Supplementary information

Development of novel *C*-nucleoside analogues for formation of antiparallel-type triplex DNA with duplex DNA that includes TA and dUA base pairs

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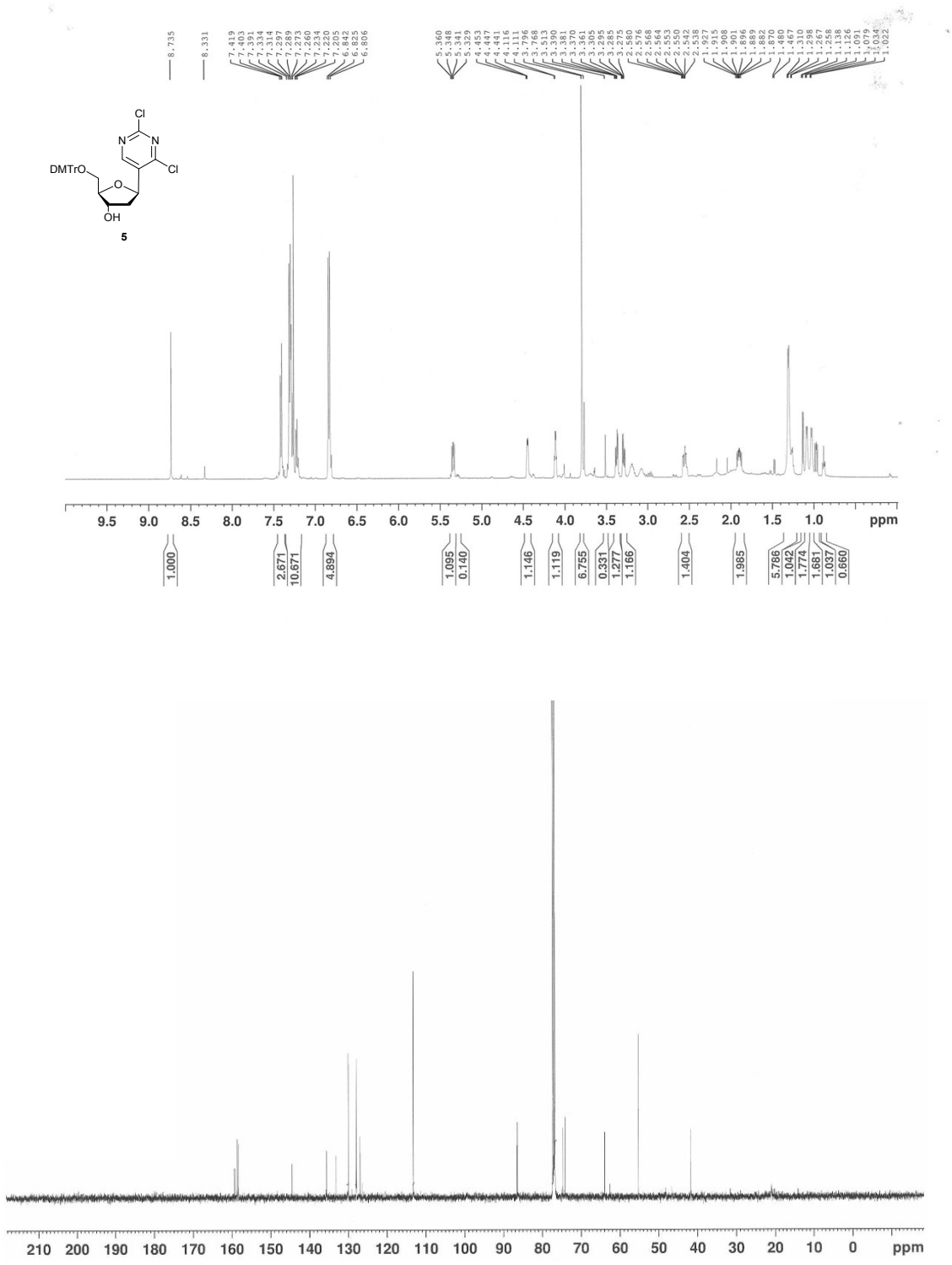


Figure S1. ^{1}H- and ^{13}C-NMR spectra of compound **5**.

