Validation of Noncompartmental Analysis Performed by NonCompart R package

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1 Introduction

NonCompart R package (Bae 2018) can conduct a noncompartmental analysis as closely as possible to the most widely used commercial software for pharmacokinetic analysis, i.e. Phoenix® WinNonlin®. This document provides validation of noncompartmental analysis performed by NonCompart R package as compared to the results from the commercial software.

2 Results

This script will be stopped if there is any difference between results from NonCompart and WinNonlin printing `Test Failed!`.

```
# install.packages("NonCompart", repos="http://pmx.amc.seoul.kr")
library(NonCompart)
RptCfg = read.csv("RptCfg.csv", as.is=TRUE)

Equal = function(Wres, Rres, Tol=0.001)
{
  Wres[,"ID"] = as.character(Wres[,"Subject"])
  ColName0 = colnames(Rres)
  rownames(RptCfg) = RptCfg[,"PPTESTCD"]
```

```
  colnames(Rres) = c(ColName0[1], RptCfg[ColName0[-1],"WNL"])
  Inter = intersect(colnames(Wres), colnames(Rres))

  IsSame = TRUE
  for (i in 1:nrow(Wres)) {
    for (j in Inter) {
      R = as.numeric(Rres[i,j])
      W = as.numeric(Wres[i,j])
      if (W != 0) {
        if(abs((R - W)/W) > Tol) {
          print(Wres[i,j])
          print(Rres[i,j])
          IsSame = FALSE
        }
      }
    }
  }
  return(IsSame)
}
```

Eight comparison tests were performed using `Theoph` and `Indometh` default datasets.

No.	Dataset	Down	Route
1	Theoph (n=12)	Linear	Extravascular
2	Theoph (n=12)	Log	Extravascular
3	Indometh (n=6)	Linear	IV Bolus
4	Indometh (n=6)	Log	IV Bolus
5	Indometh (n=6)	Linear	IV Infusion (0.25hr)
6	Indometh (n=6)	Log	IV Infusion (0.25hr)
7	Indometh (n=6)	Linear	Extravascular
8	Indometh (n=6)	Log	Extravascular

```
Theoph[,"Subject"] = as.numeric(as.character(Theoph[,"Subject"]))
Indometh[,"Subject"] = as.numeric(as.character(Indometh[,"Subject"]))

Wres = read.csv("Final_Parameters_Pivoted_Theoph_Linear.csv")
Rres = tblNCA(Theoph, "Subject", "Time", "conc", dose=320, concUnit="mg/L")
if (!Equal(Wres, Rres)) stop("Test Failed!")

Wres = read.csv("Final_Parameters_Pivoted_Theoph_Log.csv")
Rres = tblNCA(Theoph, "Subject", "Time", "conc", dose=320, down="Log",
              concUnit="mg/L")
if (!Equal(Wres, Rres)) stop("Test Failed!")

Wres = read.csv("Final_Parameters_Pivoted_Indometh_Linear.csv")
Rres = tblNCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus",
              concUnit="mg/L", R2ADJ=0.8)
if (!Equal(Wres, Rres)) stop("Test Failed!")

Wres = read.csv("Final_Parameters_Pivoted_Indometh_Log.csv")
Rres = tblNCA(Indometh, "Subject", "time", "conc", dose=25, adm="Bolus",
              down="Log", concUnit="mg/L", R2ADJ=0.8)
```

```
if (!Equal(Wres, Rres)) stop("Test Failed!")

Wres = read.csv("Final_Parameters_Pivoted_Indometh_Linear_Infusion.csv")
Rres = tblNCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion",
              dur=0.25, concUnit="mg/L", R2ADJ=0.8)
if (!Equal(Wres, Rres)) stop("Test Failed!")

Wres = read.csv("Final_Parameters_Pivoted_Indometh_Log_Infusion.csv")
Rres = tblNCA(Indometh, "Subject", "time", "conc", dose=25, adm="Infusion",
              dur=0.25, down="Log", concUnit="mg/L", R2ADJ=0.8)
if (!Equal(Wres, Rres)) stop("Test Failed!")

Wres = read.csv("Final_Parameters_Pivoted_Indometh_Linear_Wrong_Extravascular.csv")
Rres = tblNCA(Indometh, "Subject", "time", "conc", dose=25, concUnit="mg/L",
              R2ADJ=0.8)
if (!Equal(Wres, Rres)) stop("Test Failed!")

Wres = read.csv("Final_Parameters_Pivoted_Indometh_Log_Wrong_Extravascular.csv")
Rres = tblNCA(Indometh, "Subject", "time", "conc", dose=25, down="Log",
              concUnit="mg/L", R2ADJ=0.8)
if (!Equal(Wres, Rres)) stop("Test Failed!")
```

3 Conclusion

Nothing happened and it indicates that **there is no discrepancy**. Noncompartmental analyses generated by NonCompart R package are qualified and validated.

