Supplementary Information

Polypyridyl Ruthenium Complexes: Novel DNA-Intercalating Agents against Human Breast Tumor

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Table S1. The most important bands in the IR of complexes (**1-4**). Pellets, in CsI

Band / cm^{-1}	**1**	**2**	**3**	**4**
$\nu(C-H)_{arom}$	3051	3053	3060	3053
$\nu(C-H)_{aliph}$	2920, 2989	2923, 2853	2927, 2851	–
ν(C=N)	1587, 1542,	1588, 1542,	1587, 1542,	1481, 1434,
+ ν(C=C)	1494, 1434,	1496, 1469,	1500, 1471,	1419, 1384,
+ δ(C–H)	1417, 1383,	1434, 1418,	1436, 1422,	1346, 1309
	1349, 1315	1384, 1350, 1312	1397, 1386, 1351	
$\nu(P-C)_{arom}$	1114, 1090	1116, 1092	1116, 1090	1112, 1090
+ δ(C=N)				
ν(P–F)	–	–	844	–
$\gamma_{(arom\ rings)}$	699	697	697	697
δ(P–F)	–	–	558	–
ν(Ru–P)	508	507	507	518
ν(Ru–N)	425	419	427	430
ν(Ru–Cl)	317	302, 280	320	318
νCO	–	–	1996	–

