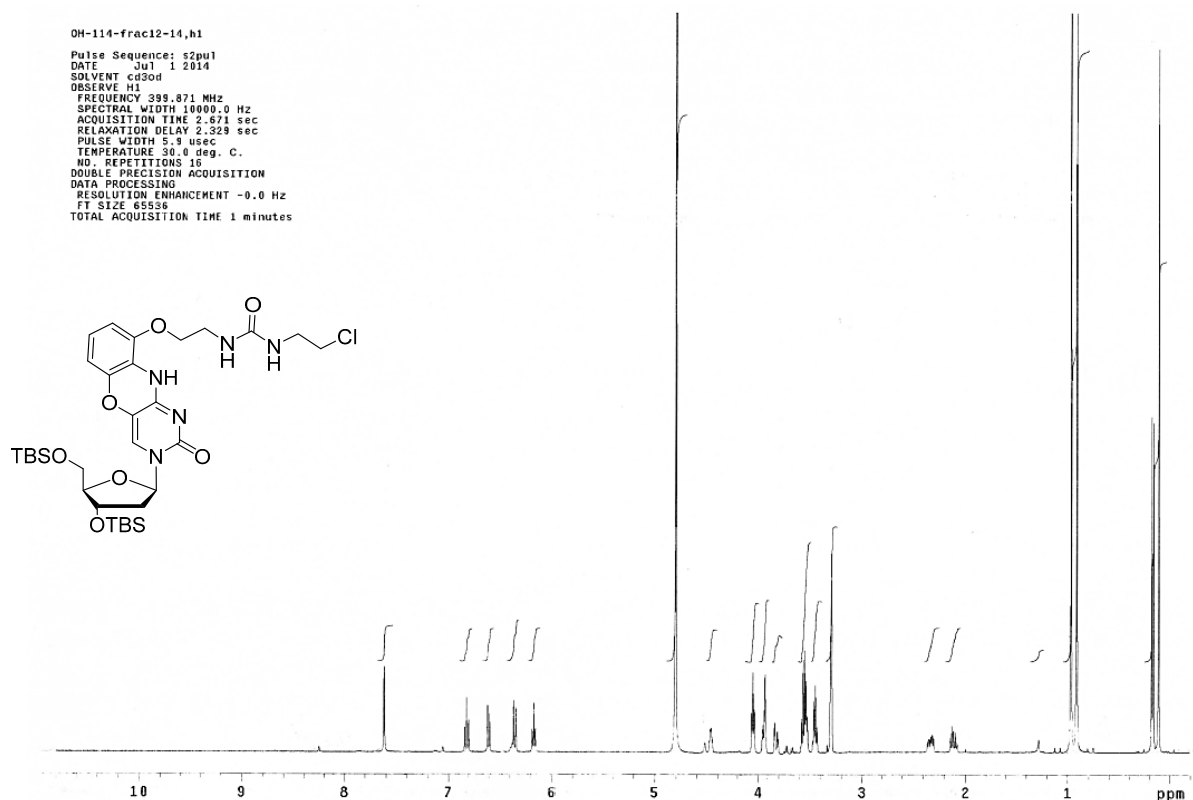
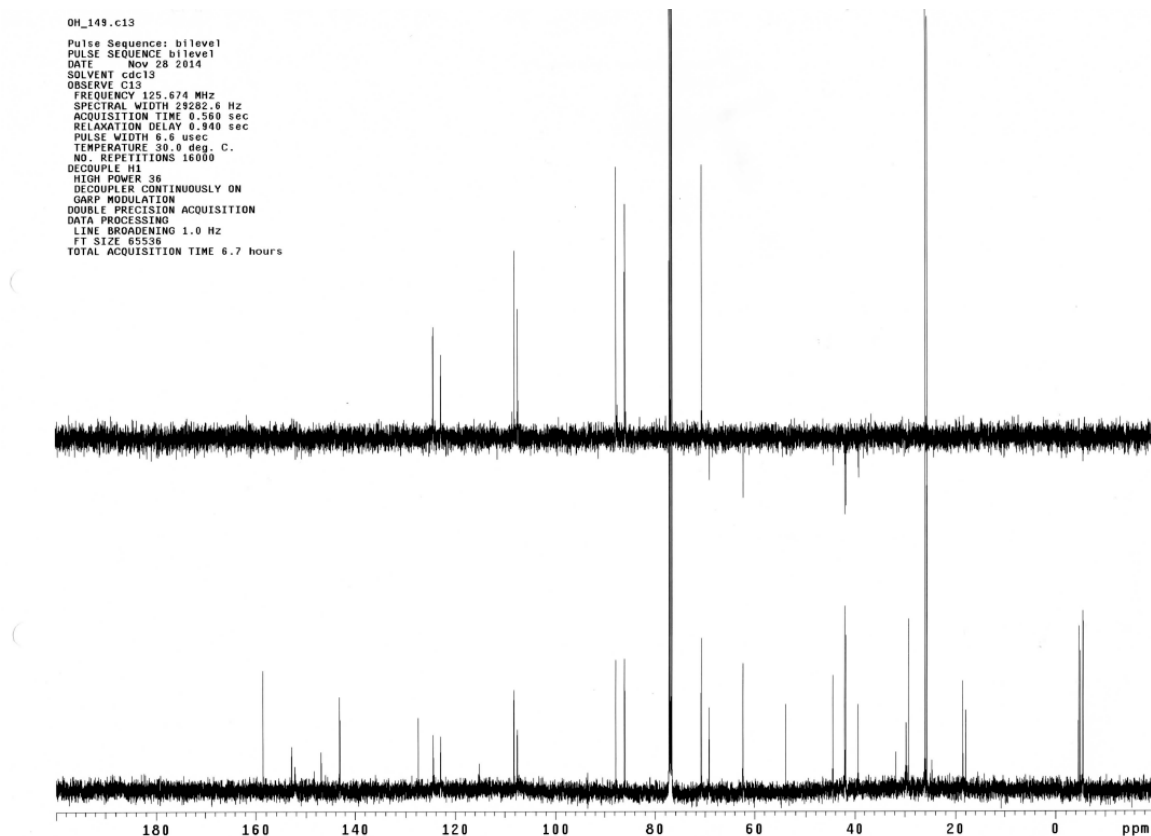


