## Supporting Information for ORIGINAL ARTICLE

Accurate construction of cell membrane biomimetic graphene nanodecoys *via* purposeful surface engineering to improve screening efficiency of active components of traditional Chinese medicine

Qi Hu<sup>a,b</sup>, Lanlan Jia<sup>a,b</sup>, Xiaolin Zhang<sup>a,b</sup>, Aihong Zhu<sup>a,b</sup>, Sicen Wang<sup>a,b</sup>, Xiaoyu Xie<sup>a,b,\*</sup>

<sup>a</sup>School of Pharmacy, Health Science Center, Xi'an Jiaotong University, Xi'an 710061, China <sup>b</sup>Shaanxi Engineering Research Center of Cardiovascular Drugs Screening & Analysis, Xi'an 710061, China

Received 6 March 2021; received in revised form 9 April 2021; accepted 12 April 2021

\*Corresponding author. Tel./fax: +86 29 82656788.

E-mail address: xiexiaoyu@xjtu.edu.cn (Xiaoyu Xie).

## **Samples preparation for TEM:**

1. 300 mesh carbon coated grids were used.

2. GO, PMGO, and HPMGO solution were prepared and ultrasonicly dispersed evenly. (GO and PMGO were dispersed in ethanol at a concentration of 0.1 mg/mL, while HPMGO was dispersed in water at the same concentration.)

3. A drop (approx. 20  $\mu$ L) of GO, PMGO, and HPMGO solution was placed on the grid, respectively.

4. Samples were dried overnight in a Petri dish and observed the next day in TEM.



Figure S1 TGA analysis results of GO and PMGO.



**Figure S2** SEM characterization of GO (scale bar=10.0  $\mu$ m), PMGO (scale bar=5.00  $\mu$ m), and HPMGO (scale bar=5.00  $\mu$ m).



Figure S3 UV/Vis spectra of MGO and PMGO.



**Figure S4** (A) Freundlich and (B) Langmuir isotherm models to fit the equilibrium adsorption data of PMGO and HPMGO.



**Figure S5** The cytotoxicity of HeLa cells incubated with the artificial mixture and *Angelica dahurica*. Data are presented as mean  $\pm$ SD (*n*=3).



**Figure S6** The apoptosis of HeLa cells incubated with the (A) artificial mixture, and (B) *Angelica dahurica*.

Isotherm model	Equation and parameters	HPMGO	PMGO	
Freundlich	$lgQ_e = lgK_F + mlgC_e$			
	$K_{\rm F}$ (L/mg)	1.9943	0.9987	
	т	0.5694	0.4530	
	r	0.9652	0.9887	
Langmuir	$\frac{C_e}{Q_e} = \frac{1}{Q_{max}K_L} + \frac{1}{Q_{max}}C_e$			
	$K_{\rm L}$ (L/mg)	0.0042	0.0075	
	$Q_{\rm max}~({ m mg/g})$	128.21	47.62	
	r	0.9963	0.9981	

**Table S1** Equations and parameters of adsorption isotherms of PMGO and HPMGO.

HPMGO, Hela CM coated PEGylated magnetic graphene oxide; PMGO, PEGylated magnetic graphene oxide.

**Table S2** Kinetic parameters for adsorption of vinorelbine ditartrate onto HPMGO and PMGO.

Kinetic model	Model parameters	HPMGO	PMGO
Pseudo-first-order	$K_1$ (min <sup>-1</sup> )	0.5516	1.9713
	$q_{\rm e} ({\rm mg/g})$	37.58	15.74
	r	0.9907	0.9835
Pseudo-second-order	$K_2$ (g/mg/min)	0.0186	0.1892
	$q_{\rm e}({\rm mg/g})$	41.23	16.36
	r	0.9915	0.9975

HPMGO, Hela CM coated PEGylated magnetic graphene oxide; PMGO, PEGylated magnetic graphene oxide.