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## Prediction of *in-vivo* permeability, solubility, BCS-classing, food interactions, fraction absorbed and oral bioavailability using new *in-silico* methods and algorithms

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**Background:** Prediction of *in-vivo* permeability (Pe), solubility, BCS-classing, food interactions, fraction absorbed (fa) and oral bioavailability(F) from *in-vitro* and animal data is a challenge, especially for compounds with low/moderate Pe, efflux and/or high lipophilicity/low solubility. For such compounds, *in-vivo* prediction from preclinical data is generally poor/uncertain and sometimes impossible. Thus, improvements are required.

**Methods:** With extensive, diverse datasets (log P -9 to 9), new algorithms and various computational chemistry methods (including machine learning) we have developed and validated prospective *in-silico* prediction models (no retrospective data fitting) for the parameters described above.

**Results & Discussion:** Models for fa and F (including compounds with low Pe, strong efflux, very low solubility, extensive gutwall and hepatic extraction) showedQ^2 of 0.77 and 0.55 and median prediction errors of 1.1- and 1.4-fold, respectively. In direct comparison, the models outperformed lab methods. For the 100 compounds with lowest solubility (including albendazole, danazol, loperamide, lovastatin, ketoconazole and troglitazone), 74% correct *in-vivo* BCS-classing and 12% average absolute prediction error for fa was obtained. The mean prediction error for AUC-changes with food was 1.4-fold.

**Conclusion:** The new *in-silico* models and algorithms enable improved and simplified prospective predictions of *in-vivo* Pe, fa, solubility, BCS-classing, food interactions and F. Benefits include reduced and defined uncertainty, reduced time and costs, and frontloaded and improved decision-making.

## Biography

He completed his PhD in pharmacokinetics/biopharmaceutics in Uppsala university in 1997. He worked as a Senior research scientist and principle scientist at AstraZeneca Sodertalje (1997-2012). Presently he is a CEO, founder and method developer at PROSILICO.

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