

# **Supporting Information**

## Decagram-scale Synthesis of Multicolor Carbon Nanodots: Self-tracking Nano-heaters with Inherent and Selective Anticancer Properties

Nicolò Mauro<sup>1\*</sup>, Mara Andrea Utzeri<sup>1</sup>, Alice Sciortino<sup>2</sup>, Fabrizio Messina<sup>2,3</sup>, Marco Cannas<sup>2</sup>, Radian Popescu<sup>4</sup>, Dagmar Gerthsen<sup>4</sup>, Gianpiero Buscarino<sup>2,3</sup>, Gennara Cavallaro<sup>1,3</sup> and Gaetano Giammona<sup>1</sup>

<sup>1</sup>Lab of Biocompatible Polymers, Department of Biological, Chemical and Pharmaceutical Sciences and Technologies (STEBICEF), University of Palermo, via Archirafi 32, 90123 Palermo, Italy;

<sup>2</sup>Department of Physics and Chemistry (DiFC) “E. Segrè”, University of Palermo, via Archirafi 36, 90123 Palermo, Italy;

<sup>3</sup>ATeN Center, University of Palermo, Viale delle Scienze – Ed. 18/A, 90128 – Palermo, Italy;

<sup>4</sup>Karlsruhe Institute of Technology | KIT · Laboratory for Electron Microscopy, Finanzmanagement  
Kaiserstraße 12 D-76131, Karlsruhe, Germany

\*Corresponding author: [nicolo.mauro@unipa.it](mailto:nicolo.mauro@unipa.it); Tel. +39-092-238-91908

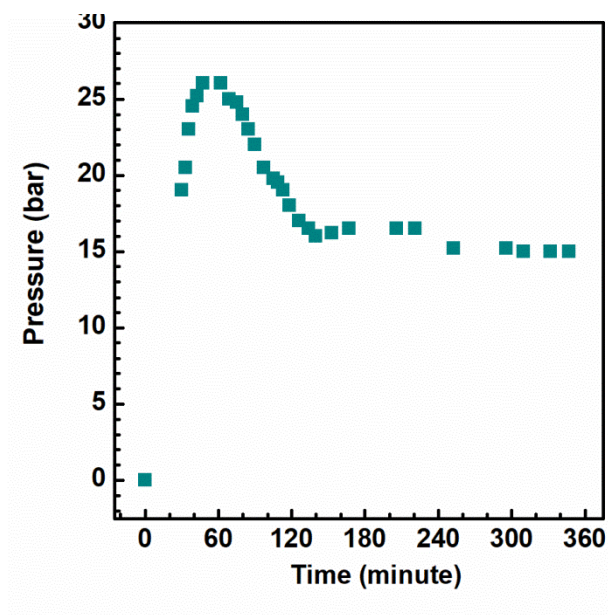


Figure S1. Pressure of the autoclave during the reaction

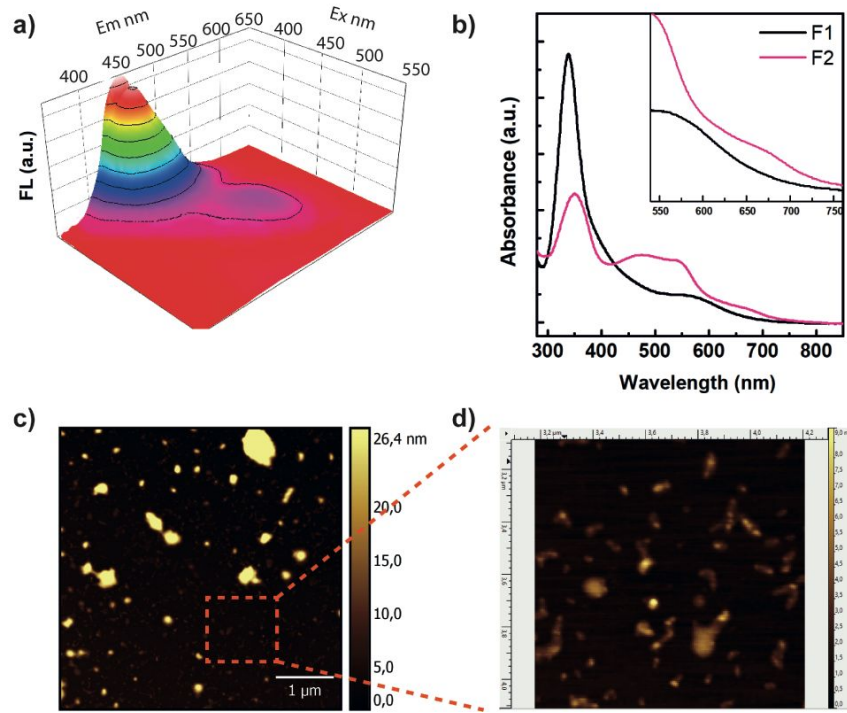


Figure S2. Preliminary characterization of the F1 fraction. a) 3D emission spectrum of the F1 fraction; b) absorption spectra of the F1 and F2 fractions. c-d) AFM micrographs of the F1 fraction

