Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry


# Design of environmentally sensitive fluorescent 8-aza-7-deaza-2'-deoxyadenosine derivative with dual fluorescence; specific detection of thymine

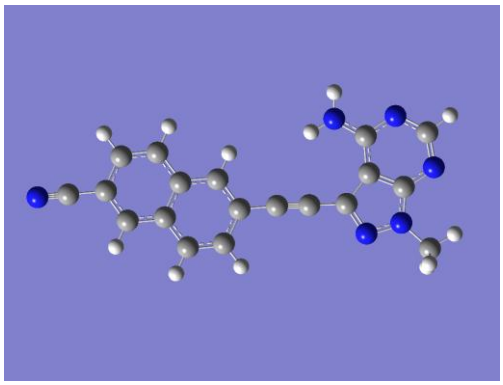
Azusa Suzuki,[†] Nobukatsu Nemoto,[†] Isao Saito[‡] and Yoshio Saito*[†]

[†]*Department of Chemical Biology and Applied Chemistry, College of Engineering, Nihon University, Koriyama, Fukushima 963-8642, Japan,* [‡]*NEWCAT Institute, College of Engineering, Nihon University, Koriyama, Fukushima 963-8642, Japan*

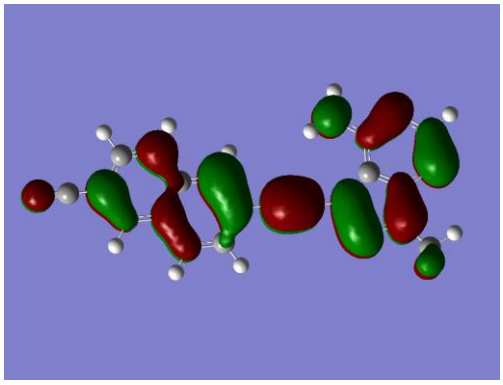
*Email Address:* saitoy@chem.ce.nihon-u.ac.jp

## List of Contents

$N^9$-methylated **$^{cna}$A**



$N^9$-methylated **$^{cna}$A** (HOMO)



$N^9$-methylated **$^{cna}$A** (LUMO)

