SUPPLEMENTARY MATERIAL

A novel ruthenium(II) gallic acid complex disrupts the actin cytoskeleton and inhibits migration, invasion and adhesion of Triple Negative Breast Tumor Cells

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Table 1S. Infrared assignments (cm^{-1}) of symmetric (vs) and asymmetric (vas) stretching of carboxyl group in free and coordinated ligand.

Compound	$\nu_{as}COO^-$	ν_sCOO^-	$\Delta(cm^{-1})$
HBAC	1688	1453	235
HGAC	1666	1468	198
HEGA	1697	1432	265
[Ru(BAC)	1619	1499	120
[Ru(GAC)	1622	1497	125
[Ru(EGA)	1624	1512	112

Table 2S. Crystallographic data and structures refinement for **Ru(BAC)** and **Ru(EGA).**

	Ru(BAC)	Ru(EGA)
Empirical formula	$C_{90}\ H_{83}\ F_{12}\ N_4\ O_{4.50}\ P_6\ Ru_2$	$C_{51}\ H_{47.50}\ F_6\ N_2\ O_{8.25}\ P_3\ Ru$
Formula weight	1908.56	1128.39
Temperature	293(2) K	293(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Monoclinic
Space group	P -1	$P2_1/a$
Unit cell dimensions	a = 11.7551(2) Å α= 110.1960(10)°. b = 17.4930(4) Å β= 97.4780(10)°. c = 22.9633(4) Å γ = 99.2730(10)°.	a = 18.6440(6) Å α= 90°. b = 31.0250(8) Å β= 110.1340(10)° c = 19.4890(7) Å γ = 90°.
Volume	4284.88(15) $Å^3$	10584.1(6) $Å^3$
Z	2	8
Density (calculated)	1.479 Mg/m^3	1.416 Mg/m^3
Absorption coefficient	0.545 mm^{-1}	0.461 mm^{-1}
F(000)	1946	4612
Crystal size	0.20 x 0.40 x 0.40 mm^3	0.12 x 0.13 x 0.34 mm^3
Theta range for data collection	3.017 to 26.093°.	1.292 to 25.598°.
Index ranges	-14≤h≤14, -21≤k≤21, -28≤l≤28	-17≤h≤22, -37≤k≤35, -23≤l≤15
Reflections collected	72618	45924
Independent reflections	16813 [R(int) = 0.0777]	18766 [R(int) = 0.0638]
Completeness to theta	(25.242) 98.9 %	(25.242°) 95.1 %
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	16813 / 0 / 1072	18766 / 0 / 1265
Goodness-of-fit on F^2	1.023	0.967
Final R indices [I>2sigma(I)]	R1 = 0.0597, wR2 = 0.1599	R1 = 0.0780, wR2 = 0.1946
R indices (all data)	R1 = 0.0931, wR2 = 0.1815	R1 = 0.1657, wR2 = 0.2515
Largest diff. peak and hole	1.009 and -0.800 $e.Å^{-3}$	0.869 and -0.995 $e.Å^{-3}$

