MetidaNCA validation report

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1 Introduction and package description

Non-compartment anlysis software.

See documentation: https://pharmcat.github.io/MetidaNCA.jl/dev/

1.1 Validation purpose

The main validation purpose is confirmation by examination and provision of objective evidence that software specifications conform to user needs and intended uses, and that the particular requirements implemented through software can be consistently fulfilled.

1.2 Requirements

- Julia 1.5.* (or higher) installed
- Julia packages from dependence list installed (see Project.toml)

1.3 Developer software life cycle

- Development stage
- Testing procedures development
- Performing testing procedures on local machine
- Push to master branch
- Performing testing procedures with GitHub Actions
- Make pull request to the official registry of general Julia packages (if nessesary)
- Make release (if previous completed)

1.3.1 Versions

- X.Y.Z - patch release (no breaking changes)

- X.Y.# - minor release (may include breaking changes)

- X.#.# - major release (breaking changes, changes in public API)

- 0.#.# - no stable public API

- ≥1.#.# - stable public API

1.4 Build support

1.4.1 Tier 1

- julia-version: 1.5, 1.6

- julia-arch: x64

- os: ubuntu-18.04, macos-10.15, windows-2019

2 Installation

2.1 System information

- Julia version: v"1.4.2"

- Current machine: "x86_64-pc-linux-gnu"

2.2 Installation method

MetidaNCA.jl can be installed by executing the following command in REPL.

```
import Pkg; Pkg.add("MetidaNCA")
```

2.3 Version check

The installation process is checking within each testing job via GitHub Actions. Also GitHub Action chek performed before merging into JuliaRegistries/General repository (see Automatic merging of pull requests).

Current package version:

"0.1.5"

3 Operation qualification

This part of validation based on testing procedures entails running software products under known conditions with defined inputs and documented outcomes that can be compared to their predefined expectations. All documented public API included in testing procedures and part of critical internal methods.

3.1 Coverage

Code coverage report available on Codecov.io. Test procedures include all public API methods check.

- Coverage goal: $\geq 90.0\%$

3.2 Data

Validation data available in the repository and included in the package. See Appendix 1.

3.3 Testing results

```
Pkg.test("MetidaNCA")
```

```
Test Summary:                                       | Pass  Total
   Simple test                                      |   8      8
Test Summary:                                       | Pass  Total
  #1 Linear trapezoidal, Dose 100, Dosetime 0, no tau  |  18     18
Test Summary:                                       | Pass  Total
  #2 Linear up Log down, Dose 100, Dosetime 0.25, tau 9  |  17     17
Test Summary:                                       | Pass  Total
  Linear up Log down, Dose 120, Dosetime 0, tau 12  |  17     17
Test Summary:                                       | Pass  Total
  Log trapezoidal ATM, Dose 120, Dosetime 0, tau 12 |   5      5
Test Summary:                                       | Pass  Total
  Linear up Log down ATM, Dose 120, Dosetime 0, tau 12 |   4      4
Test Summary:                                       | Pass  Total
  Linear trapezoidal, Dose 100, Dosetime 2.0, tau 10 |  15     15
Test Summary:                                       | Pass  Total
  Linear trapezoidal, Dose 100, Dosetime 0.0, tau 100 |  15     15
Test Summary:                                       | Pass  Total
  Linear trapezoidal, Dose 120, Dosetime 0.0, tau 12 |   4      4
Test Summary:                                       | Pass  Total
  Linear up Log down, Dose 100, Dosetime 0.25, tau 9 IV |   1      1
Test Summary:                                       | Pass  Total
  set-get*! tests                                   |   7      7
Test Summary:                                       | Pass  Total
  applylimitrule!                                   |   5      5
Test Summary:                                       |
  kel                                               | No tests
Test Summary:                                       |
  Output                                            | No tests
```

4 Performance qualification

Purpose of this testing procedures to demonstrate performance for some critical tasks. Results from MetidaNCA compared with Phoenix WinNonlin 8.0 results, see Appendix 2.

