



Supporting Information

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Catalytic Enantioselective Passerini Three-component Reaction

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General procedure for synthesis of α -acyloxyamides (Racemic)

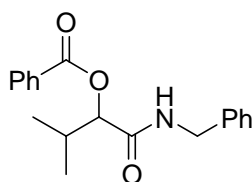
To a solution of aldehyde (0.5 mmol) in methylenechloride (1.0 mL) were added acid (0.5 mmol) and isocyanide (0.5 mmol). The reaction mixture was stirred at room temperature. After complete consumption of the isocyanide by TLC analysis (typically 24 h), the reaction mixture was quenched by addition of saturated aqueous NaHCO₃ solution, and stirred at room temperature for 0.5 h, the reaction mixture was extracted with EtOAc. The combined organic phase was washed with brine, dried over anhydrous sodium sulfate, filtered and concentrated. The crude product was then purified by flash chromatograph on silica gel to give the corresponding product.

Catalytic enantioselective Passerini reaction: synthesis of enantioenriched α -acyloxyamides

To a flame dried round bottom flask (25 mL), under argon and equipped with a stir bar, was added (salen)Al(III)Cl derived from N,N'-bis(3,5-di-*tert*-butyl-salicylidene)-*R,R*-cyclohexane-1,2-diamine (30.3 mg, 0.05 mmol) and dry toluene (0.3 mL). The mixture was stirred until the catalyst was completely dissolved. The aldehyde (in 0.1 ml toluene, 0.5 mmol) was then introduced and the resulting mixture was stirred at room temperature for 0.5 h. The mixture was cool to -40 °C, and a solution of isocyanide (0.5 mmol) in toluene (0.1 mL) was added, after stirring for 10 min, a

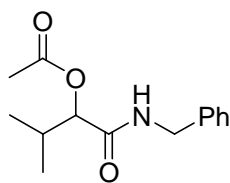
solution of acid (0.5 mmol) in toluene (1 mL) was added slowly via a syringe pump (addition time: 1 h). After being stirred at -40 °C for 48 h, the reaction mixture was quenched by addition of saturated aqueous NaHCO₃ solution, and stirred at room temperature for 0.5 h, the reaction mixture was extracted with EtOAc. The combined organic phase was washed with brine, dried over anhydrous sodium sulfate, filtered and concentrated. The crude product was then purified by flash chromatograph on silica gel to give the corresponding product.

Physical data of compound 4a-4p



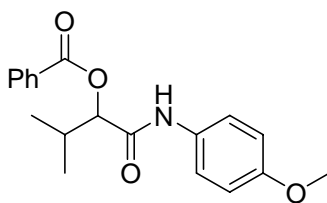
4a

White solid, mp 113-114 °C, $[\alpha]_D^{20} = +3.8^\circ$ (c = 1.07, CHCl₃); ee: 63% (chiral HPLC); IR (KBr) ν 3268, 3090, 2970, 1724, 1658, 1564, 1458, 1256, 1125 cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 1.06 (dd, $J = 7.11, 7.8$ Hz, 6H), 2.48-2.54 (m, 1H), 4.39-4.58 (m, 2H), 5.37 (d, $J = 4.2$ Hz, 1H), 6.36 (br, s, 1H), 7.23-7.33 (m, 5H), 7.44-7.47 (m, 2H), 7.58-7.63 (m, 1H), 8.05-8.08 (m, 2H); ¹³CNMR (CDCl₃, 75MHz) δ 17.1, 19.0, 30.9, 43.2, 78.7, 127.5, 127.6, 128.7(2C), 129.3, 129.8, 133.6, 137.9, 165.5, 169.4; MS (ESI) m/z 312 [M+H]⁺, 334 [M+Na]⁺.



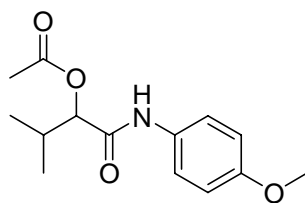
4b

White solid, mp 62-63 °C, $[\alpha]_D^{20} = -17.8^\circ$ (c = 1.35, CHCl₃); ee: 63% (chiral HPLC); IR (KBr) ν 3309, 3086, 2974, 1739, 1664, 1553, 1444, 1376, 1244, 1135cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 0.95 (dd, $J = 2.6, 6.8$ Hz, 6H), 2.13 (s, 3H), 2.29-2.35 (m, 1H), 4.39-4.55 (m, 2H), 5.08 (d, $J = 4.6$ Hz, 1H), 6.32 (br, s, 1H), 7.25-7.37 (m, 5H); ¹³CNMR (CDCl₃, 75MHz) δ 17.1, 18.7, 20.8, 30.6, 43.2, 78.2, 127.6, 127.7, 128.8, 137.9, 169.3, 169.8 ; MS (ESI) m/z 250 [M+H]⁺, 272 [M+Na]⁺; Anal. Calcd. for C₁₄H₁₉NO₃: C, 67.45; H, 7.68; N, 5.62; Found: C, 67.42; H, 7.65; N, 5.61.



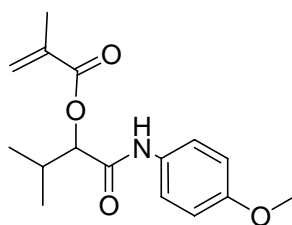
4c

White solid, mp 174-175 °C, $[\alpha]_D^{20} = +22.2^\circ$ (c = 0.94, CHCl₃); ee: 84% (chiral HPLC); IR (KBr) ν 3299, 2969, 1730, 1670, 1542, 1515, 1287, 1249, 1115 cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 1.12 (dd, $J = 6.9\text{Hz}$, $J = 12.1\text{Hz}$, 6H), 2.56-2.58 (m, 1H), 3.79 (s, 3H), 5.43 (d, $J = 4.4\text{Hz}$, 1H), 6.85 (d, $J = 8.9\text{Hz}$, 2H), 7.41 (d, $J = 8.9\text{Hz}$, 2H), 7.51-7.56 (m, 2H), 7.64-7.66 (m, 2H), 7.75 (br, s, 1H), 8.14-8.16 (m, 2H); ¹³CNMR (CDCl₃, 75MHz) δ 17.2, 19.0, 31.0, 55.5, 78.8, 114.2, 122.2, 128.8, 129.3, 129.8, 129.9, 133.8, 156.8, 163.5, 167.4; MS (ESI) m/z 328 [M+H]⁺, 350 [M+Na]⁺, 366 [M+K]⁺; Anal. Calcd. for C₁₉H₂₁NO₄: C, 69.71; H, 6.47; N, 4.28; Found: C, 69.51; H, 6.50; N, 4.26.



4d

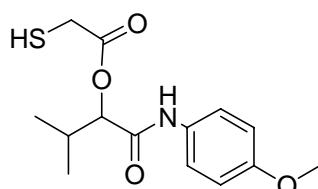
White solid, mp 120-121 °C, $[\alpha]_D^{20} = -56.9^\circ$ (c = 1.13, CHCl₃); ee: 83 % (chiral HPLC); IR (KBr) ν 3296, 2971, 1741, 1670, 1538, 1241 cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 1.00 (d, $J = 6.9\text{Hz}$, 6H), 2.21 (s, 3H), 2.35-2.40 (m, 1H), 3.78 (s, 3H), 5.14 (d, $J = 4.8\text{Hz}$, 1H), 6.85 (d, $J = 8.9\text{Hz}$, 2H), 7.40 (d, $J = 8.9\text{Hz}$, 2H), 7.62 (br, s, 1H); ¹³CNMR (CDCl₃, 75MHz) δ 17.2, 18.7, 20.9, 30.8, 55.5, 78.4, 114.2, 122.1, 130.0, 156.9, 167.3, 169.8; MS (ESI) m/z 266 [M+H]⁺, 288 [M+Na]⁺, 304 [M+K]⁺; Anal. Calcd. for C₁₄H₁₉NO₄: C, 63.38; H, 7.22; N, 5.28; Found: C, 63.32; H, 7.22; N, 5.34.



4e

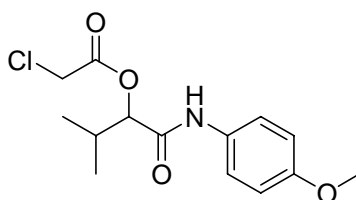
White solid, mp 124-125 °C, $[\alpha]_D^{20} = -22.3^\circ$ (c = 0.98, CHCl₃); ee: 80% (chiral HPLC); IR (KBr) ν 3253, 2970, 1719, 1662, 1610, 1550, 1515, 1301, 1240, 1167, 1029 cm⁻¹; ¹HNMR (CDCl₃,

300MHz) δ 1.03 (dd, $J = 3.1, 5.8\text{Hz}$, 6H), 2.04 (s, 3H), 2.42-2.48 (m, 1H), 3.78 (s, 3H), 5.22 (d, $J = 4.1\text{Hz}$, 1H), 5.73 (s, 1H), 6.27 (s, 1H), 6.84 (d, $J = 8.5\text{Hz}$, 2H), 7.39 (d, $J = 8.5\text{Hz}$, 2H), 7.64 (br, s, 1H); ^{13}C NMR (CDCl_3 , 75MHz) δ 17.0, 18.4, 18.9, 30.9, 55.5, 78.5, 114.2, 121.9, 122.1, 126.9, 129.9, 135.7, 156.8, 166.1, 167.4; MS (ESI) m/z 292 $[\text{M}+\text{H}]^+$, 314 $[\text{M}+\text{Na}]^+$, 330 $[\text{M}+\text{K}]^+$; Anal. Calcd. for $\text{C}_{16}\text{H}_{21}\text{NO}_4$: C, 65.96; H, 7.27; N, 4.81; Found: C, 65.92; H, 7.26; N, 4.81.



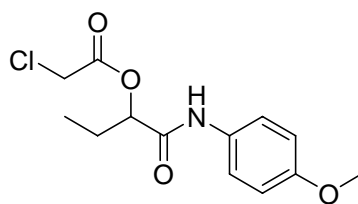
4f

White solid, mp 104-105 °C, $[\alpha]_{\text{D}}^{20} = -57.7^\circ$ ($c=1.05$, CHCl_3); ee: 75% (chiral HPLC); IR (KBr) ν 3249, 2971, 1741, 1660, 1610, 1550, 1515, 1305, 1239, 1175, 1029 cm^{-1} ; ^1H NMR (CDCl_3 , 300MHz) δ 1.02 (dd, $J = 3.8, 6.8\text{Hz}$, 6H), 2.18 (t, $J = 0.7\text{Hz}$, 1H), 2.42-2.48 (m, 1H), 3.37-3.43 (m, 2H), 3.79 (s, 1H), 5.21 (d, $J = 4.2\text{Hz}$, 1H), 6.85 (d, $J = 9.0\text{Hz}$, 2H), 7.46 (d, $J = 9.0\text{Hz}$, 2H), 7.94 (br, s, 1H); MS (ESI) m/z 298 $[\text{M}+\text{H}]^+$, 320 $[\text{M}+\text{Na}]^+$, 336 $[\text{M}+\text{K}]^+$; Anal. Calcd. for $\text{C}_{14}\text{H}_{19}\text{NO}_4\text{S}$: C, 56.55; H, 6.44; N, 4.71; Found: C, 56.33; H, 6.25; N, 4.63.



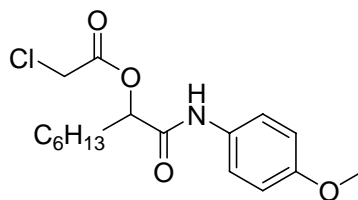
4g

White solid, mp 142-143 °C, $[\alpha]_{\text{D}}^{20} = -39.6^\circ$ ($c = 1.06$, CHCl_3); ee: >99% (chiral HPLC); IR (KBr) ν 3290, 2968, 1728, 1665, 1538, 1250 cm^{-1} ; ^1H NMR (CDCl_3 , 300MHz) δ 1.03 (d, $J = 6.8\text{Hz}$, 6H), 2.42-2.48 (m, 1H), 3.79 (s, 3H), 4.19 (dd, $J = 14.2, 22.8\text{Hz}$, 2H), 5.25 (d, $J = 4.3\text{Hz}$, 1H), 6.85 (d, $J = 8.9\text{Hz}$, 2H), 7.41 (d, $J = 8.9\text{Hz}$, 2H), 7.70 (br, s, 1H); ^{13}C NMR (CDCl_3 , 75MHz) δ 16.9, 18.7, 30.9, 40.7, 55.5, 79.7, 114.2, 122.0, 129.8, 156.9, 166.0, 166.5; MS (EI) : m/z 301 (10) $[\text{M}+2]^+$, 299 $[\text{M}]^+$ (30), 123 (100); Anal. Calcd. for $\text{C}_{14}\text{H}_{18}\text{ClNO}_4$: C, 56.10; H, 6.05; N, 4.67; Found: C, 56.18; H, 6.10; N, 4.54.



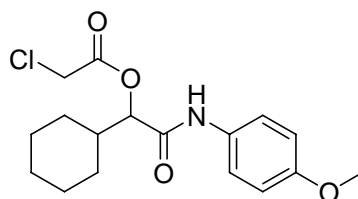
4h

White solid, mp 126-127 °C, $[\alpha]_D^{20} = -41.9^\circ$ ($c = 1.05$, CHCl_3); ee: 87% (chiral HPLC); IR (KBr) ν 3262, 3086, 1761, 1662, 1552, 1515, 1237, 1184 cm^{-1} ; ^1H NMR (CDCl_3 , 300MHz) δ 1.00 (t, $J = 7.5\text{Hz}$, 3H), 1.97-2.06 (m, 1H), 3.77 (s, 3H), 4.18 (dd, $J = 14.5, 22.1\text{Hz}$, 2H), 5.31 (t, $J = 5.1\text{Hz}$, 1H), 6.85 (d, $J = 9.0\text{Hz}$, 2H), 7.41 (d, $J = 9.0\text{Hz}$, 2H), 7.87 (br, s, 1H); ^{13}C NMR (CDCl_3 , 75MHz) δ 89.0, 25.1, 40.7, 55.5, 76.6, 114.2, 122.0, 129.9, 156.9, 165.9, 166.8; MS (ESI) m/z 286 $[\text{M}+\text{H}]^+$; Anal. Calcd. for $\text{C}_{13}\text{H}_{16}\text{ClNO}_4$: C, 54.65; H, 5.64; N, 4.90; Found: C, 54.68; H, 5.64; N, 5.14.



4i

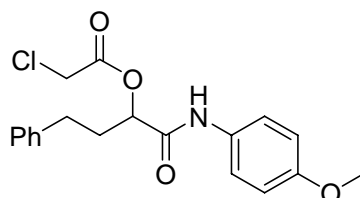
White solid, mp 90-91 °C, $[\alpha]_D^{20} = -37.2^\circ$ ($c = 1.15$, CHCl_3); ee: 73% (chiral HPLC); IR (KBr) ν 3284, 2939, 1730, 1668, 1544, 1251 cm^{-1} ; ^1H NMR (CDCl_3 , 300MHz) δ 0.85-0.89 (m, 3H), 1.28-1.39 (m, 8H), 1.93-2.01 (m, 2H), 3.79 (s, 3H), 4.17 (dd, $J = 14.4, 22.1\text{Hz}$, 2H), 5.34 (t, $J = 5.5\text{Hz}$, 1H), 6.85 (d, $J = 8.9\text{Hz}$, 2H), 7.41 (d, $J = 8.9\text{Hz}$, 2H), 7.84 (br, s, 1H); ^{13}C NMR (CDCl_3 , 75MHz) δ 14.0, 22.5, 24.6, 28.9, 31.5, 31.9, 40.8, 55.5, 75.8, 114.2, 121.9, 129.9, 156.9, 165.9, 167.0; MS (ESI) m/z 342 $[\text{M}+\text{H}]^+$, 364 $[\text{M}+\text{Na}]^+$; Anal. Calcd. for $\text{C}_{19}\text{H}_{24}\text{ClNO}_4$: C, 59.73; H, 7.08; N, 4.10; Found: C, 59.73; H, 6.97; N, 4.24.