# Supplementary Materials

## 2a $^1\text{H}$ -NMR

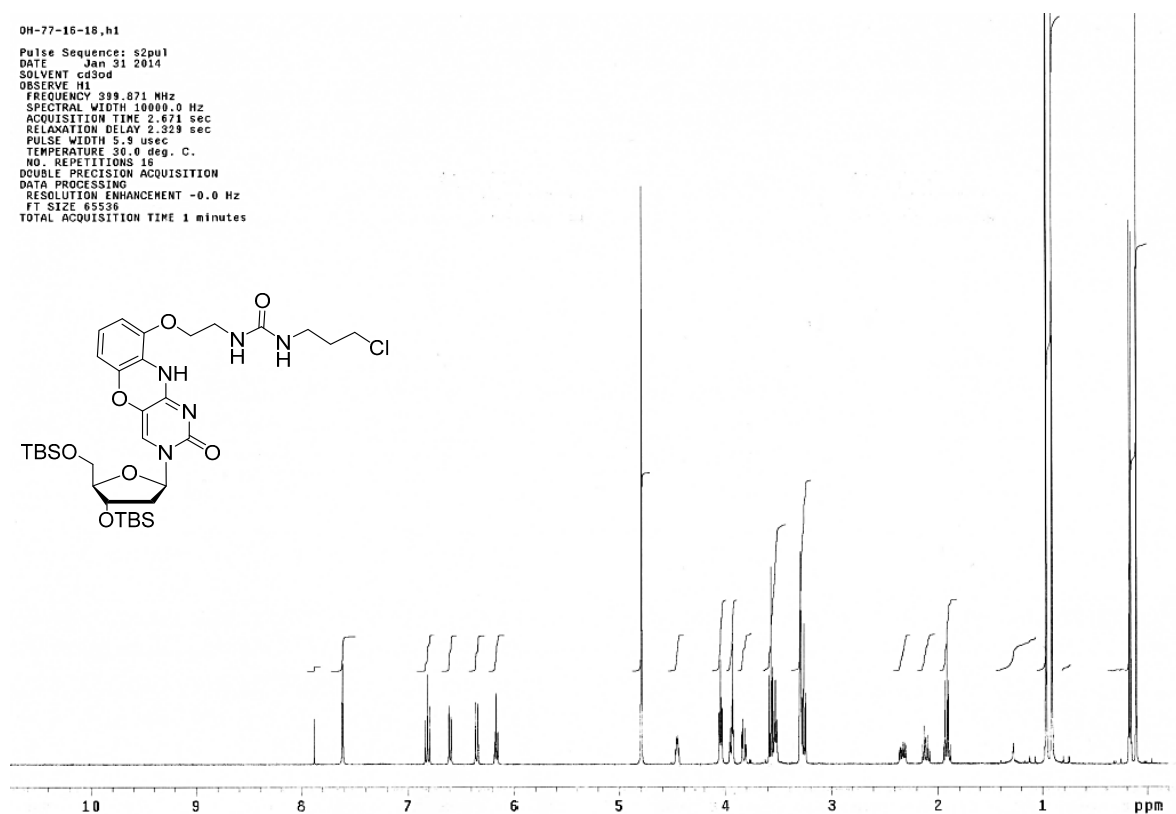
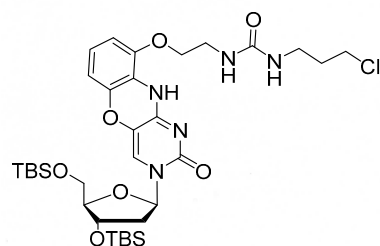