A Side by side value comparison

```
library(dplyr)
library(tidyr)

table_wres_rres <- function(wres, rres){
  wres %>%
    gather(WNL, WinNonlin, -Subject) %>%
    left_join(RptCfg %>% select(PPTESTCD, WNL), by = "WNL") %>%
    left_join(rres %>% as.data.frame() %>% gather(PPTESTCD, NonCompart, -Subject),
              by = c("Subject", "PPTESTCD")) %>%
    select(Subject, PPTESTCD, WNL, NonCompart, WinNonlin) %>%
    filter(!is.na(WinNonlin) & !is.na(NonCompart)) %>%
    knitr::kable(longtable = TRUE, booktabs = TRUE, format = "latex",
                 caption = "Longtable") %>%
    add_header_above(c(" ", "Group 1" = 2, "Group 2" = 2)) %>%
    kable_styling(latex_options = c("repeat_header"))

}
```

A.1 Test 1: Theoph (n=12), Linear, Extravascular

```
Wres = read.csv("Final_Parameters_Pivoted_Theoph_Log.csv")
Rres = tblNCA(Theoph, "Subject", "Time", "conc", dose=320, down="Log", concUnit="mg/L")

table_wres_rres(Wres, Rres)
```

Table 2: Longtable

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
1	R2	Rsq	0.9999997	0.9999997
2	R2	Rsq	0.9971954	0.9971954
3	R2	Rsq	0.9993250	0.9993250
4	R2	Rsq	0.9989241	0.9989241
5	R2	Rsq	0.9986472	0.9986472
6	R2	Rsq	0.9982413	0.9982413
7	R2	Rsq	0.9986702	0.9986702
8	R2	Rsq	0.9910124	0.9910124
9	R2	Rsq	0.9994437	0.9994437
10	R2	Rsq	0.9995087	0.9995087
11	R2	Rsq	0.9999983	0.9999983
12	R2	Rsq	0.9993968	0.9993968
1	R2ADJ	Rsq_adjusted	0.9999995	0.9999995
2	R2ADJ	Rsq_adjusted	0.9957931	0.9957931
3	R2ADJ	Rsq_adjusted	0.9986499	0.9986499
4	R2ADJ	Rsq_adjusted	0.9978483	0.9978483

Table 2: Longtable *(continued)*

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
5	R2ADJ	Rsq_adjusted	0.9979708	0.9979708
6	R2ADJ	Rsq_adjusted	0.9978896	0.9978896
7	R2ADJ	Rsq_adjusted	0.9980053	0.9980053
8	R2ADJ	Rsq_adjusted	0.9887655	0.9887655
9	R2ADJ	Rsq_adjusted	0.9988873	0.9988873
10	R2ADJ	Rsq_adjusted	0.9990174	0.9990174
11	R2ADJ	Rsq_adjusted	0.9999965	0.9999965
12	R2ADJ	Rsq_adjusted	0.9987936	0.9987936
1	CORRXY	Corr_XY	-0.9999999	-0.9999999
2	CORRXY	Corr_XY	-0.9985967	-0.9985967
3	CORRXY	Corr_XY	-0.9996624	-0.9996624
4	CORRXY	Corr_XY	-0.9994619	-0.9994619
5	CORRXY	Corr_XY	-0.9993234	-0.9993234
6	CORRXY	Corr_XY	-0.9991203	-0.9991203
7	CORRXY	Corr_XY	-0.9993349	-0.9993349
8	CORRXY	Corr_XY	-0.9954961	-0.9954961
9	CORRXY	Corr_XY	-0.9997218	-0.9997218
10	CORRXY	Corr_XY	-0.9997543	-0.9997543
11	CORRXY	Corr_XY	-0.9999991	-0.9999991
12	CORRXY	Corr_XY	-0.9996984	-0.9996984
1	LAMZNPT	No_points_lambda_z	3.0000000	3.0000000
2	LAMZNPT	No_points_lambda_z	4.0000000	4.0000000
3	LAMZNPT	No_points_lambda_z	3.0000000	3.0000000
4	LAMZNPT	No_points_lambda_z	3.0000000	3.0000000
5	LAMZNPT	No_points_lambda_z	4.0000000	4.0000000
6	LAMZNPT	No_points_lambda_z	7.0000000	7.0000000
7	LAMZNPT	No_points_lambda_z	4.0000000	4.0000000
8	LAMZNPT	No_points_lambda_z	6.0000000	6.0000000
9	LAMZNPT	No_points_lambda_z	3.0000000	3.0000000
10	LAMZNPT	No_points_lambda_z	3.0000000	3.0000000
11	LAMZNPT	No_points_lambda_z	3.0000000	3.0000000
12	LAMZNPT	No_points_lambda_z	3.0000000	3.0000000
1	LAMZ	Lambda_z	0.0484570	0.0484570
2	LAMZ	Lambda_z	0.1040864	0.1040864
3	LAMZ	Lambda_z	0.1024443	0.1024443
4	LAMZ	Lambda_z	0.0992870	0.0992870
5	LAMZ	Lambda_z	0.0866189	0.0866189
6	LAMZ	Lambda_z	0.0877957	0.0877957
7	LAMZ	Lambda_z	0.0883365	0.0883365
8	LAMZ	Lambda_z	0.0814505	0.0814505
9	LAMZ	Lambda_z	0.0824586	0.0824586
10	LAMZ	Lambda_z	0.0749598	0.0749598
11	LAMZ	Lambda_z	0.0954586	0.0954586
12	LAMZ	Lambda_z	0.1102595	0.1102595
1	LAMZLL	Lambda_z_lower	9.0500000	9.0500000

