

## Naturally available hypericin undergoing electron transfer for type I photodynamic and photothermal synergistic therapy

Zhen Ke†<sup>a</sup>, Aize Xie†<sup>b</sup>, Jianjiao Chen<sup>a</sup>, Zhenyuan Zou<sup>a</sup>, Lei Shen\*<sup>c</sup>, Yansong Dai\*<sup>d</sup>,  
Dengfeng Zou\*<sup>a</sup>

*a.* School of Pharmacy, Guilin Medical University, Guilin 541004, Guangxi, P.R. China, Email: [zdf1226@126.com](mailto:zdf1226@126.com)

*b.* The First Affiliated Hospital of Guangxi Medical University, Nanning 530021, Guangxi, P.R. China

*c.* Jiangsu Laboratory of Advanced Functional Material, Department of Chemistry and Material Engineering, Changshu Institute of Technology, Changshu 215500, Jiangsu, P.R. China Email: [leishen@cslg.edu.cn](mailto:leishen@cslg.edu.cn)

*d.* Virginia University of Integrative Medicine, Fairfax, 22031, Virginia, USA. Email: [daiyansong@gmail.com](mailto:daiyansong@gmail.com)

†: These authors contribute equally to the work

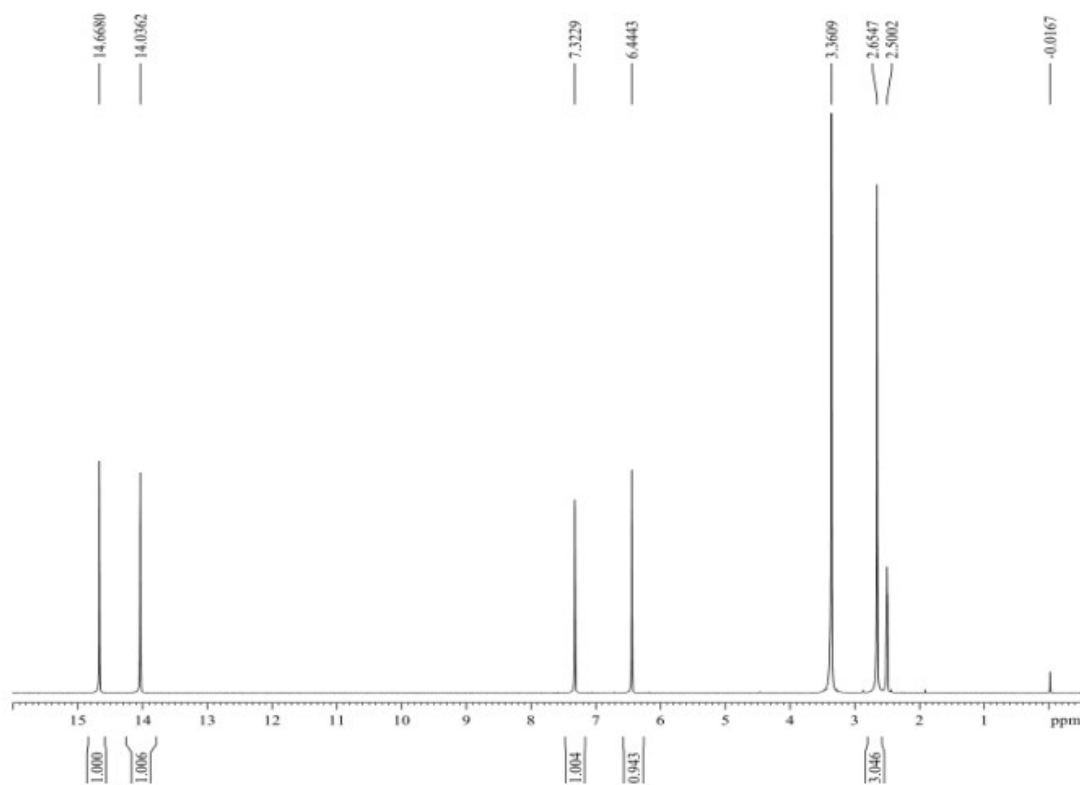


Figure S1 <sup>1</sup>H NMR spectra of **HC** in CDCl<sub>3</sub>

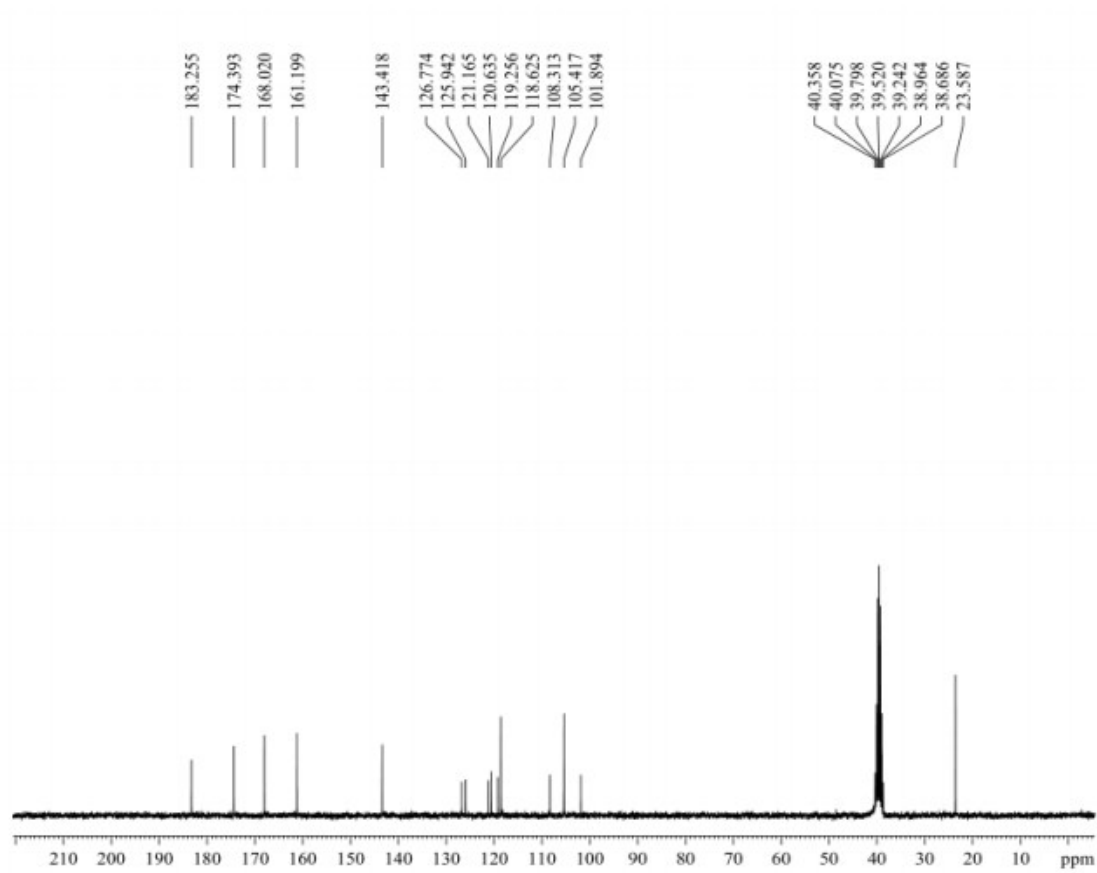
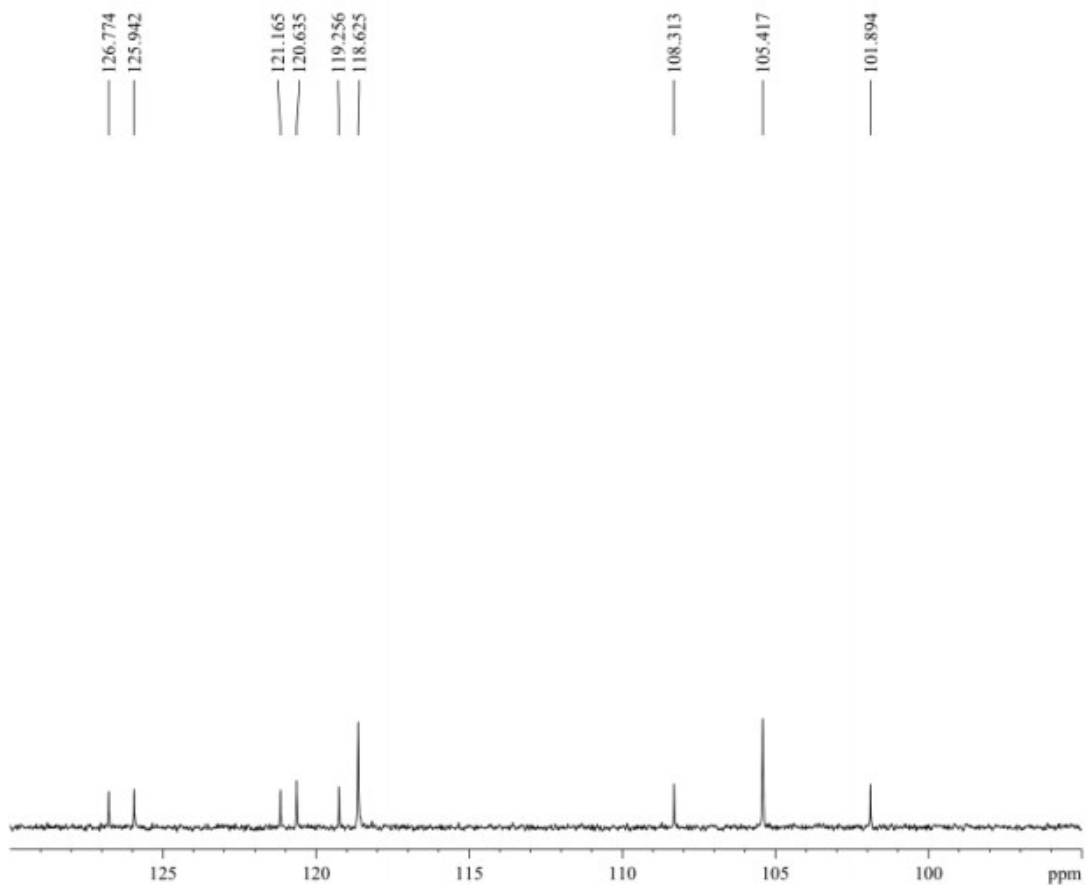
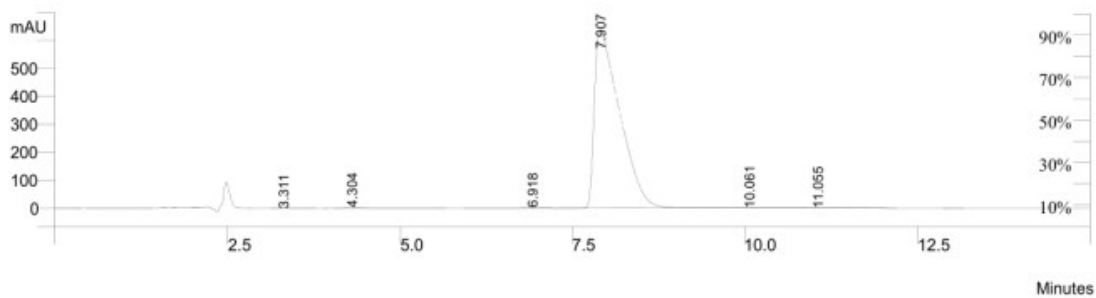


