Supporting Information For

Synthesis and evaluation of anticancer activities of novel C-28 guanidine-functionalized triterpene acid derivatives.

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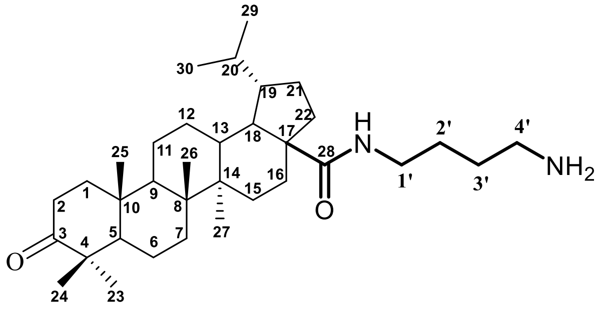
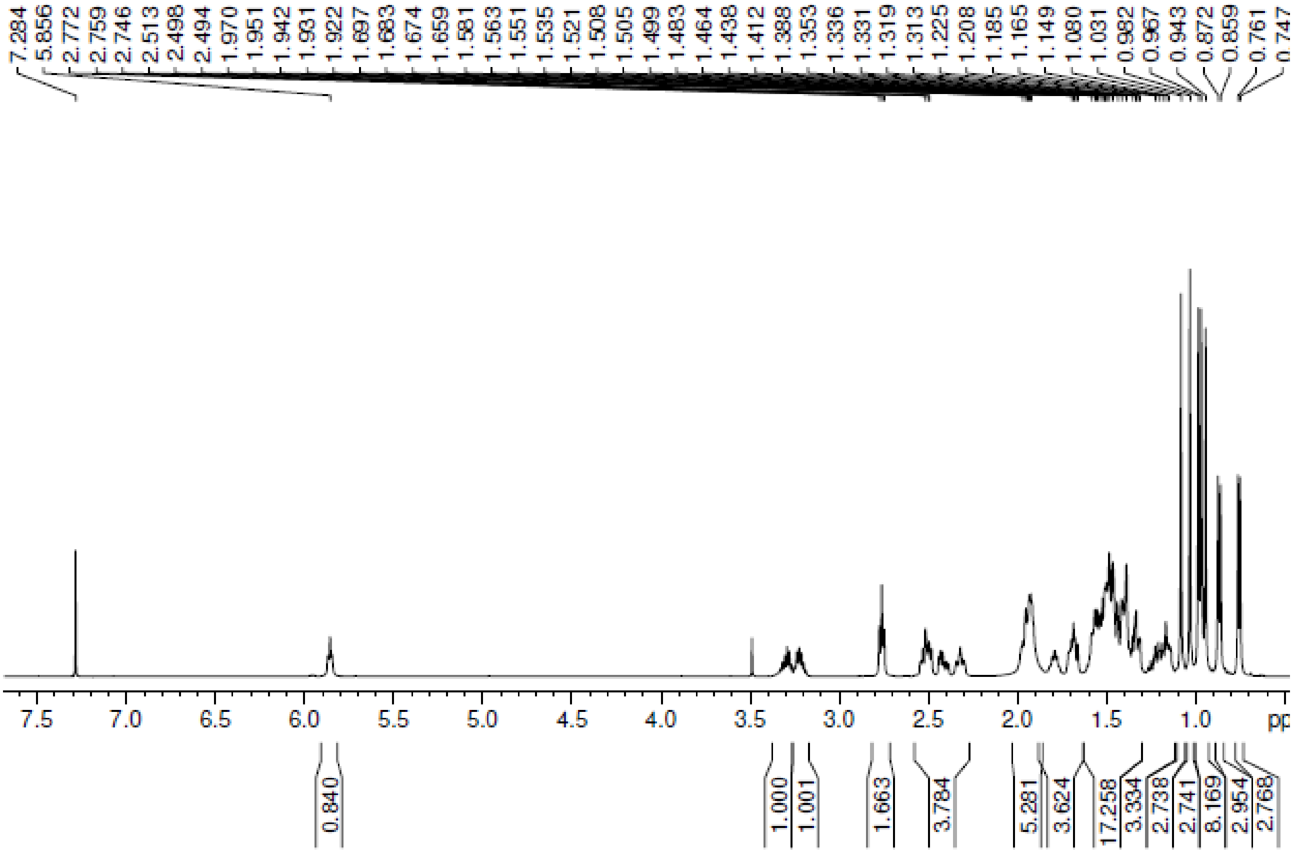
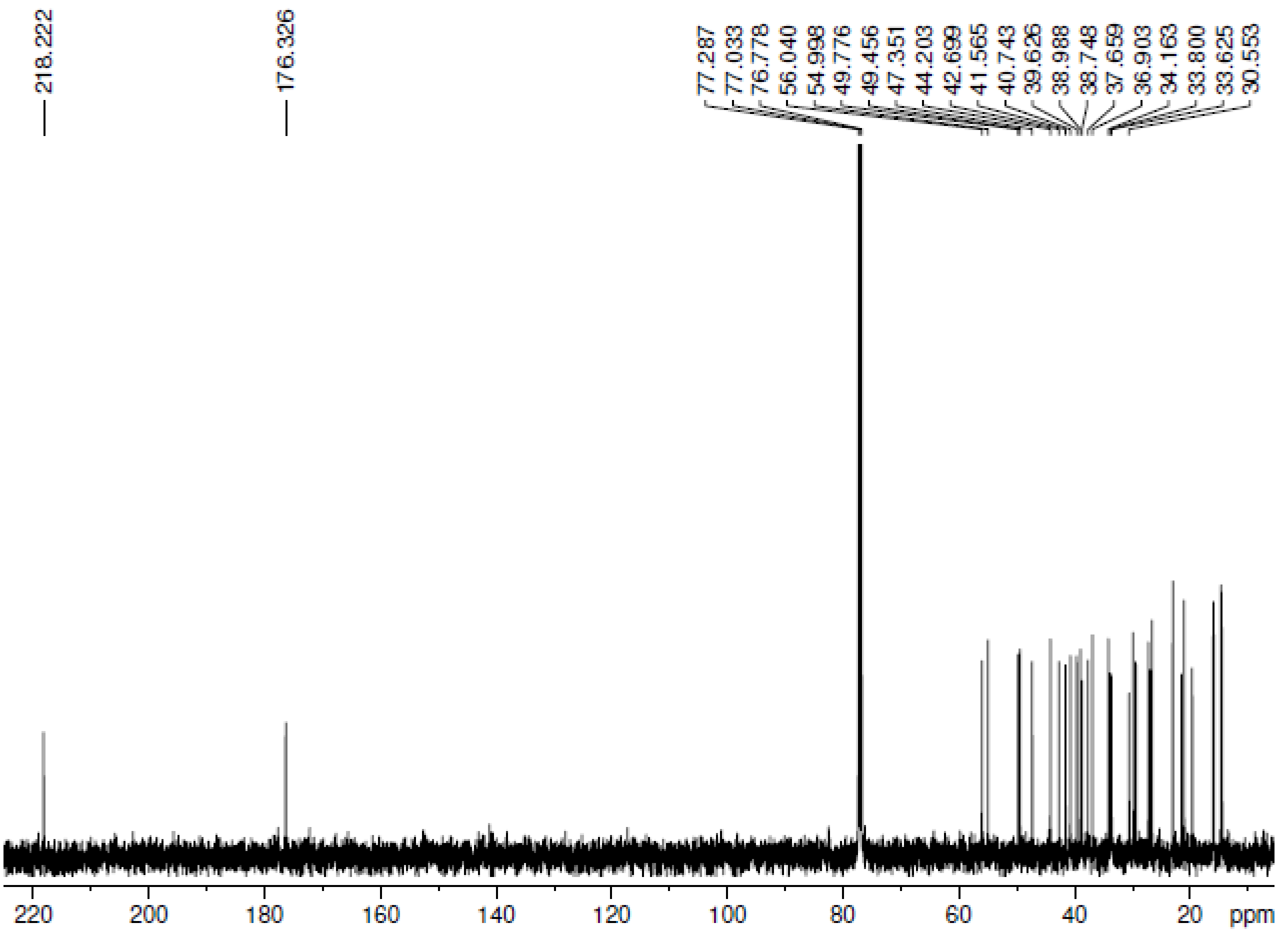
N-(4-aminobuthyl)-3-oxolupane-28-amide (4). ^{1}H NMR spectra (CDCl$_3$)

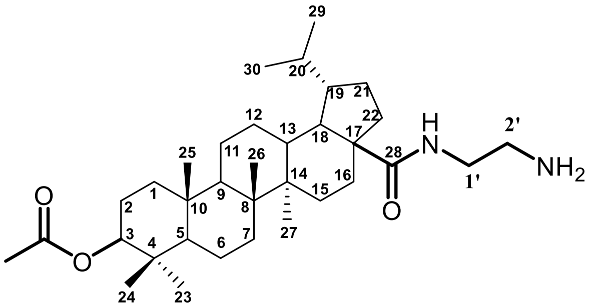


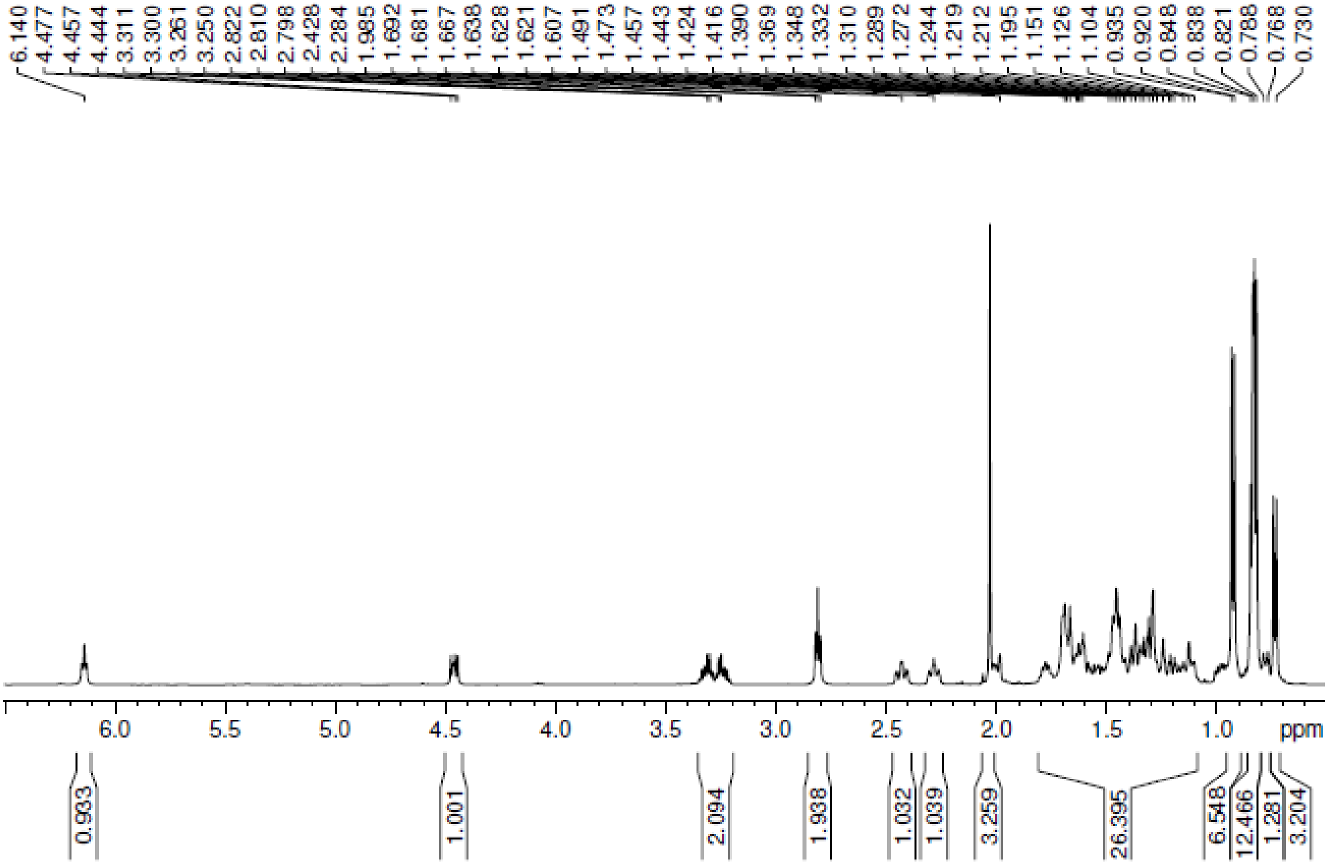


N-(4-aminobuthyl)-3-oxolupane-28-amide (4). ^{13}C NMR spectra (CDCl$_3$)



3β-N-(2-aminoethyl)-3-O-acetyl-lupane-28-amide (5). ^{1}H NMR spectra ($CDCl_3$)





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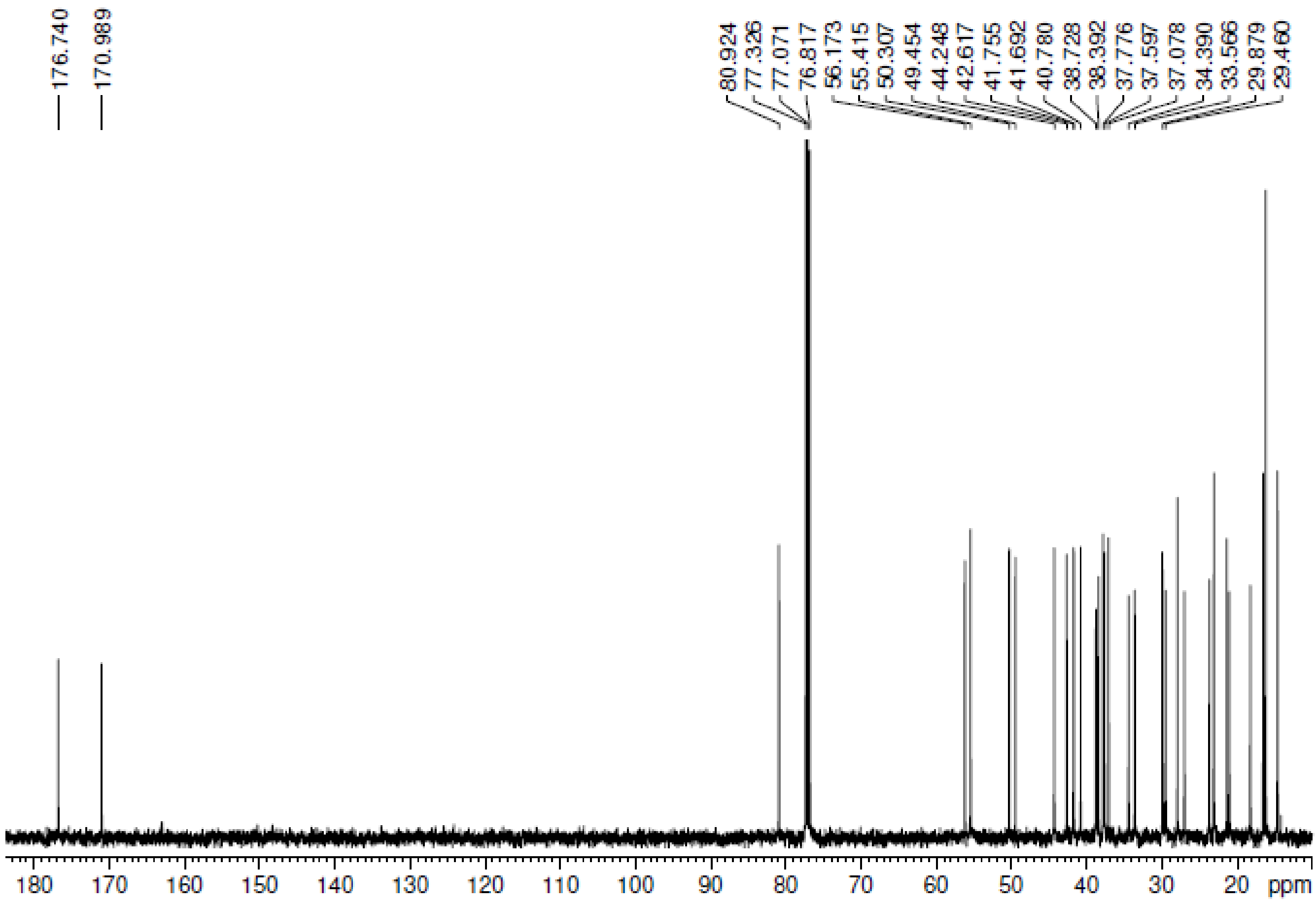
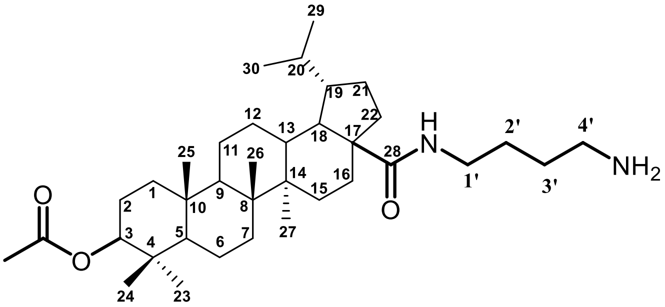
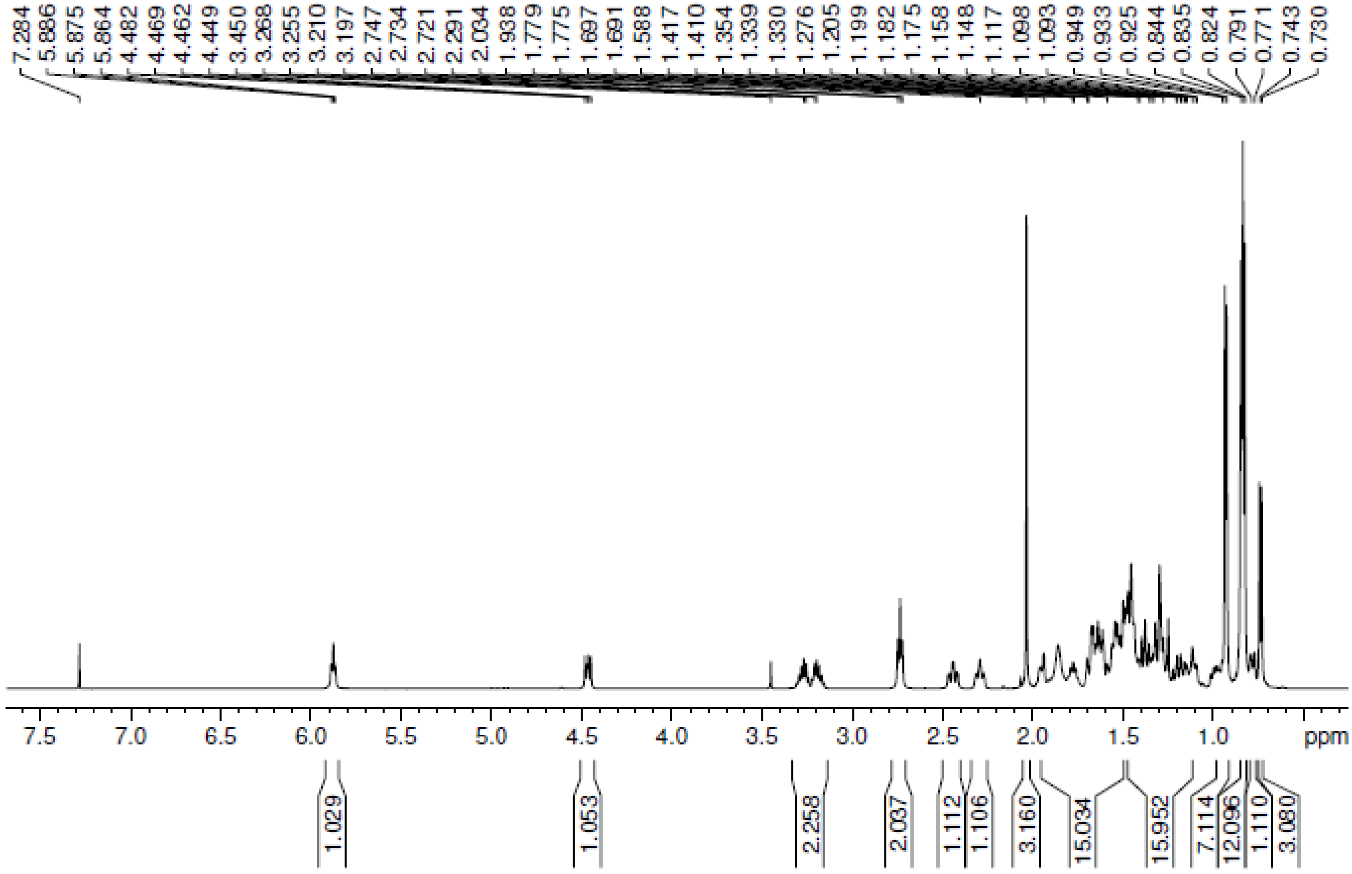
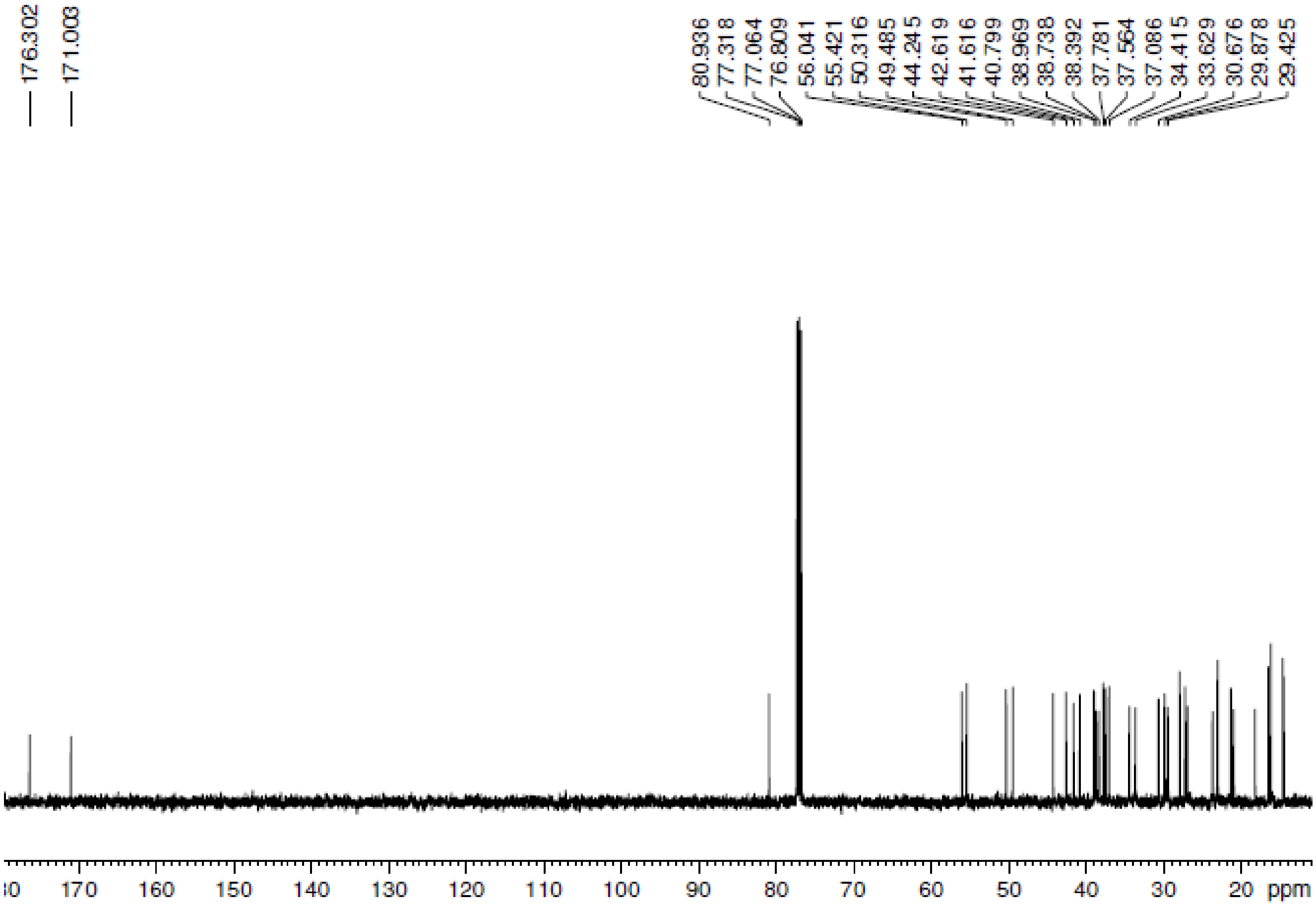


3β-N-(4-aminobuthyl)-3-O-acetyl-lupane-28-amide (6) ^{1}H NMR spectra (CDCl$_3$)



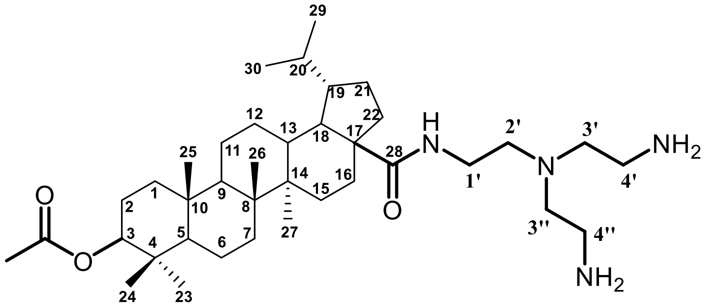


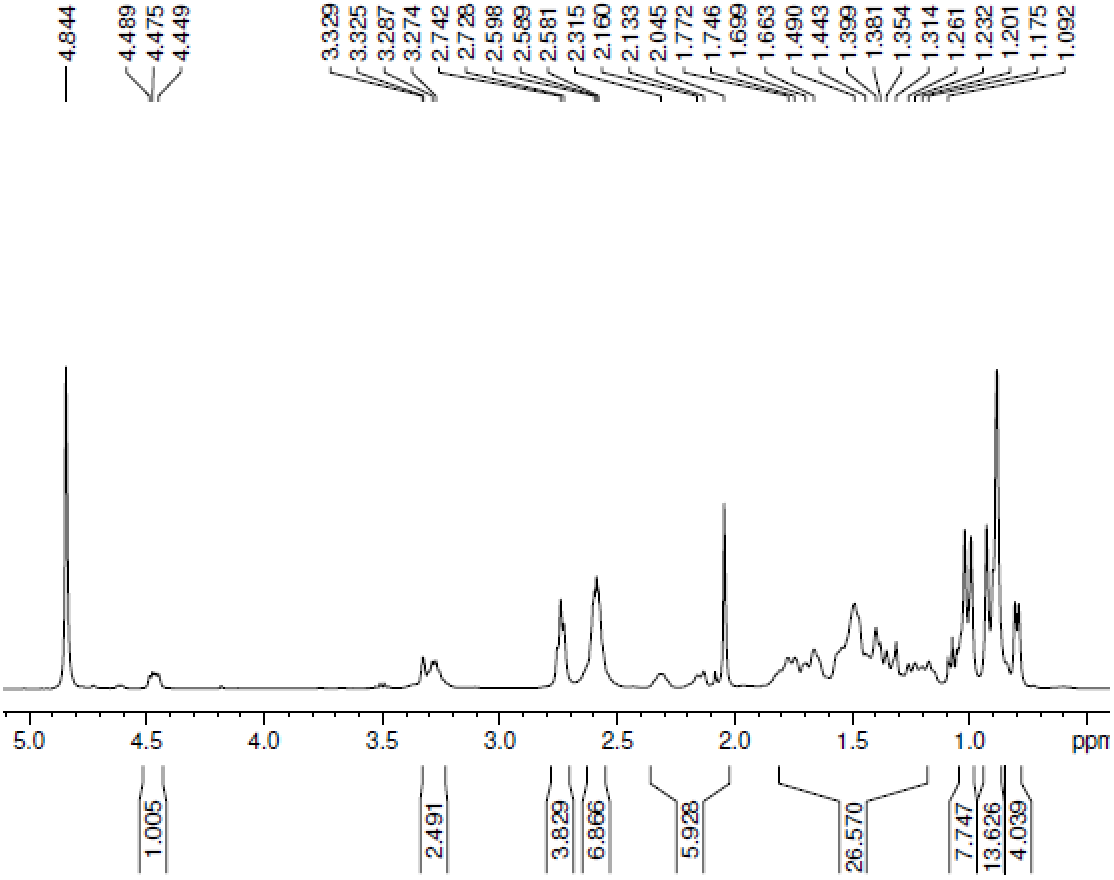
3β-N-(4-aminobuthyl)-3-O-acetyl-lupane-28-amide (6) ^{13}C NMR spectra (CDCl$_3$)



3β-N-[2-(N,N’-bis-aminoethyl)-aminoethyl]-3-O-acetyl-lupane-28-amide (7).

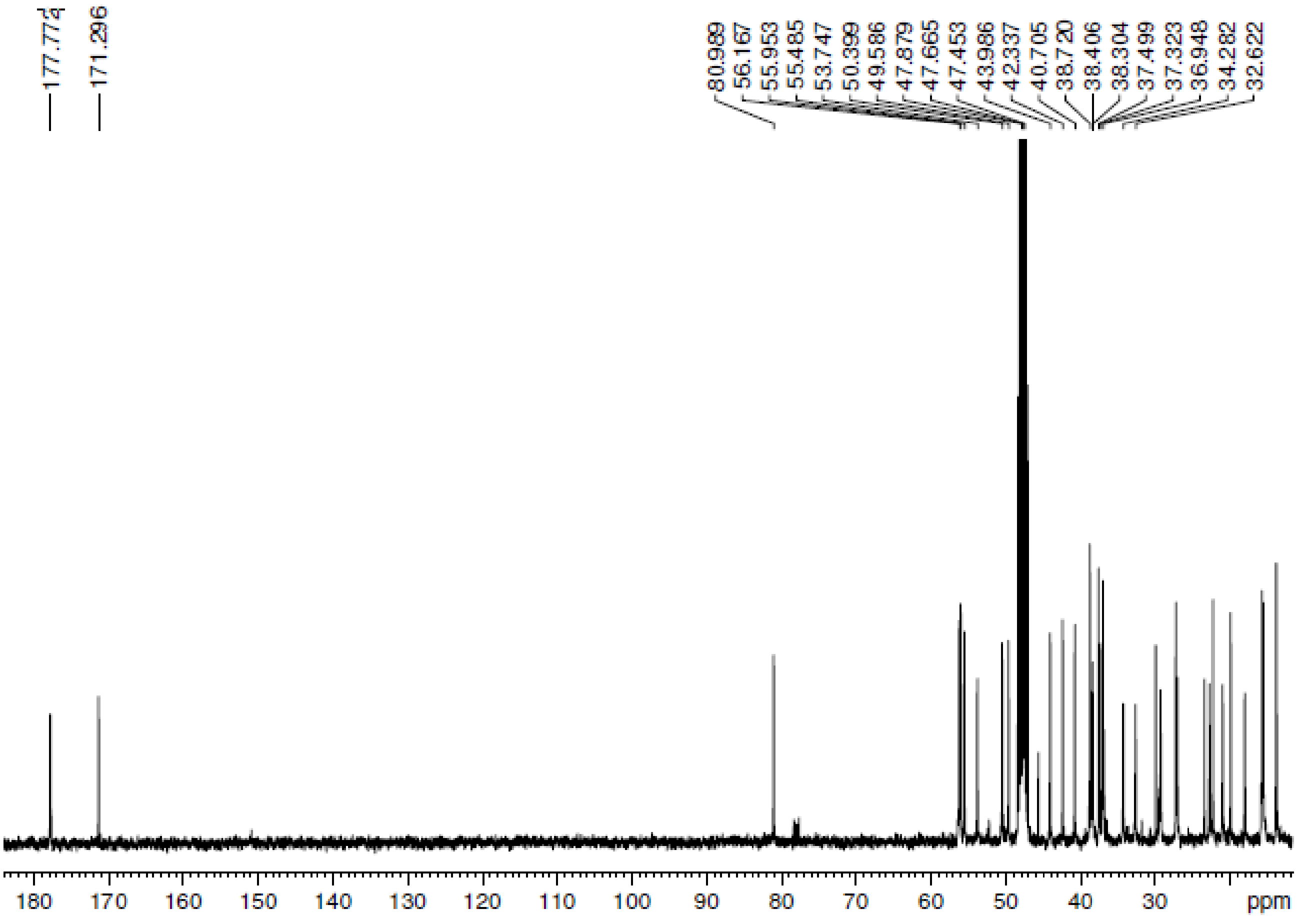
^{1}H NMR spectra (MeOD)





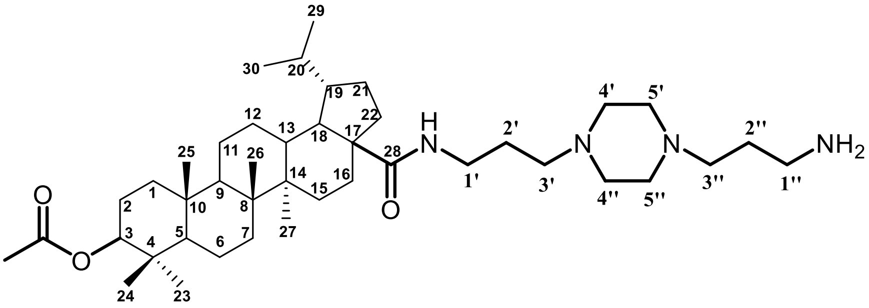
3β-N-[2-(N,N’-bis-aminoethyl)-aminoethyl]-3-O-acetyl-lupane-28-amide (7).