## 2a $^{13}\text{C}$ -NMR

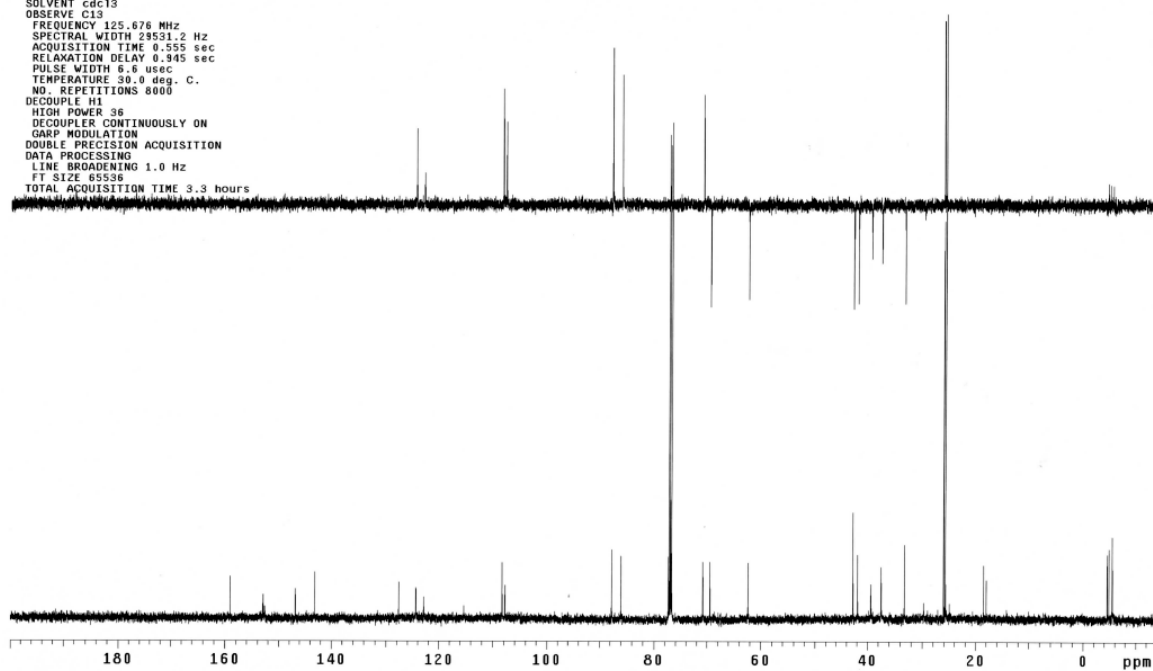


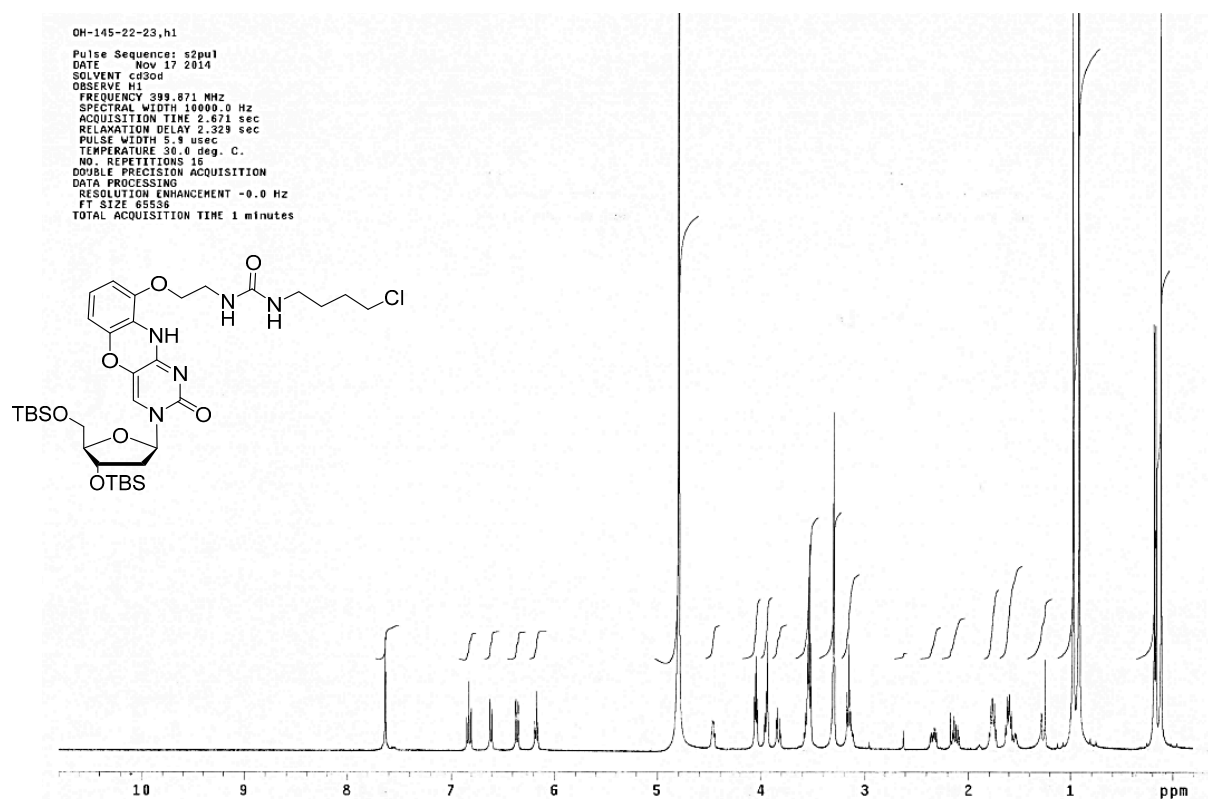
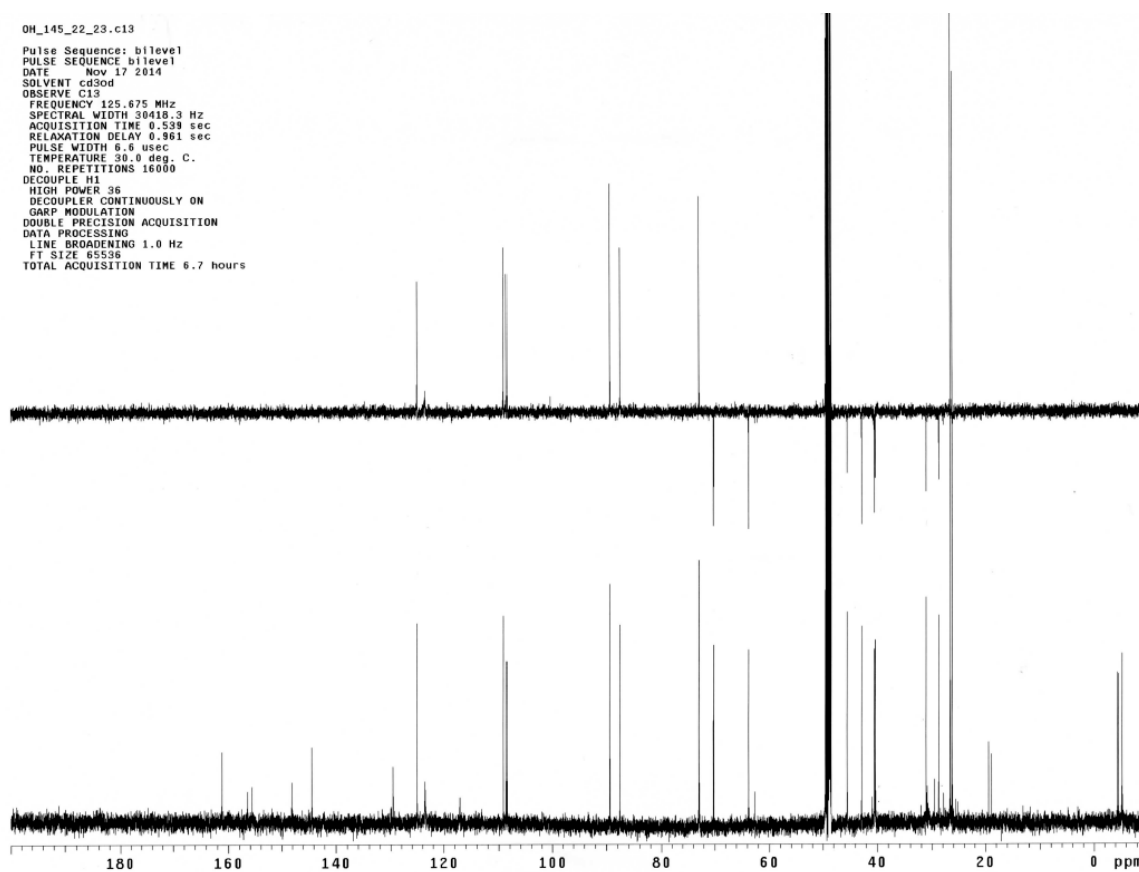
2b  $^1\text{H}$ -NMR