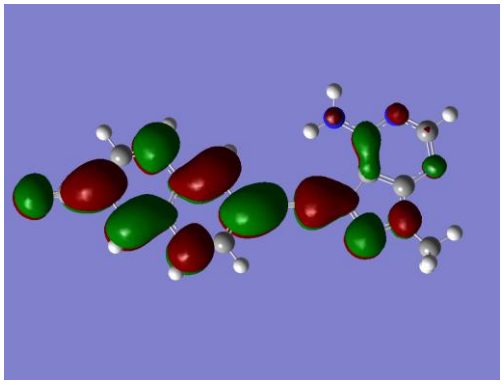


**Figure S1.** HOMO and LUMO of $N^9$-methylated **$^{cna}$A** calculated at the DFT(B3LYP)/6-31G* level.

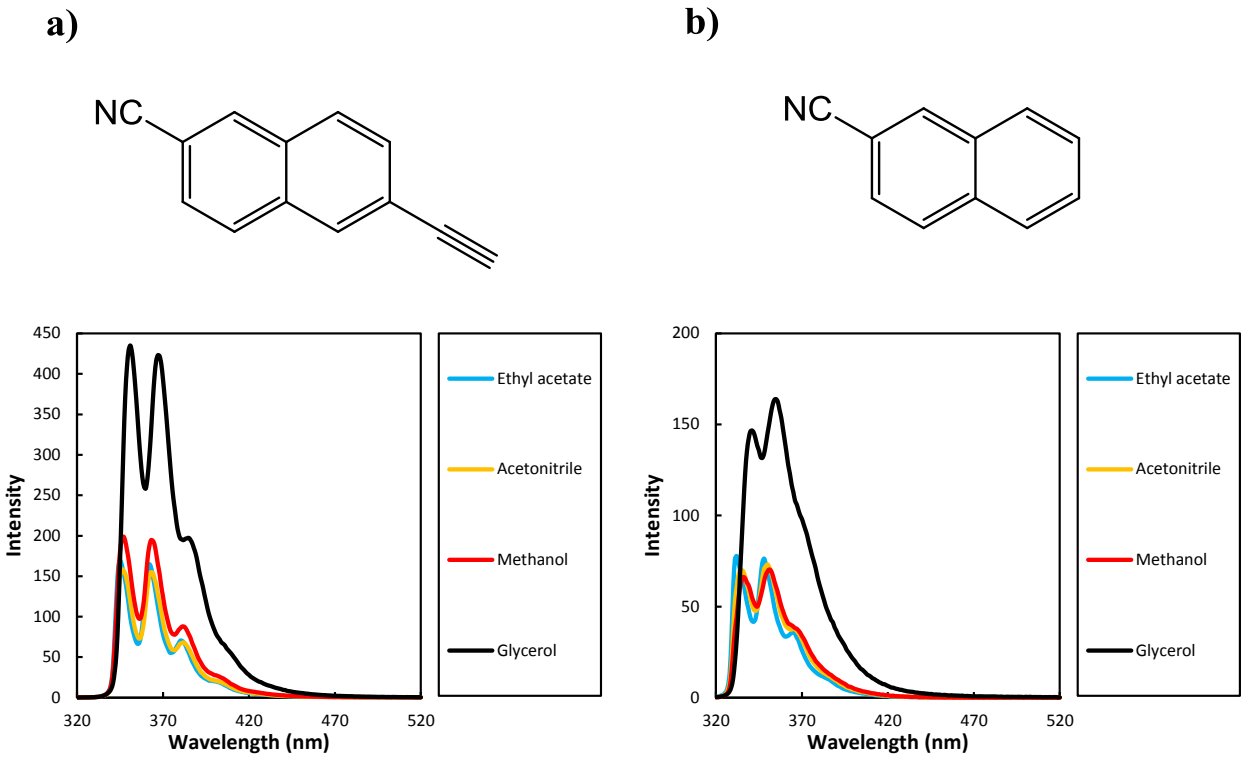
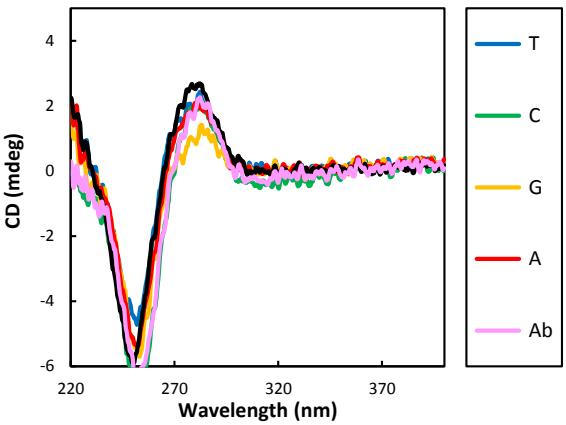


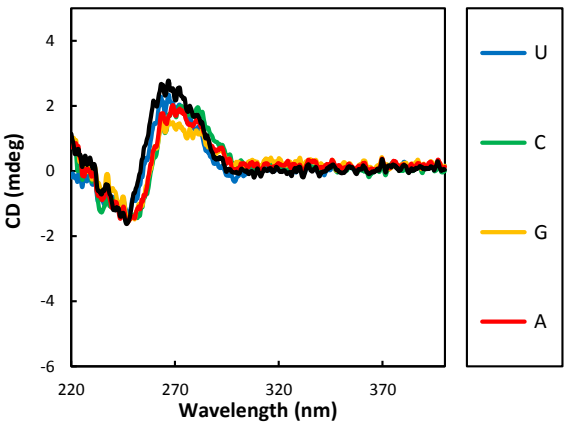

**Figure S2.** Fluorescence spectra of (a) 6-ethynyl-2-naphthonitrile (100 μM) and (b) 2-naphthonitrile (100 μM) in various solvents.

