Supplementary Information

Binding of pixantrone to DNA at CpA dinucleotide sequences and bulge structures

Shyam K. Konda[a], Haiqiang Wang[a], Suzanne M. Cutts[b*],
Don R. Phillips[b] and J. Grant Collins[a*]

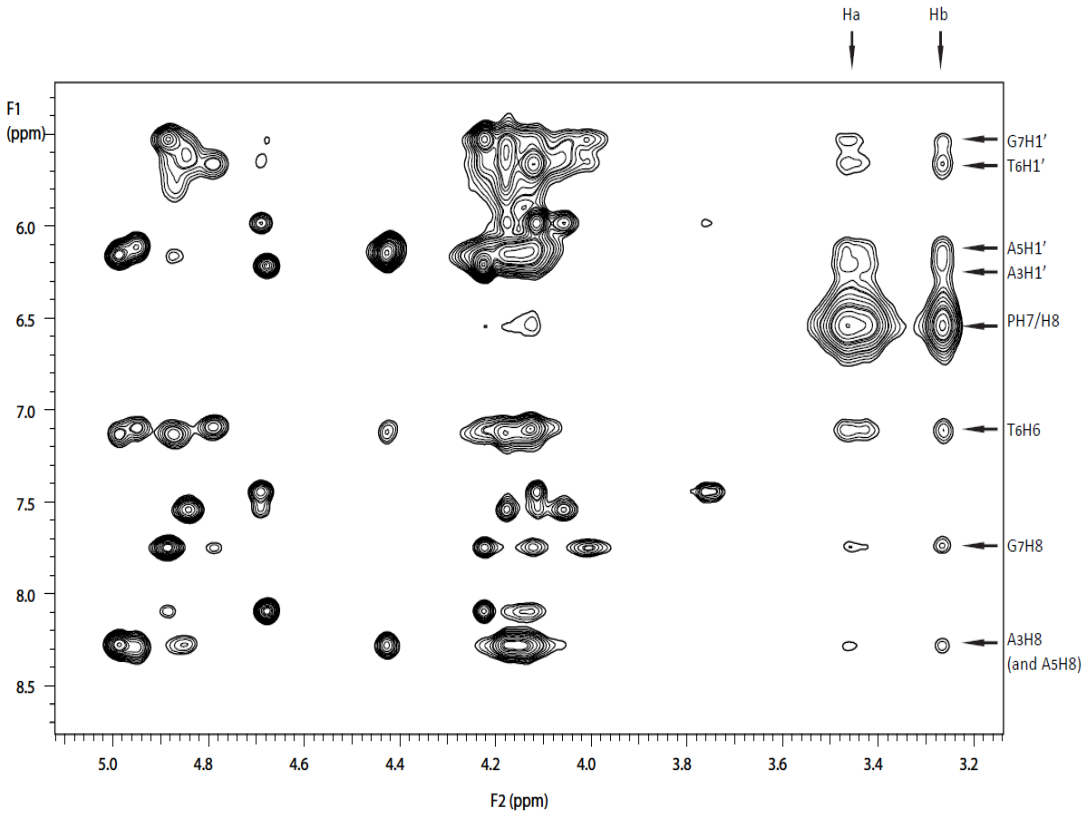

Figure S1 An expansion of a NOESY spectrum of d(TCATATGA)$_2$ with added pixantrone, at a drug to DNA duplex ratio of 2, at 30 °C in D_2O and pH 7 phosphate buffer. The expansion shows the NOE connectivities from the pixantrone H7/H8 protons to the octanucleotide H3', H4', H5' and H5" sugar protons (3.2 to 5.5 ppm), and the NOEs from the pixantrone Ha/Hb protons to the octanucleotide H8/H6 protons.