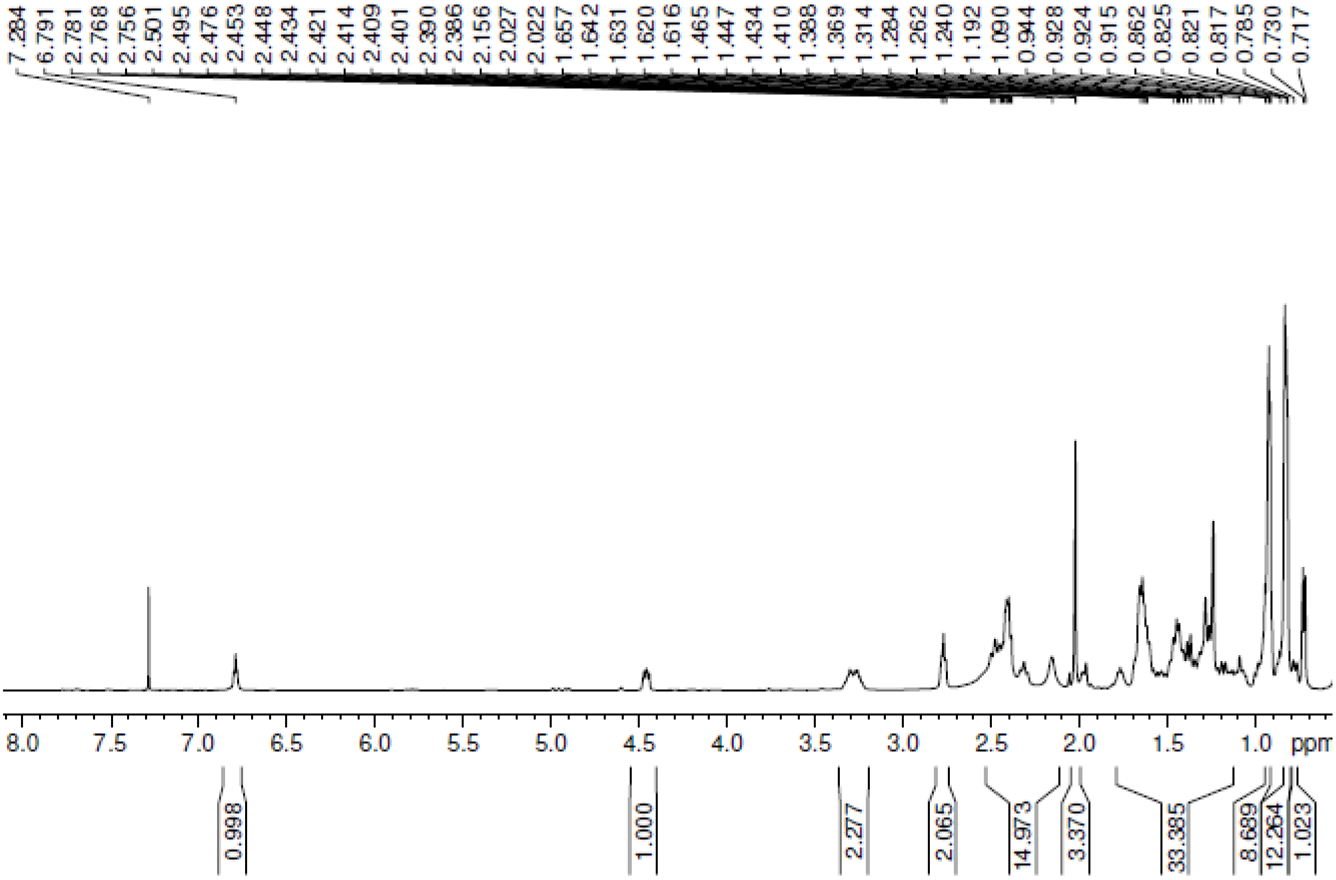
^{13}C NMR spectra (MeOD)



3β-N-{[3-(3-aminopropyl)piperazinyl]propyl}-3-O-acetyl-lupane-28-amide (8a).

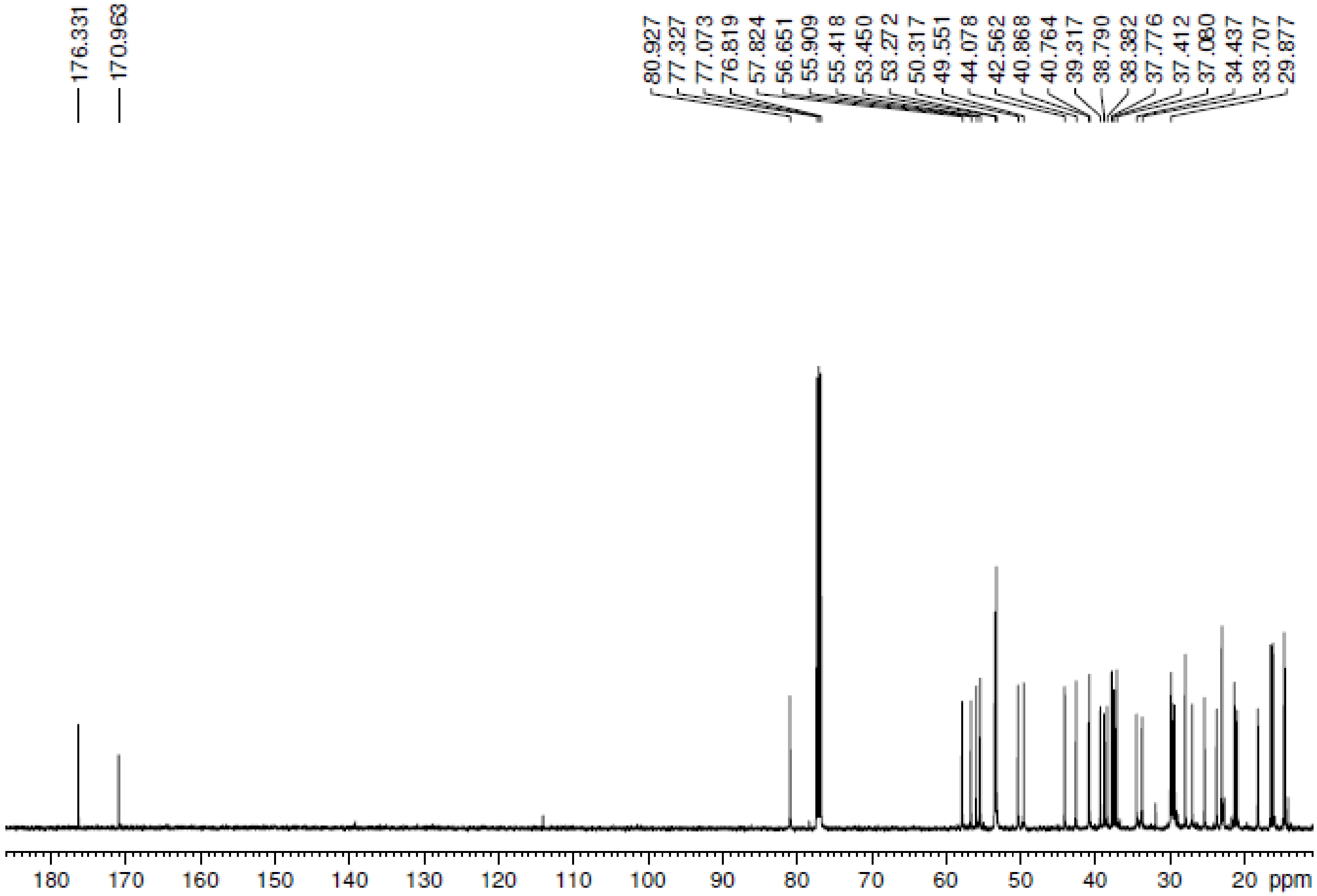
^{1}H NMR spectra ($CDCl_3$)





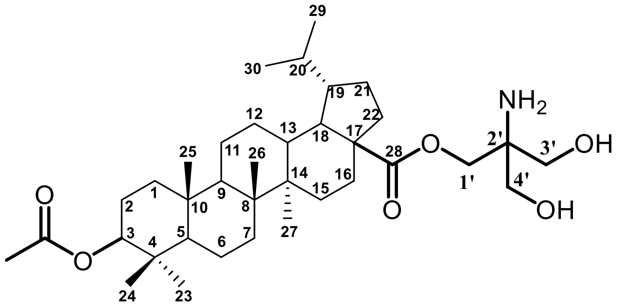
3β-N-{[3-(3-aminopropyl)piperazinyl]propyl}-3-O-acetyl-lupane-28-amide (8a).

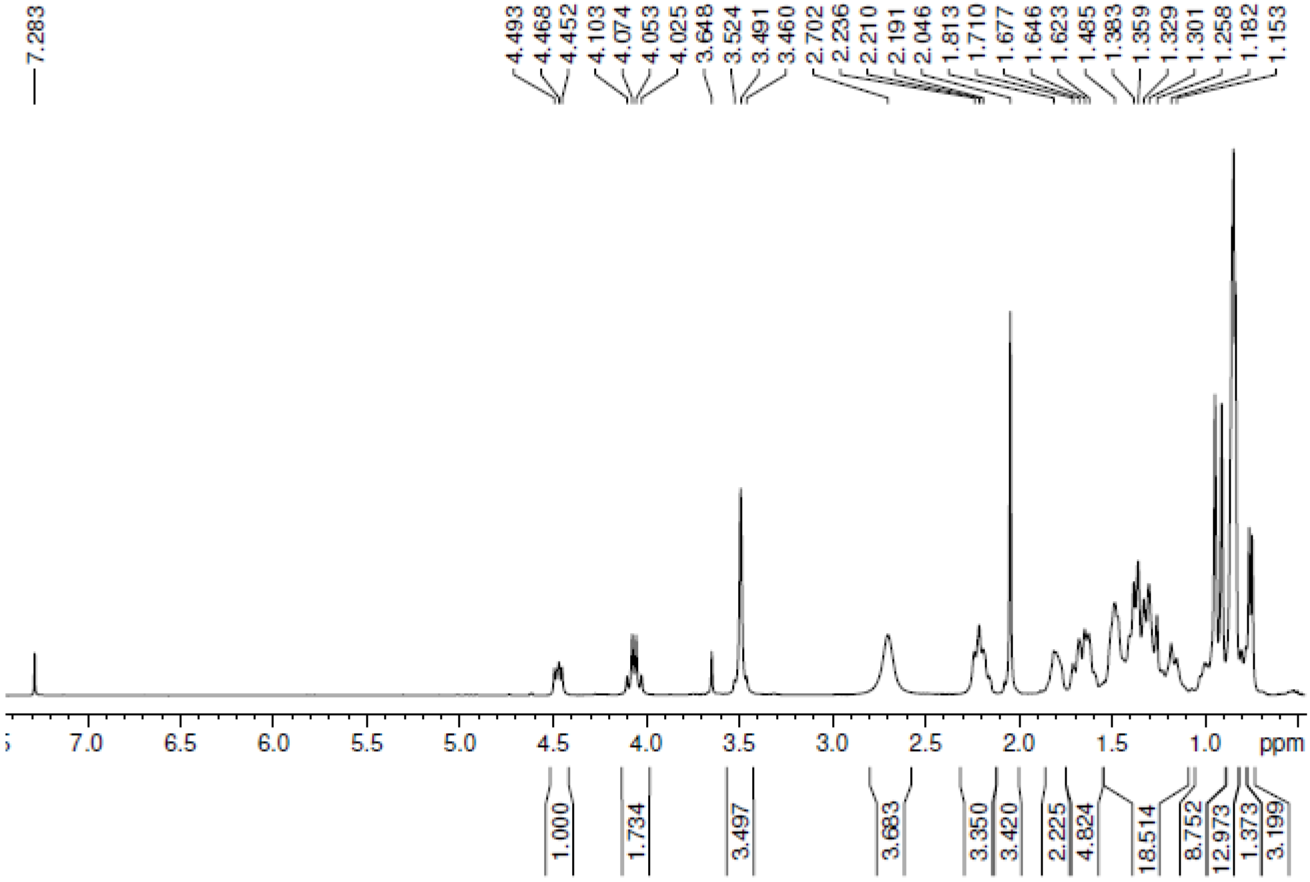
^{13}C NMR spectra (CDCl$_3$)



3β-[2-amino-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl -lupane-28-oate (15).

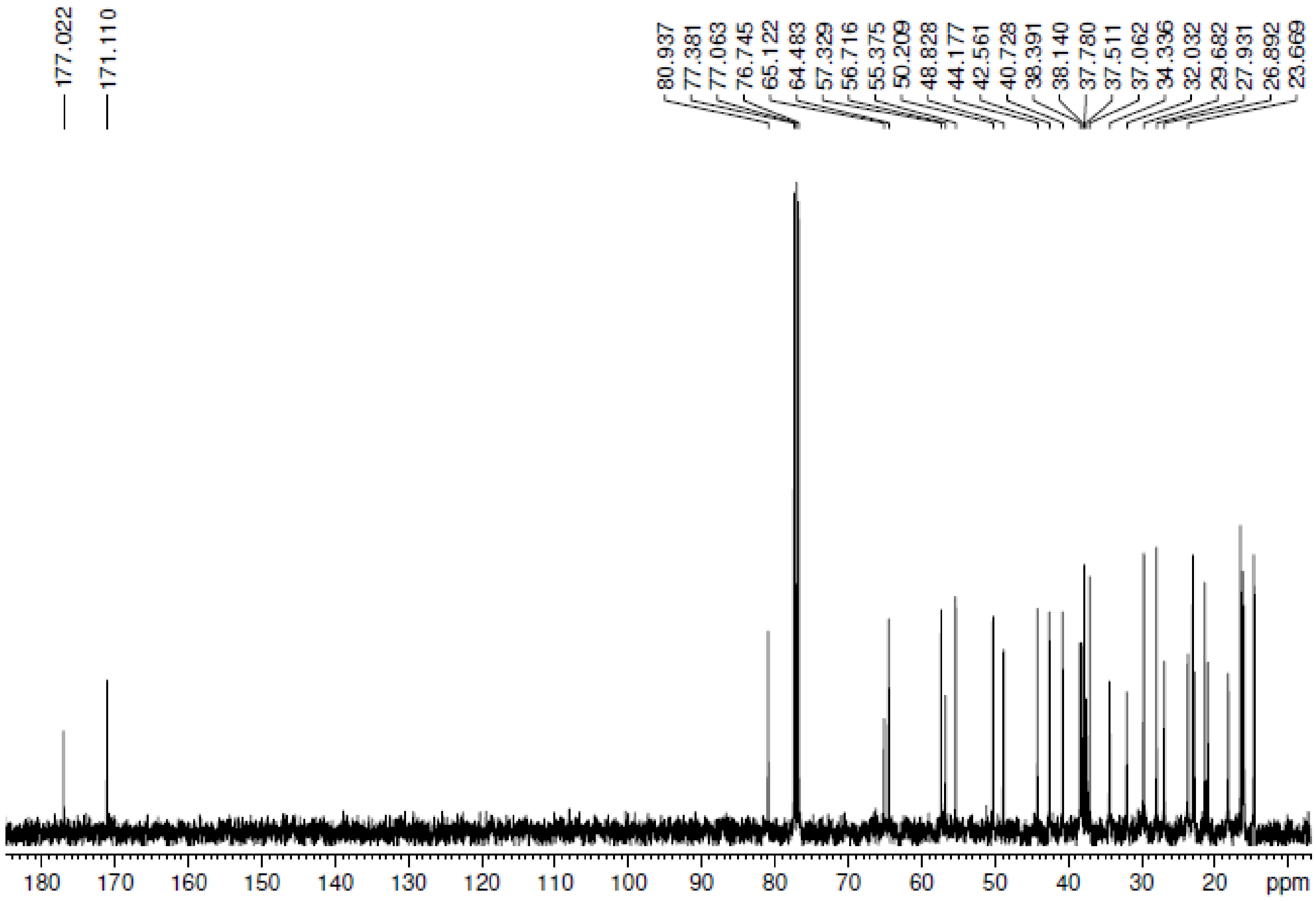
^{1}H NMR spectra ($CDCl_3$)





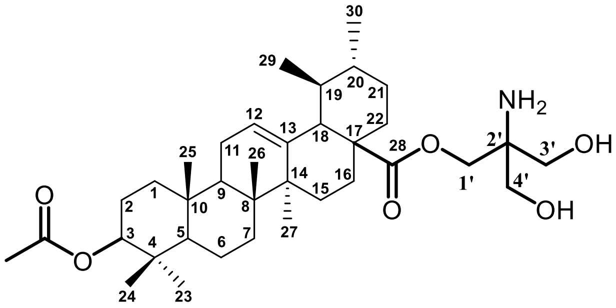
3β-[2-amino-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl -lupane-28-oate (15).

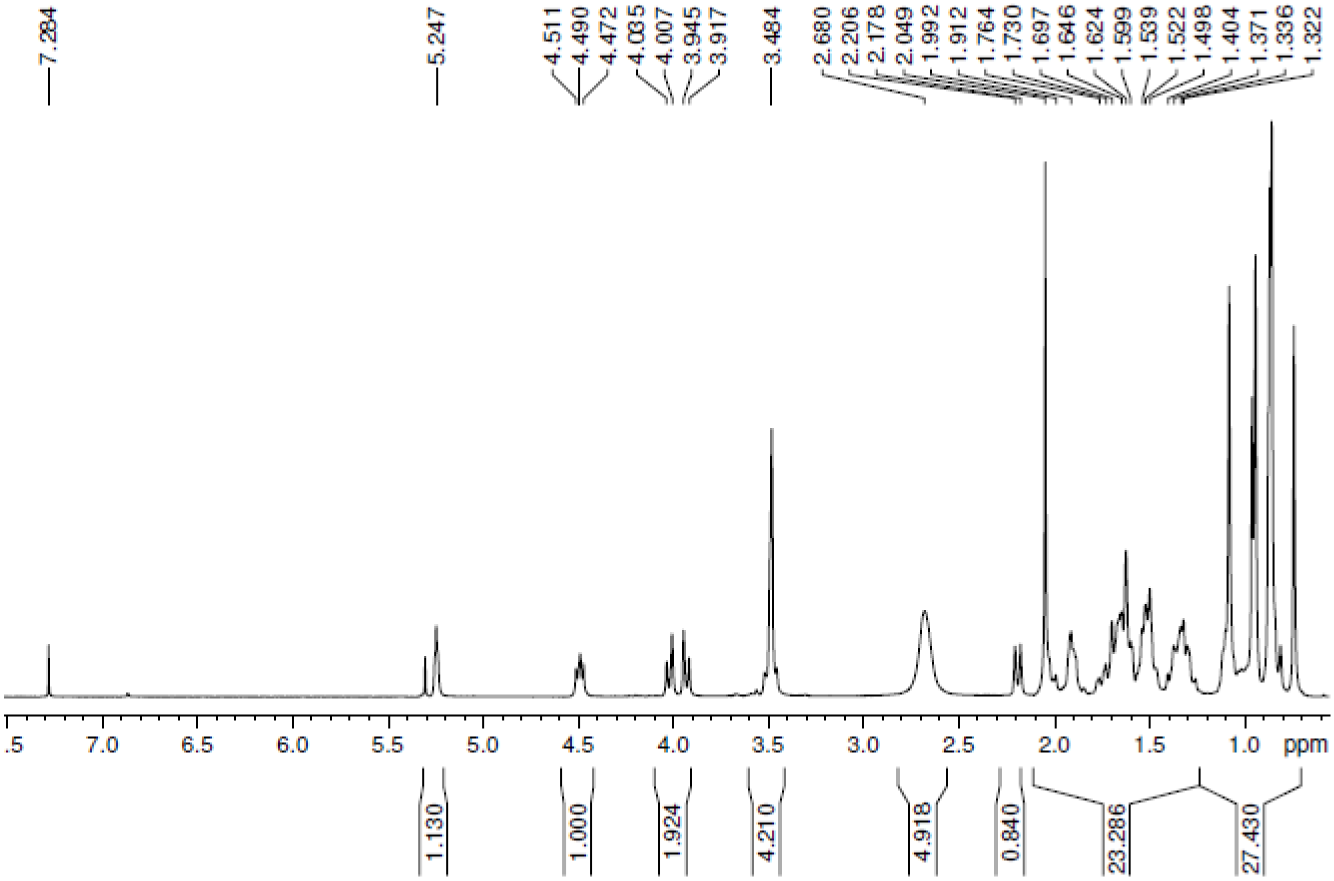
^{13}C NMR spectra (CDCl$_3$)



3β-[2-amino-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetylurs-12-en-28-oate (18).

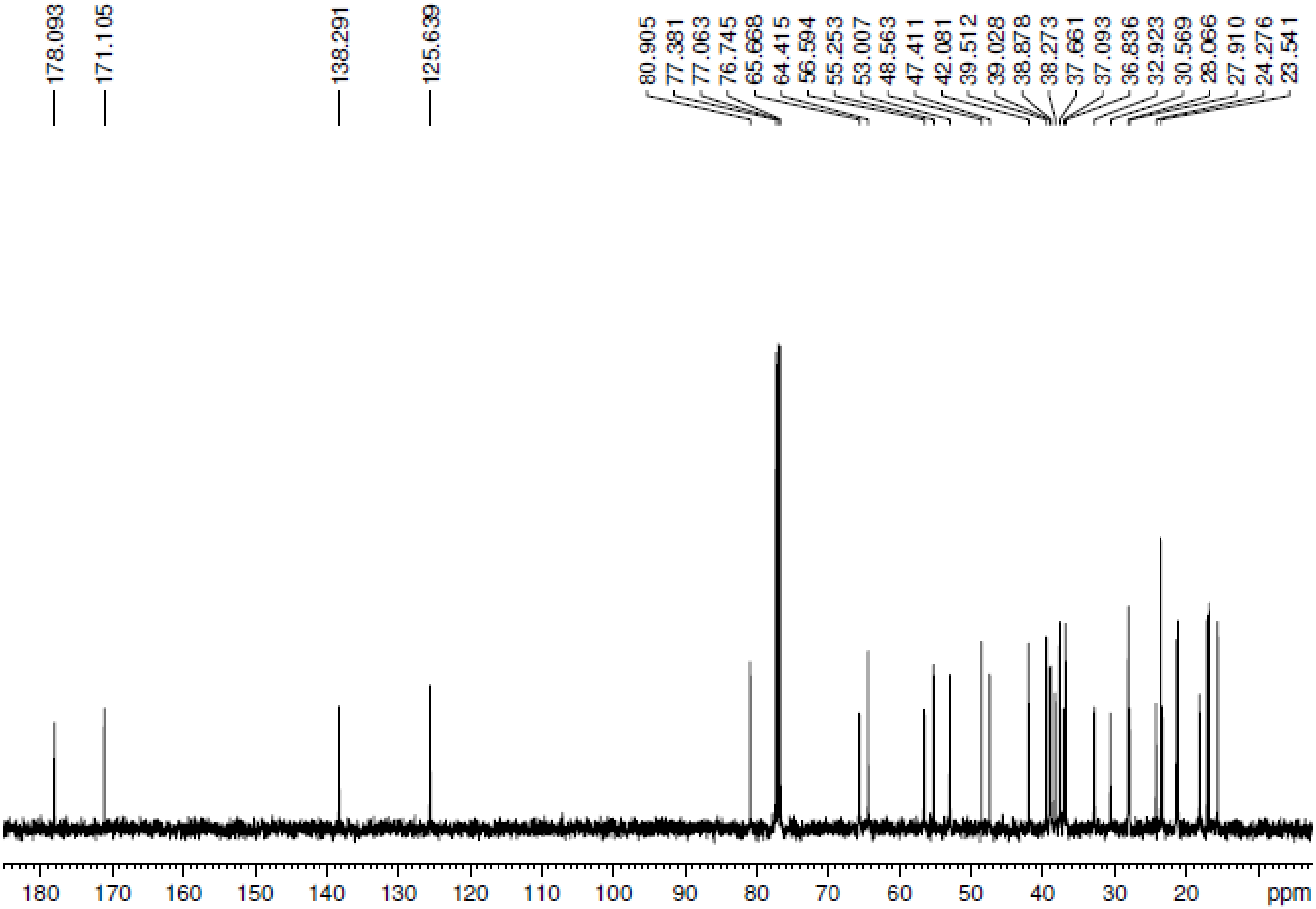
^{1}H NMR spectra (CDCl$_3$)





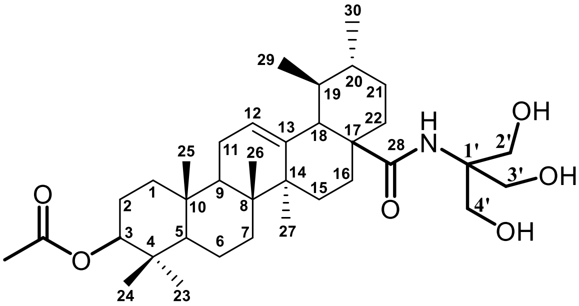
3β-[2-amino-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetylurs-12-en-28-oate (18).

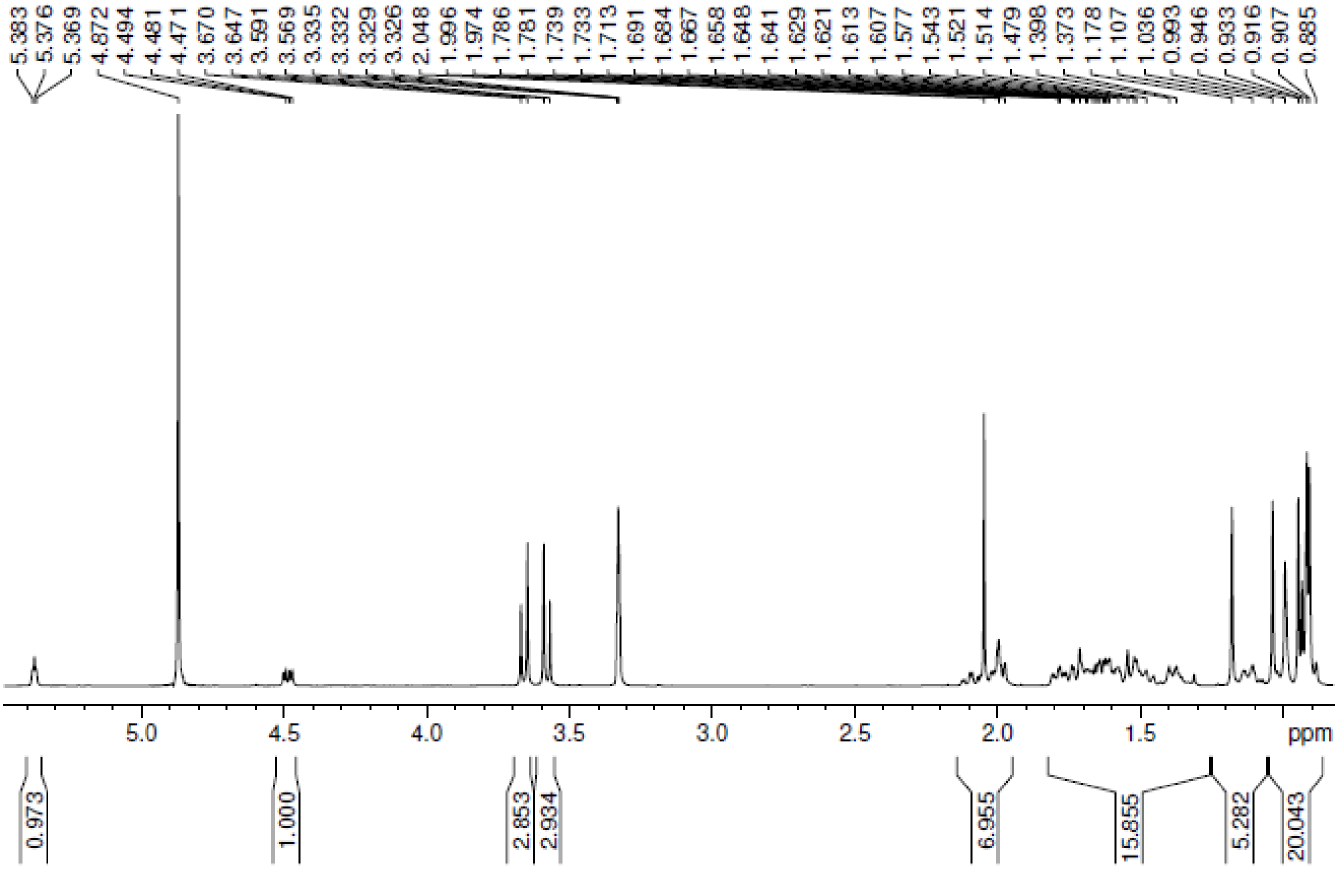
^{13}C NMR spectra (CDCl$_3$)



3β-N-[(1',1',1'-tris-hidroxymethyl)methyl]-3-O-acetyl-ursolamide (19)

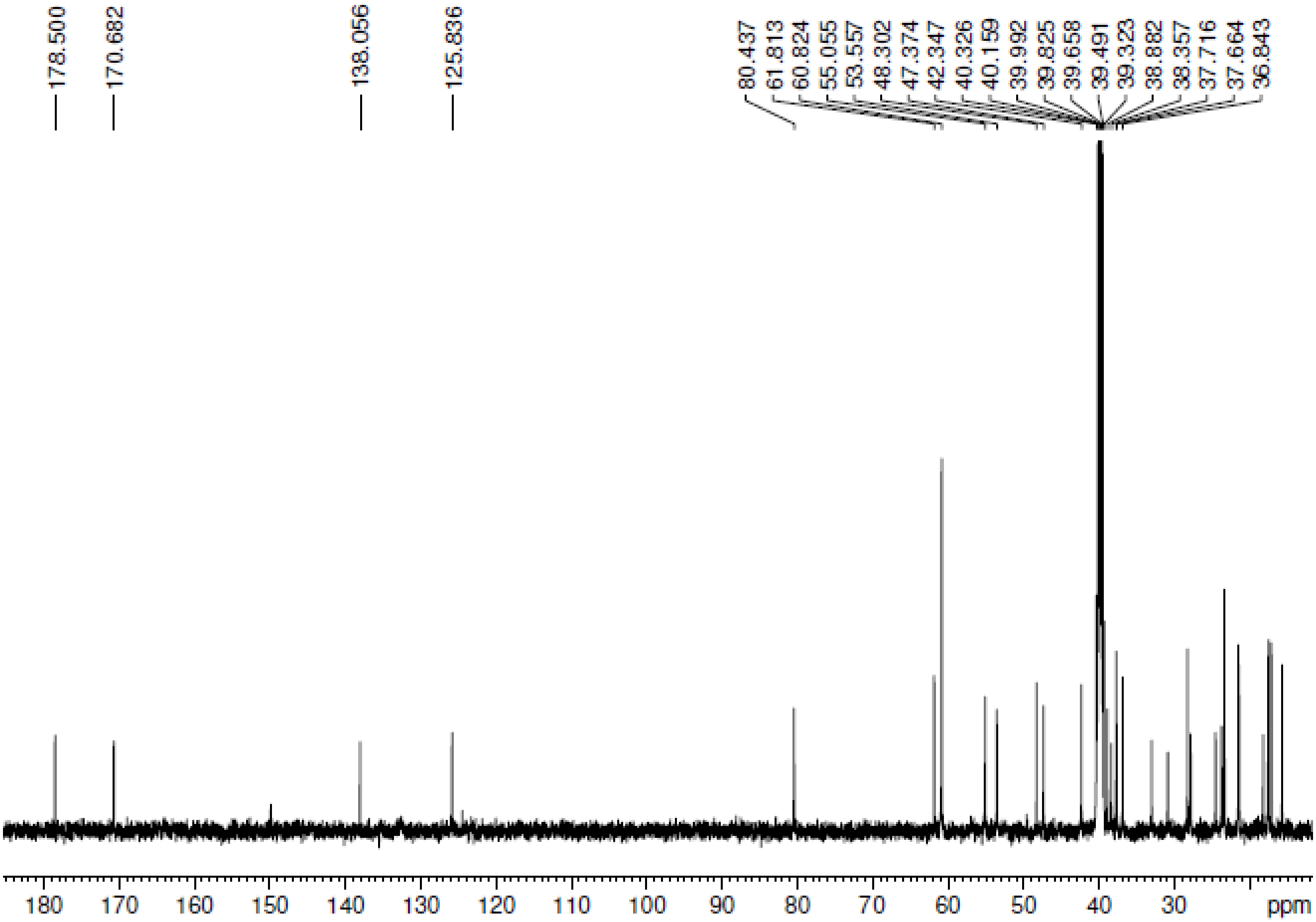
^{1}H NMR spectra (MeOD)





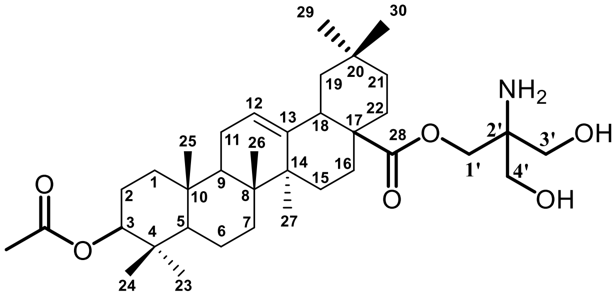
3β-N-[(1',1',1'-tris-hidroxymethyl)methyl]-3-O-acetyl-ursolamide (19)

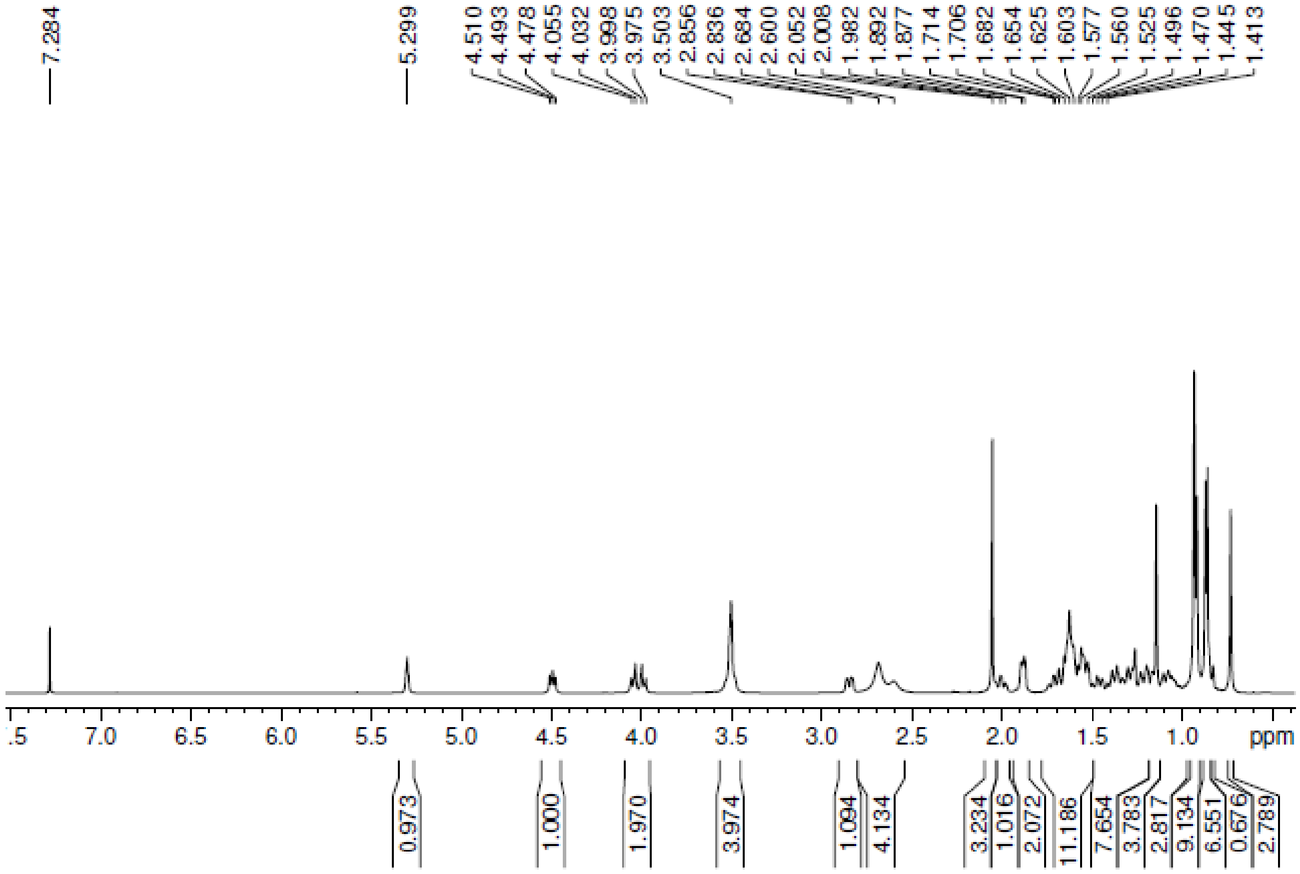
^{13}C NMR spectra (d5-DMSO)



3β-[2-amino-3-hydroxy-2(hydroxymethyl)propyl]-3-O-acetylolean-12-en-28-oate (20).

