

Electronic Supplementary Information

Distinct Photophysical Behaviour and Transport of Cell-Impermeable $[\text{Ru}(\text{bpy})_2\text{dppz}]^{2+}$ in Live Cells using Cucurbit[7]uril as Delivery System

Meenakshi N. Shinde, , Soniya S. Rao, Shridhar P. Gejji and Anupa A. Kumbhar*

Department of Chemistry, Savitribai Phule Pune University, Pune-411 007, India.

* Author to whom correspondence should be addressed.

E-mail address: aak@chemunipune.ac.in

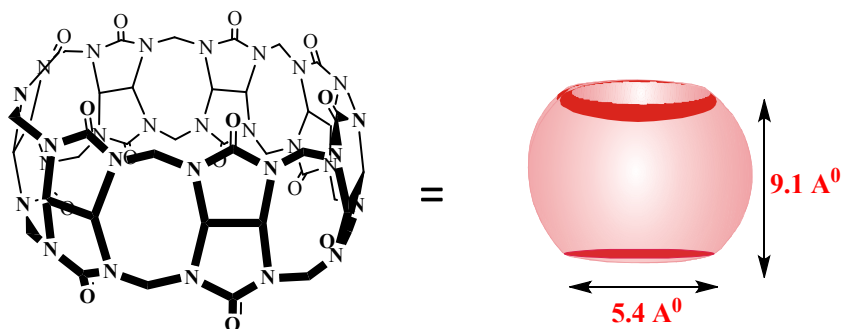


Chart S1. Structure of Cucurbit[7]uril

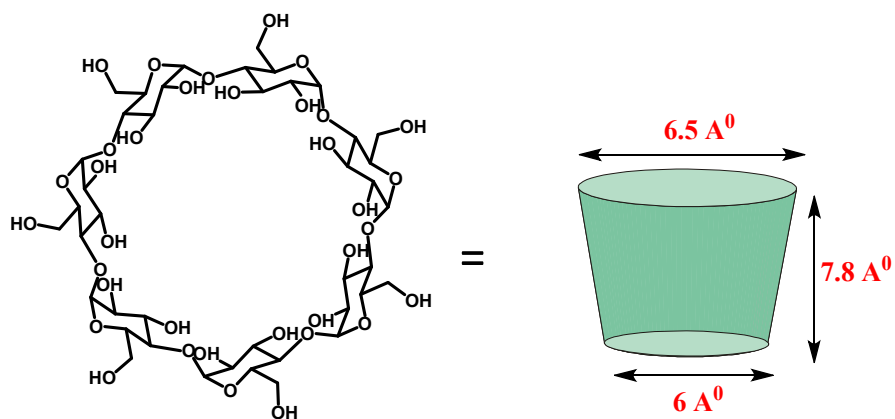


Chart S2. Structure of β -cyclodextrin

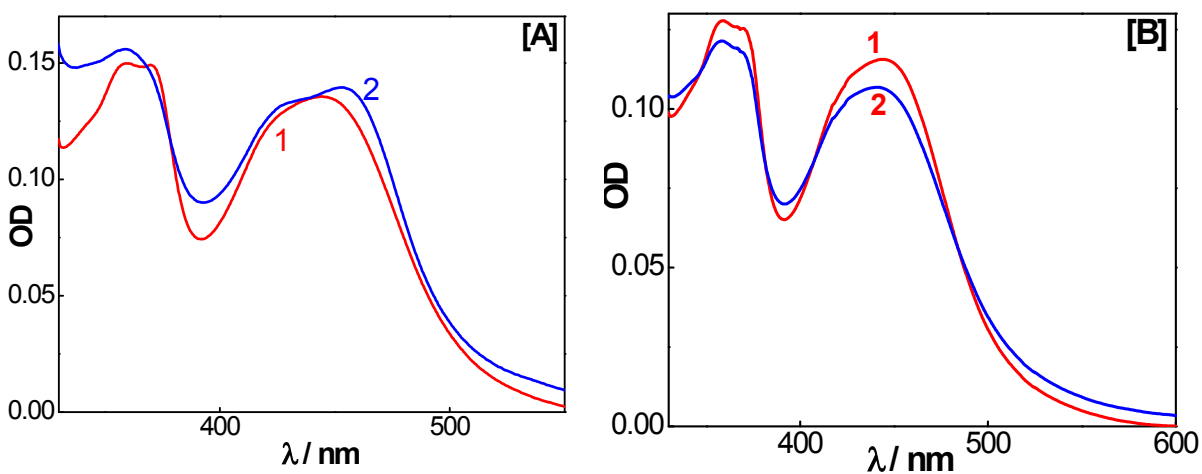


Fig. S1. Absorption spectra of complex 1 (7.5 μM) (A) in presence of CB7 (μM): 1) 0, 2) 1500 (B) in presence of β -CD (μM): 1) 0 2) 4000.

