

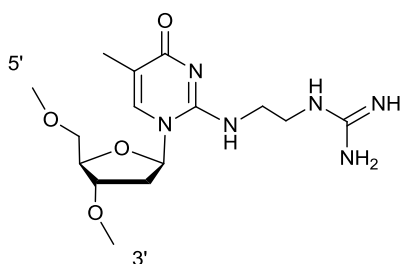
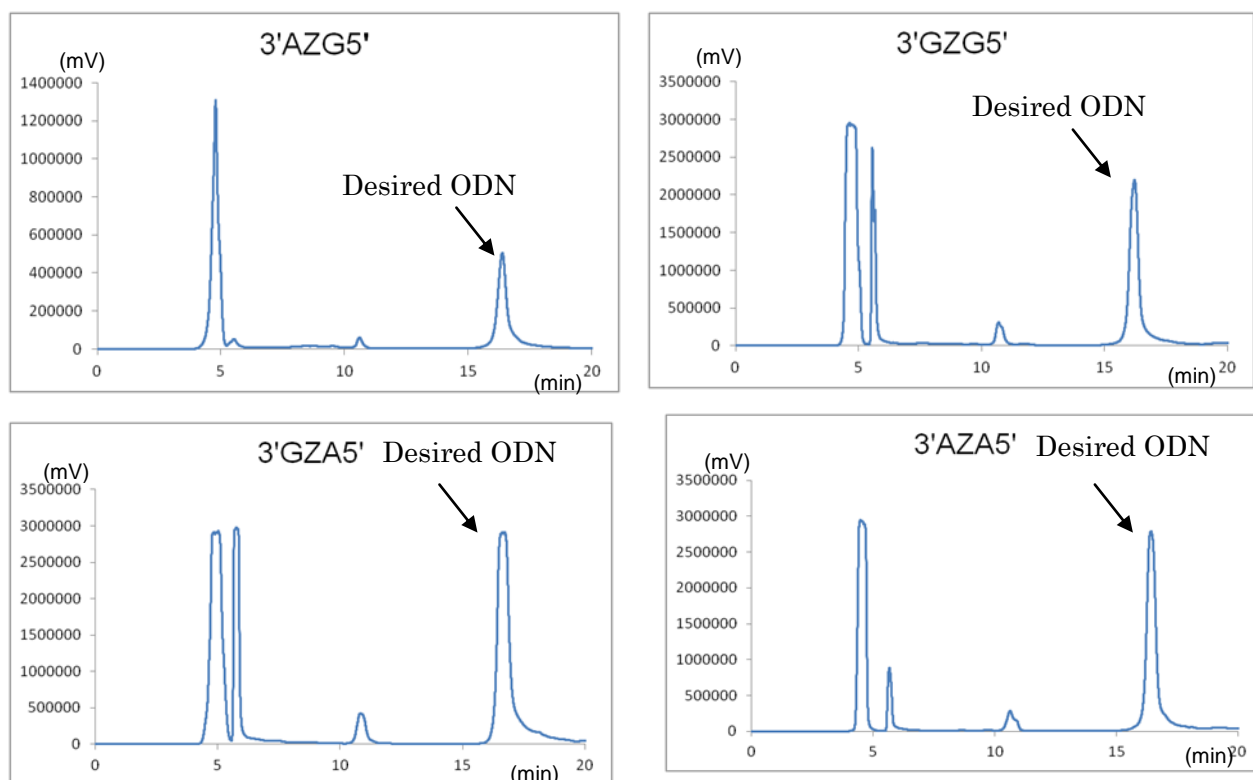
Electronic Supplementary Information

***N*-(Guanidinoethyl)-2'-deoxy-5-methylisocytidine exhibits a selective recognition of a CG interrupting site for the formation of anti-parallel triplexes†**

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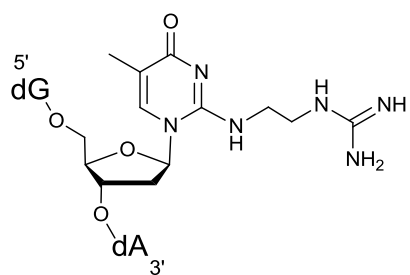


Z = et-guanidino-isodC

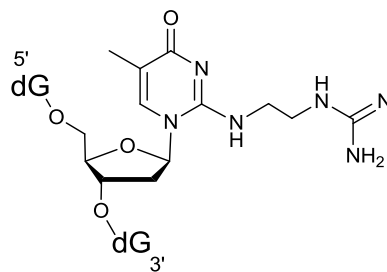
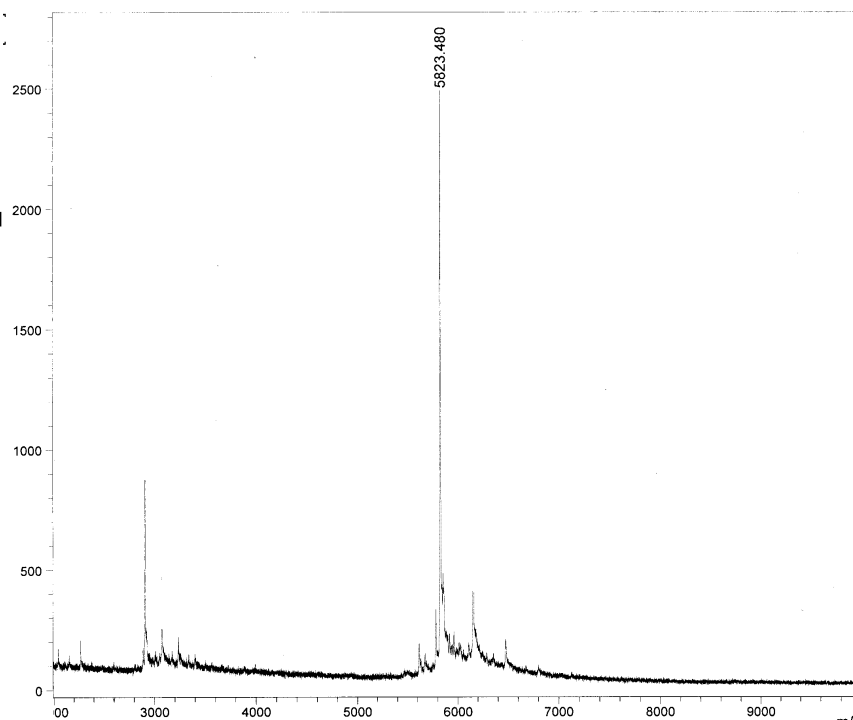
HPLC conditions:

column: Nacalai tesque COSMOSIL
5C18-ARII, 10 x 250 mm,
solvents: A: 0.1 M TEAA buffer, B: CH₃CN, B:
