Electronic Supplementary Material (ESI) for Analyst.

A new insight into the interaction of cisplatin with DNA: ROA spectroscopic studies on the therapeutic effect of the drug

M. Gąsior-Głogowska, K. Malek, G. Zajac and M. Baranska*

ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Positions (in cm^{-1}) and Tentative Assignment of Major Bands Observed in Raman and Raman Optical Activity ROA Spectra of Herring Sperm DNA and DNA-Cisplatin [1–8].

Raman spectra		ROA spectra			
DNA	DNA-cisplatin (0.01)	DNA	DNA-cisplatin (r = 0.01)	DNA-cisplatin (r = 0.02)	Assignments
wavenumber / cm^{-1}					
1660 s, br	1655 s, br	-1660 m	+1638 w	+1637 m	ν(C=O), δ(NH_2) of dT, dG, dC; δ(OH) of water
			-1625 w	-1620 m	
1579 s	1581 m	-1571 m	-1574 m	-1574 m	dG, dA
-	1556 vw, sh				dC
1513 w, sh	1511 vw, sh				dA, dC
1490 s	1489 m	+1495 w	+1497 w	+1500 w	dG, dA
1459 m	1458 w				δ(CH), dA, dT
		+1431 m	+1430 m	+1430 m/w	δ(CH)
1424 m	1423 m		-1418 w	-1417 w	δ(CH)
1380 s	1377 m	+1383 m	+1381 m	+1384 m	dT, dA, dG
		-1365 w	-1364 m	-1367 m	dT, dA, dG
1341 s	1341 m	-1342 m	-1336 m/w	-1337 w/vw	dG, dA
1315 s	1311 m	+1319 s	+1314 s	+1321 s	dG, dA
1259 m	1256 m				$\nu_{antisym}(PO_2^-)$, dC, dA, dT
1243 m	1240 m	-1257 vs	-1257 vs	-1257 vs	$\nu_{antisym}(PO_2^-)$, dT, dC
1216 m	1215 m, sh	-1214 m	-1211 s	-1213 s	$\nu_{antisym}(PO_2^-)$, dT
1185 m, sh	1185 m, sh				dT, dC
1146 w	1145 vw				ν(C-C)
		+1120 w	+ 1125 w	+1125 vw	dA
1097 s	1096 s		-1093 vw	-1093 w	$\nu_{sym}(PO_2^-)$
		+1078 w			$\nu_{sym}(PO_2^-)$
1051 vs	1050 s	+1053 w	+1055 w	+1056 w	$\nu_{sym}(PO_2^-)$, ν(C-O)
1027 m, sh	1023 m, sh				dA, d
			- 1008 m	-1010 s	ν(C-O)
		-989 m	-990 w	-987 w	ν(C-O)
981 vw, sh	976 vw	+971 w	+967 w	+966 w	ν(C-O)
		-939 m	-936 m	-936 m	d
925 vw	922 vw, sh	+918 w	+ 923 w	+924 w	d
899 vw	897 vw, sh				d
843 m, sh	839 m, sh				$\nu_{antisym}$(O-P-O)
			-826 w	-826 w	$\nu_{antisym}$(O-P-O)
815 s, sh	810 s, sh	-801 m	-800 m	-800 m	$\nu_{antisym}$(O-P-O)
795 vs	795 vs				ν_{sym}(O-P-O), dC
757 w	754 w, sh	+753 m	+755 w	+758 w	dT
734 w	734 w				dT, dA
684 w	686 vw				C2'-endo/anti, dG

r – molar ratio of Pt/nucleotide. ROA band: - negative, + - positive. Band intensity: vs – very strong, s – strong, m – medium, w – weak, vw – very weak, sh – shoulder, br – broad. Mode: ν - stretching, δ - in-plane bending, Components: dA – deoxyadenosine, dC – deoxycytidine, dG – deoxyguanosine, dT – thymidine, d – deoxyribose

