SUPPLEMENTARY MATERIAL:

The phenanthridine biguanides efficiently differentiate between dGdC, dAdT and rArU sequences by two independent, sensitive spectroscopic methods.

*Marijana Radić Stojković, Snežana Miljanić, Katarina Mišković, Ljubica Glavaš-Obrovac, Ivo Piantanida**

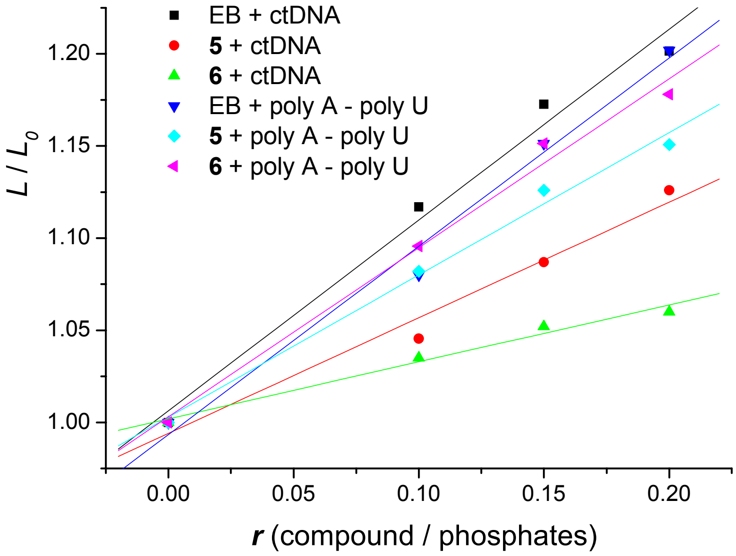

Figure S1. Relative ctDNA and poly A – poly U helix length extension (L/L_0) *vs*. ratio $r_{[compound] / [polynucleotide]}$ plot for **EB**, **5** and **6** at pH 7.0, sodium cacodylate buffer, I = 0.05 mol dm^{-3}. Results: α = 0.62 ± 0.06 (for **5**), 0.31 ± 0.03 (for **6**) and 1.04 ± 0.09 (**EB**) with ctDNA; α = 0.77 ± 0.05 (for **5**), 0.91 ± 0.06 (for **6**) and 1.02 ± 0.08 (**EB**) with poly A – poly U.

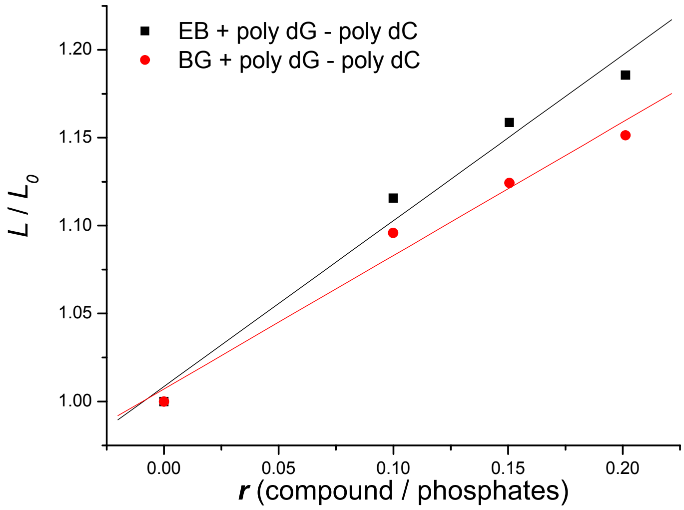

Figure S2. Relative poly dG - poly dC helix length extension (L/L_0) *vs*. ratio $r_{[compound]\ /\ [polynucleotide]}$ plot for **EB** and **5** at pH 7.0, sodium cacodylate buffer, I = 0.05 mol dm^{-3}. Result: $\alpha_{\mathbf{5}}/\alpha_{\mathbf{EB}}$= 0.805.