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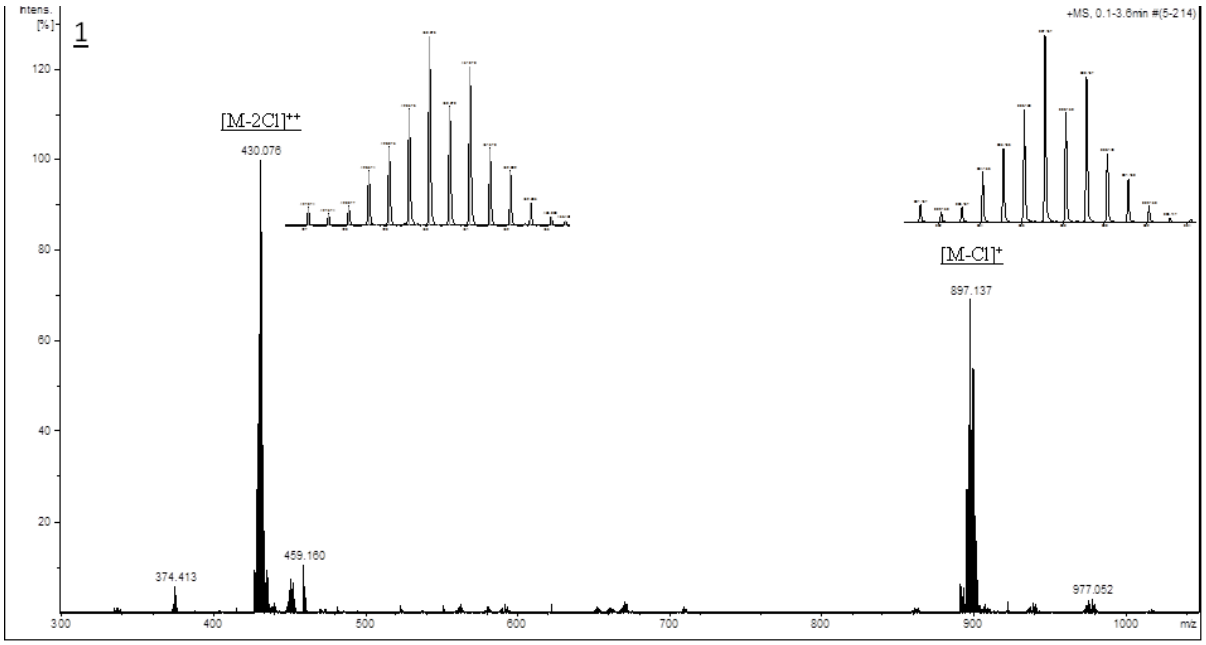
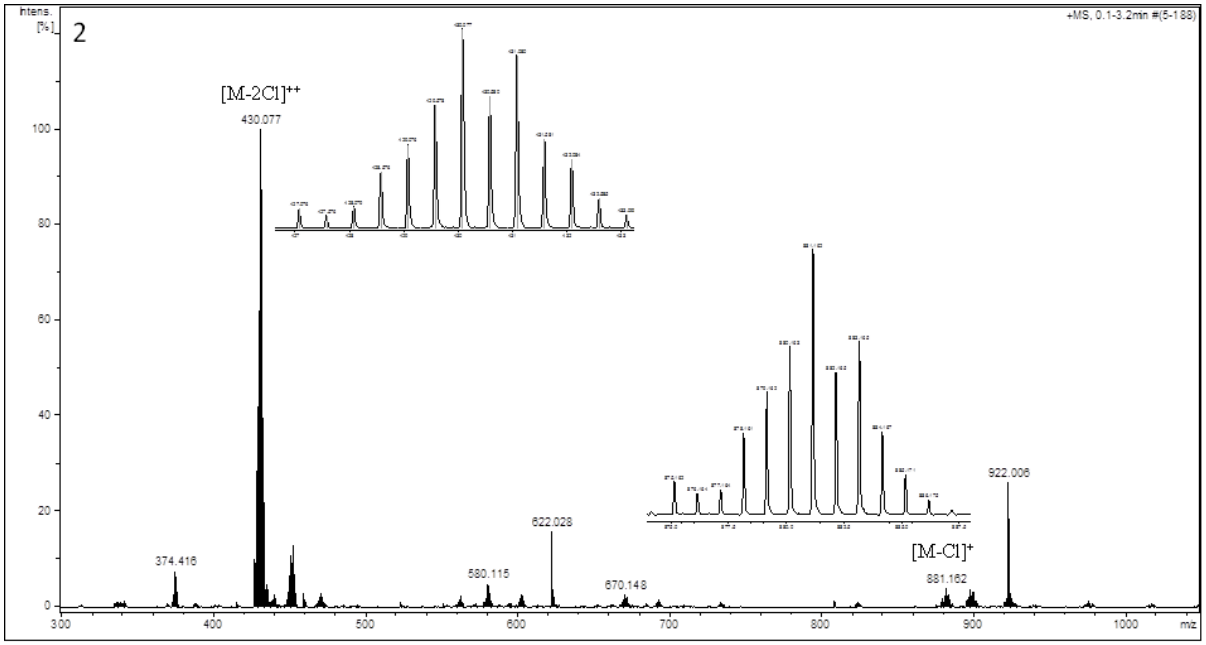
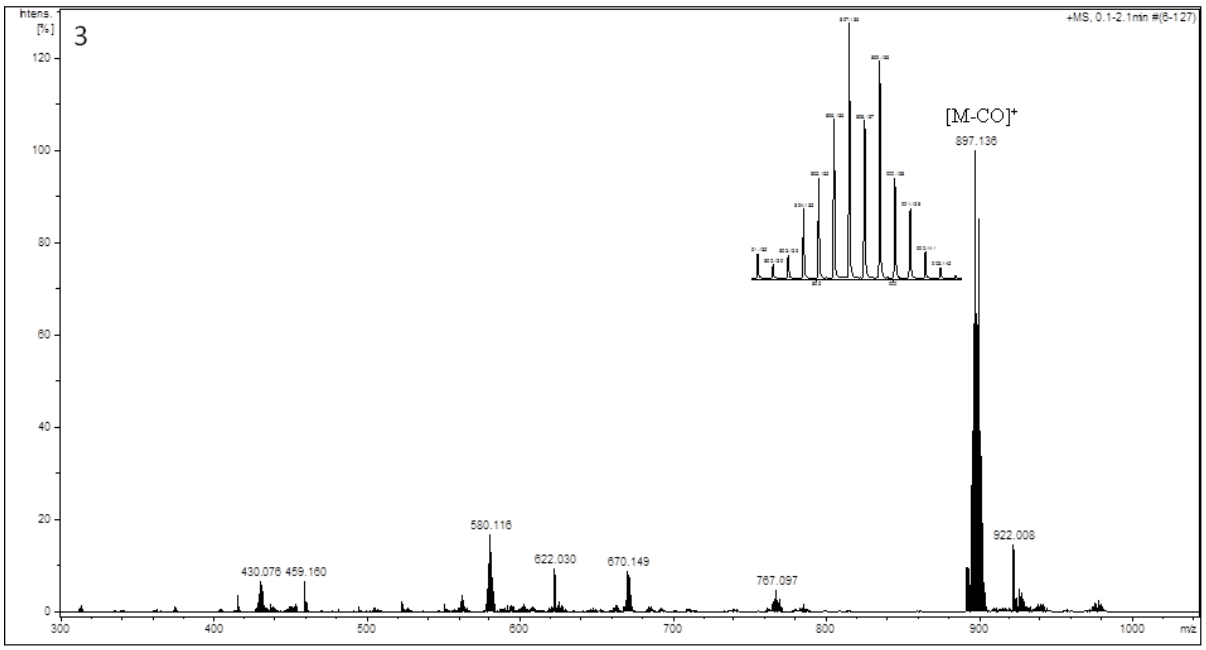