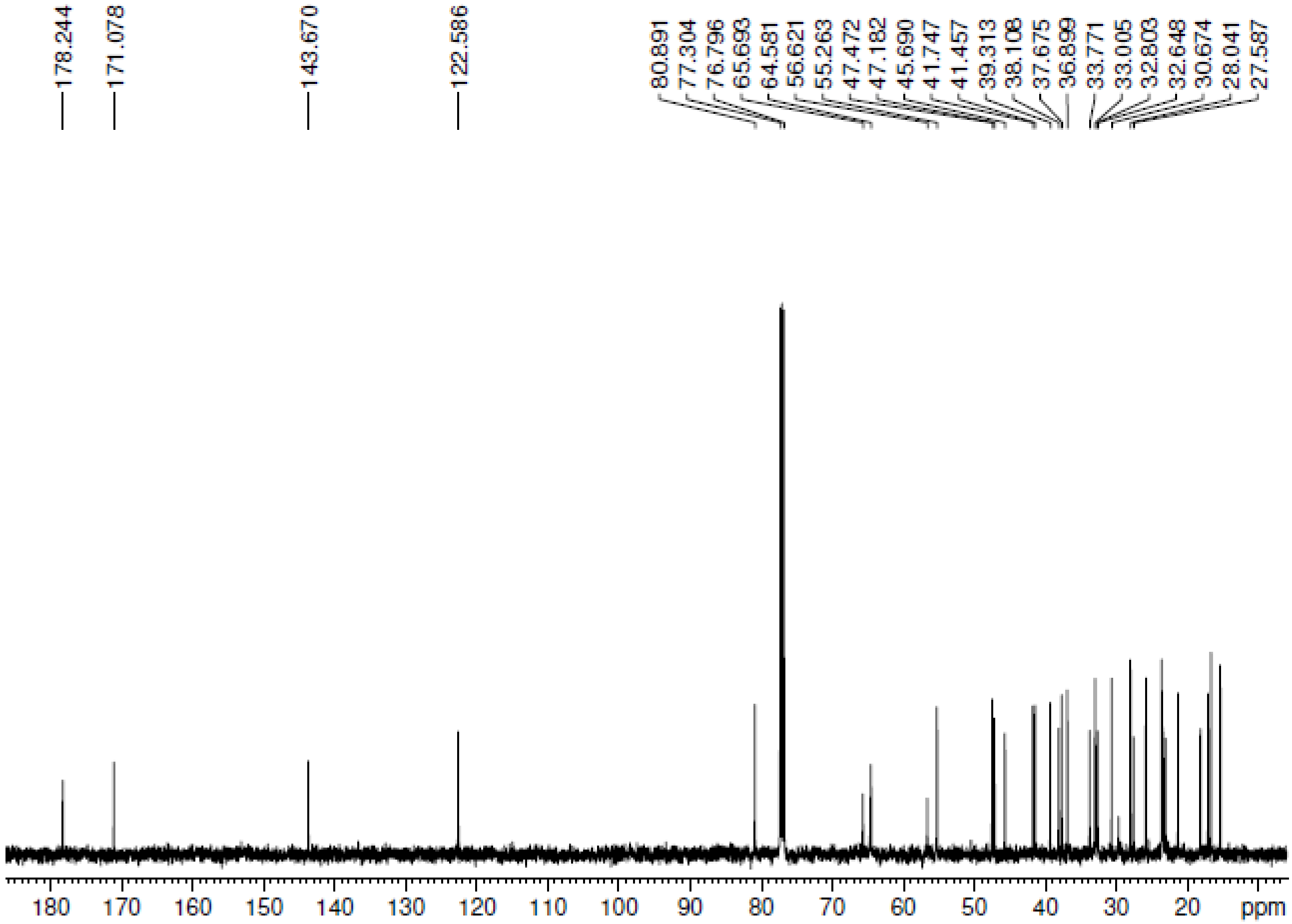
^{1}H NMR spectra ($CDCl_3$)





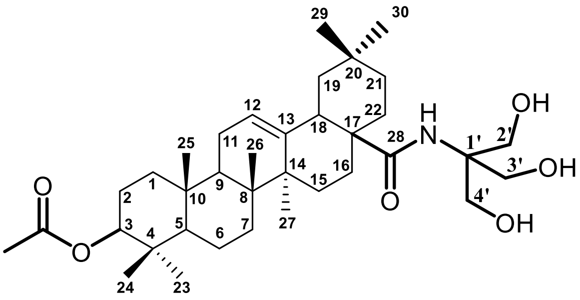
3β-[2-amino-3-hydroxy-2(hydroxymethyl)propyl]-3-O-acetylolean-12-en-28-oate (20).

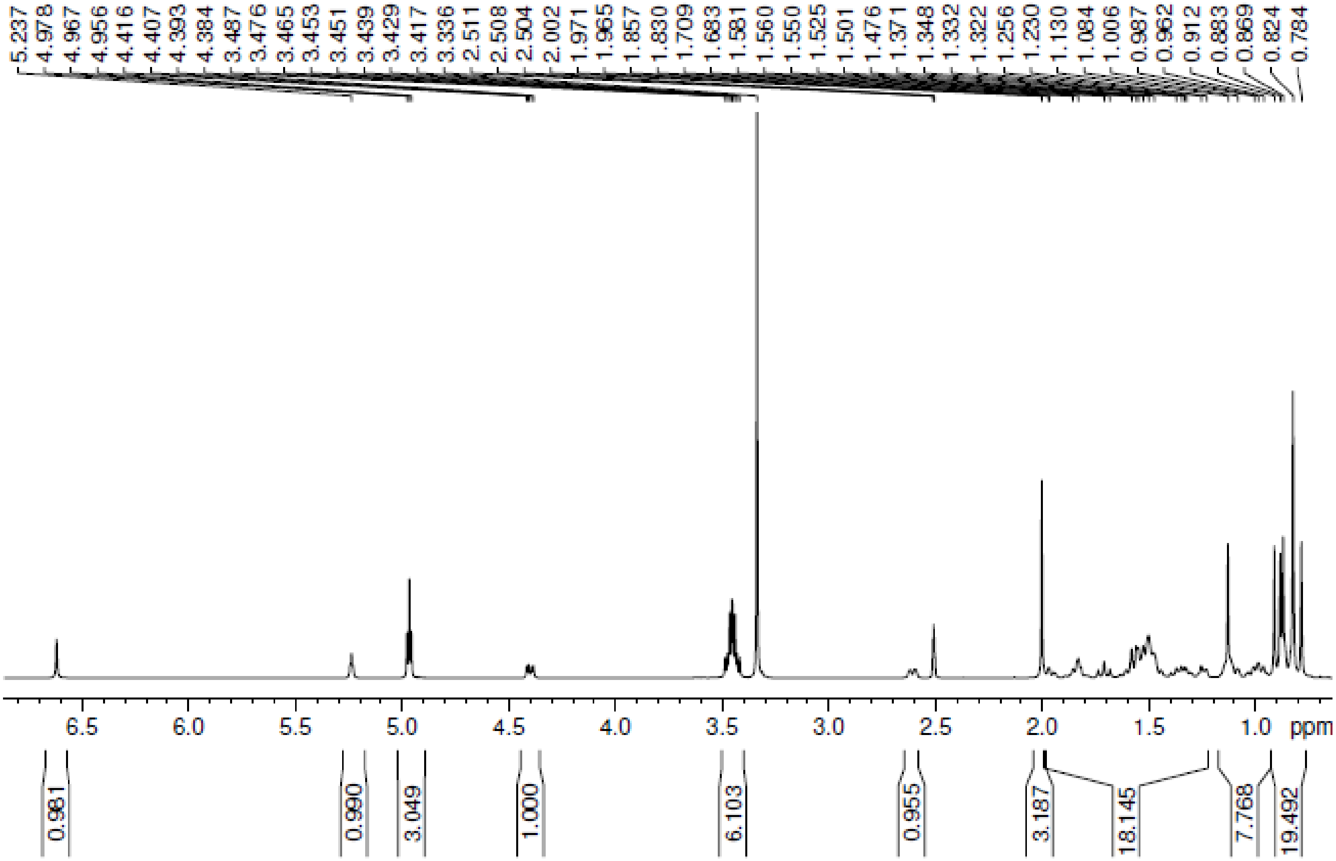
^{13}C NMR spectra ($CDCl_3$)



3β-N-[(1',1',1'-tris-hidroxymethyl)methyl]-3-O-acetyl-oleanolamide (21)

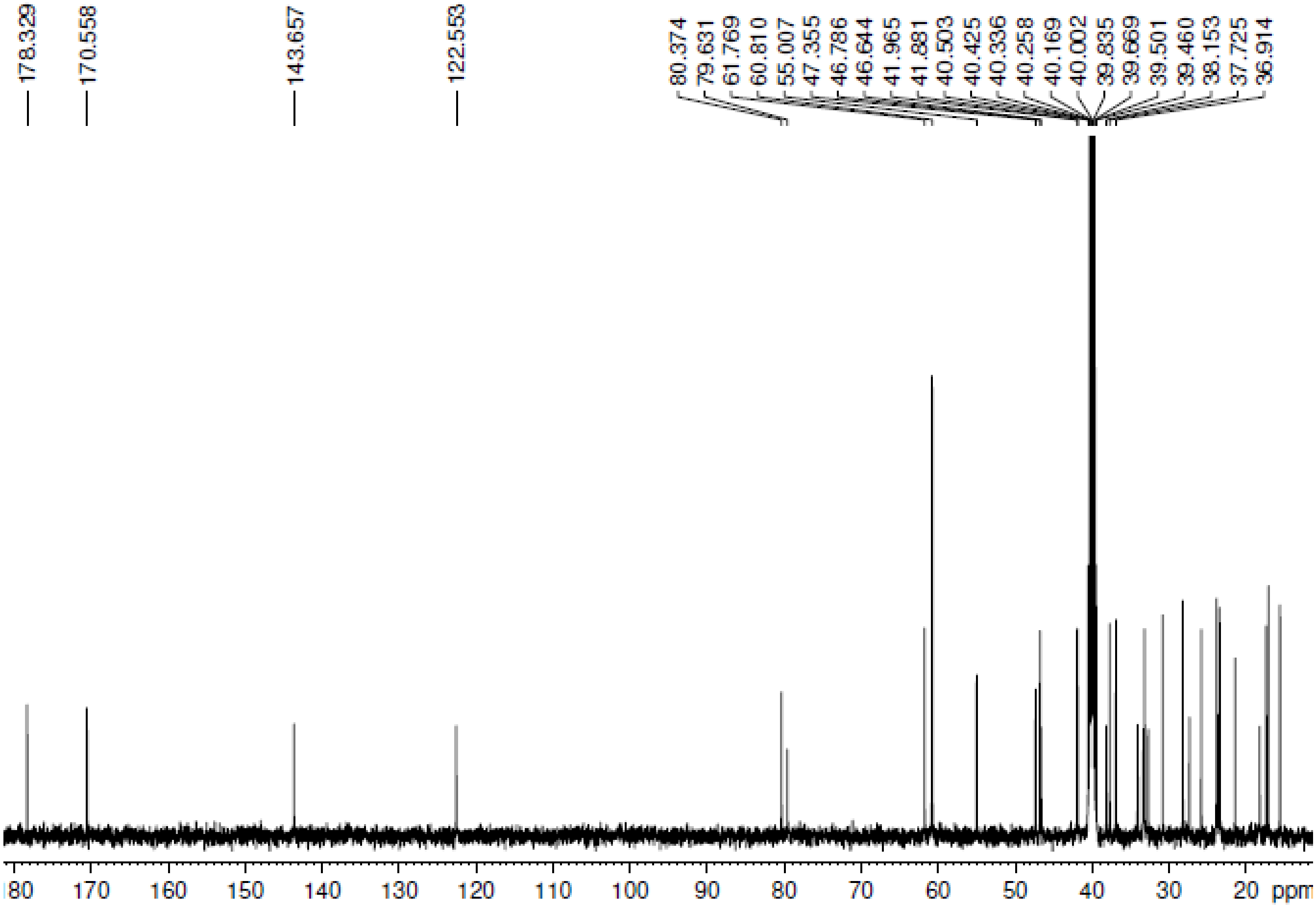
^{1}H NMR spectra (d$_6$-DMSO)





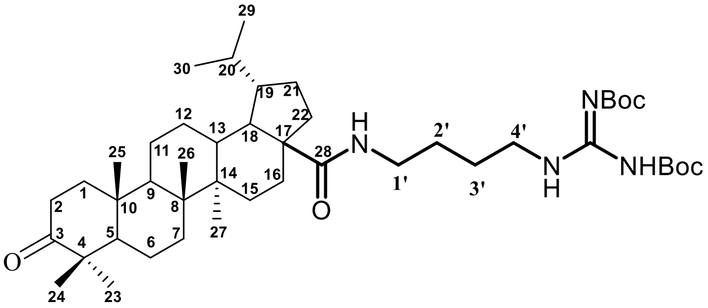
3β-N-[(1',1',1'-tris-hidroxymethyl)methyl]-3-O-acetyl-oleanolamide (21)

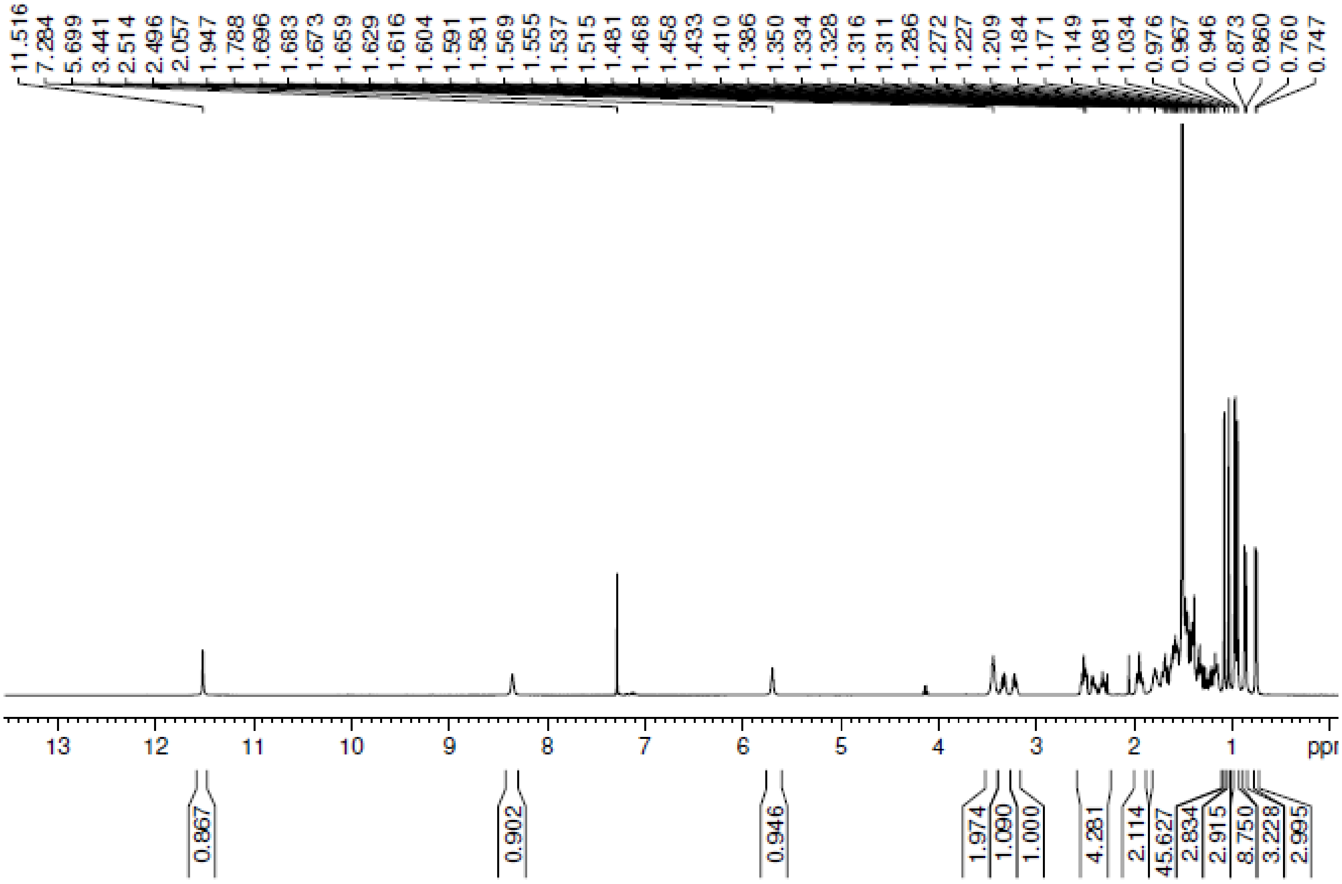
^{13}C NMR spectra (d$_6$-DMSO)



N-[4-tert-butyloxycarbonyl buthylguanidine]-3-oxo-lupane-28-amide (9)

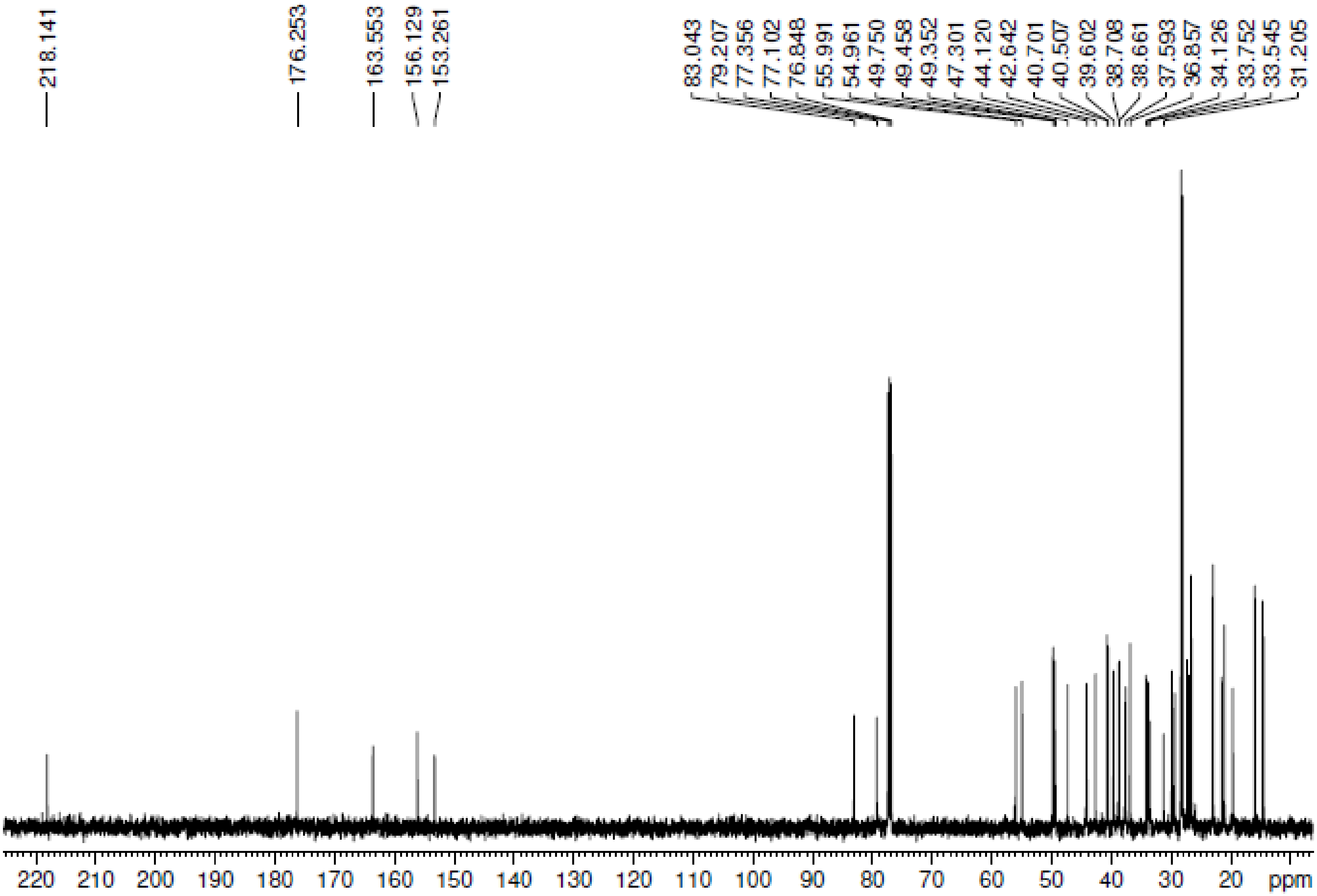
^{1}H NMR spectra ($CDCl_3$)





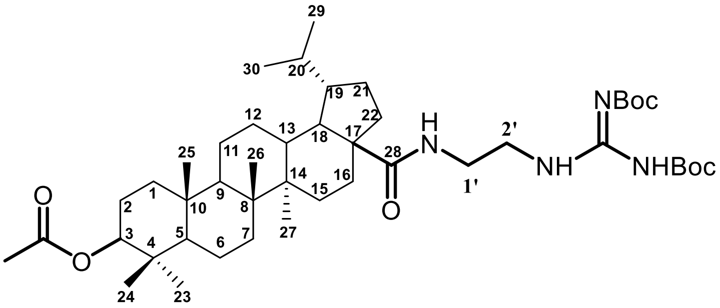
N-[4-tert-butyloxycarbonyl buthylguanidine]-3-oxo-lupane-28-amide (9)

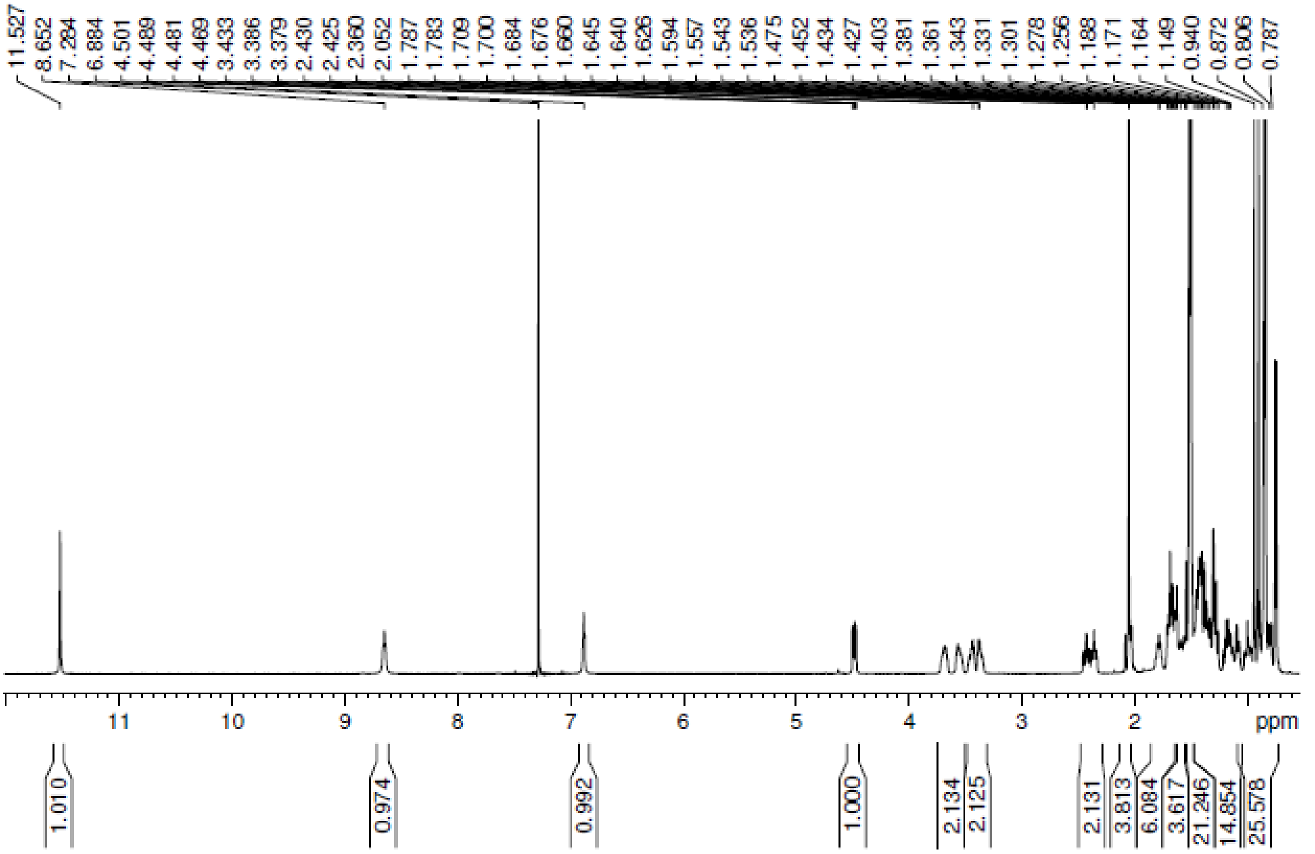
^{13}C NMR spectra ($CDCl_3$)



3β-N-(2-tert-butyloxycarbonyl ethylguanidine)-3-O-acetyl-lupane-28-amide (10).

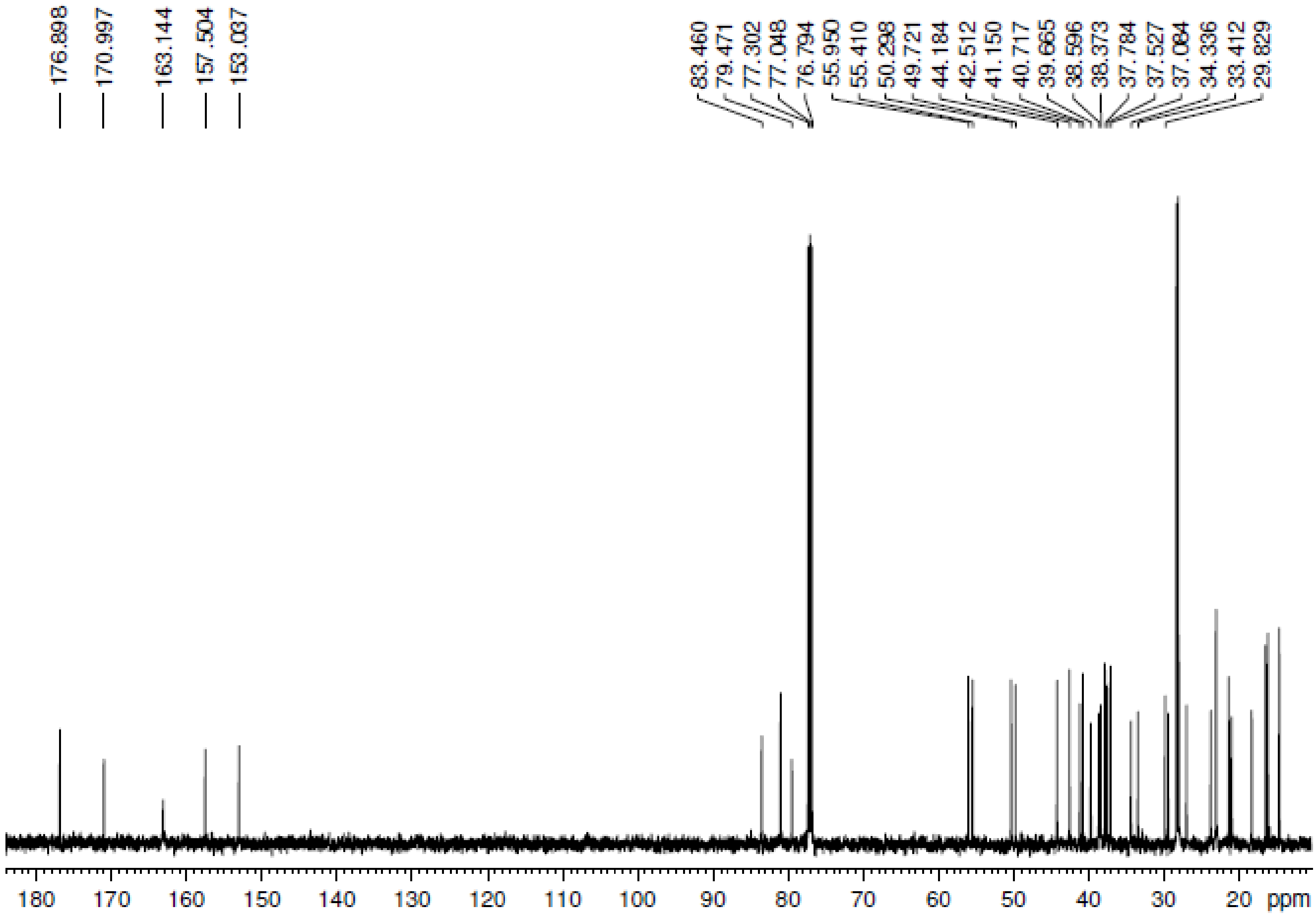
^1H NMR spectra ($CDCl_3$)





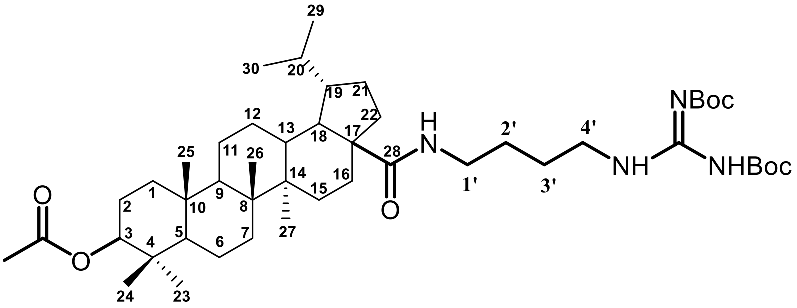
3β-N-(2-tert-butyloxycarbonyl ethylguanidine)-3-O-acetyl-lupane-28-amide (10).

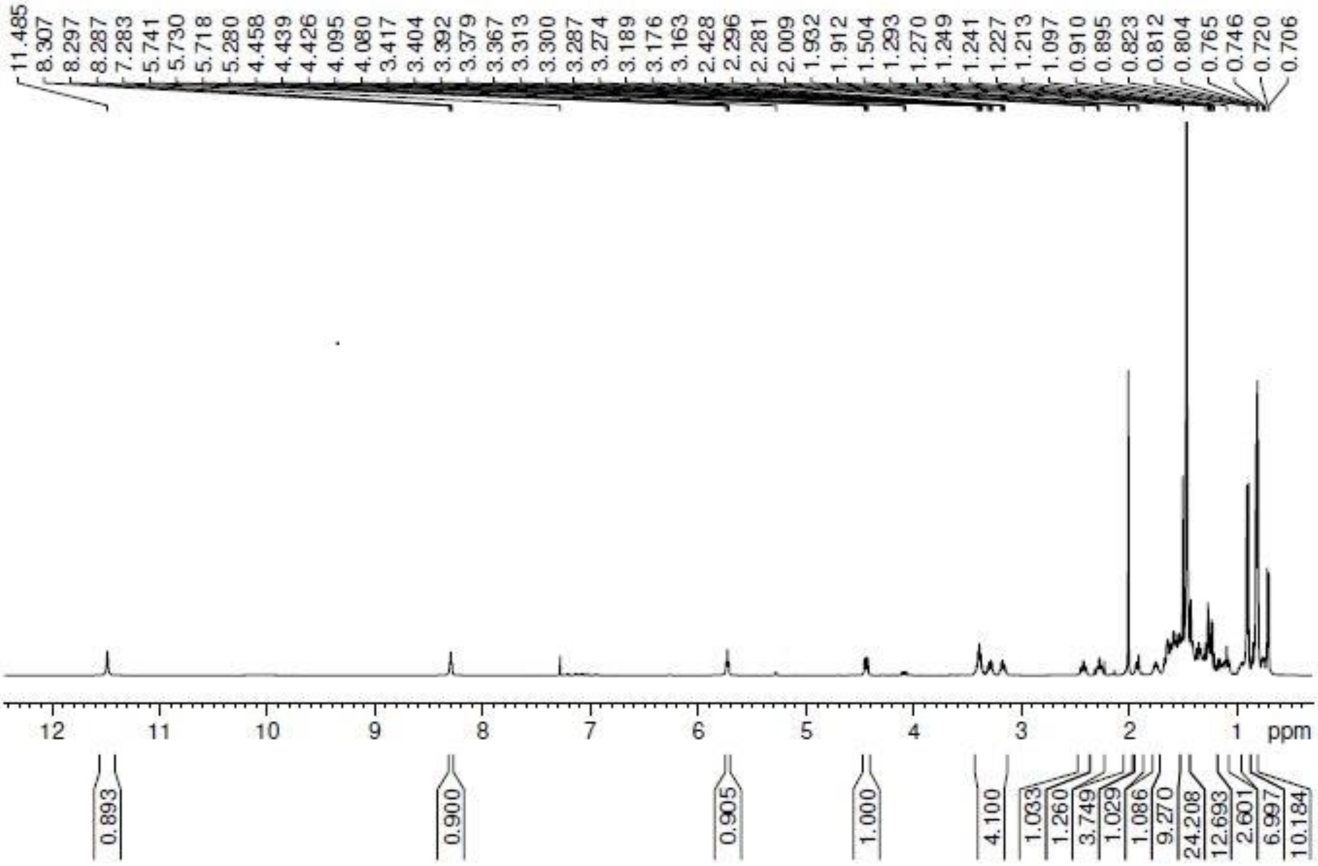
^{13}C NMR spectra (CDCl$_3$)



3β-N-[4-tert-butyloxycarbonyl buthylguanidine]-3-O-acetyl -lupane-28-amide (11).