Table 2: Longtable *(continued)*

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
2	LAMZLL	Lambda_z_lower	7.0300000	7.0300000
3	LAMZLL	Lambda_z_lower	9.0000000	9.0000000
4	LAMZLL	Lambda_z_lower	9.0200000	9.0200000
5	LAMZLL	Lambda_z_lower	7.0200000	7.0200000
6	LAMZLL	Lambda_z_lower	2.0300000	2.0300000
7	LAMZLL	Lambda_z_lower	6.9800000	6.9800000
8	LAMZLL	Lambda_z_lower	3.5300000	3.5300000
9	LAMZLL	Lambda_z_lower	8.8000000	8.8000000
10	LAMZLL	Lambda_z_lower	9.3800000	9.3800000
11	LAMZLL	Lambda_z_lower	9.0300000	9.0300000
12	LAMZLL	Lambda_z_lower	9.0300000	9.0300000
1	LAMZUL	Lambda_z_upper	24.3700000	24.3700000
2	LAMZUL	Lambda_z_upper	24.3000000	24.3000000
3	LAMZUL	Lambda_z_upper	24.1700000	24.1700000
4	LAMZUL	Lambda_z_upper	24.6500000	24.6500000
5	LAMZUL	Lambda_z_upper	24.3500000	24.3500000
6	LAMZUL	Lambda_z_upper	23.8500000	23.8500000
7	LAMZUL	Lambda_z_upper	24.2200000	24.2200000
8	LAMZUL	Lambda_z_upper	24.1200000	24.1200000
9	LAMZUL	Lambda_z_upper	24.4300000	24.4300000
10	LAMZUL	Lambda_z_upper	23.7000000	23.7000000
11	LAMZUL	Lambda_z_upper	24.0800000	24.0800000
12	LAMZUL	Lambda_z_upper	24.1500000	24.1500000
1	LAMZHL	HL_Lambda_z	14.3043776	14.3043776
2	LAMZHL	HL_Lambda_z	6.6593416	6.6593416
3	LAMZHL	HL_Lambda_z	6.7660874	6.7660874
4	LAMZHL	HL_Lambda_z	6.9812467	6.9812467
5	LAMZHL	HL_Lambda_z	8.0022640	8.0022640
6	LAMZHL	HL_Lambda_z	7.8949979	7.8949979
7	LAMZHL	HL_Lambda_z	7.8466683	7.8466683
8	LAMZHL	HL_Lambda_z	8.5100379	8.5100379
9	LAMZHL	HL_Lambda_z	8.4059988	8.4059988
10	LAMZHL	HL_Lambda_z	9.2469158	9.2469158
11	LAMZHL	HL_Lambda_z	7.2612365	7.2612365
12	LAMZHL	HL_Lambda_z	6.2865082	6.2865082
1	TLAG	Tlag	0.0000000	0.0000000
2	TLAG	Tlag	0.0000000	0.0000000
3	TLAG	Tlag	0.0000000	0.0000000
4	TLAG	Tlag	0.0000000	0.0000000
5	TLAG	Tlag	0.0000000	0.0000000
6	TLAG	Tlag	0.0000000	0.0000000
7	TLAG	Tlag	0.0000000	0.0000000
8	TLAG	Tlag	0.0000000	0.0000000
9	TLAG	Tlag	0.0000000	0.0000000
10	TLAG	Tlag	0.0000000	0.0000000

Table 2: Longtable *(continued)*

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
11	TLAG	Tlag	0.0000000	0.0000000
12	TLAG	Tlag	0.0000000	0.0000000
1	TMAX	Tmax	1.1200000	1.1200000
2	TMAX	Tmax	1.9200000	1.9200000
3	TMAX	Tmax	1.0200000	1.0200000
4	TMAX	Tmax	1.0700000	1.0700000
5	TMAX	Tmax	1.0000000	1.0000000
6	TMAX	Tmax	1.1500000	1.1500000
7	TMAX	Tmax	3.4800000	3.4800000
8	TMAX	Tmax	2.0200000	2.0200000
9	TMAX	Tmax	0.6300000	0.6300000
10	TMAX	Tmax	3.5500000	3.5500000
11	TMAX	Tmax	0.9800000	0.9800000
12	TMAX	Tmax	3.5200000	3.5200000
1	CMAX	Cmax	10.5000000	10.5000000
2	CMAX	Cmax	8.3300000	8.3300000
3	CMAX	Cmax	8.2000000	8.2000000
4	CMAX	Cmax	8.6000000	8.6000000
5	CMAX	Cmax	11.4000000	11.4000000
6	CMAX	Cmax	6.4400000	6.4400000
7	CMAX	Cmax	7.0900000	7.0900000
8	CMAX	Cmax	7.5600000	7.5600000
9	CMAX	Cmax	9.0300000	9.0300000
10	CMAX	Cmax	10.2100000	10.2100000
11	CMAX	Cmax	8.0000000	8.0000000
12	CMAX	Cmax	9.7500000	9.7500000
1	CMAXD	Cmax_D	0.0328125	0.0328125
2	CMAXD	Cmax_D	0.0260312	0.0260312
3	CMAXD	Cmax_D	0.0256250	0.0256250
4	CMAXD	Cmax_D	0.0268750	0.0268750
5	CMAXD	Cmax_D	0.0356250	0.0356250
6	CMAXD	Cmax_D	0.0201250	0.0201250
7	CMAXD	Cmax_D	0.0221562	0.0221562
8	CMAXD	Cmax_D	0.0236250	0.0236250
9	CMAXD	Cmax_D	0.0282188	0.0282188
10	CMAXD	Cmax_D	0.0319063	0.0319062
11	CMAXD	Cmax_D	0.0250000	0.0250000
12	CMAXD	Cmax_D	0.0304688	0.0304688
1	TLST	Tlast	24.3700000	24.3700000
2	TLST	Tlast	24.3000000	24.3000000
3	TLST	Tlast	24.1700000	24.1700000
4	TLST	Tlast	24.6500000	24.6500000
5	TLST	Tlast	24.3500000	24.3500000
6	TLST	Tlast	23.8500000	23.8500000
7	TLST	Tlast	24.2200000	24.2200000

