NMR Solution Structure of a DNA-Actinomycin D Complex Containing a Non-Hydrogen Bonding Pair in the Binding Site

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Supporting Information Table 1. Proton chemical shift assignments (ppm) for the G-T:ActD complex at 30°C[a].

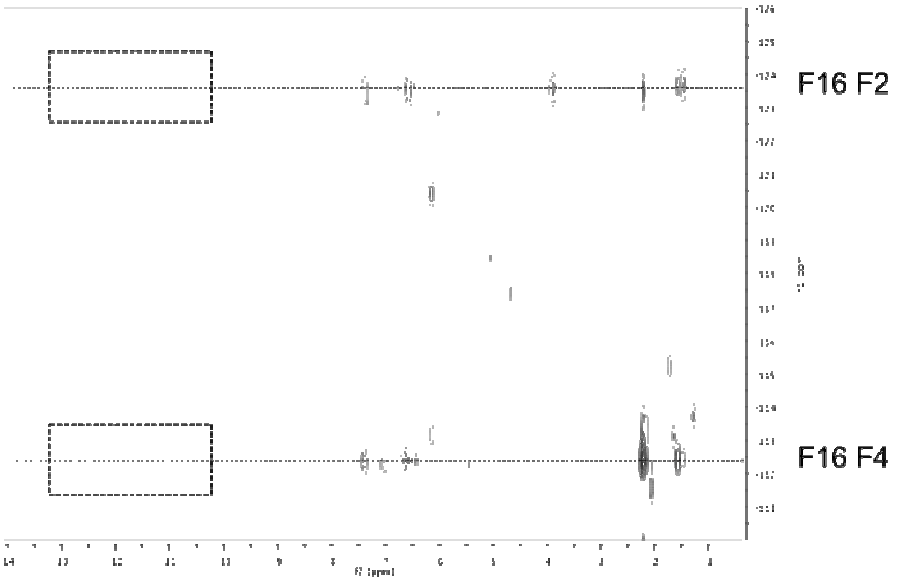
Nucleotide	H6/H8	H5	Methyl	H1'	H2'	H2''	H3'	H4'	H2	NH[b]
C1	7.92	6.13	na[c]	6.11	2.22	2.65	4.83	4.27	na	na
C2	7.75	5.92	na	5.48	2.27	2.51	5.01	4.25	na	na
A3	8.43	na	na	6.01	2.96	3.06	4.6	4.34	7.43	na
A4	8.11	na	na	5.93	2.42	2.45	5.16	4.39	7.49	na
G5	7.72	na	na	5.47	2.27	2.51	4.79	4.33	na	12.23
C6	7.73	5.93	na	6.28	2.5	2.69	4.79	4.33	na	na
T7	7.61	na	1.9	6.14	2.65	2.99	4.24	4.01	na	13.95
T8	7.4	na	1.91	5.97	2.38	2.65	4.99	4.18	na	14.22
C9	7.32	5.95	na	6.24	2.4	2.66	4.32	4.01	na	na
C10	7.81	6	na	5.97	2.4	2.64	4.99	4.18	na	na
G11	7.47	na	na	6.26	2.51	2.66	4.98	4.03	na	12.8
G12	7.71	na	na	5.92	2.22	2.51	3.99	4.31	na	12.02
A13	8.33	na	na	6.09	2.86	3.06	4.32	4.18	7.6	na
A14	8.06	na	na	5.93	2.87	3.05	4.32	4.18	7.51	na
G15	7.58	na	na	5.56	2.6	2.77	4.96	4.91	na	12.31
T16	7.75	na	1.95	6.09	2.23	2.41	4.74	4.02	na	13.86
T17	7.65	na	1.96	6.23	2.39	2.66	4.34	4.22	na	13.83
T18	7.5	na	1.96	5.79	2.07	2.39	4.94	4.2	na	14.14
G19	7.98	na	na	5.83	2.35	2.86	4.05	3.83	na	13.01
G20	7.94	na	na	6.26	2.51	2.67	4.25	4.01	na	11.89

[a]Chemical shifts are referenced to residual HOD resonance.
[b]Chemical shifts for imino protons are reported for the duplex at 10°C.
[c]Not applicable.

