Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Design of Configuration-Restricted Triazolylated β-D-Ribofuranosides: A Unique Family of Crescent-Shaped RNase A Inhibitors

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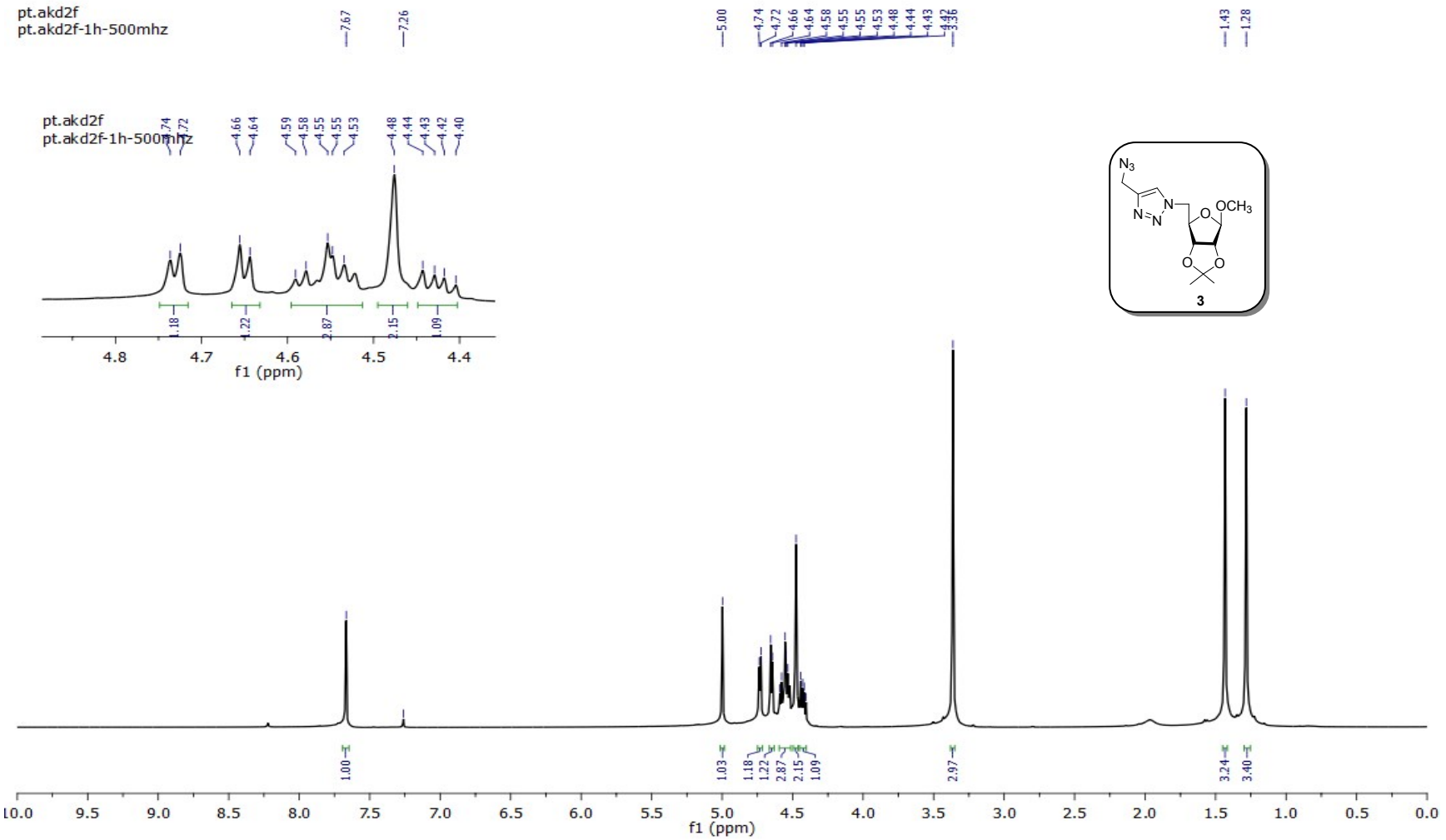

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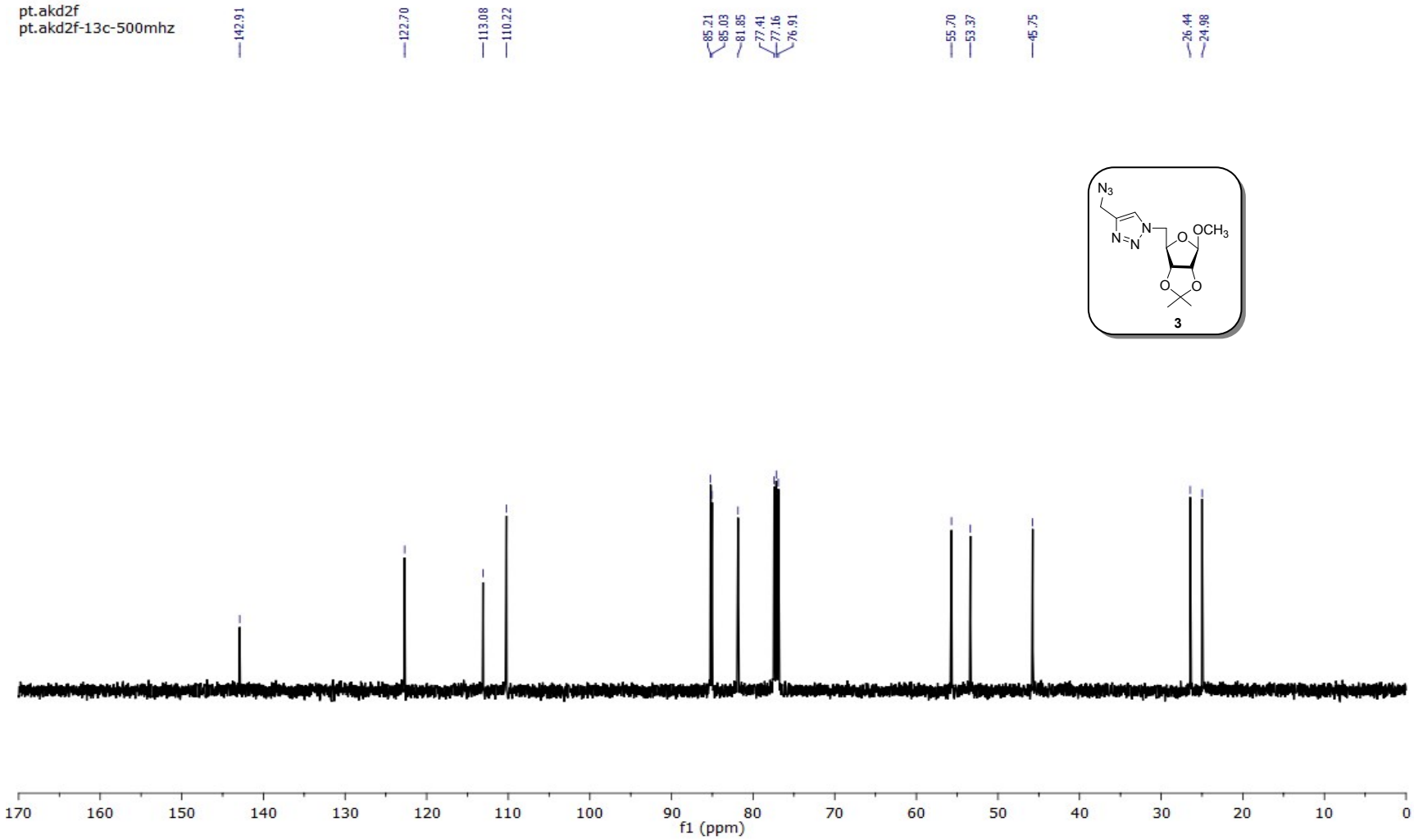

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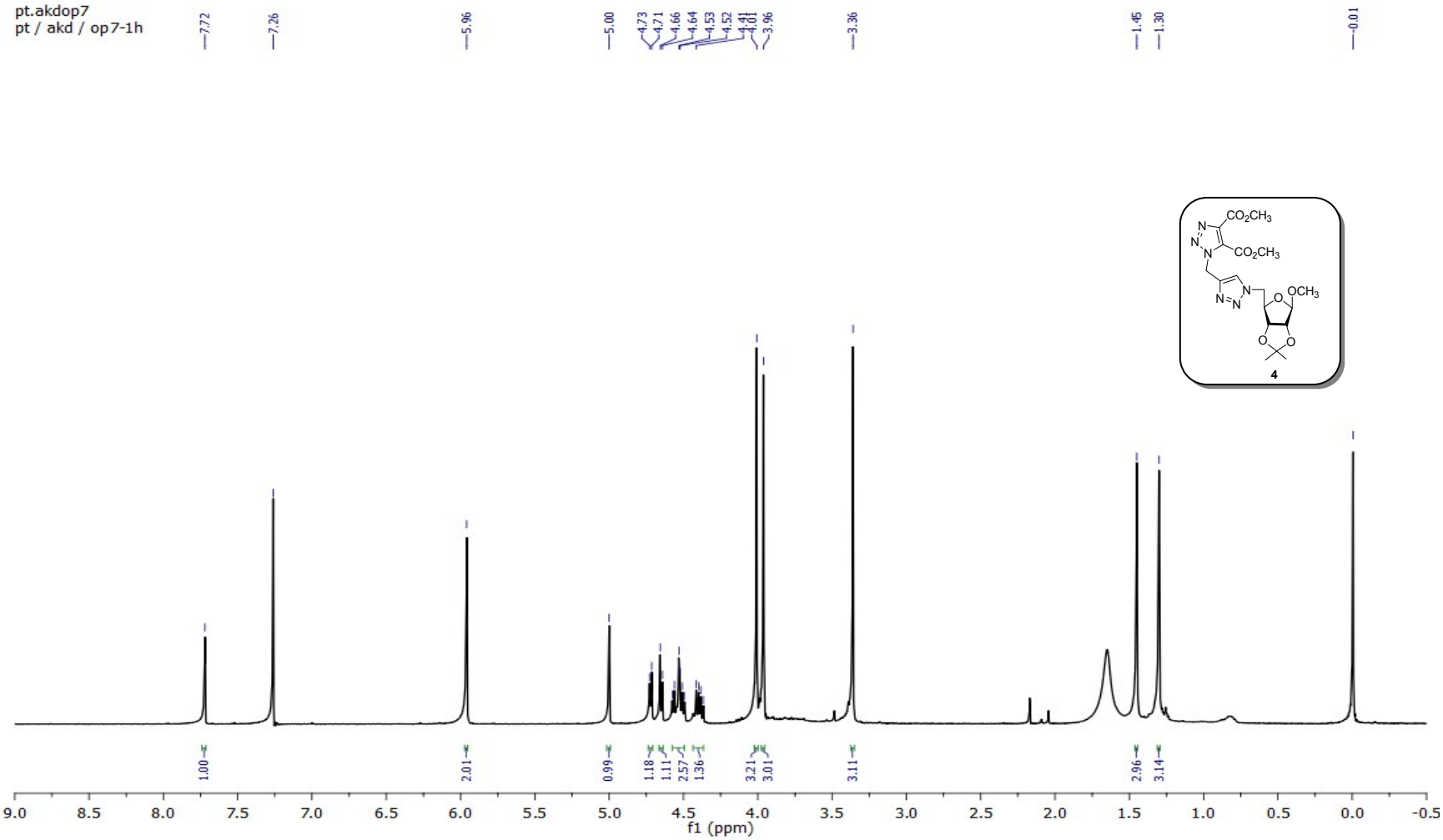

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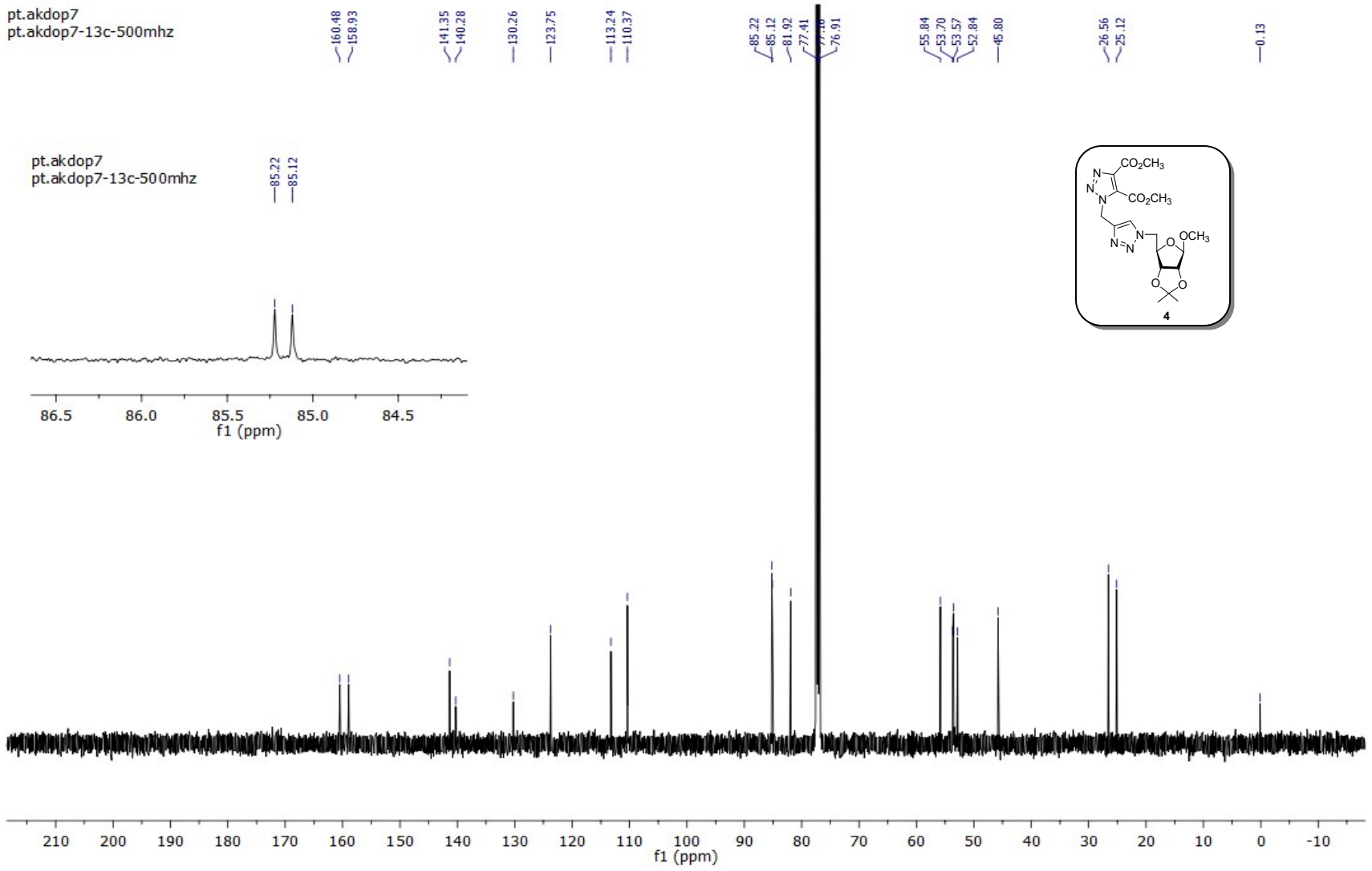

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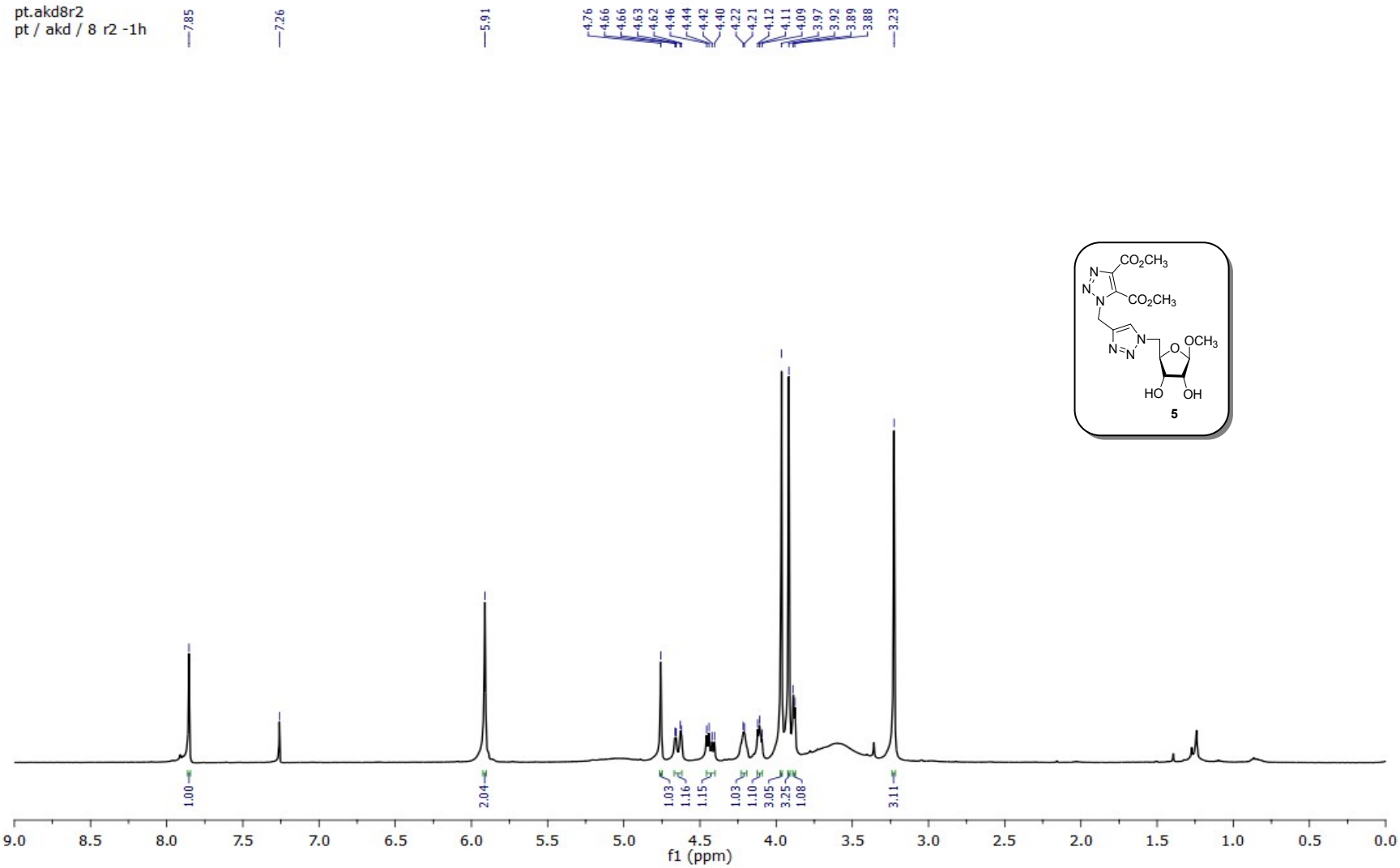

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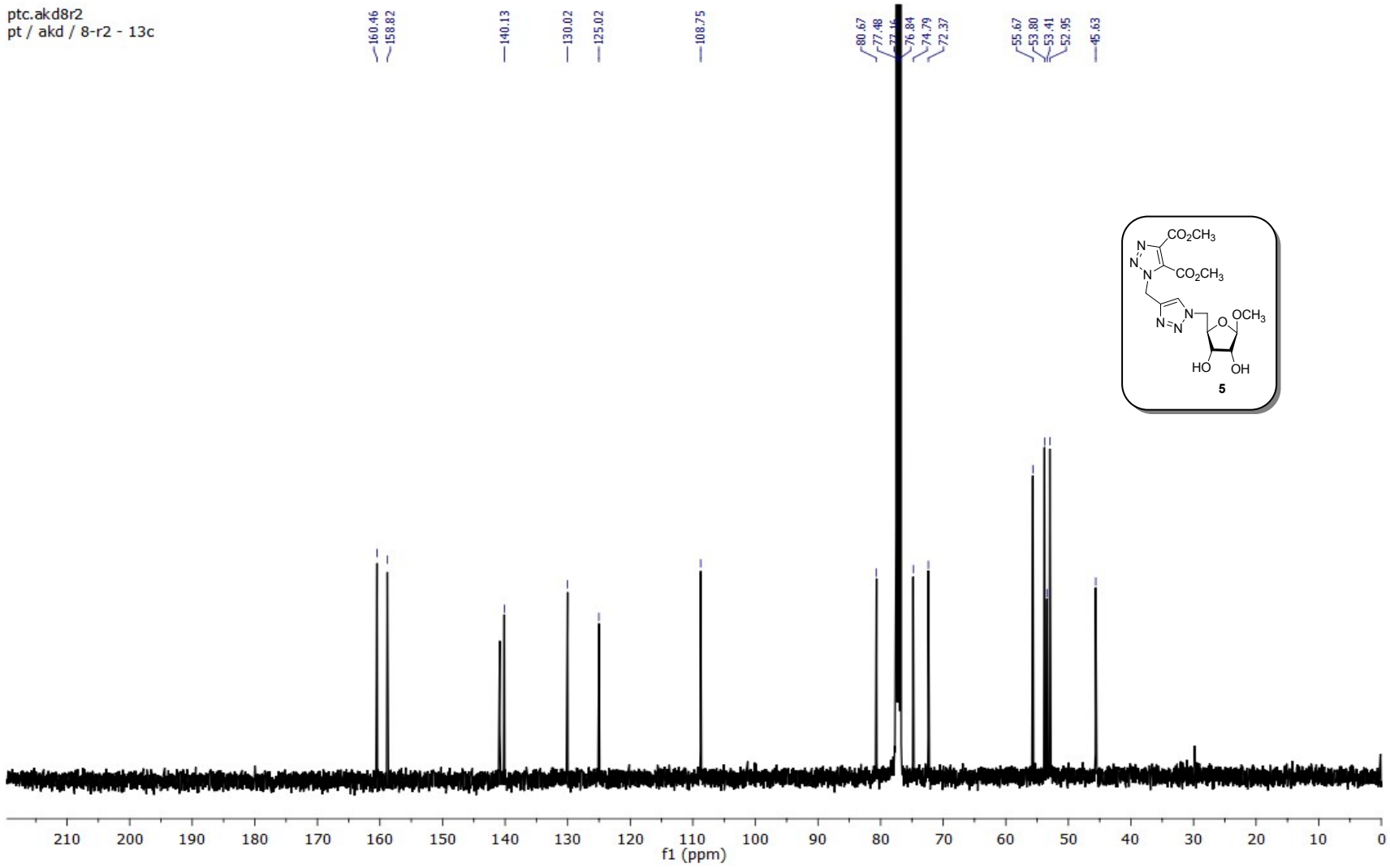

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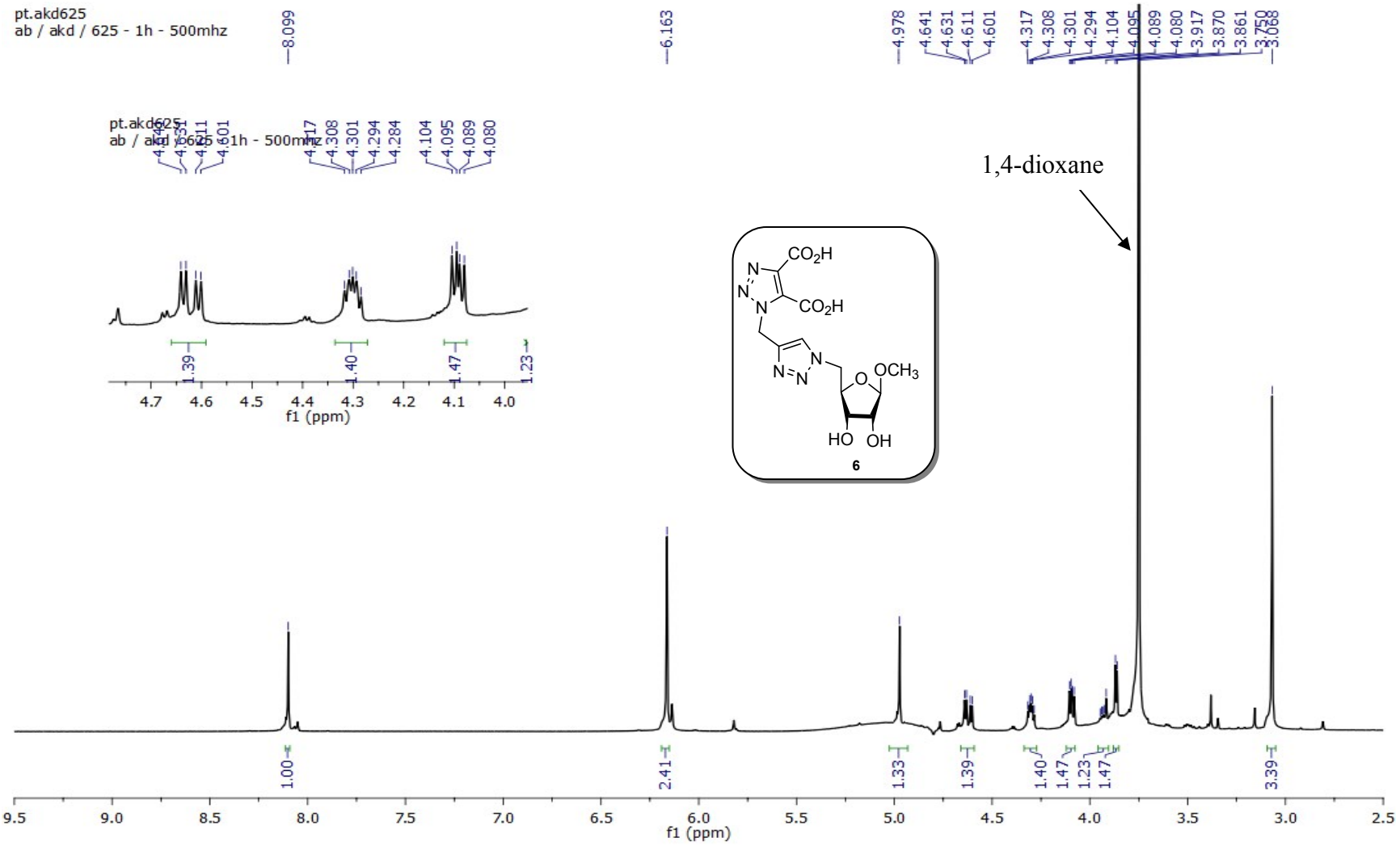

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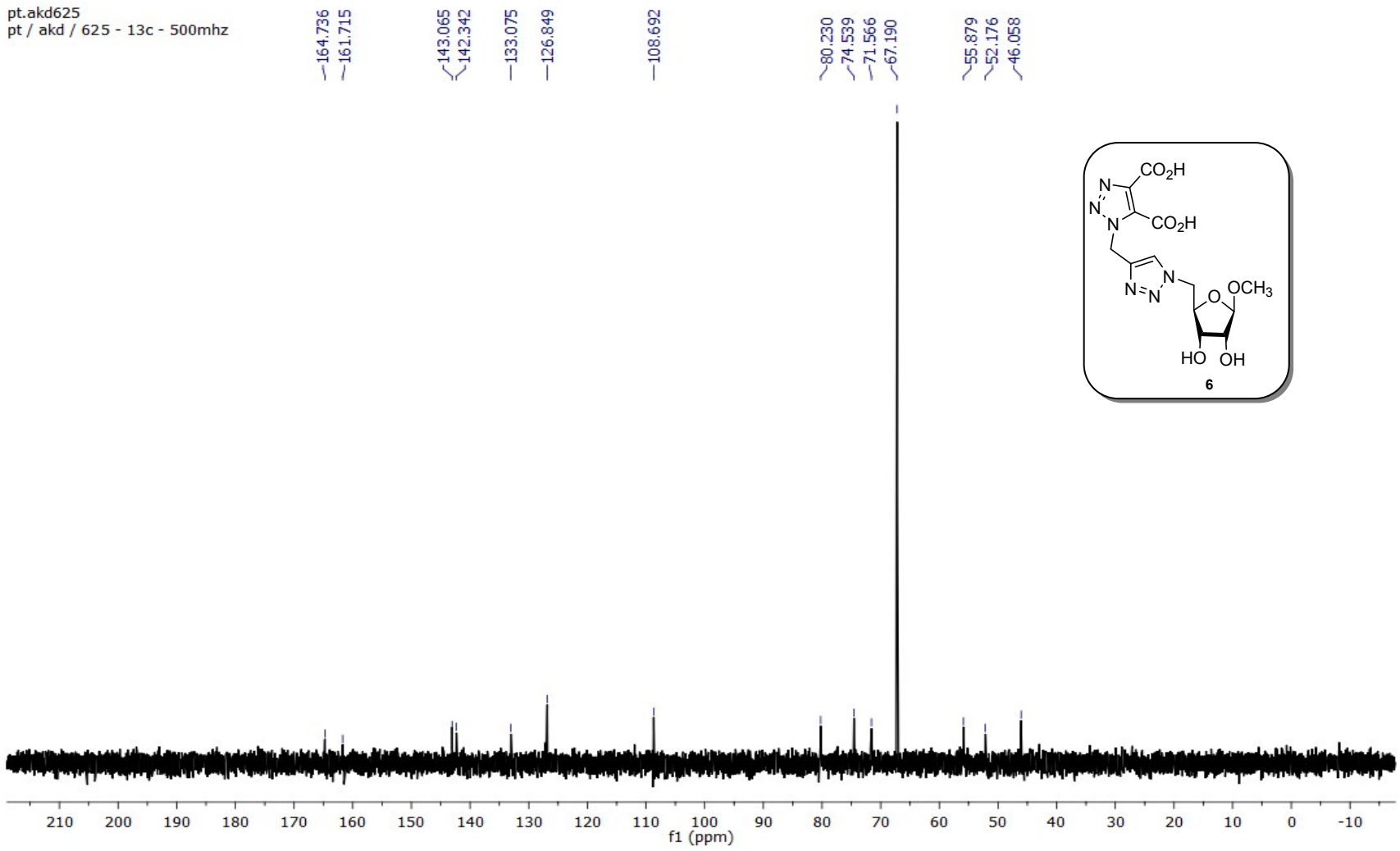

