

Electronic Supplementary Information

Encapsulation of doxorubicin within multifunctional gadolinium-loaded dendrimer nanocomplexes for targeted theranostics of cancer cells†

Jingyi Zhu,¹ Zhijuan Xiong,² Mingwu Shen,² Xiangyang Shi^{*1,2}

¹ State Key Laboratory for Modification of Chemical Fibers and Polymer Materials, College of Materials Science and Engineering, Donghua University, Shanghai 201620, People's Republic of China

² College of Chemistry, Chemical Engineering and Biotechnology, Donghua University, Shanghai 201620, People's Republic of China

* Corresponding author. Tel: +86 21 67792656; fax: +86 21 67792306 804.

E-mail address: xshi@dhu.edu.cn

Table S1. Zeta potential values of the G5.NHAc-DOTA(Gd)-PEG-FA dendrimers and G5.NHAc-DOTA(Gd)-PEG-FA/DOX complexes under different pH conditions.

Materials	Zeta potential (mV)		
	pH = 5.0	pH = 7.4	pH = 10.0
G5.NHAc-DOTA(Gd)-PEG-FA	14.7 ± 2.2	11.3 ± 2.3	-9.7 ± 1.0
G5.NHAc-DOTA(Gd)-PEG-FA/DOX	15.4 ± 1.9	8.8 ± 4.0	-10.4 ± 4.4

Table S2. Quantification of DOX loaded within the G5.NHAc-DOTA(Gd)-PEG-FA dendrimers.

Materials	Practical number of DOX loaded within each G5 dendrimer	Drug encapsulation efficiency (EE%)	Drug loading percentage (DL%)
G5.NHAc-DOTA(Gd)-PEG-FA/DOX	8.5	78.9%	5.7%

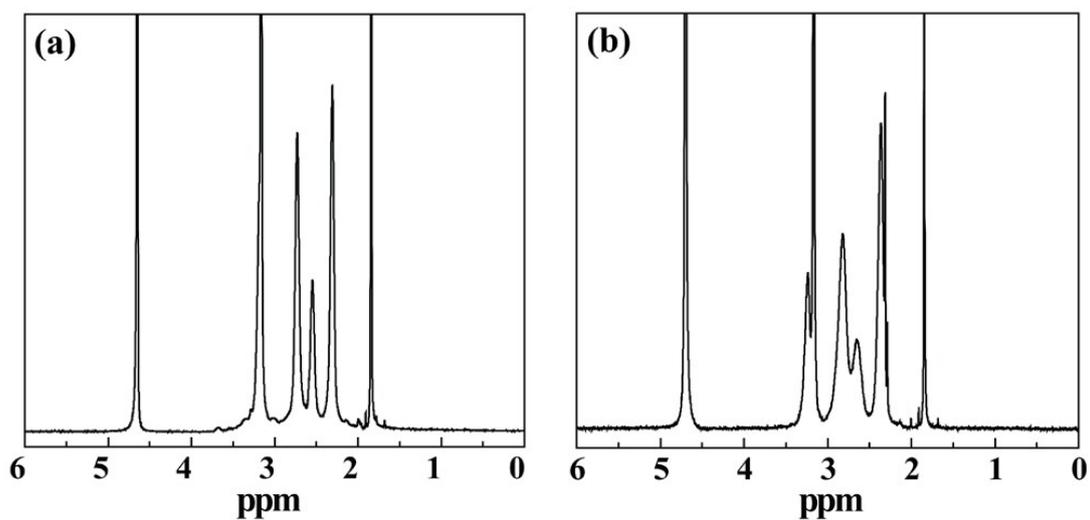


Figure S1. ^1H NMR spectrum of G5.NHAc (a) and G5.NHAc-DOTA dendrimers (b) dissolved in D_2O .

