

Electronic Supplementary Information

**Induced Cytotoxicity of Peptides with Crypto-
Thioester by Native Chemical Ligation**

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Experimental Section

Circular dichroism. Circular dichroism spectra were recorded on a Jasco J-815 spectropolarimeter (Tokyo, Japan) between 190 and 250 nm at room temperature using a quartz cell with 1 mm path length. The concentration of peptides was 30 μ M in PBS buffer (1 mM, pH 7.4) or in PBS/TFE mixed solvent (1:1, v/v). Five scans with a scan speed of 20 nm/min were averaged for each measurement. The percentage α -helicity was calculated from the mean residue ellipticity at 222 nm using following equation:

$$\% \text{helicity} = [\theta]_{222} / [\theta]_{\text{max}} \times 100$$

$$[\theta]_{\text{max}} = -40,000 \times (1 - 4 / n)$$

where $[\theta]_{222}$ is the mean residue ellipticity, $[\theta]_{\text{max}}$ is the maximal mean residue ellipticity and n is the number of amino acids.^{1,2}

Cell lines and culture conditions. H1299 human lung adenocarcinoma cells were purchased from the American Type Culture Collection (ATCC) and cultured in RPMI-1640 medium. Cells were incubated at 37 °C in a 5% CO₂-containing humidified incubator.

References

- 1 W. C. Johnson, Jr. and I. Tinoco, Jr., *J. Am. Chem. Soc.*, 1972, **94**, 4389-4390.
- 2 J. R. Kumita, O. S. Smart and G. A. Woolley, *Proc. Natl. Acad. Sci. U.S.A.*, 2000, **97**, 3803-3808.

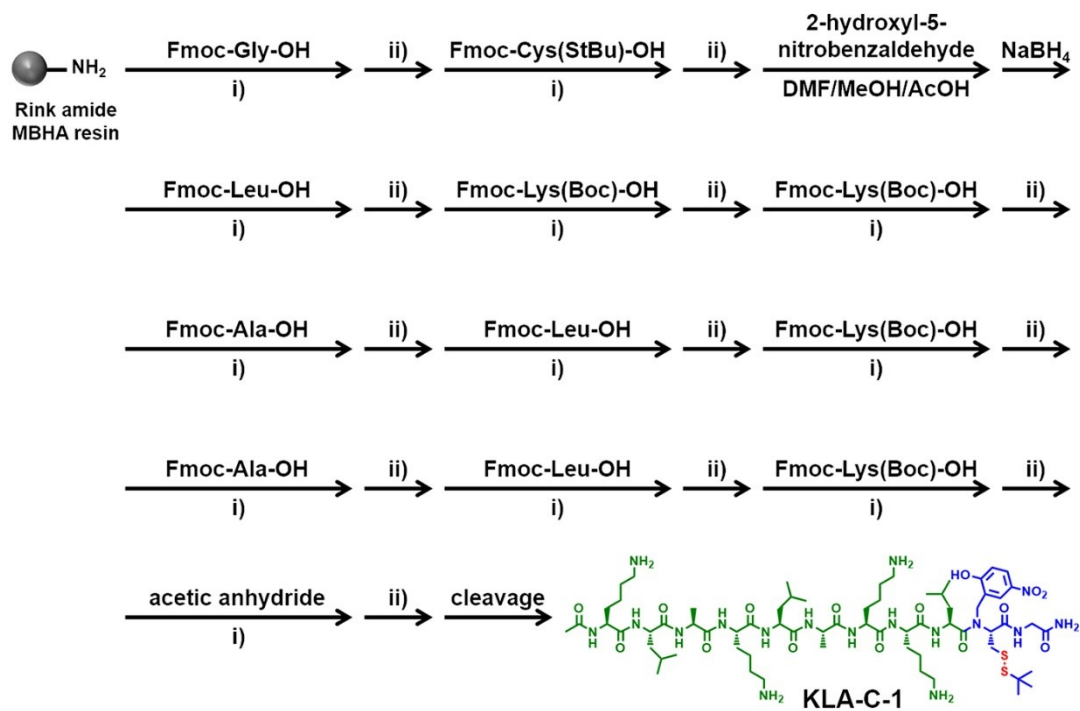


Fig. S1 Synthetic route to KLA-C-1 peptide.

