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Supplementary material

Table S1 Coupling constant values for the B and C rings of benzo[*b*]isoquino[2,3-*h*]-naphthyridines [a]

J(H, H)	**7a**	**9**	**9**[b]	**10a**		**7b**	**10b**	
5ax, 5eq	15.2	15.3	15.7	15.3		15.2	15.1	
7ax, 7eq	11.6	11.6	12.5	11.6		11.4	11.5	
8ax, 8eq	13.2	13.3	14.5	13.3		13.0	13.1	
7ax, 8ax	12.6	12.8	13.5	12.8		12.4	12.2	
7ax, 8eq	3.2	3.3	3.6	3.3		2.6	2.5[c]	
7eq, 8ax	4.1	4.1	4.4	4.1		3.8	3.8	
7eq, 8eq	3.0	2.7	2.1	2.9		3.0	3.0	
8a, 8ax	12.5	12.3	12.5	12.4	(ax, ax)	12.3	12.3	(ax, ax)
8a, 8eq	3.2	3.4	4.0	3.2	(ax, eq)	3.3	3.3	(ax, eq)
8a,14a	3.2	3.1	3.0	3.2	**(ax,eq)**	10.6	10.7	**(ax,ax)**
14a,14b	2.1	2.3	1.7	2.0	**(eq,ax)**	8.5	8.5	**(ax,ax)**
14a, NH[c,d,e]	1.5	~1.5		~2.0		≤0.5	0.7	
14b,15ax	11.3	11.3	11.8	11.3	(ax, eq)	10.5	10.5	(ax, eq)
14b,15eq	4.7	4.8	5.4	4.8	(ax, eq)	4.3	4.3	(ax, eq)
15ax,15eq	16.7	16.7	17.6	16.7		15.9	15.9	
^{5}J(5ax,15ax)[c,d]	1.0	1.1	[f]	1.1		1.2	1.3	
^{4}J(8eq,14°)[c,d]	1.2	1.3	~1.0	1.3		Zero	zero	
^{4}J(8°, NH)[c,d]	1.3	1.5		≤1.2		Zero	zero	

[a] Measured in Hz by 1D experiments, solvent $CDCl_3$, estimated accuracy within ± 0.05 Hz, unless otherwise specified. [b] In D_2O. [c] Estimated accuracy ± 0.1 Hz. [d] Proved by decoupling experiments. [e] These values may be affected by exchange due to the small amount of acid present in the unstabilized $CDCl_3$. [f] Not detected.

Table S2 ^{1}H Chemical shift assignments (δ) for **9**, **10a** and **10b** with shift variation (Δδ) in presence of oligonucleotides[a]

