FractaLPK — Drug Release Auto-Diagnose Report

Dataset: **dr_real_loperamide** · Generated: 2026-05-12 11:39 UTC · ID: dde2b0b3af

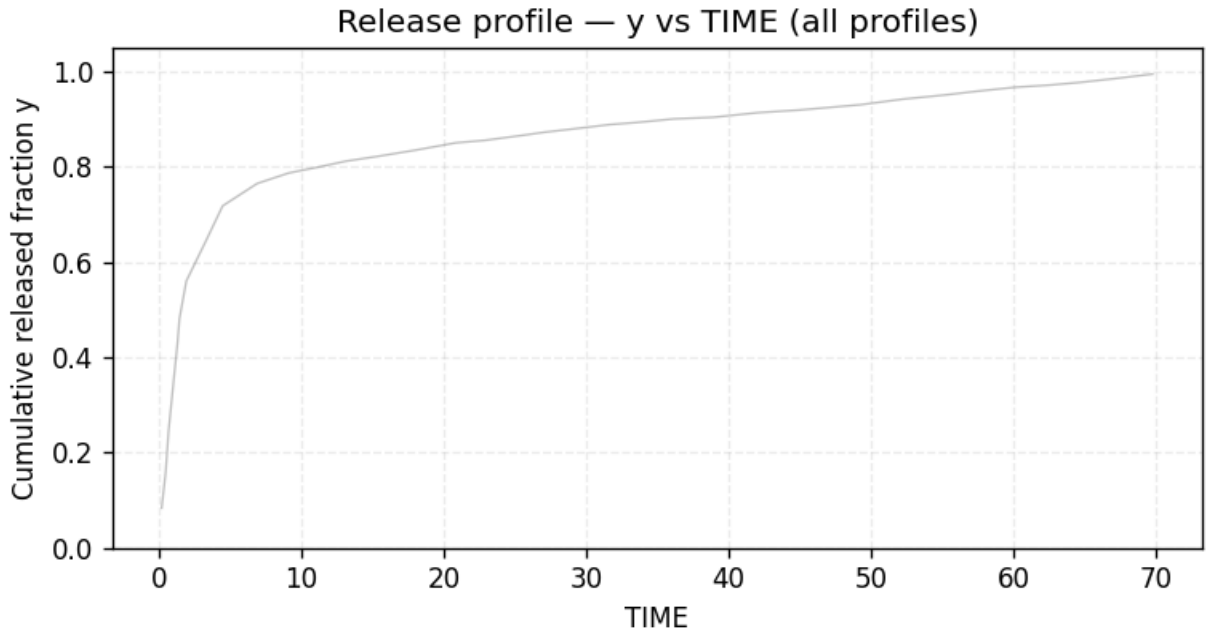
Rule applied	RULE 3 MEMORY DRIVEN
Selected model	FractaLPK ML stretched exp (R^2 = 0.979, AIC = -195.11)
ΔAIC vs runner-up	19.92
Confidence	high
Verdict	MEMORY-DRIVEN RELEASE — Best model: Mittag-Leffler fractional with α = 0.680. ΔAIC = 19.92 vs the classical alternatives indicates that integer-order release kinetics do not fit the data; sub-unit α captures memory effects in the release process. Mechanistic interpretation of α is the responsibility of the user's expert team.

Key parameters

Parameter	Estimate
alpha	0.6795
tau	3.267

Dataset overview

Profiles (N)	1
Observations	35
TIME range	0.2 – 69.75
y range	0.084 – 0.995



Single-profile study: final cumulative release y(t_max) = 0.995. Final-release histogram omitted (only one profile).

Model comparison — 5 release-profile models

#	Model	Class	n	OFV	AIC	ΔAIC	R²	Conv
1 ★	**FractaLPK ML stretched exp**	**ml_fractional**	**2**	**-199.11**	**-195.11**	**ref**	**0.979**	✓
2	Weibull	weibull	2	-179.19	-175.19	+19.92	0.963	✓
3	First-order	first_order	1	-125.47	-123.47	+71.64	0.826	✓
4	Higuchi (sqrt-t Fickian)	higuchi	1	-79.92	-77.92	+117.20	0.362	✓
5	Korsmeyer-Peppas (early window <=60%)	korsmeyer_peppas	2	-50.65	-46.65	+148.46	0.990	✓

Verdict — rule applied

Rule 3 — Mittag-Leffler fractional wins by ΔAIC ≥ 4 (or ≥ 8 in incomplete release windows). Sub-unit α captures memory effects in the release process.

