Synthesis and crystal structure of 2'-Se-modified guanosine containing DNA

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General Experimental Methods

^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded on a 400 (400 MHz ^{1}H NMR, 100 MHz ^{13}C NMR) MHz spectrometer. The chemical shifts are reported relative to TMS. ^{1}H and ^{13}C peak assignments are based on similar compounds reported in the literature and APT experiments. Analytical thin-layer chromatography (TLC) was performed on silica 60F-254 plates. Flash column chromatography was carried out on silica gel 60 (70-230 mesh). All reactions were carried out under an argon atmosphere. The starting material 9-[*β*-D-Arabino-furanosyl]guanine was purchased from *MetkinenOy*, Finland. Chemical reagents and solvents were purchased from commercial sources and were used without further purification with the exception of dimethoxytrityl chloride (DMTr-Cl), which was crystallized from hexanes.

Figure S1. ^{1}H NMR spectrum of compound **2** in DMSO-d_6

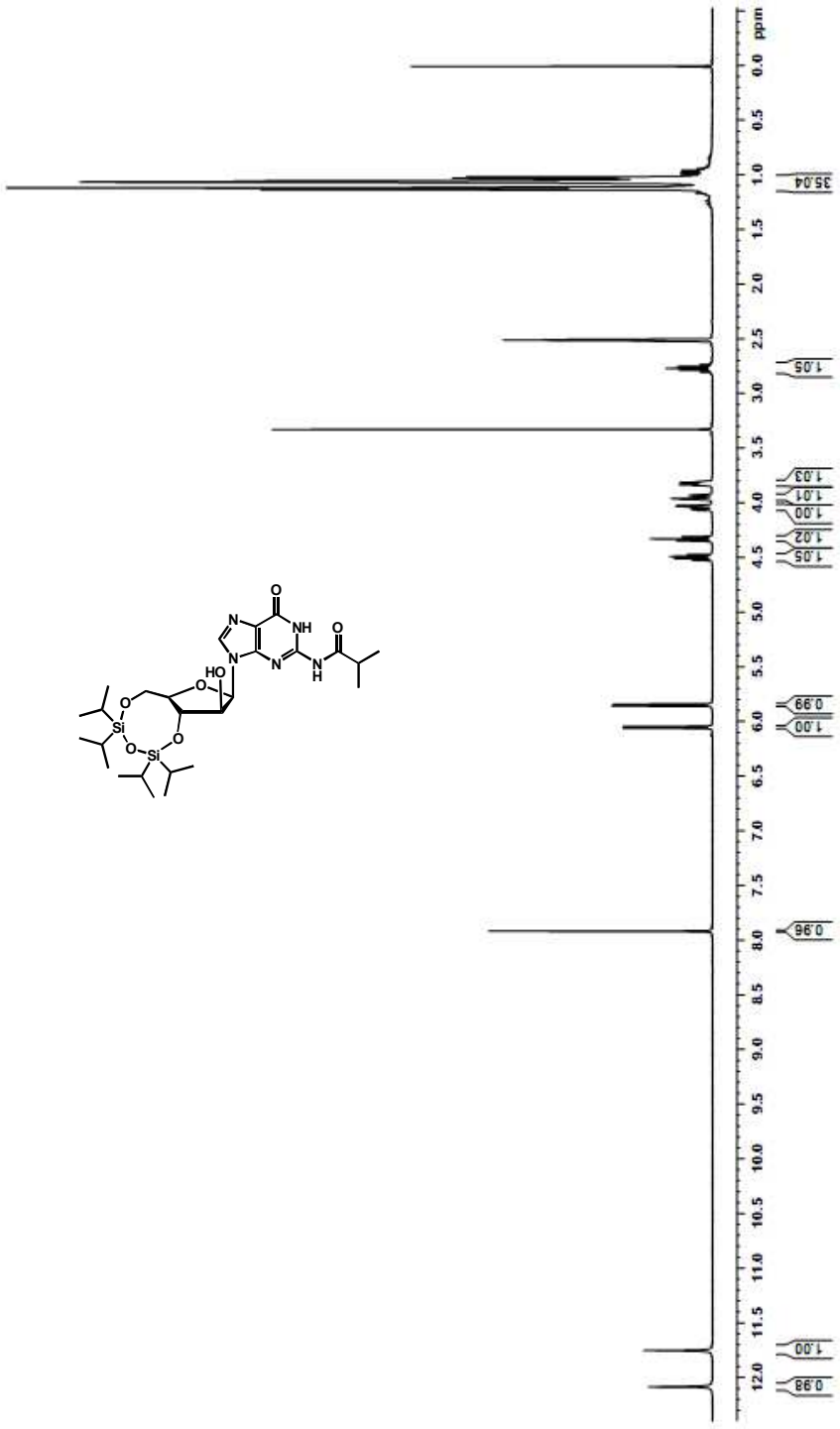

Figure S2. ^{1}H NMR spectrum of compound **3** in DMSO-d_6

