	7	0	387	400	10	-4	1	1	158	237	55	-5	8	1	0	16	1	0	15	1	79	92	78	-2	1	2	195	178	27
3	7	0	266	271	22	-3	1	1	625	619	16	-4	8	1	27	86	26	1	15	1	117	27	67	-1	1	2	339	337	7
4	7	0	0	6	1	-2	1	1	150	130	58	-3	8	1	148	153	41	2	15	1	73	75	72	1	1	2	179	131	58
5	7	0	178	189	51	-1	1	1	303	278	16	-2	8	1	401	337	34	3	15	1	77	11	76	2	1	2	238	236	31
6	7	0	109	138	108	1	1	1	189	235	26	-1	8	1	161	200	27	4	15	1	146	77	106	3	1	2	62	108	62
0	8	0	757	797	19	2	1	1	474	462	17	0	8	1	367	389	20	5	15	1	0	2	1	4	1	2	193	70	127
1	8	0	395	418	29	3	1	1	214	162	37	1	8	1	711	677	16	-5	16	1	218	183	125	5	1	2	131	64	131
2	8	0	321	287	34	4	1	1	389	382	22	2	8	1	115	103	41	-4	16	1	0	108	1	6	1	2	143	178	84
3	8	0	0	41	1	5	1	1	0	13	1	3	8	1	0	70	1	-3	16	1	78	25	78	-6	2	2	74	148	73
4	8	0	236	224	26	6	1	1	207	224	46	4	8	1	0	19	1	-2	16	1	172	53	44	-5	2	2	205	208	38
5	8	0	164	91	97	-6	2	1	205	121	65	5	8	1	0	26	1	-1	16	1	171	94	46	-4	2	2	0	91	1
6	8	0	112	73	111	-5	2	1	227	19	32	6	8	1	43	8	42	0	16	1	124	52	58	-3	2	2	256	204	22
1	9	0	380	396	17	-4	2	1	173	179	39	-6	9	1	200	43	199	1	16	1	0	23	1	-2	2	2	362	384	10
2	9	0	621	640	18	-3	2	1	798	812	16	-5	9	1	0	28	1	2	16	1	145	58	62	-1	2	2	1243	1241	27
3	9	0	0	40	1	-2	2	1	64	144	63	-4	9	1	208	175	31	3	16	1	121	92	120	1	2	2	710	704	11
4	9	0	181	147	49	-1	2	1	342	357	9	-3	9	1	80	162	79	4	16	1	117	41	117	2	2	2	0	24	1
5	9	0	0	68	1	1	2	1	466	471	14	-2	9	1	187	153	35	5	16	1	89	28	89	3	2	2	402	397	17
6	9	0	107	33	107	2	2	1	120	199	68	-1	9	1	0	111	1	-4	17	1	0	25	1	4	2	2	283	307	41
0	10	0	0	139	1	3	2	1	139	129	62	0	9	1	152	178	46	-3	17	1	210	137	122	5	2	2	142	134	105
1	10	0	364	355	16	4	2	1	166	74	42	1	9	1	285	269	30	-2	17	1	143	42	64	6	2	2	128	21	127
2	10	0	166	185	33	5	2	1	218	268	41	2	9	1	264	239	22	-1	17	1	0	30	1	-6	3	2	123	95	122
3	10	0	61	10	60	6	2	1	193	16	89	3	9	1	196	178	25	0	17	1	0	53	1	-5	3	2	84	45	84
4	10	0	80	89	80	-6	3	1	181	68	82	4	9	1	0	89	1	1	17	1	149	148	42	-4	3	2	88	101	88
5	10	0	0	65	1	-5	3	1	152	120	48	5	9	1	121	149	121	2	17	1	617	550	31	-3	3	2	452	443	20
6	10	0	146	20	145	-4	3	1	184	130	31	6	9	1	0	2	1	3	17	1	35	32	35	-2	3	2	356	355	13
1	11	0	151	74	30	-3	3	1	144	43	43	-5	10	1	23	39	23	4	17	1	0	40	1	-1	3	2	866	891	14
2	11	0	234	226	22	-2	3	1	483	497	10	-4	10	1	126	55	76	-4	18	1	197	210	73	0	3	2	288	280	8
3	11	0	120	74	46	-1	3	1	548	550	10	-3	10	1	181	91	21	-3	18	1	0	81	1	1	3	2	344	347	12
4	11	0	8	26	8	1	3	1	286	291	10	-2	10	1	290	275	31	-2	18	1	152	159	152	2	3	2	373	426	26
5	11	0	203	79	59	2	3	1	112	121	111	-1	10	1	145	26	40	-1	18	1	68	33	67	3	3	2	398	410	28
0	12	0	405	428	21	3	3	1	316	275	30	0	10	1	165	184	30	0	18	1	147	89	45	4	3	2	52	40	52
1	12	0	249	273	20	4	3	1	0	117	1	1	10	1	123	38	45	1	18	1	0	11	1	5	3	2	93	51	92
2	12	0	282	305	38	5	3	1	0	118	1	2	10	1	180	147	37	2	18	1	211	96	41	6	3	2	171	48	171
3	12	0	157	97	44	6	3	1	141	36	127	3	10	1	186	175	58	3	18	1	133	19	132	-6	4	2	123	26	122
4	12	0	164	146	31	-6	4	1	111	37	111	4	10	1	158	21	83	4	18	1	0	97	1	-5	4	2	148	51	58
5	12	0	115	118	114	-5	4	1	267	194	34	5	10	1	0	32	1	-4	19	1	113	65	112	-4	4	2	413	379	14
1	13	0	237	239	20	-4	4	1	0	6	1	6	10	1	0	11	1	-3	19	1	144	27	99	-3	4	2	311	328	14
2	13	0	176	165	135	-3	4	1	681	656	14	-6	11	1	50	13	50	-2	19	1	139	120	55	-2	4	2	405	450	17
3	13	0	87	60	87	-2	4	1	288	307	11	-5	11	1	0	44	1	-1	19	1	92	40	91	-1	4	2	1247	1242	18
4	13	0	0	75	1	-1	4	1	402	225	31	-4	11	1	114	24	68	0	19	1	0	4	1	0	4	2	472	476	33
5	13	0	114	107	113	0	4	1	49	104	49	-3	11	1	115	148	80	1	19	1	67	26	66	1	4	2	892	867	40
0	14	0	215	125	31	1	4	1	1209	1197	25	-2	11	1	99	101	98	2	19	1	53	178	53	2	4	2	265	248	19
1	14	0	205	173	27	2	4	1	0	31	1	-1	11	1	464	426	12	3	19	1	79	44	79	3	4	2	206	219	42

Table 7. Observed and calculated structure factors for 1 Page 2

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
4	4	2	63	142	63	2	11	2	652	675	37	-1	20	2	0	20	1	5	5	3	0	2	1	4	12	3	114	21	114
5	4	2	0	54	1	3	11	2	0	38	1	0	20	2	0	36	1	6	5	3	109	48	109	5	12	3	20	63	20
6	4	2	92	4	91	4	11	2	291	236	35	1	20	2	39	30	38	-6	6	3	0	162	1	-5	13	3	8	42	8
-6	5	2	0	9	1	5	11	2	168	219	72	2	20	2	89	111	88	-5	6	3	0	6	1	-4	13	3	164	195	37
-5	5	2	128	85	101	-5	12	2	159	182	61	3	20	2	0	2	1	-4	6	3	0	102	1	-3	13	3	109	37	87
-4	5	2	134	101	85	-4	12	2	0	112	1	-3	21	2	0	43	1	-3	6	3	259	196	22	-2	13	3	315	320	17
-3	5	2	215	181	19	-3	12	2	109	22	109	-2	21	2	171	59	80	-2	6	3	628	630	8	-1	13	3	124	64	123
-2	5	2	302	317	20	-2	12	2	138	51	40	-1	21	2	146	189	75	-1	6	3	116	66	74	0	13	3	168	246	79
-1	5	2	2381	2306	50	-1	12	2	120	127	61	0	21	2	75	25	63	0	6	3	1030	1093	39	1	13	3	796	794	15
0	5	2	1886	1811	42	0	12	2	218	203	30	1	21	2	169	102	60	1	6	3	735	737	33	2	13	3	77	15	76
1	5	2	1673	1672	22	1	12	2	164	182	28	2	21	2	188	121	50	2	6	3	342	287	19	3	13	3	130	96	130
2	5	2	234	266	16	2	12	2	87	116	86	3	21	2	84	75	84	3	6	3	0	112	1	4	13	3	224	215	24
3	5	2	261	226	35	3	12	2	84	14	83	-2	22	2	86	4	86	4	6	3	115	44	115	5	13	3	41	100	40
4	5	2	26	67	26	4	12	2	328	338	23	-1	22	2	109	27	109	5	6	3	196	174	62	-5	14	3	149	26	108
5	5	2	78	105	78	5	12	2	0	68	1	0	22	2	0	66	1	6	6	3	82	7	81	-4	14	3	259	243	41
6	5	2	0	15	1	-5	13	2	0	23	1	1	22	2	0	15	1	-6	7	3	220	108	91	-3	14	3	68	14	68
-6	6	2	84	23	84	-4	13	2	218	121	39	2	22	2	168	75	118	-5	7	3	179	30	36	-2	14	3	172	85	35
-5	6	2	244	219	30	-3	13	2	0	36	1	-2	23	2	237	74	67	-4	7	3	319	312	25	-1	14	3	189	59	37
-4	6	2	181	119	97	-2	13	2	119	5	69	-1	23	2	121	63	120	-3	7	3	276	143	63	0	14	3	318	311	44
-3	6	2	0	112	1	-1	13	2	257	218	27	0	23	2	0	69	1	-2	7	3	847	824	12	1	14	3	126	172	51
-2	6	2	58	36	58	0	13	2	254	239	51	1	23	2	0	61	1	-1	7	3	241	152	48	2	14	3	0	16	1
-1	6	2	519	449	158	1	13	2	450	398	22	2	23	2	109	80	108	0	7	3	577	581	41	3	14	3	274	237	45
0	6	2	406	267	47	2	13	2	244	228	32	-1	24	2	126	88	126	1	7	3	256	217	55	4	14	3	0	86	1
1	6	2	608	558	53	3	13	2	192	31	36	0	24	2	0	112	1	2	7	3	180	121	20	5	14	3	235	18	58
2	6	2	371	408	13	4	13	2	105	16	104	1	24	2	150	140	149	3	7	3	355	377	20	-5	15	3	165	145	164
3	6	2	72	165	72	5	13	2	52	36	51	-6	1	3	0	8	1	4	7	3	129	99	67	-4	15	3	0	36	1
4	6	2	306	254	41	-5	14	2	0	23	1	-5	1	3	132	57	132	5	7	3	0	58	1	-3	15	3	113	115	112
5	6	2	164	18	53	-4	14	2	147	112	45	-4	1	3	0	75	1	6	7	3	0	105	1	-2	15	3	102	95	102
6	6	2	162	15	126	-3	14	2	0	9	1	-3	1	3	221	212	19	-6	8	3	0	3	1	-1	15	3	228	207	29
-6	7	2	134	59	133	-2	14	2	226	241	42	-2	1	3	112	171	31	-5	8	3	0	154	1	0	15	3	0	64	1
-5	7	2	213	189	38	-1	14	2	0	32	1	-1	1	3	832	848	10	-4	8	3	140	79	33	1	15	3	157	154	39
-4	7	2	120	28	57	0	14	2	0	8	1	1	1	3	668	641	11	-3	8	3	155	2	29	2	15	3	161	113	46
-3	7	2	482	453	18	1	14	2	0	103	1	2	1	3	429	471	16	-2	8	3	191	27	23	3	15	3	255	298	29
-2	7	2	352	337	12	2	14	2	102	124	101	3	1	3	475	468	19	-1	8	3	0	26	1	4	15	3	0	15	1
-1	7	2	874	834	24	3	14	2	406	358	29	4	1	3	117	34	102	0	8	3	717	714	22	5	15	3	52	45	51
0	7	2	324	324	33	4	14	2	0	7	1	5	1	3	144	19	116	1	8	3	46	38	46	-5	16	3	0	68	1
1	7	2	454	443	10	5	14	2	137	17	137	6	1	3	90	74	90	2	8	3	83	116	83	-4	16	3	40	116	39
2	7	2	708	705	11	-5	15	2	0	27	1	-6	2	3	151	181	79	3	8	3	0	35	1	-3	16	3	41	146	41
3	7	2	0	67	1	-4	15	2	121	16	104	-5	2	3	229	92	51	4	8	3	99	100	99	-2	16	3	95	75	94
4	7	2	0	11	1	-3	15	2	0	73	1	-4	2	3	0	8	1	5	8	3	0	0	1	-1	16	3	117	110	116
5	7	2	136	35	81	-2	15	2	126	19	64	-3	2	3	282	246	14	6	8	3	131	20	131	0	16	3	0	86	1
6	7	2	0	73	1	-1	15	2	189	154	40	-2	2	3	85	157	84	-6	9	3	255	61	165	1	16	3	0	12	1
-6	8	2	263	11	93	0	15	2	0	95	1	-1	2	3	1052	1089	20	-5	9	3	0	34	1	2	16	3	0	111	1
-5	8	2	149	144	69	1	15	2	80	102	80	0	2	3	1053	1027	58	-4	9	3	87	137	87	3	16	3	105	91	104
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-2	8	2	871	840	14	4	15	2	152	177	152	3	2	3	192	175	36	-1	9	3	129	166	65	-3	17	3	17	97	16
-1	8	2	287	302	12	5	15	2	180	69	97	4	2	3	206	236	40	0	9	3	82	98	82	-2	17	3	87	16	86
0	8	2	654	635	18	-5	16	2	0	38	1	5	2	3	228	159	38	1	9	3	109	67	60	-1	17	3	112	175	111
1	8	2	670	665	15	-4	16	2	62	18	62	6	2	3	0	67	1	2	9	3	158	155	31	0	17	3	58	41	57
2	8	2	114	161	46	-3	16	2	0	85	1	-6	3	3	110	185	109	3	9	3	23	100	23	1	17	3	73	126	72
3	8	2	172	98	28	-2	16	2	103	37	103	-5	3	3	136	15	46	4	9	3	133	193	132	2	17	3	0	12	1
4	8	2	58	46	58	-1	16	2	144	74	87	-4	3	3	207	150	40	5	9	3	161	97	112	3	17	3	0	146	1
5	8	2	0	28	1	0	16	2	81	136	81	-3	3	3	588	561	16	6	9	3	111	1	110	4	17	3	79	107	78
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-1	9	2	199	245	21	-2	17	2	225	172	44	4	3	3	276	307	28	0	10	3	341	343	16	2	18	3	197	222	41
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2	9	2	0	127	1	1	17	2	0	120	1	-6	4	3	250	157	49	3	10	3	170	35	38	-4	19	3	175	34	174
3	9	2	101	27	101	2	17	2	131	138	131	-5	4	3	53	57	53	4	10	3	241	185	27	-3	19	3	166	108	105
4	9	2	76	34	76	3	17	2	104	249	103	-4	4	3	466	446	13	5	10	3	0	68	1	-2	19	3	4	82	3
5	9	2	0	5	1	4	17	2	198	89	80	-3	4	3	317	300	17	-6	11	3	130	17	129	-1	19	3	129	15	128
6	9	2	0	5	1	-4	18	2	0	67	1	-2	4	3	313	347	13	-5	11	3	167	187	38	0	19	3	74	63	74
-5	10	2	149	132	125	-3	18	2	145	148	69	-1	4	3	346	305	13	-4	11	3	164	50	57	1	19	3	33	51	33
-4	10	2	160	55	53	-2	18	2	0	18	1	0	4	3	552	475	17	-3	11	3	246	252	30	2	19	3	119	77	118
-3	10	2	100	186	62	-1	18	2	35	20	35	1	4	3	1552	1522	45	-2	11	3	155	155	29	3	19	3	209	66	86
-2	10	2	118	57	63	0	18	2	99	17	99	2	4	3	0	48	1	-1	11	3	173	124	23	4	19	3	0	4	1
-1	10	2	105	67	43	1	18	2	106	0	89	3	4	3	0	101	1	0	11	3	108	143	107	-3	20	3	0	67	1
0	10	2	0	94	1	2	18	2	202	178	51	4	4	3	164	113	66	1	11	3	648	618	14	-2	20	3	0	135	1
1	10	2	221	218	38	3	18	2	187	4	74	5	4	3	135	156	134	2	11	3	280	272	23	-1	20	3	0	20	1
2	10	2	557	579	17	4	18	2	0	150	1	6	4	3	182	44	119	3	11	3	149	160	76	0	20	3	132	146	115
3	10	2	225	204	20	-4	19	2	0	9	1	-6	5	3	107	2	106	4	11	3	183	206	47	1	20	3	145	17	77
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-3	11	2	136	145	45	2	19	2	79	70	79	0	5	3	1163	1049	23	-1	12	3	107	73	106	0	21	3	60	60	60
-2	11	2	450	438	28	3	19	2	143	78	142	1	5	3	456	413	20	0	12	3	434	458	22	1	21	3	31	96	31
-1	11	2	199	195	21	4	19	2	150	34	150	2	5	3	0	97	1	1	12	3	499	505	19	2	21	3	175	78	73
0	11	2	510	552	21	-3	20	2	0	93	1	3	5	3	297	281	20	2	12	3	83	17	82	3	21	3	41	118	41
1	11	2	646	702	15	-2	20	2	164	44	41	4	5	3	225	188	55	3	12	3	160	185	46	-2	22	3	203	71	62

