Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Catalytic Enantioselective Bromohydroxylation of Aryl Olefins with Flexible Functionalities

Jing Li,[a,b] Zequan Li,[a,b] Xun Zhang,[a,b] Bing Xu,[a,b] and Yian Shi*[,a,c,d]

[a]Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China.
[b]University of Academy of Sciences, Beijing 100049, P. R. China.
[c]State Key Laboratory of Coordination Chemistry, Center for Multimolecular Organic Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, P. R. China.
[d]Department of Chemistry, Colorado State University, Fort Collins, Colorado 80523, USA.

Supporting Information

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General Methods. All commercially available reagents were used without further purification unless otherwise noted. All dry solvents were freshly distilled under nitrogen from appropriate drying agents before use. Tetrahydrofuran and ethyl ether were distilled from sodium-benzophenone. Acetone AR was used directly. Column chromatography was performed on silica gel (200-300 mesh). ^{1}H NMR spectra were recorded on a 400 MHz NMR spectrometer and ^{13}C NMR spectra were recorded on a 100 MHz NMR spectrometer. IR spectra were recorded on a FT-IR spectrometer. Melting points were uncorrected. 2-Aryl allylic alcohols were prepared by reacting the corresponding aryl Grignard regents with propargyl alcohol in the presence of CuI according to the reported procedures.[1] Homoallylic alcohol **1l** was prepared by reacting 4-chloro-α-methylstyrene with paraformaldehyde and $Sc(OTf)_3$ according to the reported procedure.[2] Olefin **5a** was prepared from the corresponding alcohol (**1a**) via deprotonation with NaH and subsequent alkylation with MeI according to the reported procedures.[3] Olefin **5b** was prepared from the corresponding alcohol (**1a**) with Et_3N and AcCl in DCM at rt. Olefin **5c** was prepared by reacting the corresponding alcohol (**1a**) with pyridine and ClCOOEt.[4] Olefin **5d** was prepared by reacting the corresponding allylic bromide[5] with LiCl.[6] Allylic fluorides **5e-g** and allylic azides **5h-l** were prepared by reacting the corresponding allylic bromide[1,5] with TBAF[7] or NaN_3[1,8] according to the reported procedures. Olefins **7a, 7b**, **7d-h**, **7p-t**, **7v**, **7x,** and **7y** were purchased from commercial suppliers. Olefins **7c**, **7i-o**, and **7u** were prepared from the corresponding aldehydes or ketones by wittig reaction.[9,10] Olefin **7w** was prepared from 7-bromo-1-tetralone according to the reported procedures.[11-14]

1) Y. Kawato, A. Kubota, H. Ono, H. Egami and Y. Hamashima, *Org. Lett.* 2015, **17**, 1244.
2) S. Sultana, S. Bondalapati, K. Indukuri, P. Gogoi, P. Saha and A. K. Saikia, *Tetrahedron Lett.* 2013, **54**, 1576.
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5) C. B. Tripathi and S. Mukherjee, *Angew. Chem., Int. Ed.* 2013, **52**, 8450.
6) D. Huang, X. Liu, L. Li, Y. Cai, W. Liu and Y. Shi, *J. Am. Chem. Soc.* 2013, **135**, 8101.
7) D. P. Cox, J. Terpinski and W. Lawrynowicz, *J. Org. Chem.* 1984, **49**, 3216.

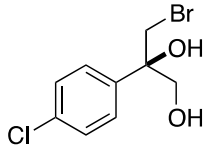
8) A. Garzan, A. Jaganathan, N. S. Marzijarani, R. Yousefi, D. C. Whitehead, J. E. Jackson and B. Borhan, *Chem. Eur. J.* 2013, **19**, 9015.
9) T. Okamoto, K. Kobayashi, S. Oka and S. Taninoto, *J. Org. Chem.* 1988, **53**, 4897.
10) X.-L. Qiu, J. Zhu, G. Wu, W.-H. Lee and A. R. Chamberlin, *J. Org. Chem.* 2009, **74**, 2018.
11) L. Li, C. Su, X. Liu, H. Tian and Y. Shi, *Org. Lett.* 2014, **16**, 3728.
12) M. F. Gross, N. A. Castle, A. Zou, A. D. Wickenden, W. Yu and K. L. Spear, *Bioorg. Med. Chem. Lett.* 2009, **19**, 3063.
13) Y. Yu, S. K. Singh, A. Liu, T.-K. Li, L. F. Liu and E. J. LaVoie, *Bioorg. Med. Chem.* 2003, **11**, 1475.
14) F. Portela-Cubillo, J. S. Scott and J. C. Walton, *J. Org. Chem.* 2008, **73**, 5558.

Representative procedure for asymmetric bromohydroxylation of allylic alcohol (Table 2, entry 1). A mixture of $(DHQD)_2PHAL$ (0.0389 g, 0.050 mmol), (+)-CSA (0.0116 g, 0.050 mmol), and *N*-bromobenzamide[1] (0.120 g, 0.60 mmol) in acetone (5.0 mL) and water (0.5 mL) was stirred at -50 ^oC for 15 min. Allylic alcohol (**1a**) (0.0843 g, 0.50 mmol) was subsequently added. Upon stirring at -50 ^oC for 72 h, the reaction mixture was quenched with saturated aqueous $Na_2S_2O_3$ (10 mL) at -50 ^oC, extracted with EtOAc (3×10 mL), dried over $MgSO_4$, filtered, concentrated, and purified by flash chromatography (silica gel, eluent: petroleum ether/ethyl acetate = 2:1) to afford bromohydrin **2a** as colorless oil (0.1102 g, 83% yield, 96% ee).

1) S. Fujisaki, S. Hamura, H. Eguchi and A. Nishida, *Bull. Chem. Soc. Jpn*. 1993, **66**, 2426.

Representative procedure for asymmetric bromohydroxylation of styrene (Table 4, entry 1). A mixture of $(DHQD)_2PHAL$ (0.0389 g, 0.050 mmol), (-)-CSA (0.0116 g, 0.050 mmol), and *N*-bromobenzamide (0.120 g, 0.60 mmol) in acetone (5.0 mL) and water (0.25 mL) was stirred at -40 ^oC for 15 min. 2-Methylstyrene (**7a**) (0.0591 g, 0.50 mmol) was subsequently added. The reaction mixture was stirred at -40 ^oC for 72 h, quenched with saturated aqueous $Na_2S_2O_3$ (10 mL) at -40 ^oC, extracted with DCM (3×10 mL), dried over $MgSO_4$, filtered, concentrated, and purified by flash chromatography (silica gel, eluent: petroleum ether/ethyl acetate = 15:1) to afford bromohydrin **8a** as pale yellow oil (0.0891 g, 83% yield, 90% ee).

Table 2, entry 1



2a

Colorless oil; $[\alpha]_D^{20}$ = +11.9 (*c* 1.1, $CHCl_3$) (96% ee); IR (film) 3465, 1492, 1074, 818 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.42-7.34 (m, 4H), 3.90 (d, *J* = 10.8 Hz, 1H), 3.86-3.81 (m, 2H), 3.78 (d, *J* = 10.8 Hz, 1H), 3.02 (br s, 1H), 2.17 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 134.3, 129.0, 127.2, 75.8, 68.4, 41.0; HRMS Calcd for $C_9H_{10}BrClNaO_2$ (M+Na): 286.9445; Found: 286.9446.

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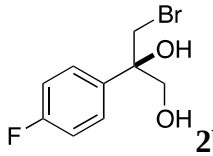
Table 2, entry 2

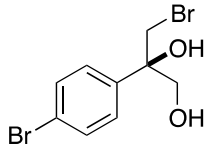


2b

Colorless oil; $[\alpha]_D^{20}$ = +11.6 (*c* 1.1, $CHCl_3$) (91% ee); IR (film) 3433, 1510, 1075, 835 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.47-7.40 (m, 2H), 7.11-7.04 (m, 2H), 3.90 (d, *J* = 10.8 Hz, 1H), 3.85-3.81 (m, 2H), 3.79 (d, *J* = 10.8 Hz, 1H), 3.05 (br s, 1H), 2.23 (t, *J* = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 161.4, 136.98, 136.95, 127.6, 127.5, 115.8, 115.6, 75.8, 68.4, 41.2; HRMS Calcd for $C_9H_{10}BrFNaO_2$ (M+Na): 270.9740; Found: 270.9741.

Y. Zhang, H. Xing, W. Xie, X. Wan, Y. Lai and D. Ma, *Adv. Synth. Catal.* 2013, **355**, 68.

Table 2, entry 3



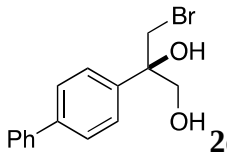
2c

Colorless oil; $[\alpha]_D^{20}$ = +12.4 (*c* 0.97, $CHCl_3$) (96% ee); IR (film) 3465, 1078, 818 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 9.2 Hz, 2H), 7.34 (d, *J* = 9.2 Hz, 2H), 3.91 (d, *J* = 10.8 Hz, 1H), 3.86-3.81 (m, 2H), 3.79 (d, *J* = 10.8 Hz, 1H), 2.97 (br s, 1H), 2.06 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 131.9, 127.5, 122.4, 75.9, 68.3, 40.9;

HRMS Calcd for $C_9H_{10}Br_2NaO_2$ (M+Na): 330.8940; Found: 330.8942.

Y. Zhang, H. Xing, W. Xie, X. Wan, Y. Lai and D. Ma, *Adv. Synth. Catal.* 2013, **355**, 68.

Table 2, entry 4



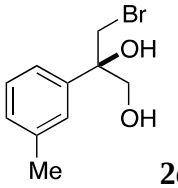
2d

(X-ray structure)

White solid; mp. 111-113 ^oC; $[\alpha]_D^{20}$ = +17.8 (*c* 0.93, $CHCl_3$) (93% ee); IR (film) 3366, 1076, 761 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.65-7.57 (m, 4H), 7.56-7.50 (m, 2H), 7.48-7.42 (m, 2H), 7.39-7.33 (m, 1H), 3.97 (d, *J* = 10.8 Hz, 1H), 3.95-3.87 (m, 2H), 3.87 (d, *J* = 10.8 Hz, 1H), 3.03 (br s, 1H), 2.13 (dd, *J* = 7.2, 5.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.2, 140.6, 140.1, 129.0, 127.7, 127.5, 127.3, 126.2, 76.0, 68.6, 41.3; HRMS Calcd for $C_{15}H_{15}BrNaO_2$ (M+Na): 329.0148; Found: 329.0147.

Y. Zhang, H. Xing, W. Xie, X. Wan, Y. Lai and D. Ma, *Adv. Synth. Catal.* 2013, **355**, 68.

Table 2, entry 5

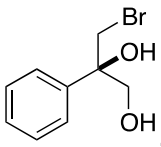


2e

Colorless oil; $[\alpha]_D^{20}$ = +12.8 (*c* 0.97, $CHCl_3$) (90% ee); IR (film) 3433, 1075, 707 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.31-7.26 (m, 2H), 7.25-7.21 (m, 1H), 7.17-7.12 (m, 1H), 3.94 (d, *J* = 10.8 Hz, 1H), 3.91-3.84 (m, 2H), 3.82 (d, *J* = 10.8 Hz, 1H), 2.93 (br s, 1H), 2.38 (s, 3H), 2.01-1.92 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 138.5, 129.0, 128.7, 126.3, 122.7, 76.1, 68.6, 41.4, 21.8; HRMS Calcd for $C_{10}H_{13}BrNaO_2$ (M+Na): 266.9991; Found: 266.9991.

Y. Zhang, H. Xing, W. Xie, X. Wan, Y. Lai and D. Ma, *Adv. Synth. Catal.* 2013, **355**, 68.

Table 2, entry 6



2f

Colorless oil; $[\alpha]_D^{20}$ = +11.2 (*c* 0.95, $CHCl_3$) (77% ee); IR (film) 3398, 1448, 1075, 700 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.48-7.43 (m, 2H), 7.43-7.37 (m, 2H), 7.36-7.30 (m, 1H), 3.94 (d, *J* = 10.8 Hz, 1H), 3.91-3.83 (m, 2H), 3.83 (d, *J* = 10.8 Hz, 1H), 3.02 (br s, 1H), 2.18-2.10 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 128.8, 128.2, 125.7, 76.1, 68.5, 41.3; HRMS Calcd for $C_9H_{11}BrNaO_2$ (M+Na): 252.9835; Found: 252.9835.

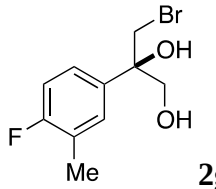
1) W. Adam and M. Heil, *J. Am. Chem. Soc.* 1992, **114**, 5591.

2) W. Adam, R. Stössel, A. Treiber, *J. Org. Chem.* 1995, **60**, 2879.

3) S.-T. Chen and J.-M. Fang, *J. Org. Chem.* 1997, **62**, 4349.

4) Y. Zhang, H. Xing, W. Xie, X. Wan, Y. Lai and D. Ma, *Adv. Synth. Catal.* 2013, **355**, 68.

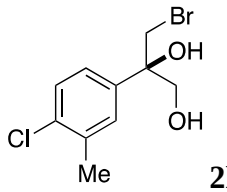
Table 2, entry 7



2g

Colorless oil; $[\alpha]_D^{20}$ = +11.3 (*c* 0.91, $CHCl_3$) (93% ee); IR (film) 3398, 1508, 1076, 818 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.30-7.25 (m, 1H), 7.25-7.19 (m, 1H), 7.01 (t, *J* = 9.2 Hz, 1H), 3.90 (d, *J* = 10.8 Hz, 1H), 3.88-3.81 (m, 2H), 3.78 (d, *J* = 10.8 Hz, 1H), 3.00 (br s, 1H), 2.29 (d, *J* = 1.6 Hz, 3H), 2.17 (t, *J* = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.4, 159.9, 136.6, 136.5, 129.0, 128.9, 125.3, 125.2, 124.75, 124.67, 115.4, 115.1, 75.7, 68.5, 41.3, 14.99, 14.96; HRMS Calcd for $C_{10}H_{12}BrFNaO_2$ (M+Na): 284.9897; Found: 284.9899.

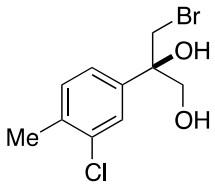
Table 2, entry 8



2h

Colorless oil; $[\alpha]_D^{20}$ = +12.3 (*c* 0.95, $CHCl_3$) (96% ee); IR (film) 3398, 1076, 821 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.4 Hz, 1H), 7.32 (d, *J* =2.0 Hz, 1H), 7.19 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.89 (d, *J* = 10.8 Hz, 1H), 3.86-3.80 (m, 2H), 3.77 (d, *J* = 10.8 Hz, 1H), 3.05 (br s, 1H), 2.39 (s, 3H), 2.25 (t, *J* = 6.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 136.5, 134.4, 129.4, 128.3, 124.5, 75.8, 68.4, 41.1, 20.5; HRMS Calcd for $C_{10}H_{12}BrClNaO_2$ (M+Na): 300.9601; Found: 300.9602.

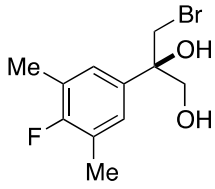
Table 2, entry 9



2i

Colorless oil; $[\alpha]_D^{20}$ = +11.2 (*c* 0.92, $CHCl_3$) (94% ee); IR (film) 3398, 1076, 824 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 2.0 Hz, 1H), 7.26 (d, *J* =8.0 Hz, 1H), 7.20 (dd, *J* = 8.0, 1.6 Hz, 1H), 3.88 (d, *J* = 10.8 Hz, 1H), 3.85-3.79 (m, 2H), 3.76 (d, *J* = 10.8 Hz, 1H), 3.10 (br s, 1H), 2.37 (s, 3H), 2.35-2.30 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 136.1, 135.0, 131.2, 126.6, 123.9, 75.8, 68.4, 41.0, 19.9; HRMS Calcd for $C_{10}H_{12}BrClNaO_2$ (M+Na): 300.9601; Found: 300.9601.

Table 2, entry 10



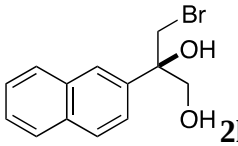
2j

(X-ray structure)

White solid; mp. 90-92 °C; $[\alpha]_D^{20}$ = +11.3 (*c* 0.97, $CHCl_3$) (83% ee); IR (film) 3433, 1491, 1076, 726 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 6.8 Hz, 2H), 3.90 (d, *J* = 10.8 Hz, 1H), 3.88-3.78 (m, 2H), 3.78 (d, *J* = 10.8 Hz, 1H), 2.89 (br s, 1H), 2.27 (d, *J* =

2.0 Hz, 6H), 1.95 (dd, *J* = 7.6, 5.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 158.5, 135.9, 135.8, 126.22, 126.17, 124.9, 124.7, 75.7, 68.5, 41.4, 15.1, 15.0; HRMS Calcd for $C_{11}H_{14}BrFNaO_2$ (M+Na): 299.0053; Found: 299.0052.

Table 2, entry 11



2k

Colorless oil; $[\alpha]_D^{20}$ = +11.5 (*c* 0.99, $CHCl_3$) (90% ee); IR (film) 3433, 1508, 1075, 752 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 1.6 Hz, 1H), 7.91-7.82 (m, 3H), 7.55-7.47 (m, 3H), 4.03 (d, *J* = 10.8 Hz, 1H), 4.01-3.91 (m, 2H), 3.95 (d, *J* = 10.8 Hz, 1H), 3.09 (br s, 1H), 2.10-2.00 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 133.3, 133.1, 128.7, 128.5, 127.8, 126.7, 126.6, 125.3, 123.2, 76.3, 68.6, 41.3; HRMS Calcd for $C_{13}H_{13}BrNaO_2$ (M+Na): 302.9991; Found: 302.9992.

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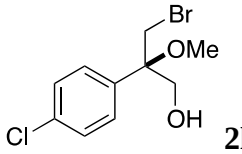
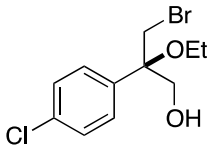
Table 2, entry 12



2l

Colorless oil; $[\alpha]_D^{20}$ = +8.7 (*c* 1.1, $CHCl_3$) (90% ee); IR (film) 3466, 1491, 1090, 827 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.31 (m, 4H), 4.00 (dd, *J* = 11.6, 5.2 Hz, 1H), 3.95 (dd, *J* = 11.6, 6.0 Hz, 1H), 3.86 (d, *J* = 11.2 Hz, 1H), 3.77 (d, *J* = 10.8 Hz, 1H), 3.19 (s, 3H), 1.80 (t, *J* = 6.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.4, 134.4, 129.0, 128.5, 79.9, 65.2, 51.2, 35.3; HRMS Calcd for $C_{10}H_{12}BrClNaO_2$ (M+Na): 300.9601; Found: 300.9600.

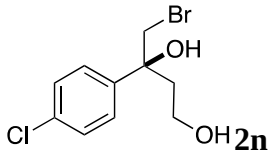
Table 2, entry 13



2m

Colorless oil; $[\alpha]_D^{20}$ = +7.6 (*c* 0.95, $CHCl_3$) (91% ee); IR (film) 3449, 1491, 1076, 831 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.41-7.31 (m, 4H), 3.99 (dd, *J* = 11.2, 5.6 Hz, 1H), 3.94 (dd, *J* = 11.2, 6.4 Hz, 1H), 3.86 (d, *J* = 10.8 Hz, 1H), 3.79 (d, *J* = 10.8 Hz, 1H), 3.43-3.34 (m, 1H), 3.33-3.24 (m, 1H), 1.75 (t, *J* = 6.4 Hz, 1H), 1.21 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 134.3, 129.0, 128.4, 79.7, 65.5, 58.9, 35.7, 15.7; HRMS Calcd for $C_{11}H_{14}BrClNaO_2$ (M+Na): 314.9758; Found: 314.9757.

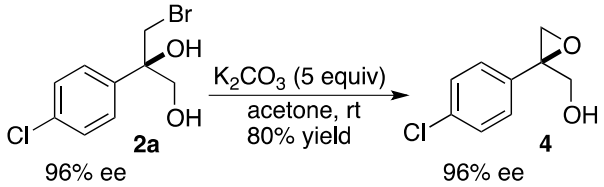
Table 2, entry 14



2n

Colorless oil; $[\alpha]_D^{20}$ = +0.22 (*c* 0.90, $CHCl_3$) (86% ee); IR (film) 3366, 1491, 1093, 829 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.41-7.31 (m, 4H), 3.84 (br s, 1H), 3.79-3.67 (m, 3H), 3.65-3.55 (m, 1H), 2.39 (ddd, *J* = 14.4, 9.6, 4.4 Hz, 1H), 2.13-2.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 133.7, 128.8, 127.2, 76.5, 59.9, 44.7, 40.7; HRMS Calcd for $C_{10}H_{16}BrClNO_2$ (M+NH_4): 296.0047; Found: 296.0049.

Determination of the absolute configuration of bromohydrin 2a (Scheme 3)

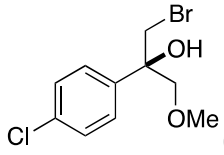


To a mixture of **2a** (0.0648 g, 0.24 mmol) in acetone (2 mL) was added K_2CO_3 (0.1659 g, 1.2 mmol). Upon stirring at rt overnight, the reaction mixture was filtered through a silica gel plug and concentrated to give epoxide **4** as colorless oil (0.0359 g, 80% yield, 96% ee). $[\alpha]_D^{20}$ = +19.8 (*c* 1.0, $CHCl_3$) (96% ee) {lit.[1] $[\alpha]_D^{20}$ = +26 (*c* 0.92, $CHCl_3$) for (*R*)-**4**}; IR (film) 3423, 1495, 1014, 827 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36-7.29

(m, 4H), 4.08 (dd, *J* = 12.4, 4.4 Hz, 1H), 3.97 (dd, *J* = 12.4, 8.4 Hz, 1H), 3.26 (d, *J* = 5.2 Hz, 1H), 2.79 (d, *J* = 5.2 Hz, 1H), 1.95 (dd, *J* = 8.8, 4.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.1, 134.2, 128.9, 127.6, 63.3, 60.1, 52.9. HRMS (EI) Calcd for $C_9H_9O_2Cl$ (M): 184.0291; Found: 184.0293.

R. H. Prager, K. Schafer, D. P. G. Hamon and R. A. Massy-Westropp, *Tetrahedron* 1995, **51**, 11465.

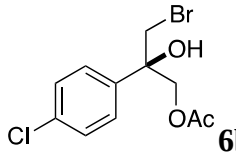
Table 3, entry 1



6a

Yellow oil; $[\alpha]_D^{20}$ = +23.9 (*c* 1.2, $CHCl_3$) (98% ee); IR (film) 3464, 1491, 1092, 834 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 9.2 Hz, 2H), 7.34 (d, *J* = 9.2 Hz, 2H), 3.78 (d, *J* = 10.8 Hz, 1H), 3.70 (d, *J* = 10.8 Hz, 1H), 3.69 (d, *J* = 9.6 Hz, 1H), 3.65 (d, *J* = 9.6 Hz, 1H), 3.40 (s, 3H), 2.99 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 134.0, 128.7, 127.3, 77.4, 74.7, 59.7, 40.7; HRMS Calcd for $C_{10}H_{12}BrClNaO_2$ (M+Na): 300.9601; Found: 300.9600.

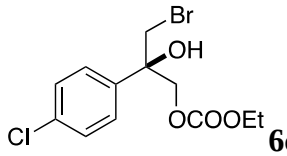
Table 3, entry 2



6b

Colorless oil; $[\alpha]_D^{20}$ = +13.7 (*c* 1.2, $CHCl_3$) (63% ee); IR (film) 3467, 1736, 1491, 1234, 829 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.8 Hz, 2H), 4.42 (d, *J* = 11.6 Hz, 1H), 4.38 (d, *J* = 11.6 Hz, 1H), 3.79 (d, *J* = 10.8 Hz, 1H), 3.73 (d, *J* = 10.8 Hz, 1H), 2.98 (br s, 1H), 2.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 139.1, 134.4, 128.9, 127.3, 74.5, 68.8, 40.5, 21.0; HRMS Calcd for $C_{11}H_{12}BrClNaO_3$ (M+Na): 328.9551; Found: 328.9550.

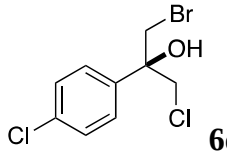
Table 3, entry 3



6c

Colorless oil; $[\alpha]_D^{20}$ = +19.4 (*c* 1.0, $CHCl_3$) (83% ee); IR (film) 3483, 1745, 1492, 1260, 830 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 4.43 (s, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.82 (d, *J* = 10.8 Hz, 1H), 3.74 (d, *J* = 10.8 Hz, 1H), 3.01 (br s, 1H), 1.28 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 138.8, 134.5, 128.9, 127.3, 74.4, 71.5, 64.8, 40.2, 14.3; HRMS Calcd for $C_{12}H_{14}BrClNaO_4$ (M+Na): 358.9656; Found: 358.9658.

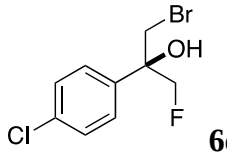
Table 3, entry 4



6d

Colorless oil; $[\alpha]_D^{20}$ = +11.2 (*c* 0.79, $CHCl_3$) (87% ee); IR (film) 3538, 1490, 1093, 829 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.47-7.41 (m, 2H), 7.41-7.35 (m, 2H), 3.95 (d, *J* = 11.6 Hz, 1H), 3.91 (d, *J* = 11.6 Hz, 1H), 3.86 (d, *J* = 10.8 Hz, 1H), 3.78 (d, *J* = 10.8 Hz, 1H), 2.89 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.9, 134.7, 129.0, 127.4, 74.9, 51.2, 40.4; HRMS (EI) Calcd for $C_9H_9BrCl_2O$ (M): 281.9214; Found: 281.9217.

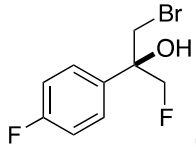
Table 3, entry 5



6e

Colorless oil; $[\alpha]_D^{20}$ = +36.4 (*c* 0.88, $CHCl_3$) (90% ee); IR (film) 3464, 1492, 1094, 829 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 4.64 (dd, *J* = 38.4, 9.2 Hz, 1H), 4.52 (dd, *J* = 38.4, 9.6 Hz, 1H), 3.90 (dd, *J* = 11.2, 1.2 Hz, 1H), 3.76 (dd, *J* = 11.2, 2.0 Hz, 1H), 2.79 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 134.7, 129.0, 127.3, 87.1, 85.3, 74.3, 74.1, 39.83, 39.80; HRMS (EI) Calcd for $C_9H_9BrClFO$ (M): 265.9509; Found: 265.9512.

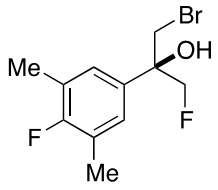
Table 3, entry 6



6f

Colorless oil; $[\alpha]_D^{20}$ = +27.0 (*c* 0.67, $CHCl_3$) (85% ee); IR (film) 3547, 1510, 1231, 836 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.53-7.44 (m, 2H), 7.13-7.04 (m, 2H), 4.65 (dd, *J* = 38.4, 9.6 Hz, 1H), 4.53 (dd, *J* = 38.0, 9.6 Hz, 1H), 3.90 (dd, *J* = 10.8, 1.2 Hz, 1H), 3.77 (dd, *J* = 11.2, 2.0 Hz, 1H), 2.79 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 161.6, 135.5, 127.8, 127.75, 127.66, 115.8, 115.6, 87.2, 85.4, 74.3, 74.1, 40.1, 40.0; HRMS (EI) Calcd for $C_9H_9BrF_2O$ (M): 249.9805; Found: 249.9807.

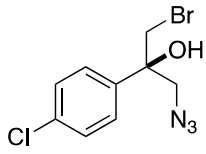
Table 3, entry 7



6g

Colorless oil; $[\alpha]_D^{20}$ = +35.0 (*c* 1.3, $CHCl_3$) (91% ee); IR (film) 3547, 1490, 1015, 727 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.13 (d, *J* = 6.8 Hz, 2H), 4.63 (dd, *J* = 32.0, 9.6 Hz, 1H), 4.52 (dd, *J* = 31.6, 9.2 Hz, 1H), 3.89 (dd, *J* = 10.8, 0.8 Hz, 1H), 3.76 (dd, *J* = 11.2, 2.0 Hz, 1H), 2.76 (br s, 1H), 2.28 (d, *J* = 1.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 158.7, 134.4, 126.4, 126.35, 126.30, 125.0, 124.8, 87.3, 85.6, 74.3, 74.1, 40.2, 40.1, 15.1, 15.0; HRMS (EI) Calcd for $C_{11}H_{13}BrF_2O$ (M): 278.0118; Found: 278.0116.

Table 3, entry 8

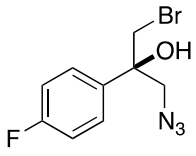


6h

Colorless oil; $[\alpha]_D^{20}$ = -22.7 (*c* 0.96, $CHCl_3$) (92% ee); IR (film) 3538, 2106, 1491, 1093, 772 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.44-7.35 (m, 4H), 3.85 (d, *J* = 10.8 Hz, 1H), 3.75 (d, *J* = 11.2 Hz, 1H), 3.70 (d, *J* = 12.8 Hz, 1H), 3.60 (d, *J* = 12.4 Hz, 1H), 2.87

(br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 134.5, 129.0, 127.1, 75.6, 58.7, 41.1; HRMS Calcd for $C_9H_9BrClN_3NaO$ (M+Na): 311.9510; Found: 311.9512.

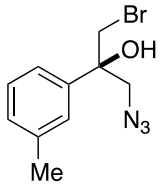
Table 3, entry 9



6i

Colorless oil; $[\alpha]_D^{20}$ = -13.1 (*c* 0.94, $CHCl_3$) (87% ee); IR (film) 3539, 2108, 1510, 1232, 836 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.40 (m, 2H), 7.13-7.05 (m, 2H), 3.86 (d, *J* = 10.8 Hz, 1H), 3.76 (d, *J* = 10.8 Hz, 1H), 3.71 (d, *J* = 12.8 Hz, 1H), 3.61 (d, *J* = 12.4 Hz, 1H), 2.83 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 161.5, 136.60, 136.57, 127.6, 127.5, 115.9, 115.7, 75.5, 58.9, 41.3; HRMS Calcd for $C_9H_9BrFN_3NaO$ (M+Na): 295.9805; Found: 295.9806.

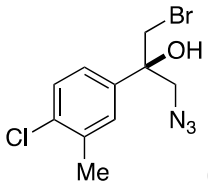
Table 3, entry 10



6j

Colorless oil; $[\alpha]_D^{20}$ = -16.9 (*c* 1.1, $CHCl_3$) (84% ee); IR (film) 3538, 2105, 1489, 1297, 706 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.27 (m, 2H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.17 (d, *J* = 7.6 Hz, 1H), 3.88 (d, *J* = 10.8 Hz, 1H), 3.78 (d, *J* = 10.8 Hz, 1H), 3.73 (d, *J* = 12.4 Hz, 1H), 3.62 (d, *J* = 12.8 Hz, 1H), 2.81 (br s, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.7, 138.6, 129.3, 128.7, 126.2, 122.5, 75.8, 58.9, 41.5, 21.8; HRMS Calcd for $C_{10}H_{12}BrN_3NaO$ (M+Na): 292.0056; Found: 292.0056.

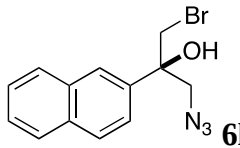
Table 3, entry 11



6k

Colorless oil; $[\alpha]_D^{20}$ = -29.3 (*c* 1.2, $CHCl_3$) (94% ee); IR (film) 3539, 2106, 1484, 1048, 827 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 2.0 Hz, 1H), 7.20 (dd, *J* = 8.0, 2.0 Hz, 1H), 3.85 (d, *J* = 10.8 Hz, 1H), 3.74 (d, *J* = 10.8 Hz, 1H), 3.69 (d, *J* = 12.4 Hz, 1H), 3.60 (d, *J* = 12.4 Hz, 1H), 2.86 (br s, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 136.6, 134.6, 129.4, 128.2, 124.3, 75.5, 58.8, 41.2, 20.5; HRMS Calcd for $C_{10}H_{11}BrClN_3NaO$ (M+Na): 325.9666; Found: 325.9669.

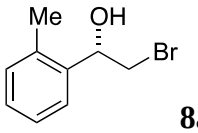
Table 3, entry 12



6l

Colorless oil; $[\alpha]_D^{20}$ = -38.9 (*c* 1.1, $CHCl_3$) (96% ee); IR (film) 3538, 2106, 1508, 1290, 750 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 1.6 Hz, 1H), 7.92-7.82 (m, 3H), 7.56-7.47 (m, 3H), 3.99 (d, *J* = 10.8 Hz, 1H), 3.90 (d, *J* = 10.8 Hz, 1H), 3.83 (d, *J* = 12.4 Hz, 1H), 3.72 (d, *J* = 12.8 Hz, 1H), 2.93 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 133.2, 133.1, 128.7, 128.5, 127.8, 126.8, 126.7, 125.2, 122.9, 76.1, 58.9, 41.4; HRMS Calcd for $C_{13}H_{12}BrN_3NaO$ (M+Na): 328.0056; Found: 328.0058.

Table 4, entry 1



8a

Pale yellow oil; $[\alpha]_D^{20}$ = +51.3 (*c* 1.07, $CHCl_3$) (90% ee); IR (film) 3388, 1460, 1064 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.55-7.49 (m, 1H), 7.29-7.19 (m, 2H), 7.18-7.14 (m, 1H), 5.14 (dt, *J* = 9.6, 2.8 Hz, 1H), 3.60 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.49 (dd, *J* = 10.8, 9.6 Hz, 1H), 2.58 (d, *J* = 2.8 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 134.9, 130.8, 128.4, 126.7, 125.5, 70.9, 39.2, 19.2.

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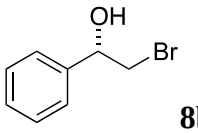
Table 4, entry 2



8b

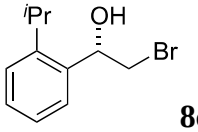
Pale yellow oil; $[\alpha]_D^{20}$ = +40.6 (*c* 0.86, $CHCl_3$) (76% ee) {lit.[1] $[\alpha]_D^{20}$ = +47.9 (c 1.6, $CHCl_3$) for (*S*)-**8b**}; IR (film) 3388, 1453, 1060 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.42-7.31 (m, 5H), 4.92 (dd, *J* = 8.8, 3.2 Hz, 1H), 3.64 (dd, *J* = 10.8, 3.6 Hz, 1H), 3.54 (dd, *J* = 10.4, 9.2 Hz, 1H), 2.76 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5, 128.9, 128.7, 126.2, 74.0, 40.4.

1) S. Wei, R. Messerer and S. B. Tsogoeva, *Chem. Eur. J.* 2011, **17**, 14380.

2) A. K. Macharla, R. C. Nappunni and N. Nama, *Tetrahedron Lett.* 2012, **53**, 1401.

3) X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 3



8c

Pale yellow oil; $[\alpha]_D^{20}$ = +44.4 (*c* 1.10, $CHCl_3$) (89% ee); IR (film) 3387, 1449, 1057 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.6 Hz, 1H), 7.33-7.26 (m, 2H), 7.26-7.18 (m, 1H), 5.25 (dd, *J* = 9.2, 3.2 Hz, 1H), 3.57 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.52 (dd, *J* = 10.4, 9.2 Hz, 1H), 3.14 (septet, *J* = 6.8 Hz, 1H), 2.66 (br s, 1H), 1.27 (d, *J* = 7.2 Hz, 3H), 1.25 (d, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 137.0, 128.8, 126.4, 125.8, 125.7, 70.4, 40.0, 28.6, 24.8, 23.8.

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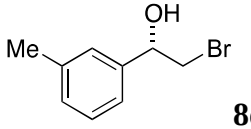
Table 4, entry 4



8d

Pale yellow oil; $[\alpha]_D^{20}$ = +38.3 (*c* 1.05, $CHCl_3$) (82% ee); IR (film) 3397, 1488, 1067 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.25 (t, *J* = 7.6 Hz, 1H), 7.21-7.10 (m, 3H), 4.86 (dd, *J* = 9.2, 3.2 Hz, 1H), 3.61 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.52 (dd, *J* = 10.4, 9.2 Hz, 1H),

2.73 (br s, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 138.6, 129.4, 128.7, 126.8, 123.2, 74.0, 40.4, 21.6.

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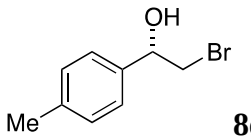
Table 4, entry 5



8e

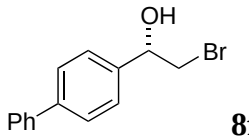
Pale yellow oil; $[\alpha]_D^{20}$ = +37.8 (*c* 0.95, $CHCl_3$) (81% ee) {lit.[1] $[\alpha]_D^{20}$ = +34.7 (c 0.63, $CHCl_3$) for (*S*)-**8e**}; IR (film) 3388, 1438, 1067 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 4.87 (dd, *J* = 8.8, 3.2 Hz, 1H), 3.59 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.52 (dd, *J* = 10.4, 8.8 Hz, 1H), 2.60 (br s, 1H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 137.6, 129.5, 126.1, 73.9, 40.4, 21.4.

1) X.-F. Wu, C. Min, E. Nyamzundui, H.-B. Zhou and C. Dong, *Tetrahedron: Asymmetry* 2011, **22**, 1640.

2) A. K. Macharla, R. C. Nappunni and N. Nama, *Tetrahedron Lett.* 2012, **53**, 1401.

3) X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 6



8f

White solid; mp. 98-100 ^{o}C; $[\alpha]_D^{20}$ = +31.1 (*c* 1.05, $CHCl_3$) (83% ee); IR (film) 3433, 1486, 1073 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.58 (m, 4H), 7.51-7.43 (m, 4H), 7.42-7.36 (m, 1H), 4.98 (dd, *J* = 8.8, 3.2 Hz, 1H), 3.69 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.60 (dd, *J* = 10.4, 9.2 Hz, 1H), 2.71 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 140.7, 139.4, 129.0, 127.7, 127.6, 127.2, 126.6, 73.7, 40.2.

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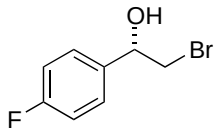
Table 4, entry 7



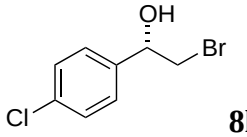
8g

Pale yellow oil; $[\alpha]_D^{20}$ = +39.9 (*c* 0.95, $CHCl_3$) (86% ee); IR (film) 3397, 1510, 1067 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.39-7.31 (m, 2H), 7.10-7.01 (m, 2H), 4.90 (dd, *J* = 8.8, 3.2 Hz, 1H), 3.60 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.50 (dd, *J* = 10.4, 8.8 Hz, 1H), 2.78 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 161.6, 136.29, 136.26, 128.0, 127.9, 115.9, 115.7, 73.3, 40.2.

1) J. Ren, W. Dong, B. Yu, Q. Wu and D. Zhu, *Tetrahedron: Asymmetry* 2012, **23**, 497.

2) X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 8



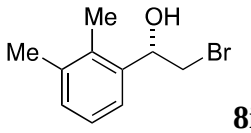
8h

Pale yellow oil; $[\alpha]_D^{20}$ = +38.3 (*c* 0.95, $CHCl_3$) (88% ee); IR (film) 3364, 1492, 1092 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.37-7.29 (m, 4H), 4.90 (dd, *J* = 8.8, 3.6 Hz, 1H), 3.60 (dd, *J* = 10.4, 3.6 Hz, 1H), 3.49 (dd, *J* = 10.4, 8.8 Hz, 1H), 2.75 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.9, 134.4, 129.0, 127.6, 73.3, 40.1.

1) A. K. Macharla, R. C. Nappunni and N. Nama, *Tetrahedron Lett.* 2012, **53**, 1401.

2) X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 9

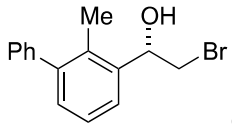


8i

Yellow oil; $[\alpha]_D^{20}$ = +46.8 (*c* 1.01, $CHCl_3$) (88% ee); IR (film) 3364, 1463, 1079 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.44-7.37 (m, 1H), 7.21-7.12 (m, 2H), 5.19 (dt, *J* = 9.6, 2.8 Hz, 1H), 3.60 (dd, *J* = 10.8, 2.8 Hz, 1H), 3.47 (dd, *J* = 10.4, 9.6 Hz, 1H), 2.84 (d, *J* = 2.8 Hz, 1H), 2.32 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 137.3, 133.4,

130.0, 126.1, 123.3, 71.2, 39.3, 20.8, 14.9; HRMS (EI) Calcd for $C_{10}H_{13}BrO$ (M): 228.0150; Found: 228.0151.

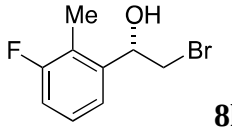
Table 4, entry 10



8j

Yellow oil; $[\alpha]_D^{20}$ = +42.0 (*c* 1.08, $CHCl_3$) (96% ee); IR (film) 3358, 1465, 1062 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.2 Hz, 1H), 7.44-7.15 (m, 7H), 5.21 (dd, *J* = 9.2, 2.0 Hz, 1H), 3.63 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.51 (dd, *J* = 10.4, 9.6 Hz, 1H), 2.77 (br s, 1H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 142.1, 139.1, 132.3, 130.2, 129.5, 128.3, 127.1, 126.2, 124.7, 71.2, 39.4, 16.4; HRMS (EI) Calcd for $C_{15}H_{15}BrO$ (M): 290.0306; Found: 290.0310.

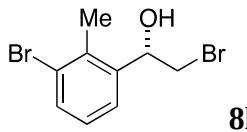
Table 4, entry 11



8k

Colorless oil; $[\alpha]_D^{20}$ = +32.0 (*c* 0.92, $CHCl_3$) (90% ee); IR (film) 3351, 1466, 1083 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 7.6 Hz, 1H), 7.25-7.17 (m, 1H), 6.99 (t, *J* = 8.8 Hz, 1H), 5.12 (dt, *J* = 9.2, 2.8 Hz, 1H), 3.57 (dd, *J* = 10.8, 3.2 Hz, 1H), 3.46 (dd, *J* = 10.4, 9.2 Hz, 1H), 2.75 (d, *J* = 2.8 Hz, 1H), 2.24 (d, *J* = 2.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.5, 160.1, 140.8, 140.7, 127.5, 127.4, 122.4, 122.2, 121.19, 121.16, 115.2, 114.9, 70.8, 70.7, 38.9, 10.4, 10.3; HRMS (EI) Calcd for $C_9H_{10}BrFO$ (M): 231.9899; Found: 231.9896.

Table 4, entry 12

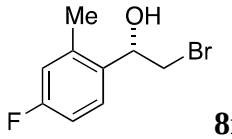


8l

Yellow oil; $[\alpha]_D^{20}$ = +18.8 (*c* 1.07, $CHCl_3$) (93% ee); IR (film) 3375, 1462, 1062 cm^{-1};

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.45 (m, 2H), 7.11 (t, *J* = 8.0 Hz, 1H), 5.18 (dd, *J* = 9.2, 2.0 Hz, 1H), 3.59 (dd, *J* = 10.8, 2.8 Hz, 1H), 3.43 (t, *J* = 10.0 Hz, 1H), 2.64 (br s, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.5, 134.5, 132.7, 127.7, 126.5, 124.9, 71.5, 38.9, 18.9; HRMS (EI) Calcd for $C_9H_{10}Br_2O$ (M): 291.9098; Found: 291.9095.

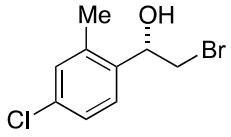
Table 4, entry 13



8m

Yellow oil; $[\alpha]_D^{20}$ = +42.5 (*c* 1.22, $CHCl_3$) (95% ee); IR (film) 3365, 1496, 1066 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 8.4, 6.0 Hz, 1H), 6.92 (td, *J* = 8.4, 2.8 Hz, 1H), 6.88 (dd, *J* = 9.6, 2.4 Hz, 1H), 5.07 (dt, *J* = 9.2, 2.8 Hz, 1H), 3.54 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.44 (dd, *J* = 10.4, 9.6 Hz, 1H), 2.81 (d, *J* = 2.8 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 161.2, 137.43, 137.35, 134.31, 134.28, 127.5, 127.4, 117.5, 117.3, 113.5, 113.3, 70.4, 39.1, 19.2; HRMS (EI) Calcd for $C_9H_{10}BrFO$ (M): 231.9899; Found: 231.9901.

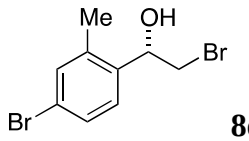
Table 4, entry 14



8n

Yellow oil; $[\alpha]_D^{20}$ = +37.1 (*c* 1.12, $CHCl_3$) (98% ee); IR (film) 3386, 1483, 1064 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.4 Hz, 1H), 7.20 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.14 (s, 1H), 5.06 (dd, *J* = 9.2, 2.8 Hz, 1H), 3.53 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.42 (dd, *J* = 10.4, 9.6 Hz, 1H), 2.85 (br s, 1H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.0, 136.7, 133.9, 130.5, 127.1, 126.7, 70.4, 38.8, 19.0; HRMS (EI) Calcd for $C_9H_{10}BrClO$ (M): 247.9604; Found: 247.9606.

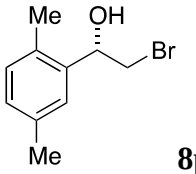
Table 4, entry 15



8o

White solid; mp. 64-66 °C; $[\alpha]_D^{20}$ = +37.3 (*c* 1.17, $CHCl_3$) (98% ee); IR (film) 3366, 1480, 1066 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.45-7.33 (m, 2H), 7.33-7.27 (m, 1H), 5.04 (dt, *J* = 9.2, 3.2 Hz, 1H), 3.53 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.42 (dd, *J* = 10.4, 9.2 Hz, 1H), 2.83 (d, *J* = 3.2 Hz, 1H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 137.0, 133.5, 129.7, 127.4, 122.2, 70.4, 38.7, 19.0; HRMS (EI) Calcd for $C_9H_{10}Br_2O$ (M): 291.9098; Found: 291.9096.

Table 4, entry 16



8p

White solid; mp. 79-81 °C; $[\alpha]_D^{20}$ = +46.7 (*c* 0.98, $CHCl_3$) (94% ee); IR (film) 3347 1499, 1065 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.34 (s, 1H), 7.08-7.01 (m, 2H), 5.11 (dd, *J* = 9.6, 2.8 Hz, 1H), 3.58 (dd, *J* = 10.8, 2.8 Hz, 1H), 3.48 (dd, *J* = 10.4, 9.6 Hz, 1H), 2.66 (br s, 1H), 2.34 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 136.2, 131.7, 130.7, 129.1, 126.1, 71.0, 39.4, 21.3, 18.8.

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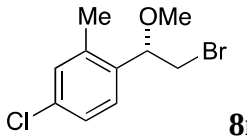
Table 4, entry 17

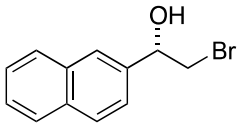


8n'

Colorless oil; $[\alpha]_D^{20}$ = +66.8 (*c* 0.95, $CHCl_3$) (97% ee); IR (film) 1481, 1119, 1103 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.0 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 7.17 (s, 1H), 4.60 (dd, *J* = 8.0, 4.0 Hz, 1H), 3.45 (dd, *J* = 10.8, 8.4 Hz, 1H), 3.40 (dd, *J* = 10.8, 4.4 Hz, 1H), 3.29 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 135.8, 133.9, 130.7, 127.6, 126.8, 79.8, 57.4, 35.1, 19.1; HRMS (EI) Calcd for

$C_{10}H_{12}BrClO$ (M): 261.9760; Found: 261.9763.

Table 4, entry 18



8q

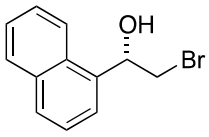
White solid; mp. 80-82 °C; $[\alpha]_D^{20}$ = +36.6 (*c* 1.01, $CHCl_3$) (72% ee), $[\alpha]_D^{20}$ = +17.6 (*c* 1.01, EtOH) (72% ee) {lit.[1] $[\alpha]_D^{20}$ = -22.3 (c 1.0, EtOH) for (*R*)-**8q**}; IR (film) 3396, 1067 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.89-7.81 (m, 4H), 7.55-7.43 (m, 3H), 5.09 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.72 (dd, *J* = 10.4, 3.2 Hz, 1H), 3.63 (dd, *J* = 10.4, 8.8 Hz, 1H), 2.73 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 133.5, 133.4, 128.7, 128.2, 127.9, 126.6, 126.5, 125.4, 123.8, 74.1, 40.2.

1) S. Wei, R. Messerer and S. B. Tsogoeva, *Chem. Eur. J.* 2011, **17**, 14380.

2) Y. Wang, J. Wang, Y. Xiong and Z. Liu, *Tetrahedron Lett.* 2014, **55**, 2734.

3) X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 19

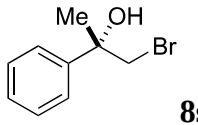


8r

Pale yellow oil; $[\alpha]_D^{20}$ = +31.8 (*c* 1.02, $CHCl_3$) (74% ee); IR (film) 3386, 1420, 1079 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 7.2 Hz, 1H), 7.59-7.47 (m, 3H), 5.70 (dd, *J* = 9.2, 2.0 Hz, 1H), 3.84 (dd, *J* = 10.4, 2.8 Hz, 1H), 3.63 (t, *J* = 10.0 Hz, 1H), 2.91 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 133.9, 130.3, 129.3, 129.1, 126.8, 126.0, 125.7, 123.7, 122.5, 71.3, 39.9.

X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 20



8s

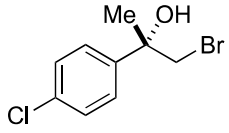
Pale yellow oil; $[\alpha]_D^{20}$ = +21.9 (*c* 0.98, $CHCl_3$) (64% ee) {lit.[1] $[\alpha]_D^{20}$ = +15.3 (c 1.15, $CHCl_3$) for (*S*)-**8s**}; IR (film) 3453, 1447, 1068 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.50-7.42 (m, 2H), 7.41-7.33 (m, 2H), 7.32-7.26 (m 1H), 3.76 (d, *J* = 10.4 Hz, 1H), 3.70 (d, *J* = 10.4 Hz, 1H), 2.59 (br s, 1H), 1.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 128.6, 127.7, 125.1, 73.4, 46.5, 28.2.

1) V. J. Forrat, D. J. Ramón and M. Yus, *Tetrahedron: Asymmetry* 2007, **18**, 400.

2) A. K. Macharla, R. C. Nappunni and N. Nama, *Tetrahedron Lett.* 2012, **53**, 1401.

3) X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 21

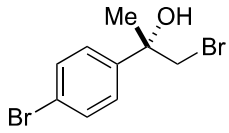


8t

Pale yellow oil; $[\alpha]_D^{20}$ = +30.7 (*c* 0.98, $CHCl_3$) (87% ee); IR (film) 3448, 1491, 1095 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.42-7.37 (m, 2H), 7.36-7.30 (m, 2H), 3.72 (d, *J* = 10.4 Hz, 1H), 3.67 (d, *J* = 10.4 Hz, 1H), 2.61 (br s, 1H), 1.66 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.0, 133.6, 128.8, 126.6, 73.1, 46.0, 28.2.

X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 22

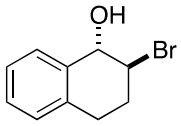


8u

Pale yellow oil; $[\alpha]_D^{20}$ = +26.6 (*c* 1.07, $CHCl_3$) (89% ee); IR (film) 3456, 1488, 1075 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.52-7.46 (m, 2H), 7.36-7.30 (m, 2H), 3.72 (d, *J* = 10.4 Hz, 1H), 3.67 (d, *J* = 10.4 Hz, 1H), 2.58 (br s, 1H), 1.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 131.7, 127.0, 121.8, 73.2, 45.9, 28.2.

X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 23



8v

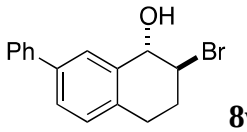
White solid; mp. 99-101 ^{o}C; $[\alpha]_D^{20}$ = -34.7 (*c* 1.06, $CHCl_3$) (71% ee) {lit.[1] $[\alpha]_D^{20}$ = +23.3 (c 0.41, $CHCl_3$) for (1*R*, 2*R*)-**8v**}; IR (film) 3232, 1492, 1213 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.44 (m, 1H), 7.30-7.17 (m, 2H), 7.13-7.04 (m, 1H), 4.86 (d, *J* = 6.4 Hz, 1H), 4.31 (ddd, *J* = 9.6, 6.8, 2.8 Hz, 1H), 3.03-2.82 (m, 2H), 2.73 (br s, 1H), 2.55-2.42 (m, 1H), 2.32-2.17 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.6, 135.2, 128.7, 128.5 128.2, 126.8, 74.2, 56.2, 29.8, 28.2.

1) M. Kasai, K.-i. Kawai, M. Imuta and H. Ziffer, *J. Org. Chem.* 1984, **49**, 675.

2) L. Li, C. Su, X. Liu, H. Tian and Y. Shi, *Org. Lett.* 2014, **16**, 3728.

3) X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 24

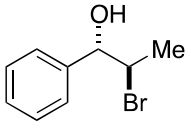


8w

White solid; mp. 111-113 ^{o}C; $[\alpha]_D^{20}$ = -18.1 (*c* 1.03, $CHCl_3$) (78% ee); IR (film) 3299, 1484, 1221 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.61 (d, *J* = 7.2 Hz, 2H), 7.54-7.40 (m, 3H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 1H), 4.94 (d, *J* = 6.8 Hz, 1H), 4.38 (ddd, *J* = 9.2, 6.8, 2.8 Hz, 1H), 3.08-2.88 (m, 2H), 2.79 (br s, 1H), 2.59-2.48 (m, 1H), 2.36-2.23 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.8, 139.9, 136.0, 134.3, 129.2, 128.9, 127.4, 127.2, 127.0, 74.2, 56.2, 29.8, 27.9.

X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 25



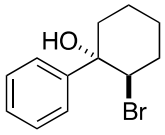
8x

Pale yellow oil; $[\alpha]_D^{20}$ = -5.9 (*c* 0.80, $CHCl_3$) (52% ee); IR (film) 3425, 1451 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.41-7.28 (m, 5H), 5.01 (d, *J* = 3.6 Hz, 1H), 4.43 (qd, *J* = 6.8, 3.6 Hz, 1H), 2.53 (br s, 1H), 1.55 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 128.6, 128.3, 126.6, 77.5, 56.4, 19.0.

1) K. Kikushima, T. Moriuchi and T. Hirao, *Chem. Asian J*. 2009, **4**, 1213.

2) X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

Table 4, entry 26



8y

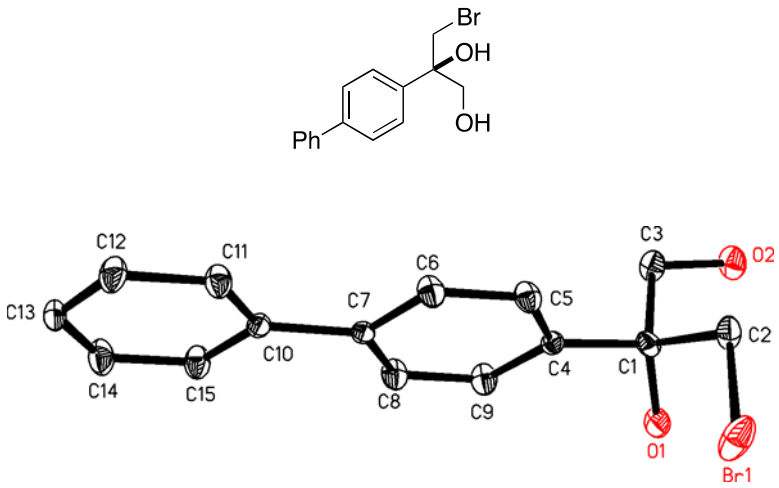
White solid; mp. 44-46 °C; $[\alpha]_D^{20}$ = -15.8 (*c* 0.65, $CHCl_3$) (56% ee); IR (film) 3425, 1447, 1008 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.2 Hz, 1H), 4.49-4.43 (m, 1H), 2.71-2.59 (m, 1H), 2.53-2.41 (m, 1H), 2.14-2.04 (m, 1H), 1.96 (br s, 1H), 1.88-1.78 (m, 3H), 1.76-1.66 (m, 1H), 1.65-1.55 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.5, 128.3, 127.9, 125.8, 74.5, 60.2, 31.5, 31.4, 21.1, 20.5.

1) L. Li, P. Cai, Q. Guo and S. Xue, *J. Org. Chem.* 2008, **73**, 3516.

2) M. Ceylan, E. Findik, E. Sahin and Z. Kazaz, *Russ. Chem. Bull., Int. Ed.* 2009, **58**, 2299.

3) X. Zhang, J. Li, H. Tian and Y. Shi, *Chem. Eur. J.* 2015, **21**, 11658.

The X-ray structure of compound **2d**



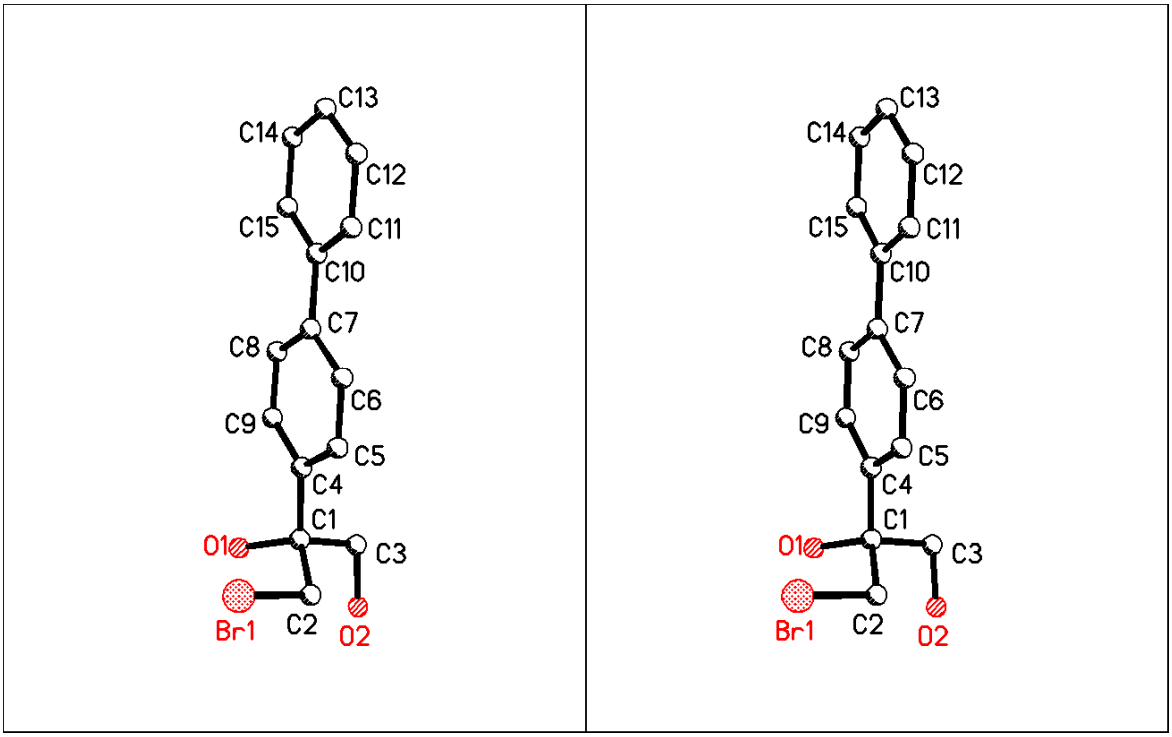


Table 1. Crystal data and structure refinement for **2d**.

Identification code	**2d**	
Empirical formula	$C_{15}H_{15}BrO_2$	
Formula weight	307.18	
Temperature	173.1500 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 7.813(4) Å	a= 90°.
	b = 5.321(3) Å	b= 91.594(8)°.
	c = 15.394(8) Å	g = 90°.
Volume	639.7(6) $Å^3$	
Z	2	
Density (calculated)	1.595 Mg/m^3	
Absorption coefficient	3.204 mm^{-1}	
F(000)	312	
Crystal size	0.25 x 0.22 x 0.05 mm^3	
Theta range for data collection	2.608 to 27.498°.	
Index ranges	-10<=h<=10, -6<=k<=6, -19<=l<=19	
Reflections collected	7124	
Independent reflections	2875 [R(int) = 0.0430]	
Completeness to theta = 26.000°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.4523	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2875 / 1 / 169	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0575, wR2 = 0.1494	
R indices (all data)	R1 = 0.0582, wR2 = 0.1501	
Absolute structure parameter	0.04(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.433 and -0.770 e.$Å^{-3}$	

Table 2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for **2d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br1	-6192(1)	-3721(3)	-3873(1)	50(1)
O1	-2498(8)	-965(9)	-3913(4)	35(1)
O2	-484(8)	-4808(11)	-4744(3)	37(1)
C1	-2494(7)	-3496(15)	-3624(4)	24(1)
C2	-3906(9)	-5009(15)	-4085(5)	31(1)
C3	-770(9)	-4747(14)	-3831(4)	29(1)
C4	-2598(7)	-3473(13)	-2637(3)	20(1)
C5	-3377(9)	-5391(13)	-2177(4)	27(1)
C6	-3344(9)	-5386(13)	-1272(4)	28(1)
C7	-2541(6)	-3489(13)	-796(3)	19(1)
C8	-1742(10)	-1607(12)	-1258(5)	29(1)
C9	-1778(10)	-1586(13)	-2158(4)	31(2)
C10	-2503(6)	-3529(15)	178(3)	21(1)
C11	-3346(9)	-5366(13)	639(4)	28(1)
C12	-3308(10)	-5378(14)	1546(4)	32(2)
C13	-2448(8)	-3515(16)	2006(4)	28(1)
C14	-1589(12)	-1655(16)	1552(5)	39(2)
C15	-1634(10)	-1651(13)	655(5)	31(2)

Table 3. Bond lengths [Å] and angles [°] for **2d**.

Br1-C2	1.949(7)
O1-C1	1.418(9)
O1-H1	0.71(9)
O2-H2	0.8200
O2-C3	1.430(8)
C1-C2	1.525(9)
C1-C3	1.543(9)
C1-C4	1.524(7)
C2-H2A	0.9700
C2-H2B	0.9700
C3-H3A	0.9700
C3-H3B	0.9700
C4-C5	1.392(9)
C4-C9	1.391(9)
C5-H5	0.9300
C5-C6	1.392(9)
C6-H6	0.9300
C6-C7	1.387(9)
C7-C8	1.387(9)
C7-C10	1.499(7)
C8-H8	0.9300
C8-C9	1.386(10)
C9-H9	0.9300
C10-C11	1.386(9)
C10-C15	1.404(9)
C11-H11	0.9300
C11-C12	1.395(9)
C12-H12	0.9300
C12-C13	1.382(10)
C13-H13	0.9300
C13-C14	1.394(11)
C14-H14	0.9300
C14-C15	1.381(10)
C15-H15	0.9300
C1-O1-H1	114(7)

C3-O2-H2	109.5
O1-C1-C2	111.1(6)
O1-C1-C3	109.8(5)
O1-C1-C4	107.8(6)
C2-C1-C3	107.5(6)
C4-C1-C2	114.2(6)
C4-C1-C3	106.3(5)
Br1-C2-H2A	109.0
Br1-C2-H2B	109.0
C1-C2-Br1	113.0(5)
C1-C2-H2A	109.0
C1-C2-H2B	109.0
H2A-C2-H2B	107.8
O2-C3-C1	112.0(6)
O2-C3-H3A	109.2
O2-C3-H3B	109.2
C1-C3-H3A	109.2
C1-C3-H3B	109.2
H3A-C3-H3B	107.9
C5-C4-C1	122.5(6)
C9-C4-C1	119.8(6)
C9-C4-C5	117.5(5)
C4-C5-H5	119.6
C4-C5-C6	120.7(6)
C6-C5-H5	119.6
C5-C6-H6	119.2
C7-C6-C5	121.7(6)
C7-C6-H6	119.2
C6-C7-C8	117.3(5)
C6-C7-C10	120.9(6)
C8-C7-C10	121.7(6)
C7-C8-H8	119.3
C9-C8-C7	121.4(6)
C9-C8-H8	119.3
C4-C9-H9	119.3
C8-C9-C4	121.4(6)
C8-C9-H9	119.3
C11-C10-C7	121.7(6)

C11-C10-C15	117.7(5)
C15-C10-C7	120.6(6)
C10-C11-H11	119.4
C10-C11-C12	121.2(6)
C12-C11-H11	119.4
C11-C12-H12	119.8
C13-C12-C11	120.4(6)
C13-C12-H12	119.8
C12-C13-H13	120.4
C12-C13-C14	119.1(6)
C14-C13-H13	120.4
C13-C14-H14	119.9
C15-C14-C13	120.2(7)
C15-C14-H14	119.9
C10-C15-H15	119.3
C14-C15-C10	121.4(6)
C14-C15-H15	119.3

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2x10^3$) for **2d**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br1	27(1)	88(1)	33(1)	13(1)	1(1)	9(1)
O1	61(4)	26(2)	19(2)	6(2)	4(2)	-1(2)
O2	36(3)	52(3)	23(2)	-2(2)	11(2)	2(2)
C1	25(3)	27(3)	22(3)	-5(3)	5(2)	2(3)
C2	27(3)	44(4)	22(3)	-5(3)	-1(2)	-1(3)
C3	21(3)	46(4)	22(3)	0(3)	7(2)	2(3)
C4	20(2)	22(3)	17(2)	1(3)	2(2)	2(3)
C5	33(3)	24(3)	26(3)	-3(2)	2(2)	-9(2)
C6	37(3)	23(3)	24(3)	-1(2)	4(3)	-10(3)
C7	17(2)	20(3)	19(2)	0(2)	2(2)	2(2)
C8	37(4)	23(3)	27(3)	-1(2)	0(3)	-13(3)
C9	40(4)	27(3)	25(3)	3(2)	4(3)	-12(3)
C10	20(2)	24(3)	19(2)	1(3)	1(2)	3(3)
C11	36(4)	27(3)	22(3)	-1(2)	1(3)	-8(3)
C12	40(4)	34(3)	22(3)	6(3)	4(3)	-8(3)
C13	34(3)	34(3)	17(2)	-1(3)	0(2)	3(3)
C14	55(5)	37(4)	24(3)	-5(3)	-2(3)	-8(3)
C15	38(4)	31(3)	24(3)	-1(3)	-1(3)	-11(3)

Table 5. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for **2d**.

	x	y	z	U(eq)
H2	-215	-3401	-4910	56
H2A	-3838	-6741	-3890	37
H2B	-3718	-4990	-4705	37
H3A	153	-3827	-3541	35
H3B	-758	-6451	-3606	35
H5	-3926	-6691	-2477	33
H6	-3874	-6688	-979	34
H8	-1169	-330	-957	35
H9	-1242	-285	-2449	37
H11	-3949	-6615	339	34
H12	-3865	-6647	1842	38
H13	-2441	-3502	2610	34
H14	-984	-413	1855	46
H15	-1077	-378	360	37
H1	-2560(100)	-840(160)	-4370(60)	20(20)

Table 6. Torsion angles [°] for **2d**.