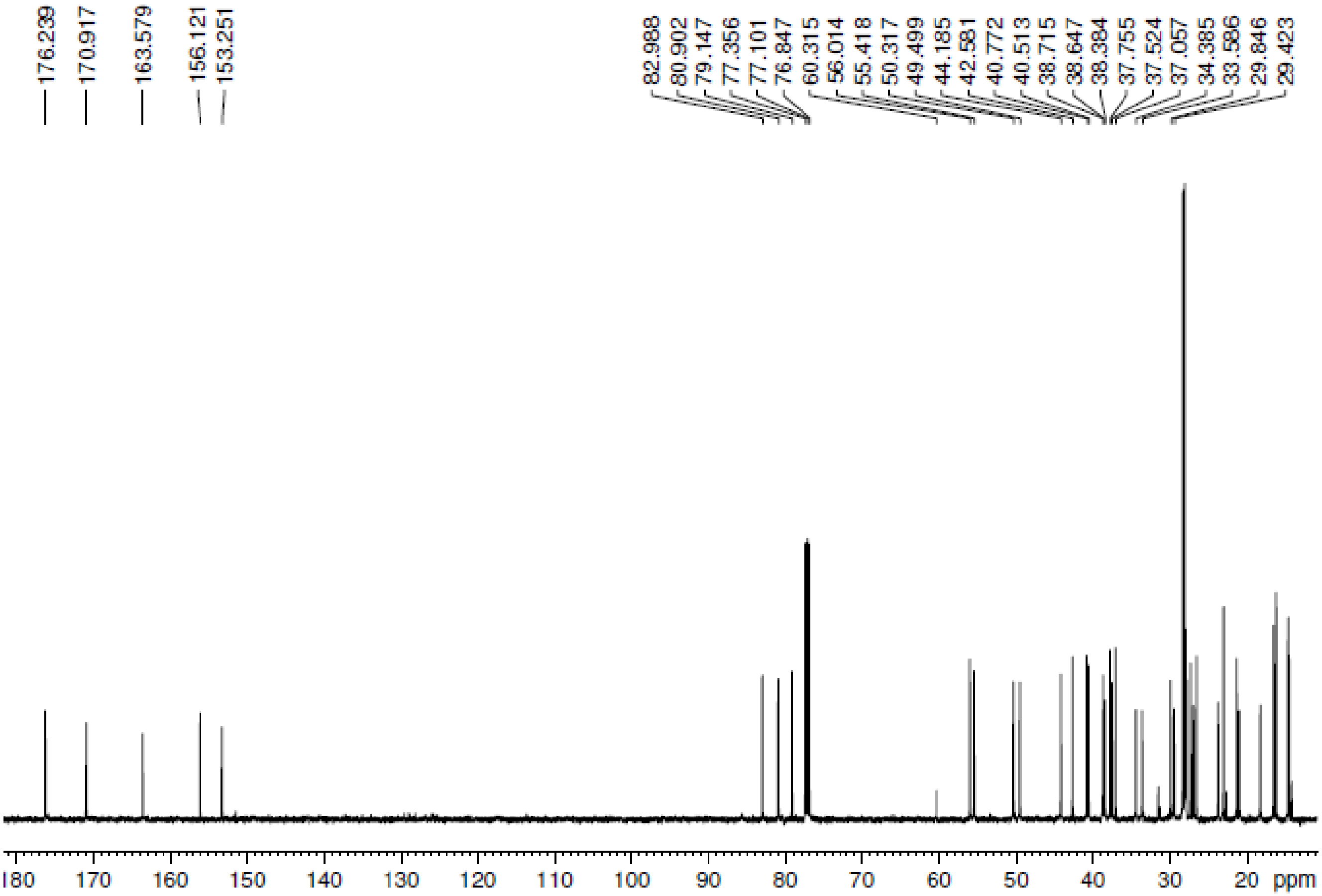
^{1}H NMR spectra ($CDCl_3$)





3β-N-[4-tert-butyloxycarbonyl buthylguanidine]-3-O-acetyl -lupane-28-amide (11).

^{13}C NMR spectra (CDCl$_3$)



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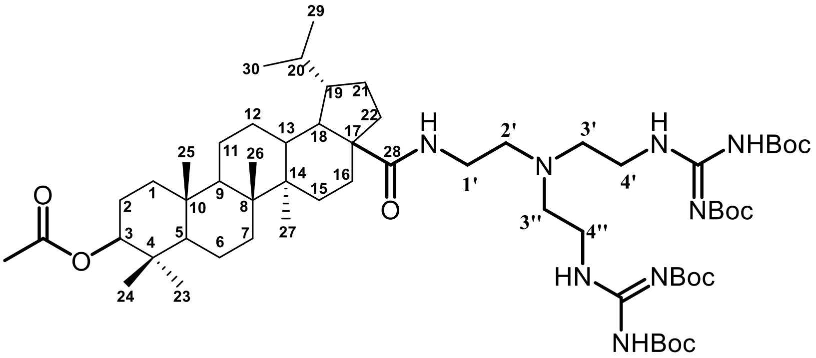
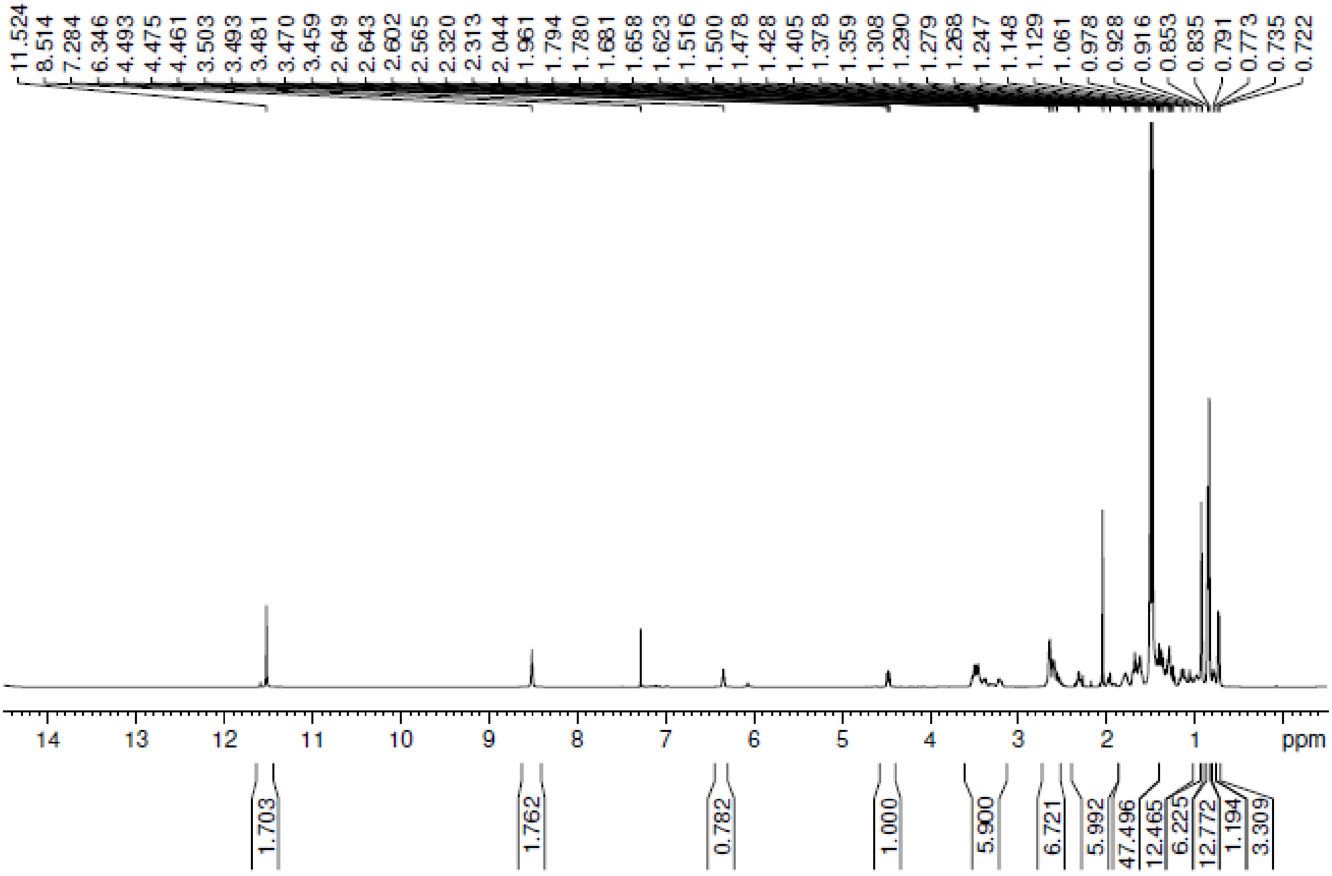
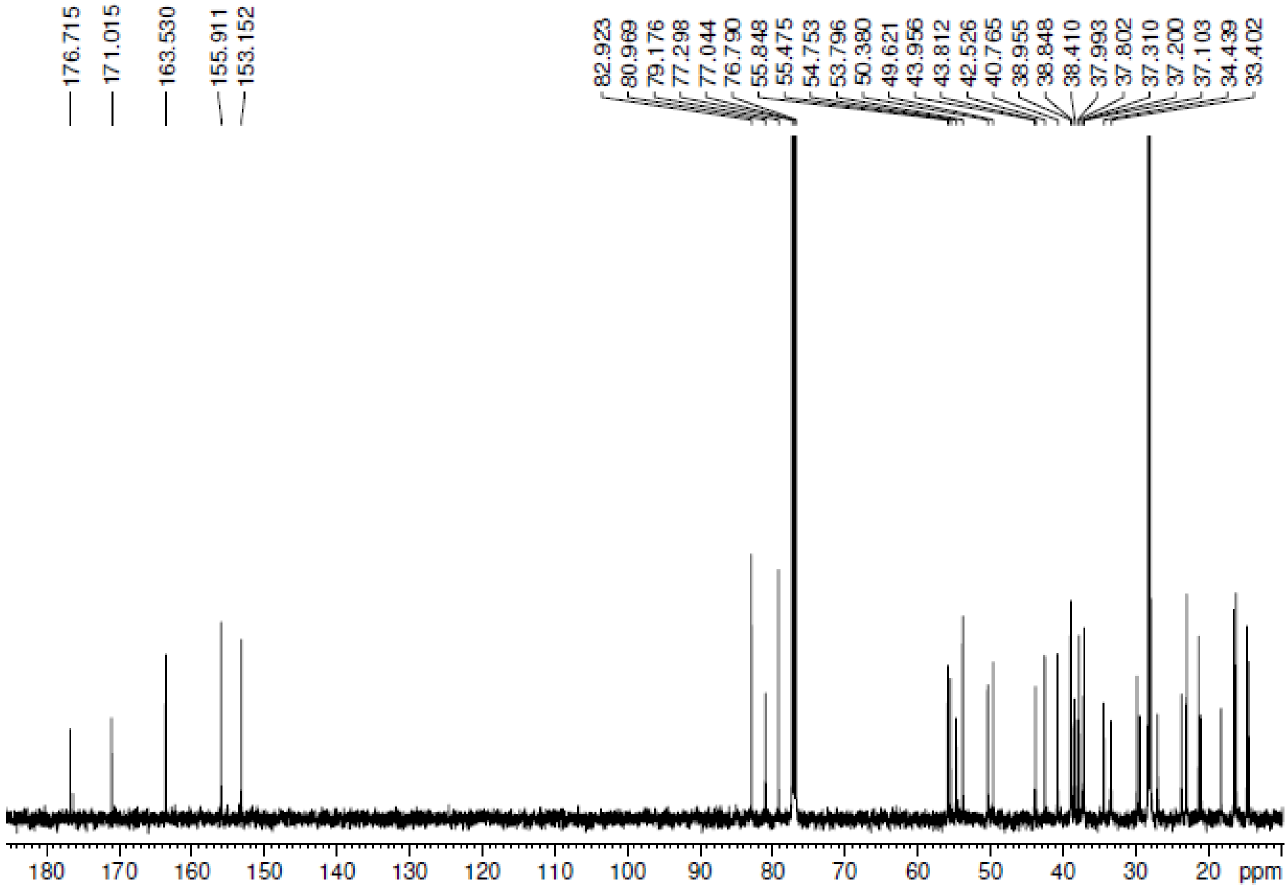
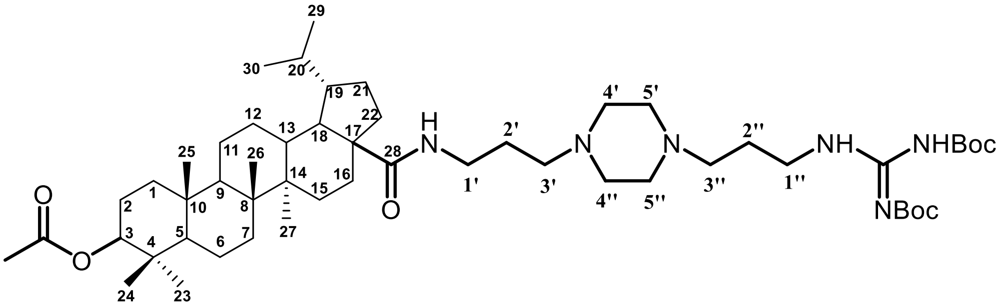


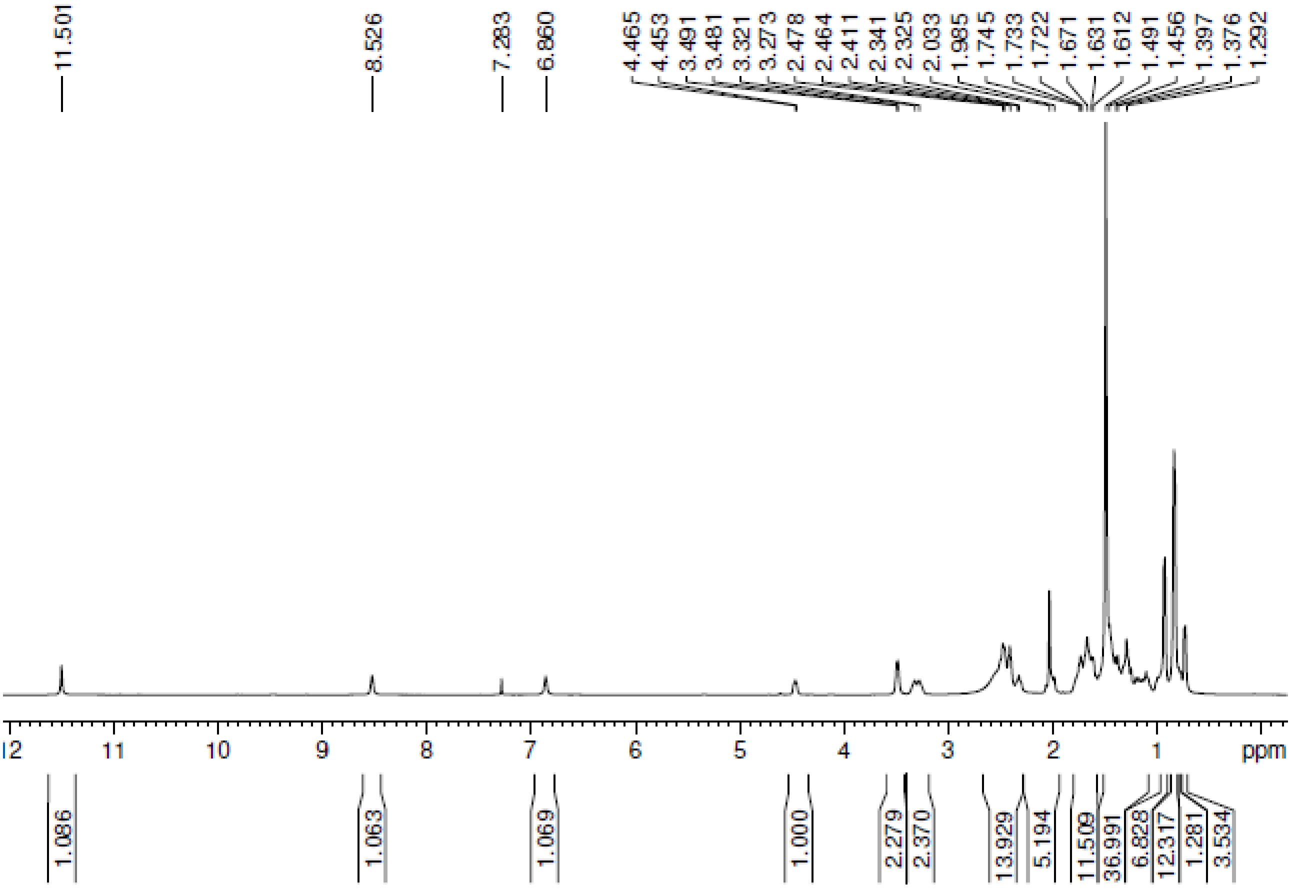


3β-N-[2-(N,N’-bis-tert-butyloxycarbonyl ethylgyanidine)-aminoethyl]-3-O-acetyl-lupane-28-amide (12). ^{13}C NMR spectra (CDCl$_3$)

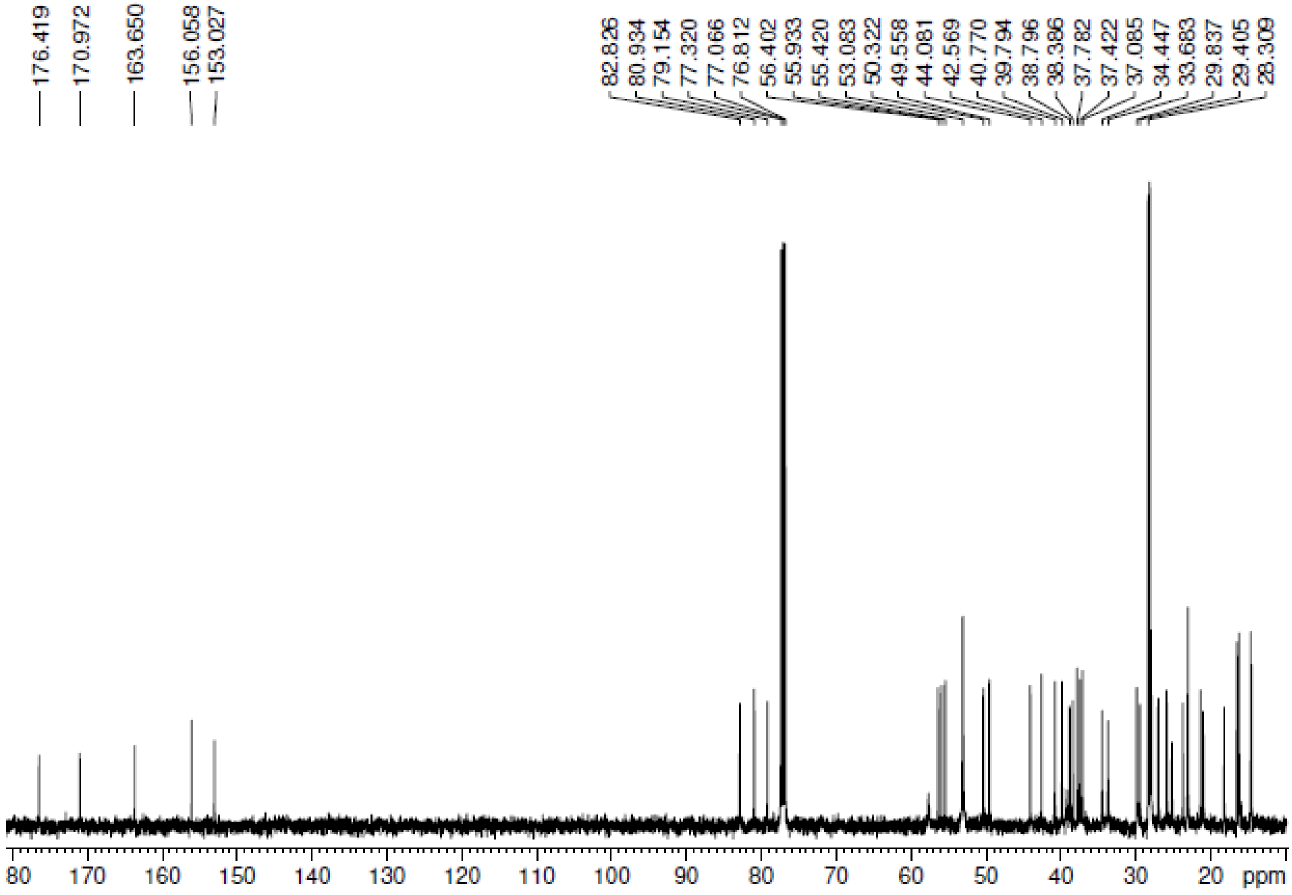


3β-N-{[3-(3-tert-butyloxycarbonyl propylgyanidine)piperazinyl]propyl}-3-O-acetyl-lupane-28-amide (13). ^{1}H NMR spectra ($CDCl_3$)

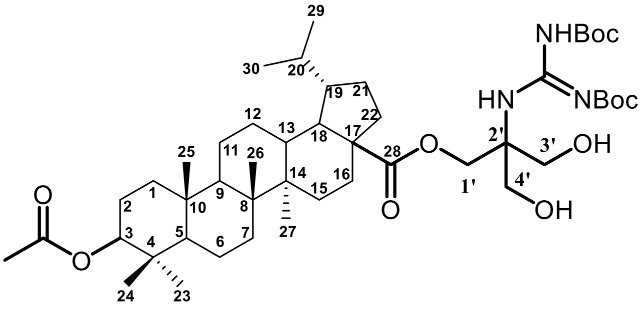


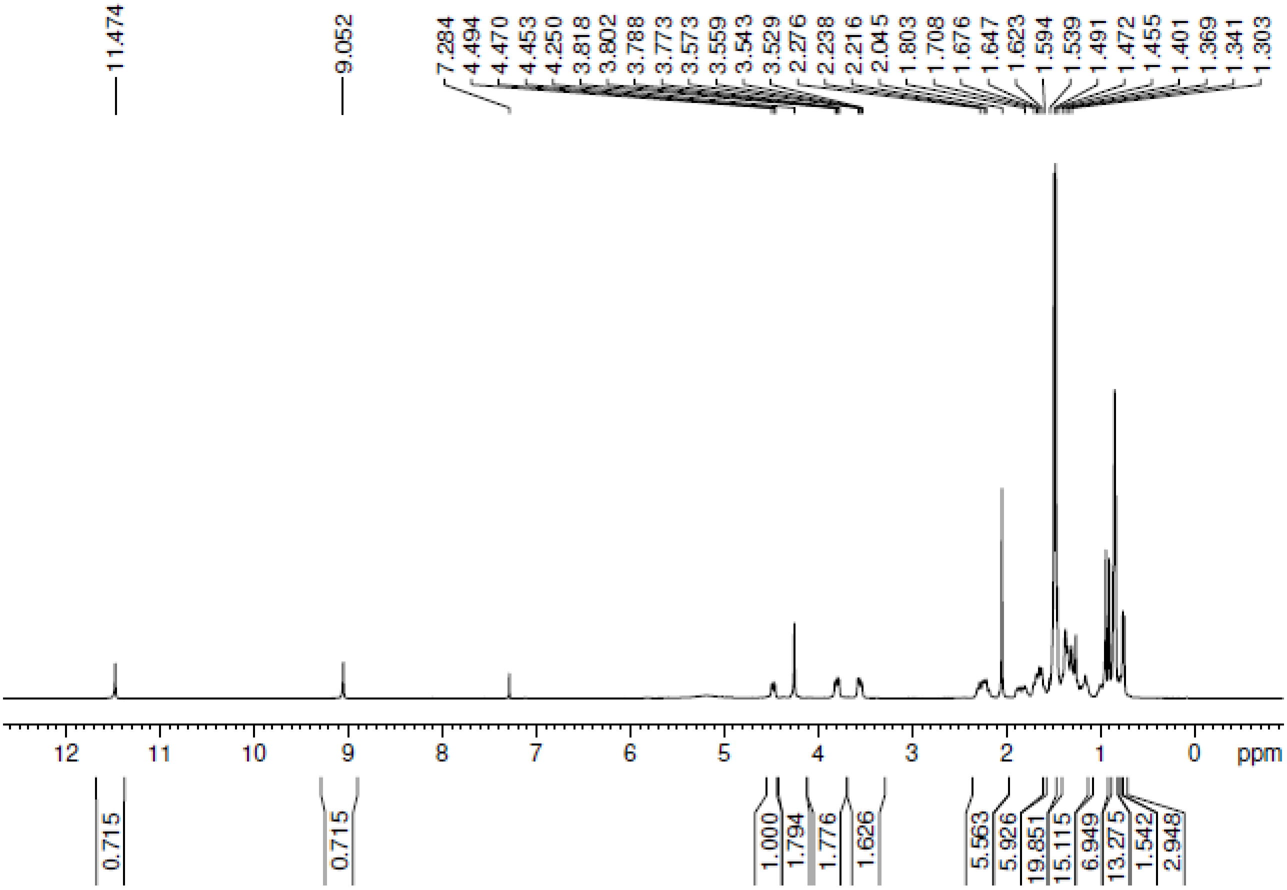


3β-N-{[3-(3- tert-butyloxycarbonyl propylgyanidine)piperazinyl]propyl}-3-O-acetyl-lupane-28-amide (13). ^{13}C NMR spectra (CDCl$_3$)

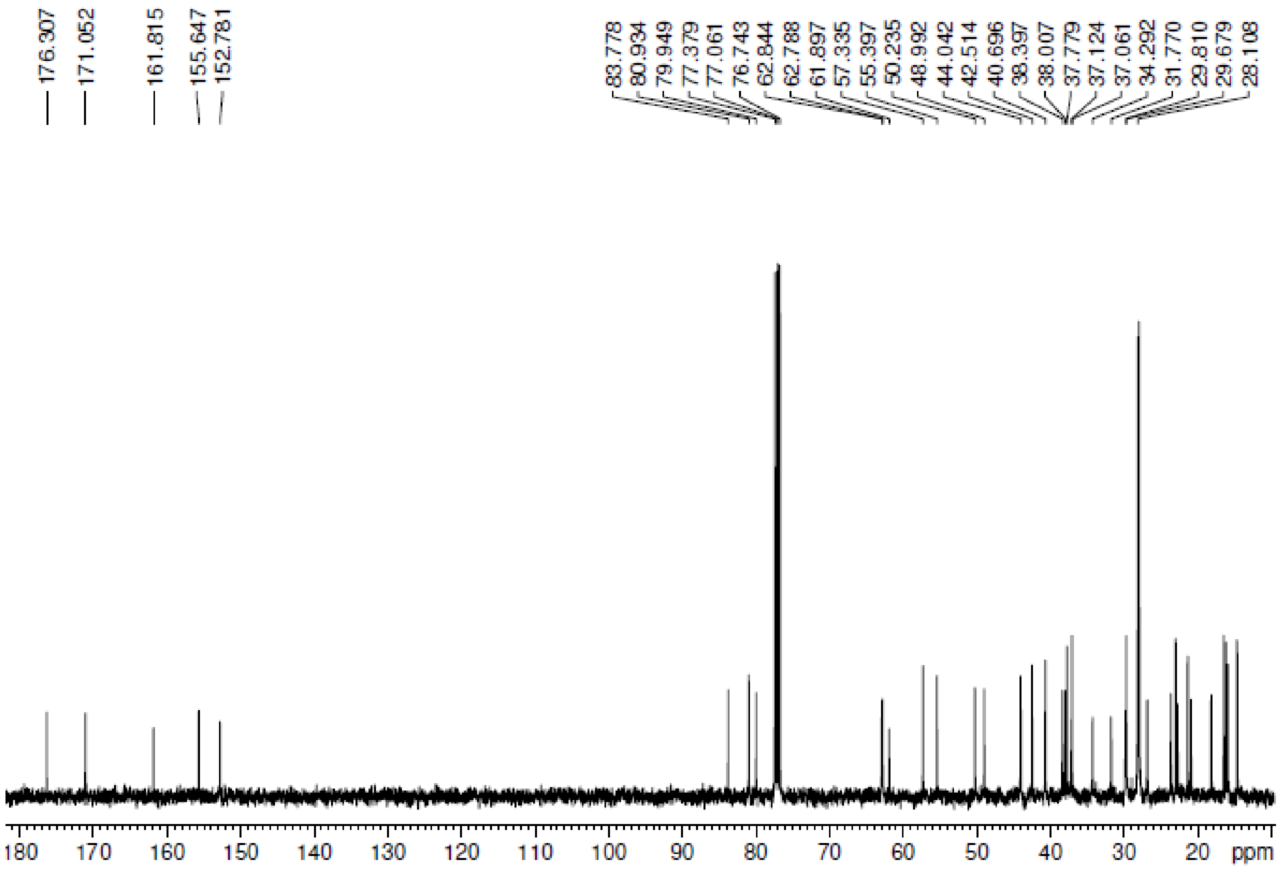


3β-[2-tert-butyloxycarbonylguanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-lupane-28-oate (15a). ^{1}H NMR spectra ($CDCl_3$)

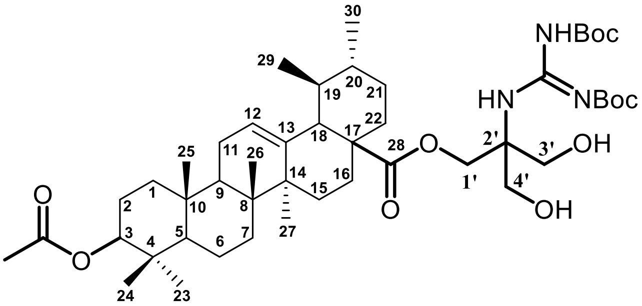


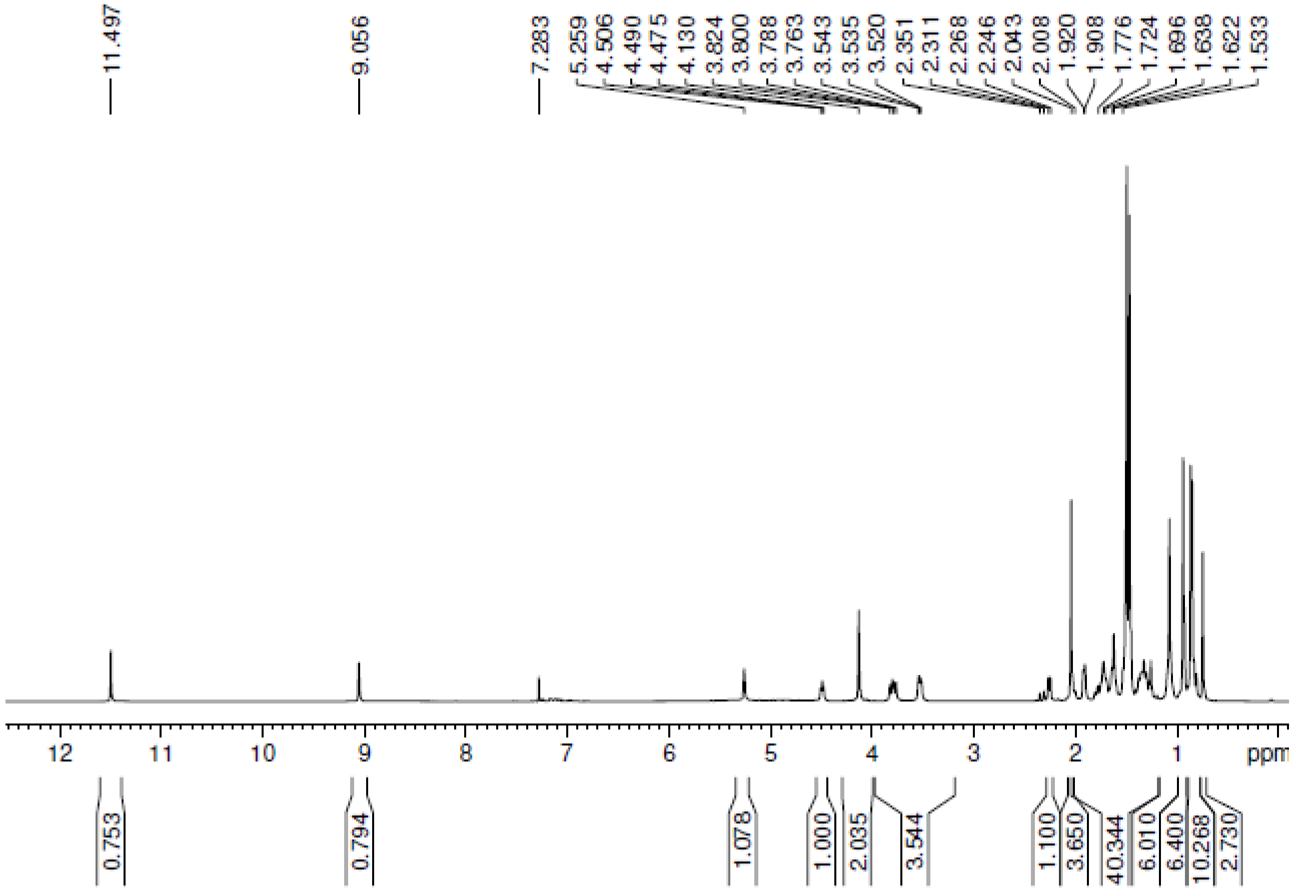


3β-[2-tert-butyloxycarbonylguanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl -lupane-28-oate (15a). ^{13}C NMR spectra (CDCl$_3$)

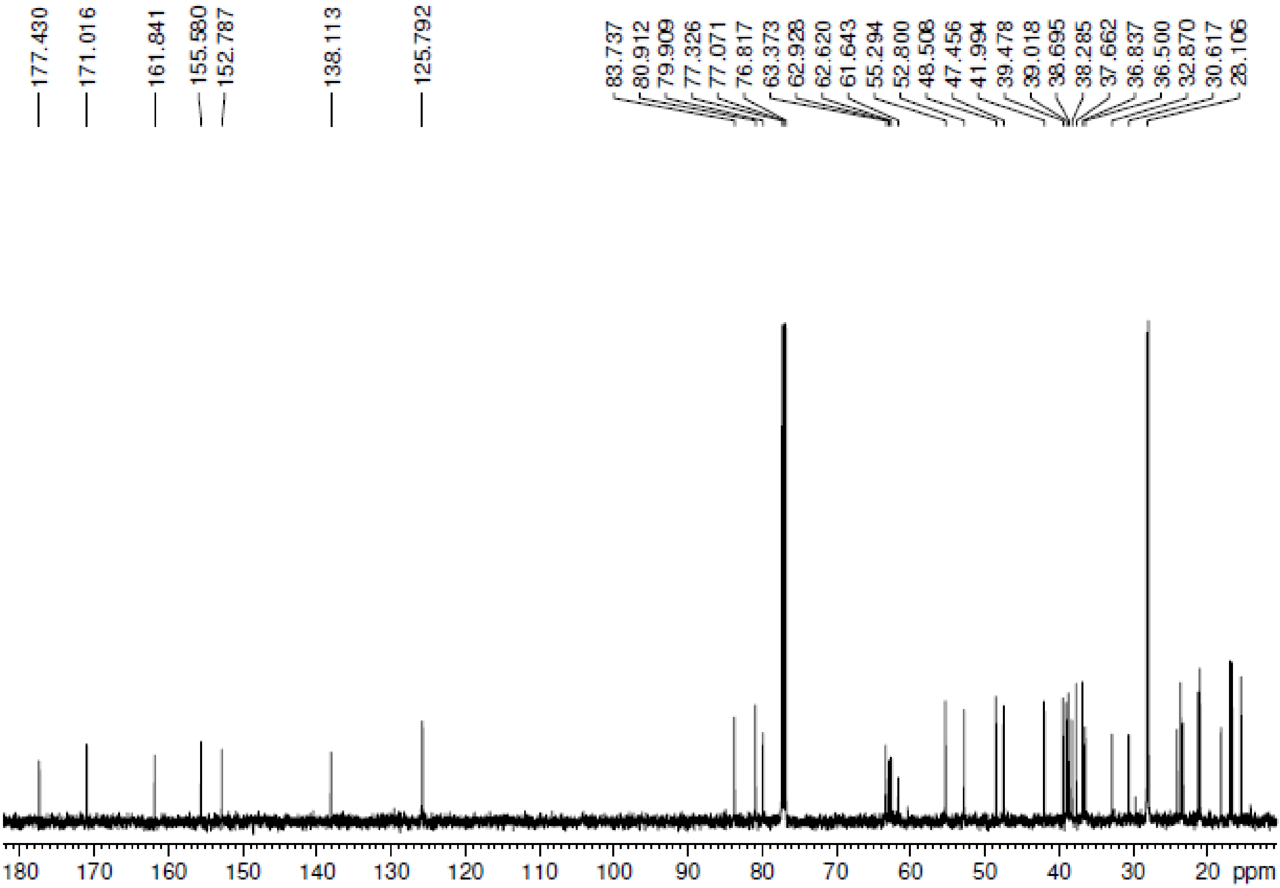


3β-[2-tert-butyloxycarbonylguanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-urs-12-en-28-oate (18a). ^{1}H NMR spectra ($CDCl_3$)

