

Supporting Information for

Diastereoselective Ireland–Claisen rearrangements of substituted allyl β -amino esters: applications in the asymmetric synthesis of C(5)-substituted transpentacins

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Myriam Y. Souleymanou, James E. Thomson and Charlotte M. Zammit

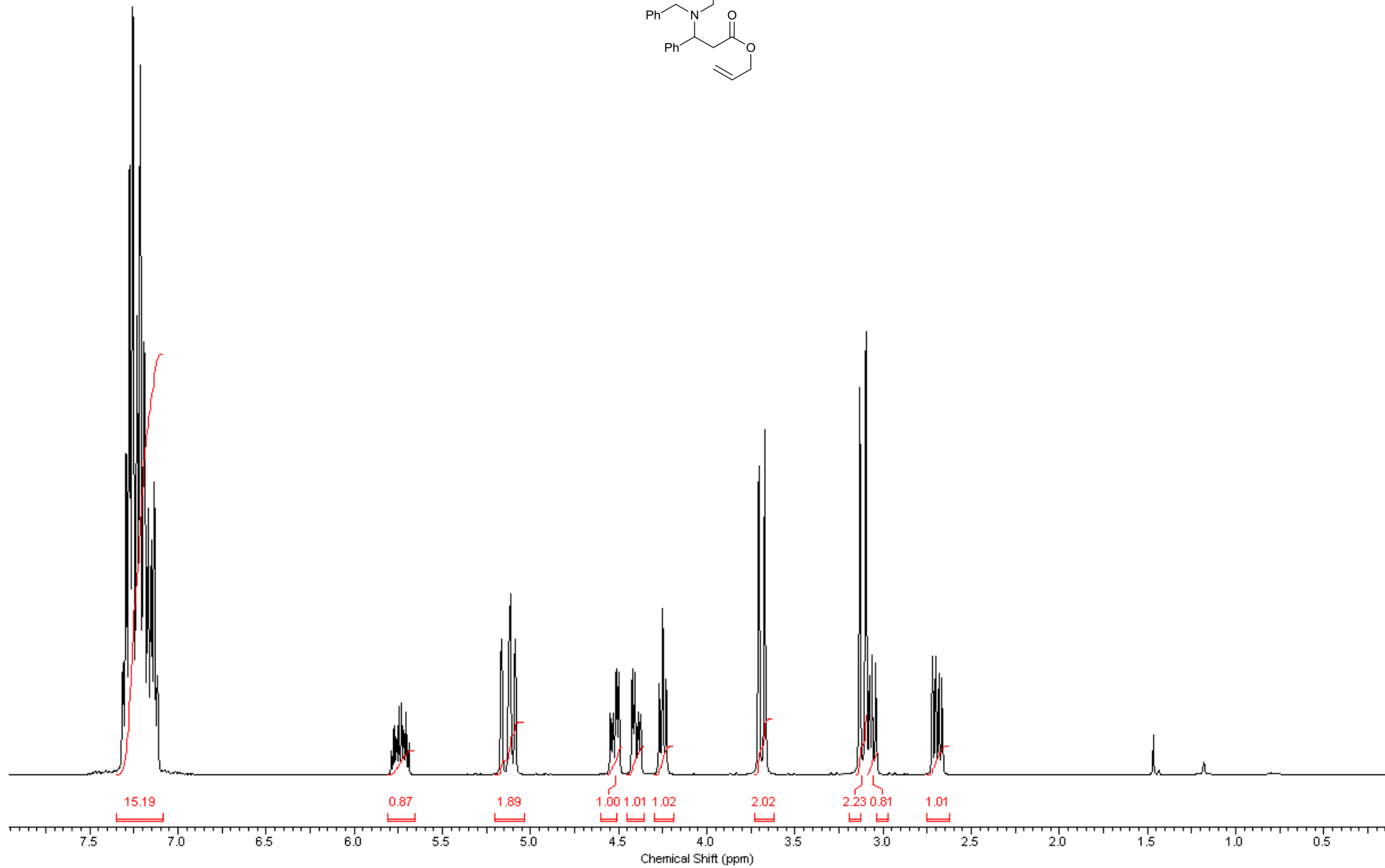
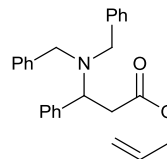
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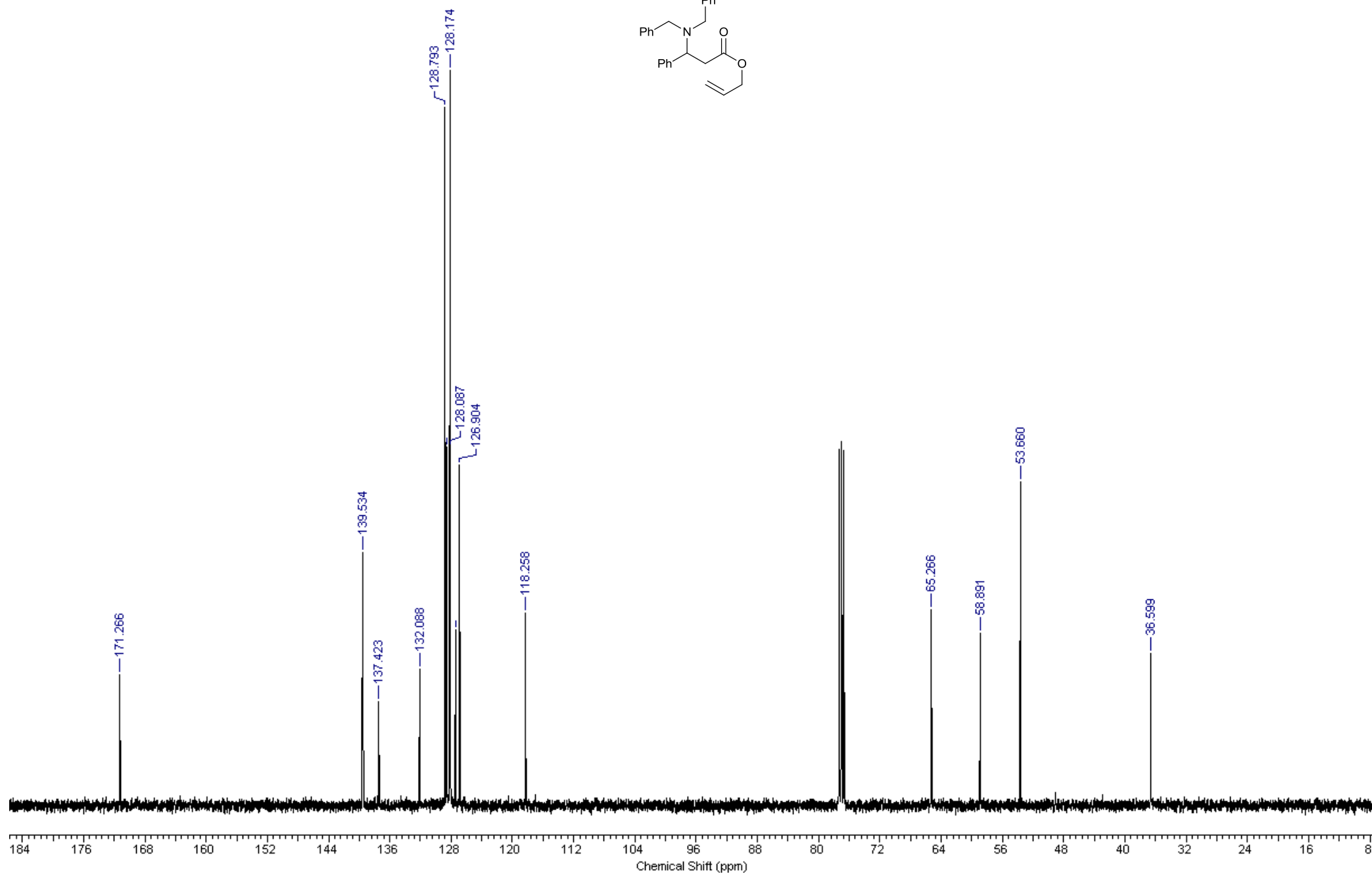
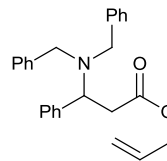
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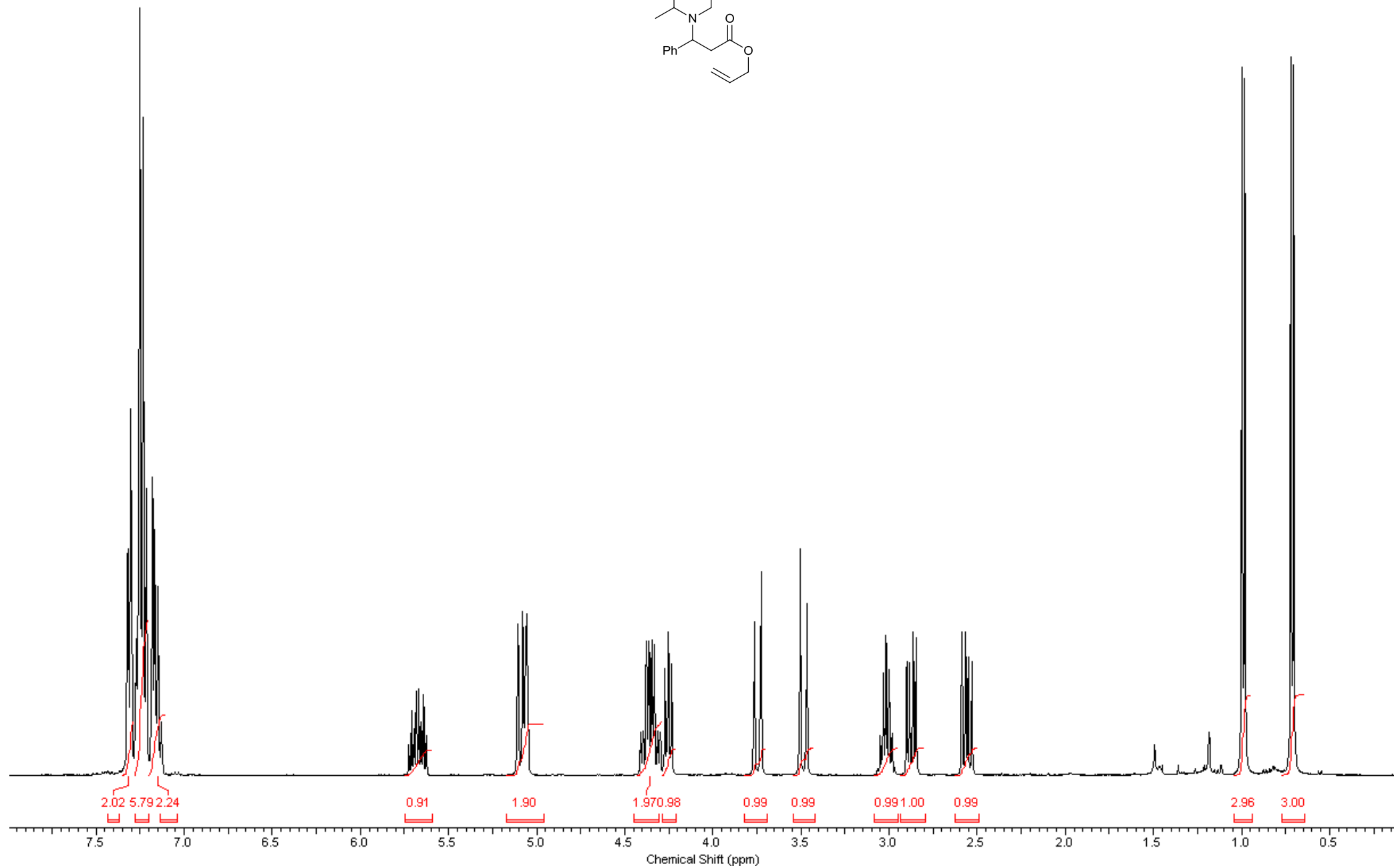
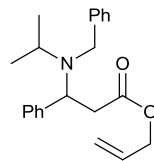
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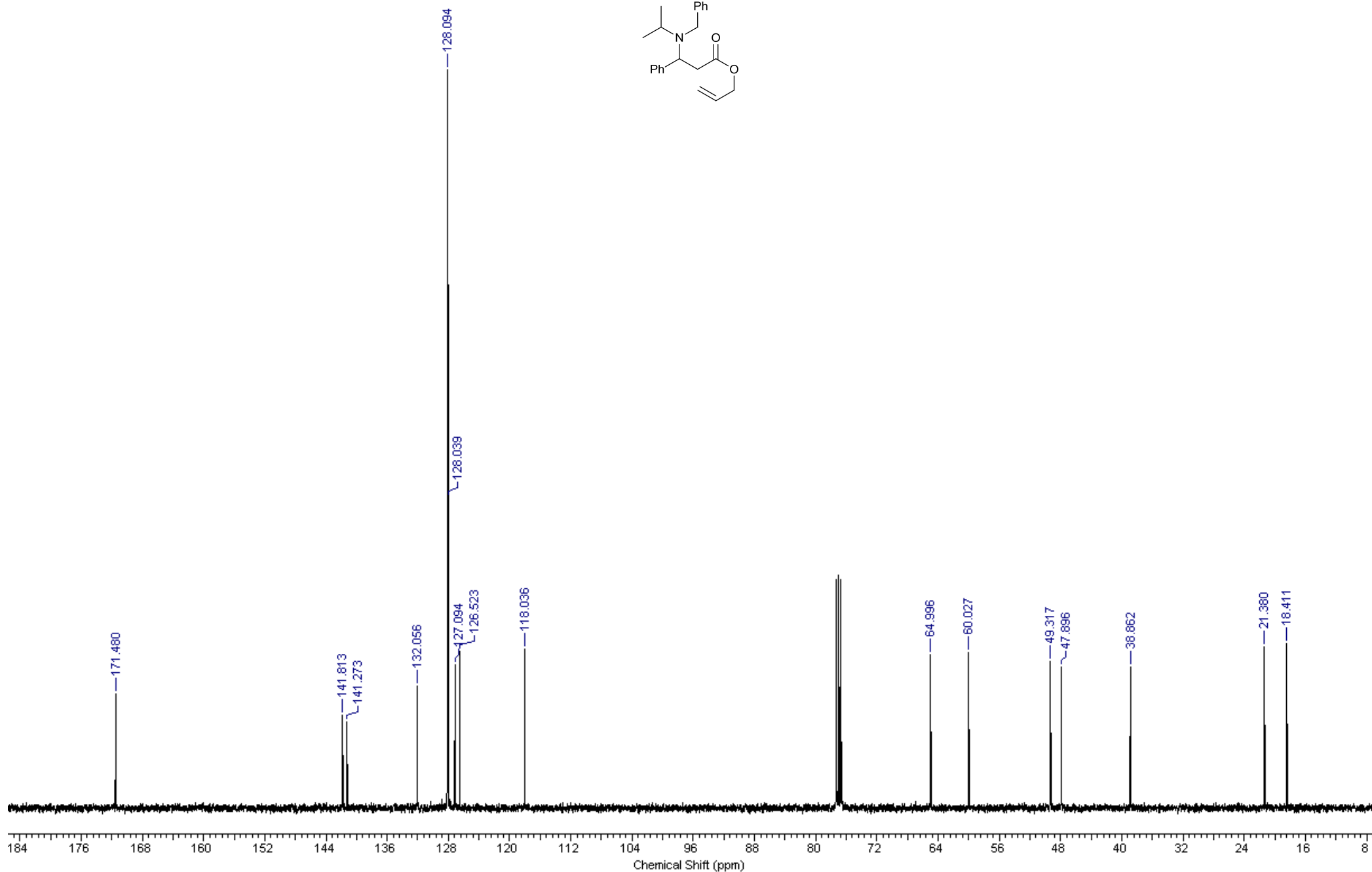
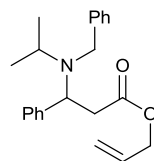
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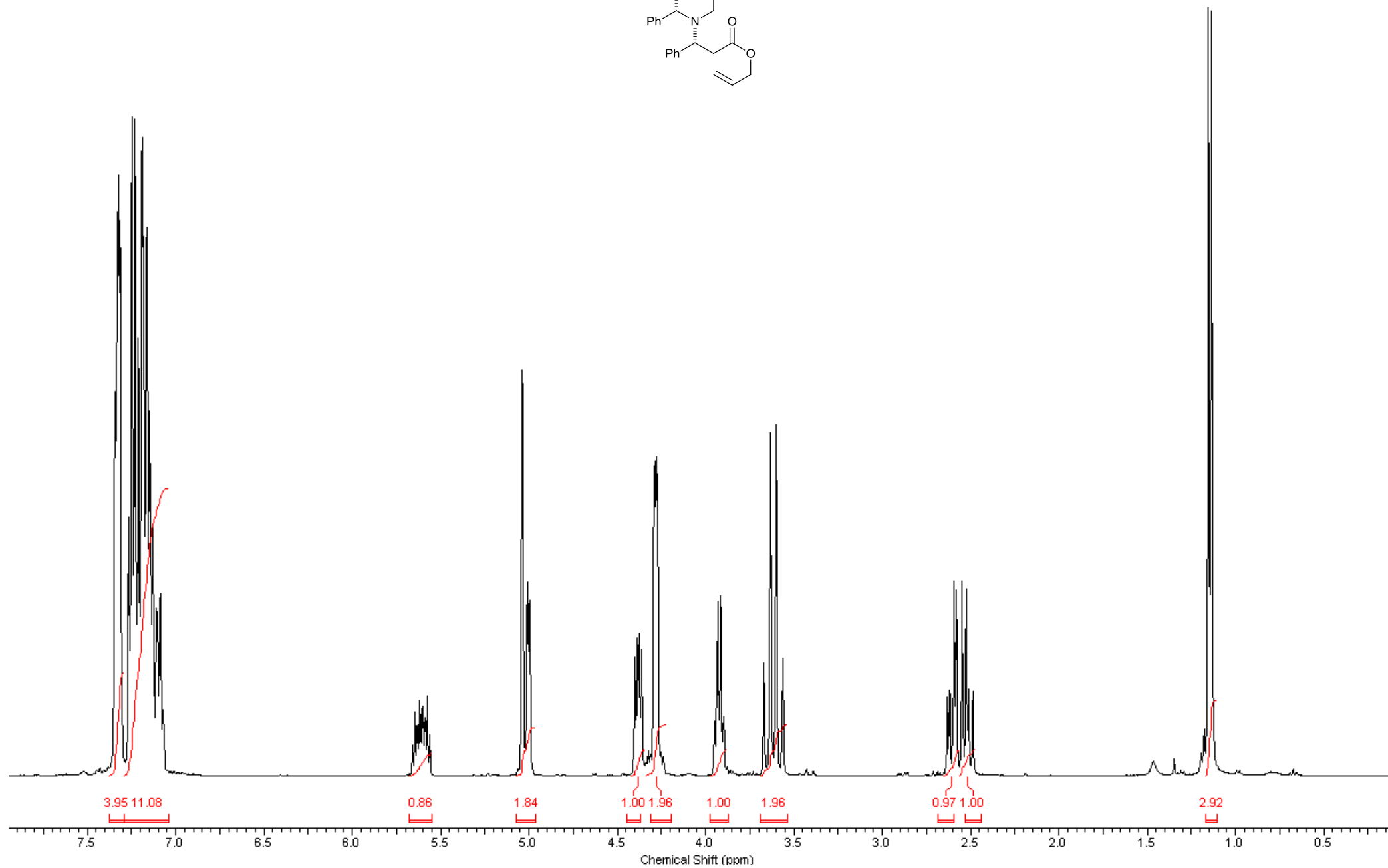
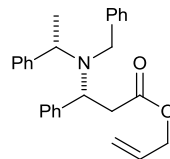
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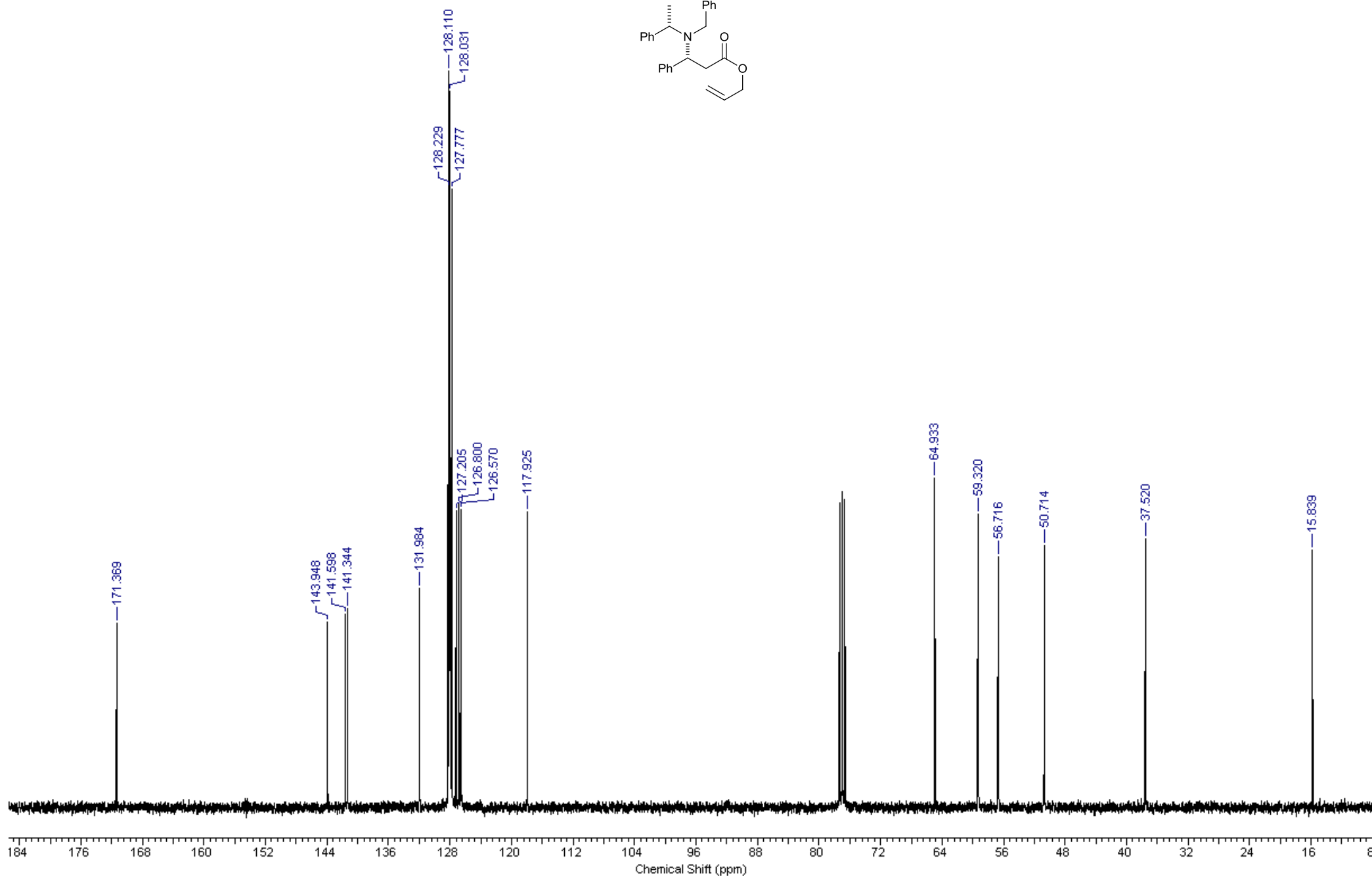
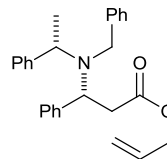
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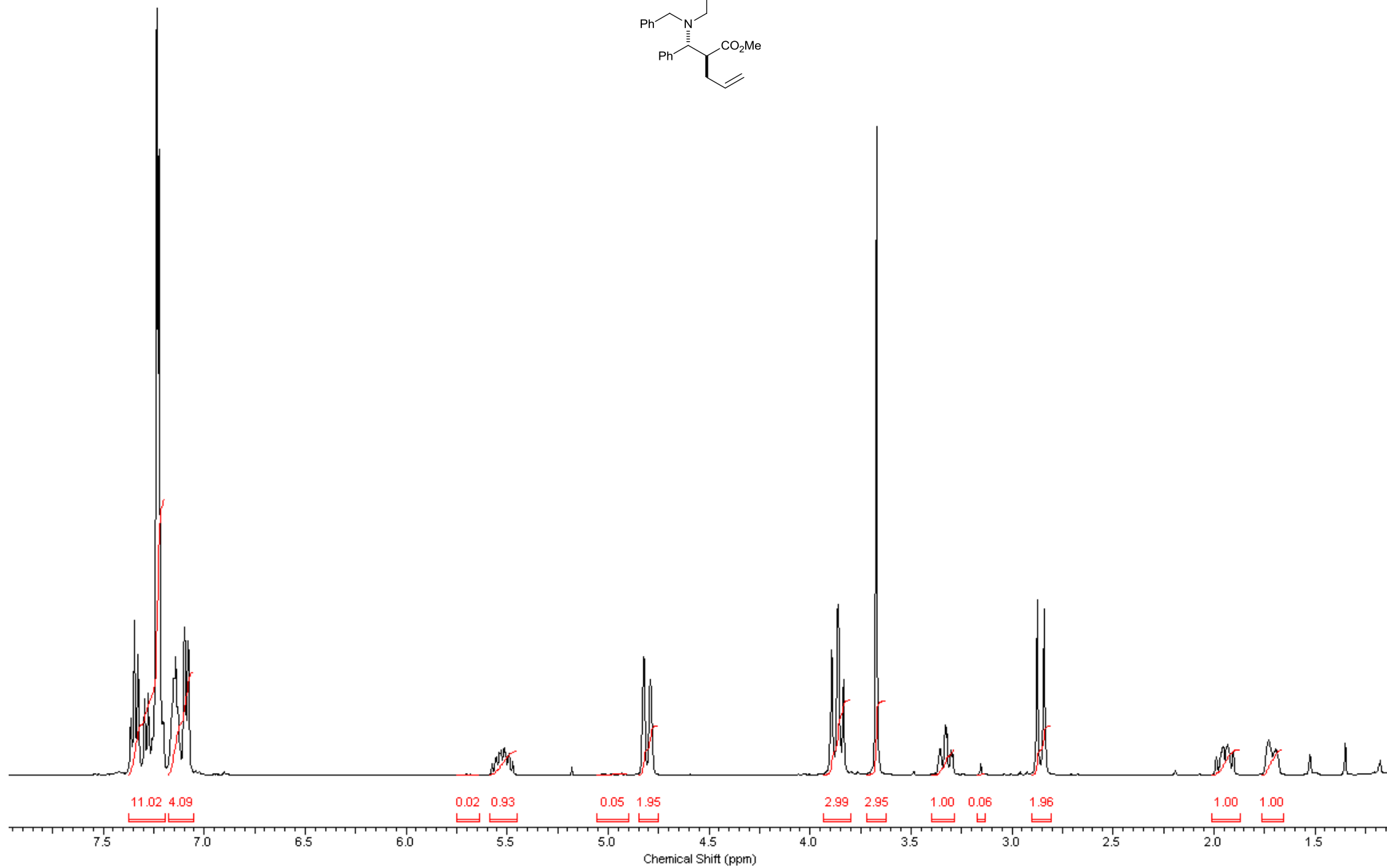
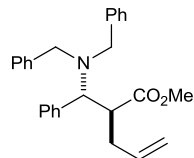
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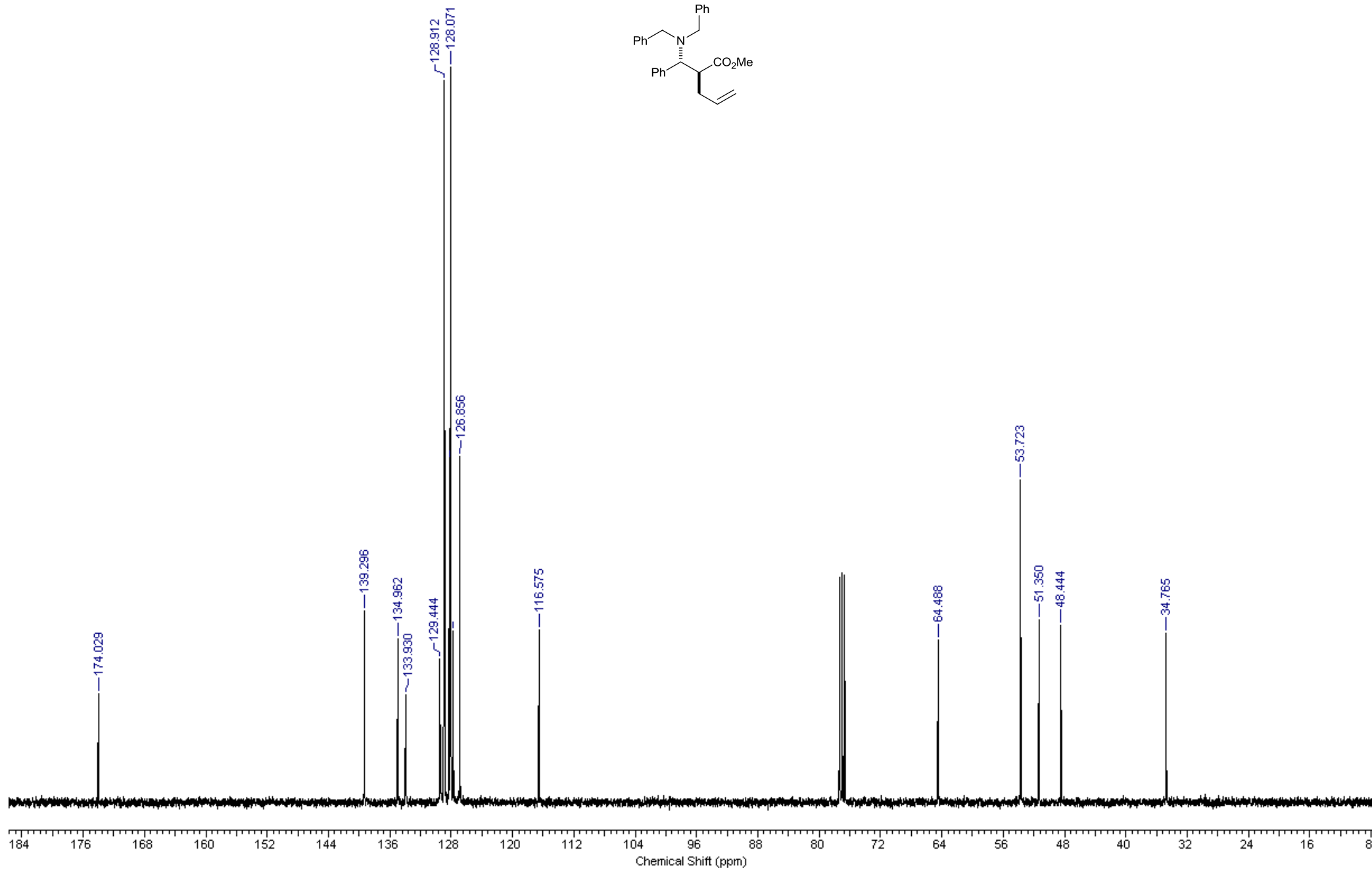
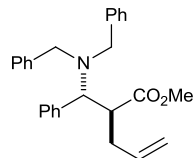
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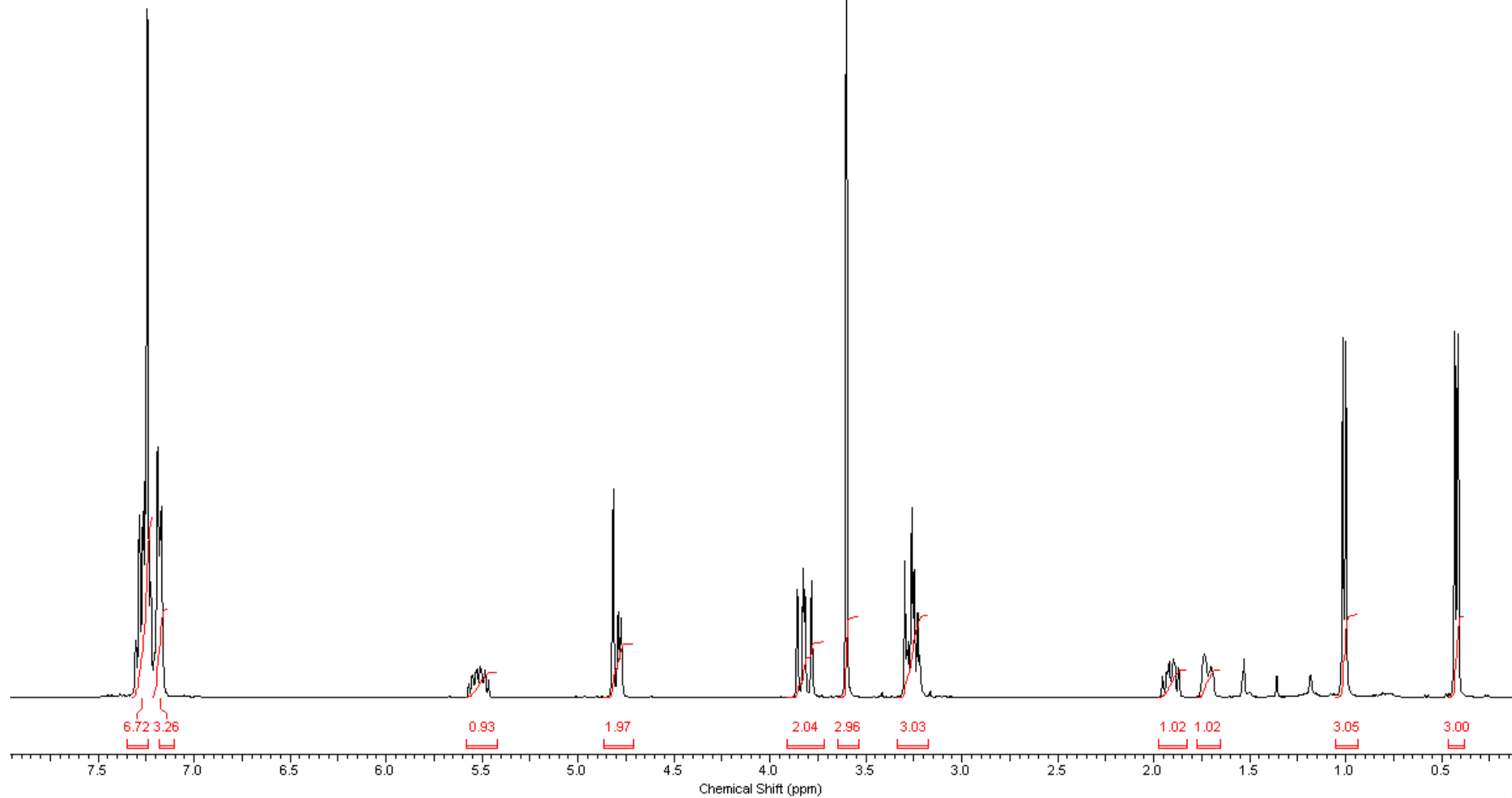
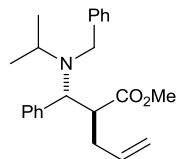
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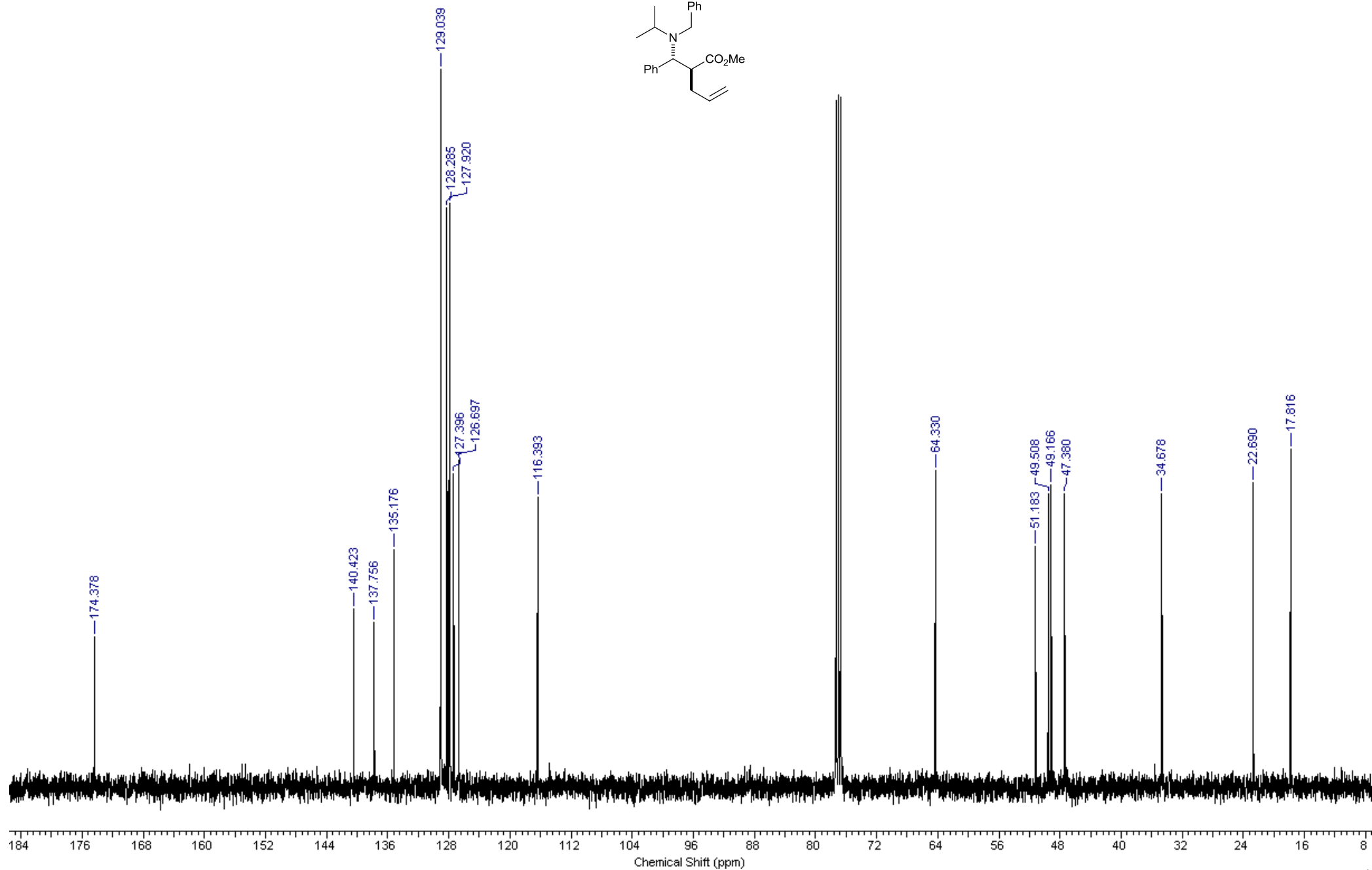
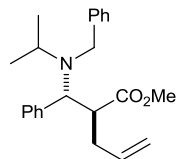
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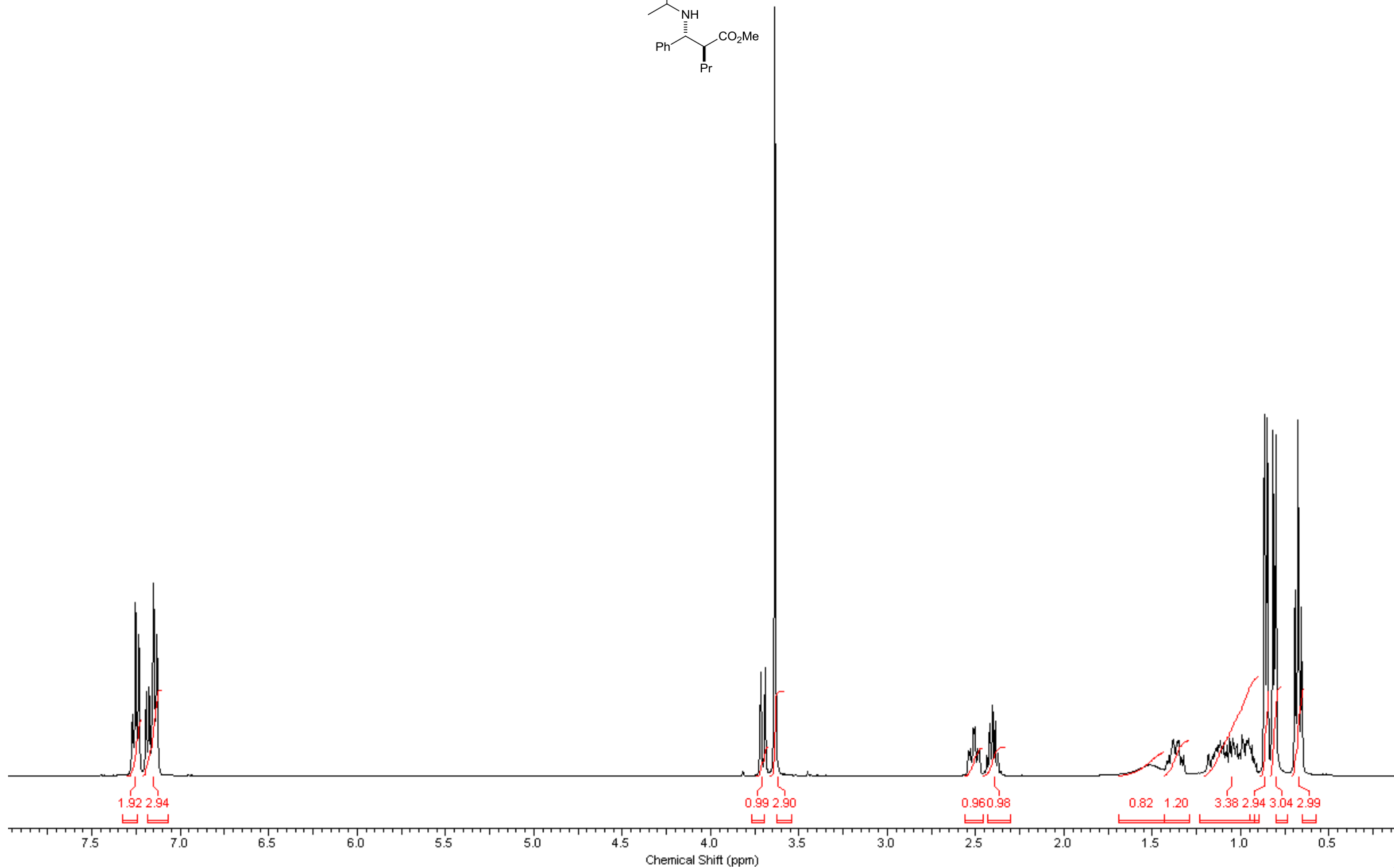
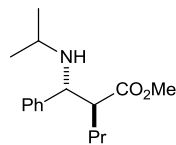
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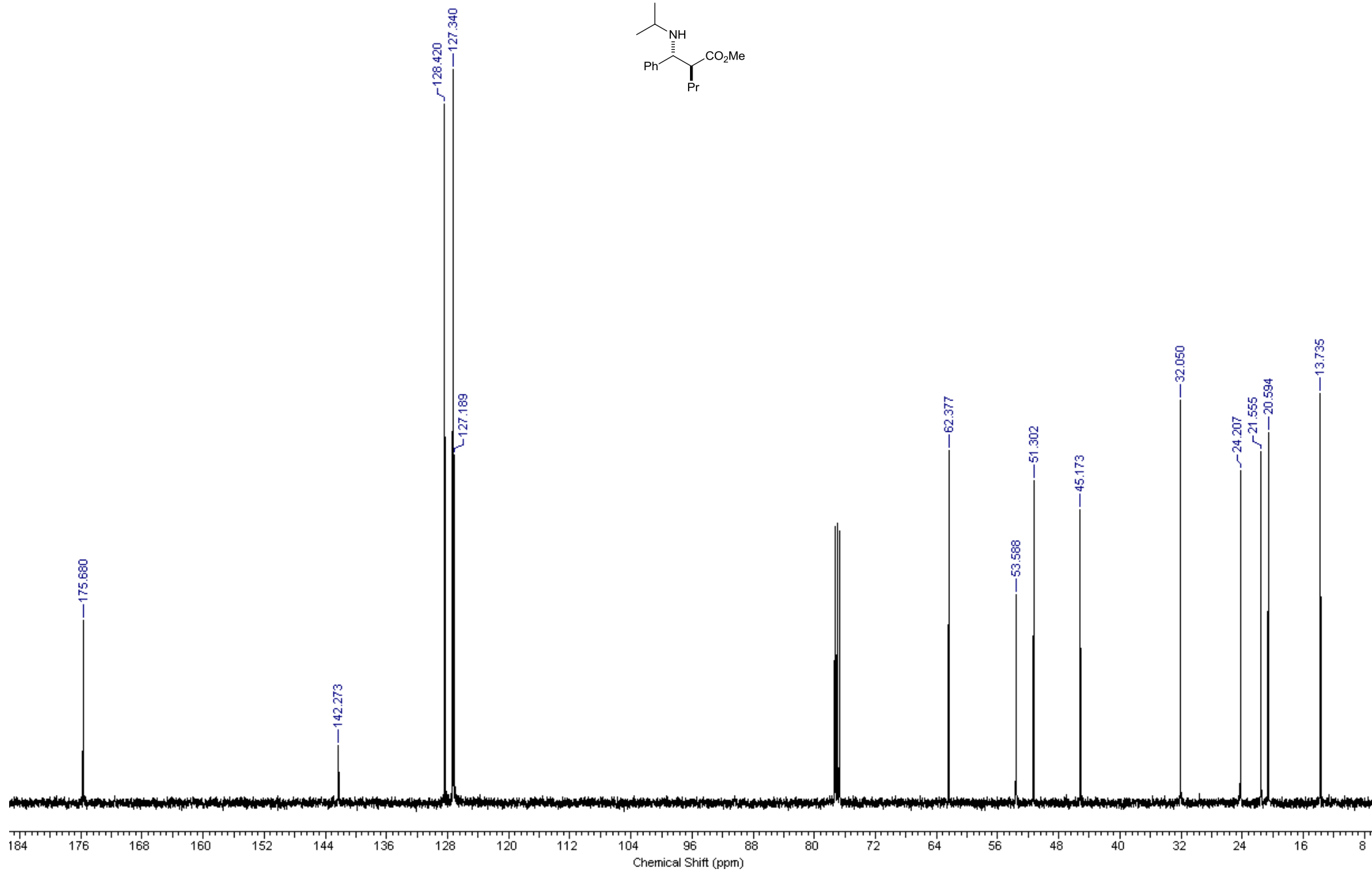
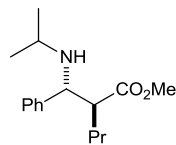
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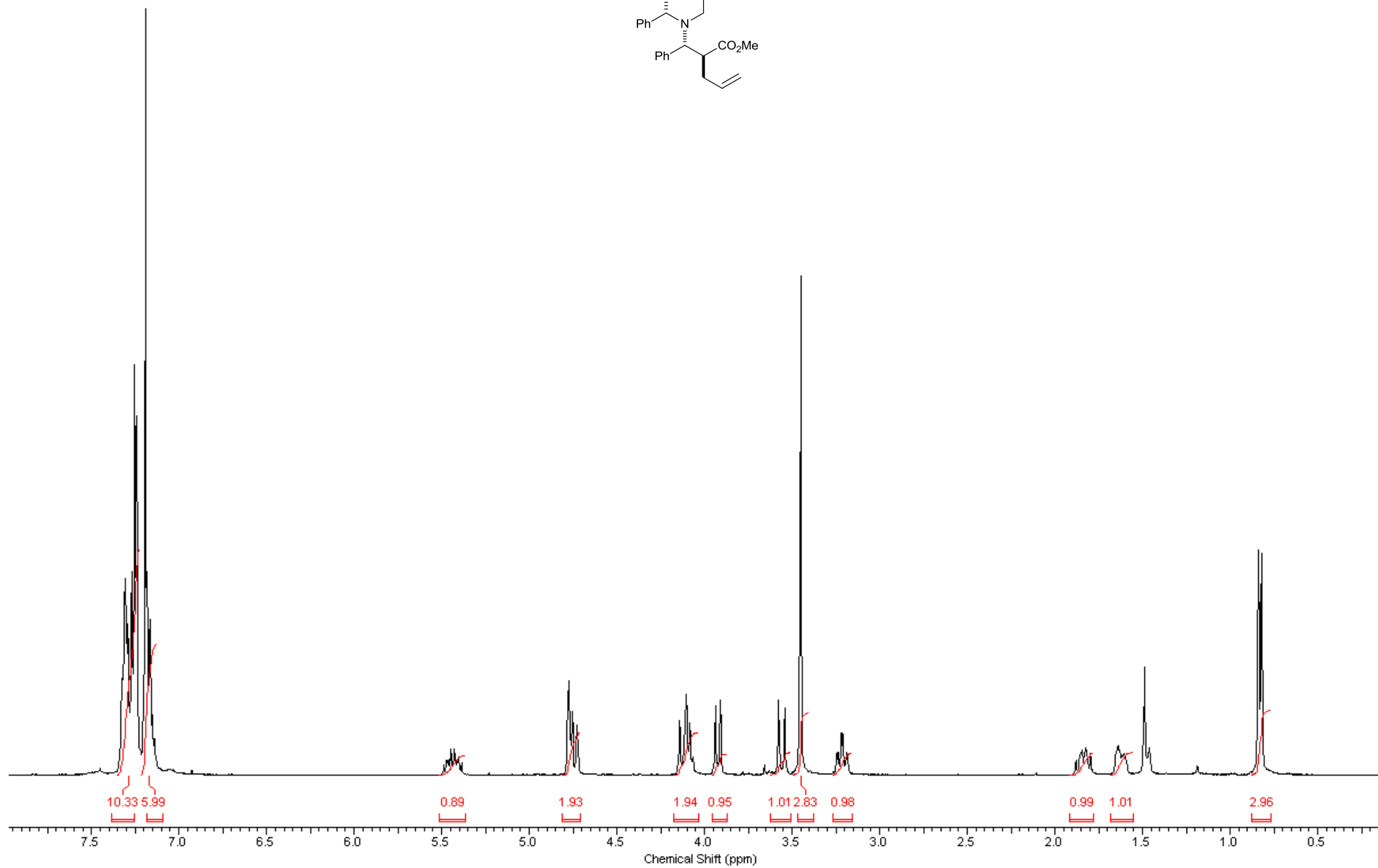
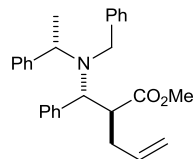
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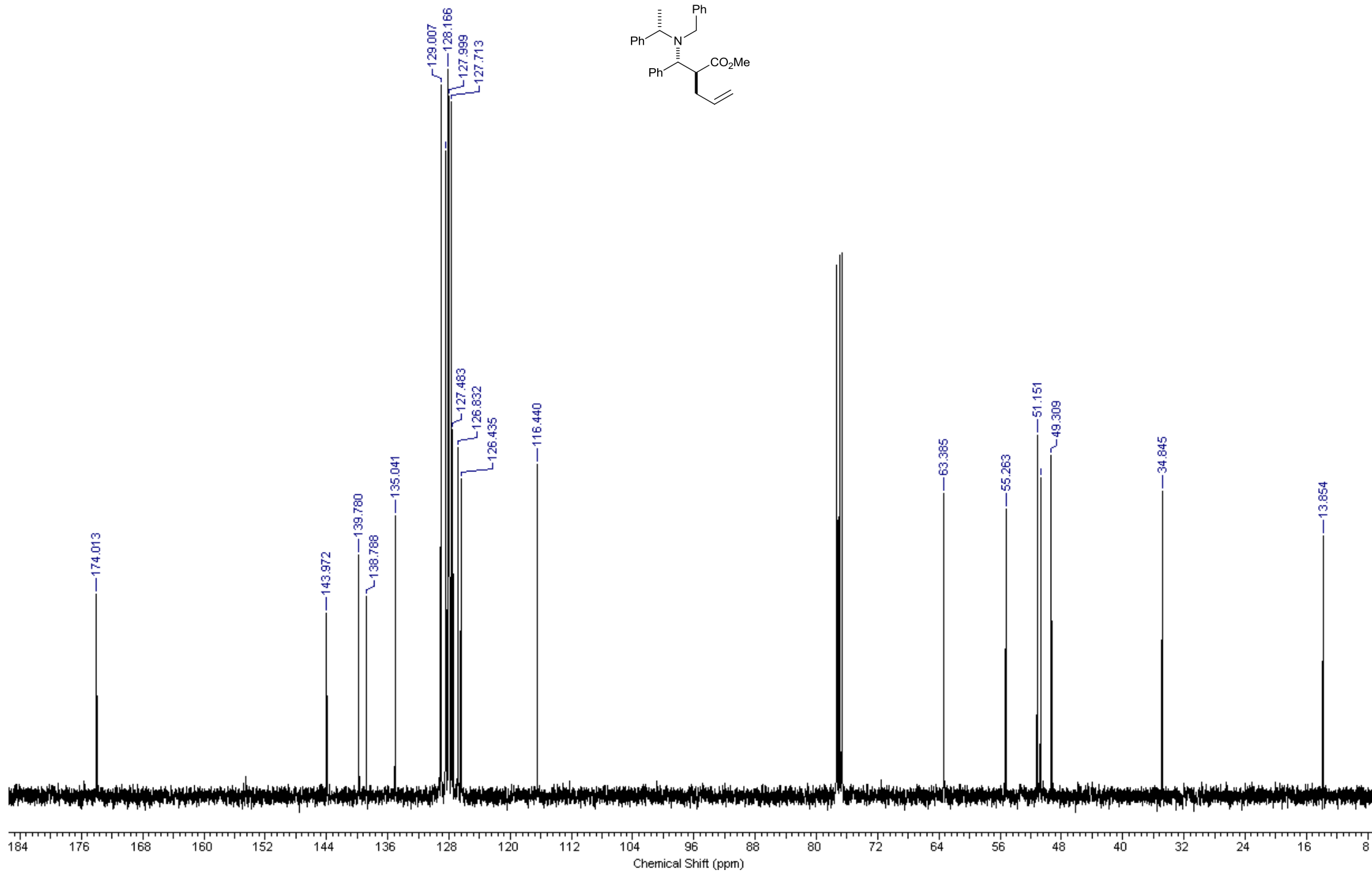
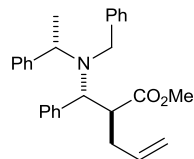
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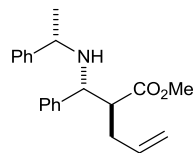
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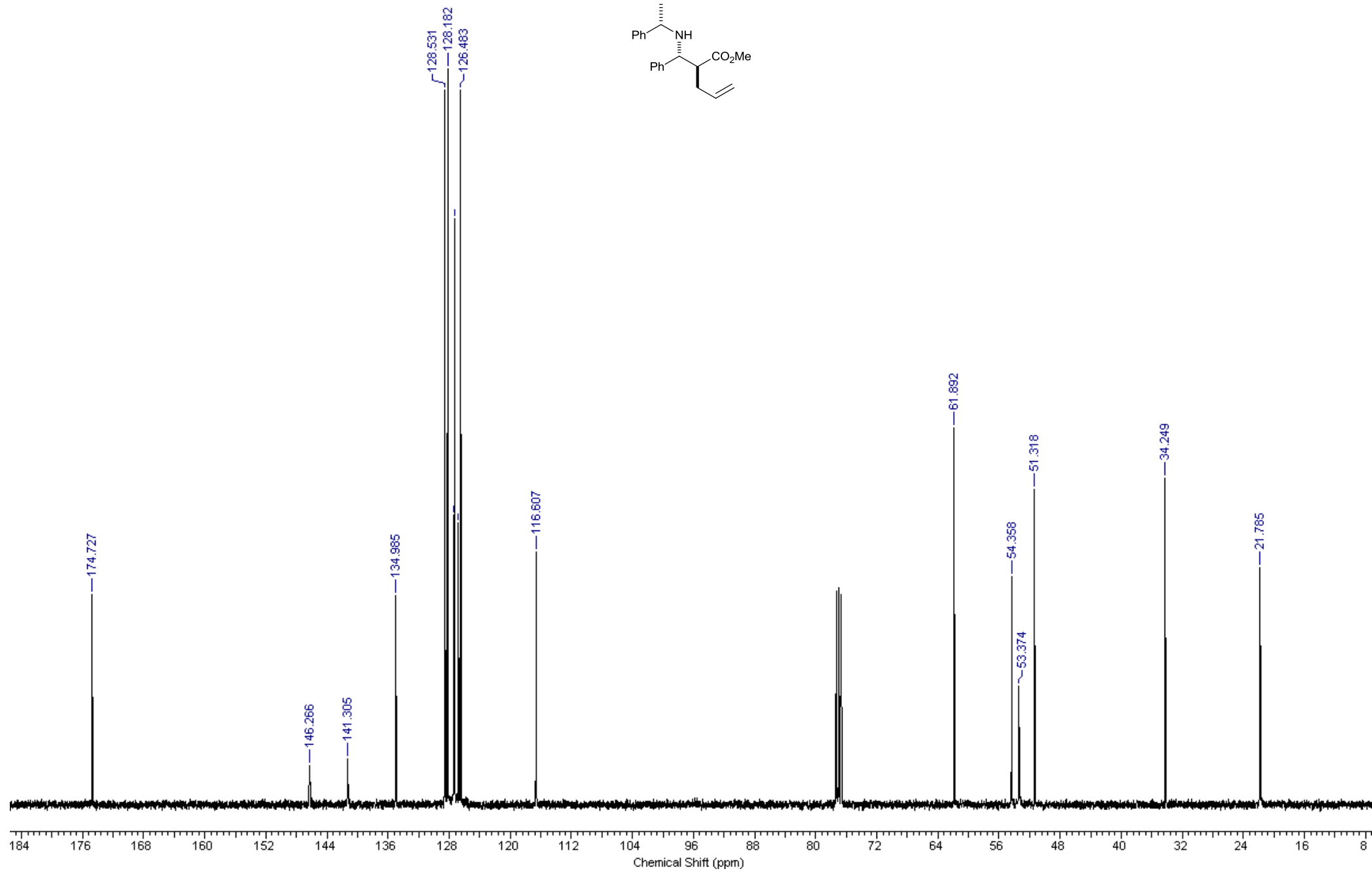
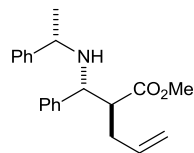
Methyl (2*S*,3*R*, α *S*)-2-(prop-2'-en-1'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate **20** (100 MHz ^{13}C , CDCl_3)



