Supplementary Data

Synthesis and Evaluation of Modified siRNA Molecules Containing a Novel Glucose Derivative

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Procedures

Procedure for LC/MS: LC/MS chromatograms were acquired on an Agilent 6545 QTOF-MS with Agilent 1260 Infinity Binary Pump HPLC using a ZORBAX Eclipse Plus C18 2.1x100mm 1.8-Micron Agilent column and a mobile phase of 5 mM ammonium acetate buffer (pH 7)/acetonitrile (95:5). Oligonucleotide samples were prepared at a concentration of 0.01 O.D/µL with an injection volume of 20 µL. Data were analysed using Agilent Technologies MassHunter Workstation Qualitative Analysis Software (Qual. 10.0).

Tables

Table S1. Sequences and mass spectrometry data of modified oligonucleotide strands

Code	*Sequence*	*Mass (predicted)*	*Mass (found)*
S1	5’ CUU ACG CUG AGU ACU UCG A**X** 3’ (S)	6796.88	6796.52
S2	5’ CUU ACG CUG AGU ACU **X**CG ATT 3’ (S)	6794.90	6795.56
S3	5’ CUU ACG CUG AG**X** ACU UCG ATT 3’ (S)	6794.90	6794.62
AS1	3’ **X**G AAU GCG ACU CAU GAA GCU 5’ (AS)	6882.94	6882.87
AS2	3’ TTG AA**X** GCG ACU CAU GAA GCU 5’ (AS)	6880.96	6880.80
AS3	3’ TTG AAU GCG AC**X** CAU GAA GCU 5’ (AS)	6880.96	6880.61

(S) corresponds to the sense strand; (AS) corresponds to the antisense strand. **X** corresponds to the position of the glucose nucleoside with a triazole-linked uracil.