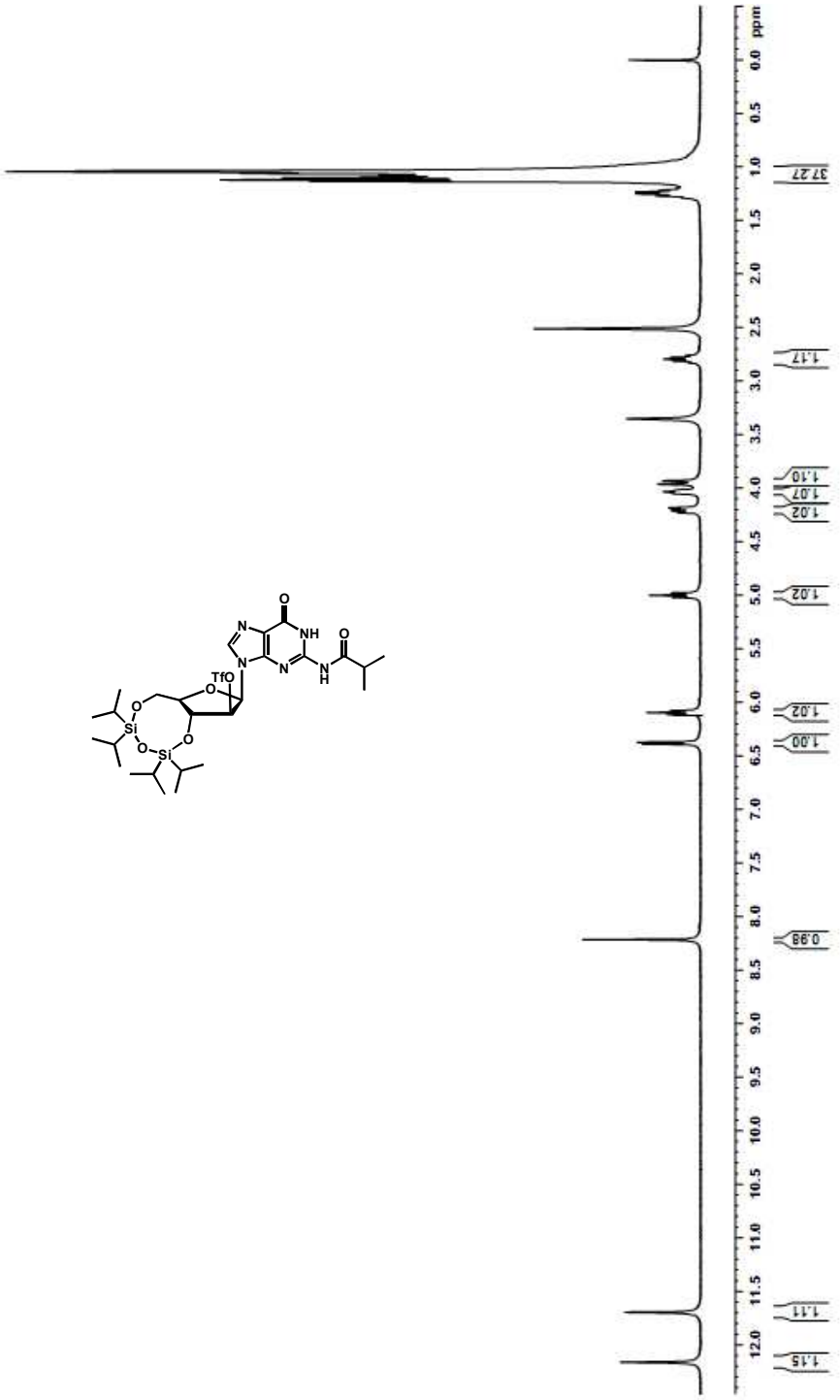

Figure S3. ^{1}H NMR spectrum of compound **4** in $CDCl_3$

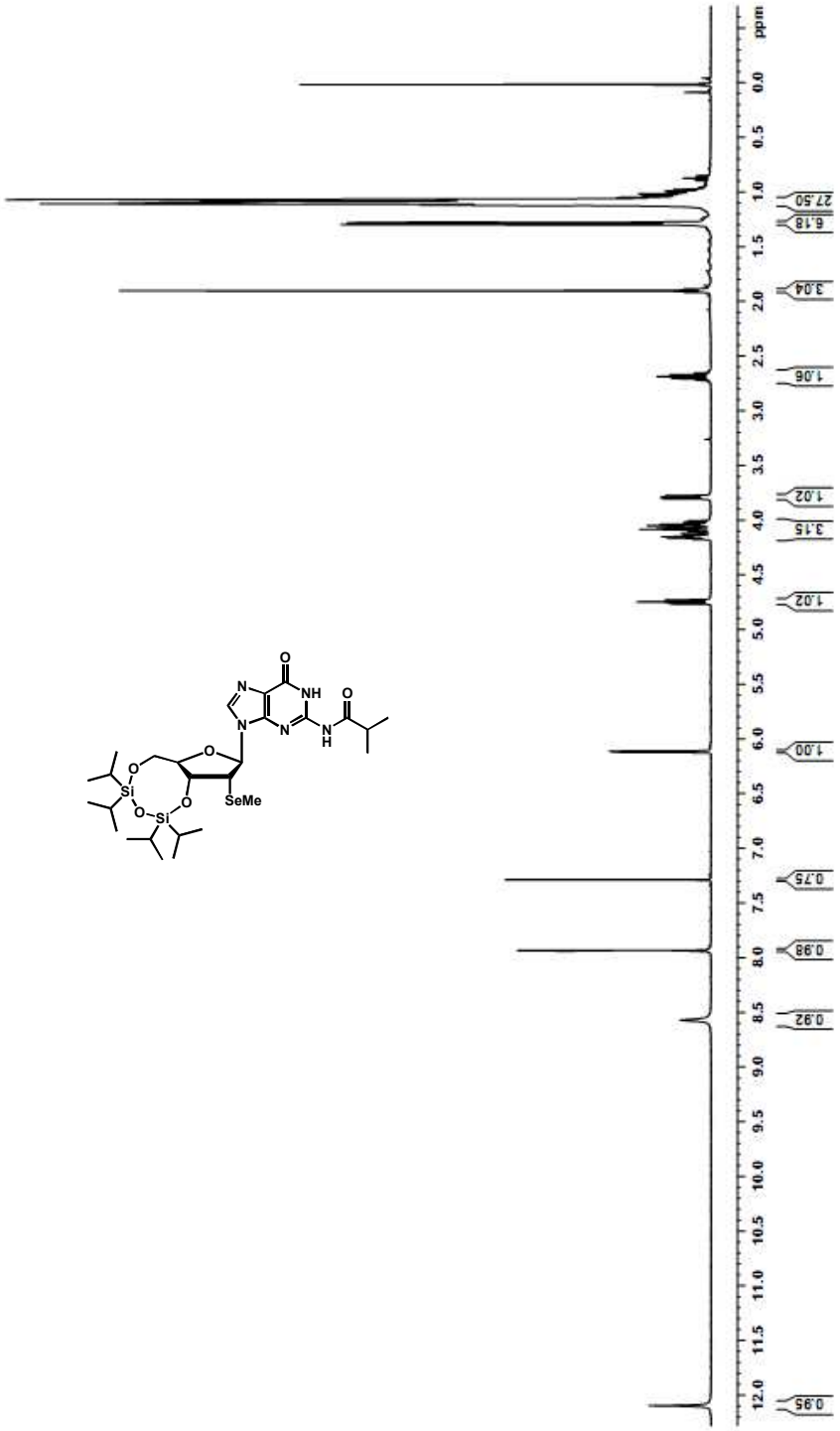

Figure S4. ^{1}H NMR spectrum of compound **5** in DMSO-d_6

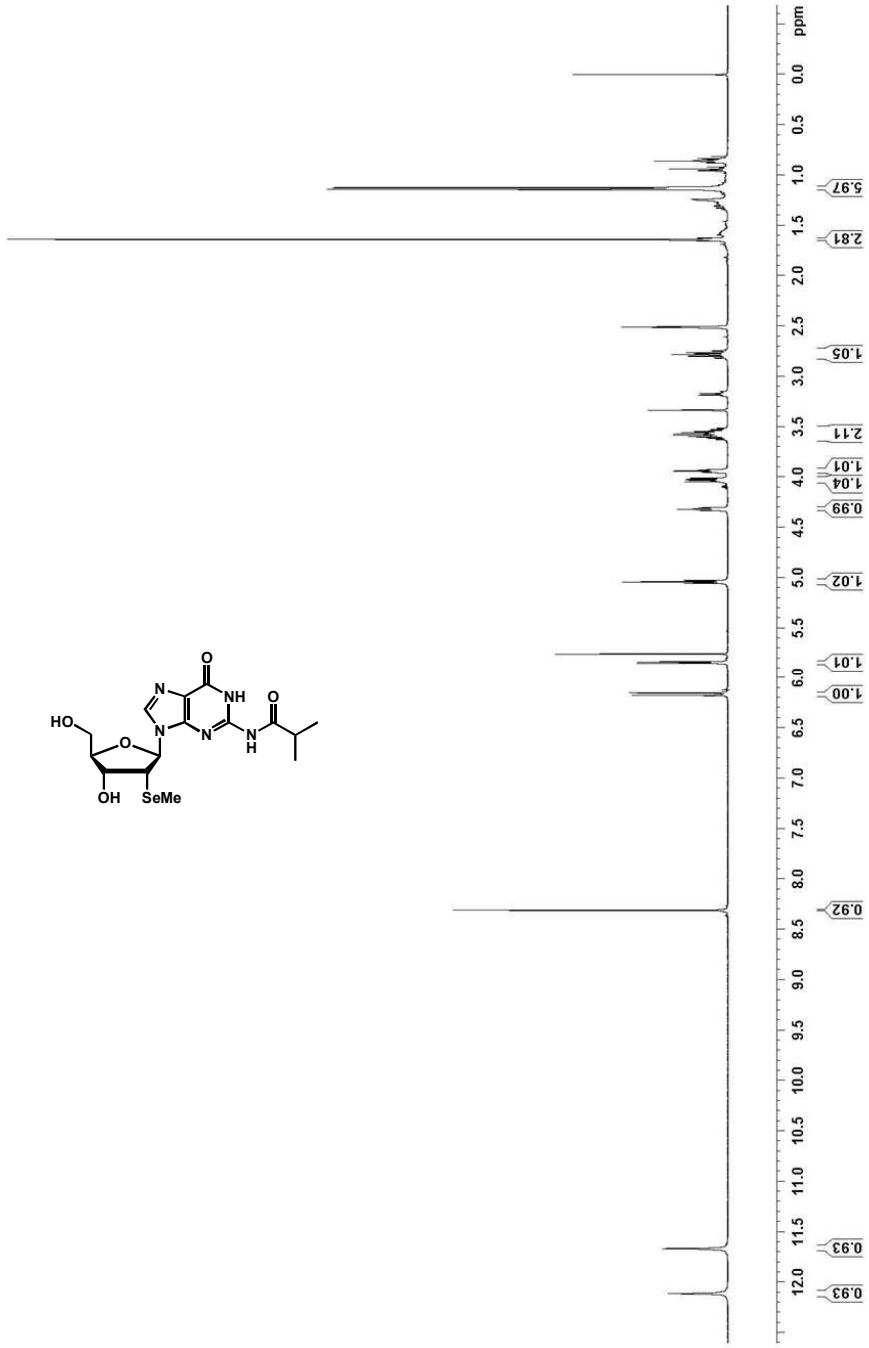

Figure S5. ^{1}H NMR spectrum of compound **6** in DMSO-d_6

Figure S6. ^{1}H NMR spectrum of compound **7** in $CDCl_3$