O1-C1-C2-Br1	-61.0(6)
O1-C1-C3-O2	-61.6(7)
O1-C1-C4-C5	149.9(6)
O1-C1-C4-C9	-35.4(8)
C1-C4-C5-C6	175.6(6)
C1-C4-C9-C8	-175.3(7)
C2-C1-C3-O2	59.3(8)
C2-C1-C4-C5	25.9(9)
C2-C1-C4-C9	-159.3(6)
C3-C1-C2-Br1	178.8(4)
C3-C1-C4-C5	-92.4(7)
C3-C1-C4-C9	82.3(8)
C4-C1-C2-Br1	61.2(8)
C4-C1-C3-O2	-177.9(6)
C4-C5-C6-C7	0.0(11)
C5-C4-C9-C8	-0.3(11)
C5-C6-C7-C8	-1.1(10)
C5-C6-C7-C10	-179.4(6)
C6-C7-C8-C9	1.5(11)
C6-C7-C10-C11	-3.8(9)
C6-C7-C10-C15	177.7(7)
C7-C8-C9-C4	-0.9(12)
C7-C10-C11-C12	-179.7(6)
C7-C10-C15-C14	179.8(7)
C8-C7-C10-C11	178.0(7)
C8-C7-C10-C15	-0.6(9)
C9-C4-C5-C6	0.7(10)
C10-C7-C8-C9	179.8(6)
C10-C11-C12-C13	1.2(11)
C11-C10-C15-C14	1.3(11)
C11-C12-C13-C14	-1.3(12)
C12-C13-C14-C15	1.4(12)
C13-C14-C15-C10	-1.4(13)
C15-C10-C11-C12	-1.2(11)

Symmetry transformations used to generate equivalent atoms:

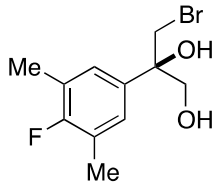
Table 7. Hydrogen bonds for **2d** [Å and °].

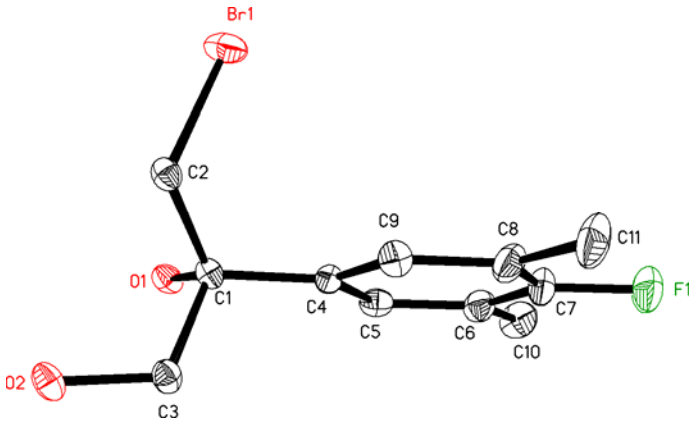
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O2-H2...O2#1	0.82	2.06	2.881(4)	176.9
O1-H1...Br1#2	0.71(9)	3.06(9)	3.727(6)	157(8)

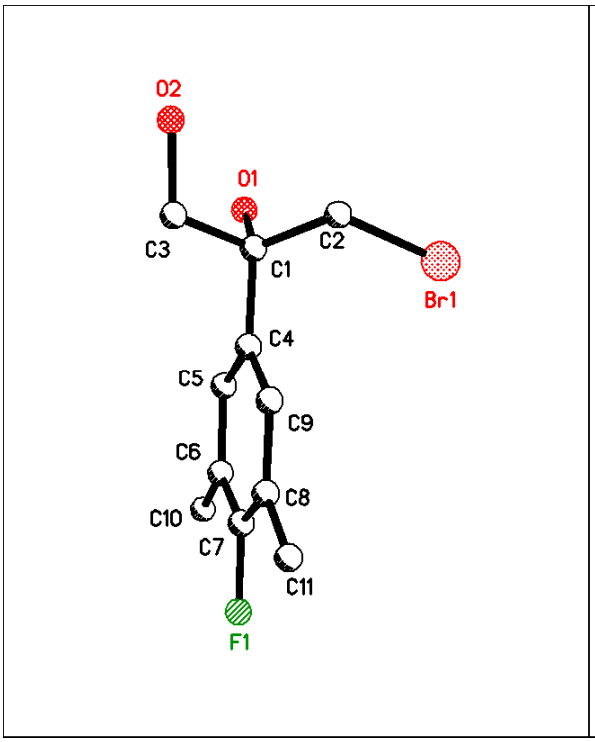
Symmetry transformations used to generate equivalent atoms:

#1 -x,y+1/2,-z-1 #2 -x-1,y+1/2,-z-1

The X-ray structure of compound **2j**







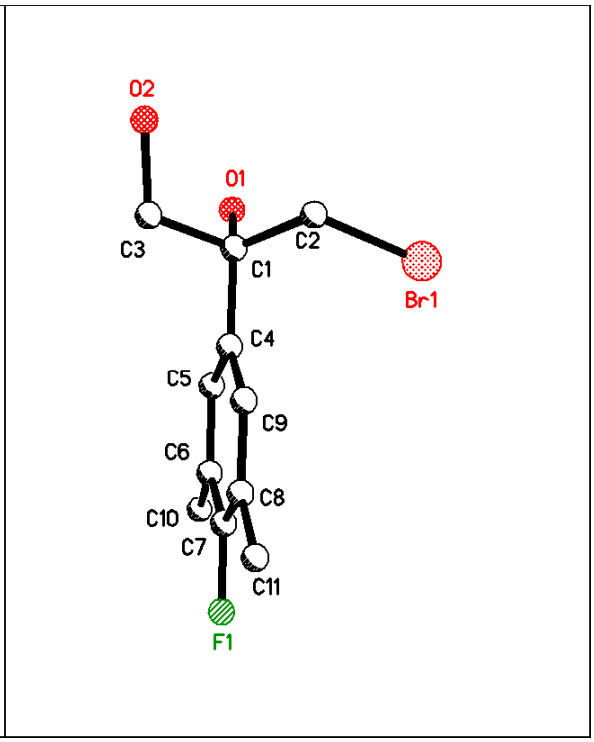


Table 1. Crystal data and structure refinement for **2j**.

Identification code	**2j**	
Empirical formula	$C_{11}H_{14}BrFO_2$	
Formula weight	277.13	
Temperature	173.1500 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 5.651(2) Å	a= 90°.
	b = 16.364(7) Å	b= 90°.
	c = 38.4918(16) Å	g = 90°.
Volume	3559(2) $Å^3$	
Z	12	
Density (calculated)	1.551 Mg/m^3	
Absorption coefficient	3.456 mm^{-1}	
F(000)	1680	
Crystal size	0.34 x 0.03 x 0.03 mm^3	
Theta range for data collection	1.352 to 27.400°.	
Index ranges	-7<=h<=7, -21<=k<=20, -49<=l<=49	
Reflections collected	34787	
Independent reflections	7939 [R(int) = 0.0853]	
Completeness to theta = 26.000°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.5903	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7939 / 0 / 418	
Goodness-of-fit on F^2	1.159	
Final R indices [I>2sigma(I)]	R1 = 0.0694, wR2 = 0.1075	
R indices (all data)	R1 = 0.0824, wR2 = 0.1135	
Absolute structure parameter	0.008(8)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.602 and -0.839 $e.Å^{-3}$	

Table 2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for **2j**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br1	8728(2)	7738(1)	4374(1)	41(1)
F1	8201(11)	9018(3)	2838(1)	54(2)
O1	10369(10)	6131(3)	3901(2)	27(1)
O2	15303(10)	6108(3)	4019(2)	30(1)
C1	11660(14)	6879(4)	3876(2)	22(2)
C2	11777(14)	7290(5)	4231(2)	26(2)
C3	14174(15)	6623(5)	3771(2)	27(2)
C4	10727(15)	7442(5)	3594(2)	24(2)
C5	9044(14)	7187(5)	3352(2)	27(2)
C6	8137(15)	7711(6)	3094(2)	34(2)
C7	9049(18)	8487(5)	3089(2)	37(2)
C8	10755(18)	8786(5)	3313(2)	37(2)
C9	11566(16)	8250(5)	3567(2)	28(2)
C10	6150(16)	7450(6)	2855(2)	45(3)
C11	11710(20)	9641(5)	3287(2)	51(3)
Br1B	5637(2)	4814(1)	2678(1)	44(1)
F1B	5611(12)	957(3)	3130(2)	56(2)
O1B	7254(10)	4708(3)	3494(1)	24(1)
O2B	12206(10)	4968(3)	3438(1)	28(1)
C1B	8581(13)	4244(5)	3244(2)	22(2)
C2B	8695(14)	4720(5)	2900(2)	25(2)
C3B	11093(15)	4191(5)	3392(2)	26(2)
C4B	7685(15)	3371(5)	3203(2)	25(2)
C5B	6068(16)	3043(5)	3437(2)	31(2)
C6B	5303(15)	2233(6)	3412(2)	32(2)
C7B	6302(19)	1753(5)	3152(2)	38(2)
C8B	7950(16)	2043(5)	2915(2)	32(2)
C9B	8628(16)	2853(5)	2947(2)	32(2)
C10B	3410(20)	1882(6)	3652(3)	53(3)
C11B	9003(18)	1478(5)	2646(2)	47(3)
Br1A	1787(2)	2810(1)	4597(1)	40(1)
F1A	520(11)	5506(4)	5743(1)	55(2)
O1A	3518(10)	4510(3)	4215(1)	25(1)

O2A	8492(11)	4290(4)	4185(1)	32(1)
C1A	4743(14)	4252(5)	4524(2)	24(2)
C2A	4896(14)	3308(5)	4531(2)	29(2)
C3A	7265(14)	4587(5)	4483(2)	27(2)
C4A	3680(14)	4618(5)	4854(2)	25(2)
C5A	1996(15)	5242(5)	4836(2)	28(2)
C6A	917(16)	5547(5)	5134(2)	33(2)
C7A	1659(16)	5226(6)	5448(2)	34(2)
C8A	3351(19)	4639(6)	5483(2)	41(2)
C9A	4361(17)	4336(5)	5180(2)	33(2)
C10A	-1016(18)	6192(6)	5118(3)	50(3)
C11A	4120(30)	4349(8)	5841(2)	79(4)

Table 3. Bond lengths [Å] and angles [°] for **2j**.

Br1-C2	1.952(8)
F1-C7	1.386(9)
O1-H1	0.8200
O1-C1	1.428(9)
O2-H2	0.8200
O2-C3	1.424(9)
C1-C2	1.524(10)
C1-C3	1.536(11)
C1-C4	1.520(10)
C2-H2A	0.9700
C2-H2B	0.9700
C3-H3A	0.9700
C3-H3B	0.9700
C4-C5	1.395(11)
C4-C9	1.408(11)
C5-H5	0.9300
C5-C6	1.409(11)
C6-C7	1.371(12)
C6-C10	1.513(12)
C7-C8	1.383(13)
C8-C9	1.391(11)
C8-C11	1.503(12)
C9-H9	0.9300
C10-H10A	0.9600
C10-H10B	0.9600
C10-H10C	0.9600
C11-H11A	0.9600
C11-H11B	0.9600
C11-H11C	0.9600
Br1B-C2B	1.933(8)
F1B-C7B	1.362(10)
O1B-H1B	0.8200
O1B-C1B	1.436(9)
O2B-H2BA	0.8200
O2B-C3B	1.430(9)
C1B-C2B	1.539(10)

C1B-C3B	1.531(11)
C1B-C4B	1.524(10)
C2B-H2BB	0.9700
C2B-H2BC	0.9700
C3B-H3BA	0.9700
C3B-H3BB	0.9700
C4B-C5B	1.392(11)
C4B-C9B	1.402(10)
C5B-H5B	0.9300
C5B-C6B	1.397(12)
C6B-C7B	1.393(12)
C6B-C10B	1.525(12)
C7B-C8B	1.385(12)
C8B-C9B	1.386(11)
C8B-C11B	1.512(11)
C9B-H9B	0.9300
C10B-H10D	0.9600
C10B-H10E	0.9600
C10B-H10F	0.9600
C11B-H11D	0.9600
C11B-H11E	0.9600
C11B-H11F	0.9600
Br1A-C2A	1.954(8)
F1A-C7A	1.386(9)
O1A-H1A	0.8200
O1A-C1A	1.438(8)
O2A-H2AA	0.8200
O2A-C3A	1.426(9)
C1A-C2A	1.547(11)
C1A-C3A	1.536(11)
C1A-C4A	1.529(10)
C2A-H2AB	0.9700
C2A-H2AC	0.9700
C3A-H3AA	0.9700
C3A-H3AB	0.9700
C4A-C5A	1.396(11)
C4A-C9A	1.393(11)
C5A-H5A	0.9300

C5A-C6A	1.392(11)
C6A-C7A	1.380(12)
C6A-C10A	1.520(13)
C7A-C8A	1.363(13)
C8A-C9A	1.389(11)
C8A-C11A	1.522(12)
C9A-H9A	0.9300
C10A-H10G	0.9600
C10A-H10H	0.9600
C10A-H10I	0.9600
C11A-H11G	0.9600
C11A-H11H	0.9600
C11A-H11I	0.9600

C1-O1-H1	109.5
C3-O2-H2	109.5
O1-C1-C2	109.9(6)
O1-C1-C3	104.9(6)
O1-C1-C4	113.0(6)
C2-C1-C3	108.5(6)
C4-C1-C2	112.8(6)
C4-C1-C3	107.3(6)
Br1-C2-H2A	109.1
Br1-C2-H2B	109.1
C1-C2-Br1	112.4(5)
C1-C2-H2A	109.1
C1-C2-H2B	109.1
H2A-C2-H2B	107.9
O2-C3-C1	113.5(6)
O2-C3-H3A	108.9
O2-C3-H3B	108.9
C1-C3-H3A	108.9
C1-C3-H3B	108.9
H3A-C3-H3B	107.7
C5-C4-C1	122.2(7)
C5-C4-C9	117.4(7)
C9-C4-C1	120.4(7)
C4-C5-H5	118.7

C4-C5-C6	122.5(8)
C6-C5-H5	118.7
C5-C6-C10	121.8(8)
C7-C6-C5	115.8(8)
C7-C6-C10	122.2(8)
C6-C7-F1	117.4(8)
C6-C7-C8	125.6(8)
C8-C7-F1	117.0(8)
C7-C8-C9	116.4(8)
C7-C8-C11	122.6(8)
C9-C8-C11	121.1(9)
C4-C9-H9	118.9
C8-C9-C4	122.2(8)
C8-C9-H9	118.9
C6-C10-H10A	109.5
C6-C10-H10B	109.5
C6-C10-H10C	109.5
H10A-C10-H10B	109.5
H10A-C10-H10C	109.5
H10B-C10-H10C	109.5
C8-C11-H11A	109.5
C8-C11-H11B	109.5
C8-C11-H11C	109.5
H11A-C11-H11B	109.5
H11A-C11-H11C	109.5
H11B-C11-H11C	109.5
C1B-O1B-H1B	109.5
C3B-O2B-H2BA	109.5
O1B-C1B-C2B	109.4(6)
O1B-C1B-C3B	105.4(6)
O1B-C1B-C4B	113.0(6)
C3B-C1B-C2B	108.1(6)
C4B-C1B-C2B	113.4(6)
C4B-C1B-C3B	107.0(6)
Br1B-C2B-H2BB	109.1
Br1B-C2B-H2BC	109.1
C1B-C2B-Br1B	112.5(5)
C1B-C2B-H2BB	109.1

C1B-C2B-H2BC	109.1
H2BB-C2B-H2BC	107.8
O2B-C3B-C1B	113.7(6)
O2B-C3B-H3BA	108.8
O2B-C3B-H3BB	108.8
C1B-C3B-H3BA	108.8
C1B-C3B-H3BB	108.8
H3BA-C3B-H3BB	107.7
C5B-C4B-C1B	120.8(7)
C5B-C4B-C9B	118.1(7)
C9B-C4B-C1B	120.9(7)
C4B-C5B-H5B	119.2
C4B-C5B-C6B	121.6(8)
C6B-C5B-H5B	119.2
C5B-C6B-C10B	122.1(8)
C7B-C6B-C5B	117.3(8)
C7B-C6B-C10B	120.6(8)
F1B-C7B-C6B	117.8(8)
F1B-C7B-C8B	118.7(8)
C8B-C7B-C6B	123.5(8)
C7B-C8B-C9B	117.0(8)
C7B-C8B-C11B	120.4(8)
C9B-C8B-C11B	122.5(8)
C4B-C9B-H9B	118.8
C8B-C9B-C4B	122.4(8)
C8B-C9B-H9B	118.8
C6B-C10B-H10D	109.5
C6B-C10B-H10E	109.5
C6B-C10B-H10F	109.5
H10D-C10B-H10E	109.5
H10D-C10B-H10F	109.5
H10E-C10B-H10F	109.5
C8B-C11B-H11D	109.5
C8B-C11B-H11E	109.5
C8B-C11B-H11F	109.5
H11D-C11B-H11E	109.5
H11D-C11B-H11F	109.5
H11E-C11B-H11F	109.5

C1A-O1A-H1A	109.5
C3A-O2A-H2AA	109.5
O1A-C1A-C2A	109.6(6)
O1A-C1A-C3A	104.9(6)
O1A-C1A-C4A	112.5(6)
C3A-C1A-C2A	107.9(7)
C4A-C1A-C2A	113.5(6)
C4A-C1A-C3A	108.0(6)
Br1A-C2A-H2AB	109.3
Br1A-C2A-H2AC	109.3
C1A-C2A-Br1A	111.6(6)
C1A-C2A-H2AB	109.3
C1A-C2A-H2AC	109.3
H2AB-C2A-H2AC	108.0
O2A-C3A-C1A	114.3(7)
O2A-C3A-H3AA	108.7
O2A-C3A-H3AB	108.7
C1A-C3A-H3AA	108.7
C1A-C3A-H3AB	108.7
H3AA-C3A-H3AB	107.6
C5A-C4A-C1A	120.9(7)
C9A-C4A-C1A	120.7(7)
C9A-C4A-C5A	118.3(7)
C4A-C5A-H5A	119.3
C6A-C5A-C4A	121.4(7)
C6A-C5A-H5A	119.3
C5A-C6A-C10A	122.1(8)
C7A-C6A-C5A	116.7(8)
C7A-C6A-C10A	121.2(8)
C6A-C7A-F1A	116.8(8)
C8A-C7A-F1A	118.4(7)
C8A-C7A-C6A	124.7(8)
C7A-C8A-C9A	117.1(8)
C7A-C8A-C11A	120.8(8)
C9A-C8A-C11A	122.1(9)
C4A-C9A-H9A	119.2
C8A-C9A-C4A	121.6(8)
C8A-C9A-H9A	119.2

C6A-C10A-H10G	109.5
C6A-C10A-H10H	109.5
C6A-C10A-H10I	109.5
H10G-C10A-H10H	109.5
H10G-C10A-H10I	109.5
H10H-C10A-H10I	109.5
C8A-C11A-H11G	109.5
C8A-C11A-H11H	109.5
C8A-C11A-H11I	109.5
H11G-C11A-H11H	109.5
H11G-C11A-H11I	109.5
H11H-C11A-H11I	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2x10^3$) for **2j**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br1	34(1)	46(1)	44(1)	-14(1)	4(1)	7(1)
F1	62(4)	57(4)	43(3)	20(3)	-6(3)	11(3)
O1	18(3)	26(3)	36(3)	2(2)	5(3)	-1(3)
O2	22(3)	25(3)	43(3)	2(3)	-4(3)	0(3)
C1	18(4)	19(4)	28(4)	-1(3)	-4(3)	-2(3)
C2	24(4)	24(4)	31(4)	-2(3)	-6(3)	1(4)
C3	23(5)	24(4)	32(4)	6(3)	1(4)	-1(4)
C4	24(4)	26(4)	22(4)	2(3)	1(3)	2(4)
C5	19(4)	30(4)	32(4)	-2(4)	5(3)	-5(4)
C6	29(5)	45(5)	28(4)	1(4)	-1(3)	4(5)
C7	43(6)	36(5)	31(4)	11(4)	-2(4)	4(5)
C8	50(6)	34(5)	28(4)	7(4)	4(4)	-5(5)
C9	24(5)	26(4)	35(4)	1(3)	-1(4)	-7(4)
C10	28(5)	69(7)	37(5)	1(4)	-8(4)	1(5)
C11	81(8)	34(5)	38(5)	13(4)	-8(5)	-17(6)
Br1B	33(1)	64(1)	36(1)	11(1)	-7(1)	0(1)
F1B	64(4)	32(3)	70(4)	-9(3)	20(3)	-22(3)
O1B	22(3)	25(3)	27(3)	-8(2)	1(2)	4(3)
O2B	19(3)	29(3)	35(3)	-7(2)	-1(2)	-6(3)
C1B	11(4)	28(4)	27(4)	-5(3)	1(3)	-3(3)
C2B	24(4)	23(4)	29(4)	1(3)	0(3)	-4(4)
C3B	25(5)	23(4)	32(4)	-3(3)	3(4)	-3(4)
C4B	24(4)	21(4)	31(4)	-2(3)	1(3)	-4(4)
C5B	34(5)	27(5)	33(4)	-6(3)	1(4)	-2(4)
C6B	27(5)	31(5)	37(4)	0(4)	4(4)	-7(4)
C7B	47(6)	25(4)	42(5)	-3(4)	9(5)	-13(5)
C8B	33(5)	29(5)	35(4)	-7(4)	-1(4)	0(4)
C9B	35(5)	25(4)	35(4)	-5(4)	4(4)	-3(5)
C10B	51(7)	48(6)	59(6)	-2(5)	21(6)	-20(6)
C11B	55(7)	34(5)	51(6)	-17(4)	19(5)	-7(5)
Br1A	37(1)	32(1)	50(1)	7(1)	4(1)	-8(1)
F1A	58(4)	68(4)	39(3)	-15(3)	18(3)	1(3)
O1A	14(3)	33(3)	27(3)	4(2)	-4(2)	0(3)

O2A	22(3)	45(4)	28(3)	5(3)	7(3)	1(3)
C1A	18(4)	31(5)	25(4)	3(3)	-5(3)	6(4)
C2A	21(4)	40(5)	25(4)	5(4)	1(3)	1(4)
C3A	23(4)	35(5)	24(4)	0(3)	0(3)	-3(4)
C4A	15(4)	32(5)	28(4)	0(3)	2(3)	-1(4)
C5A	26(5)	30(5)	28(4)	4(3)	1(3)	0(4)
C6A	24(5)	38(5)	36(4)	-5(4)	1(4)	-4(4)
C7A	34(5)	46(5)	21(4)	-13(4)	4(4)	-2(5)
C8A	55(7)	39(5)	27(4)	-6(4)	-6(4)	3(5)
C9A	36(5)	38(5)	25(4)	6(4)	2(4)	9(4)
C10A	39(6)	54(7)	56(6)	-22(5)	3(5)	13(5)
C11A	117(12)	94(10)	26(5)	9(5)	-5(7)	26(9)

Table 5. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for **2j**.

	x	y	z	U(eq)
H1	8996	6229	3956	40
H2	14613	5667	4027	45
H2A	12935	7727	4223	31
H2B	12300	6894	4402	31
H3A	14102	6339	3550	32
H3B	15127	7110	3739	32
H5	8499	6652	3362	33
H9	12700	8431	3724	34
H10A	6078	6864	2846	67
H10B	6435	7659	2625	67
H10C	4676	7660	2940	67
H11A	10444	10025	3315	76
H11B	12429	9717	3063	76
H11C	12875	9726	3465	76
H1B	5876	4745	3430	37
H2BA	11349	5264	3555	42
H2BB	9778	4445	2743	30
H2BC	9315	5263	2944	30
H3BA	11033	3913	3614	32
H3BB	12054	3862	3237	32
H5B	5483	3370	3615	37
H9B	9748	3062	2794	38
H10D	3109	2261	3838	79
H10E	3958	1374	3748	79
H10F	1984	1791	3523	79
H11D	9298	1779	2436	70
H11E	7916	1041	2598	70
H11F	10464	1257	2731	70
H1A	2091	4441	4241	37
H2AA	7988	4518	4011	48
H2AB	5937	3139	4718	35
H2AC	5571	3116	4314	35
H3AA	7188	5178	4470	33
H3AB	8168	4447	4689	33

H5A	1587	5457	4621	33
H9A	5520	3934	5196	40
H10G	-2433	5981	5223	74
H10H	-1324	6330	4880	74
H10I	-512	6671	5242	74
H11G	4654	4808	5976	118
H11H	5389	3962	5818	118
H11I	2809	4094	5957	118

Table 6. Torsion angles [°] for **2j**.

F1-C7-C8-C9	179.1(8)
F1-C7-C8-C11	-1.2(14)
O1-C1-C2-Br1	-71.4(7)
O1-C1-C3-O2	-61.3(8)
O1-C1-C4-C5	-9.7(10)
O1-C1-C4-C9	170.7(7)
C1-C4-C5-C6	178.8(7)
C1-C4-C9-C8	-179.8(8)
C2-C1-C3-O2	56.1(8)
C2-C1-C4-C5	-135.1(8)
C2-C1-C4-C9	45.3(10)
C3-C1-C2-Br1	174.5(5)
C3-C1-C4-C5	105.4(8)
C3-C1-C4-C9	-74.1(9)
C4-C1-C2-Br1	55.7(8)
C4-C1-C3-O2	178.3(6)
C4-C5-C6-C7	1.3(12)
C4-C5-C6-C10	-174.2(8)
C5-C4-C9-C8	0.6(12)
C5-C6-C7-F1	179.9(7)
C5-C6-C7-C8	0.2(14)
C6-C7-C8-C9	-1.2(15)
C6-C7-C8-C11	178.5(10)
C7-C8-C9-C4	0.7(13)
C9-C4-C5-C6	-1.7(12)
C10-C6-C7-F1	-4.6(13)
C10-C6-C7-C8	175.7(9)
C11-C8-C9-C4	-178.9(9)
F1B-C7B-C8B-C9B	-179.4(8)
F1B-C7B-C8B-C11B	-1.6(14)
O1B-C1B-C2B-Br1B	-67.0(7)
O1B-C1B-C3B-O2B	-60.9(8)
O1B-C1B-C4B-C5B	-11.8(11)
O1B-C1B-C4B-C9B	174.1(7)
C1B-C4B-C5B-C6B	-177.2(8)
C1B-C4B-C9B-C8B	176.3(8)

C2B-C1B-C3B-O2B	56.0(8)
C2B-C1B-C4B-C5B	-137.1(8)
C2B-C1B-C4B-C9B	48.8(10)
C3B-C1B-C2B-Br1B	178.7(5)
C3B-C1B-C4B-C5B	103.8(9)
C3B-C1B-C4B-C9B	-70.3(9)
C4B-C1B-C2B-Br1B	60.2(8)
C4B-C1B-C3B-O2B	178.5(6)
C4B-C5B-C6B-C7B	2.8(13)
C4B-C5B-C6B-C10B	-175.9(9)
C5B-C4B-C9B-C8B	2.1(13)
C5B-C6B-C7B-F1B	178.5(8)
C5B-C6B-C7B-C8B	-1.5(14)
C6B-C7B-C8B-C9B	0.6(14)
C6B-C7B-C8B-C11B	178.4(9)
C7B-C8B-C9B-C4B	-0.9(13)
C9B-C4B-C5B-C6B	-3.0(13)
C10B-C6B-C7B-F1B	-2.8(14)
C10B-C6B-C7B-C8B	177.2(9)
C11B-C8B-C9B-C4B	-178.6(9)
F1A-C7A-C8A-C9A	176.2(8)
F1A-C7A-C8A-C11A	-5.2(15)
O1A-C1A-C2A-Br1A	-68.1(7)
O1A-C1A-C3A-O2A	-60.4(8)
O1A-C1A-C4A-C5A	-10.6(11)
O1A-C1A-C4A-C9A	169.1(8)
C1A-C4A-C5A-C6A	176.3(8)
C1A-C4A-C9A-C8A	-177.5(9)
C2A-C1A-C3A-O2A	56.4(8)
C2A-C1A-C4A-C5A	-135.7(8)
C2A-C1A-C4A-C9A	44.0(11)
C3A-C1A-C2A-Br1A	178.2(5)
C3A-C1A-C4A-C5A	104.7(8)
C3A-C1A-C4A-C9A	-75.6(10)
C4A-C1A-C2A-Br1A	58.5(8)
C4A-C1A-C3A-O2A	179.5(6)
C4A-C5A-C6A-C7A	2.4(13)
C4A-C5A-C6A-C10A	-176.5(8)

C5A-C4A-C9A-C8A	2.2(13)
C5A-C6A-C7A-F1A	-177.5(8)
C5A-C6A-C7A-C8A	0.0(14)
C6A-C7A-C8A-C9A	-1.2(15)
C6A-C7A-C8A-C11A	177.4(10)
C7A-C8A-C9A-C4A	0.0(14)
C9A-C4A-C5A-C6A	-3.5(12)
C10A-C6A-C7A-F1A	1.5(13)
C10A-C6A-C7A-C8A	178.9(9)
C11A-C8A-C9A-C4A	-178.5(10)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **2j** [Å and °].

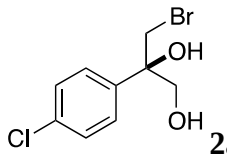
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O1-H1...O2#1	0.82	2.11	2.898(8)	161.2
O2-H2...O1A#2	0.82	2.12	2.903(8)	159.6
O1B-H1B...Br1B	0.82	2.90	3.276(5)	110.4
O1B-H1B...O2B#1	0.82	2.11	2.893(8)	160.8
O2B-H2BA...O1	0.82	2.02	2.808(8)	159.7
O2B-H2BA...O1B	0.82	2.50	2.839(8)	106.3
O1A-H1A...O2A#1	0.82	2.06	2.865(8)	167.0
O2A-H2AA...O1B	0.82	2.05	2.834(8)	158.6

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z #2 x+1,y,z

The determination of enantiomeric excess

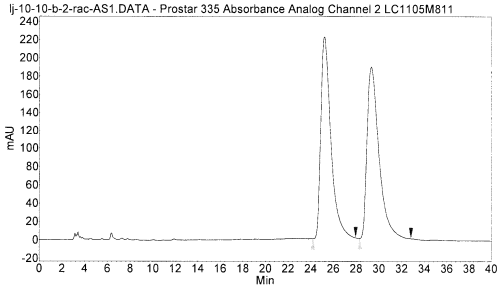
Table 2, entry 1



2a

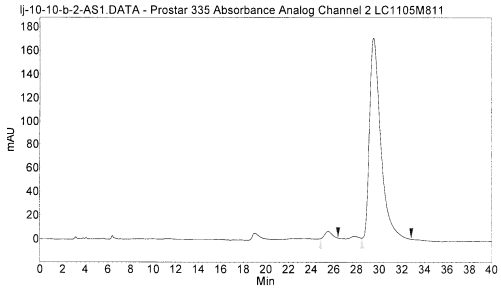
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



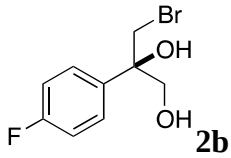
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	25.23	49.902	24.19	27.95
2	29.33	50.098	28.32	32.82
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	25.51	2.159	24.85	26.38
2	29.49	97.841	28.48	32.82
Total		100.000		

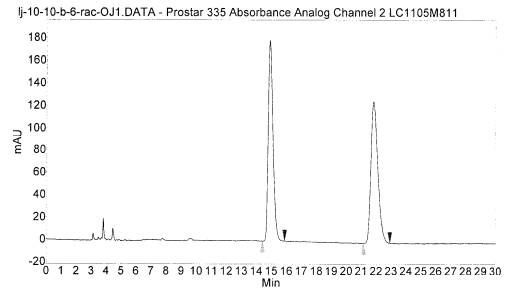
Table 2, entry 2



2b

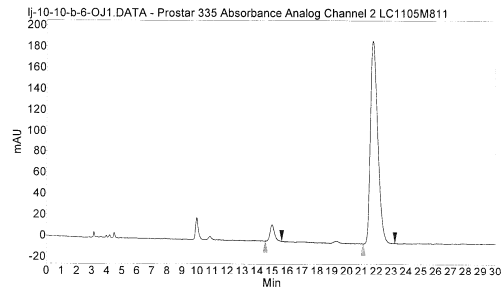
HPLC Condition: Column: Chiralpak OJ-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV215 nm.

Racemic standard



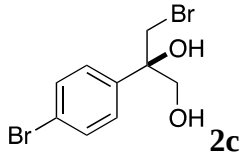
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	14.89	49.915	14.40	15.88
2	21.83	50.085	21.15	22.91
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	14.99	4.473	14.55	15.63
2	21.76	95.527	21.11	23.25
Total		100.000		

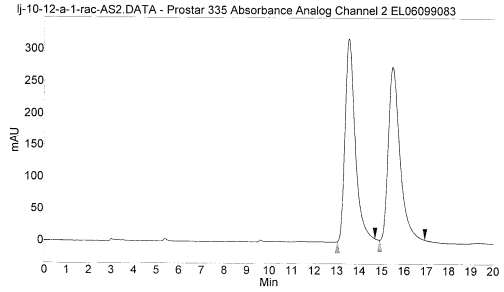
Table 2, entry 3



2c

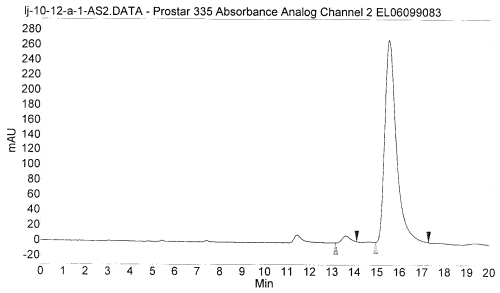
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



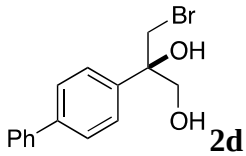
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	13.52	50.004	13.02	14.70
2	15.47	49.996	14.90	16.93
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	13.60	2.152	13.17	14.10
2	15.51	97.848	14.94	17.30
Total		100.000		

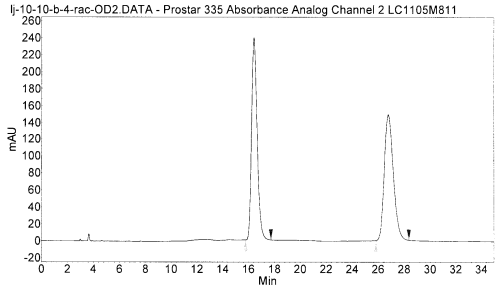
Table 2, entry 4



2d

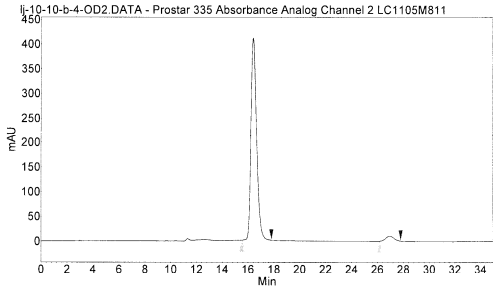
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV252 nm.

Racemic standard



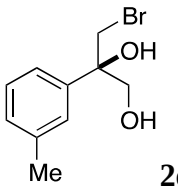
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	16.43	49.929	15.75	17.73
2	26.77	50.071	25.83	28.35
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	16.43	96.539	15.53	17.81
2	26.93	3.461	26.15	27.78
Total		100.000		

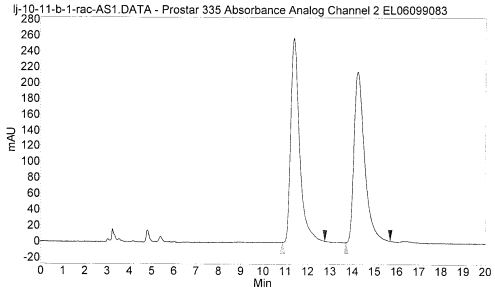
Table 2, entry 5



2e

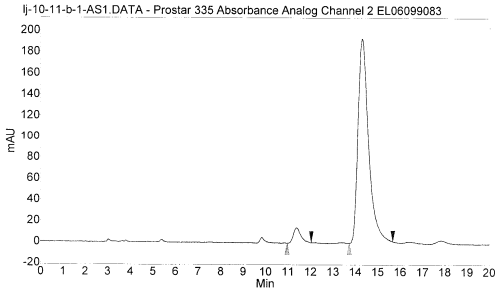
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



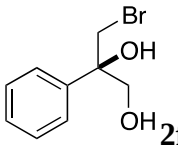
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.37	50.077	10.88	12.78
2	14.25	49.923	13.73	15.71
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.36	4.940	10.96	12.03
2	14.27	95.060	13.73	15.67
Total		100.000		

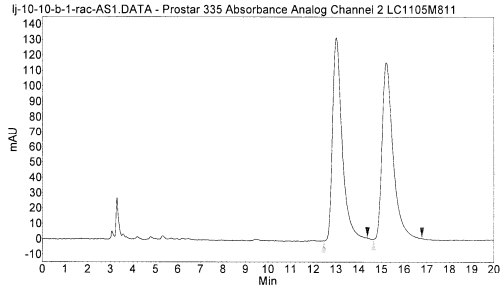
Table 2, entry 6



2f

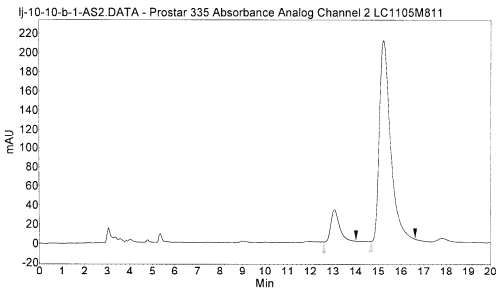
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV215 nm.

Racemic standard



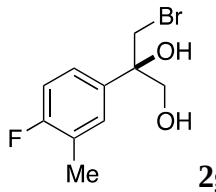
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	13.01	49.993	12.47	14.39
2	15.20	50.007	14.65	16.78
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	13.07	11.402	12.61	14.01
2	15.23	88.598	14.68	16.62
Total		100.000		

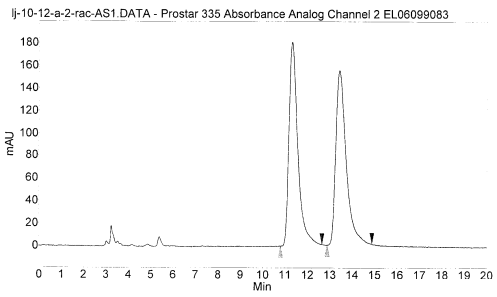
Table 2, entry 7



2g

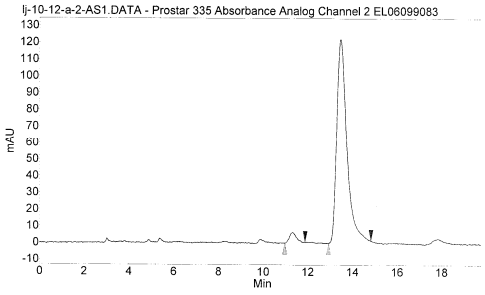
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



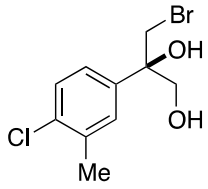
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.31	50.034	10.79	12.65
2	13.43	49.966	12.88	14.88
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.31	3.274	10.97	11.87
2	13.44	96.726	12.92	14.82
Total		100.000		

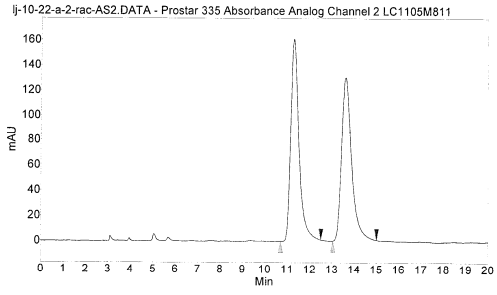
Table 2, entry 8



2h

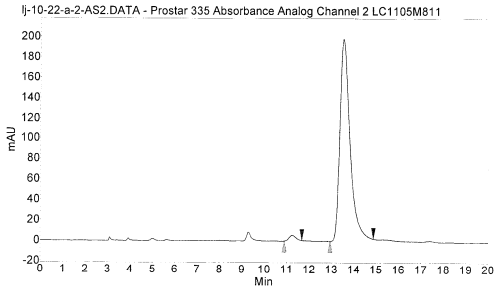
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



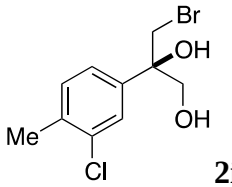
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.29	50.061	10.71	12.51
2	13.60	49.939	13.04	15.01
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.25	1.759	10.90	11.68
2	13.55	98.241	12.94	14.88
Total		100.000		

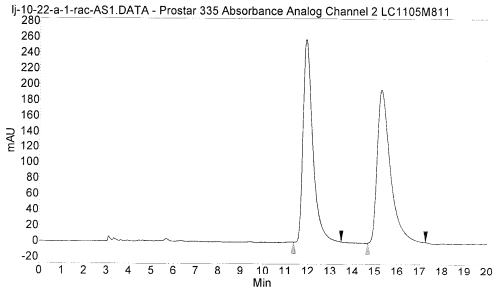
Table 2, entry 9



2i

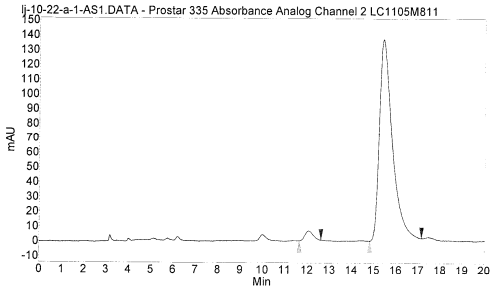
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



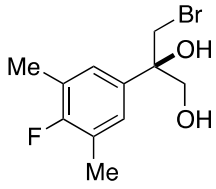
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.93	49.910	11.37	13.50
2	15.29	50.090	14.70	17.28
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	12.09	2.972	11.66	12.63
2	15.44	97.028	14.82	17.15
Total		100.000		

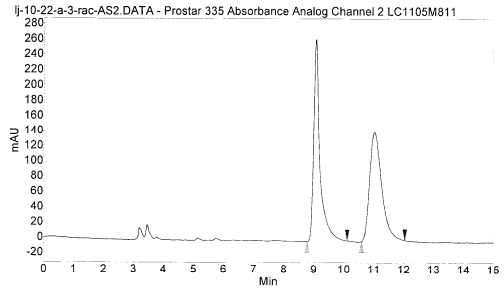
Table 2, entry 10



2j

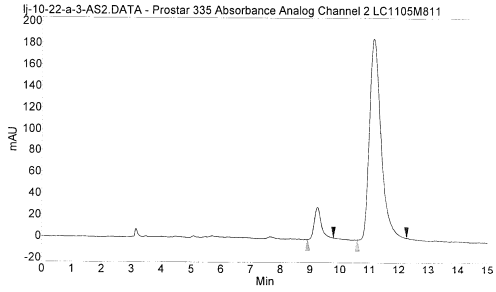
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV215 nm.

Racemic standard



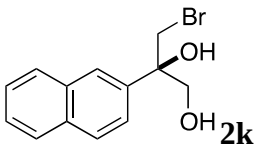
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.08	49.846	8.78	10.11
2	11.01	50.154	10.59	12.03
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.24	8.494	8.92	9.78
2	11.15	91.506	10.59	12.26
Total		100.000		

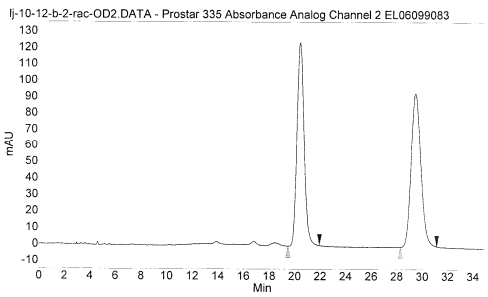
Table 2, entry 11



2k

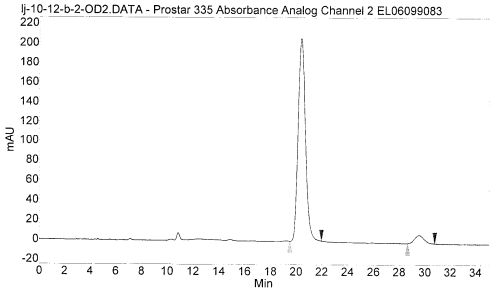
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV230 nm.

Racemic standard



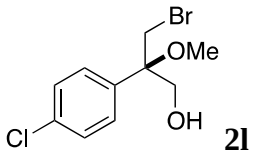
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	20.39	49.957	19.47	21.92
2	29.44	50.043	28.28	31.14
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	20.36	94.988	19.50	21.96
2	29.53	5.012	28.64	30.77
Total		100.000		

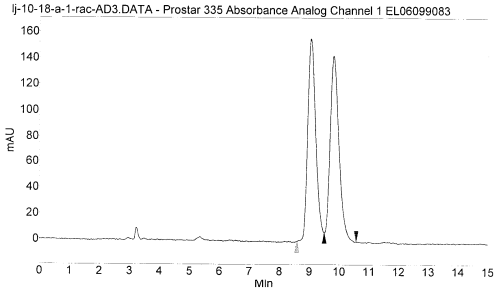
Table 2, entry 12



2l

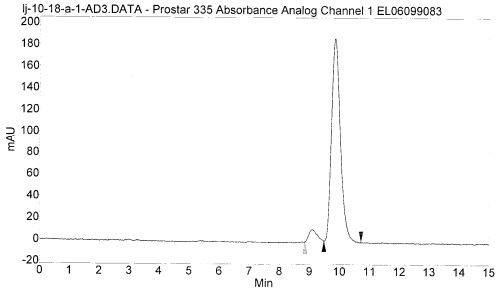
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV215 nm.

Racemic standard



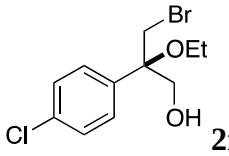
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.04	50.074	8.59	9.50
2	9.80	49.926	9.50	10.57
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.09	4.974	8.85	9.49
2	9.84	95.026	9.49	10.71
Total		100.000		

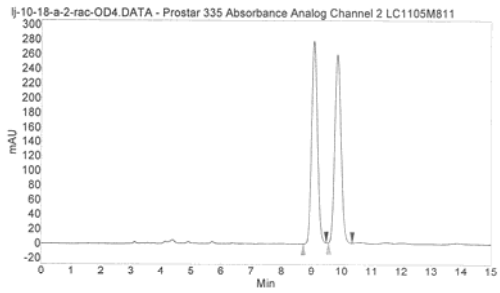
Table 2, entry 13



2m

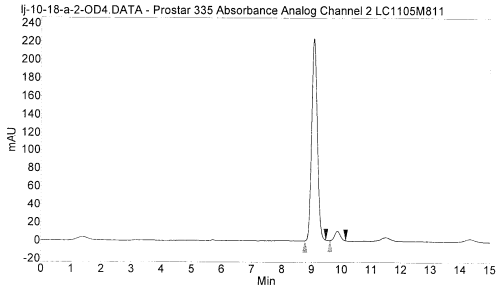
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



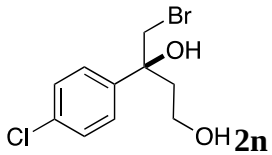
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.08	49.937	8.73	9.49
2	9.87	50.063	9.57	10.36
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.08	95.456	8.78	9.47
2	9.87	4.544	9.61	10.14
Total		100.000		

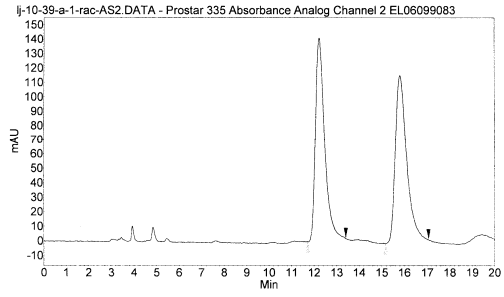
Table 2, entry 14



2n

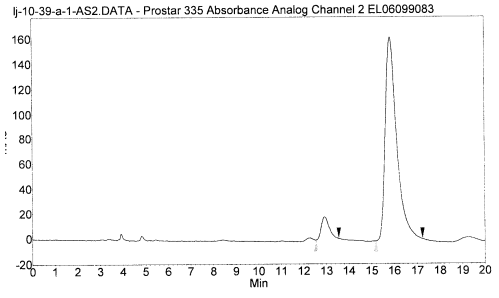
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



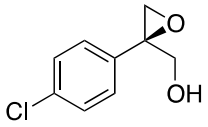
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	12.24	49.824	11.72	13.41
2	15.81	50.176	15.17	17.07
Total		100.000		

Enantio-enriched product



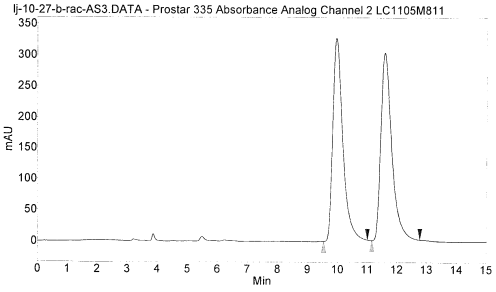
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	12.92	7.148	12.54	13.55
2	15.84	92.852	15.19	17.23
Total		100.000		

Scheme 3, epoxide 4



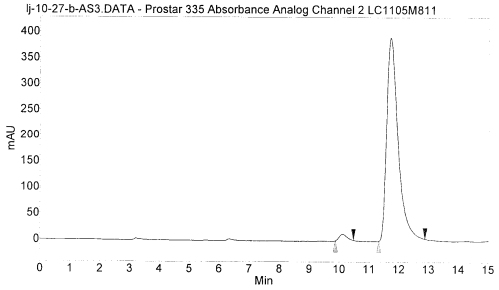
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



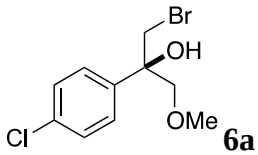
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.95	49.829	9.54	11.01
2	11.57	50.171	11.16	12.77
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.11	2.046	9.88	10.48
2	11.72	97.954	11.33	12.88
Total		100.000		

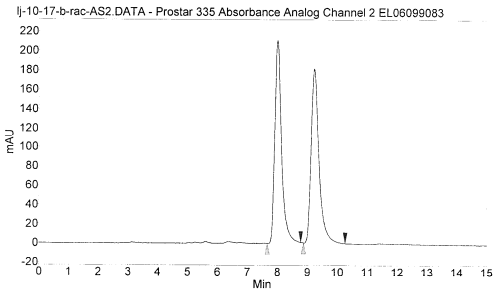
Table 3, entry 1



6a

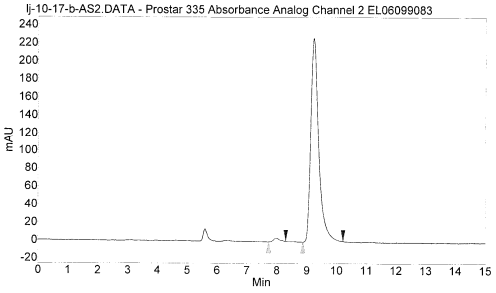
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



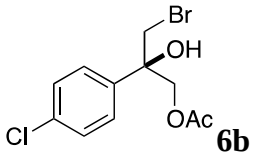
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	7.99	49.897	7.66	8.78
2	9.21	50.103	8.87	10.26
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	7.96	1.168	7.72	8.30
2	9.23	98.832	8.87	10.22
Total		100.000		

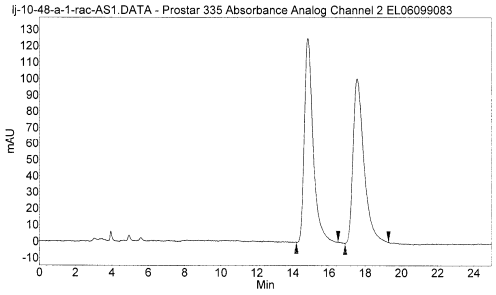
Table 3, entry 2



6b

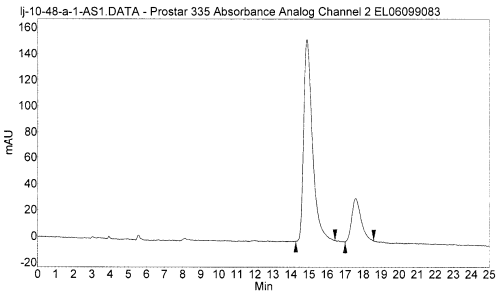
HPLC Condition: Column: Chiralpak AS-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



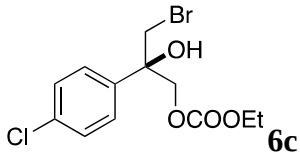
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	14.84	50.045	14.20	16.52
2	17.56	49.955	16.91	19.30
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	14.91	81.652	14.28	16.45
2	17.59	18.348	17.02	18.60
Total		100.000		

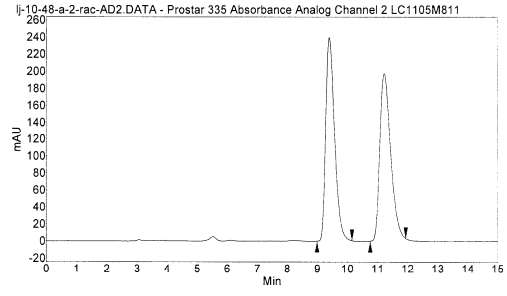
Table 3, entry 3



6c

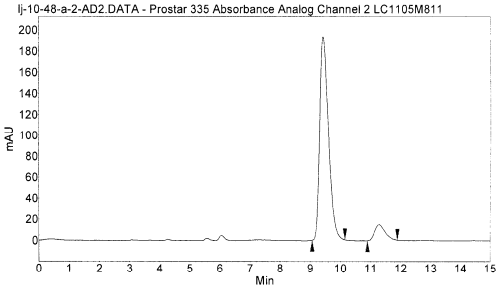
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



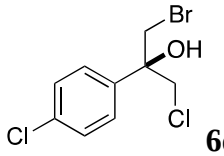
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.40	50.062	8.99	10.16
2	11.21	49.938	10.76	11.94
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.43	91.619	9.07	10.16
2	11.28	8.381	10.90	11.89
Total		100.000		

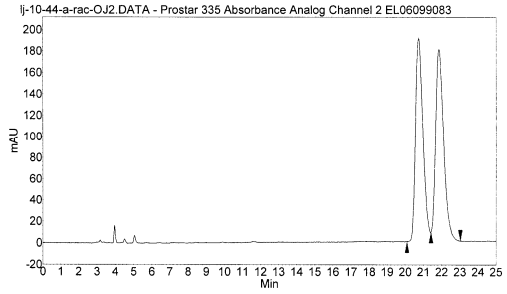
Table 3, entry 4



6d

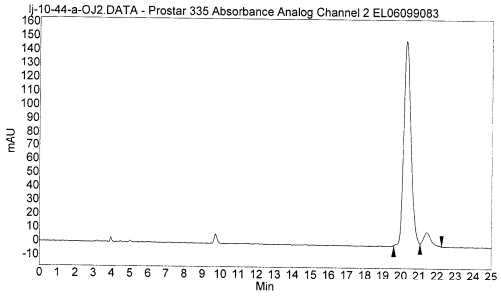
HPLC Condition: Column: Chiralpak OJ-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



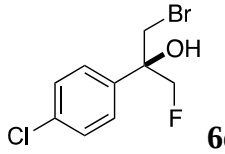
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	20.72	49.869	20.10	21.41
2	21.84	50.131	21.41	23.04
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	20.27	93.317	19.60	21.05
2	21.41	6.683	21.05	22.24
Total		100.000		

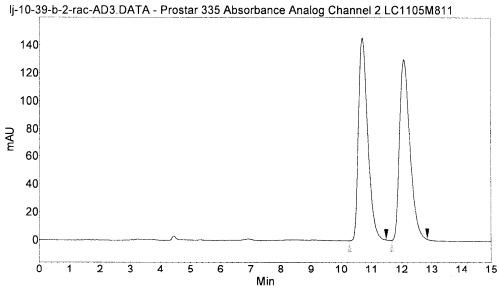
Table 3, entry 5



6e

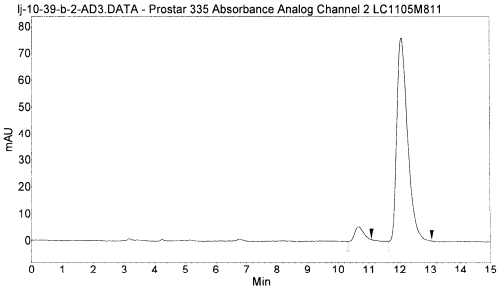
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



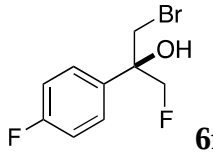
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.71	49.817	10.28	11.49
2	12.08	50.183	11.67	12.85
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.67	5.132	10.32	11.08
2	12.07	94.868	11.63	13.05
Total		100.000		

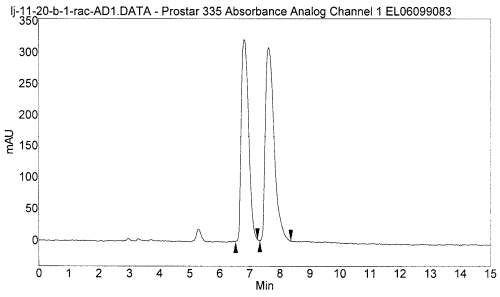
Table 3, entry 6



6f

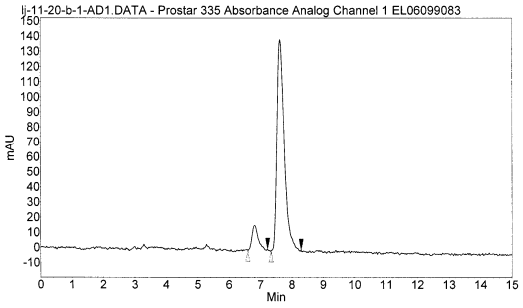
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



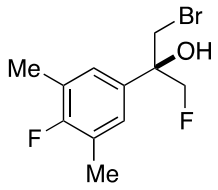
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	6.81	50.087	6.53	7.26
2	7.63	49.913	7.34	8.37
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	6.80	7.673	6.59	7.23
2	7.61	92.327	7.34	8.30
Total		100.000		

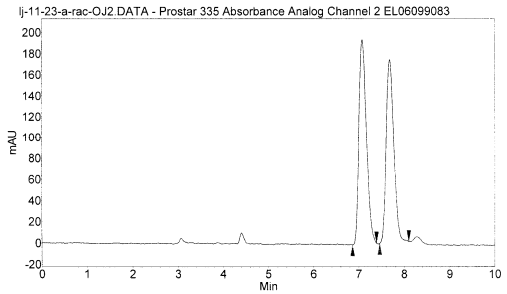
Table 3, entry 7



6g

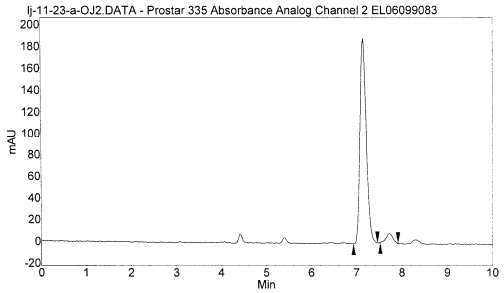
HPLC Condition: Column: Chiralpak OJ-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



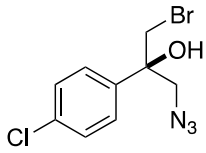
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	7.08	50.018	6.86	7.39
2	7.68	49.982	7.46	8.10
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	7.13	95.458	6.94	7.46
2	7.72	4.542	7.52	7.92
Total		100.000		

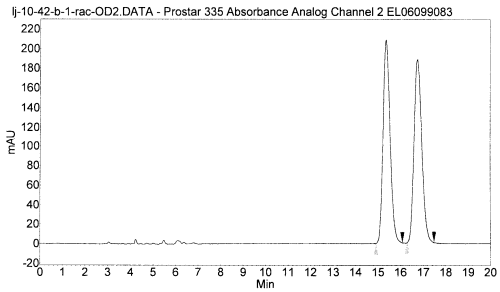
Table 3, entry 8



6h

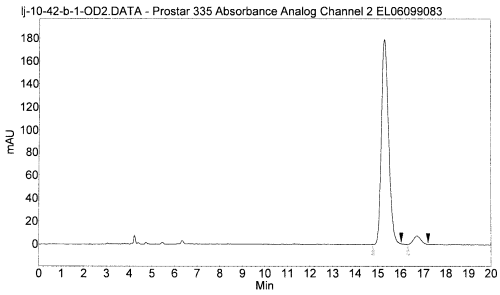
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



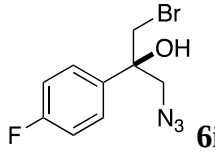
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	15.37	49.999	14.90	16.08
2	16.76	50.001	16.29	17.48
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	15.31	96.201	14.79	16.03
2	16.73	3.799	16.32	17.21
Total		100.000		

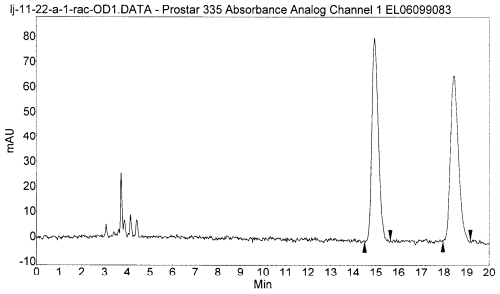
Table 3, entry 9



6i

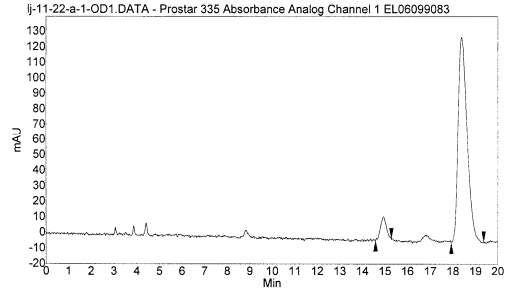
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



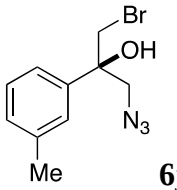
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	14.95	49.865	14.51	15.65
2	18.44	50.135	17.96	19.18
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	14.93	6.706	14.59	15.29
2	18.40	93.294	17.94	19.38
Total		100.000		

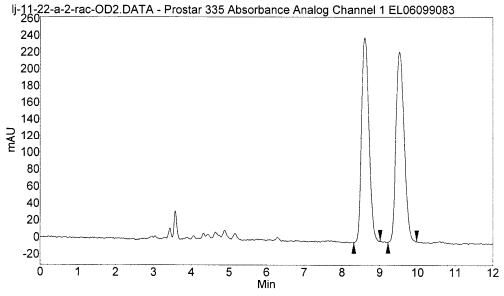
Table 3, entry 10



6j

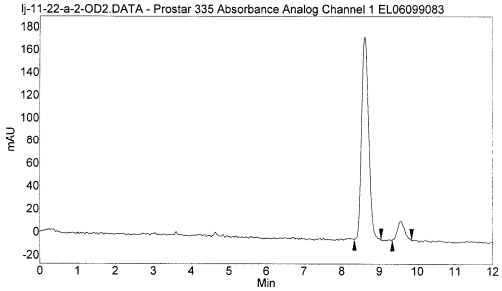
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



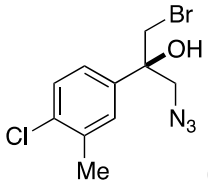
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	8.61	49.797	8.32	9.02
2	9.53	50.203	9.23	9.98
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	8.61	91.772	8.35	9.05
2	9.57	8.228	9.35	9.86
Total		100.000		

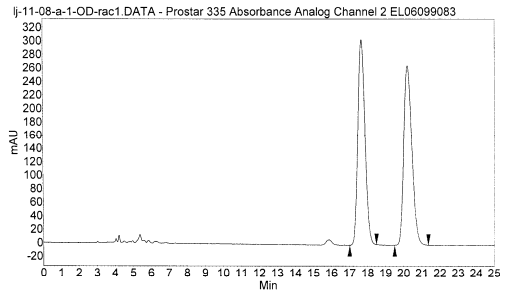
Table 3, entry 11



6k

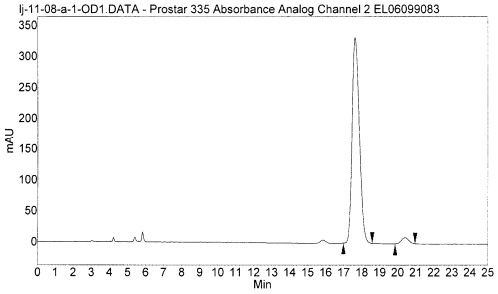
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV225 nm.

