Supplementary Material

Modeling Pharmacokinetics in Individual Patients Using Therapeutic Drug Monitoring and Artificial Population Quasi-Models: A Study with Piperacillin

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1. Source code for modeling using Pmetrics:

```
Library(Pmetrics)


# Run 1 - 1-compt, no covariate

pipdata <- PM_data$new(data = "data.csv")

pipmodel.onecompt.1 <- PM_model$new("model.txt")

pip.onecompt.1 <- PM_fit$new(model = pipmodel.onecompt.1, data =
pipdata)

pip.onecompt.1$run(cycles=5000)


# Run 2 - 2-compt, no covariate

pipmodel.twocompt.1 <- PM_model$new("model.txt")

pip.twocompt.1 <- PM_fit$new(model = pipmodel.twocompt.1, data =
pipdata)

pip.twocompt.1$run(cycles=5000)


# Run 3 - 1-compt, covariate: CRCL

pipmodel.onecompt.cov.1 <- PM_model$new("model.txt")

pip.onecompt.cov.1 <- PM_fit$new(model = pipmodel.onecompt.cov.1,
data = pipdata)

pip.onecompt.cov.1$run(cycles=5000)


# Run 4 - 2-compt, covariate: CRCL

pipmodel.twocompt.cov.1 <- PM_model$new("model.txt")

pip.twocompt.cov.1 <- PM_fit$new(model = pipmodel.twocompt.cov.1,
data = pipdata)

pip.twocompt.cov.1$run(cycles=5000)
```

```
# Evaluation of models

pip.subj=NULL

pip.1ct.data = PM_load(1)

pip.1ct.sum=pip.1ct.data$op$summary(pred.type =
"post",icen="median")

pip.1ct.post = pip.1ct.data$final$data$postMed # posteriors

pip.1ct.supp = pip.1ct.data$final$popPoints # support points

pip.1ct.stat=subset(pip.1ct.data$op$data,pip.1ct.data$op$data$pred.t
ype=="post"&pip.1ct.data$op$data$icen=="mean")

pip.1ct.stat.list=split(pip.1ct.stat,pip.1ct.stat$id) # list by
subject initials


pip.1ct.mse=NULL

pip.1ct.regr=data.frame(NA,NA,NA)


for (s in 1:length(pip.1ct.stat.list)) {

     pip.1ct.mse[[s]]=mean(pip.1ct.stat.list[[s]]$ds)

     pip.subj[[s]]=pip.1ct.stat.list[[s]][1,1]

     pip.1ct.regr[[s,1]]=lm(pip.1ct.stat.list[[s]]$pred~pip.1ct.stat
.list[[s]]$obs)$coefficients[[2]]

     pip.1ct.regr[[s,2]]=lm(pip.1ct.stat.list[[s]]$pred~pip.1ct.stat
.list[[s]]$obs)$coefficients[[1]]

     pip.1ct.regr[[s,3]]=cor(x=pip.1ct.stat.list[[s]]$pred,
     y=pip.1ct.stat.list[[s]]$obs, method="pearson")

}


pip.1ct.mse=unlist(pip.1ct.mse)

pip.subj=unlist(pip.subj)

pip.1ct.mse.wr=data.frame(pip.subj,pip.1ct.mse)

pip.1ct.regr=cbind(pip.subj, pip.1ct.regr)

colnames(pip.1ct.regr)=c("subject","slope","intercept","pearson r")


pip.2ct.data = PM_load(4)
```

```
pip.2ct.sum=pip.2ct.data$op$summary(pred.type =
"post",icen="median")

pip.2ct.post = pip.2ct.data$final$data$postMed # posteriors

pip.2ct.supp = pip.2ct.data$final$popPoints # support points

pip.2ct.stat=subset(pip.2ct.data$op$data,pip.2ct.data$op$data$pred.t
ype=="post"&pip.2ct.data$op$data$icen=="mean")

pip.2ct.stat.list=split(pip.2ct.stat,pip.2ct.stat$id) # list by
subject initials

pip.2ct.mse=NULL

pip.2ct.regr=data.frame(NA,NA,NA)



for (s in 1:length(pip.2ct.stat.list)) {

     pip.2ct.mse[[s]]=mean(pip.2ct.stat.list[[s]]$ds)

     pip.subj[[s]]=pip.2ct.stat.list[[s]][1,1]



     pip.2ct.regr[[s,1]]=lm(pip.2ct.stat.list[[s]]$pred~pip.2ct.stat
.list[[s]]$obs)$coefficients[[2]]


     pip.2ct.regr[[s,2]]=lm(pip.2ct.stat.list[[s]]$pred~pip.2ct.stat
.list[[s]]$obs)$coefficients[[1]]

     pip.2ct.regr[[s,3]]=cor(x=pip.2ct.stat.list[[s]]$pred,
     y=pip.2ct.stat.list[[s]]$obs, method="pearson")

  }


pip.2ct.mse=unlist(pip.2ct.mse)

pip.subj=unlist(pip.subj)

pip.2ct.mse.wr=data.frame(pip.subj,pip.2ct.mse)

pip.2ct.regr=cbind(pip.subj, pip.2ct.regr)

colnames(pip.2ct.regr)=c("subject","slope","intercept","pearson r")


pip.1ct.crcl.data = PM_load(3)

pip.1ct.crcl.sum=pip.1ct.crcl.data$op$summary(pred.type =
"post",icen="median")
```

```
pip.1ct.crcl.post = pip.1ct.crcl.data$final$data$postMed #
posteriors

pip.1ct.crcl.supp = pip.1ct.crcl.data$final$popPoints # support
points

pip.1ct.crcl.stat=subset(pip.1ct.crcl.data$op$data,pip.1ct.crcl.data
$op$data$pred.type=="post"&pip.1ct.crcl.data$op$data$icen=="mean")

pip.1ct.crcl.stat.list=split(pip.1ct.crcl.stat,pip.1ct.crcl.stat$id)
# list by subject initials

pip.1ct.crcl.mse=NULL

pip.1ct.crcl.regr=data.frame(NA,NA,NA)


for (s in 1:length(pip.1ct.crcl.stat.list)) {

     pip.1ct.crcl.mse[[s]]=mean(pip.1ct.crcl.stat.list[[s]]$ds)

     pip.subj[[s]]=pip.1ct.crcl.stat.list[[s]][1,1]

     pip.1ct.crcl.regr[[s,1]]=lm(pip.1ct.crcl.stat.list[[s]]$pred~pi
p.1ct.crcl.stat.list[[s]]$obs)$coefficients[[2]]

     pip.1ct.crcl.regr[[s,2]]=lm(pip.1ct.crcl.stat.list[[s]]$pred~pi
p.1ct.crcl.stat.list[[s]]$obs)$coefficients[[1]]


     pip.1ct.crcl.regr[[s,3]]=cor(x=pip.1ct.crcl.stat.list[[s]]$pred
, y=pip.1ct.crcl.stat.list[[s]]$obs, method="pearson")

}


pip.1ct.crcl.mse=unlist(pip.1ct.crcl.mse)

pip.subj=unlist(pip.subj)

pip.1ct.crcl.mse.wr=data.frame(pip.subj,pip.1ct.crcl.mse)

pip.1ct.crcl.regr=cbind(pip.subj, pip.1ct.crcl.regr)

colnames(pip.1ct.crcl.regr)=c("subject","slope","intercept","pearson
r")


pip.2ct.crcl.data = PM_load(4)

pip.2ct.crcl.sum=pip.2ct.crcl.data$op$summary(pred.type =
"post",icen="median")

pip.2ct.crcl.post = pip.2ct.crcl.data$final$data$postMed #
posteriors

pip.2ct.crcl.supp = pip.2ct.crcl.data$final$popPoints # support
points
```

```
pip.2ct.crcl.stat=subset(pip.2ct.crcl.data$op$data,pip.2ct.crcl.data
$op$data$pred.type=="post"&pip.2ct.crcl.data$op$data$icen=="mean")

pip.2ct.crcl.stat.list=split(pip.2ct.crcl.stat,pip.2ct.crcl.stat$id)
# list by subject initials

pip.2ct.crcl.mse=NULL

pip.2ct.crcl.regr=data.frame(NA,NA,NA)


for (s in 1:length(pip.2ct.crcl.stat.list)) {

     pip.2ct.crcl.mse[[s]]=mean(pip.2ct.crcl.stat.list[[s]]$ds)

     pip.subj[[s]]=pip.2ct.crcl.stat.list[[s]][1,1]

     pip.2ct.crcl.regr[[s,1]]=lm(pip.2ct.crcl.stat.list[[s]]$pred~pi
p.2ct.crcl.stat.list[[s]]$obs)$coefficients[[2]]

     pip.2ct.crcl.regr[[s,2]]=lm(pip.2ct.crcl.stat.list[[s]]$pred~pi
p.2ct.crcl.stat.list[[s]]$obs)$coefficients[[1]]

pip.2ct.crcl.regr[[s,3]]=cor(x=pip.2ct.crcl.stat.list[[s]]$pred,
y=pip.2ct.crcl.stat.list[[s]]$obs, method="pearson")

}


pip.2ct.crcl.mse=unlist(pip.2ct.crcl.mse)

pip.subj=unlist(pip.subj)

pip.2ct.crcl.mse.wr=data.frame(pip.subj,pip.2ct.crcl.mse)

pip.2ct.crcl.regr=cbind(pip.subj, pip.2ct.crcl.regr)

colnames(pip.2ct.crcl.regr)=c("subject","slope","intercept","pearson
r")


comps=PM_compare(pip.1ct.data,pip.2ct.data,pip.1ct.crcl.data,pip.2ct
.crcl.data, icen="median")

comp.2ct=PM_compare(pip.2ct.data,pip.2ct.crcl.data, icen="median")


write.csv(pip.1ct.post,file="onecompt-posts.csv")

write.csv(pip.2ct.post,file="twocompt-posts.csv")

write.csv(pip.1ct.crcl.post,file="onecompt-crcl-posts.csv")

write.csv(pip.2ct.crcl.post,file="twocompt-crcl-posts.csv")


write.csv(pip.1ct.supp,file="onecompt-suppoints.csv")
```

```
write.csv(pip.2ct.supp,file="twocompt-suppoints.csv")
write.csv(pip.1ct.crcl.supp,file="onecompt-crcl-suppoints.csv")
write.csv(pip.2ct.crcl.supp,file="twocompt-crcl-suppoints.csv")

write.csv(pip.1ct.mse.wr,file="onecompt-mse.csv")
write.csv(pip.2ct.mse.wr,file="twocompt-mse.csv")
write.csv(pip.1ct.crcl.mse.wr,file="onecompt-crcl-mse.csv")
write.csv(pip.2ct.crcl.mse.wr,file="twocompt-crcl-mse.csv")
```

2. Final model files used for nonparametric adaptive grid population pharmacokinetic modeling

- **One compartment, no covariate**

```
#pri
Ke, 0.100000, 0.750000
V, 10.000000, 100.000000

#out
Y(1)=X(1)/V

#err
L=0.100000
0.255000,0.049873,-0.000361,0.000001
```

- **Two compartments, no covariate**

```
#pri
Ke, 0.100000, 1.700000
KPC, 0.050000, 5.000000
KCP, 0.050000, 5.000000
V, 5.000000, 35.000000

#out
Y(1)=X(1)/V

#err
L=0.100000
0.255000,0.049873,-0.000361,0.000001
```

- **One compartment, creatinine clearance covariate**

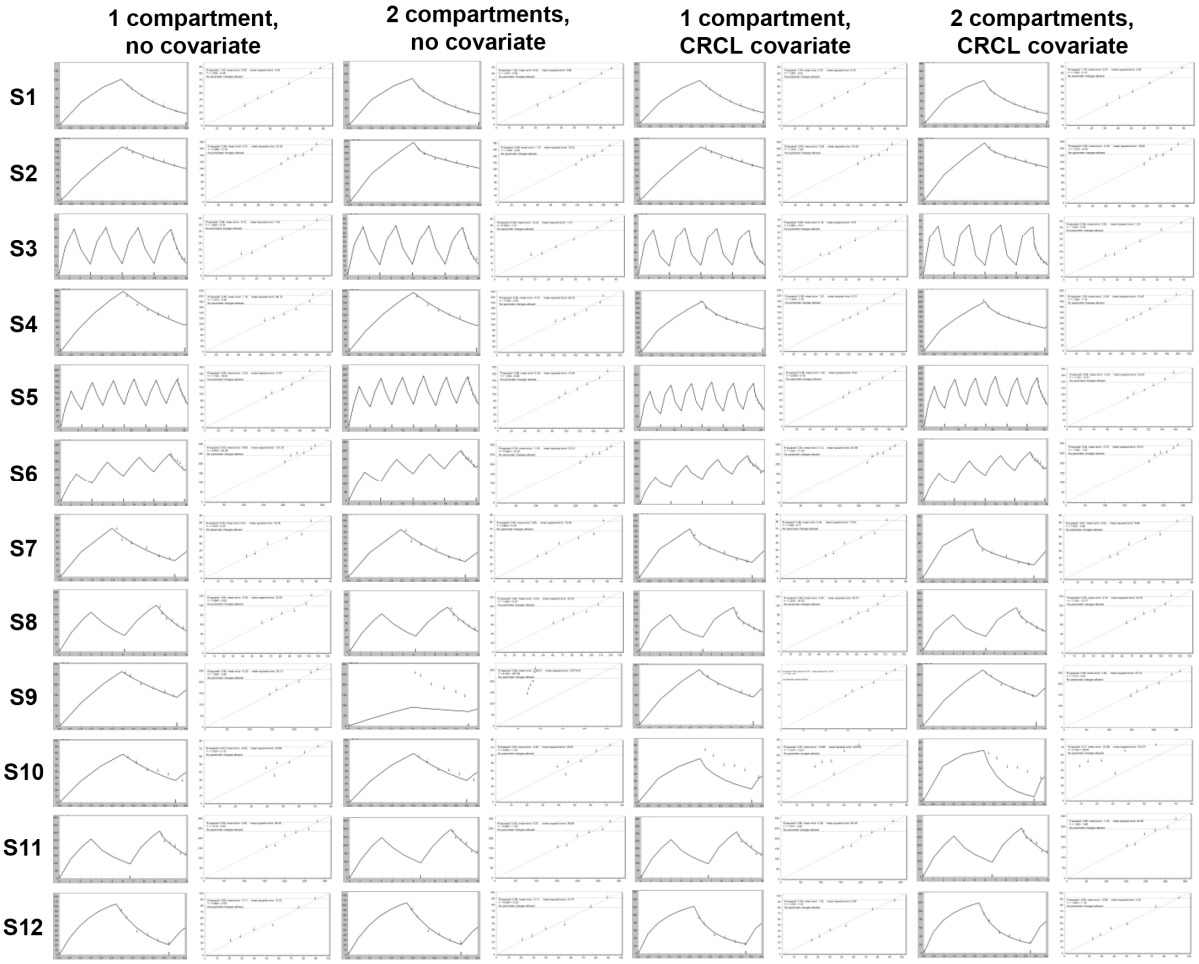
```
#pri
K, 0.001000, 0.006000
```

```
Ki, 0.005000, 0.100000
V, 15.000000, 80.000000

#cov
CRCL

#sec
Ke=K*CRCL+Ki

#out
Y(1)=X(1)/V

#err
L=0.100000
0.255000,0.049873,-0.000361,0.000001
```

- **Two compartments, creatinine clearance covariate**

```
#pri
K, 0.000500, 0.025000
Ki, 0.000000, 0.350000
V, 5.000000, 25.000000
KCP, 0.200000, 6.000000
KPC, 0.200000, 6.000000

#cov
CRCL

#sec
Ke=K*CRCL+Ki

#out
Y(1)=X(1)/V

#err
L=0.100000
0.255000,0.049873,-0.000361,0.000001
```

3. Supplementary Figure



Supplementary Figure S1. Individual concentration-time curves obtained when applying the best-performing quasi-models to the observed piperacillin concentrations. Each row shows the curves fitted, along with the correlation plots of the observed and predicted concentrations for a Subject (S1-S12). The horizontal and vertical axes of the fitted curve plots represent time (h) and piperacillin concentration (μmol/L), respectively. The origin (time=0 h) corresponds to the time of the initiation of treatment with piperacillin/tazobactam. The axes of the correlation plots are predicted and observed piperacillin concentrations (μmol/L). CRCL, creatinine clearance.

4. Supplementary tables.

Supplementary table S1. Coefficients of correlation between the values of the covariates tested, and the pharmacokinetic variables modeled. K, elimination rate constant. KCP, rate constant of the mass transfer from the central to the peripheral compartmetnt. KPC, rate constant of the mass transfer from the peripheral to the central compartment. V, Volume of distribution. V_c, volume of the central compartment.

