Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information for

A Targeted Agent with Intercalation Structure for Cancer Near-Infrared Imaging and Photothermal Therapy

Chunyang Li,[a] Ruizheng Liang,*[a] Rui Tian,[a] Shanyue Guan,[a] Dongpeng Yan,[a] Jiaoyang Luo,*[b] Min Wei,*[a] David G. Evans[a] and Xue Duan[a]

[a] *State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing 100029, P. R. China*

[b] *Institute of Medicinal Plant Development, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing 100193, P. R. China.*

E-mail: liangruizheng2000@163.com (R. Liang); luojiaoyang1986@163.com (J. Luo); weimin@mail.buct.edu.cn (M. Wei).

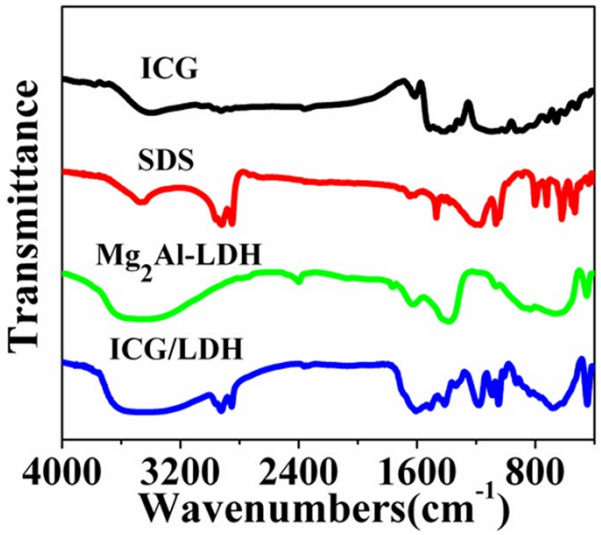

Figure S1. FT-IR spectra of ICG, SDS, Mg_2Al-LDH and ICG/LDH, respectivley.

Table S1. Chemical compositions of various ICG(*x*%)/LDH samples

Sample	Chemical Composition	M^{2+}/M^{3+}	Determined *x*%	Drug Loading Capacity (mg/mg)
ICG(1%)/LDH	$Mg_{0.611}Al_{0.389}(OH)_2ICG_{0.00284}SDS_{0.0148}$	1.62	0.73	0.0338
ICG(2%)/LDH	$Mg_{0.618}Al_{0.382}(OH)_2ICG_{0.00378}SDS_{0.0134}$	1.57	1.00	0.0464
ICG(3%)/LDH	$Mg_{0.644}Al_{0.356}(OH)_2ICG_{0.00546}SDS_{0.0147}$	1.81	1.53	0.0655
ICG(5%)/LDH	$Mg_{0.671}Al_{0.329}(OH)_2ICG_{0.00625}SDS_{0.0145}$	2.04	1.90	0.0750
ICG(10%)/LDH	$Mg_{0.683}Al_{0.317}(OH)_2ICG_{0.00880}SDS_{0.0131}$	2.15	2.78	0.1063

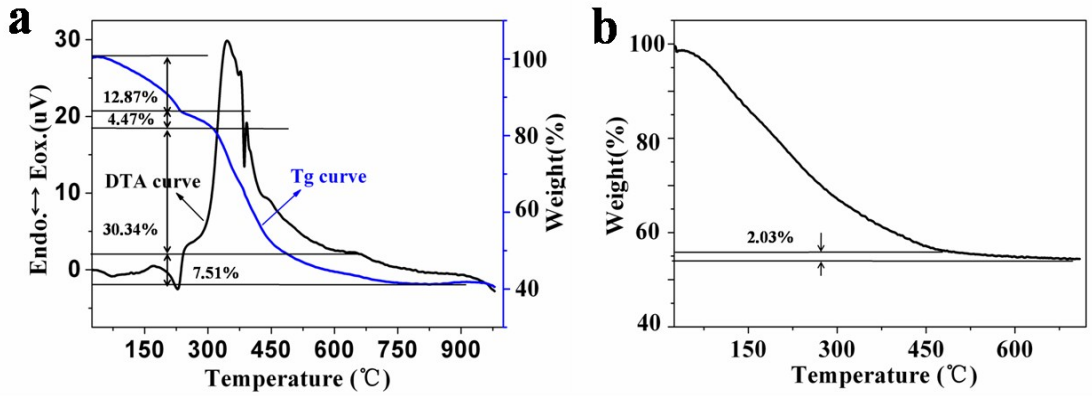

Figure S2. (a) TG and DTA curves for the sample of ICG(2%)/LDH, (b) TG curve for the sample of Mg_2Al-LDH.

