Supporting Information

for

'Incorporation of Ahc into Model Dipeptides as an Inductor of a β-Turn with a Distorted Amide Bond. Analysis of Solid State Conformation'

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CONTENTS:

Boc-L-Ser(OBn)-L-Pro-NHMe (7). ^{1}H NMR ($CDCl_3$): δ = 1.43 (s, 9H, Boc); 1.79-2.05 (m, 3H); 2.21-2.29 (m, 1H); 2.36 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, C$\underline{H}_3$NH); 3.62-3.87 (m, 4H, $2H_\beta$ + $2H_{5Pro}$); 4.52-4.59 (m, 2H, H_{Bn}); 4.60-4.67 (m, 1H, H_{2Pro}); 4.74-4.85 (m, 1H, H_α); 5.68 (d, 1H, $J_{NHBoc\text{-}H\alpha}$ = 8.1, NH_{Boc}); 6.61-6.73 (m, 1H, $\underline{NH}CH_3$); 7.22-7.40 (m, 5H, arom.). ^{13}C NMR ($CDCl_3$): δ = 24.0; 25.4 ($\underline{C}H_3NH$); 28.0 (($\underline{C}H_3)_3$); 28.2; 47.1 (C_{5Pro}); 50.8 (C_α); 59.9 (C_{2Pro}); 70.9 (C_β); 73.4 (C_{Bn}); 79.6 ($\underline{C}(CH_3)_3$); 127.0, 127.8, 128.3, 136.7 (arom.); 154.8 ($\underline{CO}OC(CH_3)_3$); 170.1, 171.0 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ser}$).

Piv-L-Ser(OBn)-L-Pro-NHMe (8). NMR data for the major conformer: ^{1}H NMR ($CDCl_3$): δ = 1.20 (s, 9H, Piv); 1.82-2.09 (m, 3H); 2.21-2.32 (m, 1H); 2.42 (d, 3H, $J_{CH3\text{-}NH}$ = 4.5, C$\underline{H}_3$NH); 3.59-3.72 (m, 2H, $H_{\beta1}$ + H_{5Pro}); 3.74-3.83 (m, 1H, H_{5Pro}); 3.90 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 9.0, $J_{H\beta2\text{-}H\alpha}$ = 5.4, $H_{\beta2}$); 4.48-4.66 (m, 3H, $2H_{Bn}$ + H_{2Pro}); 4.97-5.06 (m, 1H, H_α); 6.60-6.71 (m, 2H, $\underline{NH}CH_3$ + NH_{Piv}); 7.24-7.41 (m, 5H, arom.). ^{13}C NMR ($CDCl_3$): δ = 24.3; 25.7 ($\underline{C}H_3NH$); 27.2 (($\underline{C}H_3)_3$); 28.3; 38.5 ($\underline{C}(CH_3)_3$); 47.4 (C_{5Pro}); 50.1 (C_α); 60.2 (C_{2Pro}); 70.6 (C_β); 73.7 (C_{Bn}); 127.3, 128.1, 128.5, 136.8 (arom.); 169.8, 171.0 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ser}$); 178.1 ($\underline{CO}C(CH_3)_3$).

Piv-L-Ser-L-Pro-NHMe (2). NMR data for the major conformer: ^{1}H NMR ($CDCl_3$): δ = 1.20 (s, 9H, Piv); 1.87-2.20 (m, 4H); 2.76 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, C$\underline{H}_3$NH); 3.53-3.74 (m, 2H, $H_{\beta1}$ + H_{5Pro}); 3.84-4.02 (m, 2H, $H_{\beta2}$ + H_{5Pro}); 4.59 (dd, 1H, $J_{H2Pro\text{-}H3Pro}$ = 7.5, $J_{H2Pro\text{-}H3Pro}$ = 4.5, H_{H2Pro}); 4.77-4.96 (m, 2H, H_α + OH); 6.77 (d, 1H, $J_{NHPiv\text{-}H\alpha}$ = 7.5, NH_{Piv}); 7.14-7.24 (m, 1H, $N\underline{H}CH_3$). ^{13}C NMR ($CDCl_3$): δ = 24.6; 26.2 ($\underline{C}H_3NH$); 27.2 (($\underline{C}H_3)_3$); 29.1; 38.6 ($\underline{C}(CH_3)_3$); 47.6 (C_{5Pro}); 52.3 (C_α); 60.4 (C_{2Pro}); 63.5 (C_β); 169.8, 172.3, 178.7 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ser}$, $\underline{CO}C(CH_3)_3$).

Piv-Ahc-OBn (10). ^{1}H NMR ($CDCl_3$): δ = 1.16 (s, 9H, Piv); 1.46-1.57 (m, 2H); 1.58-1.69 (m, 2H); 1.77-1.92 (m, 2H); 2.07-2.20 (m, 2H); 4.43-4.52 (m, 1H, H_4); 5.14 (s, 2H, $C\underline{H}_2Ph$); 7.17-7.32 (m, 5H, arom.). ^{13}C NMR ($CDCl_3$): δ = 28.0, 30.6 (C_2, C_3, C_5, C_6); 31.5 ($(\underline{C}H_3)_3$); 39.6 ($\underline{C}(CH_3)_3$); 59.3 (C_4); 66.5 ($\underline{C}H_2Ph$); 68.2 (C_1); 127.7, 127.9, 128.2, 136.1 (arom.); 170.8 ($\underline{CO}OBn$); 179.2 ($\underline{CO}C(CH_3)_3$).

Piv-Ahc-OH (11). ^{1}H NMR (CD_3OD): δ = 1.25 (s, 9H, Piv); 1.55-1.74 (m, 4H); 1.80-1.95 (m, 2H); 2.03-2.19 (m, 2H); 4.59-4.67 (m, 1H, H_4). ^{13}C NMR (CD_3OD): δ = 28.4, 31.6, 33.2 (C_2, C_3, C_5, C_6, $(\underline{C}H_3)_3$); 40.9 ($\underline{C}(CH_3)_3$); 61.0 (C_4); 71.5 (C_1); 178.8, 181.2 ($\underline{CO}OH$, $\underline{CO}C(CH_3)_3$).

Boc-L-Ser(OBn)-NHMe (12). ^{1}H NMR ($CDCl_3$): δ = 1.37 (s, 9H, Boc); 2.75 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, $C\underline{H}_3NH$); 3.50 (dd, 1H, $J_{H\beta1\text{-}H\beta2}$ = 9.3, $J_{H\beta1\text{-}H\alpha}$ = 6.3, $H_{\beta1}$); 3.85 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 9.3, $J_{H\beta2\text{-}H\alpha}$ = 3.6, $H_{\beta2}$); 4.13-4.25 (m, 1H, H_α); 4.51 (d, 1H, $J_{HBn1\text{-}HBn2}$ = 11.7, H_{Bn1}); 5.33 (d, 1H, $J_{HBn2\text{-}HBn1}$ = 11.7, H_{Bn2}); 5.33 (brs, 1H, $\underline{NH}_{Boc}$); 6.31-6.42 (m, 1H, $\underline{NH}CH_3$); 7.16-7.32 (m, 5H, arom.). ^{13}C NMR ($CDCl_3$): δ = 26.3 ($\underline{C}H_3NH$); 28.2 ($(\underline{C}H_3)_3$); 53.8 (C_α); 69.8 (C_β); 73.4 (C_{Bn}); 80.2 ($\underline{C}(CH_3)_3$); 127.7, 127.9, 128.5, 137.4 (arom.); 155.5 ($\underline{CO}OC(CH_3)_3$), 170.8 ($\underline{CO}NHCH_3$).

L-Ser(OBn)-NHMe·HCl (13). ^{1}H NMR (CD_3OD): δ = 2.77 (s, 3H, $C\underline{H}_3NH$); 3.73-3.92 (m, 2H, $H_{\beta1}$ + $H_{\beta2}$); 4.08-4.20 (m, 1H, H_α); 4.57 (d, 1H, $J_{HBn1\text{-}HBn2}$ = 12.3, H_{Bn1}); 4.63 (d, 1H, $J_{HBn2\text{-}HBn1}$ = 12.3, H_{Bn2}); 7.20-7.41 (m, 5H, arom.). ^{13}C NMR (CD_3OD): δ = 26.5 ($\underline{C}H_3NH$); 54.5 (C_α); 69.0 (C_β); 74.3 (C_{Bn}); 128.9, 129.0, 129.4, 138.5 (arom.); 168.2 ($\underline{CO}NHCH_3$).

Piv-Ahc-L-Ser(OBn)-NHMe (14). ^{1}H NMR ($CDCl_3$): δ = 1.17 (s, 9H, Piv); 1.51-1.95 (m, 7H); 2.13-2.27 (m, 1H); 2.75 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, C$\underline{H}_3$NH); 3.52 (dd, 1H, $J_{H\beta1\text{-}H\beta2}$ = 9.3, $J_{H\beta1\text{-}H\alpha}$ = 3.9, $H_{\beta1}$); 4.19 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 9.3, $J_{H\beta2\text{-}H\alpha}$ = 2.7, $H_{\beta2}$); 4.36 (d, 1H, $J_{HBn1\text{-}HBn2}$ = 12.0, H_{Bn1}); 4.42-4.61 (m, 3H, H_α + H_{Bn2} + H_4); 6.23 (d, 1H, $J_{NHSer\text{-}H\alpha}$ = 8.1, NH_{Ser}); 7.13-7.31 (m, 5H, arom.); 7.80-7.90 (m, 1H, N$\underline{H}$CH$_3$). ^{13}C NMR ($CDCl_3$): δ = 26.2 ($\underline{C}H_3$NH); 27.8 (($\underline{C}H_3)_3$); 30.1, 30.2, 30.9, 33.4 (C_2, C_3, C_5, C_6); 40.2 ($\underline{C}(CH_3)_3$); 52.8 (C_α); 60.2 (C_4); 68.9 (C_β); 69.8 (C_1); 72.9 (C_{Bn}); 127.5, 127.6, 128.3, 137.7 (arom.); 170.2, 170.3 ($\underline{CO}$NHCH$_3$, $\underline{CO}_{Ahc}$); 182.0 ($\underline{CO}C(CH_3)_3$).

Piv-Ahc-(L)-Ser-NHMe (3). ^{1}H NMR ($CDCl_3$): δ = 1.18 (s, 9H, Piv); 1.53-2.02 (m, 7H); 2.13-2.26 (m, 1H); 2.69 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, C$\underline{H}_3$NH); 3.61 (dd, 1H, $J_{H\beta1\text{-}H\beta2}$ = 11.4, $J_{H\beta1\text{-}H\alpha}$ = 3.6, $H_{H\beta1}$); 4.11 ("t", 1H, $J_{OH\text{-}H\beta1}$ = $J_{OH\text{-}H\beta2}$ = 6.0, OH); 4.23 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 11.4, $J_{H\beta2\text{-}H\alpha}$ = 2.7, $H_{\beta2}$); 4.39-4.49 (m, 1H, H_α); 4.52-4.62 (m, 1H, H_4); 6.51 (d, 1H, $J_{NHSer\text{-}H\alpha}$ = 8.4, H_{NHSer}); 7.84-8.01 (m, 1H, $\underline{NH}$CH$_3$) ^{13}C NMR ($CDCl_3$): δ = 26.2 ($\underline{C}H_3$NH); 28.0 (($\underline{C}H_3)_3$); 30.3, 30.8, 30.9, 33.1 (C_2, C_3, C_5, C_6); 40.2 ($\underline{C}(CH_3)_3$); 54.6 (C_α); 60.2 (C_4); 62.2 (C_β); 69.9 (C_1); 170.7, 171.4 ($\underline{CO}$NHCH$_3$, $\underline{CO}_{Ahc}$); 181.7 ($\underline{CO}C(CH_3)_3$).

Boc-Ahc-OH (15). ^{1}H NMR ($CDCl_3$): δ = 1.19-1.38 (m, 11H, 9H Boc + 2H); 1.51-1.77 (m, 4H); 1.99-2.18 (m, 2H); 4.09-4.18 (m, 1H, H_4); ^{13}C NMR ($CDCl_3$): δ = 28.3 (($\underline{C}H_3)_3$); 29.2, 34.0 (C_2, C_3, C_5, C_6); 59.7 (C_4); 70.7 (C_1); 80.7 ($\underline{C}(CH_3)_3$); 156.9 ($\underline{CO}C(CH_3)_3$); 178.4 ($\underline{CO}$OH).

Boc-Ahc-NHMe (16). ^{1}H NMR ($CDCl_3$): δ = 1.35 (s, 9H, Boc); 1.38-1.49 (m, 2H); 1.72-1.91 (m, 4H); 1.92-2.07 (m, 2H); 2.80 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, C$\underline{H}_3$NH); 4.21-4.30 (m, 1H, H_4); 5.99-6.11 (m, 1H, $\underline{NH}$CH$_3$). ^{13}C NMR ($CDCl_3$): δ = 26.1 ($\underline{C}H_3$NH); 27.9 (($\underline{C}H_3)_3$);

28.9, 34.0 (C_2, C_3, C_5, C_6); 60.3 (C_4); 70.4 (C_1); 80.5 ($\underline{C}(CH_3)_3$); 157.0 ($\underline{CO}OC(CH_3)_3$); 172.2 ($\underline{CO}NHCH_3$).

Ahc-NHMe·HCl (17). ^{1}H NMR (CD_3OD): δ = 1.82-2.26 (m, 8H); 2.80 (s, 3H, $C\underline{H}_3NH$); 4.13-4.22 (m, 1H, H_4). ^{13}C NMR (CD_3OD): δ = 26.5 ($\underline{C}H_3NH$); 29.2, 31.7 (C_2, C_3, C_5, C_6); 59.1 (C_4); 74.7 (C_1); 170.1 ($\underline{CO}NHCH_3$).

Boc-L-Ser(OBn)-Ahc-NHMe (18). ^{1}H NMR ($CDCl_3$): δ = 1.35 (s, 9H, Boc); 1.43-2.05 (m, 8H); 2.69 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, $C\underline{H}_3NH$); 3.52-3.64 (m, 2H, $H_{\beta1}$ + $H_{\beta2}$); 4.25-4.35 (m, 1H, H_4); 4.39 (d, 1H, $J_{HBn1\text{-}HBn2}$ = 12.0, H_{Bn1}); 4.42-4.58 (m, 2H, H_α + H_{Bn2}); 5.40 (d, 1H, $J_{NHBoc\text{-}H\alpha}$ = 8.1, NH_{Boc}); 6.27-6.36 (m, 1H, $\underline{NH}CH_3$); 7.14-7.29 (m, 5H, arom.). ^{13}C NMR ($CDCl_3$): δ = 26.3 ($\underline{C}H_3NH$); 28.2 ($(\underline{C}H_3)_3$); 29.3, 30.6, 31.3, 35.0 (C_2, C_3, C_5, C_6); 52.7 (C_α); 60.0 (C_4); 69.7 (C_1); 70.9 (C_β); 73.3 (C_{Bn}); 79.8 ($\underline{C}(CH_3)_3$); 127.6, 127.7, 128.2, 137.4 (arom.); 155.2 ($\underline{CO}OC(CH_3)_3$); 171.1, 171.2 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ser}$).

Piv-L-Ser(OBn)-Ahc-NHMe (19). ^{1}H NMR ($CDCl_3$): δ = 1.12 (s, 9H, Piv); 1.31-1.57 (m, 2H); 1.58-1.82 (m, 4H); 1.83-2.11 (m, 2H); 2.70 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, $C\underline{H}_3NH$); 3.52-3.65 (m, 2H, $H_{\beta1}$ + $H_{\beta2}$); 4.26-4.34 (m, 1H, H_4); 4.40 (d, 1H, $J_{HBn1\text{-}HBn2}$ = 12.0, H_{Bn1}); 4.50 (d, 1H, $J_{HBn2\text{-}HBn1}$ = 12.0, H_{Bn2}); 4.74-4.83 (m, 1H, H_α); 6.26-6.35 (m, 1H, $\underline{NH}CH_3$); 6.61 (d, 1H, $J_{NHPiv\text{-}H\alpha}$ = 7.2, NH_{Piv}); 7.14-7.32 (m, 5H, arom.). ^{13}C NMR ($CDCl_3$): δ = 26.2 ($\underline{C}H_3NH$); 27.2 ($(\underline{C}H_3)_3$); 29.1, 30.6, 30.8, 35.2 (C_2, C_3, C_5, C_6); 38.5 ($\underline{C}(CH_3)_3$); 51.4 (C_α); 60.0 (C_4); 69.5 (C_1); 70.4 (C_β); 73.2 (C_{Bn}); 127.7, 127.8, 128.3, 137.3 (arom.); 170.8, 170.9 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ser}$); 178.1 ($\underline{CO}C(CH_3)_3$).

Piv-L-Ser-Ahc-NHMe (4). ^{1}H NMR ($CDCl_3$): δ = 1.14 (s, 9H, Piv); 1.49-1.64 (m, 2H); 1.67-1.90 (m, 3H); 1.91-2.16 (m, 3H); 2.82 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, $C\underline{H}_3NH$); 3.71 (dd, 1H,

$J_{H\beta1\text{-}H\beta2}$ = 11.4, $J_{H\beta1\text{-}H\alpha}$ = 4.5, $H_{\beta1}$); 3.80 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 11.4, $J_{H\beta2\text{-}H\alpha}$ = 4.2, $H_{\beta2}$); 4.38-4.47 (m, 1H, H_4); 4.61-4.69 (m, 1H, H_α); 6.21-6.34 (m, 1H, $\underline{NH}CH_3$); 6.82 (d, 1H, $J_{NHPiv\text{-}H\alpha}$ = 6.9, NH_{Piv}). ^{13}C NMR ($CDCl_3$): δ = 26.7 ($\underline{C}H_3NH$); 27.4 (($\underline{C}H_3)_3$); 29.6, 30.8, 35.2, 35.3 (C_2, C_3, C_5, C_6); 38.7 ($\underline{C}(CH_3)_3$); 53.6 (C_α); 59.8 (C_4); 64.8 (C_β); 69.4 (C_1); 171.0, 171.0 ($\underline{CO}NHCH_3$, $\underline{CO}C(CH_3)_3$); 179.0 ($\underline{CO}_{Ser}$).

Piv-L-(O-(+)-MTPA)Ser-L-Pro-NHMe (20). NMR data for the major isomer: ^{1}H NMR ($CDCl_3$): δ = 1.16 (s, 9H, Piv); 1.85-2.14 (m, 3H); 2.32-2.43 (m, 1H); 2.66 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, $C\underline{H}_3NH$); 3.54 (s, 3H, $O\underline{CH}_3$); 3.61-3.70 (m, 2H, $2H_{5Pro}$); 4.44-4.57 (m, 2H, $H_{\beta1}$ + H_{2Pro}); 4.69 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 11.4, $J_{H\beta2\text{-}H\alpha}$ = 4.2, $H_{\beta2}$); 4.98-5.06 (m, 1H, H_α); 6.46-6.54 (m, 1H, $\underline{NH}CH_3$); 6.62 (d, 1H, $J_{NH_{Ser}\text{-}H\alpha}$ = 7.2, NH_{Ser}); 7.38-7.51 (m, 5H, arom.). ^{19}F NMR ($CDCl_3$): δ = -78.81. ^{13}C NMR ($CDCl_3$): δ = 25.6; 26.1 ($\underline{C}H_3NH$); 27.2 (($\underline{C}H_3)_3$); 27.8; 38.7 ($\underline{C}(CH_3)_3$); 47.6 (C_{5Pro}); 50.0 (C_α); 55.5 (OCH_3); 60.8 (C_{2Pro}); 64.5 (C_β); 121.2, 125.0, 127.3, 128.6, 129.8, 131.6 (arom. + $\underline{C}CF_3$ + $C\underline{C}F_3$); 167.0 ($\underline{CO}$Mosher); 168.9, 170.9 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ser}$); 178.3 ($\underline{CO}C(CH_3)_3$).

Piv-L-(O-(-)-MTPA)Ser-L-Pro-NHMe (23). NMR data for the major isomer: ^{1}H NMR ($CDCl_3$): δ = 1.14 (s, 9H, Piv); 1.83-2.11 (m, 3H); 2.34-2.45 (m, 1H); 2.73 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, $C\underline{H}_3NH$); 3.52 (s, 3H, $O\underline{CH}_3$); 3.55-3.76 (m, 2H, $2H_{5Pro}$); 4.53-4.61 (m, 2H, $H_{\beta1}$ + H_{2Pro}); 4.69 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 11.4, $J_{H\beta2\text{-}H\alpha}$ = 4.2, $H_{\beta2}$); 4.94-5.05 (m, 1H, H_α); 6.51-6.64 (m, 2H, NH_{Ser} + $\underline{NH}CH_3$); 7.39-7.53 (m, 5H, arom.). ^{19}F NMR ($CDCl_3$): δ = -71.77. ^{13}C NMR ($CDCl_3$): δ = 24.9; 26.1 ($\underline{C}H_3NH$); 27.2 (($\underline{C}H_3)_3$); 27.8; 38.7 ($\underline{C}(CH_3)_3$); 47.5 (C_{5Pro}); 49.9 (C_α); 55.3 (OCH_3); 60.9 (C_{2Pro}); 64.3 (C_β); 121.2, 125.0, 127.2, 128.6, 129.8,

131.8 (arom. + $\underline{C}CF_3$ + $C\underline{C}F_3$); 166.8 ($\underline{CO}$Mosher); 168.9, 170.9 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ser}$); 178.3 ($\underline{CO}C(CH_3)_3$).

Piv-Ahc-L-Ser(O-(+)-MTPA)-NHMe (21). ^{1}H NMR ($CDCl_3$): δ = 1.21 (s, 9H, Piv); 1.54-2.03 (m, 7H); 2.18-2.32 (m, 1H); 2.77 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, $C\underline{H}_3NH$); 3.49 (s, 3H, $OC\underline{H}_3$); 4.37 (dd, 1H, $J_{H\beta1\text{-}H\beta2}$ = 11.1, $J_{H\beta1\text{-}H\alpha}$ = 3.3, $H_{\beta1}$); 4.57-4.66 (m, 1H, H_4); 4.92 ('dt', 1H, $J_{H\alpha\text{-}NHSer}$ = 9.3, $J_{H\alpha\text{-}H\beta1}$ = $J_{H\alpha\text{-}H\beta2}$ = 3.3 H_α); 5.20 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 11.1, $J_{H\beta2\text{-}H\alpha}$ = 3.3, $H_{\beta2}$); 5.99 (d, 1H, $J_{NHSer\text{-}H\alpha}$ = 9.3, NH_{Ser}); 7.35-7.52 (m, 5H, arom.); 7.89-8.02 (m, 1H, $\underline{NH}CH_3$). ^{19}F NMR ($CDCl_3$): δ = -71.94. ^{13}C NMR ($CDCl_3$): δ = 26.4 ($\underline{C}H_3NH$); 27.8 (($\underline{C}H_3)_3$); 30.2, 30.3, 31.0, 33.6 (C_2, C_3, C_5, C_6); 40.2 ($\underline{C}(CH_3)_3$); 51.7 (C_α); 55.2 ($O\underline{C}H_3$); 60.3 (C_4); 66.3 (C_β); 69.9 (C_1); 121.4, 125.2, 127.5, 128.6, 129.8, 131.3 (arom. + $\underline{C}CF_3$ + $C\underline{C}F_3$); 166.0 ($\underline{CO}$Mosher); 168.8, 170.4 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ahc}$); 182.0 ($\underline{CO}C(CH_3)_3$).

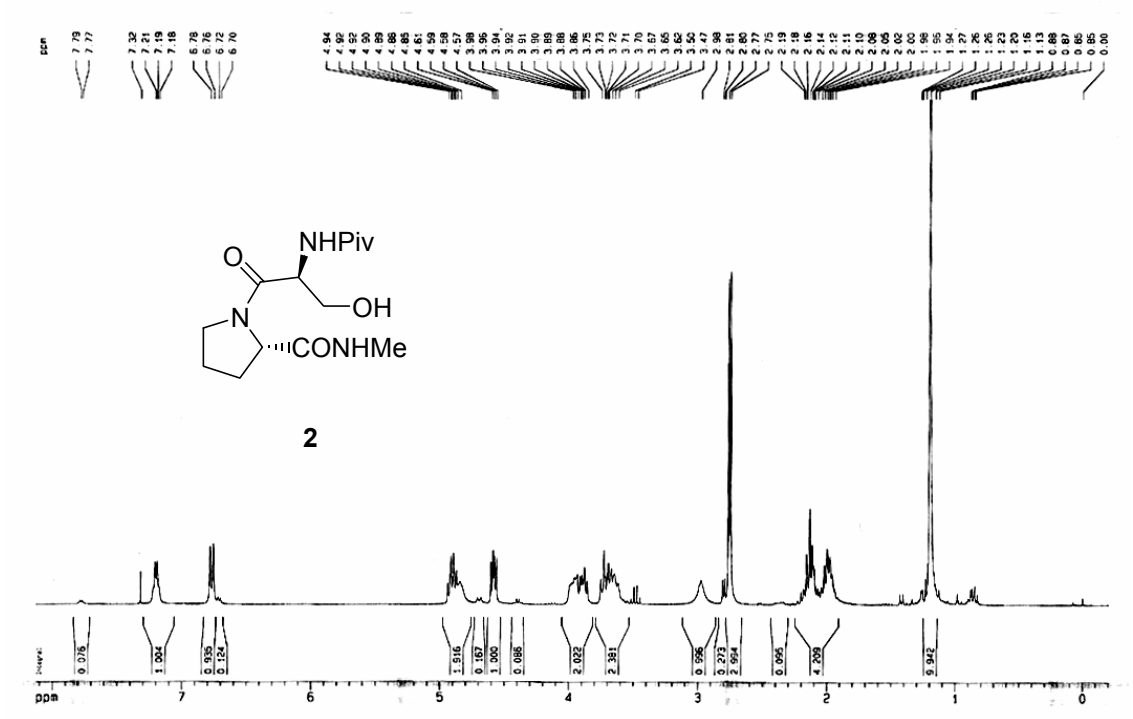
Piv-Ahc-L-(O-(-)-MTPA)Ser-NHMe (24) ^{1}H NMR ($CDCl_3$): δ = 1.24 (s, 9H, Piv); 1.56-2.06 (m, 7H); 2.19-2.33 (m, 1H); 2.77 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, $C\underline{H}_3NH$); 3.44 (s, 3H, $OC\underline{H}_3$); 4.49 (dd, 1H, $J_{H\beta1\text{-}H\beta2}$ = 11.1, $J_{H\beta1\text{-}H\alpha}$ = 3.3, $H_{\beta1}$); 4.58-4.65 (m, 1H, H_4); 4.86-4.93 (m, 1H, H_α); 5.10 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 11.1, $J_{H\beta2\text{-}H\alpha}$ = 4.2, $H_{\beta2}$); 6.11 (d, 1H, $J_{NHSer\text{-}H\alpha}$ = 9.0, NH_{Ser}); 7.33-7.52 (m, 5H, arom.); 7.88-8.03 (m, 1H, $\underline{NH}CH_3$). ^{19}F NMR ($CDCl_3$): δ = -72.50. ^{13}C NMR ($CDCl_3$): δ = 26.3 ($\underline{C}H_3NH$); 27.8 (($\underline{C}H_3)_3$); 30.1, 30.2, 31.0, 33.7 (C_2, C_3, C_5, C_6); 40.3 ($\underline{C}(CH_3)_3$); 52.1 (C_α); 55.2 ($O\underline{C}H_3$); 60.4 (C_4); 66.2 (C_β); 69.9 (C_1); 121.2, 125.0, 127.6, 128.5, 129.8, 131.3 (arom. + $\underline{C}CF_3$ + $C\underline{C}F_3$); 166.3 ($\underline{CO}$Mosher); 168.6, 170.5 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ahc}$); 182.1 ($\underline{CO}C(CH_3)_3$).