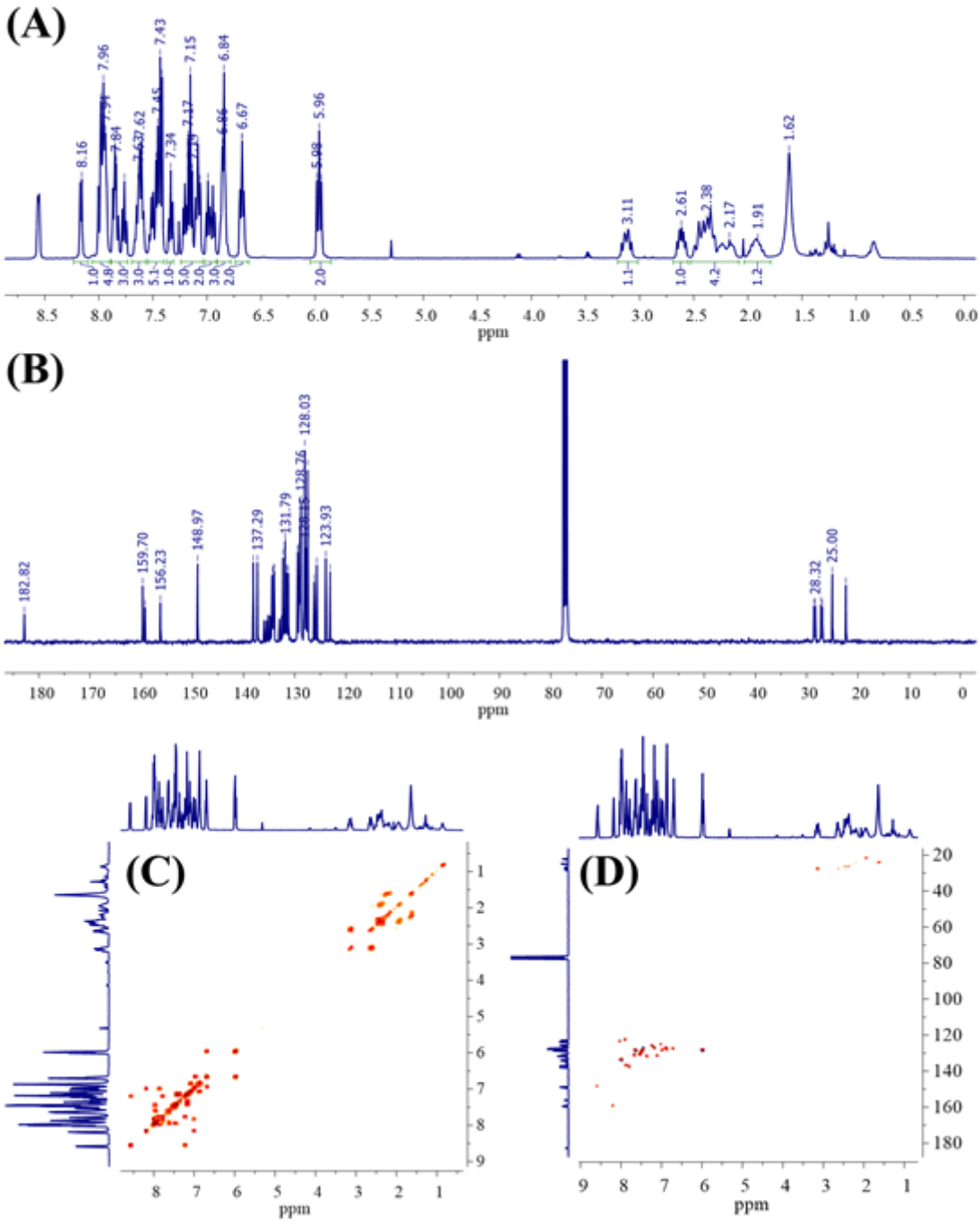


Figure 1S: ^{1}H (A), $^{13}C\{^{1}H\}$ (B), ^{1}H-^{1}H COSY (C) and ^{1}H-^{13}C HSQC (D) NMR spectra of complex **Ru(BAC)** in chloroform-d at 298 K.