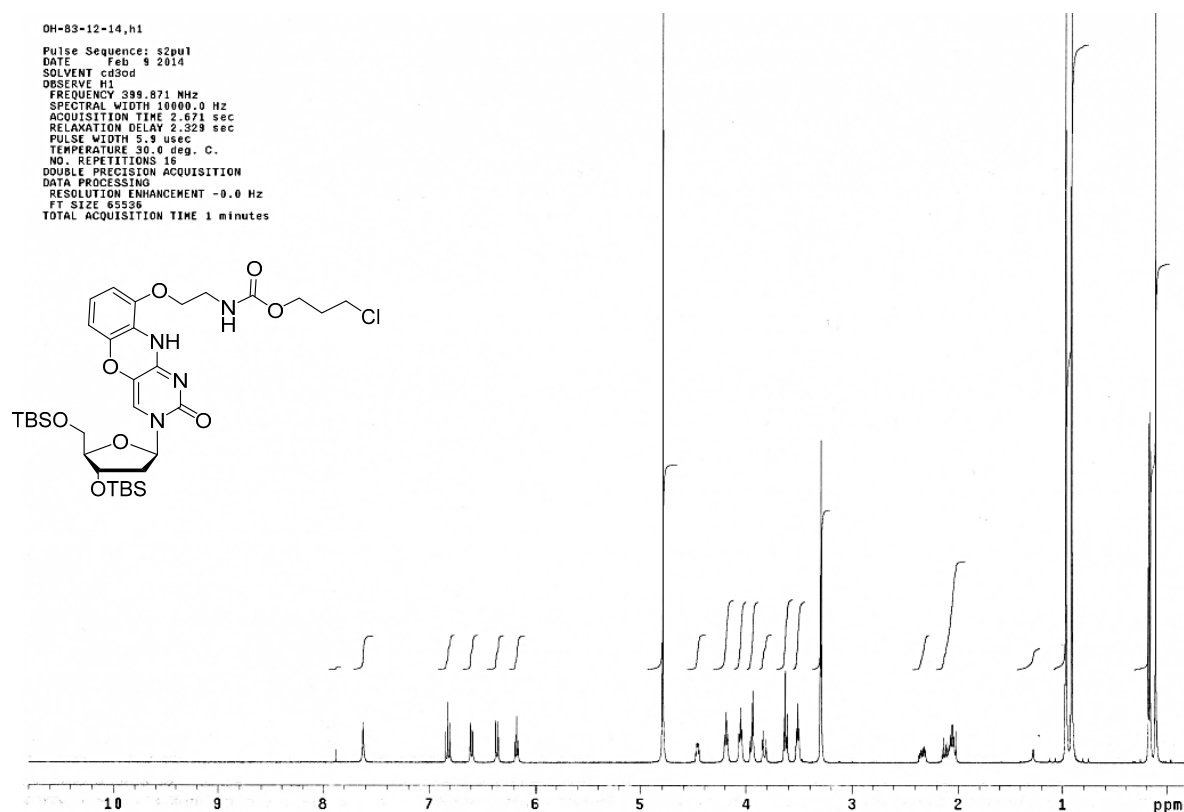
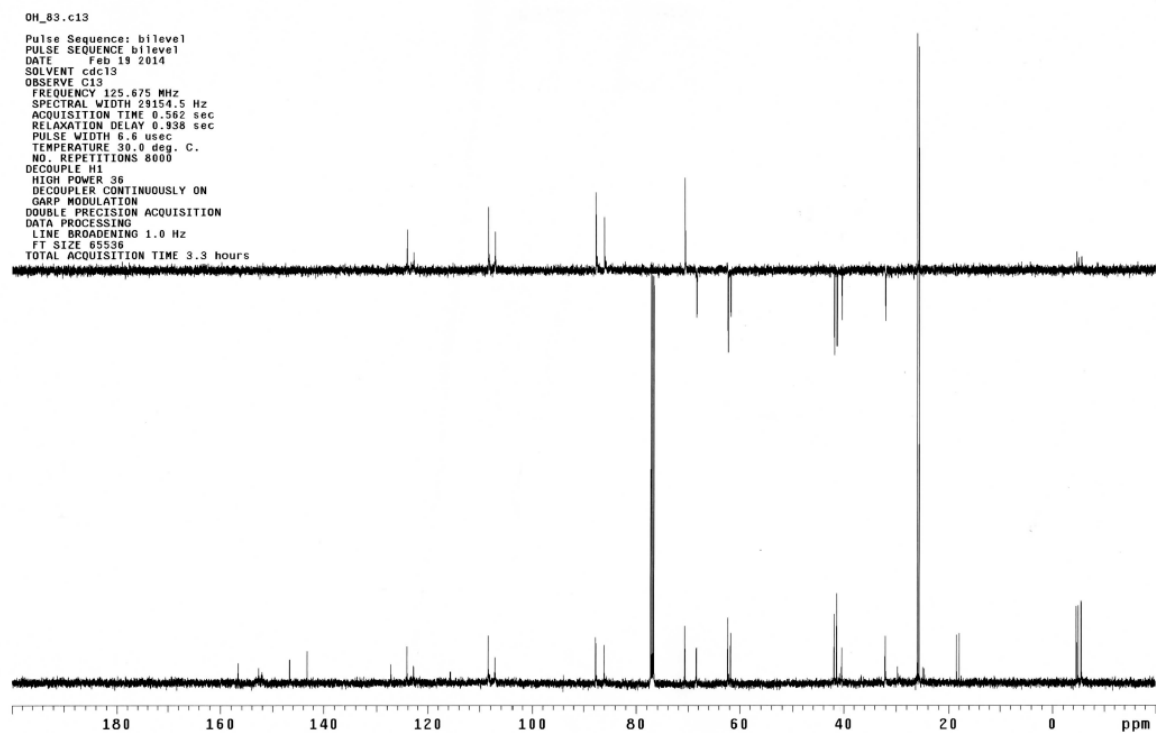
OH-77-16-16,h1  
Pulse Sequence: s2pul  
DATE Jan 31 2014  
SOLVENT cd3od  
OBSERVE H1  
FREQUENCY 399.871 MHz  
SPECTRAL WIDTH 10000.0 Hz  
ACQUISITION TIME 2.671 sec  
RELAXATION DELAY 2.359 sec  
PULSE WIDTH 5.9 usec  
TEMPERATURE 30.0 deg. C.  
NO. REPETITIONS 16  
DOUBLE PRECISION ACQUISITION  
DATA PROCESSING  
RESOLUTION ENHANCEMENT -0.0 Hz  
FT SIZE 65536  
TOTAL ACQUISITION TIME 1 minutes

