

Supplementary Material

Click chemistry-assisted synthesis of novel C-2 triazole-linked betulinic acid conjugates with azidothymidine as potential anti-HIV agents

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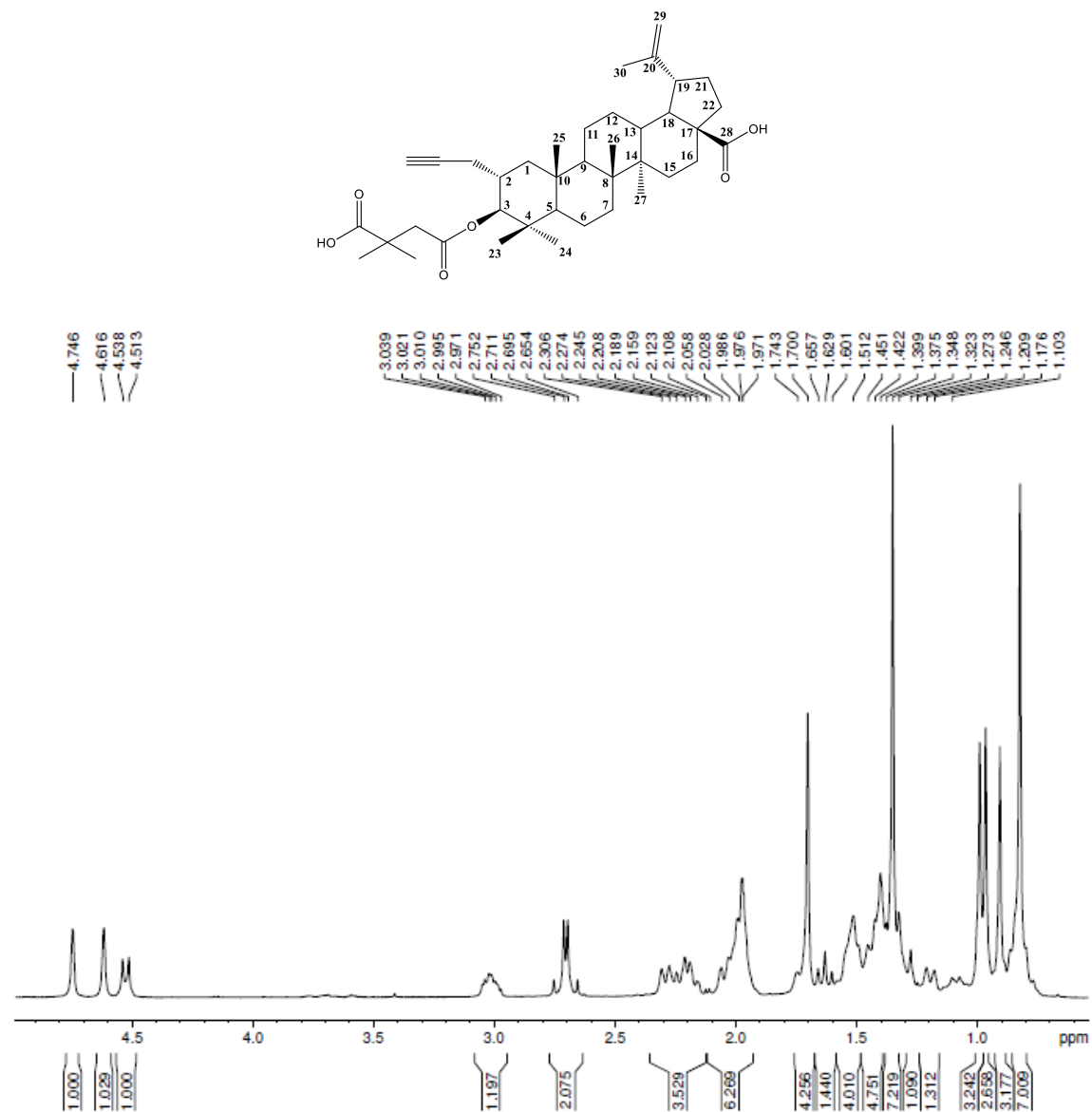
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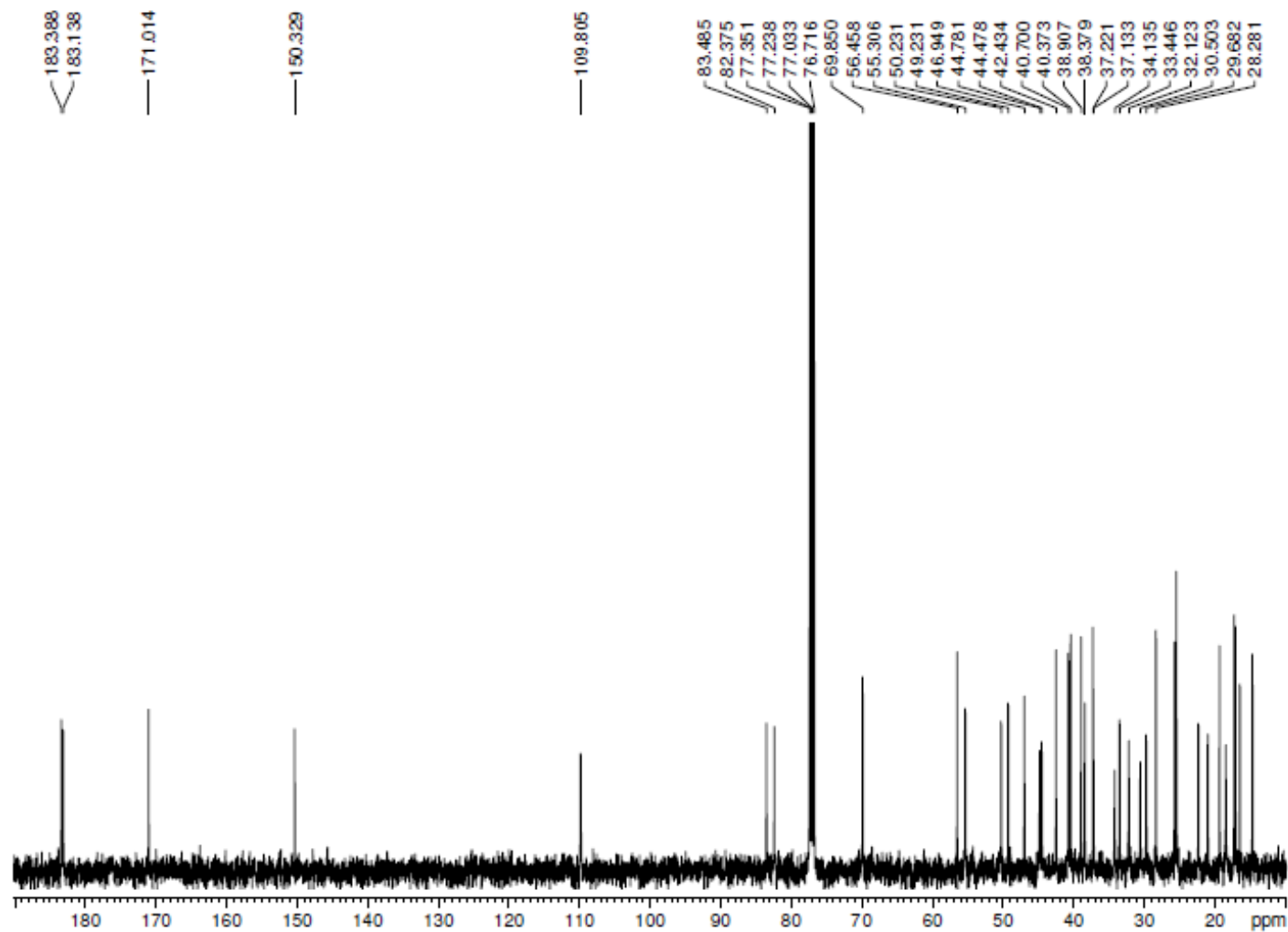
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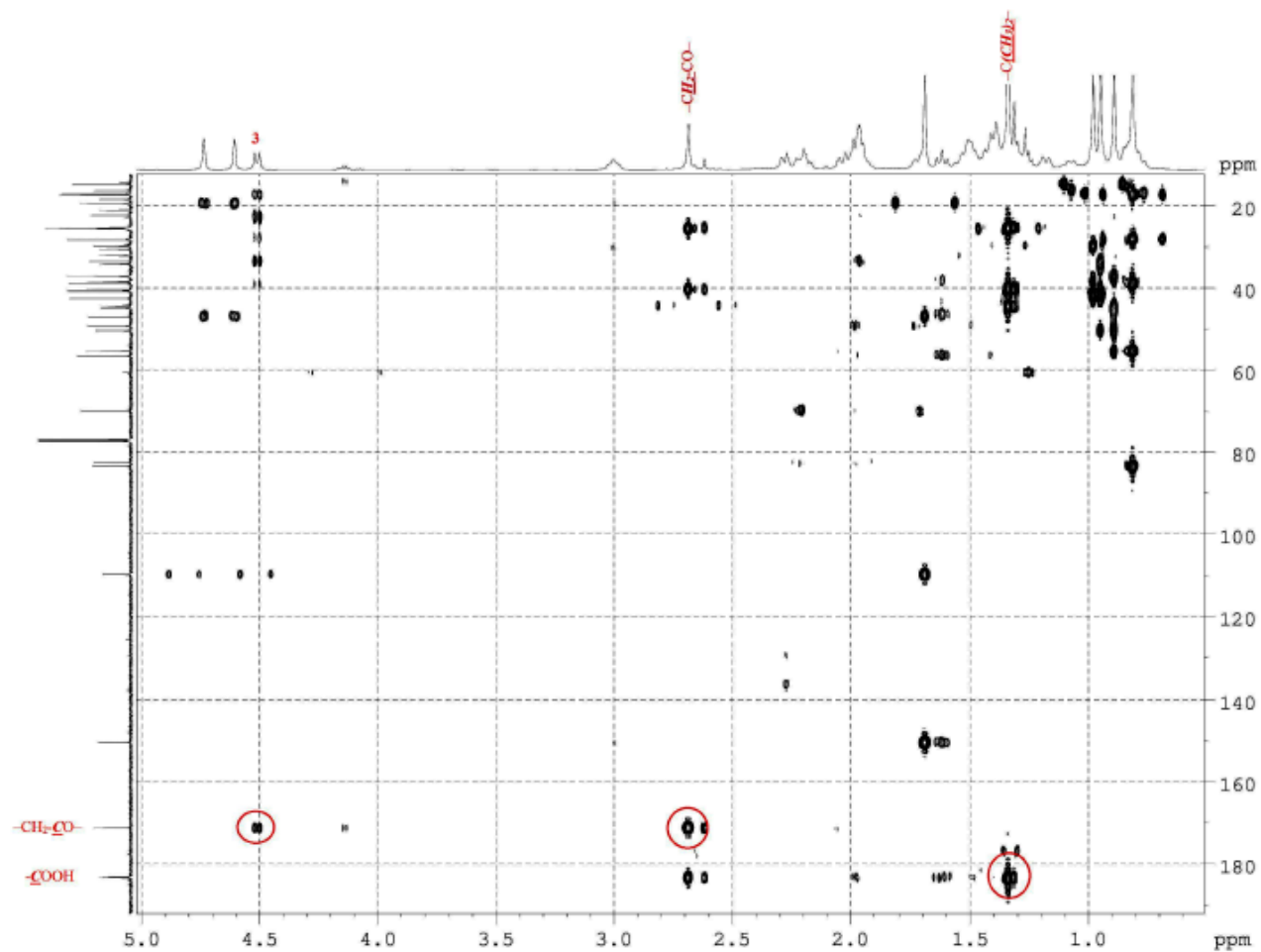
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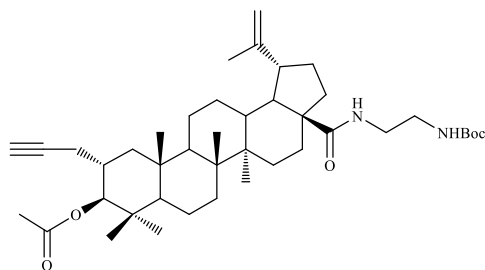
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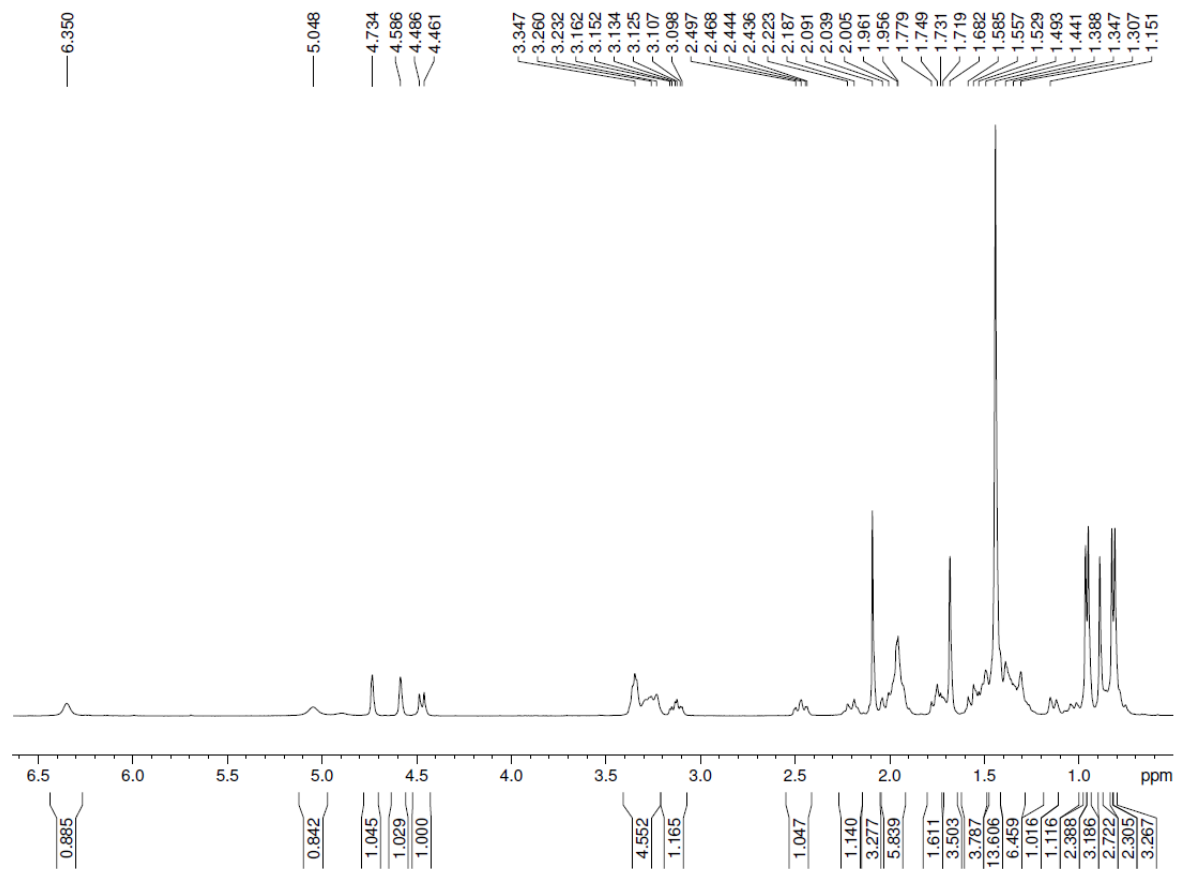


3β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oic acid **6** ^{13}C NMR spectra (CDCl_3)

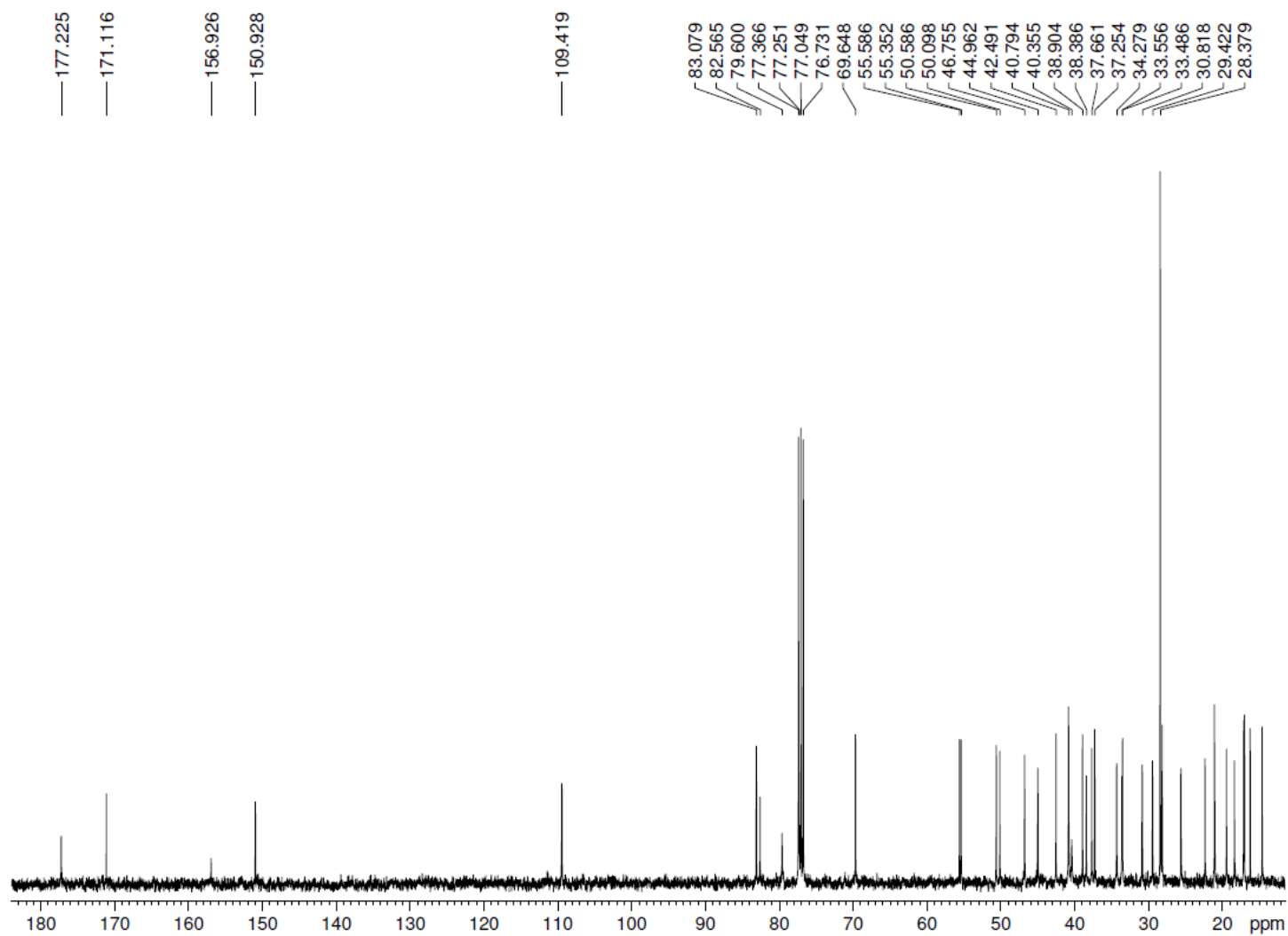


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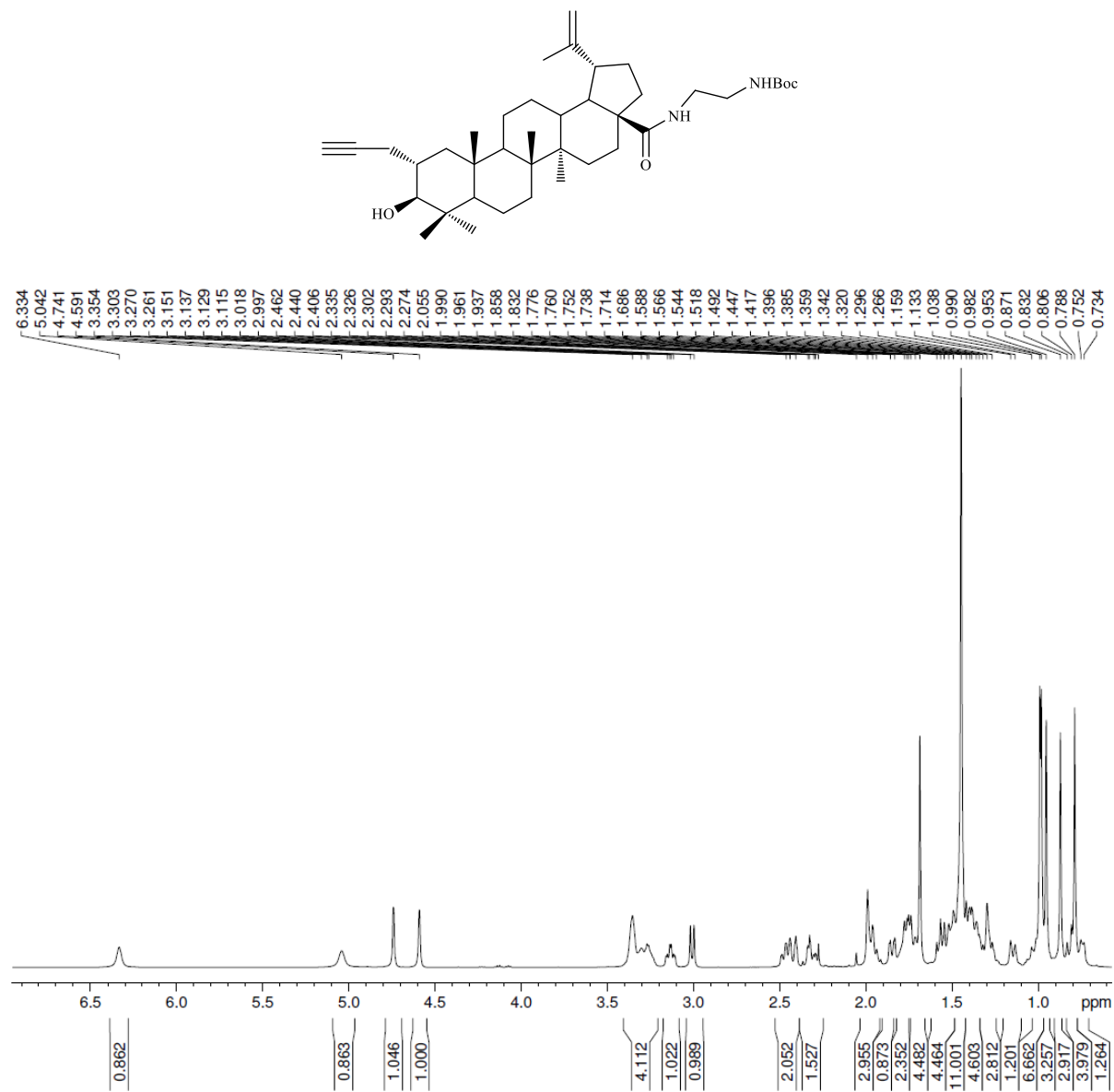