4j

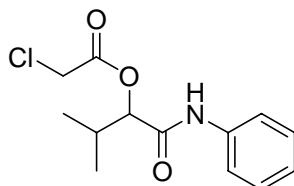
White solid, mp 179-180 °C, $[\alpha]_D^{20} = -43.7^\circ$ ($c = 1.15$, CHCl_3); ee: 87% (chiral HPLC); IR (KBr) ν 3287, 2931, 1728, 1664, 1541, 1294, 1251 cm^{-1} ; ^1H NMR (CDCl_3 , 300 MHz) δ 1.08-1.31 (m, 5H), 1.63-1.77 (m, 5H), 2.09 (m, 1H), 4.18 (dd, $J = 14.3, 23.2\text{Hz}$, 2H), 5.21 (d, $J = 4.5\text{Hz}$, 1H), 6.85 (d, J

= 8.9Hz, 2H), 7.41 (d, $J = 9.1$ Hz, 2H), 7.73 (br, s, 1H); ^{13}C NMR (CDCl_3 , 75MHz) δ 25.8, 25.9 (2C), 27.2, 29.1, 40.3, 40.7, 55.5, 79.4, 114.2, 121.9, 129.9, 156.9, 166.0, 166.4; MS (ESI) m/z 340 $[\text{M}+\text{H}]^+$; Anal. Calcd. for $\text{C}_{17}\text{H}_{22}\text{ClNO}_4$: C, 60.09; H, 6.53; N, 4.12; Found: C, 60.27; H, 6.56; N, 4.18.



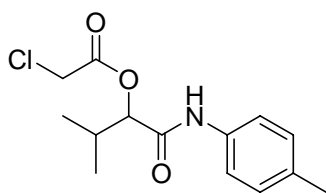
4k

White solid, mp 90-91 °C, $[\alpha]_{\text{D}}^{20} = -26.5^\circ$ ($c = 1.40$, CHCl_3); ee: 71% (chiral HPLC); IR (KBr) ν 3269, 2958, 1731, 1668, 1520, 1248 cm^{-1} ; ^1H NMR (CDCl_3 , 300MHz) δ 2.32-2.34 (m, 2H), 2.75 (t, $J = 7.0$ Hz, 2H), 3.78 (s, 3H), 4.04 (dd, $J = 14.5, 19.4$ Hz, 2H), 5.35 (t, $J = 5.5$ Hz, 1H), 6.84 (d, $J = 8.2$ Hz, 2H), 7.16-7.28 (m, 5H), 7.39 (d, $J = 8.3$ Hz, 2H), 7.82 (br, s, 1H); ^{13}C NMR (CDCl_3 , 75MHz) δ 31.1, 33.0, 40.6, 55.5, 75.3, 114.3, 122.0, 126.3, 128.4, 128.6, 129.8, 140.4, 156.9, 166.0, 166.6; MS (ESI) m/z 362 $[\text{M}+\text{H}]^+$, 384 $[\text{M}+\text{Na}]^+$; Anal. Calcd. for $\text{C}_{19}\text{H}_{20}\text{ClNO}_4$: C, 63.07; H, 5.57; N, 3.87; Found: C, 62.77; H, 5.53; N, 3.50.



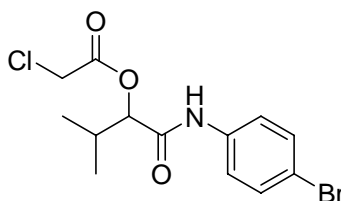
4l

White solid, mp 117-118 °C, $[\alpha]_{\text{D}}^{20} = -57.5^\circ$ ($c = 0.84$, CHCl_3); ee: 93% (chiral HPLC); IR (KBr) ν 3288, 2972, 1757, 1671, 1543, 1185 cm^{-1} ; ^1H NMR (CDCl_3 , 300MHz) δ 1.02 (d, $J = 6.8$ Hz, 6H), 2.41-2.49 (m, 1H), 4.19 (dd, $J = 14.3, 23.6$ Hz, 2H), 5.24 (d, $J = 4.4$ Hz, 1H), 7.11-7.16 (m, 1H), 7.26-7.35 (m, 2H), 7.51-7.54 (m, 2H), 7.87 (br, s, 1H); ^{13}C NMR (CDCl_3 , 75MHz) δ 16.9, 18.7, 30.9, 40.7, 79.7, 120.2, 125.0, 129.1, 136.8, 166.0, 166.7; MS (ESI) m/z 270 $[\text{M}+\text{H}]^+$, 292 $[\text{M}+\text{Na}]^+$, 308 $[\text{M}+\text{K}]^+$; Anal. Calcd. for $\text{C}_{13}\text{H}_{16}\text{ClNO}_3$: C, 57.89; H, 5.98; N, 5.19; Found: C, 57.95; H, 5.99; N, 5.14.



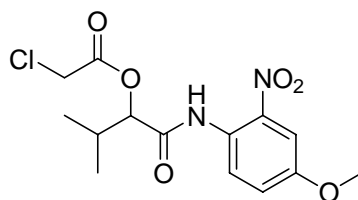
4m

White solid, mp 134-135 °C, $[\alpha]_D^{20} = -63.3^\circ$ (c = 0.79, CHCl₃); ee: 81% (chiral HPLC); IR (KBr) ν 3291, 2970, 1757, 1670, 1537, 1185 cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 1.01 (dd, *J* = 6.1, 6.8Hz, 6H), 2.31 (s, 3H), 2.40-2.44 (m, 1H), 4.18 (dd, *J* = 14.3, 22.8Hz, 2H), 5.23 (d, *J* = 4.4Hz, 1H), 7.12 (d, *J* = 8.2Hz, 2H), 7.38 (d, *J* = 8.3Hz, 2H), 7.79 (br, s, 1H); ¹³CNMR (CDCl₃, 75MHz) δ 16.9, 18.7, 30.9, 40.7, 79.7, 120.2, 129.6, 134.2, 134.7, 166.0, 166.5; MS (ESI) *m/z* 284 [M+H]⁺, 306 [M+Na]⁺, 322 [M+K]⁺; Anal. Calcd. for C₁₄H₁₈ClNO₃: C, 59.26; H, 6.39; N, 4.94; Found: C, 59.61; H, 6.47; N, 4.94.



4n

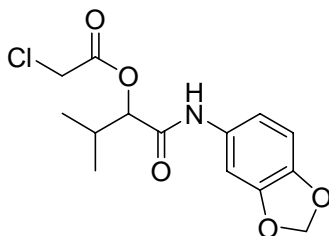
White solid, mp 118-119 °C, $[\alpha]_D^{20} = -46.1^\circ$ (c = 1.09, CHCl₃); ee: 88% (chiral HPLC); IR (KBr) ν 3298, 2970, 1761, 1678, 1532, 1183 cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 1.01 (dd, *J* = 0.9, 6.8Hz, 6H), 2.38-2.44 (m, 1H), 4.19 (dd, *J* = 14.3, 23.4Hz, 2H), 5.19 (d, *J* = 4.6Hz, 1H), 7.39-7.45 (m, 4H), 7.90 (br, s, 1H); ¹³CNMR (CDCl₃, 75MHz) δ 16.9, 18.6, 30.9, 40.7, 79.7, 117.7, 121.7, 132.1, 135.9, 166.1, 166.8; MS (ESI) *m/z* 349 [M+H]⁺, 351 [M+2+H]⁺, 372 [M+Na]⁺, 388 [M+K]⁺; Anal. Calcd. for C₁₃H₁₅BrClNO₃: C, 44.79; H, 4.34; N, 4.02; Found: C, 44.80; H, 4.29; N, 4.37.



4o

Oil, $[\alpha]_D^{20} = -93.1^\circ$ (c = 1.10, CHCl₃); ee: 75% (chiral HPLC); IR (KBr) ν 3351, 2968, 1767, 1702, 1516, 1461, 1279, 1155 cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 1.05 (dd, *J* = 6.9, 8.4Hz, 6H), 2.43-2.51 (m, 1H), 3.87 (s, 3H), 4.37 (s, 2H), 7.24-7.28 (m, 1H), 7.71 (d, *J* = 3.0Hz, 1H), 8.68 (d, *J* = 9.3Hz,

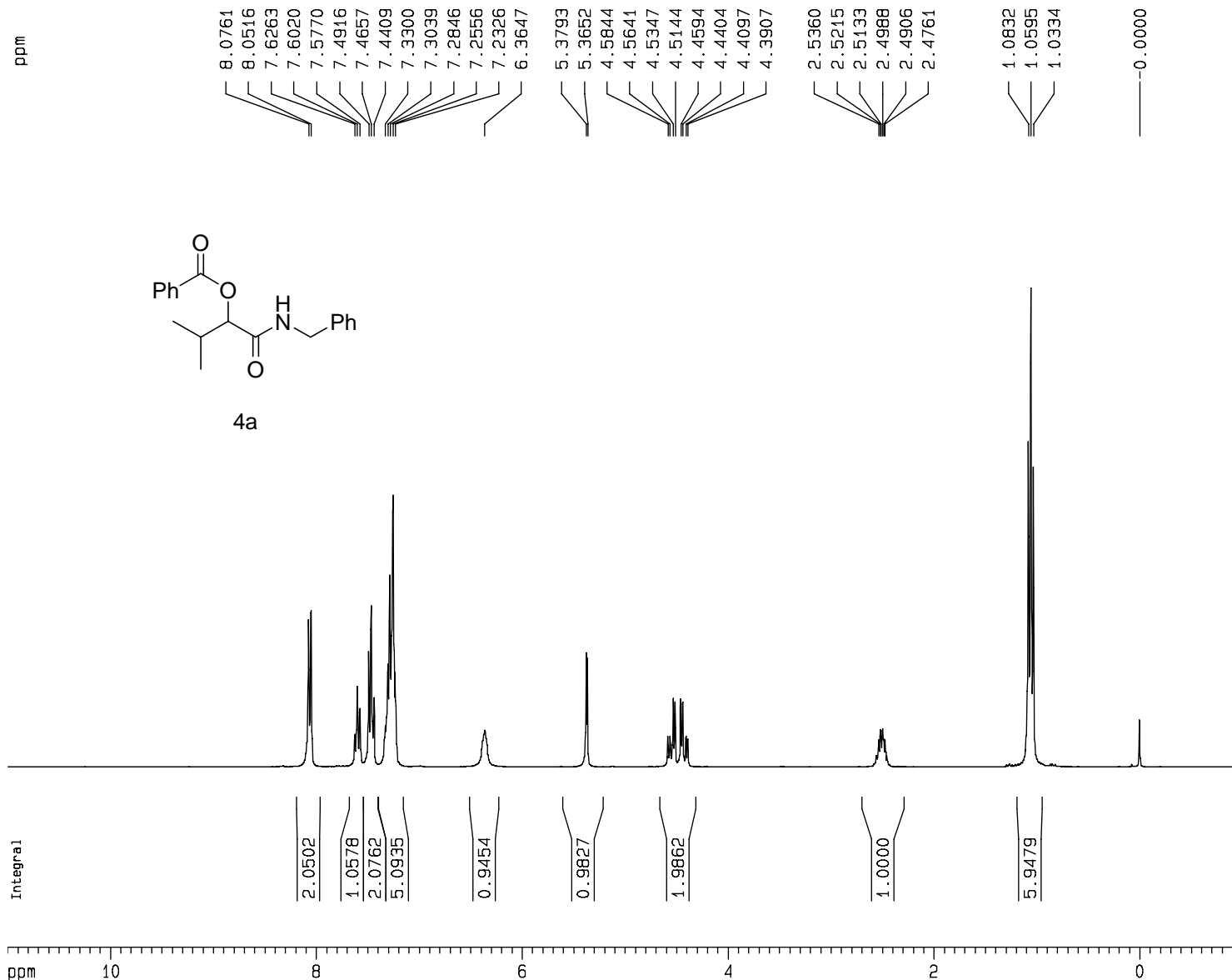
1H), 10.77 (br, s, 1H); ¹³CNMR (CDCl₃, 75MHz) δ 16.8, 18.7, 31.1, 40.6, 56.0, 79.7, 108.9, 123.5, 127.5, 137.2, 155.5, 166.4, 167.5; MS (ESI) *m/z* 345 [M+H]⁺, 367 [M+Na]⁺, 383 [M+K]⁺; Anal. Calcd. for C₁₄H₁₇ClN₂O₆: C, 48.77; H, 4.97; N, 8.13; Found: C, 48.91; H, 4.60; N, 8.15.



4p

White solid, mp 147-148 °C, [α]_D²⁰ = -43.6°(c = 1.09, CHCl₃); ee: 68% (chiral HPLC); IR (KBr) ν 3255, 3096, 2969, 1759, 1660, 1536, 1498, 1189 cm⁻¹; ¹HNMR (CDCl₃, 300MHz) δ 1.01 (d, *J* = 6.8Hz, 6H), 2.39-2.45 (m, 1H), 4.18 (dd, *J* = 14.3, 23.0Hz, 2H), 5.20 (d, *J* = 4.4Hz, 1H), 6.72 (d, *J* = 8.3Hz, 1H), 6.79 (dd, *J* = 2.1, 8.3Hz, 1H), 7.20 (d, *J* = 2.1Hz, 1H), 7.79 (br, s, 1H); ¹³CNMR (CDCl₃, 75MHz) δ 16.9, 18.6, 30.9, 40.7, 79.7, 101.4, 103.0, 108.1, 113.5, 130.9, 144.8, 147.9, 166.0, 166.6; MS (ESI) *m/z* 314 [M+H]⁺, 336 [M+Na]⁺, 352 [M+K]⁺; Anal. Calcd. for C₁₄H₁₆ClNO₅: C, 53.60; H, 5.14; N, 4.46; Found: C, 53.63; H, 5.17; N, 4.66.