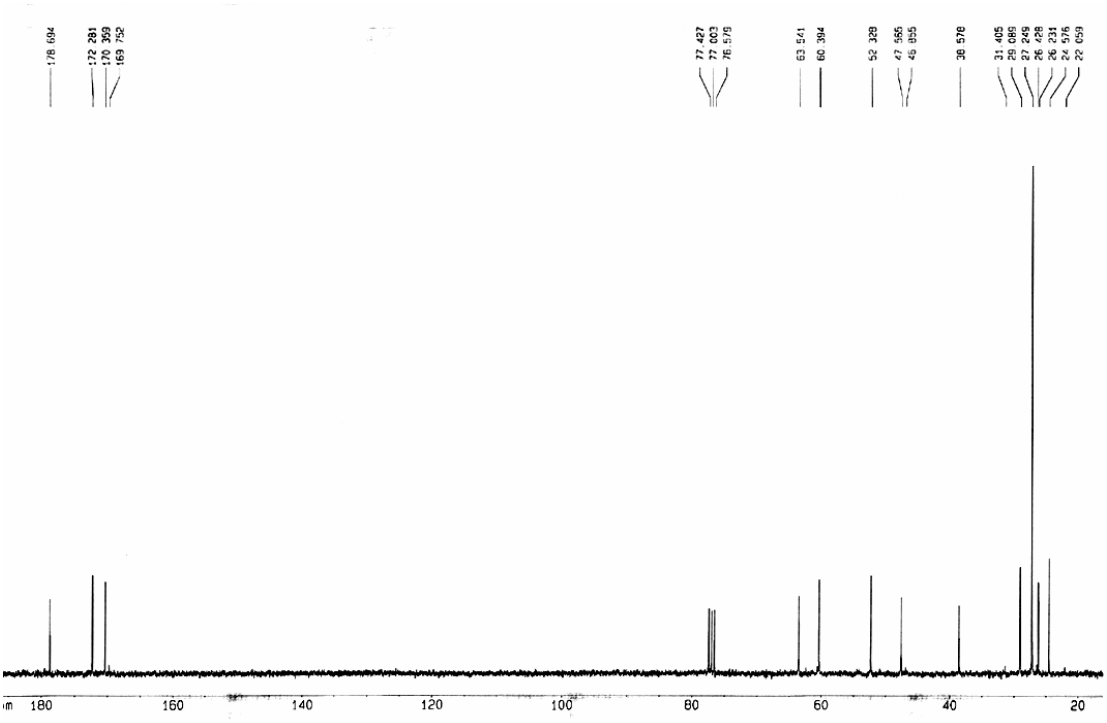
Piv-L-(O-(+)-MTPA)Ser-Ahc-NHMe (22). NMR data for the major isomer: ^{1}H NMR ($CDCl_3$): δ = 1.12 (s, 9H, Piv); 1.57-2.04 (m, 7H); 2.08-2.22 (m, 1H); 2.77 (d, 3H, $J_{CH3\text{-}NH}$

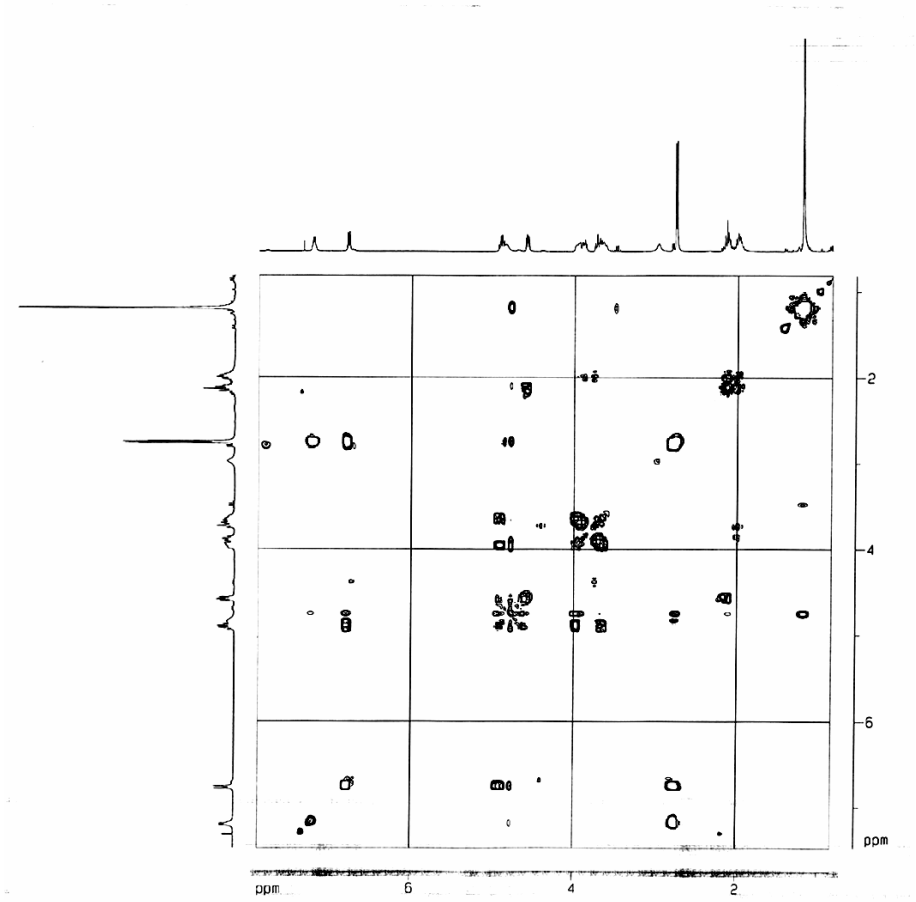
= 4.8, C$\underline{H}_3$NH); 3.51 (s, 3H, O$\underline{CH}_3$); 4.39-4.47 (m, 1H, H_4); 4.54 (dd, 1H, $J_{H\beta1\text{-}H\beta2}$ = 11.1, $J_{H\beta1\text{-}H\alpha}$ = 3.3, $H_{\beta1}$); 4.67 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 11.1, $J_{H\beta2\text{-}H\alpha}$ = 3.9, $H_{\beta2}$); 4.91-5.00 (m, 1H, H_α); 5.94-6.19 (m, 1H, $\underline{NH}CH_3$); 6.68 (d, 1H, $J_{NHSer\text{-}H\alpha}$ = 6.6, NH_{Ser}); 7.37-7.53 (m, 5H, arom.). ^{19}F NMR ($CDCl_3$): δ = -72.00. ^{13}C NMR ($CDCl_3$): δ = 26.4 ($\underline{C}H_3NH$); 27.2 (($\underline{C}H_3)_3$); 29.4, 30.7, 30.8, 35.4 (C_2, C_3, C_5, C_6); 38.7 ($\underline{C}(CH_3)_3$); 50.5 (C_α); 55.5 ($O\underline{C}H_3$); 60.4 (C_4); 66.0 (C_β); 69.8 (C_1); 121.2, 125.0, 127.4, 128.6, 129.9, 131.5 (arom. + $\underline{C}CF_3$ + $C\underline{C}F_3$); 166.7 ($\underline{CO}$Mosher); 169.5, 170.7 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ahc}$); 178.4 ($\underline{CO}C(CH_3)_3$).

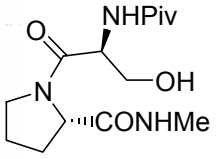
Piv-L-(O-(-)-MTPA)Ser-Ahc-NHMe (25) NMR data for the major isomer: ^{1}H NMR ($CDCl_3$): δ = 1.09 (s, 9H, Piv); 1.54-2.06 (m, 7H); 2.09-2.23 (m, 1H); 2.79 (d, 3H, $J_{CH3\text{-}NH}$ = 4.8, C$\underline{H}_3$NH); 3.53 (s, 3H, O$\underline{CH}_3$); 4.37-4.44 (m, 1H, H_4); 4.61 (dd, 1H, $J_{H\beta1\text{-}H\beta2}$ = 11.1, $J_{H\beta1\text{-}H\alpha}$ = 3.3, $H_{\beta1}$); 4.67 (dd, 1H, $J_{H\beta2\text{-}H\beta1}$ = 11.1, $J_{H\beta2\text{-}H\alpha}$ = 3.3, $H_{\beta2}$); 4.87-4.95 (m, 1H, H_α); 5.94-6.10 (m, 1H, $\underline{NH}CH_3$); 6.60 (d, 1H, $J_{NHSer\text{-}H\alpha}$ = 6.9, NH_{Ser}); 7.37-7.53 (m, 5H, arom.). ^{19}F NMR ($CDCl_3$): δ = -72.05. ^{13}C NMR ($CDCl_3$): δ = 26.4 ($\underline{C}H_3NH$); 27.2 (($\underline{C}H_3)_3$); 29.3, 30.3, 30.9, 35.8 (C_2, C_3, C_5, C_6); 38.6 ($\underline{C}(CH_3)_3$); 50.6 (C_α); 55.5 ($O\underline{C}H_3$); 60.4 (C_4); 65.8 (C_β); 69.8 (C_1); 121.2, 125.0, 127.3, 128.6, 129.9, 131.8 (arom. + $\underline{C}CF_3$ + $C\underline{C}F_3$); 166.7 ($\underline{CO}$Mosher); 169.5, 170.8 ($\underline{CO}NHCH_3$, $\underline{CO}_{Ahc}$); 178.4 ($\underline{CO}C(CH_3)_3$).

Piv-L-Ser-L-Pro-NHMe (2).









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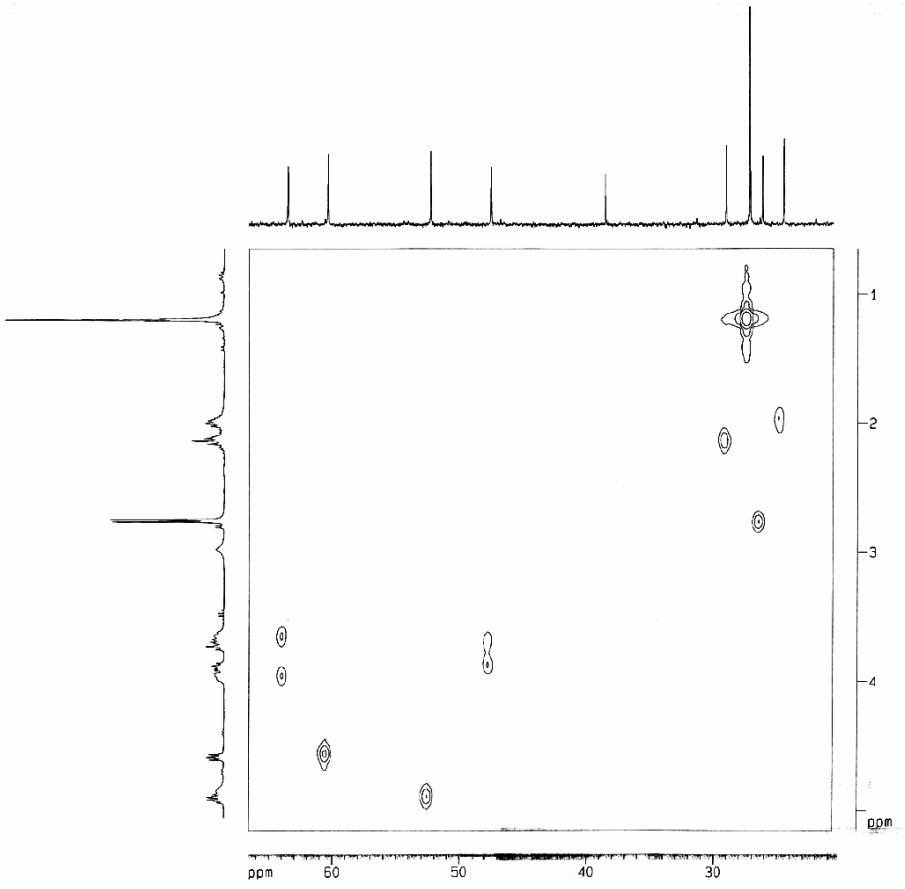
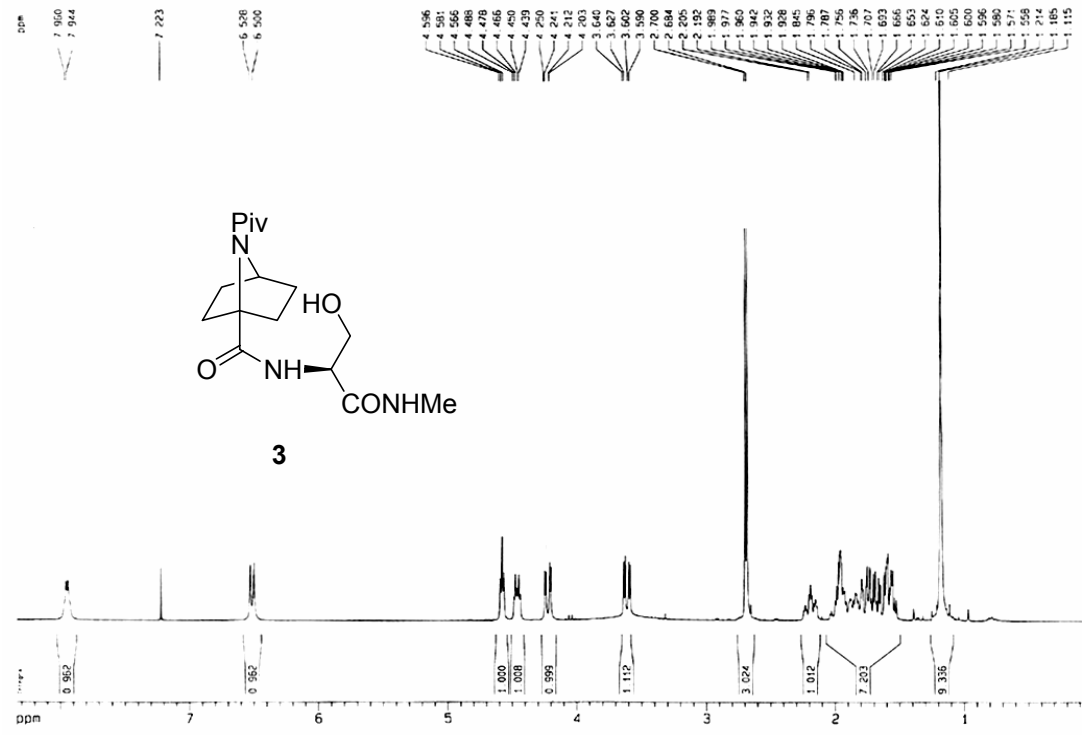
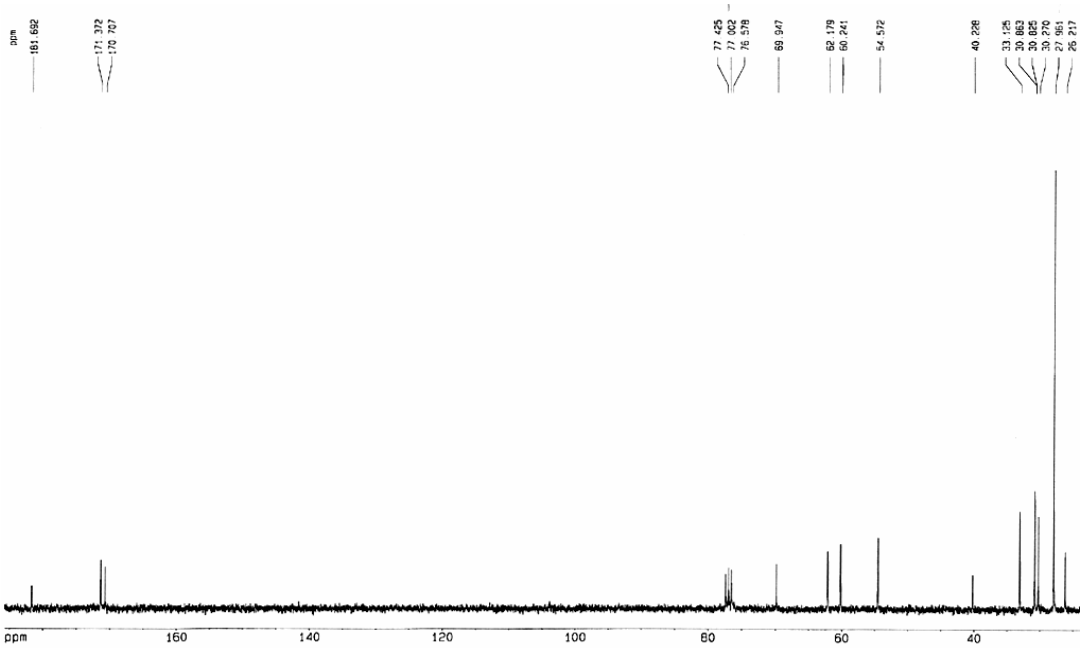
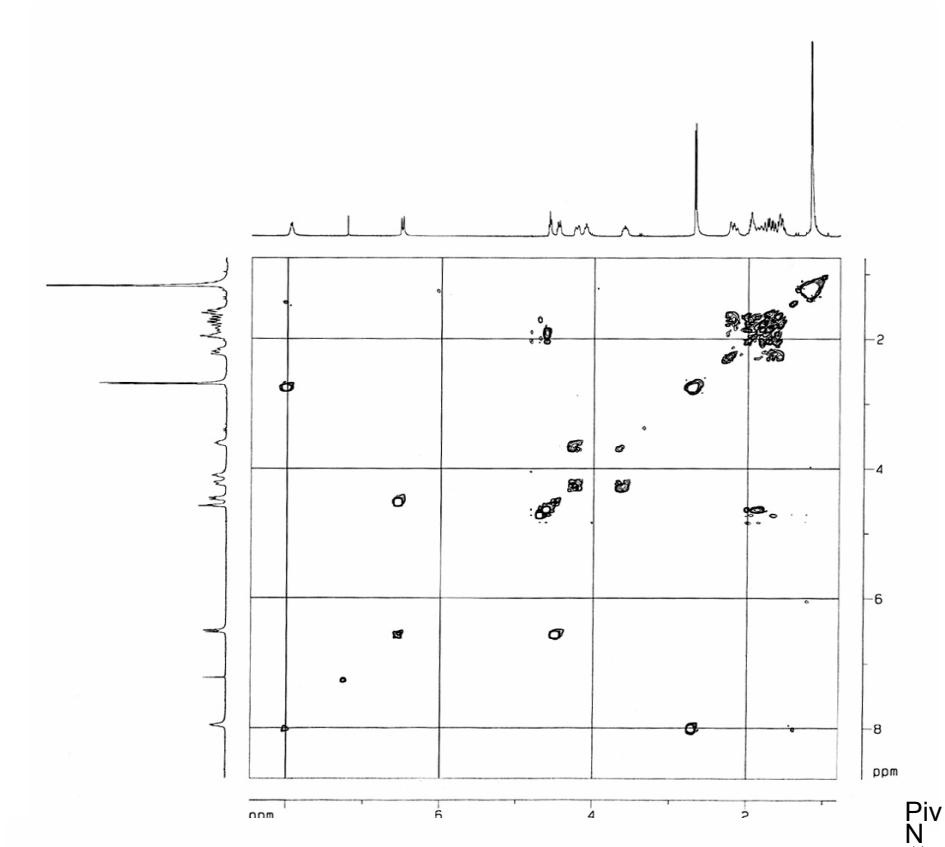
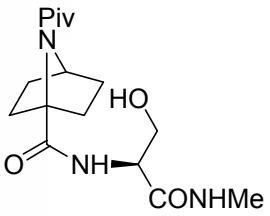


Piv-Ahc-L-Ser-NHMe (3).









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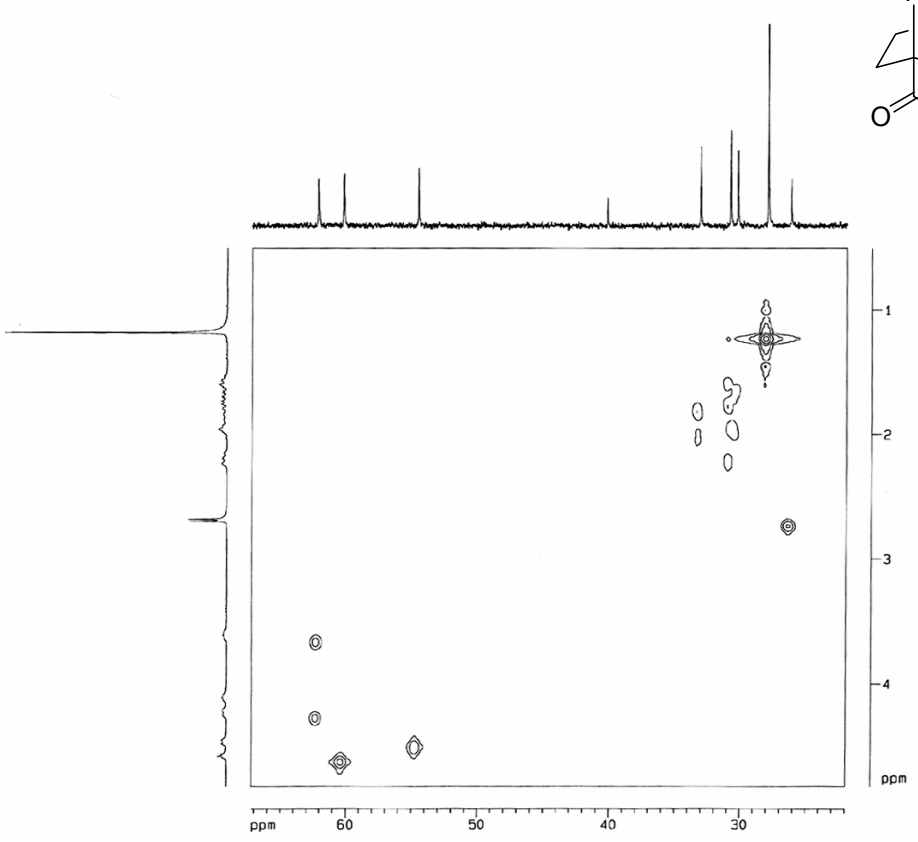
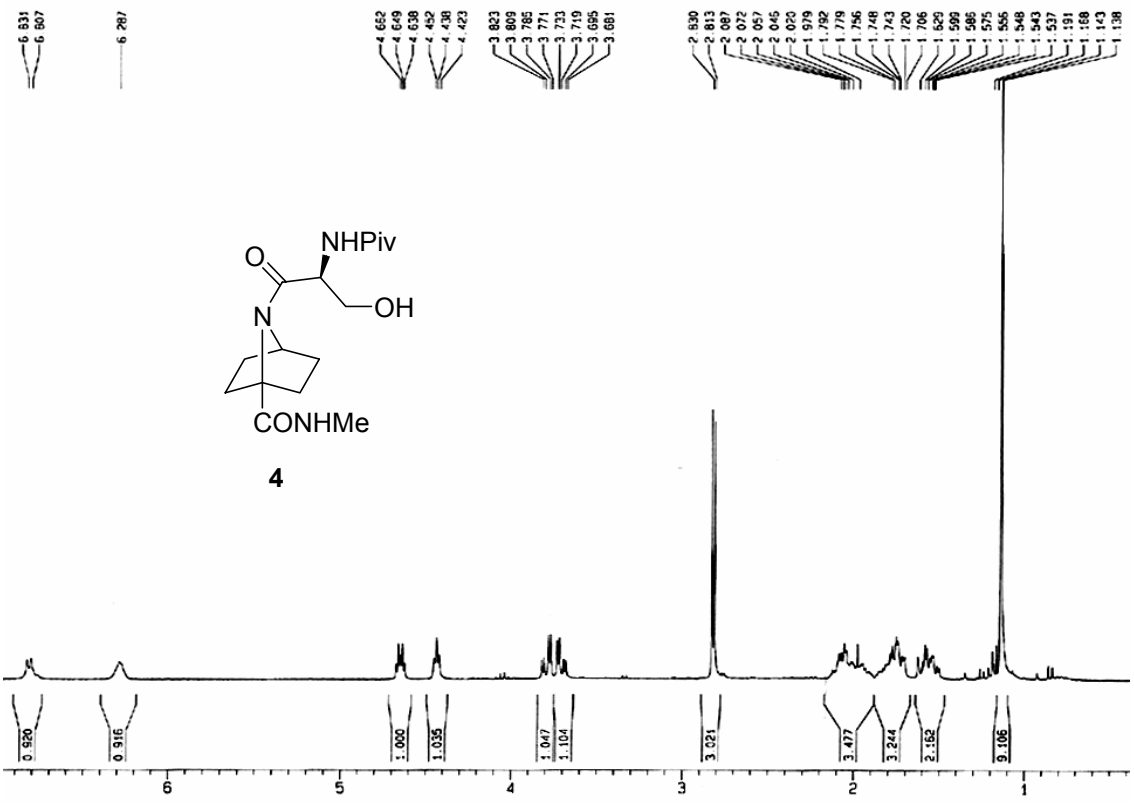
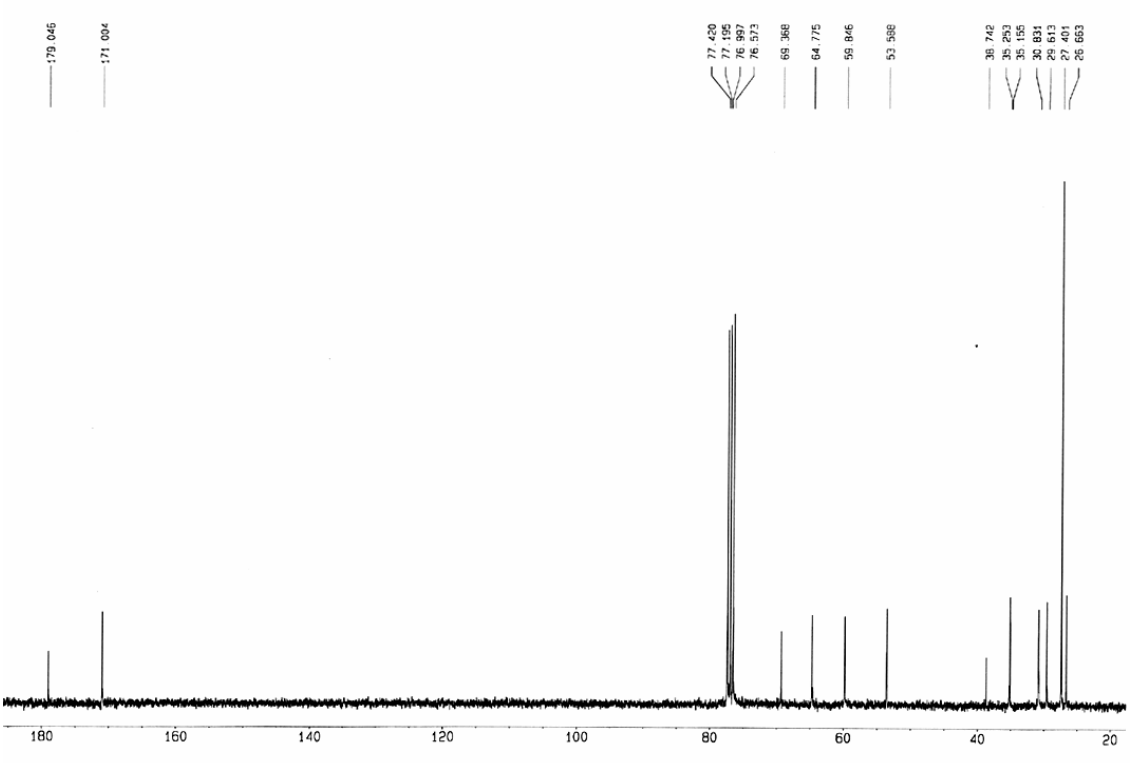
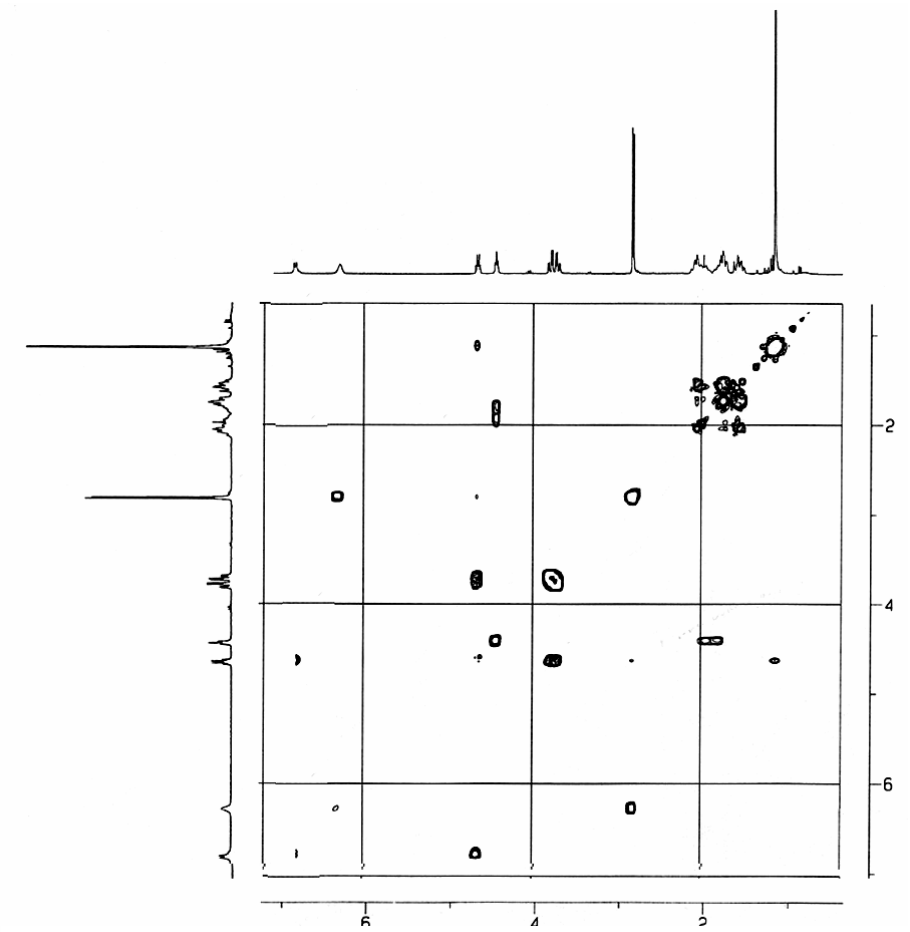
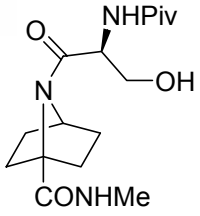


Piv-L-Ser-Ahc-NHMe (4).