### 1. Mathematical model for evaluation of the photothermal conversion efficiency

The photothermal efficiency of the  $\text{SO}_x\text{-CDs}$  carbon nanodots were calculated by considering the photothermal kinetic of a dispersion of carbon nanodots in ultrapure water () place into a 1 cm quartz cuvette and irradiated using a diode laser of proper wavelength, and the dissipation curve obtained after the heating processes during the cooling period.

Under NIR irradiation, the change in temperature  $T$  is described by the energy balance equation (1):

$$\sum m_i C_i dT dt = E_{abs} - E_{loss} \quad (1)$$

Equation (2) can be used to describe the energy transfer

$$T(t) = T_0 + \frac{A}{B}(1 - e^{-Bt}) + (T_i - T_0) \quad (2)$$

where  $A$  is the rate of energy absorption and  $B$  is the rate of heat dissipation,  $T_0$  is the ambient temperature and  $T_i$  is the initial temperature value.

In order to retrieve the photothermal conversion efficiency  $\eta$ , it is needed to measure the temperature variation of the  $\text{SO}_x\text{-CDs}$  dispersions as a function of time during both the photothermal heating (laser on,  $A \neq 0$  and  $T_i = T_0$ ) and the subsequent cooling (laser off,  $A = 0$  and  $T_i > T_0$ ).

Thus obtaining equation (3) and (4), respectively:

$$T(t) = T_0 + \frac{A}{B}(1 - e^{-Bt}) \quad (3)$$

$$T(t) = T_0 + \frac{A}{B}(1 - e^{-Bt}) + (T_i - T_0) \quad (4)$$

By fitting the experimental curve with equation (1), the values of  $A$  and  $B$  can be obtained and employed to calculate the experimental photothermal conversion efficiency  $\eta$ :

$$\eta = \frac{A \sum_i m_i C_i}{P (1 - 10^{-A_{\lambda}})} \quad (5)$$

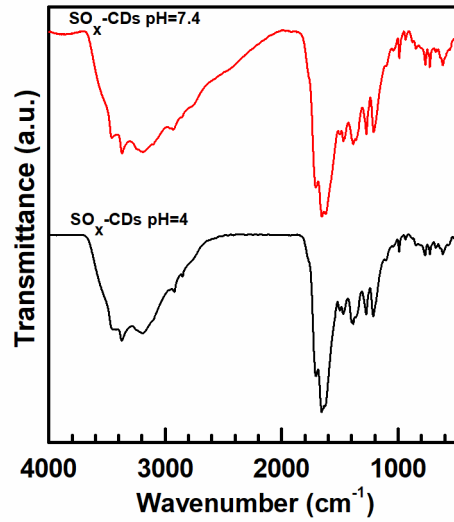


Figure S3. FTIR spectrum of  $\text{SO}_x\text{-CDs}$  at pH 7.4 and pH 4 after two days incubation.

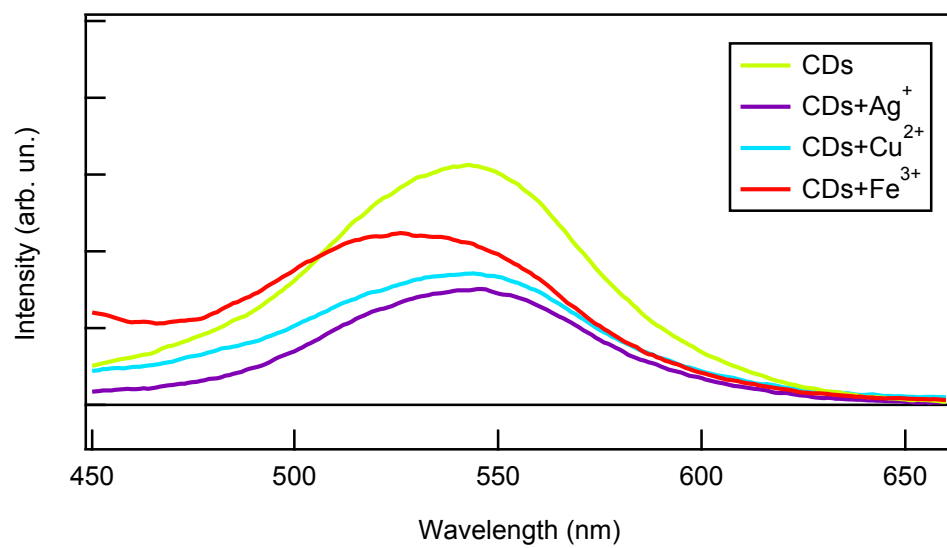


Figure S4. Fluorescence spectra of CDs in presence of metal ions.