Figures

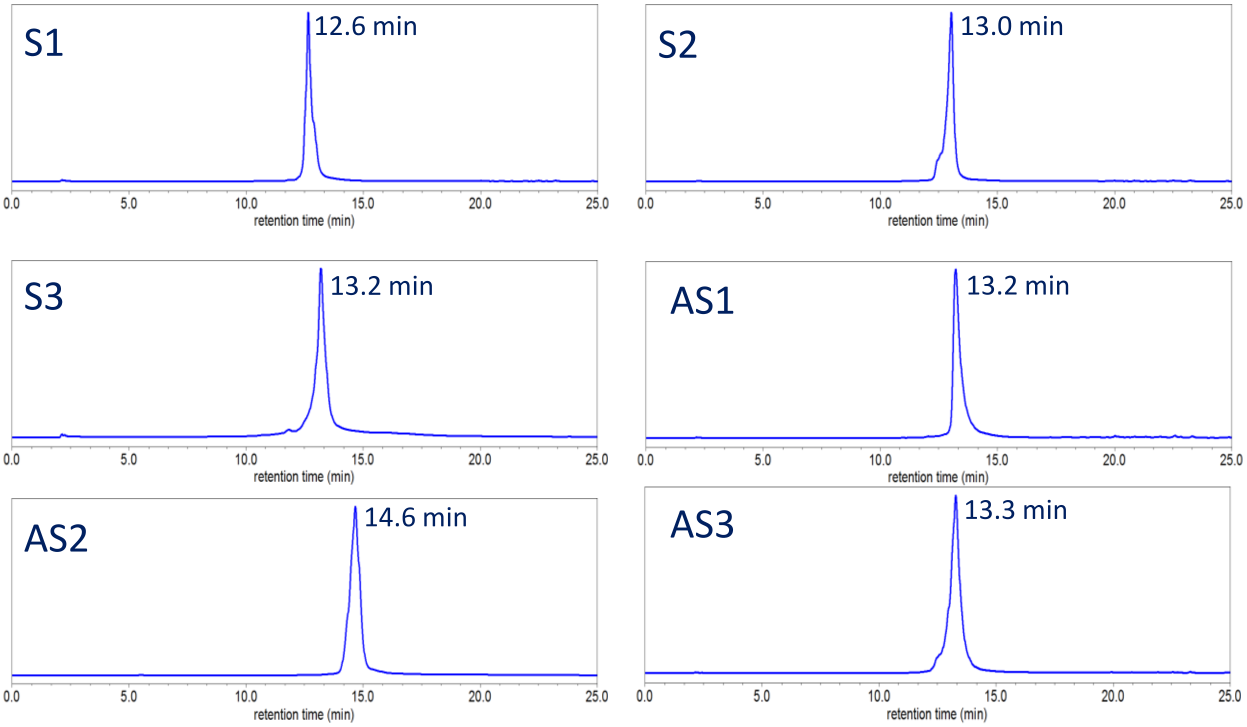


Figure S1. Analytical HPLC traces of modified oligonucleotides. Corresponding sequences can be found in Table S1. HPLC was performed on a Waters 1525 binary HPLC pump with a Waters 2489 UV/Vis detector, using a C18 4.6 x 150 mm reverse-phase column, eluting from 5 to 95% ACN in 0.1 M TEAA buffer (pH 7.0).

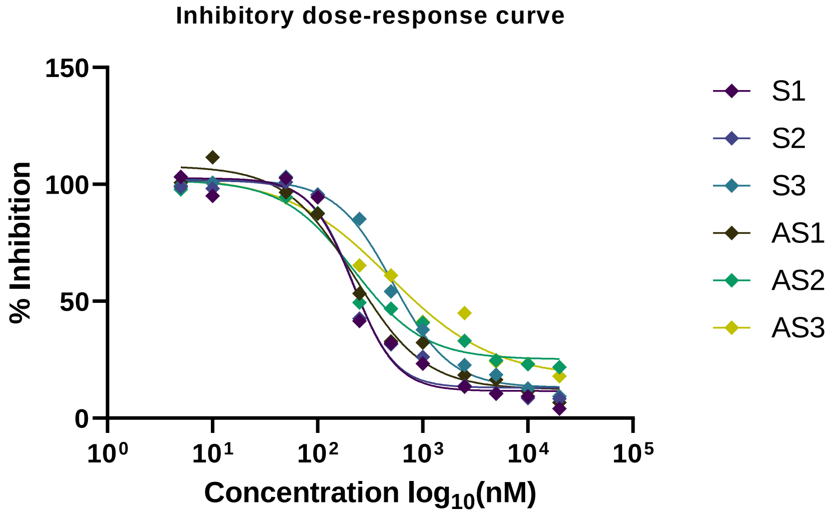
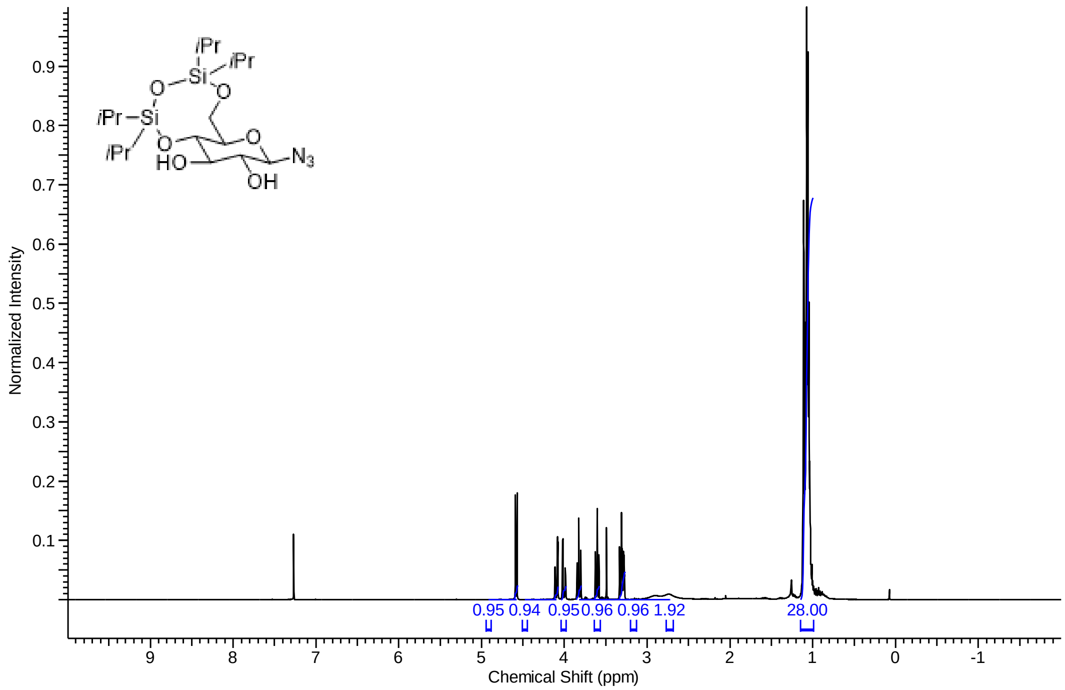


