A Sensitive Multispectroscopic Probe for Nucleic Acids

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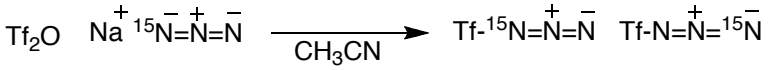
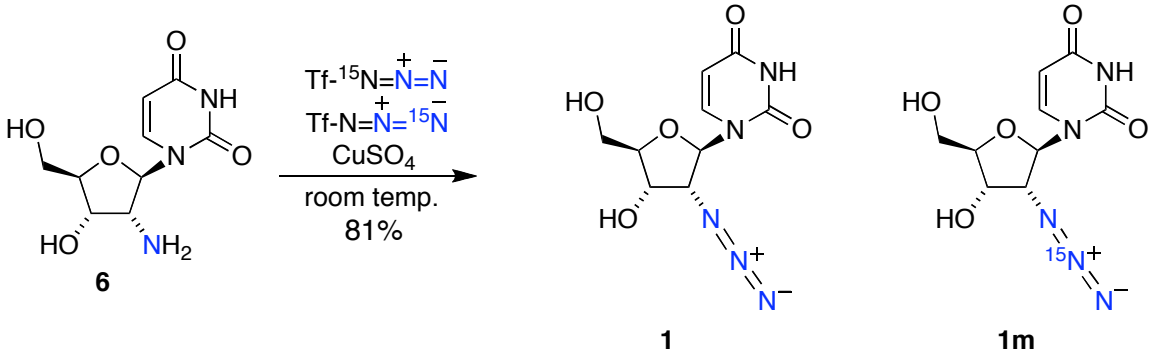
Supporting Information

1. **Synthetic Schemes** (Procedures are given in the paper.)

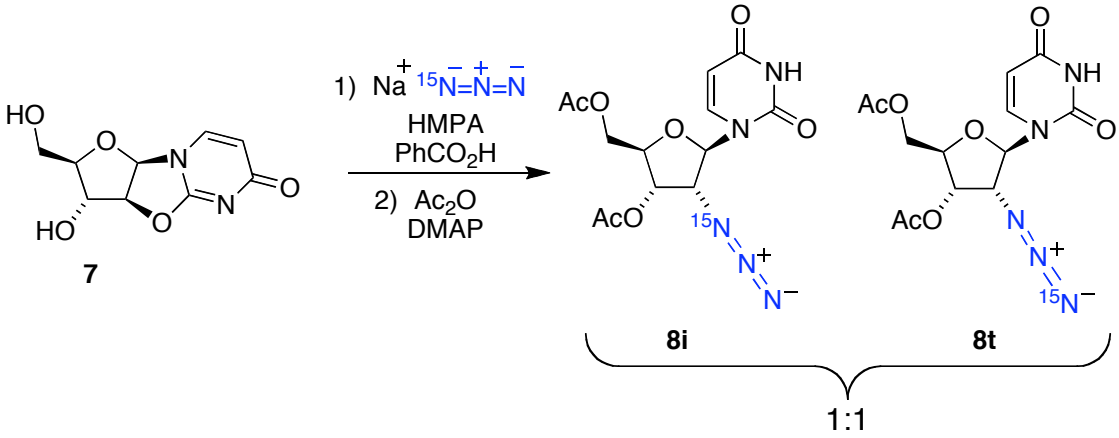
Internal and terminal labeled (1:1) trifluoromethanesulfonic azide (triflic azide).[#]



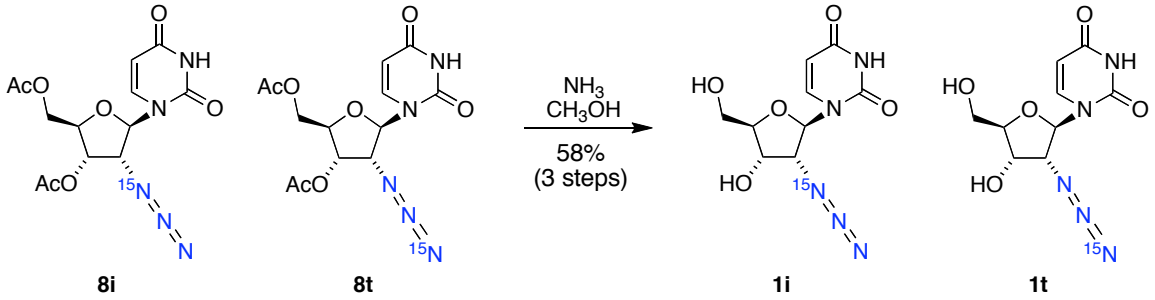
^{15}N middle labeled and unlabeled (1:1) 2′-Azido-2′-deoxyuridine (1m and 1).[1]