In the case of ICG/LDH, the thermal decomposition process is characterized by four mass loss steps. The first one from room temperature to 230 °C (mass loss: 12.87%) is due to the removal of surface adsorbed and interlayer water molecules. The second one with a gradual mass loss of 4.47% in the temperature range 230–320 °C mainly derives from the decomposition and dehydroxylation of the brucite-like layers. The third one (mass loss: 30.34%) corresponds to the decomposition/combustion of SDS and collapse of the layer, accompanied by a strong exothermic peak at 346 °C in the DTA curve.[1] The forth one with the mass loss of 7.51% is ascribed to the decomposition/combustion of ICG and further collapse of the LDH layer.[2, 3] Compared with the TG curve of Mg_2Al-LDH sample, the ICG loading on LDH is calculated to be 5.48%, close to the result obtained by elemental analysis.

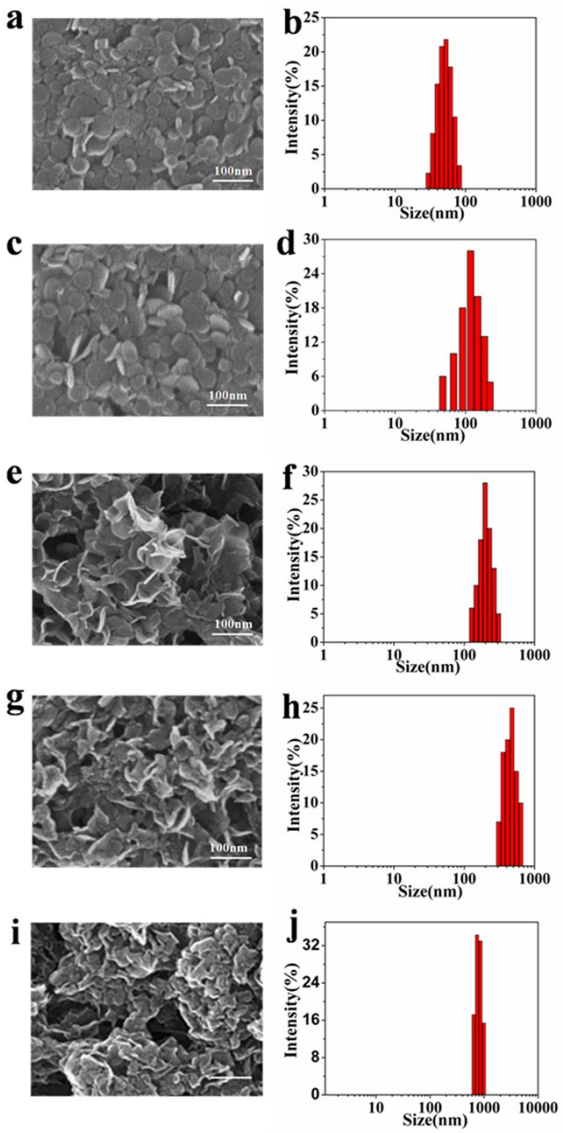

Figure S3. SEM images and particle size distribution of ICG(*x*%)/LDH samples determined by a dynamic light scattering analyzer: (a, b) ICG(1%)/LDH, (c, d) ICG(2%)/LDH, (e, f) ICG(3%)/LDH, (g, h) ICG(5%)/LDH, (i, j) ICG(10%)/LDH.

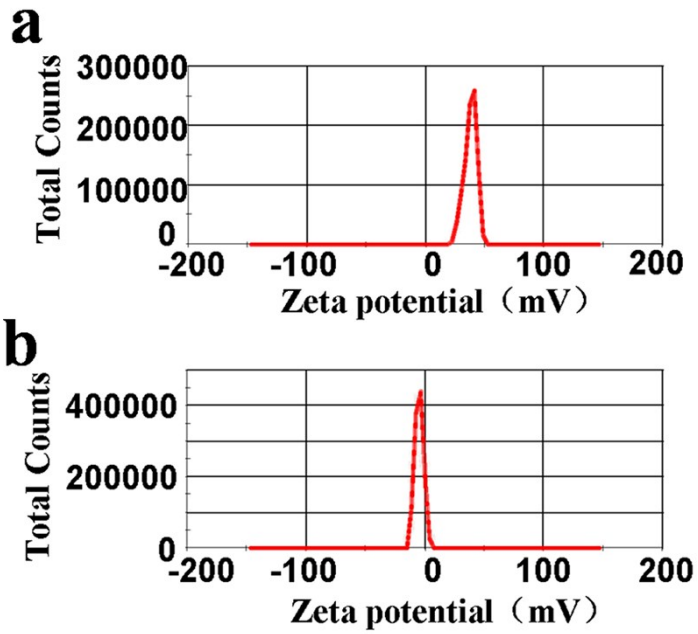

Figure S4. Zeta potential of (a) ICG(2%)/LDH and (b) ICG(2%)-FA(20%)/LDH determined by a dynamic light scattering analyzer.