Candidate covariate	Correlation coefficient					
	Single-compartment model		Two-compartment model			
	K	V	K	KPC	KCP	V_c
Serum sodium concentration	0.0637	0.0664	-0.0384	0.0895	0.0491	0.0281
Serum potassium concentration	0.5696	0.2672	0.3140	-0.2399	-0.2959	0.1741
Serum glucose concentration	-0.2127	0.1090	-0.0297	-0.2184	-0.2325	-0.0199
Serum creatinine concentration	-0.5330	-0.3787	-0.6435	0.7017	0.0507	0.2462
Serum urea concentration	-0.6462	-0.3014	-0.6294	0.7233	0.2409	0.2153
Serum total bilirubin concentration	-0.3739	-0.5302	-0.5920	0.7229	0.3923	0.0462
White blood cell count	0.2698	0.4800	0.7408	-0.4525	-0.0700	-0.1677
Platelet count	0.3196	0.1956	0.3921	-0.1077	0.1767	-0.1307
Hematocrit	0.2567	-0.0512	0.2007	-0.0058	0.2053	-0.1175
Serum procalcitonin concentration	-0.1020	-0.0974	-0.0801	-0.1923	-0.1568	-0.1217
Serum C-reactive protein concentration	0.0011	0.2121	0.2909	-0.0819	0.2523	-0.0362
Serum interleukin-6 concentration	-0.1067	-0.1398	0.0921	-0.2615	-0.1315	-0.3063
Serum cortisol concentration	-0.1809	-0.2432	-0.1134	0.1785	0.0597	-0.1148
Serum cortisone concentration	0.3626	-0.1841	0.0851	0.2288	-0.0723	0.0044
Serum 11-deoxycortisol concentration	-0.1059	-0.0985	-0.0451	-0.2089	-0.1494	-0.1556
Serum corticosterone concentration	-0.1096	-0.1329	0.0391	-0.1937	-0.1030	-0.2311
Creatinine renal clearance	0.8622	0.5002	0.8037	-0.4033	-0.0723	0.0693

Supplementary tables S2-S13. Performance of the fully artificial population quasi-models generated for describing the pharmacokinetics of piperacillin. K, elimination rate constant (models without a covariate). KCP, rate constant of mass transfer from the central to the peripheral compartment. KI, nonrenal component of the elimination rate constant. KPC, coefficient of mass transfer from the peripheral to the central compartment. KS, renal component of the elimination rate constant (models with a covariate). R^2, determination coefficient. MAP Bayesian, maximum a posteriori probability Bayesian analysis. MSE, mean squared error. NPAG, nonparametric adaptive grid modeling. Pop-PK, population pharmacokinetic model. V, apparent volume of distribution. V_c, apparent volume of the central compartment.

Supplementary table S2: Performance of the quasi-models for Subject 1

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.461	41.950	0.999	0.554
Pop-PK, MAP Bayesian	0.458	42.152	0.999	0.539
Quasi-model 1	0.437	45.560	0.999	0.579
Quasi-model 2	0.430	46.200	0.999	4.436
Quasi-model 3	0.478	41.672	0.999	0.629
Quasi-model 4	0.463	42.377	0.999	0.780
Quasi-model 5	0.476	40.436	0.999	1.203
Quasi-model 6	0.446	42.587	0.999	0.840
Quasi-model 7	0.444	43.791	0.999	1.349
Quasi-model 8	0.473	41.556	0.999	0.681
Quasi-model 9	0.450	42.835	0.999	0.598
Quasi-model 10	0.450	43.185	0.999	0.721
Quasi-model 11	0.439	43.036	0.999	2.624
Quasi-model 12	0.471	39.900	0.999	5.343
Quasi-model 13	0.462	41.661	0.999	1.299
Quasi-model 14	0.482	39.654	0.999	2.334
Quasi-model 15	0.438	42.484	0.999	0.538
Quasi-model 16	0.462	42.226	0.999	0.696
Quasi-model 17	0.438	44.408	0.999	1.312
Quasi-model 18	0.441	44.299	0.999	1.296
Quasi-model 19	0.419	45.958	0.999	1.970
Quasi-model 20	0.459	42.126	0.999	0.566
Quasi-model 21	0.429	45.285	0.999	1.586
Quasi-model 22	0.439	44.775	0.999	2.497
Quasi-model 23	0.448	43.615	0.999	1.141
Quasi-model 24	0.445	42.984	0.999	1.285
Quasi-model 25	0.451	43.652	0.999	1.864
Quasi-model 26	0.441	43.012	0.999	2.318
Quasi-model 27	0.497	38.990	0.998	3.270
Quasi-model 28	0.458	42.133	0.999	0.594

Quasi-model 29	0.453	43.137	0.999	0.944
Quasi-model 30	0.471	41.987	0.999	2.233

Model #2: Two compartments, no covariate

Model	K	KCP	KPC	V	R^2	MSE
Pop-PK, NPAG	1.287	4.663	2.982	13.492	0.999	0.508
Pop-PK, MAP Bayesian	2.982	1.287	4.663	13.492	0.999	0.508
Quasi-model 1	0.928	3.693	3.278	18.801	0.998	8.441
Quasi-model 2	0.965	3.283	3.835	20.179	0.998	1.116
Quasi-model 3	0.634	0.929	2.234	28.268	0.998	2.196
Quasi-model 4	0.826	2.359	3.622	19.802	0.998	3.422
Quasi-model 5	0.779	2.867	3.502	21.162	0.999	5.415
Quasi-model 6	1.101	3.884	3.367	15.593	0.999	11.075
Quasi-model 7	1.270	3.169	2.301	13.139	0.998	0.891
Quasi-model 8	0.725	2.218	2.803	25.357	0.998	2.915
Quasi-model 9	0.982	1.600	2.575	17.846	0.998	2.249
Quasi-model 10	0.672	1.349	3.873	26.125	0.998	3.204
Quasi-model 11	0.756	1.103	3.846	20.776	0.998	9.276
Quasi-model 12	0.797	1.659	2.907	24.150	0.997	2.566
Quasi-model 13	0.837	2.691	4.135	20.470	0.999	12.678
Quasi-model 14	0.756	2.018	2.804	23.538	0.998	0.812
Quasi-model 15	0.843	1.948	3.852	23.771	0.998	14.606
Quasi-model 16	0.974	2.797	3.093	18.894	0.998	5.690
Quasi-model 17	0.960	3.284	3.846	23.299	0.998	1.610
Quasi-model 18	0.877	1.410	2.688	19.595	0.998	2.152
Quasi-model 19	0.777	1.331	2.455	25.639	0.998	1.183
Quasi-model 20	0.783	2.855	3.493	21.156	0.999	6.011
Quasi-model 21	1.245	3.760	2.483	11.444	0.998	4.241
Quasi-model 22	1.266	3.181	2.393	12.972	0.998	0.974
Quasi-model 23	0.724	1.199	2.273	25.383	0.998	1.807
Quasi-model 24	0.641	1.354	2.719	28.709	0.998	0.867
Quasi-model 25	0.668	1.244	3.865	26.230	0.998	3.043
Quasi-model 26	0.941	3.804	3.779	18.436	0.999	6.105
Quasi-model 27	1.115	2.495	2.517	16.340	0.998	11.435
Quasi-model 28	0.881	2.411	2.628	18.750	0.998	2.530
Quasi-model 29	0.631	1.347	3.245	28.384	0.999	0.679
Quasi-model 30	1.077	2.833	2.600	15.362	0.998	21.561

Model #3: One compartment, covariate: creatinine clearance

Model	KS	KI	V_c	R^2	MSE
Pop-PK, NPAG	0.003	0.011	42.715	0.999	1.097
Pop-PK, MAP Bayesian	0.003	0.011	42.305	0.999	0.536
Quasi-model 1	0.003	0.037	39.970	0.999	1.949
Quasi-model 2	0.003	0.059	37.068	0.998	12.316

Quasi-model 3	0.003	0.096	37.729	0.998	5.686
Quasi-model 4	0.003	0.009	39.583	0.999	1.110
Quasi-model 5	0.003	0.076	44.806	0.999	3.356
Quasi-model 6	0.003	0.055	41.820	0.999	0.579
Quasi-model 7	0.003	0.097	41.570	0.999	1.439
Quasi-model 8	0.003	0.040	37.363	0.998	6.056
Quasi-model 9	0.003	0.022	43.628	0.999	0.811
Quasi-model 10	0.003	0.027	38.822	0.999	1.593
Quasi-model 11	0.003	0.028	40.104	0.999	1.816
Quasi-model 12	0.003	0.058	42.824	0.999	1.214
Quasi-model 13	0.003	0.029	42.144	0.999	1.002
Quasi-model 14	0.003	0.027	43.054	0.999	1.271
Quasi-model 15	0.003	0.074	43.158	0.999	1.183
Quasi-model 16	0.003	0.059	42.495	0.999	0.688
Quasi-model 17	0.003	0.062	42.850	0.999	0.550
Quasi-model 18	0.003	0.087	40.113	0.999	2.523
Quasi-model 19	0.003	0.048	41.281	0.999	0.950
Quasi-model 20	0.003	0.059	42.592	0.999	0.534
Quasi-model 21	0.003	0.093	43.235	0.999	2.516
Quasi-model 22	0.003	0.060	41.274	0.999	1.350
Quasi-model 23	0.002	0.065	48.180	0.999	6.872
Quasi-model 24	0.003	0.069	42.011	0.999	0.714
Quasi-model 25	0.003	0.043	44.254	0.999	2.476
Quasi-model 26	0.003	0.081	41.875	0.999	1.965
Quasi-model 27	0.003	0.070	42.252	0.999	2.036
Quasi-model 28	0.003	0.250	42.445	0.999	1.317
Quasi-model 29	0.003	0.072	44.226	0.999	1.191
Quasi-model 30	0.003	0.660	41.555	0.999	0.748

Model #4: Two compartments, covariate: creatinine clearance

Model	**KS**	**KCP**	**KPC**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.004	4.057	5.739	0.306	23.100	0.999	0.536
Pop-PK, MAP Bayesian	0.004	4.031	5.771	0.305	23.213	0.999	1.045
Quasi-model 1	0.004	2.162	2.773	0.118	23.046	0.999	1.396
Quasi-model 2	0.004	1.785	3.043	0.241	23.355	0.999	4.229
Quasi-model 3	0.004	1.816	3.178	0.334	22.270	0.999	2.269
Quasi-model 4	0.007	5.095	5.492	0.048	17.023	0.999	78.540
Quasi-model 5	0.004	4.329	5.514	0.227	20.874	0.999	29.530
Quasi-model 6	0.007	4.288	3.644	0.120	15.178	0.999	4.764
Quasi-model 7	0.005	2.701	4.783	0.041	23.481	0.999	6.970
Quasi-model 8	0.007	1.784	1.593	0.111	14.273	0.997	18.588
Quasi-model 9	0.006	3.452	2.835	0.115	18.603	0.999	0.860
Quasi-model 10	0.005	4.498	4.406	0.268	19.227	0.999	8.833
Quasi-model 11	0.005	3.729	4.272	0.206	21.661	0.999	7.773
Quasi-model 12	0.006	5.064	5.252	0.238	19.932	0.999	1.564
Quasi-model 13	0.006	2.592	2.253	0.185	20.866	0.999	1.701

Quasi-model 14	0.010	3.832	2.156	0.301	8.846	0.998	83.857
Quasi-model 15	0.006	4.312	3.532	0.263	17.411	0.999	8.206
Quasi-model 16	0.004	1.340	1.679	0.244	19.240	0.997	2.758
Quasi-model 17	0.004	4.648	5.289	0.318	23.783	0.998	4.375
Quasi-model 18	0.005	2.939	3.499	0.184	19.644	0.998	20.566
Quasi-model 19	0.006	3.539	3.698	0.139	21.156	0.999	1.055
Quasi-model 20	0.009	2.524	1.546	0.126	13.562	0.996	3.275
Quasi-model 21	0.006	4.236	3.825	0.114	19.557	0.999	9.238
Quasi-model 22	0.006	3.058	2.578	0.154	18.146	0.998	2.978
Quasi-model 23	0.004	2.737	3.262	0.256	22.370	0.999	0.764
Quasi-model 24	0.006	4.338	4.038	0.129	19.652	0.999	6.677
Quasi-model 25	0.005	2.738	2.752	0.259	19.620	0.999	0.963
Quasi-model 26	0.005	3.174	3.589	0.098	22.797	0.999	2.245
Quasi-model 27	0.006	1.770	1.974	0.197	16.605	0.998	16.036
Quasi-model 28	0.005	4.461	3.706	0.237	19.322	0.999	0.629
Quasi-model 29	0.007	3.780	3.442	0.245	18.187	0.998	7.369
Quasi-model 30	0.007	4.272	3.705	0.246	17.381	0.999	38.327

Supplementary table S3: Performance of the quasi-models for Subject 2

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.162	35.678	0.969	22.774
Pop-PK, MAP	0.165	35.289	0.938	22.597
Quasi-model 1	0.144	33.199	0.938	22.597
Quasi-model 2	0.169	36.902	0.938	47.374
Quasi-model 3	0.154	36.368	0.938	49.029
Quasi-model 4	0.163	35.190	0.938	25.111
Quasi-model 5	0.161	34.959	0.938	23.008
Quasi-model 6	0.173	33.185	0.938	31.119
Quasi-model 7	0.156	38.177	0.938	36.506
Quasi-model 8	0.174	37.787	0.938	26.485
Quasi-model 9	0.171	35.846	0.939	79.781
Quasi-model 10	0.162	35.520	0.938	23.738
Quasi-model 11	0.180	32.406	0.938	41.174
Quasi-model 12	0.156	36.063	0.939	156.513
Quasi-model 13	0.169	38.058	0.938	27.033
Quasi-model 14	0.158	35.181	0.938	116.942
Quasi-model 15	0.175	37.496	0.938	30.457
Quasi-model 16	0.161	37.216	0.938	52.015
Quasi-model 17	0.157	35.854	0.938	38.286
Quasi-model 18	0.163	34.373	0.938	40.993
Quasi-model 19	0.164	38.261	0.938	27.527
Quasi-model 20	0.178	34.271	0.938	128.264
Quasi-model 21	0.158	39.229	0.939	35.384
Quasi-model 22	0.168	32.539	0.938	77.567
Quasi-model 23	0.169	36.699	0.938	45.675
Quasi-model 24	0.168	36.511	0.938	22.552
Quasi-model 25	0.165	35.682	0.938	25.347
Quasi-model 26	0.058	37.036	0.938	26.730
Quasi-model 27	0.160	33.939	0.938	44.798
Quasi-model 28	0.154	38.564	0.938	30.223
Quasi-model 29	0.168	34.714	0.938	27.238
Quasi-model 30	0.166	35.611	0.938	24.184

Model #2: Two compartments, no covariate

Model	K	KCP	KPC	V	R^2	MSE
Pop-PK, NPAG	1.292	4.678	2.995	13.550	0.985	0.508
Pop-PK, MAP Bayesian	1.287	4.663	2.982	13.492	0.964	16.332
Quasi-model 1	0.339	3.805	3.425	16.118	0.954	55.386
Quasi-model 2	0.360	2.551	2.674	13.973	0.966	51.596
Quasi-model 3	0.270	2.945	2.773	19.548	0.954	75.722
Quasi-model 4	0.229	2.058	4.336	23.488	0.948	32.384
Quasi-model 5	0.337	2.903	2.184	15.357	0.960	32.789

Quasi-model 6	0.303	2.524	1.768	16.315	0.961	16.941
Quasi-model 7	0.319	3.210	2.144	15.931	0.956	25.224
Quasi-model 8	0.273	2.403	2.208	16.587	0.960	20.884
Quasi-model 9	0.291	2.751	3.204	16.472	0.962	227.949
Quasi-model 10	0.326	3.525	2.353	14.151	0.958	43.970
Quasi-model 11	0.312	3.174	2.233	14.482	0.966	45.001
Quasi-model 12	0.270	2.661	2.721	17.956	0.956	19.998
Quasi-model 13	0.252	3.148	3.159	20.226	0.958	47.325
Quasi-model 14	0.348	3.659	2.675	15.586	0.964	15.219
Quasi-model 15	0.252	3.536	4.394	21.920	0.952	30.874
Quasi-model 16	0.335	4.506	3.137	16.008	0.956	80.099
Quasi-model 17	0.353	3.527	1.827	14.174	0.964	65.168
Quasi-model 18	0.283	2.78	2.180	15.229	0.958	56.027
Quasi-model 19	0.247	3.262	4.415	21.589	0.948	44.119
Quasi-model 20	0.346	2.903	2.182	15.345	0.959	20.913
Quasi-model 21	0.303	2.525	1.955	16.590	0.960	26.090
Quasi-model 22	0.261	3.188	2.829	17.767	0.953	29.699
Quasi-model 23	0.274	2.571	3.082	16.561	0.956	20.516
Quasi-model 24	0.286	2.756	3.237	17.924	0.961	265.71
Quasi-model 25	0.272	2.433	3.237	22.292	0.959	318.759
Quasi-model 26	0.286	3.012	1.755	14.321	0.962	62.512
Quasi-model 27	0.285	2.69	3.076	17.929	0.951	25.184
Quasi-model 28	0.286	3.102	3.304	18.316	0.958	65.133
Quasi-model 29	0.247	3.262	4.415	21.589	0.948	44.119
Quasi-model 30	0.272	3.014	3.235	17.634	0.951	89.276

Model #3: One compartment, covariate: creatinine clearance

Model	**KS**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.001	0.054	35.475	0.969	22.530
Pop-PK, MAP Bayesian	0.001	0.054	35.449	0.938	22.564
Quasi-model 1	0.002	0.017	32.503	0.938	110.179
Quasi-model 2	0.001	0.06	32.842	0.938	29.271
Quasi-model 3	0.002	0.042	33.010	0.938	73.226
Quasi-model 4	0.001	0.063	37.996	0.938	76.828
Quasi-model 5	0.002	0.021	37.956	0.938	48.021
Quasi-model 6	0.002	0.041	34.701	0.938	51.483
Quasi-model 7	0.002	0.037	33.617	0.938	67.574
Quasi-model 8	0.002	0.033	35.870	0.938	35.730
Quasi-model 9	0.002	0.041	34.914	0.938	24.769
Quasi-model 10	0.001	0.054	31.457	0.938	123.65
Quasi-model 11	0.001	0.076	37.356	0.938	23.565
Quasi-model 12	0.001	0.045	36.624	0.938	41.761
Quasi-model 13	0.002	0.025	32.816	0.938	42.695
Quasi-model 14	0.001	0.059	37.399	0.938	22.853
Quasi-model 15	0.001	0.044	34.216	0.938	37.701
Quasi-model 16	0.001	0.058	34.990	0.938	41.866

