

Pharmacokinetic Analysis Report

Non-Compartmental Analysis (NCA) — Population Summary

Dataset: **theophylline_demo_v1.csv**

Job ID: **B3-NCA**

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Synthetic demonstration data — not real drug data. This report is generated from a synthetic CSV bundled with the FractaLPK platform for evaluation and demonstration purposes. Numerical results do not represent the named compound and must not be cited as such.

Computational non-compartmental analysis (NCA) results — informational only. FractaLPK does not issue regulatory advice; pharmacological interpretation is the responsibility of the user's expert team.

Methodology consistent with standard non-compartmental analysis practice (Gabrielsson & Weiner, Pharmacokinetic and Pharmacodynamic Data Analysis, 5th ed., 2016).

Subjects analysed: 30 · Reportable subjects: 30

Sampling regime: rich

Rich sampling — NCA reported without sampling caveat.

Unit basis: concentration: **mg/L** (dataset name inference) · time: **h** (dataset name inference) · dose basis: **mg/kg** (dataset name inference)

Population NCA parameters

| Parameter | Median | [P5, P95] | Mean ± SD | n |
|-----------------------------|--------|-------------------|-------------------|----|
| C _{max} (mg/L) | 2.197 | [1.921, 2.437] | 2.183 ± 0.18 | 30 |
| T _{max} (h) | 2 | [1, 2] | 1.833 ± 0.5921 | 30 |
| AUC _{0-t} (mg·h/L) | 18.64 | [13.57, 25.97] | 18.51 ± 4.598 | 30 |
| AUC _{0-∞} (mg·h/L) | 19.57 | [14.6, 26.26] | 20.35 ± 4.227 | 22 |
| % AUC extrapolated (%) | 0.5898 | [0.409, 0.8168] | 0.5947 ± 0.1561 | 22 |
| λ _z (1/h) | 0.1094 | [0.09777, 0.1196] | 0.1075 ± 0.008328 | 22 |
| t _{1/2} (h) | 6.336 | [5.796, 7.09] | 6.485 ± 0.5177 | 22 |
| MRT (h) | 9.437 | [8.089, 11.13] | 9.542 ± 1.099 | 22 |
| CL/F (L/h/kg) | 5.109 | [3.808, 6.849] | 5.125 ± 1.084 | 22 |
| V _z /F (L/kg) | 45.54 | [35.04, 68.19] | 48.19 ± 12.5 | 22 |

Methodology

AUC_{0-t} was computed by the trapezoidal rule (linear-up / log-down where the post-T_{max} phase was strictly decreasing, linear otherwise).

λ_z was estimated by log-linear regression over the terminal phase, selecting the consecutive subset of three or more points that maximised the adjusted coefficient of determination (adjusted R²). λ_z was reported only

when adjusted $R^2 \geq 0.90$ (canonical FractalPK threshold shared by the NCA / BE / FE / DP reports).
SPAN_INSUFFICIENT fires only when the terminal regression window covers $< 2 \times t_{1/2}$ AND %AUCext > 20 %; below 20 %, AUC0- ∞ is reliable by construction. A reinforced rule rejects λz when %AUCext > 50 % AND fewer than 4 terminal points were used in the regression.

$AUC_{0-\infty} = AUC_{0-t} + C_{last} / \lambda z$. $t_{1/2} = \ln(2) / \lambda z$. $CL/F = Dose / AUC_{0-\infty}$. $Vz/F = CL/F / \lambda z$. MRT was computed from the area under the first-moment curve.

Below-quantification-limit (BLQ) observations were handled per the convention summarised in the individual subject flags: zero before first quantifiable, log-linear interpolation between quantifiable, zero-and-excluded-from- λz after last quantifiable.

Individual subject estimates

Each row is one reportable subject. Subjects not meeting the adjusted R² threshold for λz or the minimum terminal-phase requirement are excluded from this table. Flags column: **NTP** = NO_TERMINAL_PHASE (λz not estimable; AUC_{0-∞} reported as N/A); **HIE** = HIGH_EXTRAPOLATION (%AUC_{ext} > 20 %); **EXE** = EXTREME_EXTRAPOLATION (%AUC_{ext} > 50 %); **SPI** = SPAN_INSUFFICIENT (regression window < 2 × t_{1/2} AND %AUC_{ext} > 20 %). TLT (TLAST_TRUNCATED) is a two-arm-only flag and never fires in single-arm NCA. The supplementary Excel bundle contains the unfiltered per-subject diagnostic tokens.