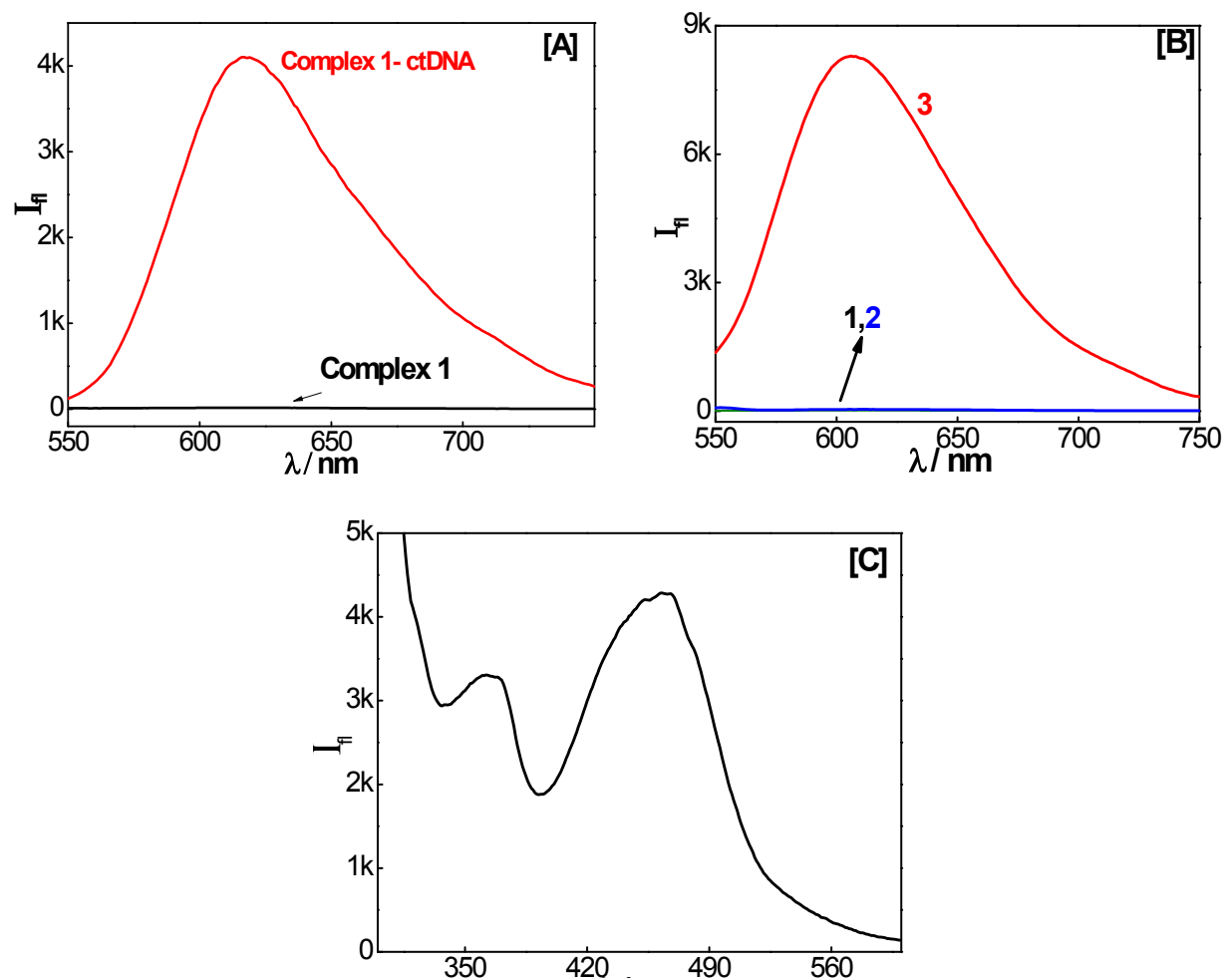


Fig. S2. (A). Emission spectra of Complex **1** (7.5 μ M) with Ct-DNA (400 μ M) (B). Emission spectra of Complex **1** (7.5 μ M) 1) in water (black line) 2) Complex **1** in β -CD (4000 μ M) (blue line) 3) Complex **1** with CB7 (1000 μ M) (red line) (C). Excitation