Table 7. Observed and calculated structure factors for 1 Page 3

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-1	22	3	65	102	64	6	5	4	0	60	1	-5	13	4	117	171	116	2	22	4	124	69	123	-2	7	5	0	52	1
0	22	3	0	5	1	-6	6	4	0	44	1	-4	13	4	96	101	96	-2	23	4	207	9	104	-1	7	5	299	320	15
1	22	3	71	91	71	-5	6	4	55	35	54	-3	13	4	329	261	20	-1	23	4	155	120	154	0	7	5	0	68	1
2	22	3	0	79	1	-4	6	4	102	130	101	-2	13	4	306	251	20	0	23	4	0	27	1	1	7	5	428	432	13
-2	23	3	0	42	1	-3	6	4	598	630	25	-1	13	4	482	436	49	1	23	4	0	119	1	2	7	5	569	573	17
-1	23	3	109	48	108	-2	6	4	301	263	27	0	13	4	354	250	27	0	24	4	109	94	109	3	7	5	80	137	80
0	23	3	171	188	170	-1	6	4	643	649	16	1	13	4	422	417	16	-6	1	5	234	75	33	4	7	5	0	85	1
1	23	3	193	13	71	0	6	4	1249	1289	33	2	13	4	227	154	34	-5	1	5	124	170	108	5	7	5	0	20	1
-1	24	3	89	77	89	1	6	4	982	956	17	3	13	4	199	162	45	-4	1	5	85	19	84	6	7	5	0	16	1
0	24	3	0	11	1	2	6	4	450	407	12	4	13	4	108	123	107	-3	1	5	179	62	20	-6	8	5	183	58	128
-6	0	4	0	1	1	3	6	4	113	73	112	5	13	4	0	29	1	-2	1	5	234	242	11	-5	8	5	171	69	108
-5	0	4	0	120	1	4	6	4	92	82	92	-5	14	4	0	35	1	-1	1	5	261	198	9	-4	8	5	141	91	59
-4	0	4	171	94	55	5	6	4	210	200	45	-4	14	4	106	108	106	0	1	5	270	84	44	-3	8	5	385	341	20
-3	0	4	491	455	14	6	6	4	115	3	115	-3	14	4	108	8	107	1	1	5	149	8	37	-2	8	5	113	135	113
-2	0	4	1628	1648	28	-6	7	4	0	74	1	-2	14	4	224	195	27	2	1	5	67	106	66	-1	8	5	203	208	21
-1	0	4	1344	1454	22	-5	7	4	282	228	34	-1	14	4	63	60	63	3	1	5	289	183	72	0	8	5	614	670	19
0	0	4	999	1074	31	-4	7	4	83	22	83	0	14	4	0	41	1	4	1	5	188	72	51	1	8	5	716	741	54
1	0	4	268	208	17	-3	7	4	156	150	75	1	14	4	222	164	31	5	1	5	138	114	70	2	8	5	387	405	13
2	0	4	236	199	53	-2	7	4	216	27	101	2	14	4	138	24	64	6	1	5	0	14	1	3	8	5	173	174	40
3	0	4	0	9	1	-1	7	4	0	53	1	3	14	4	490	465	28	-6	2	5	130	154	67	4	8	5	0	23	1
4	0	4	0	84	1	0	7	4	646	636	18	4	14	4	0	12	1	-5	2	5	201	87	26	5	8	5	78	1	77
5	0	4	0	136	1	1	7	4	176	164	25	5	14	4	132	32	132	-4	2	5	293	287	27	-6	9	5	0	67	1
6	0	4	363	191	71	2	7	4	0	58	1	-5	15	4	129	91	128	-3	2	5	130	22	41	-5	9	5	204	42	50
-6	1	4	110	22	109	3	7	4	139	202	54	-4	15	4	84	19	84	-2	2	5	451	436	12	-4	9	5	0	55	1
-5	1	4	250	115	57	4	7	4	308	192	54	-3	15	4	125	23	82	-1	2	5	716	710	28	-3	9	5	178	69	39
-4	1	4	406	420	15	5	7	4	269	186	44	-2	15	4	67	39	67	0	2	5	1447	1483	26	-2	9	5	520	495	15
-3	1	4	255	219	17	6	7	4	179	91	133	-1	15	4	314	261	28	1	2	5	31	0	30	-1	9	5	243	212	19
-2	1	4	315	295	14	-6	8	4	229	61	105	0	15	4	213	214	31	2	2	5	156	208	32	0	9	5	669	669	24
-1	1	4	979	980	13	-5	8	4	234	209	47	1	15	4	250	120	41	3	2	5	438	424	22	1	9	5	243	210	20
0	1	4	181	195	14	-4	8	4	309	344	47	2	15	4	314	339	43	4	2	5	164	139	52	2	9	5	413	439	14
1	1	4	634	627	21	-3	8	4	117	81	49	3	15	4	36	73	36	5	2	5	45	143	44	3	9	5	220	187	31
2	1	4	56	211	56	-2	8	4	820	784	14	4	15	4	126	192	126	6	2	5	164	173	109	4	9	5	0	128	1
3	1	4	129	135	71	-1	8	4	136	137	33	5	15	4	199	46	116	-6	3	5	139	142	113	5	9	5	132	226	132
4	1	4	133	187	132	0	8	4	628	562	24	-5	16	4	0	11	1	-5	3	5	172	189	29	-6	10	5	0	105	1
5	1	4	65	125	65	1	8	4	181	172	28	-4	16	4	177	90	61	-4	3	5	0	20	1	-5	10	5	64	132	63
6	1	4	171	2	171	2	8	4	150	92	48	-3	16	4	105	25	53	-3	3	5	196	198	34	-4	10	5	132	66	78
-6	2	4	0	205	1	3	8	4	138	18	46	-2	16	4	0	14	1	-2	3	5	1003	1032	14	-3	10	5	150	91	40
-5	2	4	187	123	41	4	8	4	0	65	1	-1	16	4	80	41	80	-1	3	5	333	331	27	-2	10	5	110	61	110
-4	2	4	104	61	104	5	8	4	0	10	1	0	16	4	91	95	90	0	3	5	892	890	25	-1	10	5	181	157	90
-3	2	4	261	233	12	6	8	4	0	106	1	1	16	4	262	212	64	1	3	5	225	250	18	0	10	5	213	192	30
-2	2	4	200	244	20	-6	9	4	209	67	172	2	16	4	209	219	64	2	3	5	315	358	16	1	10	5	330	318	13
-1	2	4	806	819	21	-5	9	4	282	201	52	3	16	4	104	103	103	3	3	5	119	105	70	2	10	5	238	215	43
0	2	4	484	510	12	-4	9	4	127	137	127	4	16	4	193	138	100	4	3	5	70	69	70	3	10	5	265	226	40
1	2	4	420	406	12	-3	9	4	204	201	20	-4	17	4	0	47	1	5	3	5	131	10	131	4	10	5	273	252	30
2	2	4	394	430	13	-2	9	4	58	0	57	-3	17	4	226	100	44	6	3	5	0	35	1	5	10	5	123	25	122
3	2	4	130	134	130	-1	9	4	0	74	1	-2	17	4	78	178	77	-6	4	5	35	48	35	-6	11	5	163	47	163
4	2	4	138	82	59	0	9	4	238	206	22	-1	17	4	132	39	85	-5	4	5	153	16	66	-5	11	5	0	86	1
5	2	4	157	1	87	1	9	4	173	176	39	0	17	4	0	77	1	-4	4	5	104	87	104	-4	11	5	63	83	62
6	2	4	118	122	118	2	9	4	315	293	29	1	17	4	170	182	28	-3	4	5	612	625	16	-3	11	5	128	68	58
-6	3	4	126	111	86	3	9	4	176	154	53	2	17	4	237	34	48	-2	4	5	0	56	1	-2	11	5	0	33	1
-5	3	4	156	46	35	4	9	4	377	342	40	3	17	4	199	160	47	-1	4	5	742	682	18	-1	11	5	382	319	39
-4	3	4	317	303	14	5	9	4	157	81	99	4	17	4	0	17	1	0	4	5	298	256	37	0	11	5	189	122	35
-3	3	4	390	373	11	-6	10	4	0	94	1	-4	18	4	0	21	1	1	4	5	872	913	27	1	11	5	0	15	1
-2	3	4	249	278	17	-5	10	4	0	22	1	-3	18	4	122	120	122	2	4	5	184	197	27	2	11	5	155	57	65
-1	3	4	203	5	28	-4	10	4	24	57	24	-2	18	4	78	17	78	3	4	5	0	22	1	3	11	5	137	44	136
0	3	4	719	718	14	-3	10	4	156	83	42	-1	18	4	107	10	107	4	4	5	267	256	36	4	11	5	11	26	11
1	3	4	672	691	27	-2	10	4	340	338	22	0	18	4	108	81	107	5	4	5	118	122	117	5	11	5	82	87	82
2	3	4	287	301	14	-1	10	4	244	296	33	1	18	4	146	138	65	6	4	5	121	101	120	-5	12	5	173	77	64
3	3	4	88	30	87	0	10	4	0	87	1	2	18	4	203	210	68	-6	5	5	103	150	102	-4	12	5	108	166	108
4	3	4	88	71	88	1	10	4	187	130	25	3	18	4	0	40	1	-5	5	5	172	91	65	-3	12	5	176	175	50
5	3	4	83	145	82	2	10	4	390	399	12	4	18	4	186	61	91	-4	5	5	148	28	69	-2	12	5	163	21	47
6	3	4	193	89	192	3	10	4	190	26	31	-4	19	4	203	99	202	-3	5	5	0	119	1	-1	12	5	184	51	36
-6	4	4	0	28	1	4	10	4	334	250	21	-3	19	4	179	144	62	-2	5	5	0	38	1	0	12	5	226	225	56
-5	4	4	167	123	49	5	10	4	175	113	174	-2	19	4	0	76	1	-1	5	5	254	306	21	1	12	5	322	307	20
-4	4	4	134	12	133	-6	11	4	0	44	1	-1	19	4	99	137	98	0	5	5	398	319	69	2	12	5	0	35	1
-3	4	4	235	23	63	-5	11	4	177	90	92	0	19	4	102	132	102	1	5	5	476	481	37	3	12	5	170	40	33
-2	4	4	133	156	30	-4	11	4	181	2	61	1	19	4	83	9	82	2	5	5	154	161	35	4	12	5	273	282	30
-1	4	4	200	171	33	-3	11	4	76	6	75	2	19	4	397	384	52	3	5	5	160	127	60	5	12	5	0	85	1
0	4	4	943	869	16	-2	11	4	152	144	41	3	19	4	0	11	1	4	5	5	191	70	80	-5	13	5	0	44	1
1	4	4	295	285	32	-1	11	4	308	311	32	-3	20	4	69	74	68	5	5	5	145	20	145	-4	13	5	122	105	49
2	4	4	0	74	1	0	11	4	412	412	12	-2	20	4	140	10	50	-6	6	5	0	8	1	-3	13	5	142	125	42
3	4	4	222	172	27	1	11	4	233	193	22	-1	20	4	0	59	1	-5	6	5	222	228	46	-2	13	5	148	115	41
4	4	4	63	38	62	2	11	4	25	84	24	0	20	4	0	34	1	-4	6	5	84	90	84	-1	13	5	131	96	131
5	4	4	30	28	30	3	11	4	222	87	65	1	20	4	195	66	62	-3	6	5	496	492	14	0	13	5	0	47	1
6	4	4	72	109	71	4	11	4	224	156	57	2	20	4	112	69	111	-2	6	5	114	177	68	1	13	5	219	220	36
-6	5	4	171	4	171	5	11	4	202	86	55	3	20	4	195	177	81	-1	6	5	0	3	1	2	13	5	242	234	119
-5	5	4	165	89	44	-5	12	4	0	20	1	-3	21	4	207	7	132	0	6	5	813	798	24	3	13	5	167	72	41
-4	5	4	231	268	31	-4	12	4	99	96	98	-2	21	4	0	100	1	1	6	5	564	571	10	4	13	5	125	48	80
-3	5	4	135	114	47	-3	12	4	114	29	114	-1	21	4	90	110	90	2	6	5	92	3	55	5	13	5	96	30	96
-2	5	4	40	19	39	-2	12	4	172	202	32	0	21	4	0	61	1	3	6	5	223	235	31	-5	14	5	103	152	103
-1	5	4	91	171	90	-1	12	4	346	320	26	1	21	4	65	5	64	4	6	5	0	31	1	-4	14	5	0	8	1
0	5	4	633	646	13	0	12	4	123	148	122	2	21	4	0	108	1	5	6	5	173	193	104	-3	14	5	112	118	69
1	5	4	1210	1221	15	1	12	4	101	179	60	3	21	4	62	32	61	6	6	5	126	10	126	-2	14	5	0	4	1
2	5	4	251	252	25	2	12	4	172	11	37	-2	22	4	0	23	1	-6	7	5	75	30	74	-1	14	5	122	153	122
3	5	4	193	168	32	3	12	4	71	42	70	-1	22	4	30	120	30	-5	7	5	194	89	47	0	14	5	53	6	52
4	5	4	107	58	106	4	12	4	0	75	1	0	22	4	135	94	91	-4	7	5	110	80	109	1	14	5	154	207	59
5	5	4	0	111	1	5	12	4	177	30	176	1	22	4	244	44	94	-3	7	5	118	161	72	2	14	5	186	167	42