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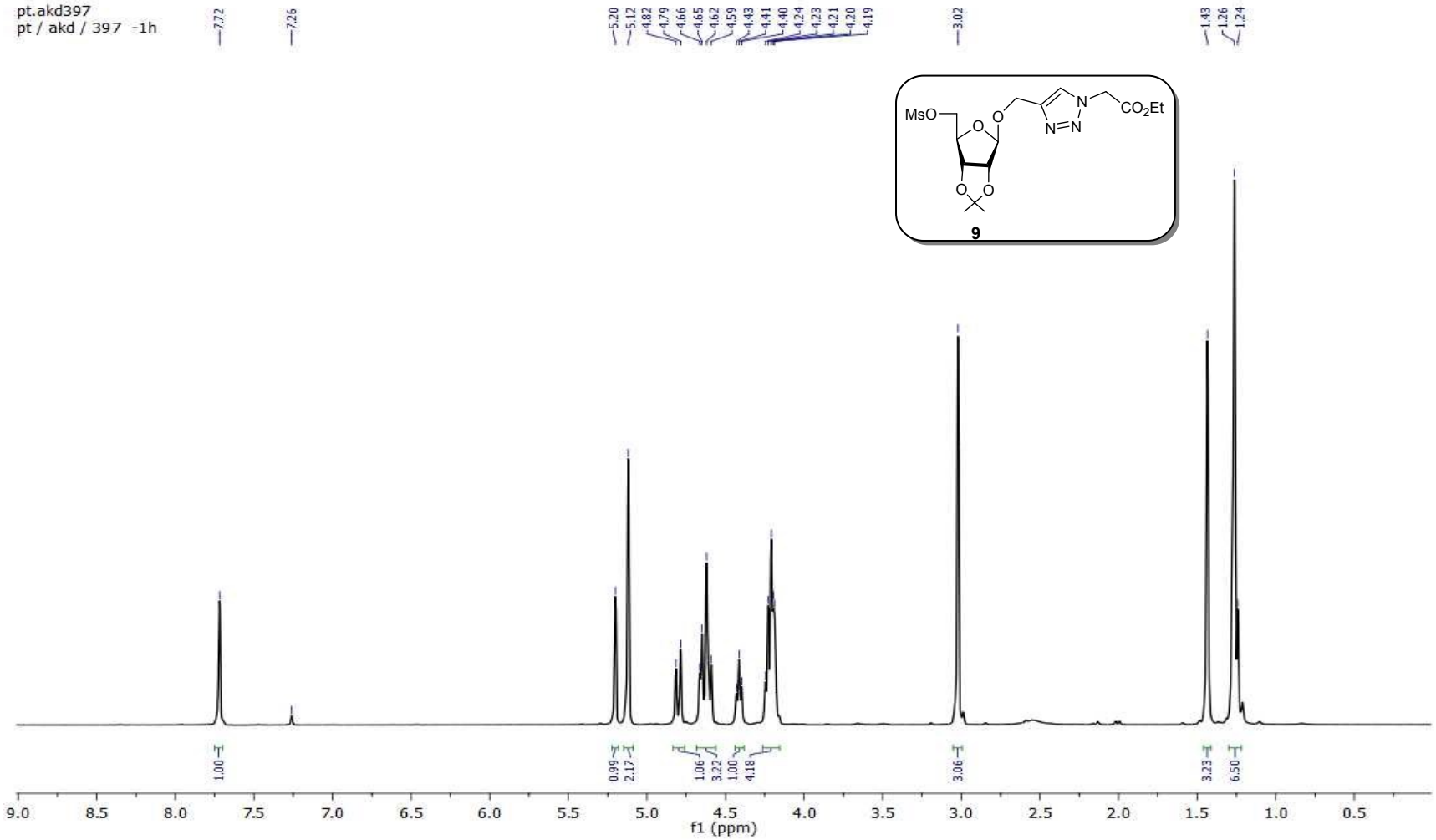

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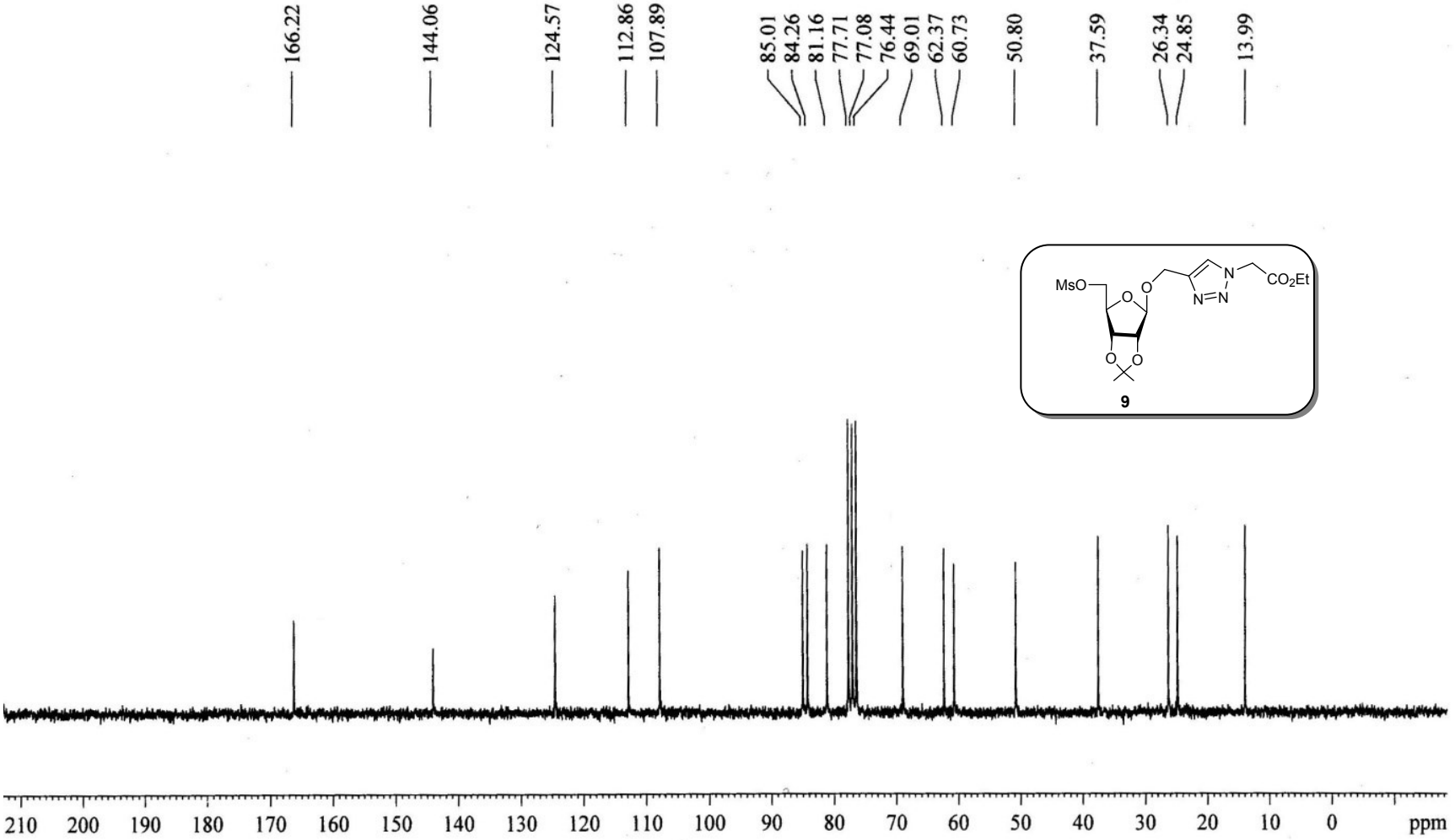

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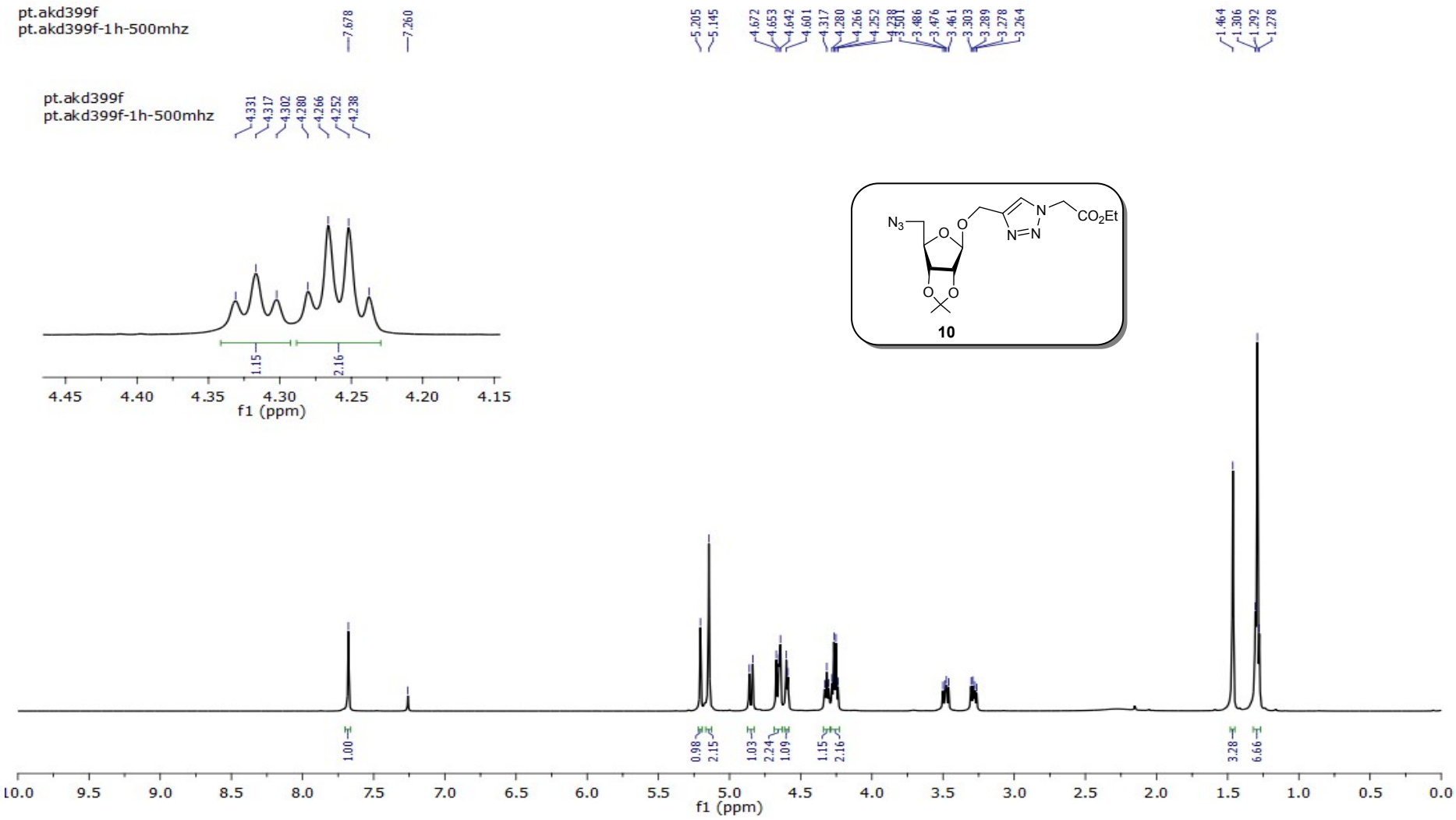

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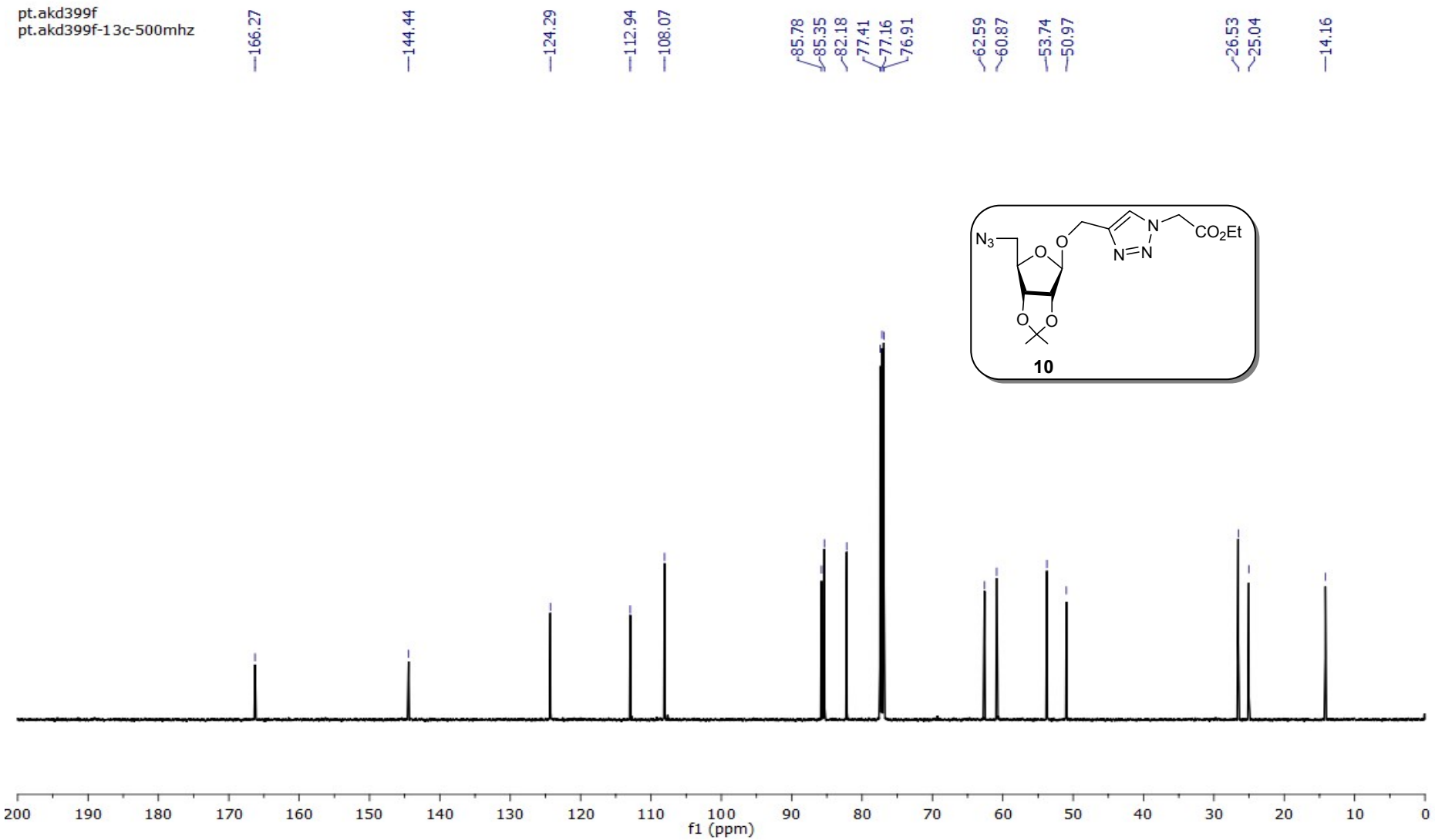

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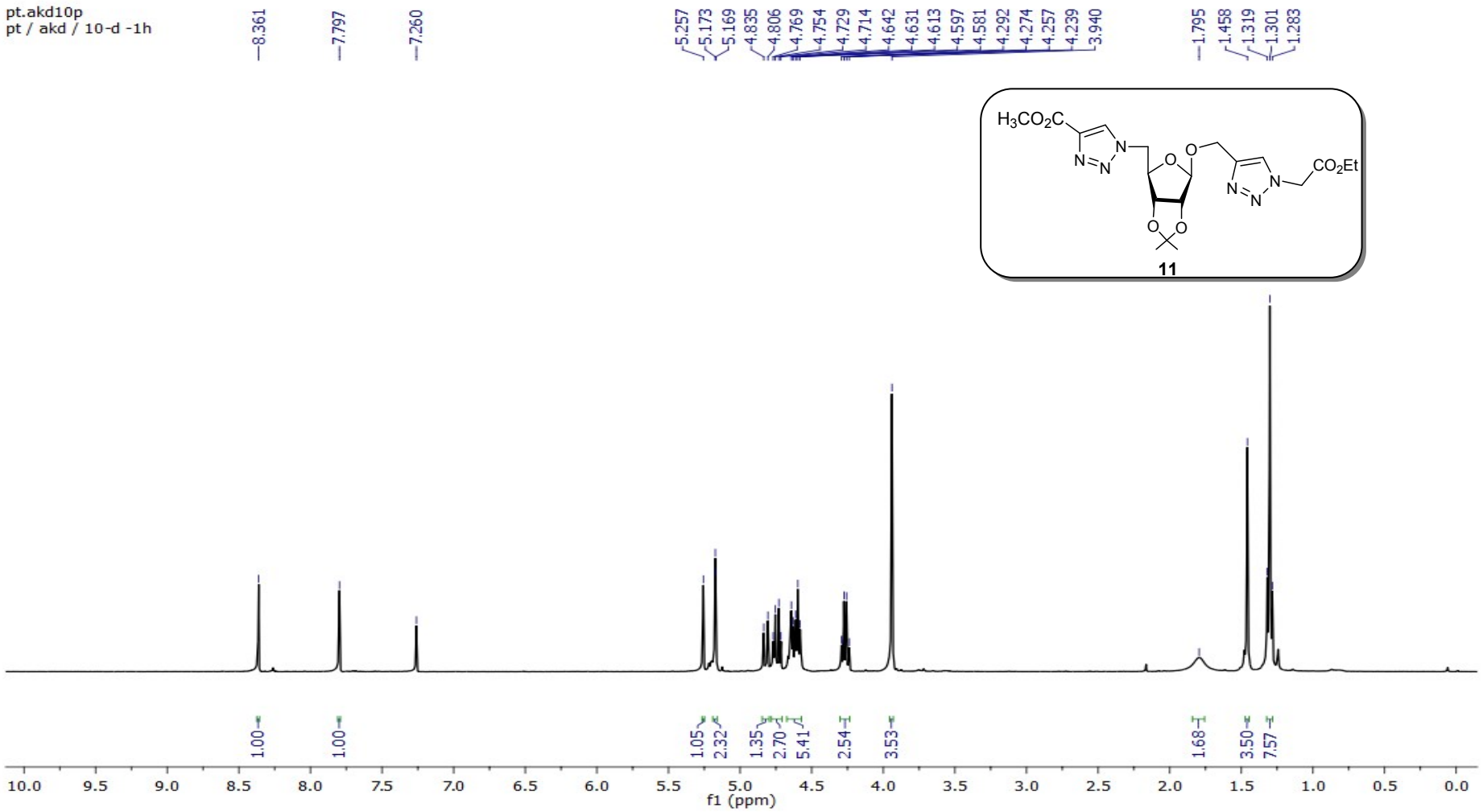

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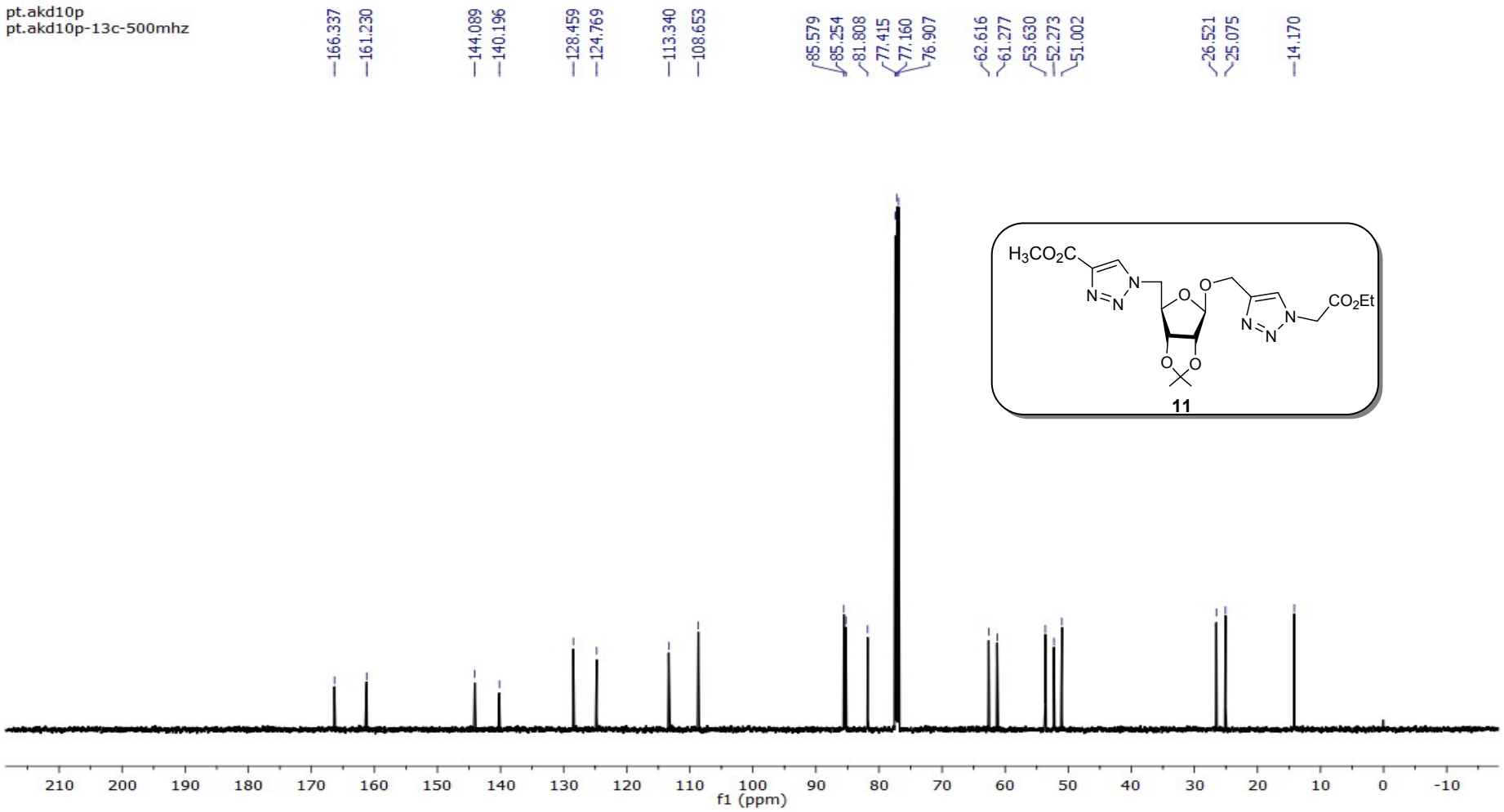

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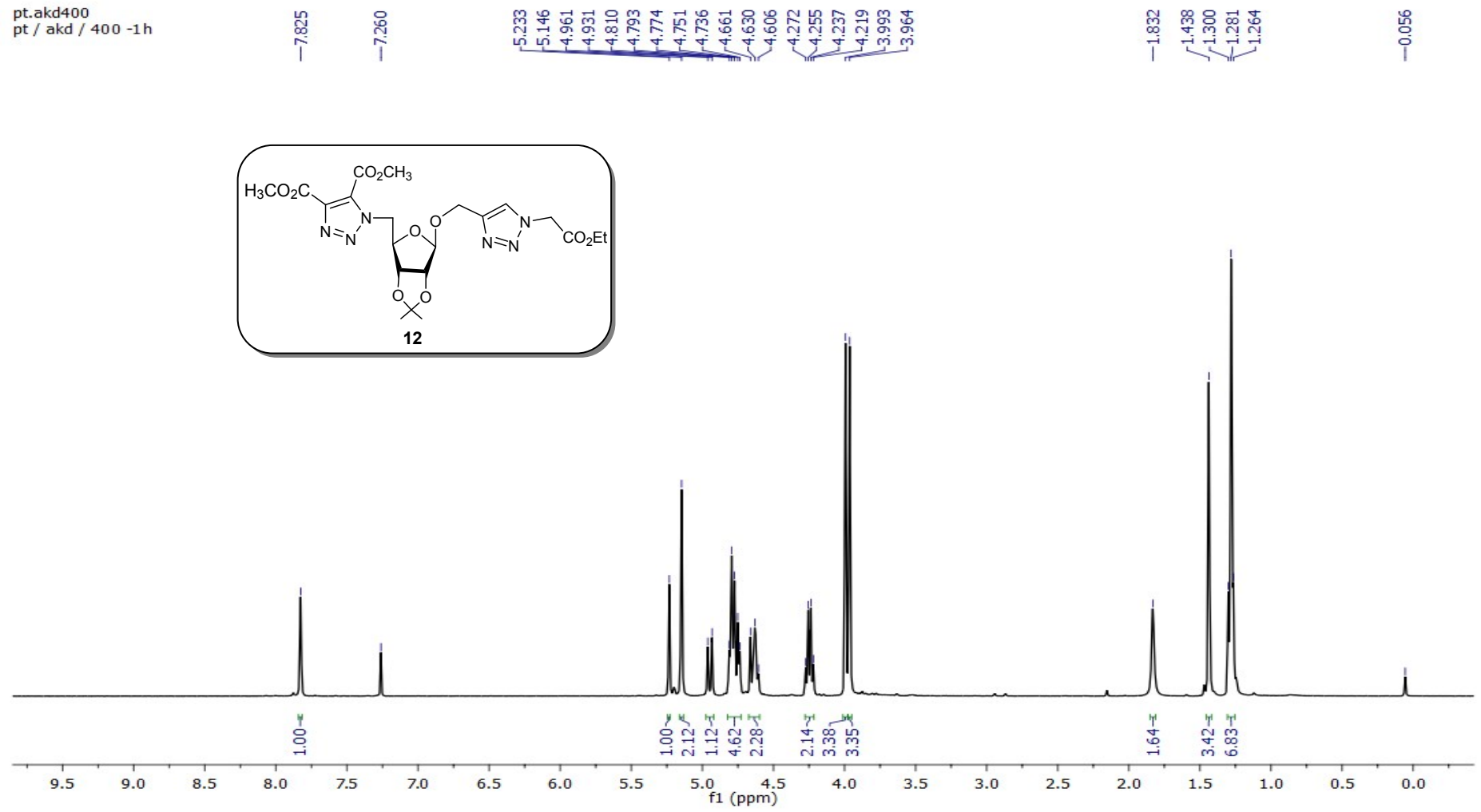

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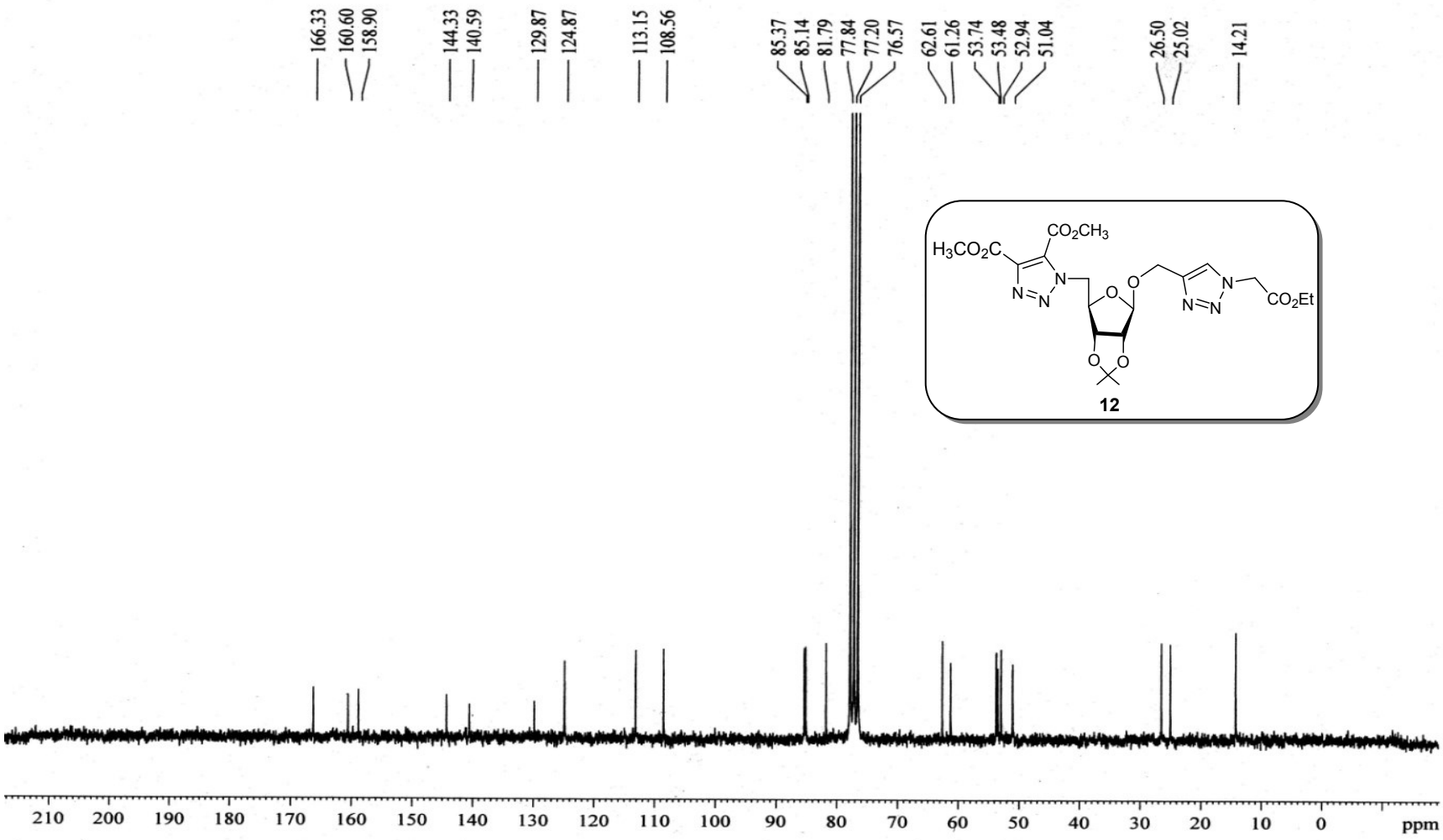

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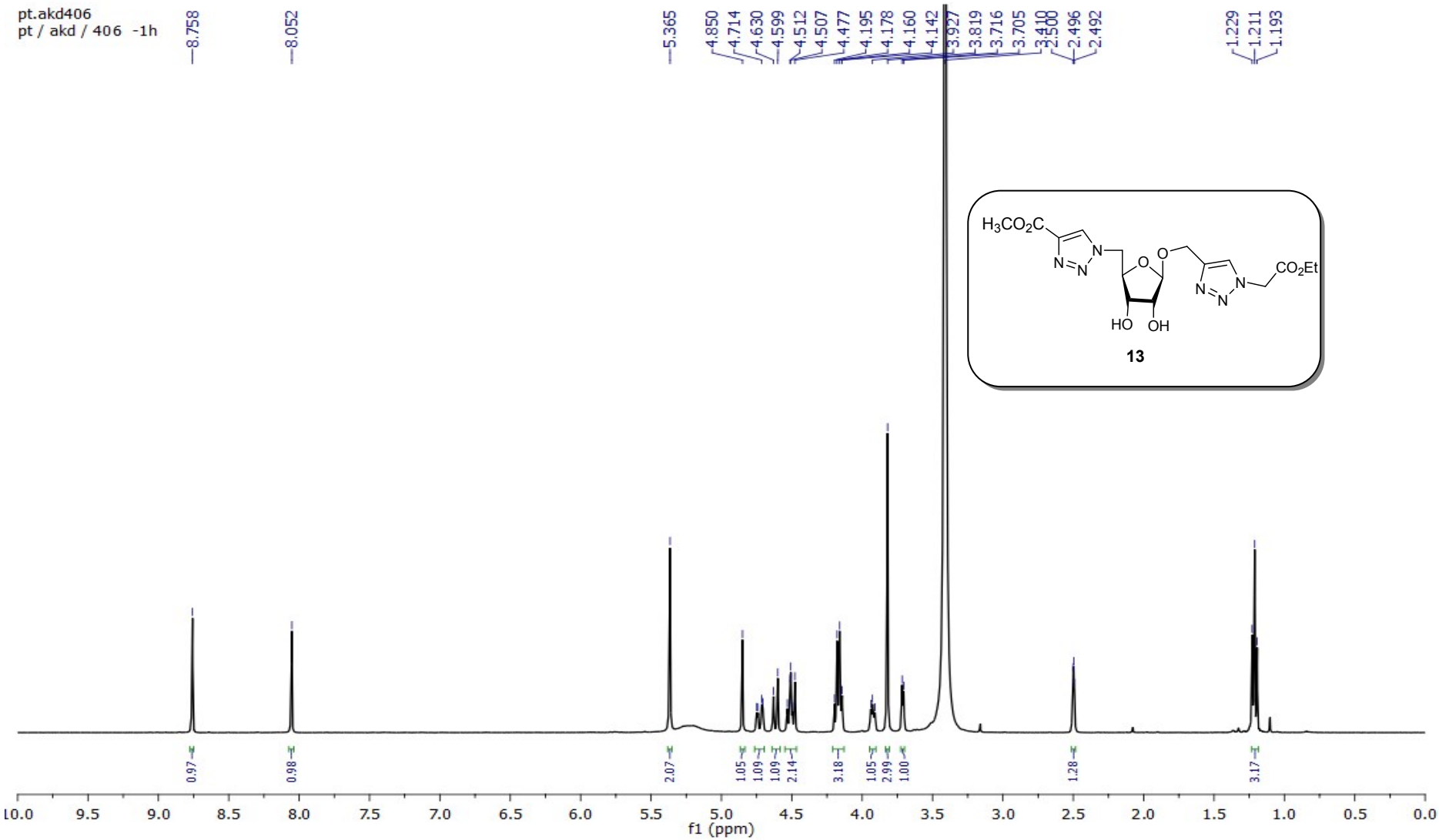

