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TITLE: InVitroInVivoCorrelation.jl: A Modular Julia Package for Level A IVIVC

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ABSTRACT: Establishing a robust in vitro-in vivo correlation (IVIVC) remains central to formulation development, clinically relevant dissolution specification setting, and post-approval change management. Level A IVIVC, the most informative correlation level, establishes a point-to-point relationship between in vitro dissolution and in vivo absorption, typically through deconvolution of plasma concentration-time profiles followed by regression of cumulative absorbed fraction against cumulative dissolved fraction. In practice, implementing a complete Level A workflow requires careful handling of asynchronous in vitro and in vivo sampling schedules, selection of unit impulse response (UIR) models, and external validation on held-out formulations. Despite the regulatory importance of IVIVC [1,2], few software tools offer a scriptable, end-to-end pipeline that is both flexible and easy to integrate into existing data analysis workflows.

InVitroInVivoCorrelation.jl is a Julia package, part of the PumasAI suite, that implements a complete Level A IVIVC workflow in five steps: (1) build a dissolution source from in vitro data via interpolation or user-provided models; (2) fit unit impulse response functions from a fast-release reference formulation; (3) deconvolve oral concentration–time profiles to estimate in vivo absorbed fractions; (4) fit the correlation model relating cumulative dissolution to cumulative absorption, with configurable timepoint strategies and optional held-out validation formulations; and (5) predict plasma concentrations for new formulations and compute validation diagnostics including percent prediction error for AUC and Cmax. The package is DataFrames-native, accepting long-format tabular inputs and returning standardized outputs. Its modular design allows the correlation function and dissolution representation to be replaced with user-defined alternatives without altering the surrounding workflow. Qualification on datasets with both uniform and asynchronous sampling demonstrated that prediction errors satisfy FDA guidance acceptance criteria.

References:
[1] Food and Drug Administration. Guidance for Industry: Extended Release Oral Dosage Forms: Development, Evaluation, and Application of In Vitro/In Vivo Correlations. 1997.
[2] Cardot JM, Beyssac E, Alric M. In vitro-in vivo correlation: importance of dissolution in IVIVC. Dissolution Technologies. 2007;14(1):15-19.

BRIEF SPEAKER BIO: Arno Strouwen holds a PhD from KU Leuven, where his doctoral research focused on optimal experimental design for dynamic systems. He previously worked at Johnson & Johnson's manufacturing and applied statistics department, designing accelerated stability studies for vaccine shelf-life prediction and optimizing chemical manufacturing conditions through high-throughput experimentation. He currently develops pharmacometric software at PumasAI, with a focus on in vitro–in vivo correlation and bioequivalence tools. His core expertise lies in optimal experimental design, Bayesian statistical modeling, and the application of scientific machine learning to pharmaceutical development.