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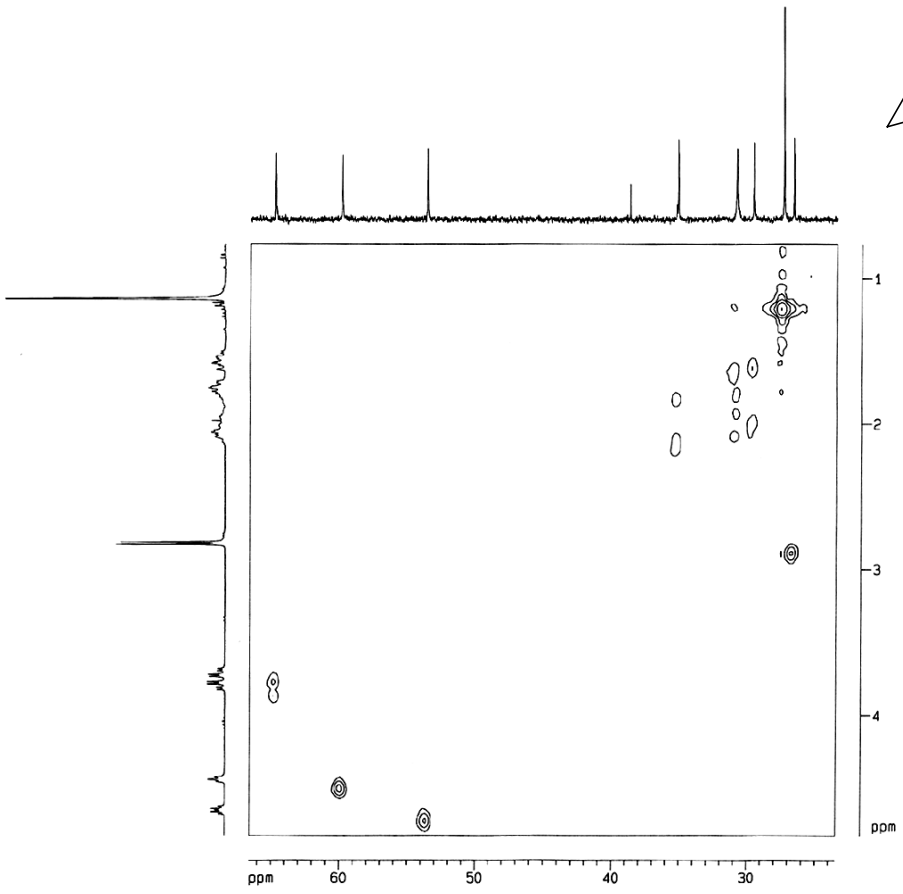
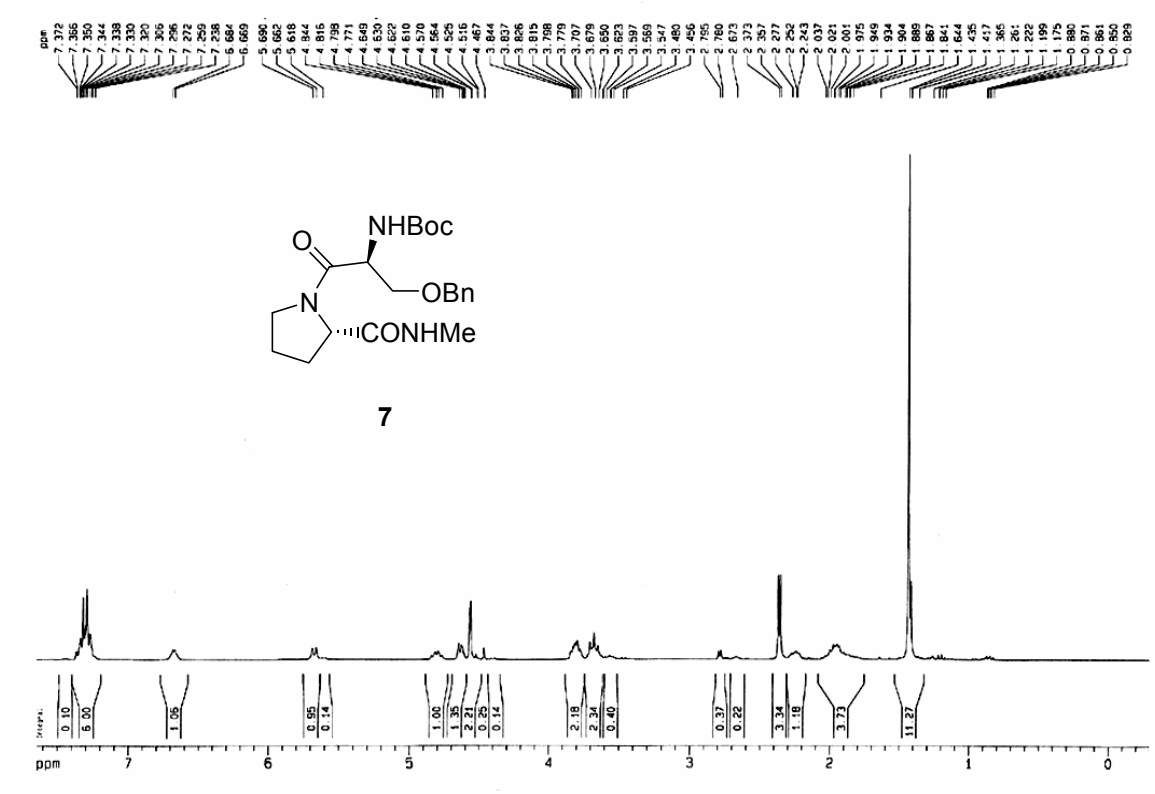
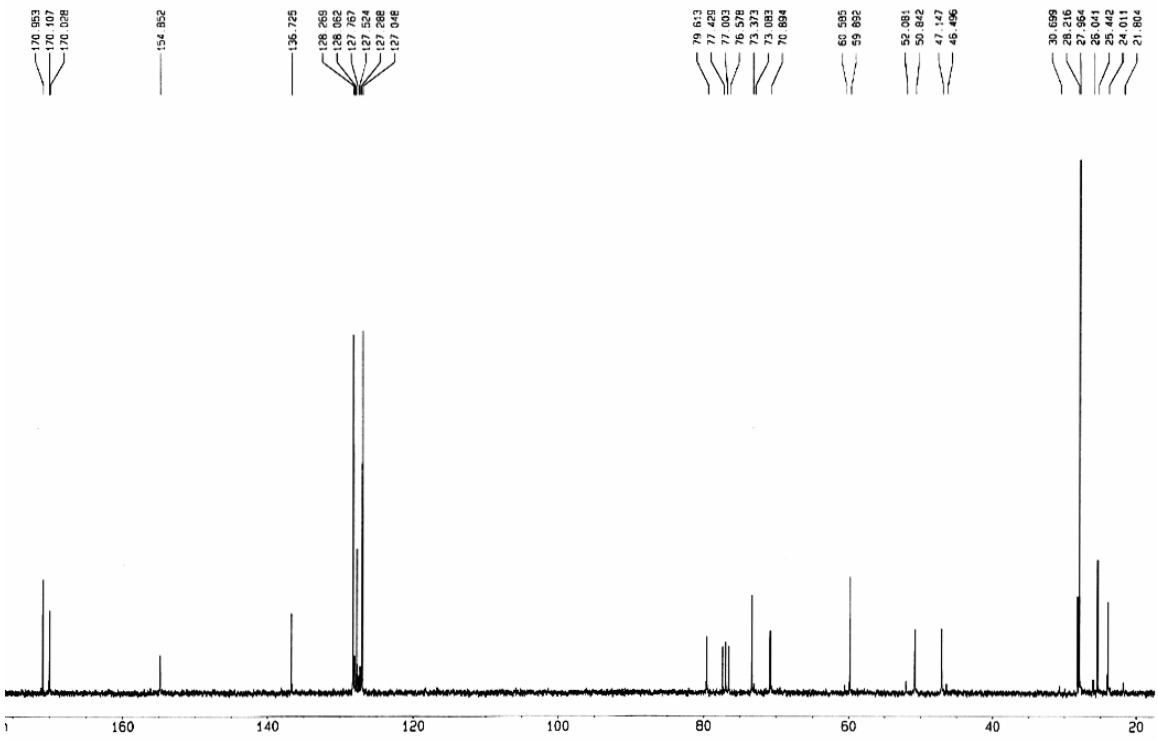
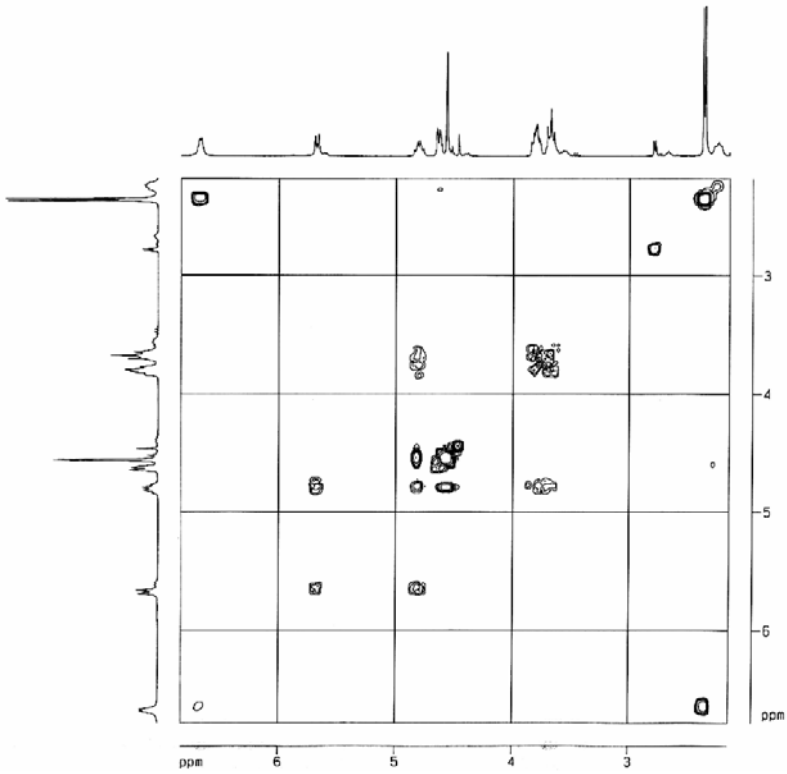
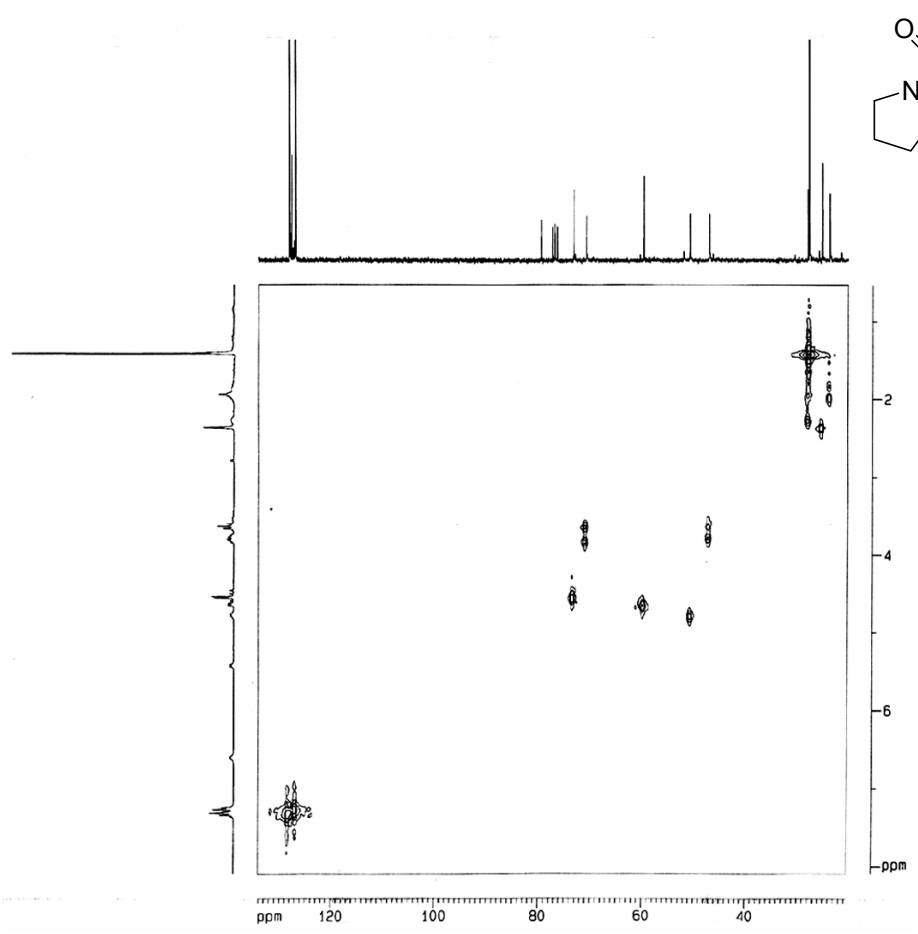


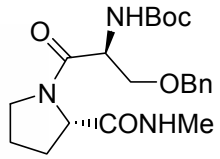
Boc-L-Ser(OBn)-L-Pro-NHMe (7).





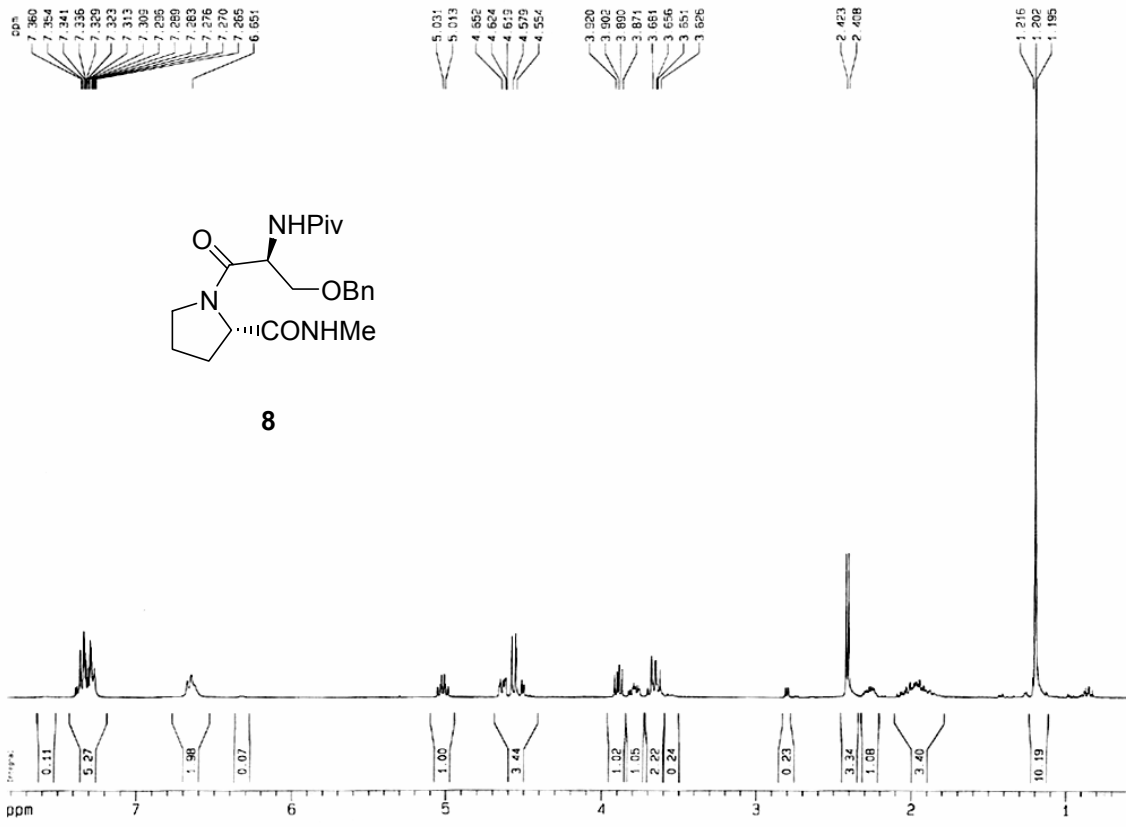

3
4
5
6
ppm
ppm
6
5
4
3

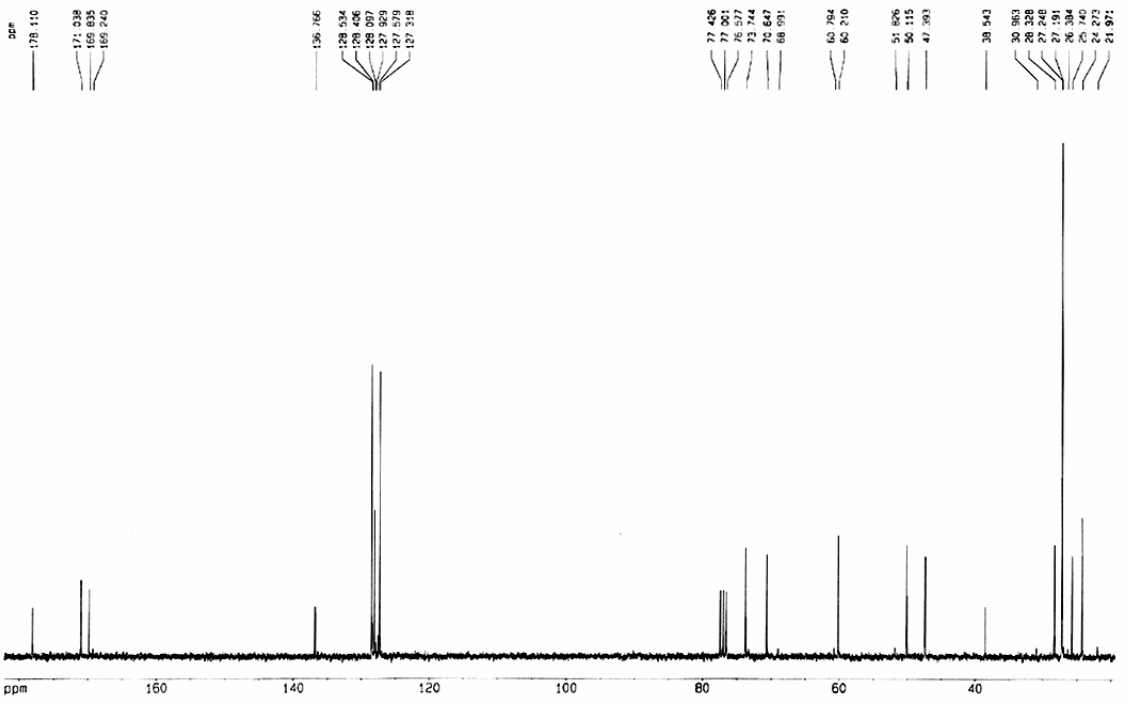

2
4
6
ppm
ppm
120
100
80
60
40

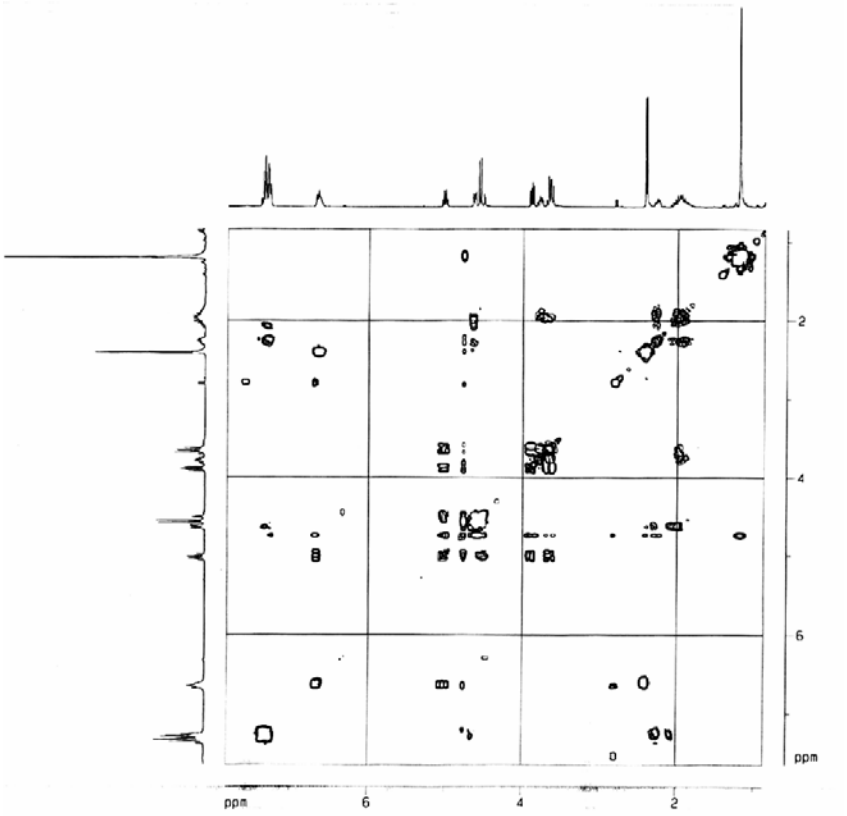

NHBoc
O
OBn
N
CONHMe

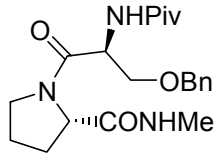
7

Piv-L-Ser(OBn)-L-Pro-NHMe (8).

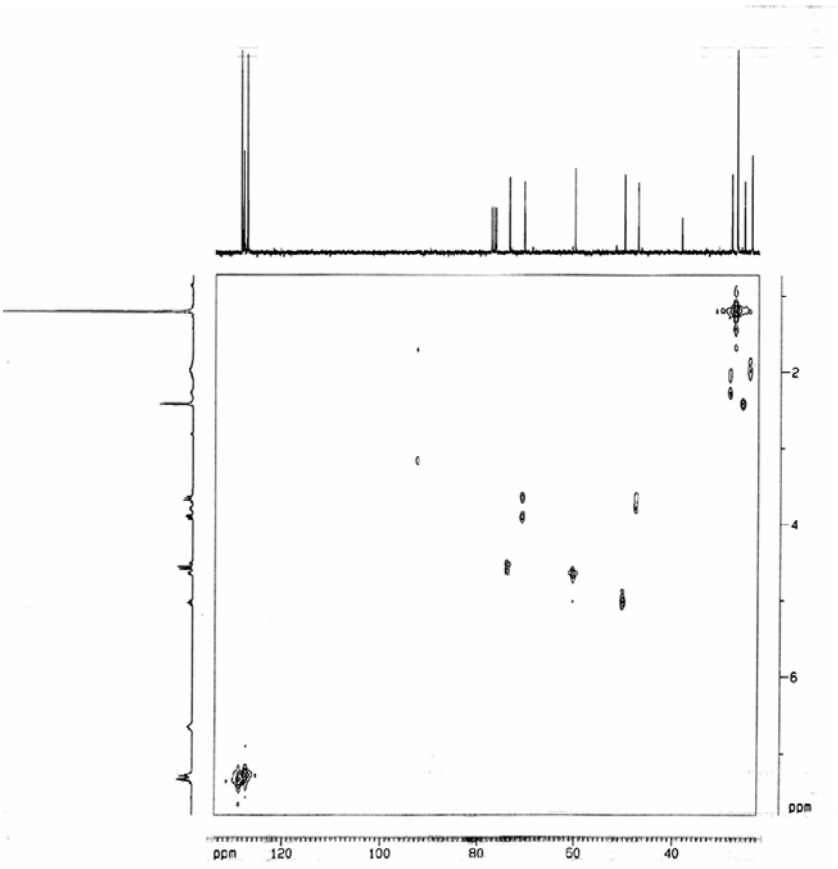




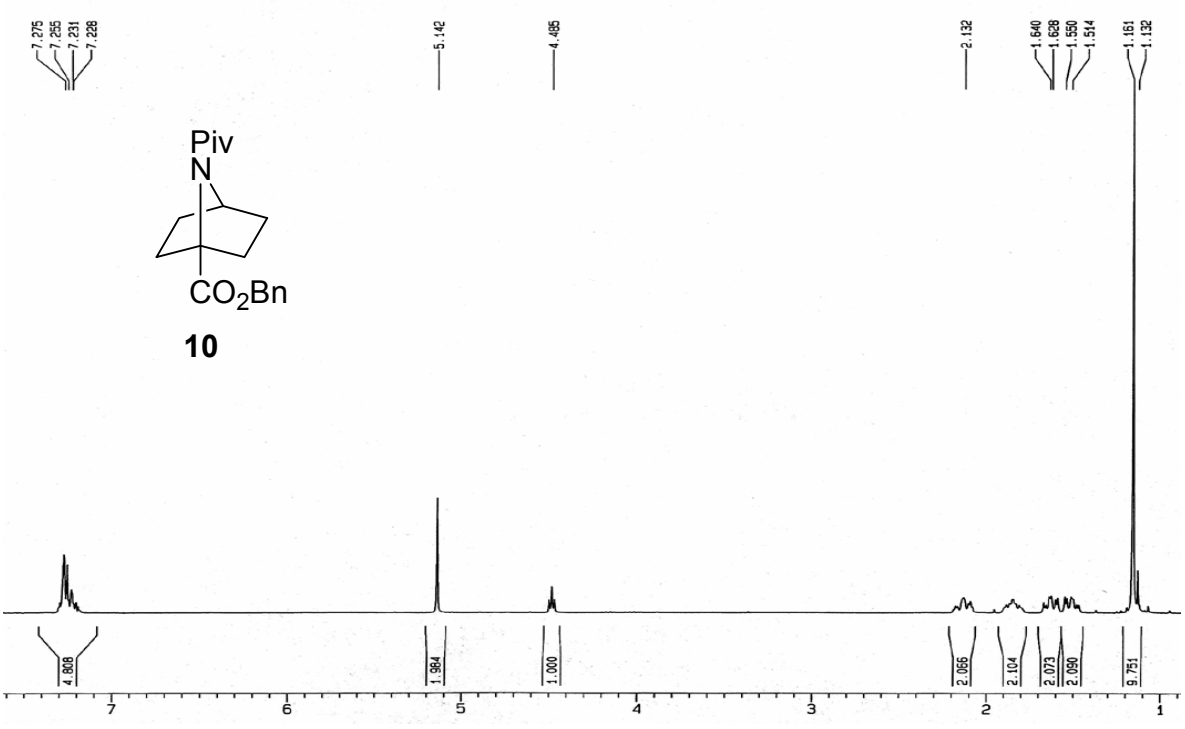


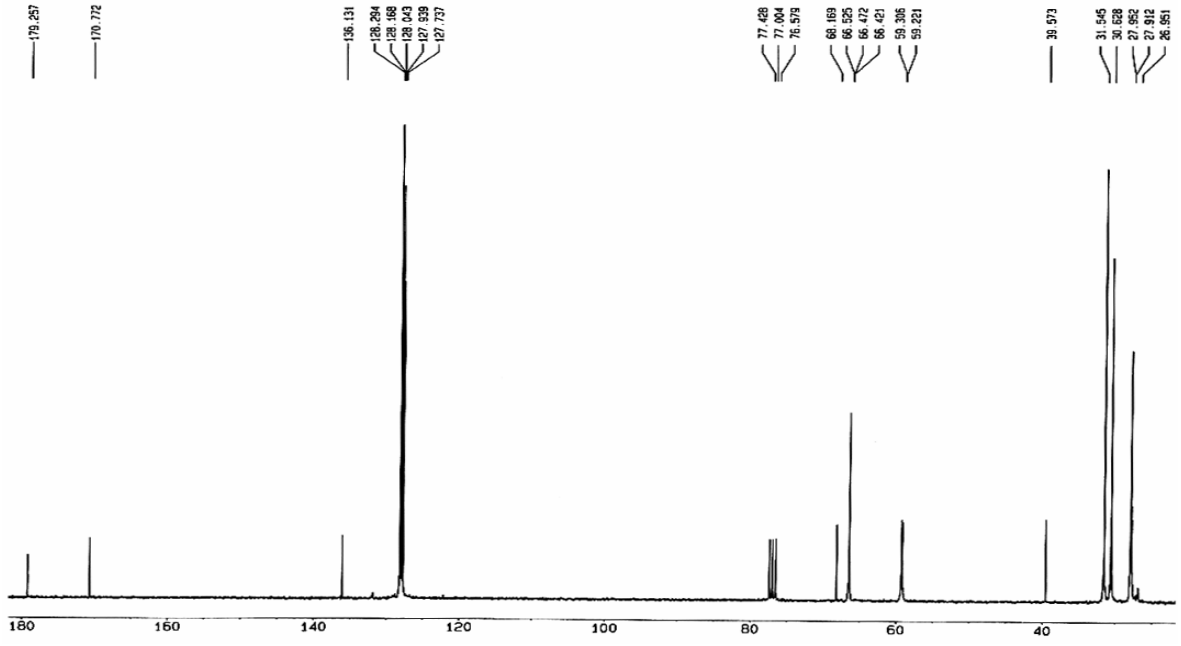


8

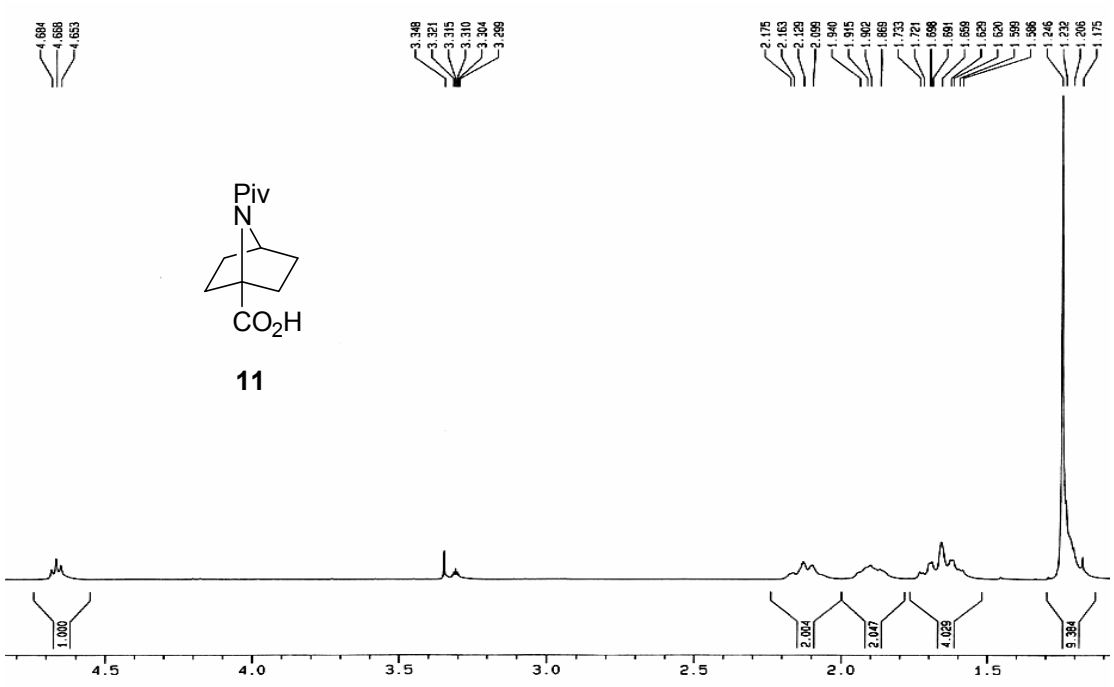


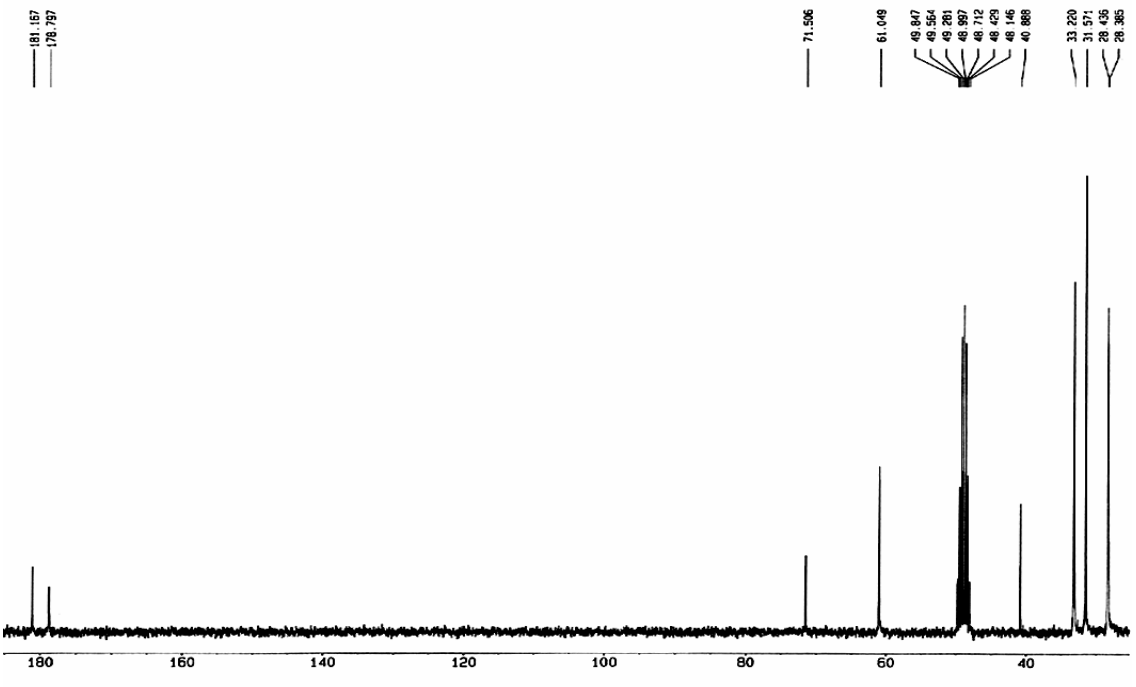
Piv-Ahc-OBn (10).



