

A hydrophilic conjugate Approach toward the design and synthesis of Ursolic acid derivatives as potential antidiabetic agent

TianMing Huang[†], PanPan Wu[†], AnMing Cheng, Jing Qin, Kun Zhang*, SuQing Zhao*

Supplementary Data

Copies of ¹H NMR and ¹³C NMR spectra of compounds **3–6, 9-11, 12-20**

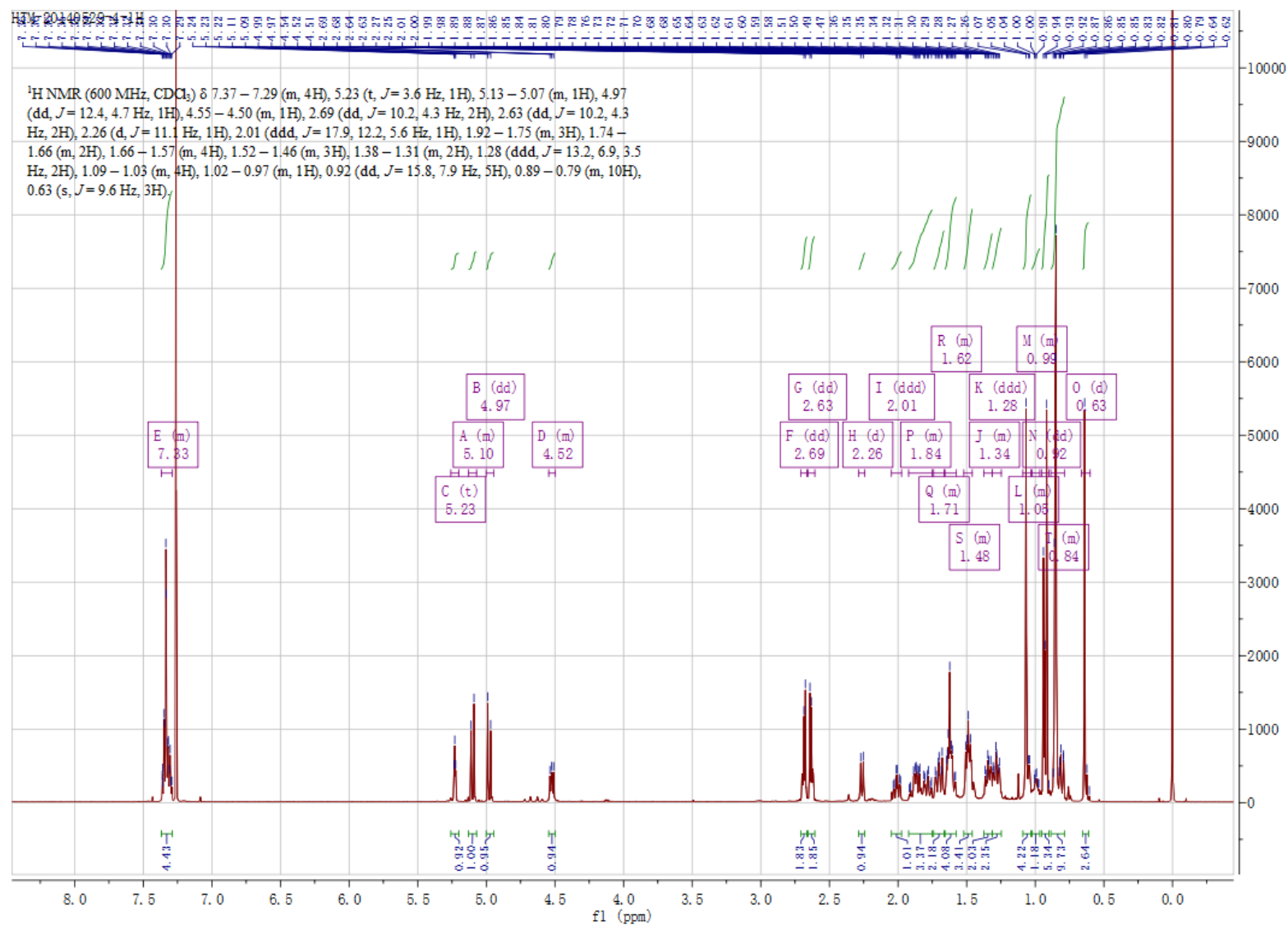


Figure 1 ¹H NMR spectrum (CDCl₃, 600 MHz) of 3β-[(3-carboxy)propionyloxy]-urs-12-en-28-oic acid benzyl ester (compound **3**)

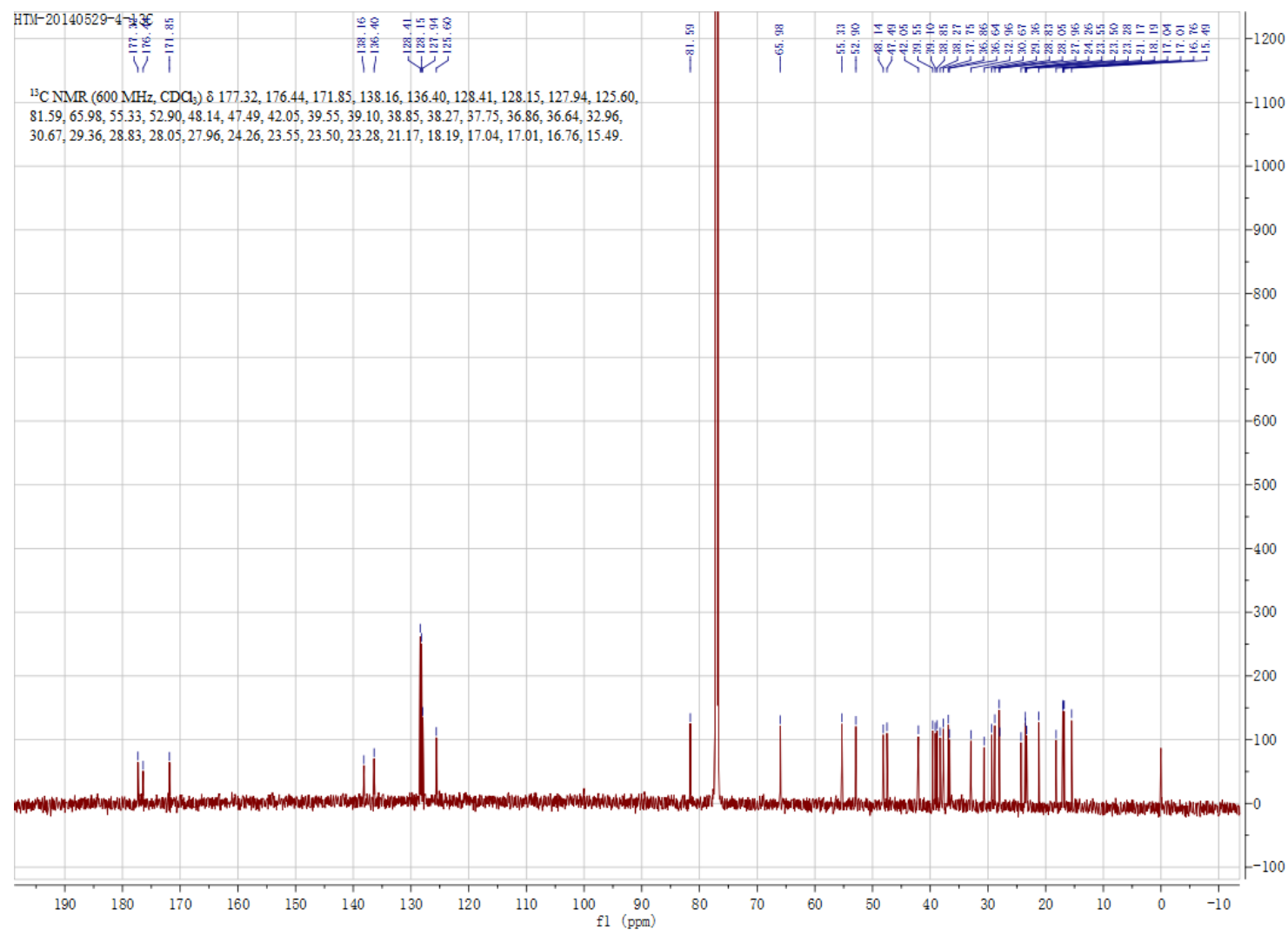


Figure 2 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of 3 β -(3-carboxy)propionyloxy]-urs-12-en-28-oic acid benzyl ester (compound 3)

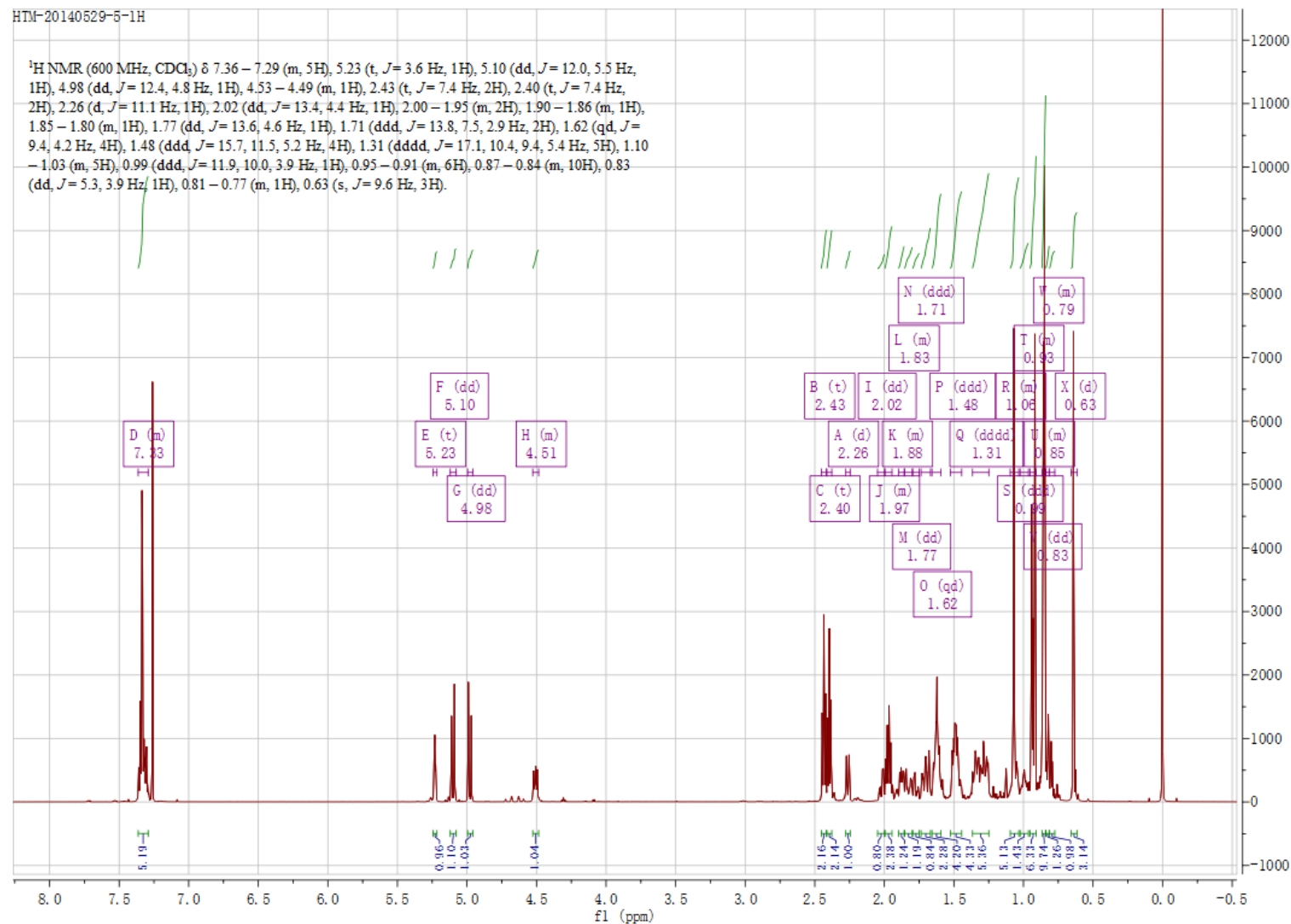


Figure 3 ¹H NMR spectrum (CDCl₃, 600 MHz) of 3β-[(3-carboxy)n-butyryloxy]-urs-12-en-28-oic acid benzyl ester (compound 4)

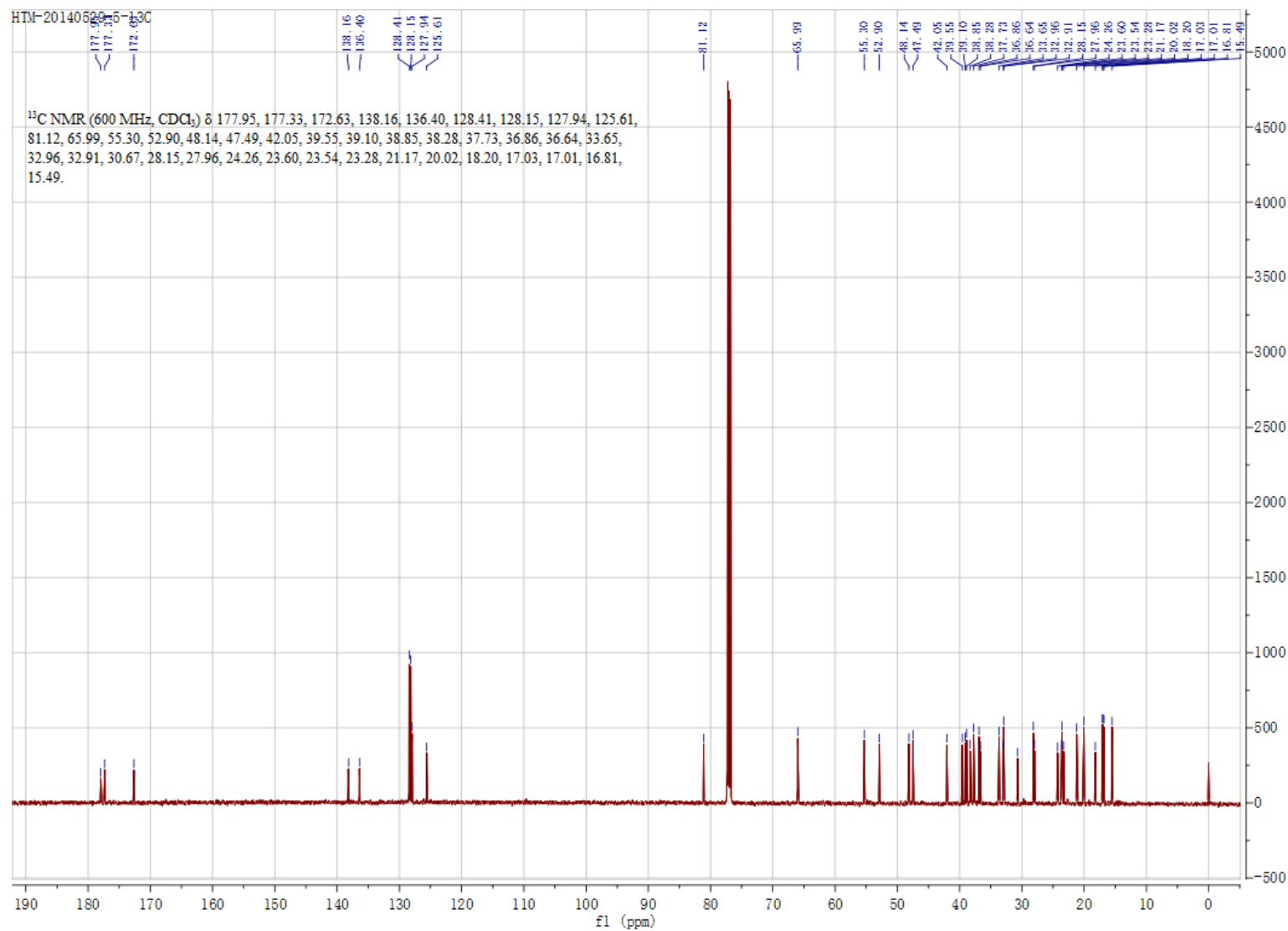


Figure 4 ¹³C NMR spectrum (CDCl₃, 600 MHz) of 3β-[(3-carboxy)n-butyryloxy]-urs-12-en-28-oic acid benzyl ester (compound **4**)

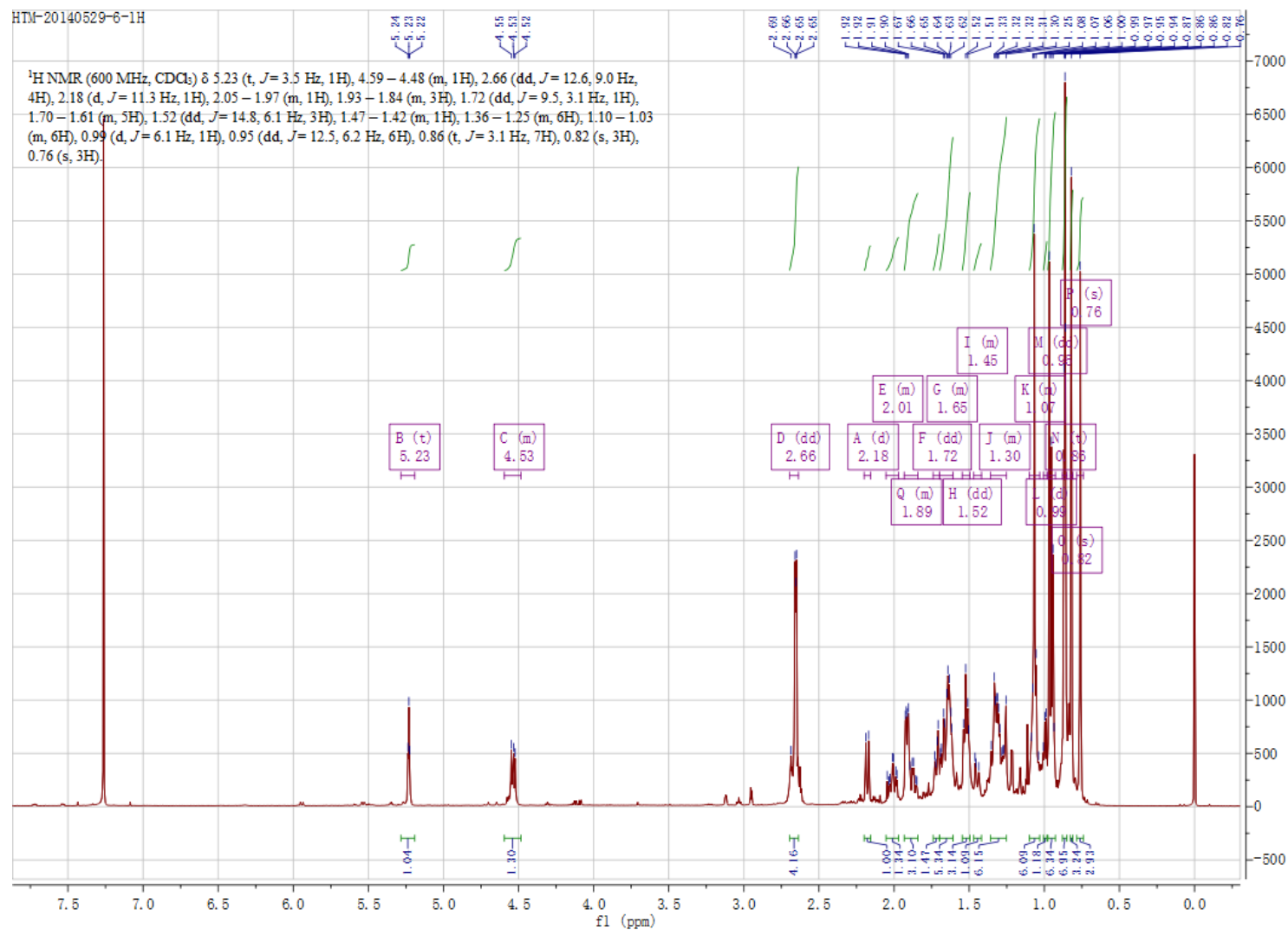


Figure 5 ¹H NMR spectrum (CDCl₃, 600 MHz) of 3β-[(3-carboxy)propionyloxy]-urs-12-en-28-oic acid (compound 5)

