

Supplementary material

Novel triazole hybrids of betulin: synthesis and biological activity profile

Ewa Bębenek, Maria Jastrzębska, Monika Kadel-Tomanek, Elwira Chrobak, Beata Orzechowska, Katarzyna Zwolińska, Małgorzata Latocha, Anna Mertas, Zenon Czuba, Stanisław Boryczka

Table of Contents

Figure S1: (a) HSQC spectrum, (b) HMBC spectrum of 28-O-(1-Benzyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5a**)

Figure S2: (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum of 28-O-(1-Benzyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5a**)

Figure S3: (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum of 28-O-{1-(4-Fluorobenzyl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5b**)

Figure S4: (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum of 28-O-{1-(4-Cyanobenzyl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5c**)

Figure S5: (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum of 28-O-(1-Phenylthiomethyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5d**)

Figure S6: (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum of 28-O-{1-(3'-Deoxythymidine-5'-yl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5e**)

Figure S7: (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum of 3,28-O,O'-Di{1-(4-fluorobenzyl-1H-[1,2,3]-triazol-4-yl)carbonyl}betulin (**6b**)

Figure S8: (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum of 3,28-O,O'-Di{1-(3-hydroxypropyl-1H-[1,2,3]-triazol-4-yl)carbonyl}betulin (**6h**)

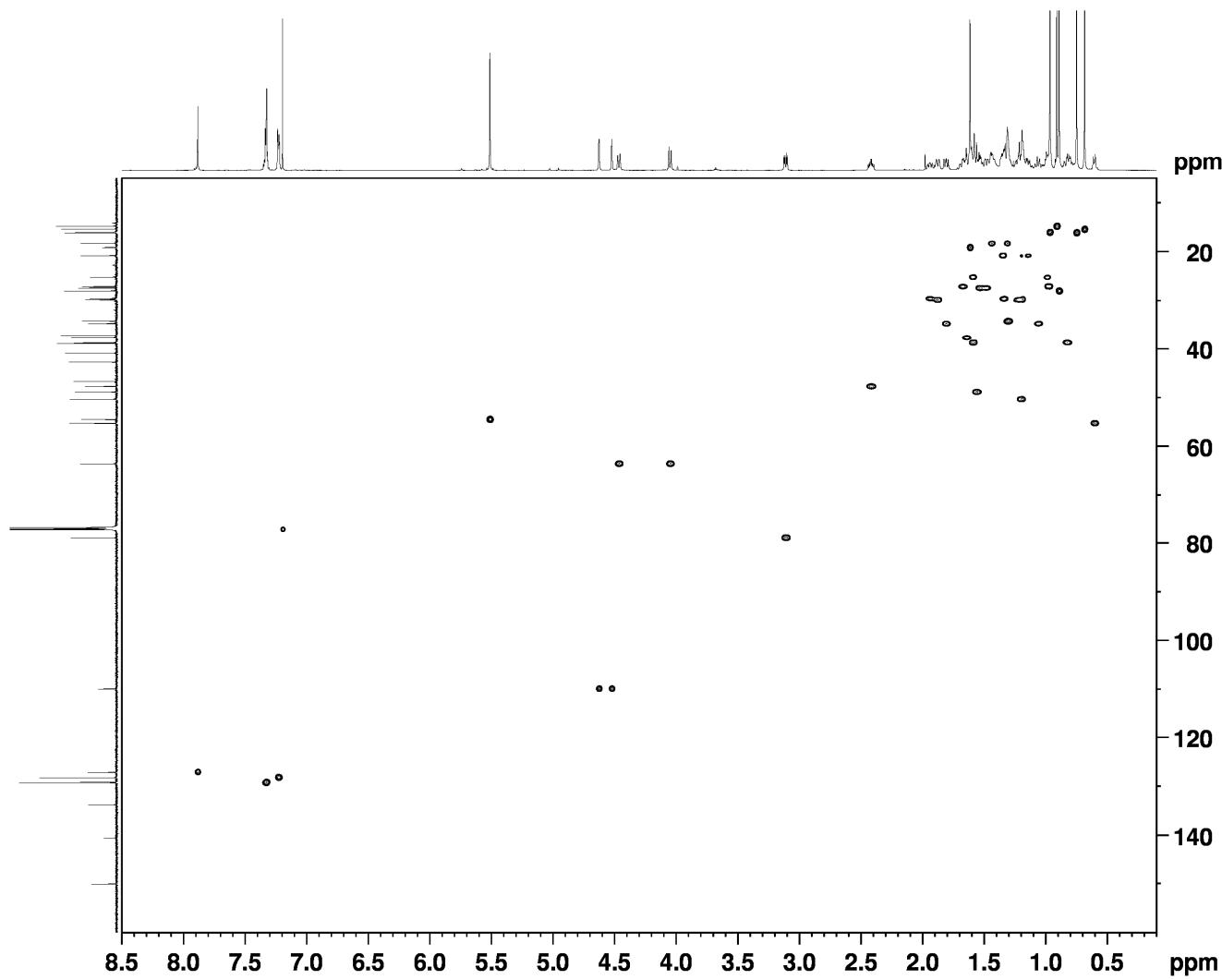


Figure S1 (a): HSQC spectrum of 28-O-(1-Benzyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5a**)

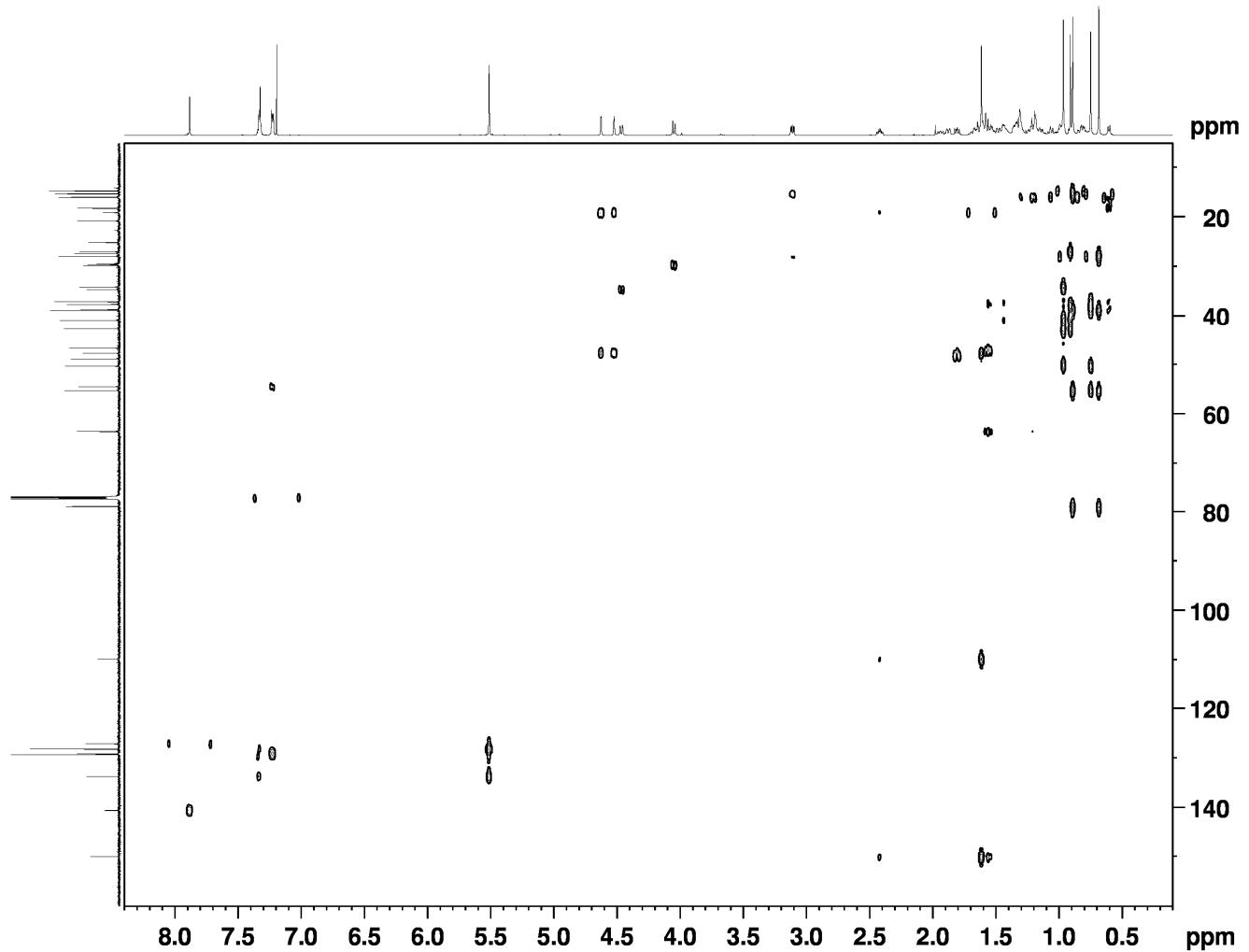


Figure S1 (b): HMBC spectrum of 28-O-(1-Benzyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5a**)

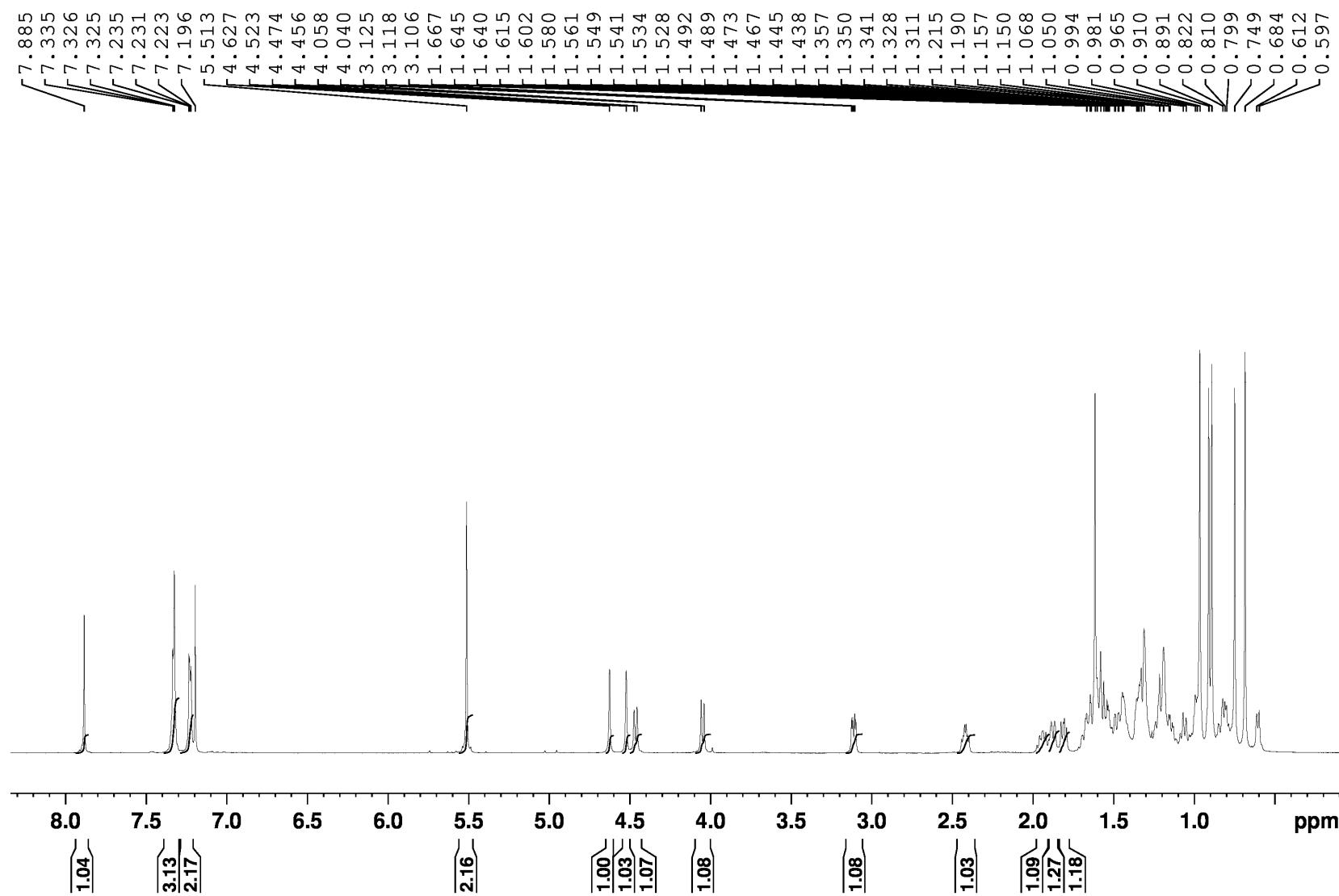


Figure S2 (a): ¹H NMR spectrum of 28-O-(1-Benzyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5a**)

