

Organocatalytic Enantioselective Synthesis of Both Diastereomers of α -Hydroxyphosphinates

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Supporting Information

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Full citation of References 4a and 4b

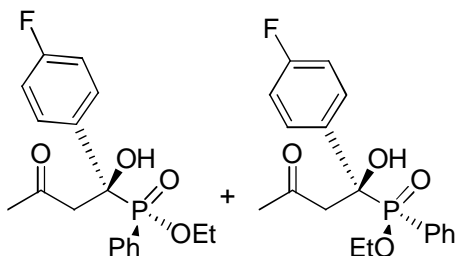
- (a) Froestl, W.; Mickel, S. J.; Hall, R. G.; von Sprecher, G.; Strub, D.; Baumann, P. A.; Brugger, F.; Gentsch, C.; Jaekel, J.; Olpe, H.-R.; Rihs, G.; Vassout, A.; Waldmeier, P. C.; Bittiger, H. *J. Med. Chem.* **1995**, *38*, 3297-

3312. (b) Froestl, W.; Mickel, S. J.; von Sprecher, G.; Diel, P. J.; Hall, R. G.; Maier, Lu.; Strub, D.; Melillo, V.; Baumann, P. A.; Bernasconi, R.; Gentsch, C.; Hauser, K.; Jaekel, J.; Karlsson's, G.; Klebs, K.; Maitre, L.; Marescaux, C.; Pozza, M. F.; Schmutz, M.; Steinmann, M. W.; van Riezen, H.; Vassout, A.; Mondadori, C.; Olpe, H.-R.; Waldmeier, P. C.; Bittiger, H. *J. Med. Chem.* **1995**, *38*, 3313-3331.

General Experimental Methods

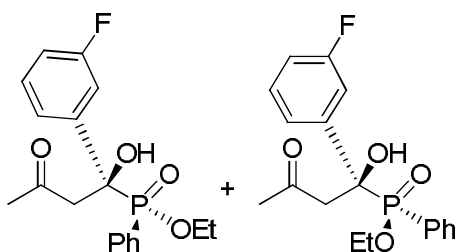
Unless otherwise noted, ^1H , ^{13}C , and ^{31}P NMR spectra were obtained on a 500 MHz spectrometer using residual solvent as the standard [^{31}P chemical shifts are reported in ppm relative to 85% H_3PO_4 (external standard)]. IR spectra were recorded on VECTOR 22 model Specac ATR instrument. Melting points were recorded on MEL-TEMP melting point apparatus in open capillaries and uncorrected. TLC was performed with silica gel GF₂₅₄ precoated on aluminum plates (EM Sciences), and spots were visualized with UV and/or iodine vapor. Flash column chromatography was performed on silica-gel. HPLC analysis was performed on a Shimadzu instrument with LC-10AT pump and SPD-10AV UV-Vis detector. ChiralCel and ChiralPak HPLC columns were purchased from Daicel Chemical Industry, Ltd. Microanalyses were conducted by Atlantic Microlab, Inc (PO Box 2288, Norcross, Georgia 30091, USA). Compounds used in this study were purchased from Aldrich, Alfa-Aesar, Acros, TCI, or Strem, and were used as received. Catalysts **2** and **3** were prepared by using the reported procedures.²⁰ THF was freshly distilled from benzophenone and sodium metal. CH_2Cl_2 and DMF were distilled from CaH_2 . Unless otherwise specified, all reactions were carried out in oven-dried glassware.

Characterization Data



Ethyl [1-(4-fluorophenyl)-1-hydroxy-3-oxobutyl](phenyl)phosphinate (7b/8b):

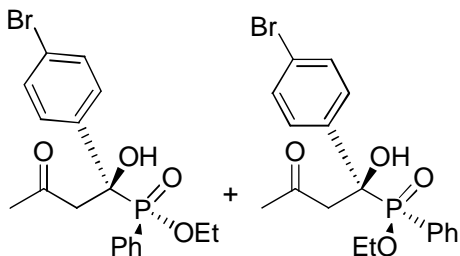
white powder, mp 89-90 °C ; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 1.27 and 1.32 (t, $J = 7.0$ Hz, 3 H), 2.03 and 2.15 (s, 3 H), 3.05 and 3.09 (d, $J = 8.0$ and 8.5 Hz, 0.5 H), 3.37-3.51 (m, 1.5 H), 3.74-4.16 (m, 2 H), 5.06 and 5.15 (d, $J = 18.0$ and 13.5 Hz, 1 H), 6.80-7.62 (m, 9 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 16.6 (q), 32.5 (q), 46.3 and 46.8 (d), 62.2 (q), 76.2 and 76.4 (d, $J_{\text{CP}} = 120.6$ and 118.8 Hz), 114.9 (q), 115.0 (q), 126.7(q), 128.0 (q), 128.4 (q), 132.8 (q), 133.7 (q), 135.2 (q), 161.3 and 163.5 (d), 210.1 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 36.0, 37.3; ν_{max} (neat, cm^{-1}): 3156, 1724, 1601, 1507, 1438, 1355; Anal. Calcd. for $\text{C}_{18}\text{H}_{20}\text{FO}_4\text{P}$: C, 61.71; H, 5.75; Found: C, 61.99; H, 5.79.



Ethyl [1-(3-fluorophenyl)-1-hydroxy-3-oxobutyl](phenyl)phosphinate (7c/8c):

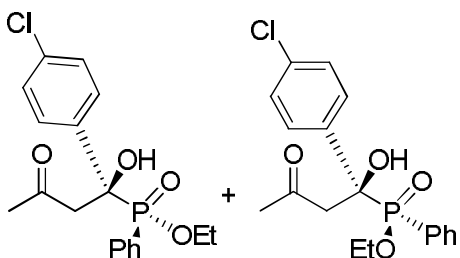
white powder, mp 75-76 °C; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 1.15 and 1.35 (t, $J = 7.0$ Hz, 3 H), 2.06 and 2.18 (s, 3 H), 3.07 and 3.10 (d, $J = 8.0$ Hz, 0.5 H), 3.39-3.53 (m, 1.5 Hz), 3.70-4.15 (m, 2 H), 5.06 and 5.16 (2 br s, 1 H), 6.81-7.65 (m, 9 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 16.6

(q), 32.4, (q), 46.7 (q), 62.3 (q), 76.3 and 76.5 (d, $J_{CP} = 121.5$ and 122.5 Hz), 113.5 (q), 114.6 (q), 121.9 (q), 126.9 (q), 128.3 (q), 129.5 (q), 132.8 (q), 133.6 (q), 142.2 (q), 161.7 and 163.8 (d), 209.8 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 38.1, 39.5; ν_{max} (neat, cm^{-1}): 3170, 1723, 1601, 1507, 1357; Anal. Calcd. for $\text{C}_{18}\text{H}_{20}\text{FO}_4\text{P}$: C, 61.71; H, 5.75; Found: C, 61.73; H, 5.82.



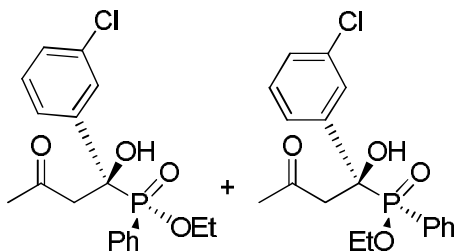
Ethyl [1-(4-bromophenyl)-1-hydroxy-3-oxobutyl](phenyl)phosphinate (7d/8d):

Colorless needles mp 95-97 °C; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 1.14 and 1.34 (t, $J = 7.0$ Hz, 3 H), 2.05 and 2.17 (s, 3 H), 3.04 and 3.08 (d, $J = 8.5$ and 7.5 Hz, 0.5 H), 3.33-3.51 (m, 1.5 H), 3.75-3.18 (m, 2 H), 5.02 and 5.14 (d, $J = 19.5$ and 17.5 Hz, 1 H), 7.15-7.65 (m, 9 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 16.6 (q), 32.5 (q), 62.3 (q), 76.4 and 76.5 (d, $J_{CP} = 120.1$ and 118.3 Hz), 122.0 (q), 126.7 (q), 128.1 (q), 128.7 (q), 131.2 (q), 132.8 (q), 133.7 (q), 138.5 (q), 210.1 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 37.8, 38.1; ν_{max} (neat, cm^{-1}): 3282, 1722, 1590, 1480, 1438, 1394, 1353; Anal. Calcd. for $\text{C}_{18}\text{H}_{20}\text{BrO}_4\text{P}$: C, 52.57; H, 4.90; Found: C, 52.63; H, 4.89.



Ethyl [1-(4-chlorophenyl)-1-hydroxy-3-oxobutyl](phenyl)phosphinate (7e/8e):

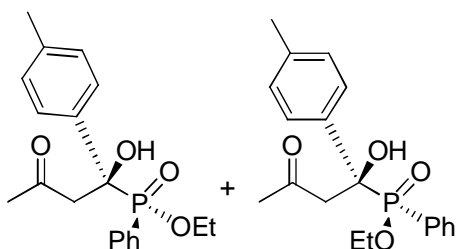
Colorless crystalline square, mp 118-119 °C; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 1.13 and 1.31 (t, $J = 7.0$ Hz, 3H), 2.02 and 2.13 (s, 3 H), 3.10 and 3.13 (d, $J = 8.5$ Hz, 0.5 H), 3.35-3.50 (m, 1.5 H), 3.75-4.15 (m, 2 H), 5.23 (br s, 1 H), 7.09-7.63 (m, 9 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 16.6 and 16.7 (d), 32.4 (q), 62.3 (q), 76.2 and 76.5 (d, $J_{\text{CP}} = 120.3$ and 123.0 Hz), 126.4 (q), 127.7 (q), 128.2 (q), 128.3 (q), 132.8 (q), 133.4 (q), 137.9 (q), 209.8 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 38.0, 39.3; ν_{max} (neat, cm^{-1}): 3147, 1723, 1591, 1489, 1439, 1406, 1356; Anal. Calcd. for $\text{C}_{18}\text{H}_{20}\text{ClO}_4\text{P}$: C, 58.94; H, 5.50; Found: C, 58.74; H, 5.47.



Ethyl [1-(3-chlorophenyl)-1-hydroxy-3-oxobutyl](phenyl)phosphinate (7f/8f):

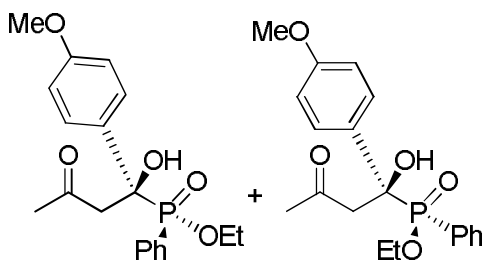
white powder, mp 110-111 °C; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 1.15 and 1.35 (t, $J = 7.0$ Hz, 3 H), 2.07 and 2.19 (s, 3 H), 3.07 and 3.11 (d, $J = 8.0$ and 8.5 Hz, 0.5 H), 3.37-3.51 (m, 1.5 H), 3.77-4.19 (m, 2 H), 5.04 and 5.16 (d, $J = 19.0$ and 16.0 Hz, 1 H), 7.10-7.65 (m, 9 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 16.5 (q), 32.4 (q), 46.6 (q), 62.4 (q), 76.3 and 76.5 (d, $J_{\text{CP}} = 120.2$ and 122.5 Hz), 124.4 and 124.8 (d), 126.6 and 127.1 (d), 127.8 and 127.9 (d), 128.0 and 128.1 (d), 128.1 and 128.2 (d), 129.3 and 129.4 (d), 132.8 and 133.0 (d), 133.4 and 133.8 (d), 141.6 and 141.9 (d), 209.9 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers)

37.8, 39.2; ν_{\max} (neat, cm^{-1}): 3144, 1721, 1591, 1489, 1440, 1410 cm^{-1} ; Anal. Calcd. for $\text{C}_{18}\text{H}_{20}\text{ClO}_4\text{P}$: C, 58.94; H, 5.50; Found: C, 58.84; H, 5.43.



Ethyl [1-hydroxy-1-(4-methylphenyl)-3-oxobutyl](phenyl)phosphinate (7g/8g):

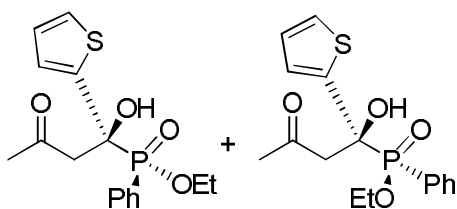
Crystalline solid, mp 101-102 °C; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 1.12 and 1.32 (t, $J = 7.0$ Hz, 3 H), 2.01 and 2.11 (s, 3 H), 2.21 and 2.30 (s, 3 H), 3.02-3.07 (m, 0.5 H), 3.36-3.54 (m, 1.5 H), 3.72-4.15 (m, 2 H), 4.94-5.03 (br s, 1 H), 6.99-7.63 (m, 9 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 16.6 (q), 32.5 (q), 46.5 and 47.0 (d), 62.1 (d), 76.4 and 76.5 (d, $J_{\text{CP}} = 120.6$ and 121.3 Hz), 126.1 (q), 126.5 (q), 127.4 (q), 128.9 (q), 132.5 (q), 133.5 (q), 136.1 (q), 137.4 (q), 210.1 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 38.2, 39.6; ν_{\max} (neat, cm^{-1}): 3228, 1702, 1592, 1510, 1474, 1439, 1411, 1388, 1356; Anal. Calcd. for $\text{C}_{19}\text{H}_{23}\text{O}_4\text{P}$: C, 65.89; H, 6.69; Found: C, 66.15; H, 6.78.



Ethyl [1-hydroxy-1-(4-methoxyphenyl)-3-oxobutyl](phenyl)phosphinate (7h/8h):

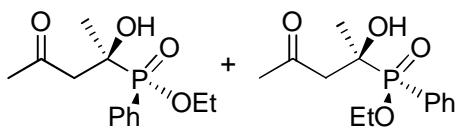
Colorless needles, mp 103-105 °C; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 1.14 and 1.34 (t, $J = 7.0$ Hz, 3 H), 2.04 and 2.15 (s, 3 H), 3.01 and 3.02 (d, $J = 8.5$ Hz, 0.5 H), 3.36-3.57 (m, 1.5 H), 3.71-4.16 (m, 5 H), 4.88 and 5.01 (d, $J = 18.0$

and 15.5 Hz, 1 H), 6.68 and 6.84 (d, $J = 8.5$ Hz, 2 H), 7.17-7.65 (m, 7 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 16.7 (q), 32.6 (d), 46.3 and 46.8 (d), 55.4 (d), 62.1 (q), 76.3 and 76.4 (d, $J_{\text{CP}} = 121.5$ and 120.3 Hz), 113.5 (q), 126.9 (q), 127.5 (q), 128.2 (q), 131.1 (q), 132.5 (q), 133.5 (q), 159.1 (q), 210.3 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 38.3, 39.7; ν_{max} (neat, cm^{-1}): 3241, 1701, 1598, 1510, 1439, 1412, 1378, 1361; Anal. Calcd. for $\text{C}_{19}\text{H}_{23}\text{O}_5\text{P}$: C, 62.98; H, 6.40; Found: C, 62.76; H, 6.41.

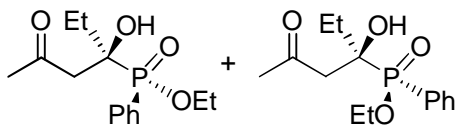


Ethyl [1-hydroxy-3-oxo-1-(thiophen-2-yl)butyl](phenyl)phosphinate (7i/8i):

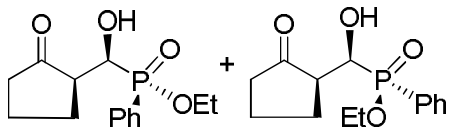
Yellowish solid, mp 89-90 °C; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 1.21 and 1.35 (t, $J = 7.0$ Hz, 3 H), 2.10 and 2.20 (s, 3 H), 3.05 (dd, $J_1 = 8.0$, $J_2 = 16.5$ Hz, 0.5 H), 3.37-3.48 (m, 1.5 H), 3.85-4.21 (m, 2 H), 5.47 and 5.53 (d, $J = 21.5$ and 18.5 Hz, 1 H), 6.84-7.71 (m 8 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 16.6 (q), 32.6 (q), 46.7 and 47.4 (d), 62.5 (q), 76.1 and 76.4 (d, $J_{\text{CP}} = 125.0$ and 123.5 Hz), 125.1 (q), 125.8 (q), 126.5 (q), 127.3 (q), 128.4 (q), 132.9 (q), 133.7 (q), 144.1 (q), 210.2 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 36.5, 37.9; ν_{max} (neat, cm^{-1}): 3219, 1715, 1591, 1442; Anal. Calcd. for $\text{C}_{16}\text{H}_{19}\text{O}_4\text{PS}$: C, 56.80; H, 5.66. Found: C, 56.81; H, 5.65.



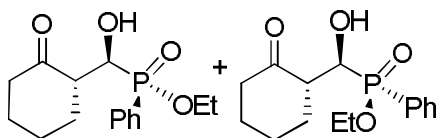
Ethyl (1-hydroxy-1-methyl-3-oxobutyl)(phenyl)phosphinate (7j/8j): Colorless oil; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 1.26 and 1.48 (d, $J = 16.5$ and 14.0 Hz, 3 H), 1.28 and 1.32 (t, $J = 7.5$ and 7.0 Hz, 3 H), 2.17 and 2.26 (s, 3 H), 2.54-2.66 (m, 1 H), 2.92 and 3.20 (dd, $J_1 = 8.5$, $J_2 = 16.5$ Hz, 1 H), 3.85-4.16 (m, 2 H), 4.62 and 4.88 (d, $J = 11.5$ and 9.0 Hz, 1 H), 7.45-7.56 (m, 3 H), 7.80-7.86 (m, 2 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 16.7 (q), 23.0 (q), 32.5 (q), 46.9 (q), 61.8 (q), 72.6 and 72.7 (d, $J_{\text{CP}} = 120.3$ and 122.5 Hz), 127.8 (q), 128.6 (q), 132.8 (q), 133.7 (q), 210.3 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 39.6, 40.6; ν_{max} (neat, cm^{-1}): 3191, 1712, 1592, 1479, 1439, 1368; Anal. Calcd. for $\text{C}_{13}\text{H}_{19}\text{O}_4\text{P}$: C, 57.77; H, 7.09; Found: C, 58.19; H, 7.36.



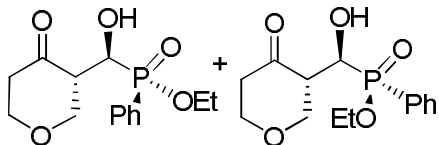
Ethyl (1-ethyl-1-hydroxy-3-oxobutyl)(phenyl)phosphinate (7k/8k): Colorless oil; ^1H NMR (500 MHz, CDCl_3) δ (mixture of two diastereomers) 0.85 and 1.00 (t, $J = 7.00$ Hz, 3 H), 1.26 and 1.33 (t, $J = 7.0$ Hz, 3 H), 2.18 and 2.34 (s, 3 H), 1.45-1.92 (m, 2 H), 2.55-2.70 (m, 1 H), 2.87 and 3.19 (dd, $J_1 = 8.0$, 18.0 and $J_2 = 5.5$, 16.3 Hz, 1 H), 3.79-4.15 (m, 2 H), 4.84 and 5.19 (d, $J = 7.5$ and 4.0 Hz, 1 H), 7.45-7.58 (m, 3 H), 7.80-7.89 (m, 2 H); ^{13}C NMR (125 MHz, CDCl_3) δ (mixture of two diastereomers) 7.2 and 7.8 (q), 16.6 and 16.8 (q), 28.9 (q), 32.4 (q), 61.6 (q), 75.4 & 75.7 (d, $J_{\text{CP}} = 118.8$ and 120.1 Hz), 127.8 (q), 128.6 (q), 132.8 (q), 133.7 (q), 211.8 (q); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 40.8, 41.4; ν_{max} (neat, cm^{-1}): 3210, 1708, 1592, 1439, 1398; Anal. Calcd. for $\text{C}_{14}\text{H}_{21}\text{O}_4\text{P}$: C, 59.15; H, 7.45; Found: C, 59.03; H, 7.64.



Ethyl [hydroxy(2-oxocyclopentyl)methyl](phenyl)phosphinate (10b/11b) Colorless gummy liquid; ^1H NMR (500 MHz, CDCl_3) δ (*syn*, mixture of two diastereomers) 1.30 (m, 3 H), 1.65-1.72(m, 1 H), 1.86-2.06 (m, 4 H), 2.22-2.48 (m, 2 H), 3.88-4.16 (m, 2 H), 4.57-4.67 (m, 1 H), 7.44-7.57 (m, 3 H), 7.80-7.85 (m, 2 H); ^{13}C NMR (125 MHz, CDCl_3) δ (*syn*, mixture of two diastereomers) 16.7 (q), 20.9 (t), 23.2 (d), 38.3 (q), 49.9 (q), 61.7 (q), 68.1 and 68.5 (d, $J_{\text{CP}} = 120.6$ and 118.3 Hz), 128.3 and 129.3 (d, $J_{\text{CP}} = 14.8$ and 14.9 Hz), 128.8 (q), 132.7 (q), 132.9 (q), 219.5 (t); ^{31}P NMR (CDCl_3) δ (mixture of two diastereomers) 39.3, 39.4; ν_{max} (neat, cm^{-1}): 3226, 1732, 1591, 1439 1390; Anal. Calcd. for $\text{C}_{14}\text{H}_{19}\text{O}_4\text{P}$: C, 59.57; H, 6.78; Found: C, 59.60; H, 6.79.



Ethyl [hydroxy(2-oxocyclohexyl)methyl](phenyl)phosphinate (10c/11c): Colorless oil; ^1H NMR (500 MHz, CDCl_3) δ (mixture of diastereomers) 1.29 (m, 3 H), 1.53-1.93 (m, 5 H), 2.14-2.32 (m, 3 H), 2.70-2.94 (m, 1 H), 3.73-4.09 (m, 2 H), 4.15-4.73 (m, 1 H), 7.35-7.40 (m, 2 H), 7.43-7.49 (m, 1 H), 7.73-7.78 (m, 2 H); ^{13}C NMR (125 MHz, CDCl_3) (major isomer, mixture of two diastereomers) δ 16.6 (q), 24.8 (q), 27.5 (q), 31.5 (q), 42.2 (q), 52.2 (q), 61.2 (q), 70.6 and 71.4 (d, $J_{\text{CP}} = 116.1$ and 113.5 Hz), 128.0 (q), 128.7 (q), 132.5 (q), 132.9 (q), 214.1 (d); ^{31}P NMR (CDCl_3) δ (mixture of diastereomers) 38.7, 39.1; 39.6; 40.9; ν_{max} (neat, cm^{-1}): 3246, 1706, 1591, 1439, 1390, 1313; Anal. Calcd. for $\text{C}_{15}\text{H}_{21}\text{O}_4\text{P}$: C, 60.80; H, 7.14; Found: C, 61.01; H, 7.35.



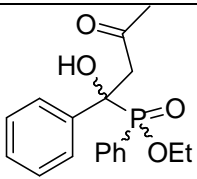
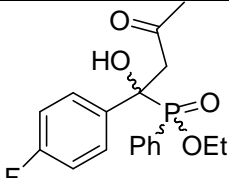
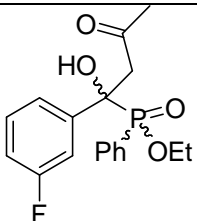
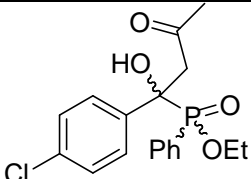
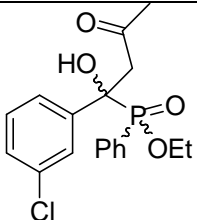
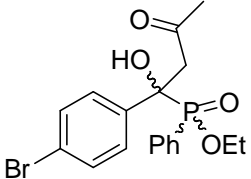
Ethyl [hydroxy(4-oxotetrahydro-2H-pyran-3-yl)methyl](phenyl)phosphinate

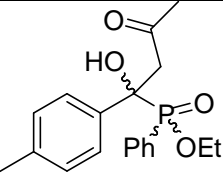
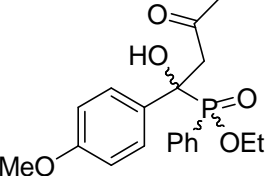
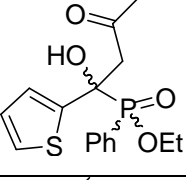
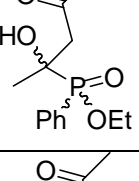
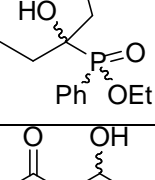
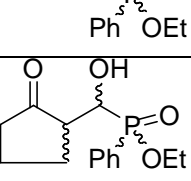
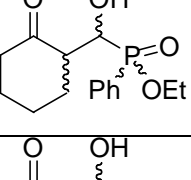
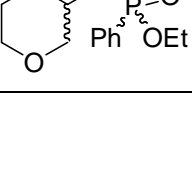

(10d/11d): Colorless oil; ^1H NMR (500 MHz, CDCl_3) δ (mixture of diastereomers) 1.28-1.38 (m, 3H), 2.42-2.64 (m, 1H), 3.57 (br s, 1H), 3.66-4.18 (m, 5H), 4.23-4.77 (m, 2H), 7.47-7.58 (m, 3H), 7.77-7.93 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) (major isomer, mixture of two diastereomers) δ 16.7 (d), 42.8 (d), 52.2 (d), 53.1 (d), 61.7 (d), 66.1 & 66.6 (d, $J_{\text{CP}} = 122.12$ and 120.62 Hz), 68.7 (q), 127.3 (q), 128.7 (q), 132.8 (q), 133.1 (d), 206.5 (q); ^{31}P NMR (CDCl_3) δ (mixture of diastereomers) 37.7, 38.8, 38.9, 39.5; ν_{max} (neat, cm^{-1}): 3245, 1715, 1591, 1476, 1439, 1373 cm^{-1} ; Anal. Calcd. for $\text{C}_{14}\text{H}_{19}\text{O}_5\text{P}$: C, 56.37; H, 6.42. Found: C, 56.38; H, 6.50.

Additional Reference

- (20) (a) Almquist, R. G.; Chao, W. R.; Jennings-White, C. *J. Med. Chem.* **1985**, *28*, 1067-1071. (b) Berkessel, A.; Koch, B.; Lex, J. *Adv. Syn. Catal.* **2004**, *346*, 1141-1146.

HPLC Conditions

Compound	Eluent <i>i</i> -PrOH/Hexane	Column	UV Det. (nm)	Flow rate (mL/min)
	5/95	AD-H	220	0.5
	5/95	AD-H	220	1
	5/95	AD-H	220	0.8
	5/95	AD-H	220	1
	5/95	AD-H	220	1
	5/95	AD-H	220	0.8

Compound	Eluent <i>i</i> -PrOH/Hexane	Column	UV Det. (nm)	Flow rate (mL/min)
	5/95	AD-H	220	0.8
	5/95	AD-H	220	1
	4/96	OJ-H	220	0.4
	3/97	OJ-H	220	0.3
	3/97	OJ-H & AD-H	220	0.3
	5/95	AS	220	0.8
	5/95	AD-H	220	1
	5/95	AD-H	220	1
	7/93	OJ-H	220	1

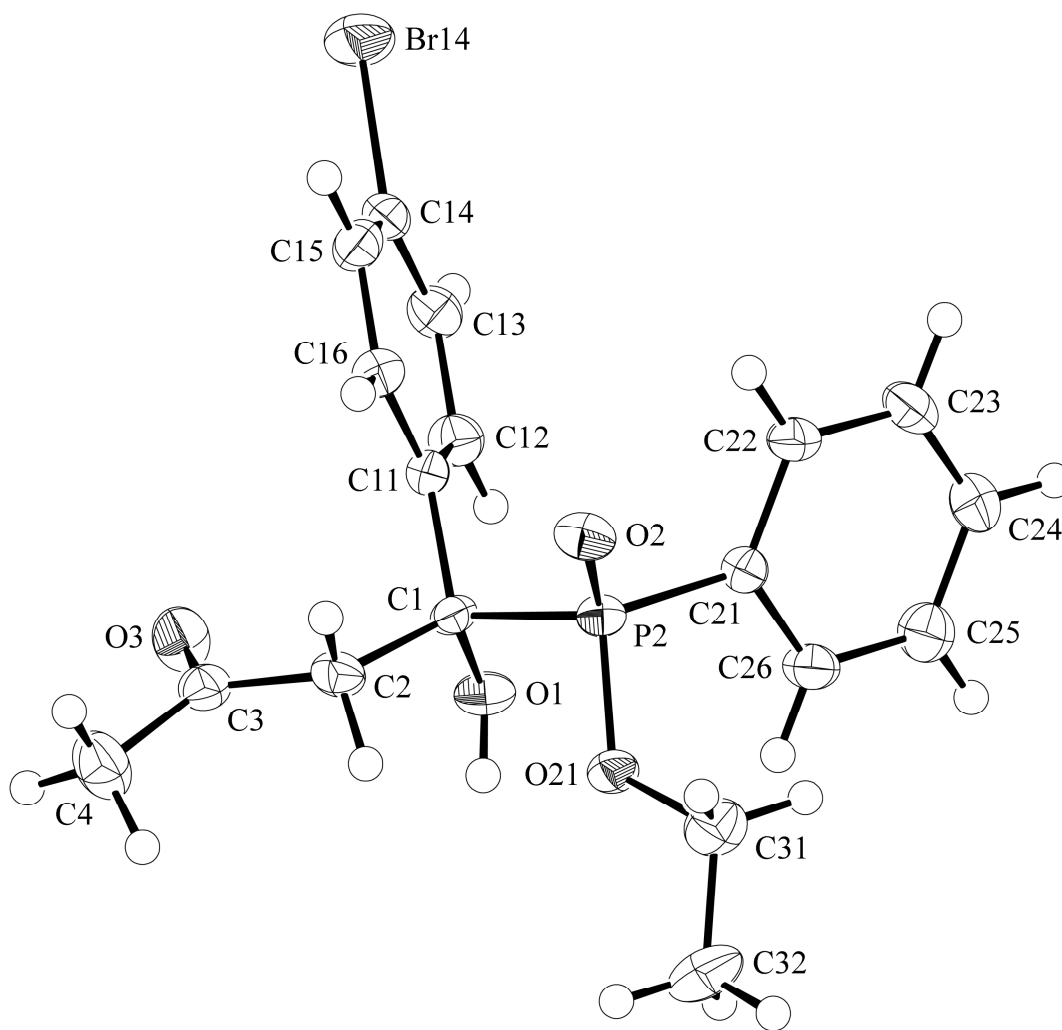
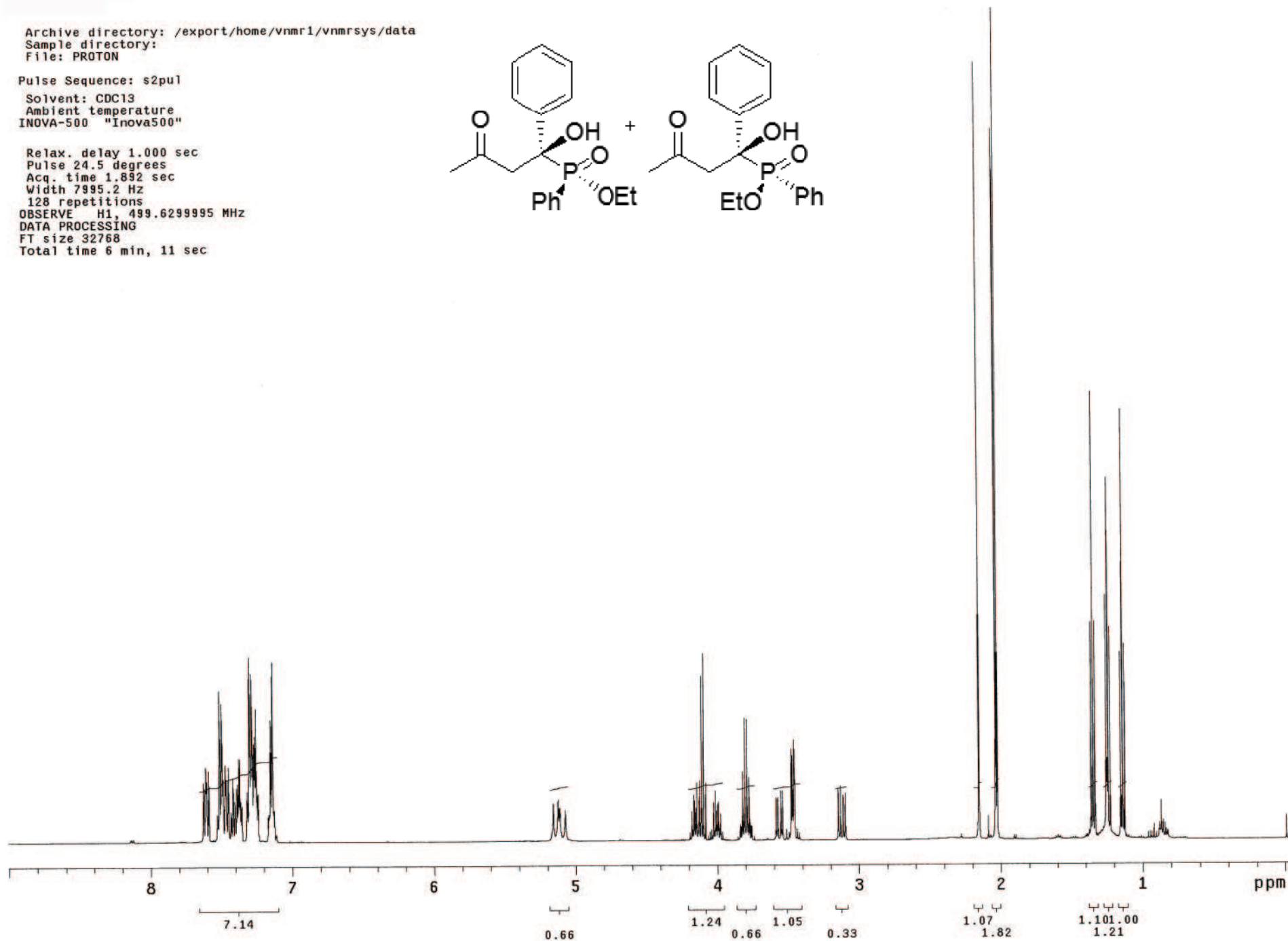
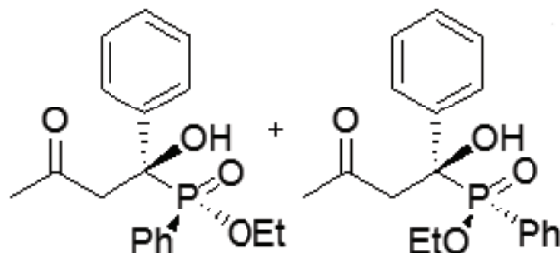


Figure 2. ORTEP Drawing of Compound *ent-7d*

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
128 repetitions
OBSERVE H1, 499.6299995 MHz
DATA PROCESSING
FT size 32768
Total time 6 min, 11 sec

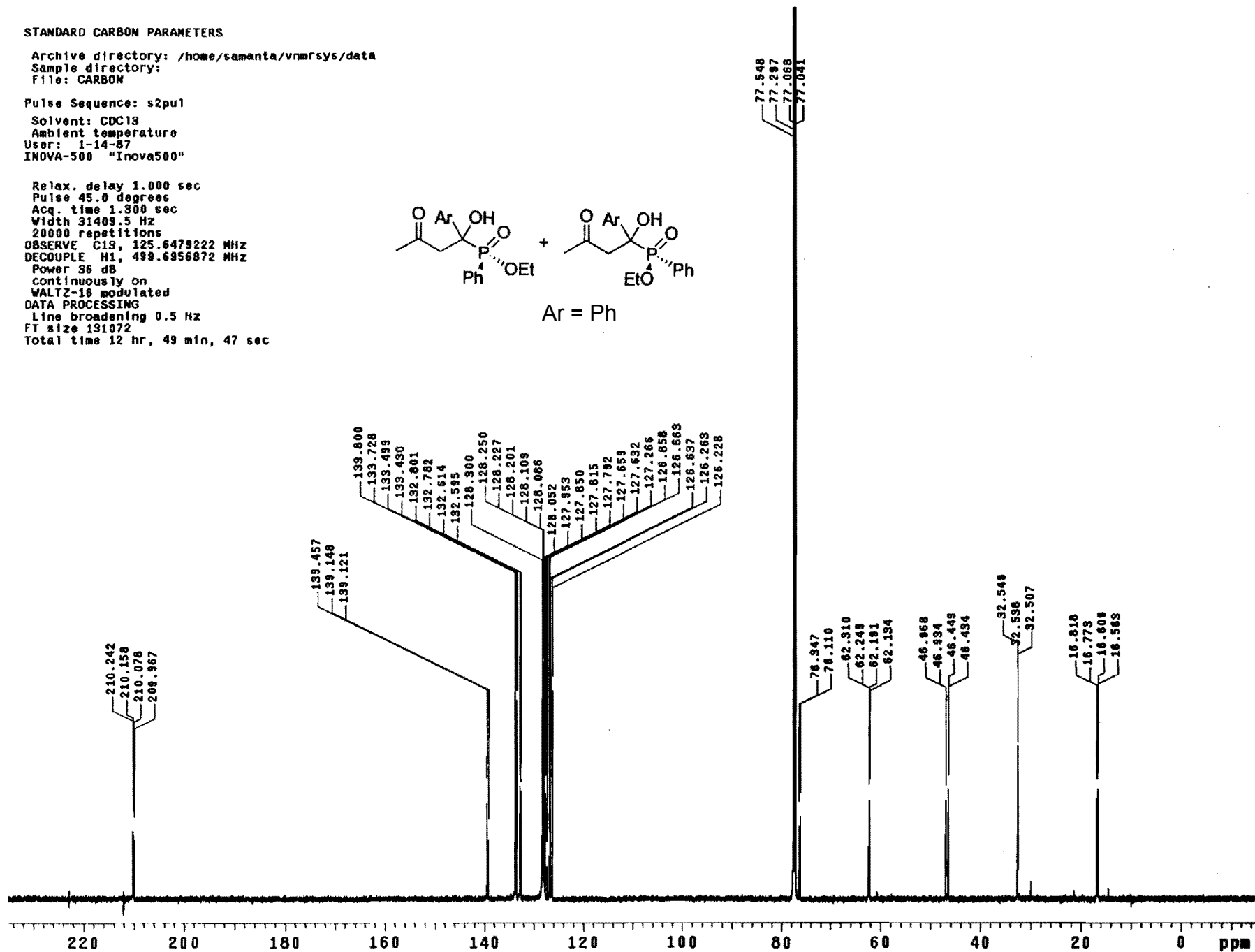
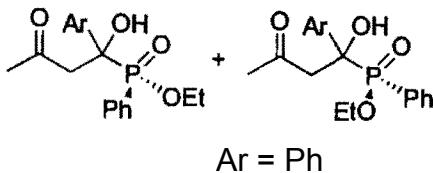