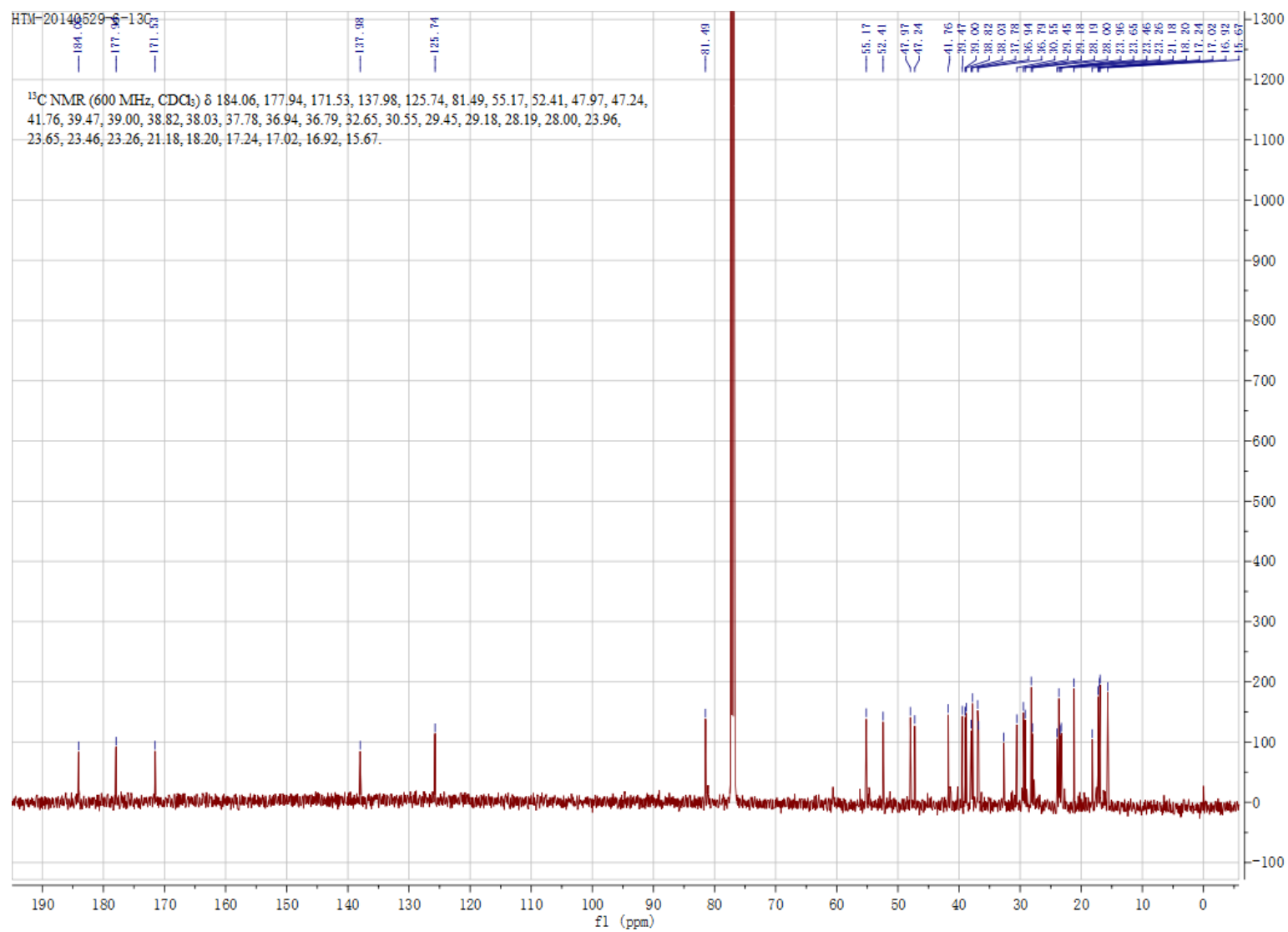


Figure 6 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of 3 β -[(3-carboxy)propionyloxy]-urs-12-en-28-oic acid (compound 5)

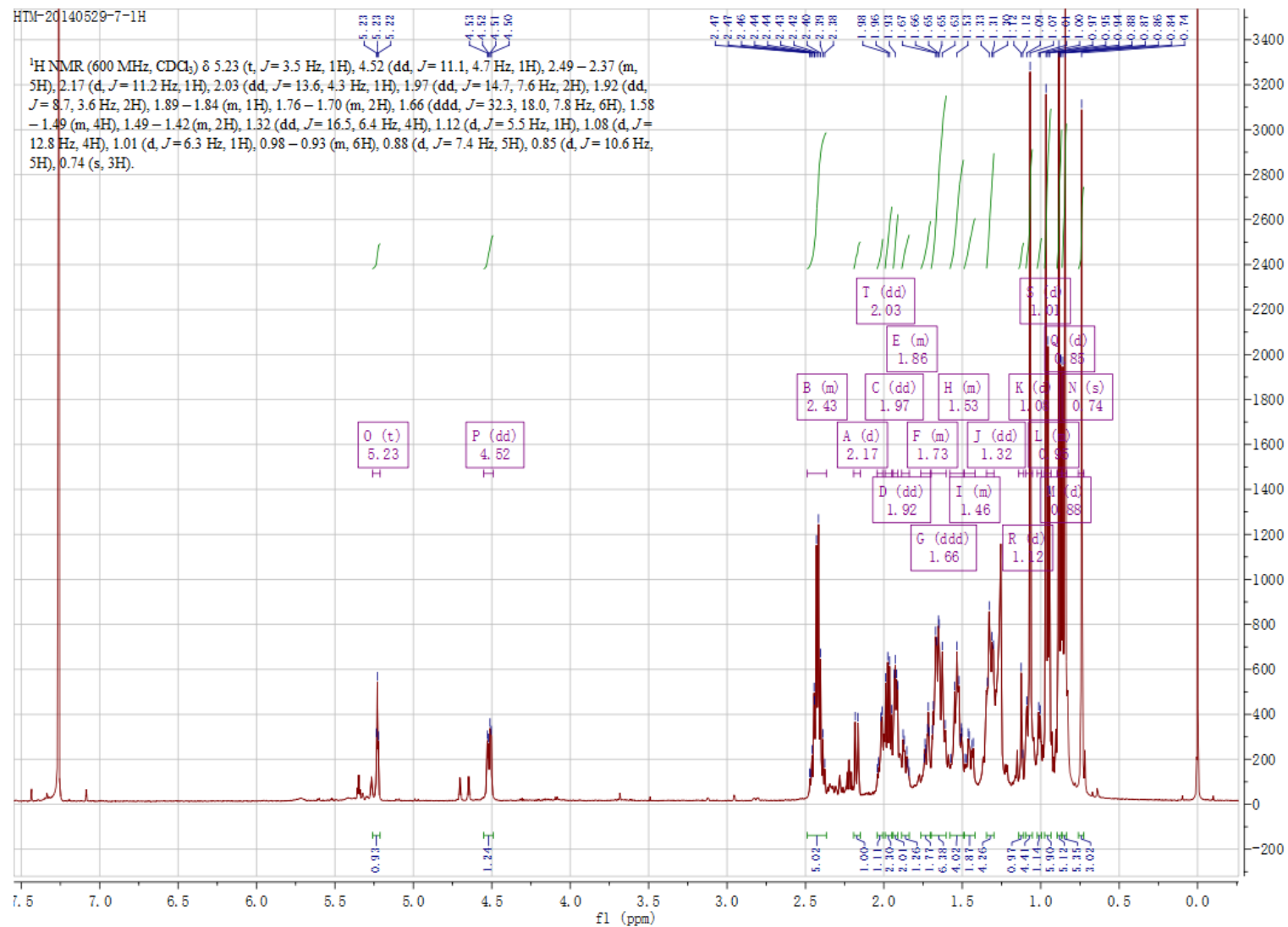


Figure 7 ¹H NMR spectrum (CDCl₃, 600 MHz) of 3β-[(3-carboxy)n-butyryloxy]-urs-12-en-28-oic acid (compound **6**)

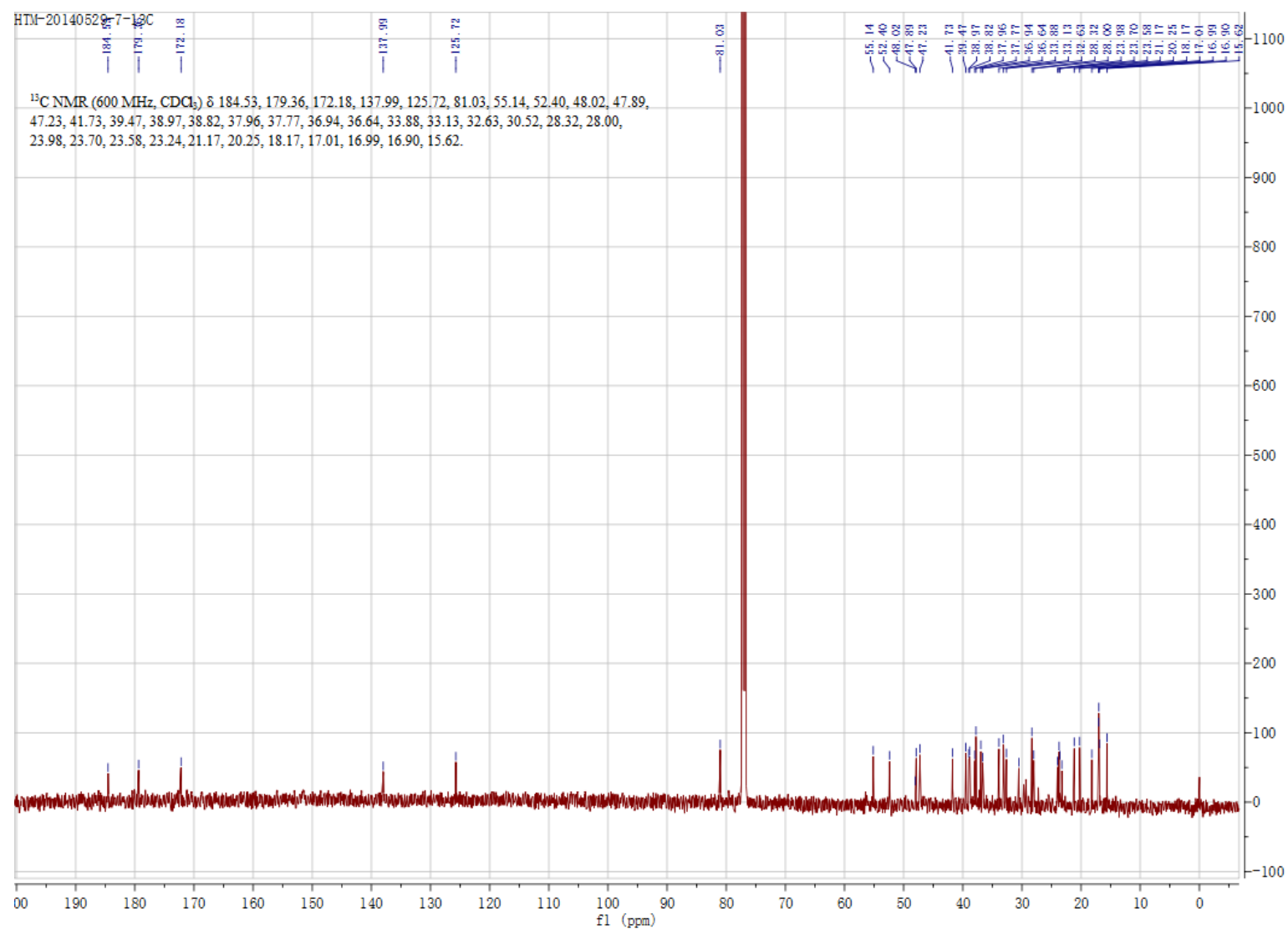


Figure 8 ¹³C NMR spectrum (CDCl₃, 600 MHz) of 3β-[(3-carboxy)n-butyryloxy]-urs-12-en-28-oic acid (compound 6)

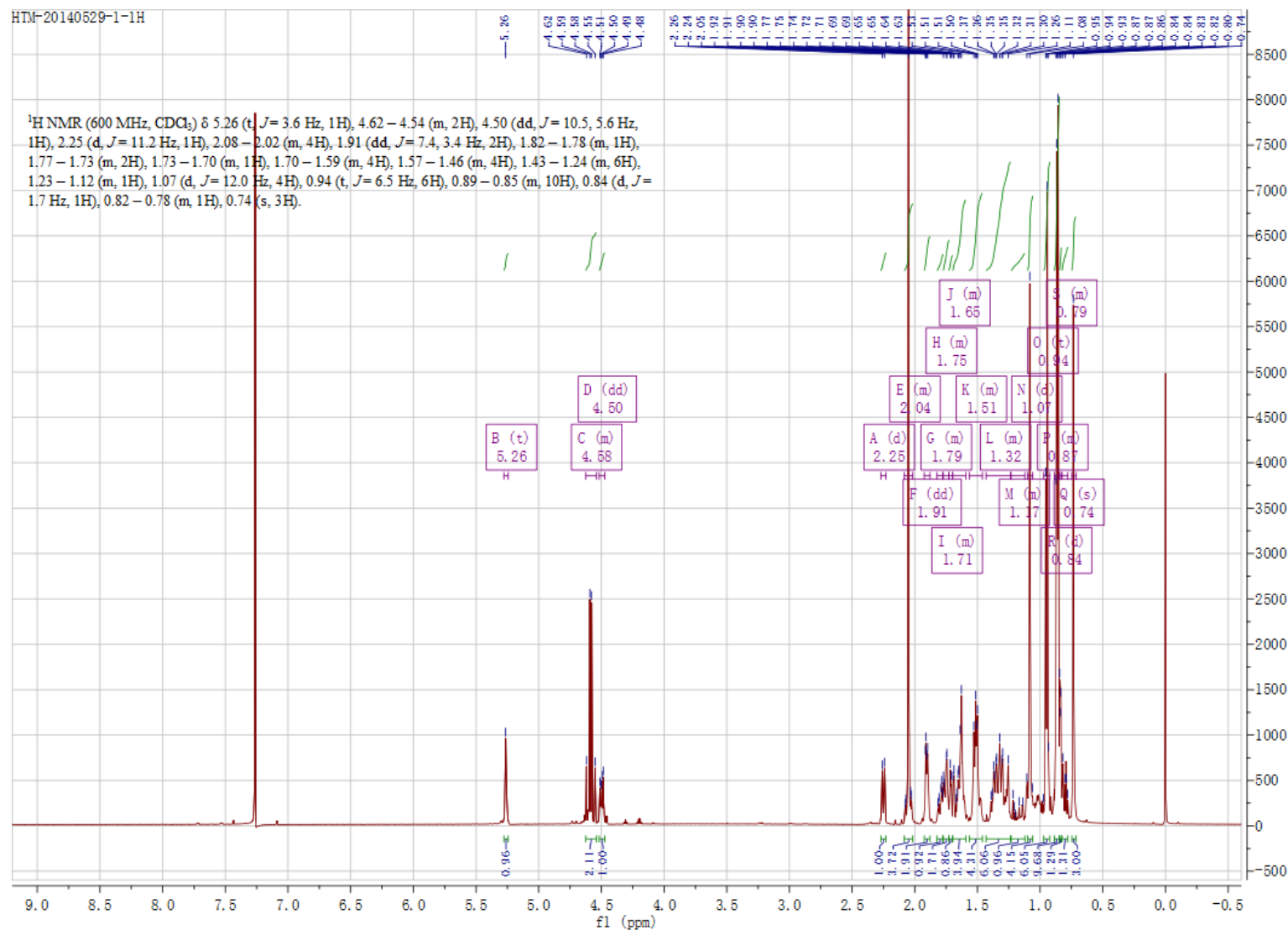


Figure 9 ¹H NMR spectrum (CDCl₃, 600 MHz) of Carboxymethyl-3β-Acetoxy-urs-12-en-28-oate (compound **9**)

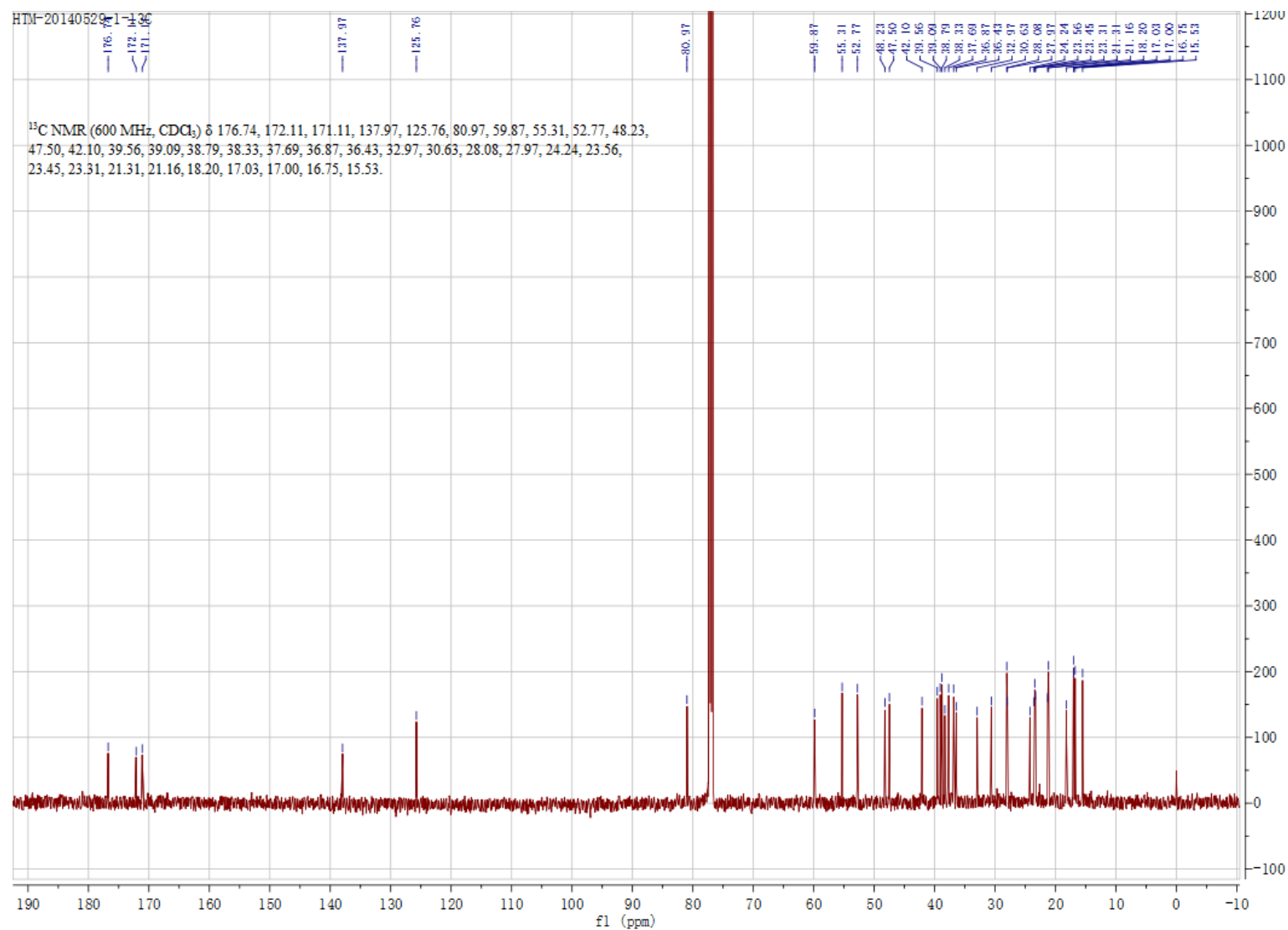


Figure 10 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of Carboxymethyl-3 β -Acetoxy-urs-12-en-28-oate (compound **9**)