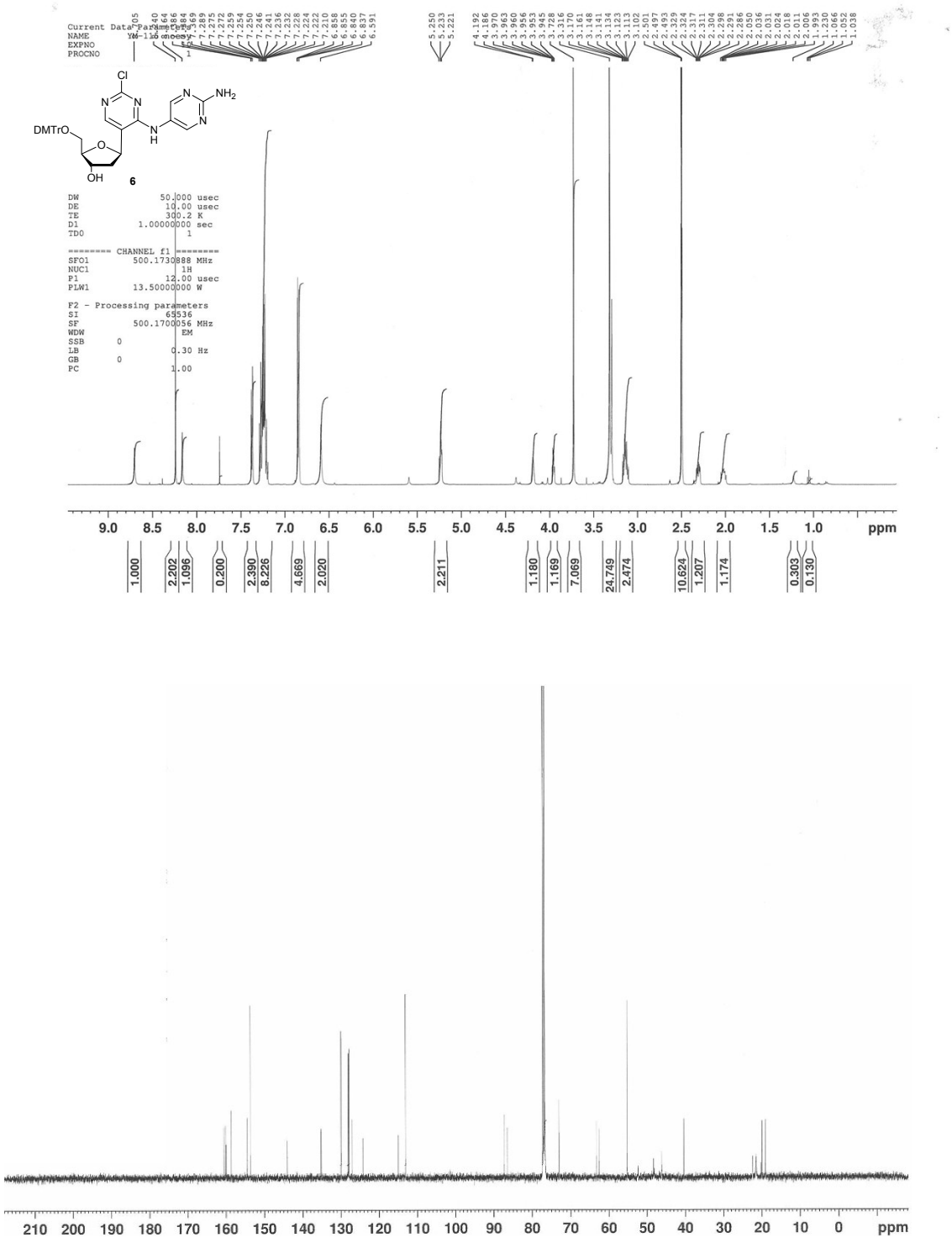


Figure S2. ^{1}H- and ^{13}C-NMR spectra of compound **6**.

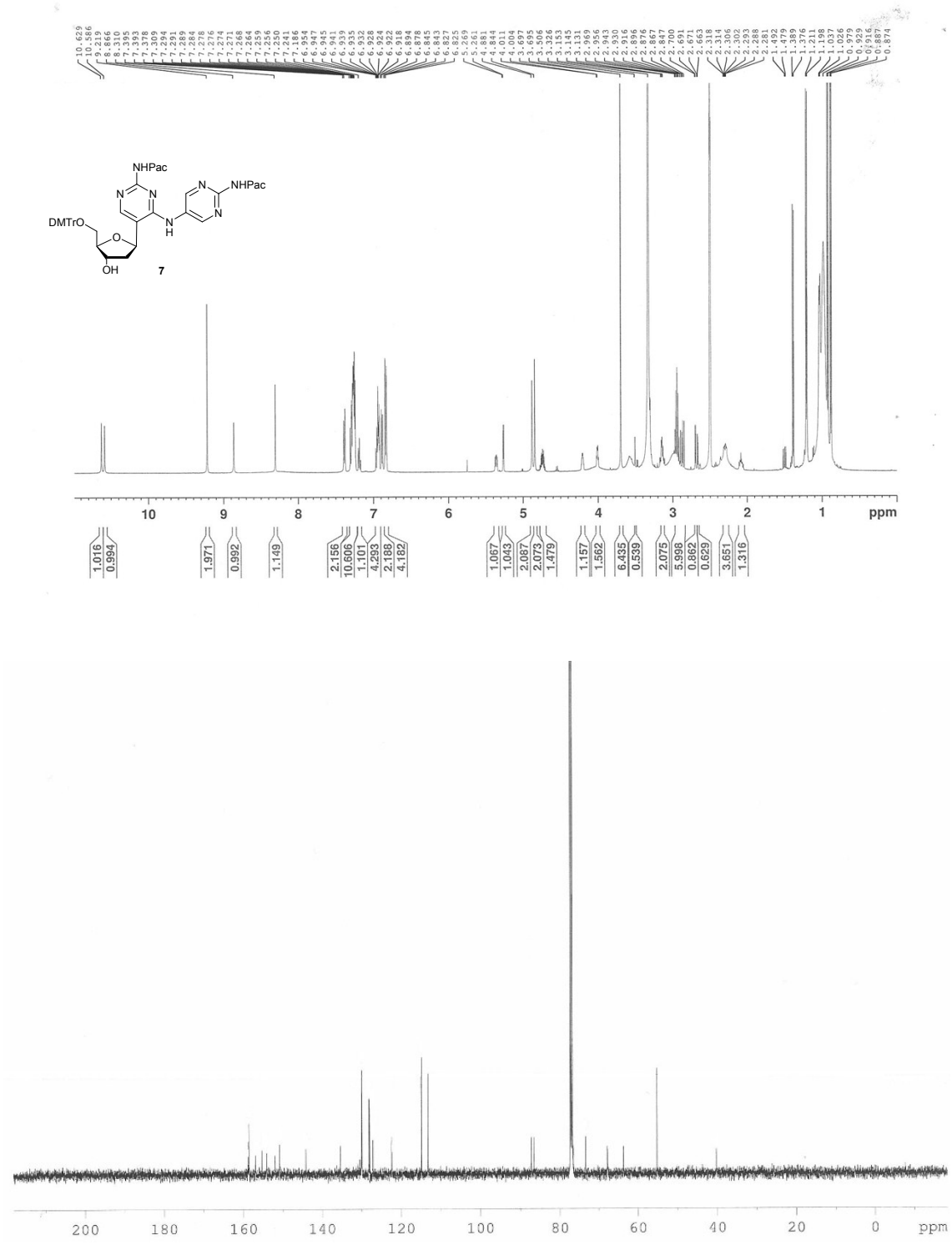


Figure S3. ^{1}H- and ^{13}C-NMR spectra of compound **7**.