¹H NMR spectra of compounds 4a-4p



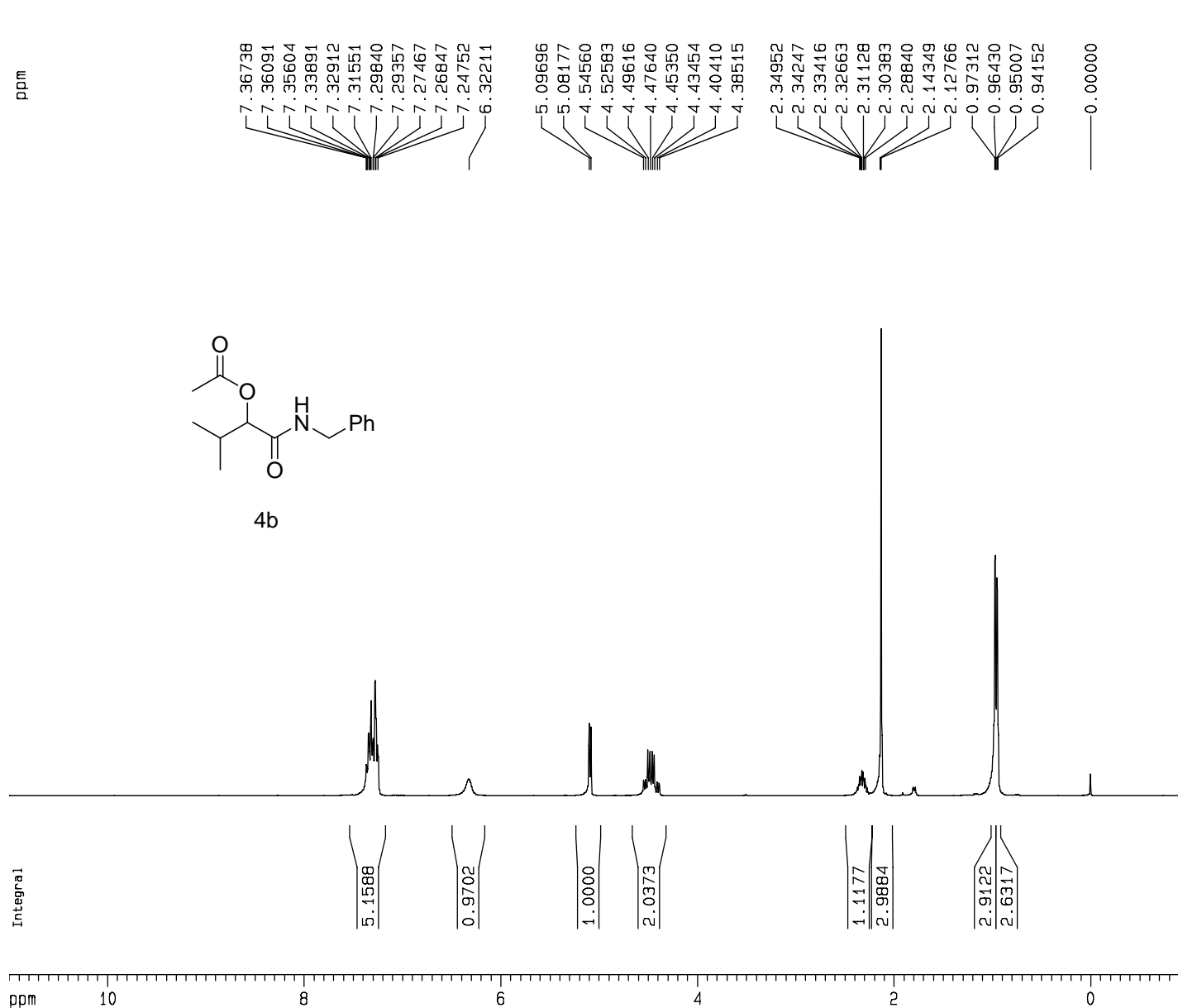
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 RG 143.7
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 DE 6.00 usec
 TE 298.2 K
 D1 5.00000000 sec

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1D NMR plot parameters
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 CY 8.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
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Current Data Parameters

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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

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PULPROG zg30
TD 65536
SOLVENT CDC13
NS 9
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
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RG 143.7
DW 81.000 usec
DE 6.00 usec
TE 300.4 K
D1 2.00000000 sec

===== CHANNEL f1 =====

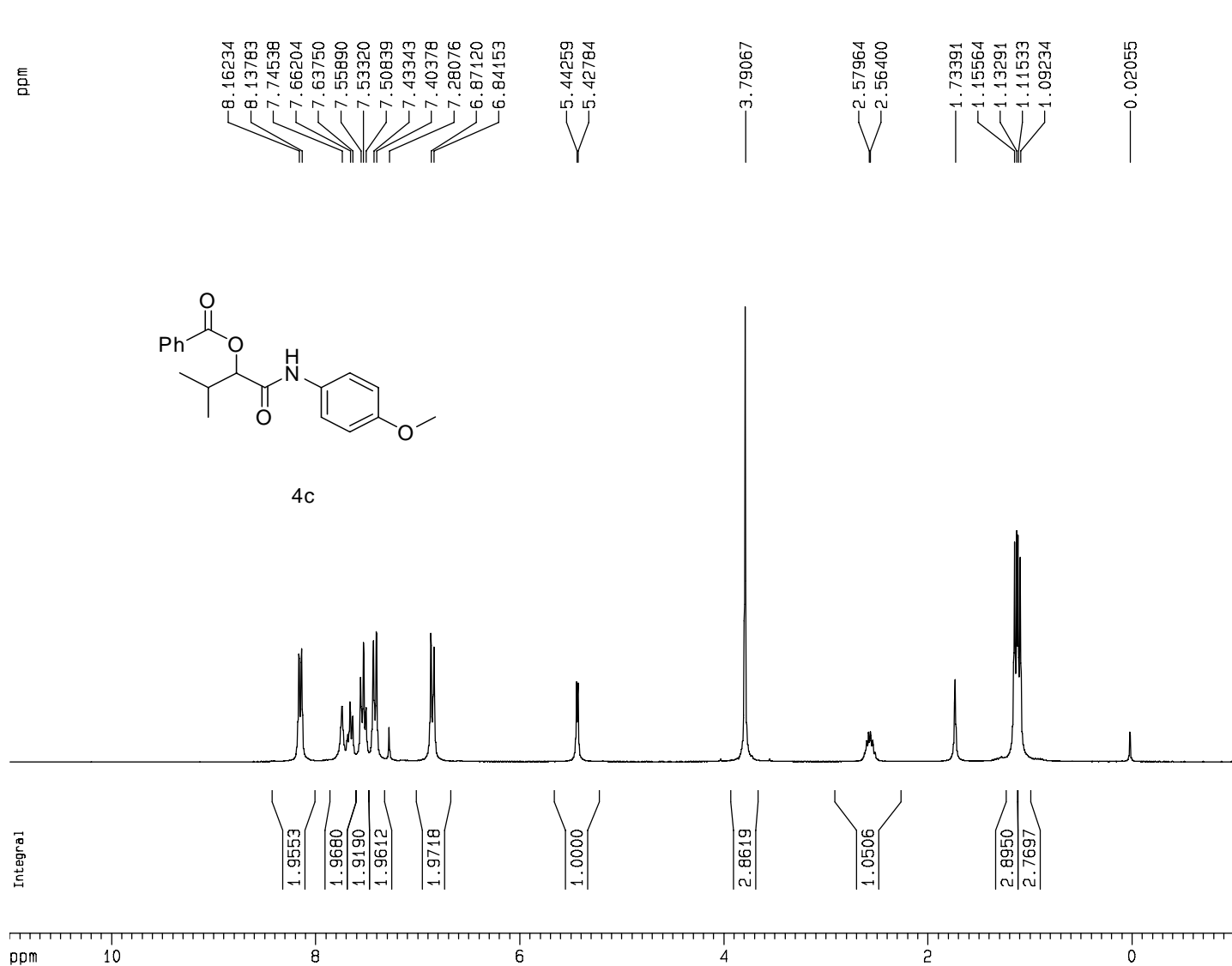
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F2 - Processing parameters

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LB 0.30 Hz
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PC 1.00

1D NMR plot parameters

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CY 8.00 cm
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F2P -1.000 ppm
F2 -300.13 Hz
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HZCM 163.70728 Hz/cm



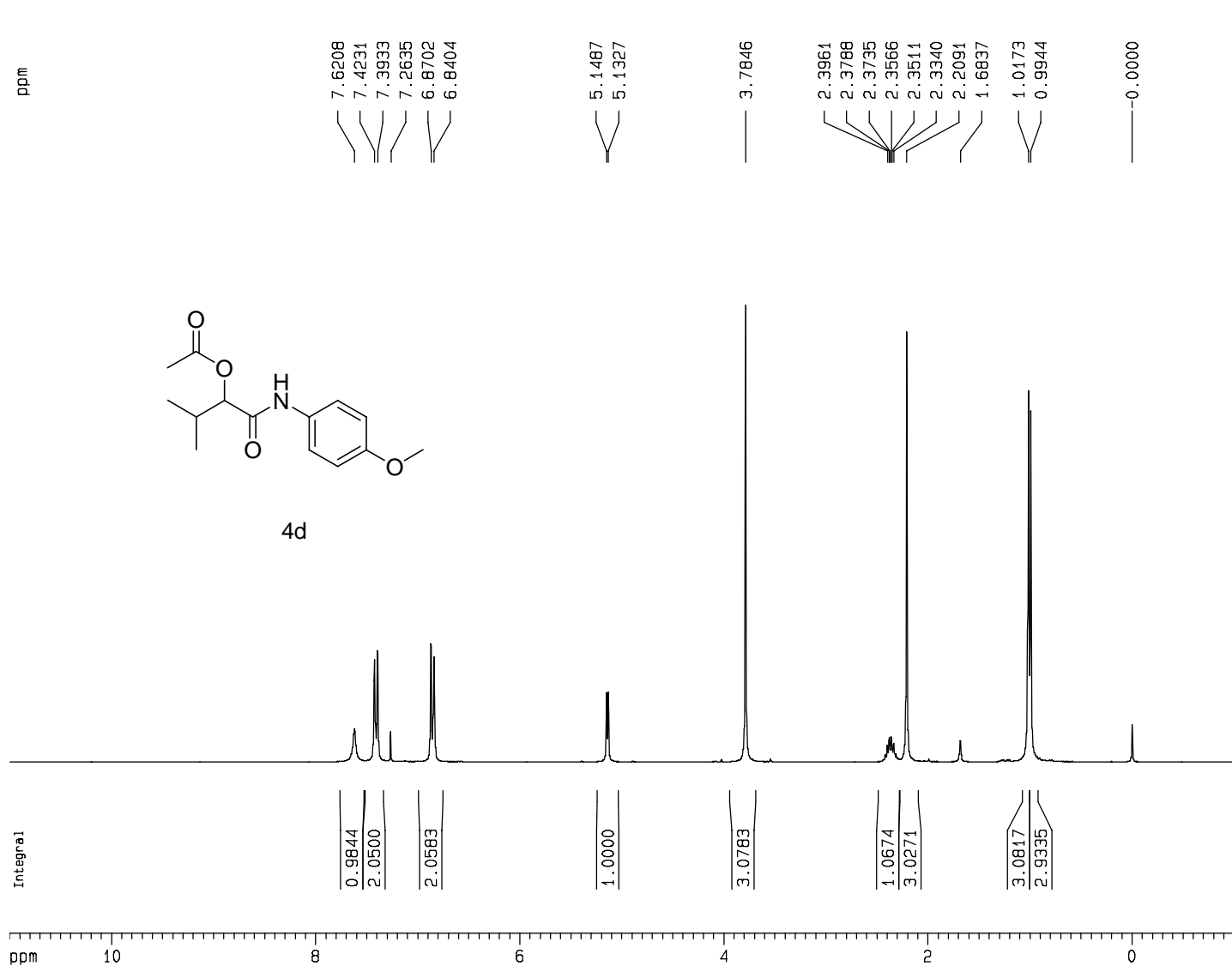
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 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
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 DW 81.000 usec
 DE 6.00 usec
 TE 299.0 K
 D1 2.00000000 sec

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 P1 9.30 usec
 PL1 -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
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 WDW EM
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1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
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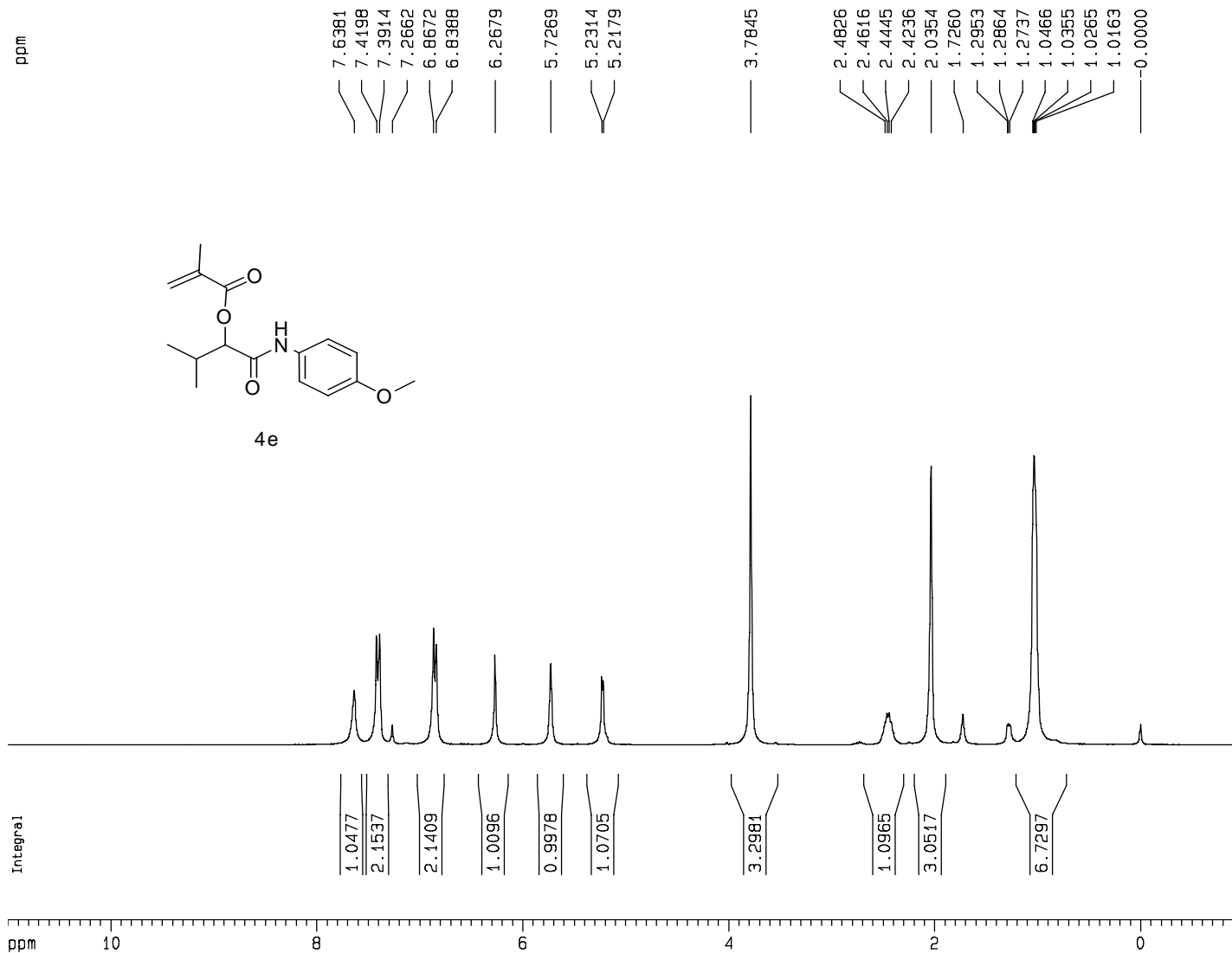
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 NS 9
 DS 2
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 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 228.1
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 TE 303.2 K
 D1 2.00000000 sec

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 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
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Current Data Parameters

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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

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PULPROG zg30
TD 65536
SOLVENT CDC13
NS 14
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 143.7
DW 55.600 usec
DE 6.00 usec
TE 297.2 K
D1 5.00000000 sec