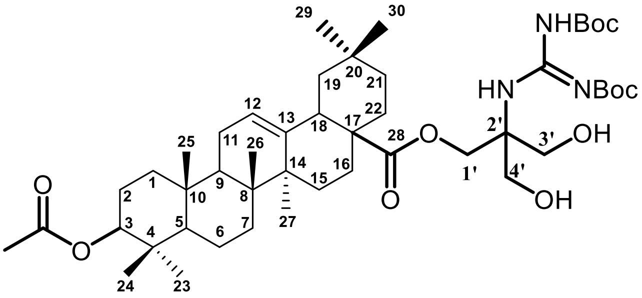


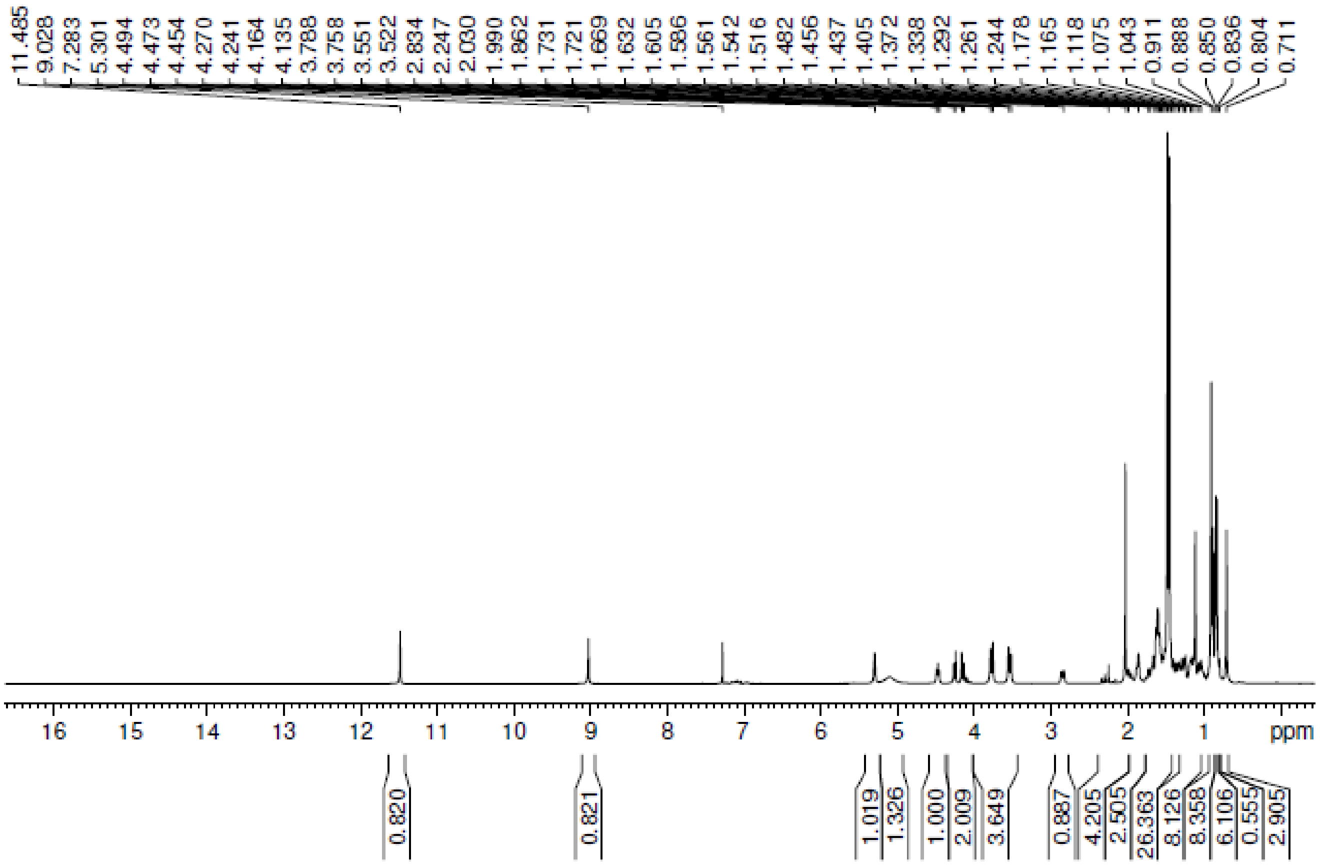


3β-[2-tert-butyloxycarbonylguanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-urs-12-en-28-oate (18a). ^{13}C NMR spectra ($CDCl_3$)

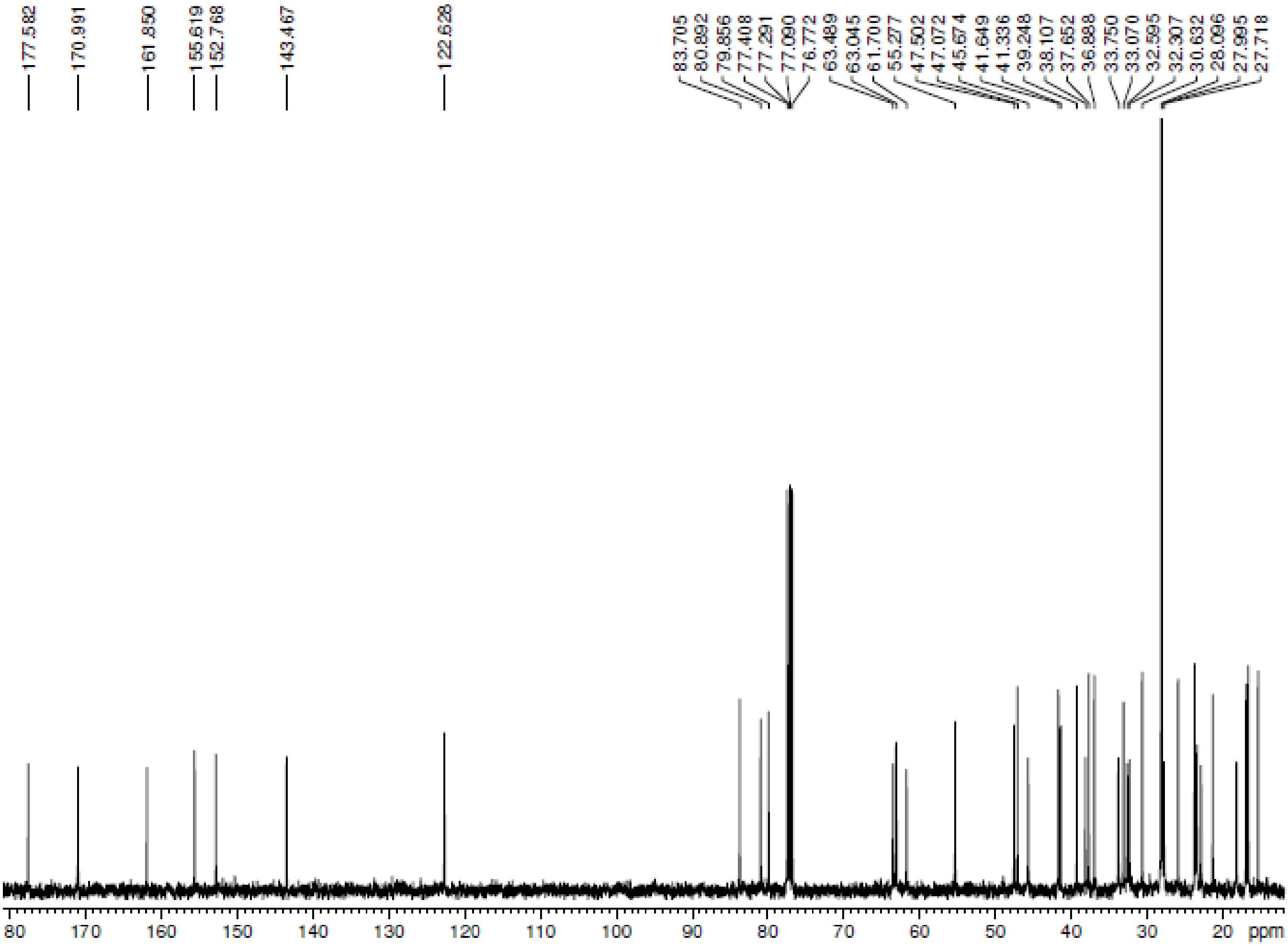


3β-[2-tert-butyloxycarbonylguanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-olean-12-en-28-oate (20a). ^{1}H NMR spectra (CDCl$_3$)

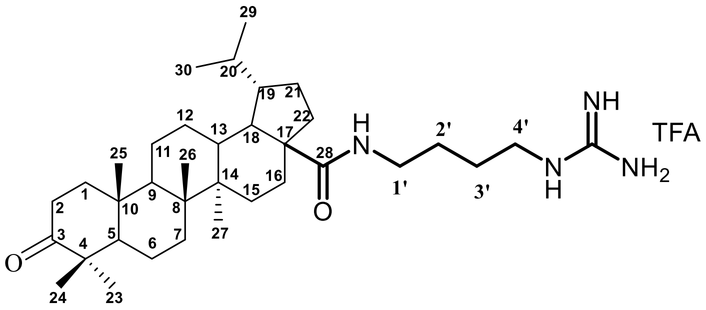


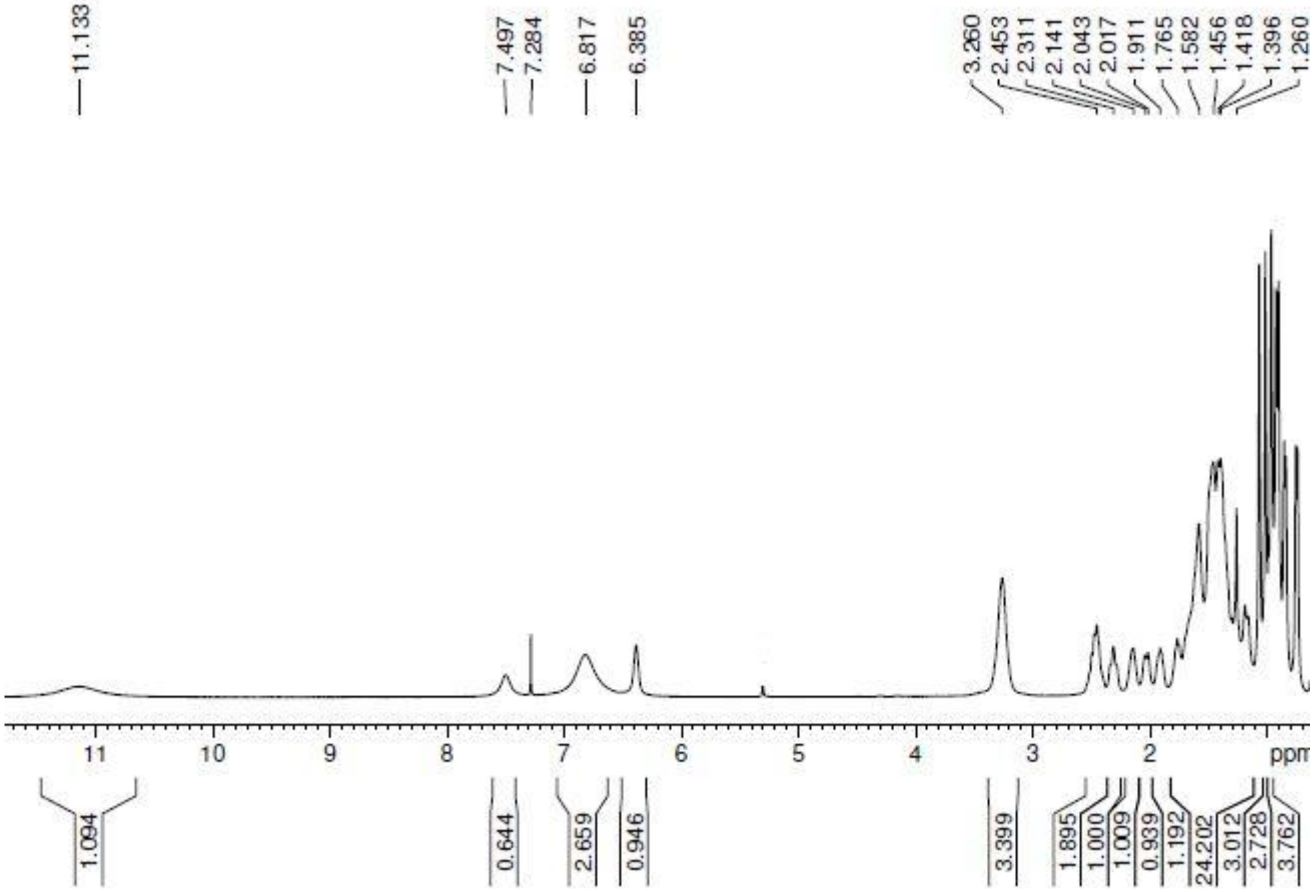


3β-[2-tert-butyloxycarbonylguanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl - olean-12-en-28-oate (20a). ^{13}C NMR spectra (CDCl$_3$)

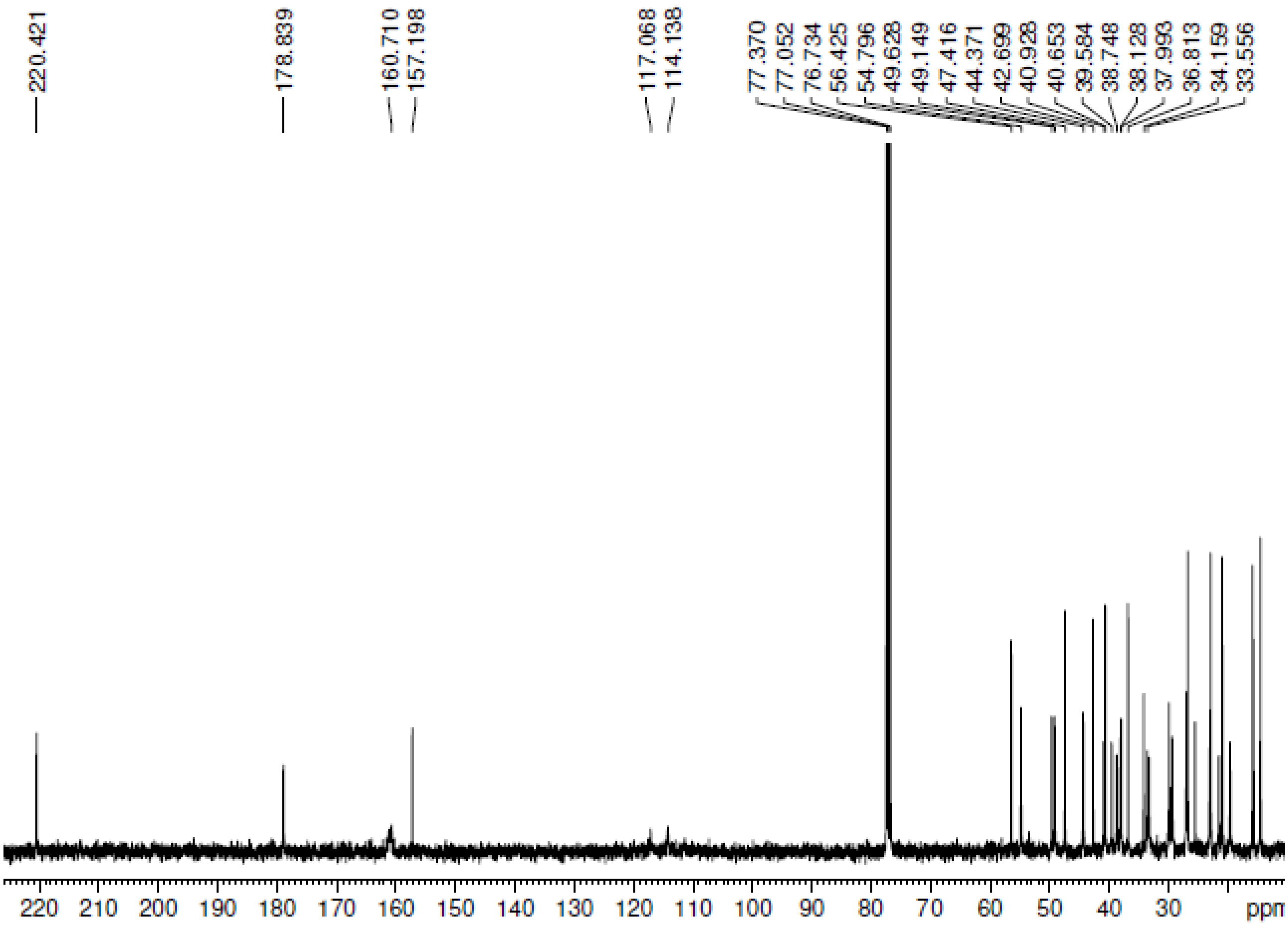


N-(4-buthylgyanidine)-3-oxolupane-28-amide trifluoroacetate (9a). ^{1}H NMR spectra ($CDCl_3$)

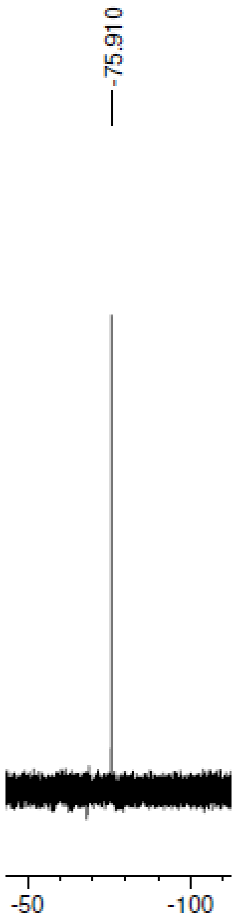




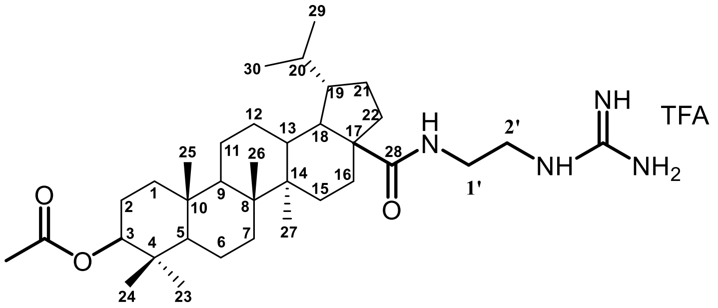
N-(4-buthylgyanidine)-3-oxolupane-28-amide trifluoroacetate (9a). ^{13}C NMR spectra ($CDCl_3$)

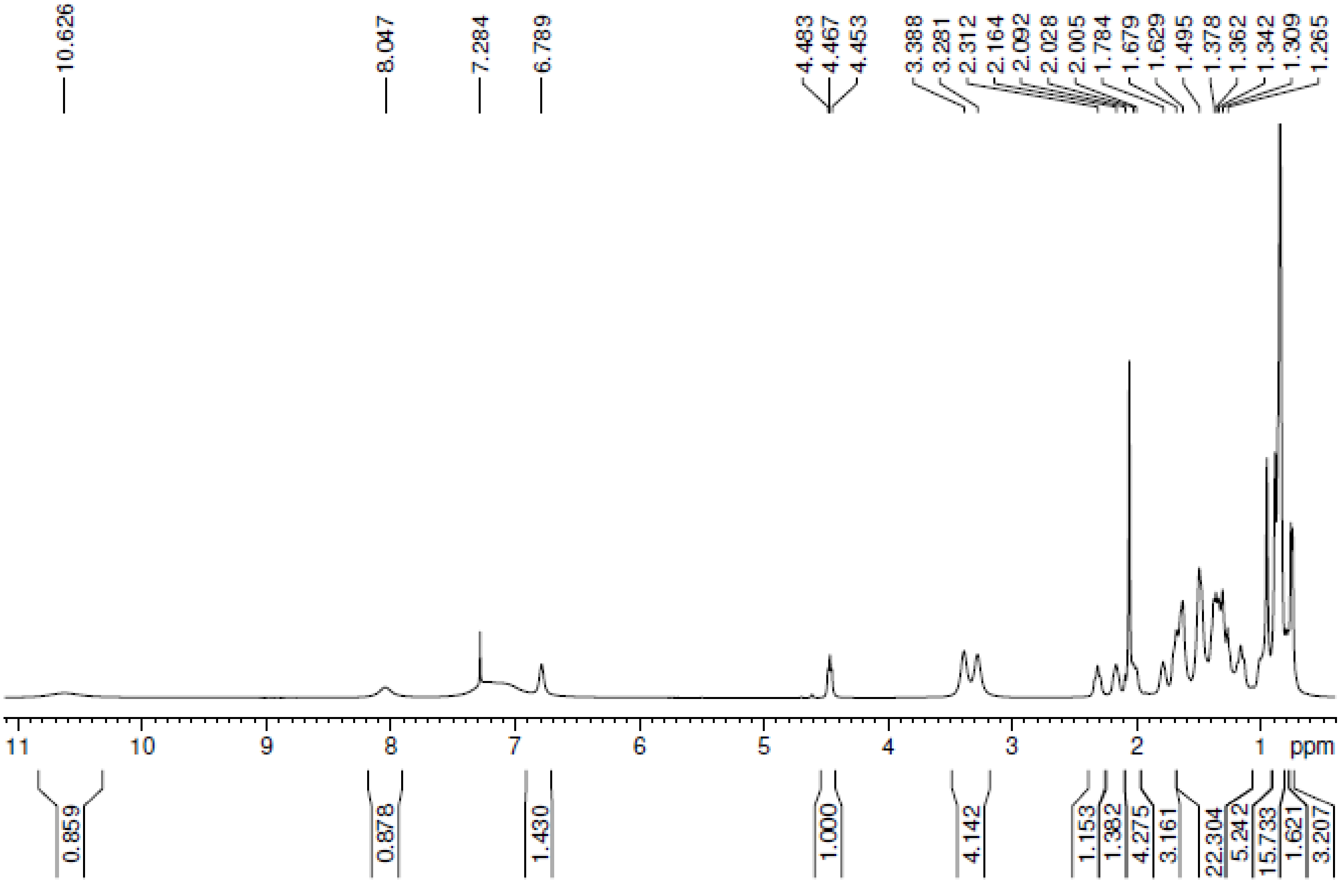


N-(4-buthylgyanidine)-3-oxolupane-28-amide trifluoroacetate (9a). ^{19}F NMR spectra (CDCl$_3$)

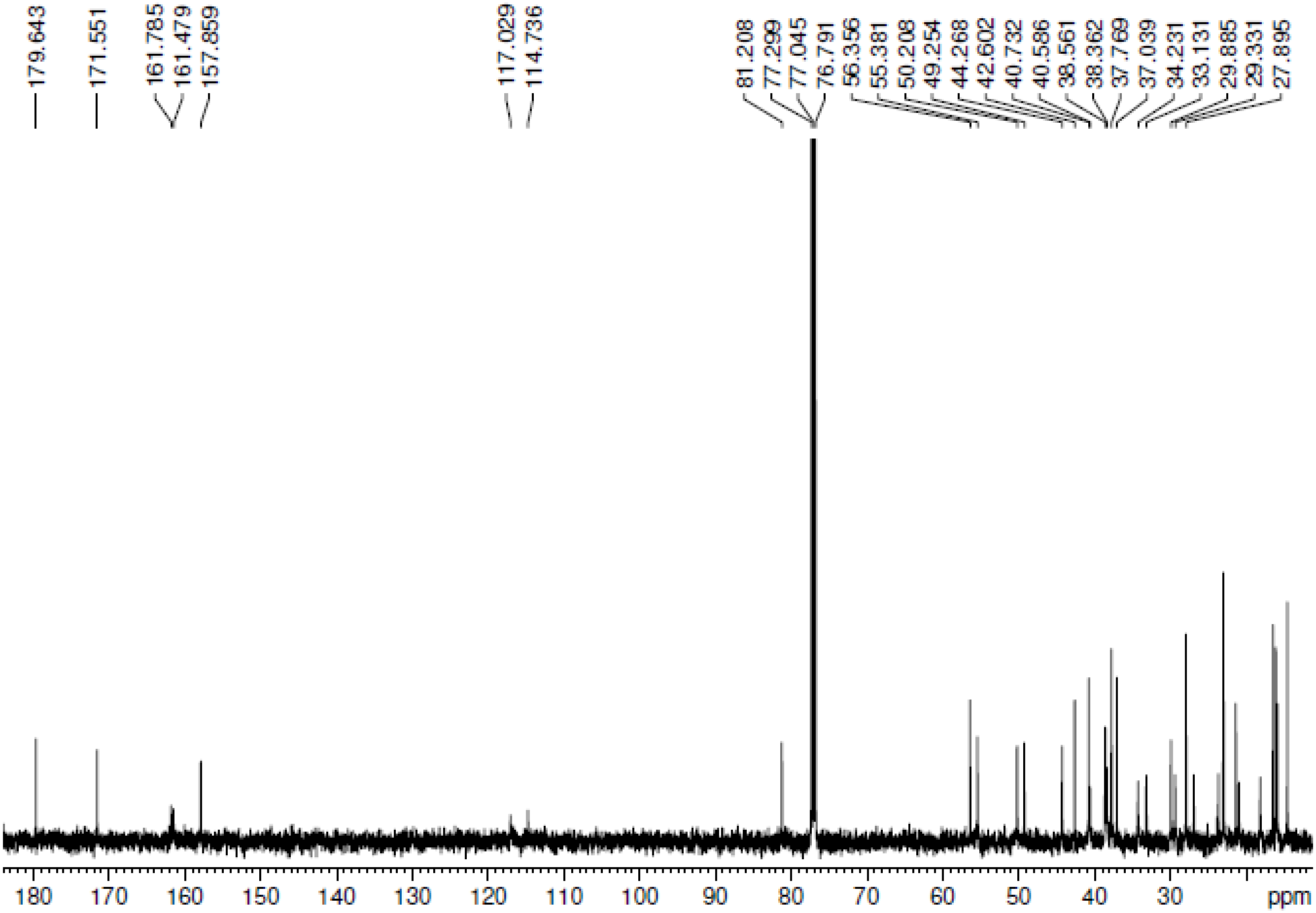


3β-N-(2-ethylgyanidine)-3-O-acetyl-lupane-28-amide trifluoroacetate (10a). ^{1}H NMR spectra ($CDCl_3$)

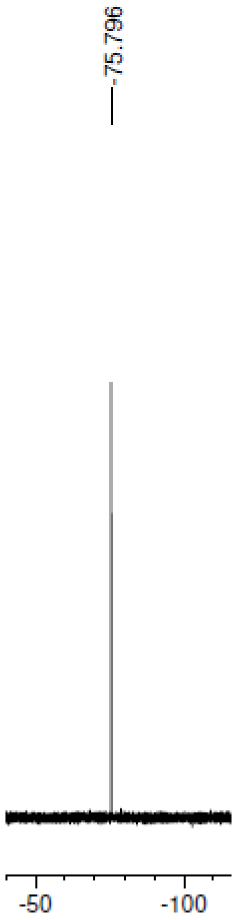




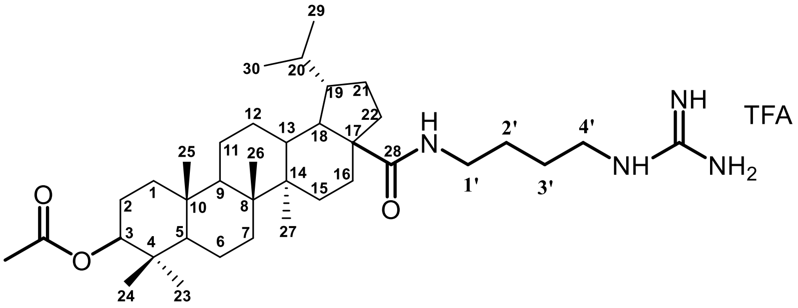
3β-N-(2-ethylgyanidine)-3- O-acetyl-lupane-28-amide trifluoroacetate (10a). ^{13}C NMR spectra (CDCl$_3$)

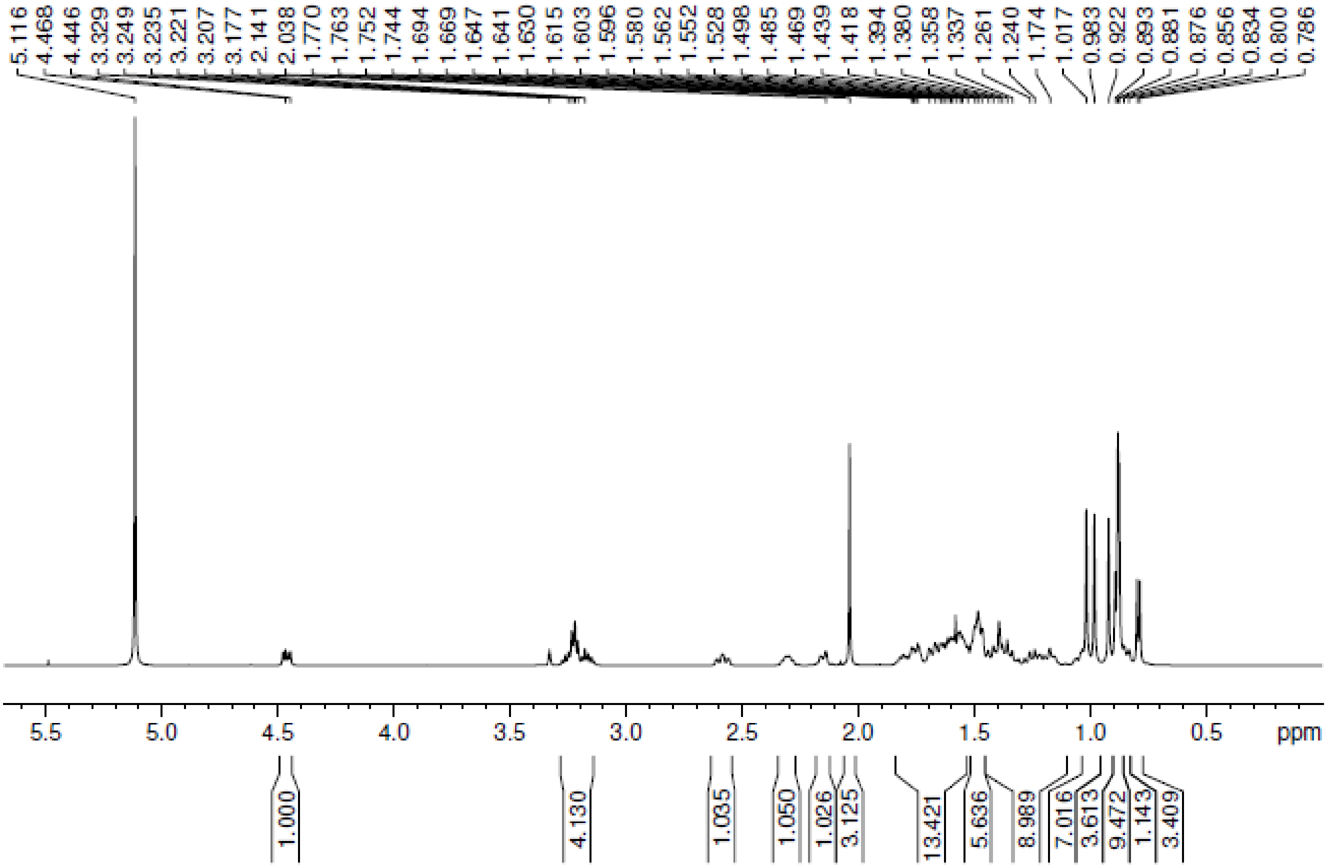


3β-N-(2-ethylgyanidine)-3- O-acetyl-lupane-28-amide trifluoroacetate (10a). ^{13}F NMR spectra (CDCl$_3$)

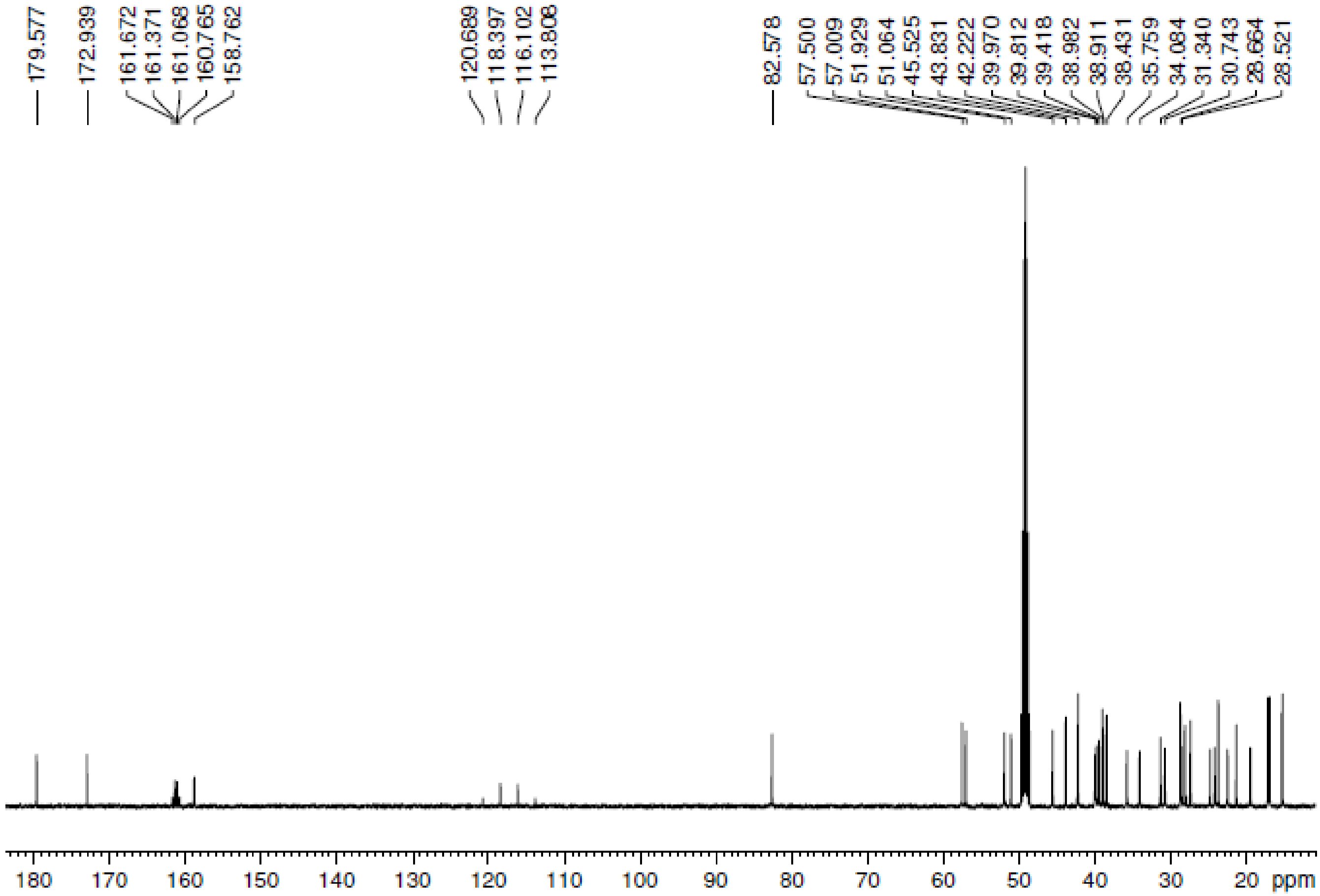


3β-N-(4-buthylgyanidine)-3-O-acetyl-lupane-28-amide trifluoroacetate (11a). ^{1}H NMR spectra (MeOD)

