

**Electronic Supplementary Information**

**Stimulus-Responsive Conformational  
Transformation of Peptide with Cell  
Penetrating Motif for Triggered Cytotoxicity**

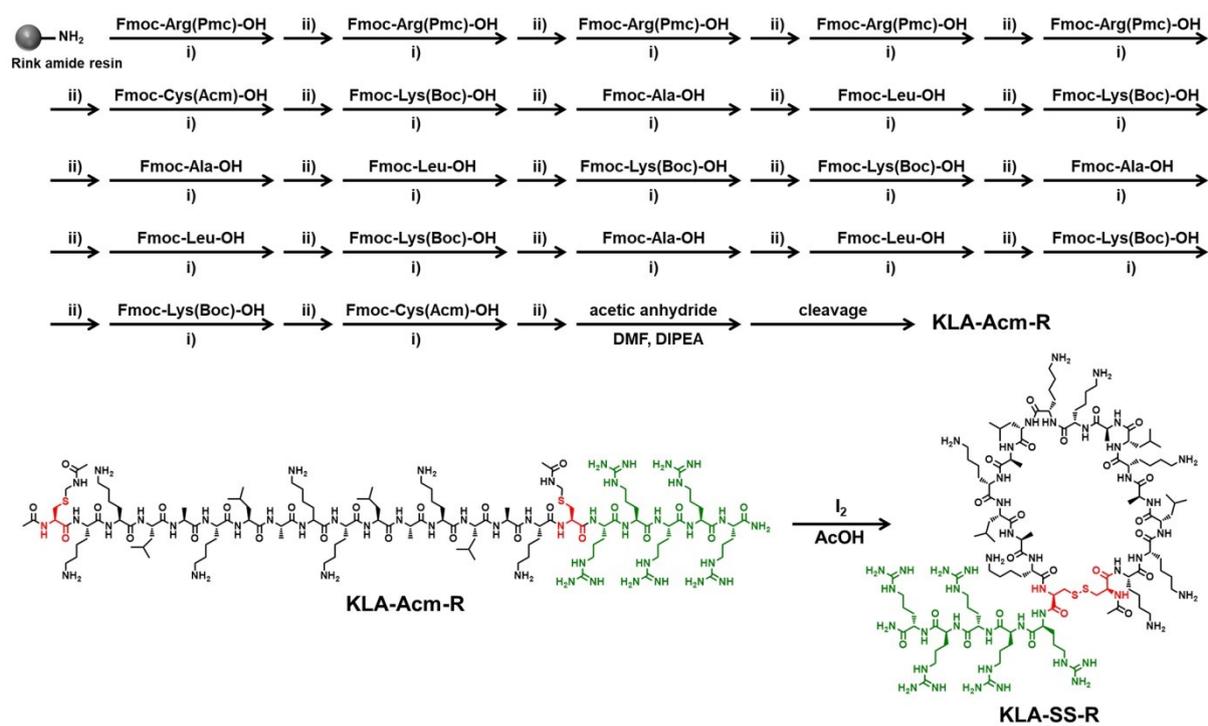
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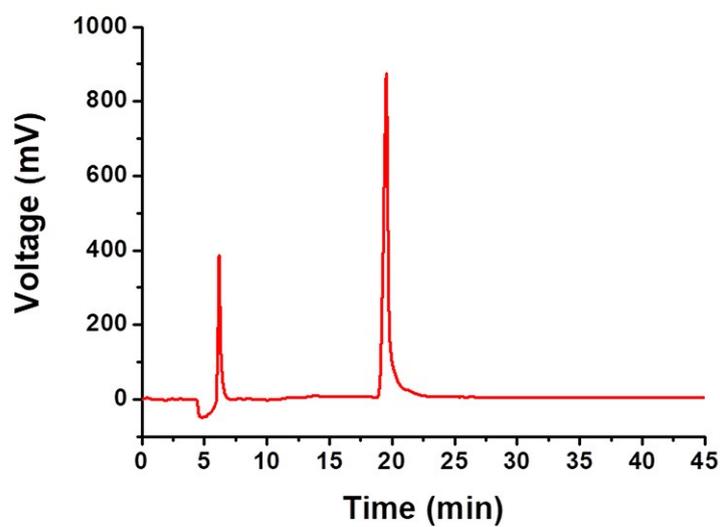
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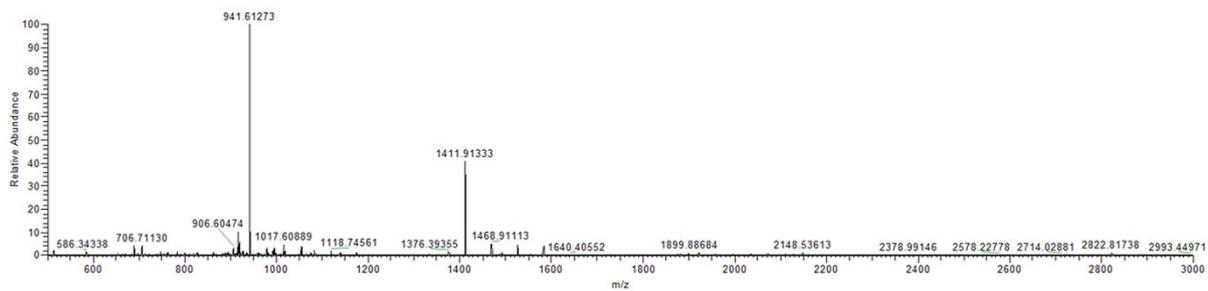
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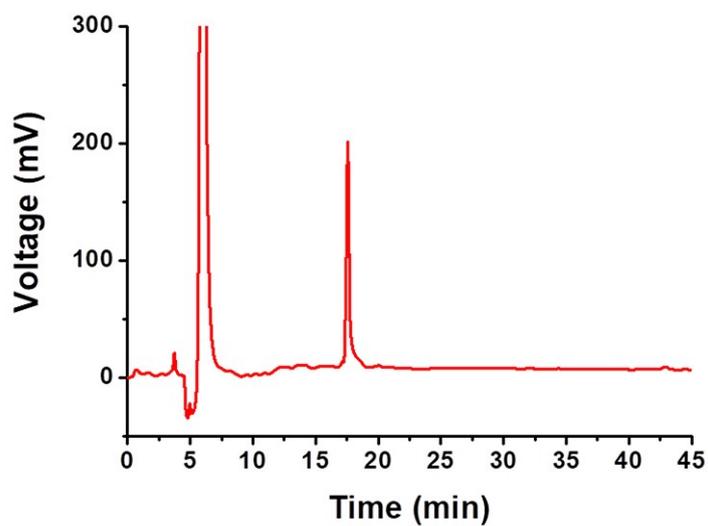
**Fig. S1.** Synthetic route to KLA-SS-R. Conditions: i) HBTU, HOBT, DIPEA and DMF; ii) 20% piperidine in DMF.