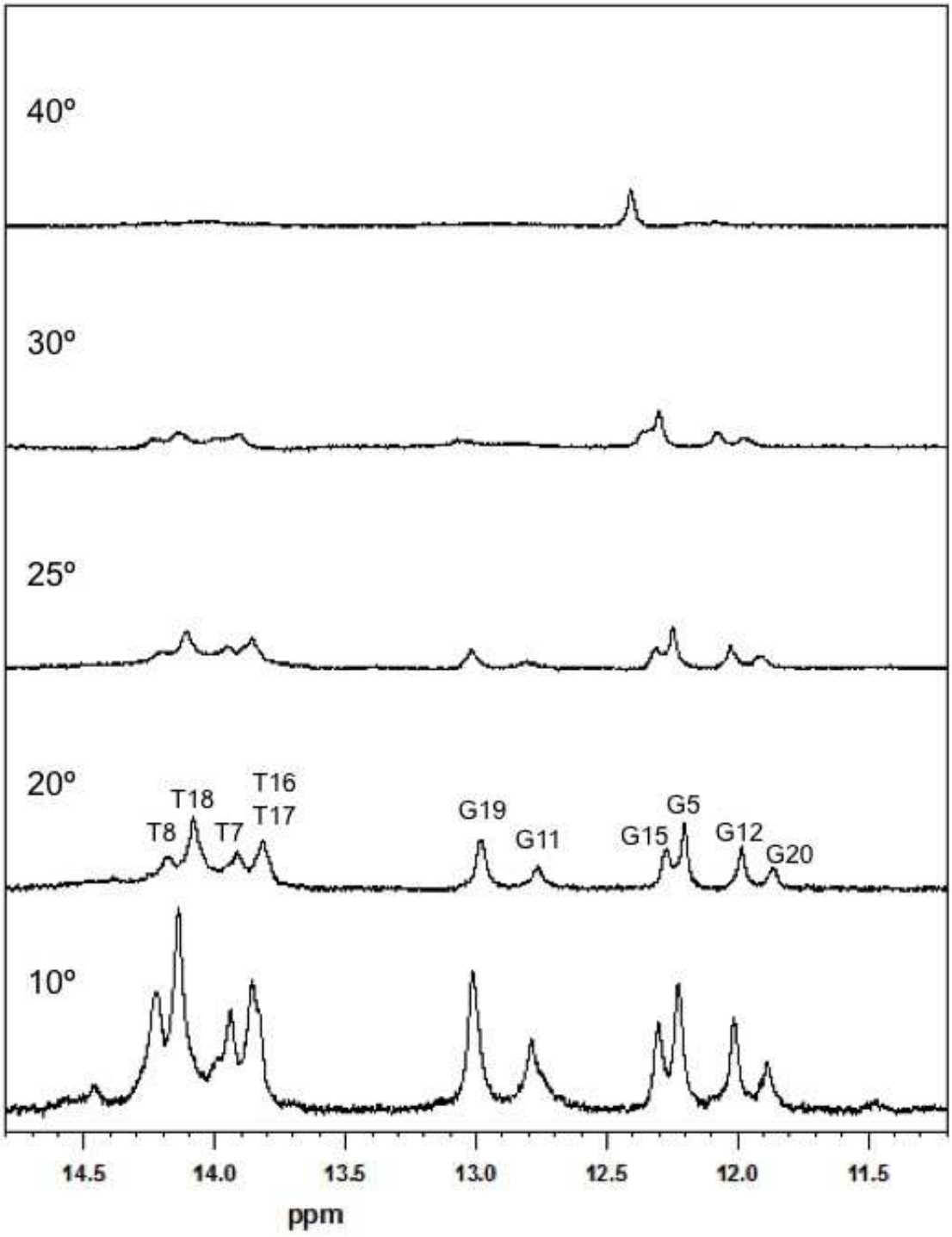
Supporting Information Table 2. Proton chemical shift assignments (ppm) for the G-F:ActD complex at 25°C[a].

Nucleotide	H6/H8	H5	Methyl	H1'	H2'	H2''	H3'	H4'	H2	NH[b]
C1	7.76	5.97	na[c]	5.95	2.06	2.5	4.68	4.00	na	Na
C2	7.51	5.84	na	5.94	2.06	2.48	4.67	4.10	na	Na
A3	8.28	na	na	5.69	2.71	2.82	4.92	4.27	7.51	Na
A4	8.04	na	na	5.80	2.26	2.50	4.82	3.97	7.59	Na
G5	7.43	na	na	5.55	2.46	2.69	5.01	3.83	na	12.27
C6	7.56	5.86	na	6.25	2.27	2.54	4.50	3.93	na	Na
T7	7.32	na	1.79	6.11	2.29	2.52	4.18	4.07	na	13.85
T8	7.46	na	1.83	6.27	2.30	2.43	4.91	4.22	na	14.16
C9	7.86	6.06	na	5.87	2.71	2.83	4.92	4.28	na	Na
C10	7.84	6.1	na	6.27	2.29	2.53	4.3	4.10	na	Na
G11	7.75	na	na	5.78	2.07	2.50	4.93	4.17	na	12.79
G12	7.53	na	na	5.86	2.71	2.82	4.92	4.28	na	12.02
A13	8.25	na	na	5.67	2.68	2.70	5.02	4.33	7.46	Na
A14	8.00	na	na	5.76	2.4	2.70	4.84	4.25	7.49	Na
G15	7.52	na	na	5.56	2.45	2.69	4.56	3.82	na	12.21
F16	6.93	na	1.72	6.22	2.30	2.43	4.91	4.22	na	Na
T17	7.41	na	1.80	6.11	2.13	2.53	4.89	4.23	na	14.01
T18	7.32	na	1.79	5.70	2.25	2.70	4.26	3.90	na	13.95
G19	7.86	na	na	5.72	2.25	2.69	4.91	3.97	na	13.06
G20	7.80	na	na	6.12	2.03	2.35	4.63	4.15	na	11.92