Racemic standard



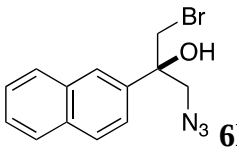
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	17.64	50.117	17.03	18.50
2	20.19	49.883	19.51	21.36
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	17.67	96.962	17.00	18.60
2	20.40	3.038	19.87	20.98
Total		100.000		

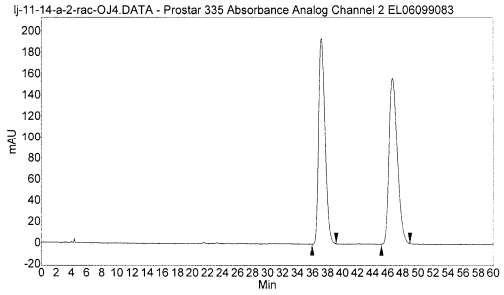
Table 3, entry 12



6l

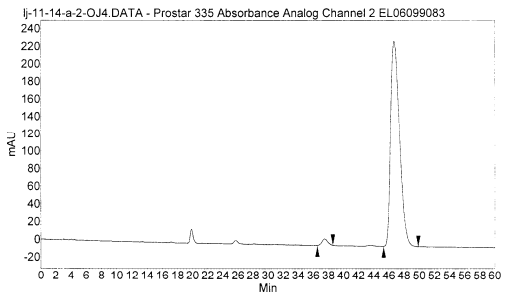
HPLC Condition: Column: Chiralpak OJ-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV230 nm.

Racemic standard



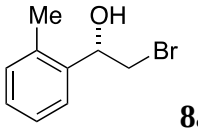
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	37.21	49.705	35.99	39.19
2	46.65	50.295	45.21	48.99
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	37.51	1.961	36.56	38.61
2	46.69	98.039	45.34	49.88
Total		100.000		

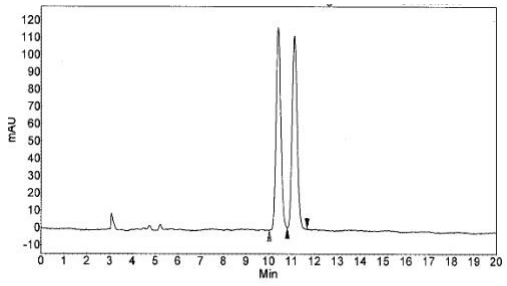
Table 4, entry 1



8a

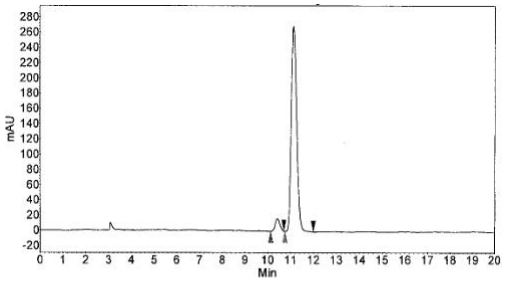
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



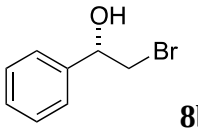
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.41	49.967	10.03	10.82
2	11.13	50.033	10.82	11.68
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.43	4.897	10.13	10.71
2	11.15	95.103	10.75	11.99
Total		100.000		

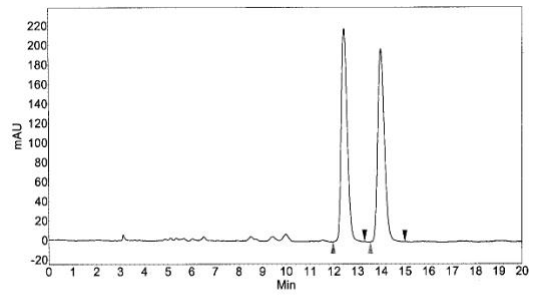
Table 4, entry 2



8b

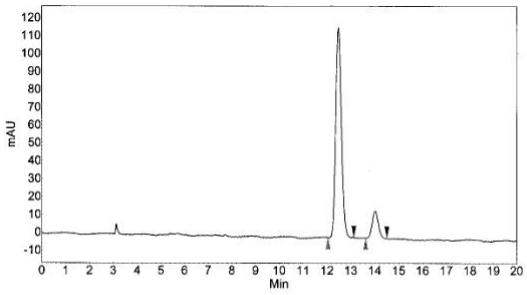
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



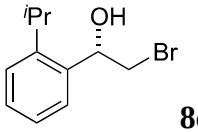
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	12.44	49.846	11.97	13.29
2	13.99	50.154	13.54	14.99
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	12.48	87.851	12.05	13.13
2	14.01	12.149	13.62	14.51
Total		100.000		

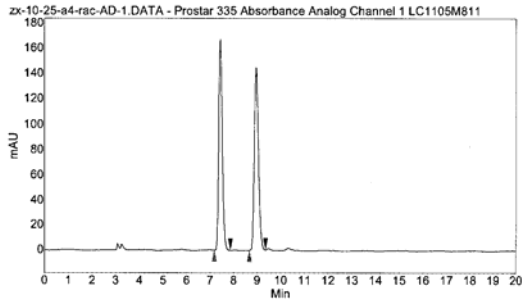
Table 4, entry 3



8c

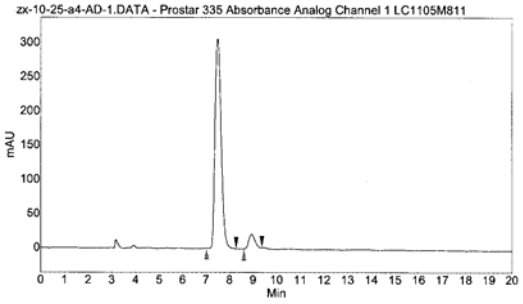
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



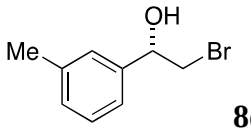
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	7.44	49.985	7.18	7.86
2	8.96	50.015	8.67	9.35
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	7.48	94.321	7.02	8.28
2	8.93	5.679	8.61	9.37
Total		100.000		

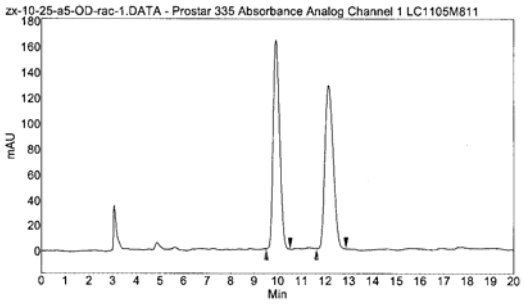
Table 4, entry 4



8d

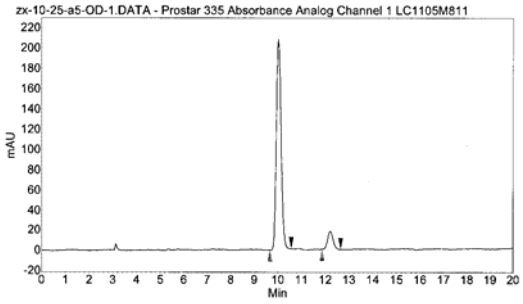
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



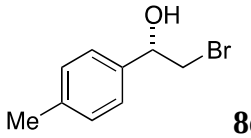
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.92	49.899	9.51	10.53
2	12.13	50.101	11.64	12.88
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.03	91.134	9.66	10.57
2	12.21	8.866	11.87	12.65
Total		100.000		

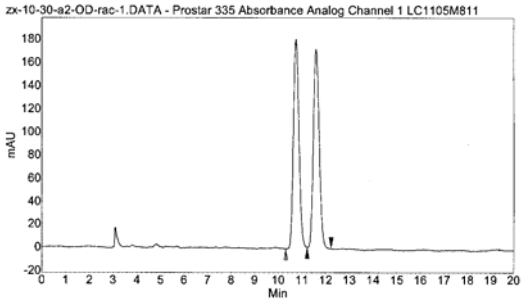
Table 4, entry 5



8e

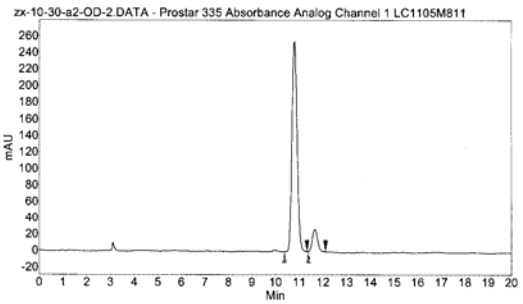
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



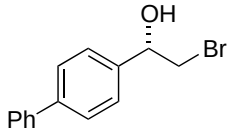
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.75	49.872	10.32	11.23
2	11.60	50.128	11.23	12.24
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.79	90.408	10.38	11.33
2	11.67	9.592	11.39	12.12
Total		100.000		

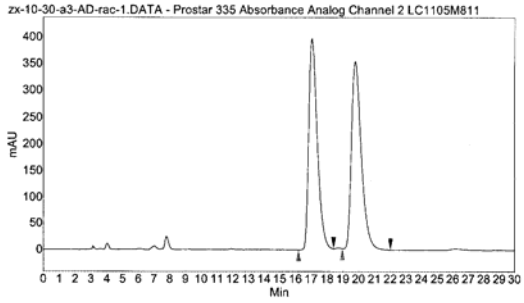
Table 4, entry 6



8f

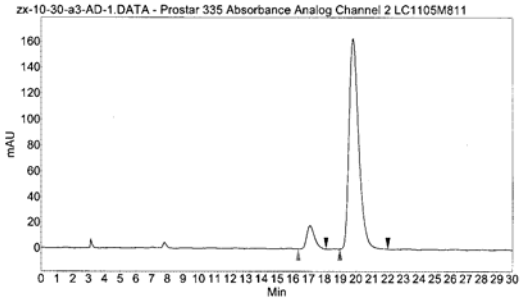
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



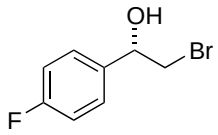
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	17.05	49.825	16.19	18.42
2	19.79	50.175	18.98	22.01
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	17.08	8.341	16.35	18.11
2	19.80	91.659	18.98	22.01
Total		100.000		

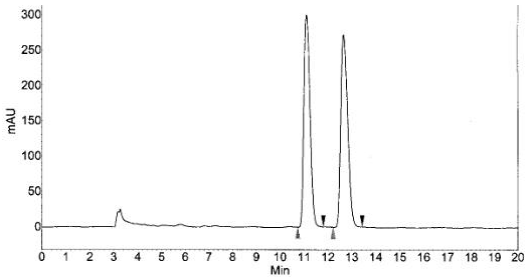
Table 4, entry 7



8g

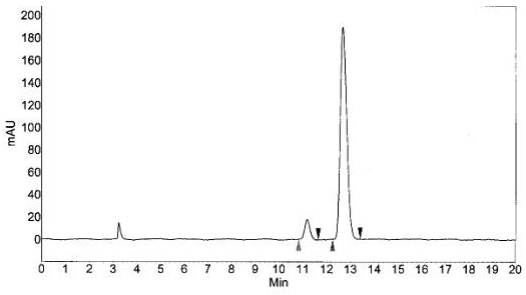
HPLC Condition: Column: Chiralpak OB-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



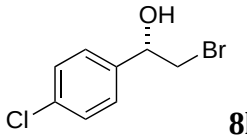
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.09	49.333	10.73	11.81
2	12.65	50.667	12.22	13.44
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.20	7.031	10.84	11.66
2	12.69	92.969	12.26	13.42
Total		100.000		

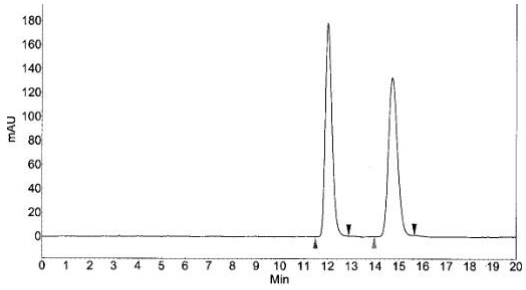
Table 4, entry 8



8h

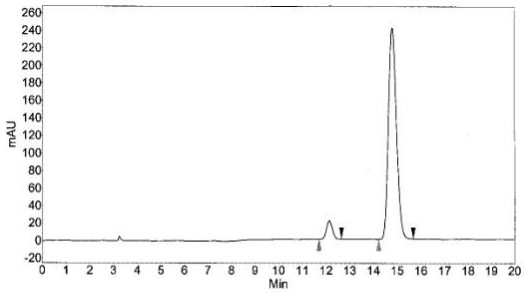
HPLC Condition: Column: Chiralpak OB-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



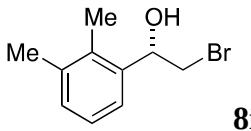
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	12.15	50.060	11.72	12.84
2	14.85	49.940	14.03	15.57
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	12.13	6.159	11.70	12.65
2	14.76	93.841	14.22	15.67
Total		100.000		

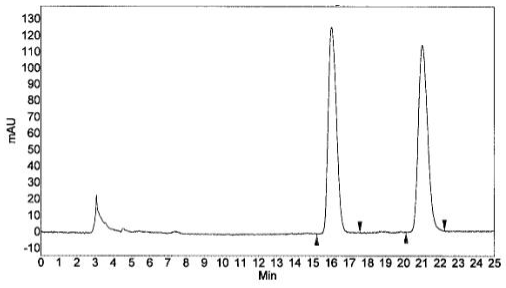
Table 4, entry 9



8i

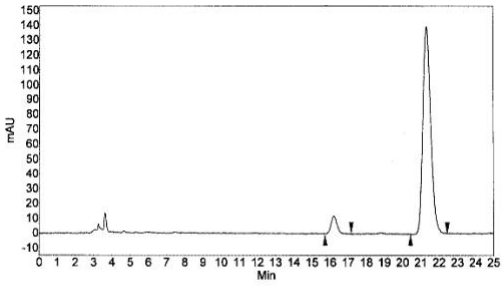
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



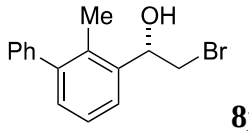
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	16.04	49.719	15.21	17.59
2	21.03	50.281	20.12	22.24
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	16.21	6.113	15.73	17.17
2	21.31	93.887	20.43	22.44
Total		100.000		

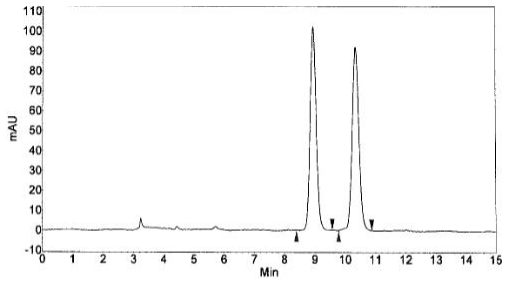
Table 4, entry 10



8j

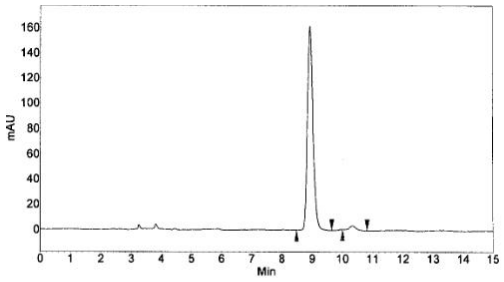
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



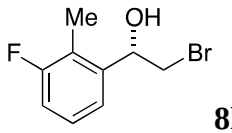
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	8.93	50.005	8.39	9.57
2	10.33	49.995	9.78	10.87
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	8.93	97.958	8.48	9.64
2	10.33	2.042	10.00	10.81
Total		100.000		

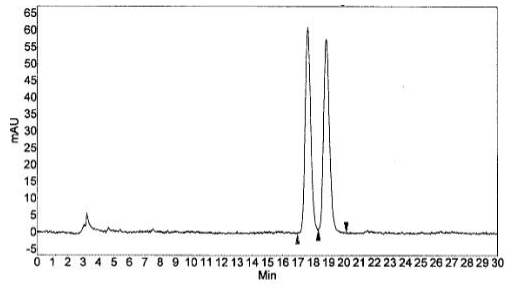
Table 4, entry 11



8k

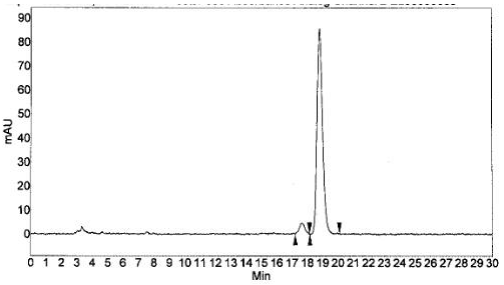
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



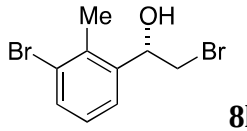
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	17.65	49.771	16.97	18.33
2	18.85	50.229	18.33	20.16
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	17.67	4.880	17.21	18.14
2	18.80	95.120	18.17	20.09
Total		100.000		

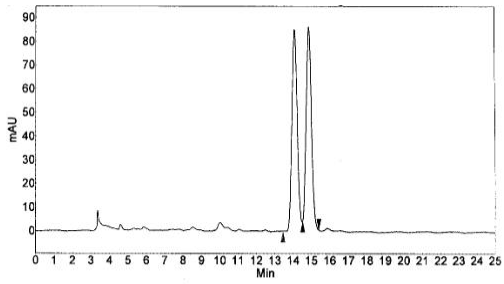
Table 4, entry 12



8l

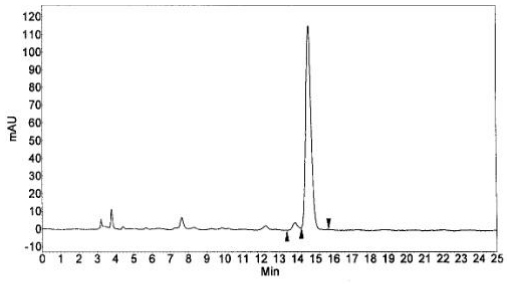
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



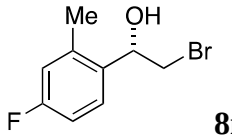
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	14.07	49.773	13.44	14.53
2	14.85	50.227	14.53	15.40
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	13.87	3.506	13.42	14.22
2	14.60	96.494	14.22	15.71
Total		100.000		

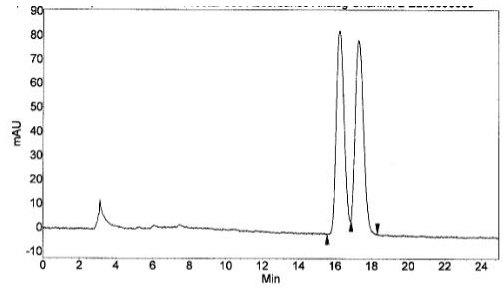
Table 4, entry 13



8m

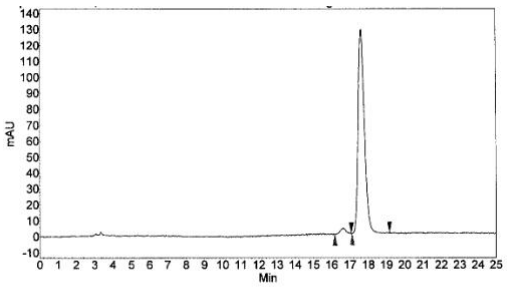
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



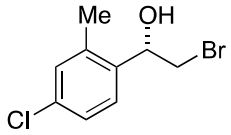
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	16.27	49.751	15.57	16.88
2	17.31	50.249	16.88	18.32
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	16.65	2.496	16.18	17.08
2	17.64	97.504	17.13	19.17
Total		100.000		

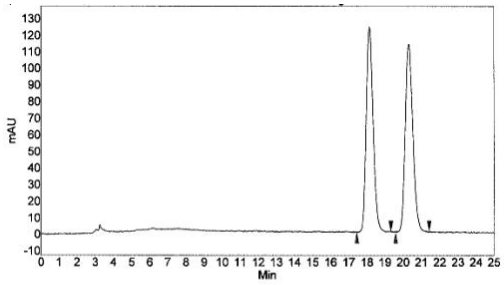
Table 4, entry 14



8n

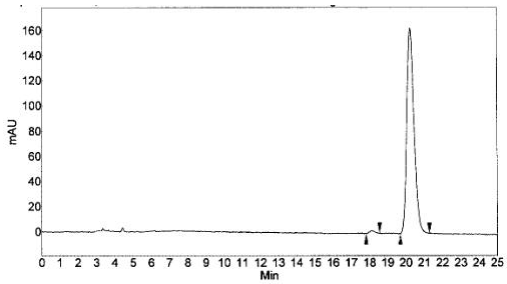
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



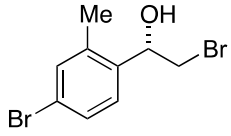
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	18.15	49.941	17.44	19.32
2	20.31	50.059	19.58	21.41
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	18.16	0.947	17.82	18.56
2	20.24	99.053	19.70	21.27
Total		100.000		

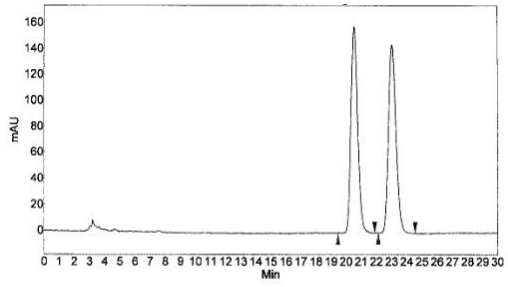
Table 4, entry 15



8o

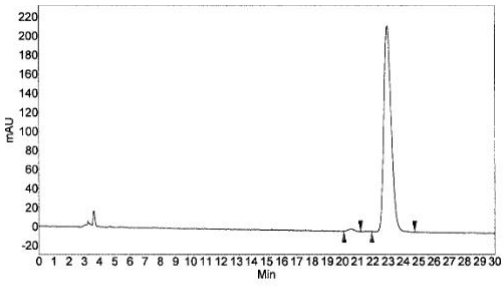
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



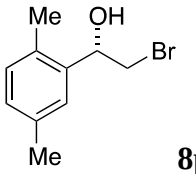
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	20.53	50.091	19.46	21.88
2	23.03	49.909	22.13	24.55
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	20.57	0.906	20.11	21.20
2	22.96	99.094	21.94	24.73
Total		100.000		

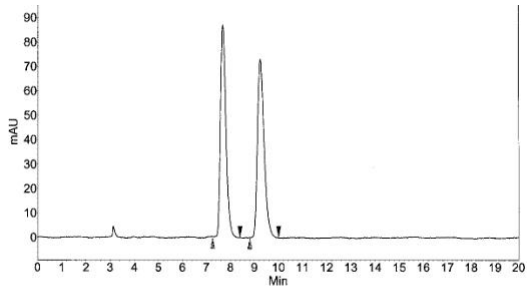
Table 4, entry 16



8p

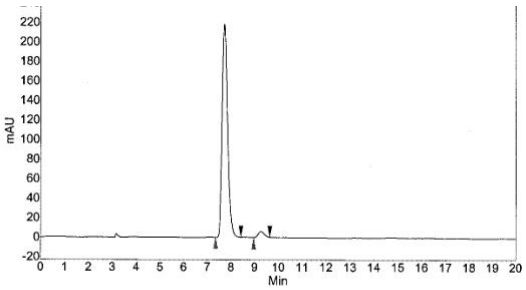
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



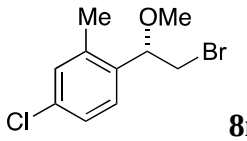
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	7.68	49.599	7.26	8.40
2	9.24	50.401	8.81	10.01
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	7.71	96.994	7.35	8.42
2	9.25	3.006	8.96	9.64
Total		100.000		

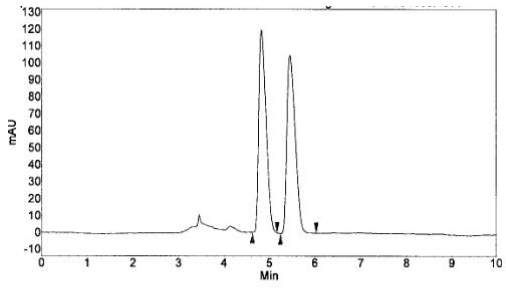
Table 4, entry 17



8n'

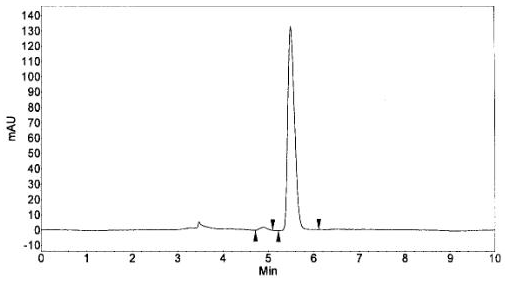
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



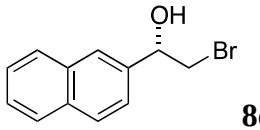
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	4.83	50.131	4.62	5.17
2	5.45	49.869	5.24	6.03
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	4.89	1.535	4.72	5.10
2	5.49	98.465	5.22	6.11
Total		100.000		

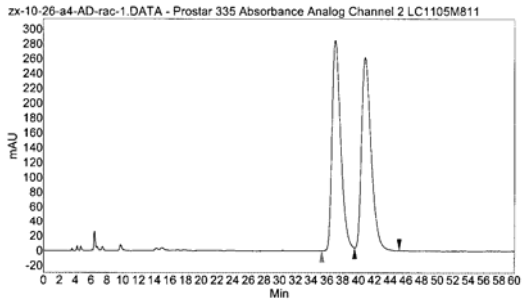
Table 4, entry 18



8q

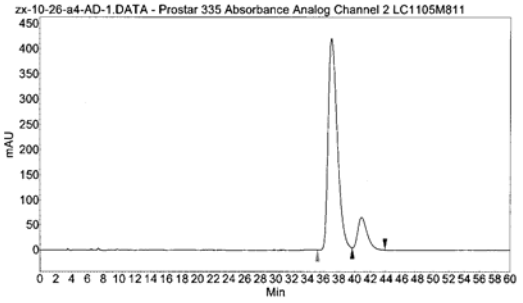
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



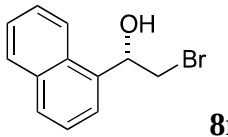
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	37.08	49.604	35.36	39.50
2	40.85	50.396	39.50	45.14
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	37.11	86.055	35.29	39.69
2	40.87	13.945	39.69	43.84
Total		100.000		

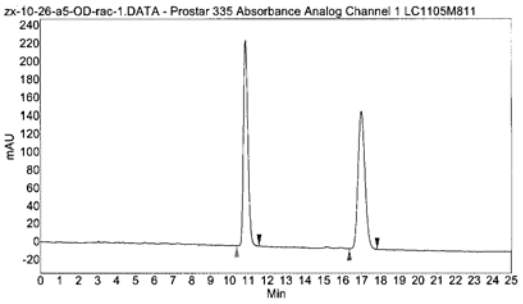
Table 4, entry 19



8r

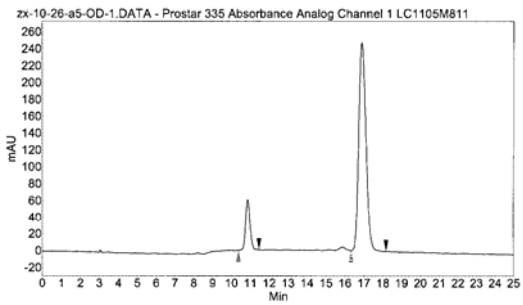
HPLC Condition: Column: Chiralpak OD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (90/10); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



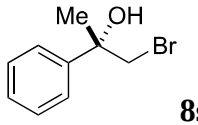
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.87	49.801	10.40	11.58
2	17.00	50.199	16.36	17.83
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.85	13.052	10.37	11.46
2	16.91	86.948	16.33	18.16
Total		100.000		

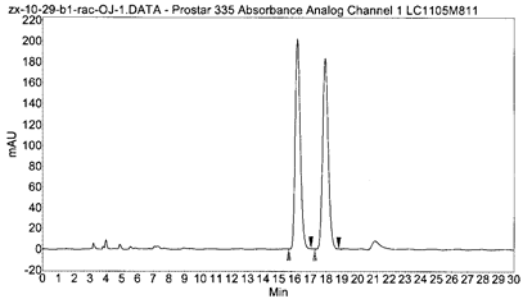
Table 4, entry 20



8s

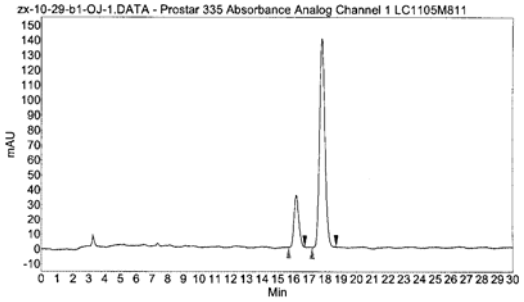
HPLC Condition: Column: Chiralpak OJ-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



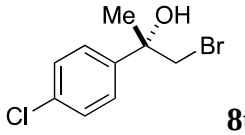
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	16.17	49.844	15.63	17.06
2	17.80	50.156	17.14	18.66
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	16.17	18.003	15.70	16.72
2	17.81	81.997	17.18	18.70
Total		100.000		

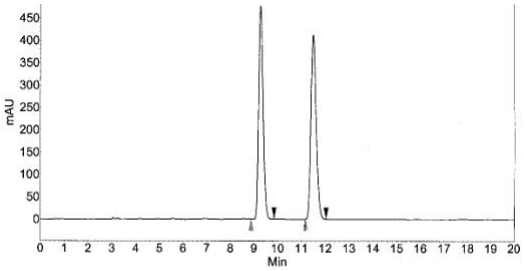
Table 4, entry 21



8t

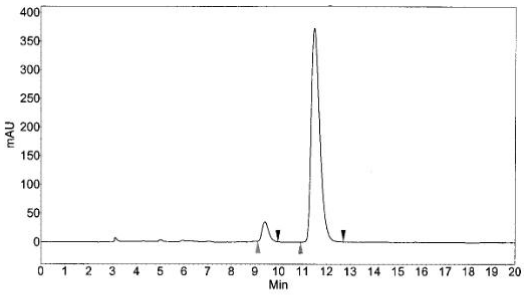
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



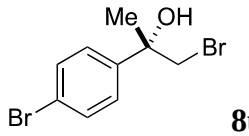
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.28	49.901	8.88	9.85
2	11.49	50.099	11.17	12.04
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	9.41	6.632	9.12	9.97
2	11.51	93.368	10.92	12.71
Total		100.000		

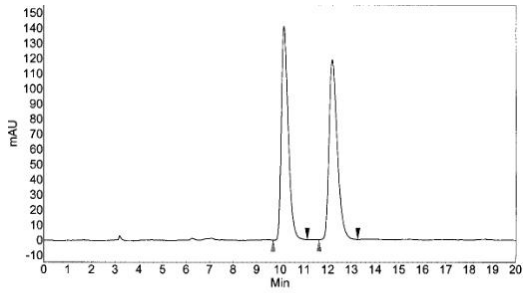
Table 4, entry 22



8u

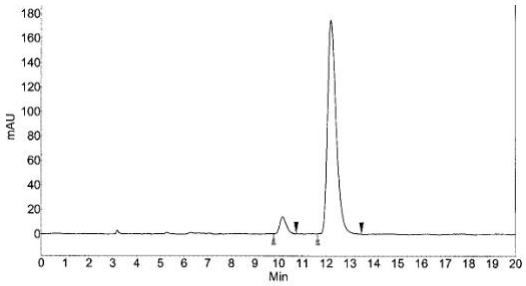
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV220 nm.

Racemic standard



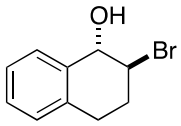
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.17	49.926	9.70	11.15
2	12.21	50.074	11.64	13.27
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	10.16	5.678	9.78	10.73
2	12.20	94.322	11.64	13.48
Total		100.000		

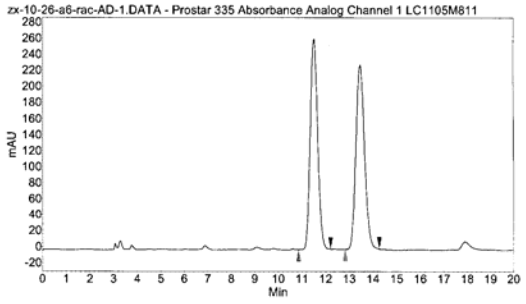
Table 4, entry 23



8v

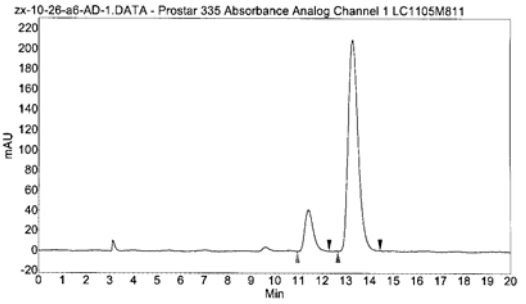
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



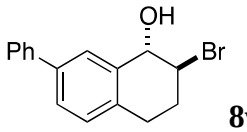
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.45	49.748	11.04	12.20
2	13.43	50.252	12.98	14.16
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	11.41	14.433	10.96	12.30
2	13.27	85.567	12.67	14.45
Total		100.000		

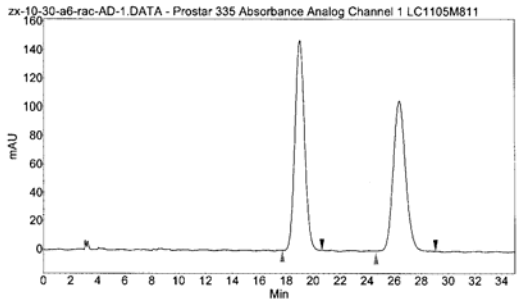
Table 4, entry 24



8w

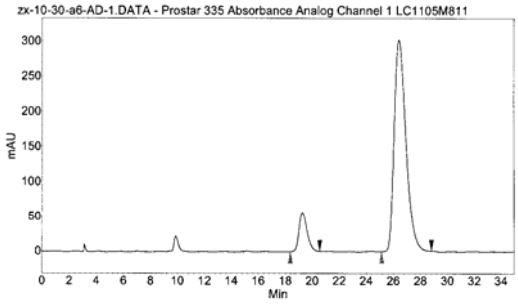
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (95/5); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



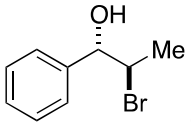
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	19.31	49.961	17.85	20.34
2	26.39	50.039	24.75	29.17
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	19.28	11.089	18.38	20.55
2	26.37	88.911	25.14	28.82
Total		100.000		

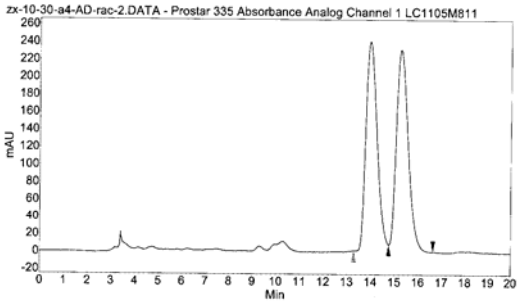
Table 4, entry 25



8x

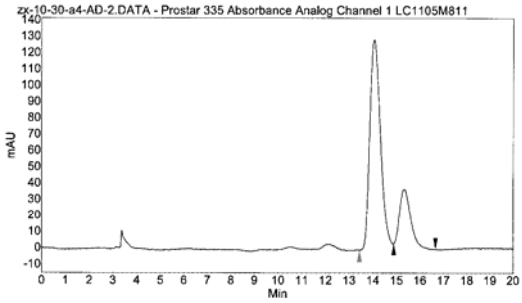
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



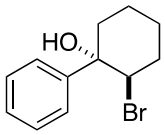
Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	13.97	49.994	13.29	14.76
2	15.28	50.006	14.76	16.64
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	14.07	76.043	13.44	14.88
2	15.32	23.957	14.88	16.66
Total		100.000		

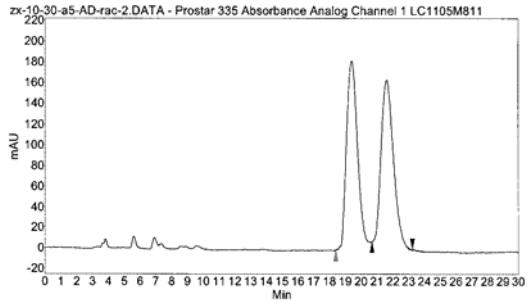
Table 4, entry 26



8y

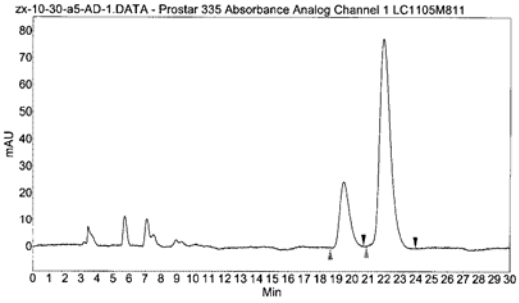
HPLC Condition: Column: Chiralpak AD-H, Daicel Chemical Industries, Ltd.; **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 1.0 mL/min; **Detection:** UV210 nm.

Racemic standard



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	19.53	50.033	18.48	20.85
2	21.91	49.967	20.85	23.42
Total		100.000		

Enantio-enriched product



Index	Time [Min]	Area % [%]	Start [Min]	End [Min]
1	19.48	21.888	18.64	20.71
2	21.99	78.112	20.90	23.96
Total		100.000		

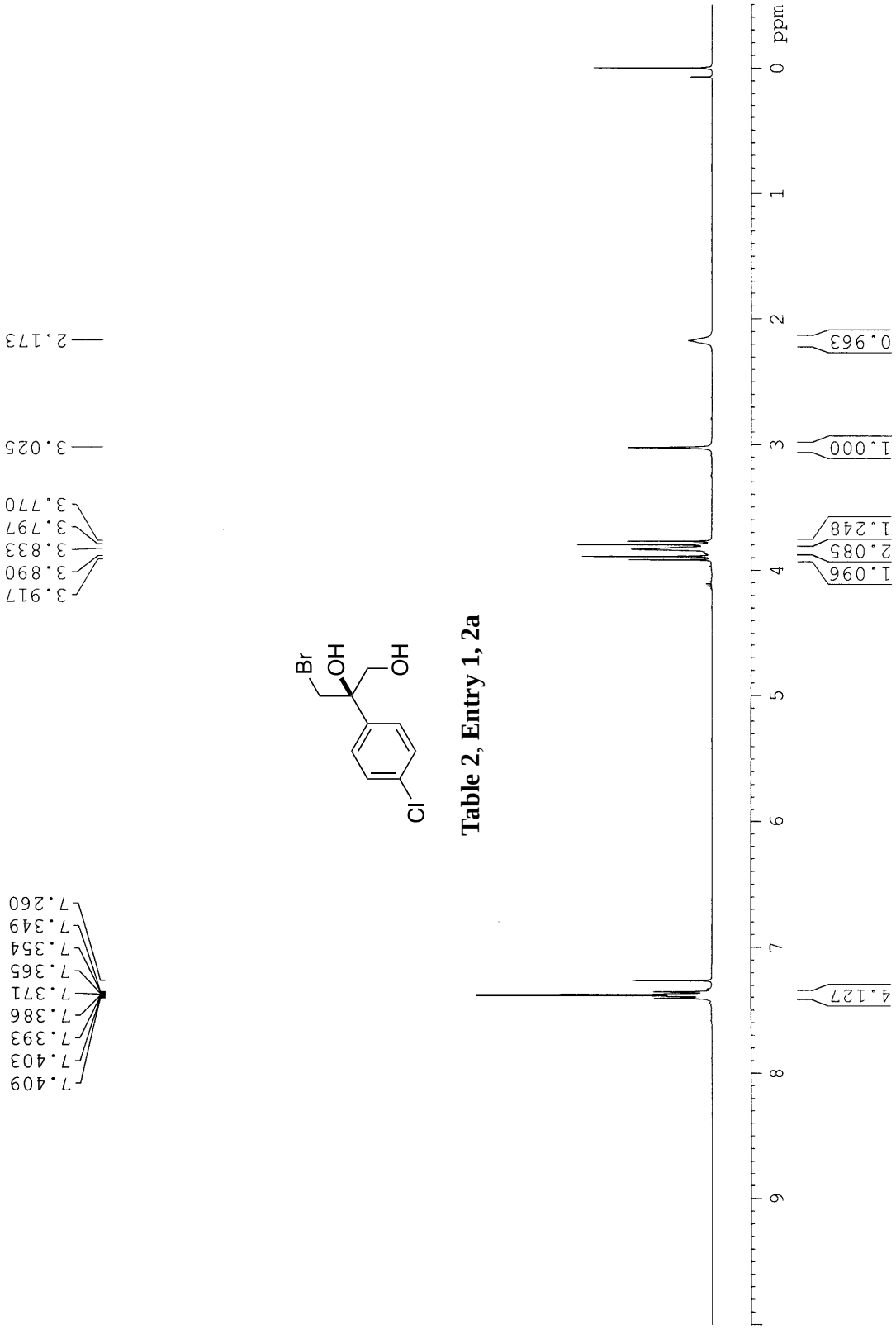


Table 2, Entry 1, 2a

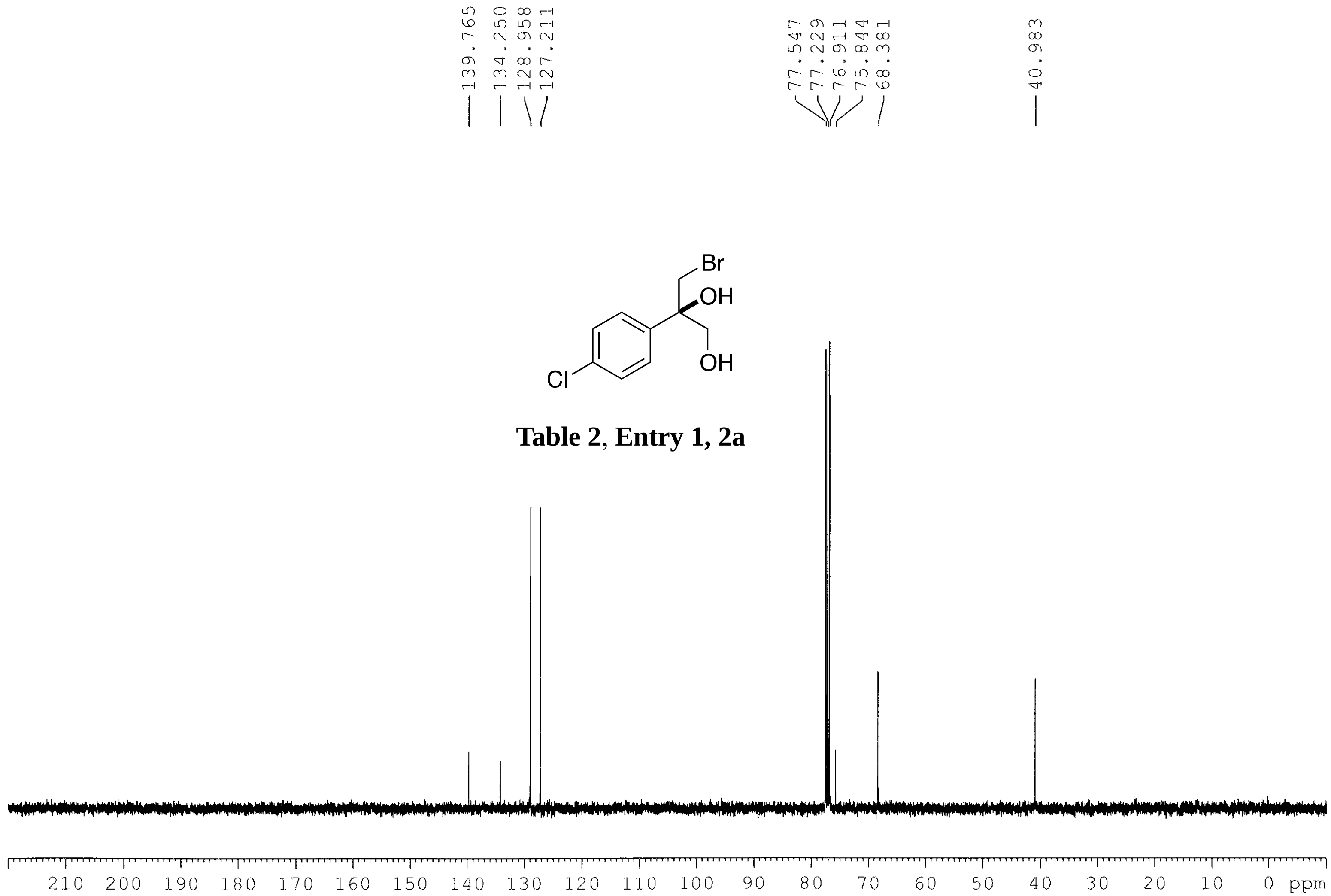
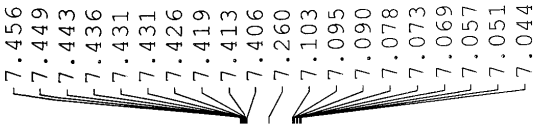
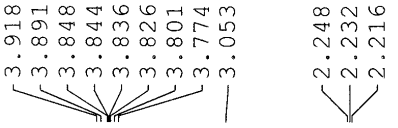


Table 2, Entry 1, 2a





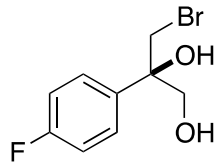
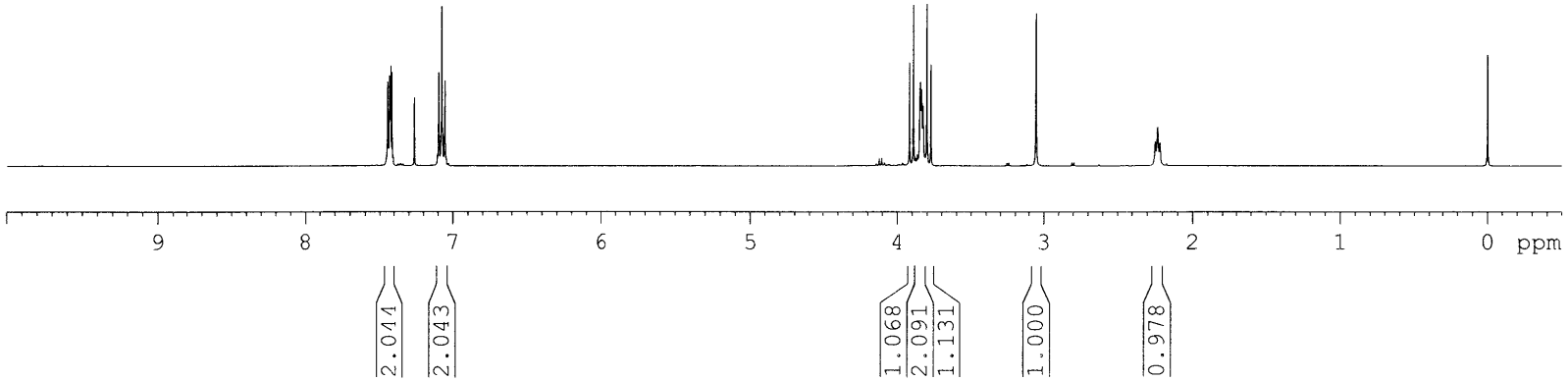


Table 2, **Entry 2, 2b**



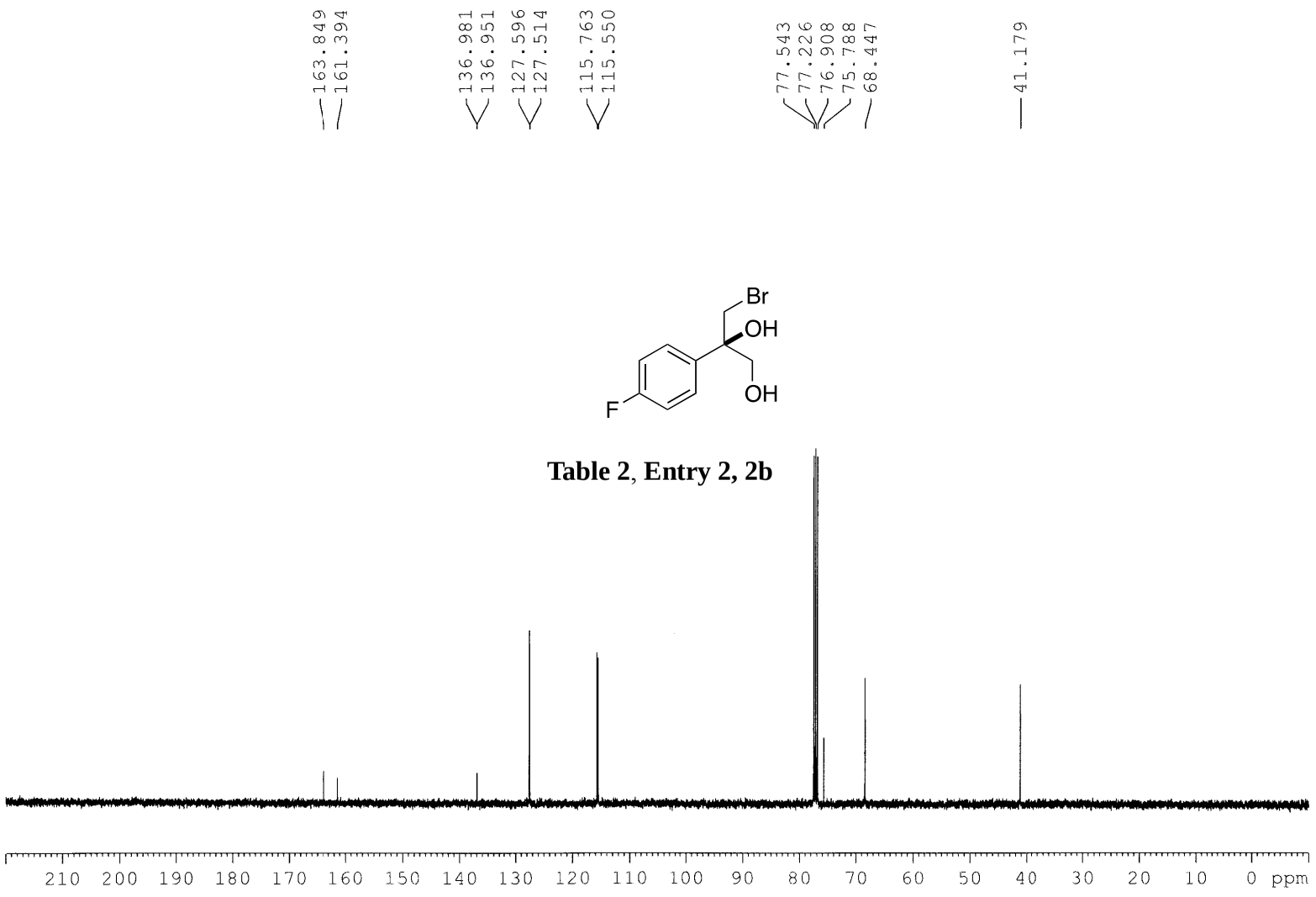


Table 2, Entry 2, 2b

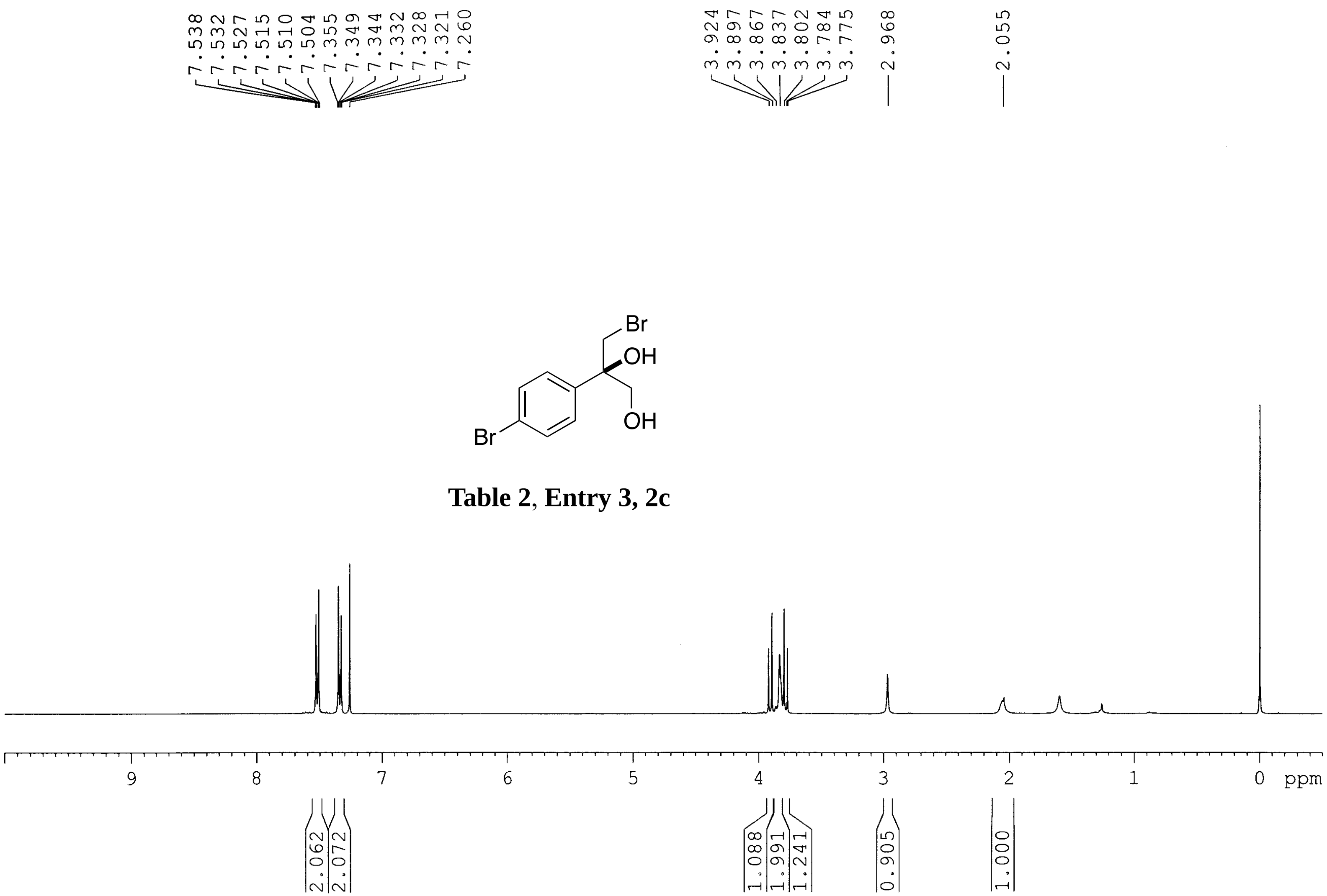


Table 2, Entry 3, 2c

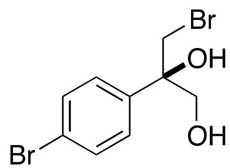
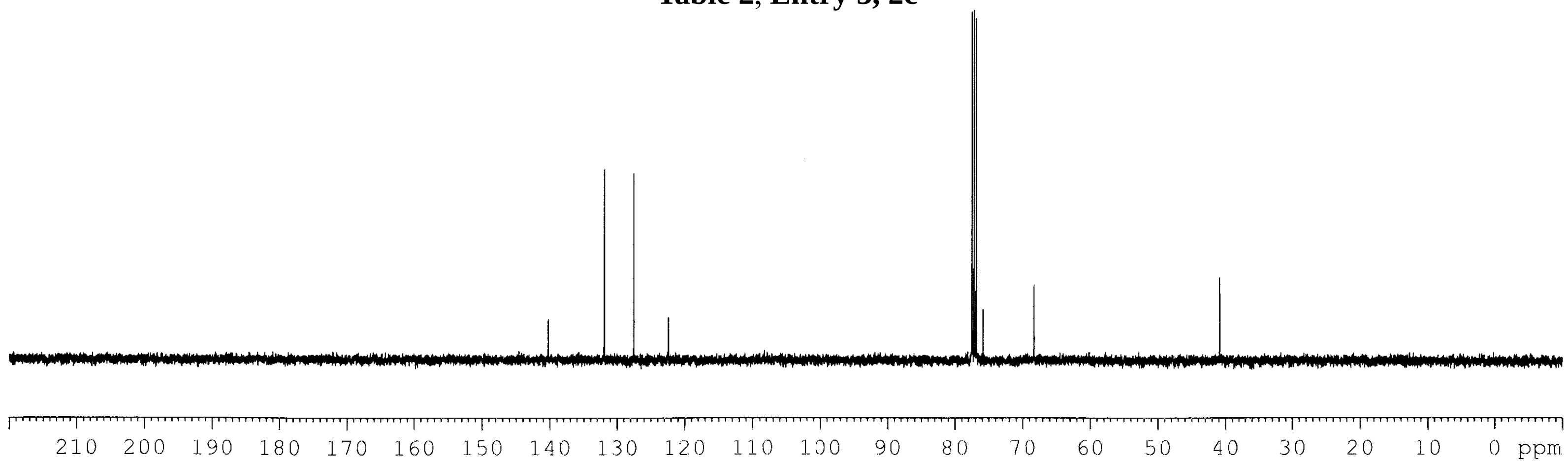
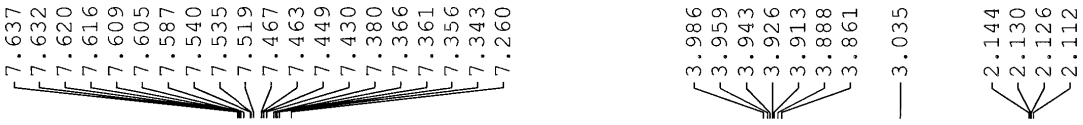


Table 2, **Entry 3, 2c**





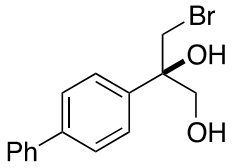
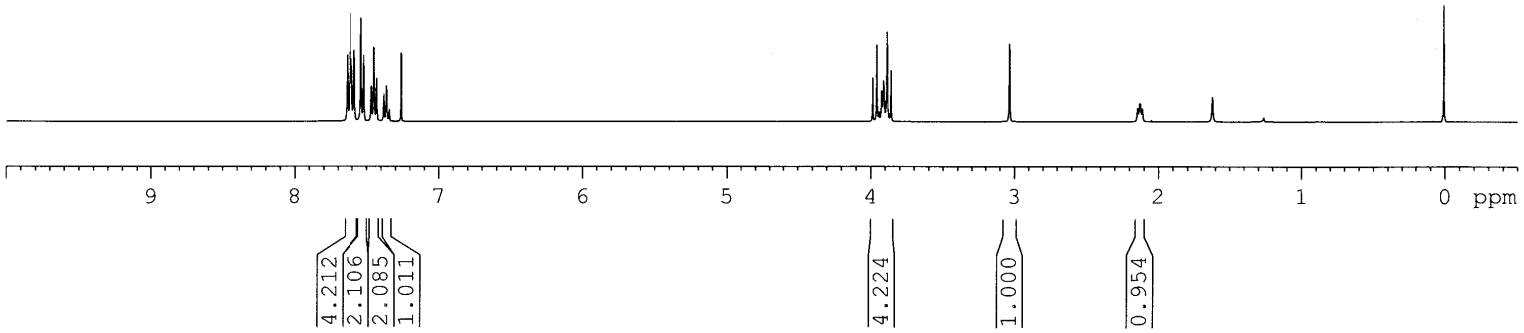


Table 2, **Entry 4, 2d**



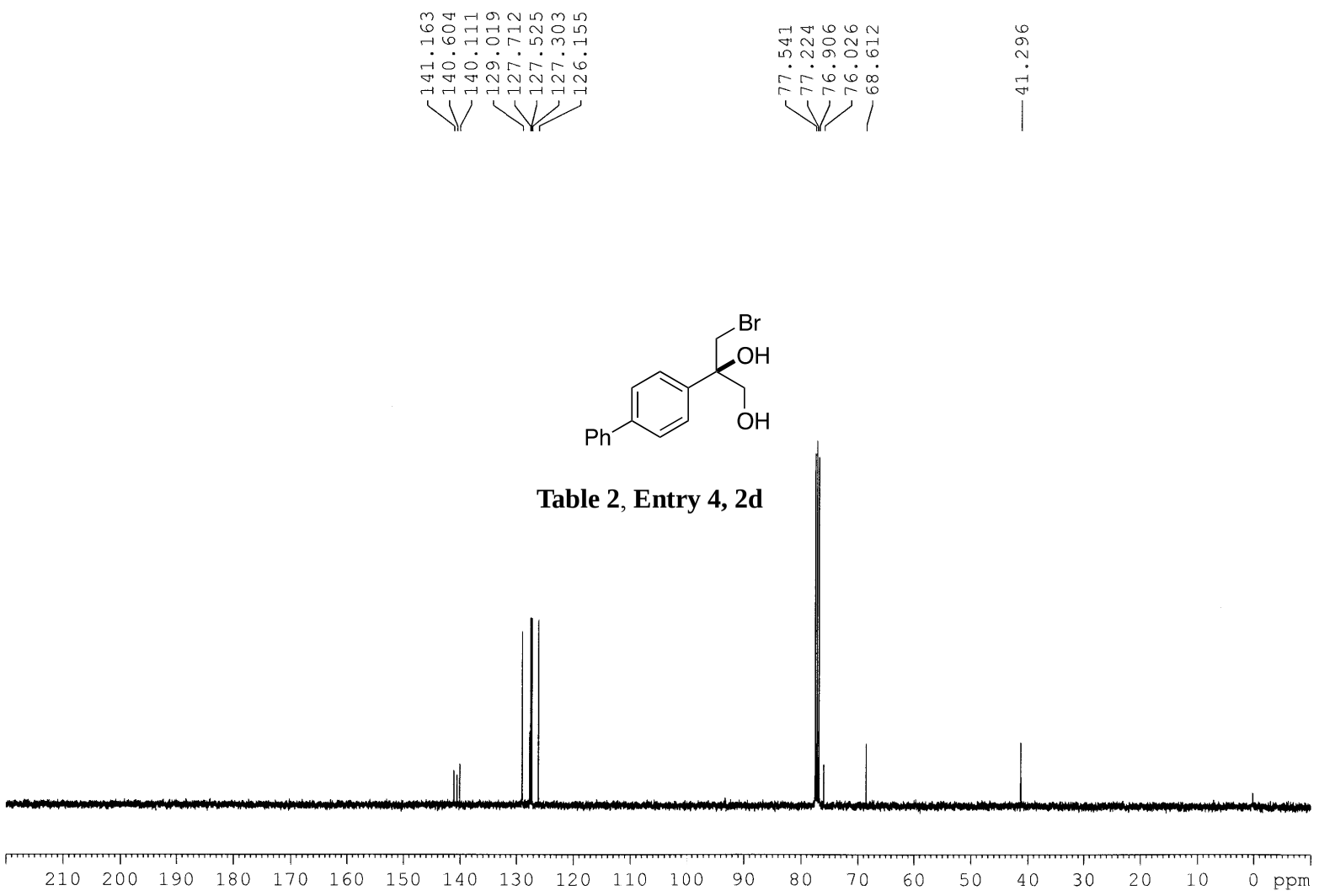


Table 2, Entry 4, 2d

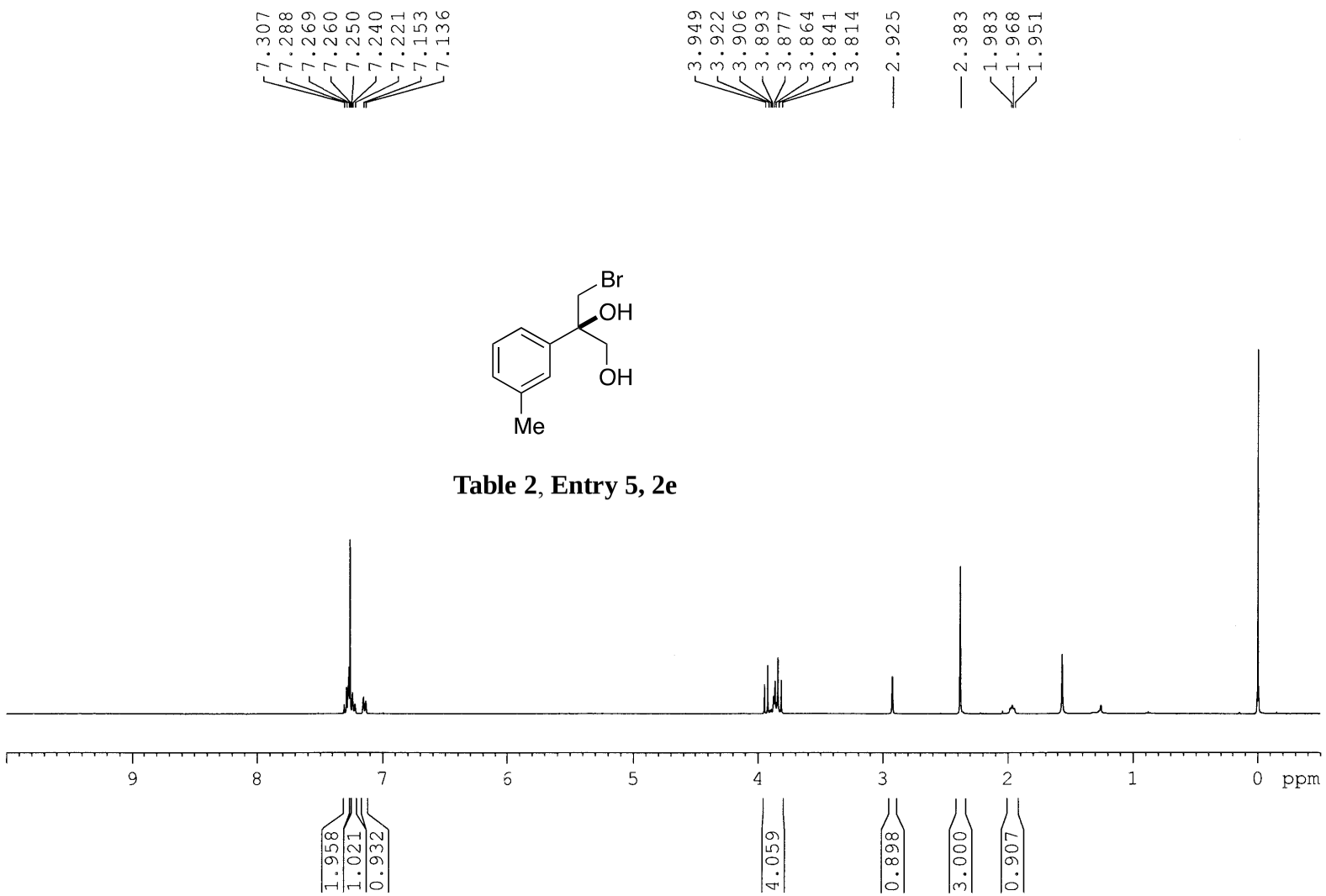
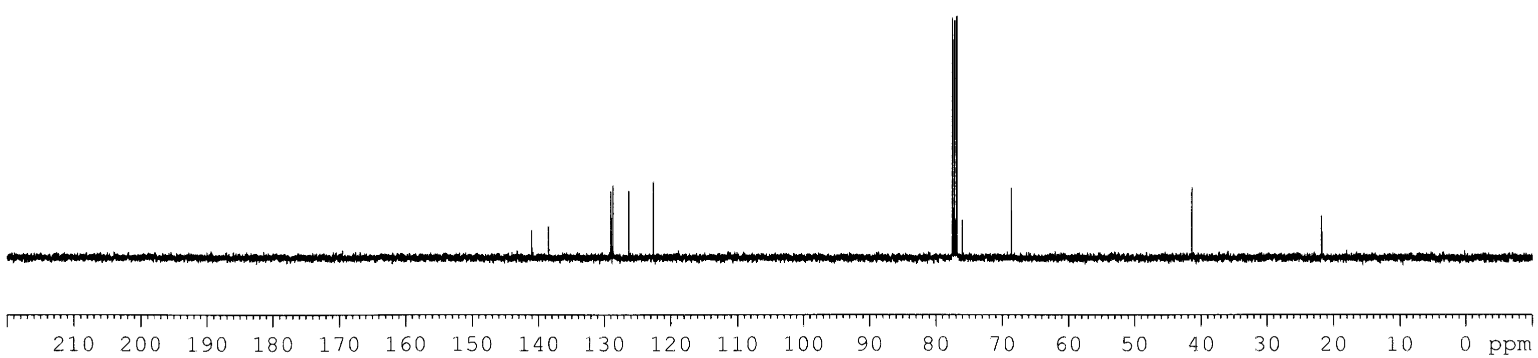
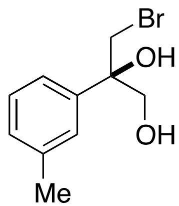


