# Bio- and Chemoinformatics: Key Technologies within the Drug Discovery Process.

Paul M. Selzer

Intervet Innovation GmbH, Zur Propstei, D-55270 Schwabenheim, Germany

Systematic *Drug Discovery* approaches started at around the second half of the 19th century with random screenings of chemical substances towards biological systems. One of the best known examples is acetylsalicylic-acid, which was discovered in 1897 by the chemist Felix Hoffmann and achieved world fame under its trade name Aspirin. By today, the sequencing of entire genomes and the generation of related biological and chemical information, inverted this classic research approach. Moreover, the overlapping computer-aided technologies of *bioinformatics* and *chemoinformatics* have become essential tools within the modern drug discovery process. This is especially true for the identification and validation of drug targets as well as for the screening and design of potential active substances. Of special importance in this context are three-dimensional protein structures, which are key elements in understanding biological processes and play a central role for structure-based rational drug-design approaches. At present, an international initiative, the *Structural Genomics Initiative*, is under way to deduce the three-dimensional structures of all proteins encoded in the sequenced genomes of the most important organisms. In addition to the overview of the Drug Discovery process, an example of a cyclin dependent kinase (EtCRK2) of an economically important parasite (*Eimeria tenella* the causative agent of coccidiosis, a disease of the colon of poultry) will be presented. In this study bioinformatics and molecular biology approaches were used to identify the target protein, which was then used by chemoinformatics approaches to identify small chemical lead structures as potential inhibitors of EtCRK2.