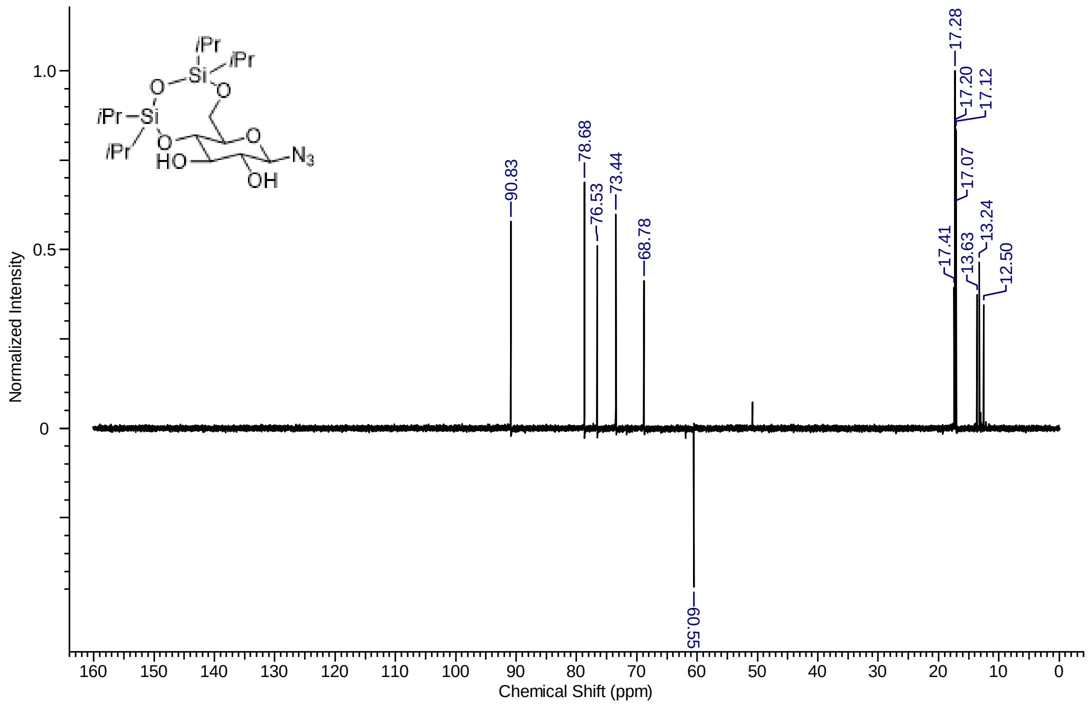
Figure S2. Inhibitory dose-response curves for modified anti-luciferase siRNAs, tested in HeLa at concentrations from 5 to 20,000 pM.

