



## Expert Systems and Knowledge Bases for pharmaceutical research

PharmaInformatic provides ADME/Tox knowledge bases and predictive tools (expert systems) to improve drug discovery and development. We have developed PACT-F, the largest and most annotated knowledge base on bioavailability worldwide.

**PACT-F (Preclinical And Clinical Trials Knowledge Base on Bioavailability)** contains experimental bioavailability results of clinical trials in humans and preclinical trials in animals. The results and conditions of those trials have been taken manually from reliable scientific publications. PACT-F contains the knowledge from more than 5000 scientific research articles related to bioavailability.



The development of PACT-F commenced in 2005. PACT-F is now the largest knowledge base on bioavailability worldwide. It contains 8296 records, which are extensively annotated: up to 17 fields describe in detail the results and conditions of a trial. PACT-F is now available for licensing.

Every record contains the investigated chemical structure. This enables scientists to build relationships between structures and properties and to select drug candidates with sufficient oral bioavailability for human clinical trials. The knowledge base has been used to develop [IMPACT-F](#), which estimates human oral bioavailability much more precisely than animal trials.

PACT-F is the fundamental knowledge base to analyse the factors and conditions which influence bioavailability. It provides scientists with the results and knowledge of 100 years of bioavailability research in order to improve future drug design and drug development.

**PharmaInformatic's expert systems** help to identify and prioritise promising drug candidates for clinical trials in humans. Our products select compounds which display a high probability of becoming a successful drug:



**IMPACT-F** calculates oral bioavailability of future drug candidates in humans. Predictions were shown to be much more precise than animal trials: they were as accurate as the common deviation between individual humans taking part in the same clinical trial. Read our [current research results](#) on drug bioavailability.



**MolScore-Drugs** helps to identify and prioritise promising drug candidates with the maximum possibility of success in human trials. The expert system prioritises drug candidates in multiple therapeutic areas.



**MolScore-Antibiotics** detects antibacterial drug candidates. The expert system recognises structural patterns of every type of antibiotics, even new antibiotic substances with unknown mechanism of action which are now in clinical trials.



**MolScore-Antivirals** detects antiviral drug candidates. The expert system combines different strategies of drug research, so that structural patterns of virus-specific and target-specific inhibitors will be recognised.

PharmaInformatic was founded in 2004 by Dr Wolfgang Boomgaarden. He has invented several drug design and virtual screening products, which have been successfully used in pharmaceutical research. Before he founded the company, he worked as a professor in bioinformatics at the University of Applied Science in Emden, Germany.



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