spectra of Complex **1** (7.5 μ M) with CB7 (1000 μ M).

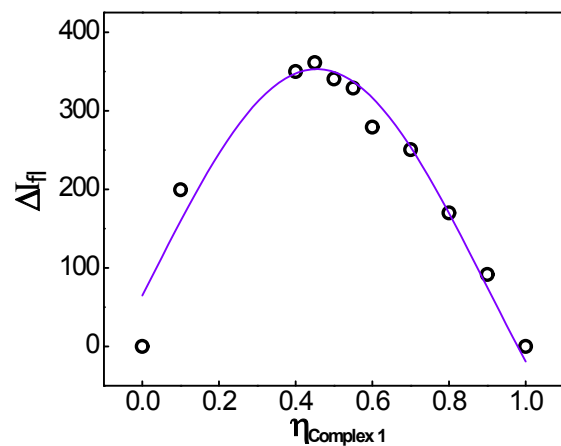


Fig. S3. Job's Plot for Complex 1-CB7

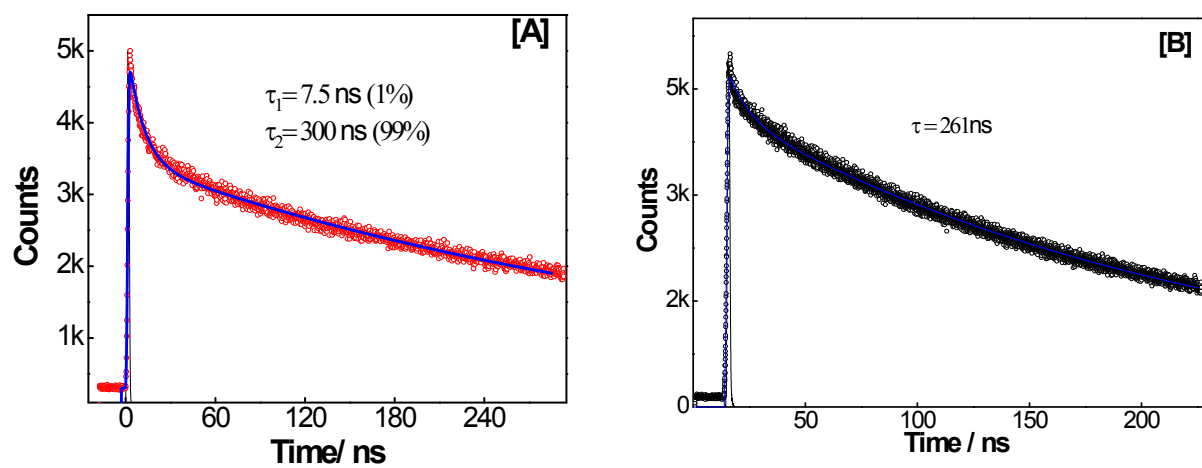


Fig. S4. Fluorescence lifetime decay of Complex **1** (7.5 μ M) (A) in CB7 (1mM) and (B) in n-octanol solvent

