

Supplementary information:

An in-vitro cytotoxicity study of 5-Fluorouracil encapsulated chitosan/gold nanocomposite towards MCF7 cells

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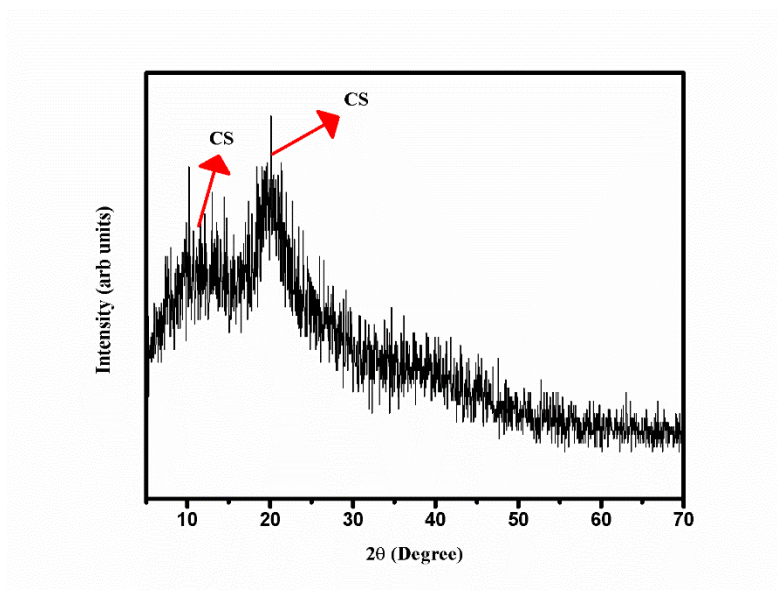


Figure S1. XRD pattern of Pure Chitosan.

Figure S1 shows the XRD pattern of pure chitosan. The occurrence of two peaks at $2\theta \sim 11.8^\circ$ and 21° shows the semi-crystalline nature of chitosan. The nature of peaks (broadness) is also indicative of the semi-crystallinity of chitosan. The obtained result is in agreement to the results already reported in the literature.

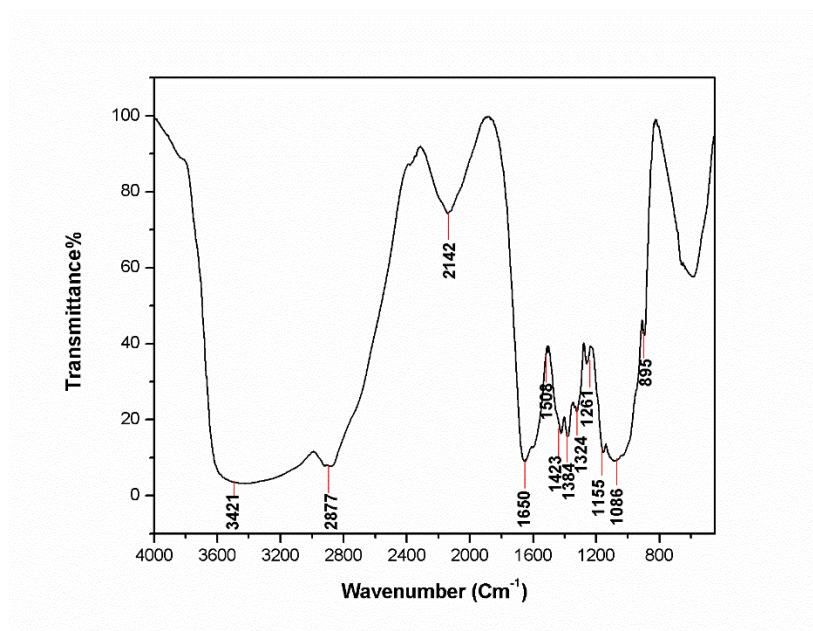


Figure S2. FTIR spectrum of pure chitosan.

The various vibrations obtained in the FTIR spectrum of chitosan are tabulated below.

Table S1. Various Vibrations in the FTIR spectrum of pure chitosan.

Wavenumber (cm ⁻¹)	Vibrations
895	NH ₂ twisting
1086	C-O stretching
1261	C-O-C stretching
1324	C-N stretching
1384	C-H bending
1423	CH ₂ bending
1508	Peak of NH ₃ ⁺
1650	C=O stretching & N-H bending
3421	O-H stretching

EDAX

The EDAX spectrum of CS/Au nanocomposite shows peaks corresponding to gold, carbon, oxygen and copper. The appearance of Cu is due to the use of Cu grids, on which the sample has been dispersed. Hence the presence of carbon and oxygen, the major components of chitosan and gold confirm the presence of chitosan and silver in the nanocomposite. The absence of peaks corresponding to other elements clearly shows the nonexistence of impurities in the prepared composite.