4.1 Parameter's names description

```
.-----------.-----------------------------------.
|       Name |                        Description |
|     String |                             String |
:-----------+-----------------------------------:
|       Cmax |              Maximum concentration |
|       Tmax |                       Time at Cmax |
|      Cdose |            Concentration at dose time |
|      Clast |           Last non-zero concentration |
|    AUClast |                        AUC to Clast |
|   AUMClast |                       AUMC to Clast |
|     AUCall |                   AUC with all values |
|        Rsq |                           r square |
|       ARsq |                  Adjusted r square |
|        Kel |        Terminal elimination constant |
|         HL |                   Half live or T1/2 |
|      LZint |                          Intercept |
| Clast_pred |                    Predicted Clast |
|     AUCinf |           AUC extrapolated to infinity |
|     AUCpct |        Percentage AUClast from AUCinf |
|    MRTlast |             Mean Residence Time (last) |
|     MRTinf |              Mean Residence Time (inf) |
|      Clinf |                          Clearence |
|      Vzinf |              Volume of distribution |
|     AUCtau |                   AUC in Tau range |
|    AUMCtau |                  AUMC in Tau range |
|  MRTtauinf |                  MRT based on Tau |
|      Cltau |             Clearence in Tau range |
|      Vztau | Volume of distribution in Tau range |
'-----------'-----------------------------------'
```

4.2 Results

4.2.1 Linear-trapezoidal rule; Extravascular

Cmax

```
  Subjct      Value   Reference   Difference
 Float64    Float64     Float64      Float64

     1.0    190.869     190.869          0.0
     2.0    261.177     261.177          0.0
     3.0    105.345     105.345          0.0
     4.0    208.542     208.542          0.0
     5.0    169.334     169.334          0.0
     6.0    154.648     154.648          0.0
     7.0    153.254     153.254          0.0
     8.0    138.327     138.327          0.0
     9.0    167.347     167.347          0.0
```

```
    10.0    125.482      125.482            0.0
```

Tmax

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	1.0	1.0	0.0
2.0	1.0	1.0	0.0
3.0	1.5	1.5	0.0
4.0	1.0	1.0	0.0
5.0	4.0	4.0	0.0
6.0	2.5	2.5	0.0
7.0	2.5	2.5	0.0
8.0	4.0	4.0	0.0
9.0	3.0	3.0	0.0
10.0	2.0	2.0	0.0

Cdose

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	0.0	0.0	0.0
2.0	0.0	0.0	0.0
3.0	0.0	0.0	0.0
4.0	0.0	0.0	0.0
5.0	0.0	0.0	0.0
6.0	0.0	0.0	0.0
7.0	0.0	0.0	0.0
8.0	0.0	0.0	0.0
9.0	0.0	0.0	0.0
10.0	0.0	0.0	0.0

Clast

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	112.846	112.846	0.0
2.0	85.241	85.241	0.0
3.0	67.901	67.901	0.0
4.0	97.625	97.625	0.0
5.0	110.778	110.778	0.0
6.0	69.501	69.501	0.0
7.0	58.051	58.051	0.0
8.0	74.437	74.437	0.0
9.0	93.44	93.44	0.0
10.0	42.191	42.191	0.0

AUClast

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64

```
  1.0    9585.42     9585.42          0.0
  2.0    10112.2     10112.2          0.0
  3.0    5396.55     5396.55          0.0
  4.0    9317.84     9317.84          0.0
  5.0    9561.26     9561.26          0.0
  6.0     6966.6      6966.6          0.0
  7.0    7029.57     7029.57          0.0
  8.0    7110.67     7110.67          0.0
  9.0    8315.08     8315.08          0.0
 10.0    5620.89     5620.89          0.0
```