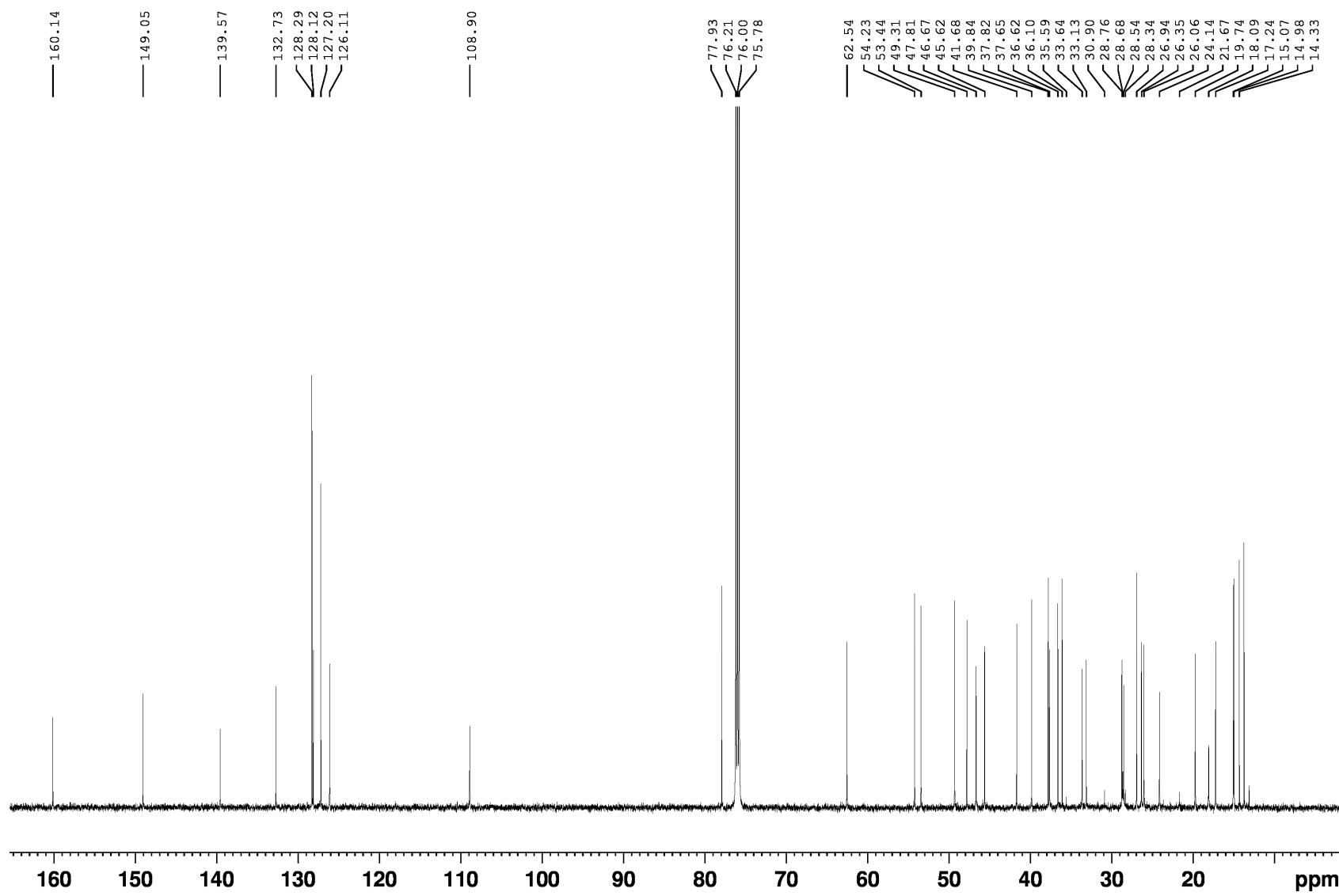


Figure S2 (b): ^{13}C NMR spectrum of 28-O-(1-Benzyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5a**)

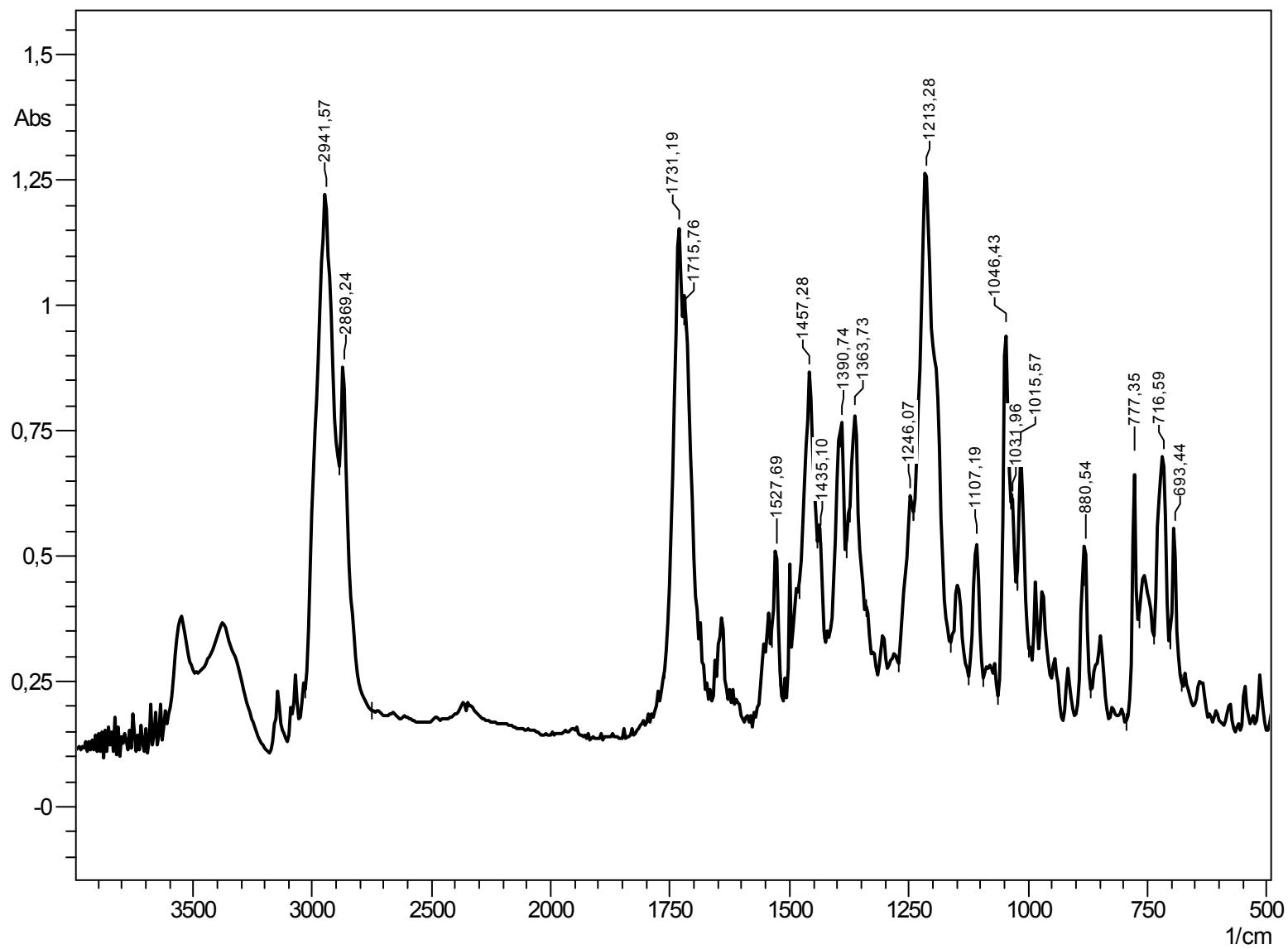


Figure S2 (c): IR spectrum of 28-O-(1-Benzyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5a**)

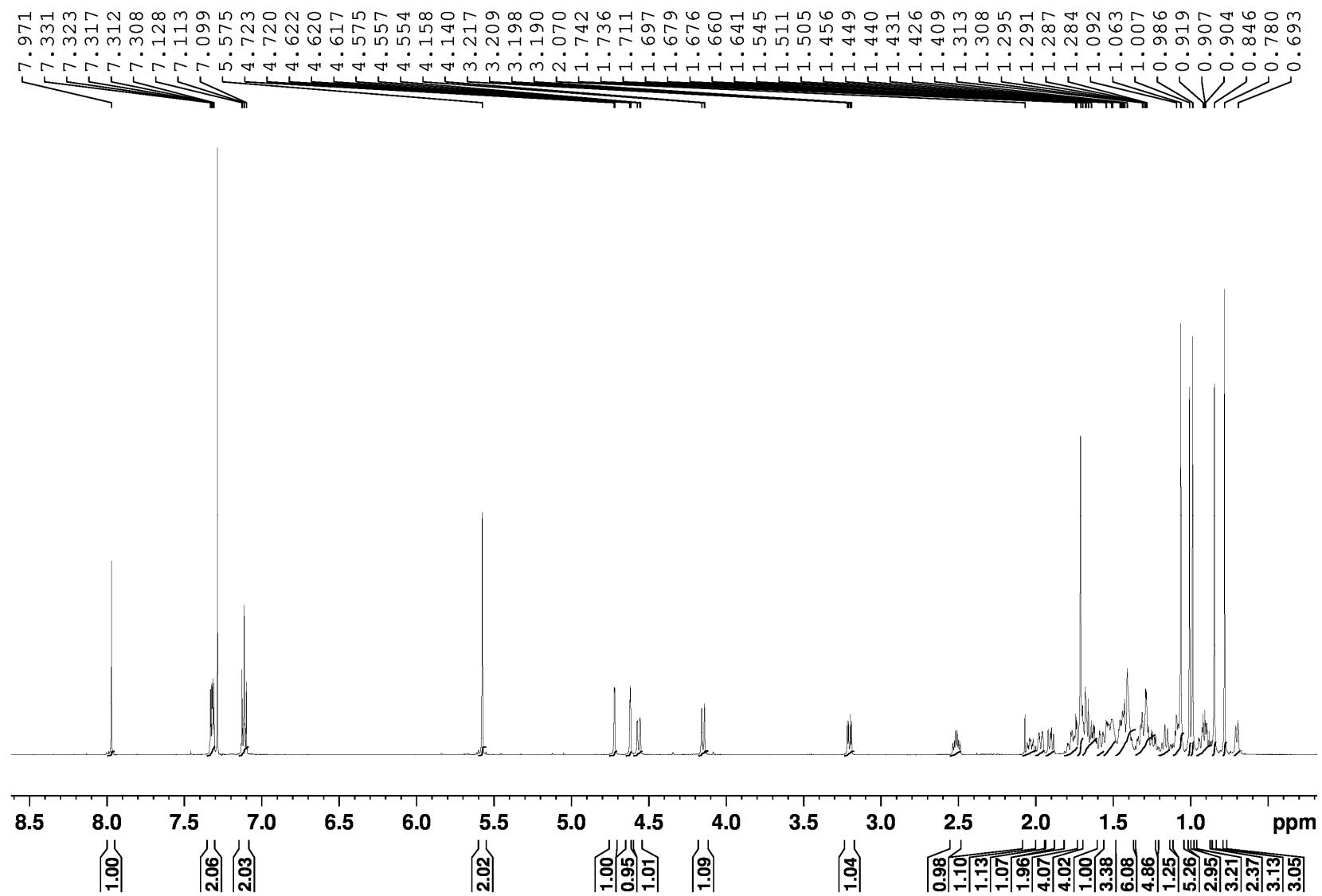


Figure S3 (a): ¹H NMR spectrum of 28-O-{1-(4-Fluorobenzyl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5b**)