Table 2, **Entry 5, 2e**





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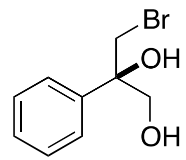
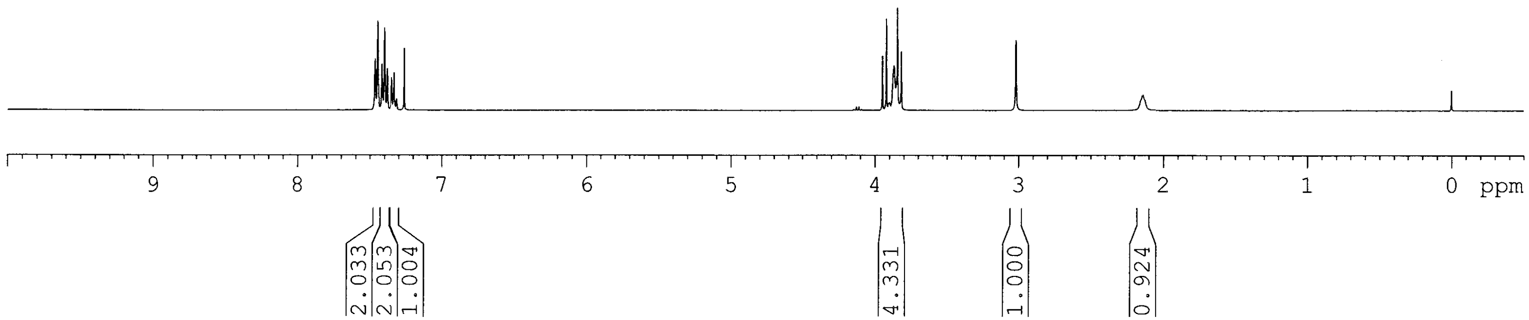


Table 2, Entry 6, 2f



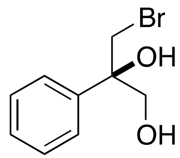
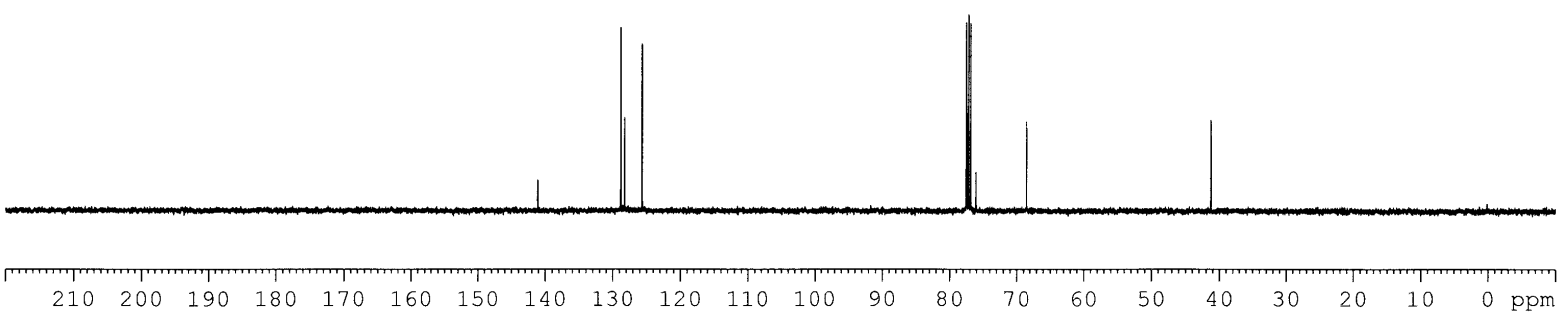


Table 2, Entry 6, 2f



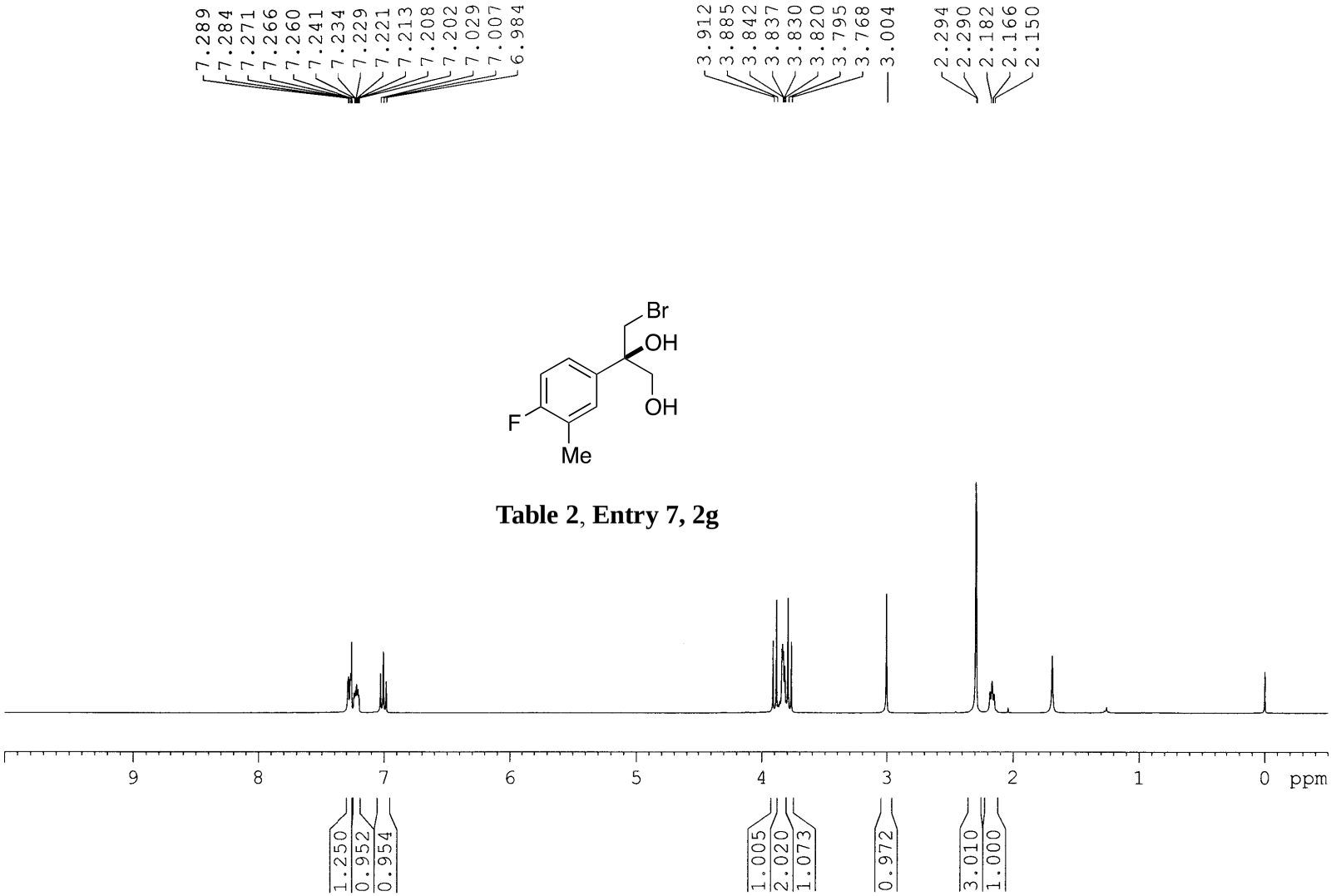
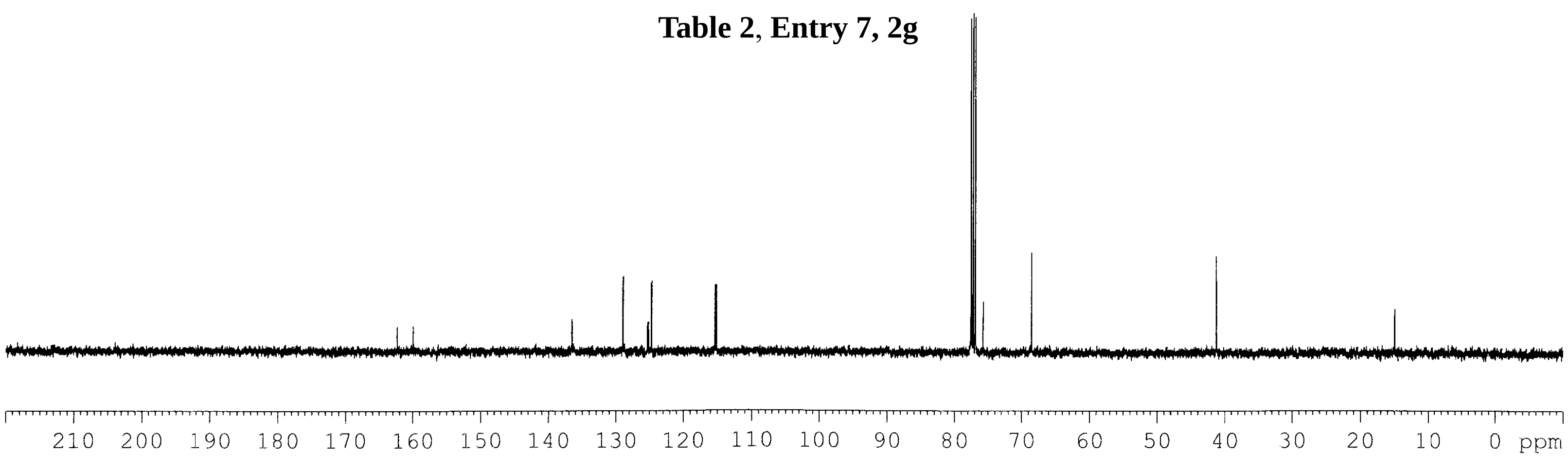


Table 2, **Entry 7, 2g**



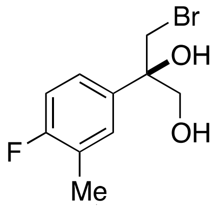


Table 2, Entry 7, 2g

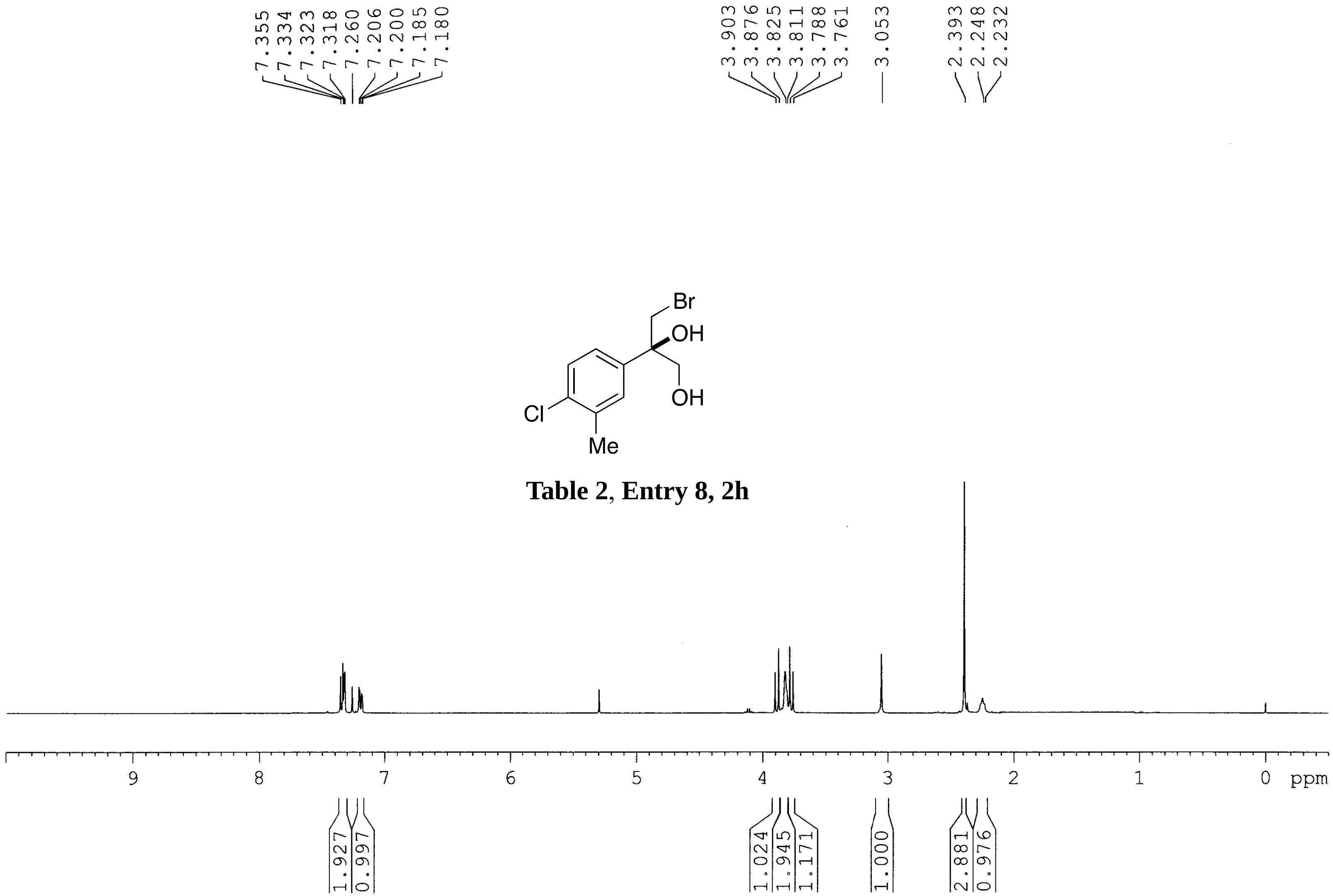


Table 2, Entry 8, 2h

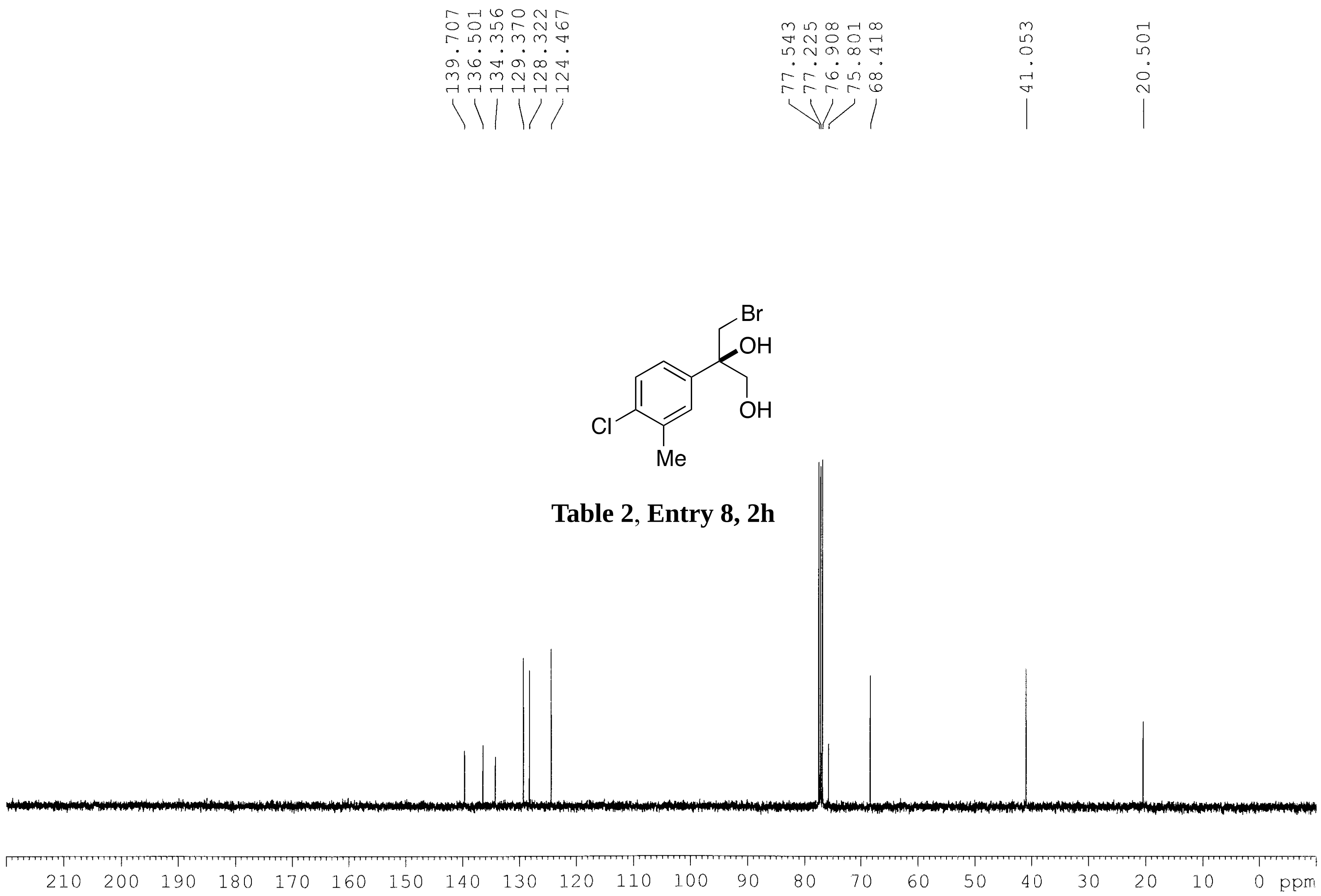


Table 2, Entry 8, 2h

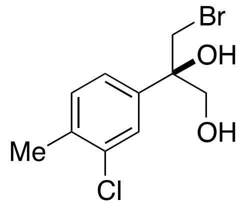
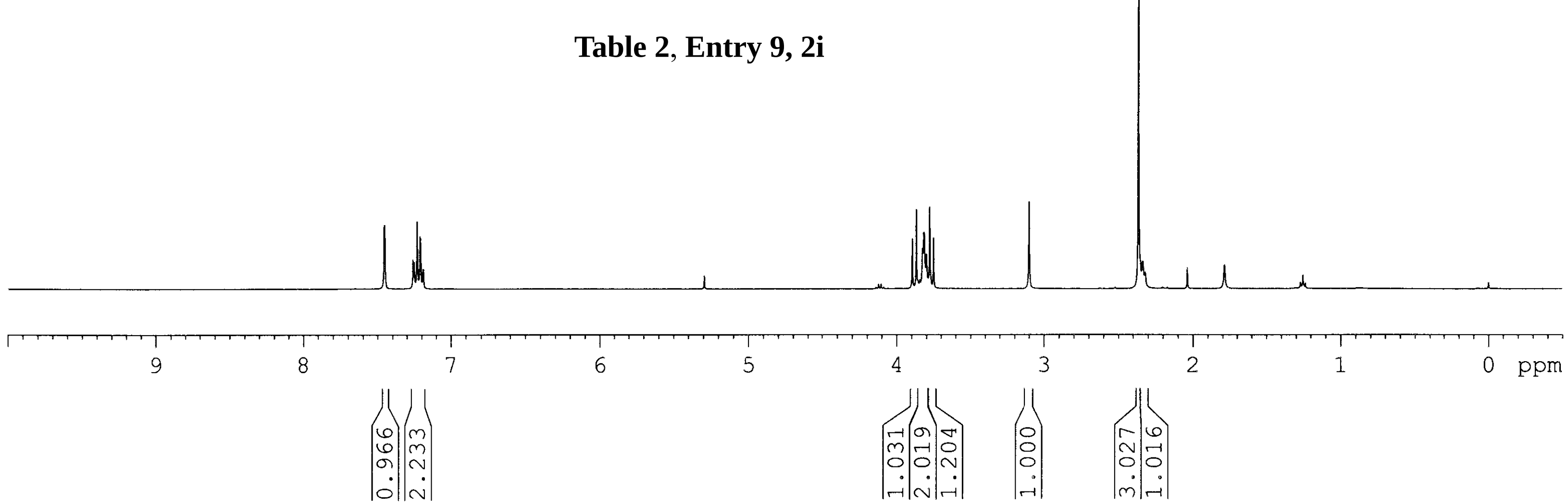


Table 2, Entry 9, 2i



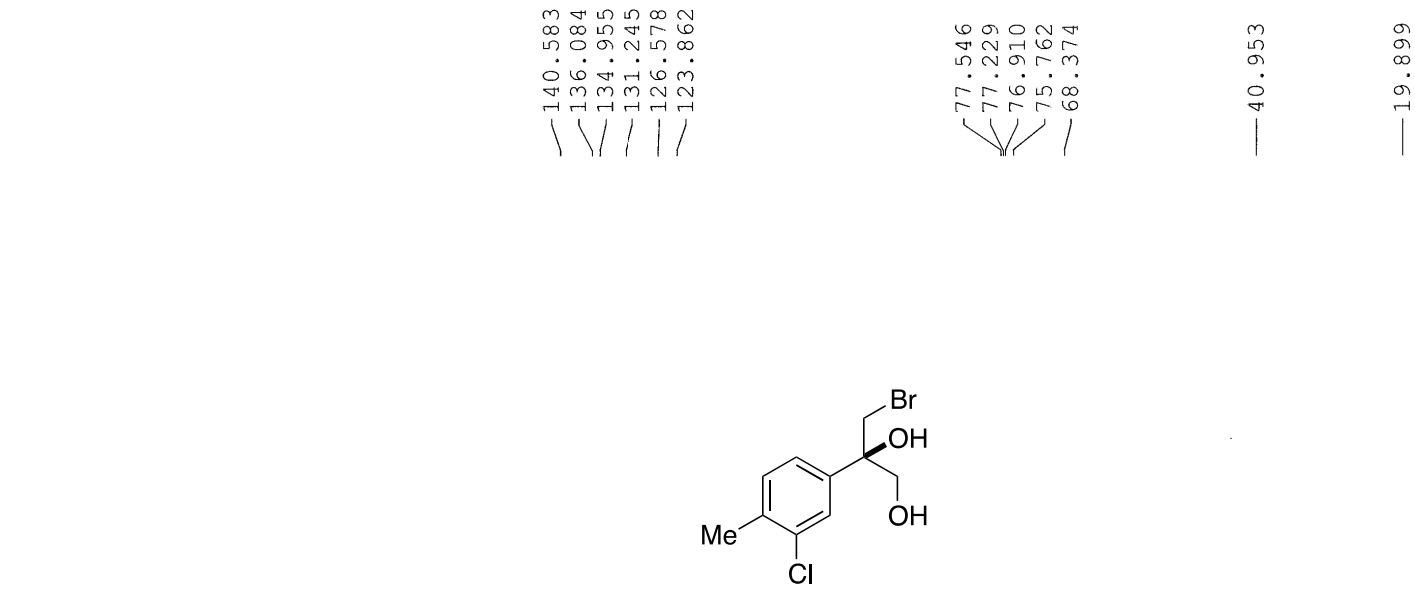
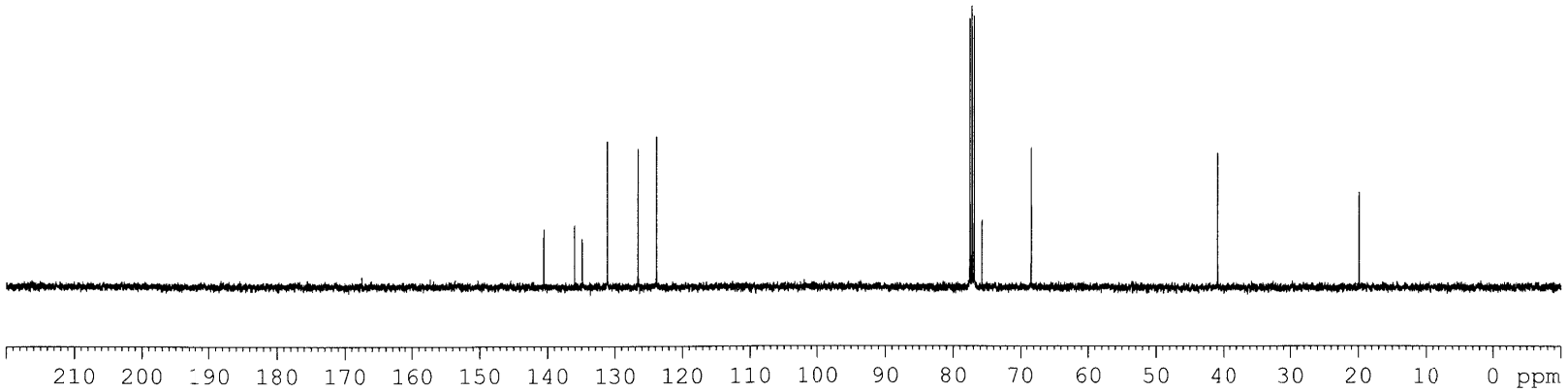
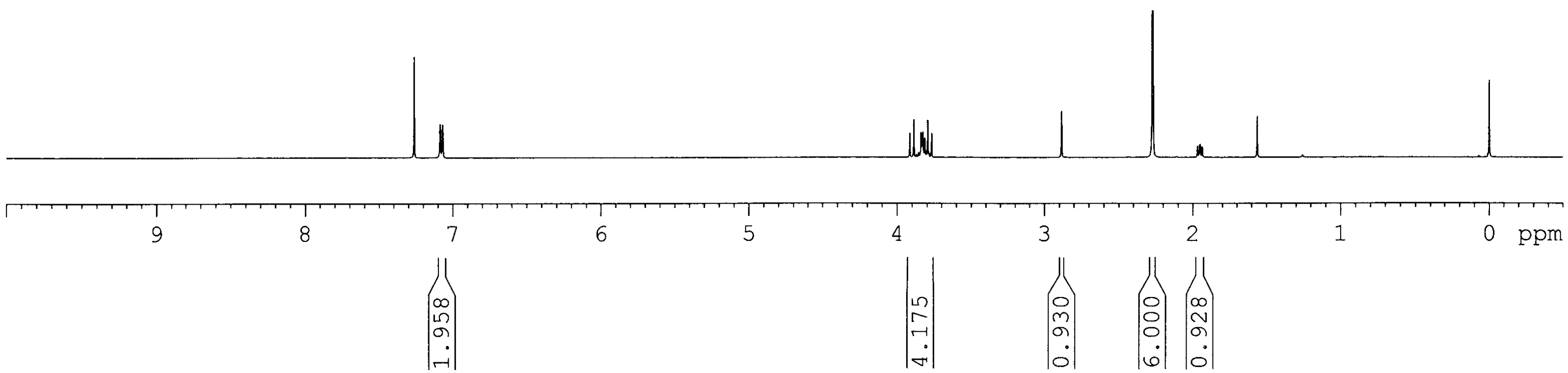


Table 2, **Entry 9, 2i**





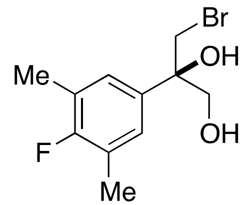


Table 2, Entry 10, 2j

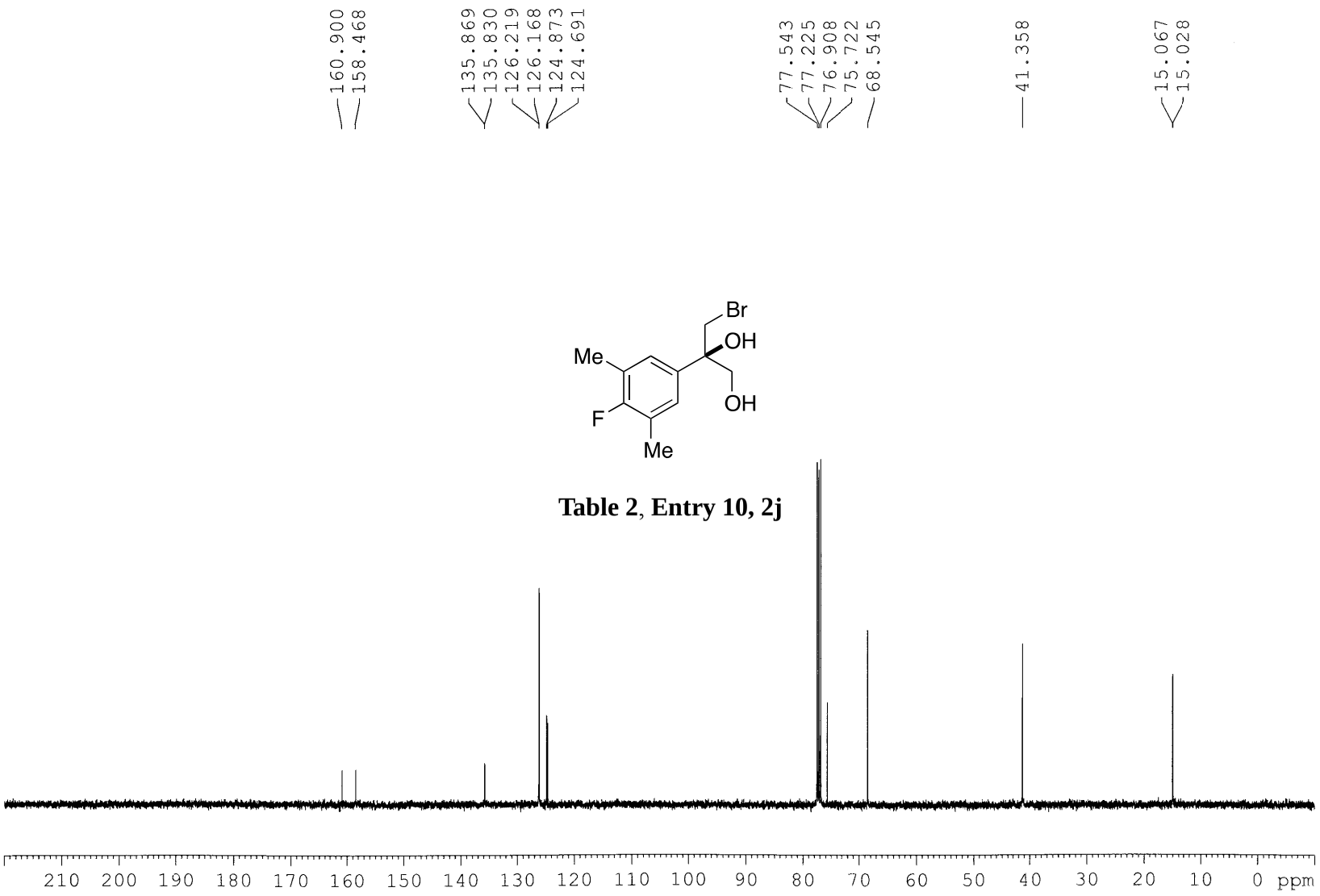


Table 2, Entry 10, 2j

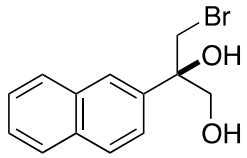
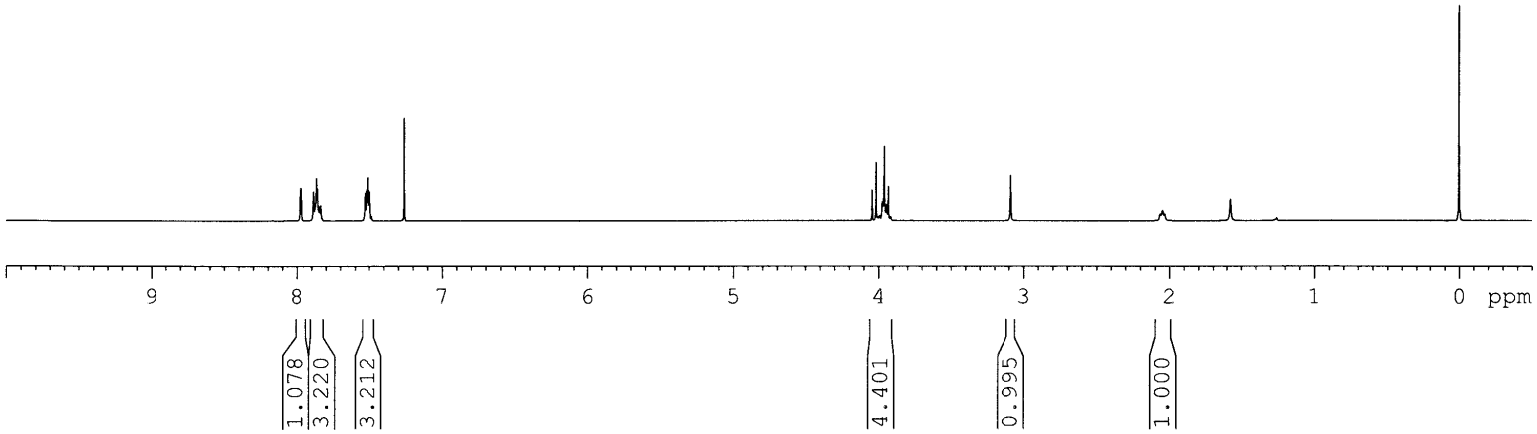


Table 2, Entry 11, 2k



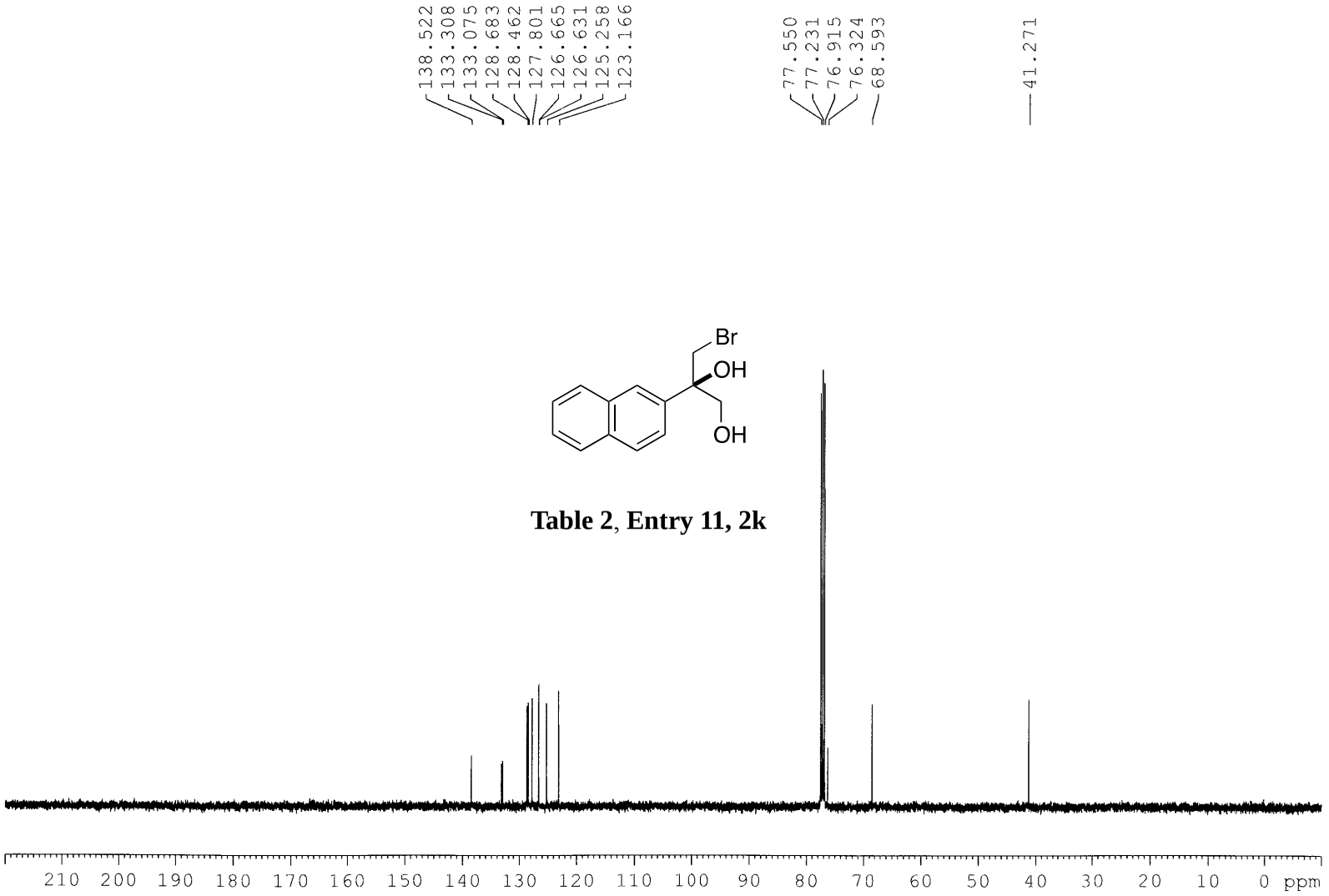


Table 2, **Entry 11, 2k**

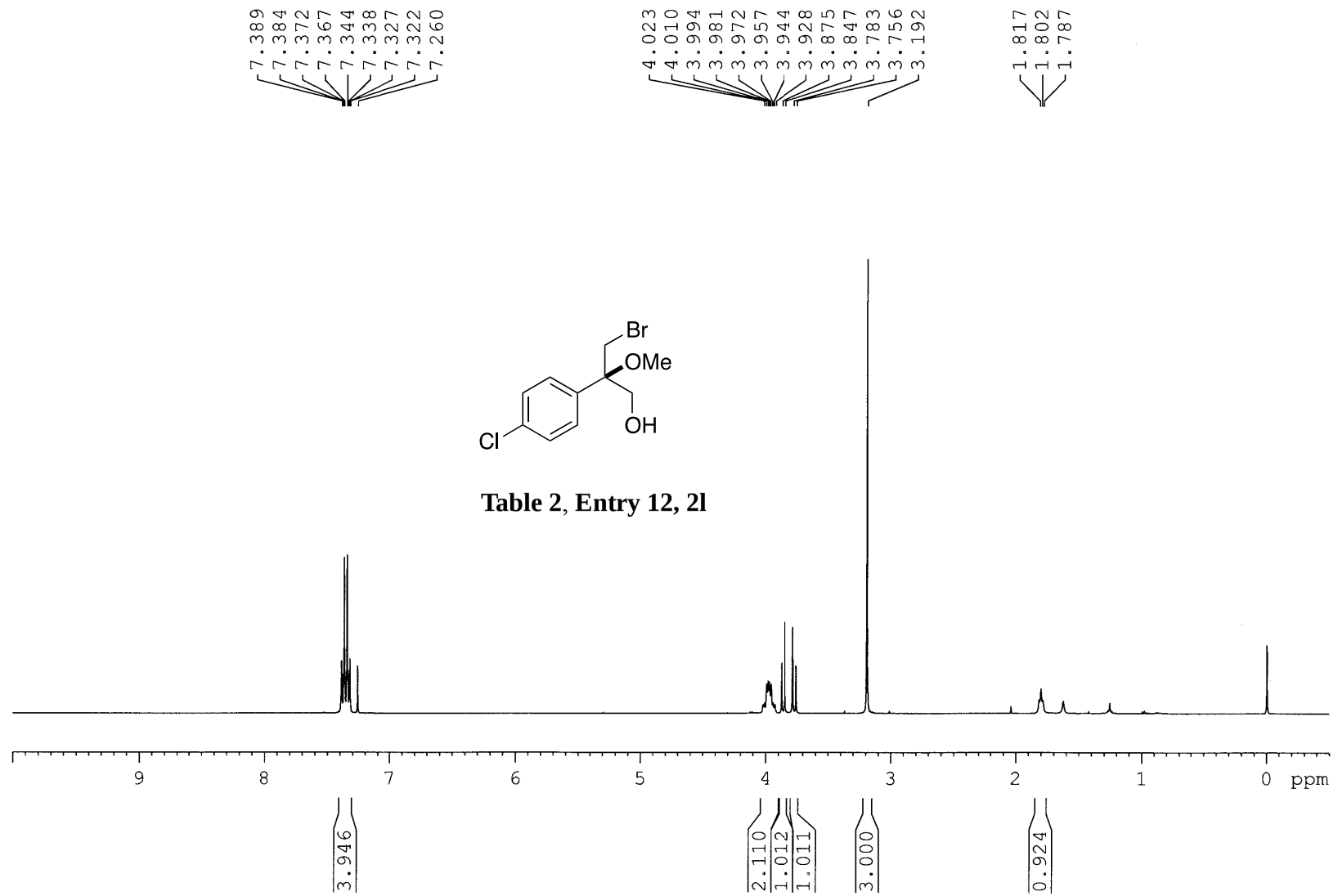


Table 2, Entry 12, 2l

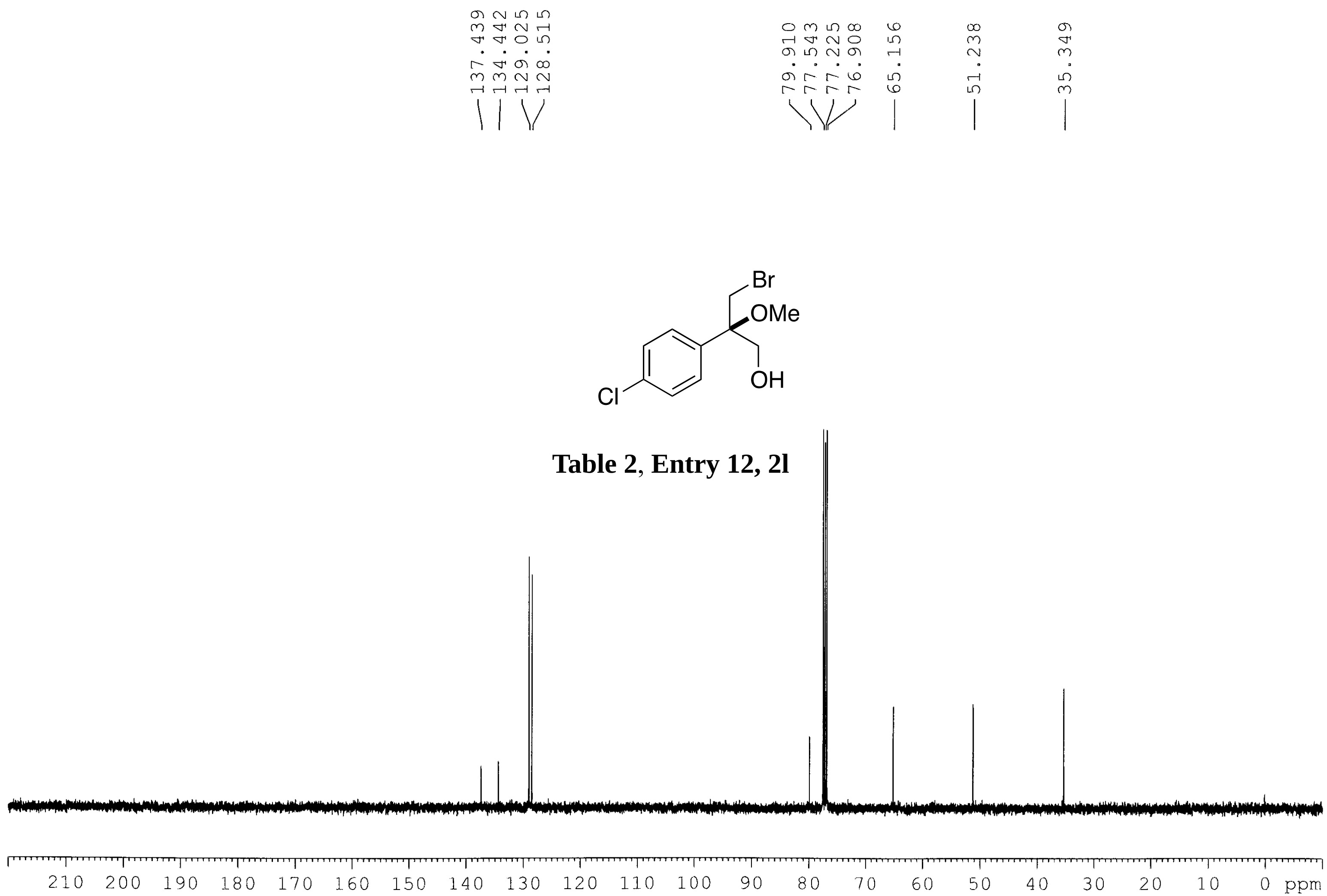
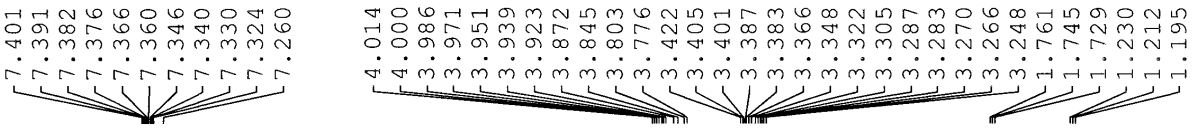


Table 2, Entry 12, 2l



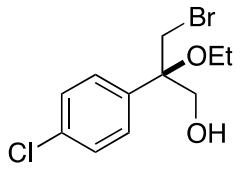
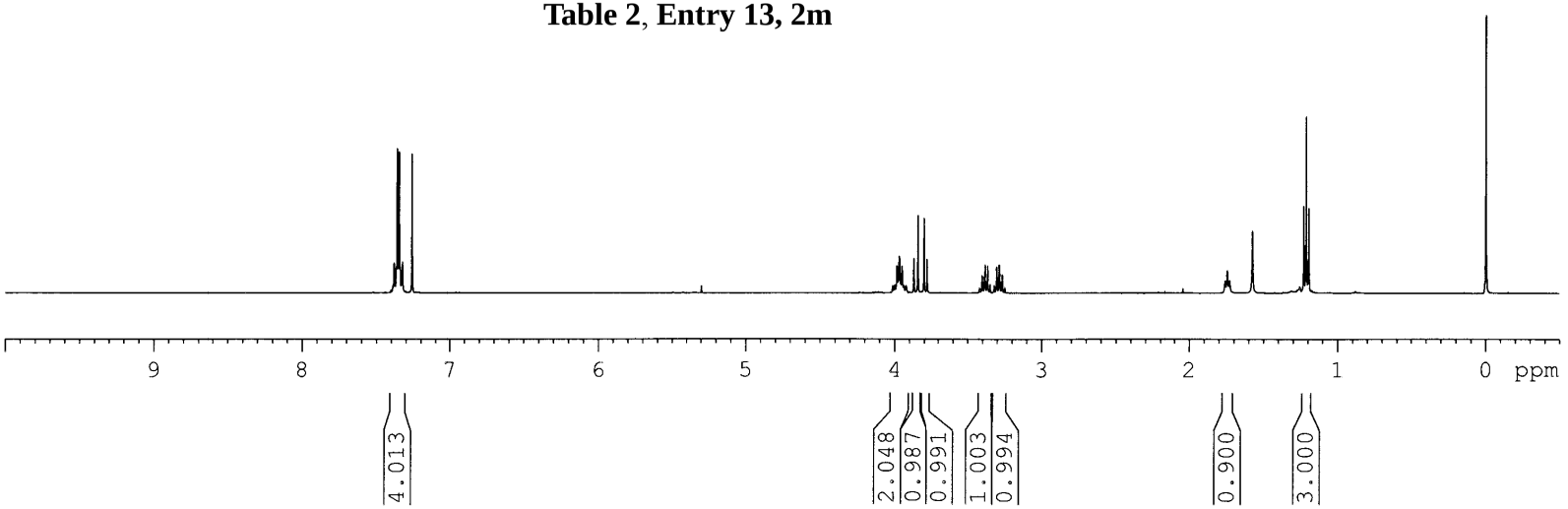


Table 2, **Entry 13, 2m**



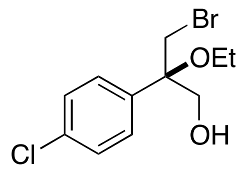
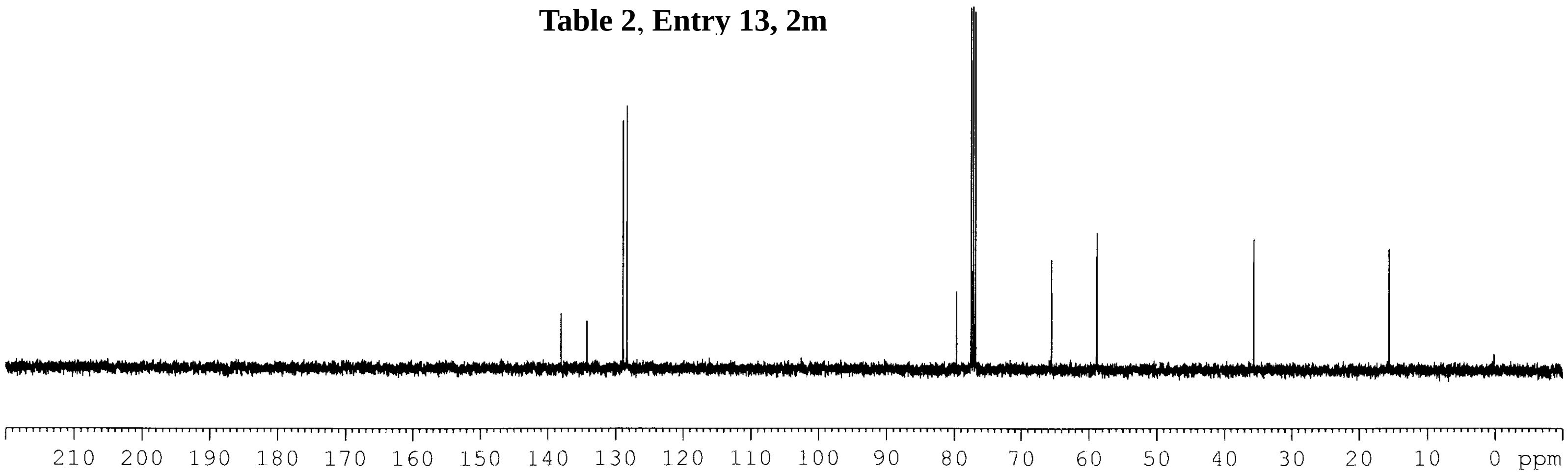
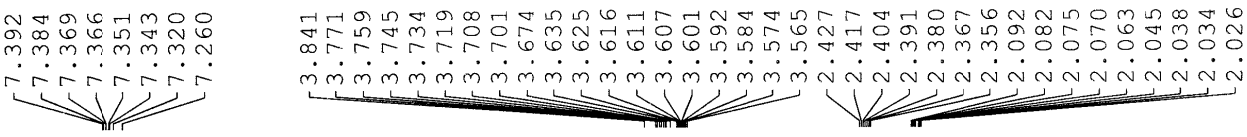


Table 2, Entry 13, 2m





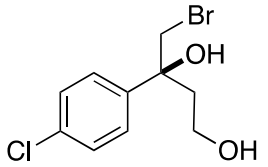
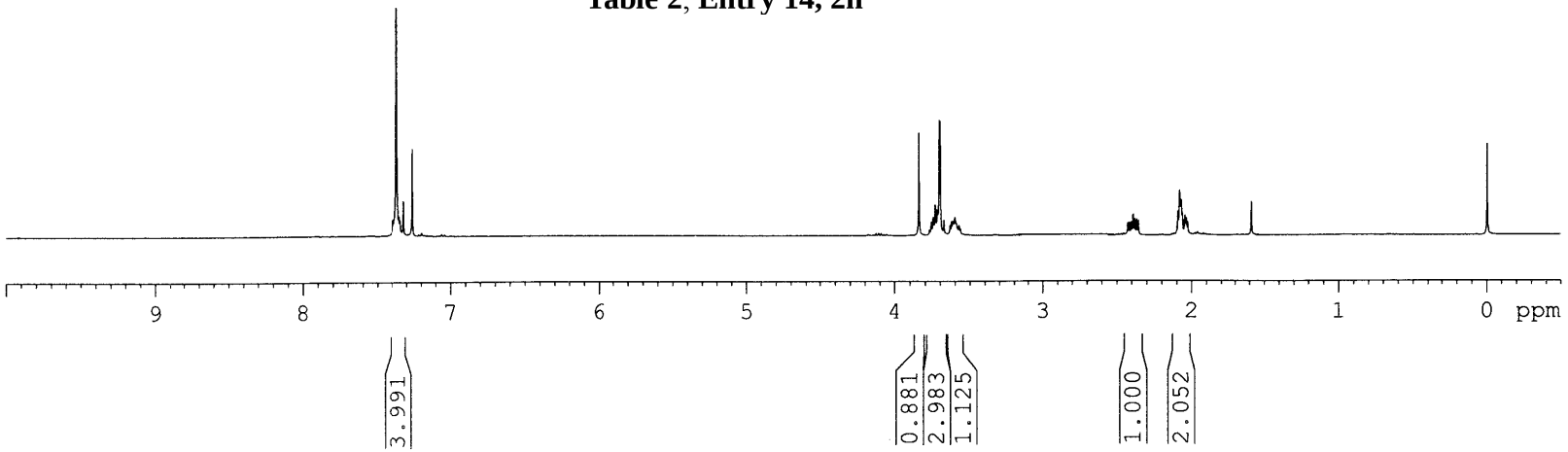


Table 2, **Entry 14, 2n**



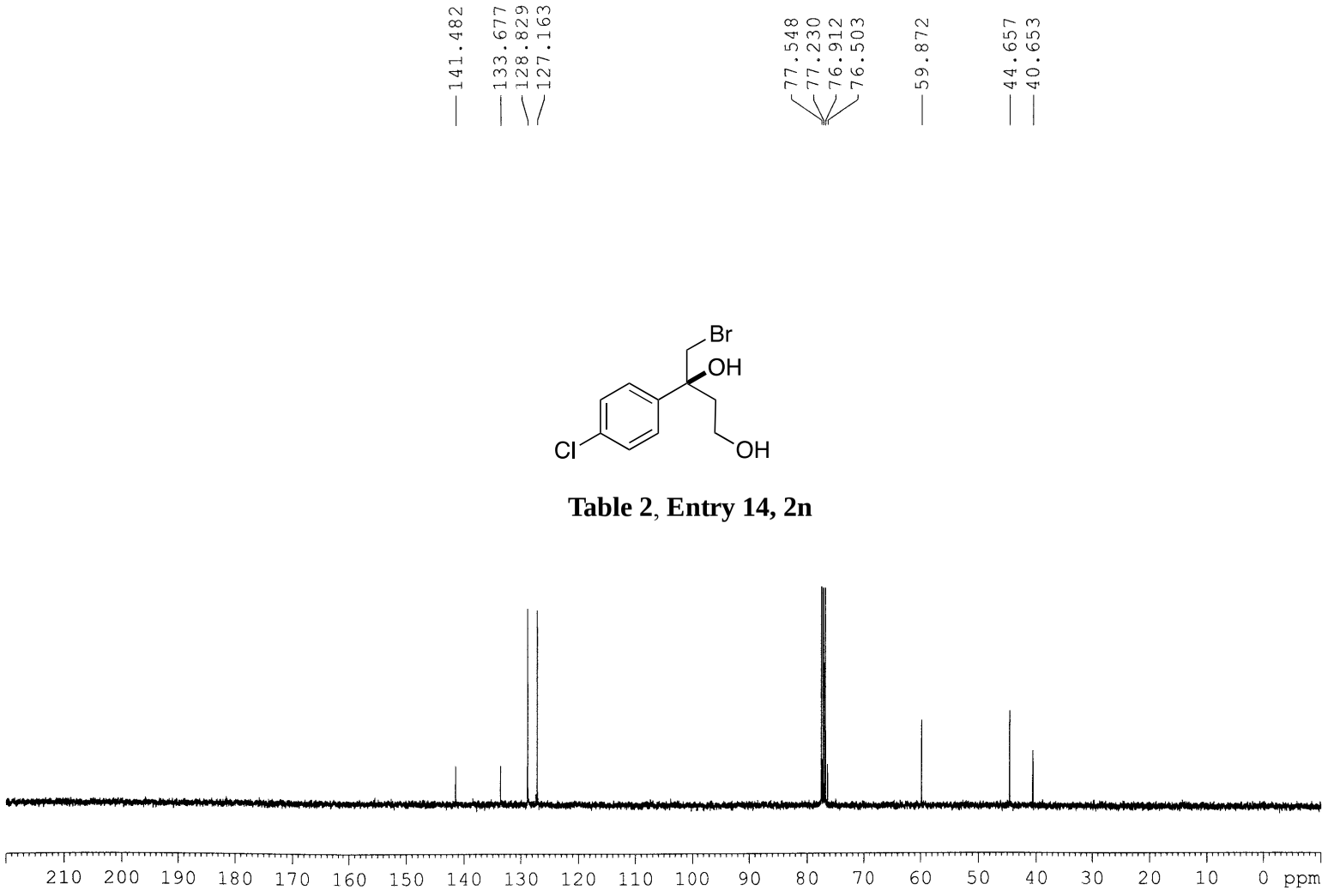
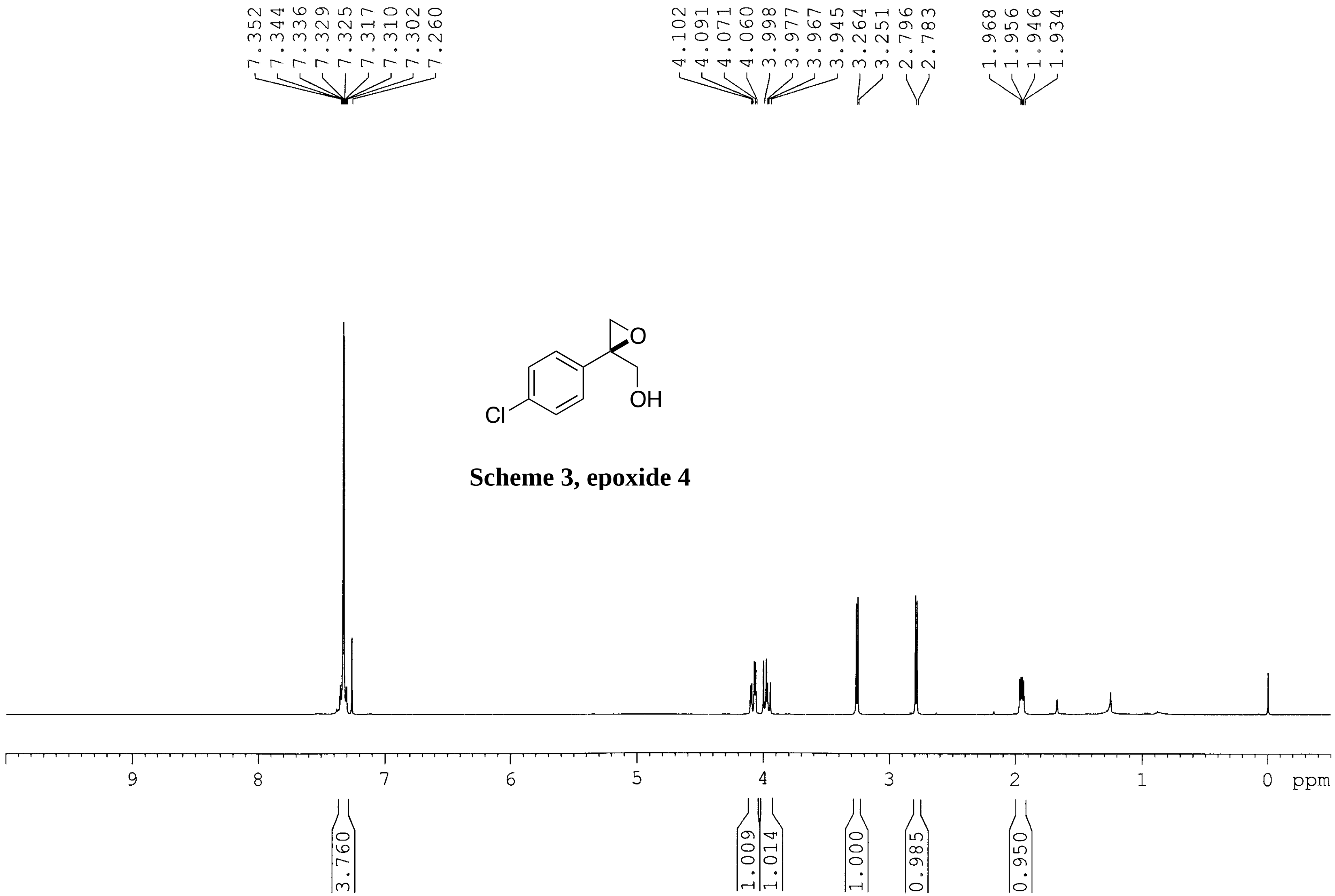
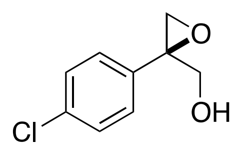


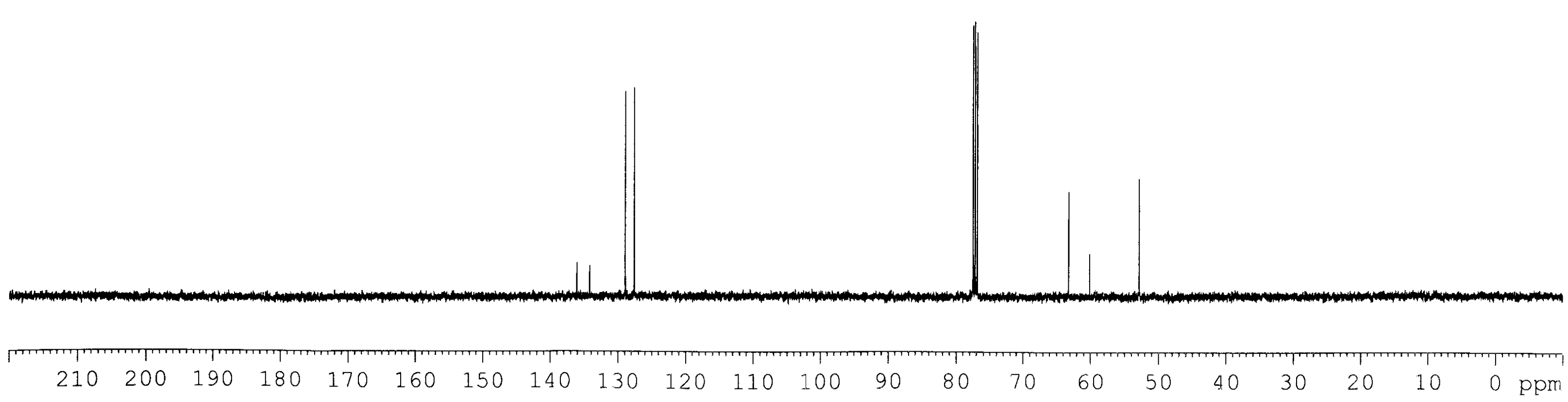
Table 2, **Entry 14, 2n**

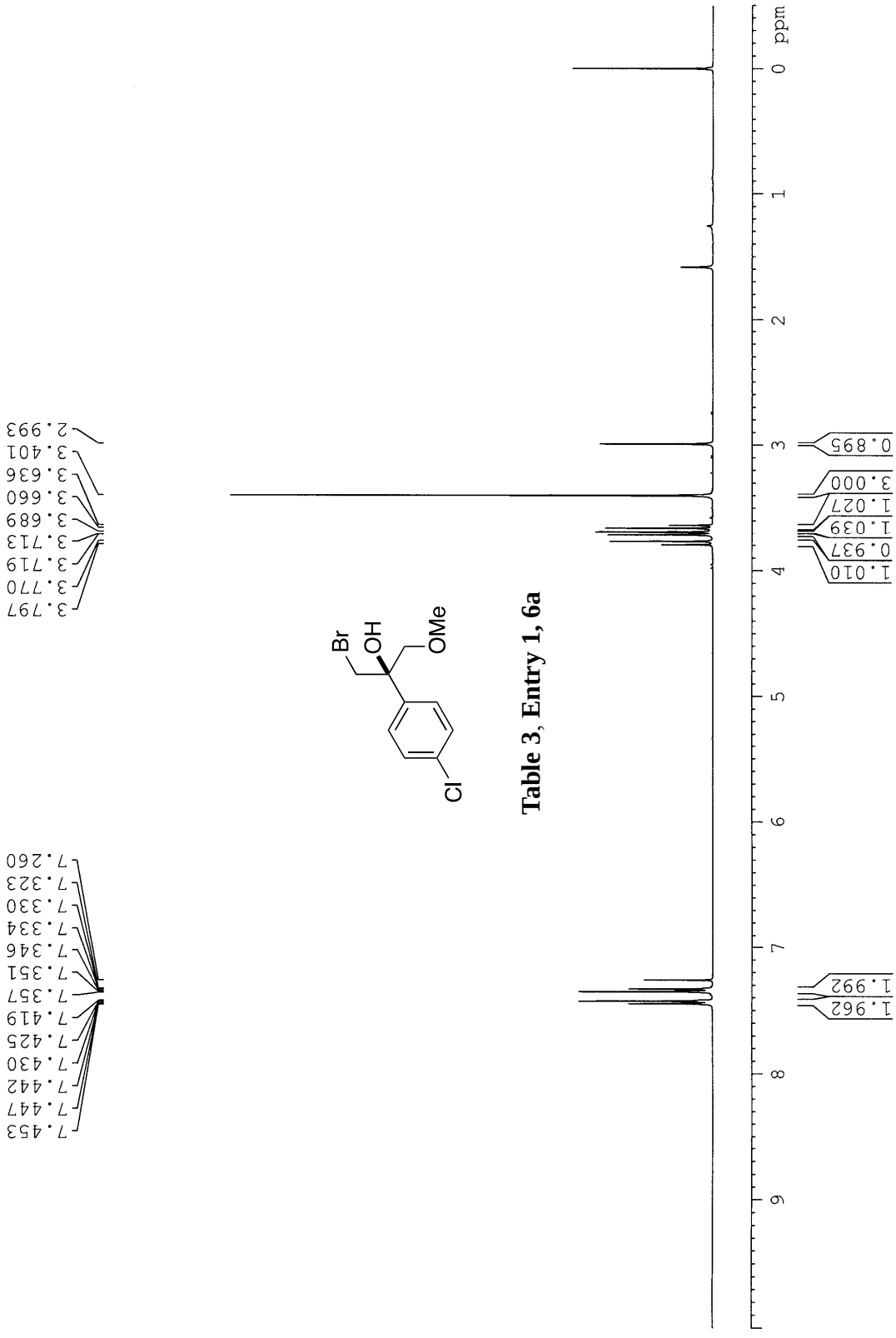


Scheme 3, epoxide 4



Scheme 3, epoxide 4

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7.447
7.442
7.430
7.425
7.419
7.357
7.351
7.346
7.334
7.330
7.323
7.260
3.797
3.770
3.719
3.713
3.689
3.660
3.636
3.401
2.993
Br
OH
OMe
Cl
Table 3, Entry 1, 6a
1.962
1.992
0.895
3.000
1.027
1.039
0.937
1.010
0 ppm