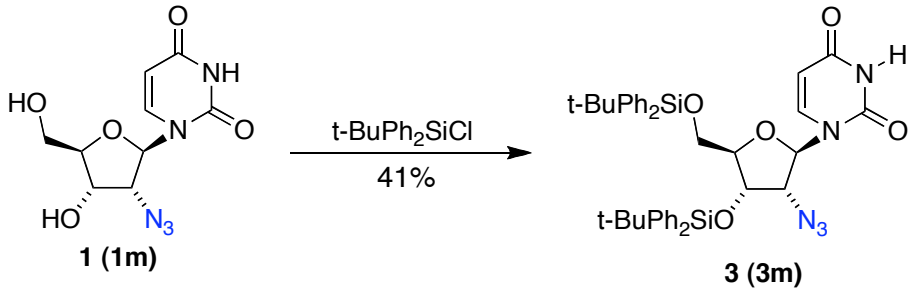
^{15}N internal and terminal labeled (1:1) 3′, 5′-Bis-*O*-(acetyl)-2′-Azido-2′-deoxyuridine (8i and 8t).[3]



^{15}N internal and terminal labeled (1:1) 2′-Azido-2′-deoxyuridine (1i and 1t).



3′,5′-Bis-O-(tert-butyldiphenylsilyl)-2′-azido-2′-deoxyuridine (3).
^{15}N middle labeled and unlabeled 3′,5′-Bis-O-(tert-butyldiphenylsilyl)-2′-azido-2′-deoxyuridine (3m and 3). (Same procedure as used to prepare **3**.)



2. Experimental IR Data

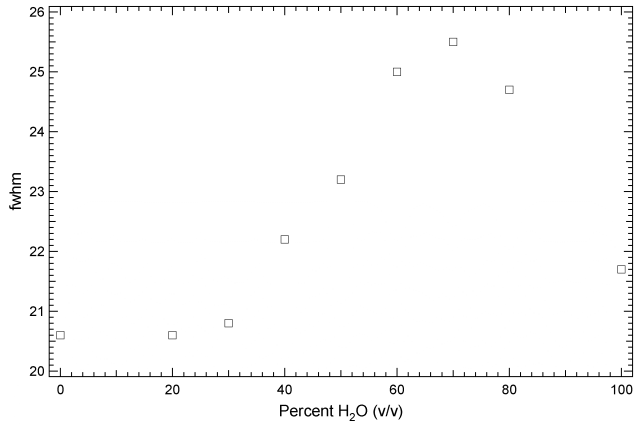


Figure S1. The dependence of the full-width half-maximum (fwhm) of the IR absorbance band of the azide stretch of **1** on the amount of water in the water-THF solvent mixtures (open squares).

3. DFT Calculations Figures and Table

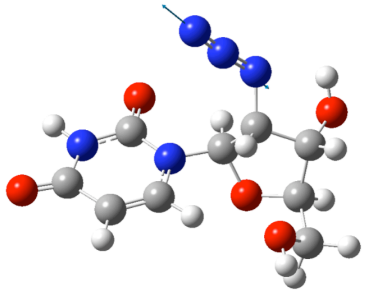


Figure S2. Eigenvector projection for the 2297.58 cm^{-1} vibrational mode of **1** as a monomer comprised primarily of an N_3 asymmetric stretch.

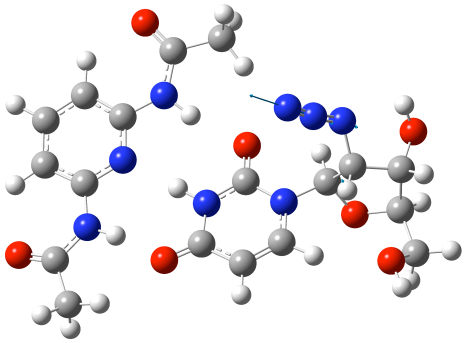
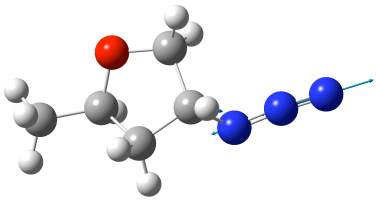


Figure S3. DFT calculation model for the 2297.23 cm^{-1} vibrational mode of **1** forming a dimer with compound **4** comprised primarily of an N_3 asymmetric stretch.



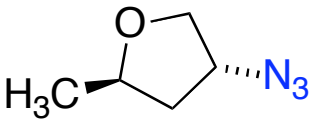


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Figure S4. DFT calculation model for the 2274.9 cm^{-1} vibrational mode of (*2R, 4R*) 2-methyl-4-azidotetrahydrofuran (**9**) comprised primarily of an N_3 asymmetric stretch.