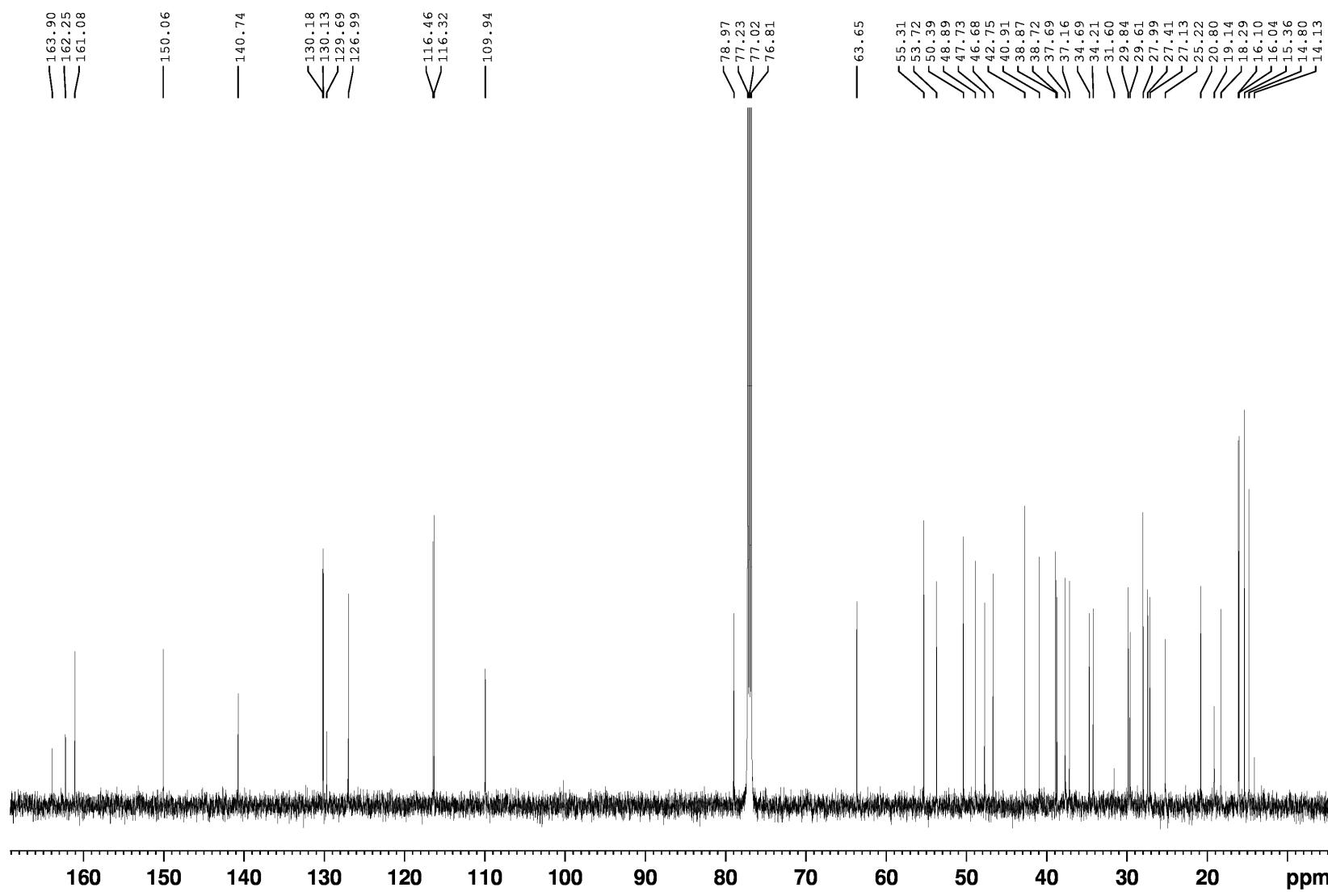


Figure S3 (b): ¹³C NMR spectrum of 28-O-{1-(4-Fluorobenzyl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5b**)

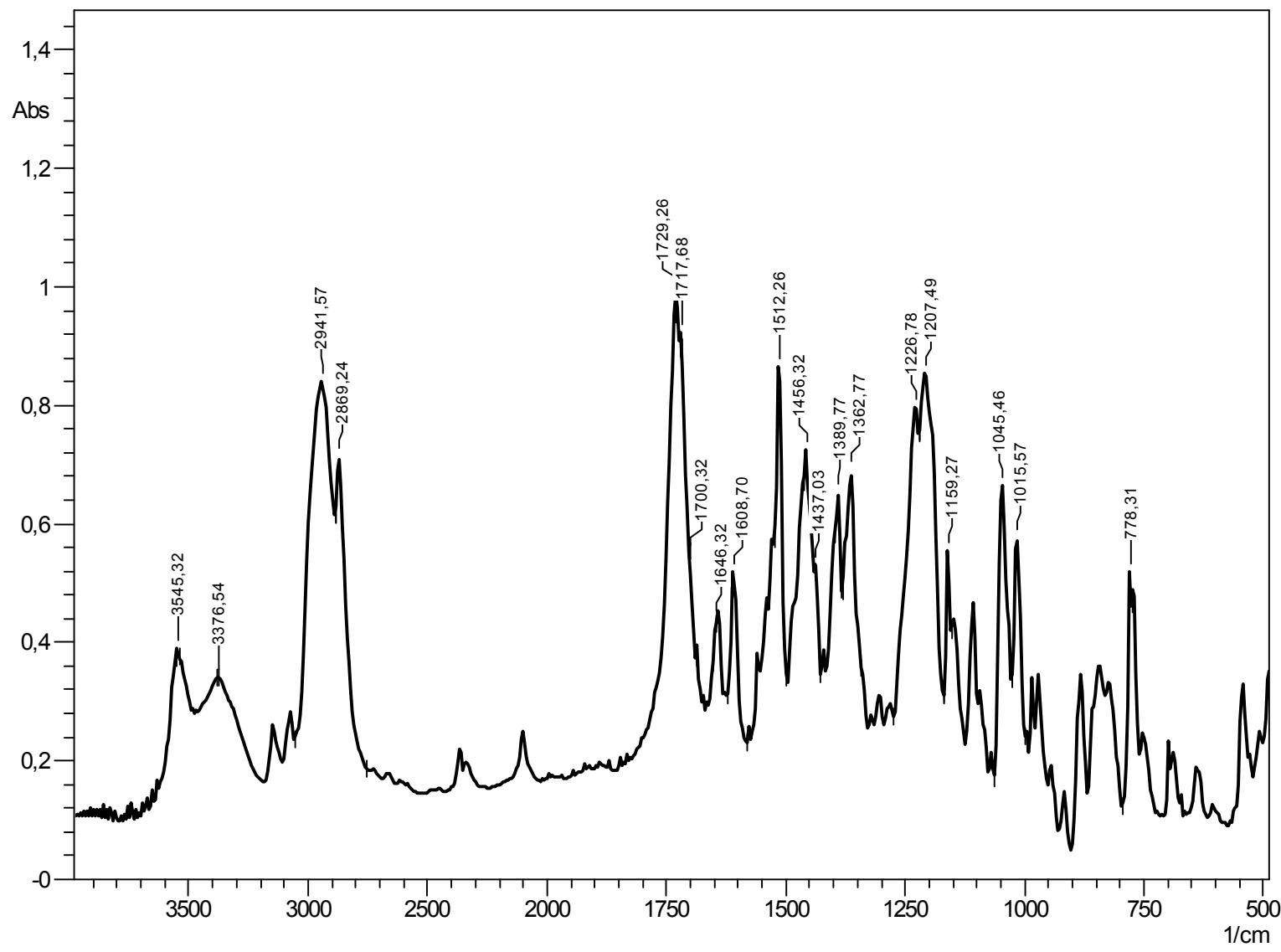


Figure S3 (c): IR spectrum of 28-O-{1-(4-Fluorobenzyl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5b**)