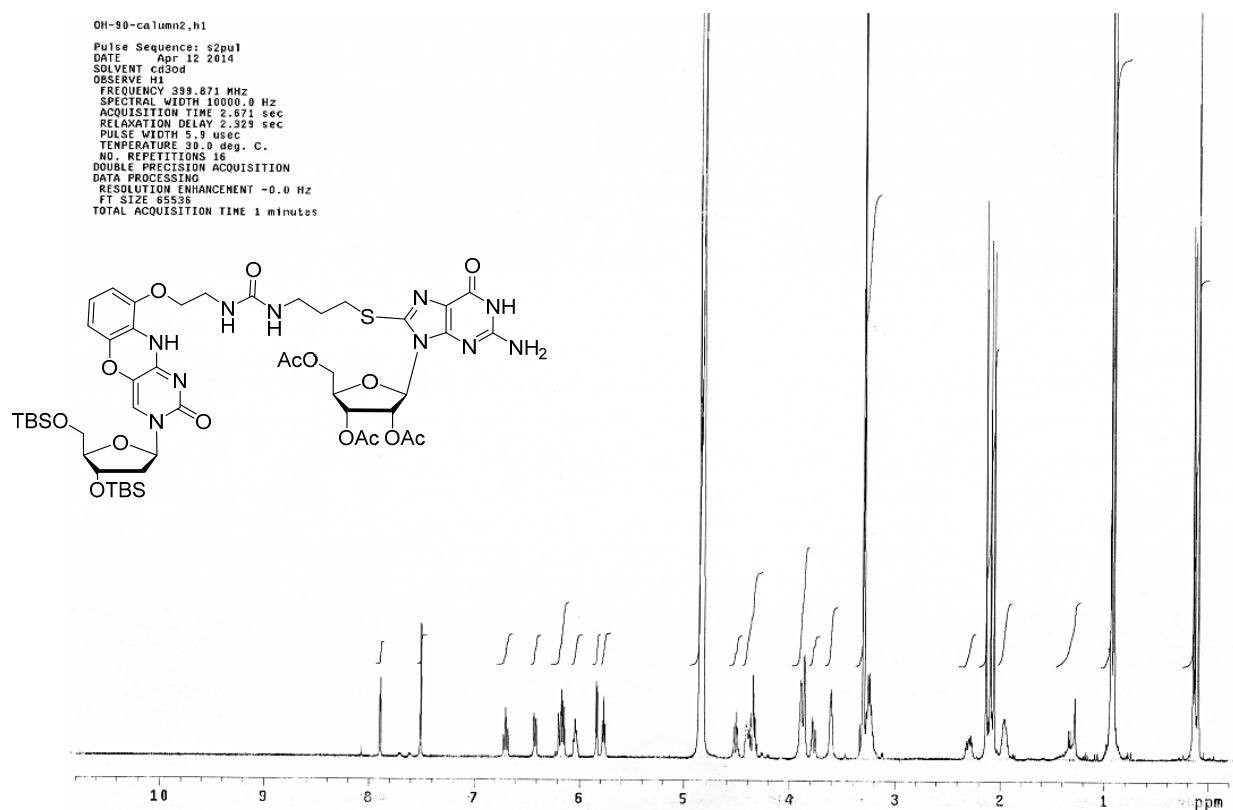
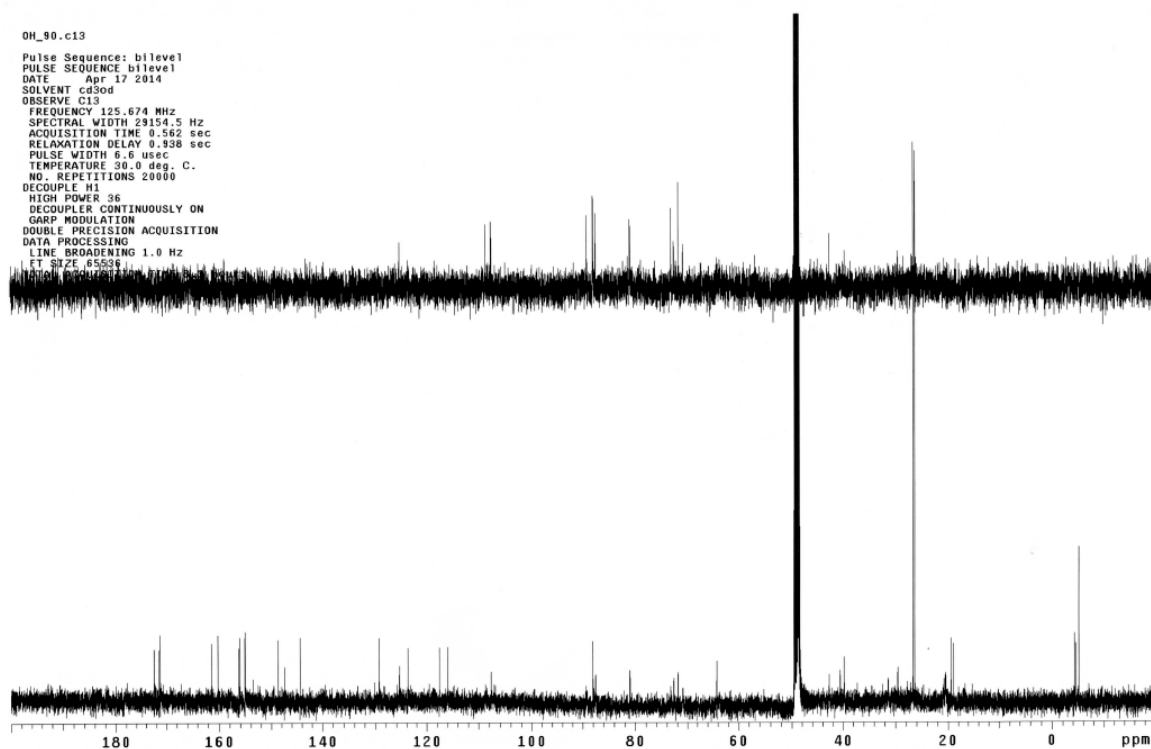
2b  $^{13}\text{C}$ -NMR