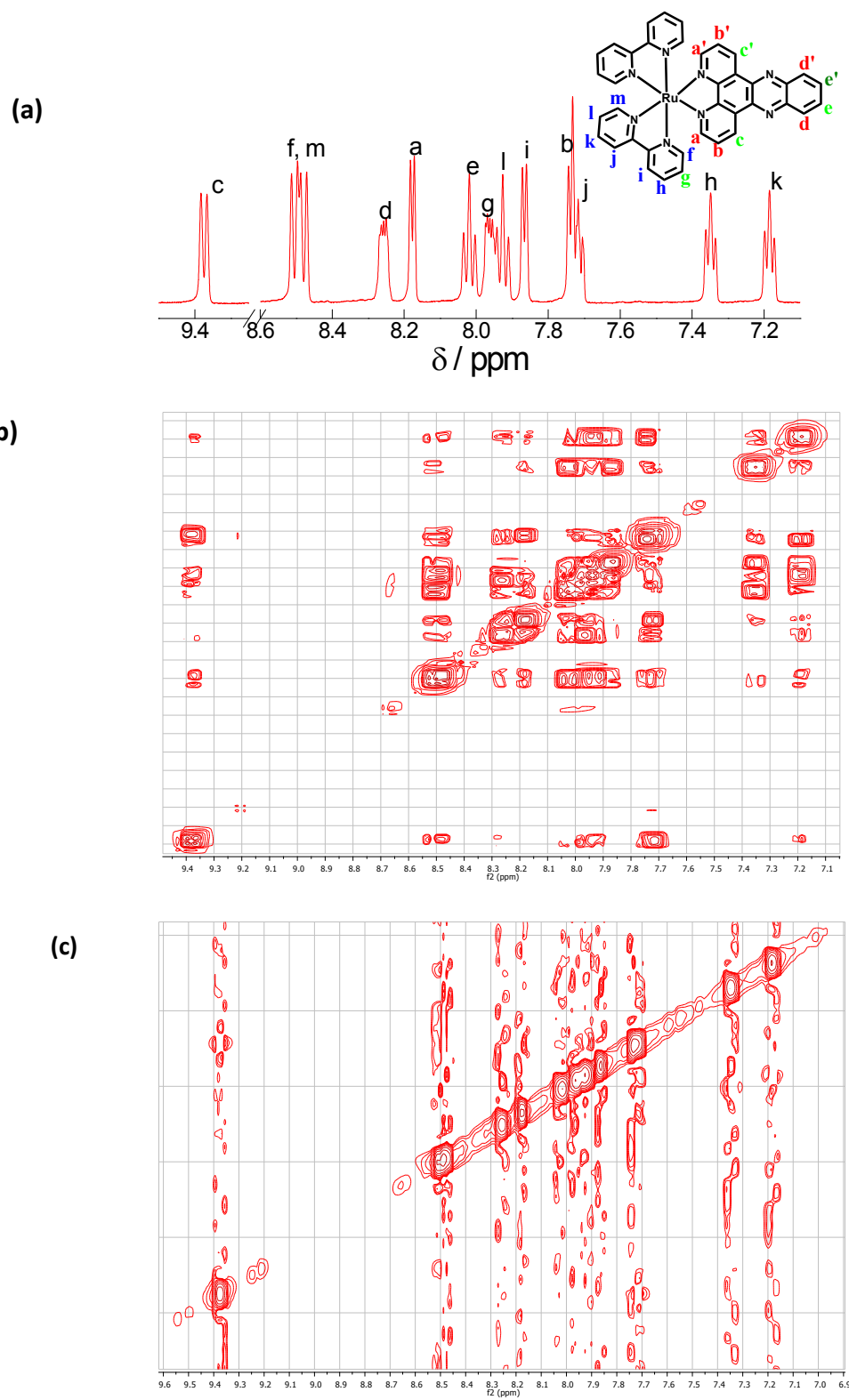


Fig. S5. (a) ^1H -NMR of free Complex **1** (b) ^1H -COSY NMR of free Complex **1** (c) ^1H -NOESY NMR of free Complex **1**