AUMClast

```
 Subjct      Value   Reference   Difference
 Float64    Float64     Float64      Float64

  1.0    333582.0    333582.0          0.0
  2.0    298701.0    298701.0          0.0
  3.0    186032.0    186032.0          0.0
  4.0    313956.0    313956.0          0.0
  5.0    315182.0    315182.0          0.0
  6.0    226977.0    226977.0          0.0
  7.0    219798.0    219798.0          0.0
  8.0    240526.0    240526.0          0.0
  9.0    277614.0    277614.0          0.0
 10.0    154893.0    154893.0          0.0
```

AUCall

```
 Subjct      Value   Reference   Difference
 Float64    Float64     Float64      Float64

  1.0    9585.42     9585.42          0.0
  2.0    10112.2     10112.2          0.0
  3.0    5396.55     5396.55          0.0
  4.0    9317.84     9317.84          0.0
  5.0    9561.26     9561.26          0.0
  6.0     6966.6      6966.6          0.0
  7.0    7029.57     7029.57          0.0
  8.0    7110.67     7110.67          0.0
  9.0    8315.08     8315.08          0.0
 10.0    5620.89     5620.89          0.0
```

Rsq

```
 Subjct      Value   Reference   Difference
 Float64    Float64     Float64      Float64

  1.0    0.786077    0.786077          0.0
  2.0    0.992764    0.992764          0.0
  3.0    0.813589    0.813589          0.0
  4.0    0.918859    0.918859          0.0
  5.0     0.85336     0.85336          0.0
  6.0    0.950119    0.950119          0.0
  7.0    0.970312    0.970312          0.0
  8.0    0.947969    0.947969          0.0
```

| | 9.0 | 0.947538 | 0.947538 | 0.0 |
| | 10.0 | 0.880923 | 0.880923 | 0.0 |

ARsq

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	0.714769	0.714769	0.0
2.0	0.990351	0.990351	0.0
3.0	0.776307	0.776307	0.0
4.0	0.837717	0.837717	0.0
5.0	0.82892	0.82892	0.0
6.0	0.925179	0.925179	0.0
7.0	0.960416	0.960416	0.0
8.0	0.921954	0.921954	0.0
9.0	0.921307	0.921307	0.0
10.0	0.863912	0.863912	0.0

Kel

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	0.00338474	0.00338474	0.0
2.0	0.0141063	0.0141063	0.0
3.0	0.00329143	0.00329143	0.0
4.0	0.00769534	0.00769534	0.0
5.0	0.00681333	0.00681333	0.0
6.0	0.00769228	0.00769228	0.0
7.0	0.012459	0.012459	0.0
8.0	0.00893008	0.00893008	0.0
9.0	0.00564586	0.00564586	0.0
10.0	0.0171897	0.0171897	0.0

HL

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	204.786	204.786	0.0
2.0	49.1374	49.1374	0.0
3.0	210.591	210.591	0.0
4.0	90.0736	90.0736	0.0
5.0	101.734	101.734	0.0
6.0	90.1095	90.1094	0.0001
7.0	55.6345	55.6345	0.0
8.0	77.6194	77.6194	0.0
9.0	122.771	122.771	0.0
10.0	40.3233	40.3233	0.0

Clast_pred

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64

```
    1.0   117.306    117.306         0.0
    2.0   82.5367    82.5367         0.0
    3.0   66.9311    66.9311         0.0
    4.0   100.768    100.768         0.0
    5.0   105.298    105.298         0.0
    6.0   71.9399    71.9399         0.0
    7.0   61.1727    61.1727         0.0
    8.0   75.6043    75.6043         0.0
    9.0   93.7618    93.7618         0.0
   10.0   38.8109    38.8109         0.0
```

AUCinf

```
  Subjct     Value   Reference  Difference
 Float64    Float64     Float64     Float64

    1.0    42925.0     42925.0         0.0
    2.0    16154.9     16154.9         0.0
    3.0    26026.2     26026.2         0.0
    4.0    22004.1     22004.1         0.0
    5.0    25820.3     25820.3         0.0
    6.0    16001.8     16001.8         0.0
    7.0    11689.0     11689.0         0.0
    8.0    15446.2     15446.2         0.0
    9.0    24865.2     24865.2         0.0
   10.0    8075.32     8075.32         0.0
```