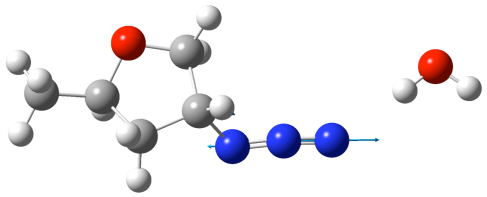

Figure S5. DFT calculation model for the 2283.39 cm^{-1} vibrational mode of (*2R, 4R*) 2-methyl-4-azidotetrahydrofuran (**9**) with one explicit water molecule comprised primarily of an N_3 asymmetric stretch.

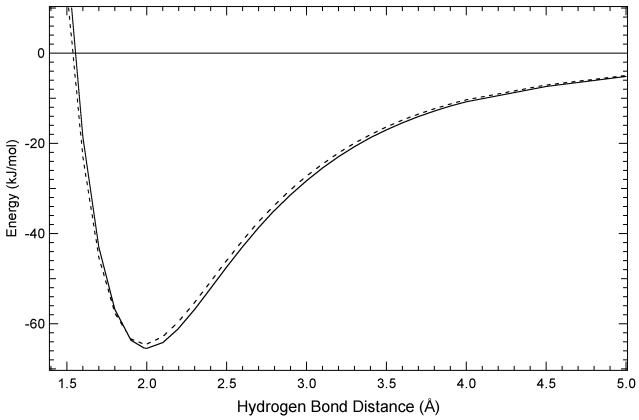

Figure S6. Potential energy surface (PES) corresponding to the energy of interaction between **N_3-dU** (**1**) and **5** (dashed line) and 2′-deoxyuridine and **5** (solid line) formed by modulating the distance between the imino N-H group of **N_3-dU** /2′-deoxyuridine and the pyridine nitrogen of **5** allowing all other coordinates to be optimized. The energy at a hydrogen bond distance of 10 Å was subtracted from all other calculated energies to determine the energy of interaction between the molecules.

Table S1. DFT calculation results of the change in ^{15}N NMR chemical shift of triply-labeled **N_3-dU** upon heterodimer formation with **4**

	Terminal N atom (ppm)	Middle N atom (ppm)	Internal N atom (ppm)
$\Delta\delta$	0.292	0.469	0.3923

4. Experimental Isotopic Shifts of 1m/1 and 1t/1i

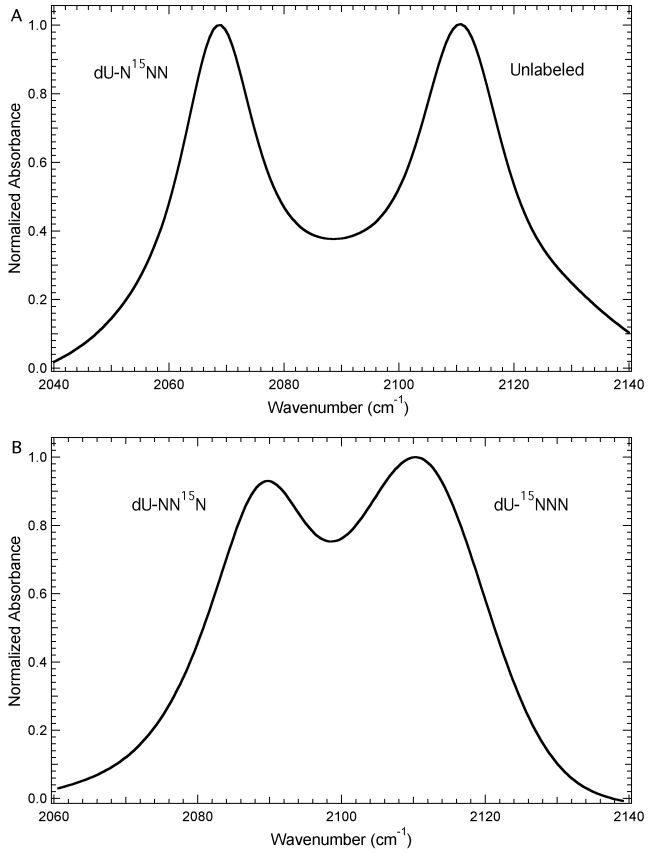

Figure S7. FTIR absorbance spectra of (A) **1m** and **1**, and (B) **1t** and **1i** in THF recorded at 293 K. The spectra were normalized to a maximum absorbance of unity. The concentrations were 50 mM.