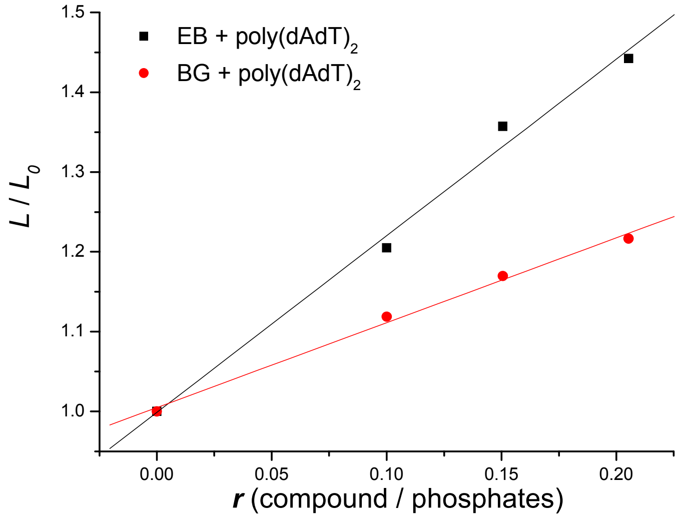

Figure S3. Relative poly$(dAdT)_2$ helix length extension (L/L_0) *vs*. ratio $r_{[compound]\ /\ [polynucleotide]}$ plot for **EB** and **5** at pH 7.0, sodium cacodylate buffer, I = 0.05 mol dm^{-3}. Result: $\alpha_{\mathbf{5}}/\alpha_{\mathbf{EB}}$= 0.48.

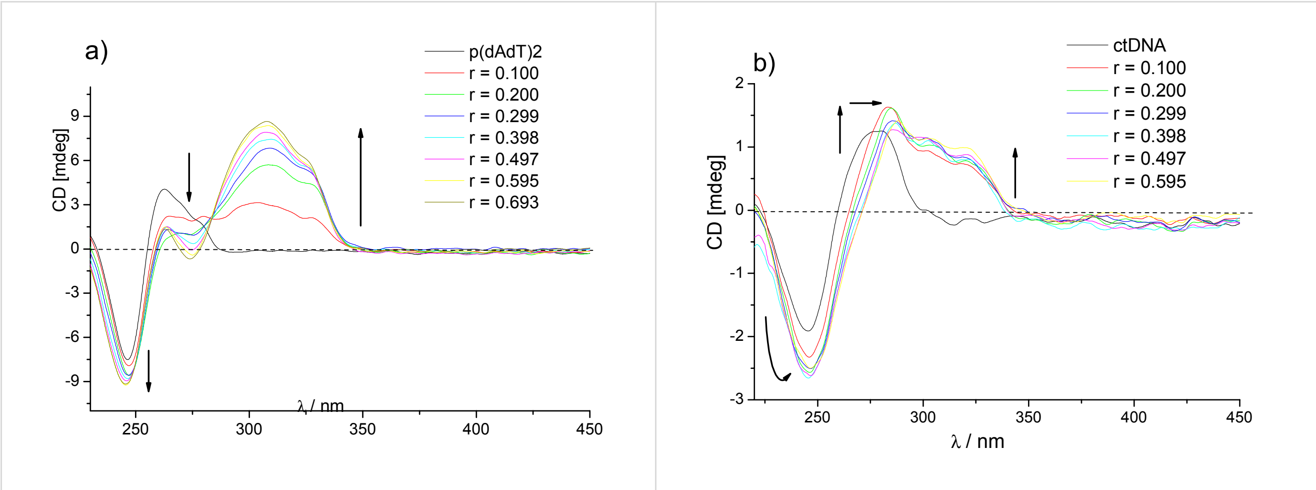

Figure S4. CD titrations of a) poly (dAdT)$_2$ and b) ctDNA ($c = 3.0 \times 10^{-5}$ mol dm^{-3}) with **6** at molar ratios ***r*** = [compound] / [polynucleotide] (pH 5.0, citric acid/NaOH buffer, I = 0.03 mol dm^{-3}).