Table 7. Observed and calculated structure factors for 1 Page 4

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	14	5	140	32	63	-2	1	6	251	245	10	-5	8	6	161	205	94	3	15	6	0	7	1	-2	3	7	210	199	17
4	14	5	224	290	47	-1	1	6	661	666	9	-4	8	6	118	147	94	4	15	6	103	2	102	-1	3	7	71	69	70
5	14	5	62	6	61	0	1	6	479	492	27	-3	8	6	111	32	72	-5	16	6	109	63	109	0	3	7	160	145	15
-5	15	5	0	33	1	1	1	6	869	870	16	-2	8	6	620	602	12	-4	16	6	0	10	1	1	3	7	209	220	18
-4	15	5	139	93	57	2	1	6	561	504	27	-1	8	6	238	231	18	-3	16	6	16	28	16	2	3	7	423	440	15
-3	15	5	15	46	15	3	1	6	73	68	72	0	8	6	368	350	24	-2	16	6	133	73	50	3	3	7	238	264	57
-2	15	5	0	22	1	4	1	6	190	150	39	1	8	6	905	833	21	-1	16	6	160	24	53	4	3	7	125	78	87
-1	15	5	156	102	100	5	1	6	108	177	108	2	8	6	366	385	31	0	16	6	201	182	39	5	3	7	184	185	67
0	15	5	130	111	130	6	1	6	203	55	202	3	8	6	182	145	38	1	16	6	108	46	58	6	3	7	0	88	1
1	15	5	141	142	44	-6	2	6	0	171	1	4	8	6	213	189	45	2	16	6	198	255	73	-6	4	7	0	69	1
2	15	5	125	92	125	-5	2	6	119	131	57	5	8	6	0	55	1	3	16	6	184	193	55	-5	4	7	177	150	67
3	15	5	258	304	27	-4	2	6	0	40	1	-6	9	6	355	33	72	4	16	6	0	72	1	-4	4	7	62	3	62
4	15	5	0	78	1	-3	2	6	368	377	14	-5	9	6	155	114	88	-4	17	6	200	77	148	-3	4	7	0	60	1
-5	16	5	0	73	1	-2	2	6	435	436	14	-4	9	6	89	76	88	-3	17	6	0	53	1	-2	4	7	67	71	66
-4	16	5	185	73	70	-1	2	6	139	28	53	-3	9	6	137	140	41	-2	17	6	0	106	1	-1	4	7	601	594	15
-3	16	5	64	24	64	0	2	6	150	34	16	-2	9	6	346	364	15	-1	17	6	3	120	2	0	4	7	0	33	1
-2	16	5	109	106	83	1	2	6	465	485	28	-1	9	6	200	167	21	0	17	6	111	55	111	1	4	7	0	16	1
-1	16	5	0	16	1	2	2	6	135	111	55	0	9	6	266	287	23	1	17	6	155	115	46	2	4	7	153	222	62
0	16	5	143	54	143	3	2	6	0	36	1	1	9	6	0	84	1	2	17	6	144	113	55	3	4	7	109	38	109
1	16	5	112	43	112	4	2	6	0	39	1	2	9	6	477	396	34	3	17	6	0	11	1	4	4	7	32	52	32
2	16	5	0	16	1	5	2	6	92	91	91	3	9	6	271	269	23	4	17	6	115	18	115	5	4	7	213	110	94
3	16	5	97	151	97	6	2	6	32	52	32	4	9	6	401	415	28	-4	18	6	365	11	82	6	4	7	63	41	63
4	16	5	0	32	1	-6	3	6	0	33	1	5	9	6	180	72	97	-3	18	6	158	45	82	-6	5	7	135	110	135
-4	17	5	113	129	113	-5	3	6	105	97	104	-6	10	6	0	4	1	-2	18	6	102	96	102	-5	5	7	197	167	42
-3	17	5	129	22	128	-4	3	6	137	60	54	-5	10	6	0	4	1	-1	18	6	0	26	1	-4	5	7	223	234	36
-2	17	5	86	89	86	-3	3	6	493	576	39	-4	10	6	105	114	104	0	18	6	217	203	63	-3	5	7	95	135	95
-1	17	5	129	57	71	-2	3	6	375	373	13	-3	10	6	35	90	35	1	18	6	126	30	53	-2	5	7	100	138	100
0	17	5	234	338	49	-1	3	6	181	169	22	-2	10	6	211	261	27	2	18	6	100	154	100	-1	5	7	0	40	1
1	17	5	164	137	44	0	3	6	234	220	14	-1	10	6	284	271	21	3	18	6	204	202	74	0	5	7	646	654	12
2	17	5	246	292	32	1	3	6	148	72	148	0	10	6	130	137	130	-4	19	6	0	55	1	1	5	7	623	632	16
3	17	5	149	8	85	2	3	6	467	477	14	1	10	6	68	31	68	-3	19	6	0	35	1	2	5	7	371	354	14
4	17	5	82	28	81	3	3	6	91	11	90	2	10	6	432	421	28	-2	19	6	0	115	1	3	5	7	230	235	33
-4	18	5	163	48	163	4	3	6	0	17	1	3	10	6	318	274	22	-1	19	6	166	142	72	4	5	7	165	191	55
-3	18	5	154	66	77	5	3	6	0	110	1	4	10	6	339	347	31	0	19	6	140	73	51	5	5	7	189	160	58
-2	18	5	0	53	1	6	3	6	232	236	146	5	10	6	251	220	82	1	19	6	248	270	40	-6	6	7	167	36	167
-1	18	5	105	61	45	-6	4	6	227	189	78	-5	11	6	73	117	73	2	19	6	142	202	68	-5	6	7	0	81	1
0	18	5	49	211	49	-5	4	6	171	121	79	-4	11	6	68	13	67	3	19	6	113	29	113	-4	6	7	141	149	56
1	18	5	184	202	45	-4	4	6	214	170	50	-3	11	6	114	68	114	-3	20	6	133	28	132	-3	6	7	0	99	1
2	18	5	93	137	93	-3	4	6	287	311	16	-2	11	6	127	148	44	-2	20	6	164	26	65	-2	6	7	261	247	36
3	18	5	342	257	52	-2	4	6	126	138	18	-1	11	6	0	45	1	-1	20	6	0	6	1	-1	6	7	143	144	33
4	18	5	0	7	1	-1	4	6	162	213	28	0	11	6	215	211	33	0	20	6	0	2	1	0	6	7	403	405	16
-4	19	5	258	166	184	0	4	6	339	344	10	1	11	6	223	191	28	1	20	6	86	24	86	1	6	7	187	189	20
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-1	19	5	93	150	92	3	4	6	0	25	1	4	11	6	184	160	40	-3	21	6	89	11	89	4	6	7	150	56	149
0	19	5	87	114	86	4	4	6	200	137	36	5	11	6	203	90	82	-2	21	6	130	63	130	5	6	7	0	69	1
1	19	5	71	87	71	5	4	6	163	120	86	-5	12	6	80	17	80	-1	21	6	22	113	22	-5	7	7	69	48	68
2	19	5	179	189	178	6	4	6	63	26	63	-4	12	6	190	9	51	0	21	6	0	7	1	-4	7	7	12	44	11
3	19	5	182	35	93	-6	5	6	0	56	1	-3	12	6	0	13	1	1	21	6	62	84	61	-3	7	7	151	203	40
-3	20	5	0	13	1	-5	5	6	32	73	31	-2	12	6	200	140	25	2	21	6	0	63	1	-2	7	7	249	254	26
-2	20	5	144	86	72	-4	5	6	398	377	20	-1	12	6	241	206	25	-2	22	6	155	31	154	-1	7	7	97	87	87
-1	20	5	85	159	85	-3	5	6	125	18	43	0	12	6	293	281	18	-1	22	6	0	81	1	0	7	7	106	169	105
0	20	5	0	55	1	-2	5	6	439	435	12	1	12	6	674	694	23	0	22	6	0	38	1	1	7	7	1120	1104	24
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0	21	5	0	193	1	5	5	6	0	105	1	-3	13	6	232	198	52	-4	1	7	269	267	25	-3	8	7	188	177	35
1	21	5	0	56	1	6	5	6	0	43	1	-2	13	6	0	38	1	-3	1	7	422	405	16	-2	8	7	425	418	19
2	21	5	198	144	65	-6	6	6	136	131	135	-1	13	6	520	384	67	-2	1	7	0	42	1	-1	8	7	169	96	27
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-1	22	5	71	13	71	-4	6	6	112	79	105	1	13	6	0	30	1	0	1	7	343	360	12	1	8	7	26	135	26
0	22	5	171	31	58	-3	6	6	0	4	1	2	13	6	93	86	92	1	1	7	315	338	25	2	8	7	634	617	13
1	22	5	149	109	148	-2	6	6	150	183	57	3	13	6	153	113	56	2	1	7	336	320	15	3	8	7	178	102	40
2	22	5	0	47	1	-1	6	6	131	177	35	4	13	6	26	26	25	3	1	7	145	35	51	4	8	7	327	178	54
-1	23	5	171	144	170	0	6	6	89	117	89	5	13	6	103	50	103	4	1	7	126	30	125	5	8	7	264	225	63
0	23	5	0	26	1	1	6	6	763	793	14	-5	14	6	167	71	167	5	1	7	117	128	117	-6	9	7	0	0	1
1	23	5	0	69	1	2	6	6	327	315	14	-4	14	6	113	101	112	6	1	7	196	0	196	-5	9	7	0	123	1
-6	0	6	304	303	118	3	6	6	127	161	53	-3	14	6	91	63	90	-6	2	7	138	15	138	-4	9	7	0	8	1
-5	0	6	435	412	66	4	6	6	235	205	29	-2	14	6	145	197	53	-5	2	7	305	267	15	-3	9	7	291	268	28
-4	0	6	0	115	1	5	6	6	0	119	1	-1	14	6	170	23	64	-4	2	7	156	129	50	-2	9	7	0	41	1
-3	0	6	57	104	56	6	6	6	36	29	36	0	14	6	223	227	29	-3	2	7	0	4	1	-1	9	7	515	500	18
-2	0	6	442	424	10	-6	7	6	85	31	85	1	14	6	250	277	28	-2	2	7	198	261	15	0	9	7	527	504	15
-1	0	6	268	213	12	-5	7	6	150	139	89	2	14	6	0	76	1	-1	2	7	72	47	72	1	9	7	357	356	14
0	0	6	776	920	51	-4	7	6	0	57	1	3	14	6	265	274	23	0	2	7	659	671	11	2	9	7	375	365	29
1	0	6	1001	978	16	-3	7	6	368	309	16	4	14	6	92	107	91	1	2	7	590	609	9	3	9	7	122	124	84
2	0	6	353	343	20	-2	7	6	362	383	18	5	14	6	7	21	7	2	2	7	190	64	39	4	9	7	120	117	119
3	0	6	263	42	63	-1	7	6	408	423	13	-5	15	6	233	123	130	3	2	7	148	57	148	5	9	7	0	28	1
4	0	6	144	49	82	0	7	6	456	454	14	-4	15	6	87	136	87	4	2	7	145	7	64	-6	10	7	179	18	179
5	0	6	155	47	72	1	7	6	375	382	40	-3	15	6	100	31	70	5	2	7	94	1	94	-5	10	7	135	40	135
6	0	6	96	54	96	2	7	6	125	86	40	-2	15	6	0	75	1	6	2	7	0	57	1	-4	10	7	0	62	1
-6	1	6	71	55	70	3	7	6	245	240	29	-1	15	6	186	37	138	-6	3	7	99	59	98	-3	10	7	230	207	19
-5	1	6	212	208	27	4	7	6	312	245	36	0	15	6	206	218	38	-5	3	7	0	23	1	-2	10	7	268	304	23
-4	1	6	186	178	71	5	7	6	166	133	64	1	15	6	143	128	46	-4	3	7	4	5	4	-1	10	7	115	121	44
-3	1	6	200	227	17	-6	8	6	242	170	115	2	15	6	304	276	25	-3	3	7	296	281	16	0	10	7	278	289	17

