

Electronic Supplementary Information(†ESI)

pH-responsive Magnetic Nanocarriers for Chelator-free Bimodal (MRI/SPECT-CT) Image Guided Chemo-hyperthermia Therapy in Human Breast Carcinoma

Bijaideep Dutta^{a,b}, Neena G. Shetake^{b,c}, Sourav Patra^{b,d}, Rubel Chakravarty^{b,d}, K. V. Vimalnath^d, Avik Chakraborty^{b,e}, Sudipta Chakraborty^{b,d}, B. N. Pandey^{b,c}, P. A. Hassan^{a,b,*}, K. C. Barick^{a,b,*}

^aChemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, India

^bHomi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India

^cRadiation Biology and Health Sciences Division, Bhabha Atomic Research Centre, Mumbai 400085, India

^dRadiopharmaceutical Division, Bhabha Atomic Research Centre, Mumbai 400085, India

^eRadiation Medicine Centre, Bhabha Atomic Research Centre, Mumbai 400012, India

*Corresponding authors: hassan@barc.gov.in (P. A. Hassan), kcbarick@barc.gov.in (K. C. Barick)

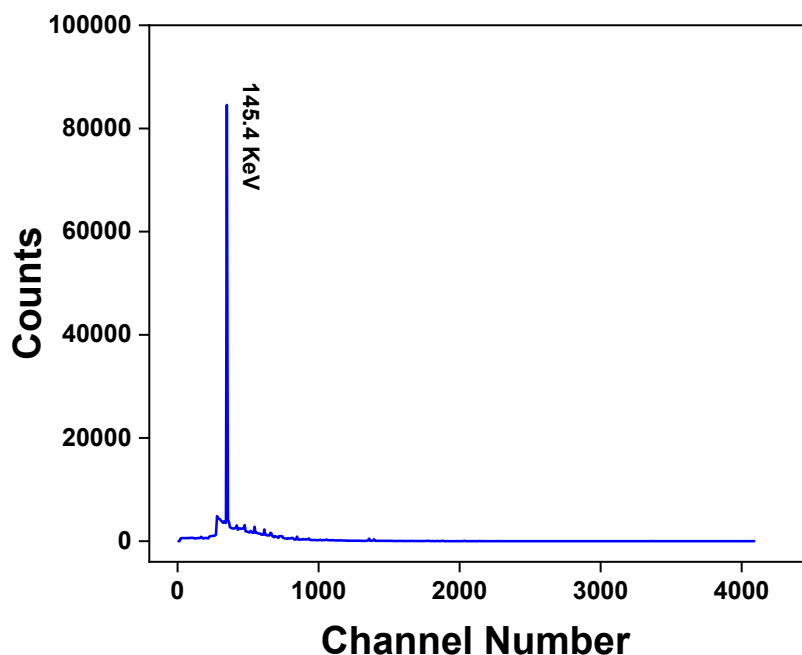


Fig. S1. γ - spectrum of ^{141}Ce recorded in HPGe detector.