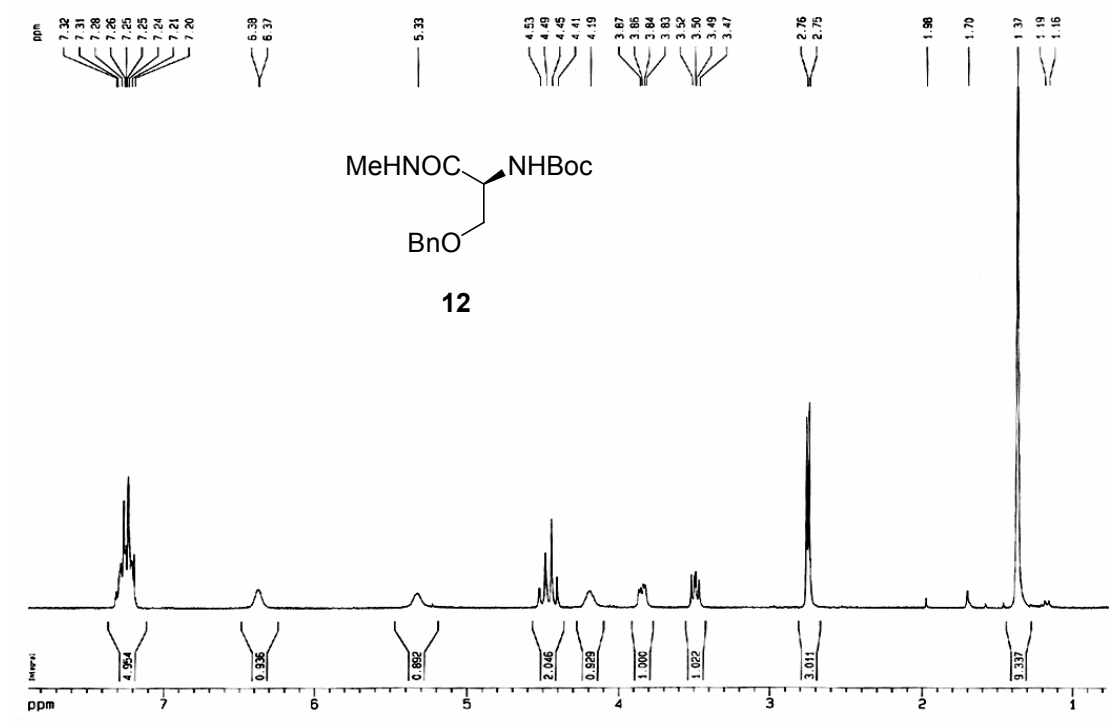


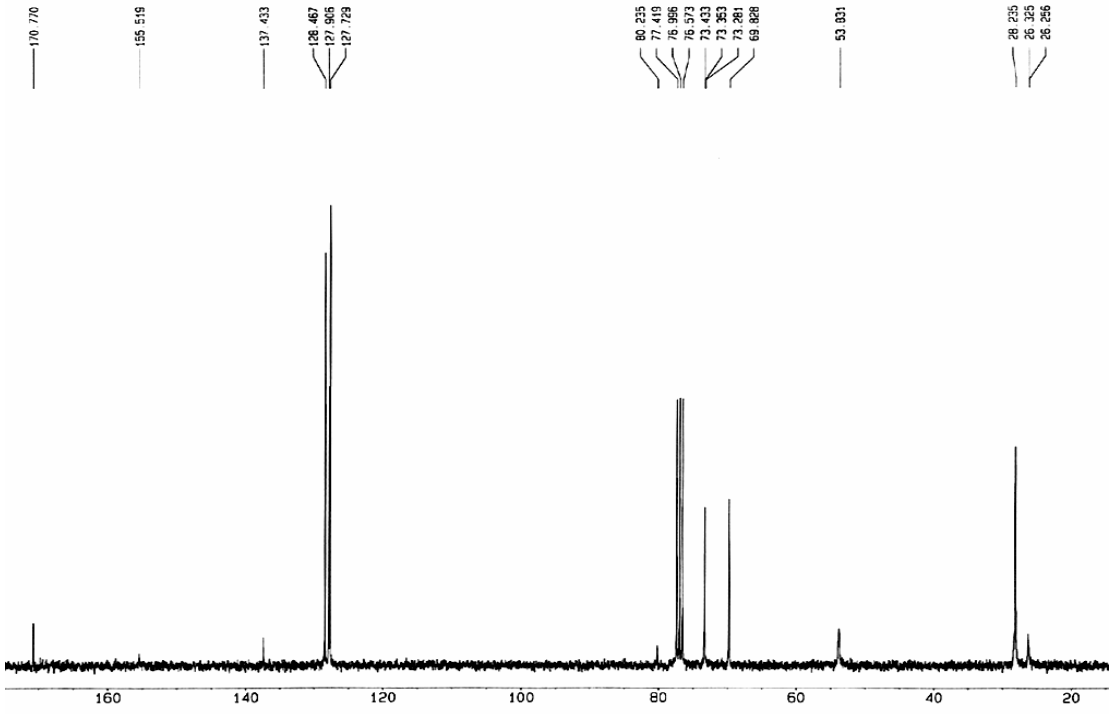
Piv-Ahc-OH (11).

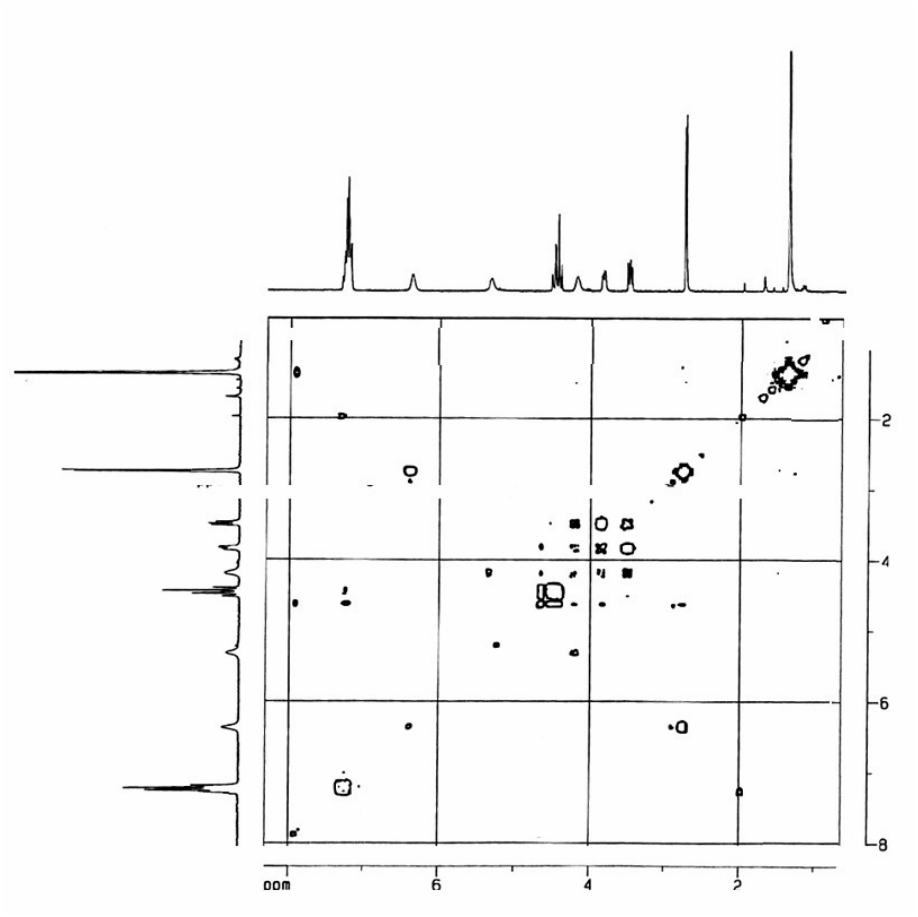


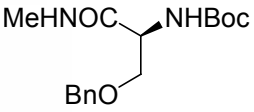


Boc-L-Ser(OBn)-NHMe (12).

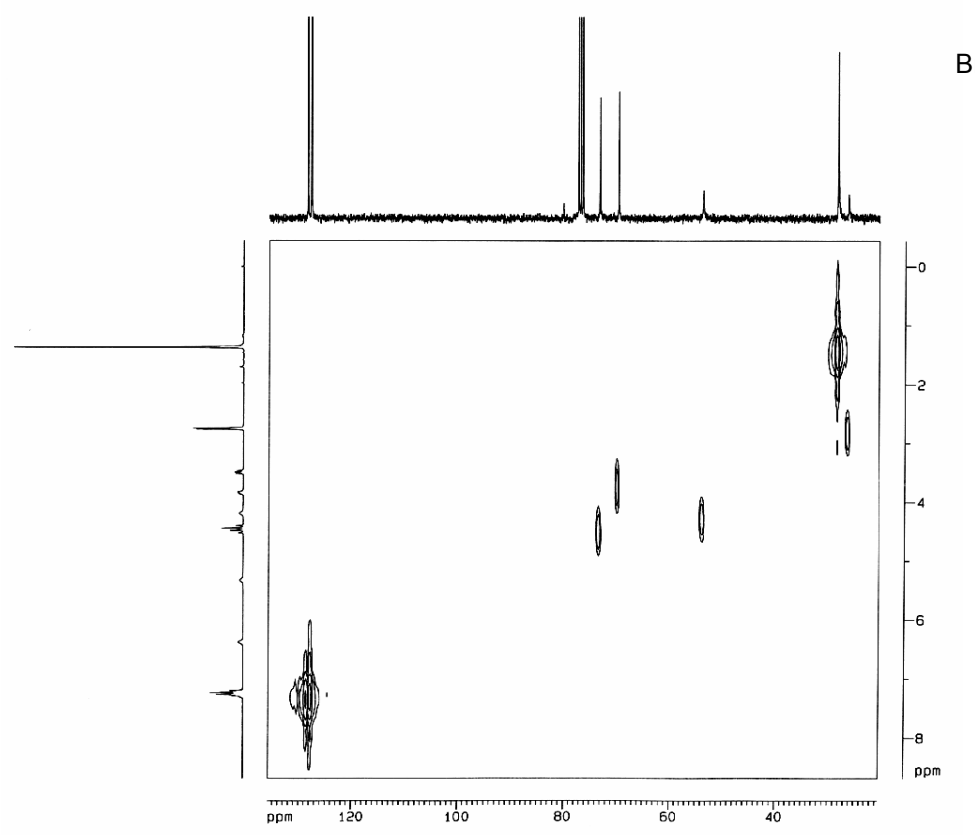




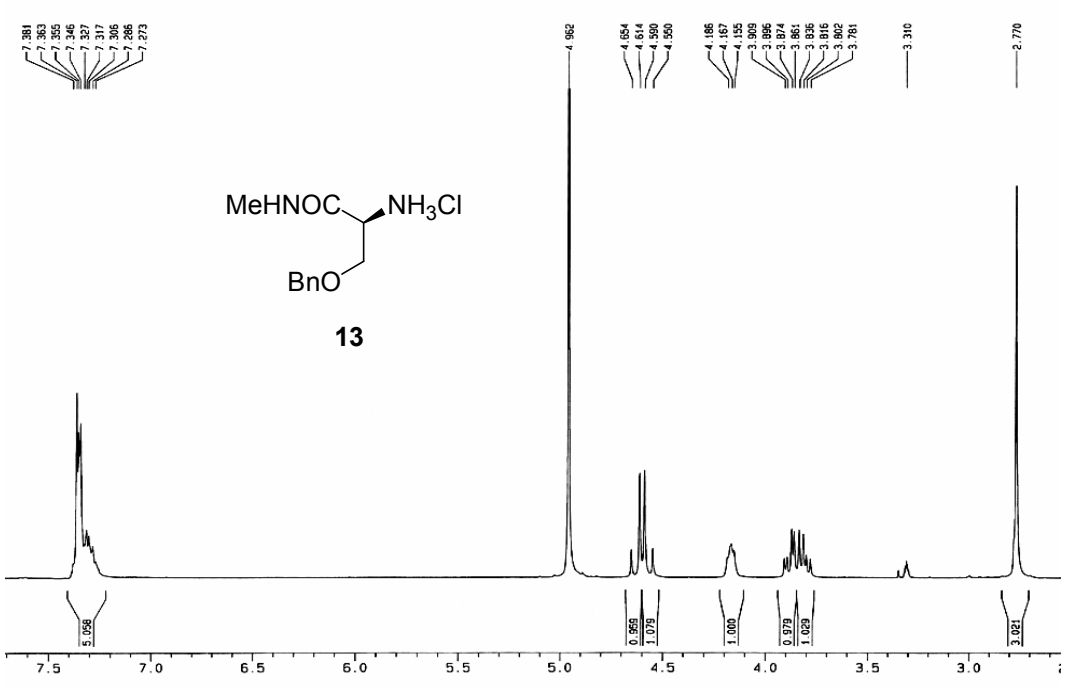


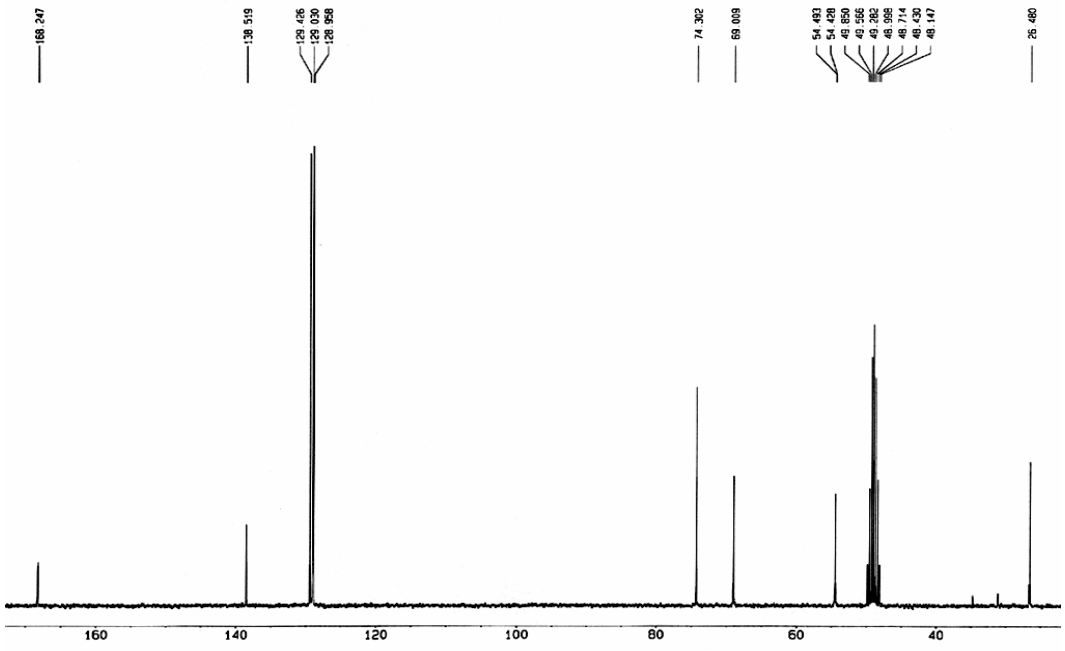


12

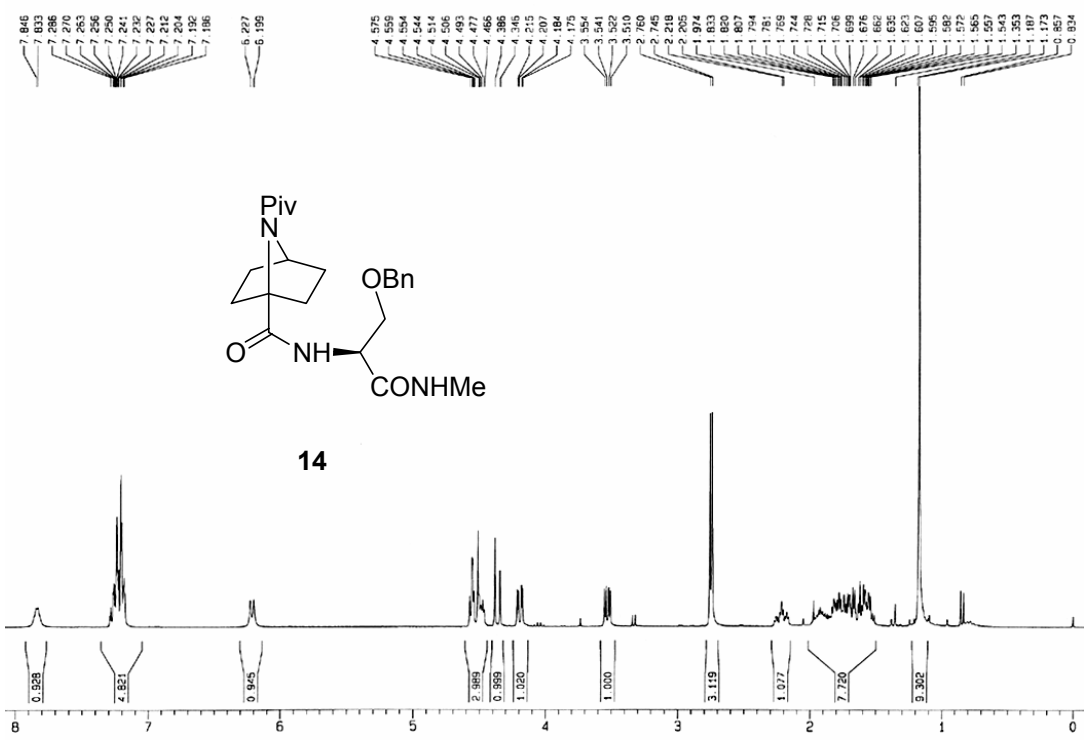


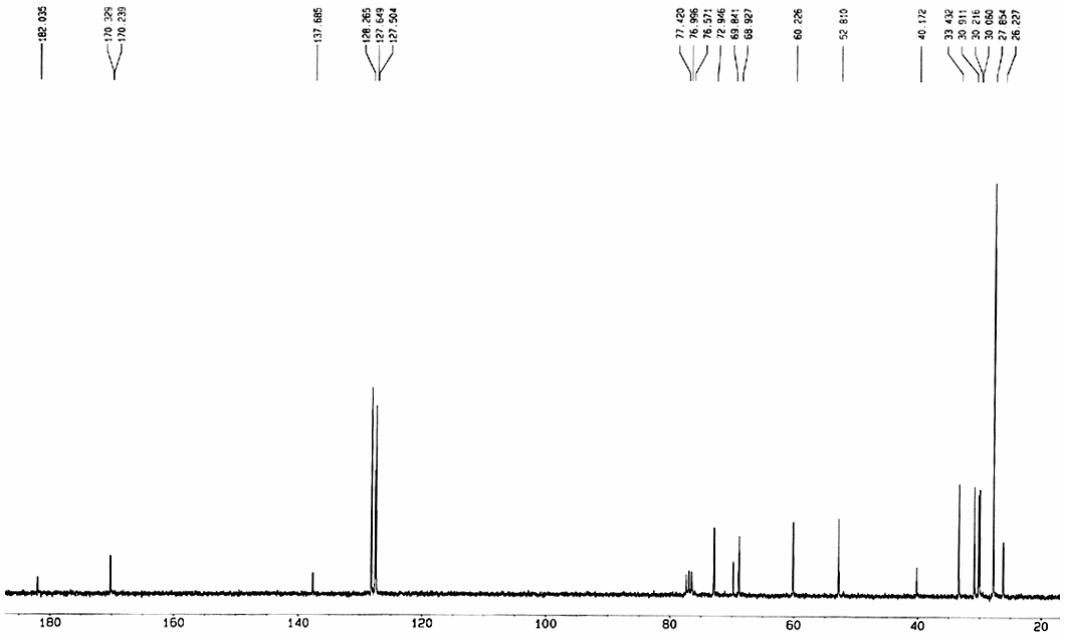
L-Ser(OBn)-NHMe·HCl (13).

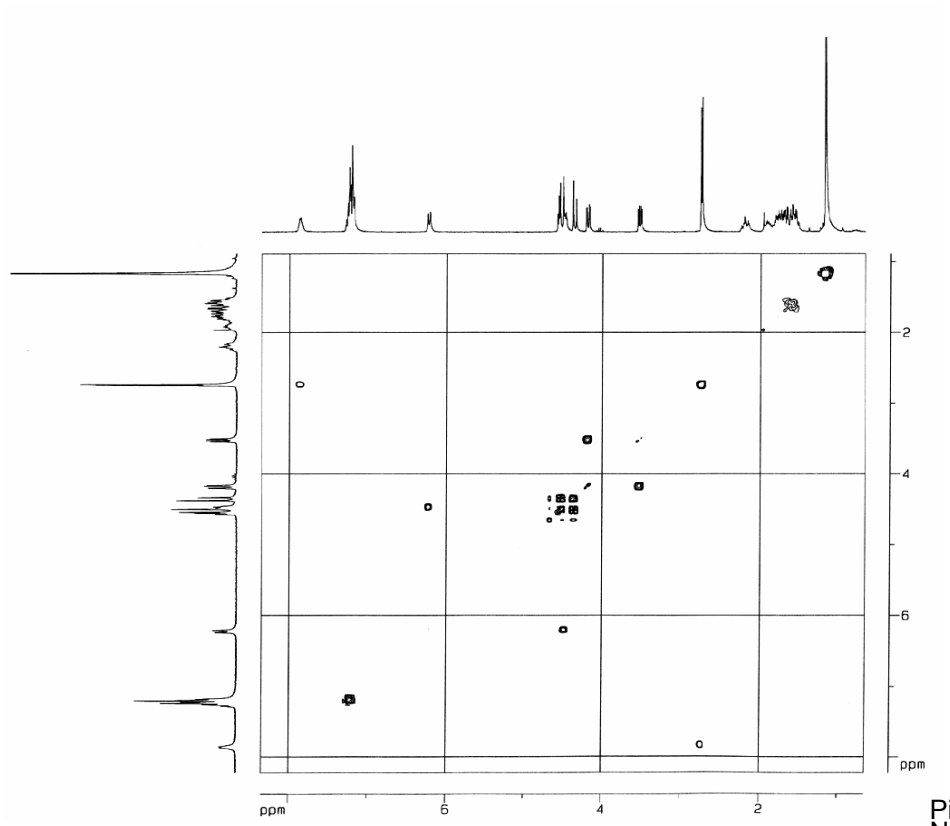


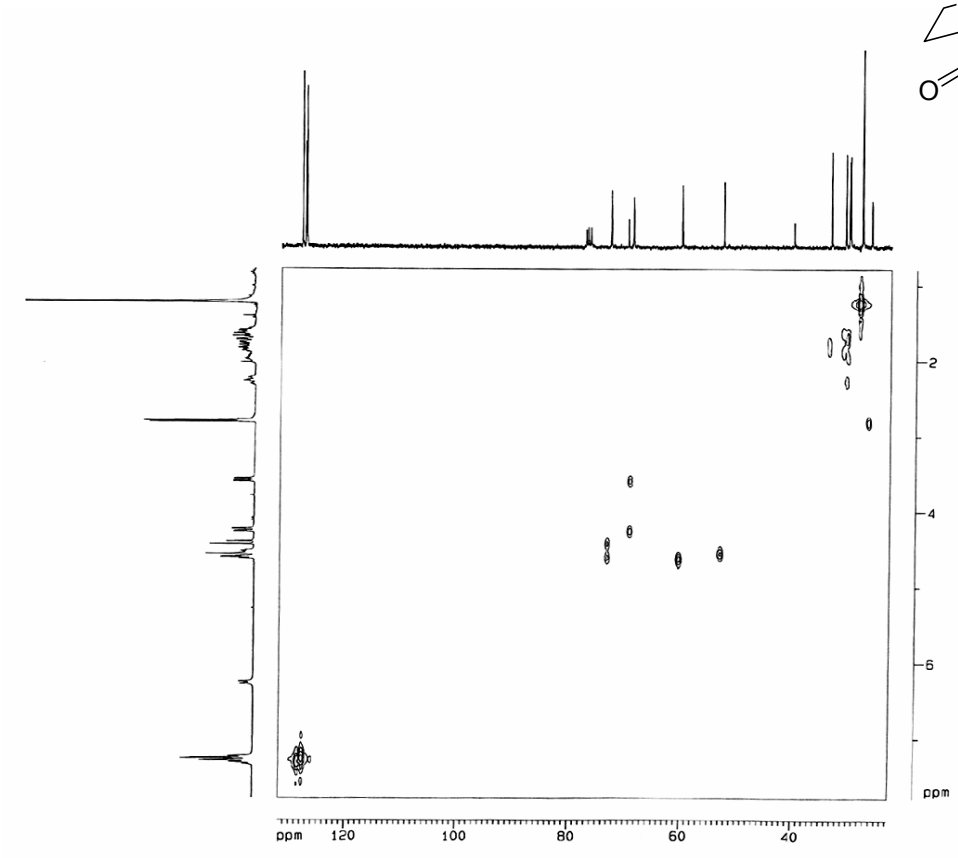


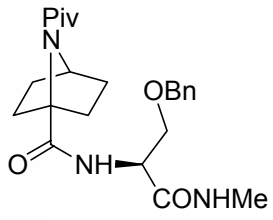
Piv-Ahc-L-Ser(OBn)-NHMe (14).





