J|A|C|S COMMUNICATIONS

Published on Web 07/04/2003

Use of Abasic Site Containing DNA Strands for Nucleobase Recognition in Water

Keitaro Yoshimoto, Seiichi Nishizawa, Masakazu Minagawa, and Norio Teramae

J. Am. Chem. Soc., ***125***, 8982-8983 (2003).

Abstract

Nucleobase recognition in water is successfully achieved by the use of an abasic site (AP site) as the molecular recognition field. We intentionally construct the AP site in DNA duplex so as to orient the AP site toward a target nucleobase, and examine the complexation of 2-amino-7-methylnaphthyridine (AMND) with nucleobases at the AP site. AMND is found to selectively bind to cytosine (C) base with a 1:1 binding constant of > 10^6 M^{-1}, accompanied by remarkable quenching of its fluorescence. In addition to hydrogen-bonding, stacking interaction with nucleobases flanking the AP site seems responsible for the binding properties of AMND at the AP site. Possible use of AMND is also presented for selective and visible detection of a single-base alternation related to the cytosine base.

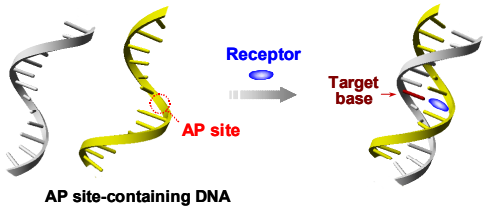

Figure 1. Schematic illustration of nucleobase recognition in water using an abasic site (AP site)-containing DNA strand

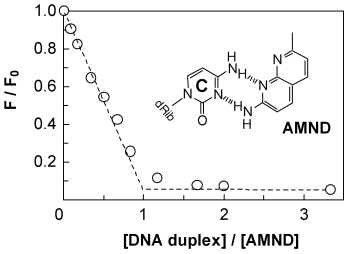

Figure 2. Fluorescence intensity of AMND at 405 nm in a titration with the AP site-containing duplex (5'-TCCAGXGCAAC-3' / 5'-GTTGCCCT GGA-3', X = dSpacer) in water. F and F_0 denote the fluorescence of AMND with and without DNA duplexes, respectively. [AMND]: 30 μM, [NaCl]: 100 mM, [Sodium cacodylate buffer]: 10 mM, [EDTA]: 1 mM, at pH 7.0, excitation wavelength: 355 nm.

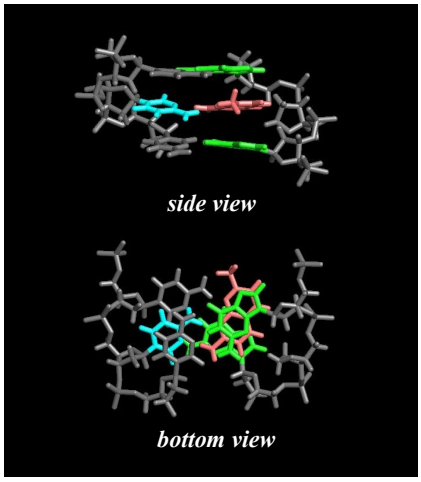

Figure 3. Energy-minimized structure, obtained using MacroModel (version 7.2), for the complex between AMND and the AP site-containing duplex with cytosine base opposite the AP site (5'-TCCAGXGCAAC-3' / 5'-GTTGCCCTGGA-3', X = dSpacer). AMND and the cytosine base opposite an AP site are colored red and blue, respectively. The guanine bases flanking the AP site are colored green.

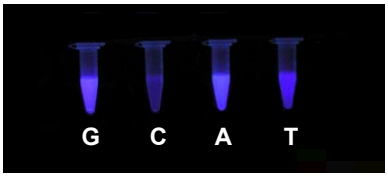

Figure 4. Changes in fluorescence of AMND in the presence of AP site-containing duplexes (5'-TCCAG**X**GCAAC-3' / 5'-GTTGC**Y**CTGGA -3', X = dSpacer, left to right: Y = G, C, A, and T) in water. The samples are excited with a UV lamp at 302 nm. [DNA duplex]: 60 μM, [AMND]: 30μM, [NaCl]: 100 mM, [Sodium cacodylate buffer]: 10 mM, [EDTA]: 1 mM, at pH 7.0.