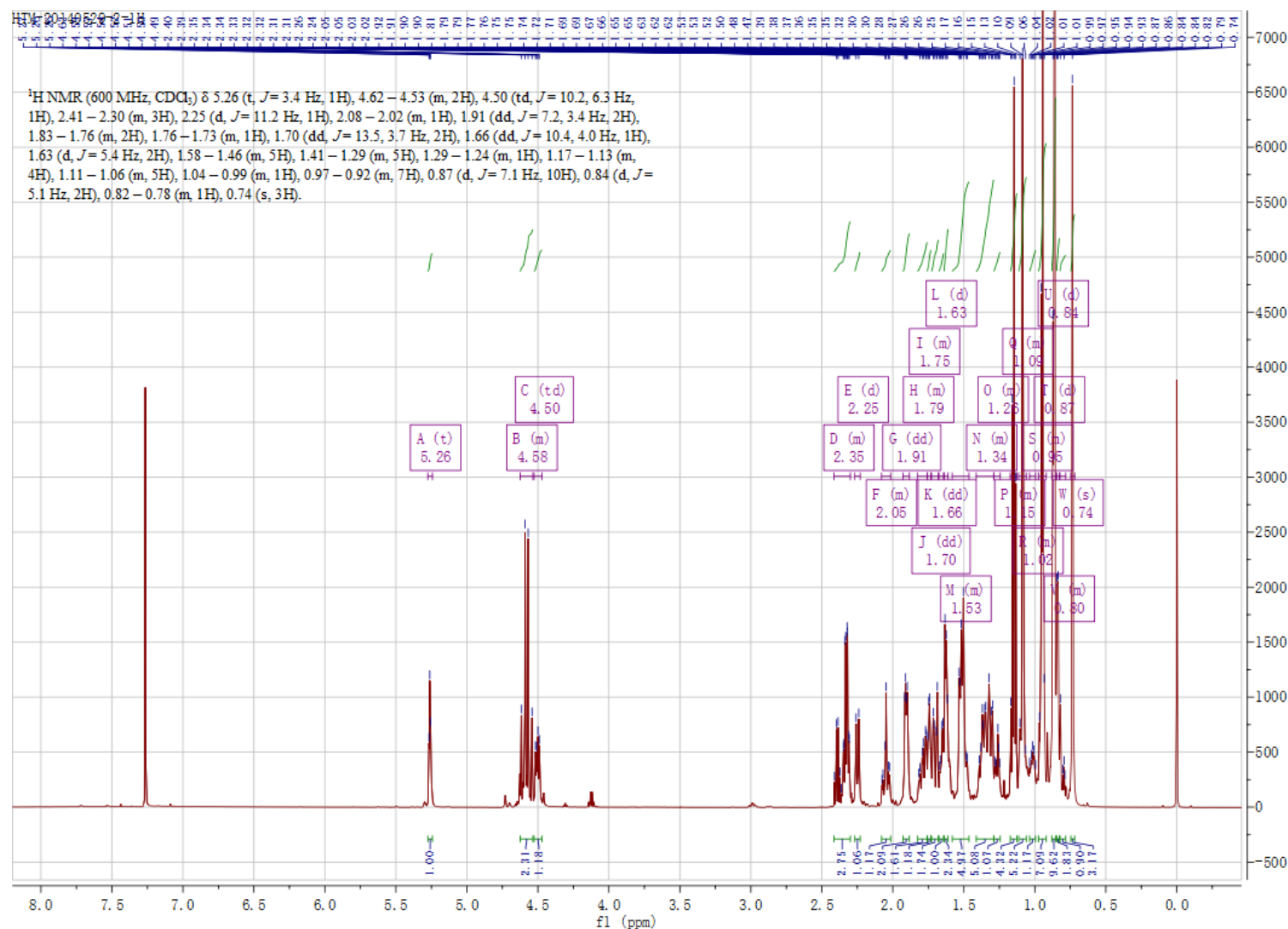
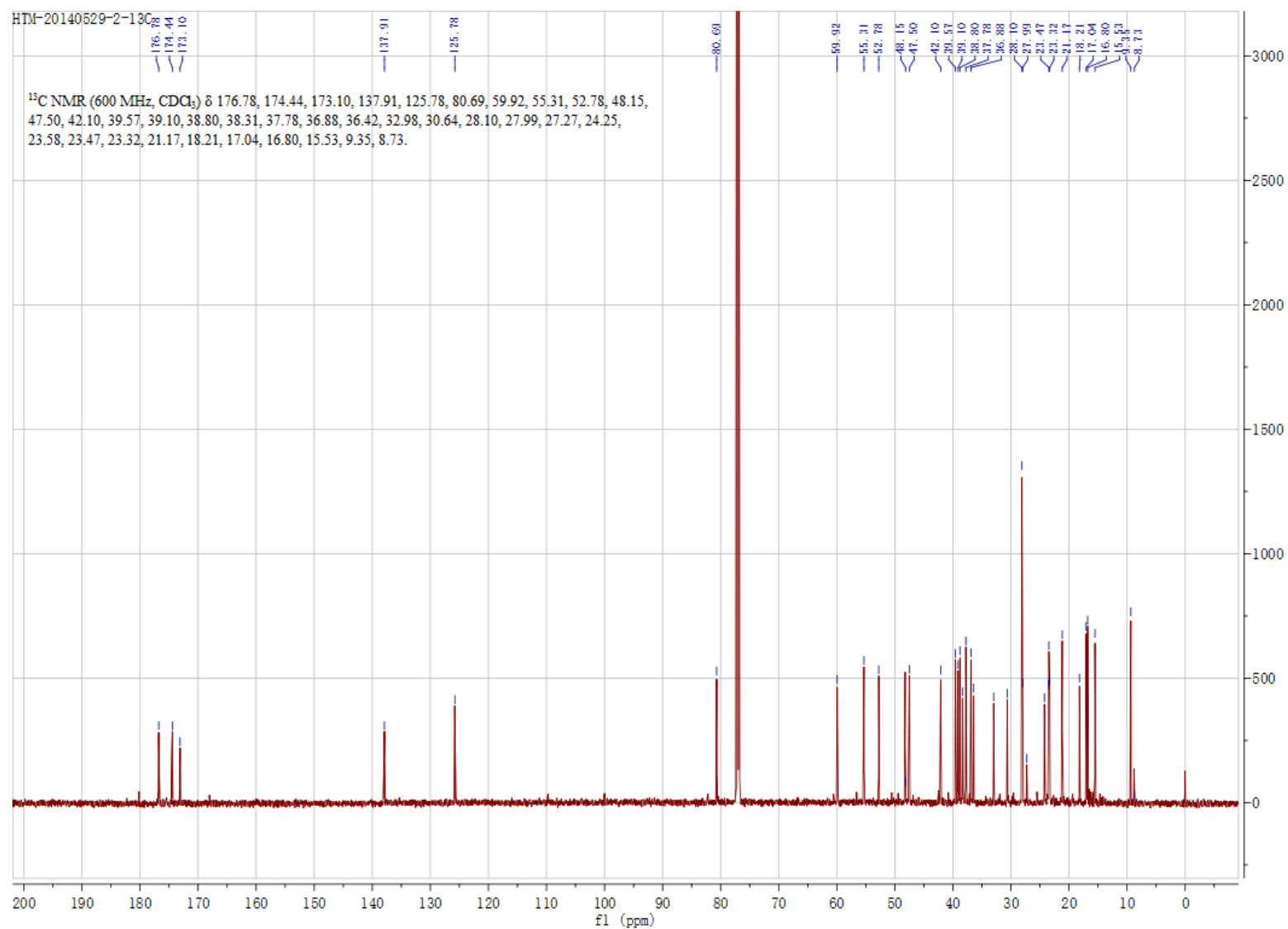


Figure 11 ¹H NMR spectrum (CDCl₃, 600 MHz) of Carboxymethyl-3β-propionyloxy-urs-12-en-28-oate (compound 10)



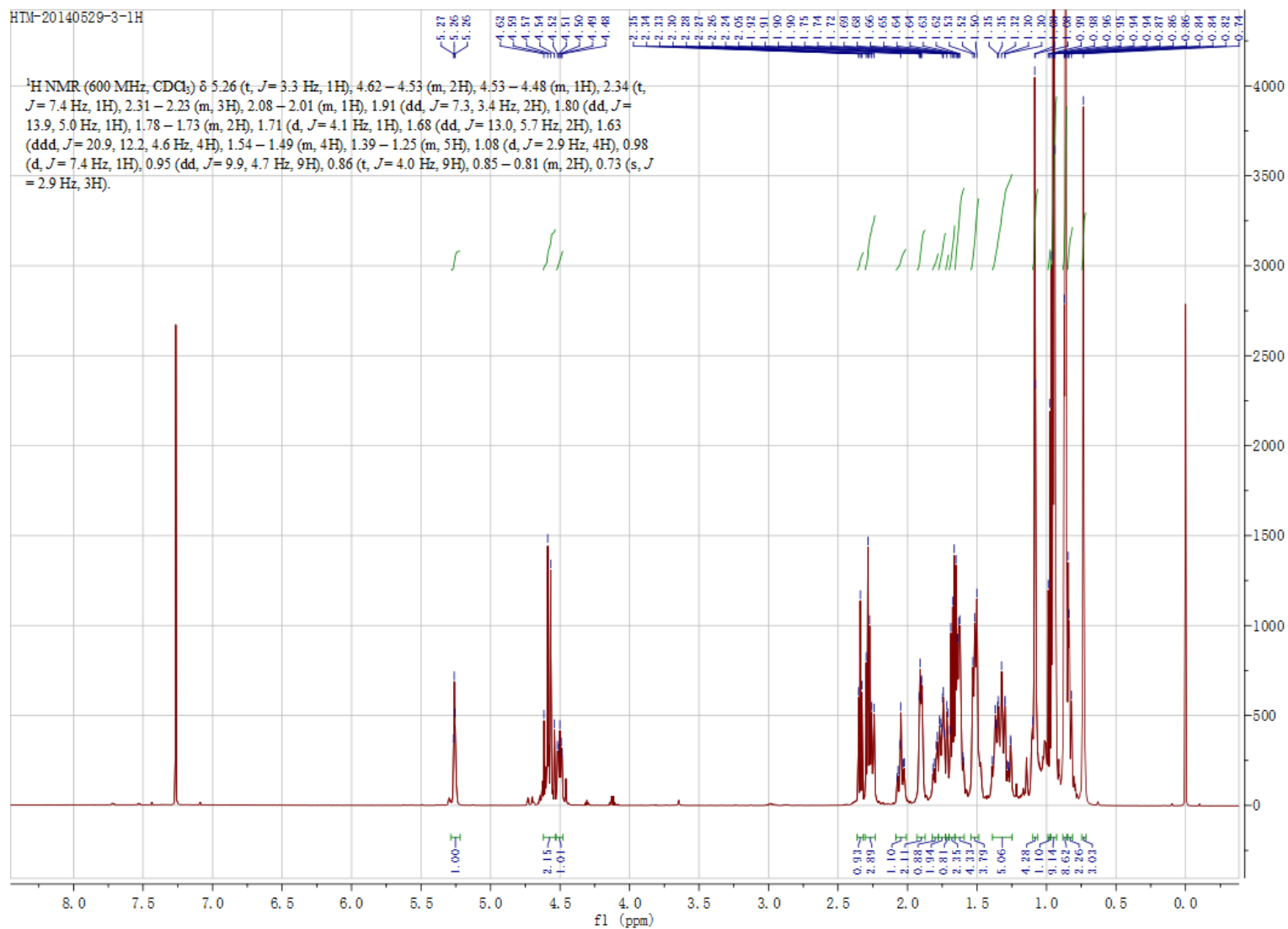


Figure 13 ¹H NMR spectrum (CDCl₃, 600 MHz) of Carboxymethyl-3β-n-Butyryloxy-urs-12-en-28-oate (compound **11**)

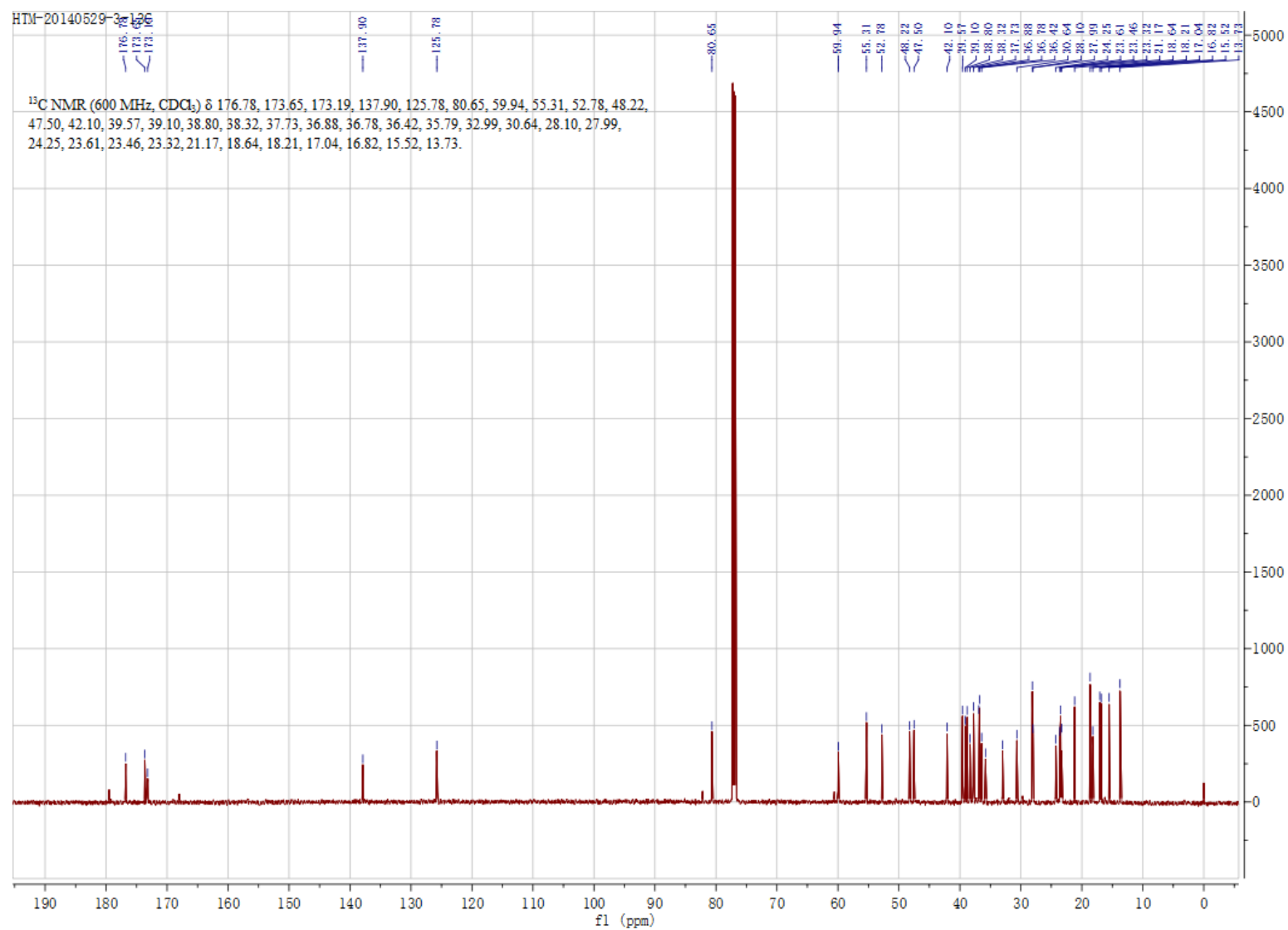


Figure 14 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of Carboxymethyl-3 β -n-Butyryloxy-urs-12-en-28-oate (compound **11**)

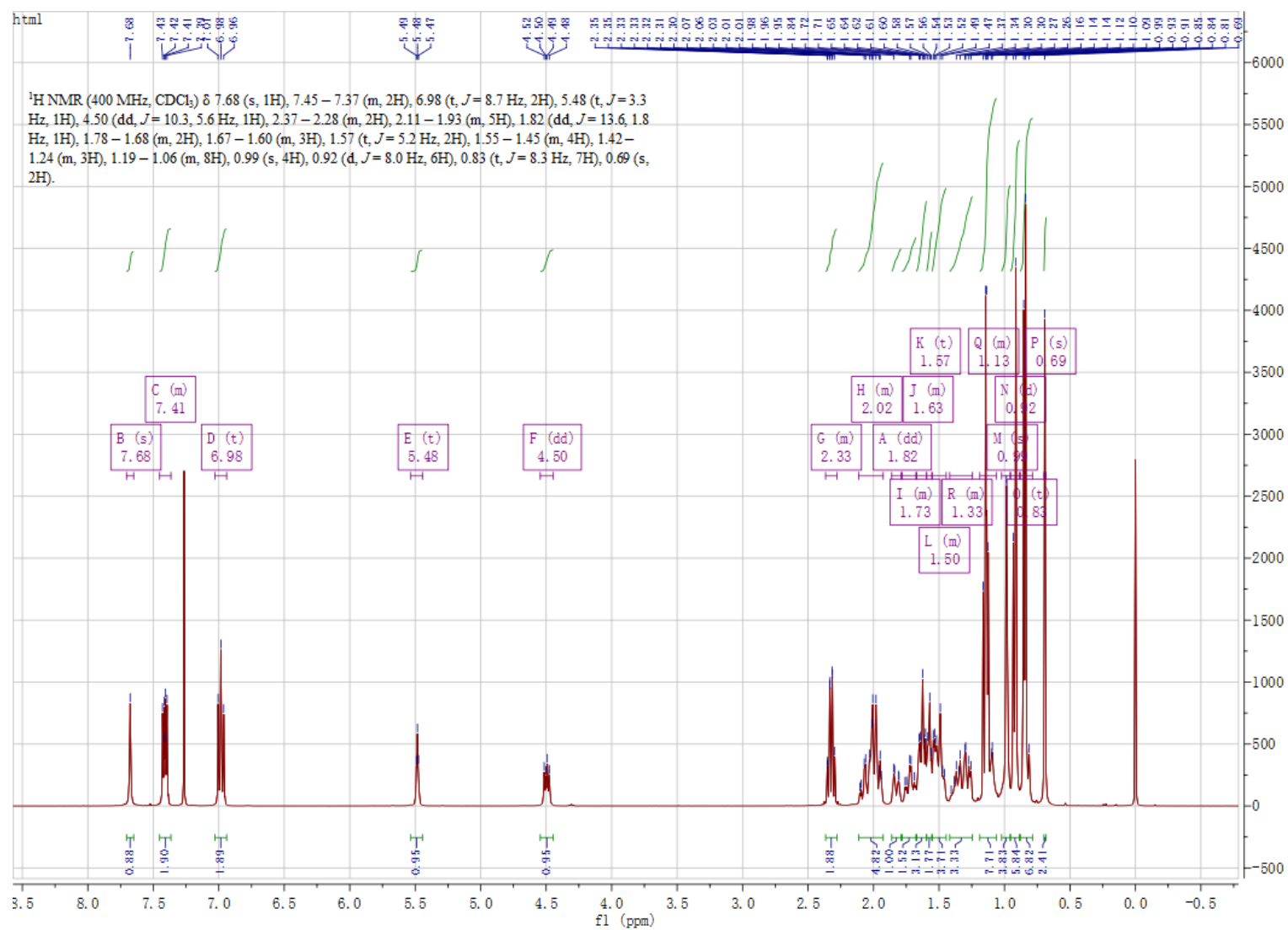


Figure 15 ¹H NMR spectrum (CDCl₃, 400 MHz) of N-[3β-propionyloxy-urs-12-en-28-oyl]-para-fluoroaniline (compound **13**)

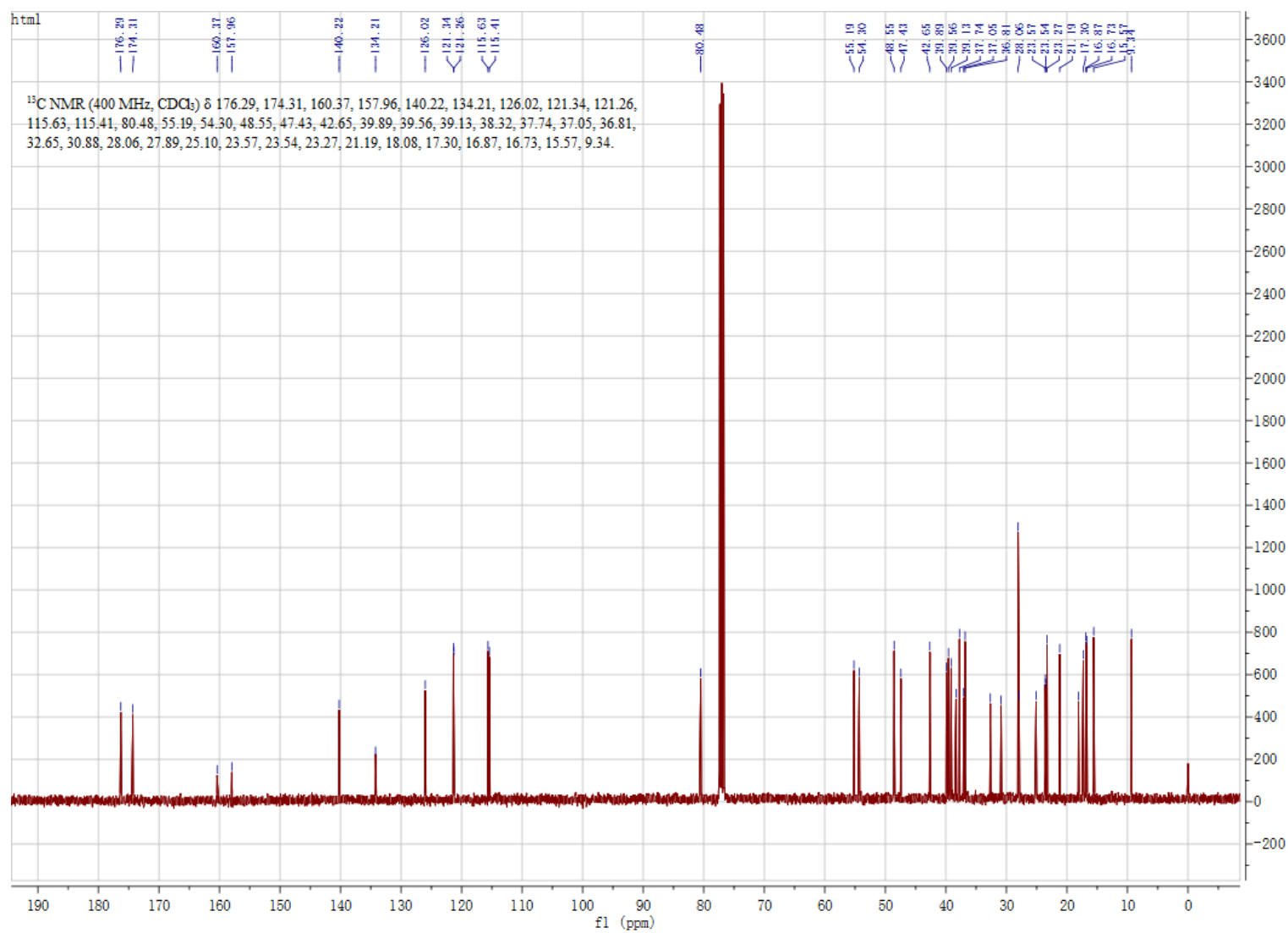


Figure 16 ^{13}C NMR spectrum (CDCl_3 , 400 MHz) of N-[3 β -propionyloxy-urs-12-en-28-oyl]-para-fluoroaniline (compound 13)