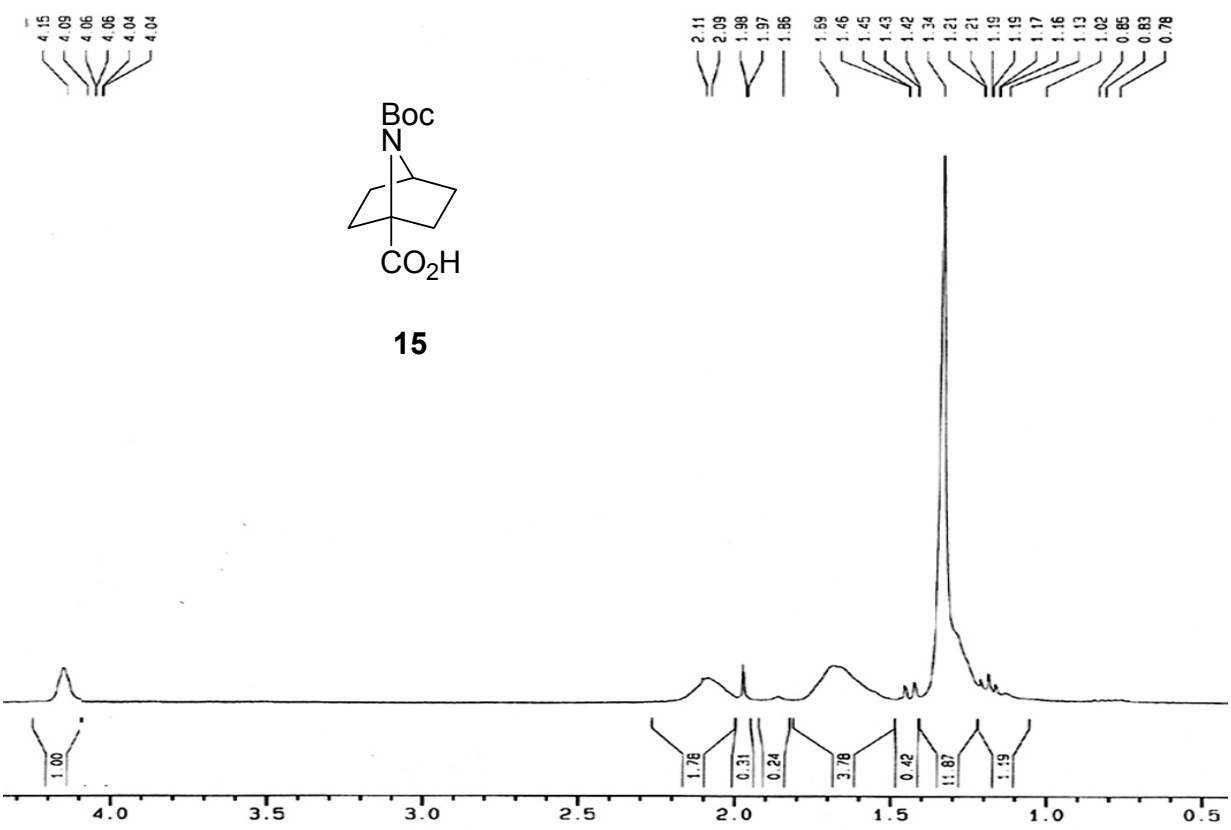






14

Boc-Ahc-OH (15).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4.06
4.06
4.04
4.04
2.11
2.09
1.98
1.97
1.86
1.69
1.46
1.45
1.43
1.42
1.34
1.21
1.21
1.19
1.19
1.17
1.16
1.13
1.02
0.85
0.83
0.78
Boc
N
CO2H
15
1.00
1.78
0.31
0.24
3.78
0.42
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1.19
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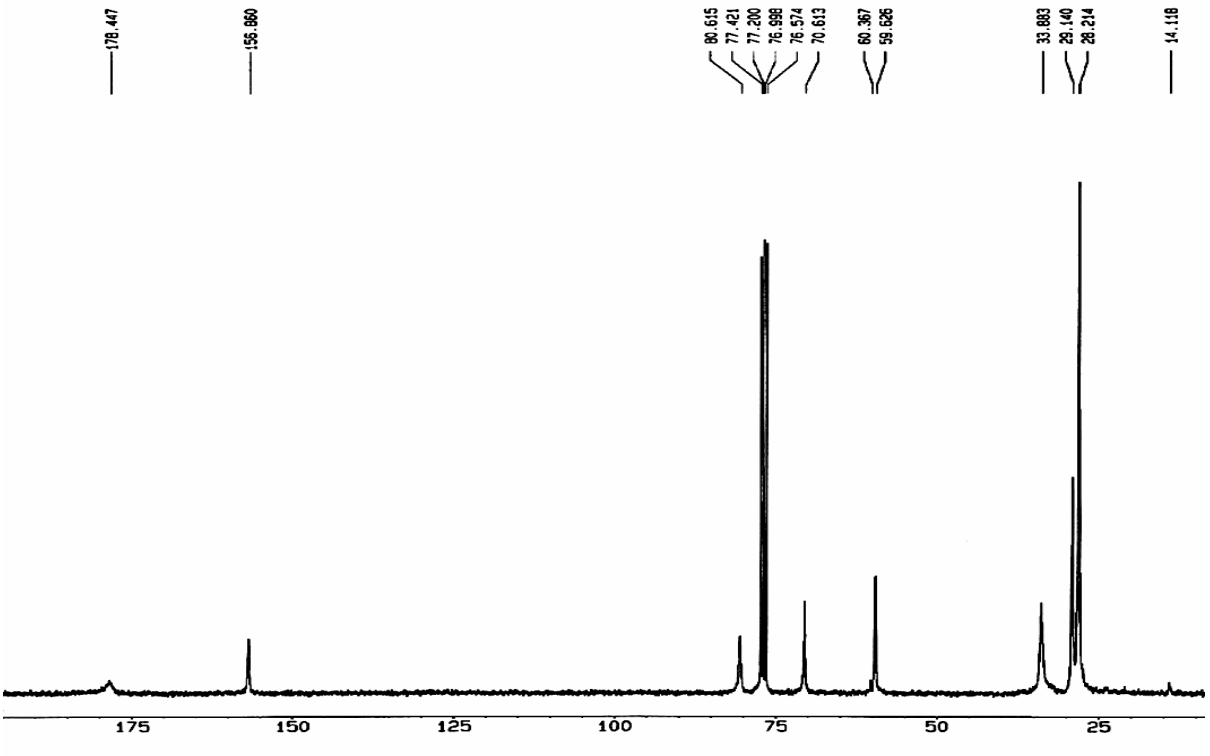
3.5
3.0
2.5
2.0
1.5
1.0
0.5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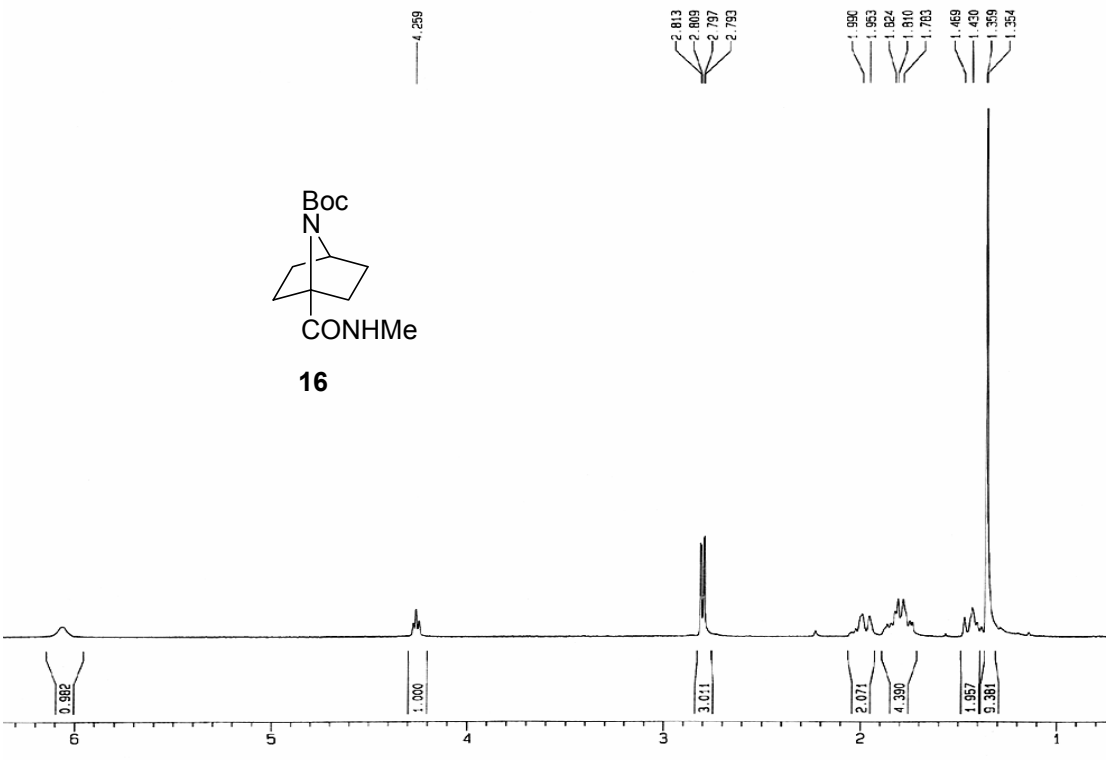
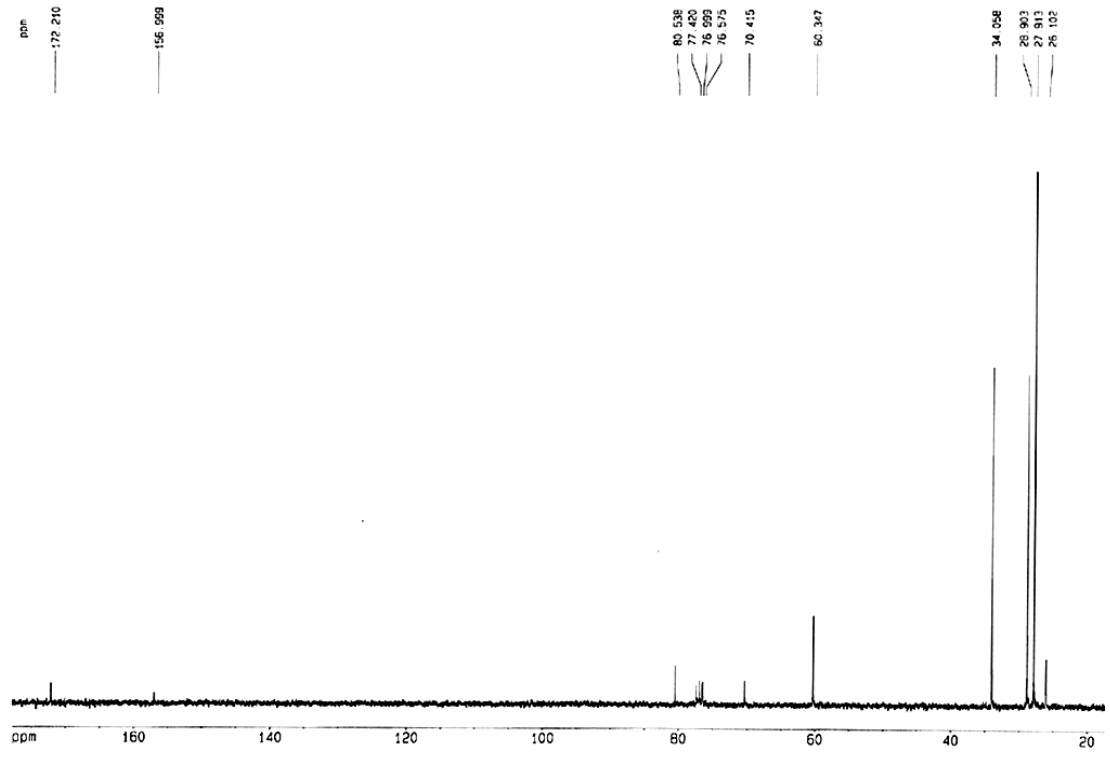
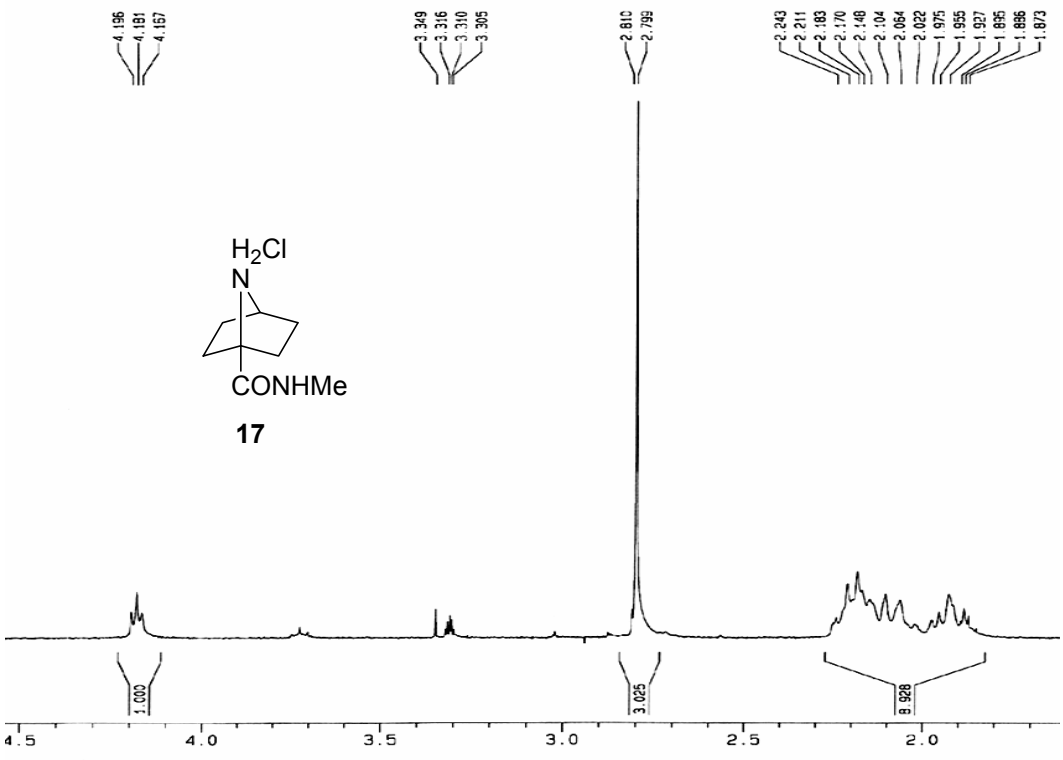
80.615
77.421
77.200
76.998
76.574
70.613
60.367
59.626
33.883
29.140
28.214
14.118
175
150
125
100
75
50
25

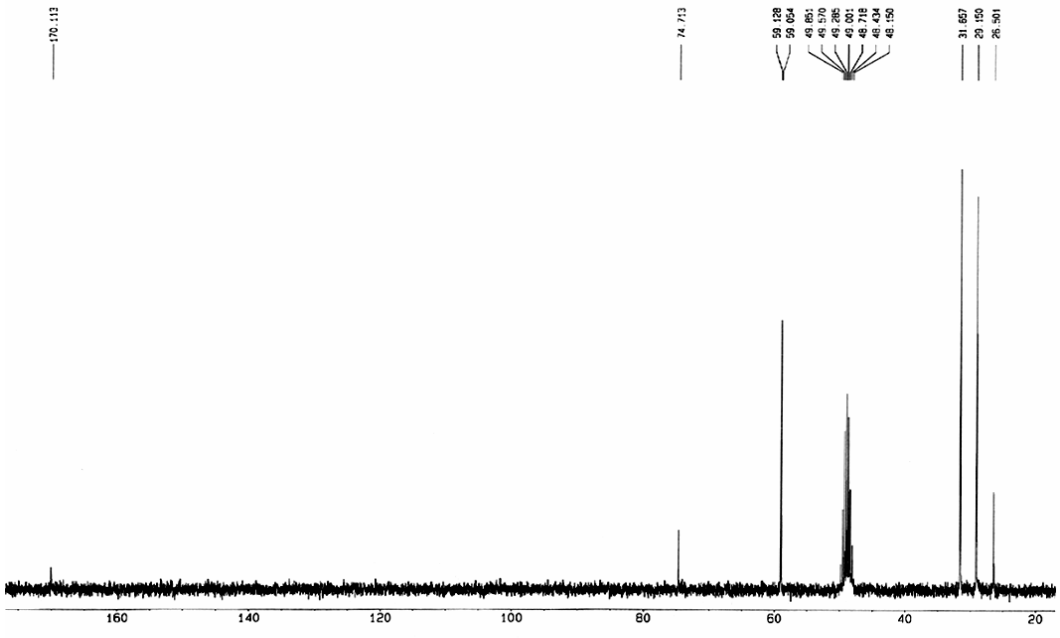
Boc-Ahc-NHMe (16).



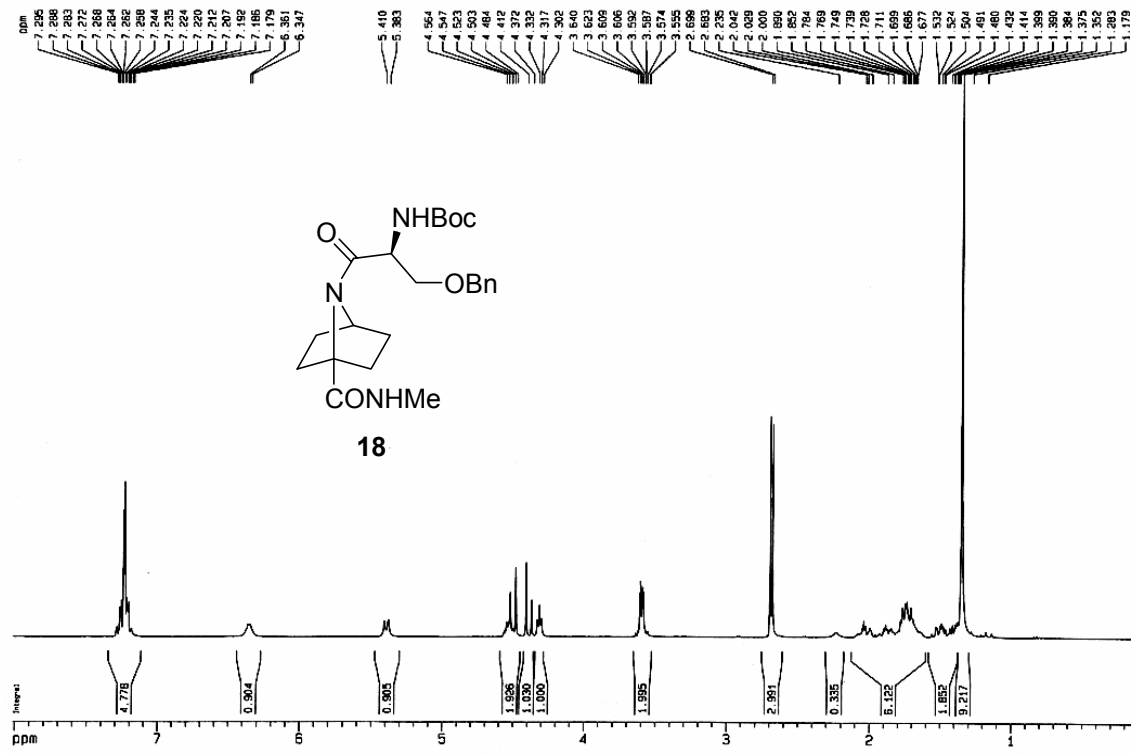


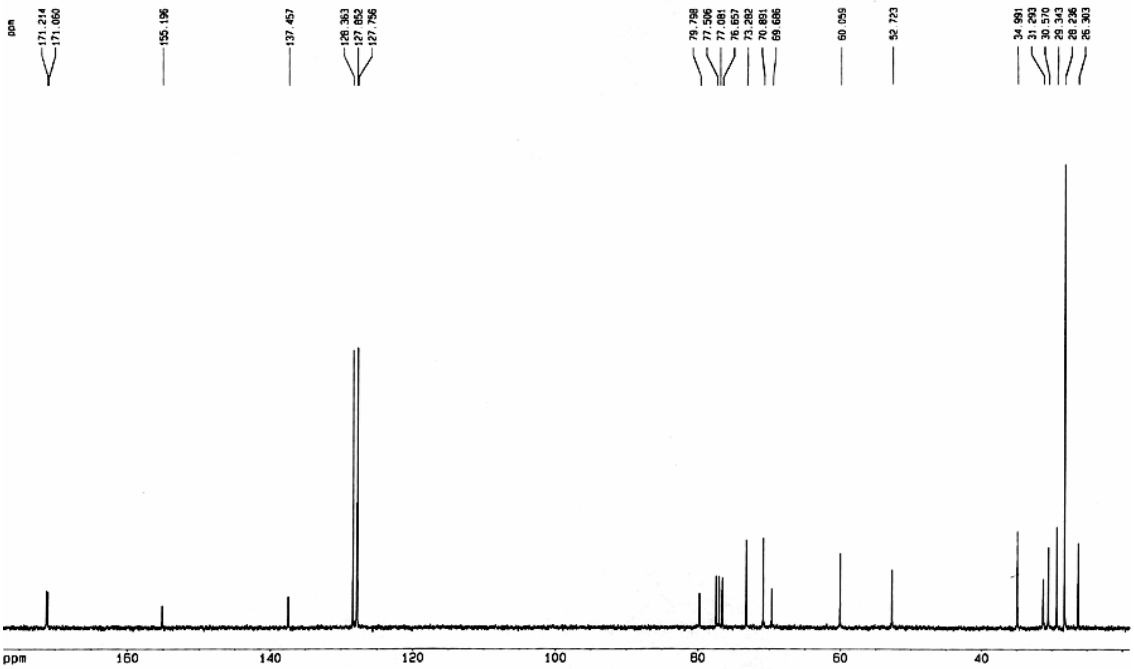
Ahc-NHMe·HCl (17).

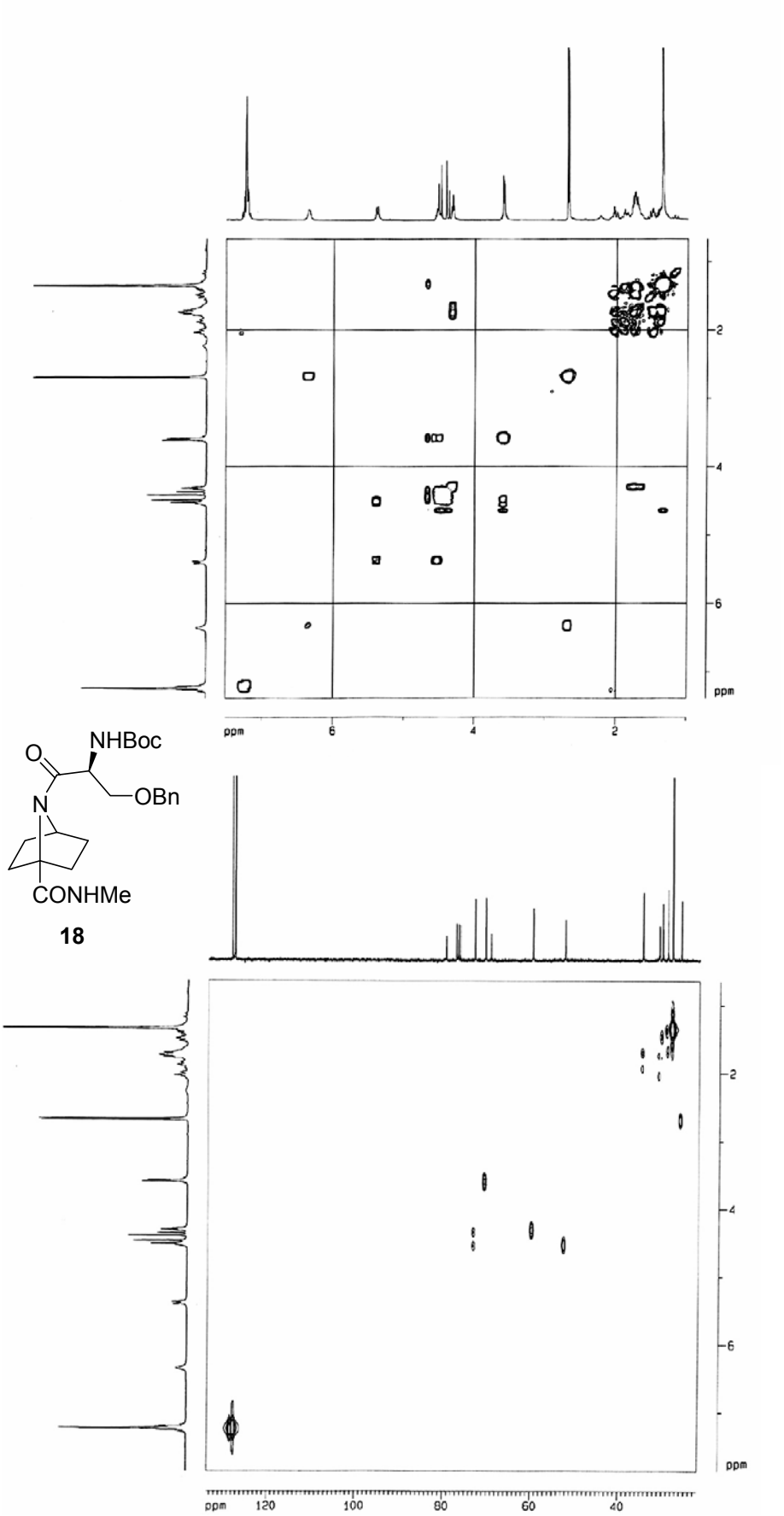




Boc-L-Ser(OBn)-Ahc-NHMe (18).

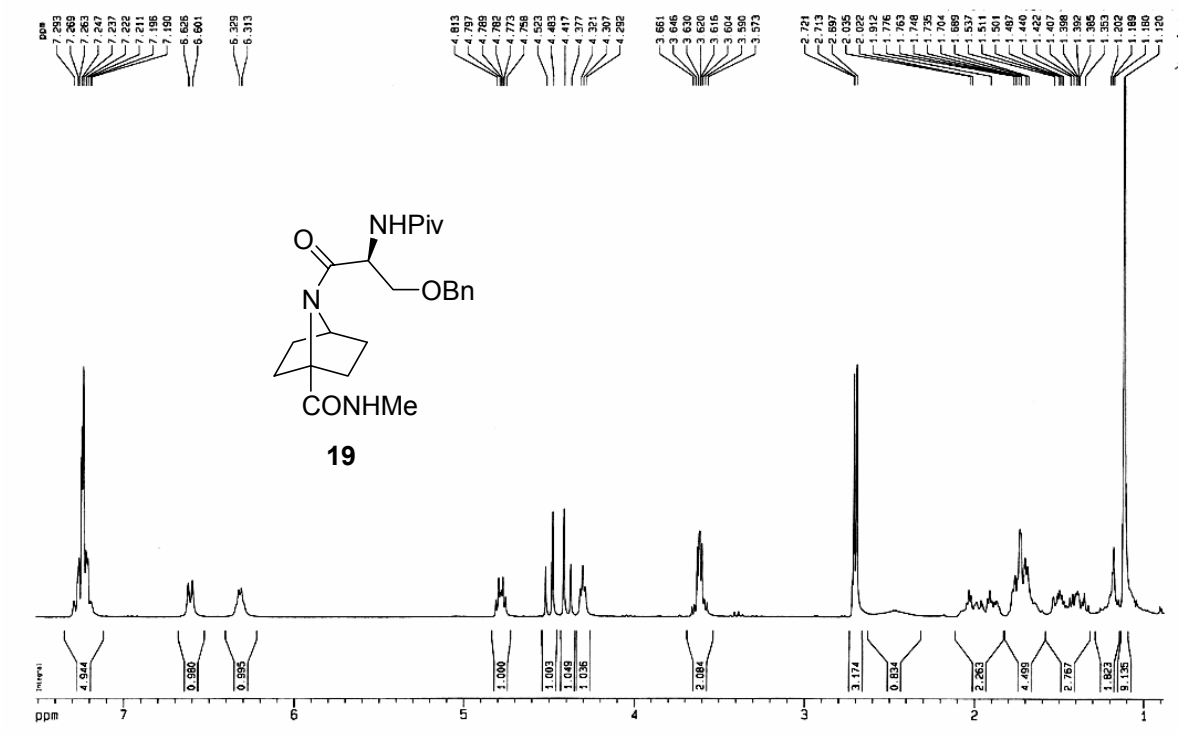


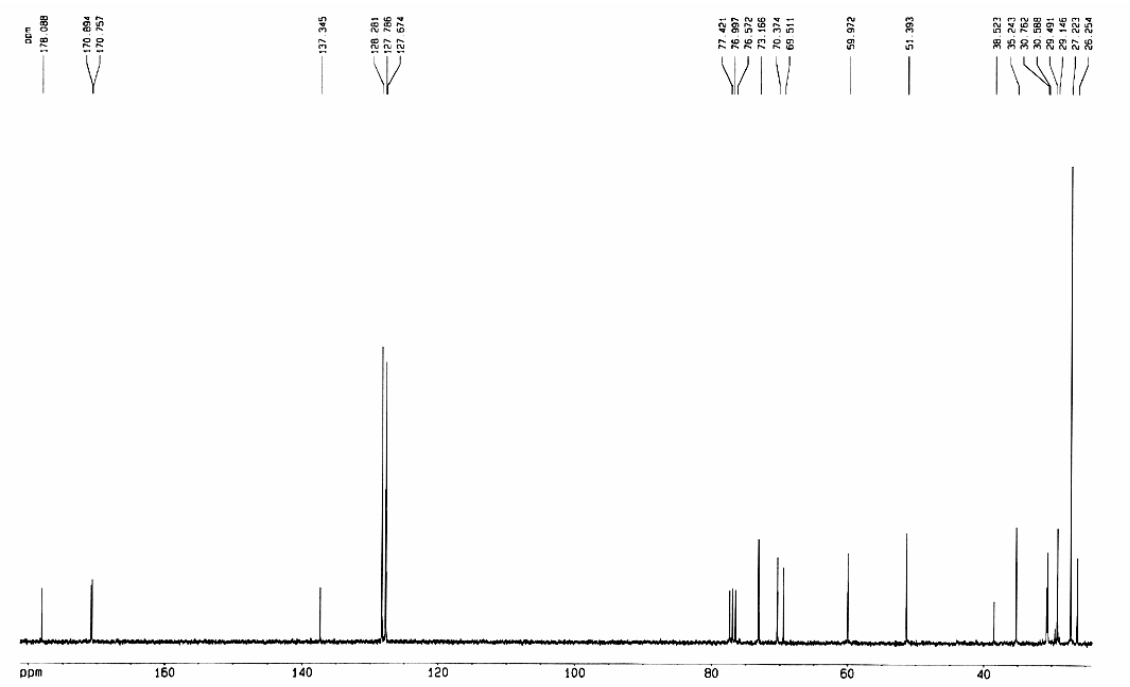


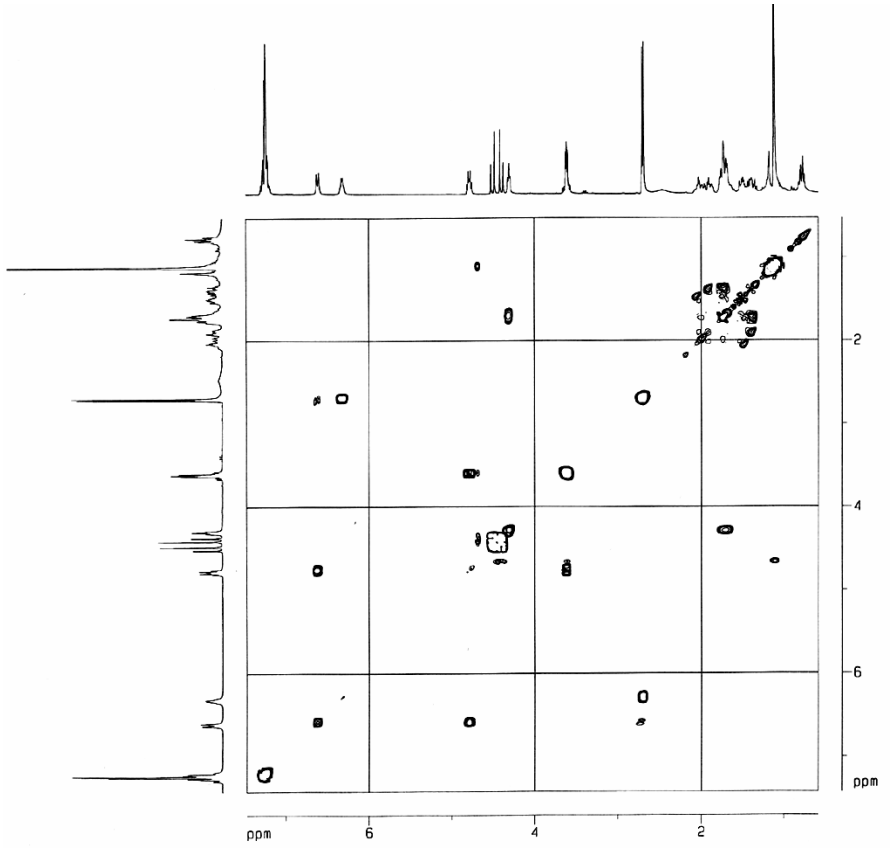


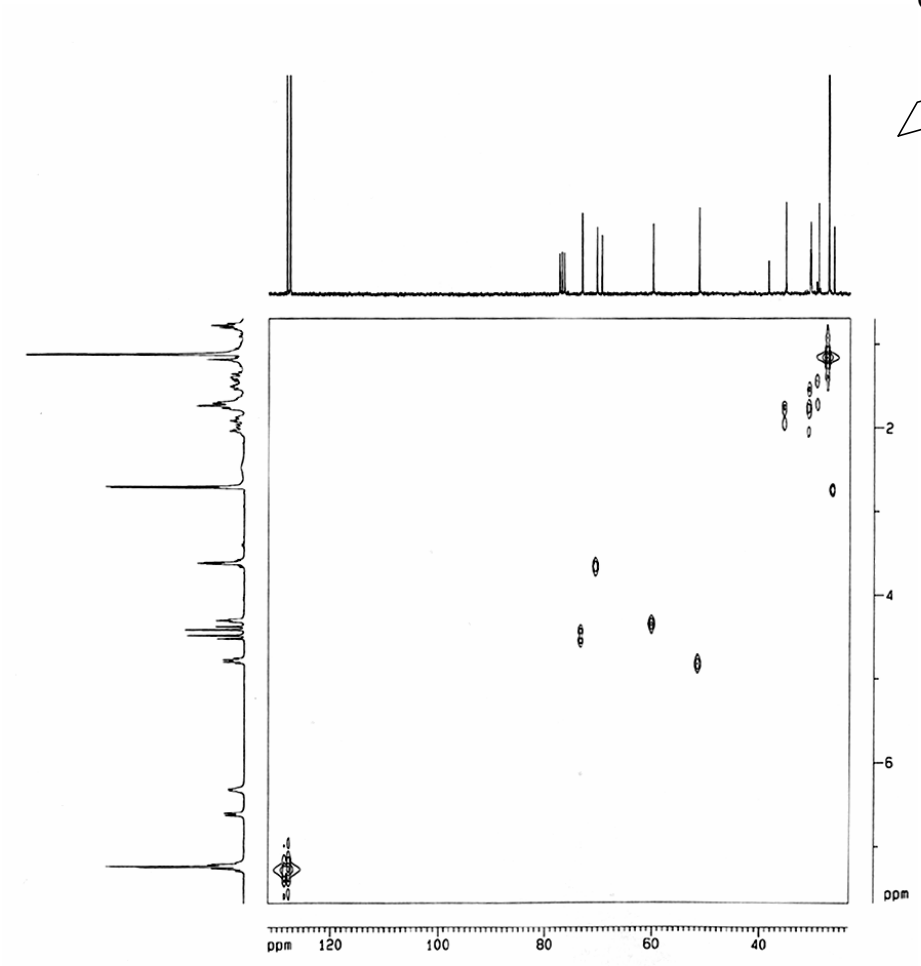
18

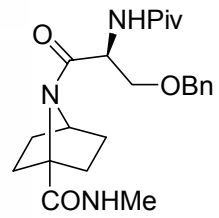
Piv-L-Ser(OBn)-Ahc-NHMe (19).