===== CHANNEL f1 =====

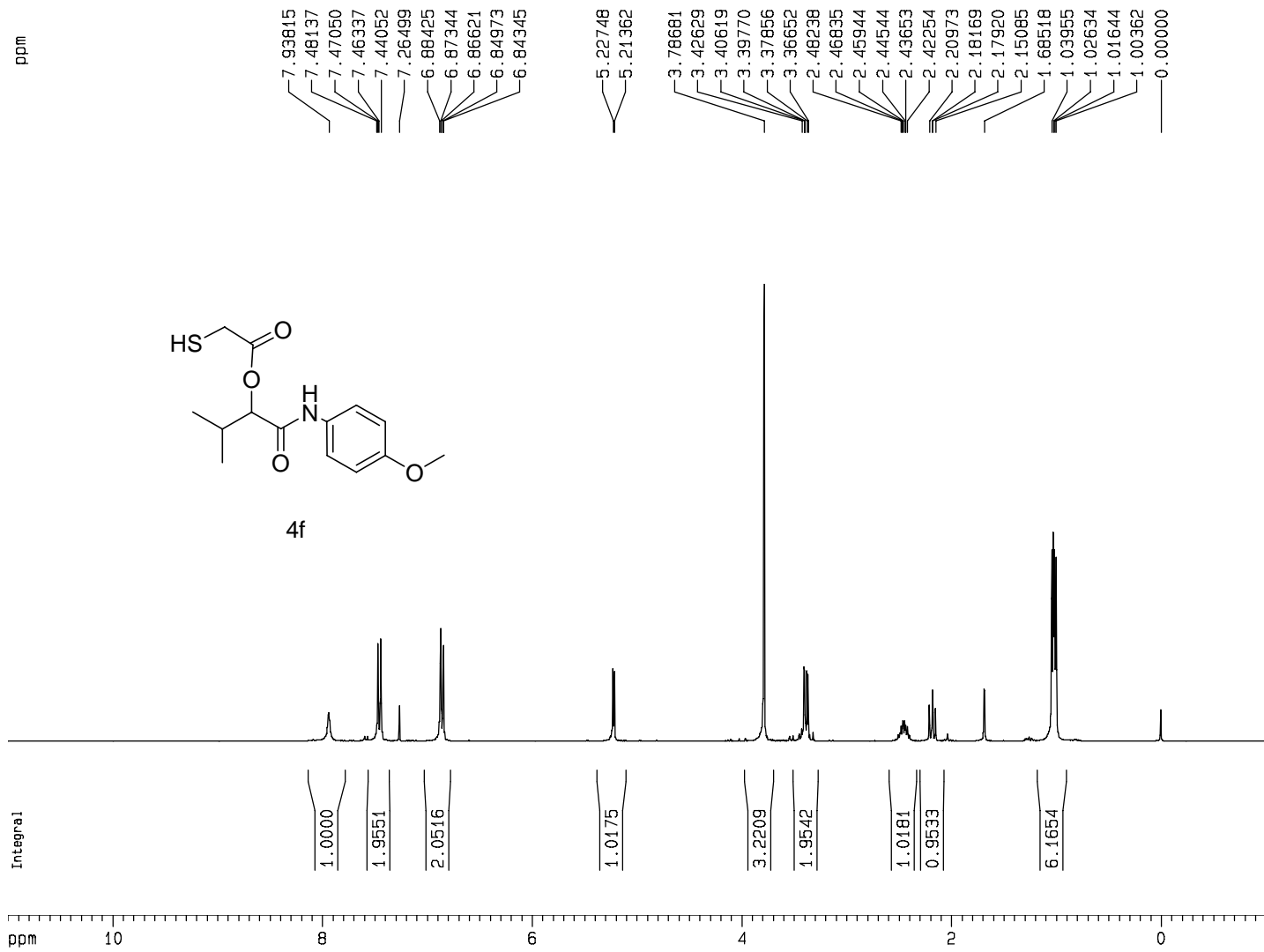
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SSB 0
LB 0.35 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 22.00 cm
CY 6.00 cm
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F2P -1.000 ppm
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PPMCM 0.54545 ppm/cm
HZCM 163.70728 Hz/cm



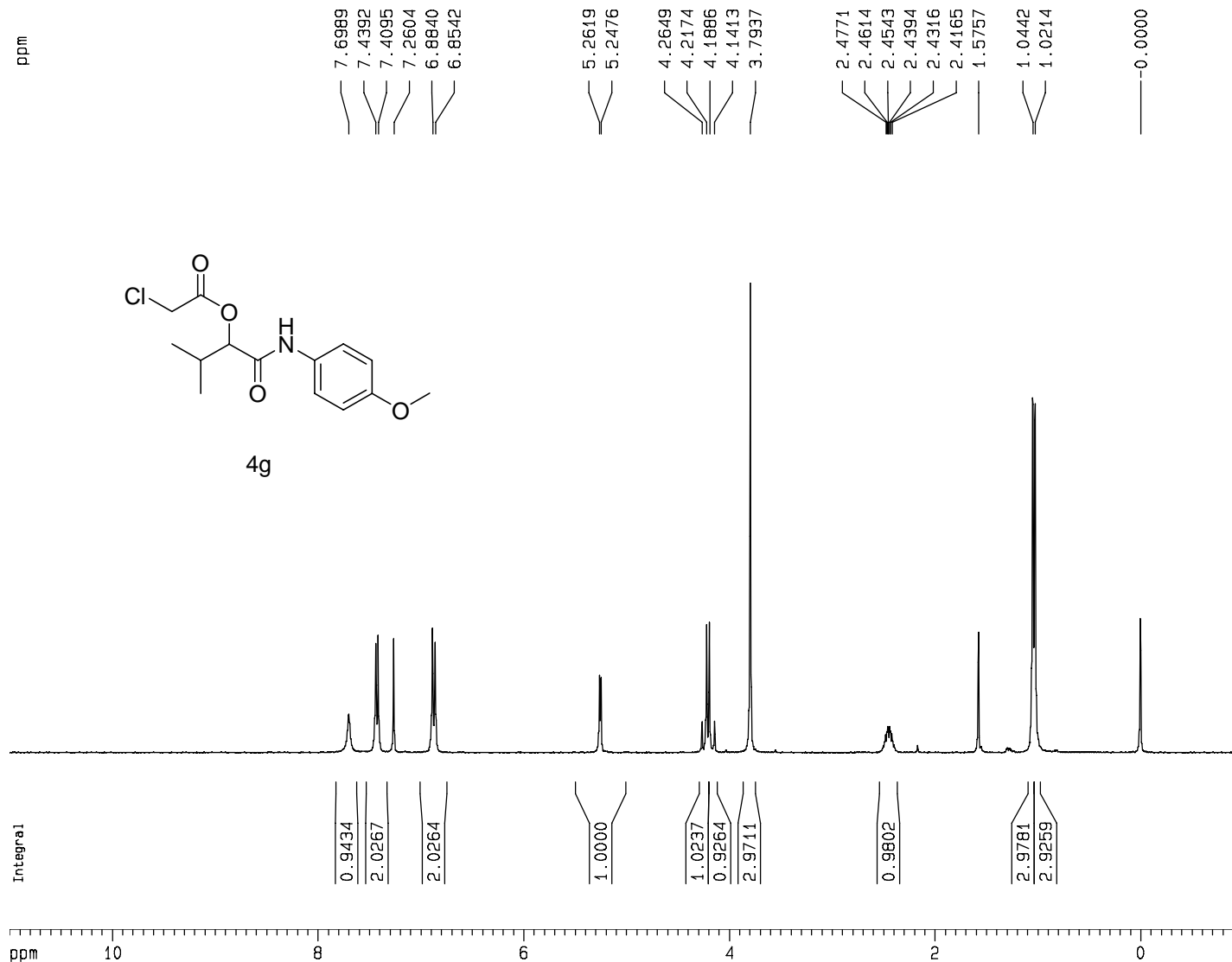
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F2 - Acquisition Parameters
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 INSTRUM av300
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 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 14
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 203.2
 DW 55.600 usec
 DE 6.00 usec
 TE 299.4 K
 D1 5.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.60 usec
 PL1 -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300045 MHz
 WDW EM
 SSB 0
 LB 0.35 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
 F1P 11.000 ppm
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 F2P -1.000 ppm
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 PPMCM 0.54545 ppm/cm
 HZCM 163.70728 Hz/cm



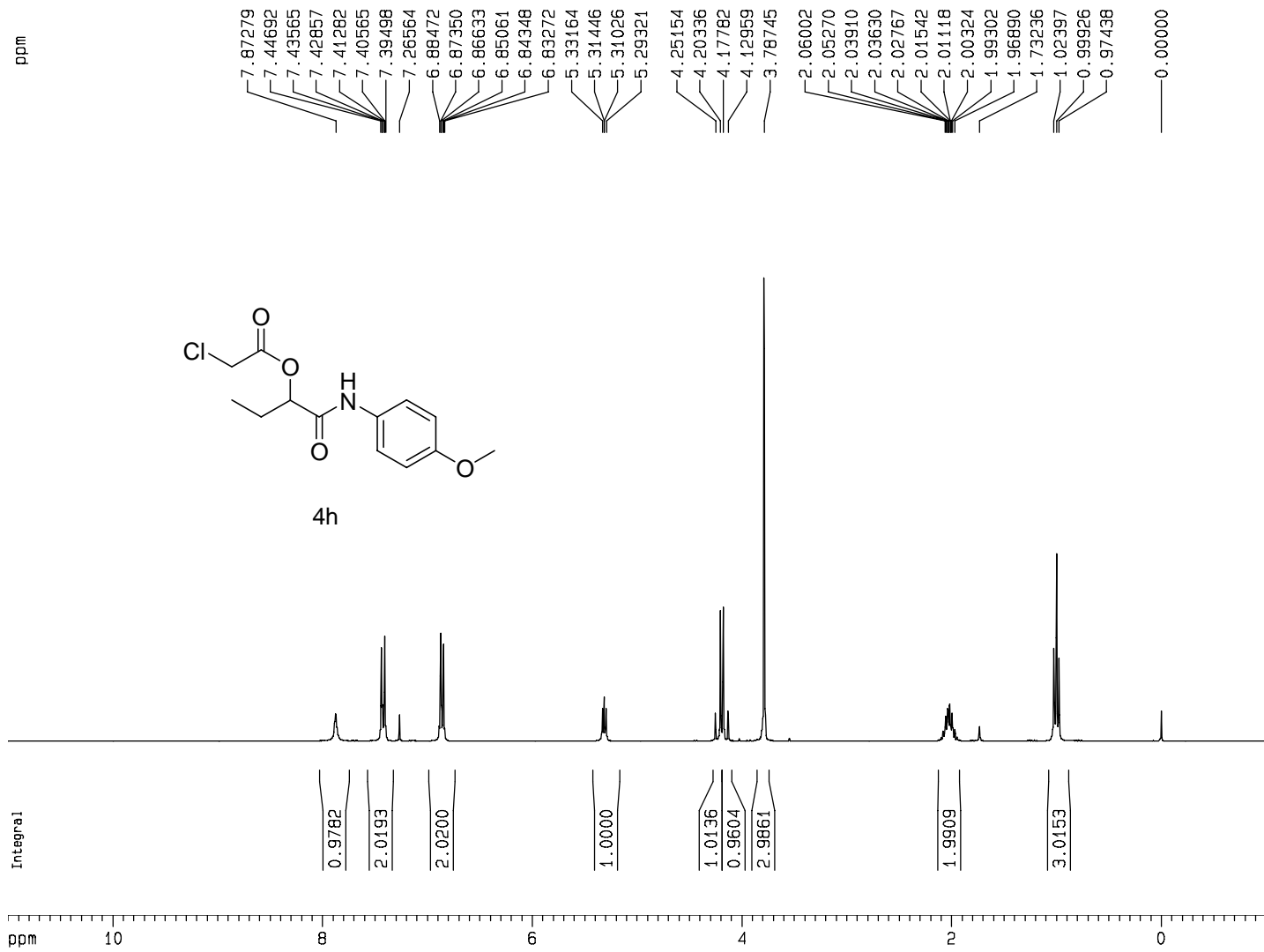
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 TD 65536
 SOLVENT CDCl3
 NS 13
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 322.5
 DW 81.000 usec
 DE 6.00 usec
 TE 300.1 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.30 usec
 PL1 -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300063 MHz
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1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
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 F2P -1.000 ppm
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 PPMCM 0.54545 ppm/cm
 HZCM 163.70728 Hz/cm



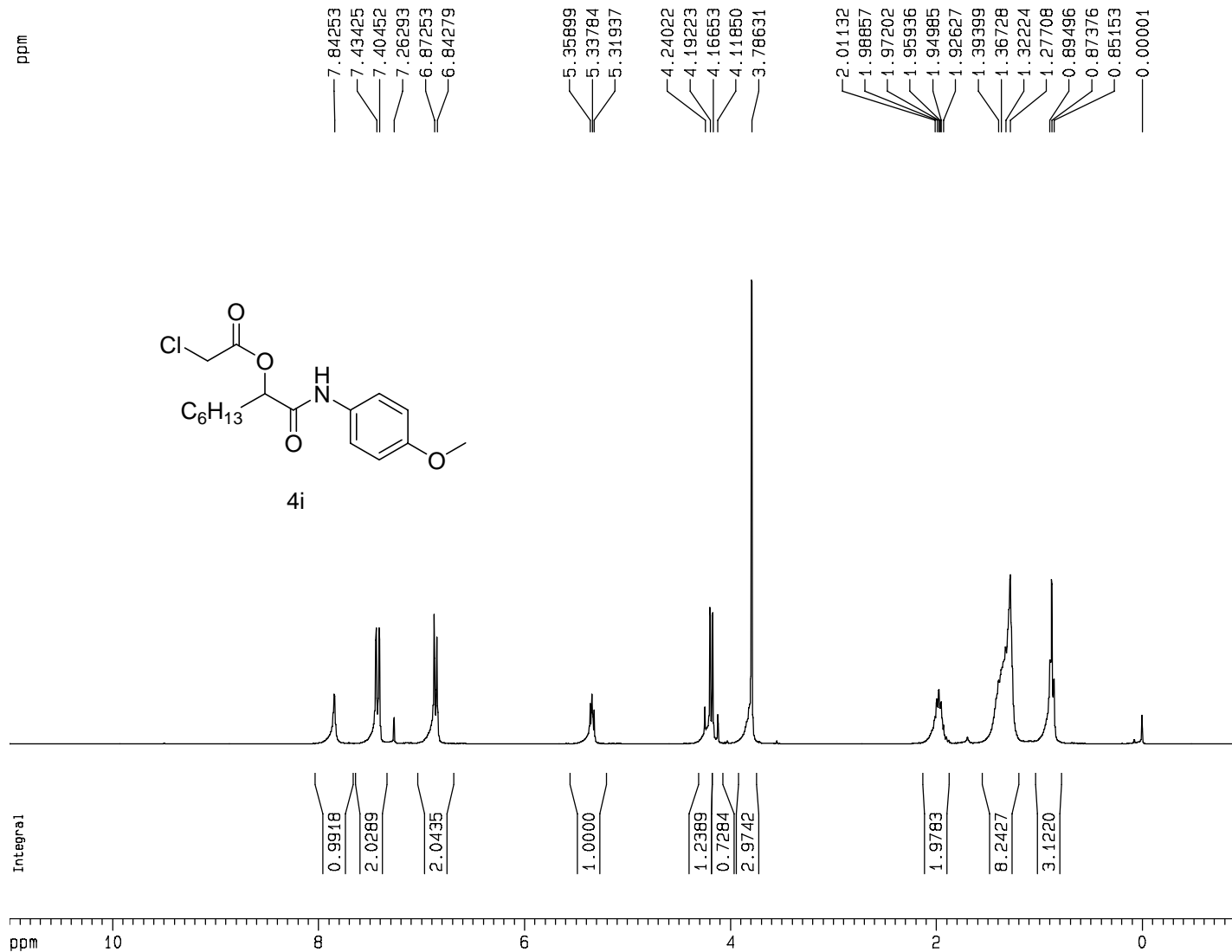
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 TD 65536
 SOLVENT CDC13
 NS 9
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 161.3
 DW 55.600 usec
 DE 6.00 usec
 TE 297.7 K
 D1 5.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.30 usec
 PL1 -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300045 MHz
 WDW EM
 SSB 0
 LB 0.35 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.54545 ppm/cm
 HZCM 163.70728 Hz/cm