AUCpct

```
  Subjct     Value   Reference  Difference
 Float64    Float64     Float64     Float64

    1.0    77.6694     77.6694         0.0
    2.0     37.405      37.405         0.0
    3.0    79.2649     79.2649         0.0
    4.0    57.6541     57.6541         0.0
    5.0      62.97       62.97         0.0
    6.0    56.4636     56.4636         0.0
    7.0    39.8614     39.8614         0.0
    8.0    53.9649     53.9649         0.0
    9.0    66.5594     66.5594         0.0
   10.0    30.3942     30.3942         0.0
```

MRTlast

```
  Subjct     Value   Reference  Difference
 Float64    Float64     Float64     Float64

    1.0     34.801      34.801         0.0
    2.0    29.5388     29.5388         0.0
    3.0    34.4724     34.4724         0.0
    4.0    33.6941     33.6941         0.0
    5.0    32.9644     32.9644         0.0
    6.0    32.5808     32.5808         0.0
    7.0    31.2676     31.2676         0.0
```

```
   8.0  33.8261    33.8261          0.0
   9.0  33.3868    33.3868          0.0
  10.0  27.5567    27.5567          0.0
```

MRTinf

```
 Subjct    Value   Reference  Difference
Float64   Float64    Float64     Float64

   1.0   293.162    293.162          0.0
   2.0   71.9379    71.9379          0.0
   3.0   305.041    305.041          0.0
   4.0     130.7      130.7          0.0
   5.0   149.967    149.967          0.0
   6.0   128.241    128.241          0.0
   7.0   79.4983    79.4983          0.0
   8.0   114.857    114.857          0.0
   9.0   176.978    176.978          0.0
  10.0   58.7464    58.7464          0.0
```

Clinf

```
 Subjct      Value    Reference  Difference
Float64     Float64      Float64     Float64

   1.0   0.00232964   0.00232964          0.0
   2.0   0.00619006   0.00619006          0.0
   3.0   0.00384228   0.00384228          0.0
   4.0   0.00454461   0.00454461          0.0
   5.0   0.00387293   0.00387293          0.0
   6.0   0.00624931   0.00624931          0.0
   7.0   0.00855509   0.00855509          0.0
   8.0   0.00647408   0.00647408          0.0
   9.0   0.00402168   0.00402168          0.0
  10.0    0.0123834    0.0123834          0.0
```

Vzinf

```
 Subjct     Value   Reference  Difference
Float64    Float64     Float64     Float64

   1.0   0.688278   0.688278          0.0
   2.0   0.438815   0.438815          0.0
   3.0    1.16736    1.16736          0.0
   4.0   0.590566   0.590566          0.0
   5.0   0.568434   0.568434          0.0
   6.0   0.812414   0.812414          0.0
   7.0   0.686662   0.686662          0.0
   8.0   0.724974   0.724974          0.0
   9.0   0.712323   0.712323          0.0
  10.0   0.720395   0.720395          0.0
```

4.2.2 Linear-Up Log-Down; Extravascular; Dosetime 0.25; Tau 9

Cmax

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	190.869	190.869	0.0
2.0	261.177	261.177	0.0
3.0	105.345	105.345	0.0
4.0	208.542	208.542	0.0
5.0	169.334	169.334	0.0
6.0	154.648	154.648	0.0
7.0	153.254	153.254	0.0
8.0	138.327	138.327	0.0
9.0	167.347	167.347	0.0
10.0	125.482	125.482	0.0

Tmax

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	1.0	1.0	0.0
2.0	1.0	1.0	0.0
3.0	1.5	1.5	0.0
4.0	1.0	1.0	0.0
5.0	4.0	4.0	0.0
6.0	2.5	2.5	0.0
7.0	2.5	2.5	0.0
8.0	4.0	4.0	0.0
9.0	3.0	3.0	0.0
10.0	2.0	2.0	0.0