Table 2: Longtable *(continued)*

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
8	TLST	Tlast	24.1200000	24.1200000
9	TLST	Tlast	24.4300000	24.4300000
10	TLST	Tlast	23.7000000	23.7000000
11	TLST	Tlast	24.0800000	24.0800000
12	TLST	Tlast	24.1500000	24.1500000
1	CLST	Clast	3.2800000	3.2800000
2	CLST	Clast	0.9000000	0.9000000
3	CLST	Clast	1.0500000	1.0500000
4	CLST	Clast	1.1500000	1.1500000
5	CLST	Clast	1.5700000	1.5700000
6	CLST	Clast	0.9200000	0.9200000
7	CLST	Clast	1.1500000	1.1500000
8	CLST	Clast	1.2500000	1.2500000
9	CLST	Clast	1.1200000	1.1200000
10	CLST	Clast	2.4200000	2.4200000
11	CLST	Clast	0.8600000	0.8600000
12	CLST	Clast	1.1700000	1.1700000
1	AUCLST	AUClast	147.2347485	147.2347485
2	AUCLST	AUClast	88.7312755	88.7312755
3	AUCLST	AUClast	95.8781978	95.8781978
4	AUCLST	AUClast	102.6336232	102.6336232
5	AUCLST	AUClast	118.1793538	118.1793538
6	AUCLST	AUClast	71.6970150	71.6970150
7	AUCLST	AUClast	87.9692274	87.9692274
8	AUCLST	AUClast	86.8065635	86.8065635
9	AUCLST	AUClast	83.9374360	83.9374360
10	AUCLST	AUClast	135.5760701	135.5760701
11	AUCLST	AUClast	77.8934723	77.8934723
12	AUCLST	AUClast	115.2202082	115.2202082
1	AUCALL	AUCall	147.2347485	147.2347485
2	AUCALL	AUCall	88.7312755	88.7312755
3	AUCALL	AUCall	95.8781978	95.8781978
4	AUCALL	AUCall	102.6336232	102.6336232
5	AUCALL	AUCall	118.1793538	118.1793538
6	AUCALL	AUCall	71.6970150	71.6970150
7	AUCALL	AUCall	87.9692274	87.9692274
8	AUCALL	AUCall	86.8065635	86.8065635
9	AUCALL	AUCall	83.9374360	83.9374360
10	AUCALL	AUCall	135.5760701	135.5760701
11	AUCALL	AUCall	77.8934723	77.8934723
12	AUCALL	AUCall	115.2202082	115.2202082
1	AUCIFO	AUCINF_obs	214.9236316	214.9236316
2	AUCIFO	AUCINF_obs	97.3779346	97.3779346
3	AUCIFO	AUCINF_obs	106.1276685	106.1276685
4	AUCIFO	AUCINF_obs	114.2162046	114.2162046

