

Report of *ncappc*^{*} package

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1 Summary of the data set and the results

```
## Name of the file with the observed data: "Theoph.csv"  
## Route of administration: extravascular  
## Dose type: non-steady-state  
## No. of population stratification level: 0
```

Summary table

Dose (M)	No. of individuals
	12

2 Command-line arguments passed to ncappc function

```
## ncappc(obsFile = "Theoph.csv", psnOut = FALSE, method = "linear-log",  
##      evid = FALSE, noPlot = TRUE, printOut = TRUE)
```

3 Description of the tabular output

3.1 Table 1 (ncaOutput.tsv)

The **ncappc** functionality produces this table to report the estimated values of the NCA metrics described in the documentation for each individual along with other stratifiers (eg. population group ID, dose ID, etc.) if specified in the input command. The extension "tsv" stands for "tab separated variable", *i.e.*, the columns in this table are separated by tabs. "NaN" or "NA" is produced for the NCA metrics which are irrelevant for the specified data type. Below is an excerpt of selected columns of top 100 rows.

Table 1. ncaOutput.tsv (selected columns of top 100 rows)

ID	Dose (M)	AUClast (T*M.L ⁻³)	Cmax (M.L ⁻³)	Tmax (T)	AUCINF_obs (T*M.L ⁻³)	Vz_obs (M/M.L ⁻³)	Cl_obs (M/(T*M.L ⁻³))	HL_Lambda_z (T)
1	NA	147.2347	10.5000	1.1200	214.9236	NA	NA	14.3044
2	NA	88.7313	8.3300	1.9200	97.3779	NA	NA	6.6593
3	NA	95.8782	8.2000	1.0200	106.1277	NA	NA	6.7661
4	NA	102.6336	8.6000	1.0700	114.2162	NA	NA	6.9812
5	NA	118.1794	11.4000	1.0000	136.3047	NA	NA	8.0023
6	NA	71.6970	6.4400	1.1500	82.1759	NA	NA	7.8950
7	NA	87.9692	7.0900	3.4800	100.9876	NA	NA	7.8467
8	NA	86.8066	7.5600	2.0200	102.1533	NA	NA	8.5100
9	NA	83.9374	9.0300	0.6300	97.5200	NA	NA	8.4060
10	NA	135.5761	10.2100	3.5500	167.8600	NA	NA	9.2469
11	NA	77.8935	8.0000	0.9800	86.9026	NA	NA	7.2612
12	NA	115.2202	9.7500	3.5200	125.8315	NA	NA	6.2865

3.2 Table 2 (Obs_Stat.tsv)

A set of statistical parameters calculated for the entire population or the stratified population for the mean values of the following NCA metrics estimated from the simulated data: Tmax, Cmax, AUClast, AUClower_upper, AUCINF_obs, AUC_pExtrap_obs, AUCINF_pred, AUC_pExtrap_pred, AUMClast, AUMCINF_obs, AUMC_pExtrap_obs, AUMCINF_pred, AUMC_pExtrap_pred, HL_Lambda_z, Rsq, Rsq_adjusted, No_points_Lambda_z obtained from the observed data. Brief description of the calculated statistical parameters: **Ntot** = Total number of data points, **Nunique** = number of unique data points, **Min** = minimum value, **Max** = maximum value, **Mean** = mean/average value, **SD** = standard deviation, **SE** = standard error, **CVp** = coefficient of variation %, **a95CIu** = upper limit of 95% arithmetic confidence interval, **a95Cil** = lower limit of 95% arithmetic confidence interval, **gMean** = geometric mean, **gCVp** = geometric coefficient of variation %.

4 Description of the graphical output

4.1 Figure 1. [Individual level] Concentration *vs.* time profile

```
## [1] "No concentration vs time plot is available."
```

Concentration vs time profile for each individual stratified by dose or population group, if any, as obtained from the observed data. The left panels represent the raw data, while the right panels represent the semi-logarithmic form of the concentration data. Each of the lines represents individual data.

4.2 Figure 2. [Population level] Histogram of the selected NCA metrics estimated from the observed data

```
## No histogram is available as the number of individuals is less than 5 in  
## all population strata!
```

Histogram of four selected NCA metrics (AUClast, AUCINF_obs, Cmax, Tmax) estimated from the observed data. The solid blue vertical and dotted lines represent the population mean and the "spread" of the data. The "spread" is defined by 95% nonparametric prediction interval of the NCA metrics obtained from the observed data.