Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

69451 Weinheim, Germany

"Control of the yeast cell cycle with a photocleavable α-factor analog"

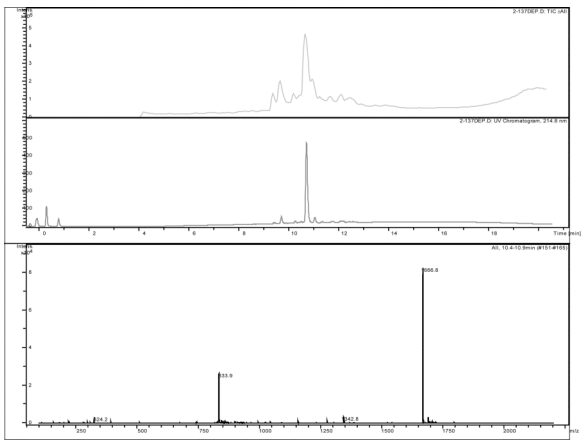
Laurie L. Parker, Josh Kurutz, Stephen B. H. Kent, Stephen J. Kron*

Contents

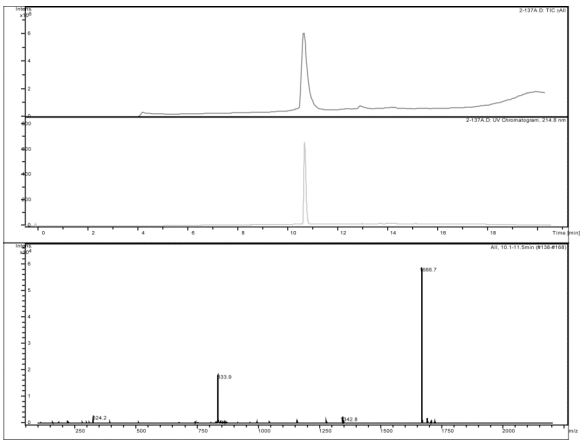
A. Peptide characterization data

Supp. Fig. 1. a) crude peptide **1**; b) purified peptide **1**; c) crude peptide **2**; d) purified diastereomer **2a**; e) purified diastereomer **2b**.

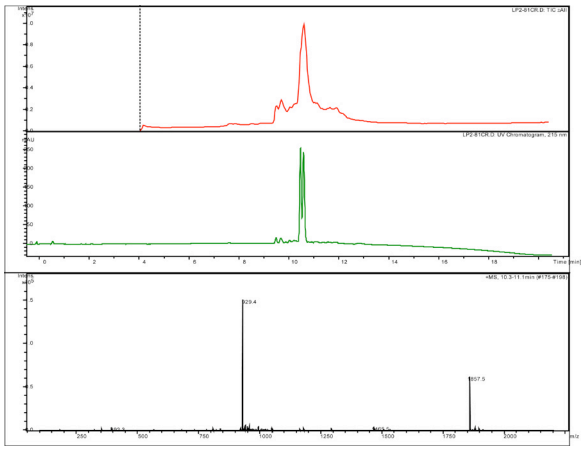
a)



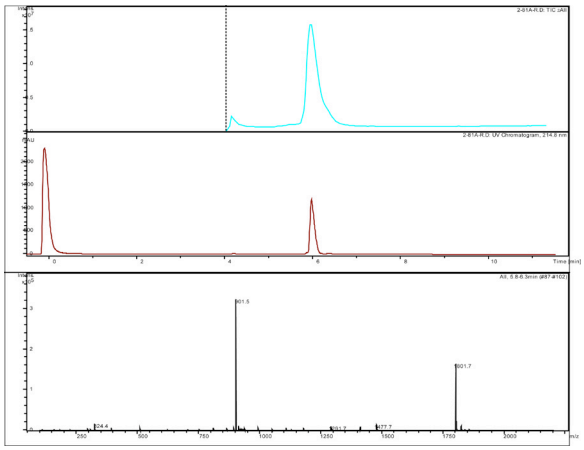
b)



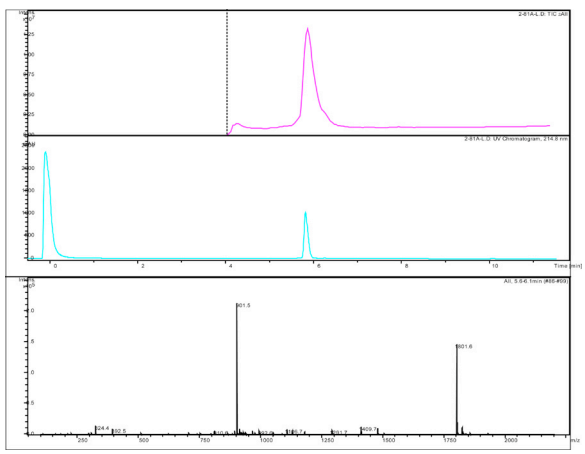
c)



d)