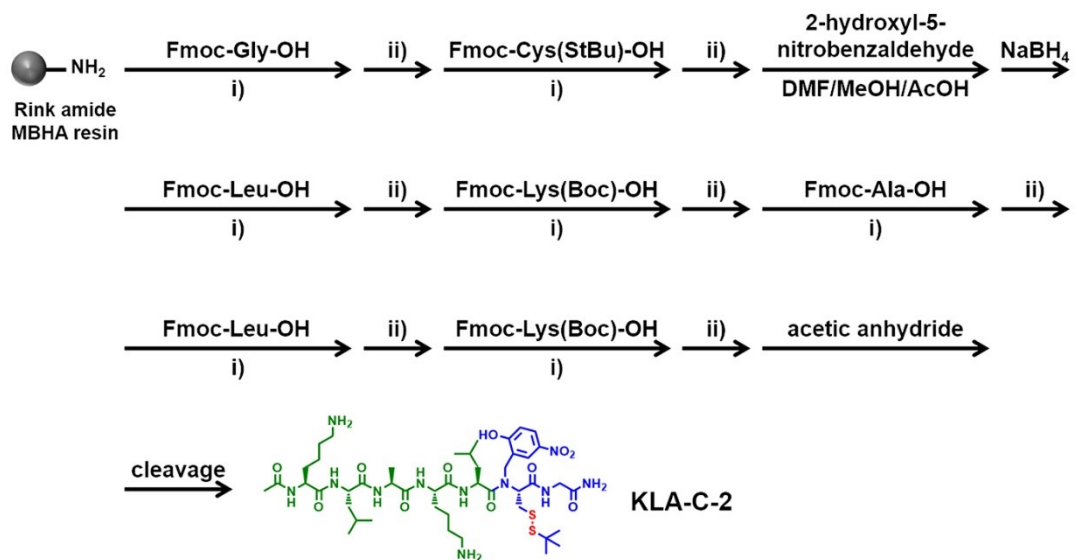


Fig. S2 Synthetic route to KLA-C-2 peptide.

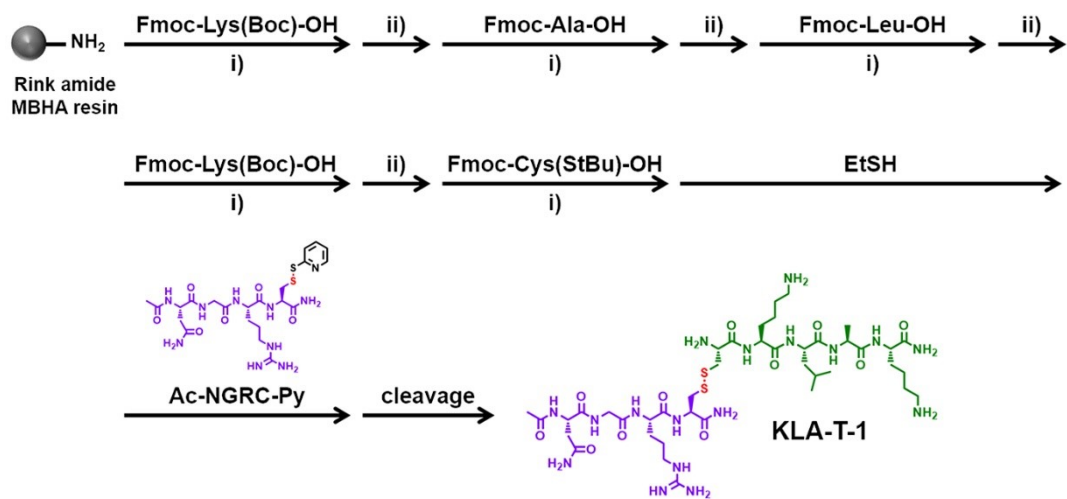


Fig. S3 Synthetic route to KLA-T-1 peptide.