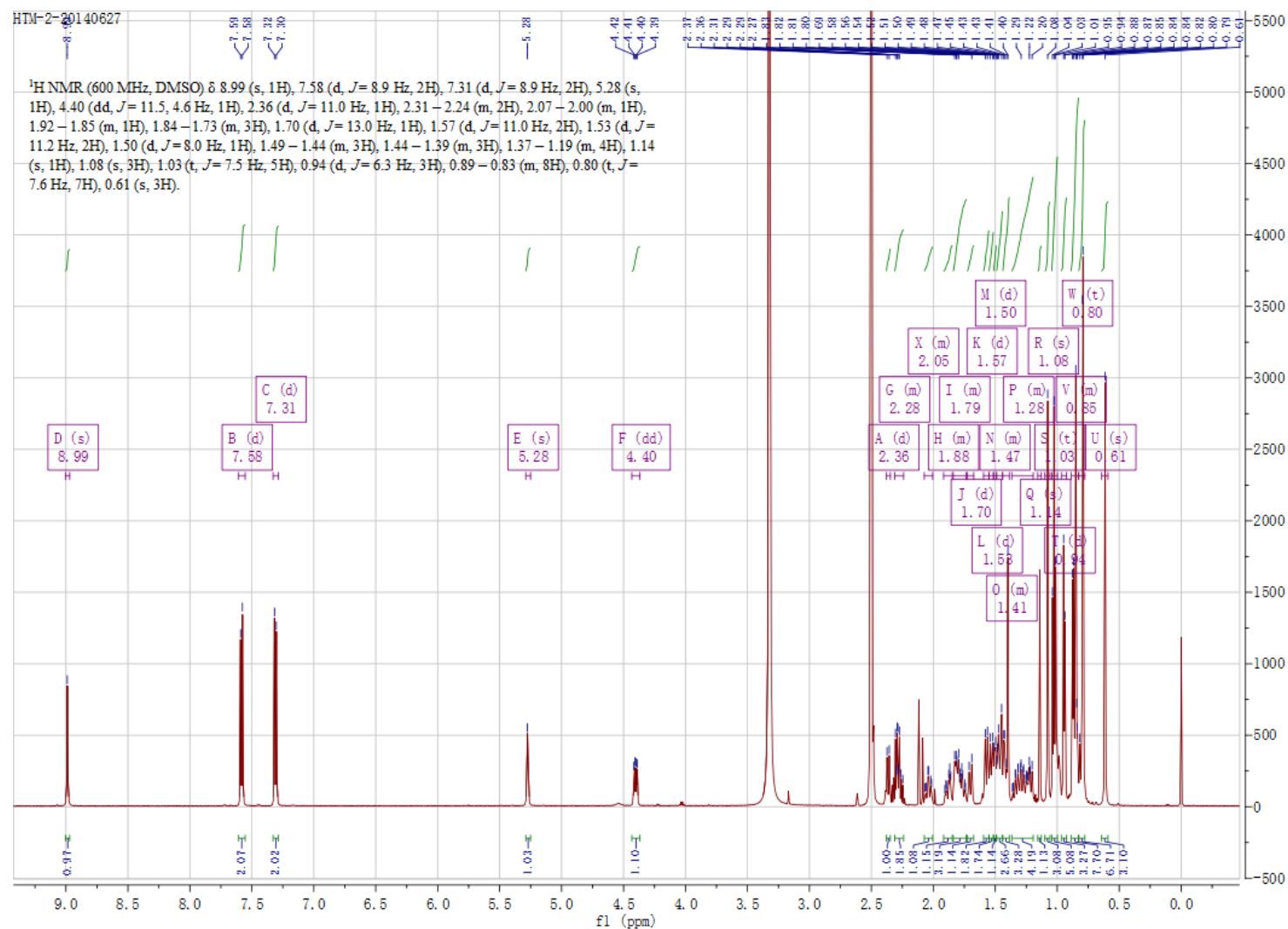


Figure 17 ¹H NMR spectrum (CDCl₃, 600 MHz) of N-[3β-propionyloxy-urs-12-en-28-oyl]-para-chloroaniline (compound 14)

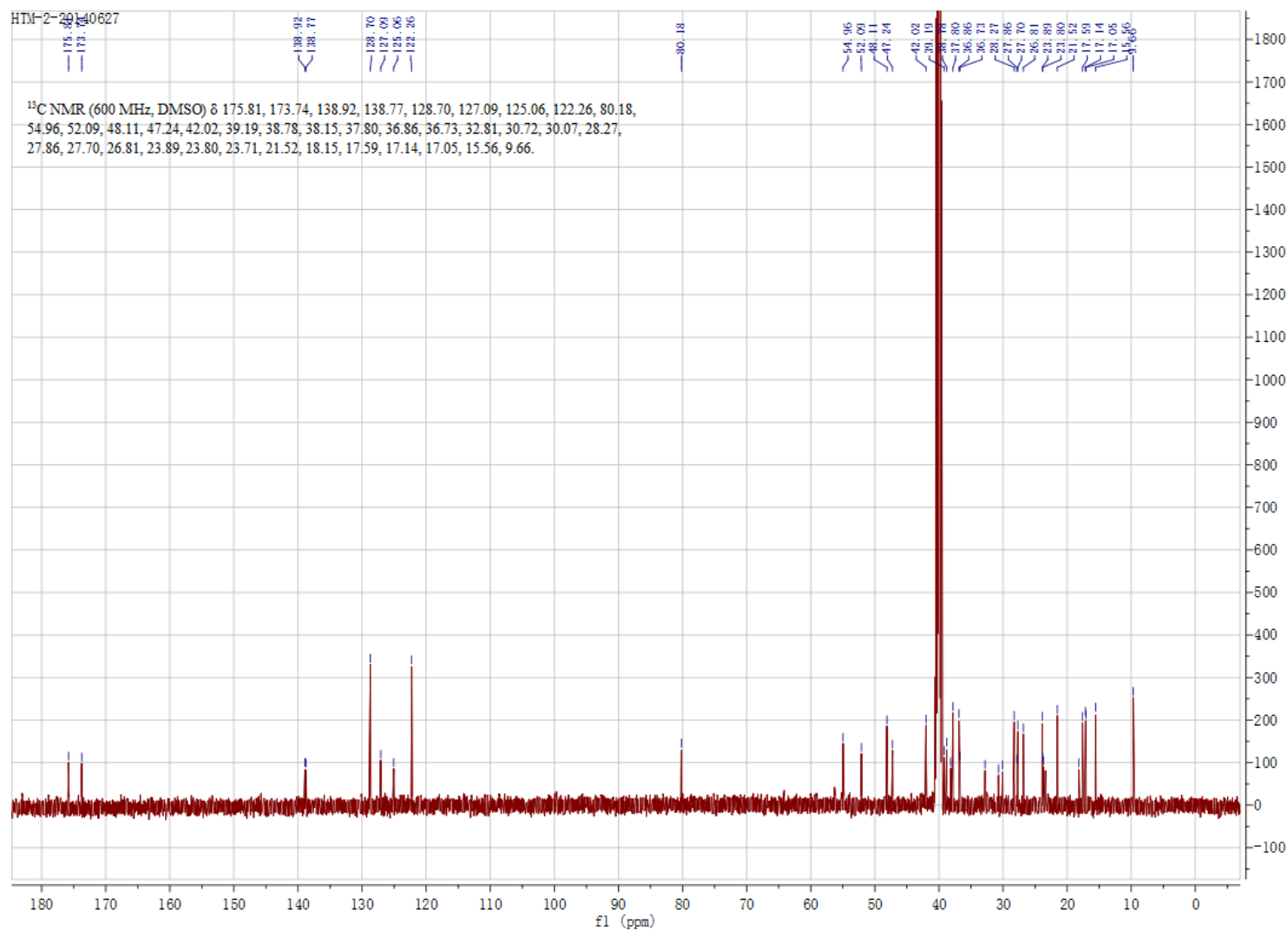


Figure 18 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of N-[3 β -propionyloxy-urs-12-en-28-oyl]-para-chloroaniline (compound **14**)

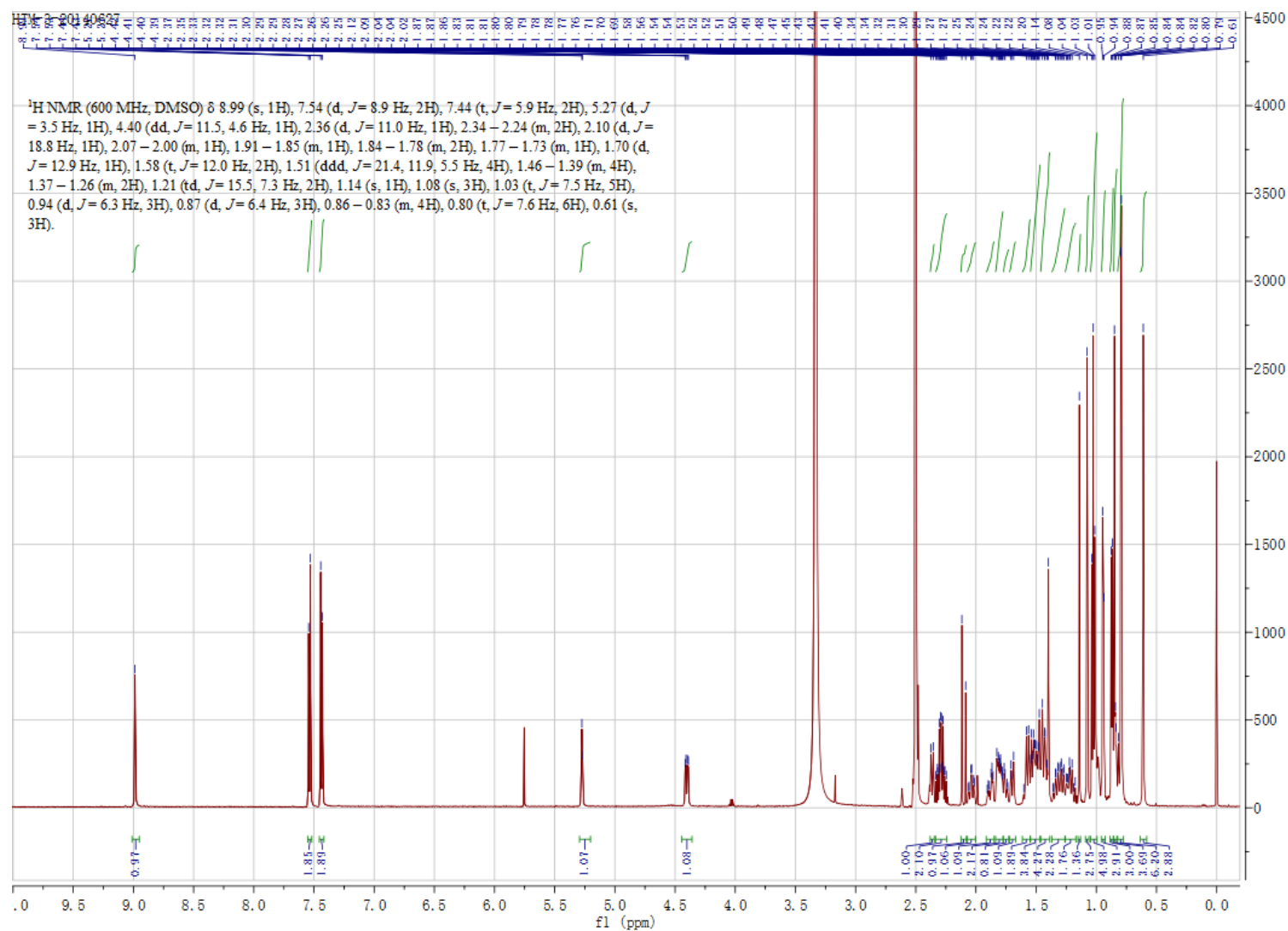


Figure 19 ¹H NMR spectrum (CDCl₃, 600 MHz) of N-[3β-propionyloxy-urs-12-en-28-oyl]-para-bromoaniline (compound 15)

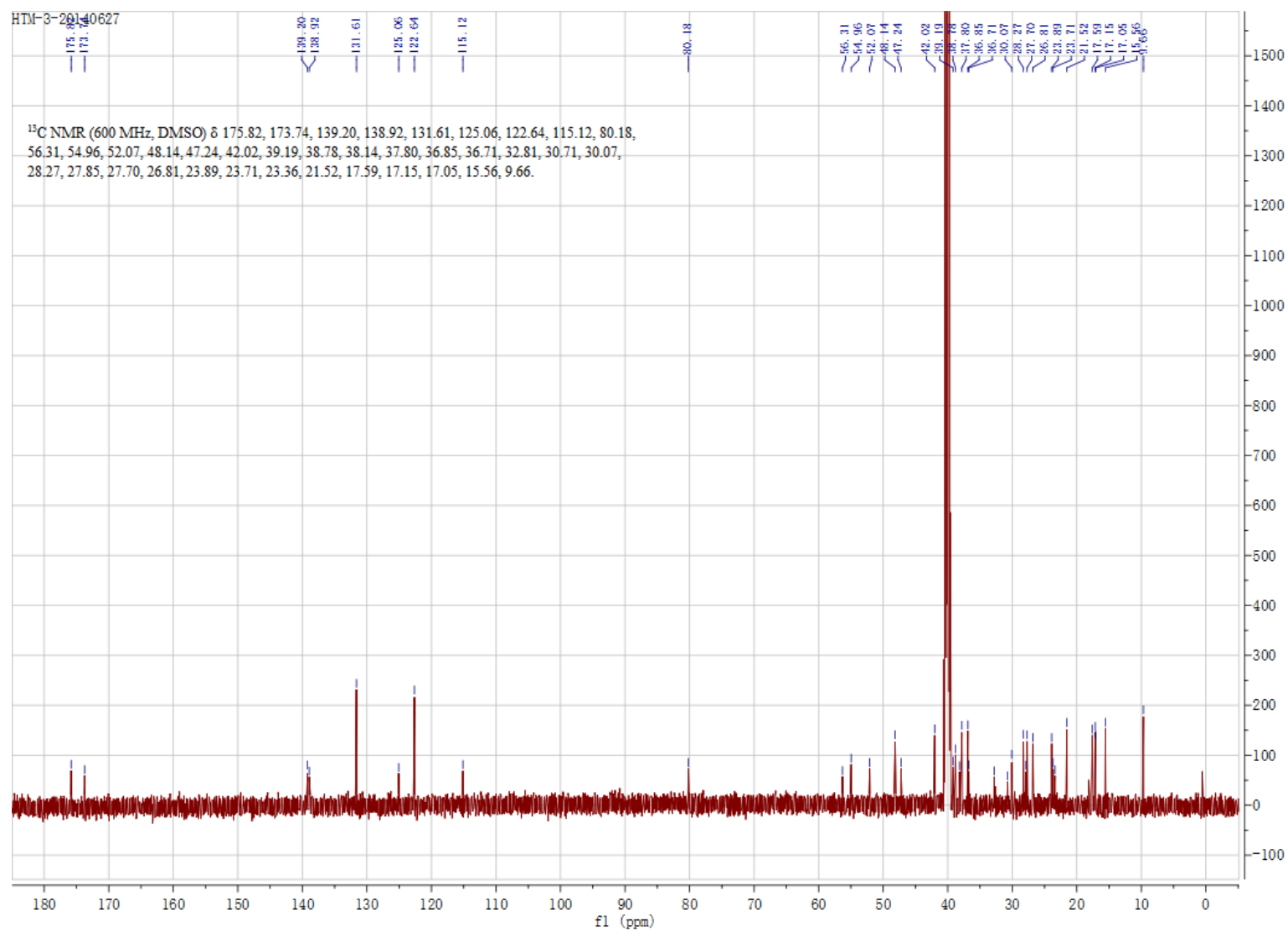


Figure 20 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of N-[3 β -propionyloxy-urs-12-en-28-oyl]-para-bromoaniline (compound 15)

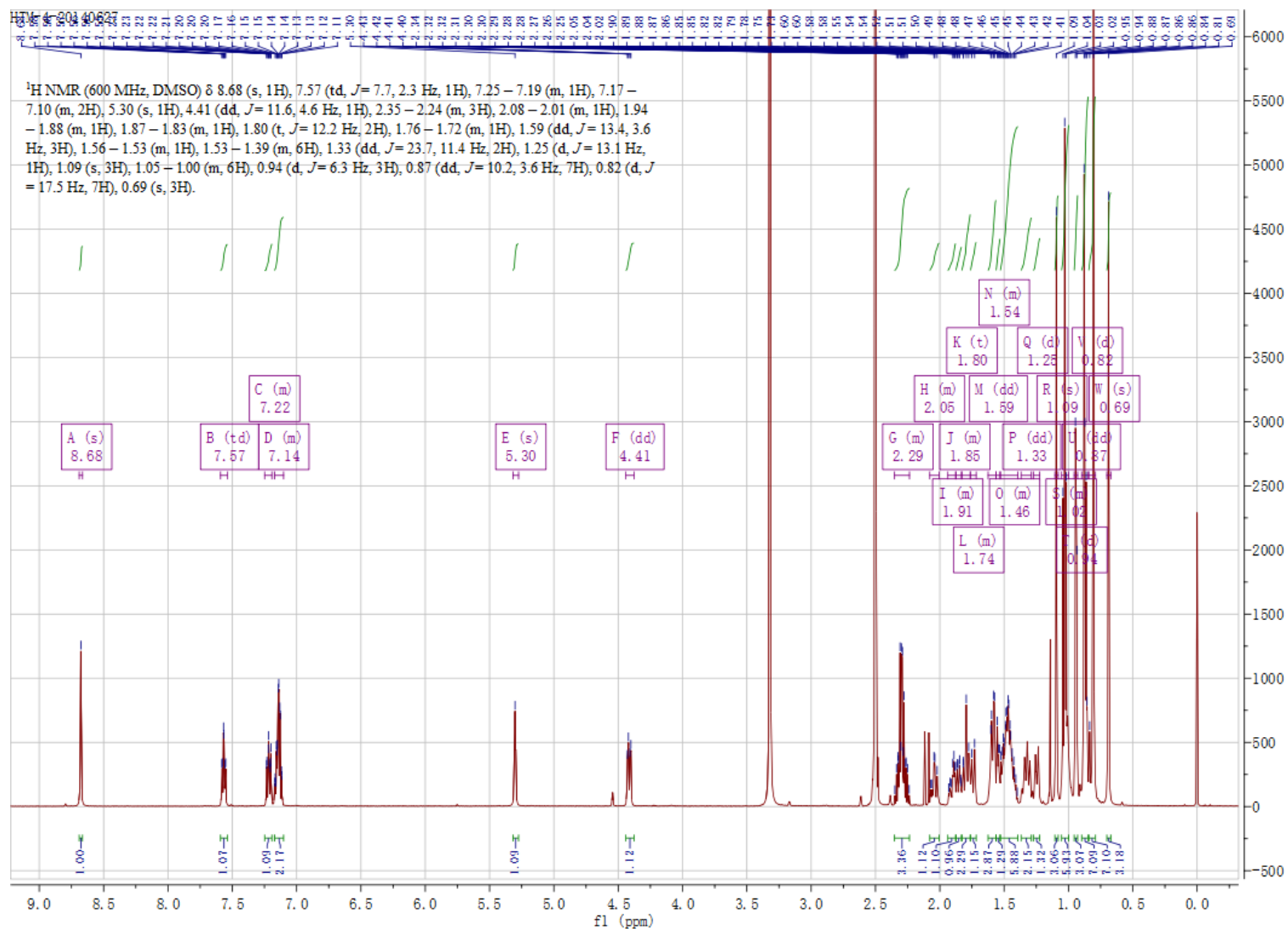


Figure 21 ¹H NMR spectrum (CDCl₃, 600 MHz) of N-[3β-propionyloxy-urs-12-en-28-oyl]-ortho-fluoroaniline (compound 16)

