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REGIONE AUTONOMA DELLA SARDEGNA

SARDEGNA RICERCHE

MAURIZIO BOTTA

THE FIGHT AGAINST AIDS: THE "OLD" REVERSE TRANSCRIPTASE (RT) AND THE "NEW" DDX3

22 February 2011 - 11:00

SARDEGNA RICERCHE
Loc. Piscinamanna – Edificio 2 - Pula

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A multi-target approach to fight the HIV-1 virus is presented. It is focused on the inhibition of the viral Reverse Transcriptase (RT) and the cellular helicase DDX3. Innovative molecular modeling and synthetic techniques were successfully applied to improve the activity of a class S-DABOs toward wt RT and some clinically relevant mutants and to the identification of the first RT dimerization inhibitor. Furthermore, the identification of a new class of inhibitors (namely 6-vinylpyrimidines) endowed with an unprecedented mechanism of action is reported.

Enzymological and computational studies, followed by the crystallization of the complex between RT and a 6-vinylpyrimidine, has been conducted to elucidate their unique mechanism of action.

Finally, a structure-based pharmacophoric model based on the X-ray crystallographic structure of human helicase DDX3 was inserted in a virtual screening approach leading to the discovery of the first small molecule inhibiting HIV-1 replication by targeting DDX3. It represents a hit compound for a completely new class of antiviral agents.

Information and registration available at www.sardegnaricerche.it/agenda/eventi

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