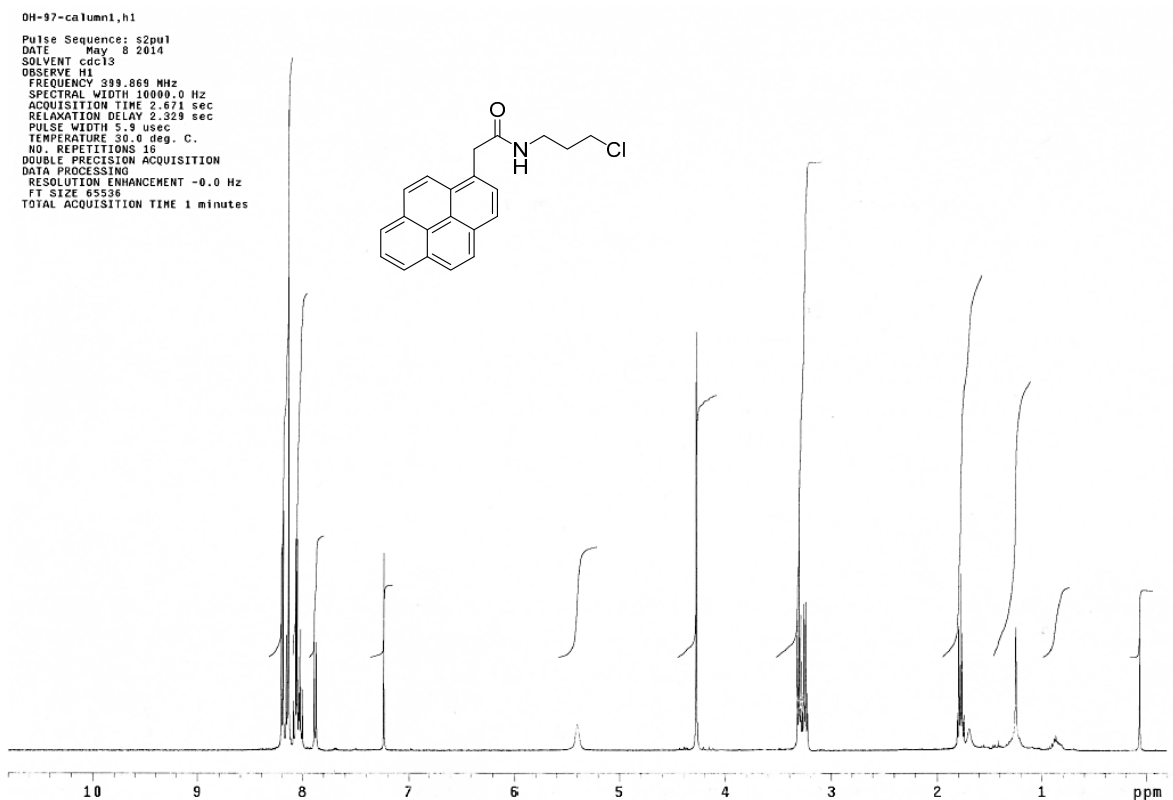
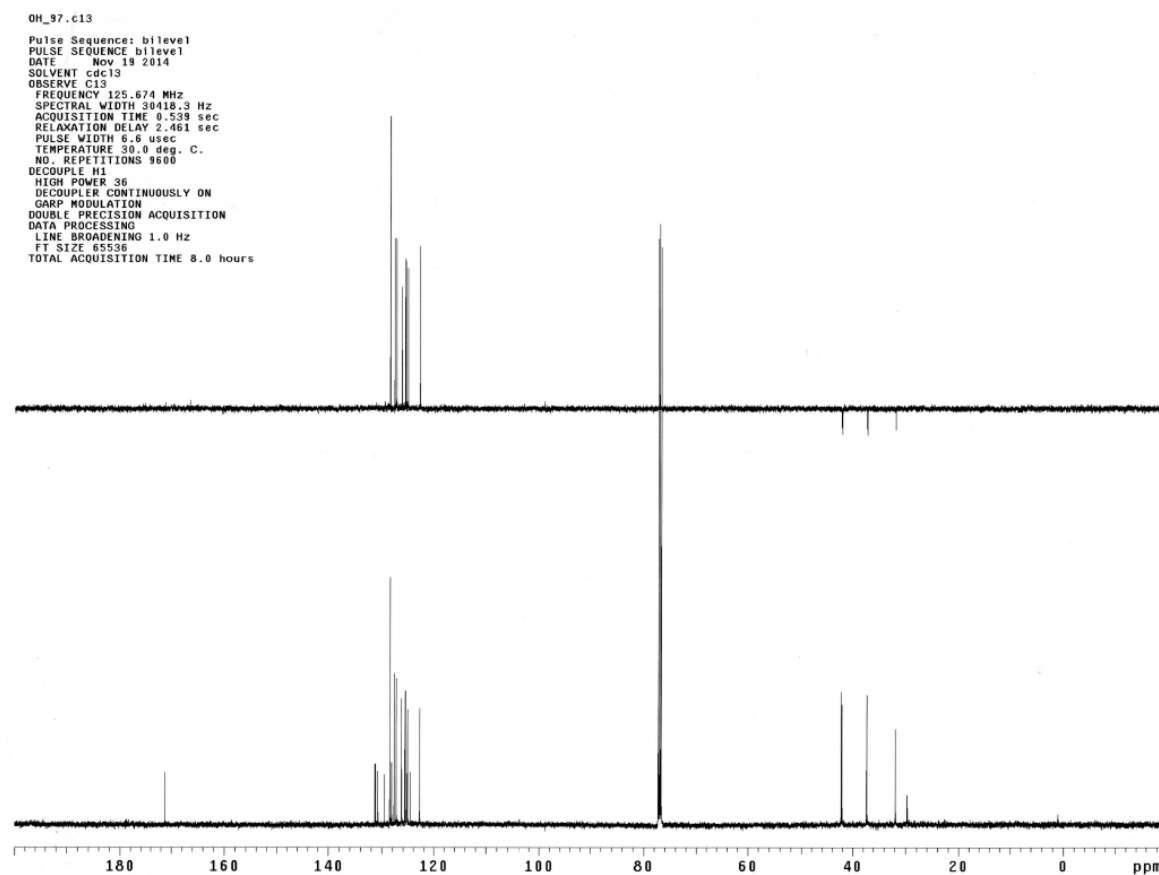
OH\_77.c13  
Pulse Sequence: bilevel1  
PULSE SEQUENCE bilevel1  
DATE Feb 4 2014  
SOLVENT cdc13  
OBSERVE C13  
FREQUENCY 125.676 MHz  
SPECTRAL WIDTH 29531.2 Hz  
ACQUISITION TIME 0.555 sec  
RELAXATION DELAY 0.945 sec  
PULSE WIDTH 8.6 usec  
TEMPERATURE 30.0 deg. C.  
NO. REPETITIONS 8000  
DECOUPLE H1  
HIGH POWER 36  
DECOUPLER CONTINUOUSLY ON  
GARP MODULATION  
DOUBLE PRECISION ACQUISITION  
DATA PROCESSING  
LINE BROADENING 1.0 Hz  
FT SIZE 65536  
TOTAL ACQUISITION TIME 3.3 hours