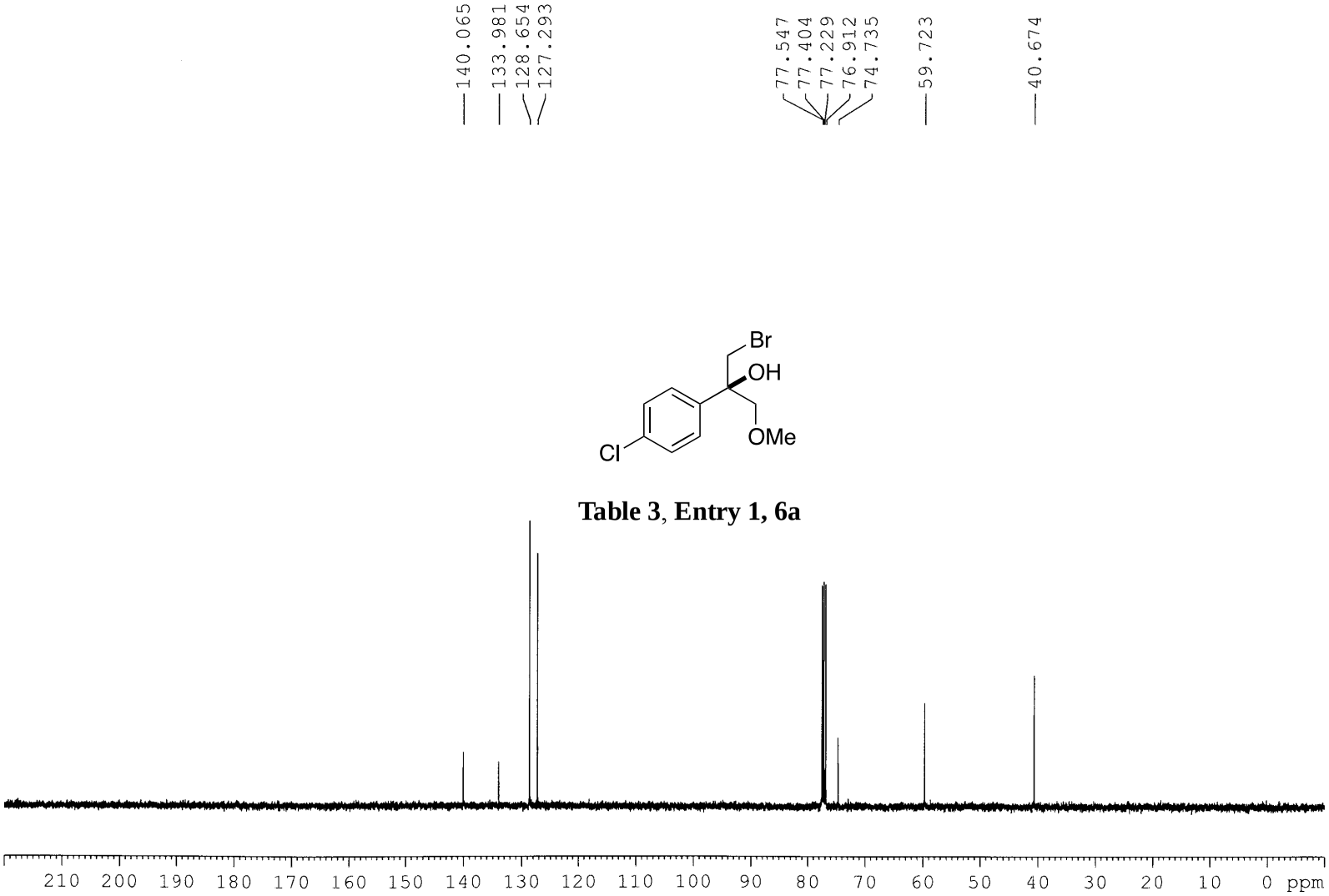
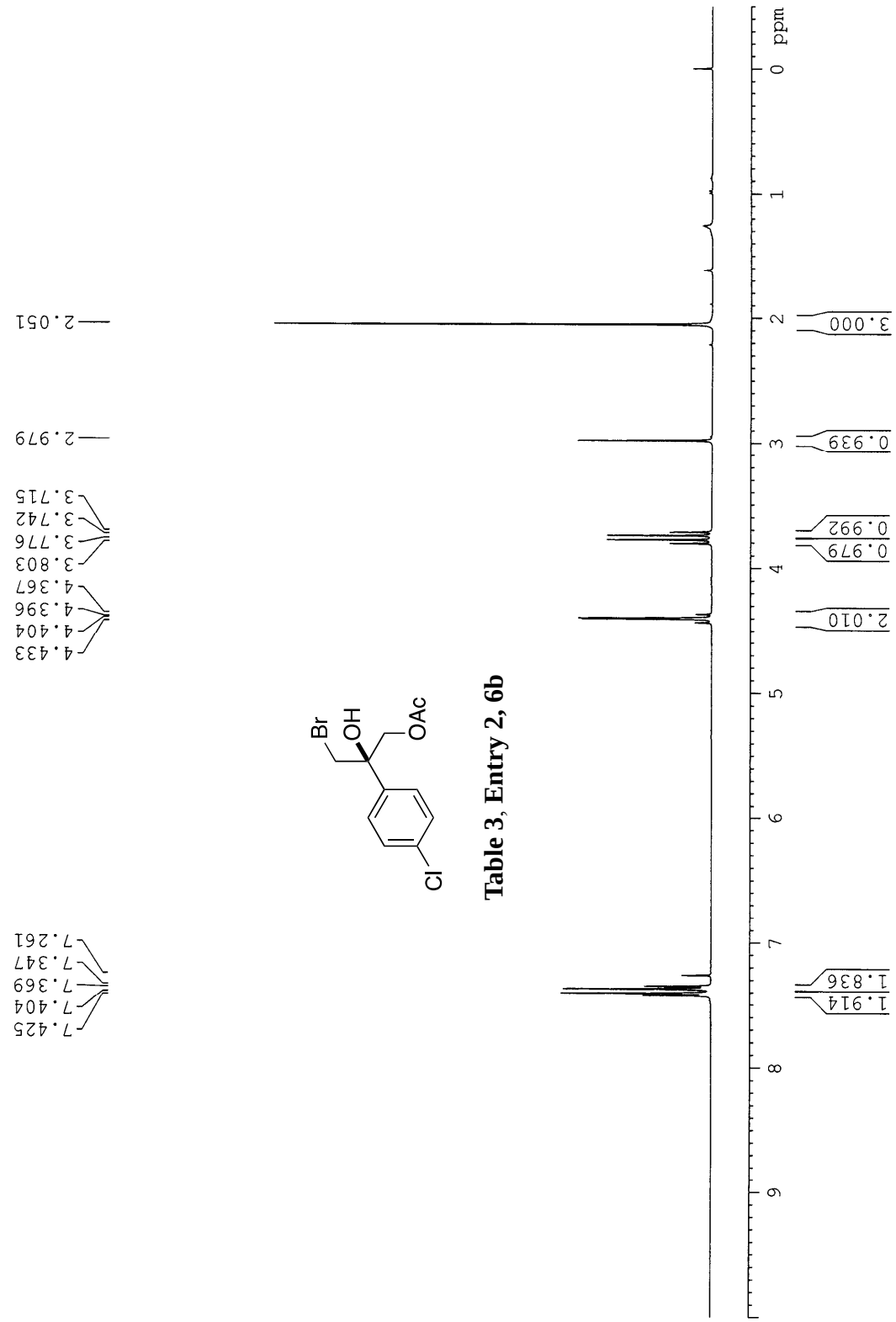


Table 3, Entry 1, 6a


Br
OH
OAc
Cl
Table 3, Entry 2, 6b
2.051
2.979
3.715
3.742
3.776
3.803
4.367
4.396
4.404
4.433
7.261
7.347
7.369
7.404
7.425
3.000
0.939
0.992
0.979
2.010
1.914
1.836
ppm

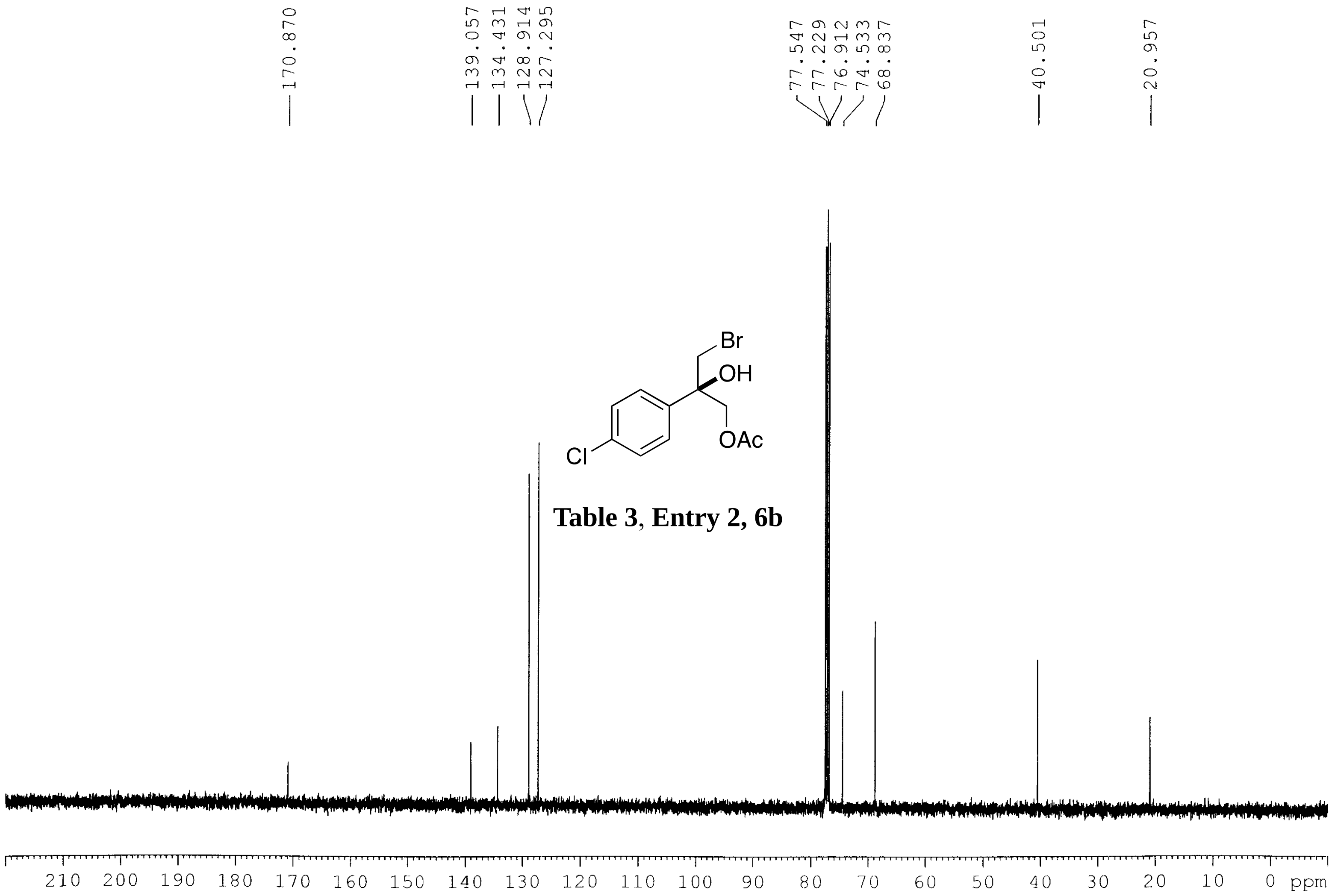


Table 3, Entry 2, 6b

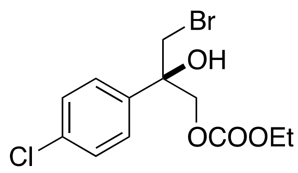
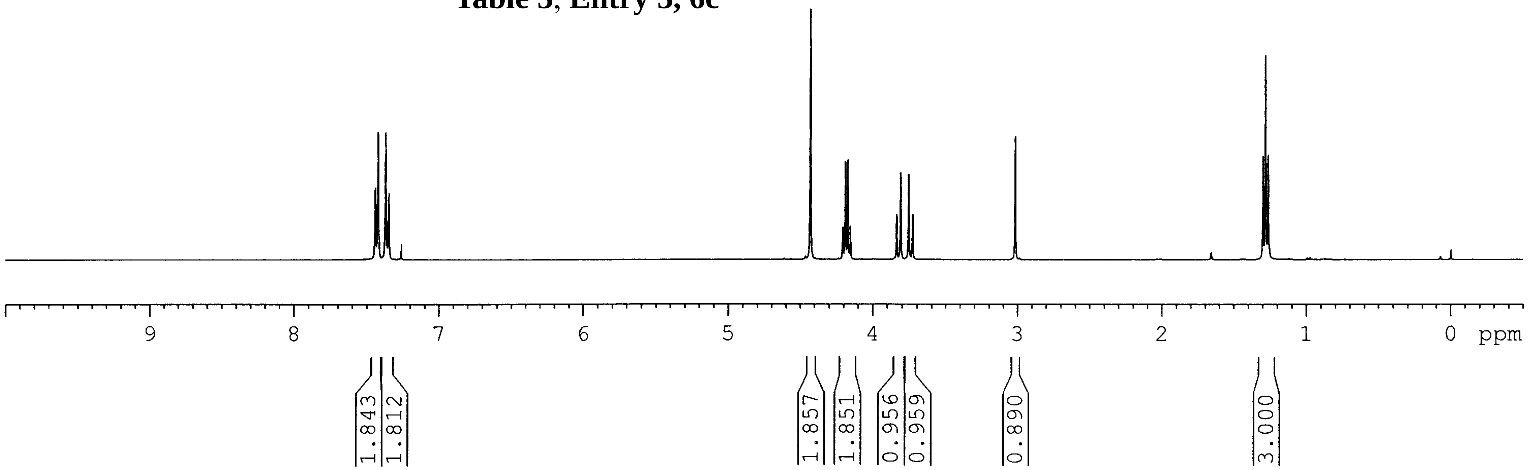


Table 3, Entry 3, 6c



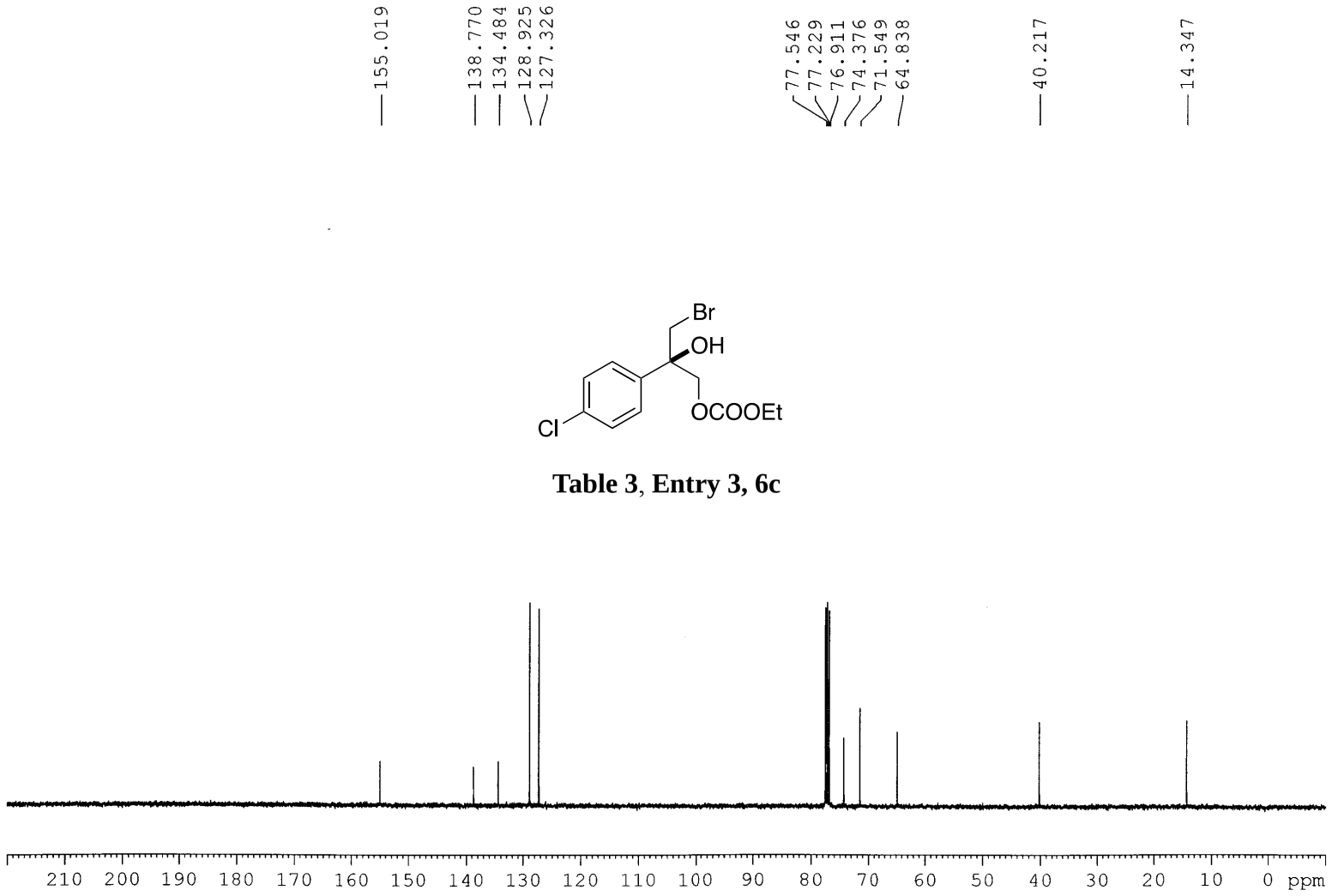


Table 3, Entry 3, 6c

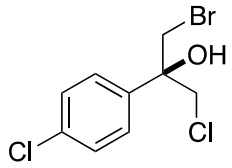
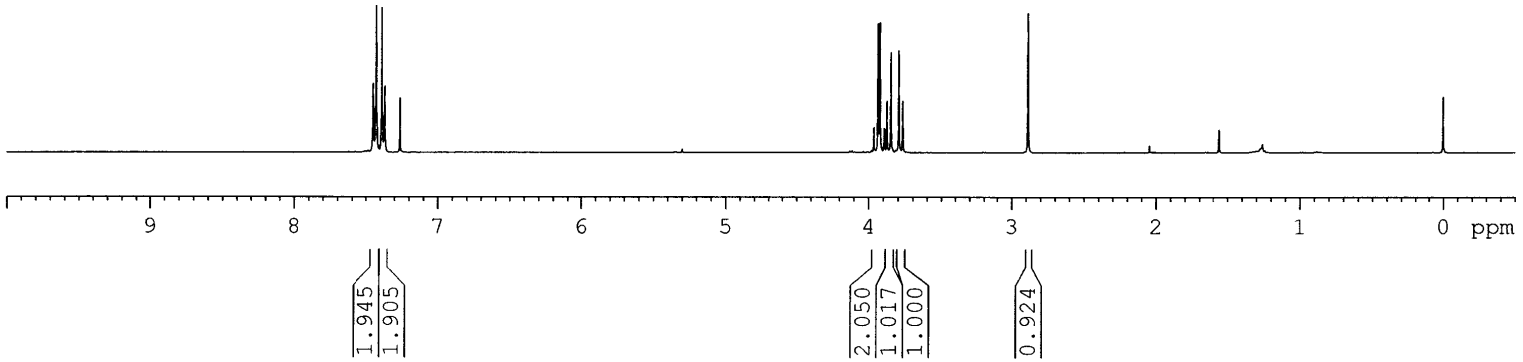


Table 3, **Entry 4, 6d**



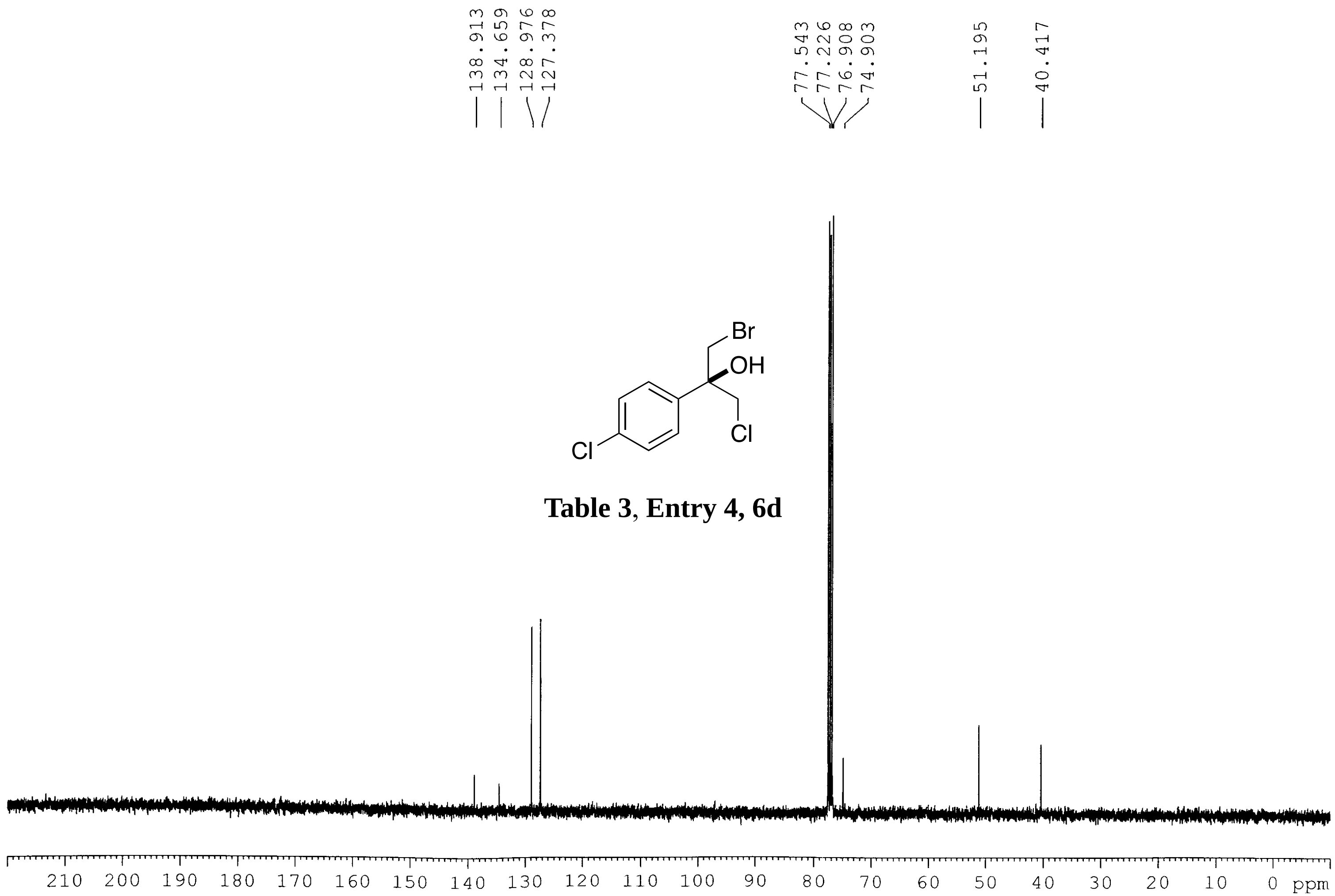


Table 3, Entry 4, 6d

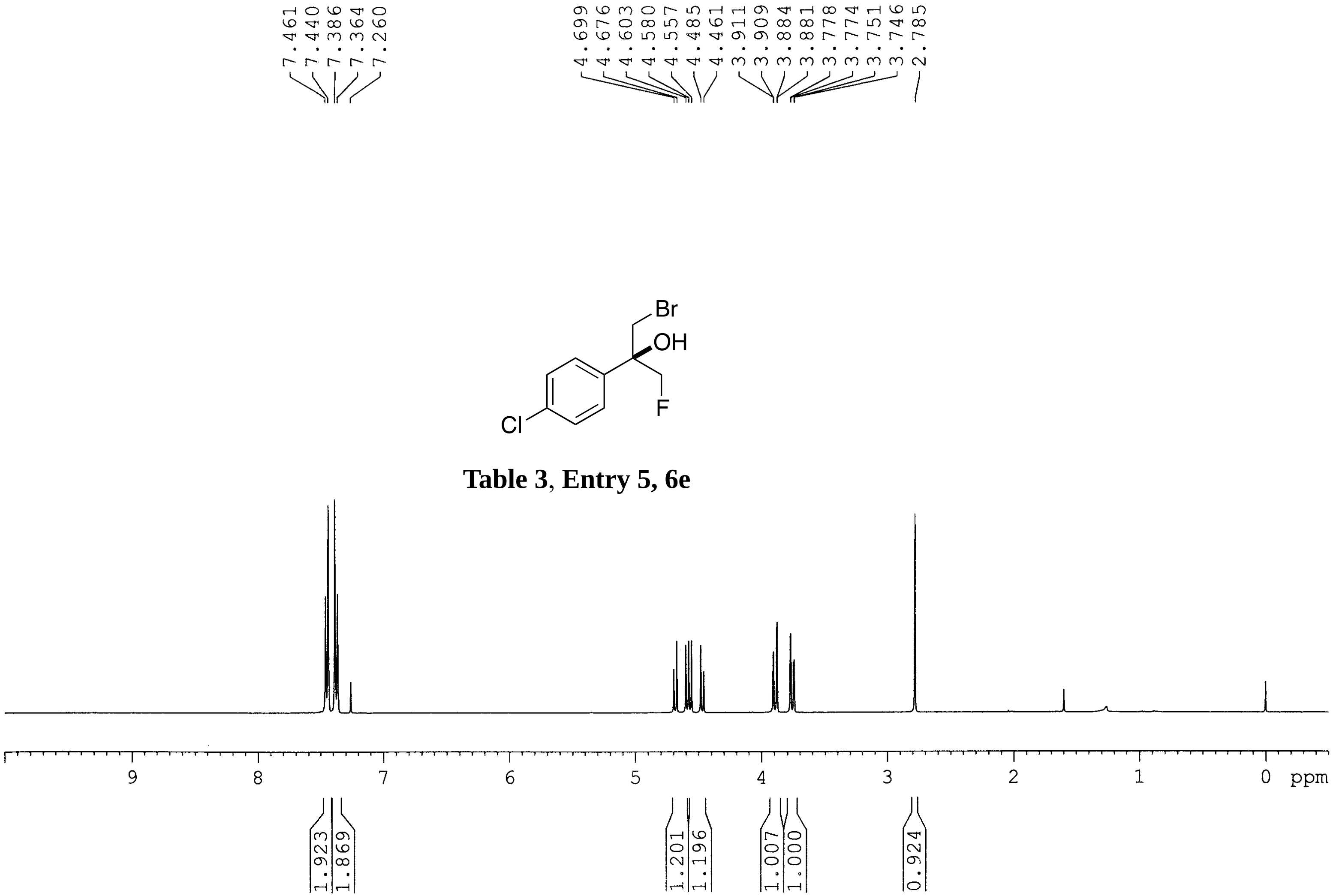


Table 3, Entry 5, 6e

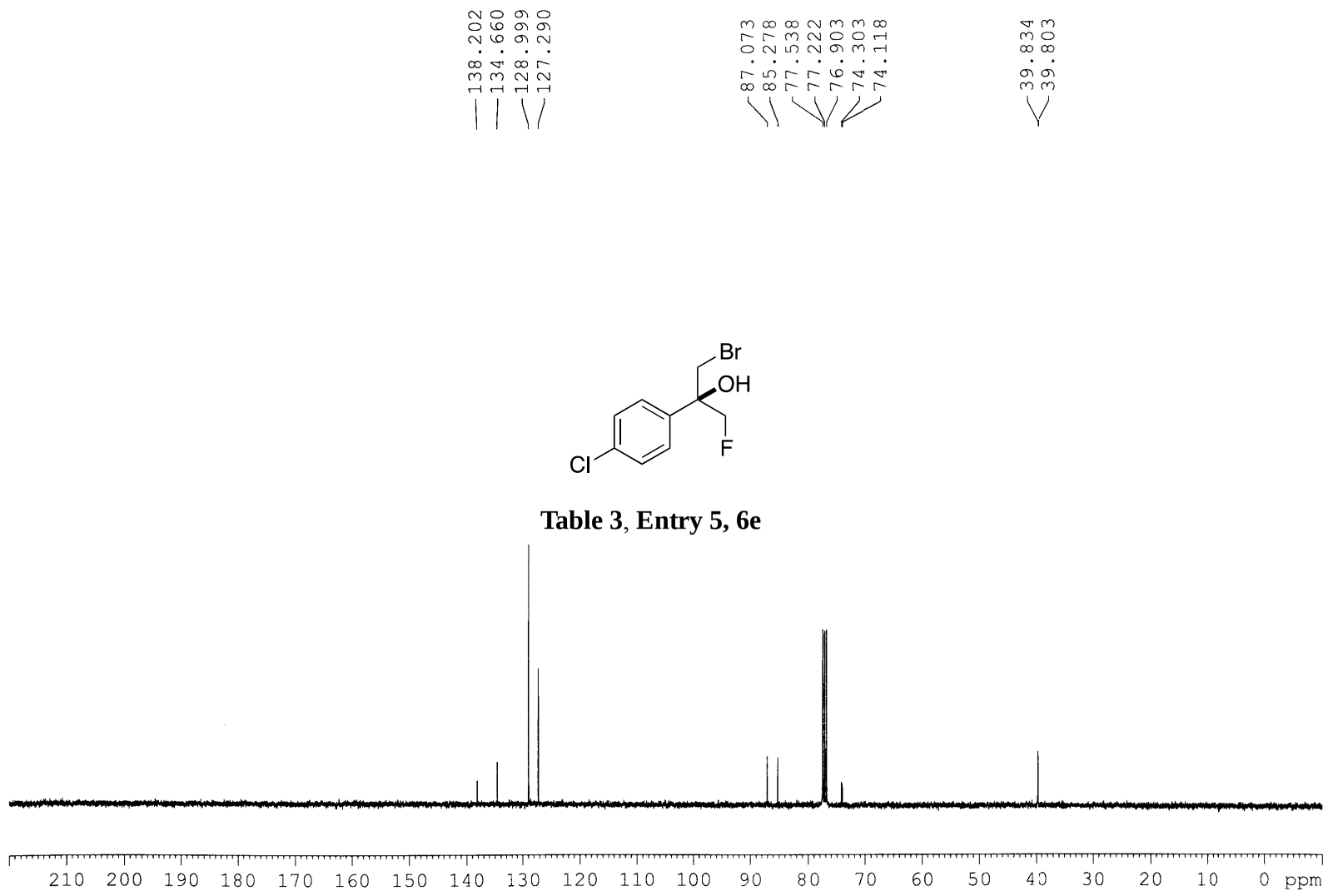
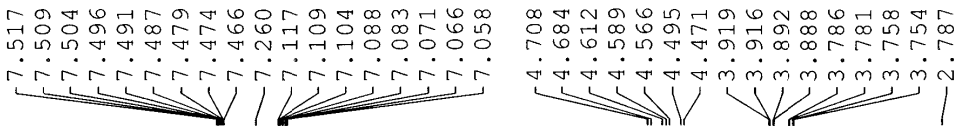


Table 3, Entry 5, 6e



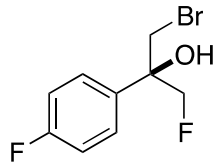
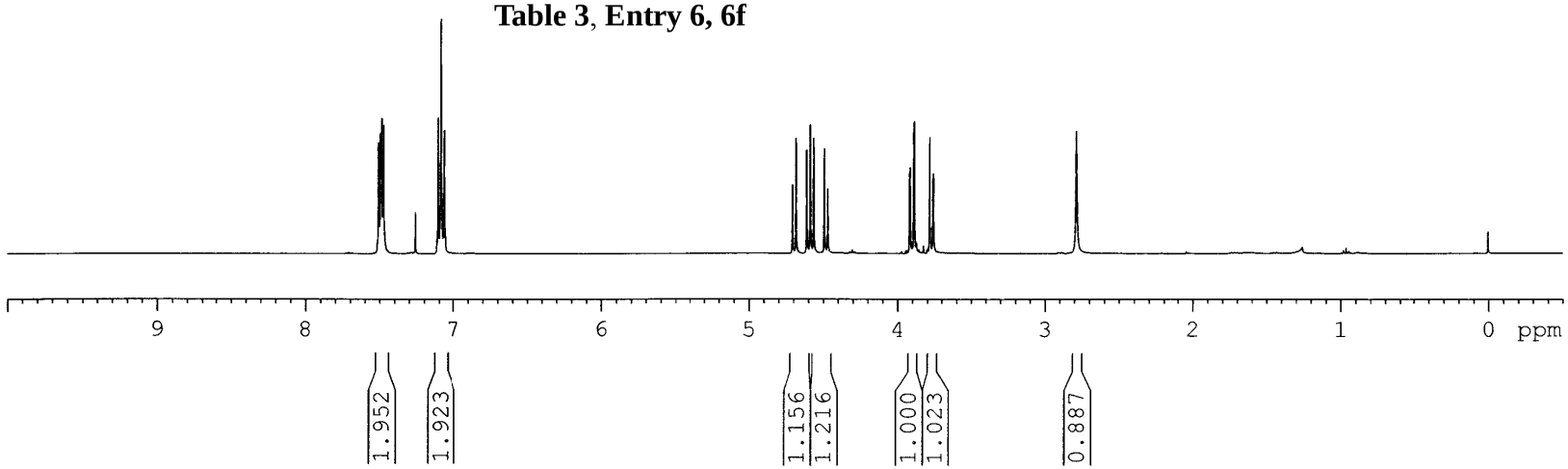


Table 3, **Entry 6, 6f**



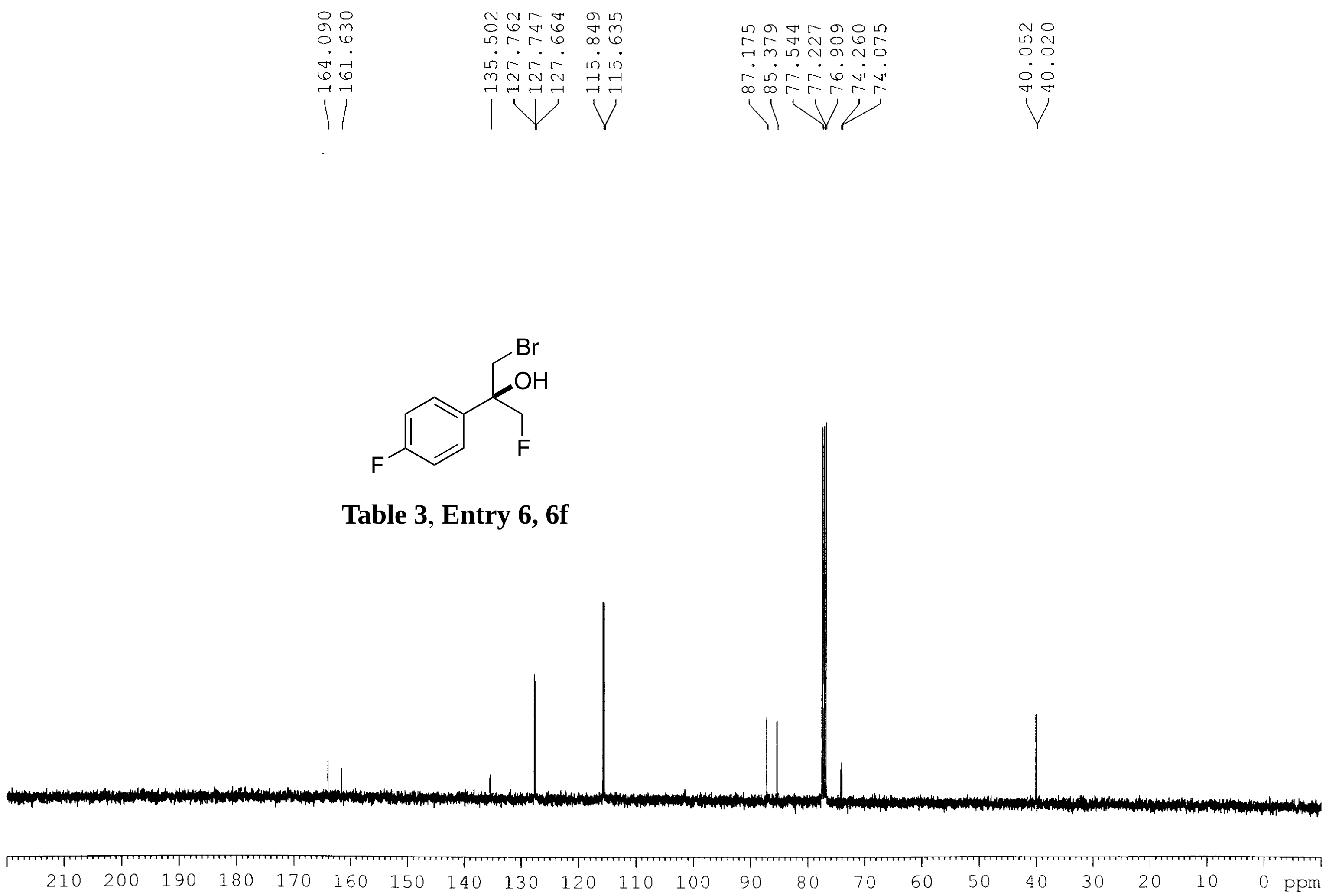


Table 3, Entry 6, 6f

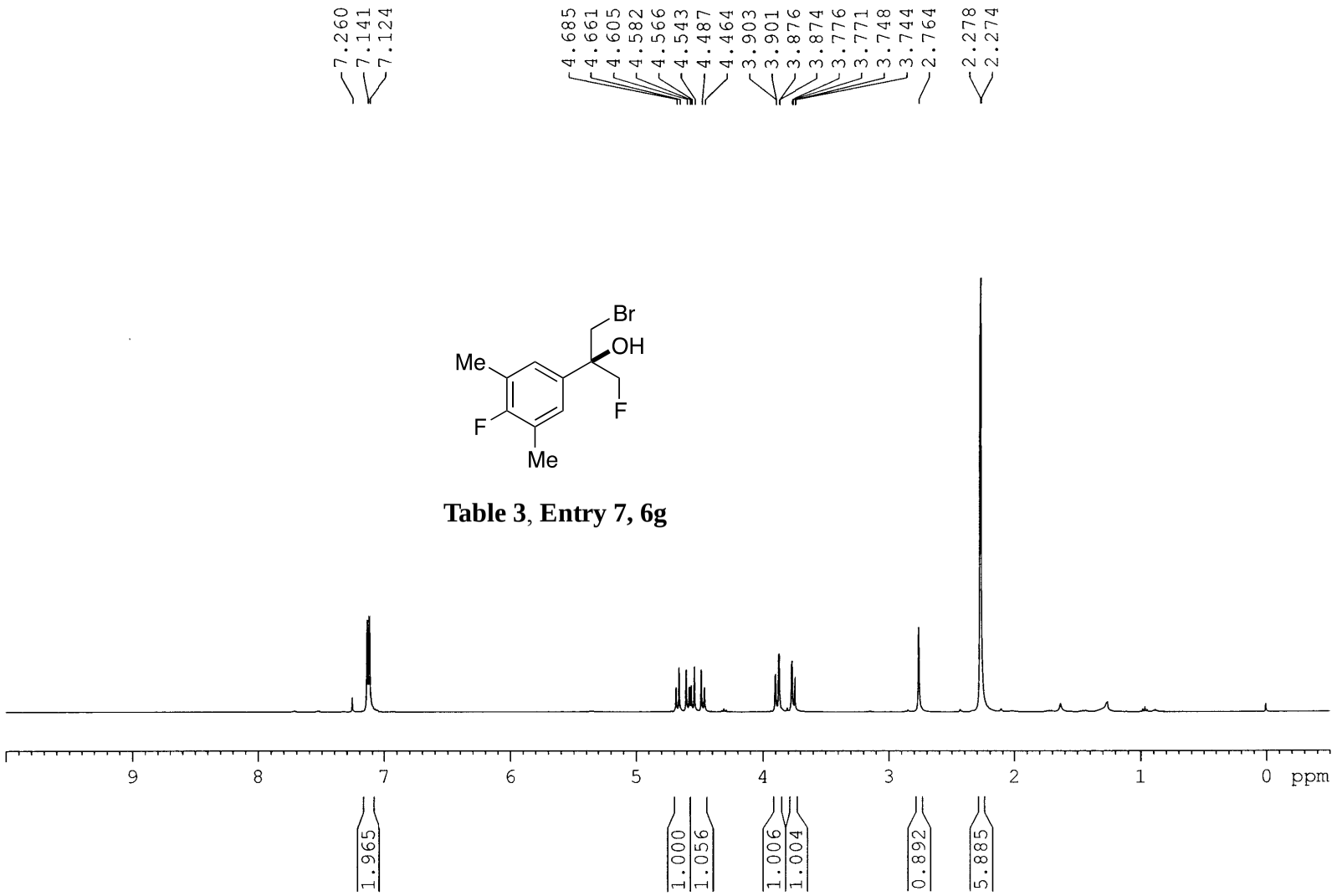


Table 3, **Entry 7, 6g**

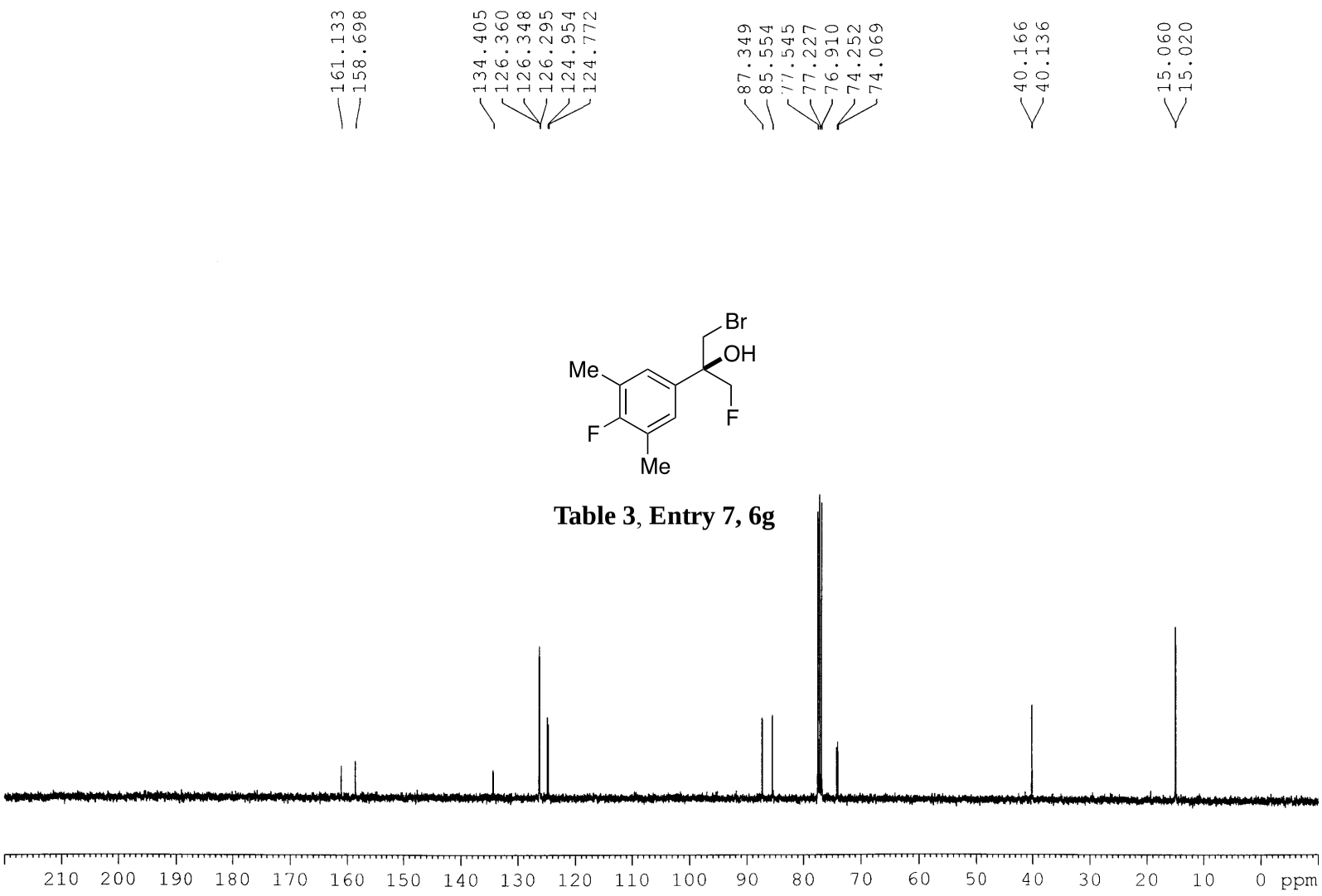
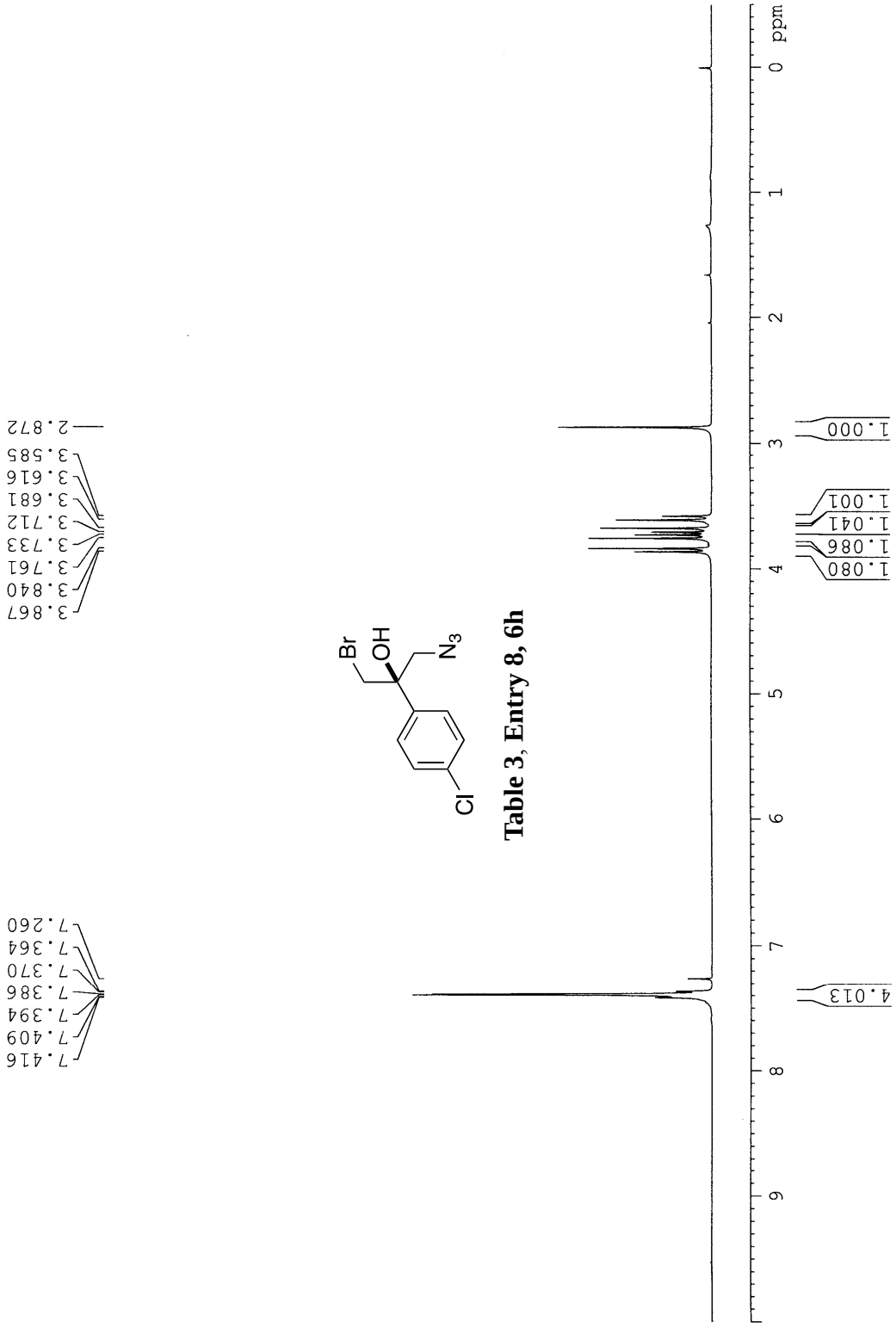


Table 3, Entry 7, 6g


2.872
3.585
3.616
3.681
3.712
3.733
3.761
3.840
3.867
7.260
7.364
7.370
7.386
7.394
7.409
7.416
Br
OH
N3
Cl
Table 3, Entry 8, 6h
1.000
1.001
1.041
1.086
1.080
4.013
ppm

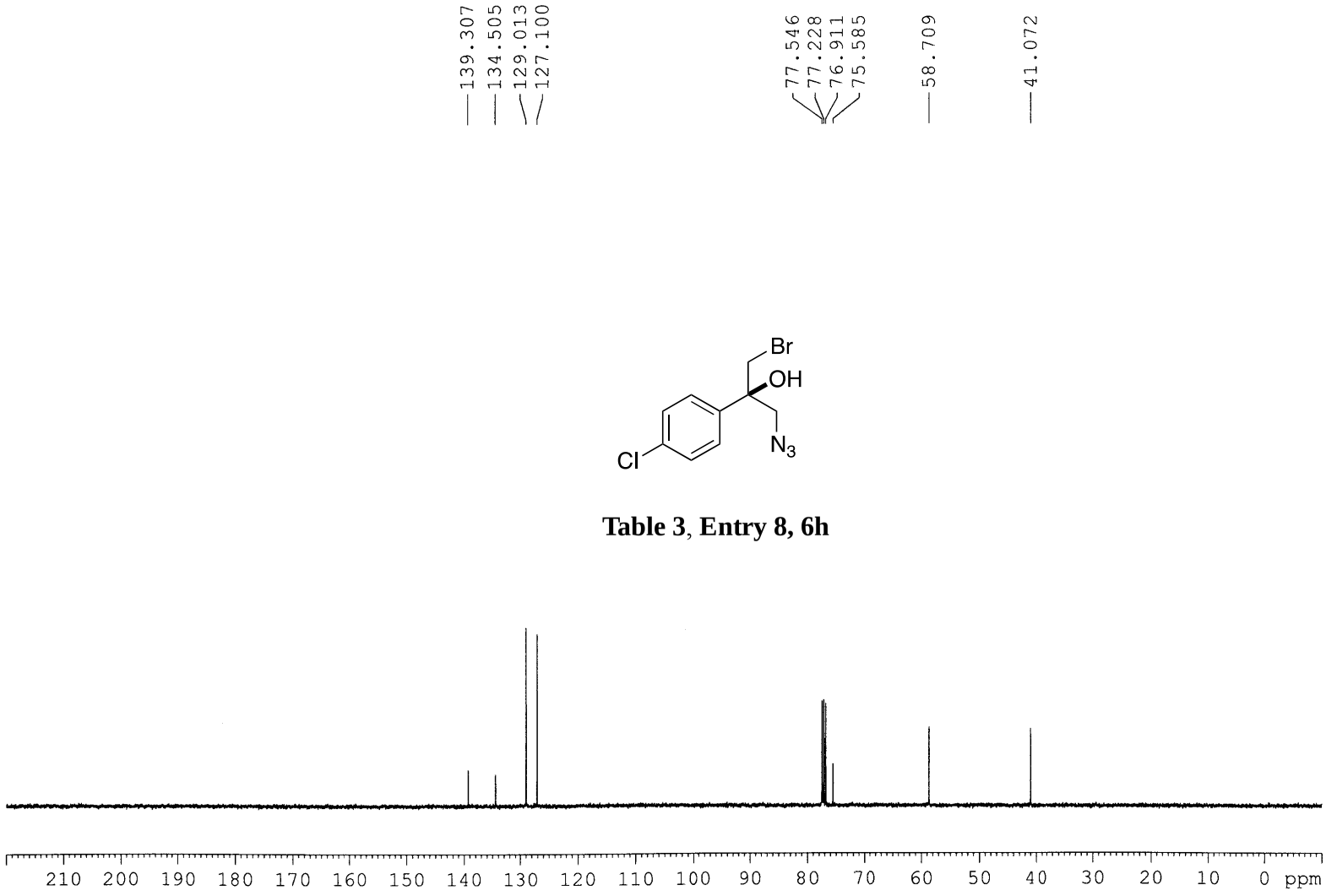
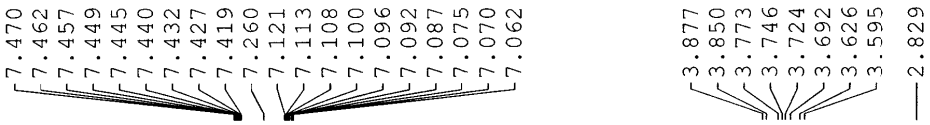


Table 3, Entry 8, 6h



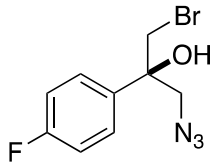
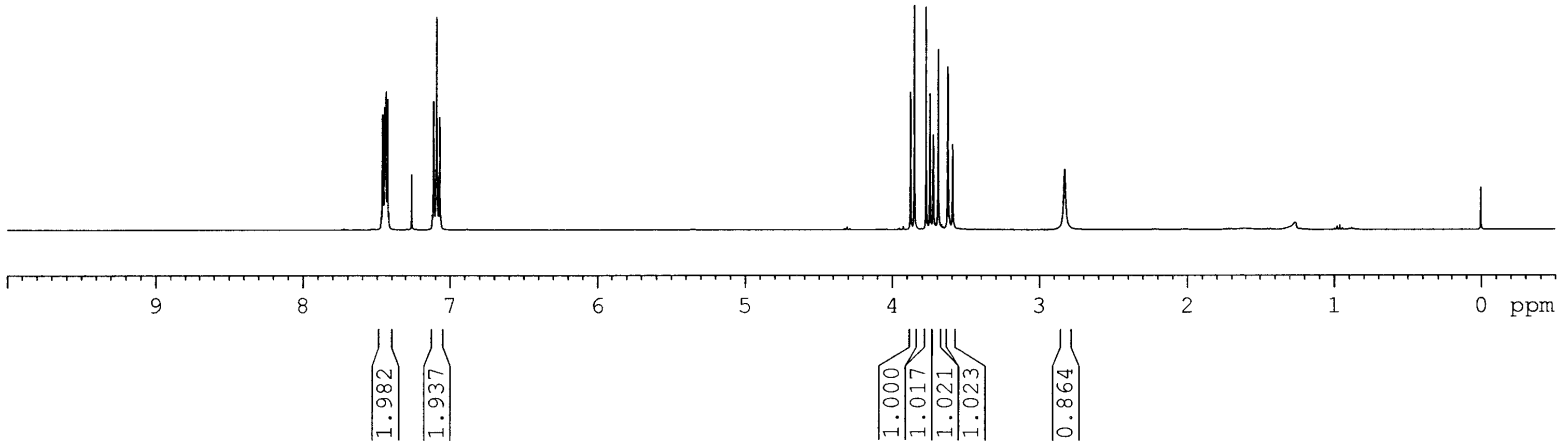


Table 3, **Entry 9, 6i**



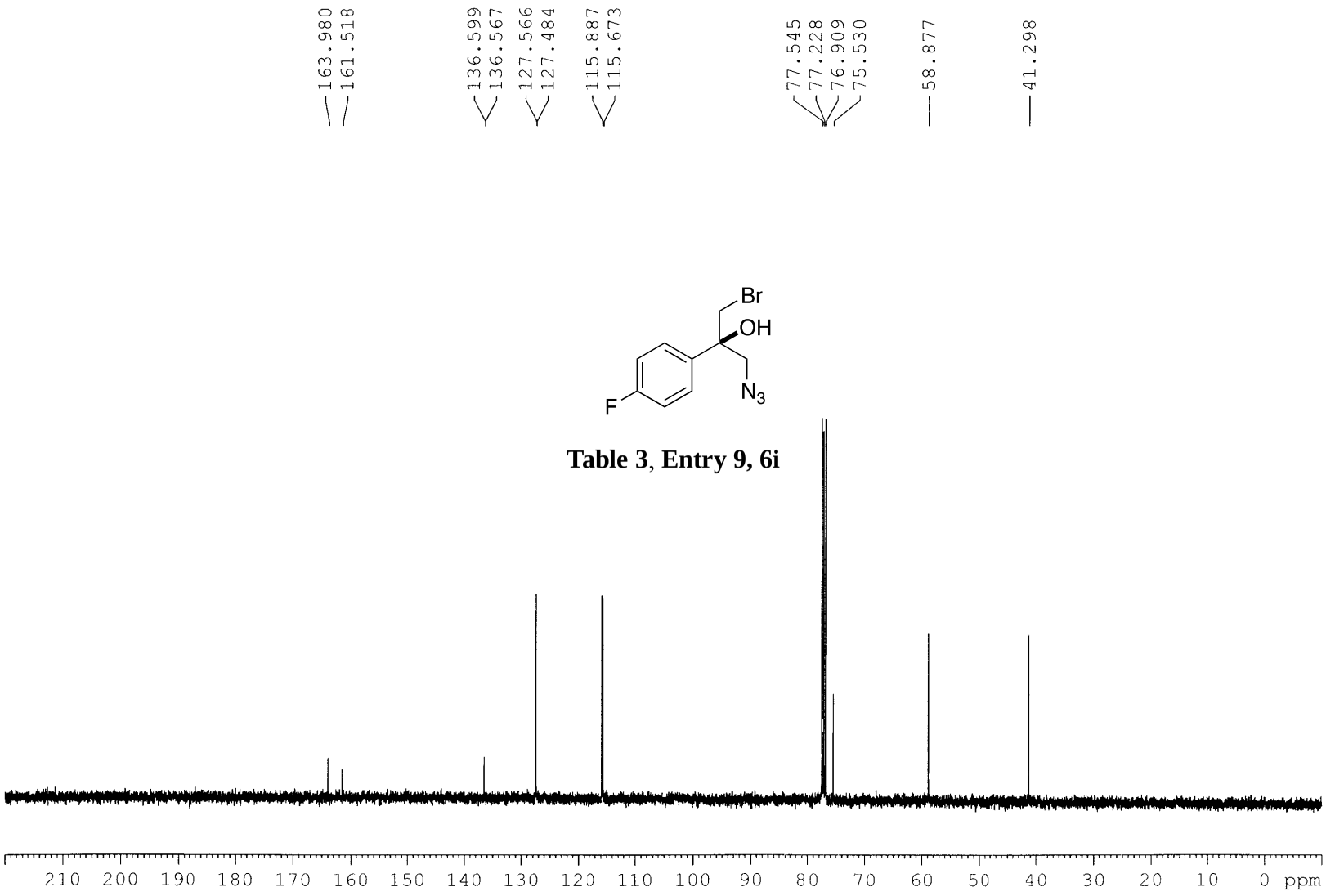


Table 3, Entry 9, 6i

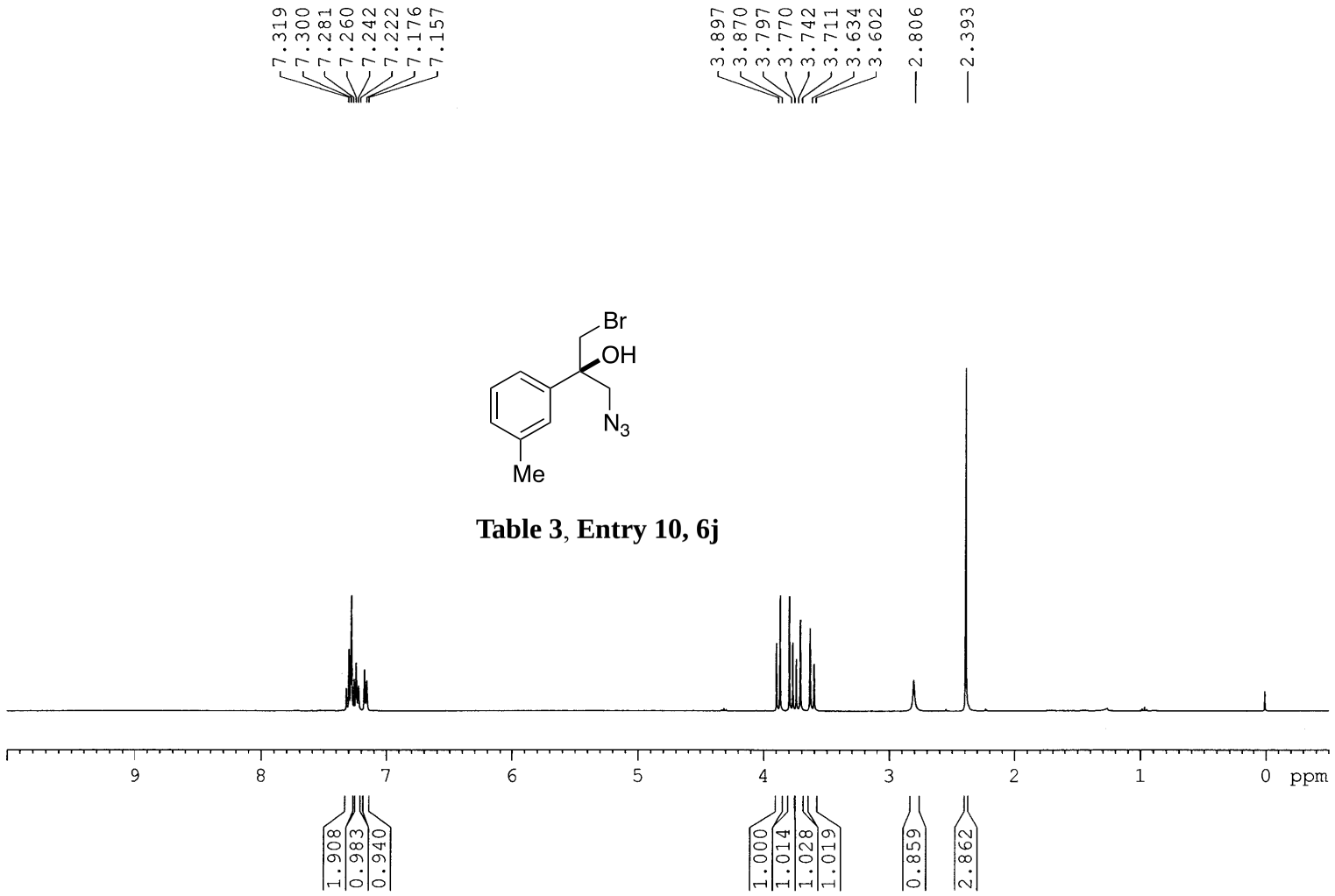


Table 3, Entry 10, 6j

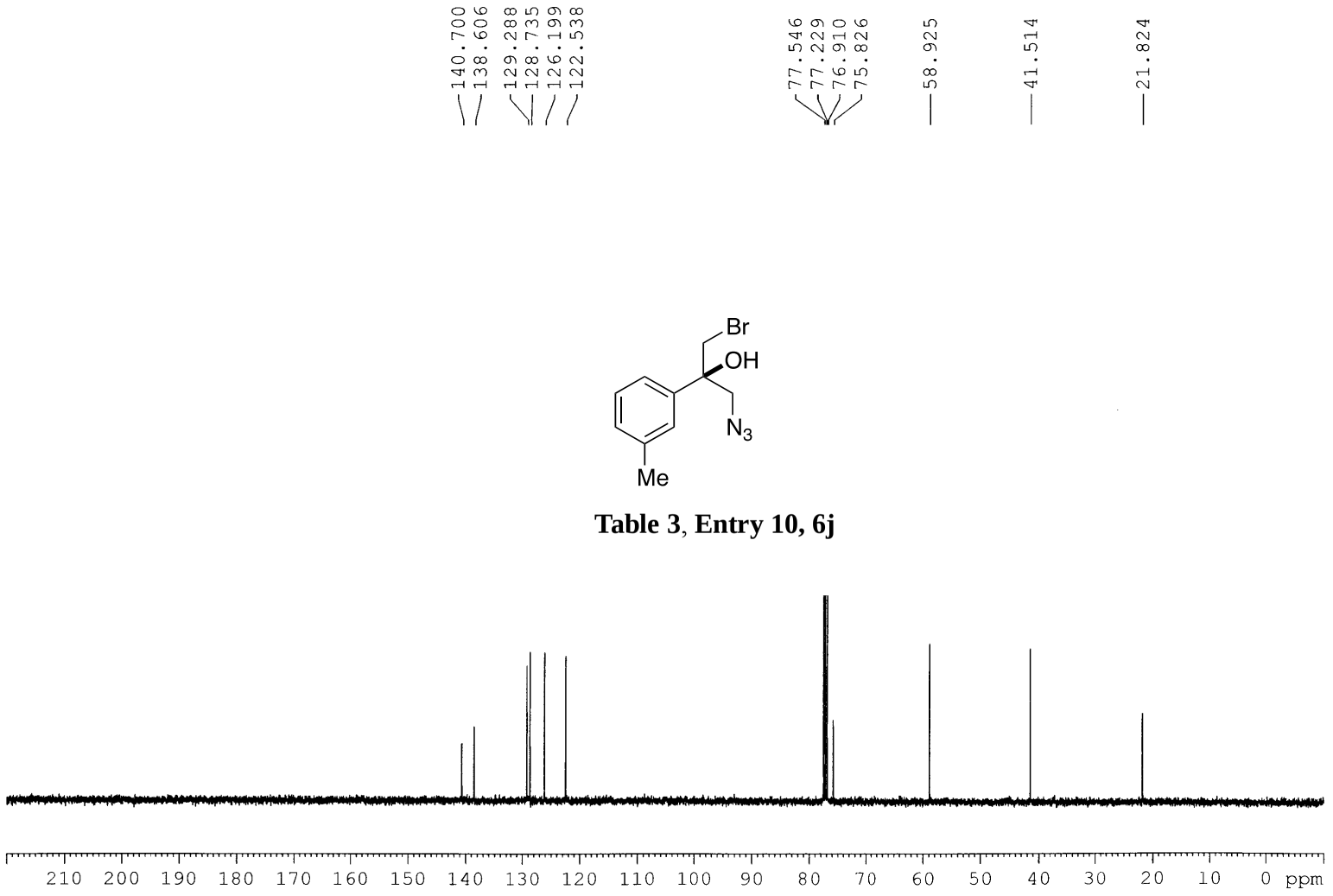
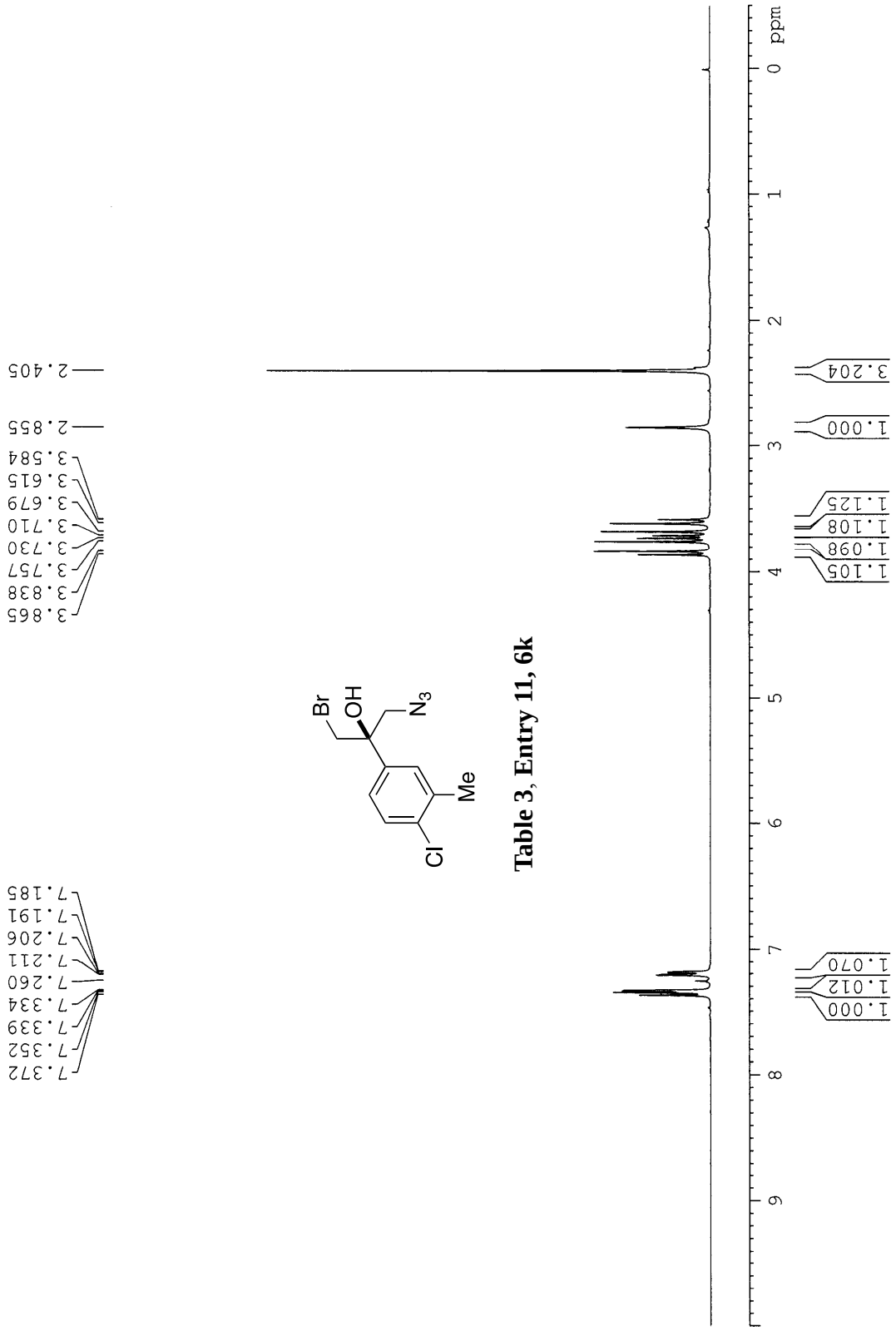