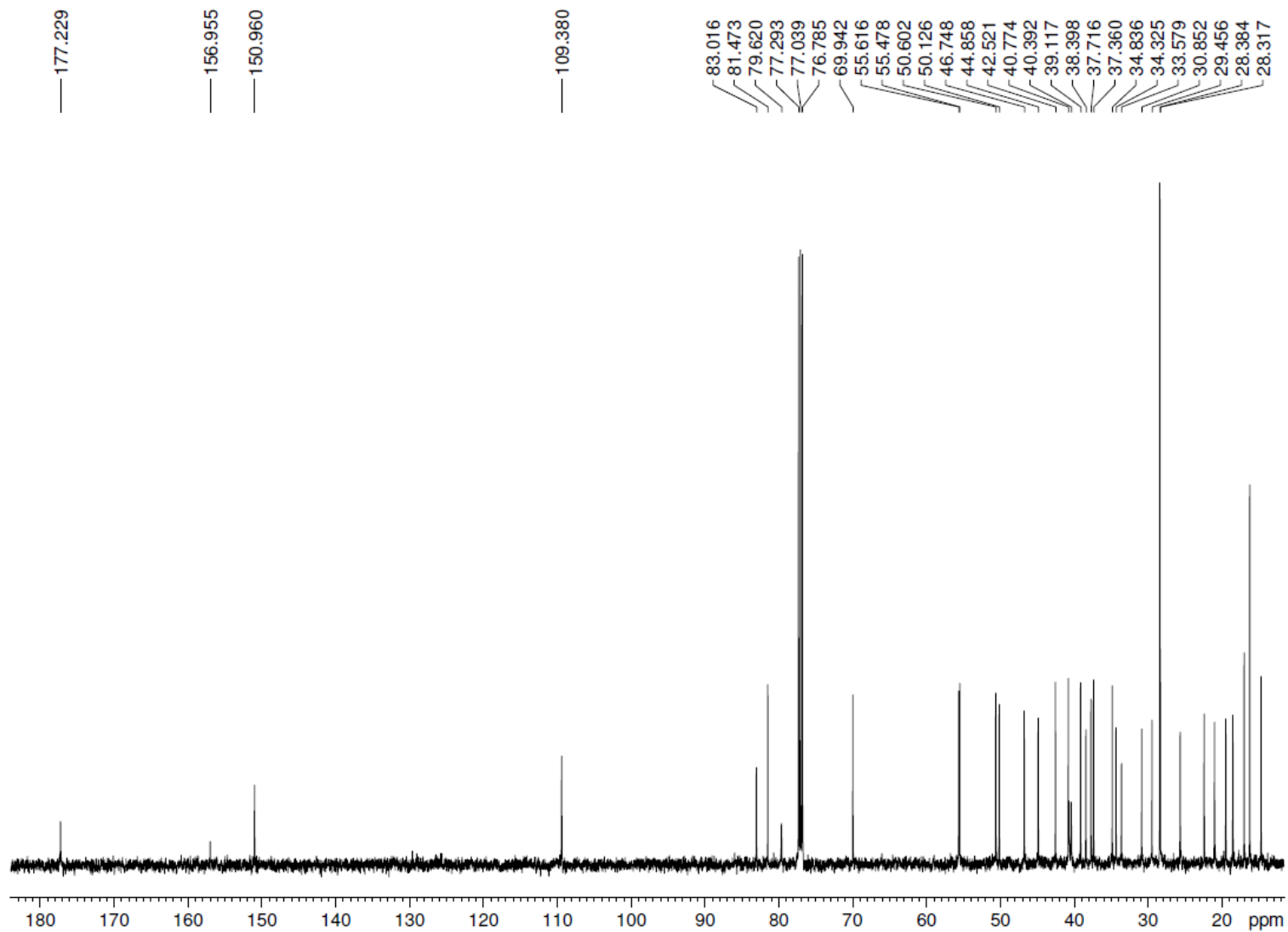
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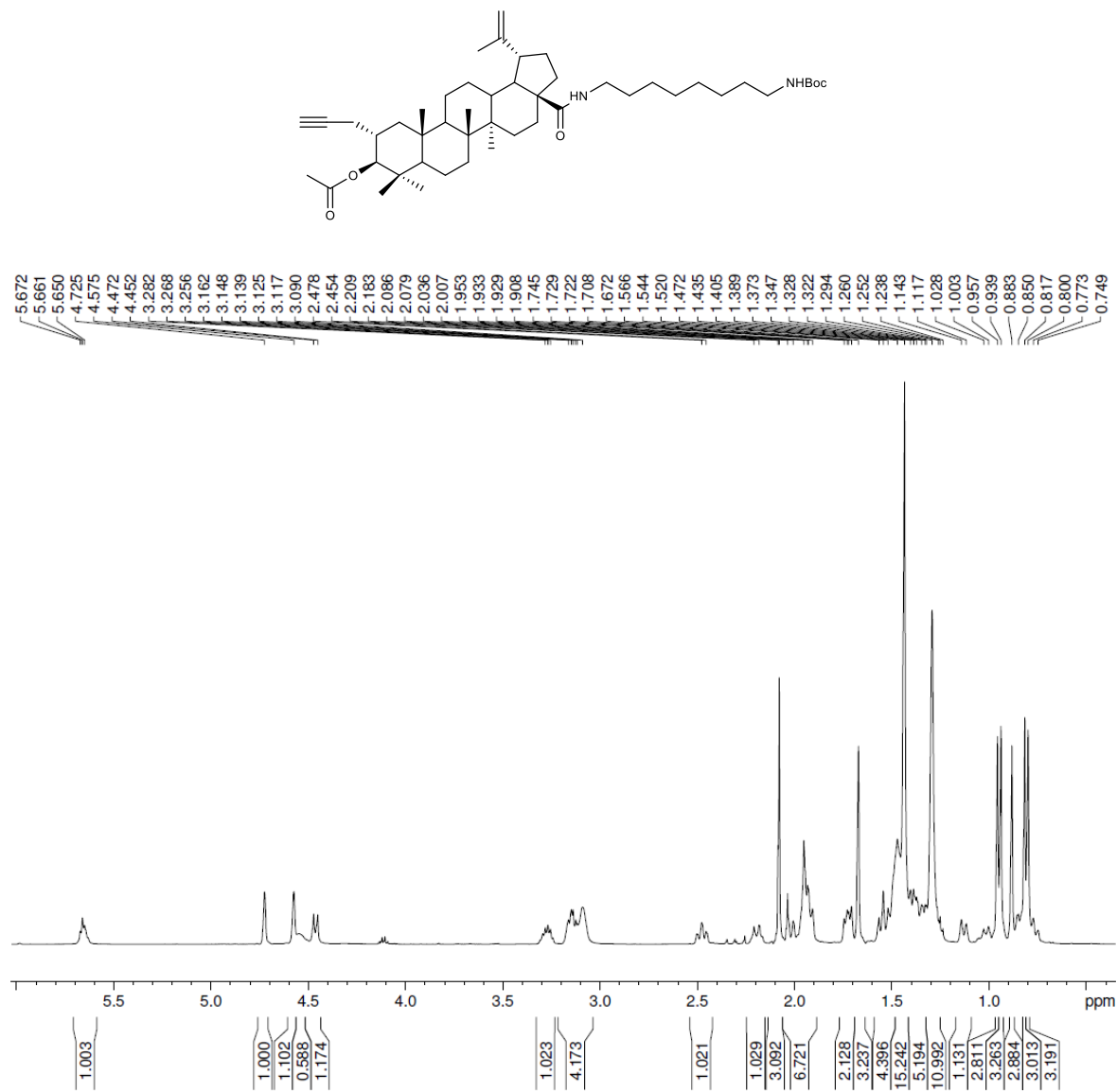
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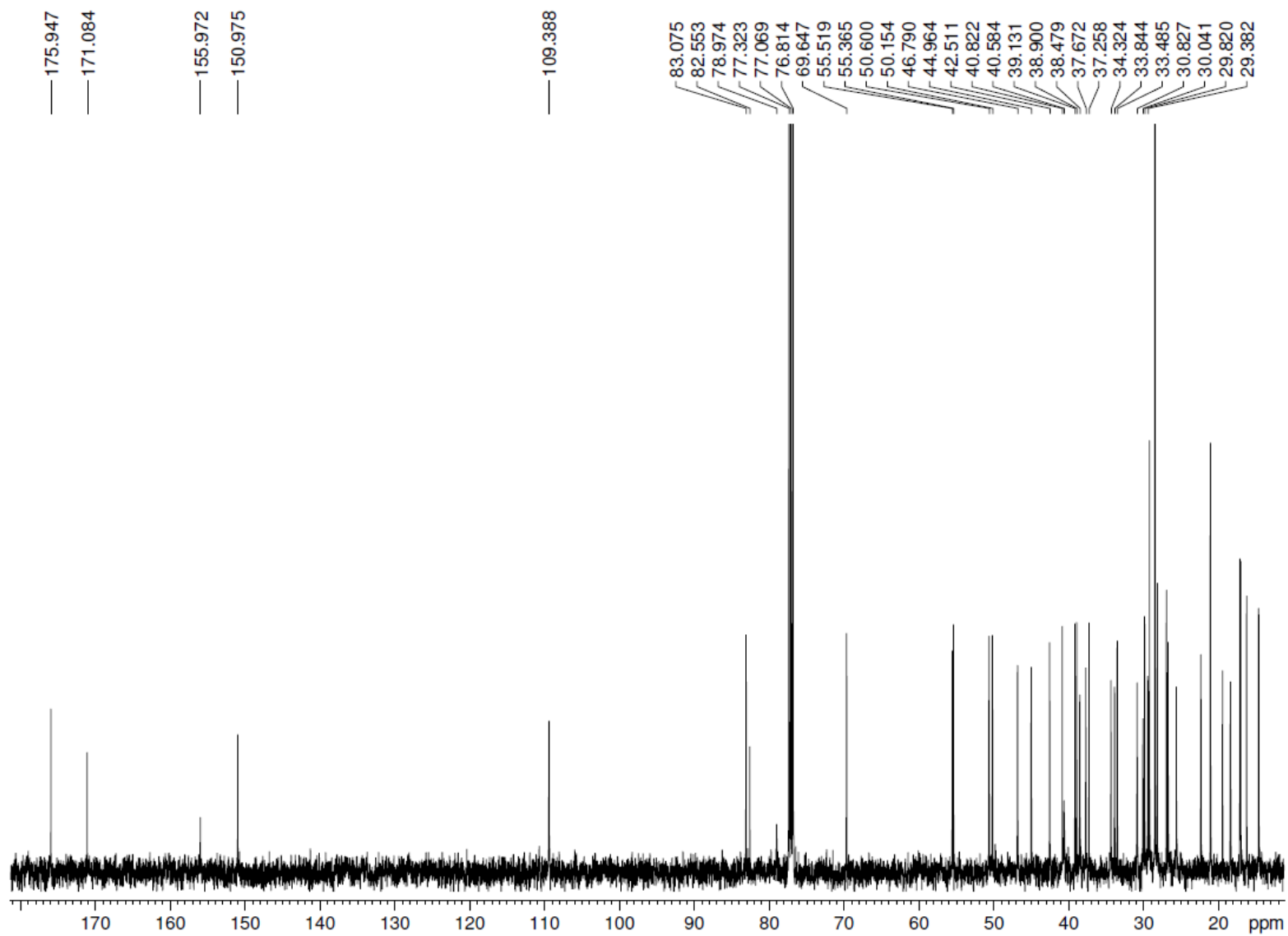
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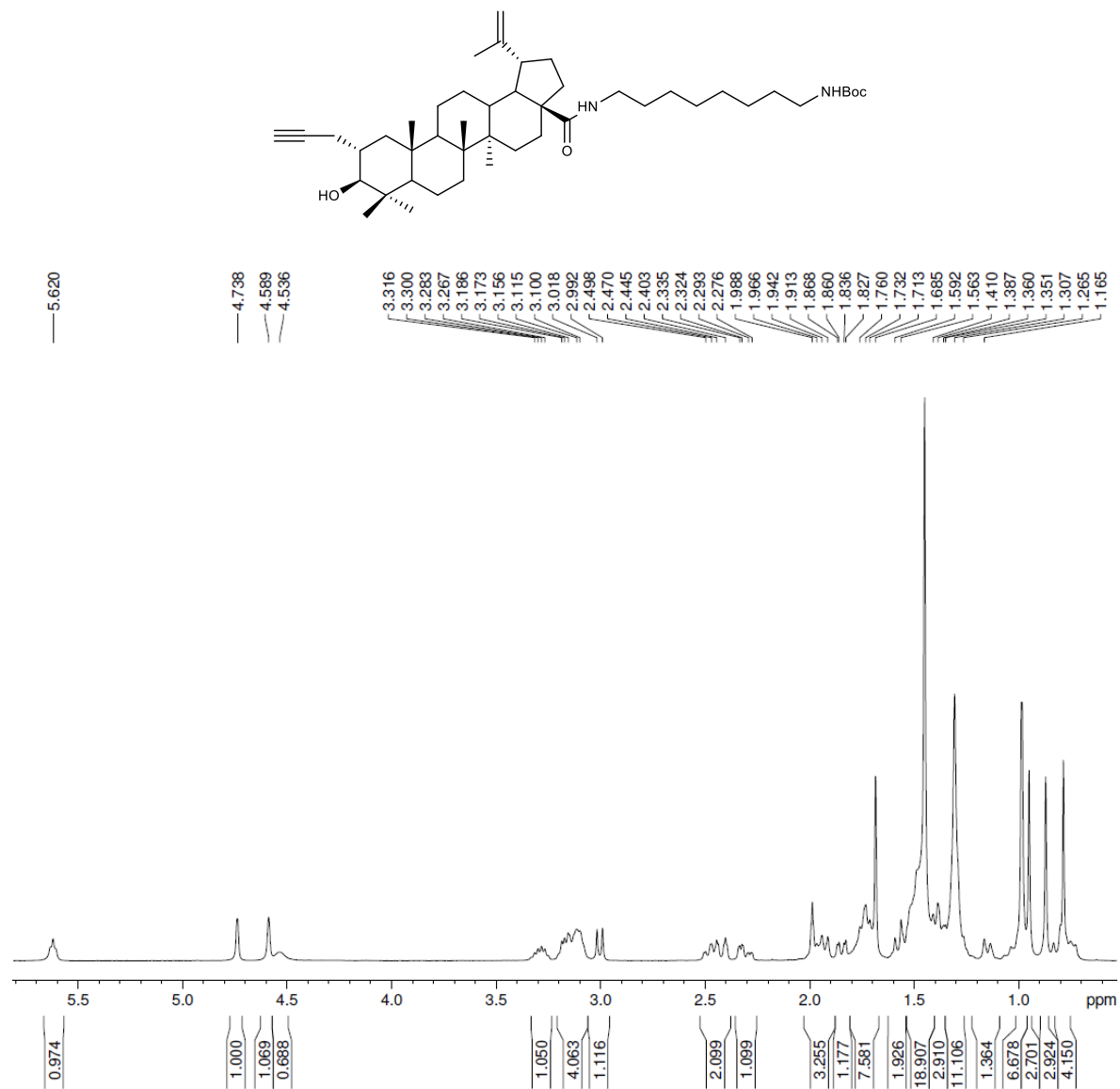
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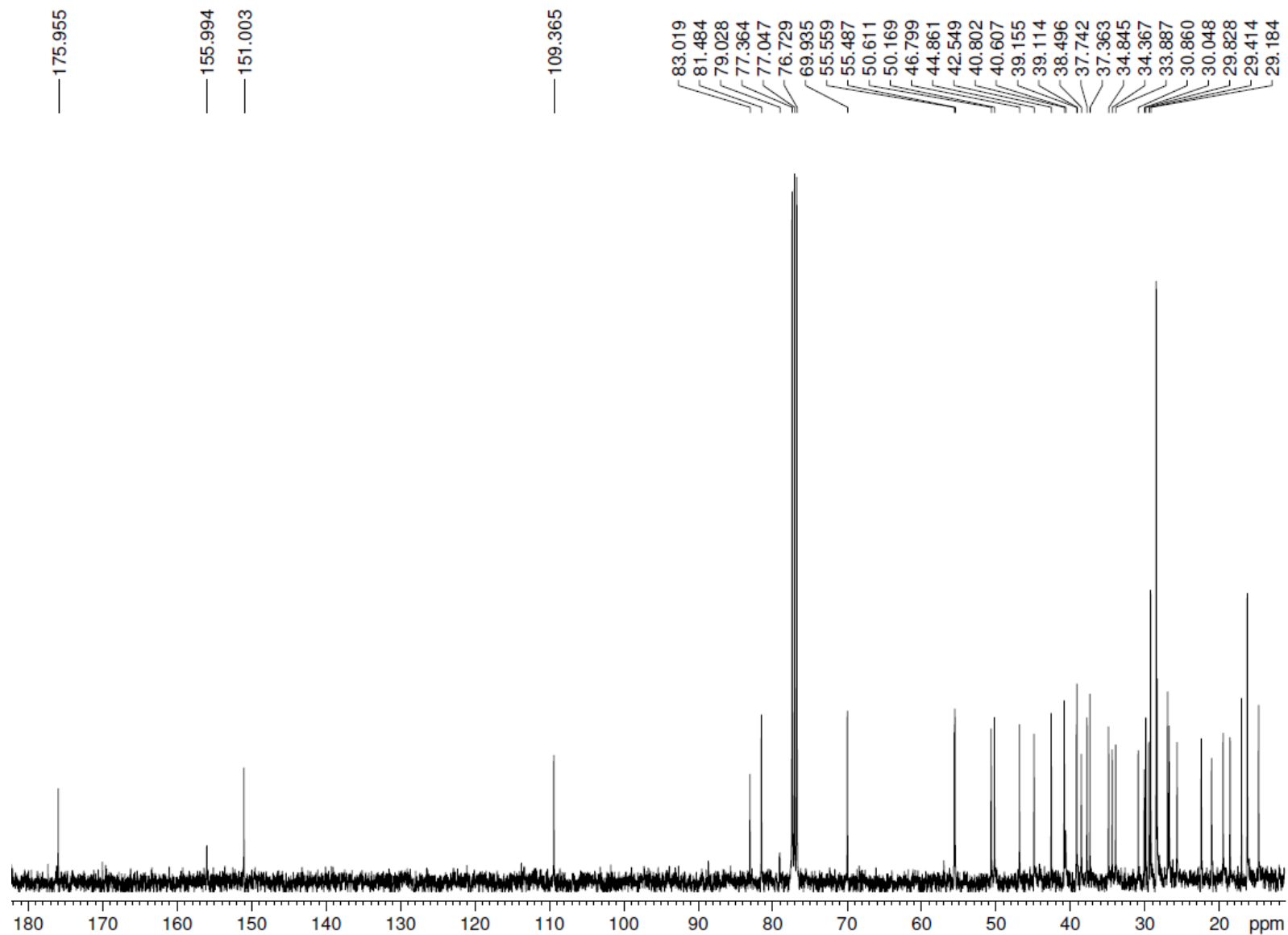
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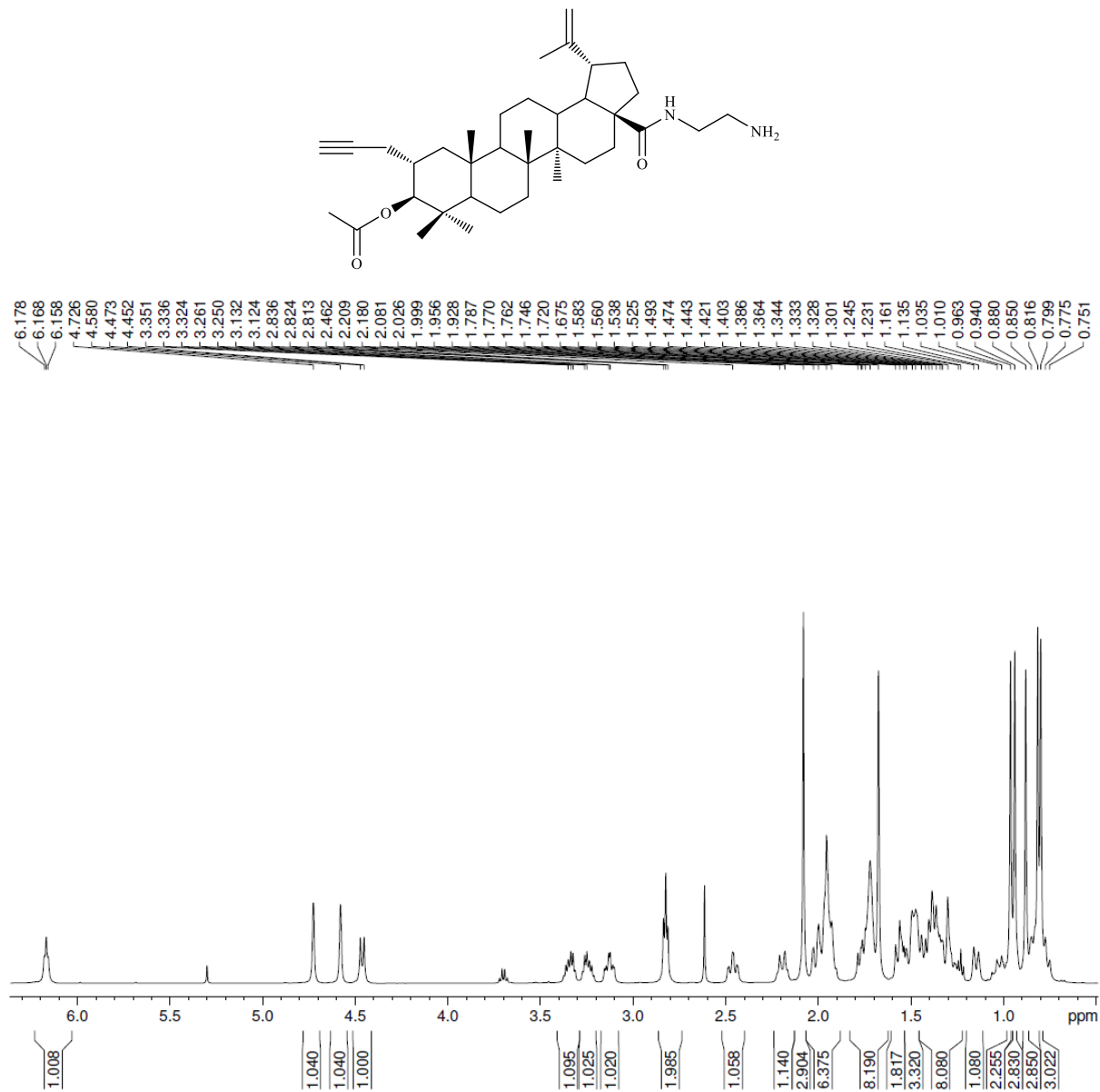
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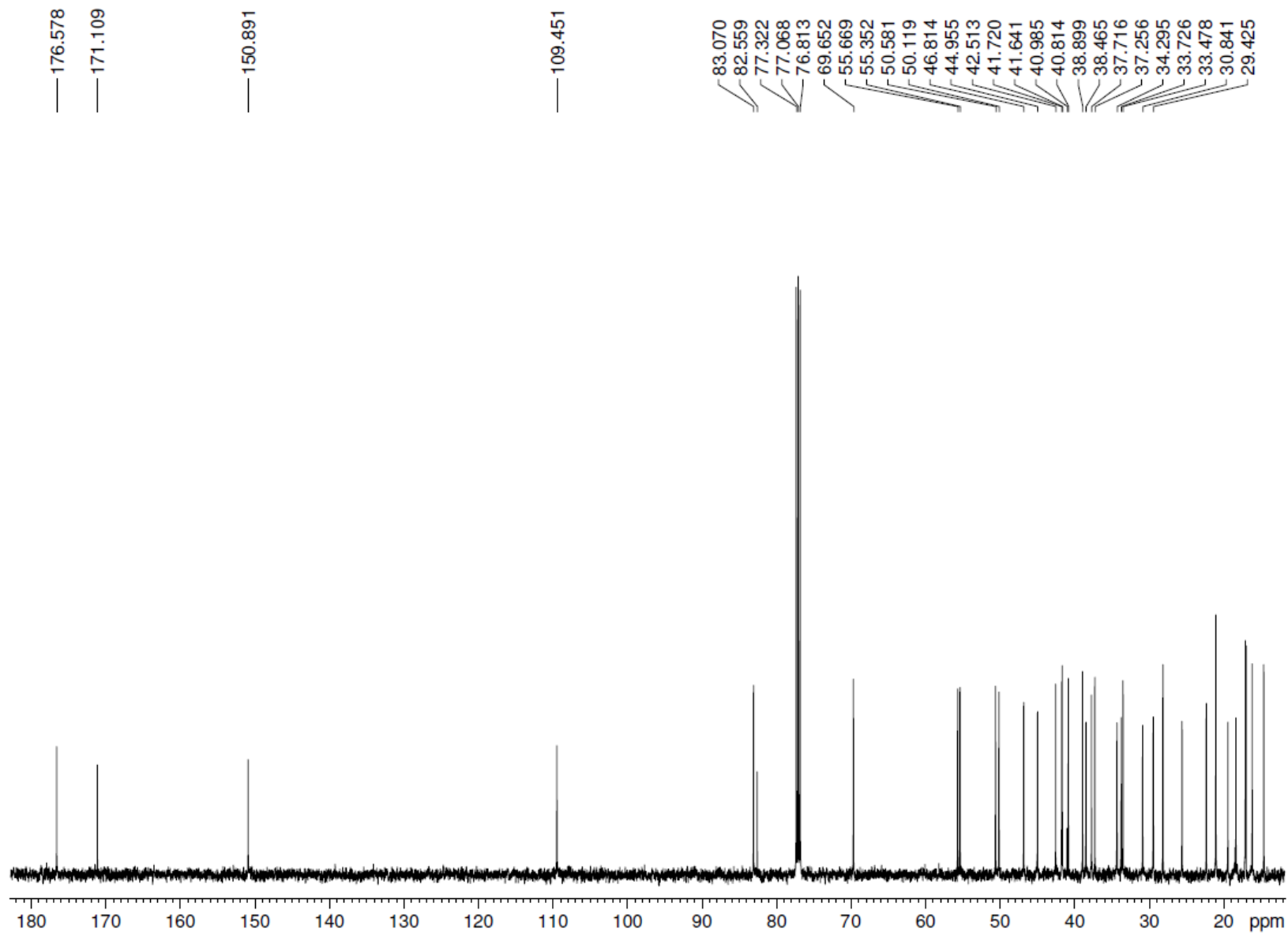


N-[3 β -hydroxy-2 α -propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-8-octylamine **9b** ^1H NMR spectra (CDCl_3)

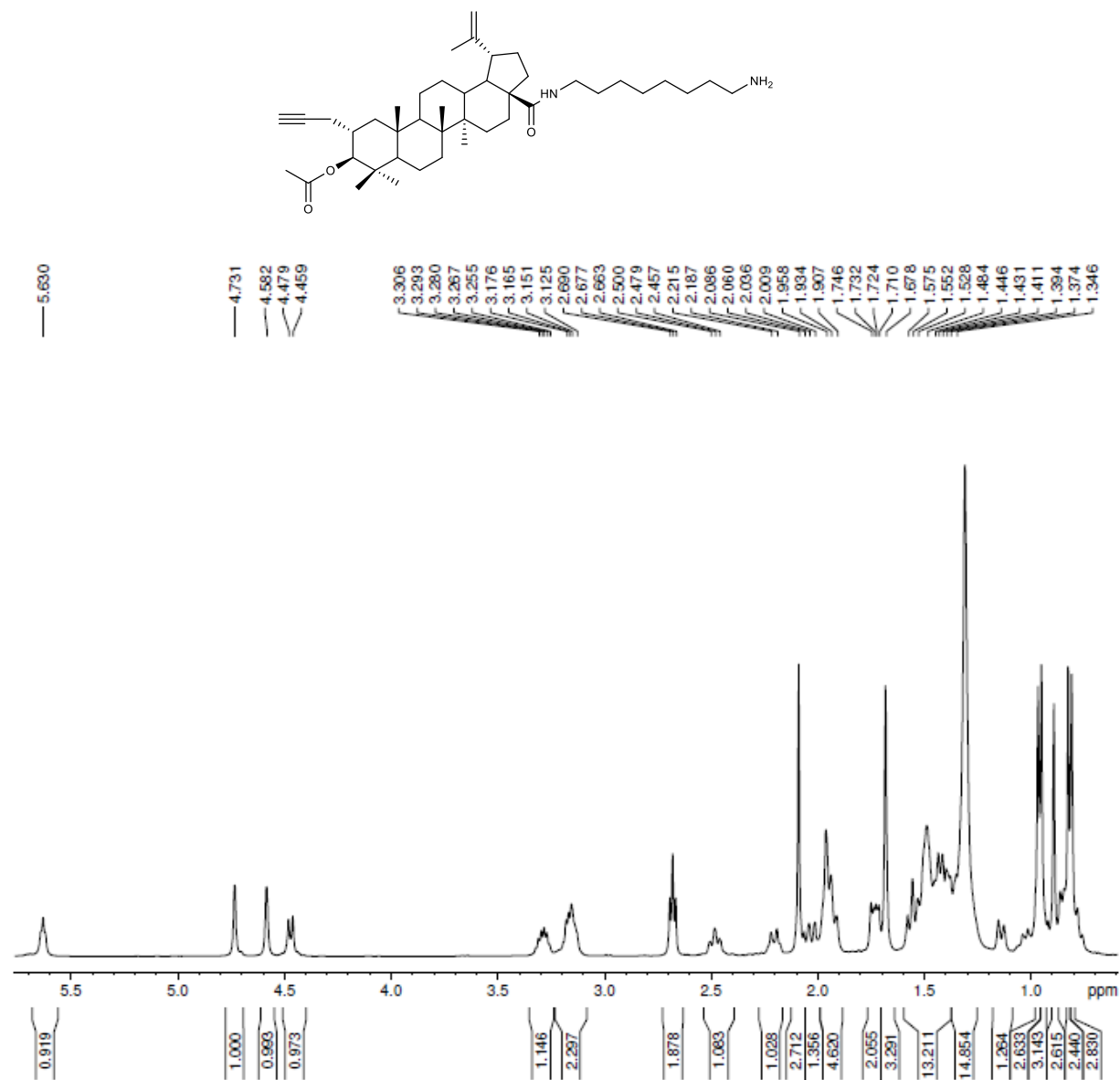


N-[3 β -hydroxy-2 α -propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-8-octylamine **9b** ^{13}C NMR spectra (CDCl_3)