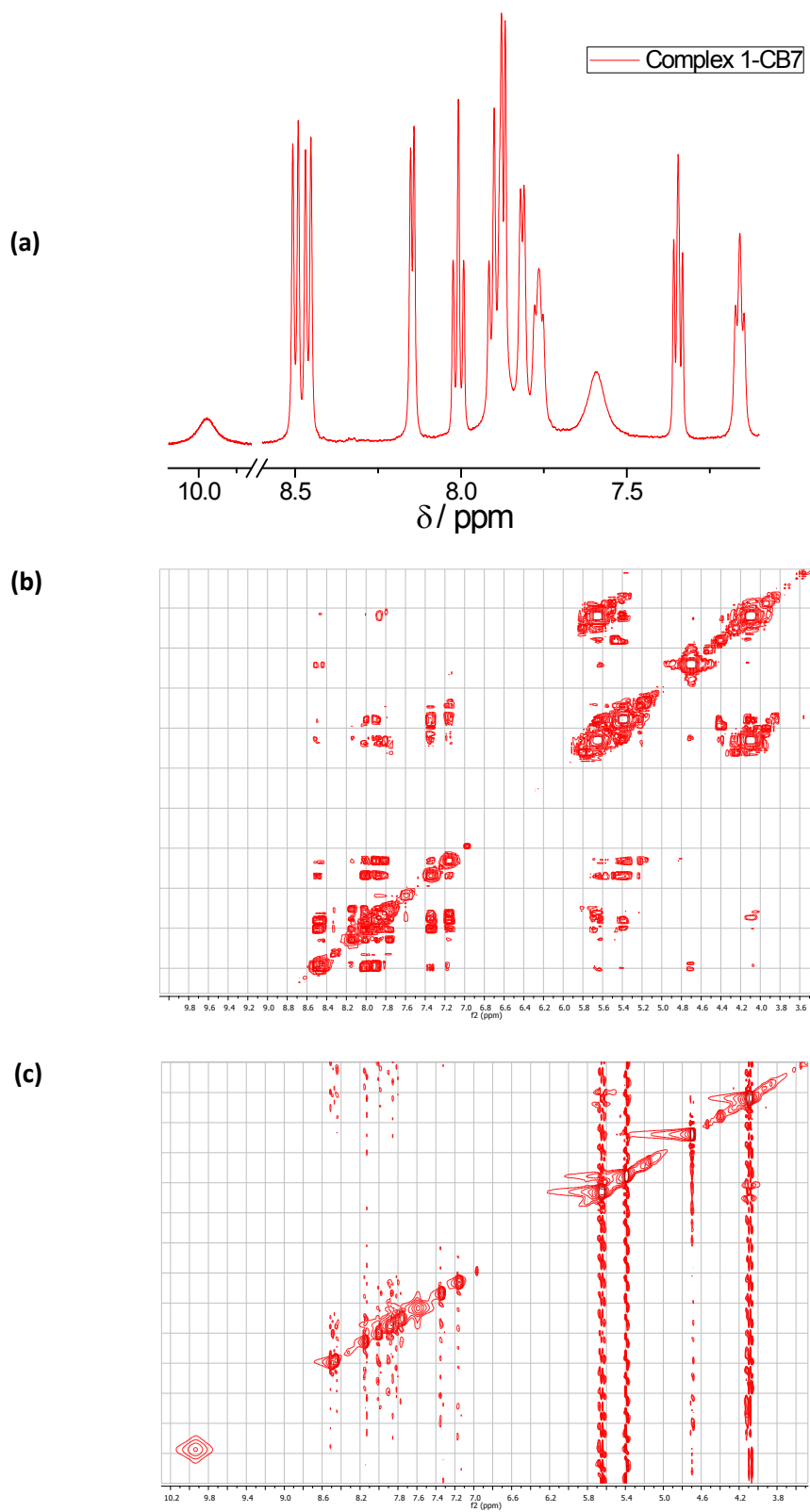


Fig. S6. (a) ^1H -NMR of complex **1**-CB7 (b) ^1H -COSY NMR of complex **1**-CB7 (c) ^1H -NOESY NMR of complex **1**-CB7

