Table S2. ^{1}H NMR Chemical Shift Assignments for the 1:2 DNA–Drug Complex $[d(GGAGCTCC)_2(ACRAMTU)_2]^a$

residue	H6/H8	H2/H5/ CH_3	H1'	H2'	H2"	H3'	H4'	H5 H5"
G1	7.71 (-0.10)		5.54 (-0.10)	2.33 (-0.01)	2.51 (0.01)	4.78 (-0.03)	4.14 (-0.02)	3.68 (0.02) 3.58 (0.08)
G2	7.69 (-0.18)		5.38 (-0.12)	2.57 (-0.13)	2.57 (-0.21)	4.96 (-0.05)	4.31 (-0.03)	4.10 (-0.05) 4.03 (-0.09)
A3	8.05 (-0.09)	7.39 (-0.42)	5.91 (-0.21)	2.57 (-0.15)	2.75 (-0.18)	5.04 (-0.05)	4.40 (-0.06)	4.22 (0.00) 4.17 (0.01)
G4	7.64 (-0.01)		5.69 (-0.10)	2.51 (0.07)	2.61 (-0.13)	4.94 (-0.03)	4.39 (-0.03)	n.a.[c] 4.21 (-0.03)
C5	7.32 (-0.05)	5.23 (0.01)	5.90 (-0.01)	2.12 (0.02)	2.43 (-0.09)	4.80 (0.11)	4.22 (-0.09)	n. a. n. a.
T6	7.34 (-0.17)	1.66 (0.04)	6.07 (-0.05)	2.23 (-0.04)	2.53 (-0.03)	4.85 (-0.05)	4.22 (-0.00)	4.15 (-0.08) 4.04 (-0.08)
C7	7.76 (0.12)	5.76 (-0.05)	6.07 (-0.07)	2.23 (-0.00)	2.51 (-0.01)	4.87 (-0.01)	4.22 (-0.03)	4.15 (-0.01) 4.08 (-0.04)
C8	7.65 (-0.10)	5.78 (-0.12)	6.21 (-0.07)	2.49 (0.00)	2.31 (-0.03)	4.57 (-0.00)	4.180 (-0.02)	n. a. 4.07 (-0.01)
ACR	H1/H8	H2/H7	H3/H6	H4/H5	H9	H10	H11	H12
	7.88 (-0.52)[b]	6.68 (-0.87)	7.15 (-0.80)	7.04 (-0.72)	4.14 (-0.30)	4.04 (-0.34)	3.13 (0.25)	3.09 (0.24)

[a] 500 MHz, D_2O, 308 K, pH* 7.0; shifts are relative to DSS. The noticeable upfield shifts for G1 and C8 base protons is probably caused by the slight excess of drug stacking to the ends of the duplex. [b] Numbers in parentheses are $\Delta\delta = \delta_{\text{adduct}} - \delta_{\text{free DNA/free ACRAMTU}}$ (ppm). [c] Not assigned due to signal overlap.