Comprehensive bioinformatic analysis of HIV-1 protease

Presented at Biosapiens-viRgil Workshop on Bioinformatics for Viral Infections(HIV-HCV2005),

Inhibitors of the protease of human immunodeficiency virus type 1 (HIV-1) are today an important part of highly active antiretroviral therapy (HAART) for HIV-infected individuals and AIDS patients. However, rapidly developing viral resistance to antiretroviral therapy is an increasing problem worldwide and accurate models for predicting protease cleavage specificity are needed for a rational design of more effective protease inhibitors. We have previously analyzed the specificity of HIV-1 protease using bioinformatic machine learning methods [1]. In the present work, we have extended these studies and used a new, extensive 746 peptide dataset for analysis of the specificity of HIV-1 protease [2]. We show that the best predictor is a nonlinear predictor using two physicochemical peptide residue parameters (hydrophobicity and size), indicating that these properties are key features

recognized by the HIV-1 protease. Our cleavage prediction model provides new, important insights into the function of HIV-1 protease.

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