Cdose

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	121.239	121.239	0.0
2.0	62.222	62.222	0.0
3.0	49.849	49.849	0.0
4.0	52.421	52.421	0.0
5.0	0.0	0.0	0.0
6.0	57.882	57.882	0.0
7.0	19.95	19.95	0.0
8.0	22.724	22.724	0.0
9.0	105.438	105.438	0.0
10.0	13.634	13.634	0.0

Clast

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	112.846	112.846	0.0
2.0	85.241	85.241	0.0
3.0	67.901	67.901	0.0
4.0	97.625	97.625	0.0

```
   5.0   110.778    110.778         0.0
   6.0    69.501     69.501         0.0
   7.0    58.051     58.051         0.0
   8.0    74.437     74.437         0.0
   9.0     93.44      93.44         0.0
  10.0    42.191     42.191         0.0
```

AUClast

```
 Subjct     Value   Reference   Difference
Float64    Float64     Float64      Float64

   1.0    9566.6     9566.6          0.0
   2.0   10054.3    10054.3          0.0
   3.0   5392.46    5392.46          0.0
   4.0    9297.1     9297.1          0.0
   5.0   9519.18    9519.18          0.0
   6.0   6948.99    6948.99          0.0
   7.0   6988.77    6988.77          0.0
   8.0   7058.82    7058.82          0.0
   9.0   8302.37    8302.37          0.0
  10.0   5486.84    5486.84          0.0
```

AUCtau

```
 Subjct     Value   Reference   Difference
Float64    Float64     Float64      Float64

   1.0   1268.28    1268.28          0.0
   2.0   1831.82    1831.82          0.0
   3.0   754.649    754.649          0.0
   4.0   1336.48    1336.48          0.0
   5.0    1310.9     1310.9          0.0
   6.0   1114.24    1114.24          0.0
   7.0   1079.37    1079.37          0.0
   8.0    766.62     766.62          0.0
   9.0   1219.63    1219.63          0.0
  10.0   970.306    970.306          0.0
```

AUMCtau

```
 Subjct     Value   Reference   Difference
Float64    Float64     Float64      Float64

   1.0    5477.2     5477.2          0.0
   2.0   8367.57    8367.57          0.0
   3.0   3455.35    3455.35          0.0
   4.0   6014.65    6014.65          0.0
   5.0   6609.79    6609.79          0.0
   6.0   5064.72    5064.72          0.0
   7.0   4976.96    4976.96          0.0
   8.0   2863.01    2863.01          0.0
   9.0   5386.88    5386.88          0.0
  10.0   4713.48    4713.48          0.0
```

AUCall

Subjct	Value	Reference	Difference
Float64	Float64	Float64	Float64
1.0	9566.6	9566.6	0.0
2.0	10054.3	10054.3	0.0
3.0	5392.46	5392.46	0.0
4.0	9297.1	9297.1	0.0
5.0	9519.18	9519.18	0.0
6.0	6948.99	6948.99	0.0
7.0	6988.77	6988.77	0.0
8.0	7058.82	7058.82	0.0
9.0	8302.37	8302.37	0.0
10.0	5486.84	5486.84	0.0

Rsq

Subjct	Value	Reference	Difference
Float64	Float64	Float64	Float64
1.0	0.786077	0.786077	0.0
2.0	0.992764	0.992764	0.0
3.0	0.813589	0.813589	0.0
4.0	0.918859	0.918859	0.0
5.0	0.85336	0.85336	0.0
6.0	0.950119	0.950119	0.0
7.0	0.970312	0.970312	0.0
8.0	0.947969	0.947969	0.0
9.0	0.947538	0.947538	0.0
10.0	0.880923	0.880923	0.0

ARsq

Subjct	Value	Reference	Difference
Float64	Float64	Float64	Float64
1.0	0.714769	0.714769	0.0
2.0	0.990351	0.990351	0.0
3.0	0.776307	0.776307	0.0
4.0	0.837717	0.837717	0.0
5.0	0.82892	0.82892	0.0
6.0	0.925179	0.925179	0.0
7.0	0.960416	0.960416	0.0
8.0	0.921954	0.921954	0.0
9.0	0.921307	0.921307	0.0
10.0	0.863912	0.863912	0.0

