Structure of the Isolated Pin1 WW Domain *via* Racemic Crystallization (Supplementary Material)

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Materials

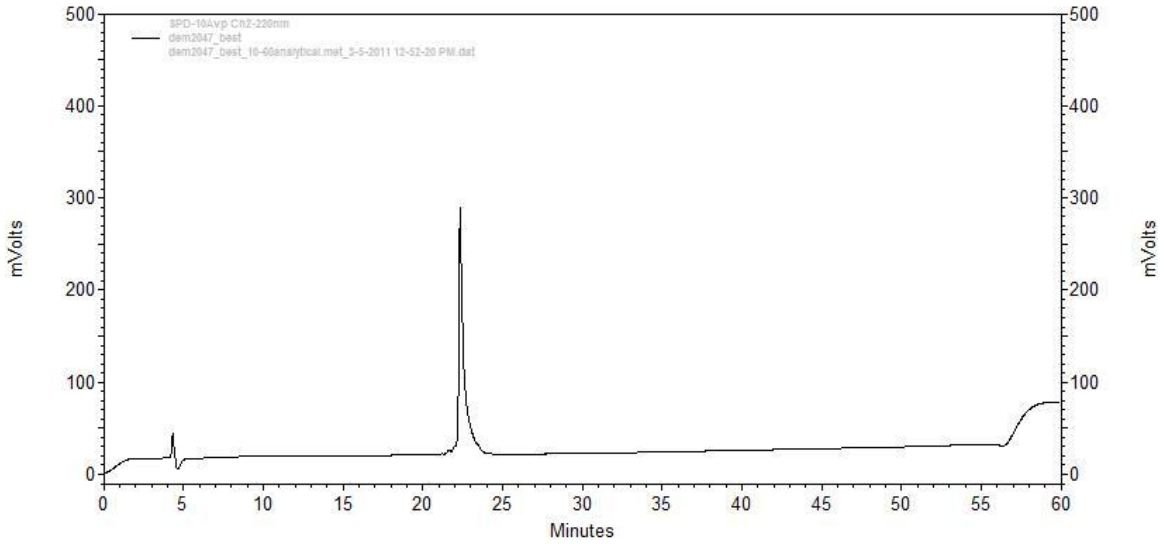
Peptides were synthesized on solid-phase using N-terminal Fmoc protection. Amino acids were activated using 2-(6-chloro-1H-benzotriazole-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HCTU) and 6-chloro-1-hydroxybenzotriazole (Cl-HOBt). Fmoc-protected amino acids with trifluoroacetic acid-labile side-chain protecting groups, HCTU, and Cl-HOBt were purchased from ChemImpex. N,N-dimethylformamide (DMF) and N,N-diisopropylethylamine (DIEA) were purchased from Sigma-Aldrich. NovaPEG Wang resin was purchased from Novabiochem and preloaded with Fmoc-Gly-OH by combining 5 equivalents of the protected amino acid with 1-(mesitylene-2-sulfonyl)-3-nitro-1H-1,2,4-triazole (MSNT; 5 equivalents) and N-methylimidazole (3.75 equivalents) in methylene chloride, and adding of this solution to the pre-swelled resin for at least 4 hours with agitation. The resin was drained, washed with dimethyl formamide and then methylene chloride, and subjected to the same reaction conditions again to ensure adequate loading of the resin.

HPLC Purification and Characterization of Pin1 WW Domain Peptides

Peptides were purified on a Shimadzu SCL-10A liquid chromatograph fitted with a C_{18}-functionalized reverse-phase column. The binary solvent system used in purifications used H_2O:CF_3CO_2H (100:0.1 v/v) as A solvent and CH_3CN:CF_3CO_2H (100:0.1 v/v) as B solvent. Following purification, fractions were pooled and lyophilized to dryness. Polypeptide identity was confirmed using matrix-assisted laser desorption ionization-time of flight (MALDI-TOF) mass spectrometry. Purity was determined by analytical HPLC.

L-Pin1 WW Domain

C_{18} analytical column (250 X 4.6 mm, Supelco), flow rate 1 mL/min, gradient 10-60% B solvent (CH_3CN:CF_3CO_2H, 100:0.1 v/v) in A (H_2O:CF_3CO_2H, 100:0.1 v/v) over 50 minutes, retention time of 22.5 minutes. MALDI-TOF $[M+H]^+$ calculated 4167.6, observed 4169.3.



D-Pin1 WW domain

C_{18} analytical column (250 X 4.6 mm, Supelco), flow rate 1 mL/min, gradient 10-60% B solvent (CH_3CN:CF_3CO_2H, 100:0.1 v/v) in A (H_2O:CF_3CO_2H, 100:0.1 v/v) over 50 minutes, retention time of 22.5 minutes. MALDI-TOF $[M+H]^+$ calculated 4167.6, observed 4169.3.