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## **Electronic Supplementary Information**

## Heat shock protein-guided dual-mode CT/MR imaging of orthotropic

## hepatocellular carcinoma tumor

Ruizhi Wang<sup>1</sup><sup>§</sup>, Yu Luo<sup>2</sup><sup>§</sup>, Xin Li<sup>3</sup><sup>§</sup>, Aihua Ji<sup>1</sup>, Rongfang Guo<sup>1</sup>, Xiangyang Shi<sup>3</sup>\*, Xiaolin Wang<sup>1</sup>\*

<sup>a</sup> Department of Interventional, Zhongshan Hospital, Fudan University, Shanghai Institute of Medical Imaging, Shanghai 200032, P. R. China

<sup>b</sup> State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, 1295 Ding-Xi Road, Shanghai 200050, P. R. China.

<sup>c</sup> College of Chemistry, Chemical Engineering and Biotechnology, Donghua University, Shanghai 201620, P. R. China

\*To whom correspondence should be addressed. E-mail: xshi@dhu.edu.cn (X. Shi), fduwangxiaolin@hotmail.com (X. Wang).

<sup>§</sup> Authors contributed equally to this work.

**Table S1.** Zeta potential and hydrodynamic size of the Au@PEI-Gd-AAG.

Sample	Zeta potential (mV)	Hydrodynamic size (nm)	PDI
Au@PEI-Gd-AAG	$+ 6.1 \pm 0.6$	$245.1 \pm 8.8$	$0.209 \pm 0.047$

Table S2. The Au and Gd content of the Au@PEI-Gd-AAG, respectively.

Sample	Au (µg/mg)	Gd (µg/mg)
Au@PEI-Gd-AAG	89.5 <mark>± 3.8</mark>	17.9 <mark>± 2.9</mark>



Figure S1. <sup>1</sup>H NMR of COOH-PEG-(17-AAG).



**Figure S2.** Photographs of the Au@PEI-Gd-AAG (1 mg/mL) dispersed in water, PBS, and cell culture medium (with FBS) for 28 days. Cell culture medium (without FBS) was used as control.



Figure S3. Hydrodynamic size of the Au@PEI-Gd-AAG, 1 mg/mL, dispersed in water within

<mark>28 days.</mark>



Figure S4. Photo micrographs of HCCLM3 cells treated with PBS (a), the Au@PEI-Gd-AAG NPs

at the Gd concentrations of 10 (b), 20 (c), 40 (d), 80 (e), and 100 (f)  $\mu$ g/mL for 24 h.



**Figure S5.** The live/dead staining photos were observed by laser confocal microscopy, and HCCLM3 cells treated with PBS (a), the Au@PEI-Gd-AAG NPs at the Gd concentrations of 10 (b), 20 (c), 40 (d), 80 (e), and 100 (f) µg/mL for 24 h.



Figure S6. Flow cytometry analysis of HCCLM3 cells treated with PBS (a, l), Au@PEI-Gd-AAG at the Gd concentration 10 (b), 25 (c), 50 (d), 75 (e) (Hsp90 blocked by free 17-AAG), and 100 (f)

 $\mu$ g/mL, and Au@PEI-Gd-AAG at the Gd concentration 10 (g), 25 (h), 50 (i), 75 (j), and 100 (k)  $\mu$ g/mL for 4 h, respectively.



Figure S7. CT signal of tumor at different time points postinjection of the Au@PEI-Gd-AAG (0.3 mL in PBS, [Au] = 120 mM, mean  $\pm$  S.D., n = 3).



**Figure S8.** MR signal/noise ratio (SNR) of tumor at different time points postinjection of the Au@PEI-Gd-AAG (0.3 mL in PBS, [Au] = 120 mM, mean  $\pm$  S.D., n = 3). The MR signal intensity of blank was used as the background (noise). (\*<0.05, \*\*<0.01, \*\*\*<0.001)