Figure S2 (a)  $^{13}\text{C}$ NMR of **HC** in  $\text{CDCl}_3$



(b)  $^{13}\text{C}$ NMR of **HC** in  $\text{CDCl}_3$  from 130 to 90 ppm



Peak No	Peak Name	Area (counts)	Result ()	Ret. Time (min)	Width 1/2 (sec)
1		115754	0.0705	3.311	8.6
2		468341	0.2852	4.304	9.7
3		501820	0.3056	6.918	12.4
4		162519536	98.9725	7.907	24.0
5		209014	0.1273	10.061	0.0
6		392380	0.2390	11.055	0.0
<b>Totals</b>		<b>164206848</b>	<b>100.0001</b>		

Figure S3 HPLC of **HC**

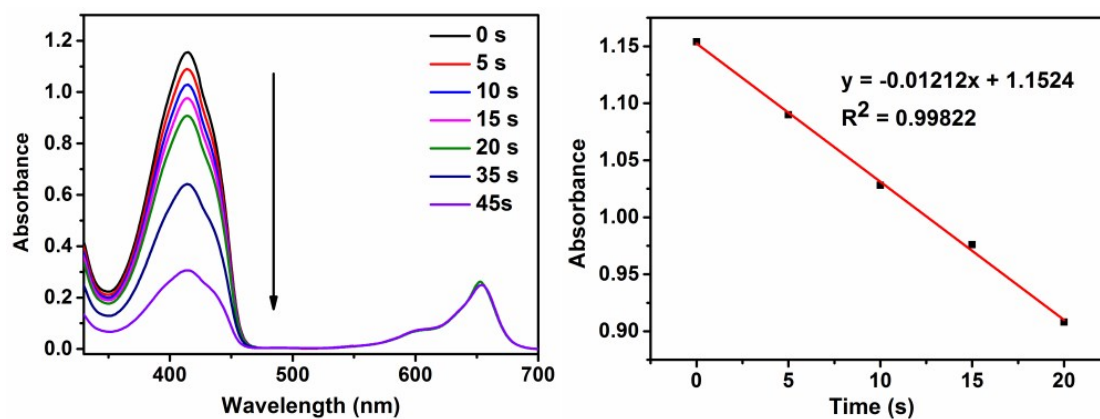


Figure S4 (a) Degradation of DPBF under the presence of **MB** with irradiation; (b) linear fitting of the absorbance.