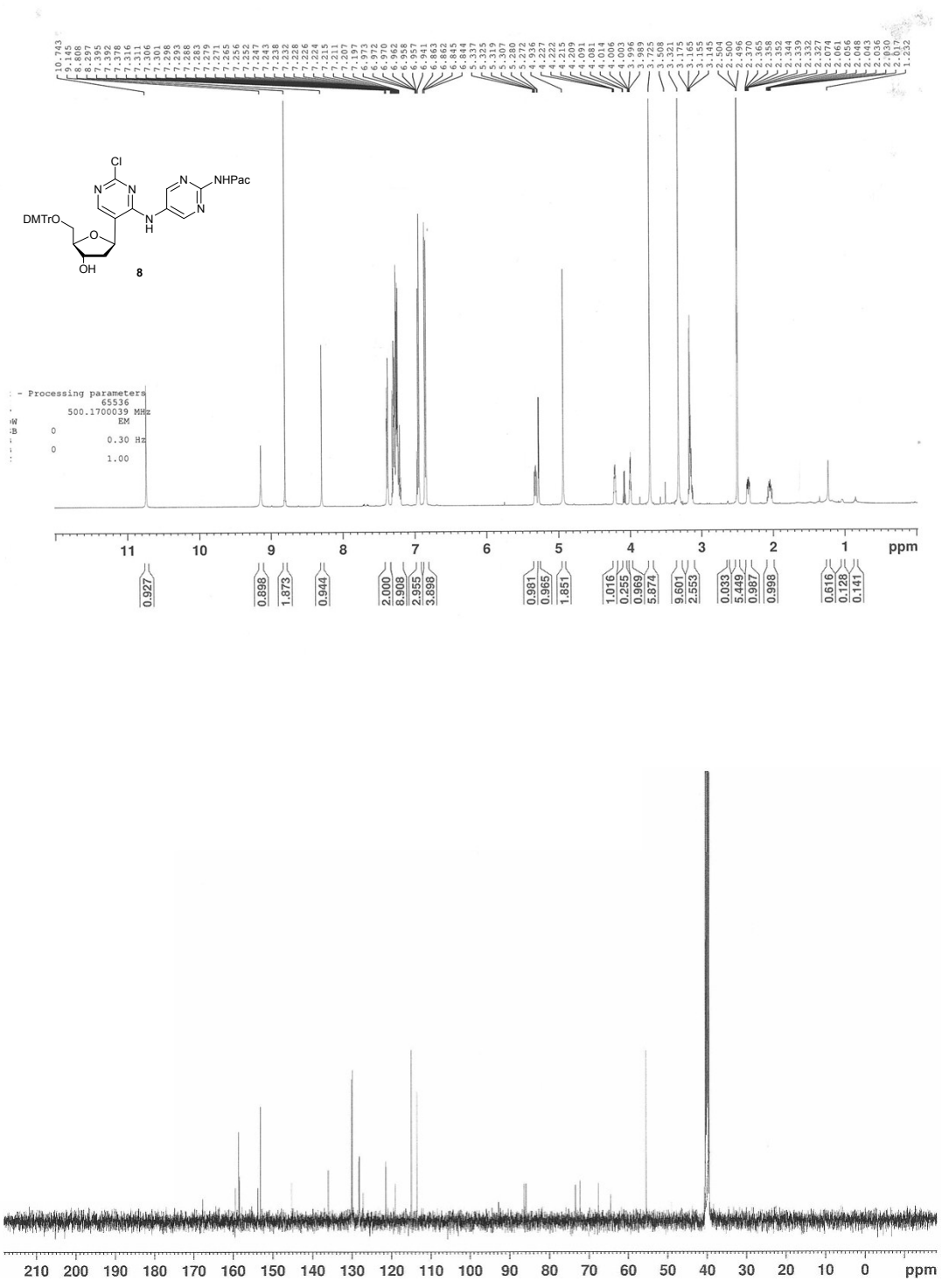


Figure S4. ^{1}H- and ^{13}C-NMR spectra of compound **8**.

