

Evaluation of Serum Phosphopeptides as Potential Biomarkers of Gastric Cancer

Guijin Zhai,^{ad} Liping Yang,^b Qun Luo,^{a,c} Kui Wu,^a Yao Zhao,^a Jianan Liu,^a Shaoxiang Xiong,^a Fuyi Wang^{*a,c}

a: Beijing National Laboratory for Molecular Sciences; National Centre for Mass Spectrometry in Beijing; CAS Key Laboratory of Analytical Chemistry for Living Biosystems, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, PR China; E-mail: fuyi.wang@iccas.ac.cn

b: Cancer Research Centre, Tumour Hospital Affiliated to Nantong University, Nantong 226361, Jiangsu, PR China; E-mail: liping.yang@ntu.edu.cn

c: University of Chinese Academy of Sciences

d: Present address: Department of Biochemistry and Molecular Biology; Tianjin Key Laboratory of Medical Epigenetics, Tianjin Medical University, Tianjin, 300070, PR China

Supporting Information

Tables S1 –S2

Figures

Table S1. Calibration equations corresponding to the calibration curves shown in Fig. 4 and Fig. S2 – S4 for determination of phosphopeptides F1 – F4.

Phosphopeptides	Square	R ²
F1	$Y = 1.0000 X + 0.0011$	0.998
F2	$Y = 1.0482 X + 0.0016$	0.999
F3	$Y = 0.9578 X - 0.0060$	0.999
F4	$Y = 0.9435 X - 0.0054$	0.999

F1: ADpSGEGDFLAEGGGV; F2: DpSGEGDFLAEGGGV;

F3: DpSGEGDFLAEGGGVR; F4: ADpSGEGDFLAEGGGVR.

Table S2. Descriptive characteristics of participants in this work.

	Controls		GC		<i>P</i> Value (TS vs VS for GC)
	TS	VS*	TS	VS	
Age(years)	24.5±3.4	24.5±3.4	63.2±8.9	62.5±8.2	0.71
Male/Female	10/20	10/20	23/17	11/9	0.85
Stage I	NA	NA	6	3	
Stage II, III, IV	NA	NA	32	17	
Unknown	NA	NA	2	0	

*Validation set is identical with training set for controls.