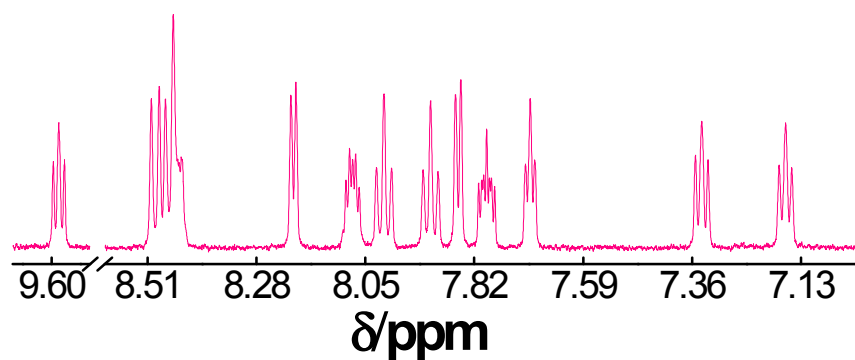


Fig. S7. ^1H -NMR of Complex **1**- β -CD

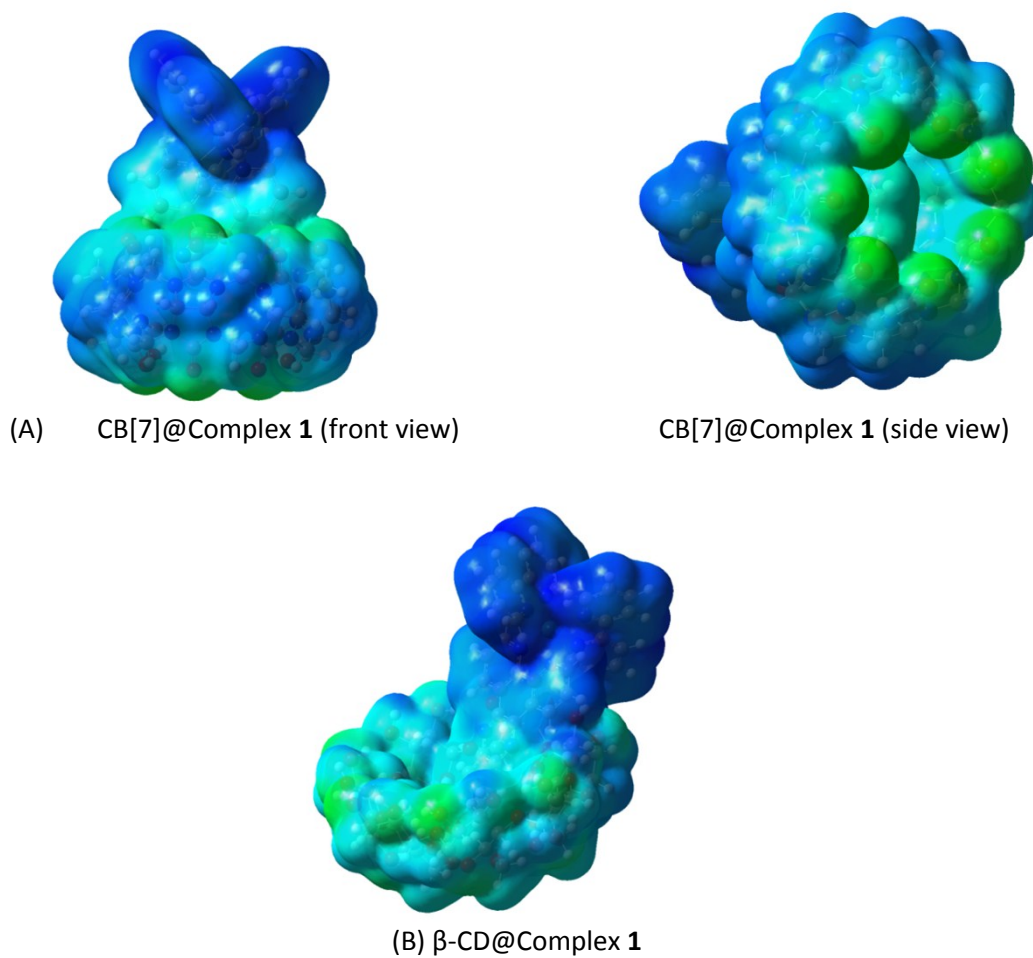


Fig. S8: Electron density isosurfaces (0.001 au) overlaid with MESP (from +0.045 to -0.045 au) in (A) **1**-CB7, (B) **1**- β -CD.

Table S1. Theoretical ^1H -NMR shifts in ppm

Protons	Free complex	Complex 1 @CB[7]	Complex 1 @ β -CD
H _e	9.63	9.27	10.37
H _d	9.77	9.34	9.93
H _c	9.63	9.18	8.03
H _g	8.66	8.36	9.374

Loading Efficiency: The loading efficiency was calculated considering that **1** is completely encapsulated (~100%) when emission titration attains saturation at 1.2mM of CB7 against 7.5 μM of **1**. Hence for cell imaging experiments, 