The faculty of Biotechnology and Food Engineering

Seminar

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Quantitative Prediction of Nanoparticle Assembly for Personalized Nanomedicine

Abstract

Development of targeted nanoparticle for personalized cancer therapeutics often requires complex synthetic schemes involving both supramolecular self-assembly and multiple chemical modifications. These processes are generally difficult to predict, execute, and control. I will describe a new method to accurately and quantitatively predict self-assembly of kinase inhibitors drug molecules into nanoparticles based on their molecular structures. The drugs assemble with the aid of new kind of excipient comprised of highly conjugated sulfated molecule into particles with ultra-high drug loadings of up to 90%. Using quantitative structure-nanoparticle assembly prediction (QSNAP) calculations and machine learning, a new algorithm was developed as highly predictive indicators of both nano-self assembly and nanoparticle size with unprecedented accuracy. The resulting nanoparticles selectively targeted the kinase inhibitors to caveolin-1-expressing human colon cancer and autochthonous c-Myc driven liver cancer models to yield striking therapeutic effects while completely avoiding pERK inhibition in healthy skin. I will also talk about additional polymeric coating of nanoparticles that enables radiation guided drug delivery to achieve significant response in multiple cancer models in vivo.

Wednesday, 29.5.19, 14:00 – 15:00, Room 300

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