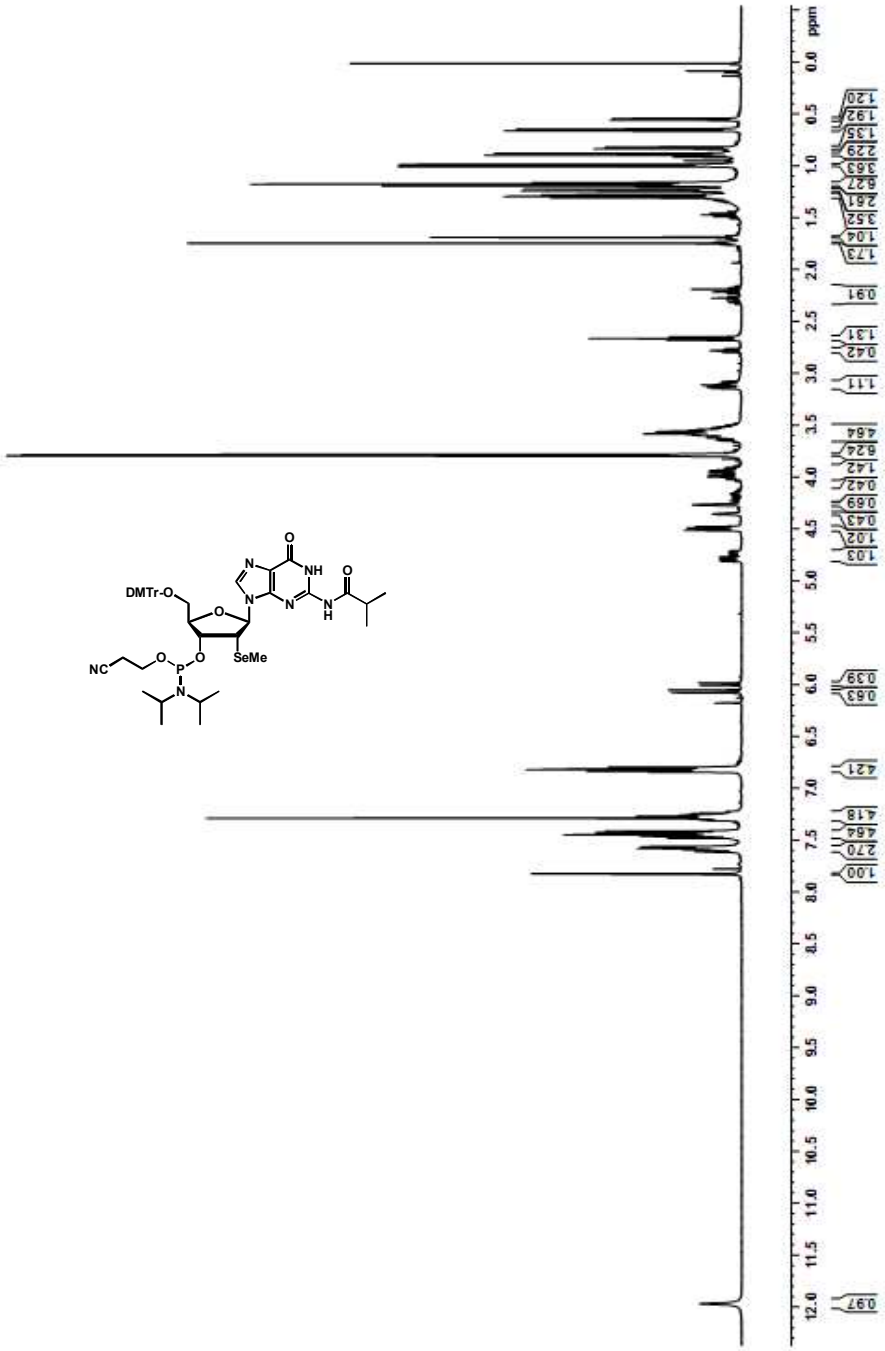

Figure S7. ^{13}C NMR (APT) spectrum of compound **4** in $CDCl_3$

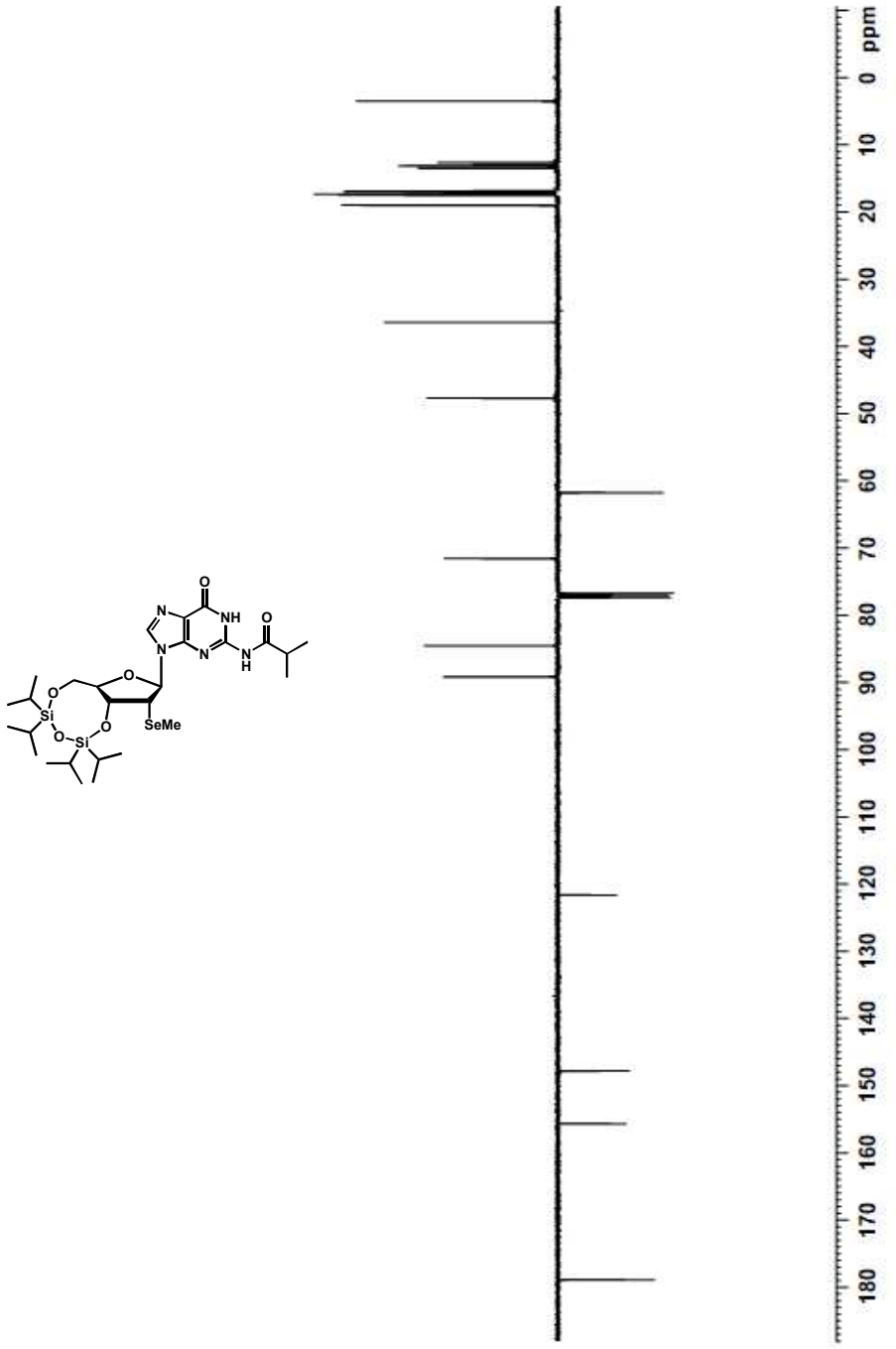

Figure S8. ^{13}C NMR (APT) spectrum of compound **5** in DMSO-d_6

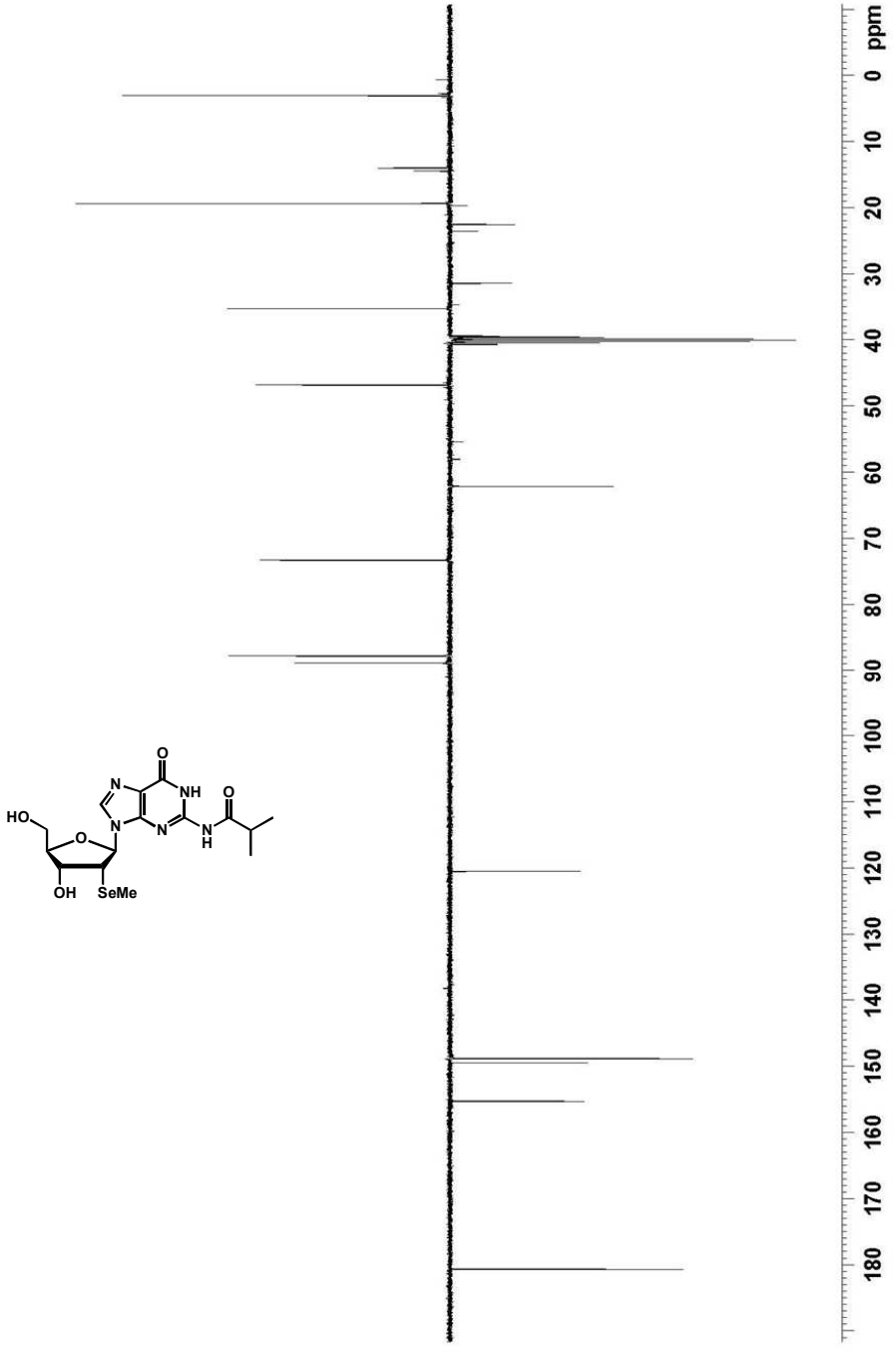

Figure S9. ^{13}C NMR (APT) spectrum of compound **6** in $CDCl_3$

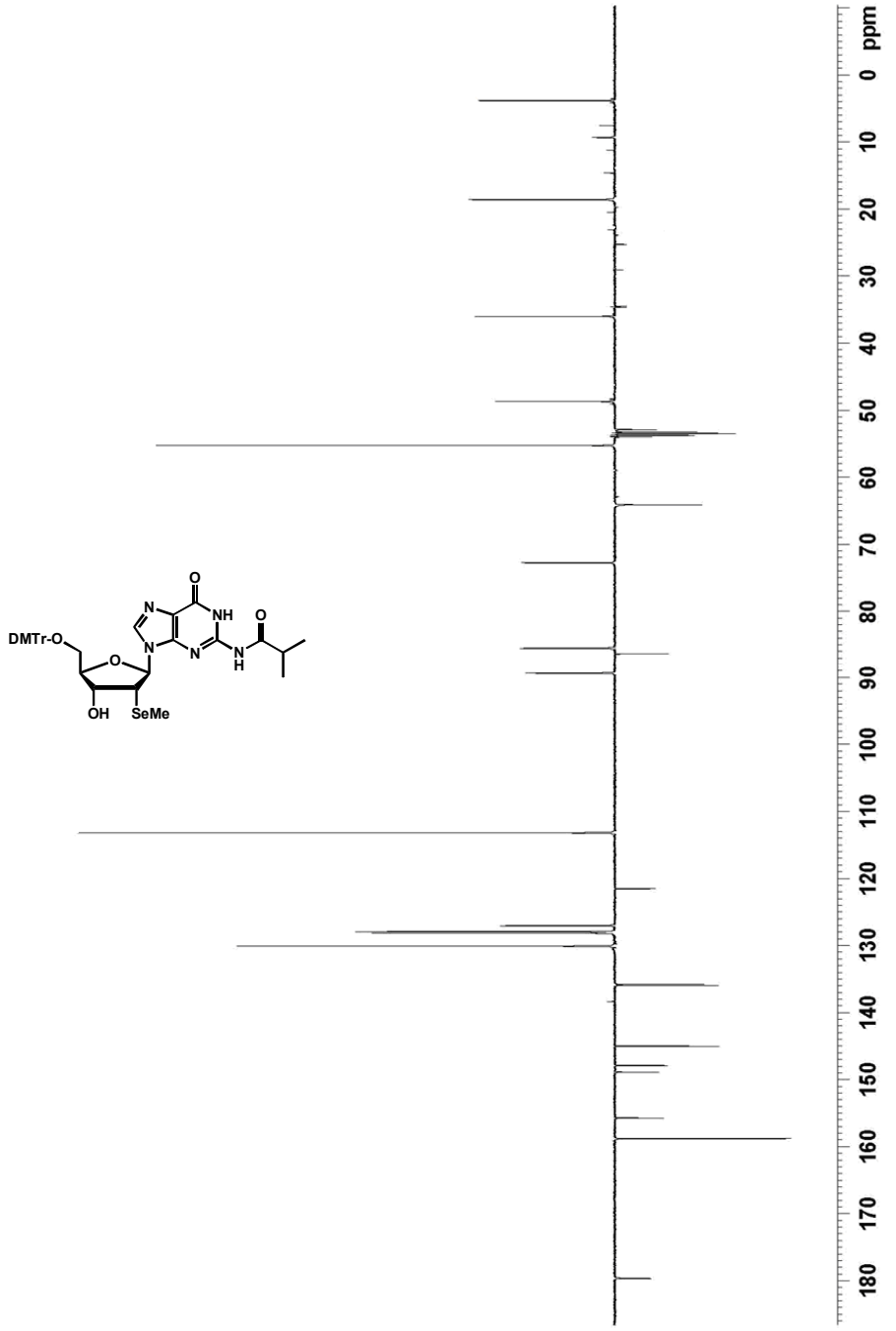