Quasi-model 17	0.002	0.028	37.158	0.938	64.372
Quasi-model 18	0.002	0.038	33.073	0.938	65.665
Quasi-model 19	0.002	0.044	35.424	0.938	25.573
Quasi-model 20	0.002	0.013	32.029	0.938	253.216
Quasi-model 21	0.001	0.064	33.307	0.938	40.453
Quasi-model 22	0.002	0.049	38.053	0.938	44.842
Quasi-model 23	0.002	0.04	38.323	0.938	45.101
Quasi-model 24	0.001	0.053	40.584	0.938	214.218
Quasi-model 25	0.002	0.045	33.557	0.938	23.568
Quasi-model 26	0.002	0.046	38.011	0.938	30.580
Quasi-model 27	0.002	0.056	34.010	0.938	32.331
Quasi-model 28	0.002	0.52	35.402	0.938	50.117
Quasi-model 29	0.001	0.081	34.733	0.938	24.320
Quasi-model 30	0.001	0.048	36.134	0.938	23.489

Model #4: Two compartments, covariate: creatinine clearance

Model	**KS**	**KCP**	**KPC**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.007	4.405	1.157	0.201	6.300	0.986	10.245
Pop-PK, MAP Bayesian	0.007	4.398	1.144	0.200	6.303	0.972	10.328
Quasi-model 1	0.002	4.963	2.945	0.155	11.105	0.952	70.987
Quasi-model 2	0.002	3.358	5.881	0.083	20.999	0.943	266.620
Quasi-model 3	0.002	3.980	3.410	0.158	18.613	0.950	27.805
Quasi-model 4	0.001	2.605	2.394	0.175	17.639	0.959	100.505
Quasi-model 5	0.002	5.313	5.626	0.146	16.227	0.946	270.863
Quasi-model 6	0.003	4.114	4.194	0.076	20.590	0.949	184.376
Quasi-model 7	0.002	4.314	3.839	0.153	18.524	0.957	46.081
Quasi-model 8	0.003	2.801	1.834	0.180	13.867	0.960	40.052
Quasi-model 9	0.003	3.800	3.935	0.050	18.593	0.949	125.268
Quasi-model 10	0.002	3.921	3.080	0.118	18.009	0.962	152.032
Quasi-model 11	0.003	3.631	2.203	0.130	12.166	0.957	60.456
Quasi-model 12	0.003	4.123	3.806	0.078	16.880	0.954	35.214
Quasi-model 13	0.003	4.386	2.526	0.123	16.047	0.959	199.367
Quasi-model 14	0.003	3.903	2.885	0.135	13.045	0.954	83.213
Quasi-model 15	0.002	3.993	2.179	0.193	20.058	0.954	57.918
Quasi-model 16	0.003	2.990	3.153	0.080	20.138	0.955	114.024
Quasi-model 17	0.001	3.906	1.680	0.204	16.134	0.960	16.599
Quasi-model 18	0.003	4.675	3.644	0.158	18.128	0.956	168.955
Quasi-model 19	0.003	3.892	2.884	0.140	21.547	0.958	23.92
Quasi-model 20	0.003	4.312	2.804	0.208	14.872	0.955	71.574
Quasi-model 21	0.003	4.800	5.511	0.035	18.554	0.945	54.664
Quasi-model 22	0.002	4.002	1.938	0.249	13.879	0.960	87.428
Quasi-model 23	0.001	4.276	2.298	0.202	17.760	0.959	130.169
Quasi-model 24	0.002	4.480	3.128	0.165	17.306	0.951	24.091
Quasi-model 25	0.003	2.492	2.663	0.077	17.791	0.955	63.028
Quasi-model 26	0.003	4.593	3.714	0.079	16.473	0.950	74.783
Quasi-model 27	0.003	4.342	3.488	0.154	16.953	0.957	32.449

Quasi-model 28	0.003	4.144	3.909	0.085	15.519	0.956	45.901
Quasi-model 29	0.003	2.865	3.254	0.059	18.562	0.952	34.382
Quasi-model 30	0.005	4.810	2.470	0.158	11.095	0.957	105.791

Supplementary table S4: Performance of the quasi-models for Subject 3

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.474	91.450	0.987	2.317
Pop-PK, MAP	0.476	92.001	0.984	6.067
Quasi-model 1	0.461	89.607	0.982	2.238
Quasi-model 2	0.470	90.449	0.983	1.949
Quasi-model 3	0.481	82.046	0.984	2.294
Quasi-model 4	0.483	83.816	0.984	1.704
Quasi-model 5	0.454	89.465	0.984	1.724
Quasi-model 6	0.512	78.904	0.986	1.740
Quasi-model 7	0.480	84.732	0.983	1.782
Quasi-model 8	0.487	83.046	0.985	1.639
Quasi-model 9	0.486	83.262	0.984	1.668
Quasi-model 10	0.475	84.334	0.983	1.820
Quasi-model 11	0.480	83.990	0.984	1.675
Quasi-model 12	0.494	81.344	0.984	1.657
Quasi-model 13	0.451	91.323	0.983	2.029
Quasi-model 14	0.454	92.637	0.983	2.105
Quasi-model 15	0.478	85.830	0.984	1.623
Quasi-model 16	0.453	91.849	0.982	2.276
Quasi-model 17	0.470	87.035	0.984	1.800
Quasi-model 18	0.463	87.917	0.983	1.817
Quasi-model 19	0.482	83.777	0.984	1.738
Quasi-model 20	0.466	90.453	0.984	1.789
Quasi-model 21	0.458	88.865	0.983	2.070
Quasi-model 22	0.485	85.101	0.984	1.685
Quasi-model 23	0.466	89.013	0.983	2.257
Quasi-model 24	0.450	93.472	0.982	2.399
Quasi-model 25	0.454	91.701	0.983	2.127
Quasi-model 26	0.460	90.304	0.983	1.917
Quasi-model 27	0.470	84.822	0.984	1.684
Quasi-model 28	0.500	79.364	0.985	1.626
Quasi-model 29	0.459	91.201	0.983	1.978
Quasi-model 30	0.464	85.779	0.984	1.703

Model #2: Two compartments, no covariate

Model	K	KCP	KPC	V	R^2	MSE
Pop-PK, NPAG	1.356	1.263	0.718	23.750	0.997	8.441
Pop-PK, MAP Bayesian	1.360	1.282	0.719	23.853	0.986	5.530

Quasi-model 1	1.236	3.145	1.622	27.474	0.991	1.800
Quasi-model 2	1.204	2.626	2.008	31.969	0.987	3.801
Quasi-model 3	1.140	1.987	1.886	31.165	0.987	1.783
Quasi-model 4	1.253	1.882	1.419	23.788	0.992	6.220
Quasi-model 5	1.267	2.483	1.539	28.146	0.989	1.479
Quasi-model 6	1.376	2.932	1.852	26.581	0.989	1.715
Quasi-model 7	1.205	3.117	2.102	33.801	0.985	6.858
Quasi-model 8	1.079	2.460	2.104	31.573	0.988	3.686
Quasi-model 9	1.062	1.878	1.738	32.105	0.988	2.131
Quasi-model 10	1.434	3.538	1.952	27.547	0.986	3.412
Quasi-model 11	1.185	1.349	0.817	24.079	0.992	0.920
Quasi-model 12	1.316	1.237	0.983	24.066	0.992	2.307
Quasi-model 13	1.407	3.838	2.064	27.801	0.989	1.553
Quasi-model 14	1.174	3.736	2.259	29.337	0.988	7.468
Quasi-model 15	1.210	2.005	1.447	29.446	0.990	1.922
Quasi-model 16	1.240	2.151	1.383	25.735	0.991	2.419
Quasi-model 17	1.237	1.817	1.775	27.038	0.990	1.682
Quasi-model 18	1.137	1.982	1.887	31.240	0.987	1.540
Quasi-model 19	1.302	2.332	1.803	27.301	0.989	2.430
Quasi-model 20	1.268	2.799	1.933	28.163	0.987	1.705
Quasi-model 21	1.313	2.934	1.860	26.586	0.989	1.412
Quasi-model 22	1.190	3.123	2.113	33.777	0.985	5.164
Quasi-model 23	1.259	2.764	2.074	28.195	0.987	1.824
Quasi-model 24	1.384	3.608	2.268	27.569	0.986	1.812
Quasi-model 25	1.435	3.520	1.940	26.895	0.988	2.440
Quasi-model 26	1.248	3.419	2.008	29.059	0.988	1.217
Quasi-model 27	1.197	3.862	1.870	28.681	0.993	0.755
Quasi-model 28	1.332	3.287	2.187	27.393	0.987	2.134
Quasi-model 29	1.430	2.473	1.369	26.282	0.99	2.702
Quasi-model 30	1.216	2.612	2.201	29.627	0.989	1.163

Model #3: One compartment, covariate: creatinine clearance

Model	**KS**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.004	0.022	72.525	0.990	4.721
Pop-PK, MAP Bayesian	0.004	0.022	72.608	0.990	5.930
Quasi-model 1	0.003	0.016	78.576	0.986	1.953
Quasi-model 2	0.003	0.018	77.008	0.987	1.917
Quasi-model 3	0.003	0.066	74.390	0.986	3.815
Quasi-model 4	0.003	0.086	73.844	0.987	2.253
Quasi-model 5	0.003	0.065	79.137	0.985	2.258
Quasi-model 6	0.003	0.055	75.168	0.987	2.207
Quasi-model 7	0.003	0.015	78.107	0.986	2.092
Quasi-model 8	0.003	0.071	73.997	0.987	2.229
Quasi-model 9	0.003	0.076	72.904	0.987	2.760
Quasi-model 10	0.003	0.017	78.528	0.986	1.756
Quasi-model 11	0.003	0.045	78.020	0.986	2.876

Quasi-model 12	0.003	0.073	76.698	0.986	2.134
Quasi-model 13	0.003	0.086	75.113	0.987	2.066
Quasi-model 14	0.003	0.038	74.868	0.988	2.320
Quasi-model 15	0.003	0.078	79.764	0.986	1.727
Quasi-model 16	0.003	0.059	80.031	0.986	2.045
Quasi-model 17	0.003	0.031	76.413	0.987	1.926
Quasi-model 18	0.003	0.027	75.678	0.987	2.147
Quasi-model 19	0.003	0.082	75.270	0.987	2.083
Quasi-model 20	0.003	0.018	76.956	0.986	2.045
Quasi-model 21	0.003	0.024	78.633	0.986	1.905
Quasi-model 22	0.003	0.028	71.143	0.987	4.298
Quasi-model 23	0.003	0.062	78.368	0.986	1.770
Quasi-model 24	0.003	0.090	74.923	0.986	2.775
Quasi-model 25	0.003	0.074	78.269	0.986	2.285
Quasi-model 26	0.003	0.053	77.809	0.986	2.121
Quasi-model 27	0.003	0.073	76.735	0.987	1.998
Quasi-model 28	0.003	0.087	75.819	0.986	3.062
Quasi-model 29	0.003	0.012	77.417	0.986	1.989
Quasi-model 30	0.003	0.096	77.643	0.986	1.888

Model #4: Two compartments, covariate: creatinine clearance

Model	**KS**	**KCP**	**KPC**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.010	1.679	0.751	0.222	17.100	0.997	0.603
Pop-PK, MAP Bayesian	0.010	1.703	0.755	0.222	17.132	0.989	1.733
Quasi-model 1	0.009	3.917	1.923	0.229	20.842	0.990	13.678
Quasi-model 2	0.013	2.834	1.374	0.08	15.025	0.990	1.256
Quasi-model 3	0.01	1.282	0.76	0.343	13.680	0.987	7.555
Quasi-model 4	0.009	3.162	1.464	0.112	20.206	0.992	5.846
Quasi-model 5	0.008	1.452	0.092	0.288	16.691	0.991	11.324
Quasi-model 6	0.011	2.388	1.045	0.149	16.744	0.989	8.551
Quasi-model 7	0.013	1.084	0.550	0.175	9.765	0.978	16.063
Quasi-model 8	0.010	4.493	1.563	0.183	20.605	0.989	1.286
Quasi-model 9	0.015	3.745	1.638	0.192	13.544	0.989	6.612
Quasi-model 10	0.007	3.005	1.788	0.336	24.893	0.987	1.801
Quasi-model 11	0.011	4.511	1.495	0.158	20.617	0.989	2.478
Quasi-model 12	0.009	4.408	2.036	0.292	23.484	0.986	3.349
Quasi-model 13	0.009	1.147	0.815	0.039	18.808	0.990	4.236
Quasi-model 14	0.010	5.238	1.844	0.253	20.063	0.986	1.879
Quasi-model 15	0.011	1.738	0.956	0.020	19.679	0.988	4.105
Quasi-model 16	0.011	3.598	1.596	0.064	19.977	0.988	7.132
Quasi-model 17	0.008	2.618	1.553	0.296	22.582	0.989	2.714
Quasi-model 18	0.009	3.365	1.436	0.146	22.287	0.989	2.739
Quasi-model 19	0.014	2.930	1.077	0.284	12.765	0.988	1.830
Quasi-model 20	0.012	3.079	1.230	0.169	13.076	0.989	8.693
Quasi-model 21	0.010	2.962	0.967	0.170	21.292	0.989	1.196
Quasi-model 22	0.009	2.146	1.001	0.009	19.502	0.993	10.474

Quasi-model 23	0.010	1.379	0.790	0.283	13.746	0.989	15.076
Quasi-model 24	0.009	1.942	0.940	0.201	20.221	0.989	1.607
Quasi-model 25	0.009	2.644	1.408	0.209	22.548	0.989	2.302
Quasi-model 26	0.010	4.394	1.342	0.217	21.345	0.990	5.602
Quasi-model 27	0.013	4.052	1.276	0.057	16.367	0.988	1.754
Quasi-model 28	0.010	2.370	1.139	0.275	20.511	0.990	1.352
Quasi-model 29	0.016	2.819	1.005	0.119	9.349	0.989	5.352
Quasi-model 30	0.011	4.456	1.589	0.174	19.170	0.988	4.812

Supplementary table S5: Performance of the quasi-models for Subject 4

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.272	26.650	0.984	36.060
Pop-PK, MAP	0.273	26.255	0.939	101.22
Quasi-model 1	0.268	28.396	0.938	71.117
Quasi-model 2	0.259	32.883	0.937	304.078
Quasi-model 3	0.279	26.564	0.940	131.192
Quasi-model 4	0.271	28.638	0.939	118.108
Quasi-model 5	0.286	26.488	0.941	91.942
Quasi-model 6	0.276	29.649	0.939	238.243
Quasi-model 7	0.273	28.075	0.939	159.972
Quasi-model 8	0.283	28.618	0.940	109.114
Quasi-model 9	0.266	29.921	0.939	157.863
Quasi-model 10	0.276	29.716	0.939	193.094
Quasi-model 11	0.276	28.866	0.940	87.607
Quasi-model 12	0.272	27.526	0.938	71.739
Quasi-model 13	0.284	25.140	0.939	72.167
Quasi-model 14	0.267	28.829	0.939	78.059
Quasi-model 15	0.290	27.995	0.941	116.547
Quasi-model 16	0.266	27.716	0.938	77.563
Quasi-model 17	0.268	30.310	0.938	244.136
Quasi-model 18	0.290	29.988	0.940	110.571
Quasi-model 19	0.254	28.255	0.937	129.064
Quasi-model 20	0.284	27.348	0.941	66.147
Quasi-model 21	0.290	29.618	0.940	177.571
Quasi-model 22	0.270	27.571	0.939	75.959
Quasi-model 23	0.268	26.334	0.939	200.753
Quasi-model 24	0.261	30.449	0.939	257.478
Quasi-model 25	0.271	30.019	0.939	120.036
Quasi-model 26	0.278	30.482	0.939	208.885
Quasi-model 27	0.272	26.544	0.939	87.027
Quasi-model 28	0.269	28.143	0.939	80.276
Quasi-model 29	0.288	28.909	0.941	193.378
Quasi-model 30	0.281	25.781	0.940	199.467