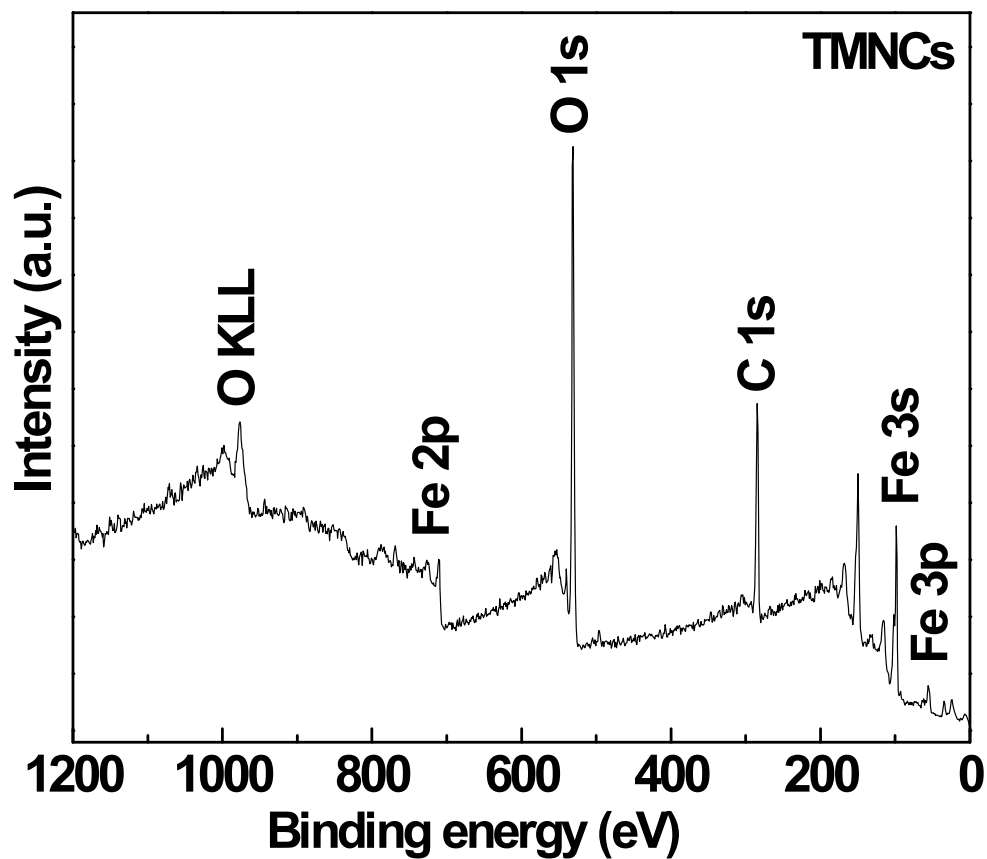


Fig. S2. Fig. S1. XPS survey scan of TMNCs. The peaks corresponding to Fe (Fe 2p, Fe 3p, Fe 3s), O (O 1s) and C (C1s) are observed on TMNCs. In addition, auger peak corresponding to O KLL transition is also found [1].