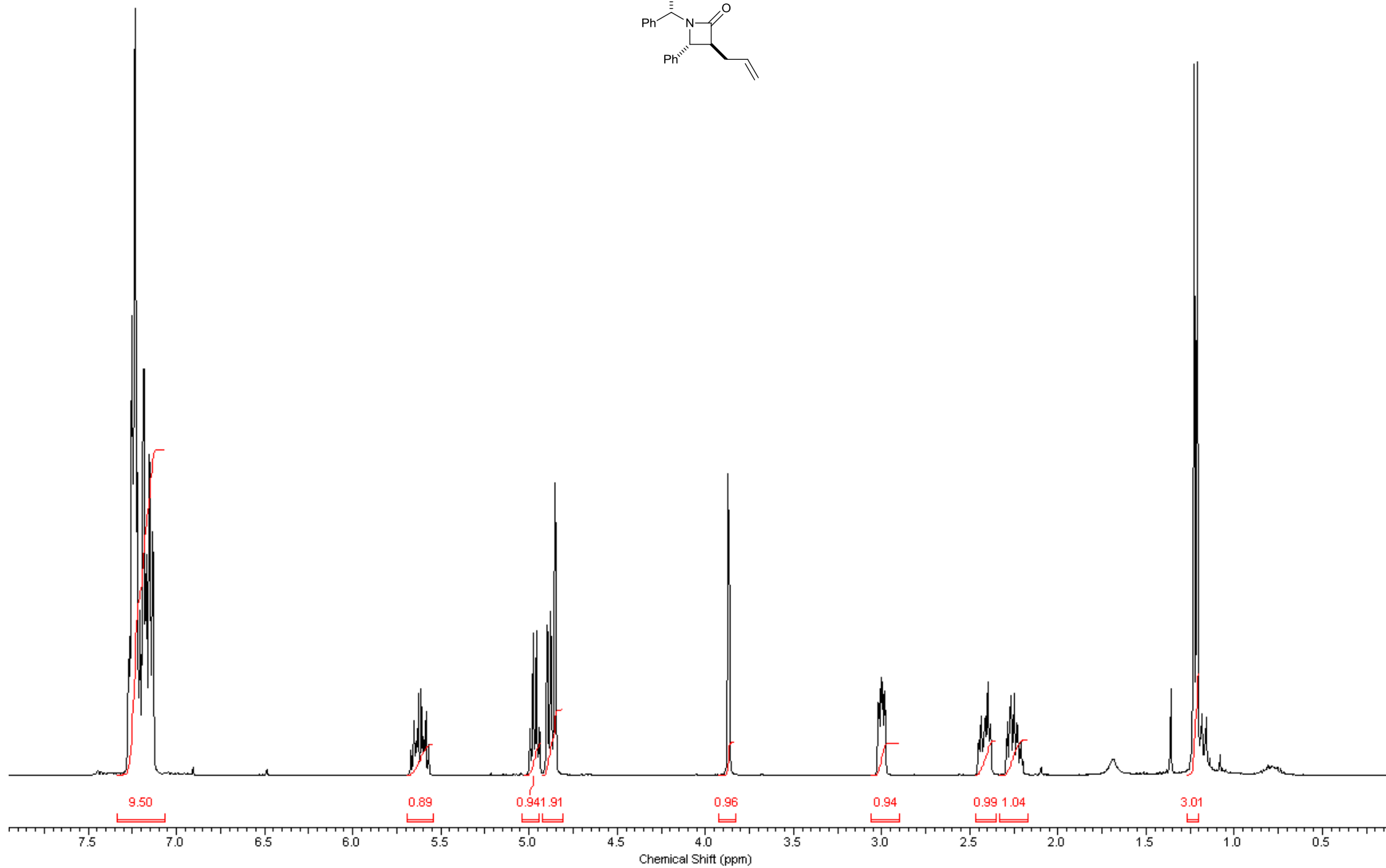
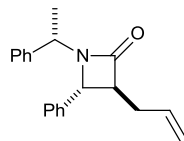
Methyl (2*S*,3*R*, α *S*)-2-(prop-2'-en-1'-yl)-3-[*N*-(α -methylbenzyl)amino]-3-phenylpropanoate **22** (400 MHz ^1H , CDCl_3)



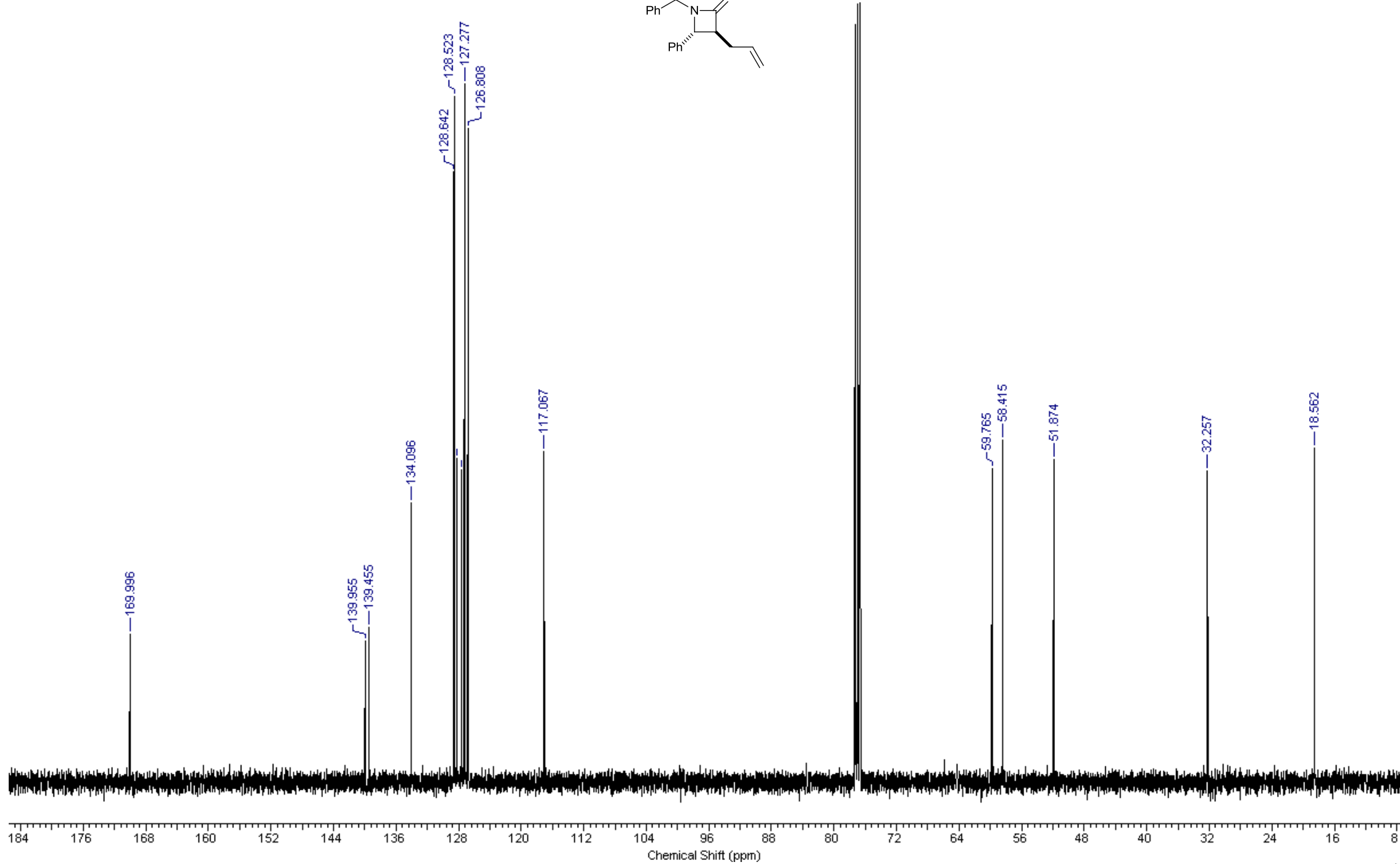
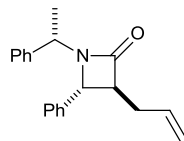
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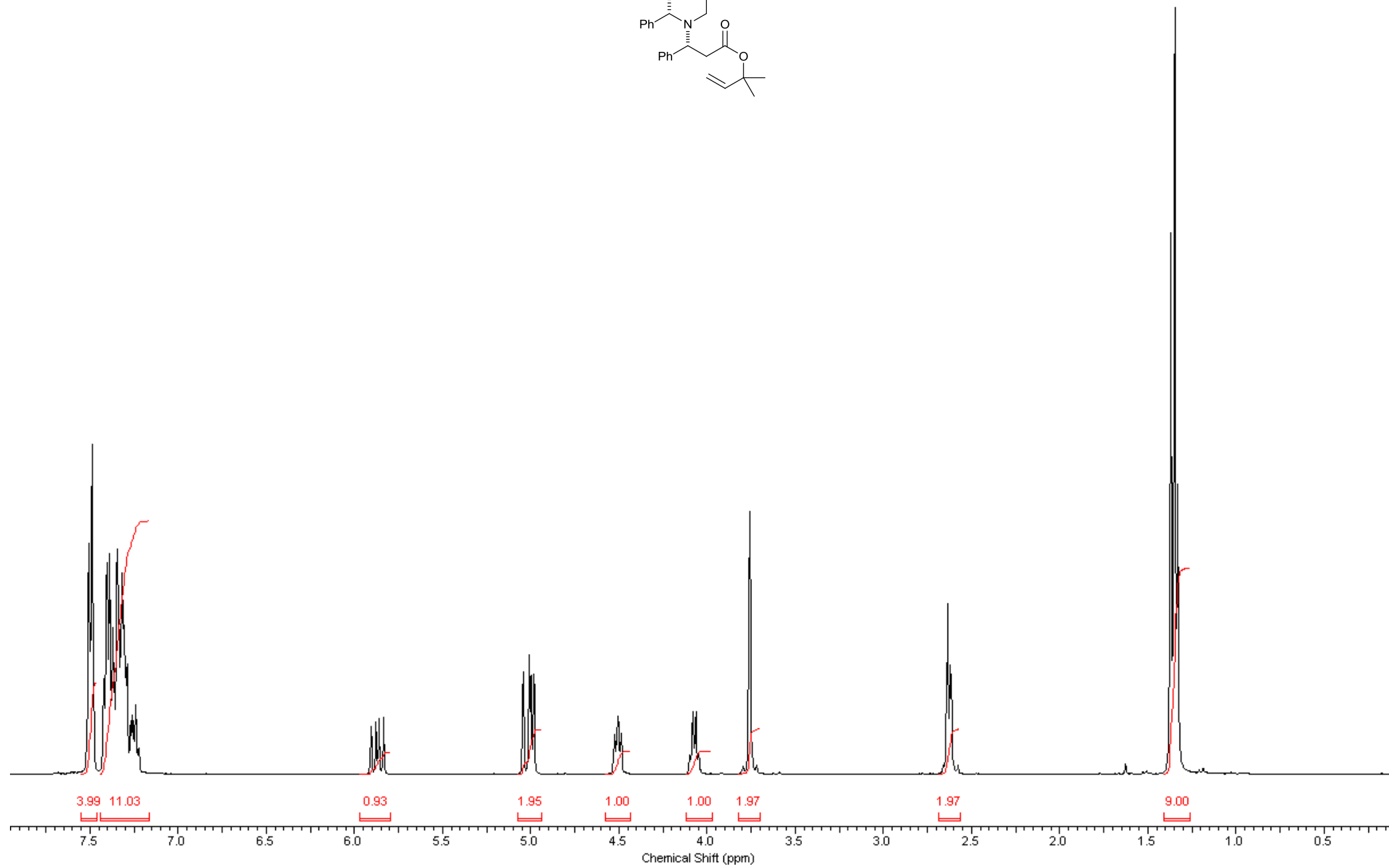
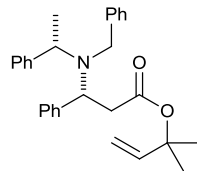
(3*S*,4*R*, α *S*)-*N*(1)-(α -Methylbenzyl)-3-(prop-2'-en-1'-yl)-4-phenylazetid-2-one 23 (400 MHz ^1H , CDCl_3)



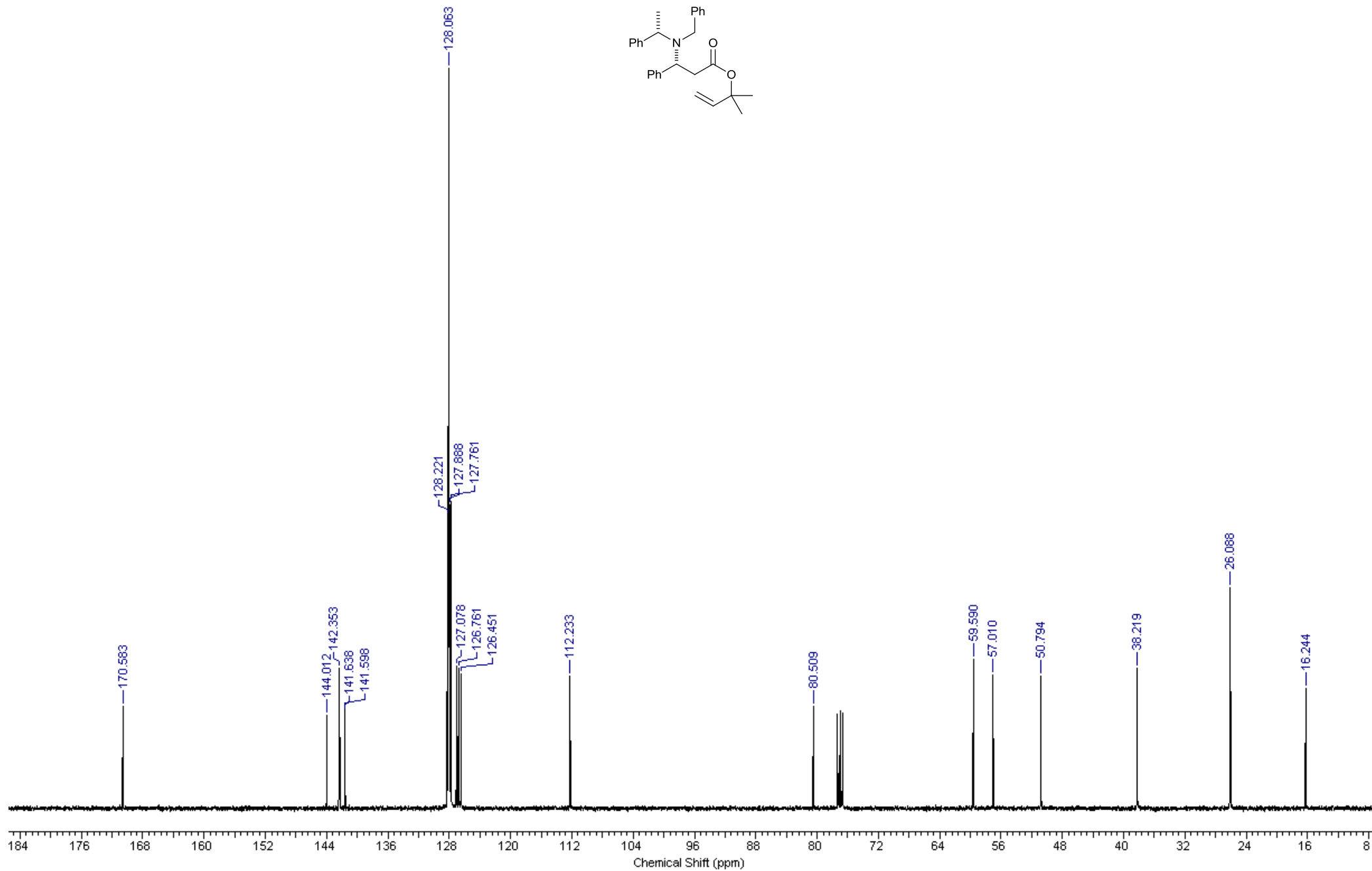
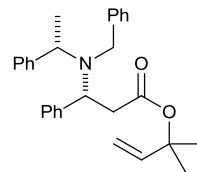
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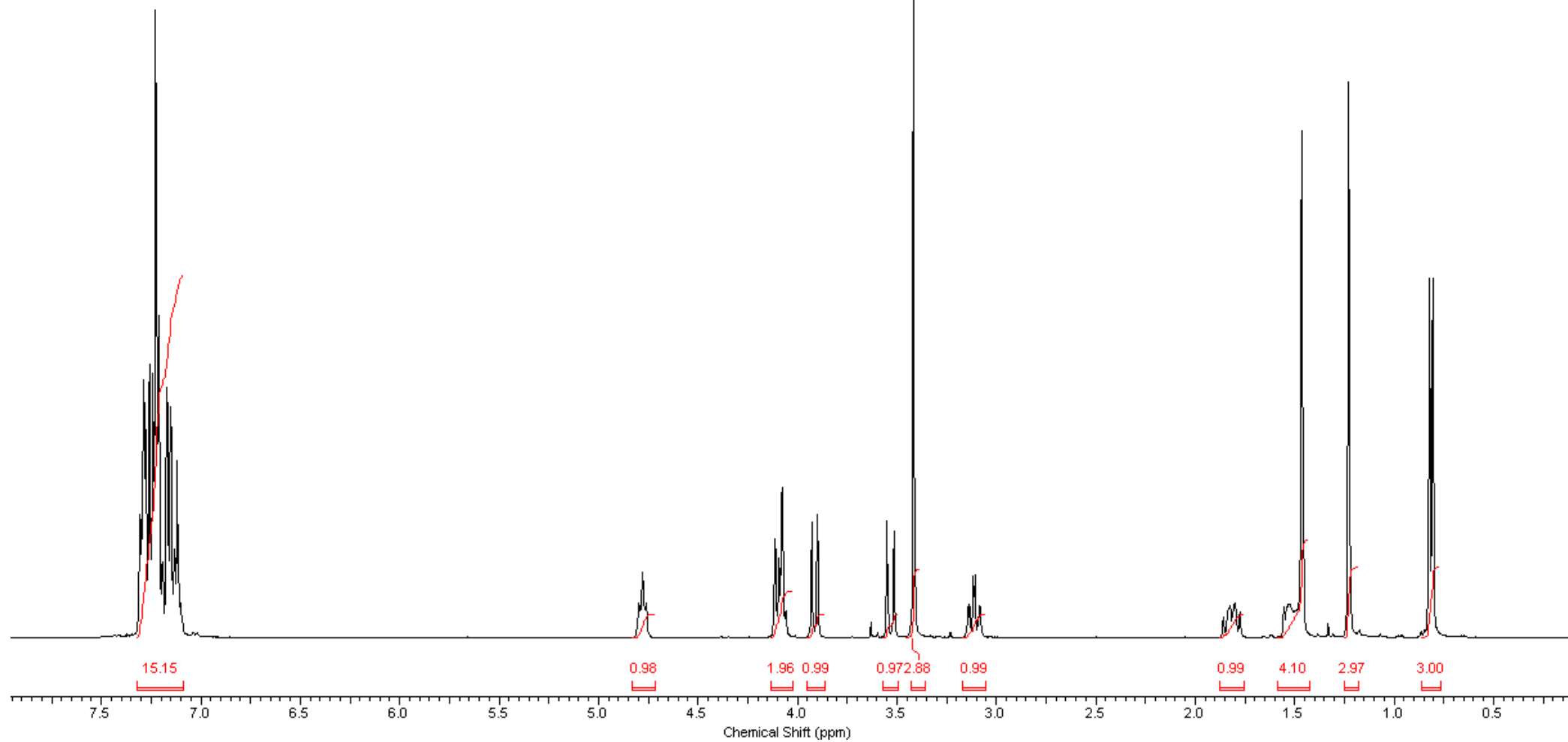
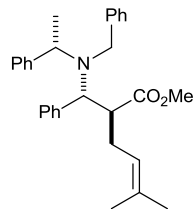
2'-Methylbut-3'-en-2'-yl (3*R*, α *S*)-3-[*N*-benzyl-*N*-(α -methyl-benzyl)amino]-3-phenylpropanoate 25 (400 MHz ^1H , CDCl_3)