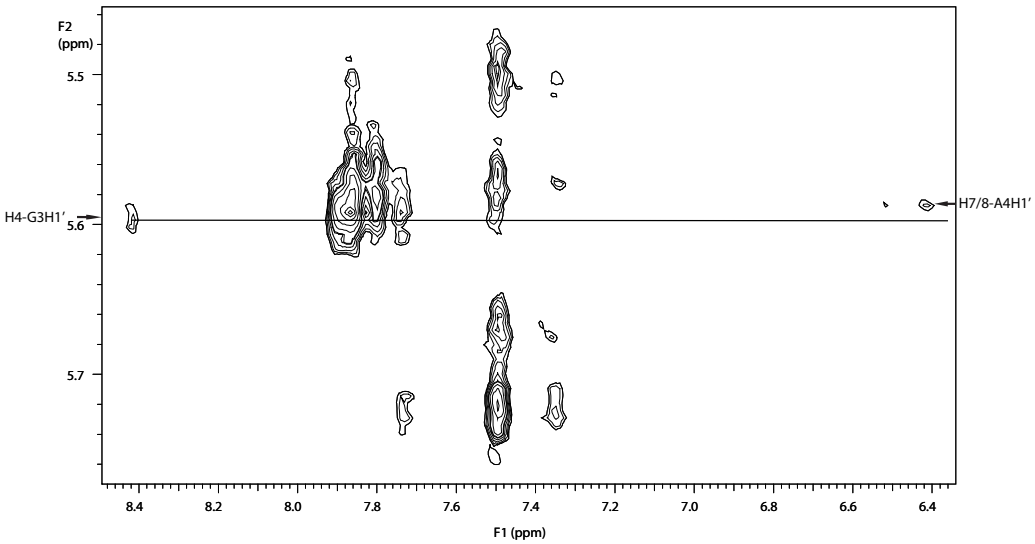

Figure S2 An expansion of a NOESY spectrum of DB with added pixantrone, at a drug to DNA duplex ratio of 1, in pH 7 phosphate buffer at 5 °C. In this case, the FID was processed with a shifted sine bell function in both dimensions to allow the resolution of the resonances from the G_3H1' and A_4H1' protons of DB. The G_3H1' and A_4H1' resonances were assigned from their connectivities to their own and 5'- sugar H2'/H2" resonances.

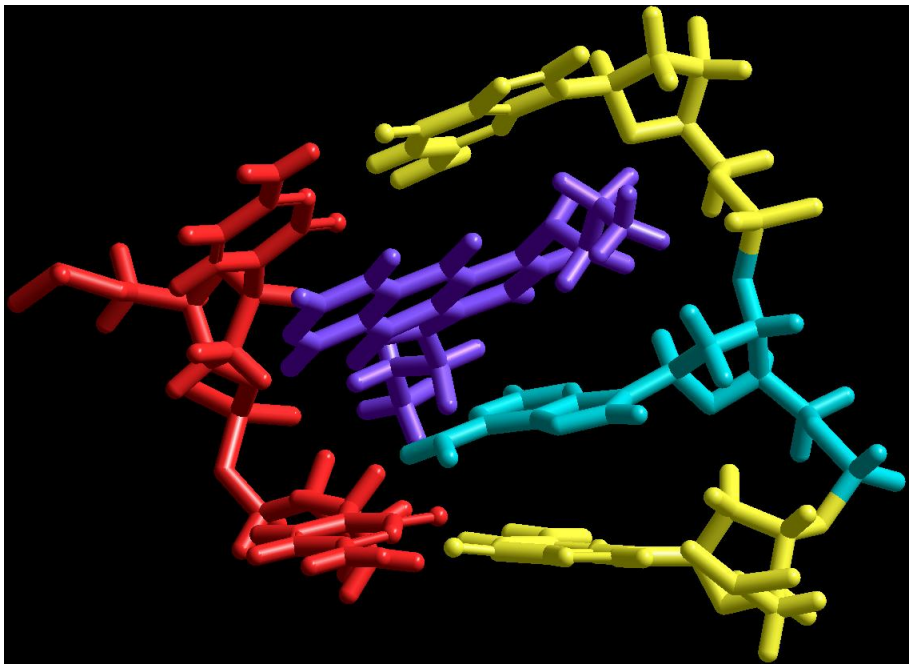

Figure S3 Energy minimised HyperChem molecular model of pixantrone-bound SB generated using HyperChem 7.5. The pixantrone is inserted from minor groove at the A_8pG_9 site. The bases are colour coded: adenine (cyan), guanine (yellow) and cytosine (red) and pixantrone is in violet.