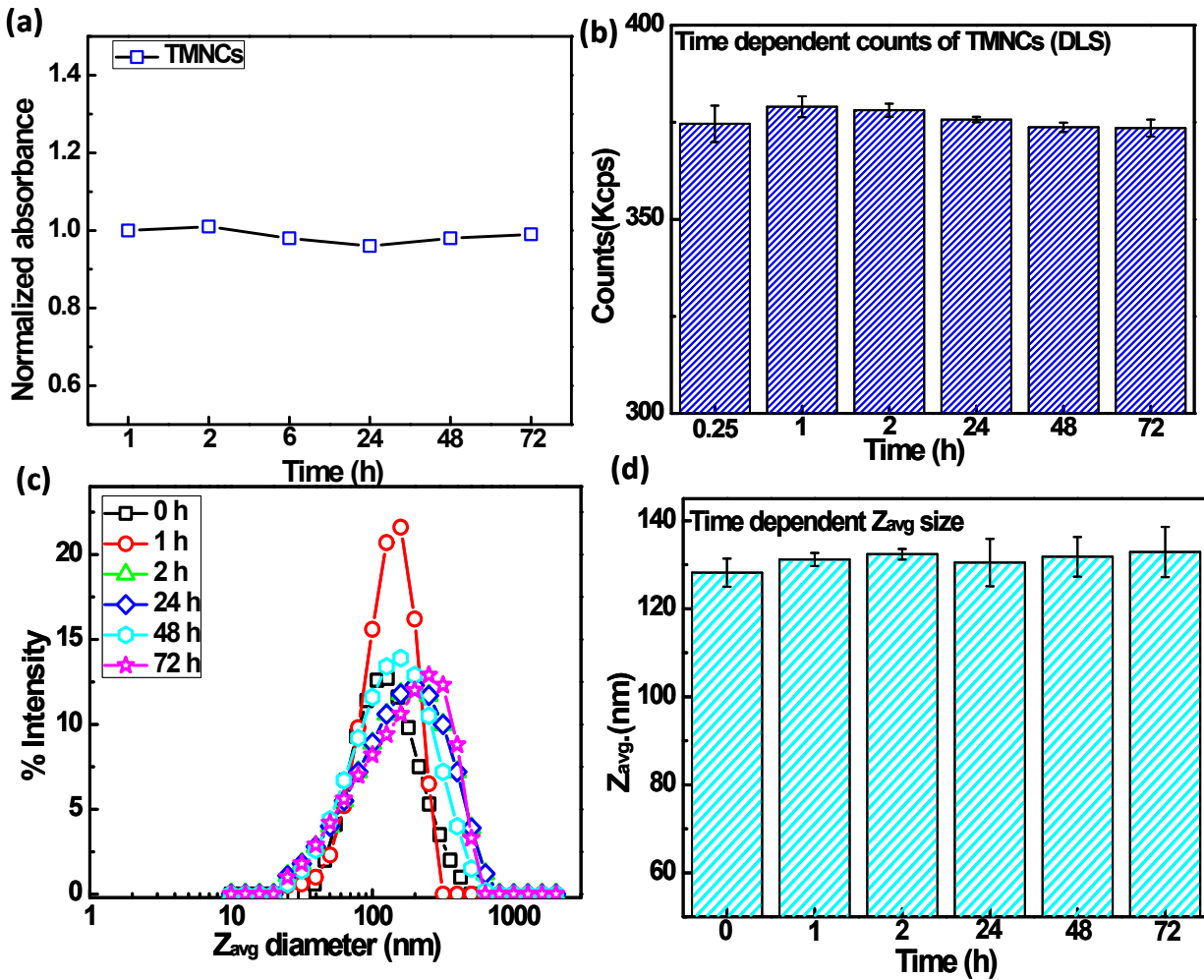


Fig. S3. Colloidal stability studies of TMNCs by (a) time dependent absorbance measurement using UV-vis spectrophotometer, time dependent DLS measurement by monitoring the (b) counts, (c) and (d) average hydrodynamic diameter.

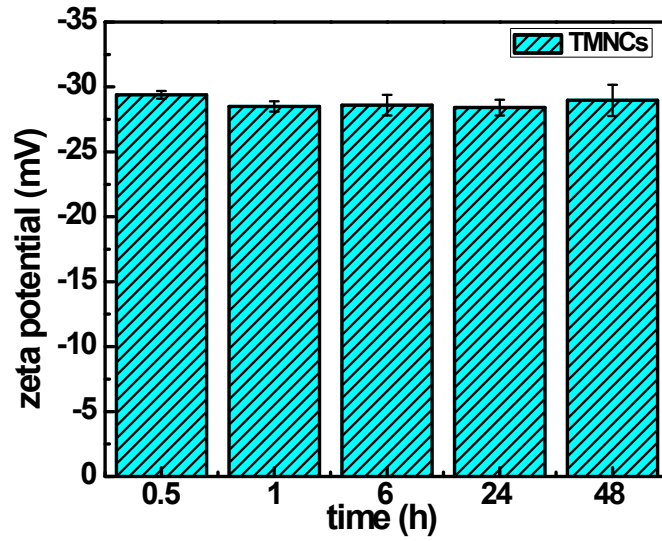


Fig. S4. Time dependent surface charge measurement for TMNCs and BSA interaction.

