KEMIJSKI INŠTITUT

Vabilo na Forum40 / Invitation to the Forum40

dr. Andrej Perdih

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Četrtek / Thursday, 14.9.2017 ob / at 13:00

Velika predavalnica Kemijskega inštituta/ Great Lecture Hall, National Institute of Chemistry; Hajdrihova 19, Ljubljana

Anticancer target human DNA topoisomerase IIα revisited: Computational insights and design of catalytic inhibitors

Human DNA topoisomerase IIα is one of the major anticancer targets. It catalyzes topological changes of the DNA molecule, essential for cell replication and its concentration is higher in rapidly dividing cells. Several possibilities exist to tackle this target: an established group of topoisomerase poisons already used in clinical practice and an emerging group of catalytic inhibitors that provide new unexplored possibilities to tackle this enzyme via different mechanisms potentially leading to new molecules with anticancer properties and improved toxicity profile.

In the talk, we will demonstrate how we coupled computational approaches such as pharmacophore modeling, docking, molecular dynamics and QM/MM simulations with biochemical, biophysical and cancer cell-based experiments to gain more mechanistic insights into the function of this enzyme and discover potential new catalytic inhibitors targeting its ATP binding site.

Vljudno vabljeni / Kindly invited