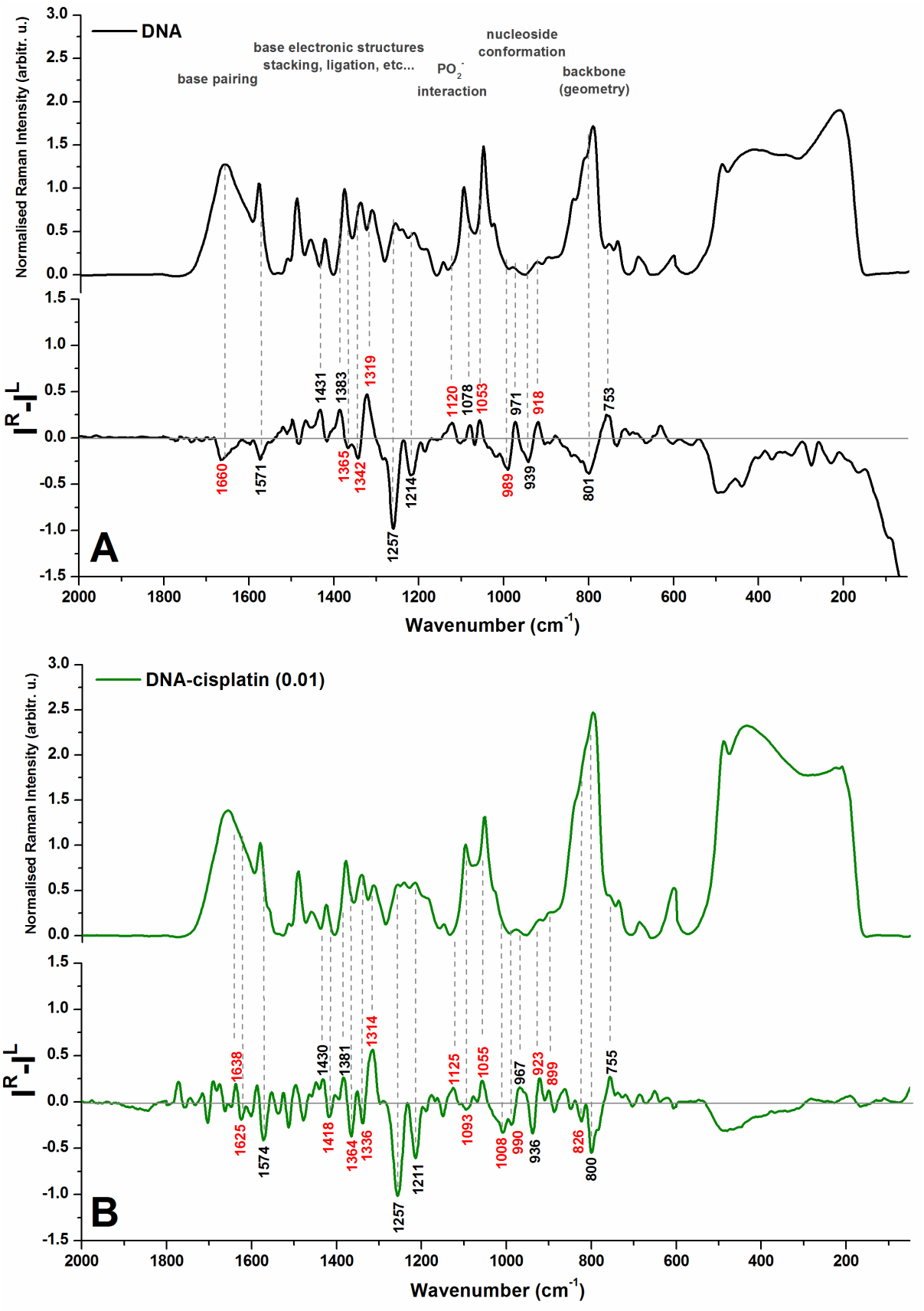

Figure S1. Backscattered SCP Raman and Raman optical activity (ROA) spectra of DNA (A) and DNA complex with cisplatin at 0.01 molar ratio of Pt/nucleotide (B) in the range 2000-50 cm^{-1}.

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