Table 2: Longtable *(continued)*

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
5	AUCIFO	AUCINF_obs	136.3047316	136.3047316
6	AUCIFO	AUCINF_obs	82.1758833	82.1758833
7	AUCIFO	AUCINF_obs	100.9876292	100.9876292
8	AUCIFO	AUCINF_obs	102.1533003	102.1533003
9	AUCIFO	AUCINF_obs	97.5200039	97.5200039
10	AUCIFO	AUCINF_obs	167.8600307	167.8600307
11	AUCIFO	AUCINF_obs	86.9026173	86.9026173
12	AUCIFO	AUCINF_obs	125.8315397	125.8315397
1	AUCIFOD	AUCINF_D_obs	0.6716363	0.6716363
2	AUCIFOD	AUCINF_D_obs	0.3043060	0.3043060
3	AUCIFOD	AUCINF_D_obs	0.3316490	0.3316490
4	AUCIFOD	AUCINF_D_obs	0.3569256	0.3569256
5	AUCIFOD	AUCINF_D_obs	0.4259523	0.4259523
6	AUCIFOD	AUCINF_D_obs	0.2567996	0.2567996
7	AUCIFOD	AUCINF_D_obs	0.3155863	0.3155863
8	AUCIFOD	AUCINF_D_obs	0.3192291	0.3192291
9	AUCIFOD	AUCINF_D_obs	0.3047500	0.3047500
10	AUCIFOD	AUCINF_D_obs	0.5245626	0.5245626
11	AUCIFOD	AUCINF_D_obs	0.2715707	0.2715707
12	AUCIFOD	AUCINF_D_obs	0.3932236	0.3932236
1	AUCPEO	AUC_.Extrap_obs	31.4943883	31.4943883
2	AUCPEO	AUC_.Extrap_obs	8.8794850	8.8794850
3	AUCPEO	AUC_.Extrap_obs	9.6576801	9.6576801
4	AUCPEO	AUC_.Extrap_obs	10.1409266	10.1409266
5	AUCPEO	AUC_.Extrap_obs	13.2976879	13.2976879
6	AUCPEO	AUC_.Extrap_obs	12.7517562	12.7517562
7	AUCPEO	AUC_.Extrap_obs	12.8910857	12.8910857
8	AUCPEO	AUC_.Extrap_obs	15.0232413	15.0232413
9	AUCPEO	AUC_.Extrap_obs	13.9279813	13.9279813
10	AUCPEO	AUC_.Extrap_obs	19.2326669	19.2326669
11	AUCPEO	AUC_.Extrap_obs	10.3669431	10.3669432
12	AUCPEO	AUC_.Extrap_obs	8.4329665	8.4329665
1	VZFO	Vz_F_obs	30.7262325	30.7262325
2	VZFO	Vz_F_obs	31.5715024	31.5715024
3	VZFO	Vz_F_obs	29.4329299	29.4329299
4	VZFO	Vz_F_obs	28.2182304	28.2182304
5	VZFO	Vz_F_obs	27.1035678	27.1035677
6	VZFO	Vz_F_obs	44.3539348	44.3539348
7	VZFO	Vz_F_obs	35.8708471	35.8708471
8	VZFO	Vz_F_obs	38.4594978	38.4594978
9	VZFO	Vz_F_obs	39.7942323	39.7942323
10	VZFO	Vz_F_obs	25.4316257	25.4316257
11	VZFO	Vz_F_obs	38.5746722	38.5746722
12	VZFO	Vz_F_obs	23.0645237	23.0645237
1	CLFO	Cl_F_obs	1.4889010	1.4889010

Table 2: Longtable *(continued)*

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
2	CLFO	Cl_F_obs	3.2861654	3.2861654
3	CLFO	Cl_F_obs	3.0152363	3.0152363
4	CLFO	Cl_F_obs	2.8017040	2.8017040
5	CLFO	Cl_F_obs	2.3476808	2.3476808
6	CLFO	Cl_F_obs	3.8940865	3.8940865
7	CLFO	Cl_F_obs	3.1687049	3.1687049
8	CLFO	Cl_F_obs	3.1325469	3.1325469
9	CLFO	Cl_F_obs	3.2813780	3.2813780
10	CLFO	Cl_F_obs	1.9063502	1.9063502
11	CLFO	Cl_F_obs	3.6822827	3.6822827
12	CLFO	Cl_F_obs	2.5430826	2.5430826
1	AUCIFP	AUCINF_pred	214.9266543	214.9266543
2	AUCIFP	AUCINF_pred	97.2687931	97.2687931
3	AUCIFP	AUCINF_pred	106.1774195	106.1774195
4	AUCIFP	AUCINF_pred	114.2808818	114.2808818
5	AUCIFP	AUCINF_pred	136.1395842	136.1395842
6	AUCIFP	AUCINF_pred	82.4181636	82.4181636
7	AUCIFP	AUCINF_pred	101.1089745	101.1089745
8	AUCIFP	AUCINF_pred	101.8896649	101.8896649
9	AUCIFP	AUCINF_pred	97.4773537	97.4773537
10	AUCIFP	AUCINF_pred	167.7758826	167.7758826
11	AUCIFP	AUCINF_pred	86.9005913	86.9005913
12	AUCIFP	AUCINF_pred	125.8817762	125.8817762
1	AUCIFPD	AUCINF_D_pred	0.6716458	0.6716458
2	AUCIFPD	AUCINF_D_pred	0.3039650	0.3039650
3	AUCIFPD	AUCINF_D_pred	0.3318044	0.3318044
4	AUCIFPD	AUCINF_D_pred	0.3571278	0.3571278
5	AUCIFPD	AUCINF_D_pred	0.4254362	0.4254362
6	AUCIFPD	AUCINF_D_pred	0.2575568	0.2575568
7	AUCIFPD	AUCINF_D_pred	0.3159655	0.3159655
8	AUCIFPD	AUCINF_D_pred	0.3184052	0.3184052
9	AUCIFPD	AUCINF_D_pred	0.3046167	0.3046167
10	AUCIFPD	AUCINF_D_pred	0.5242996	0.5242996
11	AUCIFPD	AUCINF_D_pred	0.2715643	0.2715643
12	AUCIFPD	AUCINF_D_pred	0.3933806	0.3933806
1	AUCPEP	AUC_.Extrap_pred	31.4953518	31.4953518
2	AUCPEP	AUC_.Extrap_pred	8.7772423	8.7772423
3	AUCPEP	AUC_.Extrap_pred	9.7000114	9.7000114
4	AUCPEP	AUC_.Extrap_pred	10.1917822	10.1917822
5	AUCPEP	AUC_.Extrap_pred	13.1925116	13.1925116
6	AUCPEP	AUC_.Extrap_pred	13.0082352	13.0082352
7	AUCPEP	AUC_.Extrap_pred	12.9956288	12.9956288
8	AUCPEP	AUC_.Extrap_pred	14.8033674	14.8033674
9	AUCPEP	AUC_.Extrap_pred	13.8903213	13.8903213
10	AUCPEP	AUC_.Extrap_pred	19.1921580	19.1921580