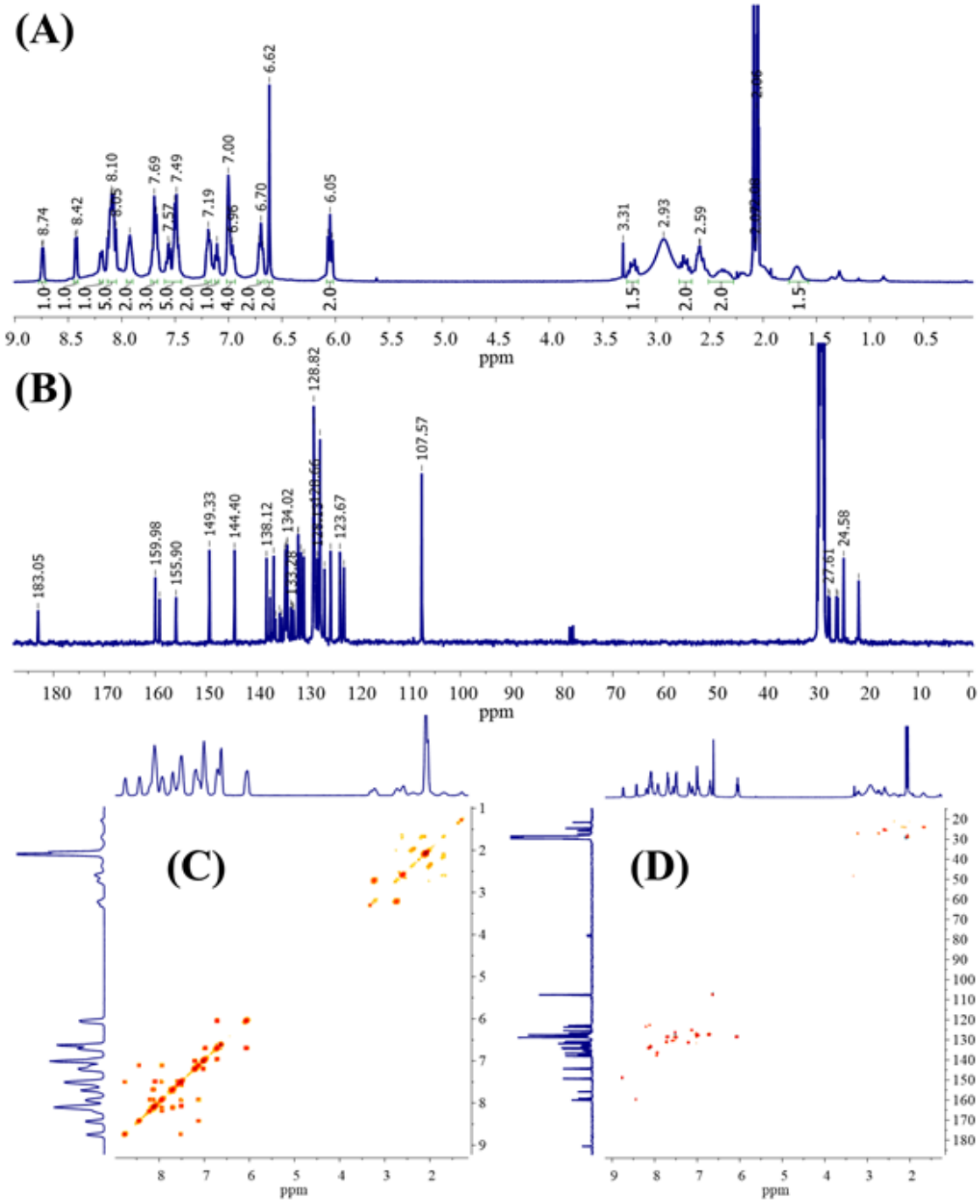


Figure 2S: ^{1}H (A), $^{13}C\{^{1}H\}$ (B), ^{1}H-^{1}H COSY (C) and ^{1}H-^{13}C HSQC (D) NMR spectra of complex **Ru(GAC)** in chloroform-d at 298 K.