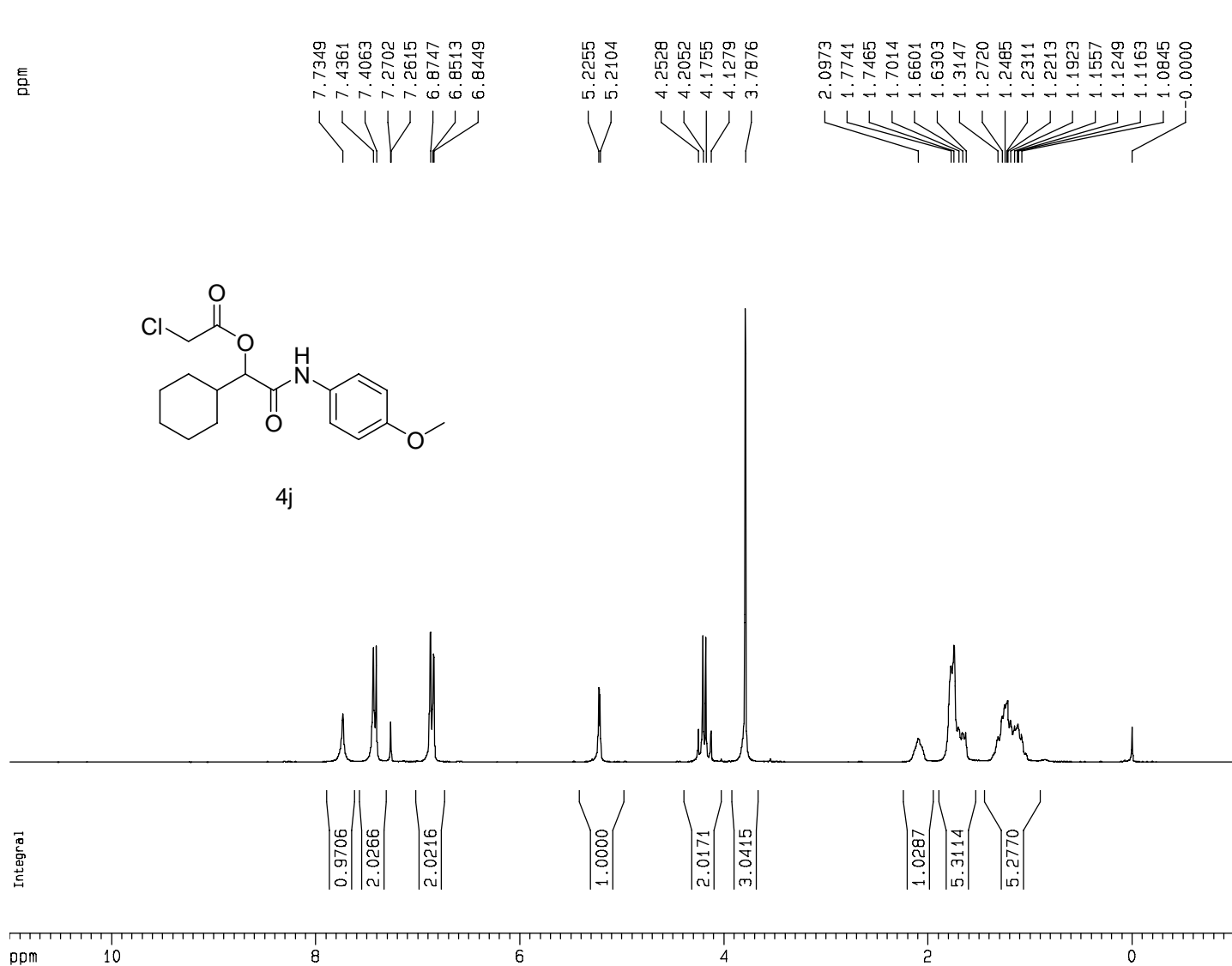
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 SOLVENT CDC13
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 DS 2
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 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 143.7
 DW 81.000 usec
 DE 6.00 usec
 TE 297.2 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.30 usec
 PL1 -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300049 MHz
 WDW EM
 SSB 0
 LB 0.35 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.54545 ppm/cm
 HZCM 163.70728 Hz/cm



Current Data Parameters

NAME wsx-0321-pcr20
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20070321
Time 20.23
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 5
DS 0
SWH 8992.806 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 228.1
DW 55.600 usec
DE 6.00 usec
TE 298.4 K
D1 5.00000000 sec

===== CHANNEL f1 =====

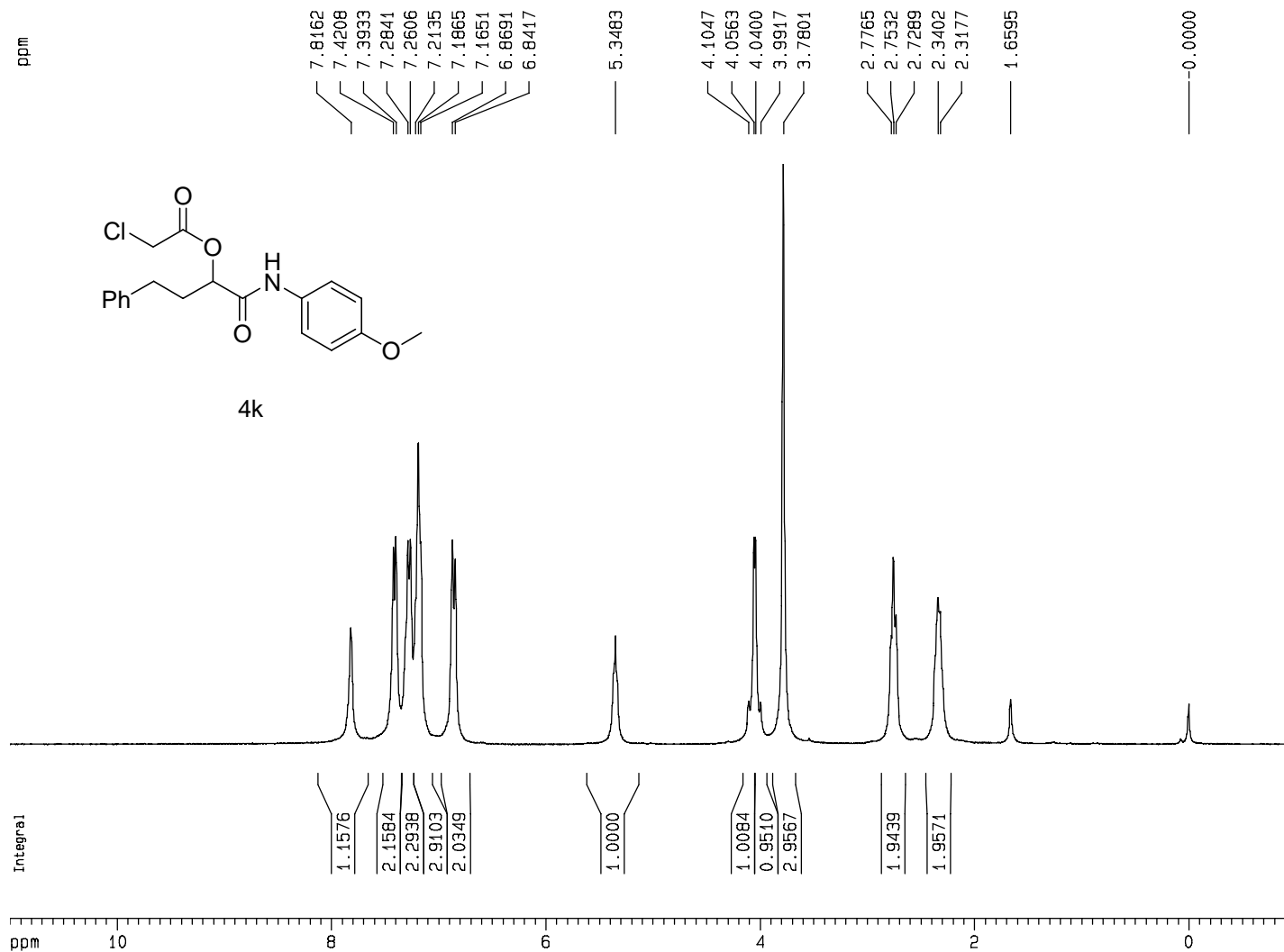
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F2 - Processing parameters

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SSB 0
LB 0.35 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 22.00 cm
CY 8.00 cm
F1P 11.000 ppm
F1 3301.43 Hz
F2P -1.000 ppm
F2 -300.13 Hz
PPMCM 0.54545 ppm/cm
HZCM 163.70728 Hz/cm



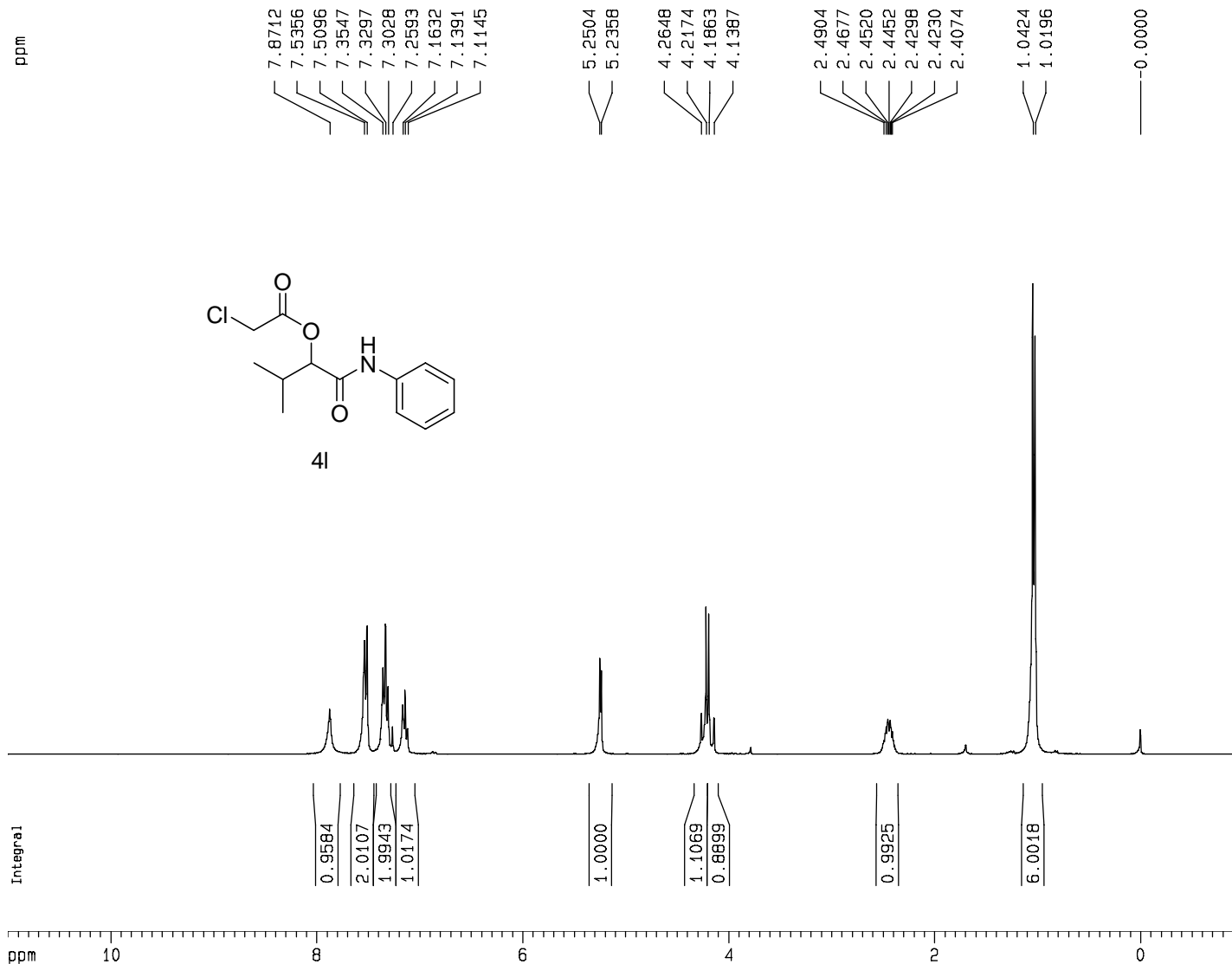
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 10
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 143.7
 DW 55.600 usec
 DE 6.00 usec
 TE 298.2 K
 D1 5.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.30 usec
 PL1 -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
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1D NMR plot parameters
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 CY 10.00 cm
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 F2P -1.000 ppm
 F2 -300.13 Hz
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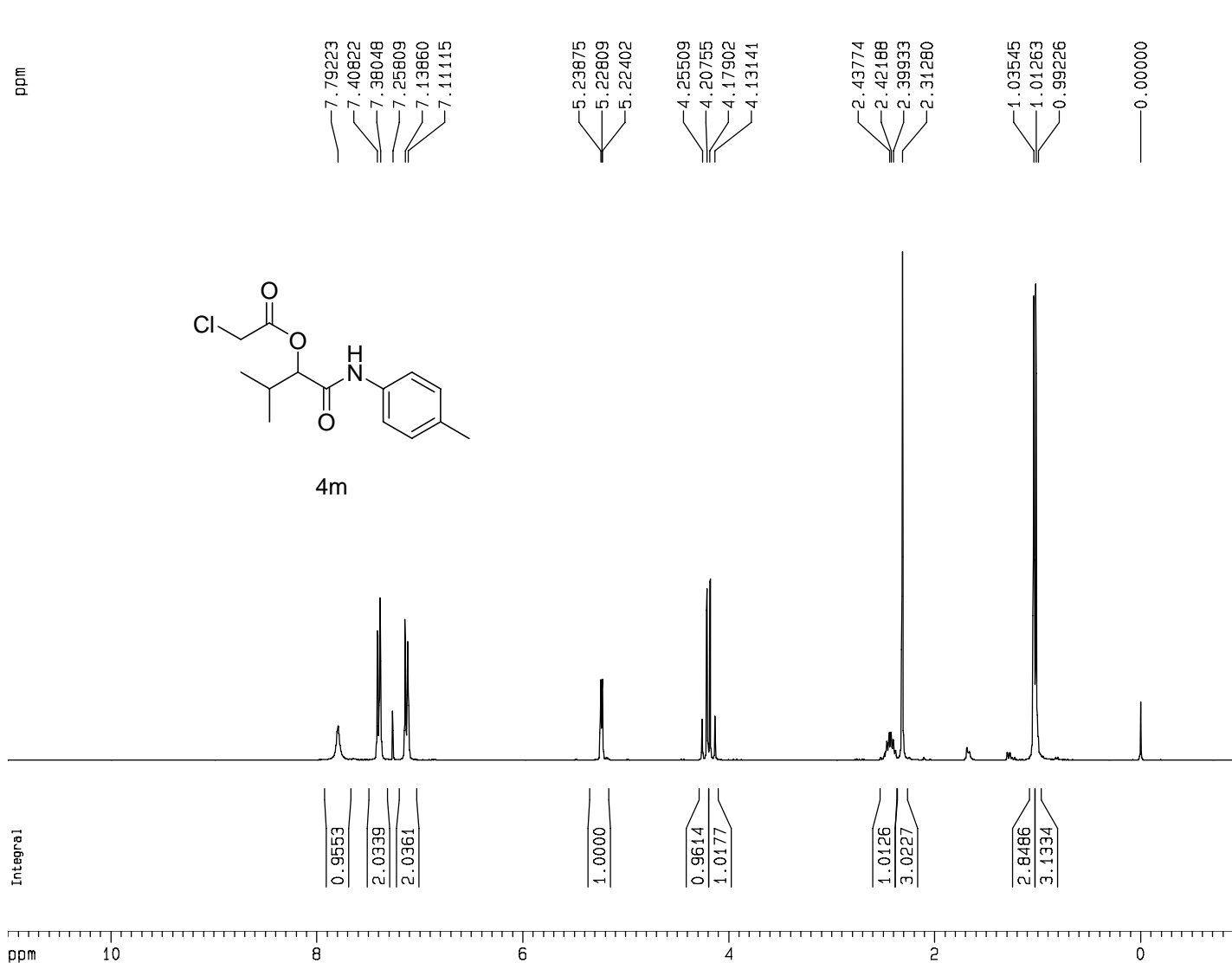
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 6
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 181
 DW 81.000 usec
 DE 6.00 usec
 TE 296.2 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
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 P1 9.30 usec
 PL1 -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
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 GB 0
 PC 1.00

1D NMR plot parameters
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 CY 8.00 cm
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 F2P -1.000 ppm
 F2 -300.13 Hz
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 HZCM 163.70728 Hz/cm