1
Intens.
[%]
+MS, 0.1-3.6min #(5-214)
[M-2Cl]++
430.076
[M-Cl]+
897.137
374.413
459.160
977.052
300
400
500
600
700
800
900
1000
m/z


2
Intens.
[%]
+MS, 0.1-3.2min #(5-188)
[M-2Cl]++
430.077
[M-Cl]+
922.006
622.028
374.416
580.115
670.148
881.162
300
400
500
600
700
800
900
1000
m/z



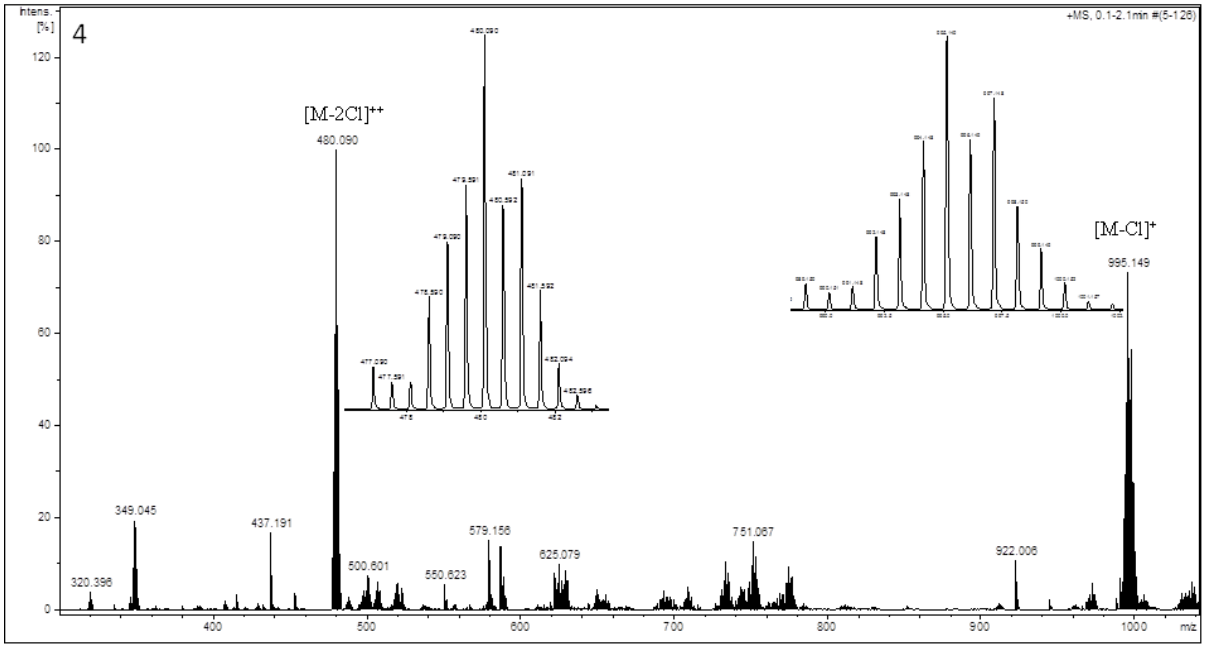
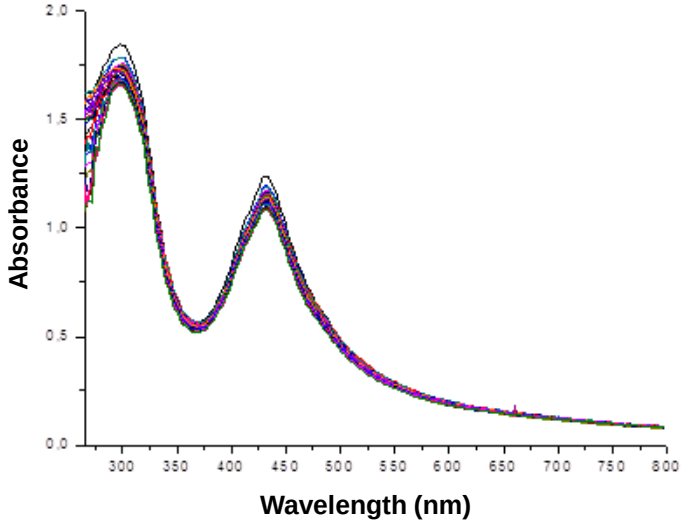
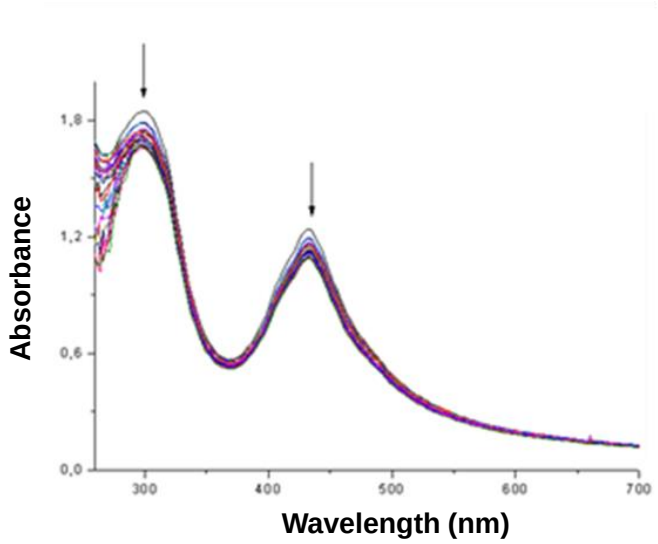
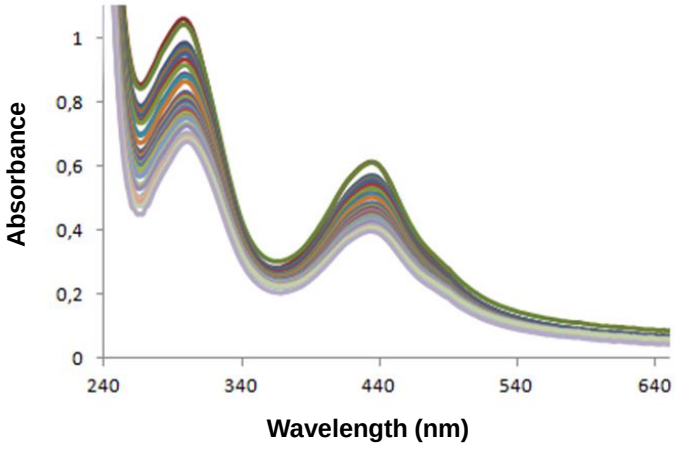