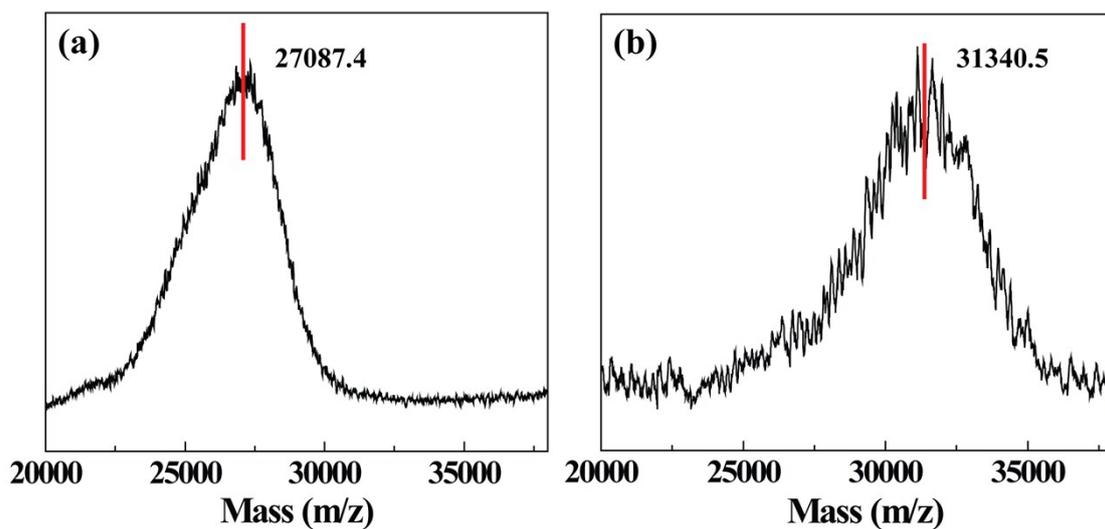


Figure S2. MALDI-TOF mass spectrum of G5.NH₂ (a) and G5.NH₂-DOTA (b) dendrimers.

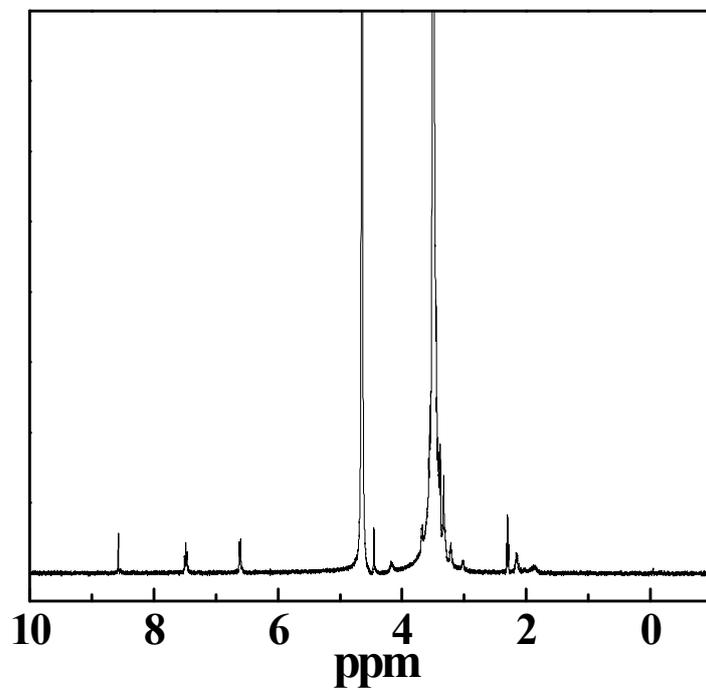


Figure S3. ¹H NMR spectrum of FA-PEG-COOH dissolved in D₂O.

