



TITLE: A Unified Bayesian Framework for AI Uncertainty and Reliability in Pharmaceutical Development

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ABSTRACT: AI-based tools are increasingly embedded in pharmaceutical development - from spectroscopic and image-based bioassays, to soft sensors in bioprocesses, to AI-supported analytical procedures under ICH Q2(R2) and ICH Q14. Yet the question of how to measure their reliability remains open. The field uses overlapping but disconnected terminology - Personalized Uncertainty Quantification (PUQ), conformal prediction, calibration, total analytical error (TAE), predictive values - that lacks a shared conceptual foundation. This makes it difficult for developers, quality units, and regulators to specify acceptance criteria or to qualify AI components within established CMC and analytical lifecycle frameworks.

This presentation proposes a formal, Bayesian-grounded definition of AI uncertainty in which the **predictive distribution $p(\mathbf{y}_{\text{new}} \mid \mathbf{x}_{\text{new}}, \mathbf{D})$** is the single fundamental object, and every reliability or performance metric is a functional of it. Treating an AI system as a **measurement instrument**, the framework shows that the relevant determinant of reliability is not model complexity but the **domain coverage of the training data** - the AI analogue of the validated operating range of an analytical method.

From this foundation, we derive a unified scheme connecting concepts that today live in separate vocabularies: precision and trueness (ICH Q2, GUM), total analytical error, PUQ and conformal prediction sets, calibration, and predictive values - and we map them onto the lifecycle concepts introduced in ICH Q14 (Analytical Target Profile, established conditions, performance characteristics). The same scheme provides a transparent basis for qualifying adaptive AI systems that evolve over their lifecycle, by recasting model updating as Bayesian sequential method re-verification.

The result is a single statistically coherent roadmap - bridging analytical, machine-learning, and decision-theoretic vocabularies - for specifying, validating, and monitoring AI-augmented measurement and decision systems across pharmaceutical development.