**a)**



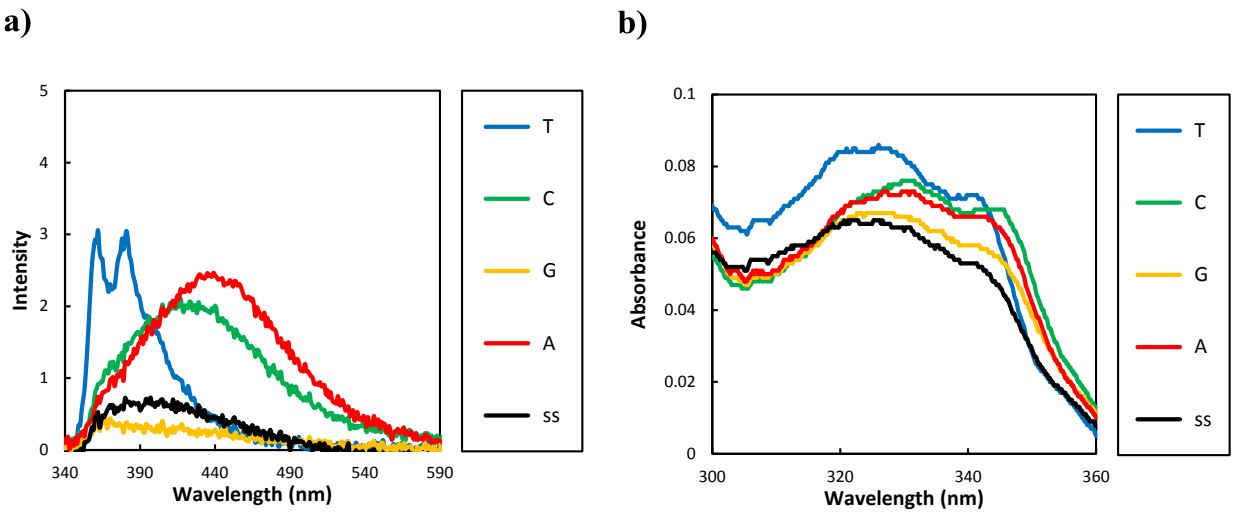

DNA 1: 5'-d(CGCAAT **X** TAACGC)-3' (**X** = $^{cna}$**A** or A)
DNA 2: 3'-d(GCGTTA **N** ATTGCG)-5'
(**N** = T, C, G, A, Abasic site)

**b)**




DNA 1: 5'-d(CGCAAT **X** TAACGC)-3' (**X** = $^{cna}$**A** or A)
RNA 1: 3'-r(GCGUUA **N** AUUGCG)-5'
(**N** = U, C, G, A)

**Figure S3.** CD spetra of DNA 1 (**X** = $^{cna}$**A**) hybridized (a) with DNA 2 (**N** = T, C, G, A, Ab) and (b) with RNA 1 (N = U, C, G, A). black line: (a) DNA 1 (**X** = A) / DNA 2 (**N** = T), (b) DNA 1 (**X** = A) / RNA 1 (**N** = U). "Ab" denotes abasic site (2.5 uM ODNs, 50 mM sodium phoshate, 0.1 M sodium chloride, pH 7.0, rt).




DNA 3: 5'-CGCAAT **X** AAACGC-3' (**X** = $^{cna}$**A** or A)
DNA 4: 3'-GCGTTA **N** TTTGCG-5' (**N** = T, C, G, A)

**Figure S4.** (a) Fluorescence and (b) UV absorption spectra of DNA 3 (**X** = $^{cna}$**A**) hybridized with DNA 4 (**N** = T, C, G, A). "Ab" denotes abasic site and "ss" denotes a single-strand DNA 3 (2.5 μM duplex, 0.1 M sodium chloride, 50 mM sodium phosphate buffer, pH 7.0, rt).