STANDARD CARBON PARAMETERS

Archive directory: /home/samanta/vnmrsys/data
 Sample directory:
 File: CARBON

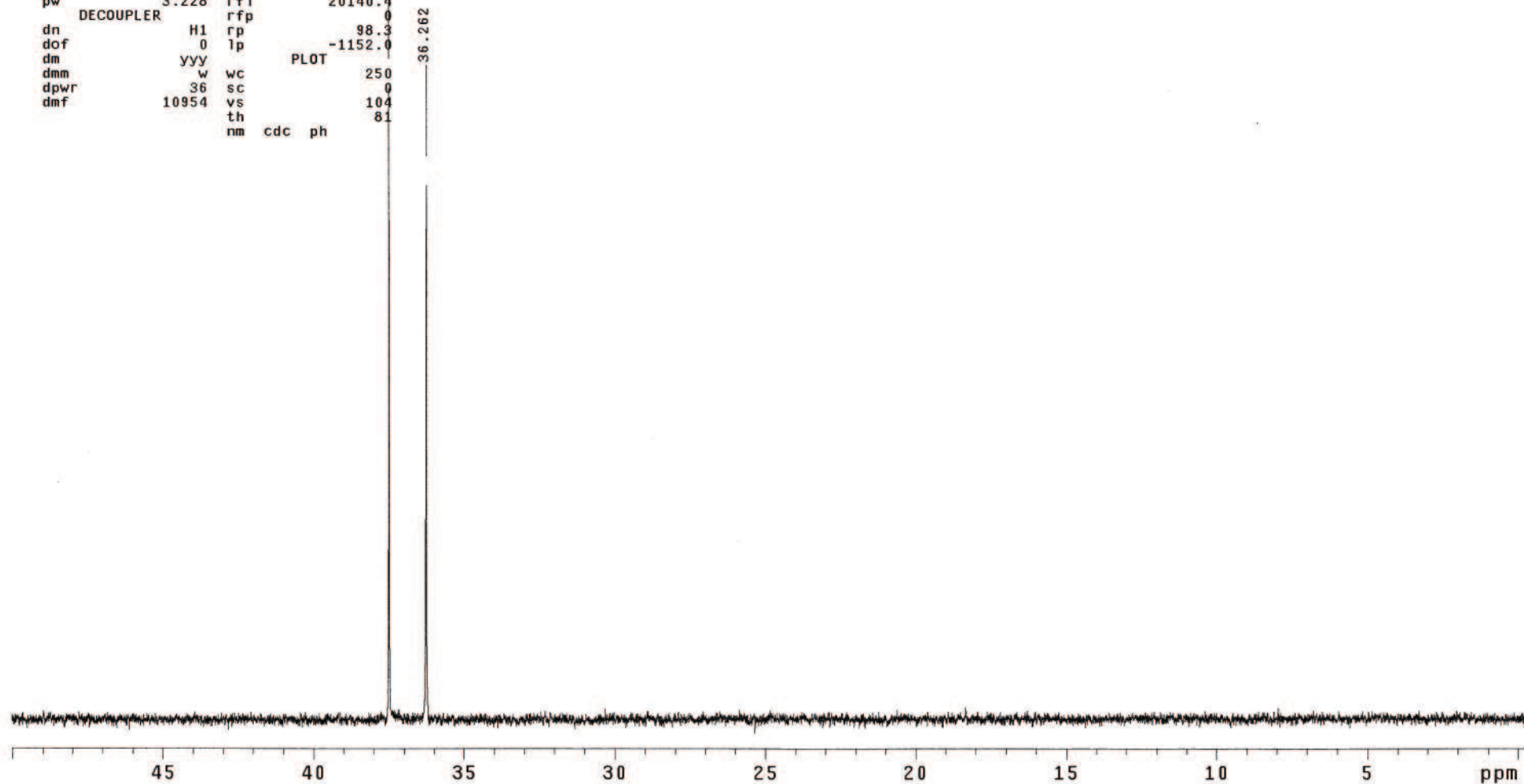
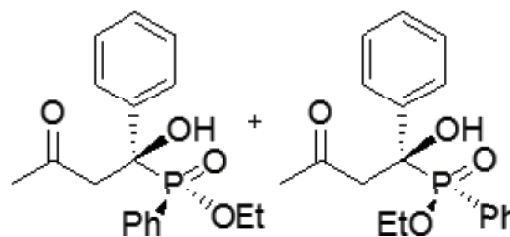
Pulse Sequence: s2pu1
 Solvent: CDC13
 Ambient temperature
 User: 1-14-87
 INOVA-500 "Inova500"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31409.5 Hz
 20000 repetitions
 OBSERVE C13, 125.6479222 MHz
 DECOUPLE H1, 499.6956872 MHz
 Power 36 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 131072
 Total time 12 hr, 49 min, 47 sec



exp3 s2pu1

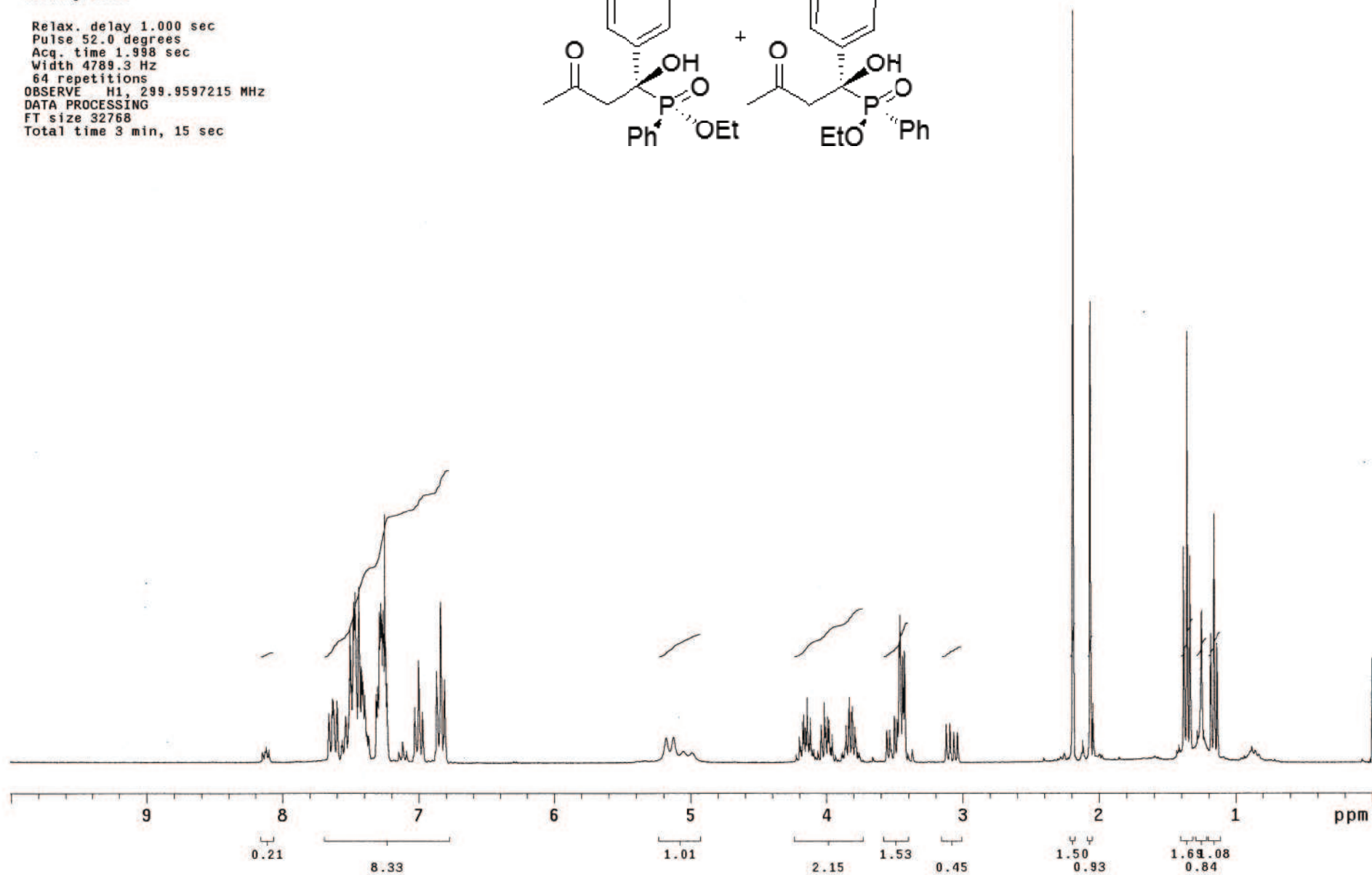
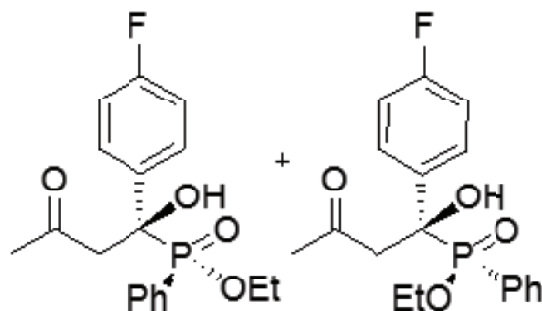
SAMPLE		SPECIAL	
date	Nov 24 2009	temp	not used
solvent	D2O	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	40140.5	pw90	8.300
at	1.600	alfa	10.000
np	128450	FLAGS	
fb	22000	il	n
bs	64	in	n
d1	1.000	dp	y
nt	4	hs	ny
ct	4	PROCESSING	
TRANSMITTER		lb	1.00
tn	P31	fn	not used
sfrq	202.254	DISPLAY	
tof	5050.4	sp	-47.2
tpwr	54	wp	10162.7
pw	3.228	rfl	20140.4
DECOUPLER		rfp	0
dn	H1	rp	98.3
dof	0	lp	-1152.0
dm	yyy	PLOT	
dmm	w	wc	250
dpwr	36	sc	0
dmf	10954	vs	104
		th	81
		nm	cdc ph



Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
Mercury-300BB "varian300"

Relax. delay 1.000 sec
Pulse 52.0 degrees
Acq. time 1.998 sec
Width 4789.3 Hz
64 repetitions
OBSERVE H1, 299.9597215 MHz
DATA PROCESSING
FT size 32768
Total time 3 min, 15 sec



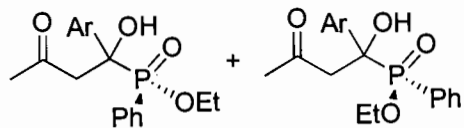
STANDARD CARBON PARAMETERS
v-ss-79c

Archive directory: /home/samanta/vnmrsys/data
Sample directory:

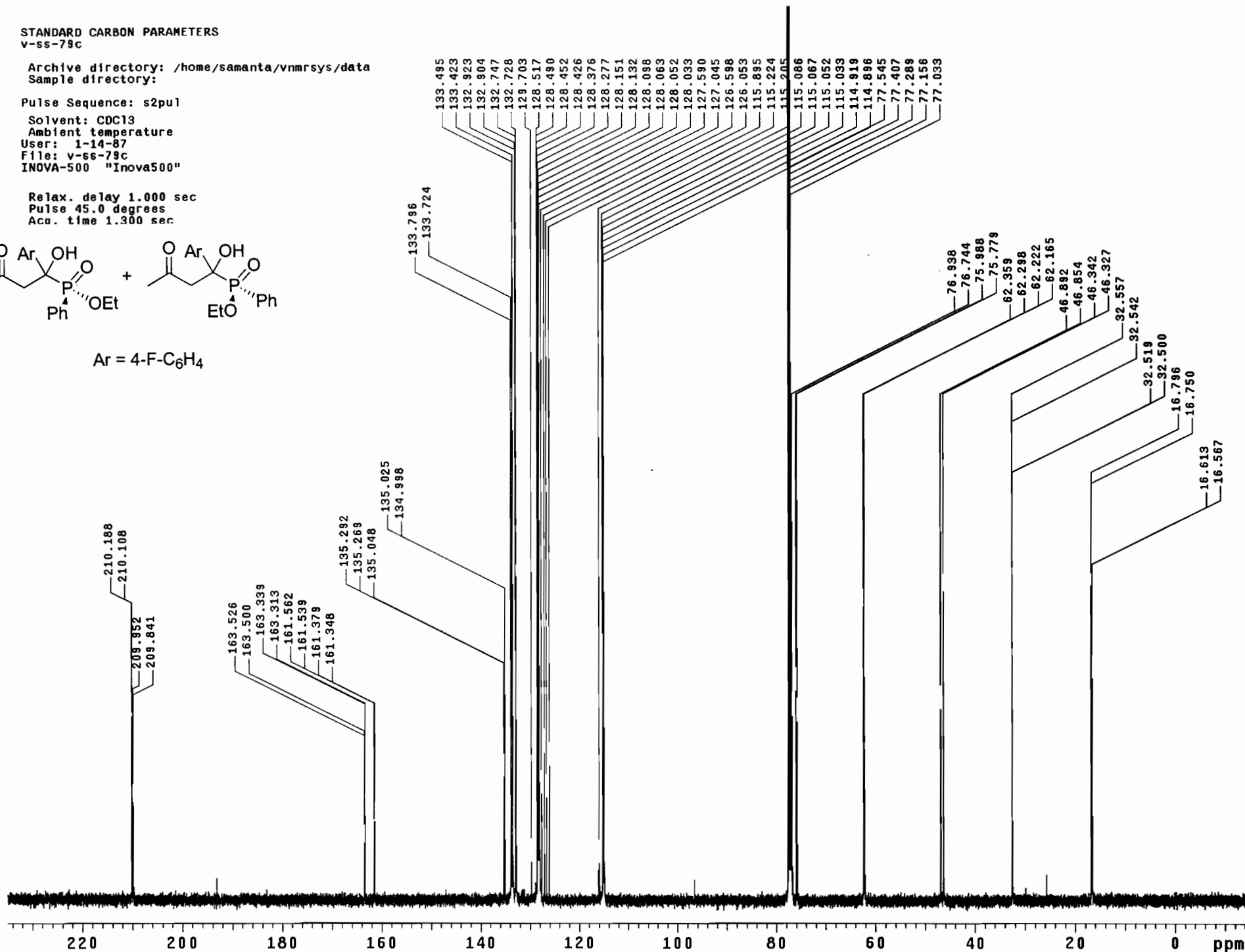
Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: v-ss-79c
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Aca. time 1.300 sec

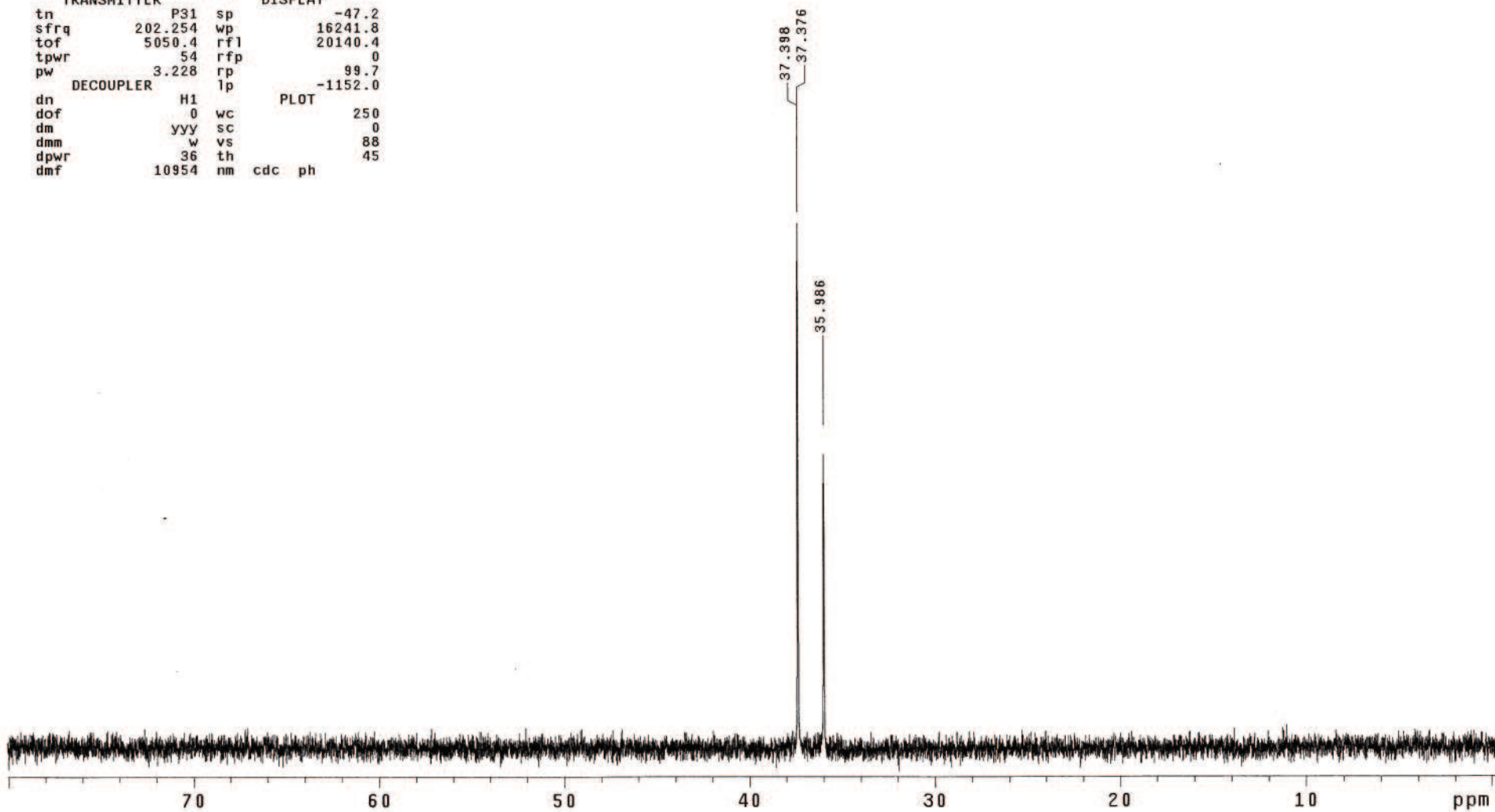
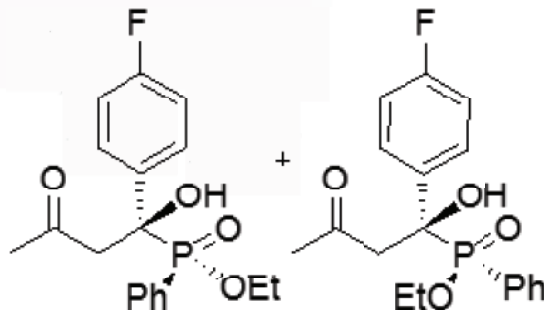


Ar = 4-F-C₆H₄



exp3 s2pu1

SAMPLE		SPECIAL	
date	Nov 24 2009	temp	not used
solvent	D2O	gain	not used
file	/export2/home~	spin	not used
/sperera/3-sp-7P31~		hst	0.008
.fid		pw90	8.300
		alfa	10.000
ACQUISITION		FLAGS	
sw	40140.5		
at	1.600	il	n
np	128450	in	n
fb	22000	dp	y
bs	64	hs	ny
d1	1.000	PROCESSING	
nt	100	lb	1.00
ct	100	fn	not used
TRANSMITTER		DISPLAY	
tn	P31	sp	-47.2
sfrq	202.254	wp	16241.8
tof	5050.4	rf1	20140.4
tpwr	54	rfp	0
pw	3.228	rp	99.7
DECOUPLER		lp	-1152.0
dn	H1	PLOT	
dof	0	wc	250
dm	yyy	sc	0
dmm	w	vs	88
dpwr	36	th	45
dmf	10954	nm	cdc ph

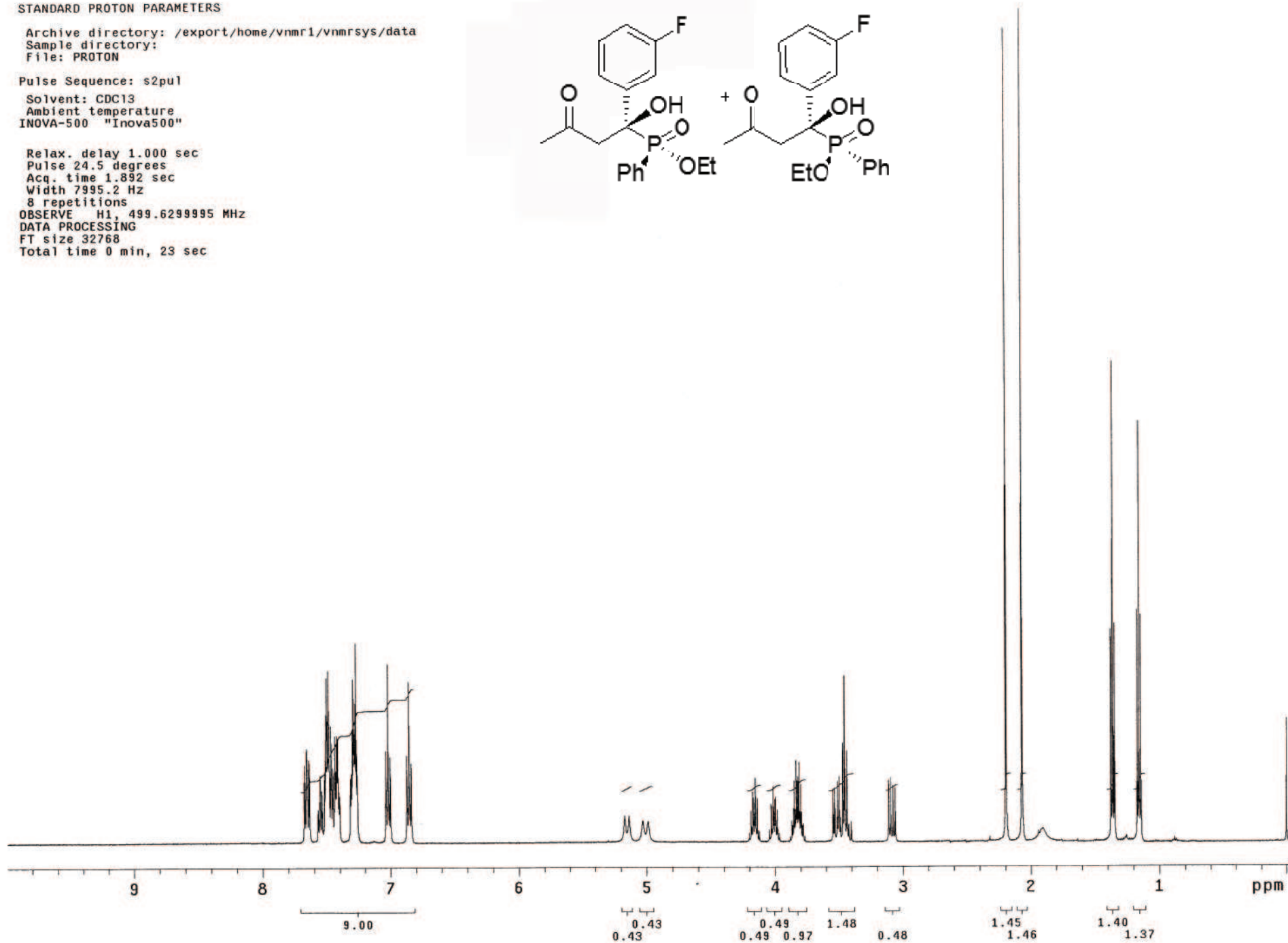
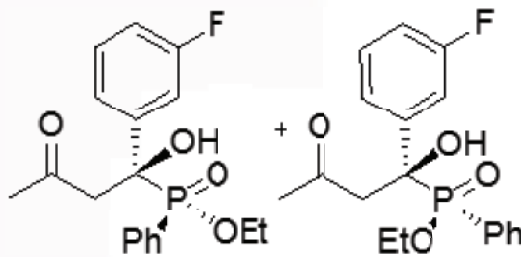


STANDARD PROTON PARAMETERS

Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory:
 File: PROTON

Pulse Sequence: s2pu1
 Solvent: CDC13
 Ambient temperature
 INOVA-500 "Inova500"

Relax. delay 1.000 sec
 Pulse 24.5 degrees
 Acq. time 1.892 sec
 Width 7995.2 Hz
 8 repetitions
 OBSERVE H1, 499.6299995 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min, 23 sec



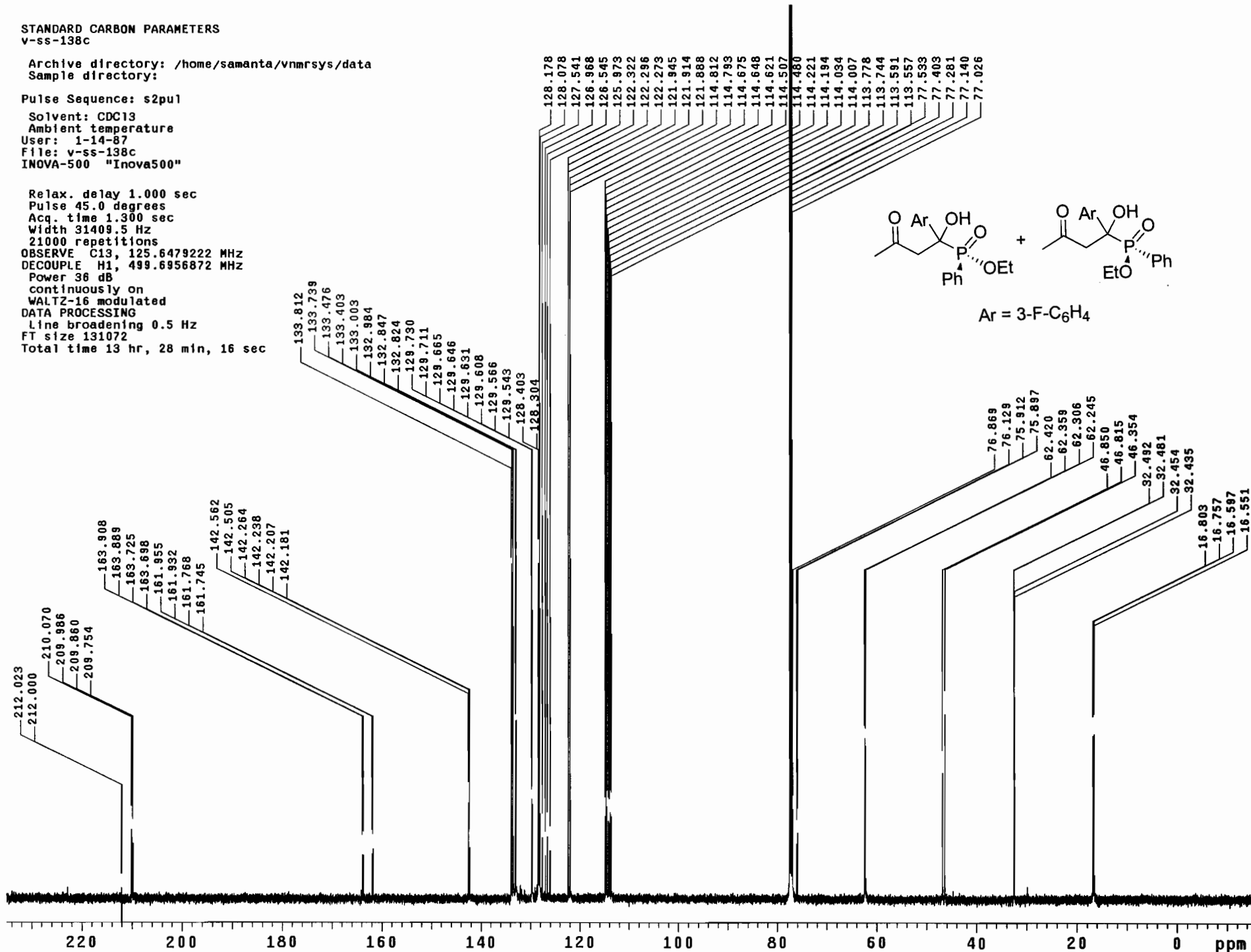
STANDARD CARBON PARAMETERS
v-ss-138c

Archive directory: /home/samanta/vnmrSYS/data
Sample directory:

Pulse Sequence: s2pul1

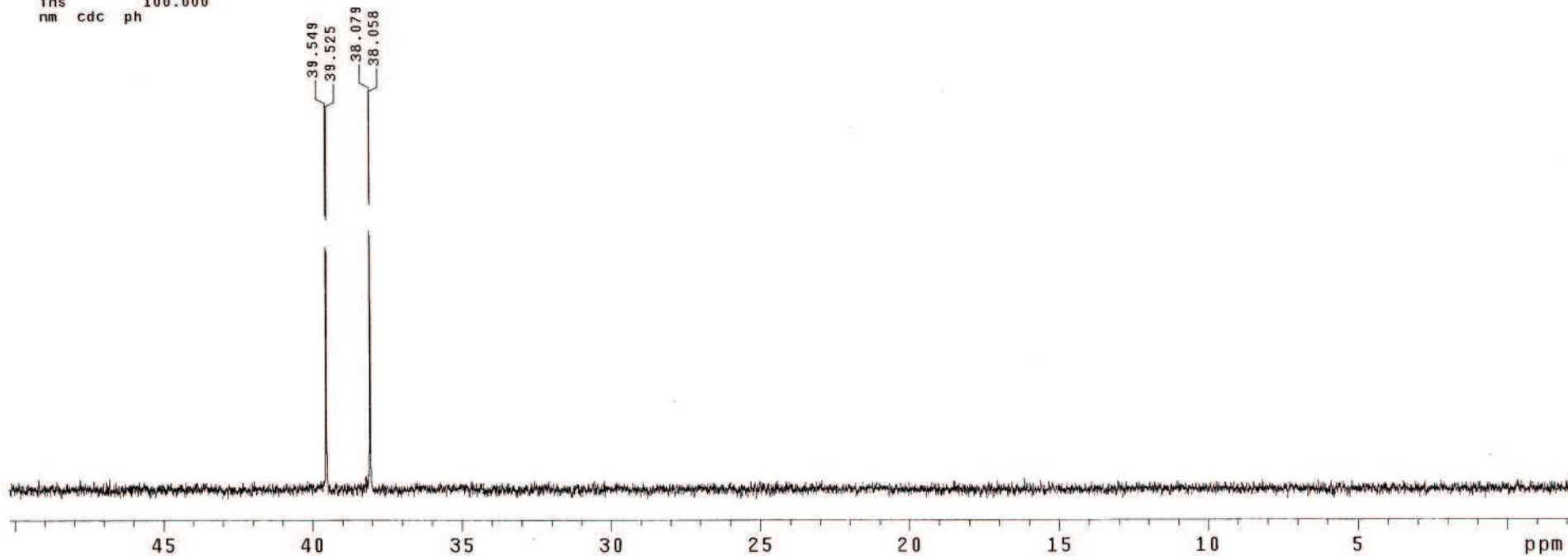
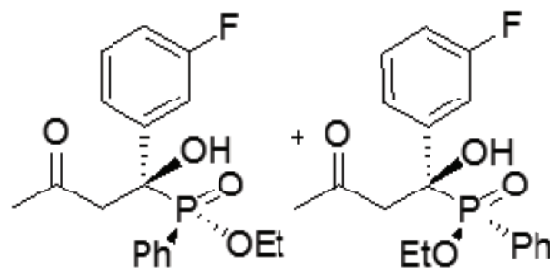
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: v-ss-138c
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
21000 repetitions
OBSERVE C13, 125.6479222 MHz
DECOUPLE H1, 499.6956872 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 13 hr, 28 min, 16 sec



exp1 s2pu1

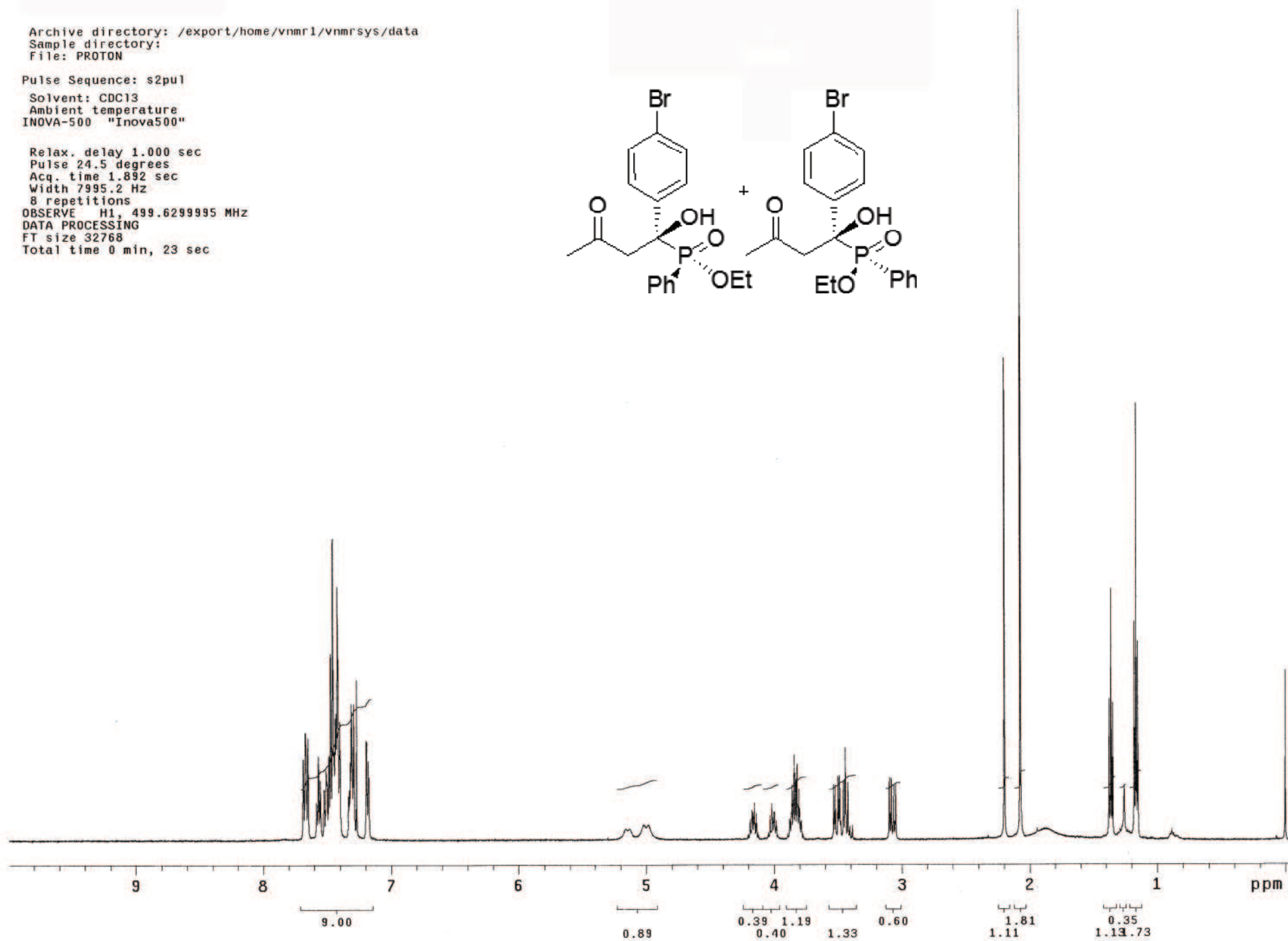
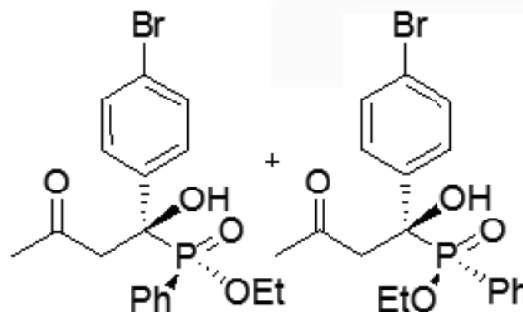
```
SAMPLE          DEC. & VT
date    Dec 30 2009  dfrq    499.632
solvent  CDC13      dn      H1
file     exp       dpwr    36
ACQUISITION
sfrq    202.258    dm      nny
tn      P31       dmm     w
at      1.600     dmf    10954
np      64000     dseq
sw      20000.0   dres   1.0
fb      11000    homo   n
tpwr    54       temp   26.0
pw      4.0      PROCESSING
d1      5.000    lb     1.00
tof     9000.0   wtfile
nt      16      proc
ct      16      fn     not used
alock   n       math   f
gain    not used
FLAGS
il      n       werr
in      n       wexp
dp      y       wbs
hs      ny      wnt
DISPLAY
sp      -427.9
wp      10578.9
vs      42
sc      0
wc      250
hzmm    42.32
is      500.00
rfl     6186.7
rfp     0
th      37
ins     100.000
nm      cdc ph
```



Archive directory: /export/home/vnmr1/vnmr/sys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
8 repetitions
OBSERVE H1, 499.6299995 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 23 sec



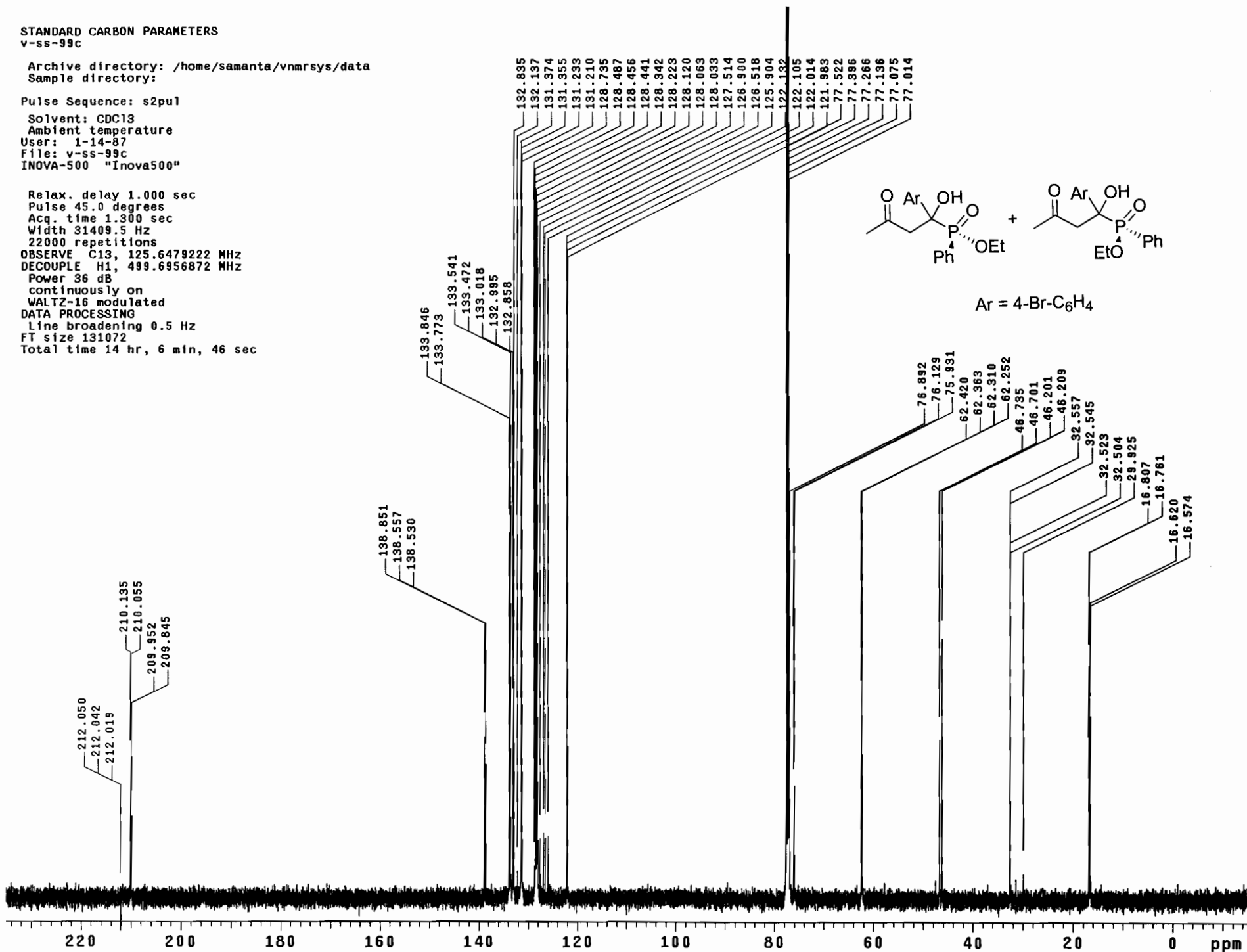
STANDARD CARBON PARAMETERS
v-ss-99c

Archive directory: /home/samanta/vnmrSYS/data
Sample directory:

Pulse Sequence: s2pul

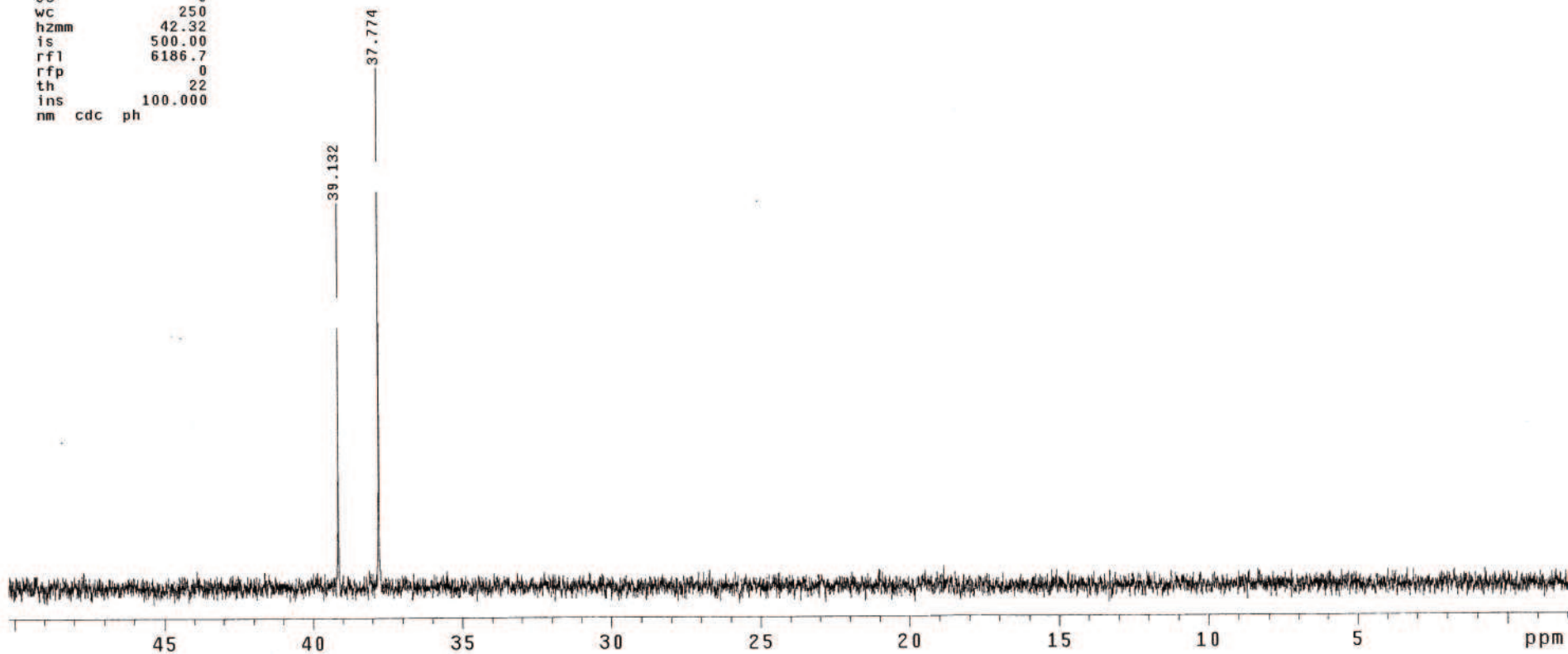
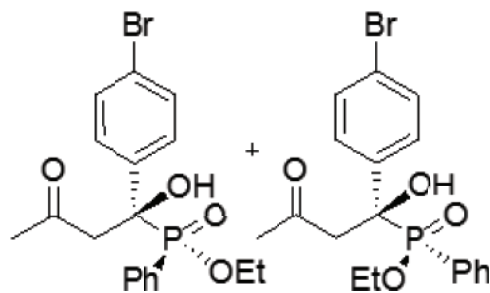
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: v-ss-99c
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
22000 repetitions
OBSERVE C13, 125.6479222 MHz
DECOUPLE H1, 499.6956872 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 14 hr, 6 min, 46 sec



exp1 s2pu1

```
SAMPLE          DEC. & VT
date   Dec 30 2009  dfrq      499.632
solvent CDC13      dn        H1
file    exp        dpwr      36
          ACQUISITION  dof        0
sfrq    202.258    dm         nny
tn       P31       dmm        w
at       1.600     dmf       10954
np       64000     dseq
sw       20000.0   dres      1.0
fb       11000    homo      n
tpwr     54        temp     26.0
pw       4.0      PROCESSING
d1       5.000     lb        1.00
tof      9000.0   wtfile
nt       16       proc
ct       16       fn        not used
alock    not used math
gain     not used
          FLAGS    werr
il       n        wexp
in       n        wbs
dp       y        wnt
hs       ny
          DISPLAY
sp      -427.9
wp      10578.9
vs       63
sc       0
wc       250
h2mm    42.32
is       500.00
rfl     6186.7
rfp     0
th       22
ins     100.000
nm      cdc  ph
```

