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

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

<table>
<thead>
<tr>
<th>LNCaP cell</th>
<th>TSTO</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.0 ng mL⁻¹</td>
<td>5.0 ng mL⁻¹</td>
<td>50.0 ng mL⁻¹</td>
</tr>
<tr>
<td></td>
<td>Recovery (%)</td>
<td>RSD (%)</td>
<td>Recovery (%)</td>
</tr>
<tr>
<td>Intra-day</td>
<td>102.1</td>
<td>4.7</td>
<td>99.8</td>
</tr>
<tr>
<td>Inter-day</td>
<td>103.2</td>
<td>5.1</td>
<td>100.7</td>
</tr>
</tbody>
</table>
Fig. S4 Chromatograms of the human prostate cancer LNCaP cell spiked with TSTO at the concentration of 5.0 ng mL⁻¹ (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) μg mL⁻¹ of MCNTs@TSTO-MIPs for 48 h.