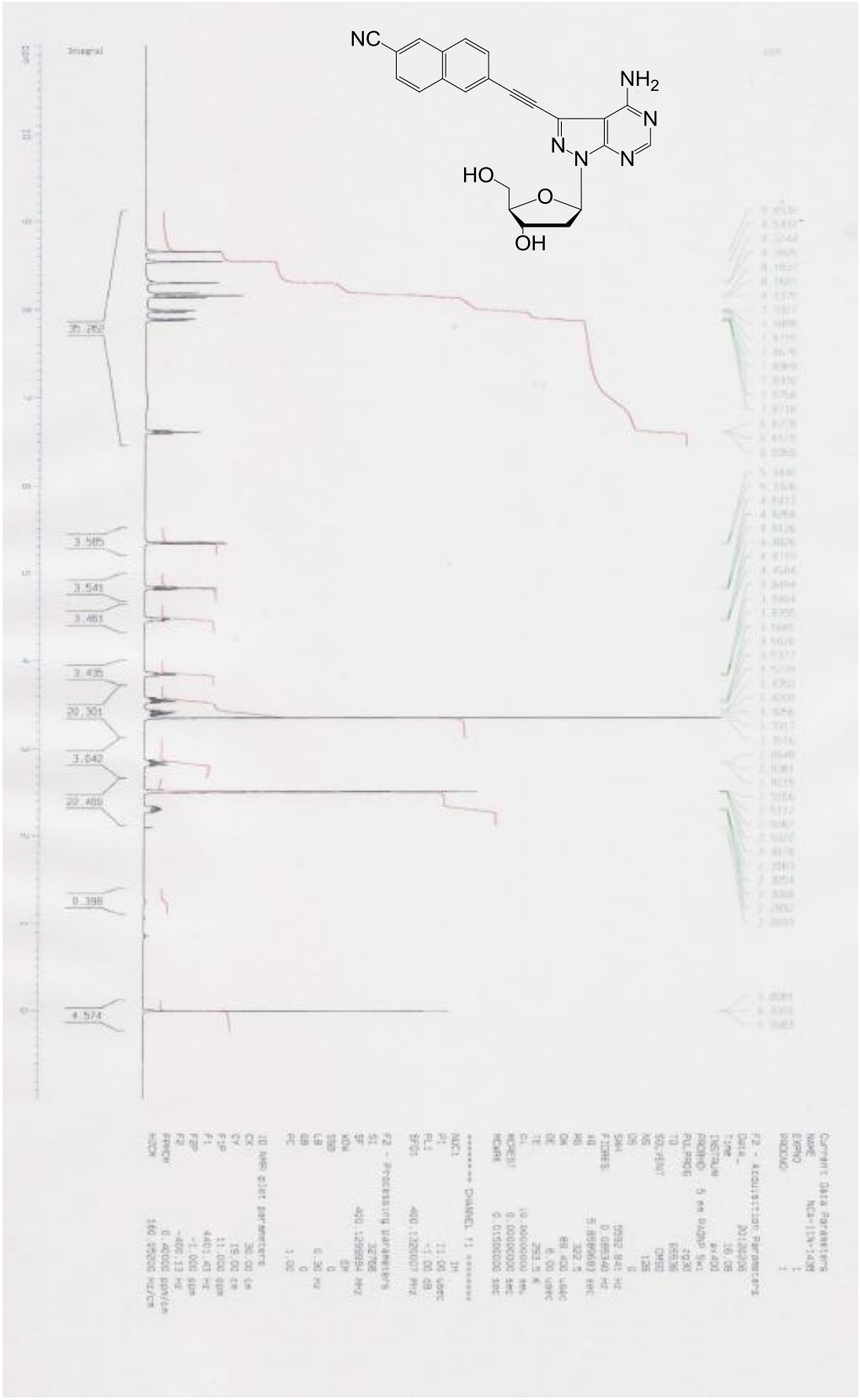



**Figure S5.** $^{1}$H-NMR spectra of $^{cna}$**A** (**1**)