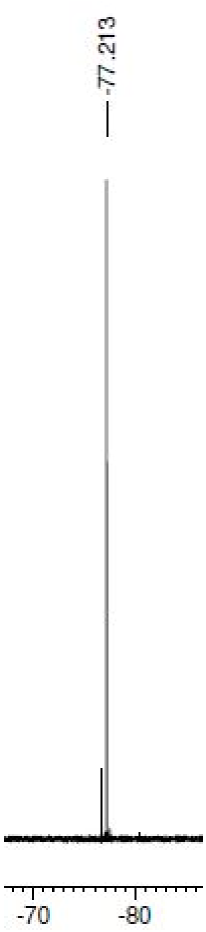




3β-N-(4-buthylgyanidine)-3- O-acetyl-lupane-28-amide trifluoroacetate (11a). ^{13}C NMR spectra (MeOD)

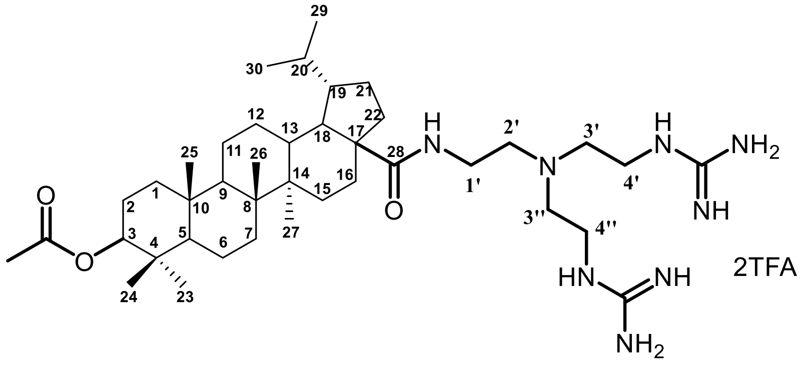


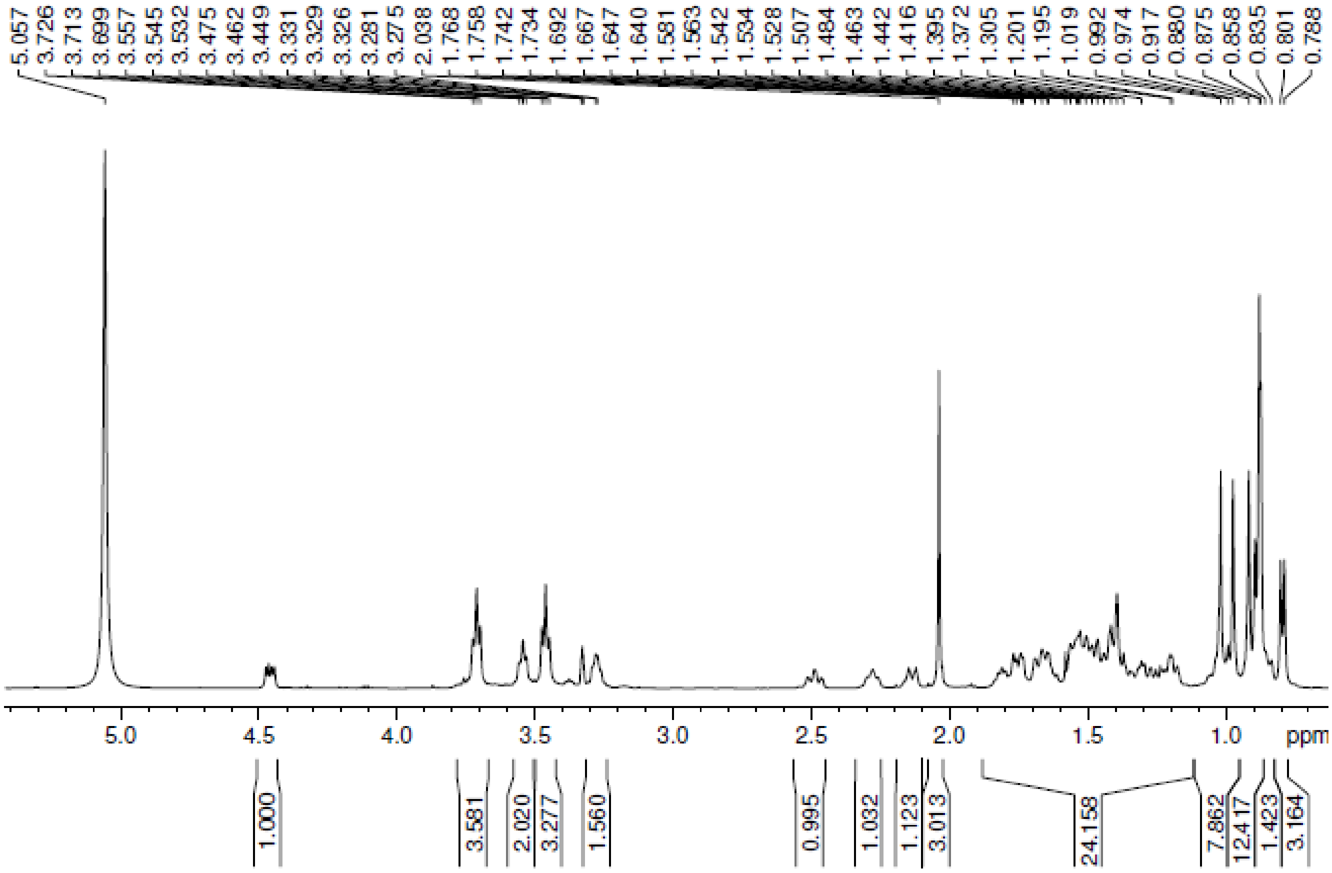
3β-N-(4-buthylgyanidine)-3- O-acetyl-lupane-28-amide trifluoroacetate (11a). ^{19}F NMR spectra (MeOD)



3β-N-[2-(N,N’-bis-ethylgyanidine)-ethyl]-3-O-acetyl-lupane-28-amide trifluoroacetate (12a)

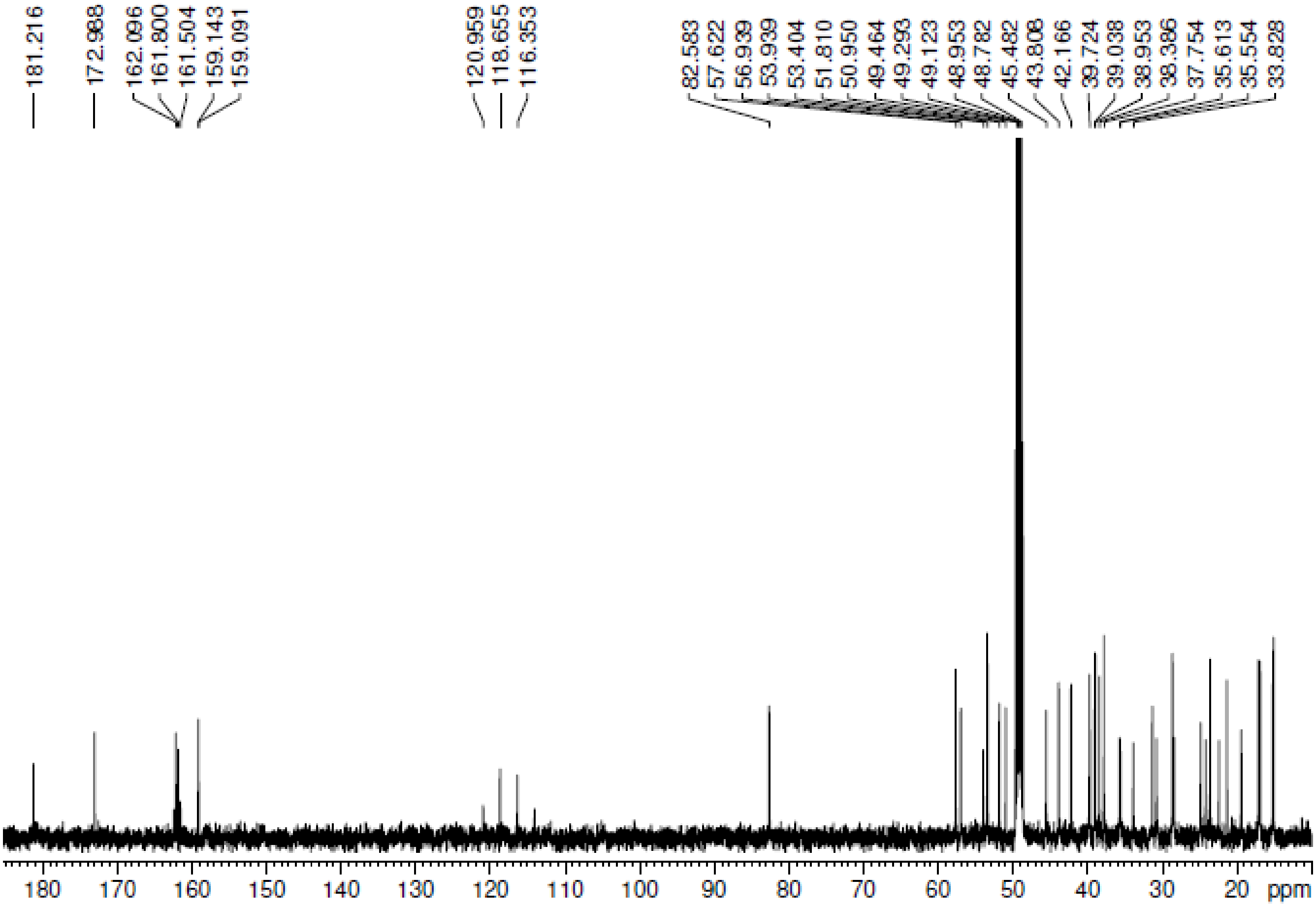
^{1}H NMR spectra (MeOD)





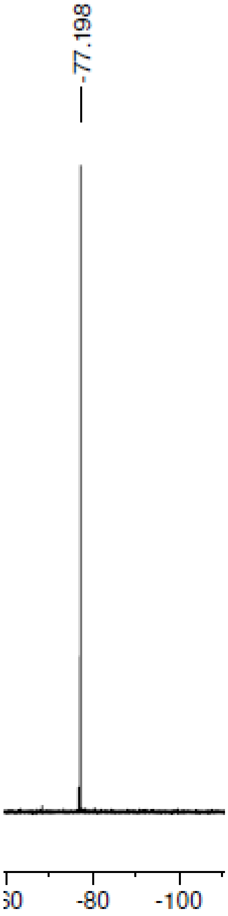
3β-N-[2-(N,N’-bis-ethylgyanidine)-ethyl]-3- O-acetyl -lupane-28-amide trifluoroacetate (12a).

^{13}C NMR spectra (MeOD)



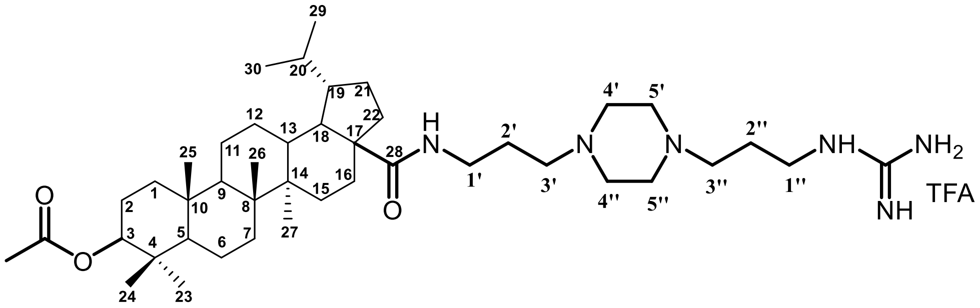
3β-N-[2-(N,N’-bis-ethylgyanidine)-ethyl]-3- O-acetyl -lupane-28-amide trifluoroacetate (12a).

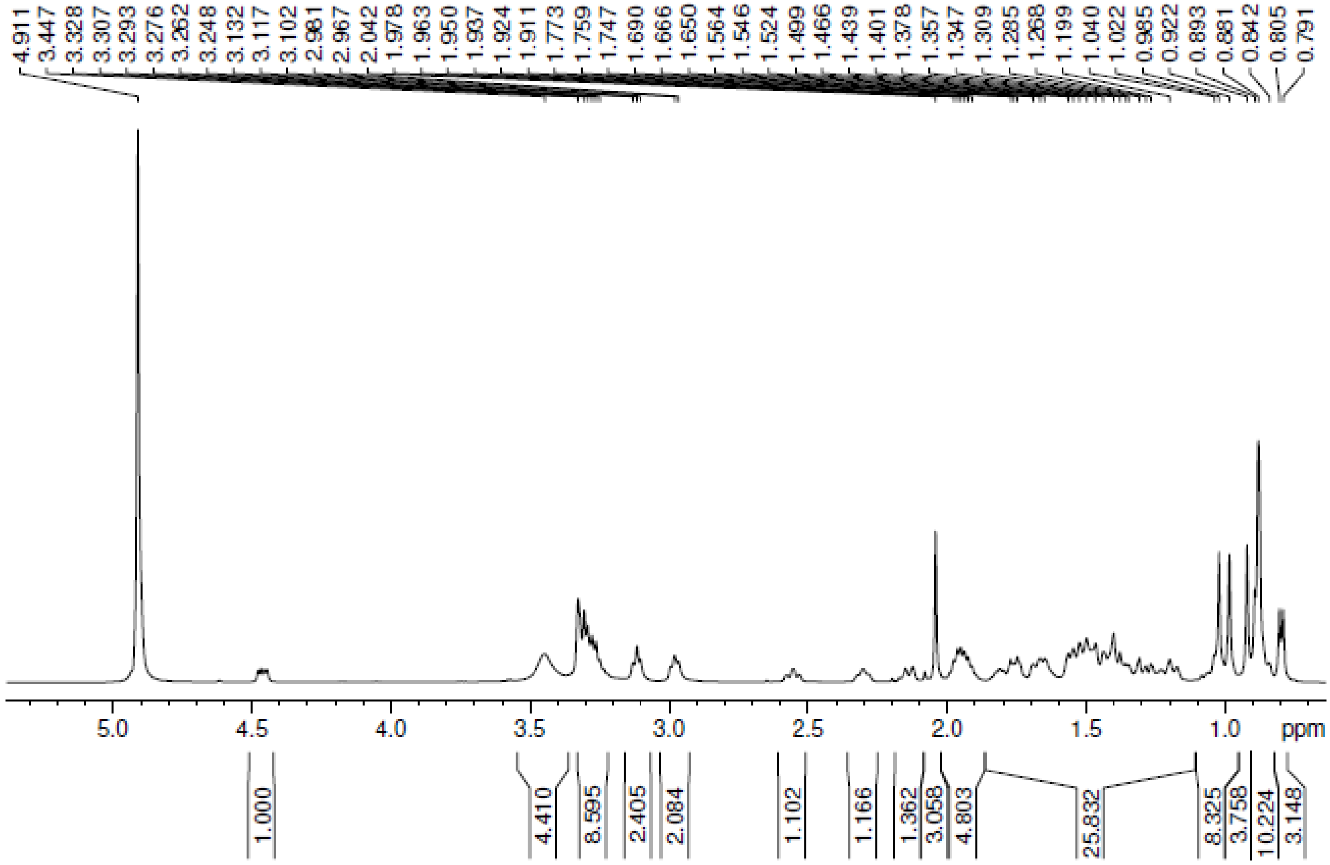
^{19}F NMR spectra (MeOD)



3β-N-{[3-(3-propylguanidine)piperazinyl]propyl}-3-O-acetyl-lupane-28-amide trifluoroacetate (13a).

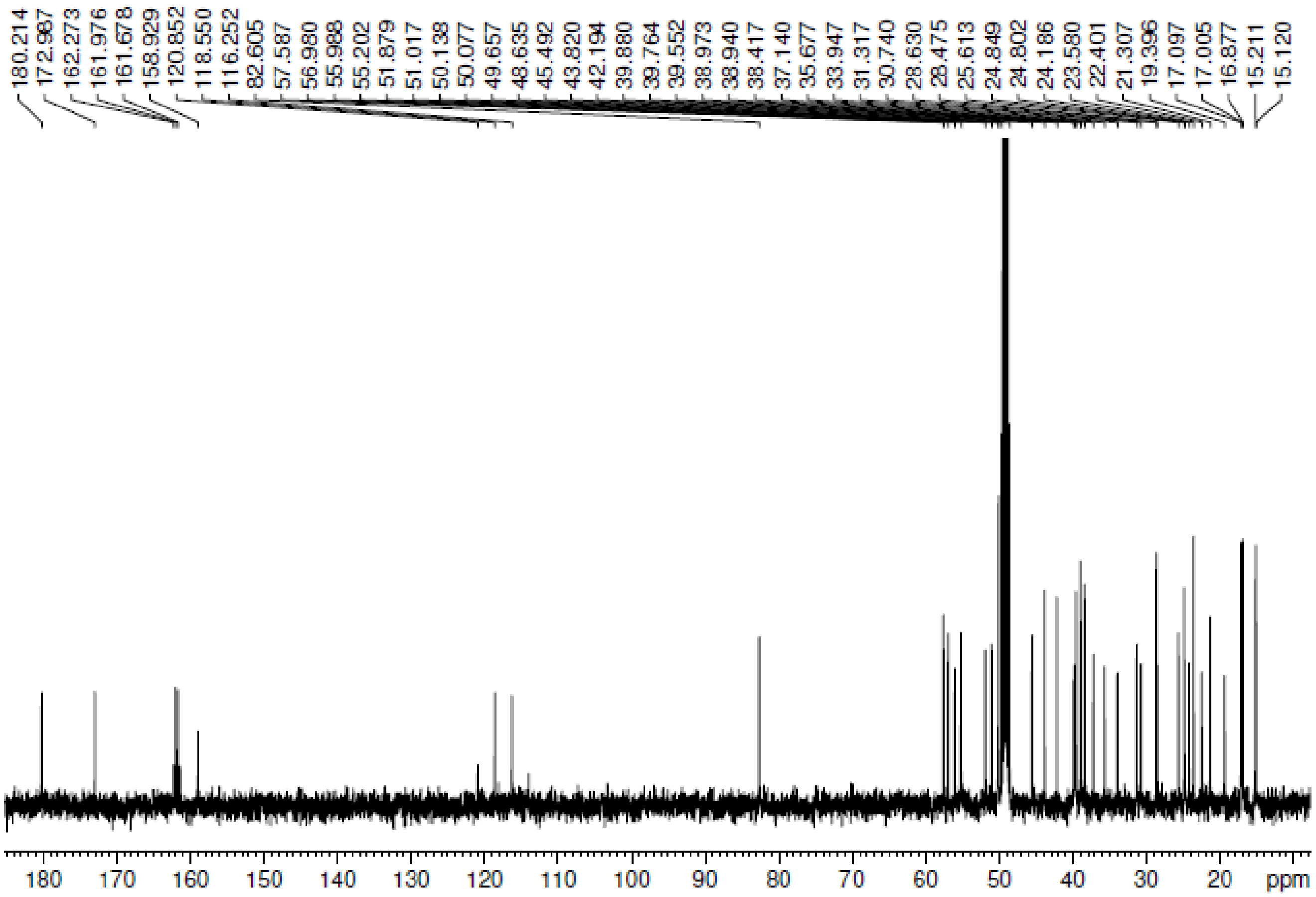
^{1}H NMR spectra (MeOD)





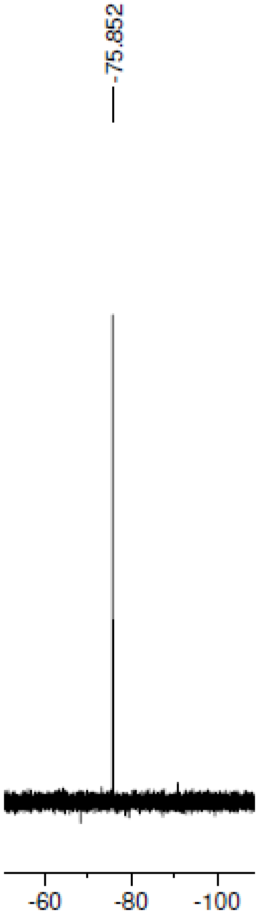
3β-N-{[3-(3-propylguanidine)piperazinyl]propyl}-3-O-acetyl-lupane-28-amide trifluoroacetate (13a).

^{13}C NMR spectra (MeOD)

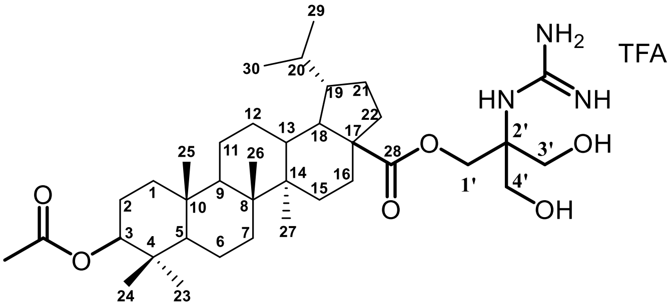


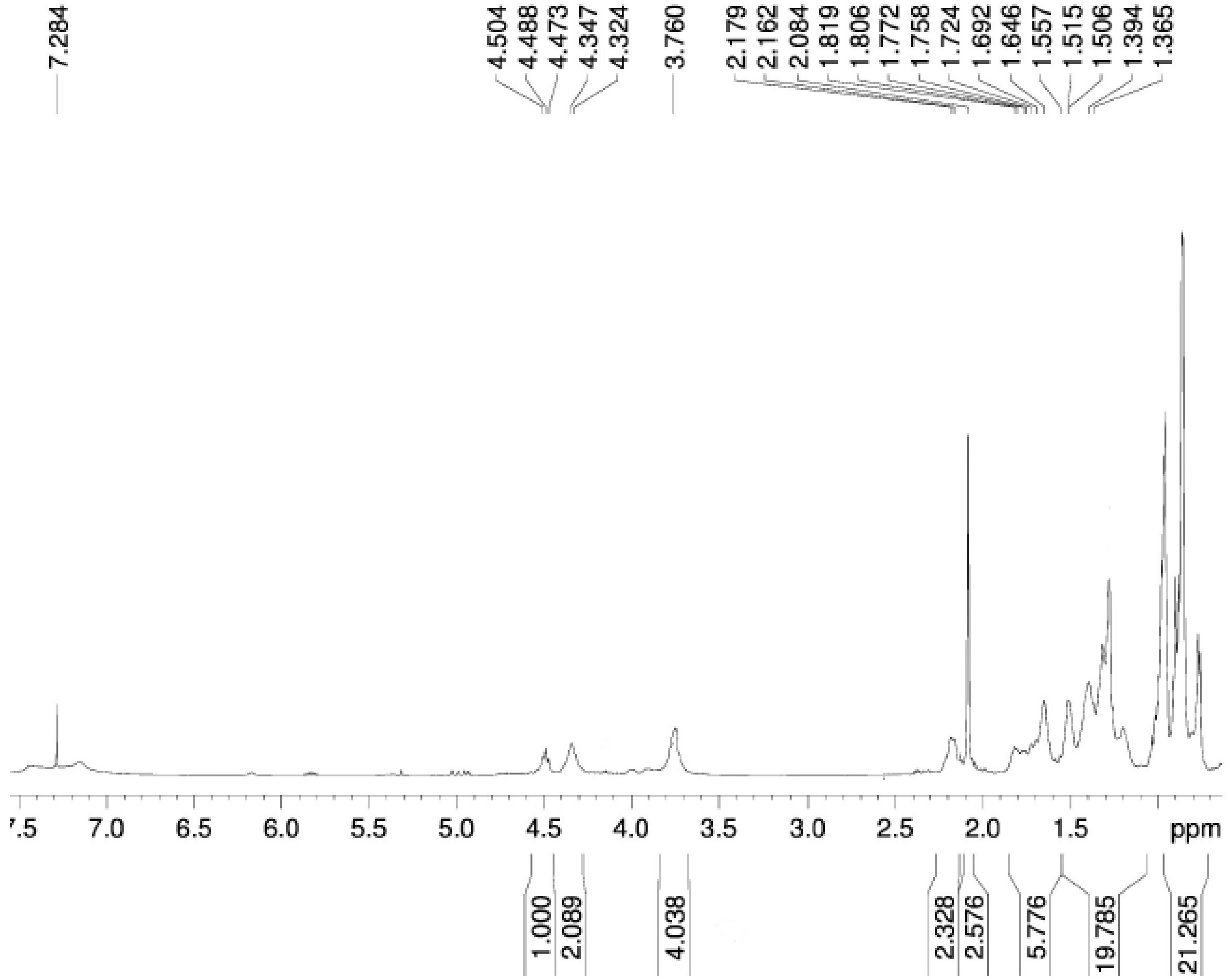
3β-N-{[3-(3-propylguanidine)piperazinyl]propyl}-3-O-acetyl-lupane-28-amide trifluoroacetate (13a).

^{19}F NMR spectra (MeOD)

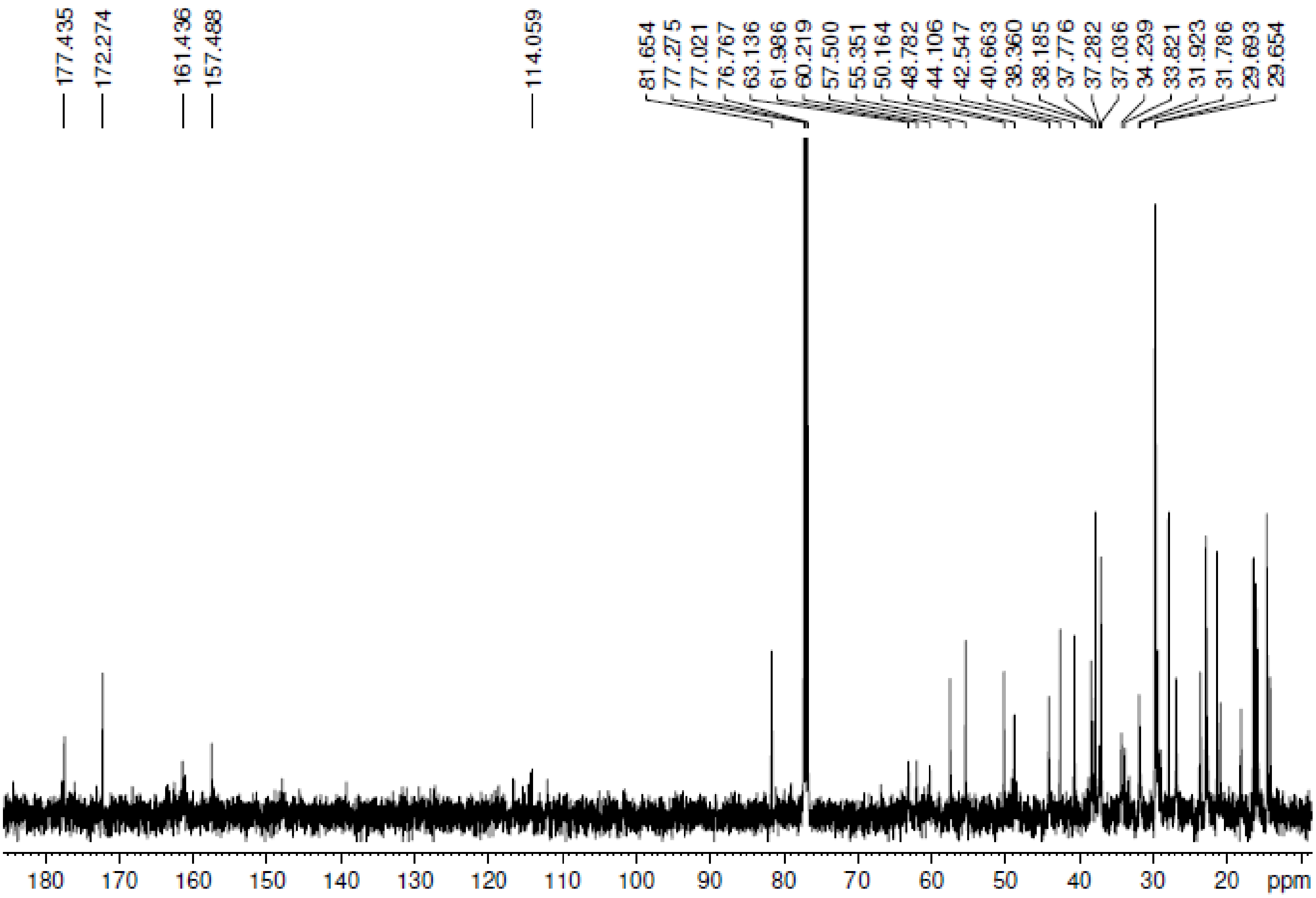


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-lupane-28-oate trifluoroacetate (15b). ^{1}H NMR spectra (CDCl$_3$)

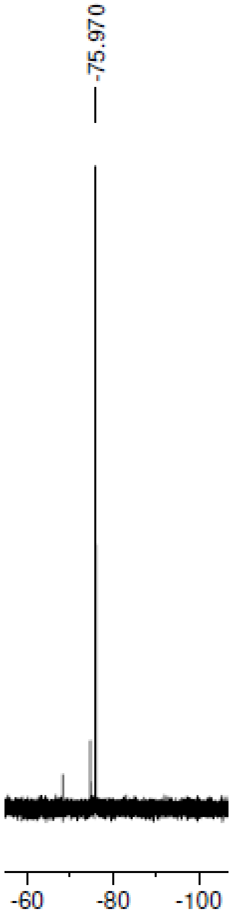




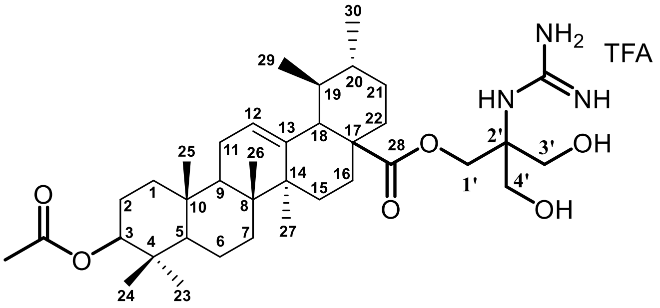
3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-lupane-28-oate trifluoroacetate (15b).^{13}C NMR spectra (CDCl$_3$)

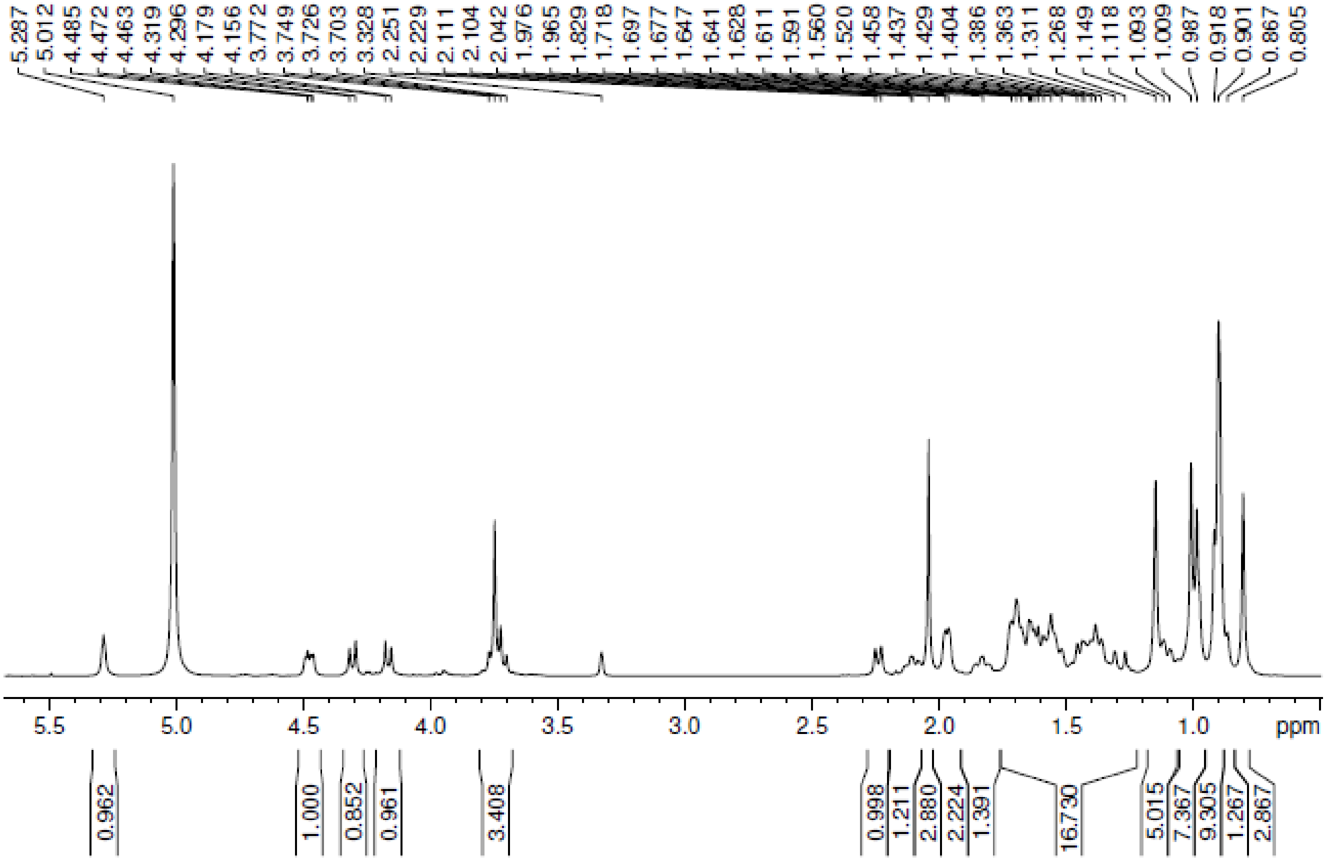


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-lupane-28-oate trifluoroacetate (15b). ^{19}F NMR spectra (CDCl$_3$)