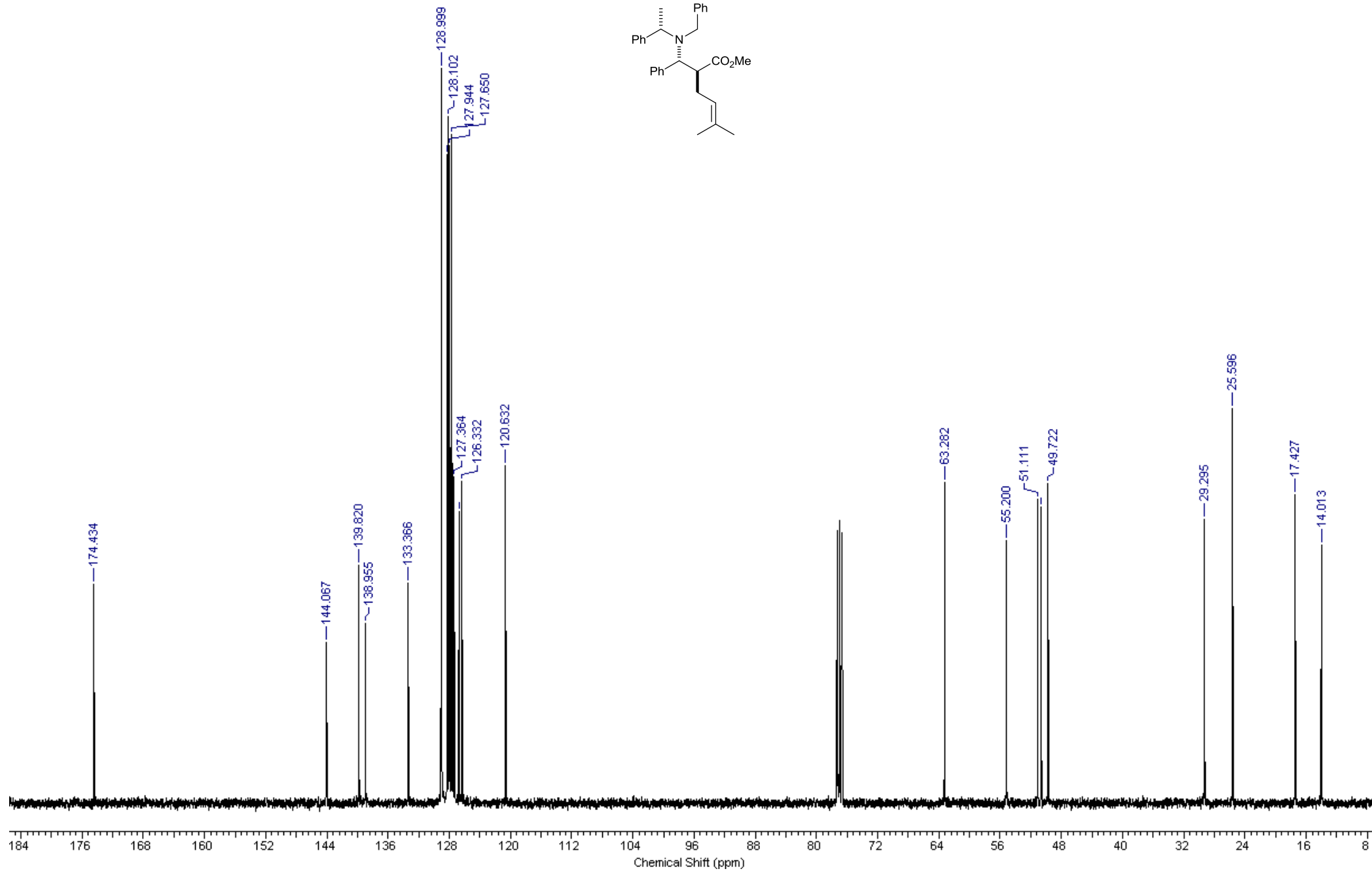
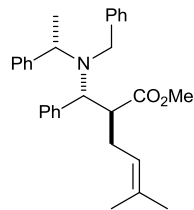
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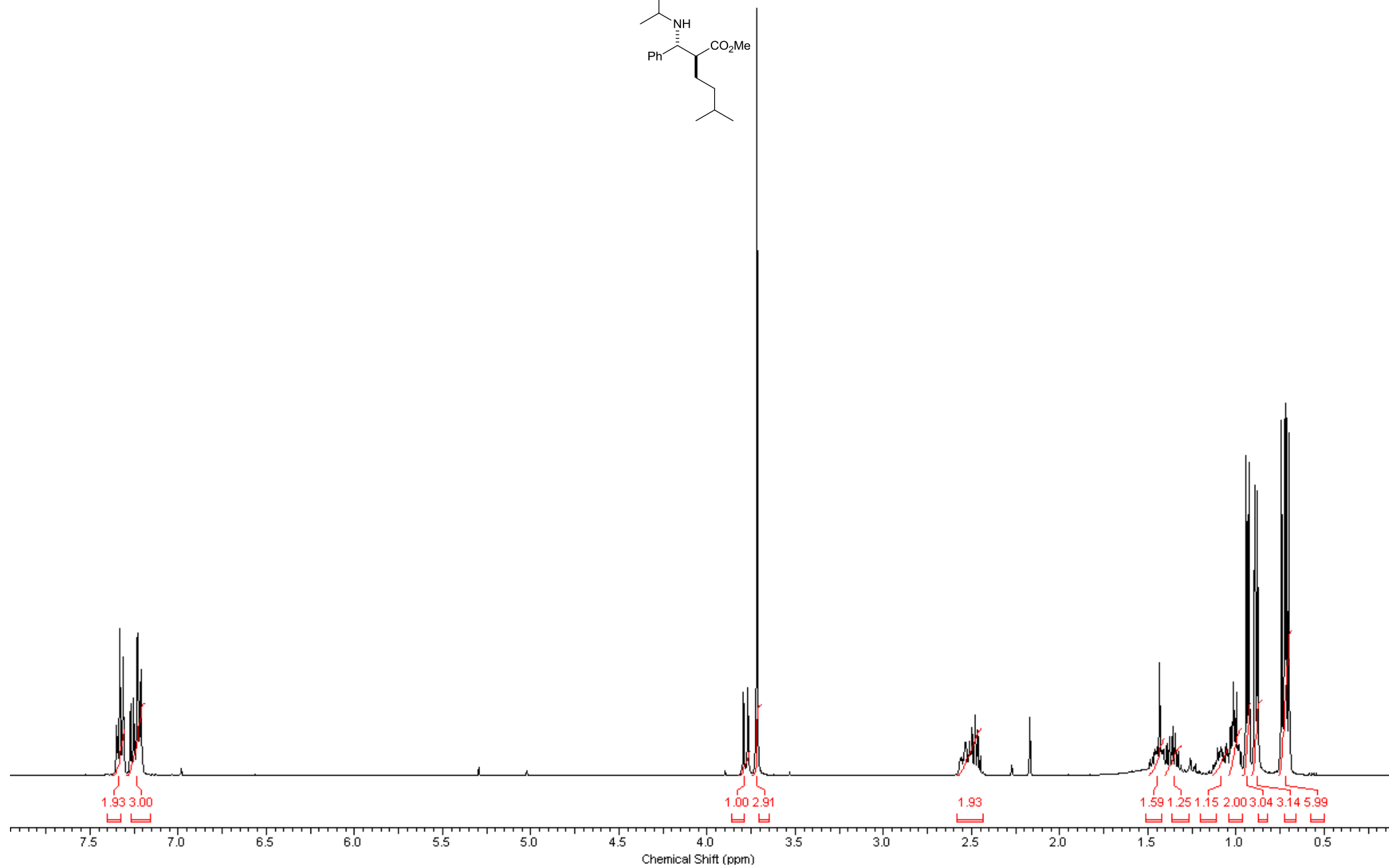
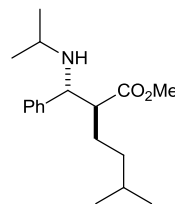
Methyl (2*S*,3*R*, α *S*)-2-(3'-methylbut-2'-en-1'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate 27 (400 MHz ^1H , CDCl_3)



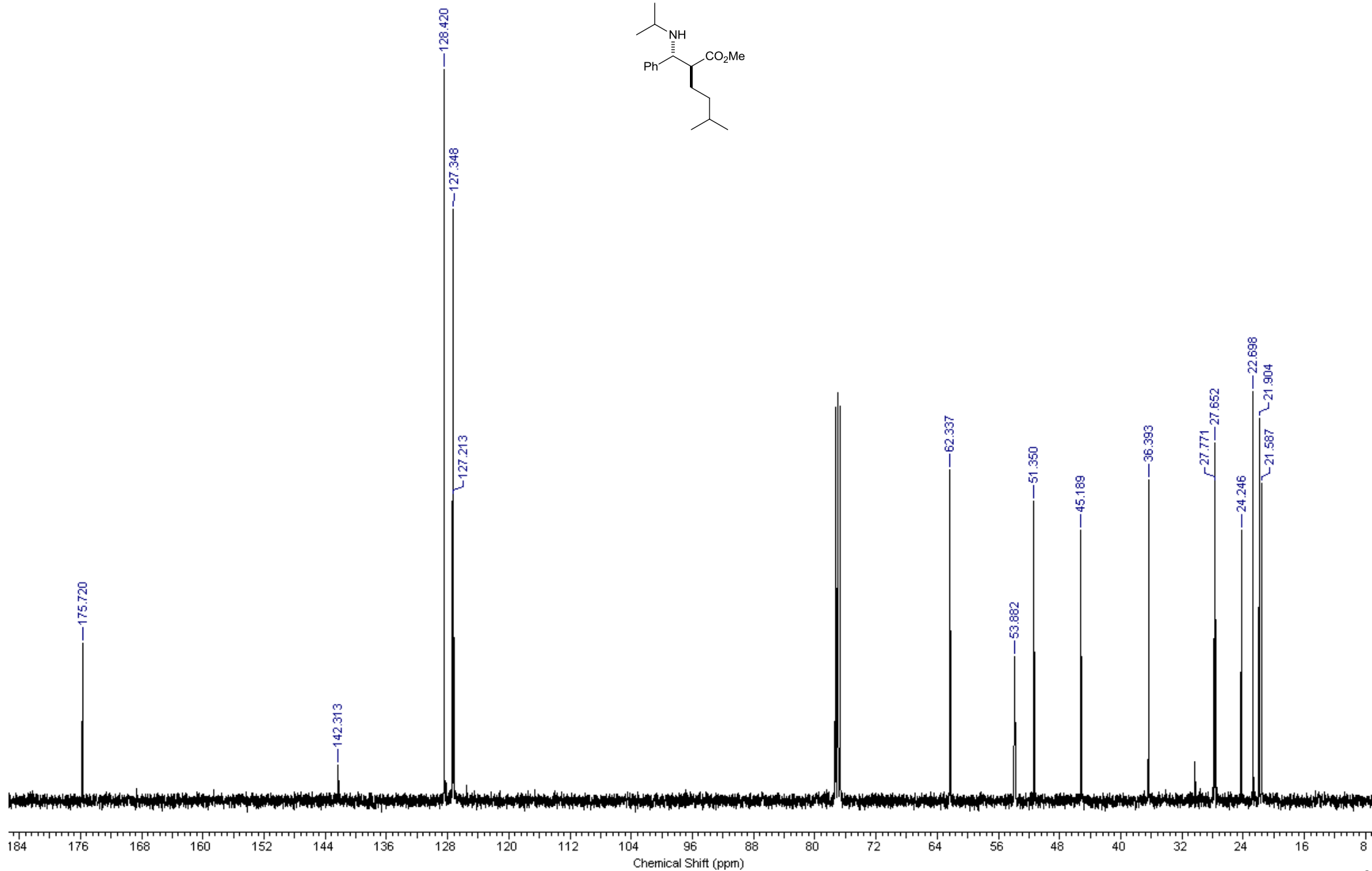
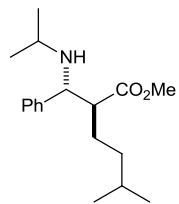
Methyl (2*S*,3*R*, α *S*)-2-(3'-methylbut-2'-en-1'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate **27** (100 MHz ^{13}C , CDCl_3)



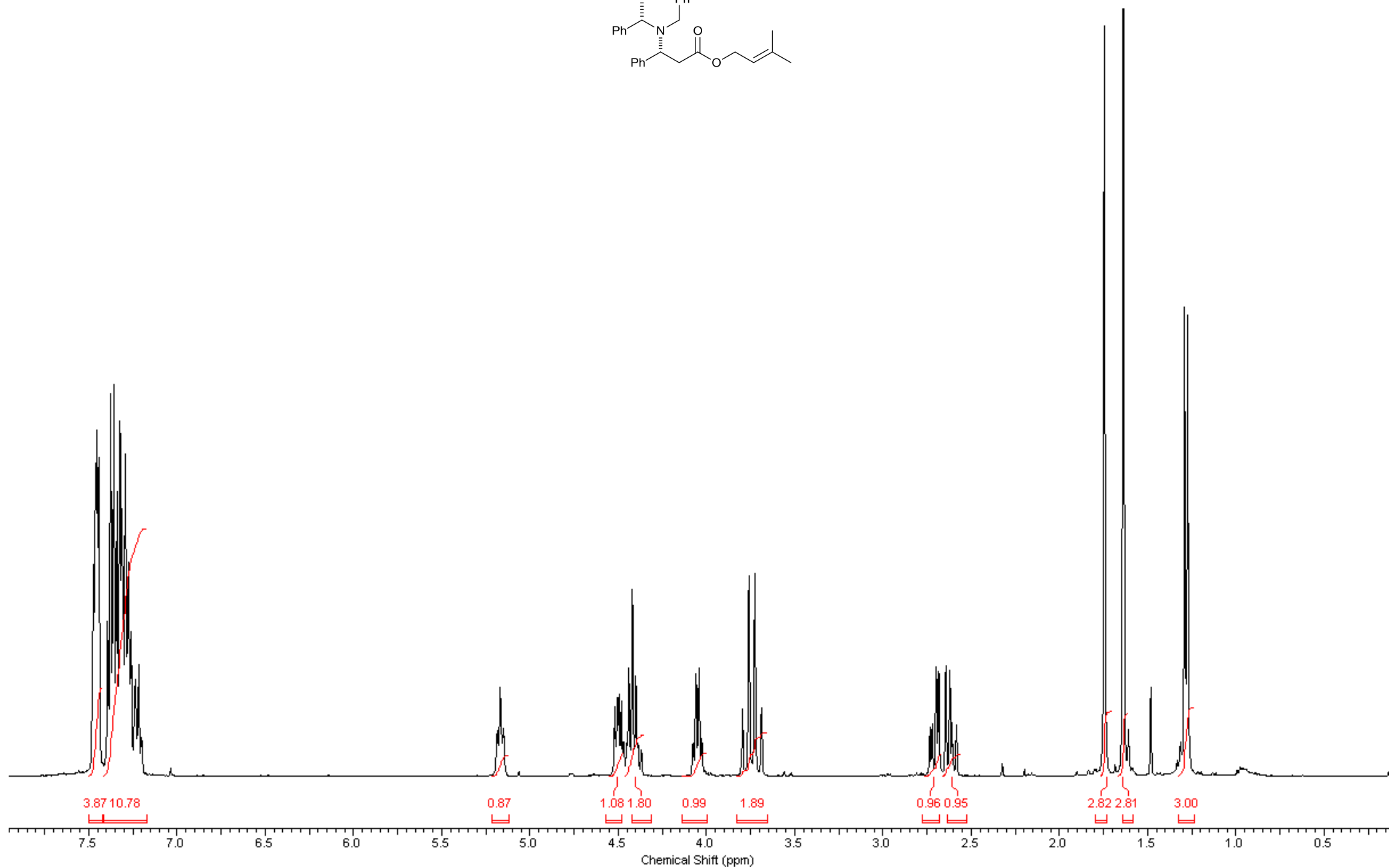
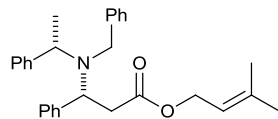
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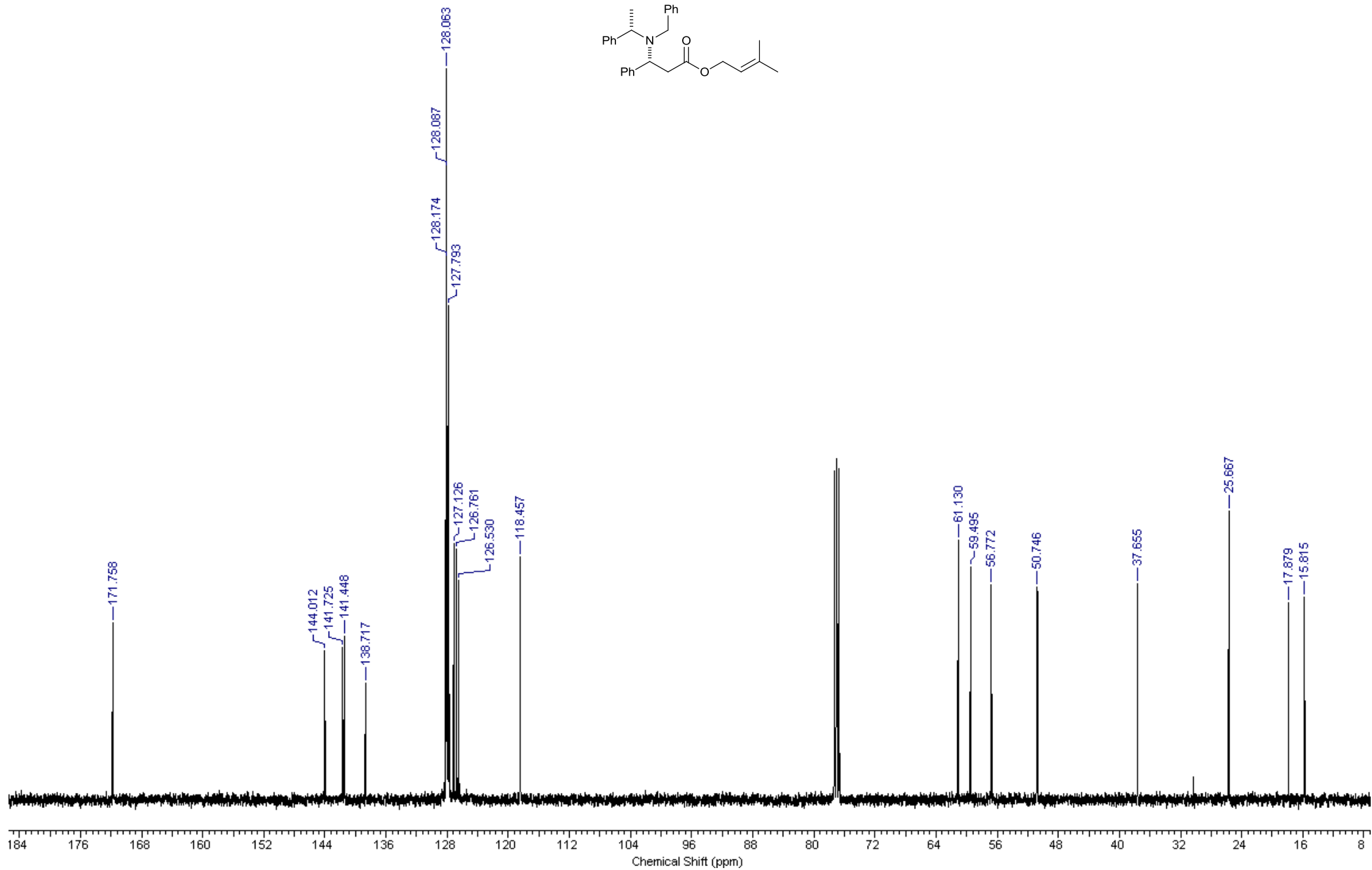
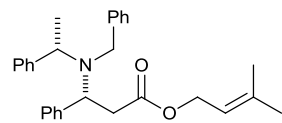
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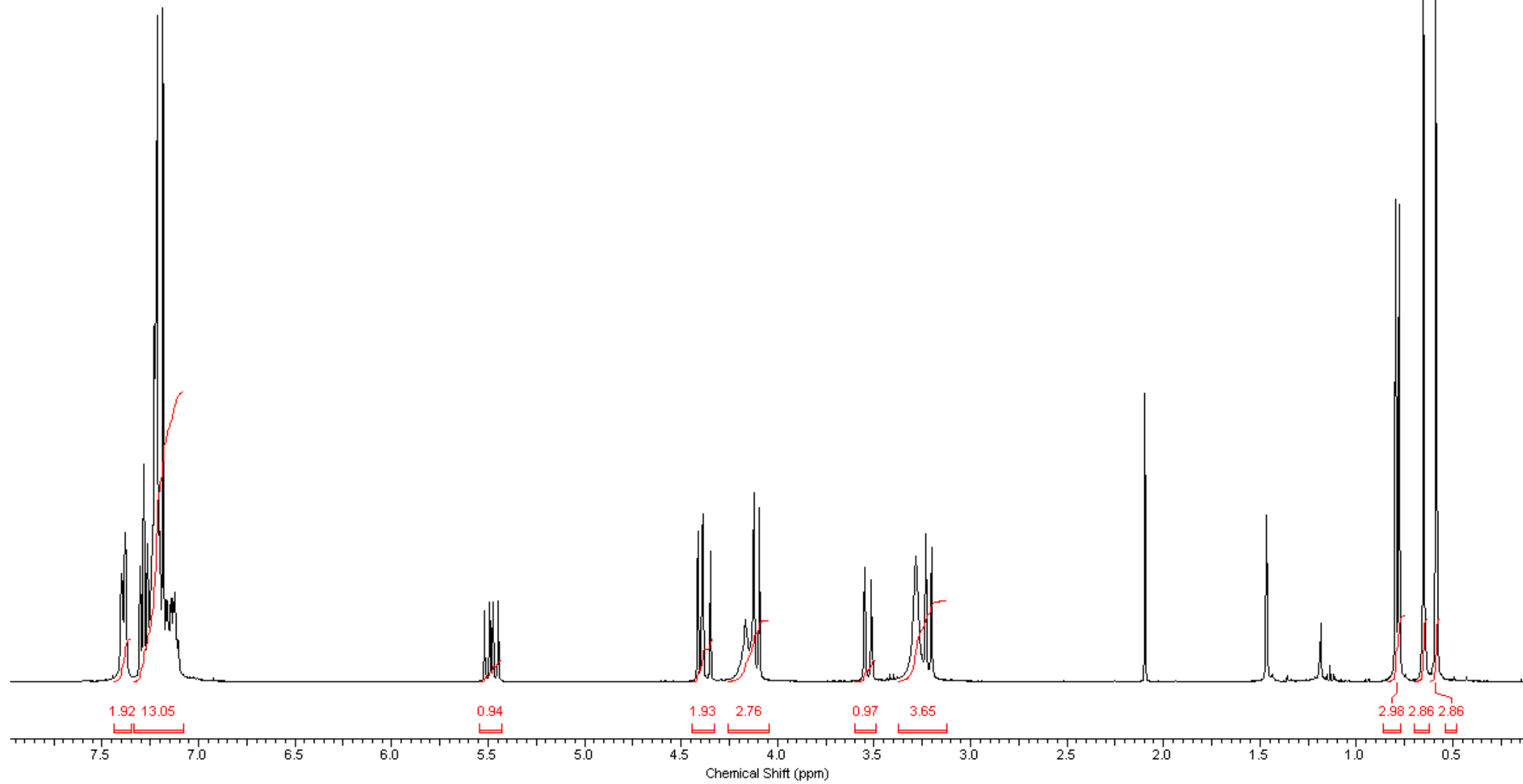
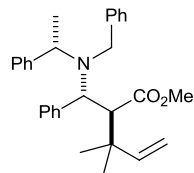
3'-Methylbut-2'-en-1'-yl (3*R*, α *S*)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate 30 (400 MHz ^1H , CDCl_3)



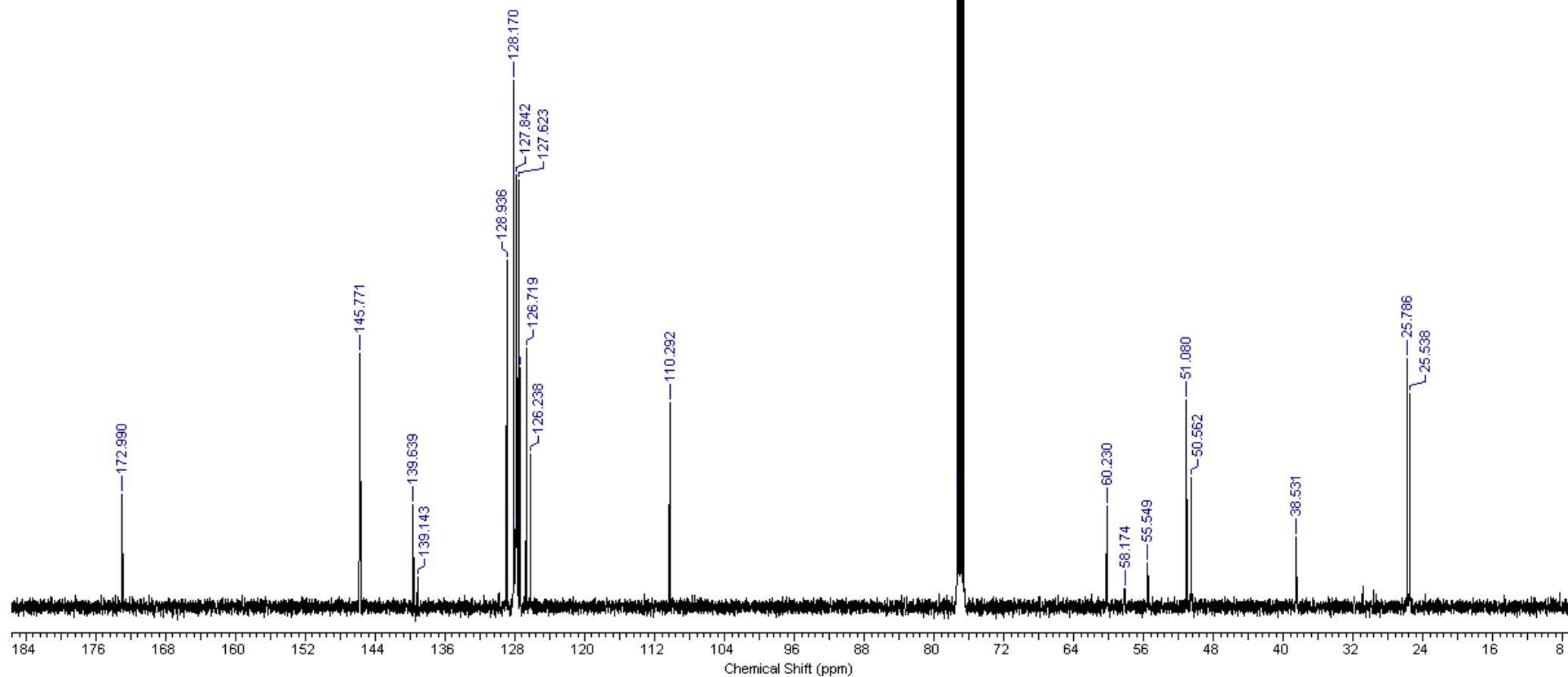
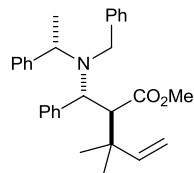
3'-Methylbut-2'-en-1'-yl (3*R*, α *S*)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate 30 (100 MHz ^{13}C , CDCl_3)



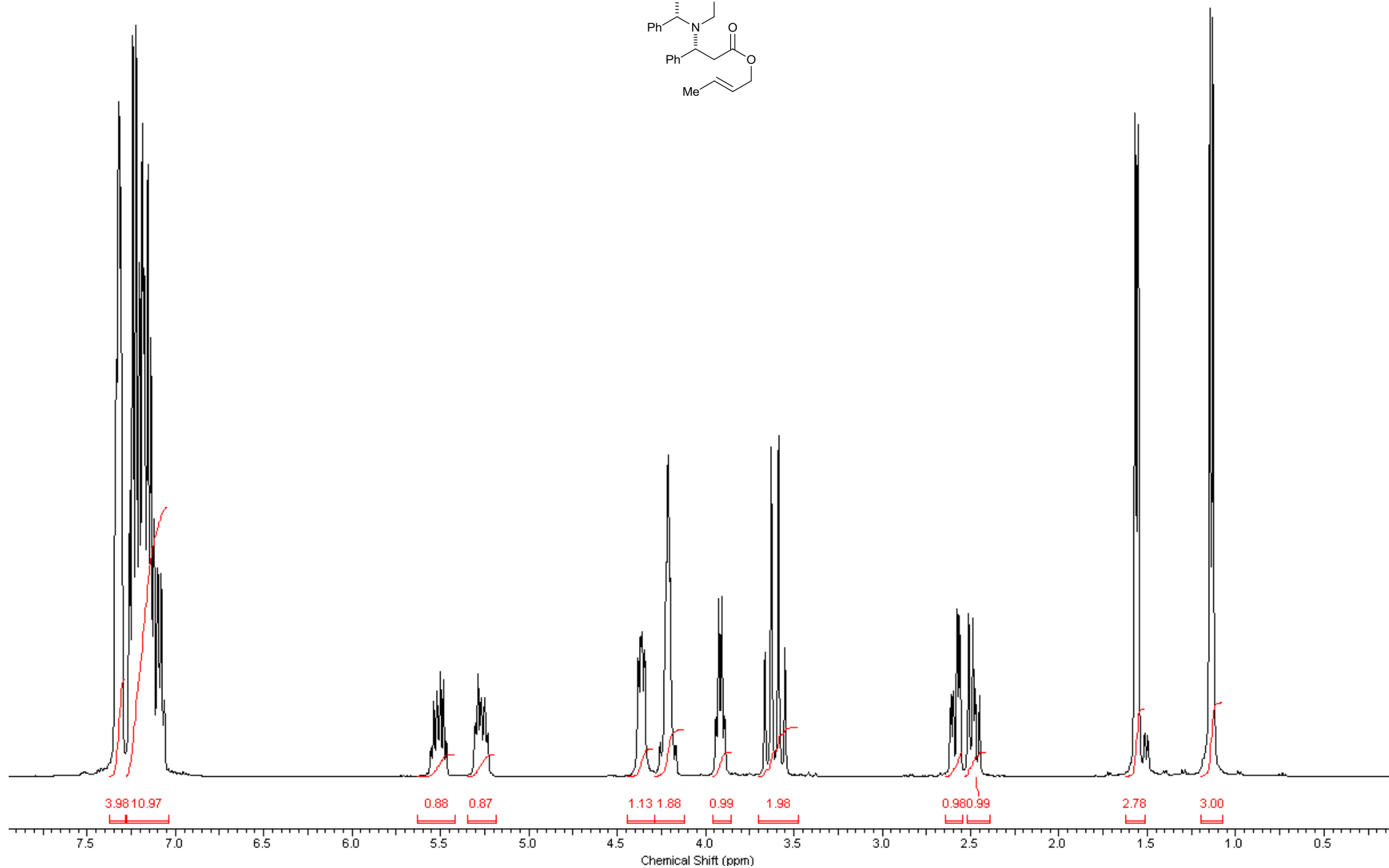
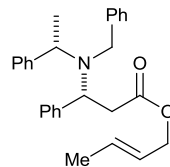
Methyl (2*S*,3*R*, α *S*)-2-(2'-methylbut-3'-en-2'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate **32** (400 MHz ^1H , CDCl_3)



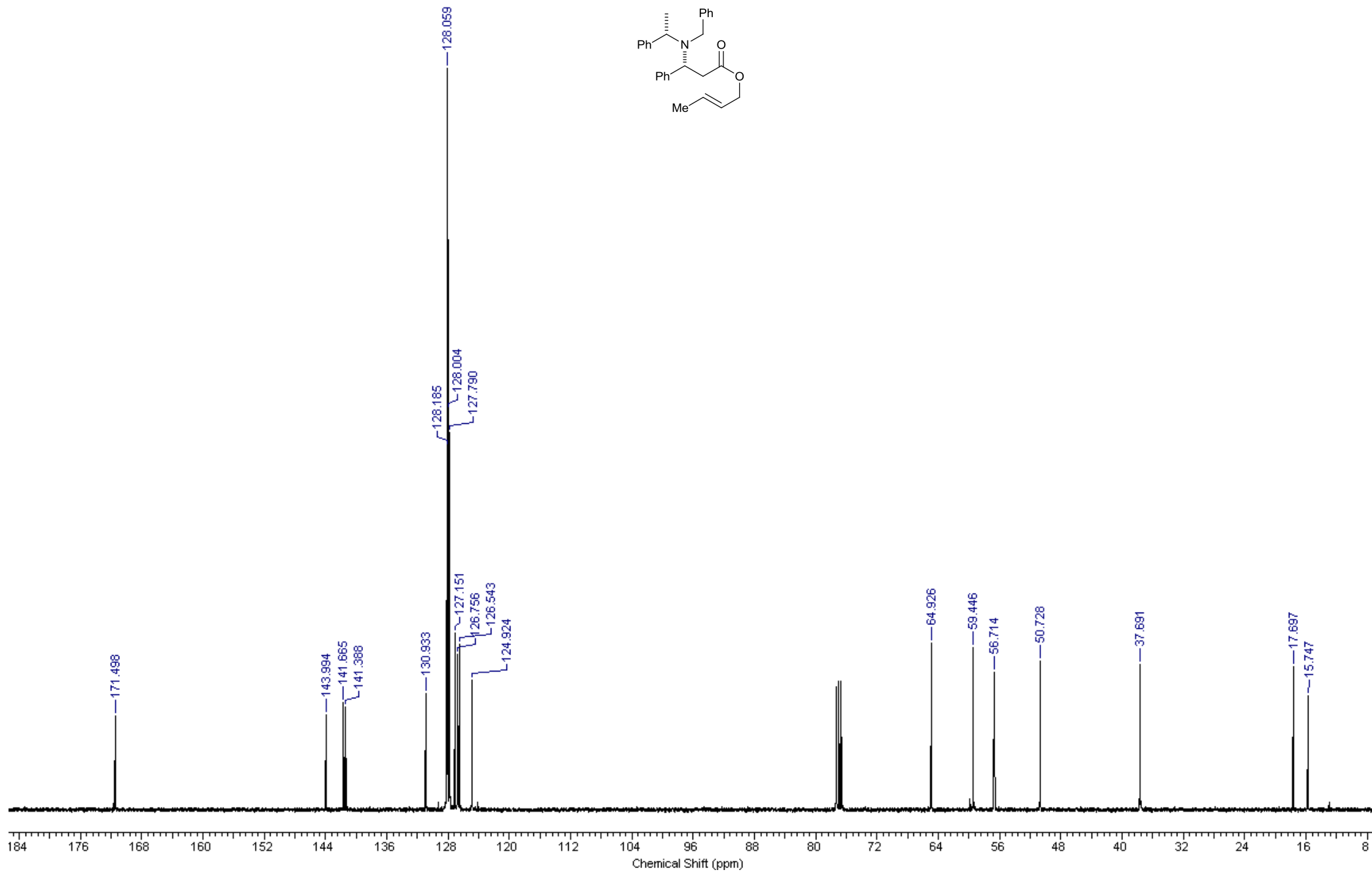
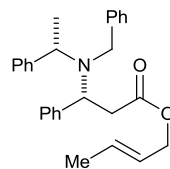
Methyl (2*S*,3*R*, α *S*)-2-(2'-methylbut-3'-en-2'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate **32** (100 MHz ^{13}C , CDCl_3)



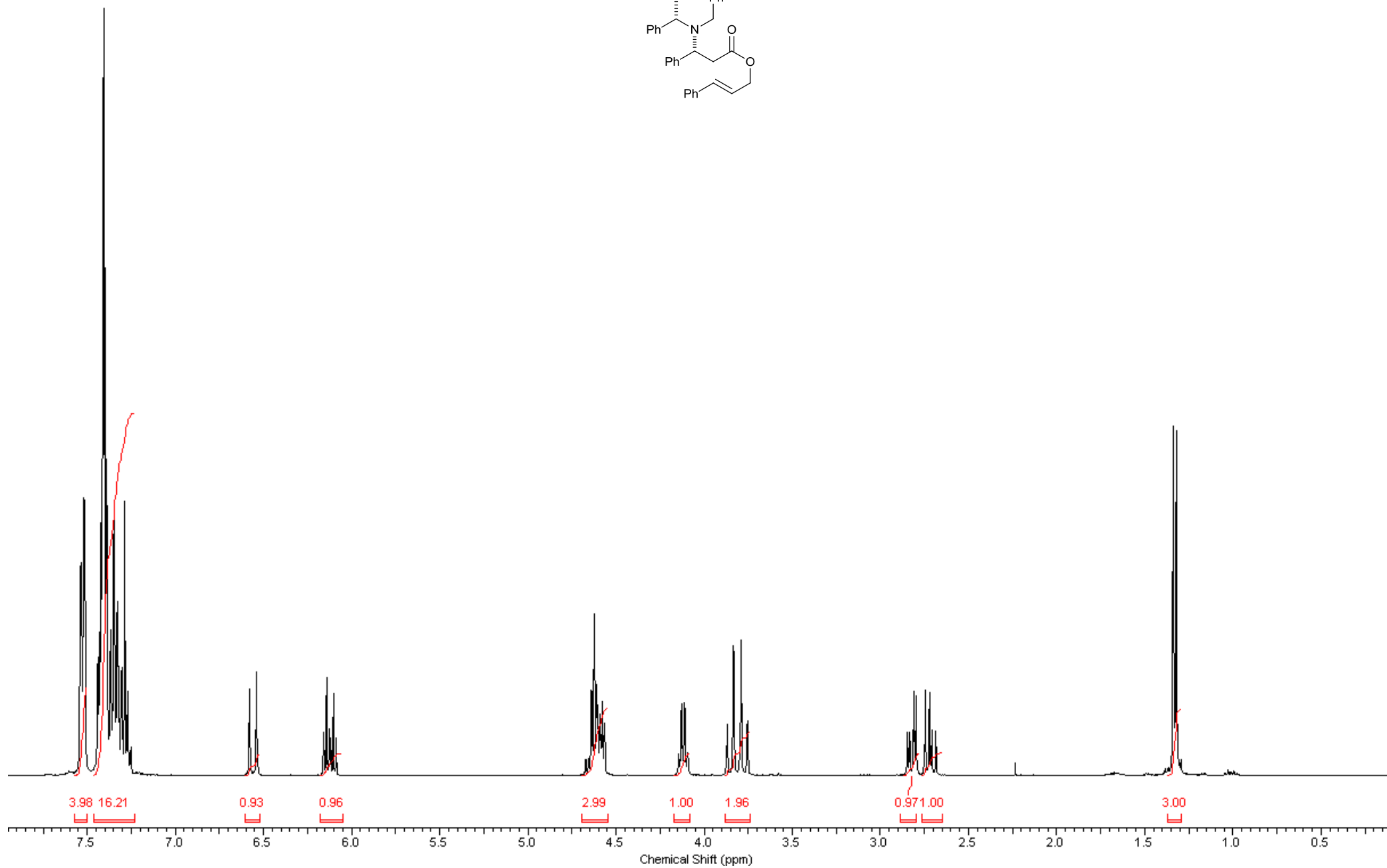
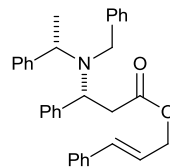
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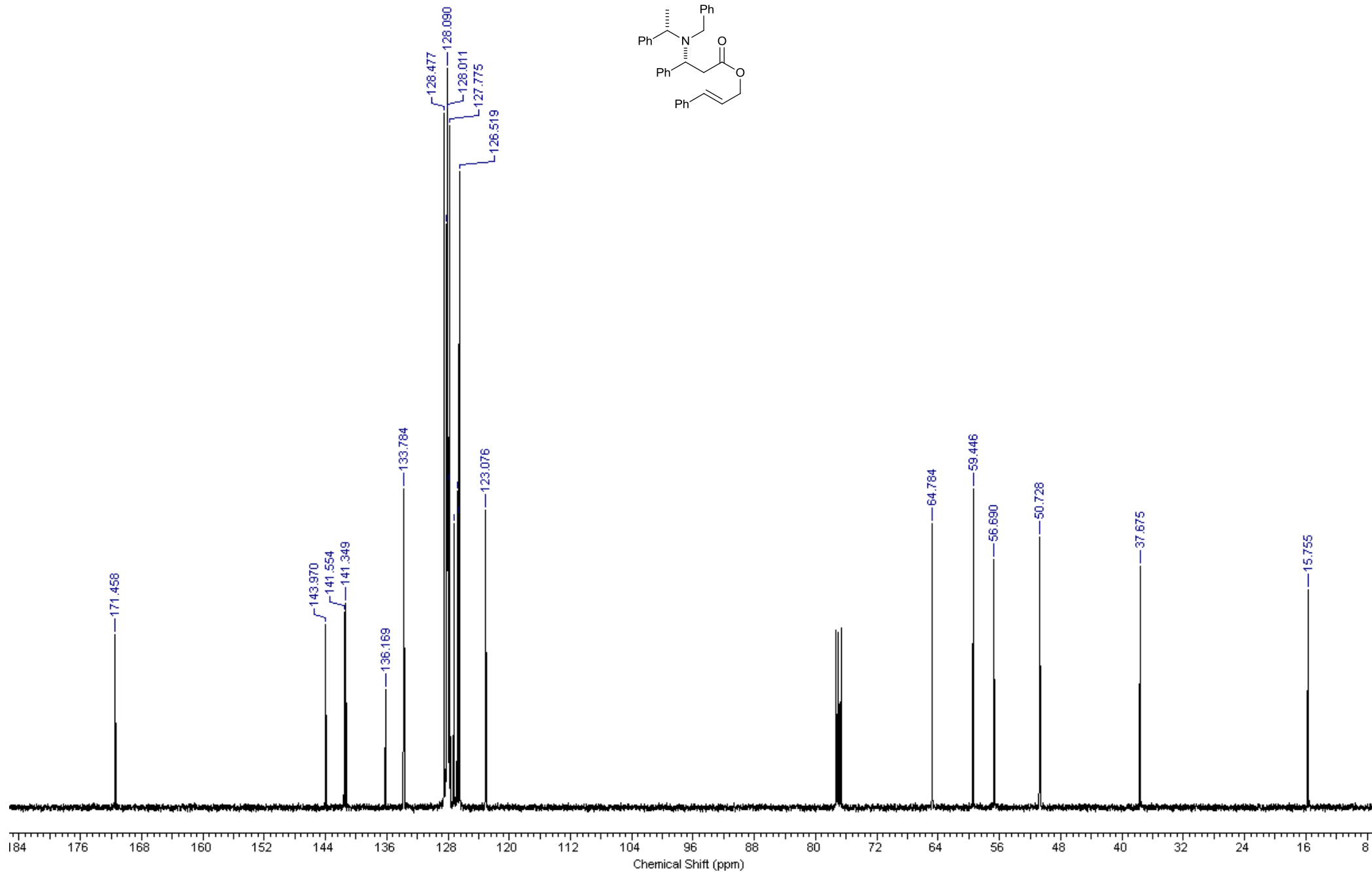
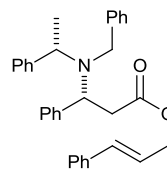
(E)-But-2'-en-1'-yl (3R, α S)-3-[N-benzyl-N-(α -methylbenzyl)amino]-3-phenylpropanoate 33 (100 MHz ^{13}C , CDCl_3)