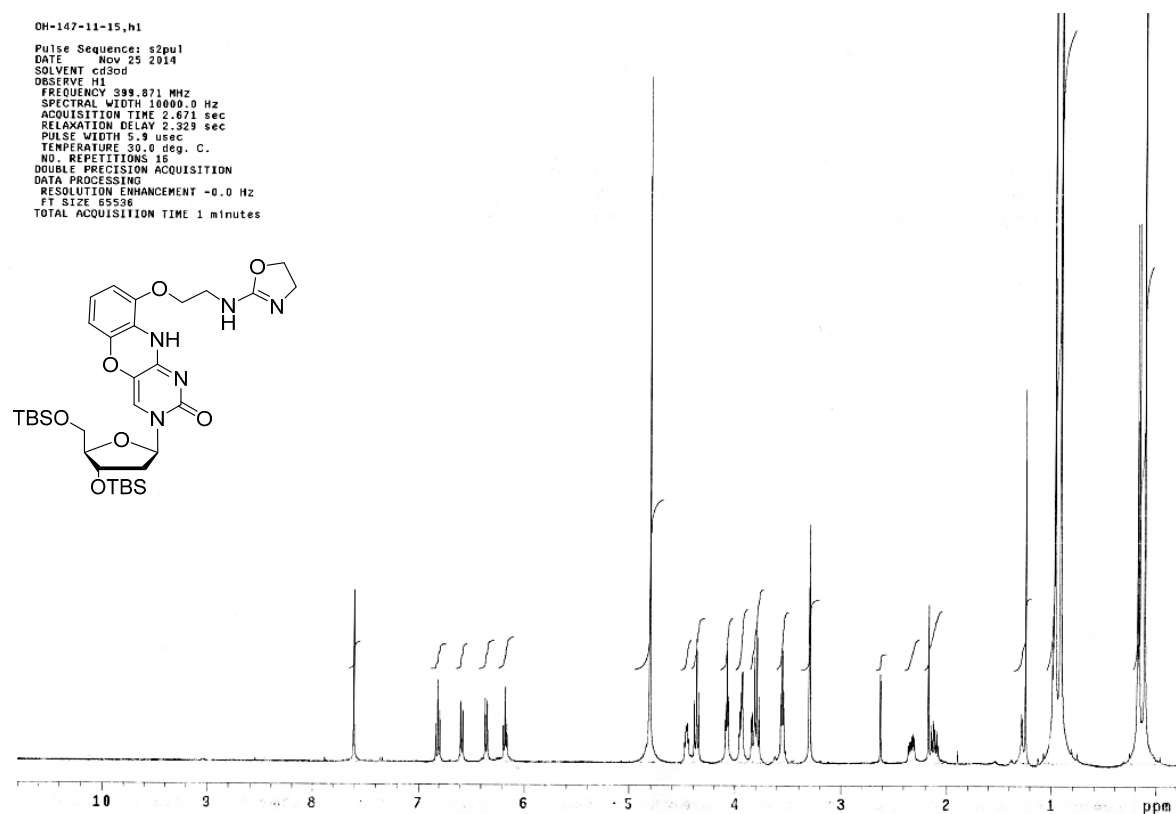
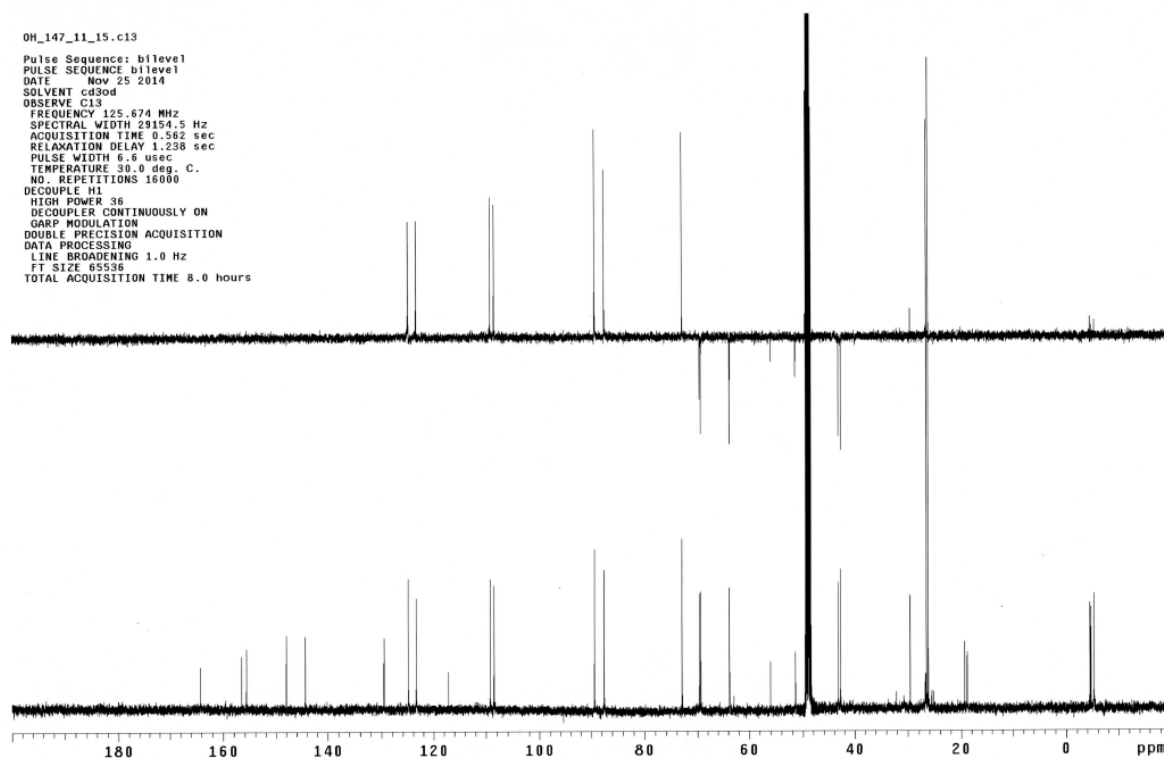