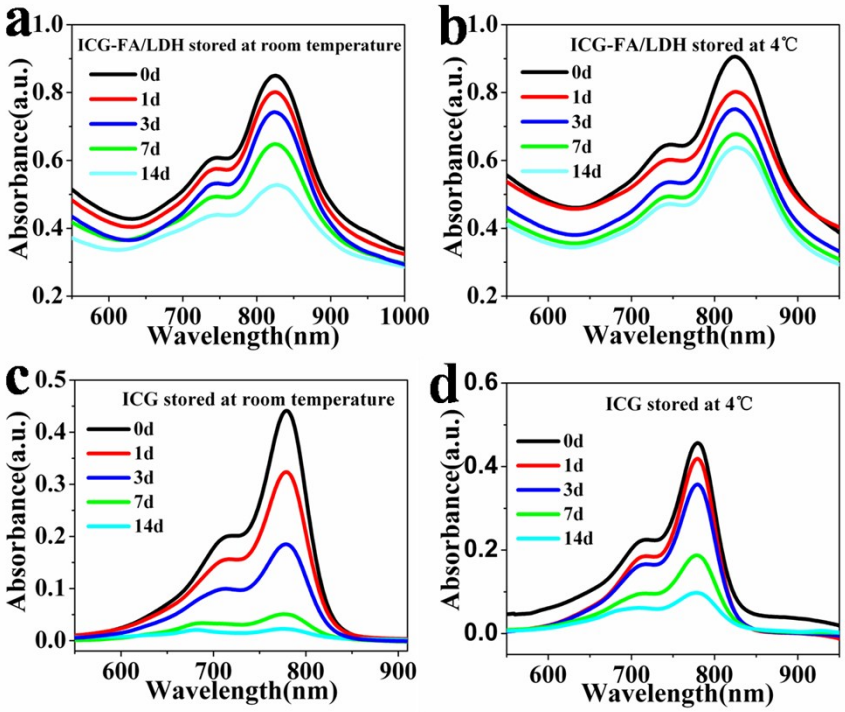

Figure S5. UV-vis-NIR absorption spectra of ICG-FA/LDH stored at (a) room temperature and (b) 4 °C within 14 days; UV-vis-NIR absorption spectra of pristine ICG stored at (c) room temperature and (d) 4 °C within 14 days.

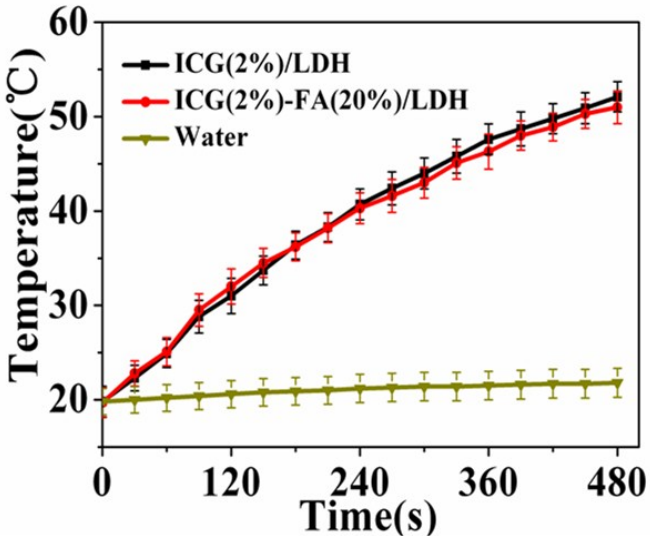

Figure S6. Temperature increase as a function of NIR laser irradiation time (wavelength: 808 nm; power density: 1.1 W/cm^2) over samples of ICG(2%)/LDH and ICG(2%)-FA(20%)/LDH, respectively (ICG concentration in solution: 10 μg/mL).