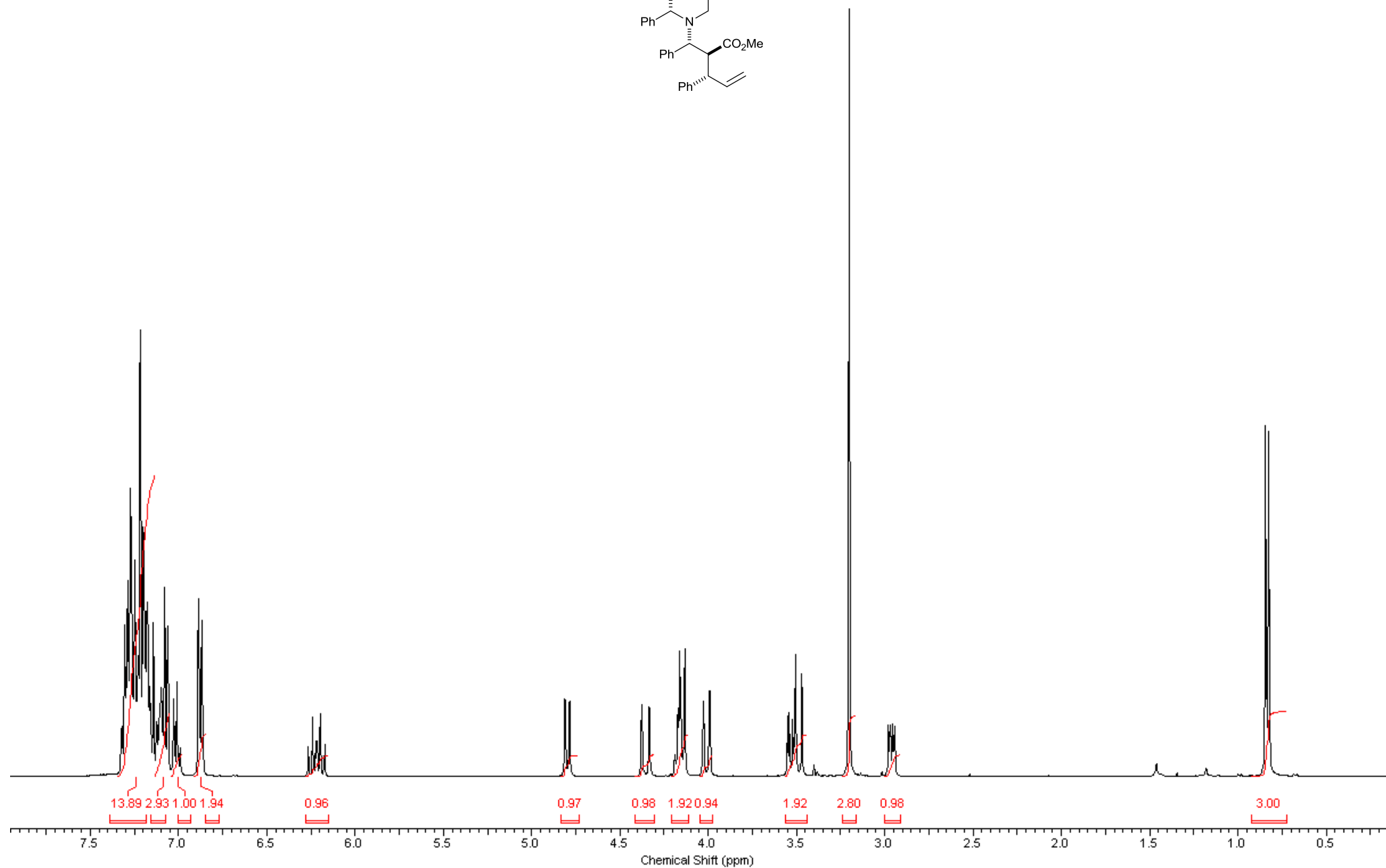
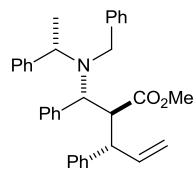
(E)-3'-Phenylprop-2'-en-1'-yl (3R, α S)-3-[N-benzyl-N-(α -methylbenzyl)amino]-3-phenylpropanoate 34 (400 MHz ^1H , CDCl_3)



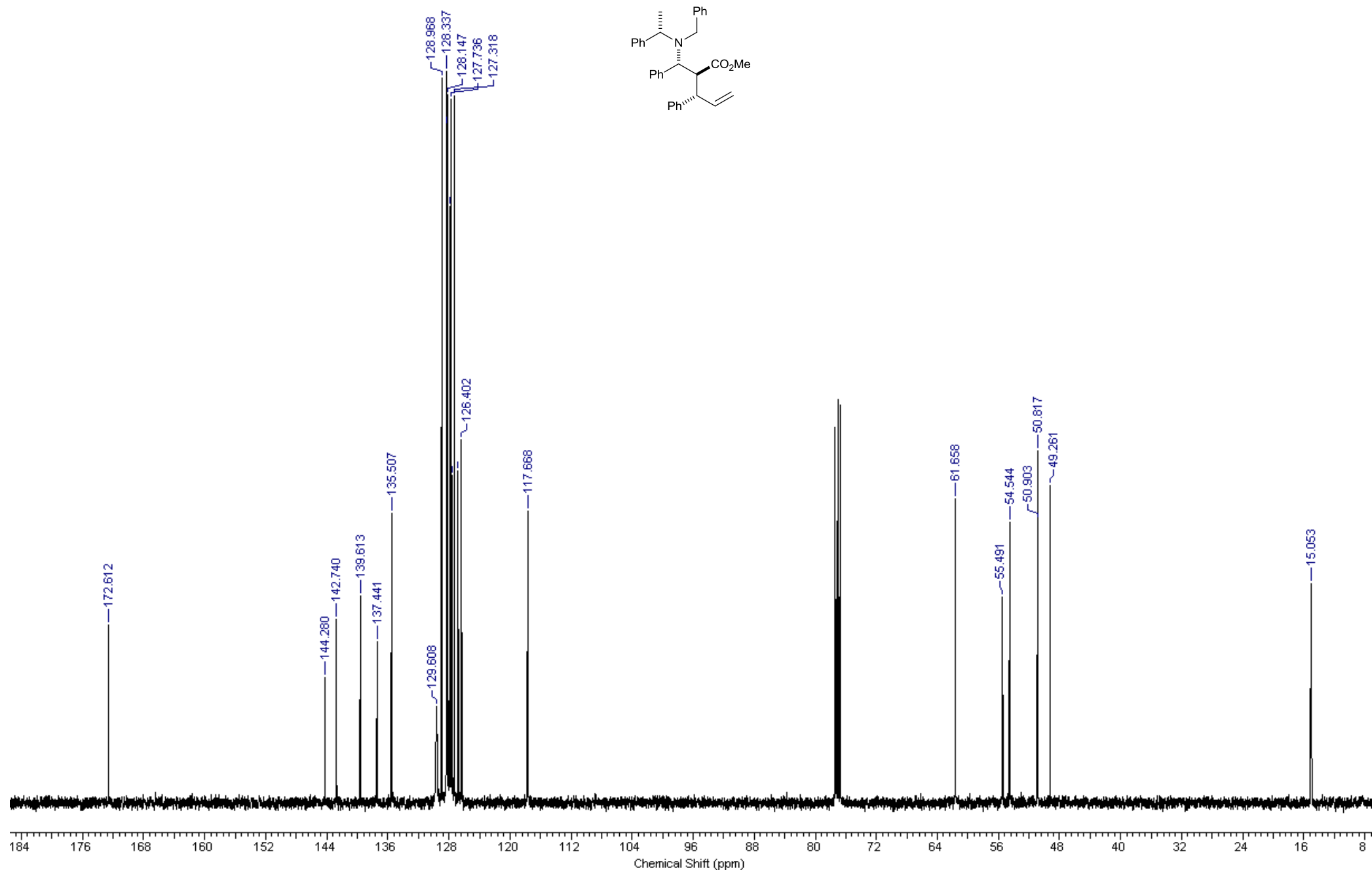
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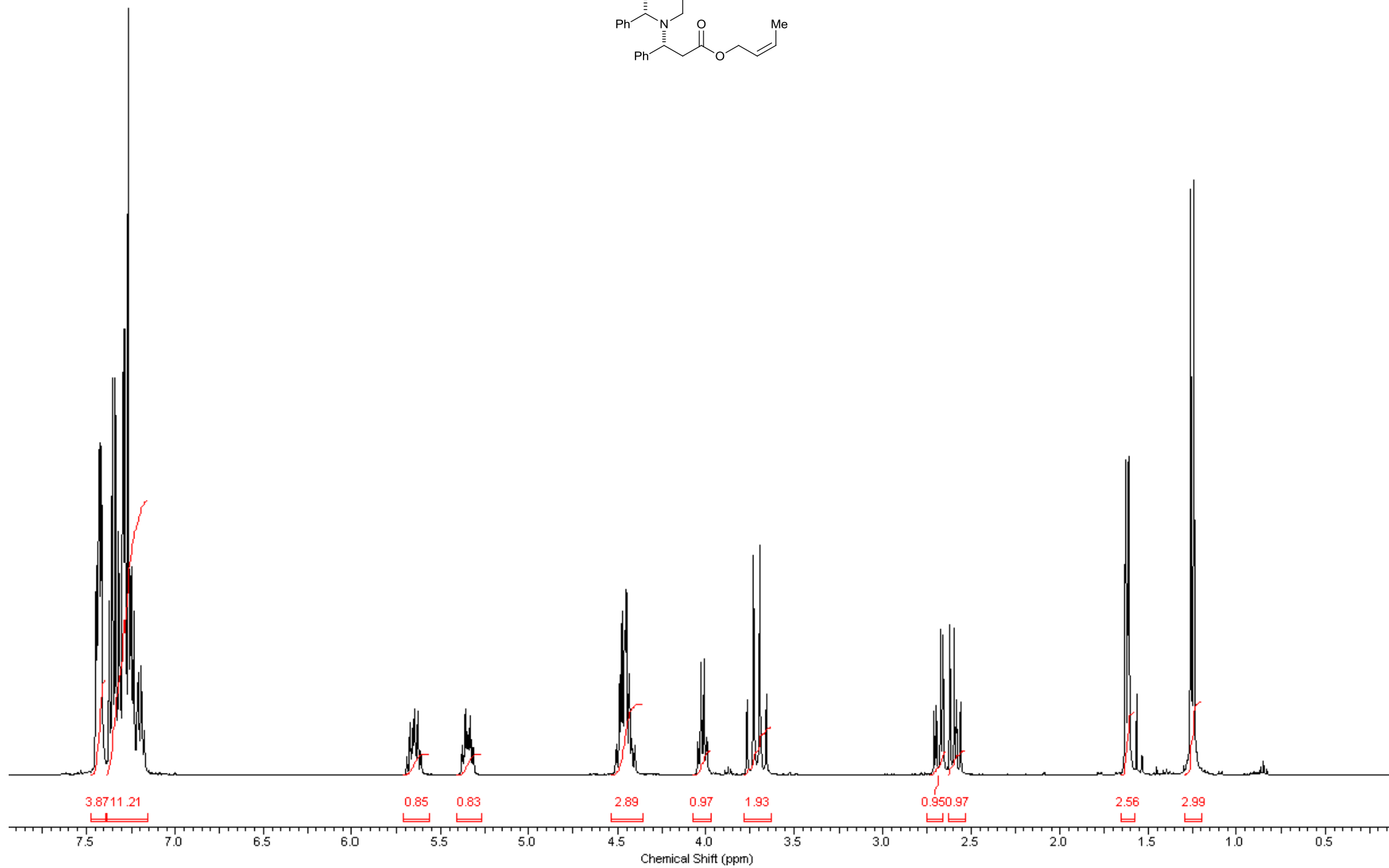
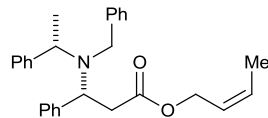
Methyl (2*S*,3*R*,1'*S*, α *S*)-2-(1'-phenylprop-2'-en-1'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate 39 (400 MHz ^1H , CDCl_3)



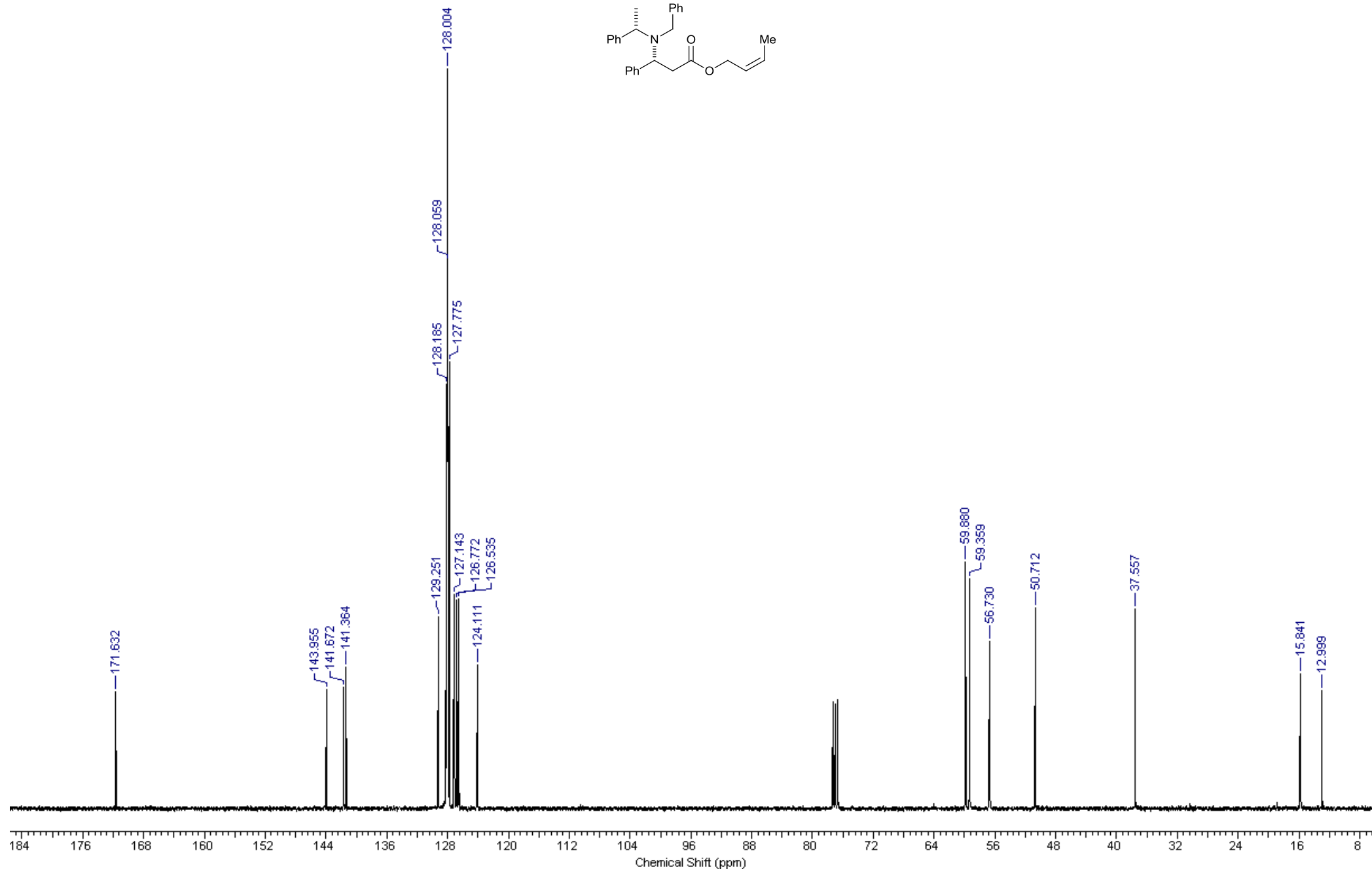
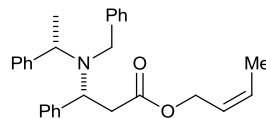
Methyl (2*S*,3*R*,1'*S*, α *S*)-2-(1'-phenylprop-2'-en-1'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate **39** (100 MHz ^{13}C , CDCl_3)



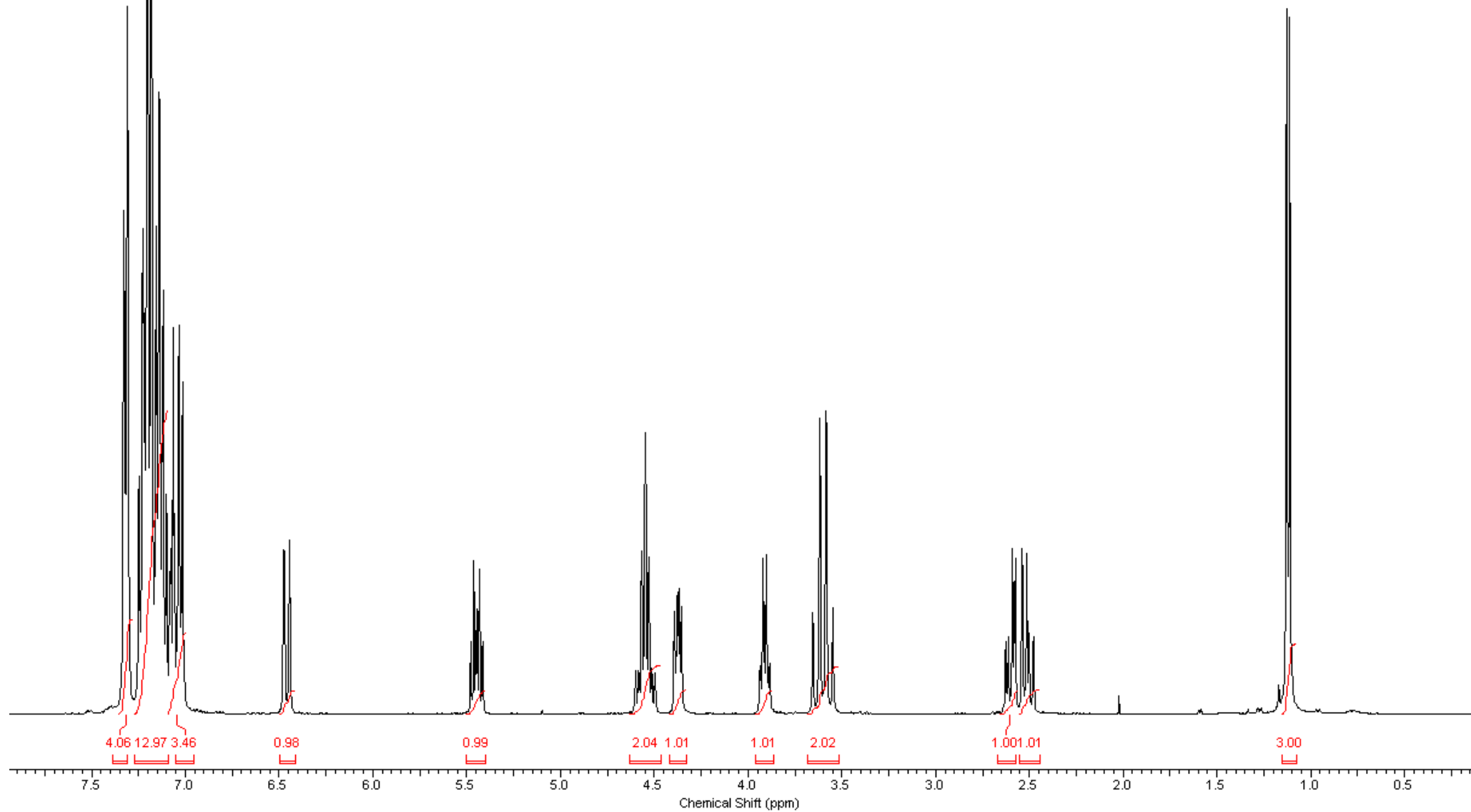
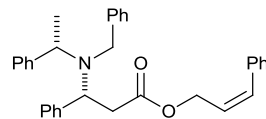
(Z)-But-2'-en-1'-yl (3R, α S)-3-[N-benzyl-N-(α -methylbenzyl)amino]-3-phenylpropanoate 41 (400 MHz ^1H , CDCl_3)



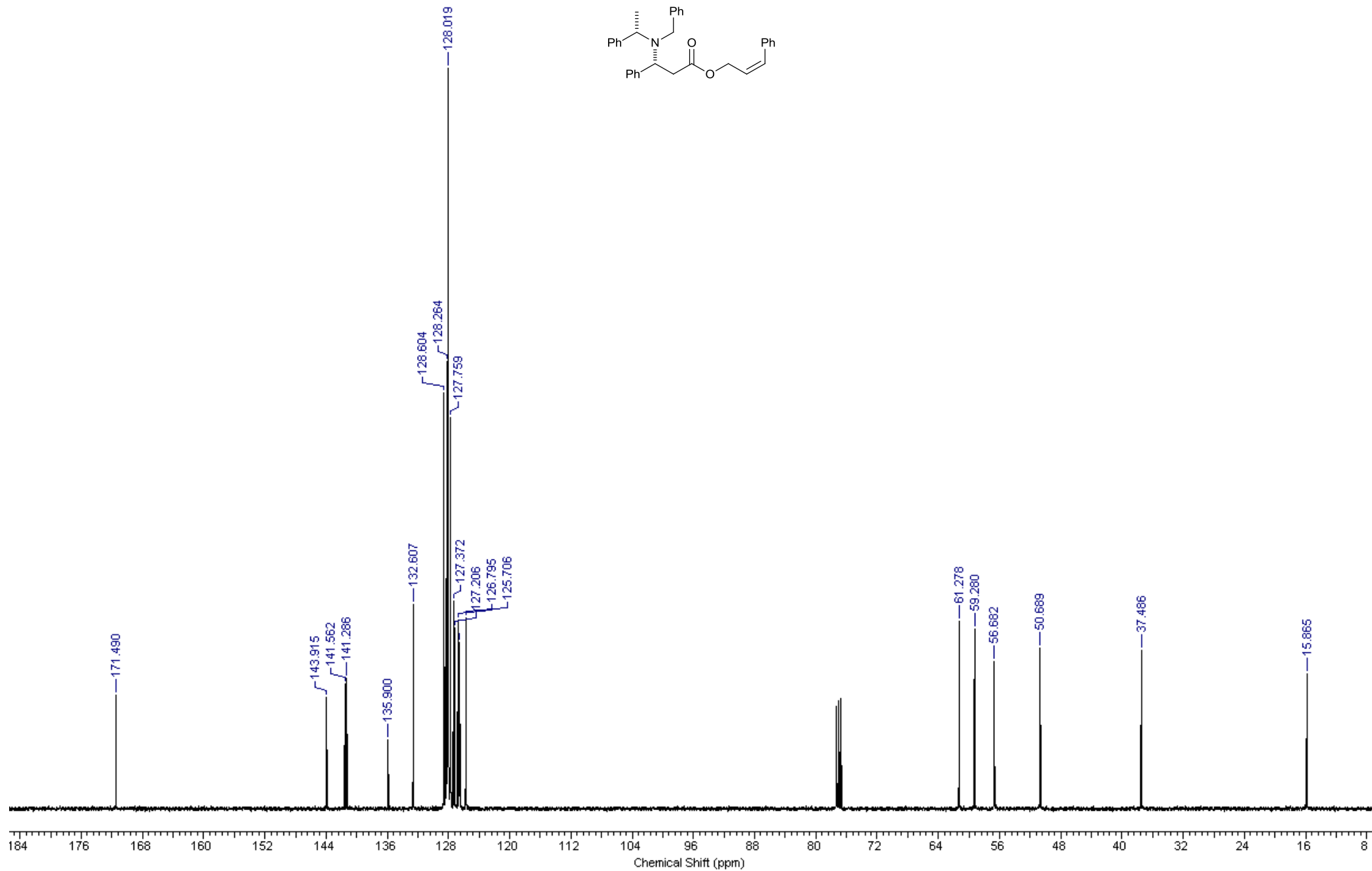
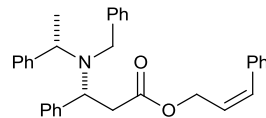
(Z)-But-2'-en-1'-yl (3R, α S)-3-[N-benzyl-N-(α -methylbenzyl)amino]-3-phenylpropanoate 41 (100 MHz ^{13}C , CDCl_3)



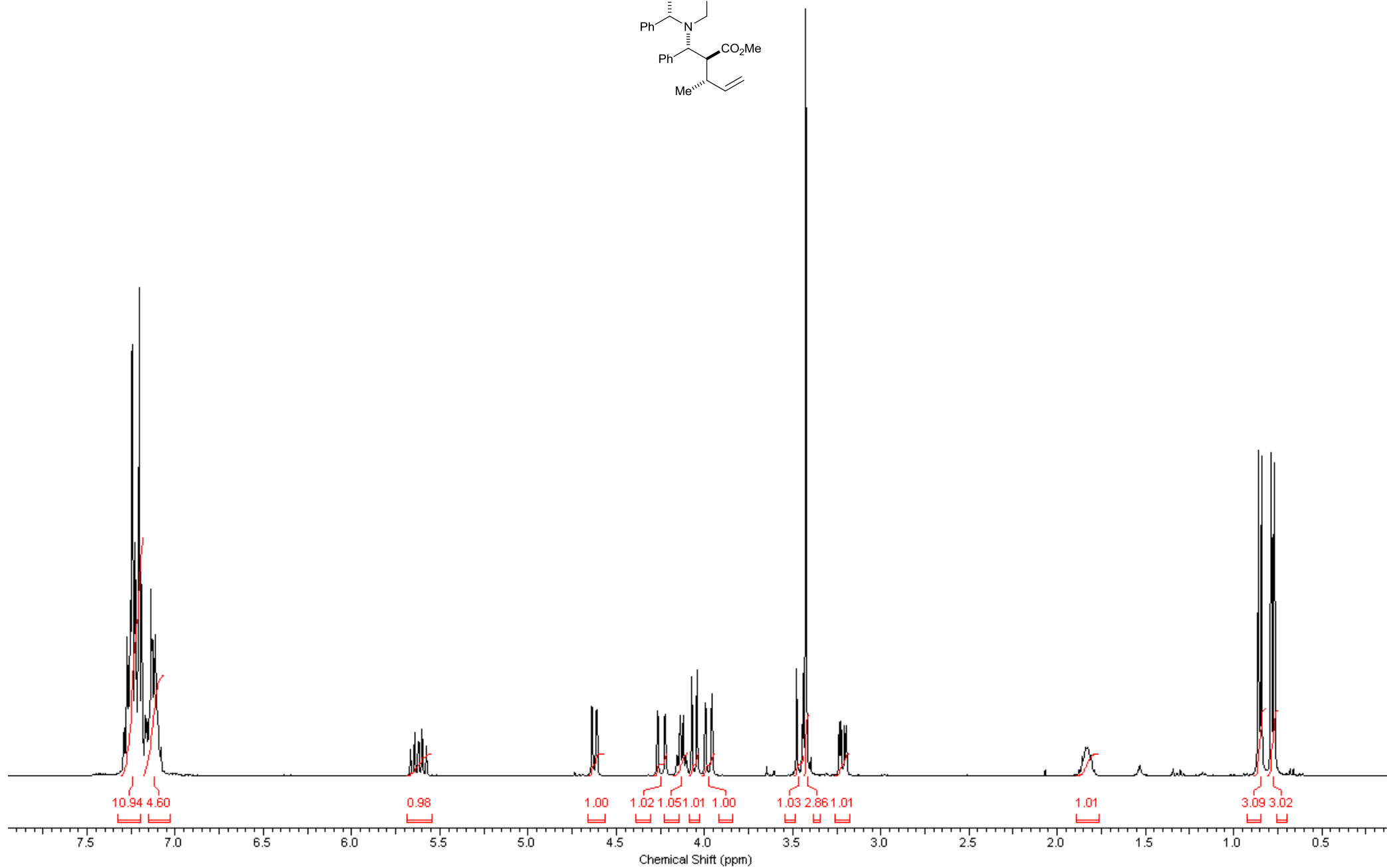
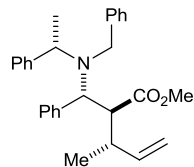
(Z)-3'-Phenylprop-2'-en-1'-yl (3R, α S)- 3-[N-benzyl-N-(α -methylbenzyl)amino]-3-phenylpropanoate 42 (400 MHz ^1H , CDCl_3)



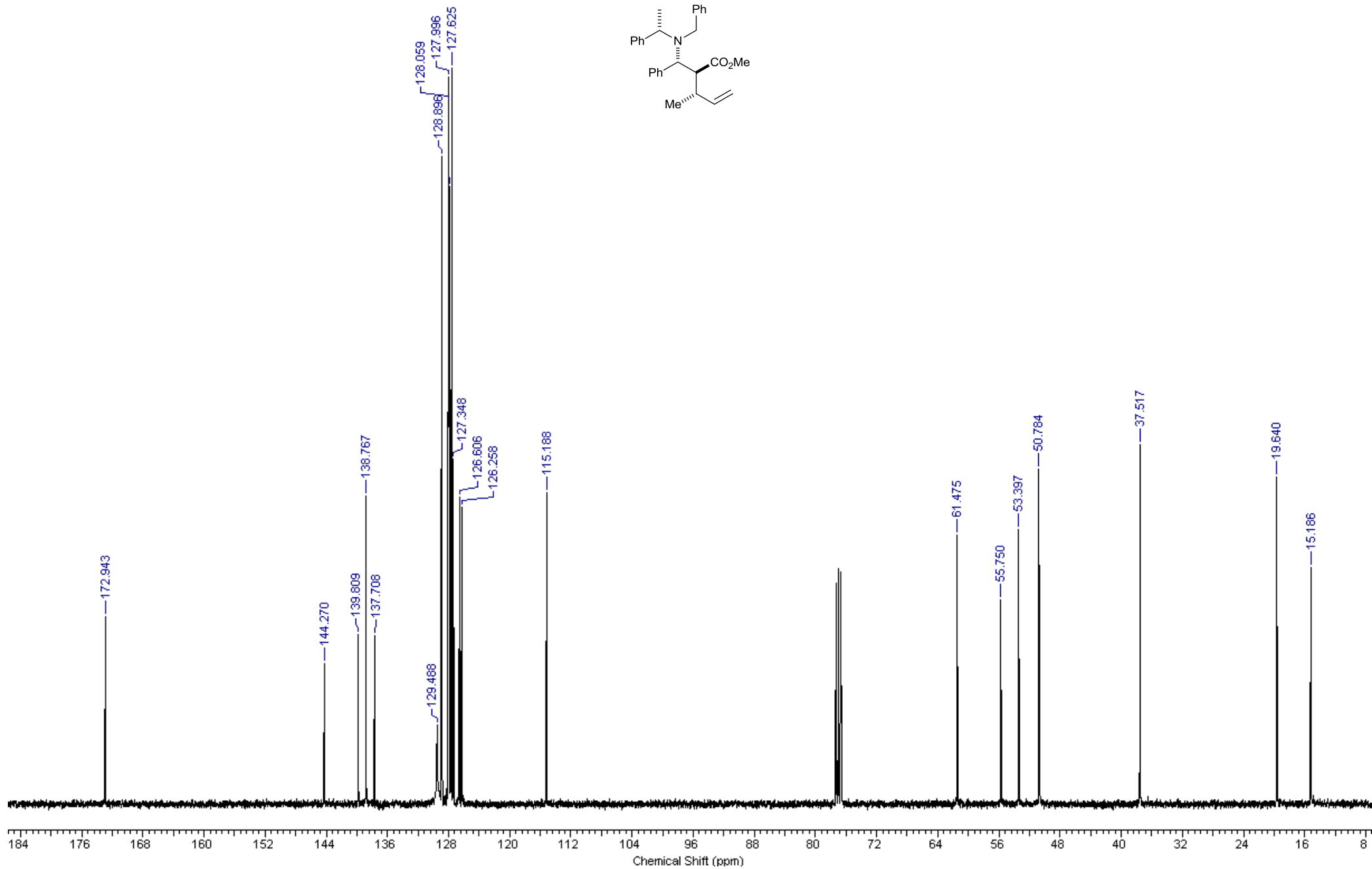
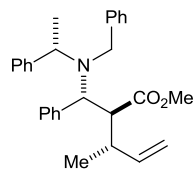
(Z)-3'-Phenylprop-2'-en-1'-yl (3R, α S)- 3-[N-benzyl-N-(α -methylbenzyl)amino]-3-phenylpropanoate 42 (100 MHz ^{13}C , CDCl_3)



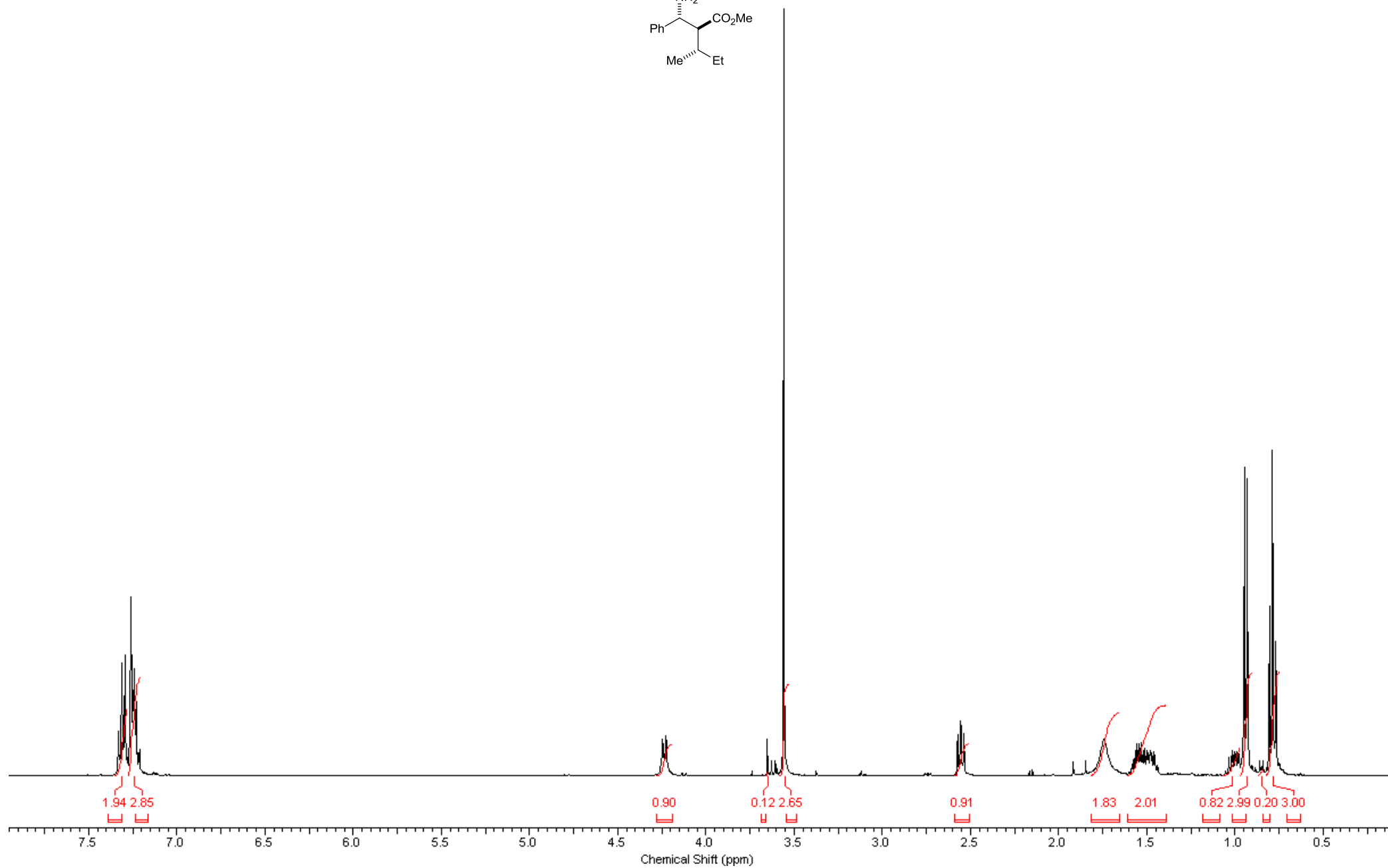
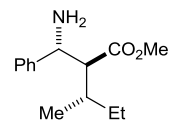
Methyl (2*S*,3*R*,1'*S*, α *S*)-2-(but-3'-en-2'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate 44 (400 MHz ^1H , CDCl_3)