Table 7. Observed and calculated structure factors for 1 Page 5

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	10	7	575	557	19	-1	19	7	150	123	45	-2	5	8	0	102	1	5	12	8	163	58	163	3	1	9	182	106	50
2	10	7	27	13	27	0	19	7	151	159	63	-1	5	8	203	84	81	-5	13	8	249	127	170	4	1	9	0	28	1
3	10	7	358	322	29	1	19	7	92	103	91	0	5	8	374	379	11	-4	13	8	92	62	92	5	1	9	122	38	122
4	10	7	123	158	74	2	19	7	159	42	75	1	5	8	707	705	24	-3	13	8	116	129	56	-6	2	9	182	7	60
5	10	7	0	1	1	3	19	7	117	38	117	2	5	8	140	36	84	-2	13	8	107	16	72	-5	2	9	279	273	42
-5	11	7	200	88	82	-3	20	7	0	7	1	3	5	8	162	12	61	-1	13	8	457	354	60	-4	2	9	140	96	139
-4	11	7	122	31	121	-2	20	7	103	8	103	4	5	8	121	28	121	0	13	8	134	103	38	-3	2	9	0	56	1
-3	11	7	131	92	131	-1	20	7	0	34	1	5	5	8	198	171	153	1	13	8	136	211	135	-2	2	9	95	61	94
-2	11	7	153	91	43	0	20	7	55	180	54	-6	6	8	0	173	1	2	13	8	58	94	58	-1	2	9	49	106	48
-1	11	7	81	18	81	1	20	7	0	37	1	-5	6	8	278	257	29	3	13	8	292	266	46	0	2	9	0	43	1
0	11	7	346	245	35	2	20	7	170	129	170	-4	6	8	0	142	1	4	13	8	0	12	1	1	2	9	0	44	1
1	11	7	127	75	46	3	20	7	101	27	100	-3	6	8	255	198	51	-5	14	8	0	24	1	2	2	9	507	535	18
2	11	7	129	66	64	-3	21	7	0	23	1	-2	6	8	475	479	30	-4	14	8	0	43	1	3	2	9	114	67	113
3	11	7	161	189	36	-2	21	7	174	123	113	-1	6	8	0	16	1	-3	14	8	222	285	50	4	2	9	0	46	1
4	11	7	141	50	61	-1	21	7	216	45	142	0	6	8	331	367	18	-2	14	8	0	16	1	5	2	9	100	64	99
5	11	7	167	87	167	0	21	7	0	48	1	1	6	8	316	348	15	-1	14	8	161	8	122	-6	3	9	0	85	1
-5	12	7	292	77	56	1	21	7	0	70	1	2	6	8	158	152	32	0	14	8	48	74	48	-5	3	9	213	224	51
-4	12	7	73	126	72	2	21	7	154	6	153	3	6	8	175	182	35	1	14	8	187	170	27	-4	3	9	77	14	76
-3	12	7	0	79	1	-2	22	7	73	26	72	4	6	8	230	243	106	2	14	8	186	35	43	-3	3	9	166	161	21
-2	12	7	201	159	33	-1	22	7	91	77	90	5	6	8	0	38	1	3	14	8	416	361	51	-2	3	9	392	377	10
-1	12	7	228	272	42	0	22	7	0	12	1	-5	7	8	63	46	62	4	14	8	105	24	104	-1	3	9	122	143	69
0	12	7	118	202	51	1	22	7	0	8	1	-4	7	8	258	278	48	-5	15	8	0	22	1	0	3	9	14	90	14
1	12	7	166	190	30	-1	23	7	265	59	115	-3	7	8	240	237	25	-4	15	8	97	88	97	1	3	9	262	297	33
2	12	7	244	276	48	0	23	7	0	82	1	-2	7	8	436	409	28	-3	15	8	44	38	44	2	3	9	142	90	59
3	12	7	358	305	26	-6	0	8	179	179	88	-1	7	8	262	261	17	-2	15	8	137	116	46	3	3	9	101	61	101
4	12	7	0	82	1	-5	0	8	251	245	94	0	7	8	220	202	49	-1	15	8	51	92	50	4	3	9	212	215	107
5	12	7	0	15	1	-4	0	8	411	357	32	1	7	8	149	158	26	0	15	8	87	93	86	5	3	9	229	104	70
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-4	13	7	0	16	1	-2	0	8	386	403	12	3	7	8	257	168	28	2	15	8	237	222	31	-5	4	9	371	410	49
-3	13	7	0	63	1	-1	0	8	126	107	36	4	7	8	368	350	24	3	15	8	0	124	1	-4	4	9	164	24	83
-2	13	7	119	84	118	0	0	8	356	349	25	5	7	8	215	213	50	4	15	8	91	107	91	-3	4	9	145	208	31
-1	13	7	97	25	97	1	0	8	199	213	22	-6	8	8	0	2	1	-4	16	8	167	75	167	-2	4	9	146	141	57
0	13	7	284	283	33	2	0	8	291	2	291	-5	8	8	0	85	1	-3	16	8	155	114	28	-1	4	9	532	540	23
1	13	7	89	146	88	3	0	8	0	3	1	-4	8	8	0	15	1	-2	16	8	212	238	64	0	4	9	0	8	1
2	13	7	0	49	1	4	0	8	91	59	90	-3	8	8	143	172	84	-1	16	8	0	95	1	1	4	9	662	621	16
3	13	7	171	13	48	-6	1	8	224	134	33	-2	8	8	135	6	33	0	16	8	70	62	69	2	4	9	101	163	101
4	13	7	164	143	47	-5	1	8	148	138	56	-1	8	8	433	444	14	1	16	8	21	144	20	3	4	9	343	259	27
5	13	7	66	15	66	-4	1	8	129	22	40	0	8	8	728	710	16	2	16	8	103	30	103	4	4	9	92	100	92
-5	14	7	0	85	1	-3	1	8	88	23	41	1	8	8	91	72	51	3	16	8	0	96	1	5	4	9	91	143	90
-4	14	7	0	76	1	-2	1	8	36	31	36	2	8	8	269	261	18	4	16	8	0	129	1	-6	5	9	107	119	106
-3	14	7	157	189	52	-1	1	8	195	188	30	3	8	8	295	260	22	-4	17	8	0	13	1	-5	5	9	182	177	54
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0	14	7	329	287	61	2	1	8	1143	1141	72	-6	9	8	0	85	1	-1	17	8	30	31	29	-2	5	9	247	253	25
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3	14	7	217	139	52	5	1	8	331	424	49	-3	9	8	68	31	68	2	17	8	0	141	1	1	5	9	162	164	30
4	14	7	118	147	118	-6	2	8	141	108	132	-2	9	8	0	23	1	3	17	8	124	90	123	2	5	9	65	9	64
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-3	15	7	146	120	54	-3	2	8	0	42	1	1	9	8	149	70	65	-2	18	8	127	10	127	5	5	9	153	216	153
-2	15	7	0	60	1	-2	2	8	338	351	12	2	9	8	521	467	19	-1	18	8	75	85	74	-6	6	9	253	21	97
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1	16	7	135	127	52	-3	3	8	301	295	16	3	10	8	149	189	44	-3	20	8	0	39	1	-6	7	9	52	55	51
2	16	7	137	179	39	-2	3	8	139	105	29	4	10	8	155	147	47	-2	20	8	0	2	1	-5	7	9	0	101	1
3	16	7	0	59	1	-1	3	8	366	399	23	5	10	8	0	105	1	-1	20	8	0	68	1	-4	7	9	290	228	21
4	16	7	114	23	114	0	3	8	502	516	10	-5	11	8	138	62	137	0	20	8	0	29	1	-3	7	9	0	69	1
-4	17	7	188	79	112	1	3	8	108	38	41	-4	11	8	210	74	37	1	20	8	49	13	48	-2	7	9	212	211	18
-3	17	7	129	99	39	2	3	8	202	173	60	-3	11	8	281	273	19	2	20	8	183	127	69	-1	7	9	529	510	35
-2	17	7	0	64	1	3	3	8	0	53	1	-2	11	8	88	147	88	-2	21	8	159	38	158	0	7	9	128	2	55
-1	17	7	120	37	119	4	3	8	144	142	60	-1	11	8	211	216	25	-1	21	8	35	24	34	1	7	9	172	31	171
0	17	7	191	63	41	5	3	8	107	83	107	0	11	8	69	0	68	0	21	8	105	10	105	2	7	9	425	435	13
1	17	7	93	20	93	-6	4	8	0	108	1	1	11	8	189	179	24	1	21	8	0	32	1	3	7	9	334	296	22
2	17	7	0	21	1	-5	4	8	102	26	101	2	11	8	116	18	61	2	21	8	195	35	79	4	7	9	106	69	106
3	17	7	0	105	1	-4	4	8	238	210	31	3	11	8	107	137	96	-2	22	8	0	10	1	5	7	9	89	82	89
4	17	7	0	4	1	-3	4	8	163	188	27	4	11	8	159	193	55	0	22	8	90	10	90	-6	8	9	63	119	63
-4	18	7	159	60	158	-2	4	8	125	54	41	5	11	8	0	0	1	1	22	8	206	100	68	-5	8	9	103	90	102
-3	18	7	148	82	148	-1	4	8	192	221	50	-5	12	8	0	101	1	0	23	8	0	38	1	-4	8	9	0	17	1
-2	18	7	73	107	72	0	4	8	221	256	18	-4	12	8	97	134	97	-6	1	9	0	18	1	-3	8	9	95	72	95
-1	18	7	144	32	70	1	4	8	36	9	35	-3	12	8	57	62	57	-5	1	9	105	29	105	-2	8	9	0	91	1
0	18	7	0	99	1	2	4	8	338	340	20	-2	12	8	0	51	1	-4	1	9	167	137	80	-1	8	9	110	38	70
1	18	7	0	11	1	3	4	8	176	108	50	-1	12	8	348	400	78	-3	1	9	0	21	1	0	8	9	63	43	63
2	18	7	45	41	44	4	4	8	0	22	1	0	12	8	127	54	38	-2	1	9	166	188	17	1	8	9	250	204	40
3	18	7	116	72	115	5	4	8	131	138	130	1	12	8	323	299	14	-1	1	9	0	3	1	2	8	9	242	223	28
-4	19	7	228	63	146	-5	5	8	99	67	99	2	12	8	89	112	88	0	1	9	318	400	41	3	8	9	241	112	36
-3	19	7	178	126	63	-4	5	8	44	14	44	3	12	8	367	381	21	1	1	9	0	88	1	4	8	9	171	186	64
-2	19	7	0	22	1	-3	5	8	113	84	53	4	12	8	69	156	69	2	1	9	136	243	136	5	8	9	231	114	94