Figure S10. ^{13}C NMR (APT) spectrum of compound **7** in $CDCl_3$

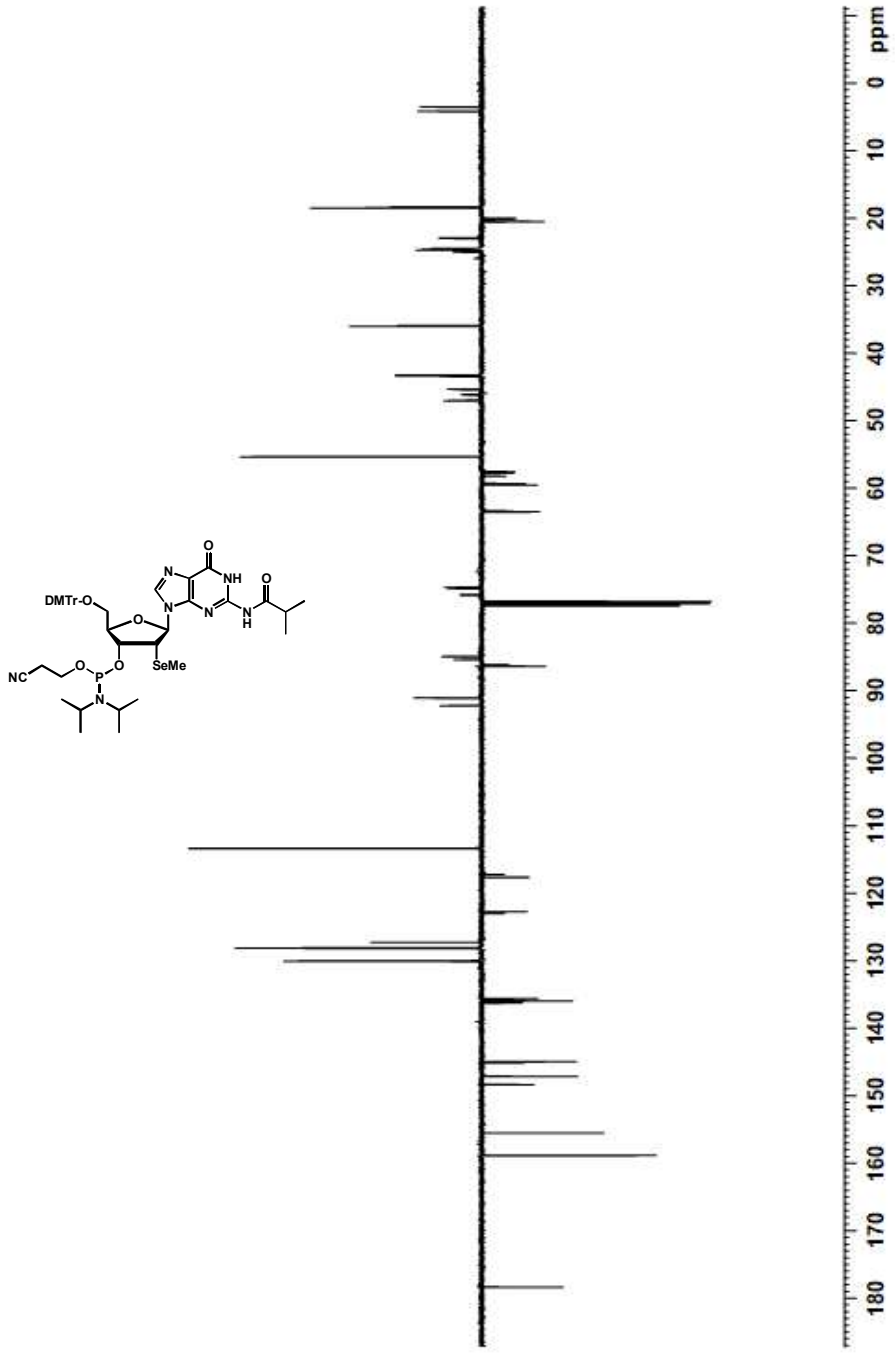

Figure S11. ^{31}P NMR spectrum of compound **7** in $CDCl_3$

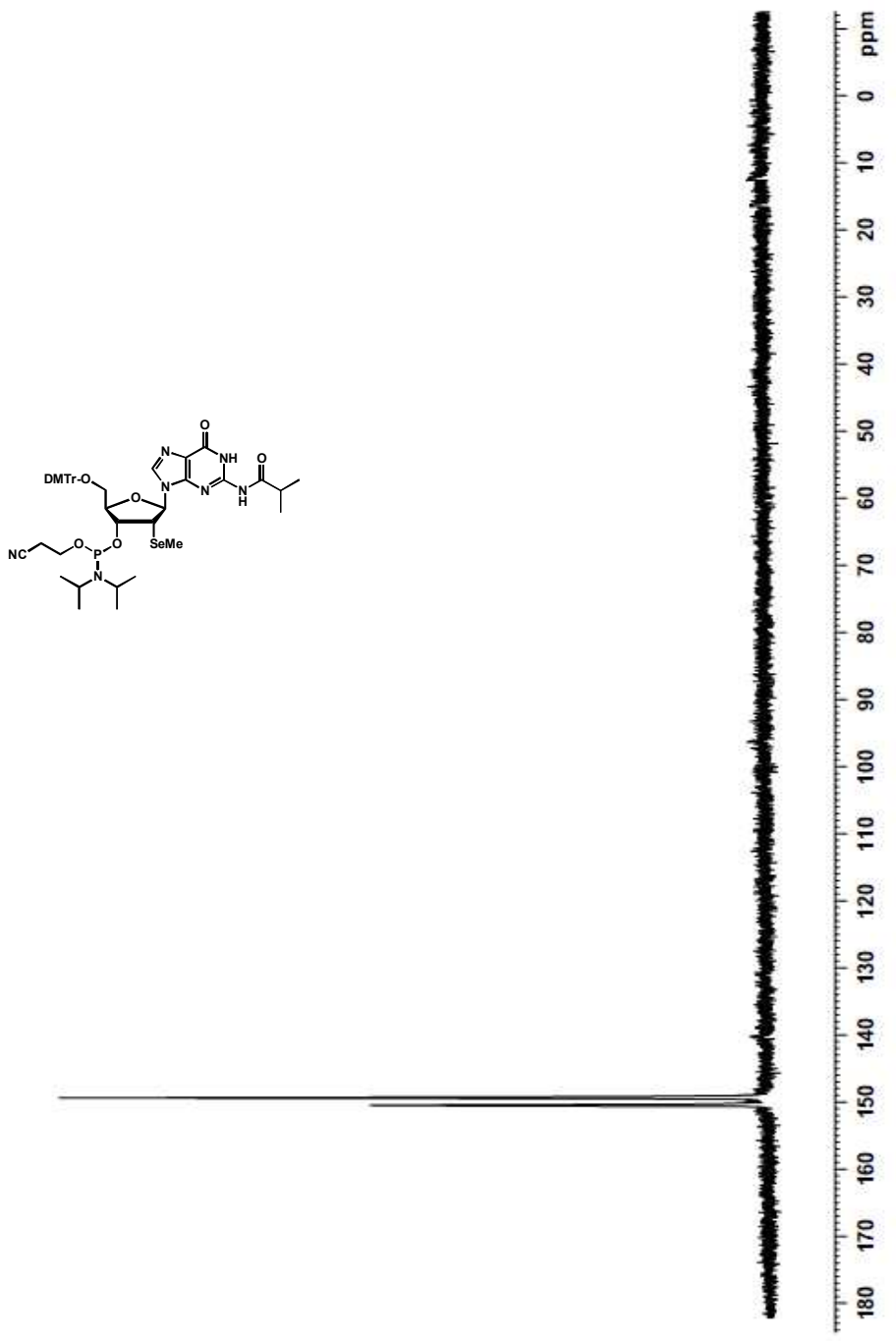

Figure S12. ESI-TOF high-acc spectrum of compound **4**, calcd for $C_{27}H_{47}N_5O_6SeSi_2$ $[M + H]^+$ 674.2303, found 674.2304, $[M + Na]^+$ 696.2122, found 696.2126.