Figure S1. Mass spectra of *trans*-[$RuCl_2$(dppb)(dpqQX)] (**1**), *cis*-[$RuCl_2$(dppb)(dpqQX)] (**2**), *ct*-[RuCl(CO)(dppb)(dpqQX)]PF_6 (**3**) and *ct*-[$RuCl_2(PPh_3)_2$(dpqQX)] (**4**).


Absorbance
2,0
1,5
1,0
0,5
0,0
300
350
400
450
500
550
600
650
700
750
800
Wavelength (nm)


Absorbance
1,8
1,2
0,6
0,0
300
400
500
600
700
Wavelength (nm)


Absorbance
1
0,8
0,6
0,4
0,2
0
240
340
440
540
640
Wavelength (nm)

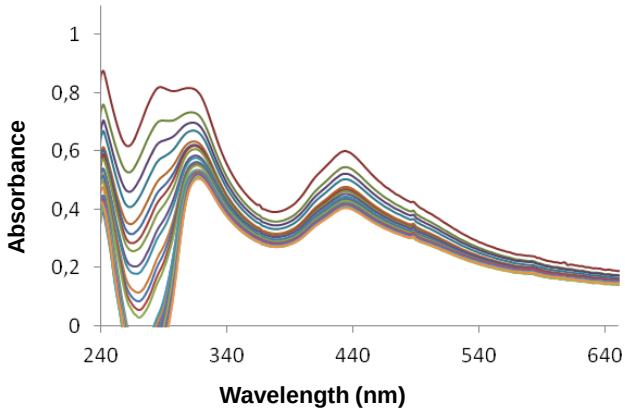


Figure S2. Electronic absorption spectra of (**1**), (**2**), (**3**) and (**4**) with increasing amounts of CT DNA in Tris-HCl buffer (5 mM Tris-HCl and 50 mM NaCl, pH 7.4).