10% to 40% / 20 min, 40% to 100% / 30 min,
Flow rate: 3.0 mL / min,
UV: 254 nm
Column oven: at 35°C

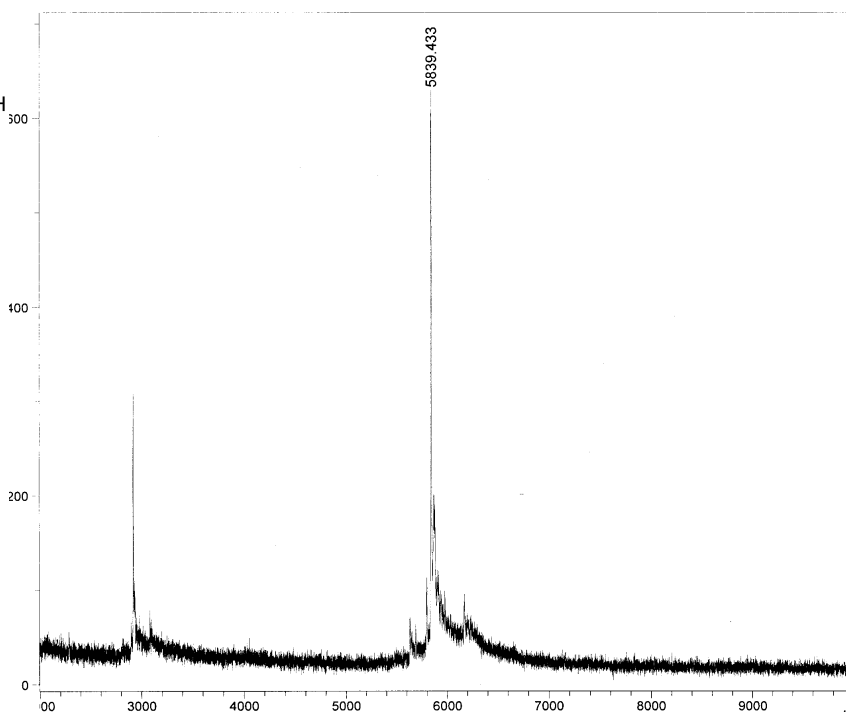
Figure S1. HPLC chart of guanidineethyl-isodC in TFO (3'-N³ZN⁵-5'). A suspension of the support-bound TFO in 250 μL of CH₃CN was treated with 1H-pyrazole-1-carboxamide hydrochloride (1.0 mg) and DBU (50 μl) for overnight at room temperature. The support was washed two times with CH₃CN, and the resulting TFO was treated with 28% aqueous ammonia for overnight at 55°C followed by HPLC purification. The major peak around 16 min was collected.