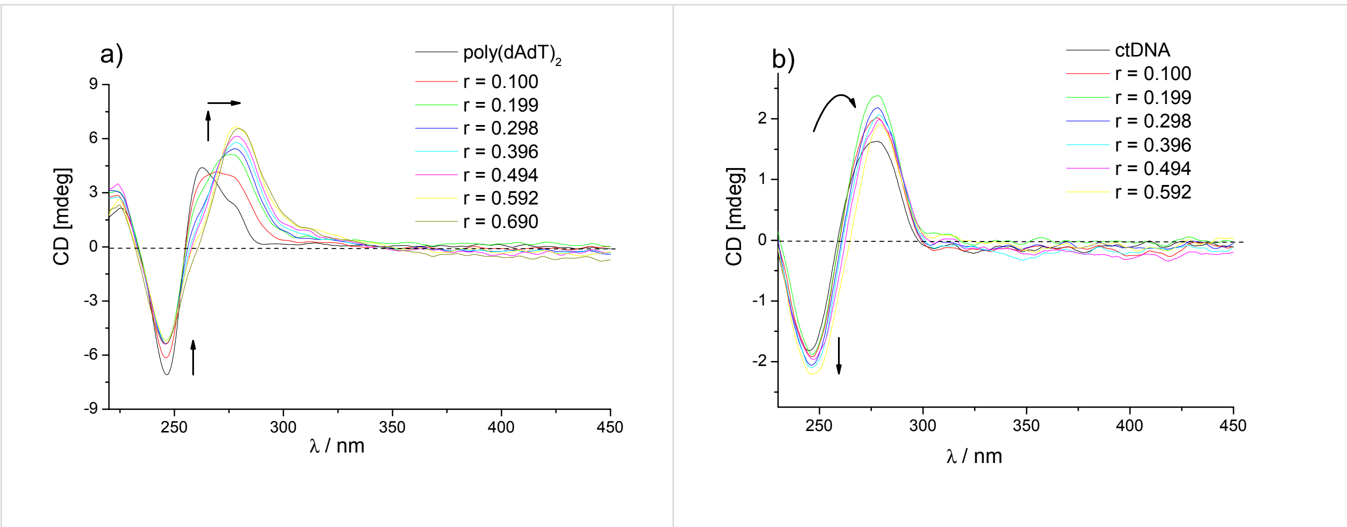

Figure S5. CD titrations of a) poly (dAdT)$_2$ and b) ctDNA ($c = 3.0 \times 10^{-5}$ mol dm^{-3}) with **5** at molar ratios ***r*** = [compound] / [polynucleotide] (pH 5.0, citric acid/NaOH buffer, I = 0.03 mol dm^{-3}).

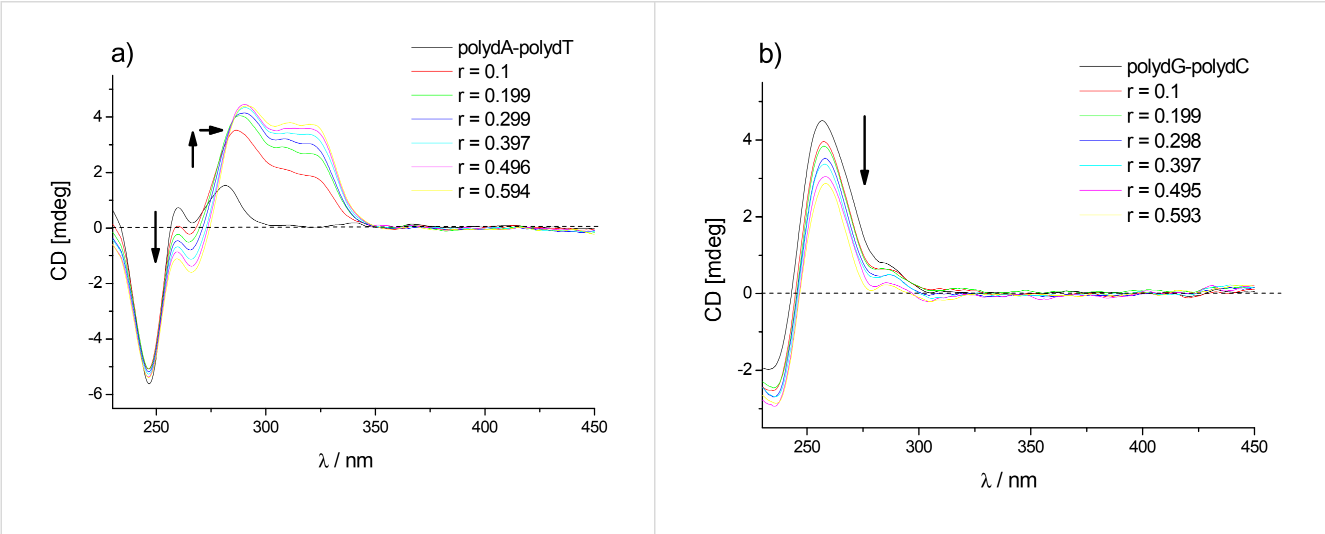

Figure S6. CD titrations of a) poly dA – poly dT and b) poly dG – poly dC ($c = 3.0 \times 10^{-5}$ mol dm^{-3}) with **6** at molar ratios $\boldsymbol{r}$ = [compound] / [polynucleotide] (pH 7.0, buffer sodium cacodylate, I=0.05 moldm^{-3}).