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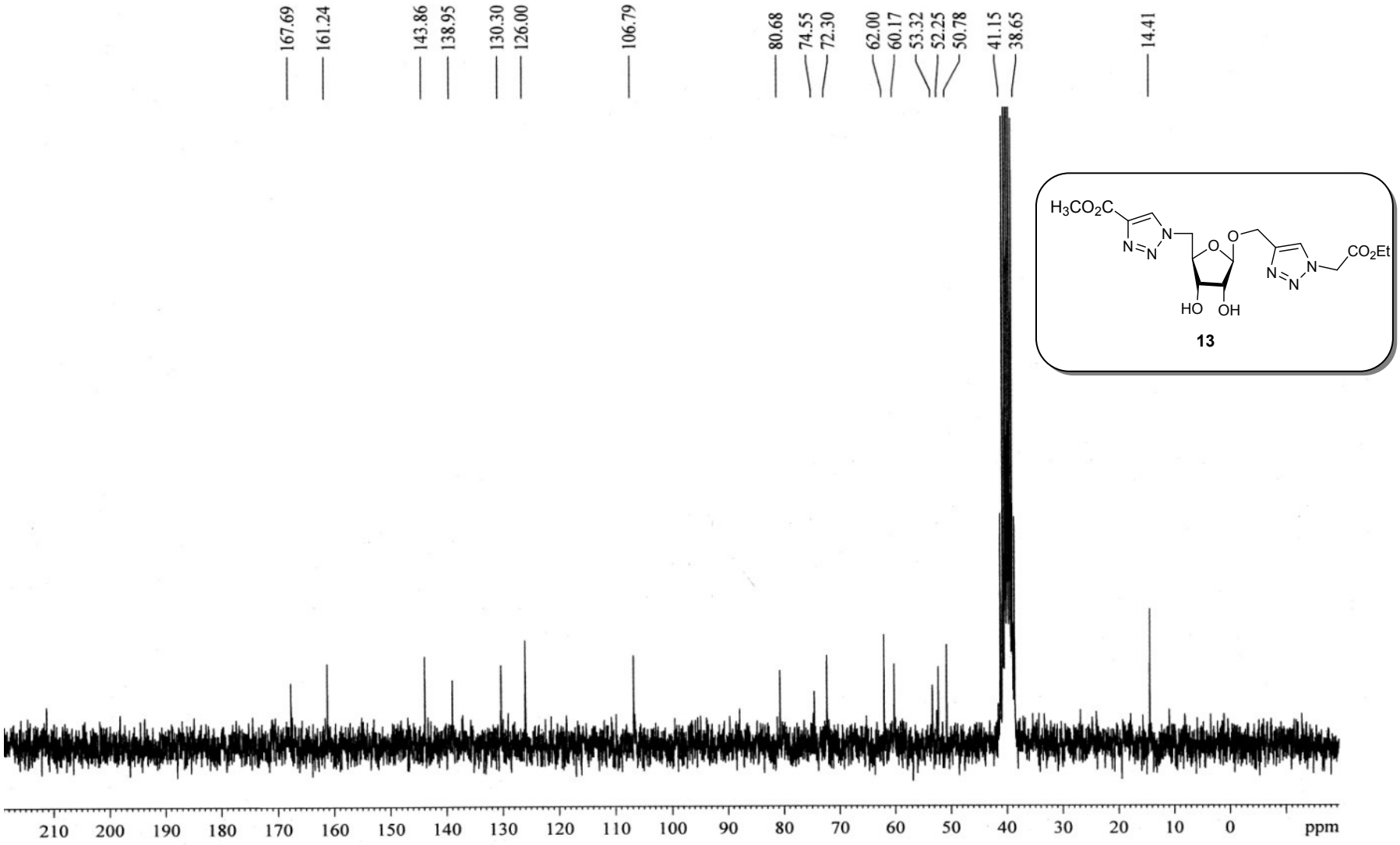

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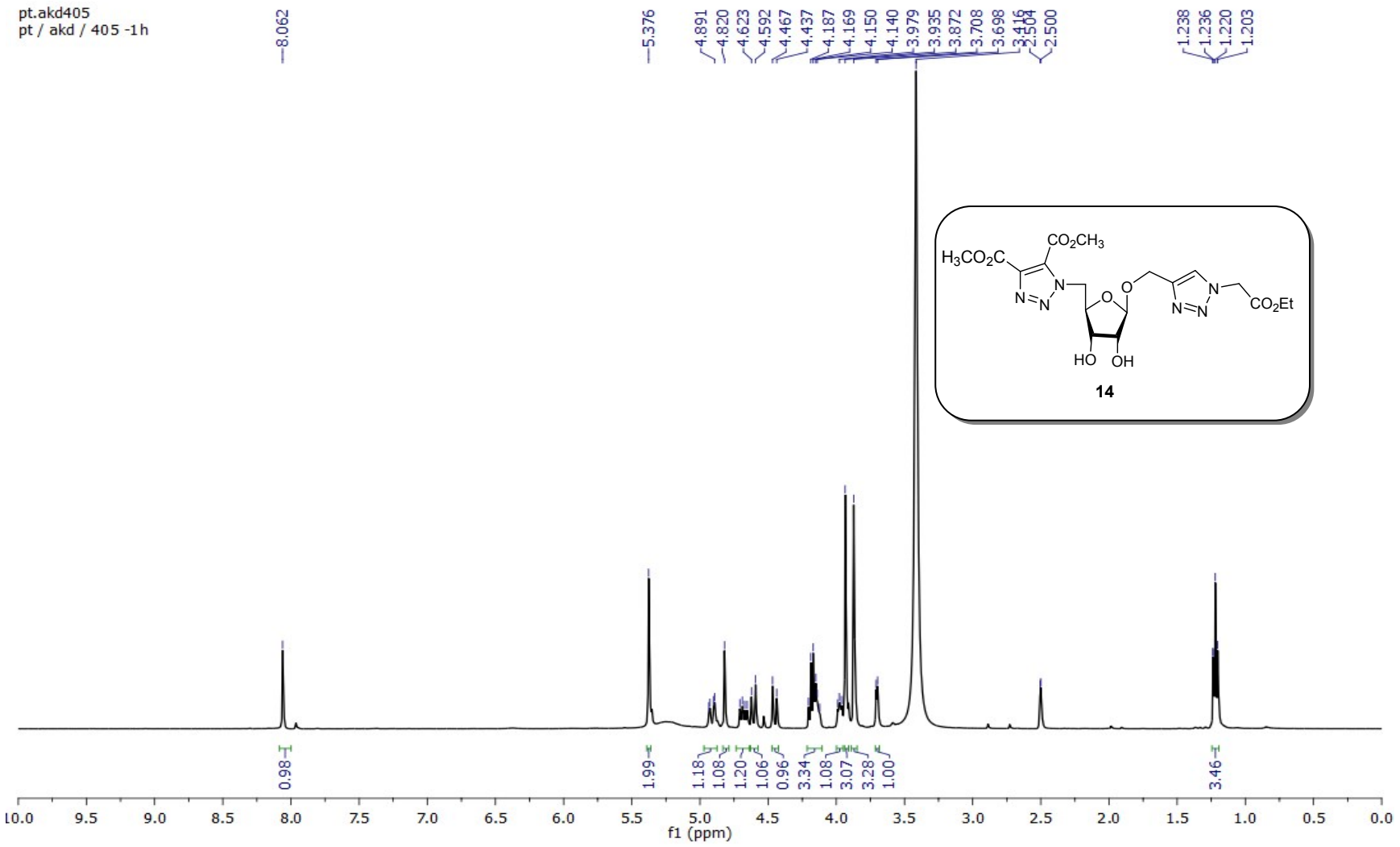

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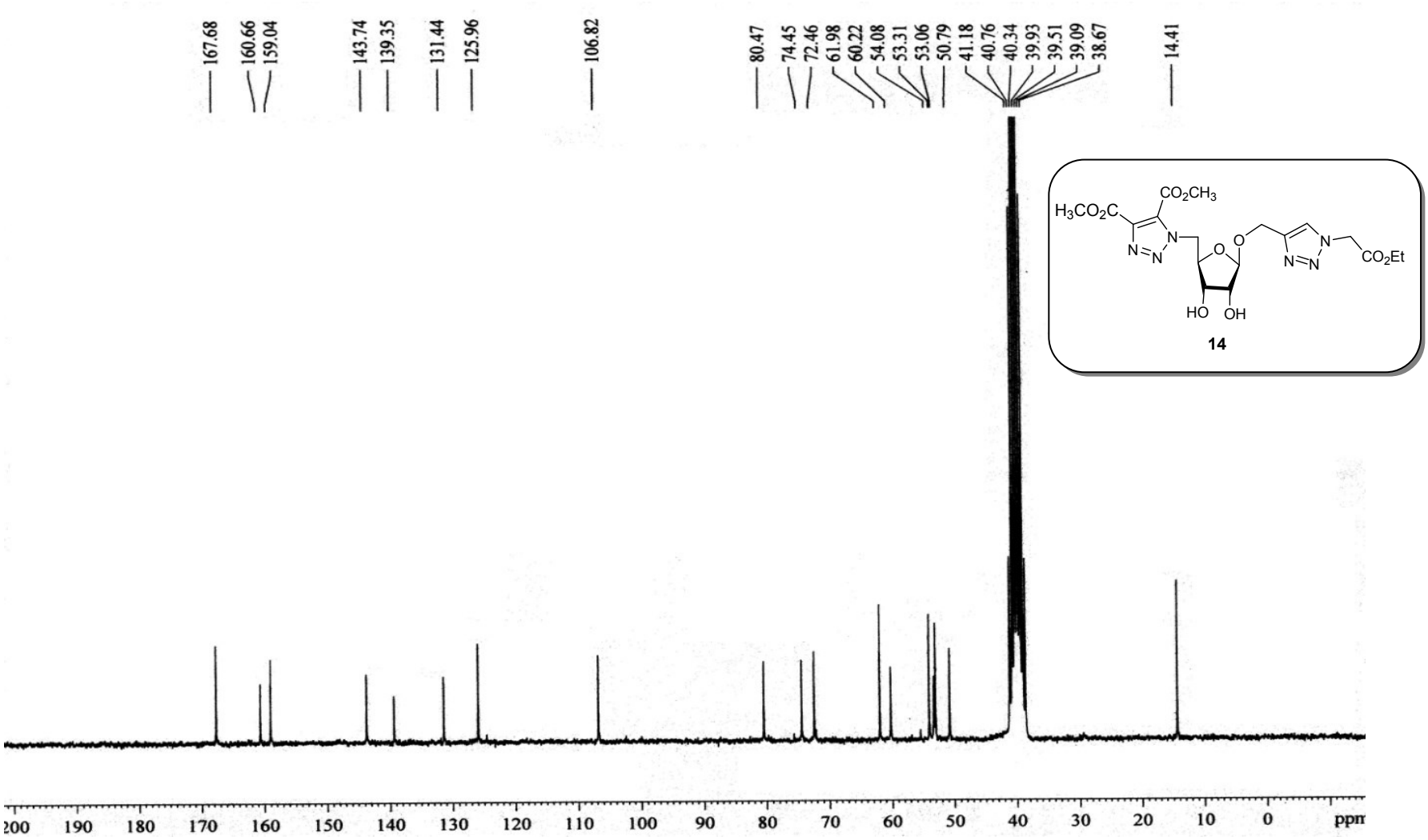

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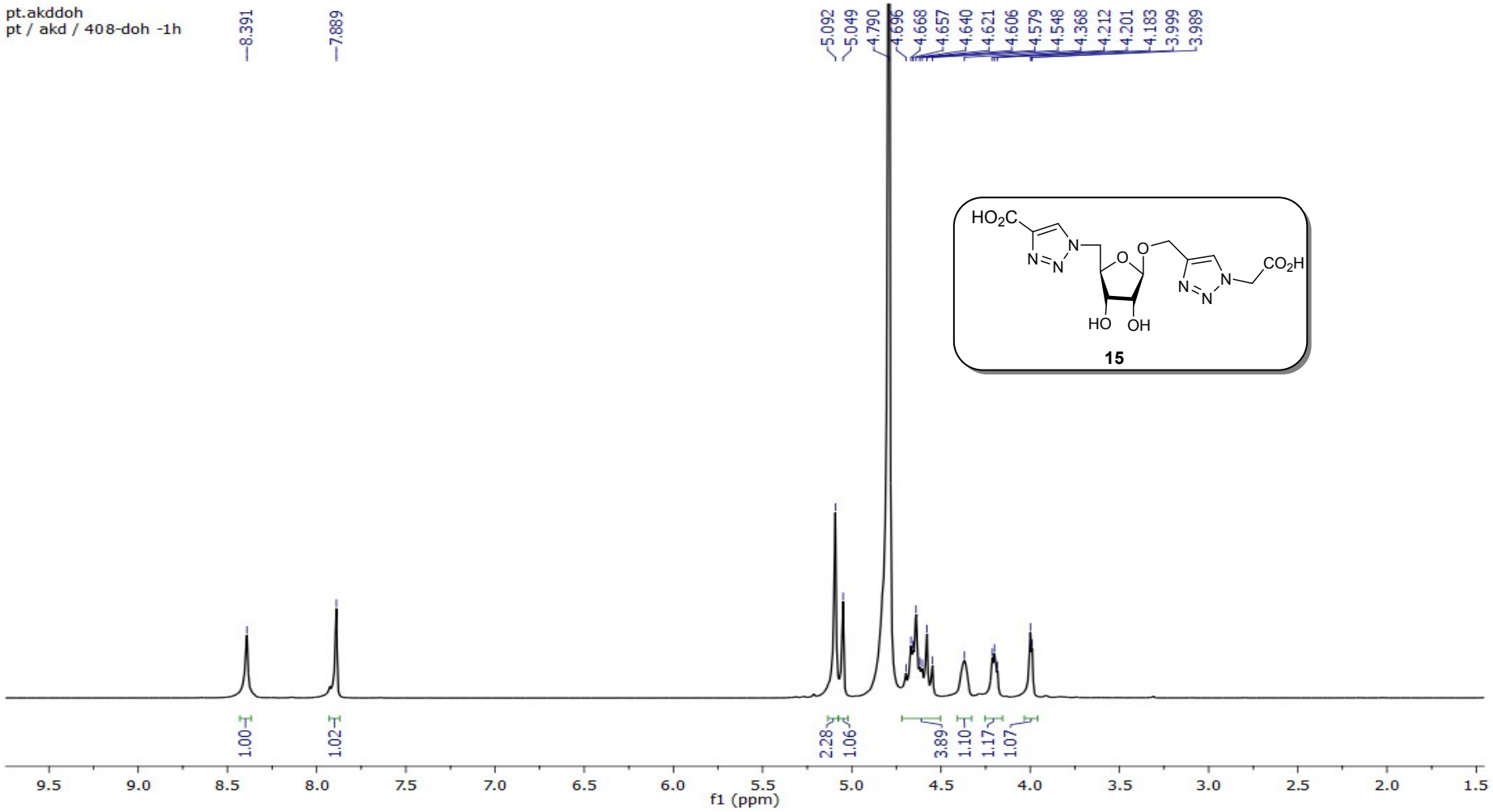

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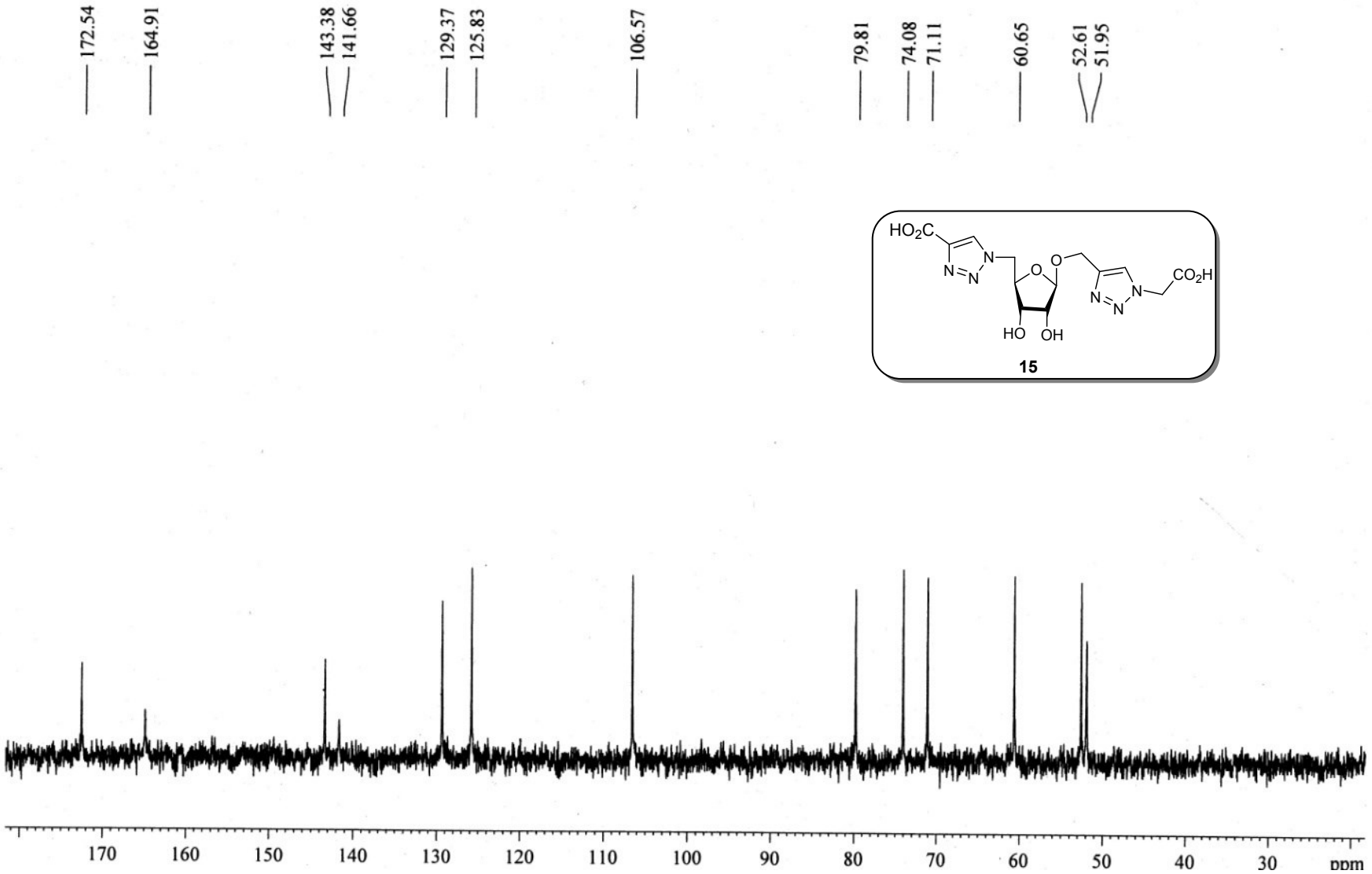

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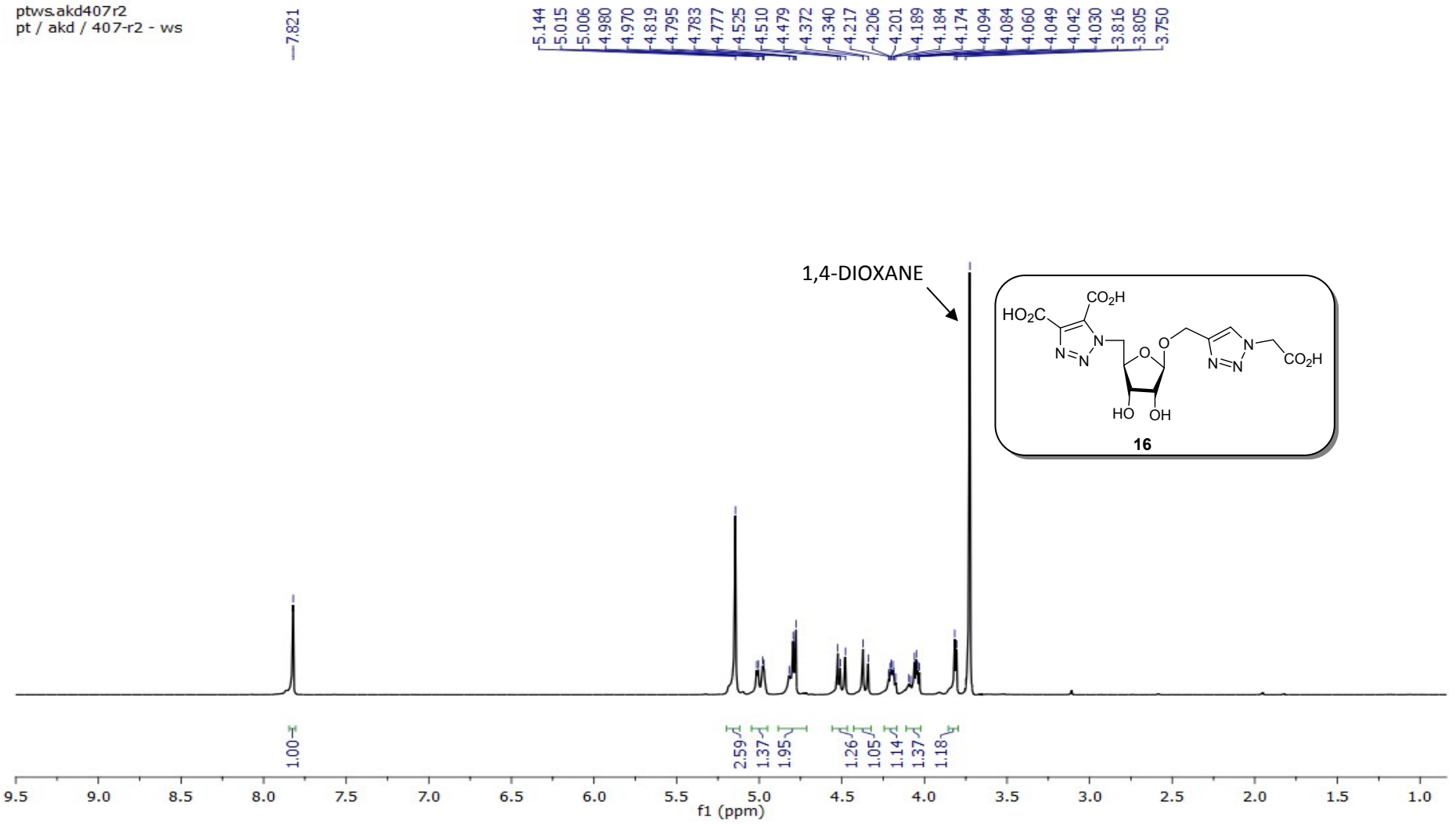

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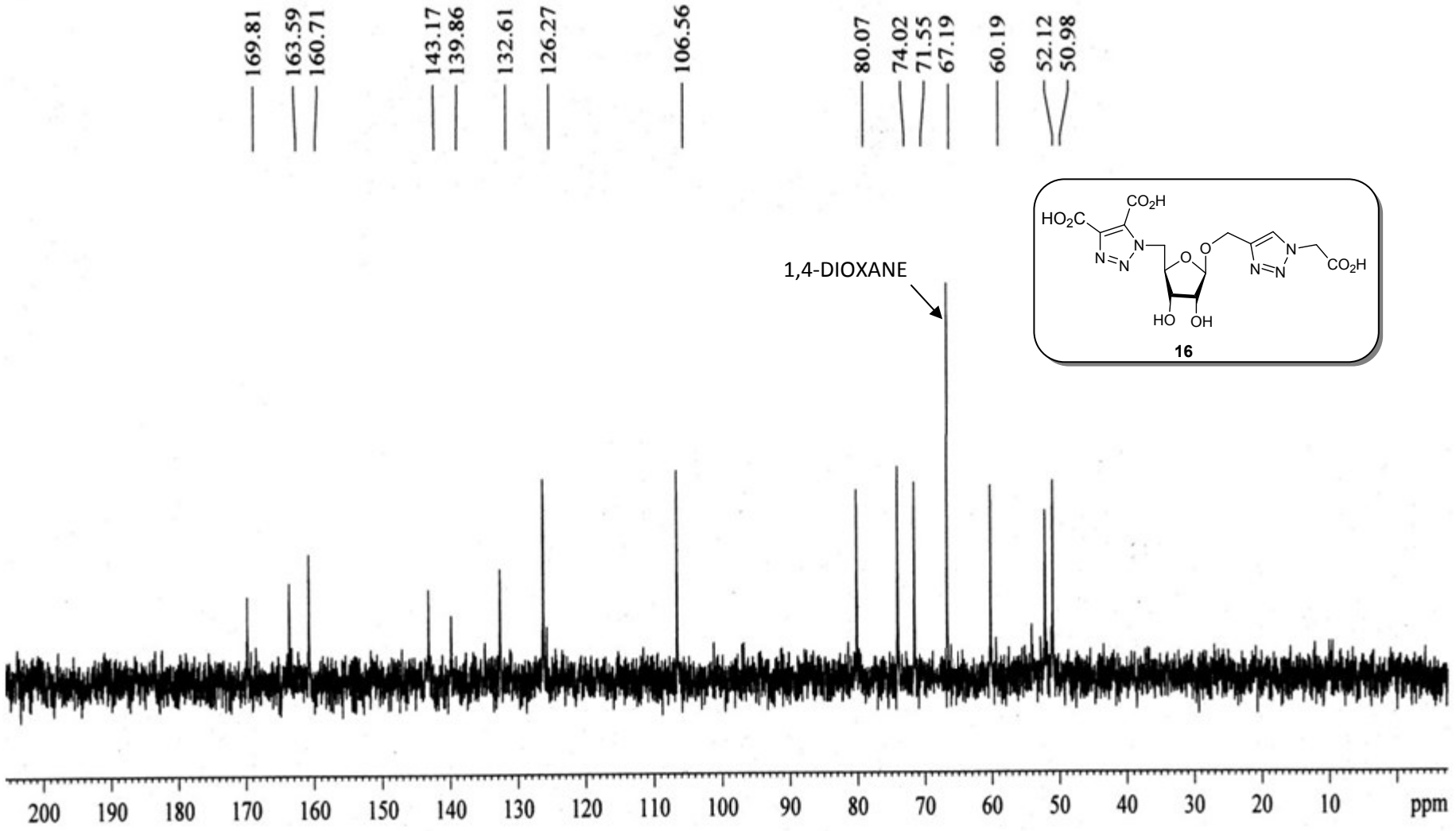

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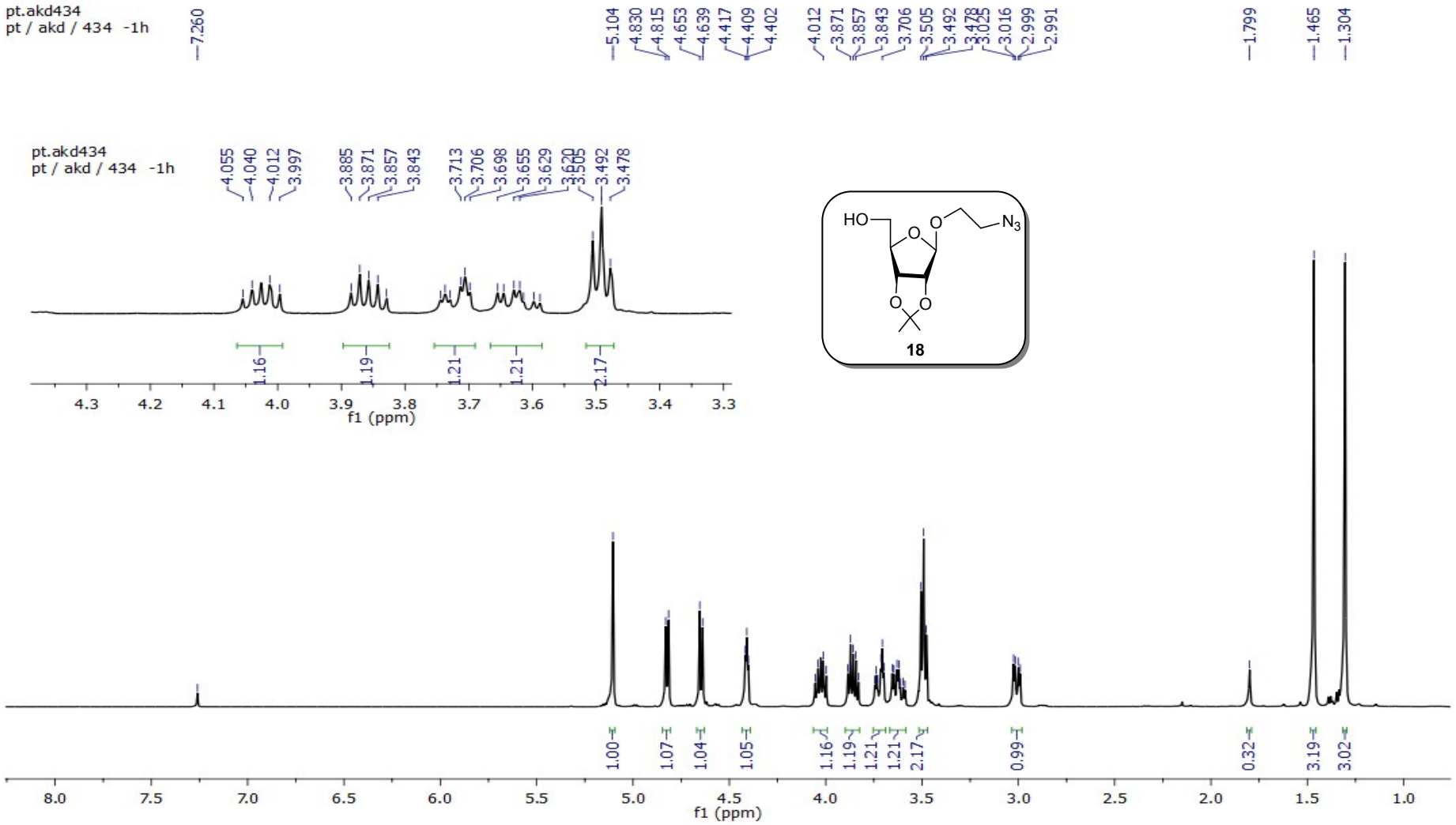