Table 3, Entry 10, 6j


7.372
7.352
7.339
7.334
7.260
7.211
7.206
7.191
7.185
3.865
3.838
3.757
3.730
3.710
3.679
3.615
3.584
2.855
2.405
Br
OH
N3
Me
Cl
Table 3, Entry 11, 6k
1.105
1.098
1.108
1.125
3.204
1.000
1.000
1.012
1.070
0 ppm

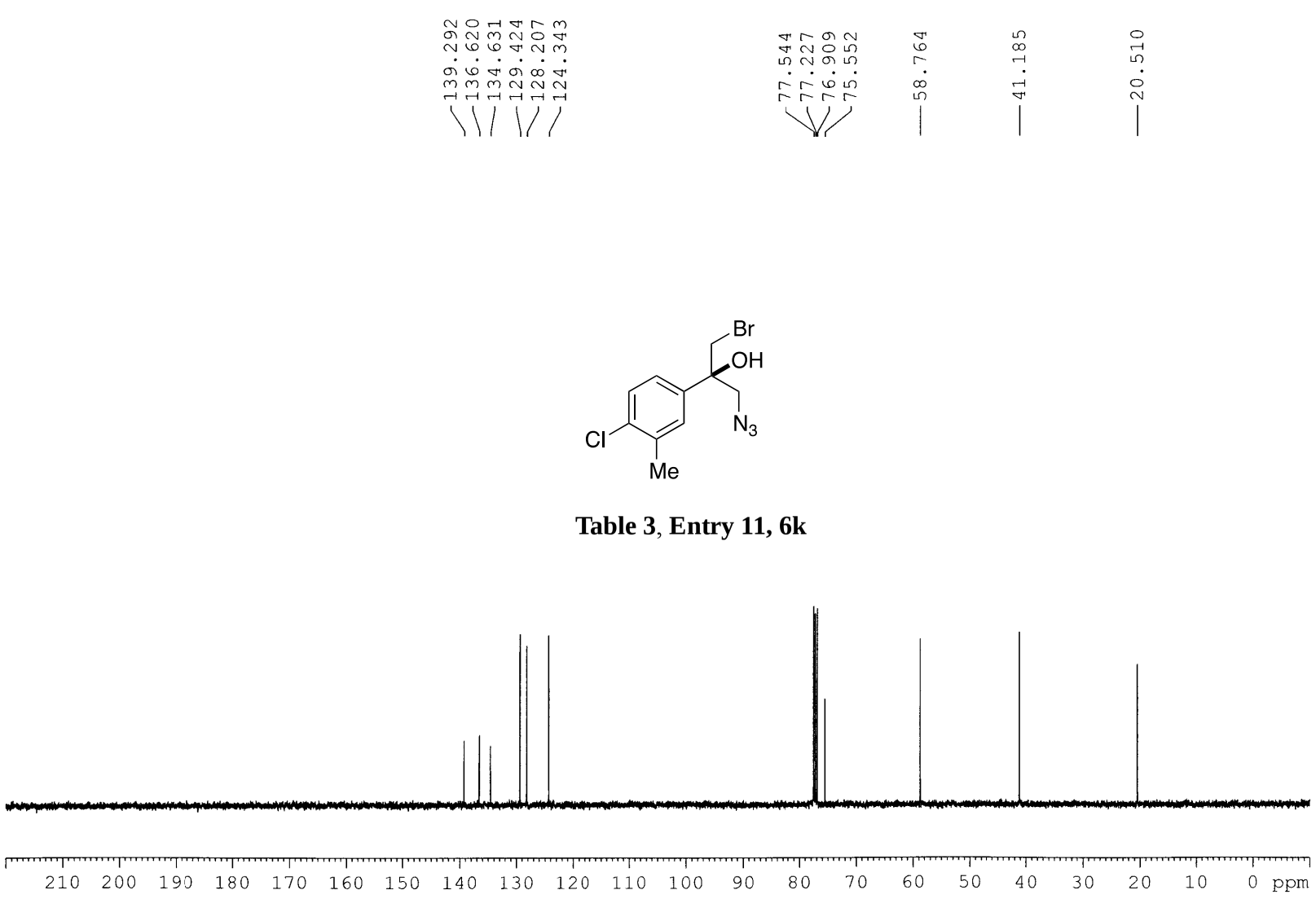
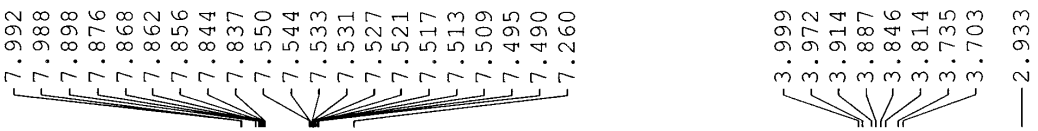


Table 3, Entry 11, 6k



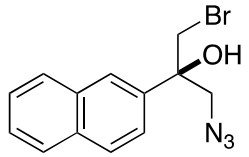
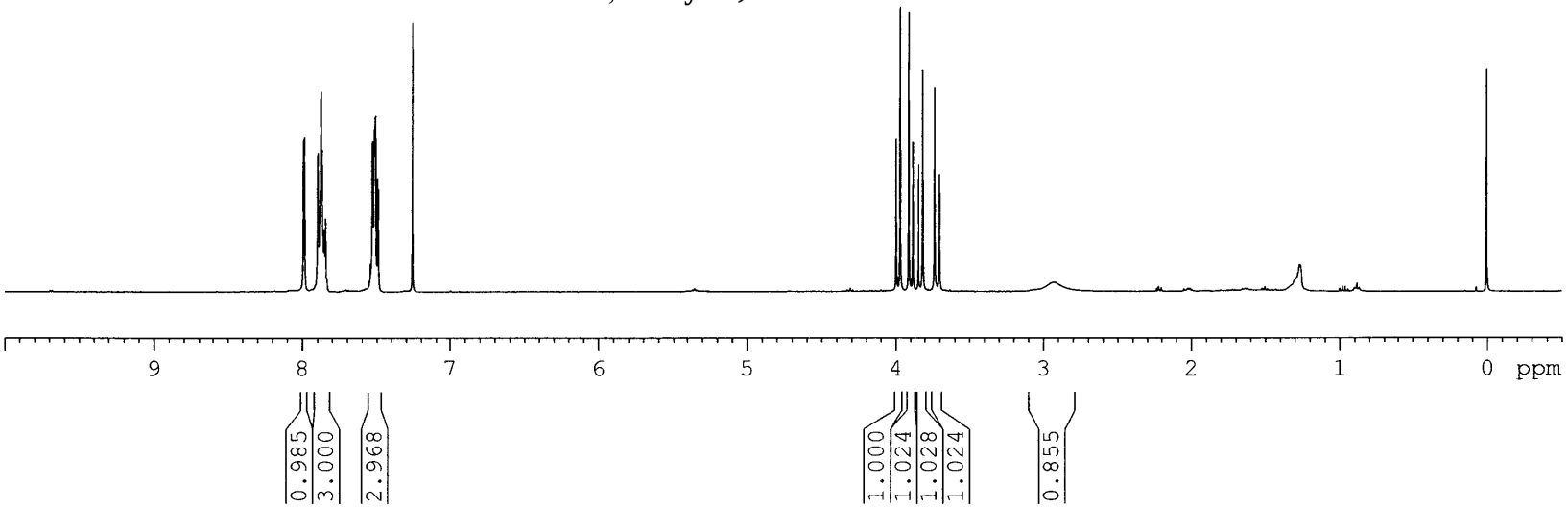


Table 3, **Entry 12, 6l**



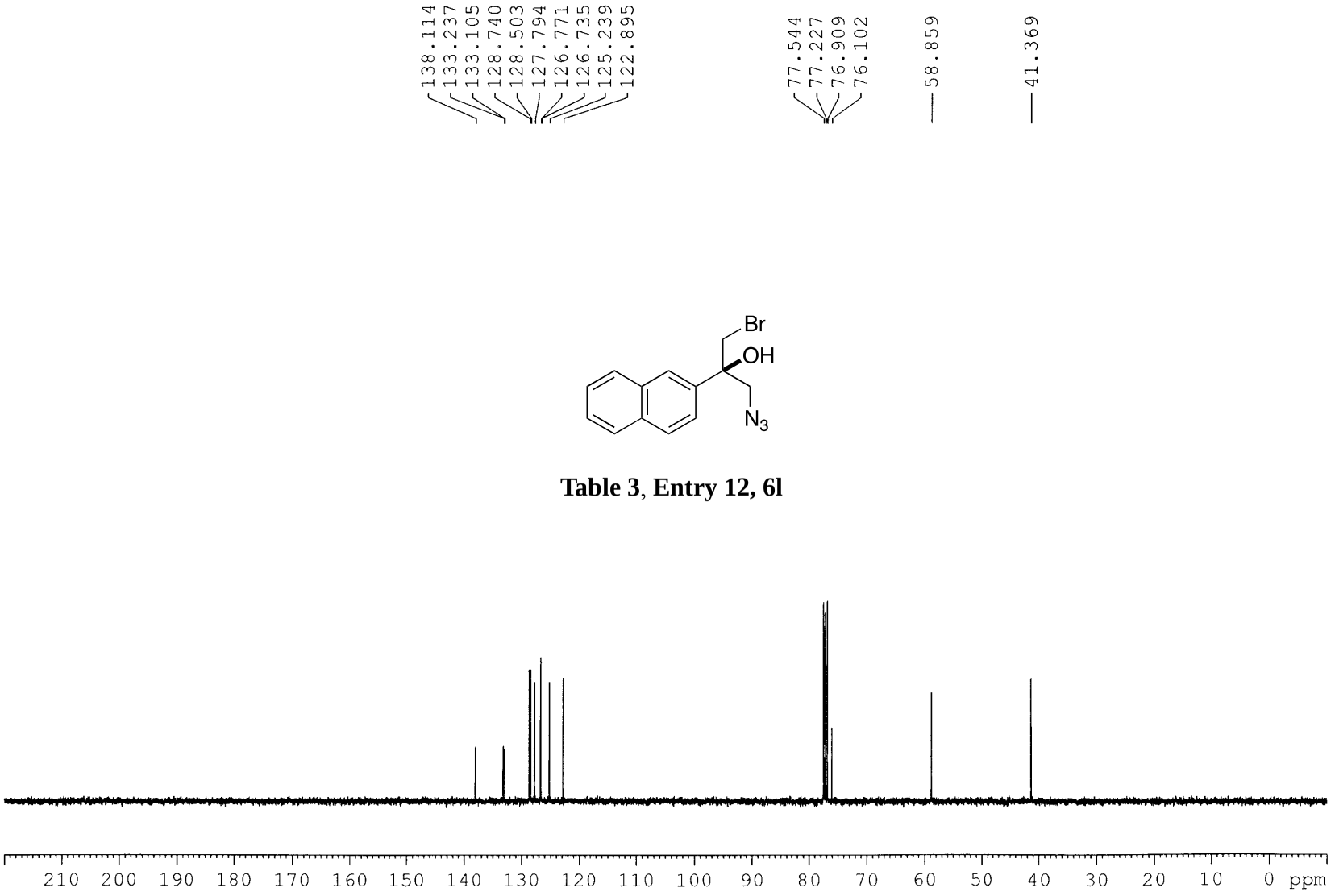


Table 3, **Entry 12, 6l**

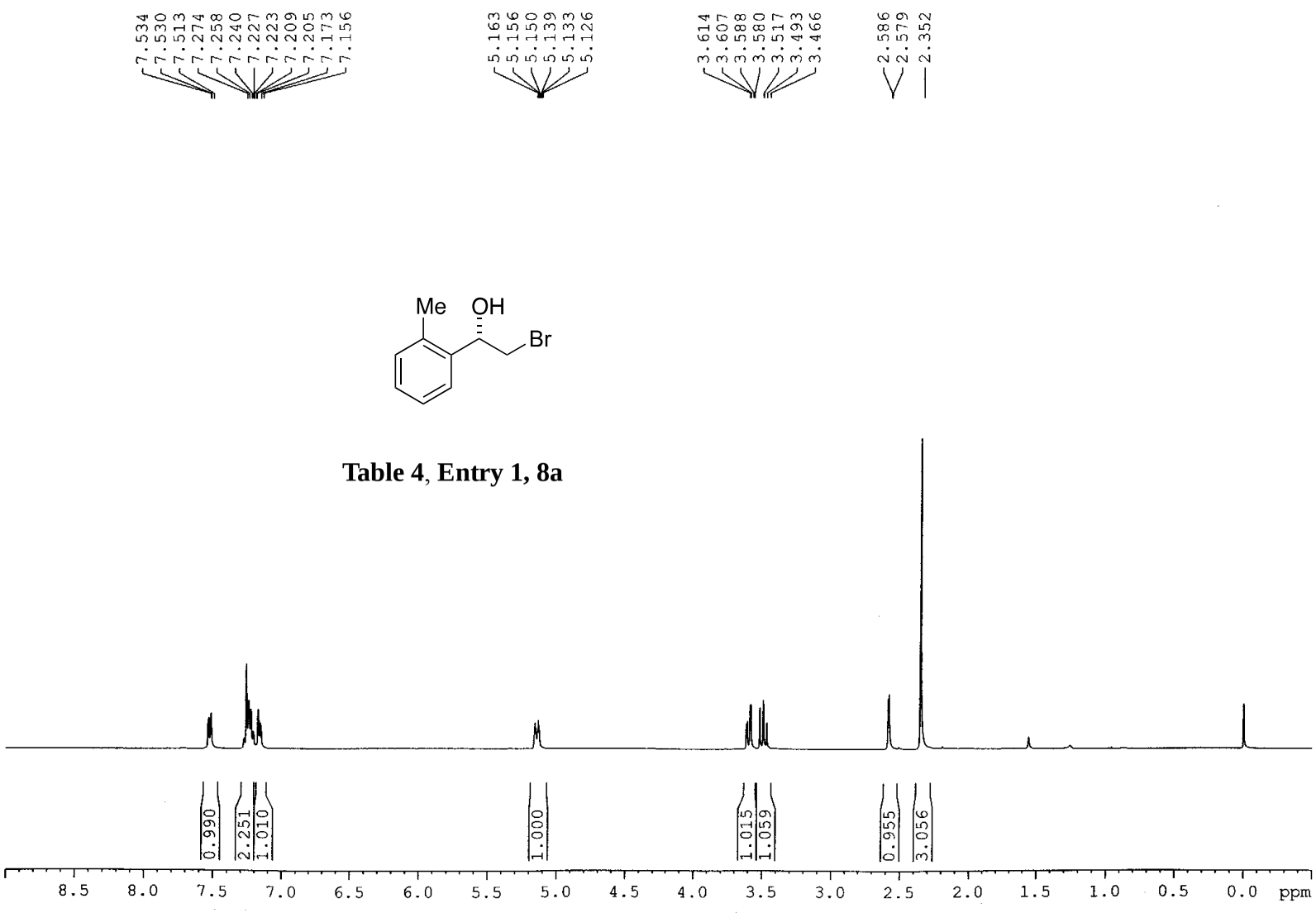


Table 4, **Entry 1, 8a**

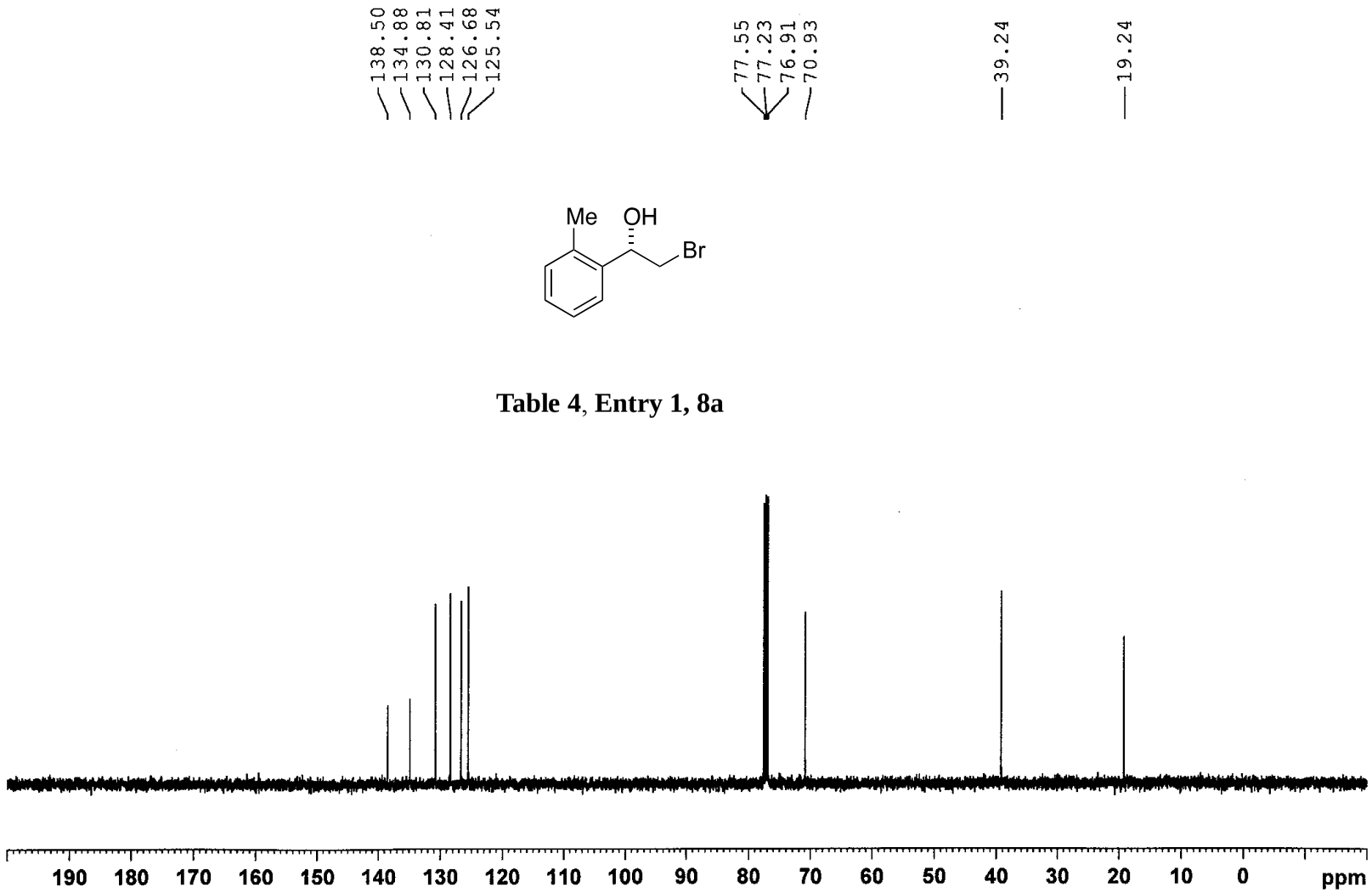
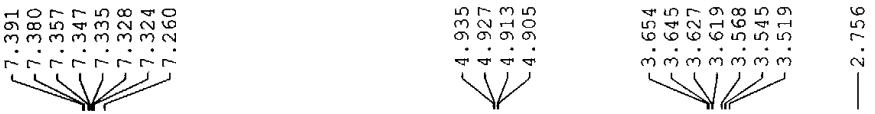


Table 4, Entry 1, 8a



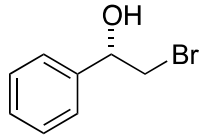
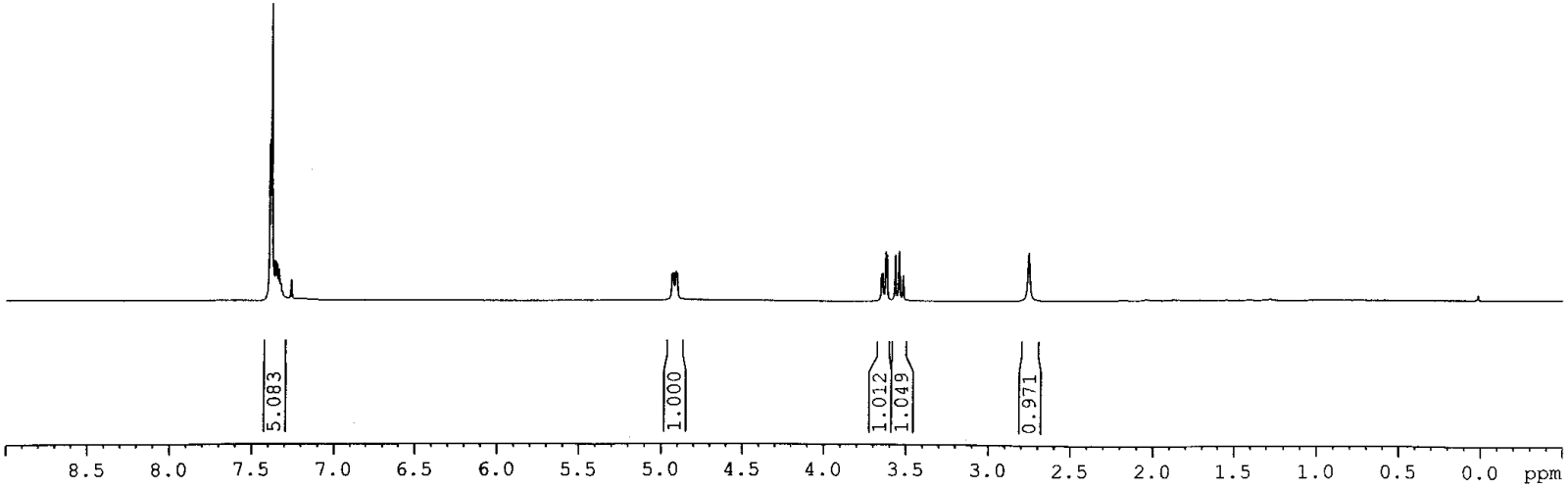


Table 4, **Entry 2, 8b**



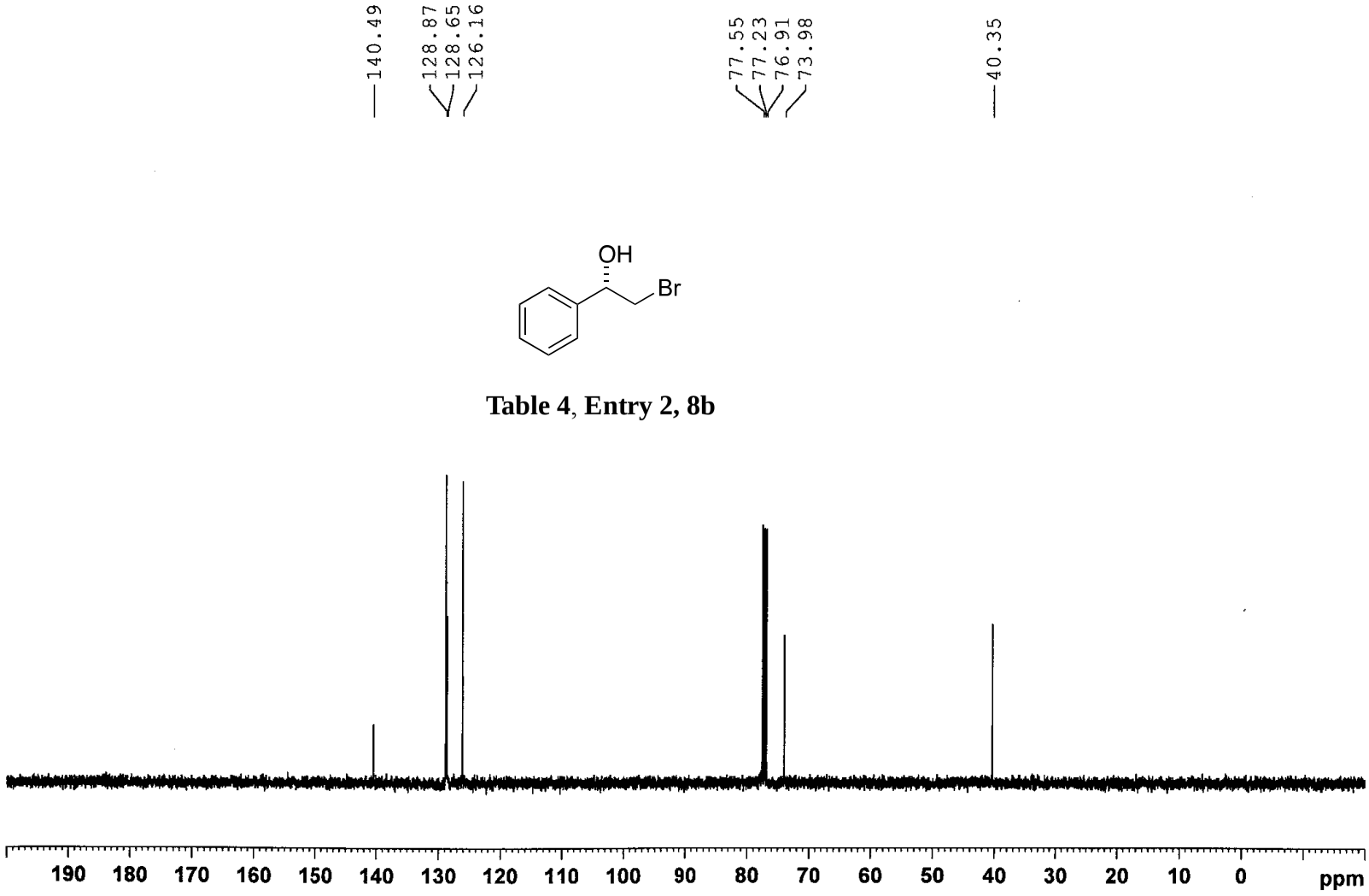


Table 4, Entry 2, 8b

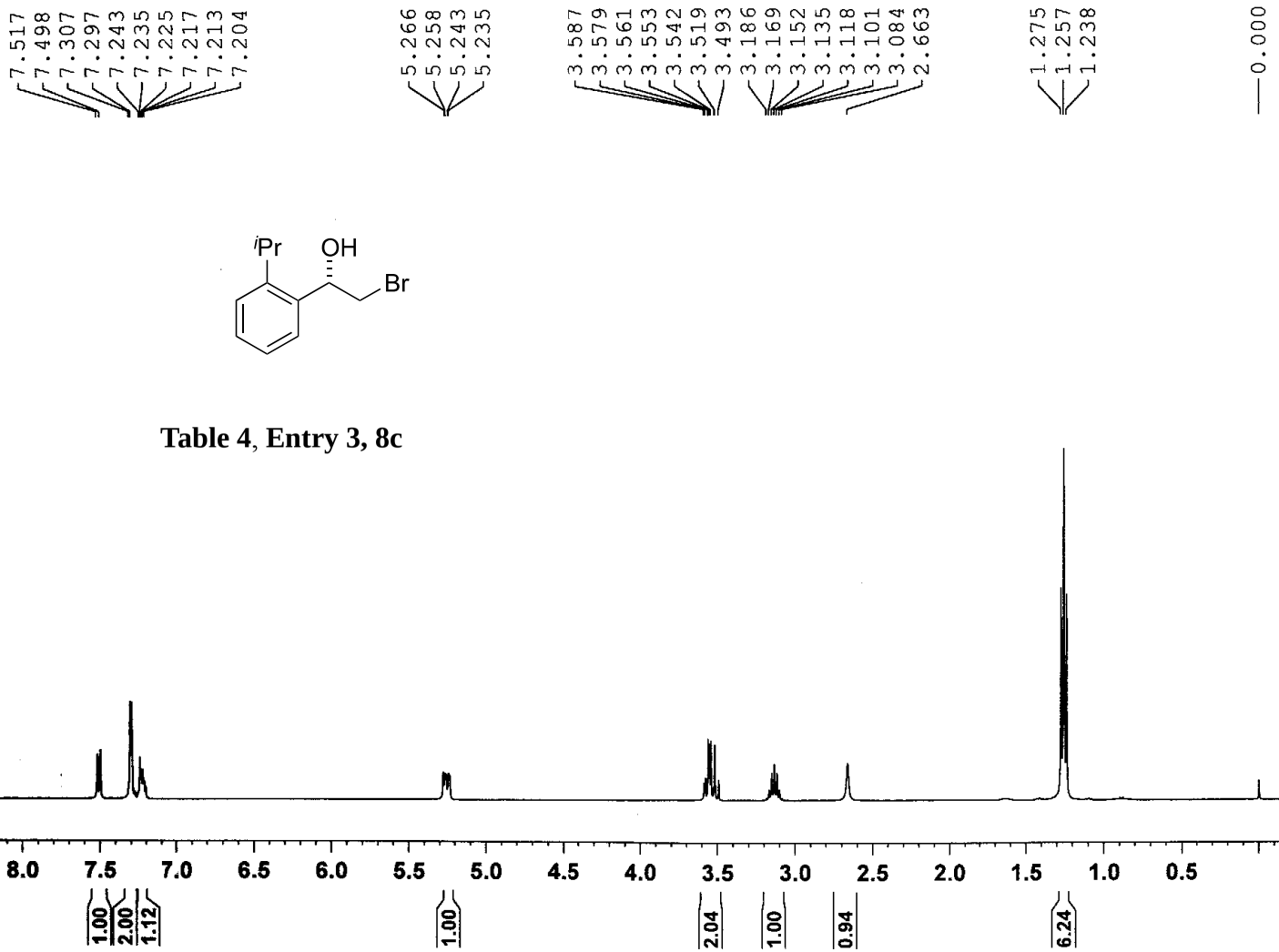


Table 4, **Entry 3, 8c**

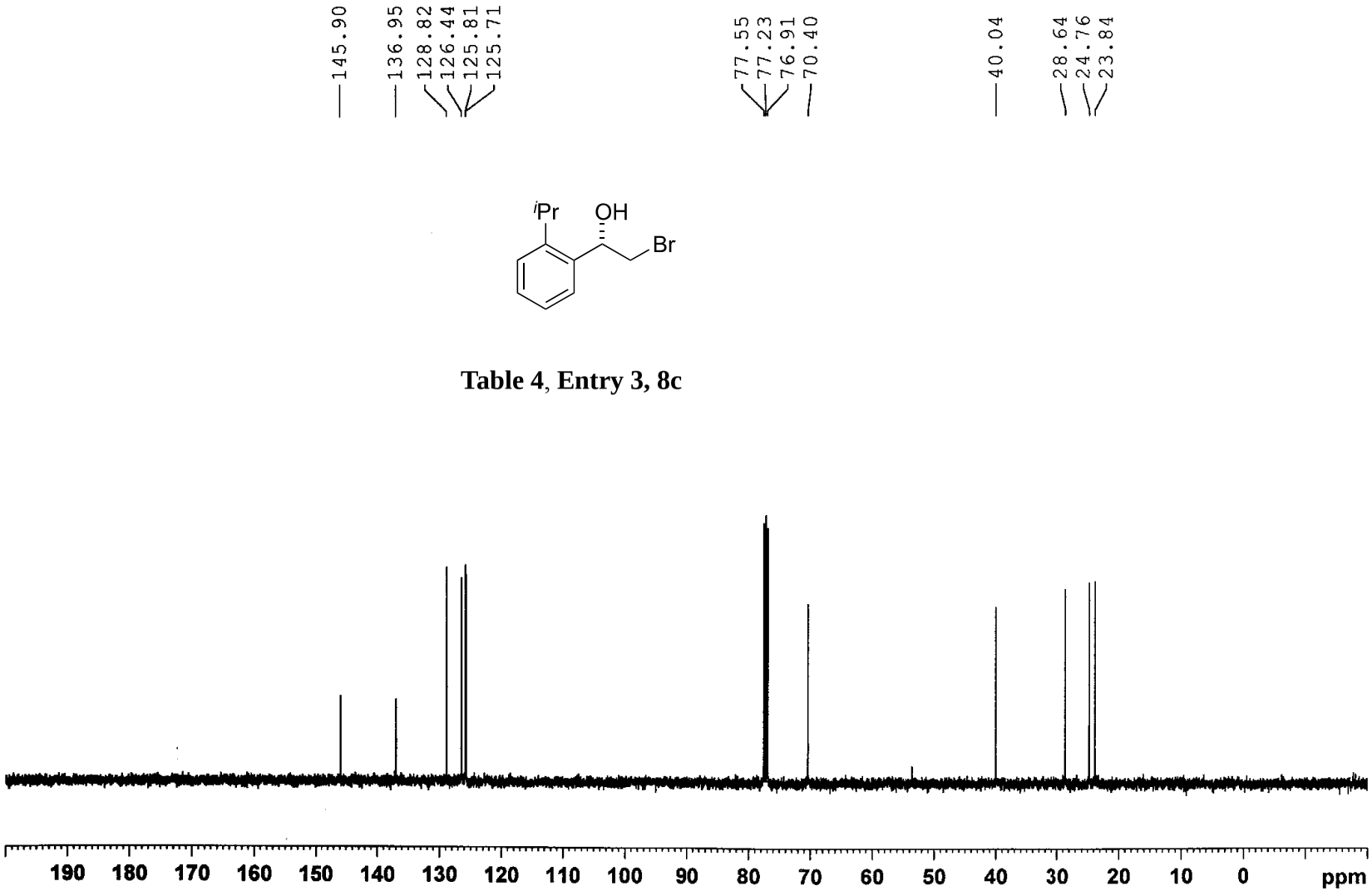


Table 4, **Entry 3, 8c**

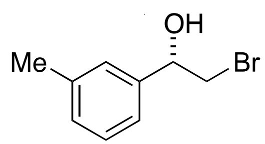
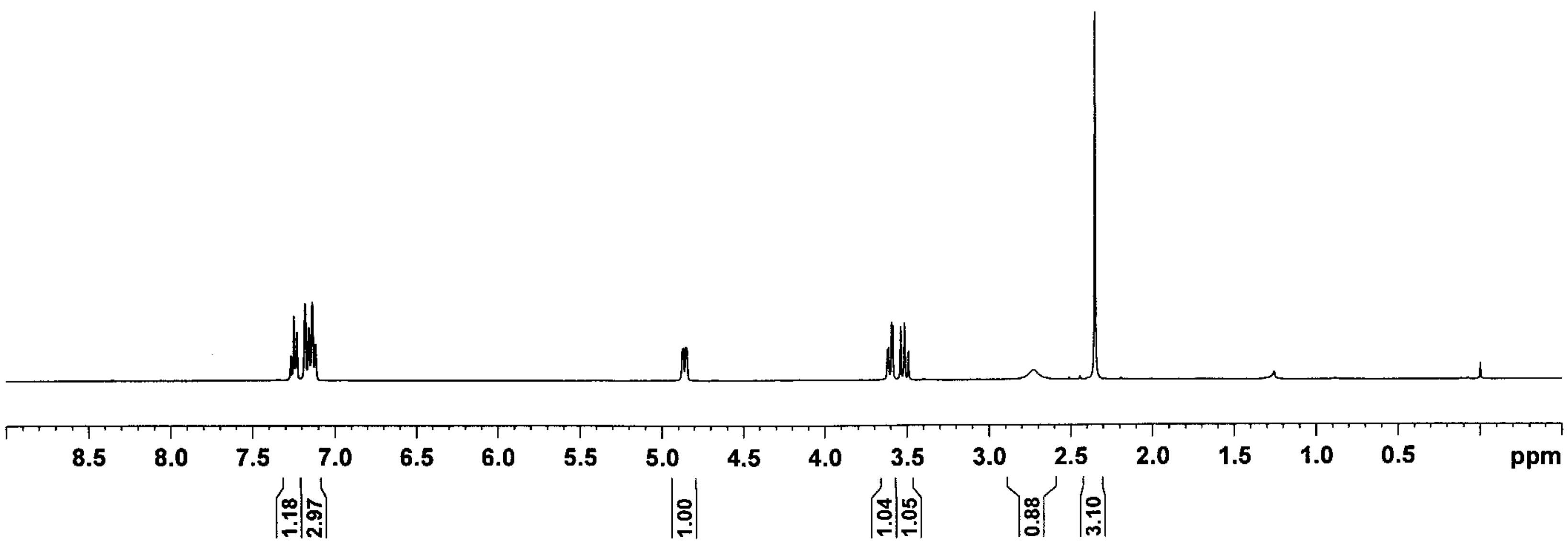


Table 4, Entry 4, 8d



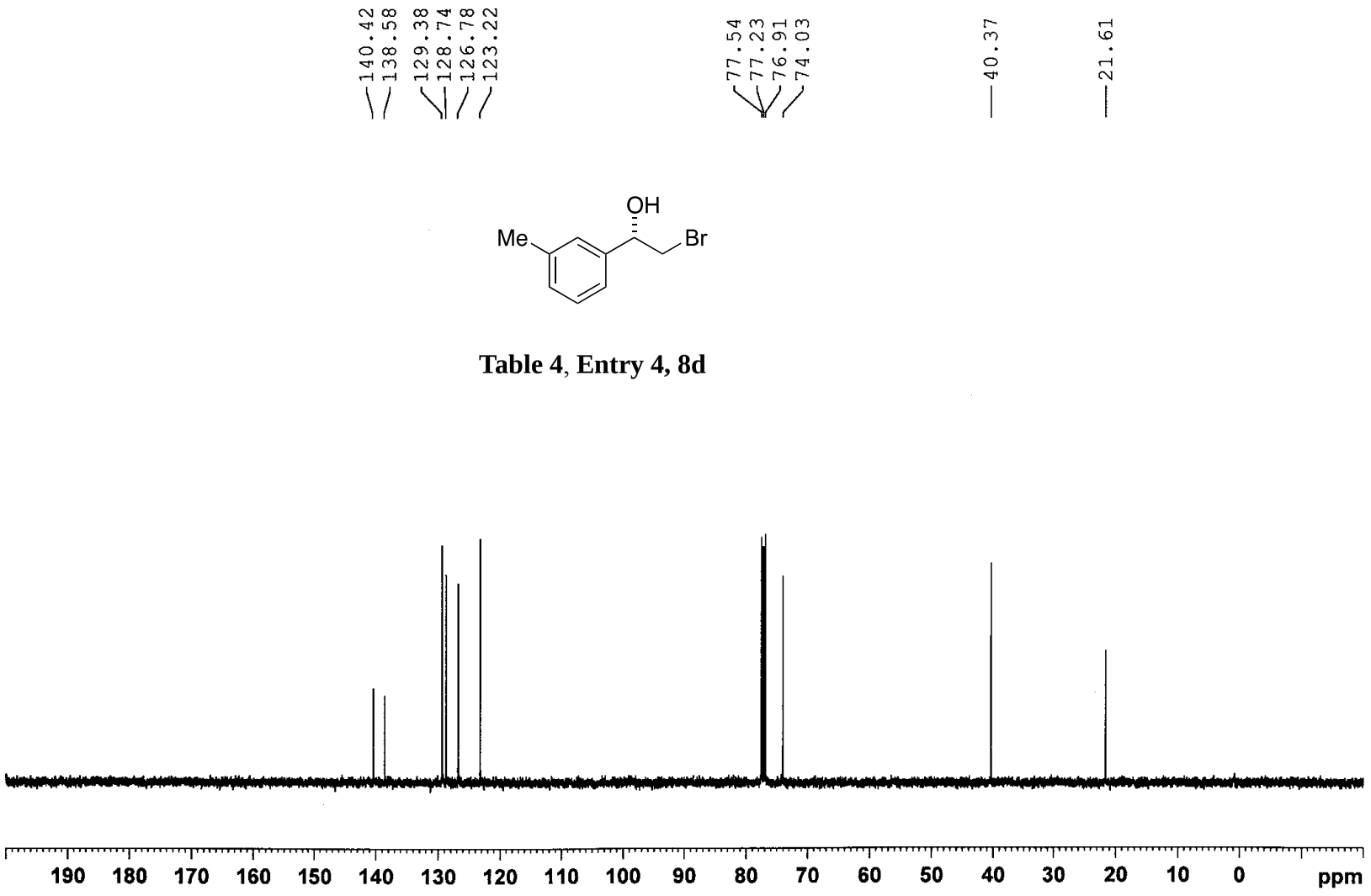


Table 4, **Entry 4, 8d**

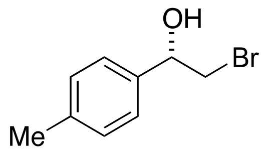
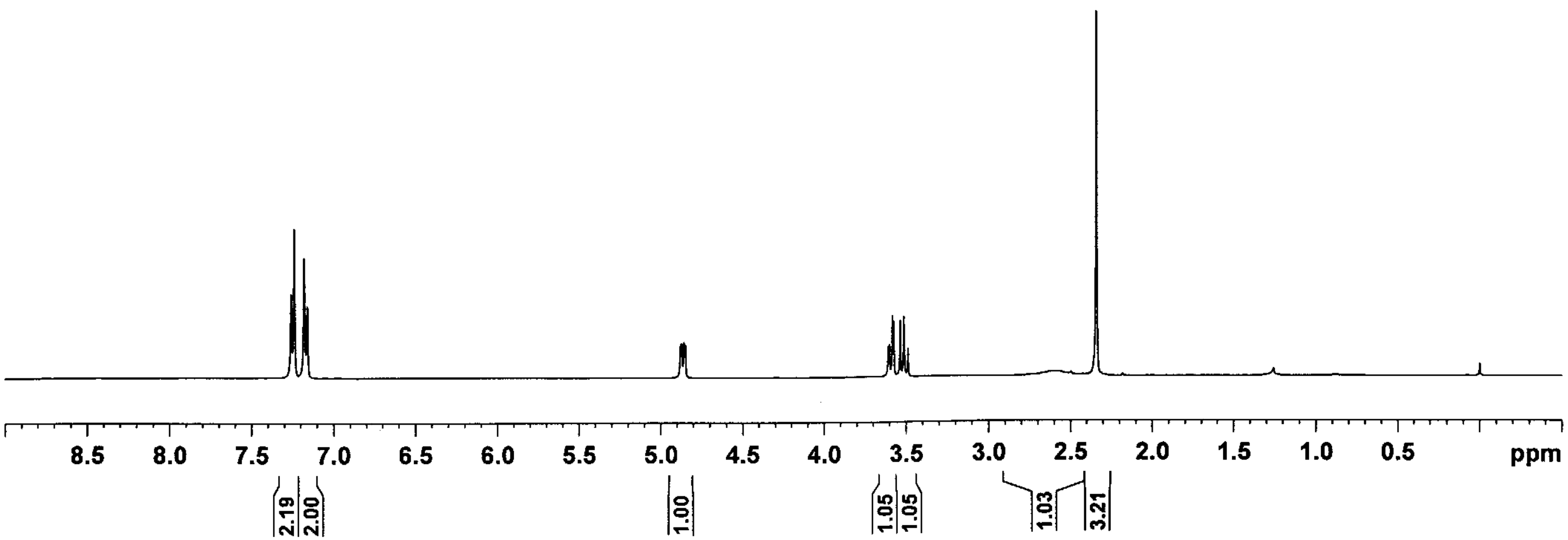


Table 4, Entry 5, 8e



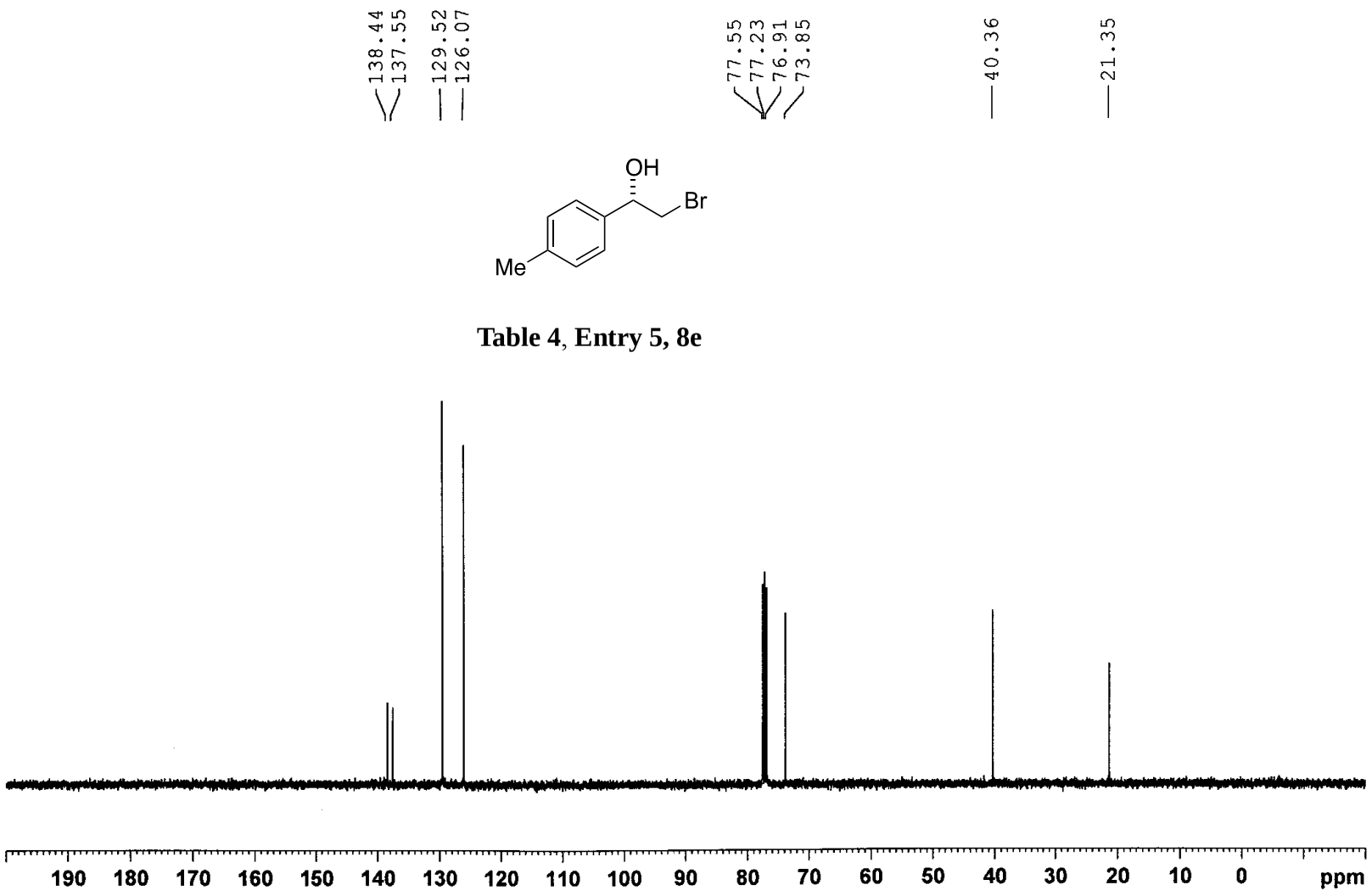


Table 4, **Entry 5, 8e**

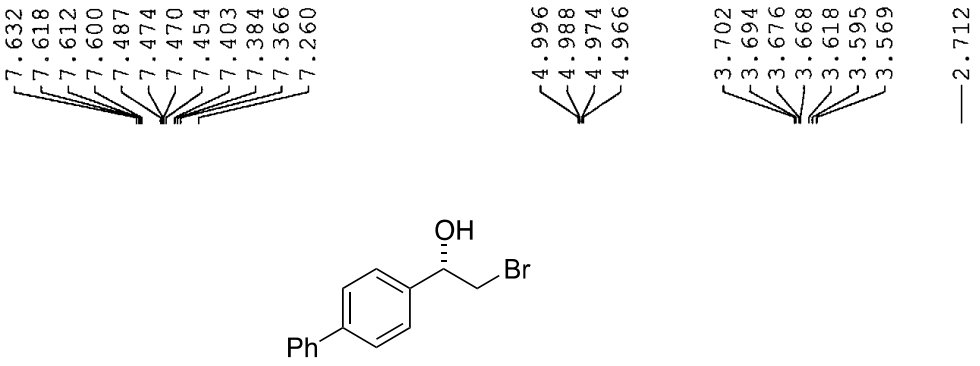
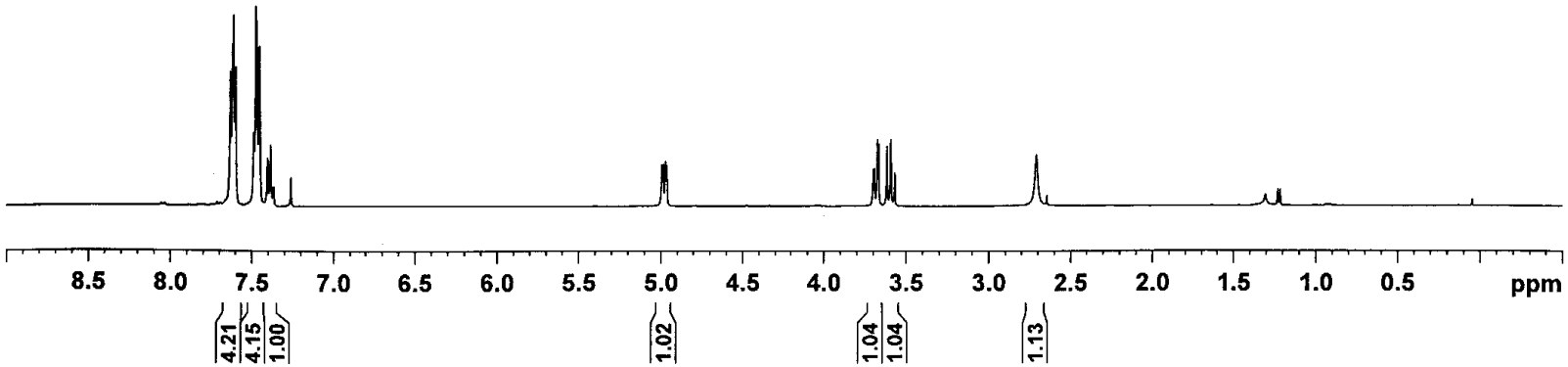


Table 4, **Entry 6, 8f**



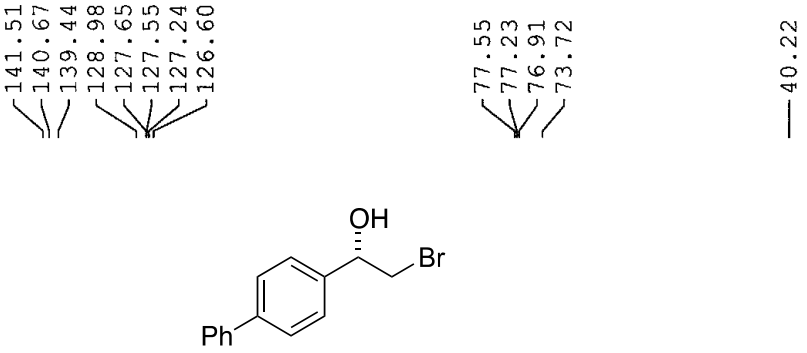
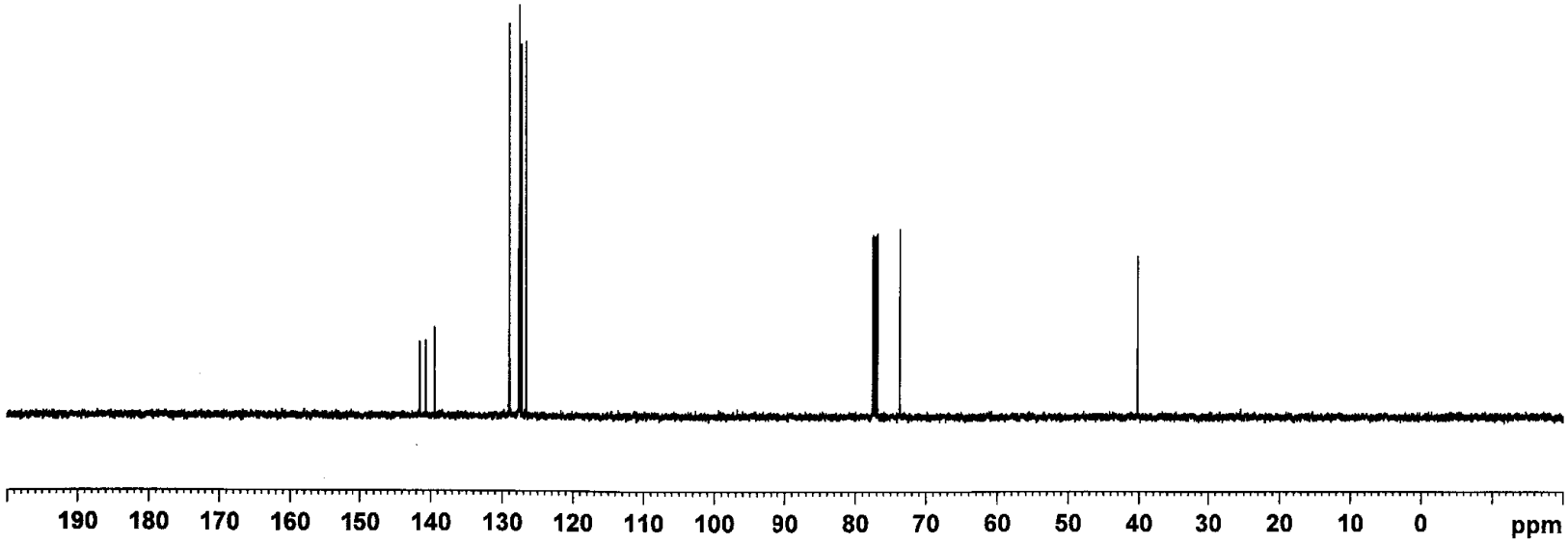
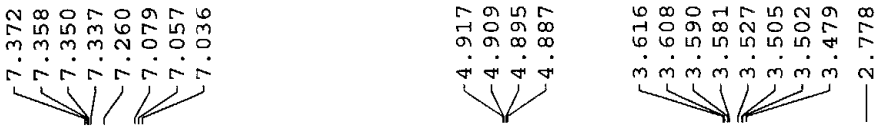


Table 4, **Entry 6, 8f**





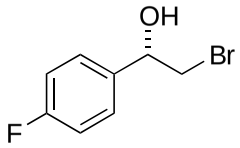
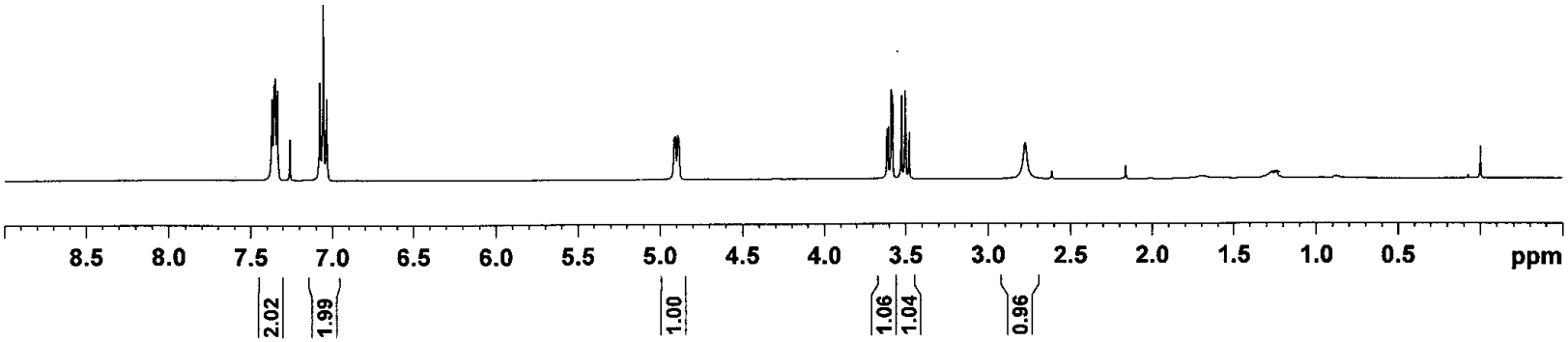


Table 4, **Entry 7, 8g**



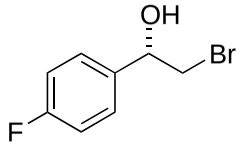
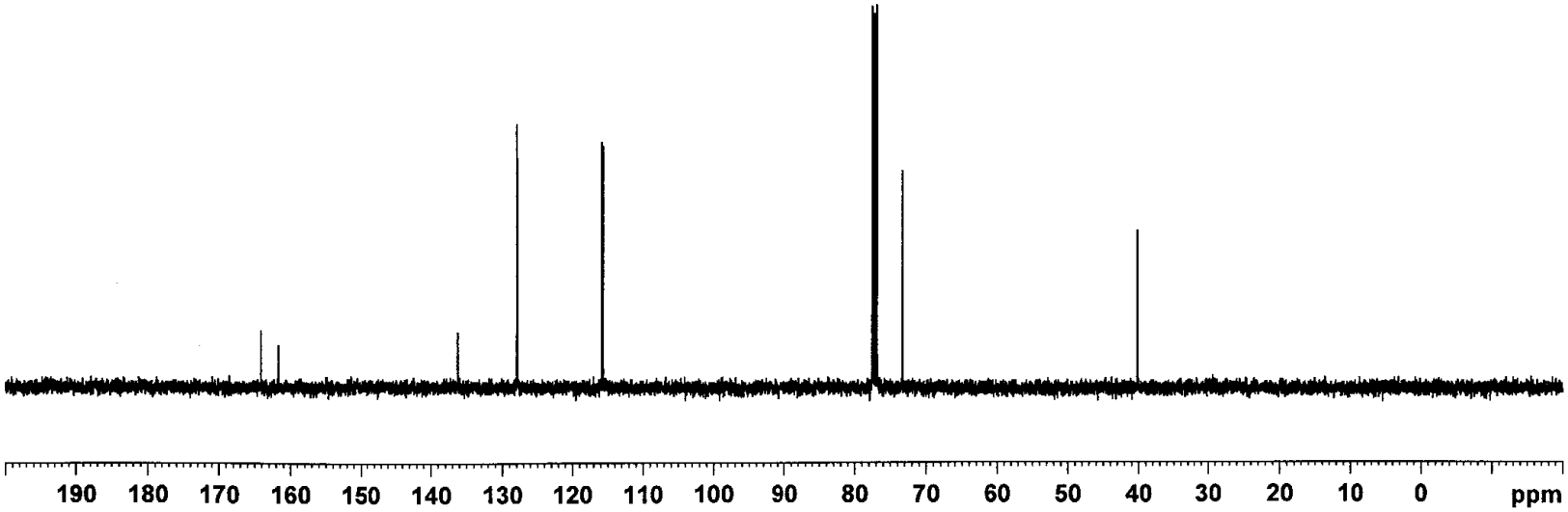


Table 4, Entry 7, 8g



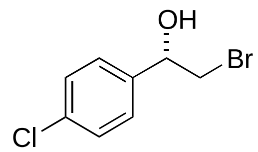
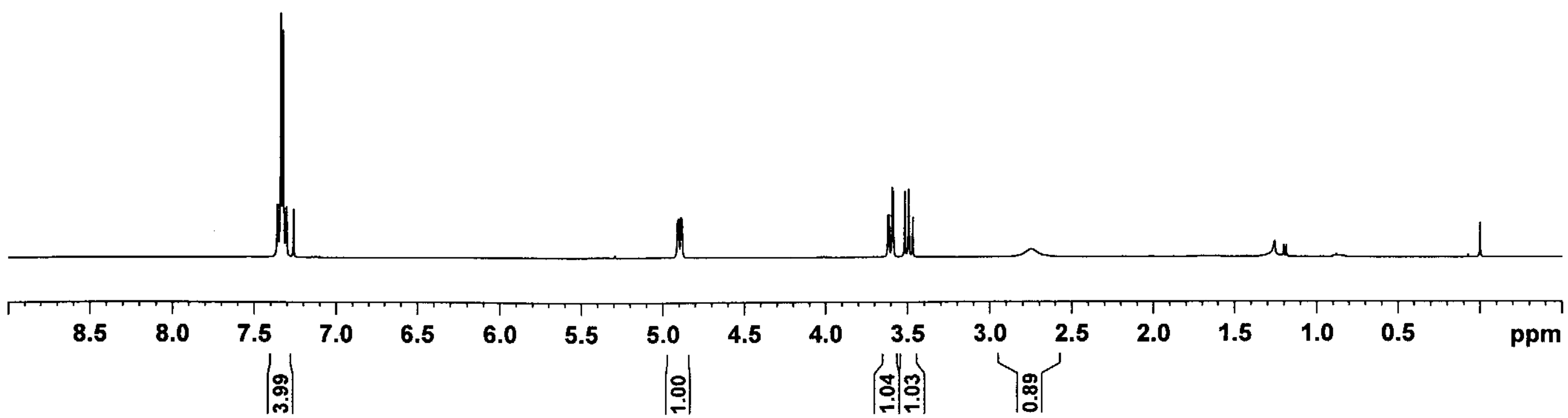