Table 7. Observed and calculated structure factors for 1 Page 6

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-6	9	9	150	26	150	0	17	9	100	126	71	1	4	10	233	211	18	1	12	10	58	65	58	-4	2	11	0	30	1
-5	9	9	0	15	1	1	17	9	0	64	1	2	4	10	301	300	29	2	12	10	138	104	57	-3	2	11	84	12	55
-4	9	9	0	13	1	2	17	9	0	18	1	3	4	10	0	15	1	3	12	10	0	43	1	-2	2	11	513	498	10
-3	9	9	23	71	22	3	17	9	0	92	1	4	4	10	111	1	111	4	12	10	105	83	104	-1	2	11	316	285	45
-2	9	9	220	225	44	-4	18	9	209	158	209	5	4	10	0	27	1	-5	13	10	0	9	1	0	2	11	146	99	42
-1	9	9	205	195	29	-3	18	9	0	8	1	-6	5	10	14	35	14	-4	13	10	0	19	1	1	2	11	62	99	62
0	9	9	372	352	20	-2	18	9	0	46	1	-5	5	10	194	163	52	-3	13	10	133	89	45	2	2	11	171	164	29
1	9	9	88	62	87	-1	18	9	0	130	1	-4	5	10	510	488	18	-2	13	10	121	133	76	3	2	11	0	87	1
2	9	9	203	54	39	0	18	9	0	98	1	-3	5	10	269	295	26	-1	13	10	105	51	105	4	2	11	180	62	51
3	9	9	151	83	47	1	18	9	63	128	63	-2	5	10	263	178	33	0	13	10	170	161	34	5	2	11	0	0	1
4	9	9	0	139	1	2	18	9	124	70	102	-1	5	10	235	171	29	1	13	10	98	11	98	-6	3	11	151	90	104
5	9	9	155	19	154	3	18	9	0	18	1	0	5	10	511	514	24	2	13	10	112	99	111	-5	3	11	0	22	1
-5	10	9	0	105	1	-3	19	9	0	59	1	1	5	10	307	343	14	3	13	10	59	173	58	-4	3	11	352	350	32
-4	10	9	195	86	36	-2	19	9	0	118	1	2	5	10	0	10	1	4	13	10	185	16	170	-3	3	11	311	303	19
-3	10	9	190	178	34	-1	19	9	96	65	96	3	5	10	0	56	1	-5	14	10	142	65	141	-2	3	11	113	38	112
-2	10	9	246	224	24	0	19	9	0	63	1	4	5	10	208	161	52	-4	14	10	70	112	69	-1	3	11	309	293	25
-1	10	9	286	293	24	1	19	9	0	26	1	-6	6	10	113	149	113	-3	14	10	0	27	1	0	3	11	299	271	12
0	10	9	284	241	16	2	19	9	187	106	78	-5	6	10	0	58	1	-2	14	10	153	63	71	1	3	11	174	180	25
1	10	9	99	23	99	3	19	9	57	43	56	-4	6	10	187	163	39	-1	14	10	90	0	89	2	3	11	318	308	17
2	10	9	34	72	33	-3	20	9	0	33	1	-3	6	10	167	172	18	0	14	10	150	147	35	3	3	11	0	166	1
3	10	9	156	38	77	-2	20	9	0	32	1	-2	6	10	76	73	76	1	14	10	120	96	59	4	3	11	77	99	77
4	10	9	0	12	1	-1	20	9	174	1	55	-1	6	10	173	152	76	2	14	10	121	40	121	5	3	11	26	102	25
5	10	9	96	93	96	0	20	9	0	78	1	0	6	10	183	166	20	3	14	10	79	88	78	-6	4	11	0	129	1
-5	11	9	126	101	126	1	20	9	0	28	1	1	6	10	449	438	12	4	14	10	0	133	1	-5	4	11	185	109	53
-4	11	9	0	22	1	2	20	9	120	54	120	2	6	10	221	231	17	-4	15	10	0	86	1	-4	4	11	208	212	29
-3	11	9	112	34	112	-2	21	9	0	52	1	3	6	10	218	236	25	-3	15	10	0	143	1	-3	4	11	143	104	50
-2	11	9	75	83	75	-1	21	9	0	21	1	4	6	10	0	73	1	-2	15	10	140	59	38	-2	4	11	378	351	14
-1	11	9	0	22	1	0	21	9	0	39	1	5	6	10	228	129	138	-1	15	10	173	142	62	-1	4	11	45	22	45
0	11	9	102	0	102	1	21	9	134	98	134	-5	7	10	0	41	1	0	15	10	0	31	1	0	4	11	138	143	34
1	11	9	143	127	42	2	21	9	126	51	125	-4	7	10	179	154	42	1	15	10	107	115	69	1	4	11	301	312	22
2	11	9	223	171	28	0	22	9	132	29	132	-3	7	10	202	202	12	2	15	10	82	47	82	2	4	11	139	97	80
3	11	9	174	142	32	1	22	9	0	38	1	-2	7	10	0	68	1	3	15	10	0	81	1	3	4	11	184	202	36
4	11	9	195	189	70	-6	0	10	0	148	1	-1	7	10	235	191	38	4	15	10	103	66	102	4	4	11	0	129	1
5	11	9	36	11	36	-5	0	10	150	82	61	0	7	10	489	480	19	-4	16	10	0	26	1	5	4	11	0	106	1
-5	12	9	103	89	103	-4	0	10	282	225	111	1	7	10	384	414	30	-3	16	10	167	66	166	-6	5	11	222	63	86
-4	12	9	39	1	39	-3	0	10	403	333	33	2	7	10	448	434	16	-2	16	10	121	27	44	-5	5	11	0	33	1
-3	12	9	235	267	24	-2	0	10	890	857	17	3	7	10	63	38	62	-1	16	10	85	115	84	-4	5	11	175	79	175
-2	12	9	268	114	31	-1	0	10	150	49	47	4	7	10	0	65	1	0	16	10	51	8	51	-3	5	11	132	118	132
-1	12	9	294	260	38	0	0	10	409	289	32	5	7	10	186	79	149	1	16	10	148	91	48	-2	5	11	261	242	48
0	12	9	324	339	19	1	0	10	118	15	57	-5	8	10	93	74	93	2	16	10	170	40	55	-1	5	11	526	549	24
1	12	9	176	47	48	2	0	10	200	148	42	-4	8	10	194	160	53	3	16	10	229	110	64	0	5	11	140	110	20
2	12	9	0	41	1	3	0	10	234	282	53	-3	8	10	327	323	16	-4	17	10	0	27	1	1	5	11	0	39	1
3	12	9	123	35	97	4	0	10	123	14	122	-2	8	10	221	202	36	-3	17	10	0	24	1	2	5	11	296	305	37
4	12	9	64	51	64	5	0	10	0	49	1	-1	8	10	413	382	47	-2	17	10	0	54	1	3	5	11	61	81	61
-5	13	9	0	59	1	-6	1	10	0	83	1	0	8	10	179	28	159	-1	17	10	194	231	63	4	5	11	133	124	80
-4	13	9	170	1	107	-5	1	10	260	235	20	1	8	10	219	199	26	0	17	10	252	233	31	5	5	11	0	102	1
-3	13	9	219	184	32	-4	1	10	416	411	64	2	8	10	360	337	40	1	17	10	205	155	51	-6	6	11	0	142	1
-2	13	9	170	121	36	-3	1	10	0	70	1	3	8	10	0	30	1	2	17	10	0	102	1	-5	6	11	111	69	110
-1	13	9	180	197	77	-2	1	10	701	612	36	4	8	10	0	114	1	3	17	10	190	54	76	-4	6	11	0	21	1
0	13	9	0	16	1	-1	1	10	681	710	14	5	8	10	136	6	136	-3	18	10	0	54	1	-3	6	11	63	8	63
1	13	9	125	108	51	0	1	10	244	261	19	-5	9	10	98	131	97	-2	18	10	88	33	88	-2	6	11	354	334	18
2	13	9	187	216	58	1	1	10	664	640	33	-4	9	10	133	48	64	-1	18	10	28	21	28	-1	6	11	113	128	33
3	13	9	102	50	101	2	1	10	110	93	67	-3	9	10	89	70	89	0	18	10	11	17	11	0	6	11	331	346	19
4	13	9	168	118	66	3	1	10	146	8	81	-2	9	10	304	308	28	1	18	10	60	103	59	1	6	11	451	446	14
-5	14	9	99	1	99	4	1	10	320	342	30	-1	9	10	231	232	25	2	18	10	106	1	105	2	6	11	23	30	22
-4	14	9	0	62	1	5	1	10	116	110	116	0	9	10	194	188	41	3	18	10	76	88	75	3	6	11	37	0	36
-3	14	9	111	91	37	-6	2	10	133	153	133	1	9	10	340	316	28	-3	19	10	141	59	140	4	6	11	77	32	76
-2	14	9	101	75	87	-5	2	10	178	66	53	2	9	10	285	182	24	-2	19	10	89	19	89	5	6	11	159	184	158
-1	14	9	227	236	59	-4	2	10	259	225	32	3	9	10	148	58	71	-1	19	10	0	48	1	-6	7	11	0	72	1
0	14	9	94	71	94	-3	2	10	155	117	20	4	9	10	162	123	73	0	19	10	81	36	80	-5	7	11	0	30	1
1	14	9	99	64	67	-2	2	10	255	156	45	5	9	10	236	99	81	1	19	10	112	29	111	-4	7	11	0	26	1
2	14	9	69	68	69	-1	2	10	231	150	65	-5	10	10	117	217	116	2	19	10	159	10	159	-3	7	11	444	449	19
3	14	9	86	127	85	0	2	10	130	207	44	-4	10	10	0	72	1	-3	20	10	65	27	64	-2	7	11	210	183	37
4	14	9	70	48	69	1	2	10	505	532	27	-3	10	10	54	29	53	-2	20	10	0	121	1	-1	7	11	343	300	16
-5	15	9	186	31	185	2	2	10	86	40	86	-2	10	10	255	260	26	-1	20	10	127	13	126	0	7	11	261	255	19
-4	15	9	123	32	123	3	2	10	148	183	69	-1	10	10	0	90	1	0	20	10	54	67	54	1	7	11	141	79	67
-3	15	9	94	73	93	4	2	10	165	17	48	0	10	10	161	161	38	1	20	10	123	50	123	2	7	11	224	149	24
-2	15	9	80	131	80	5	2	10	67	15	66	1	10	10	258	224	16	2	20	10	192	81	90	3	7	11	0	3	1
-1	15	9	163	41	163	-6	3	10	122	0	122	2	10	10	181	94	38	-2	21	10	0	54	1	4	7	11	215	9	73
0	15	9	164	110	38	-5	3	10	180	116	47	3	10	10	185	191	39	-1	21	10	246	117	79	5	7	11	128	22	128
1	15	9	145	33	49	-4	3	10	186	109	92	4	10	10	234	116	35	0	21	10	63	73	63	-5	8	11	0	15	1
2	15	9	164	145	43	-3	3	10	51	57	50	-5	11	10	0	12	1	1	21	10	122	1	122	-4	8	11	170	76	52
3	15	9	0	26	1	-2	3	10	235	208	20	-4	11	10	98	133	98	0	22	10	0	79	1	-3	8	11	273	259	31
4	15	9	26	2	25	-1	3	10	90	222	89	-3	11	10	91	33	91	-6	1	11	134	168	133	-2	8	11	105	91	105
-4	16	9	78	38	77	0	3	10	147	130	16	-2	11	10	376	387	21	-5	1	11	124	120	94	-1	8	11	219	153	34
-3	16	9	85	15	85	1	3	10	350	348	27	-1	11	10	214	233	47	-4	1	11	276	295	23	0	8	11	189	224	37
-2	16	9	0	95	1	2	3	10	179	167	83	0	11	10	235	207	24	-3	1	11	62	6	61	1	8	11	53	12	52
-1	16	9	112	9	112	3	3	10	177	26	34	1	11	10	98	103	98	-2	1	11	314	283	13	2	8	11	266	200	21
0	16	9	146	129	79	4	3	10	213	171	54	2	11	10	214	188	65	-1	1	11	327	331	13	3	8	11	0	41	1
1	16	9	197	162	39	5	3	10	301	259	97	3	11	10	130	32	59	0	1	11	19	1	18	4	8	11	79	45	79
2	16	9	147	80	57	-6	4	10	0	137	1	4	11	10	60	175	59	1	1	11	219	221	13	5	8	11	146	37	145
3	16	9	188	6	187	-5	4	10	166	212	48	-5	12	10	0	5	1	2	1	11	0	30	1	-5	9	11	0	31	1
4	16	9	0	85	1	-4	4	10	333	273	42	-4	12	10	33	17	33	3	1	11	134	25	69	-4	9	11	155	164	51
-4	17	9	89	111	89	-3	4	10	290	267	22	-3	12	10	0	55	1	4	1	11	69	28	68	-3	9	11	421	420	30
-3	17	9	0	95	1	-2	4	10	304	285	26	-2	12	10	143	136	86	5	1	11	0	75	1	-2	9	11	220	204	34
-2	17	9	0	91	1	-1	4	10	316	308	26	-1	12	10	0	55	1	-6	2	11	231	63	70	-1	9	11	99	39	99
-1	17	9	67	60	67	0	4	10	600	519	31	0	12	10	133	41	45	-5	2	11	153	146	61	0	9	11	0	16	1