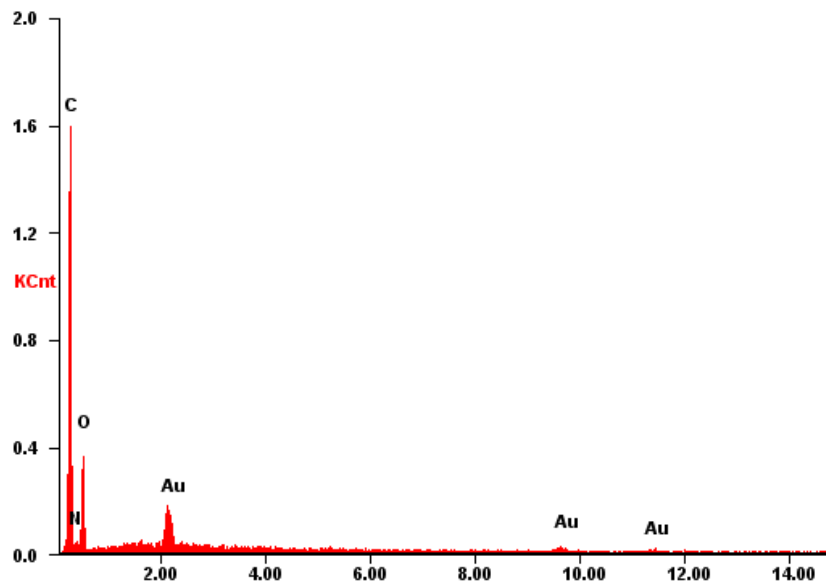


Figure S3. EDAX spectrum of CS-Au nanocomposite.

Formula for the calculation of loading efficiency

$$\text{Drug loading efficiency} = \left(\frac{\text{Drug total} - \text{Drug free}}{\text{total weight of nanoparticles}} \right) \times 100$$

Release kinetics:

The diffusion exponent “n” is got from the slope of the graph plotted between log (time in hours) versus log (% Drug release). The value of n is indicative of the process controlling the release of the drug. In general, if $n \leq 0.45$ then the process responsible for release is the Fickian diffusion. $0.45 < n < 0.89$ indicates anomalous diffusion or non-Fickian diffusion to be the process behind the release. If $n = 0.89$ and above, then the process responsible for release is the super case II transport which refers to the erosion of the polymeric chain.

Region 1: 1 to 6 hours

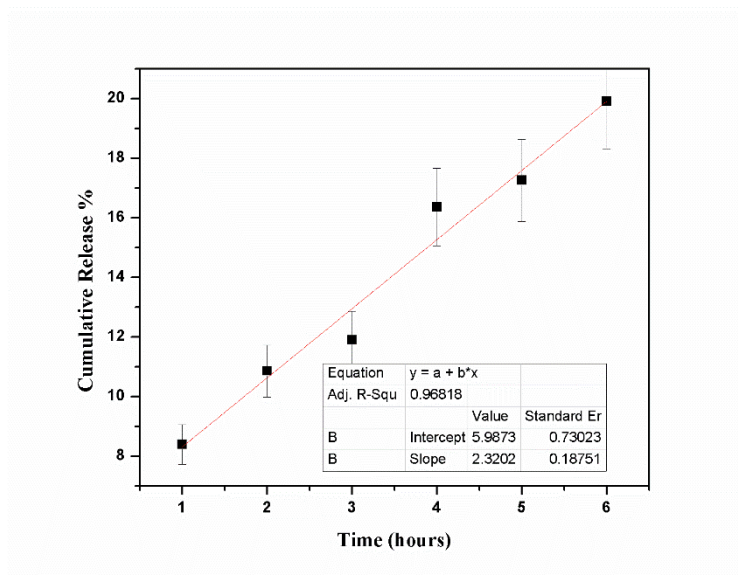


Figure S4. Zero order kinetics for region 1.

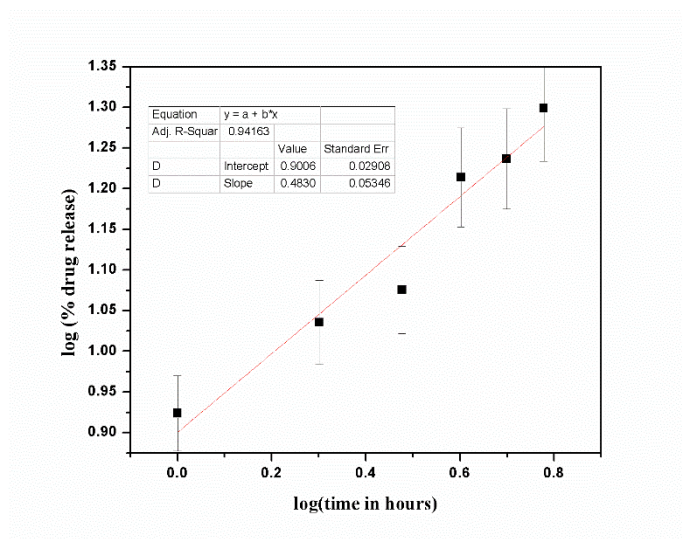


Figure S5. Korsmeyer-Peppas Kinetics for region 1.