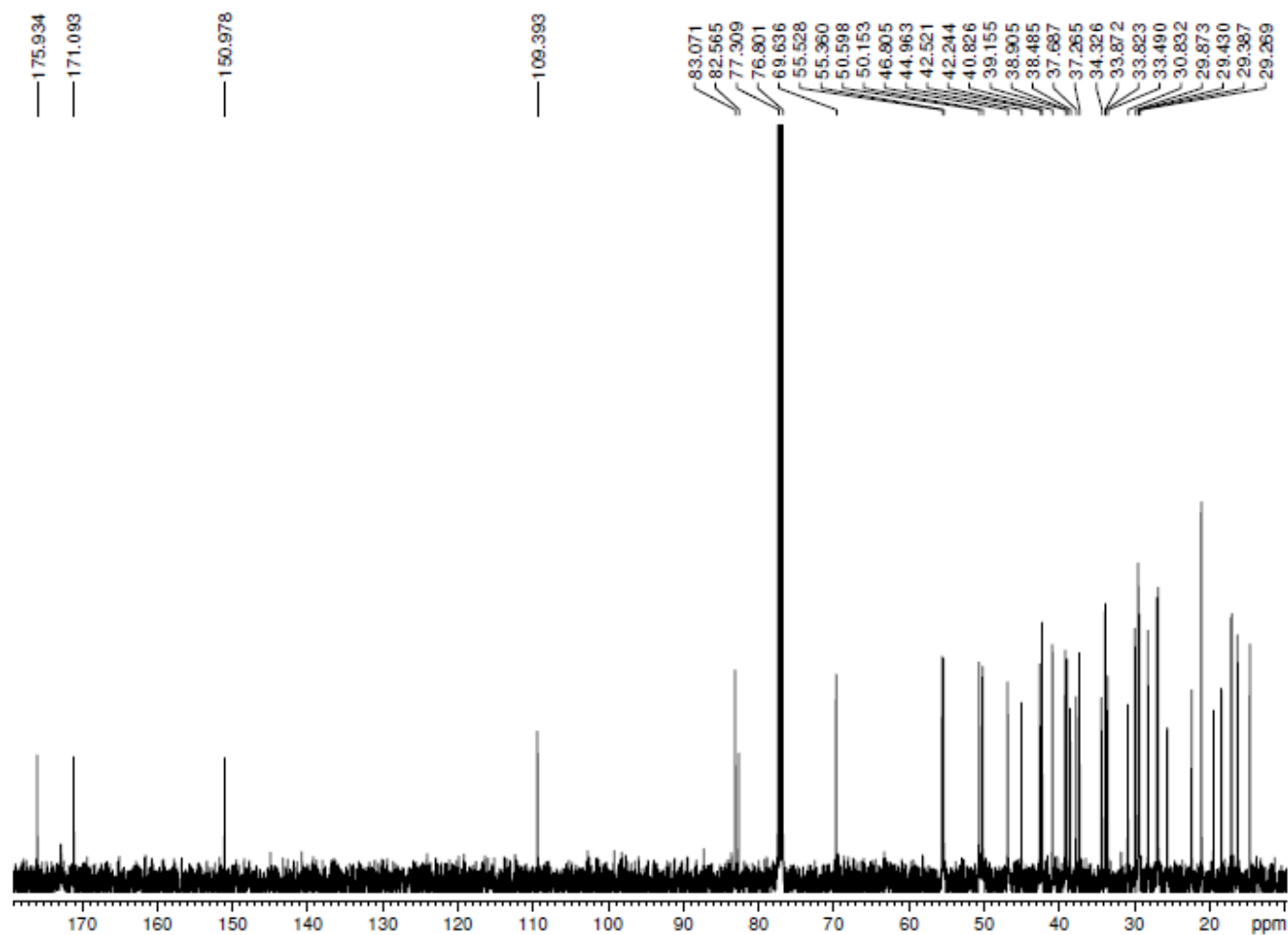
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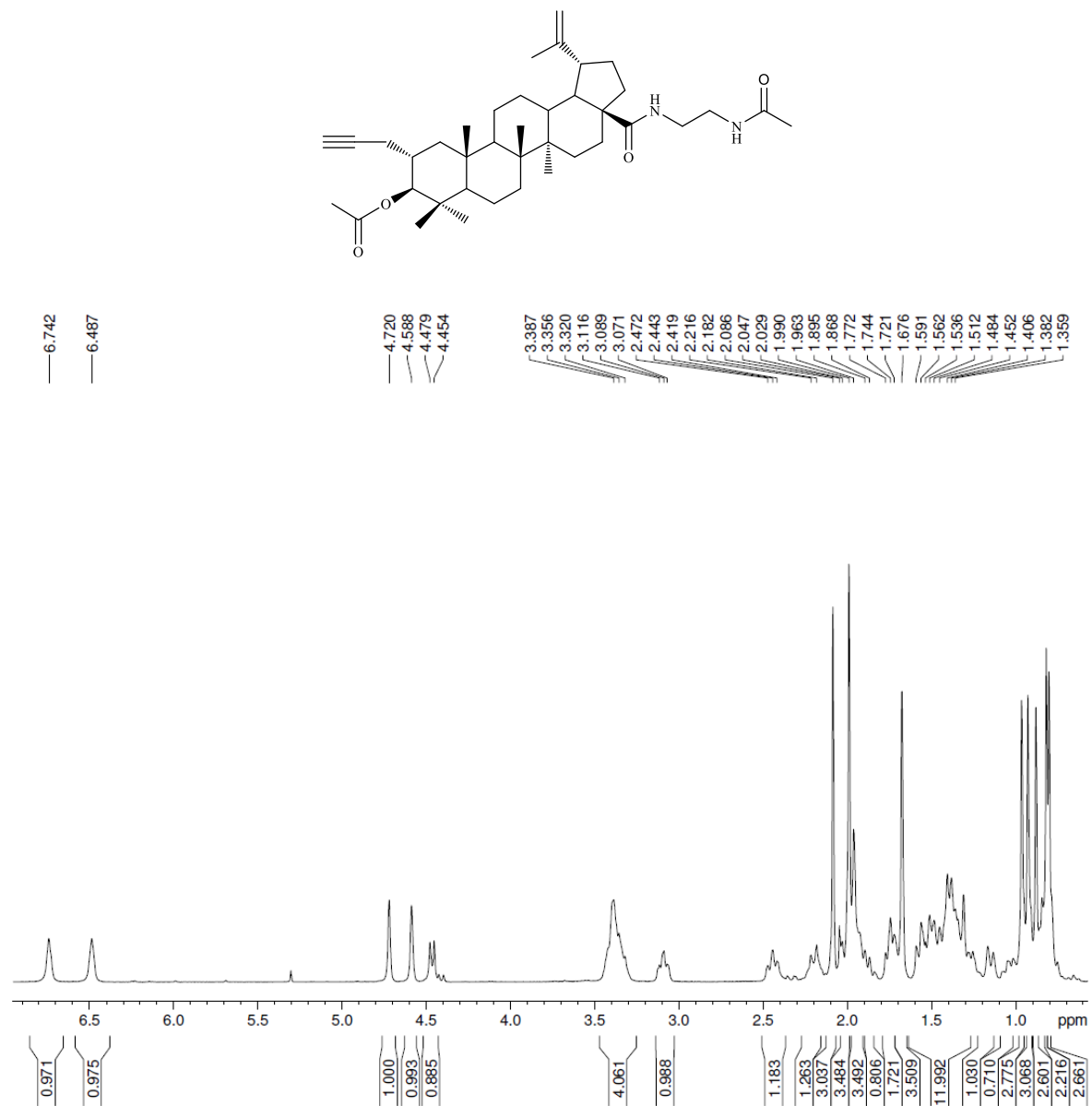
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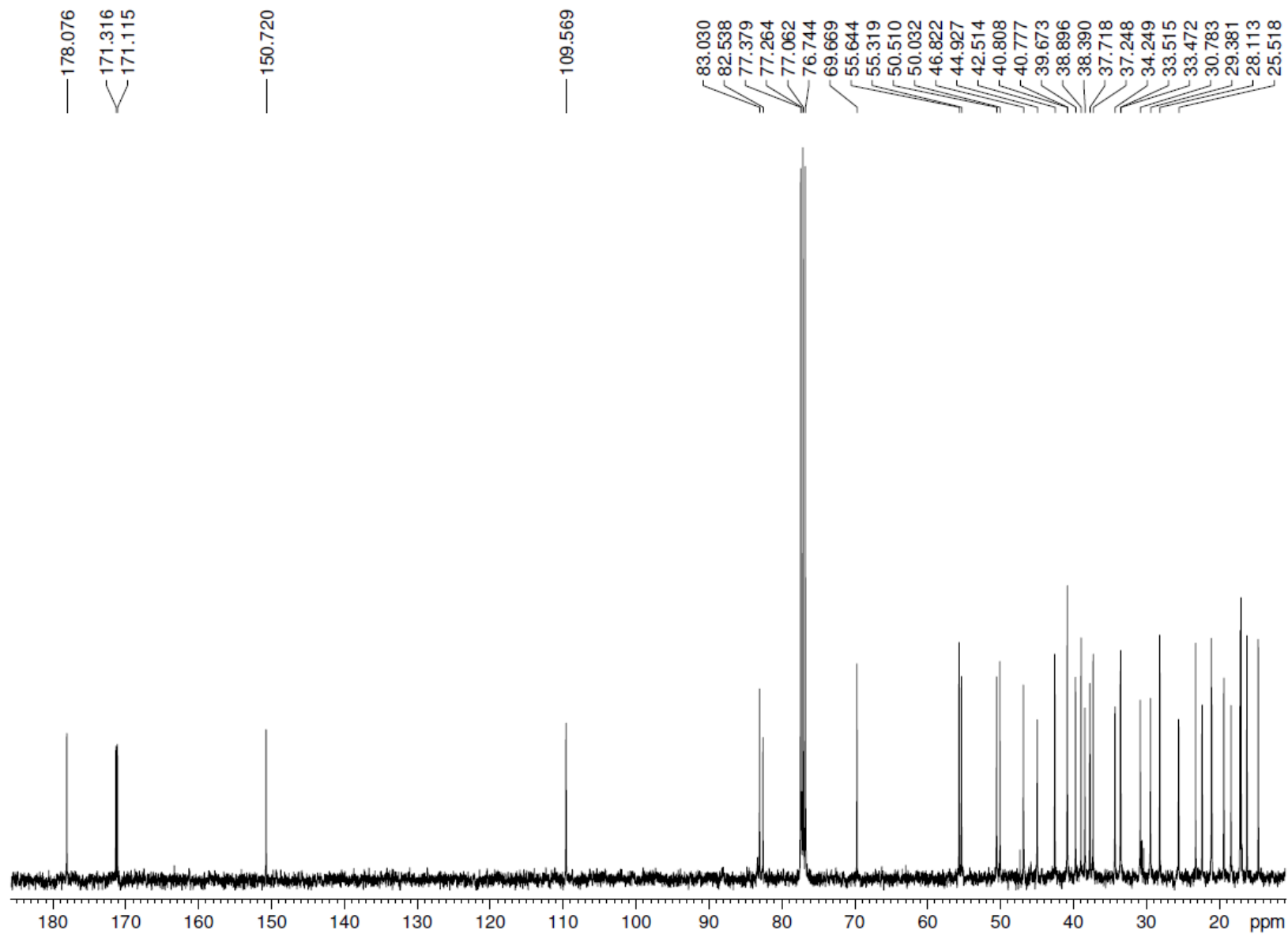
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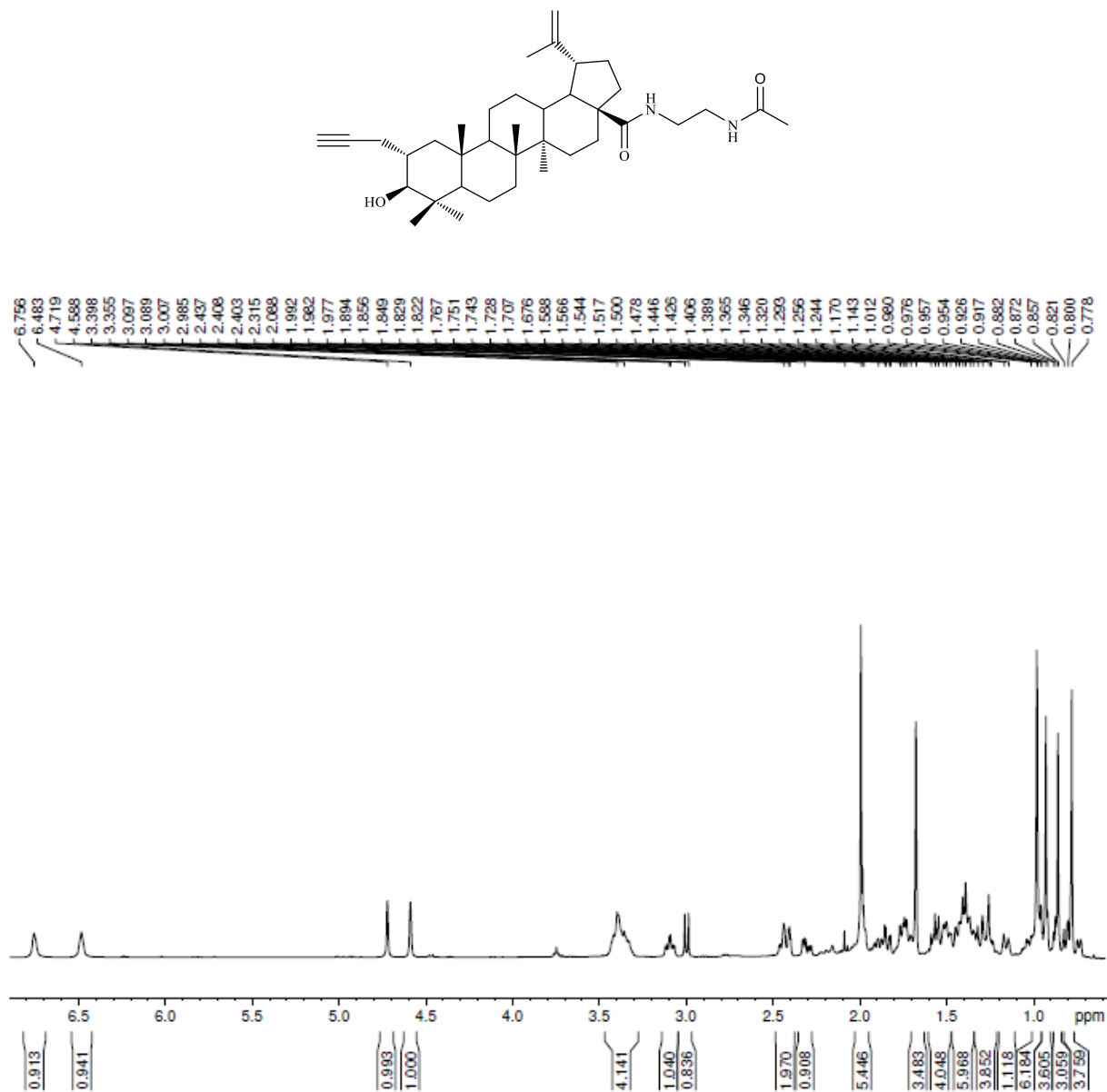
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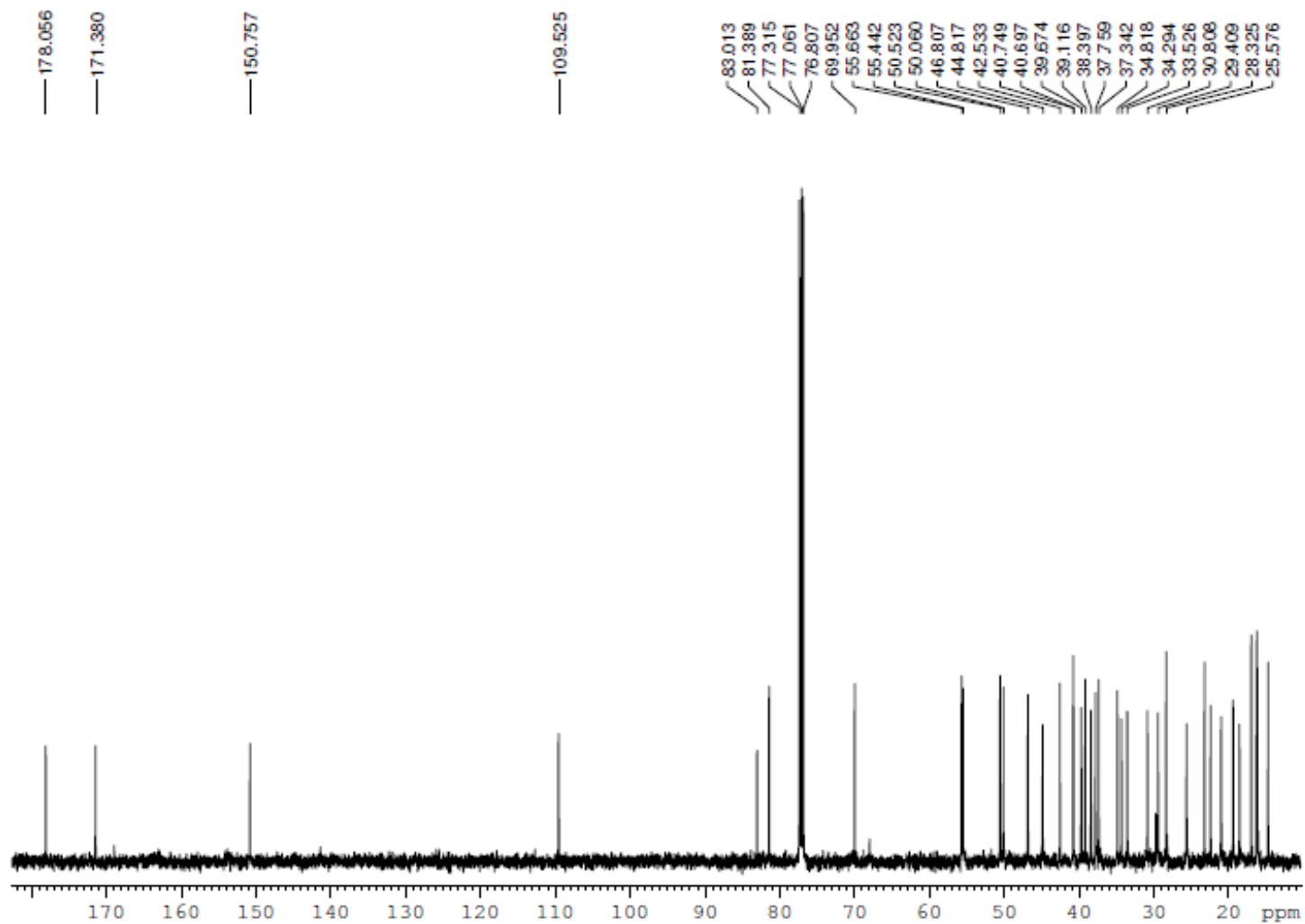
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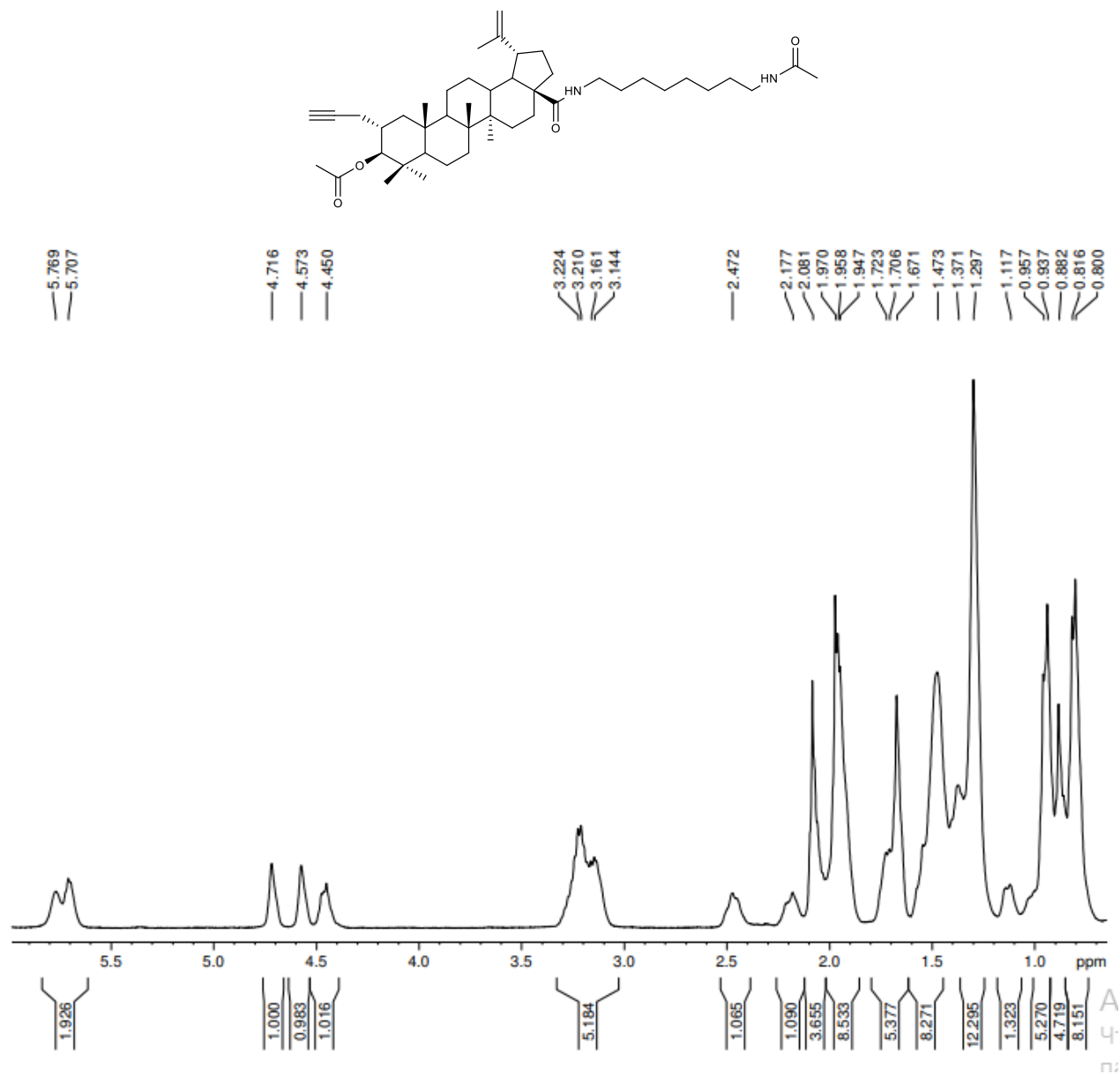
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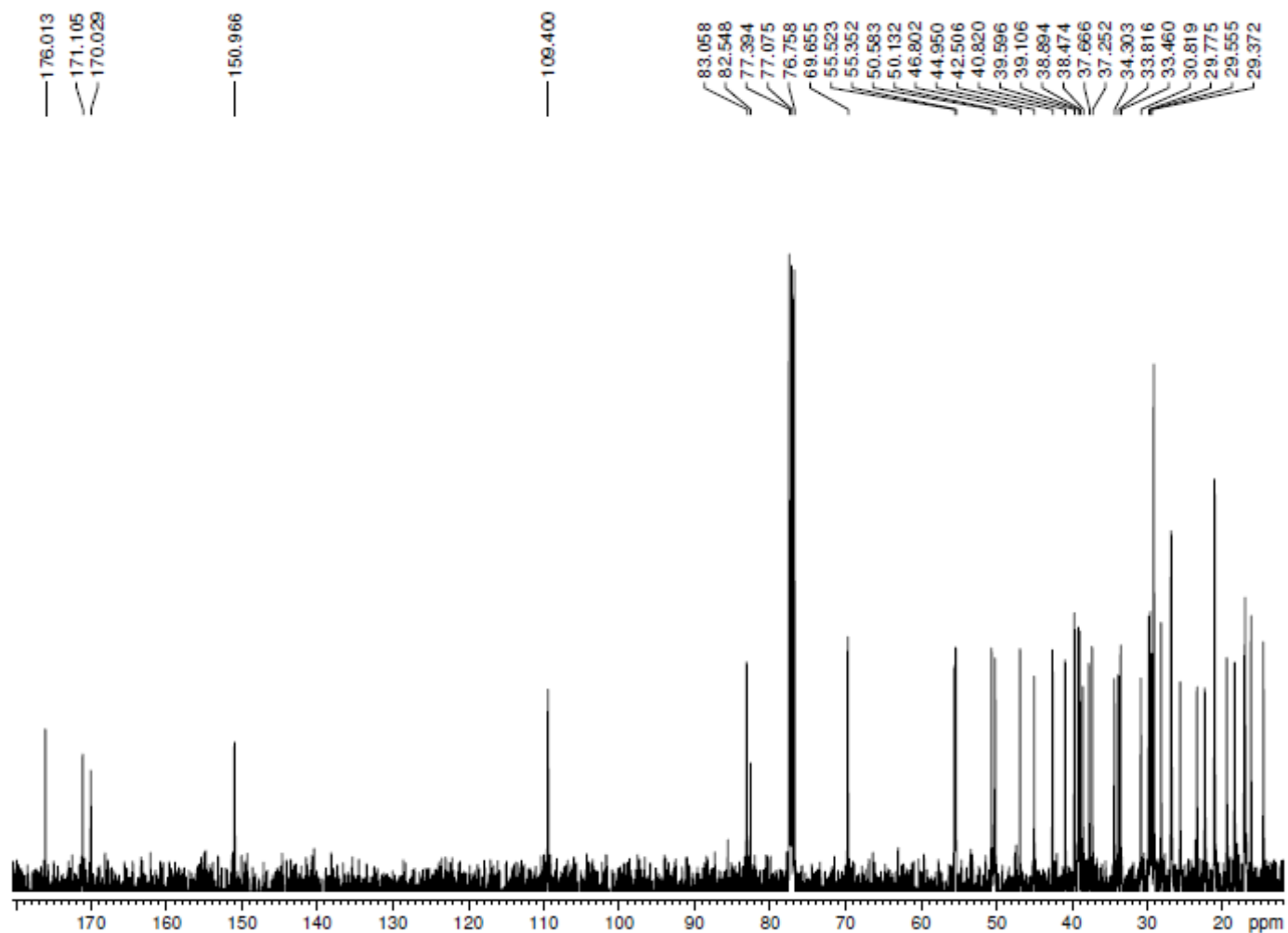
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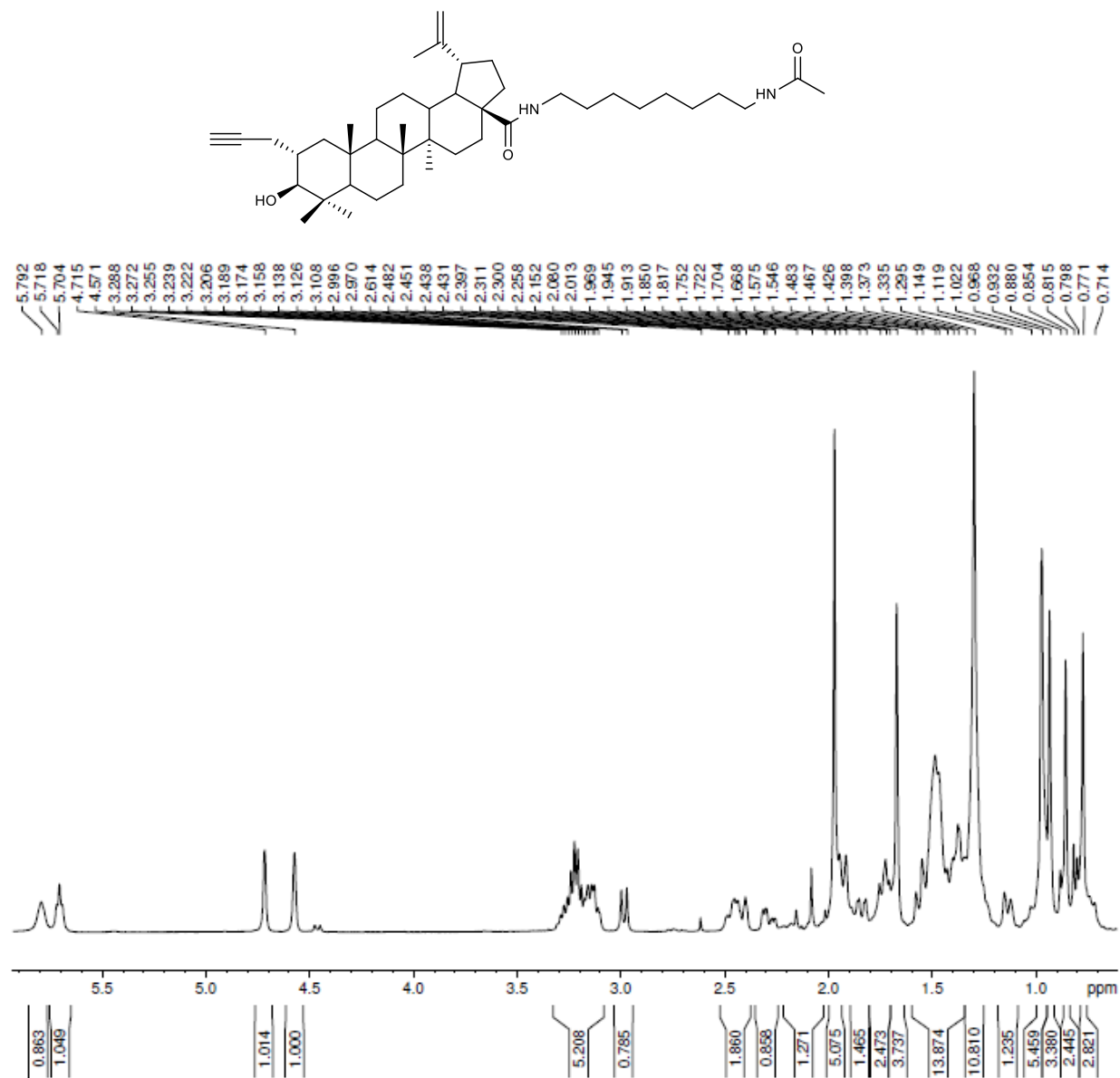
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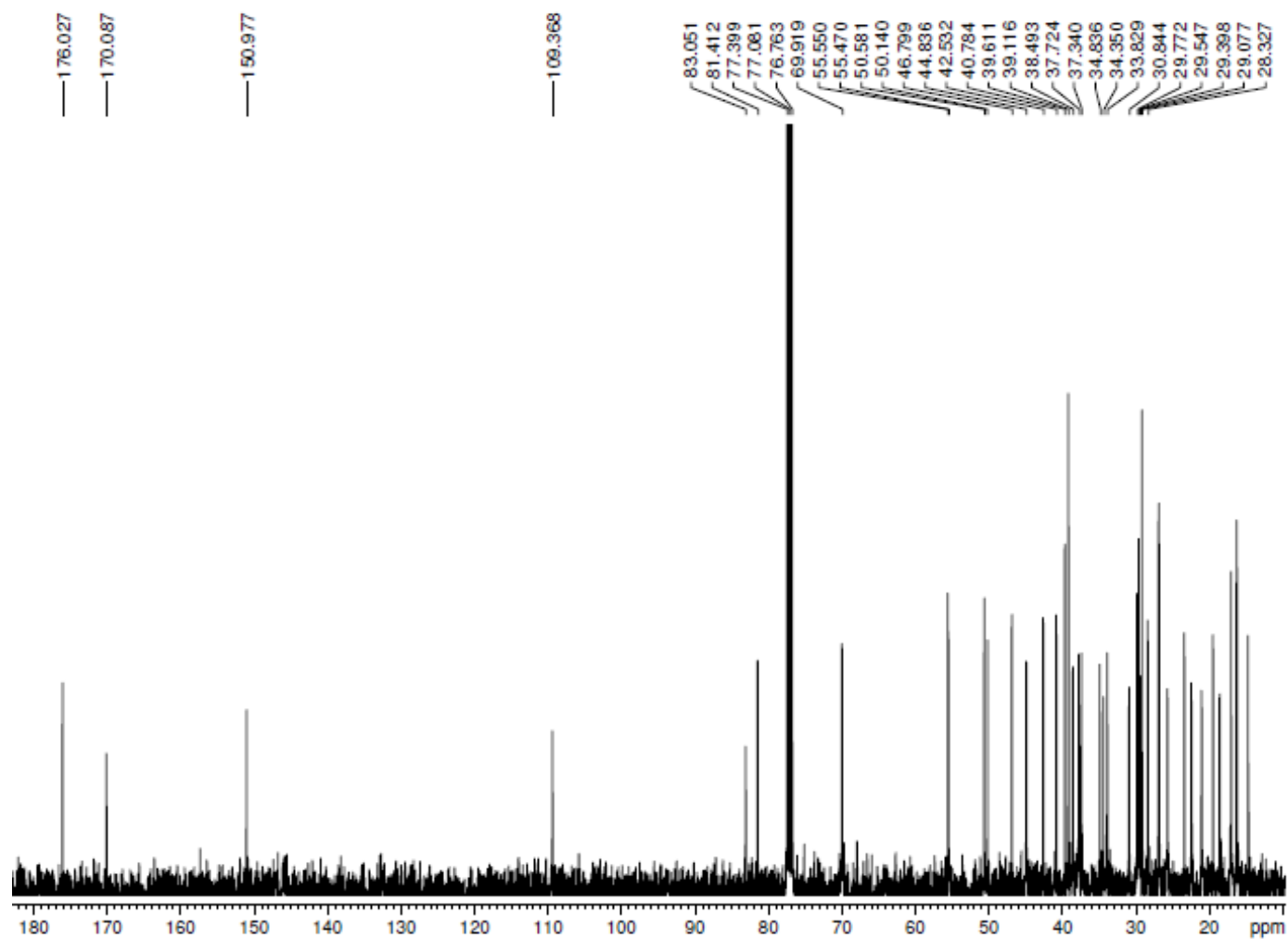
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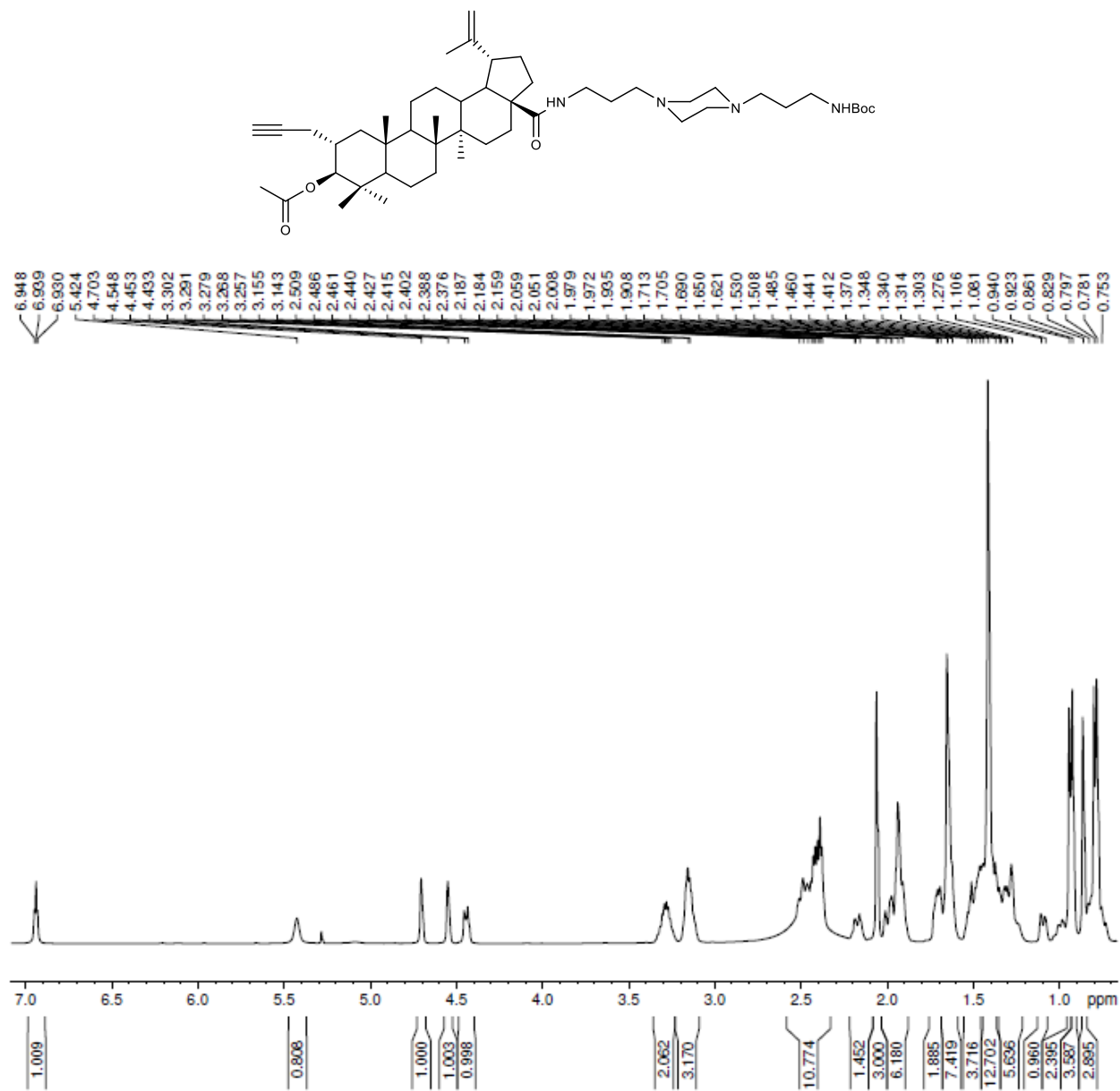
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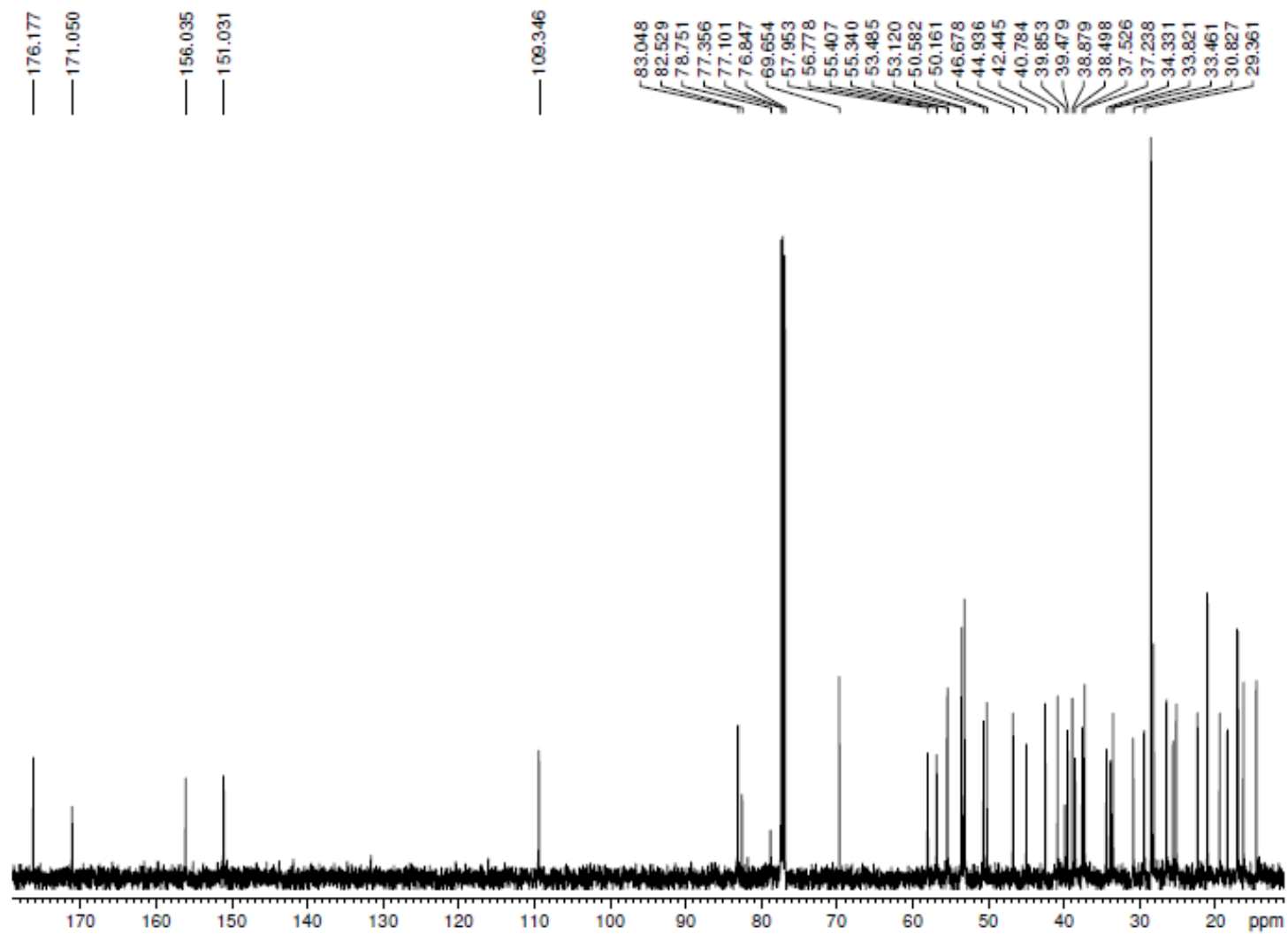
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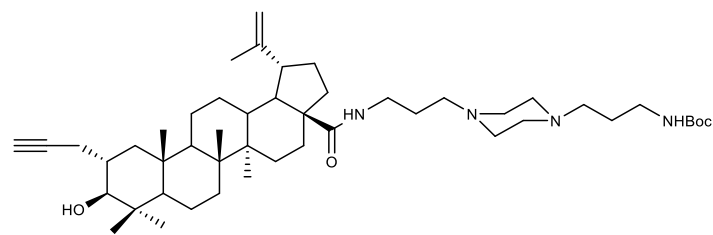
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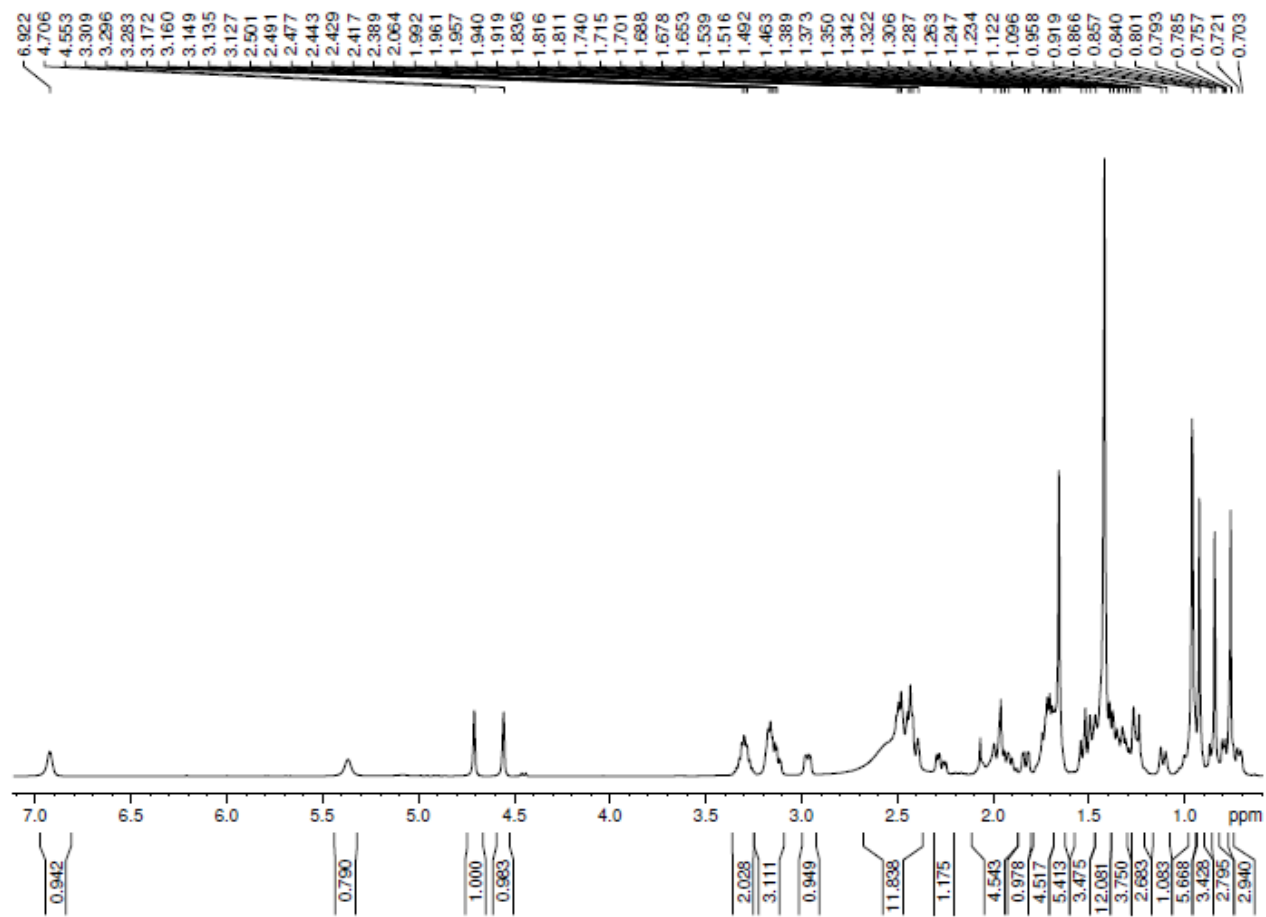