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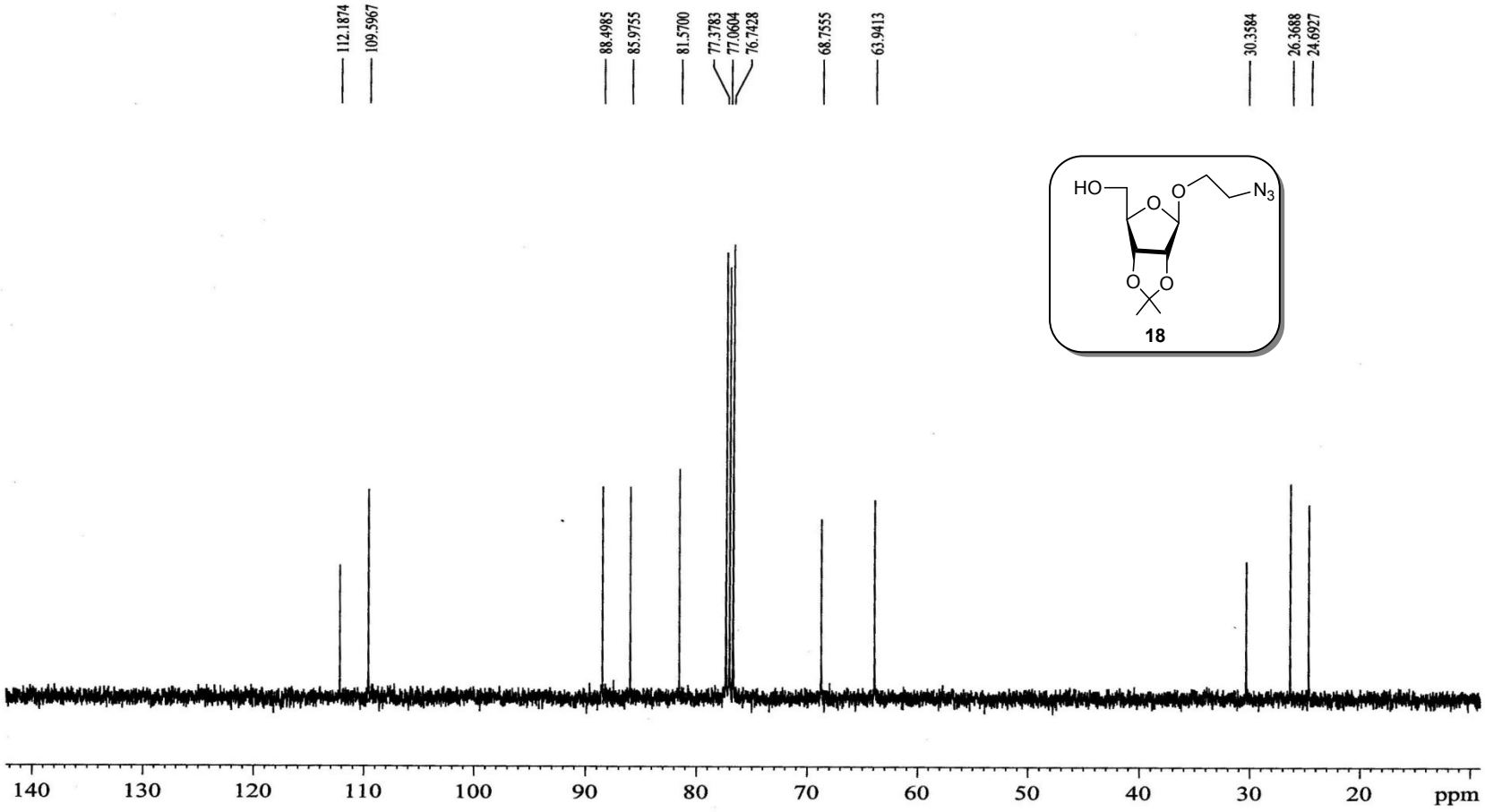

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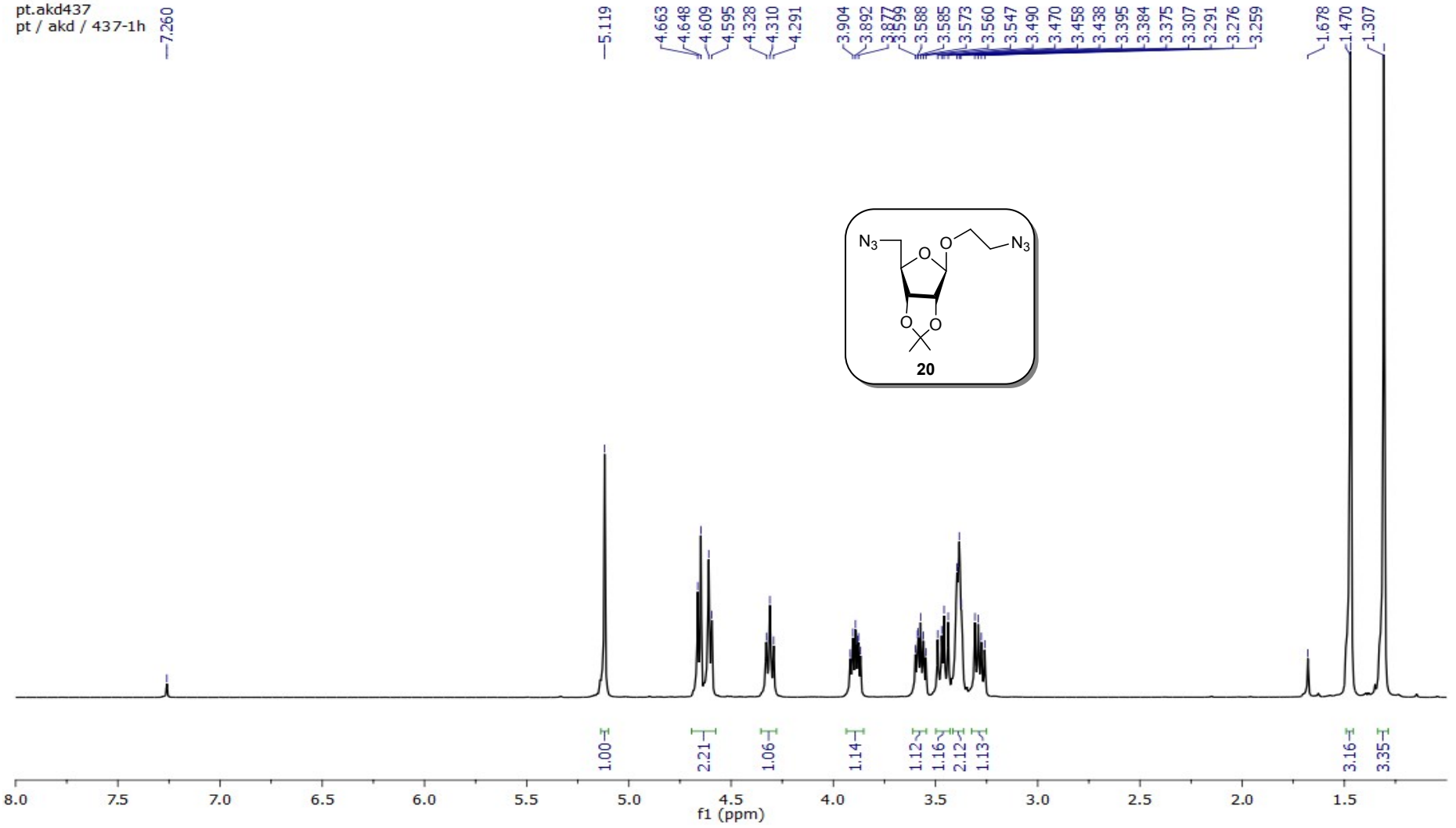

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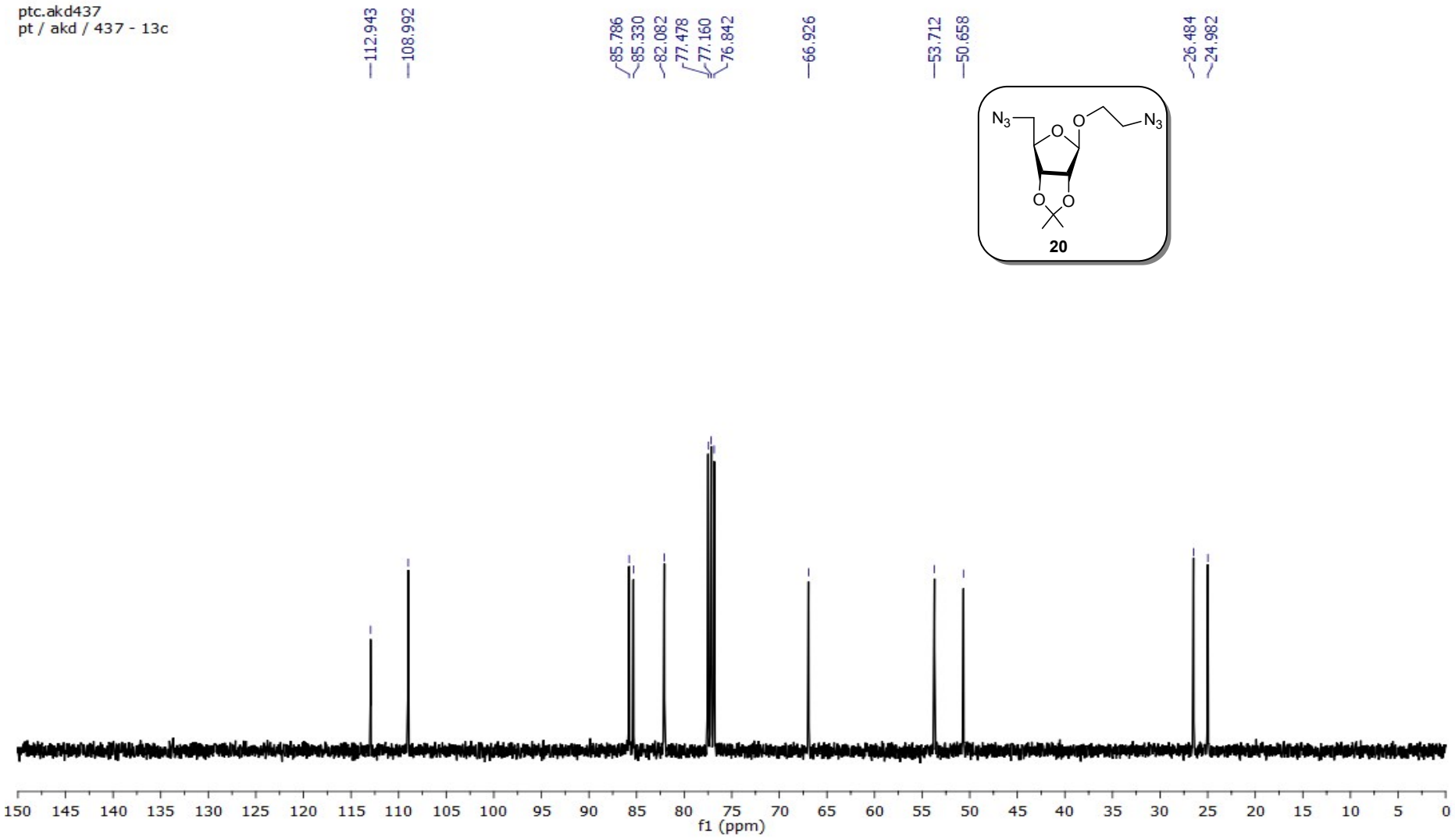

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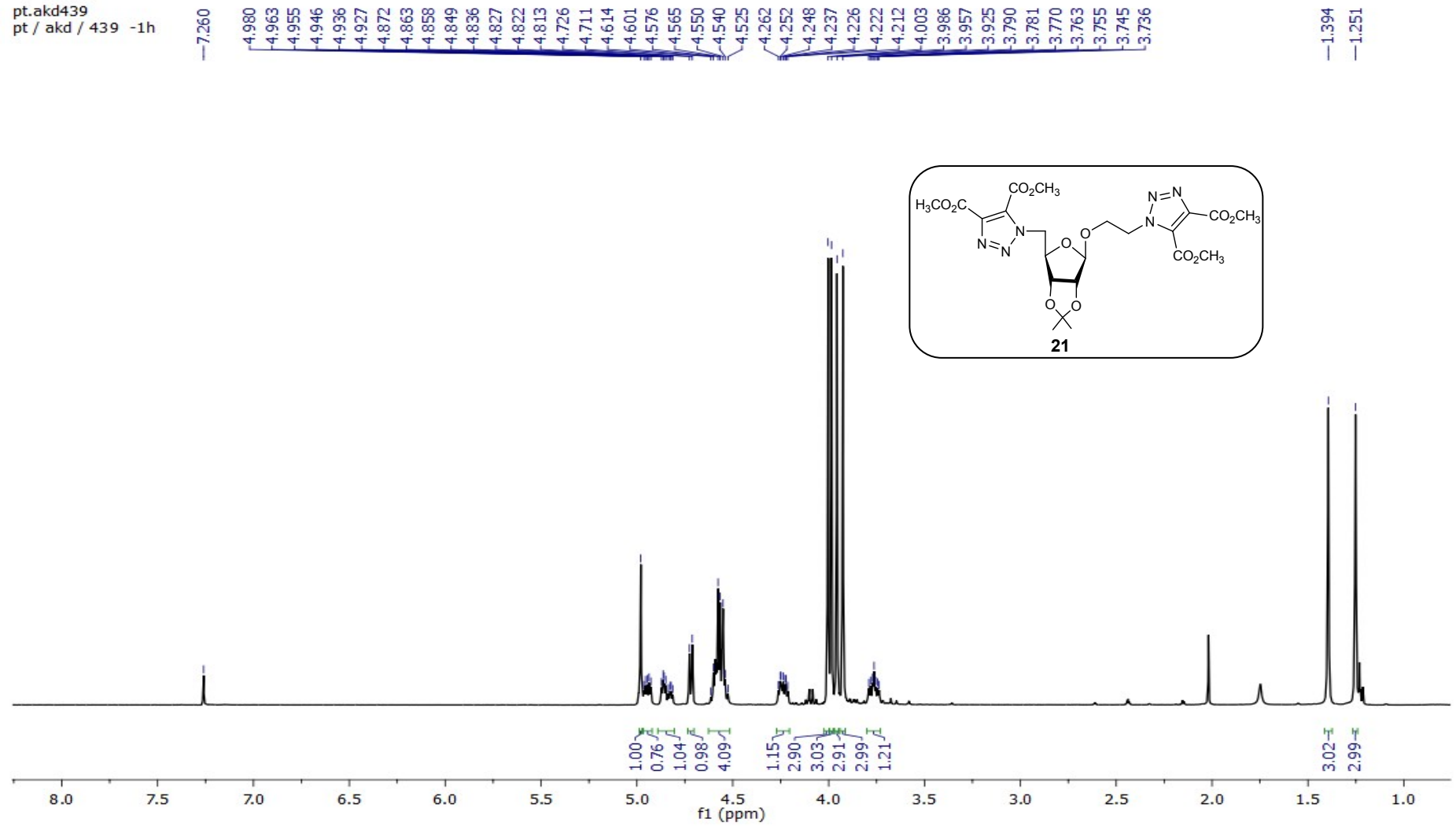

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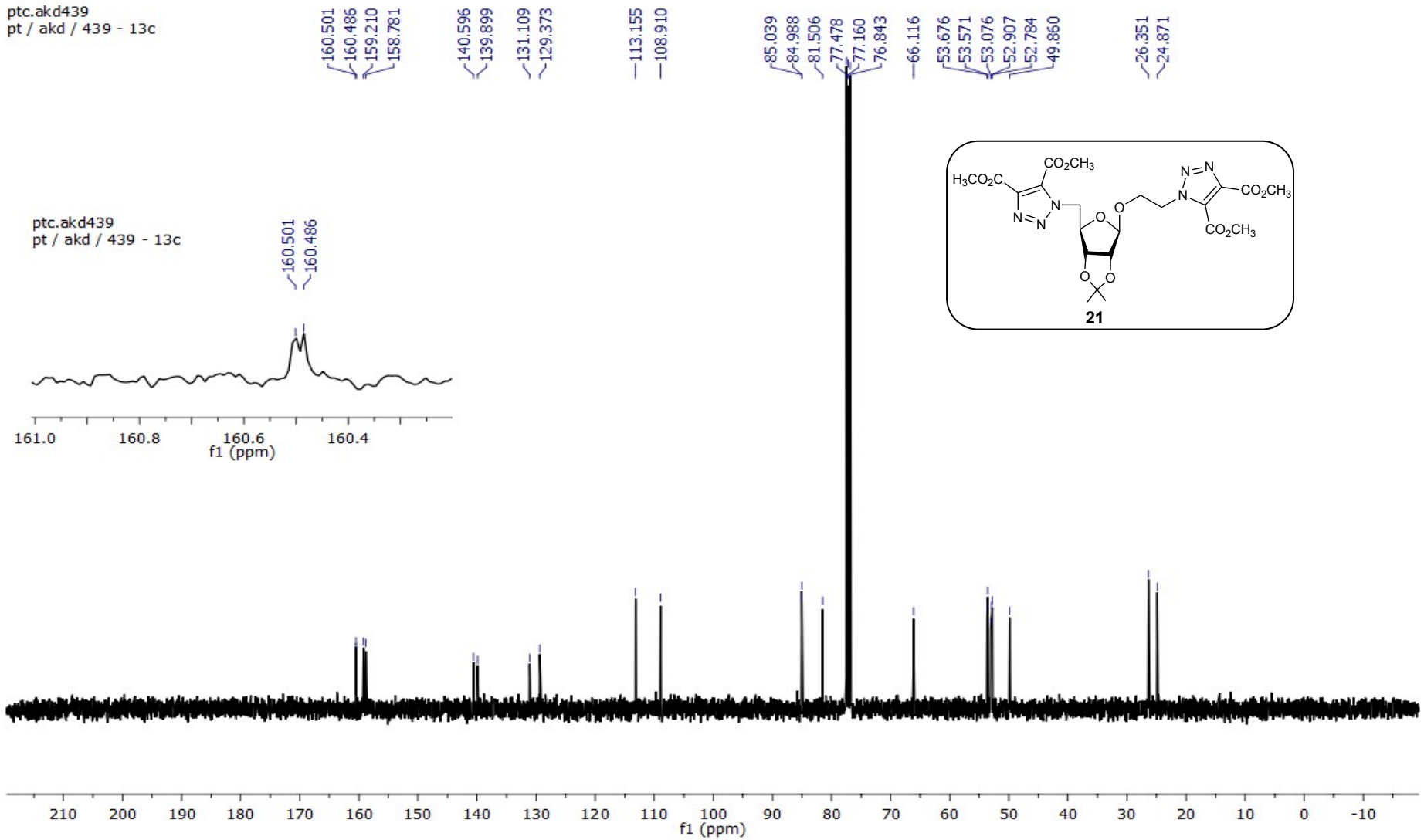

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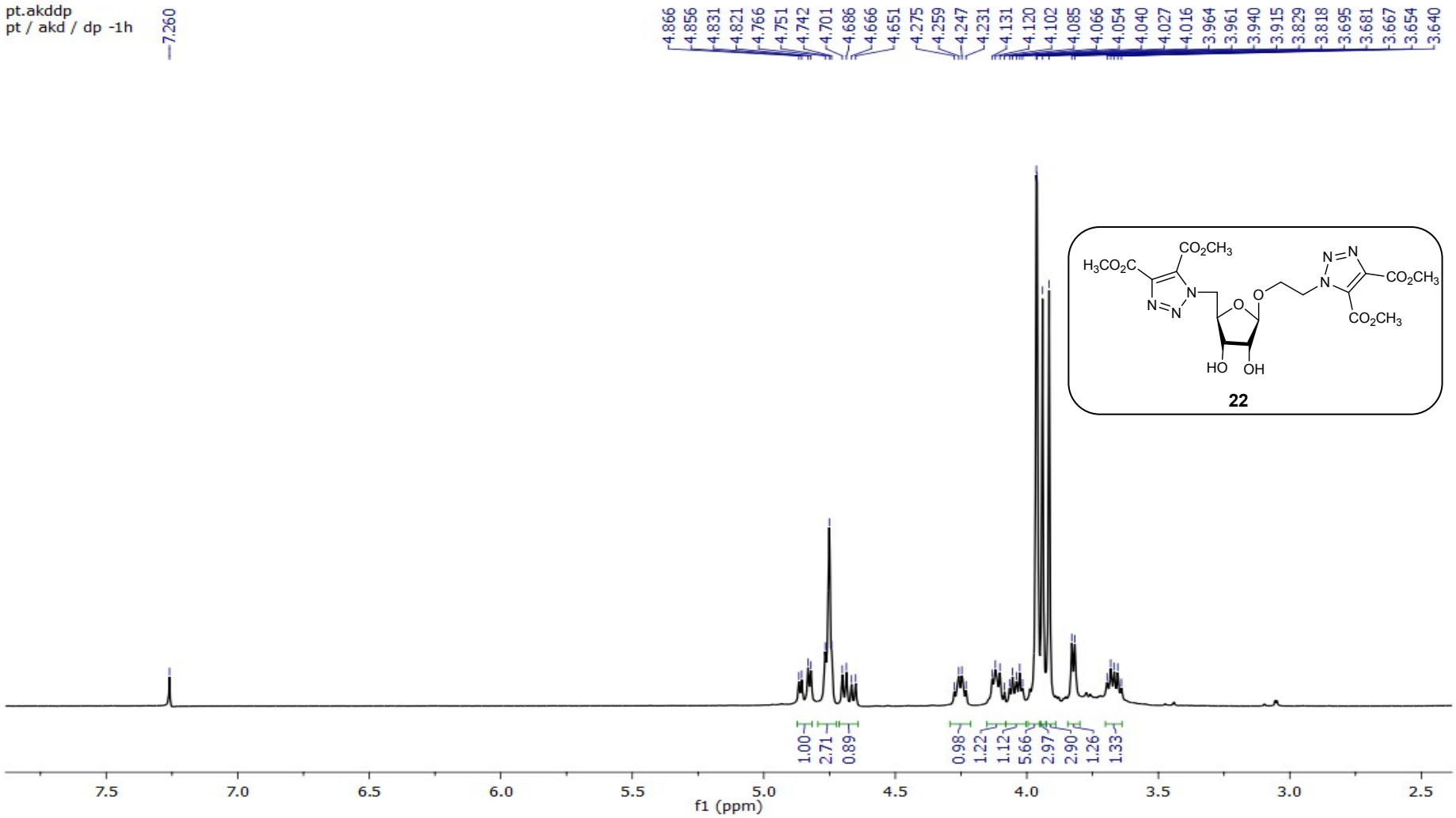

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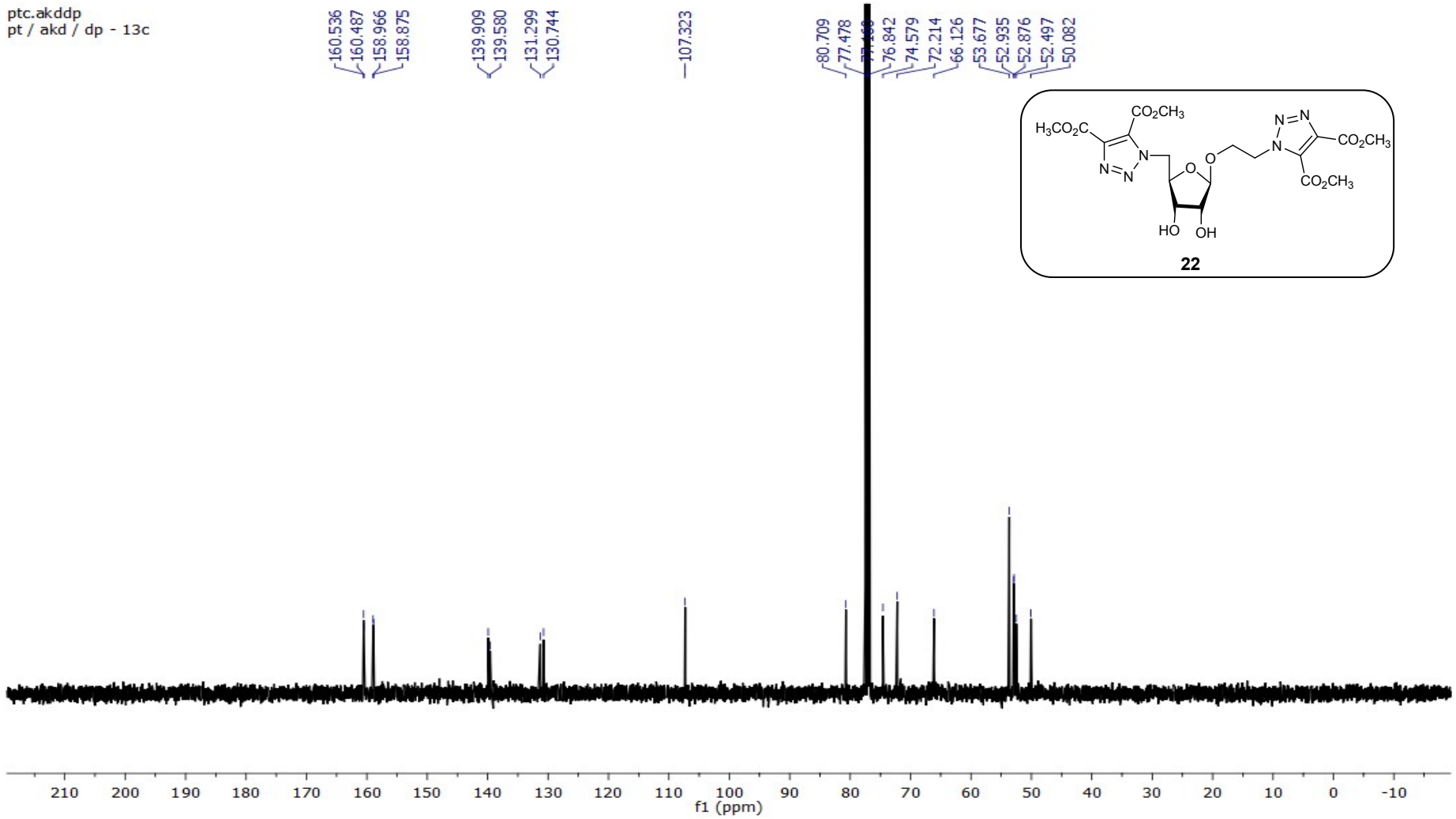

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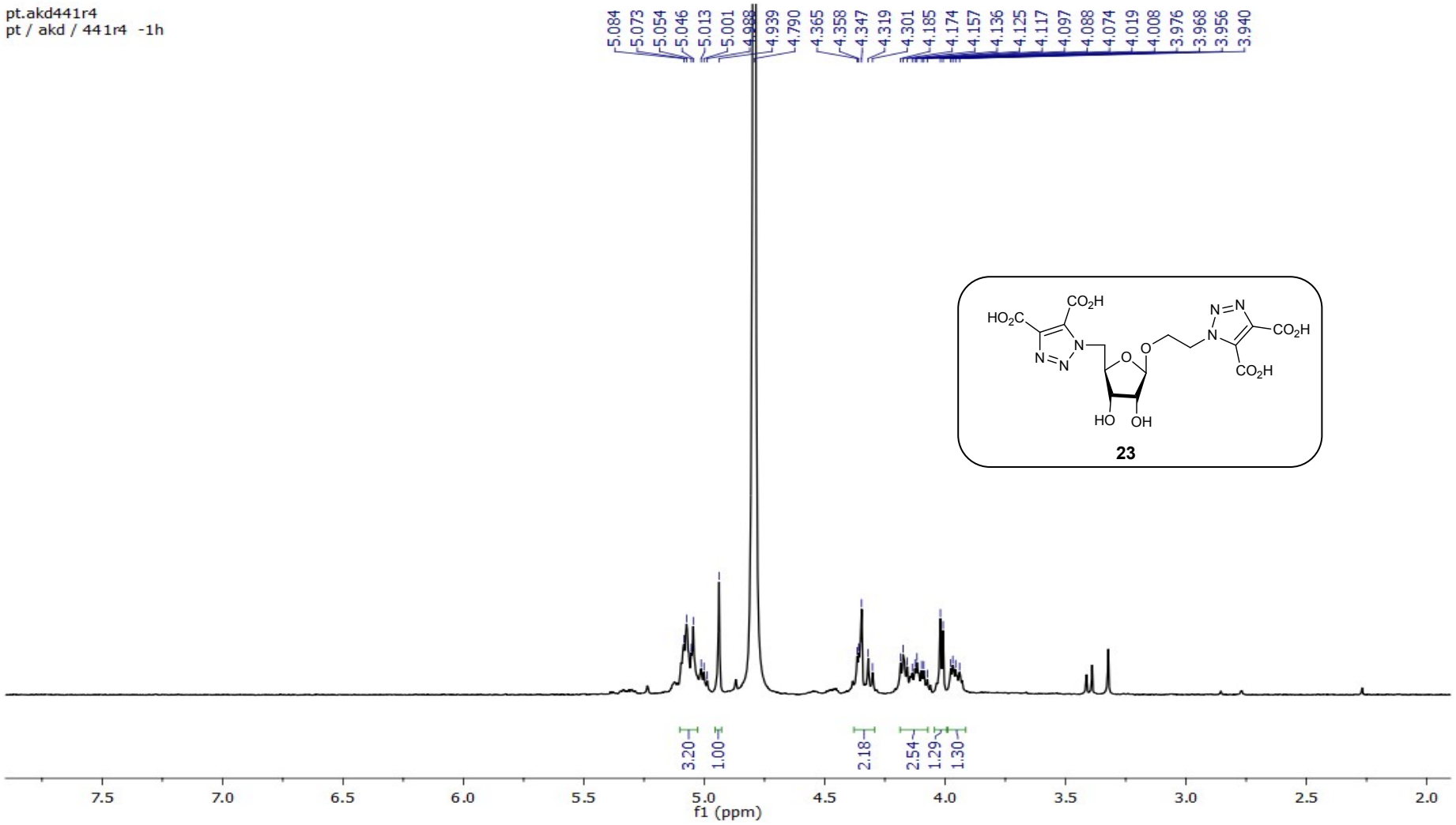

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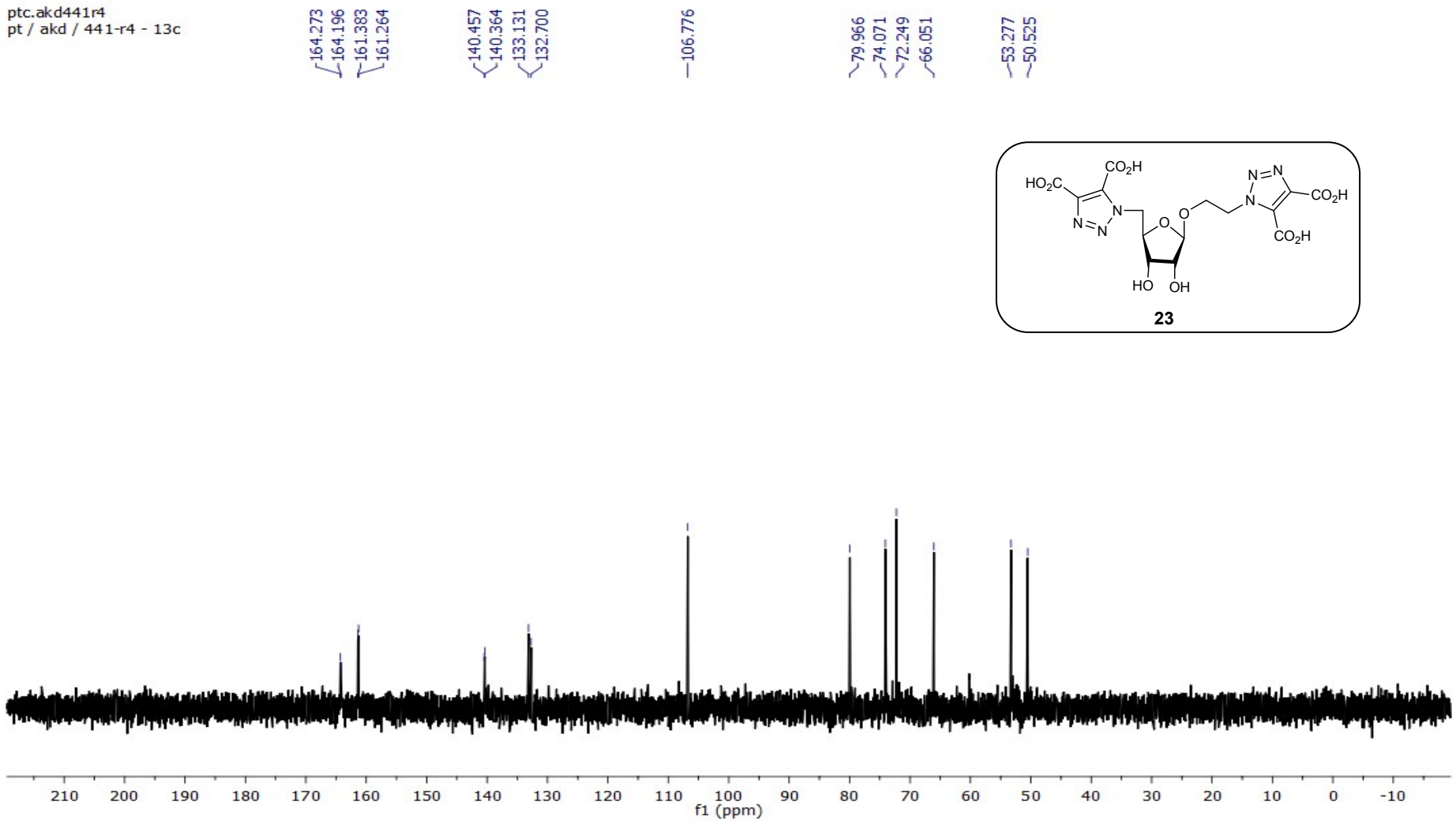