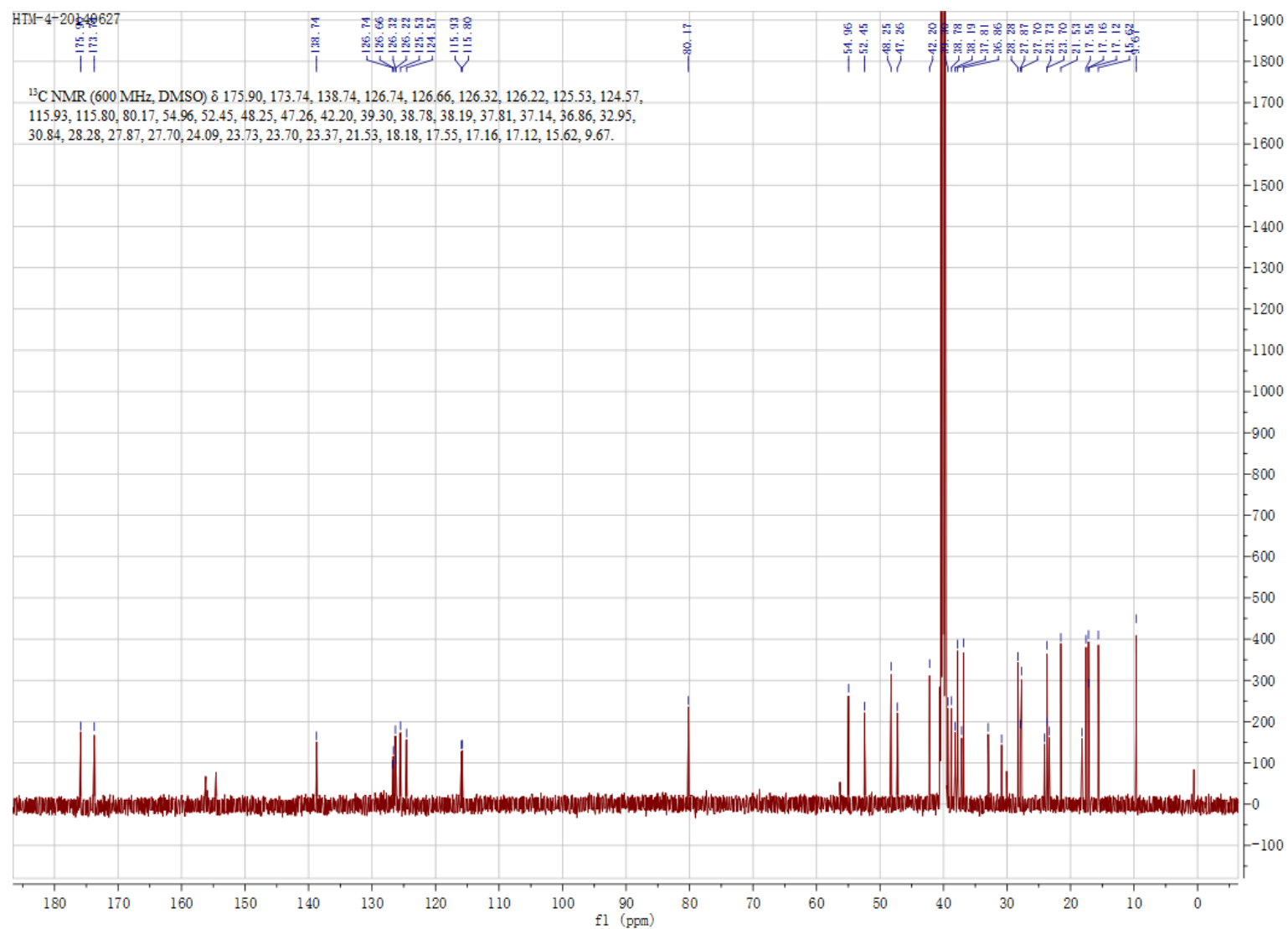


Figure 22 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of N-[3 β -propionyloxy-urs-12-en-28-oyl]-ortho-fluoroaniline (compound **16**)

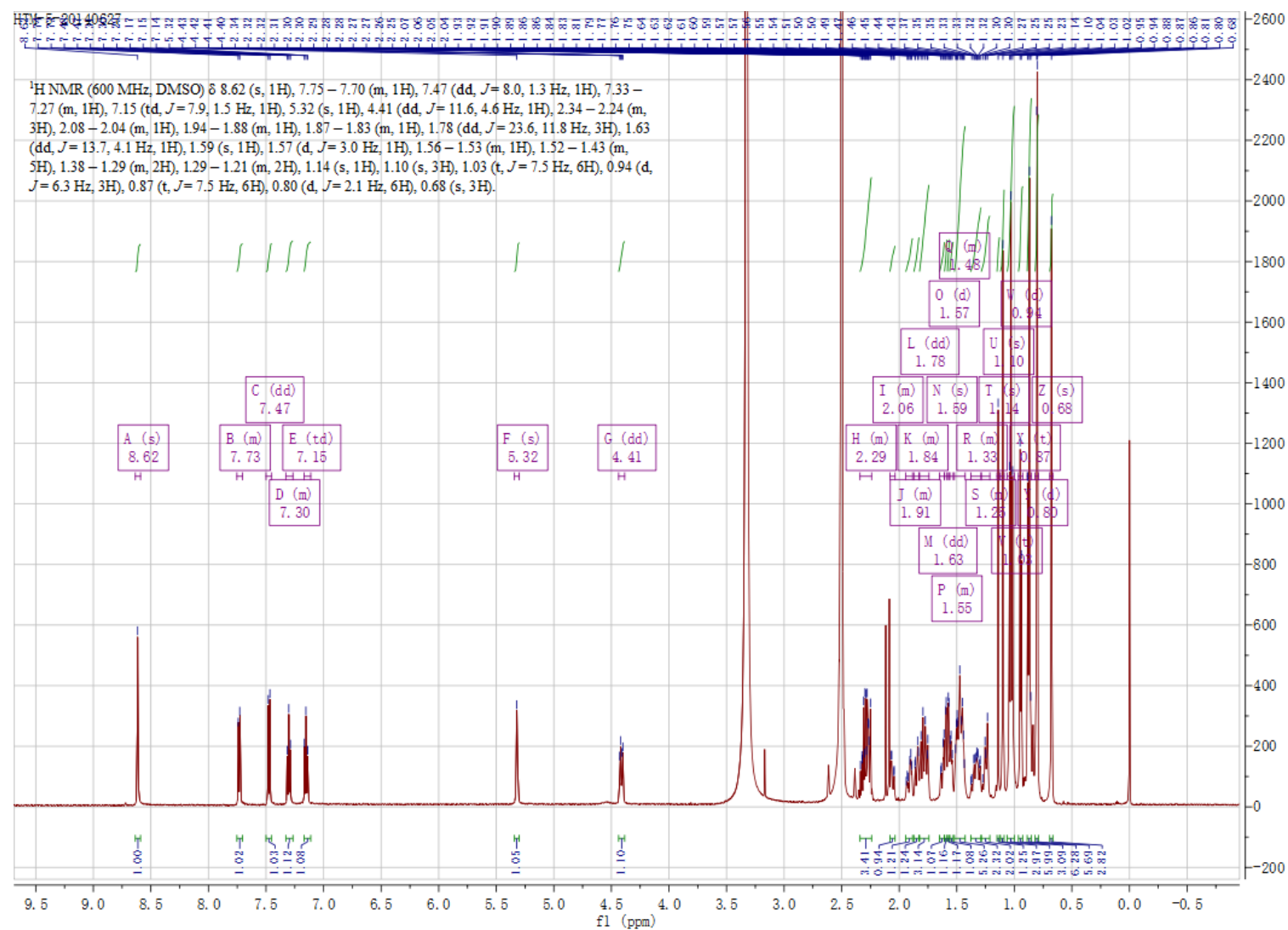


Figure 23 ¹H NMR spectrum (CDCl₃, 600 MHz) of N-[3β-propionyloxy-urs-12-en-28-oyl]-ortho-chloroaniline (compound 17)

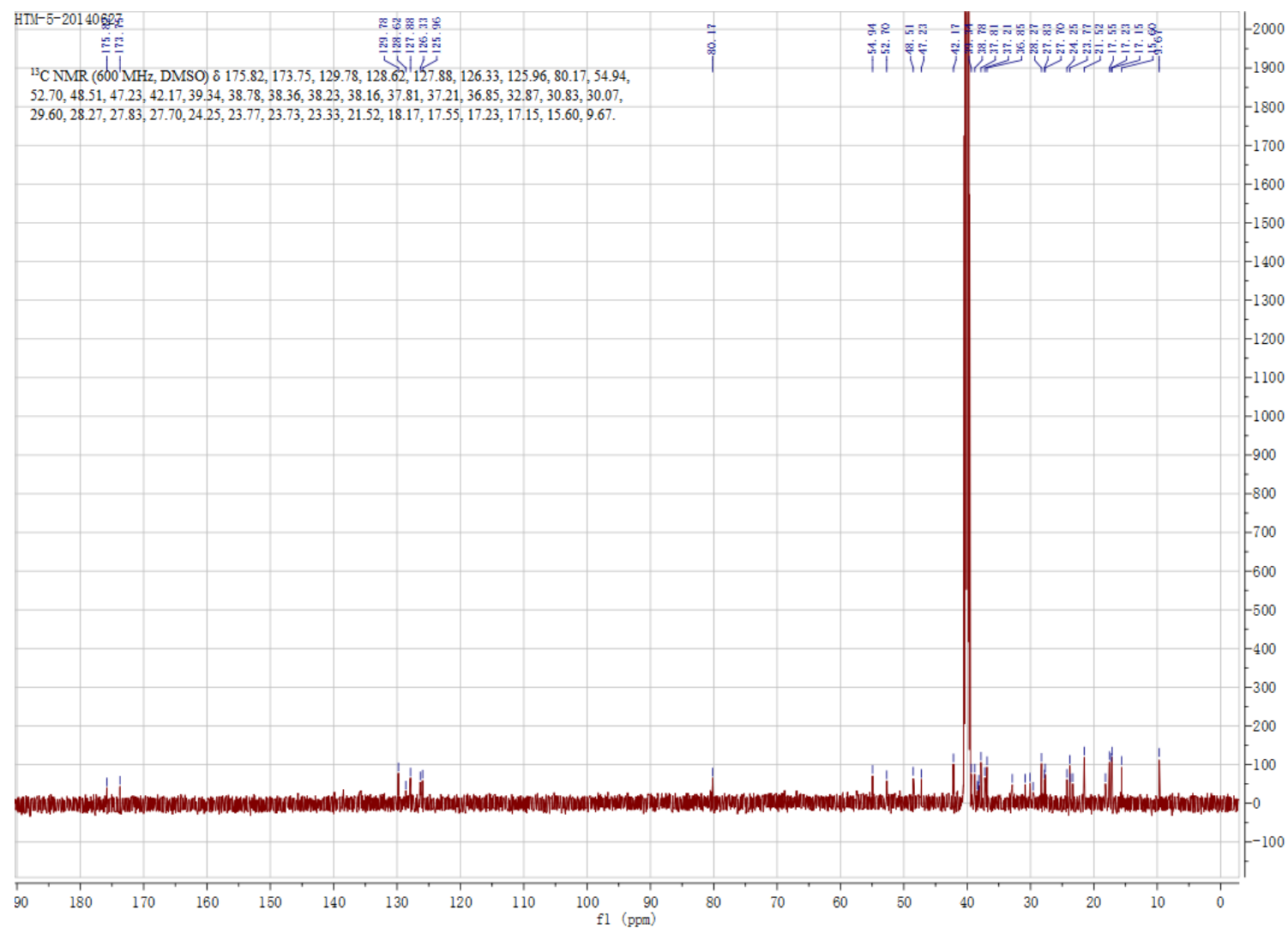


Figure 24 ¹³C NMR spectrum (CDCl₃, 600 MHz) of N-[3β-propionyloxy-urs-12-en-28-oyl]-ortho-chloroaniline (compound 17)

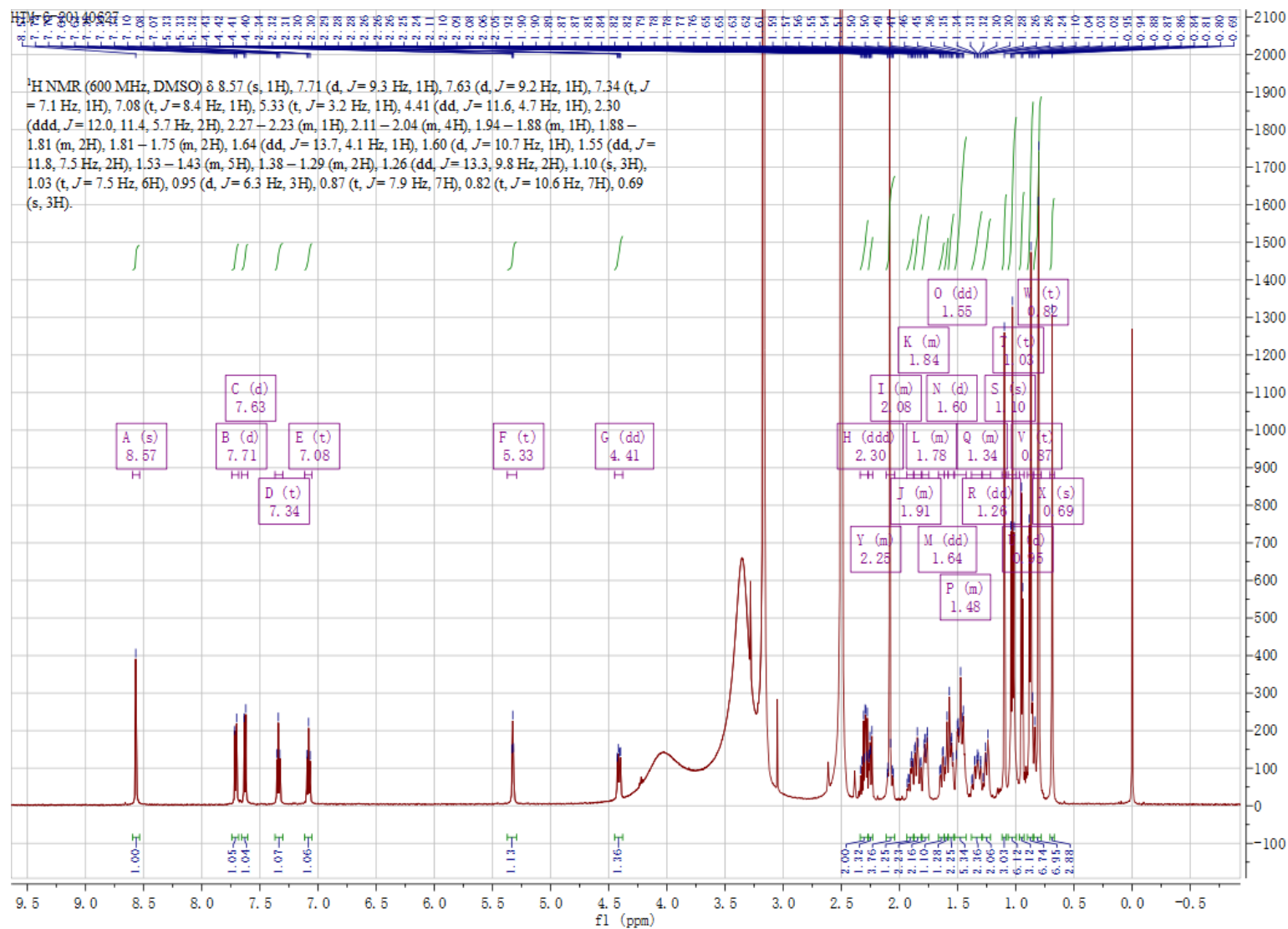


Figure 25 ¹H NMR spectrum (CDCl₃, 600 MHz) of N-[3β-propionyloxy-urs-12-en-28-oyl]-ortho-bromoaniline (compound **18**)

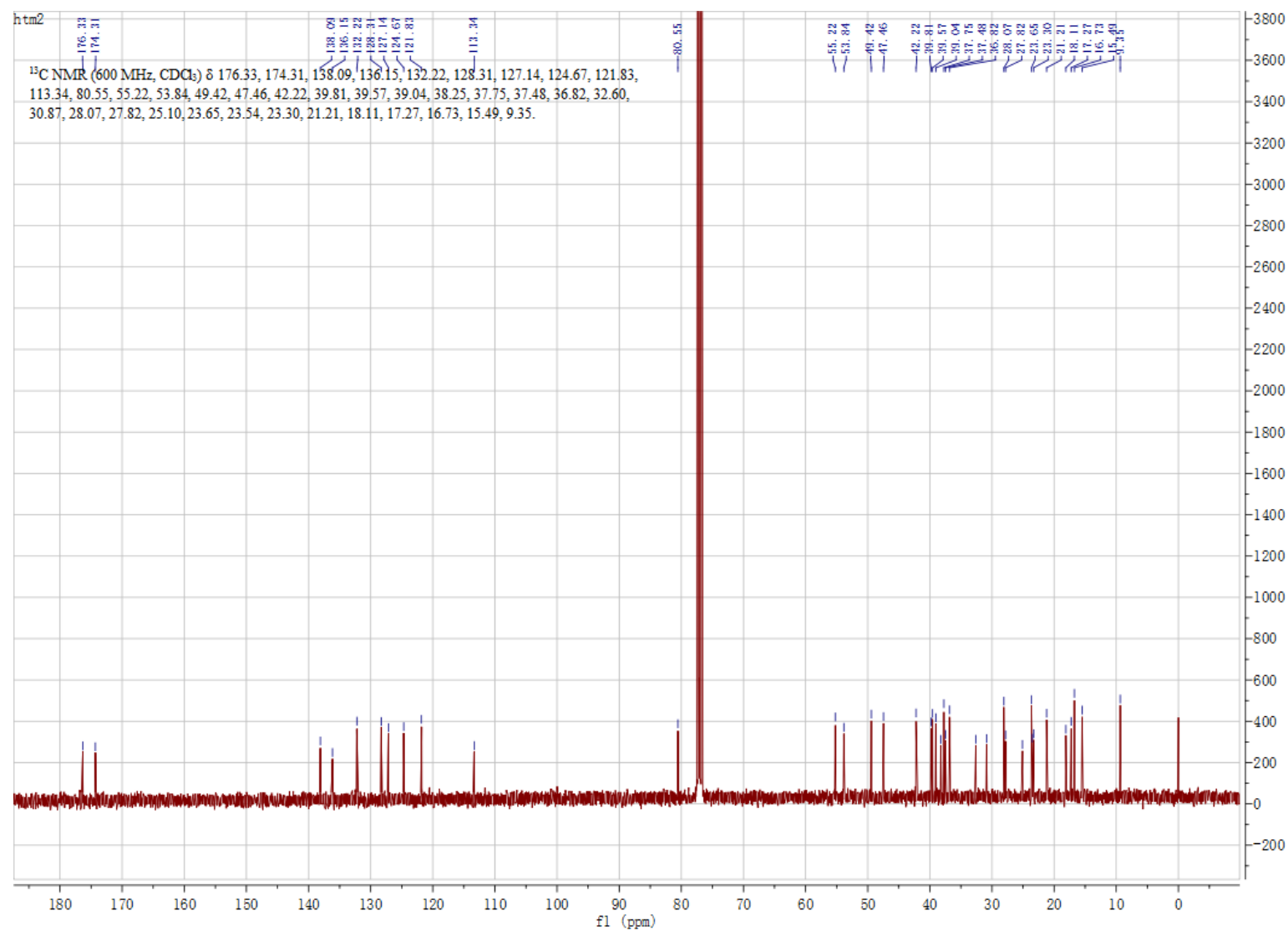


Figure 26 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of N-[3 β -propionyloxy-urs-12-en-28-oyl]-ortho-bromoaniline (compound **18**)



Figure 27 ¹H NMR spectrum (CDCl₃, 600 MHz) of N-[3β-propionyloxy-urs-12-en-28-oyl]-aminobenzene (compound **19**)

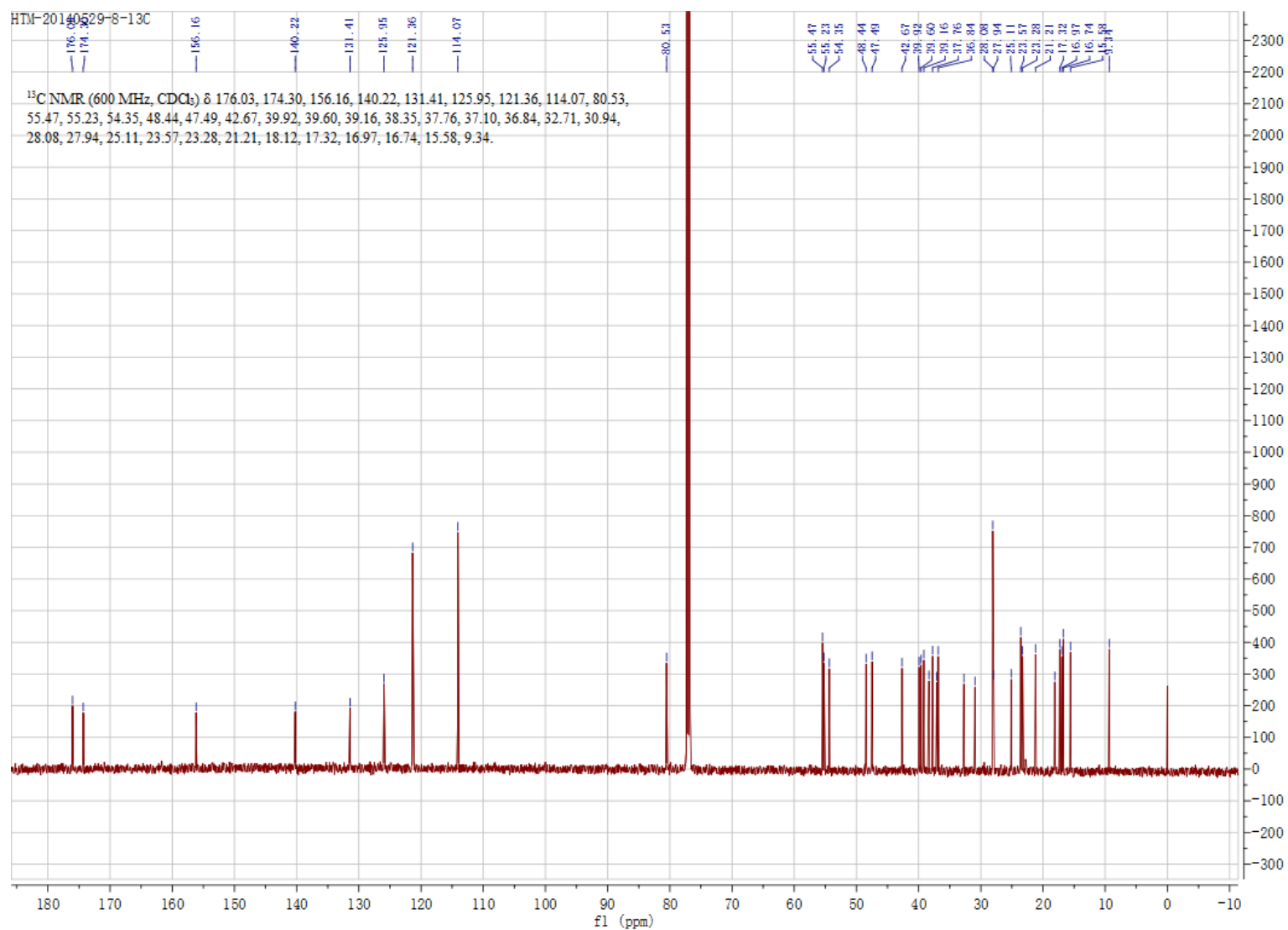


Figure 28 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of N-[3 β -propionyloxy-urs-12-en-28-oyl]-aminobenzene (compound **19**)

