

PuMaS NCA Tutorial - Single dose IV administration

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```
using Pumas, PumasTutorials, CSV
```

1 Introduction

In this tutorial, we will cover the fundamentals of performing an NCA analysis with PuMaS of an example dataset in which a single intravenous (IV) bolus dose was administered.

2 The dataset

A single IV bolus dose of 2000 mg was administered to 24 different subjects. Samples were collected every 30 minutes until 21 hours after dose administration. Two different datasets are available, one with 7% of the samples below the limit of quantification (BLQ) and the other with 18% of the samples BLQ.

Let's start reading the dataset. By using the `missingstring` option we are specifying how the missing values are labeled in our dataset.

```
data7BLQ =  
    CSV.read("./tutorials/nca/data/single_dose_IVbolus_7BLQ.csv",missingstring="NA")
```

```
Error: ArgumentError: "./tutorials/nca/data/single_dose_IVbolus_7BLQ.csv" is  
not a valid file
```

```
data7BLQ
```

```
Error: UndefVarError: data7BLQ not defined
```

```
data18BLQ =  
    CSV.read("./tutorials/nca/data/single_dose_IVbolus_18BLQ.csv",missingstring="NA")
```

```
Error: ArgumentError: "./tutorials/nca/data/single_dose_IVbolus_18BLQ.csv"  
is not a valid file
```

```
data18BLQ
```

```
Error: UndefVarError: data18BLQ not defined
```

3 Defining the units

Next we can define time, concentration and dose units so the report includes the units for the pharmacokinetic parameters.

```
timeu = u"hr"  
concu = u"mg/L"  
amtu  = u"mg"
```

mg

4 Defining the population object

Using the `read_nca` function, the next step would be to define the population that we are going to use for the NCA. Within this function we need to specify the dataset, the name of the column with the subject identifier (`id=`), name of the time column (`time=`), name of the concentration column (`conc=`), name of the dose column (`amt=`), the interdose interval (`ii=`) multiplied by the time units, and the route of administration (`route=`).

```
pop7 = read_nca(data7BLQ, id=:ID, time=:time, conc=:DV, amt=:DOSE, ii=24timeu,  
               route=:Formulation,timeu=timeu, concu=concu, amtu=amtu)
```

Error: UndefVarError: data7BLQ not defined

```
pop18 = read_nca(data18BLQ, id=:ID, time=:time, conc=:DV, amt=:DOSE, ii=24timeu,  
                route=:Formulation, timeu=timeu, concu=concu, amtu=amtu)
```

Error: UndefVarError: data18BLQ not defined

Please, note that in the `route=` option the name between quotes should match the name of the route of administration in the dataset. Routes include "iv" or "ev".

Also note that in the function above by default the lower limit of quantification (LLQ) is 0 and concentrations that are below LLQ (BLQ) are dropped.

Let's say we want to specify an LLQ value of 0.4 mg/L, then we need to add `llq=0.4concu` to the function above:

```
pop7 = read_nca(data7BLQ, id=:ID, time=:time, conc=:DV, amt=:DOSE, ii=24timeu,  
               route=:Formulation,timeu=timeu, concu=concu, amtu=amtu,llq=0.4concu)
```

Error: UndefVarError: data7BLQ not defined

```
pop18 = read_nca(data18BLQ, id=:ID, time=:time, conc=:DV, amt=:DOSE, ii=24timeu,  
                route=:Formulation,timeu=timeu, concu=concu, amtu=amtu,llq=0.4concu)
```

Error: UndefVarError: data18BLQ not defined

5 Single PK parameter calculation

We can use different functions to calculate single PK parameters. For example, we can calculate the area under the concentration-time curve from time 0 to the last observation using the linear trapezoidal rule by writing the following code.