N-[3 β -acetoxy-2 α -propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-{3-[4-(3-aminopropyl)piperazinyl]}propylamine **14a** ¹H NMR spectra (CDCl₃)

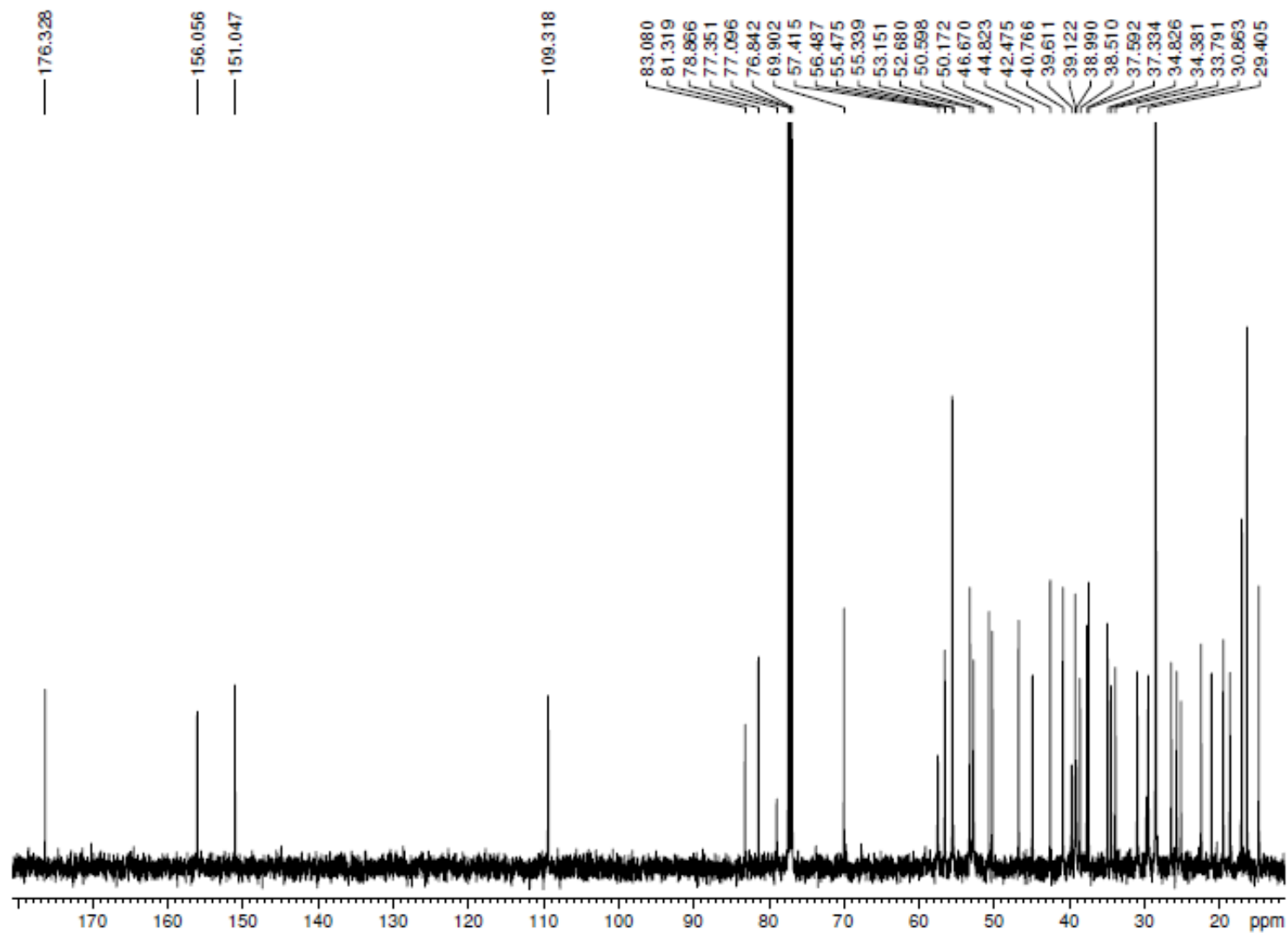


N-[3 β -acetoxy-2 α -propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-{3-[4-(3-aminopropyl)piperazinyl]}propylamine **14a** ^{13}C NMR spectra (CDCl_3)

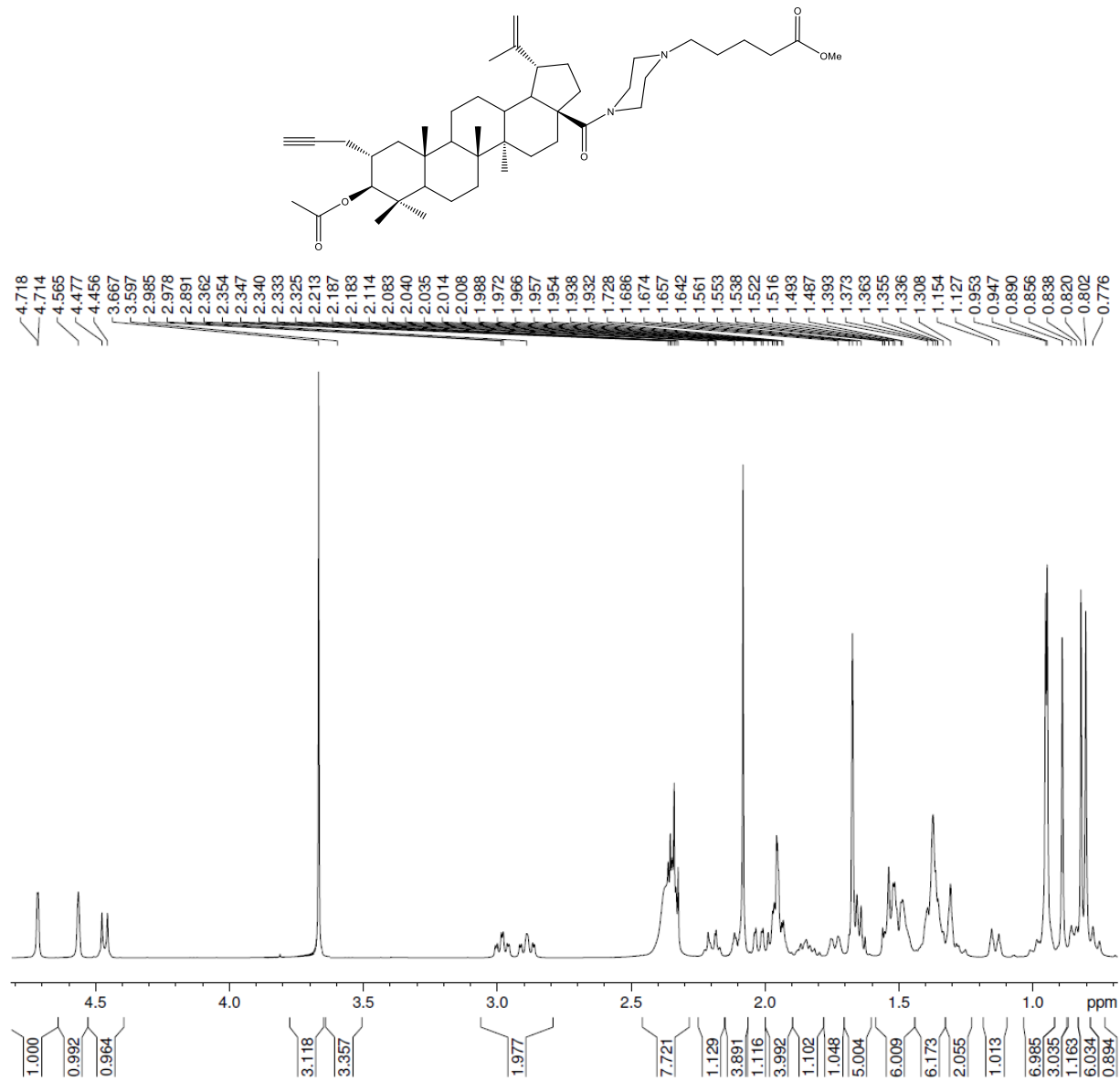


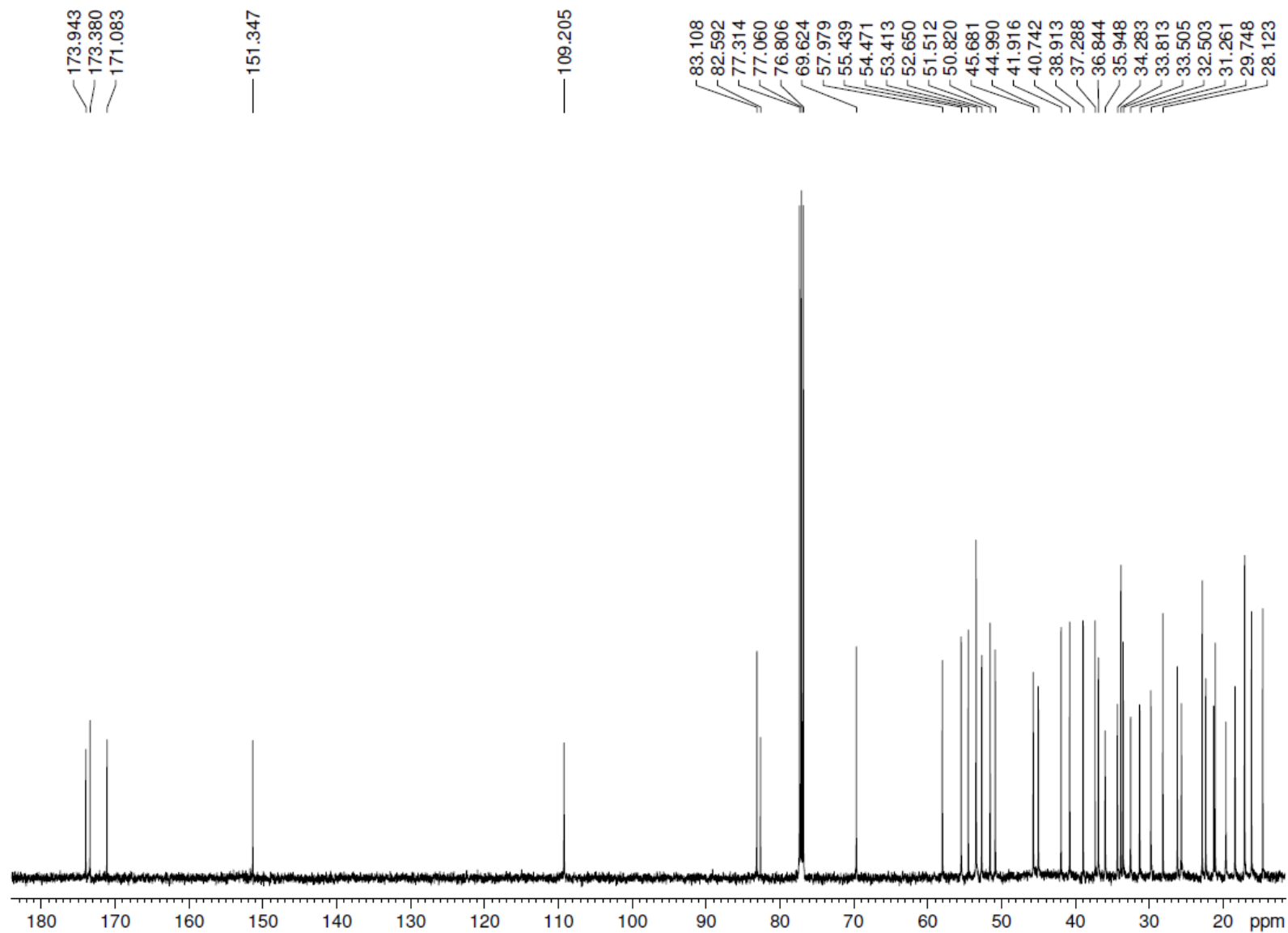


N-[3 β -hydroxy-2 α -propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-{3-[4-(3-aminopropyl)piperazinyl]}propylamine **14b** ^1H NMR spectra (CDCl_3)

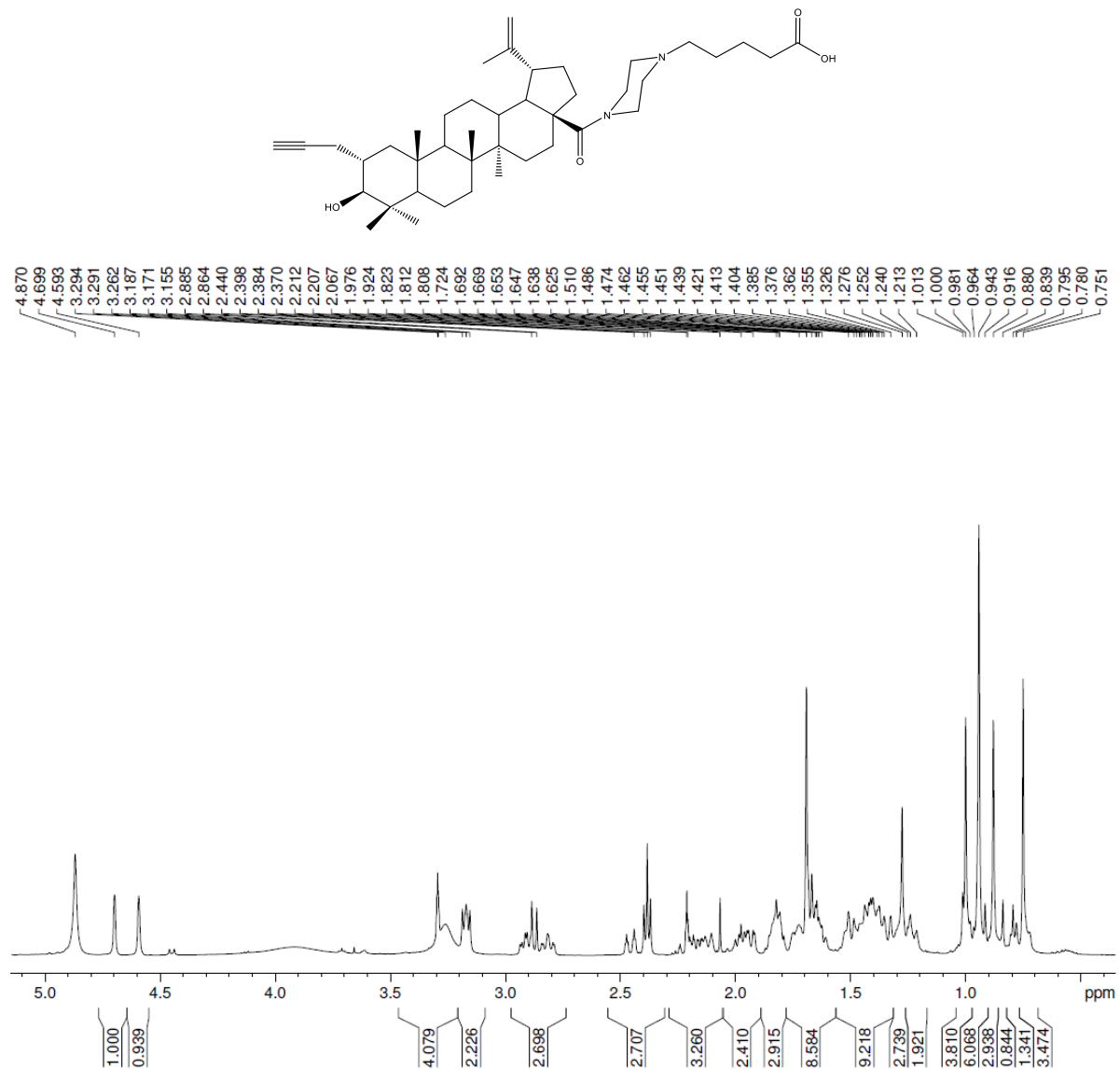


N-[3 β -hydroxy-2 α -propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-{3-[4-(3-aminopropyl)piperazinyl]}propylamine **14b** ^{13}C NMR spectra (CDCl_3)

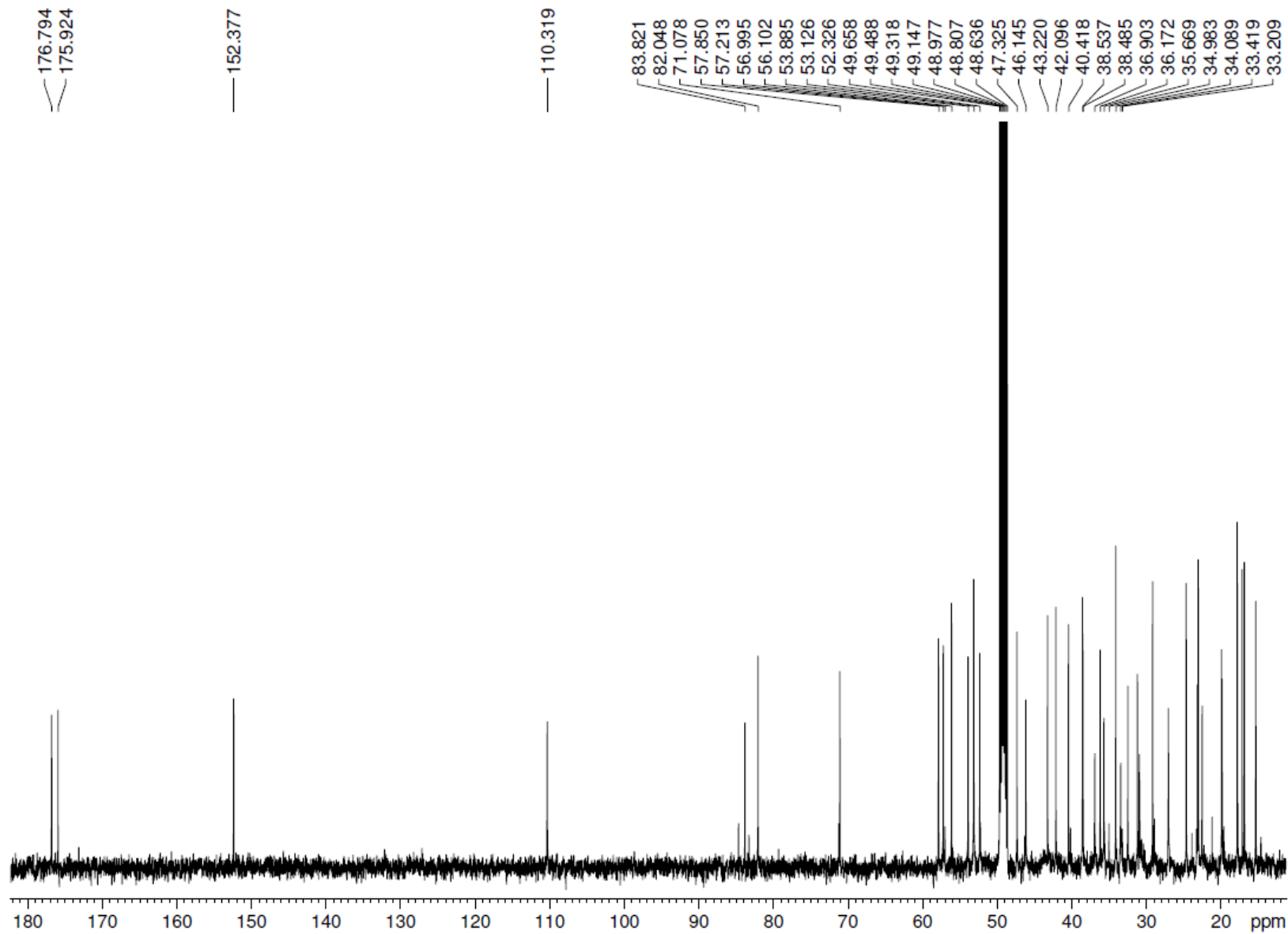
Methyl N-[3 β -acetoxy-2 α -propargyl-lup-20(29)-en-28-oyl]-5-piperazine-pentanoate **15a** ^1H NMR spectra (CDCl_3)



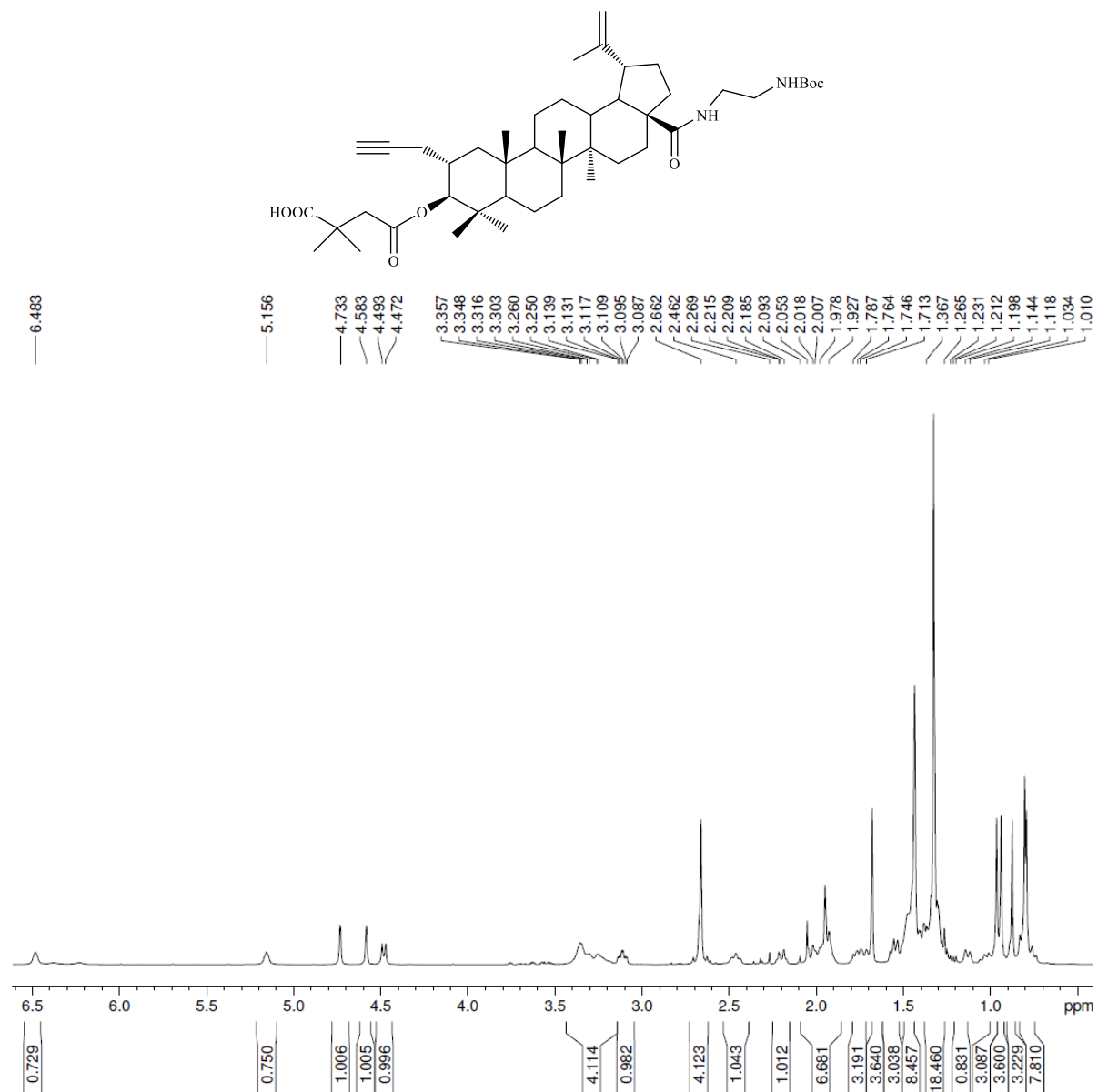
Methyl N-[3 β -acetoxy-2 α -propargyl-lup-20(29)-en-28-oyl]-5-piperazine-pentanoate **15a** ^{13}C NMR spectra (CDCl_3)