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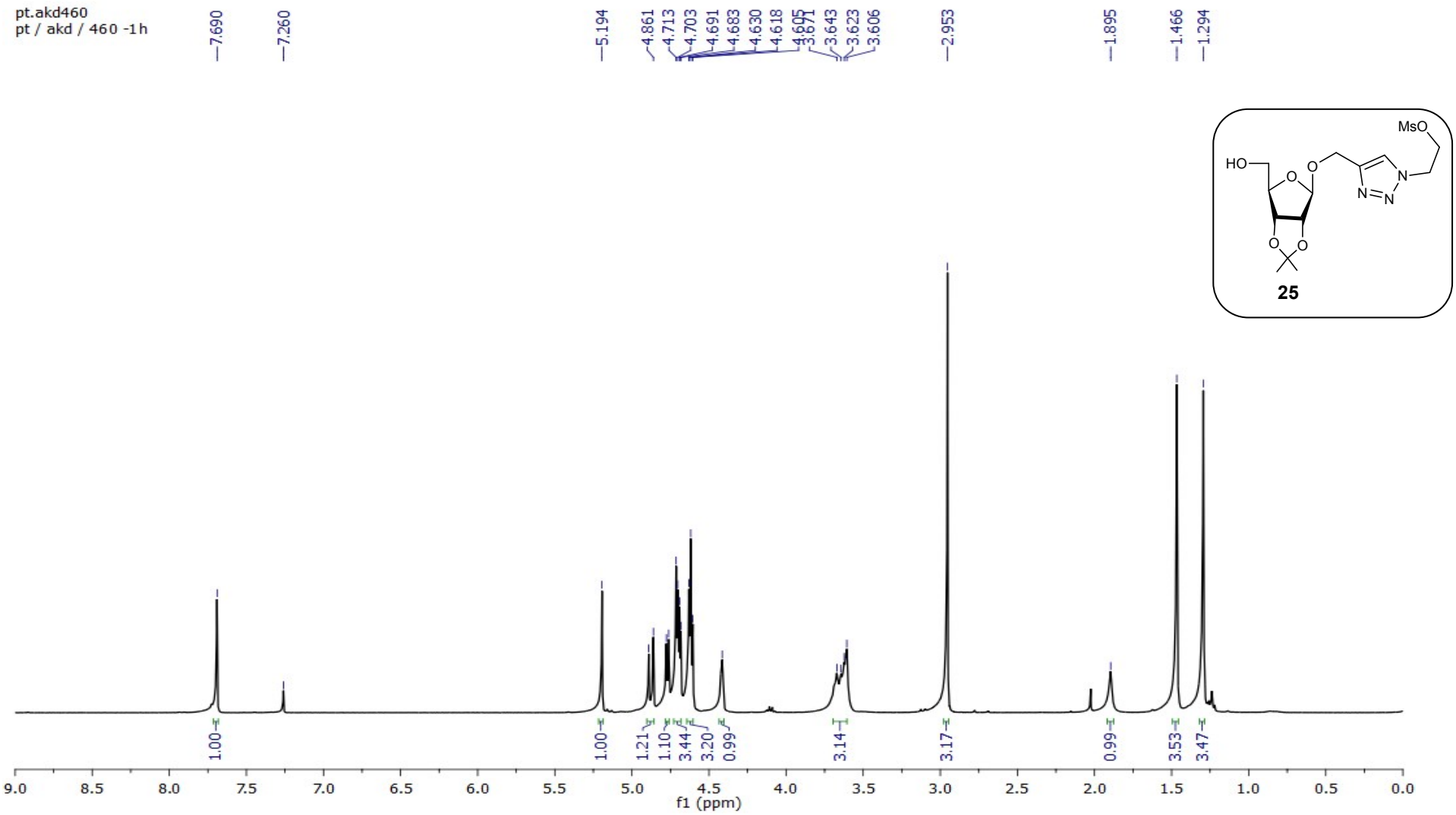

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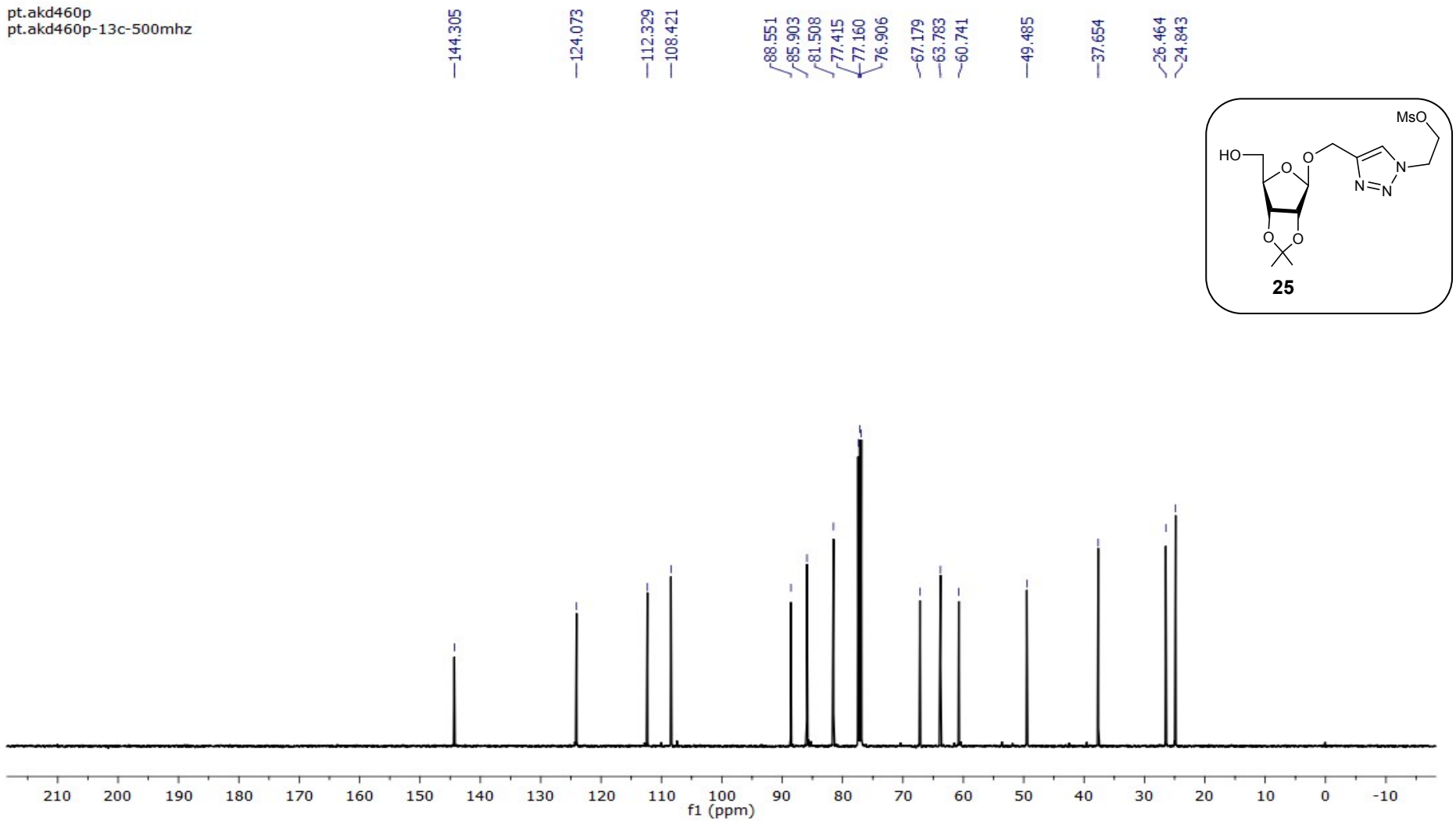

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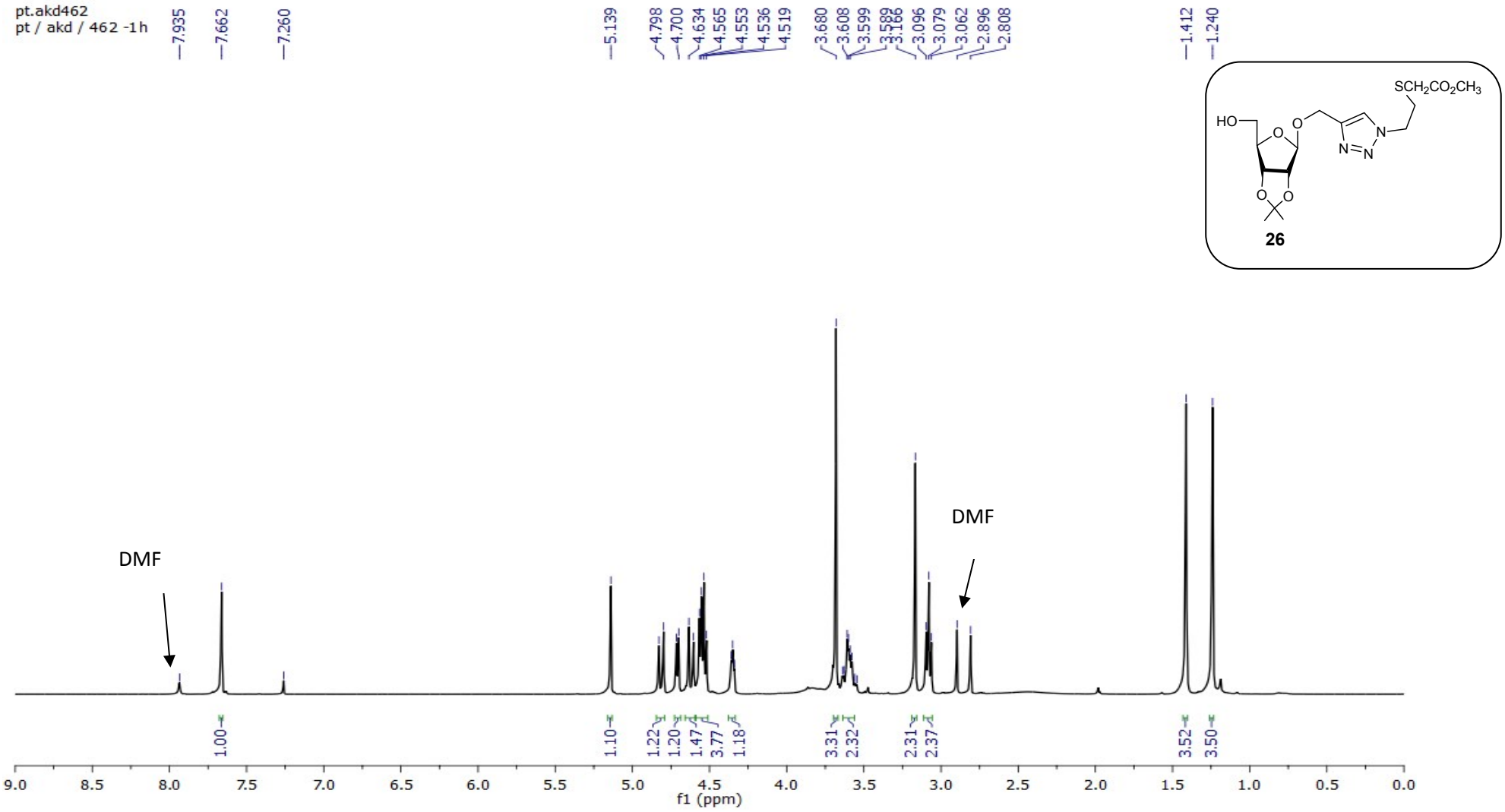

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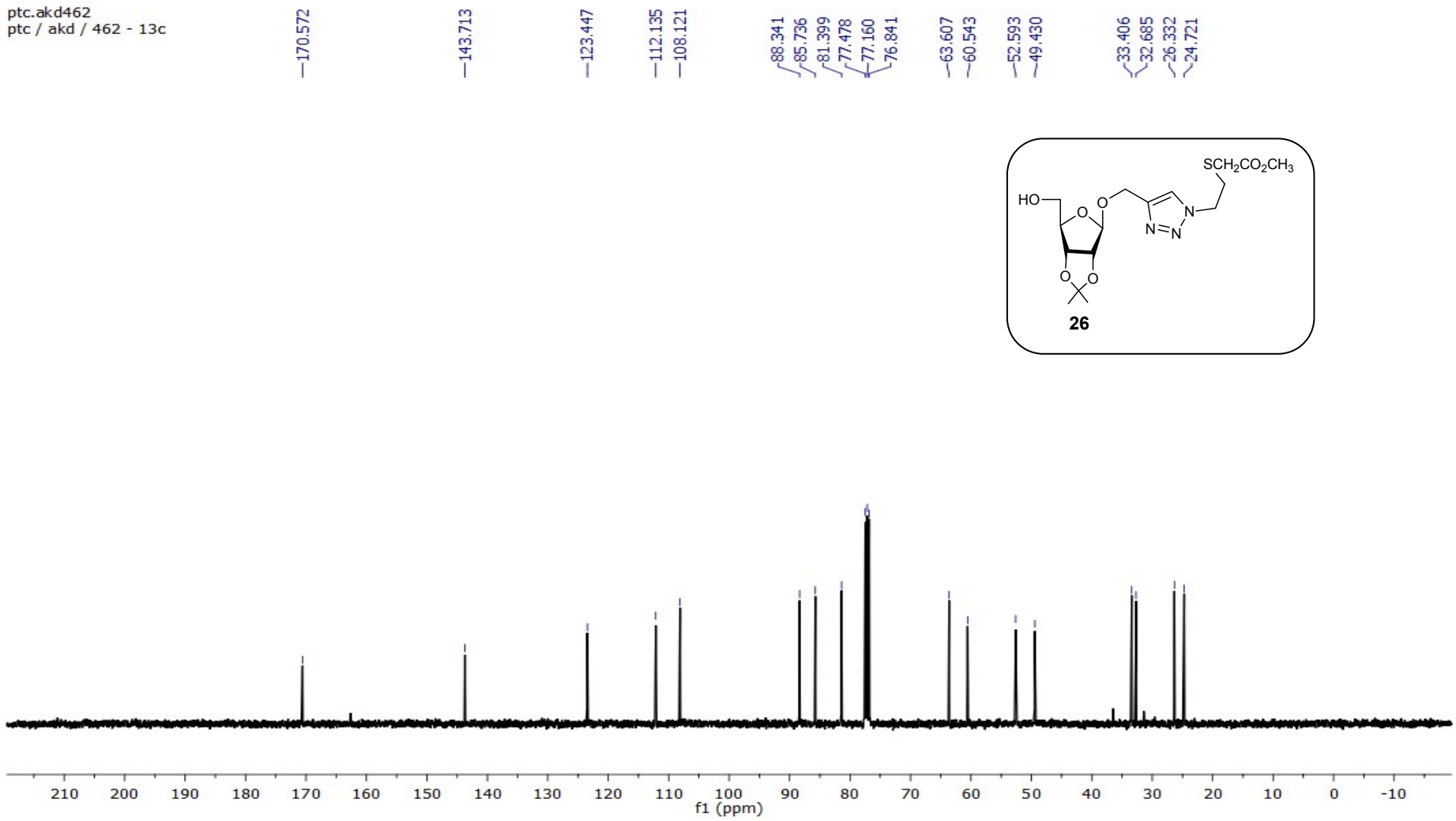

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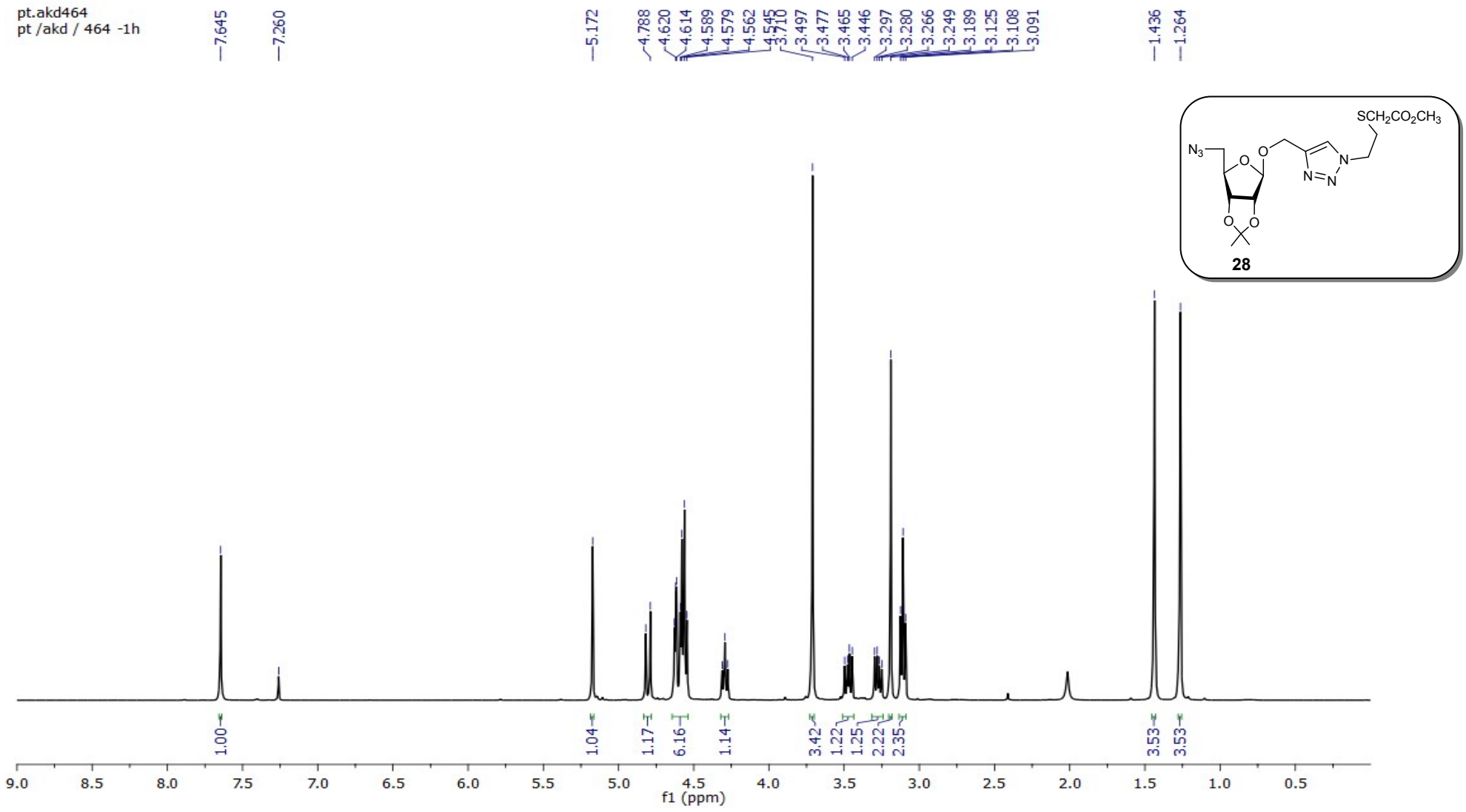

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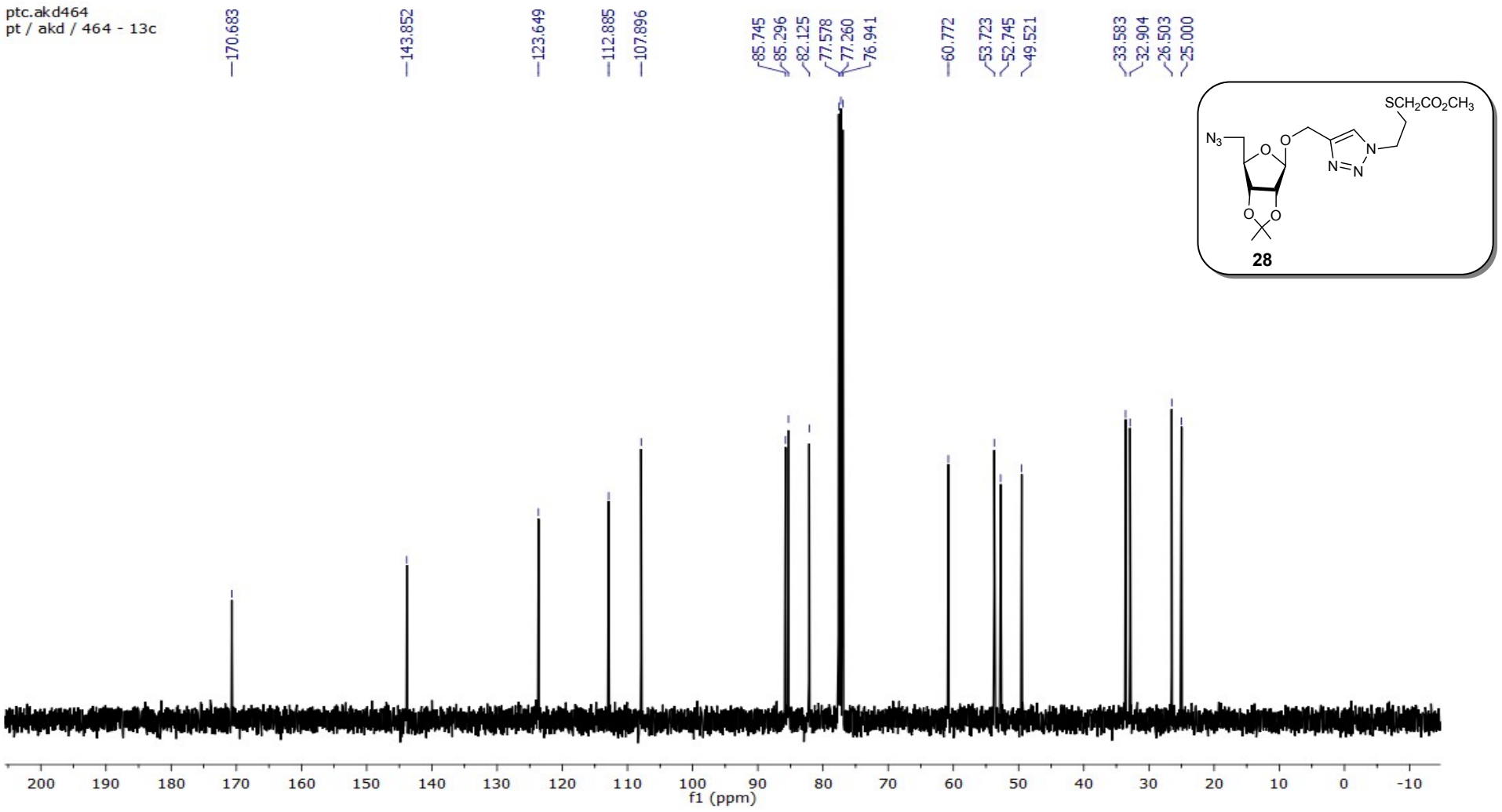

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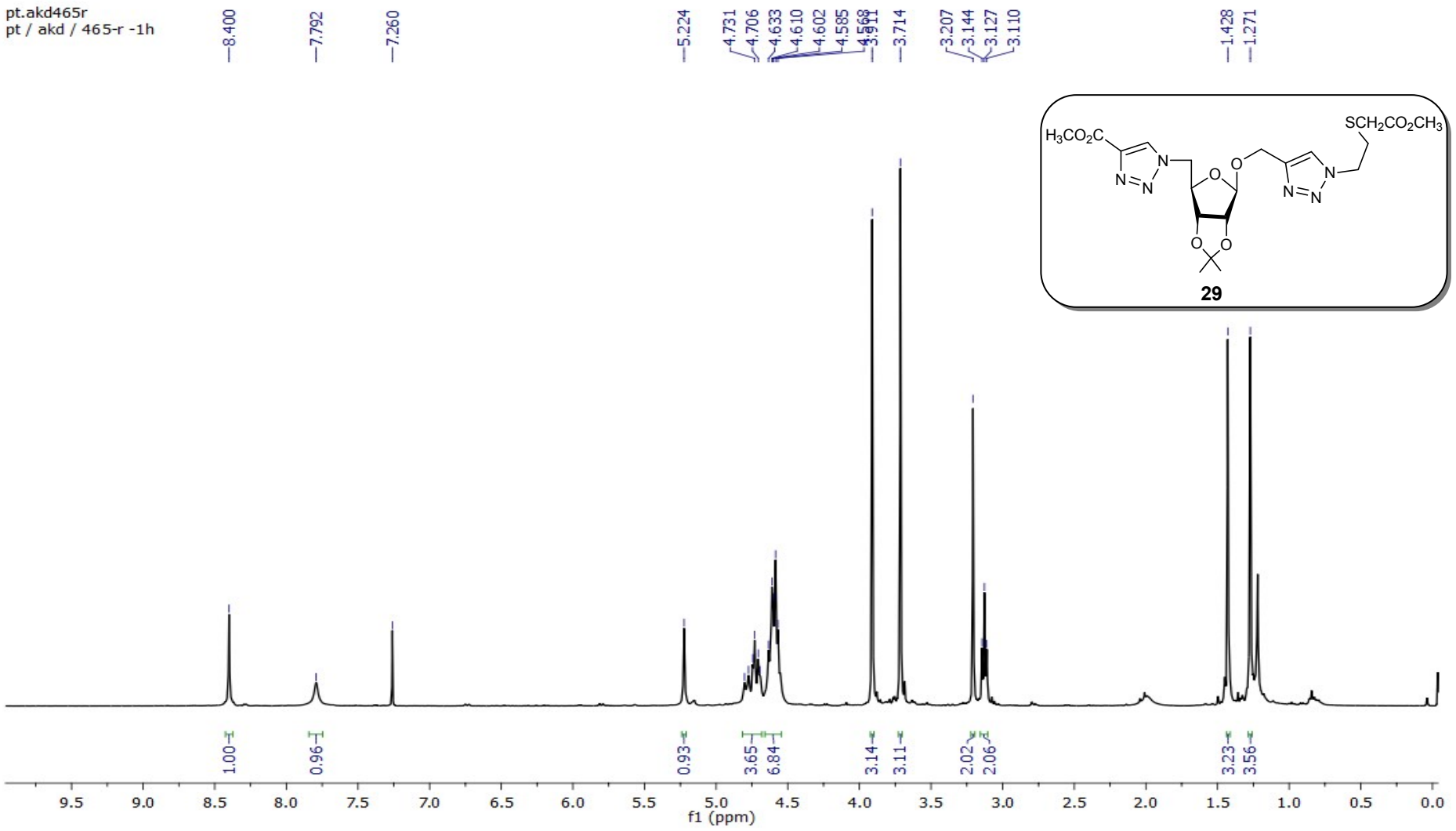

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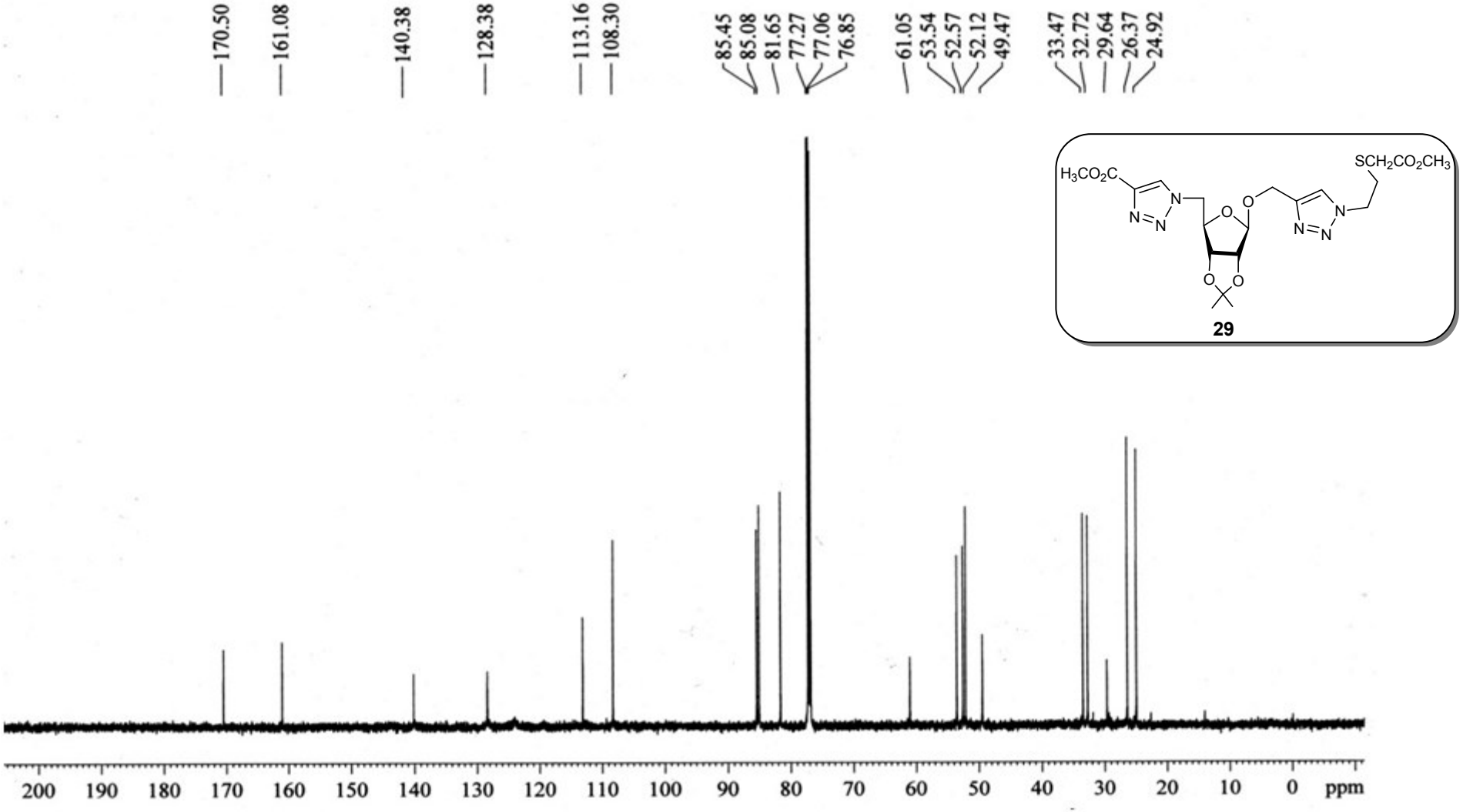