MALDI-TOF Mass (negative)
calcd. for 5824.08
found 5823.48



MALDI-TOF Mass (negative)
calcd. for 5840.07
found 5839.43



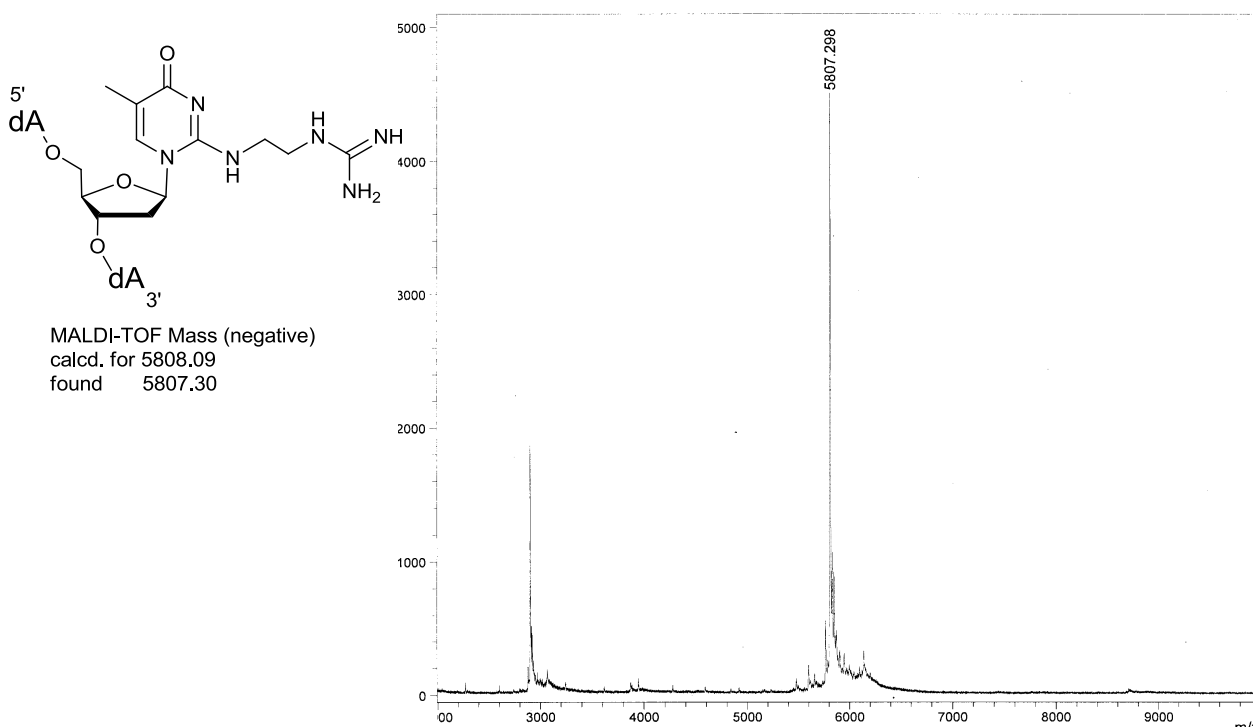
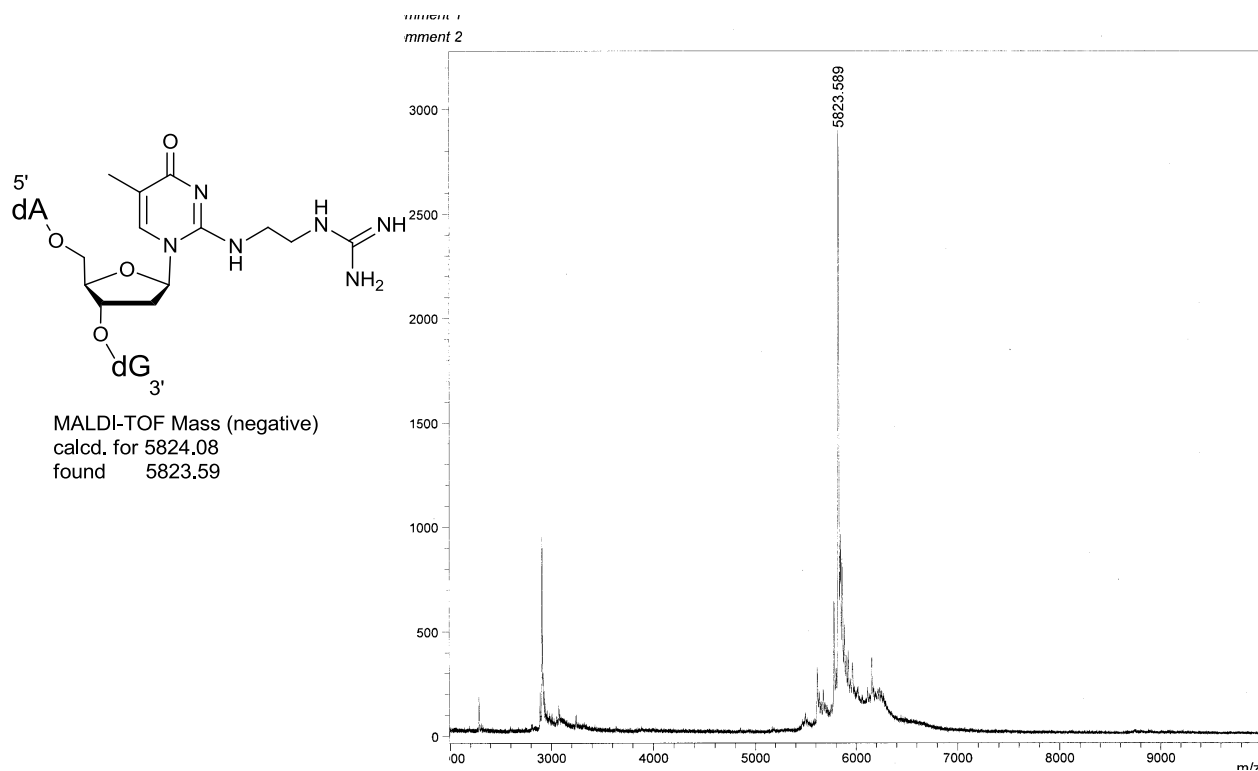
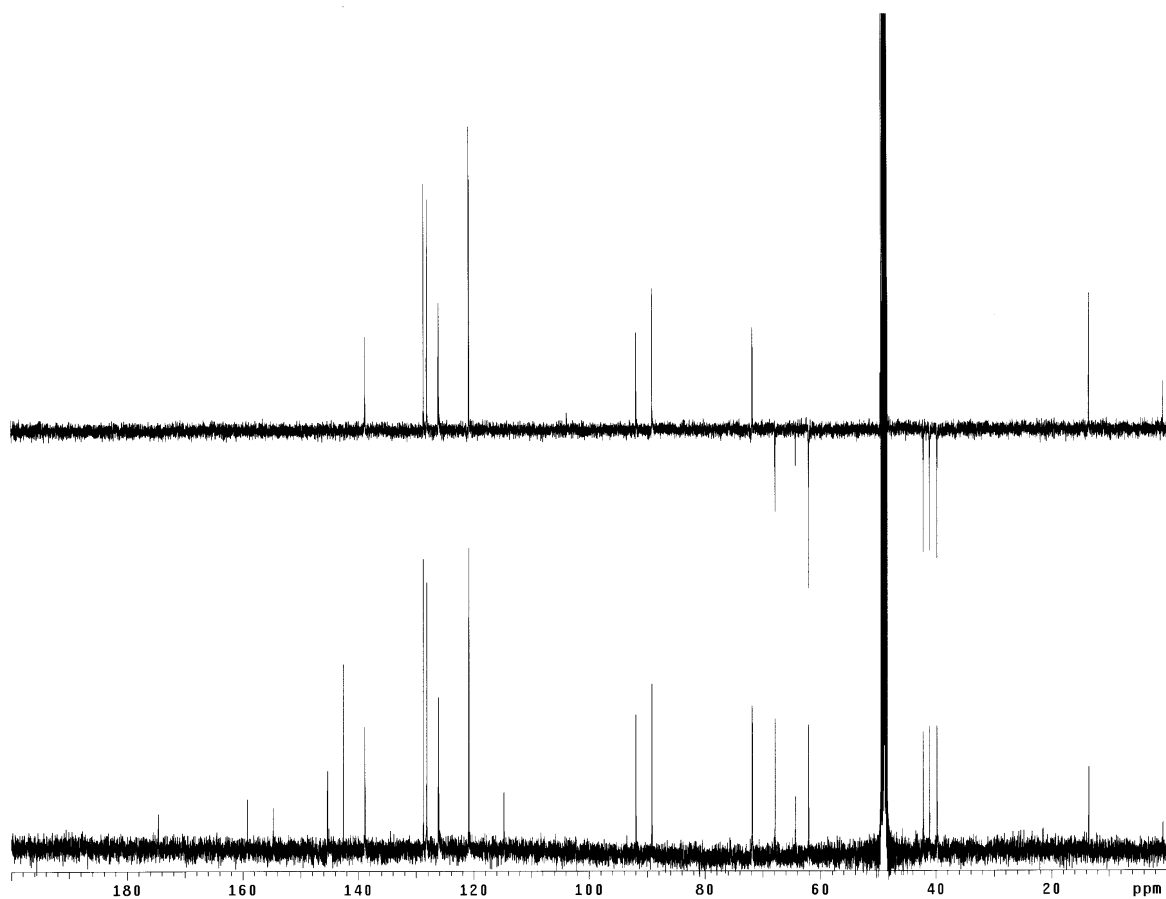
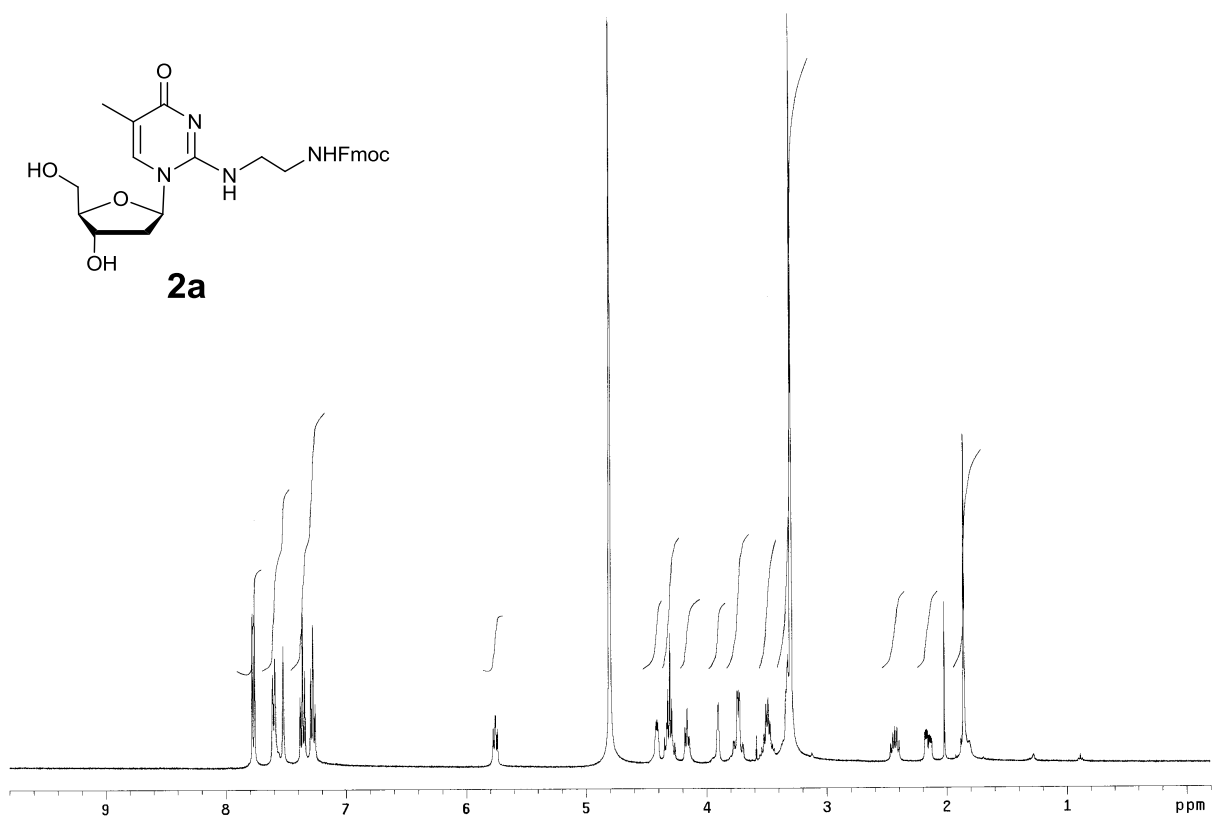