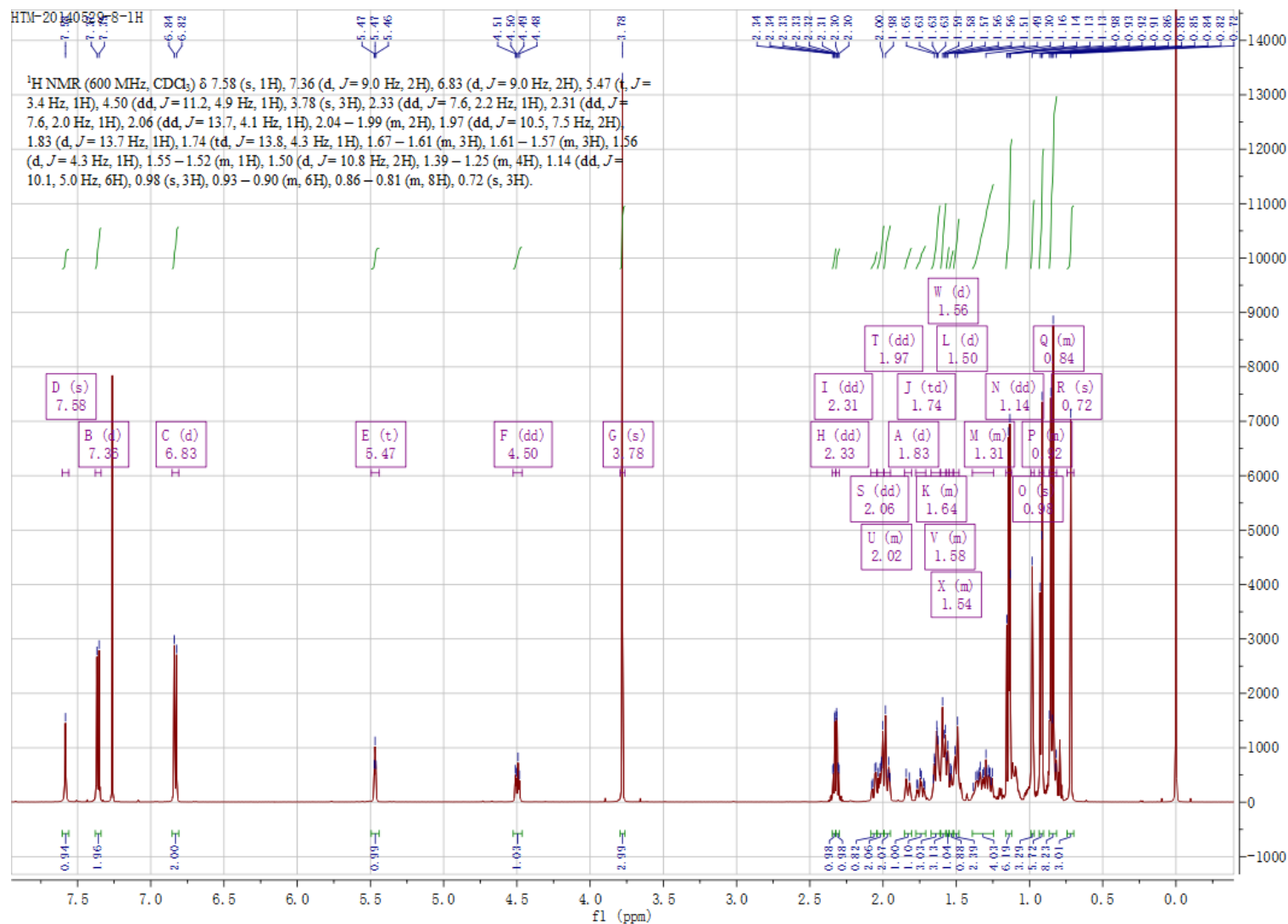


Figure 29 ¹H NMR spectrum (CDCl₃, 600 MHz) of N-[3β-propionyloxy-urs-12-en-28-oyl]-para-methoxyaniline (compound **20**)

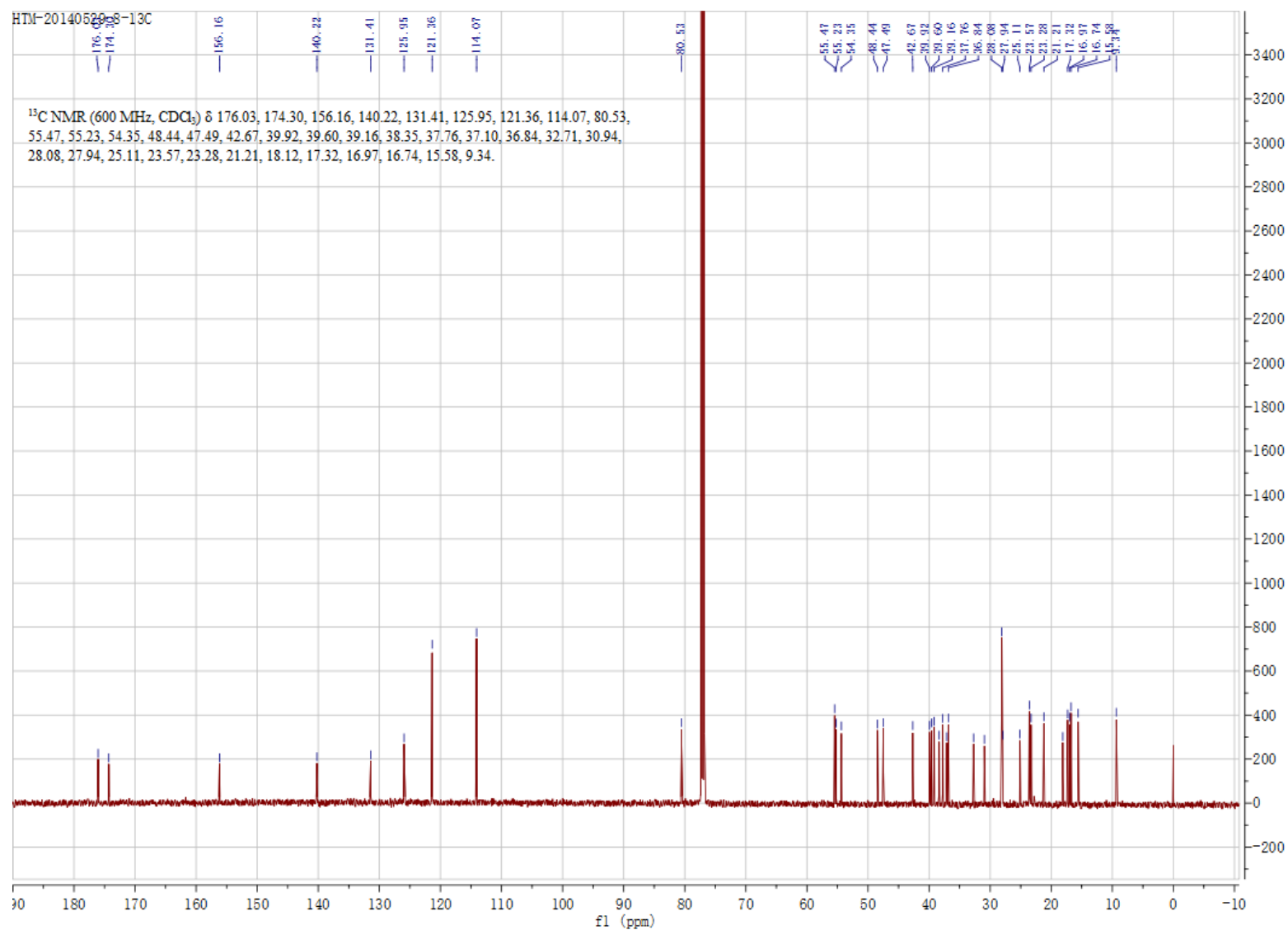


Figure 30 ^{13}C NMR spectrum (CDCl_3 , 600 MHz) of N-[3 β -propionyloxy-urs-12-en-28-oyl]-para-methoxyaniline (compound **20**)

A hydrophilic conjugate Approach toward the design and synthesis of Ursolic acid derivatives as potential antidiabetic agent

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Supplementary Data

Copies of **HRMS (ESI)** spectra of compounds **3–6, 9-11, 12-20**

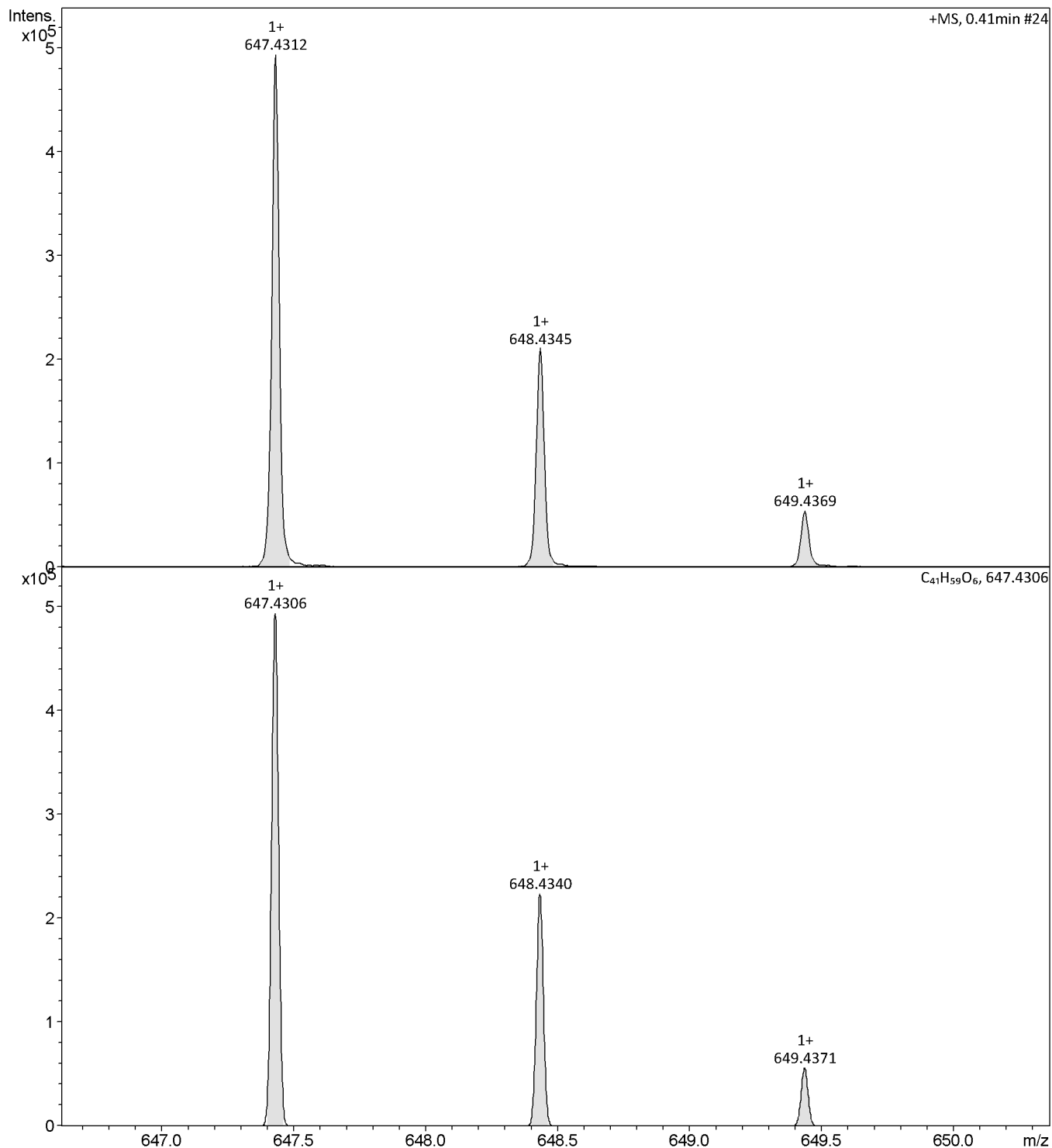
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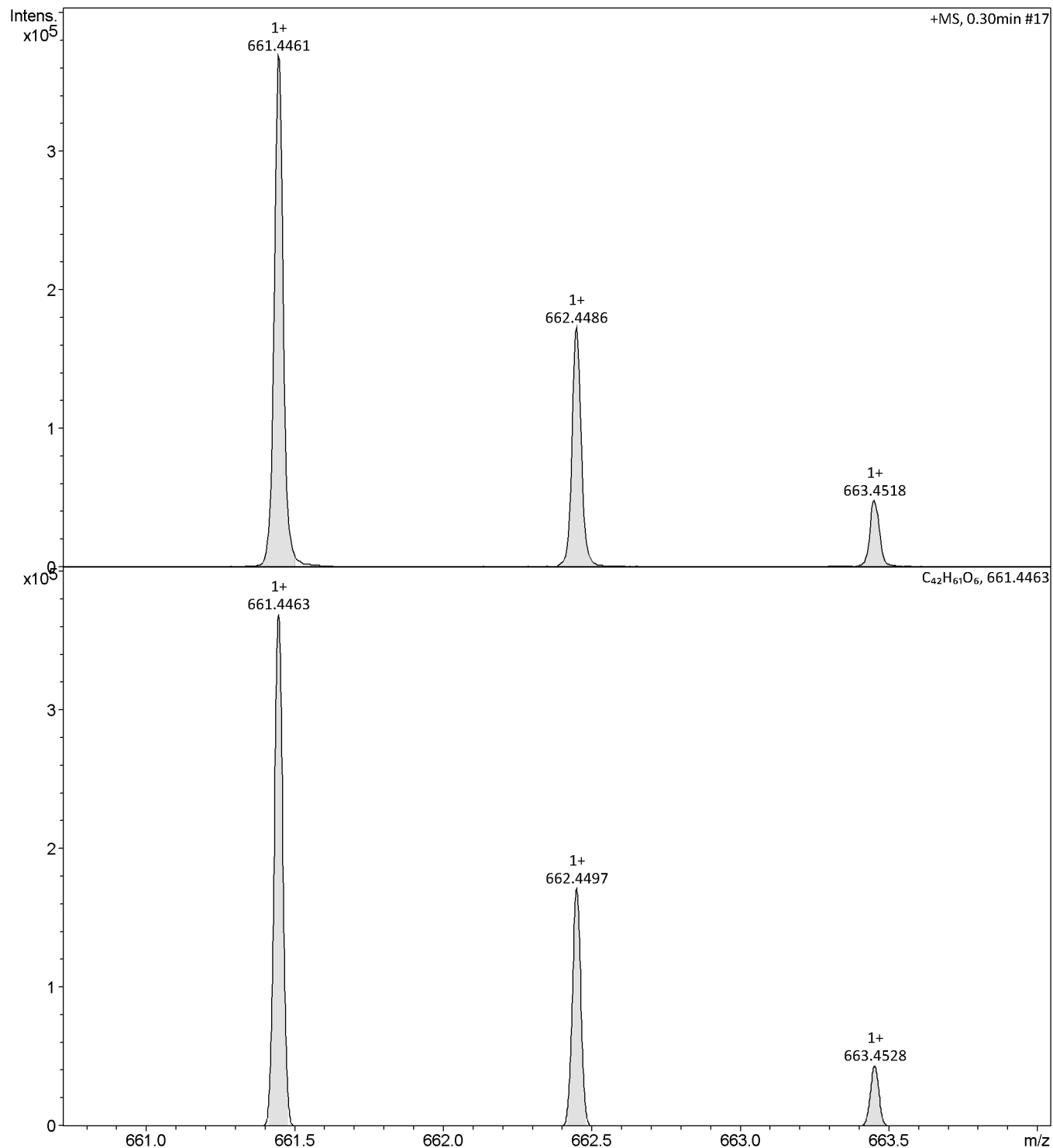
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3 β -[(3-carboxy)propionyloxy]-urs-12-en-28-oic acid (compound 5)

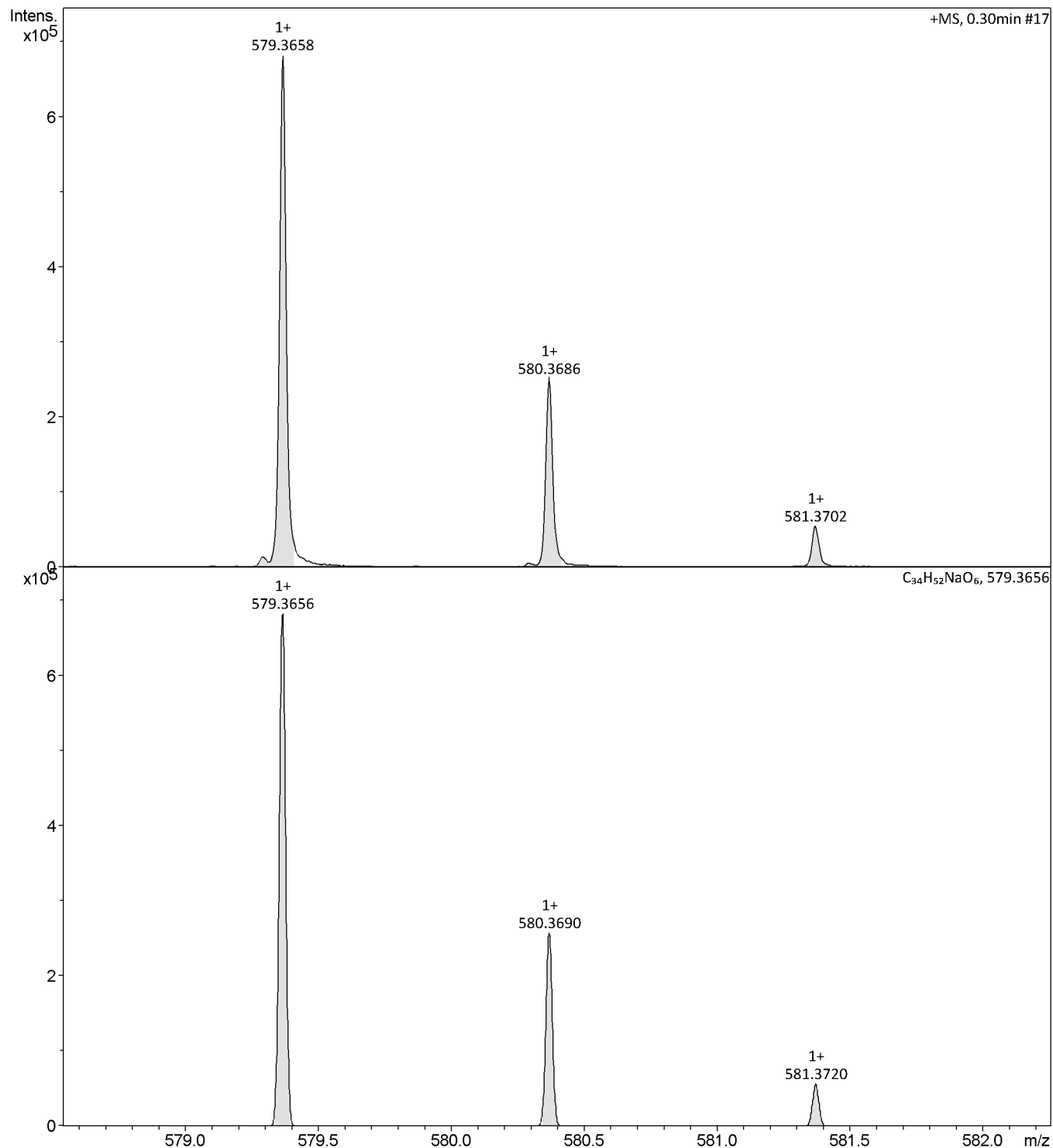
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3β-[(3-carboxy)n-butyryloxy]-urs-12-en-28-oic acid (compound 6)