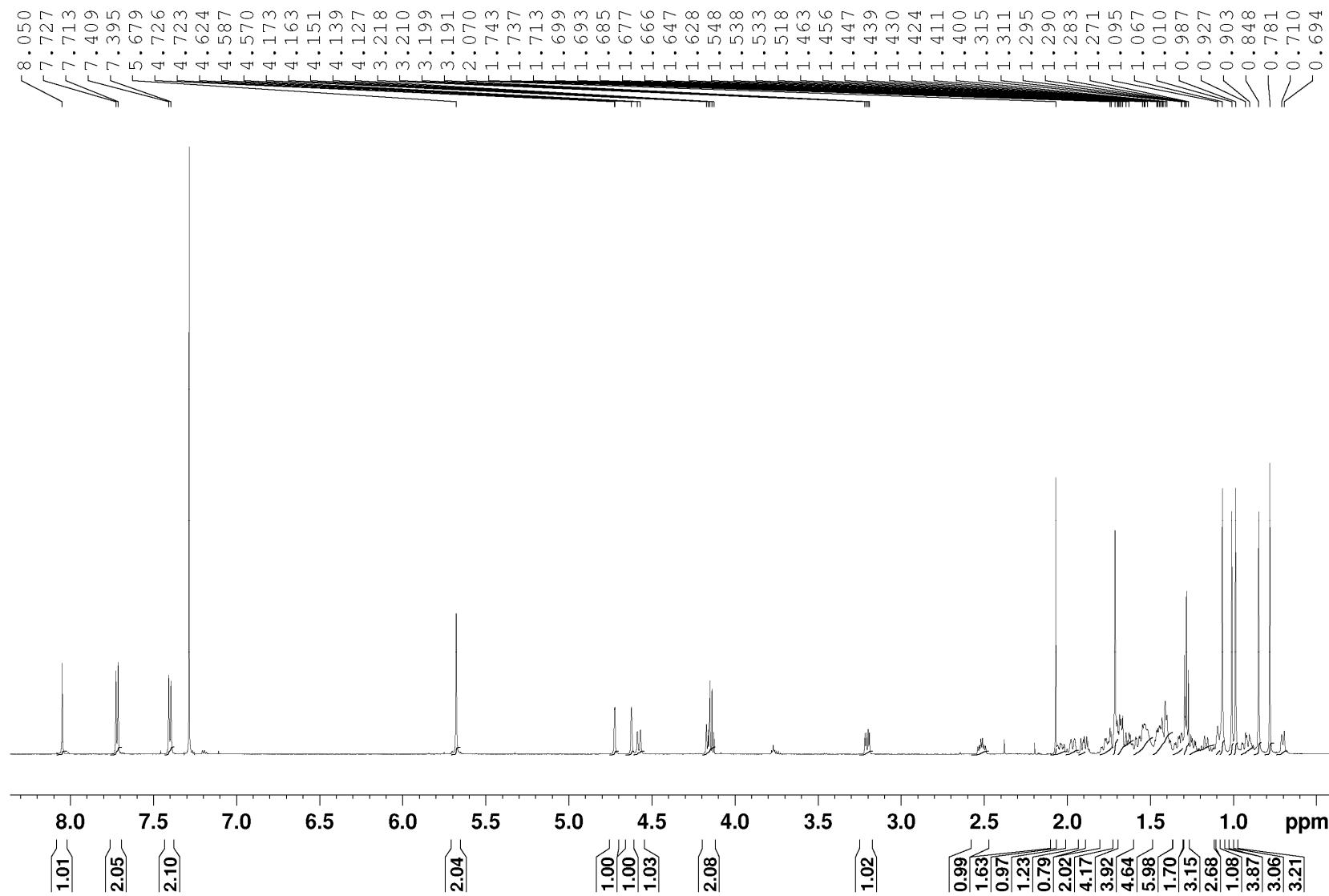


Figure S4 (a): ¹H NMR spectrum of 28-O-{1-(4-Cyanobenzyl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5c**)

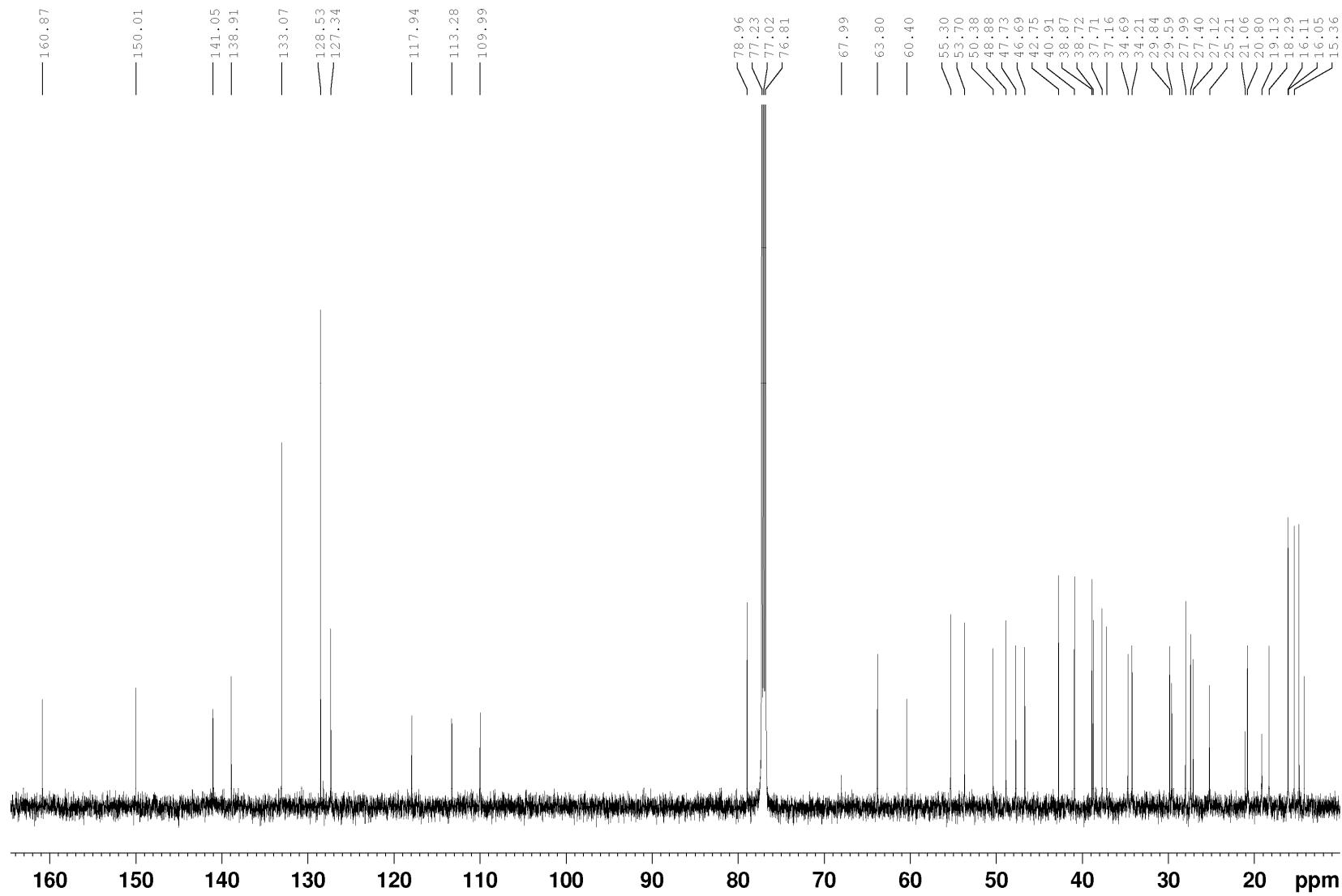


Figure S4 (b): ^{13}C NMR spectrum of 28-O-{1-(4-Cyanobenzyl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5c**)

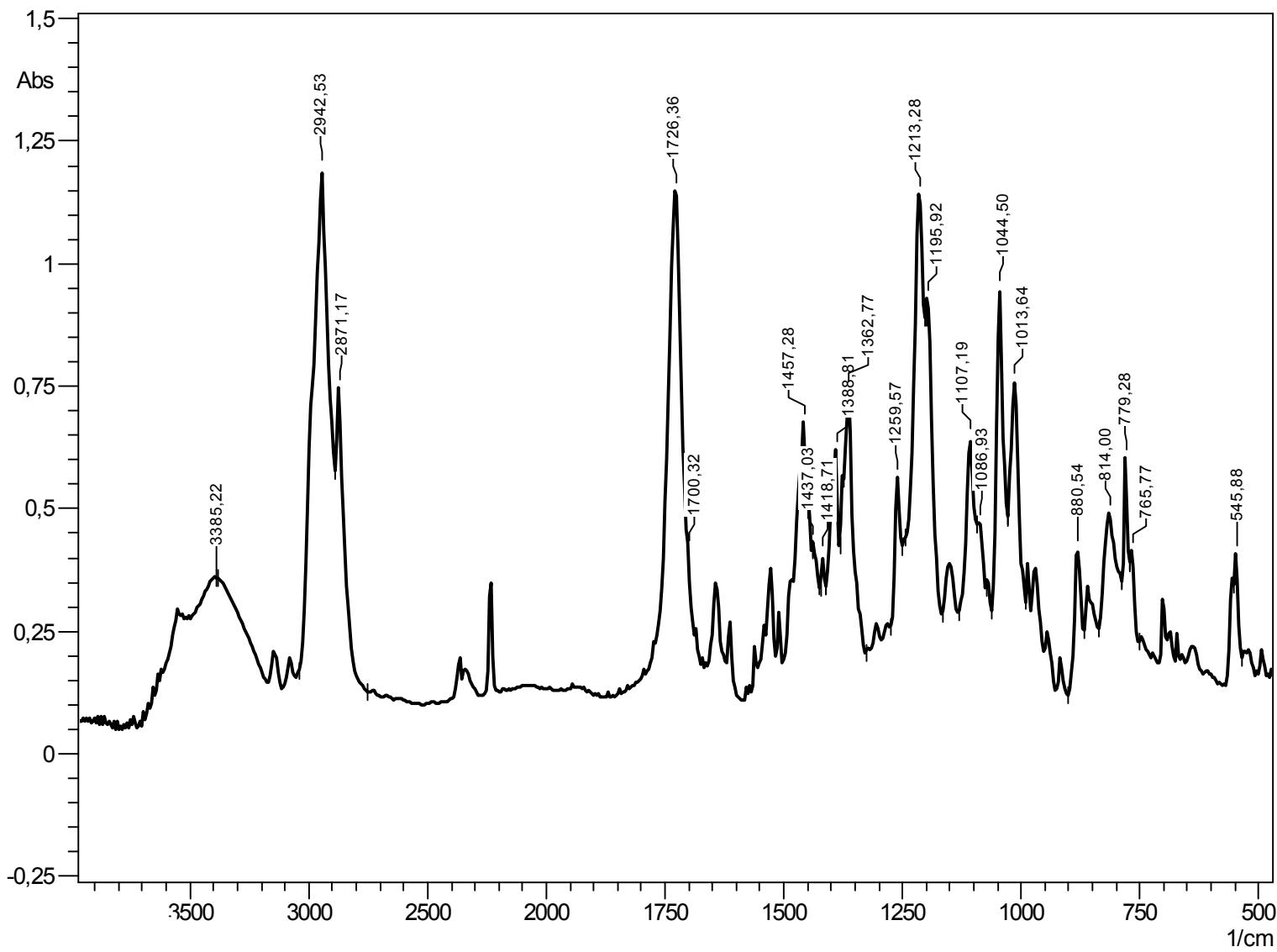


Figure S4 (c): IR spectrum of 28-O-{1-(4-Cyanobenzyl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5c**)

