

Supporting Information for

"Efficient Guest Inclusion by β -Cyclodextrin Attached to the Ends of DNA Oligomers upon Hybridization to Various DNA Conjugates"

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Supporting Table 1. Thermodynamic parameters of the duplexes that do not involve β -CyD.

Supporting Table 2. Thermodynamic parameters of the duplexes of β -CyD–DNA conjugate (**1b**) and its complementary strands (**3**).

Supporting Table 3. Thermodynamic parameters of the duplexes of β -CyD–DNA conjugate (**1c**) and its complementary strands (**3**).

Supporting Table 4. Thermodynamic parameters of the 7-mer duplexes.

Supporting Table 1. Thermodynamic parameters of the duplexes that do not involve β -CyD.

	ΔH	$\Delta\Delta H$	ΔS	$\Delta\Delta S$	ΔG_{37}	$\Delta\Delta G_{37}$
	(kcal/mol)	(kcal/mol)	(cal/mol·K)	(cal/mol·K)	(kcal/mol)	(kcal/mol)
1a/3a	-98.3		-275.6		-12.8	
1a/3b	-97.6	0.7	-272.5	3.1	-13.1	-0.3
1a/3c	-113.4	-15.1	-321.3	-45.7	-13.8	-1.0
1a/3d	-77.5	20.8	-208.2	67.4	-12.9	-0.1
1a/3e	-97.2	1.0	-271.3	4.4	-13.1	-0.3
1a/2f	-92.4	5.9	-257.4	18.3	-12.6	0.2

Supporting Table 2. Thermodynamic parameters of the duplexes of β -CyD–DNA conjugate (**1b**) and its complementary strands (**3**).

	ΔH	$\Delta\Delta H$	ΔS	$\Delta\Delta S$	ΔG_{37}	$\Delta\Delta G_{37}$
	(kcal/mol)	(kcal/mol)	(cal/mol·K)	(cal/mol·K)	(kcal/mol)	(kcal/mol)
1b/3a	-76.6	-	-209.2	-	-11.7	-
1b/3b	-116.3	-39.7	-318.8	-109.6	-17.5	-5.8
1b/3c	-93.0	-16.4	-258.2	-49.0	-12.9	-1.2
1b/3d	-71.3	5.3	-189.5	19.7	-12.5	-0.8
1b/3e	-67.9	8.7	-180.2	29.0	-12.0	-0.3
1b/3f	-68.5	8.1	-183.9	25.3	-11.5	0.2

Supporting Table 3. Thermodynamic parameters of the duplexes of β -CyD–DNA conjugate (**1c**) and its complementary strands (**3**).

	ΔH	$\Delta\Delta H$	ΔS	$\Delta\Delta S$	ΔG_{37}	$\Delta\Delta G_{37}$
	(kcal/mol)	(kcal/mol)	(cal/mol·K)	(cal/mol·K)	(kcal/mol)	(kcal/mol)
1c/3a	-79.5	-	-216.1	-	-12.5	-
1c/3b	-111.2	-31.7	-292.3	-76.2	-20.6	-8.1
1c/3c	-84.4	-4.9	-228.7	-12.6	-13.6	-1.0
1c/3d	-110.7	-31.2	-95.2	120.9	-15.5	-3.0
1c/3e	-89.1	-9.6	-237.2	-21.1	-15.6	-3.1
1c/3f	-75.5	4.0	-201.0	15.1	-13.2	-0.7

Supporting Table 4. Thermodynamic parameters of the 7-mer duplexes.

	ΔH	ΔS	ΔG_{37}
	(kcal/mol)	(cal/mol·K)	(kcal/mol)
2a/4a	-39.3	-107.9	-5.9
2a/4b	-36.8	-316.5	-6.4
2a/4c	-48.2	-136.6	-5.9
2b/4a	-45.5	-129.5	-5.3
2b/4b	-67.6	-187.2	-9.6
2b/4c	-19.2	-39.0	-7.1
2c/4a	-59.3	-173.2	-5.6
2c/4b	-90.0	-245.6	-13.9
2c/4c	-55.0	-153.3	-7.5