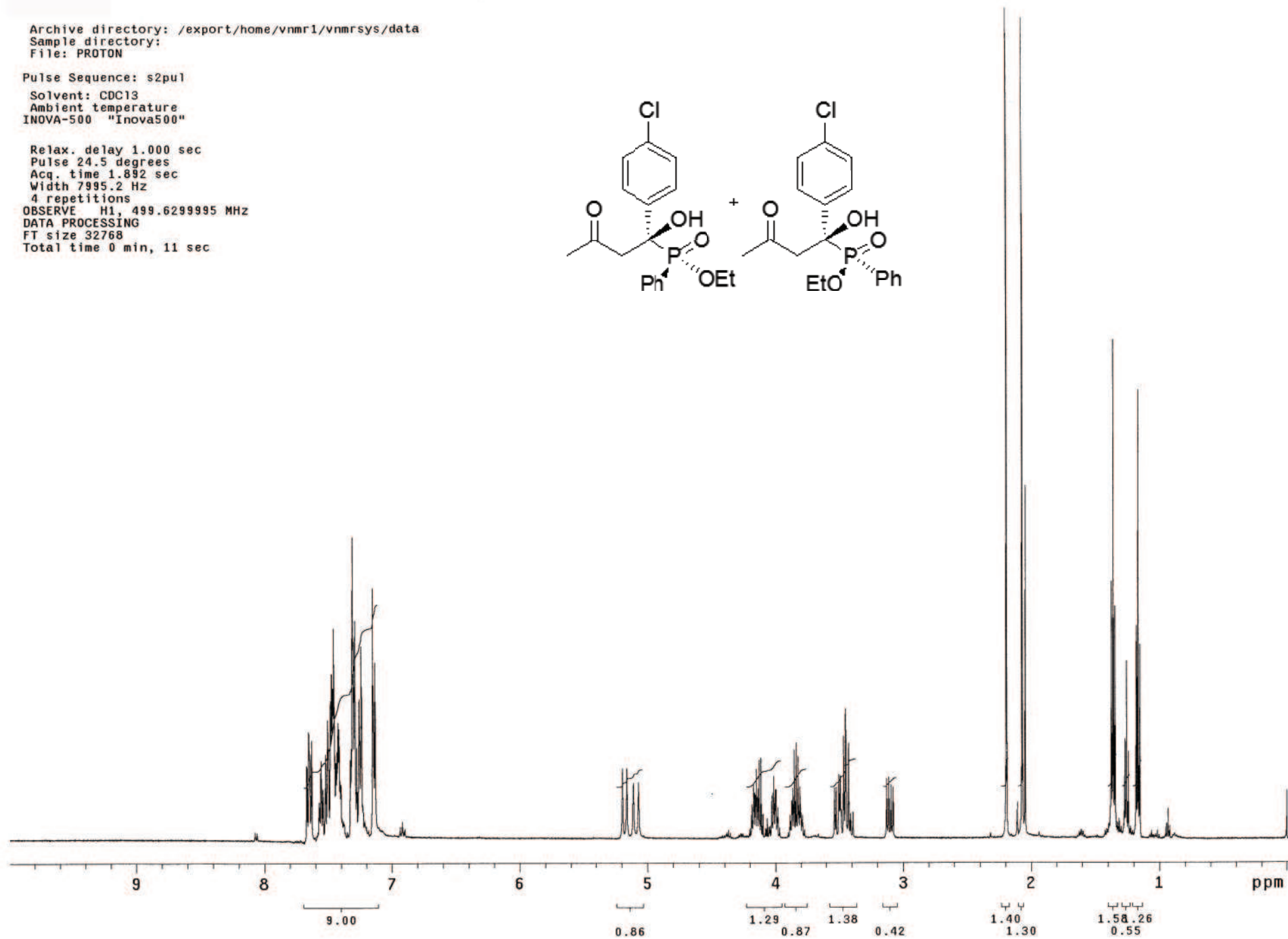
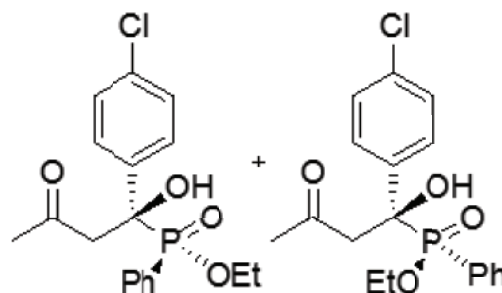


Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
4 repetitions
OBSERVE H1, 499.6299995 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 11 sec



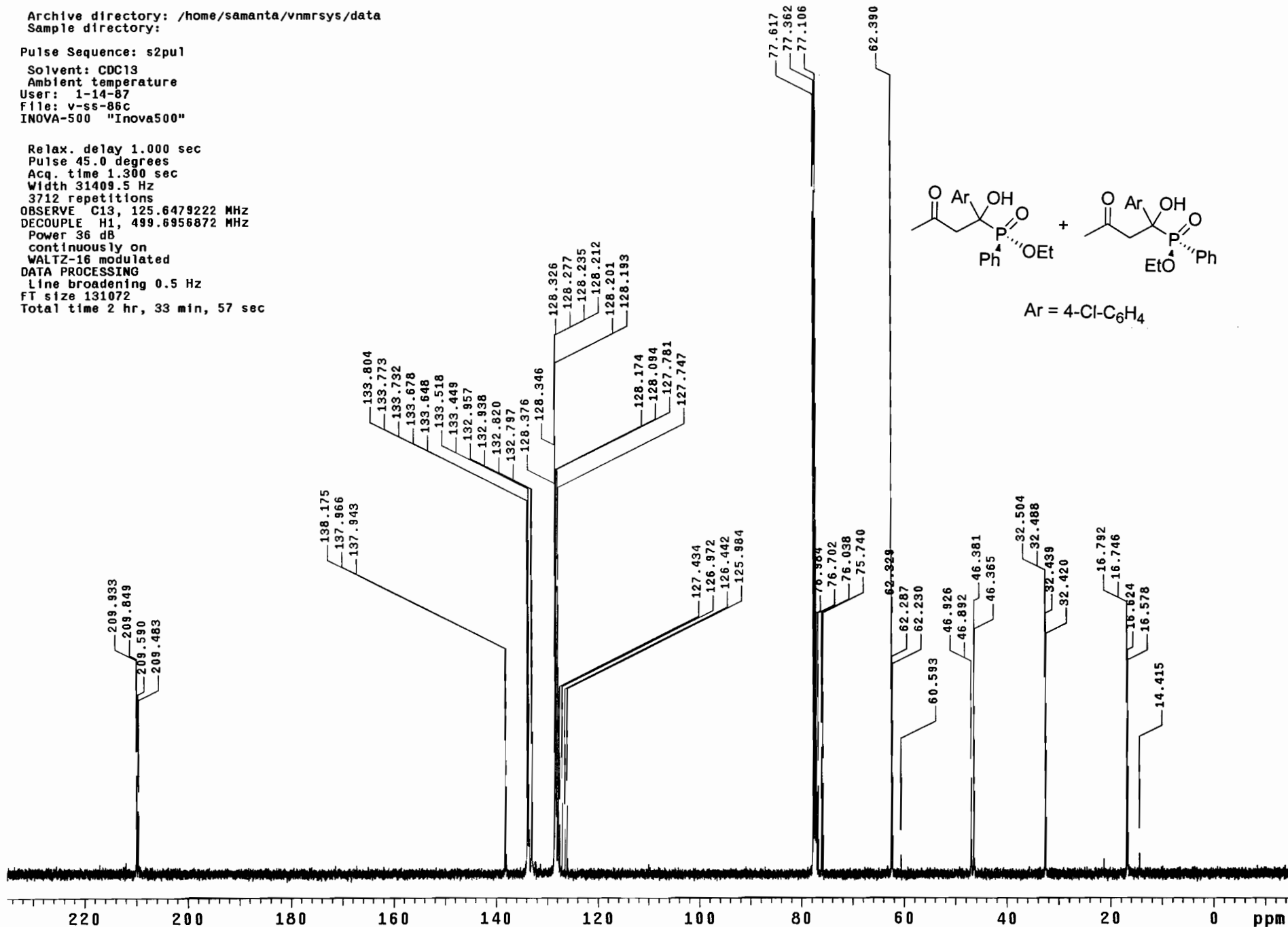
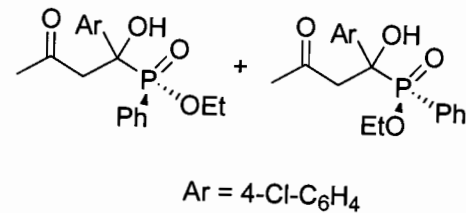
STANDARD CARBON PARAMETERS
v-ss-86c

Archive directory: /home/samanta/vnmrsys/data
Sample directory:

Pulse Sequence: s2pu1

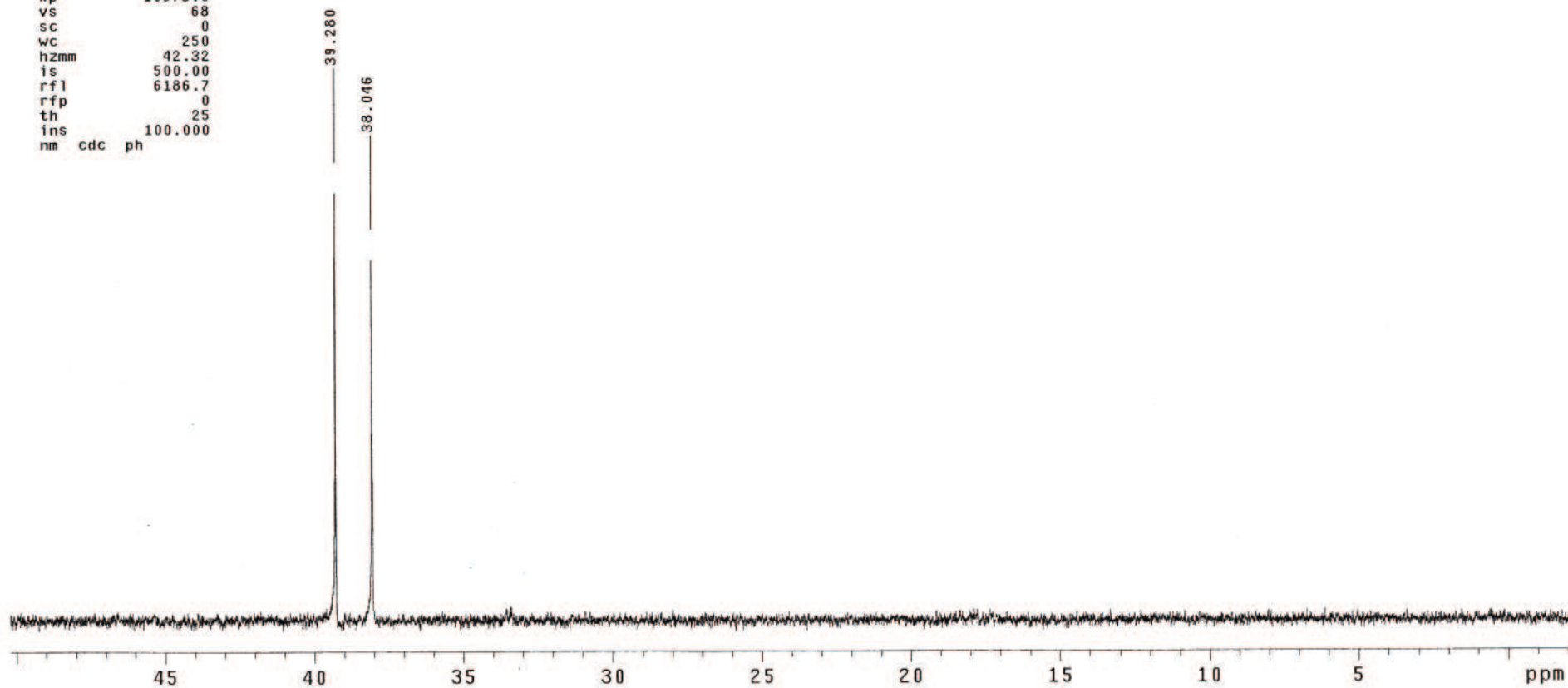
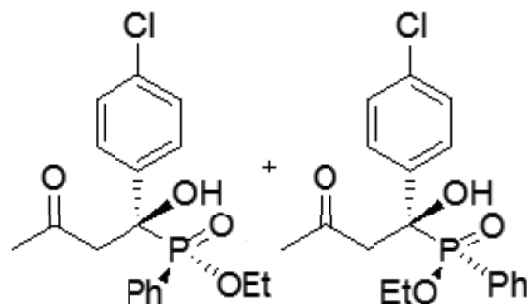
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: v-ss-86c
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
3712 repetitions
OBSERVE C13, 125.6479222 MHz
DECOUPLE H1, 499.6956872 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 2 hr, 33 min, 57 sec



exp1 s2pu1

SAMPLE		DEC. & VT	
date	Dec 30 2009	dfrq	499.632
solvent	CDC13	dn	H1
file	exp	dpwr	36
ACQUISITION		DOF	
sfrq	202.258	dm	nny
tn	P31	dmm	w
at	1.600	dmf	10954
np	64000	dseq	
sw	20000.0	dres	1.0
fb	11000	homo	n
tpwr	54	temp	26.0
pw	4.0	PROCESSING	
d1	5.000	lb	1.00
tof	9000.0	wtfile	
nt	16	proc	ft
ct	16	fn	not used
alock	n	math	f
gain	not used		
FLAGS		werr	
il	n	wexp	
in	n	wbs	
dp	y	wnt	
hs	ny		
DISPLAY			
sp	-427.9		
wp	10578.9		
vs	68		
sc	0		
wc	250		
hzmm	42.32		
is	500.00		
rfl	6186.7		
rfp	0		
th	25		
ins	100.000		
nm	cdc ph		

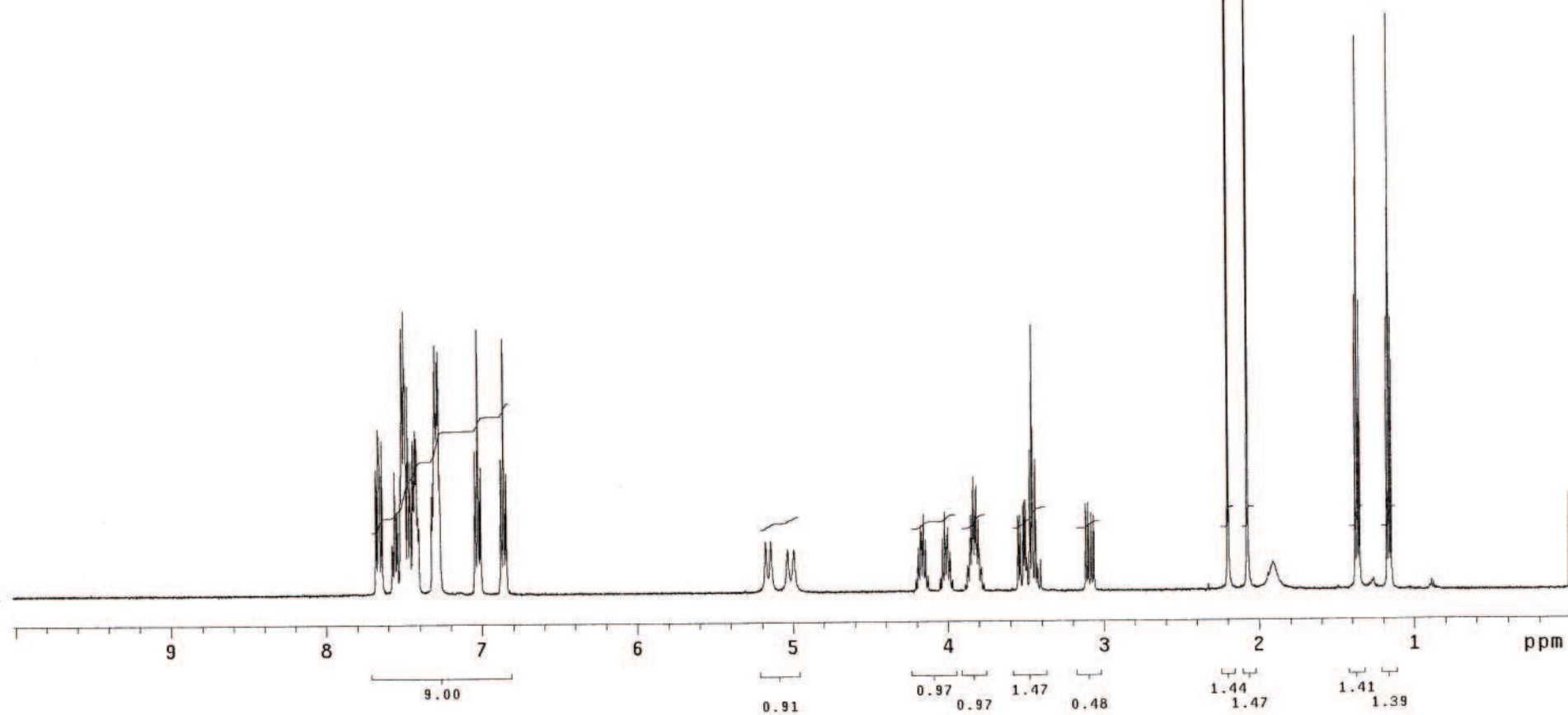
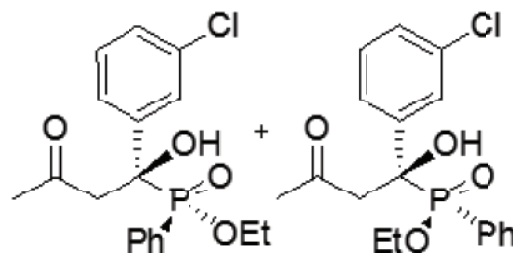


Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
4 repetitions
OBSERVE H1, 499.6299995 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 11 sec



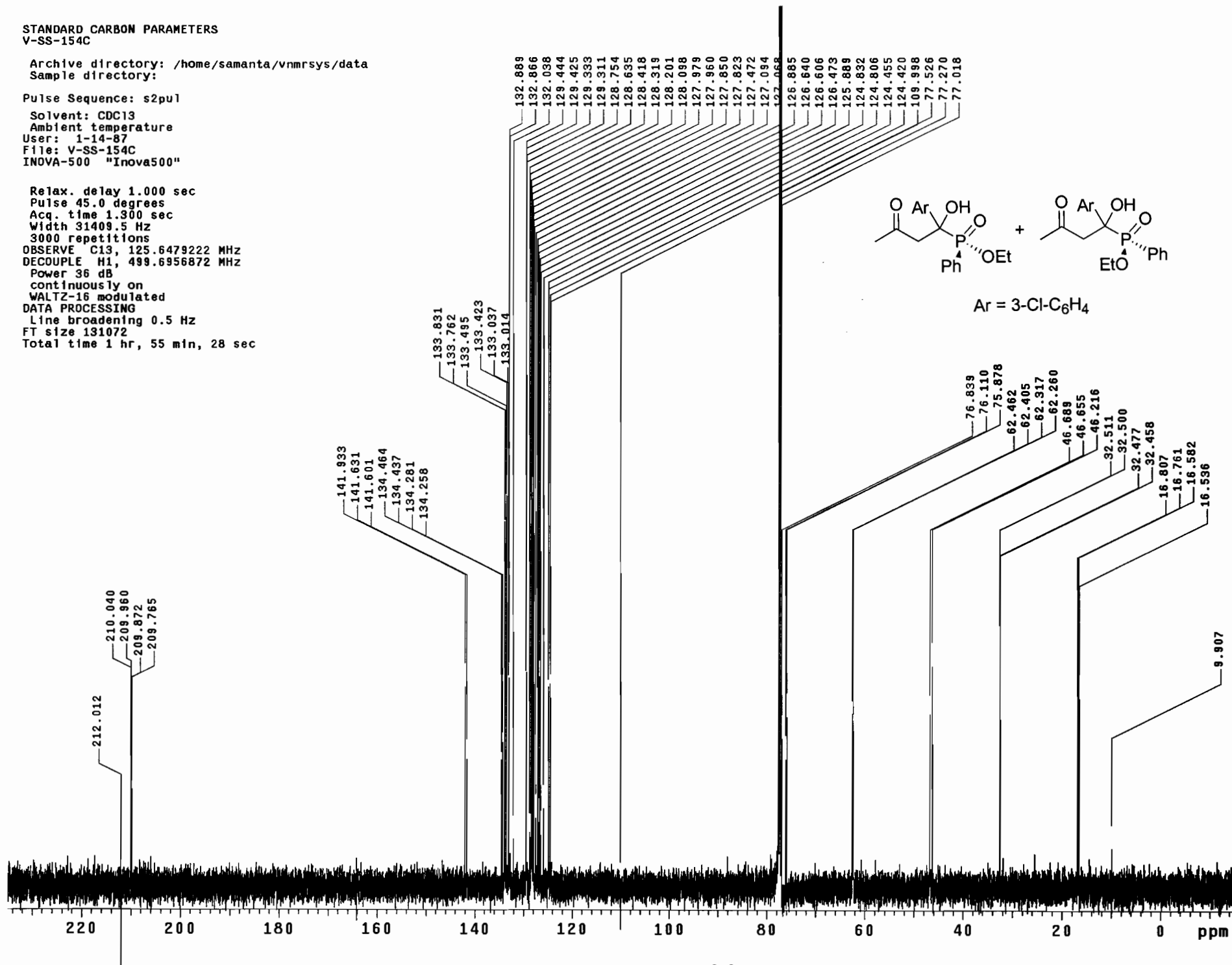
STANDARD CARBON PARAMETERS
V-SS-154C

Archive directory: /home/samanta/vnmrsys/data
Sample directory:

Pulse Sequence: s2pu1

Solvent: CDC13
Ambient temperature
User: 1-14-87
File: V-SS-154C
INOVA-500 "Inova500"

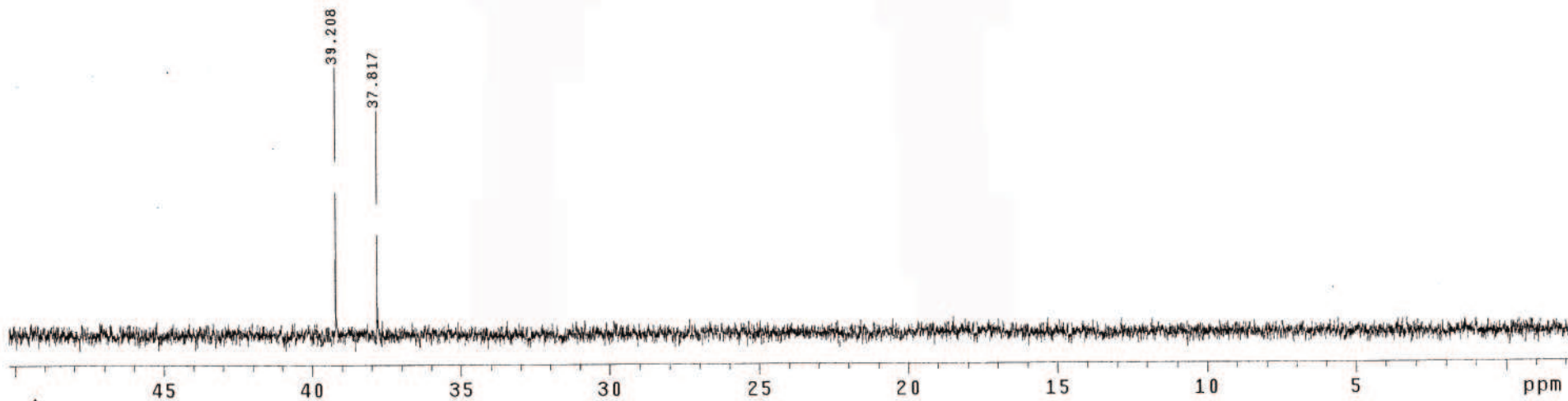
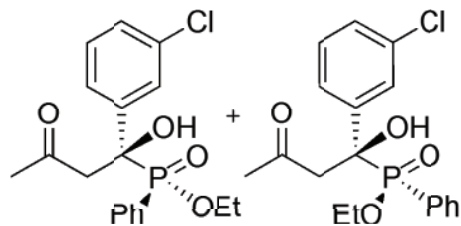
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
3000 repetitions
OBSERVE C13, 125.6479222 MHz
DECOUPLE H1, 499.6956872 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 1 hr, 55 min, 28 sec



3-sp-24

exp1 s2pu1

SAMPLE		DEC. & VT	
date	Dec 30 2009	dfrq	499.632
solvent	CDC13	dn	H1
file	exp	dpwr	36
ACQUISITION		dof	0
sfrq	202.258	dm	nny
tn	P31	dmm	w
at	1.600	dmf	10954
np	64000	dseq	
sw	20000.0	dres	1.0
fb	11000	homo	n
tpwr	54	temp	26.0
pw	4.0	PROCESSING	
d1	5.000	lb	1.00
tof	9000.0	wtfile	
nt	16	proc	ft
ct	16	fn	not used
alock	n	math	f
gain	not used		
FLAGS		werr	n
il	n	wexp	n
in	n	wbs	n
dp	y	wnt	y
hs	ny		
DISPLAY			
sp	-427.9		
wp	10578.9		
vs	80		
sc	0		
wc	250		
hzmm	42.32		
is	500.00		
rfl	6186.7		
rfp	0		
th	5		
ins	100.000		
nm	cdc ph		

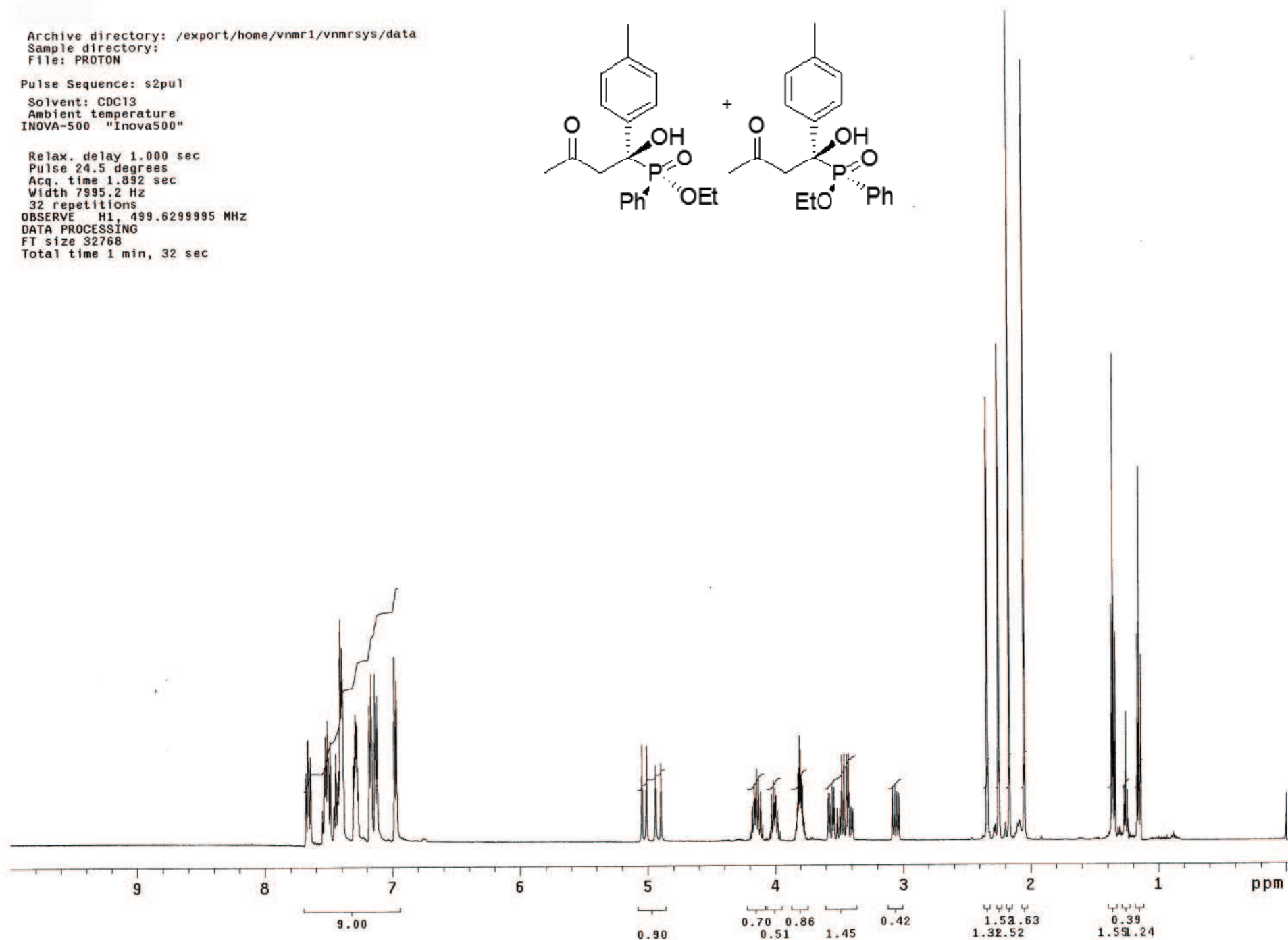
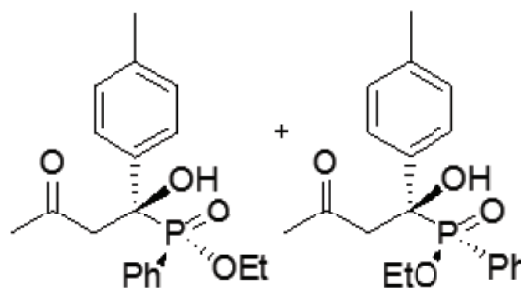


Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDC13
Ambient temperature
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
32 repetitions
OBSERVE H1, 499.6299995 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 32 sec



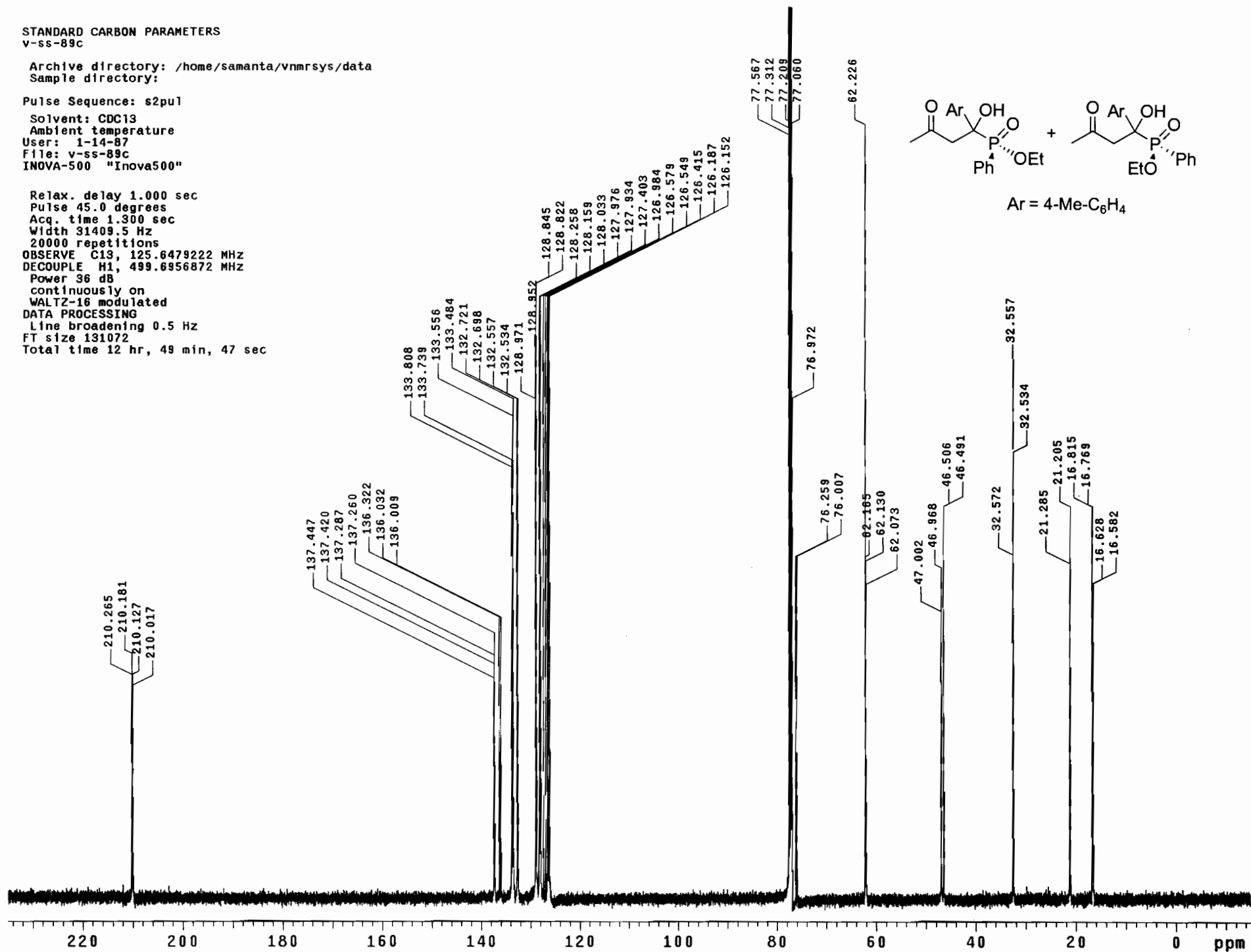
STANDARD CARBON PARAMETERS
v-ss-89c

Archive directory: /home/samanta/vnmrSYS/data
Sample directory:

Pulse Sequence: s2pu1

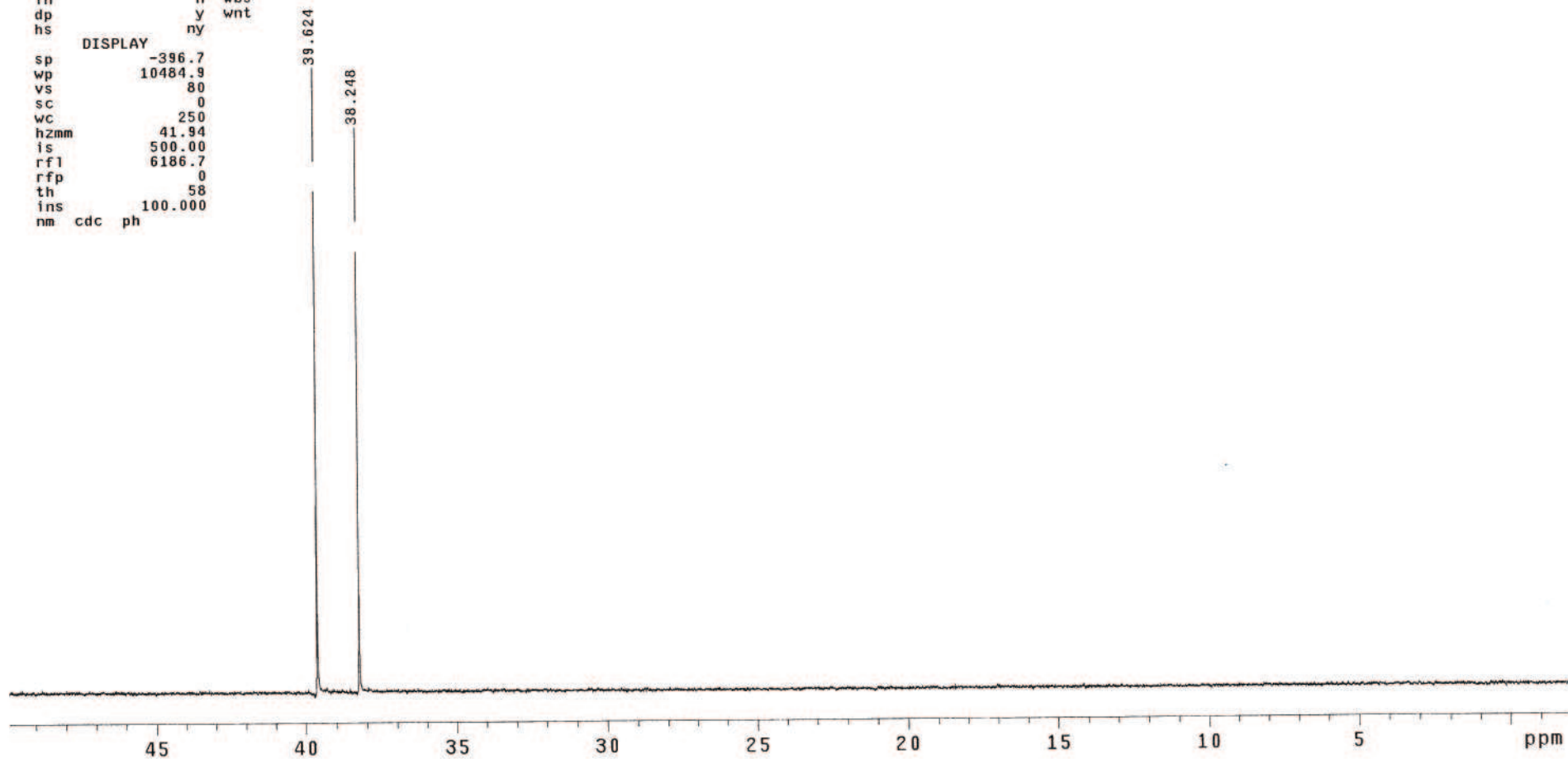
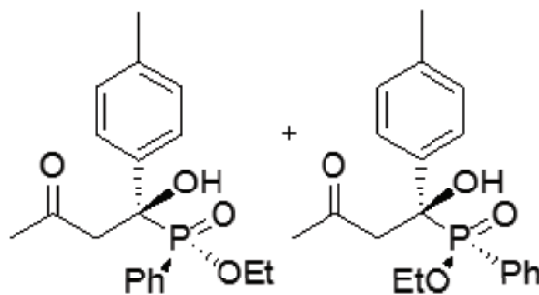
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: v-ss-89c
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
20000 repetitions
OBSERVE C13, 125.6479222 MHz
DECOUPLE H1, 499.6956872 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 12 hr, 49 min, 47 sec



exp1 s2pul

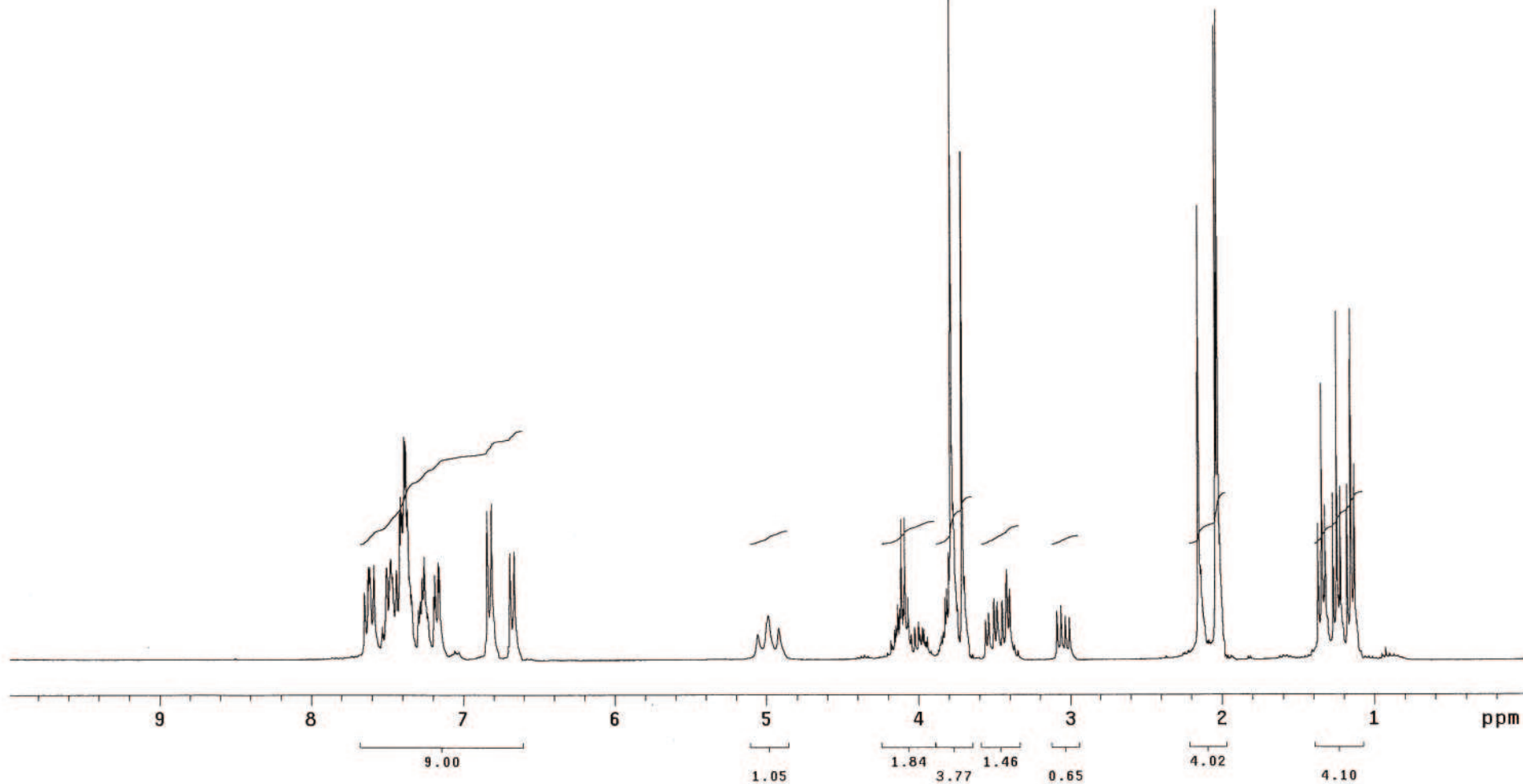
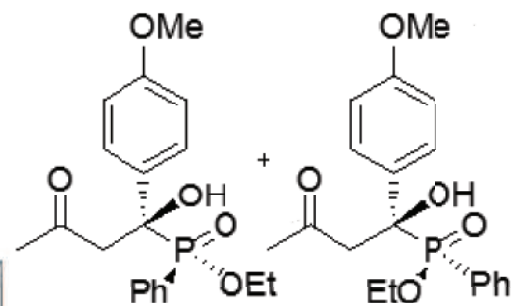
SAMPLE		DEC. & VT	
date	Dec 30 2009	dfrq	499.632
solvent	CDC13	dn	H1
file	exp	dpwr	36
ACQUISITION		dof	0
sfrq	202.258	dm	nny
tn	P31	dmm	w
at	1.600	dmf	10954
np	64000	dseq	
sw	20000.0	dres	1.0
fb	11000	homo	n
tpwr	54	temp	26.0
PROCESSING		lb	1.00
pw	4.0	wtfile	
d1	5.000	proc	ft
tof	9000.0	fn	not used
nt	16	math	f
ct	16		
alock	n		
gain	not used		
FLAGS		werr	
il	n	wexp	
in	n	wbs	
dp	y	wnt	
hs	ny		
DISPLAY			
sp	-396.7		
wp	10484.9		
vs	80		
sc	0		
wc	250		
hzmm	41.94		
is	500.00		
rfl	6186.7		
rfp	0		
th	58		
ins	100.000		
nm	cdc ph		



Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "varian300"

Relax. delay 1.000 sec
Pulse 52.0 degrees
Acq. time 1.998 sec
Width 4789.3 Hz
64 repetitions
OBSERVE H1, 299.9597215 MHz
DATA PROCESSING
FT size 32768
Total time 3 min, 15 sec



STANDARD CARBON PARAMETERS
v-ss-94paramethoxycarbon

Archive directory: /home/samanta/vnmrsys/data
Sample directory:

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

User: 1-14-87

File: v-ss-94paramethoxycarbon

INOVA-500 "Inova500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 31409.5 Hz

10000 repetitions

OBSERVE C13, 125.6479222 MHz

DECOUPLE H1, 499.6956872 MHz

Power 36 dB

continuously on

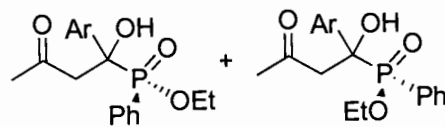
WALTZ-16 modulated

DATA PROCESSING

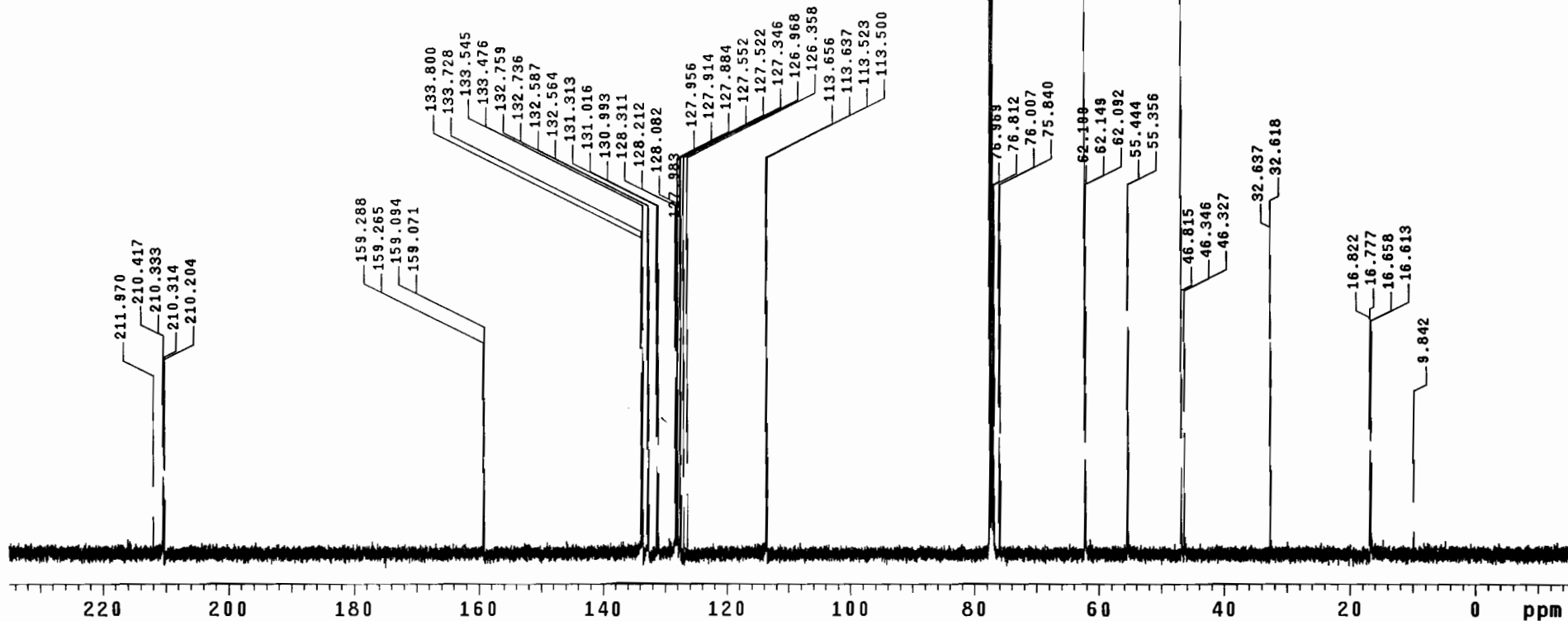
Line broadening 0.5 Hz

FT size 131072

Total time 6 hr, 24 min, 53 sec



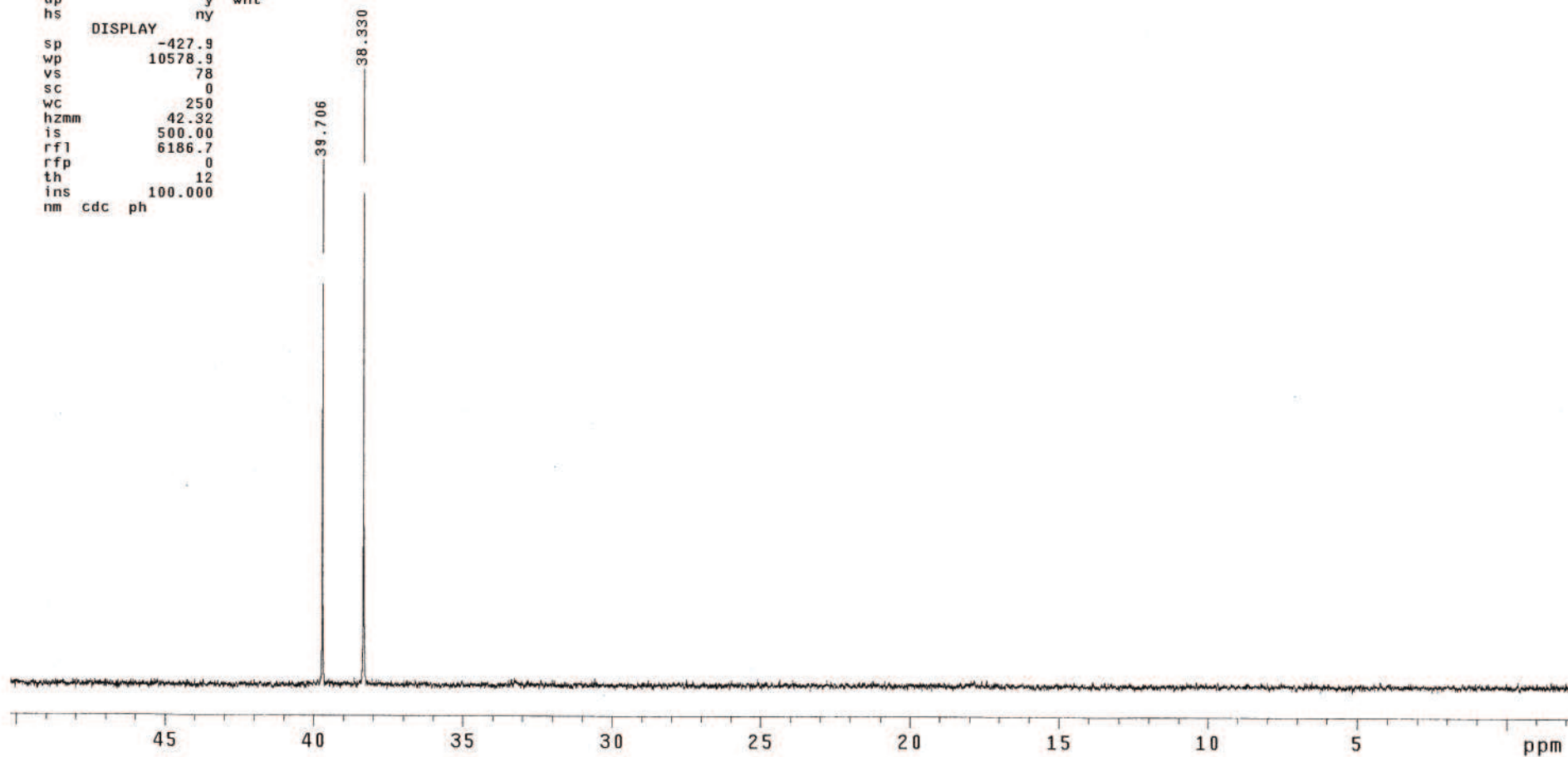
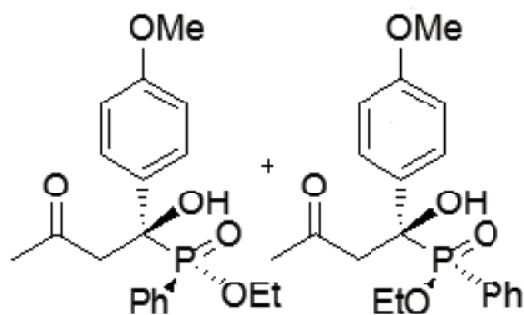
Ar = 4-MeO-C₆H₄



```

exp1 s2pul
SAMPLE DEC. & VT
date Dec 30 2009 dfrq 499.632
solvent CDC13 dn H1
file exp dpwr 36
ACQUISITION dof 0
sfrq 202.258 dm nny
tn P31 dmm w
at 1.600 dmf 10954
np 64000 dseq
sw 20000.0 dres 1.0
fb 11000 homo n
tpwr 54 temp 26.0
pw 4.0
d1 5.000 lb PROCESSING 1.00
tof 9000.0 wtfile
nt 16 proc ft
ct 16 fn not used f
alock n math
gain not used
FLAGS werr
il n wexp
in n wbs
dp y wnt
hs ny
DISPLAY
sp -427.9
wp 10578.9
vs 78
sc 0
wc 250
hzmm 42.32
is 500.00
rfl 6186.7
rfp 0
th 12
ins 100.000
nm cdc ph

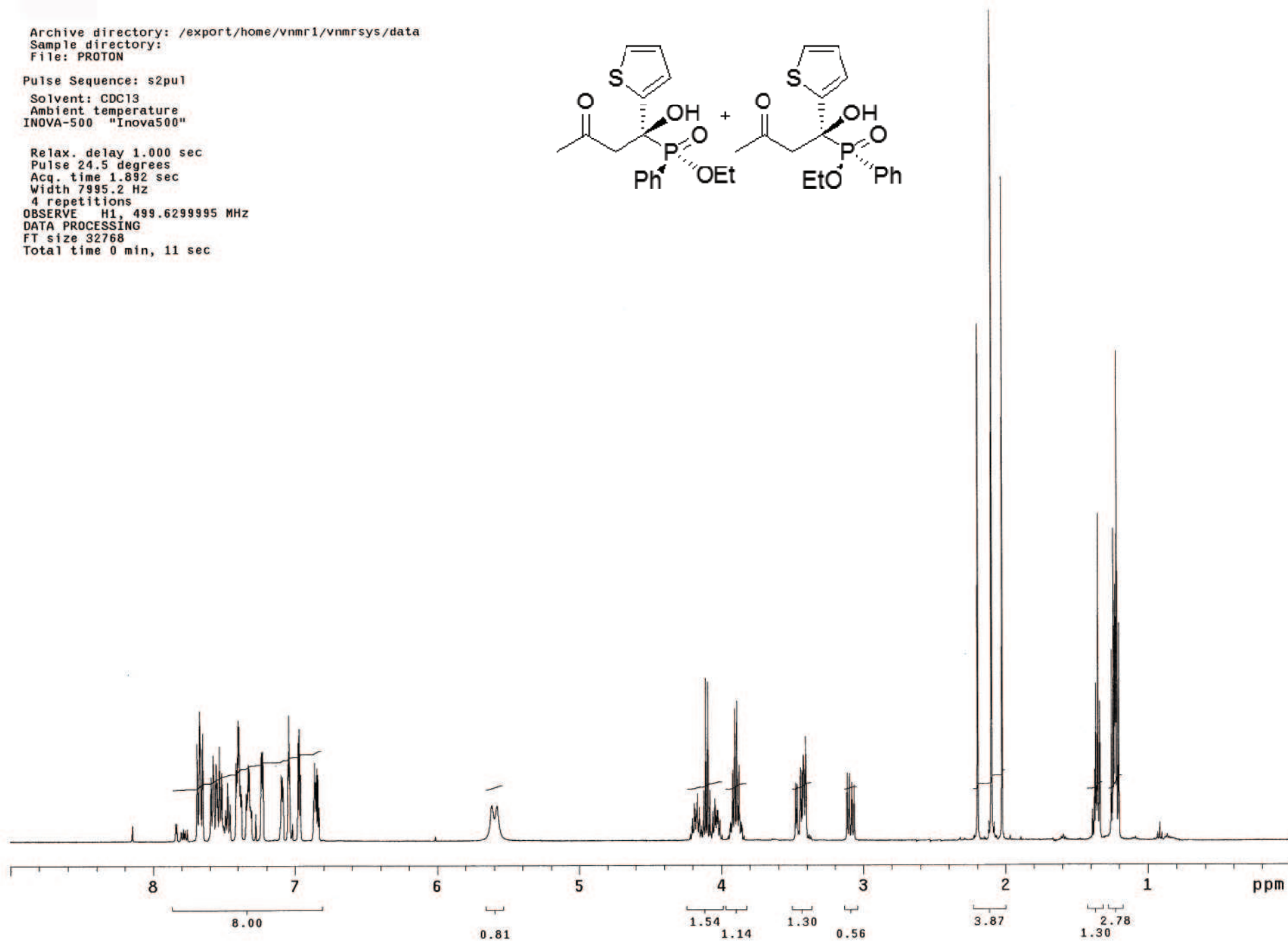
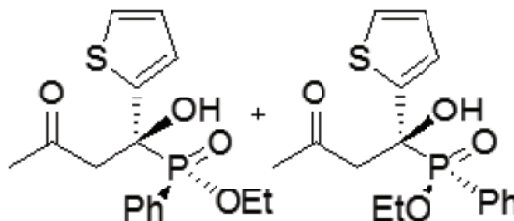
```



Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
4 repetitions
OBSERVE H1, 499.6299995 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 11 sec



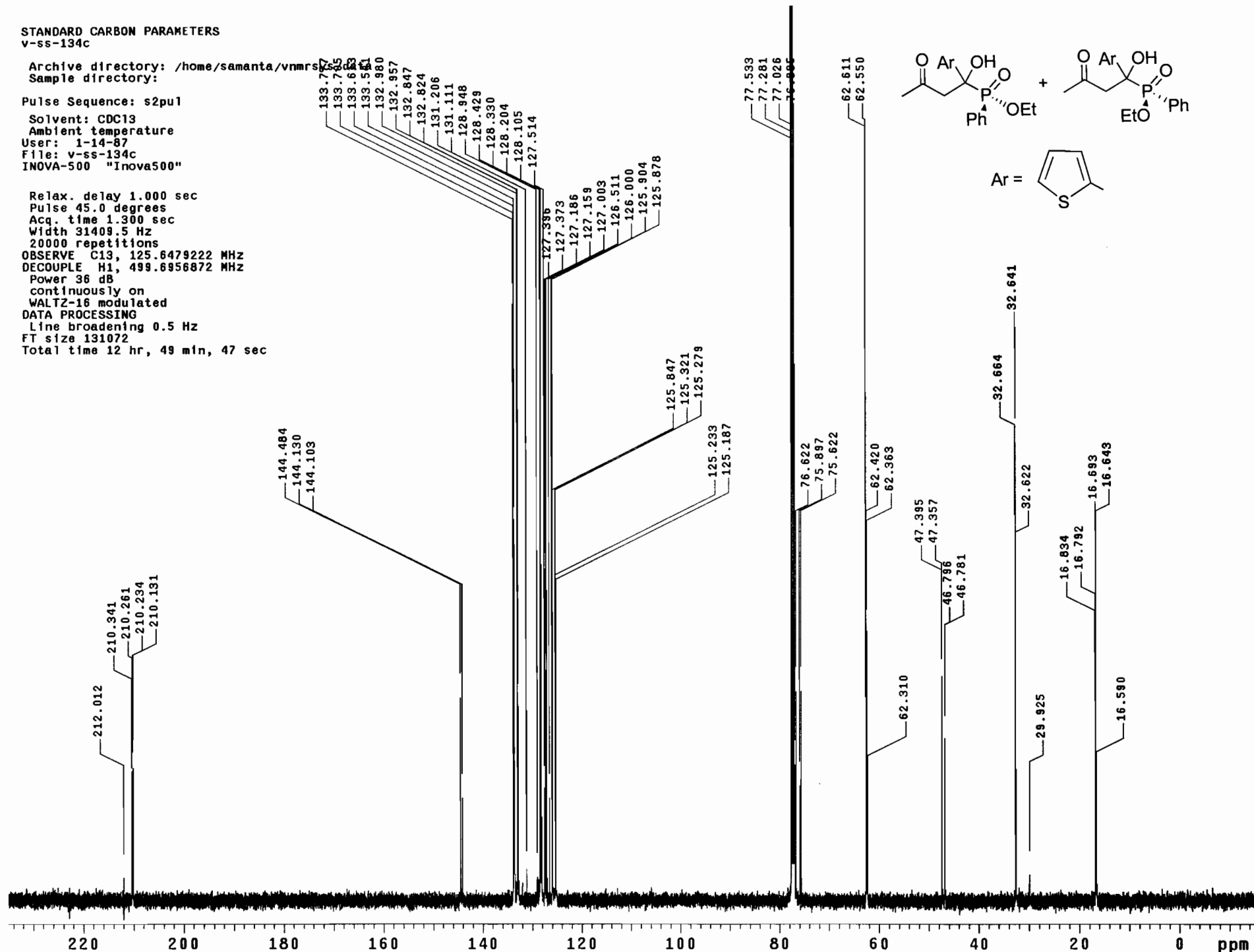
STANDARD CARBON PARAMETERS
v-ss-134c

Archive directory: /home/samanta/vnmrsv
Sample directory:

Pulse Sequence: s2pu1

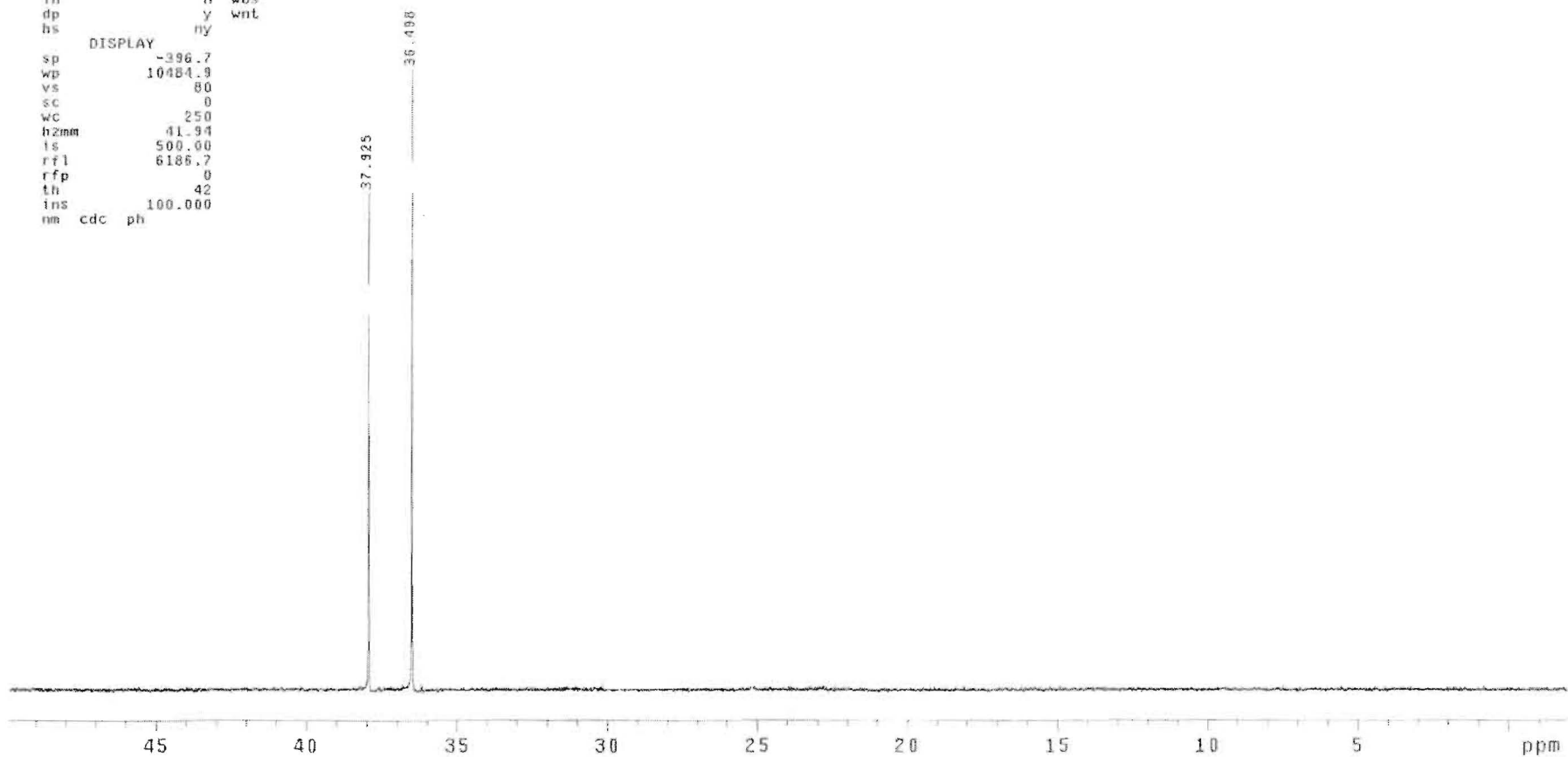
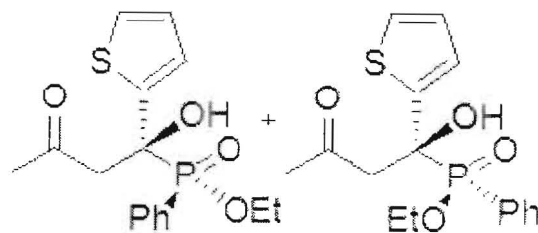
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: v-ss-134c
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
20000 repetitions
OBSERVE C13, 125.6479222 MHz
DECOUPLE H1, 499.6956872 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 12 hr, 49 min, 47 sec



exp1 s2pul

SAMPLE		DEC. & VT	
date	Dec 30 2009	dfrq	499.632
solvent	CDCl3	dn	H1
file	exp	dpwr	36
ACQUISITION			
sfrq	202.258	dm	ny
tn	P31	dmm	w
at	1.600	daf	10954
np	64000	dsq	
sw	20000.0	dres	1.0
fb	11000	homo	n
tpwr	54	temp	26.0
pw	4.0	PROCESSING	
d1	5.000	tb	1.00
tof	9000.0	wtfile	
nt	8	proc	ft
ct	8	in	not used
alock	n	math	f
gain	not used		
FLAGS			
il	n	werr	
in	n	wexp	
dp	y	wbs	
hs	ny	wnt	
DISPLAY			
sp	-396.7		
wp	10484.9		
vs	80		
sc	0		
wc	250		
h2mm	41.94		
ts	500.00		
rfl	6186.2		
rfp	0		
th	42		
ins	100.000		
nm	cdc ph		

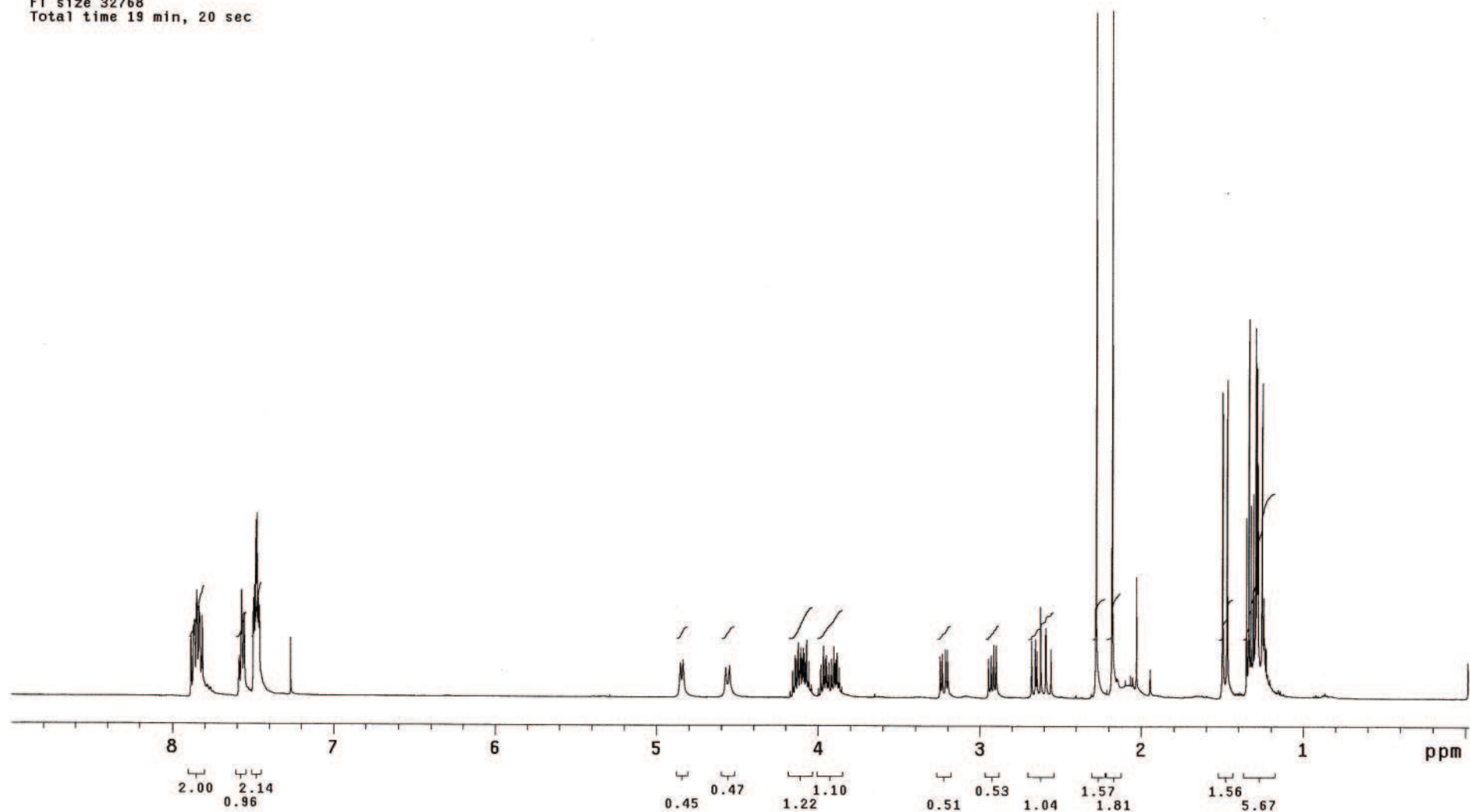
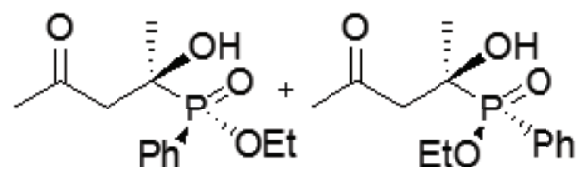


Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pul

Solvent: CDC13
Ambient temperature
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
400 repetitions
OBSERVE H1, 499.6391196 MHz
DATA PROCESSING
FT size 32768
Total time 19 min, 20 sec



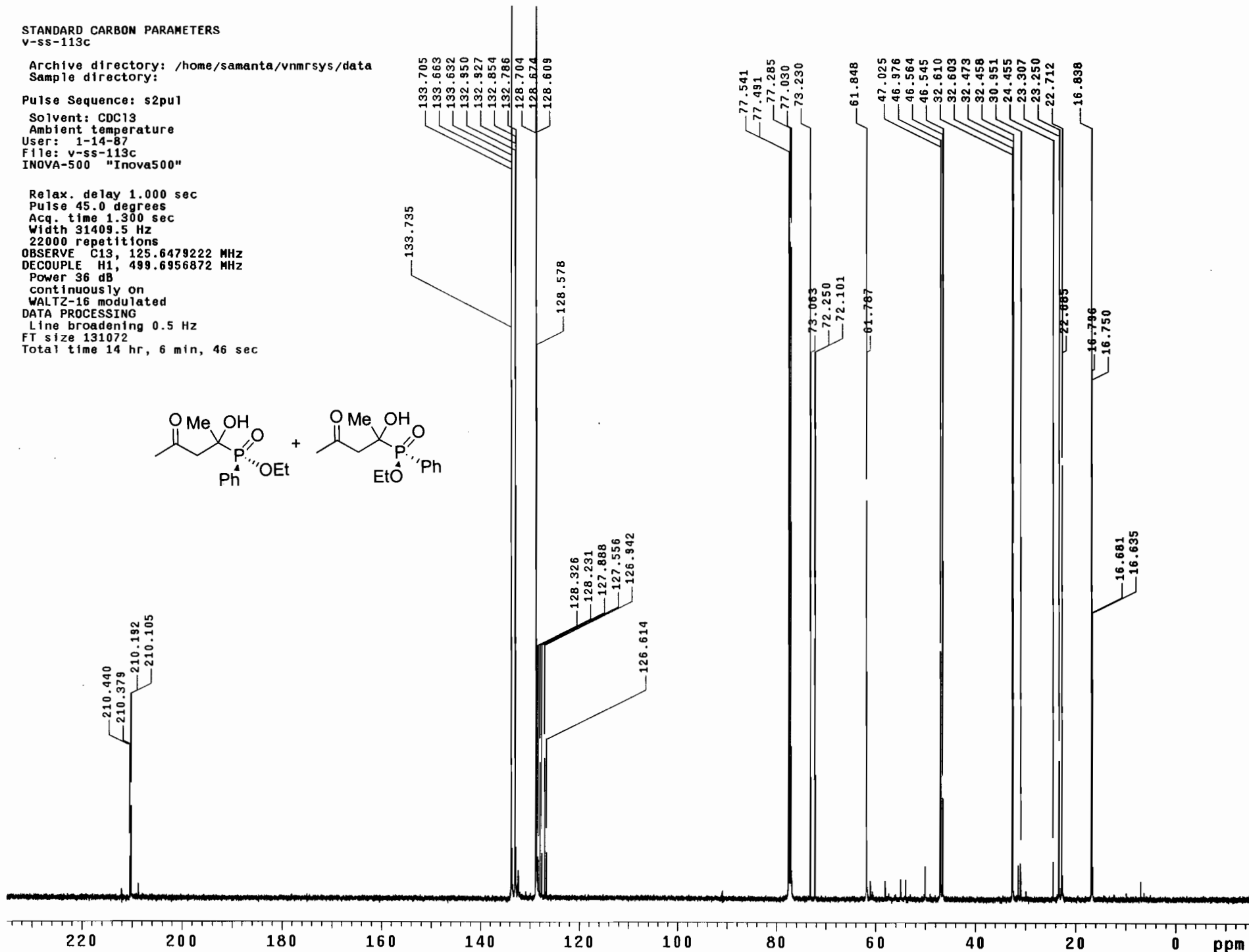
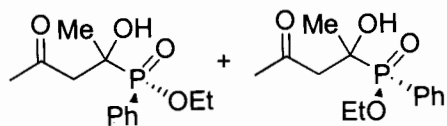
STANDARD CARBON PARAMETERS
v-ss-113c

Archive directory: /home/samanta/vnmrsys/data
Sample directory:

Pulse Sequence: s2pu1

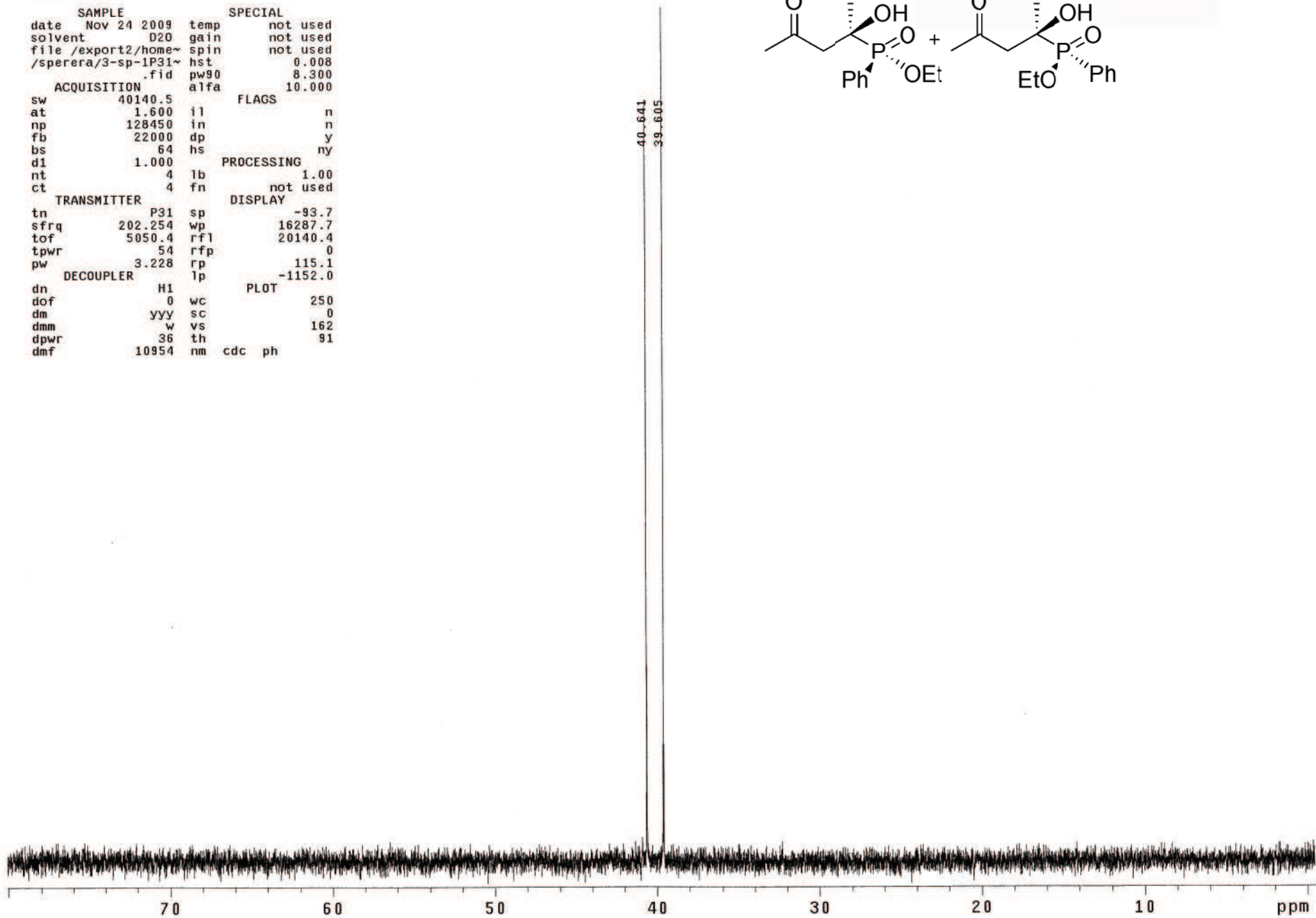
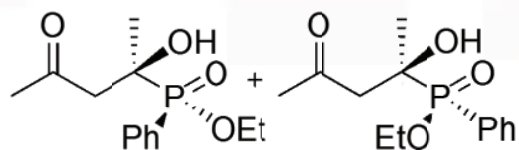
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: v-ss-113c
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
22000 repetitions
OBSERVE C13, 125.6479222 MHz
DECOUPLE H1, 499.6956872 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 14 hr, 6 min, 46 sec



exp3 s2pu1

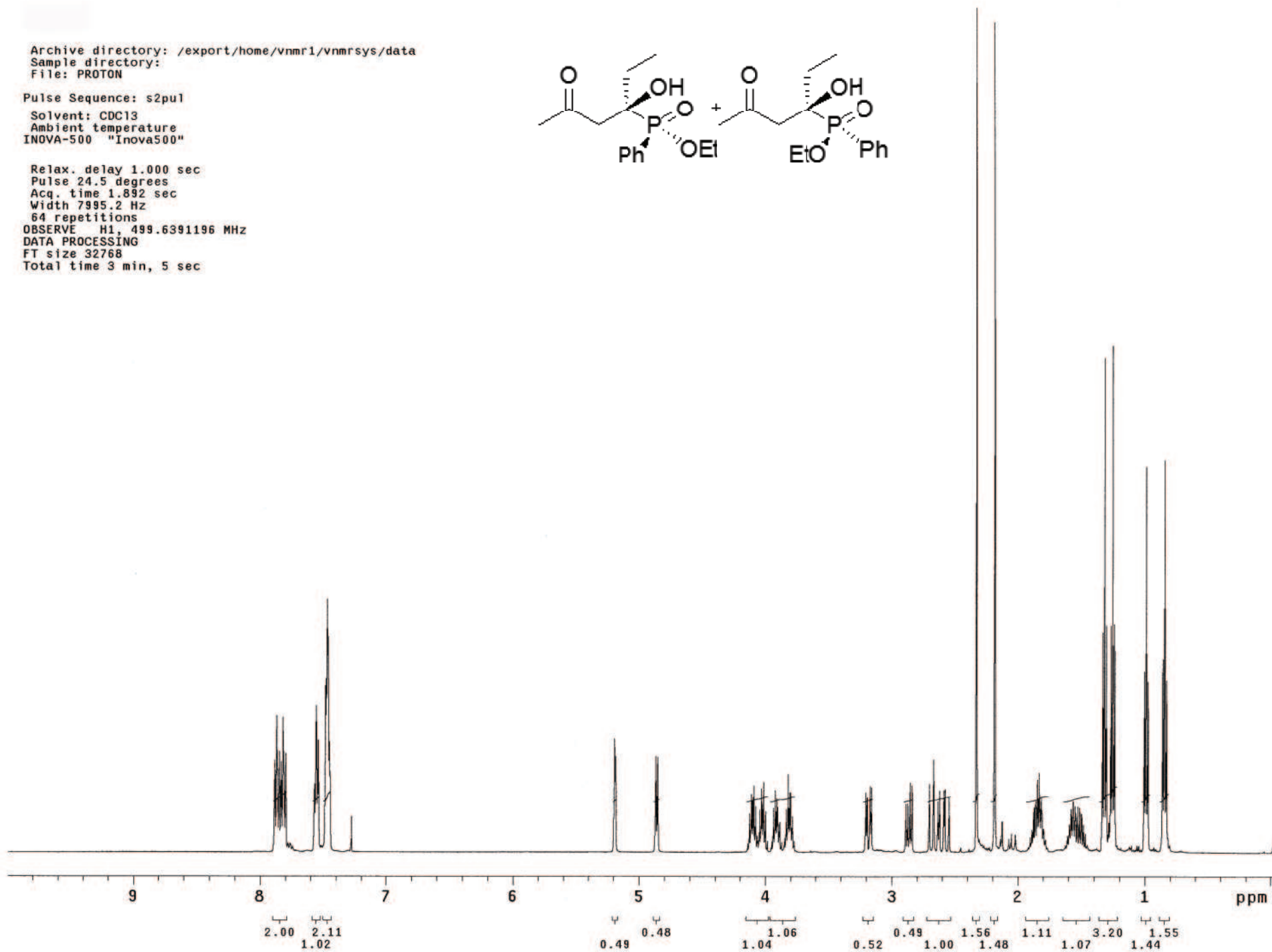
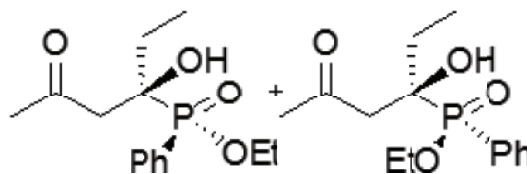
SAMPLE		SPECIAL	
date	Nov 24 2009	temp	not used
solvent	D2O	gain	not used
file	/export2/home~	spin	not used
/sperera/3-sp-1P31~		hst	0.008
.fid		pw90	8.300
alfa			10.000
ACQUISITION		FLAGS	
sw	40140.5		
at	1.600	il	n
np	128450	in	n
fb	22000	dp	y
bs	64	hs	ny
d1	1.000	PROCESSING	
nt	4	lb	1.00
ct	4	fn	not used
TRANSMITTER		DISPLAY	
tn	P31	sp	-93.7
sfrq	202.254	wp	16287.7
tof	5050.4	rfl	20140.4
tpwr	54	rffp	0
pw	3.228	rp	115.1
		lp	-1152.0
DECOUPLER		PLOT	
dn	H1		
dof	0	wc	250
dm	yyy	sc	0
dmm	w	vs	162
dpwr	36	th	91
dmf	10954	nm	cdc ph



Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pul
Solvent: CDC13
Ambient temperature
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
64 repetitions
OBSERVE H1, 499.6391196 MHz
DATA PROCESSING
FT size 32768
Total time 3 min, 5 sec



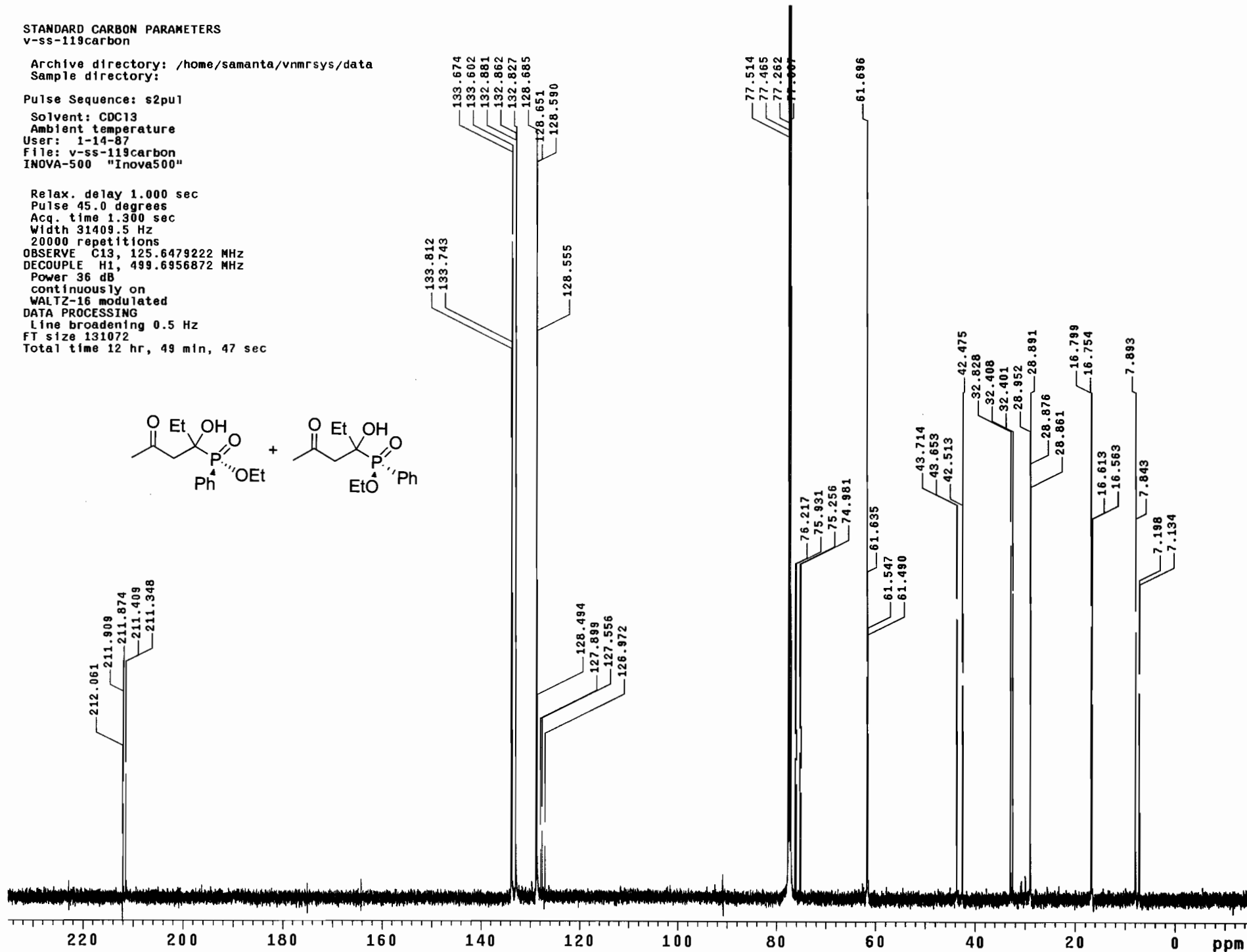
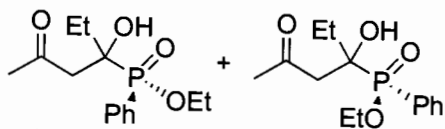
STANDARD CARBON PARAMETERS
v-ss-119carbon

Archive directory: /home/samanta/vnmr/sys/data
Sample directory:

Pulse Sequence: s2pu1

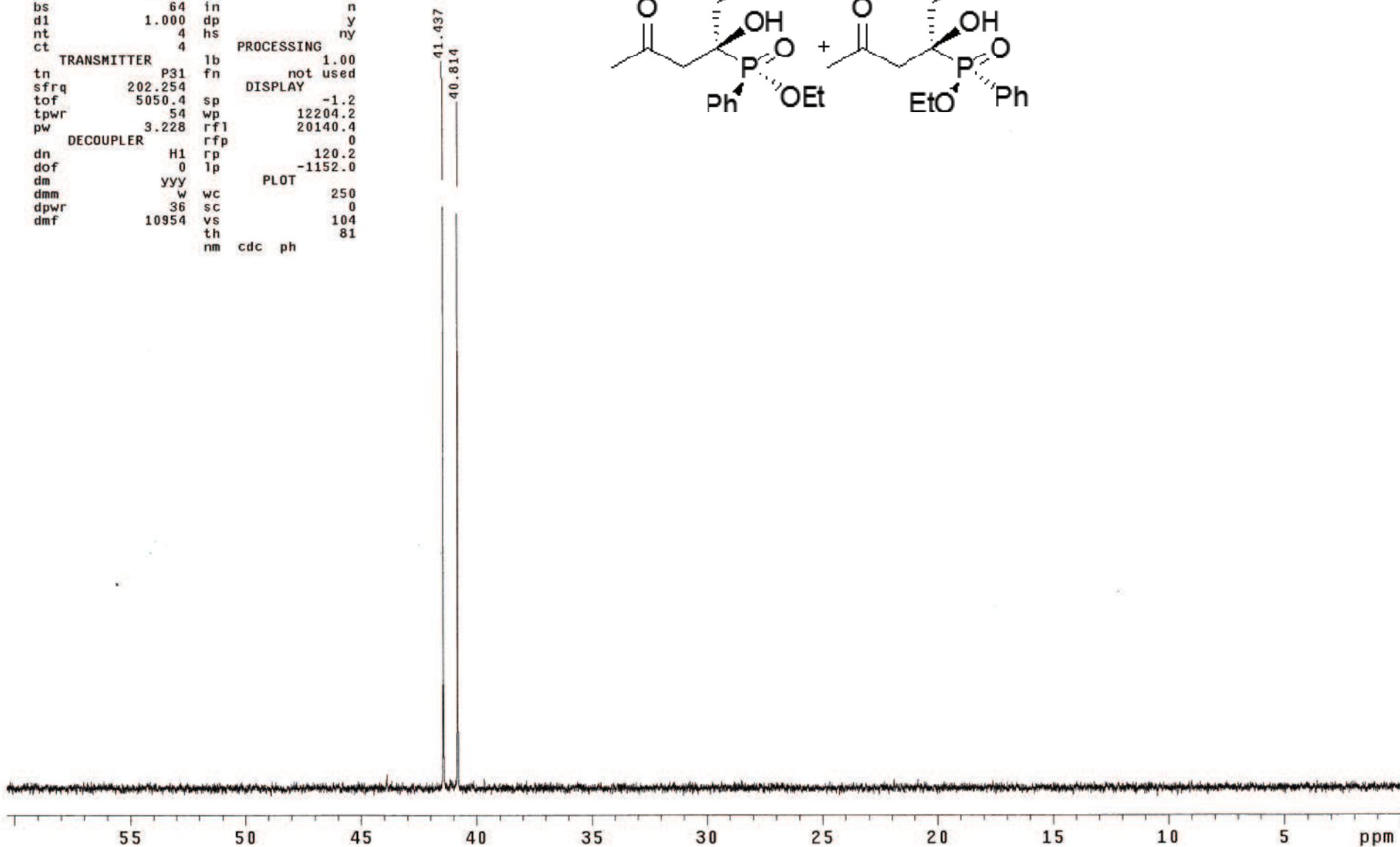
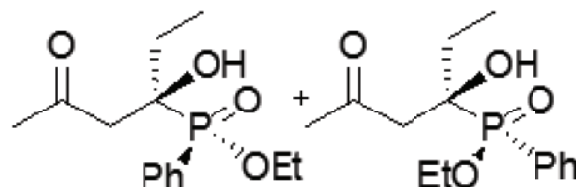
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: v-ss-119carbon
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
20000 repetitions
OBSERVE C13, 125.6479222 MHz
DECOUPLE H1, 499.6956872 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 12 hr, 49 min, 47 sec



exp3 s2pu1

SAMPLE		SPECIAL	
date	Nov 24 2009	temp	not used
solvent	D2O	gain	not used
file	exp	spin	not used
ACQUISITION		SPECIAL	
sw	40140.5	hst	0.008
at	1.600	pw90	8.300
np	128450	alfa	10.000
fb	22000	FLAGS	
bs	64	il	n
d1	1.000	in	n
nt	4	dp	y
ct	4	hs	ny
TRANSMITTER		PROCESSING	
tn	P31	lb	1.00
sfrq	202.254	fn	not used
tof	5050.4	DISPLAY	
tpwr	54	sp	-1.2
pw	3.228	wp	12204.2
DECOUPLER		rfl	20140.4
dn	H1	rfp	0
dof	0	rp	120.2
dm	YYY	lp	-1152.0
dmm	36	PLOT	
dpwr	10954	wc	250
dmf		sc	0
		vs	104
		th	81
		nm	cdc ph

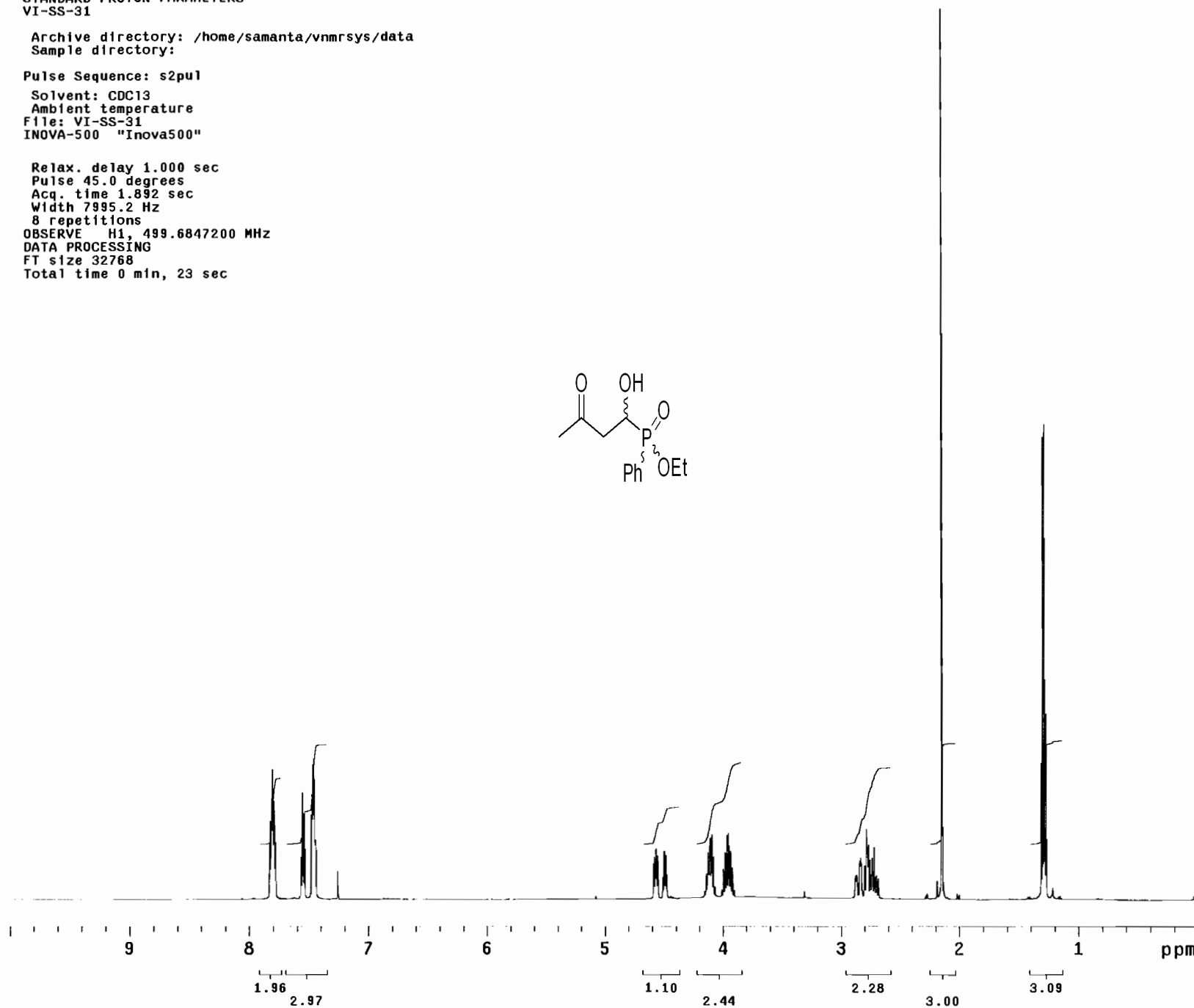
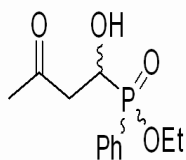


STANDARD PROTON PARAMETERS
VI-SS-31

Archive directory: /home/samanta/vnmrsys/data
Sample directory:

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
File: VI-SS-31
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
8 repetitions
OBSERVE H1, 499.6847200 MHz
DATA PROCESSING
FT size 32768
Total time 0 min, 23 sec



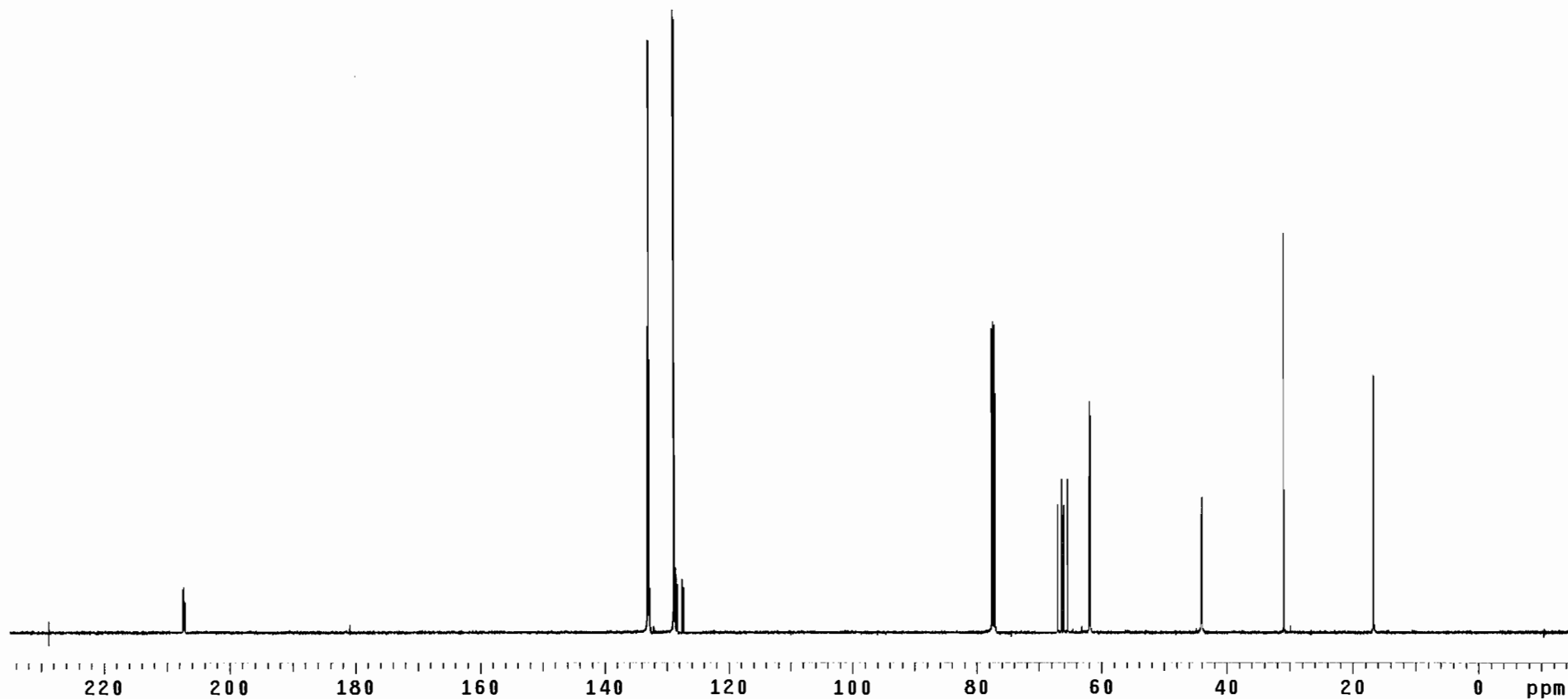
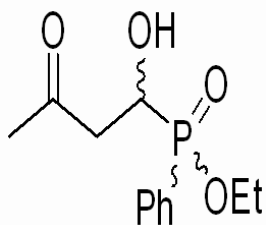
STANDARD CARBON PARAMETERS
VI-SS-31c

Archive directory: /home/samanta/vnmrsys/data
Sample directory:

Pulse Sequence: s2pu1

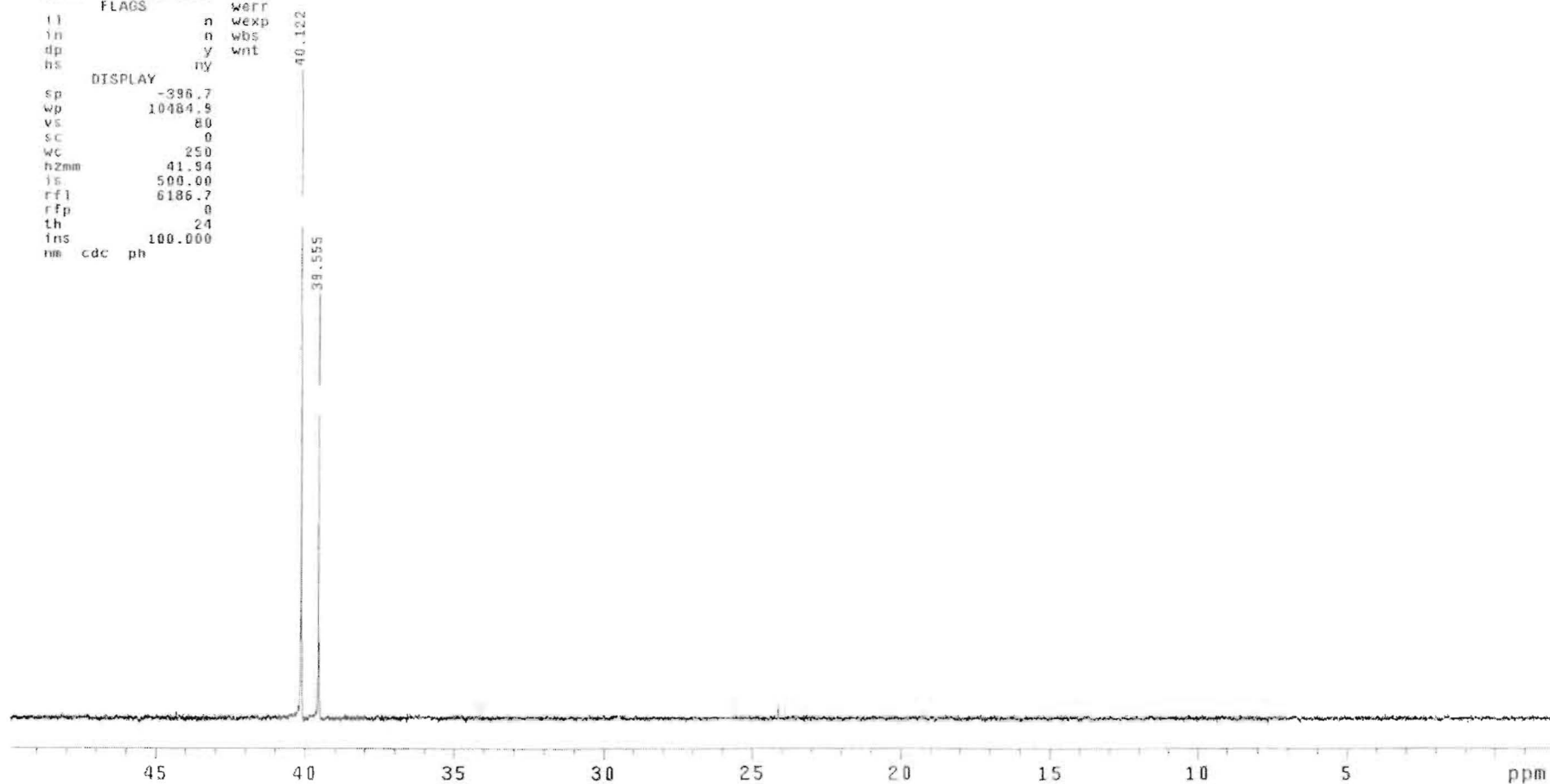
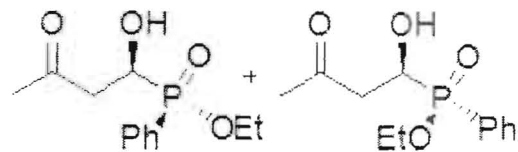
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: VI-SS-31carbon
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
8000 repetitions
OBSERVE C13, 125.6457928 MHz
DECOUPLE H1, 499.6872185 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 5 hr, 7 min, 54 sec



expi s2pu1

```
SAMPLE          DEC. & VT
date    Dec 30 2009  dfrq      499.632
solvent  CDC13      dn        h1
file     exp        dpwr      35
          ACQUISITION  dof        0
sfrq    202.258    dm         nny
tn       P31       dnm        w
at       1.600     dmf       10954
np       64000     dseq
sw       20000.0   dres      1.0
fb       11000    homo      n
tpwr     54       temp     25.0
pw       4.0      PROCESSING
dl       5.000    lb        1.00
tof      9000.0   utfile
nt       8        proc      ft
ct       8        fn        not used
alock    n        math      f
gain     not used
          FLAGS
ll       n        werr
ln       n        wexp
dp       y        wbs
hs       ny       wnt
          DISPLAY
sp       -396.7
wp       10484.5
vs       80
sc       0
wc       250
hzmm     41.94
js       500.00
rf1      6186.7
rfp      0
th       24
lms     100.000
nm      cdc ph
```

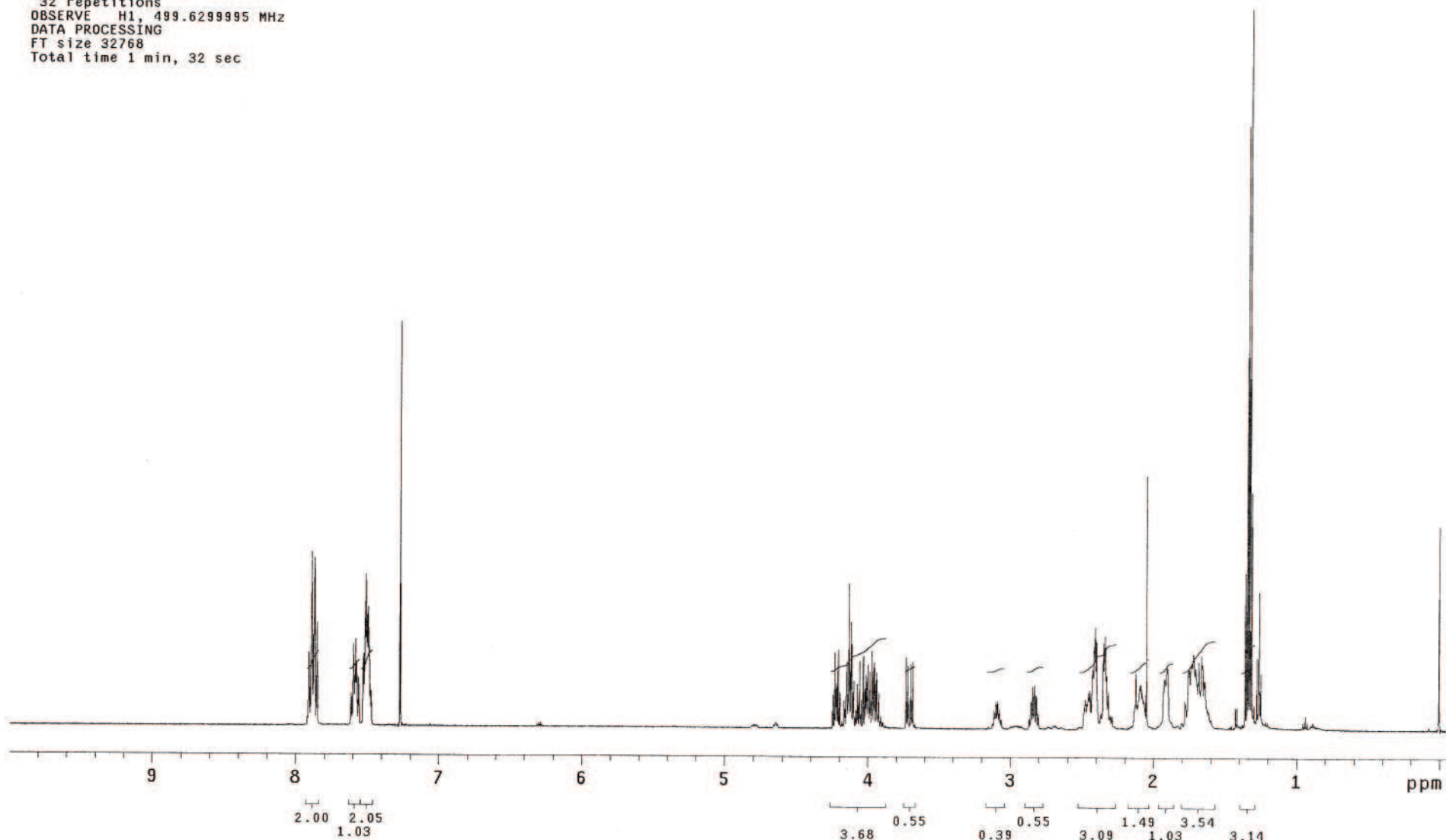
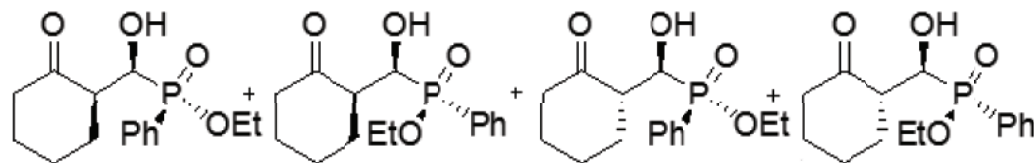


STANDARD PROTON PARAMETERS

Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory:
 File: PROTON

Pulse Sequence: s2pu1
 Solvent: CDC13
 Ambient temperature
 INOVA-500 "Inova500"

Relax. delay 1.000 sec
 Pulse 24.5 degrees
 Acq. time 1.892 sec
 Width 7995.2 Hz
 32 repetitions
 OBSERVE H1, 499.6299995 MHz
 DATA PROCESSING
 FT size 32768
 Total time 1 min, 32 sec



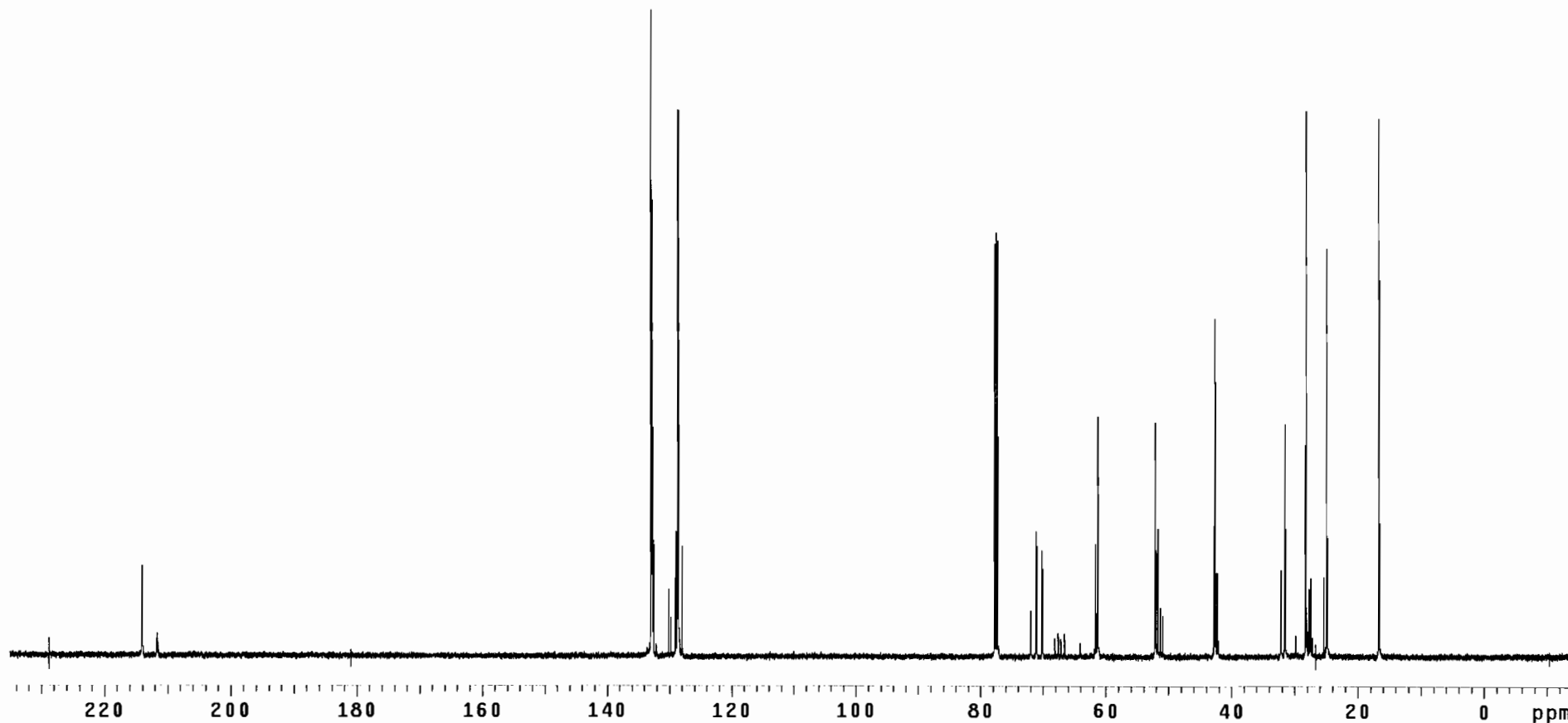
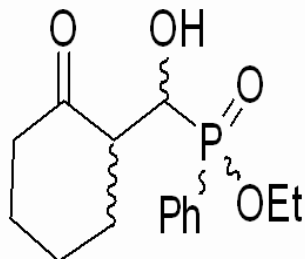
STANDARD CARBON PARAMETERS
VI-SS-53c

Archive directory: /home/samanta/vnmrsys/data
Sample directory:

Pulse Sequence: s2pu1

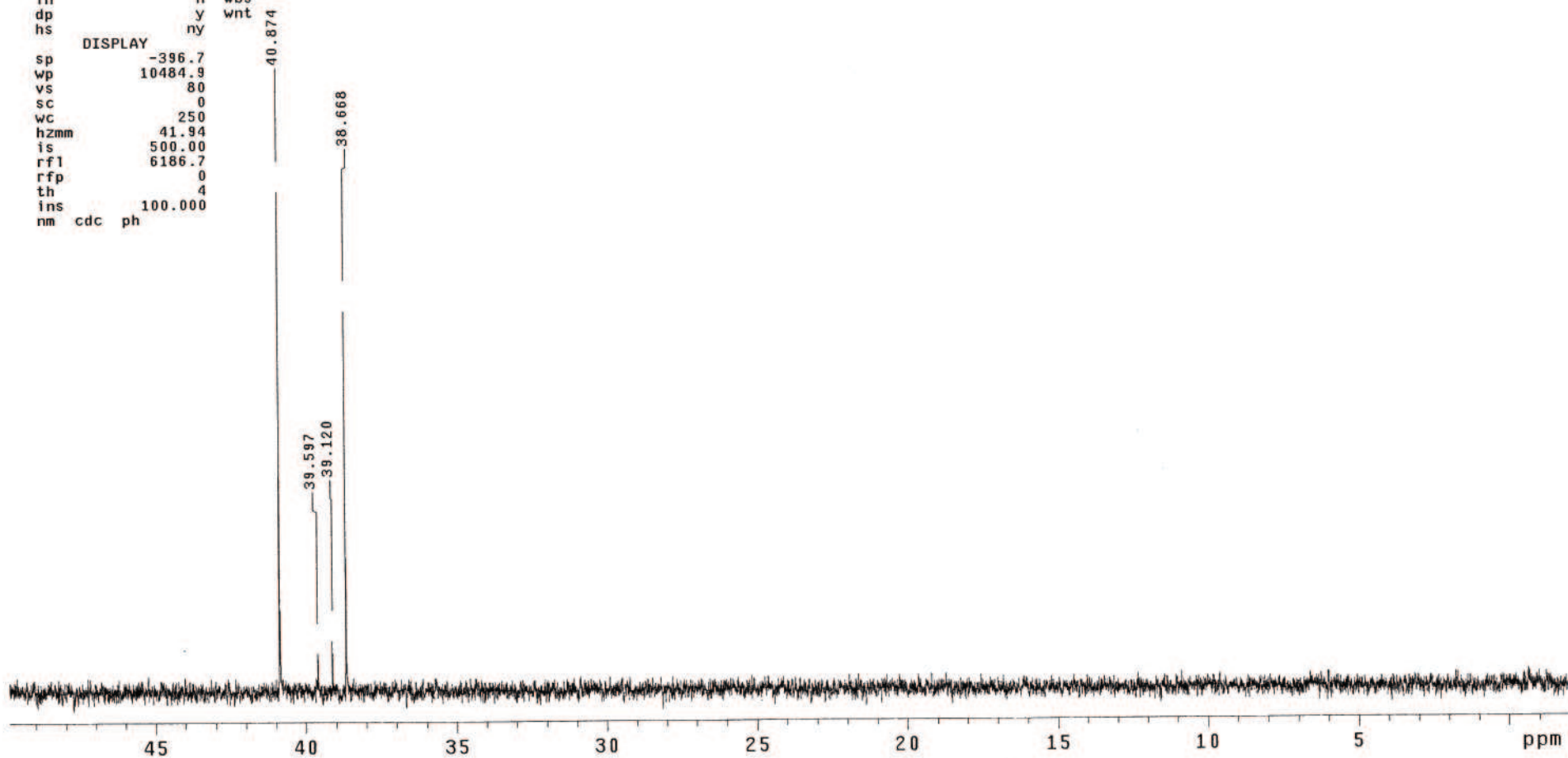
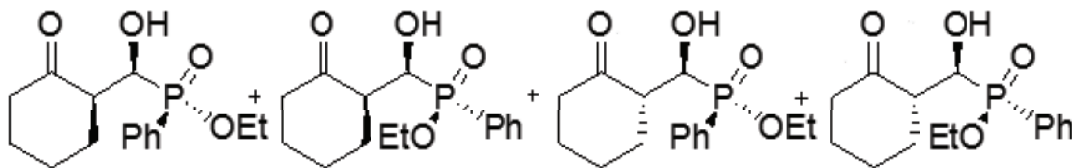
Solvent: CDC13
Ambient temperature
User: 1-14-87
File: VI-SS-53c
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
6900 repetitions
OBSERVE C13, 125.6457928 MHz
DECOUPLE H1, 499.6872185 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 4 hr, 25 min, 34 sec



exp1 s2pu1

SAMPLE		DEC. & VT	
date	Dec 30 2009	dfrq	499.632
solvent	CDC13	dn	H1
file	exp	dpwr	36
ACQUISITION		dof	0
sfrq	202.258	dm	nny
tn	P31	dmm	w
at	1.600	dmf	10954
np	64000	dseq	
sw	20000.0	dres	1.0
fb	11000	homo	n
tpwr	54	temp	26.0
pw	4.0	PROCESSING	
d1	5.000	lb	1.00
tof	9000.0	wtfile	
nt	8	proc	ft
ct	8	fn	not used
alock	n	math	f
gain	not used		
FLAGS		werr	n
il	n	wexp	n
in	n	wbs	n
dp	y	wnt	n
hs	ny		
DISPLAY			
sp	-396.7		
wp	10484.9		
vs	80		
sc	0		
wc	250		
hzmm	41.94		
is	500.00		
rf1	6186.7		
rfp	0		
th	4		
ins	100.000		
nm	cdc ph		

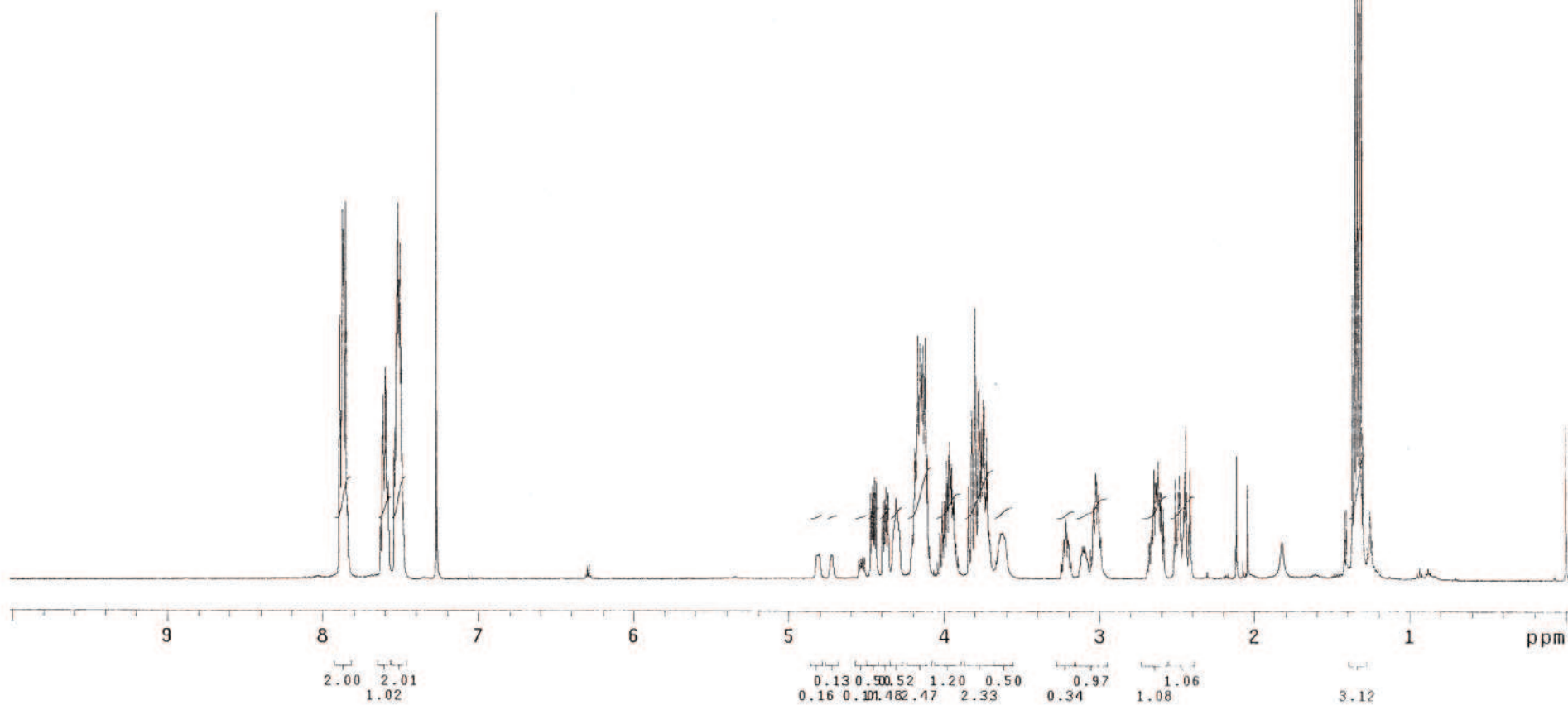
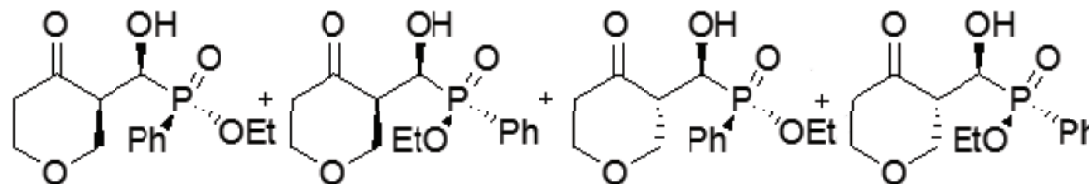


Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
64 repetitions
OBSERVE H1, 499.6299995 MHz
DATA PROCESSING
FT size 32768
Total time 3 min, 5 sec



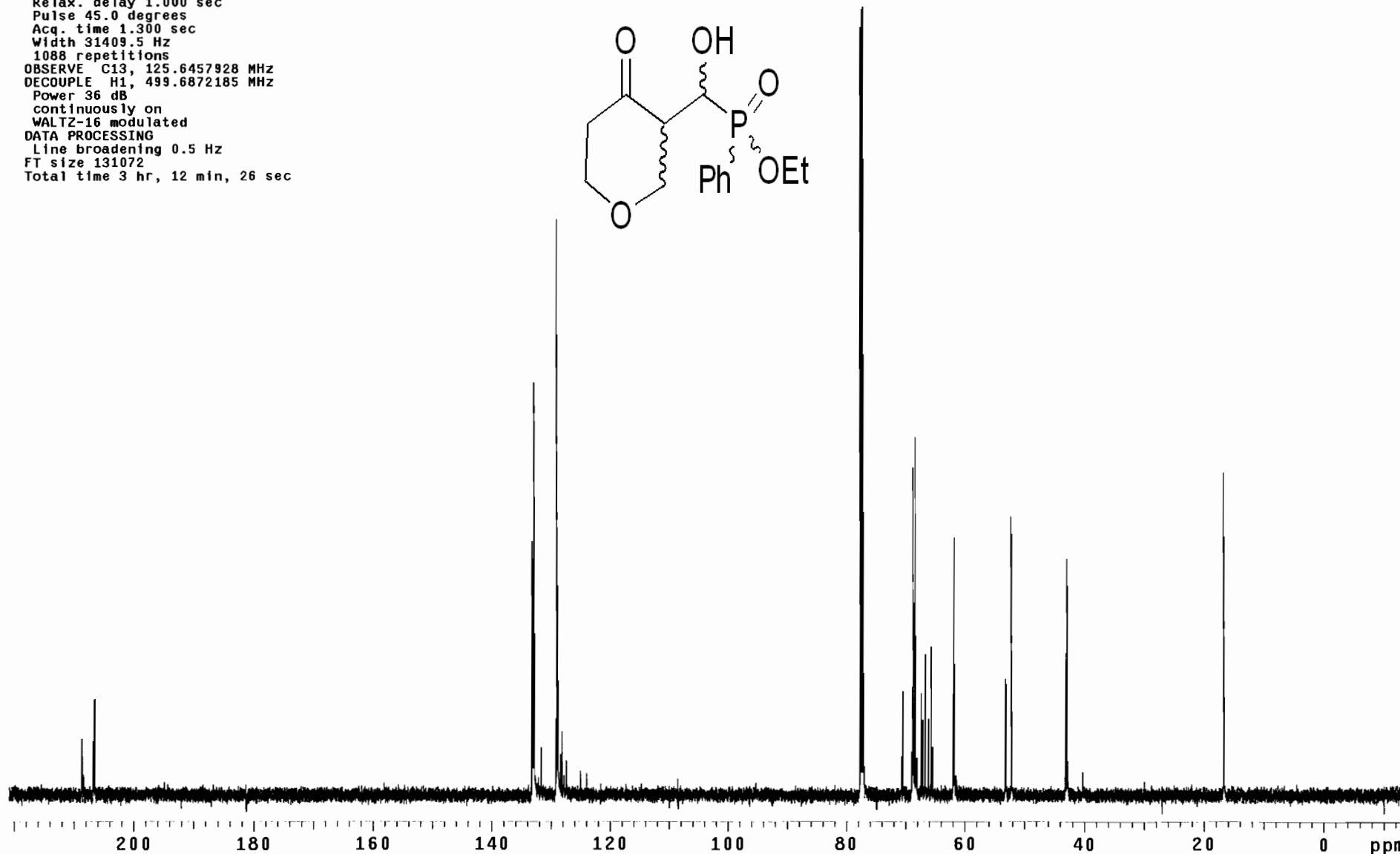
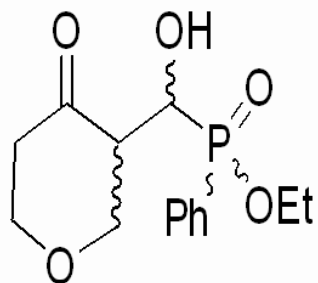
STANDARD CARBON PARAMETERS
VI-SS-78c

Archive directory: /home/samanta/vnmrSYS/data
Sample directory:

Pulse Sequence: s2pu1

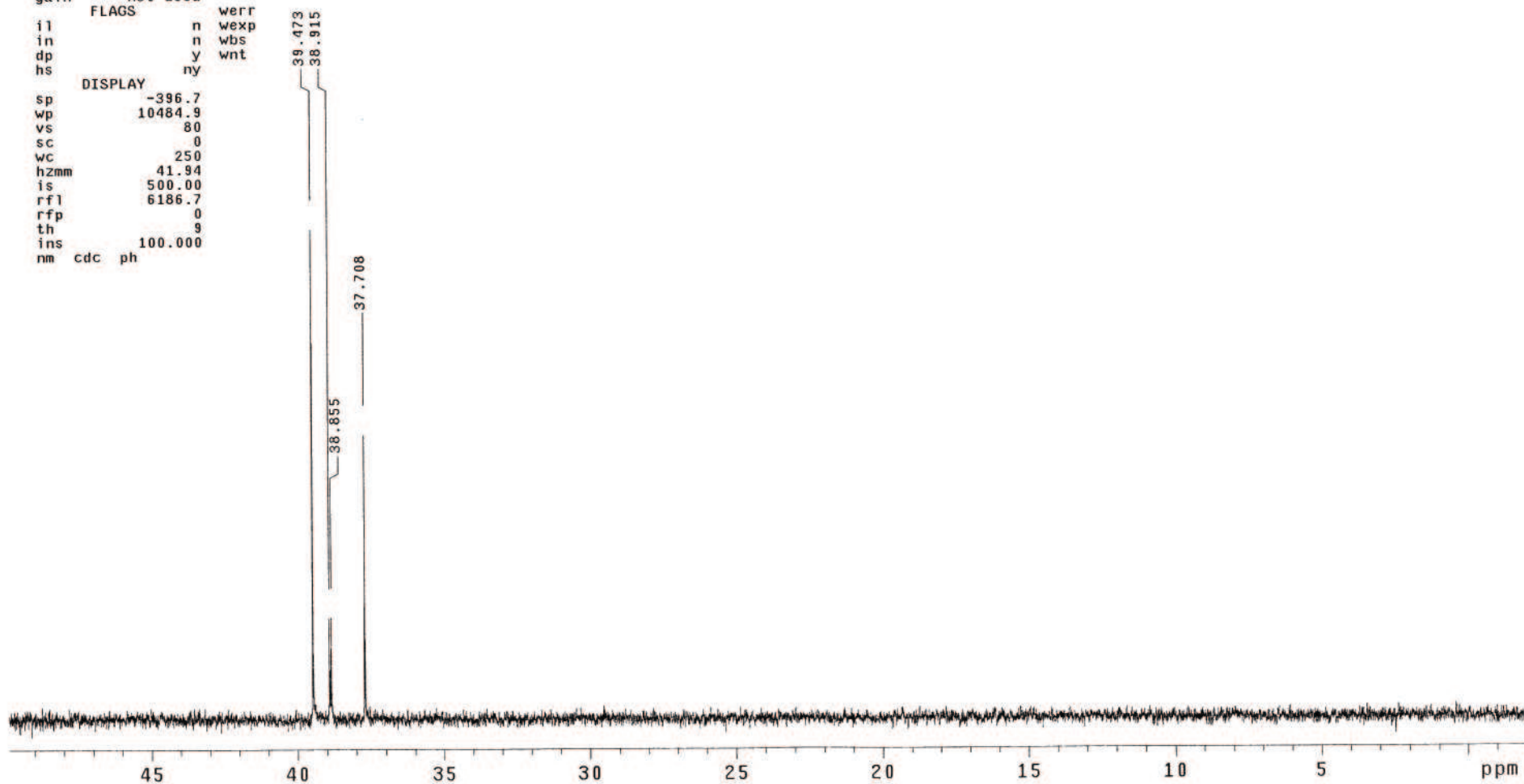
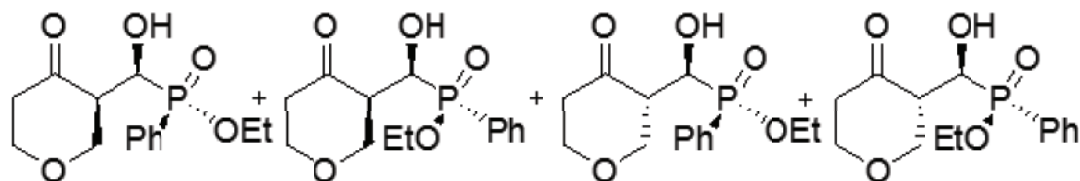
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: VI-SS-78C
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
1088 repetitions
OBSERVE C13, 125.6457928 MHz
DECOUPLE H1, 499.6872185 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 3 hr, 12 min, 26 sec



exp1 s2pul

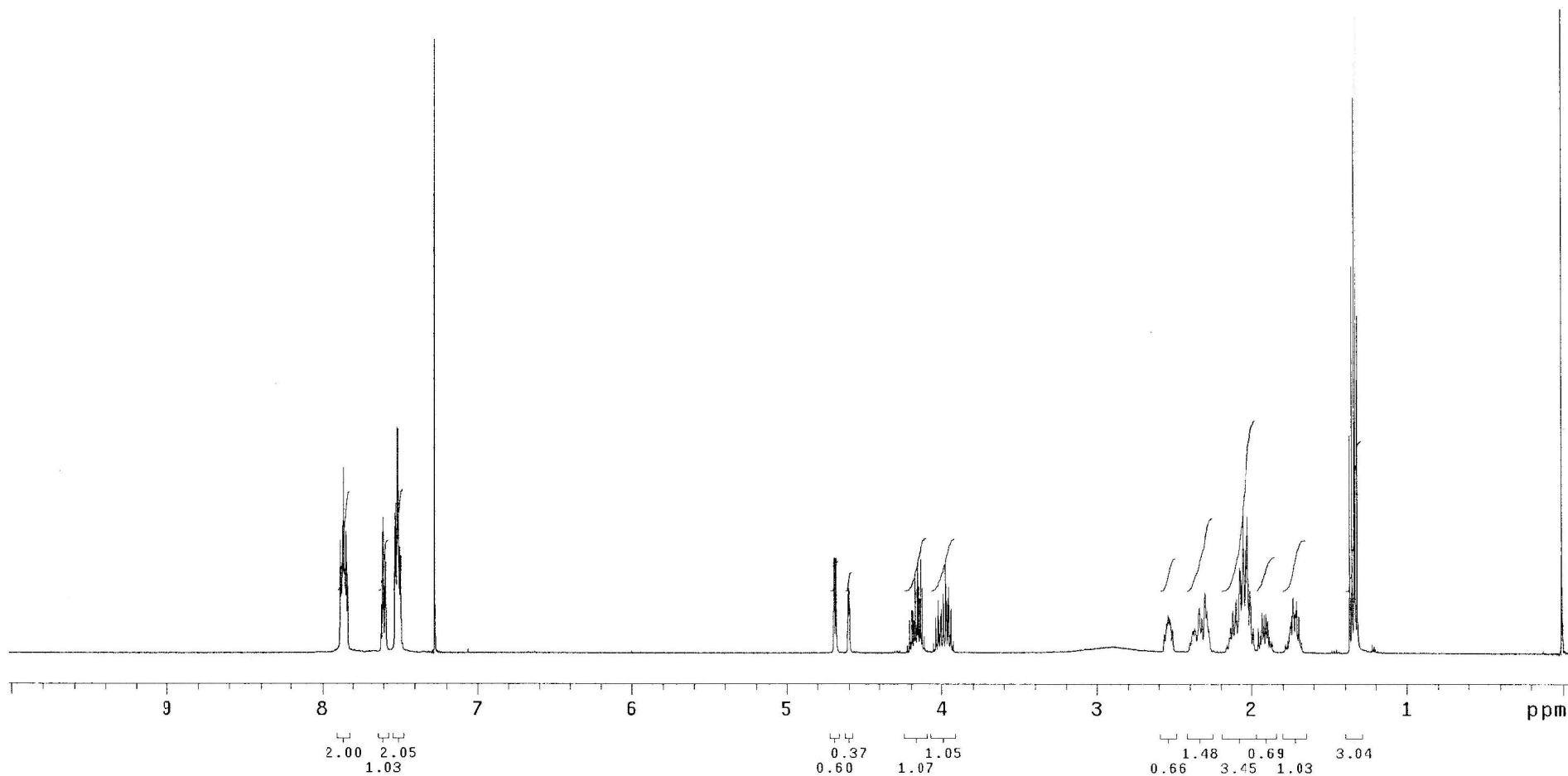
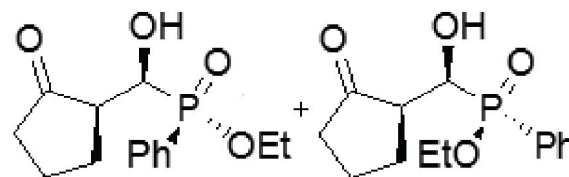
SAMPLE		DEC. & VT	
date	Dec 30 2009	dfrq	499.632
solvent	CDC13	dn	H1
file	exp	dpwr	36
ACQUISITION			
sfrq	202.258	dm	nny
tn	P31	dmm	w
at	1.600	dmf	10954
np	64000	dseq	
sw	20000.0	dres	1.0
fb	11000	homo	n
tpwr	54	temp	26.0
pw	4.0	PROCESSING	
d1	5.000	lb	1.00
tof	9000.0	wtfile	
nt	8	proc	ft
ct	8	fn	not used
alock	n	math	f
gain	not used		
FLAGS		werr	n
il	n	wexp	n
in	n	wbs	n
dp	y	wnt	n
hs	ny		
DISPLAY			
sp	-396.7		
wp	10484.9		
vs	80		
sc	0		
wc	250		
hzmm	41.94		
is	500.00		
rfl	6186.7		
rfp	0		
th	9		
ins	100.000		
nm	cdc ph		



Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul
Solvent: CDC13
Ambient temperature
File: 3-sp-28cyclopentane
INOVA-500 "Inova500"

Relax. delay 1.000 sec
Pulse 24.5 degrees
Acq. time 1.892 sec
Width 7995.2 Hz
32 repetitions
OBSERVE H1, 499.6299995 MHz
DATA PROCESSING
FT size 32768
Total time 1 min, 32 sec



STANDARD CARBON PARAMETERS
VI-SS-cyclopentanonecarbon

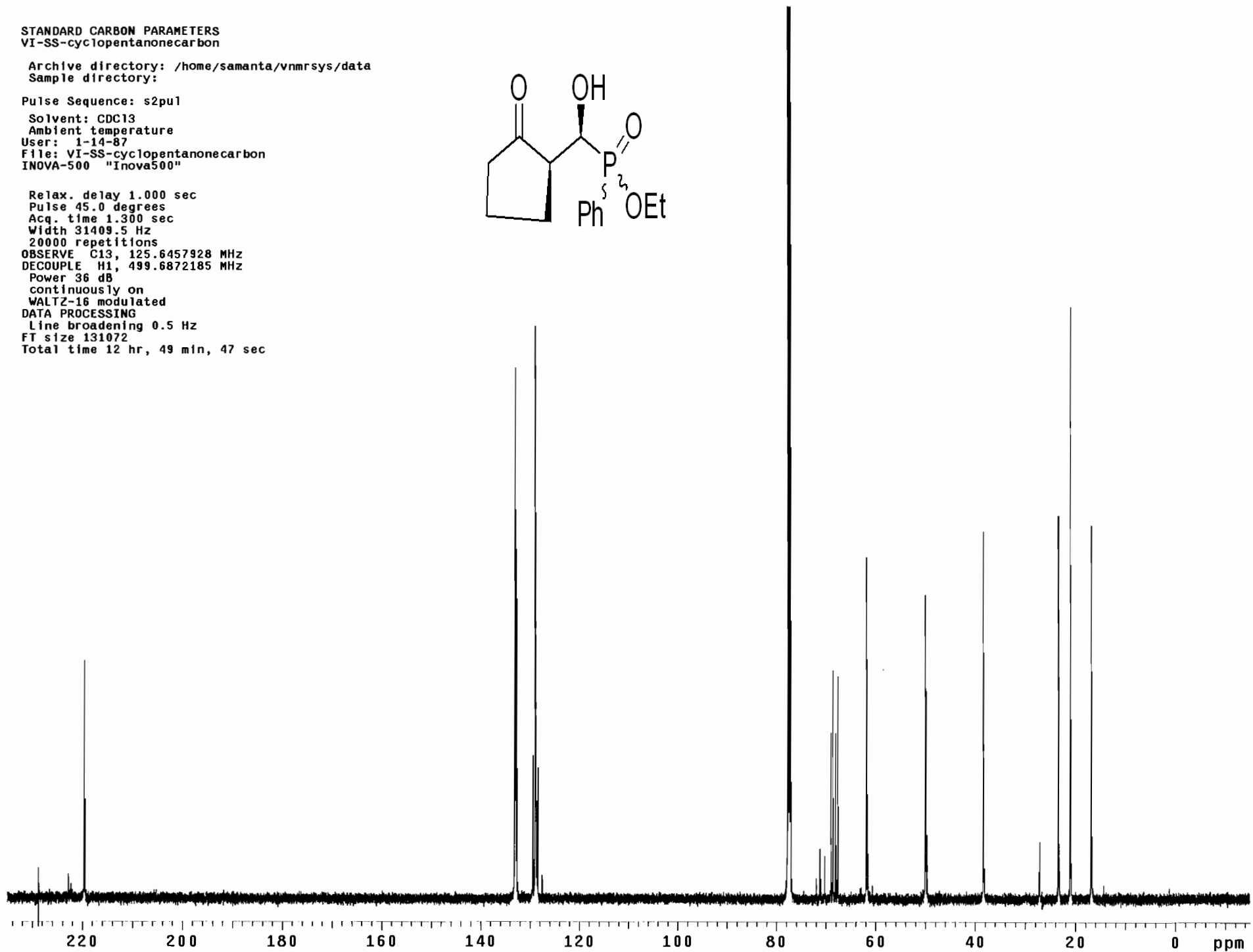
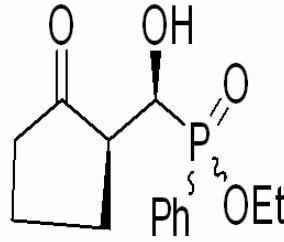
Archive directory: /home/samanta/vnmrsys/data
Sample directory:

Pulse Sequence: s2pu1

Solvent: CDC13
Ambient temperature
User: 1-14-87

File: VI-SS-cyclopentanonecarbon
INOVA-500 "Inova500"

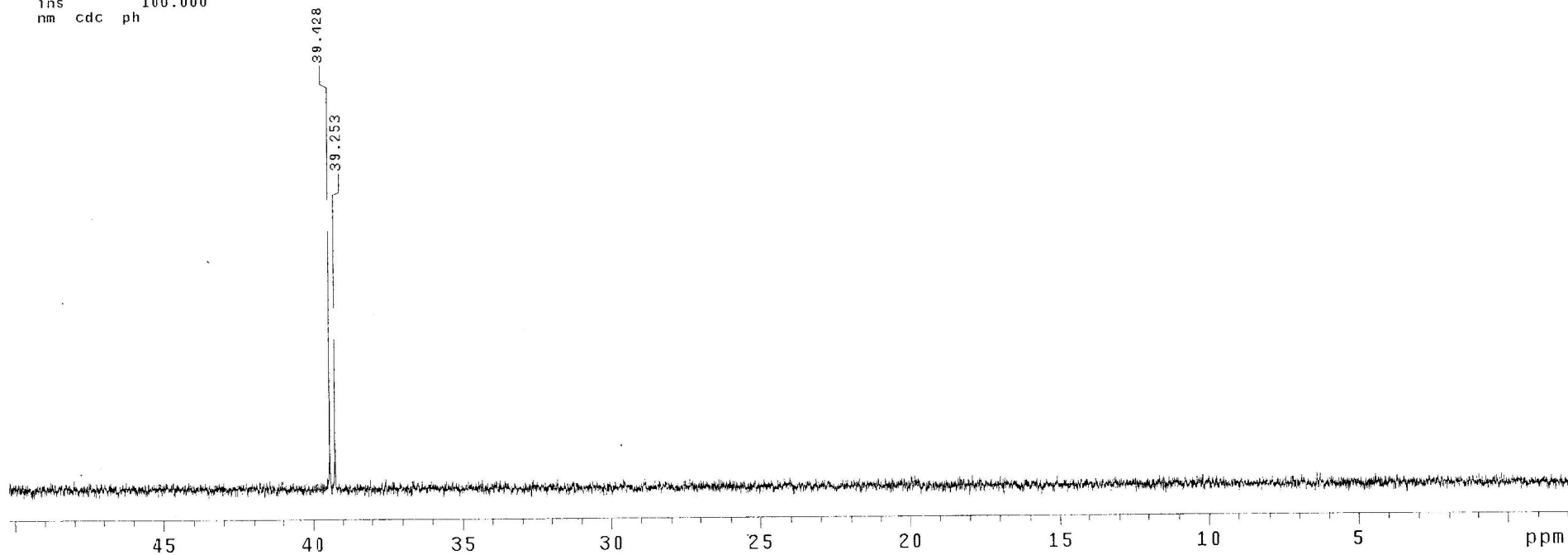
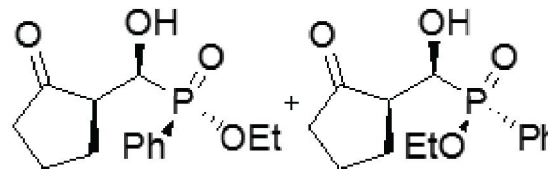
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31409.5 Hz
20000 repetitions
OBSERVE C13, 125.6457928 MHz
DECOUPLE H1, 499.6872185 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 12 hr, 49 min, 47 sec



```

expl s2pu1
SAMPLE          DEC. & VT
date   Dec 30 2009  dfrq   499.632
solvent CDC13      dn     H1
file   exp        dpwr   36
ACQUISITION    dof     0
sfrq   202.258   dm     nny
tn     P31       dmm    w
at     1.600    dmf    10954
np     64000    dseq
sw     20000.0  dres   1.0
fb     11000   homo   n
tpwr   54      temp   26.0
pw     4.0     PROCESSING
d1     5.000   lb     1.00
tof    9000.0 wtfile
nt     16     proc   ft
ct     16     fn     not used
alock  n      math   f
gain   not used
FLAGS
il     n      werr
in     n      wexp
dp     y      wbs
hs     ny     wnt
DISPLAY
sp     -427.9
wp     10578.9
vs     42
sc     0
wc     250
hzmm   42.32
is     500.00
rfl    6186.7
rfp    0
th     17
ins    100.000
nm     cdc ph

```

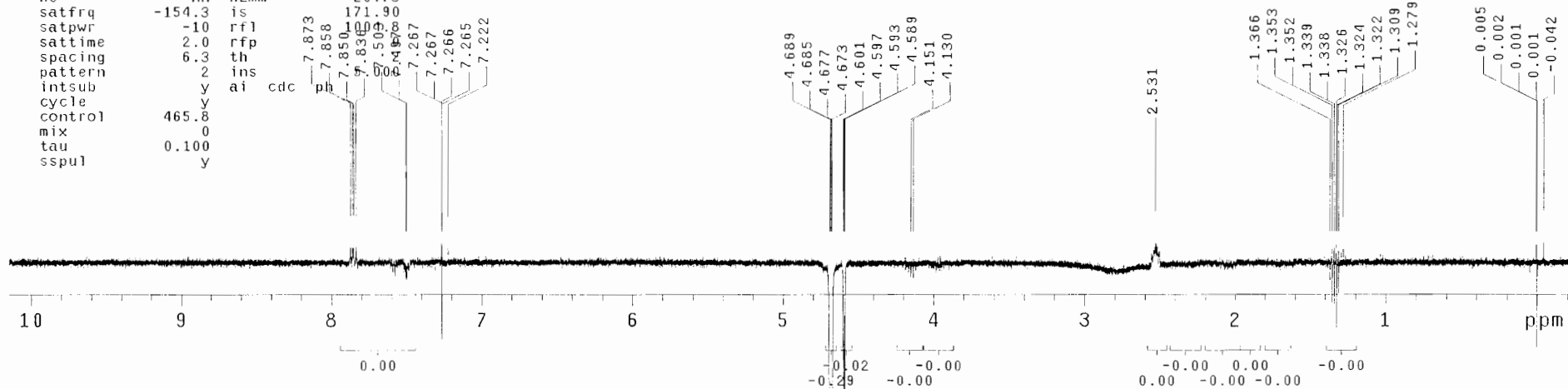
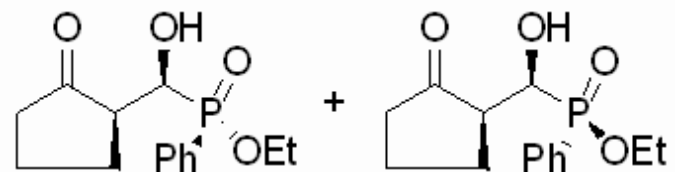


3-sp29_NOE01F

exp3 cyclenoe

```
SAMPLE          DEC. & VI
date Jan 4 2010  dn          C13
solvent CDC13    dof          -154.3
file          exp          dm          nnn
ACQUISITION     dmm          c
sfrq          499.633     dpwr          0
tn            H1          dpwrf         undefined
at            4.378       homo          n
np            70000       temp          26.0
sw            7995.2      PROCESSING
fb            4000        fn          not used
bs            32          math          f
pw            12.5
d1            4.000       werr
tof           499.5       wexp          process
nt            344        wbs
ct            344        wnt
alock         n          DISPLAY
gain          40         sp           -112.3
FLAGS         wp           5182.9
il            n          vs           9707
in            n          sc           0
dp            y          wc           250
hs            nn         hzmm         20.73
satfrq        -154.3     is           171.90
satpwr        -10       rfl
sattime       2.0        rfp
spacing       6.3        th
pattern       2          ins
intsub        y          ai
cycle         y          cdc
control       465.8      ph
mix           0
tau           0.100
sspul        y
```

NOE experiment for

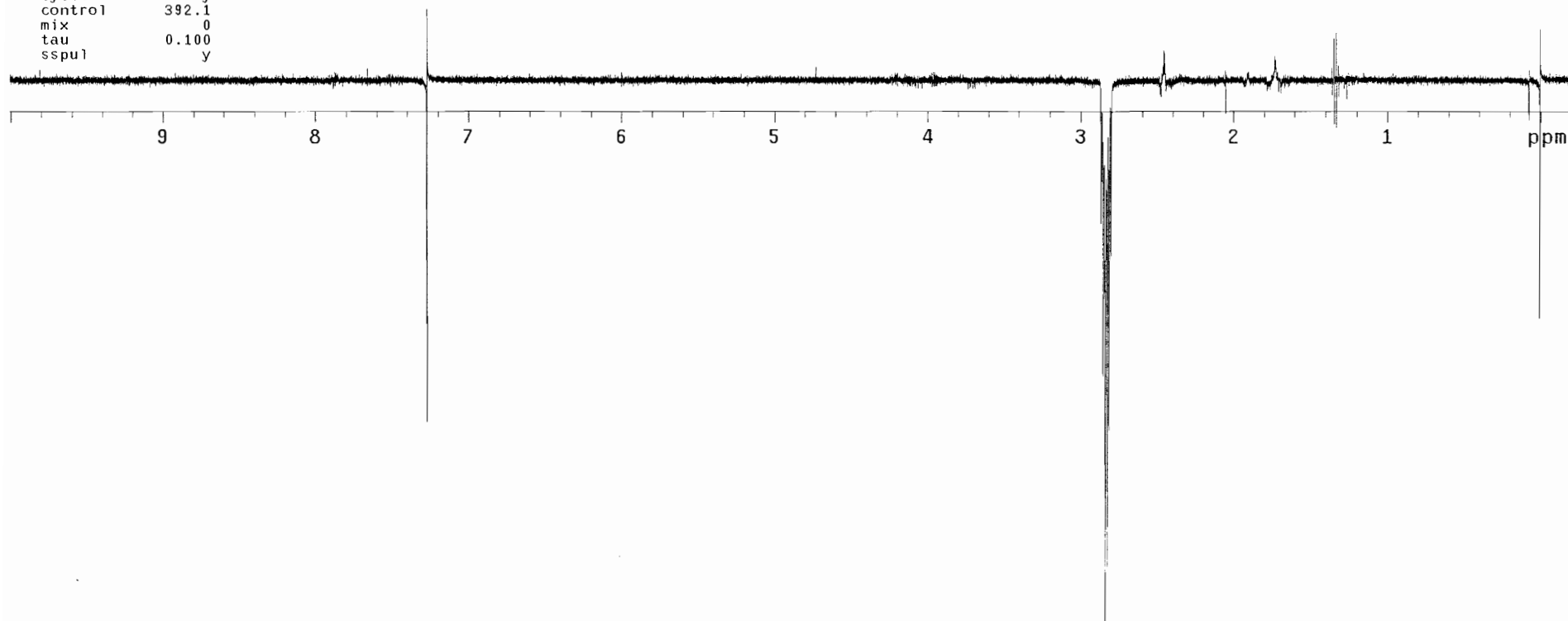
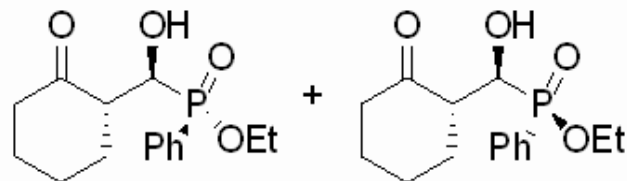


3-sp-30_NOE_Difference

exp3 cyclenoe

SAMPLE		DEC. & VT	
date	Jan 6 2010	dn	C13
solvent	CDC13	dof	392.1
file	exp	dm	nnn
ACQUISITION			
sfrq	499.633	dmm	c
tn	H1	dpwr	undefined
at	4.378	homo	n
np	70000	PROCESSING	
sw	7995.2	fn	not used
fb	4000	math	f
bs	32		
pw	3.4	werr	
d1	2.000	wexp	process
tof	499.5	wbs	
nt	512	wnt	
ct	512	DISPLAY	
alock	n	sp	-109.3
gain	58	wp	5108.2
FLAGS			
il	n	sc	0
in	n	wc	250
dp	y	hzmm	20.43
hs	nn	is	33.57
satfrq	-1081.0	rfl	999.9
satpwr	-10	rfp	0
sattime	1.0	th	7
spacing	9.1	ins	100.000
pattern	6	nm	cdc ph
intsub	y		
cycle	y		
control	392.1		
mix	0		
tau	0.100		
sspul	y		

NOE experiment for



Area % Report

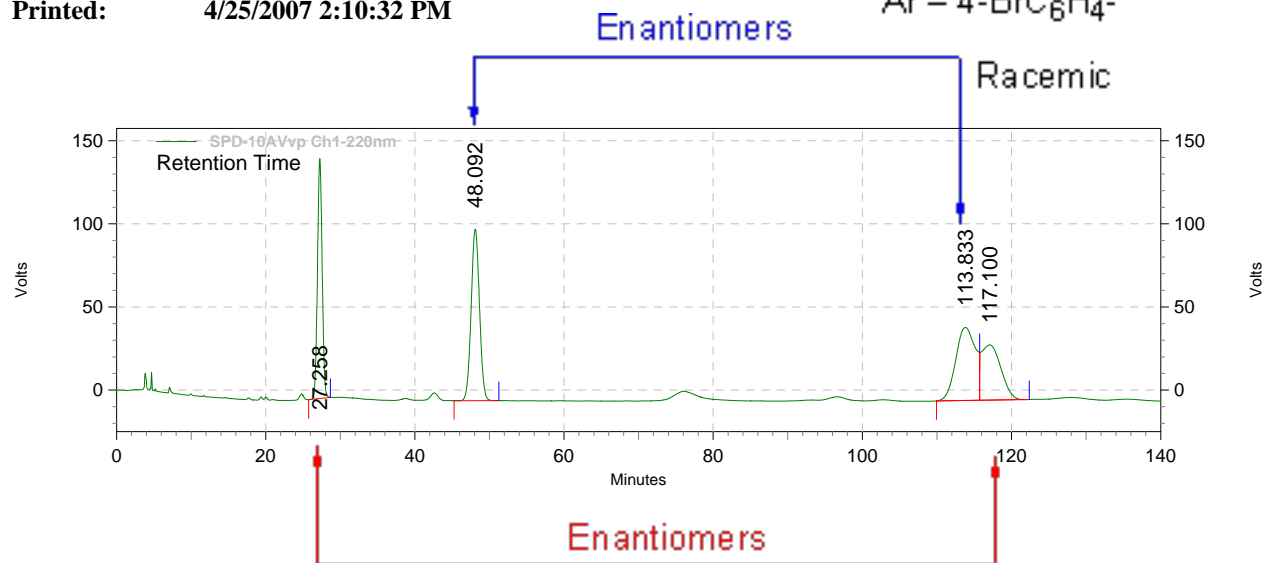
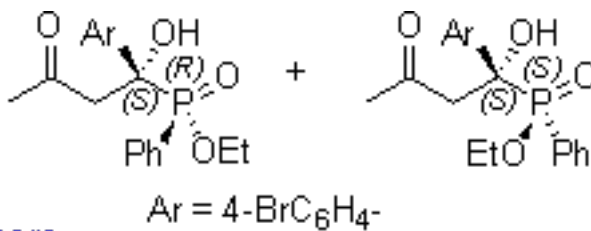
Method Name: C:\EZStart\Projects\Default\Methods\AS.met

Data: C:\EZStart\Projects\Default\Data\v-ss-92l

User: System

Acquired: 4/27/2006 2:23:27 PM

Printed: 4/25/2007 2:10:32 PM



SPD-10AVvp

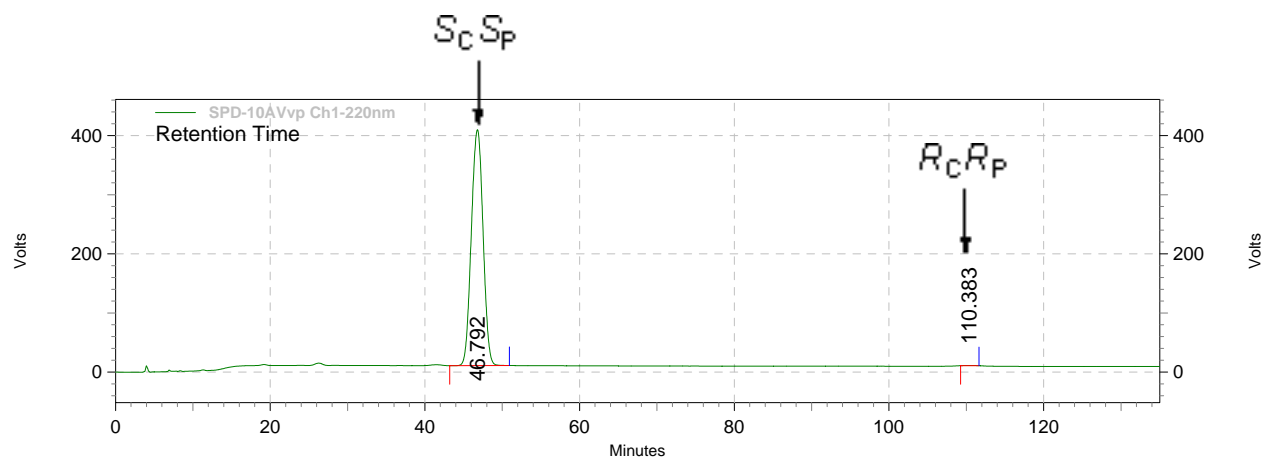
Ch1-220nm

Results

Retention Time	Area	Area %	Height	Height %
27.258	6307405	22.20	144252	44.42
48.092	8022192	28.24	103296	31.81
113.833	8053997	28.35	43919	13.52
117.100	6026061	21.21	33258	10.24
Totals	28409655	100.00	324725	100.00

Area % Report

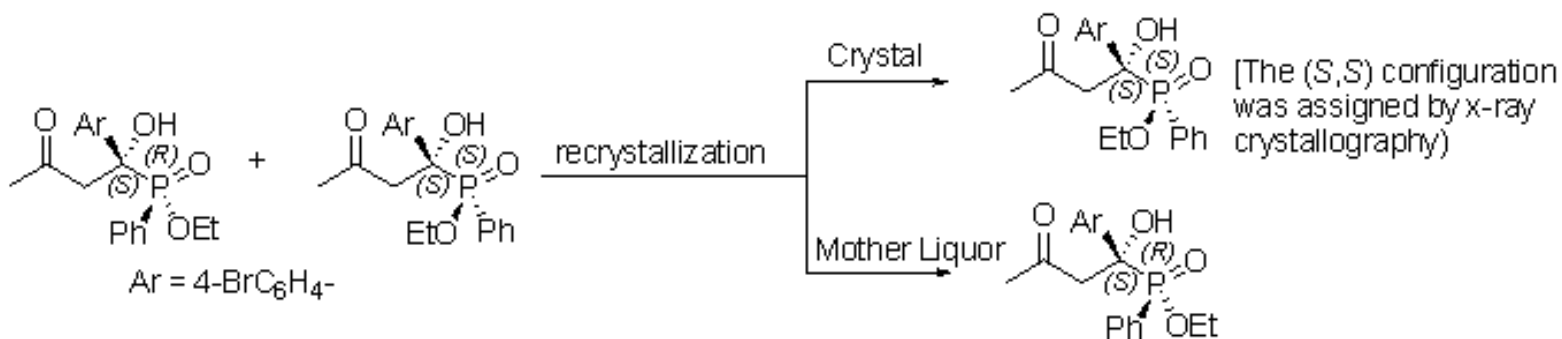
Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\VIII-SS-35b
 User: System
 Acquired: 12/20/2006 3:20:15 PM
 Printed: 4/26/2007 3:00:02 PM



SPD-10AVvp Ch1-220nm Results

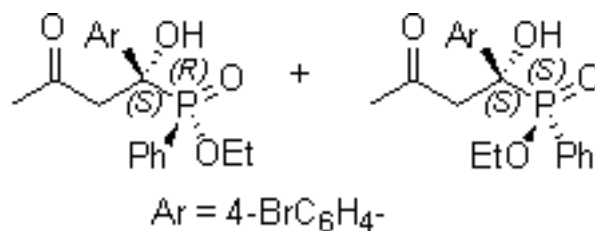
Retention Time	Area	Area %	Height	Height %
46.792	41985162	99.92	398934	99.91
110.383	34943	0.08	379	0.09

Totals	Area	Area %	Height	Height %
	42020105	100.00	399313	100.00

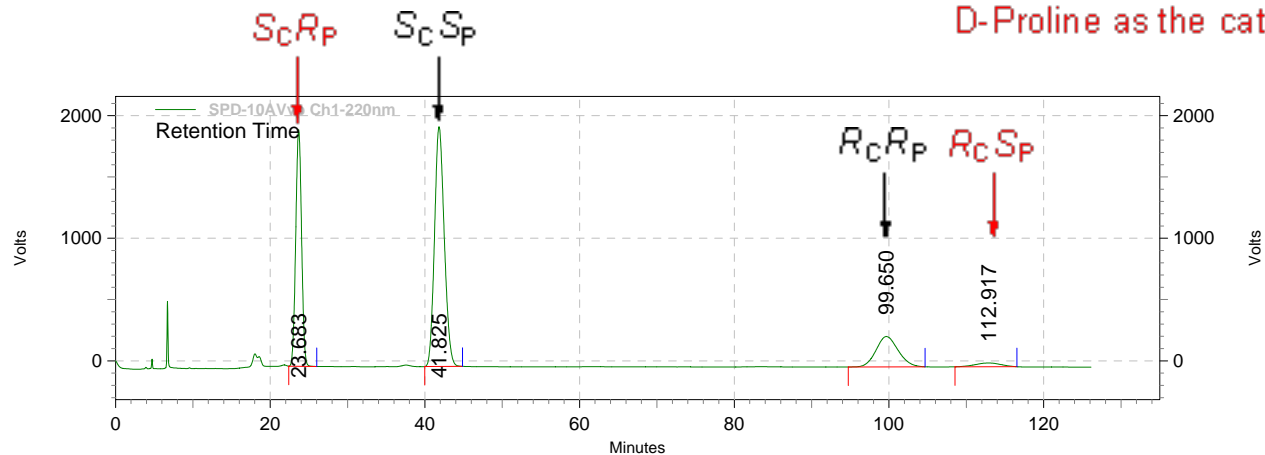


Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\vi-ss-100
 User: System
 Acquired: 10/10/2006 9:59:16 AM
 Printed: 4/25/2007 2:12:24 PM