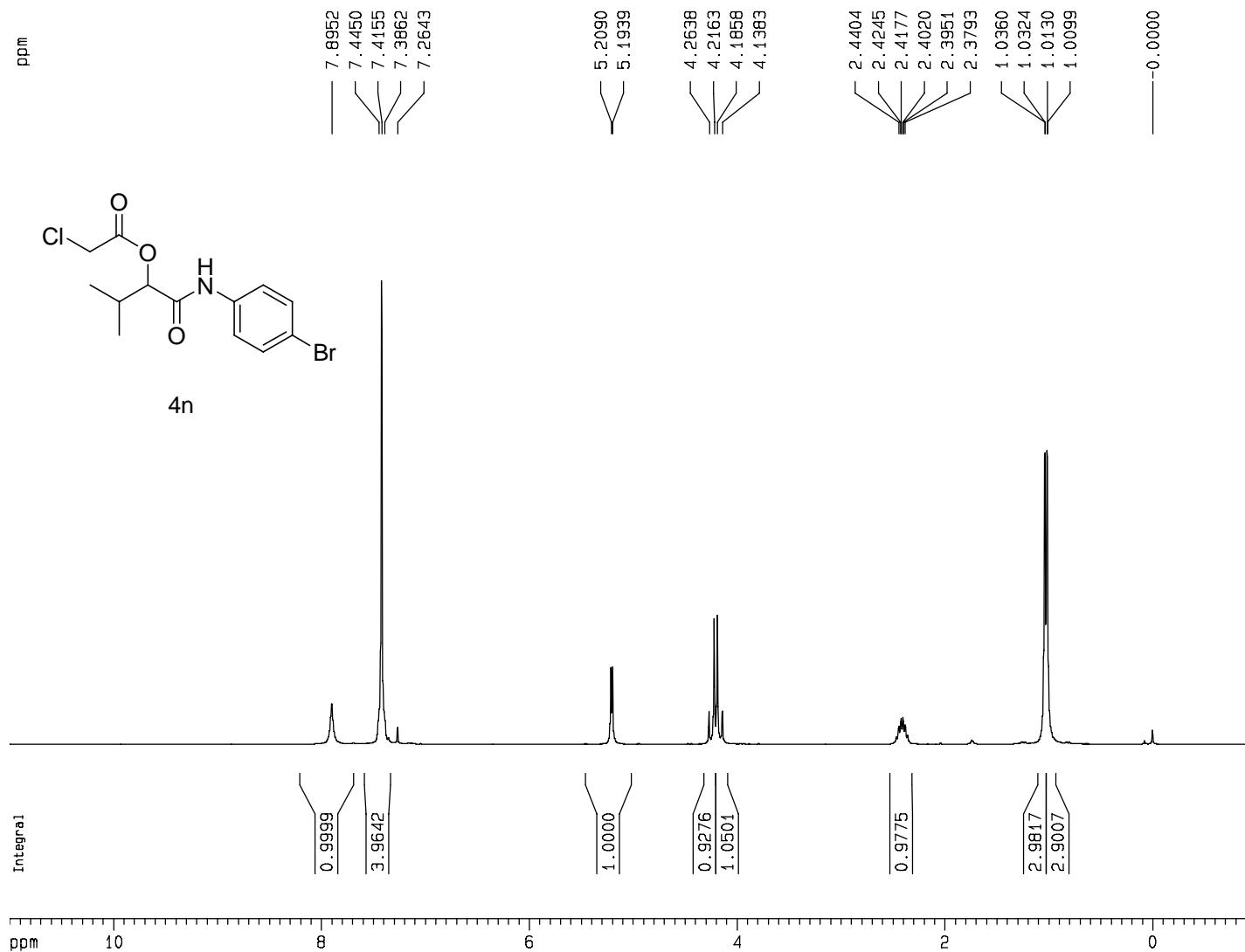
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 TD 65536
 SOLVENT CDC13
 NS 10
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 143.7
 DW 55.600 usec
 DE 6.00 usec
 TE 299.1 K
 D1 5.00000000 sec

===== CHANNEL f1 =====
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 P1 9.30 usec
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 SFO1 300.1318534 MHz

F2 - Processing parameters
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 WDW EM
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 PC 1.00

1D NMR plot parameters
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 CY 9.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.54545 ppm/cm
 HZCM 163.70728 Hz/cm



Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
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 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 181
 DW 81.000 usec
 DE 6.00 usec
 TE 302.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.30 usec
 PL1 -1.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
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 SF 300.1300049 MHz
 WDW EM
 SSB 0
 LB 0.35 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
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 CY 8.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
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 PPMCM 0.54545 ppm/cm
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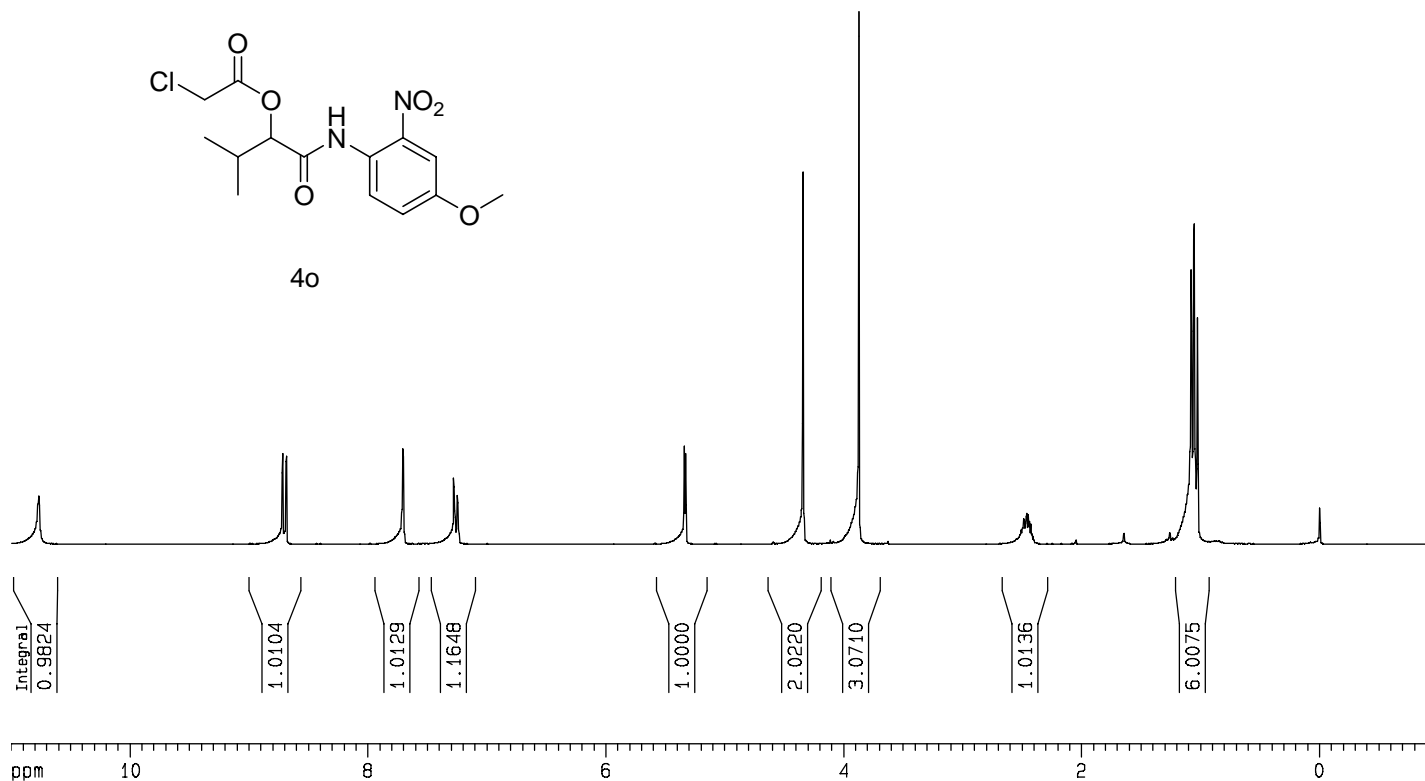
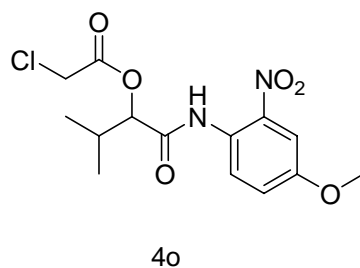
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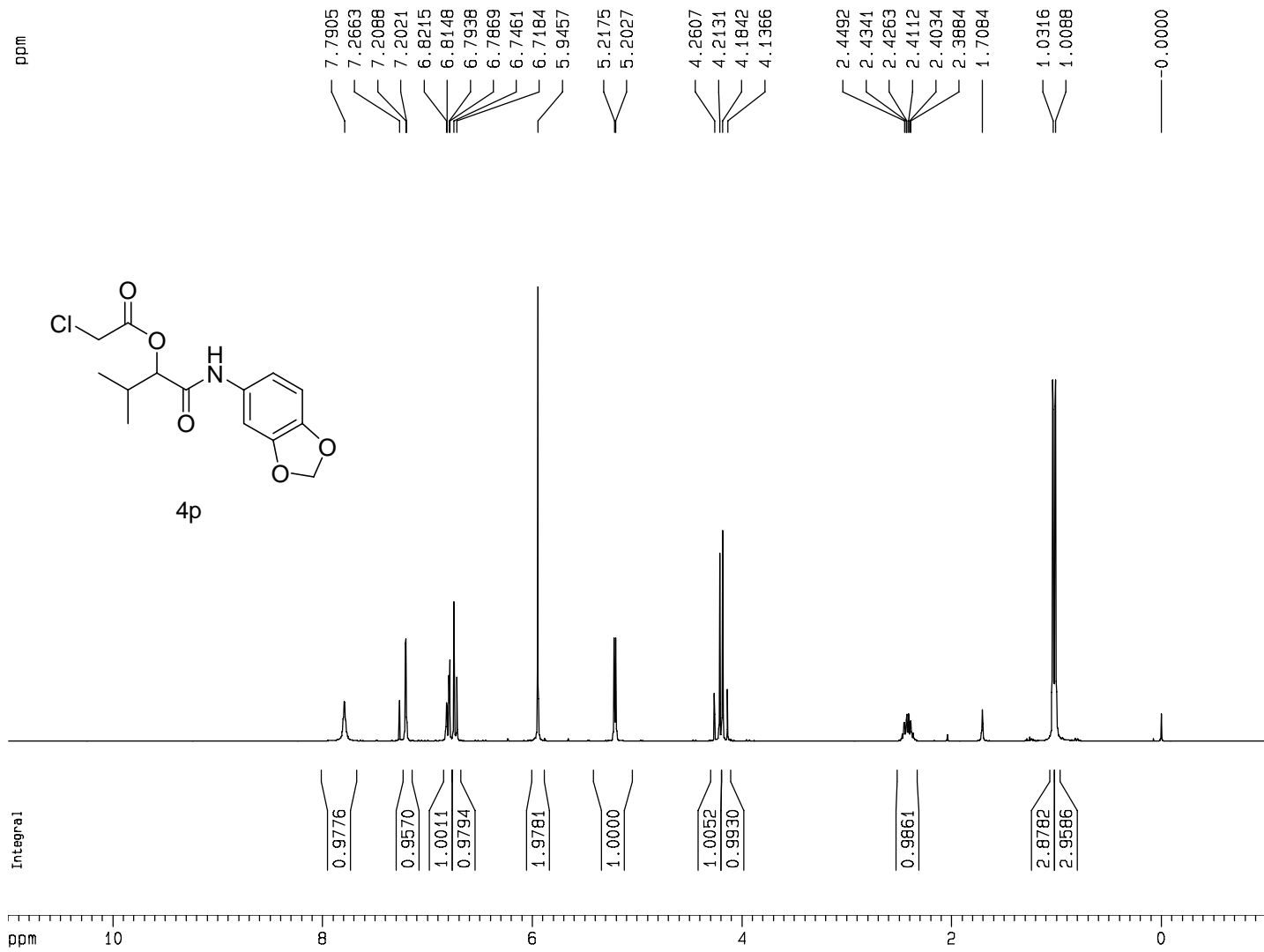
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TD 65536
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NS 6
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.30 usec
PL1 -1.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
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SF 300.1300020 MHz
WDW EM
SSB 0
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GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 11.000 ppm
F1 3301.43 Hz
F2P -1.000 ppm
F2 -300.13 Hz
PPMCM 0.54545 ppm/cm
HZCM 163.70728 Hz/cm



Current Data Parameters
 NAME wsx-0329-pcr27
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20070329
 Time 11.24
 INSTRUM av300
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 5
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 203.2
 DW 55.600 usec
 DE 6.00 usec
 TE 297.8 K
 D1 5.00000000 sec

===== CHANNEL f1 =====
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 P1 9.30 usec
 PL1 -1.00 dB
 SFO1 300.1318534 MHz

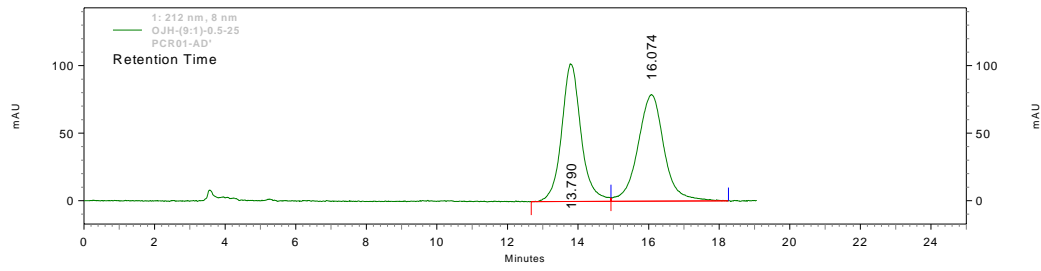
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1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.54545 ppm/cm
 HZCM 163.70728 Hz/cm

Chiral HPLC trace of 4a-4p

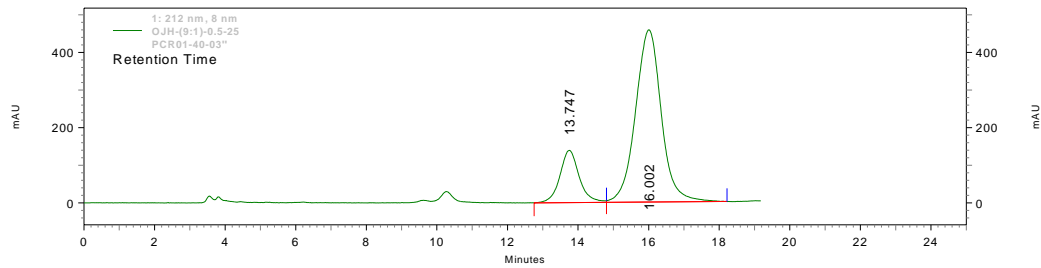
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4c	AD	Hex:IPA 9:1	0.8	25	24.2	43.4
4d	AD	Hex:IPA 9:1	0.8	25	14.6	19.6
4e	AD	Hex:IPA 9:1	0.8	25	19.7	34.9
4f	AD	Hex:IPA 9:1	0.8	25	24.1	47.2
4g	AD	Hex:IPA 9:1	0.8	25	19.0	32.0
4h	AD	Hex:IPA 9:1	0.8	25	23.2	37.5
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4j	AD	Hex:IPA 9:1	0.8	25	18.7	34.5
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4l	AD	Hex:IPA 9:1	0.8	25	10.0	14.2
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4n	AD	Hex:IPA 9:1	0.8	25	12.8	23.8
4o	AD	Hex:IPA 9:1	0.8	25	15.6	19.8
4p	AD	Hex:IPA 9:1	0.8	25	17.7	28.8

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4a	AD	Hex:IPA 9:1	0.8	25	13.8	16.1



1: 212 nm, 8 nm

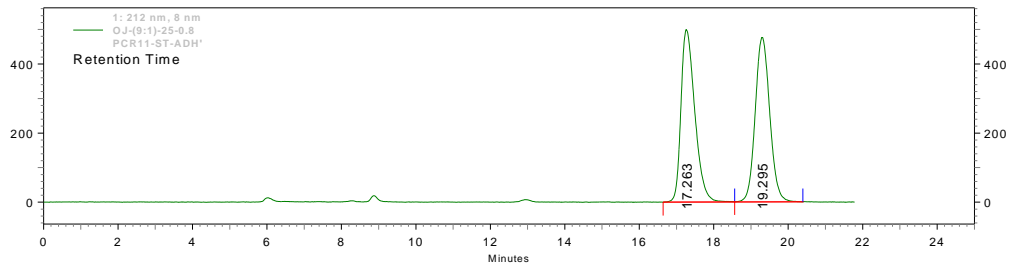
Pk #	Retention Time	Area	Area %
1	13.790	4881272	49.084
2	16.074	5063531	50.916
Totals		9944803	100.000