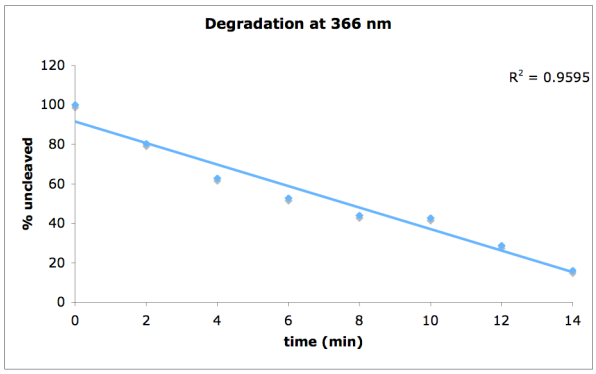


e)



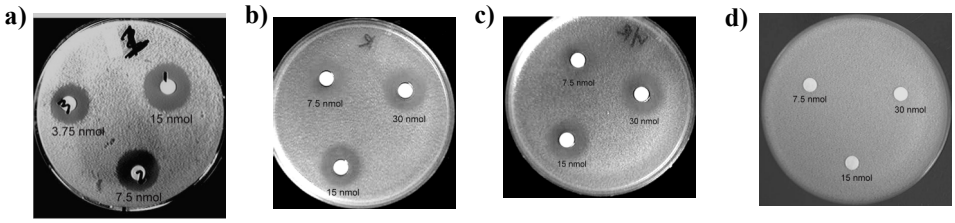
B. Peptide photocleavage data

Supp. Fig. 2. UV-induced degradation (366 nm, 5 mW/cm^2) of **2** monitored by HPLC



C. Halo assay

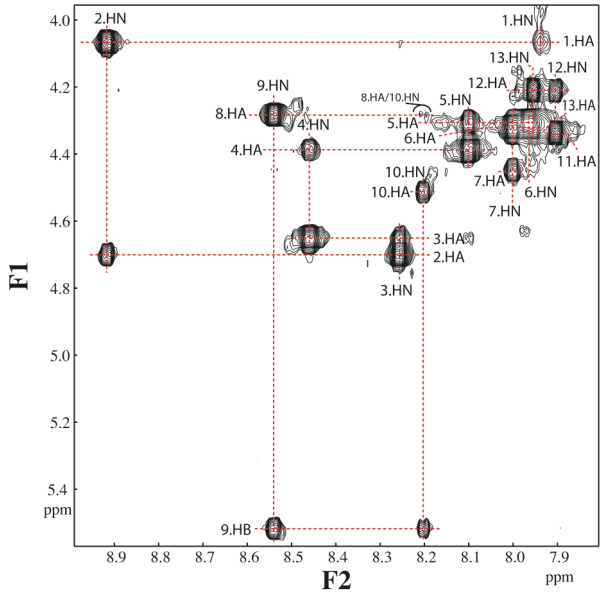
Supp. Fig. 3. Representative plate images from disc diffusion assay to measure growth arrest halos.
a) peptide **1**; b) peptide **2a** (D); c) peptide **2** (D/L); d) peptide **2b** (L)



D. Conformational analysis by NMR

The active peptide was analyzed by NOESY NMR to determine the configuration of the photocleavable residue. A potion of the NOESY spectrum and backbone assignments are given in Supp. Fig. 4. The spectrum was analyzed to identify key cross peaks that, based on molecular modeling, indicate the D-configuration at the photocleavable residue. The results of this analysis are summarized in Supp. Table 1.

Supp. Fig. 4. Sequential backbone assignments in the HN/HA region of the NOESY spectrum of the active peptide.



Supp. Table 1. Table summarizing the cross peaks identified to support the assignment of D-configuration for the photocleavable residue in the active peptide isomer.

^{1}H-^{1}H pair	NOESY crosspeak volume	D model ^{1}H-^{1}H distance (Å, average)	L model ^{1}H-^{1}H distance (Å, average)	difference | D-L |, Å	Supports D or L
9.HA – 10.HA	3.67 (weak)	4.64	5.96	1.32	D: would expect no xpk from L
9.HA – 10.HB1	Not observed	3.70	5.81	2.11	L: but absence of NOE is not a good indicator of distance
9.HD1 – 10.HA	Not observed	6.65	3.95	2.70	D: but absence of NOE is not a good indicator of distance
9.HD1 – 10.HB1	4.51 (weak)	5.96	2.77	3.19	D: L would be more likely associated w/ stronger xpk
9.HD1 – 10.HN	10.49 (weak)	5.06	2.79	2.27	D: L would be more likely associated w/ stronger xpk
9.HD1 – 8.HB1	31.64 (medium)	3.24	5.03	1.79	D: moderately strong xpk associated w/ medium-short distance
9.HD1 – 8.HB2	13.02 (weak)	4.82	6.52	1.60	D: would expect no xpk from L