200 μM of CB7 will guarantee 3.25 % encapsulation of loaded 100 μM of **1**. From that, we calculated the amount of encapsulated and free ruthenium. Then by using following equation, we calculated the loading efficiency:

Loading efficiency = (total amount of Ru encapsulated-free Ru)/(wt of complex **1**+wt of CB7)

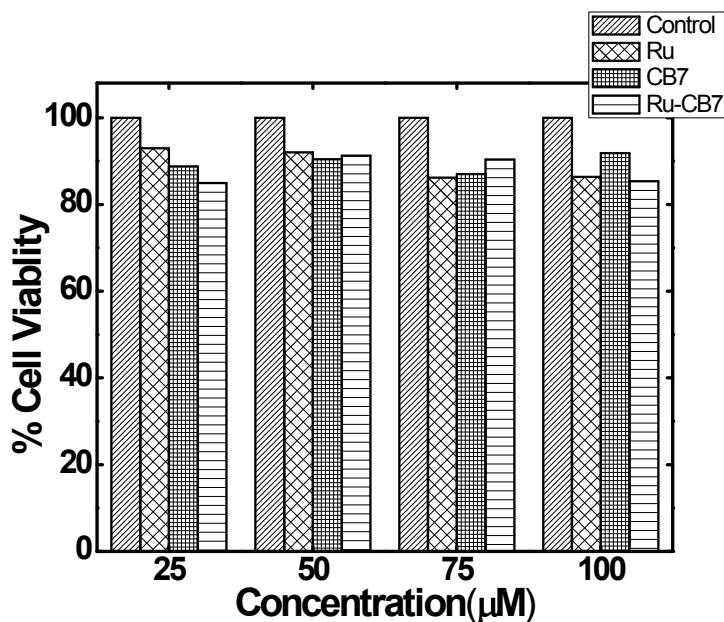


Fig. S9: Effect of concentration on cytotoxicity of complex **1**, CB7 and adduct of **1**-CB7 complex on MCF-7 cell line after 24 h incubation at 37°C. [**1**] = 25, 50, 75 and 100 μM and corresponding [CB7] = 50, 100, 150 and 200 μM . For [**1**-CB7 complex] = 25-50; 50-100; 75-150 and 100-200 μM respectively.