Kel

Subjct	Value	Reference	Difference
Float64	Float64	Float64	Float64
1.0	0.00338474	0.00338474	0.0
2.0	0.0141063	0.0141063	0.0
3.0	0.00329143	0.00329143	0.0

```
    4.0   0.00769534   0.00769534              0.0
    5.0   0.00681333   0.00681333              0.0
    6.0   0.00769228   0.00769228              0.0
    7.0     0.012459     0.012459              0.0
    8.0   0.00893008   0.00893008              0.0
    9.0   0.00564586   0.00564586              0.0
   10.0    0.0171897    0.0171897              0.0
```

HL

```
  Subjct      Value   Reference   Difference
 Float64    Float64     Float64      Float64

    1.0     204.786     204.786          0.0
    2.0     49.1374     49.1374          0.0
    3.0     210.591     210.591          0.0
    4.0     90.0736     90.0736          0.0
    5.0     101.734     101.734          0.0
    6.0     90.1095     90.1095          0.0
    7.0     55.6345     55.6345          0.0
    8.0     77.6194     77.6194          0.0
    9.0     122.771     122.771          0.0
   10.0     40.3233     40.3233          0.0
```

Clast_pred

```
  Subjct      Value   Reference   Difference
 Float64    Float64     Float64      Float64

    1.0     117.306     117.306          0.0
    2.0     82.5367     82.5367          0.0
    3.0     66.9311     66.9311          0.0
    4.0     100.768     100.768          0.0
    5.0     105.298     105.298          0.0
    6.0     71.9399     71.9399          0.0
    7.0     61.1727     61.1727          0.0
    8.0     75.6043     75.6043          0.0
    9.0     93.7618     93.7618          0.0
   10.0     38.8109     38.8109          0.0
```

AUCinf

```
  Subjct      Value   Reference   Difference
 Float64    Float64     Float64      Float64

    1.0     42906.2     42906.2          0.0
    2.0     16097.0     16097.0          0.0
    3.0     26022.1     26022.1          0.0
    4.0     21983.3     21983.3          0.0
    5.0     25778.2     25778.2          0.0
    6.0     15984.1     15984.1          0.0
    7.0     11648.2     11648.2          0.0
    8.0     15394.4     15394.4          0.0
    9.0     24852.5     24852.5          0.0
   10.0     7941.27     7941.27          0.0
```

AUCpct

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	77.7035	77.7035	0.0
2.0	37.5395	37.5395	0.0
3.0	79.2774	79.2774	0.0
4.0	57.7084	57.7084	0.0
5.0	63.0727	63.0727	0.0
6.0	56.5258	56.5258	0.0
7.0	40.001	40.001	0.0
8.0	54.1467	54.1467	0.0
9.0	66.5935	66.5935	0.0
10.0	30.9073	30.9073	0.0

MRTtauinf

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	299.792	299.792	0.0
2.0	74.655	74.655	0.0
3.0	305.92	305.92	0.0
4.0	143.538	143.538	0.0
5.0	173.022	173.022	0.0
6.0	124.653	124.653	0.0
7.0	92.7359	92.7359	0.0
8.0	175.462	175.462	0.0
9.0	178.811	178.811	0.0
10.0	69.5163	69.5163	0.0

Cltau

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	0.0788472	0.0788472	0.0
2.0	0.0545905	0.0545905	0.0
3.0	0.132512	0.132512	0.0
4.0	0.0748234	0.0748234	0.0
5.0	0.0762832	0.0762832	0.0
6.0	0.0897472	0.0897472	0.0
7.0	0.0926469	0.0926469	0.0
8.0	0.130443	0.130443	0.0
9.0	0.081992	0.081992	0.0
10.0	0.10306	0.10306	0.0