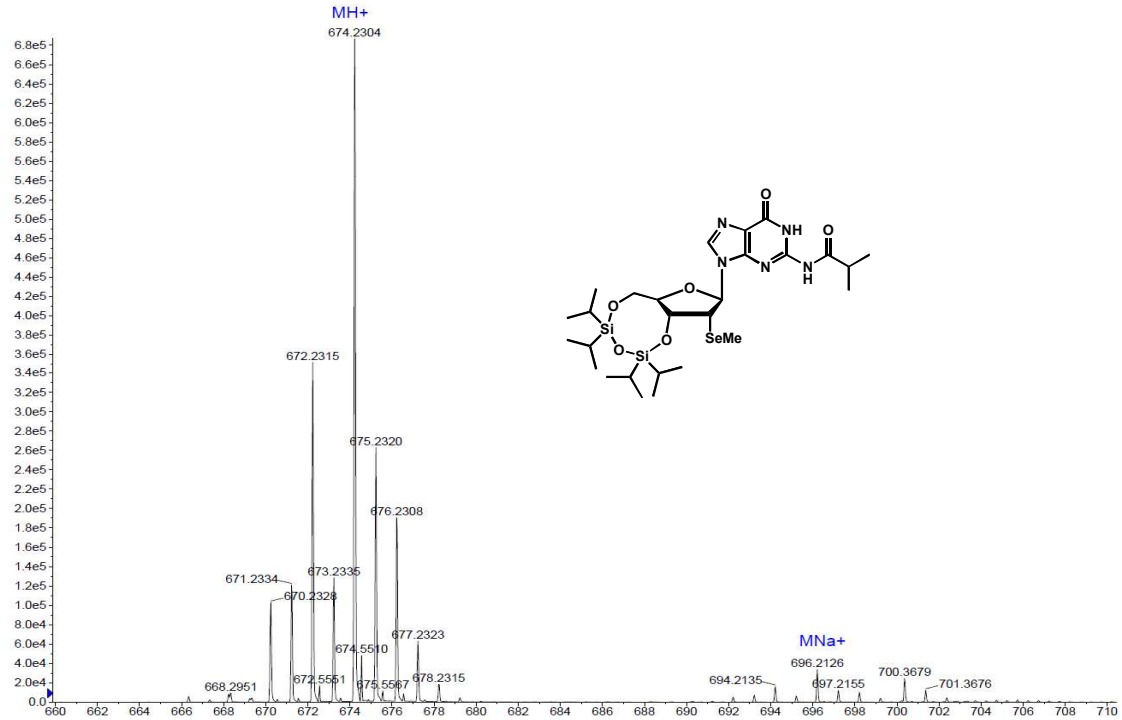

Figure S13. ESI-TOF high-acc spectrum of compound **5**, calcd for $C_{15}H_{21}N_5O_5Se$ $[M + H]^+$ 432.0781, found 432.0777; $[M + Na]^+$ 454.06, found 454.0601.

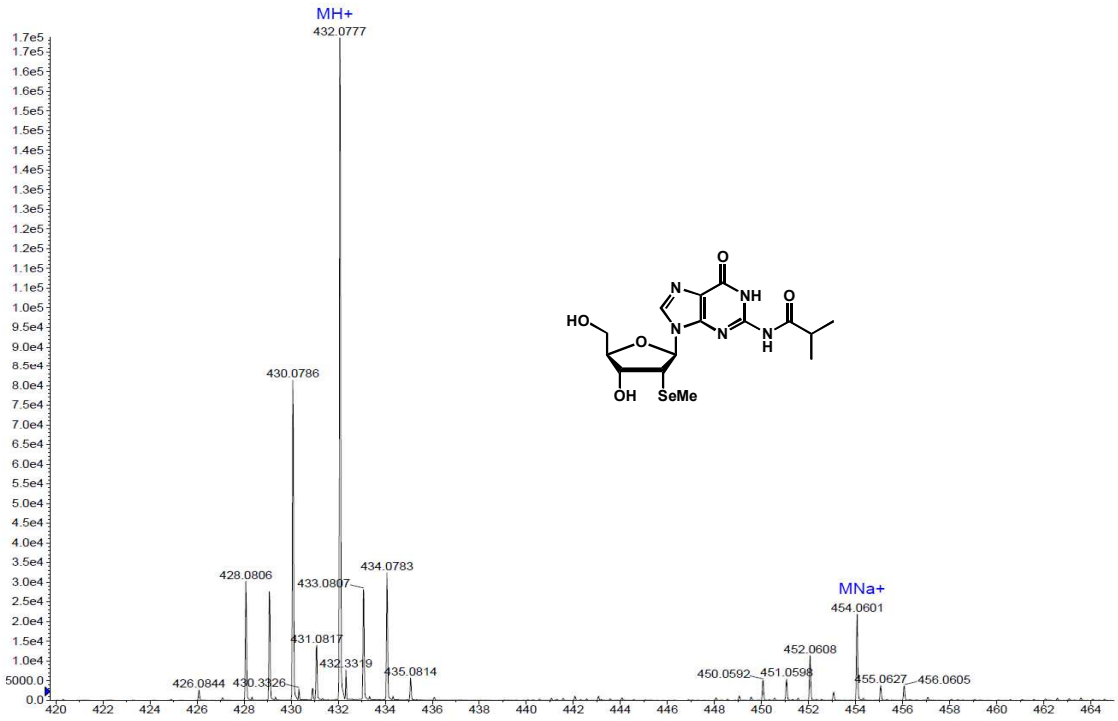

Figure S14. ESI-TOF high-acc spectrum of compound **6**, calcd for $C_{36}H_{39}N_5O_7Se$ $[M + H]^+$ 734.2087, found 734.2085; $[M + Na]^+$ 756.1907, found 756.1908.