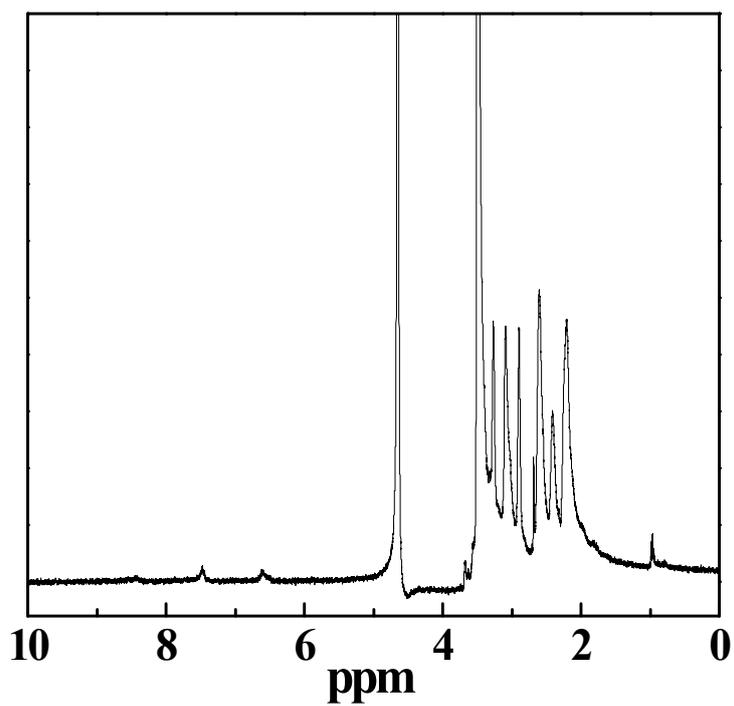


Figure S4. ¹H NMR spectrum of G5.NH₂-DOTA-PEG-FA dissolved in D₂O.

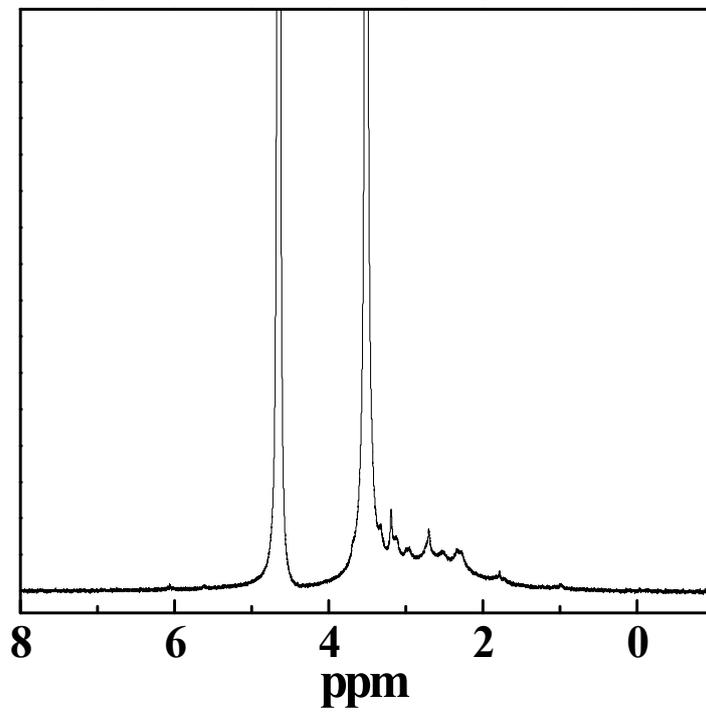


Figure S5. ^1H NMR spectrum of G5.NH₂-DOTA-*m*PEG dissolved in D₂O.