Table 2: Longtable *(continued)*

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
11	AUCPEP	AUC_.Extrap_pred	10.3648535	10.3648535
12	AUCPEP	AUC_.Extrap_pred	8.4695087	8.4695087
1	VZFP	Vz_F_pred	30.7258003	30.7258003
2	VZFP	Vz_F_pred	31.6069275	31.6069275
3	VZFP	Vz_F_pred	29.4191386	29.4191386
4	VZFP	Vz_F_pred	28.2022603	28.2022603
5	VZFP	Vz_F_pred	27.1364464	27.1364464
6	VZFP	Vz_F_pred	44.2235499	44.2235499
7	VZFP	Vz_F_pred	35.8277969	35.8277969
8	VZFP	Vz_F_pred	38.5590101	38.5590101
9	VZFP	Vz_F_pred	39.8116439	39.8116439
10	VZFP	Vz_F_pred	25.4443810	25.4443809
11	VZFP	Vz_F_pred	38.5755715	38.5755715
12	VZFP	Vz_F_pred	23.0553192	23.0553192
1	CLFP	Cl_F_pred	1.4888800	1.4888800
2	CLFP	Cl_F_pred	3.2898527	3.2898527
3	CLFP	Cl_F_pred	3.0138235	3.0138235
4	CLFP	Cl_F_pred	2.8001184	2.8001184
5	CLFP	Cl_F_pred	2.3505287	2.3505287
6	CLFP	Cl_F_pred	3.8826393	3.8826393
7	CLFP	Cl_F_pred	3.1649020	3.1649020
8	CLFP	Cl_F_pred	3.1406522	3.1406522
9	CLFP	Cl_F_pred	3.2828138	3.2828138
10	CLFP	Cl_F_pred	1.9073063	1.9073063
11	CLFP	Cl_F_pred	3.6823685	3.6823685
12	CLFP	Cl_F_pred	2.5420677	2.5420677
1	AUMCLST	AUMClast	1499.1290852	1499.1290850
2	AUMCLST	AUMClast	716.2787279	716.2787279
3	AUMCLST	AUMClast	810.8726830	810.8726830
4	AUMCLST	AUMClast	911.7828093	911.7828093
5	AUMCLST	AUMClast	1038.8799844	1038.8799840
6	AUMCLST	AUMClast	618.6659191	618.6659191
7	AUMCLST	AUMClast	795.6267785	795.6267785
8	AUMCLST	AUMClast	756.3619816	756.3619816
9	AUMCLST	AUMClast	723.3794155	723.3794155
10	AUMCLST	AUMClast	1306.7406149	1306.7406150
11	AUMCLST	AUMClast	626.6357849	626.6357849
12	AUMCLST	AUMClast	982.6343023	982.6343023
1	AUMCIFO	AUMCINF_obs	4545.5928011	4545.5928010
2	AUMCIFO	AUMCINF_obs	1009.4644499	1009.4644500
3	AUMCIFO	AUMCINF_obs	1158.6515817	1158.6515820
4	AUMCIFO	AUMCINF_obs	1313.9510002	1313.9510000
5	AUMCIFO	AUMCINF_obs	1689.4872798	1689.4872800
6	AUMCIFO	AUMCINF_obs	987.9420173	987.9420173
7	AUMCIFO	AUMCINF_obs	1258.3053268	1258.3053270