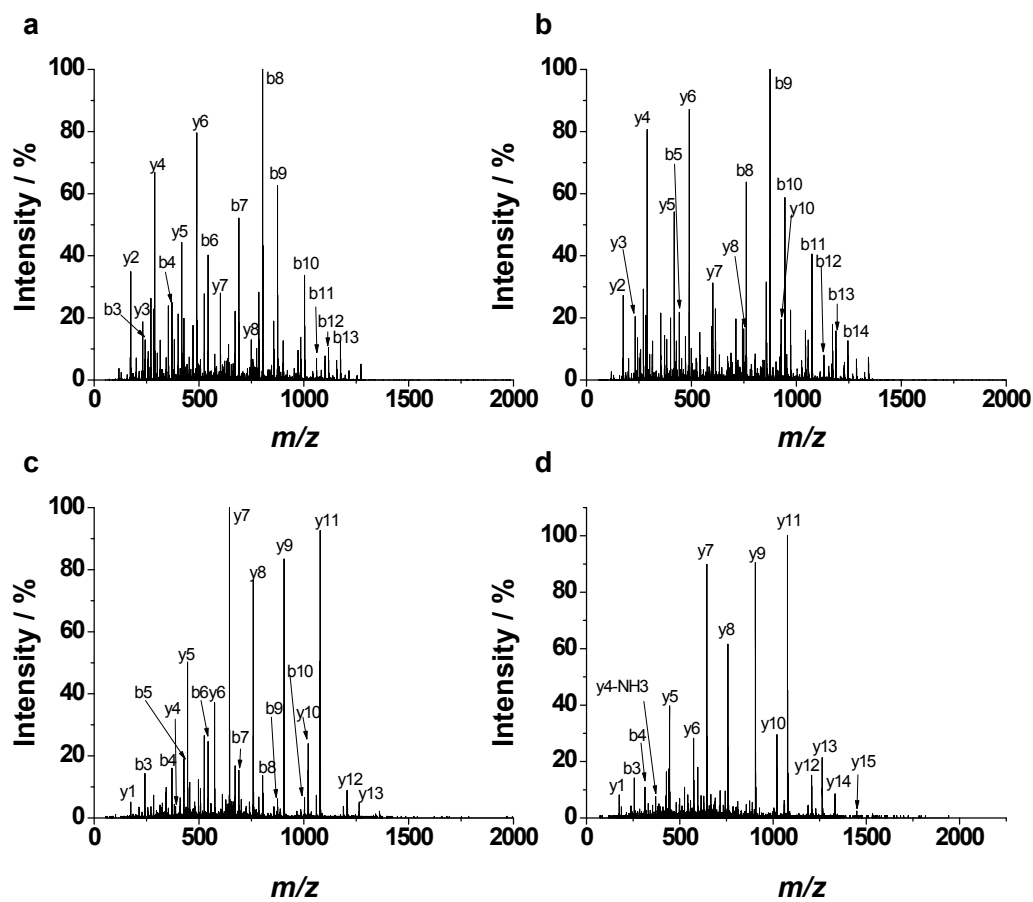


Fig. S1 ESI-Q-TOF MS/MS spectra of the phosphopeptides in human serum: (a) F1 = ADpSGEGDFLAEGGGV; (b) F2 = DpSGEGDFLAEGGGV; (c) F3 = DpSGEGDFLAEGGGVR and (d) F4 = ADpSGEGDFLAEGGGVR.

