Table S1. ^{1}H NMR Chemical Shift Assignments for the 1:1 DNA–Drug Complex [d(GGACGTCC)$_2$ACRAMTU][a]

residue	H6/H8	H2/H5/ CH_3	H1'	H2'	H2"	H3'	H4'	H5 H5"
G1	7.75 (-0.08)[b]		5.57 (-0.09)	2.37 (-0.09)	2.54 (-0.07)	4.79 (-0.03)	n.a.[c]	3.66 (-0.01) 3.56 (-0.01)
G2	7.76 (-0.09)		5.45 (-0.13)	2.63 (-0.08)	2.63 (-0.17)	4.98 (-0.05)	4.33 (-0.05)	4.11 (-0.04) 4.04 (-0.05)
A3	8.13 (-0.08)	7.42 (-0.50)	6.13 (-0.14)	2.67 (-0.05)	2.81 (-0.12)	5.03 (-0.05)	4.44 (-0.05)	4.21 (-0.05) 4.19 (-0.02)
C4	7.19 (-0.04)	5.22 (-0.02)	5.60 (-0.04)	2.05 (0.03)	2.31 (-0.07)	4.81 (-0.03)	n. a.	n. a. n. a.
G5	7.82 (-0.01)		5.86 (-0.13)	2.63 (0.00)	2.70 (-0.09)	4.96 (0.00)	4.39 (0.00)	4.12 (-0.03) 4.01 (-0.09)
T6	7.21 (-0.09)	1.42 (0.00)	6.05 (-0.02)	2.18 (0.01)	2.51 (-0.02)	4.88 (-0.01)	4.23 (-0.02)	4.21 (-0.05) 4.21 (0.01)
C7	7.57 (-0.03)	5.74 (0.00)	6.07 (-0.03)	2.48 (-0.24)	2.21 (-0.28)	4.84 (0.00)	4.19 (0.01)	4.11 (0.05) 4.04 (0.02)
C8	7.64 (-0.01)	5.76 (0.01)	6.21 (-0.05)	2.28 (-0.02)	n. a.	4.55 (-0.02)	4.15 (0.09)	n. a. 4.05 (0.00)
ACR	H1/H8	H2/H7	H3/H6	H4/H5	H9	H10	H11	H12
	7.86 (-0.54)[b]	6.61 (-0.95)	7.08 (-0.87)	7.01 (-0.75)	4.15 (-0.29)	4.03 (-0.35)	3.14 (0.26)	3.12 (0.27)

[a] 500 MHz, D_2O, 308 K, pH* 7.0; shifts are relative to DSS. [b] Numbers in parentheses are $\Delta\delta = \delta_{\text{adduct}} - \delta_{\text{free DNA/free ACRAMTU}}$ (ppm). [c] Not assigned due to signal overlap.