Table 7. Observed and calculated structure factors for 1 Page 7

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	9	11	361	358	16	0	19	11	140	33	99	0	6	12	70	28	69	-1	15	12	58	43	57	-1	5	13	123	45	123
2	9	11	22	90	22	1	19	11	114	118	114	1	6	12	236	226	21	0	15	12	72	150	71	0	5	13	395	328	20
3	9	11	96	95	96	2	19	11	54	81	54	2	6	12	78	8	78	1	15	12	0	20	1	1	5	13	0	0	1
4	9	11	0	48	1	-2	20	11	115	6	115	3	6	12	164	32	61	2	15	12	70	133	69	2	5	13	199	195	35
5	9	11	0	41	1	-1	20	11	121	49	120	4	6	12	0	45	1	3	15	12	0	7	1	3	5	13	221	176	47
-5	10	11	79	17	79	0	20	11	44	26	44	5	6	12	142	165	141	-4	16	12	0	22	1	4	5	13	120	167	119
-4	10	11	0	6	1	1	20	11	192	12	68	-5	7	12	85	56	84	-3	16	12	78	114	77	-5	6	13	101	19	100
-3	10	11	0	82	1	2	20	11	0	2	1	-4	7	12	230	205	36	-2	16	12	0	18	1	-4	6	13	128	107	57
-2	10	11	98	62	97	-2	21	11	160	93	160	-3	7	12	94	52	76	-1	16	12	0	182	1	-3	6	13	224	189	18
-1	10	11	176	96	66	0	21	11	0	36	1	-2	7	12	78	48	77	0	16	12	26	7	26	-2	6	13	169	180	39
0	10	11	246	234	18	1	21	11	0	147	1	-1	7	12	277	242	33	1	16	12	0	40	1	-1	6	13	182	119	49
1	10	11	24	23	23	-6	0	12	156	58	156	0	7	12	218	244	30	2	16	12	145	53	94	0	6	13	0	51	1
2	10	11	111	110	111	-5	0	12	746	753	28	1	7	12	383	373	14	3	16	12	0	19	1	1	6	13	0	19	1
3	10	11	145	36	67	-4	0	12	200	202	49	2	7	12	543	523	15	-3	17	12	0	29	1	2	6	13	75	99	74
4	10	11	132	222	131	-3	0	12	444	413	47	3	7	12	198	207	38	-2	17	12	0	33	1	3	6	13	143	58	57
-5	11	11	0	65	1	-2	0	12	146	150	42	4	7	12	0	15	1	-1	17	12	35	2	35	4	6	13	171	87	47
-4	11	11	68	68	67	-1	0	12	96	92	33	5	7	12	155	214	154	0	17	12	140	228	49	-5	7	13	262	216	37
-3	11	11	129	122	34	0	0	12	179	196	32	-5	8	12	95	125	95	1	17	12	0	86	1	-4	7	13	185	232	41
-2	11	11	142	0	46	1	0	12	0	52	1	-4	8	12	221	239	34	2	17	12	0	5	1	-3	7	13	0	48	1
-1	11	11	97	38	97	2	0	12	0	3	1	-3	8	12	94	122	93	3	17	12	150	31	150	-2	7	13	164	117	43
0	11	11	161	173	51	3	0	12	224	183	59	-2	8	12	203	206	27	-3	18	12	207	98	83	-1	7	13	334	321	42
1	11	11	169	138	37	4	0	12	0	16	1	-1	8	12	51	75	51	-2	18	12	0	127	1	0	7	13	102	145	102
2	11	11	139	130	84	-6	1	12	0	85	1	0	8	12	36	26	36	-1	18	12	124	80	123	1	7	13	131	102	131
3	11	11	48	16	48	-5	1	12	297	266	38	1	8	12	162	13	36	0	18	12	0	25	1	2	7	13	39	20	38
4	11	11	0	9	1	-4	1	12	69	62	69	2	8	12	89	148	88	1	18	12	0	141	1	3	7	13	139	105	139
-5	12	11	0	46	1	-3	1	12	159	10	79	3	8	12	0	118	1	2	18	12	0	34	1	4	7	13	201	91	39
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-3	12	11	122	139	45	-1	1	12	80	40	56	-5	9	12	140	71	139	-2	19	12	112	32	111	-4	8	13	80	58	79
-2	12	11	310	309	24	0	1	12	59	10	58	-4	9	12	157	224	83	-1	19	12	95	43	95	-3	8	13	104	94	103
-1	12	11	104	73	104	1	1	12	289	291	27	-3	9	12	301	305	17	0	19	12	117	41	69	-2	8	13	147	117	35
0	12	11	133	15	115	2	1	12	0	28	1	-2	9	12	380	361	25	1	19	12	141	11	141	-1	8	13	0	12	1
1	12	11	63	36	63	3	1	12	224	190	49	-1	9	12	441	437	45	2	19	12	87	59	87	0	8	13	0	70	1
2	12	11	0	55	1	4	1	12	179	175	75	0	9	12	296	261	19	-2	20	12	0	11	1	1	8	13	143	143	51
3	12	11	159	128	158	5	1	12	136	20	136	1	9	12	169	161	45	-1	20	12	0	6	1	2	8	13	223	154	30
4	12	11	101	15	100	-6	2	12	0	28	1	2	9	12	118	33	73	1	20	12	96	30	96	3	8	13	0	83	1
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-4	13	11	0	90	1	-4	2	12	193	151	25	4	9	12	21	113	21	-6	1	13	0	30	1	-5	9	13	159	188	64
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-2	13	11	132	132	74	-2	2	12	116	19	50	-4	10	12	268	261	27	-4	1	13	98	83	64	-3	9	13	121	137	52
-1	13	11	0	2	1	-1	2	12	193	248	56	-3	10	12	420	422	14	-3	1	13	111	66	44	-2	9	13	226	224	28
0	13	11	82	70	82	0	2	12	145	155	38	-2	10	12	141	136	83	-2	1	13	283	280	14	-1	9	13	0	0	1
1	13	11	215	145	21	1	2	12	150	170	23	-1	10	12	207	197	47	-1	1	13	313	306	19	0	9	13	205	249	74
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3	13	11	0	133	1	3	2	12	121	144	92	1	10	12	158	95	44	1	1	13	107	118	36	2	9	13	75	64	74
4	13	11	138	22	138	4	2	12	170	209	81	2	10	12	0	28	1	2	1	13	153	85	35	3	9	13	72	85	72
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-3	14	11	171	94	42	-6	3	12	193	138	74	4	10	12	175	72	174	4	1	13	227	222	49	-5	10	13	82	61	81
-2	14	11	202	146	34	-5	3	12	332	428	47	-5	11	12	0	13	1	-6	2	13	143	23	142	-4	10	13	0	53	1
-1	14	11	0	54	1	-4	3	12	0	118	1	-4	11	12	0	10	1	-5	2	13	61	76	61	-3	10	13	193	134	35
0	14	11	111	82	73	-3	3	12	208	182	22	-3	11	12	0	5	1	-4	2	13	135	133	36	-2	10	13	136	123	135
1	14	11	84	64	83	-2	3	12	548	517	13	-2	11	12	315	293	32	-3	2	13	173	114	34	-1	10	13	119	77	49
2	14	11	0	50	1	-1	3	12	170	181	49	-1	11	12	0	47	1	-2	2	13	201	51	83	0	10	13	0	15	1
3	14	11	106	76	106	0	3	12	310	307	15	0	11	12	165	82	30	-1	2	13	134	150	33	1	10	13	156	22	40
4	14	11	0	91	1	1	3	12	128	139	36	1	11	12	181	1	40	0	2	13	146	186	84	2	10	13	112	77	105
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0	15	11	112	29	69	-5	4	12	0	76	1	-4	12	12	0	31	1	5	2	13	175	17	174	-3	11	13	176	70	33
1	15	11	82	102	82	-4	4	12	113	50	112	-3	12	12	211	209	30	-6	3	13	0	30	1	-2	11	13	330	272	27
2	15	11	0	38	1	-3	4	12	228	188	27	-2	12	12	198	158	30	-5	3	13	155	127	93	-1	11	13	144	139	31
3	15	11	192	43	71	-2	4	12	160	113	23	-1	12	12	110	0	77	-4	3	13	108	66	107	0	11	13	0	82	1
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-3	16	11	171	83	59	0	4	12	273	252	16	1	12	12	103	52	102	-2	3	13	197	167	26	2	11	13	0	69	1
-2	16	11	71	62	71	1	4	12	349	367	16	2	12	12	138	116	78	-1	3	13	357	331	37	3	11	13	0	9	1
-1	16	11	89	47	88	2	4	12	166	78	45	3	12	12	138	147	138	0	3	13	117	15	116	4	11	13	96	5	96
0	16	11	205	231	33	3	4	12	65	8	64	4	12	12	200	6	45	1	3	13	264	268	20	-5	12	13	0	45	1
1	16	11	14	92	13	4	4	12	188	143	46	-5	13	12	113	32	113	2	3	13	231	261	30	-4	12	13	109	147	108
2	16	11	0	7	1	5	4	12	88	14	87	-4	13	12	158	61	65	3	3	13	85	59	84	-3	12	13	122	123	121
3	16	11	198	133	99	-6	5	12	70	35	70	-3	13	12	123	22	122	4	3	13	22	36	22	-2	12	13	106	86	79
-4	17	11	0	42	1	-5	5	12	133	162	64	-2	13	12	189	161	34	5	3	13	0	7	1	-1	12	13	82	62	81
-3	17	11	214	119	85	-4	5	12	195	4	46	-1	13	12	271	229	34	-6	4	13	0	103	1	0	12	13	74	73	73
-2	17	11	107	15	106	-3	5	12	169	29	49	0	13	12	110	29	70	-5	4	13	163	190	62	1	12	13	153	190	59
-1	17	11	0	26	1	-2	5	12	106	96	60	1	13	12	71	138	71	-4	4	13	316	307	38	2	12	13	0	6	1
0	17	11	0	58	1	-1	5	12	274	249	34	2	13	12	0	34	1	-3	4	13	174	117	27	3	12	13	0	54	1
1	17	11	0	78	1	0	5	12	217	194	25	3	13	12	0	17	1	-2	4	13	0	26	1	4	12	13	0	15	1
2	17	11	0	20	1	1	5	12	143	186	36	-4	14	12	0	29	1	-1	4	13	131	182	131	-4	13	13	0	90	1
3	17	11	0	0	1	2	5	12	95	75	48	-3	14	12	136	35	56	0	4	13	159	146	24	-3	13	13	0	33	1
-3	18	11	158	130	158	3	5	12	247	221	50	-2	14	12	206	303	56	1	4	13	77	50	77	-2	13	13	0	67	1
-2	18	11	200	13	199	4	5	12	153	59	68	-1	14	12	108	92	76	2	4	13	132	87	34	-1	13	13	147	184	147
-1	18	11	92	71	91	5	5	12	74	125	73	0	14	12	179	127	33	3	4	13	0	37	1	0	13	13	40	33	40
0	18	11	118	55	78	-6	6	12	0	69	1	1	14	12	153	134	88	4	4	13	127	106	96	1	13	13	69	74	68
1	18	11	136	141	135	-5	6	12	123	113	122	2	14	12	118	74	61	5	4	13	159	22	158	2	13	13	66	28	66
2	18	11	118	47	117	-4	6	12	195	103	47	3	14	12	154	190	97	-5	5	13	0	138	1	3	13	13	81	47	81
-3	19	11	0	8	1	-3	6	12	269	253	17	-4	15	12	70	78	69	-4	5	13	126	73	53	-4	14	13	175	176	174
-2	19	11	71	21	70	-2	6	12	91	92	90	-3	15	12	0	114	1	-3	5	13	83	10	83	-3	14	13	257	289	28
-1	19	11	160	62	159	-1	6	12	144	178	109	-2	15	12	0	87	1	-2	5	13	193	133	59	-2	14	13	0	30	1

