Supporting information

Figure S1. DF-STD spectra of the 10–DNA complex. A, B) STD spectra recorded upon saturation in the aromatic (9.2 ppm) and deoxyribose/backbone (1.3 ppm) spectral regions, respectively. C) Reference STD spectrum with an off-resonance irradiation (-16 ppm).
**Figure S2.** DF-STD spectra of the 9–DNA complex. A, B) STD spectra recorded upon saturation in the aromatic (9.8 ppm) and deoxyribose/backbone (5.5 ppm) spectral regions, respectively. C) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

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**Figure S3.** DF-STD spectra of the 16–DNA complex. A, B) STD spectra recorded upon saturation in the aromatic (9.4 ppm) and deoxyribose/backbone (1.2 ppm) spectral regions, respectively. C) Reference STD spectrum with an off-resonance irradiation (-16 ppm).

**Table S1:** Calculated inhibition constants ($K_i$) by the software Autodock 3.0.5, for 7-12 and 16, interacting with two DNA models A and B.
**Figure S4.** 3D interactions of 7-Model A (a and b) and 7-Model B (c and d) complexes. In a) a c) the DNA is represented by molecular surface, and sticks and balls (coloured by atom type: O, red; C, grey; polar H, sky blue; N, blue), whereas in b) and d) only by sticks and balls. The ligand is depicted in sticks (yellow) and balls (coloured as for DNA). In a) and c), the figure highlights the intercalation between two adjacent base pairs and the hydrogen bonds (yellow line) between ester functionality and NH$_2$ of guanine. In b) and d), beside the intercalation, the hydrogen bonds (yellow line) formed by OH group are showed.

**Figure S5.** 3D interactions of 9-Model A (a and b) and 9-Model B (c and d) complexes. In a) a c) the DNA is represented by molecular surface, and sticks and balls (coloured by atom type: O, red;
C, grey; polar H, sky blue; N, blue), whereas in b) and d) only by sticks and balls. The ligand is depicted in sticks (green) and balls (coloured as for DNA). In a) and c), the figure highlights the intercalation between two adjacent base pairs and the hydrogen bonds (yellow line) between ester functionality and NH$_2$ of guanine. In b) and d), beside the intercalation, the hydrogen bonds (yellow line) formed by OH group are showed.

**Figure S6.** 3D interactions of 12-Model A (a and b) and 12-Model B (c and d) complexes. In a) a c) the DNA is represented by molecular surface, and sticks and balls (coloured by atom type: O, red; C, grey; polar H, sky blue; N, blue), whereas in b) and d) only by sticks and balls. The ligand is depicted in sticks (cyan) and balls (coloured as for DNA). In a) and c), the figure highlights the intercalation between two adjacent base pairs and the hydrogen bonds (yellow line) between ester functionality and NH$_2$ of guanine. In b) and d), beside the intercalation, the hydrogen bonds (yellow line) formed by OH group are showed.
Figure S7. 3D interactions of 8-Model A (a and b) and 8-Model B (c and d) complexes. In a) a c) the DNA is represented by molecular surface, and sticks and balls (coloured by atom type: O, red; C, grey; polar H, sky blue; N, blue), whereas in b) and d) only by sticks and balls. The ligand is depicted in sticks (white) and balls (coloured as for DNA). In a) and c), the figure highlights the intercalation between two adjacent base pairs and the hydrogen bonds (yellow line) between ester functionality and NH₂ of guanine. In b) and d), beside the intercalation, the hydrogen bonds (yellow line) formed by OH group are showed.

Figure S8. 3D interactions of 11-Model A (a and b) and 11-Model B (c and d) complexes. In a) a c) the DNA is represented by molecular surface, and sticks and balls (coloured by atom type: O,
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**Figure S9.** 3D interactions of 16-Model A (a and b) and 16-Model B (c and d) complexes. In a) a c) the DNA is represented by molecular surface, and sticks and balls (coloured by atom type: O, red; C, grey; polar H, sky blue; N, blue), whereas in b) and d) only by sticks and balls. The ligand is depicted in sticks (purple) and balls (coloured as for DNA). In a) and c), the figure highlights the intercalation between two adjacent base pairs and the hydrogen bonds (yellow line) between ester functionality and NH$_2$ of guanine. In b) and d), beside the intercalation, the hydrogen bonds (yellow line) formed by OH group are showed.
Figure S10. Graphical representation of SW480 and HepG2 cell percentages related to the untreated control cells after a 48 h treatment with 8, 9, 11 and 12. Counting is realized with a haemocytometer after dead cells exclusion by Trypan Blue staining.
Figure S11. Phase contrast microscopy observation of SW480 colon cancer cells treated for 48 hours with 10, 11 and 12.

Three dimensional Cartesian coordinates of Model A, used in docking calculations.

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**Figure S13.** $^{13}$C NMR (125 MHz, CDCl$_3$) of 8.
**Figure S14.** ESI MS of 8.
Figure S15. $^1$H NMR (500 MHz, CDCl$_3$) of 9.
Figure S16. $^{13}$C NMR (125 MHz, acetone-d$_6$) of 9.
Figure S17. ESI MS of 9.
Figure S18. $^1$H NMR (500 MHz, acetone-d$_6$) of 11.
Figure S19. $^{13}$C NMR (125 MHz, acetone-$d_6$) of 11.
Figure S20 ESI MS of 11.