	δ	Δδ	δ	Δδ	Δδ	δ	Δδ	Δδ	Δδ	Δδ
	9	**9** /AATT	**10a**	**10a**/AATT	**10a**/GATC	**10b**	**10b**/GATC[c]	**10b**/ACGT	**10b**/CGCG	**10b**/AATT
H-1[b]	7.37	-0.10	7.37	-0.10	-0.06	7.32	-0.11	-0.21	-0.12	-0.05
H-2[b]	7.39	-0.12	7.37	-0.10	-0.06	7.32	-0.11	-0.14	-0.12	-0.05
H-3[b]	7.34	-0.10	7.33	-0.11	-0.06	7.28	-0.10	-0.10	-0.12	-0.04
H-4[b]	7.22	-0.10	7.25	-0.10	-0.05	7.18	-0.11	-0.08	-0.11	-0.05
H-5eq	4.52	-0.20	4.40	-0.18	-0.09	4.28	-0.17	-0.18	-0.20	-0.07
H-5ax	4.38	-0.15	4.15	-0.12	-0.10	3.95	-0.14	-0.15	-0.16	-0.08
H-7eq	3.70	-0.10	3.55	-0.10	-0.08	3.55	-0.10	-0.12	-0.12	-0.06
H-7ax	3.25	-0.11	3.00	-0.09	-0.07	2.97	-0.09	-0.10	-0.11	-0.05
H-8eq	2.00	-0.15	1.94	-0.09	-0.06	2.18	-0.12	-0.15	-0.14	-0.04
H-8ax	1.44	-0.04	1.47	-0.05	-0.02	1.60	-0.07	-0.07	-0.08	-0.02
H-8a	2.05	-0.20	1.97	≤-0.12	-0.04	1.68	-0.18	-0.20	-0.21	-0.04
H-10	7.94	-0.10	7.76	-0.09	-0.07	7.80	-0.09	-0.12	-0.12	-0.07
H-12	7.74	-0.15	7.55	-0.11	-0.09	7.47	-0.10	-0.15	-0.14	-0.09
H-13	6.78	-0.10	6.82	-0.12	-0.07	6.79	-0.11	-0.12	-0.11	-0.07
H-14a	4.13	-0.20	4.04	-0.14	-0.10	3.54	-0.15	-0.18	-0.18	-0.08
H-14b	3.81	-0.10	3.52	-0.11	-0.09	3.25	-0.10	-0.12	-0.12	-0.08
H-15ax	3.48	-0.09	3.45	-0.08	-0.08	2.84	-0.10	-0.11	-0.10	-0.06
H-15eq	3.22	-0.07	3.14	≤-0.1	-0.06	3.54	-0.09	-0.10	-0.12	-0.05
9-Me	1.44	-0.04	1.47	-0.04	-0.03	1.42	-0.03	-0.05	-0.04	-0.03
9-Me	1.27	-0.05	1.31	-0.05	-0.05	1.17	-0.04	-0.04	-0.03	-0.03
OCH_2	4.64	-0.08	3.75	-0.10	-0.08	3.74	-0.09	-0.10	-0.10	-0.04
NCH_2	3.62	-0.22	3.53	-0.18	-0.07	3.48	-0.15	-0.18	-0.19	-0.05
N-Me	3.00	-0.20								

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[a] Measured at 20°C in D_2O, pH 5.9-6.0, 0.02 M NaCl, R = [drug]/ [DNA] = 1, δ_{free} were measured at the concentration of 10^{-5} M. AATT is $d(AAGAATTCTT)_2$, GATC is $d(GCGATCGC)_2$, ACGT is $d(CGACGTCG)_2$, CGCG is $d(GCATCGCGATGC)_2$. [b] Assigned by ROESY experiments. [c] In H_2O/D_2O (90:10) at 5°C the NH signals are: A4:T5 13.44 (free), 13.35 (bound); C2:G7 12.89 (free), 12.77 (bound); G3:C6 12.59 (free), 12.48 (bound); G1:C8 12.94 (free), ca. 12.6-12.7 (bound).

Table S3 ^{31}P Chemical shift values (δ) for the phosphates of $d(AAGAATTCTT)_2$ free and bound to **10a**[a]

	Free	Bound	$\Delta\delta^b$
	δ	Δ	
A_1pA_2	-1.31	-1.26	+0.05
A_2pG_3	-1.00	-0.98	+0.02
G_3pA_4	-1.14	-1.21	-0.07
A_4pA_5	-1.40	-1.35	+0.06
A_5pT_6	-1.37	-1.46	-0.09
T_6pT_7	(-1.18)	-1.14	+0.04
T_7pC_8	(-1.11)	-1.14	-0.05
C_8pT_9	(-1.14)	-1.14	0.00
T_9pT_{10}	(-1.04)	-1.14	-0.04

[a] Spectra measured at 20°C in ppm from methylenediphosphonic acid (MDA), as external reference, solvent D_2O, pH 5.8, 0.02 M NaCl. Similar values in parentheses may be interchanged. For the assignments see Ref. 8.
[b] $\Delta\delta = \delta_{bound} - \delta_{free}$