The best fit for this region of the release profile was obtained while using zero order kinetics. The slope of the linear fit of the Korsmeyer- Peppas kinetics is 0.42 which shows Fickian diffusion is the process due to which release occurs in this region.

Region 2: 10 to 40 hours

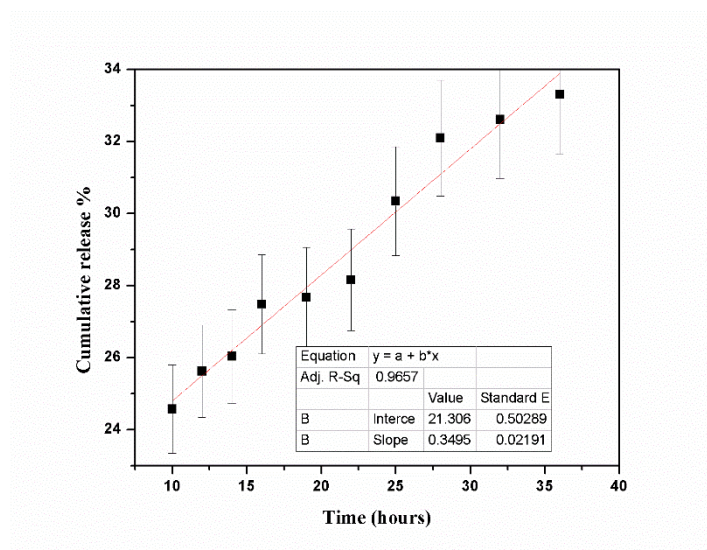


Figure S6. Zero order kinetics for region 2.

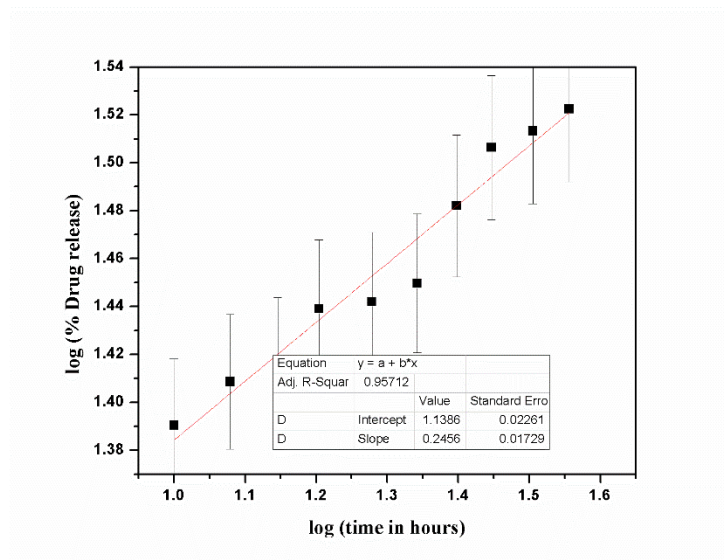


Figure S7. Korsmeyer-Peppas Kinetics for region 2.

Figure S6 and S7 show the Zero order kinetics and Korsmeyer-Peppas kinetics for the region 2. This best fit for this region was obtained for the zero order kinetics. The slope value from the

Korsmeyer-Peppas equation is equal to 0.24, which indicates that the phenomenon responsible for the release in this region to be Fickian diffusion.

Region 3: 40 to

72 hours

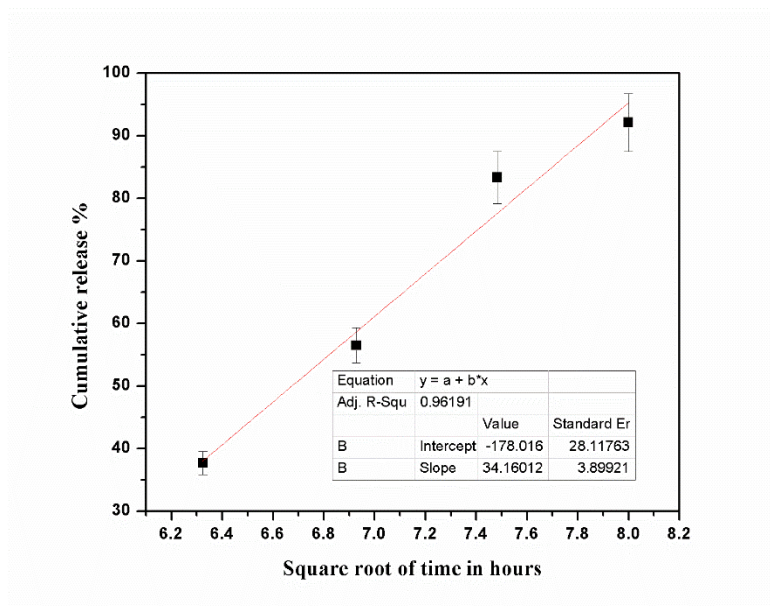


Figure S8. Higuchi kinetics for region 3.