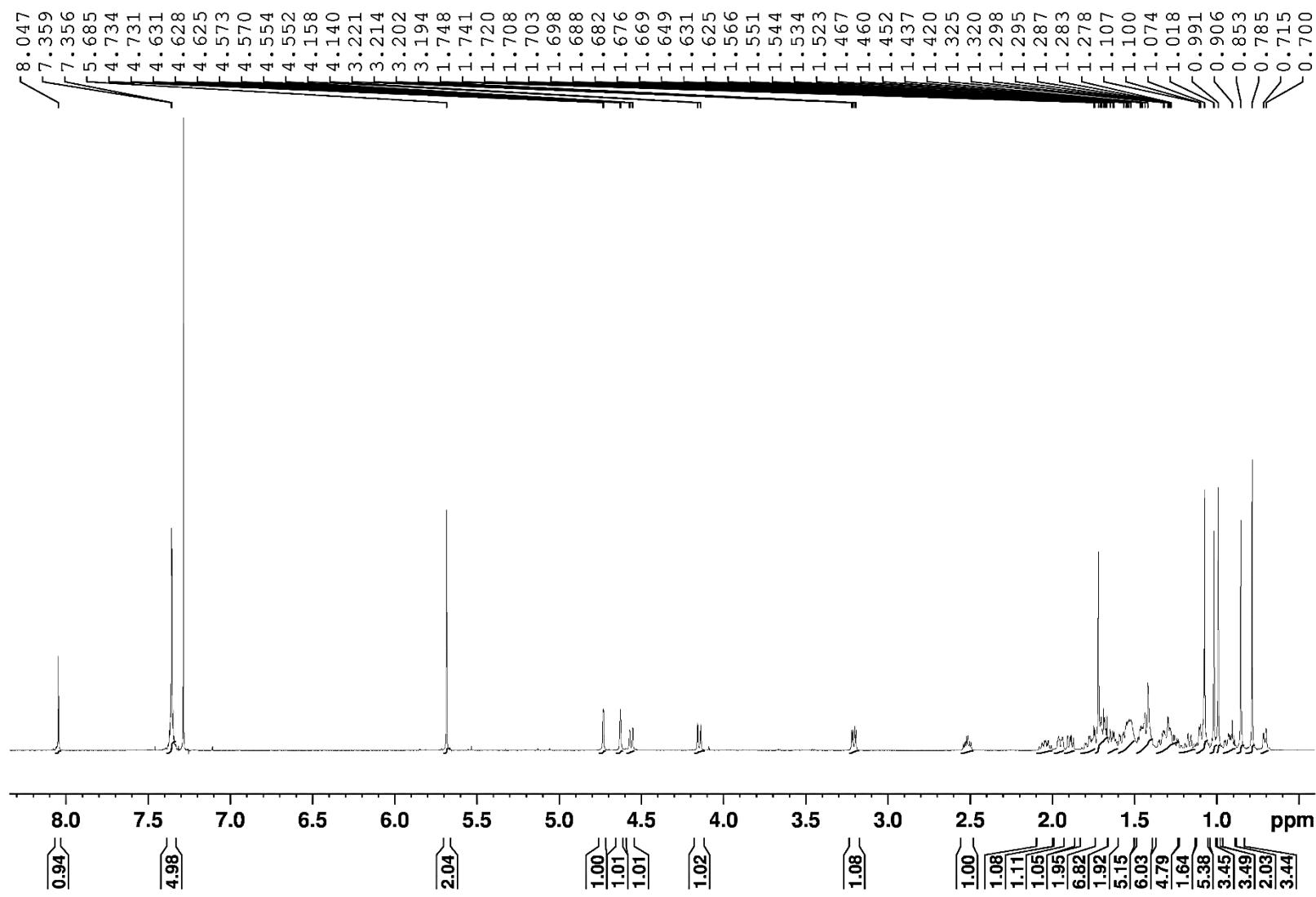


Figure S5 (a): ¹H NMR spectrum of 28-O-(1-Phenylthiomethyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5d**)

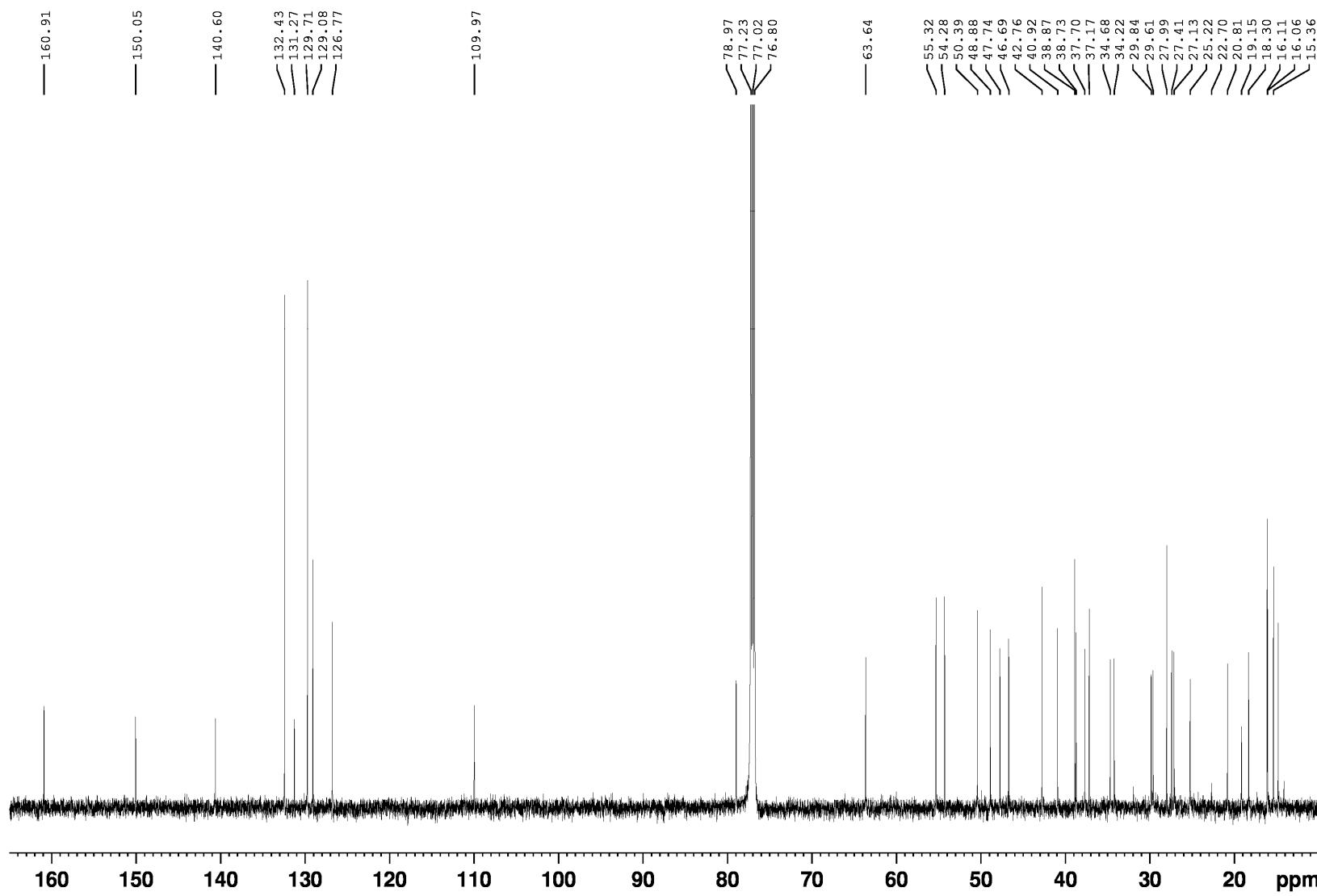


Figure S5 (b): ^{13}C NMR spectrum of 28-O-(1-Phenylthiomethyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5d**)

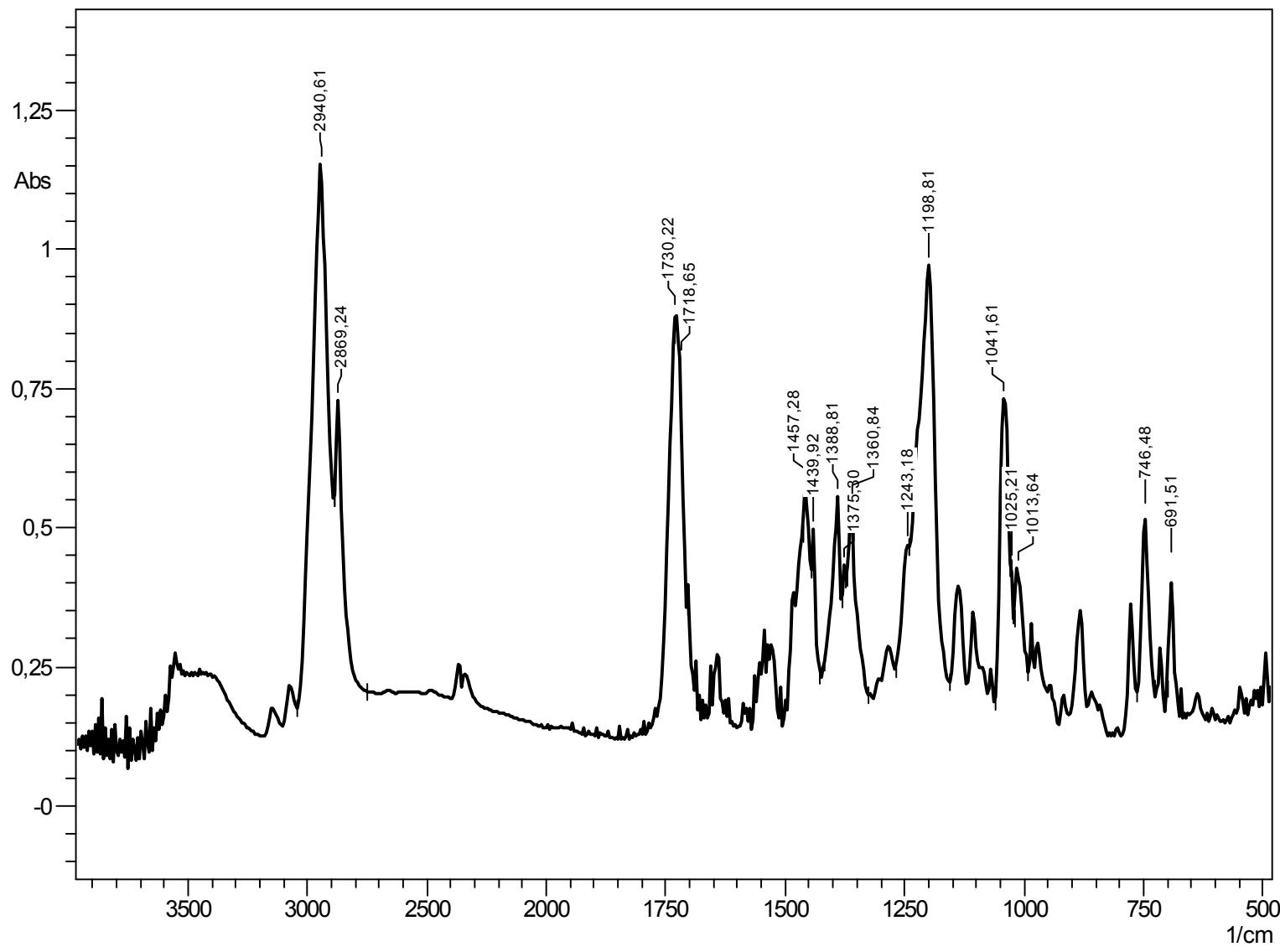


Figure S5 (c): IR spectrum of 28-O-(1-Phenylthiomethyl-1H-[1,2,3]-triazol-4-yl)carbonylbetulin (**5d**)