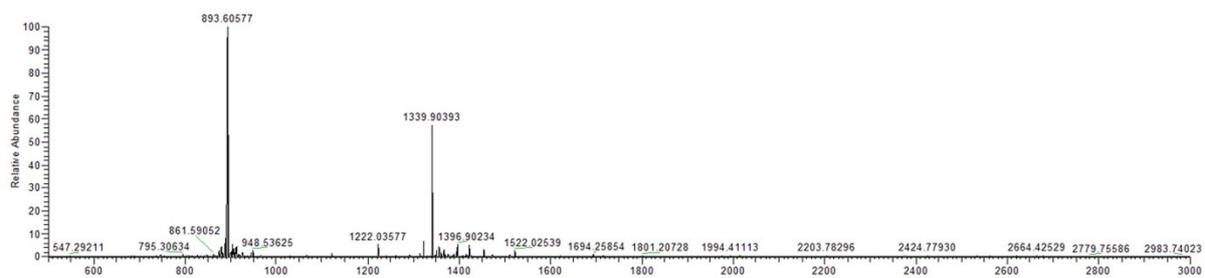
**Fig. S2.** HPLC chromatogram of KLA-Acm-R.



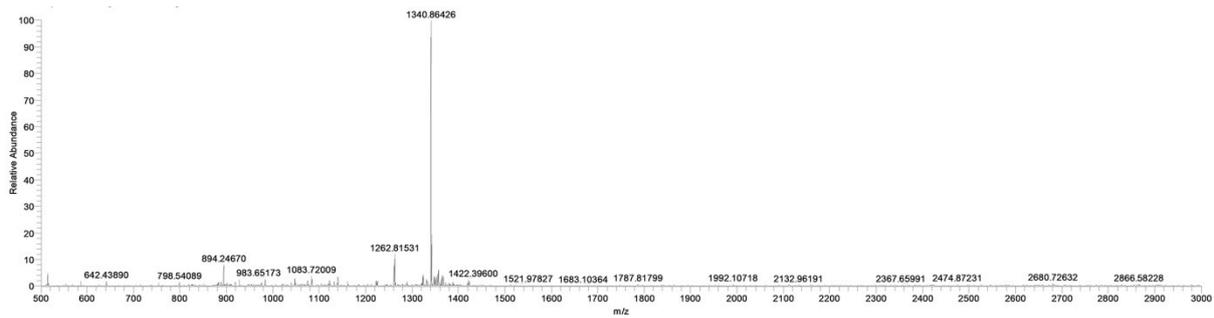
**Fig. S3.** LC-Mass spectrum of KLA-Acm-R.