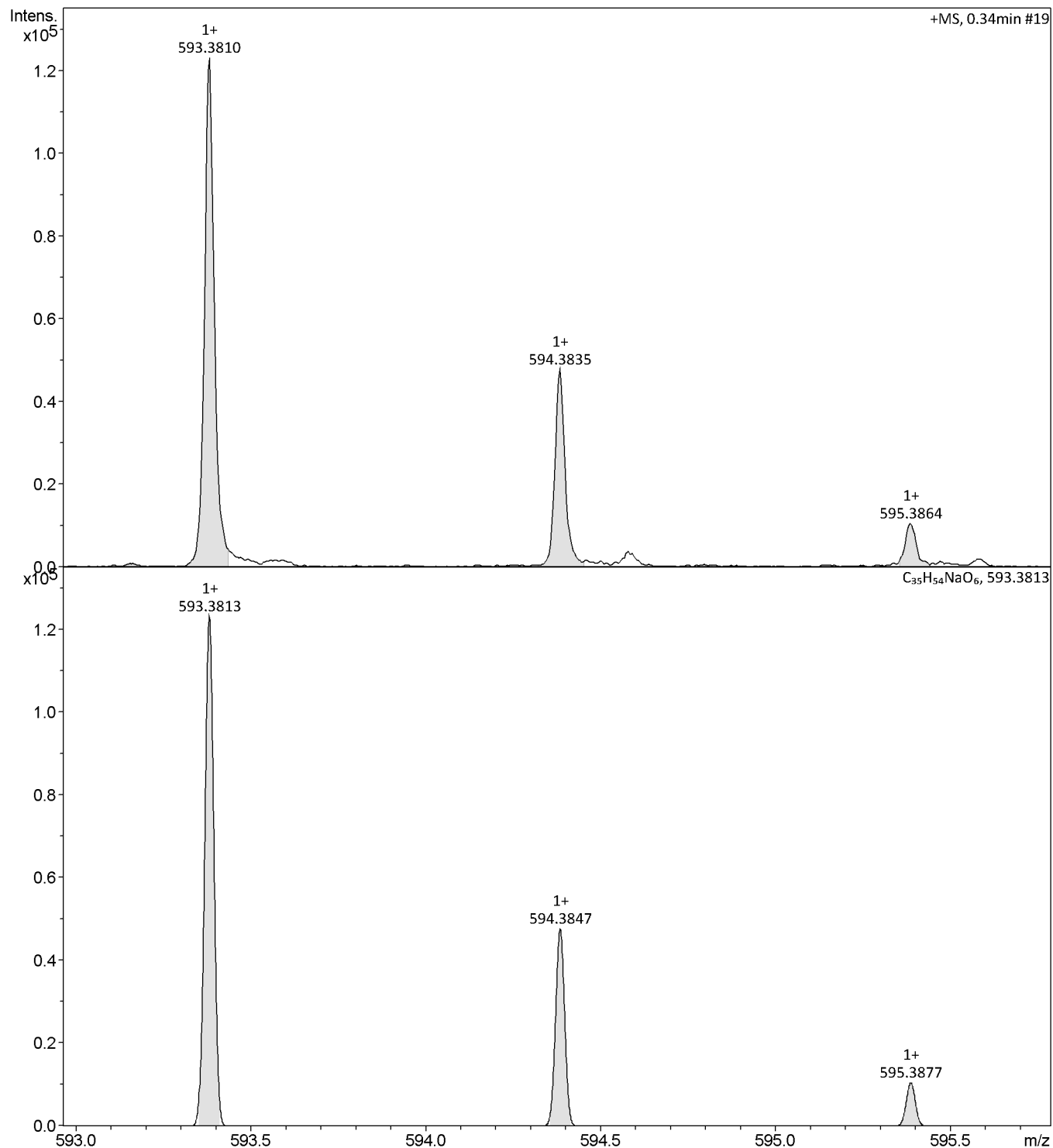
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Carboxymethyl-3 β -Acetoxy-urs-12-en-28-oate (compound 9)

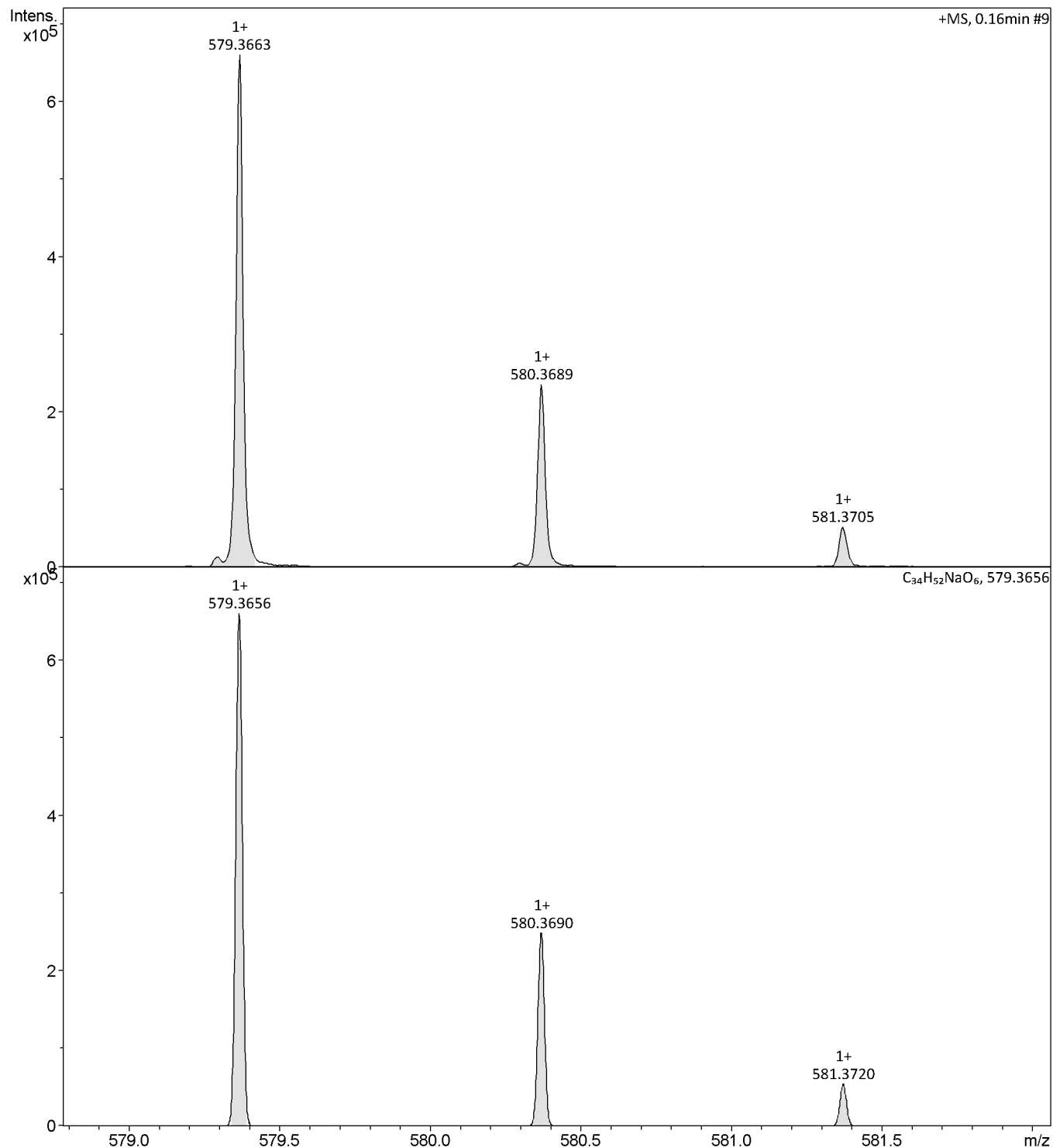
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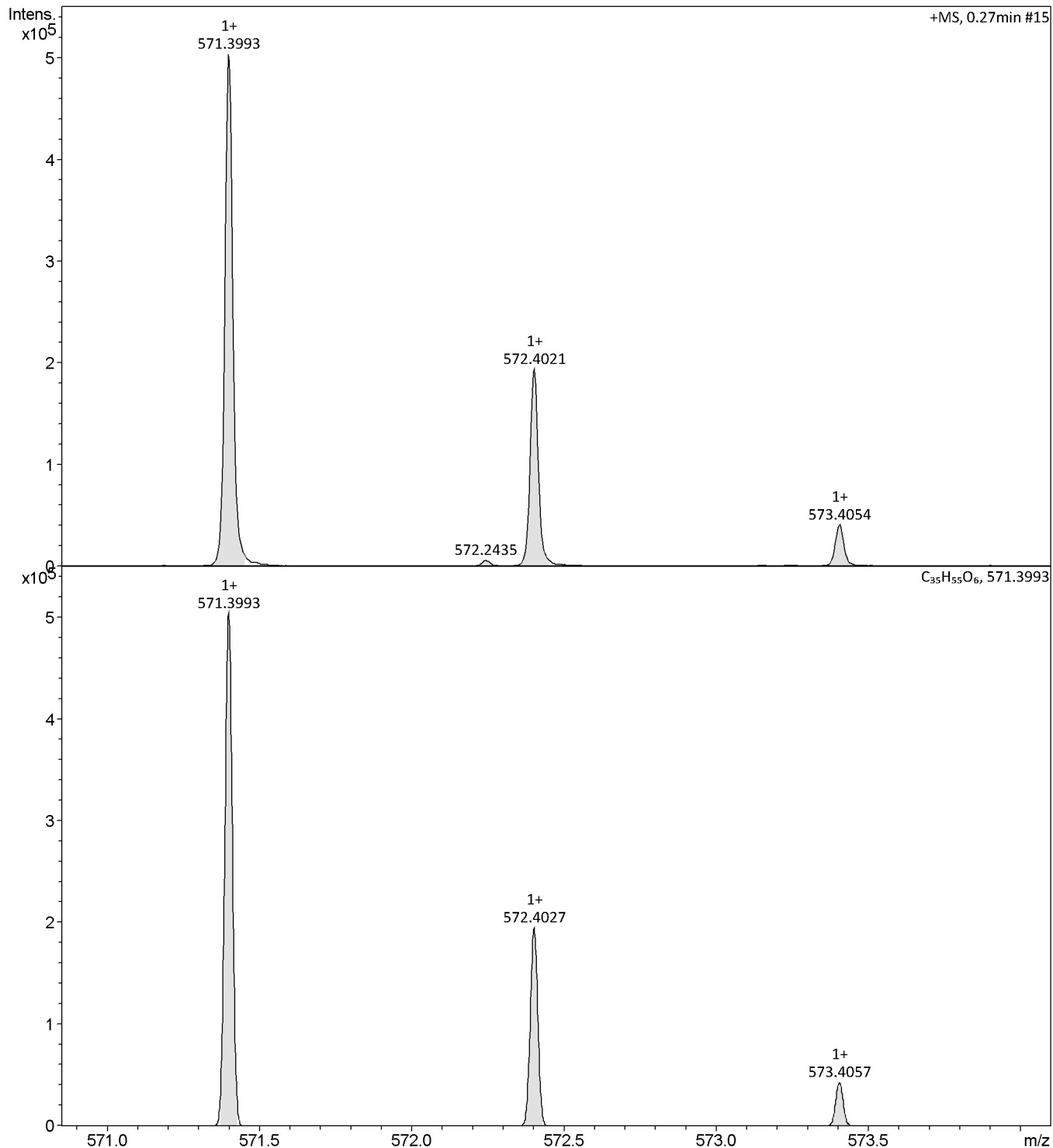
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Carboxymethyl-3 β -n-Butyryloxy-urs-12-en-28-oate (compound 11)