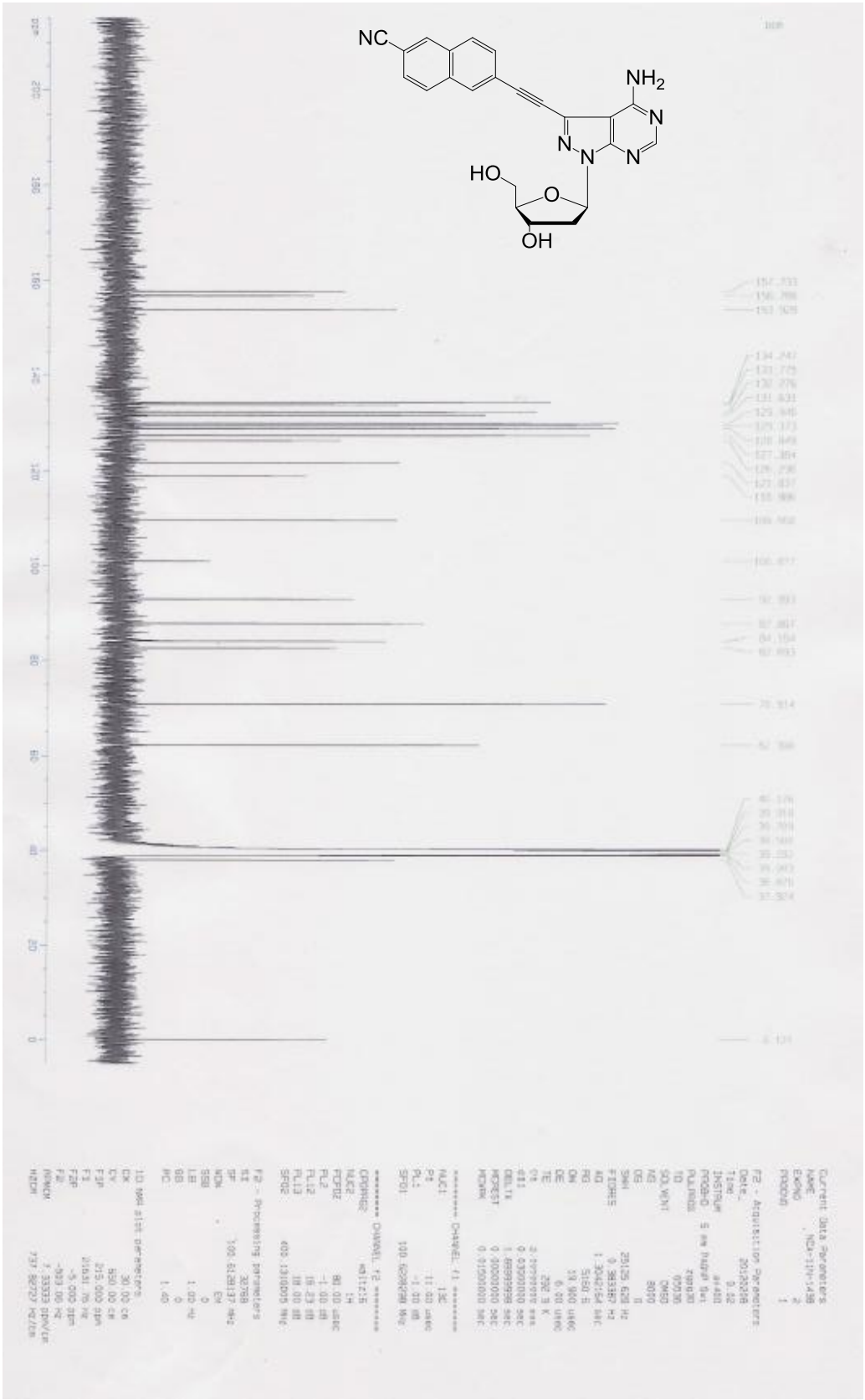



**Figure S6.** $^{13}$C-NMR spectra of $^{cna}$**A** (**1**)

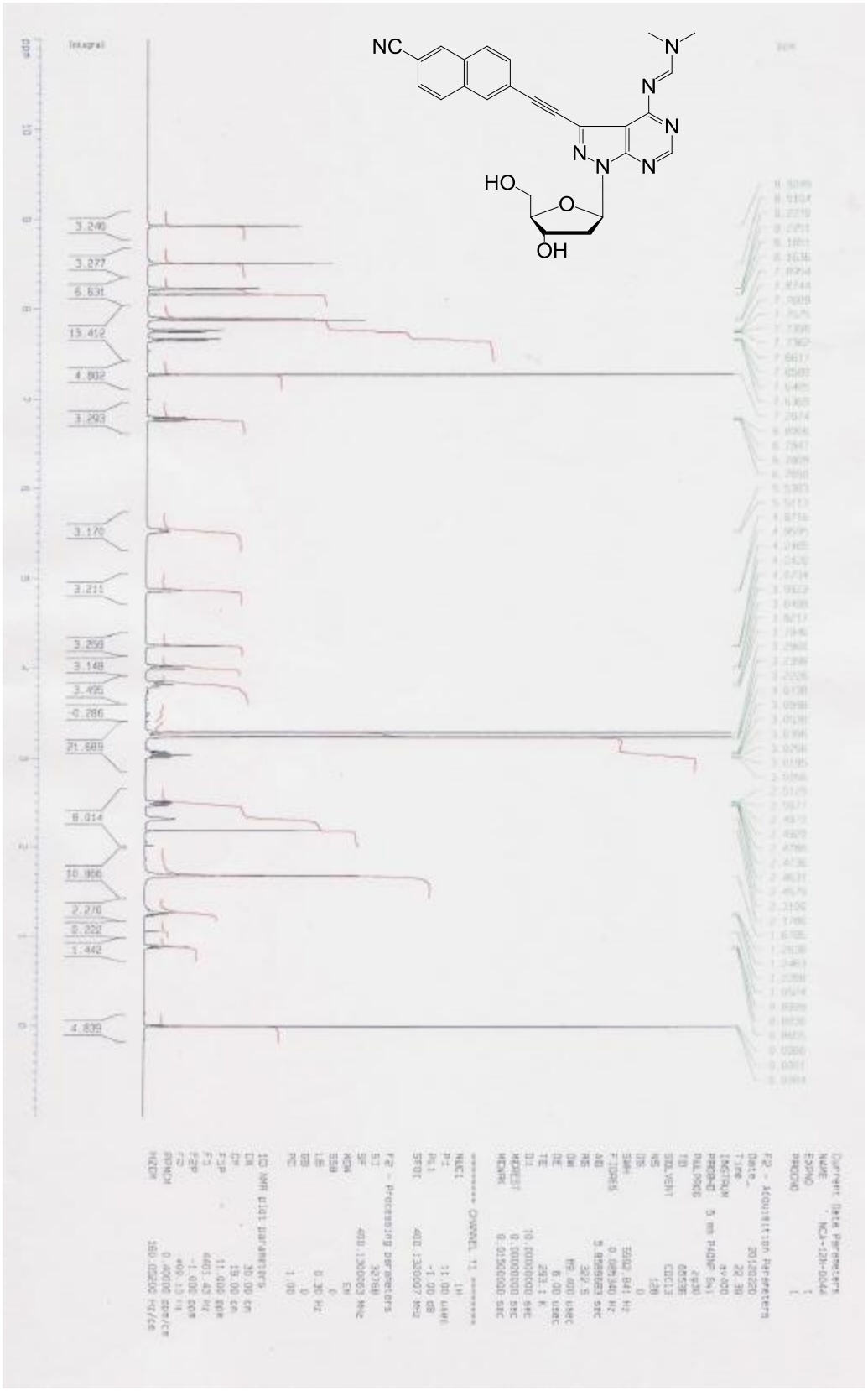