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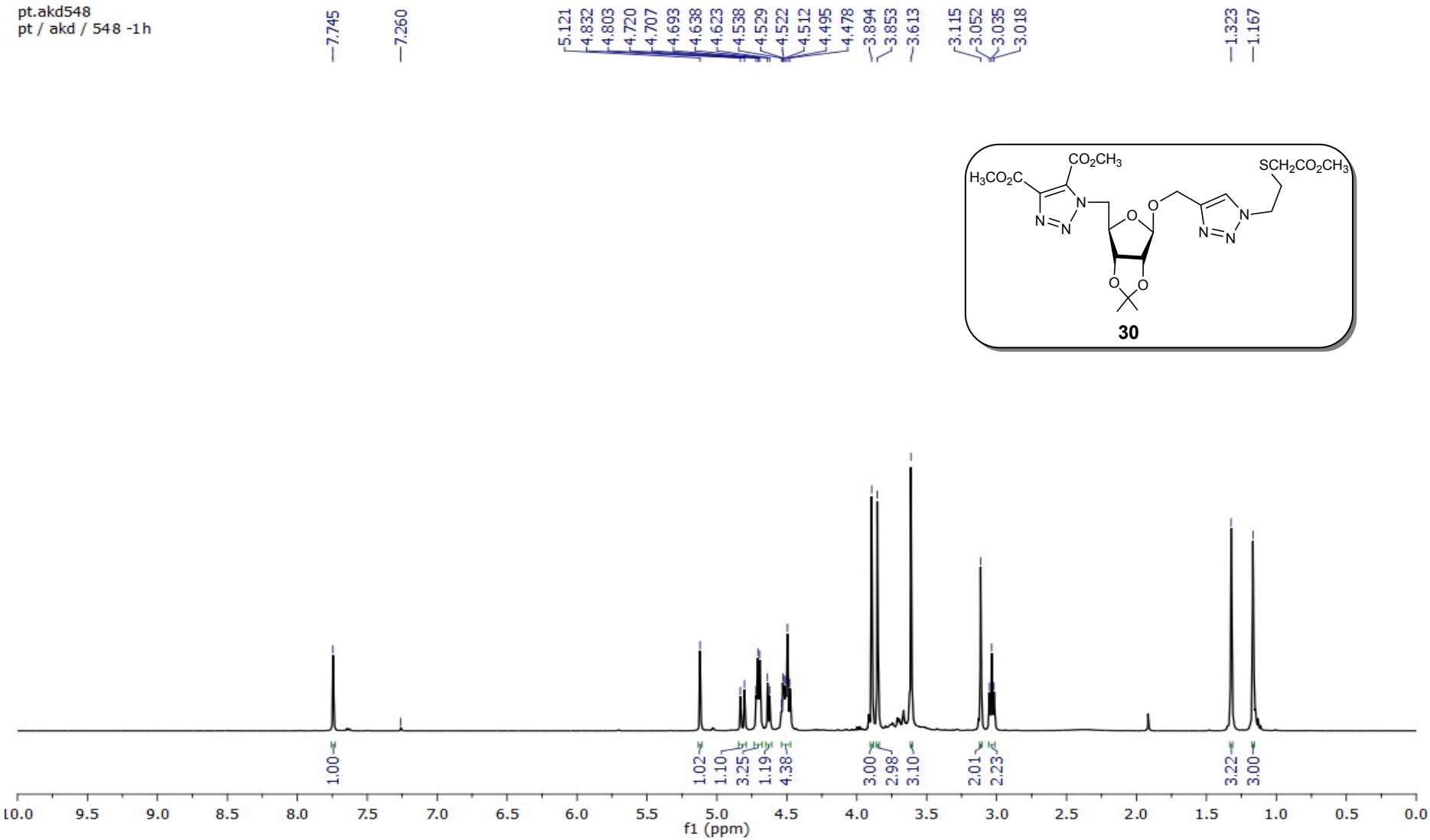

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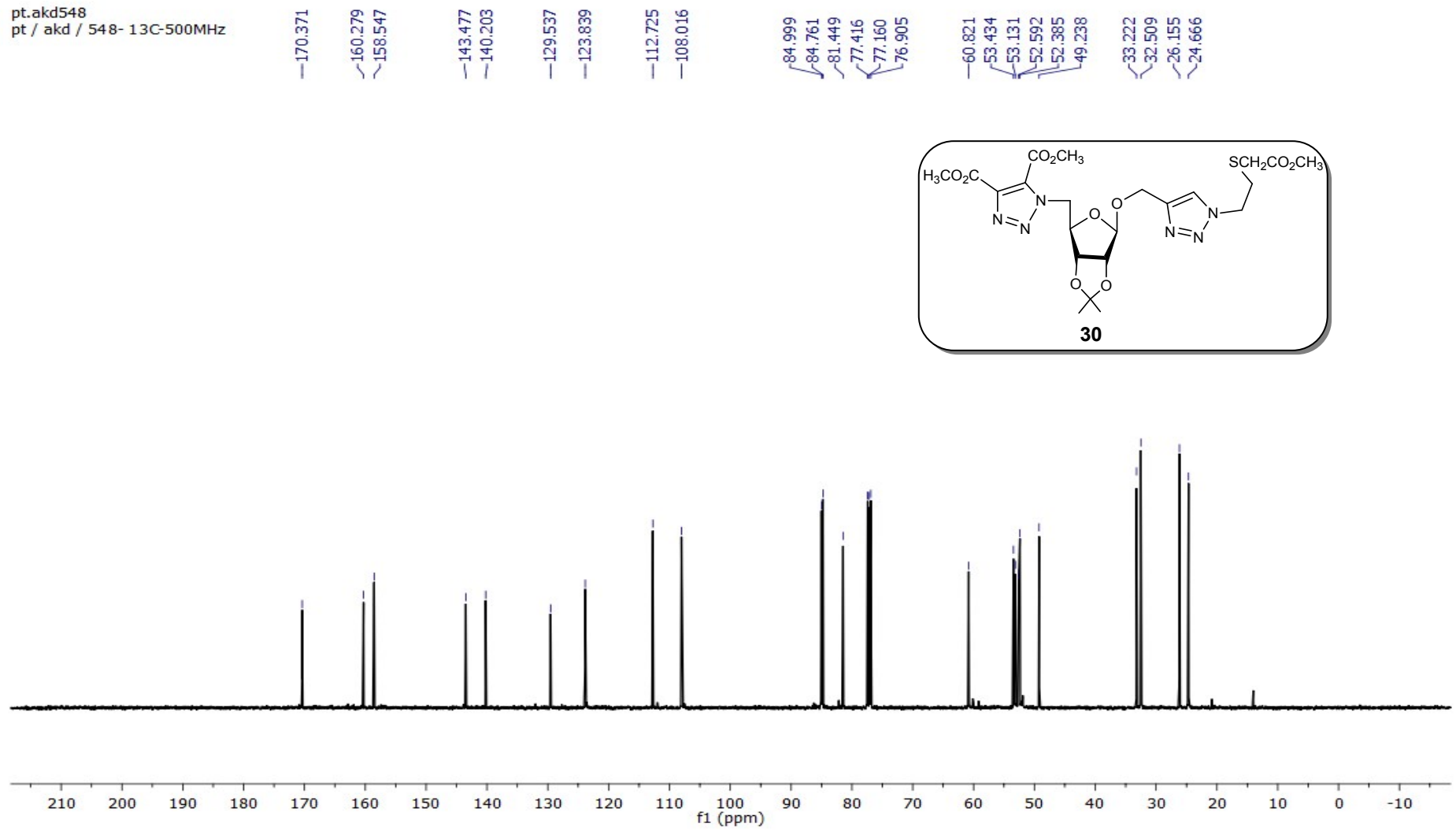

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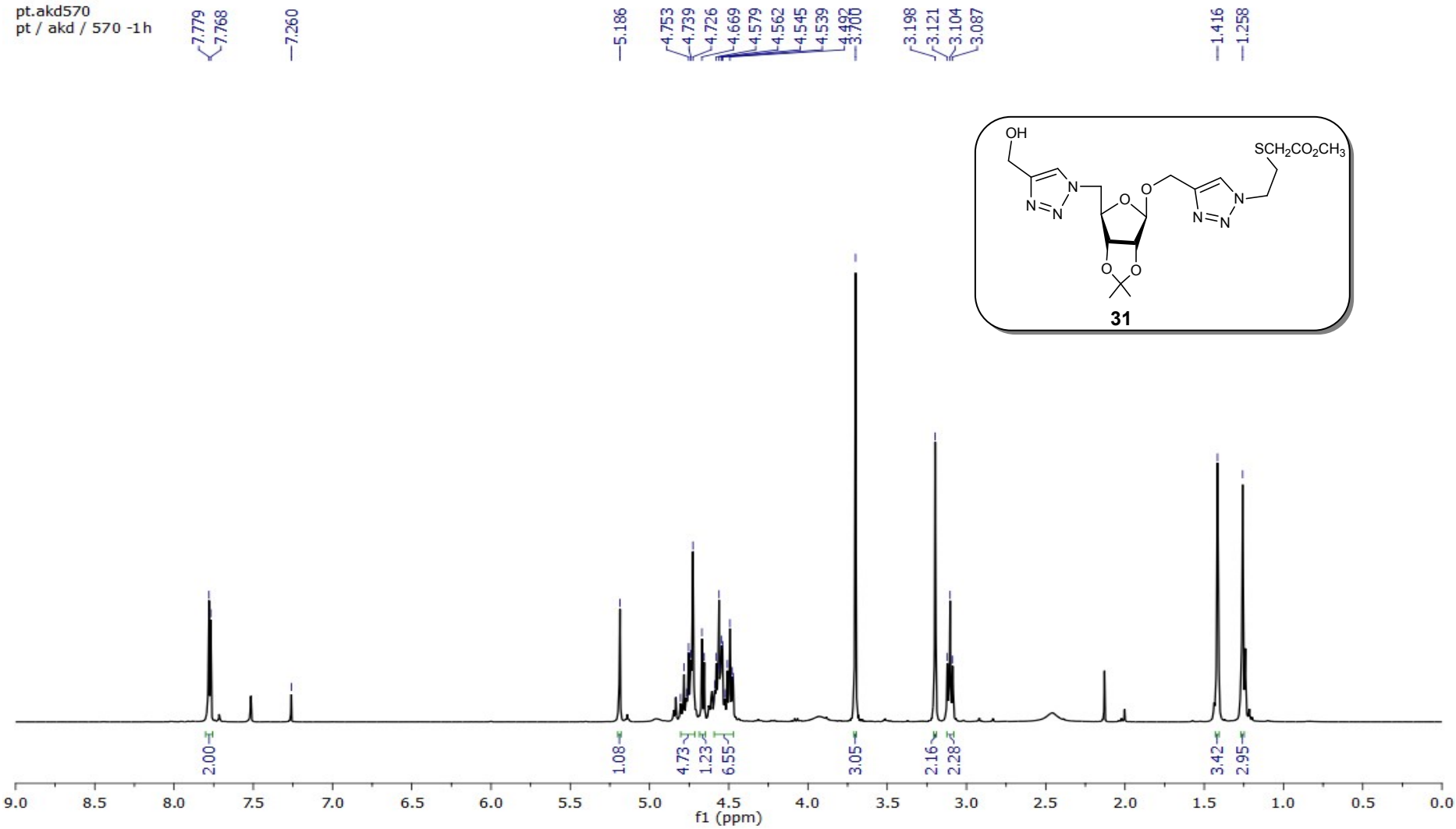

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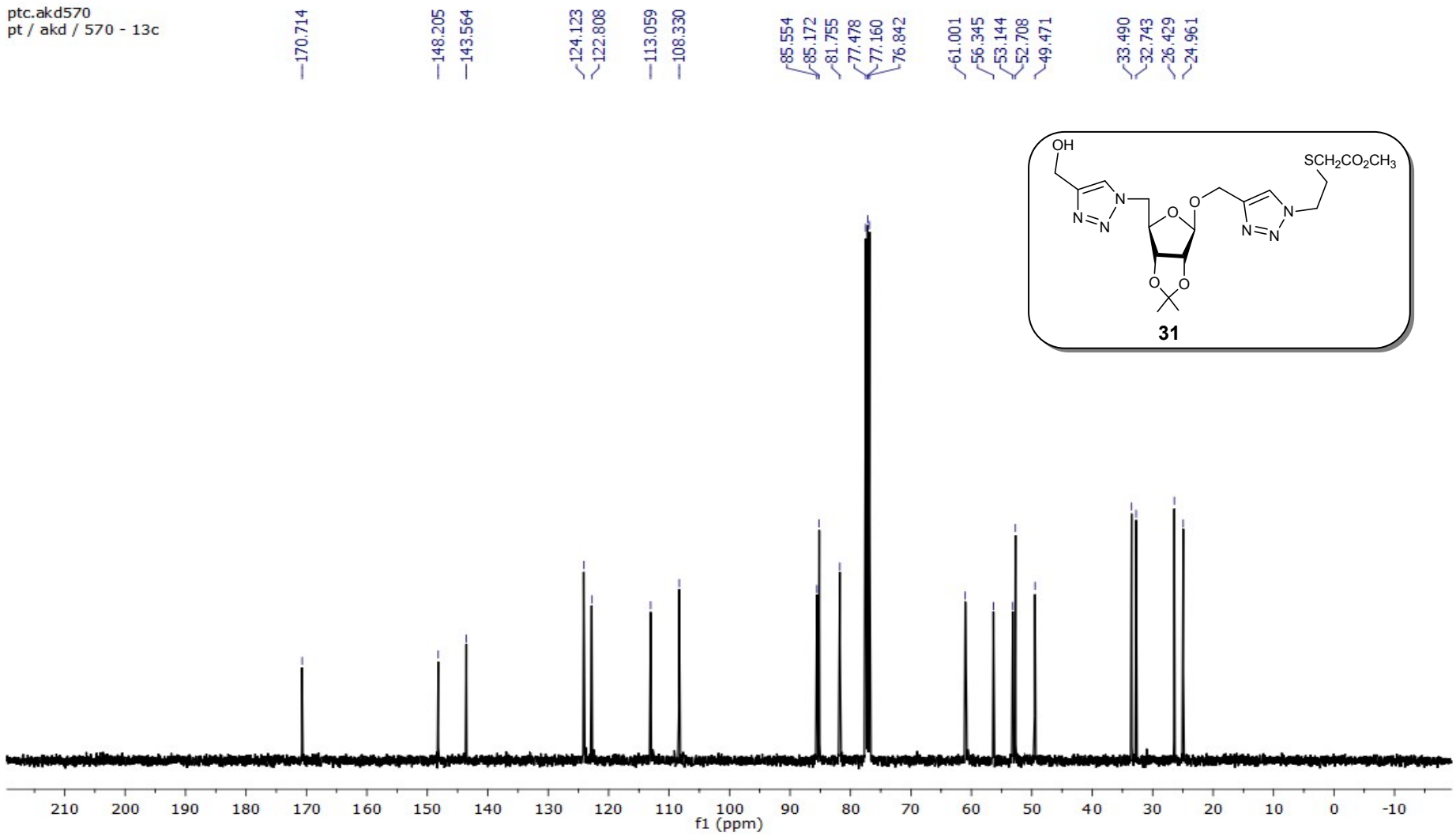

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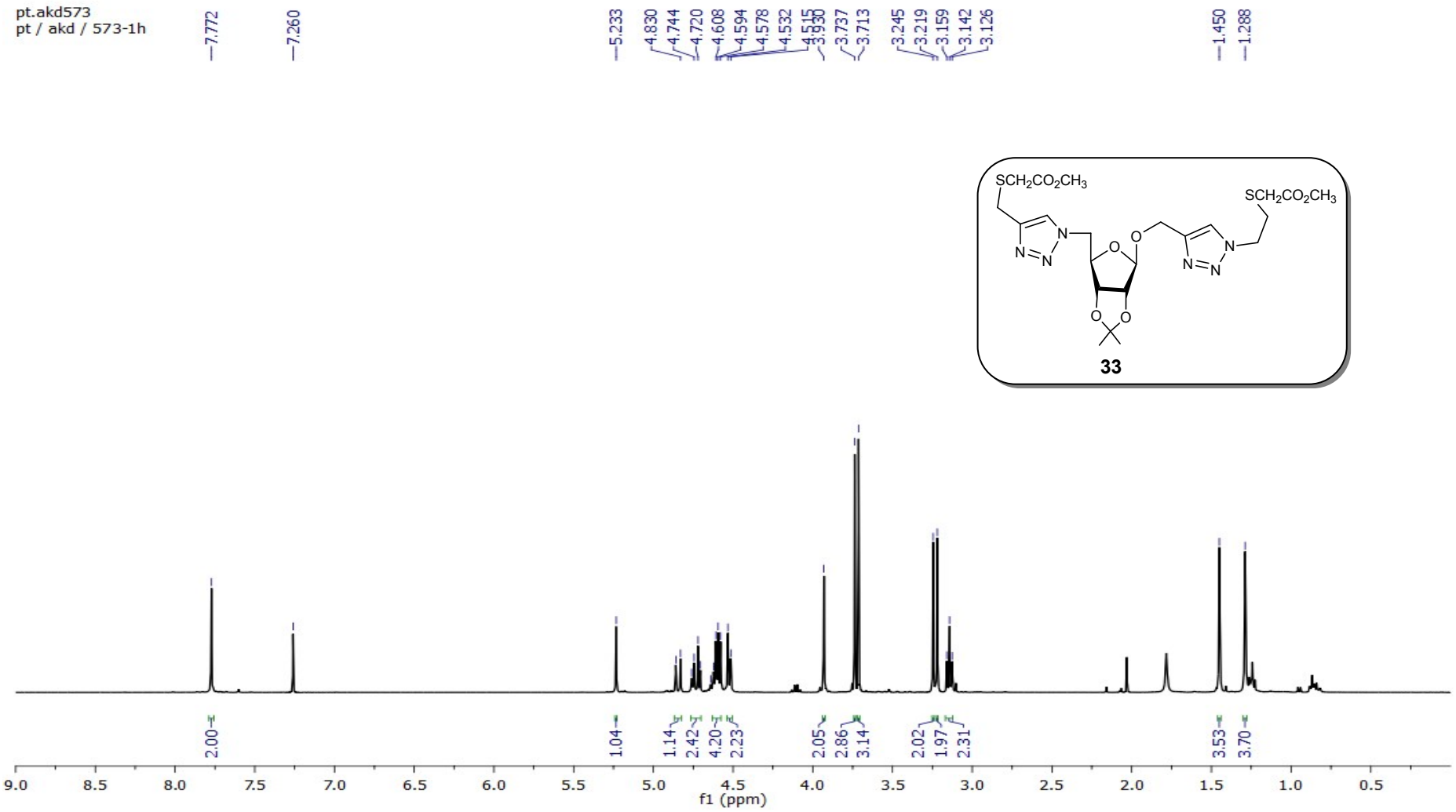

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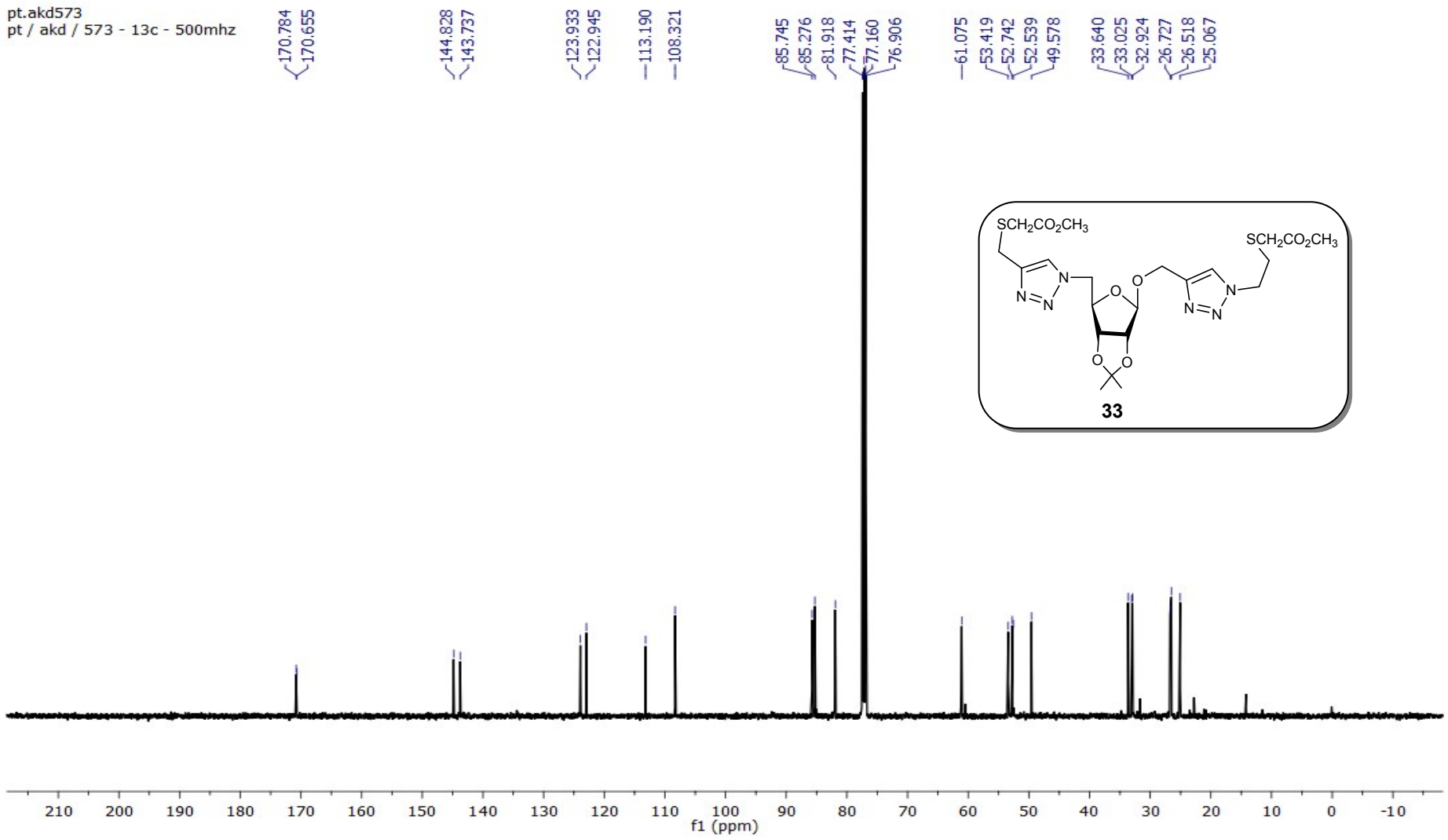

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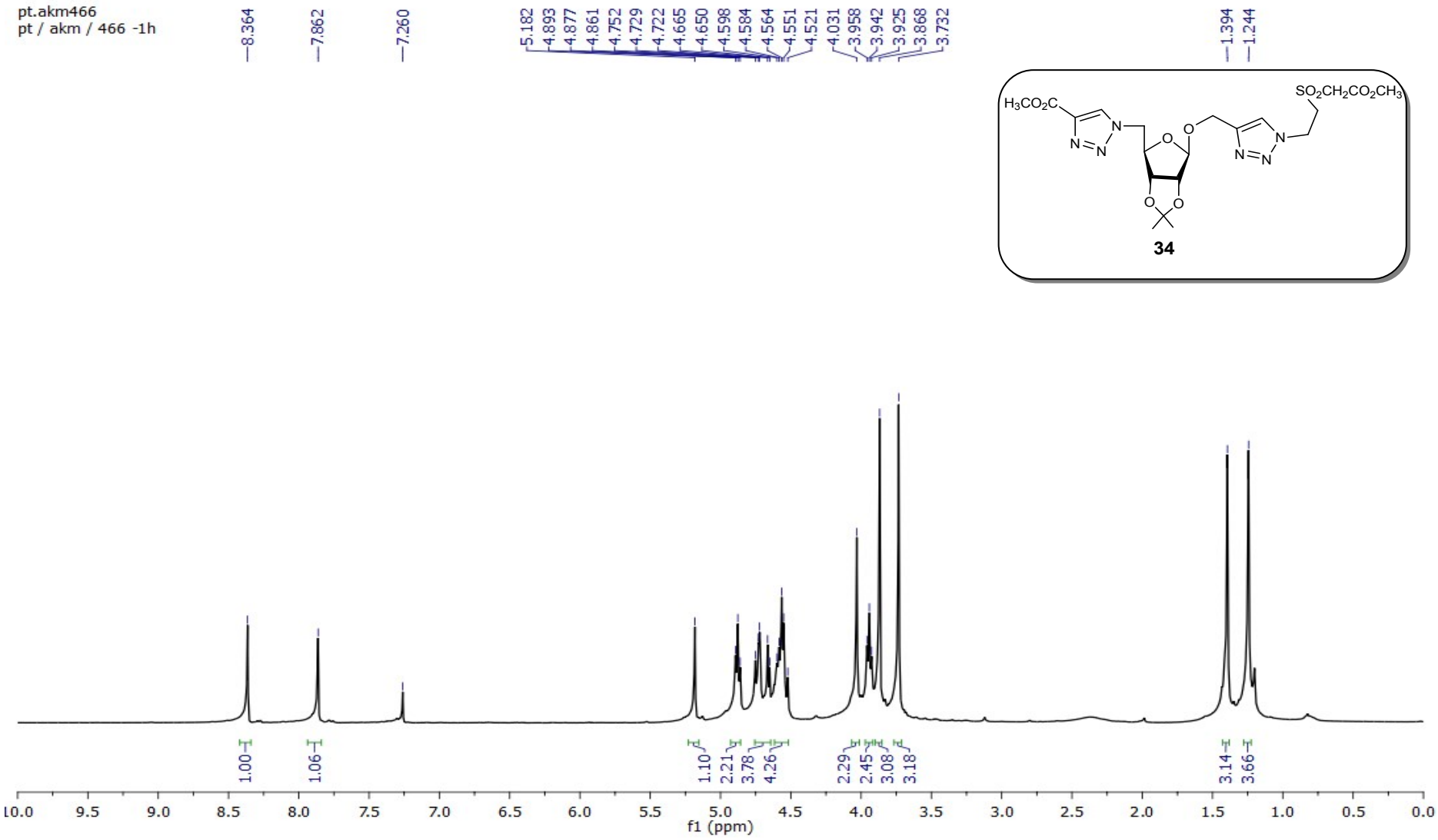

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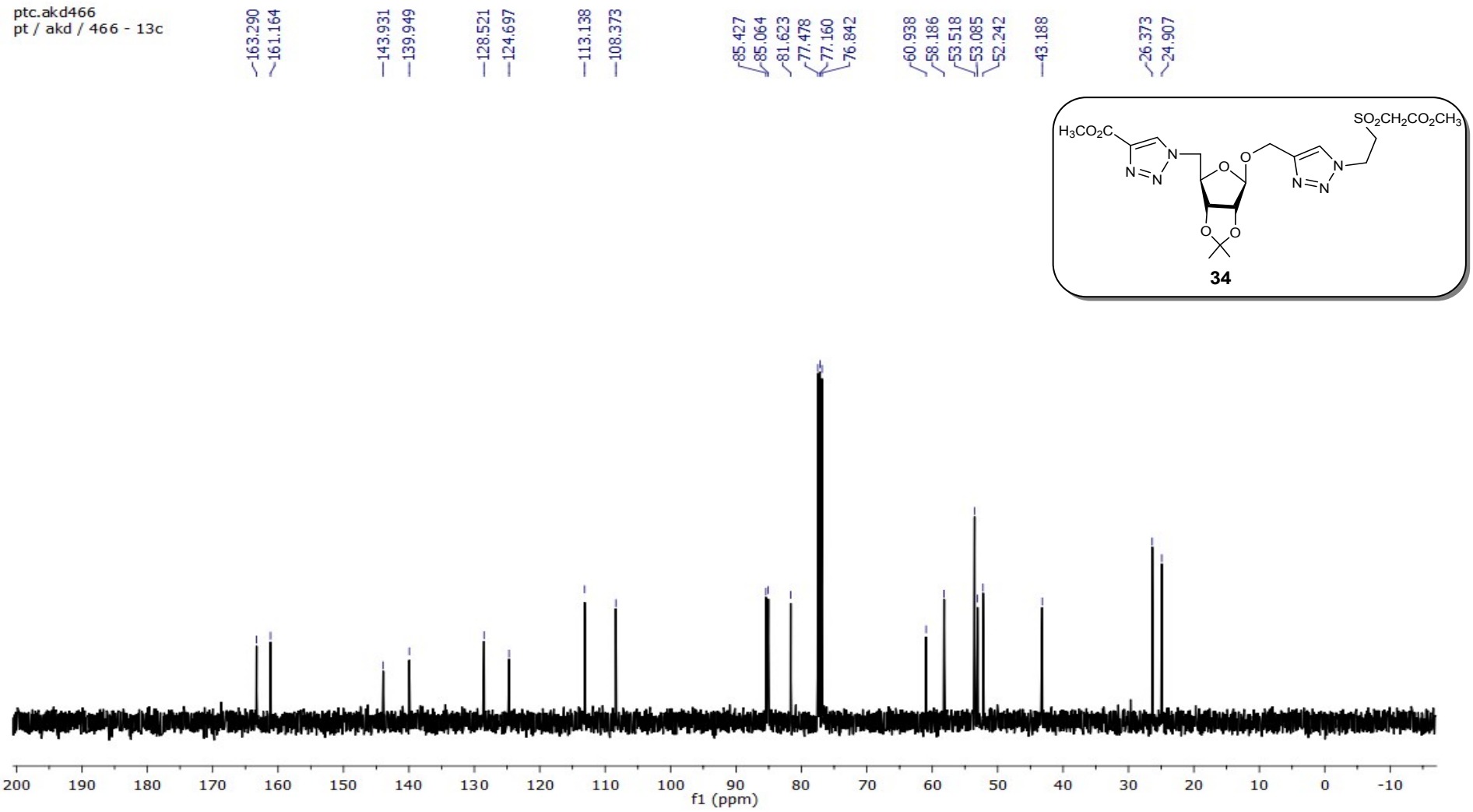