NMR Spectra

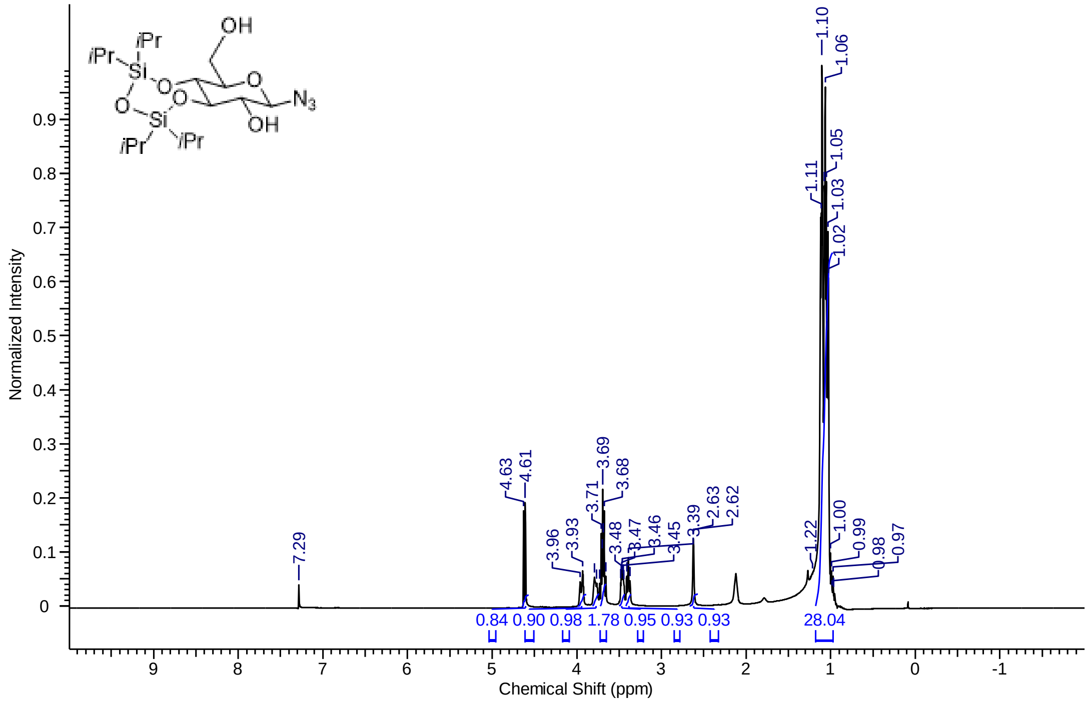
^{1}H NMR Spectrum of Compound **1**



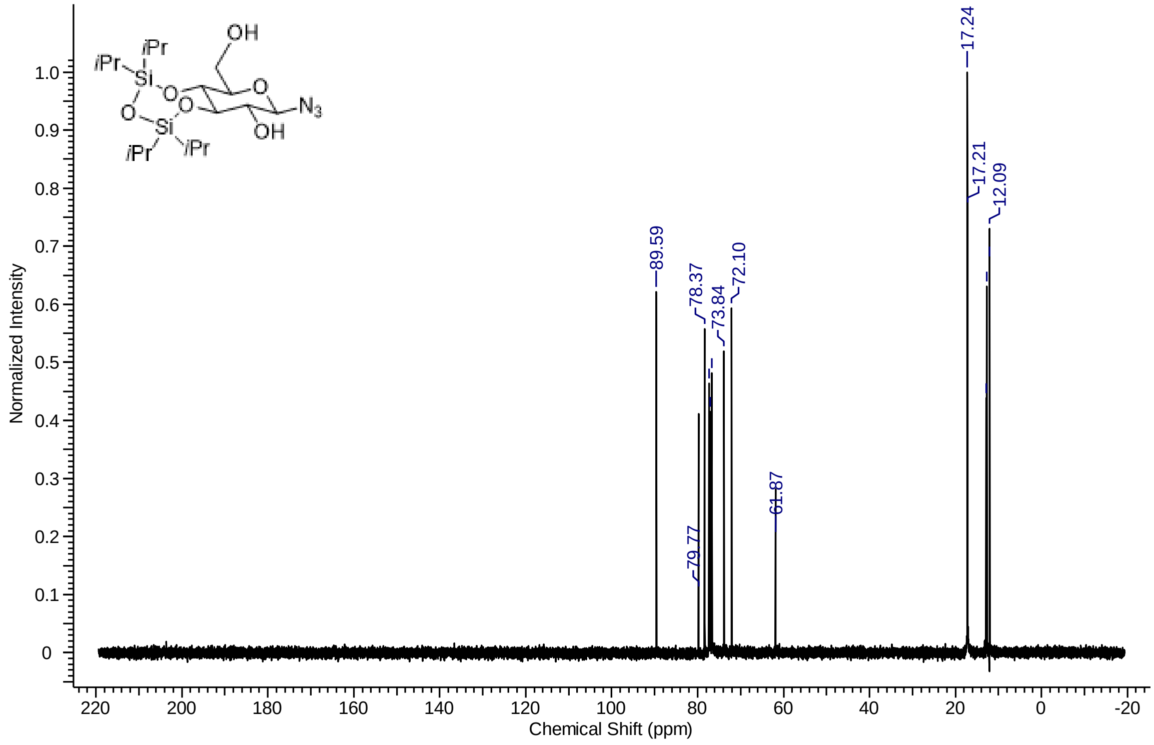