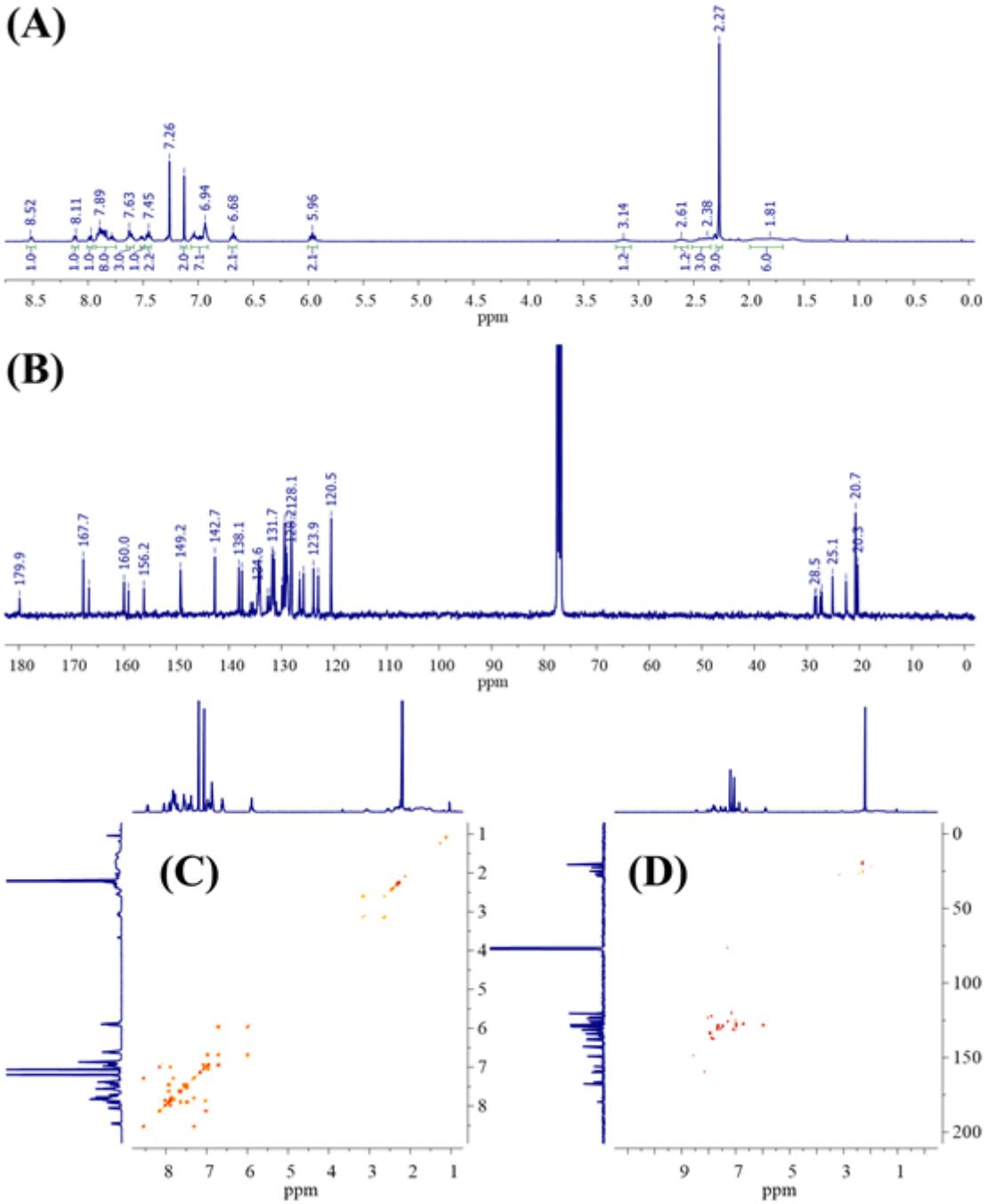


Figure 3S: ^{1}H (A), $^{13}C\{^{1}H\}$ (B), ^{1}H-^{1}H COSY (C) and ^{1}H-^{13}C HSQC (D) NMR spectra of complex **Ru(EGA)** in chloroform-d at 298 K.