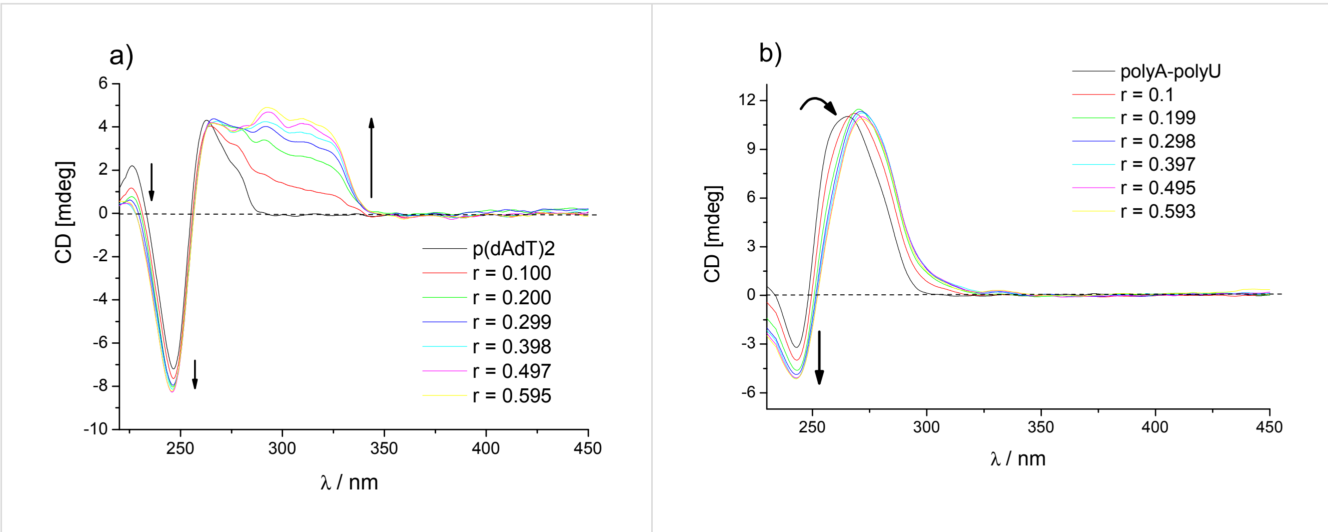

Figure S7. CD titrations of a) poly (dAdT)$_2$ and b) poly A – poly U ($c = 3.0 \times 10^{-5}$ mol dm^{-3}) with **6** at molar ratios $\boldsymbol{r}$ = [compound] / [polynucleotide] (pH 7.0, buffer sodium cacodylate, I=0.05 moldm^{-3}).