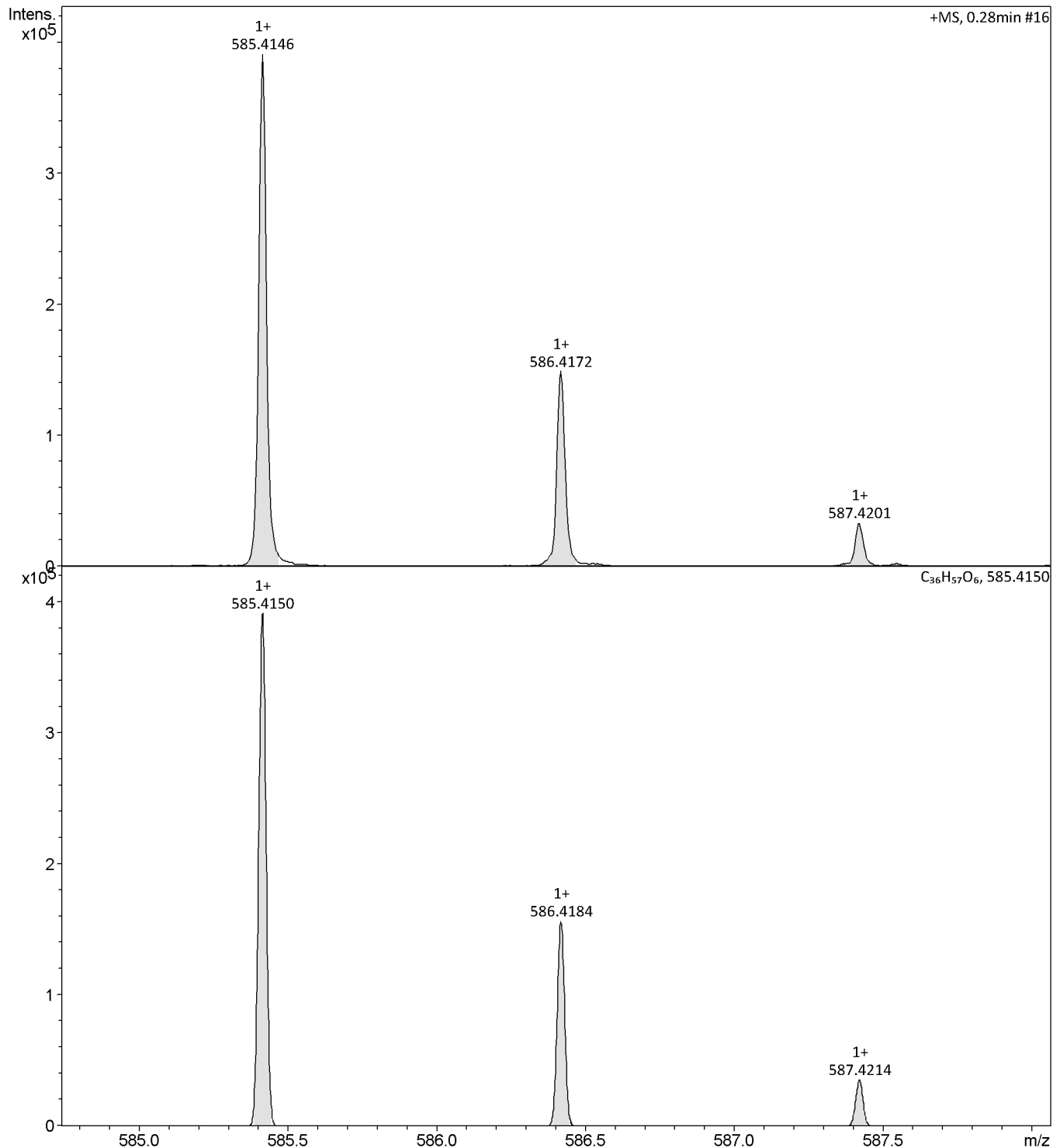
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Operator BDAL@DE
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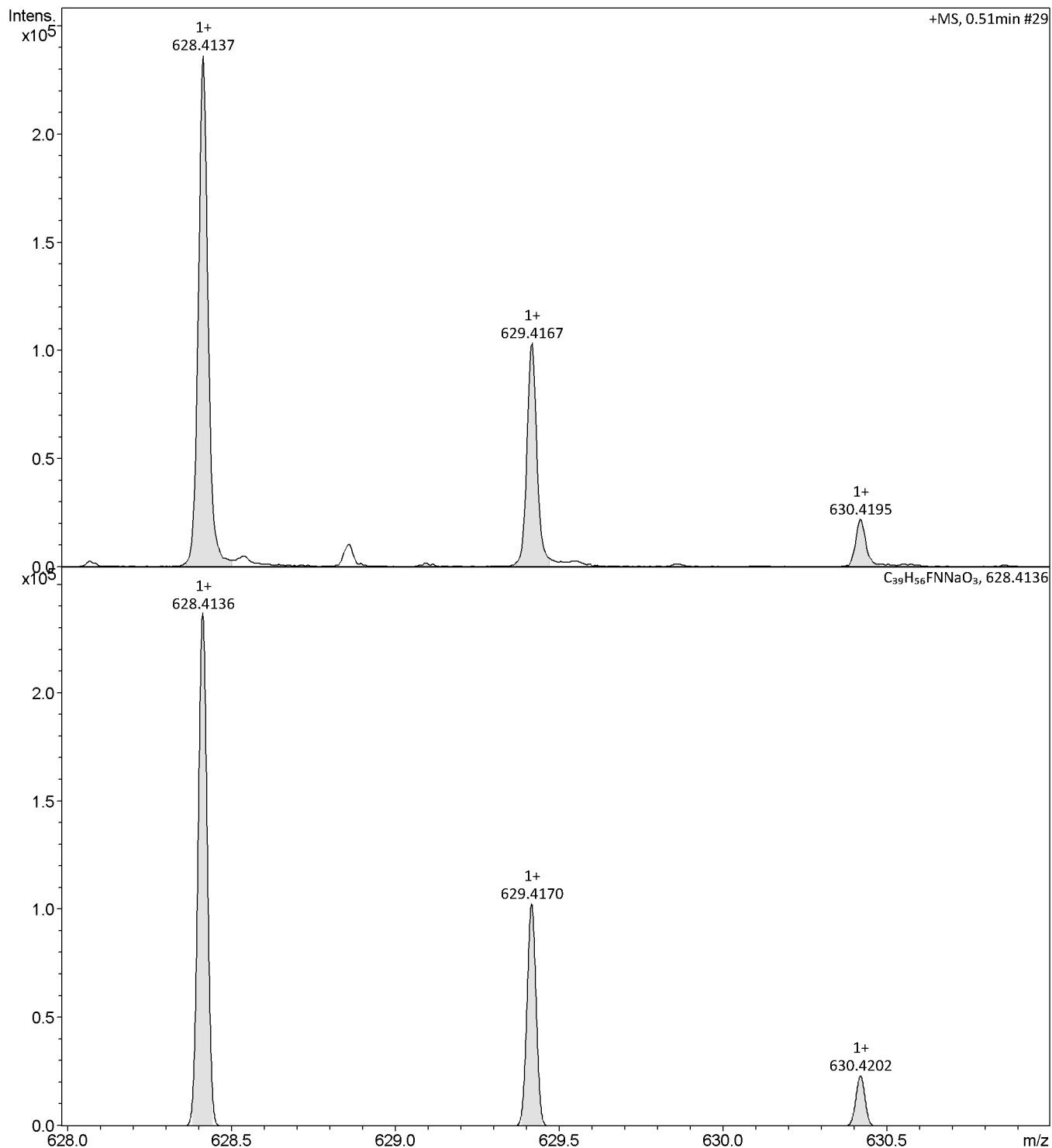
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Operator BDAL@DE
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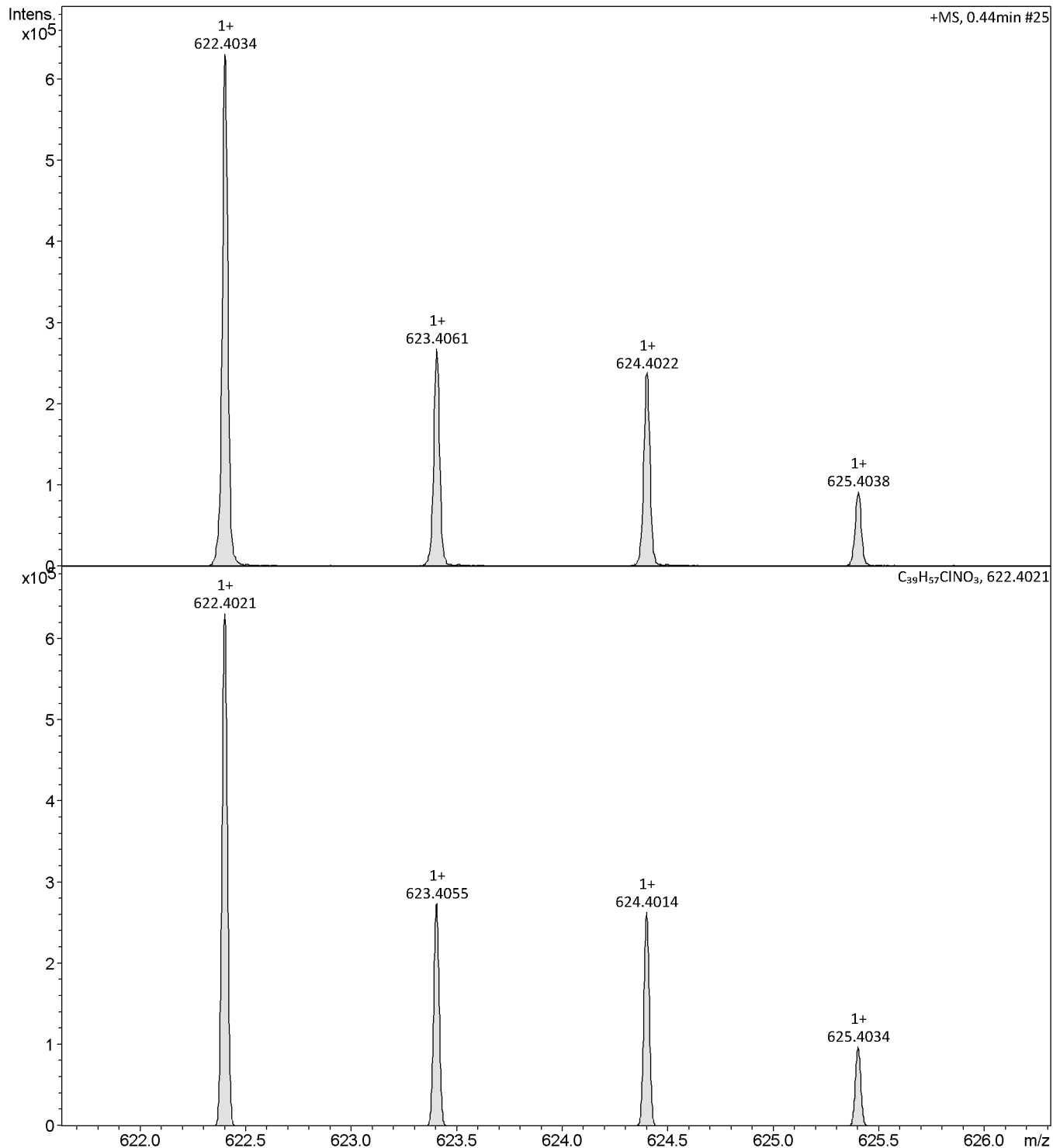
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Operator BDAL@DE
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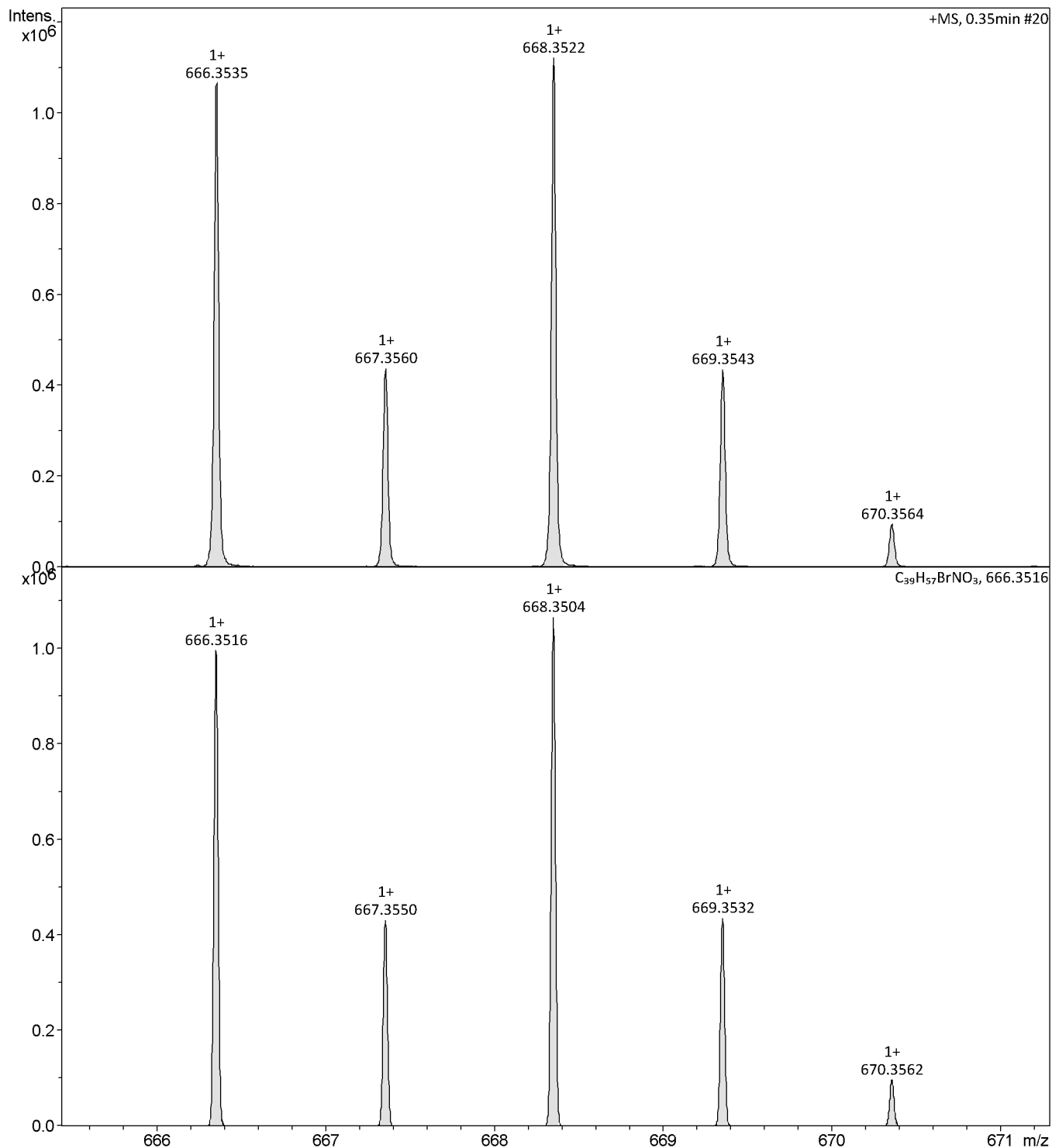
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Operator BDAL@DE
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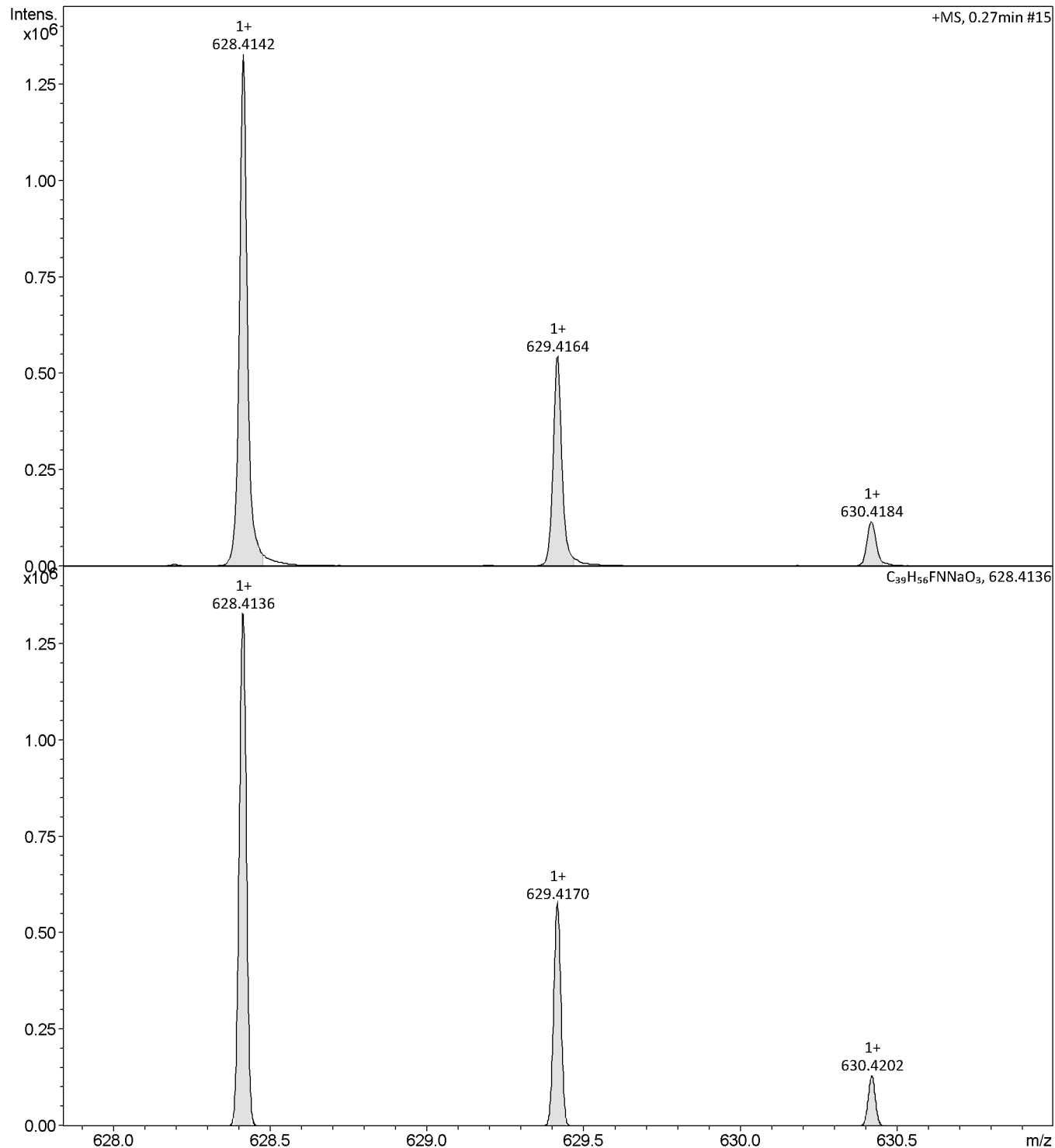
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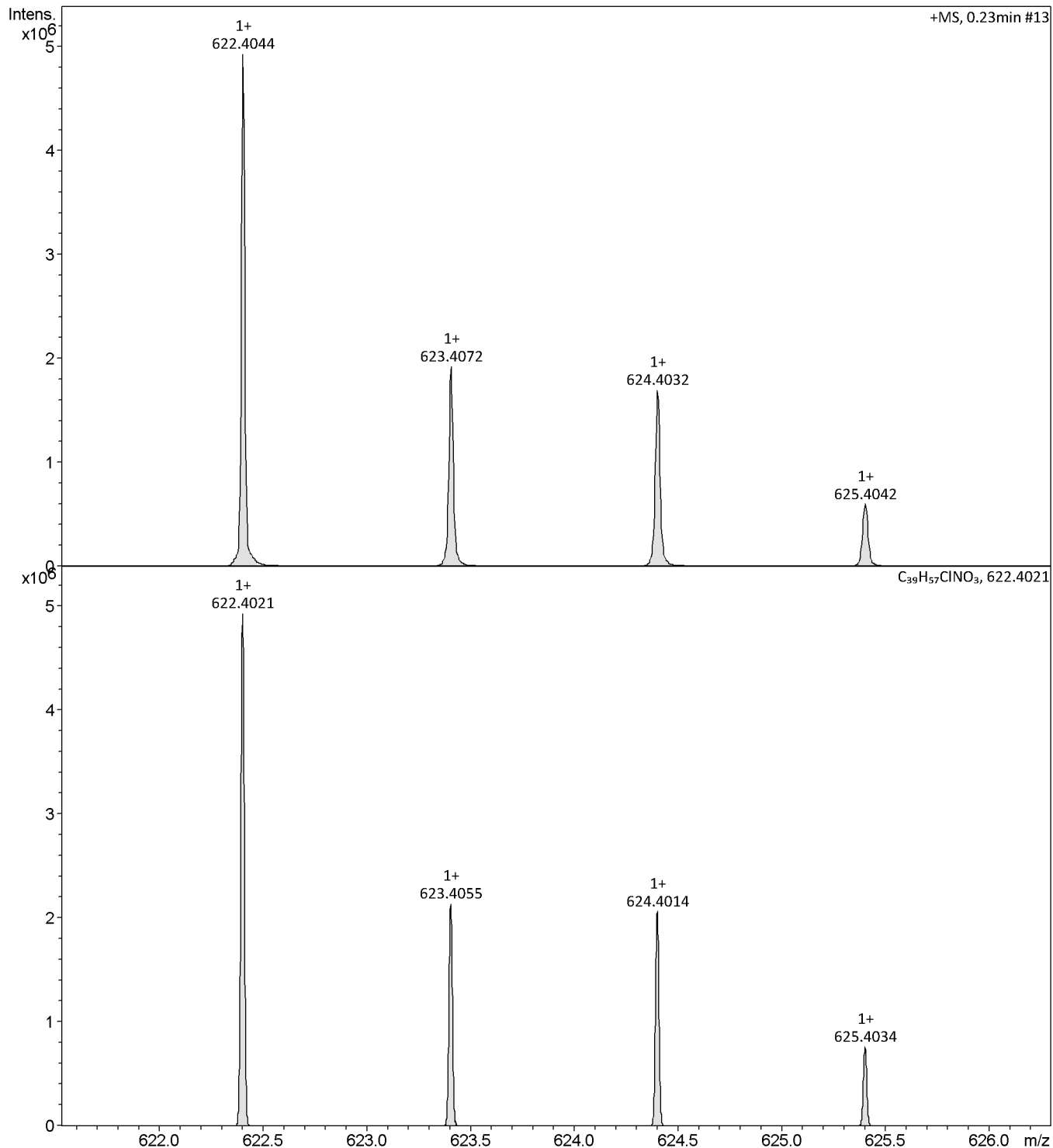
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Operator BDAL@DE
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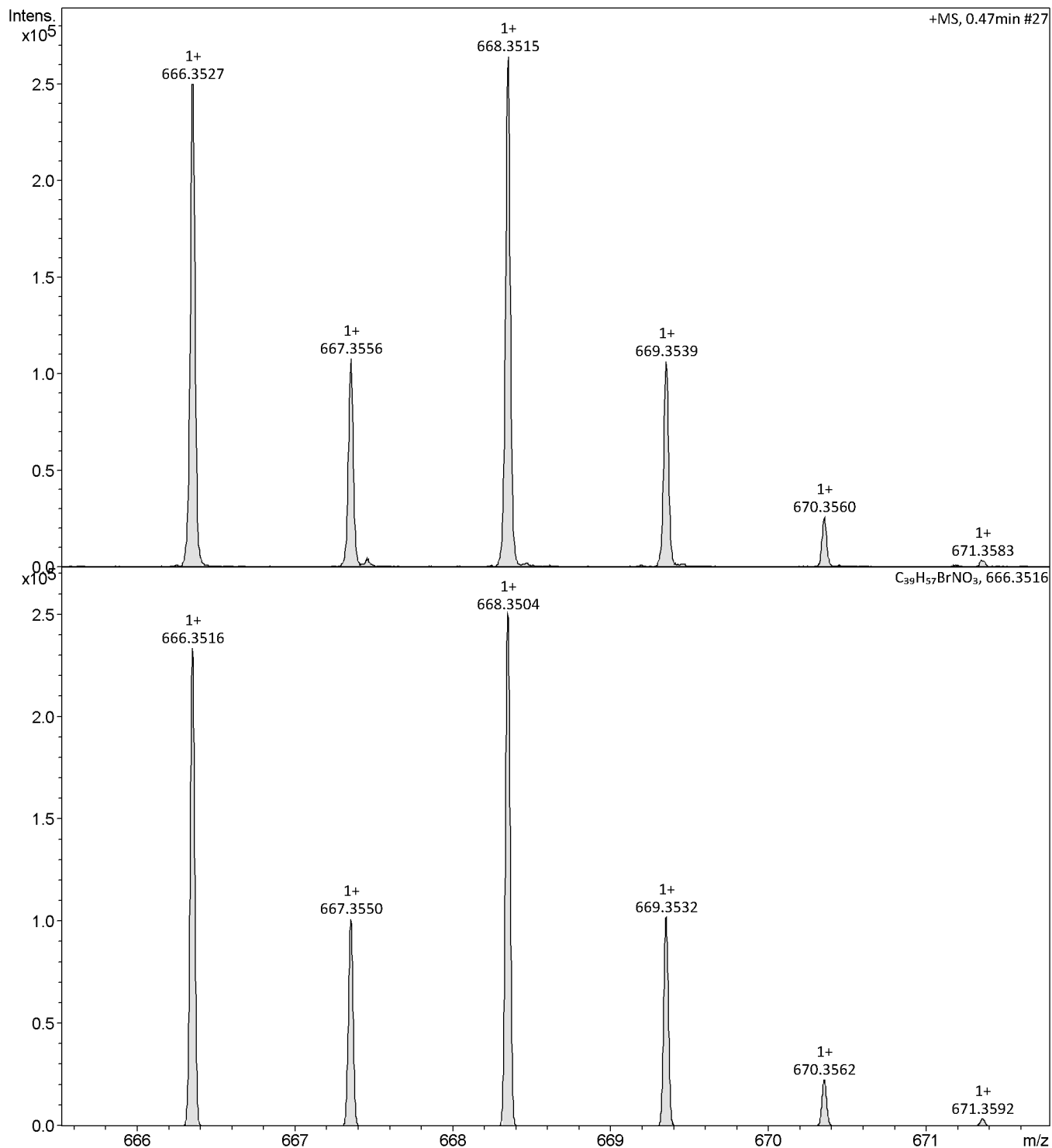
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Operator BDAL@DE
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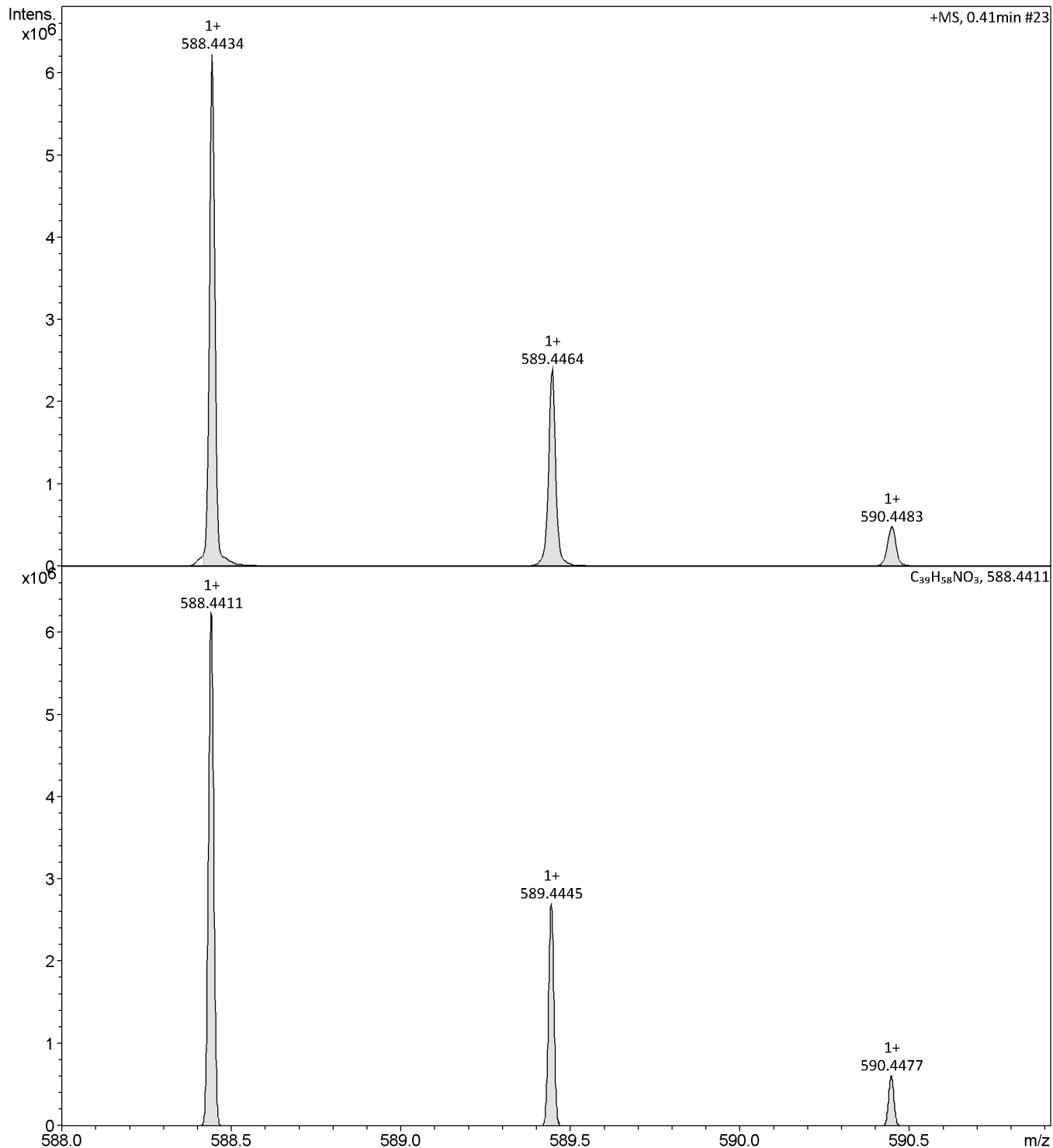
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Operator BDAL@DE
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