Table 4, Entry 8, 8h



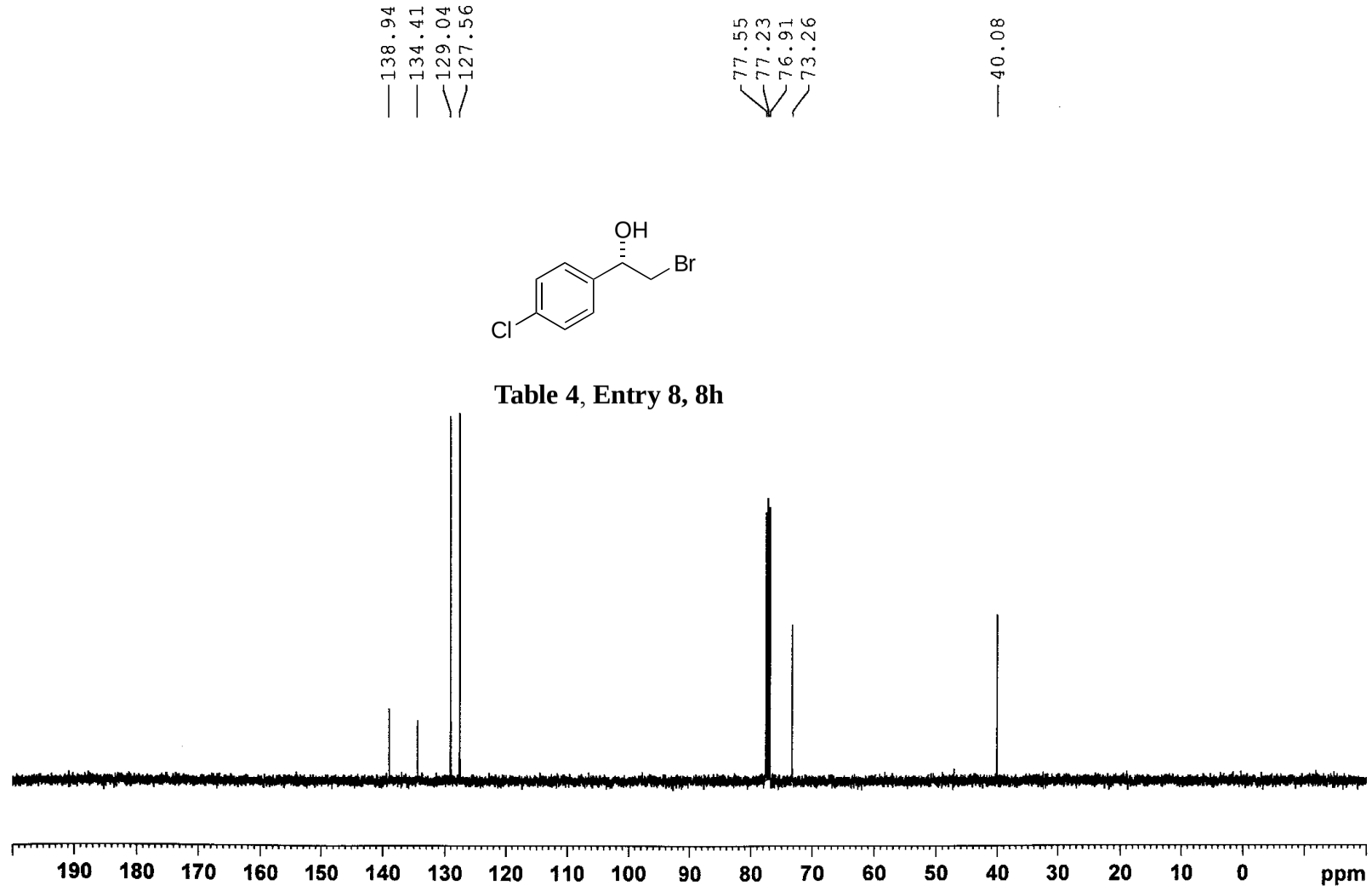


Table 4, Entry 8, 8h

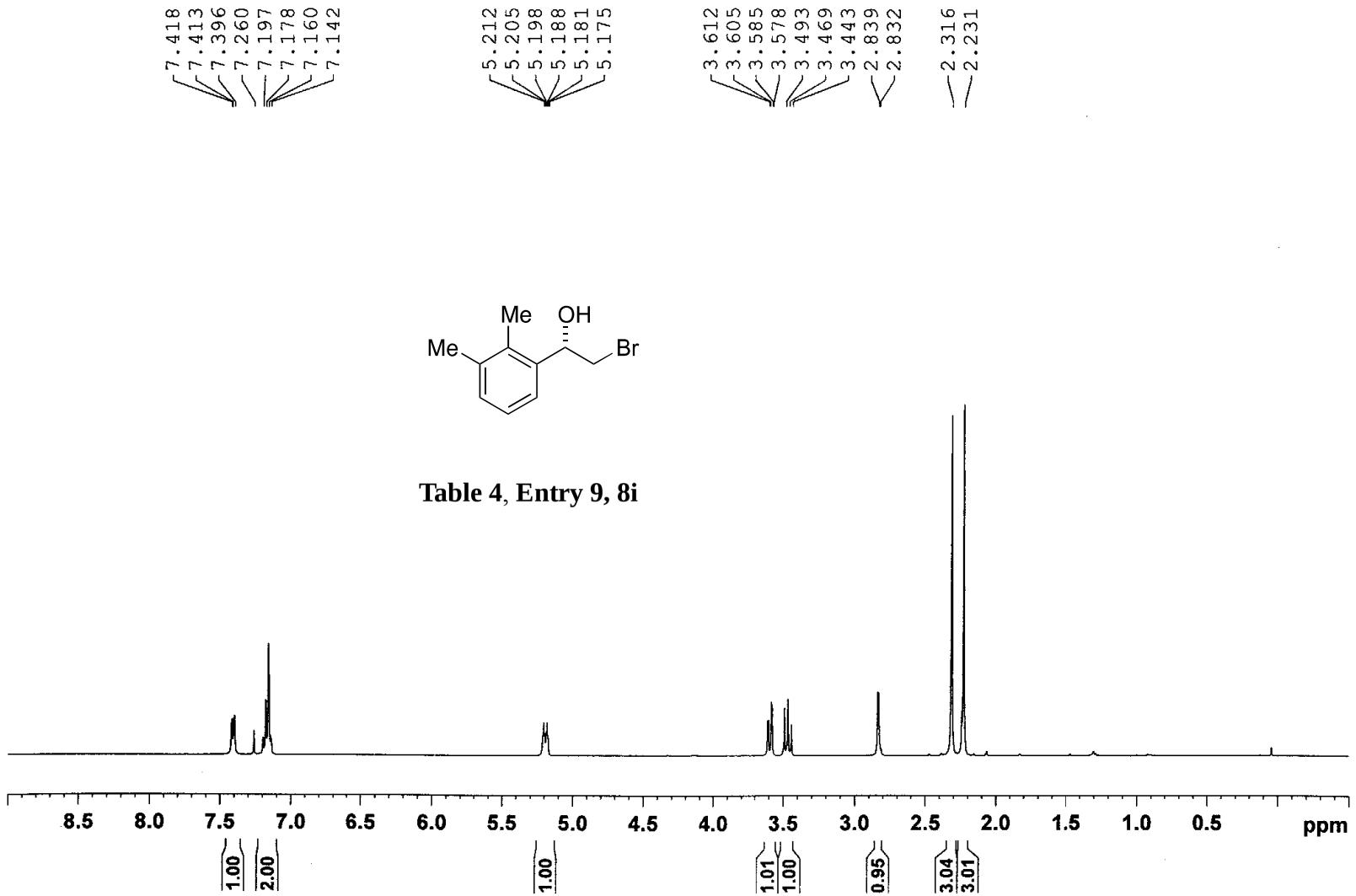
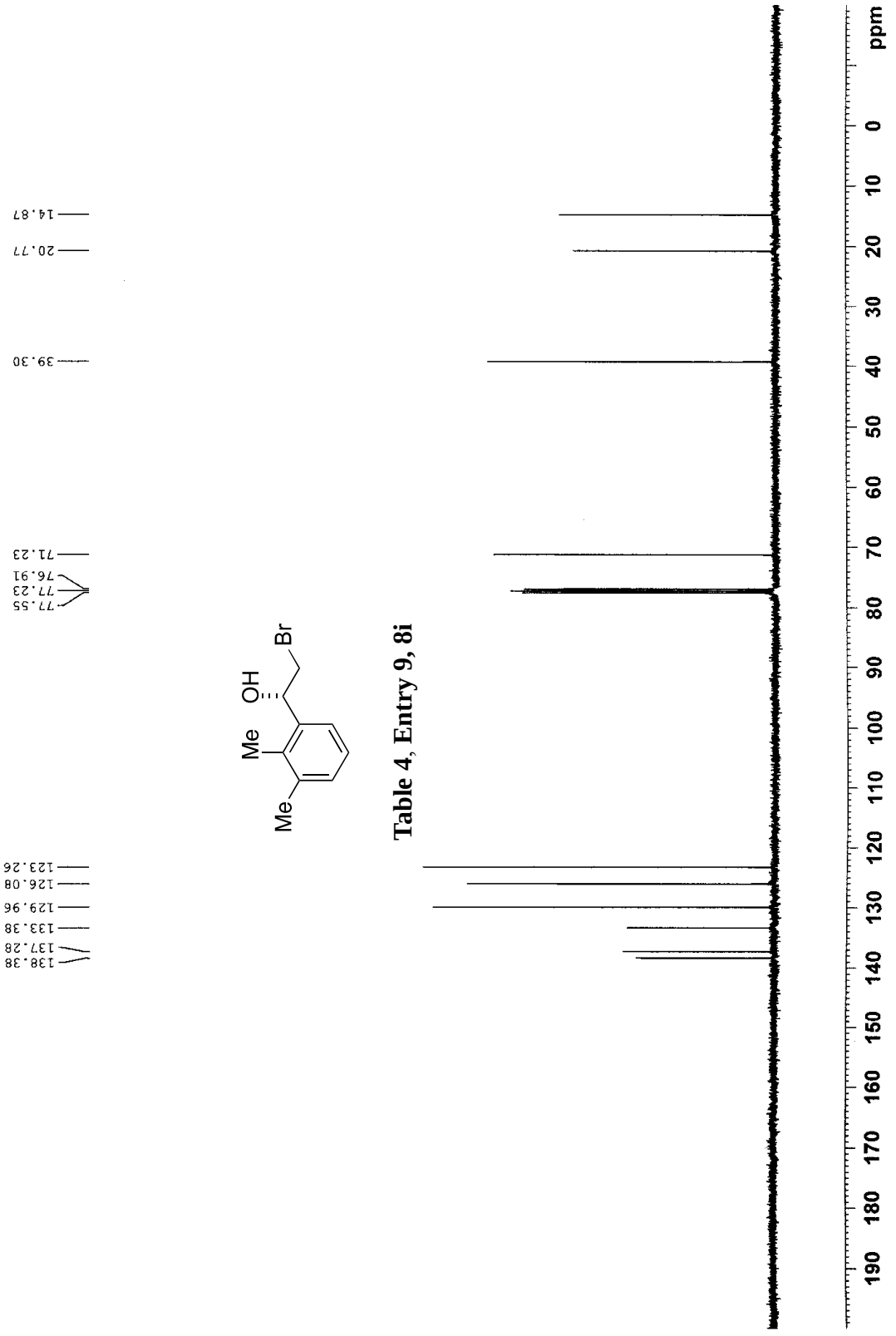


Table 4, **Entry 9, 8i**


14.87
20.77
39.30
71.23
76.91
77.23
77.55
123.26
126.08
129.96
133.38
137.28
138.38
Me
OH
Br
Me
Table 4, Entry 9, 8i
ppm
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

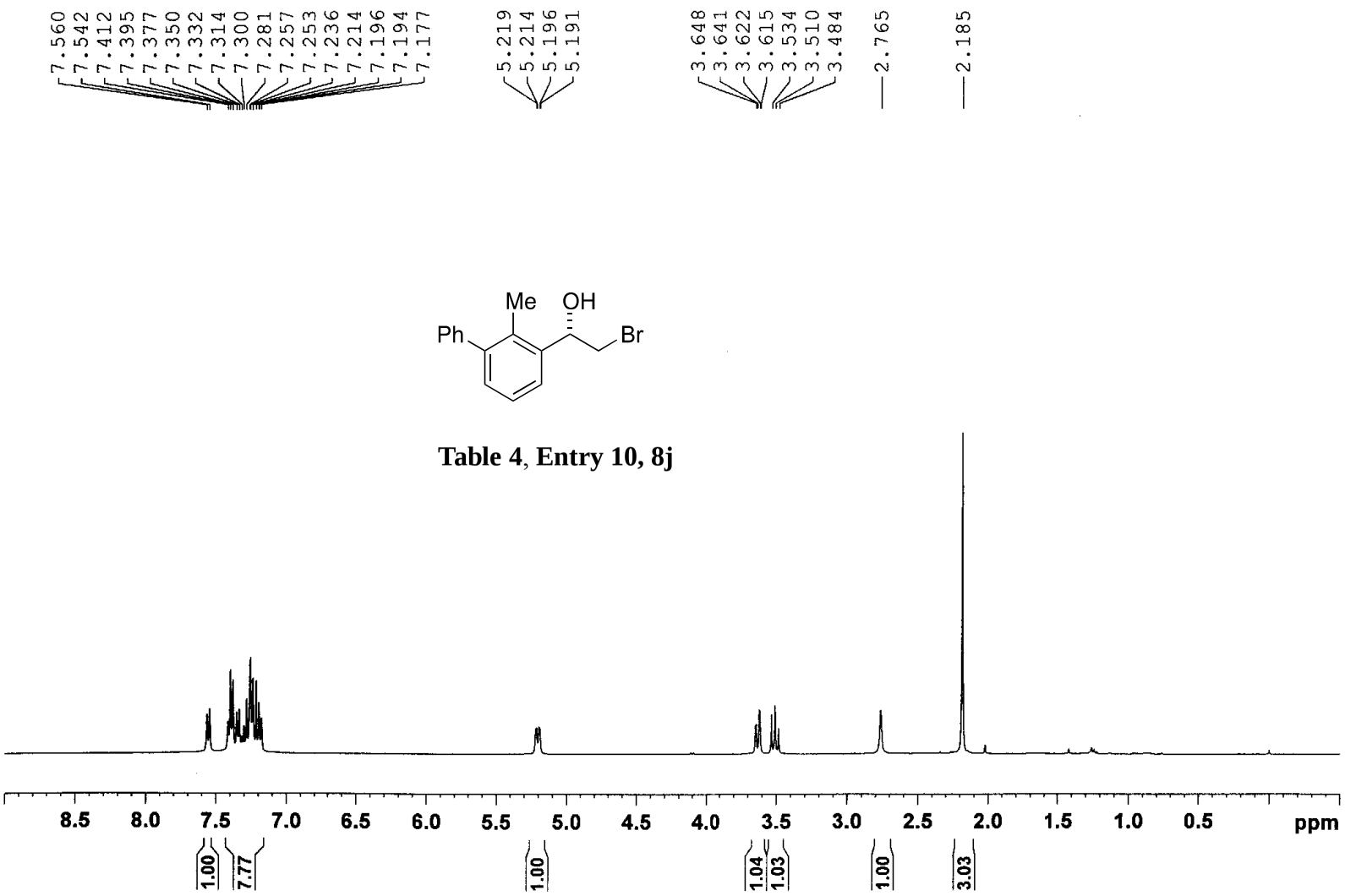


Table 4, **Entry 10, 8j**

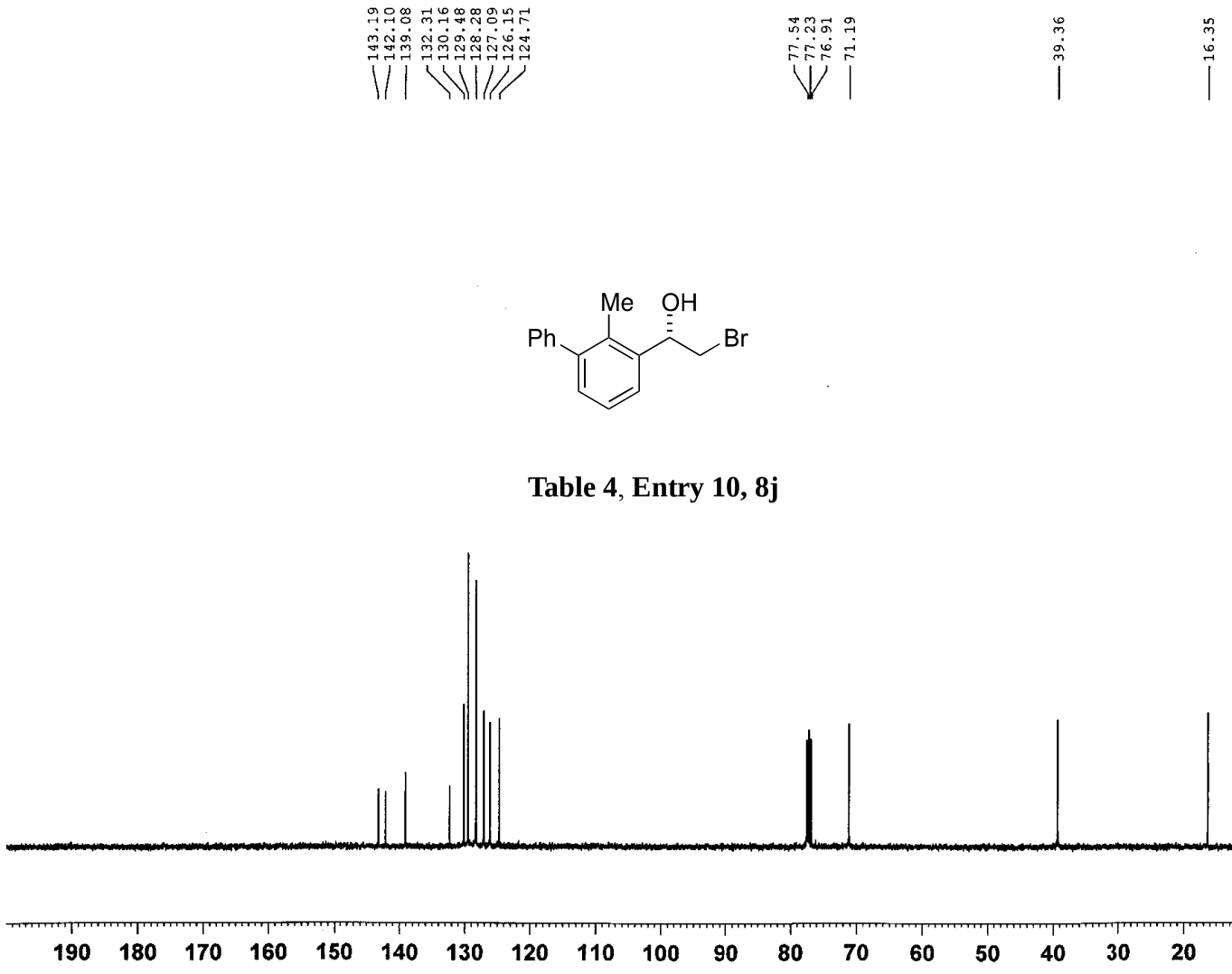


Table 4, **Entry 10, 8j**

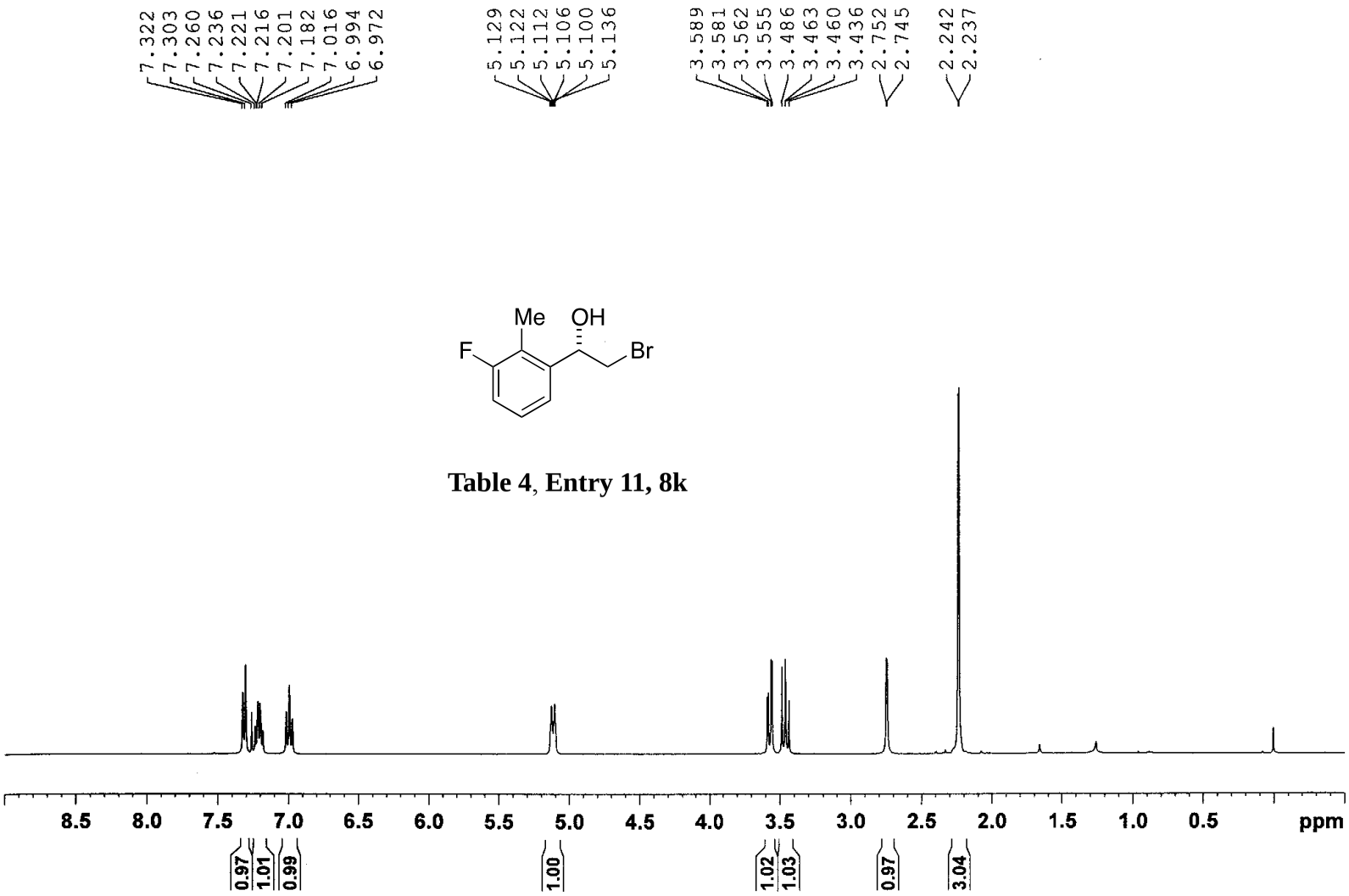


Table 4, **Entry 11, 8k**

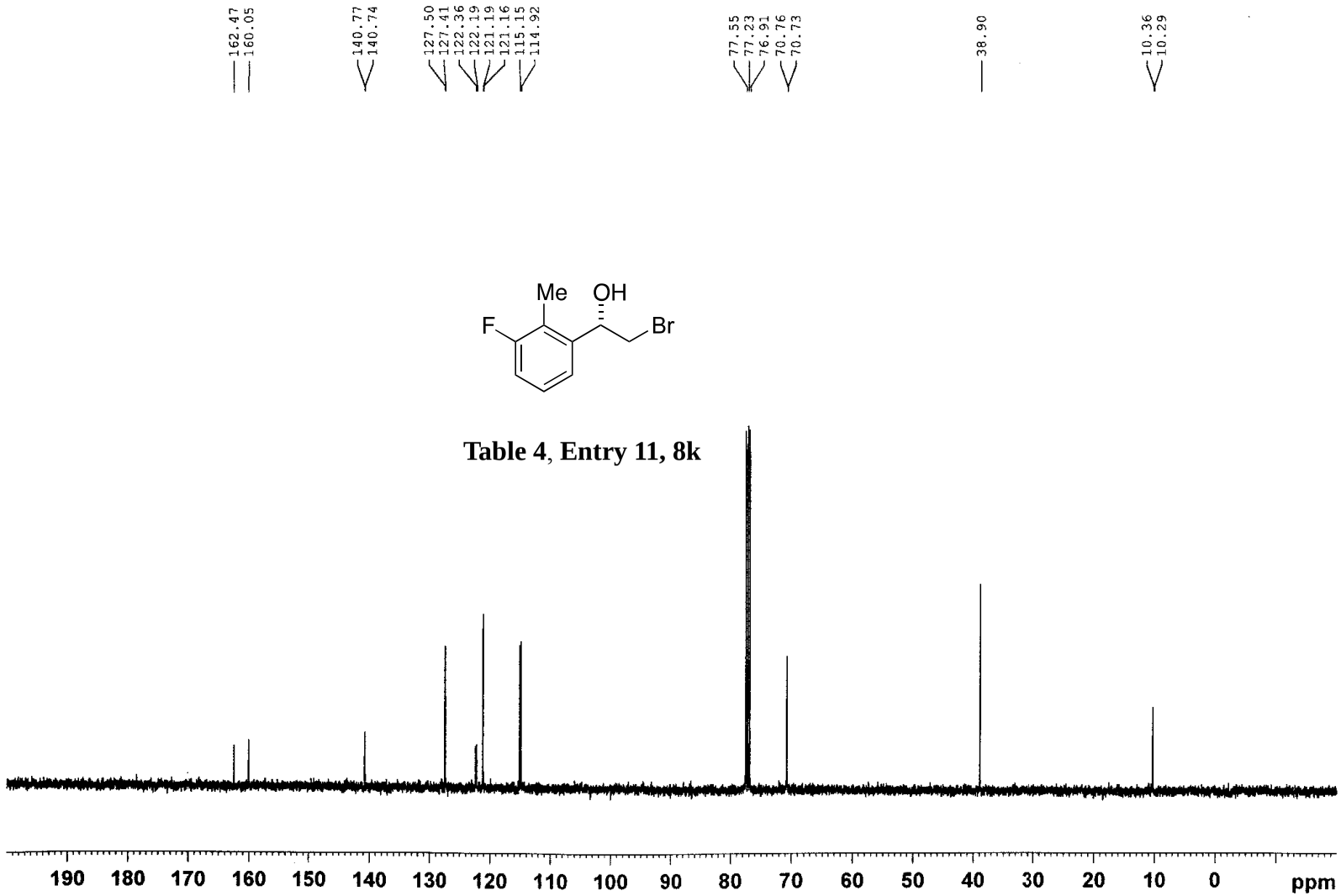
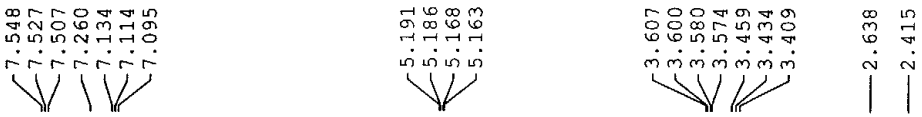


Table 4, Entry 11, 8k



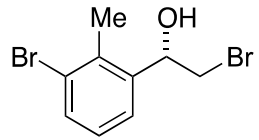
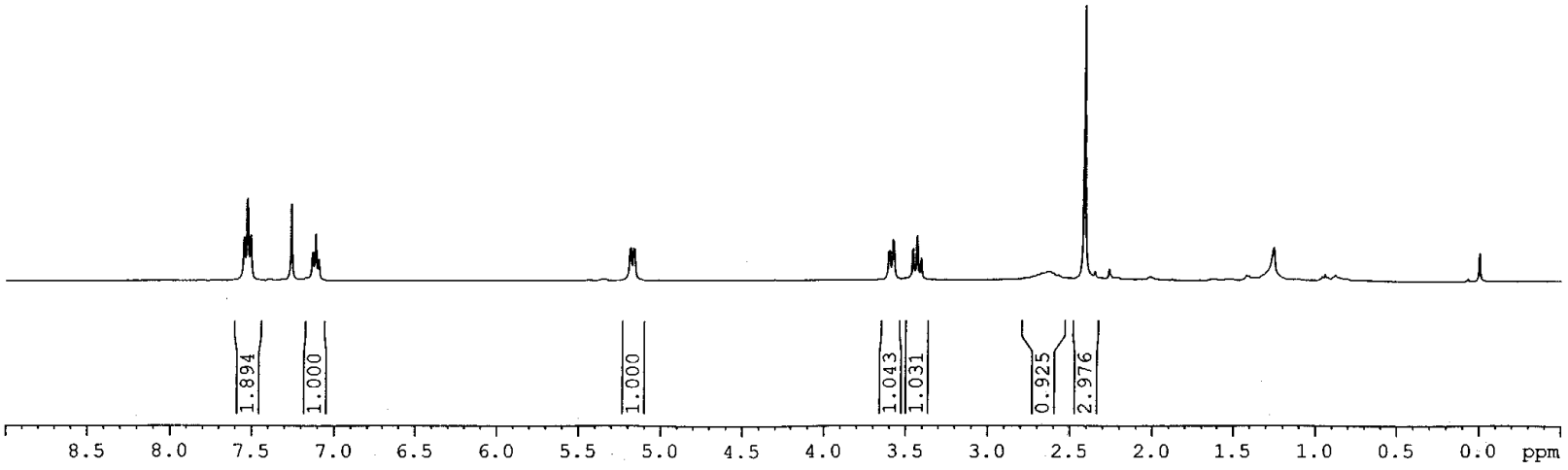


Table 4, **Entry 12, 8l**



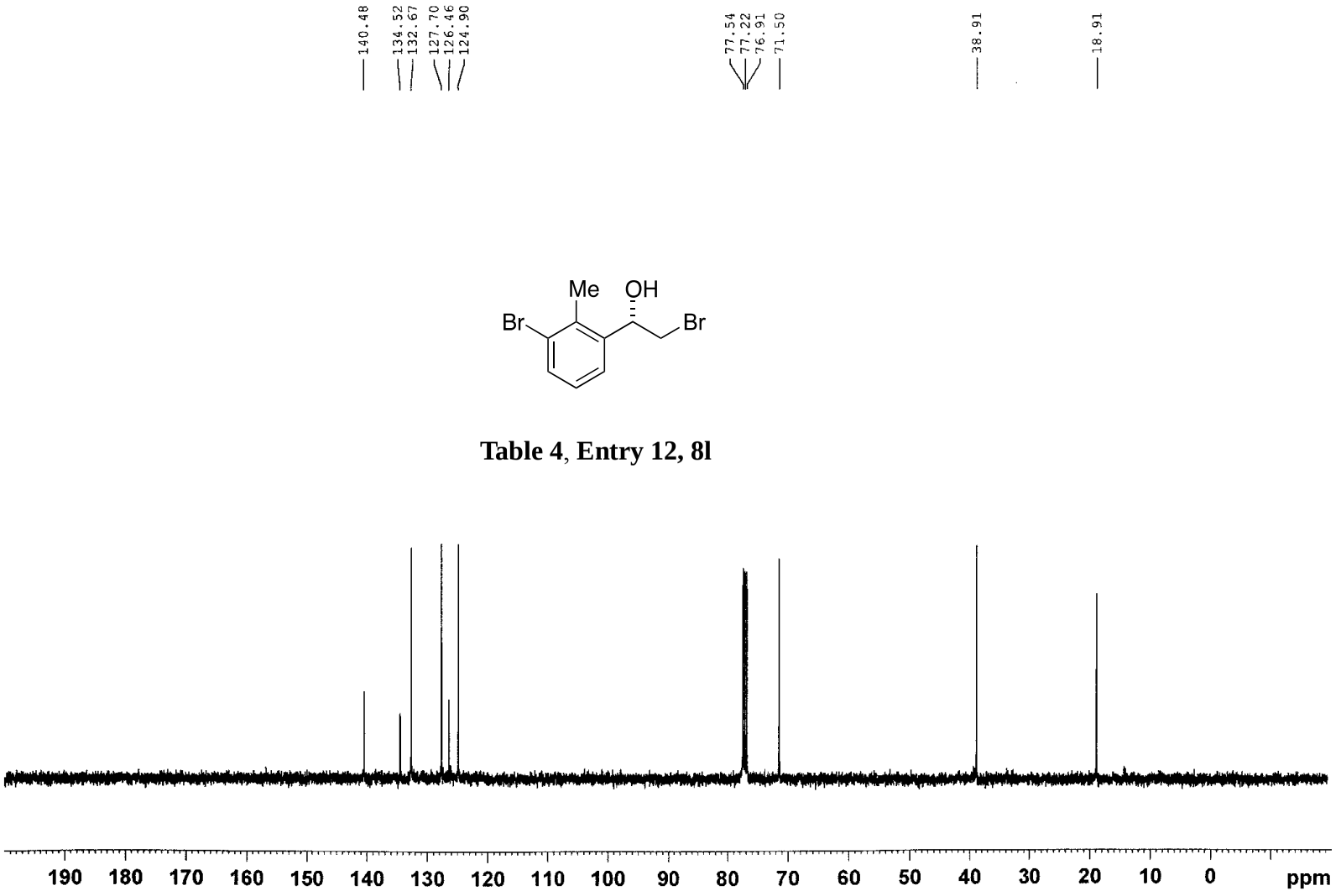


Table 4, Entry 12, 8l

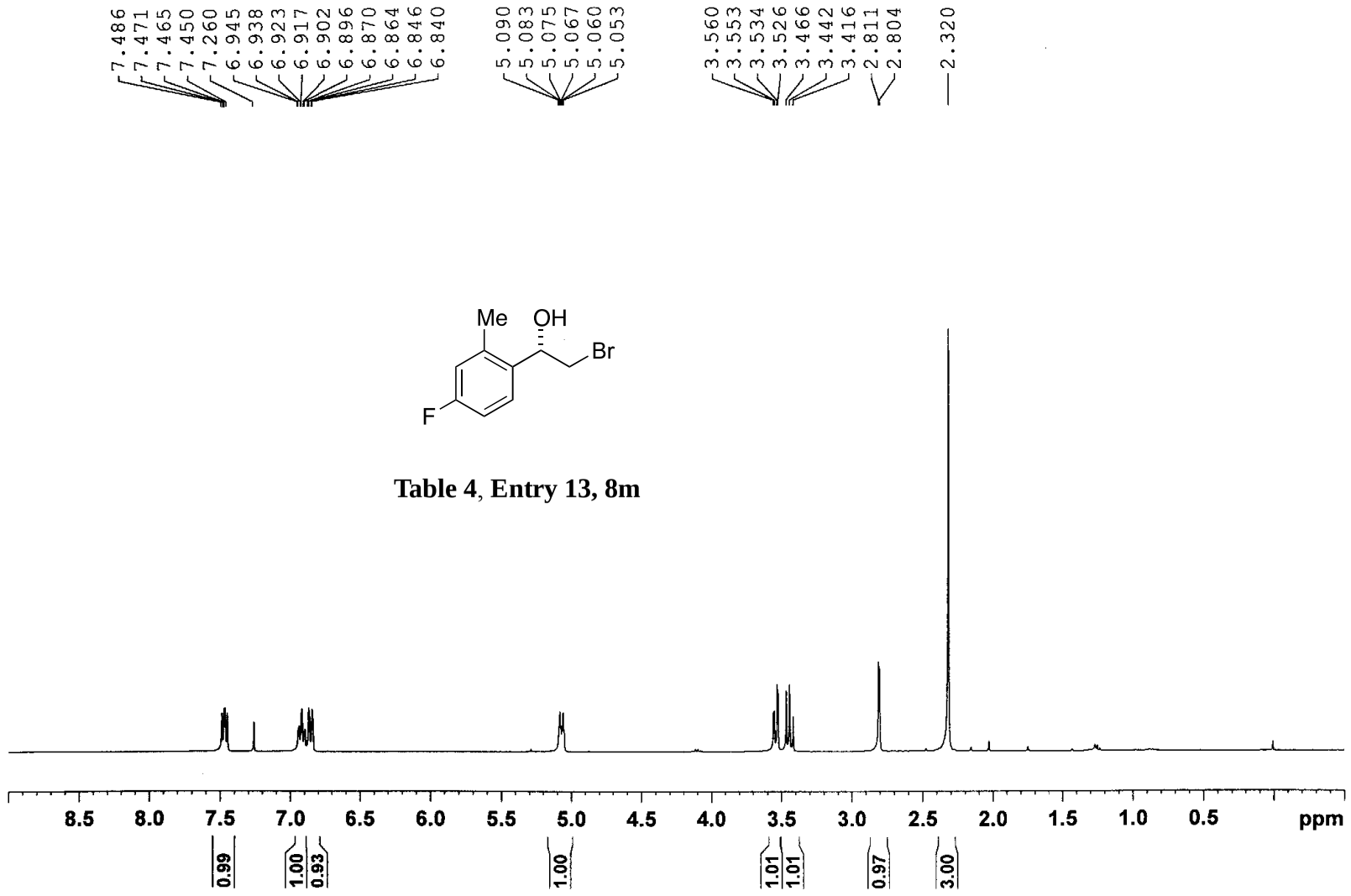


Table 4, **Entry 13, 8m**

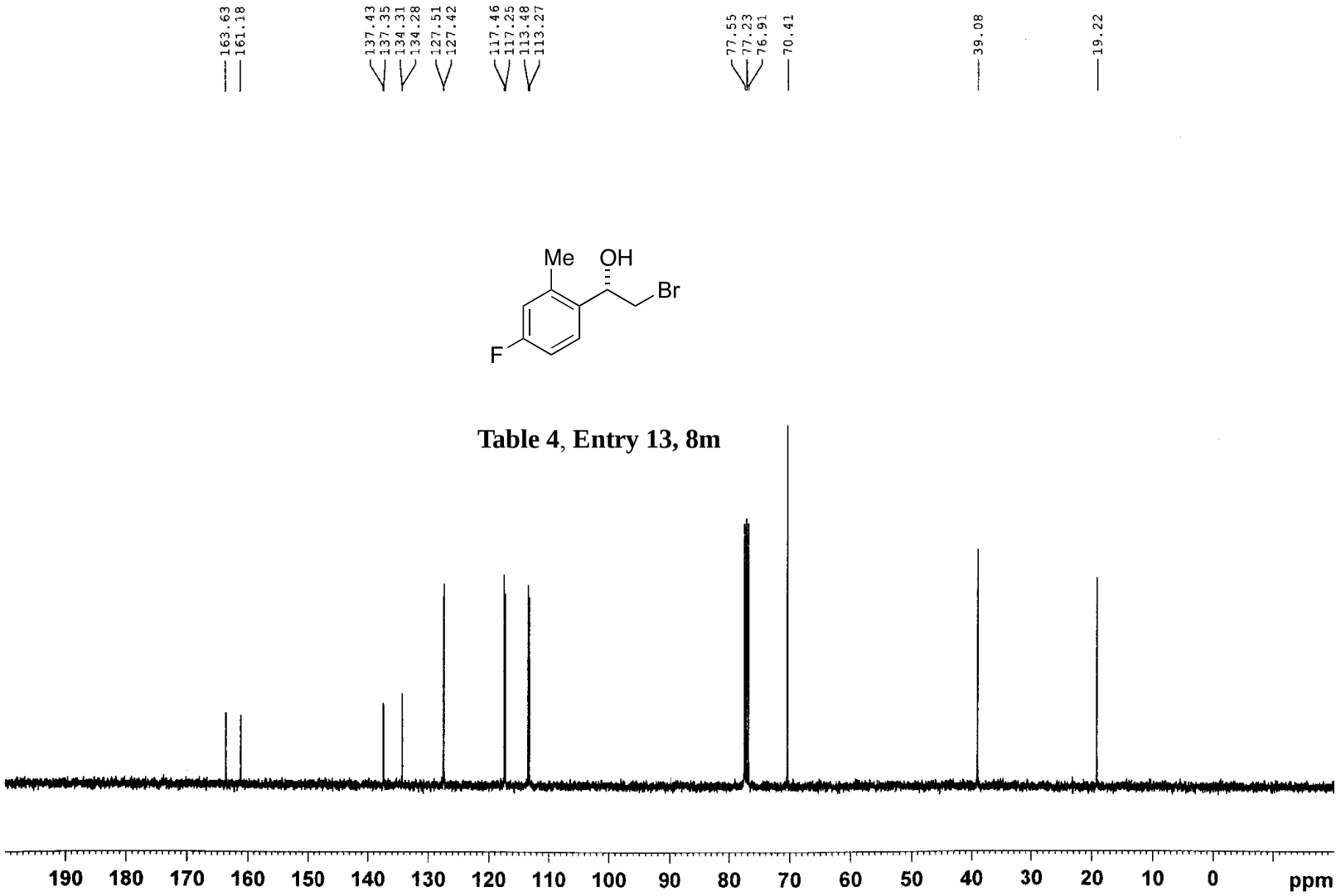


Table 4, Entry 13, 8m

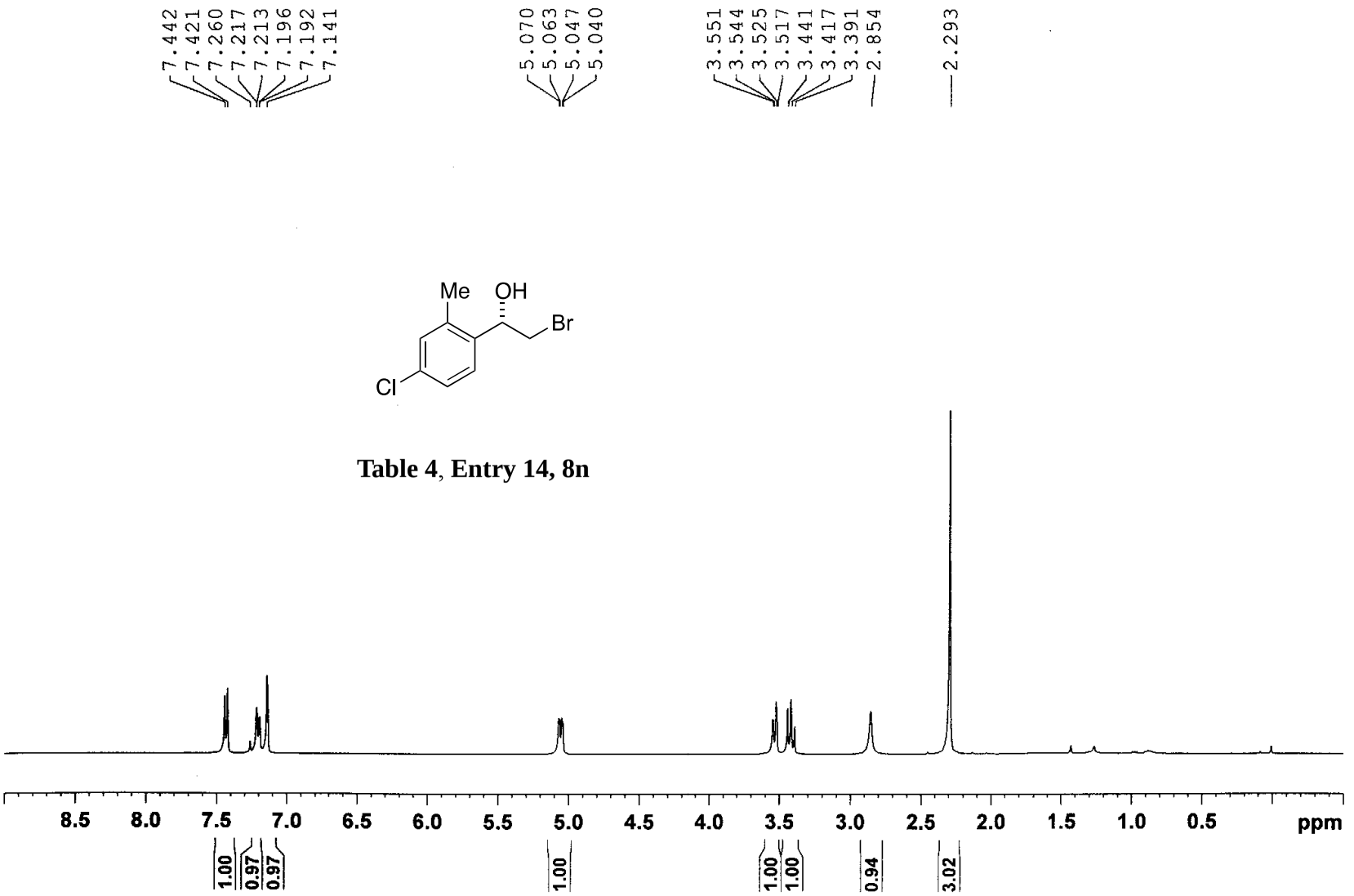


Table 4, **Entry 14, 8n**

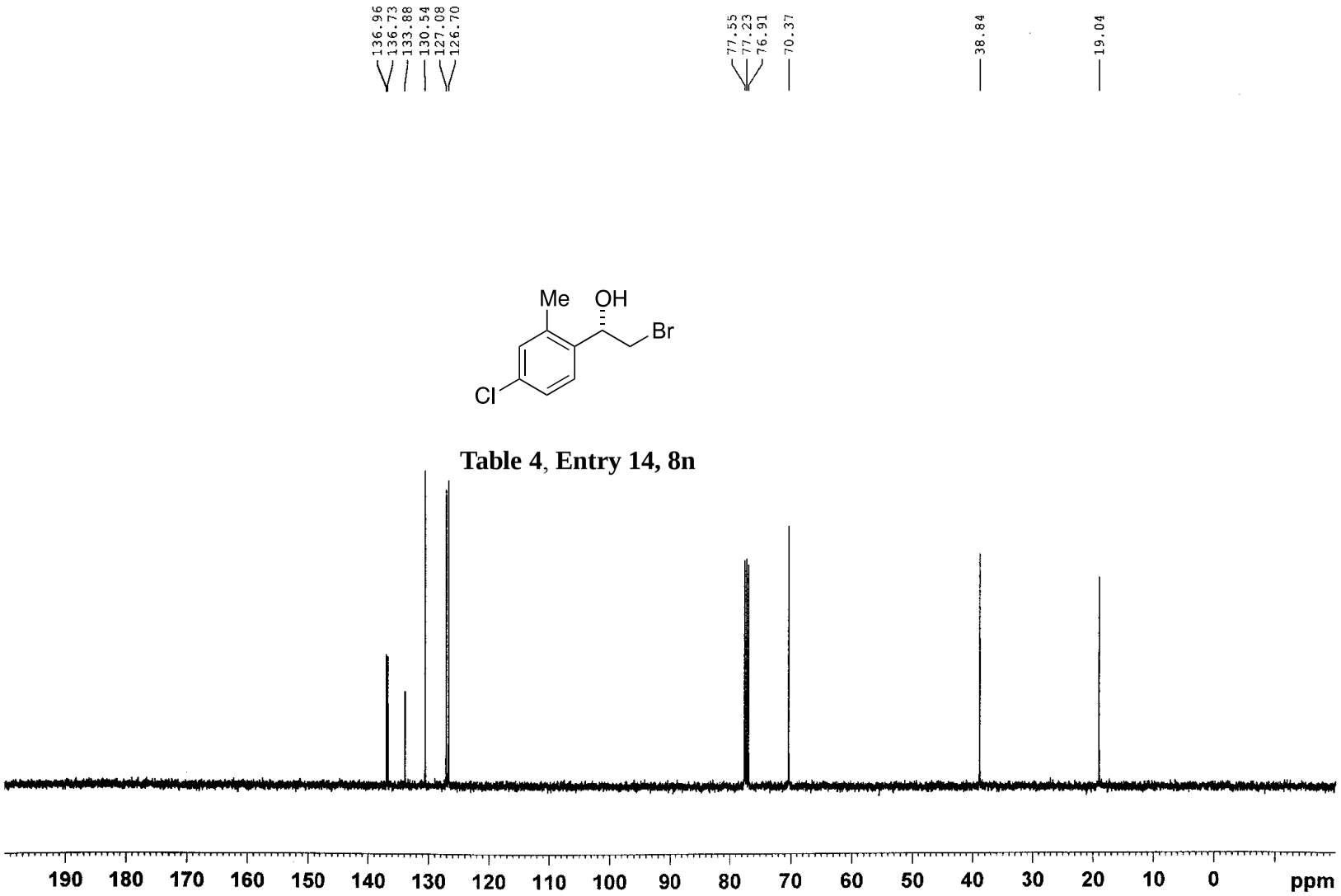


Table 4, Entry 14, 8n

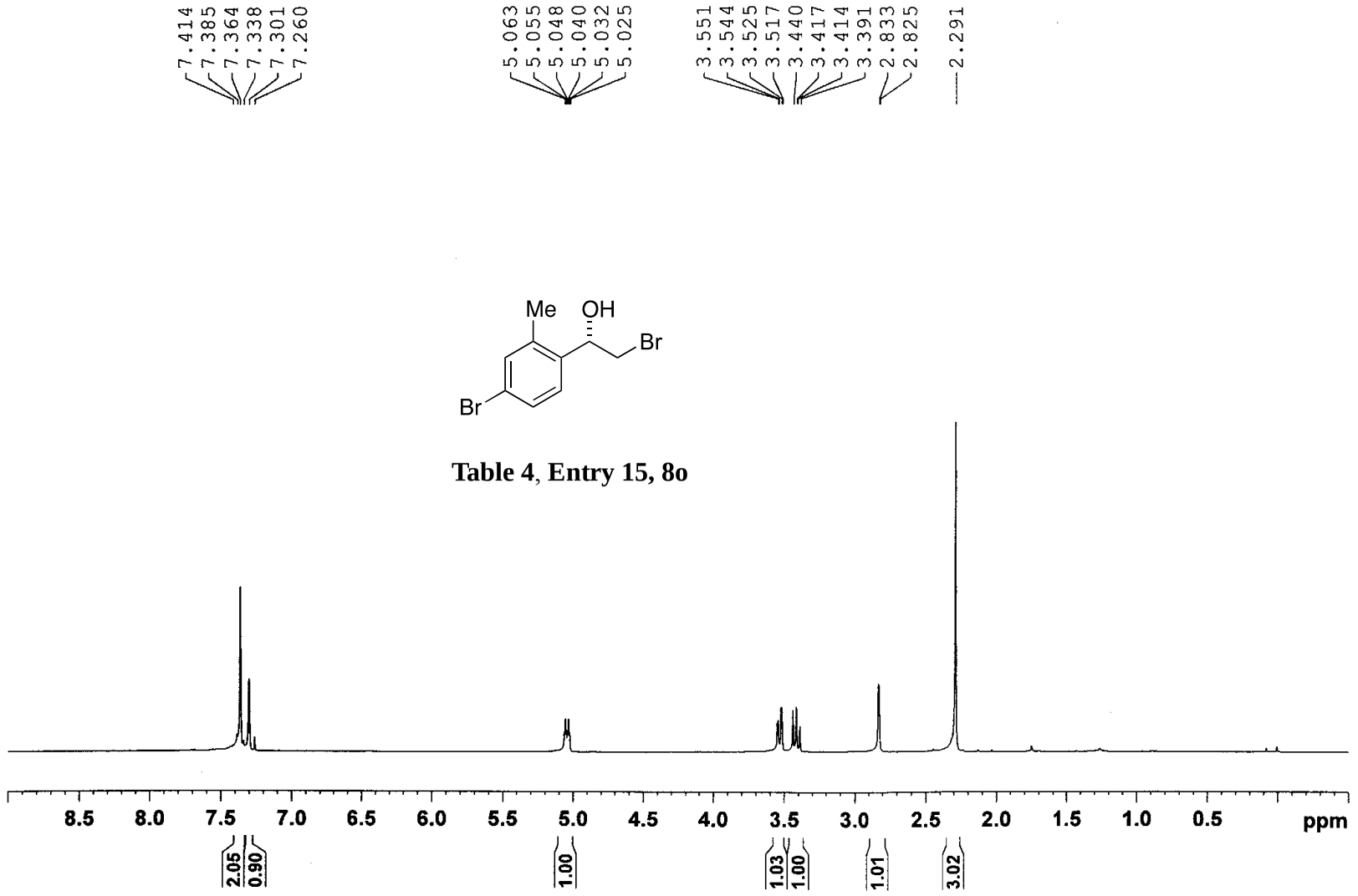


Table 4, **Entry 15, 8o**

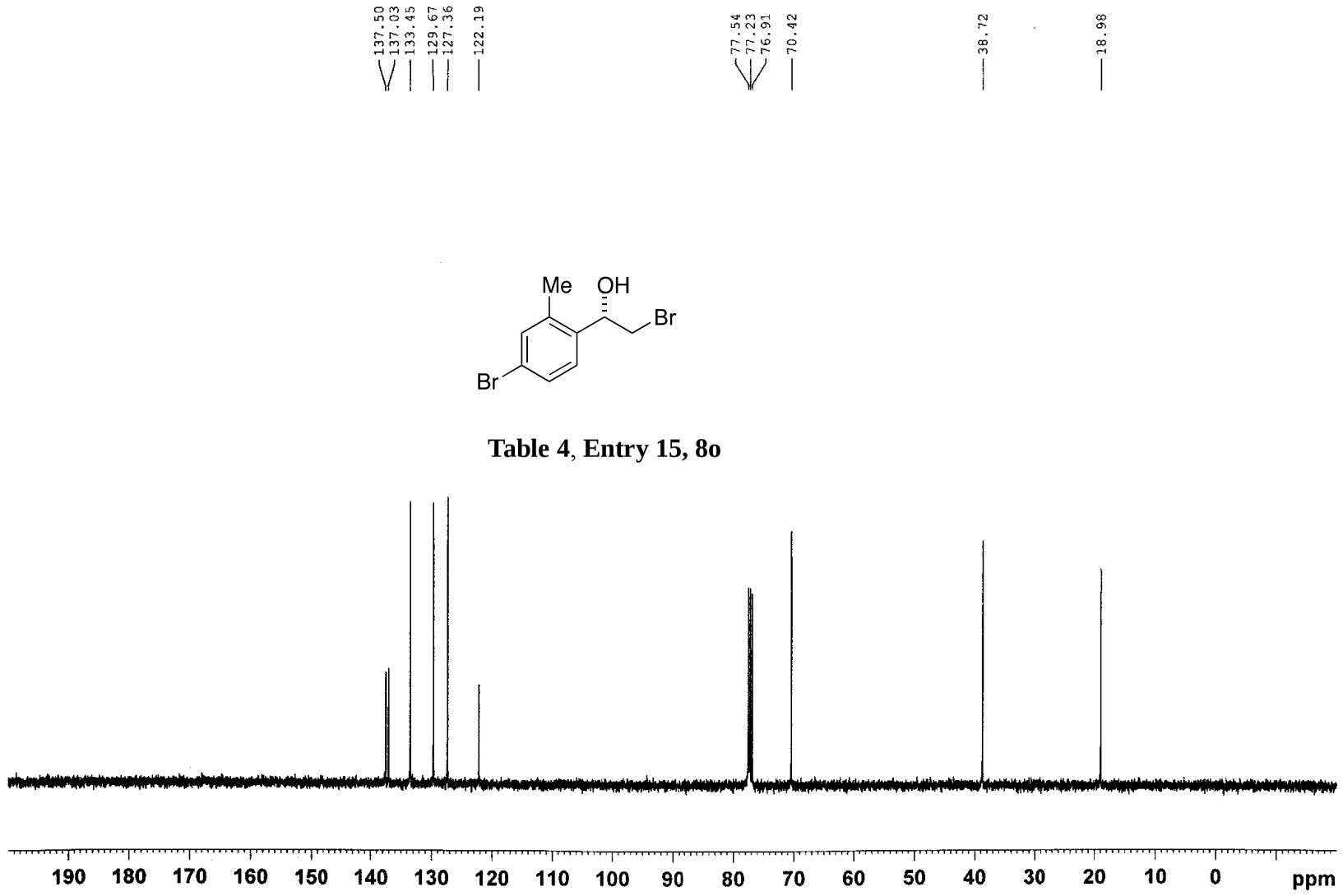


Table 4, Entry 15, 8o

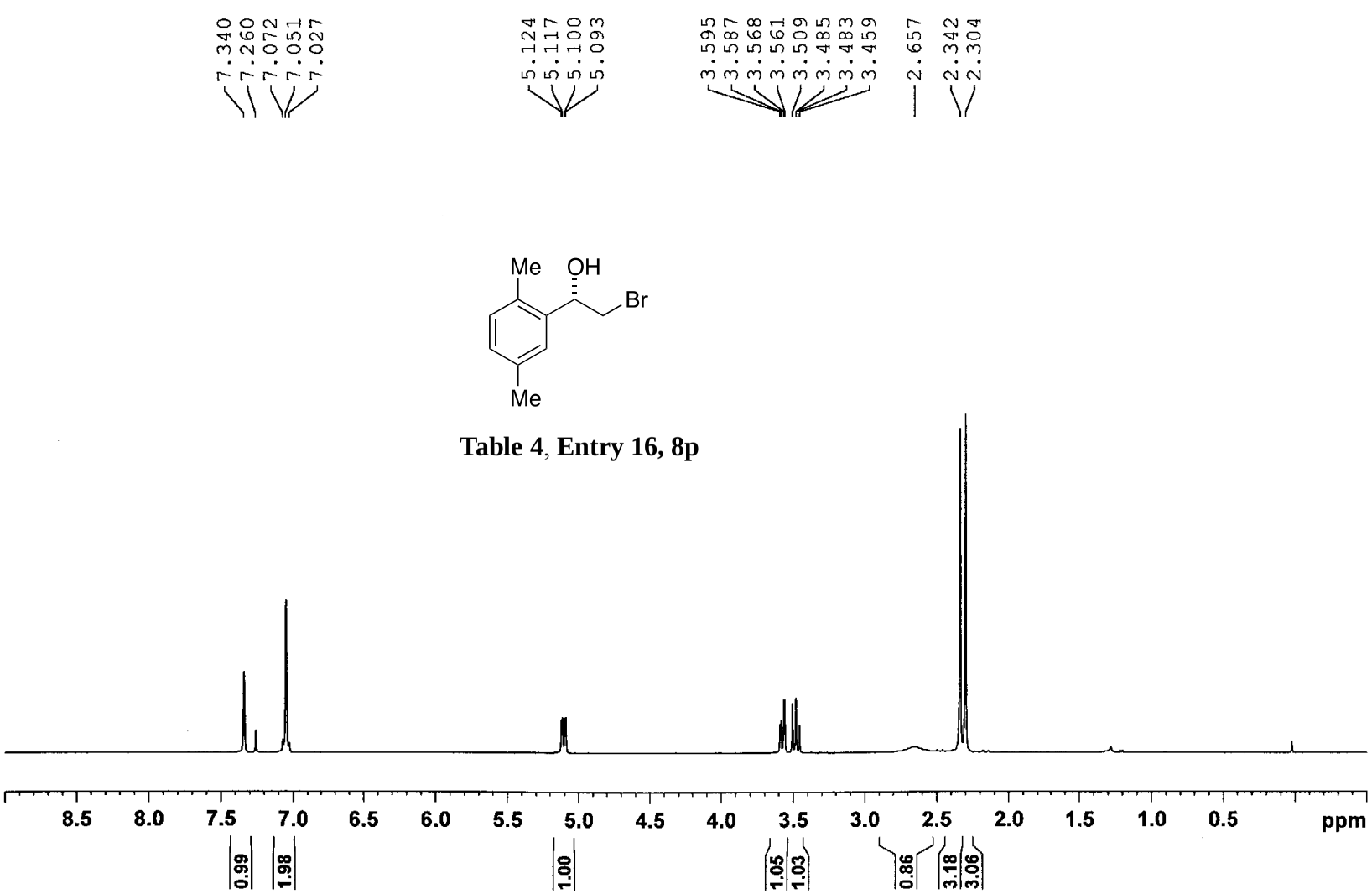


Table 4, **Entry 16, 8p**

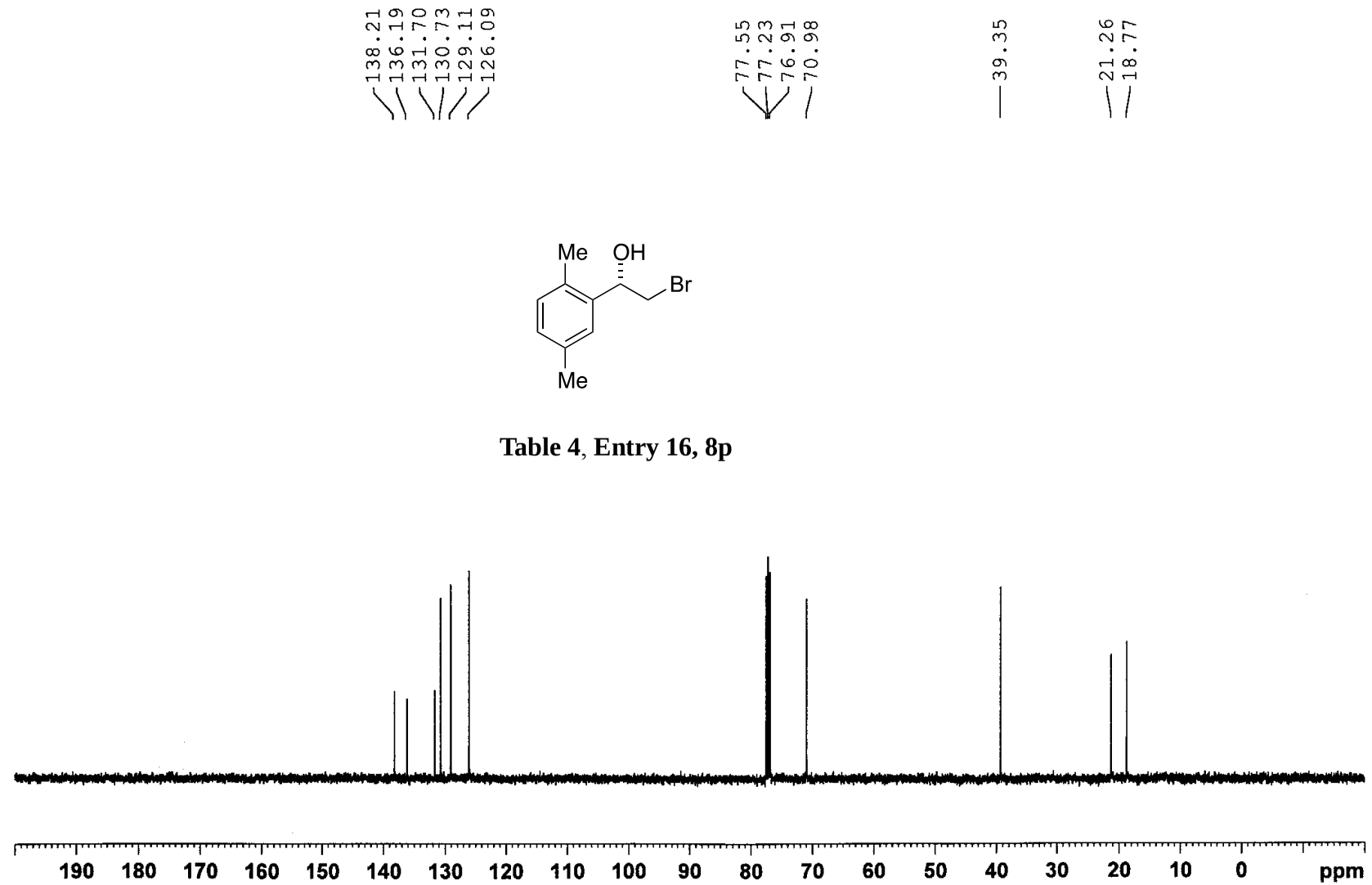


Table 4, **Entry 16, 8p**

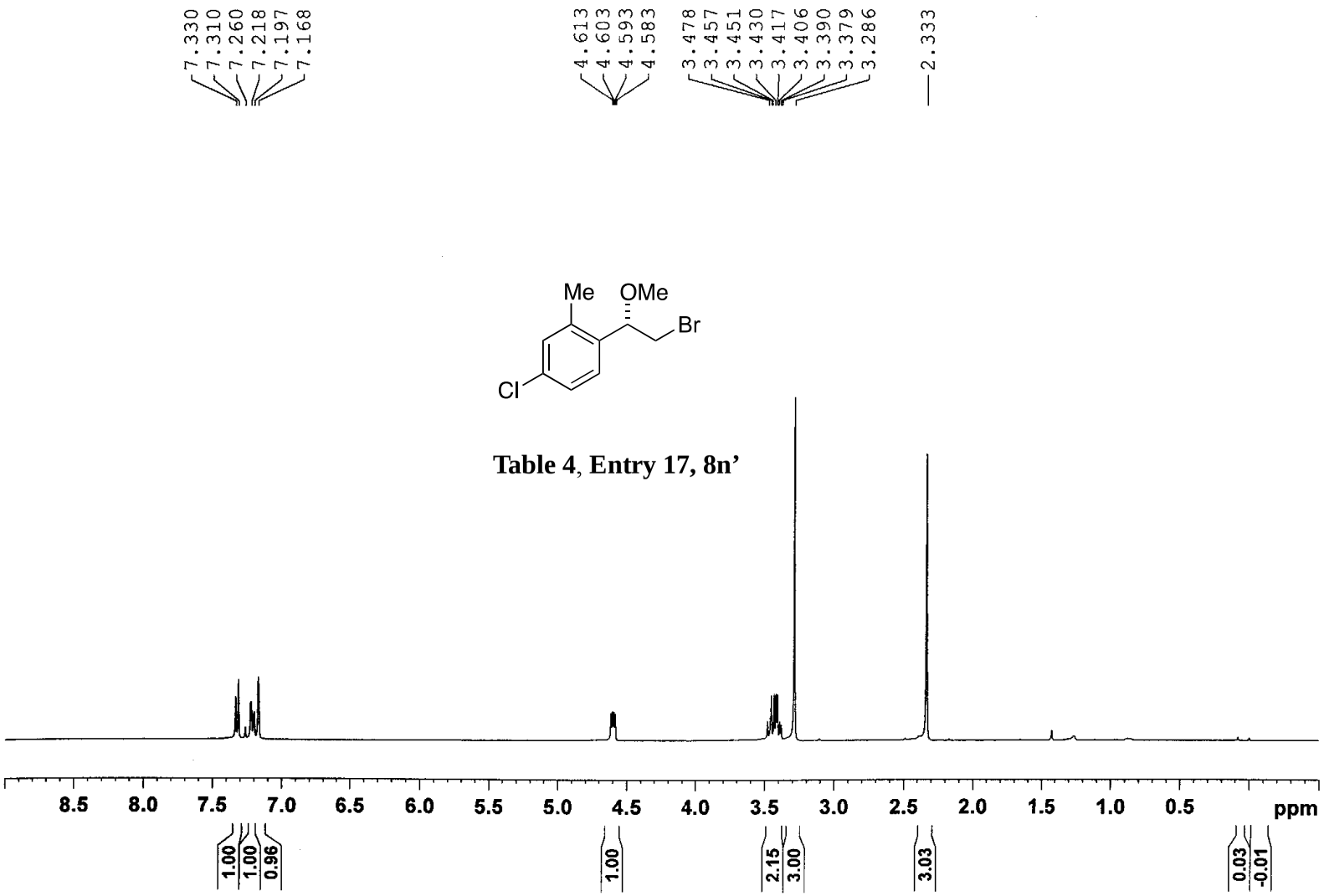
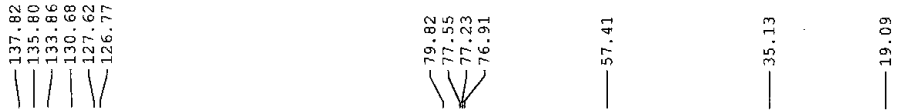


