

acslXtreme[®]

Case Study: Modeling Drug Dispersion

Topical antibiotics are used to treat a variety of skin infections and dermatological reactions. Effectiveness of a topical antibiotic is dependent on a number of factors including drug dispersion through the skin. The skin is a multi-layered and complex organ with its outermost layer, the stratum corneum, typically being the most difficult to penetrate and is hence, usually the rate-limiting step of topically applied drug products.

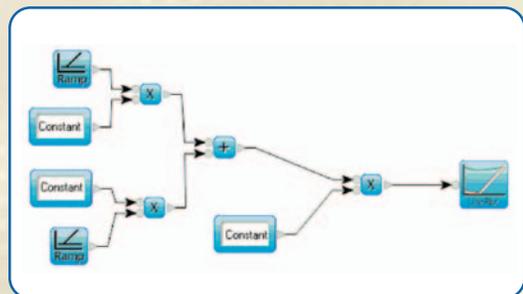
acslXtreme has been utilized in evaluating topically applied antibiotics and predicting efficiency of dispersion. Three models of dispersion have been created with acslXtreme representing drug penetration, variance in skin permeability, and diffusability. The models quickly and accurately predict and evaluate their respective parameters. They have been created utilizing a drag-and-drop method of ready-to-use blocks of code from the acslXtreme libraries. The blocks are easily connected for quick building of a system model and are saved for later use with actual data.

Model 1: Drug penetration

Drug dispersion is dependent on skin permeability. Too much drug product or too quick of delivery can result in toxic levels of drug product and produce harmful effects. Accordingly, too little drug product or too slow of delivery may produce sub-therapeutic dose delivery and result in antibiotic resistant pathogens and persistent infection. Hence, proper drug penetration is essential to effectiveness of a drug product. acslXtreme has been utilized to predict drug penetration distance as a function of the skin permeability coefficient (K_p) and time in hours. Collected data are imported into acslXtreme and the resulting plot depicts similarity of drug dispersion among the agents tested.

Model 2: Variance of skin permeability and diffusability

Skin permeability is highly variable from one compound to the next. Even compounds that appear similar in structure can have different permeability coefficients (K_p). Often, it is necessary to prove similarity between compounds for manufacturing purposes and FDA regulations. acslXtreme has been utilized to model variance in the skin permeability coefficient (K_p) between molecularly similar compounds based on formula weight and log K_{ow} and to predict similarity. acslXtreme accurately models and predicts the similarity of the variance in K_p among the agents tested as verified by imported data.



Diffusability of the skin is variable from one region to the next and between individuals. The variance in the diffusability constant (D) is tested for a compound to demonstrate uniform and proper delivery of a drug product from various sites on the body. acslXtreme has been utilized to model variance in the diffusability constant (D) as a function of formula weight and thickness of the stratum corneum for predictive measures of drug delivery. Imported data verifies the accuracy of the predicted model that has been generated by acslXtreme.

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Work Cited

Bartzatt R. University of Nebraska. Evaluation of a simple carrier molecule which enhances drug penetration of dermal layers by utilizing multivariate methods, structure property correlations, and continuous system modeling. Submitted for publication.

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