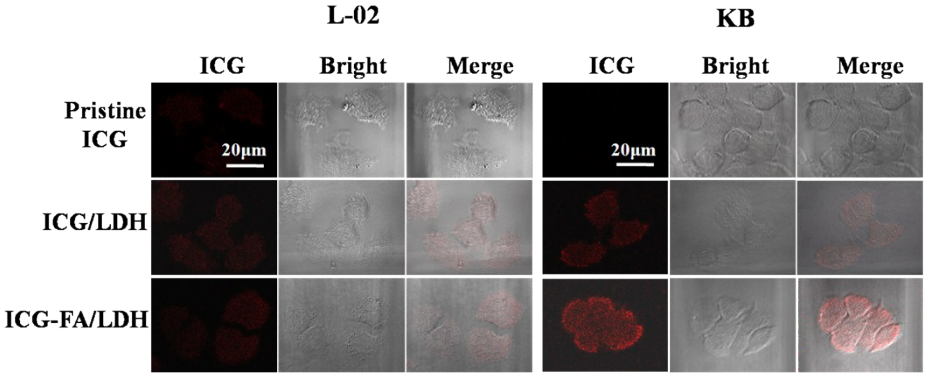

Figure S7. *In vitro* confocal analysis images of L-02 cells and KB cells treated with various samples: pristine ICG, ICG(20%)/LDH and ICG(2%)-FA(20%)/LDH, respectively (ICG concentration in solution: 8 μg/mL, 3 h incubation). The red fluorescence comes from ICG; the scale bar is 20 μm.

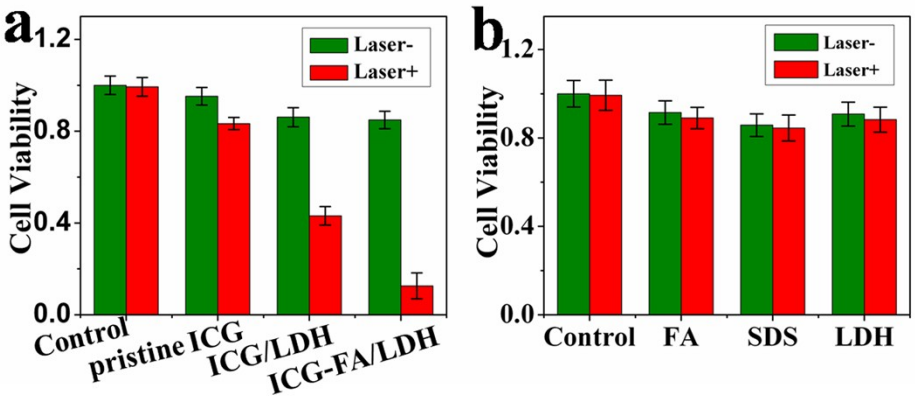

Figure S8. PTT performance of (a) pristine ICG, ICG(2%)/LDH, ICG(2%)-FA(20%)/LDH (ICG dosage: 8 μg/mL) and (b) pristine FA (0.5 mg/mL), SDS (0.5 mg/mL), LDH (0.5 mg/mL) with irradiation for 12 min. NIR irradiation conditions: 808 nm; 1.1 W/cm^2.

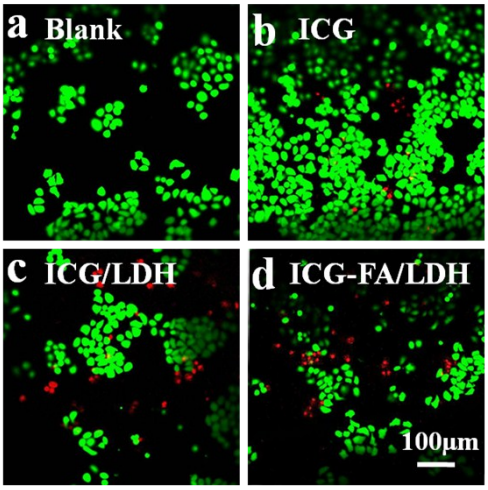

Figure S9. Confocal fluorescence images of KB cells stained by Calcein AM/PI after treated with various drugs (equivalent ICG: 8 μg/mL; incubation time: 3 h) without irradiation: (a) blank, (b) pristine ICG, (c) ICG(2%)/LDH, (d) ICG(2%)-FA(20%)/LDH. The scale bar is 100 μm.

References

1. S. Li, J. Lu, M. Wei, D. G. Evans and X. Duan, *Adv. Funct. Mater.*, 2010, **20**, 2848–2856.
2. X. Zhao, F. Zhang, S. Xu, D. G. Evans and X. Duan, *Chem. Mater.*, 2010, **22**,

3933–3942.

3. D. Yan, J. Lu, M. Wei, D. G. Evans and X. Duan, *J. Phys. Chem. B*, 2009, **113**, 1381–1388.