D-Proline as the catalyst

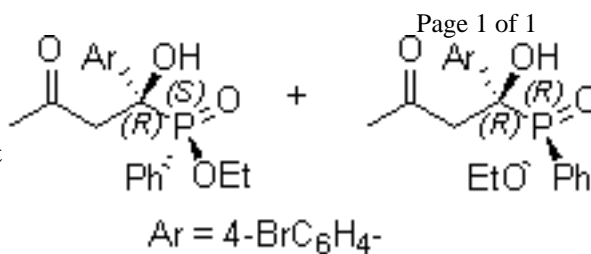


SPD-10AVvp
 Ch1-220nm
 Results

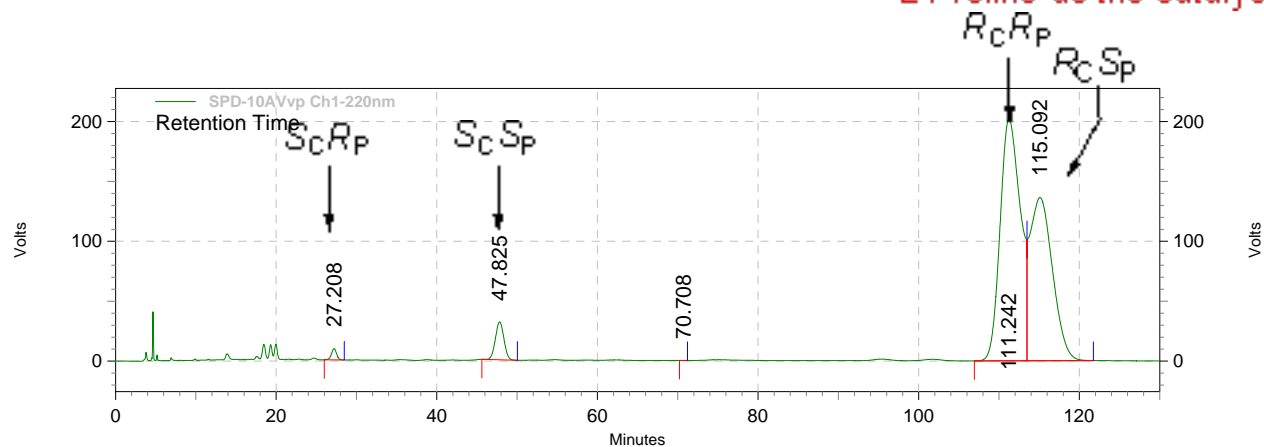
Retention Time	Area	Area %	Height	Height %
23.683	101402953	30.78	1929494	46.34
41.825	171735609	52.14	1955603	46.97
99.650	49182378	14.93	247436	5.94
112.917	7077277	2.15	30915	0.74
Totals	329398217	100.00	4163448	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\V-SS-99A
User: System
Acquired: 5/3/2006 10:44:43 AM
Printed: 4/25/2007 2:11:19 PM



L-Proline as the catalyst



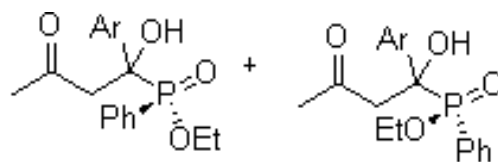
SPD-10AVvp
Ch1-220nm
Results

Retention Time	Area	Area %	Height	Height %
27.208	419158	0.65	9420	2.48
47.825	2332862	3.61	31592	8.33
70.708	834	0.00	28	0.01
111.242	35326343	54.61	202051	53.27
115.092	26614828	41.14	136197	35.91

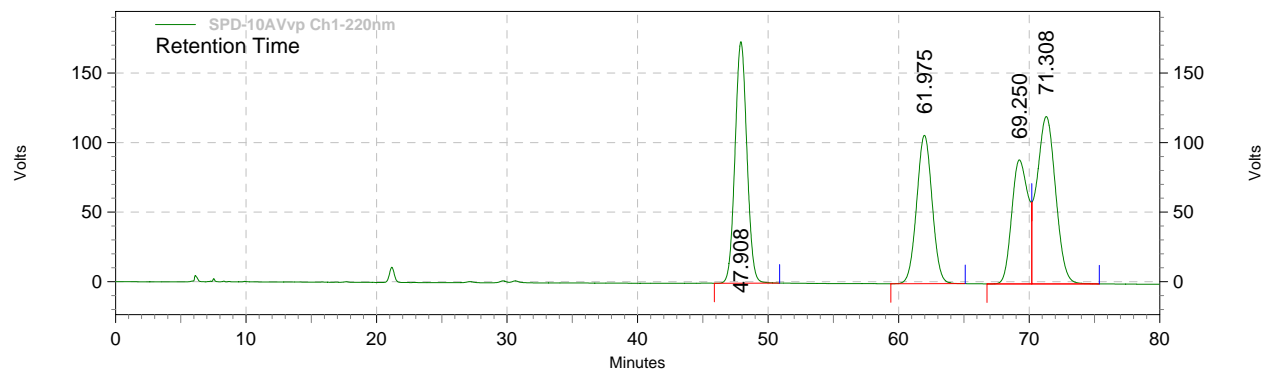
Totals	64694025	100.00	379288	100.00
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Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\VI-SS-8A
User: System
Acquired: 6/19/2006 11:15:05 AM
Printed: 4/25/2007 2:03:09 PM



Ar = Ph racemic

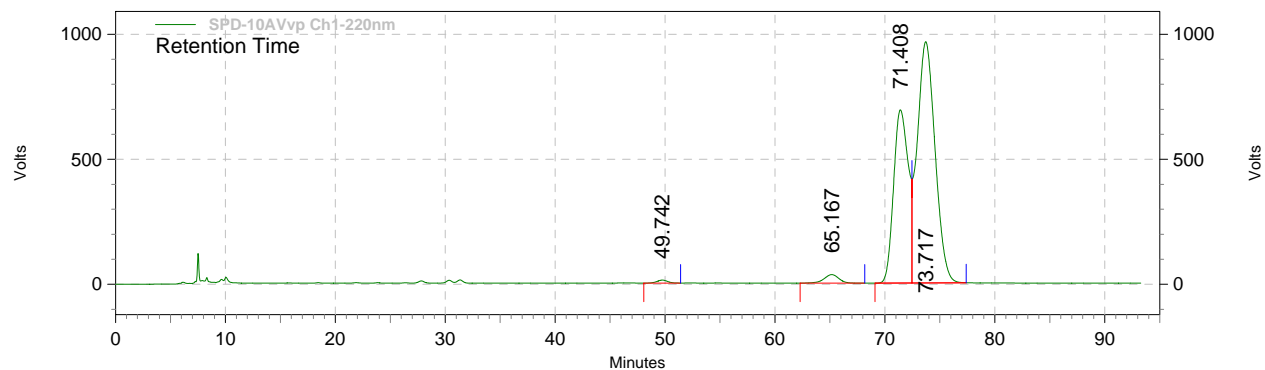
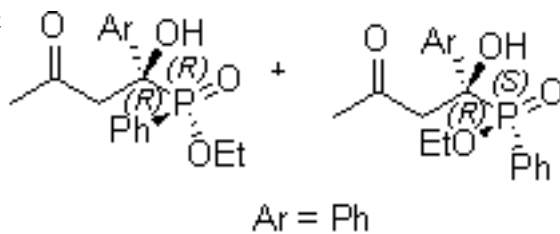


SPD-10AVvp
Ch1-220nm
Results

Retention Time	Area	Area %	Height	Height %
47.908	10981114	27.73	173608	35.44
61.975	8793983	22.20	106738	21.79
69.250	7775129	19.63	89132	18.20
71.308	12053502	30.44	120347	24.57
Totals	39603728	100.00	489825	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-75
 User: System
 Acquired: 4/17/2006 12:06:24 PM
 Printed: 4/25/2007 2:04:43 PM

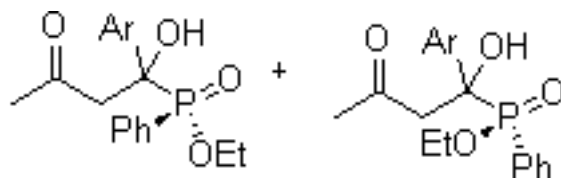


SPD-10AVvp Ch1-220nm Results

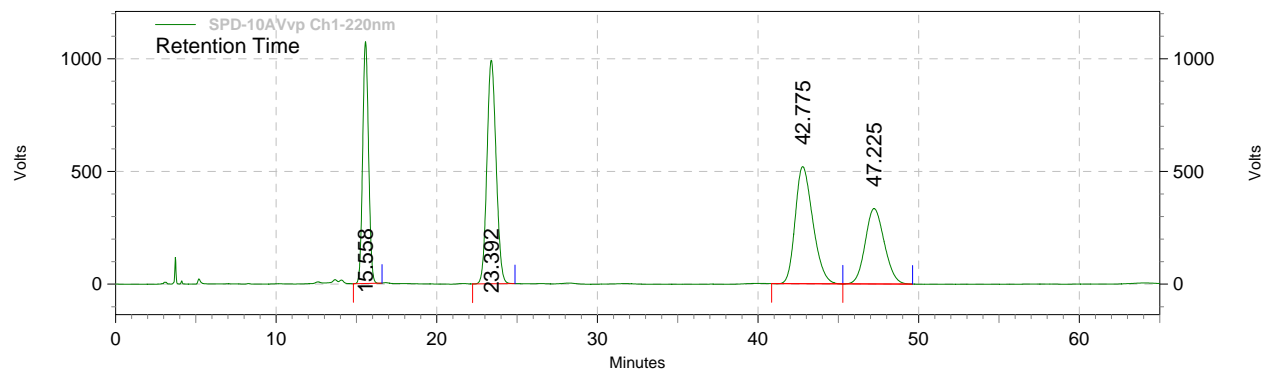
Retention Time	Area	Area %	Height	Height %
49.742	799069	0.45	11878	0.70
65.167	3157296	1.78	34035	2.00
71.408	64541546	36.36	692571	40.67
73.717	108989234	61.41	964603	56.64
Totals	177487145	100.00	1703087	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-79C
 User: System
 Acquired: 4/20/2006 12:39:20 PM
 Printed: 4/25/2007 2:07:12 PM



Ar = 4-F-Ph racemic

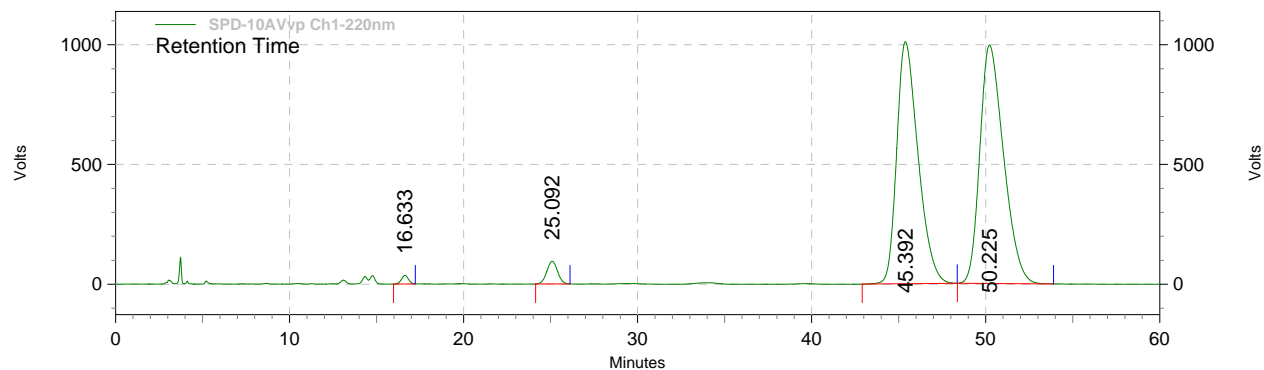
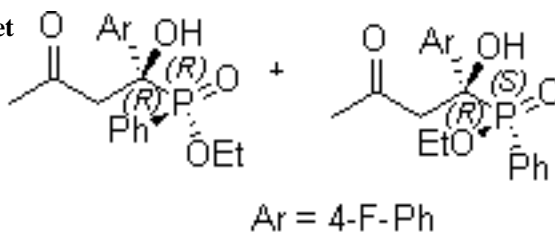


SPD-10AVvp
 Ch1-220nm
 Results

Retention Time	Area	Area %	Height	Height %
15.558	27434842	20.44	1072464	36.74
23.392	39490664	29.43	992036	33.99
42.775	39609775	29.52	519744	17.81
47.225	27662953	20.61	334696	11.47
Totals	134198234	100.00	2918940	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-81B
 User: System
 Acquired: 4/24/2006 11:56:20 AM
 Printed: 4/25/2007 2:06:24 PM

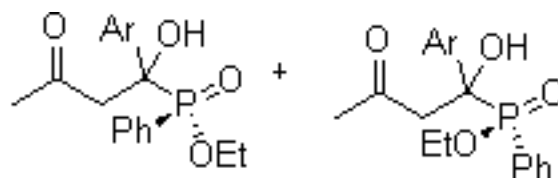


**SPD-10AVvp
 Ch1-220nm
 Results**

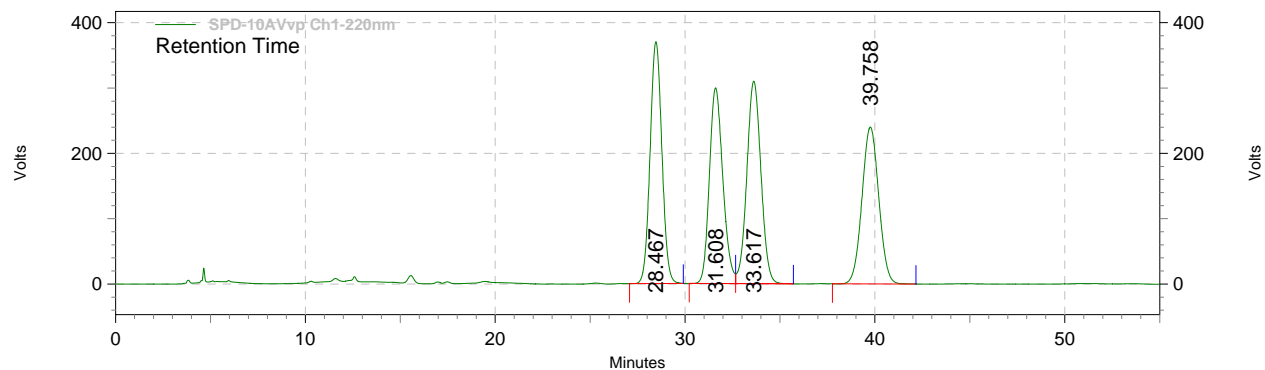
Retention Time	Area	Area %	Height	Height %
16.633	999895	0.54	35489	1.66
25.092	4061528	2.19	94515	4.43
45.392	86176162	46.44	1010200	47.30
50.225	94307892	50.83	995574	46.61
Totals	185545477	100.00	2135778	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-138A
 User: System
 Acquired: 5/31/2006 2:02:20 PM
 Printed: 4/25/2007 2:08:09 PM



Ar = 3-F-Ph racemic

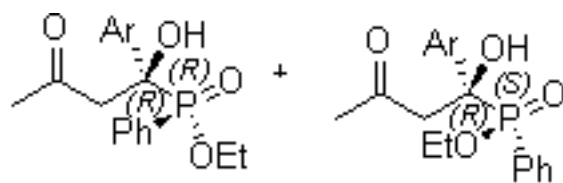


SPD-10AVvp
Ch1-220nm
Results

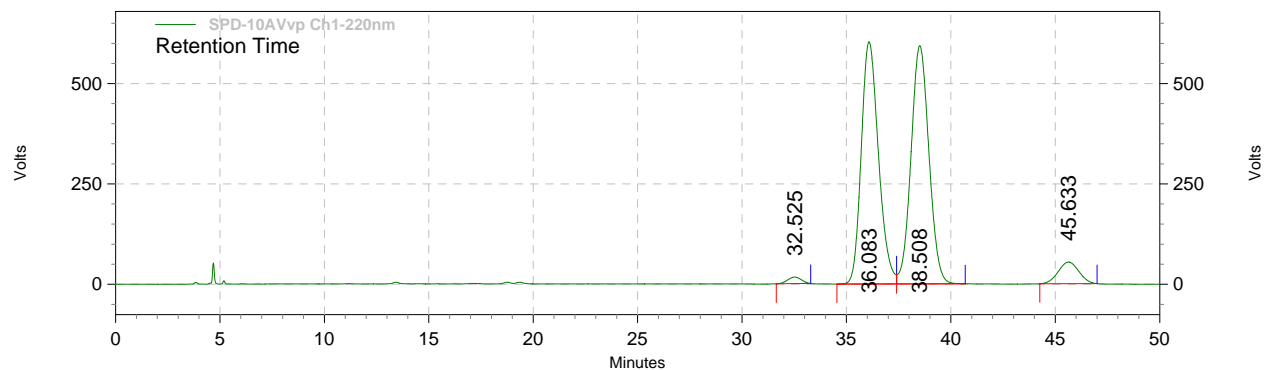
Retention Time	Area	Area %	Height	Height %
28.467	15945462	25.92	369993	30.34
31.608	14739673	23.96	299485	24.56
33.617	16067412	26.12	309925	25.41
39.758	14760819	24.00	240148	19.69
Totals	61513366	100.00	1219551	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\V-SS-140F
User: System
Acquired: 6/6/2006 2:09:37 PM
Printed: 4/25/2007 2:09:20 PM



Ar = 3-F-Ph

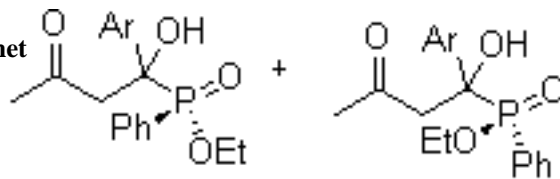


SPD-10AVvp Ch1-220nm Results

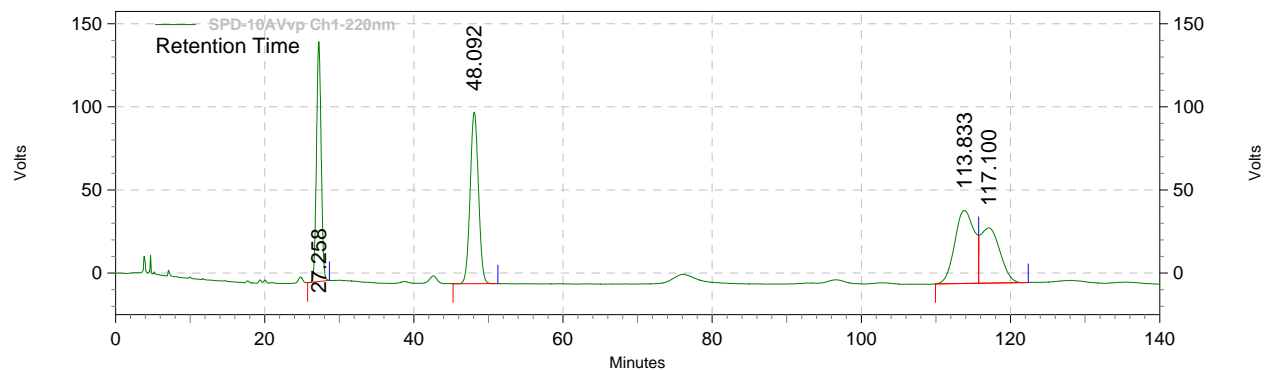
Retention Time	Area	Area %	Height	Height %
32.525	745767	1.00	16276	1.28
36.083	34534551	46.45	603361	47.63
38.508	35366780	47.57	593345	46.84
45.633	3701735	4.98	53844	4.25
Totals	74348833	100.00	1266826	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\v-ss-92l
 User: System
 Acquired: 4/27/2006 2:23:27 PM
 Printed: 4/25/2007 2:10:32 PM

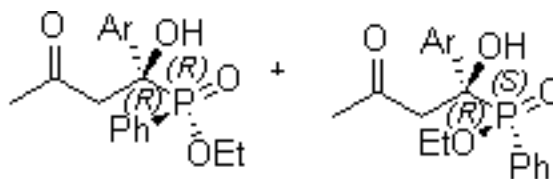


Ar = 4-Br-Ph racemic



SPD-10AVvp
 Ch1-220nm
 Results

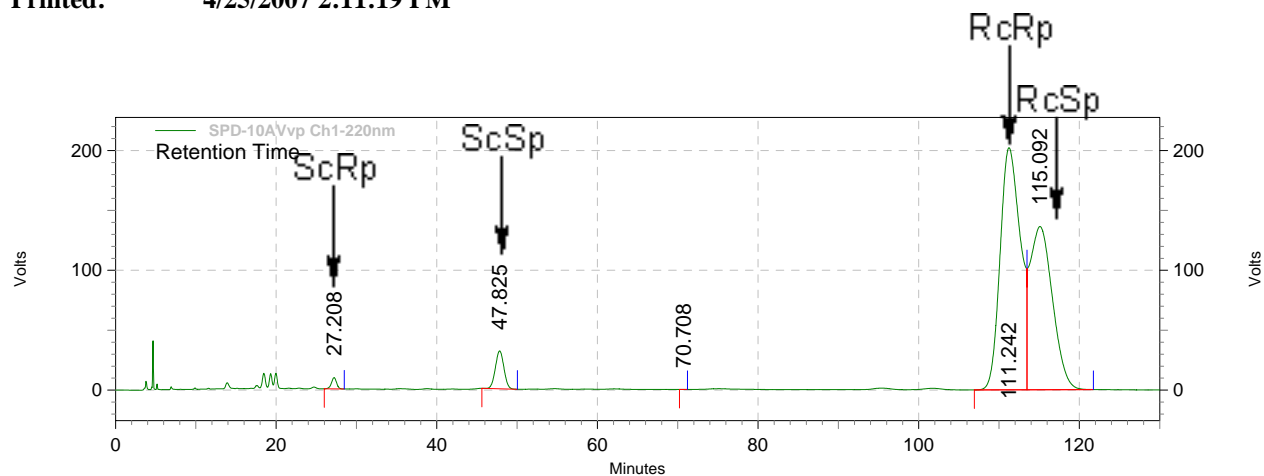
Retention Time	Area	Area %	Height	Height %
27.258	6307405	22.20	144252	44.42
48.092	8022192	28.24	103296	31.81
113.833	8053997	28.35	43919	13.52
117.100	6026061	21.21	33258	10.24
Totals	28409655	100.00	324725	100.00



Area % Report

Ar = 4-Br-Ph; L-Proline

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-99A
 User: System
 Acquired: 5/3/2006 10:44:43 AM
 Printed: 4/25/2007 2:11:19 PM



SPD-10AVvp
 Ch1-220nm
 Results

Retention Time	Area	Area %	Height	Height %
27.208	419158	0.65	9420	2.48
47.825	2332862	3.61	31592	8.33
70.708	834	0.00	28	0.01
111.242	35326343	54.61	202051	53.27
115.092	26614828	41.14	136197	35.91

Totals	64694025	100.00	379288	100.00
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Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met

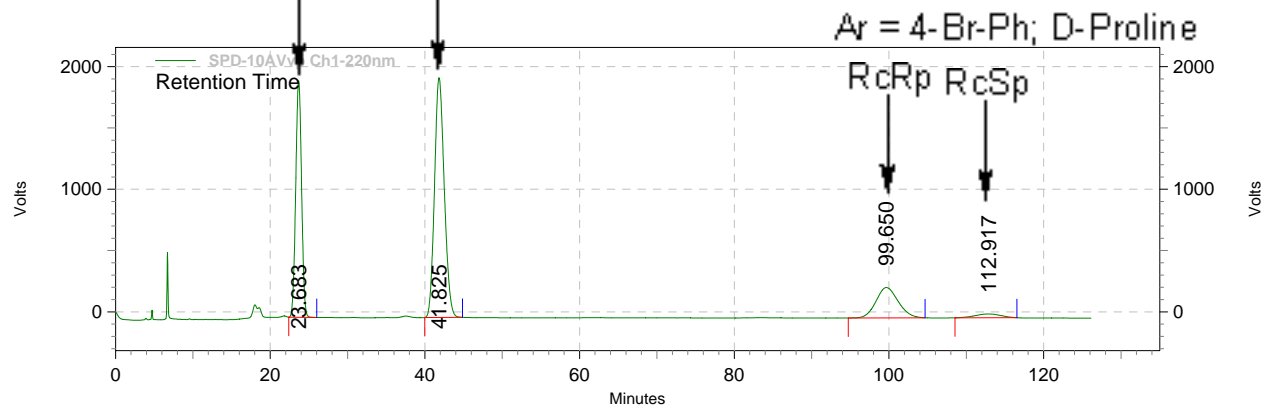
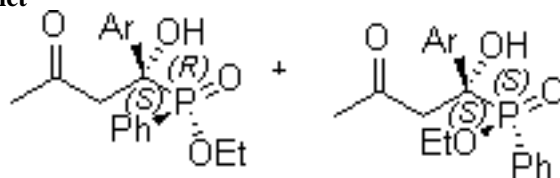
Data: C:\EZStart\Projects\Default\Data\vi-ss-100

User: System

Acquired: 10/10/2006 9:59:16 AM

Printed: 4/25/2007 2:12:24 PM

ScRp ScSp



SPD-10AVvp

Ch1-220nm

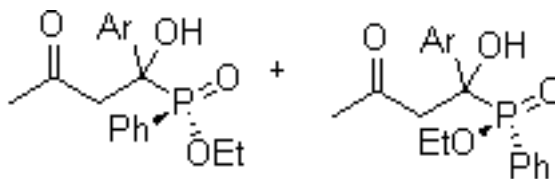
Results

Retention Time	Area	Area %	Height	Height %
23.683	101402953	30.78	1929494	46.34
41.825	171735609	52.14	1955603	46.97
99.650	49182378	14.93	247436	5.94
112.917	7077277	2.15	30915	0.74

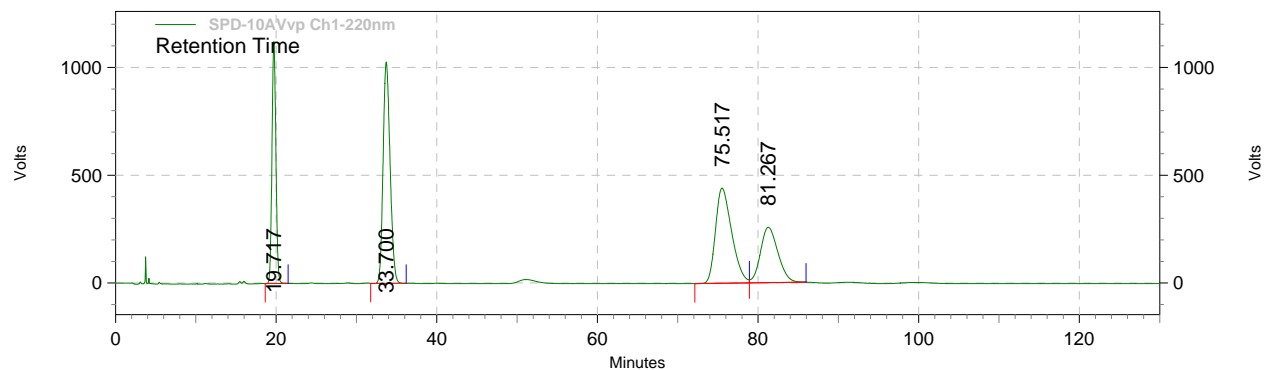
Totals	329398217	100.00	4163448	100.00
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Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\v-ss-861
 User: System
 Acquired: 4/25/2006 1:03:52 PM
 Printed: 4/25/2007 2:17:34 PM



Ar = 4-Cl-Ph racemic

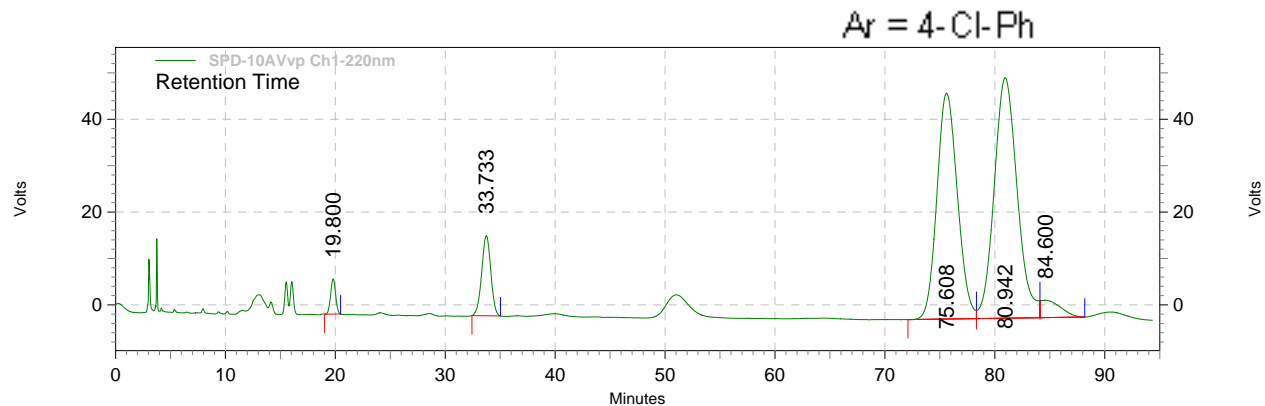
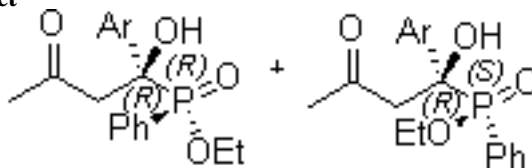


SPD-10AVvp
Ch1-220nm
Results

Retention Time	Area	Area %	Height	Height %
19.717	38032132	18.96	1121651	39.40
33.700	62068400	30.95	1026667	36.07
75.517	61763941	30.80	441468	15.51
81.267	38690976	19.29	256714	9.02
Totals	200555449	100.00	2846500	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-88E
 User: System
 Acquired: 4/30/2006 1:37:19 PM
 Printed: 4/25/2007 2:18:59 PM

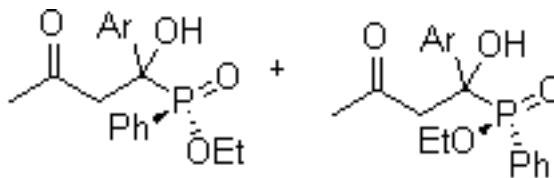


SPD-10AVvp Ch1-220nm Results

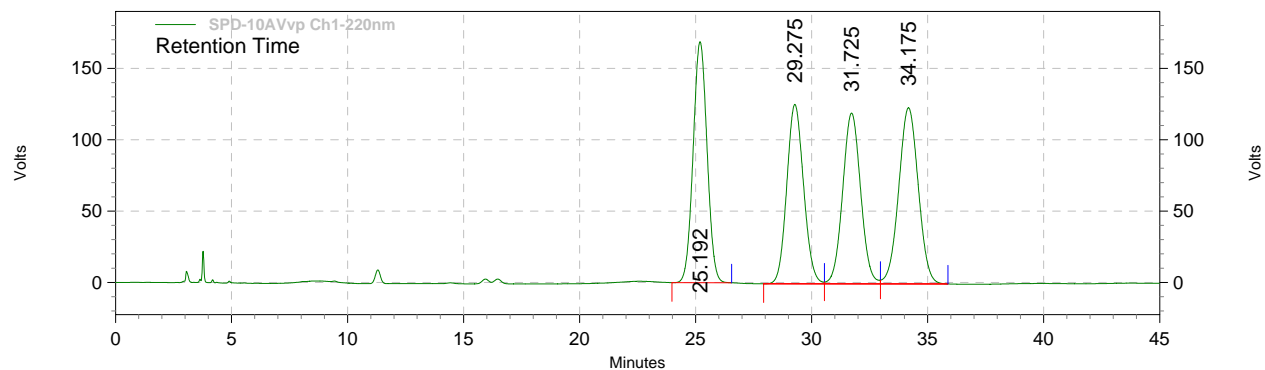
Retention Time	Area	Area %	Height	Height %
19.800	240142	1.54	7583	5.87
33.733	994355	6.39	17251	13.36
75.608	6314780	40.59	48672	37.71
80.942	7538385	48.46	51830	40.15
84.600	468849	3.01	3746	2.90
Totals	15556511	100.00	129082	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-154L
 User: System
 Acquired: 6/13/2006 10:56:50 AM
 Printed: 4/25/2007 2:19:47 PM



Ar = 3-Cl-Ph racemic

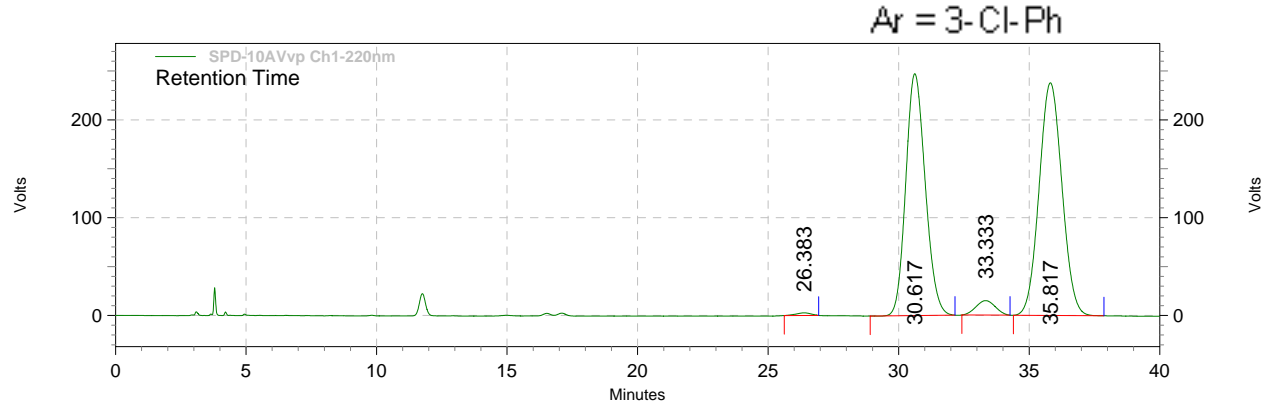
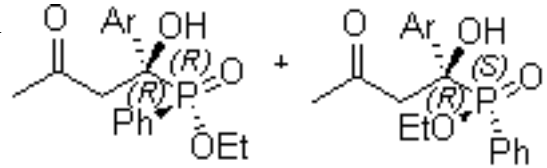


SPD-10AVvp
Ch1-220nm
Results

Retention Time	Area	Area %	Height	Height %
25.192	7062498	26.10	168784	31.40
29.275	6333169	23.40	125683	23.38
31.725	6432760	23.77	119636	22.26
34.175	7235102	26.73	123404	22.96
Totals	27063529	100.00	537507	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\V-SS-156L1
User: System
Acquired: 6/15/2006 12:32:36 PM
Printed: 4/25/2007 2:20:28 PM

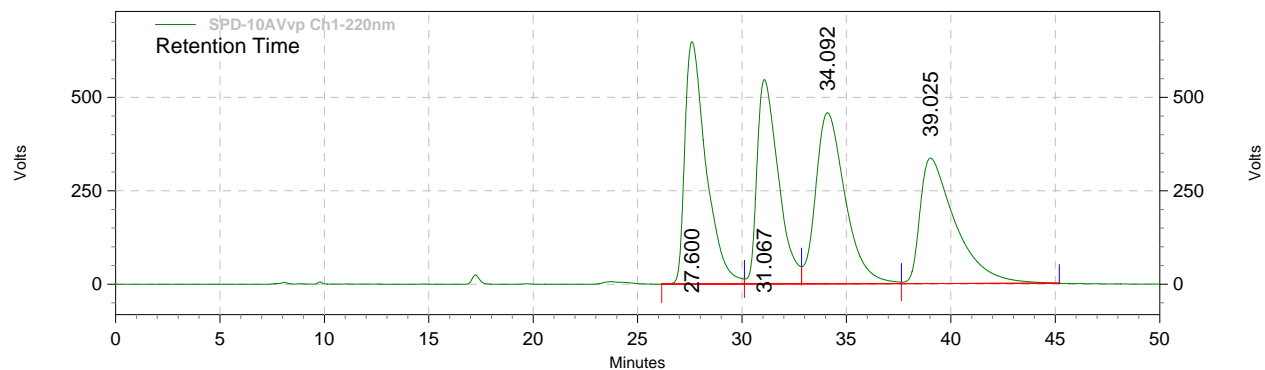
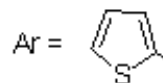
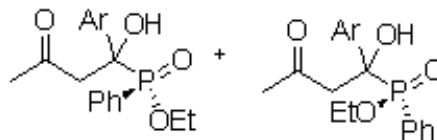


SPD-10AVvp
Ch1-220nm
Results

Retention Time	Area	Area %	Height	Height %
26.383	104686	0.37	2609	0.52
30.617	12843101	45.54	247344	49.20
33.333	758992	2.69	14771	2.94
35.817	14492010	51.39	238012	47.34
Totals	28198789	100.00	502736	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\v-ss-13411
User: System
Acquired: 5/29/2006 12:21:34 PM
Printed: 4/25/2007 2:23:51 PM

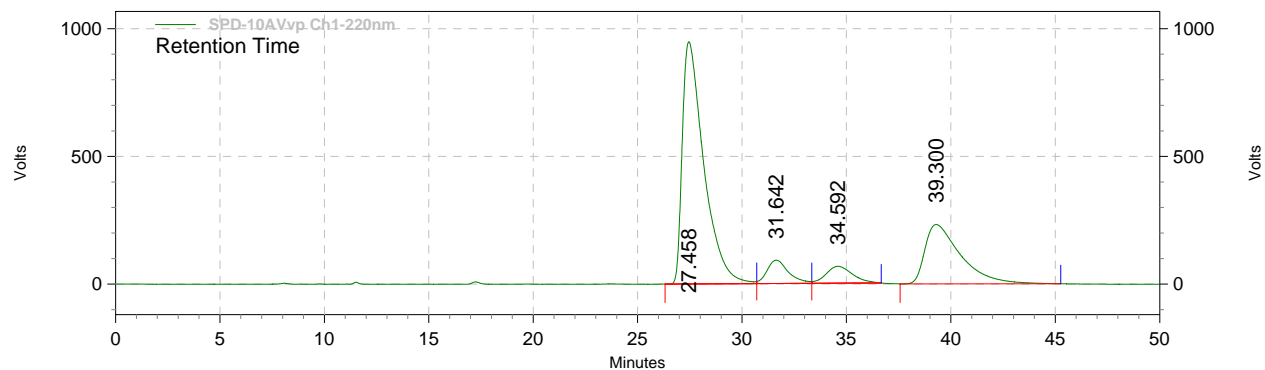
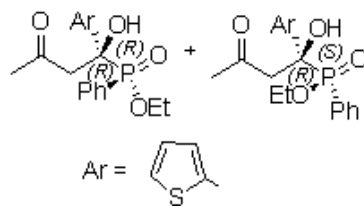


SPD-10AVvp Ch1-220nm Results

Retention Time	Area	Area %	Height	Height %
27.600	45630886	27.04	648373	32.61
31.067	38918762	23.06	546719	27.49
34.092	44731312	26.51	457695	23.02
39.025	39464526	23.39	335664	16.88
Totals	168745486	100.00	1988451	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\v-ss-137
User: System
Acquired: 5/31/2006 10:27:36 AM
Printed: 4/25/2007 2:24:30 PM

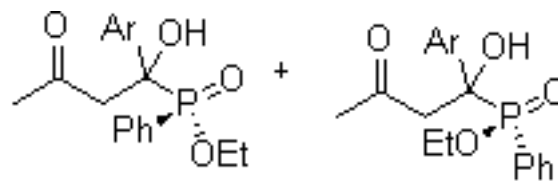


SPD-10AVvp Ch1-220nm Results

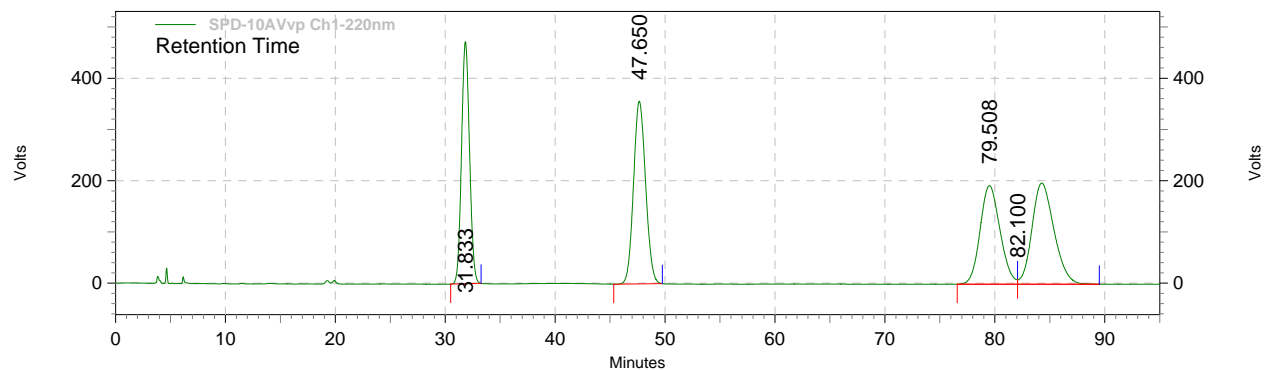
Retention Time	Area	Area %	Height	Height %
27.458	67944771	62.94	948585	70.85
31.642	6534725	6.05	91604	6.84
34.592	5826399	5.40	66246	4.95
39.300	27651497	25.61	232393	17.36
Totals	107957392	100.00	1338828	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-89B
 User: System
 Acquired: 5/2/2006 11:59:38 AM
 Printed: 4/25/2007 2:21:08 PM