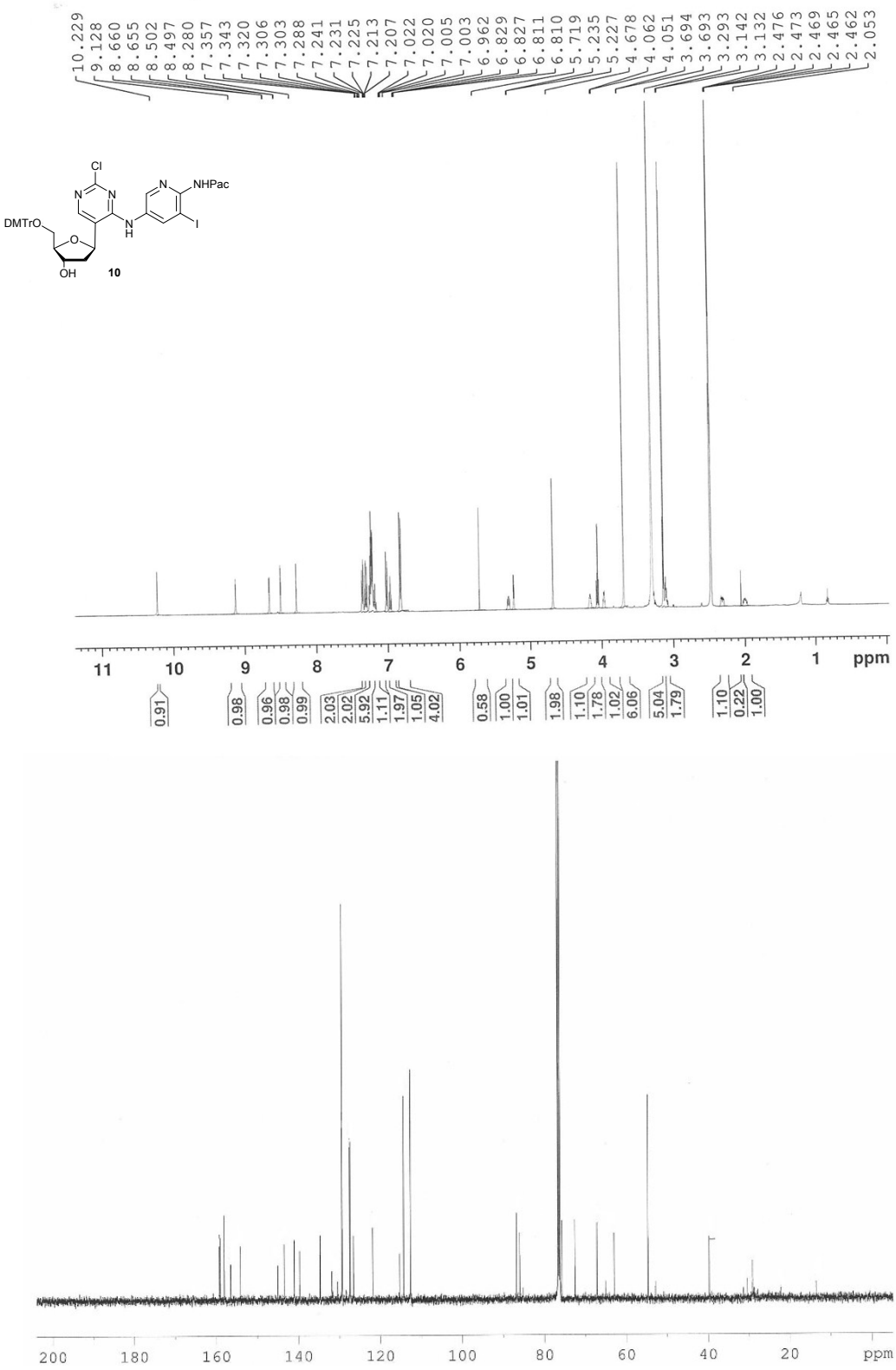
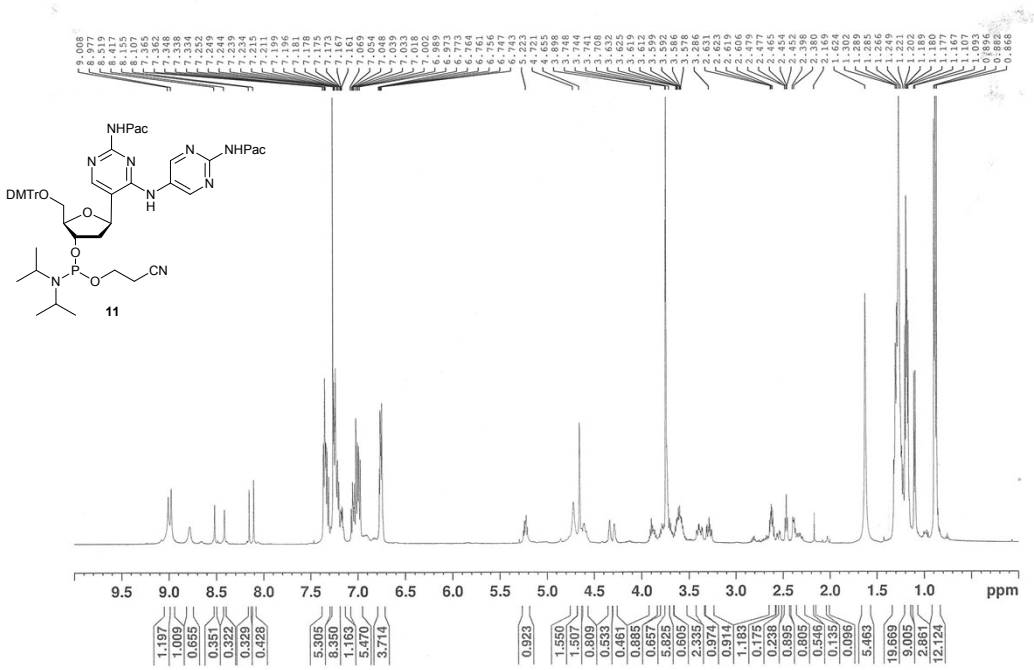
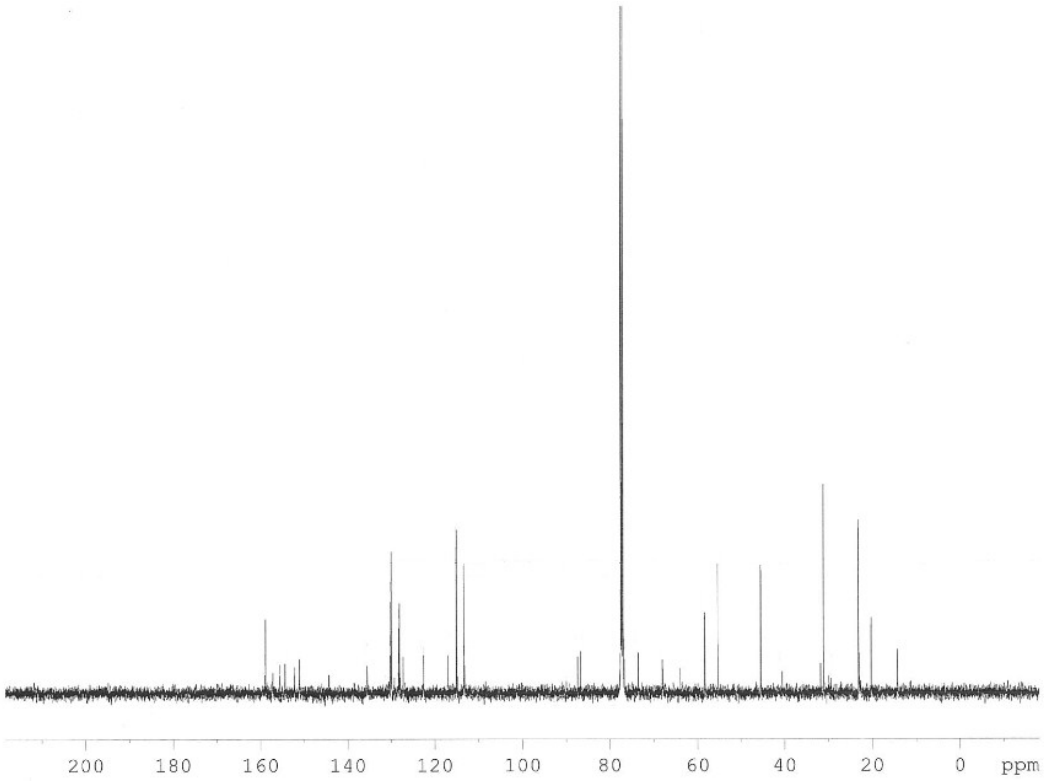


Figure S5. ^{1}H- and ^{13}C-NMR spectra of compound **10**.