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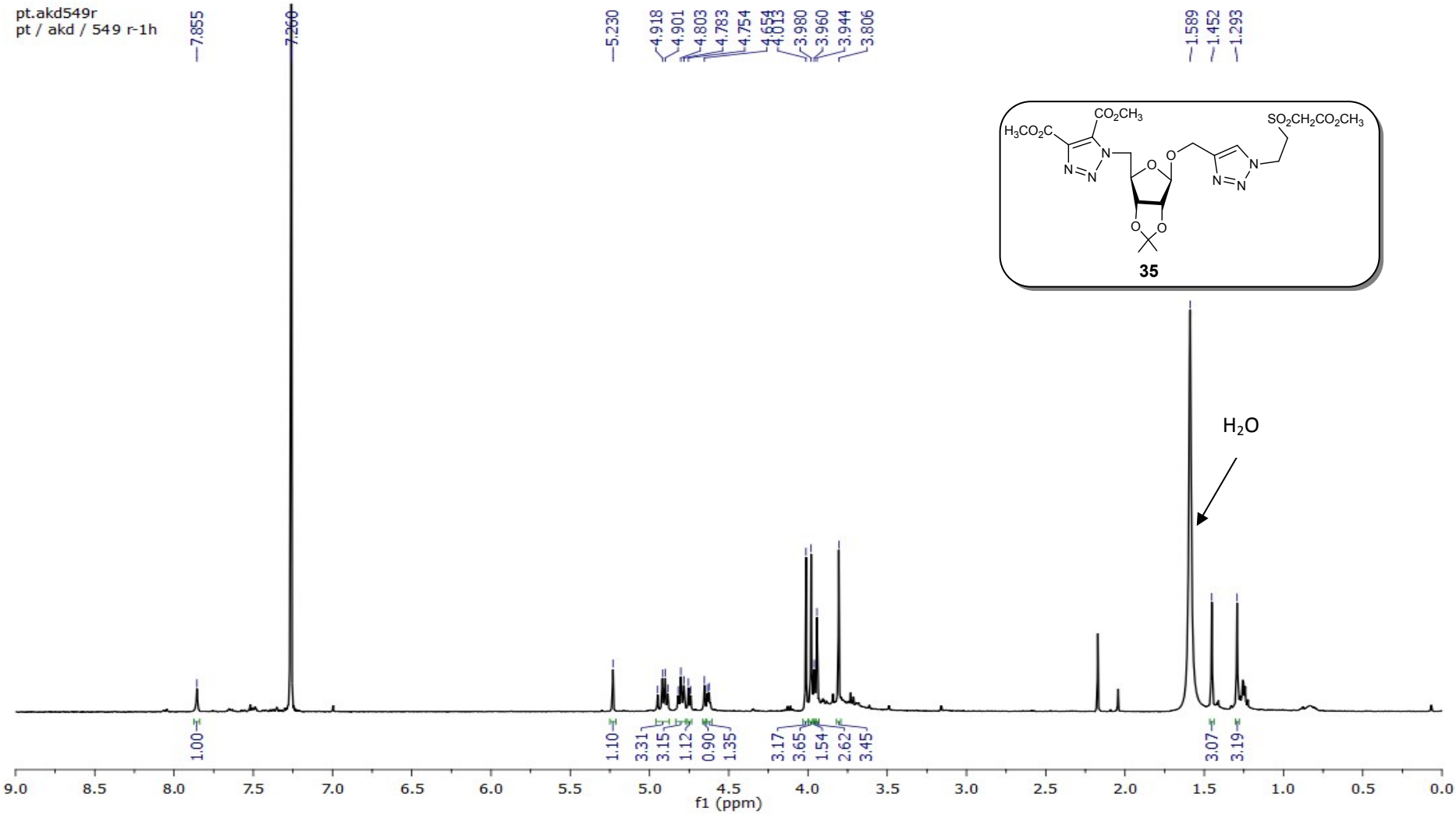

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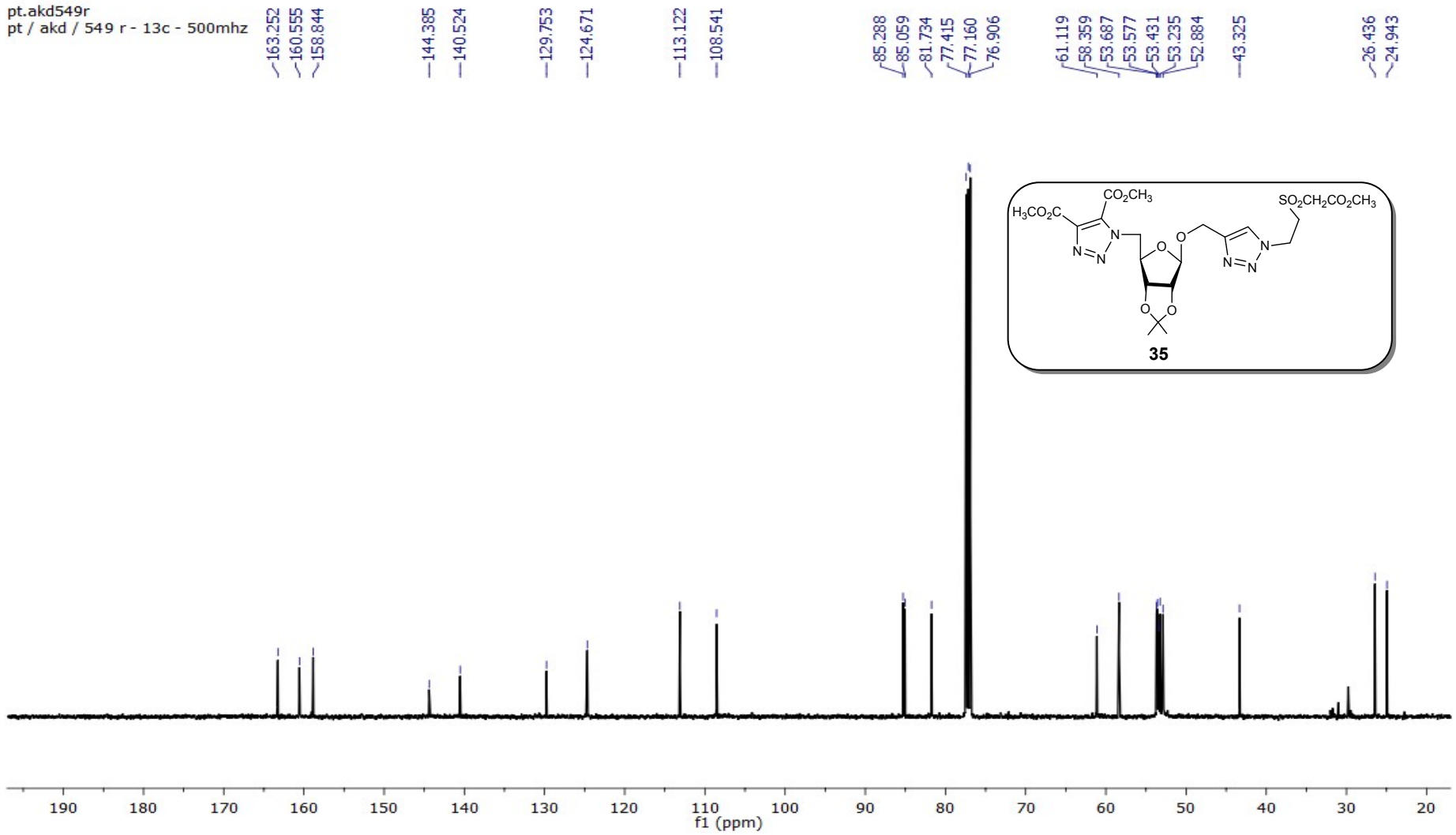

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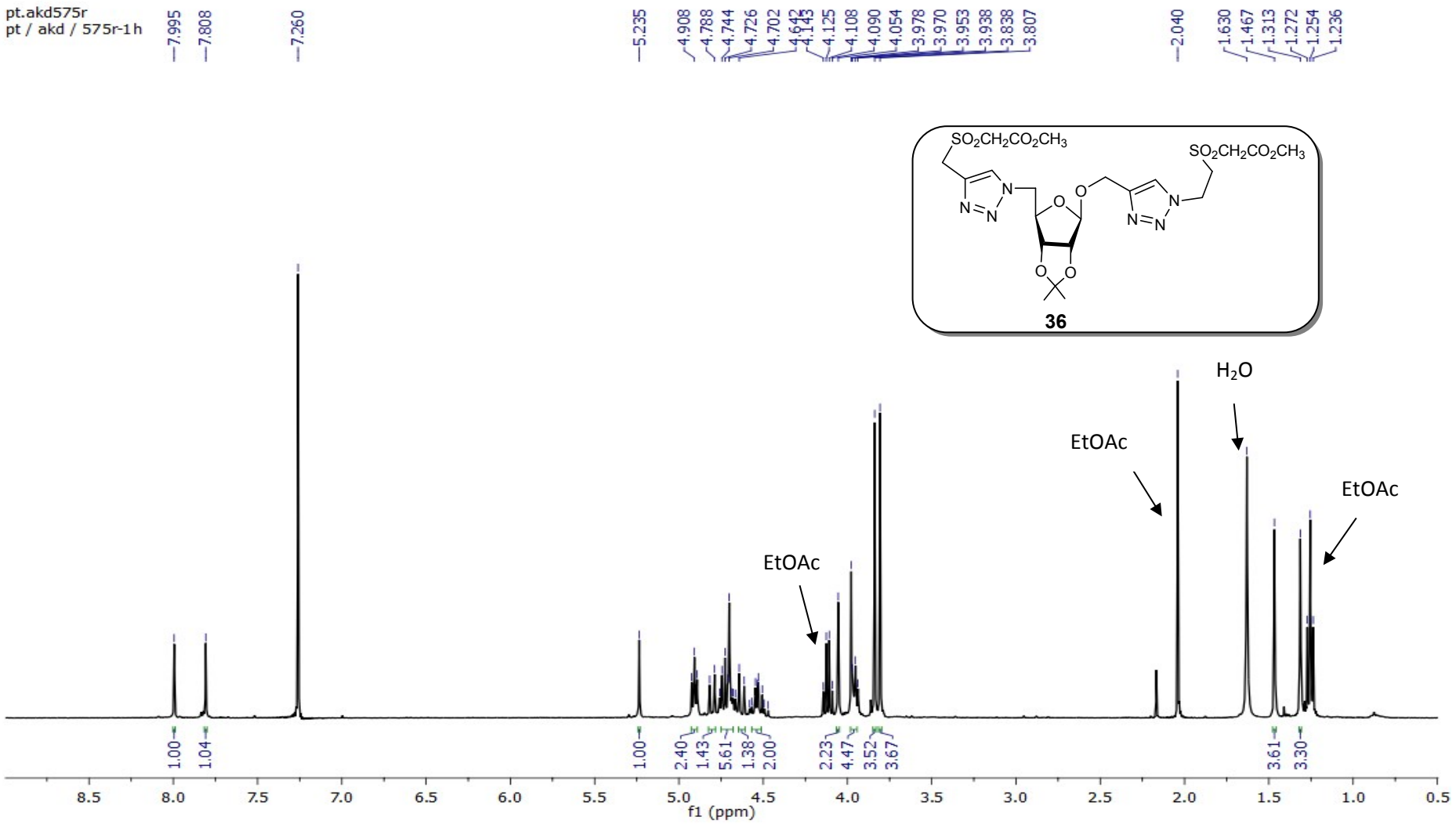

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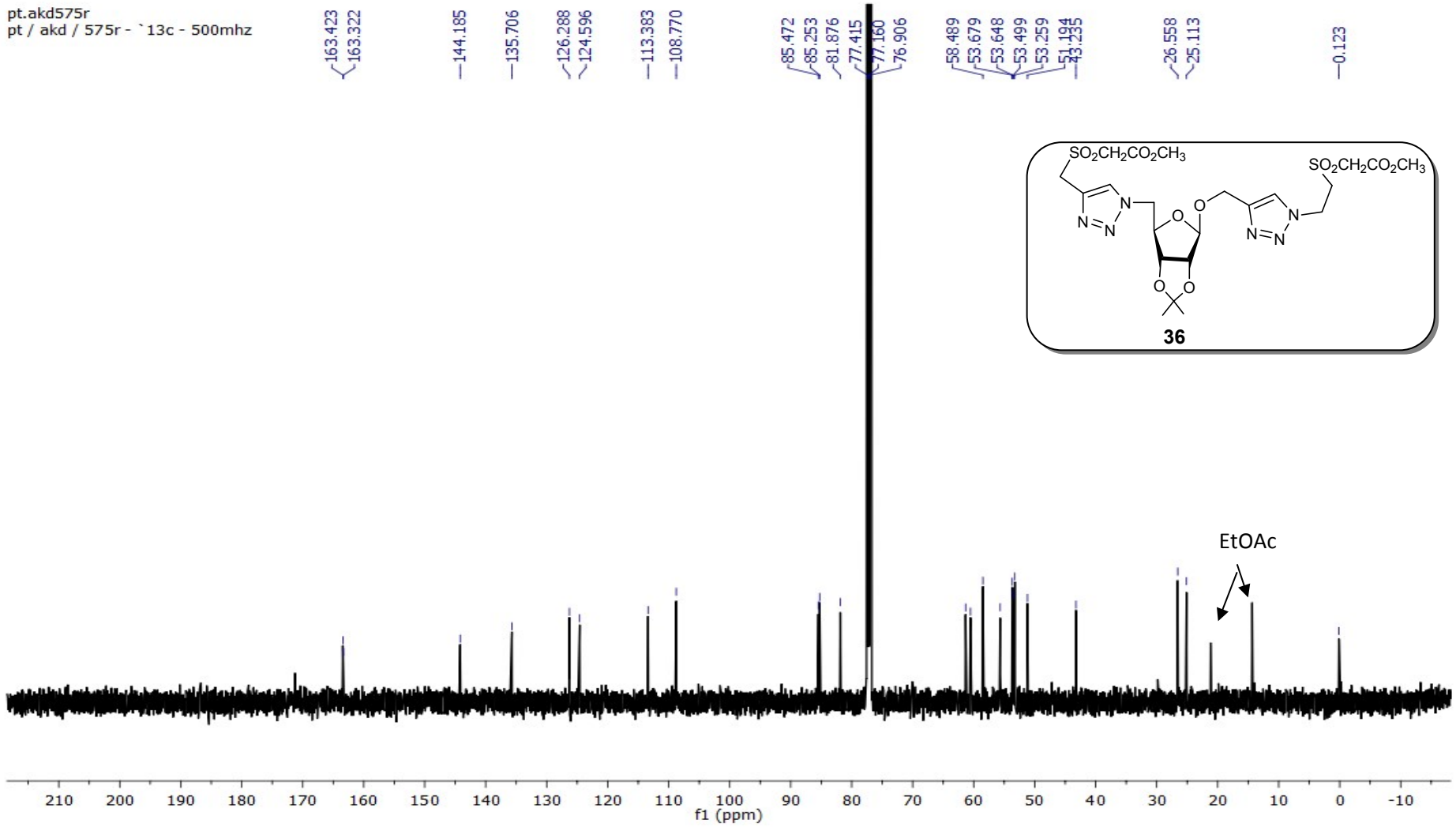

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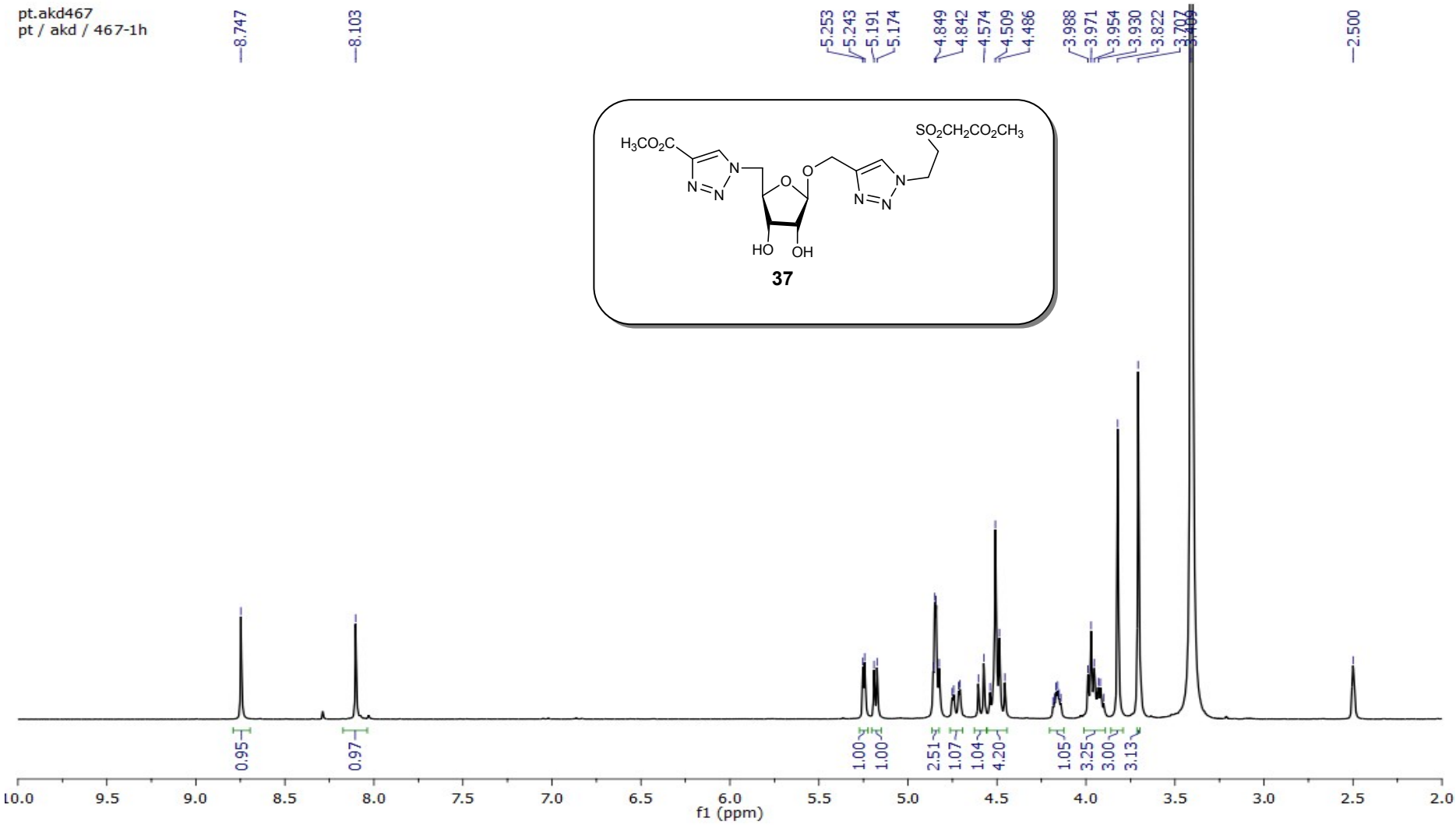

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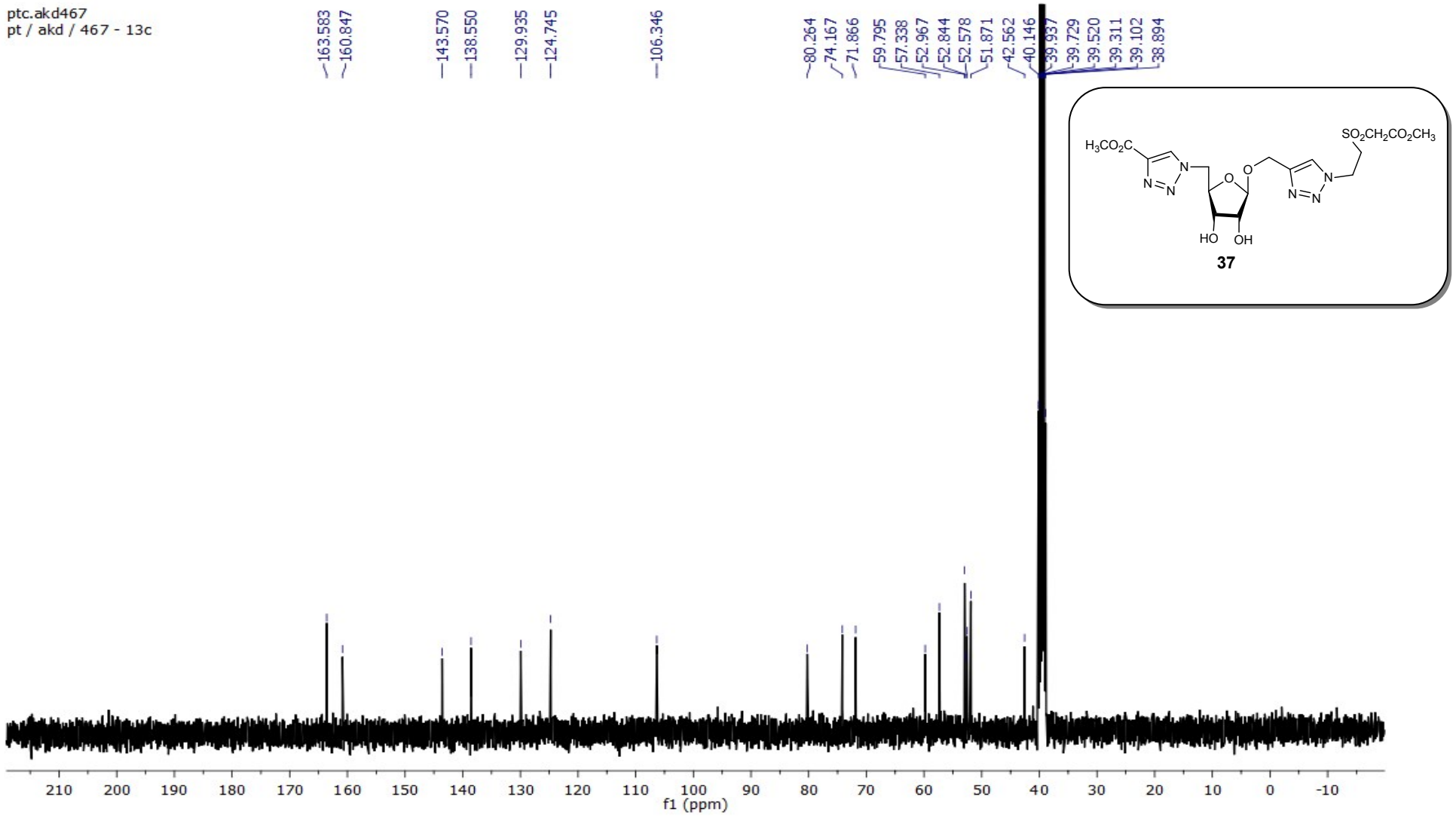

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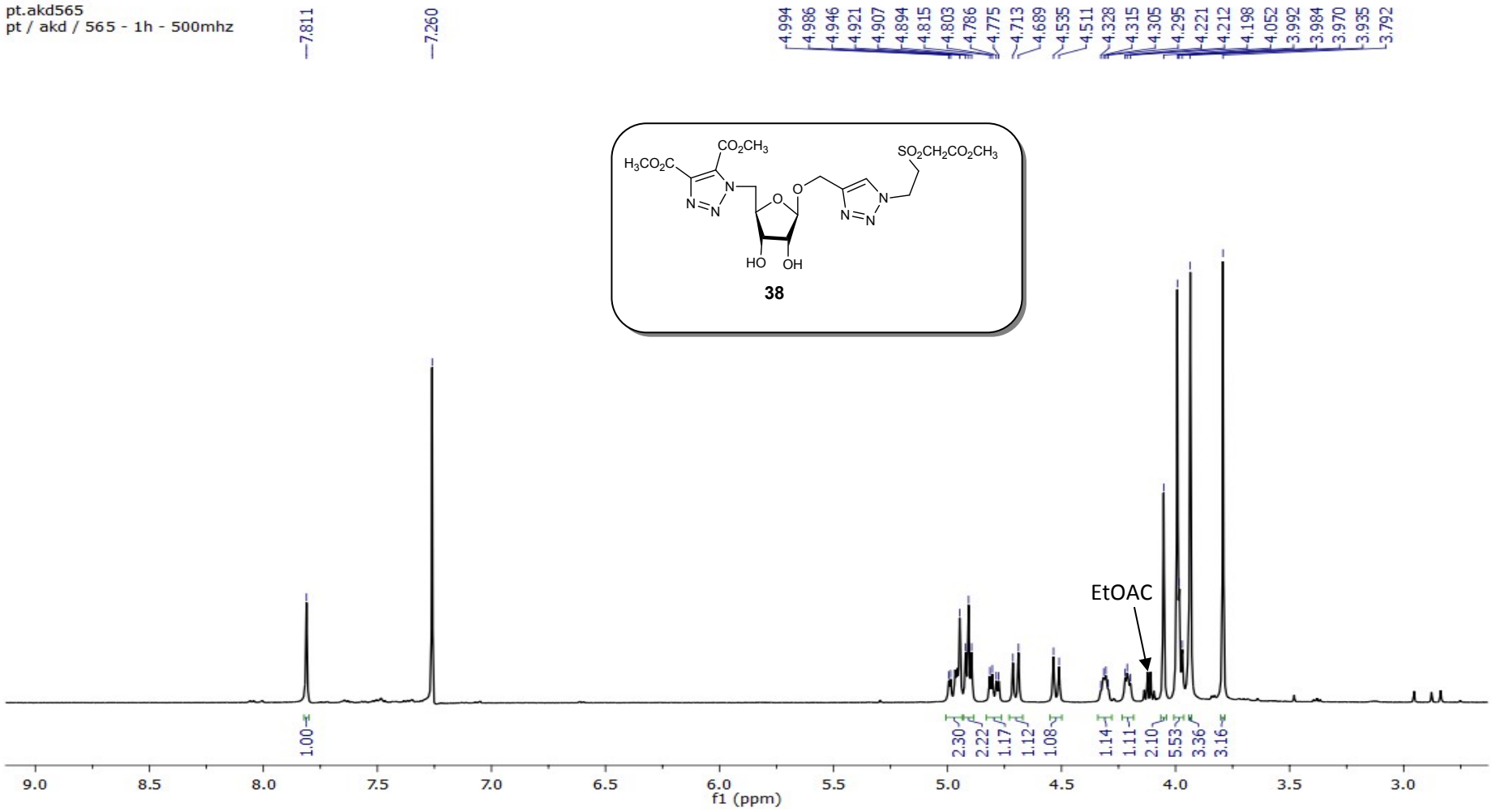
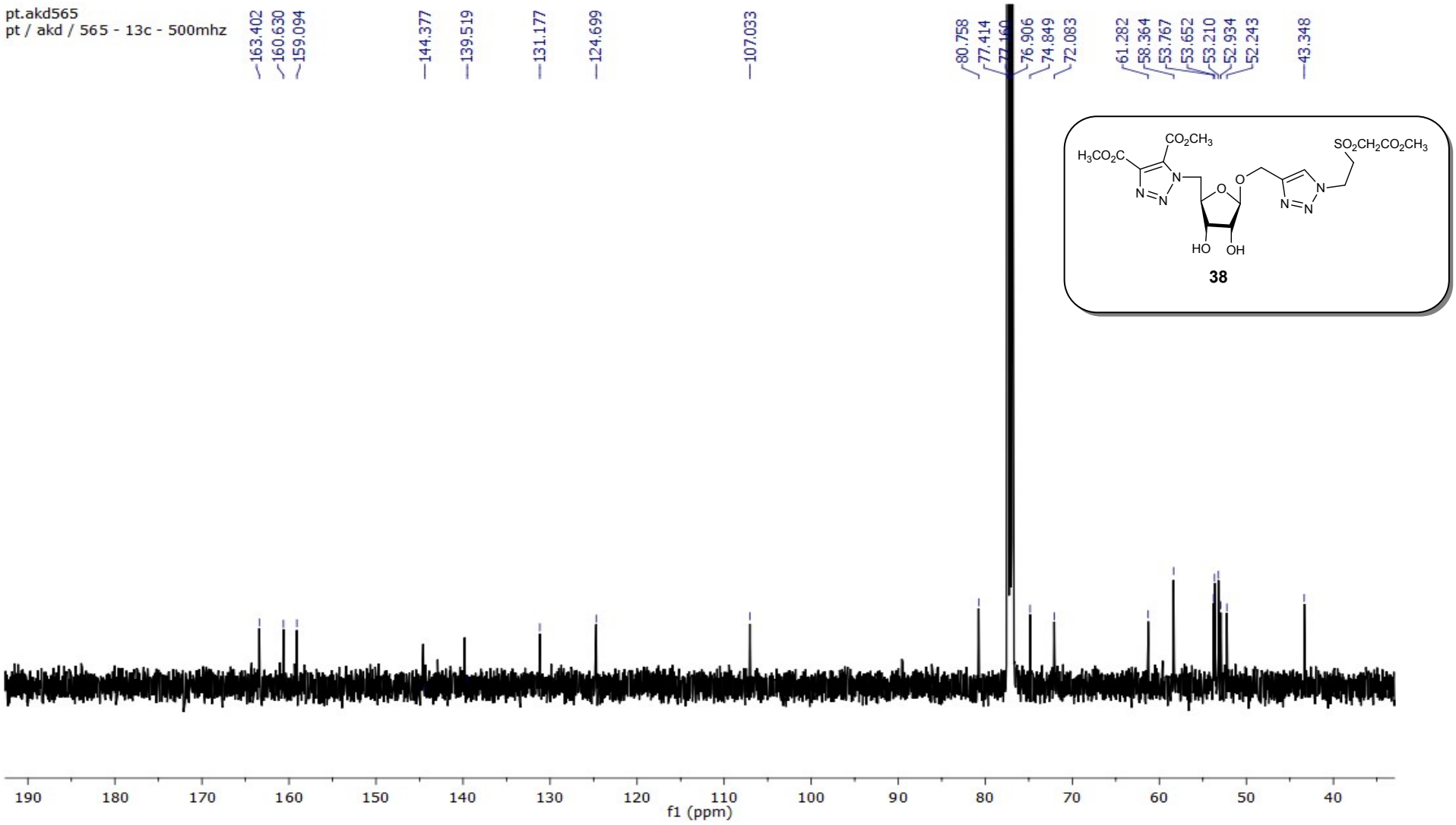
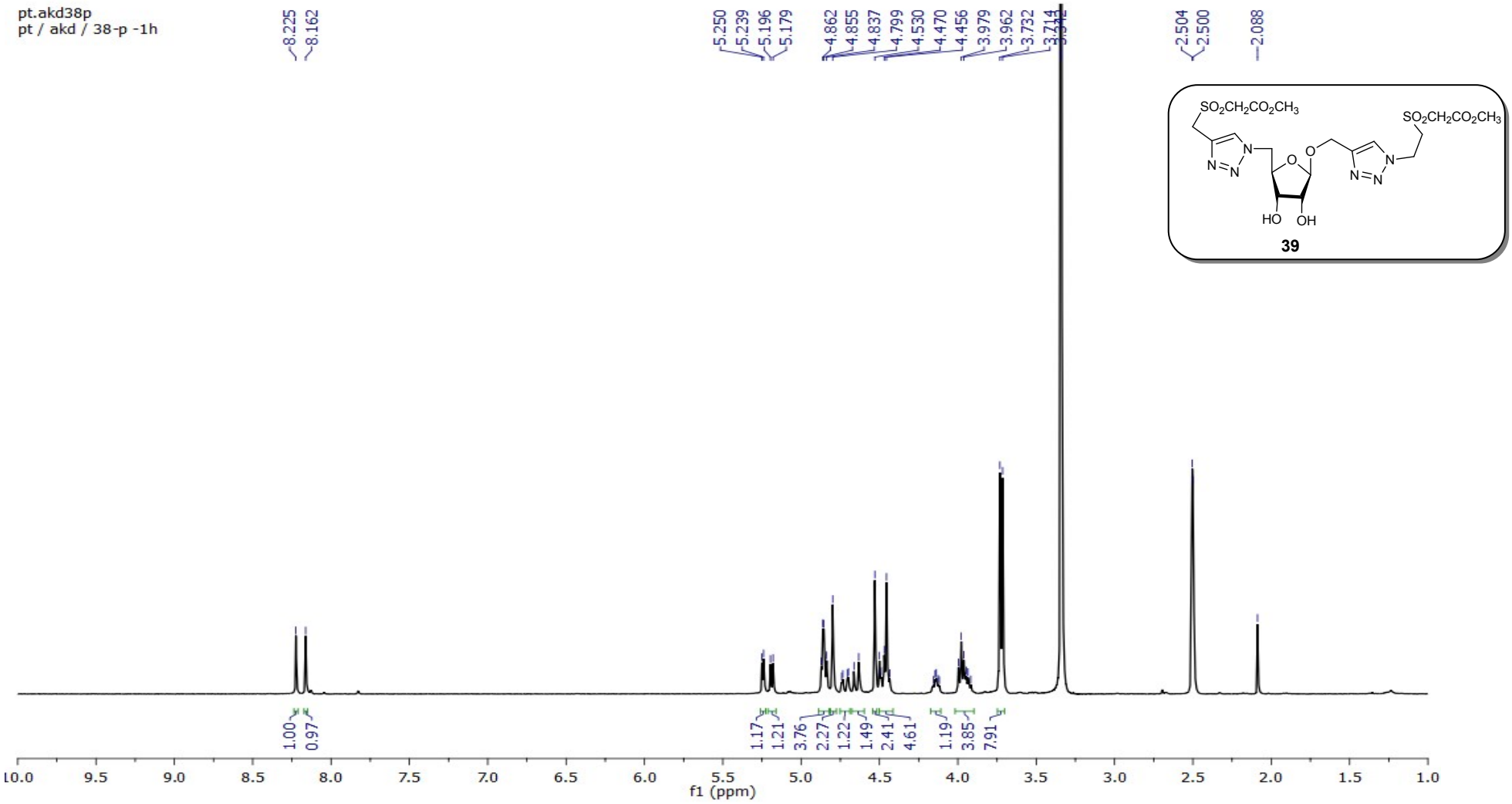