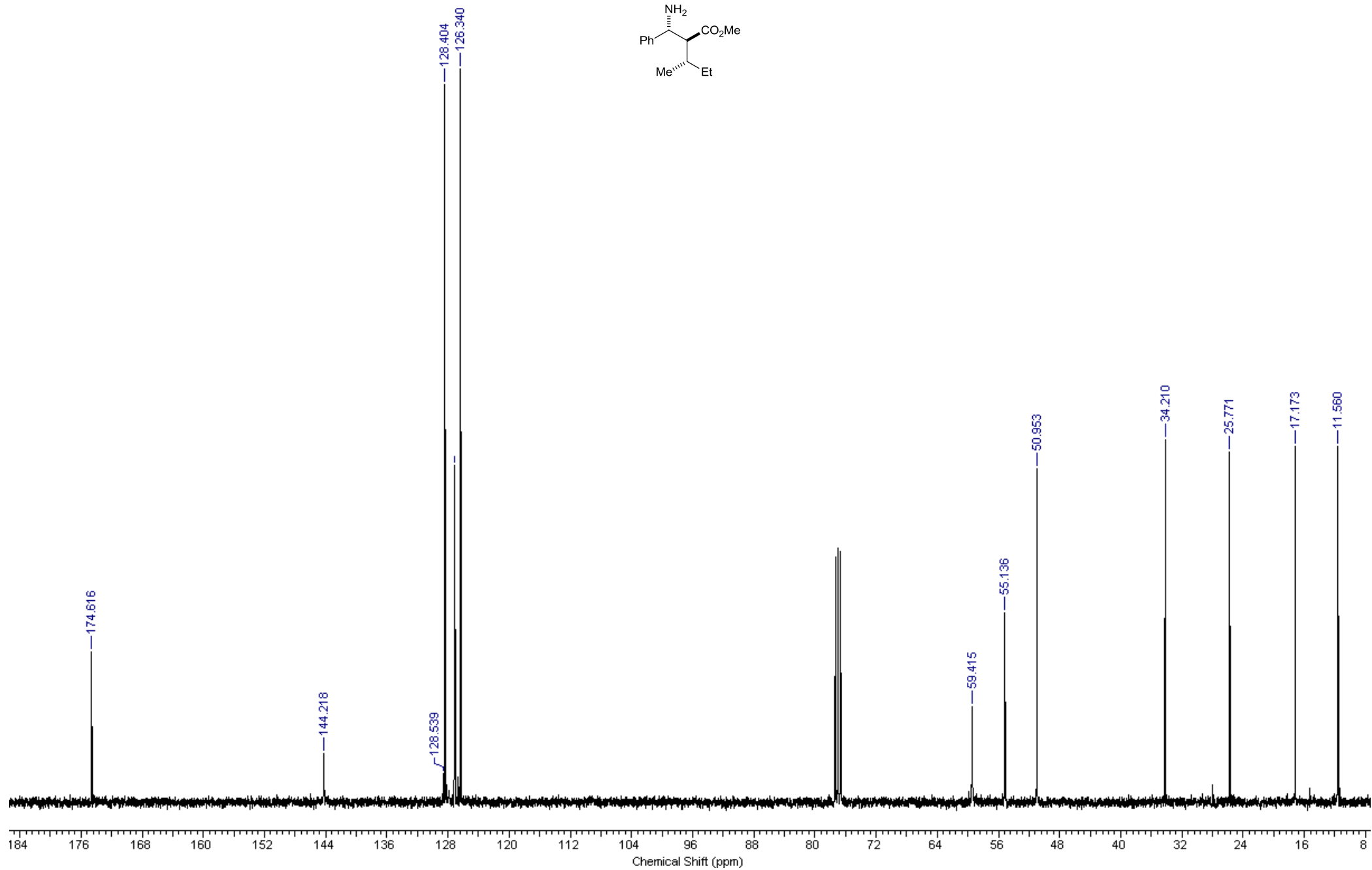
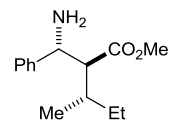
Methyl (2*S*,3*R*,1'*S*, α *S*)-2-(but-3'-en-2'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-3-phenylpropanoate 44 (100 MHz ^{13}C , CDCl_3)



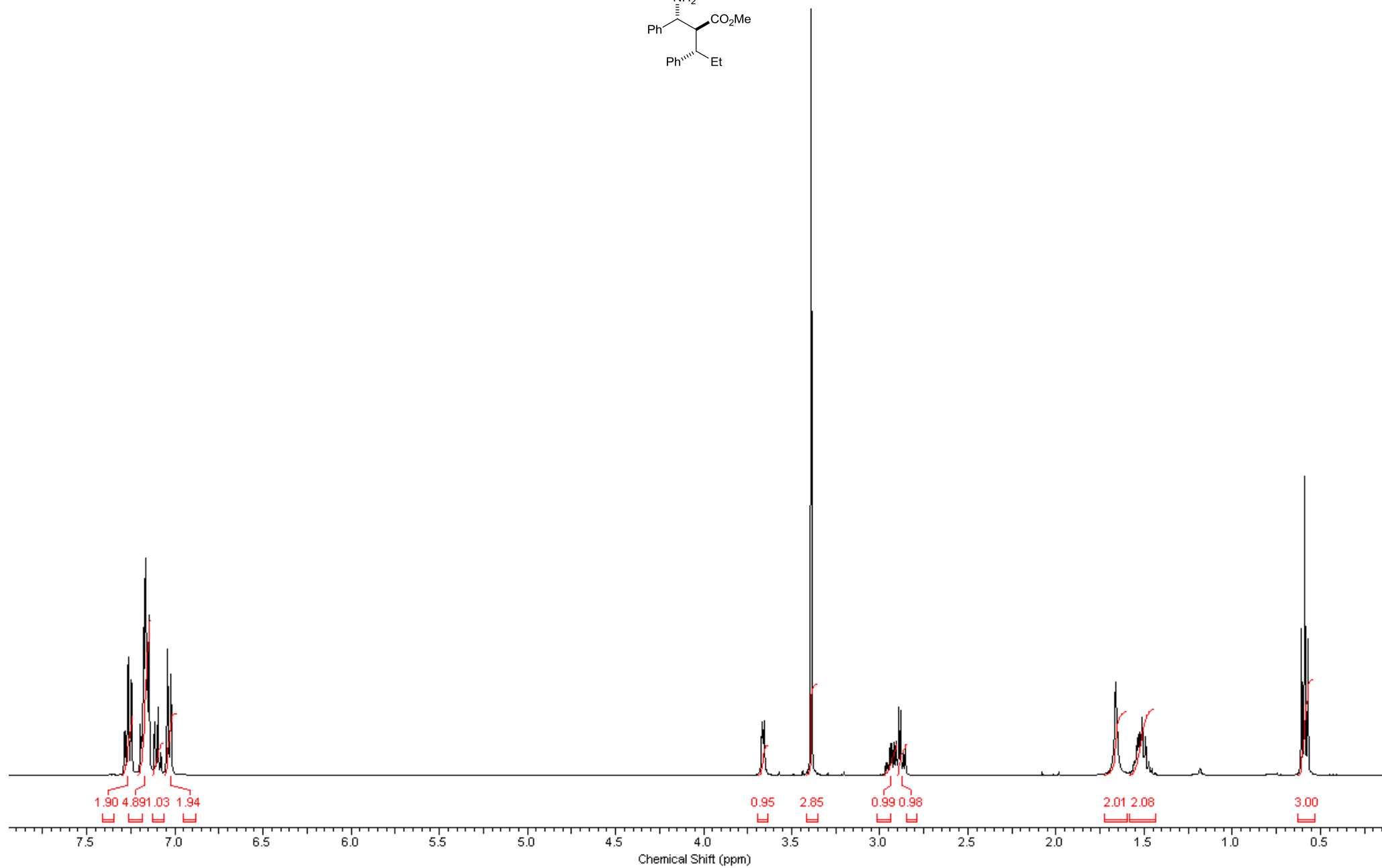
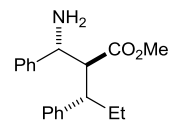
Methyl (2*S*,3*R*,1'*S*)-2-(but-2'-yl)-3-amino-3-phenylpropanoate 45 (400 MHz ¹H, CDCl₃)



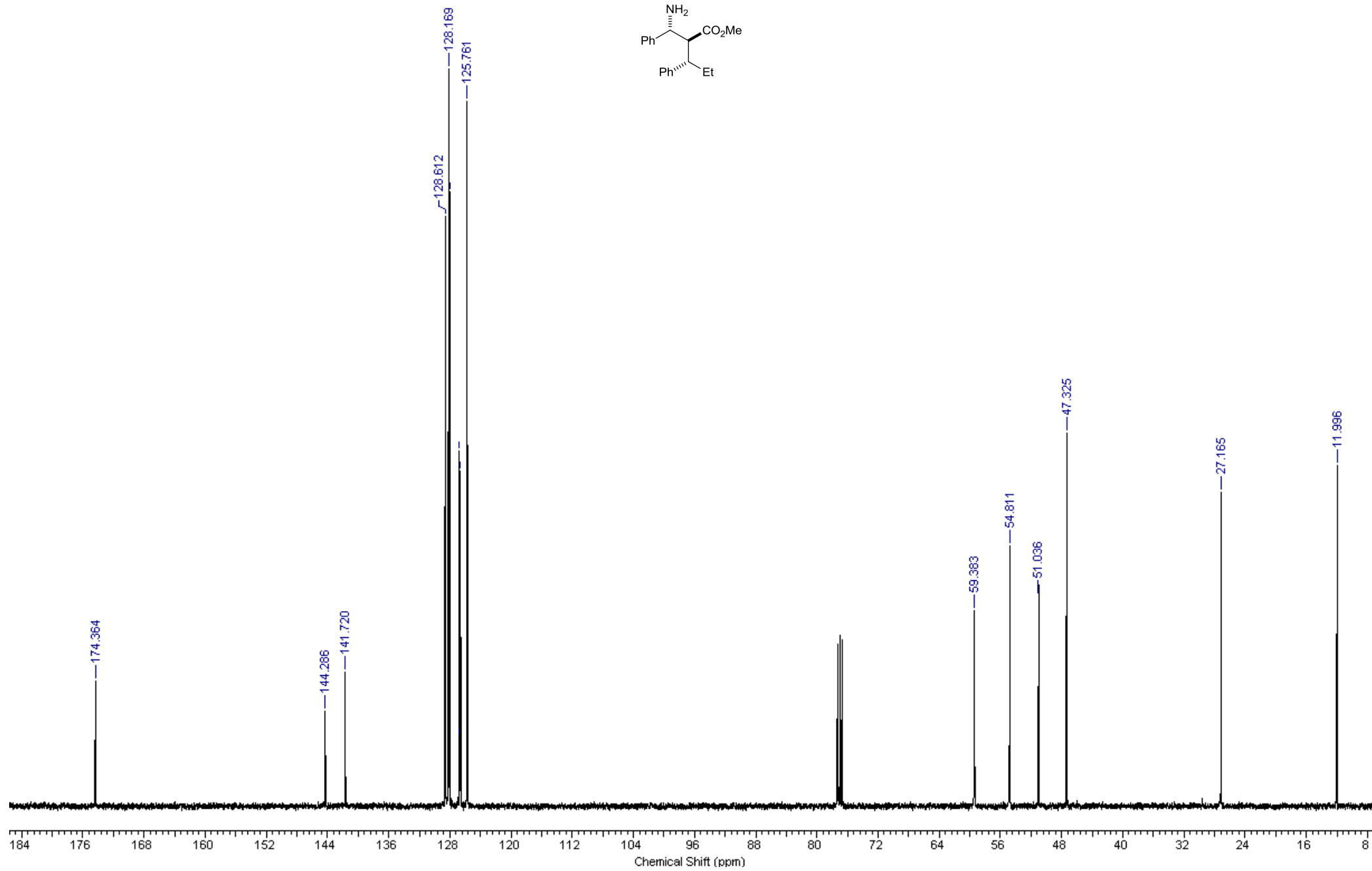
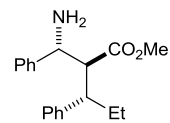
Methyl (2*S*,3*R*,1'*S*)-2-(but-2'-yl)-3-amino-3-phenylpropanoate 45 (100 MHz ¹³C, CDCl₃)



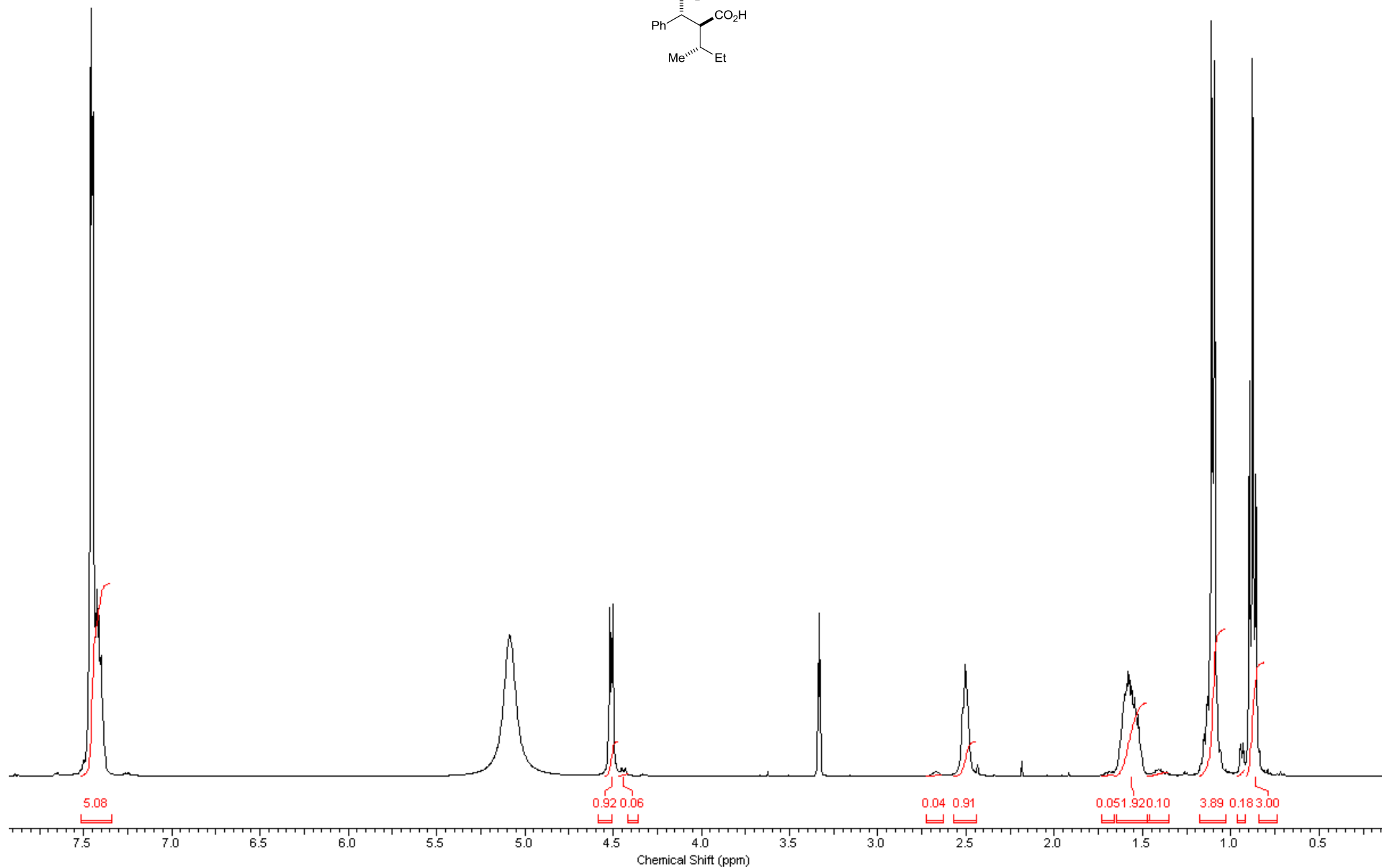
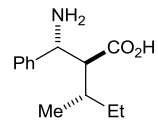
Methyl (2*S*,3*R*,1'*S*)-2-(1'-phenylpropyl)-3-amino-3-phenylpropanoate **46** (400 MHz ¹H, CDCl₃)



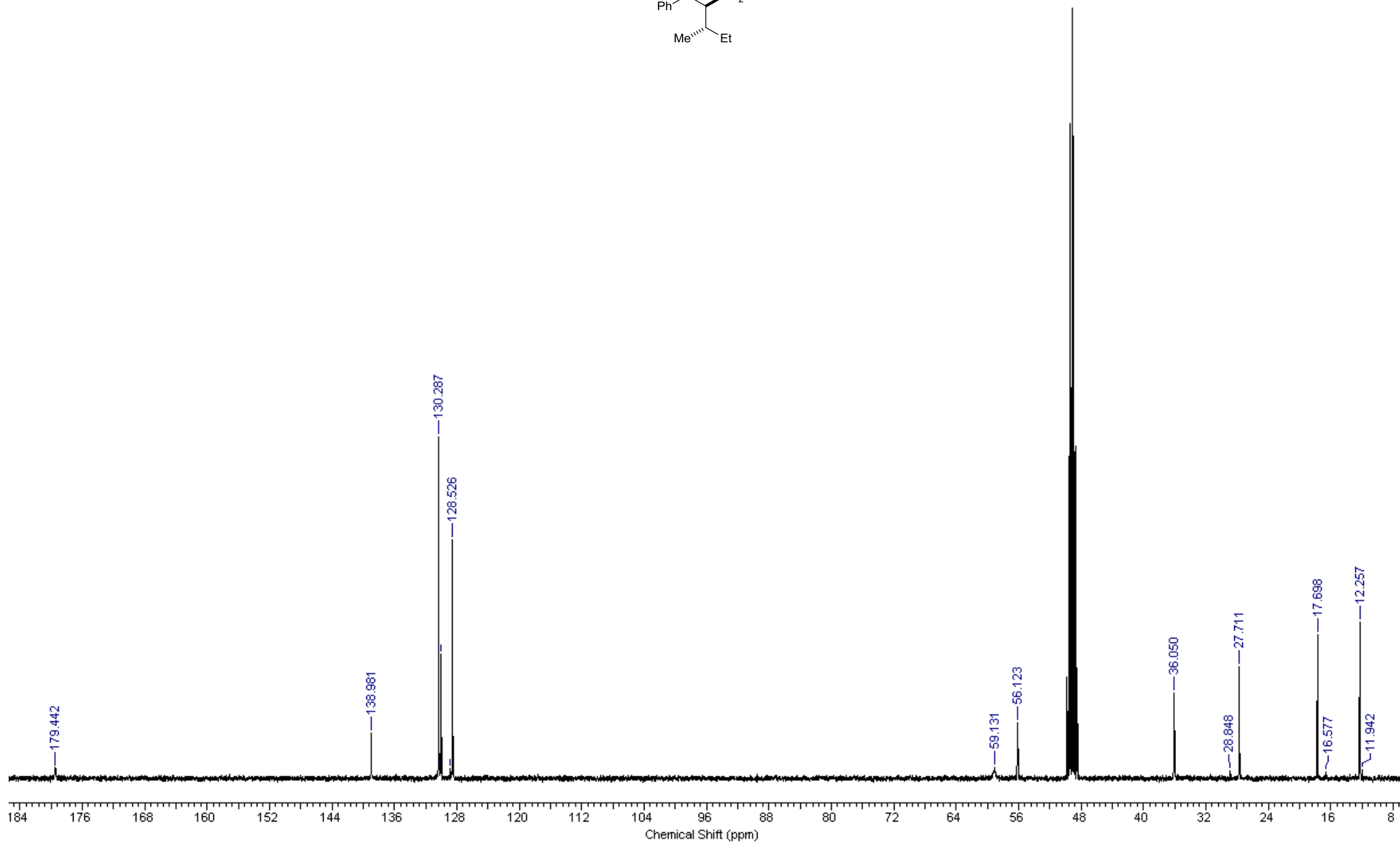
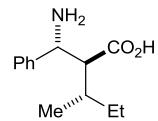
Methyl (2*S*,3*R*,1'*S*)-2-(1'-phenylpropyl)-3-amino-3-phenylpropanoate **46** (100 MHz ^{13}C , CDCl_3)



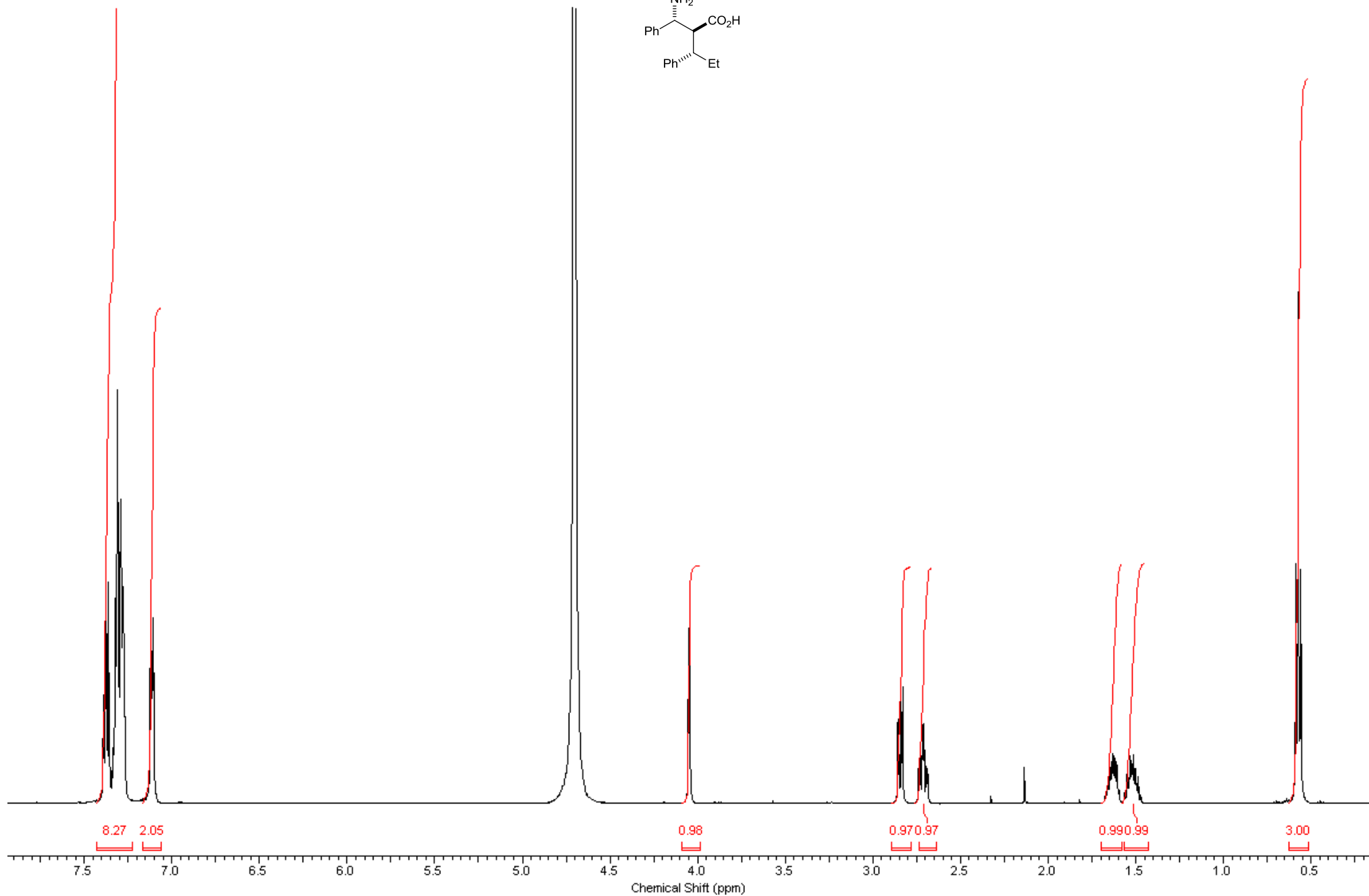
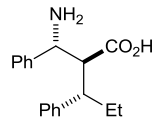
(2*S*,3*R*,1'*S*)-2-(But-2'-yl)-3-amino-3-phenylpropanoic acid 47 (400 MHz ¹H, MeOH-*d*₄)



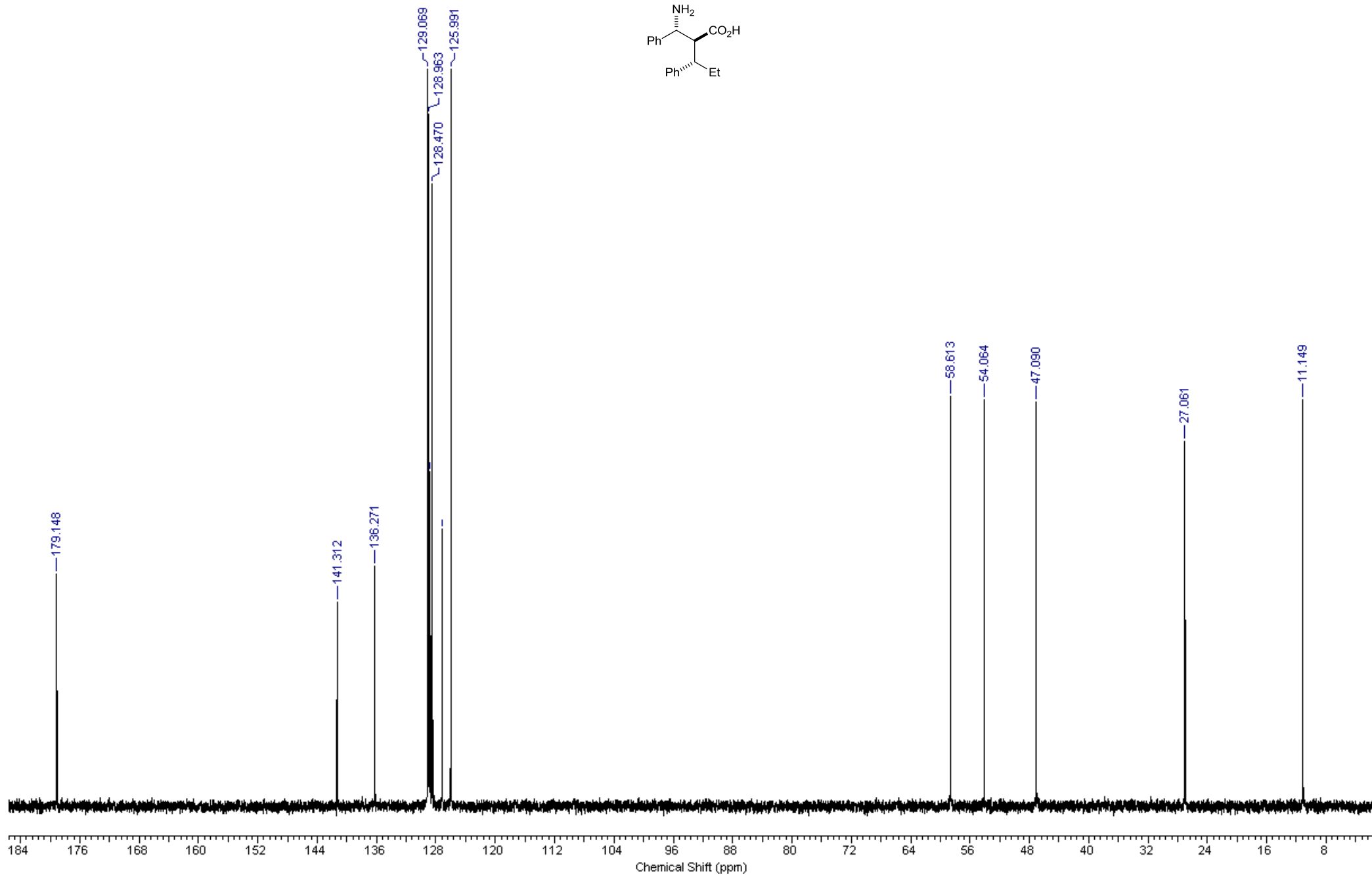
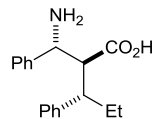
(2*S*,3*R*,1'*S*)-2-(But-2'-yl)-3-amino-3-phenylpropanoic acid **47** (100 MHz ¹H, MeOH-*d*₄)



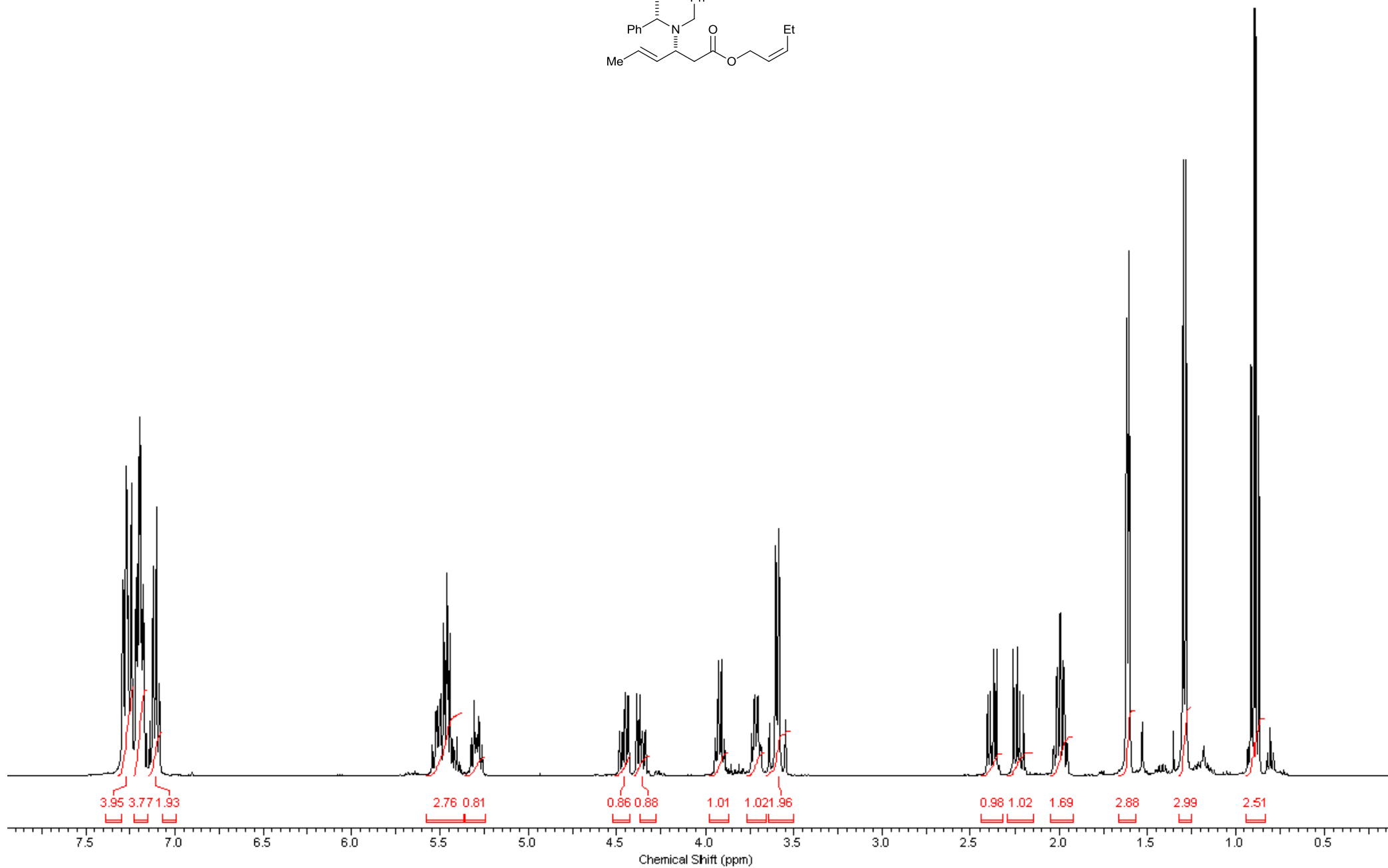
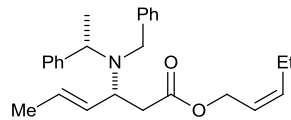
(2*S*,3*R*,1'*S*)-2-(1'-Phenylpropyl)-3-amino-3-phenylpropanoic acid 48 (500 MHz ¹H, D₂O)



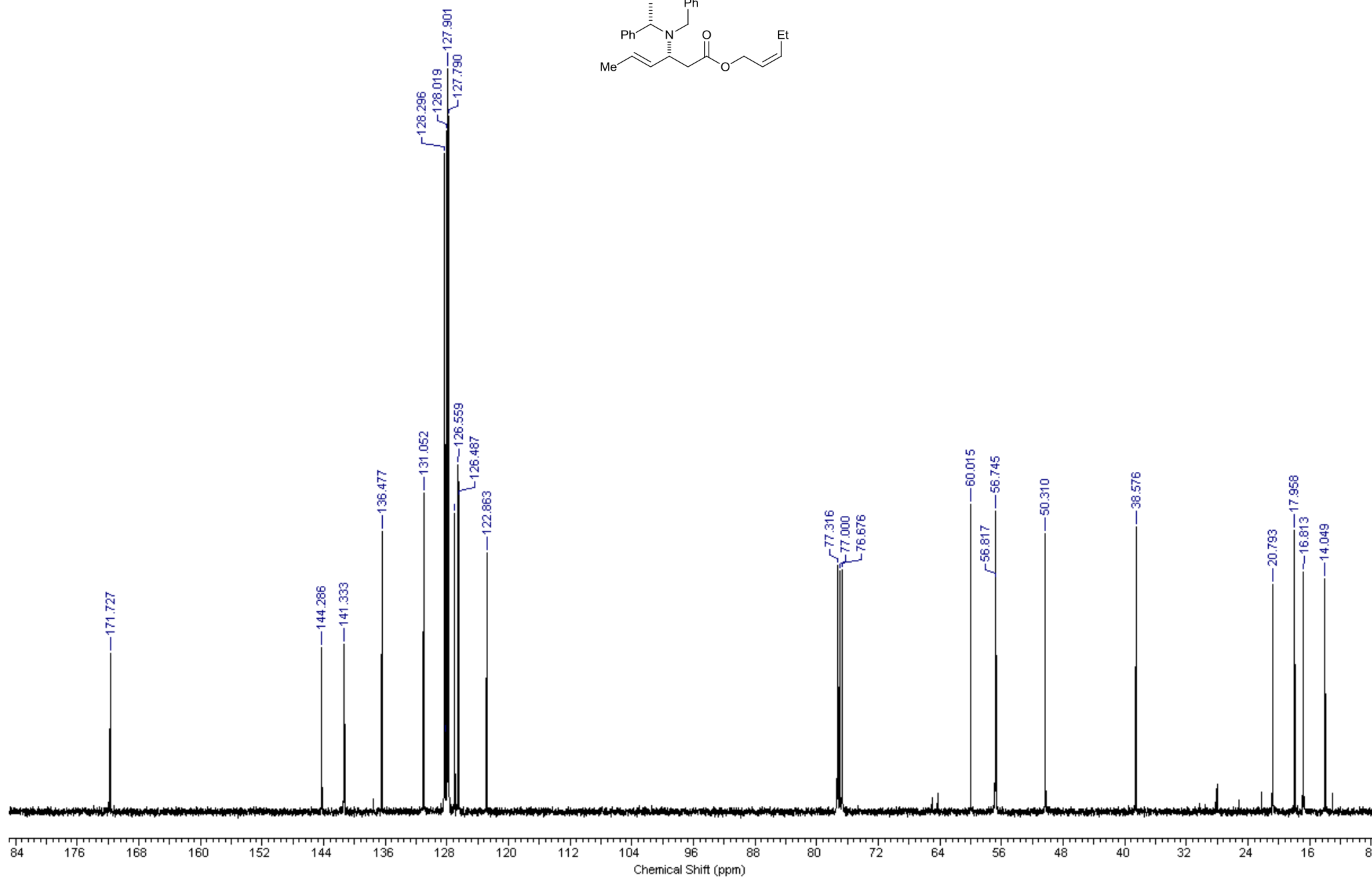
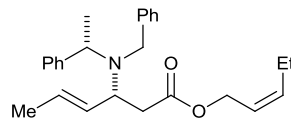
(2*S*,3*R*,1'*S*)-2-(1'-Phenylpropyl)-3-amino-3-phenylpropanoic acid 48 (125 MHz ¹³C, D₂O)



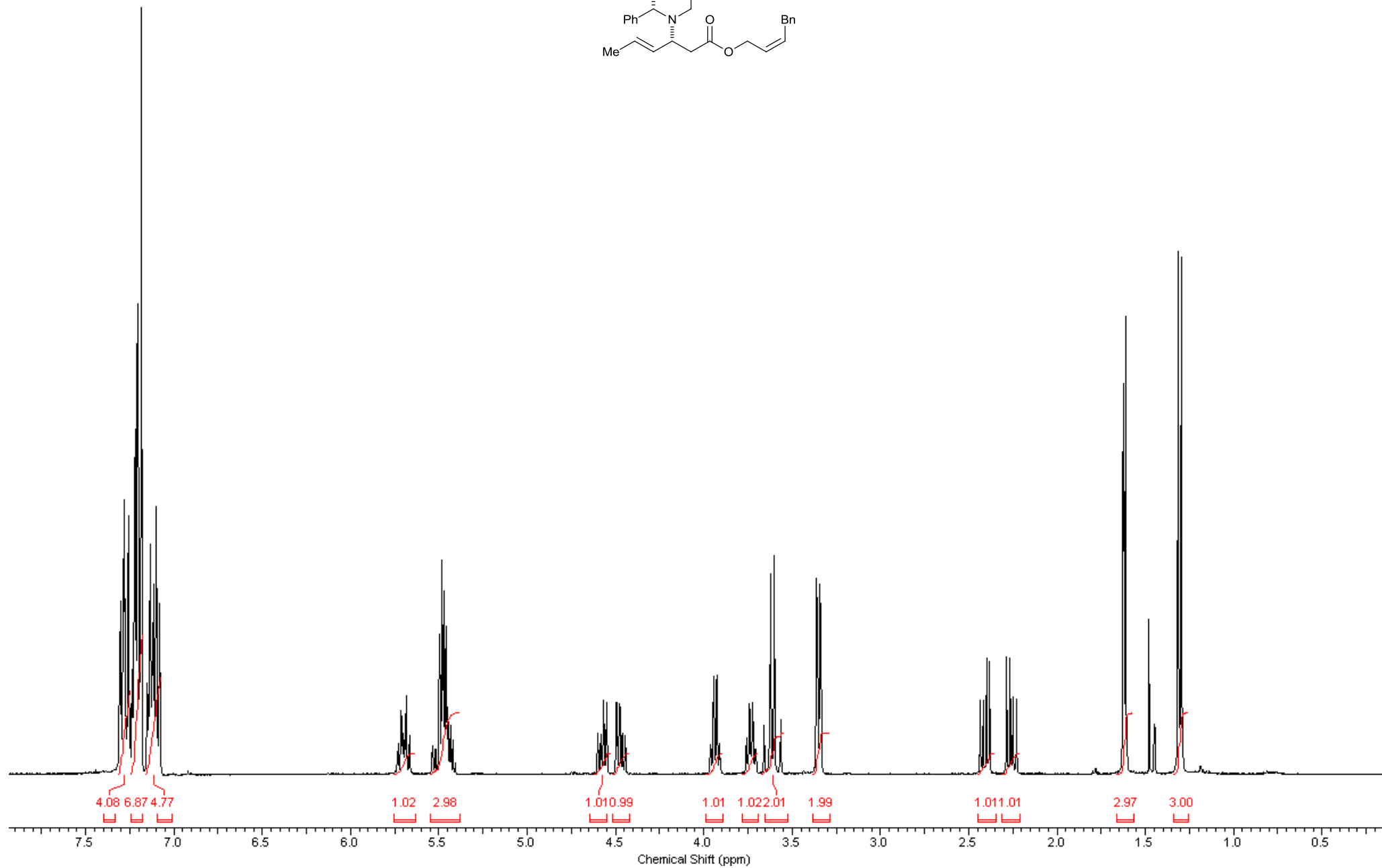
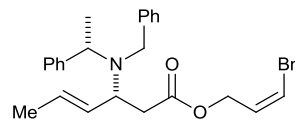
(Z)-Pent-2'-en-1'-yl (3R, α S,E)-3-[N-benzyl-N-(α -methylbenzyl)amino]hex-4-enoate 66 (400 MHz ^1H , CDCl_3)