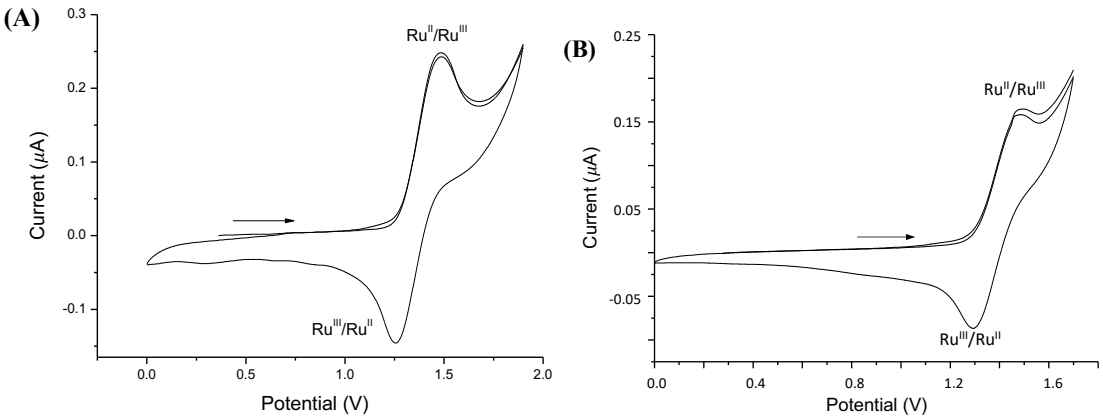


Figure 4S: Cyclic voltammograms for complexes (A) **Ru(BAC),** (B) **Ru(EGA)** in Pt disc electrode (0.1 M PTBA, 100 mV s^{-1}, reference electrode: Ag/AgCl).

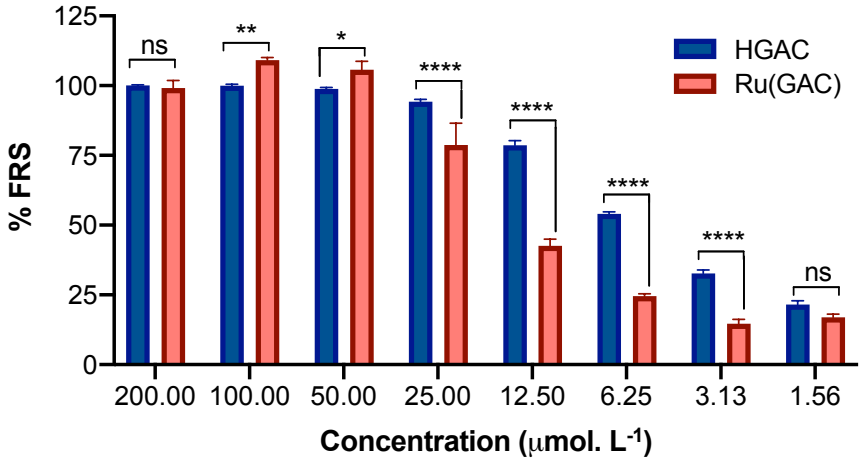


Figure 5S: % FRS of the ligand **HGAC** and the complex **Ru(GAC)** after 30 minutes of reaction. Data represents mean ± SD from three independent assays in triplicate. Significance at the *p < 0.05; **p < 0.01and ****p < 0.0001 levels using 2way ANOVA and Sidak's test.