**Figure S7.** $^{1}$H-NMR spectra of compound **3**

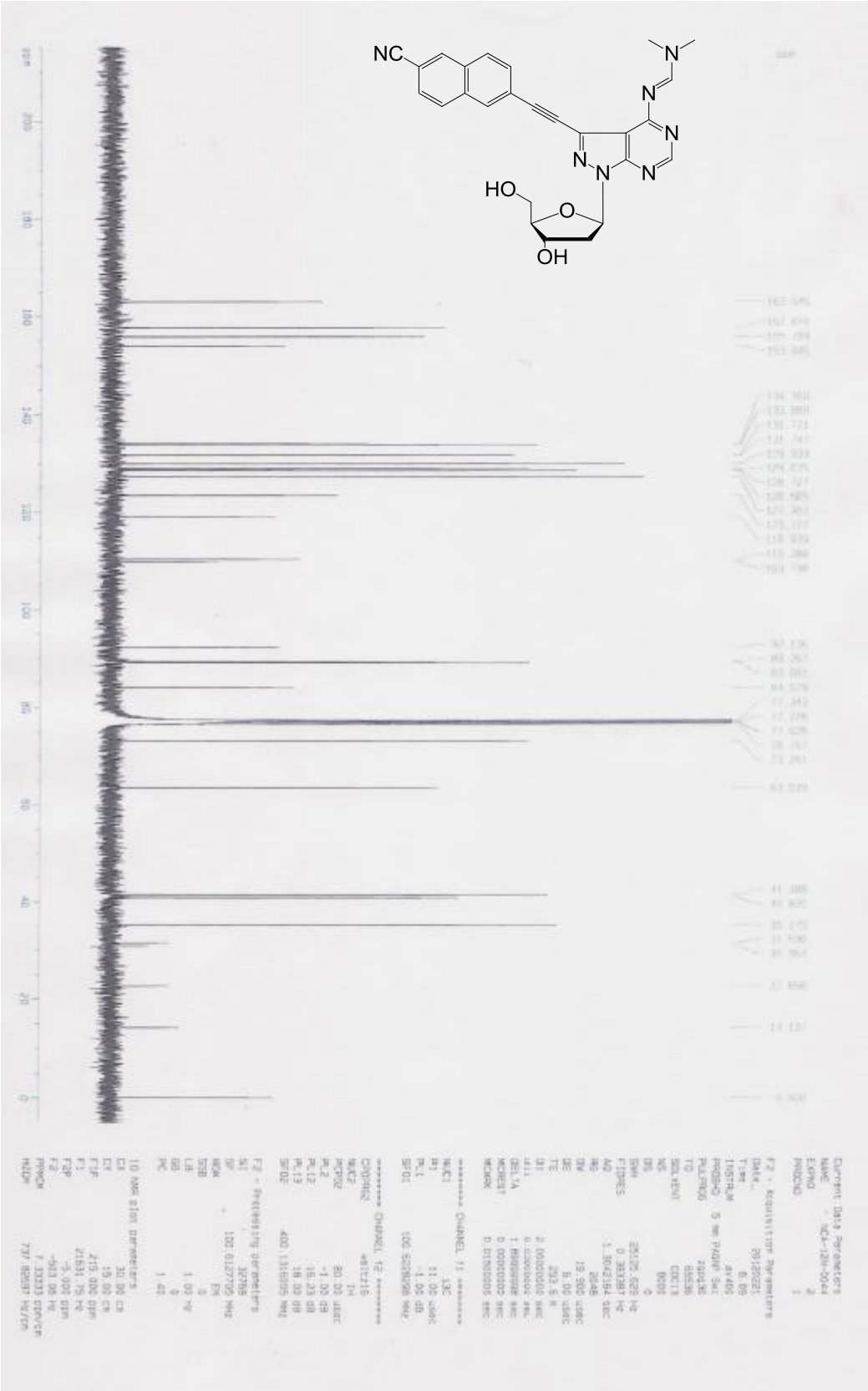