Ar = 4-Me-Ph, Racemic

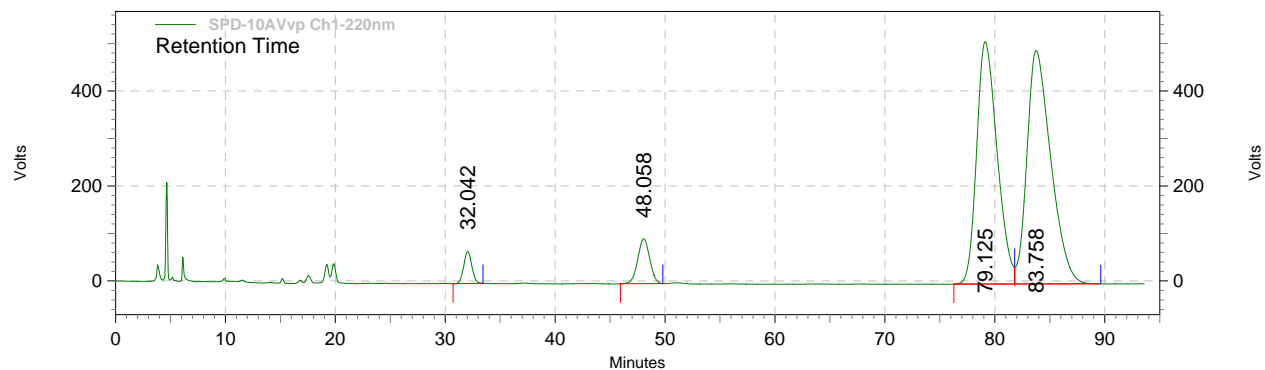
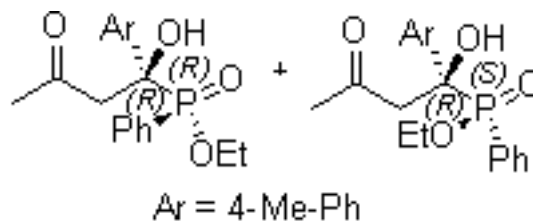


**SPD-10AVvp
 Ch1-220nm
 Results**

Retention Time	Area	Area %	Height	Height %
31.833	23980714	23.32	472371	45.85
47.650	27232695	26.48	356842	34.63
79.508	24184872	23.52	192378	18.67
82.100	27444434	26.69	8773	0.85
Totals	102842715	100.00	1030364	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-90
 User: System
 Acquired: 5/2/2006 10:25:08 AM
 Printed: 4/25/2007 2:21:34 PM

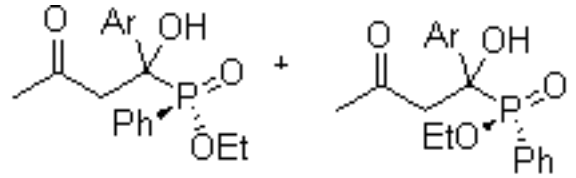


SPD-10AVvp
Ch1-220nm
Results

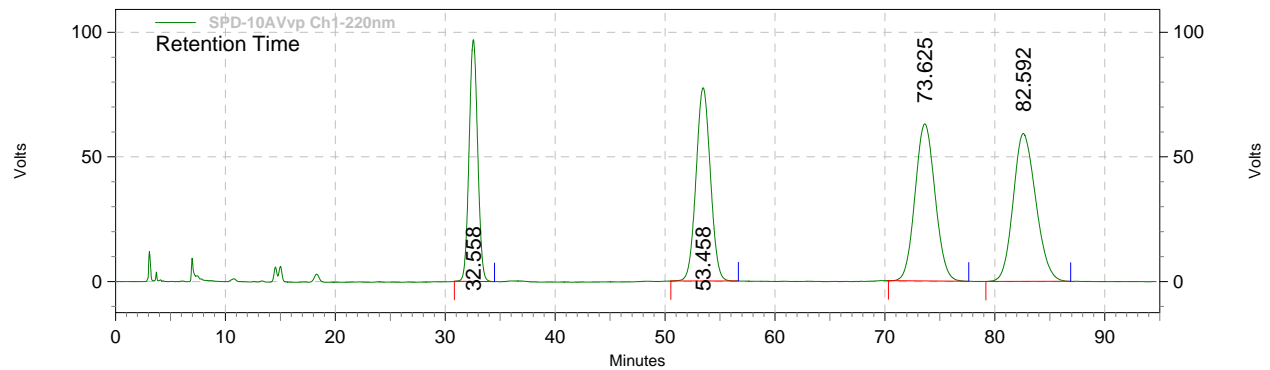
Retention Time	Area	Area %	Height	Height %
32.042	3468253	2.30	67253	5.78
48.058	7193972	4.76	94558	8.13
79.125	66117640	43.79	510403	43.86
83.758	74215288	49.15	491404	42.23
Totals	150995153	100.00	1163618	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\V-SS-94L
User: System
Acquired: 5/1/2006 2:11:41 PM
Printed: 4/25/2007 2:22:27 PM



Ar = 4-MeO-Ph, Racemic

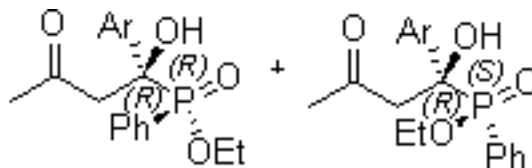


SPD-10AVvp
Ch1-220nm
Results

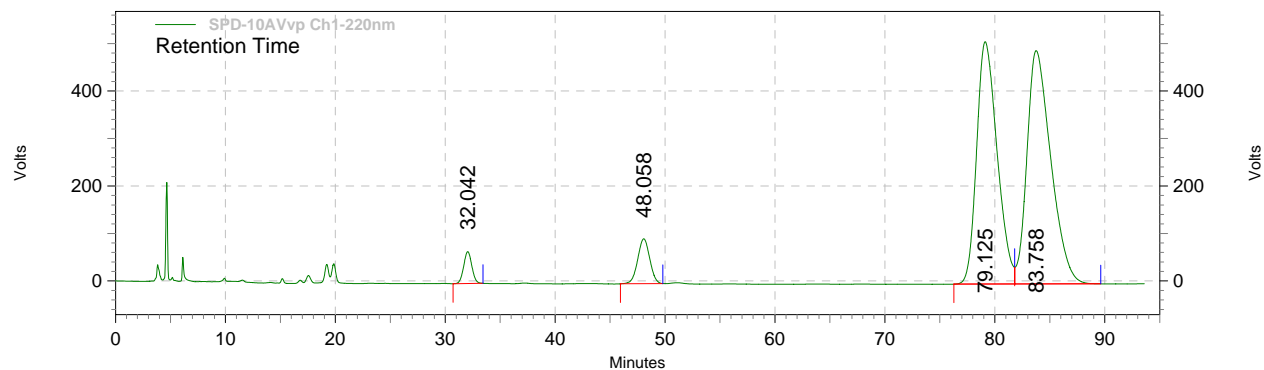
Retention Time	Area	Area %	Height	Height %
32.558	5287035	18.38	96981	32.68
53.458	7033213	24.45	77522	26.12
73.625	7963523	27.69	62982	21.22
82.592	8480119	29.48	59319	19.99
Totals	28763890	100.00	296804	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\V-SS-90
User: System
Acquired: 5/2/2006 10:25:08 AM
Printed: 4/25/2007 2:21:34 PM



Ar = 4-MeO-Ph

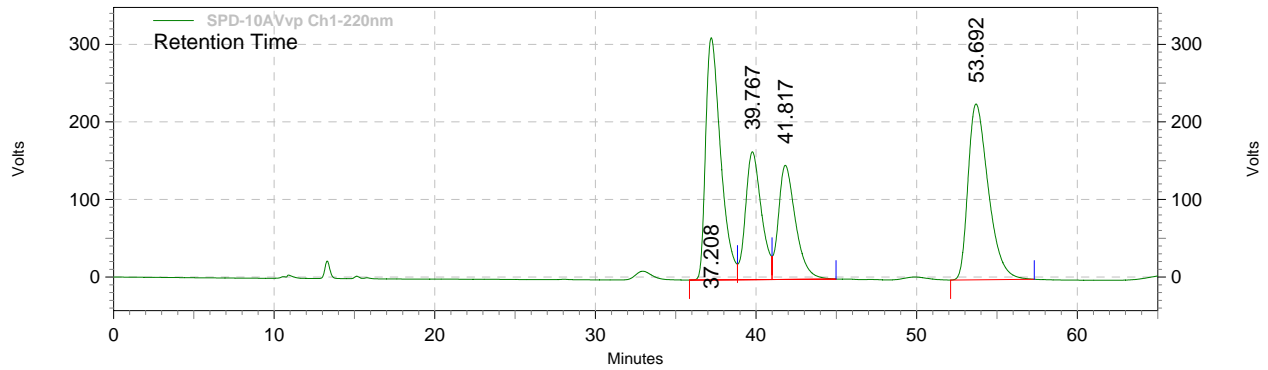
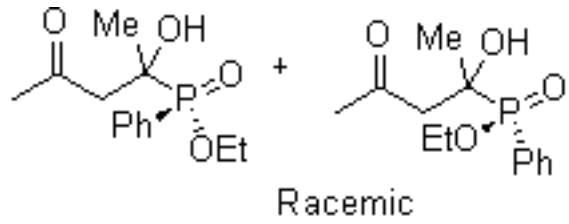


SPD-10AVvp Ch1-220nm Results

Retention Time	Area	Area %	Height	Height %
32.042	3468253	2.30	67253	5.78
48.058	7193972	4.76	94558	8.13
79.125	66117640	43.79	510403	43.86
83.758	74215288	49.15	491404	42.23
Totals	150995153	100.00	1163618	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-113L1
 User: System
 Acquired: 5/17/2006 2:41:11 PM
 Printed: 4/25/2007 2:25:32 PM

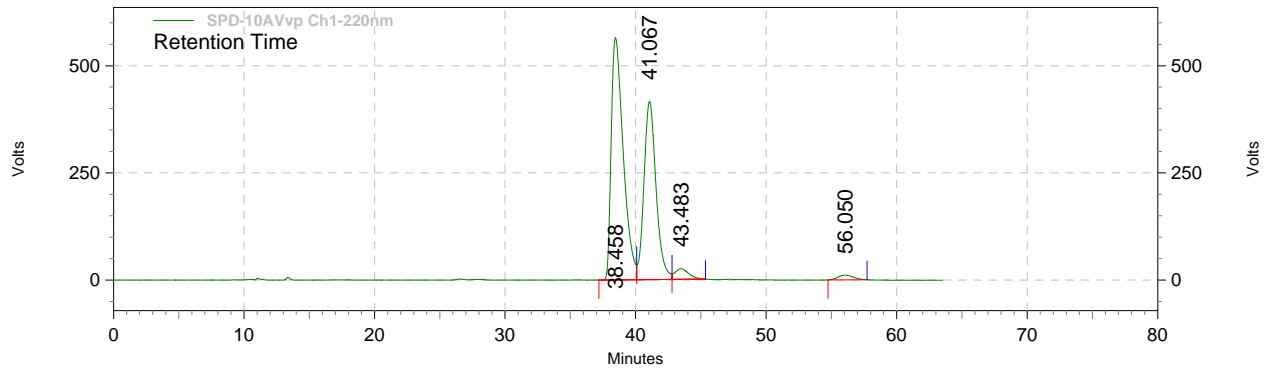
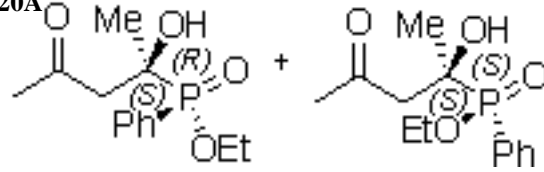


**SPD-10AVvp
 Ch1-220nm
 Results**

Retention Time	Area	Area %	Height	Height %
37.208	20294461	32.50	312190	36.70
39.767	11365945	18.20	164745	19.37
41.817	10938901	17.52	147105	17.29
53.692	19840435	31.78	226670	26.64
Totals	62439742	100.00	850710	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\V-SS-120A
 User: System
 Acquired: 5/23/2006 2:42:19 PM
 Printed: 4/25/2007 2:26:08 PM

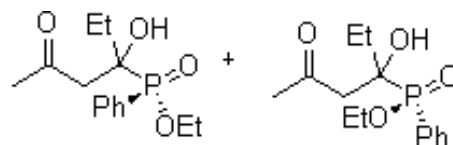


SPD-10AVvp Ch1-220nm Results

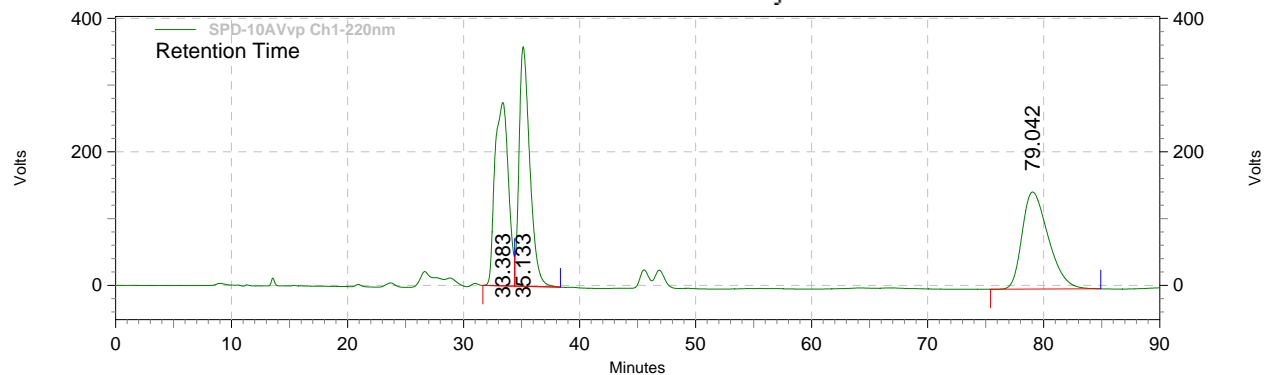
Retention Time	Area	Area %	Height	Height %
38.458	36110687	54.96	565118	55.59
41.067	26860891	40.88	415656	40.89
43.483	1833955	2.79	24696	2.43
56.050	899373	1.37	11089	1.09
Totals	65704906	100.00	1016559	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\V-SS-119L
User: System
Acquired: 5/19/2006 12:37:16 PM
Printed: 4/25/2007 2:27:17 PM



Racemic compounds are separated by two different columns.



SPD-10AVvp Ch1-220nm Results

Retention Time	Area	Area %	Height	Height %
33.383	22240491	32.61	274797	35.26
35.133	23080693	33.84	358959	46.06
79.042	22878779	33.55	145521	18.67
Totals	68199963	100.00	779277	100.00

Area % Report

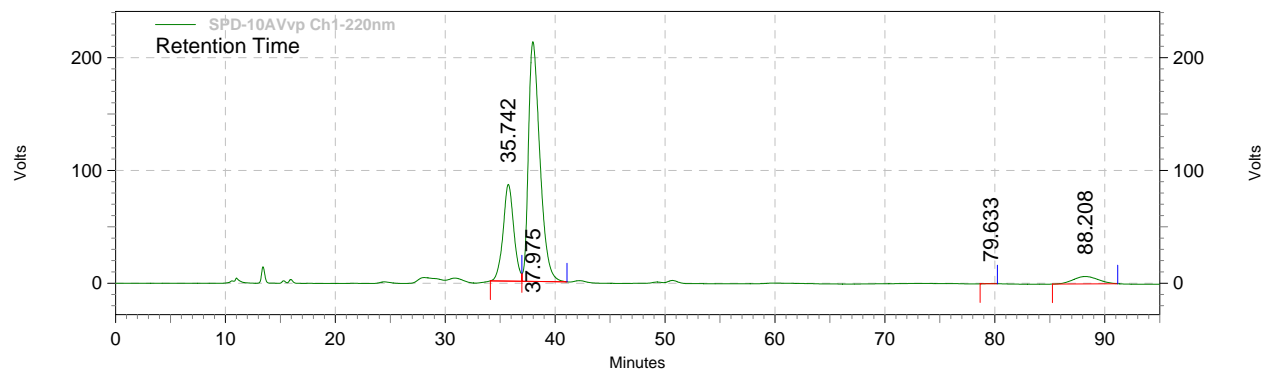
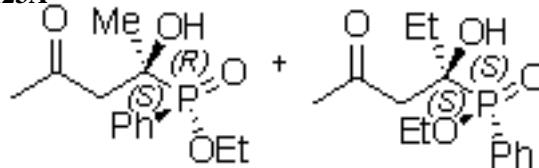
Method Name: C:\EZStart\Projects\Default\Methods\AS.met

Data: C:\EZStart\Projects\Default\Data\V-SS-123A

User: System

Acquired: 5/22/2006 11:36:04 AM

Printed: 4/25/2007 2:30:43 PM



SPD-10AVvp

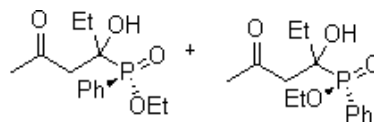
Ch1-220nm

Results

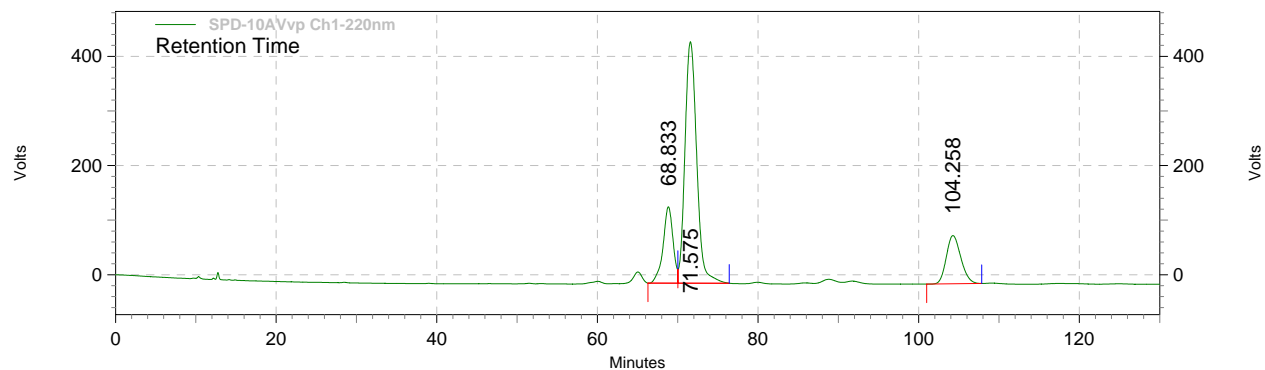
Retention Time	Area	Area %	Height	Height %
35.742	5805011	26.05	85806	28.12
37.975	15425090	69.22	212565	69.67
79.633	7828	0.04	133	0.04
88.208	1045787	4.69	6597	2.16
Totals	22283716	100.00	305101	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\V-SS-119L2
User: System
Acquired: 5/19/2006 4:08:50 PM
Printed: 4/25/2007 2:32:07 PM



Racemic compounds are separated by two different columns.

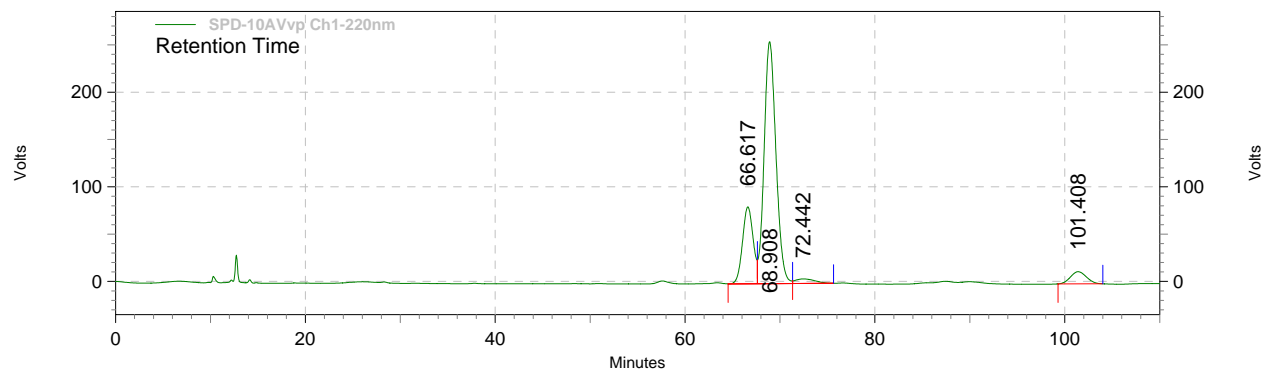
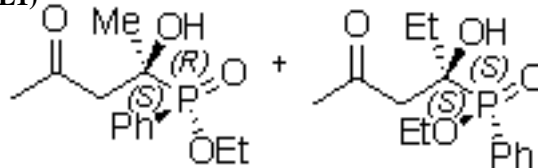


SPD-10AVvp
Ch1-220nm
Results

Retention Time	Area	Area %	Height	Height %
68.833	12086724	17.73	139921	20.87
71.575	45002937	66.01	442116	65.94
104.258	11088654	16.26	88443	13.19
Totals	68178315	100.00	670480	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\V-SS-123(AD-L1)
User: System
Acquired: 5/24/2006 4:24:44 PM
Printed: 4/25/2007 2:33:43 PM

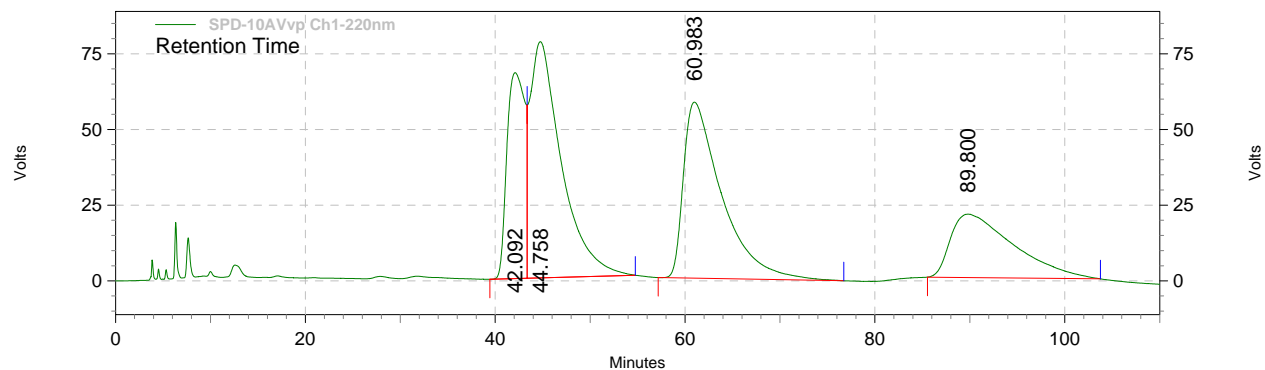
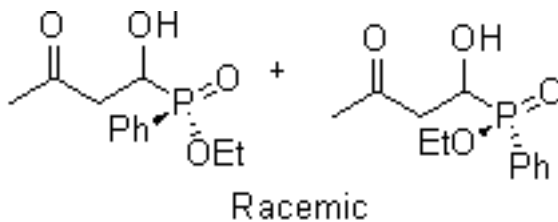


SPD-10AVvp Ch1-220nm Results

Retention Time	Area	Area %	Height	Height %
66.617	6327760	20.61	81314	22.92
68.908	22171556	72.23	255721	72.09
72.442	680911	2.22	4810	1.36
101.408	1517160	4.94	12891	3.63
Totals	30697387	100.00	354736	100.00

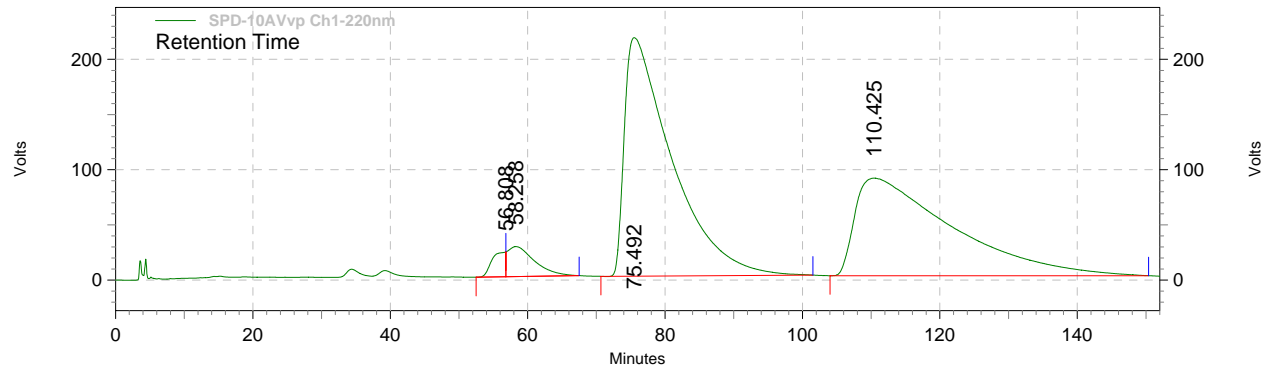
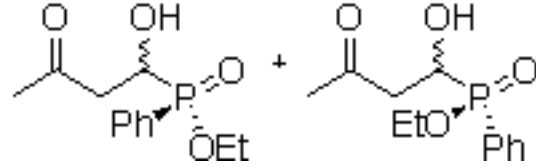
Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\VI-SS-L
User: System
Acquired: 7/13/2006 10:06:27 AM
Printed: 4/25/2007 2:35:10 PM



SPD-10AVvp Ch1-220nm Results

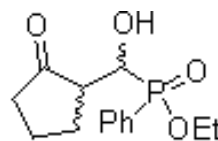
Retention Time	Area	Area %	Height	Height %
42.092	8863777	16.82	68017	30.22
44.758	17920164	34.00	77983	34.65
60.983	16289168	30.90	58138	25.83
89.800	9636855	18.28	20934	9.30
Totals	52709964	100.00	225072	100.00

Area % Report**Method Name:** C:\EZStart\Projects\Default\Methods\AS.met**Data:** C:\EZStart\Projects\Default\Data\vi-ss-391**User:** System**Acquired:** 7/19/2006 11:13:20 AM**Printed:** 4/25/2007 2:36:06 PM**SPD-10AVvp****Ch1-220nm****Results**

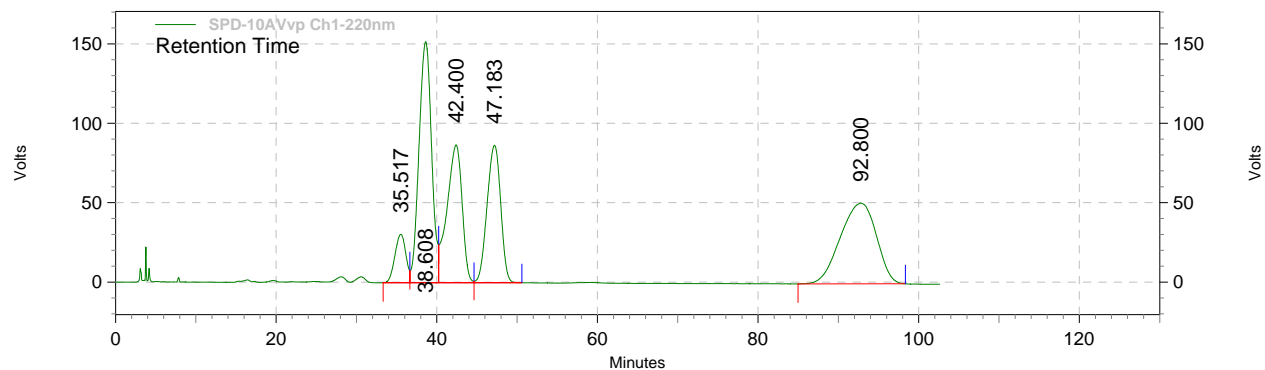
Retention Time	Area	Area %	Height	Height %
56.808	3079080	1.53	22484	6.35
58.258	7413595	3.68	27251	7.69
75.492	103989510	51.62	216098	60.99
110.425	86982472	43.18	88508	24.98
Totals	201464657	100.00	354341	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\VI-SS-46L1
User: System
Acquired: 8/5/2006 1:28:42 PM
Printed: 4/25/2007 2:37:19 PM



Racemic, Syn

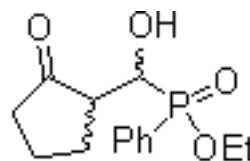


SPD-10AVvp
Ch1-220nm
Results

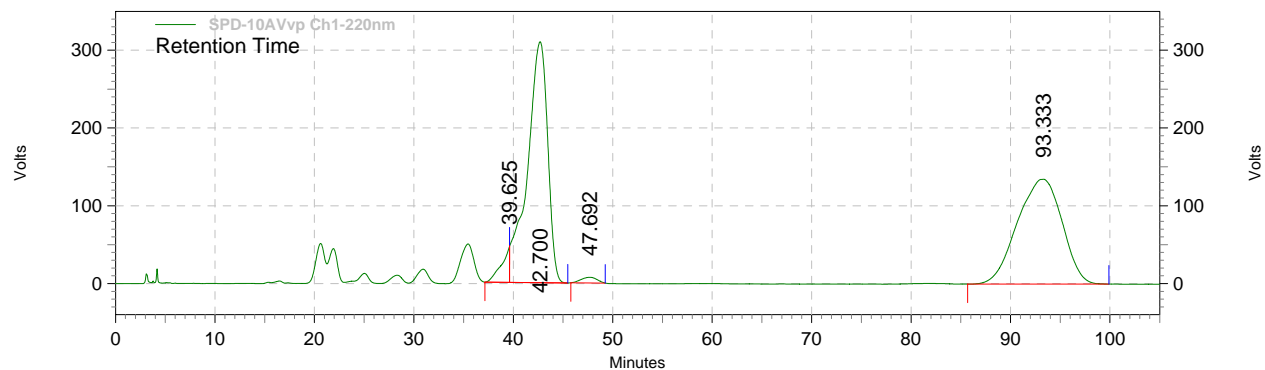
Retention Time	Area	Area %	Height	Height %
35.517	2865142	5.04	30496	7.50
38.608	16533169	29.11	151729	37.33
42.400	11352432	19.99	86837	21.37
47.183	10195706	17.95	86535	21.29
92.800	15850187	27.91	50847	12.51
Totals	56796636	100.00	406444	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\VI-SS-63L1
User: System
Acquired: 8/5/2006 3:13:30 PM
Printed: 4/25/2007 2:39:18 PM



Chiral, Syn

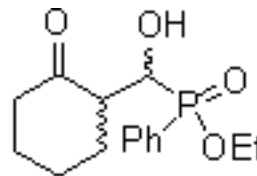


SPD-10AVvp Ch1-220nm Results

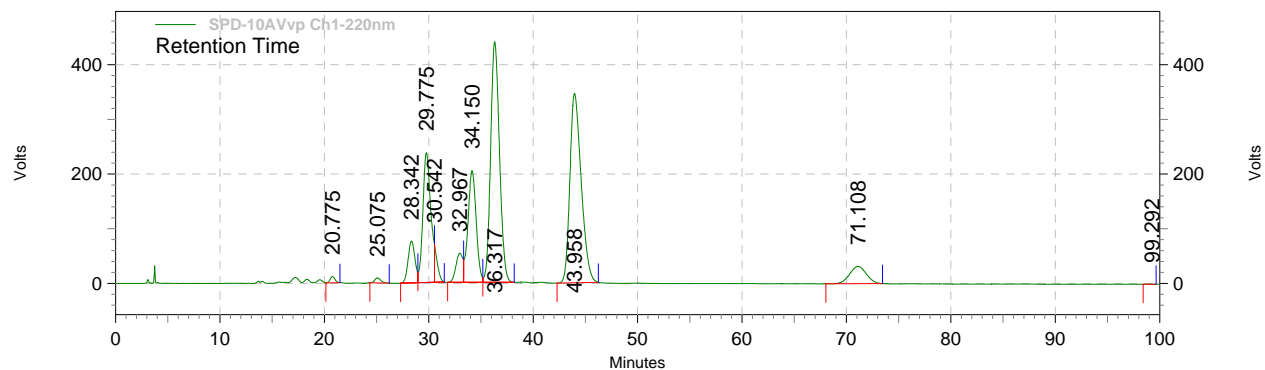
Retention Time	Area	Area %	Height	Height %
39.625	2543288	2.84	46373	9.31
42.700	43906765	49.10	309751	62.19
47.692	795505	0.89	7192	1.44
93.333	42186405	47.17	134726	27.05
Totals	89431963	100.00	498042	100.00

Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
 Data: C:\EZStart\Projects\Default\Data\VI-SS-53
 User: System
 Acquired: 7/28/2006 10:08:57 AM
 Printed: 4/25/2007 2:40:23 PM



Racemic, anti + syn



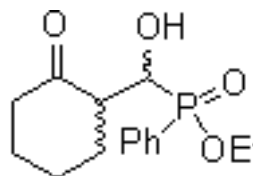
**SPD-10AVvp
 Ch1-220nm
 Results**

Retention Time	Area	Area %	Height	Height %
20.775	359468	0.41	11427	0.77
25.075	364734	0.42	9243	0.62
28.342	3491966	4.00	76574	5.17
29.775	12440202	14.27	237420	16.04
30.542	1314901	1.51	69656	4.70
32.967	2451333	2.81	53372	3.60
34.150	11194228	12.84	204414	13.81
36.317	25994095	29.81	440277	29.74
43.958	26027264	29.85	346457	23.40
71.108	3560556	4.08	31644	2.14
99.292	816	0.00	24	0.00

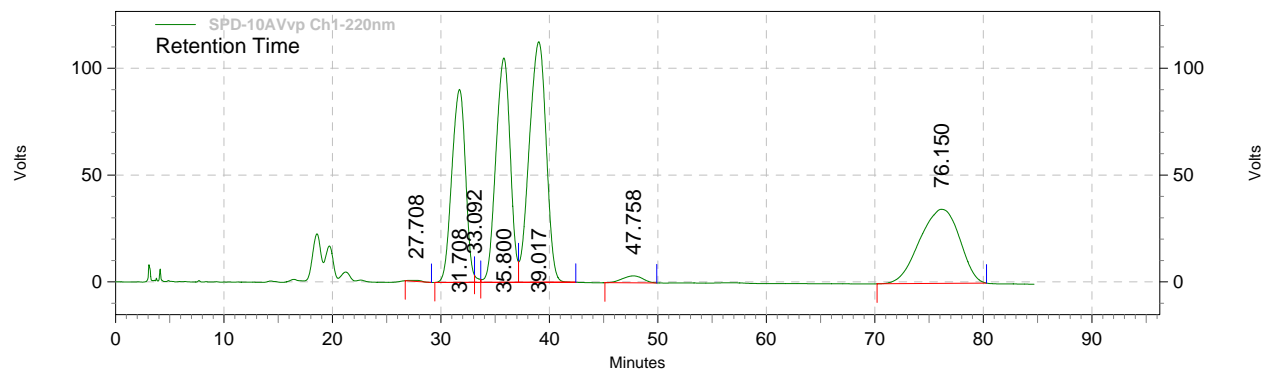
Totals	87199563	100.00	1480508	100.00
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Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\VI-SS-62
User: System
Acquired: 8/7/2006 11:14:26 AM
Printed: 4/25/2007 2:40:57 PM



Chiral, anti + syn



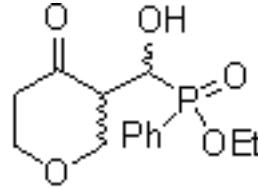
SPD-10AVvp Ch1-220nm Results

Retention Time	Area	Area %	Height	Height %
27.708	33965	0.09	511	0.15
31.708	7932167	20.23	90359	25.82
33.092	69246	0.18	3361	0.96
35.800	9663671	24.64	105077	30.03
39.017	12228688	31.18	112664	32.20
47.758	421693	1.08	3236	0.92
76.150	8866306	22.61	34686	9.91

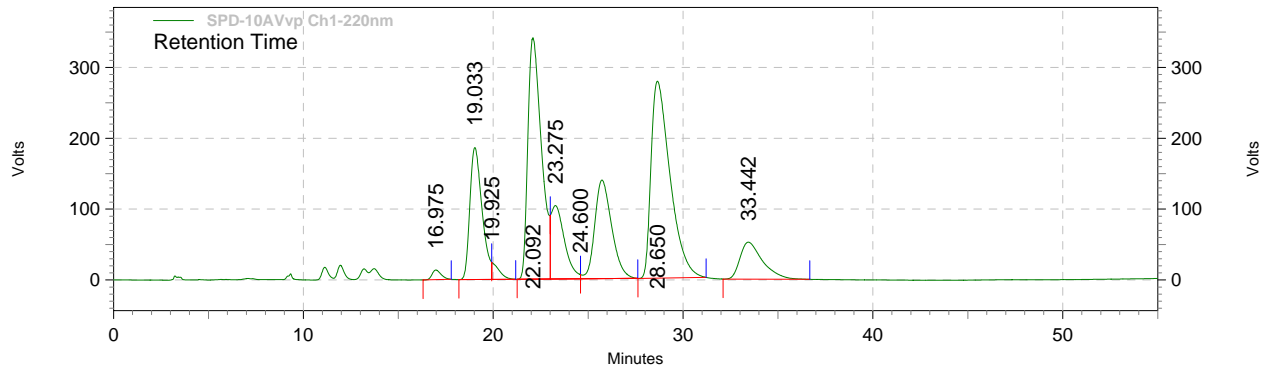
Totals	39215736	100.00	349894	100.00
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Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\VI-SS-78F
User: System
Acquired: 8/15/2006 1:19:05 PM
Printed: 4/25/2007 2:41:32 PM



Racemic, anti + syn



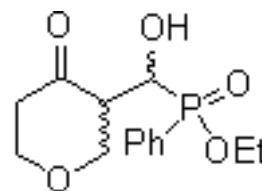
SPD-10AVvp
Ch1-220nm
Results

Retention Time	Area	Area %	Height	Height %
16.975	446247	0.70	13652	1.36
19.033	8305161	13.03	186364	18.55
19.925	627444	0.98	24132	2.40
22.092	17022499	26.70	340873	33.92
23.275	5068369	7.95	103684	10.32
24.600	8644698	13.56	5890	0.59
28.650	19343407	30.34	278106	27.68
33.442	4301600	6.75	52180	5.19

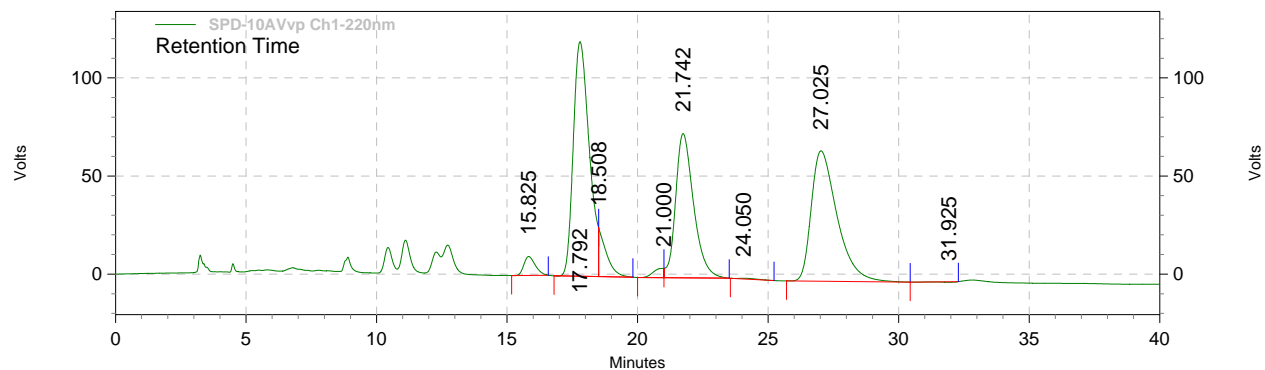
Totals	63759425	100.00	1004881	100.00
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Area % Report

Method Name: C:\EZStart\Projects\Default\Methods\AS.met
Data: C:\EZStart\Projects\Default\Data\VI-SS-80E
User: System
Acquired: 8/16/2006 1:59:53 PM
Printed: 4/25/2007 2:42:13 PM



Chiral, anti + syn



SPD-10AVvp
Ch1-220nm
Results

Retention Time	Area	Area %	Height	Height %
15.825	292638	2.07	9641	3.22
17.792	5060293	35.88	119527	39.93
18.508	506020	3.59	24884	8.31
21.000	129091	0.92	4758	1.59
21.742	3530618	25.03	73535	24.56
24.050	18531	0.13	338	0.11
27.025	4555852	32.30	66441	22.19
31.925	10474	0.07	248	0.08

Totals	14103517	100.00	299372	100.00
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