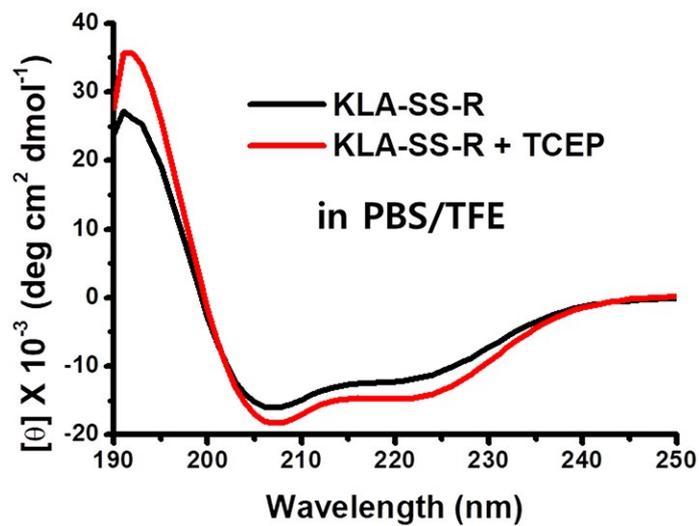
**Fig. S4.** HPLC chromatogram of KLA-SS-R.



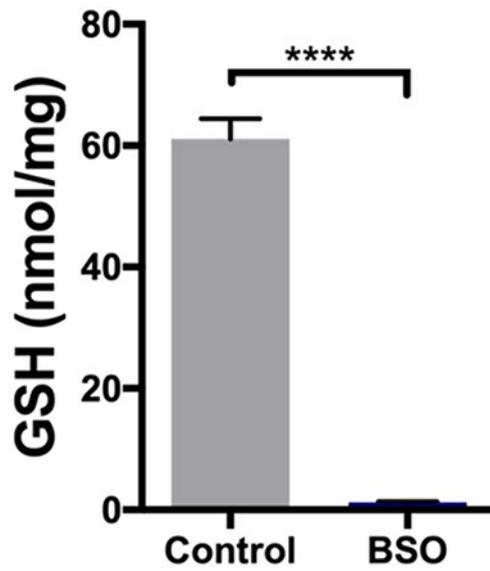
**Fig. S5.** LC-Mass spectrum of KLA-SS-R.



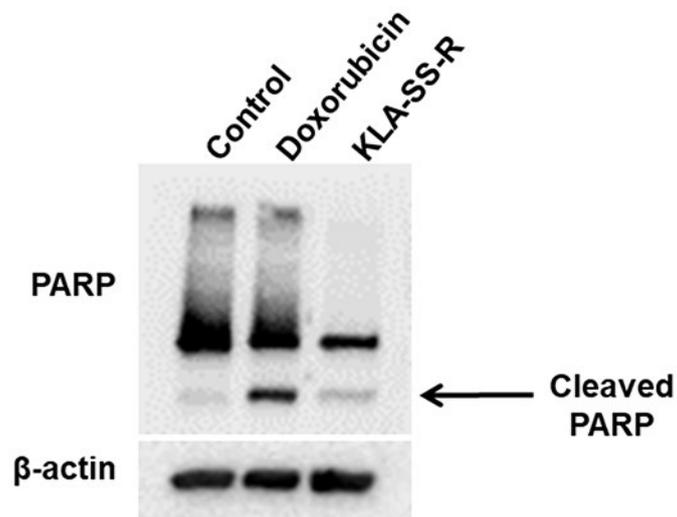
**Fig. S6.** LC-Mass spectrum of KLA-SS-R after TCEP treatment (10 equiv).  $m/z$  calculated for  $[M+2H]^{2+}$  1340.87, found 1340.86.



**Fig. S7.** CD spectra of KLA-SS-R without and with TCEP in PBS/TFE mixed solvent in the wavelength range from 190 to 250 nm.



**Fig. S8.** Depletion of GSH in MDA-MB-231 cells. Columns represent compiled data (means  $\pm$  standard deviation) derived from three independent experiments. \*\*\*\*:  $P < 0.0001$ .



**Fig. S9.** Effect of KLA-SS-R on PARP cleavage in MDA-MB-231 cells. Cells were treated with 3  $\mu$ M doxorubicin or 30  $\mu$ M KLA-SS-R, and PARP cleavage was determined by immunoblot analysis.