Model #2: Two compartments, no covariate

Model	K	KCP	KPC	V	R^2	MSE
Pop-PK, NPAG	0.428	0.966	0.867	12.95	1.000	1.116
Pop-PK, MAP Bayesian	0.454	1.838	1.411	11.060	0.994	1434.563
Quasi-model 1	0.521	3.837	2.134	9.934	0.997	177.345
Quasi-model 2	0.469	2.156	1.362	10.780	0.994	33.283
Quasi-model 3	0.573	3.975	2.836	11.512	0.987	288.82
Quasi-model 4	0.482	2.787	2.545	15.576	0.992	42.556
Quasi-model 5	0.497	1.594	1.562	14.041	0.993	20.523
Quasi-model 6	0.442	1.379	1.564	14.871	0.989	22.169
Quasi-model 7	0.416	1.212	1.104	13.371	0.994	70.384
Quasi-model 8	0.591	2.951	1.275	13.543	0.998	360.764
Quasi-model 9	0.374	1.341	1.455	13.190	0.992	629.852
Quasi-model 10	0.472	2.282	2.646	16.211	0.990	398.170
Quasi-model 11	0.385	1.923	2.316	16.546	0.978	334.610
Quasi-model 12	0.700	2.982	1.082	10.238	0.998	36.567
Quasi-model 13	0.483	2.925	3.223	13.230	0.986	70.965
Quasi-model 14	0.357	2.141	1.575	14.042	0.995	42.072
Quasi-model 15	0.57	2.738	1.736	12.755	0.992	20.030
Quasi-model 16	0.521	2.088	1.551	12.001	0.996	47.791
Quasi-model 17	0.567	3.100	1.545	10.167	0.995	9.096
Quasi-model 18	0.530	3.985	2.831	11.489	0.992	138.501
Quasi-model 19	0.481	2.564	2.569	15.567	0.987	23.439
Quasi-model 20	0.498	1.582	1.556	14.054	0.994	23.695
Quasi-model 21	0.439	1.380	1.565	14.875	0.989	20.764
Quasi-model 22	0.416	1.206	1.116	13.266	0.994	79.353
Quasi-model 23	0.591	3.264	1.288	13.546	0.998	373.423
Quasi-model 24	0.404	1.506	1.685	14.967	0.990	268.341
Quasi-model 25	0.471	2.295	2.639	13.750	0.989	157.614
Quasi-model 26	0.430	1.715	2.192	15.047	0.985	86.466
Quasi-model 27	0.425	3.098	3.314	14.478	0.977	65.843
Quasi-model 28	0.238	0.572	0.488	19.163	0.990	72.704
Quasi-model 29	0.404	2.113	2.171	11.990	0.989	81.648
Quasi-model 30	0.488	1.768	1.039	12.580	0.997	128.298

Model #3: One compartment, covariate: creatinine clearance

Model	KS	KI	V_c	R^2	MSE
Pop-PK, NPAG	0.003	0.027	26.375	0.984	35.757
Pop-PK, MAP Bayesian	0.003	0.027	26.225	0.939	100.592
Quasi-model 1	0.003	0.060	28.983	0.939	89.518
Quasi-model 2	0.002	0.048	27.770	0.941	110.379
Quasi-model 3	0.003	0.059	27.318	0.940	67.853
Quasi-model 4	0.003	0.045	26.135	0.940	82.869
Quasi-model 5	0.003	0.074	26.643	0.941	76.017
Quasi-model 6	0.003	0.081	27.027	0.941	65.318
Quasi-model 7	0.003	0.034	28.422	0.939	84.036

Quasi-model 8	0.003	0.023	29.055	0.940	152.749
Quasi-model 9	0.003	0.045	27.216	0.938	72.328
Quasi-model 10	0.003	0.048	27.513	0.940	107.703
Quasi-model 11	0.003	0.046	27.307	0.940	100.119
Quasi-model 12	0.003	0.054	30.371	0.940	109.210
Quasi-model 13	0.003	0.044	27.892	0.940	101.274
Quasi-model 14	0.003	0.901	30.312	0.939	198.963
Quasi-model 15	0.003	0.058	28.544	0.940	167.230
Quasi-model 16	0.003	0.043	30.074	0.938	159.524
Quasi-model 17	0.003	0.047	27.757	0.939	84.826
Quasi-model 18	0.003	0.069	27.877	0.940	100.184
Quasi-model 19	0.003	0.062	26.170	0.939	72.858
Quasi-model 20	0.003	0.053	25.835	0.941	68.281
Quasi-model 21	0.002	0.098	28.958	0.939	124.591
Quasi-model 22	0.003	0.034	28.909	0.940	67.671
Quasi-model 23	0.003	0.061	27.912	0.940	102.970
Quasi-model 24	0.003	0.058	28.854	0.939	106.295
Quasi-model 25	0.003	0.075	31.053	0.938	262.235
Quasi-model 26	0.003	0.043	28.190	0.940	72.171
Quasi-model 27	0.003	0.070	27.356	0.939	69.345
Quasi-model 28	0.003	0.058	29.637	0.939	133.678
Quasi-model 29	0.003	0.037	29.374	0.940	109.575
Quasi-model 30	0.003	0.077	28.309	0.940	73.815

Model #4: Two compartments, covariate: creatinine clearance

Model	**KS**	**KCP**	**KPC**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.009	2.375	1.041	0.180	6.900	0.999	2.772
Pop-PK, MAP Bayesian	0.007	4.395	1.146	0.200	6.313	0.990	151.068
Quasi-model 1	0.008	4.850	3.155	0.170	9.067	0.991	345.149
Quasi-model 2	0.006	3.193	1.981	0.237	12.751	0.993	57.430
Quasi-model 3	0.003	3.625	3.504	0.153	13.221	0.975	220.867
Quasi-model 4	0.003	2.736	2.239	0.286	10.268	0.994	274.017
Quasi-model 5	0.003	3.052	2.152	0.095	15.211	0.987	149.965
Quasi-model 6	0.004	3.240	2.019	0.241	13.120	0.990	48.408
Quasi-model 7	0.004	1.491	1.238	0.207	12.191	0.996	34.988
Quasi-model 8	0.009	3.001	1.590	0.013	10.470	0.997	56.405
Quasi-model 9	0.004	3.87	2.486	0.181	11.023	0.986	124.68
Quasi-model 10	0.005	1.915	1.847	0.053	13.444	0.990	31.199
Quasi-model 11	0.007	3.925	1.988	0.177	10.810	0.996	13.452
Quasi-model 12	0.001	1.166	1.553	0.306	15.882	0.986	20.044
Quasi-model 13	0.002	2.771	3.591	0.247	13.760	0.977	175.738
Quasi-model 14	0.004	2.335	2.550	0.145	14.835	0.988	22.226
Quasi-model 15	0.003	2.893	2.795	0.218	14.892	0.981	56.153
Quasi-model 16	0.004	2.071	1.861	0.144	12.190	0.989	288.210
Quasi-model 17	0.004	2.154	1.887	0.128	12.560	0.992	81.225
Quasi-model 18	0.004	1.871	2.371	0.178	16.418	0.984	59.429

Quasi-model 19	0.003	1.077	1.236	0.142	13.470	0.988	860.981
Quasi-model 20	0.006	3.507	2.315	0.166	10.295	0.996	84.763
Quasi-model 21	0.006	4.105	2.300	0.073	10.827	0.991	405.058
Quasi-model 22	0.003	1.636	2.011	0.190	14.451	0.988	290.924
Quasi-model 23	0.006	2.749	1.657	0.124	9.723	0.995	45.009
Quasi-model 24	0.004	1.136	0.903	0.144	15.660	0.994	276.014
Quasi-model 25	0.004	1.350	1.659	0.207	17.544	0.991	15.733
Quasi-model 26	0.005	2.588	1.601	0.113	11.186	0.997	98.008
Quasi-model 27	0.004	2.264	1.778	0.055	13.148	0.992	72.788
Quasi-model 28	0.007	4.541	2.238	0.205	10.722	0.995	20.486
Quasi-model 29	0.003	4.686	5.265	0.222	13.625	0.979	363.393
Quasi-model 30	0.002	1.233	1.271	0.260	15.320	0.993	20.060

Supplementary table S6: Performance of the quasi-models for Subject 5

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.272	37.450	0.991	13.523
Pop-PK, MAP	0.276	37.093	0.982	13.386
Quasi-model 1	0.241	43.447	0.98	31.829
Quasi-model 2	0.259	40.664	0.981	27.391
Quasi-model 3	0.261	41.444	0.981	42.235
Quasi-model 4	0.278	38.216	0.982	28.478
Quasi-model 5	0.284	34.600	0.982	19.969
Quasi-model 6	0.329	31.392	0.984	39.915
Quasi-model 7	0.324	31.560	0.984	22.123
Quasi-model 8	0.289	35.061	0.982	15.065
Quasi-model 9	0.247	43.113	0.981	14.631
Quasi-model 10	0.269	38.894	0.982	18.737
Quasi-model 11	0.256	38.088	0.98	50.876
Quasi-model 12	0.266	38.270	0.981	14.362
Quasi-model 13	0.305	34.536	0.983	29.327
Quasi-model 14	0.265	38.734	0.981	15.066
Quasi-model 15	0.229	45.445	0.979	33.753
Quasi-model 16	0.312	32.763	0.984	23.709
Quasi-model 17	0.301	32.309	0.983	64.636
Quasi-model 18	0.267	38.728	0.981	15.632
Quasi-model 19	0.288	35.495	0.982	14.644
Quasi-model 20	0.749	99.849	0.979	67.223
Quasi-model 21	0.262	39.629	0.981	16.207
Quasi-model 22	0.301	32.341	0.983	66.004
Quasi-model 23	0.288	35.491	0.982	14.49
Quasi-model 24	0.284	36.943	0.982	20.465
Quasi-model 25	0.243	41.753	0.98	24.581
Quasi-model 26	0.254	39.814	0.981	17.548
Quasi-model 27	0.324	31.506	0.984	27.805
Quasi-model 28	0.315	32.308	0.983	19.241

Quasi-model 29	0.268	38.342	0.981	14.681
Quasi-model 30	0.290	33.477	0.982	15.012

Model #2: Two compartments, no covariate

Model	K	KCP	KPC	V	R^2	MSE
Pop-PK, NPAG	0.748	1.906	1.065	12.05	0.998	2.196
Pop-PK, MAP Bayesian	0.745	1.883	1.085	12.039	0.995	3.557
Quasi-model 1	0.669	3.668	2.097	15.963	0.989	30.629
Quasi-model 2	0.699	3.868	2.486	14.215	0.987	20.513
Quasi-model 3	0.541	1.030	0.887	17.357	0.993	6.822
Quasi-model 4	0.528	2.781	3.245	16.751	0.989	23.12
Quasi-model 5	0.588	3.138	2.501	17.421	0.986	32.766
Quasi-model 6	0.444	2.315	4.044	22.292	0.99	23.108
Quasi-model 7	0.486	1.759	2.140	19.214	0.987	27.305
Quasi-model 8	0.441	2.503	3.603	22.292	0.987	12.049
Quasi-model 9	0.449	3.103	4.774	24.328	0.983	112.095
Quasi-model 10	0.641	2.819	1.540	15.505	0.993	55.511
Quasi-model 11	0.404	2.184	3.410	24.322	0.986	22.510
Quasi-model 12	0.741	2.478	1.496	12.377	0.995	8.027
Quasi-model 13	0.741	3.689	2.290	13.420	0.990	39.204
Quasi-model 14	0.339	0.756	2.208	29.366	0.987	21.405
Quasi-model 15	0.492	2.588	3.288	18.893	0.987	16.103
Quasi-model 16	0.712	3.658	2.099	14.718	0.989	23.919
Quasi-model 17	0.688	3.977	2.495	14.270	0.985	15.565
Quasi-model 18	0.508	1.743	2.501	19.080	0.992	5.975
Quasi-model 19	0.574	2.920	3.252	19.226	0.989	14.742
Quasi-model 20	0.587	3.130	2.497	17.429	0.986	37.192
Quasi-model 21	0.441	2.313	4.044	22.297	0.990	21.123
Quasi-model 22	0.485	1.748	2.143	19.283	0.987	15.108
Quasi-model 23	0.44	2.503	3.589	22.298	0.987	12.468
Quasi-model 24	0.451	3.621	3.768	24.286	0.983	138.902
Quasi-model 25	0.639	2.826	1.569	15.546	0.992	58.993
Quasi-model 26	0.430	0.675	0.779	21.874	0.993	5.292
Quasi-model 27	0.479	3.377	3.128	21.261	0.985	83.252
Quasi-model 28	0.477	2.018	1.840	21.648	0.990	56.173
Quasi-model 29	0.545	4.333	4.057	19.156	0.984	52.471
Quasi-model 30	0.506	2.158	2.106	20.049	0.988	37.232

Model #3: One compartment, covariate: creatinine clearance

Model	KS	KI	V_c	R^2	MSE
Pop-PK, NPAG	0.004	0.096	36.775	0.991	13.498
Pop-PK, MAP Bayesian	0.004	0.096	36.503	0.982	13.435
Quasi-model 1	0.004	0.084	36.695	0.982	13.509
Quasi-model 2	0.004	0.087	35.247	0.982	14.299

Quasi-model 3	0.004	0.070	40.651	0.981	15.377
Quasi-model 4	0.003	0.098	43.134	0.980	24.080
Quasi-model 5	0.005	0.049	36.791	0.982	13.593
Quasi-model 6	0.004	0.082	34.268	0.982	15.006
Quasi-model 7	0.005	0.018	35.899	0.982	14.365
Quasi-model 8	0.005	0.055	35.445	0.982	13.305
Quasi-model 9	0.004	0.082	37.044	0.982	13.484
Quasi-model 10	0.005	0.041	36.854	0.982	16.240
Quasi-model 11	0.004	0.074	37.402	0.982	14.896
Quasi-model 12	0.004	0.184	39.915	0.981	15.866
Quasi-model 13	0.005	0.021	36.651	0.982	13.346
Quasi-model 14	0.004	0.031	39.164	0.981	14.009
Quasi-model 15	0.005	0.020	39.394	0.981	18.806
Quasi-model 16	0.005	0.027	35.886	0.982	13.737
Quasi-model 17	0.005	0.071	35.592	0.982	14.921
Quasi-model 18	0.005	0.032	34.675	0.983	16.370
Quasi-model 19	0.005	0.048	38.372	0.981	14.578
Quasi-model 20	0.003	0.097	38.685	0.981	13.920
Quasi-model 21	0.005	0.053	34.847	0.983	15.383
Quasi-model 22	0.003	0.087	36.639	0.981	15.840
Quasi-model 23	0.004	0.061	39.344	0.981	21.607
Quasi-model 24	0.005	0.020	37.724	0.982	13.555
Quasi-model 25	0.004	0.062	35.741	0.982	19.907
Quasi-model 26	0.004	0.098	37.213	0.982	13.477
Quasi-model 27	0.005	0.036	37.307	0.982	13.516
Quasi-model 28	0.004	0.067	38.411	0.981	14.572
Quasi-model 29	0.003	0.092	41.728	0.980	23.205
Quasi-model 30	0.005	0.007	40.736	0.981	27.077

Model #4: Two compartments, covariate: creatinine clearance

Model	**KS**	**KCP**	**KPC**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.014	2.375	1.099	0.212	9.900	0.998	3.321
Pop-PK, MAP Bayesian	0.014	2.385	1.093	0.211	9.827	0.995	4.272
Quasi-model 1	0.007	2.790	3.097	0.226	18.247	0.985	79.112
Quasi-model 2	0.009	3.135	2.703	0.175	18.023	0.989	10.961
Quasi-model 3	0.007	3.958	3.443	0.145	21.966	0.983	20.953
Quasi-model 4	0.008	2.830	2.814	0.227	20.188	0.993	5.968
Quasi-model 5	0.010	3.666	2.051	0.124	15.751	0.99	31.248
Quasi-model 6	0.010	5.048	3.13	0.139	15.351	0.985	39.013
Quasi-model 7	0.007	4.226	4.101	0.162	20.614	0.986	16.744
Quasi-model 8	0.003	2.473	2.384	0.335	19.038	0.985	15.612
Quasi-model 9	0.011	3.813	2.063	0.106	16.476	0.987	23.050
Quasi-model 10	0.006	4.108	2.567	0.307	17.584	0.985	21.175
Quasi-model 11	0.008	2.031	1.995	0.118	18.710	0.988	38.798
Quasi-model 12	0.011	4.195	2.804	0.166	15.762	0.968	11.775
Quasi-model 13	0.008	3.596	2.368	0.185	17.477	0.989	17.494

Quasi-model 14	0.008	4.757	4.276	0.123	21.208	0.982	119.62
Quasi-model 15	0.009	3.714	2.115	0.096	15.053	0.989	40.202
Quasi-model 16	0.004	1.338	1.685	0.294	19.241	0.989	15.409
Quasi-model 17	0.008	4.426	3.943	0.150	17.987	0.986	41.253
Quasi-model 18	0.007	2.627	2.739	0.121	18.818	0.986	94.956
Quasi-model 19	0.005	2.994	3.475	0.238	21.165	0.985	36.229
Quasi-model 20	0.013	3.634	1.862	0.207	12.597	0.990	19.157
Quasi-model 21	0.007	3.963	3.236	0.122	20.111	0.988	19.966
Quasi-model 22	0.008	4.932	3.952	0.152	16.173	0.985	27.756
Quasi-model 23	0.008	2.742	3.267	0.217	22.360	0.984	31.997
Quasi-model 24	0.012	3.120	2.391	0.159	13.294	0.990	62.133
Quasi-model 25	0.006	3.556	4.105	0.269	19.596	0.985	15.464
Quasi-model 26	0.010	4.536	3.064	0.178	14.088	0.985	24.234
Quasi-model 27	0.009	4.008	2.690	0.225	15.683	0.986	21.684
Quasi-model 28	0.005	3.783	2.200	0.235	19.356	0.988	28.555
Quasi-model 29	0.007	2.814	1.487	0.296	14.979	0.990	20.875
Quasi-model 30	0.007	3.782	3.227	0.260	18.919	0.986	13.797