Table 2: Longtable *(continued)*

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
8	AUMCIFO	AUMCINF_obs	1314.9431383	1314.9431380
9	AUMCIFO	AUMCINF_obs	1219.9213281	1219.9213280
10	AUMCIFO	AUMCINF_obs	2502.5540002	2502.5540000
11	AUMCIFO	AUMCINF_obs	937.9535438	937.9535438
12	AUMCIFO	AUMCINF_obs	1335.1375811	1335.1375810
1	AUMCPEO	AUMC_.Extrap_obs	67.0201632	67.0201632
2	AUMCPEO	AUMC_.Extrap_obs	29.0436897	29.0436897
3	AUMCPEO	AUMC_.Extrap_obs	30.0158308	30.0158308
4	AUMCPEO	AUMC_.Extrap_obs	30.6075486	30.6075486
5	AUMCPEO	AUMC_.Extrap_obs	38.5091562	38.5091562
6	AUMCPEO	AUMC_.Extrap_obs	37.3783169	37.3783169
7	AUMCPEO	AUMC_.Extrap_obs	36.7699745	36.7699745
8	AUMCPEO	AUMC_.Extrap_obs	42.4794913	42.4794914
9	AUMCPEO	AUMC_.Extrap_obs	40.7027815	40.7027815
10	AUMCPEO	AUMC_.Extrap_obs	47.7837196	47.7837196
11	AUMCPEO	AUMC_.Extrap_obs	33.1911704	33.1911704
12	AUMCPEO	AUMC_.Extrap_obs	26.4020191	26.4020191
1	AUMCIFP	AUMCINF_pred	4545.7288462	4545.7288460
2	AUMCIFP	AUMCINF_pred	1005.7637454	1005.7637450
3	AUMCIFP	AUMCINF_pred	1160.3397033	1160.3397030
4	AUMCIFP	AUMCINF_pred	1316.1967080	1316.1967080
5	AUMCIFP	AUMCINF_pred	1683.5593423	1683.5593420
6	AUMCIFP	AUMCINF_pred	996.4799913	996.4799913
7	AUMCIFP	AUMCINF_pred	1262.6179786	1262.6179790
8	AUMCIFP	AUMCINF_pred	1305.3474998	1305.3475000
9	AUMCIFP	AUMCINF_pred	1218.3621498	1218.3621500
10	AUMCIFP	AUMCINF_pred	2499.4371146	2499.4371150
11	AUMCIFP	AUMCINF_pred	937.8835360	937.8835360
12	AUMCIFP	AUMCINF_pred	1336.8064129	1336.8064130
1	AUMCPEP	AUMC_.Extrap_pred	67.0211503	67.0211503
2	AUMCPEP	AUMC_.Extrap_pred	28.7826061	28.7826061
3	AUMCPEP	AUMC_.Extrap_pred	30.1176474	30.1176474
4	AUMCPEP	AUMC_.Extrap_pred	30.7259467	30.7259467
5	AUMCPEP	AUMC_.Extrap_pred	38.2926424	38.2926424
6	AUMCPEP	AUMC_.Extrap_pred	37.9148679	37.9148679
7	AUMCPEP	AUMC_.Extrap_pred	36.9859457	36.9859457
8	AUMCPEP	AUMC_.Extrap_pred	42.0566568	42.0566568
9	AUMCPEP	AUMC_.Extrap_pred	40.6268969	40.6268969
10	AUMCPEP	AUMC_.Extrap_pred	47.7186040	47.7186040
11	AUMCPEP	AUMC_.Extrap_pred	33.1861835	33.1861835
12	AUMCPEP	AUMC_.Extrap_pred	26.4938967	26.4938967
1	MRTEVLST	MRTlast	10.1818973	10.1818973
2	MRTEVLST	MRTlast	8.0724494	8.0724494
3	MRTEVLST	MRTlast	8.4573209	8.4573209
4	MRTEVLST	MRTlast	8.8838607	8.8838607

Table 2: Longtable *(continued)*

	Group 1		Group 2	
Subject	PPTESTCD	WNL	NonCompart	WinNonlin
5	MRTEVLST	MRTlast	8.7907063	8.7907063
6	MRTEVLST	MRTlast	8.6288937	8.6288937
7	MRTEVLST	MRTlast	9.0443761	9.0443761
8	MRTEVLST	MRTlast	8.7131889	8.7131889
9	MRTEVLST	MRTlast	8.6180785	8.6180785
10	MRTEVLST	MRTlast	9.6384311	9.6384311
11	MRTEVLST	MRTlast	8.0447792	8.0447792
12	MRTEVLST	MRTlast	8.5283156	8.5283156
1	MRTEVIFO	MRTINF_obs	21.1498046	21.1498045
2	MRTEVIFO	MRTINF_obs	10.3664599	10.3664599
3	MRTEVIFO	MRTINF_obs	10.9175260	10.9175260
4	MRTEVIFO	MRTINF_obs	11.5040681	11.5040681
5	MRTEVIFO	MRTINF_obs	12.3949276	12.3949276
6	MRTEVIFO	MRTINF_obs	12.0222866	12.0222866
7	MRTEVIFO	MRTINF_obs	12.4599947	12.4599947
8	MRTEVIFO	MRTINF_obs	12.8722531	12.8722531
9	MRTEVIFO	MRTINF_obs	12.5094471	12.5094471
10	MRTEVIFO	MRTINF_obs	14.9085758	14.9085758
11	MRTEVIFO	MRTINF_obs	10.7931564	10.7931564
12	MRTEVIFO	MRTINF_obs	10.6105161	10.6105161
1	MRTEVIFP	MRTINF_pred	21.1501401	21.1501401
2	MRTEVIFP	MRTINF_pred	10.3400455	10.3400455
3	MRTEVIFP	MRTINF_pred	10.9283095	10.9283095
4	MRTEVIFP	MRTINF_pred	11.5172082	11.5172082
5	MRTEVIFP	MRTINF_pred	12.3664205	12.3664205
6	MRTEVIFP	MRTINF_pred	12.0905386	12.0905386
7	MRTEVIFP	MRTINF_pred	12.4876944	12.4876944
8	MRTEVIFP	MRTINF_pred	12.8113828	12.8113828
9	MRTEVIFP	MRTINF_pred	12.4989252	12.4989252
10	MRTEVIFP	MRTINF_pred	14.8974756	14.8974756
11	MRTEVIFP	MRTINF_pred	10.7926025	10.7926025
12	MRTEVIFP	MRTINF_pred	10.6195388	10.6195388