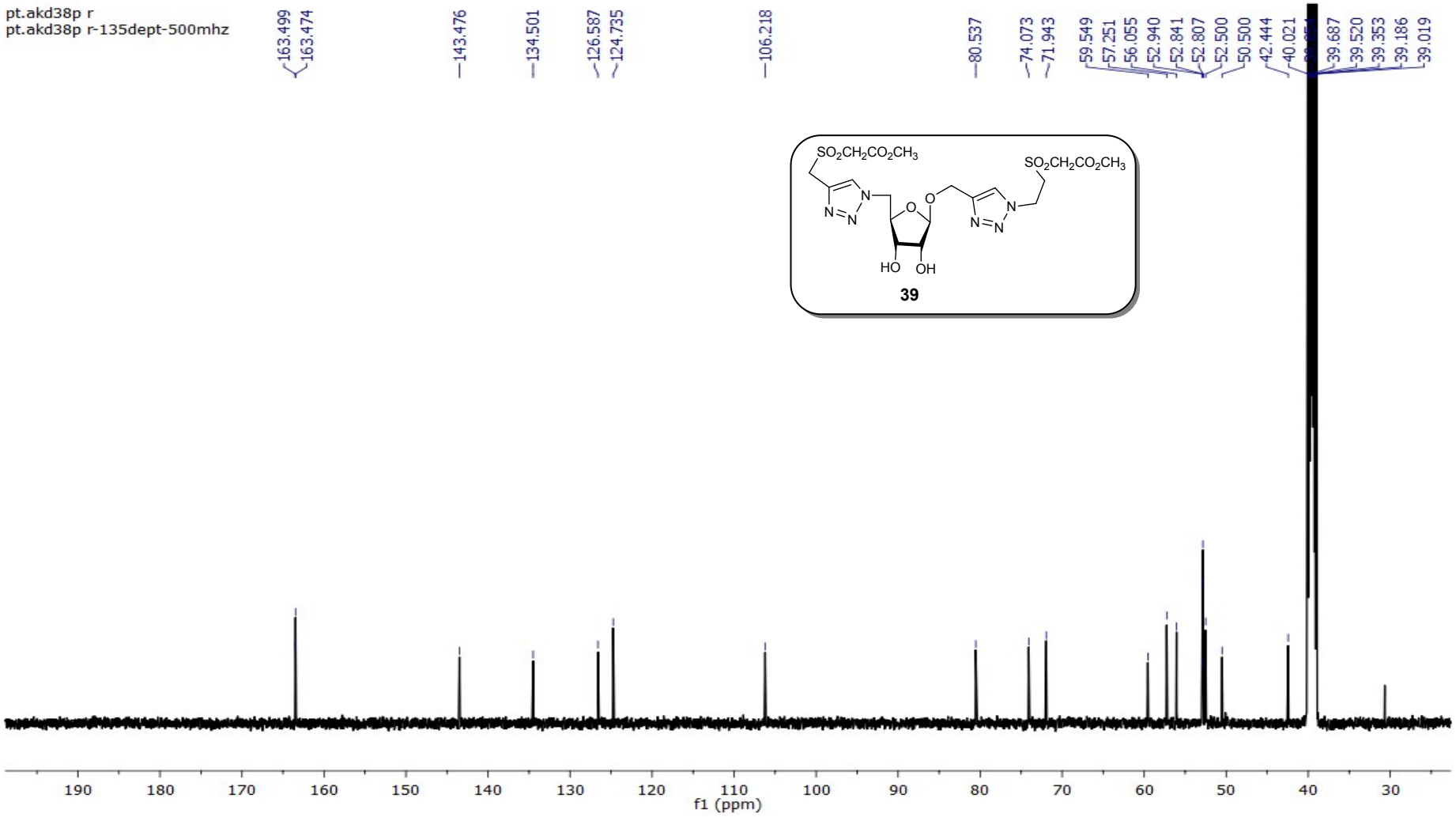
^{13}C -NMR spectra of compound **38**



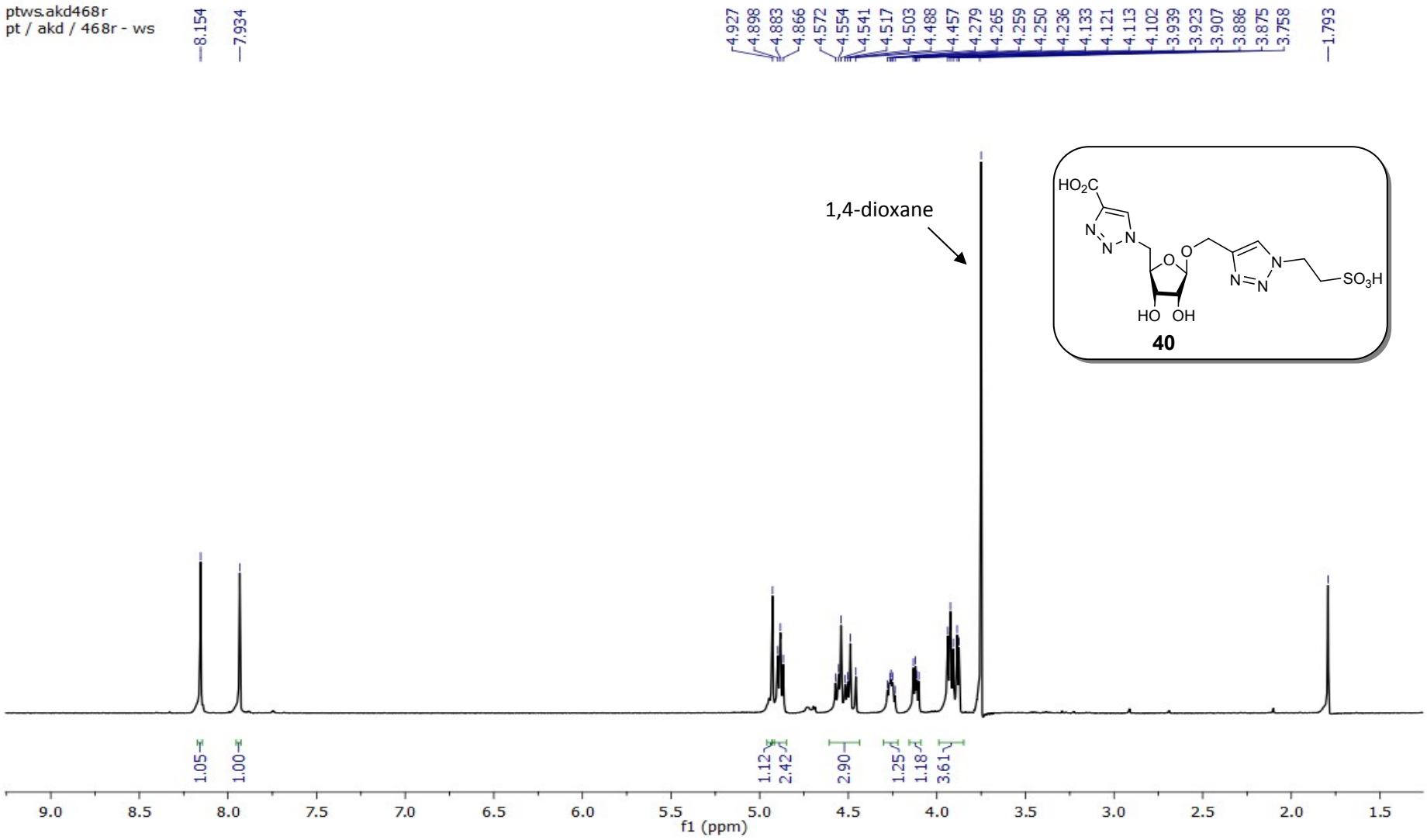
^{1}H -NMR spectra of compound **39**



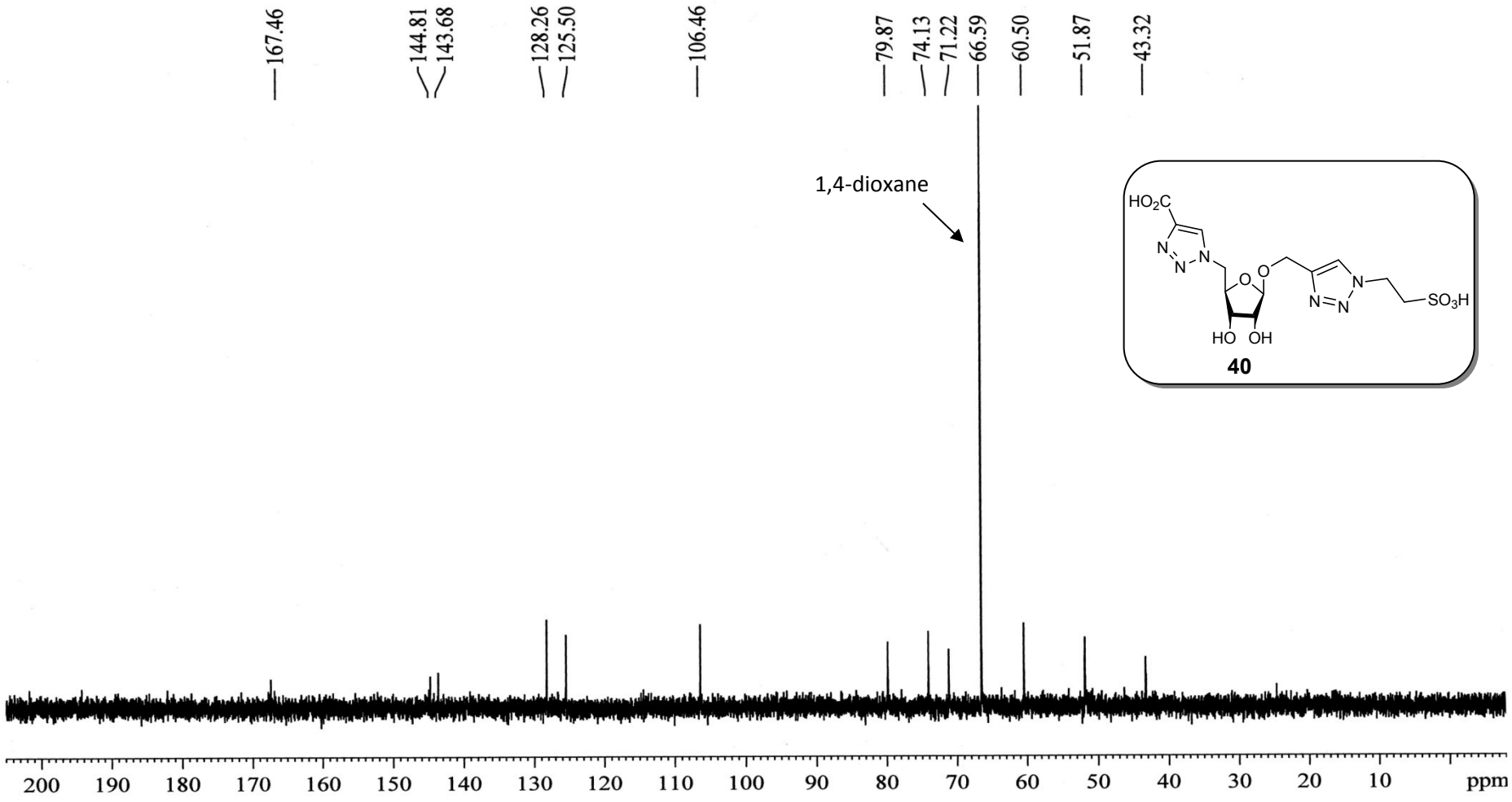
^{13}C -NMR spectra of compound **39**



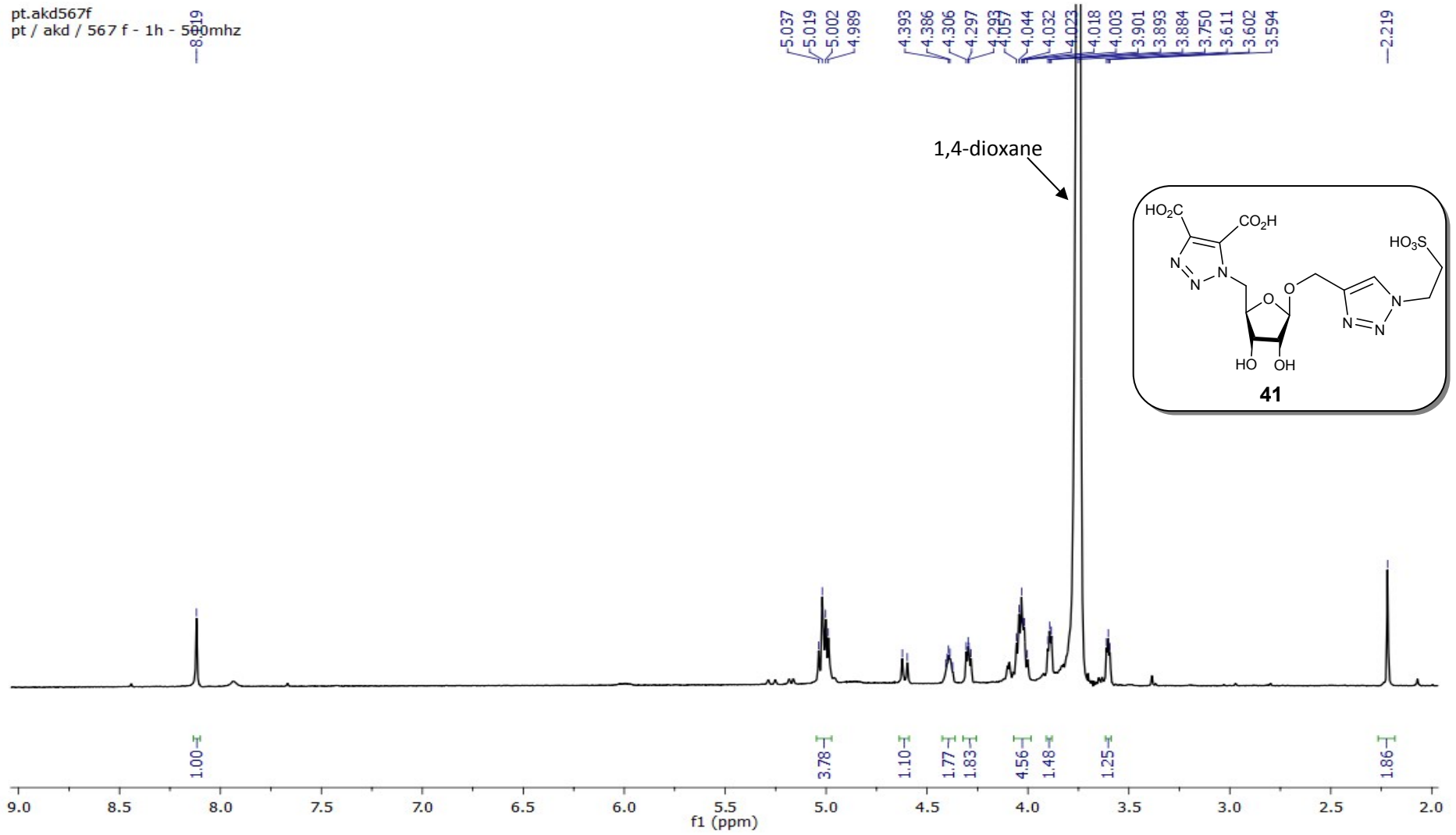
^{1}H -NMR spectra of compound **40**



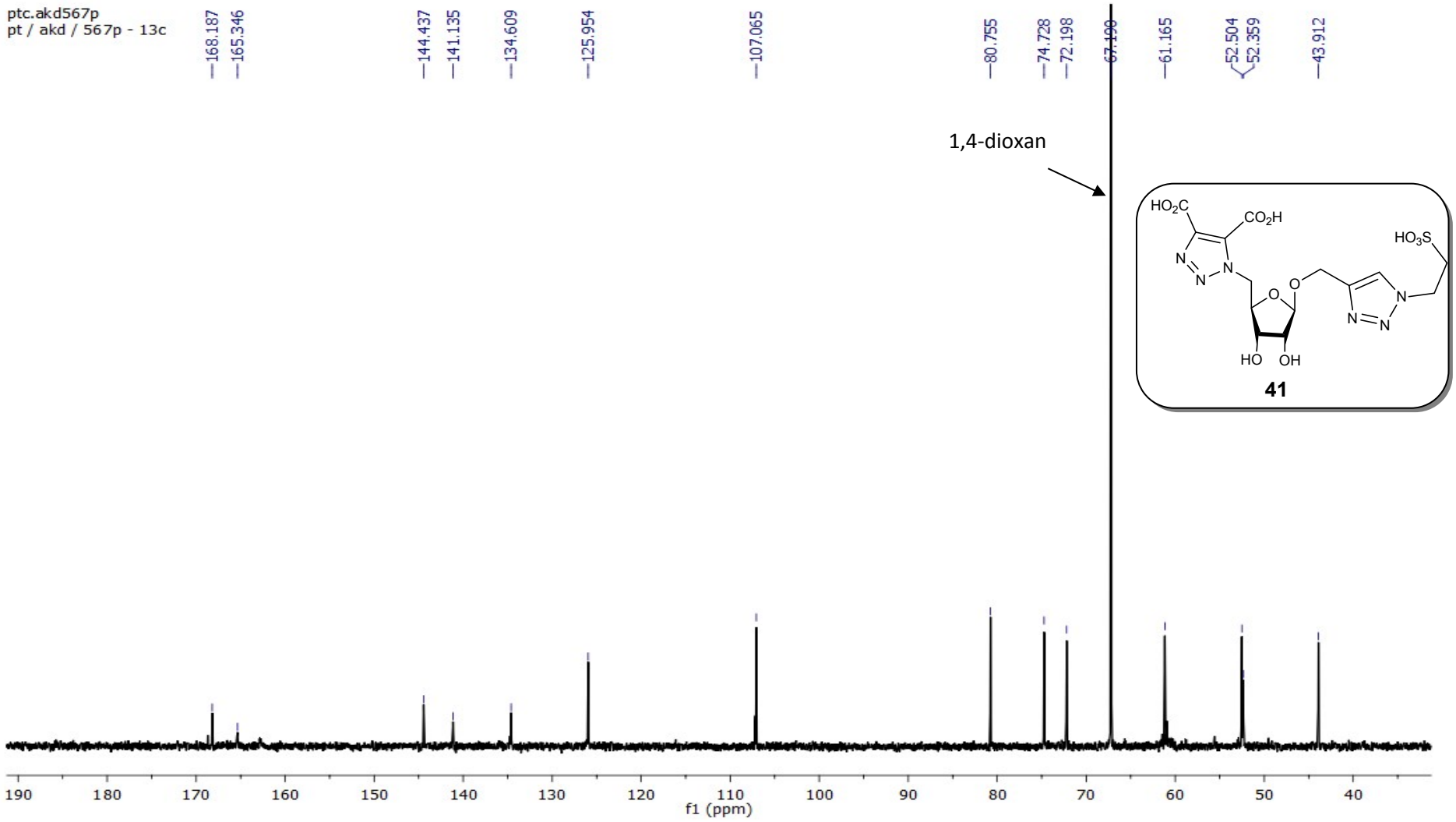
^{13}C -NMR spectra of compound **40**



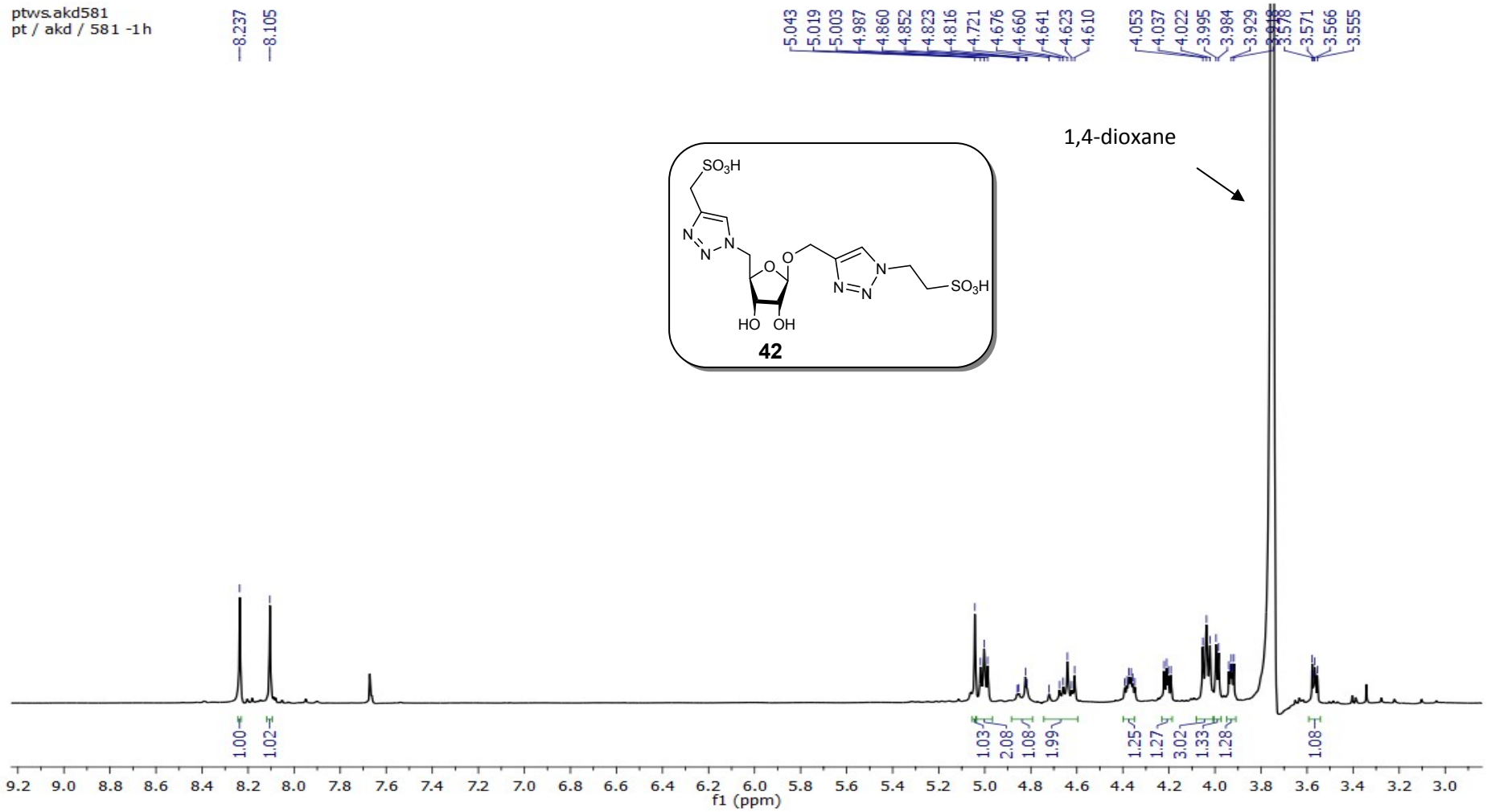
^{1}H -NMR spectra of compound **41**



^{13}C -NMR spectra of compound **41**



^{1}H -NMR spectra of compound **42**



^{13}C -NMR spectra of compound **42**

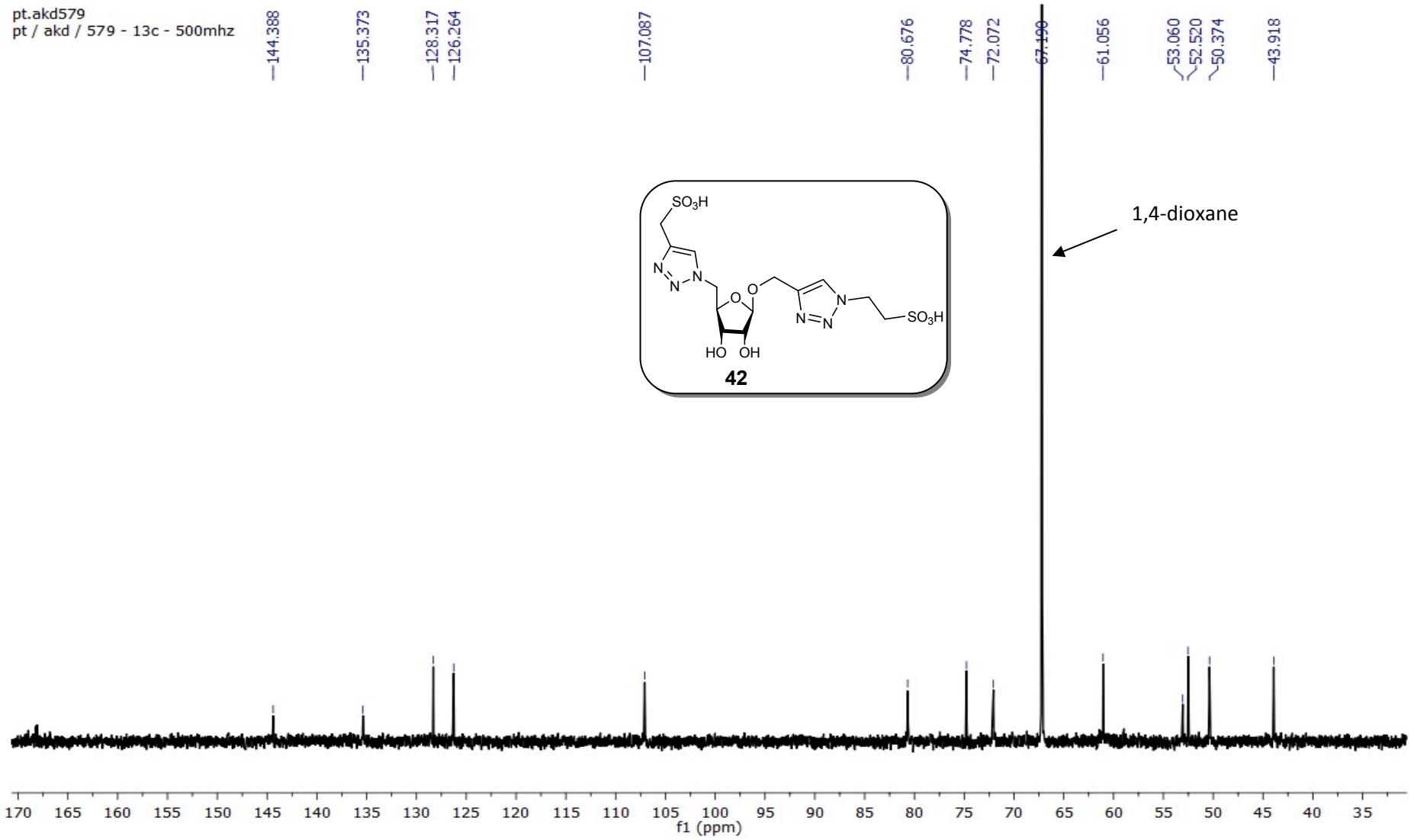
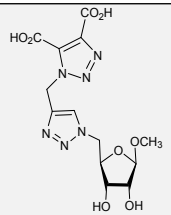
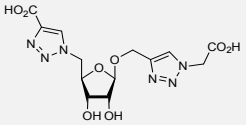
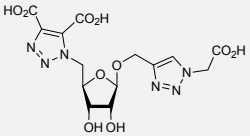
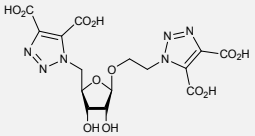
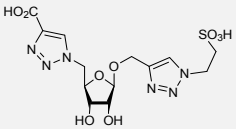
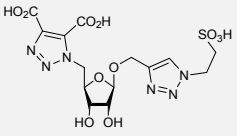
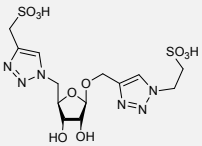


Table S1: H-bonding Distance (Å) measurement from Docking Studies

RNase A (PDB ID: 1FS3) Amino acid residues	 6	 15	 16	 23	 40	 41	 42
Lys7 NHζ			2.2 [CO]of CO_2H	1.9 [OH] of CO_2H 2.2 [3′-OH] of sugar	2.1 [OH] of SO_3H 2.2 [O] of SO_3H	2.5 [OH] of CO2H 2.5 [3′-OH] of sugar	1.9 [O] of SO_3H
Gln11 COε^1				2.3[OH] of CO_2H		2.3 [OH] of CO_2H	
Gln11 NHε^2	3.0 [OCH_3]	2.5 [OH] of CO_2H	2.7 [N] of triazole	1.6 [O] of sugar	2.1 [OH] of SO_3H 2.7 [O] of SO_3H	1.9 [O] of sugar ring	2.4 [O] of SO_3H 2.0 [N] of nitrogen ring
His12 NHε^2		1.9 [OH] of CO_2H	2.2 [N] of triazole		3.1 [N] of triazole ring	2.7 [O] of glycoside	2.6 [N] of triazole ring 3.2 [N] of triazole ring
Arg39 Nη^1				1.6 [CO] of CO_2H		2.0 [CO] of CO_2H	
Arg39 Nη^2				2.1 [OH] of CO_2H			
Lys41 NHζ	2.3 [O] of sugar ring	2.3 [N] of triazole 2.2 [N] of triazole	2.3 [N] of triazole 1.8 [N] of triazole		1.7 [N] of triazole ring 2.0 [N] of triazole ring	2.3 [OH] of CO_2H 2.3 [N] of triazole 1.9 [O] of glycoside	2.3 [N] of triazole
Asn44 δ^1							3.2 [3′-OH] of sugar ring
Thr45 OHγ^1		2.0 [O] of sugar 2.3 [O] of glycoside	3.3 [O] of sugar	2.4 [CO] of CO_2H		2.5 [O] of SO_3H 3.1 [O] of SO_3H	2.4 [2′-OH] of sugar ring
Thr45 amide NH							1.8 [3′-OH] of sugar ring
Asp83 CO_2^-γ		3.2 [O] of sugar ring				2.8 [O] of SO_3H	
Arg85	3.1 [CO]of	2.9 [3′-OH] of sugar					

NHη^1	CO_2H						
Arg85 NHε^1	2.8 [CO] of CO_2H						
Lys104 NHζ					2.7 [OH] of CO_2H		2.7 [O] of SO_3H
Val118 amide CO				2.5 [2′-OH] of sugar			2.1 [OH] of SO_3H 3.0 [O] of SO_3H
His119 NHδ^1	1.9 [3′-OH] of sugar	2.1 [CO] of CO_2H	2.1 [OH] of CO_2H		2.8 [O] of SO_3H	2.2[2′-OH] of sugar	
Phe120 amide NH	2.9 [3′-OH] of sugar			2.7 [2′-OH] of sugar		2.4 [2′-OH] of sugar	
Phe120 amide CO	1.9 [3′-OH] of sugar						
Asp121 CO_2^-δ							
Asp121 amide CO			1.9 [OH] of CO_2H	2.1 [OH] of CO_2H 2.2 [OH] of CO_2H	1.9 [2′-OH] of sugar ring 2.0 [3′-OH] of sugar ring		
Ser123 OHγ	3.2 [CO] of CO_2H		2.0 [OH] of CO_2H		2.2 [OH] of CO_2H		3.0 [O] of SO_3H
Ser123 amide CO		2.2 [OH] of CO_2H					2.8 [O] of SO_3H 3.1 [O] of SO_3H
Ser123 amide NH	3.3 [CO] of CO_2H	2.2 [N] of triazole	2.2 [CO] of CO_2H				1.9 [O] of SO_3H