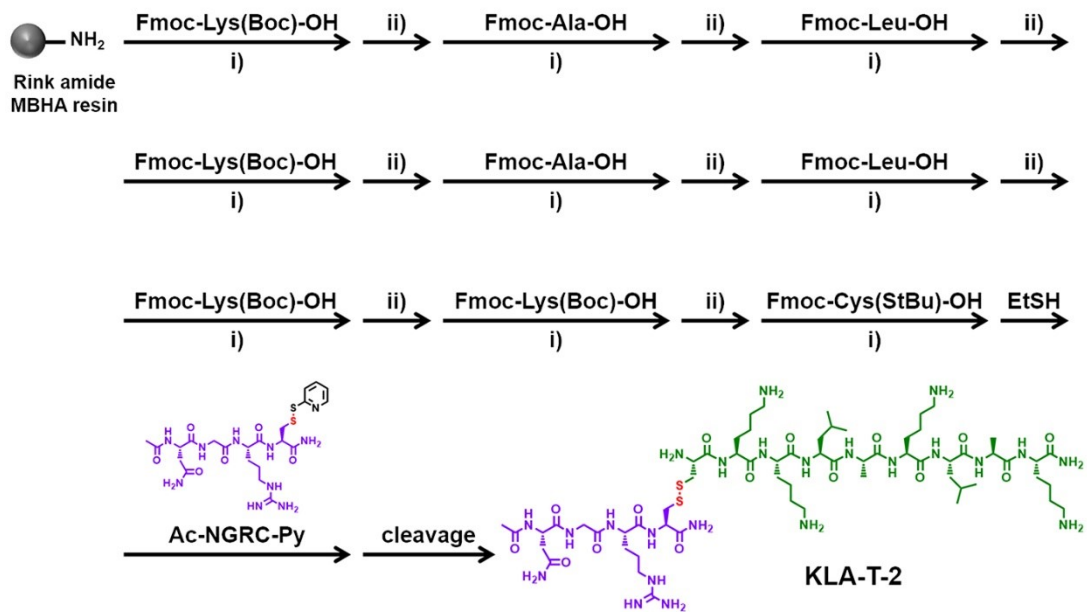


Fig. S4 Synthetic route to KLA-T-2 peptide.

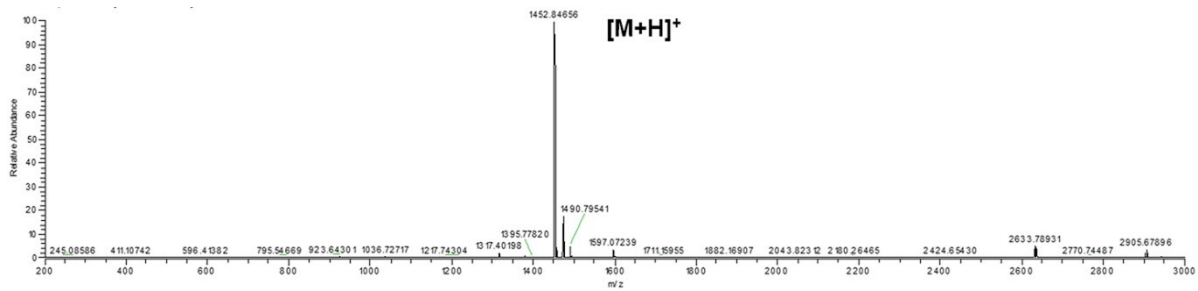


Fig. S5 LC-Mass spectrum of KLA-C-1.

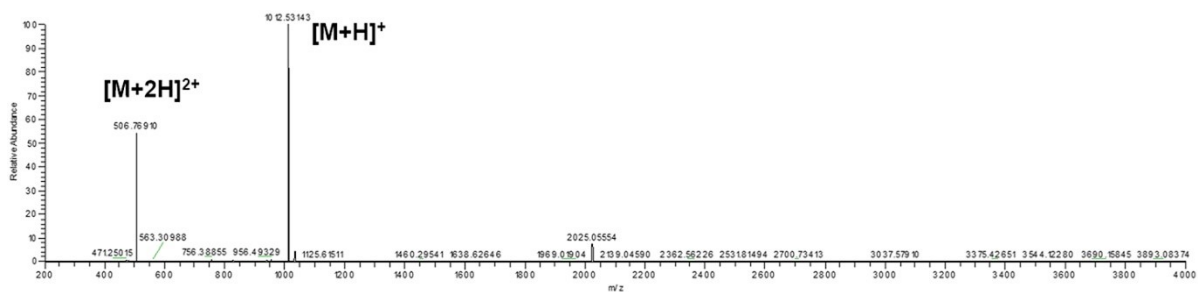


Fig. S6 LC-Mass spectrum of KLA-C-2.