**Figure S8.** $^{13}$C-NMR spectra of compound **3**

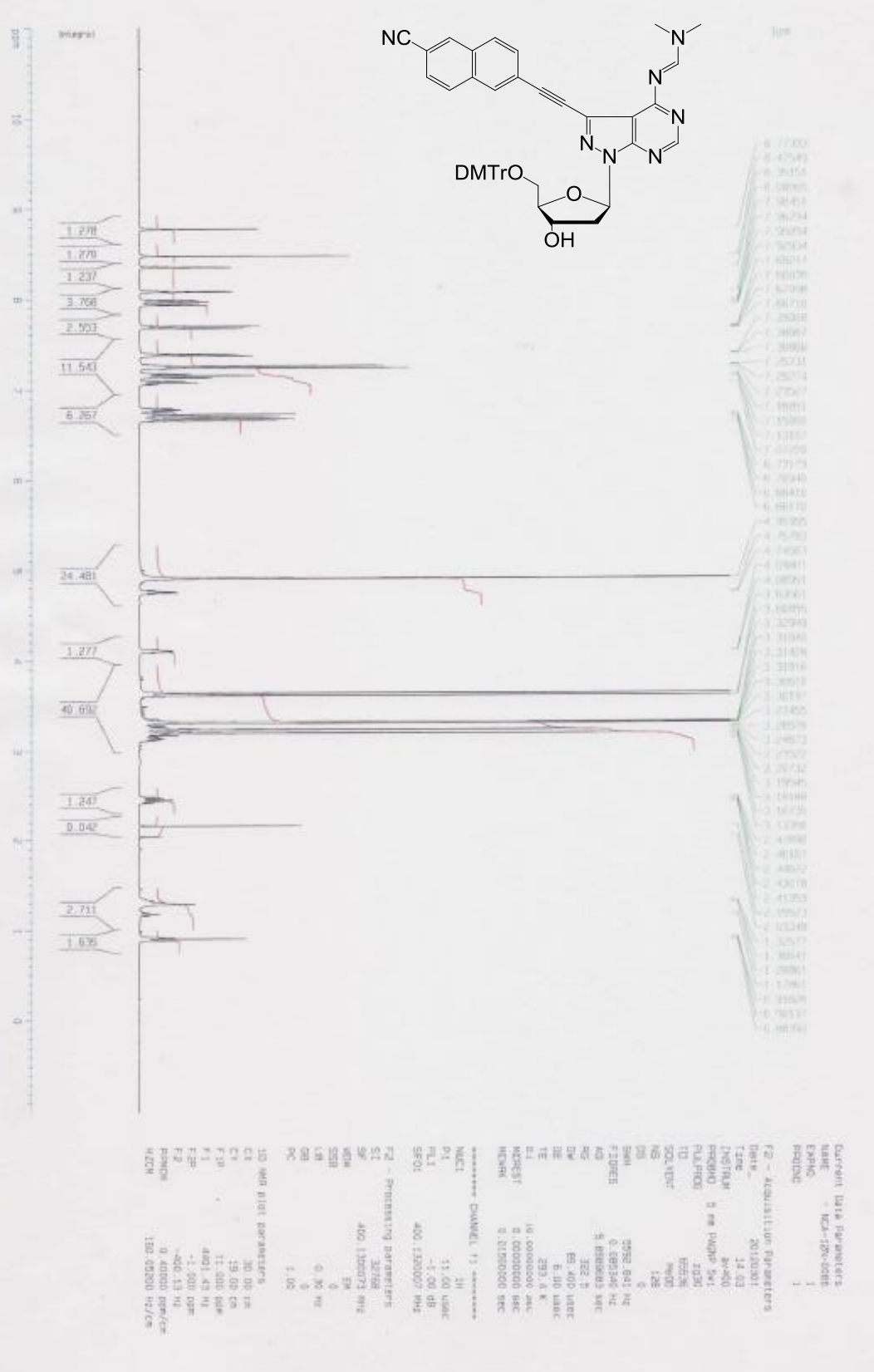



**Figure S9.** $^{1}$H-NMR spectra