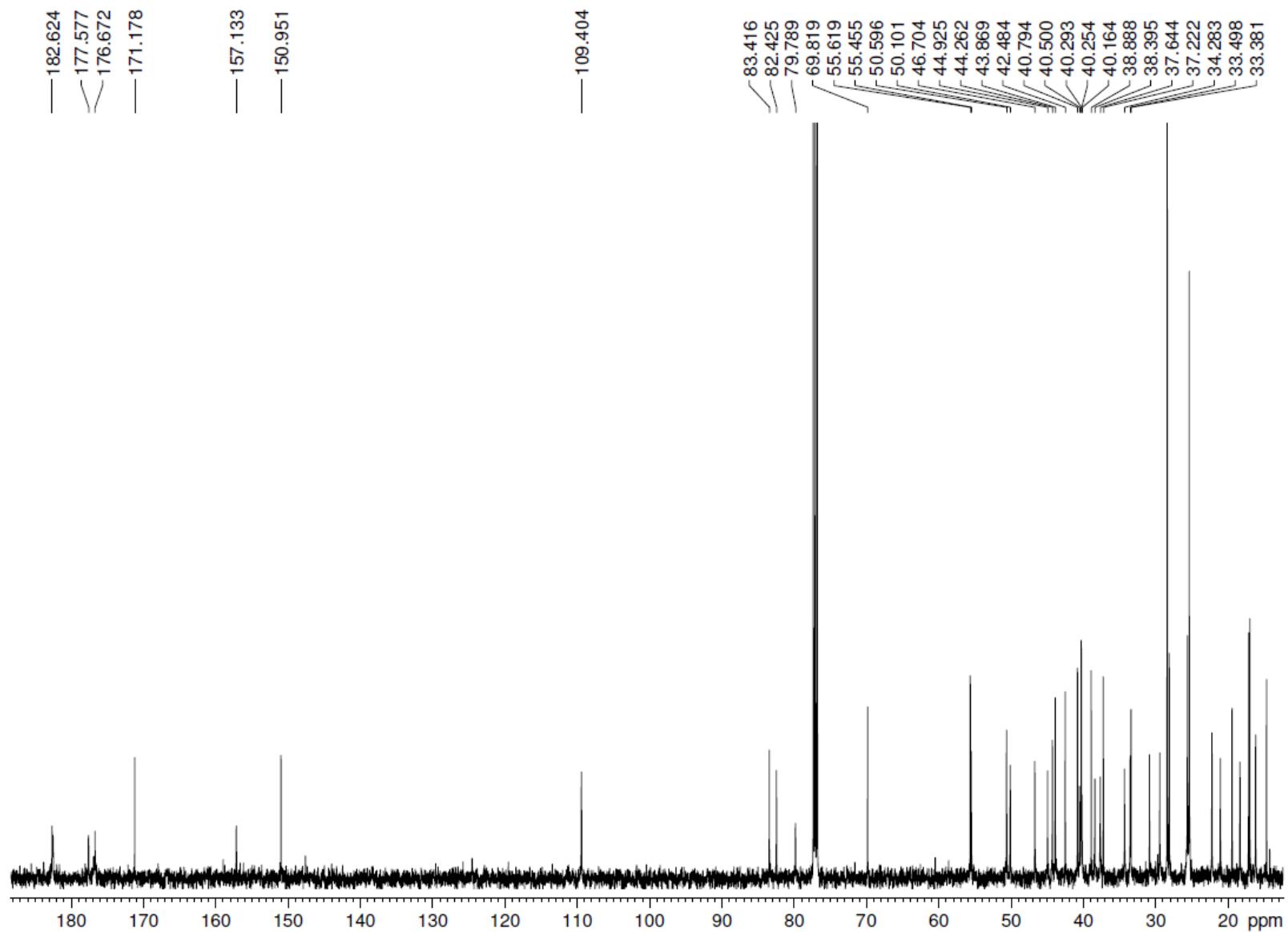
N-[3β-Hydroxy-2α-propargyl-lup-20(29)-en-28-oyl]-5-piperazine-pentanoic acid **15b** ¹H NMR spectra (CD₃OD)



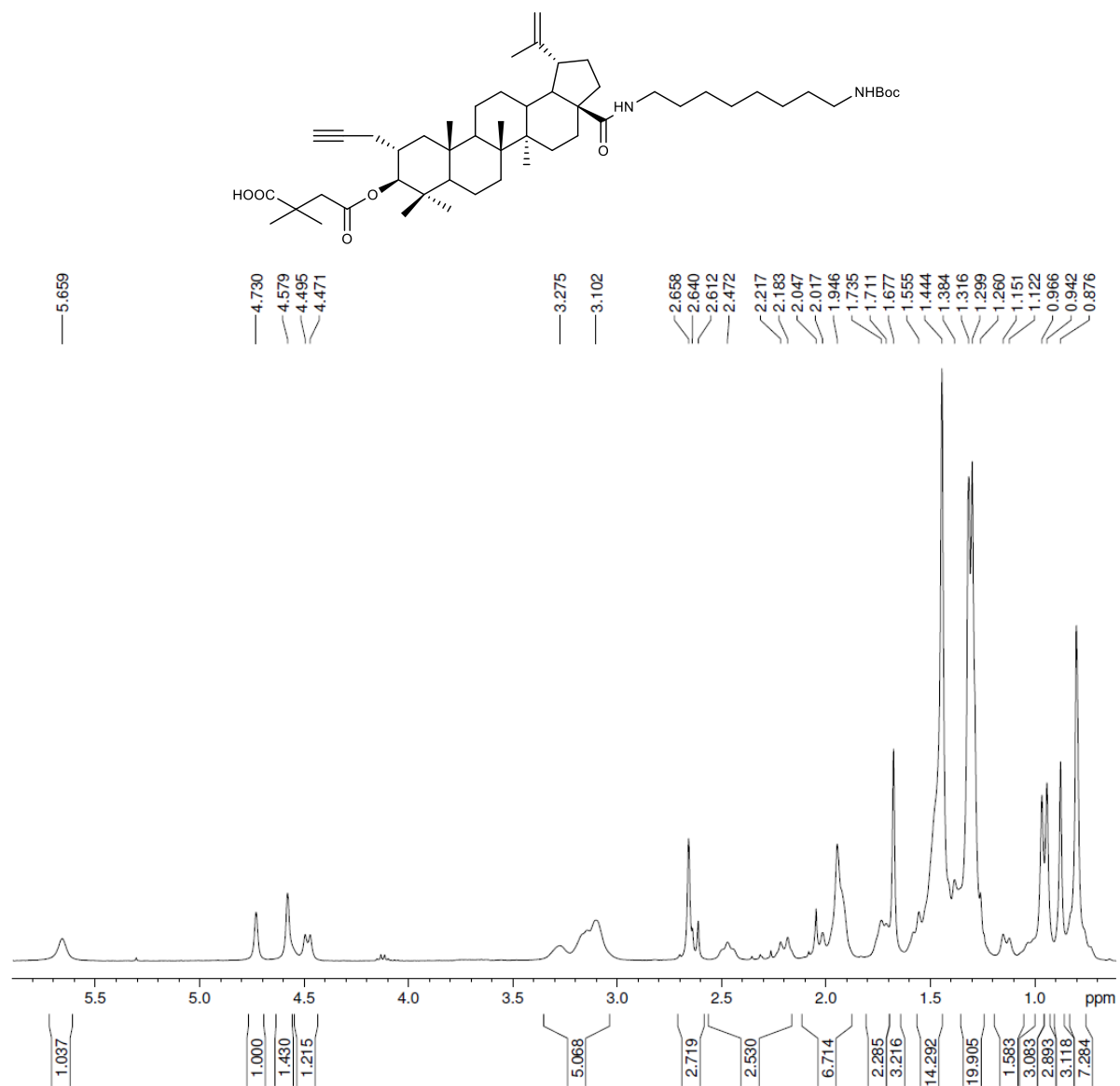
N-[3 β -Hydroxy-2 α -propargyl-lup-20(29)-en-28-oyl]-5-piperazine-pentanoic acid **15b** ^{13}C NMR spectra (CD_3OD)



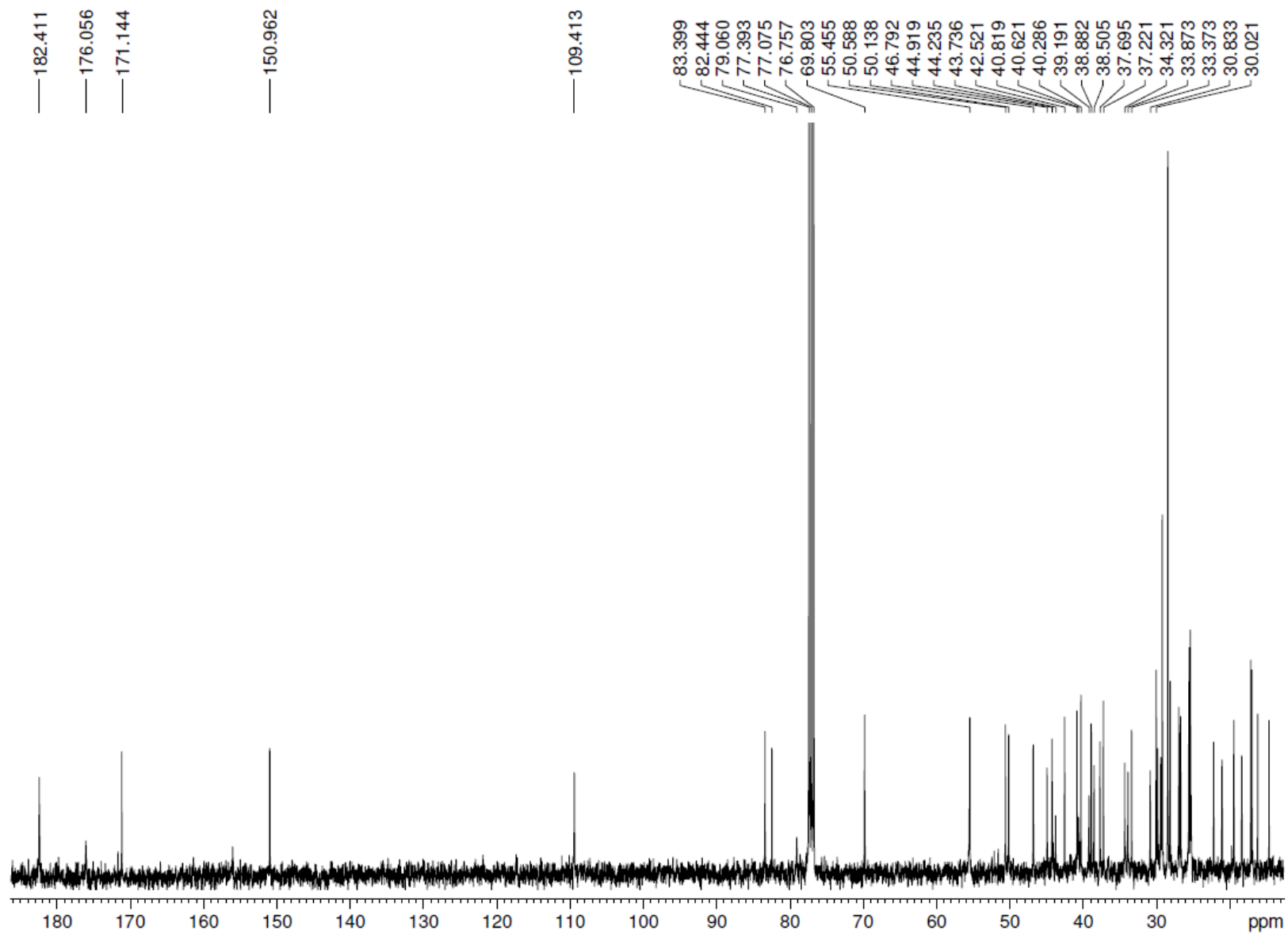
N-[3β-O-(3',3'-dimethylsuccinyl)-2α-propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-2-ethylamine **16** ¹H NMR spectra (CDCl₃)



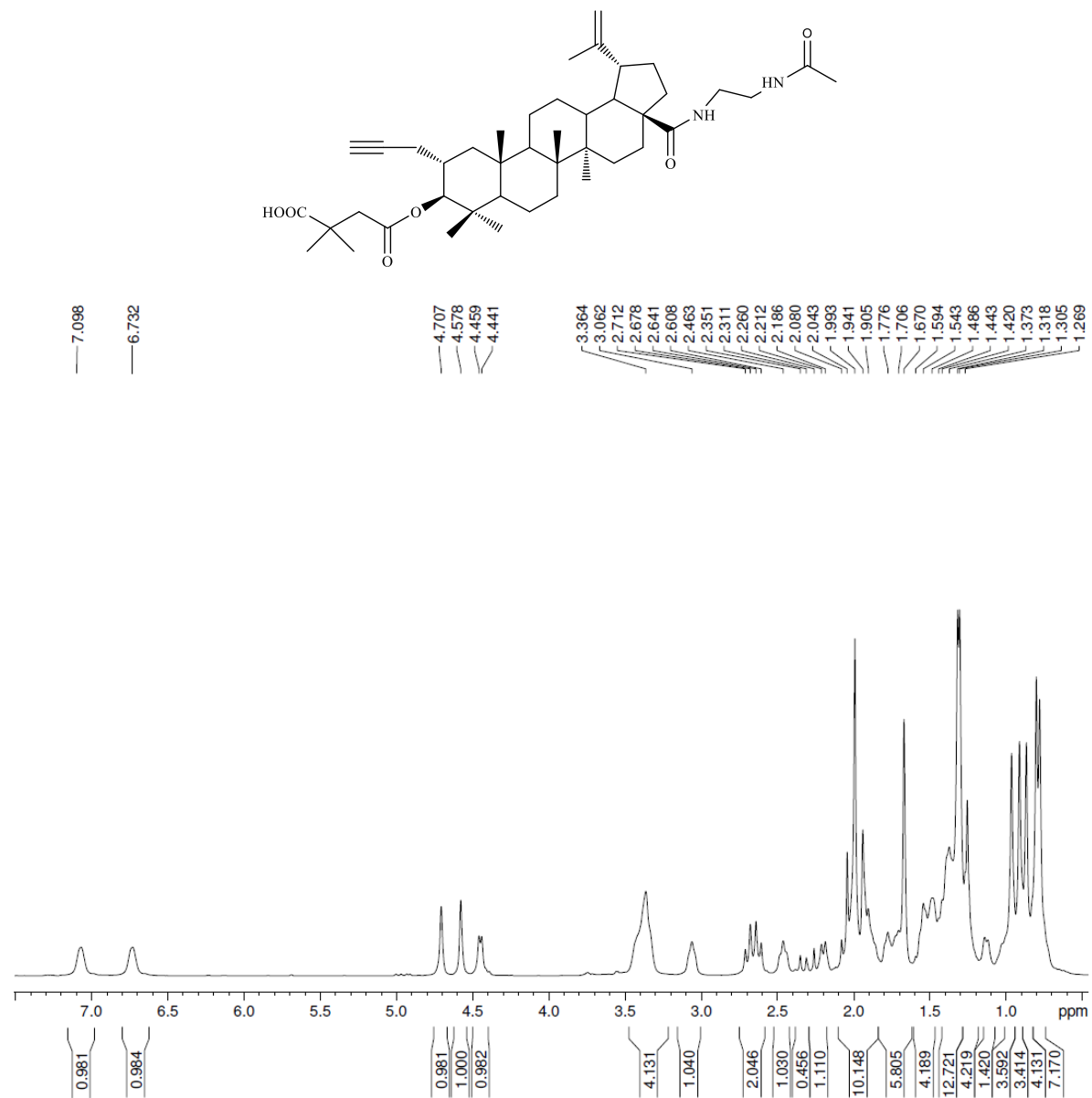
N-[3 β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-2-ethylamine **16** ^{13}C NMR spectra (CDCl_3)



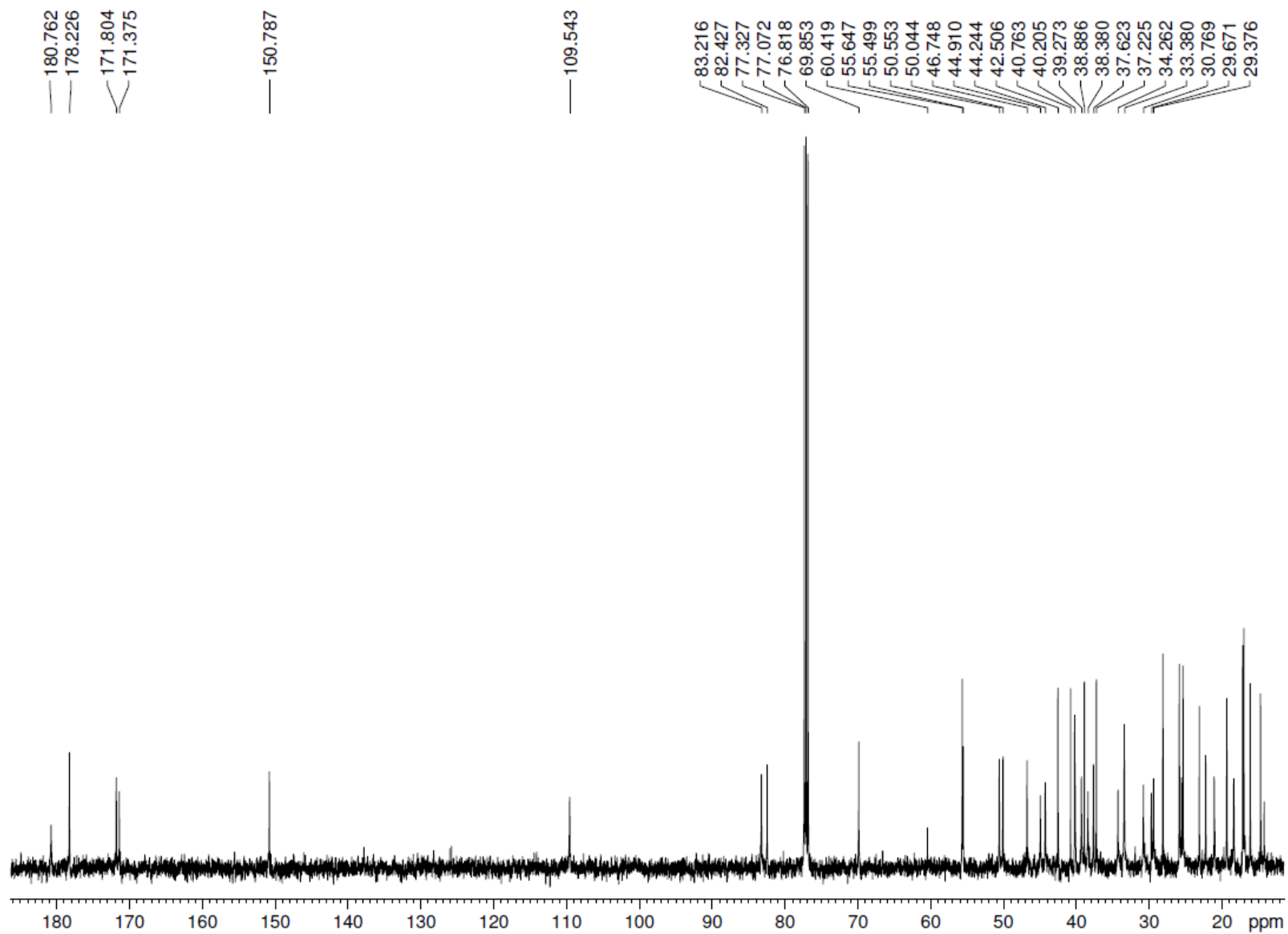
N-[3 β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-8-octylamine **17** ¹H NMR spectra (CDCl₃)



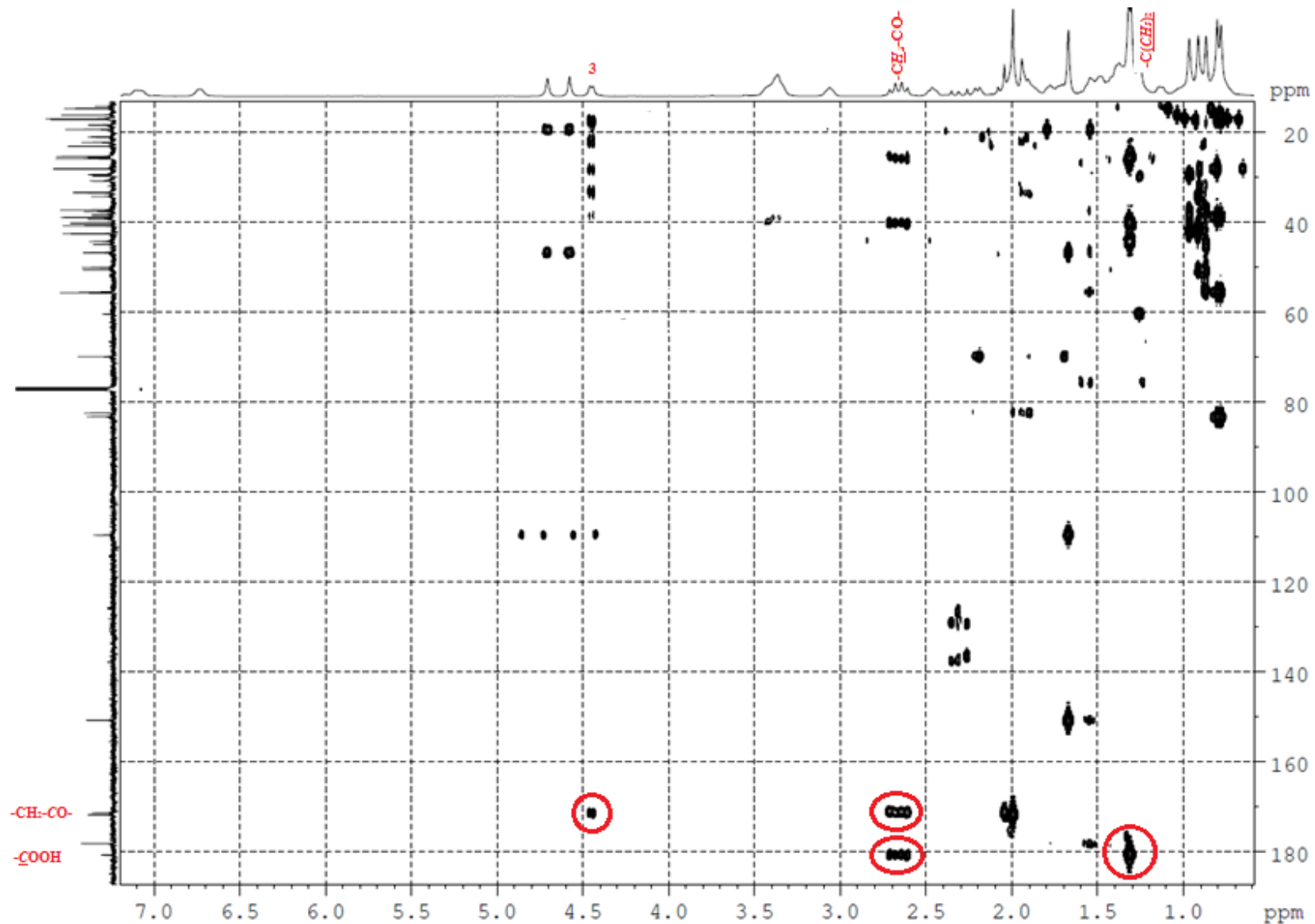
N-[3 β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oyl]-N'-(tert-butoxycarbonyl)-8-octylamine **17** ^{13}C NMR spectra (CDCl_3)



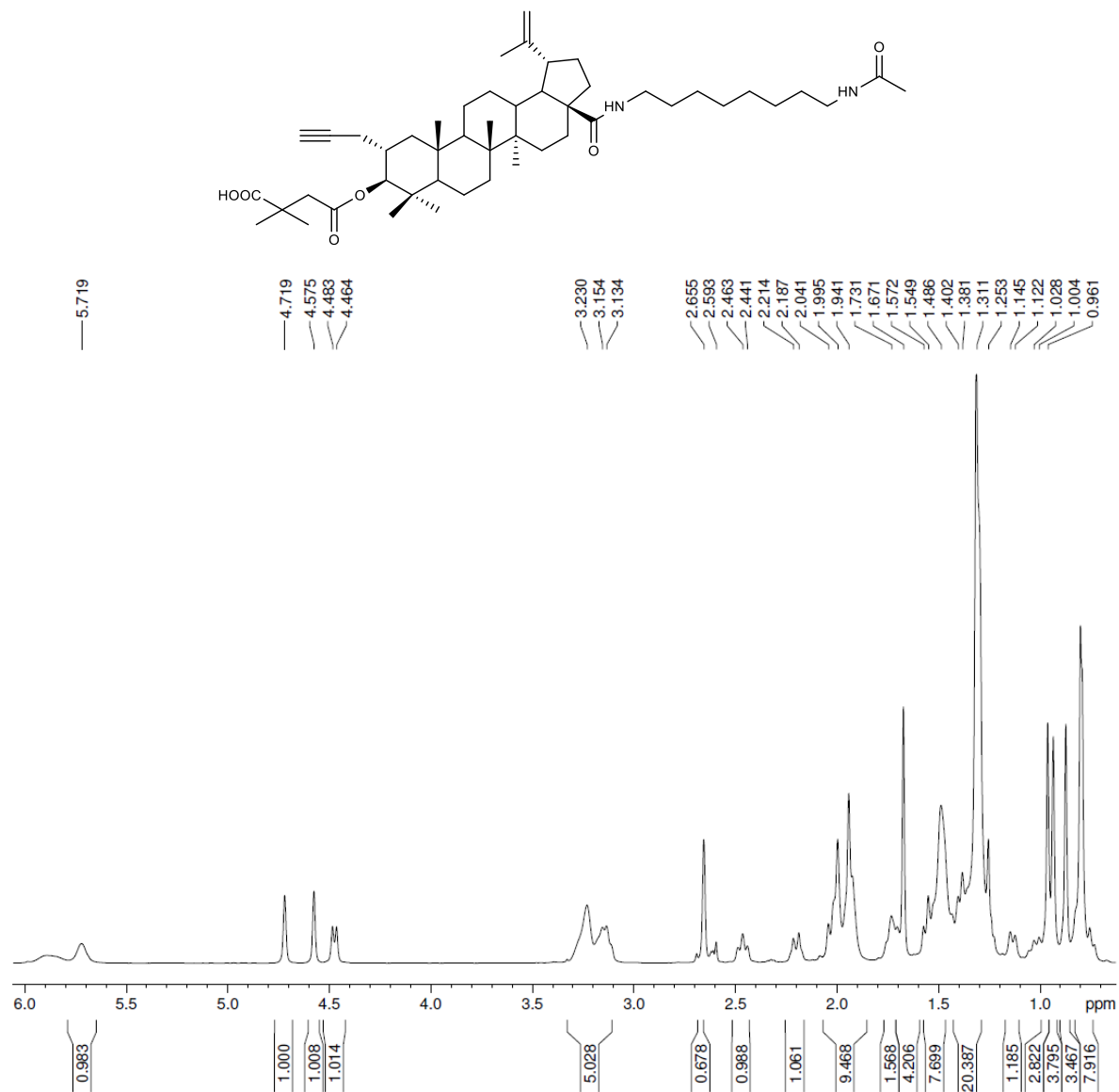
{[N-(3 β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oyl)-2-aminoethyl]-carbamoyl}methane **18** ^1H NMR spectra (CDCl_3)



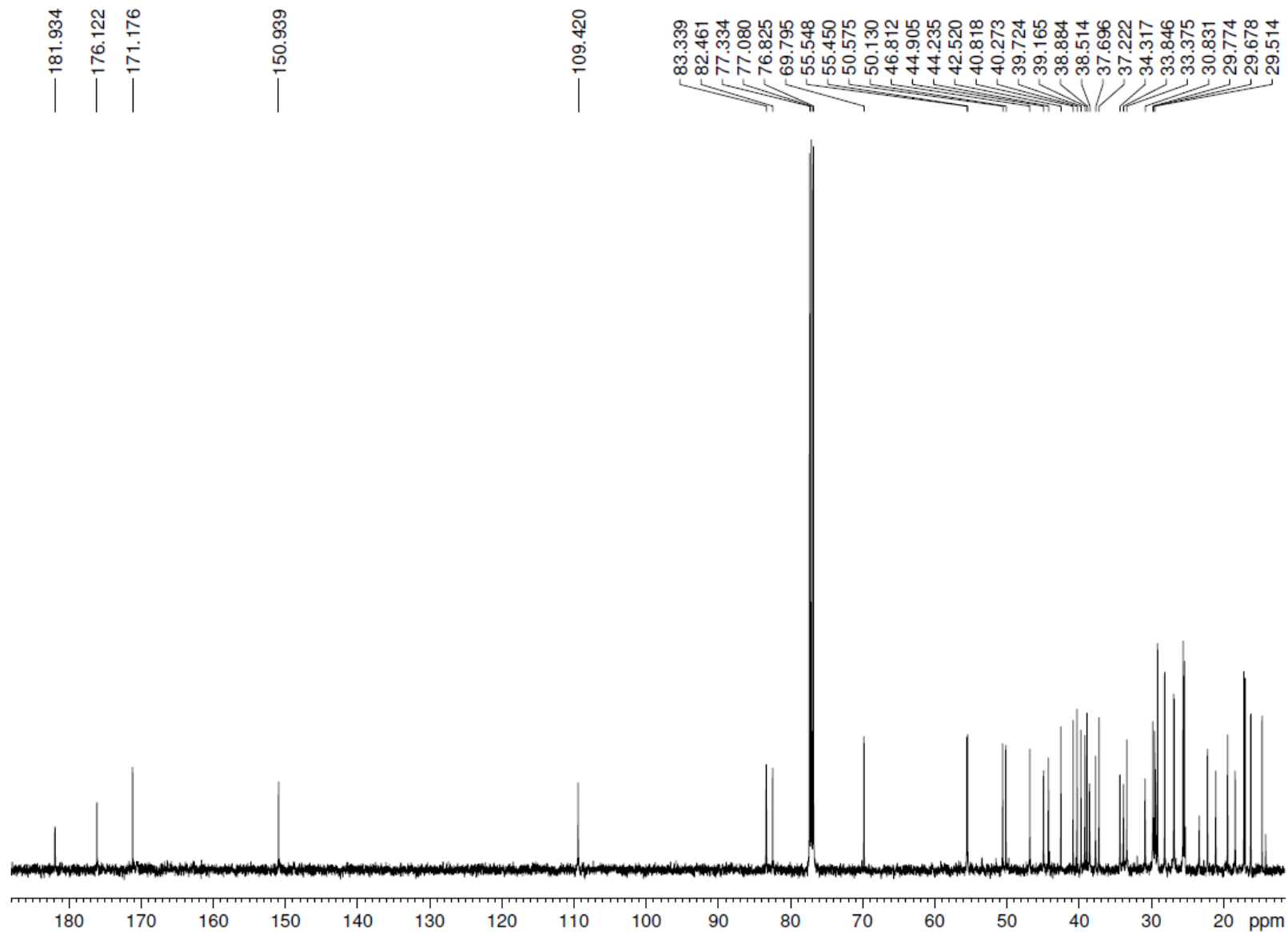
{[N-(3 β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oyl)-2-aminoethyl]-carbamoyl}methane **18** ^{13}C NMR spectra (CDCl_3)