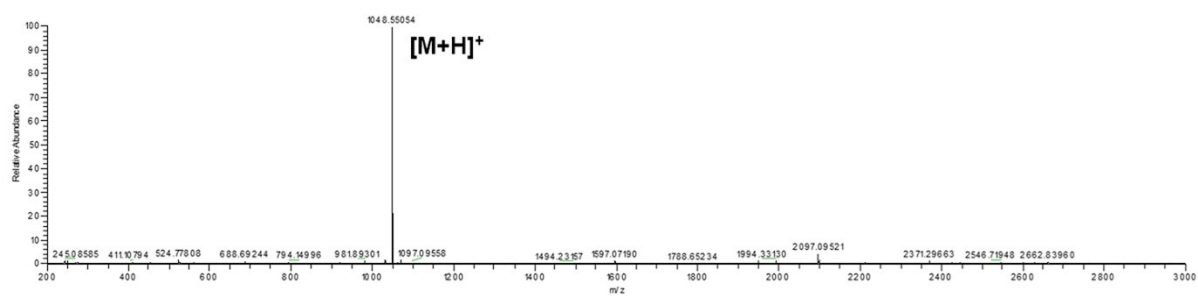


Fig. S7 LC-Mass spectrum of KLA-T-1.

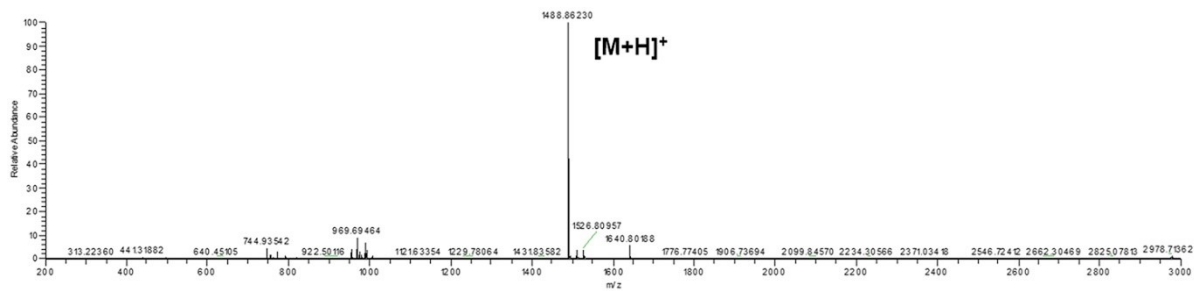


Fig. S8 LC-Mass spectrum of KLA-T-2.

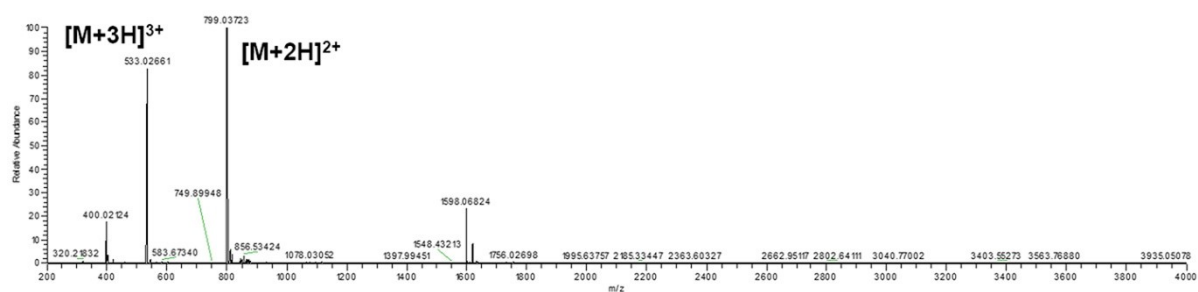


Fig. S9 LC-Mass spectrum of KLA-1.

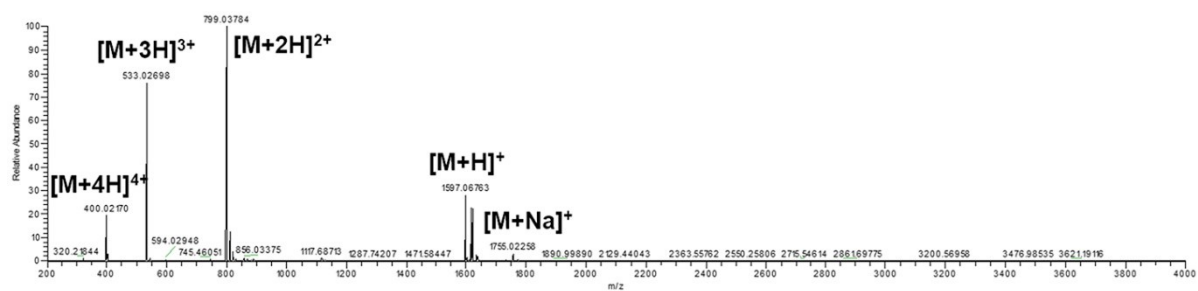


Fig. S10 LC-Mass spectrum of KLA-2.