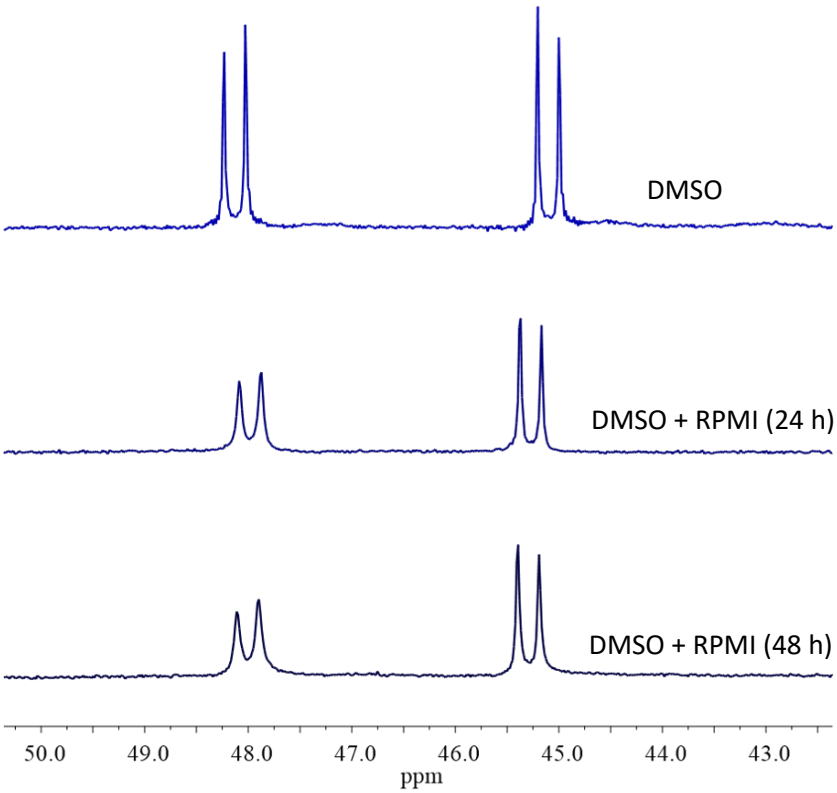
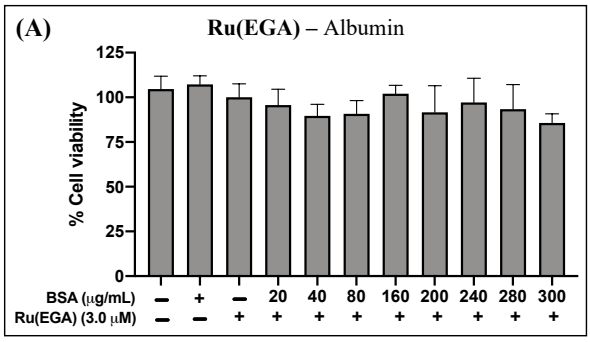


Figure 6S: $^{31}P\{^{1}H\}$ NMR spectra of stability studies of complex **Ru(GAC)** under physiological conditions DMSO/RPMI medium (2:1).



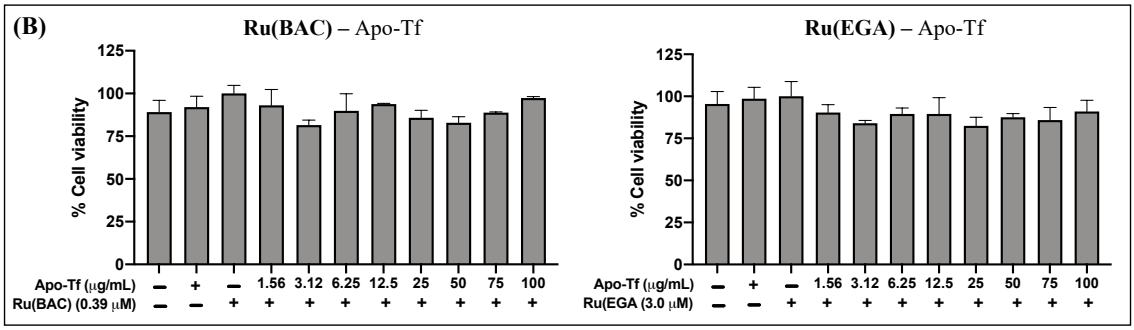


Figure 7S: Transport of ruthenium complex by albumin and transferrin in MDA-MB-231. The complexes, with fixed concentrations, were incubated with increasing concentrations of bovine serum albumin (A) or apo-Tf (B) for 48 h. Viable cells were estimated by MTT assay, and results were compared to cells treated with the complexes but in the absence of the proteins. Data represents mean ± SD from two independent assays in triplicate. Significance at the *p < 0.05; **p < 0.01; ***p < 0.001 and ****p < 0.0001 levels using ANOVA and Dunnet's test.