Table 7. Observed and calculated structure factors for 1 Page 8

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-1	14	13	0	200	1	2	4	14	193	46	47	2	13	14	73	96	72	4	5	15	0	20	1	-3	16	15	0	27	1
0	14	13	252	210	29	3	4	14	87	33	86	3	13	14	0	11	1	-5	6	15	163	40	70	-2	16	15	0	5	1
1	14	13	0	35	1	4	4	14	0	36	1	-4	14	14	0	105	1	-4	6	15	233	255	27	-1	16	15	108	118	108
2	14	13	0	48	1	-5	5	14	294	278	38	-3	14	14	0	101	1	-3	6	15	88	50	87	0	16	15	152	123	151
3	14	13	0	18	1	-4	5	14	197	218	50	-2	14	14	324	305	71	-2	6	15	0	21	1	1	16	15	0	6	1
-4	15	13	98	1	97	-3	5	14	111	92	110	-1	14	14	96	49	96	-1	6	15	0	17	1	2	16	15	0	24	1
-3	15	13	157	187	49	-2	5	14	0	91	1	0	14	14	93	158	93	0	6	15	115	4	115	-3	17	15	52	72	51
-2	15	13	23	13	23	-1	5	14	163	143	126	1	14	14	147	2	147	1	6	15	115	63	53	-2	17	15	0	37	1
-1	15	13	113	149	62	0	5	14	103	78	24	2	14	14	40	148	40	2	6	15	46	69	45	-1	17	15	109	62	109
0	15	13	104	105	103	1	5	14	138	148	40	3	14	14	0	1	1	3	6	15	63	84	63	0	17	15	185	89	68
1	15	13	130	65	102	2	5	14	108	18	108	-4	15	14	82	39	81	4	6	15	169	7	62	1	17	15	70	59	70
2	15	13	0	14	1	3	5	14	29	43	28	-3	15	14	105	74	105	-5	7	15	0	22	1	-2	18	15	0	60	1
3	15	13	98	16	98	4	5	14	0	88	1	-2	15	14	0	34	1	-4	7	15	0	40	1	-1	18	15	82	88	81
-4	16	13	0	15	1	-5	6	14	114	116	114	-1	15	14	234	281	45	-3	7	15	61	101	60	1	18	15	0	47	1
-3	16	13	197	64	197	-4	6	14	149	173	46	0	15	14	193	197	46	-2	7	15	140	101	139	-1	19	15	96	54	96
-2	16	13	0	23	1	-3	6	14	52	29	51	1	15	14	59	29	58	-1	7	15	319	190	27	0	19	15	35	11	35
-1	16	13	40	34	39	-2	6	14	135	104	105	2	15	14	213	68	109	0	7	15	104	139	104	-5	0	16	0	46	1
0	16	13	96	136	95	-1	6	14	87	7	86	3	15	14	0	13	1	1	7	15	66	40	65	-4	0	16	87	39	86
1	16	13	163	3	163	0	6	14	107	97	107	-3	16	14	124	33	114	2	7	15	220	136	42	-3	0	16	0	75	1
2	16	13	0	38	1	1	6	14	182	184	40	-2	16	14	0	57	1	3	7	15	106	39	106	-2	0	16	134	83	50
3	16	13	0	82	1	2	6	14	0	43	1	-1	16	14	138	189	65	4	7	15	0	57	1	-1	0	16	187	22	132
-3	17	13	36	117	36	3	6	14	0	61	1	0	16	14	135	176	59	-5	8	15	138	48	78	0	0	16	247	256	25
-2	17	13	68	32	68	4	6	14	0	14	1	1	16	14	75	9	75	-4	8	15	0	8	1	1	0	16	0	32	1
-1	17	13	164	55	49	-5	7	14	0	31	1	2	16	14	121	37	120	-3	8	15	78	42	78	2	0	16	0	88	1
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1	17	13	159	17	158	-3	7	14	103	29	62	-2	17	14	0	66	1	-1	8	15	282	146	46	4	0	16	167	23	167
2	17	13	250	12	99	-2	7	14	44	16	44	-1	17	14	59	58	58	0	8	15	125	32	45	-5	1	16	0	57	1
-3	18	13	126	65	126	-1	7	14	222	162	46	0	17	14	63	31	63	1	8	15	0	94	1	-4	1	16	179	198	26
-2	18	13	234	116	49	0	7	14	0	74	1	1	17	14	0	93	1	2	8	15	124	100	72	-3	1	16	101	72	101
-1	18	13	48	116	47	1	7	14	0	54	1	2	17	14	0	7	1	3	8	15	0	73	1	-2	1	16	138	117	40
0	18	13	0	95	1	2	7	14	138	97	47	-2	18	14	0	21	1	4	8	15	121	185	120	-1	1	16	154	50	59
1	18	13	0	64	1	3	7	14	0	36	1	-1	18	14	175	95	101	-5	9	15	40	18	39	0	1	16	71	75	71
2	18	13	0	13	1	4	7	14	56	53	56	0	18	14	0	78	1	-4	9	15	0	6	1	1	1	16	148	89	75
-2	19	13	158	6	91	-5	8	14	97	54	97	1	18	14	108	52	108	-3	9	15	176	5	49	2	1	16	250	327	31
-1	19	13	95	55	94	-4	8	14	155	216	78	-2	19	14	136	19	136	-2	9	15	110	197	110	3	1	16	136	146	51
1	19	13	0	55	1	-3	8	14	134	58	39	-1	19	14	159	157	112	-1	9	15	73	35	73	4	1	16	0	1	1
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1	20	13	164	108	100	-1	8	14	179	40	142	-1	20	14	0	37	1	1	9	15	134	4	55	-4	2	16	136	113	58
-6	0	14	185	19	184	0	8	14	141	80	70	-5	1	15	210	133	42	2	9	15	111	103	88	-3	2	16	130	125	90
-5	0	14	286	254	30	1	8	14	51	128	51	-4	1	15	102	11	78	3	9	15	59	103	58	-2	2	16	0	56	1
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-3	0	14	0	62	1	3	8	14	175	160	43	-2	1	15	181	59	64	-4	10	15	0	38	1	0	2	16	149	128	51
-2	0	14	216	117	26	4	8	14	127	69	127	-1	1	15	324	267	25	-3	10	15	0	53	1	1	2	16	275	243	61
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2	0	14	177	99	48	-2	9	14	102	149	71	3	1	15	134	185	68	1	10	15	221	192	41	-5	3	16	0	41	1
3	0	14	115	146	114	-1	9	14	98	29	98	4	1	15	0	120	1	2	10	15	0	83	1	-4	3	16	111	82	111
4	0	14	72	87	72	0	9	14	95	127	94	-5	2	15	162	10	50	3	10	15	0	7	1	-3	3	16	0	73	1
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2	1	14	127	100	44	-1	10	14	307	252	49	4	2	15	87	51	86	-4	12	15	52	3	51	-4	4	16	0	58	1
3	1	14	250	183	25	0	10	14	121	109	56	-5	3	15	0	49	1	-3	12	15	0	103	1	-3	4	16	92	91	79
4	1	14	173	20	47	1	10	14	89	115	88	-4	3	15	153	131	33	-2	12	15	96	133	95	-2	4	16	0	83	1
-5	2	14	0	95	1	2	10	14	0	80	1	-3	3	15	0	61	1	-1	12	15	145	144	36	-1	4	16	106	135	105
-4	2	14	150	67	43	3	10	14	48	140	47	-2	3	15	319	315	35	0	12	15	158	90	37	0	4	16	93	124	92
-3	2	14	0	17	1	4	10	14	186	71	185	-1	3	15	89	55	89	1	12	15	0	101	1	1	4	16	91	52	91
-2	2	14	283	237	21	-5	11	14	0	3	1	0	3	15	126	11	51	2	12	15	58	32	57	2	4	16	273	87	27
-1	2	14	406	405	31	-4	11	14	20	183	20	1	3	15	164	146	73	3	12	15	0	10	1	3	4	16	0	18	1
0	2	14	301	296	19	-3	11	14	179	138	39	2	3	15	266	273	27	-4	13	15	167	207	64	-5	5	16	0	96	1
1	2	14	253	223	21	-2	11	14	175	154	53	3	3	15	154	100	62	-3	13	15	68	45	67	-4	5	16	158	175	47
2	2	14	217	259	49	-1	11	14	0	48	1	4	3	15	0	39	1	-2	13	15	0	16	1	-3	5	16	107	62	107
3	2	14	171	55	55	0	11	14	71	12	70	-5	4	15	0	119	1	-1	13	15	216	208	40	-2	5	16	147	64	49
4	2	14	0	72	1	1	11	14	79	97	79	-4	4	15	119	116	51	0	13	15	82	14	82	-1	5	16	76	123	76
-5	3	14	101	106	100	2	11	14	0	35	1	-3	4	15	125	64	40	1	13	15	174	93	56	0	5	16	267	274	42
-4	3	14	206	163	25	3	11	14	165	74	112	-2	4	15	204	42	44	2	13	15	96	31	95	1	5	16	198	199	26
-3	3	14	194	189	37	4	11	14	179	24	178	-1	4	15	332	308	22	3	13	15	13	10	12	2	5	16	0	44	1
-2	3	14	211	144	36	-4	12	14	59	108	58	0	4	15	49	90	48	-4	14	15	216	50	84	3	5	16	65	110	64
-1	3	14	340	355	24	-3	12	14	36	8	36	1	4	15	71	3	70	-3	14	15	178	13	48	4	5	16	0	55	1
0	3	14	194	141	115	-2	12	14	109	104	109	2	4	15	118	111	118	-2	14	15	135	136	53	-5	6	16	113	53	112
1	3	14	0	30	1	-1	12	14	307	278	24	3	4	15	75	105	75	-1	14	15	90	102	90	-4	6	16	203	217	22
2	3	14	110	1	110	0	12	14	107	62	107	4	4	15	138	79	137	0	14	15	80	31	79	-3	6	16	72	17	72
3	3	14	180	214	51	1	12	14	123	147	122	-5	5	15	69	1	68	1	14	15	0	10	1	-2	6	16	0	55	1
4	3	14	0	12	1	2	12	14	192	224	59	-4	5	15	197	213	23	2	14	15	180	28	179	-1	6	16	0	84	1
-5	4	14	175	169	50	3	12	14	203	8	64	-3	5	15	115	61	66	3	14	15	0	4	1	0	6	16	121	127	71
-4	4	14	281	260	16	-4	13	14	59	128	58	-2	5	15	54	102	54	-3	15	15	55	5	54	1	6	16	183	52	52
-3	4	14	97	81	97	-3	13	14	159	191	71	-1	5	15	163	148	36	-2	15	15	112	44	111	2	6	16	121	151	85
-2	4	14	0	14	1	-2	13	14	250	254	25	0	5	15	288	263	61	-1	15	15	0	106	1	3	6	16	200	60	46
-1	4	14	152	158	34	-1	13	14	0	50	1	1	5	15	121	149	51	0	15	15	0	64	1	4	6	16	17	74	16
0	4	14	196	207	78	0	13	14	149	98	53	2	5	15	142	148	62	1	15	15	50	123	49	-5	7	16	125	35	125
1	4	14	0	10	1	1	13	14	161	7	47	3	5	15	98	20	98	2	15	15	0	8	1	-4	7	16	0	24	1

Table 7. Observed and calculated structure factors for 1 Page 9

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-3	7	16	98	116	63	2	1	17	213	220	25	-1	11	17	303	222	37	3	5	18	199	3	81	2	3	19	0	2	1
-2	7	16	159	64	129	3	1	17	147	177	41	0	11	17	146	70	56	-4	6	18	0	118	1	3	3	19	168	84	77
-1	7	16	208	170	27	4	1	17	155	19	154	1	11	17	50	5	50	-3	6	18	181	67	58	-4	4	19	118	180	118
0	7	16	253	241	22	-5	2	17	207	53	48	2	11	17	0	59	1	-2	6	18	68	79	68	-3	4	19	121	24	76
1	7	16	157	140	156	-4	2	17	121	127	63	3	11	17	0	30	1	-1	6	18	129	117	129	-2	4	19	0	22	1
2	7	16	126	67	84	-3	2	17	142	95	65	-4	12	17	0	103	1	0	6	18	93	37	92	-1	4	19	182	142	54
3	7	16	0	43	1	-2	2	17	76	54	75	-3	12	17	71	73	70	1	6	18	220	213	33	0	4	19	258	247	18
4	7	16	0	6	1	-1	2	17	74	17	74	-2	12	17	0	12	1	2	6	18	54	64	53	1	4	19	0	32	1
-5	8	16	125	71	124	0	2	17	119	21	94	-1	12	17	0	65	1	3	6	18	0	47	1	2	4	19	0	140	1
-4	8	16	50	86	50	1	2	17	170	107	44	0	12	17	0	102	1	-4	7	18	103	29	103	3	4	19	100	55	99
-3	8	16	208	137	27	2	2	17	155	74	87	1	12	17	51	27	51	-3	7	18	68	0	68	-4	5	19	0	134	1
-2	8	16	0	82	1	3	2	17	8	88	7	2	12	17	0	173	1	-2	7	18	91	75	90	-3	5	19	67	141	67
-1	8	16	294	280	31	-5	3	17	147	50	90	-3	13	17	59	119	59	-1	7	18	248	240	59	-2	5	19	104	144	104
0	8	16	171	161	64	-4	3	17	78	103	77	-2	13	17	77	39	76	0	7	18	0	59	1	-1	5	19	142	147	141
1	8	16	81	79	80	-3	3	17	115	41	114	-1	13	17	0	15	1	1	7	18	153	28	67	0	5	19	326	369	26
2	8	16	123	32	56	-2	3	17	0	27	1	0	13	17	102	93	101	2	7	18	0	96	1	1	5	19	166	67	50
3	8	16	144	98	75	-1	3	17	0	52	1	1	13	17	0	6	1	3	7	18	173	129	173	2	5	19	0	39	1
-5	9	16	146	81	145	0	3	17	117	91	50	2	13	17	0	84	1	-4	8	18	100	189	99	3	5	19	0	57	1
-4	9	16	166	34	66	1	3	17	0	88	1	-3	14	17	80	51	80	-3	8	18	657	131	258	-4	6	19	136	53	136
-3	9	16	0	77	1	2	3	17	93	106	92	-2	14	17	133	114	132	-2	8	18	179	65	59	-3	6	19	90	36	90
-2	9	16	89	13	89	3	3	17	69	153	68	-1	14	17	84	15	84	-1	8	18	196	162	60	-2	6	19	222	179	67
-1	9	16	146	215	94	4	3	17	0	22	1	0	14	17	39	2	38	0	8	18	132	134	132	-1	6	19	200	181	60
0	9	16	125	98	57	-5	4	17	0	50	1	1	14	17	77	7	76	1	8	18	0	56	1	0	6	19	0	47	1
1	9	16	88	44	88	-4	4	17	33	69	32	2	14	17	39	21	39	2	8	18	28	8	27	1	6	19	0	147	1
2	9	16	100	103	100	-3	4	17	305	265	28	-3	15	17	63	13	63	3	8	18	56	26	56	2	6	19	0	19	1
3	9	16	0	69	1	-2	4	17	219	107	40	-2	15	17	332	219	52	-4	9	18	0	61	1	3	6	19	0	38	1
-4	10	16	0	97	1	-1	4	17	0	64	1	-1	15	17	61	10	61	-3	9	18	0	60	1	-4	7	19	36	119	36
-3	10	16	0	168	1	0	4	17	103	6	103	0	15	17	59	45	58	-2	9	18	0	8	1	-3	7	19	0	27	1
-2	10	16	108	81	34	1	4	17	75	38	74	1	15	17	171	20	99	-1	9	18	592	480	85	-2	7	19	140	181	89
-1	10	16	247	221	30	2	4	17	101	76	101	-1	16	17	0	71	1	0	9	18	129	39	44	-1	7	19	105	107	104
0	10	16	0	29	1	3	4	17	0	65	1	0	16	17	0	17	1	1	9	18	0	35	1	0	7	19	73	14	73
1	10	16	156	172	48	4	4	17	0	39	1	1	16	17	178	7	59	2	9	18	0	11	1	1	7	19	20	44	20
2	10	16	0	35	1	-5	5	17	119	118	105	-1	17	17	0	108	1	-4	10	18	146	36	145	2	7	19	0	5	1
3	10	16	112	70	112	-4	5	17	178	172	34	0	17	17	260	63	60	-3	10	18	182	142	67	3	7	19	89	70	89
-4	11	16	0	138	1	-3	5	17	56	24	56	-5	0	18	263	55	91	-2	10	18	131	167	131	-4	8	19	37	14	36
-3	11	16	239	253	33	-2	5	17	175	117	175	-4	0	18	0	80	1	-1	10	18	0	7	1	-3	8	19	45	94	45
-2	11	16	60	78	59	-1	5	17	143	44	84	-3	0	18	95	122	94	0	10	18	202	162	38	-2	8	19	171	190	51
-1	11	16	76	45	75	0	5	17	0	4	1	-2	0	18	242	131	70	1	10	18	14	6	14	-1	8	19	123	19	122
0	11	16	210	220	34	1	5	17	0	81	1	-1	0	18	171	181	39	2	10	18	198	30	198	0	8	19	101	82	100
1	11	16	0	12	1	2	5	17	192	193	62	0	0	18	270	365	45	-4	11	18	0	18	1	1	8	19	35	126	35
2	11	16	133	74	132	3	5	17	123	58	42	1	0	18	800	741	21	-3	11	18	134	56	110	2	8	19	159	161	54
3	11	16	52	31	51	4	5	17	159	78	158	2	0	18	163	127	163	-2	11	18	0	57	1	-4	9	19	216	60	152
-4	12	16	0	36	1	-5	6	17	135	98	134	3	0	18	238	188	52	-1	11	18	240	229	45	-3	9	19	0	45	1
-3	12	16	159	140	51	-4	6	17	0	98	1	-5	1	18	0	41	1	0	11	18	0	44	1	-2	9	19	165	182	70
-2	12	16	0	64	1	-3	6	17	104	28	104	-4	1	18	107	43	106	1	11	18	0	59	1	-1	9	19	33	94	32
-1	12	16	240	203	29	-2	6	17	202	30	53	-3	1	18	0	10	1	2	11	18	0	5	1	0	9	19	22	0	21
0	12	16	107	121	107	-1	6	17	190	72	57	-2	1	18	149	111	23	-3	12	18	222	127	41	1	9	19	163	92	111
1	12	16	0	13	1	0	6	17	0	90	1	-1	1	18	130	115	40	-2	12	18	63	42	63	2	9	19	0	81	1
2	12	16	0	122	1	1	6	17	100	60	70	0	1	18	290	192	47	-1	12	18	0	13	1	-3	10	19	0	15	1
3	12	16	204	32	203	2	6	17	0	46	1	1	1	18	162	101	39	0	12	18	140	105	53	-2	10	19	0	106	1
-4	13	16	121	4	121	3	6	17	209	148	49	2	1	18	142	113	60	1	12	18	0	69	1	-1	10	19	198	140	197
-3	13	16	93	116	92	-5	7	17	0	5	1	3	1	18	0	59	1	2	12	18	311	69	118	0	10	19	115	26	114
-2	13	16	247	238	45	-4	7	17	0	64	1	-5	2	18	0	47	1	-3	13	18	173	129	56	1	10	19	117	105	117
-1	13	16	152	188	72	-3	7	17	136	152	136	-4	2	18	158	29	37	-2	13	18	63	96	63	2	10	19	0	4	1
0	13	16	162	106	58	-2	7	17	164	12	63	-3	2	18	0	20	1	-1	13	18	144	127	143	-3	11	19	103	6	103
1	13	16	0	18	1	-1	7	17	416	288	34	-2	2	18	157	206	66	0	13	18	90	68	89	-2	11	19	216	164	56
2	13	16	0	56	1	0	7	17	108	46	108	-1	2	18	91	11	91	1	13	18	202	110	64	-1	11	19	0	104	1
3	13	16	0	30	1	1	7	17	158	46	66	0	2	18	131	162	45	2	13	18	0	69	1	0	11	19	0	47	1
-3	14	16	131	48	131	2	7	17	166	20	77	1	2	18	47	19	47	-3	14	18	0	41	1	1	11	19	172	18	49
-2	14	16	295	282	25	3	7	17	182	64	53	2	2	18	78	9	78	-1	14	18	213	141	38	2	11	19	377	26	76
-1	14	16	120	110	119	-4	8	17	87	65	87	3	2	18	73	7	73	0	14	18	104	55	104	-3	12	19	101	197	100
0	14	16	100	74	99	-3	8	17	174	172	39	-5	3	18	219	13	64	1	14	18	130	30	129	-2	12	19	0	81	1
1	14	16	0	7	1	-2	8	17	121	200	120	-4	3	18	57	65	57	-1	15	18	146	24	145	-1	12	19	36	52	36
2	14	16	66	72	65	-1	8	17	151	12	80	-3	3	18	0	17	1	0	15	18	171	53	170	0	12	19	236	35	61
-3	15	16	163	131	81	0	8	17	140	67	42	-2	3	18	117	88	83	1	15	18	141	80	141	1	12	19	0	38	1
-2	15	16	301	313	31	1	8	17	119	6	72	-1	3	18	0	34	1	-4	1	19	57	20	57	2	12	19	193	8	111
-1	15	16	192	155	38	2	8	17	0	33	1	0	3	18	311	287	37	-3	1	19	80	83	80	-3	13	19	0	6	1
0	15	16	0	155	1	3	8	17	148	92	147	1	3	18	186	213	43	-2	1	19	99	30	98	-2	13	19	0	100	1
1	15	16	0	45	1	-4	9	17	126	108	126	2	3	18	105	41	104	-1	1	19	0	42	1	-1	13	19	0	27	1
2	15	16	0	10	1	-3	9	17	109	23	108	3	3	18	0	158	1	0	1	19	59	115	59	1	13	19	0	22	1
-3	16	16	222	30	221	-2	9	17	0	103	1	-5	4	18	146	87	145	1	1	19	209	94	28	-1	14	19	163	19	163
-2	16	16	157	146	71	-1	9	17	355	316	23	-4	4	18	159	65	122	2	1	19	235	207	36	-1	15	19	0	40	1
-1	16	16	245	161	41	0	9	17	251	272	46	-3	4	18	160	12	61	3	1	19	0	86	1	-4	0	20	0	14	1
0	16	16	0	39	1	1	9	17	105	62	105	-2	4	18	0	2	1	-4	2	19	124	30	124	-3	0	20	237	244	132
1	16	16	19	50	19	2	9	17	269	175	48	-1	4	18	0	4	1	-3	2	19	167	166	41	-2	0	20	0	29	1
-2	17	16	55	21	55	3	9	17	0	13	1	0	4	18	199	131	35	-2	2	19	136	91	91	-1	0	20	0	160	1
-1	17	16	103	74	103	-4	10	17	0	45	1	1	4	18	187	117	37	-1	2	19	286	247	52	0	0	20	282	316	27
0	17	16	203	37	106	-3	10	17	111	150	110	2	4	18	131	131	131	0	2	19	95	81	52	1	0	20	242	166	45
1	17	16	232	87	58	-2	10	17	82	10	81	3	4	18	18	87	18	1	2	19	455	407	47	2	0	20	193	137	58
0	18	16	169	8	131	-1	10	17	263	318	32	-5	5	18	0	33	1	2	2	19	0	158	1	3	0	20	196	45	86
-5	1	17	0	91	1	0	10	17	151	149	75	-4	5	18	0	68	1	3	2	19	0	12	1	-4	1	20	171	39	170
-4	1	17	94	98	94	1	10	17	0	12	1	-3	5	18	110	67	110	-4	3	19	0	88	1	-3	1	20	178	175	39
-3	1	17	128	73	57	2	10	17	0	0	1	-2	5	18	0	32	1	-3	3	19	125	82	125	-2	1	20	0	18	1
-2	1	17	157	54	56	3	10	17	150	40	150	-1	5	18	155	112	113	-2	3	19	0	76	1	-1	1	20	96	155	96
-1	1	17	0	58	1	-4	11	17	0	60	1	0	5	18	163	142	86	-1	3	19	202	176	28	0	1	20	198	236	25
0	1	17	159	181	35	-3	11	17	0	24	1	1	5	18	85	62	84	0	3	19	197	228	48	1	1	20	57	159	57
1	1	17	173	108	33	-2	11	17	135	59	87	2	5	18	0	73	1	1	3	19	161	162	54	2	1	20	0	69	1