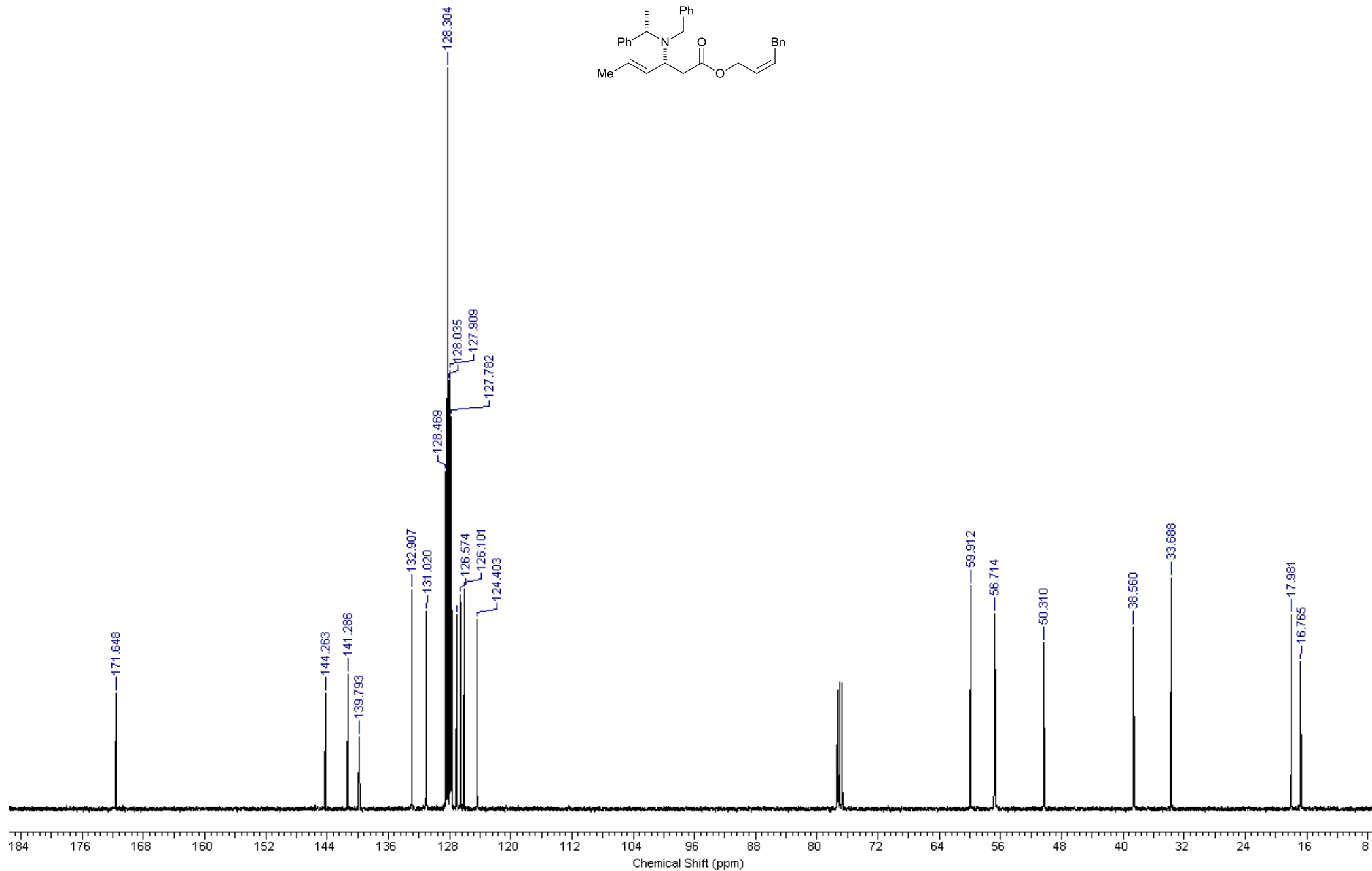
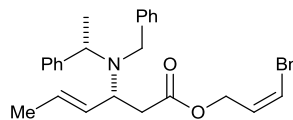
(Z)-Pent-2'-en-1'-yl (3R,αS,E)- 3-[N-benzyl-N-(α-methylbenzyl)amino]hex-4-enoate 66 (100 MHz ¹³C, CDCl₃)



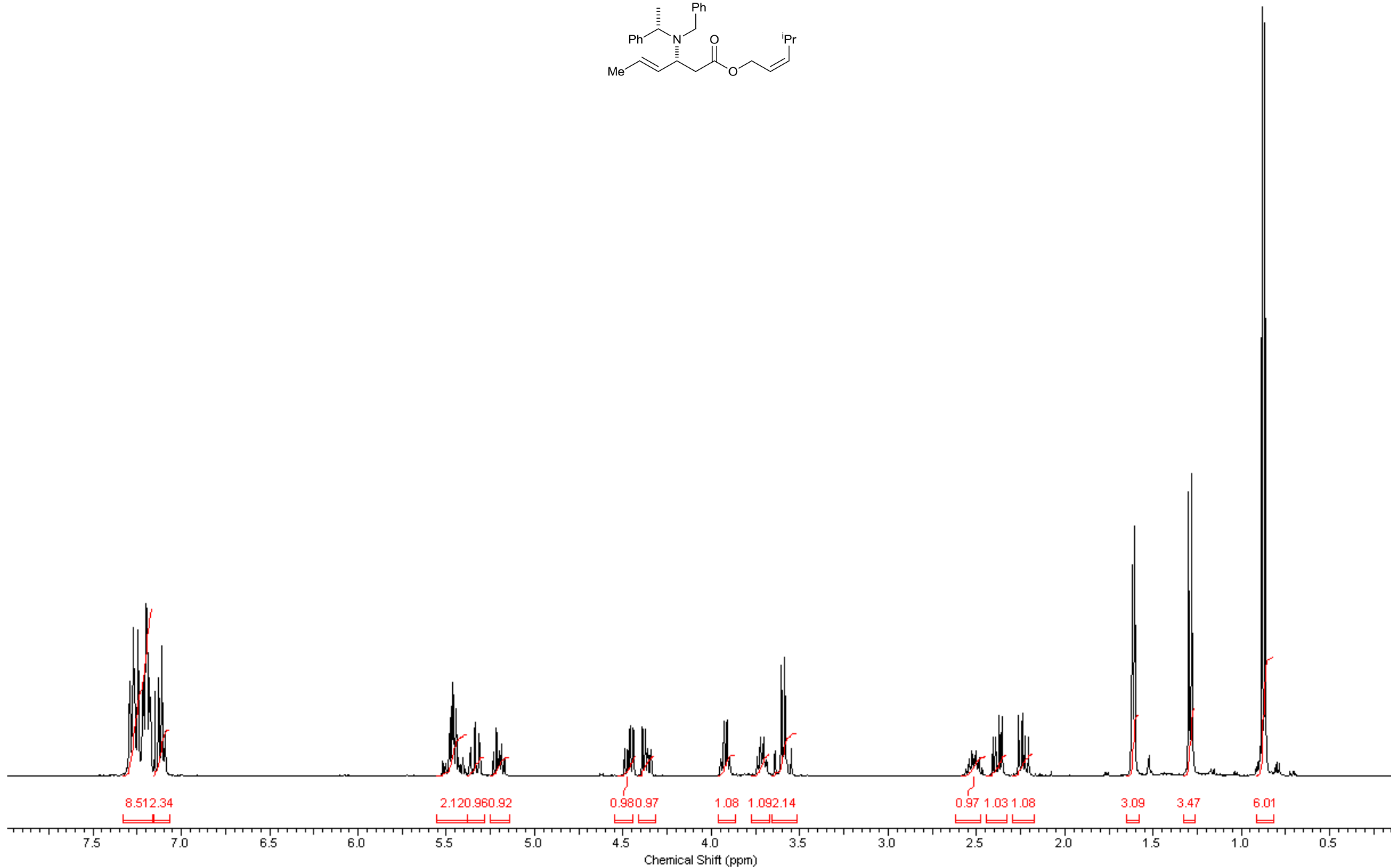
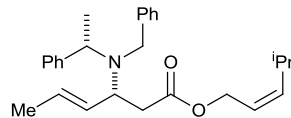
(Z)-4'-Phenylbut-2'-en-1'-yl (3R, α S,E)-3-[N-benzyl-N-(α -methylbenzyl)amino]hex-4-enoate **67** (400 MHz ^1H , CDCl_3)



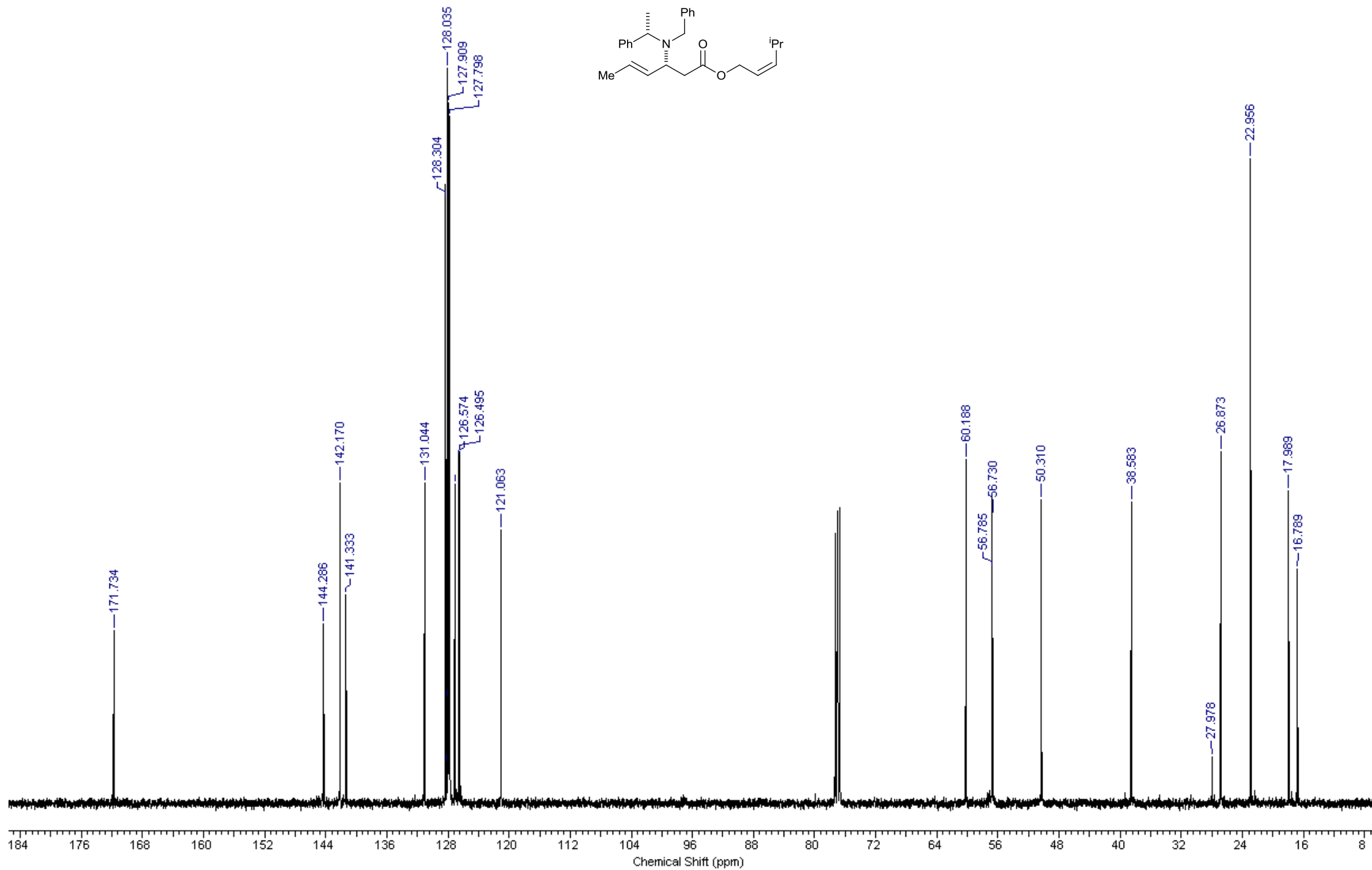
(Z)-4'-Phenylbut-2'-en-1'-yl (3R, α S,E)-3-[N-benzyl-N-(α -methylbenzyl)amino]hex-4-enoate **67** (100 MHz ^{13}C , CDCl_3)



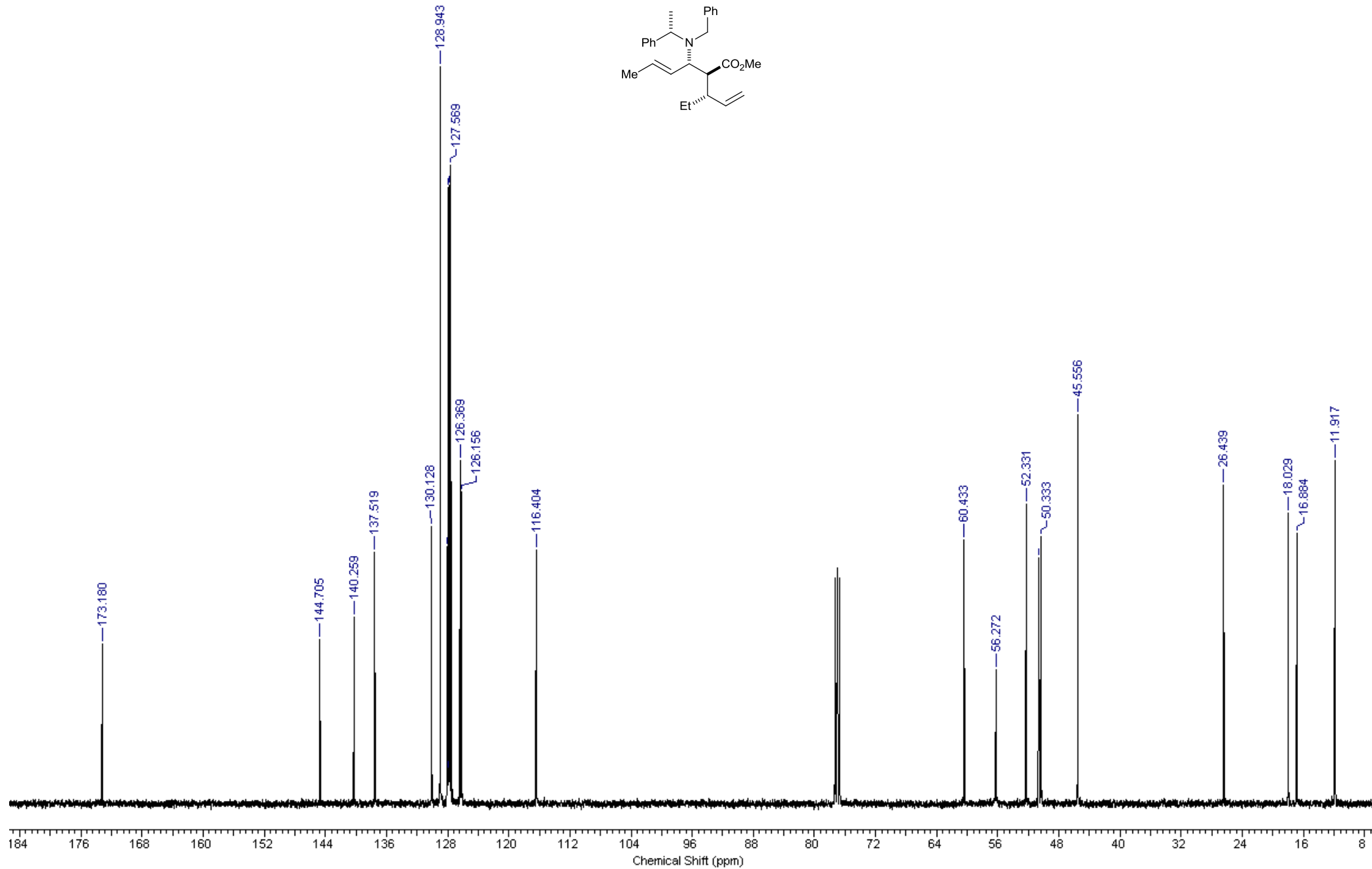
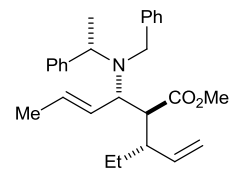
(Z)-4'-Methylpent-2'-en-1'-yl (3R, α S,E)-3-[N-benzyl-N-(α -methylbenzyl)amino]hex-4-enoate 68 (400 MHz ^1H , CDCl_3)



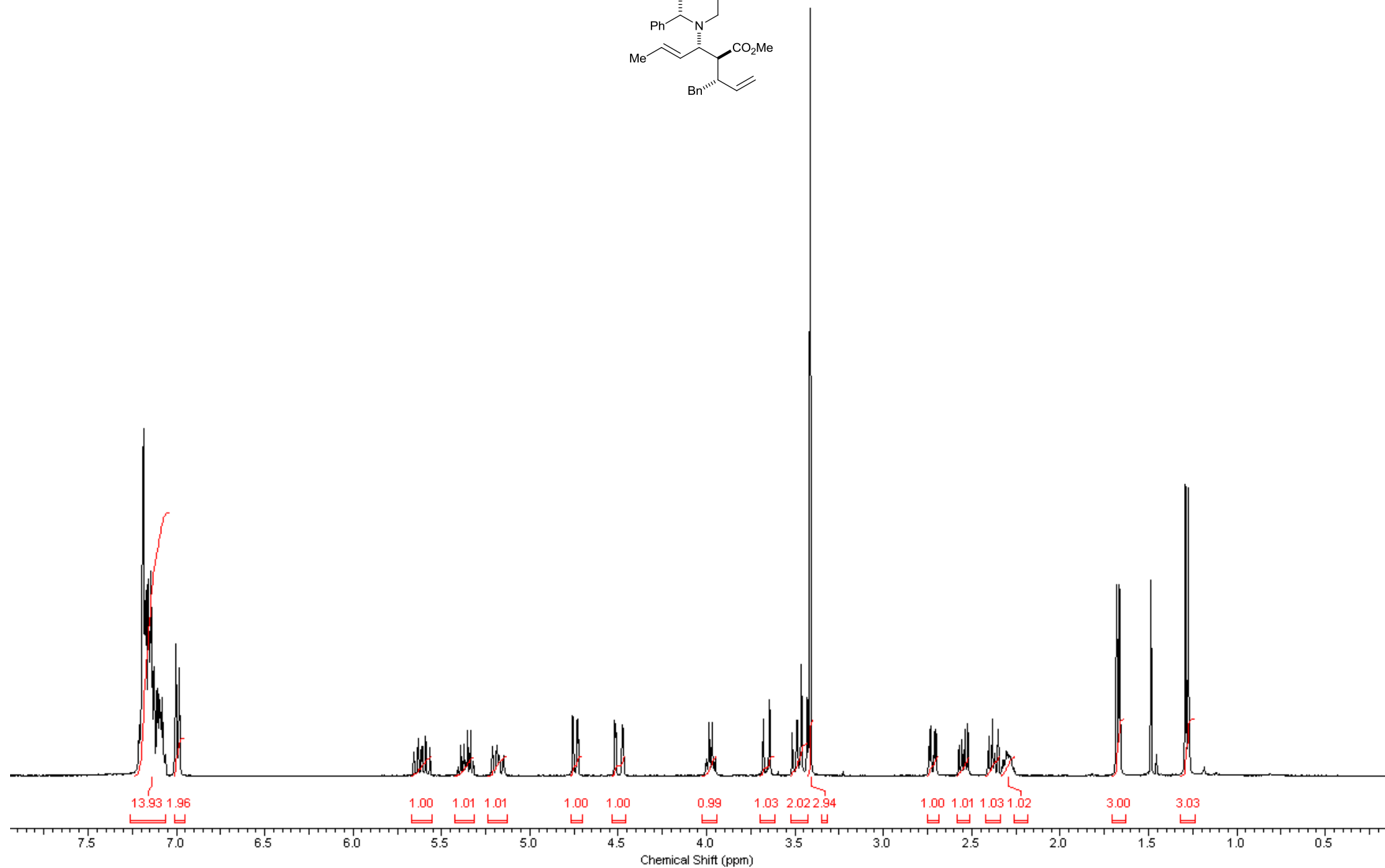
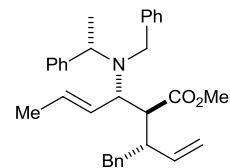
(Z)-4'-Methylpent-2'-en-1'-yl (3R, α S,E)-3-[N-benzyl-N-(α -methylbenzyl)amino]hex-4-enoate 68 (100 MHz 13 C, CDCl $_3$)



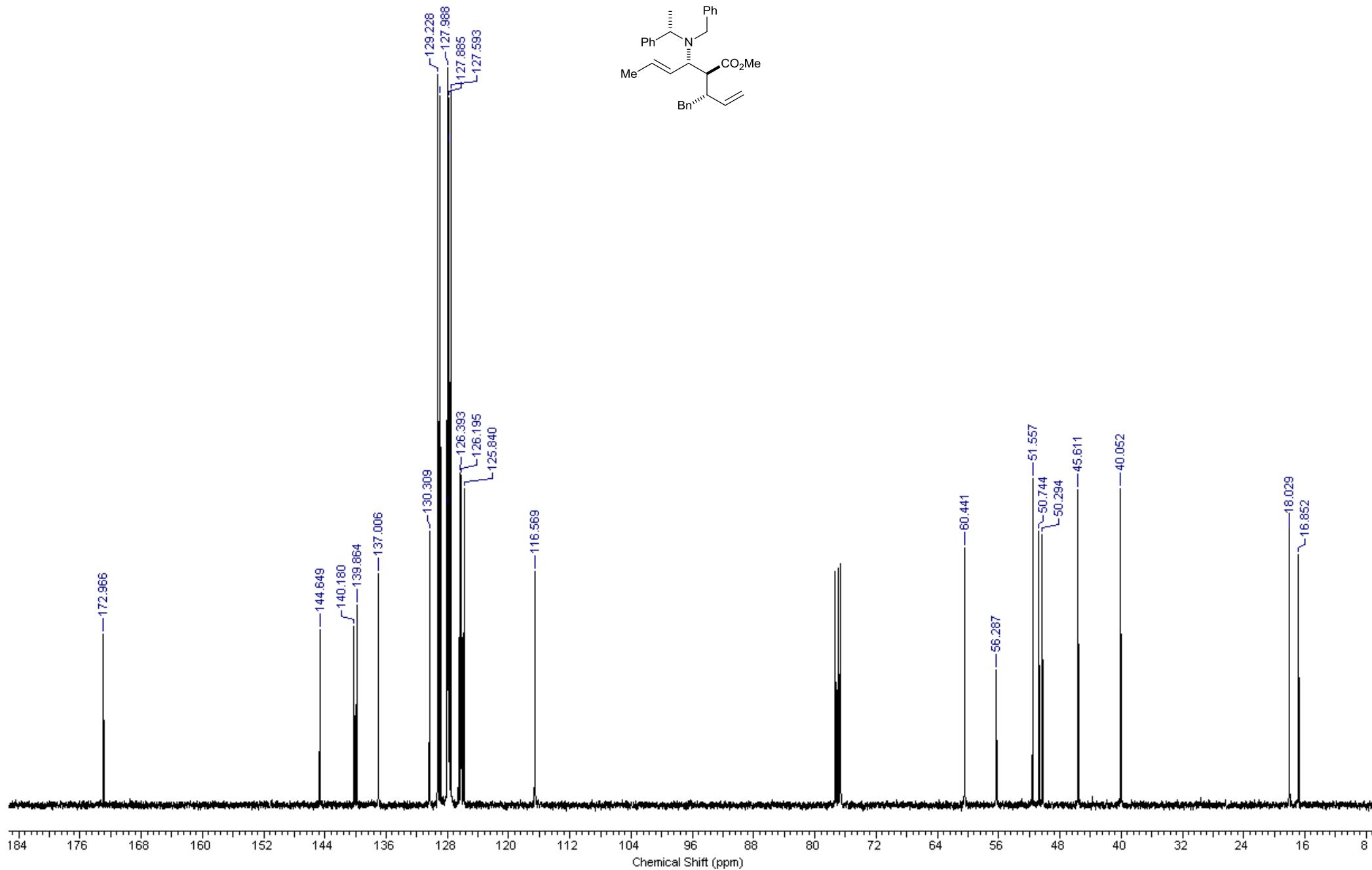
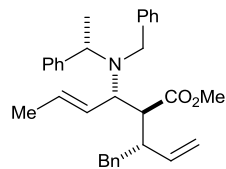
Methyl (*S,S,S,S,E*)-2-(pent-1'-en-3'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]hex-4-enoate **81** (100 MHz ^{13}C , CDCl_3)



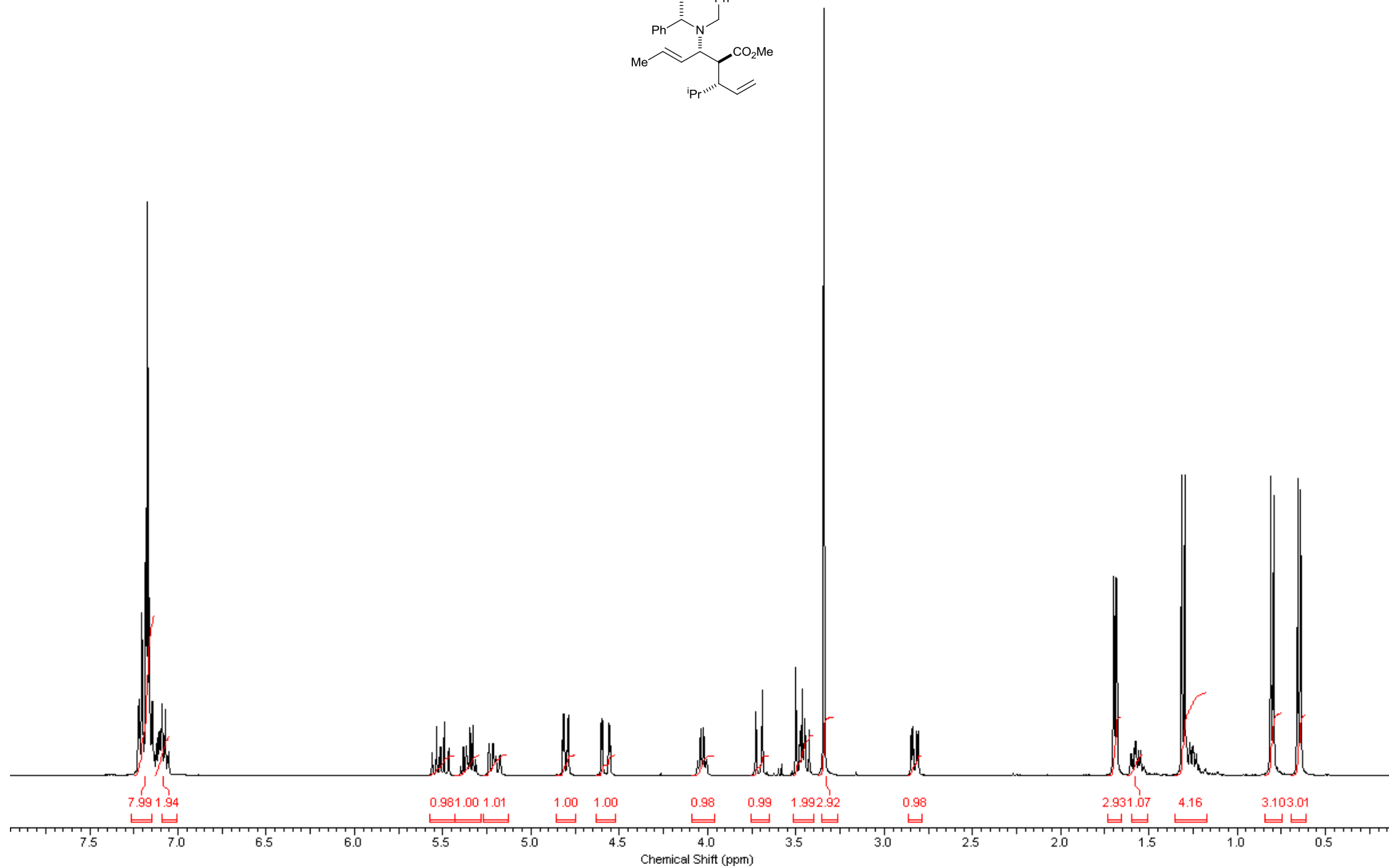
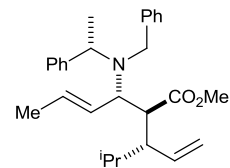
Methyl (*S,S,S,S,E*)-2-(1'-phenylbut-3'-en-2'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]hex-4-enoate **82** (400 MHz ^1H , CDCl_3)



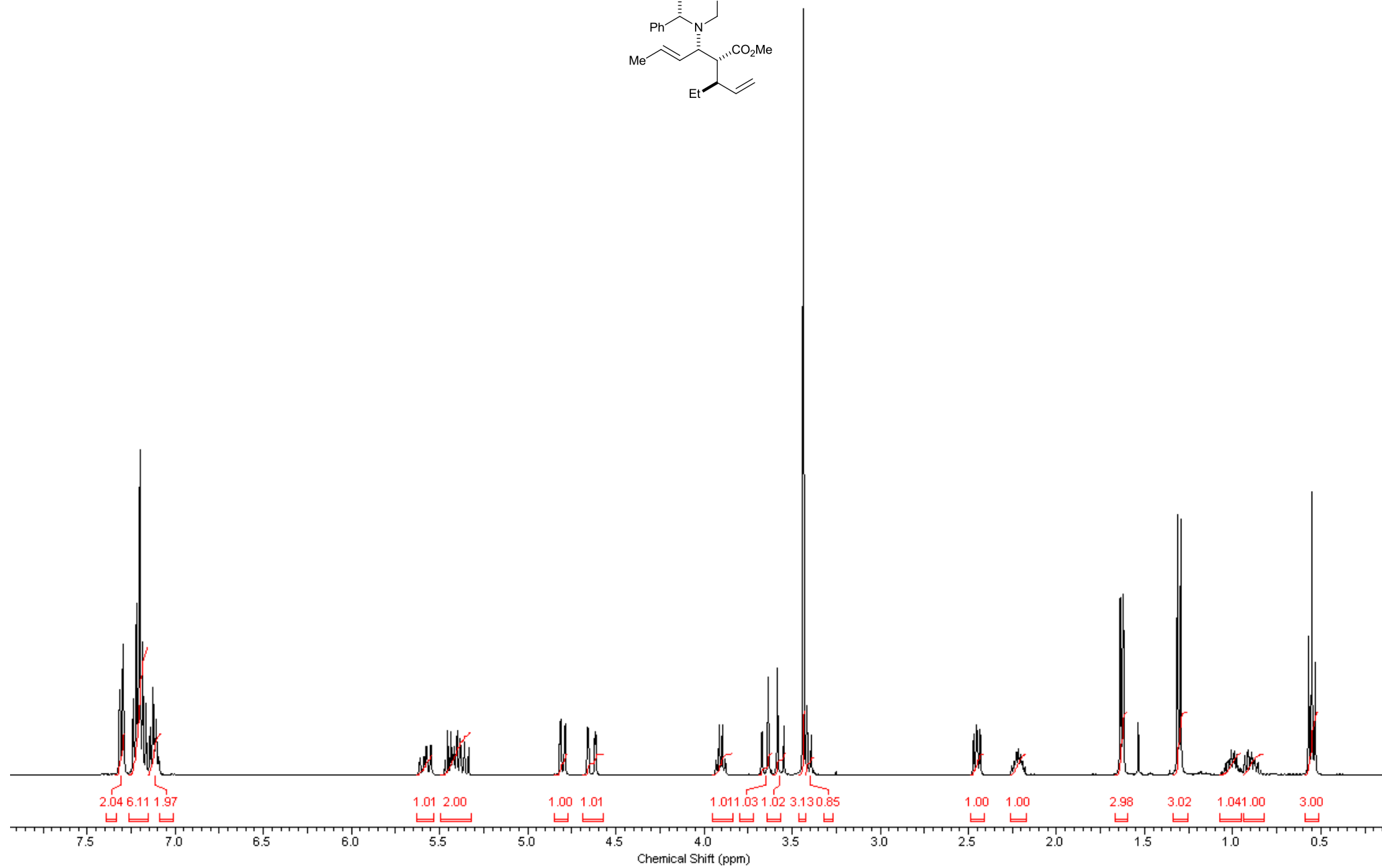
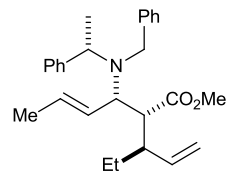
Methyl (*S,S,S,S,E*)-2-(1'-phenylbut-3'-en-2'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]hex-4-enoate **82** (100 MHz ^{13}C , CDCl_3)



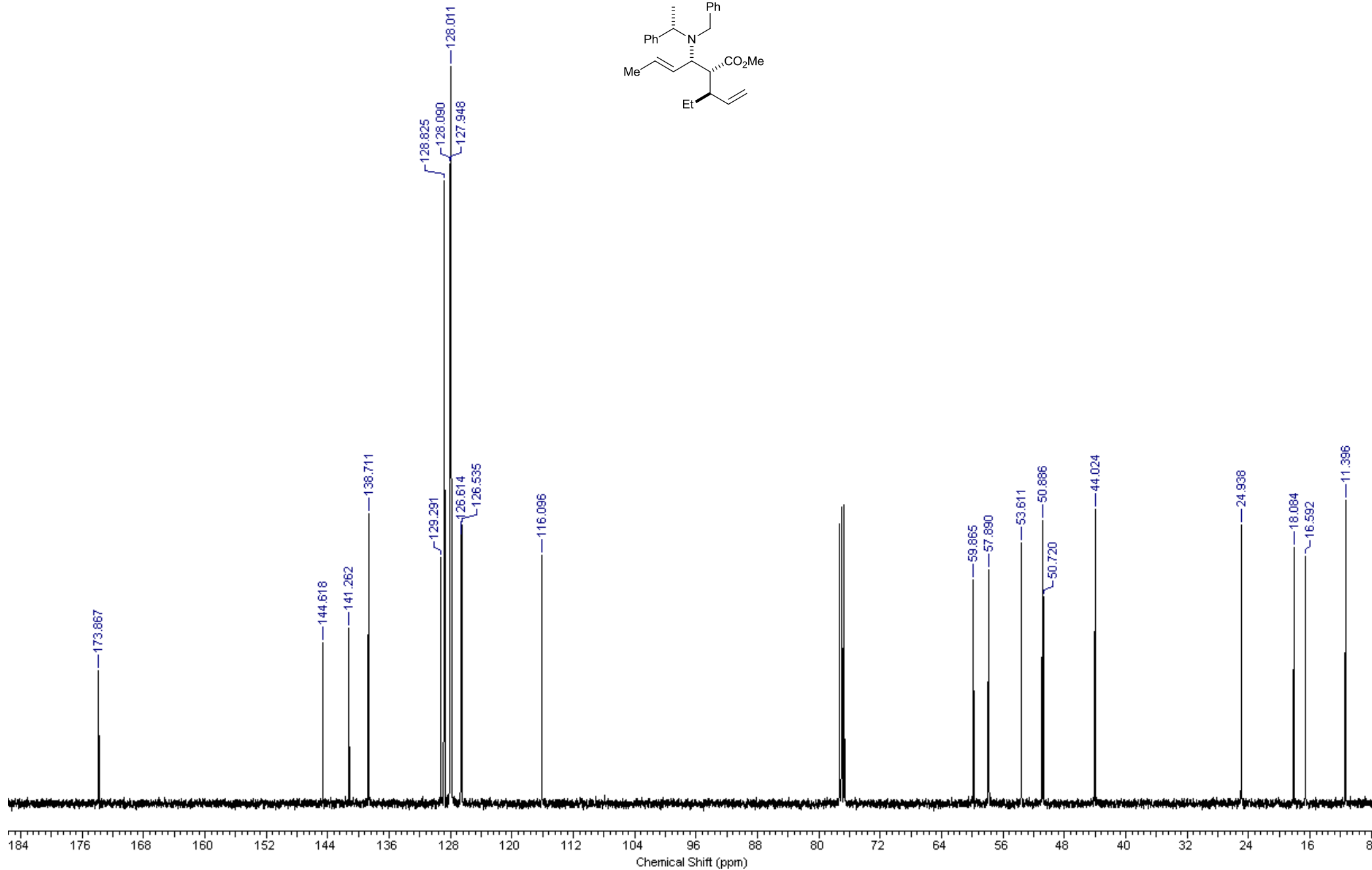
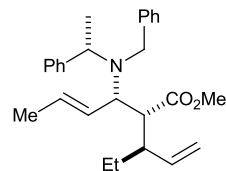
Methyl (*S,S,S,S,E*)-2-(4'-methylpent-1'-en-3'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]hex-4-enoate 83 (400 MHz ^1H , CDCl_3)