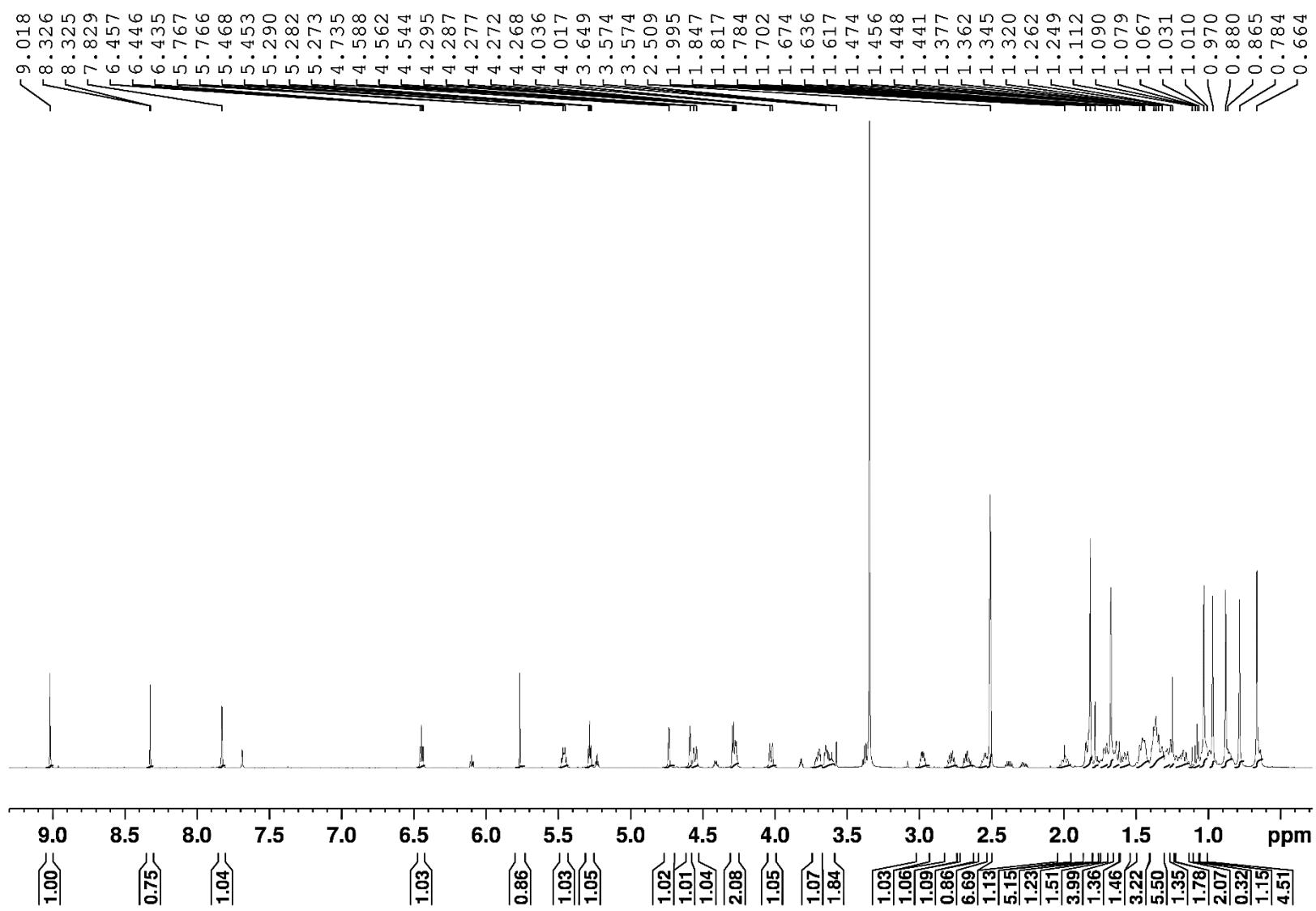


Figure S6 (a): ¹H NMR spectrum of 28-O-{1-(3'-Deoxythymidine-5'-yl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5e**)

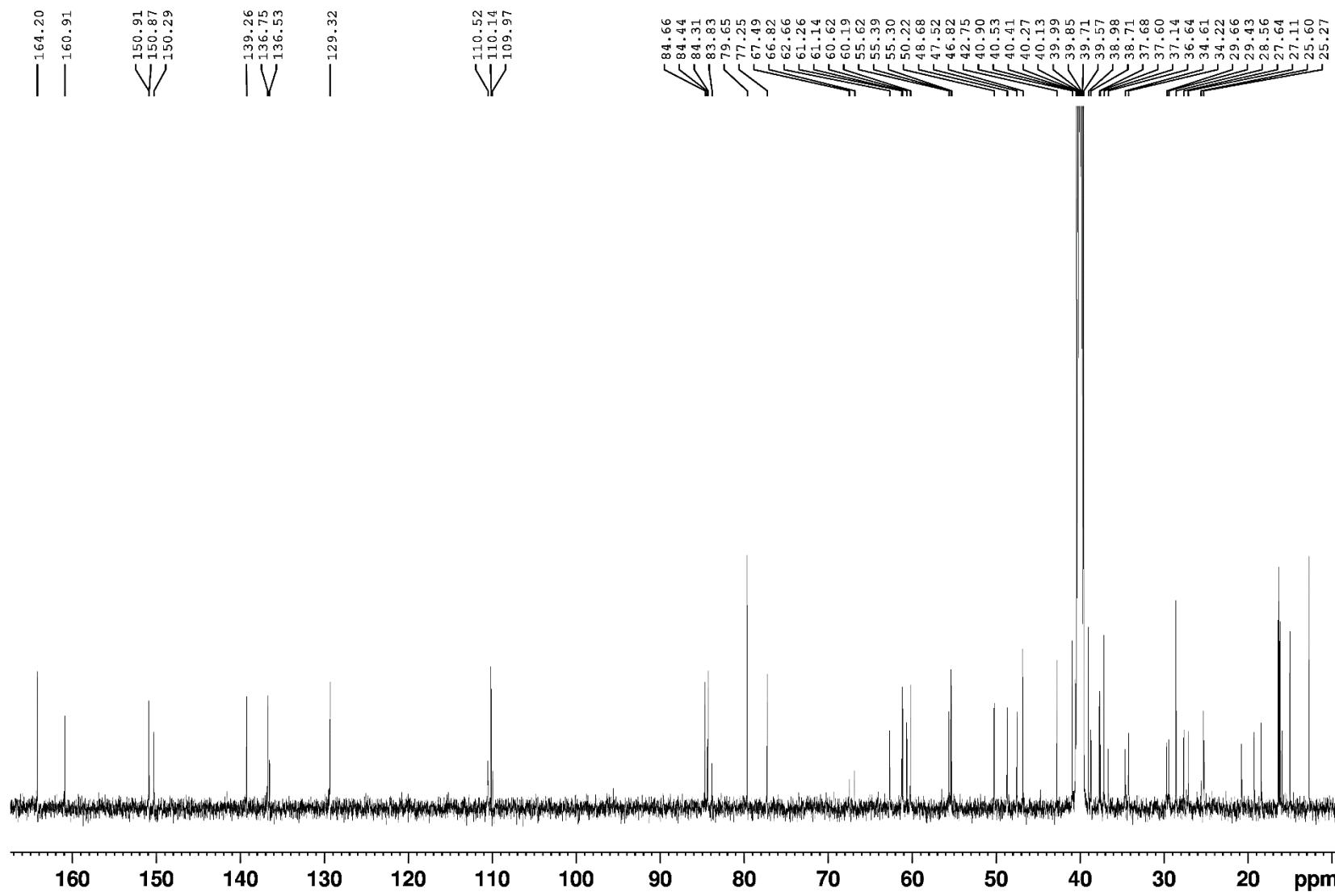


Figure S6 (b): ¹³C NMR spectrum of 28-O-{1-(3'-Deoxythymidine-5'-yl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5e**)

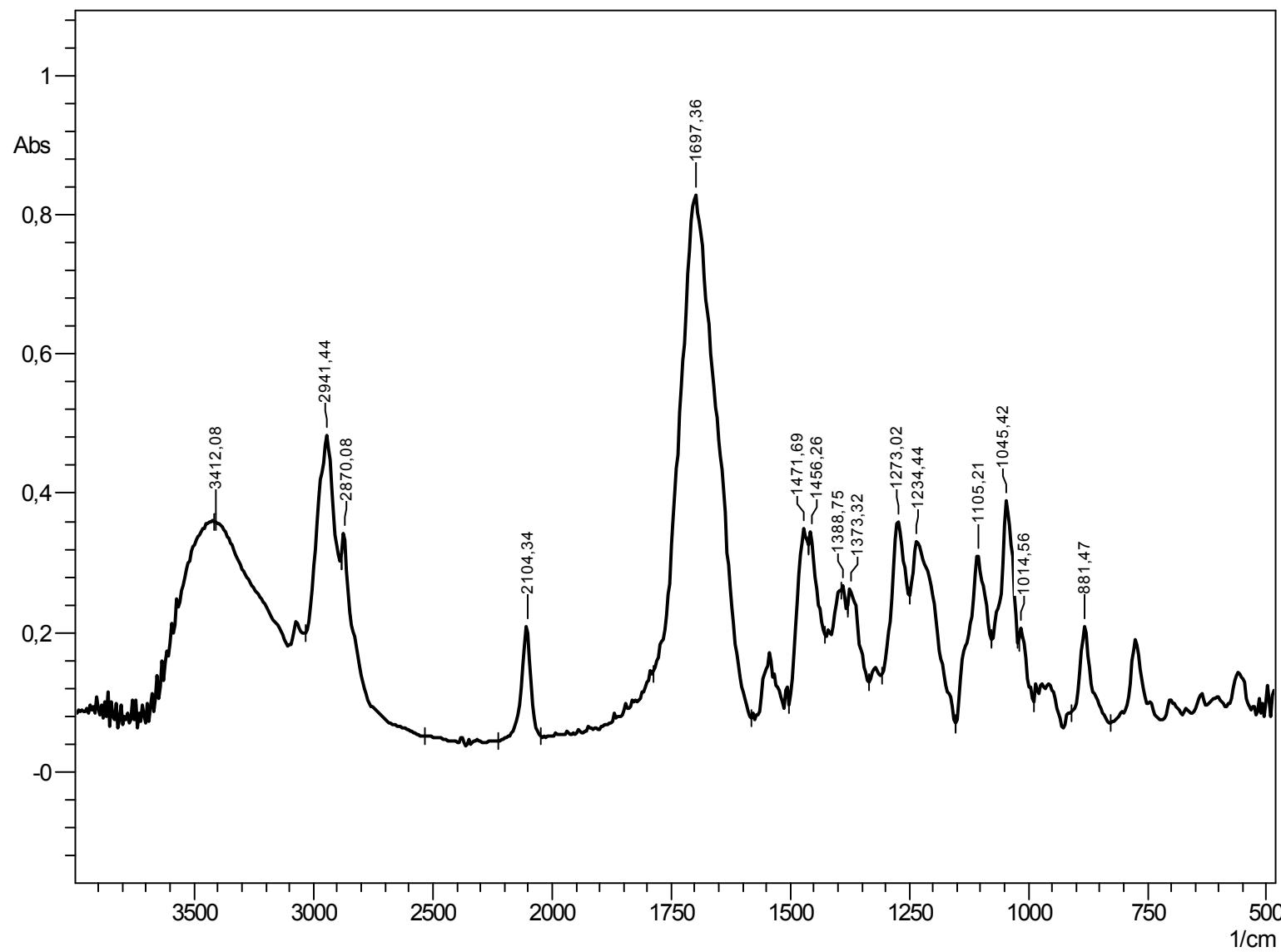


Figure S6 (c): IR spectrum of 28-O-{1-(3'-Deoxythymidine-5'-yl)-1H-[1,2,3]-triazol-4-yl}carbonylbetulin (**5e**)