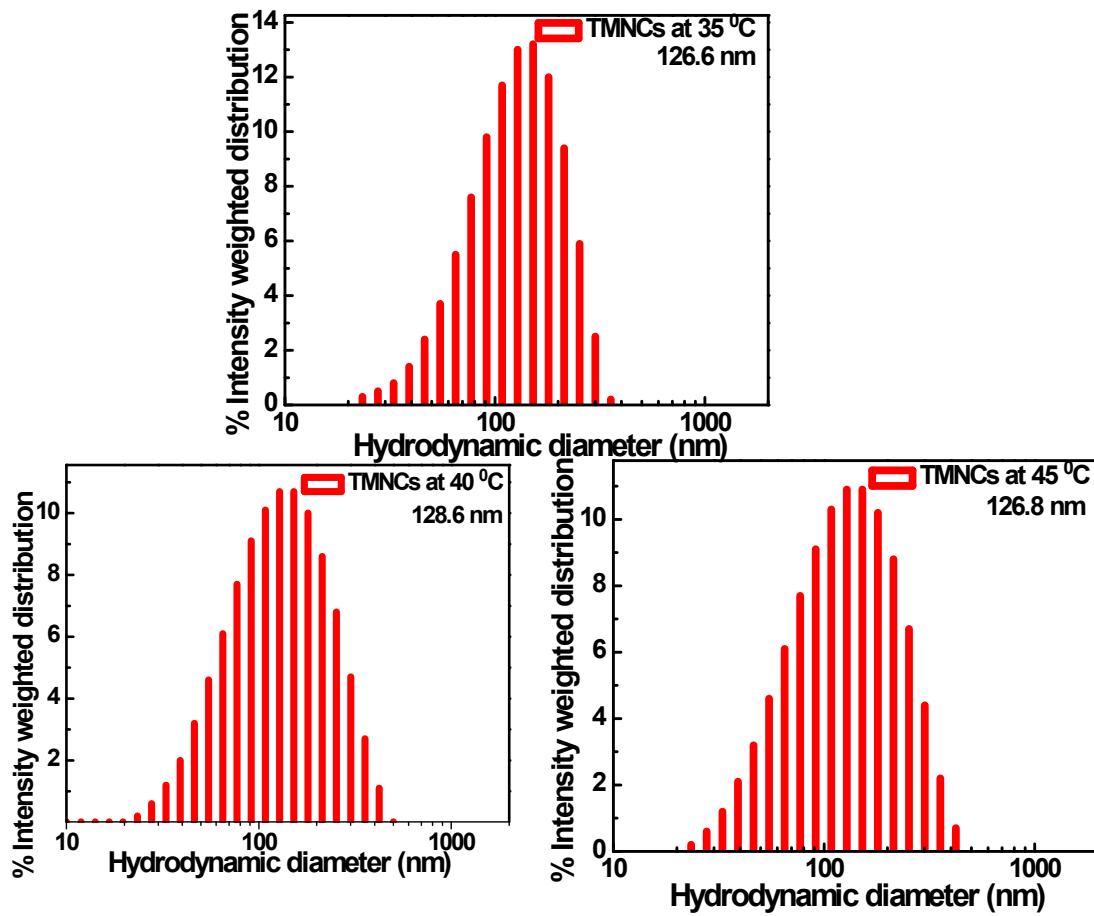


Fig. S5. Temperature dependent DLS size distribution.

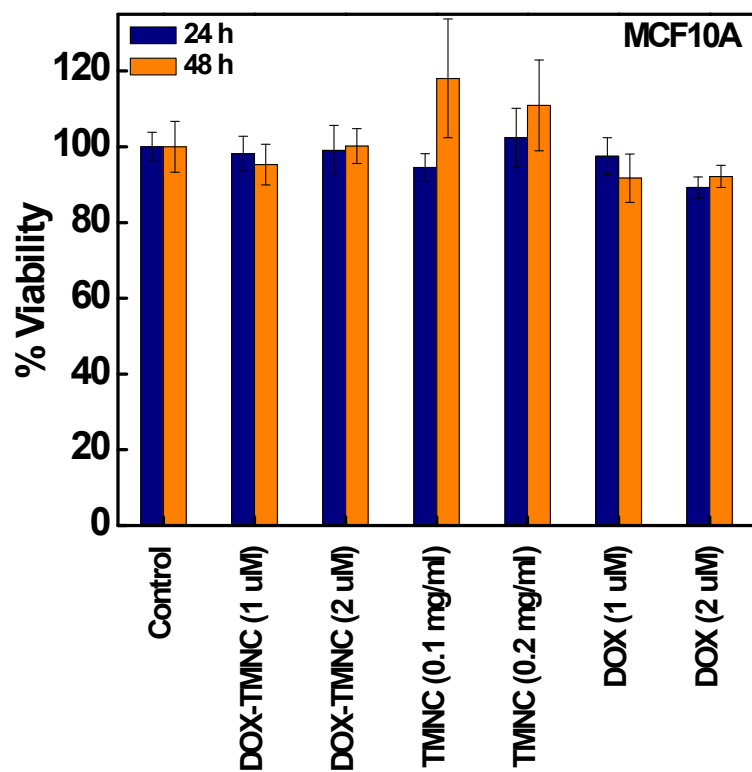


Fig. S6. Cell viability of MCF10A cell lines at 24 h and 48 h upon treatment with Pure DOX and DOX-TMNC.