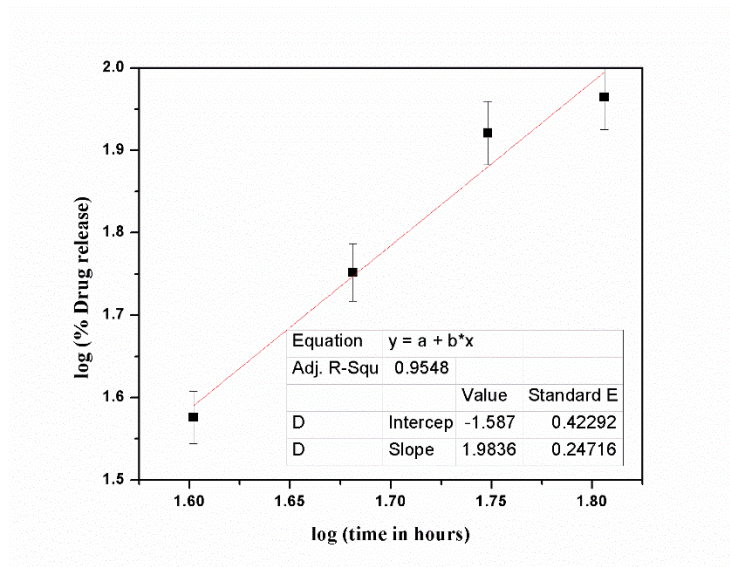


Figure S9. Korsmeyer-Peppas Kinetics for region 3.

The third region of the obtain release profile was found to adhere well to the Higuchi kinetics. The value of diffusion exponent for this region from the Kormeyer-peppas kinetics was~1.8 which shows super case II transport to be the process controlling the drug release in this zone.

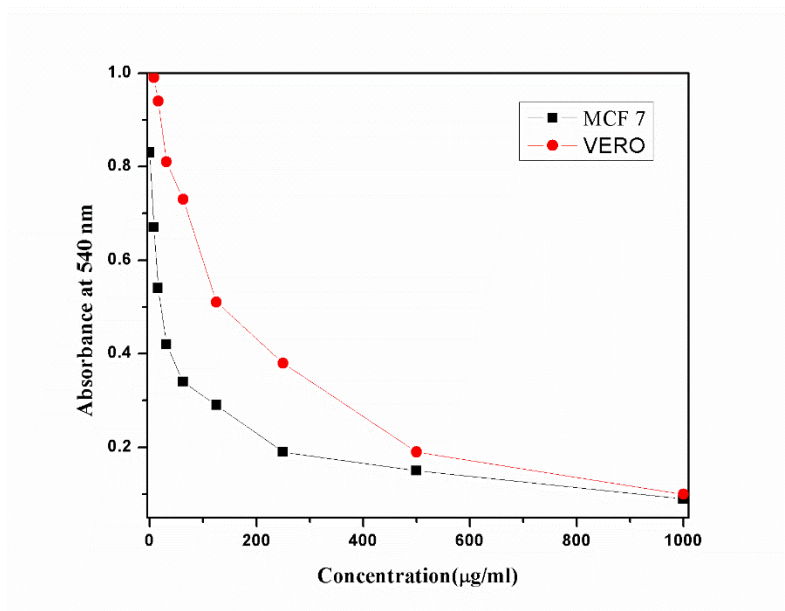


Figure S10. A plot of concentration versus absorbance for the normal VERO and carcinogenic MCF7 cells.

The absorbance at 540 nm for the addition of various concentrations of the drug loaded nanocomposite to the VERO and MCF7 cell lines are shown in figure S10. It is evident from the graph that the absorbance decreases with increase in concentration and also that the absorbance values obtained for the control as well as for the cells treated with the sample of VERO cell line are more than the values obtained for MCF7 cell line showing that 5FU loaded nanocomposite is effective towards the destruction of carcinogenic cells while being less harmful towards the normal cells. As the absorbance at 540 nm is directly proportional to cell viability it is evident that % cell viability decreases with increase in concentration. Thus, by choosing proper concentration 5FU loaded CS/Au nanocomposite can be used for the destruction of MCF7 cells without affecting the normal cells.