1: 212 nm, 8 nm

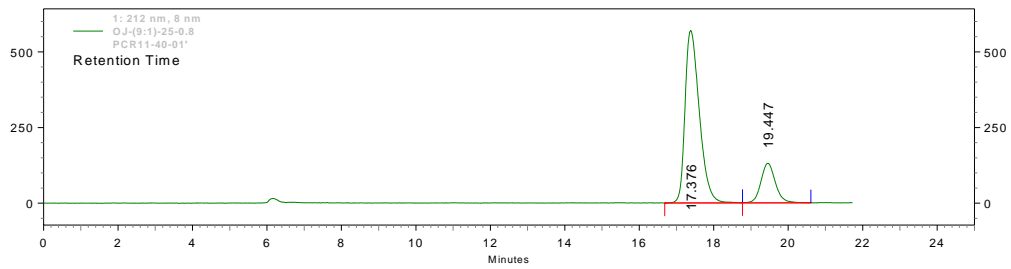
Pk #	Retention Time	Area	Area %
1	13.747	5258977	18.465
2	16.002	23221178	81.535
Totals		28480155	100.000

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4b	ADH	Hex:IPA 9:1	0.5	25	17.3	19.3



1: 212 nm, 8 nm

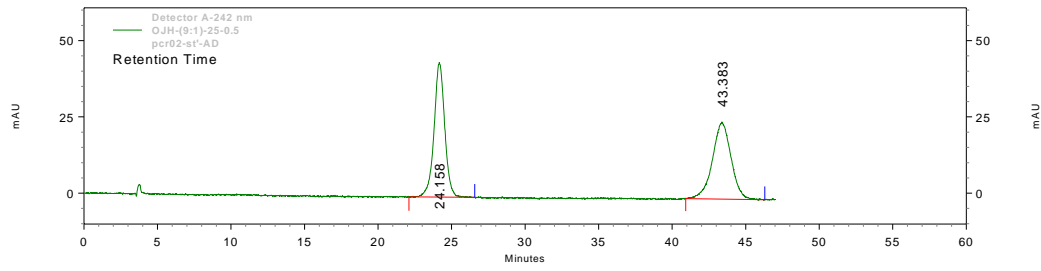
Pk #	Retention Time	Area	Area %
1	17.263	12907091	49.939
2	19.295	12938879	50.061
Totals		25845969	100.000



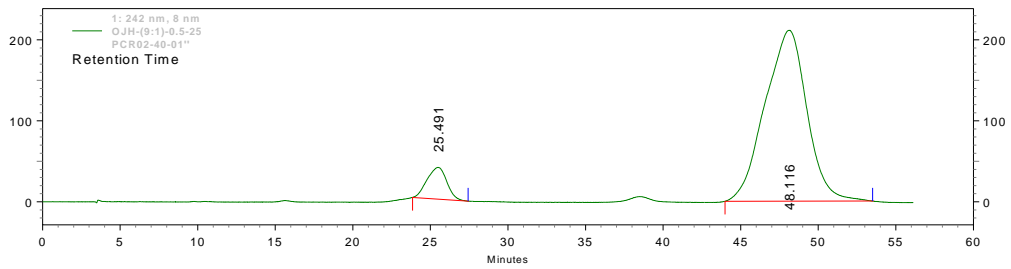
1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area %
1	17.376	15210639	81.182
2	19.447	3525863	18.818
Totals		18736501	100.000

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4c	ADH	Hex:IPA 9:1	0.5	25	24.2	43.4

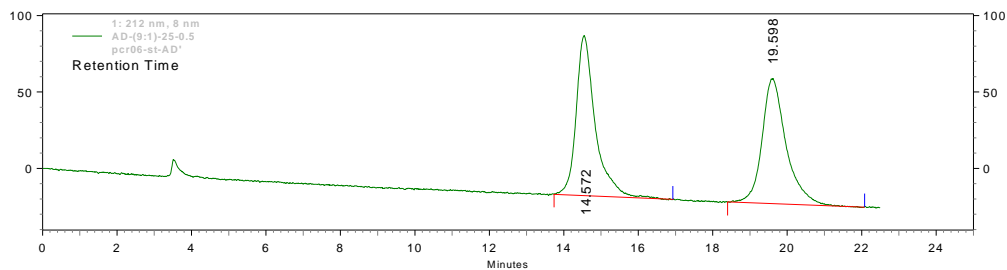


Detector A-242 nm			
Pk #	Retention Time	Area	Area %
1	24.158	2791172	50.201
2	43.383	2768770	49.799
Totals		5559943	100.000



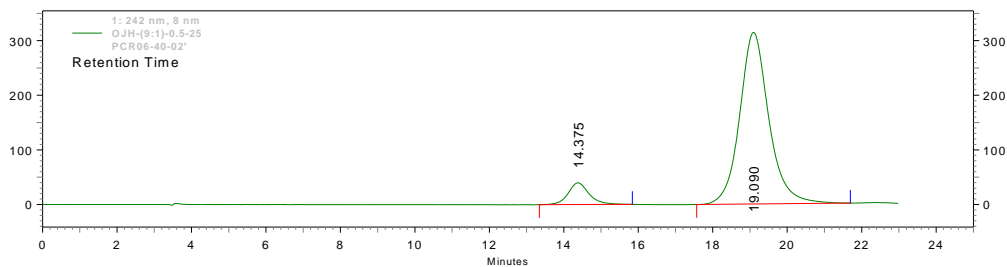
1: 242 nm, 8 nm			
Pk #	Retention Time	Area	Area %
1	25.491	3473069	8.059
2	48.116	39620287	91.941
Totals		43093356	100.000

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4d	AD	Hex:IPA 9:1	0.8	25	14.6	19.6



1: 212 nm, 8 nm

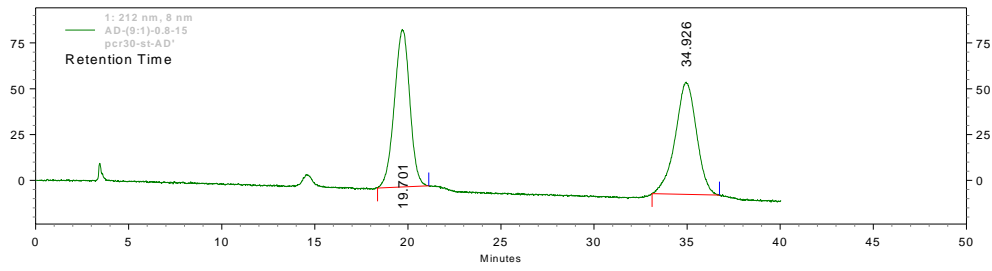
Pk #	Retention Time	Area	Area %
1	14.572	3732783	50.419
2	19.598	3670773	49.581
Totals		7403556	100.000



1: 212 nm, 8 nm

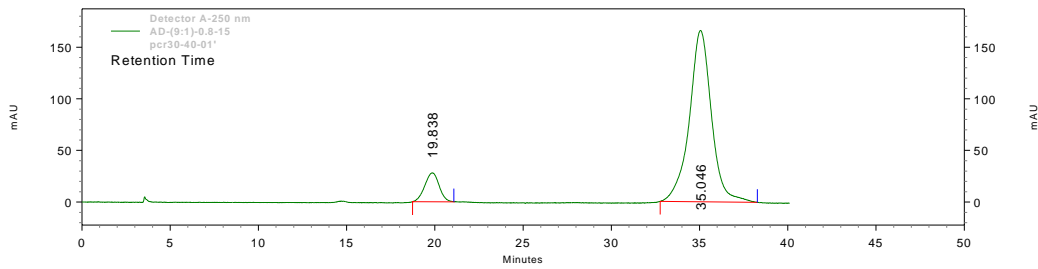
Pk #	Retention Time	Area	Area %
1	14.375	1563036	8.361
2	19.090	17130784	91.639
Totals		18693820	100.000

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4e	AD	Hex:IPA 9:1	0.8	25	19.7	34.9



1: 250 nm, 8 nm

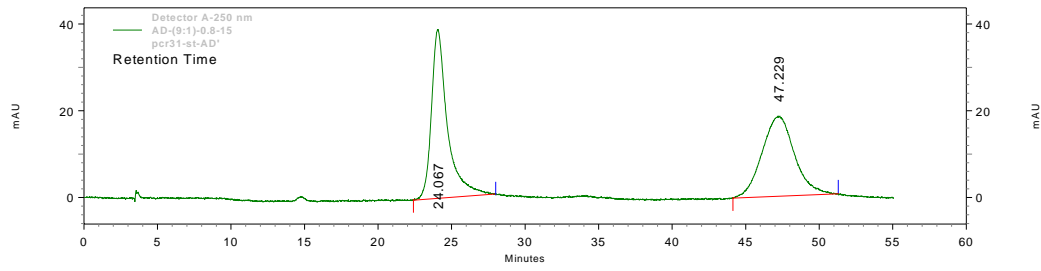
Pk #	Retention Time	Area	Area %
1	19.701	4939185	50.347
2	34.926	4871053	49.653
Totals		9810239	100.000



Detector A-250 nm

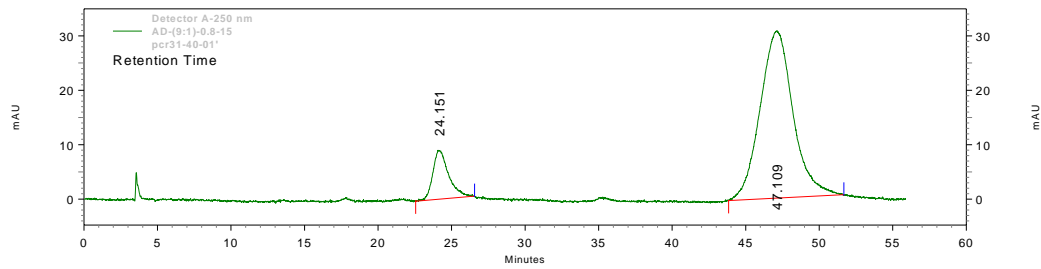
Pk #	Retention Time	Area	Area %
1	19.838	1587460	9.914
2	35.046	14425188	90.086
Totals		16012647	100.000

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4f	AD	Hex:IPA 9:1	0.8	25	24.1	47.2



Detector A-250 nm

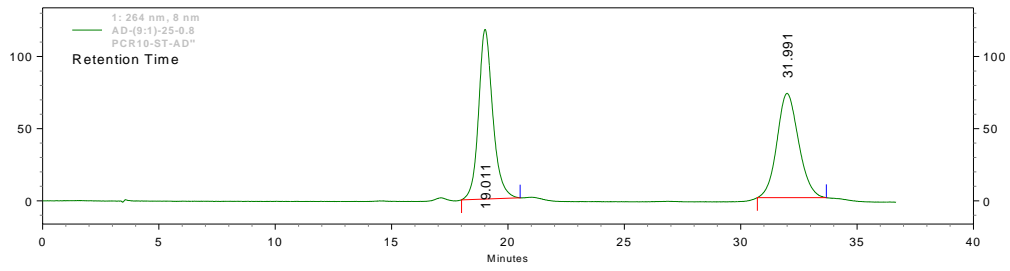
Pk #	Retention Time	Area	Area %
1	24.067	2932848	50.938
2	47.229	2824814	49.062
Totals		5757662	100.000



Detector A-250 nm

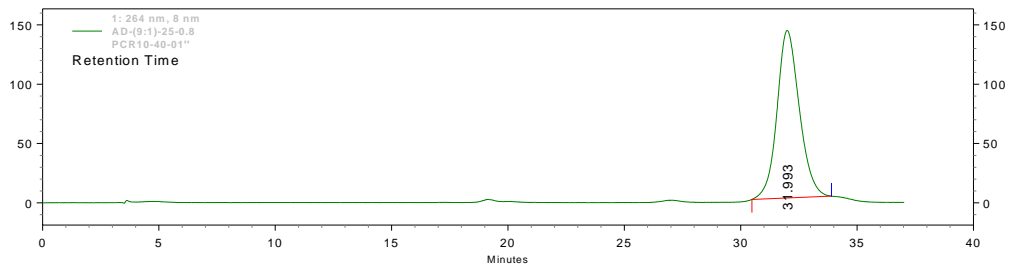
Pk #	Retention Time	Area	Area %
1	24.151	668451	12.302
2	47.109	4765085	87.698
Totals		5433536	100.000

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4g	AD	Hex:IPA 9:1	0.8	25	19.0	32.0



1: 254 nm, 8 nm

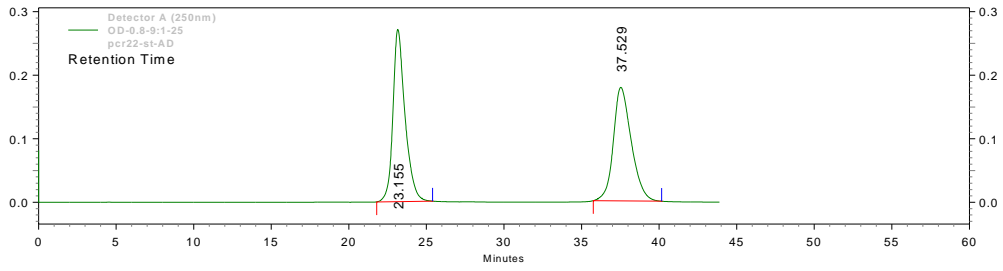
Pk #	Retention Time	Area	Area %
1	19.0	4988111	51.7
2	32.0	4664467	48.3
Totals		9652578	100.0



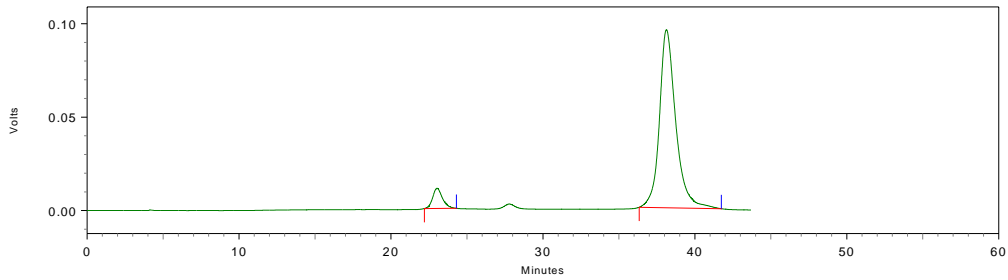
1: 254 nm, 8 nm

Pk #	Retention Time	Area	Area %
1	32.0	9422383	100.0
Totals		9422383	100.0

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4h	AD	Hex:IPA 9:1	0.8	25	23.2	37.5

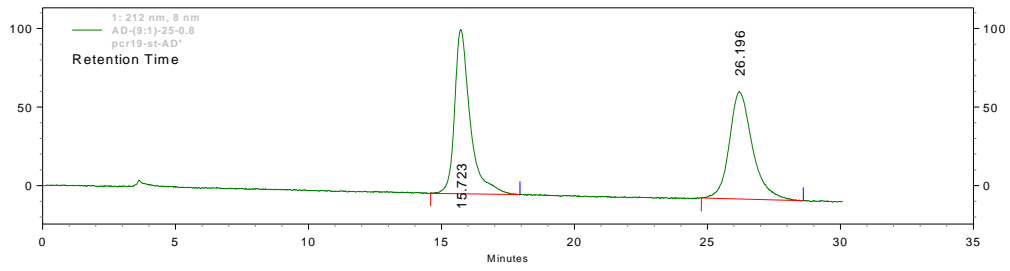


Detector A (250nm)		Pk #	Retention Time	Area	Area %
	1	23.155	14748792	50.641	
	2	37.529	14375651	49.359	
Totals			29124443	100.000	