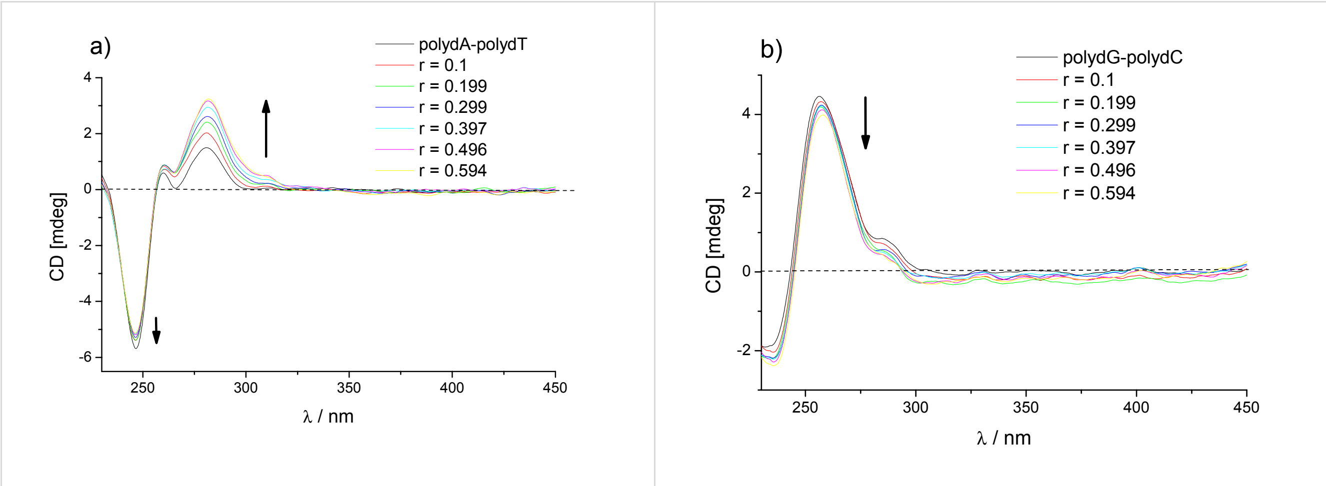

Figure S8. CD titrations of a) poly dA – poly dT b) poly dG – poly dC ($c = 3.0 \times 10^{-5}$ mol dm^{-3}) with **5** at molar ratios ***r*** = [compound] / [polynucleotide] (pH 7.0, buffer sodium cacodylate, I=0.05 moldm^{-3}).

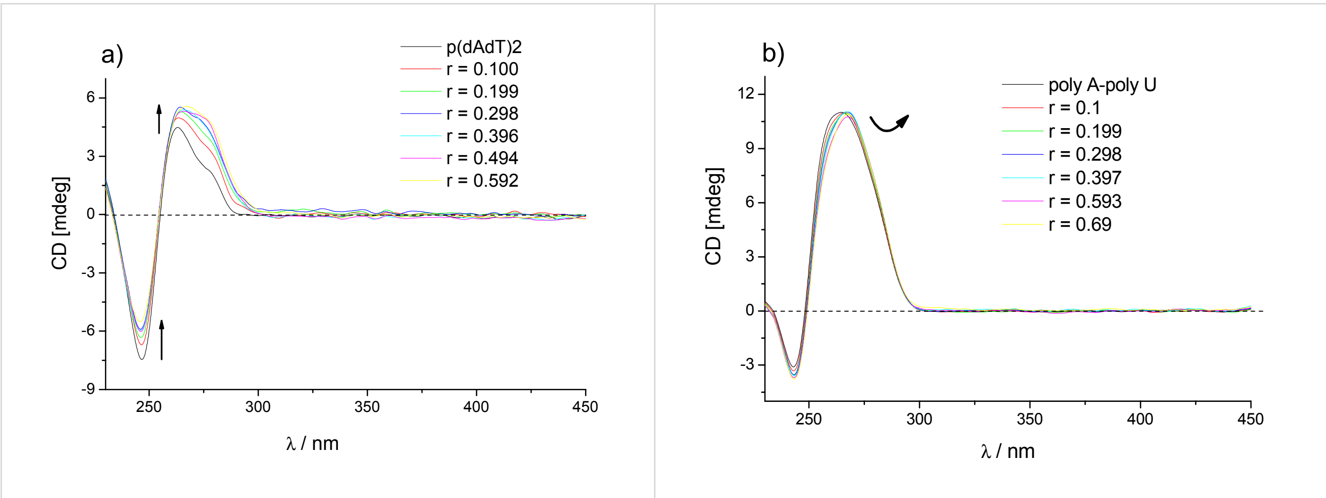

Figure S9. CD titrations of a) poly (dAdT)$_2$ and b) poly A – poly U ($c = 3.0 \times 10^{-5}$ mol dm^{-3}) with **5** at molar ratios ***r*** = [compound] / [polynucleotide] (pH 7.0, buffer sodium cacodylate, I=0.05 moldm^{-3}).