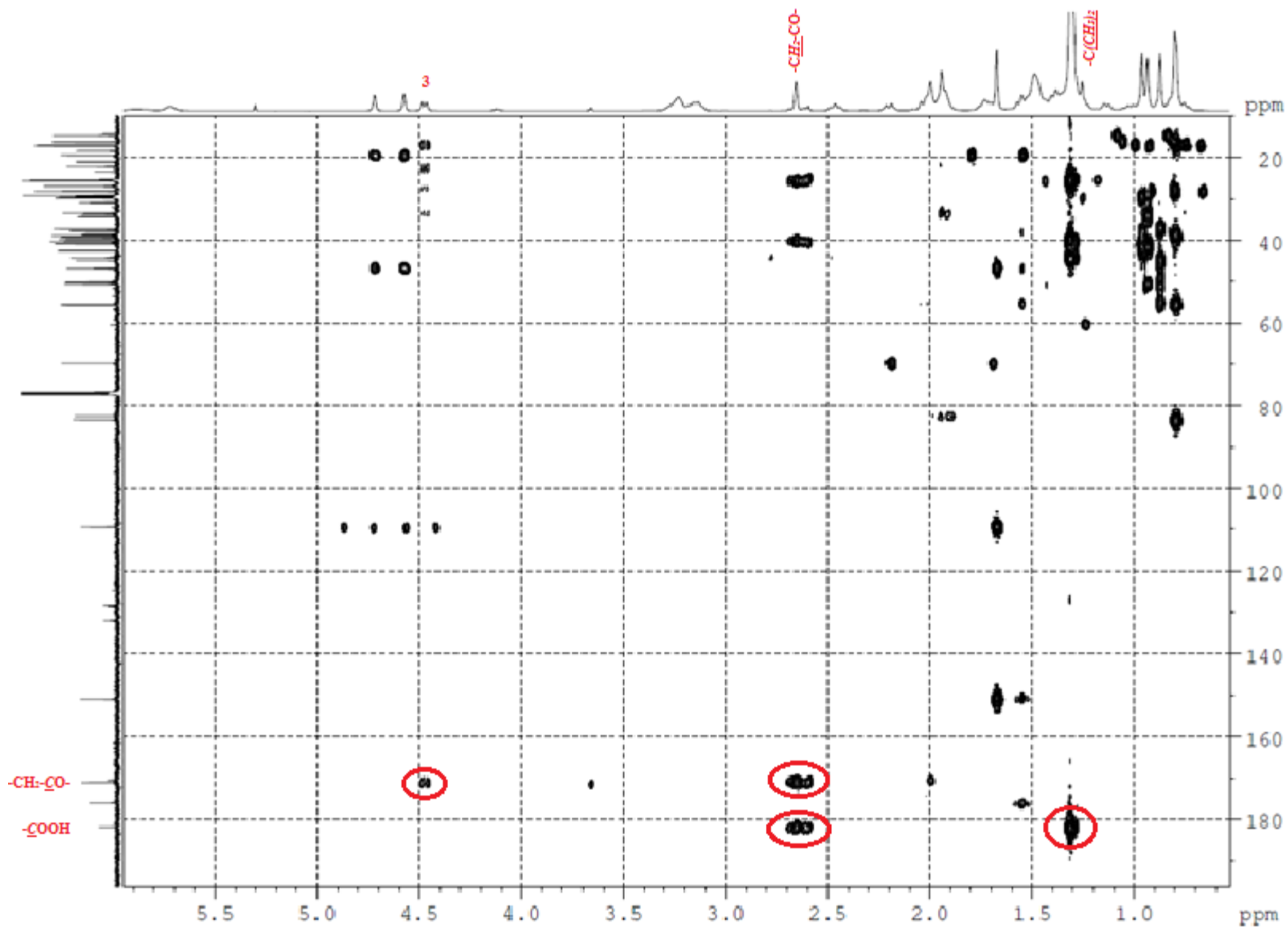
{[N-(3 β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oyl)-2-aminoethyl]-carbamoyl}methane **18** HMBC NMR spectra (CDCl₃)



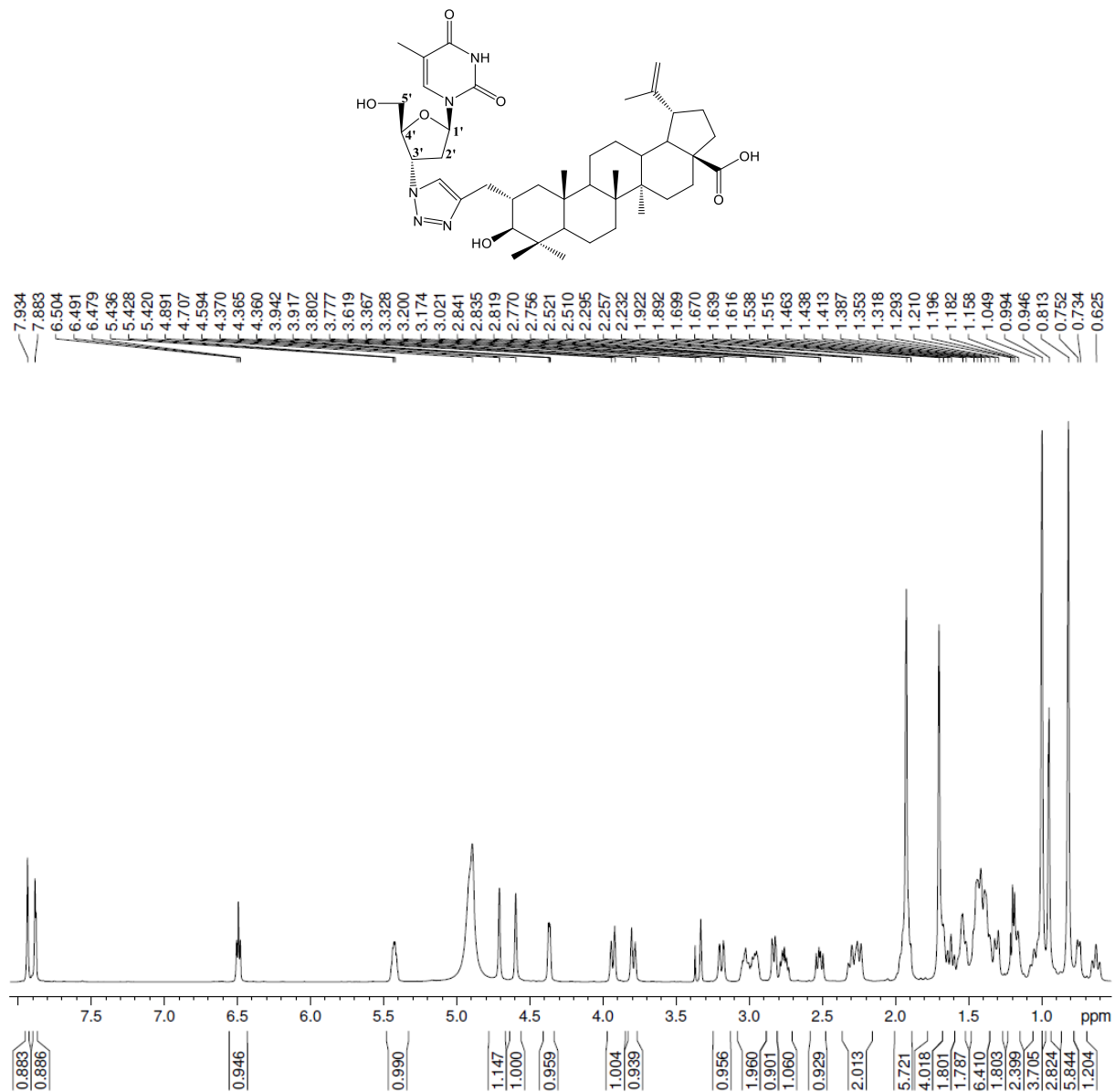
{[N-(3 β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oyl)-8-aminooctyl]-carbamoyl}methane **19** ¹H NMR spectra (CDCl₃)



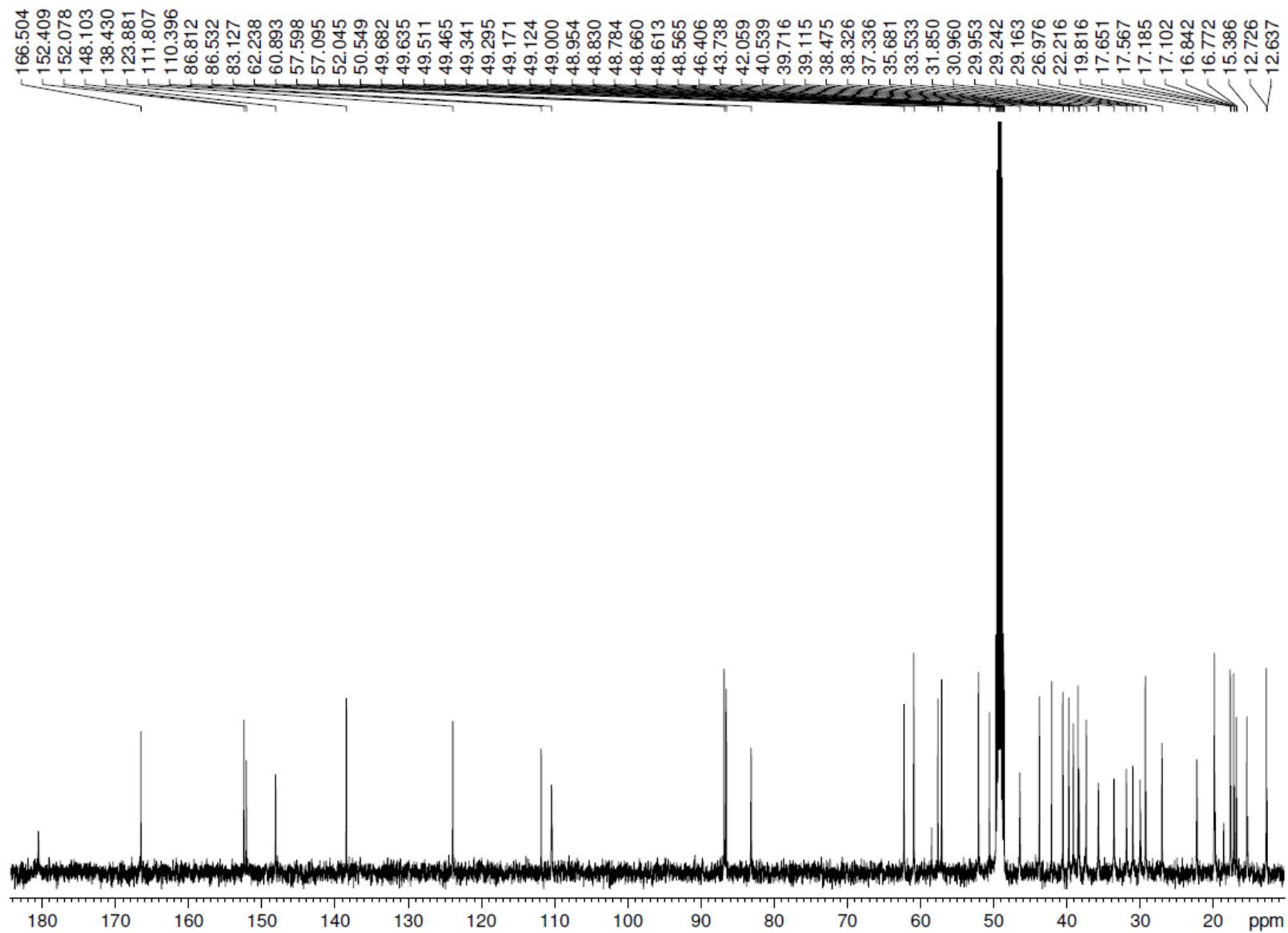
{[N-(3 β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oyl)-8-aminoctyl]-carbamoyl}methane **19** ^{13}C NMR spectra (CDCl_3)



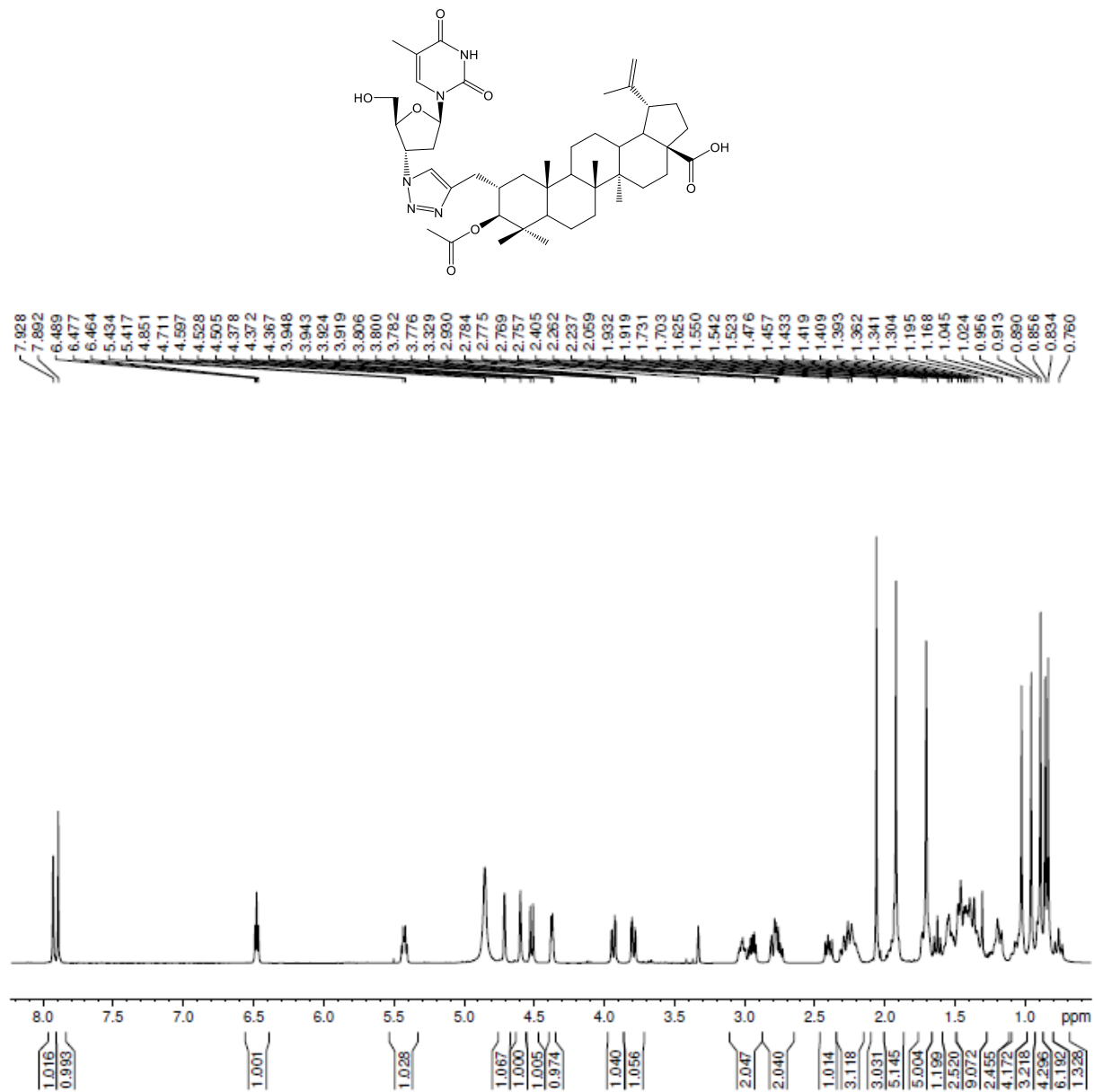
{[N-(3 β -O-(3',3'-dimethylsuccinyl)-2 α -propargyl-lup-20(29)-en-28-oyl)-8-aminoctyl]-carbamoyl}methane **19** HMBC NMR spectra (CDCl₃)



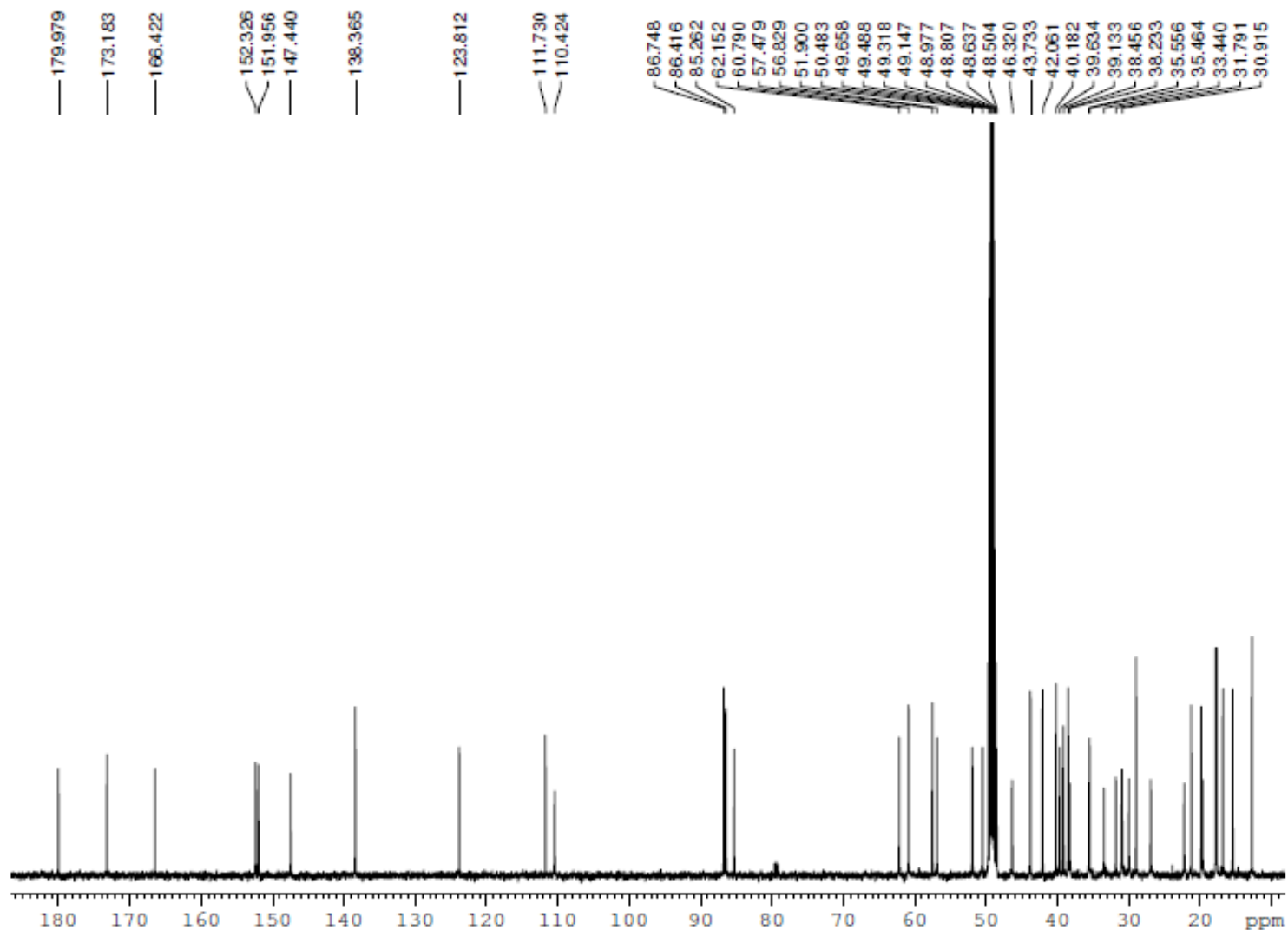
[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-2 α -methyl-3 β -hydroxylup-20(29)-en-28-oic acid **20** ^1H NMR spectra (CD_3OD)



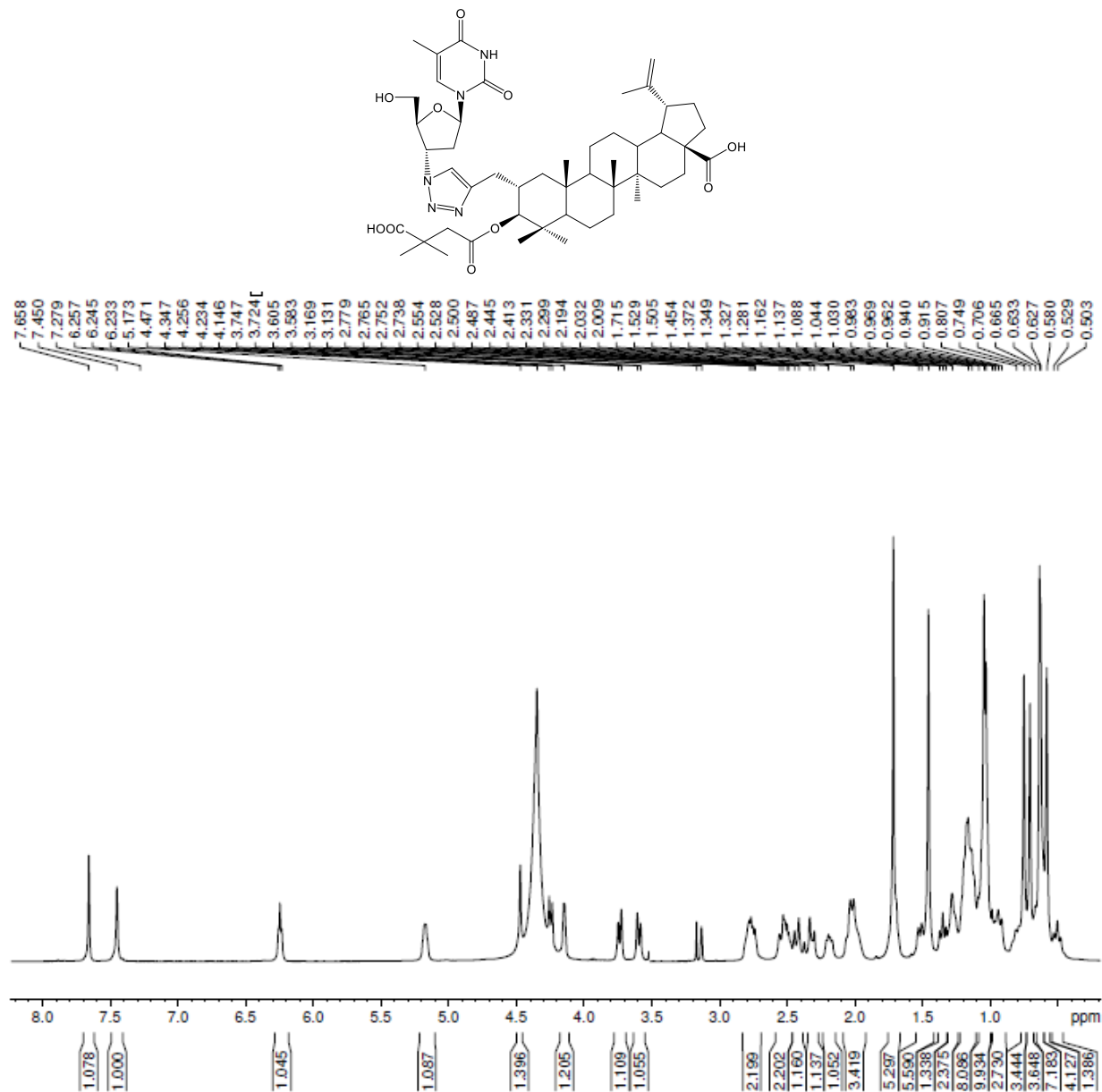
[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-2 α -methyl-3 β -hydroxylup-20(29)-en-28-oic acid **20** ^{13}C NMR spectra (CD_3OD)



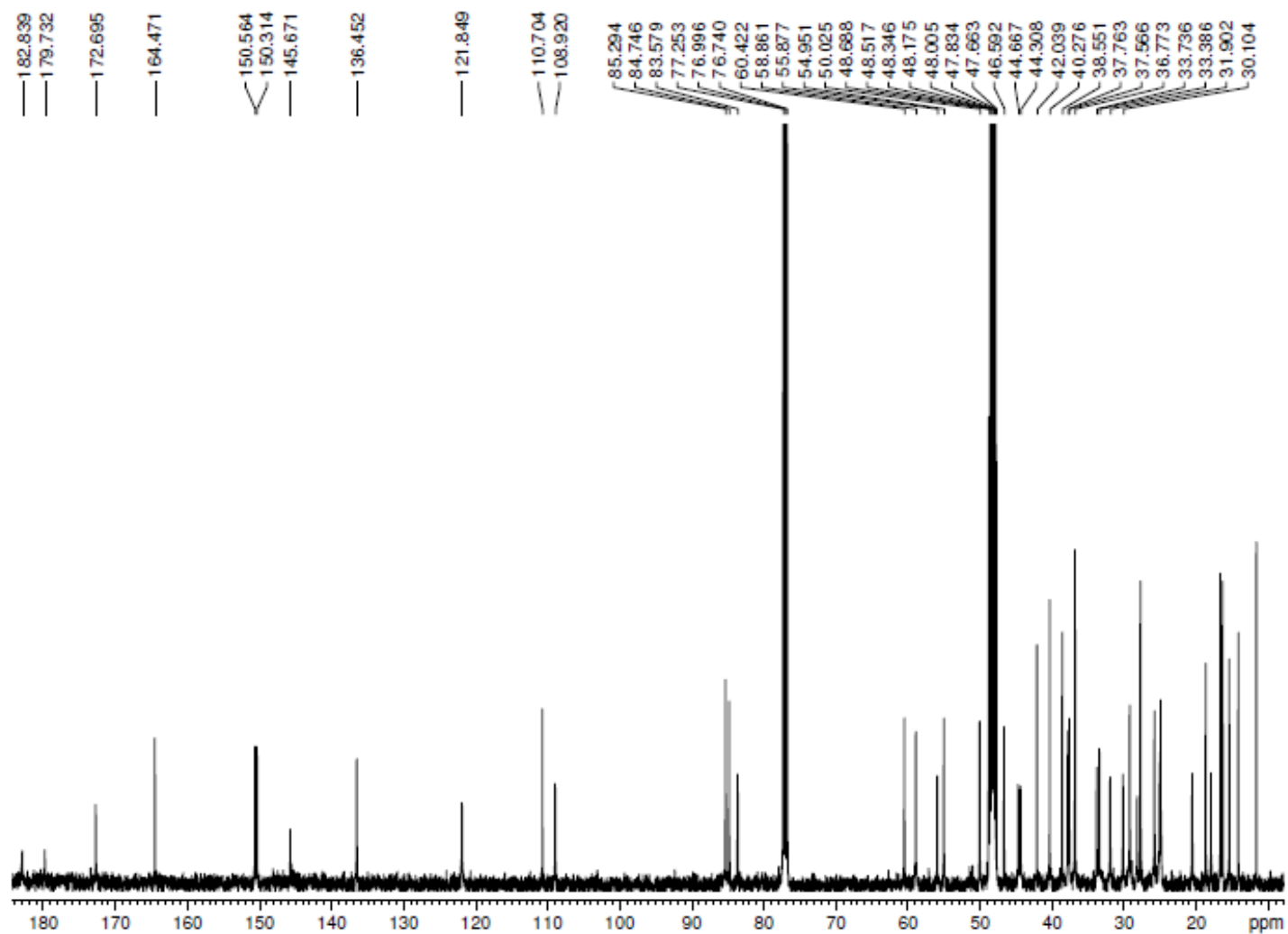
[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-2 α -methyl-3 β -acetoxy-20(29)-en-28-oic acid **21** ¹H NMR spectra (CD₃OD)



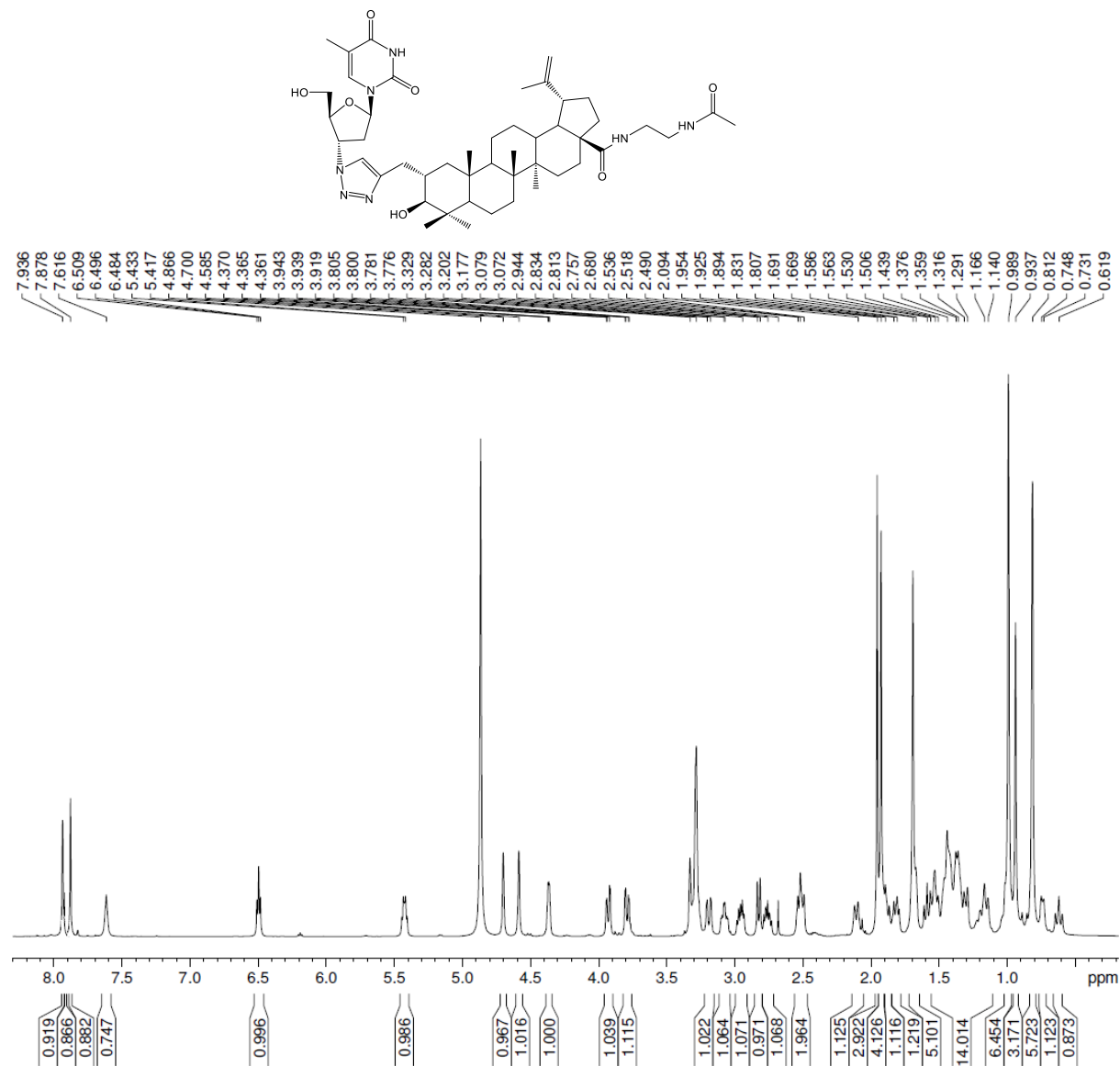
[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-2 α -methyl-3 β -acetoxylup-20(29)-en-28-oic acid **21** ^{13}C NMR spectra (CD_3OD)