Supplementary table S7: Performance of the quasi-models for Subject 6

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.129	38.35	0.968	45.317
Pop-PK, MAP	0.128	38.538	0.935	48.281
Quasi-model 1	0.122	39.807	0.936	49.163
Quasi-model 2	0.107	46.602	0.936	225.889
Quasi-model 3	0.118	40.116	0.936	69.622
Quasi-model 4	0.121	41.008	0.936	79.005
Quasi-model 5	0.156	32.727	0.934	72.591
Quasi-model 6	0.105	46.462	0.936	104.960
Quasi-model 7	0.152	33.333	0.935	67.003
Quasi-model 8	0.187	29.076	0.933	252.746
Quasi-model 9	0.136	35.951	0.935	64.245
Quasi-model 10	0.145	35.439	0.935	63.187
Quasi-model 11	0.180	27.586	0.933	211.478
Quasi-model 12	0.143	36.112	0.935	127.302
Quasi-model 13	0.120	43.737	0.936	342.101
Quasi-model 14	0.139	36.451	0.935	72.985
Quasi-model 15	0.150	34.486	0.935	73.008
Quasi-model 16	0.180	28.182	0.933	140.035
Quasi-model 17	0.162	31.848	0.934	104.782
Quasi-model 18	0.122	40.115	0.936	51.145
Quasi-model 19	0.121	41.193	0.935	70.073
Quasi-model 20	0.121	37.553	0.936	249.717
Quasi-model 21	0.146	36.418	0.935	272.057
Quasi-model 22	0.131	40.000	0.935	63.023

Quasi-model 23	0.130	37.117	0.936	50.216
Quasi-model 24	0.178	28.729	0.934	118.164
Quasi-model 25	0.106	46.060	0.936	99.051
Quasi-model 26	0.157	31.458	0.934	153.182
Quasi-model 27	0.143	34.687	0.935	67.861
Quasi-model 28	0.128	38.951	0.935	64.144
Quasi-model 29	0.139	37.007	0.935	88.566
Quasi-model 30	0.130	36.494	0.935	209.178

Model #2: Two compartments, no covariate

Model	**K**	**KCP**	**KPC**	**V**	**R^2**	**MSE**
Pop-PK, NPAG	0.204	2.500	4.777	24.050	0.968	45.728
Pop-PK, MAP Bayesian	0.204	2.504	4.792	24.042	0.936	50.773
Quasi-model 1	0.319	2.205	2.288	16.035	0.937	158.016
Quasi-model 2	0.470	2.164	1.283	9.843	0.935	94.458
Quasi-model 3	0.254	2.963	4.266	20.309	0.937	52.552
Quasi-model 4	0.222	2.066	4.341	23.369	0.936	118.055
Quasi-model 5	0.211	3.053	2.863	21.910	0.938	75.657
Quasi-model 6	0.160	1.053	4.175	31.169	0.937	47.349
Quasi-model 7	0.318	3.697	2.256	15.966	0.938	60.548
Quasi-model 8	0.233	2.392	3.842	21.913	0.937	81.124
Quasi-model 9	0.331	2.346	3.207	14.015	0.937	173.002
Quasi-model 10	0.193	2.331	0.547	27.863	0.931	51.615
Quasi-model 11	0.159	0.498	3.013	31.341	0.937	54.124
Quasi-model 12	0.271	2.665	2.715	17.946	0.937	46.657
Quasi-model 13	0.251	3.215	3.161	20.182	0.936	57.740
Quasi-model 14	0.345	3.680	2.689	15.664	0.938	187.323
Quasi-model 15	0.346	1.844	1.740	13.854	0.936	158.478
Quasi-model 16	0.334	4.509	3.126	14.924	0.937	95.392
Quasi-model 17	0.351	3.524	1.799	14.176	0.937	82.048
Quasi-model 18	0.463	4.270	1.810	10.148	0.939	60.628
Quasi-model 19	0.252	3.788	4.421	19.438	0.936	47.772
Quasi-model 20	0.211	3.073	2.858	21.918	0.938	67.938
Quasi-model 21	0.158	1.054	4.177	31.162	0.937	48.389
Quasi-model 22	0.223	2.695	3.755	21.738	0.937	48.326
Quasi-model 23	0.233	2.392	3.855	21.912	0.937	83.004
Quasi-model 24	0.331	2.345	3.227	14.015	0.937	172.843
Quasi-model 25	0.146	0.380	0.507	29.240	0.923	56.522
Quasi-model 26	0.236	1.734	1.612	19.422	0.938	63.684
Quasi-model 27	0.287	2.691	3.072	17.894	0.937	126.656
Quasi-model 28	0.213	1.097	2.150	23.413	0.936	73.842
Quasi-model 29	0.194	2.527	3.025	25.023	0.938	73.125
Quasi-model 30	0.346	4.603	3.014	14.055	0.936	172.926

Model #3: One compartment, covariate: creatinine clearance

Model	KS	KI	V_c	R^2	MSE
Pop-PK, NPAG	0.004	0.017	36.798	0.968	47.115
Pop-PK, MAP Bayesian	0.004	0.017	36.769	0.935	48.476
Quasi-model 1	0.003	0.04	39.952	0.935	48.594
Quasi-model 2	0.002	0.067	37.622	0.935	47.667
Quasi-model 3	0.005	0.012	36.878	0.935	48.273
Quasi-model 4	0.003	0.063	35.662	0.935	49.477
Quasi-model 5	0.003	0.049	37.569	0.935	48.077
Quasi-model 6	0.004	0.033	34.312	0.935	58.788
Quasi-model 7	0.004	0.015	39.319	0.935	51.642
Quasi-model 8	0.003	0.04	37.353	0.935	51.810
Quasi-model 9	0.003	0.035	37.083	0.935	55.580
Quasi-model 10	0.003	0.068	37.135	0.935	49.116
Quasi-model 11	0.002	0.062	37.795	0.935	50.202
Quasi-model 12	0.004	0.034	34.048	0.935	57.099
Quasi-model 13	0.004	0.033	35.075	0.935	52.143
Quasi-model 14	0.003	0.045	35.685	0.935	48.954
Quasi-model 15	0.002	0.064	38.637	0.935	61.942
Quasi-model 16	0.003	0.042	36.337	0.935	54.814
Quasi-model 17	0.002	0.075	38.865	0.936	48.478
Quasi-model 18	0.003	0.073	35.960	0.935	51.910
Quasi-model 19	0.003	0.076	37.833	0.935	47.589
Quasi-model 20	0.002	0.073	35.982	0.935	53.317
Quasi-model 21	0.003	0.038	36.147	0.935	50.950
Quasi-model 22	0.002	0.072	36.765	0.935	47.331
Quasi-model 23	0.004	0.029	36.582	0.935	48.941
Quasi-model 24	0.004	0.039	34.894	0.935	49.733
Quasi-model 25	0.002	0.076	36.200	0.935	54.791
Quasi-model 26	0.003	0.068	34.611	0.935	62.083
Quasi-model 27	0.004	0.038	35.709	0.935	52.683
Quasi-model 28	0.005	0.012	35.117	0.935	52.367
Quasi-model 29	0.002	0.079	36.196	0.935	142.621
Quasi-model 30	0.002	0.073	40.908	0.935	49.133

Model #4: Two compartments, covariate: creatinine clearance

Model	KS	KCP	KPC	KI	V_c	R^2	MSE
Pop-PK, NPAG	0.013	5.797	2.143	0.159	9.300	0.964	44.527
Pop-PK, MAP Bayesian	0.013	5.798	2.149	0.161	9.308	0.938	46.682
Quasi-model 1	0.011	4.182	2.689	0.121	14.421	0.937	63.638
Quasi-model 2	0.007	3.102	3.051	0.108	17.712	0.937	64.023
Quasi-model 3	0.004	2.572	3.298	0.109	19.321	0.937	61.082
Quasi-model 4	0.004	2.602	3.029	0.175	21.889	0.937	53.008
Quasi-model 5	0.002	2.377	2.610	0.144	16.826	0.936	93.821
Quasi-model 6	0.007	4.307	2.027	0.121	13.654	0.938	49.713
Quasi-model 7	0.001	2.263	4.720	0.177	23.167	0.937	56.471

Quasi-model 8	0.002	3.547	3.215	0.207	17.224	0.937	90.736
Quasi-model 9	0.006	1.760	1.972	0.116	18.276	0.937	46.923
Quasi-model 10	0.007	3.925	2.639	0.186	12.776	0.938	52.709
Quasi-model 11	0.002	2.796	5.991	0.141	23.065	0.936	147.315
Quasi-model 12	0.009	4.340	3.295	0.092	15.014	0.937	86.037
Quasi-model 13	0.009	4.175	1.863	0.097	11.058	0.937	46.938
Quasi-model 14	0.005	5.270	3.745	0.127	18.475	0.937	80.216
Quasi-model 15	0.001	4.725	5.154	0.225	20.061	0.937	48.920
Quasi-model 16	0.007	4.221	3.995	0.146	18.023	0.937	55.013
Quasi-model 17	0.007	1.450	1.672	0.063	19.569	0.935	69.714
Quasi-model 18	0.008	4.813	2.910	0.116	12.711	0.938	91.572
Quasi-model 19	0.007	3.439	5.392	0.066	21.554	0.936	55.346
Quasi-model 20	0.002	3.183	4.684	0.209	18.767	0.937	47.621
Quasi-model 21	0.008	3.064	3.473	0.066	17.093	0.936	66.364
Quasi-model 22	0.002	2.137	4.054	0.173	22.253	0.936	130.062
Quasi-model 23	0.006	2.820	3.300	0.060	18.414	0.937	52.216
Quasi-model 24	0.004	4.458	4.473	0.164	18.236	0.937	55.354
Quasi-model 25	0.004	5.046	3.489	0.209	13.130	0.936	92.622
Quasi-model 26	0.007	4.045	2.453	0.103	12.765	0.938	47.532
Quasi-model 27	0.003	4.350	4.023	0.199	20.000	0.937	56.952
Quasi-model 28	0.003	4.118	3.275	0.247	15.319	0.937	71.938
Quasi-model 29	0.004	1.531	3.950	0.107	24.394	0.936	67.269
Quasi-model 30	0.004	4.789	4.836	0.154	16.174	0.937	105.683

Supplementary table S8: Performance of the quasi-models for Subject 7

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.370	61.750	0.972	16.136
Pop-PK, MAP	0.368	61.296	0.946	16.061
Quasi-model 1	0.369	61.281	0.946	16.346
Quasi-model 2	0.375	60.379	0.946	16.102
Quasi-model 3	0.361	63.788	0.946	16.660
Quasi-model 4	0.349	65.248	0.945	17.792
Quasi-model 5	0.366	63.268	0.946	16.121
Quasi-model 6	0.385	60.202	0.946	16.500
Quasi-model 7	0.344	65.096	0.945	16.925
Quasi-model 8	0.378	61.597	0.946	17.490
Quasi-model 9	0.358	63.897	0.946	16.271
Quasi-model 10	0.372	60.699	0.946	16.244
Quasi-model 11	0.368	61.286	0.946	16.094
Quasi-model 12	0.377	61.576	0.946	16.598
Quasi-model 13	0.369	62.252	0.946	16.352
Quasi-model 14	0.360	61.233	0.946	16.857
Quasi-model 15	0.422	55.203	0.946	15.952
Quasi-model 16	0.360	63.403	0.946	16.463
Quasi-model 17	0.353	61.129	0.945	19.735

Quasi-model 18	0.378	59.905	0.946	16.242
Quasi-model 19	0.367	60.546	0.946	16.210
Quasi-model 20	0.358	62.375	0.946	16.046
Quasi-model 21	0.316	68.328	0.945	17.500
Quasi-model 22	0.358	63.528	0.946	17.301
Quasi-model 23	0.371	58.782	0.946	21.280
Quasi-model 24	0.351	64.795	0.946	17.530
Quasi-model 25	0.372	60.916	0.946	16.278
Quasi-model 26	0.340	65.831	0.945	18.326
Quasi-model 27	0.388	57.875	0.946	16.226
Quasi-model 28	0.388	64.570	0.945	17.181
Quasi-model 29	0.350	63.557	0.945	16.756
Quasi-model 30	0.392	57.988	0.947	17.298

Model #2: Two compartments, no covariate

Model	**K**	**KCP**	**KPC**	**V**	**R^2**	**MSE**
Pop-PK, NPAG	1.212	2.7	1.263	15.05	0.986	8.299
Pop-PK, MAP Bayesian	1.214	2.71	1.279	15.138	0.973	8.128
Quasi-model 1	0.871	4.626	3.002	24.667	0.957	15.684
Quasi-model 2	0.701	3.568	3.016	24.837	0.959	25.198
Quasi-model 3	0.786	3.126	2.222	29.534	0.962	17.267
Quasi-model 4	0.813	3.775	2.491	26.299	0.959	27.863
Quasi-model 5	0.907	3.708	2.549	24.884	0.962	14.395
Quasi-model 6	0.696	4.667	3.113	31.205	0.957	19.676
Quasi-model 7	0.813	4.524	3.559	27.552	0.958	23.303
Quasi-model 8	0.865	3.956	2.668	22.398	0.961	13.438
Quasi-model 9	0.801	3.483	2.858	27.630	0.958	28.607
Quasi-model 10	0.957	3.532	2.239	23.593	0.962	63.851
Quasi-model 11	0.658	3.510	3.680	29.670	0.438	13.018
Quasi-model 12	0.971	4.344	2.601	24.135	0.963	30.846
Quasi-model 13	0.694	3.404	3.665	29.088	0.958	34.910
Quasi-model 14	0.722	3.350	2.950	27.800	0.722	21.295
Quasi-model 15	0.891	3.143	2.456	26.086	0.963	23.371
Quasi-model 16	0.871	4.635	3.001	24.671	0.957	16.927
Quasi-model 17	0.788	3.566	1.995	23.205	0.96	21.467
Quasi-model 18	0.638	3.294	3.462	33.287	0.958	15.769
Quasi-model 19	0.778	3.774	3.219	28.711	0.958	30.320
Quasi-model 20	0.704	3.868	2.772	29.077	0.959	19.687
Quasi-model 21	1.329	4.412	1.772	14.169	0.964	14.376
Quasi-model 22	0.812	4.527	3.567	27.615	0.959	27.725
Quasi-model 23	0.804	3.943	2.376	25.123	0.84	16.059
Quasi-model 24	0.766	3.729	2.857	29.500	0.958	32.075
Quasi-model 25	0.953	3.516	2.247	23.664	0.959	26.056
Quasi-model 26	0.824	3.740	2.945	28.309	0.958	22.751
Quasi-model 27	0.794	4.265	2.485	25.430	0.958	26.994
Quasi-model 28	0.839	3.157	2.825	28.196	0.961	14.064

Quasi-model 29	0.79	4.117	3.230	27.730	0.955	32.327
Quasi-model 30	0.753	4.558	3.802	29.217	0.959	17.839

Model #3: One compartment, covariate: creatinine clearance

Model	**KS**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.003	0.092	61.475	0.972	16.138
Pop-PK, MAP Bayesian	0.003	0.091	61.540	0.946	16.064
Quasi-model 1	0.003	0.05	60.139	0.946	16.053
Quasi-model 2	0.002	0.079	63.332	0.946	16.172
Quasi-model 3	0.002	0.098	63.754	0.946	16.346
Quasi-model 4	0.003	0.078	63.247	0.946	16.323
Quasi-model 5	0.003	0.066	60.351	0.946	15.458
Quasi-model 6	0.003	0.086	63.034	0.946	16.493
Quasi-model 7	0.003	0.031	61.955	0.946	16.521
Quasi-model 8	0.003	0.043	66.005	0.946	17.228
Quasi-model 9	0.003	0.040	67.122	0.945	18.641
Quasi-model 10	0.003	0.051	61.892	0.946	16.358
Quasi-model 11	0.003	0.018	63.165	0.946	16.420
Quasi-model 12	0.003	0.067	61.659	0.946	16.075
Quasi-model 13	0.003	0.051	60.631	0.946	16.295
Quasi-model 14	0.003	0.066	62.961	0.946	16.474
Quasi-model 15	0.003	0.081	64.431	0.946	20.421
Quasi-model 16	0.003	0.046	58.505	0.946	17.873
Quasi-model 17	0.003	0.024	63.926	0.946	16.206
Quasi-model 18	0.003	0.018	63.229	0.946	18.498
Quasi-model 19	0.003	0.025	57.893	0.946	17.373
Quasi-model 20	0.003	0.039	59.837	0.947	17.664
Quasi-model 21	0.003	0.016	63.082	0.946	16.393
Quasi-model 22	0.003	0.078	61.438	0.946	16.383
Quasi-model 23	0.003	0.095	57.699	0.946	16.424
Quasi-model 24	0.003	0.078	62.387	0.946	16.610
Quasi-model 25	0.003	0.044	59.928	0.947	16.691
Quasi-model 26	0.003	0.038	61.514	0.946	16.041
Quasi-model 27	0.003	0.084	62.554	0.946	16.245
Quasi-model 28	0.003	0.075	63.662	0.946	16.301
Quasi-model 29	0.003	0.032	64.773	0.946	16.523
Quasi-model 30	0.003	0.017	62.326	0.946	16.837

Model #4: Two compartments, covariate: creatinine clearance

Model	**KS**	**KCP**	**KPC**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.014	3.419	1.099	0.180	10.300	0.988	7.315
Pop-PK, MAP Bayesian	0.014	3.391	1.118	0.181	10.252	0.976	7.363
Quasi-model 1	0.009	5.397	3.345	0.010	23.179	0.963	19.228
Quasi-model 2	0.110	3.859	1.586	0.025	16.575	0.966	14.710

