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 $Fig. S1 \ Molecular \ structures \ of \ template \ and \ other \ analogues.$ 



Fig.S2 The selective adsorption capacity of MCNTs@TSTO-MIPs and MCNTs@NIPs to TSTO, PROG, MTSTO, and TSTOP in the mixture solution.



Fig.S3 The reusability of MCNTs@TSTO-MIPs and MCNTs@NIPs towards TSTO.

## Table S1

	TSTO					
LNCaP cell	1.0 ng mL <sup>-1</sup>		5.0 ng mL <sup>-1</sup>		50.0 ng mL <sup>-1</sup>	
	Recovery (%)	RSD (%)	Recovery (%)	RSD (%)	Recovery (%)	RSD (%)
Intra-day	102.1	4.7	99.8	3.9	98.7	2.3
Inter-day	103.2	5.1	100.7	4.8	99.3	3.4

Recoveries of MCNTs@TSTO-MIPs absorbing TSTO for spiked LNCaP cell samples. (n=5)



Fig. S4 Chromatograms of the human prostate cancer LNCaP cell spiked with TSTO at the concentration of 5.0 ng mL<sup>-1</sup> (A), elution of absorbed MCNTs@TSTO-MIPs (B), and TSTO standard sample (C).



Fig. S5 The inhibitory effects of different amounts of MCNTs@TSTO-MIPs and different incubation times on the proliferation of LNCaP cells.



Fig. S6 The flow cytometry of control (A), 10 (B), 20 (C), and 40 (D)  $\mu$ g mL<sup>-1</sup> of MCNTs@TSTO-MIPs for 48 h.