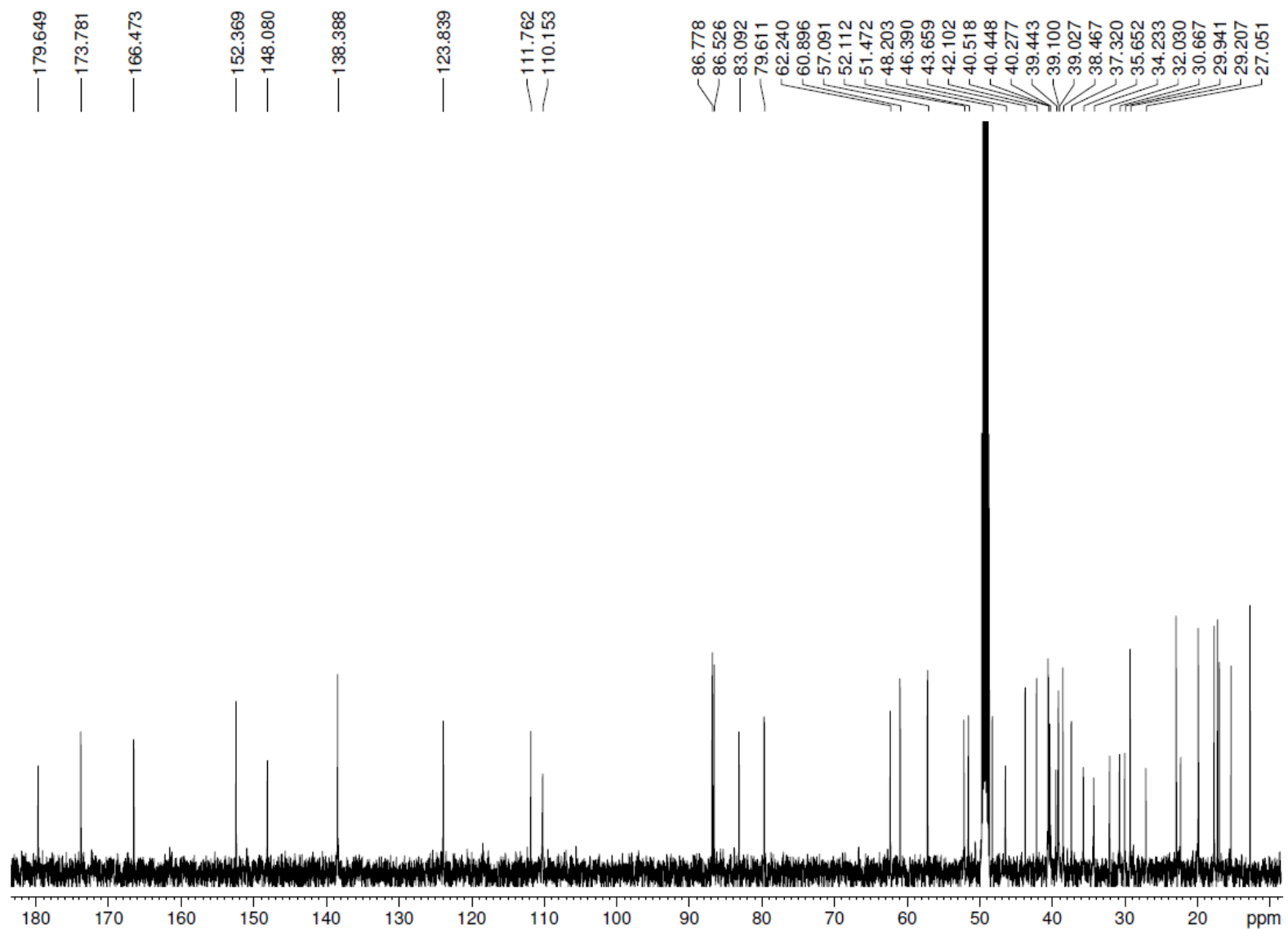
[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)lup-20(29)-en-28-oic acid **22** ¹H NMR spectra (CD₃OD)



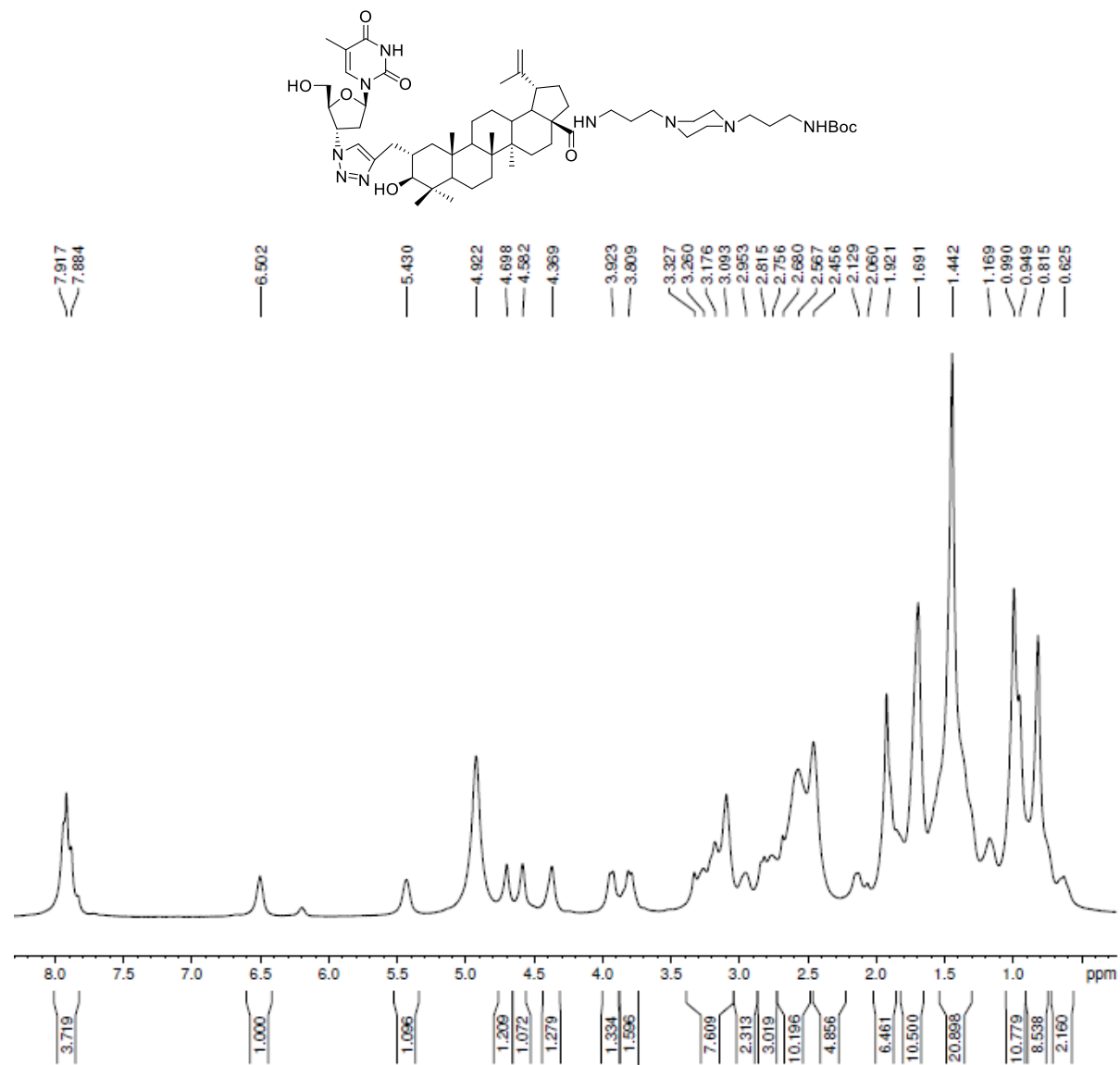
[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)lup-20(29)-en-28-oic acid **22** ^{13}C NMR spectra (CD_3OD)



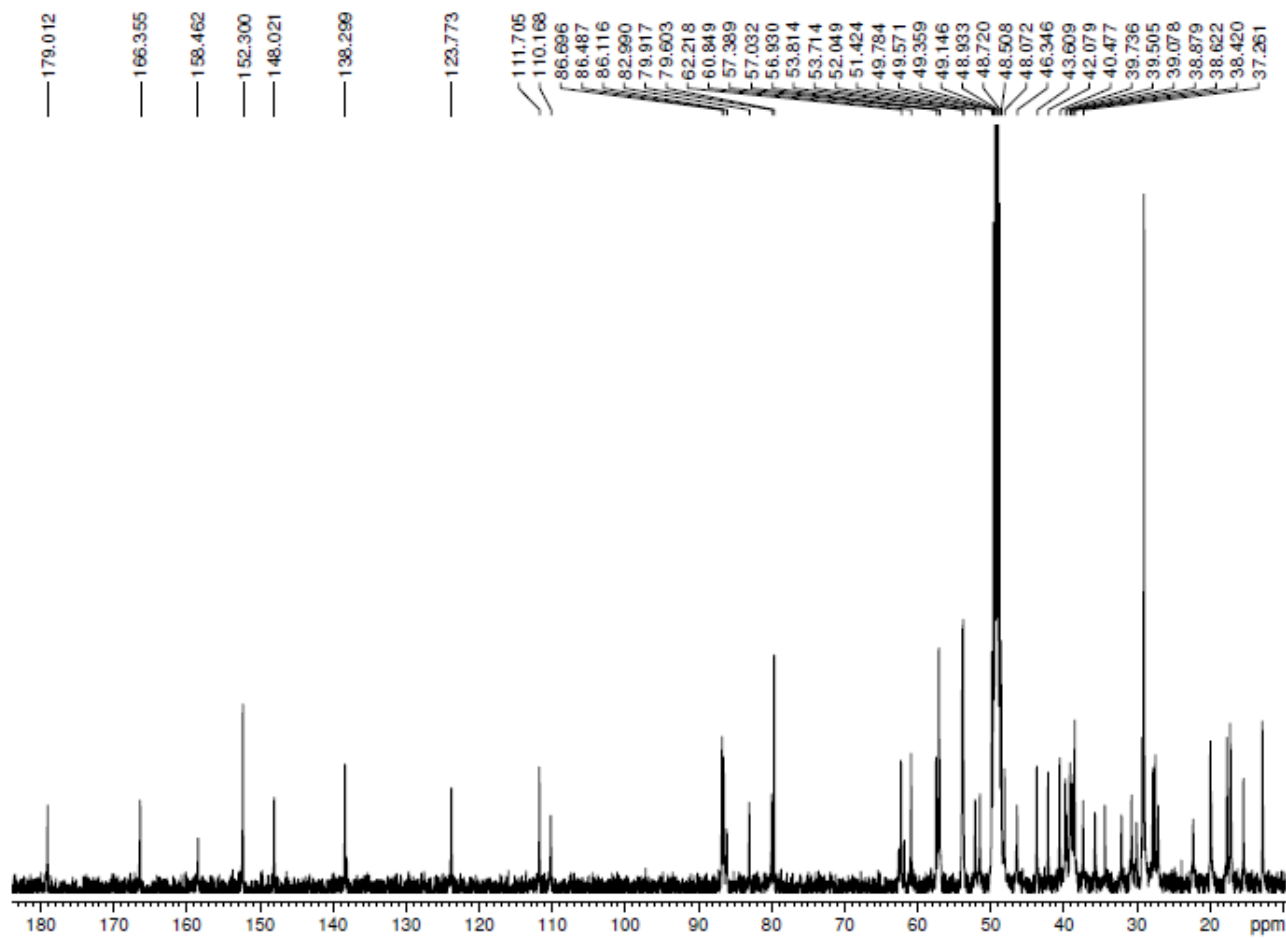
[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-{[N-(2 α -methyl-3 β -hydroxy-lup-20(29)-en-28-oyl)-2-aminoethyl]-carbomoyl}methane **23** ^1H NMR spectra (CD_3OD)



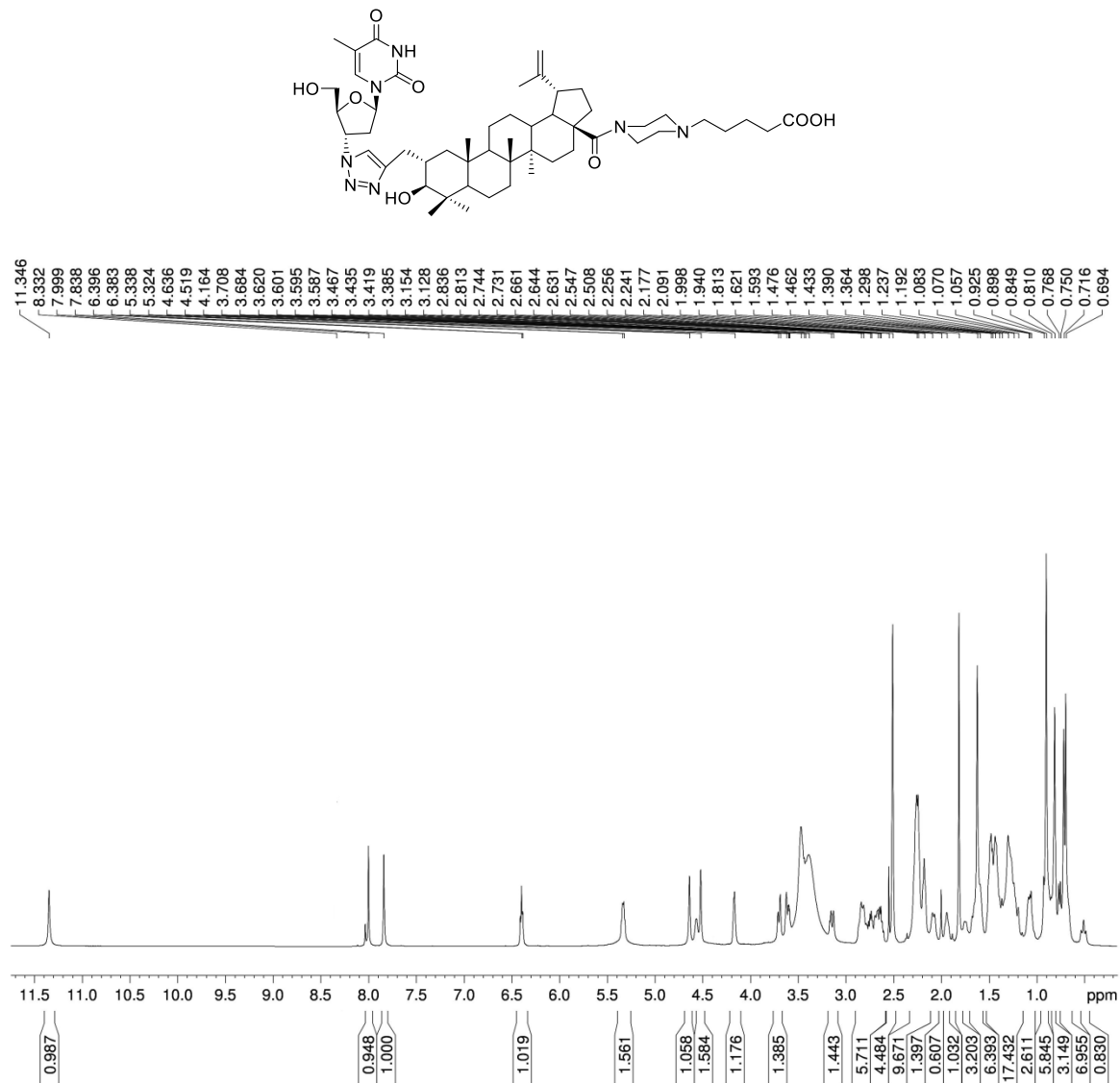
[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-[N-(2 α -methyl-3 β -hydroxy-lup-20(29)-en-28-oyl)-2-aminoethyl]-carbomoyl}methane **23** ^{13}C NMR spectra (CD_3OD)



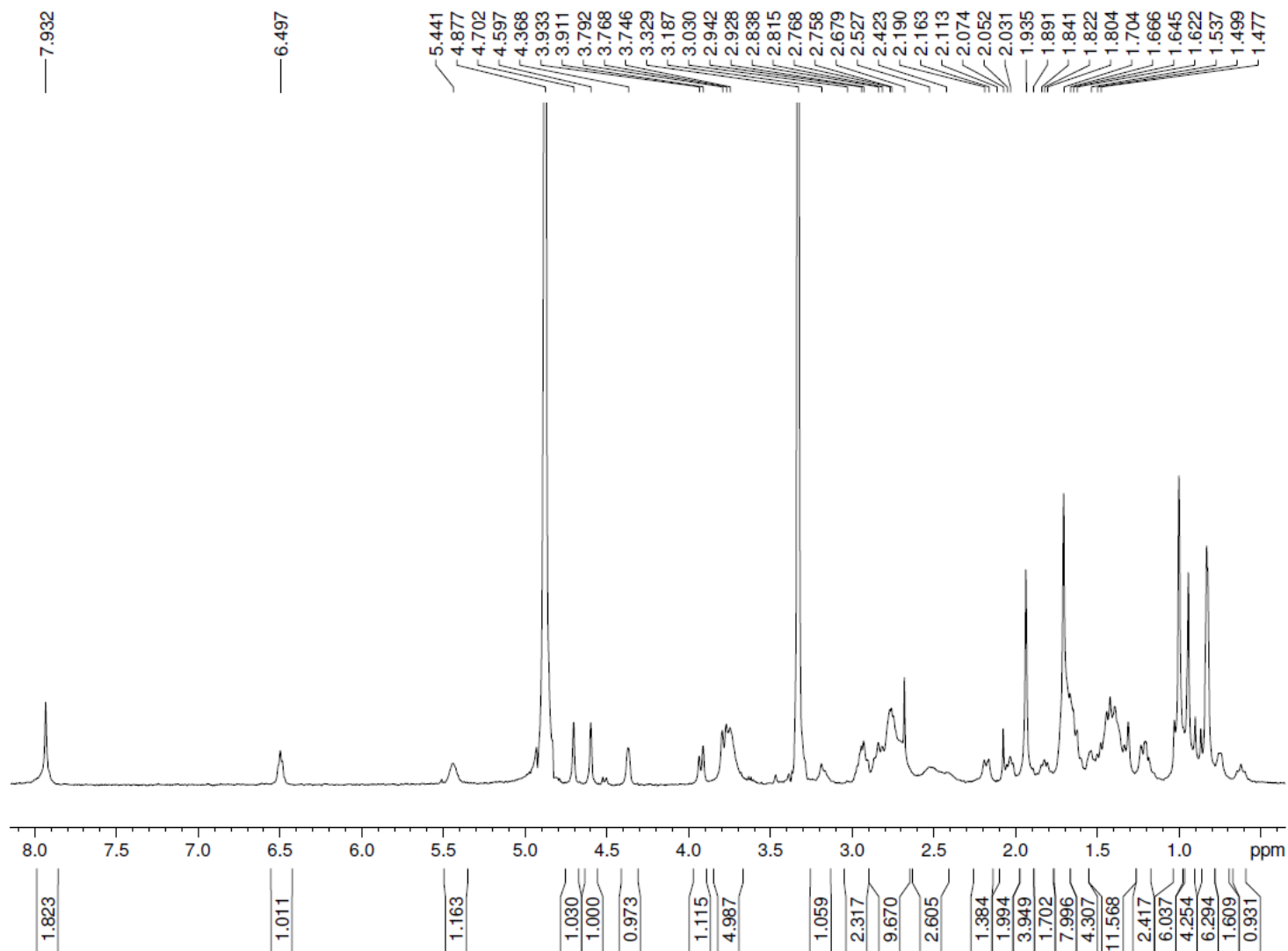
{[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-N-[N'-(tert-butoxycarbonyl)-{3-[4-(3-aminopropyl)piperazine]propyl}]}-2 α -methyl betulinic acid amide **24** ¹H NMR spectra (CD₃OD)



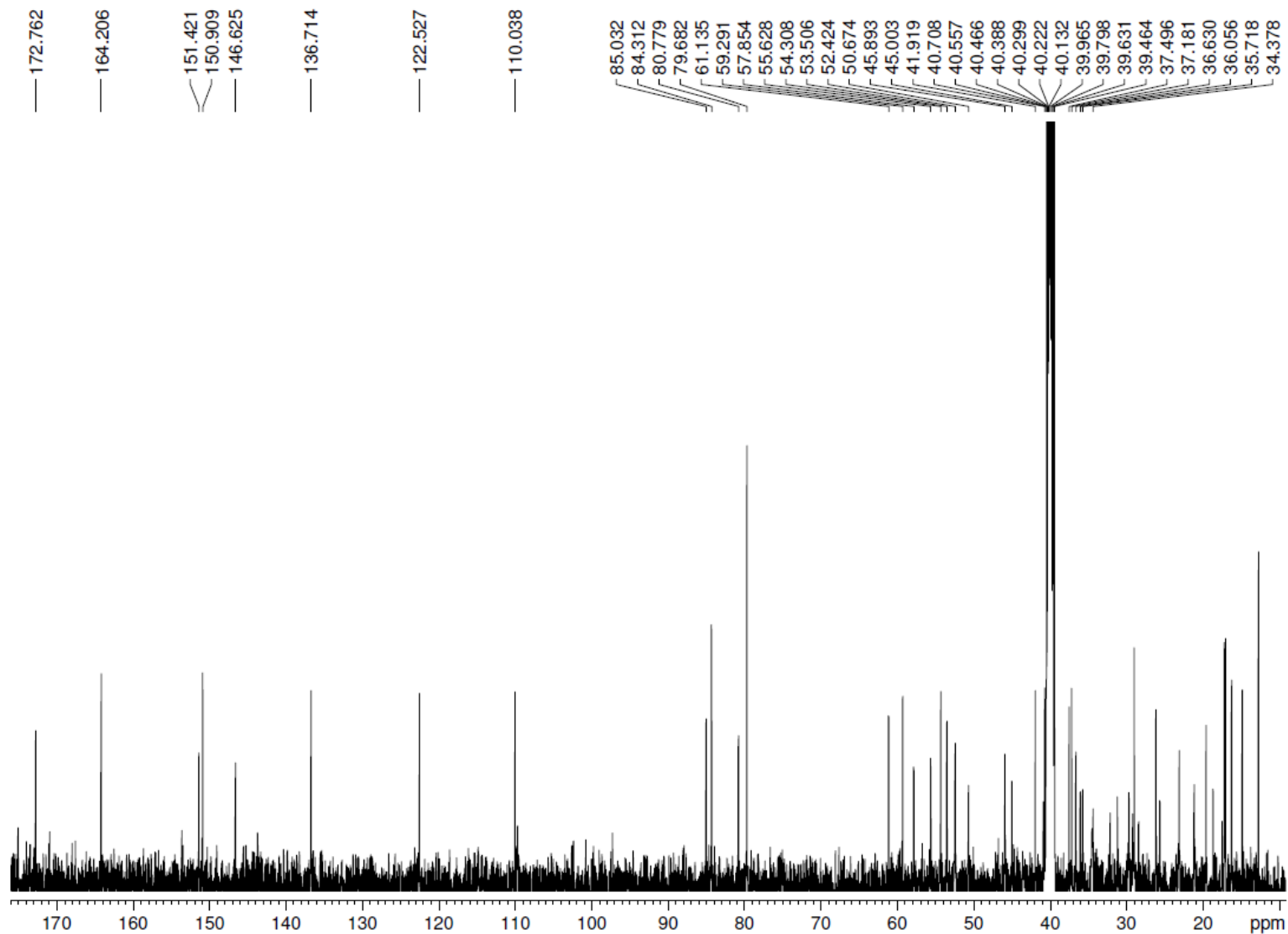
{[1-(3'-Deoxythimidine)-1H-1,2,3-triazole-4-yl]-N-[N'-(tert-butoxycarbonyl)-{3-[4-(3-aminopropyl)piperazinyl]propyl}]-2 α -methyl betulinic acid amide **24** ^{13}C NMR spectra
(CD_3OD)



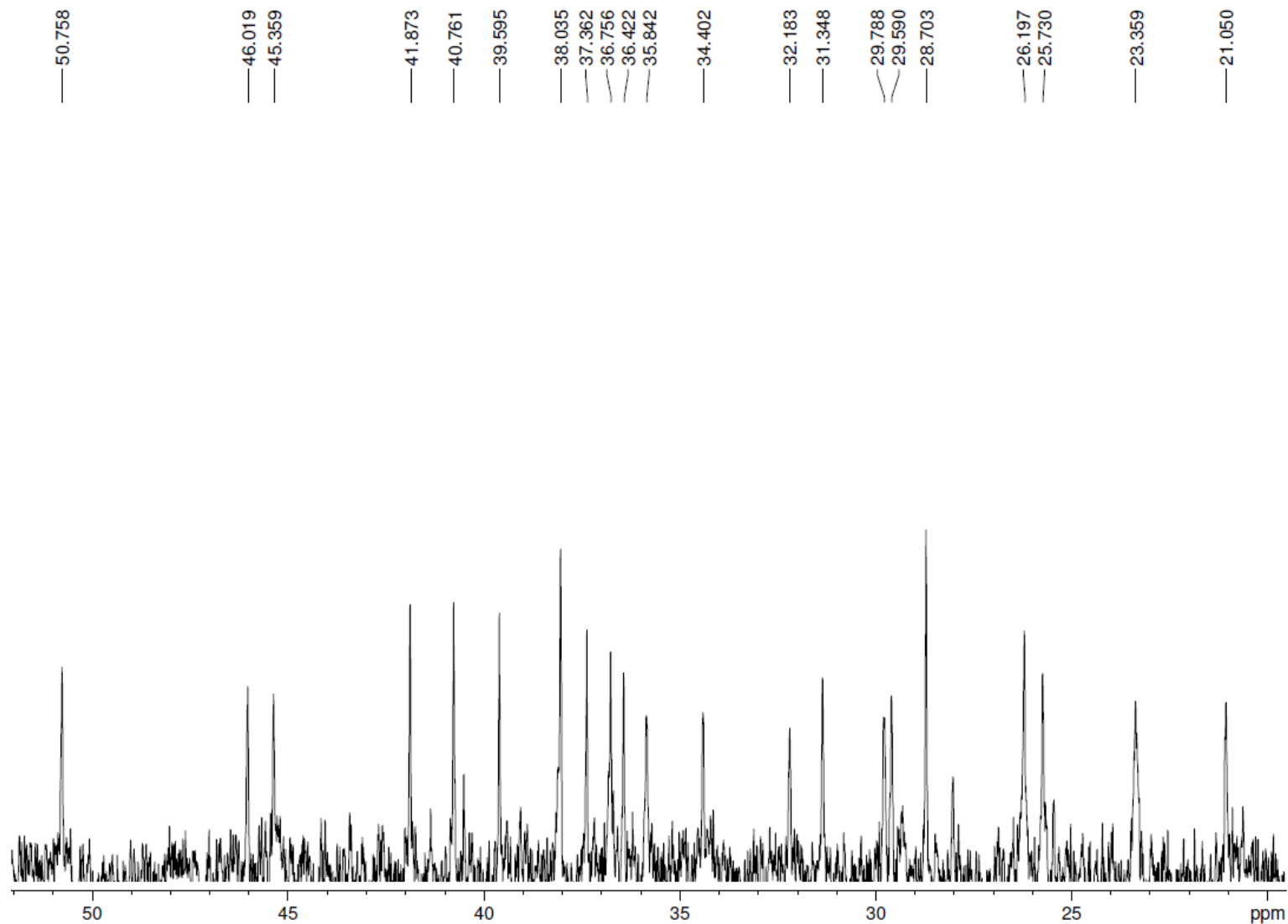
{[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-[N-2 α -methyl-3 β -hydroxy-lup-20(29)-en-28-oyl]}-5-piperazine-pentanoic acid **25** ¹H NMR spectra (DMSO)