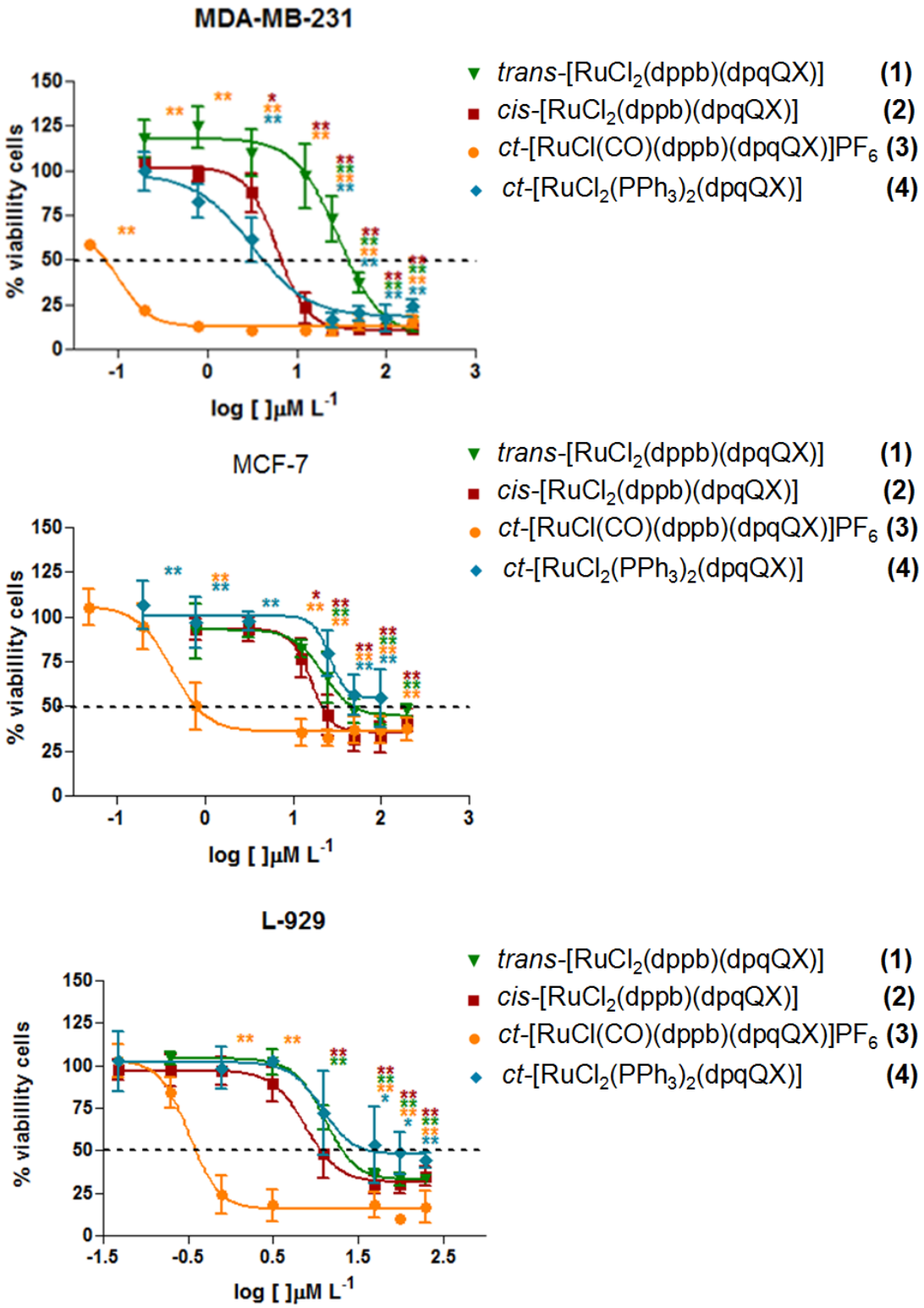


Figure S3. Effect of the compounds (**1-4**) on the viability of tumor cell lines MDA-MB 231, MCF-7 and on mouse fibroblasts L929 cells. Activity represented by IC_{50} values; *p*-values determined by Dunnett's test, compared to the control; (*) $p < 0.05$ and (**) $p < 0.01$.