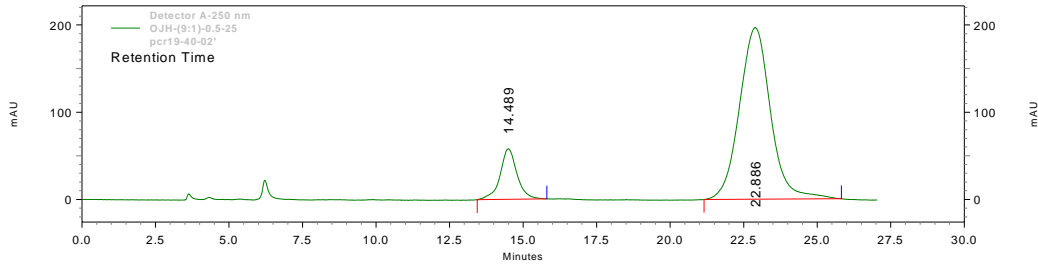
Detector A (250nm)		Pk #	Retention Time	Area	Area %
	1	23.153	810893	6.412	
	2	38.126	11836533	93.588	
Totals			12647427	100.000	

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4i	AD	Hex:IPA 9:1	0.8	25	15.7	26.2



1: 250 nm, 8 nm

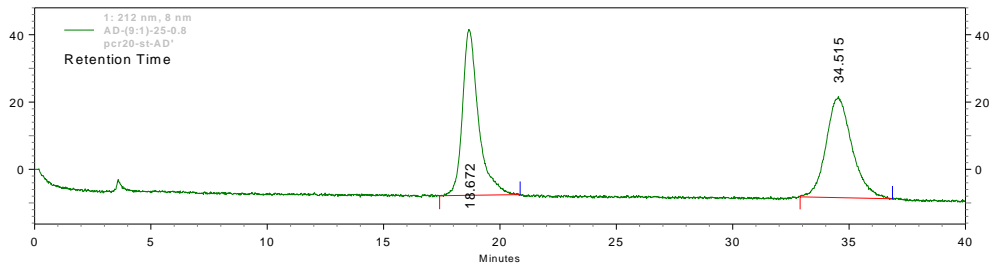
Pk #	Retention Time	Area	Area %
1	15.723	4241107	50.739
2	26.196	4117589	49.261
Totals		8358696	100.000



Detector A-250 nm

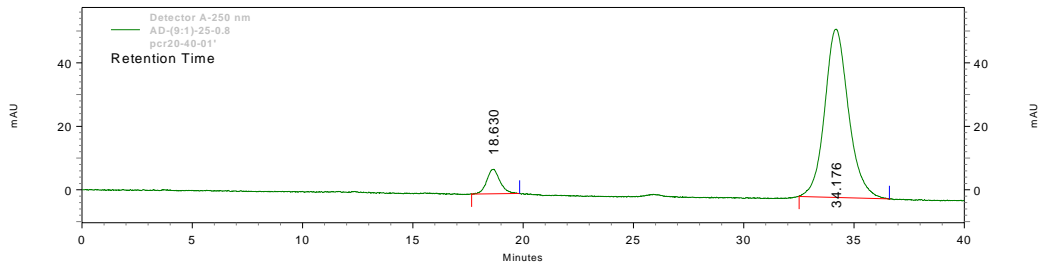
Pk #	Retention Time	Area	Area %
1	14.5	2318017	13.8
2	22.9	14466452	86.2
Totals		16784468	100.0

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4j	AD	Hex:IPA 9:1	0.8	25	18.7	34.5



1: 250 nm, 8 nm

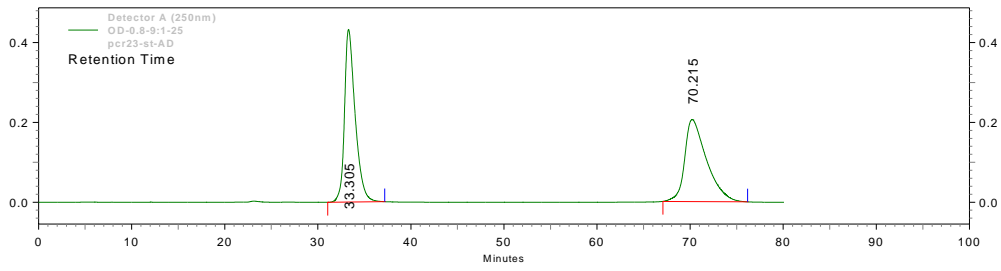
Pk #	Retention Time	Area	Area %
1	18.672	2355186	50.458
2	34.515	2312388	49.542
Totals		4667574	100.000



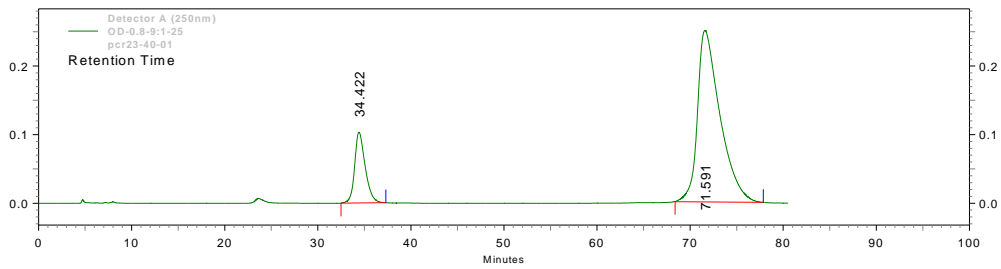
Detector A-250 nm

Pk #	Retention Time	Area	Area %
1	18.630	323199	7.500
2	34.176	3986296	92.500
Totals		4309495	100.000

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4k	AD	Hex:IPA 9:1	0.8	25	33.3	70.2

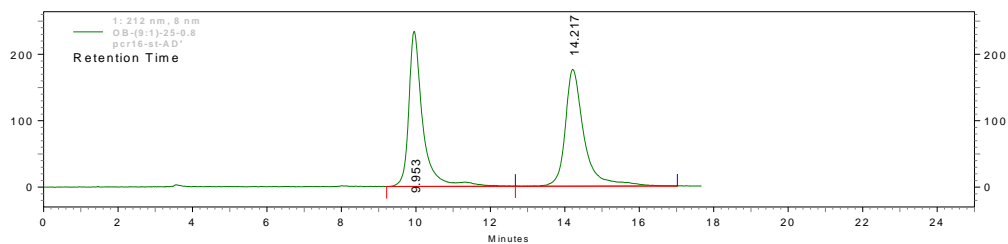


Detector A (250nm)				
	Pk #	Retention Time	Area	Area %
	1	33.305	34512363	50.647
	2	70.215	33630600	49.353
Totals			68142962	100.000



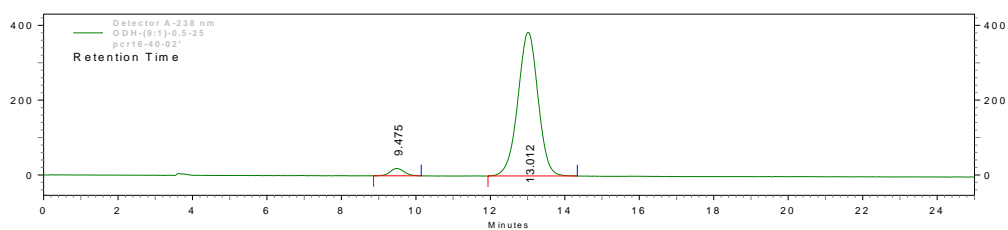
Detector A (250nm)				
	Pk #	Retention Time	Area	Area %
	1	34.422	8147607	16.267
	2	71.591	41937841	83.733
Totals			50085448	100.000

Compound	Column	chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4I	AD		Hex:IPA 9:1	0.8	25	10.0	14.2



1: 238nm, 8 nm

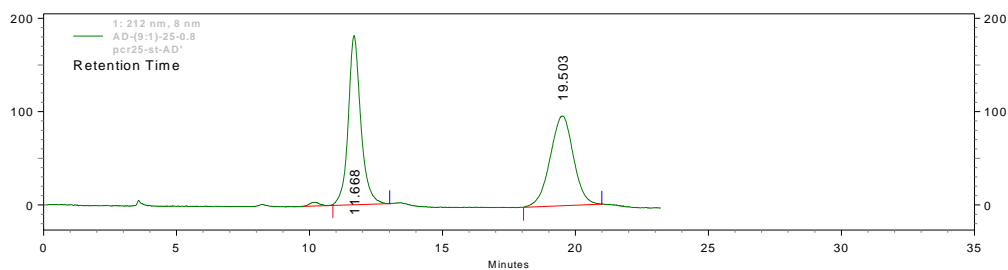
Pk #	Retention Time	Area	Area %
1	9.953	6099220	49.728
2	14.217	6165953	50.272
Totals		12265173	100.000



1: 238 nm, 8 nm

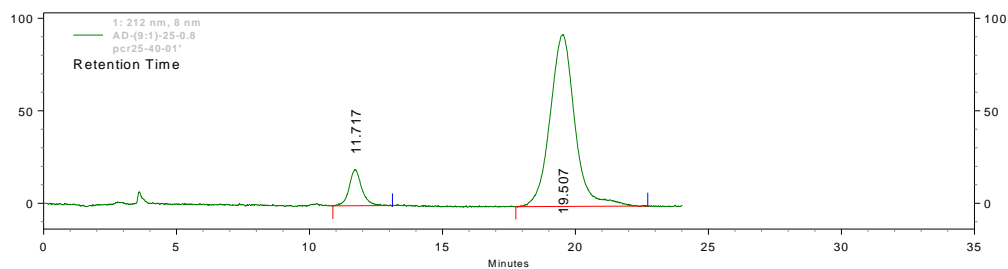
Pk #	Retention Time	Area	Area %
1	9.5	507462	3.4
2	13.0	14328718	96.6
Totals		14836180	100.0

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4m	AD	Hex:IPA 9:1	0.8	25	11.7	19.5



1: 212 nm, 8 nm

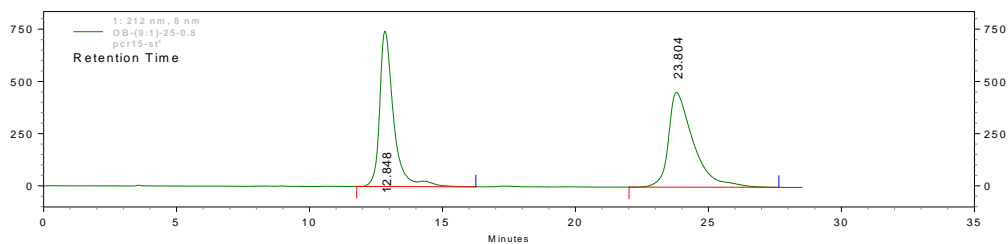
Pk #	Retention Time	Area	Area %
1	11.668	5951047	50.451
2	19.503	5844601	49.549
Totals		11795648	100.000



1: 212 nm, 8 nm

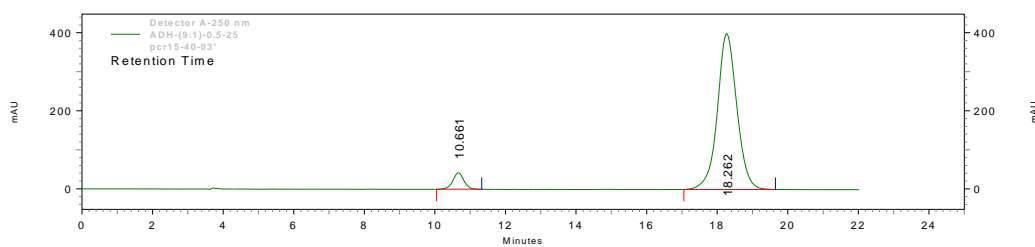
Pk #	Retention Time	Area	Area %
1	11.717	643961	9.715
2	19.507	5984493	90.285
Totals		6628454	100.000

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4n	AD	Hex:IPA 9:1	0.8	25	12.8	23.8



1: 250 nm, 8 nm

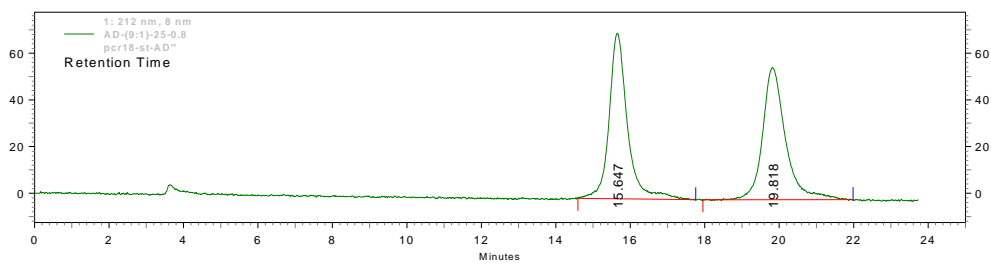
Pk #	Retention Time	Area	Area %
1	12.848	27197580	47.963
2	23.804	29508336	52.037
Totals		56705916	100.000



Detector A-250 nm

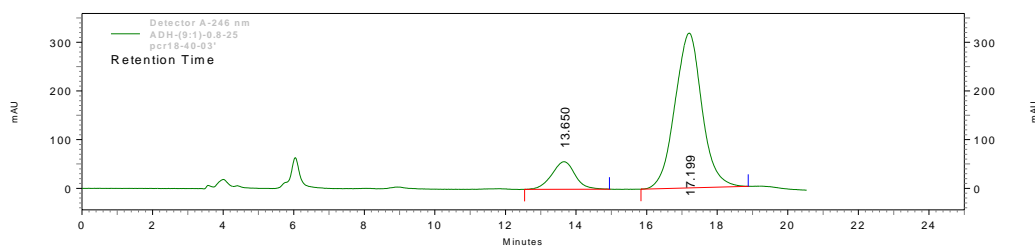
Pk #	Retention Time	Area	Area %
1	10.7	922826	5.7
2	18.3	15315058	94.3
Totals		16237884	100.0

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4o	AD	Hex:IPA 9:1	0.8	25	15.6	19.8



1: 246 nm, 8 nm

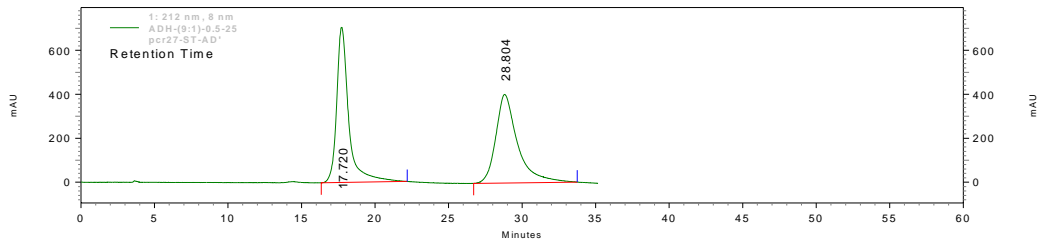
Pk #	Retention Time	Area	Area %
1	15.647	2426032	50.047
2	19.818	2421487	49.953
Totals		4847519	100.000



Detector A-246 nm

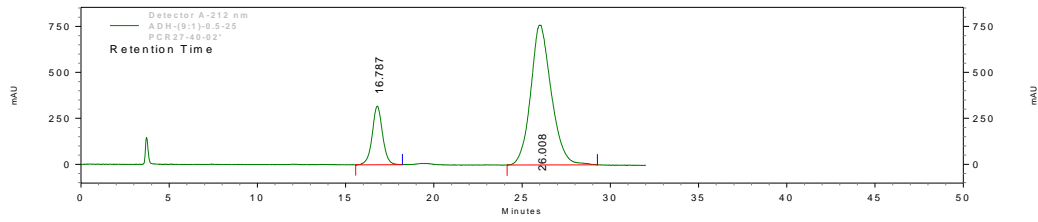
Pk #	Retention Time	Area	Area %
1	13.6	2593074	13.3
2	17.2	16896950	86.7
Totals		19490024	100.0

Compound	Column chiralcel	Mobile phase	MI / min	T °C	t ₁ min	t ₂ min
4p	AD	Hex:IPA 9:1	0.8	25	17.7	28.8



1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area %
1	17.741	36844770	49.709
2	28.818	37275504	50.291
Totals		74120275	100.000



1: 212 nm, 8 nm

Pk #	Retention Time	Area	Area %
1	16.8	2968221	16.4
2	26.0	15172772	83.6
Totals		18140993	100.0