Quasi-model 3	0.009	5.346	1.990	0.161	14.615	0.967	10.873
Quasi-model 4	0.008	4.567	2.507	0.243	21.391	0.961	14.206
Quasi-model 5	0.007	4.138	2.006	0.332	18.953	0.966	16.106
Quasi-model 6	0.010	4.779	1.861	0.139	17.647	0.964	24.715
Quasi-model 7	0.005	3.285	1.948	0.312	23.582	0.967	22.098
Quasi-model 8	0.009	5.056	2.094	0.044	17.747	0.962	18.951
Quasi-model 9	0.007	5.784	3.289	0.084	24.905	0.966	21.761
Quasi-model 10	0.009	4.605	2.201	0.253	19.819	0.961	18.809
Quasi-model 11	0.007	4.933	2.479	0.200	18.612	0.959	15.101
Quasi-model 12	0.007	4.135	1.848	0.199	19.724	0.985	25.489
Quasi-model 13	0.008	4.039	2.278	0.153	20.016	0.983	16.313
Quasi-model 14	0.010	4.891	2.266	0.148	21.323	0.959	14.537
Quasi-model 15	0.005	5.101	2.727	0.199	20.440	0.957	34.369
Quasi-model 16	0.009	4.936	2.020	0.121	15.208	0.966	57.147
Quasi-model 17	0.014	5.006	1.626	0.034	12.503	0.963	12.290
Quasi-model 18	0.008	3.450	1.325	0.120	19.935	0.970	43.492
Quasi-model 19	0.008	4.649	2.765	0.248	16.700	0.957	39.407
Quasi-model 20	0.006	4.676	3.547	0.169	24.590	0.960	15.092
Quasi-model 21	0.008	4.470	2.780	0.146	21.595	0.956	13.626
Quasi-model 22	0.008	4.695	1.958	0.162	20.499	0.963	13.866
Quasi-model 23	0.006	4.639	3.172	0.220	22.645	0.957	17.566
Quasi-model 24	0.012	3.565	1.228	0.147	11.201	0.974	8.677
Quasi-model 25	0.007	5.746	5.257	0.053	24.586	0.954	98.285
Quasi-model 26	0.011	4.268	1.366	0.185	13.171	0.973	9.163
Quasi-model 27	0.008	4.169	1.975	0.142	20.067	0.967	20.792
Quasi-model 28	0.007	5.545	3.026	0.220	22.227	0.957	17.053
Quasi-model 29	0.009	2.624	1.392	0.035	19.045	0.969	10.19
Quasi-model 30	0.010	5.254	2.007	0.265	16.607	0.959	26.476

Supplementary table S9: Performance of the quasi-models for Subject 8

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.279	49.15	0.968	23.591
Pop-PK, MAP	0.281	49.737	0.939	23.026
Quasi-model 1	0.274	48.002	0.939	36.485
Quasi-model 2	0.289	47.524	0.939	23.979
Quasi-model 3	0.255	53.331	0.938	24.342
Quasi-model 4	0.306	45.752	0.940	23.322
Quasi-model 5	0.292	47.310	0.939	23.093
Quasi-model 6	0.245	59.564	0.939	31.349
Quasi-model 7	0.282	46.373	0.940	50.850
Quasi-model 8	0.302	46.050	0.940	24.441
Quasi-model 9	0.252	53.850	0.936	28.967
Quasi-model 10	0.249	53.539	0.936	29.828
Quasi-model 11	0.273	52.046	0.938	23.426

Quasi-model 12	0.282	48.778	0.939	23.626
Quasi-model 13	0.252	54.734	0.936	28.012
Quasi-model 14	0.275	49.734	0.938	25.445
Quasi-model 15	0.271	50.546	0.938	23.464
Quasi-model 16	0.299	46.925	0.94	23.125
Quasi-model 17	0.297	45.614	0.94	23.935
Quasi-model 18	0.278	49.638	0.939	23.260
Quasi-model 19	0.282	51.913	0.939	24.283
Quasi-model 20	0.264	52.006	0.937	26.156
Quasi-model 21	0.284	48.912	0.939	22.919
Quasi-model 22	0.274	51.250	0.938	23.909
Quasi-model 23	0.259	52.961	0.937	25.278
Quasi-model 24	0.270	47.516	0.938	51.556
Quasi-model 25	0.277	49.354	0.938	25.197
Quasi-model 26	0.261	51.702	0.937	25.035
Quasi-model 27	0.287	48.064	0.939	24.030
Quasi-model 28	0.267	52.032	0.939	23.261
Quasi-model 29	0.254	54.208	0.938	24.289
Quasi-model 30	0.291	47.721	0.940	23.055

Model #2: Two compartments, no covariate

Model	**K**	**KCP**	**KPC**	**V**	**R^2**	**MSE**
Pop-PK, NPAG	1.644	1.906	1.065	5.75	0.994	4.138
Pop-PK, MAP Bayesian	1.646	2.466	0.546	5.648	0.99	3.877
Quasi-model 1	0.667	3.817	1.579	19.524	0.954	78.711
Quasi-model 2	0.960	4.135	1.282	12.431	0.954	56.993
Quasi-model 3	0.682	3.171	1.629	17.746	0.961	34.189
Quasi-model 4	0.662	4.542	1.749	18.348	0.957	44.053
Quasi-model 5	0.634	2.161	1.332	18.559	0.965	33.378
Quasi-model 6	0.673	3.598	2.128	23.817	0.952	82.834
Quasi-model 7	0.830	3.058	1.995	13.991	0.959	32.429
Quasi-model 8	0.450	4.192	2.897	30.497	0.952	39.076
Quasi-model 9	0.466	4.875	4.555	30.118	0.947	68.414
Quasi-model 10	0.798	4.470	2.142	16.781	0.956	53.407
Quasi-model 11	0.814	4.255	1.896	14.647	0.952	32.713
Quasi-model 12	0.581	4.251	2.022	23.983	0.951	63.422
Quasi-model 13	0.588	4.106	2.417	22.673	0.941	94.283
Quasi-model 14	0.668	4.279	2.546	21.652	0.941	105.975
Quasi-model 15	0.578	4.371	2.863	25.943	0.941	142.364
Quasi-model 16	0.670	3.692	1.568	19.455	0.959	95.754
Quasi-model 17	0.735	4.145	1.289	20.222	0.953	65.380
Quasi-model 18	0.680	3.184	1.639	17.671	0.951	34.981
Quasi-model 19	0.661	4.396	1.750	18.345	0.957	58.888
Quasi-model 20	0.544	2.903	2.423	26.090	0.946	53.361
Quasi-model 21	0.473	3.947	3.624	28.903	0.942	91.278
Quasi-model 22	0.827	3.574	1.763	14.090	0.957	28.703

Quasi-model 23	0.448	4.199	4.253	30.150	0.948	44.587
Quasi-model 24	0.518	4.789	4.329	23.945	0.946	54.089
Quasi-model 25	0.605	4.493	3.136	22.655	0.951	41.854
Quasi-model 26	0.482	3.745	3.436	28.213	0.955	50.368
Quasi-model 27	0.657	4.790	2.265	19.975	0.942	61.208
Quasi-model 28	0.592	4.435	2.997	22.677	0.953	38.801
Quasi-model 29	0.569	4.012	3.631	23.276	0.946	33.948
Quasi-model 30	0.467	4.144	4.306	30.144	0.942	49.258

Model #3: One compartment, covariate: creatinine clearance

Model	**KS**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.003	0.023	47.824	0.969	23.766
Pop-PK, MAP Bayesian	0.004	0.096	36.560	0.946	56.184
Quasi-model 1	0.003	0.051	50.347	0.938	23.675
Quasi-model 2	0.003	0.029	47.086	0.939	22.991
Quasi-model 3	0.003	0.081	52.840	0.938	23.528
Quasi-model 4	0.003	0.037	49.473	0.939	24.631
Quasi-model 5	0.003	0.033	55.297	0.937	26.292
Quasi-model 6	0.002	0.096	50.015	0.939	23.023
Quasi-model 7	0.003	0.011	48.808	0.939	22.997
Quasi-model 8	0.003	0.053	50.539	0.938	27.035
Quasi-model 9	0.003	0.035	50.548	0.938	23.467
Quasi-model 10	0.003	0.079	48.320	0.939	22.909
Quasi-model 11	0.003	0.026	52.617	0.938	25.563
Quasi-model 12	0.003	0.072	64.592	0.94	23.044
Quasi-model 13	0.003	0.048	49.439	0.939	23.163
Quasi-model 14	0.003	0.036	52.636	0.938	23.976
Quasi-model 15	0.003	0.092	49.705	0.94	24.756
Quasi-model 16	0.003	0.086	47.594	0.939	23.137
Quasi-model 17	0.003	0.044	51.398	0.939	23.258
Quasi-model 18	0.003	0.026	48.505	0.939	23.666
Quasi-model 19	0.003	0.027	52.786	0.939	23.818
Quasi-model 20	0.003	0.064	51.879	0.937	26.801
Quasi-model 21	0.003	0.057	51.173	0.939	23.316
Quasi-model 22	0.003	0.059	48.812	0.939	23.019
Quasi-model 23	0.003	0.022	49.142	0.939	22.911
Quasi-model 24	0.003	0.072	53.461	0.939	23.186
Quasi-model 25	0.003	0.075	45.627	0.940	23.351
Quasi-model 26	0.003	0.055	50.046	0.939	26.182
Quasi-model 27	0.003	0.060	48.366	0.939	22.987
Quasi-model 28	0.003	0.051	47.495	0.940	23.064
Quasi-model 29	0.003	0.056	48.691	0.939	25.840
Quasi-model 30	0.003	0.009	51.691	0.937	25.368

Model #4: Two compartments, covariate: creatinine clearance

Model	KS	KCP	KPC	KI	V_c	R^2	MSE
Pop-PK, NPAG	0.015	2.375	0.577	0.079	6.300	0.994	4.431
Pop-PK, MAP Bayesian	0.014	3.391	1.118	0.181	10.251	0.967	86.877
Quasi-model 1	0.012	4.489	1.365	0.221	13.073	0.953	55.227
Quasi-model 2	0.008	3.86	1.594	0.104	16.573	0.953	52.373
Quasi-model 3	0.008	4.344	1.778	0.238	14.625	0.958	33.516
Quasi-model 4	0.007	4.571	3.425	0.069	21.918	0.953	34.163
Quasi-model 5	0.008	4.681	2.036	0.171	15.542	0.946	78.297
Quasi-model 6	0.005	3.621	2.187	0.199	22.434	0.95	36.385
Quasi-model 7	0.008	4.166	1.526	0.265	18.064	0.951	173.209
Quasi-model 8	0.006	5.101	2.686	0.105	19.324	0.941	42.983
Quasi-model 9	0.008	4.558	1.602	0.084	16.002	0.946	85.586
Quasi-model 10	0.011	4.582	1.536	0.240	15.635	0.954	69.444
Quasi-model 11	0.007	4.871	2.487	0.199	18.661	0.948	30.265
Quasi-model 12	0.007	3.505	1.844	0.189	19.765	0.954	146.328
Quasi-model 13	0.010	4.325	1.605	0.086	15.354	0.95	102.499
Quasi-model 14	0.006	4.084	2.010	0.192	19.585	0.945	57.984
Quasi-model 15	0.005	4.484	2.729	0.162	20.426	0.942	73.442
Quasi-model 16	0.008	2.400	1.208	0.145	17.496	0.967	27.066
Quasi-model 17	0.011	4.953	1.095	0.040	14.573	0.946	39.911
Quasi-model 18	0.005	4.854	2.230	0.143	21.081	0.950	56.700
Quasi-model 19	0.009	4.222	1.792	0.114	16.699	0.951	60.435
Quasi-model 20	0.006	4.595	1.969	0.169	18.049	0.946	79.587
Quasi-model 21	0.005	3.568	1.866	0.274	19.966	0.951	60.527
Quasi-model 22	0.006	4.797	2.980	0.300	20.256	0.942	39.818
Quasi-model 23	0.006	5.387	3.581	0.157	22.467	0.943	34.263
Quasi-model 24	0.013	3.546	1.218	0.146	11.164	0.973	49.977
Quasi-model 25	0.005	4.991	4.043	0.214	22.371	0.950	24.227
Quasi-model 26	0.010	3.688	1.365	0.191	12.801	0.962	69.528
Quasi-model 27	0.007	4.030	2.219	0.151	18.741	0.957	45.340
Quasi-model 28	0.006	4.800	1.945	0.282	17.921	0.944	36.518
Quasi-model 29	0.009	5.589	1.610	0.036	18.753	0.951	93.079
Quasi-model 30	0.008	2.916	0.883	0.176	14.019	0.971	61.228

Supplementary table S10: Performance of the quasi-models for Subject 9

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.240	21.250	0.992	27.606
Pop-PK, MAP	0.240	21.050	0.984	26.543
Quasi-model 1	0.250	20.239	0.984	92.895
Quasi-model 2	0.262	17.743	0.985	156.758
Quasi-model 3	0.226	22.622	0.984	29.618
Quasi-model 4	0.236	22.273	0.984	55.678
Quasi-model 5	0.245	20.063	0.984	31.392
Quasi-model 6	0.234	22.083	0.984	30.370

Quasi-model 7	0.239	26.885	0.985	748.721
Quasi-model 8	0.226	24.622	0.984	552.465
Quasi-model 9	0.247	20.536	0.984	61.980
Quasi-model 10	0.240	18.952	0.984	99.625
Quasi-model 11	0.230	22.501	0.984	37.301
Quasi-model 12	0.235	17.749	0.984	65.405
Quasi-model 13	0.255	16.665	0.985	1869.622
Quasi-model 14	0.241	18.219	0.984	293.096
Quasi-model 15	0.219	22.199	0.983	44.871
Quasi-model 16	0.243	22.133	0.984	33.596
Quasi-model 17	0.235	20.760	0.984	104.395
Quasi-model 18	0.227	23.572	0.984	107.300
Quasi-model 19	0.252	21.990	0.985	88.908
Quasi-model 20	0.254	23.190	0.985	52.625
Quasi-model 21	0.252	23.582	0.985	771.321
Quasi-model 22	0.230	21.958	0.984	150.082
Quasi-model 23	0.235	19.995	0.984	241.024
Quasi-model 24	0.238	21.255	0.984	26.125
Quasi-model 25	0.228	23.013	0.984	247.559
Quasi-model 26	0.236	23.174	0.984	115.670
Quasi-model 27	0.222	22.320	0.984	33.348
Quasi-model 28	0.214	24.808	0.984	155.909
Quasi-model 29	0.238	22.496	0.984	78.532
Quasi-model 30	0.228	24.052	0.984	469.683

Model #2: Two compartments, no covariate

Model	**K**	**KCP**	**KPC**	**V**	**R^2**	**MSE**
Pop-PK, NPAG	0.492	1.857	1.659	9.350	0.995	16.700
Pop-PK, MAP Bayesian	0.489	1.845	1.667	9.234	0.988	22.156
Quasi-model 1	0.360	1.668	3.75	14.449	0.988	52.244
Quasi-model 2	0.404	1.404	3.043	12.886	0.988	145.299
Quasi-model 3	0.578	1.807	1.719	11.287	0.986	325.073
Quasi-model 4	0.471	3.464	3.769	10.237	0.987	136.782
Quasi-model 5	0.340	1.874	3.411	13.811	0.988	23.082
Quasi-model 6	0.472	2.83	3.274	11.693	0.988	64.569
Quasi-model 7	0.368	1.234	1.958	10.196	0.99	1322.221
Quasi-model 8	0.285	0.572	2.087	19.260	0.99	102.488
Quasi-model 9	0.349	1.303	2.064	13.156	0.99	248.914
Quasi-model 10	0.388	2.901	4.678	11.857	0.986	186.467
Quasi-model 11	0.365	1.449	2.635	14.546	0.989	18.442
Quasi-model 12	0.342	1.044	4.030	16.168	0.987	23.909
Quasi-model 13	0.356	2.234	3.220	13.057	0.989	56.026
Quasi-model 14	0.372	2.349	3.613	10.655	0.987	45.648
Quasi-model 15	0.432	2.317	2.903	11.036	0.988	30.522
Quasi-model 16	0.360	1.114	2.005	13.099	0.9900	39.862
Quasi-model 17	0.406	1.409	3.035	12.855	0.989	223.929

Quasi-model 18	0.673	1.801	0.932	6.957	0.979	195.212
Quasi-model 19	0.471	3.456	3.767	10.384	0.987	142.640
Quasi-model 20	0.339	1.868	3.919	13.789	0.988	36.921
Quasi-model 21	0.467	2.828	3.266	11.660	0.988	106.967
Quasi-model 22	0.431	3.599	3.974	11.458	0.988	38.406
Quasi-model 23	0.285	0.572	2.108	19.260	0.990	119.557
Quasi-model 24	0.372	1.341	2.242	10.954	0.990	64.256
Quasi-model 25	0.390	2.898	4.566	11.819	0.987	221.401
Quasi-model 26	0.366	2.202	3.288	12.330	0.989	121.609
Quasi-model 27	0.394	2.042	1.861	11.682	0.988	391.949
Quasi-model 28	0.354	0.935	1.915	13.469	0.990	49.764
Quasi-model 29	0.330	1.191	3.215	15.741	0.988	35.015
Quasi-model 30	0.382	1.766	2.256	13.942	0.990	18.822