NHPac
NHPac
DMTrO
CN
11
ppm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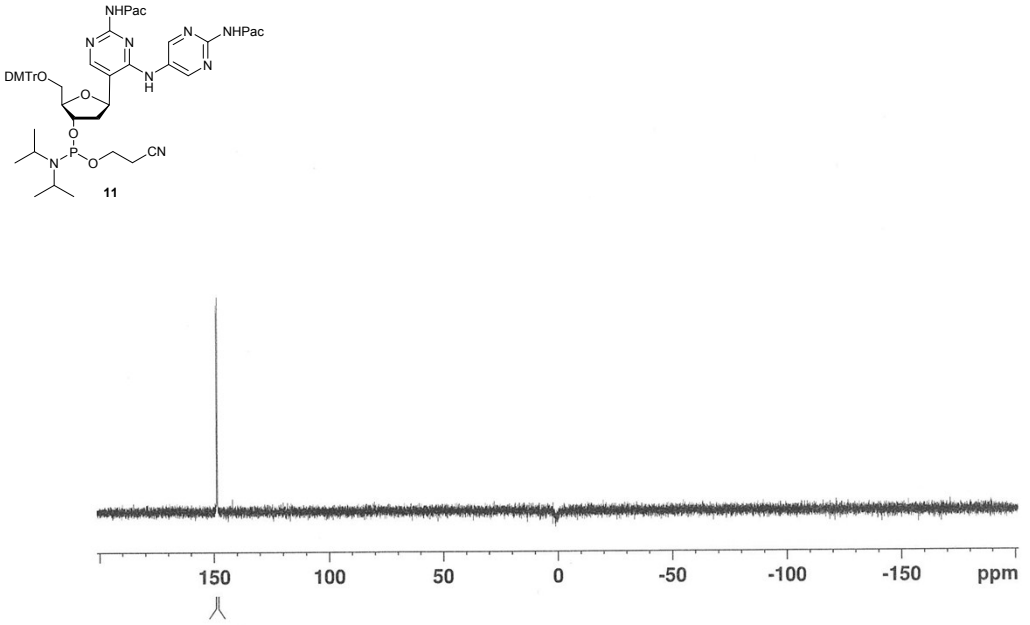
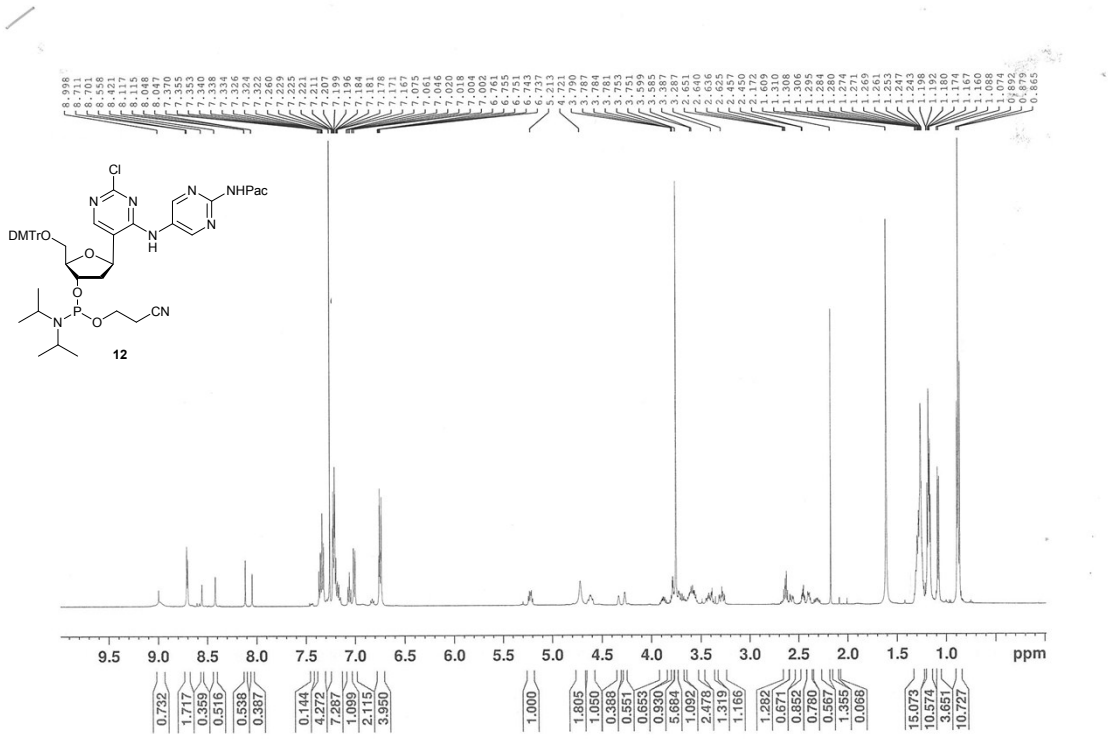


Figure S6. ^{1}H-, ^{13}C- and ^{31}P-NMR spectra of compound **11**. (^{13}C spectrum is not assigned due to the presence of diastereomers.)



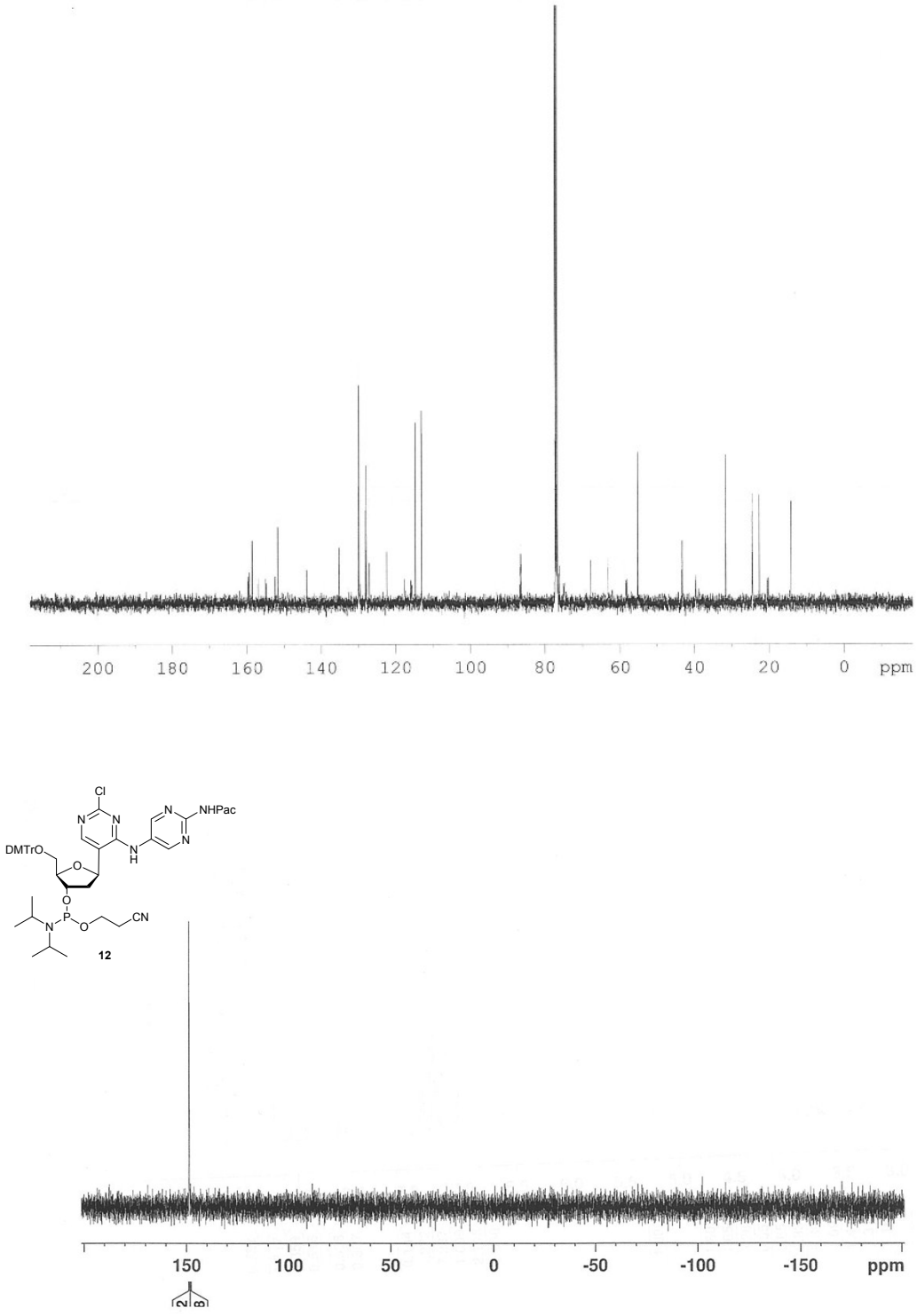


Figure S7. ^{1}H-, ^{13}C- and ^{31}P-NMR spectra of compound **12**. (^{13}C spectrum is not assigned due to the presence of diastereomers.)