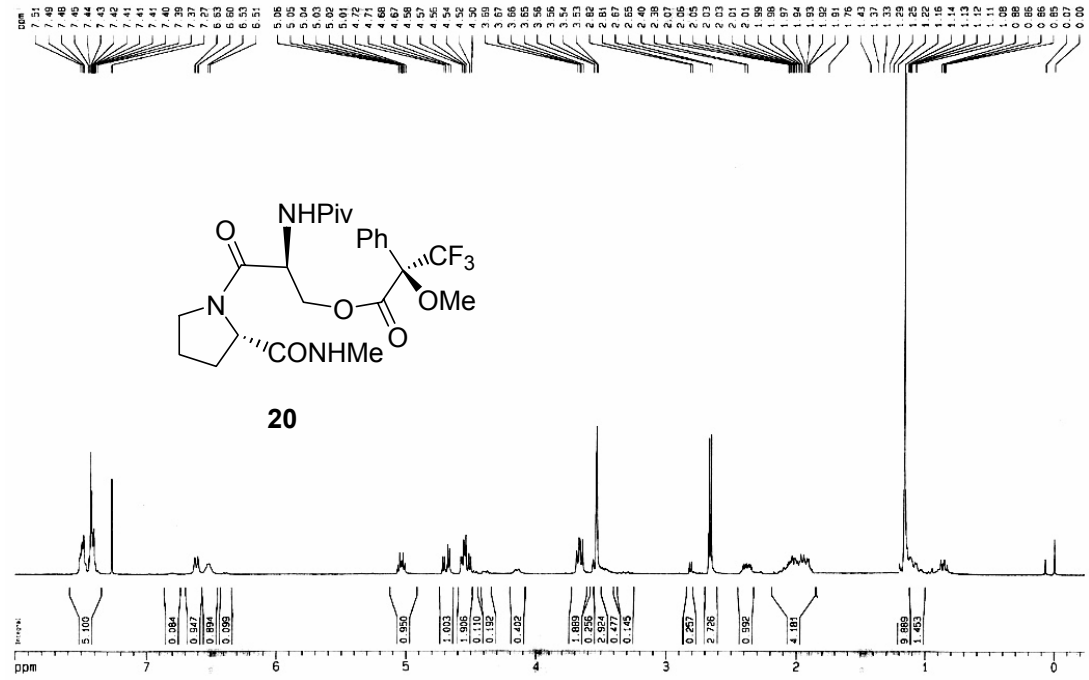






19

Piv-L-Ser(O-(+)-MTPA)-L-Pro-NHMe (20).



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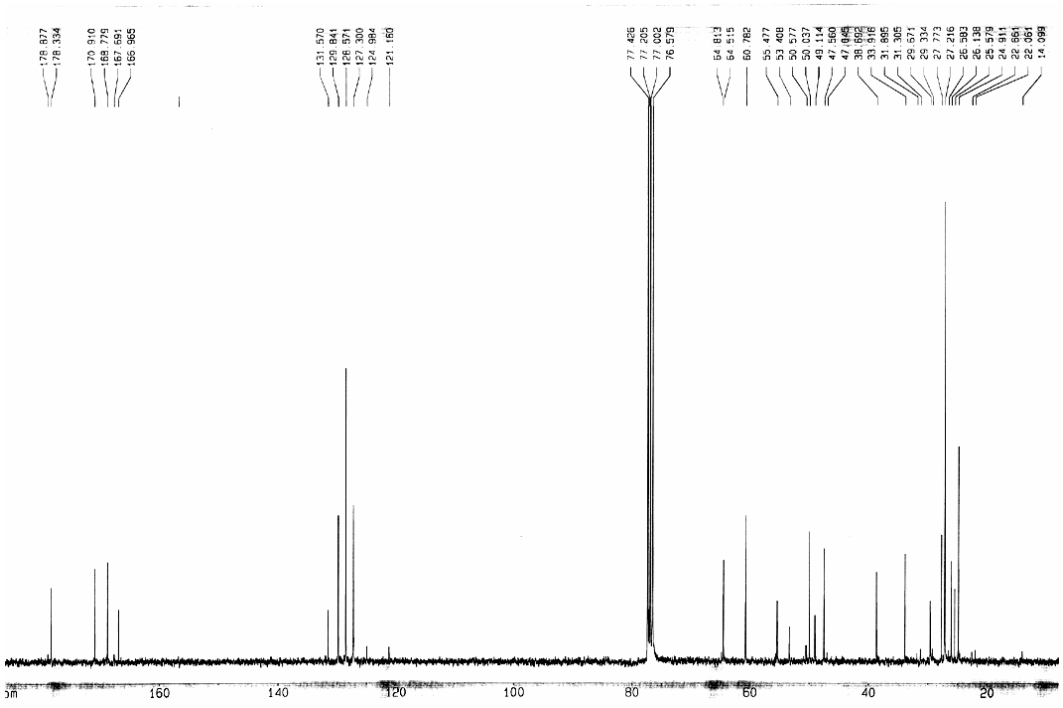

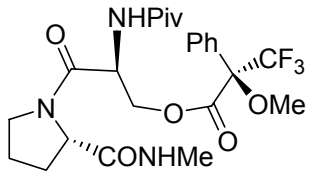

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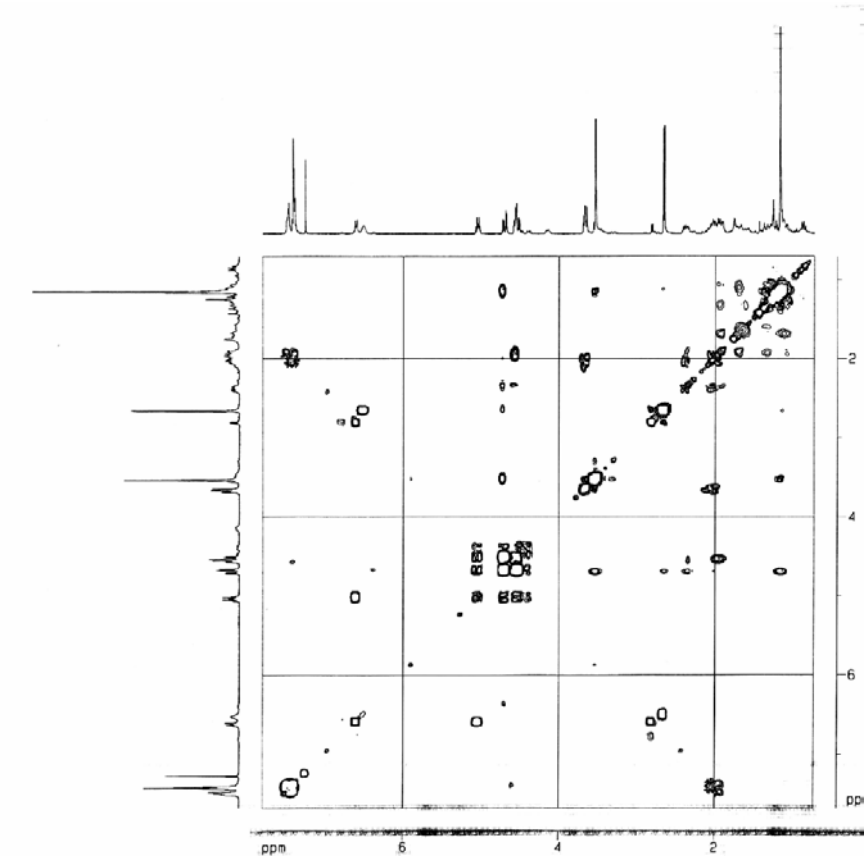
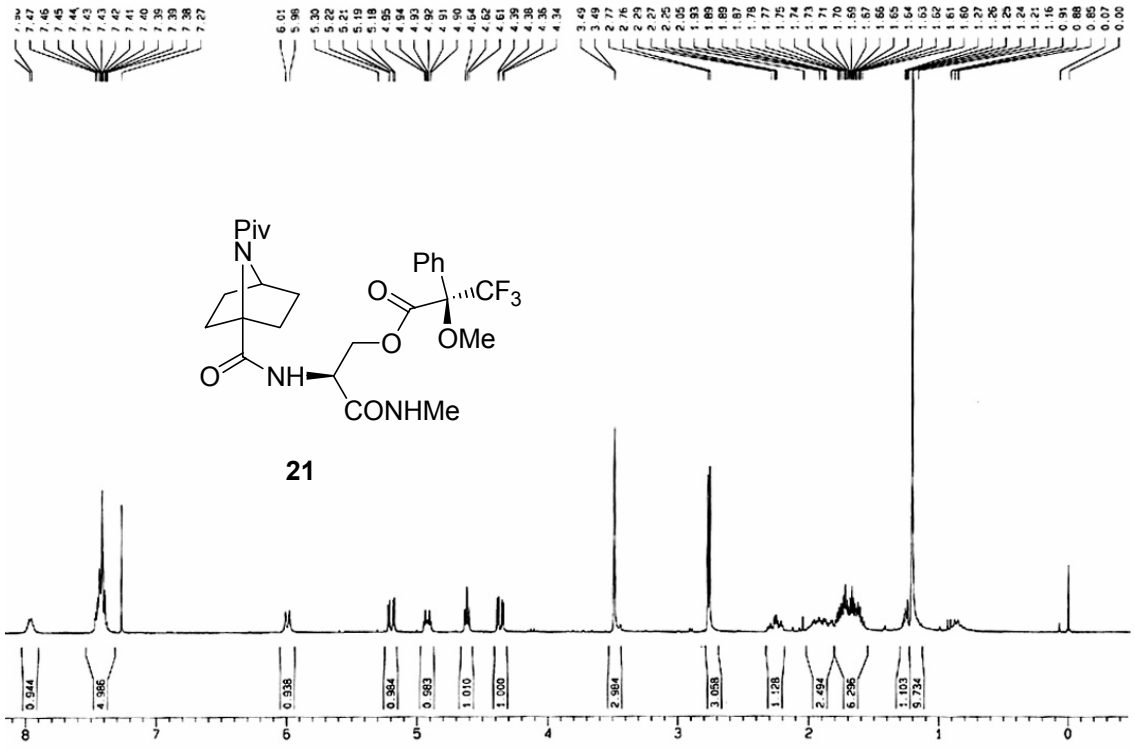


Piv-Ahc-L-Ser(O-(+)-MTPA)-NHMe (21).



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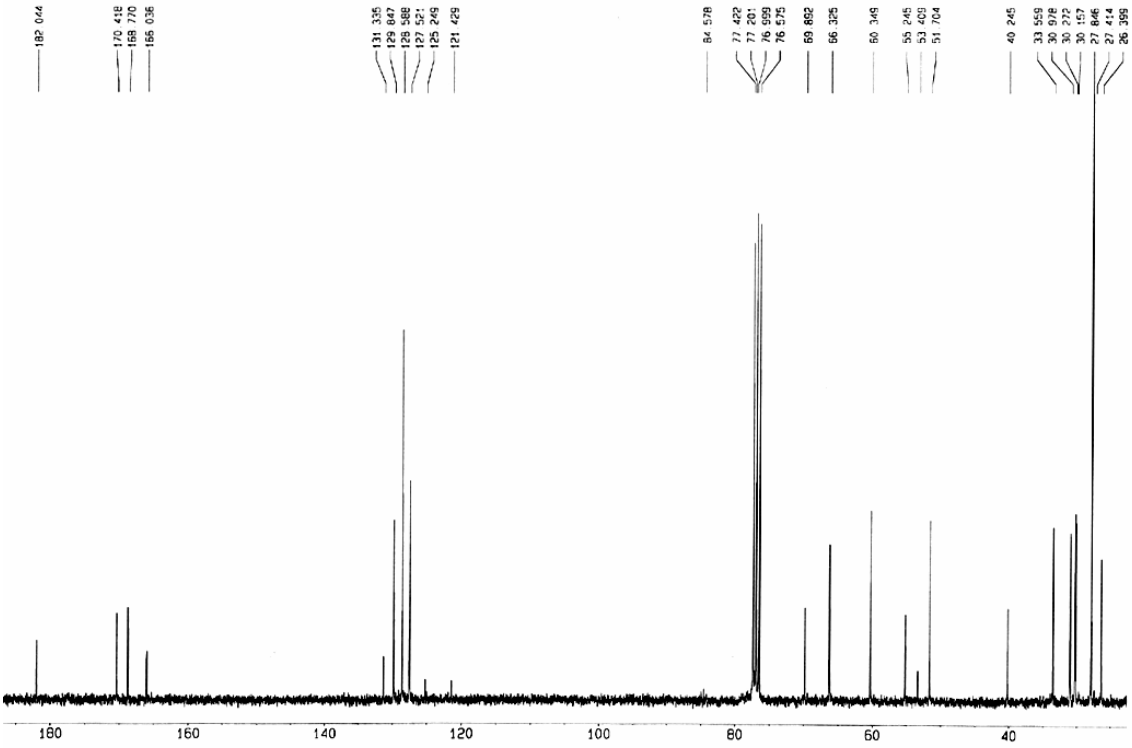

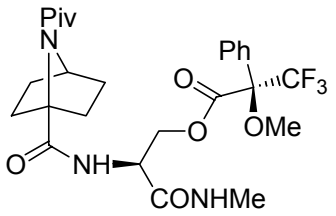

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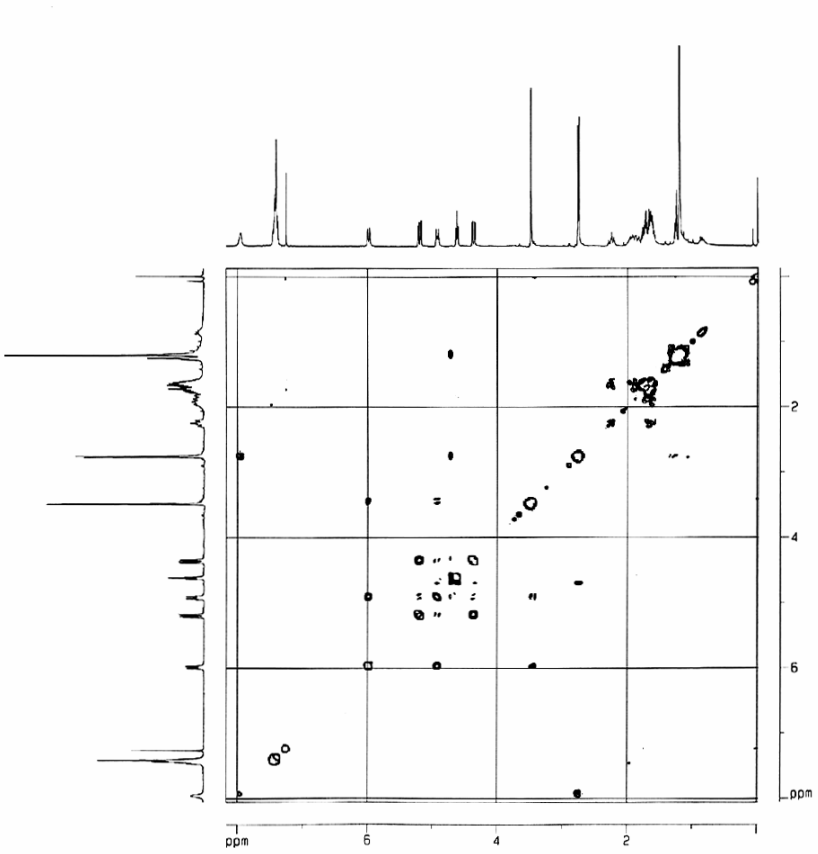
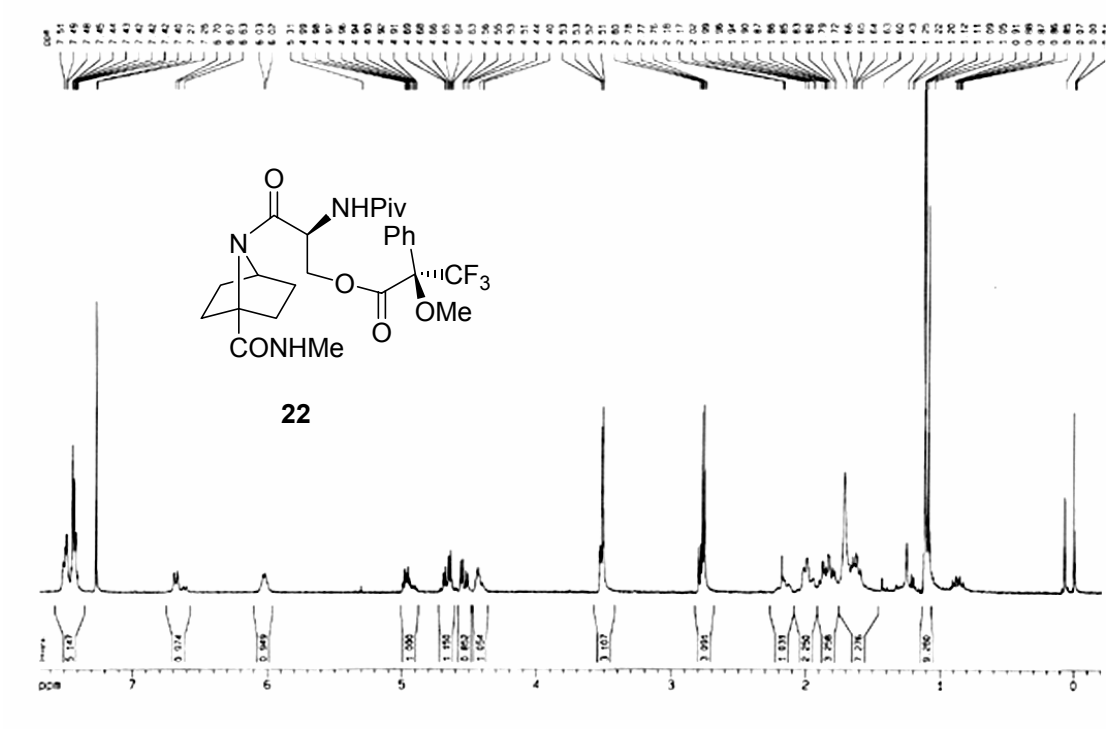
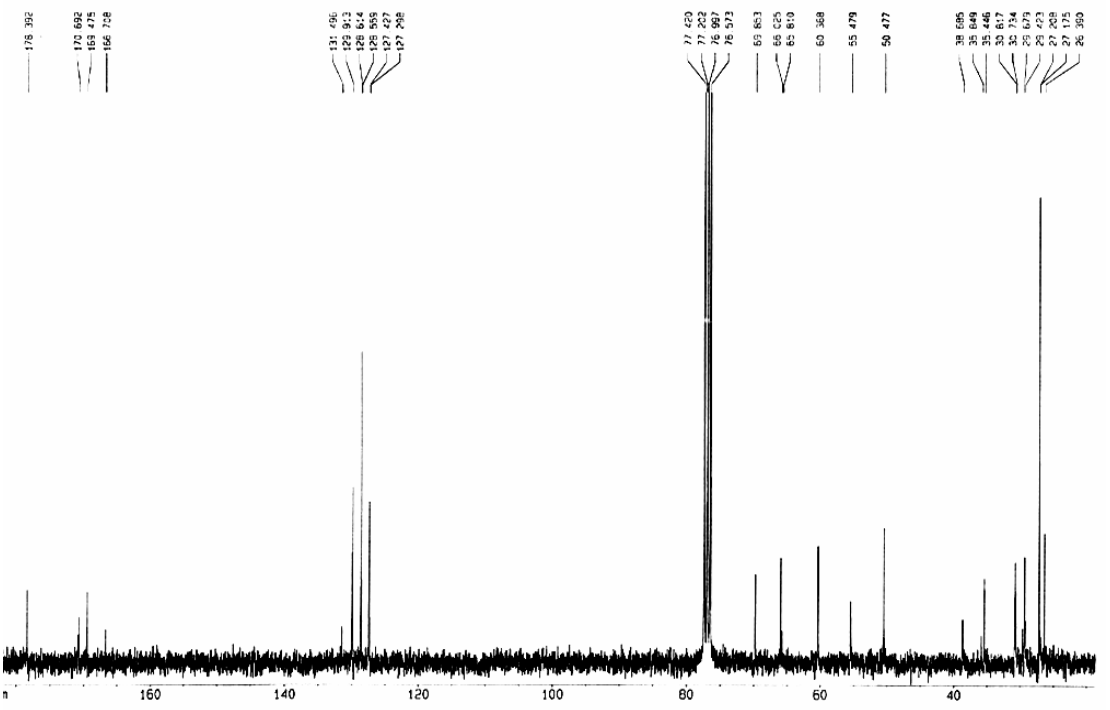
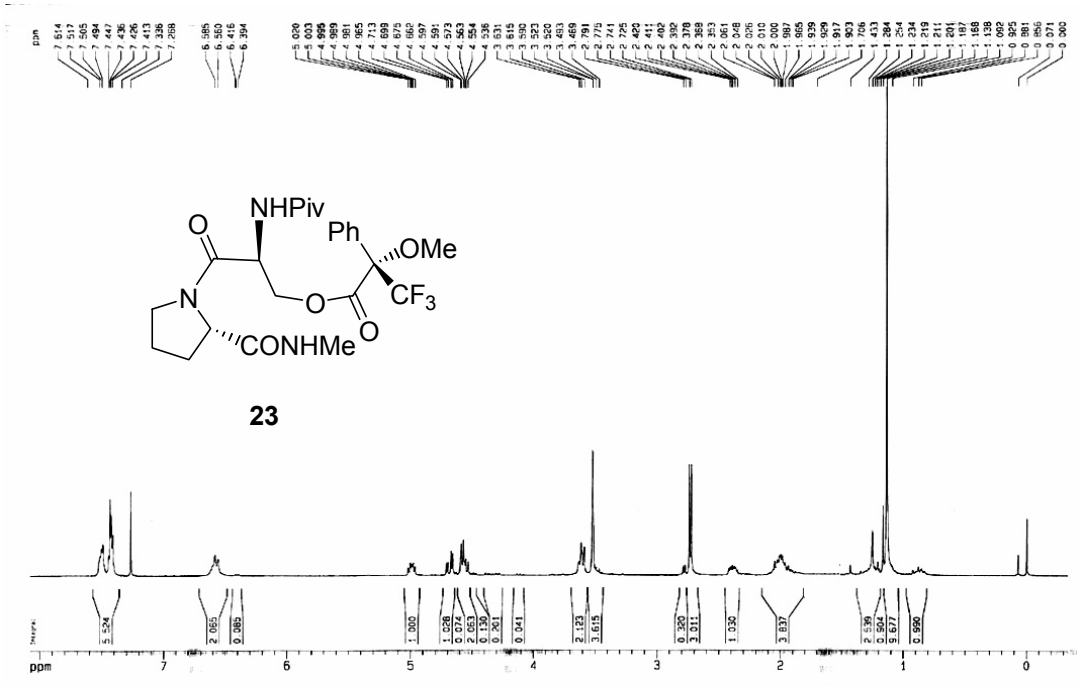


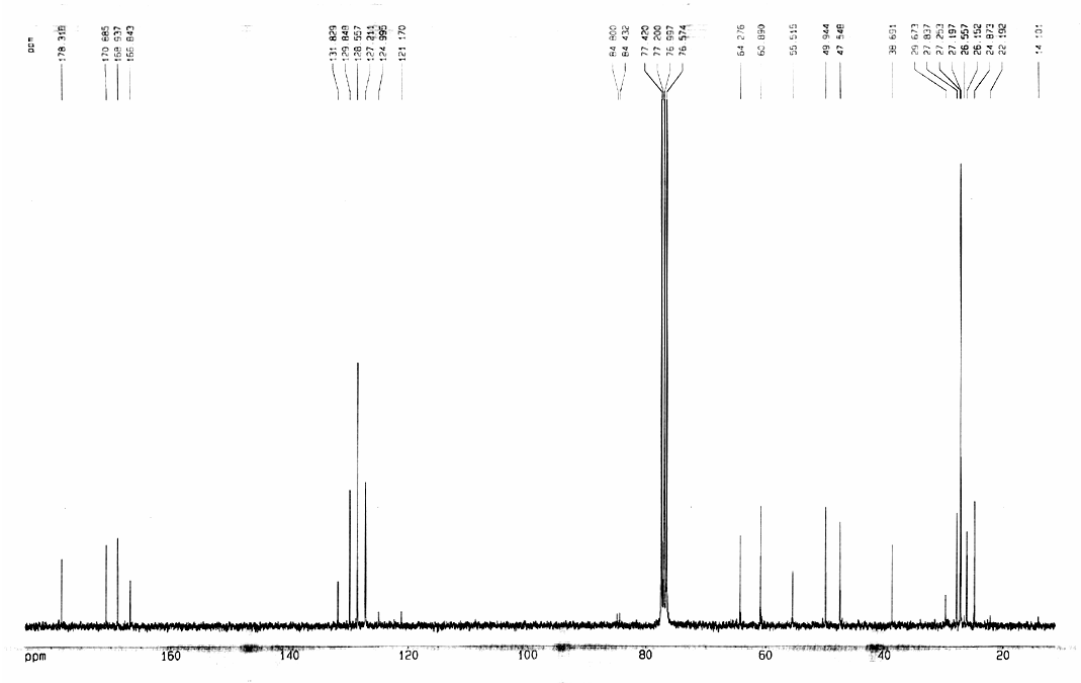
Piv-L-Ser(O-(+)-MTPA)-Ahc-NHMe (22).

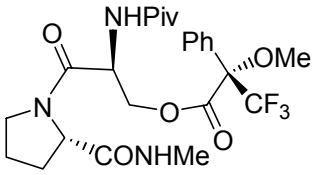




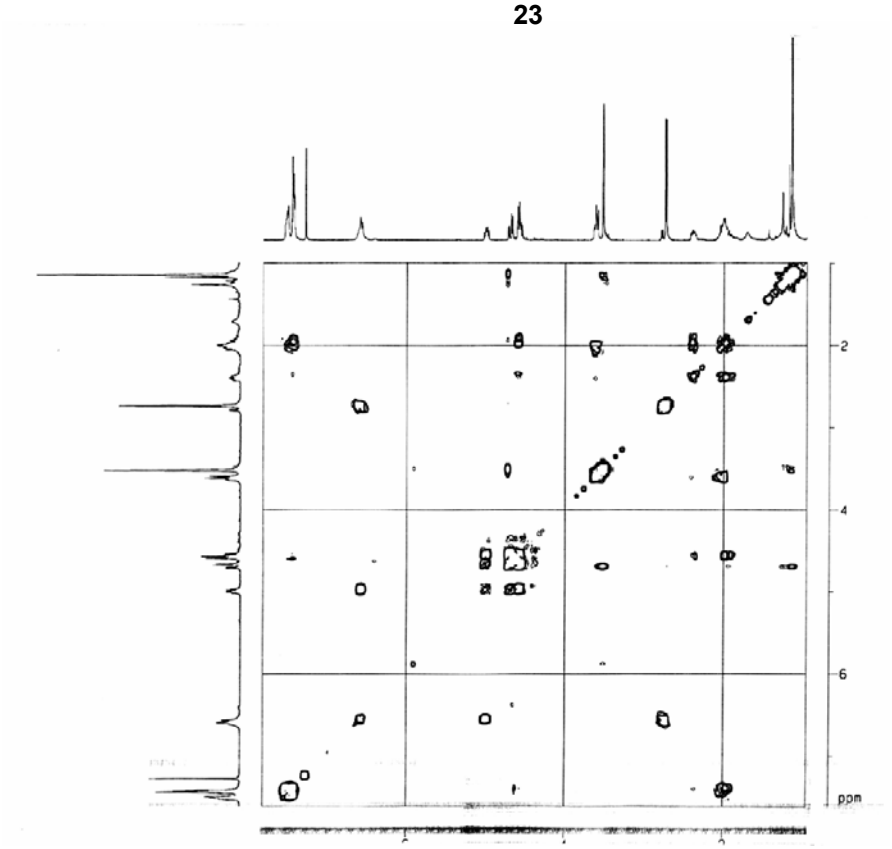
Piv-L-Ser(O-(-)-MTPA)-L-Pro-NHMe (23).