^{13}C NMR Spectrum of Compound **1**



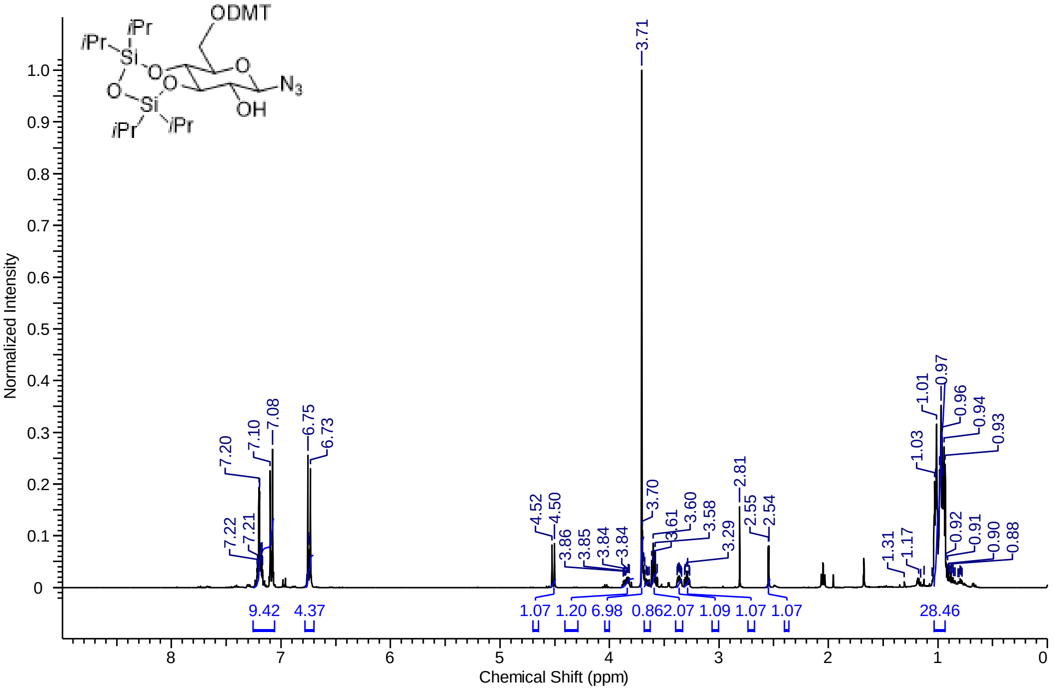
^{1}H NMR Spectrum of Compound **2**



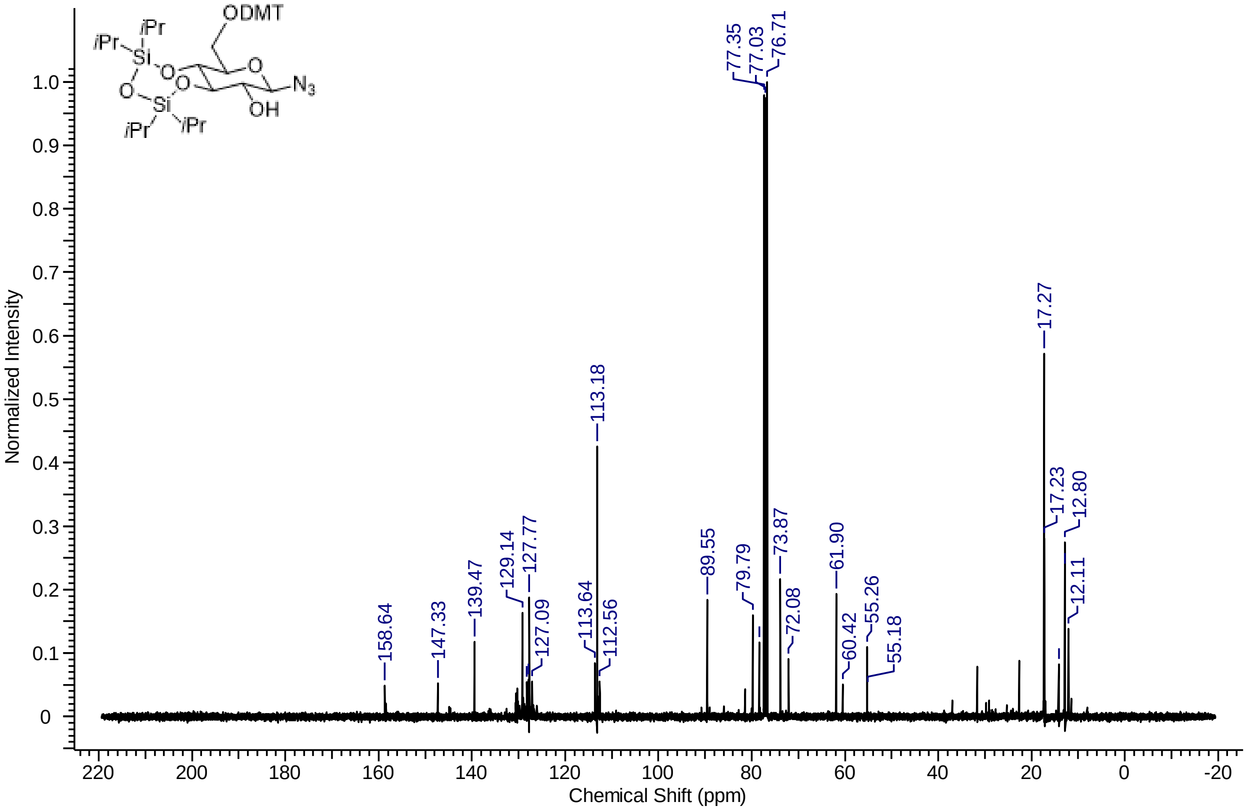