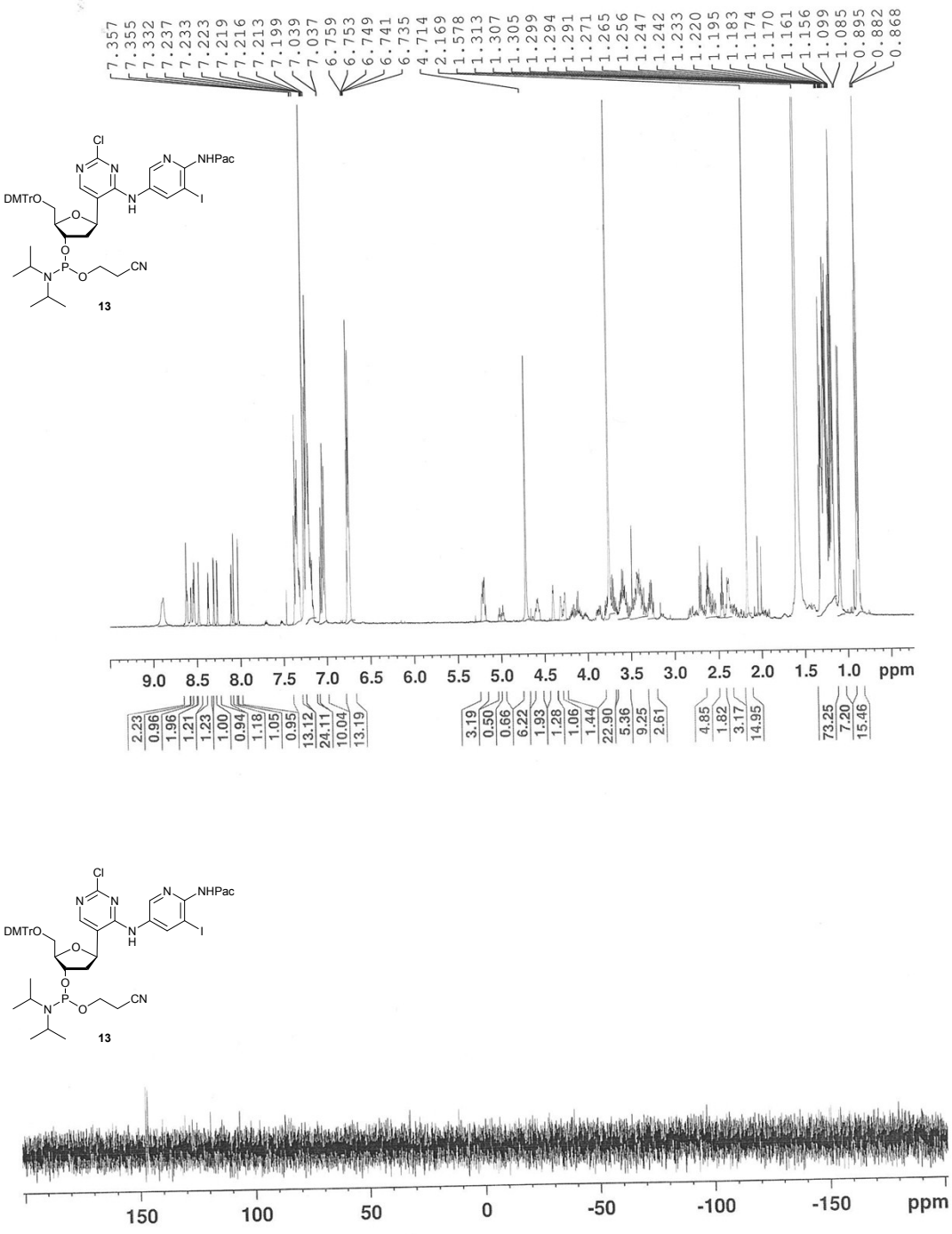


Figure S8. ^{1}H- and ^{31}P-NMR spectra of compound **13**. (Due to the low yield of the amidite compound, sufficient amounts could not be used for spectral measurements.)

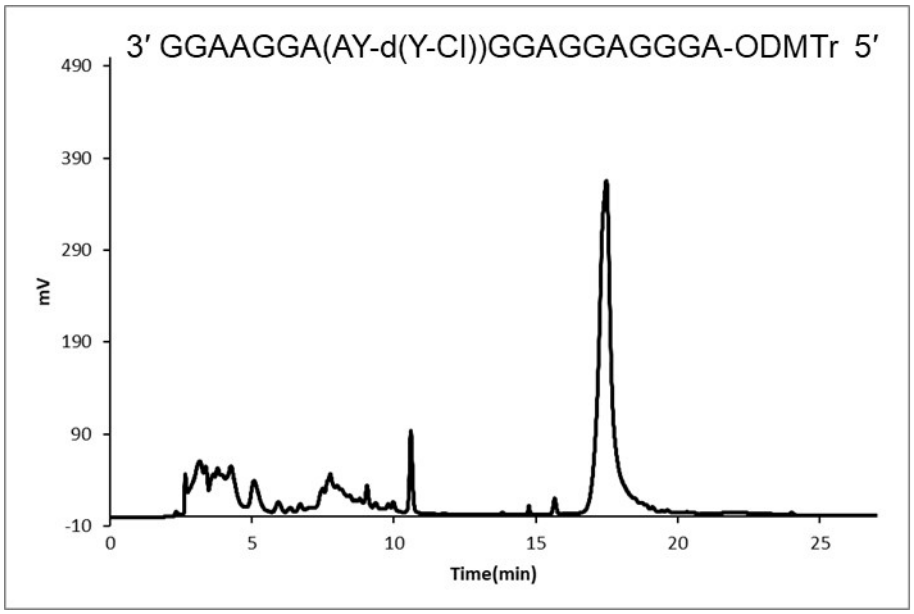


Figure S9. The representative HPLC chart of DMTr-TFO having AY-d(Y-Cl) in the 3'-A and 5'-G sequence.