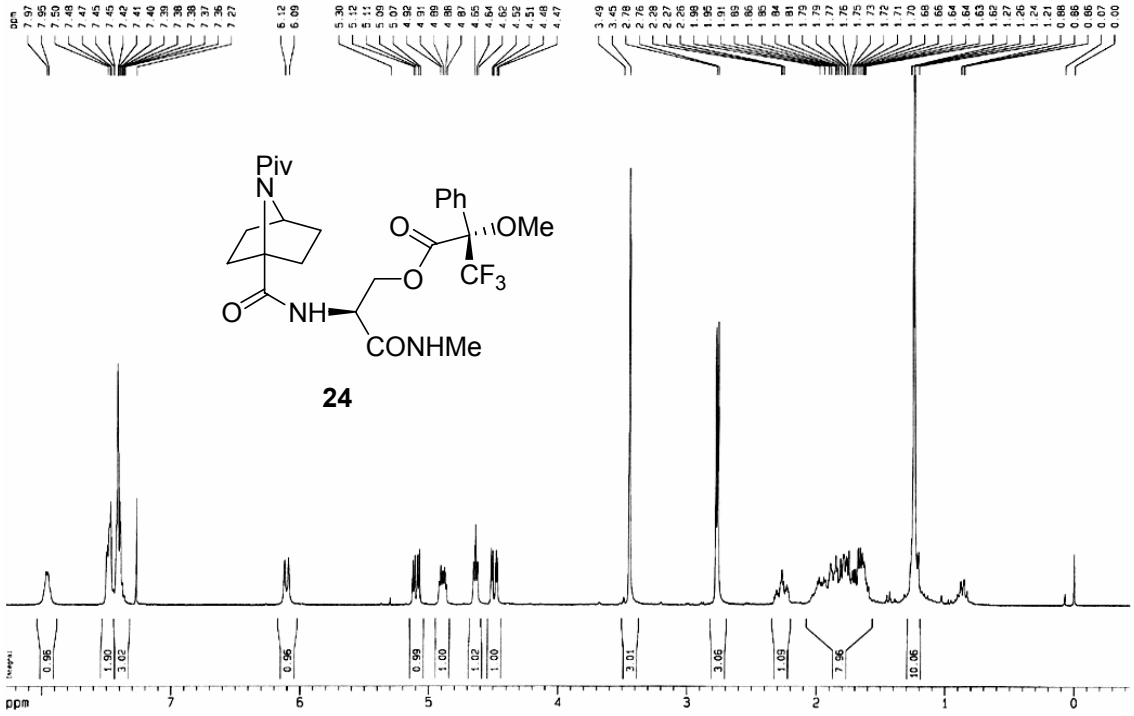


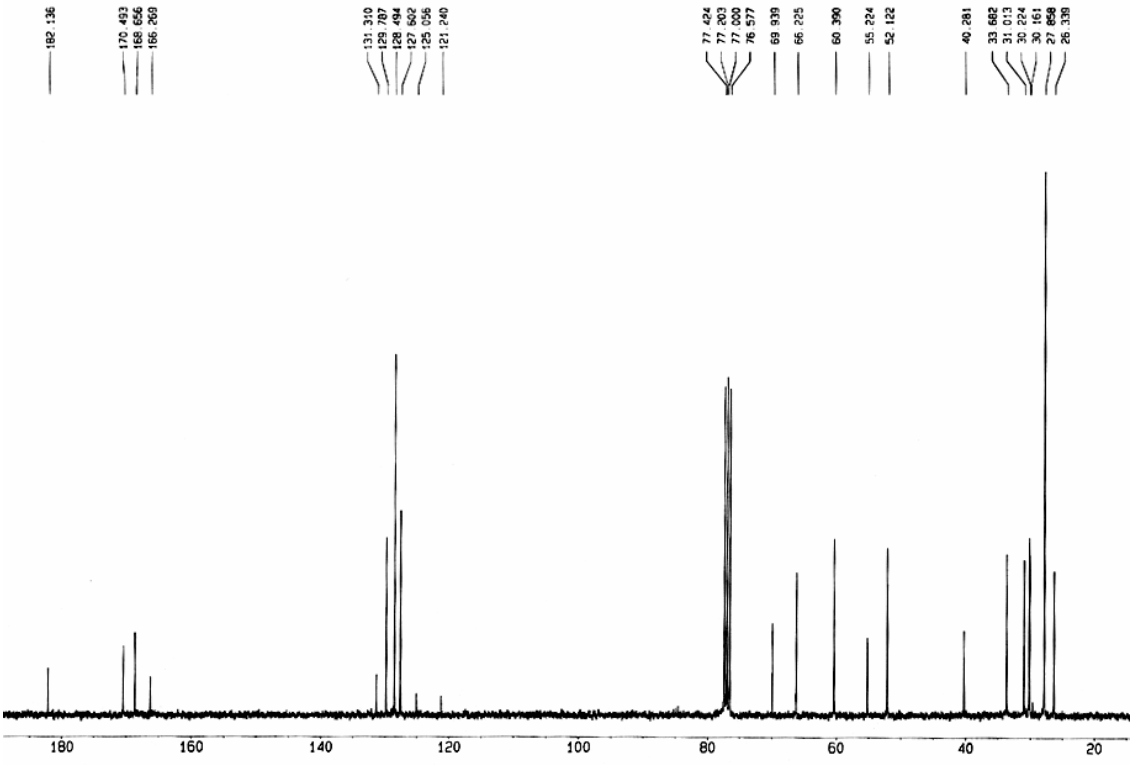


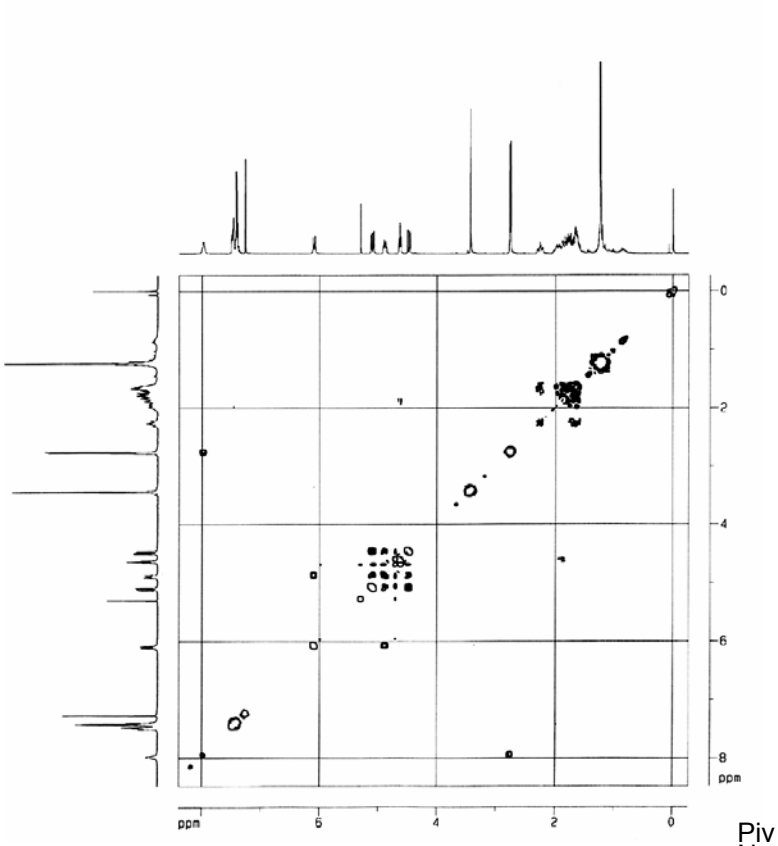
23

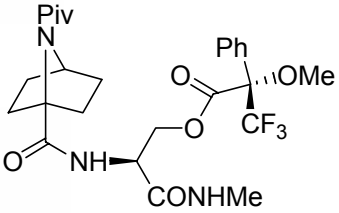


Piv-Ahc-L-Ser(O-(-)-MTPA)-NHMe (24).

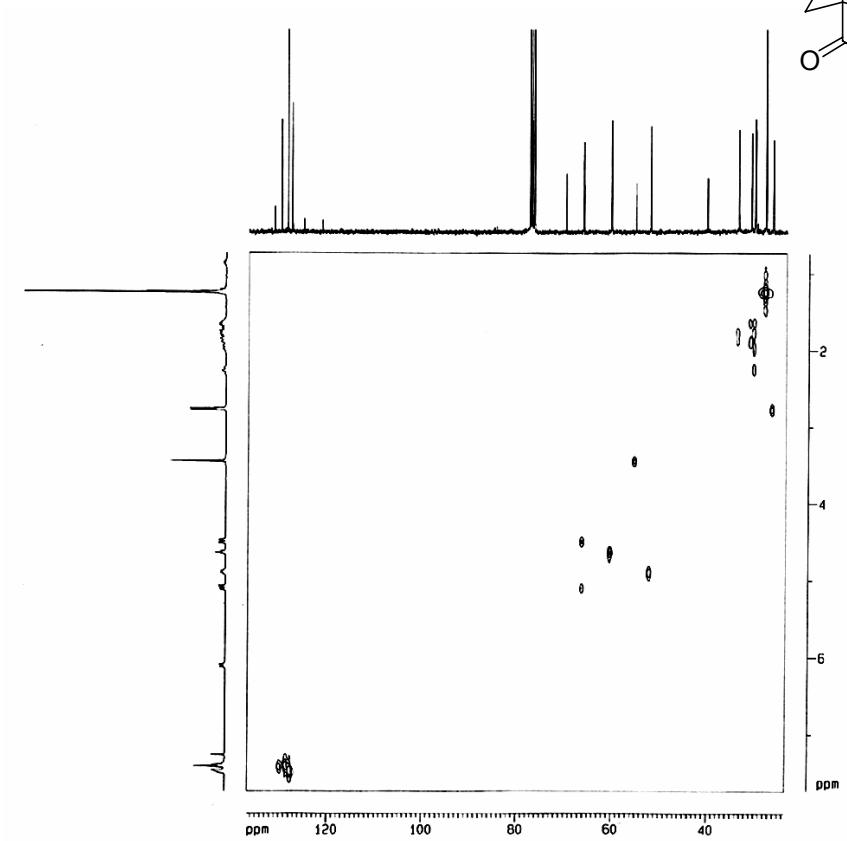




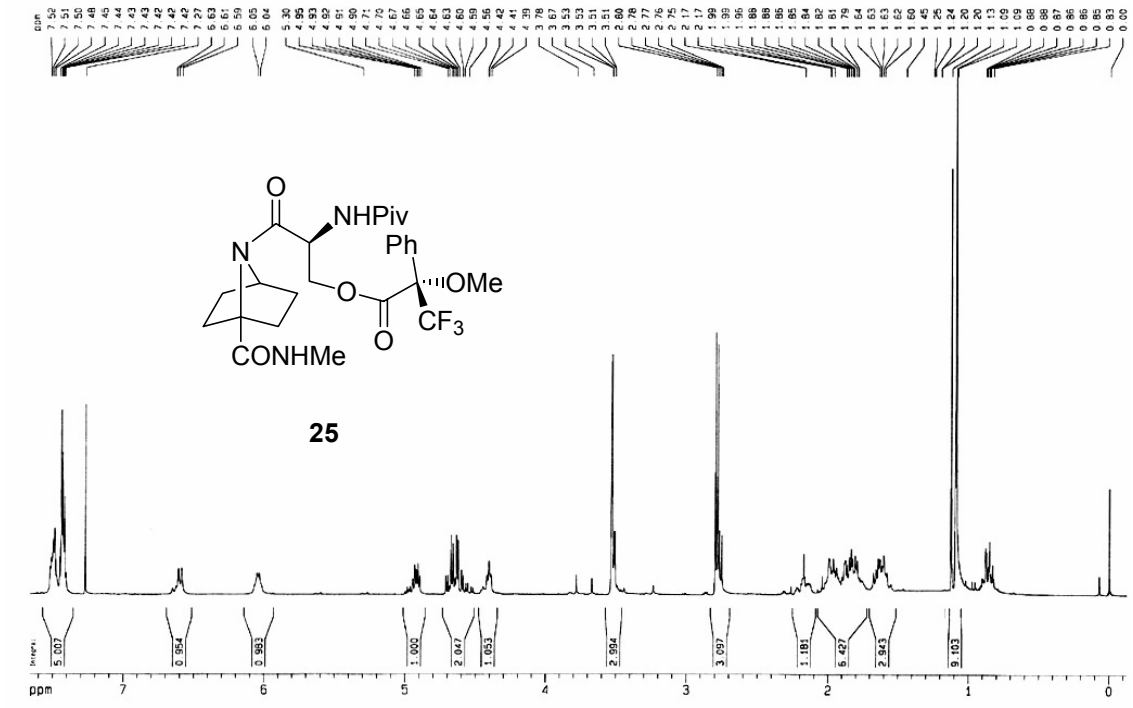

ppm
6
4
2
0
ppm

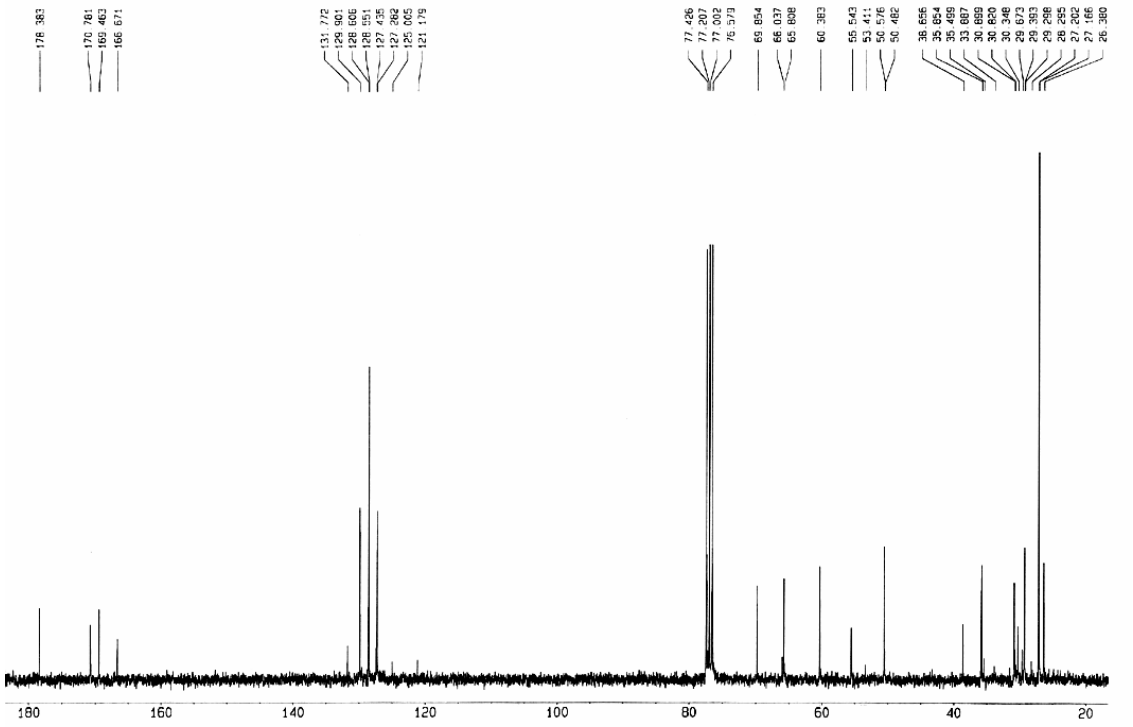

Piv
N
O
NH
CONHMe
O
O
Ph
OMe
CF3

24


ppm
120
100
80
60
40
ppm

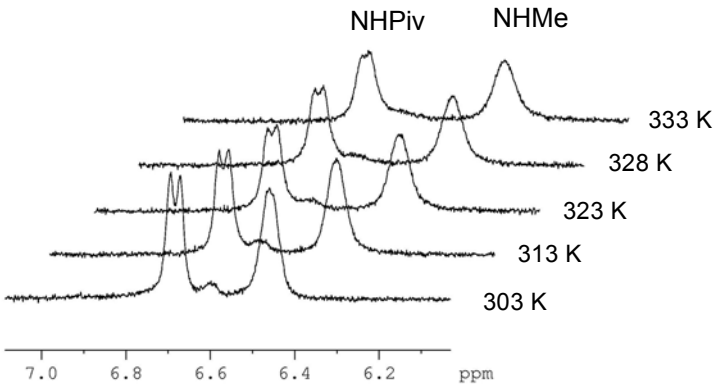
Piv-L-Ser(O-(-)-MTPA)-Ahc-NHMe (25).



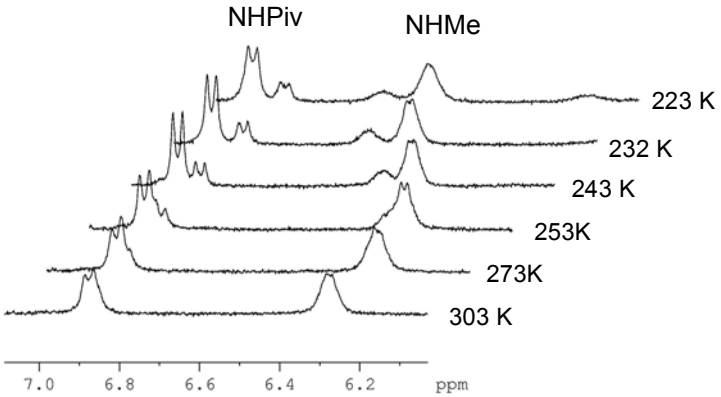


Equilibrium *cis-trans* in peptides (**2**) and (**4**) by ^{1}H NMR

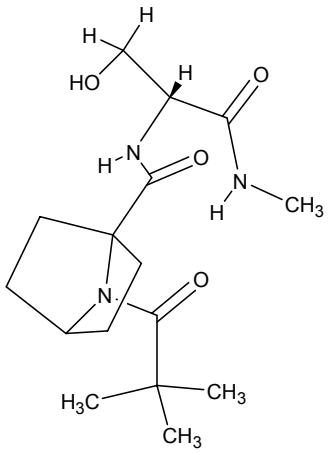
Piv-L-Ser-L-Pro-NHMe (2)



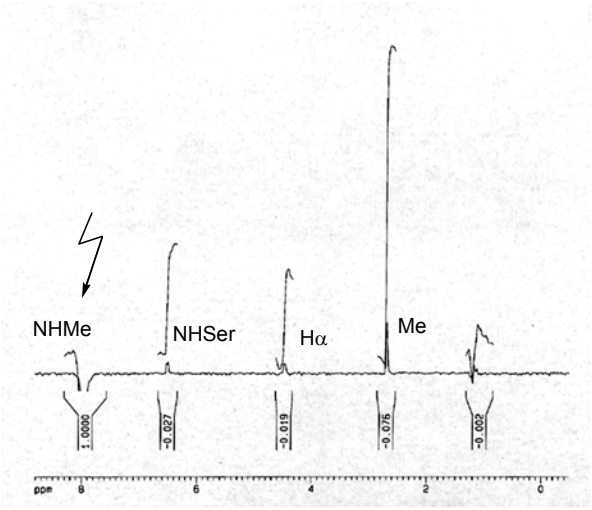
Piv-L-Ser-Ahc-NHMe (4)

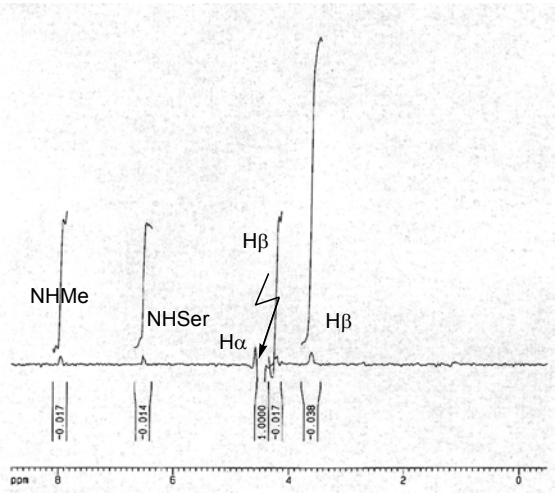


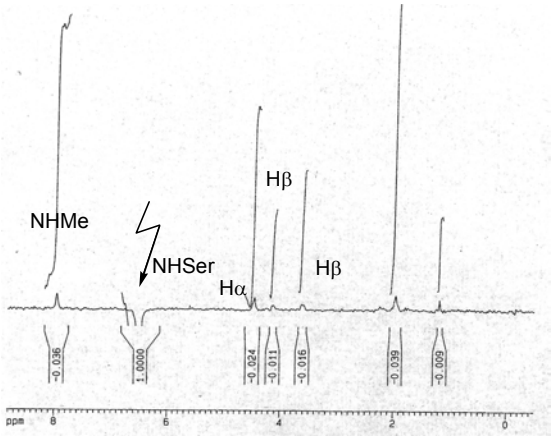
SIGNIFICANT NOE ENHANCEMENTS FOR COMPOUND 3.

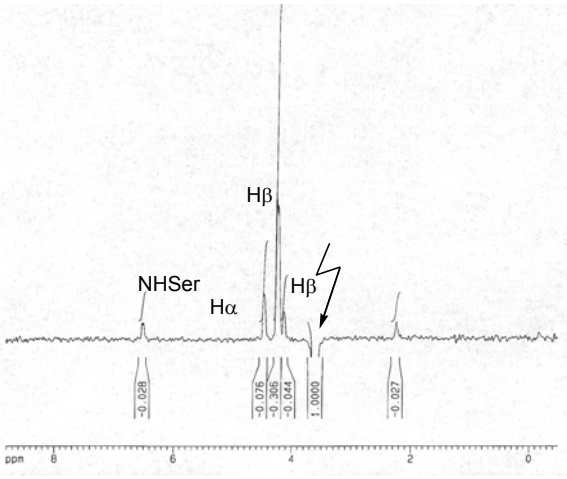


Raws extracted from noesy of compound **3**.

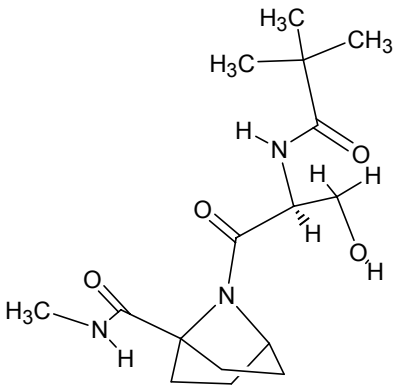




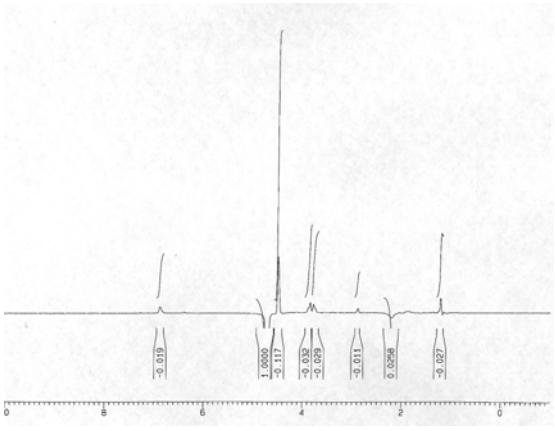


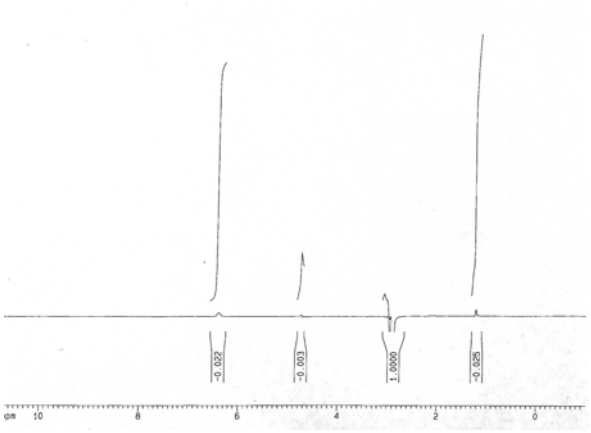


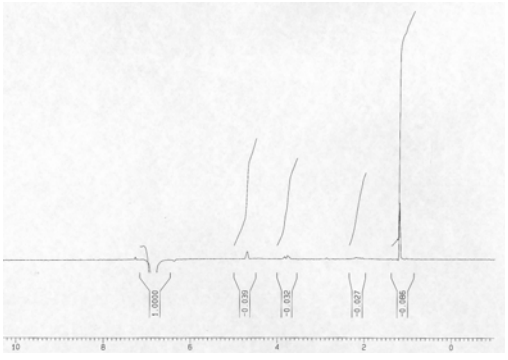
SIGNIFICANT NOE ENHANCEMENTS FOR COMPOUND 4.



Raws extracted from noesy of compound **4**.







Piv-Ahc-L-Ser-NHMe (3)

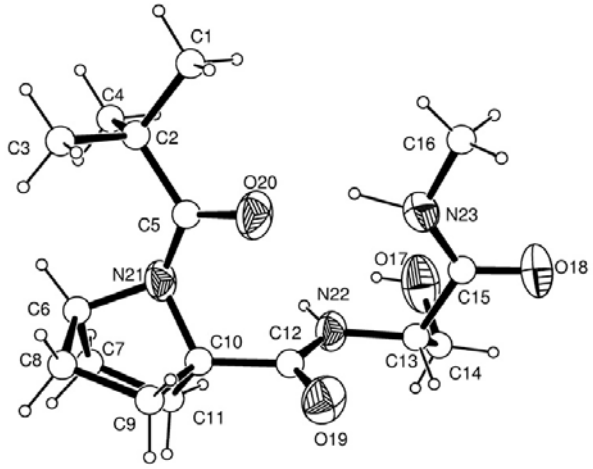


Table 1. Crystal data and structure refinement for Piv-Ahc-L-Ser-NHMe.

Identification code	AhcSer
Empirical formula	C16 H27 N3 O4
Formula weight	325.41
Temperature	130(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P 21 21 21

Unit cell dimensions	a = 10.6897(2) A alpha = 90 deg. b = 11.3502(3) A beta = 90 deg. c = 14.3201(3) A gamma = 90 deg.
Volume	1737.47(7) A^3
Z, Calculated density	4, 1.244 Mg/m^3
Absorption coefficient	0.090 mm^-1
F(000)	704
Crystal size	0.55 x 0.42 x 0.4 mm
Theta range for data collection	2.29 to 27.88 deg.
Limiting indices	-14<=h<=13, -14<=k<=14, -18<=l<=18
Reflections collected / unique	4058 / 4058 [R(int) = 0.0000]
Completeness to theta = 27.88	98.1 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4058 / 0 / 208
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0409, wR2 = 0.0984
R indices (all data)	R1 = 0.0495, wR2 = 0.1035
Absolute structure parameter	-0.6(10)
Largest diff. peak and hole	0.186 and -0.174 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ahcser.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	3518(1)	1389(1)	1498(1)	29(1)
O(4)	15(1)	-1182(1)	2437(1)	30(1)
O(3)	-1183(1)	1625(1)	2610(1)	36(1)
O(2)	3197(1)	684(1)	3614(1)	29(1)
N(5)	3678(1)	3163(1)	2181(1)	23(1)
N(6)	1530(1)	1610(1)	2989(1)	24(1)
C(12)	3810(2)	2441(1)	1431(1)	22(1)
C(14)	2955(2)	3769(1)	3641(1)	28(1)
C(17)	5530(2)	3625(2)	2994(1)	31(1)
C(20)	701(2)	611(1)	3147(1)	24(1)
C(13)	3517(2)	2684(1)	3143(1)	23(1)
N(7)	1413(1)	-95(1)	1626(1)	26(1)
C(22)	692(2)	-291(1)	2357(1)	24(1)
C(8)	5673(2)	3175(2)	529(1)	31(1)
C(18)	4892(2)	2553(1)	3457(1)	30(1)
C(16)	4457(2)	4203(1)	2445(1)	28(1)
C(15)	3592(2)	4821(1)	3137(1)	29(1)
C(10)	4264(2)	2924(1)	487(1)	27(1)
C(21)	-626(2)	1019(1)	3362(1)	31(1)
C(19)	2747(2)	1564(1)	3249(1)	23(1)
C(23)	1477(2)	-912(2)	846(1)	32(1)
C(11)	4078(2)	1958(2)	-251(1)	33(1)
C(9)	3523(2)	4026(2)	199(1)	37(1)

Table 3. Bond lengths [A] and angles [deg] for ahcser.

O(1)-C(12)	1.2378(18)
O(4)-C(22)	1.2488(19)
O(3)-C(21)	1.409(2)
O(3)-H(3)	0.8200
O(2)-C(19)	1.2262(19)
N(5)-C(12)	1.359(2)
N(5)-C(13)	1.491(2)
N(5)-C(16)	1.4935(19)
N(6)-C(19)	1.353(2)
N(6)-C(20)	1.4570(19)
N(6)-H(6)	0.8207
C(12)-C(10)	1.537(2)
C(14)-C(13)	1.544(2)
C(14)-C(15)	1.552(2)
C(14)-H(14A)	0.9599
C(14)-H(14B)	0.9603
C(17)-C(16)	1.538(2)
C(17)-C(18)	1.544(2)
C(17)-H(17A)	0.8475
C(17)-H(17B)	0.9073
C(20)-C(21)	1.523(2)
C(20)-C(22)	1.526(2)
C(20)-H(20)	0.9599
C(13)-C(19)	1.523(2)
C(13)-C(18)	1.543(2)
N(7)-C(22)	1.318(2)
N(7)-C(23)	1.454(2)
N(7)-H(7)	0.9239
C(8)-C(10)	1.534(2)
C(8)-H(8A)	0.9602
C(8)-H(8B)	0.9601
C(8)-H(8C)	0.9600
C(18)-H(18A)	0.9443
C(18)-H(18B)	0.9698
C(16)-C(15)	1.526(2)

C(16)-H(16)	0.9600
C(15)-H(15A)	0.9599
C(15)-H(15B)	0.9601
C(10)-C(11)	1.535(2)
C(10)-C(9)	1.537(2)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9599
C(23)-H(23A)	0.9601
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9598
C(11)-H(11A)	0.9602
C(11)-H(11B)	0.9601
C(11)-H(11C)	0.9599
C(9)-H(9A)	0.9601
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9602
C(21)-O(3)-H(3)	109.5
C(12)-N(5)-C(13)	121.53(12)
C(12)-N(5)-C(16)	128.22(14)
C(13)-N(5)-C(16)	96.80(12)
C(19)-N(6)-C(20)	120.80(12)
C(19)-N(6)-H(6)	126.2
C(20)-N(6)-H(6)	112.9
O(1)-C(12)-N(5)	119.57(15)
O(1)-C(12)-C(10)	119.50(14)
N(5)-C(12)-C(10)	120.88(13)
C(13)-C(14)-C(15)	103.19(13)
C(13)-C(14)-H(14A)	109.2
C(15)-C(14)-H(14A)	112.6
C(13)-C(14)-H(14B)	109.4
C(15)-C(14)-H(14B)	112.8
H(14A)-C(14)-H(14B)	109.5
C(16)-C(17)-C(18)	103.09(13)
C(16)-C(17)-H(17A)	110.6
C(18)-C(17)-H(17A)	110.0
C(16)-C(17)-H(17B)	109.6
C(18)-C(17)-H(17B)	107.5

H(17A)-C(17)-H(17B)	115.3
N(6)-C(20)-C(21)	111.21(12)
N(6)-C(20)-C(22)	114.24(13)
C(21)-C(20)-C(22)	110.35(13)
N(6)-C(20)-H(20)	104.2
C(21)-C(20)-H(20)	106.4
C(22)-C(20)-H(20)	110.0
N(5)-C(13)-C(19)	117.27(12)
N(5)-C(13)-C(18)	101.24(13)
C(19)-C(13)-C(18)	113.94(13)
N(5)-C(13)-C(14)	100.40(12)
C(19)-C(13)-C(14)	114.16(13)
C(18)-C(13)-C(14)	108.23(13)
C(22)-N(7)-C(23)	122.05(14)
C(22)-N(7)-H(7)	121.8
C(23)-N(7)-H(7)	115.8
O(4)-C(22)-N(7)	123.22(15)
O(4)-C(22)-C(20)	118.62(15)
N(7)-C(22)-C(20)	118.15(13)
C(10)-C(8)-H(8A)	109.3
C(10)-C(8)-H(8B)	109.9
H(8A)-C(8)-H(8B)	109.5
C(10)-C(8)-H(8C)	109.3
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(13)-C(18)-C(17)	102.68(13)
C(13)-C(18)-H(18A)	107.7
C(17)-C(18)-H(18A)	117.9
C(13)-C(18)-H(18B)	112.8
C(17)-C(18)-H(18B)	116.4
H(18A)-C(18)-H(18B)	99.6
N(5)-C(16)-C(15)	100.91(13)
N(5)-C(16)-C(17)	102.01(12)
C(15)-C(16)-C(17)	108.41(15)
N(5)-C(16)-H(16)	119.0
C(15)-C(16)-H(16)	115.9
C(17)-C(16)-H(16)	109.3

C(16)-C(15)-C(14)	102.38(12)
C(16)-C(15)-H(15A)	112.8
C(14)-C(15)-H(15A)	109.5
C(16)-C(15)-H(15B)	113.1
C(14)-C(15)-H(15B)	109.3
H(15A)-C(15)-H(15B)	109.5
C(8)-C(10)-C(11)	106.67(14)
C(8)-C(10)-C(9)	111.43(14)
C(11)-C(10)-C(9)	109.28(14)
C(8)-C(10)-C(12)	109.94(14)
C(11)-C(10)-C(12)	108.00(13)
C(9)-C(10)-C(12)	111.34(14)
O(3)-C(21)-C(20)	112.82(14)
O(3)-C(21)-H(21A)	107.6
C(20)-C(21)-H(21A)	109.4
O(3)-C(21)-H(21B)	108.1
C(20)-C(21)-H(21B)	109.4
H(21A)-C(21)-H(21B)	109.5
O(2)-C(19)-N(6)	121.71(14)
O(2)-C(19)-C(13)	120.69(14)
N(6)-C(19)-C(13)	117.42(13)
N(7)-C(23)-H(23A)	109.8
N(7)-C(23)-H(23B)	109.0
H(23A)-C(23)-H(23B)	109.5
N(7)-C(23)-H(23C)	109.7
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(10)-C(11)-H(11A)	109.3
C(10)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.8
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(9)-H(9A)	109.9
C(10)-C(9)-H(9B)	109.9
H(9A)-C(9)-H(9B)	109.5
C(10)-C(9)-H(9C)	108.6