B Session Information

```
devtools::session_info()
```

```
##  setting  value
##  version  R version 3.4.4 (2018-03-15)
##  system   x86_64, mingw32
##  ui       RTerm
```

```
##  language en
##  collate  Korean_Korea.949
##  tz       Asia/Seoul
##  date     2018-03-20
##
##  package     * version    date       source
##  assertthat    0.2.0      2017-04-11 CRAN (R 3.4.0)
##  backports     1.1.2      2017-12-13 CRAN (R 3.4.3)
##  base        * 3.4.4      2018-03-15 local
##  bindr         0.1.1      2018-03-13 CRAN (R 3.4.3)
##  bindrcpp    * 0.2.0.9000 2018-02-08 Github (krlmlr/bindrcpp@7553d4f)
##  bookdown      0.7        2018-02-18 CRAN (R 3.4.3)
##  colorspace    1.3-2      2016-12-14 CRAN (R 3.4.0)
##  compiler      3.4.4      2018-03-15 local
##  datasets    * 3.4.4      2018-03-15 local
##  devtools      1.13.5     2018-02-18 CRAN (R 3.4.3)
##  digest        0.6.15     2018-01-28 CRAN (R 3.4.3)
##  dplyr       * 0.7.4.9000 2018-02-08 Github (tidyverse/dplyr@0a2c208)
##  evaluate      0.10.1     2017-06-24 CRAN (R 3.4.1)
##  glue          1.2.0      2017-10-29 CRAN (R 3.4.2)
##  graphics    * 3.4.4      2018-03-15 local
##  grDevices   * 3.4.4      2018-03-15 local
##  hms           0.4.2      2018-03-10 CRAN (R 3.4.3)
##  htmltools     0.3.6      2017-04-28 CRAN (R 3.4.0)
##  httr          1.3.1      2017-08-20 CRAN (R 3.4.1)
##  kableExtra  * 0.7.0      2018-01-15 CRAN (R 3.4.3)
##  knitr       * 1.20       2018-02-20 CRAN (R 3.4.3)
##  magrittr      1.5        2014-11-22 CRAN (R 3.4.0)
##  memoise       1.1.0      2017-04-21 CRAN (R 3.4.0)
##  methods     * 3.4.4      2018-03-15 local
##  munsell       0.4.3      2016-02-13 CRAN (R 3.4.0)
##  NonCompart  * 0.4.1      2018-03-19 CRAN (R 3.4.4)
##  pillar        1.2.1      2018-02-27 CRAN (R 3.4.3)
##  pkgconfig     2.0.1      2017-03-21 CRAN (R 3.4.0)
##  plyr          1.8.4      2016-06-08 CRAN (R 3.4.0)
##  purrr         0.2.4.9000 2018-03-02 Github (tidyverse/purrr@84ce1ad)
##  R6            2.2.2      2017-06-17 CRAN (R 3.4.1)
##  Rcpp          0.12.16    2018-03-13 CRAN (R 3.4.4)
##  readr         1.1.1      2017-05-16 CRAN (R 3.4.0)
##  rlang         0.2.0      2018-02-20 CRAN (R 3.4.3)
##  rmarkdown     1.9        2018-03-01 CRAN (R 3.4.3)
##  rprojroot     1.3-2      2018-01-03 CRAN (R 3.4.3)
##  rvest         0.3.2      2016-06-17 CRAN (R 3.4.0)
##  scales        0.5.0      2017-08-24 CRAN (R 3.4.1)
##  stats       * 3.4.4      2018-03-15 local
##  stringi       1.1.7      2018-03-12 CRAN (R 3.4.4)
##  stringr       1.3.0      2018-02-19 CRAN (R 3.4.3)
##  tibble        1.4.2      2018-01-22 CRAN (R 3.4.3)
##  tidyr       * 0.8.0      2018-01-29 CRAN (R 3.4.3)
##  tidyselect    0.2.4      2018-02-26 CRAN (R 3.4.3)
##  tools         3.4.4      2018-03-15 local
##  utils       * 3.4.4      2018-03-15 local
##  viridisLite   0.3.0      2018-02-01 CRAN (R 3.4.3)
##  withr         2.1.2      2018-03-15 CRAN (R 3.4.4)
```

```
##  xfun          0.1        2018-01-22 CRAN (R 3.4.3)
##  xml2          1.2.0      2018-01-24 CRAN (R 3.4.3)
##  yaml          2.1.18     2018-03-08 CRAN (R 3.4.3)
```

References

Bae, Kyun-Seop. 2018. *NonCompart: Noncompartmental Analysis for Pharmacokinetic Data.* https://CRAN.R-project.org/package=NonCompart.