Selected model — parameter estimates

FractaLPK ML stretched exp · ml_fractional · 2 free parameters

Parameters

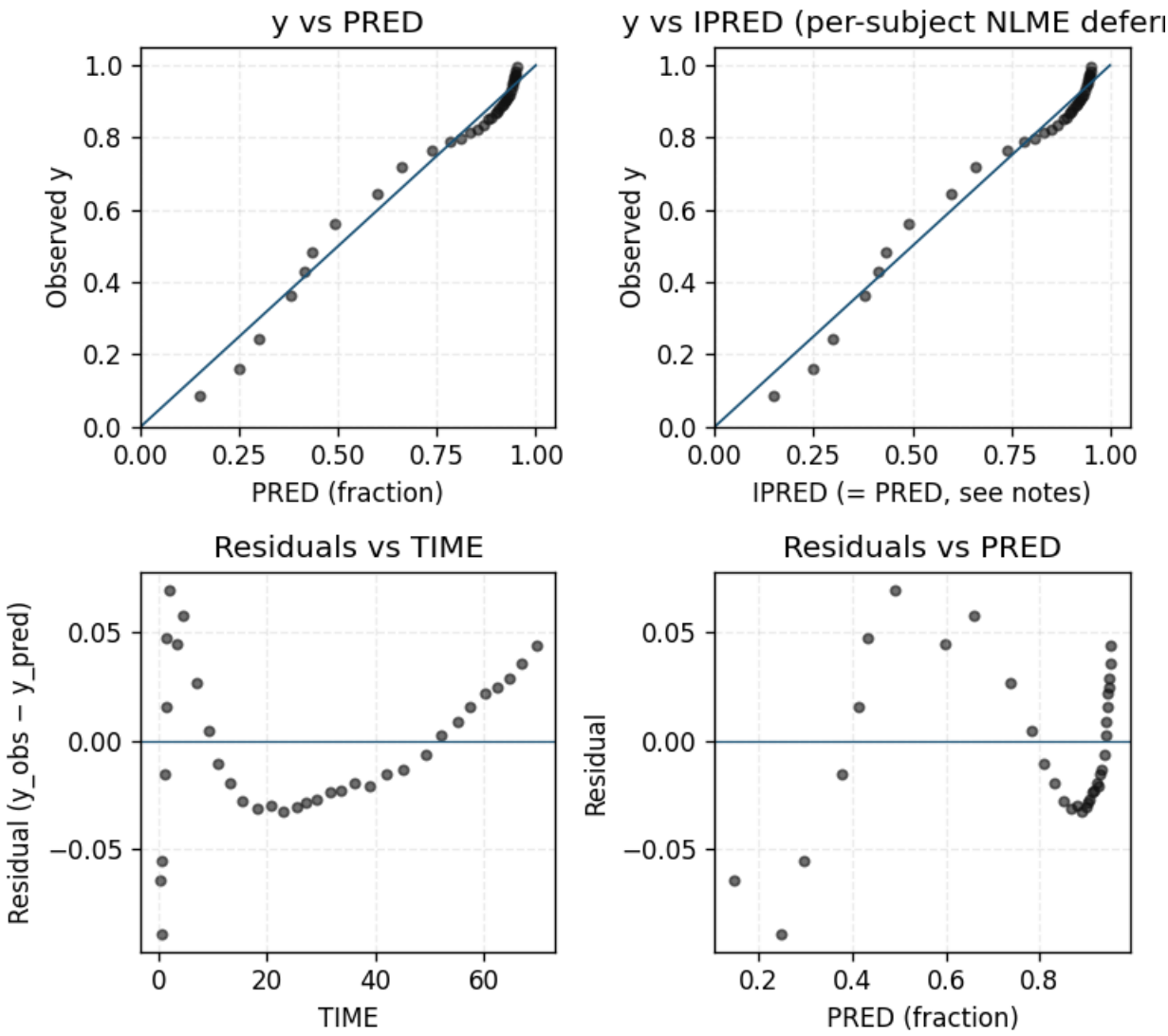
Parameter	Estimate
alpha	0.6795
tau	3.267

Fractional kinetics — interpretation

α = 0.680 (synthetic validation accuracy ±0.10; reported 95% range [0.580, 0.780]).