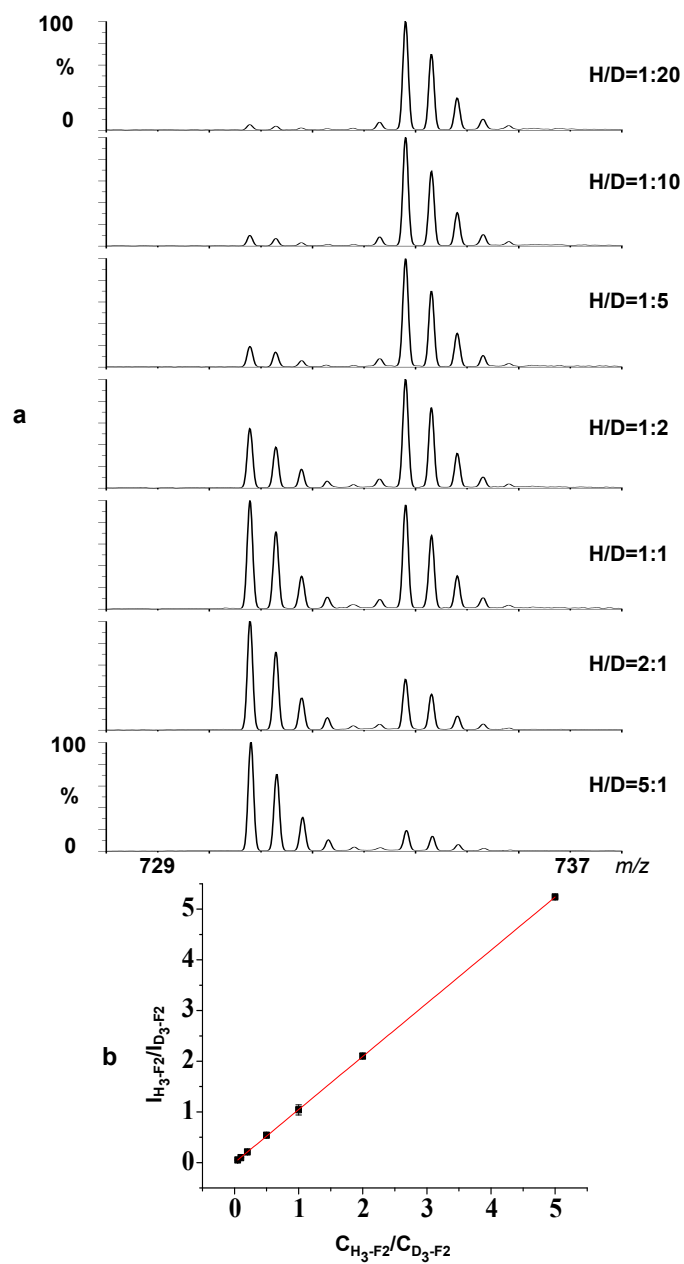


Fig. S2 (a) Mass spectra of standard samples containing various ratios of H₆- and D₆-phosphpeptide standard F2 after enrichment by ZrAs-Fe₃O₄@SiO₂ nanoparticles. (b) Calibration curve plotted by the intensity ratio vs. the molar ratio of H-/D-F2.

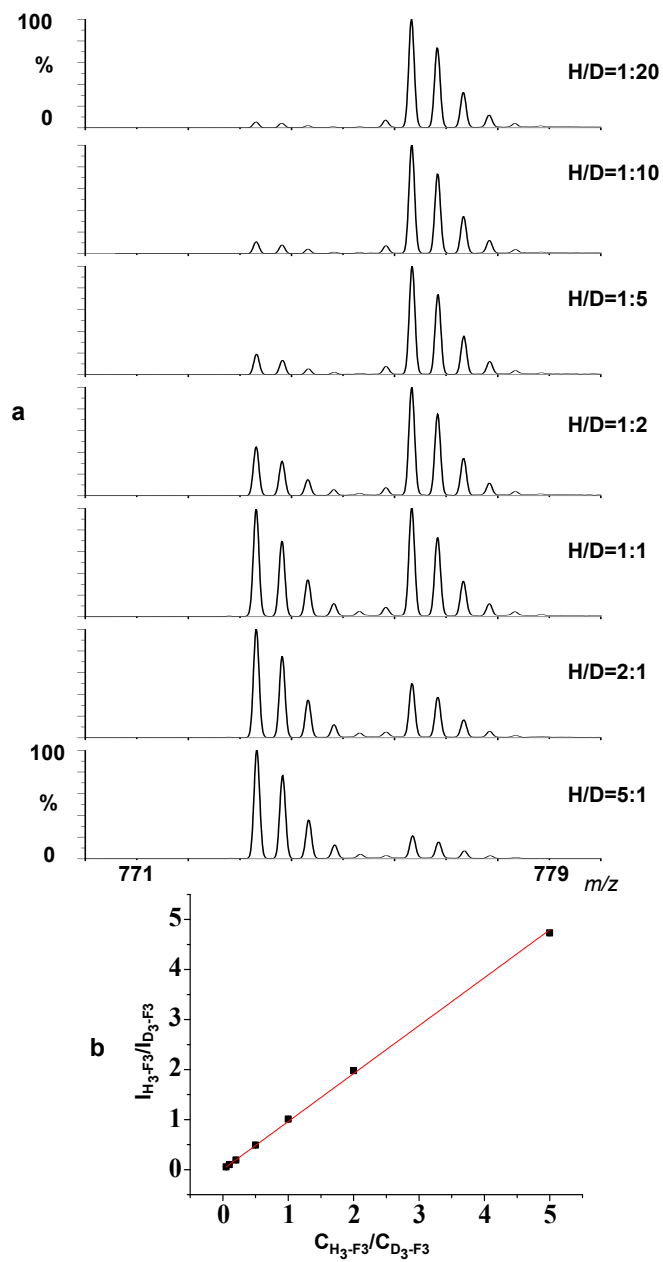


Fig. S3 (a) Mass spectra of standard samples containing various ratios of H₆- and D₆-phosphpeptide standard F3 after enrichment by ZrAs-Fe₃O₄@SiO₂ nanoparticles. (b) Calibration curve plotted by the intensity ratio vs. the molar ratio of H-/D-F3.