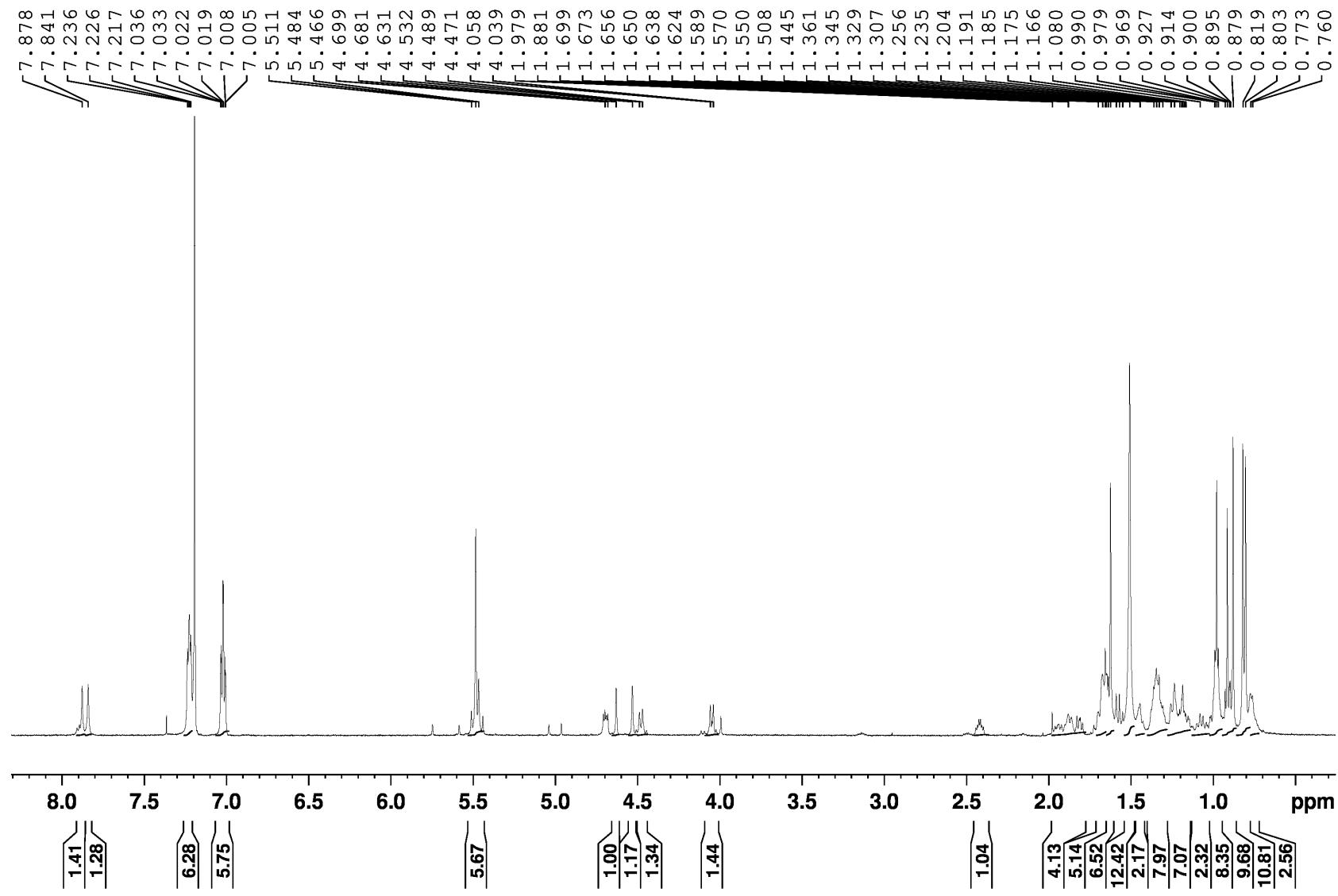


Figure S7 (a): ^1H NMR spectrum of 3,28-O,O'-Di{1-(4-fluorobenzyl-1H-[1,2,3]-triazol-4-yl)carbonyl}betulin (**6b**)

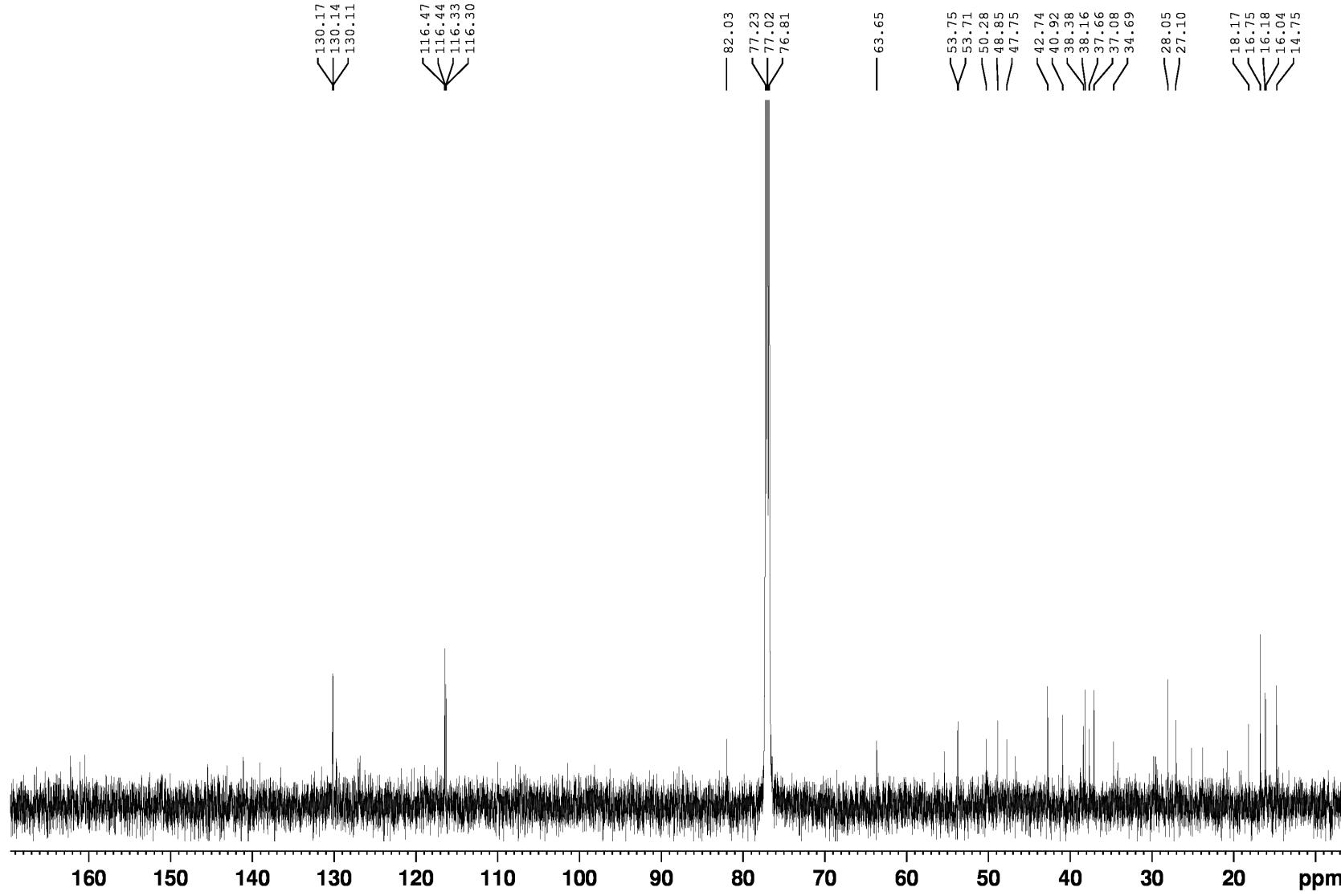


Figure S7 (b): ^{13}C NMR spectrum of 3,28-O,O'-Di{1-(4-fluorobenzyl-1H-[1,2,3]-triazol-4-yl)carbonyl}betulin (**6b**)

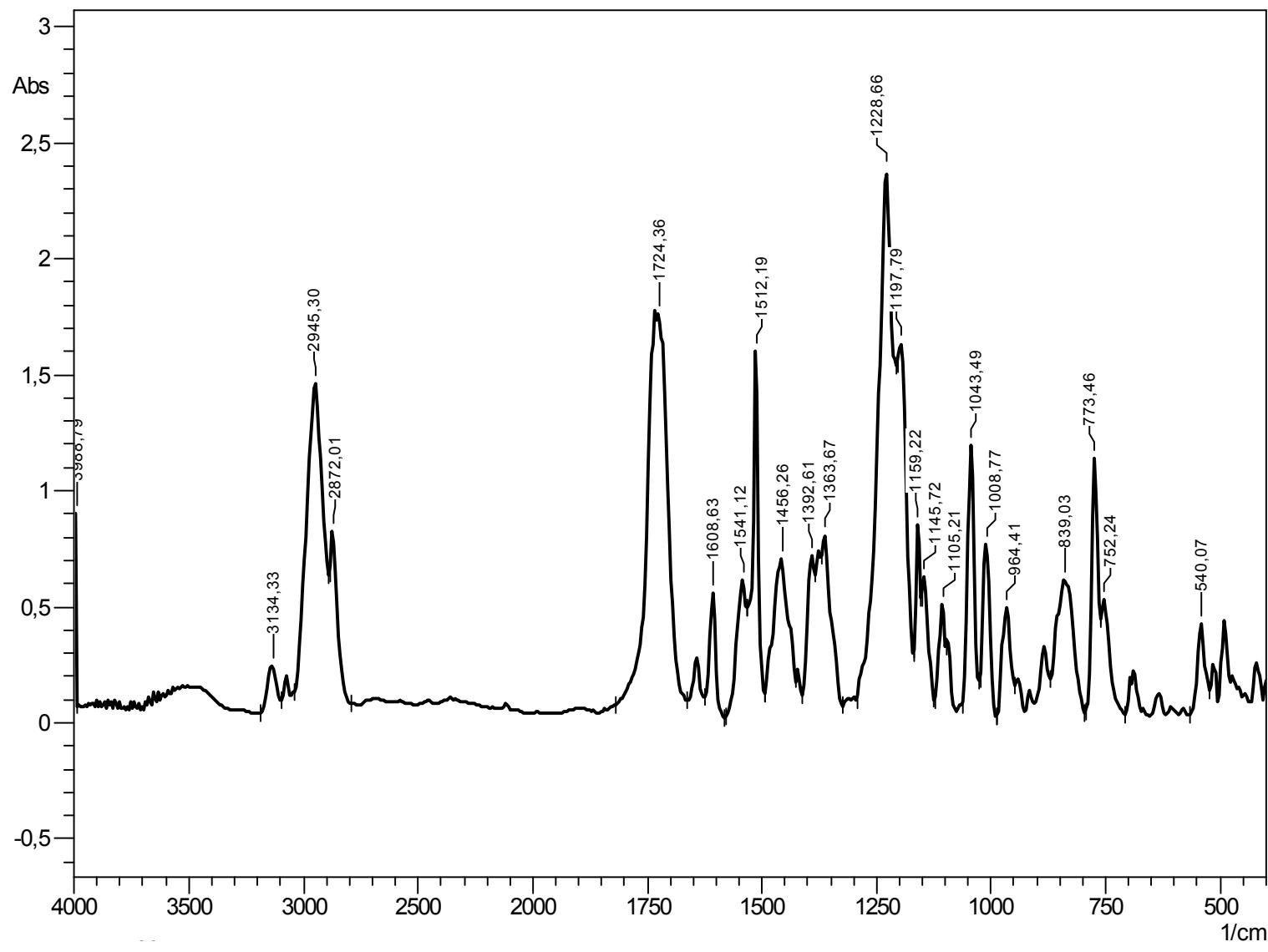


Figure S7 (c): IR spectrum of 3,28-O,O'-Di{1-(4-fluorobenzyl-1H-[1,2,3]-triazol-4-yl)carbonyl}betulin (**6b**)