Table 4, Entry 17, 8n'



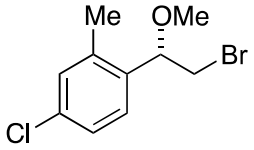
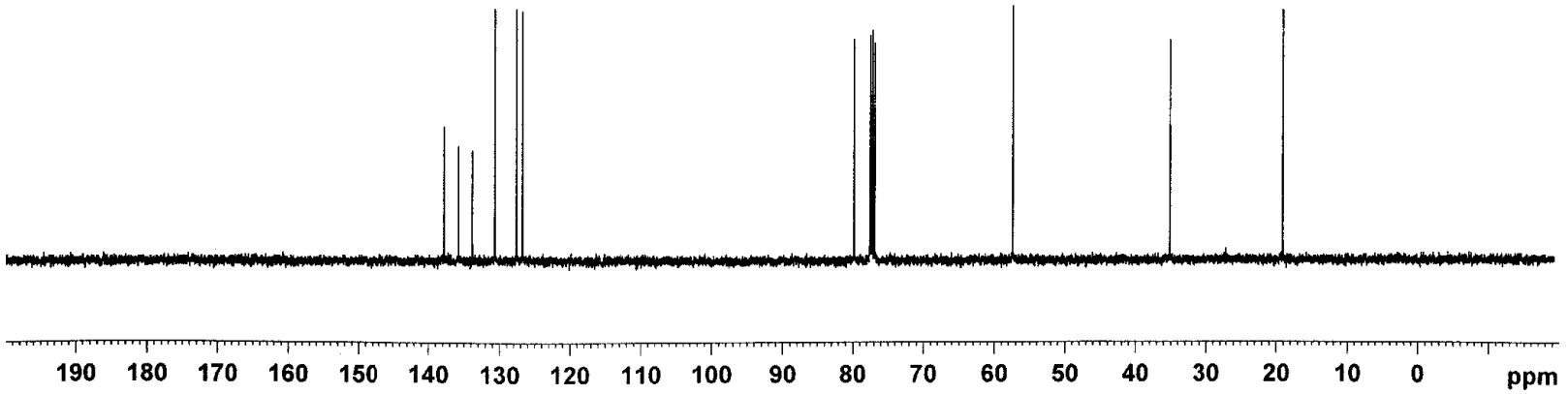


Table 4, **Entry 17, 8n'**



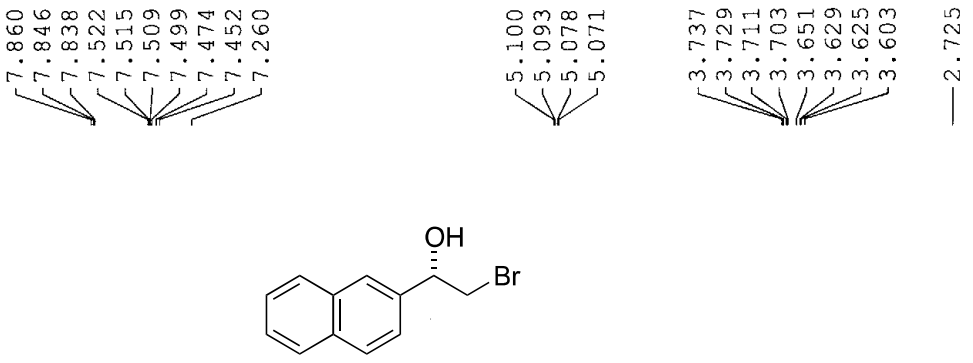
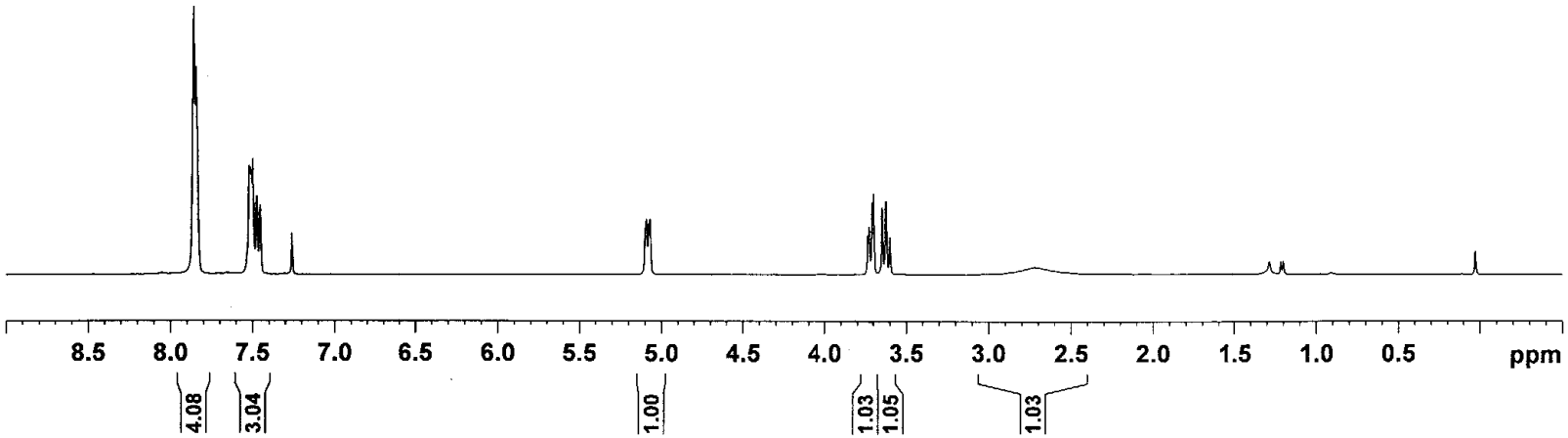


Table 4, **Entry 18, 8q**



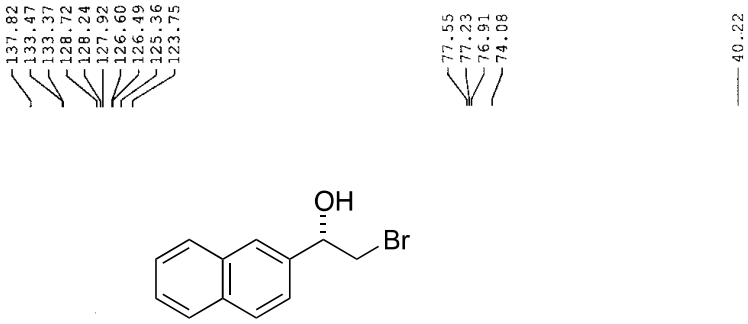
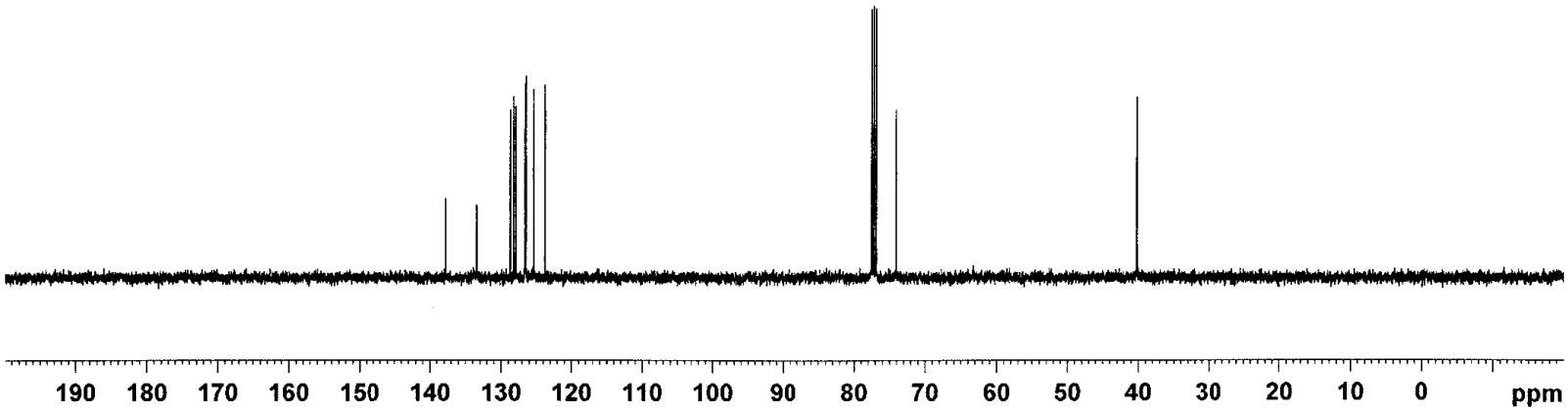


Table 4, **Entry 18, 8q**



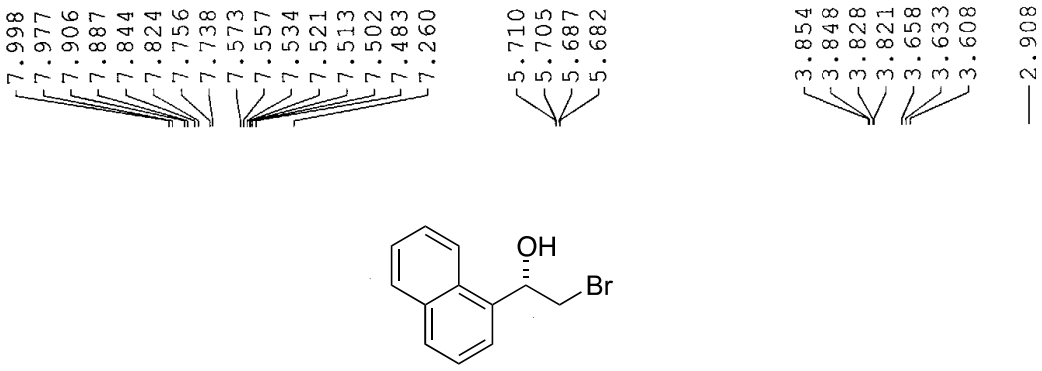
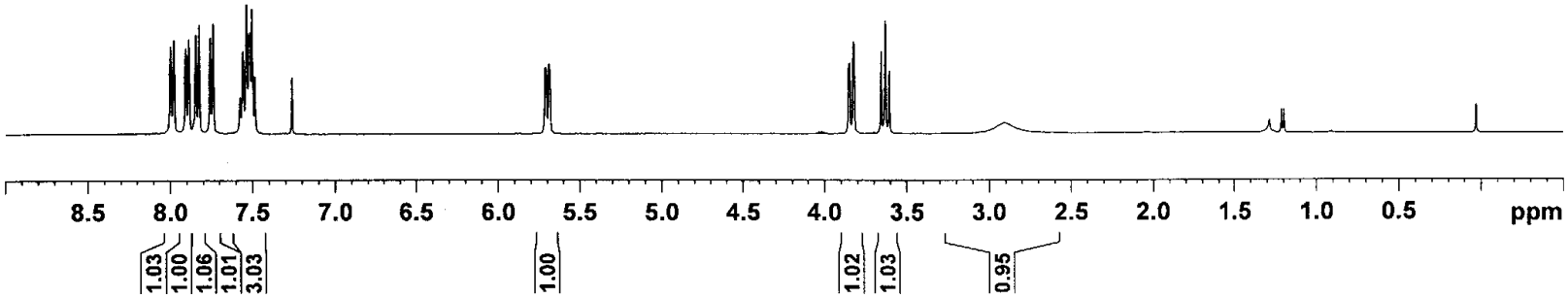


Table 4, **Entry 19, 8r**



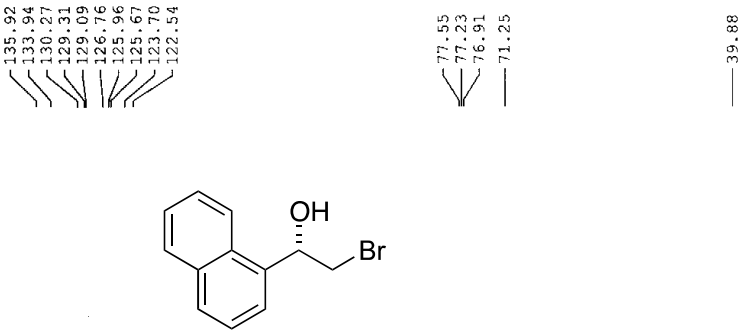
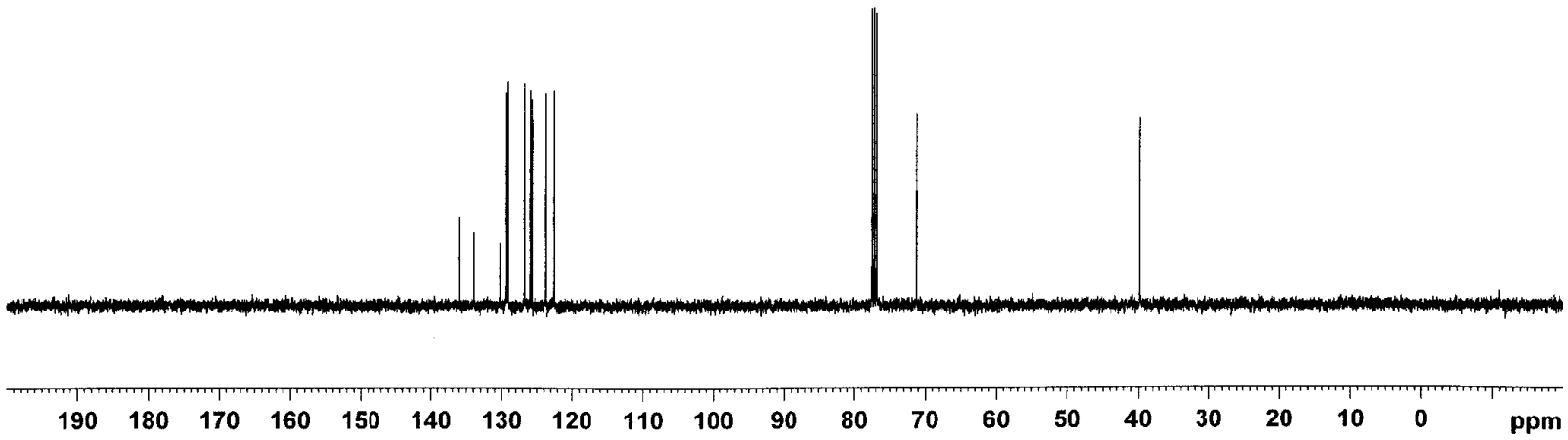


Table 4, Entry 19, 8r



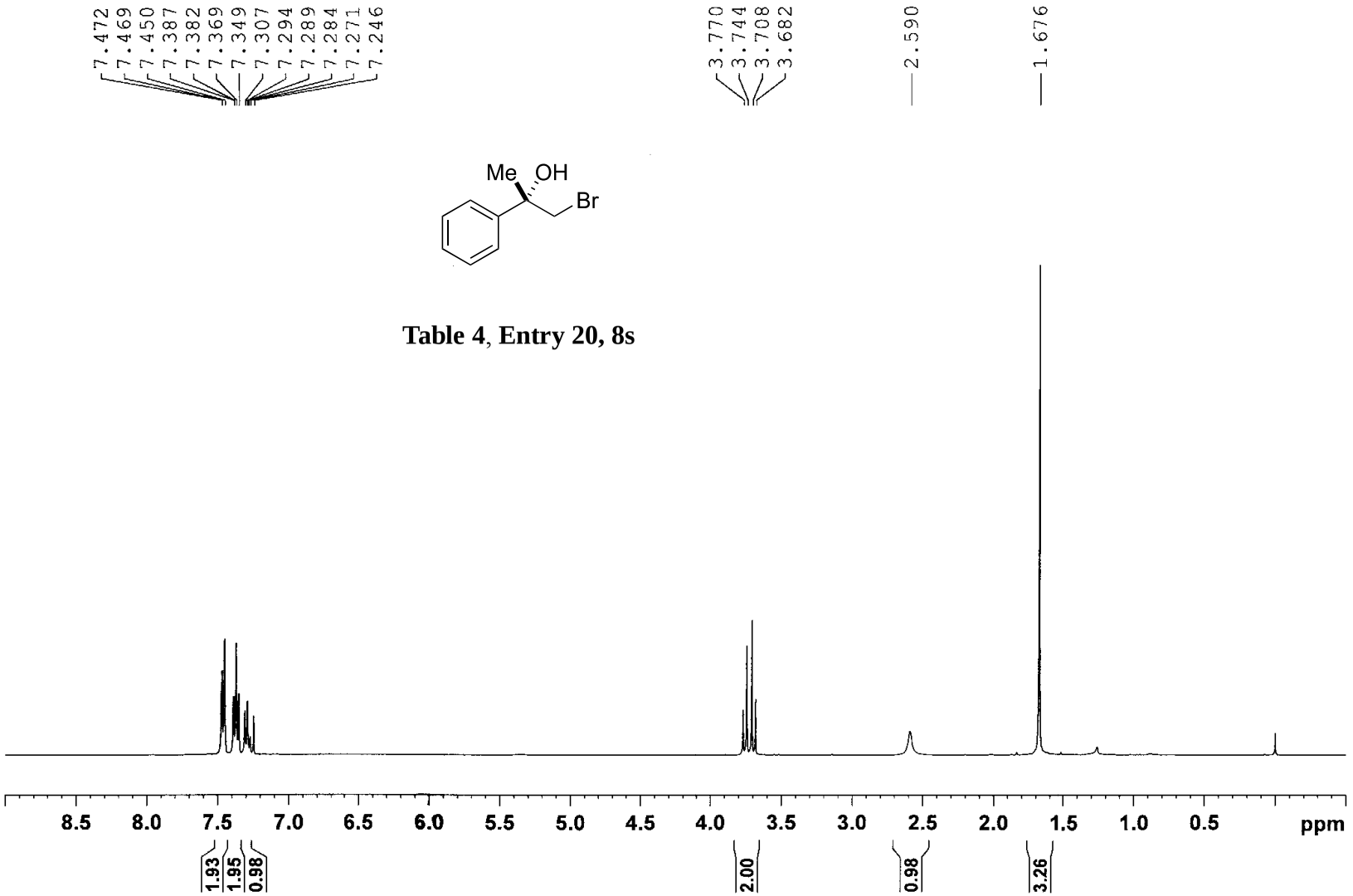


Table 4, **Entry 20, 8s**

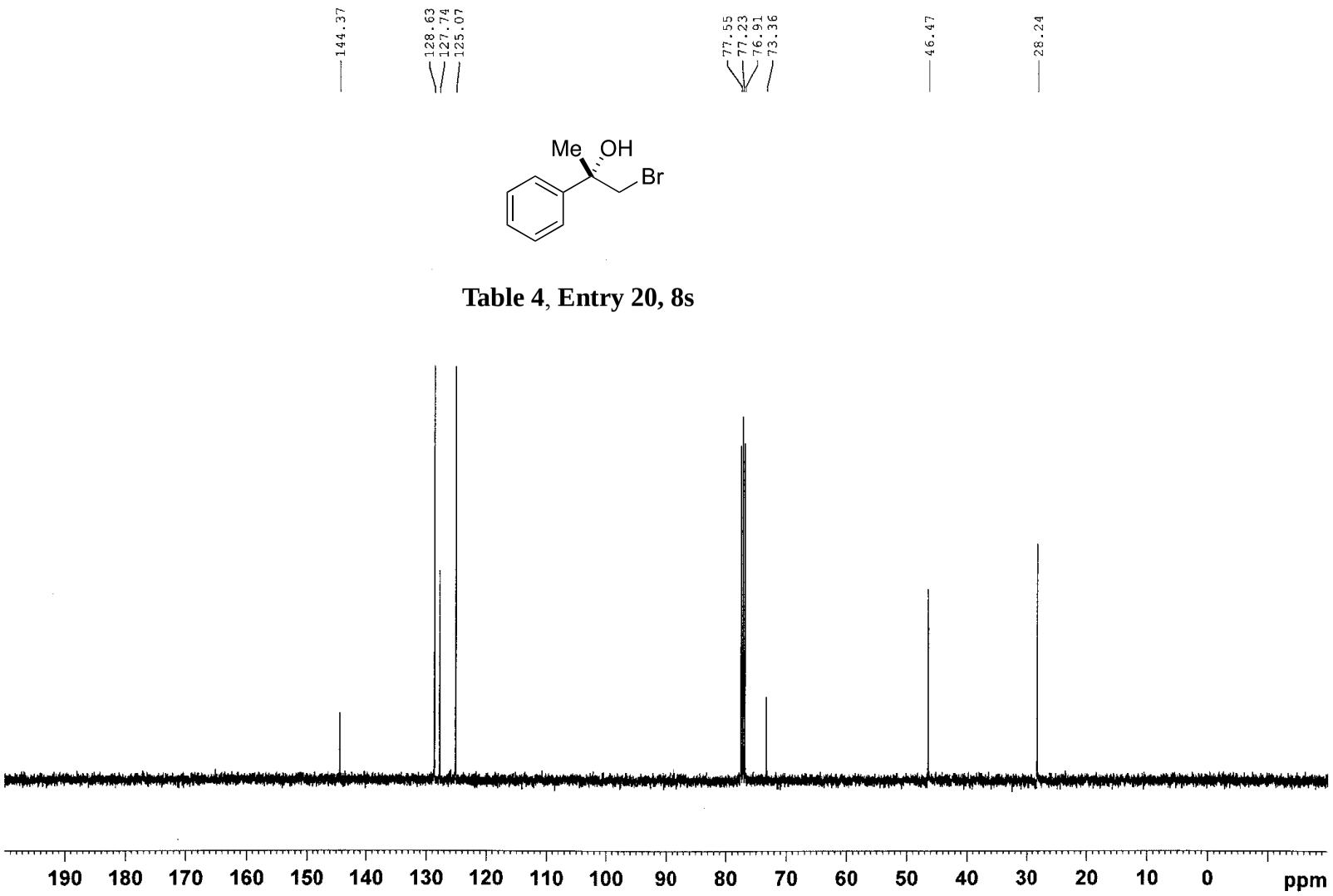


Table 4, **Entry 20, 8s**

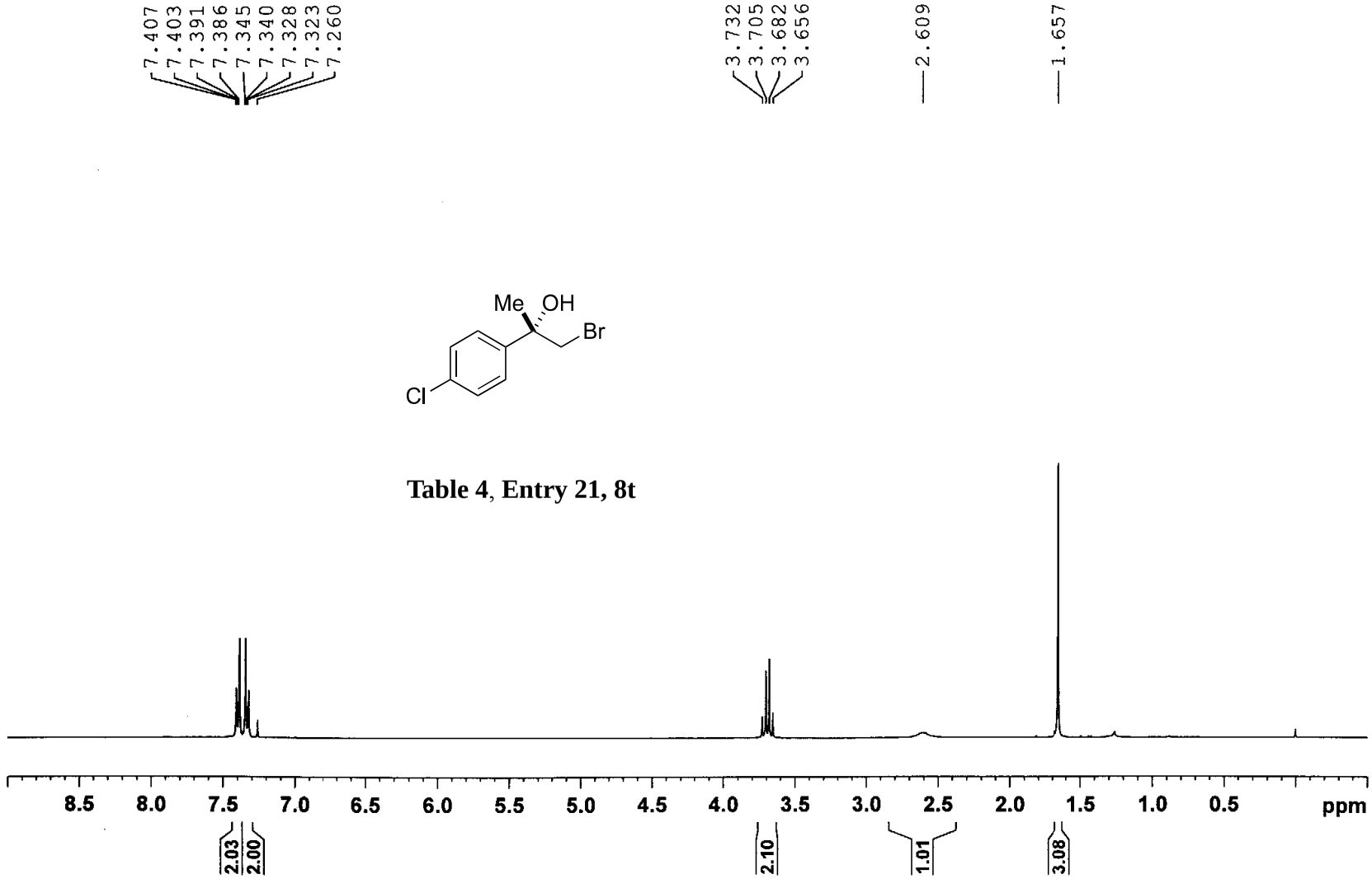


Table 4, **Entry 21, 8t**

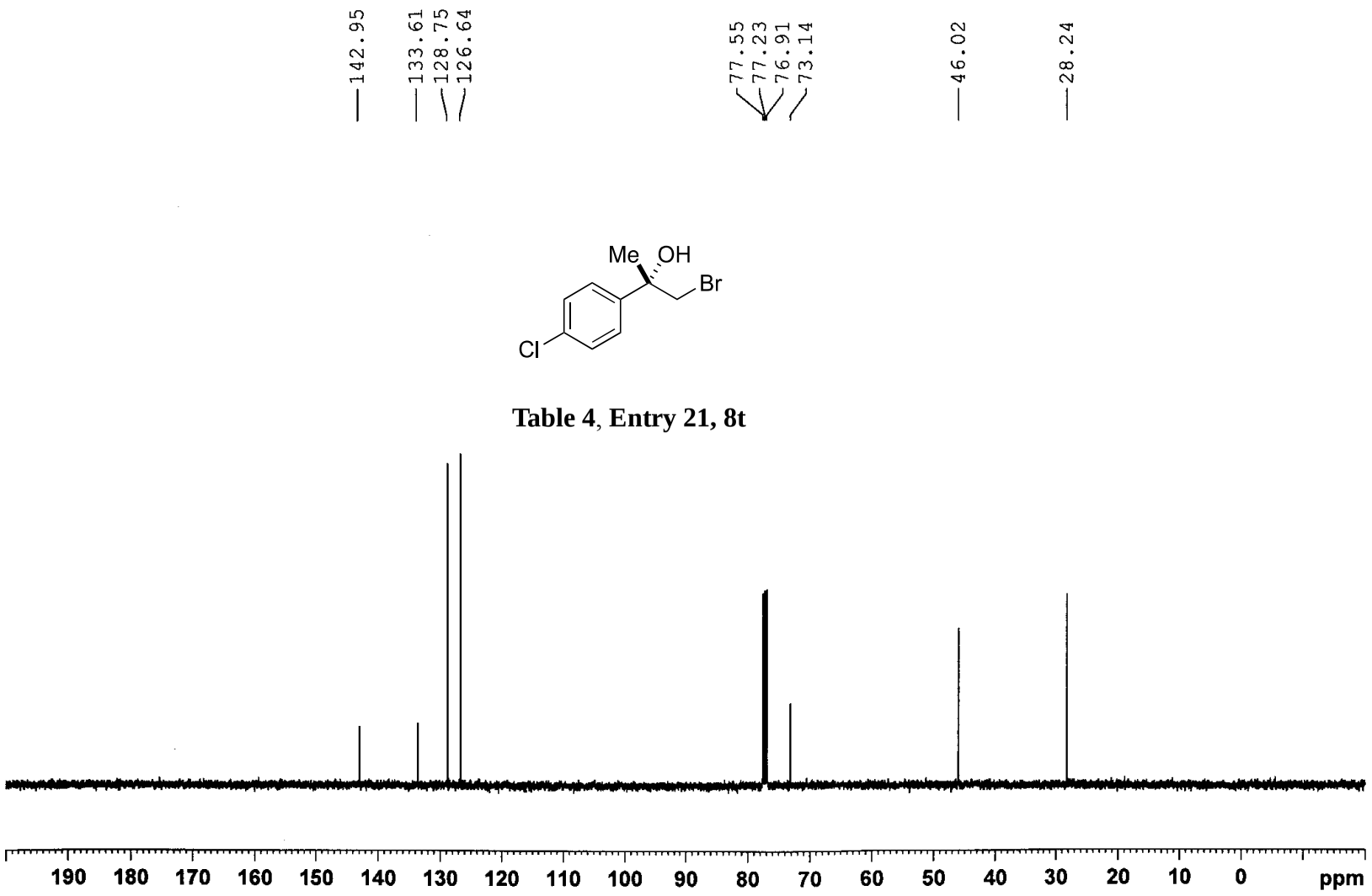


Table 4, Entry 21, 8t

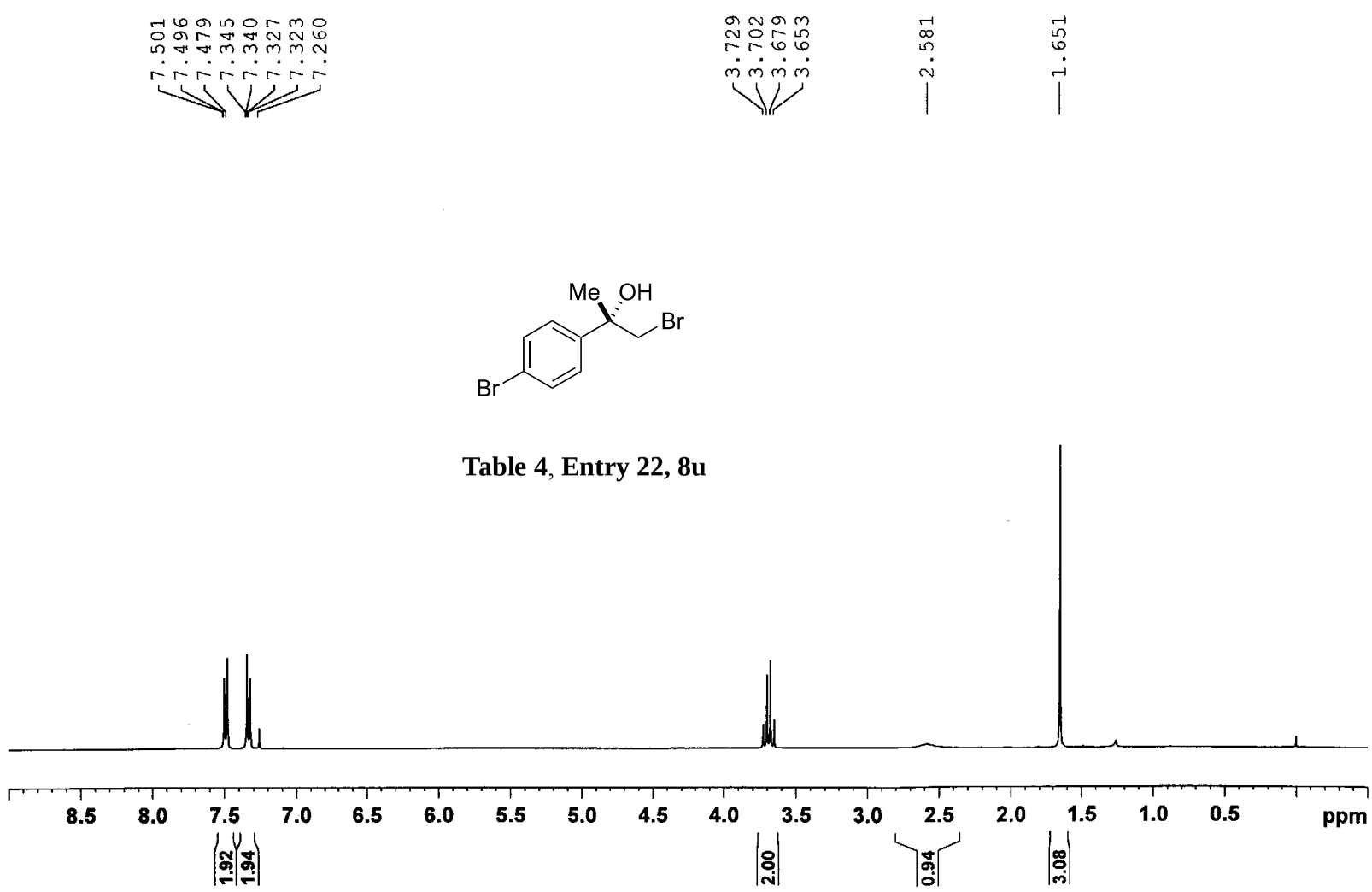


Table 4, Entry 22, 8u

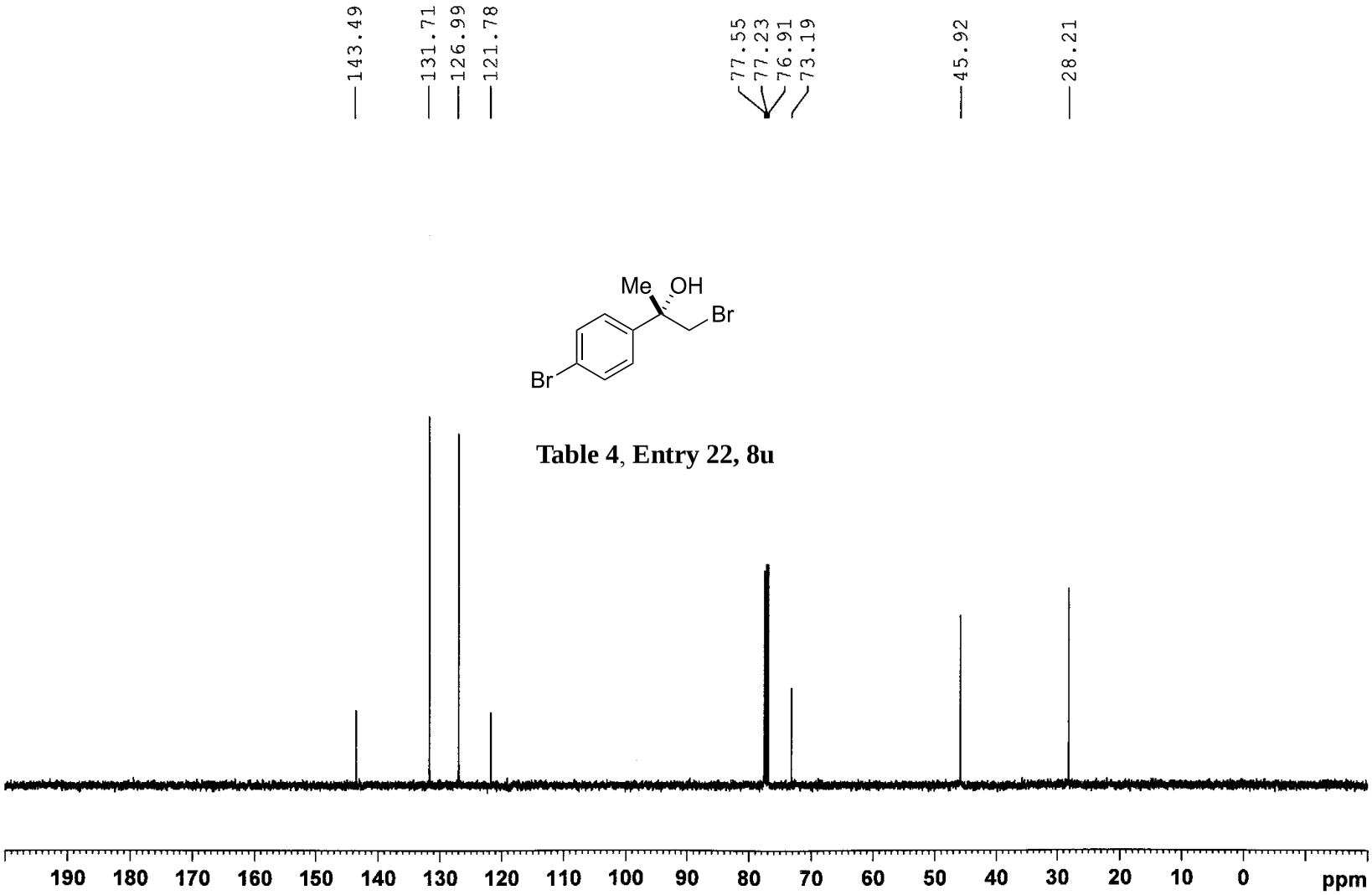
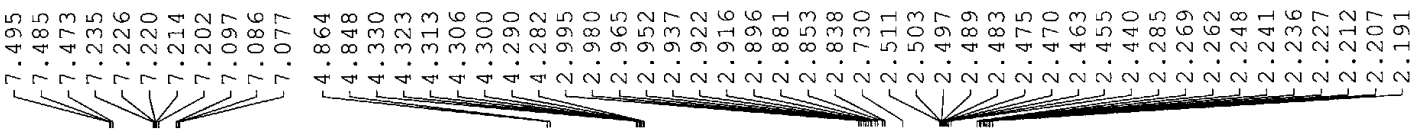


Table 4, Entry 22, 8u



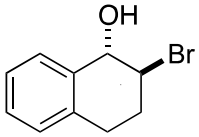
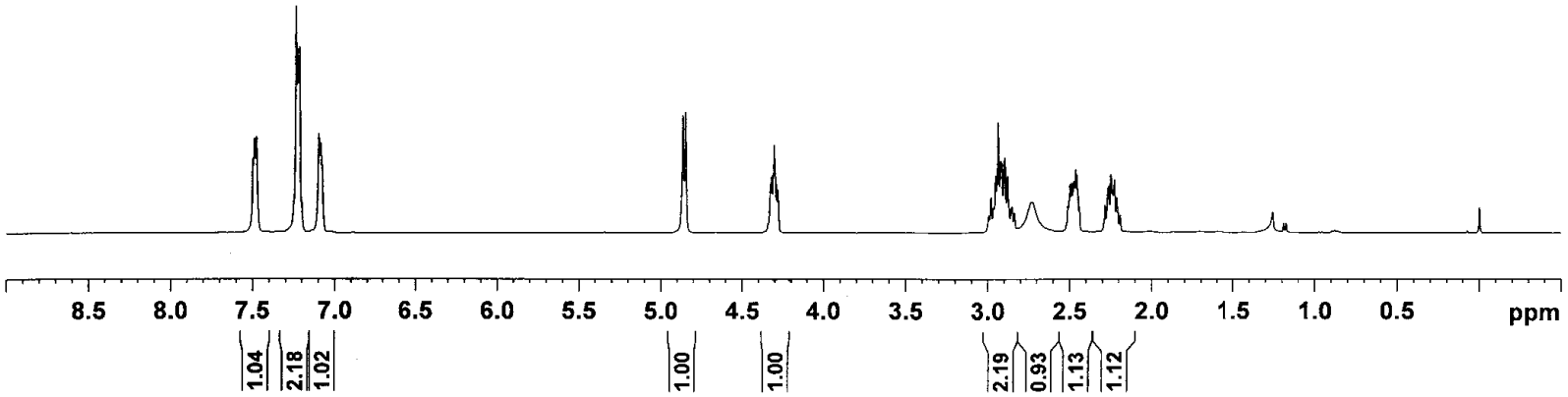


Table 4, **Entry 23, 8v**



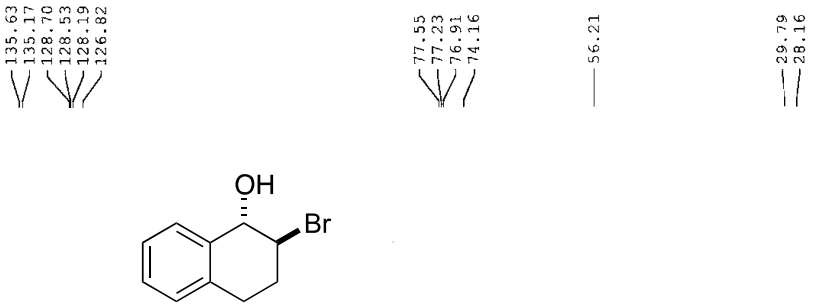
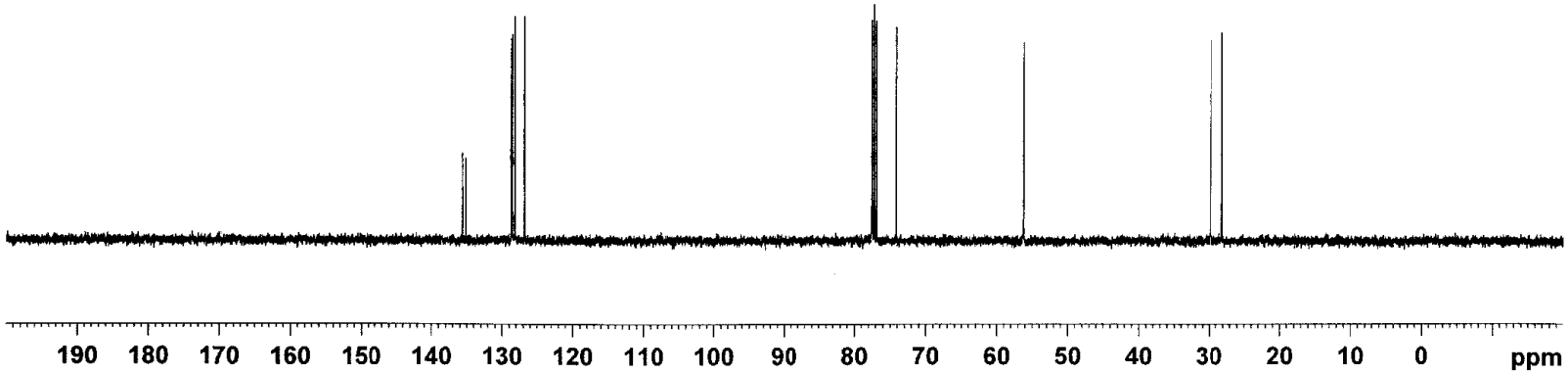
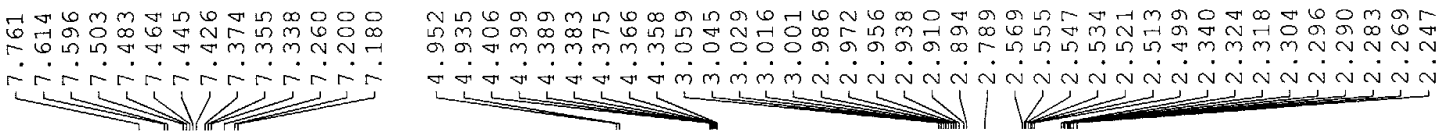


Table 4, **Entry 23, 8v**





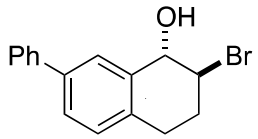
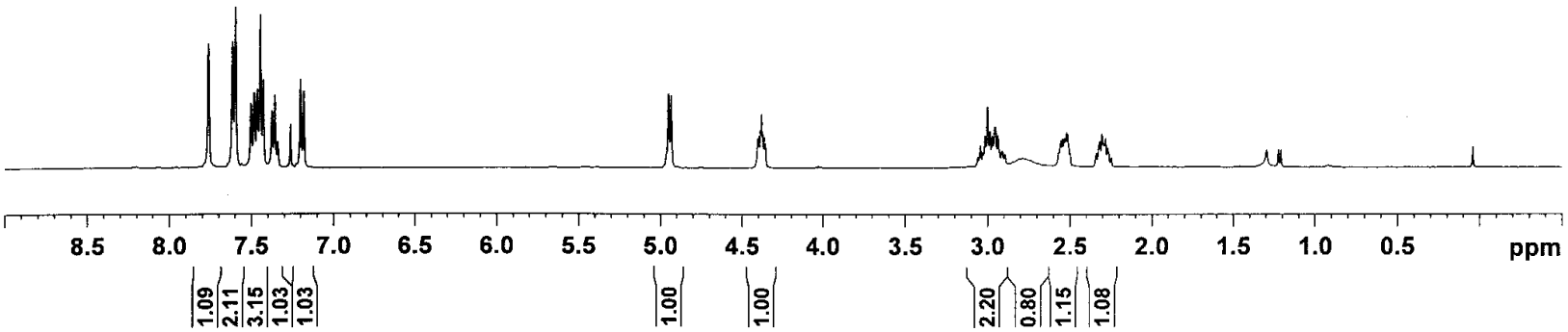


Table 4, **Entry 24, 8w**



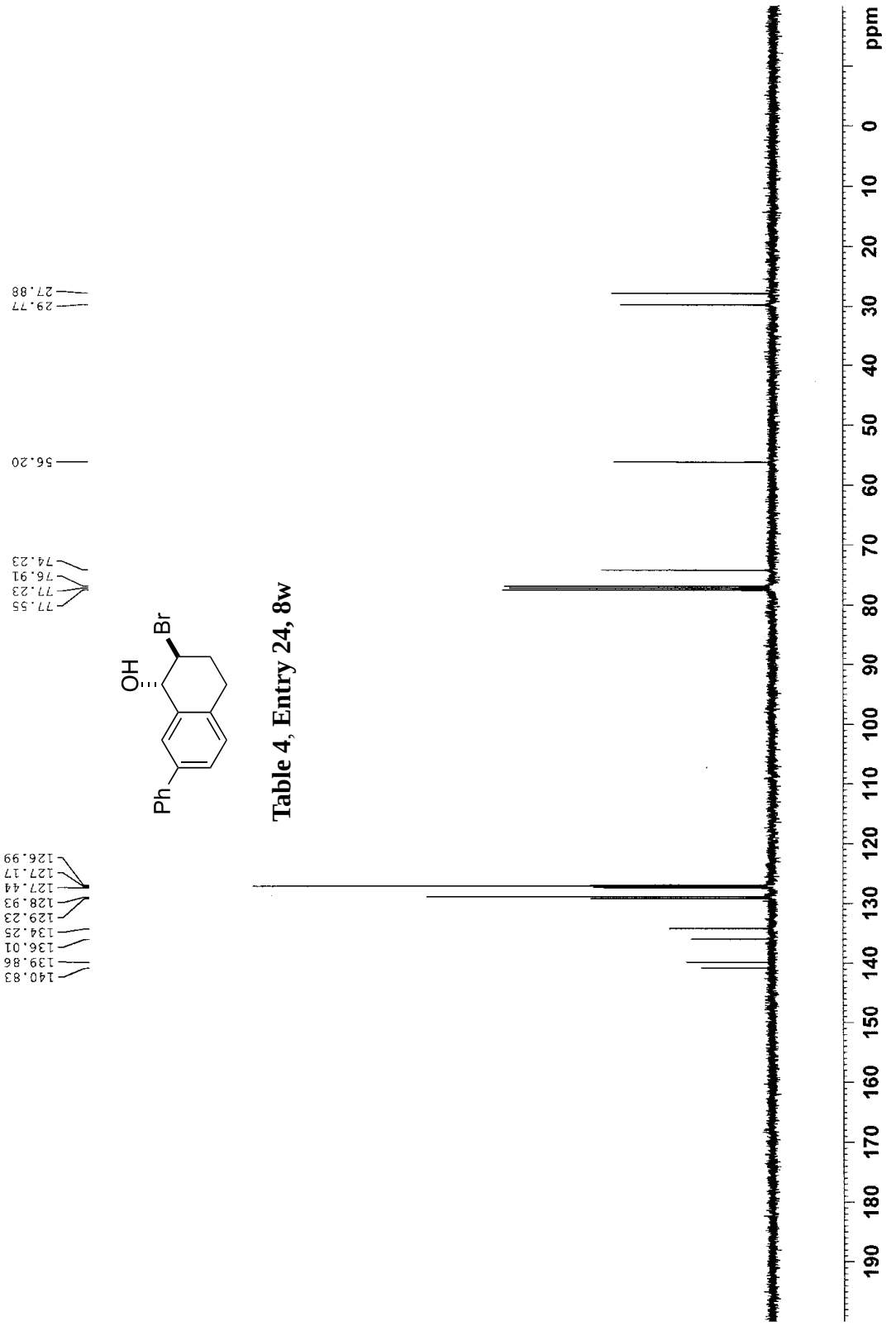


Table 4, Entry 24, 8w
OH
Br
Ph
140.83
139.86
136.01
134.25
129.23
128.93
127.44
127.17
126.99
77.55
77.23
76.91
74.23
56.20
29.77
27.88
ppm

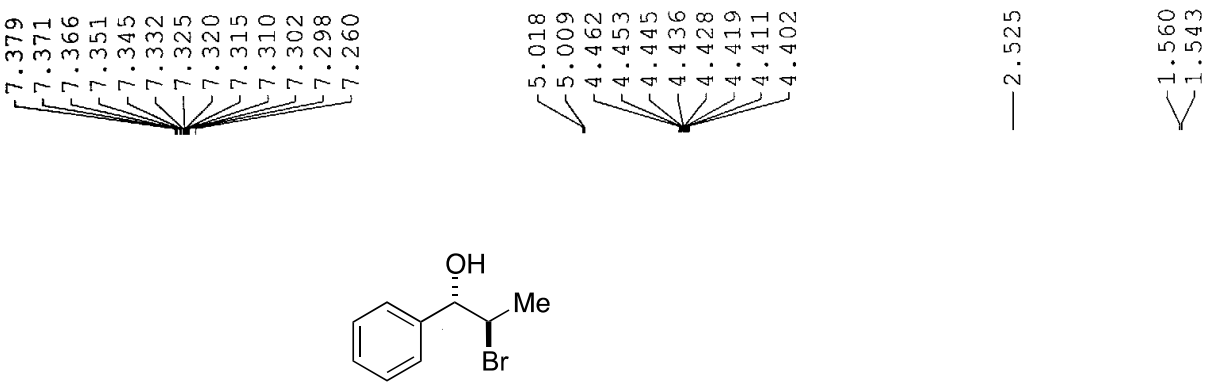
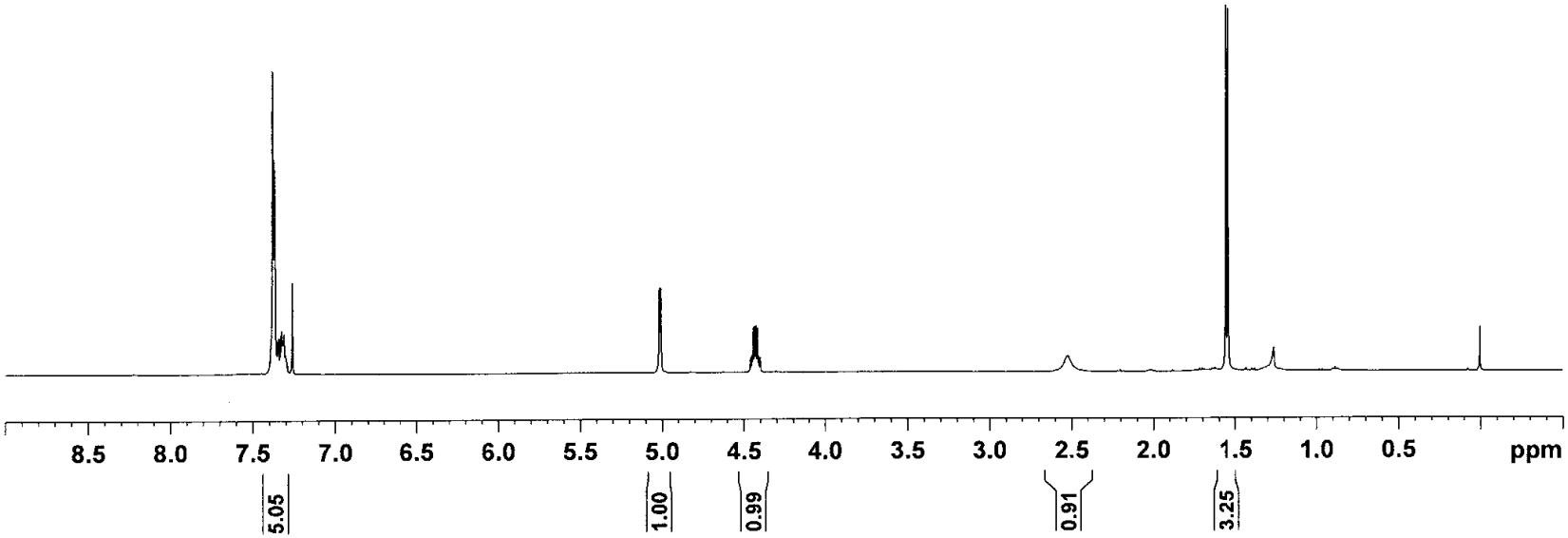


Table 4, **Entry 25, 8x**



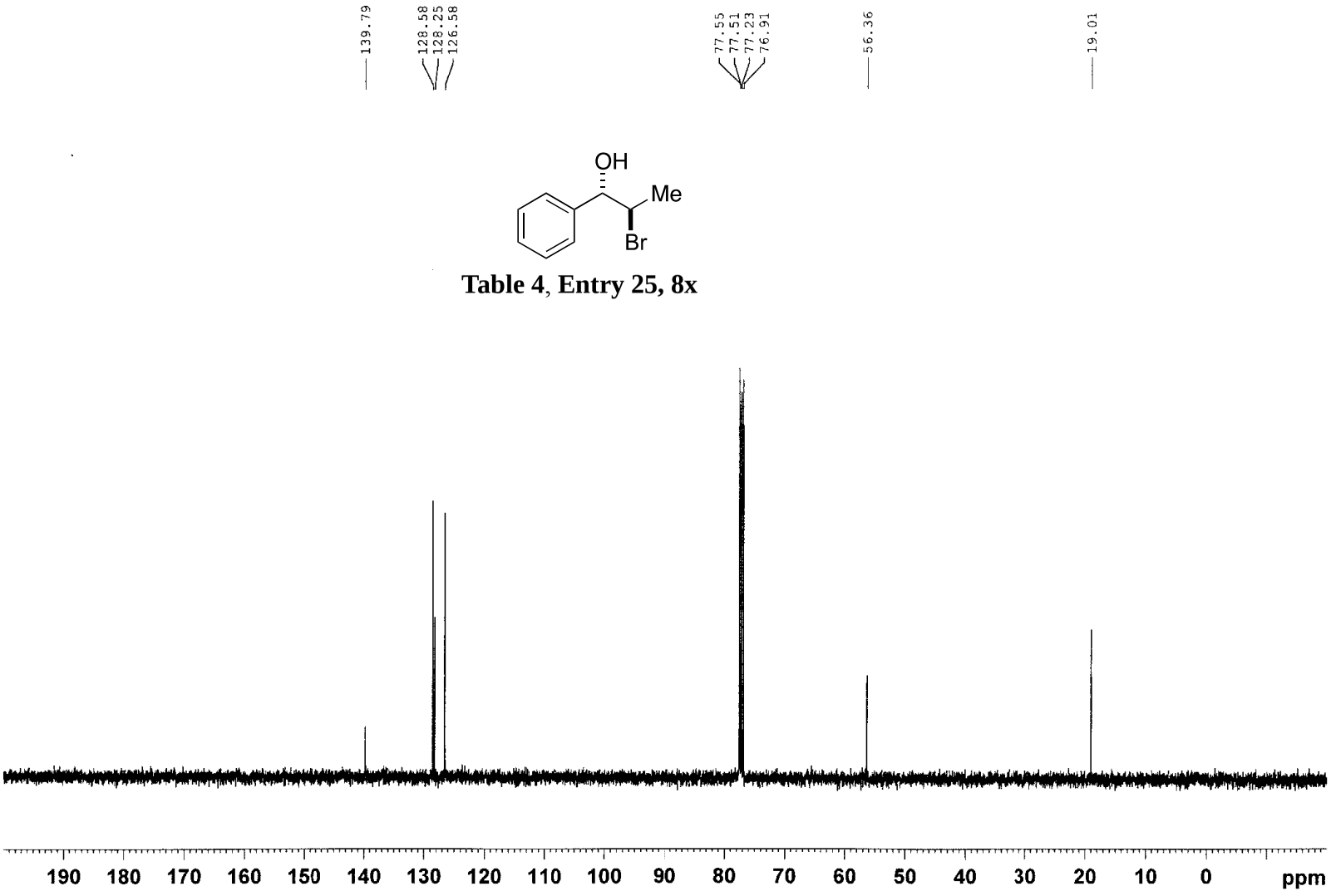


Table 4, Entry 25, 8x

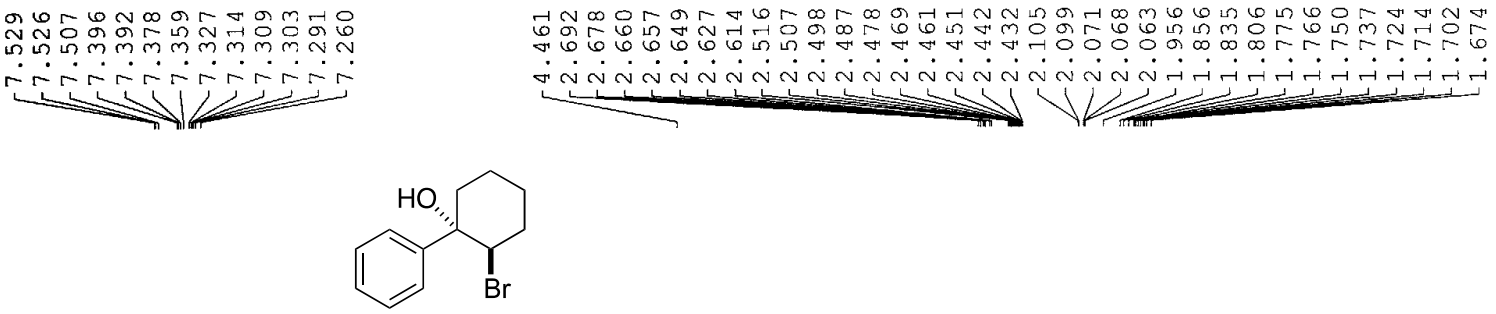
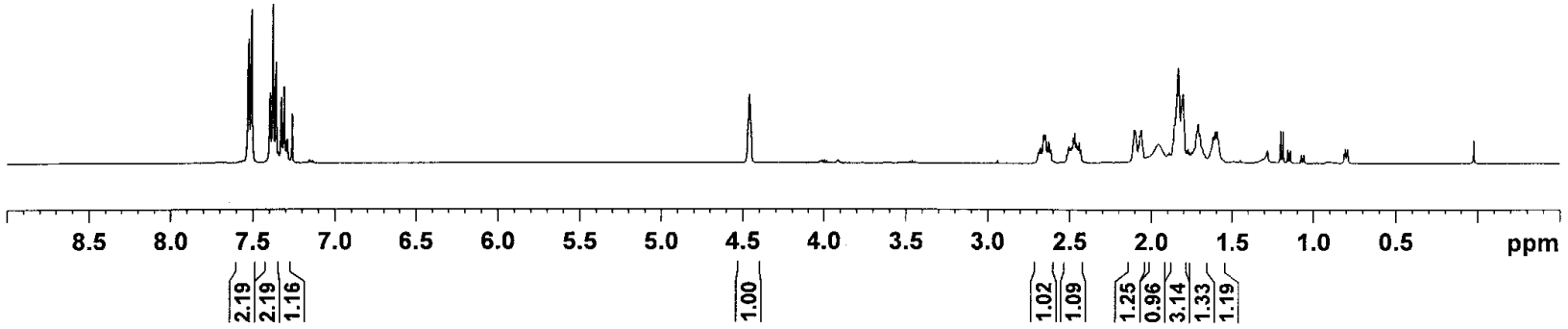


Table 4, **Entry 26, 8y**



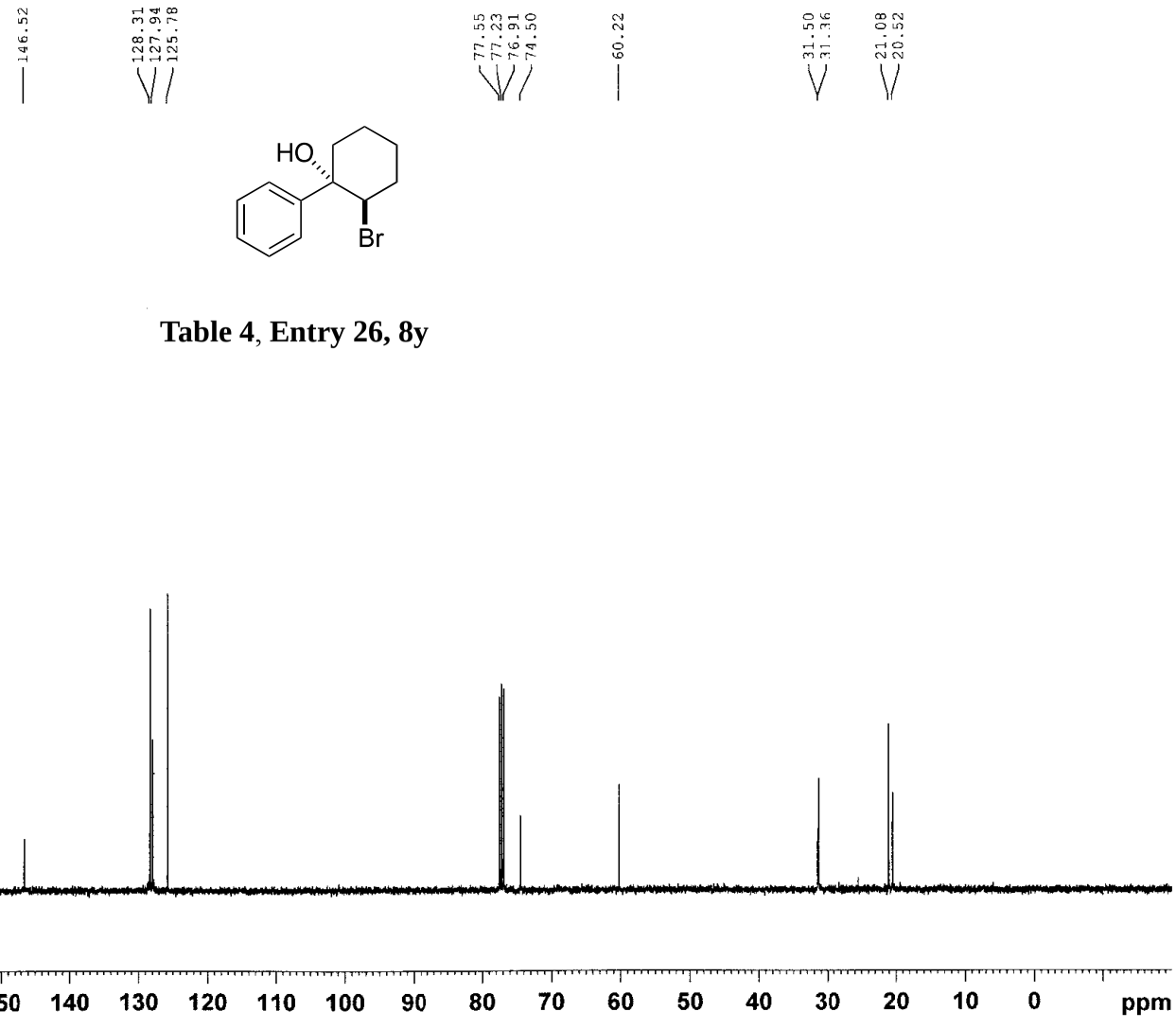


Table 4, Entry 26, 8y