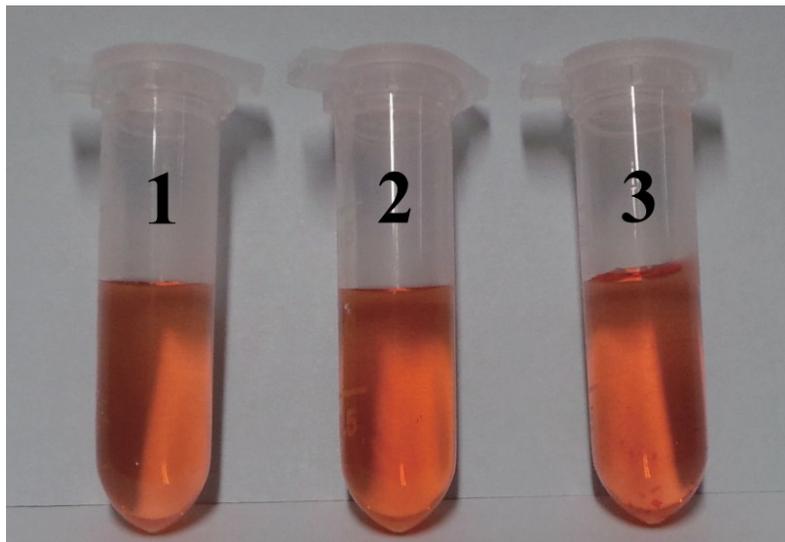


Figure S6. Photograph of the aqueous solutions of G5.NHAc-DOTA(Gd)-PEG-FA/DOX complexes (a) under different pH conditions (pH = 5.0 (1), 7.4 (2), and 10.0 (3)).