H(9A)-C(9)-H(9C)	109.4
H(9B)-C(9)-H(9C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for ahcser.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	36(1)	19(1)	33(1)	-2(1)	8(1)	-4(1)
O(4)	29(1)	21(1)	40(1)	-1(1)	0(1)	-5(1)
O(3)	30(1)	25(1)	52(1)	1(1)	-5(1)	0(1)
O(2)	31(1)	23(1)	33(1)	5(1)	-1(1)	3(1)
N(5)	25(1)	18(1)	27(1)	1(1)	-1(1)	-2(1)
N(6)	26(1)	17(1)	28(1)	2(1)	-2(1)	-2(1)
C(12)	19(1)	20(1)	28(1)	0(1)	-2(1)	2(1)
C(14)	30(1)	23(1)	30(1)	-6(1)	2(1)	-1(1)
C(17)	23(1)	28(1)	40(1)	-5(1)	-3(1)	-1(1)
C(20)	27(1)	18(1)	27(1)	2(1)	-1(1)	-3(1)
C(13)	24(1)	19(1)	25(1)	-1(1)	-1(1)	-1(1)
N(7)	30(1)	23(1)	26(1)	-2(1)	-1(1)	-4(1)
C(22)	25(1)	18(1)	30(1)	2(1)	-5(1)	1(1)
C(8)	30(1)	28(1)	35(1)	-2(1)	8(1)	-8(1)
C(18)	27(1)	25(1)	38(1)	1(1)	-8(1)	0(1)
C(16)	26(1)	19(1)	38(1)	-3(1)	-1(1)	-4(1)
C(15)	29(1)	20(1)	38(1)	-3(1)	-2(1)	-1(1)
C(10)	29(1)	23(1)	29(1)	1(1)	1(1)	-2(1)
C(21)	31(1)	24(1)	37(1)	0(1)	8(1)	-2(1)
C(19)	27(1)	21(1)	20(1)	-2(1)	-1(1)	2(1)
C(23)	38(1)	29(1)	28(1)	-5(1)	-1(1)	-4(1)
C(11)	37(1)	34(1)	27(1)	-1(1)	1(1)	-2(1)
C(9)	45(1)	30(1)	36(1)	7(1)	-3(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ahcser.

	x	y	z	U(eq)
H(3)	-767	2211	2485	54
H(6)	1189	2152	2707	28
H(14A)	2064	3765	3562	33
H(14B)	3153	3734	4295	33
H(17A)	6101	3395	2627	37
H(17B)	5783	4115	3458	37
H(20)	1014	256	3709	29
H(7)	1973	524	1610	31
H(8A)	5947	3471	-65	37
H(8B)	6119	2464	674	37
H(8C)	5833	3753	1004	37
H(18A)	5164	1794	3280	36
H(18B)	4978	2487	4129	36
H(16)	4800	4690	1960	33
H(15A)	2967	5294	2836	35
H(15B)	4034	5290	3587	35
H(21A)	-1139	347	3499	37
H(21B)	-613	1538	3891	37
H(23A)	2051	-620	385	38
H(23B)	660	-986	574	38
H(23C)	1753	-1668	1062	38
H(11A)	4357	2241	-847	39
H(11B)	3206	1759	-287	39
H(11C)	4550	1270	-81	39
H(9A)	3819	4310	-393	44
H(9B)	3621	4631	661	44
H(9C)	2655	3819	147	44

Piv-L-Ser-Ahc-NHMe (4)

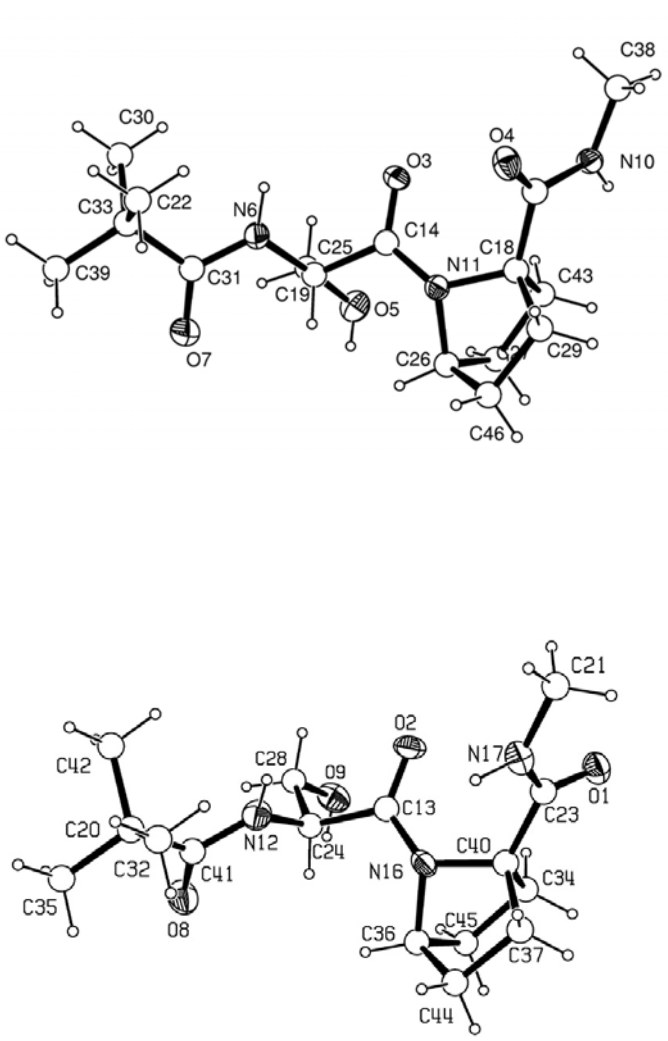


Table 1. Crystal data and structure refinement for Piv-L-Ser-Ahc-NHMe.

Identification code	sahc
Empirical formula	C16 H27 N3 O4
Formula weight	325.41

Temperature 123(2) K

Wavelength 0.71070 A

Crystal system, space group Monoclinic, P 21

Unit cell dimensions a = 9.7429(5) A alpha = 90 deg.
b = 17.4021(9) A beta = 94.368(2) deg.
c = 9.9842(6) A gamma = 90 deg.

Volume 1687.87(16) A^3

Z, Calculated density 4, 1.281 Mg/m^3

Absorption coefficient 0.092 mm^-1

F(000) 704

Crystal size 0.33 x 0.2 x 0.1 mm

Theta range for data collection 2.05 to 27.95 deg.

Limiting indices 0<=h<=12, -22<=k<=14, -13<=l<=13

Reflections collected / unique 5600 / 5600 [R(int) = 0.0000]

Completeness to theta = 27.95 97.3 %

Refinement method Full-matrix least-squares on F^2

Data / restraints / parameters 5600 / 0 / 462

Goodness-of-fit on F^2 1.031

Final R indices [I>2sigma(I)] R1 = 0.0804, wR2 = 0.2183

R indices (all data) R1 = 0.1188, wR2 = 0.2507

Absolute structure parameter -2(2)

Largest diff. peak and hole 0.460 and -0.407 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for sahc.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	-6720(4)	-4110	-10379(4)	31(1)
O(2)	-7352(4)	-2601(3)	-8232(4)	31(1)
O(8)	-10636(4)	-1941(4)	-4713(4)	39(1)
O(9)	-9824(4)	-1336(4)	-8684(4)	37(1)
N(12)	-8623(5)	-2284(4)	-5498(5)	31(1)
N(16)	-8837(5)	-3543(4)	-7785(5)	26(1)
N(17)	-6039(5)	-4187(4)	-8181(5)	30(1)
C(13)	-8394(5)	-2808(4)	-7729(6)	26(1)
C(20)	-8675(6)	-2056(4)	-3096(6)	27(1)
C(21)	-4564(6)	-4272(4)	-8356(6)	31(1)
C(23)	-6986(6)	-4113(4)	-9186(5)	24(1)
C(24)	-9175(5)	-2241(4)	-6877(6)	26(1)
C(28)	-9096(6)	-1429(4)	-7422(6)	32(1)
C(32)	-7988(7)	-2835(4)	-2727(7)	37(2)
C(34)	-9539(6)	-3888(5)	-9991(6)	35(2)
C(35)	-9708(6)	-1862(5)	-2089(6)	33(1)
C(36)	-10316(5)	-3781(4)	-7768(6)	29(1)
C(37)	-8911(6)	-4868(4)	-8225(7)	33(1)
C(40)	-8464(6)	-4097(4)	-8830(5)	27(1)
C(41)	-9403(6)	-2094(4)	-4494(6)	31(1)
C(42)	-7557(7)	-1434(5)	-3083(7)	38(2)

C(44)	-10133(7)	-4636(5)	-7453(7)	38(2)
C(45)	-10824(6)	-3678(5)	-9229(6)	40(2)
O(3)	-5919(4)	-2950(3)	-5288(4)	30(1)
O(4)	-6482(4)	-4623(3)	-5457(4)	30(1)
O(5)	-3216(5)	-1767(4)	-3737(4)	34(1)
O(7)	-2347(4)	-1801(4)	-7833(4)	38(1)
N(6)	-4391(4)	-2218(4)	-7251(5)	25(1)
N(10)	-6830(4)	-4578(4)	-3259(4)	23(1)
N(11)	-3990(4)	-3641(4)	-4799(5)	23(1)
C(14)	-4663(6)	-3008(4)	-5280(5)	25(1)
C(15)	-6077(5)	-4468(4)	-4312(6)	23(1)
C(18)	-4567(5)	-4245(4)	-3939(5)	22(1)
C(19)	-3811(5)	-2378(4)	-5902(5)	23(1)
C(22)	-4720(6)	-2383(4)	-10285(6)	35(1)
C(25)	-3859(6)	-1656(4)	-5036(6)	28(1)
C(26)	-2554(5)	-3689(4)	-4197(6)	28(1)
C(27)	-2729(6)	-3568(4)	-2709(6)	32(1)
C(29)	-3609(6)	-4919(4)	-4243(6)	32(1)
C(30)	-5469(6)	-1127(4)	-9331(6)	33(1)
C(31)	-3578(5)	-1894(4)	-8131(5)	24(1)
C(33)	-4247(6)	-1658(4)	-9503(6)	26(1)
C(38)	-8246(6)	-4858(5)	-3488(6)	33(1)
C(39)	-3189(6)	-1235(5)	-10283(6)	34(1)
C(43)	-4161(6)	-3944(4)	-2532(5)	28(1)
C(46)	-2218(6)	-4529(4)	-4459(7)	34(1)

Table 3. Bond lengths [A] and angles [deg] for sahc.

O(1)-C(23)	1.238(6)
O(2)-C(13)	1.220(7)
O(8)-C(41)	1.234(7)
O(9)-C(28)	1.407(7)
O(9)-H(9)	0.8200
N(12)-C(41)	1.345(8)

N(12)-C(24)	1.442(7)
N(12)-H(12)	0.9603
N(16)-C(13)	1.350(7)
N(16)-C(40)	1.486(7)
N(16)-C(36)	1.500(7)
N(17)-C(23)	1.317(7)
N(17)-C(21)	1.468(7)
N(17)-H(17)	0.9596
C(13)-C(24)	1.541(8)
C(20)-C(35)	1.514(8)
C(20)-C(41)	1.518(8)
C(20)-C(42)	1.534(9)
C(20)-C(32)	1.544(8)
C(21)-H(21A)	0.9607
C(21)-H(21B)	0.9601
C(21)-H(21C)	0.9600
C(23)-C(40)	1.510(7)
C(24)-C(28)	1.518(8)
C(24)-H(24)	0.9606
C(28)-H(28A)	0.9602
C(28)-H(28B)	0.9602
C(32)-H(32A)	0.9454
C(32)-H(32B)	0.9648
C(32)-H(32C)	0.9705
C(34)-C(40)	1.545(8)
C(34)-C(45)	1.557(8)
C(34)-H(34A)	0.9613
C(34)-H(34B)	0.9834
C(35)-H(35A)	0.9581
C(35)-H(35B)	0.9823
C(35)-H(35C)	0.9580
C(36)-C(45)	1.514(9)
C(36)-C(44)	1.529(9)
C(36)-H(36)	0.9802
C(37)-C(44)	1.521(8)
C(37)-C(40)	1.547(8)
C(37)-H(37A)	0.9574

C(37)-H(37B)	0.9698
C(42)-H(42A)	0.9715
C(42)-H(42B)	0.9784
C(42)-H(42C)	0.9605
C(44)-H(44A)	0.9459
C(44)-H(44B)	0.9467
C(45)-H(45A)	0.9620
C(45)-H(45B)	0.9752
O(3)-C(14)	1.227(6)
O(4)-C(15)	1.211(7)
O(5)-C(25)	1.410(7)
O(5)-H(5)	0.8194
O(7)-C(31)	1.224(7)
N(6)-C(31)	1.350(7)
N(6)-C(19)	1.448(7)
N(6)-H(6)	0.9517
N(10)-C(15)	1.341(7)
N(10)-C(38)	1.465(7)
N(10)-H(10)	0.9600
N(11)-C(14)	1.351(7)
N(11)-C(26)	1.483(7)
N(11)-C(18)	1.495(7)
C(14)-C(19)	1.535(8)
C(15)-C(18)	1.540(7)
C(18)-C(43)	1.523(8)
C(18)-C(29)	1.544(8)
C(19)-C(25)	1.528(8)
C(19)-H(19)	0.9565
C(22)-C(33)	1.535(8)
C(22)-H(22A)	0.9512
C(22)-H(22B)	0.9580
C(22)-H(22C)	0.9641
C(25)-H(25A)	0.9603
C(25)-H(25B)	0.9711
C(26)-C(27)	1.523(8)
C(26)-C(46)	1.524(9)
C(26)-H(26)	0.9884

C(27)-C(43)	1.563(8)
C(27)-H(27A)	0.9611
C(27)-H(27B)	0.9619
C(29)-C(46)	1.545(9)
C(29)-H(29A)	0.9810
C(29)-H(29B)	0.9602
C(30)-C(33)	1.527(9)
C(30)-H(30A)	0.9450
C(30)-H(30B)	0.9572
C(30)-H(30C)	0.9770
C(31)-C(33)	1.528(8)
C(33)-C(39)	1.528(8)
C(38)-H(38A)	0.9531
C(38)-H(38B)	0.9583
C(38)-H(38C)	0.9775
C(39)-H(39A)	0.9893
C(39)-H(39B)	0.9626
C(39)-H(39C)	0.9474
C(43)-H(43A)	0.9658
C(43)-H(43B)	0.9671
C(46)-H(46A)	0.9575
C(46)-H(46B)	0.9459

C(28)-O(9)-H(9)	109.0
C(41)-N(12)-C(24)	120.6(5)
C(41)-N(12)-H(12)	120.6
C(24)-N(12)-H(12)	118.9
C(13)-N(16)-C(40)	123.3(4)
C(13)-N(16)-C(36)	124.4(5)
C(40)-N(16)-C(36)	96.6(4)
C(23)-N(17)-C(21)	123.7(5)
C(23)-N(17)-H(17)	119.4
C(21)-N(17)-H(17)	116.9
O(2)-C(13)-N(16)	122.4(5)
O(2)-C(13)-C(24)	120.0(5)
N(16)-C(13)-C(24)	117.3(5)
C(35)-C(20)-C(41)	109.4(4)

C(35)-C(20)-C(42)	110.1(5)
C(41)-C(20)-C(42)	108.7(5)
C(35)-C(20)-C(32)	109.6(5)
C(41)-C(20)-C(32)	110.2(5)
C(42)-C(20)-C(32)	108.8(5)
N(17)-C(21)-H(21A)	110.3
N(17)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.4
N(17)-C(21)-H(21C)	108.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
O(1)-C(23)-N(17)	123.2(5)
O(1)-C(23)-C(40)	120.0(5)
N(17)-C(23)-C(40)	116.6(5)
N(12)-C(24)-C(28)	111.3(5)
N(12)-C(24)-C(13)	109.3(4)
C(28)-C(24)-C(13)	110.9(5)
N(12)-C(24)-H(24)	109.4
C(28)-C(24)-H(24)	107.4
C(13)-C(24)-H(24)	108.5
O(9)-C(28)-C(24)	113.1(5)
O(9)-C(28)-H(28A)	107.6
C(24)-C(28)-H(28A)	109.0
O(9)-C(28)-H(28B)	108.5
C(24)-C(28)-H(28B)	109.2
H(28A)-C(28)-H(28B)	109.4
C(20)-C(32)-H(32A)	110.1
C(20)-C(32)-H(32B)	109.2
H(32A)-C(32)-H(32B)	110.3
C(20)-C(32)-H(32C)	109.0
H(32A)-C(32)-H(32C)	109.9
H(32B)-C(32)-H(32C)	108.3
C(40)-C(34)-C(45)	102.3(5)
C(40)-C(34)-H(34A)	114.3
C(45)-C(34)-H(34A)	109.9
C(40)-C(34)-H(34B)	113.3
C(45)-C(34)-H(34B)	109.5

H(34A)-C(34)-H(34B)	107.5
C(20)-C(35)-H(35A)	110.8
C(20)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	107.7
C(20)-C(35)-H(35C)	110.9
H(35A)-C(35)-H(35C)	109.8
H(35B)-C(35)-H(35C)	107.9
N(16)-C(36)-C(45)	101.6(4)
N(16)-C(36)-C(44)	100.0(5)
C(45)-C(36)-C(44)	109.7(5)
N(16)-C(36)-H(36)	107.5
C(45)-C(36)-H(36)	118.9
C(44)-C(36)-H(36)	116.2
C(44)-C(37)-C(40)	102.9(5)
C(44)-C(37)-H(37A)	109.9
C(40)-C(37)-H(37A)	113.7
C(44)-C(37)-H(37B)	109.4
C(40)-C(37)-H(37B)	112.0
H(37A)-C(37)-H(37B)	108.9
N(16)-C(40)-C(23)	117.8(5)
N(16)-C(40)-C(34)	100.7(5)
C(23)-C(40)-C(34)	115.6(4)
N(16)-C(40)-C(37)	101.4(4)
C(23)-C(40)-C(37)	112.2(5)
C(34)-C(40)-C(37)	107.6(5)
O(8)-C(41)-N(12)	121.2(5)
O(8)-C(41)-C(20)	122.3(5)
N(12)-C(41)-C(20)	116.4(5)
C(20)-C(42)-H(42A)	111.1
C(20)-C(42)-H(42B)	110.3
H(42A)-C(42)-H(42B)	107.1
C(20)-C(42)-H(42C)	111.8
H(42A)-C(42)-H(42C)	108.5
H(42B)-C(42)-H(42C)	107.9
C(37)-C(44)-C(36)	103.7(5)
C(37)-C(44)-H(44A)	109.5
C(36)-C(44)-H(44A)	111.6

C(37)-C(44)-H(44B)	109.3
C(36)-C(44)-H(44B)	110.6
H(44A)-C(44)-H(44B)	111.8
C(36)-C(45)-C(34)	103.1(4)
C(36)-C(45)-H(45A)	111.2
C(34)-C(45)-H(45A)	112.6
C(36)-C(45)-H(45B)	109.7
C(34)-C(45)-H(45B)	112.2
H(45A)-C(45)-H(45B)	107.9
C(25)-O(5)-H(5)	109.3
C(31)-N(6)-C(19)	118.6(4)
C(31)-N(6)-H(6)	120.5
C(19)-N(6)-H(6)	120.8
C(15)-N(10)-C(38)	119.3(5)
C(15)-N(10)-H(10)	118.9
C(38)-N(10)-H(10)	121.7
C(14)-N(11)-C(26)	127.5(5)
C(14)-N(11)-C(18)	125.7(4)
C(26)-N(11)-C(18)	96.4(4)
O(3)-C(14)-N(11)	121.8(5)
O(3)-C(14)-C(19)	120.5(5)
N(11)-C(14)-C(19)	117.6(5)
O(4)-C(15)-N(10)	123.4(5)
O(4)-C(15)-C(18)	121.4(5)
N(10)-C(15)-C(18)	114.6(5)
N(11)-C(18)-C(43)	101.9(4)
N(11)-C(18)-C(15)	115.6(4)
C(43)-C(18)-C(15)	119.1(4)
N(11)-C(18)-C(29)	99.3(4)
C(43)-C(18)-C(29)	108.9(5)
C(15)-C(18)-C(29)	110.0(5)
N(6)-C(19)-C(25)	109.9(4)
N(6)-C(19)-C(14)	109.2(4)
C(25)-C(19)-C(14)	108.6(4)
N(6)-C(19)-H(19)	109.6
C(25)-C(19)-H(19)	109.3
C(14)-C(19)-H(19)	110.3

C(33)-C(22)-H(22A)	109.5
C(33)-C(22)-H(22B)	109.1
H(22A)-C(22)-H(22B)	110.4
C(33)-C(22)-H(22C)	108.7
H(22A)-C(22)-H(22C)	109.8
H(22B)-C(22)-H(22C)	109.3
O(5)-C(25)-C(19)	112.1(4)
O(5)-C(25)-H(25A)	108.7
C(19)-C(25)-H(25A)	109.6
O(5)-C(25)-H(25B)	108.8
C(19)-C(25)-H(25B)	109.0
H(25A)-C(25)-H(25B)	108.5
N(11)-C(26)-C(27)	102.4(4)
N(11)-C(26)-C(46)	101.1(5)
C(27)-C(26)-C(46)	110.0(5)
N(11)-C(26)-H(26)	109.3
C(27)-C(26)-H(26)	114.9
C(46)-C(26)-H(26)	117.1
C(26)-C(27)-C(43)	102.7(4)
C(26)-C(27)-H(27A)	111.9
C(43)-C(27)-H(27A)	109.9
C(26)-C(27)-H(27B)	112.5
C(43)-C(27)-H(27B)	110.6
H(27A)-C(27)-H(27B)	109.2
C(18)-C(29)-C(46)	104.1(5)
C(18)-C(29)-H(29A)	111.5
C(46)-C(29)-H(29A)	109.2
C(18)-C(29)-H(29B)	113.2
C(46)-C(29)-H(29B)	111.0
H(29A)-C(29)-H(29B)	107.8
C(33)-C(30)-H(30A)	109.9
C(33)-C(30)-H(30B)	109.8
H(30A)-C(30)-H(30B)	110.9
C(33)-C(30)-H(30C)	108.6
H(30A)-C(30)-H(30C)	109.3
H(30B)-C(30)-H(30C)	108.3
O(7)-C(31)-N(6)	120.7(5)

O(7)-C(31)-C(33)	121.7(5)
N(6)-C(31)-C(33)	117.7(5)
C(30)-C(33)-C(39)	109.2(5)
C(30)-C(33)-C(31)	110.2(4)
C(39)-C(33)-C(31)	109.1(5)
C(30)-C(33)-C(22)	110.4(5)
C(39)-C(33)-C(22)	109.0(5)
C(31)-C(33)-C(22)	109.0(5)
N(10)-C(38)-H(38A)	110.2
N(10)-C(38)-H(38B)	110.5
H(38A)-C(38)-H(38B)	110.2
N(10)-C(38)-H(38C)	109.2
H(38A)-C(38)-H(38C)	108.6
H(38B)-C(38)-H(38C)	108.2
C(33)-C(39)-H(39A)	109.8
C(33)-C(39)-H(39B)	110.7
H(39A)-C(39)-H(39B)	106.8
C(33)-C(39)-H(39C)	111.0
H(39A)-C(39)-H(39C)	108.0
H(39B)-C(39)-H(39C)	110.3
C(18)-C(43)-C(27)	102.2(4)
C(18)-C(43)-H(43A)	113.9
C(27)-C(43)-H(43A)	108.8
C(18)-C(43)-H(43B)	113.8
C(27)-C(43)-H(43B)	109.4
H(43A)-C(43)-H(43B)	108.4
C(26)-C(46)-C(29)	101.3(4)
C(26)-C(46)-H(46A)	112.4
C(29)-C(46)-H(46A)	108.6
C(26)-C(46)-H(46B)	112.8
C(29)-C(46)-H(46B)	110.3
H(46A)-C(46)-H(46B)	110.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for sahc.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	36(2)	33(2)	26(2)	-2(2)	8(2)	2(2)
O(2)	21(2)	29(2)	45(3)	1(2)	9(2)	-3(2)
O(8)	29(2)	53(3)	33(2)	-6(2)	1(2)	6(2)
O(9)	32(2)	45(3)	35(2)	8(2)	5(2)	2(2)
N(12)	20(2)	38(3)	35(3)	-7(2)	-3(2)	4(2)
N(16)	26(2)	28(3)	25(2)	-1(2)	11(2)	0(2)
N(17)	33(3)	32(3)	27(3)	-1(2)	6(2)	4(2)
C(13)	22(3)	28(3)	27(3)	-2(2)	-3(2)	0(2)
C(20)	23(3)	25(3)	33(3)	3(3)	5(2)	3(2)
C(21)	32(3)	33(3)	28(3)	-2(3)	1(2)	7(3)
C(23)	35(3)	17(3)	22(3)	3(2)	10(2)	0(2)
C(24)	22(3)	28(3)	28(3)	-10(2)	0(2)	2(2)
C(28)	27(3)	26(3)	43(4)	-9(3)	0(3)	-1(2)
C(32)	45(4)	25(3)	40(4)	6(3)	2(3)	10(3)
C(34)	31(3)	46(4)	28(3)	-3(3)	1(3)	-3(3)
C(35)	35(3)	35(3)	30(3)	-9(3)	-1(2)	12(3)
C(36)	23(3)	31(3)	35(3)	-4(3)	6(2)	-4(2)
C(37)	31(3)	28(3)	40(3)	-2(3)	9(3)	-8(3)
C(40)	33(3)	28(3)	21(3)	-2(2)	7(2)	-9(3)
C(41)	34(3)	24(3)	34(3)	-10(3)	2(2)	5(2)
C(42)	38(3)	41(4)	33(3)	-6(3)	-10(3)	-5(3)
C(44)	36(3)	34(4)	46(4)	-6(3)	20(3)	-9(3)
C(45)	25(3)	47(4)	48(4)	-8(3)	1(3)	2(3)
O(3)	20(2)	28(2)	43(2)	10(2)	5(2)	-1(2)
O(4)	36(2)	33(2)	21(2)	-1(2)	3(2)	-8(2)
O(5)	41(2)	36(3)	24(2)	-5(2)	-2(2)	1(2)
O(7)	27(2)	53(3)	35(2)	10(2)	1(2)	-3(2)

N(6)	24(2)	27(3)	24(2)	4(2)	-1(2)	-4(2)
N(10)	21(2)	27(2)	21(2)	0(2)	5(2)	3(2)
N(11)	22(2)	19(2)	27(2)	2(2)	4(2)	1(2)
C(14)	26(3)	26(3)	21(3)	3(2)	1(2)	-1(2)
C(15)	27(3)	18(3)	25(3)	0(2)	3(2)	4(2)
C(18)	23(3)	19(3)	24(3)	7(2)	6(2)	0(2)
C(19)	24(3)	19(3)	27(3)	5(2)	0(2)	3(2)
C(22)	38(3)	29(3)	35(3)	-3(3)	-6(3)	-6(3)
C(25)	27(3)	20(3)	37(3)	1(3)	1(2)	2(2)
C(26)	21(3)	32(3)	30(3)	9(3)	0(2)	3(2)
C(27)	29(3)	35(4)	31(3)	3(3)	-3(2)	-7(3)
C(29)	33(3)	24(3)	38(3)	2(3)	8(3)	7(3)
C(30)	38(3)	28(3)	33(3)	5(3)	2(3)	1(3)
C(31)	27(3)	17(3)	26(3)	0(2)	2(2)	4(2)
C(33)	32(3)	24(3)	24(3)	0(2)	3(2)	-4(2)
C(38)	26(3)	37(4)	36(3)	-10(3)	6(3)	-6(3)
C(39)	36(3)	41(4)	25(3)	8(3)	0(2)	-11(3)
C(43)	35(3)	28(3)	19(3)	-1(2)	0(2)	-5(2)
C(46)	28(3)	23(3)	51(4)	9(3)	8(3)	11(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for sahc.

	x	y	z	U(eq)
H(9)	-10638	-1436	-8615	12(14)
H(12)	-7681	-2437	-5310	41(19)
H(17)	-6310	-4194	-7277	140(50)
H(21A)	-4054	-4320	-7498	100(30)
H(21B)	-4419	-4721	-8886	170(60)
H(21C)	-4257	-3825	-8811	170(60)
H(24)	-10129	-2386	-6933	50

H(28A)	-8150	-1303	-7523	50
H(28B)	-9465	-1078	-6800	50
H(32A)	-8663	-3225	-2721	31(17)
H(32B)	-7329	-2955	-3370	110(40)
H(32C)	-7499	-2794	-1846	16(13)
H(34A)	-9285	-3459	-10526	50(20)
H(34B)	-9764	-4319	-10606	23(15)
H(35A)	-10405	-2250	-2081	24(15)
H(35B)	-9238	-1837	-1184	36(18)
H(35C)	-10125	-1372	-2283	50(20)
H(36)	-10728	-3470	-7085	50(20)
H(37A)	-9189	-5247	-8886	11(13)
H(37B)	-8197	-5084	-7607	39(19)
H(42A)	-7061	-1396	-2204	34(17)
H(42B)	-6882	-1562	-3725	50(20)
H(42C)	-7937	-939	-3320	90(30)
H(44A)	-9921	-4722	-6525	80(30)
H(44B)	-10919	-4917	-7785	21(15)
H(45A)	-11136	-3161	-9405	70(30)
H(45B)	-11595	-4024	-9452	35(17)
H(5)	-2407	-1881	-3795	70(30)
H(6)	-5320	-2348	-7521	26(15)
H(10)	-6433	-4456	-2375	28(16)
H(19)	-2876	-2540	-5930	50
H(22A)	-5376	-2651	-9803	190(70)
H(22B)	-5118	-2236	-11155	29(16)
H(22C)	-3931	-2705	-10387	40(18)
H(25A)	-4800	-1509	-4958	50
H(25B)	-3396	-1240	-5469	50
H(26)	-1987	-3297	-4612	41(19)
H(27A)	-2027	-3827	-2151	32(17)
H(27B)	-2739	-3033	-2467	3(11)
H(29A)	-3487	-5274	-3480	60(30)
H(29B)	-3934	-5211	-5019	40(20)
H(30A)	-6135	-1385	-8857	70(30)
H(30B)	-5161	-669	-8870	50(20)
H(30C)	-5877	-983	-10220	31(17)

H(38A)	-8656	-4905	-2655	60(20)
H(38B)	-8779	-4517	-4076	90(30)
H(38C)	-8238	-5363	-3914	21(15)
H(39A)	-3613	-1076	-11172	24(15)
H(39B)	-2883	-773	-9821	38(18)
H(39C)	-2428	-1556	-10424	60(20)
H(43A)	-4775	-3556	-2229	24(15)
H(43B)	-4058	-4342	-1856	60(20)
H(46A)	-2003	-4617	-5366	70(30)
H(46B)	-1519	-4725	-3844	40(19)