Table 7. Observed and calculated structure factors for 1 Page 10

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	1	20	51	7	51	2	7	20	134	45	127	-1	3	21	230	203	27	-3	0	22	0	10	1	1	8	22	225	126	83
-4	2	20	103	145	103	-3	8	20	0	86	1	0	3	21	89	71	88	-2	0	22	82	25	81	-2	9	22	0	15	1
-3	2	20	134	143	53	-2	8	20	109	143	109	1	3	21	46	65	46	0	0	22	82	48	81	-1	9	22	0	61	1
-2	2	20	0	48	1	-1	8	20	202	211	38	2	3	21	0	14	1	1	0	22	0	45	1	0	9	22	141	86	140
-1	2	20	103	147	103	0	8	20	0	4	1	-4	4	21	231	81	115	2	0	22	186	51	112	-2	10	22	0	61	1
0	2	20	173	164	29	1	8	20	57	99	56	-3	4	21	39	56	39	-3	1	22	75	114	74	-1	10	22	189	80	152
1	2	20	81	135	80	2	8	20	0	142	1	-2	4	21	168	181	49	-2	1	22	0	0	1	0	10	22	0	24	1
2	2	20	52	46	51	-3	9	20	0	58	1	-1	4	21	0	23	1	-1	1	22	115	176	115	-3	1	23	0	49	1
3	2	20	0	39	1	-2	9	20	0	89	1	0	4	21	263	167	63	0	1	22	126	66	74	-2	1	23	0	68	1
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2	3	20	189	28	92	1	10	20	127	5	126	1	5	21	138	39	76	1	2	22	32	33	31	1	2	23	147	32	146
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0	6	20	248	152	36	-3	2	21	0	57	1	0	9	21	0	23	1	0	6	22	0	47	1	-2	0	24	103	54	103
1	6	20	0	99	1	-2	2	21	103	70	44	1	9	21	101	28	101	1	6	22	0	153	1	-2	1	24	0	14	1
2	6	20	0	49	1	-1	2	21	137	35	35	-2	10	21	105	44	105	-3	7	22	163	15	113	-1	1	24	89	26	89
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-1	7	20	178	152	178	-4	3	21	0	76	1	-2	11	21	162	15	82	-2	8	22	189	26	81	0	4	24	0	33	1
0	7	20	97	26	97	-3	3	21	0	18	1	0	11	21	0	57	1	-1	8	22	163	92	163	-1	5	24	36	12	36
1	7	20	167	124	51	-2	3	21	118	111	55	-1	12	21	109	45	109	0	8	22	263	142	136						

Figure 1. View of **1** showing the atom labeling scheme. Displacement ellipsoids are scaled to the 30% probability level. Most hydrogen atoms have been removed for clarity. The minor component of the disordered p-nitrobenzoate is not shown.

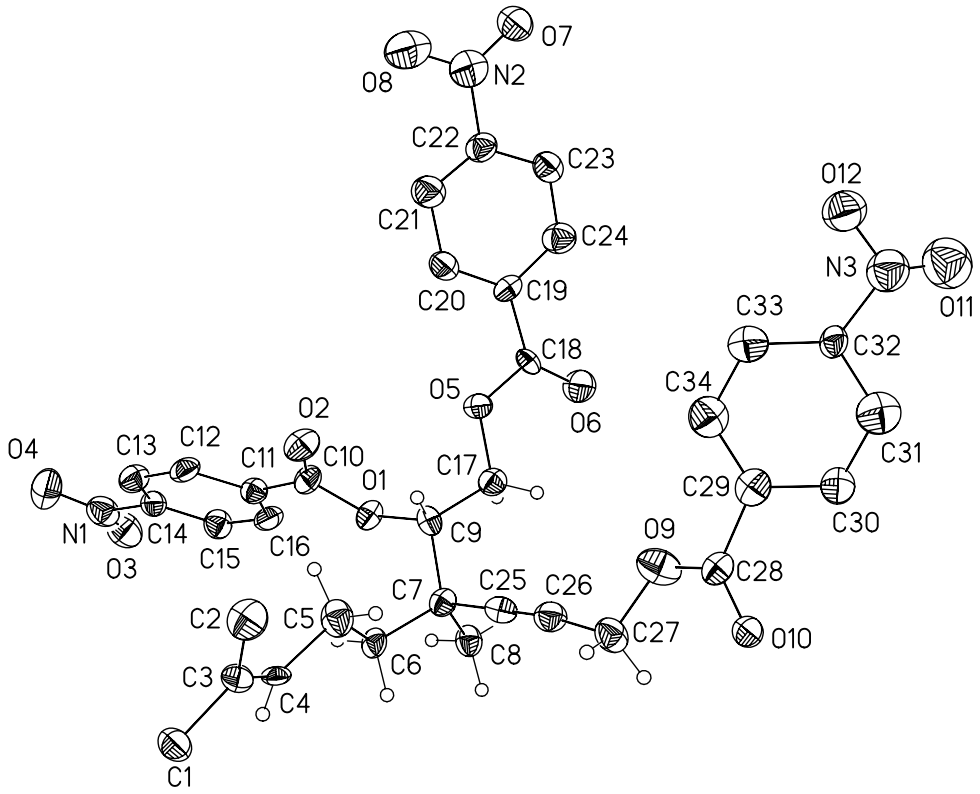

Figure 2. View of **1** showing a partial atom labeling scheme. Atoms from the minor component of the disordered p-nitrobenzoate have labels appended by an A. The site occupancy factor for the minor component refined to 44(2)%.

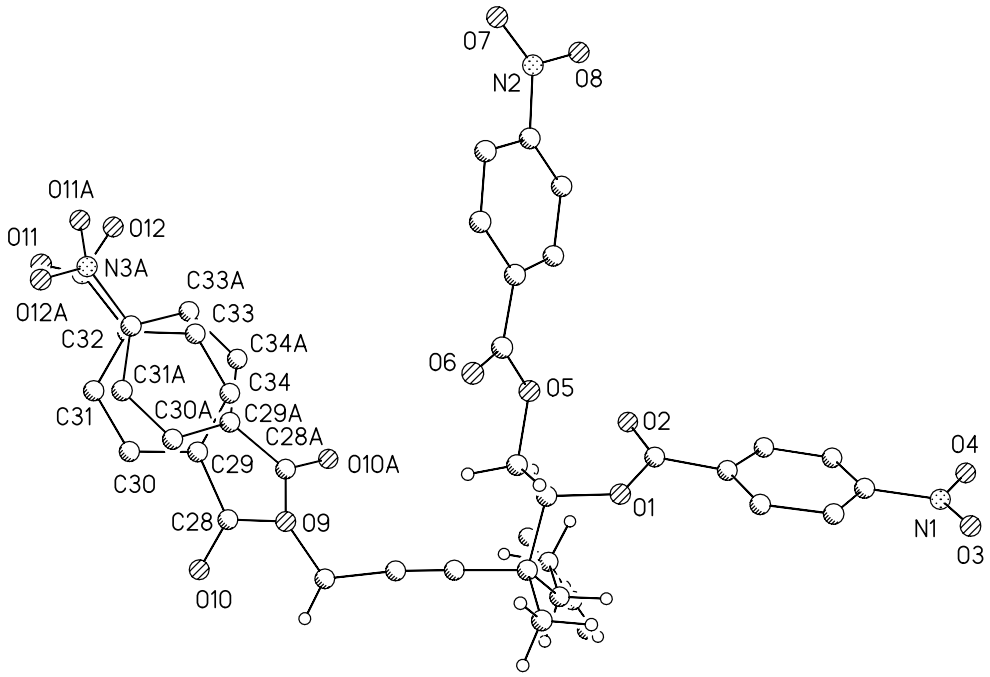

Figure 3. Unit cell packing diagram for **1**. The view is approximately down the **a** axis.