FractaLPK

Drug Release Auto-Diagnose Report

Dataset **Loperamide PLGA microspheres (O'Donnell 2015, public benchmark)** · Generated 2026-05-26 10:32 UTC · ID 5dafff82f8

Quality assessment: Standard quality

This report summarises the drug release analysis of Loperamide PLGA microspheres (O'Donnell 2015, public benchmark), comprising 1 subject and 35 observations. 5 structural models were evaluated; the FractaLPK ML stretched exp model was selected based on AIC ranking (ΔAIC = 19.92 vs runner-up). Model converged in a standard iteration count. Release profile is consistent with memory-driven kinetics (α = 0.680).

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.

Selected model: FractaLPK ML stretched exp (R^2 = 0.979, AIC = -195.11)

ΔAIC vs runner-up	R^2	Confidence
19.92	**0.979**	**high**

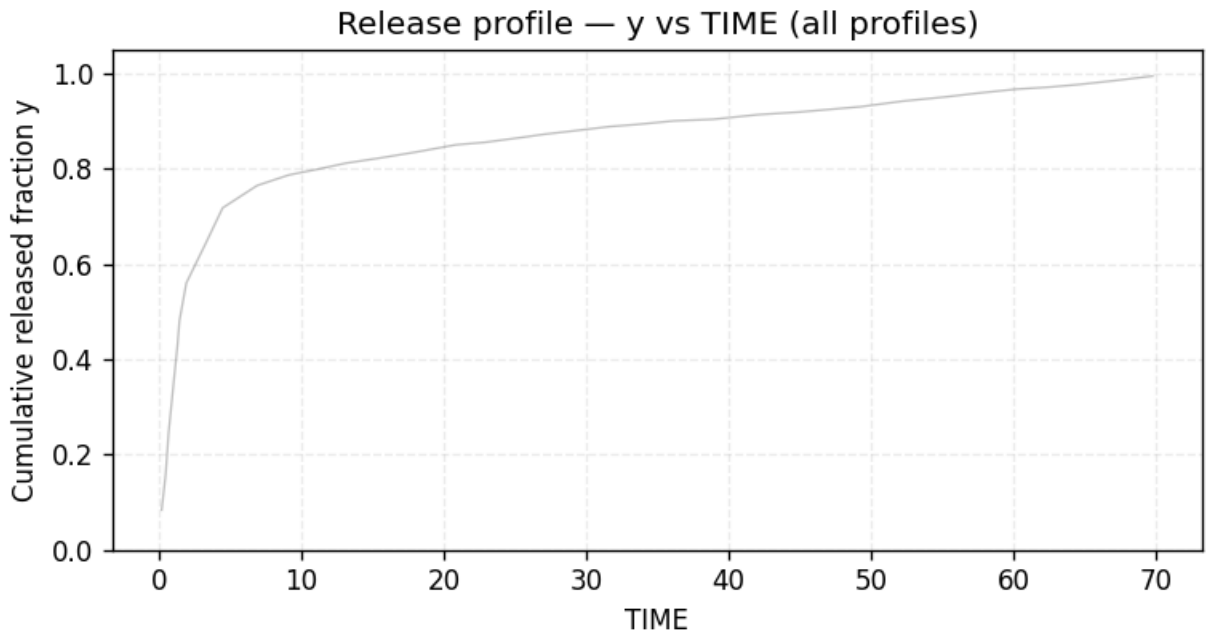
Rule applied: **RULE 3 MEMORY DRIVEN**

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).

Top-3 candidates by AIC: FractaLPK ML stretched exp, Weibull, First-order. Winner ★ selected by parsimony when ΔAIC < 4 (see verdict rules). Full comparison on next page.