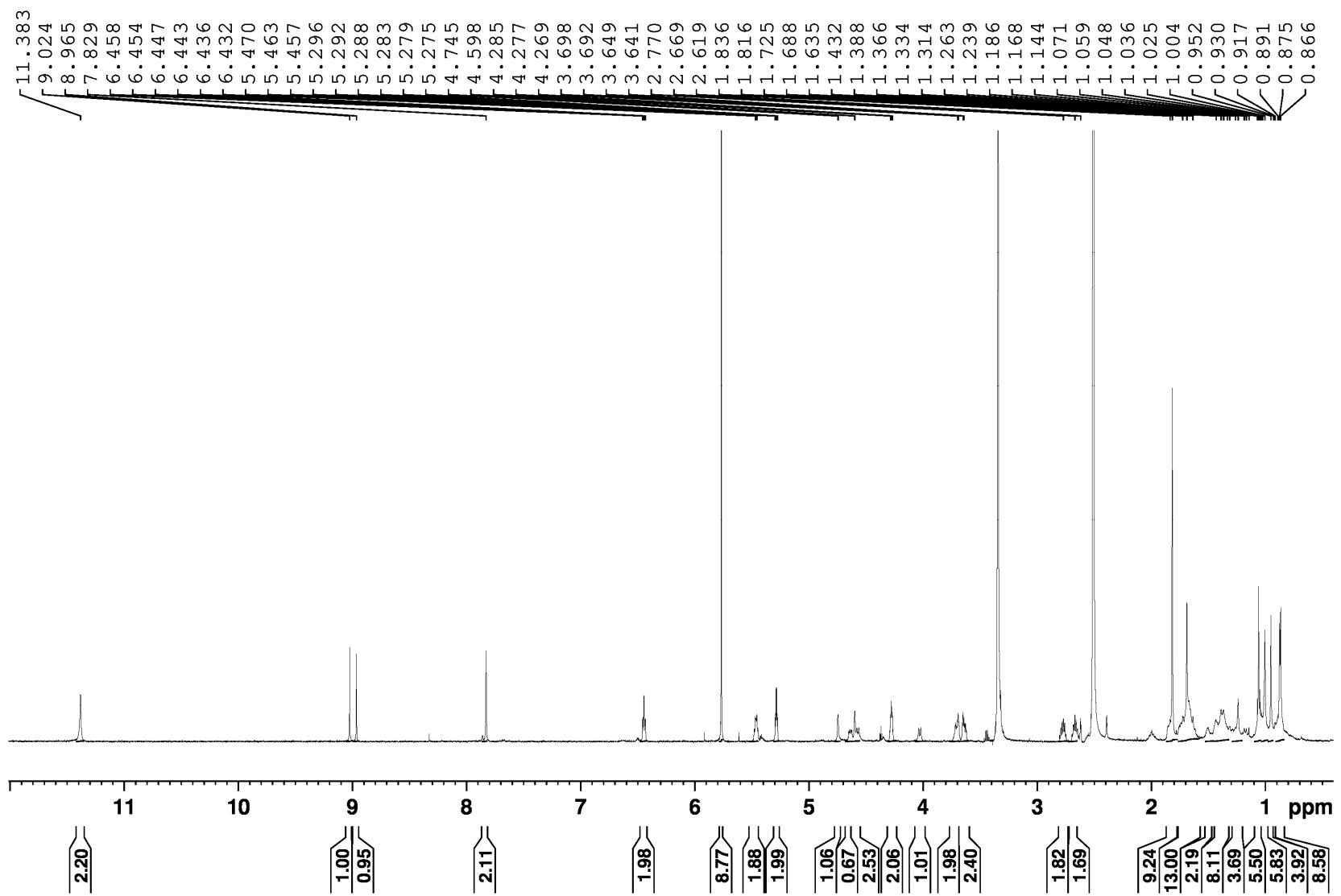


Figure S8 (a): ¹H NMR spectrum of 3,28-O,O'-Di{1-(3-hydroxypropyl-1H-[1,2,3]-triazol-4-yl)carbonyl}betulin (**6h**)

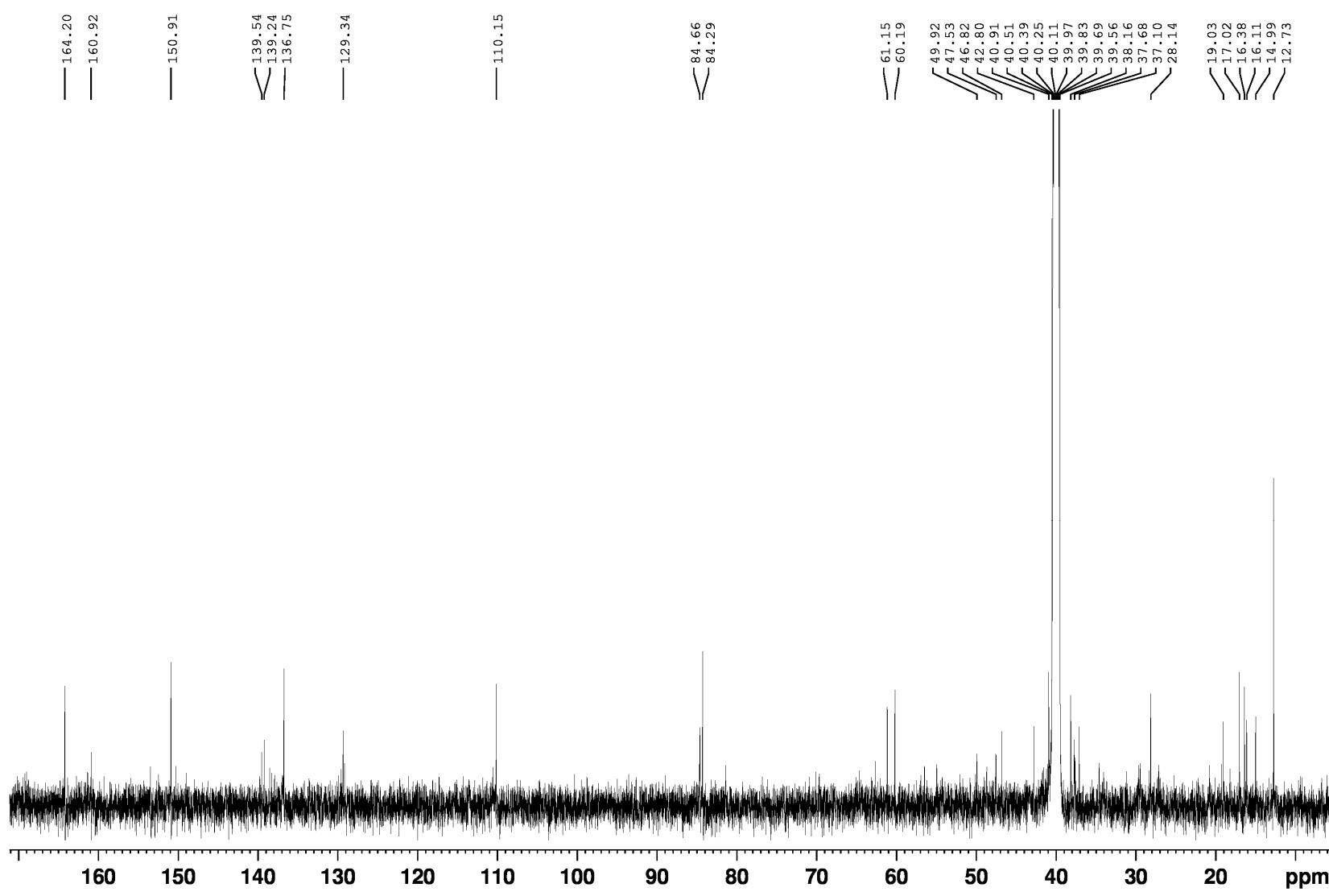


Figure S8 (b): ^{13}C NMR spectrum of 3,28-O,O'-Di{1-(3-hydroxypropyl-1H-[1,2,3]-triazol-4-yl)carbonyl}betulin (**6h**)

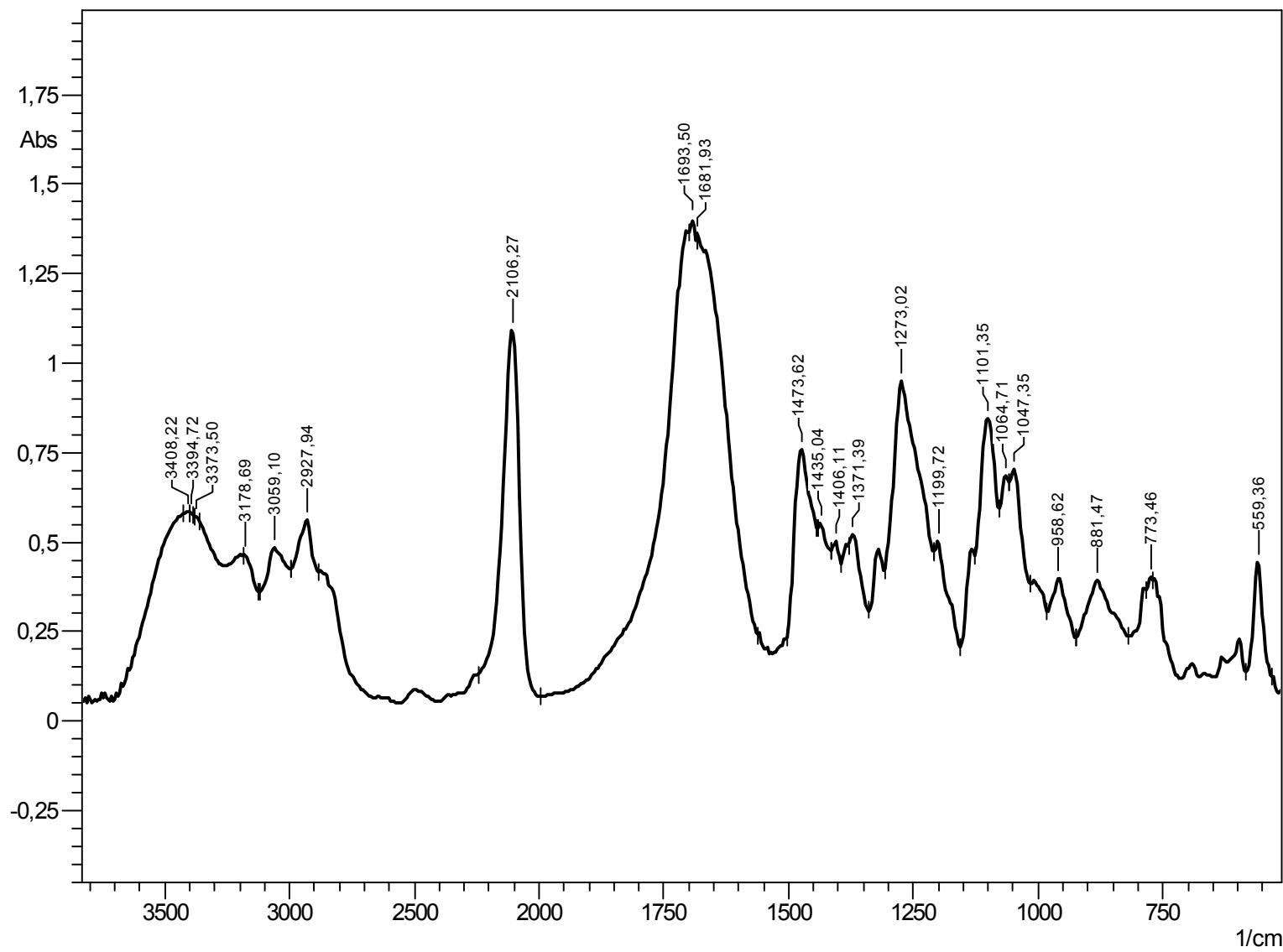


Figure S8 (c): IR spectrum of 3,28-O,O'-Di{1-(3-hydroxypropyl-1H-[1,2,3]-triazol-4-yl)carbonyl]betulin (**6h**)