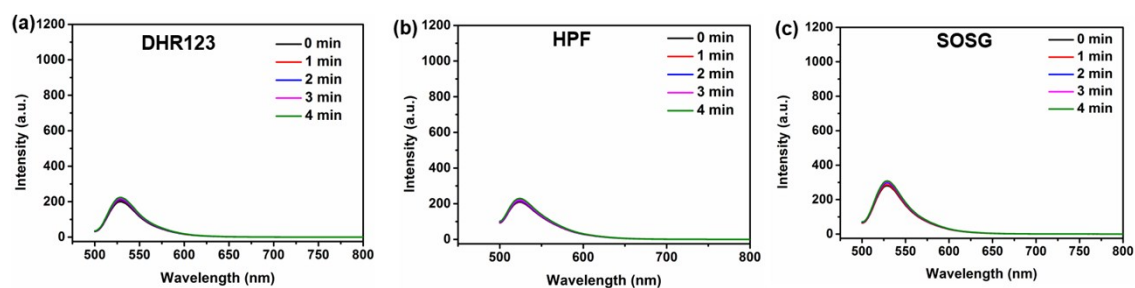


Figure S5 Fluorescence change of (a) DHR123; (b) HPF and (c) SOSG with irradiation. (660 nm, 0.1 W/cm<sup>2</sup>).

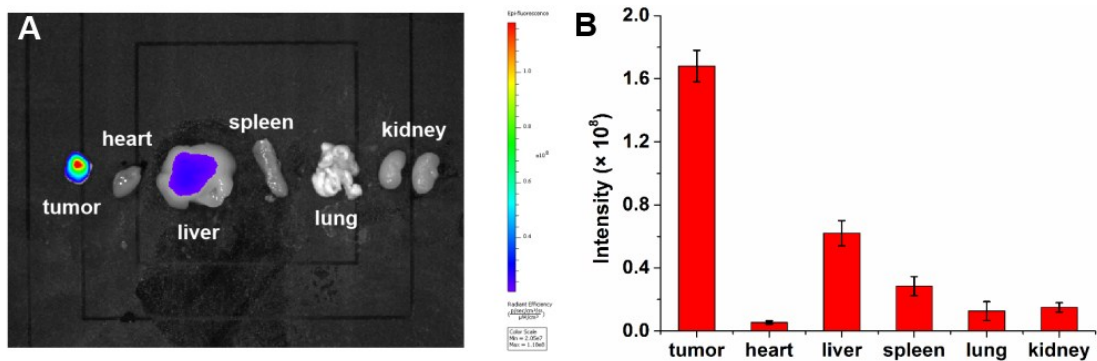


Figure S6 (A) Biodistribution of HC NPs in tumor, heart, liver, spleen, lung and kidney after 48 h post injection; (B) Fluorescence intensity of tumor, heart, liver, spleen, lung and kidney. (n = 3)

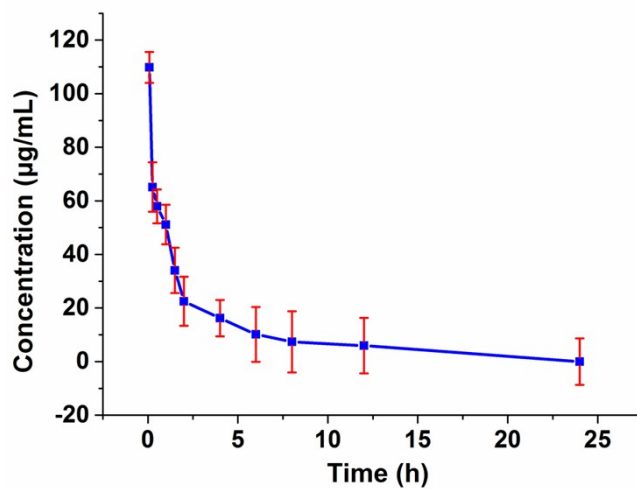


Figure S7 Time dependent drug concentration of HC NPs in mice (n = 6)