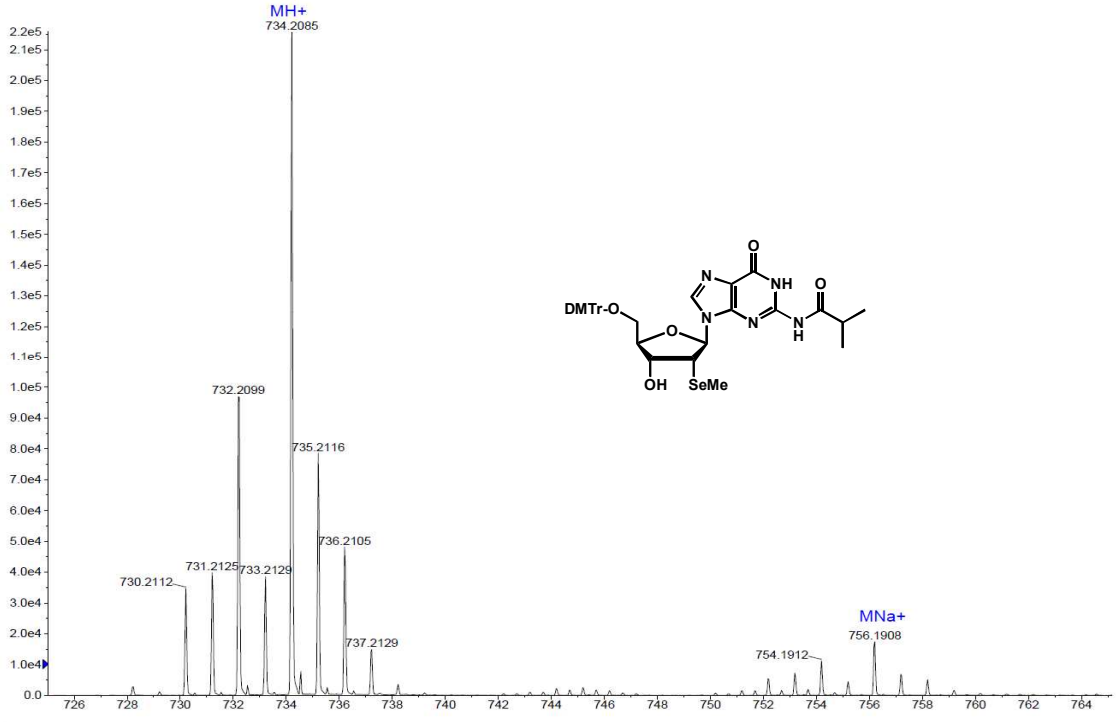

Figure S15. ESI-TOF high-acc spectrum of compound **7**, calcd for $C_{45}H_{56}N_7O_8PSe$ $[M + H]^+$ 934.3166, found 934.3170, $[M + Na]^+$ 956.2985, found 956.2983.

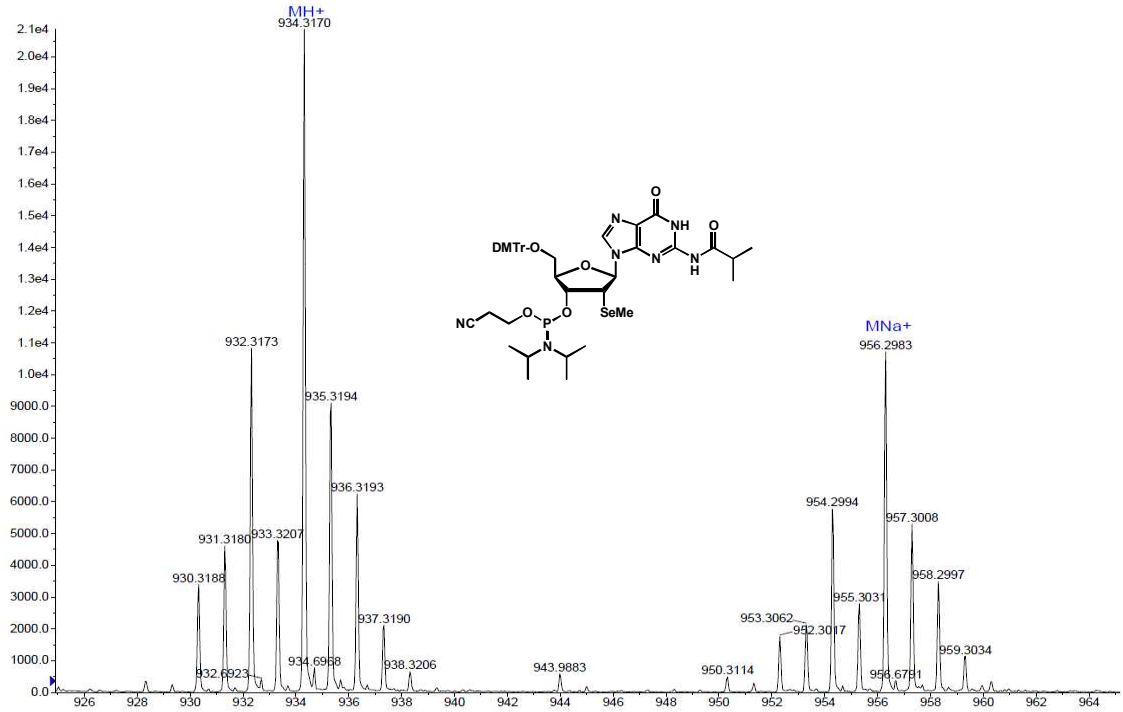

Table S1. Data collection and refinement statistics of the 2'-SeMe-modified DNA (dGTG_{Se}TACAC)

Structure (PDB ID)	dGTG_{Se}TACAC (3IFI)	**Structure (PDB ID)**	dGTG_{Se}TACAC (3IFI)
Data collection		**Refinement**	
Space Group	$P4_32_12$	Resolution range, Å (last shell)	29.5– 1.20
Cell dimensions: *a*,*b*,*c* (Å),	41.641, 41.641, 24.112,	R_{work} , %	20.2
α, β, γ (°C)	90, 90, 90		
Resolution range, Å (last shell)	50.0 – 1.20	R_{free} , %	22.1
Unique reflections	6376 (160)	Number of reflections	5901
Completeness, %	90.2 (63.9)	**Number of atoms**	
R_{merge} , %	6.5 (31.9)	Nucleic Acid (single)	210
I/σ(I)	52.8 (4.2)	Heavy Atoms and Ion	1 Se
Redundancy	13.0 (3.2)	Water	24
R.m.s. deviations			
Bond length, Å	0.004		
Bond angle	1.144		

$R_{merge}=\Sigma|I-\langle I\rangle|/\Sigma I$