FractaLPK

PopPK Auto-Diagnose Report

Dataset **PopPK NONMEM (12 subjects, oral)** · Generated 2026-05-26 10:16 UTC · ID 9019c69dd0

Quality assessment: Review recommended

This report summarises the population pharmacokinetic analysis of PopPK NONMEM (12 subjects, oral), comprising 12 subjects and 96 observations. 8 structural models were evaluated; the 1-CMT classical model was selected based on AIC ranking with parsimony rule (ΔAIC < 4) (ΔAIC = 0.32 vs runner-up). Model converged in a standard iteration count. Classical compartmental kinetics adequately describe the data.

VERDICT

STATISTICALLY EQUIVALENT — Top 2 models (1-CMT monofractional and 1-CMT classical) have ΔAIC = 0.32 < 4. They are statistically indistinguishable for this dataset. Reporting [1-CMT classical] selected by parsimony (fewer parameters). Both top candidates fit equivalently well within ΔAIC < 4; reporting the parsimonious choice per Occam's principle.

Selected model: 1-CMT classical (R^2 = 0.737, AIC = -5.50)

ΔAIC vs runner-up	R^2	Confidence
0.32	0.737	medium

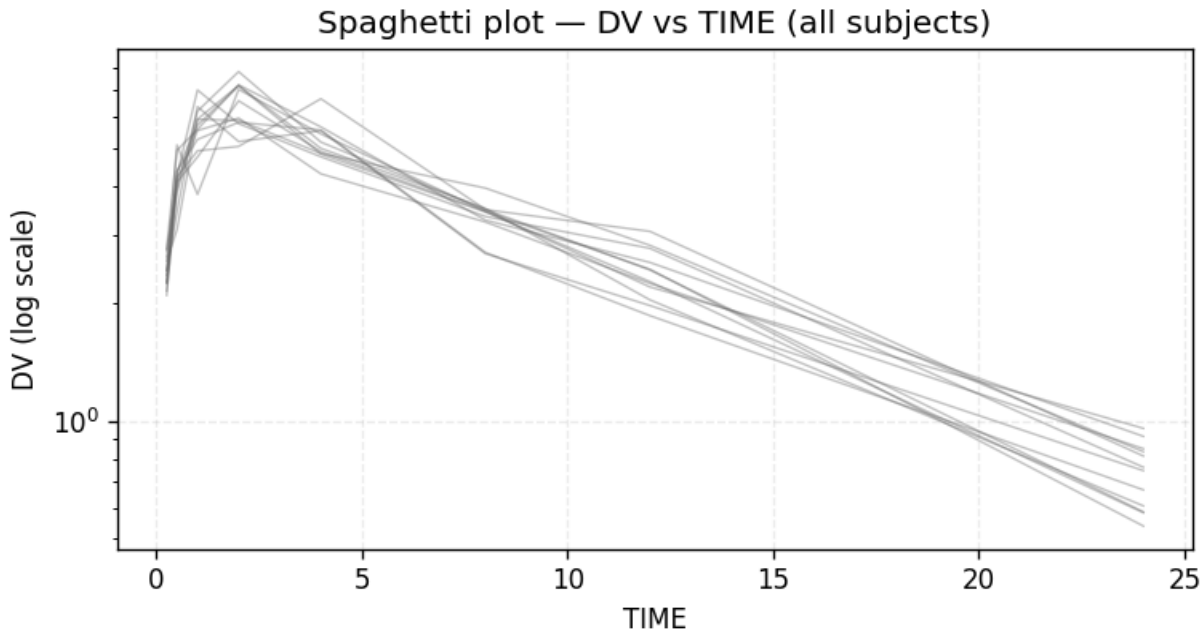
Rule applied: **RULE 2 EQUIVALENT**

Key parameters

Parameter	Estimate
A_1	5.123
k_1	0.07302

Dataset overview

Subjects (N)	12
Observations	96
TIME range	0.25 – 24.0
DV range	0.539 – 7.82
DV median	3.49
BLQ count	0
AMT min/max	320.0 / 320.0
Distinct doses	1



Single-dose study: AMT = 320 (all subjects). Dose histogram omitted (only one distinct value).

Top-3 candidates by AIC: 1-CMT monofractional, 1-CMT classical, 2-CMT monofractional. Winner ★ selected by parsimony when ΔAIC < 4 (see verdict rules). Full comparison on next page.