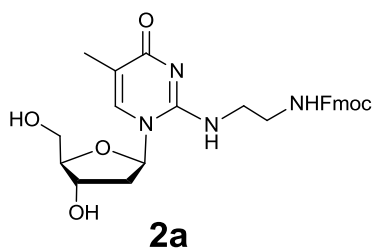
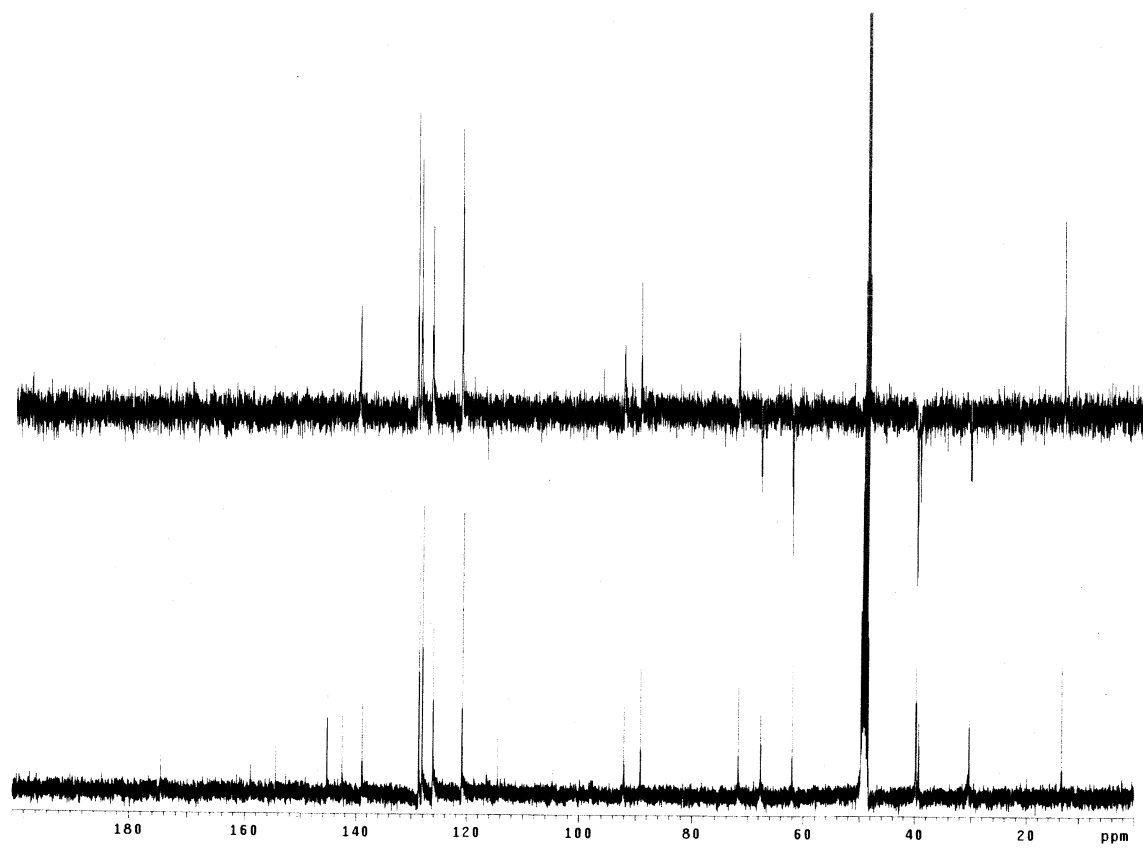
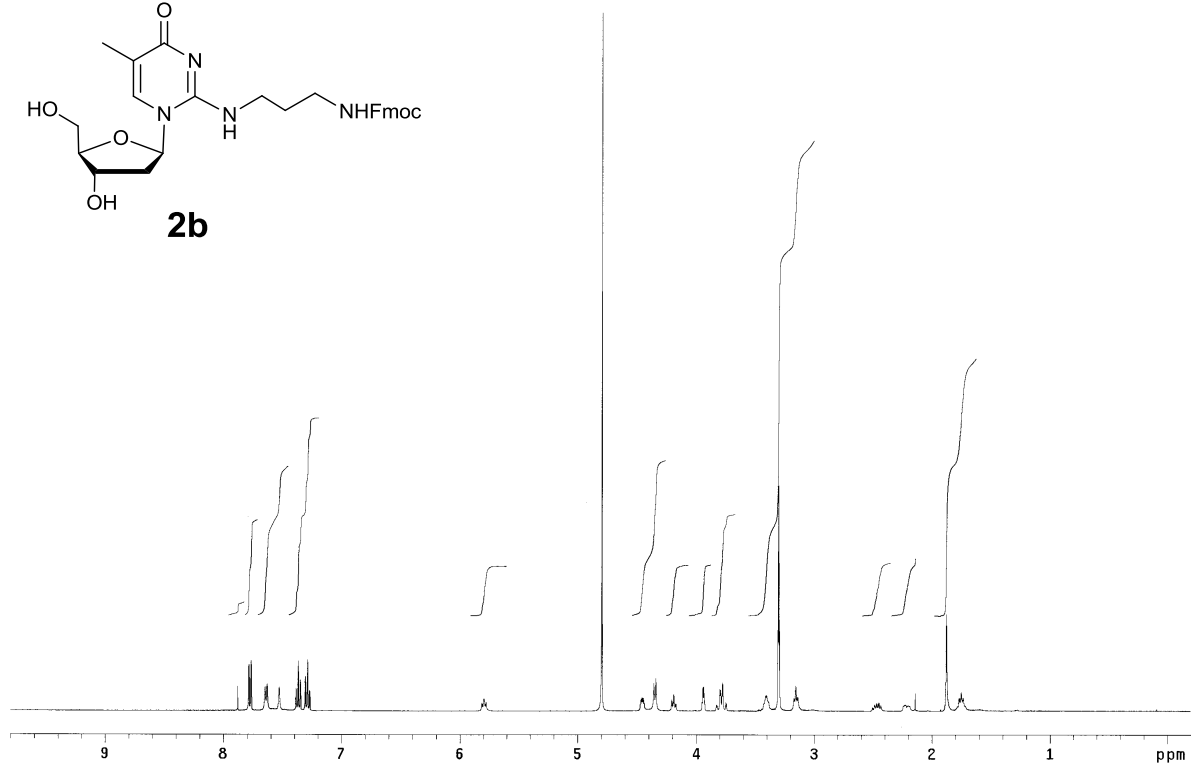
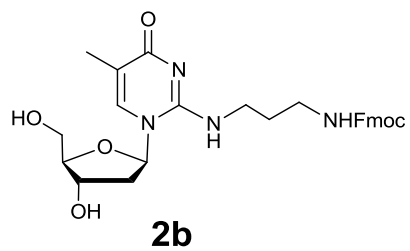


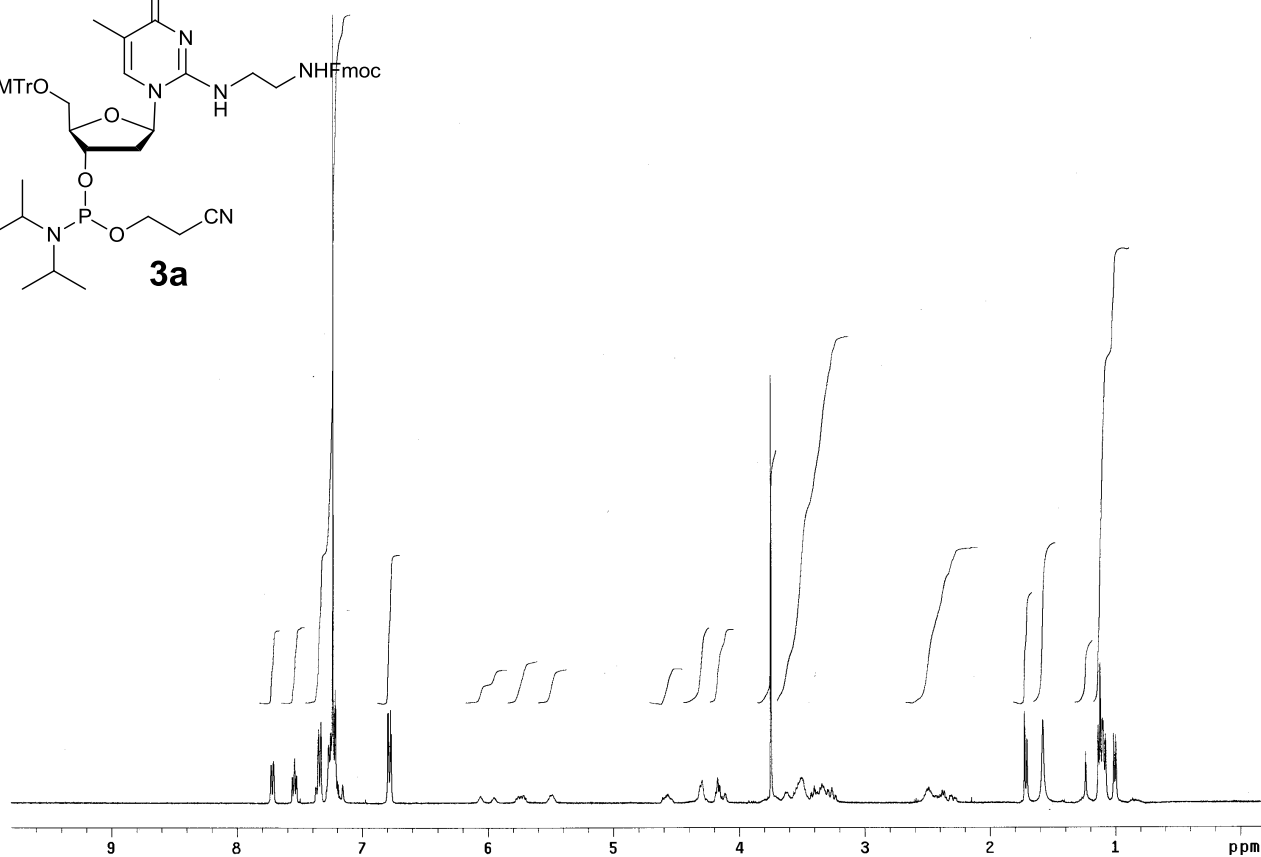
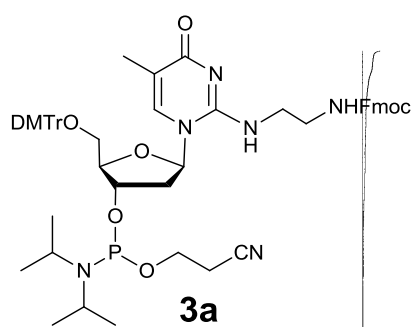