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

Derived quantities

Quantity	Value	Units	Formula
t_50 (time to 50% released)	2.05	time units	interpolated from y(t)
t_80 (time to 80% released)	10.4	time units	interpolated from y(t)
MDT (mean dissolution time)	5.7	time units	integral from 0 to t_max of (1 – y/y_inf) dt
Fraction released at t_max (t=60.5)	99.5 % (observed: 99.5 %)	%	model prediction vs observed

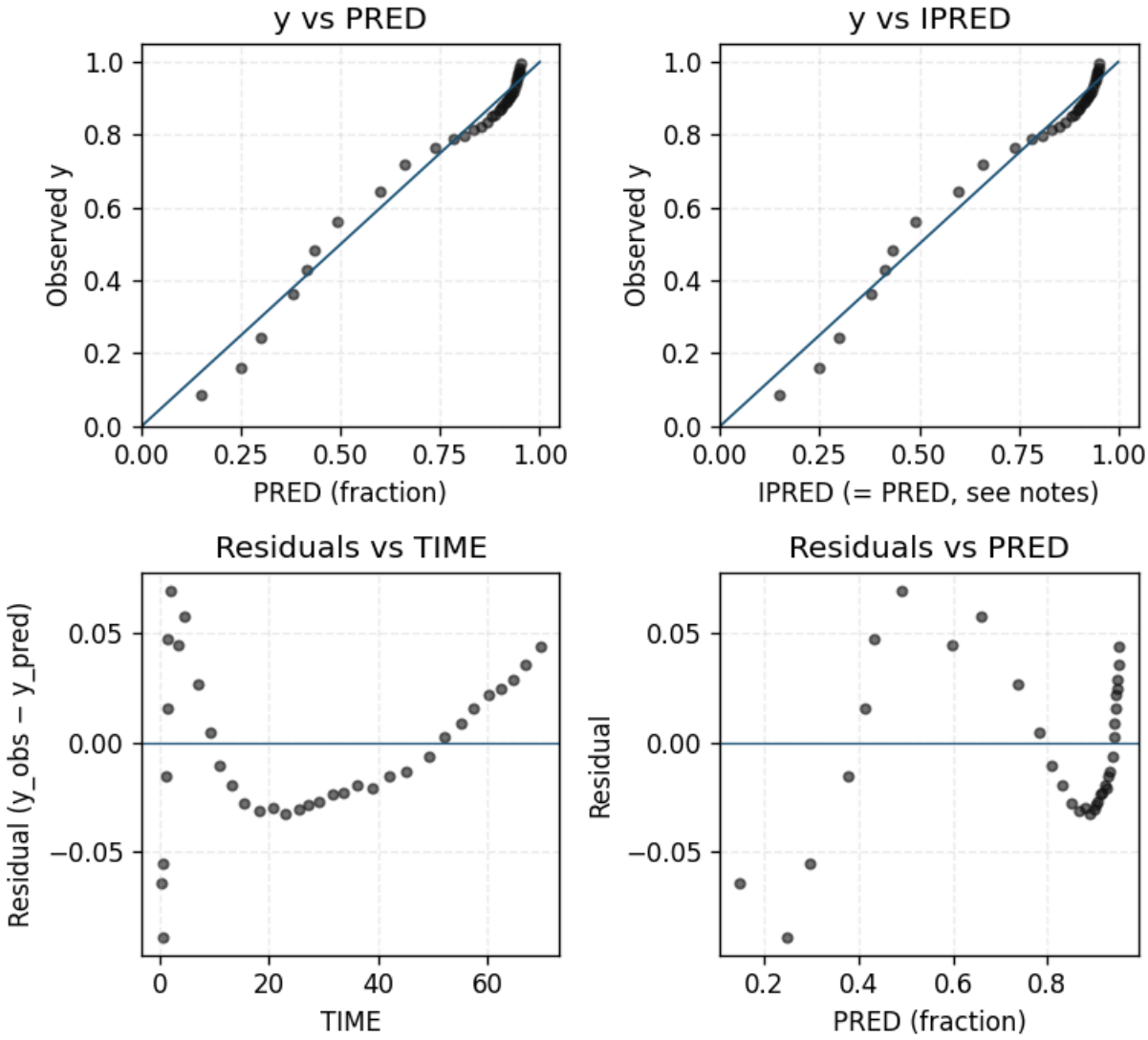
Computed from fitted parameters. Numerical values only; pharmacological interpretation is the responsibility of the user's clinical/formulation team.

