

SUPPLEMENTARY MATERIAL

Table S1. Drug–DNA NOEs in the d(GGTAATTACC)₂ complex with Hoechst 43254

Drug residue	DNA proton	Distance (Å)
bz1 H4	T6 H1'	3.18
bz1 H4	T6* H1'	3.31
bz1 H4	A5* H1'	5.00
ph H6	A5 H1'	5.00
ph H6	T3 H1'	3.87
ph H6	C9* H1'	4.10
ph H6	A4 H1'	3.73
bz1 H7	T7 H5'	3.73
bz2 H7	T7 H5'	3.52
bz2 H6	T7 H5'	3.02
bz2 H6	T7* H5'	3.38
ph H6	A4 H2	3.17
ph H5	A4 H2	2.65
bz1 H4	A5* H2	2.63
bz1 H4	A8 H2	3.54
tp H3/5	C9 H1'	3.58
tp H3/5	A4* H1'	5.00
tp H3/5	A5* H1'	2.81
tp H3/5	A4* H2	2.43
tp H3/5	A8 H2	3.28
bz2 H6	T7 H4'	3.33
bz2 H6	T7* H4'	3.76
bz1 H7	A8 H5'	4.46
bz1 H6	A8 H5'	2.92
bz1 H6	A8 H5''	2.89
bz1 H6	T7 H5'	5.00
bz2 H4	A8* H1'	4.92
ph H5	A8* H1'	5.05
tp H4	A4* H2	3.93
tp H4	A5* H1'	3.21
tp H3/5	A8 H2'	5.23
tp H3/5	A8 H2''	5.00
tp H3/5	A8 H5'	2.98
tp H3/5	A8 H4'	4.00
ph H6	A5 H2	5.95
tp H3/5	A5* H2	3.56
ph H5	A4 H2	3.71
ph H6	A4 H2	3.25
bz1 H4	A4* H2	2.71
tp NH	A5* H2	5.59
tp NH	A4* H2	4.38
bz1 NH	A5* H2	5.11
bz1 NH	A4* H2	4.65
bz2 H4	T7* NH	4.56
ph H5	T7* NH	4.07
bz1 H4	T6 NH	4.60
bz2 NH	T6* NH	4.49
bz1 NH	T6 H2'	5.08
bz1 NH	T6 H2''	4.74
tp H3/5	T7 NH	4.85

Strands run from G1 to C10 and from G1* to C10*.