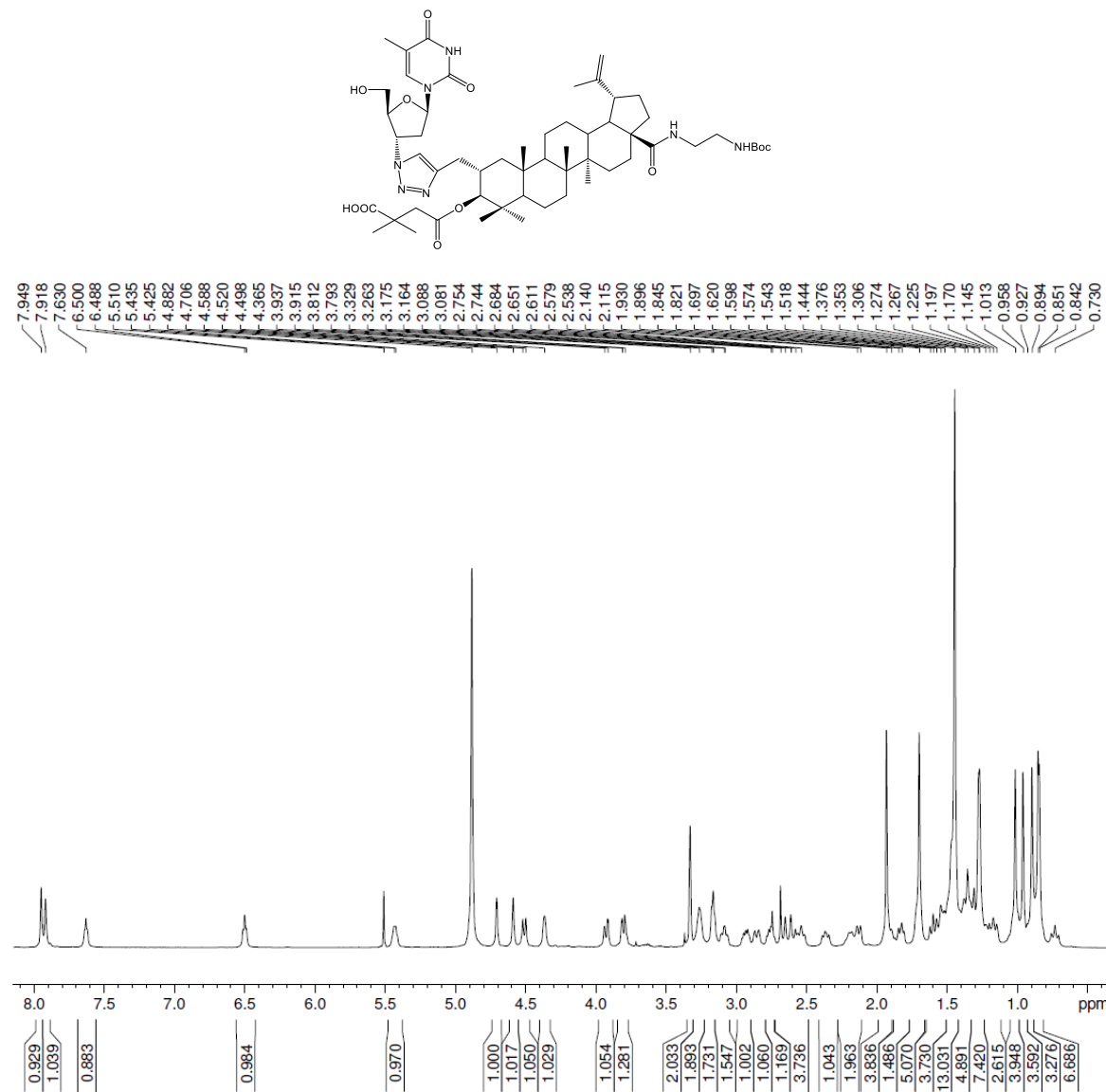
{[1-(3'-Deoxythimidine)-1H-1,2,3-triazole-4-yl]-[N-2 α -methyl-3 β -hydroxy-lup-20(29)-en-28-oyl]}-5-piperazine-pentanoic acid **25** ^1H NMR spectra (CD_3OD)



{[1-(3'-Deoxythimidine)-1H-1,2,3-triazole-4-yl]-[N-2 α -methyl-3 β -hydroxy-lup-20(29)-en-28-oyl]}-5-piperazine-pentanoic acid **25** ^{13}C NMR spectra (DMSO)

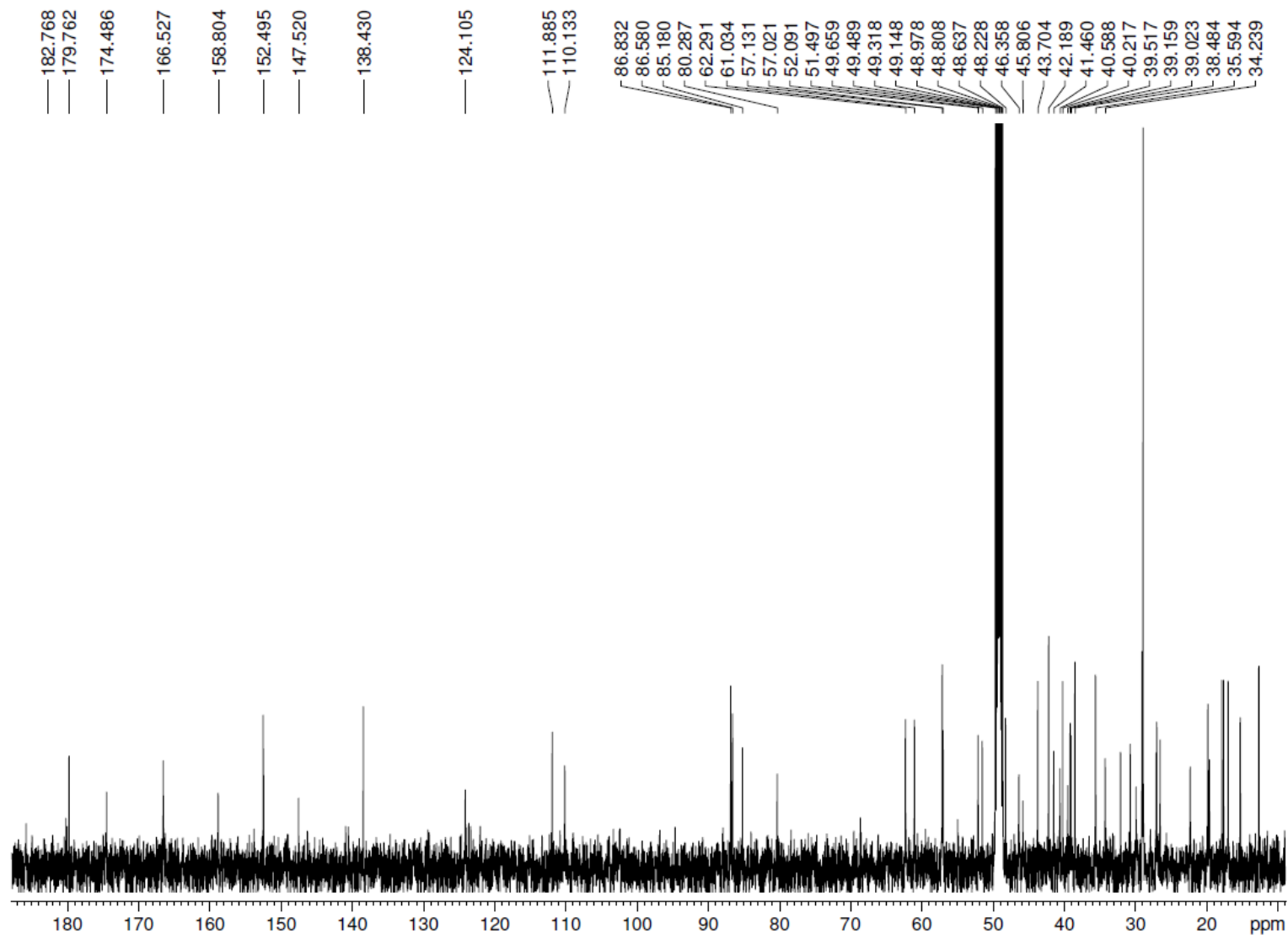


{[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-[N-2 α -methyl-3 β -hydroxy-lup-20(29)-en-28-oyl]}-5-piperazine-pentanoic acid **25** ^{13}C NMR spectra (d-Pyridine)

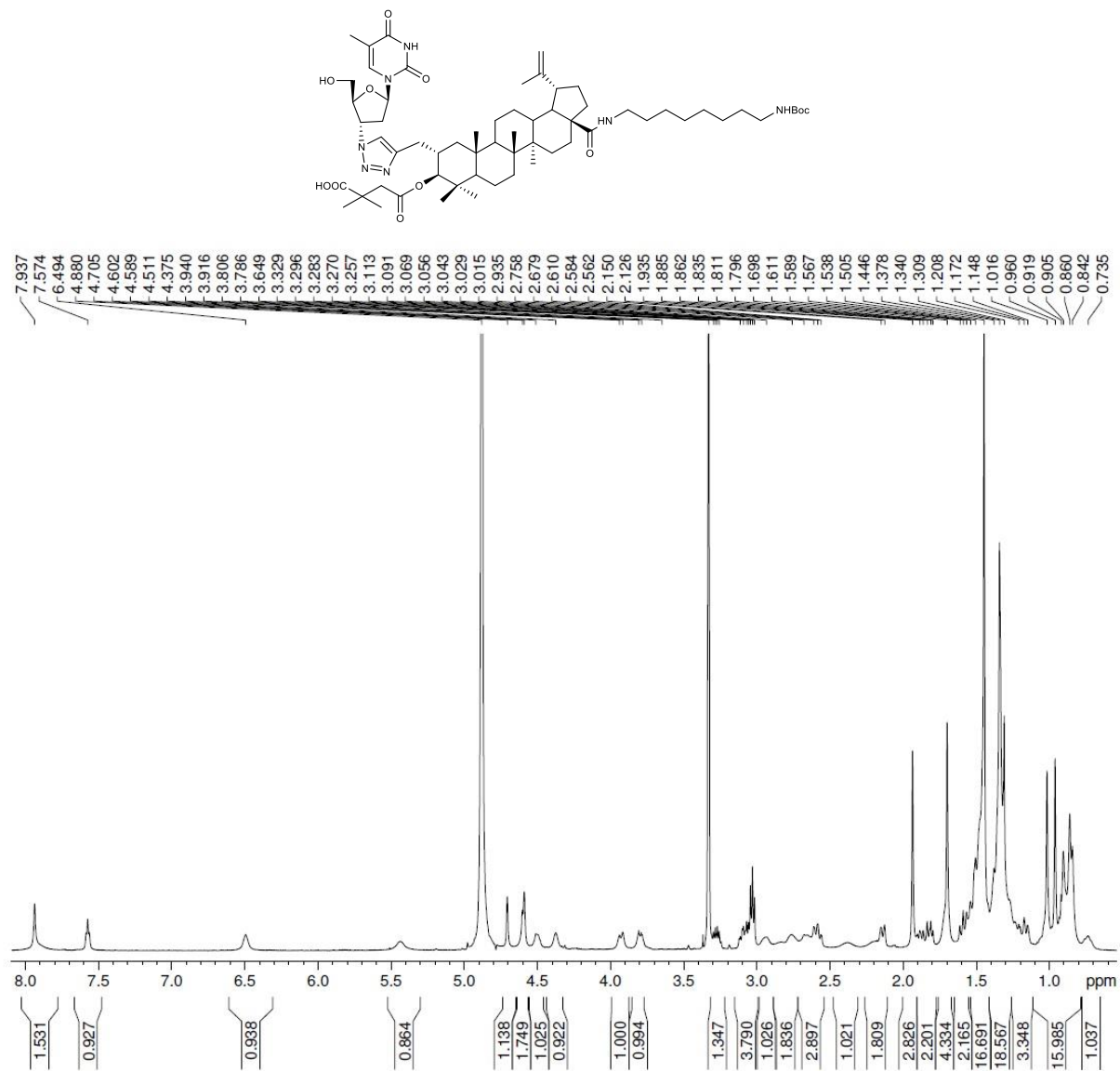


[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-[[N-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)-lup-20,29-en-28-oyl]-N'-(tert-butoxycarbonyl)]-2-ethylamine

26 ^1H NMR spectra (CD_3OD)

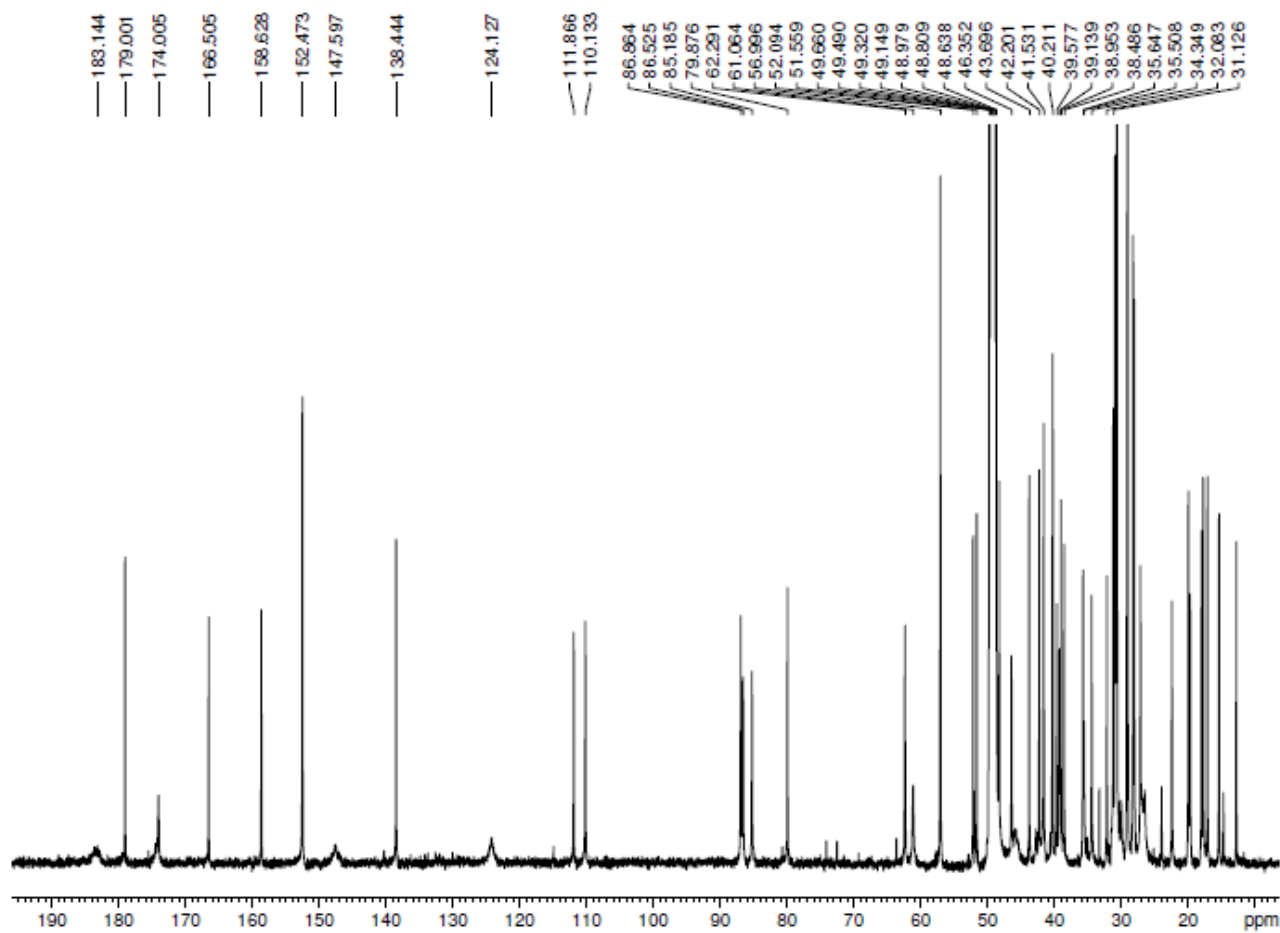


[1-(3'-Deoxythimidine)-1H-1,2,3-triazole-4-yl]-{[N-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)-lup-20,29-en-28-oyl]-N'-(tert-butoxycarbonyl)}-2-ethylamine
26 ^{13}C NMR spectra (CD_3OD)



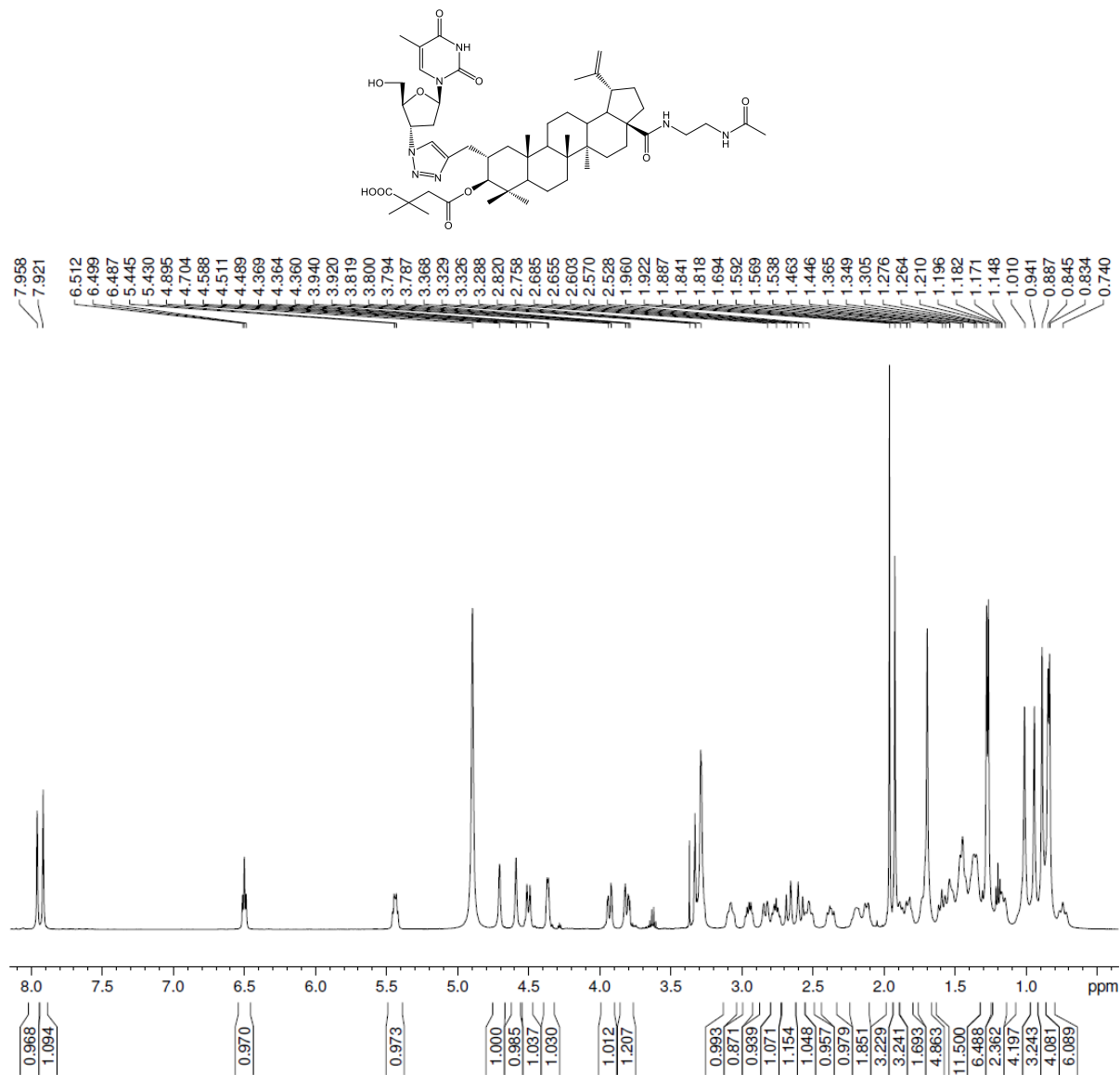
[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-[N-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)-lup-20,29-en-28-oyl]-N'-(tert-butoxycarbonyl)-8-octylamine

27 ¹H NMR spectra (CD₃OD)



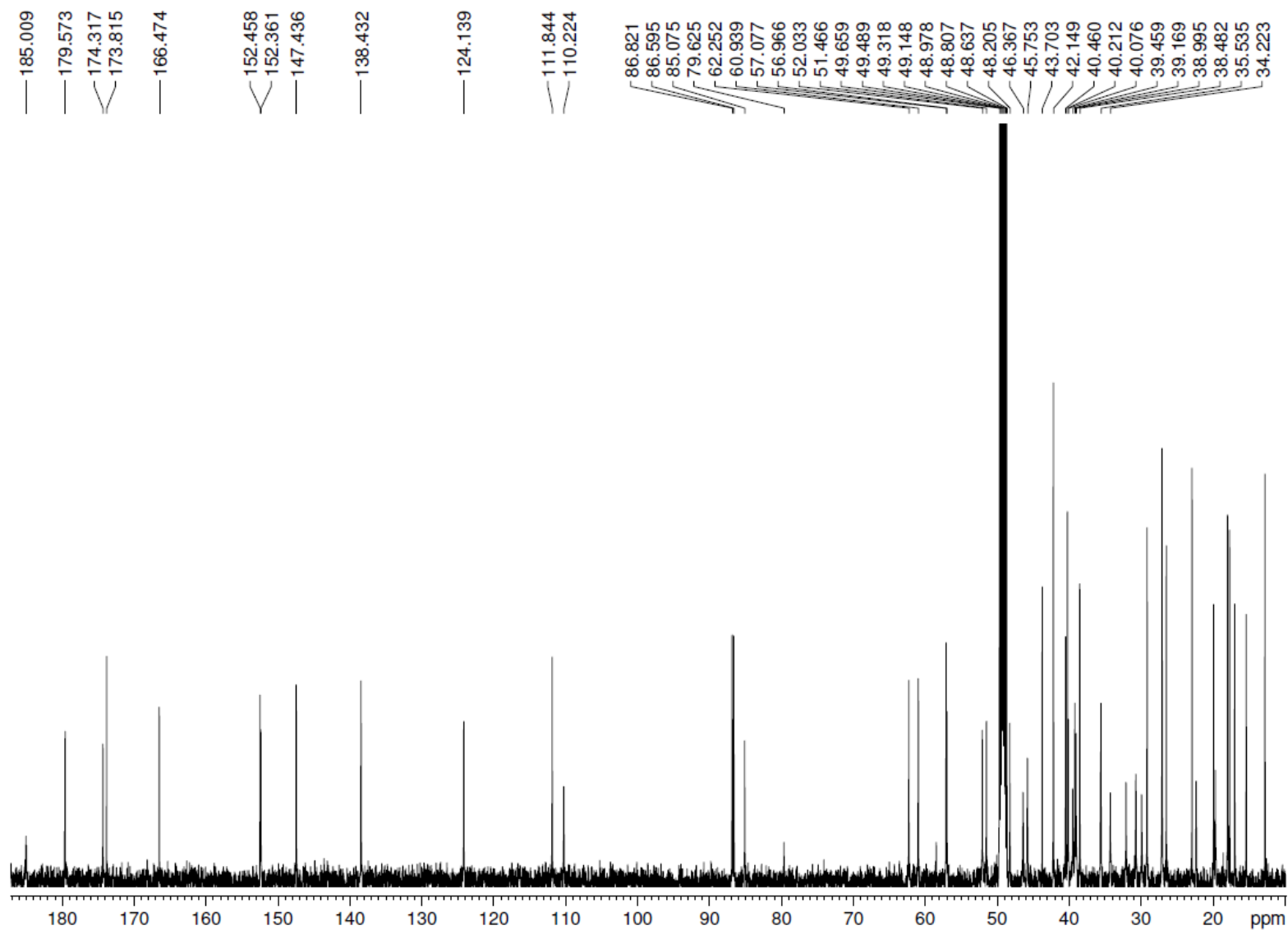
[1-(3'-Deoxythimidine)-1H-1,2,3-triazole-4-yl]-{[N-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)-lup-20,29-en-28-oyl]-N'-(tert-butoxycarbonyl)}-8-octylamine

27 ^{13}C NMR spectra (CD_3OD)

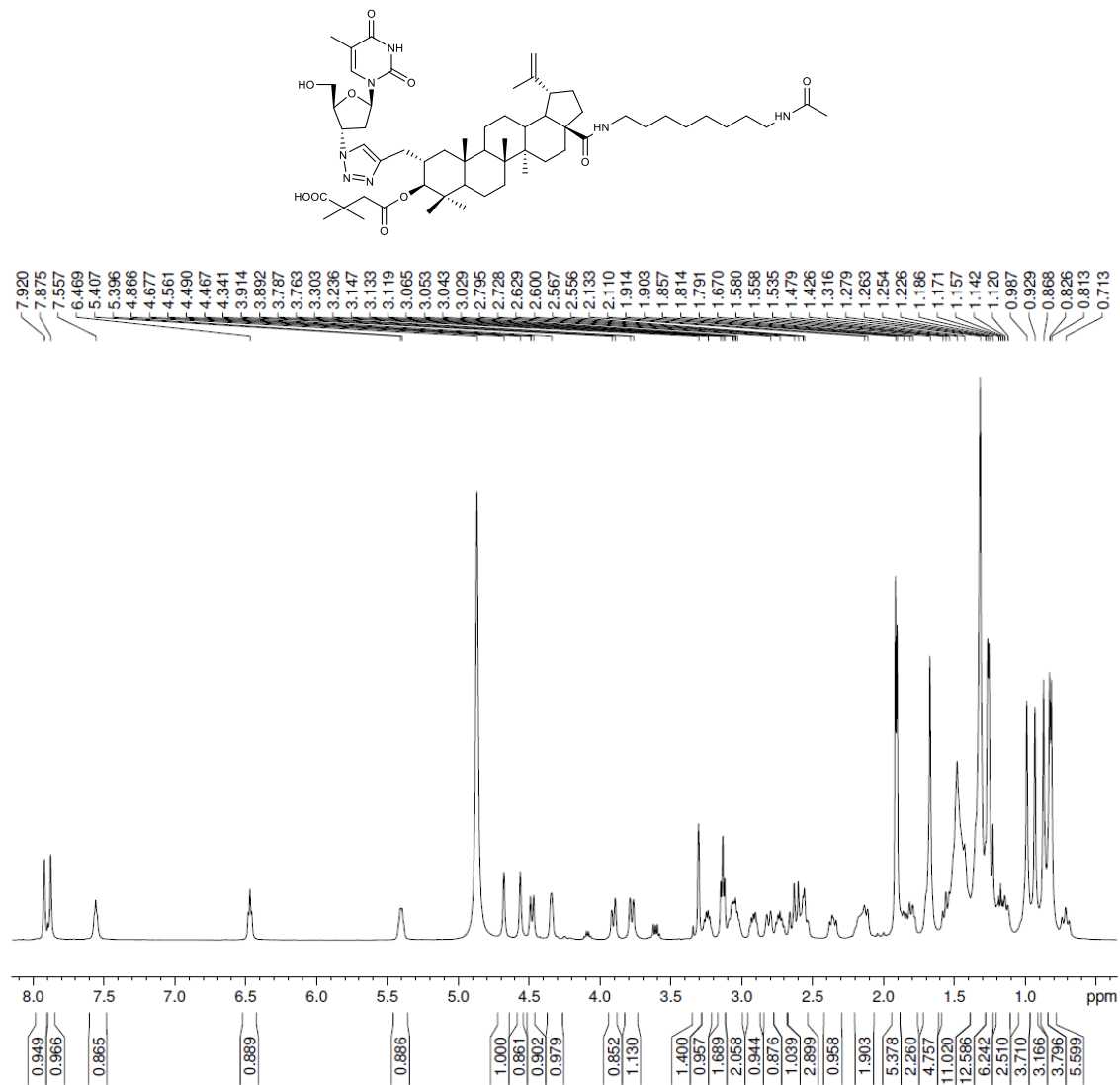


[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-[[N-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)-lup-20,29-en-28-oyl]-2-aminoethyl]-carbamoyl}methane

28 ¹H NMR spectra (CD₃OD)

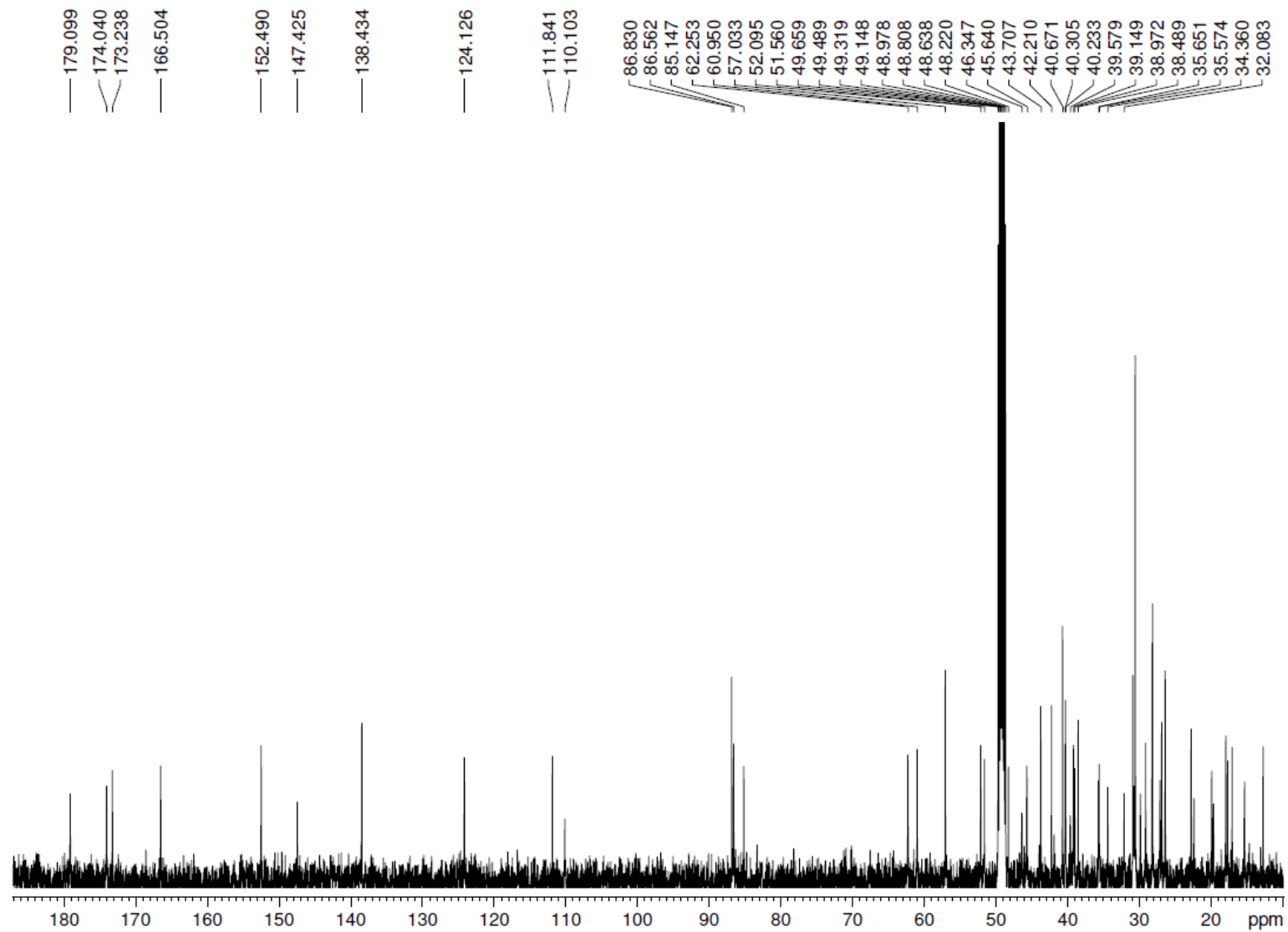


[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-{[N-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)-lup-20,29-en-28-oyl]-2-aminoethyl}-carbamoyl}methane
28 ^{13}C NMR spectra (CD_3OD)



[1-(3'-Deoxythymidine)-1H-1,2,3-triazole-4-yl]-{[N-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)-lup-20,29-en-28-oyl]-8-amino-octyl}-carbonyl}methane

29 ¹H NMR spectra (CD₃OD)



[1-(3'-Deoxythimidine)-1H-1,2,3-triazole-4-yl]-[[N-2 α -methyl-3 β -O-(3',3'-dimethylsuccinyl)-lup-20,29-en-28-oyl]-8-aminooctyl]-carbamoyl}methane

29 ^{13}C NMR spectra (CD_3OD)