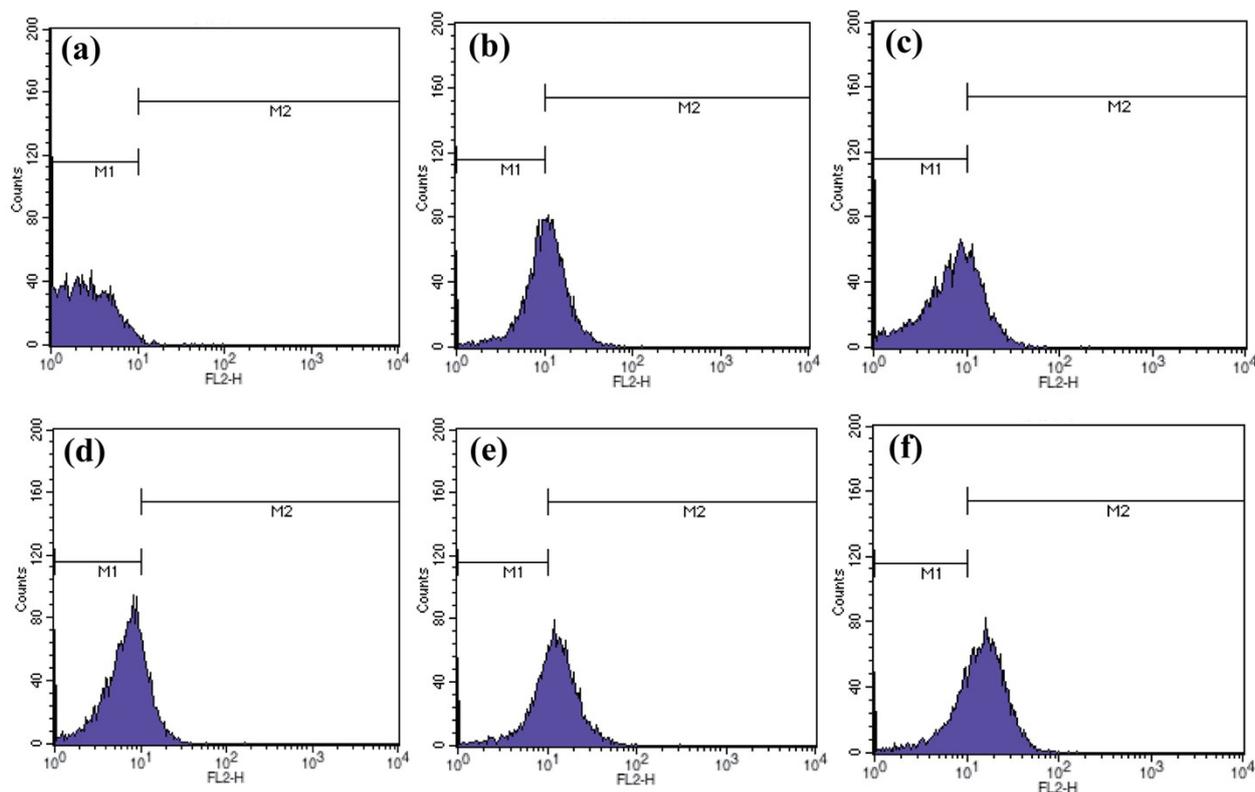


Figure S7. Flow cytometric analysis of KB-HFAR cells treated with (a) PBS and (b) free DOX; KB-LFAR cells treated with the G5.NHAc-DOTA(Gd)-*m*PEG/DOX (c) and G5.NHAc-DOTA(Gd)-PEG-FA/DOX (e) complexes; KB-HFAR cells treated with G5.NHAc-DOTA(Gd)-*m*PEG/DOX (d) and G5.NHAc-DOTA(Gd)-PEG-FA/DOX (f) complexes, respectively.

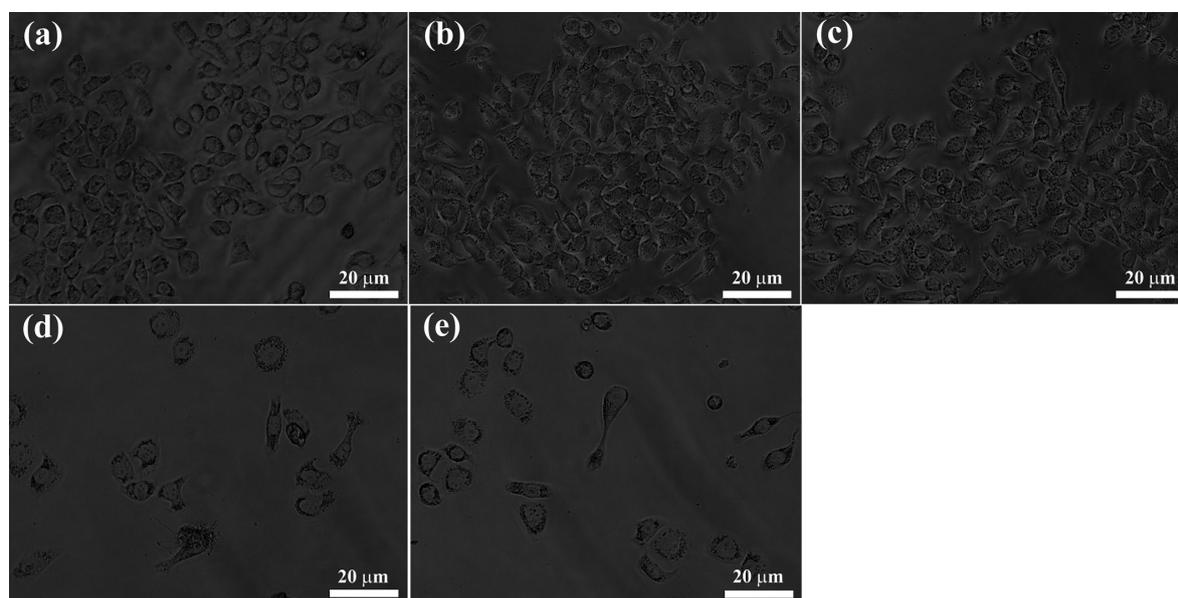


Figure S8. Phase contrast microscopic images of KB-HFAR cells without treatment (a) and treated with PBS (b), G5.NHAc-DOTA(Gd)-PEG-FA dendrimers without DOX but with the same concentration as those used to encapsulate 600 nM DOX (c), free DOX (600 nM) (d), and G5.NHAc-DOTA(Gd)-PEG-FA/DOX complexes ([DOX] = 600 nM) (e), respectively. The cells were treated for 24 h before observation.