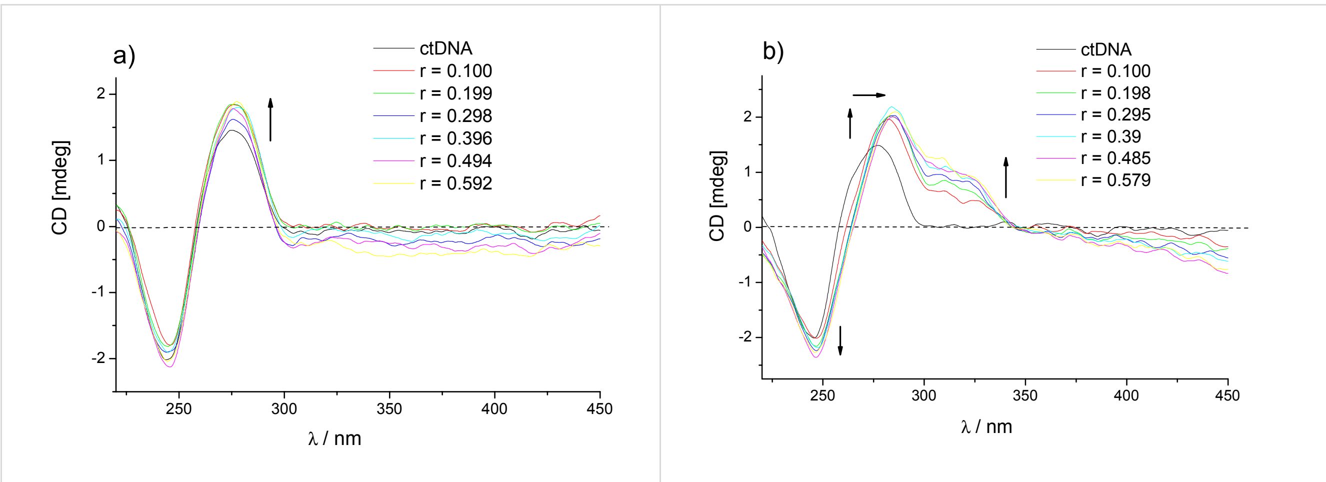

Figure S10. CD titrations of ctDNA ($c = 3.0 \times 10^{-5}$ mol dm^{-3}) with a) **5** and b) **6** at molar ratios ***r*** = [compound] / [polynucleotide] (pH 7.0, buffer sodium cacodylate, I=0.05 moldm^{-3}).

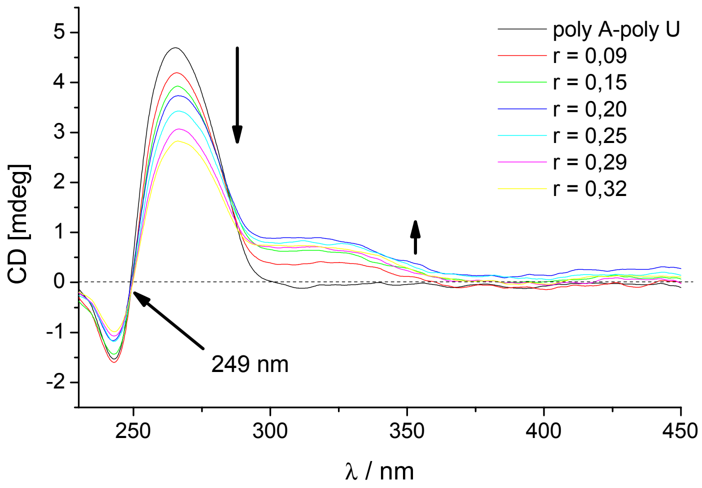

Figure S11. CD titration[1] of poly A-poly U (c = 1.5 × 10^{-5} mol dm^{-3}) with **9** at molar ratios ***r*** = [compound] / [polynucleotide] (pH 5.0, citric acid buffer, I = 0.03 mol dm^{-3}).