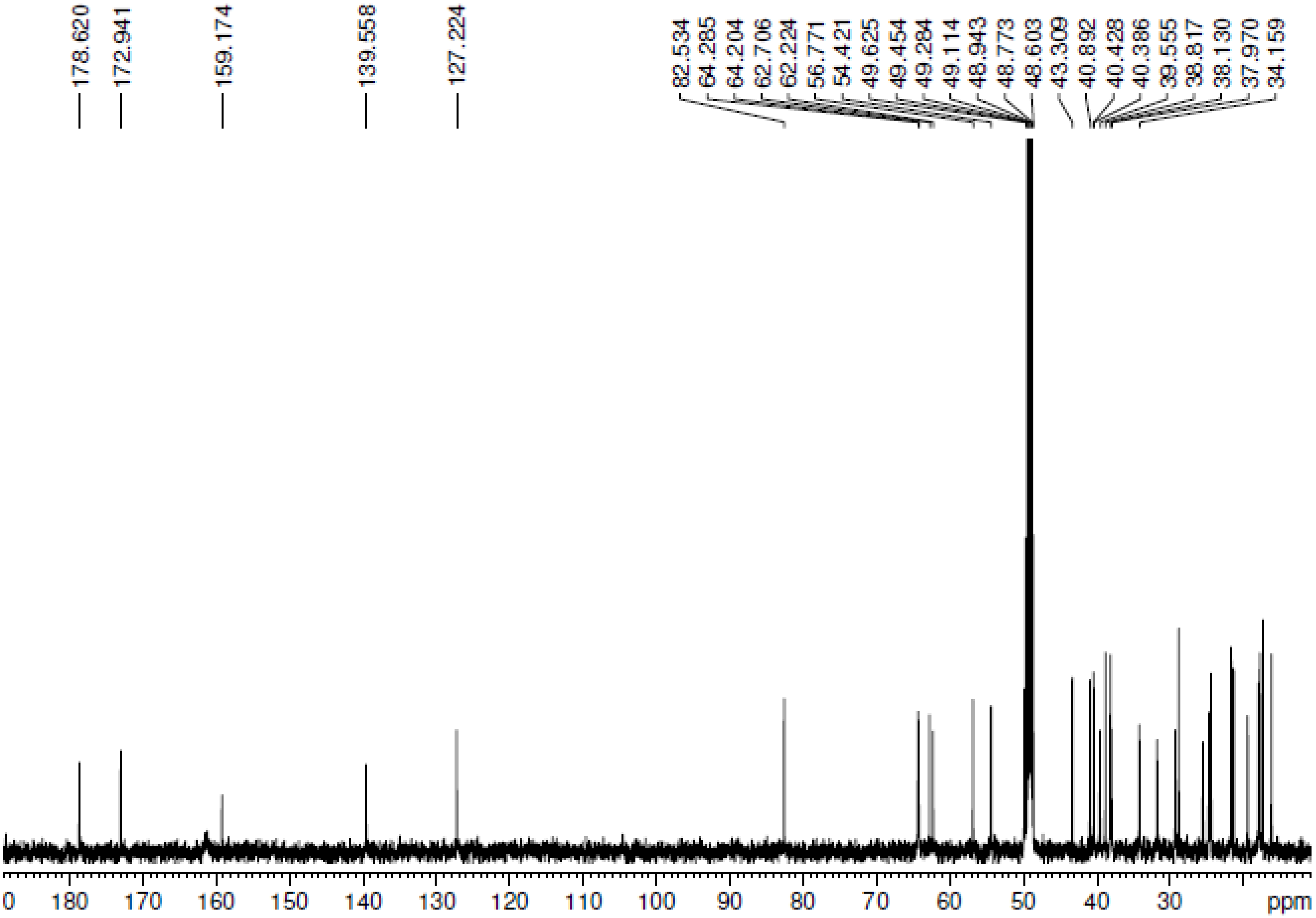


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-urs-12-en-28-oate trifluoroacetate (18b). ^{1}H NMR spectra (MeOD)

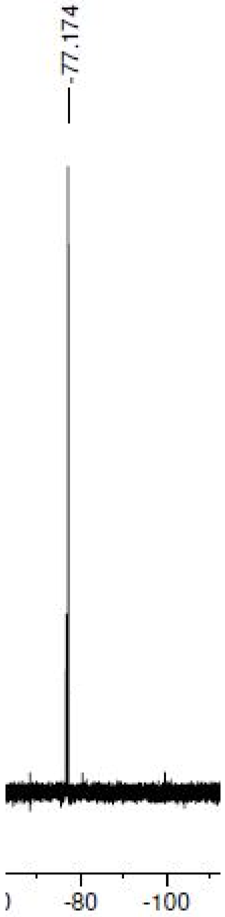




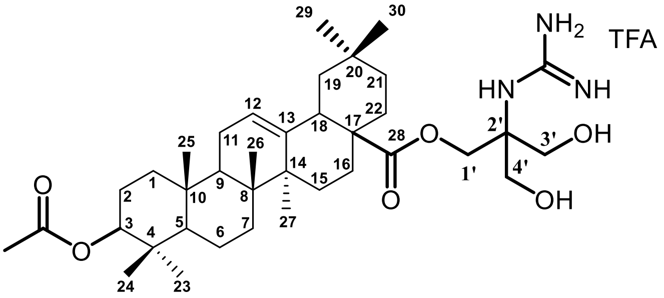
3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-urs-12-en-28-oate trifluoroacetate (18b). ^{13}C NMR spectra (MeOD)

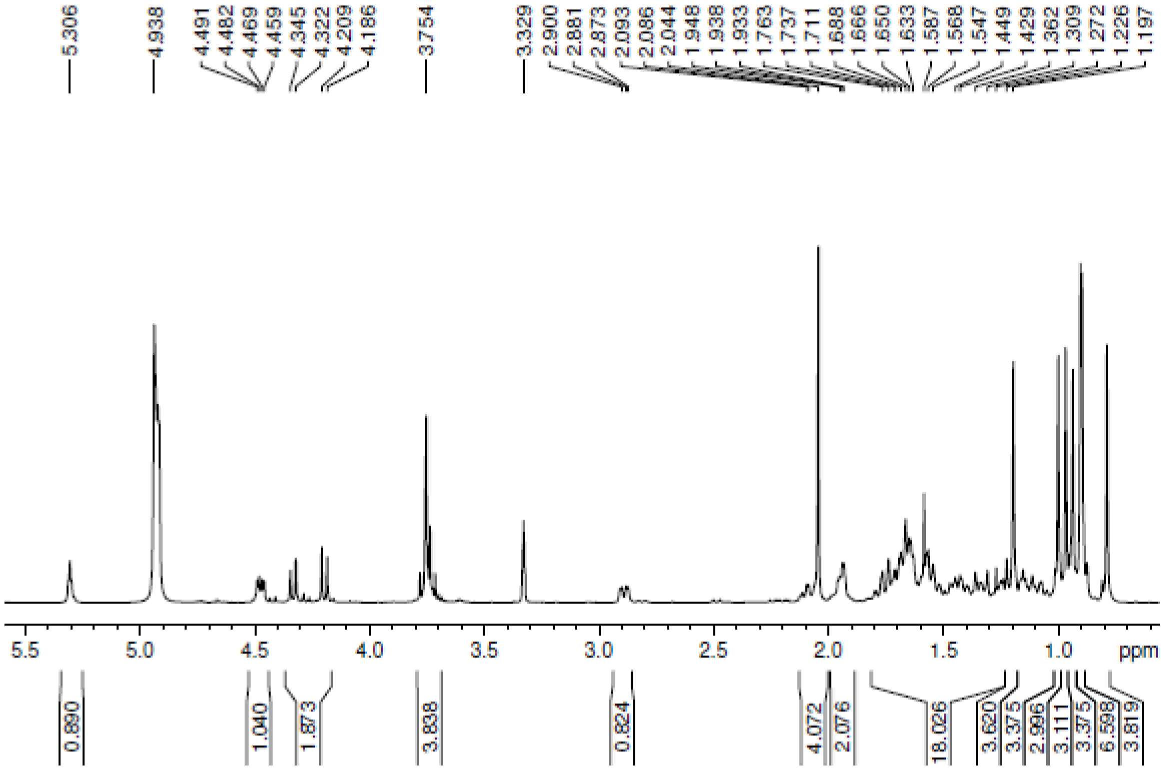


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-urs-12-en-28-oate trifluoroacetate (18b). ^{19}F NMR spectra (MeOD)

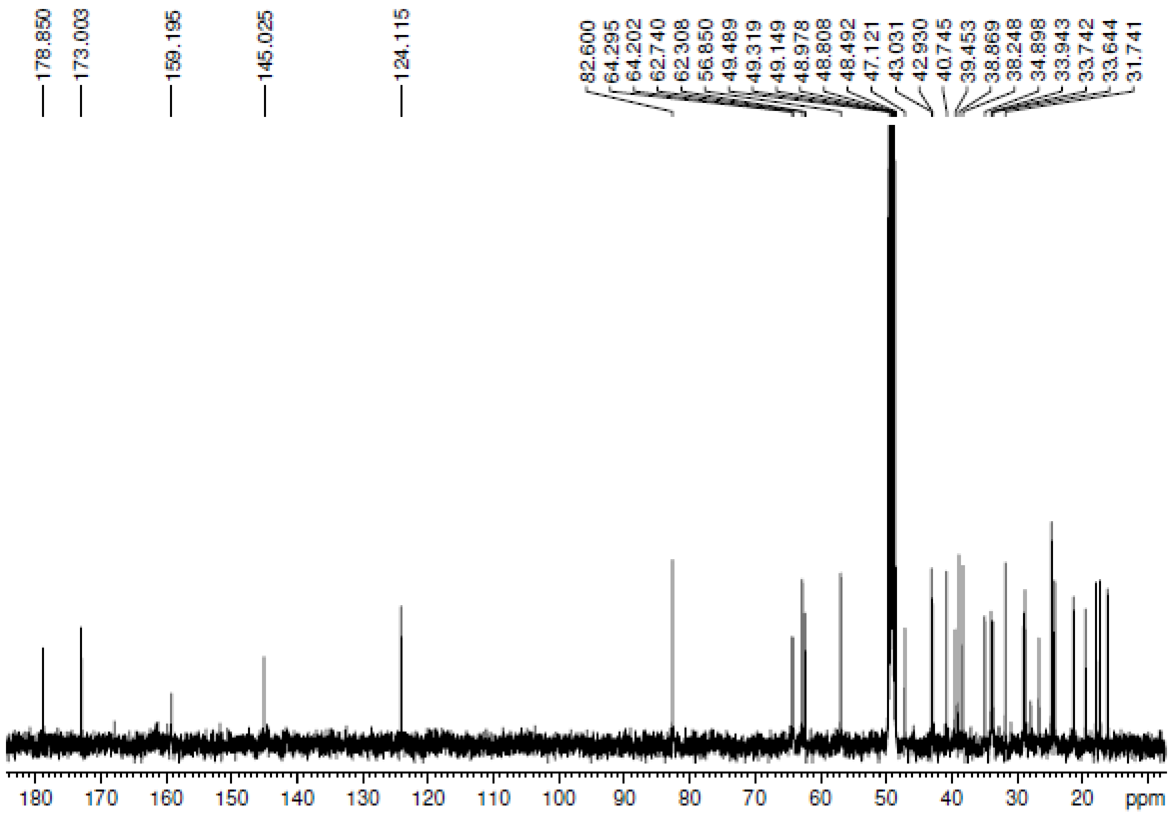


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-olean-12-en-28-oate trifluoroacetate (20b). ^{1}H NMR spectra (MeOD)

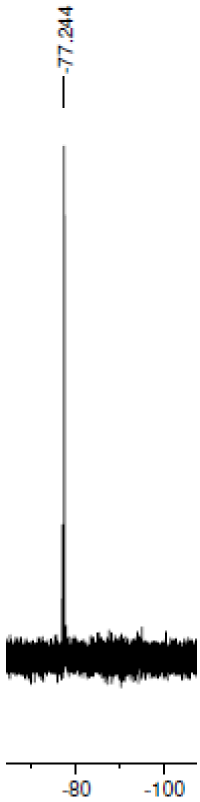




3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-olean-12-en-28-oate trifluoroacetate (20b). ^{13}C NMR spectra (MeOD)

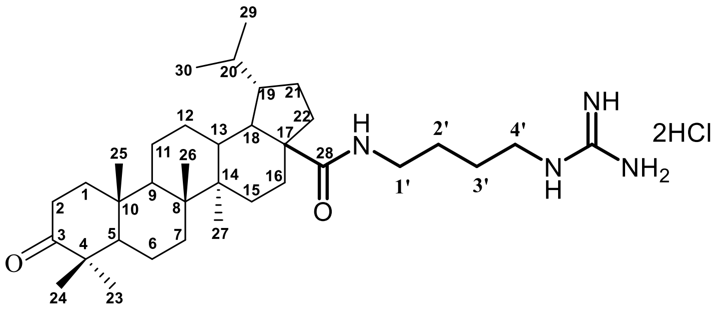


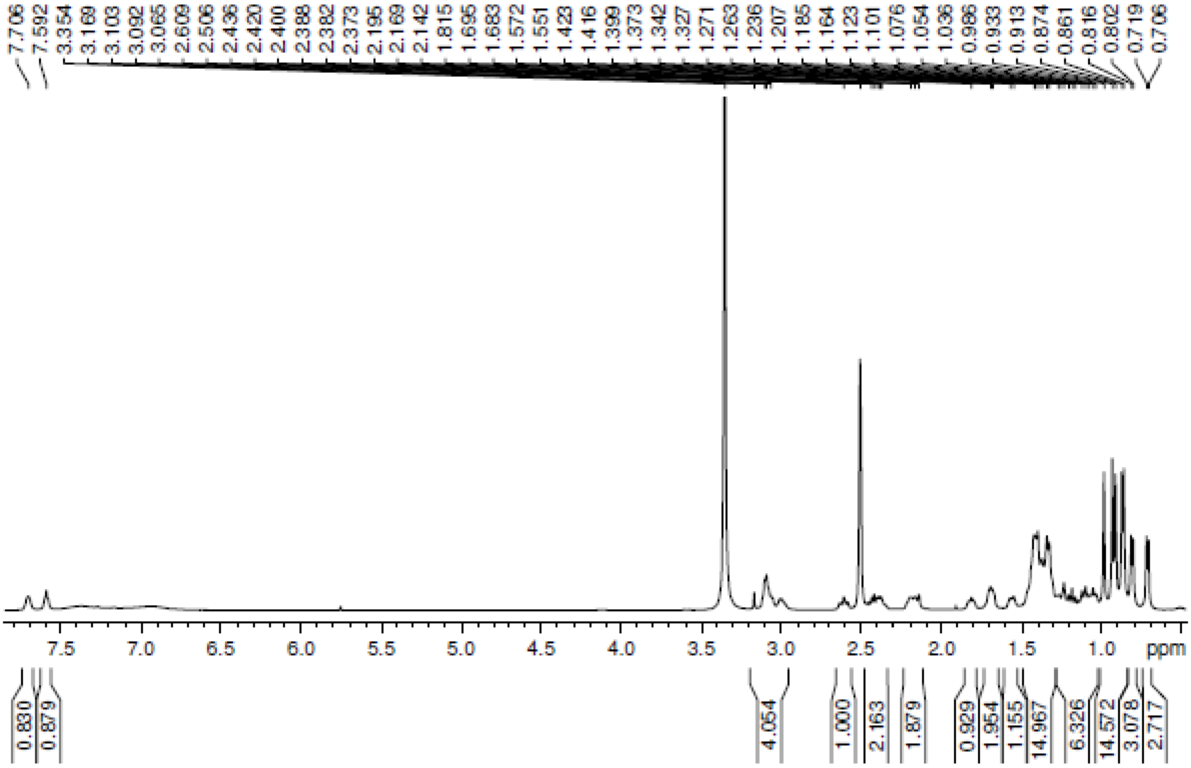
3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl- olean -12-en-28-oate trifluoroacetate (20b). ^{19}F NMR spectra (MeOD)



N-(4-buthylgyanidine)-3-oxolupane-28-amide dihydrochloride (9b).

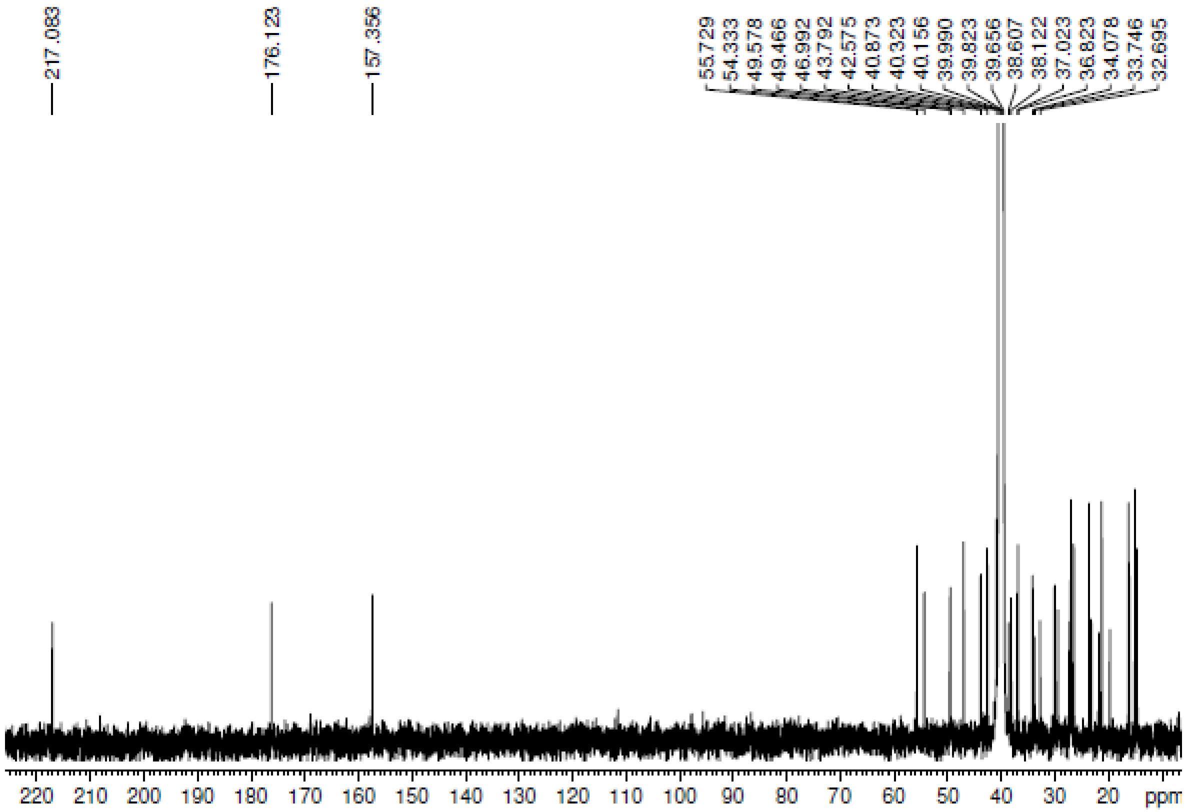
^{1}H NMR spectra (d$_6$-DMSO)





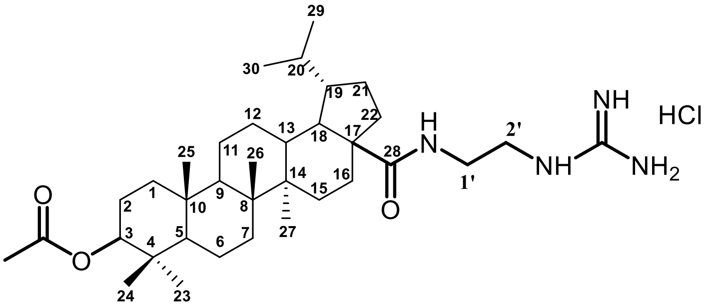
N-(4-buthylgyanidine)-3-oxolupane-28-amide dihydrochloride (9b).

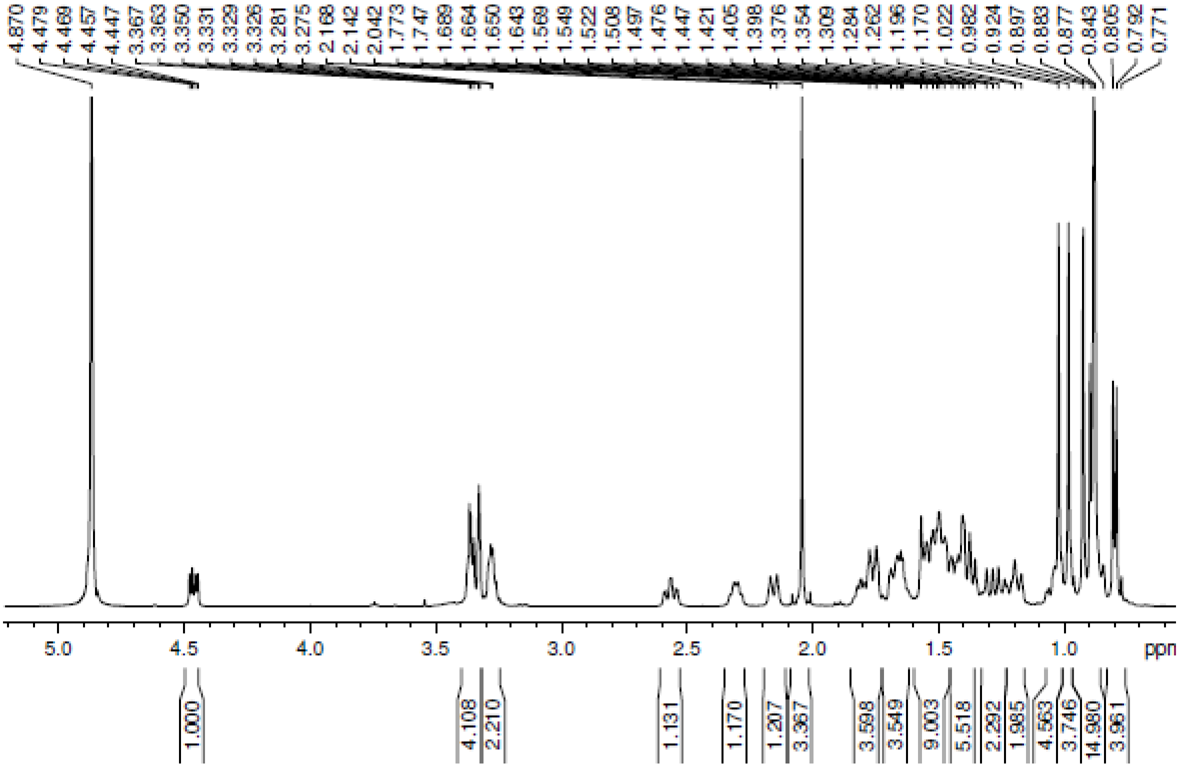
^{13}C NMR spectra (d$_6$-DMSO)



3β-N-(2-ethylgyanidine)-3-O-acetyl-lupane-28-amide hydrochloride (10b).

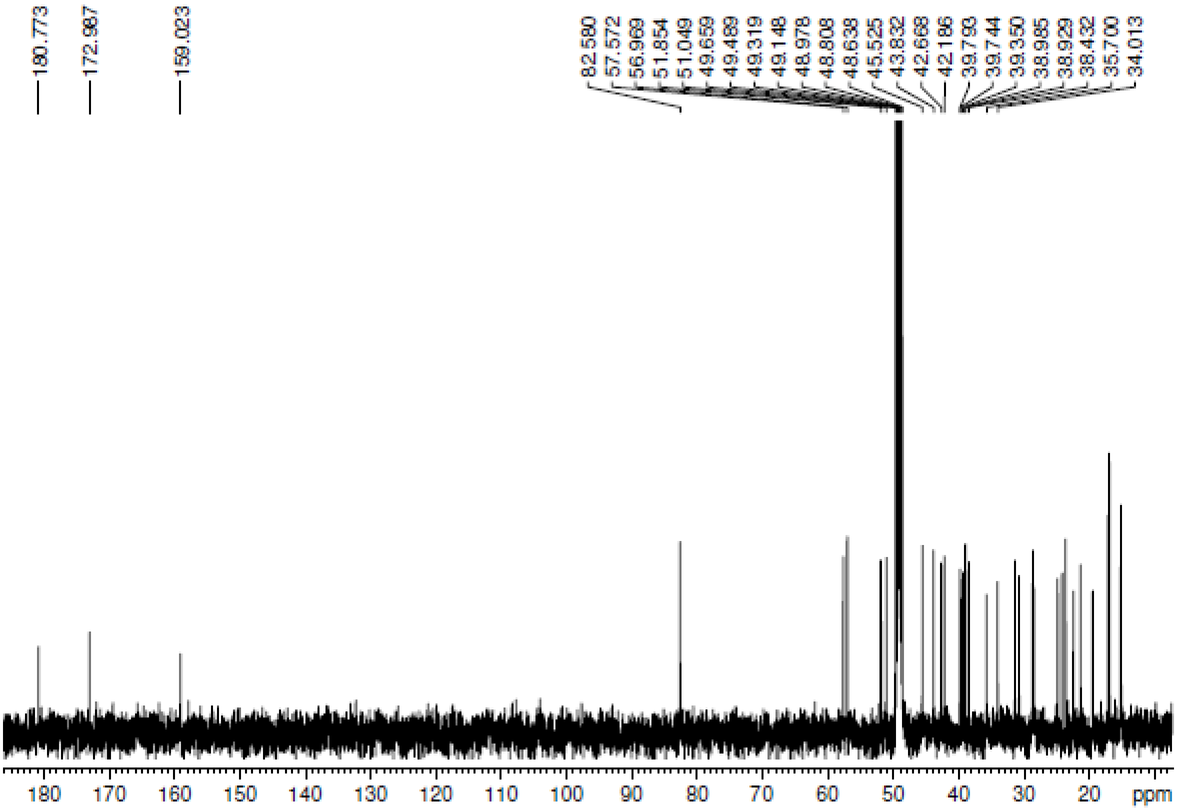
^{1}H NMR spectra (MeOD)





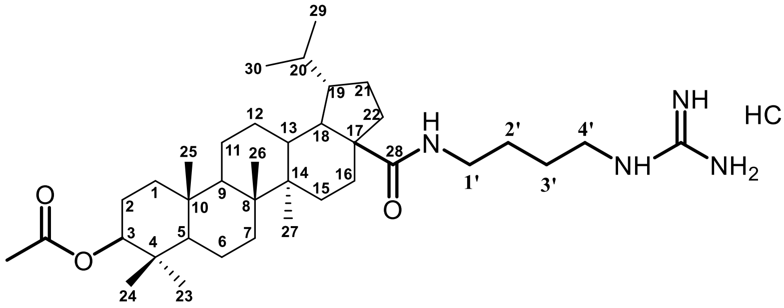
3β-N-(2-ethylgyanidine)-3-O-acetyl-lupane-28-amide hydrochloride (10b).

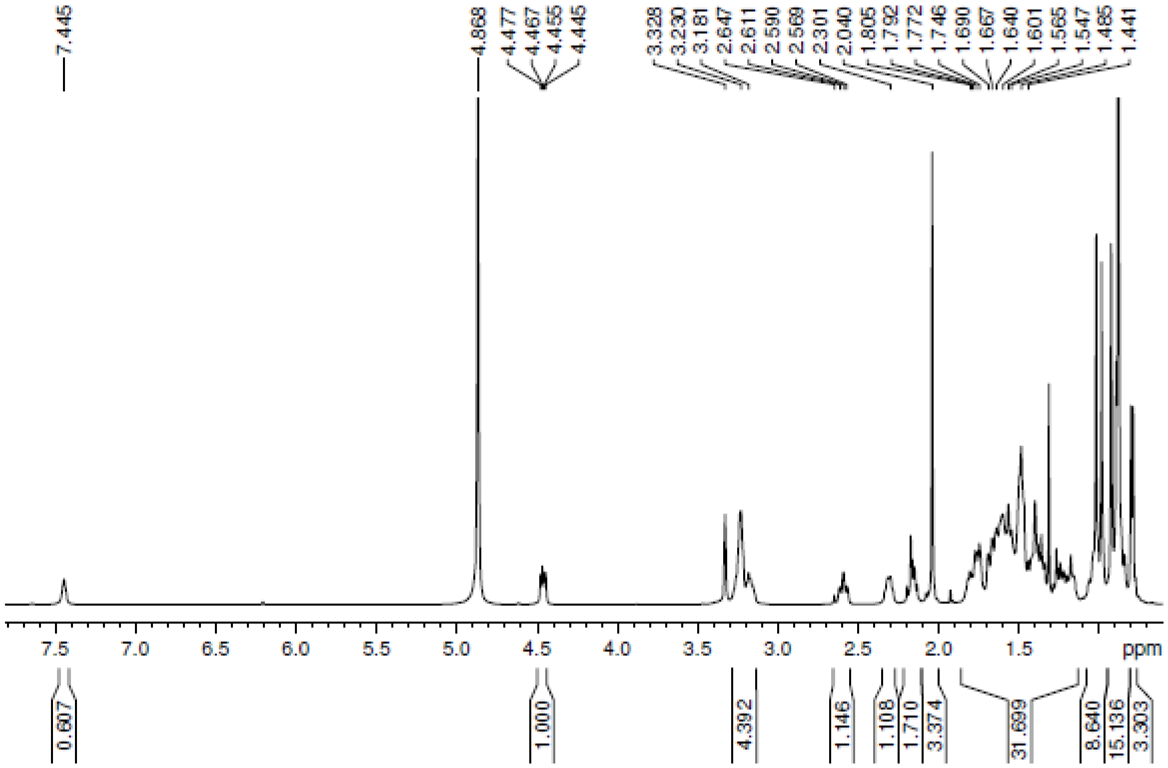
^{1}H NMR spectra (MeOD)



3β-N-(4-buthylgyanidine)-3-O-acetyl-lupane-28-amide hydrochloride (11b).

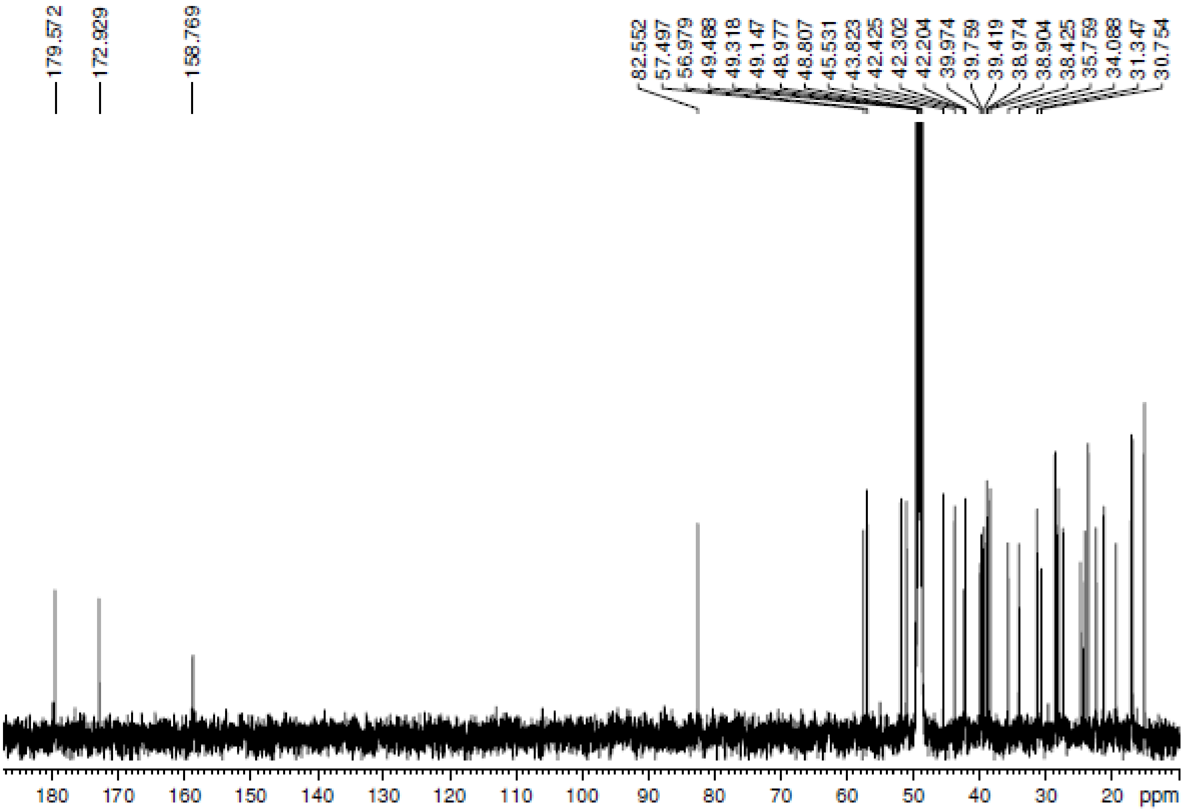
^{1}H NMR spectra (MeOD)





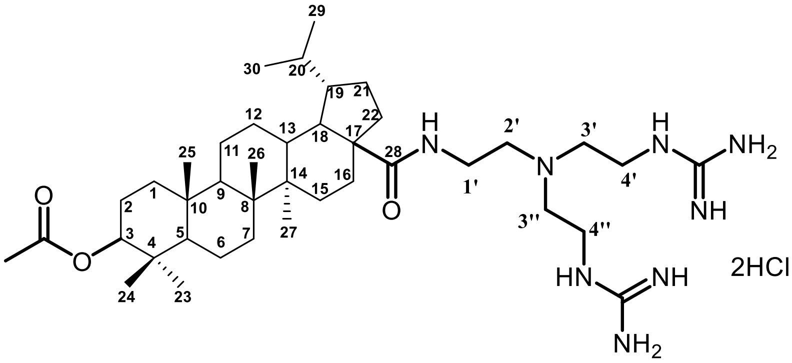
3β-N-(4-buthylgyanidine)-3-O-acetyl-lupane-28-amide hydrochloride (11b).