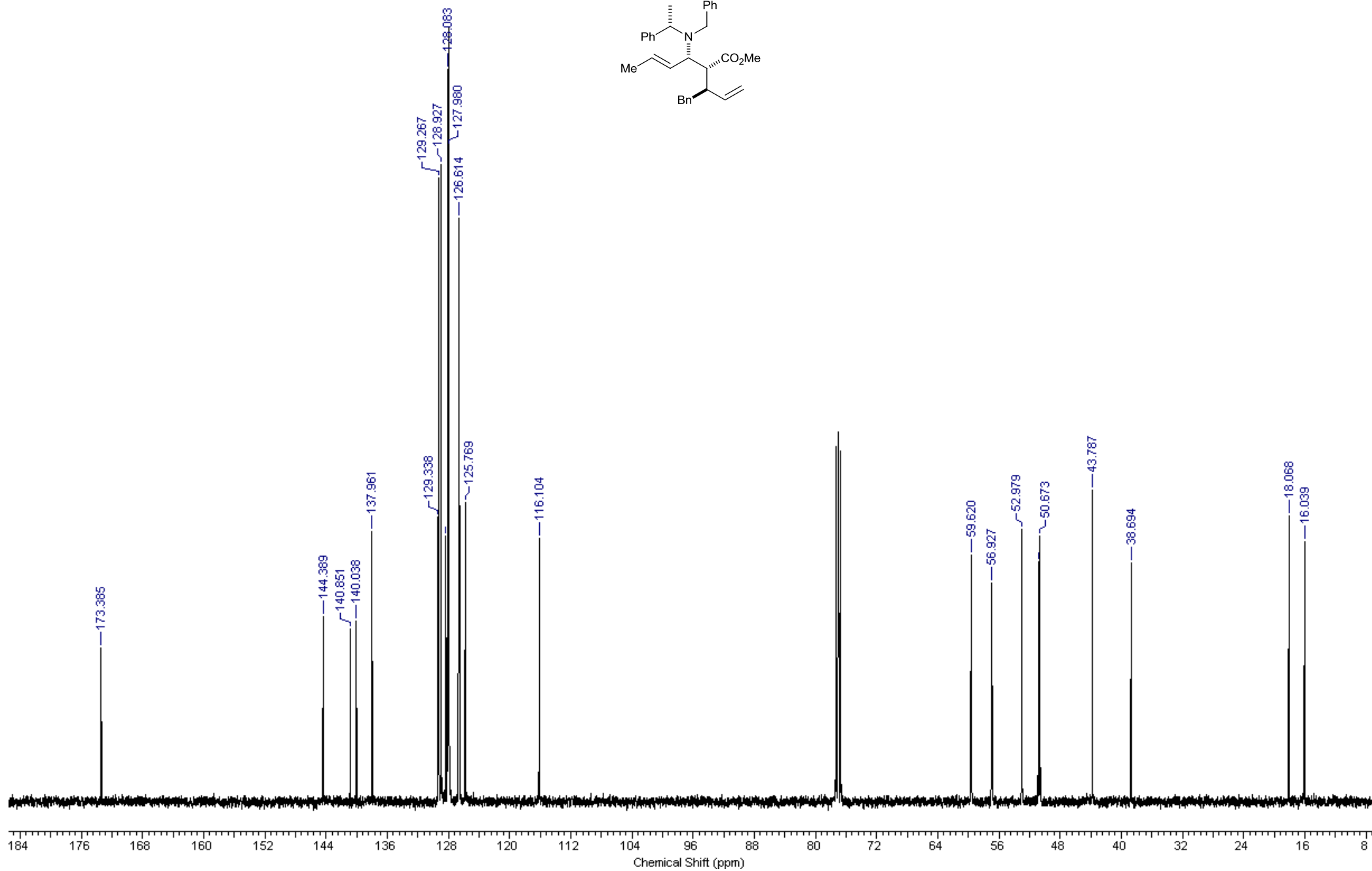
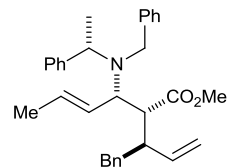
Methyl (2*R*,3*S*,1'*R*, α *S*,*E*)-2-(pent-1'-en-3'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]hex-4-enoate 86 (400 MHz ^1H , CDCl_3)



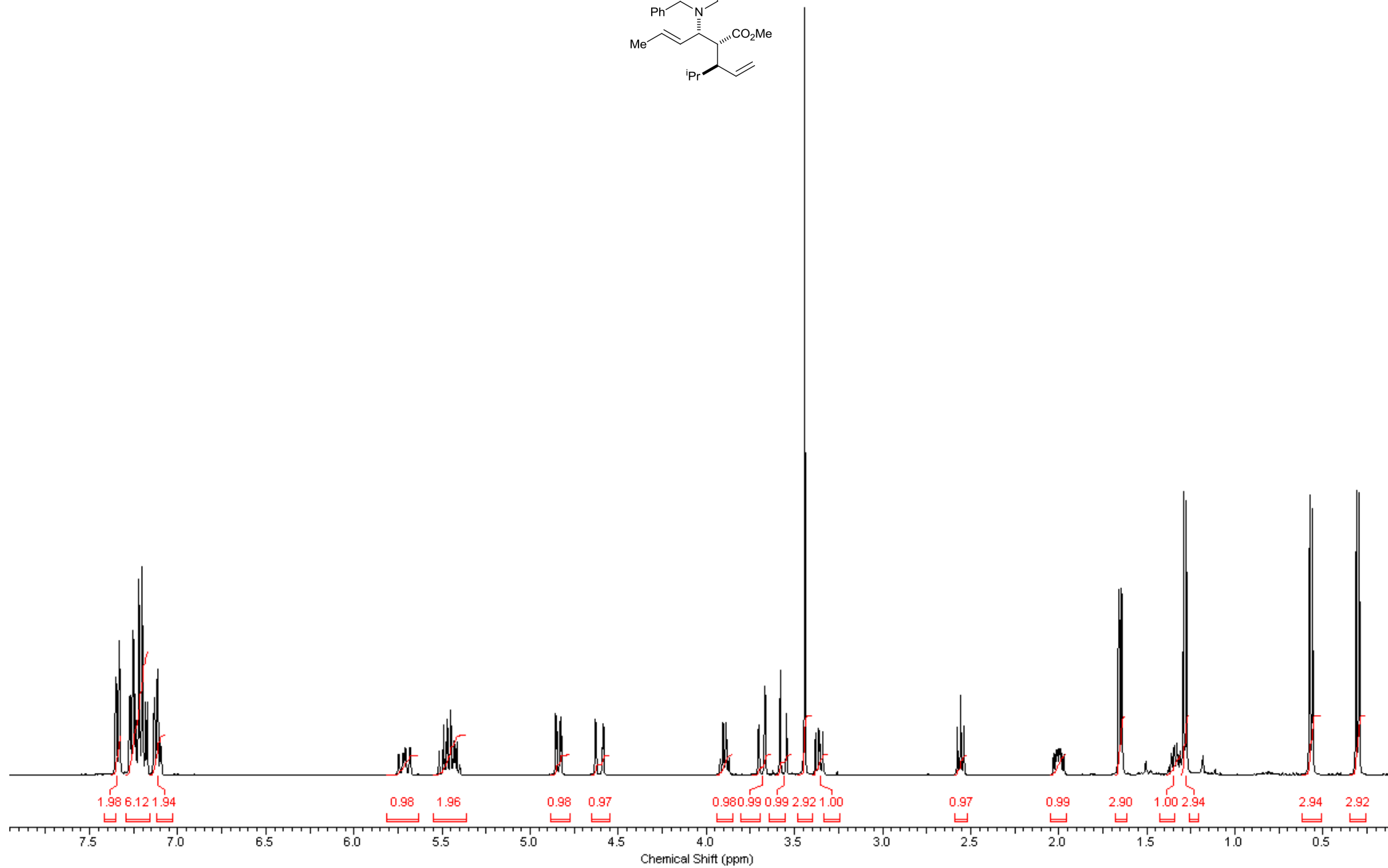
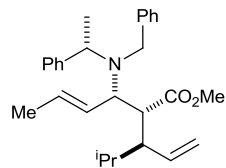
Methyl (2*R*,3*S*,1'*R*, α *S*,*E*)-2-(pent-1'-en-3'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]hex-4-enoate 86 (100 MHz ^{13}C , CDCl_3)



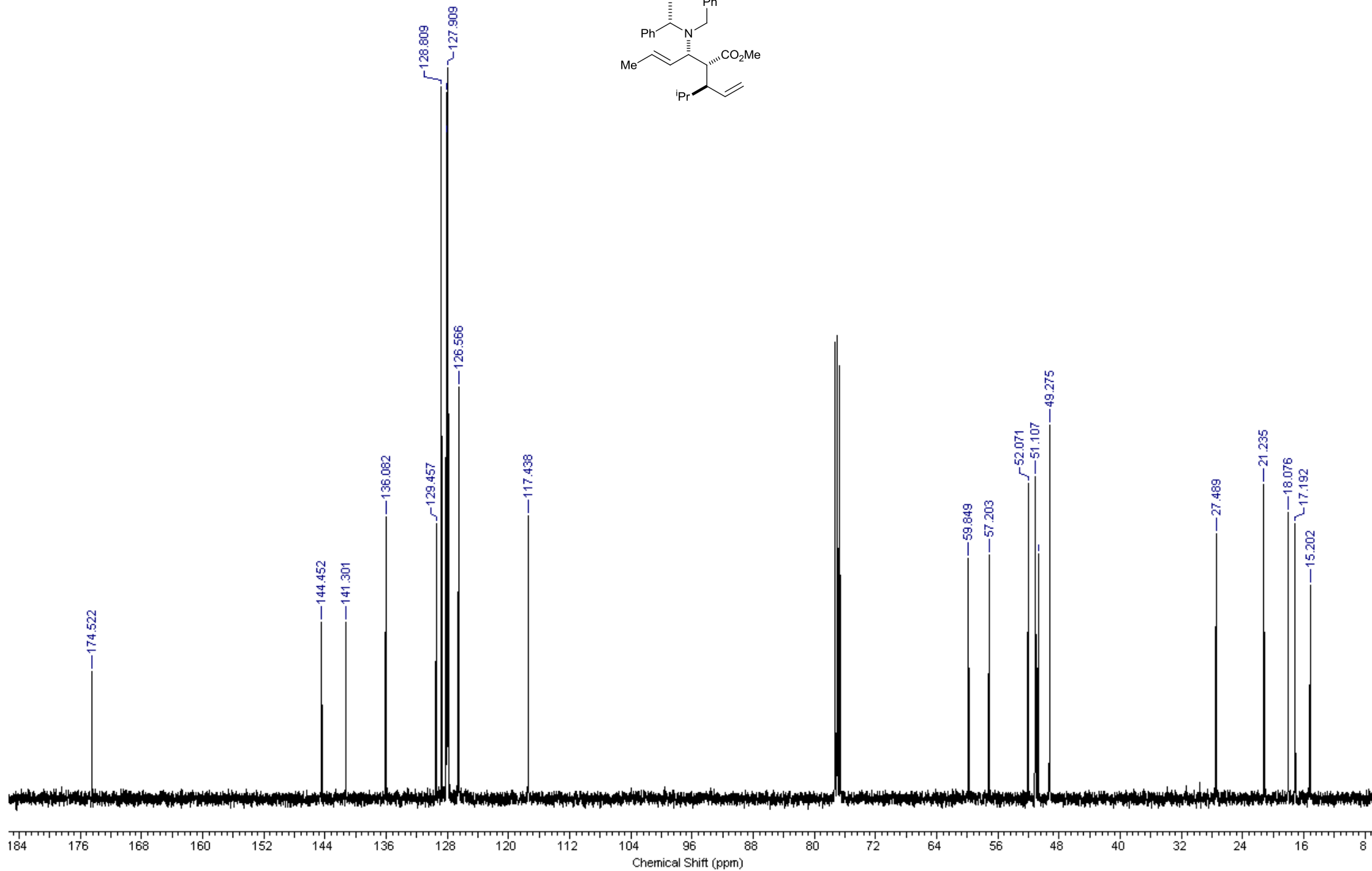
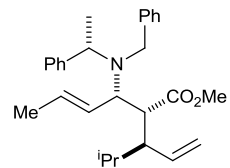
Methyl (2*R*,3*S*,1'*R*, α *S*,*E*)-2-(1'-phenylbut-3'-en-2'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]hex-4-enoate 87 (100 MHz ^{13}C , CDCl_3)



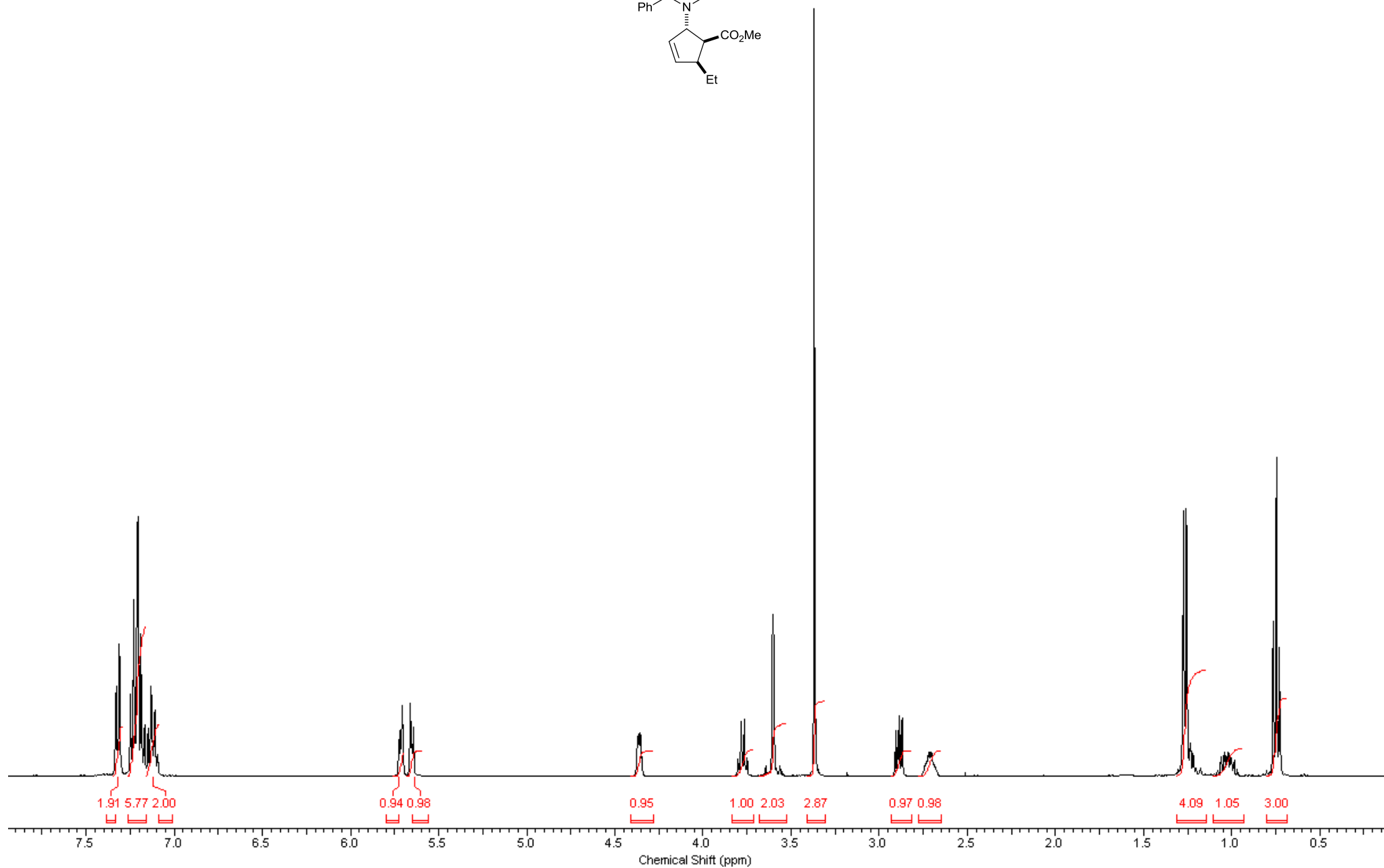
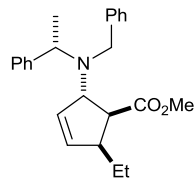
Methyl (2*R*,3*S*,1'*R*, α *S*,*E*)-2-(4'-methylpent-1'-en-3'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]hex-4-enoate 88 (400 MHz ^1H , CDCl_3)



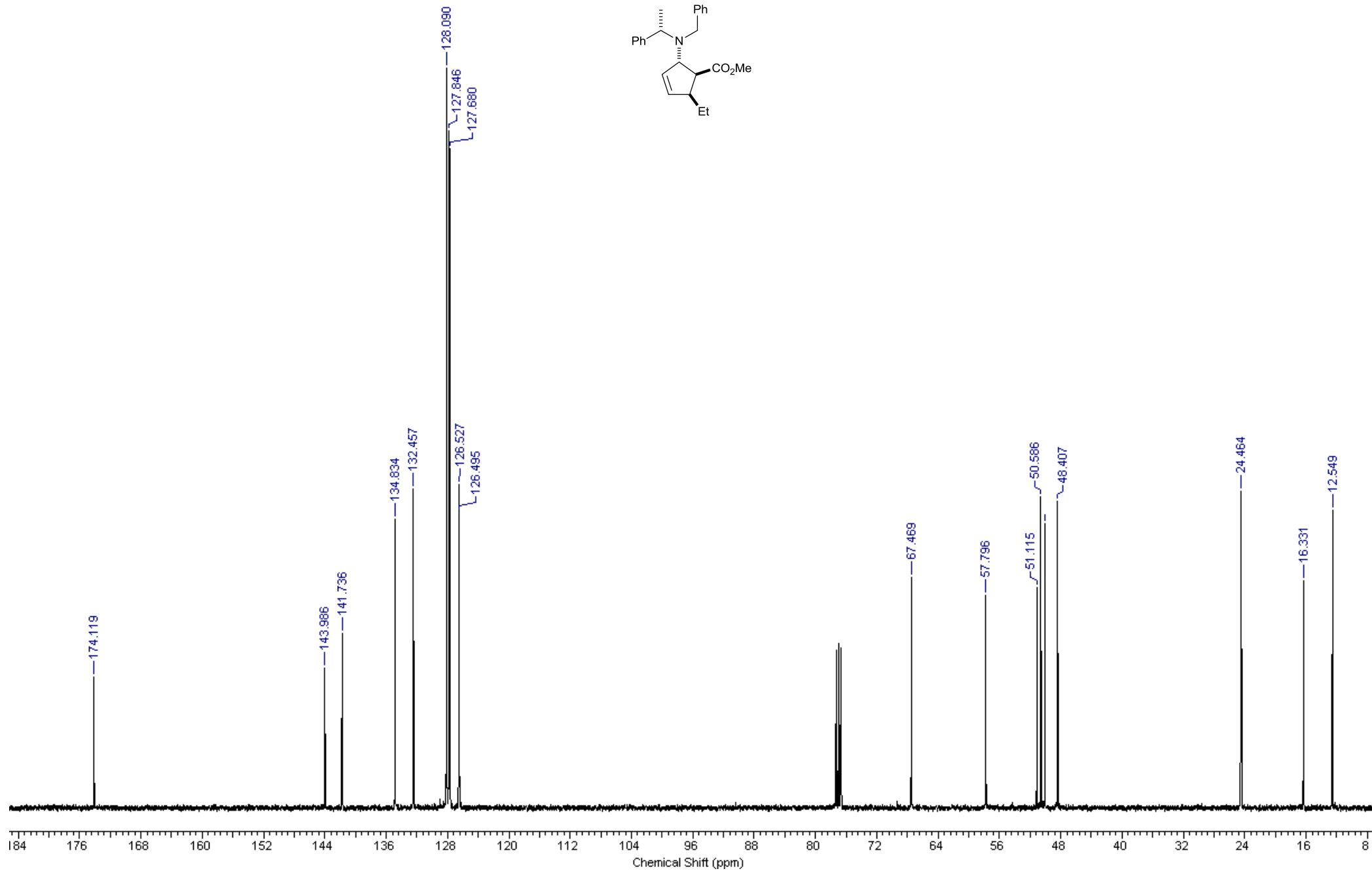
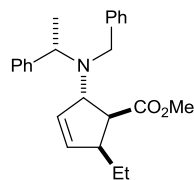
Methyl (2*R*,3*S*,1'*R*, α *S*,*E*)-2-(4'-methylpent-1'-en-3'-yl)-3-[*N*-benzyl-*N*-(α -methylbenzyl)amino]hex-4-enoate 88 (100 MHz ^{13}C , CDCl_3)



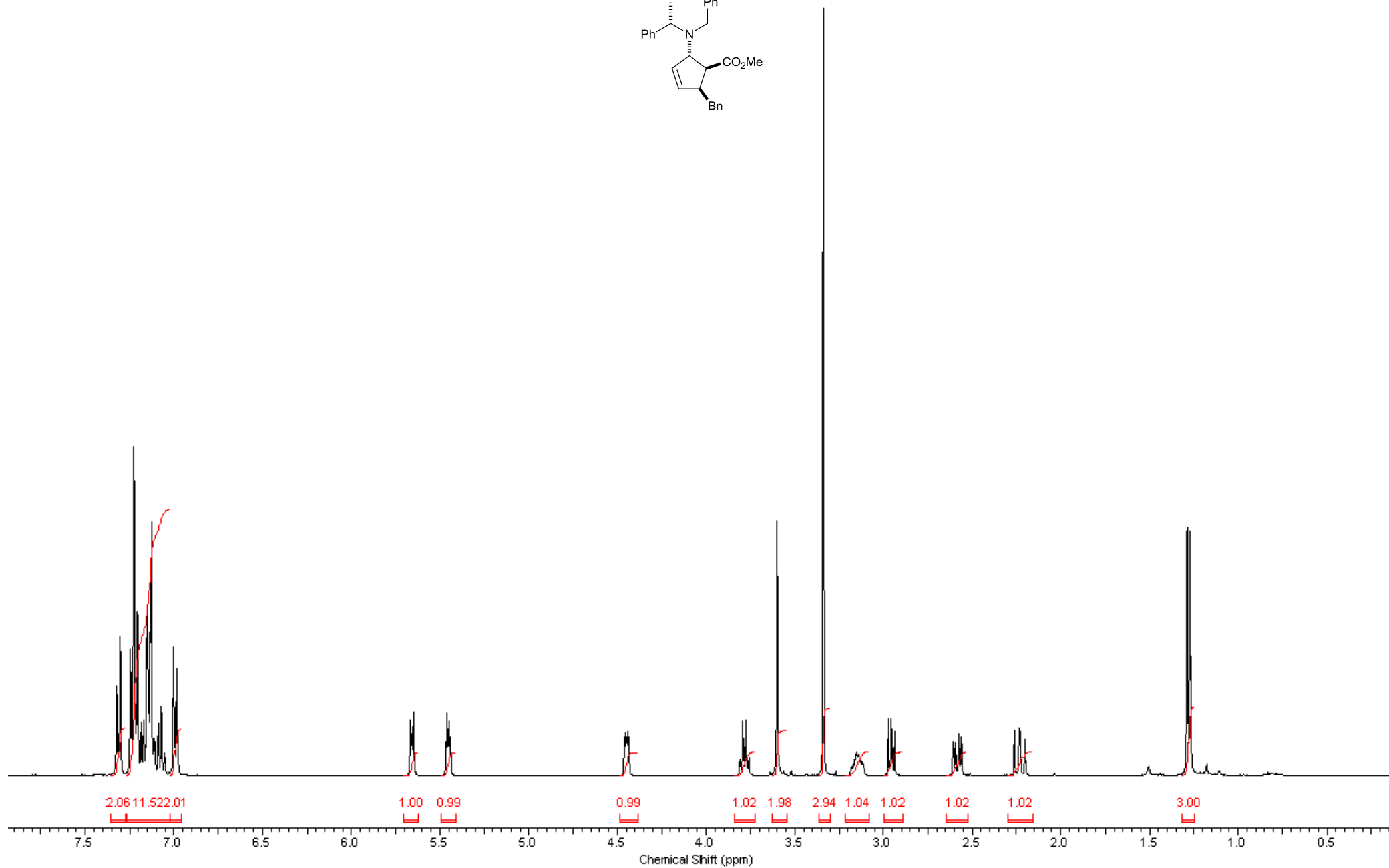
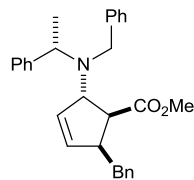
Methyl (*S,S,S,S*)-2-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-5-ethylcyclopent-3-ene-1-carboxylate **91** (400 MHz ^1H , CDCl_3)



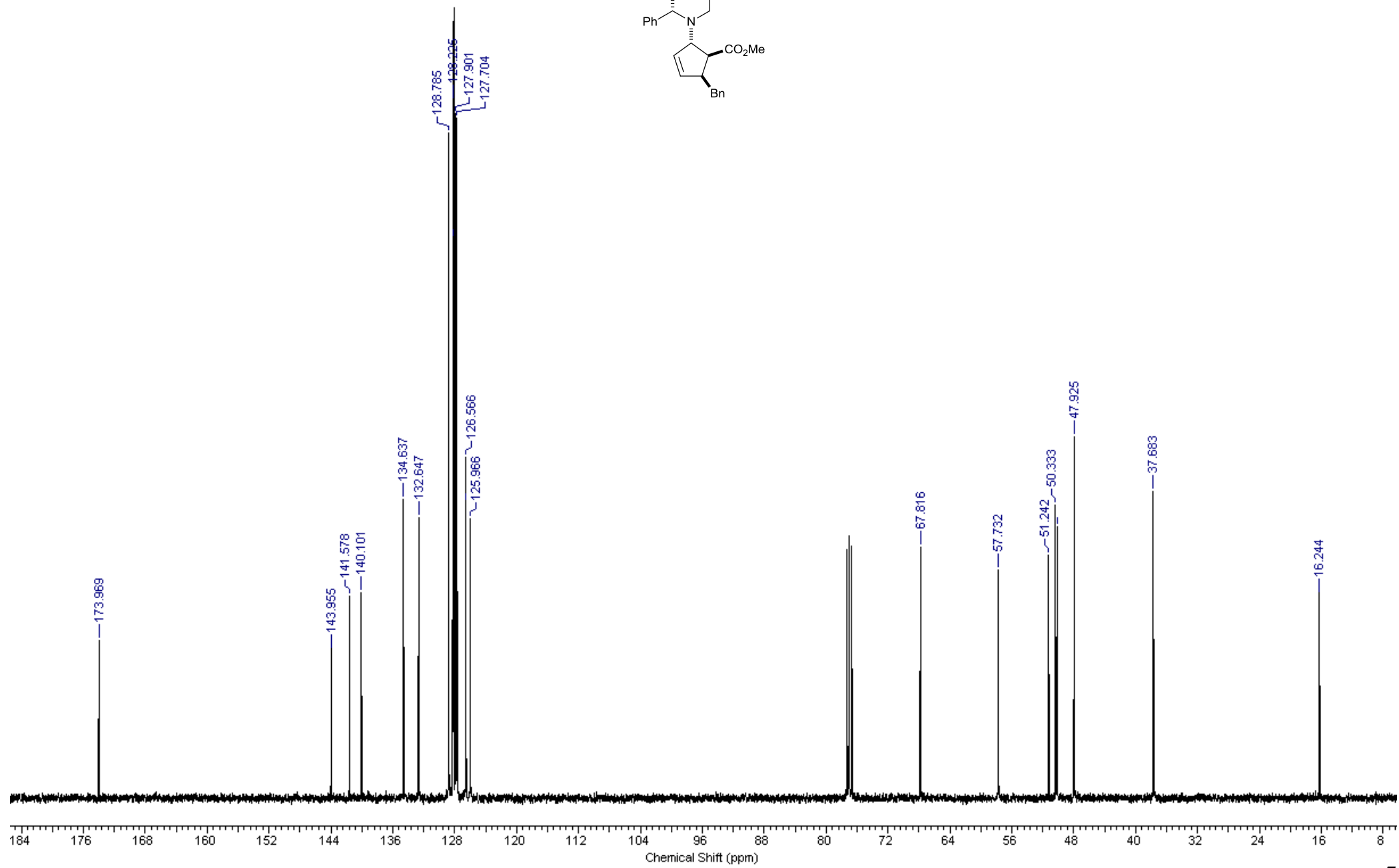
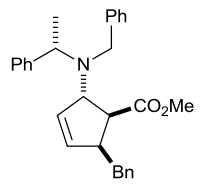
Methyl (*S,S,S,S*)-2-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-5-ethylcyclopent-3-ene-1-carboxylate **91** (100 MHz ^{13}C , CDCl_3)



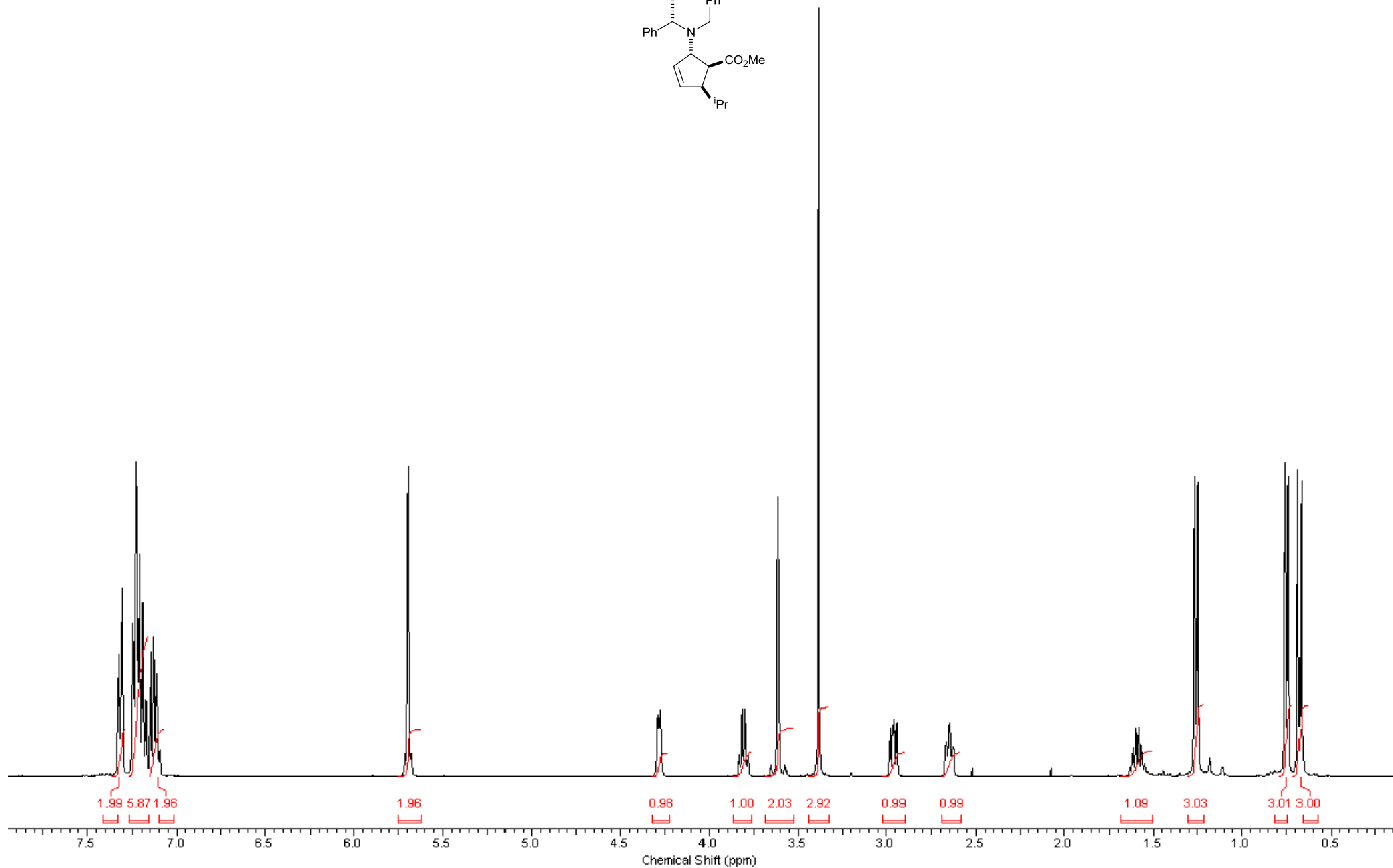
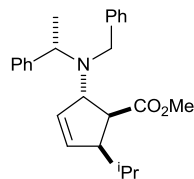
Methyl (*S,S,S,S*)-2-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-5-benzylcyclopent-3-ene-1-carboxylate **92** (400 MHz ^1H , CDCl_3)



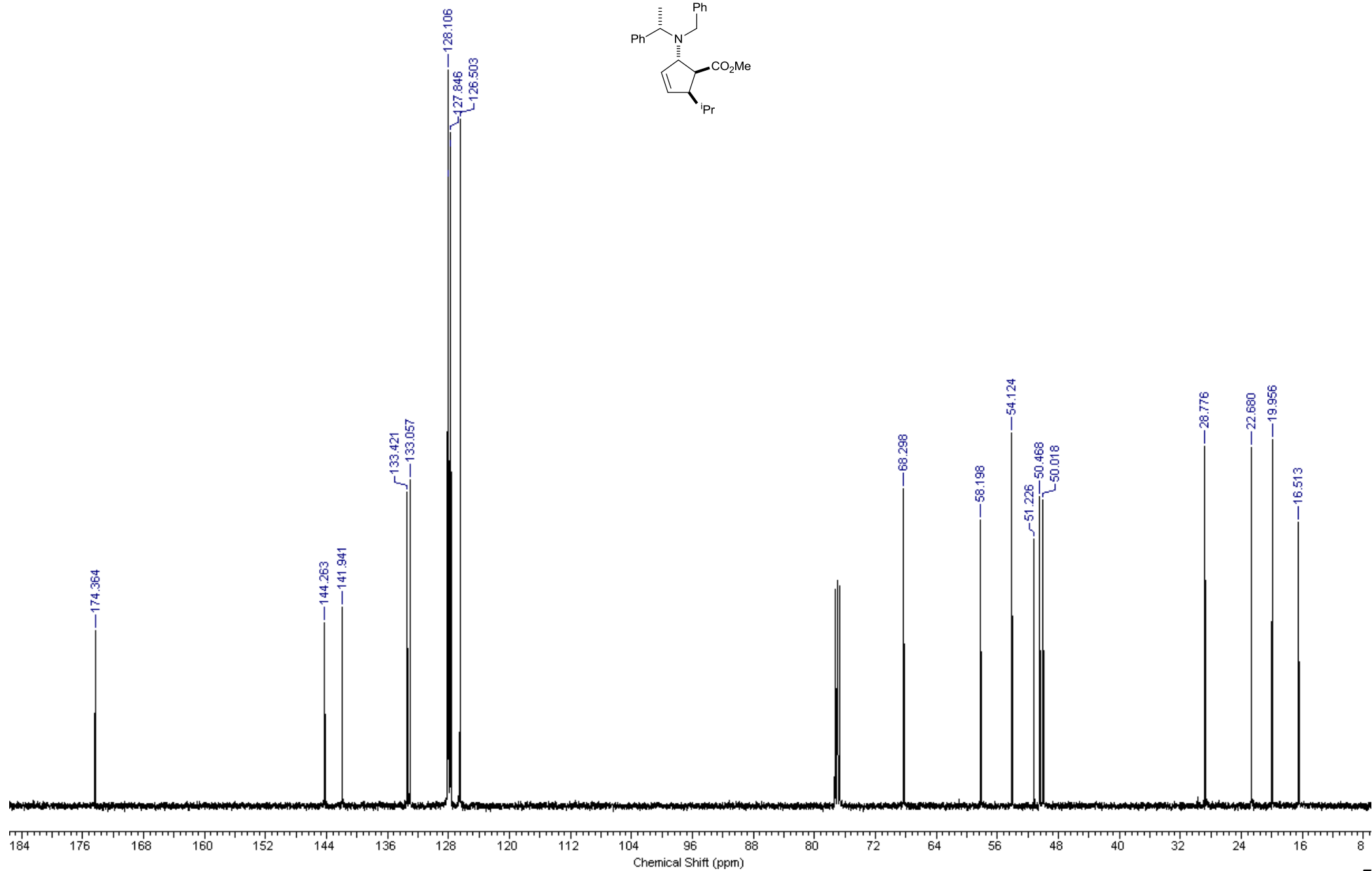
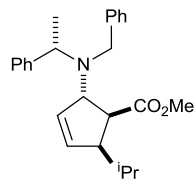
Methyl (*S,S,S,S*)-2-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-5-benzylcyclopent-3-ene-1-carboxylate **92** (100 MHz ^{13}C , CDCl_3)



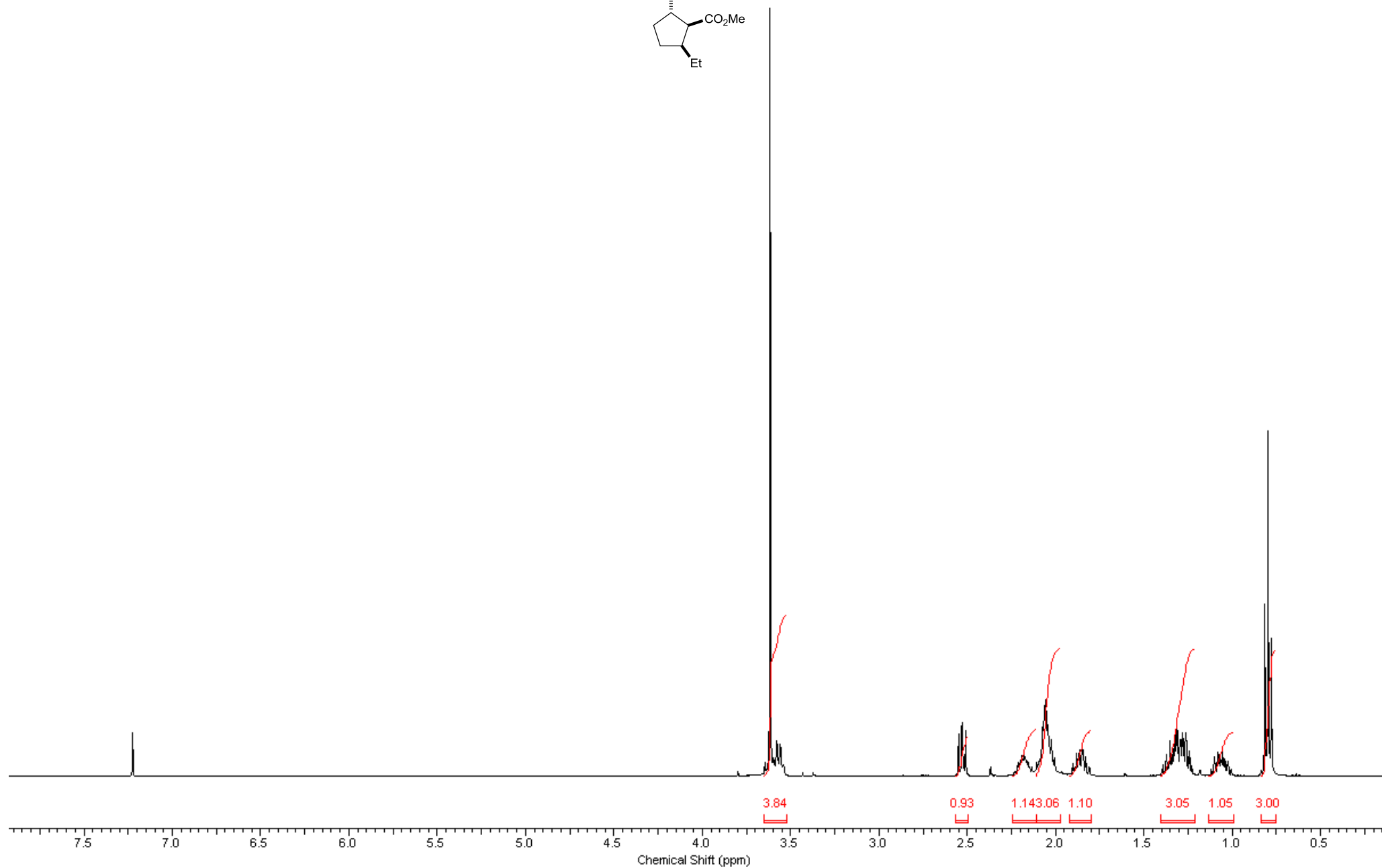
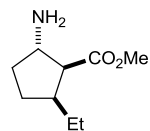
Methyl (*S,S,S,S*)-2-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-5-isopropylcyclopent-3-ene-1-carboxylate 93 (400 MHz ^1H , CDCl_3)