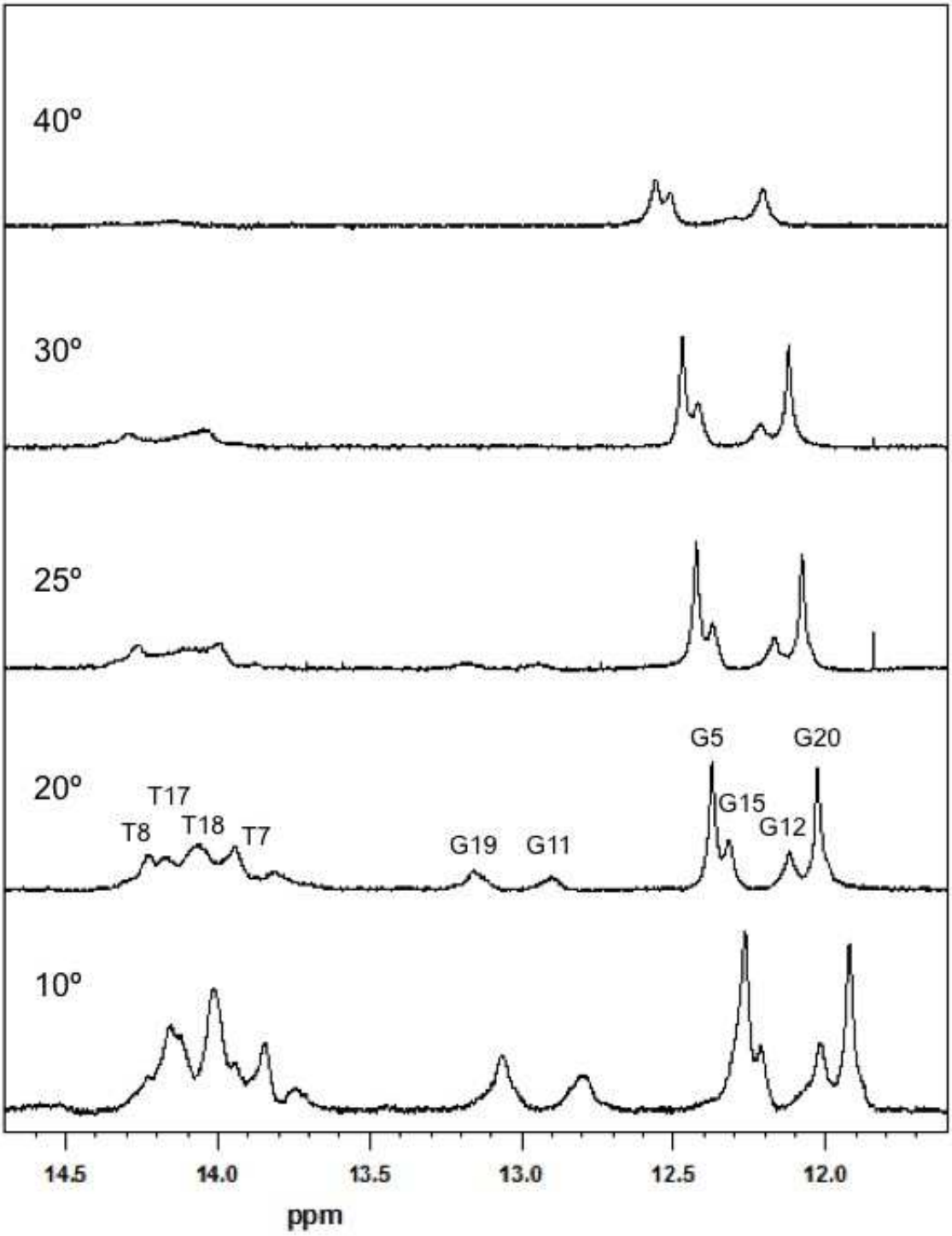
[a]Chemical shifts are referenced to residual HOD resonance.
[b]Chemical shifts for imino protons are reported for the duplex at 10°C.
[c]Not applicable.



Supporting Information Figure 1. Heteronuclear ^{1}H—^{19}F NOESY spectrum of G-F:ActD at 10°C (acquisition parameters described in Experimental Methods). The chemical shifts of F2 and F4 of the difluorotoluene are -123.7 ppm and -112.3 ppm, respectively. The boxes indicate the regions we expect to see NOEs between F16 F2 and F4 and DNA imino protons, if they existed.



Supporting Information Figure 2. Imino proton spectra of 1:1 G-T:ActD complex (**2** mM in 10 mM sodium phosphate buffer, pH 7.0, 100 mM NaCl, 0.1 mM EDTA in 600 μL 90%H_20/10%D_20) at various temperatures as indicated.



Supporting Information Figure 3. Imino proton spectra of 1:1 G-F:ActD complex (**2** mM in 10 mM sodium phosphate buffer, pH 7.0, 100 mM NaCl, 0.1 mM EDTA in 600 μL 90%H_20/10%D_20) at various temperatures as indicated.

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