Figure S2. MALDI-TOF Mass chart of guanidineethyl-isodC in TFO (3'-N³ZN⁵-5').

Table S1. MALDI-TOF mass Results of synthesized TFOs in this study (negative mode, m/z)

TFOs	calcd. [M-H] ⁻	found
TFO $N^{\beta}ZN^{\delta} = A-Z-G$		
TFO (isodC)	5739.02	5738.10
TFO (et-guanidino)	5824.08	5823.48
TFO (et-ureido)	5825.06	5823.95
TFO (et-amino)	5782.06	5781.60
TFO (propyl)	5781.06	5780.02
TFO (pr-guanidino)	5838.10	5837.27
TFO (pr-ureido)	5839.08	5838.06
TFO (pr-amino)	5796.07	5795.16
TFO $N^{\beta}ZN^{\delta} = G-Z-G$		
TFO (isodC)	5755.01	5754.30
TFO (et-guanidino)	5840.07	5839.43
TFO (et-ureido)	5841.05	5840.67
TFO (et-amino)	5798.05	5797.44
TFO (propyl)	5797.05	5796.95
TFO $N^{\beta}ZN^{\delta} = G-Z-A$		
TFO (isodC)	5739.02	5738.25
TFO (et-guanidino)	5824.08	5823.59
TFO (et-ureido)	5825.06	5824.79
TFO (et-amino)	5782.06	5781.68
TFO (propyl)	5781.06	5780.00
TFO $N^{\beta}ZN^{\delta} = A-Z-A$		
TFO (isodC)	5723.03	5722.62
TFO (et-guanidino)	5808.09	5807.30
TFO (et-ureido)	5809.07	5808.14
TFO (et-amino)	5766.07	5765.42
TFO (propyl)	5765.07	5764.16







Internal standard
(0 ppm)