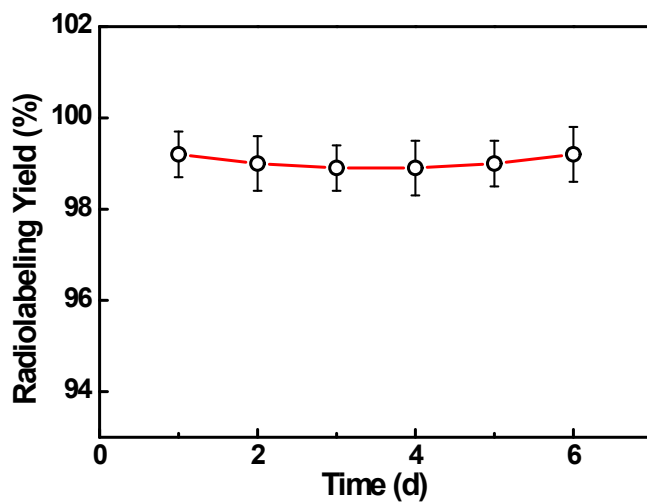


Fig. S7. Determination of the radiochemical stability of ^{141}Ce -TMNCs at different time intervals.

Sorption characteristics:

The linear fitting formula for the aforementioned isotherms are given bellow

(A) Langmuir isotherm

The linear form of the Langmuir isotherm is given as

$$\frac{C_e}{q_e} = \frac{C_e}{Q_0} + \frac{1}{Q_0 b}$$

Where Q_0 is monolayer adsorption capacity (mg g^{-1}) and b (L/mg) is the constant and C_e is the equilibrium concentration of Ce^{+3} ions (gL^{-1}).

(B) Freundlich Isotherm

The Freundlich isotherm is rely on multilayer adsorption of the adsorbates on the surface of adsorbents and the linear form of the isotherm could be written as

$$\log(q_e) = \log K_F + \frac{1}{n} \ln(C_e)$$

Where K_F (mg/g) and n (dimensionless) are Freundlich constant.

(C) Langmuir-Freundlich (L-F) isotherm

The combination of Langmuir and Freundlich isotherm is known as Langmuir-Freundlich isotherm which is an empirical model. The linear form of the model is given as

$$q_e = \frac{Q_{max} K_{LF} C_e^{\frac{1}{n_{LF}}}}{1 + K_{LF} C_e^{\frac{1}{n_{LF}}}}$$

Where K_{LF} ($\text{mg} \cdot \text{L}^{-1}$) $^{-1/n_{LF}}$ is L-F constant, Q_{max} ($\text{mg} \cdot \text{g}^{-1}$) is maximum adsorption capacity and n_{LF} ($0 < n_{LF} \leq 1$) is an exponent.