HPLC conditions: column: Nacalai tesque COSMOSIL 5C18-ARII, 10 × 250 mm, solvents: A: 0.1 M TEAA buffer, B: CH_3CN, Liner gradient: B for 10% to 40%/20 min, 40 to 100%/27 min, flow rate: 3.0 mL/min, UV: 254 nm, column oven: 35°C. The peak of around 17 min was collected.

Table S1. MALDI-TOF-MASS (Negative mode) results of the 18 mer TFOs containing dY derivatives (Z = AY-d(Y-NH_2), AY-d(Y-Cl), ^{I}AP-d(Y-Cl)).

	3’-GGAAGG **NZN’** GAGGAGGGA-5’			
Z	3’-AZG-5’		3’-GZG-5’	
	Calcd.([M-H]$^-$)	Found	Calcd.([M-H]$^-$)	Found
AY-d(Y-NH_2)	5816.05	5818.28	5832.05	5834.99
AY-d(Y-Cl)	5835.00	5836.84	5851.00	5851.65
^{I}AP-d(Y-Cl)	5959.90	5961.76	5975.90	5976.05
Z	3’-GZA-5’		3’-AZA-5’	
	Calcd.([M-H]$^-$)	Found	Calcd.([M-H]$^-$)	Found
AY-d(Y-NH_2)	5816.05	5818.86	5800.06	5802.08
AY-d(Y-Cl)	5835.00	5835.61	5819.01	5820.63
^{I}AP-d(Y-Cl)	5959.90	5960.76	5943.91	5943.70

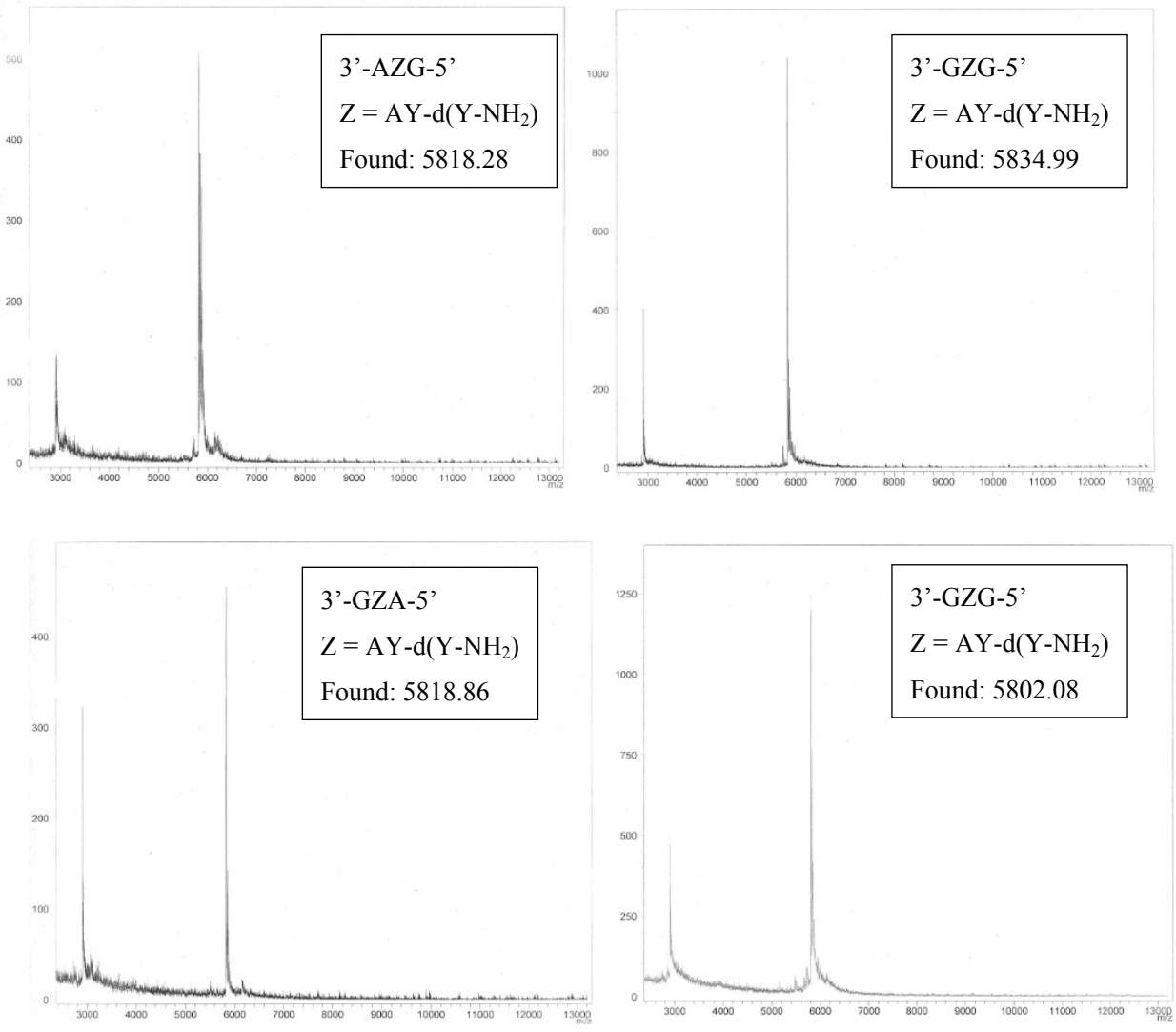


Figure S10 MALDI-TOF MS charts of TFOs containing AY-d(Y-NH_2)

