

EXPERT SYSTEM Bioavailability IMPACT-F

Expert System to predict oral bioavailability in humans

The expert system IMPACT-F predicts oral bioavailability of novel drug candidates in humans. The calculation is based on reliable computational models, which have been derived from the largest knowledge base on bioavailability worldwide ([PACT-F](#)). The computational prediction of human oral bioavailability has several advantages:

- ✓ selection of bioavailable drug candidates ==> reduces clinical failures
- ✓ much more reliable than animal trials & results almost immediately available
- ✓ confidential and reliable (no data or information leaves your company)
- ✓ unrivalled method to evaluate efficiency of drugs *before* advanced clinical trials

[Oral bioavailability](#) is one of the most important properties in drug design and development. Low oral bioavailability in clinical trials is a major reason for drug candidates failing to reach the market.

The expert system [IMPACT-F](#) is composed of several reliable models to predict oral bioavailability in humans. The performance and quality of these models, validated with large, independent and diverse sets of drugs, was shown to be remarkably better compared to preclinical trials in animals.

IMPACT-F reliably estimates bioavailability of entirely novel drug structures. The expert system was validated with novel drug candidates coming from different therapeutic areas such as cancer, CNS, inflammation, infectious disease, gastrointestinal and cardiovascular diseases.

A low error (MAE=15.968) and a good correlation ($r=0.798$) between predicted and experimental results from human clinical trials was found ([details](#)). IMPACT-F calculates oral bioavailability in humans much more precisely compared to animal models.

The expert system can forecast oral bioavailability of novel drugs reliable. Bioavailability predictions of IMPACT-F were as accurate as the common deviation between individual humans taking part in the same clinical trial ([inter-subject variability in humans](#)).

IMPACT-F has been used by several [pharmaceutical companies](#) in different therapeutic areas (cancer, inflammation, autoimmune diseases, diabetes, antivirals) for selection and prioritisation of drug candidates, to optimise prodrugs and to evaluate oral bioavailability before advanced clinical trials in humans. For licensing, please contact: licensing@pharmainformatic.com.

About Pharmainformatic

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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