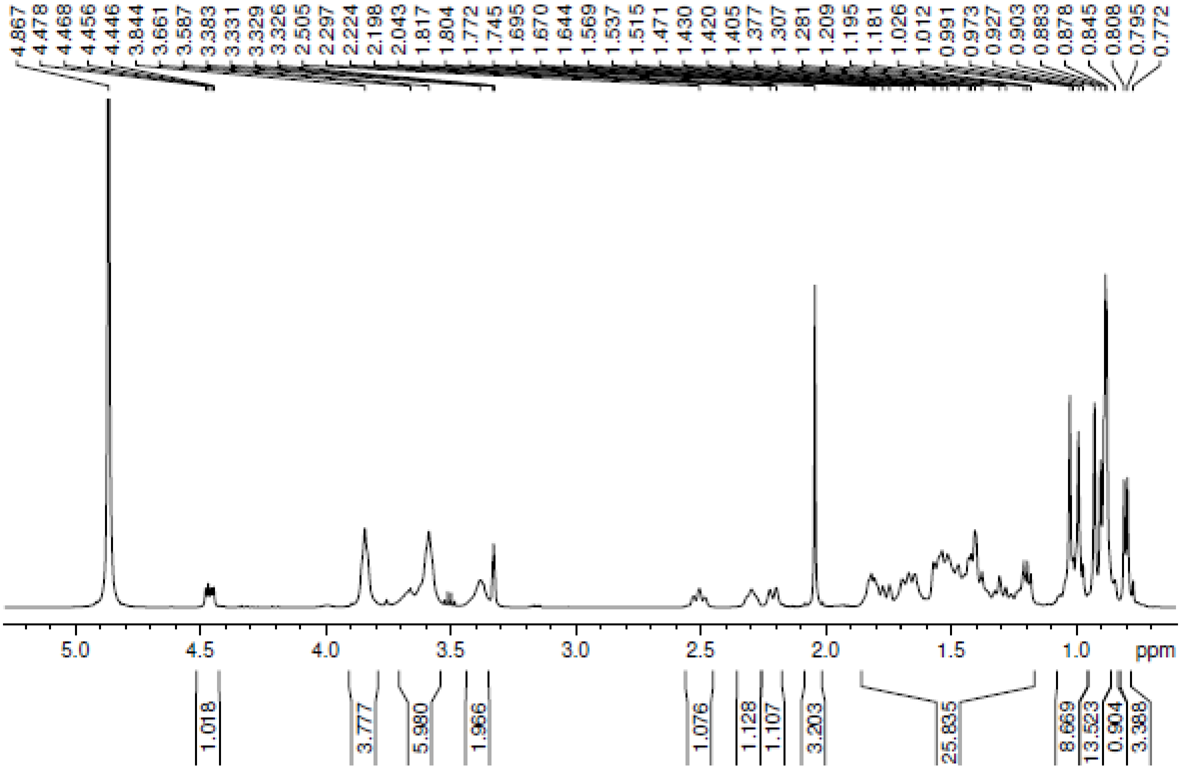
^{13}C NMR spectra (MeOD)



3β-N-[2-(N,N’-bis-ethylgyanidine)-ethyl]-3-O-acetyl-lupane-28-amide dihydrochloride (12b).

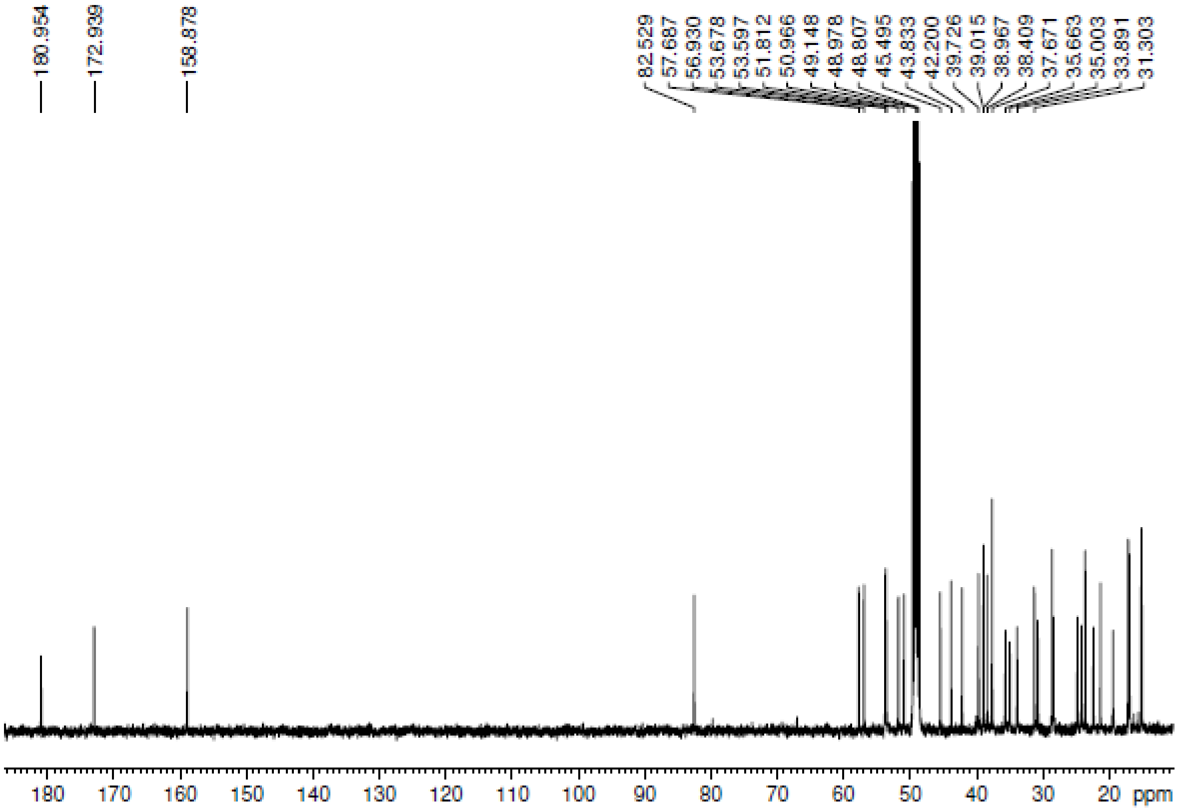
^{1}H NMR spectra (MeOD)



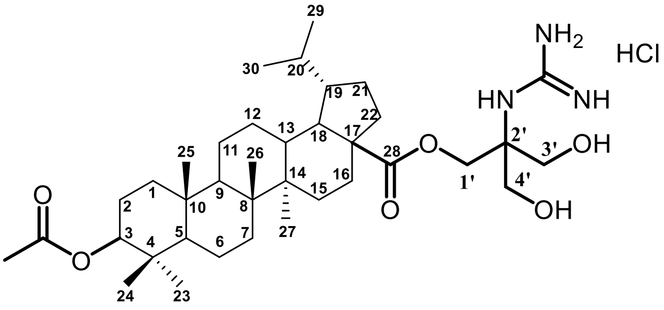


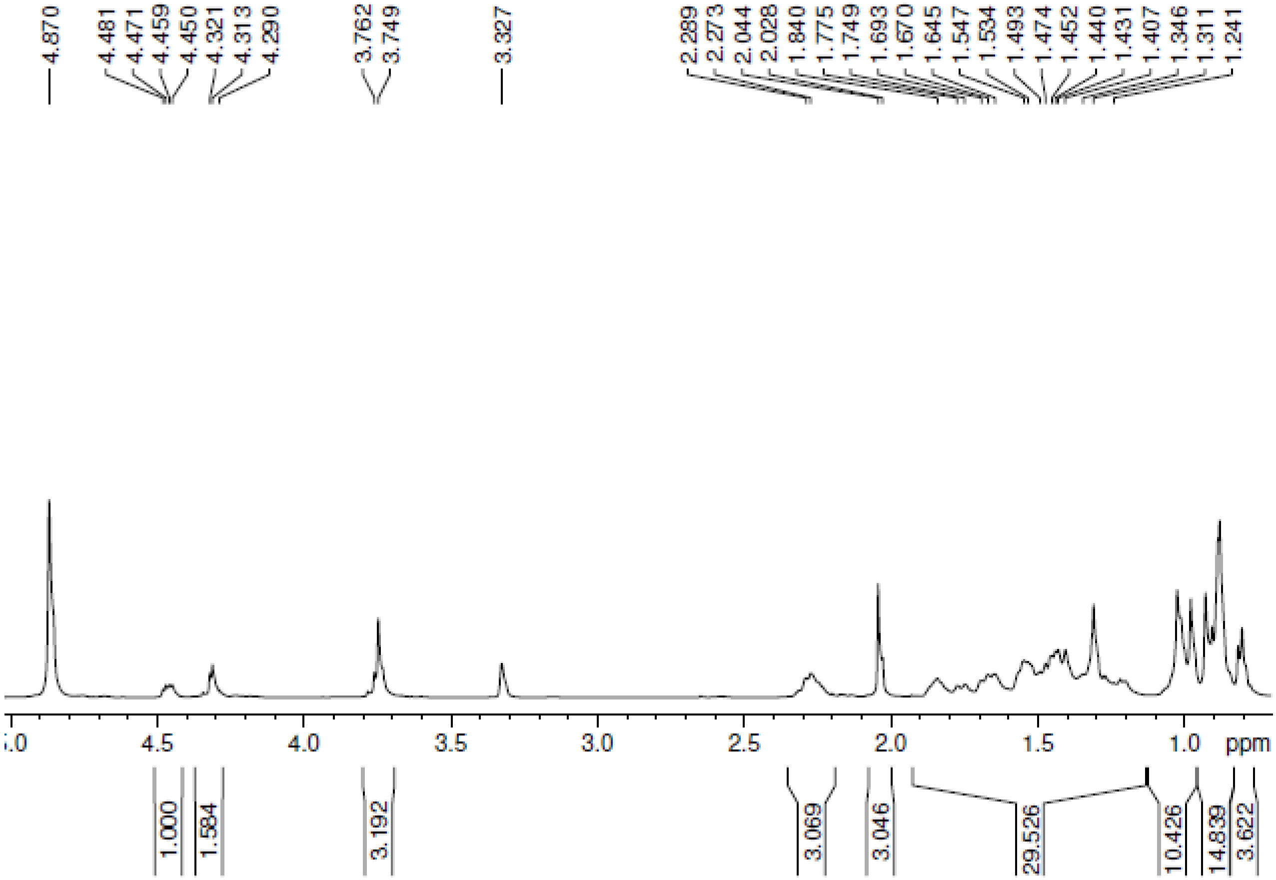
3β-N-[2-(N,N’-bis-ethylgyanidine)-ethyl]-3-O-acetyl-lupane-28-amide dihydrochloride (12b).

^{13}C NMR spectra (MeOD)

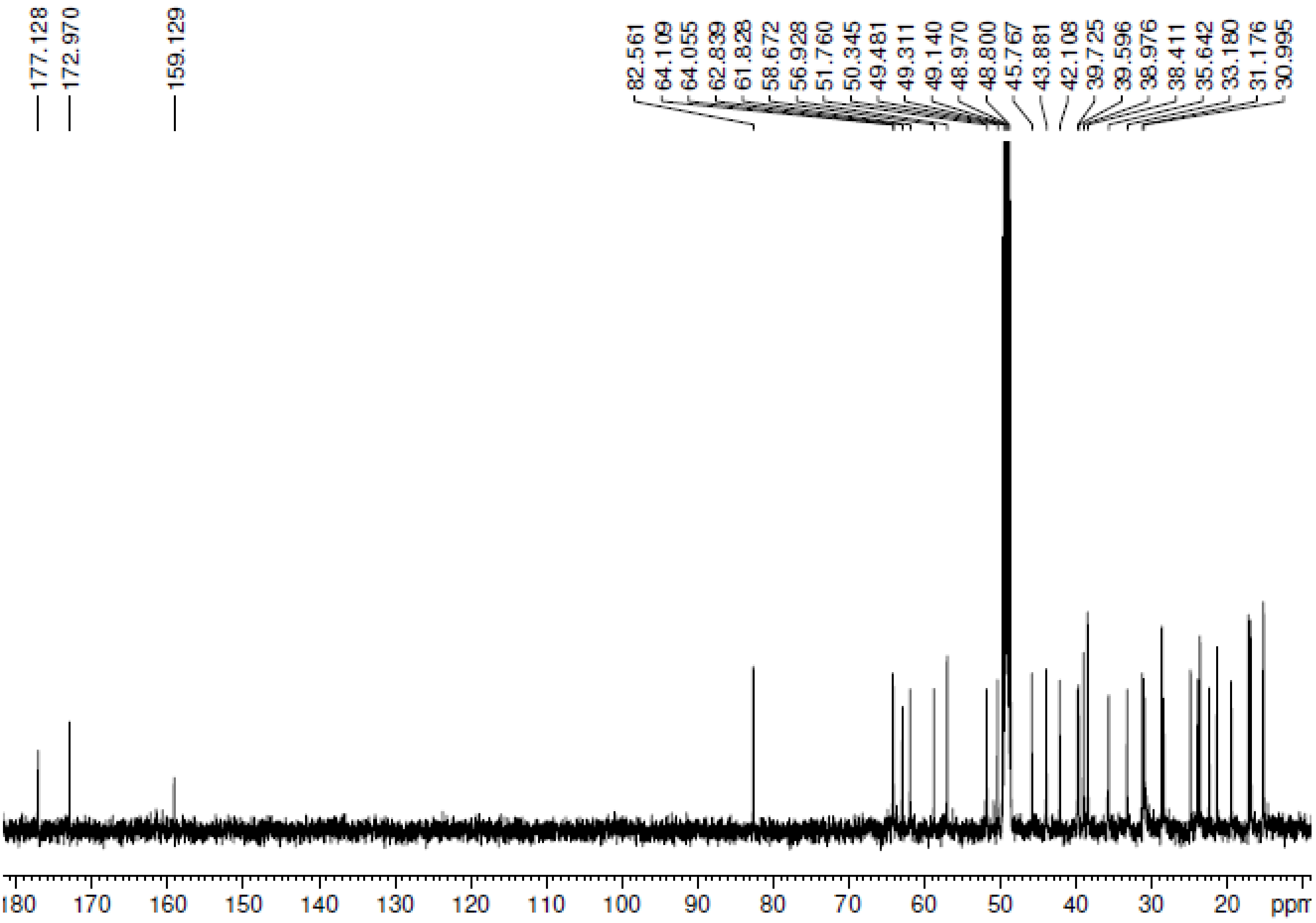


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-lupane-28-oate hydrochloride (15c). ^{1}H NMR spectra (MeOD)

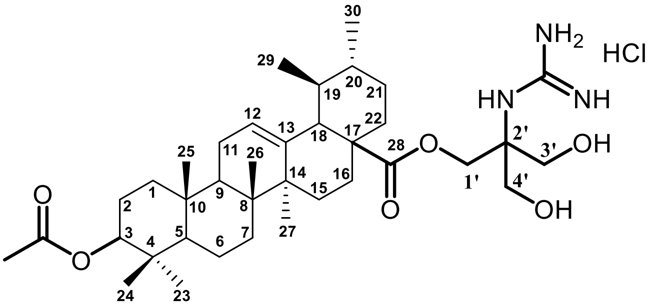


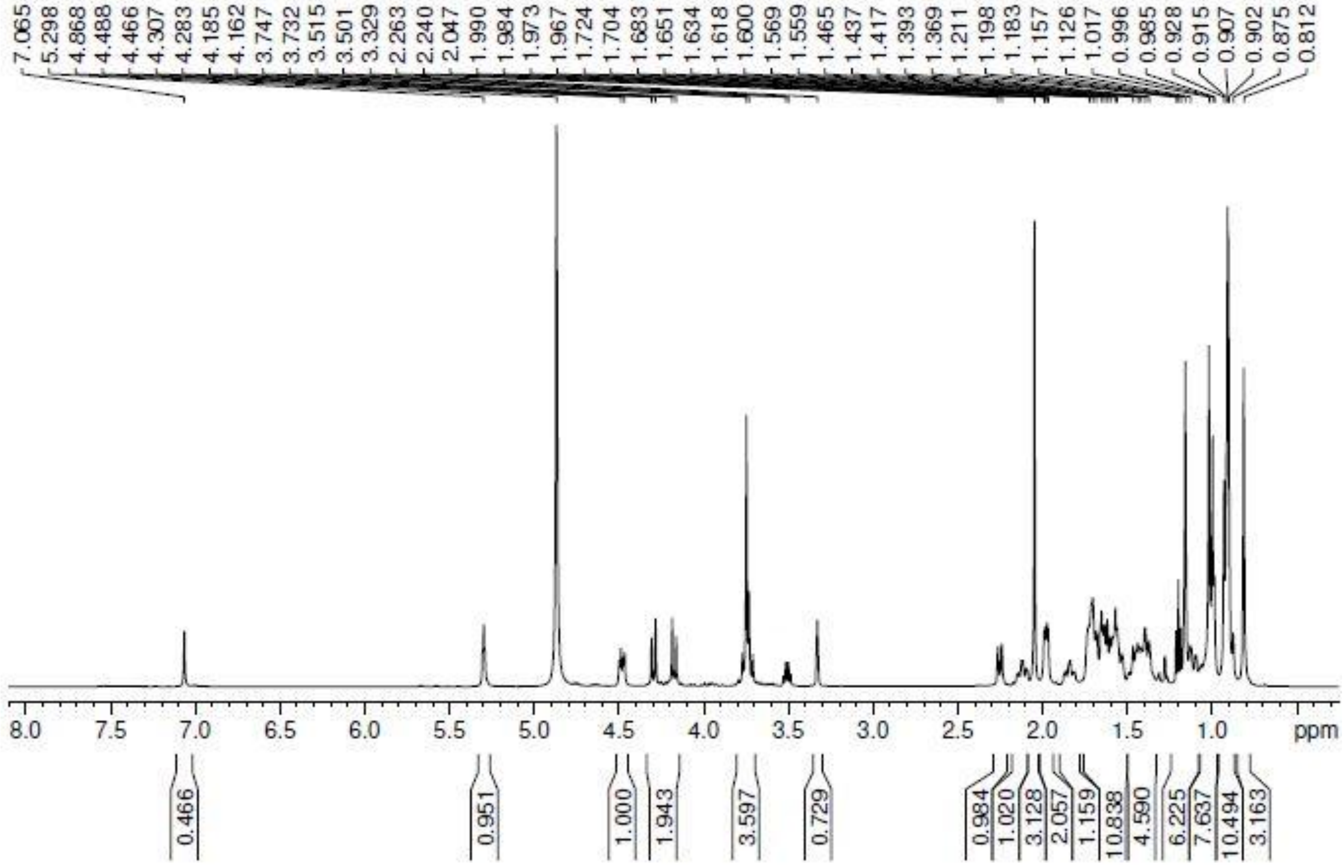


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-lupane-28-oate hydrochloride (15c).^{13}C NMR spectra (MeOD)

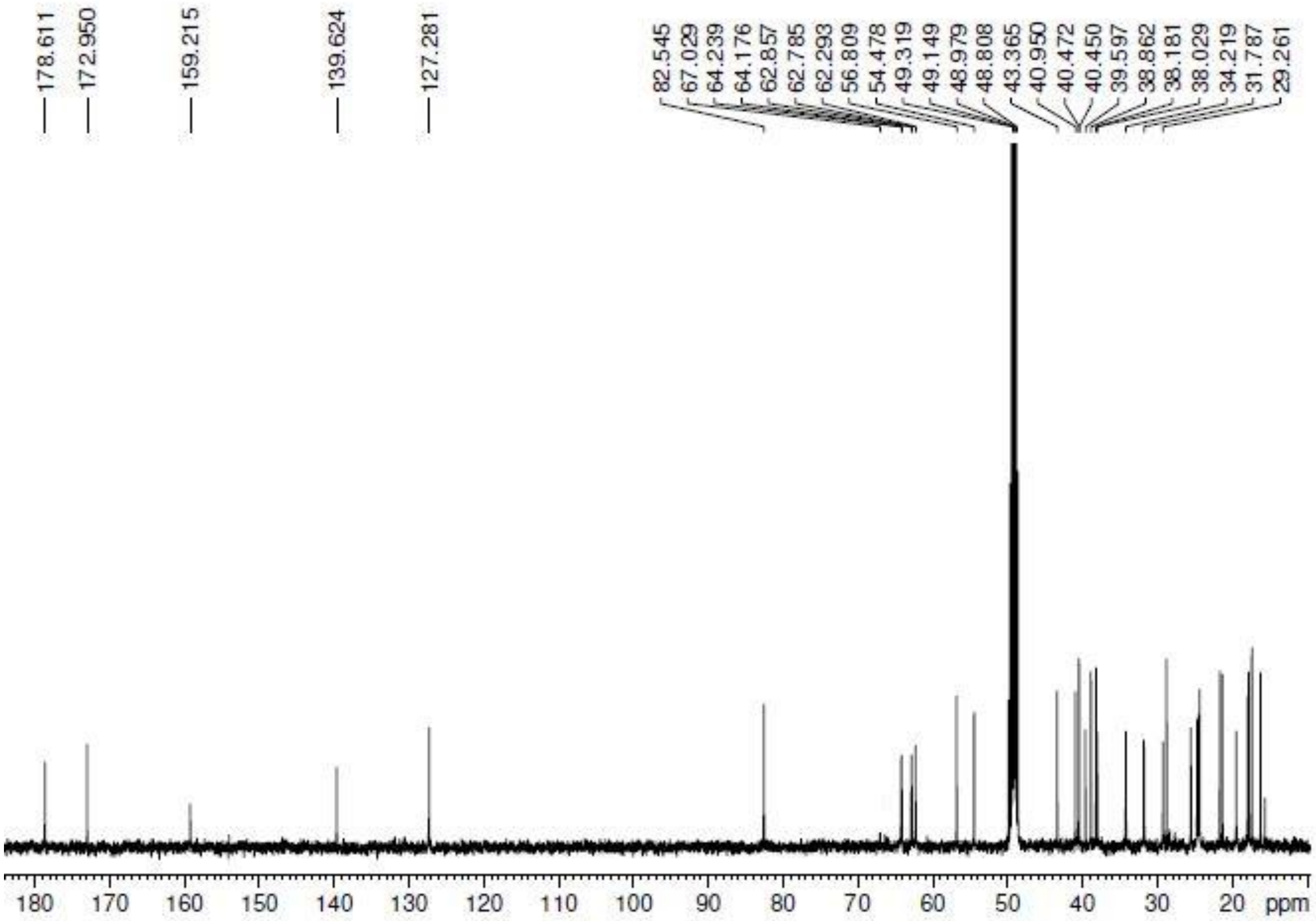


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-urs-12-en-28-oate hydrochloride (18c). ^{1}H NMR spectra (MeOD)

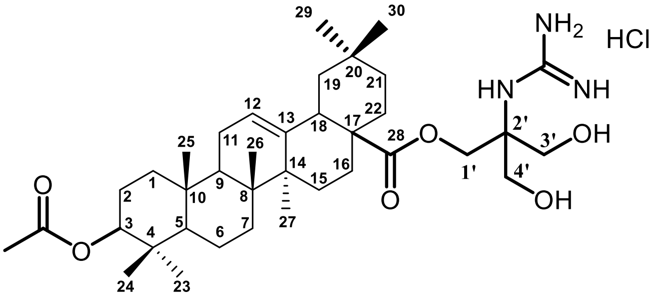


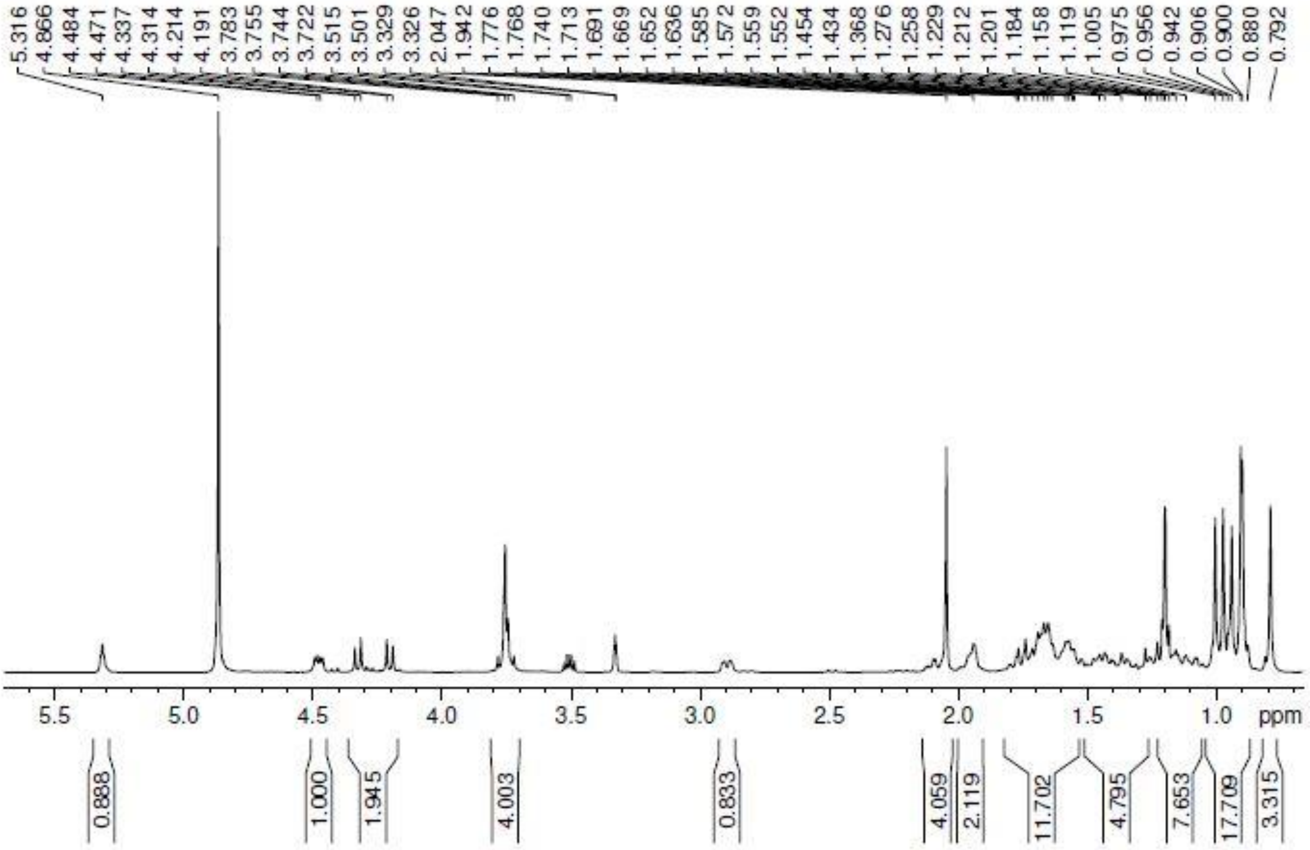


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-urs-12-en-28-oate hydrochloride (18c). ^{13}C NMR spectra (MeOD)

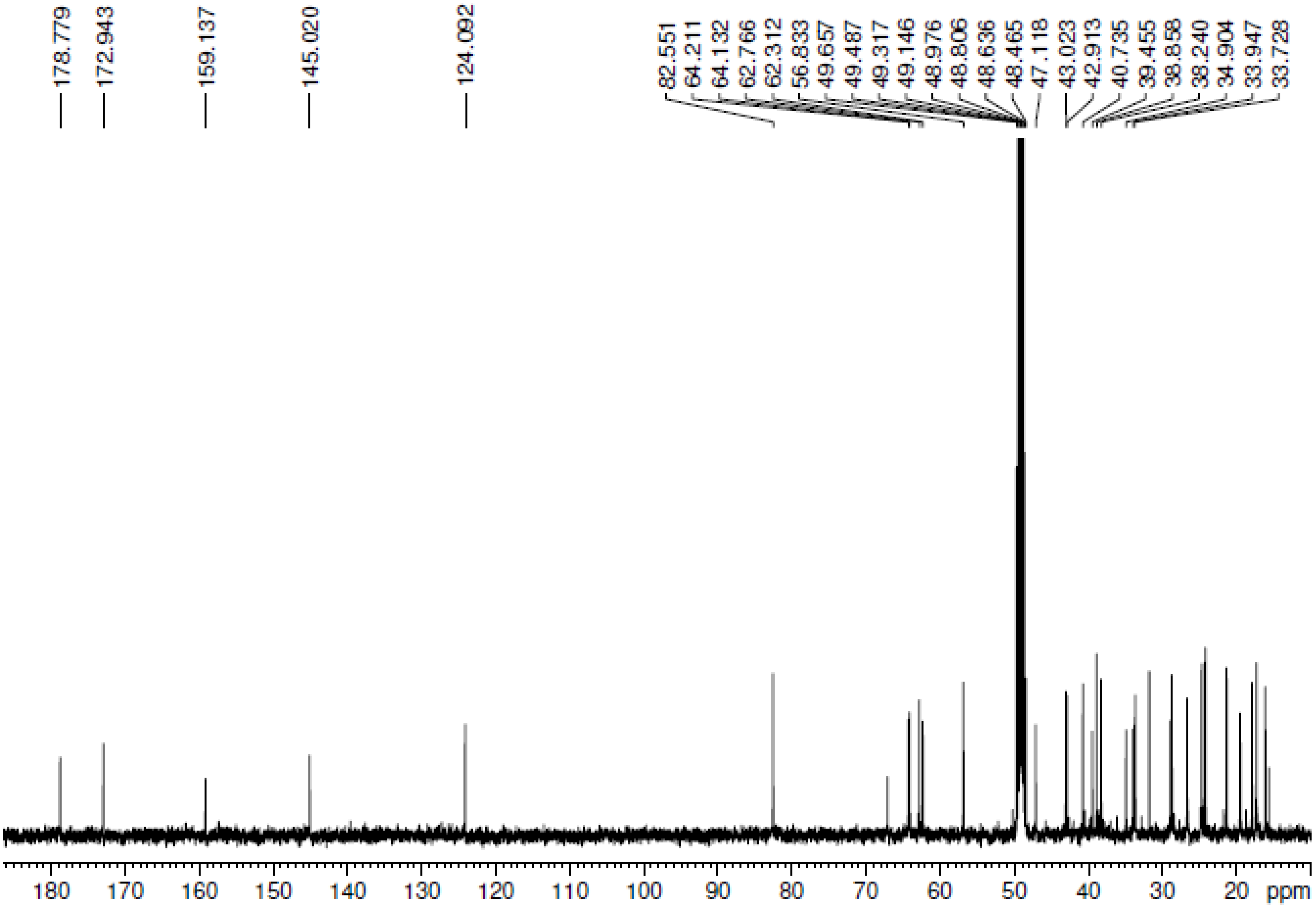


3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-olean-12-en-28-oate hydrochloride (20c). ^{1}H NMR spectra (MeOD)



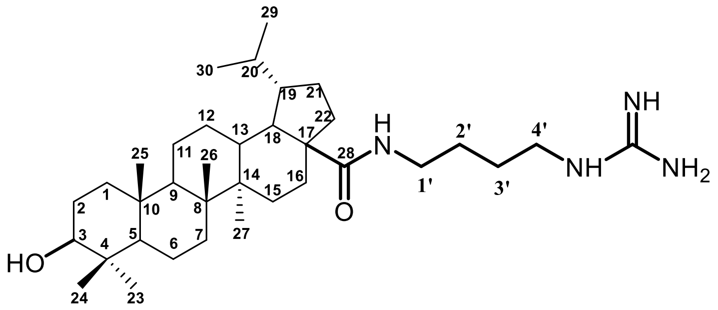


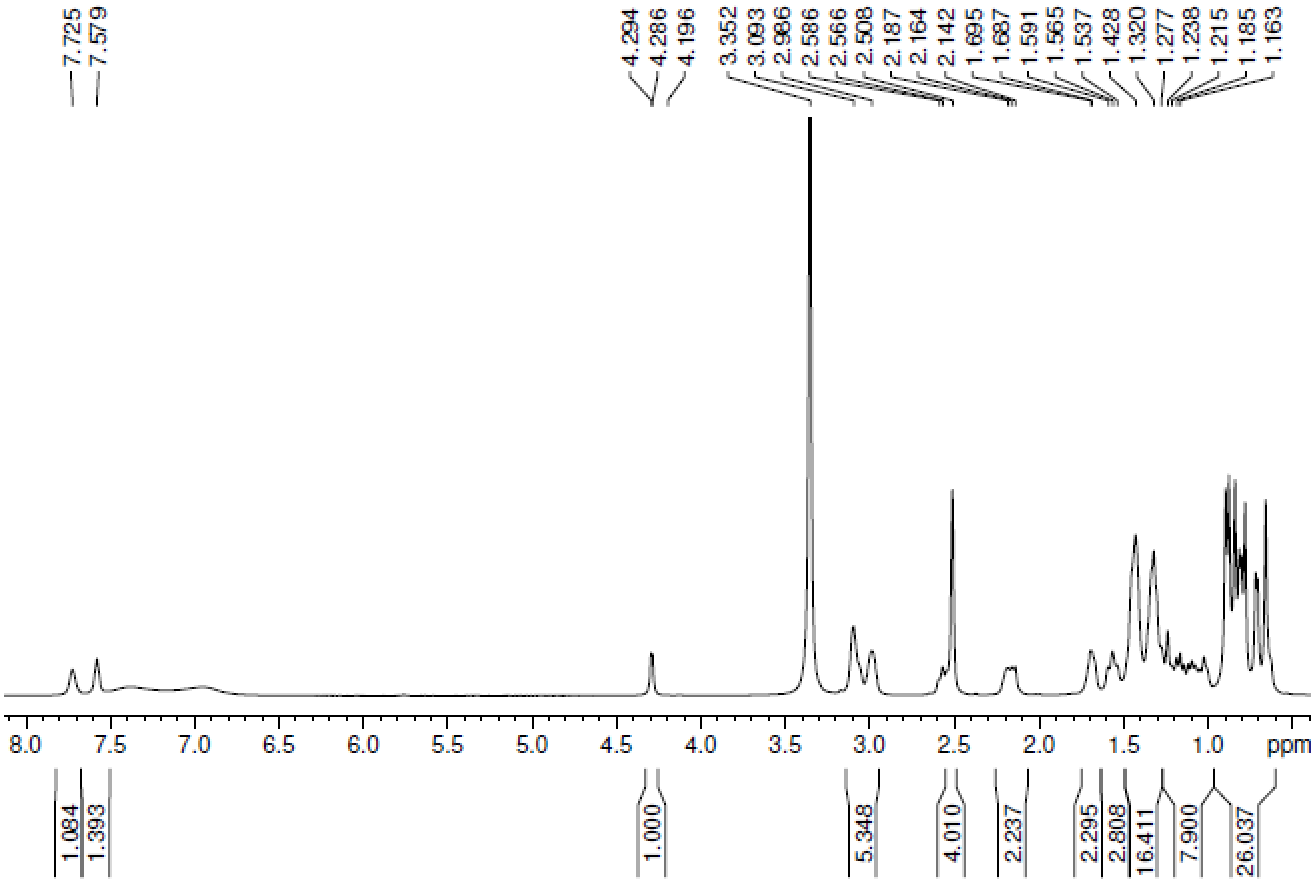
3β-[2-guanidine-3-hydroxy-2-(hydroxymethyl)propyl]-3-O-acetyl-olean-12-en-28-oate hydrochloride (20c). ^{13}C NMR spectra (MeOD)



3β-N-(4-buthylgyanidine)-3-hydroxy-lupane-28-amide (14).

^{1}H NMR spectra (d$_6$-DMSO)





3β-N-(4-buthylgyanidine)-3-hydroxy-lupane-28-amide (14).

^{13}C NMR spectra (d_6-DMSO)