^{13}C NMR Spectrum of Compound **2**



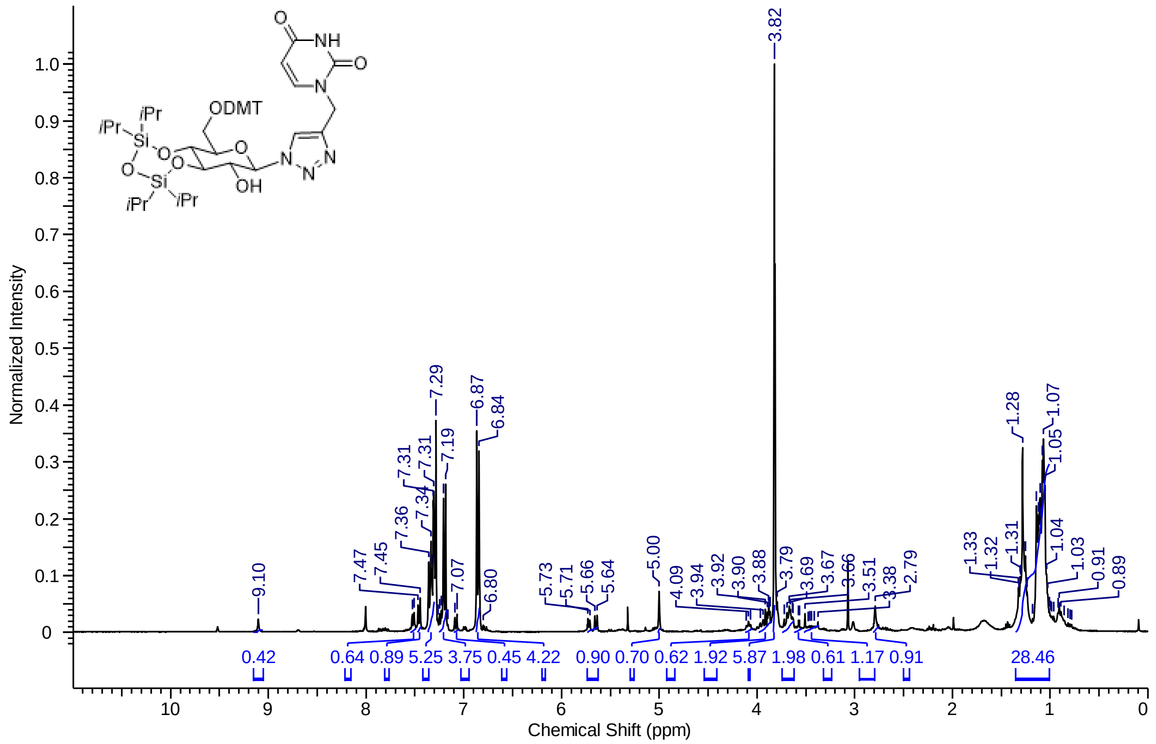
^{1}H NMR Spectrum of Compound **3**



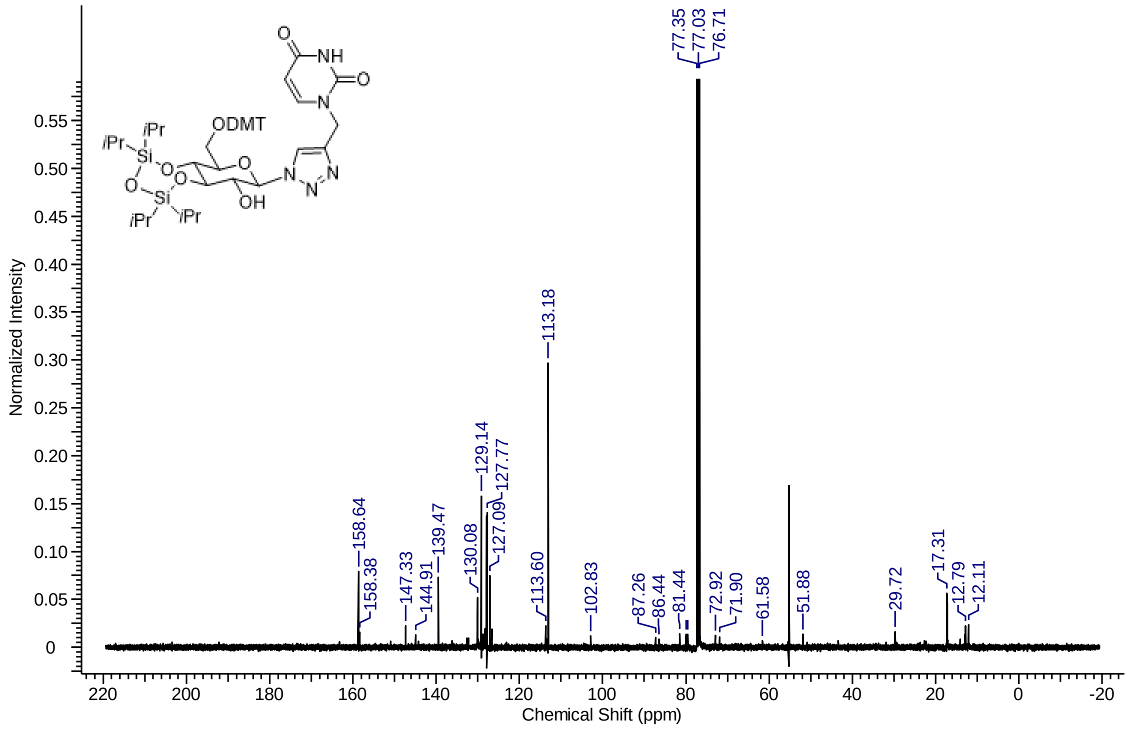
^{13}C NMR Spectrum of Compound **3**



^{1}H NMR Spectrum of Compound **4**



^{13}C NMR Spectrum of Compound **4**



^{31}P NMR Spectrum of Compound **5**