**2c**  $^1\text{H}$ -NMR**2c**  $^{13}\text{C}$ -NMR

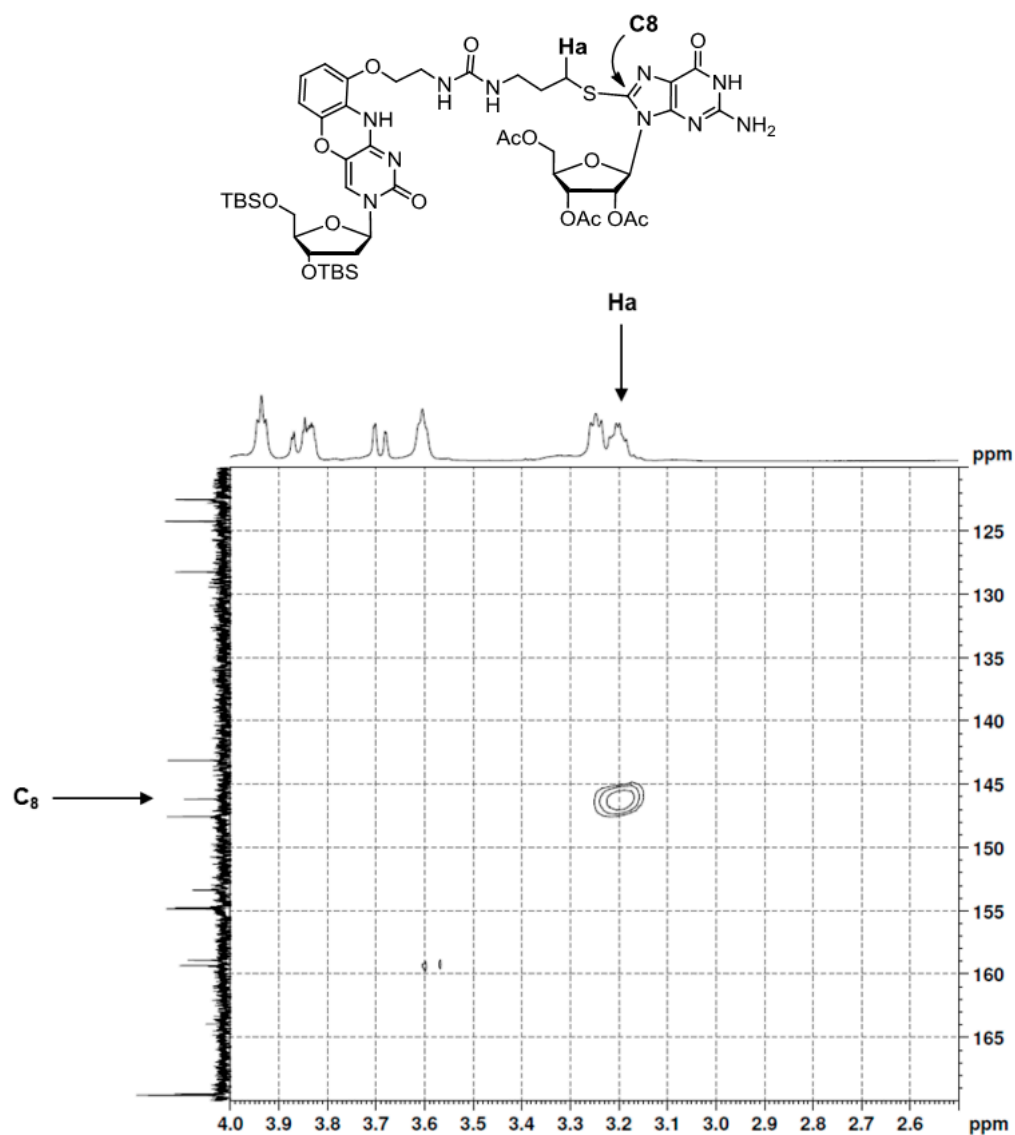
$^1\text{H}$ -NMR $^{13}\text{C}$ -NMR

7b <sup>1</sup>H-NMR7b <sup>13</sup>C-NMR

$^1\text{H}$ -NMR $^{13}\text{C}$ -NMR

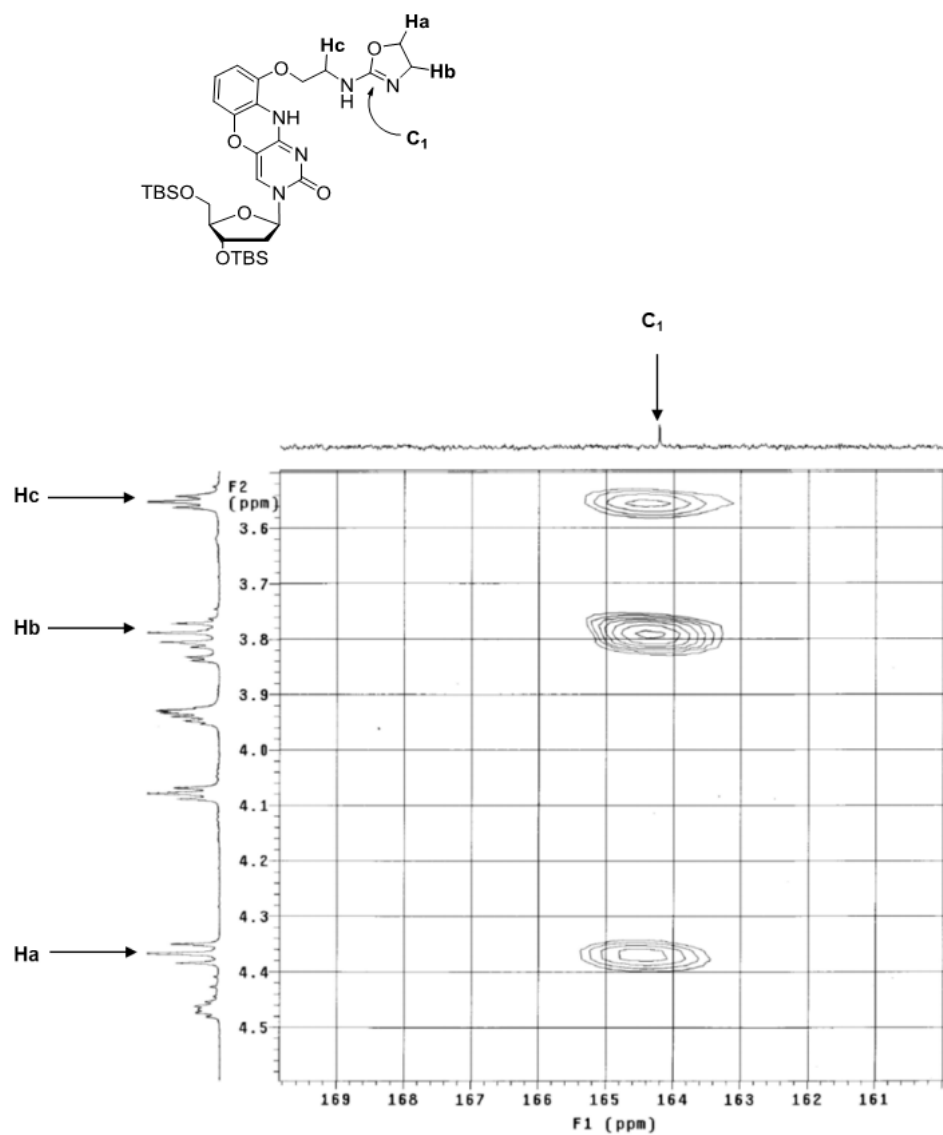
8  $^1\text{H}$ -NMR8  $^{13}\text{C}$ -NMR

## 7b 2D-HMBC





## 8 2D-HMBC



### **pK<sub>a</sub> Determination of 8-thioguanosine**

A quartz cell containing a solution of 8-thioguanosine (20  $\mu$ M) in 4 M NaOH (pH 12) was placed in a UV spectrometer and the spectrum was measured at 25 °C. A small portion of 2 M HCl was added to a quartz cell and pH was measured, and the UV spectrum was measured. This procedure was repeated. UV absorbance at 280 nm was plotted against pH and the pK<sub>a</sub> value was determined by curve-fitting method.