Fractional kinetics — interpretation

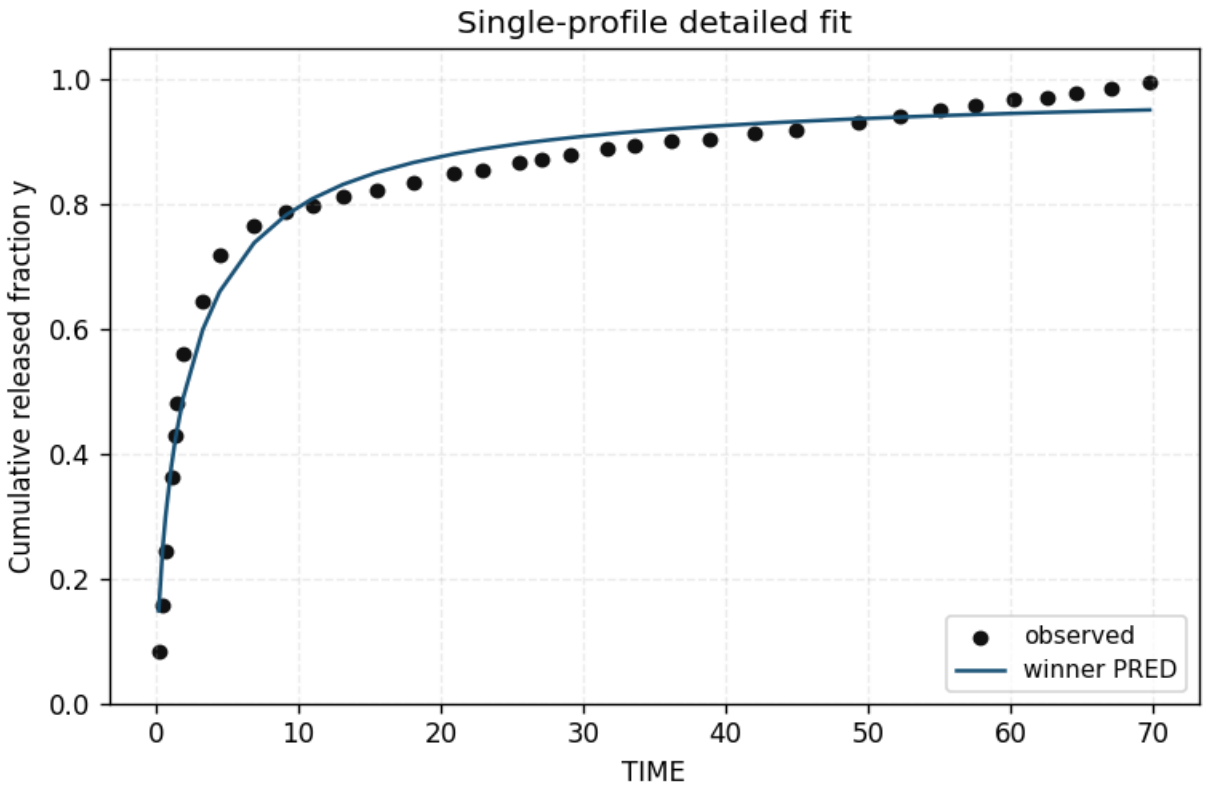
α = 0.680 (synthetic validation accuracy ±0.10; expected accuracy band [0.580, 0.780] — not a statistical confidence interval).

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.

Goodness-of-fit



Individual fits



Diagnostics & methodological notes

Metric	Value
Winner wall time (s)	654.16
Winner converged	yes
Optimizer	grid-search (multi-start)
Total wall time (s)	654.4
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.

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 outside the scope of this report. 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. Estimates are at the population (mean-profile) level; individual-profile variance components and geometry-aware / surface-erosion models are part of the extended analysis tier.

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.

Your analysis is complete.

Need a deeper analysis? Contact us at contact@fractalpk.es.

Want to share these results? Cite as: *FractaLPK drug_release_fitter (Fase B.3, plga_profile reuse + first_order), generated 2026-05-26 10:32 UTC, ID 5dafff82f8*.