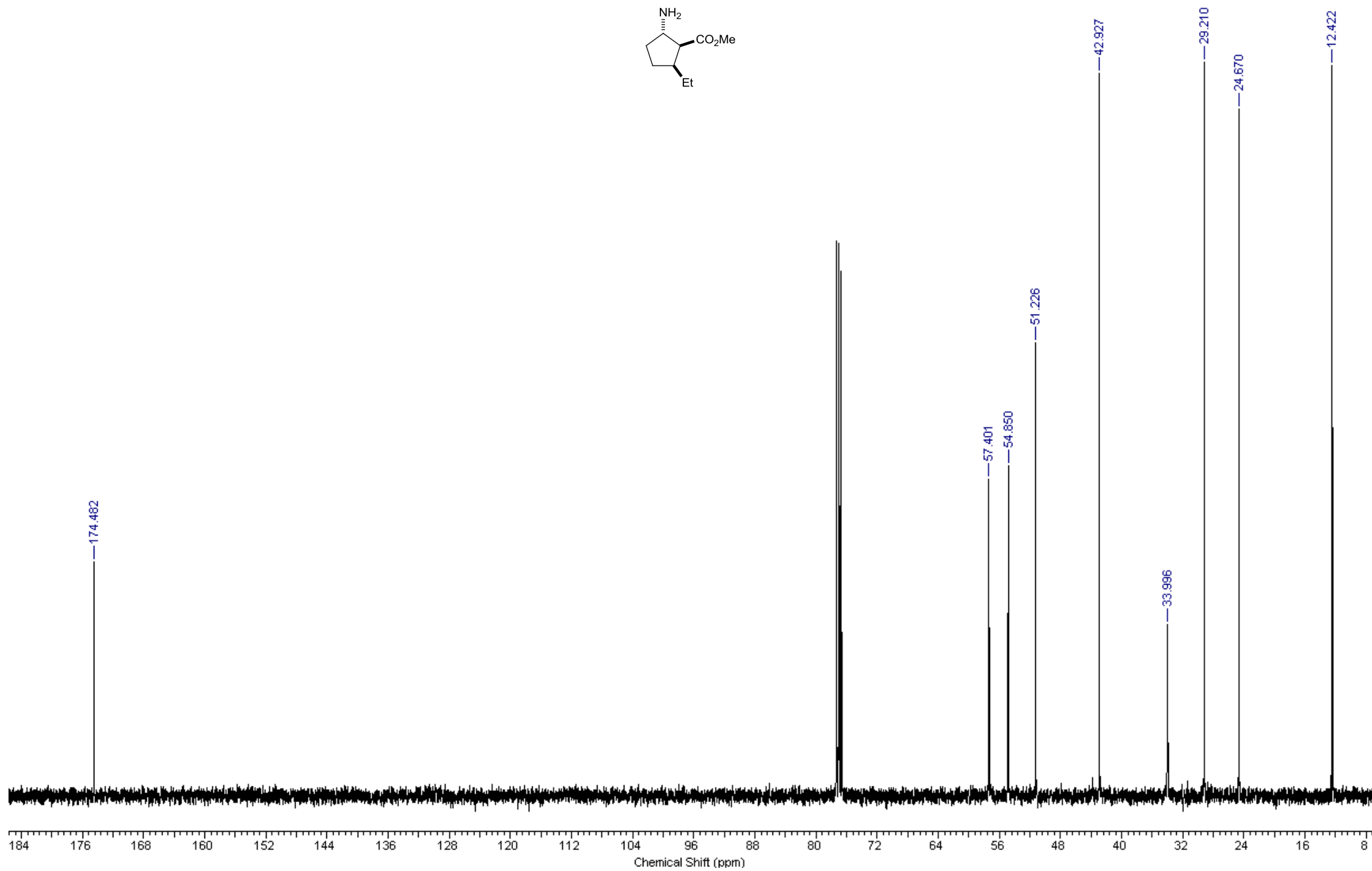
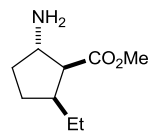
Methyl (*S,S,S,S*)-2-[*N*-benzyl-*N*-(α -methylbenzyl)amino]-5-isopropylcyclopent-3-ene-1-carboxylate 93 (100 MHz ^{13}C , CDCl_3)



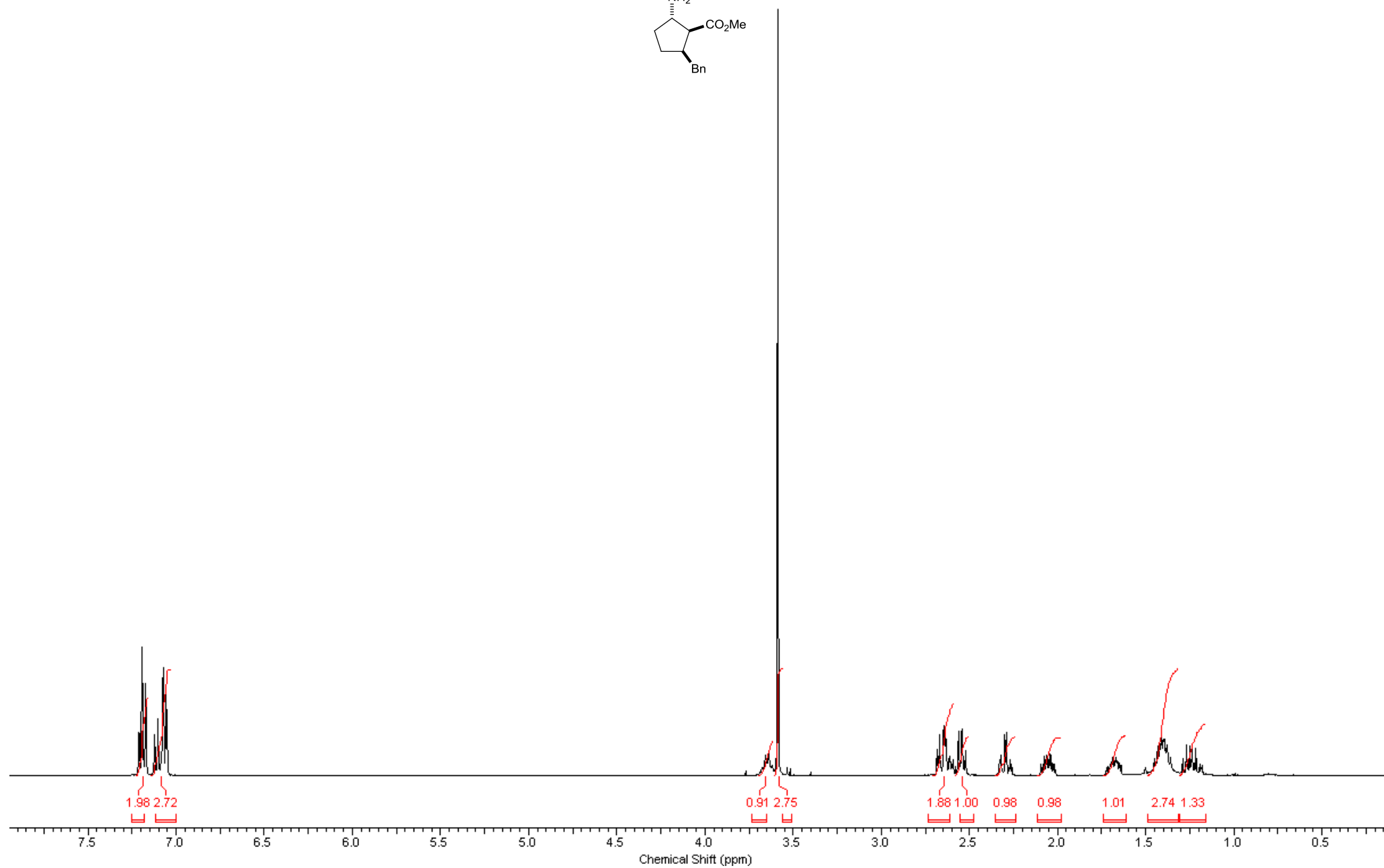
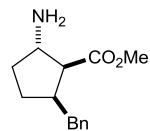
Methyl (*S,S,S*)-2-amino-5-ethylcyclopentane-1-carboxylate **96** (400 MHz ^1H , CDCl_3)



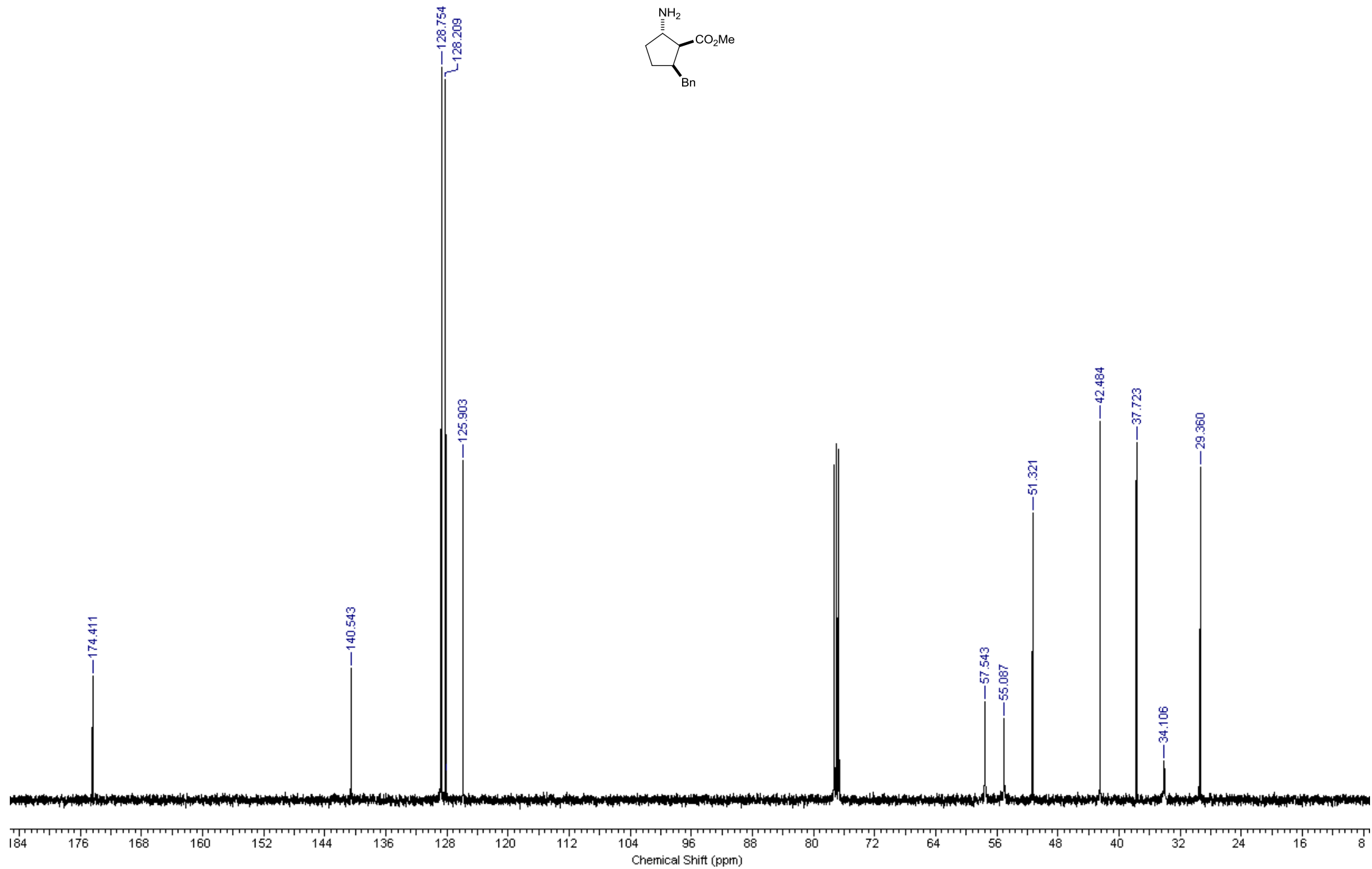
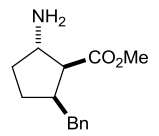
Methyl (*S,S,S*)-2-amino-5-ethylcyclopentane-1-carboxylate **96** (100 MHz ^{13}C , CDCl_3)



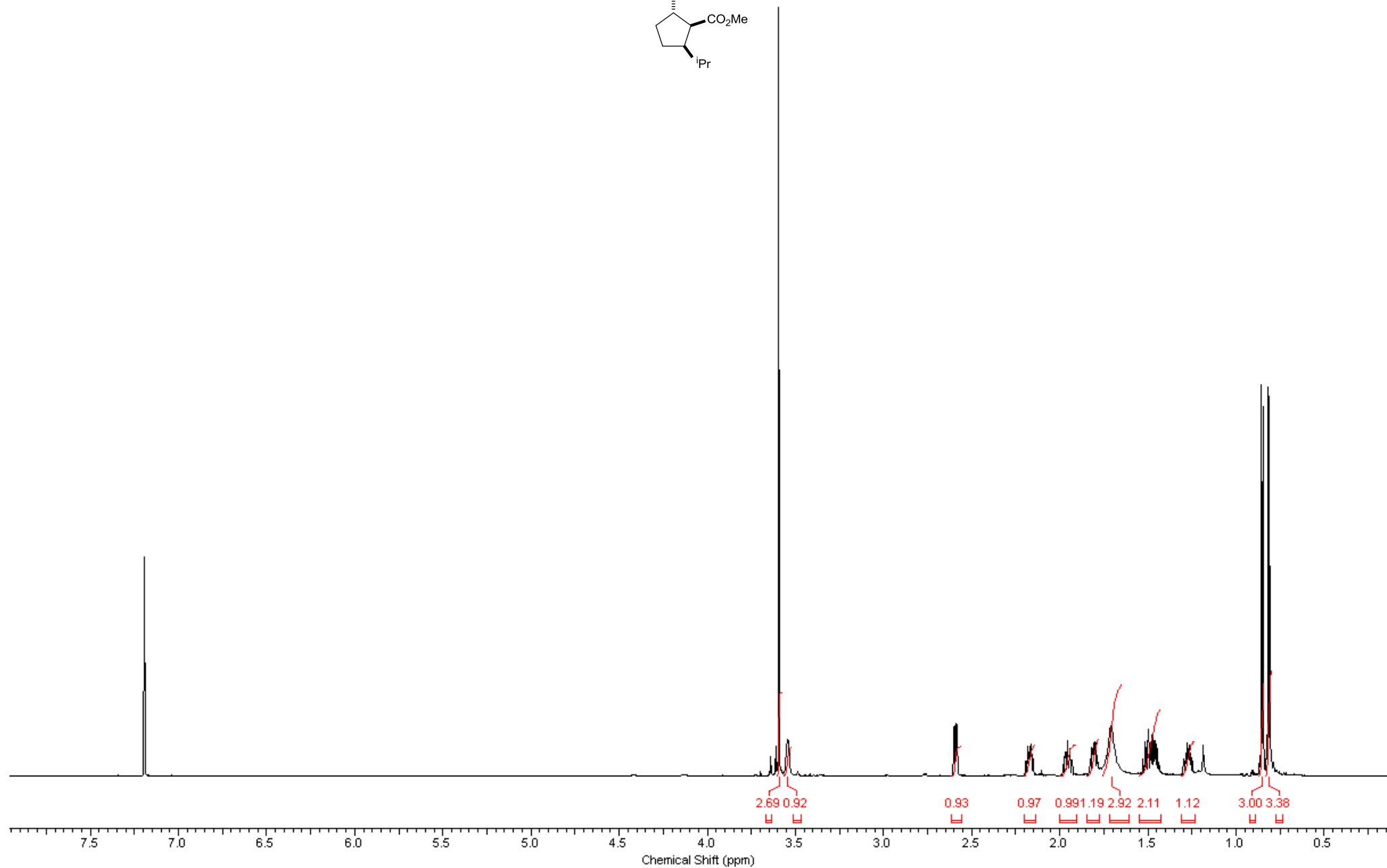
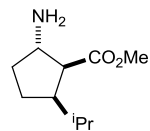
Methyl (1*S*,2*S*,5*R*)-2-amino-5-benzylcyclopentane-1-carboxylate **97** (400 MHz ^1H , CDCl_3)



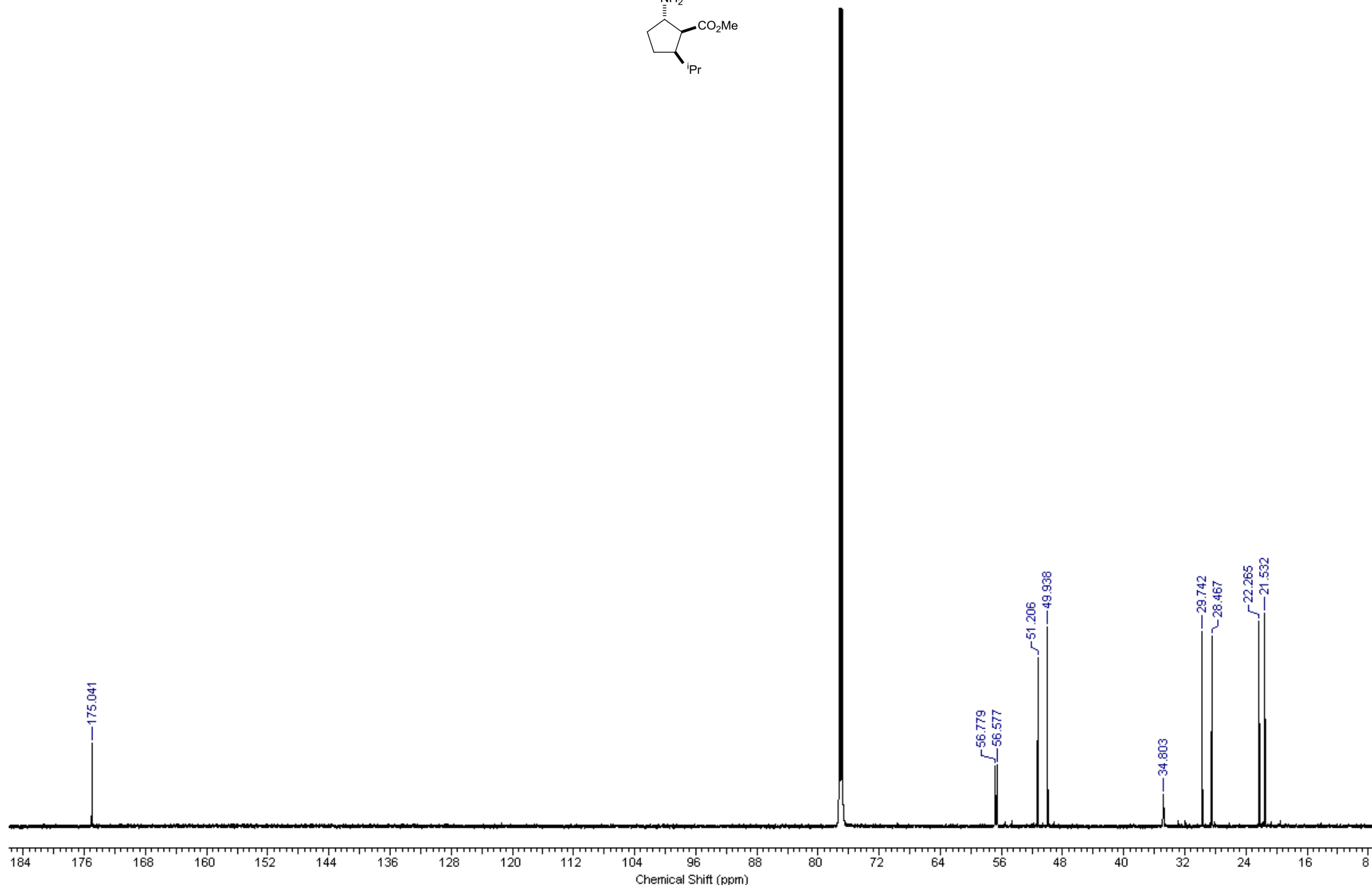
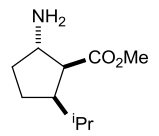
Methyl (1*S*,2*S*,5*R*)-2-amino-5-benzylcyclopentane-1-carboxylate **97** (100 MHz ¹³C, CDCl₃)



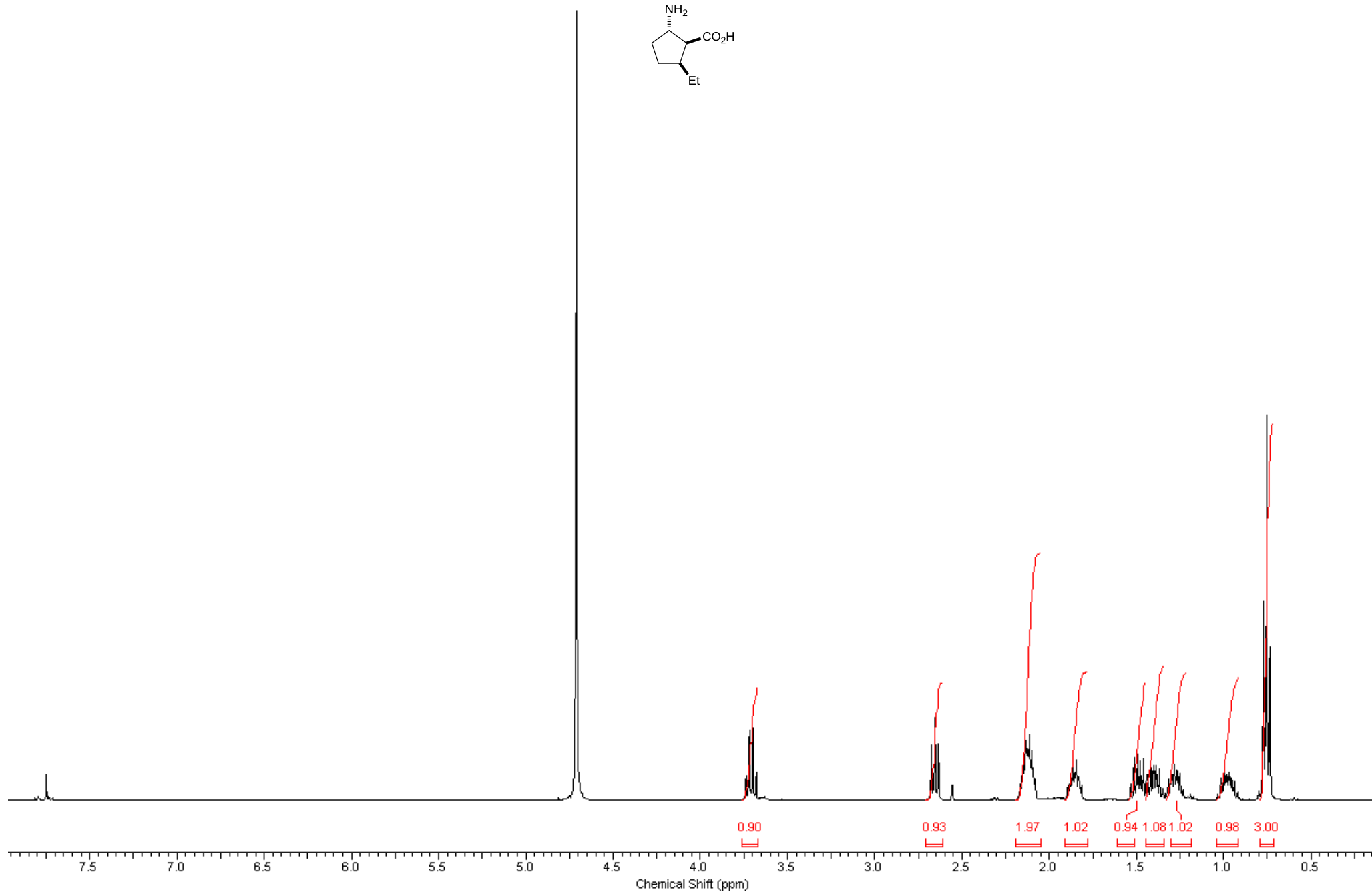
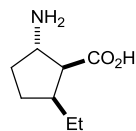
Methyl (1*S*,2*S*,5*R*)-2-amino-5-isopropylcyclopentane-1-carboxylate **98** (700 MHz ¹H, CDCl₃)



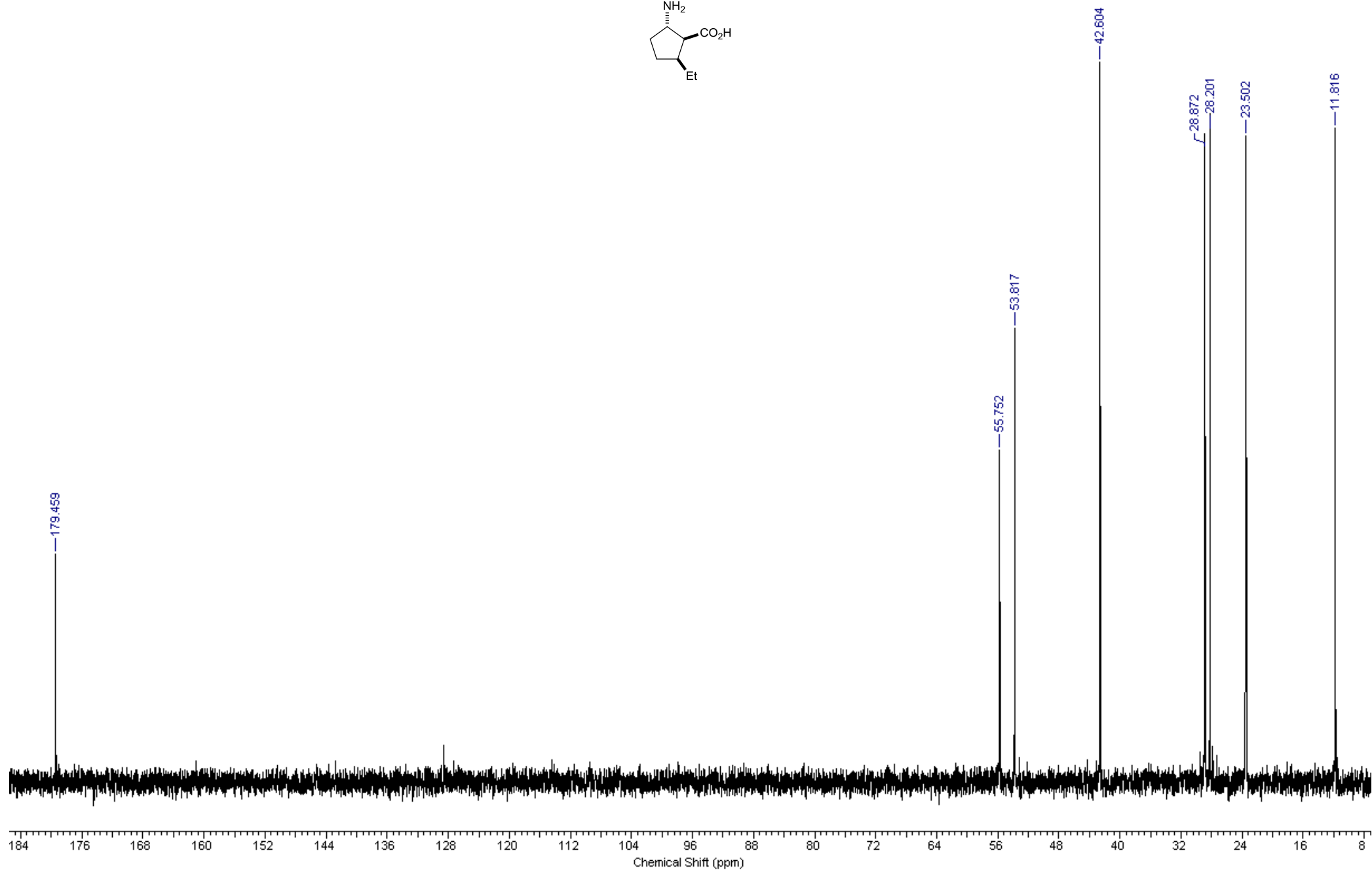
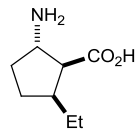
Methyl (1*S*,2*S*,5*R*)-2-amino-5-isopropylcyclopentane-1-carboxylate **98** (176 MHz ^{13}C , CDCl_3)



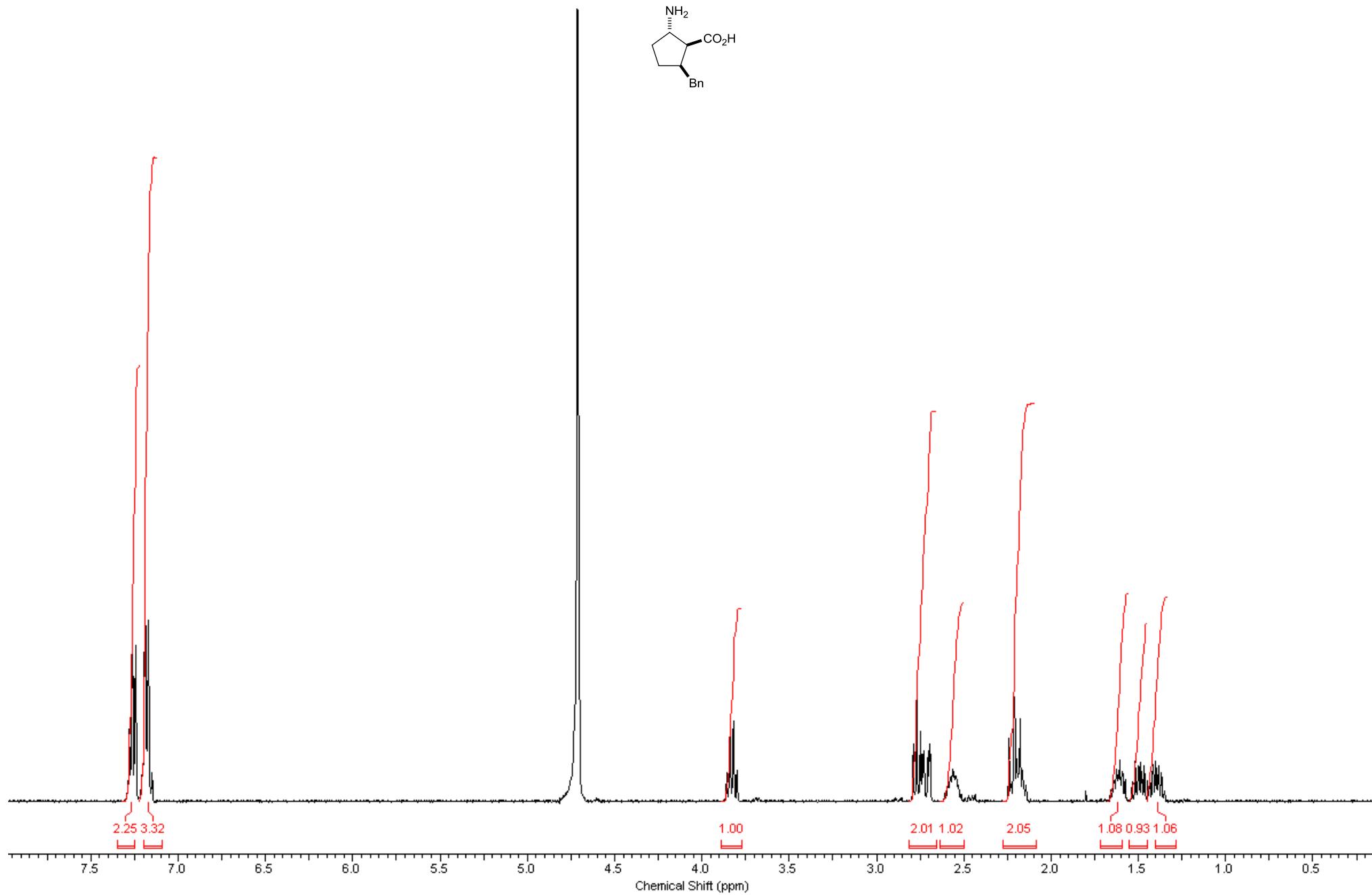
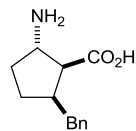
(*S,S,S*)-2-Amino-5-ethylcyclopentane-1-carboxylic acid 101 (400 MHz ^1H , D_2O)



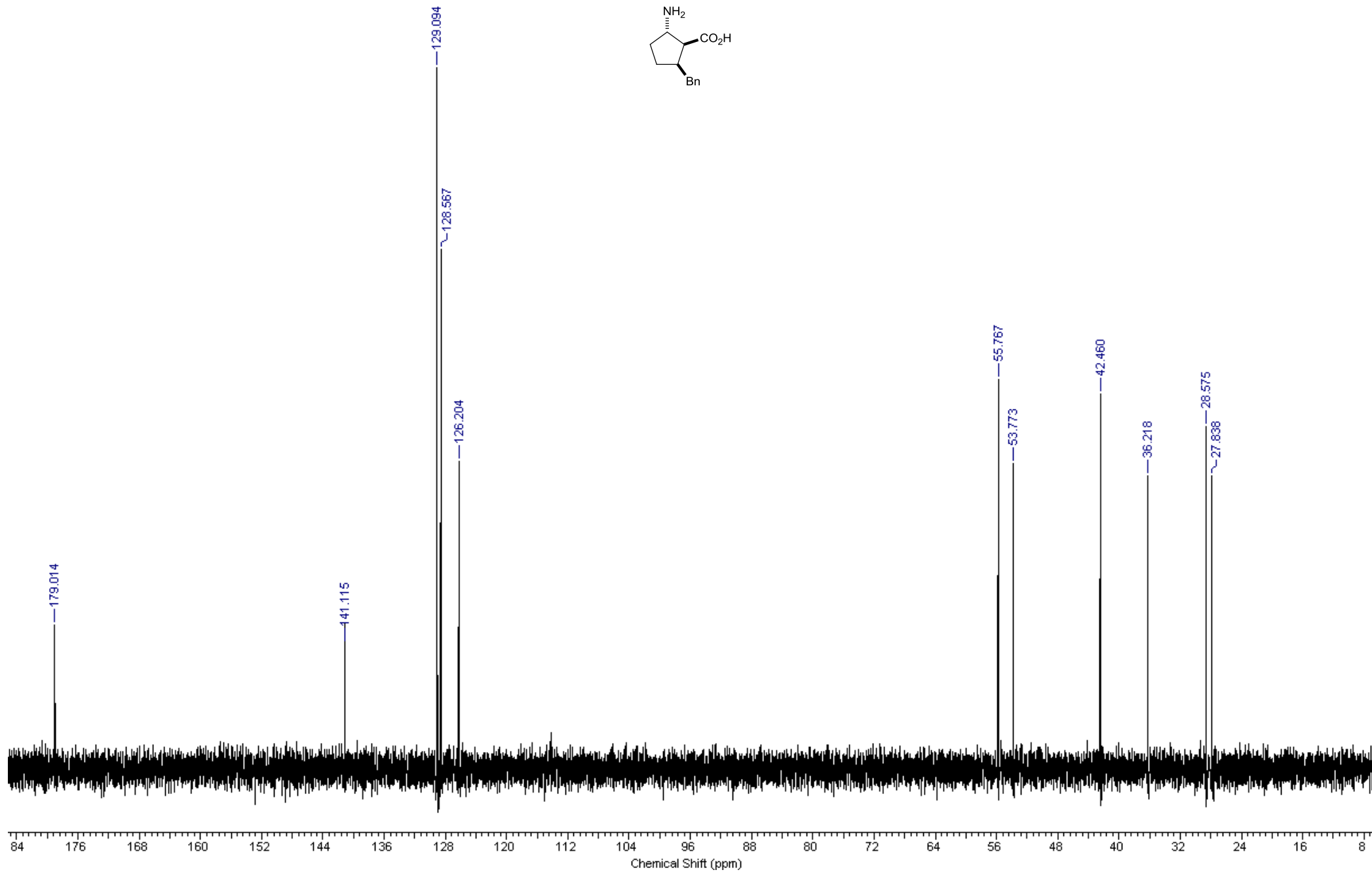
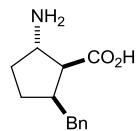
(*S,S,S*)-2-Amino-5-ethylcyclopentane-1-carboxylic acid 101 (100 MHz ^{13}C , D_2O)



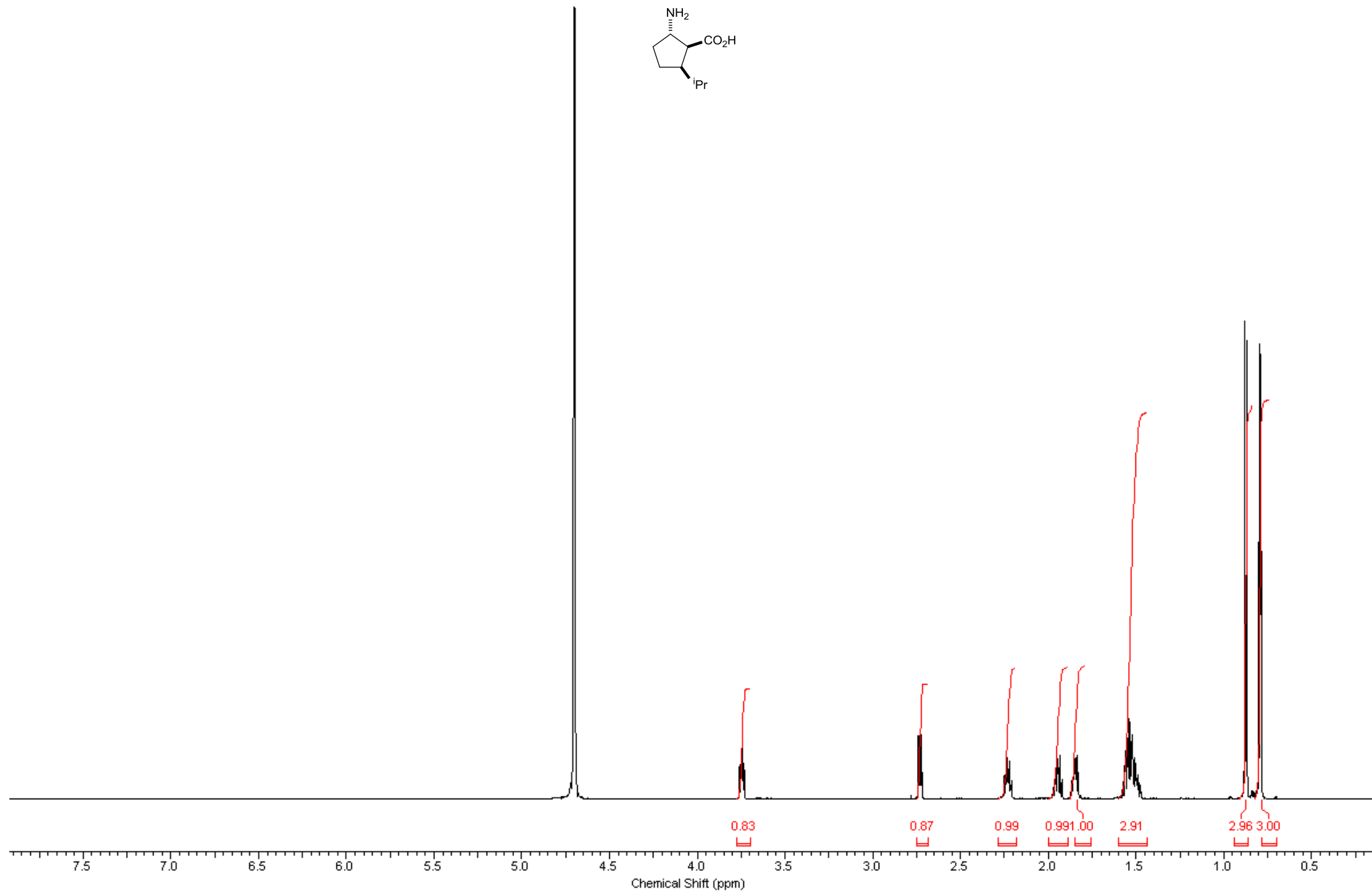
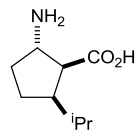
(1*S*,2*S*,5*R*)-2-Amino-5-benzylcyclopentane-1-carboxylic acid 102 (400 MHz ¹H, D₂O)



(1*S*,2*S*,5*R*)-2-Amino-5-benzylcyclopentane-1-carboxylic acid 102 (176 MHz ^{13}C , D_2O)



(1*S*,2*S*,5*R*)-2-Amino-5-isopropylcyclopentane-1-carboxylic acid 103 (700 MHz ¹H, D₂O)



(1*S*,2*S*,5*R*)-2-Amino-5-isopropylcyclopentane-1-carboxylic acid 103 (176 MHz ¹³C, D₂O)