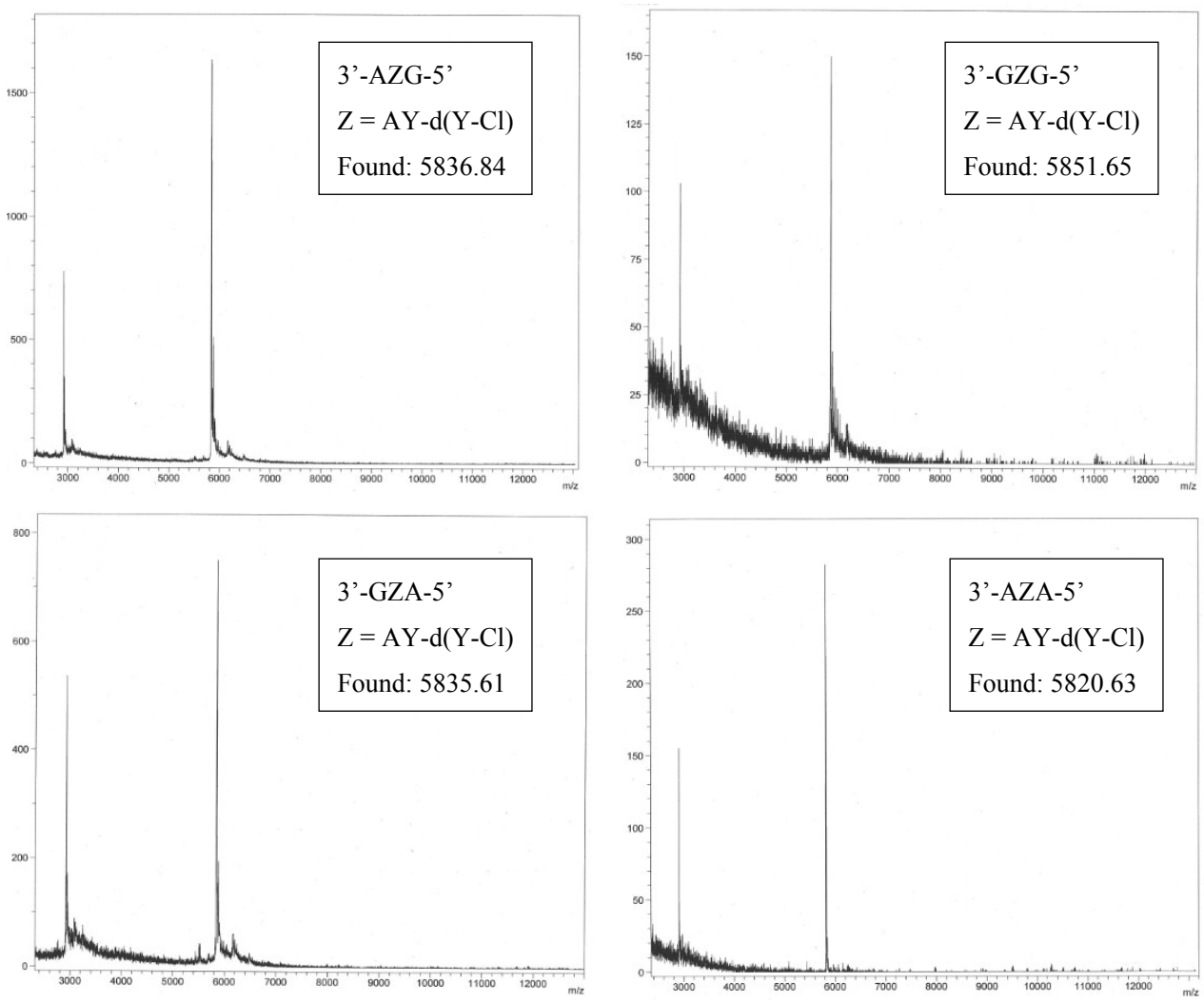


Figure S11 MALDI-TOF MS charts of TFOs containing AY-d(Y-Cl)

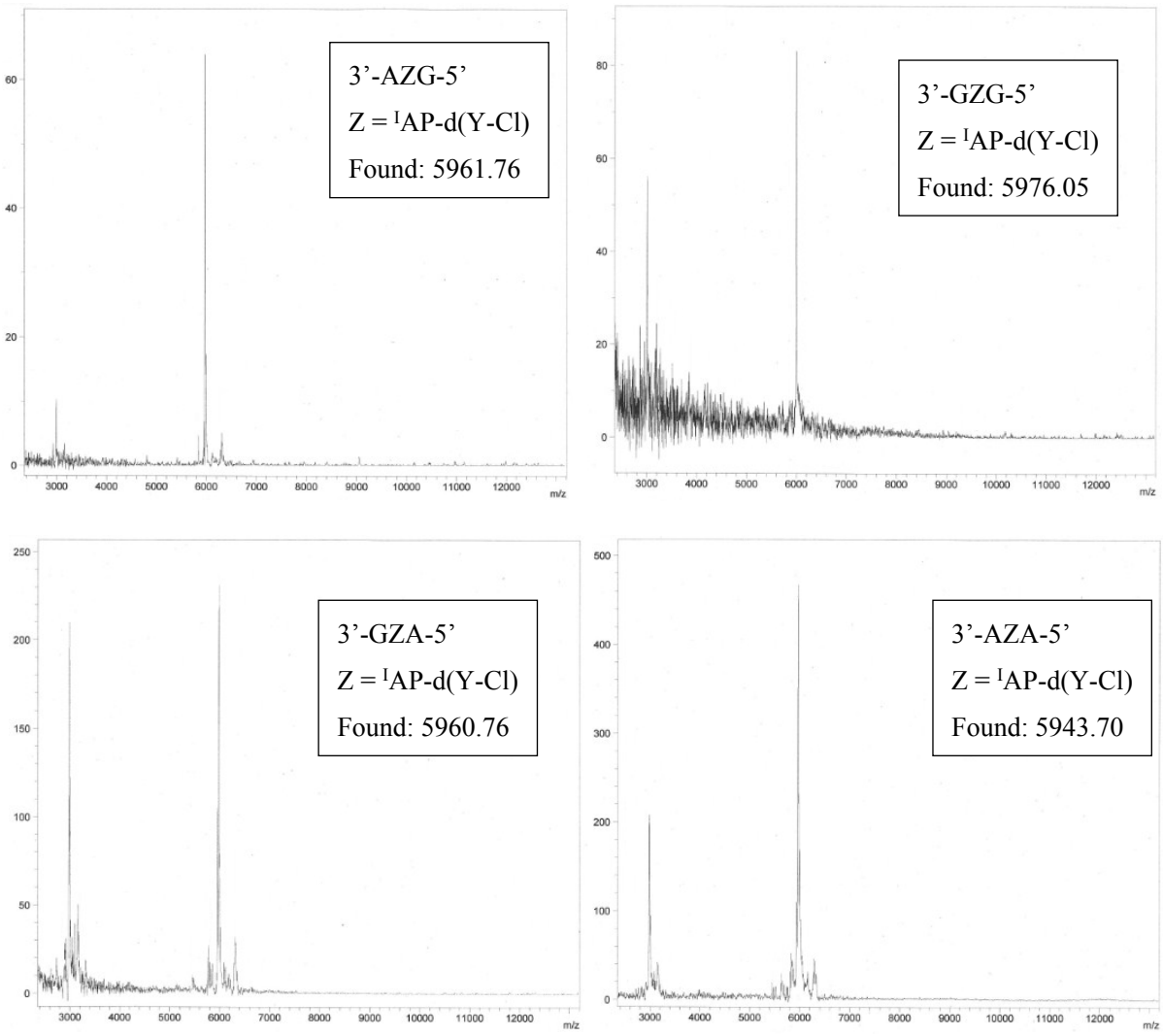


Figure S12 MALDI-TOF MS charts of TFOs containing IAP-d(Y-Cl)