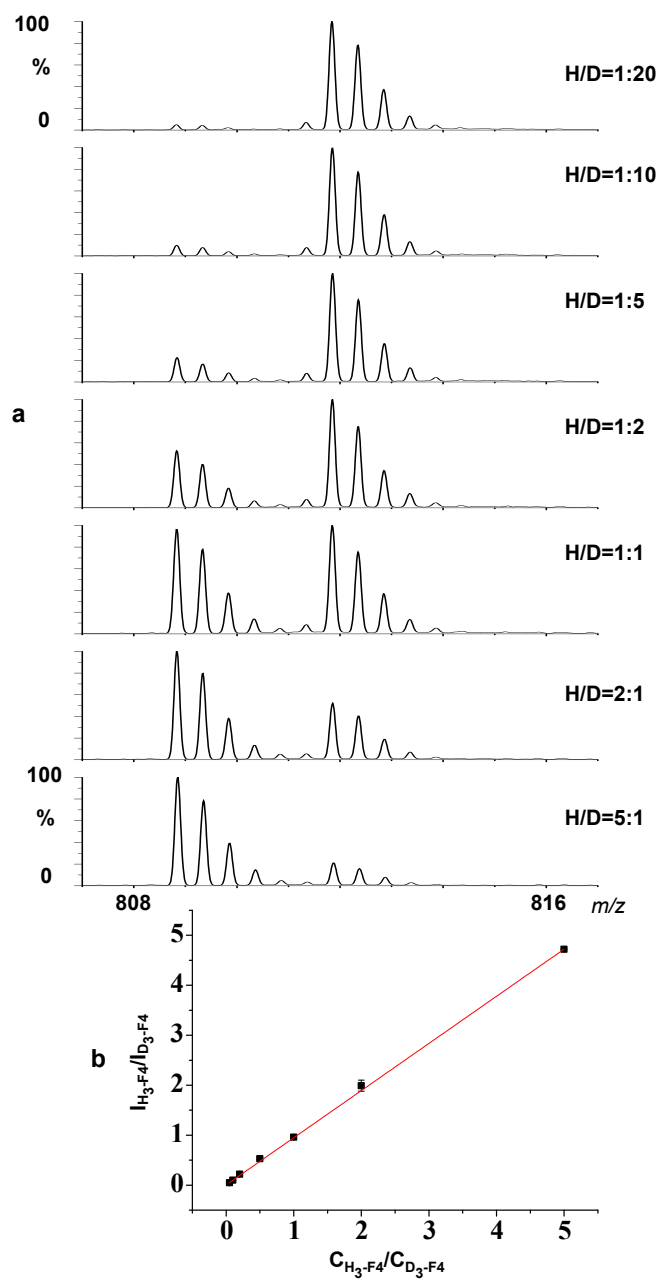


Fig. S4 (a) Mass spectra of standard samples containing various ratios of H₆- and D₆-phosphopeptide standard F4 after enrichment by ZrAs-Fe₃O₄@SiO₂ nanoparticles. (b) Calibration curve plotted by the intensity ratio vs. the molar ratio of H-/D-F4.

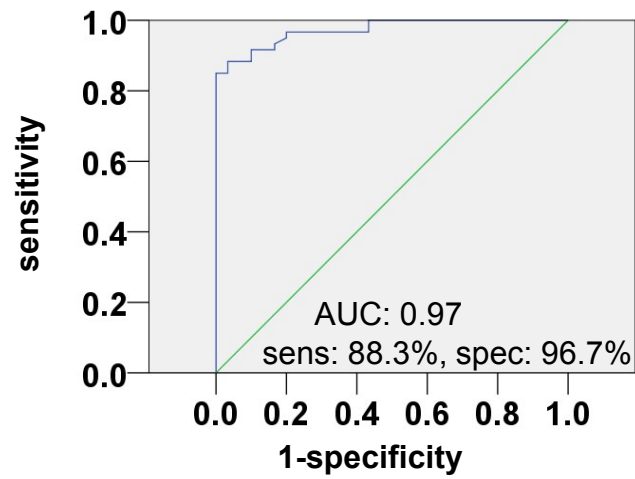


Fig. S5 ROC curve for F3 showing the comparison of controls and GC cases in both training set and validate set. The inserts sens, spec and AUC represent sensitivity, specificity and area under the curve, respectively.