

Analysis of SAR Patterns Observed Within a Series of Common Consumer Drugs

Fumie Koyoshi, Dr. Lynn Everett, Dr. Malcolm J. D'Souza*, Science Department, Wesley College, Dover, DE

Background: In a previous study we looked at 75 FDA drug profiles that contained empirical data for various pharmacokinetic properties and used this information to create a FDA Consumer Drug database[®] with a commercially available platform, called the KnowItAll[®] Informatics System.

Methods: KnowItAll[®] contains a collection of *in silico* ADME/Tox predictors that could be utilized to reduce the high attrition rates in the drug discovery process although a predictor's reliability is of major concern.

Results: Here we investigate SAR properties by separating the drugs in our database into different categories on the basis of their functional groups; extract physiological properties from the FDA drug profiles for each drug; and search for any consistencies in physiological properties (such as bioavailability and plasma protein binding) among the drugs sharing the same functional group.

Conclusions: Initial ProfileIt[®] output accurately predicts bioavailability and plasma protein binding by the drugs.

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