| Subject | Cmax | Tmax | AUC _{0-∞} | λz | t _{1/2} | adj R ² | %ext | CL/F | Flags |
|---------|-------|------|--------------------|-------------|------------------|--------------------|-------|-------|-------|
| 1 | 2.339 | 2 | 24.13 | 0.1022 | 6.784 | 0.991 | 0.811 | 4.145 | — |
| 2 | 2.203 | 2 | 19.43 | 0.1122 | 6.176 | 0.994 | 0.459 | 5.148 | — |
| 3 | 2.027 | 2 | — | — | — | 0.841 | — | — | NTP |
| 4 | 2.201 | 2 | 14.7 | 0.09959 | 6.96 | 0.936 | 0.683 | 6.802 | — |
| 5 | 1.807 | 1 | 19.72 | 0.1111 | 6.236 | 0.985 | 0.456 | 5.07 | — |
| 6 | 1.981 | 2 | — | — | — | 0.848 | — | — | NTP |
| 7 | 1.872 | 2 | 14.6 | 0.1158 | 5.986 | 0.92 | 0.592 | 6.851 | — |
| 8 | 2.422 | 2 | 20.26 | 0.1117 | 6.203 | 0.985 | 0.442 | 4.936 | — |
| 9 | 2.626 | 2 | 26.31 | 0.1088 | 6.369 | 1 | 0.594 | 3.801 | — |
| 10 | 2.065 | 2 | 16.75 | 0.1015 | 6.827 | 0.987 | 0.588 | 5.971 | — |
| 11 | 2.245 | 2 | — | — | — | 0.895 | — | — | NTP |
| 12 | 2.268 | 2 | 26.02 | 0.1013 | 6.839 | 0.999 | 0.834 | 3.843 | — |
| 13 | 2.117 | 2 | — | — | — | 0.832 | — | — | NTP |
| 14 | 2.058 | 1 | 18.77 | 0.1172 | 5.913 | 0.992 | 0.455 | 5.329 | — |
| 15 | 2.191 | 2 | 18.81 | 0.112 | 6.187 | 0.996 | 0.475 | 5.317 | — |
| 16 | 2.194 | 2 | 15.68 | 0.09794 | 7.078 | 0.94 | 0.651 | 6.378 | — |
| 17 | 2.449 | 1 | 26.27 | 0.1007 | 6.886 | 0.999 | 0.794 | 3.806 | — |
| 18 | 2.276 | 2 | 18.7 | 0.11 | 6.303 | 0.988 | 0.486 | 5.348 | — |
| 19 | 2.203 | 1 | 21.39 | 0.1202 | 5.768 | 0.994 | 0.389 | 4.675 | — |
| 20 | 2.138 | 2 | — | — | — | 0.857 | — | — | NTP |
| 21 | 2.105 | 1 | — | — | — | 0.896 | — | — | NTP |
| 22 | 2.324 | 2 | 25.1 | 0.1197 | 5.791 | 0.998 | 0.433 | 3.984 | — |

| Subject | Cmax | Tmax | AUC _{0-∞} | λ _z | t _{1/2} | adj R ² | %ext | CL/F | Flags |
|---------|-------|------|--------------------|----------------|------------------|--------------------|-------|-------|-------|
| 23 | 2.409 | 2 | 25.72 | 0.103 | 6.729 | 1 | 0.793 | 3.888 | — |
| 24 | 2.242 | 1 | 14.19 | 0.08905 | 7.783 | 0.946 | 0.791 | 7.047 | — |
| 25 | 2.247 | 2 | 20.86 | 0.1176 | 5.896 | 1 | 0.408 | 4.793 | — |
| 26 | 2.026 | 2 | 26.07 | 0.1033 | 6.71 | 0.989 | 0.817 | 3.837 | — |
| 27 | 2.074 | 2 | 15.47 | 0.09776 | 7.09 | 0.941 | 0.661 | 6.462 | — |
| 28 | 1.99 | 2 | — | — | — | 0.883 | — | — | NTP |
| 29 | 2 | 4 | 18.79 | 0.1125 | 6.164 | 0.966 | 0.473 | 5.323 | — |
| 30 | 2.38 | 1 | — | — | — | 0.835 | — | — | NTP |

Limitations and scope

This report summarises non-compartmental pharmacokinetic parameters. Structural-model parameter estimation, covariate analysis, and bioequivalence assessment are outside the scope of this report and should be addressed in the corresponding dedicated sections of the dossier.

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