Model #3: One compartment, covariate: creatinine clearance

Model	**KS**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.004	0.052	20.525	0.992	26.005
Pop-PK, MAP Bayesian	0.004	0.096	36.503	0.977	1930.343
Quasi-model 1	0.003	0.100	78.121	0.977	16163.582
Quasi-model 2	0.004	0.100	77.032	0.977	15867.909
Quasi-model 3	0.005	0.099	76.452	0.977	15798.651
Quasi-model 4	0.002	0.099	79.390	0.977	16320.148
Quasi-model 5	0.002	0.097	79.442	0.977	16225.541
Quasi-model 6	0.002	0.100	79.479	0.977	16435.030
Quasi-model 7	0.002	0.097	79.155	0.977	16232.114
Quasi-model 8	0.005	0.097	79.514	0.977	16254.626
Quasi-model 9	0.004	0.100	79.357	0.977	16439.949
Quasi-model 10	0.003	0.100	77.089	0.977	15813.633
Quasi-model 11	0.003	0.100	72.783	0.977	14741.318
Quasi-model 12	0.003	0.097	79.571	0.977	16291.543
Quasi-model 13	0.003	0.098	77.461	0.977	15908.973
Quasi-model 14	0.001	0.099	73.635	0.977	15188.758
Quasi-model 15	0.004	0.099	74.543	0.977	15075.430
Quasi-model 16	0.003	0.096	78.022	0.977	15691.112
Quasi-model 17	0.004	0.095	79.382	0.976	16130.073
Quasi-model 18	0.005	0.099	79.734	0.977	16462.576
Quasi-model 19	0.002	0.097	79.733	0.977	16383.775
Quasi-model 20	0.005	0.099	74.661	0.977	15282.424
Quasi-model 21	0.003	0.097	76.989	0.977	15695.800
Quasi-model 22	0.005	0.097	78.009	0.977	16008.559
Quasi-model 23	0.002	0.100	79.421	0.977	16501.559
Quasi-model 24	0.003	0.094	79.653	0.977	15797.891
Quasi-model 25	0.004	0.094	78.279	0.976	15874.993
Quasi-model 26	0.004	0.099	74.898	0.977	15275.141
Quasi-model 27	0.005	0.095	79.405	0.976	16141.837
Quasi-model 28	0.002	0.092	79.424	0.976	15865.659

Quasi-model 29	0.005	0.091	79.676	0.976	15525.113
Quasi-model 30	0.001	0.099	77.762	0.977	16027.284

Model #4: Two compartments, covariate: creatinine clearance

Model	KS	KCP	KPC	KI	V_c	R^2	MSE
Pop-PK, NPAG	0.014	3.419	1.099	0.18	10.300	0.988	7.315
Pop-PK, MAP Bayesian	0.014	3.391	1.118	0.181	10.252	0.976	7.363
Quasi-model 1	0.013	3.157	3.189	0.201	16.414	0.989	529.846
Quasi-model 2	0.013	3.182	3.262	0.193	17.159	0.989	607.965
Quasi-model 3	0.012	0.458	4.627	0.264	17.574	0.987	35.319
Quasi-model 4	0.012	3.077	3.089	0.198	16.868	0.989	524.862
Quasi-model 5	0.012	2.919	3.024	0.182	16.356	0.989	508.390
Quasi-model 6	0.013	3.112	3.120	0.191	16.108	0.989	519.691
Quasi-model 7	0.013	2.888	3.021	0.182	15.417	0.989	519.748
Quasi-model 8	0.014	2.980	3.250	0.191	16.680	0.989	552.896
Quasi-model 9	0.014	3.142	3.086	0.188	16.514	0.989	629.830
Quasi-model 10	0.012	3.185	3.049	0.198	16.276	0.989	538.061
Quasi-model 11	0.001	0.826	2.628	0.280	16.033	0.989	32.942
Quasi-model 12	0.009	0.706	2.694	0.298	18.400	0.988	293.612
Quasi-model 13	0.022	0.947	4.729	0.289	16.667	0.986	82.486
Quasi-model 14	0.006	0.545	1.738	0.304	18.070	0.989	167.200
Quasi-model 15	0.007	1.029	3.482	0.294	15.798	0.989	178.237
Quasi-model 16	0.015	0.887	4.643	0.277	17.035	0.986	96.474
Quasi-model 17	0.006	0.572	3.511	0.254	20.238	0.986	26.113
Quasi-model 18	0.011	0.360	1.052	0.284	16.531	0.989	23.742
Quasi-model 19	0.021	0.693	2.532	0.291	18.019	0.988	50.920
Quasi-model 20	0.009	1.041	3.646	0.312	16.488	0.988	33.384
Quasi-model 21	0.007	1.463	4.085	0.310	13.917	0.986	88.063
Quasi-model 22	0.015	1.260	5.075	0.291	17.021	0.986	31.053
Quasi-model 23	0.014	1.018	3.413	0.304	15.571	0.987	44.687
Quasi-model 24	0.013	0.222	4.129	0.253	20.159	0.987	186.474
Quasi-model 25	0.007	1.265	4.339	0.293	16.523	0.986	29.710
Quasi-model 26	0.008	0.550	2.730	0.284	16.723	0.989	57.429
Quasi-model 27	0.013	1.202	3.542	0.314	16.159	0.987	26.736
Quasi-model 28	0.010	0.832	4.231	0.290	13.840	0.986	462.577
Quasi-model 29	0.016	1.940	5.403	0.313	15.823	0.985	35.517
Quasi-model 30	0.012	0.476	1.749	0.319	15.729	0.989	37.328

Supplementary table S11: Performance of the quasi-models for Subject 10

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.266	68.95	0.985	4.579
Pop-PK, MAP	0.367	61.445	0.831	28.284
Quasi-model 1	0.336	60.789	0.834	26.685

Quasi-model 2	0.367	57.237	0.832	28.923
Quasi-model 3	0.318000	64.675	0.834	27.269
Quasi-model 4	0.294	68.053	0.834	27.010
Quasi-model 5	0.298	68.454	0.833	27.770
Quasi-model 6	0.354	59.167	0.833	27.689
Quasi-model 7	0.293	68.609	0.833	27.783
Quasi-model 8	0.298	66.901	0.834	28.364
Quasi-model 9	0.318	63.089	0.833	26.429
Quasi-model 10	0.349	59.702	0.833	28.762
Quasi-model 11	0.332	61.26	0.834	26.617
Quasi-model 12	0.309	65.944	0.834	26.142
Quasi-model 13	0.356	60.359	0.833	26.864
Quasi-model 14	0.332	61.948	0.834	27.499
Quasi-model 15	0.367	57.874	0.832	26.897
Quasi-model 16	0.322	62.970	0.834	25.978
Quasi-model 17	0.319	63.644	0.834	26.057
Quasi-model 18	0.294	68.011	0.834	27.089
Quasi-model 19	0.326	64.117	0.834	27.527
Quasi-model 20	0.318	67.011	0.832	28.593
Quasi-model 21	0.321	62.971	0.834	26.025
Quasi-model 22	0.334	63.292	0.834	26.704
Quasi-model 23	0.293	69.726	0.833	27.56
Quasi-model 24	0.308	65.294	0.834	26.543
Quasi-model 25	0.309	65.437	0.834	26.879
Quasi-model 26	0.321	62.620	0.834	26.018
Quasi-model 27	0.334	63.852	0.834	30.776
Quasi-model 28	0.336	62.327	0.834	26.696
Quasi-model 29	0.319	62.919	0.834	26.313
Quasi-model 30	0.303	65.486	0.834	26.604

Model #2: Two compartments, no covariate

Model	**K**	**KCP**	**KPC**	**V**	**R^2**	**MSE**
Pop-PK, NPAG	0.684	3.292	2.203	24.65	0.987	4.103
Pop-PK, MAP Bayesian	1.360	1.282	0.719	23.853	0.136	864.826
Quasi-model 1	0.818	4.498	4.533	33.334	0.568	525.761
Quasi-model 2	1.230	2.434	3.412	29.031	0.447	879.033
Quasi-model 3	1.346	2.182	3.505	27.282	0.490	802.525
Quasi-model 4	1.337	2.857	2.949	30.042	0.408	929.952
Quasi-model 5	1.349	3.050	3.093	29.675	0.483	842.914
Quasi-model 6	0.844	4.543	4.544	34.768	0.554	455.938
Quasi-model 7	1.411	2.183	2.829	29.552	0.419	936.534
Quasi-model 8	1.378	1.805	3.387	29.303	0.439	881.256
Quasi-model 9	1.437	2.681	2.761	27.428	0.372	1029.35
Quasi-model 10	1.389	2.405	2.777	25.669	0.369	994.131
Quasi-model 11	1.360	1.822	2.986	28.435	0.474	784.102
Quasi-model 12	1.234	2.053	3.429	30.236	0.446	901.496

Quasi-model 13	1.320	2.970	3.234	28.982	0.482	835.738
Quasi-model 14	1.475	2.353	3.119	25.159	0.370	966.538
Quasi-model 15	1.481	2.374	3.465	25.594	0.386	920.791
Quasi-model 16	0.818	4.482	4.533	33.335	0.563	528.200
Quasi-model 17	1.291	2.475	2.914	29.038	0.400	954.121
Quasi-model 18	1.341	2.138	3.236	27.223	0.481	795.990
Quasi-model 19	1.333	2.284	2.909	30.031	0.429	906.854
Quasi-model 20	1.297	2.531	3.022	30.828	0.467	847.032
Quasi-model 21	1.308	2.640	2.710	29.886	0.407	928.141
Quasi-model 22	1.393	2.175	3.018	29.539	0.424	907.659
Quasi-model 23	1.386	1.799	3.361	29.052	0.434	910.633
Quasi-model 24	1.376	2.477	2.470	27.246	0.292	1107.884
Quasi-model 25	1.396	3.743	2.911	28.128	0.409	944.231
Quasi-model 26	1.333	2.363	3.524	30.360	0.494	873.237
Quasi-model 27	1.348	3.171	3.437	29.579	0.480	882.499
Quasi-model 28	1.358	2.990	2.951	27.813	0.469	855.140
Quasi-model 29	1.242	1.464	3.193	27.988	0.427	882.819
Quasi-model 30	1.425	2.351	3.085	28.259	0.492	827.174

Model #3: One compartment, covariate: creatinine clearance

Model	**KS**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.004	0.022	72.525	0.985	5.318
Pop-PK, MAP Bayesian	0.004	0.022	72.608	0.827	33.910
Quasi-model 1	0.005	0.028	65.105	0.834	26.792
Quasi-model 2	0.005	0.049	61.456	0.833	26.455
Quasi-model 3	0.004	0.048	67.713	0.834	26.704
Quasi-model 4	0.005	0.020	62.854	0.834	26.190
Quasi-model 5	0.004	0.076	63.912	0.834	26.835
Quasi-model 6	0.004	0.065	64.453	0.834	25.999
Quasi-model 7	0.004	0.054	64.778	0.834	26.900
Quasi-model 8	0.004	0.046	64.613	0.834	26.490
Quasi-model 9	0.004	0.580	63.437	0.833	26.868
Quasi-model 10	0.005	0.016	65.495	0.834	26.781
Quasi-model 11	0.004	0.055	65.421	0.834	27.089
Quasi-model 12	0.004	0.040	62.381	0.834	26.316
Quasi-model 13	0.004	0.046	65.518	0.833	26.534
Quasi-model 14	0.004	0.052	65.008	0.834	26.425
Quasi-model 15	0.004	0.073	62.997	0.834	27.309
Quasi-model 16	0.004	0.043	65.569	0.834	26.832
Quasi-model 17	0.004	0.080	65.072	0.834	26.789
Quasi-model 18	0.004	0.043	63.366	0.834	26.433
Quasi-model 19	0.004	0.089	63.666	0.834	27.128
Quasi-model 20	0.004	0.078	61.999	0.833	26.826
Quasi-model 21	0.004	0.077	66.500	0.834	26.893
Quasi-model 22	0.004	0.039	64.727	0.833	26.528
Quasi-model 23	0.004	0.048	66.078	0.834	27.004

Quasi-model 24	0.004	0.042	64.934	0.833	27.409
Quasi-model 25	0.004	0.066	65.472	0.834	26.195
Quasi-model 26	0.004	0.057	62.382	0.834	26.178
Quasi-model 27	0.005	0.019	61.785	0.834	27.284
Quasi-model 28	0.004	0.039	65.083	0.833	27.236
Quasi-model 29	0.004	0.069	63.231	0.834	27.150
Quasi-model 30	0.004	0.042	62.769	0.834	27.056

Model #4: Two compartments, covariate: creatinine clearance

Model	**KS**	**KCP**	**KPC**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.009	3.709	2.027	0.212	21.300	0.987	4.110
Pop-PK, MAP Bayesian	0.009	3.736	2.046	0.214	21.337	0.513	139.395
Quasi-model 1	0.021	2.535	4.806	0.197	21.674	0.415	898.005
Quasi-model 2	0.020	1.927	4.889	0.251	22.297	0.457	805.901
Quasi-model 3	0.020	2.195	3.627	0.215	23.853	0.469	818.374
Quasi-model 4	0.023	3.582	4.945	0.068	24.107	0.469	801.018
Quasi-model 5	0.023	1.819	4.654	0.242	22.653	0.425	892.293
Quasi-model 6	0.023	1.651	4.322	0.205	21.620	0.393	940.515
Quasi-model 7	0.021	1.975	4.369	0.231	23.975	0.465	798.546
Quasi-model 8	0.022	2.226	4.272	0.255	22.442	0.453	837.403
Quasi-model 9	0.023	2.392	4.422	0.178	20.746	0.410	882.119
Quasi-model 10	0.023	2.297	4.527	0.219	21.905	0.433	850.569
Quasi-model 11	0.021	1.216	4.372	0.135	22.506	0.467	743.067
Quasi-model 12	0.022	1.666	4.299	0.247	22.430	0.433	862.366
Quasi-model 13	0.023	0.850	3.794	0.221	21.070	0.359	971.746
Quasi-model 14	0.023	3.233	4.811	0.283	21.865	0.390	980.739
Quasi-model 15	0.021	1.450	4.592	0.191	21.724	0.428	827.373
Quasi-model 16	0.020	0.804	4.135	0.216	21.986	0.421	844.144
Quasi-model 17	0.022	1.517	4.171	0.235	20.869	0.396	892.871
Quasi-model 18	0.023	2.438	5.500	0.230	21.753	0.471	828.392
Quasi-model 19	0.022	3.208	4.101	0.184	23.119	0.443	889.972
Quasi-model 20	0.023	2.628	4.830	0.201	21.977	0.424	883.104
Quasi-model 21	0.021	3.430	4.793	0.208	23.227	0.457	843.163
Quasi-model 22	0.021	2.918	3.960	0.180	23.475	0.416	910.886
Quasi-model 23	0.021	1.406	4.012	0.161	22.332	0.440	824.754
Quasi-model 24	0.023	2.513	4.270	0.230	21.915	0.371	999.343
Quasi-model 25	0.022	3.272	3.886	0.284	22.014	0.437	820.329
Quasi-model 26	0.023	1.811	4.151	0.236	23.377	0.428	894.251
Quasi-model 27	0.023	1.284	3.976	0.201	21.936	0.409	882.167
Quasi-model 28	0.022	2.341	4.587	0.239	22.039	0.450	855.283
Quasi-model 29	0.021	0.823	4.001	0.112	23.394	0.411	850.15
Quasi-model 30	0.021	0.871	4.629	0.114	23.019	0.454	810.809

Supplementary table S12: Performance of the quasi-models for Subject 11

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.266	22.150	0.976	101.473
Pop-PK, MAP	0.262	21.921	0.953	99.635
Quasi-model 1	0.292	19.809	0.953	127.756
Quasi-model 2	0.341	16.506	0.952	328.750
Quasi-model 3	0.290	19.783	0.953	127.756
Quasi-model 4	0.258	23.160	0.953	169.809
Quasi-model 5	0.219	24.984	0.953	156.335
Quasi-model 6	0.253	22.311	0.953	103.246
Quasi-model 7	0.301	18.856	0.953	164.157
Quasi-model 8	0.269	20.863	0.953	113.778
Quasi-model 9	0.265	21.264	0.953	142.134
Quasi-model 10	0.253	24.250	0.953	276.879
Quasi-model 11	0.269	20.755	0.953	133.241
Quasi-model 12	0.288	20.699	0.953	142.558
Quasi-model 13	0.285	20.796	0.953	105.865
Quasi-model 14	0.288	19.990	0.953	126.849
Quasi-model 15	0.302	19.007	0.953	213.777
Quasi-model 16	0.299	19.106	0.953	206.347
Quasi-model 17	0.299	20.148	0.953	159.781
Quasi-model 18	0.227	23.748	0.953	153.461
Quasi-model 19	0.255	22.214	0.953	106.674
Quasi-model 20	0.267	22.033	0.953	104.162
Quasi-model 21	0.274	20.899	0.953	99.281
Quasi-model 22	0.266	21.161	0.953	146.851
Quasi-model 23	0.255	22.719	0.953	110.761
Quasi-model 24	0.225	24.442	0.953	121.492
Quasi-model 25	0.225	25.719	0.953	213.263
Quasi-model 26	0.236	23.217	0.953	159.168
Quasi-model 27	0.268	20.566	0.953	248.588
Quasi-model 28	0.208	26.117	0.953	195.461
Quasi-model 29	0.237	23.276	0.953	148.983
Quasi-model 30	0.242	24.146	0.953	131.155

Model #2: Two compartments, no covariate

Model	K	KCP	KPC	V	R^2	MSE
Pop-PK, NPAG	0.732	4.579	2.847	7.550	0.978	92.405
Pop-PK, MAP Bayesian	0.723	4.551	2.826	7.488	0.958	89.197
Quasi-model 1	0.527	2.713	3.859	10.246	0.957	96.929
Quasi-model 2	0.334	0.444	1.908	17.242	0.954	103.233
Quasi-model 3	0.487	2.805	4.543	10.589	0.955	235.215
Quasi-model 4	0.456	3.015	4.670	13.026	0.955	155.442
Quasi-model 5	0.464	3.305	3.891	13.189	0.956	610.397
Quasi-model 6	0.474	2.838	3.276	11.667	0.957	168.720
Quasi-model 7	0.831	4.853	2.307	6.054	0.959	124.397
Quasi-model 8	0.797	4.948	2.506	7.981	0.958	889.947