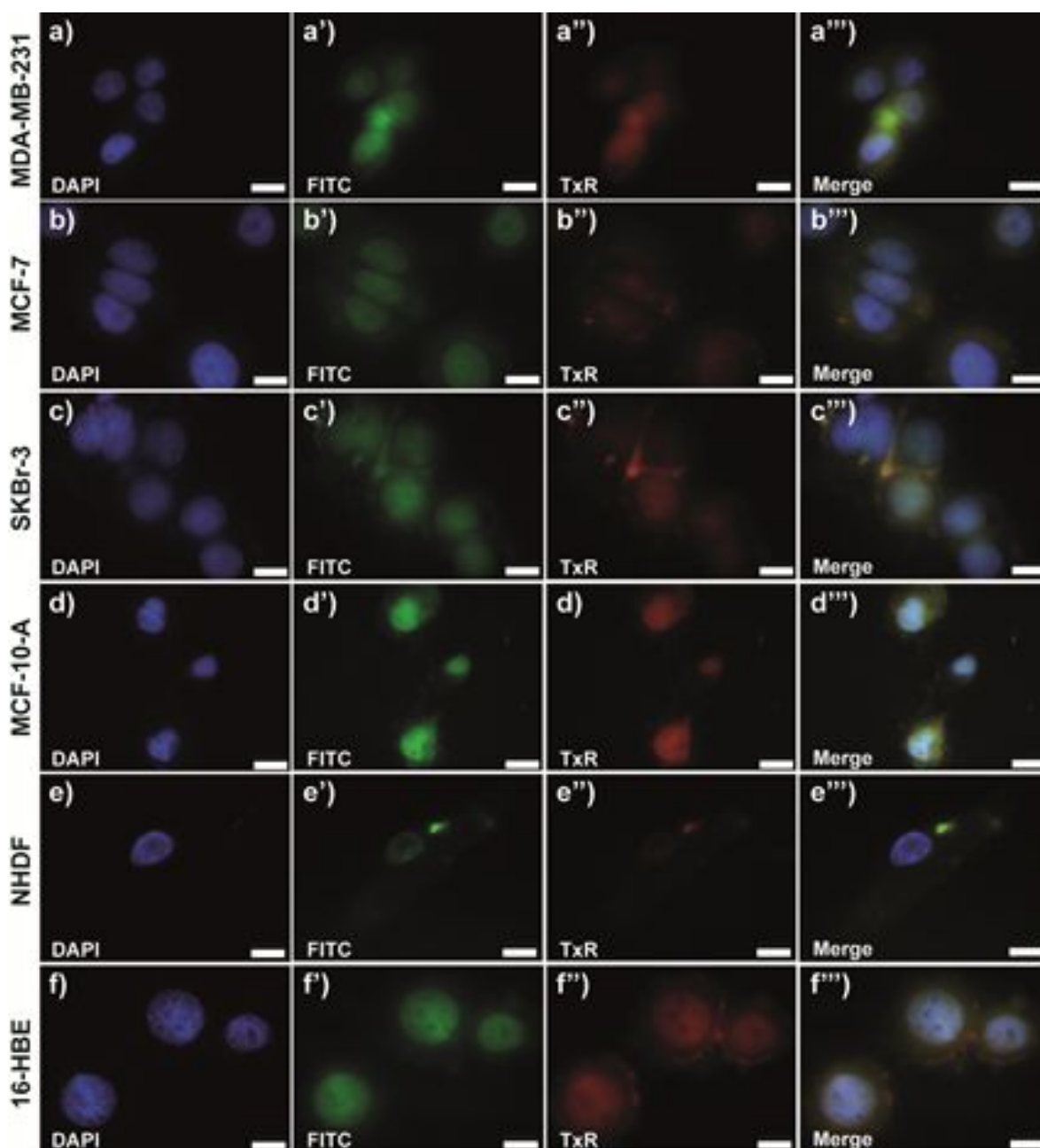


Figure S5. Fluorescence imaging of cancerous breast cell lines (MDA-MB-231, **a-a'''**; MCF-7, **b-b'''**; and SKBr-3, **c-c'''**), pre-cancerous (MCF-10A, **e-e'''**) and healthy (16-HBE, **f-f'''**) cell lines treated with SO<sub>x</sub>-CDs (0.25 mg ml<sup>-1</sup>) for 2 h. Nuclei are marked with DAPI (**a-f**), SO<sub>x</sub>-CDs self-fluorescence in the green (**a'-f'**) and red (**a''-f''**) region, and merge channels (**a'''-f'''**). Scale bar: 10  $\mu$ m.