Model comparison — 8 structures

#	Model	Class	n	OFV	AIC	ΔAIC	R^2	Conv
1	1-CMT monofractional	monofractional	3	-11.82	-5.82	-0.32	0.803	✓
2 ★	**1-CMT classical**	**classical**	**2**	**-9.50**	**-5.50**	**ref**	**0.737**	✓
3	2-CMT monofractional	monofractional	5	-12.44	-2.44	+3.07	0.817	✓
4	2-CMT classical	classical	4	-9.50	-1.50	+4.00	0.737	✓
5	2-CMT multifractional	multifractional	6	-12.44	-0.44	+5.07	0.817	✓
6	3-CMT monofractional	monofractional	7	-12.44	1.56	+7.07	0.817	✗
7	3-CMT classical	classical	6	-9.50	2.50	+8.00	0.737	✗
8	3-CMT multifractional	multifractional	9	-12.44	5.56	+11.07	0.817	✓

Verdict — rule applied

Rule 2 — Top 2 models within ΔAIC < 4. Statistically equivalent. Both top candidates fit equivalently well within ΔAIC < 4; reporting the parsimonious choice per Occam's principle.

Selected model — parameter estimates

1-CMT classical · classical · 2 parameters

THETA — population estimates

Parameter	Estimate	%RSE
A_1	5.123	N/A
k_1	0.07302	N/A

Derived quantities

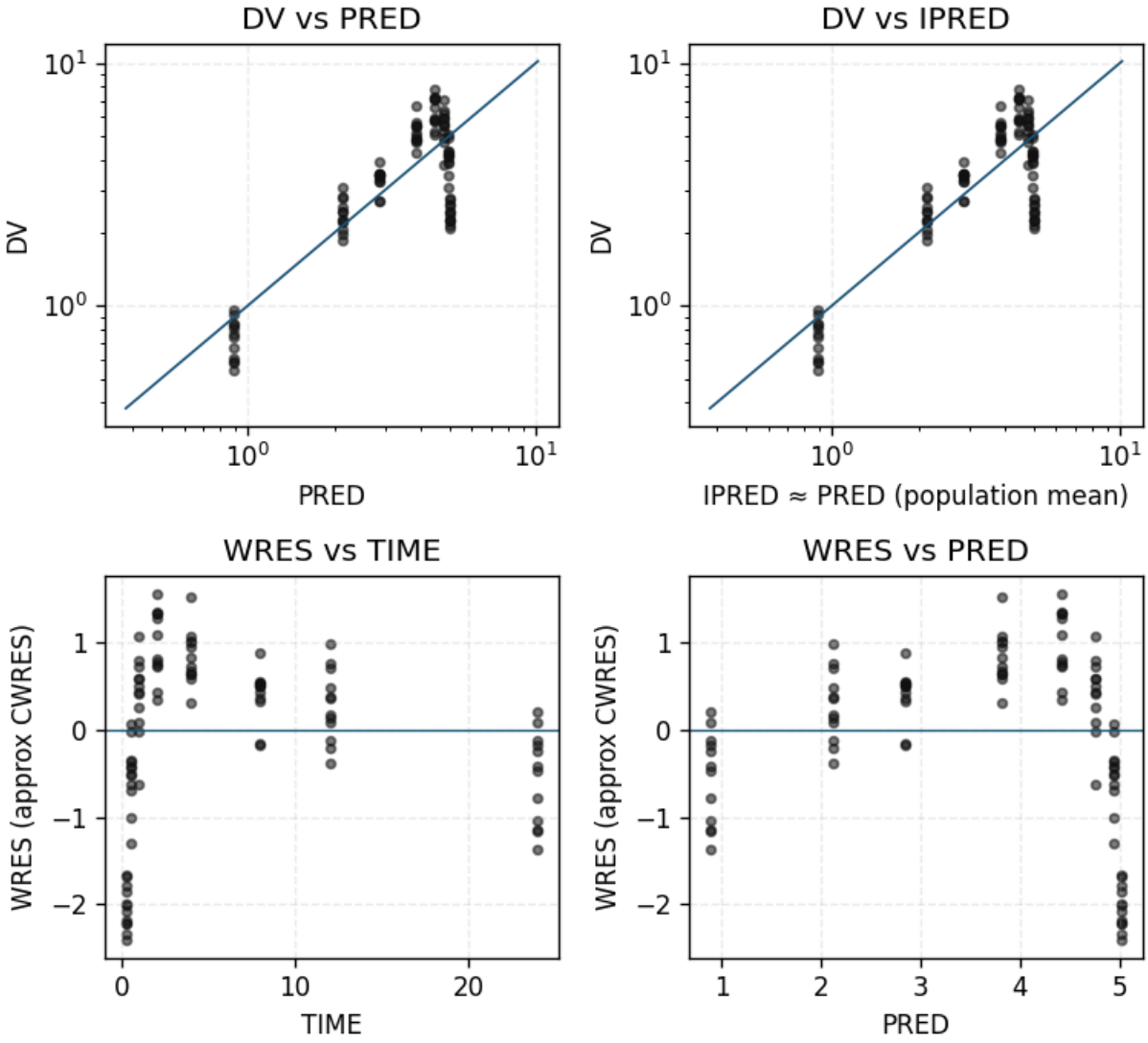
Quantity	Value	Units	Formula
Half-life (terminal)	9.49	h	ln(2) / k_terminal
Time to steady state	47.5	h	5 · t½
AUC 0→inf (apparent)	70.1	conc·h	Σ A_i / k_i
Apparent clearance	4.56	(dose units / h) / conc	dose / AUC