Quasi-model 9	0.448	2.171	3.607	12.719	0.956	123.976
Quasi-model 10	0.505	3.081	3.829	11.330	0.956	163.962
Quasi-model 11	0.361	0.996	2.244	15.008	0.955	100.766
Quasi-model 12	0.347	1.060	2544.000	17.864	0.956	528.255
Quasi-model 13	0.801	3.838	2.132	6.489	0.959	104.945
Quasi-model 14	0.549	4.378	3.609	10.597	0.957	258.327
Quasi-model 15	0.409	1.841	4.650	14.060	0.955	127.912
Quasi-model 16	0.635	2.734	2.331	8.383	0.957	150.945
Quasi-model 17	0.334	0.440	1.908	17.242	0.954	103.227
Quasi-model 18	0.486	2.802	4.547	10.658	0.955	146.014
Quasi-model 19	0.456	3.008	4.674	13.017	0.955	154.793
Quasi-model 20	0.464	3.298	3.907	13.189	0.956	611.578
Quasi-model 21	0.471	2.838	3.277	11.664	0.956	150.691
Quasi-model 22	0.529	4.358	4.350	10.377	0.956	179.500
Quasi-model 23	0.795	4.953	2.511	8.015	0.958	815.489
Quasi-model 24	0.448	2.171	3.602	12.716	0.956	115.852
Quasi-model 25	0.505	373.000	3.842	11.330	0.956	163.945
Quasi-model 26	0.607	3.662	2.713	10.036	0.958	683.446
Quasi-model 27	0.487	2.779	3.719	12.314	0.956	281.181
Quasi-model 28	0.686	2.697	1.964	7.249	0.957	179.951
Quasi-model 29	0.619	3.365	2.891	9.518	0.957	237.014
Quasi-model 30	0.971	4.912	2.082	6.209	0.959	917.214

Model #3: One compartment, covariate: creatinine clearance

Model	**KS**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.004	0.026	21.825	0.976	101.110
Pop-PK, MAP Bayesian	0.003	0.027	26.123	0.953	146.414
Quasi-model 1	0.004	0.013	24.500	0.953	170.588
Quasi-model 2	0.004	0.066	22.198	0.953	124.029
Quasi-model 3	0.004	0.028	20.592	0.953	122.371
Quasi-model 4	0.003	0.095	21.022	0.953	102.489
Quasi-model 5	0.004	0.063	20.301	0.953	102.558
Quasi-model 6	0.004	0.031	24.312	0.953	214.268
Quasi-model 7	0.005	0.019	20.998	0.953	115.970
Quasi-model 8	0.005	0.008	22.186	0.953	107.427
Quasi-model 9	0.004	0.044	22.531	0.953	103.386
Quasi-model 10	0.003	0.100	19.528	0.953	128.274
Quasi-model 11	0.003	0.066	25.328	0.953	183.048
Quasi-model 12	0.003	0.084	23.259	0.953	118.236
Quasi-model 13	0.004	0.058	20.936	0.953	121.303
Quasi-model 14	0.004	0.039	21.455	0.953	171.447
Quasi-model 15	0.004	0.024	22.180	0.953	100.296
Quasi-model 16	0.003	0.075	21.687	0.953	106.323
Quasi-model 17	0.003	0.072	23.252	0.953	108.526
Quasi-model 18	0.004	0.049	20.302	0.953	117.863
Quasi-model 19	0.003	0.071	21.048	0.953	99.798

Quasi-model 20	0.005	0.014	22.622	0.953	151.291
Quasi-model 21	0.004	0.071	19.804	0.953	124.283
Quasi-model 22	0.004	0.035	23.531	0.953	116.217
Quasi-model 23	0.004	0.076	19.260	0.953	142.133
Quasi-model 24	0.004	0.015	22.844	0.953	116.793
Quasi-model 25	0.004	0.024	21.988	0.953	100.736
Quasi-model 26	0.004	0.010	21.970	0.953	108.947
Quasi-model 27	0.003	0.077	21.900	0.953	119.534
Quasi-model 28	0.004	0.021	22.876	0.953	108.982
Quasi-model 29	0.004	0.046	21.188	0.953	99.517
Quasi-model 30	0.003	0.077	20.530	0.953	161.467

Model #4: Two compartments, covariate: creatinine clearance

Model	**KS**	**KCP**	**KPC**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.004	2.085	2.375	0.264	10.500	0.978	92.342
Pop-PK, MAP Bayesian	0.004	2.089	2.361	0.264	10.510	0.957	161.934
Quasi-model 1	0.004	4.928	5.426	0.301	11.511	0.955	237.251
Quasi-model 2	0.003	2.793	4.378	0.251	12.629	0.955	197.933
Quasi-model 3	0.005	2.058	4.461	0.120	14.446	0.956	100.612
Quasi-model 4	0.002	4.060	4.818	0.344	12.883	0.955	520.767
Quasi-model 5	0.004	3.744	5.307	0.137	13.476	0.956	117.756
Quasi-model 6	0.008	3.149	2.381	0.173	8.334	0.958	108.690
Quasi-model 7	0.004	0.525	4.412	0.046	18.994	0.954	104.869
Quasi-model 8	0.003	2.268	3.442	0.227	14.085	0.955	103.936
Quasi-model 9	0.008	5.137	4.453	0.105	10.106	0.955	223.256
Quasi-model 10	0.004	1.322	4.558	0.113	15.932	0.955	123.264
Quasi-model 11	0.006	2.055	4.036	0.051	14.150	0.956	127.437
Quasi-model 12	0.007	4.374	5.189	0.060	10.126	0.956	117.745
Quasi-model 13	0.005	0.795	5.335	0.007	18.366	0.954	97.326
Quasi-model 14	0.006	3.957	5.348	0.155	12.243	0.956	133.900
Quasi-model 15	0.003	1.661	5.781	0.136	18.660	0.55	133.122
Quasi-model 16	0.008	3.071	3.888	0.036	11.825	0.956	130.281
Quasi-model 17	0.007	4.818	4.453	0.048	11.958	0.955	171.460
Quasi-model 18	0.006	3.509	2.954	0.196	10.400	0.957	94.461
Quasi-model 19	0.002	1.577	5.591	0.227	15.890	0.954	108.326
Quasi-model 20	0.004	2.743	4.418	0.324	11.393	0.955	114.088
Quasi-model 21	0.004	5.765	5.184	0.325	9.721	0.956	96.681
Quasi-model 22	0.006	2.427	5.278	0.074	14.883	0.956	111.772
Quasi-model 23	0.001	1.723	3.699	0.321	13.575	0.956	102.592
Quasi-model 24	0.006	3.605	3.199	0.132	10.018	0.957	422.481
Quasi-model 25	0.005	3.343	4.942	0.138	12.800	0.955	199.790
Quasi-model 26	0.004	2.052	3.712	0.170	14.204	0.957	147.176
Quasi-model 27	0.007	4.007	4.197	0.185	9.658	0.956	97.329
Quasi-model 28	0.001	2.167	4.675	0.244	13.112	0.954	312.944
Quasi-model 29	0.003	1.320	3.389	0.181	15.005	0.955	98.360
Quasi-model 30	0.003	2.501	4.309	0.286	14.642	0.956	195.419

Supplementary table S13: Performance of the quasi-models for Subject 12

Model #1: One compartment, no covariate

Model	K	V	R^2	MSE
Pop-PK, NPAG	0.649	34.750	0.991	10.729
Pop-PK, MAP	0.648	34.565	0.982	10.744
Quasi-model 1	0.598	37.946	0.980	13.619
Quasi-model 2	0.622	34.816	0.981	11.621
Quasi-model 3	0.632	36.479	0.981	13.548
Quasi-model 4	0.657	34.588	0.983	10.873
Quasi-model 5	0.602	39.011	0.981	17.660
Quasi-model 6	0.654	35.563	0.982	14.504
Quasi-model 7	0.599	38.806	0.980	17.077
Quasi-model 8	0.652	33.686	0.982	11.051
Quasi-model 9	0.668	34.189	0.982	11.879
Quasi-model 10	0.652	34.096	0.982	10.755
Quasi-model 11	0.627	37.331	0.981	13.242
Quasi-model 12	0.675	32.031	0.984	13.457
Quasi-model 13	0.653	32.323	0.982	16.079
Quasi-model 14	0.587	40.240	0.979	17.839
Quasi-model 15	0.652	34.940	0.983	11.406
Quasi-model 16	0.581	38.914	0.979	17.276
Quasi-model 17	0.639	35.714	0.981	11.327
Quasi-model 18	0.631	37.362	0.982	21.058
Quasi-model 19	0.633	36.307	0.981	11.496
Quasi-model 20	0.648	35.428	0.983	10.846
Quasi-model 21	0.641	35.073	0.982	11.048
Quasi-model 22	0.603	37.123	0.980	13.544
Quasi-model 23	0.599	36.916	0.980	14.809
Quasi-model 24	0.645	36.012	0.982	13.768
Quasi-model 25	0.644	34.716	0.982	10.852
Quasi-model 26	0.587	39.618	0.980	14.791
Quasi-model 27	0.637	36.732	0.981	12.821
Quasi-model 28	0.604	37.401	0.981	12.017
Quasi-model 29	0.633	37.365	0.982	17.743
Quasi-model 30	0.613	36.678	0.980	13.557

Model #2: Two compartments, no covariate

Model	K	KCP	KPC	V	R^2	MSE
Pop-PK, NPAG	1.276	1.065	1.164	14.150	0.996	5.119
Pop-PK, MAP Bayesian	1.280	1.075	1.150	14.170	0.992	5.127
Quasi-model 1	0.922	1.480	2.899	25.251	0.984	28.250
Quasi-model 2	1.088	1.465	1.579	19.831	0.985	37.796
Quasi-model 3	0.960	1.006	1.540	23.310	0.988	29.109

Quasi-model 4	1.185	1.734	2.353	19.390	0.991	14.472
Quasi-model 5	0.860	1.553	2.060	29.240	0.985	30.400
Quasi-model 6	1.083	2.836	2.841	18.286	0.983	28.561
Quasi-model 7	0.837	0.509	1.206	25.907	0.990	20.565
Quasi-model 8	1.475	2.276	1.777	13.534	0.985	21.145
Quasi-model 9	1.254	2.915	2.762	20.810	0.985	21.821
Quasi-model 10	1.207	1.968	1.725	17.360	0.992	16.738
Quasi-model 11	0.997	0.839	0.794	16.882	0.992	6.882
Quasi-model 12	0.997	1.838	2.302	23.721	0.986	32.366
Quasi-model 13	1.086	1.515	2.628	21.830	0.985	43.573
Quasi-model 14	0.926	0.967	1.073	20.652	0.992	22.490
Quasi-model 15	1.254	0.981	1.277	14.257	0.992	7.032
Quasi-model 16	1.442	1.482	3.085	21.006	0.985	17.549
Quasi-model 17	1.086	1.472	1.589	19.881	0.986	57.780
Quasi-model 18	0.922	2.447	4.012	23.225	0.982	25.618
Quasi-model 19	1.183	1.728	2.370	19.379	0.991	16.029
Quasi-model 20	0.788	0.998	2.055	29.463	0.985	26.904
Quasi-model 21	1.078	2.843	3.069	20.066	0.982	29.050
Quasi-model 22	0.837	0.502	1.219	25.917	0.989	22.148
Quasi-model 23	1.475	2.276	1.770	13.556	0.985	28.514
Quasi-model 24	1.130	2.187	2.720	18.367	0.986	15.305
Quasi-model 25	1.207	1.816	1.715	1.207	0.992	18.943
Quasi-model 26	1.146	2.300	2.913	17.087	0.984	13.165
Quasi-model 27	0.910	1.012	2.330	22.130	0.985	13.181
Quasi-model 28	1.112	2.439	3.563	22.838	0.987	34.958
Quasi-model 29	1.163	2.996	2.543	17.569	0.983	21.672
Quasi-model 30	1.360	2.369	2.036	16.591	0.990	13.906

Model #3: One compartment, covariate: creatinine clearance

Model	**KS**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.004	0.095	36.775	0.990	12.167
Pop-PK, MAP Bayesian	0.004	0.096	36.623	0.981	12.193
Quasi-model 1	0.004	0.061	36.875	0.980	12.984
Quasi-model 2	0.004	0.072	38.016	0.980	13.424
Quasi-model 3	0.004	0.047	35.408	0.982	11.319
Quasi-model 4	0.004	0.035	35.817	0.983	11.974
Quasi-model 5	0.004	0.029	39.303	0.981	13.007
Quasi-model 6	0.004	0.045	37.772	0.981	12.051
Quasi-model 7	0.004	0.060	34.553	0.982	11.502
Quasi-model 8	0.004	0.085	35.762	0.981	12.646
Quasi-model 9	0.004	0.083	36.332	0.981	11.991
Quasi-model 10	0.004	0.059	38.352	0.981	14.999
Quasi-model 11	0.004	0.039	34.239	0.982	13.480
Quasi-model 12	0.004	0.018	39.121	0.979	16.365
Quasi-model 13	0.004	0.051	36.548	0.982	11.400
Quasi-model 14	0.004	0.060	38.717	0.980	17.248

Quasi-model 15	0.004	0.048	36.366	0.980	13.665
Quasi-model 16	0.004	0.023	36.200	0.980	13.499
Quasi-model 17	0.004	0.060	38.022	0.981	11.917
Quasi-model 18	0.004	0.073	35.671	0.982	11.232
Quasi-model 19	0.004	0.055	34.501	0.982	11.242
Quasi-model 20	0.004	0.050	36.135	0.981	11.743
Quasi-model 21	0.004	0.041	37.695	0.981	12.304
Quasi-model 22	0.004	0.053	35.672	0.982	11.336
Quasi-model 23	0.005	0.011	36.488	0.981	14.846
Quasi-model 24	0.004	0.016	38.272	0.981	12.133
Quasi-model 25	0.004	0.081	33.770	0.983	10.732
Quasi-model 26	0.004	0.095	37.058	0.981	11.595
Quasi-model 27	0.004	0.033	37.743	0.981	16.902
Quasi-model 28	0.004	0.076	39.605	0.980	16.634
Quasi-model 29	0.004	0.036	36.738	0.981	12.287
Quasi-model 30	0.004	0.042	36.378	0.981	12.499

Model #4: Two compartments, covariate: creatinine clearance

Model	**KS**	**KCP**	**KPC**	**KI**	**V_c**	**R^2**	**MSE**
Pop-PK, NPAG	0.008	0.983	1.099	0.128	15.100	0.996	4.900
Pop-PK, MAP Bayesian	0.008	0.959	1.118	0.128	15.062	0.992	4.905
Quasi-model 1	0.005	1.528	2.096	0.286	21.534	0.986	57.322
Quasi-model 2	0.007	1.623	2.471	0.089	17.712	0.986	12.424
Quasi-model 3	0.008	2.314	3.072	0.145	18.693	0.988	19.290
Quasi-model 4	0.007	0.514	0.858	0.030	19.653	0.993	5.302
Quasi-model 5	0.008	1.824	1.438	0.264	13.673	0.990	11.158
Quasi-model 6	0.006	2.376	3.074	0.303	20.720	0.984	19.492
Quasi-model 7	0.009	2.852	2.827	0.018	17.697	0.985	24.487
Quasi-model 8	0.007	0.782	1.120	0.291	12.602	0.992	56.124
Quasi-model 9	0.007	2.929	4.347	0.203	16.343	0.984	13.000
Quasi-model 10	0.007	2.926	1.672	0.265	17.760	0.988	25.874
Quasi-model 11	0.009	1.792	1.466	0.291	10.942	0.990	10.156
Quasi-model 12	0.008	3.702	3.598	0.166	16.816	0.984	45.995
Quasi-model 13	0.005	0.998	1.961	0.217	22.645	0.987	24.551
Quasi-model 14	0.008	4.128	3.215	0.123	14.196	0.984	14.264
Quasi-model 15	0.008	3.993	3.766	0.098	18.565	0.986	18.156
Quasi-model 16	0.008	2.389	2.608	0.156	18.938	0.989	9.869
Quasi-model 17	0.007	1.005	1.120	0.044	19.570	0.991	29.703
Quasi-model 18	0.006	1.877	2.765	0.232	21.686	0.986	25.206
Quasi-model 19	0.009	3.414	2.687	0.209	15.029	0.986	43.277
Quasi-model 20	0.005	2.627	4.169	0.300	21.240	0.982	16.273
Quasi-model 21	0.007	2.353	2.790	0.122	17.154	0.985	14.533
Quasi-model 22	0.009	3.500	3.107	0.191	14.462	0.985	33.624
Quasi-model 23	0.010	2.293	1.673	0.169	12.638	0.987	29.671
Quasi-model 24	0.007	2.508	2.412	0.220	20.311	0.987	30.340
Quasi-model 25	0.008	1.788	2.231	0.004	18.217	0.985	13.796

Quasi-model 26	0.005	1.169	2.238	0.313	21.319	0.986	11.211
Quasi-model 27	0.005	0.652	1.061	0.231	23.553	0.990	30.115
Quasi-model 28	0.007	2.753	3.219	0.132	20.645	0.984	11.313
Quasi-model 29	0.012	1.206	1.070	0.004	8.239	0.991	80.837
Quasi-model 30	0.009	2.969	3.061	0.067	16.684	0.985	36.019