of compound **4**

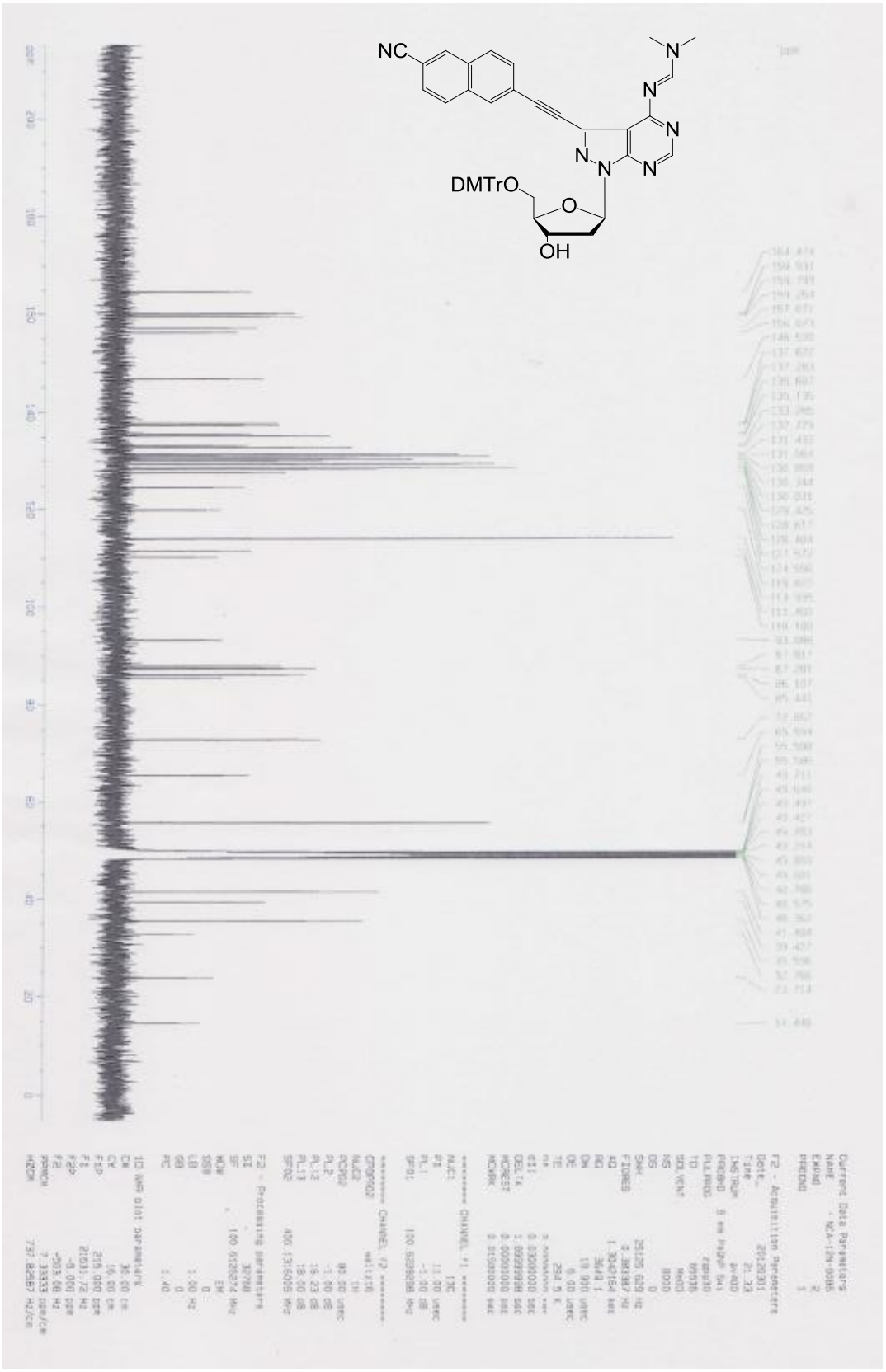



**Figure S10.** $^{13}$C-NMR spectra of compound **4**