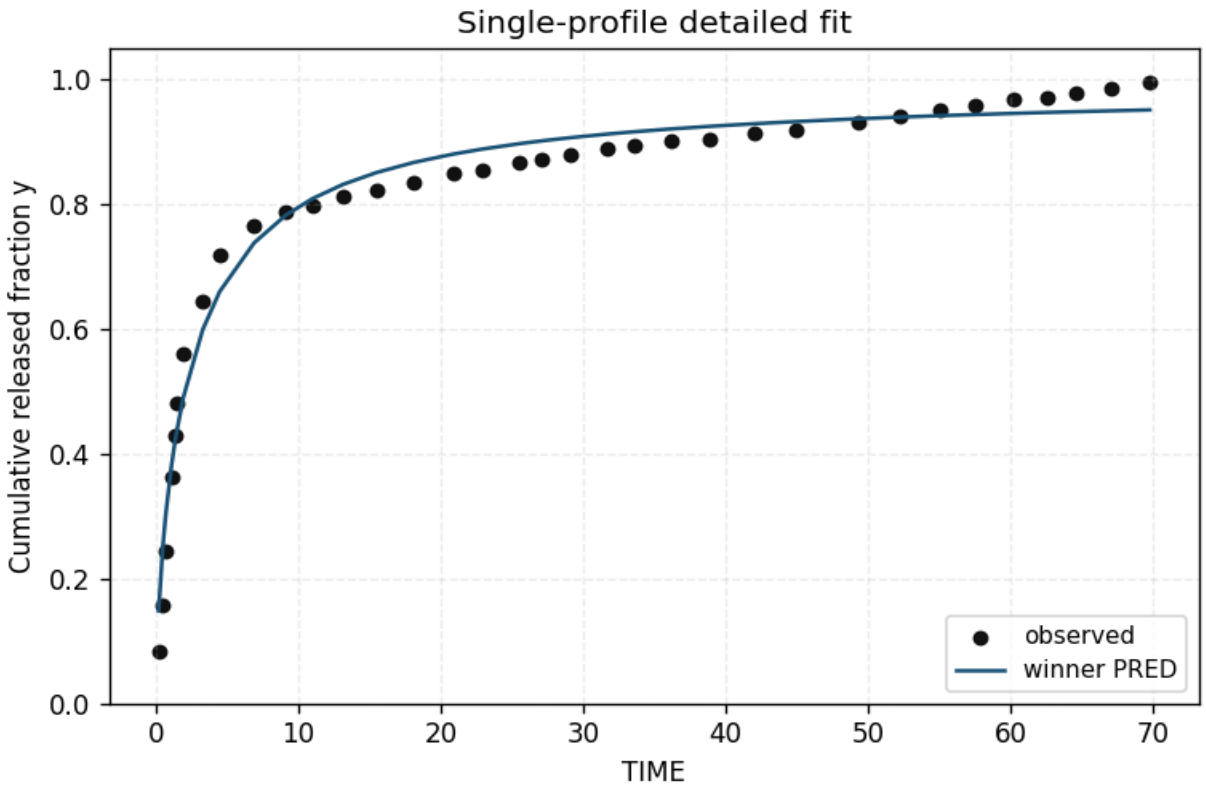
Fractional order α is estimated from the data; based on synthetic validation in the related Tumor Auto-Diagnose module, accuracy is expected within ±0.10. Drug Release-specific synthetic validation is part of B.3.

Goodness-of-fit



IPRED equals PRED because the engine fits the population mean profile only. Per-subject NLME is deferred to a later phase.

Individual fits



Diagnostics & methodological notes

Metric	Value
Winner wall time (s)	559.47
Winner converged	yes
Optimizer	grid-search (multi-start)
Total wall time (s)	564.6
Engine	drug_release_fitter (Fase B.3, plga_profile reuse + first_order)
N observations (mean curve)	35
t range	0.2-69.75
y_max observed	0.995

Methodological notes

Five candidate models are compared on a single release profile: First-order, Higuchi, Weibull, Korsmeyer-Peppas, and ML fractional (proprietary, Mittag-Leffler stretched exponential). Korsmeyer-Peppas is fitted only on the early-release window ($y \leq 60\%$) per the standard usage convention.

Primary verdict criterion: $\Delta AIC \geq 4$ against the next-best model. The regime-detection layer (regime-B) raises this to $\Delta AIC \geq 8$ only for ML fractional when the dataset covers less than 60% of release.

The verdict logic includes a regime-detection layer: when the observation window covers only the early-release phase (y_max < 60%), ML fractional verdicts require stronger statistical evidence ($\Delta AIC \geq 8$) to override simpler power-law / matrix models. This protects against overfitting in incomplete release windows.

Fractional order α is estimated from the data; based on synthetic validation in the related Tumor Auto-Diagnose module, accuracy is expected within ±0.10. Drug Release-specific synthetic validation is part of B.3.

Korsmeyer-Peppas exponent n is reported as a mathematical descriptor of the power-law behaviour in the early-release window. Mechanistic interpretation (Fickian, anomalous, Case-II, zero-order) is the responsibility of the user's formulation team.

Real validation profiles were sourced from publications in the PLGA release literature (refs: Householder et al. 2015; Malathi et al. 2015; O'Donnell et al. 2015; Kolate et al. 2015). The numerical values were obtained from a public digitization of figures provided by the g2706/plga GitHub repository (accompanying Bao et al., neural-network paper). Original measurements correspond to the cited publications.

Geometry-aware models for cylindrical implants (e.g. Nexplanon) and spherical microspheres with surface erosion (Hopfenberg) are planned for a later version (Phase 2.B roadmap). The current report uses geometry-agnostic kinetic descriptors.

Limitations

Current scope: classifying which structural model best describes the release profile among the 5 candidates. The report does NOT make pharmacological, formulation, or regulatory decisions. Per-subject variability (OMEGA / shrinkage) is not estimated; the engine fits the population mean profile. Geometry-aware models, surface-erosion (Hopfenberg) and treatment-effect terms are out of scope and planned for a later phase.

Disclaimer (extended)

This report contains computational results. Pharmacological interpretation and clinical decisions are the responsibility of the client's expert team. FractaLPK does not provide medical, pharmacological, or regulatory advice. Models compared by AIC; statistical equivalence threshold $\Delta AIC \geq 4$ (raised to ≥ 8 for ML fractional in incomplete release windows). Verdict is a diagnostic indication, not a regulatory conclusion.