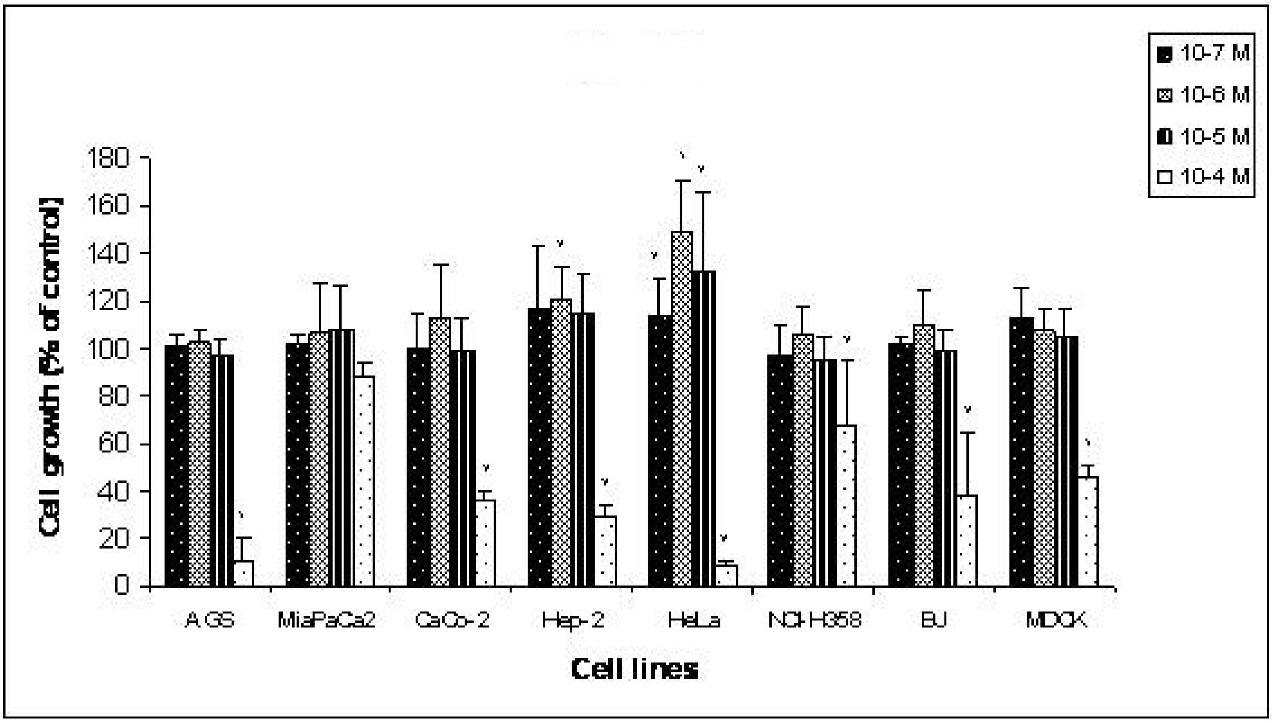

Figure S12: Cytotoxic effects of compound **5** on tumor and normal cell lines growth after 72 h of incubation in final concentration range (10^{-4}– 10^{-7} mol/dm^3).Data are presented as mean value ± SD of three independent experiments done in three plicate. Statistically significant change ($p < 0.05$) is presented by (*).