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

Variability & residual error

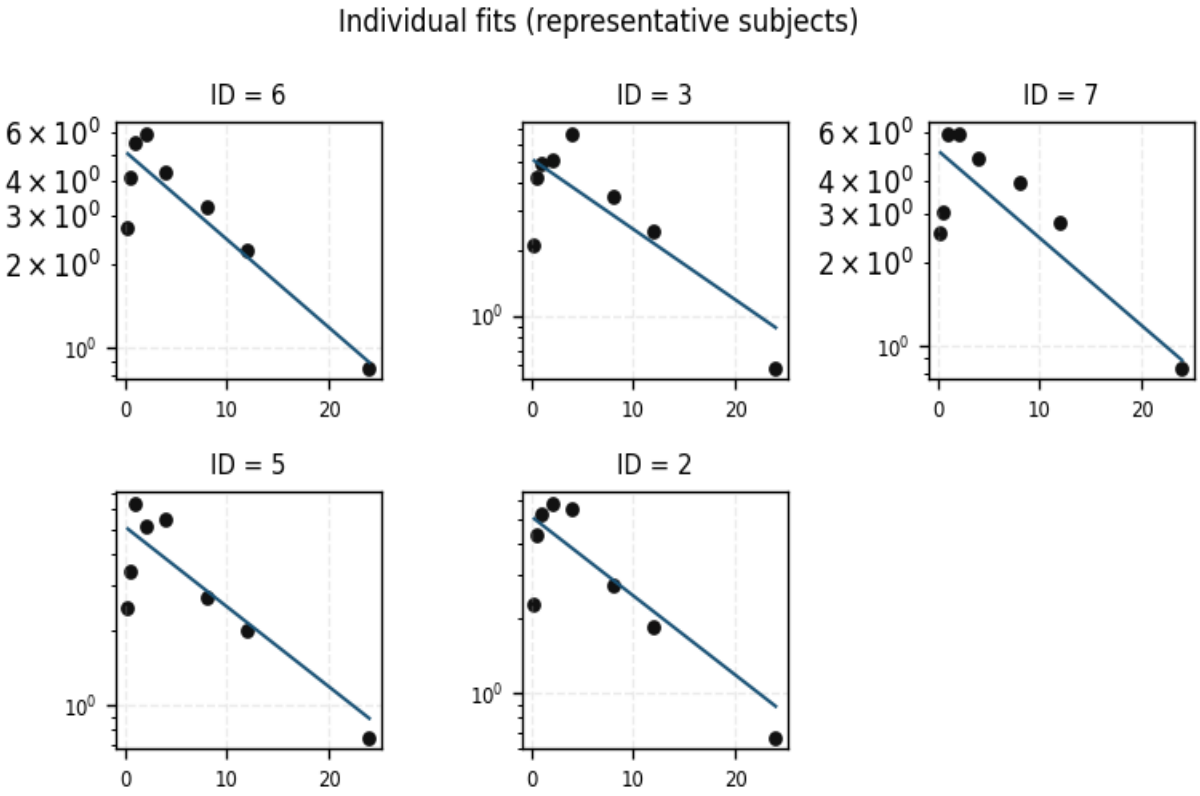
Population-level estimates. Individual-subject variance components (OMEGA / shrinkage) are part of the extended analysis tier. Residual error: single proportional model.

Goodness-of-fit



Individual fits

Representative subjects (best-fit, worst-fit, median, plus spread): 6, 3, 7, 5, 2



Diagnostics & computational details

Metric	Value
Winner iterations	37
Winner wall time (s)	0.05
Winner converged	yes
Total wall time (s)	34.5
Engine version	v2-fase1B
Fit engine	multi_cmt_fitter (numpy ML series)
N observations	8
Dose (form input)	320.0
Route	oral

Numerical diagnostics (top 2 candidates)

Top-2 candidates converged within typical parameter ranges. No numerical concerns flagged.

Methodological note

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 $\Delta AIC \geq 4$. Verdict is a diagnostic indication, not a regulatory conclusion. Estimates are reported at the population level; individual-subject variance components are part of the extended analysis tier.

Your analysis is complete.

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

Want to share these results? Cite as: *FractaLPK v2-fase1B, generated 2026-05-26 10:16 UTC, ID 9019c69dd0*.