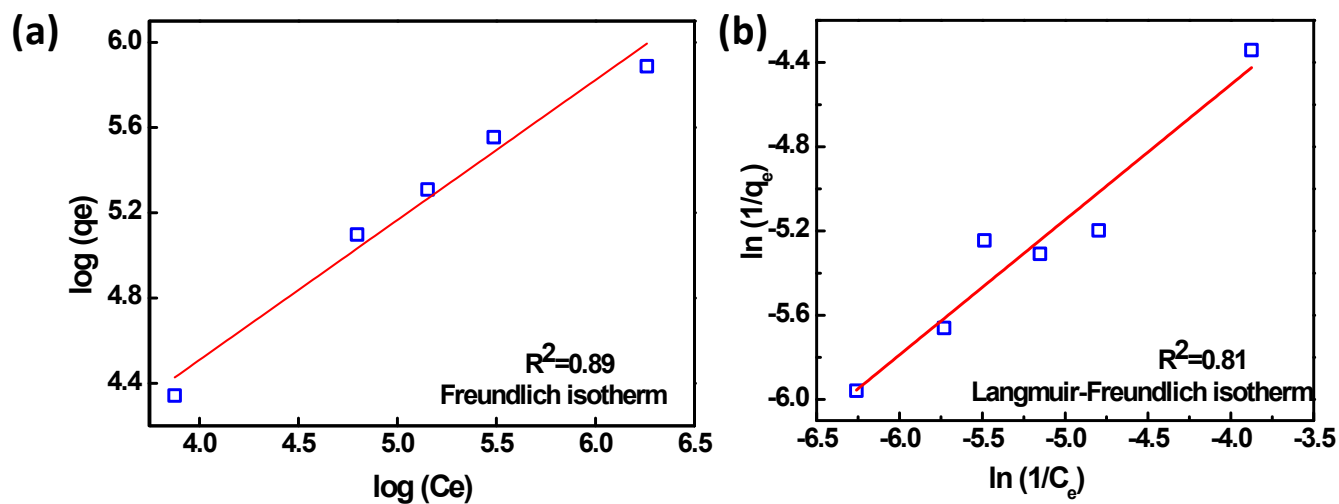


Fig. S8. Fitting of the data to the (a) Freundlich isotherm model (b) Langmuir-Freundlich isotherm model for adsorption of ^{141}Ce on TMNC.

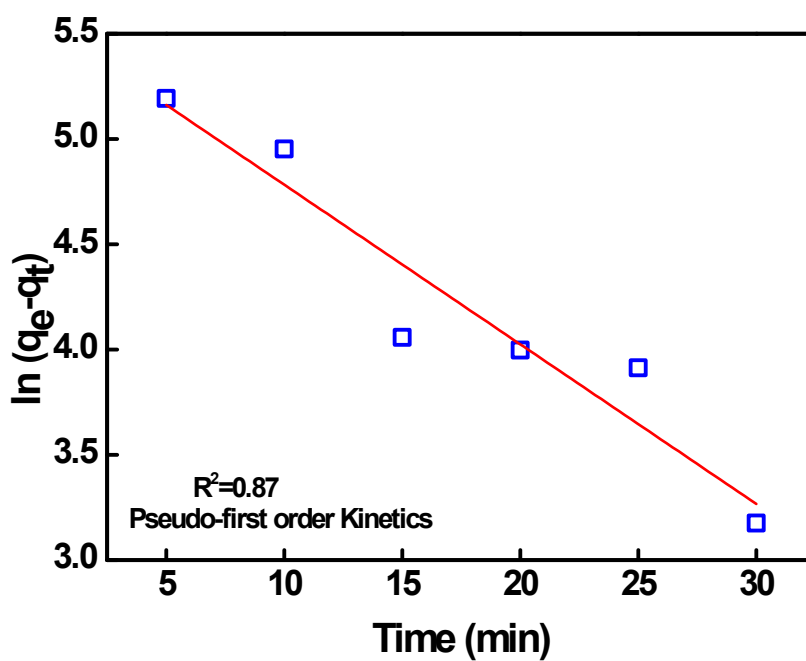


Fig. S9. Fitting of the data to the kinetics model for adsorption of ^{141}Ce on TMNC (A) pseudo-first order kinetics model.

Kinetic models:

(A) Pseudo-first-order reaction

The linear model for pseudo-first order kinetics is given bellow

$$\log (q_e - q_t) = \log q_e - \frac{k_1 t}{2.303}$$

Where k_1 (min^{-1}) is the rate constant for the pseudo first order kinetics and q_t (mg g^{-1}) is the sorption capacity of TMNC at time t (min).

(B) Pseudo-second-order reaction

The linear model for pseudo-second order kinetics is given bellow

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$$

Where k_2 ($\text{g mg}^{-1} \text{min}^{-1}$) is the rate constant for the pseudo first order kinetics and the calculated rate constant was found to be $2.45 \times 10^{-3} \text{ g mg}^{-1} \text{min}^{-1}$.

References:

1. G. Carraro, D. Barreca, D. Bekermann, T. Montini, A. Gasparotto, V. Gombac, C. Maccato, P. Fornasiero; J. Nanosci. Nanotechnol. 2013, **13**,4962-4968.