

Title (en)

STRUCTURE-BASED RATIONAL DESIGN OF COMPOUNDS TO INHIBIT PAPILLOMAVIRUS INFECTION

Title (de)

AUF DER STRUKTUR BASIERENDER RATIONALER ENTWURF VON VERBINDUNGEN ZUR HEMMUNG DER PAPILLOMAVIRUSINFEKTION

Title (fr)

CONCEPTION RATIONNELLE DE COMPOSES PERMETTANT DE LUTTER CONTRE LES INFECTIONS PAR PAPILLOMAVIRUS, FONDEE SUR LEUR STRUCTURE

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Application

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Abstract (en)

[origin: WO9917616A1] The invention provides methods of evaluating a compound for the ability to interact with the HPV E6 transforming protein. The invention also provides a machine-readable data storage medium, comprising a data storage material encoded with a set of NMR derived coordinates which define the three-dimensional structure of the E6bp molecule as well as a machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when used with a machine programmed with instructions for using the data, is capable of displaying a graphical three-dimensional representation of the E6bp molecule. The invention further provides a method of treating a subject at risk for infection by a HPV. A compound having a three-dimensional structure substantially similar to the three-dimensional structure of E6bp and a composition comprising the candidate compound and a carrier macromolecule are also provided. Finally a method of evaluating the ability of a compound to associate with an E6bp molecule is provided.

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