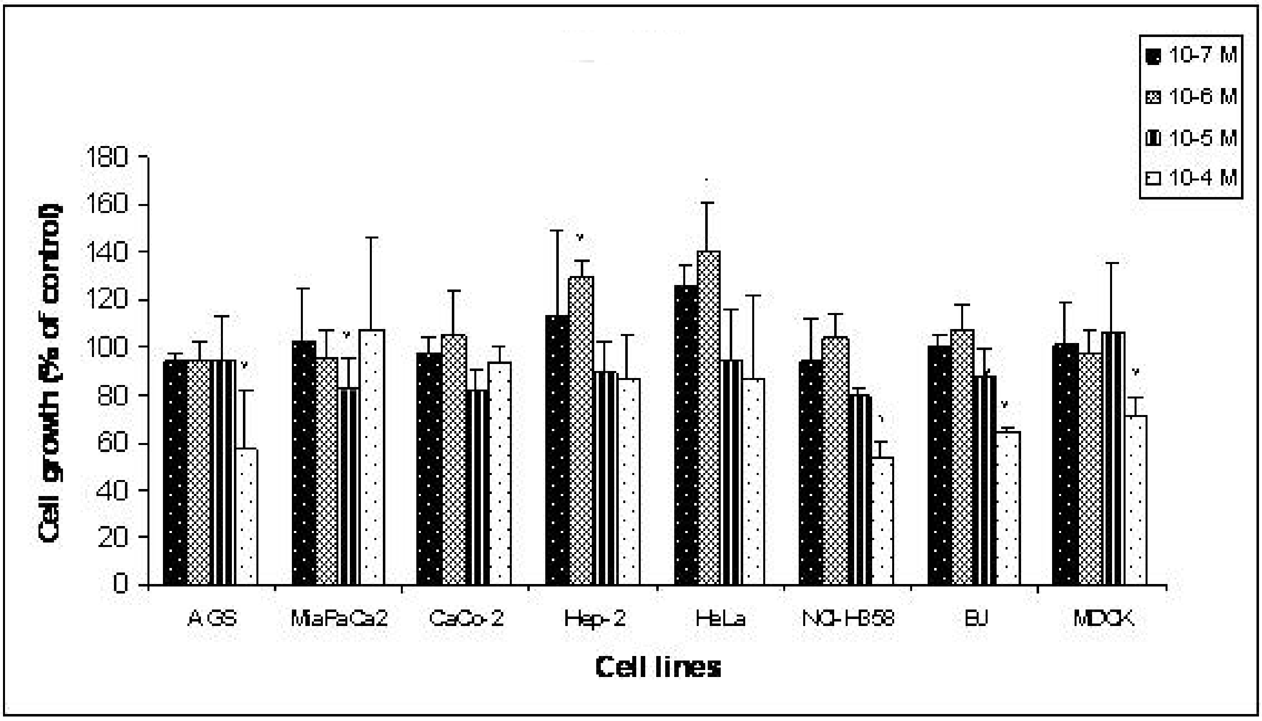

Figure S13: Cytotoxic effects of compound **6** on tumor and normal cell lines growth after 72 h of incubation in final concentration range (10^{-4}– 10^{-7} mol/dm^3).Data are presented as mean value ± SD of three independent experiments done in three plicate. Statistically significant change ($p < 0.05$) is presented by (*).

Table S1. Preliminary assignment of the vibrational bands observed in the SERS spectra of the **5** and **6** and their complexes with ctDNA, [**5**,**6**]/[DNA] 1/20

Wavenumber / cm^{-1}				Assignment
5	**5**/DNA 1/20	**6**	**6**/DNA 1/20	
1623	1624	1621	1620	ν ring (ν CC/CN), ν CN
1616 sh	1612			ν CN, δ NH_2
1582	1583	1591 sh	1592 sh	ν ring (ν CC/CN)
1536	1537	1543	1542	ν ring (ν CC)
1467	1466	1465 sh	1465 sh	δ_{as} CH_3
		1449	1448	ν ring (ν CC)
1422	1419 sh	1426	1419 sh	ν_s CNC, ν CN_3, δ NH_2
			1414	ν ring (ν CC)
1391	1392	1389	1388	ν ring (ν CC)
1365	1366	1361	1362	ν ring (ν CC), δ_s CH_3
1345	1346	1328 sh	1328 sh	ν ring (ν CC)
1298	1300	1277	1284	δ_{ip} CH, δ NH
1258	1257			δ_{ip} CH
1229	1227	1221	1222	δ_{ip} CH, ν_{as} CNC, ν CN_3

1210	1212			δ_{ip} CH, δ NH
		1185		δ_{ip} CH
1154	1157	1154	1154	δ_{ip} CH
		1138	1137	δ_{ip} CH
1076	1081	1079	1080	δ NH_2, ν CN_3
1039	1039			ν ring (ν CC)
1007	1004			ν CN_3, δ NH_2
		971	966 sh	δ ring
952	952	952 sh	954	δ ring
923	924	911	911	δ CNC, ν CN, δ NH_2
893	891			ν ring (ν CC)
869	870	870	867	ν ring (ν CC), δ_{oop} CH
837				δ ring
		797	797	δ ring, δ CNC
727	729	722	729	δ ring
		706 sh	708	δ ring
		696	696	δ ring
655	655	679	679	δ ring
617	618 sh			δ ring
588	600			δ NH_2, δ NH, δ ring
513 sh	516	520	520	δ CNC, δ ring
506	504			δ ring
462	460 sh	463	459	δ_{as} CNC
448	447	435	435	δ ring
421	421	395	395	δ CN_3, δ NH_2
341	339	328	326 sh	δ_s CNC
227	224	227	223	ν Ag–N

Abbreviations: sh, shoulder; ν, stretching; δ, deformation; s, symmetrical; as, antisymmetrical; ip, in plane; oop, out of plane.

[1] M. Radić Stojković, I. Piantanida, Tetrahedron 64 (2008) 7807-7814