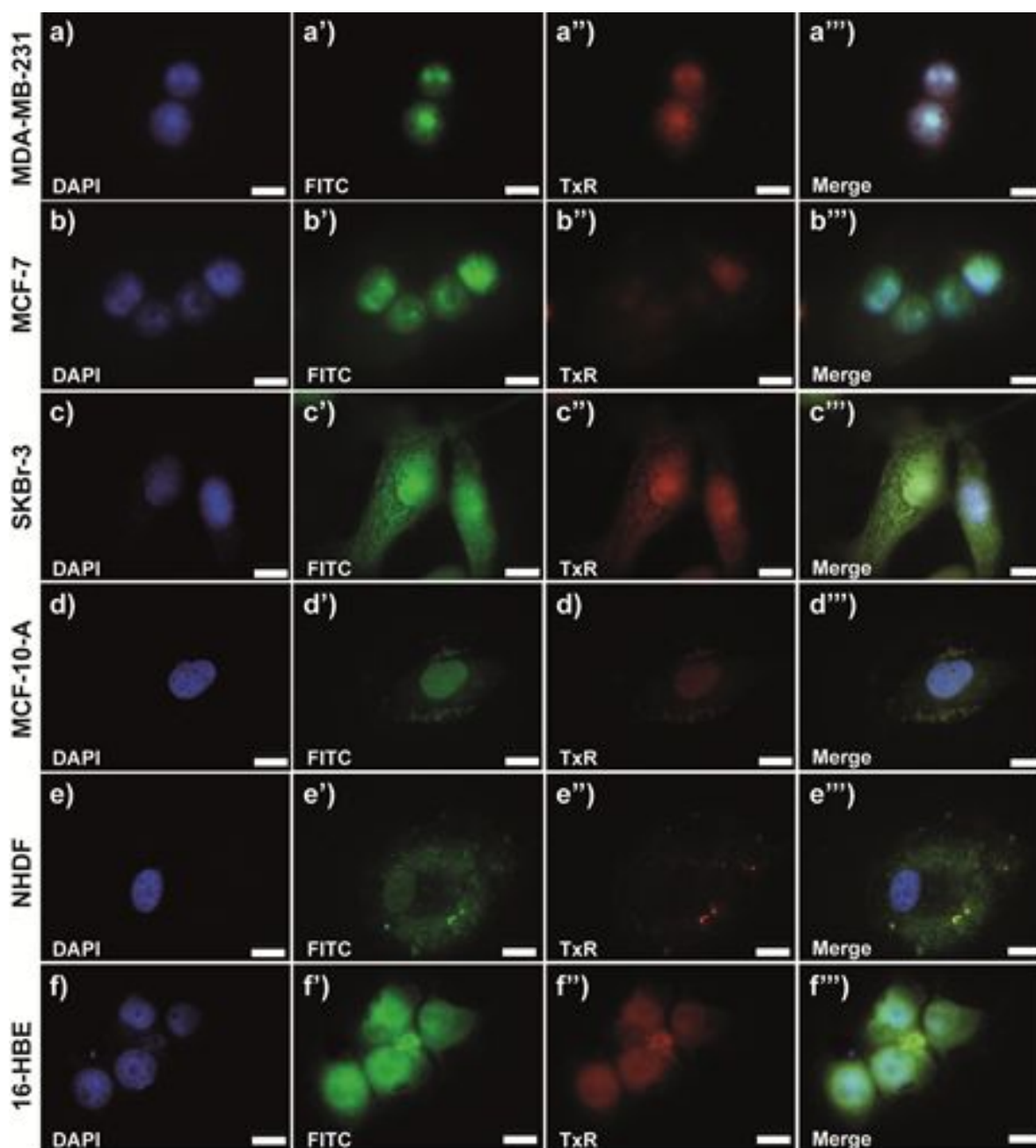


Figure S6. Fluorescence imaging of cancerous breast cell lines (MDA-MB-231, **a-a'''**; MCF-7, **b-b'''**; and SKBr-3, **c-c'''**), pre-cancerous (MCF-10A, **e-e'''**) and healthy (16-HBE, **f-f'''**) cell lines treated with SO<sub>x</sub>-CDs (0.25 mg ml<sup>-1</sup>) for 6 h. Nuclei are marked with DAPI (**a-f**), SO<sub>x</sub>-CDs self-fluorescence in the green (**a'-f'**) and red (**a''-f''**) region, and merge channels (**a'''-f'''**). Scale bar: 10  $\mu$ m.