Vztau

| Subjct | Value | Reference | Difference |
Float64	Float64	Float64	Float64
1.0	23.2949	23.2949	0.0
2.0	3.86993	3.86993	0.0

```
 3.0   40.2597    40.2597         0.0
 4.0    9.7232     9.7232         0.0
 5.0   11.1962    11.1962         0.0
 6.0   11.6672    11.6672         0.0
 7.0    7.43617    7.43617        0.0
 8.0   14.6071    14.6071         0.0
 9.0   14.5225    14.5225         0.0
10.0    5.99545    5.99545        0.0
```

5   Glossary

- Installation qualification (IQ) - Establishing confidence that process equipment and ancillary systems are compliant with appropriate codes and approved design intentions, and that manufacturer's recommendations are suitably considered.

- Operational qualification (OQ) Establishing confidence that process equipment and sub-systems are capable of consistently operating within established limits and tolerances.

- Product performance qualification (PQ) - Establishing confidence through appropriate testing that the finished product produced by a specified process meets all release requirements for functionality and safety.

- Repository - GitHub repository: https://github.com/PharmCat/MetidaNCA.jl

- Master branch - main branch on GitHub (link).

- Current machine - pc that used for validation report generating.

6   Reference

- [General Principles of Software Validation; Final Guidance for Industry and FDA Staff](#)

- [Guidance for Industry Process Validation: General Principles and Practices](#)

- [Glossary of Computer System Software Development Terminology](#)

7   Appendix 1

| Subject | Formulation | Time | Concentration |
Int64	String	Float64	Float64
1	T	0.0	0.0
1	T	0.5	178.949
1	T	1.0	190.869
1	T	1.5	164.927
1	T	2.0	139.962
1	T	2.5	129.59
1	T	3.0	131.369
1	T	4.0	150.854
1	T	5.0	121.239

	1		T	6.0	139.229
	1		T	8.0	128.52
	1		T	10.0	143.243
	1		T	12.0	144.964
	1		T	24.0	133.16
	1		T	48.0	137.271
	1		T	72.0	112.846
	2		R	0.0	0.0
	2		R	0.5	62.222
	2		R	1.0	261.177
	2		R	1.5	234.063
	2		R	2.0	234.091
	2		R	2.5	222.881
	2		R	3.0	213.896
	2		R	4.0	196.026
	2		R	5.0	199.634
	2		R	6.0	196.037
	2		R	8.0	213.352
	2		R	10.0	200.088
	2		R	12.0	196.035
	2		R	24.0	160.338
	2		R	48.0	110.28
	2		R	72.0	85.241
	3		R	0.0	0.0
	3		R	0.5	49.849
	3		R	1.0	77.367
	3		R	1.5	105.345
	3		R	2.0	100.943
	3		R	2.5	72.746
	3		R	3.0	69.985
	3		R	4.0	93.565
	3		R	5.0	91.981
	3		R	6.0	82.71
	3		R	8.0	84.205
	3		R	10.0	85.342
	3		R	12.0	76.027
	3		R	24.0	81.259
	3		R	48.0	70.107
	3		R	72.0	67.901
	4		R	0.0	0.0
	4		R	0.5	52.421
	4		R	1.0	208.542
	4		R	1.5	188.923
	4		R	2.0	165.177
	4		R	2.5	146.996
	4		R	3.0	152.701
	4		R	4.0	154.345
	4		R	5.0	128.398
	4		R	6.0	149.807
	4		R	8.0	151.066
	4		R	10.0	136.819
	4		R	12.0	132.257
	4		R	24.0	141.247
	4		R	48.0	129.138
	4		R	72.0	97.625
	5		T	0.0	0.0
	5		T	0.5	0.0
	5		T	1.0	9.545
	5		T	1.5	153.964

5	T	2.0	152.34
5	T	2.5	151.452
5	T	3.0	161.312
5	T	4.0	169.334
5	T	5.0	162.907
5	T	6.0	166.651
5	T	8.0	168.668
5	T	10.0	155.103
5	T	12.0	154.066
5	T	24.0	162.974
5	T	48.0	109.814
5	T	72.0	110.778
6	T	0.0	0.0
6	T	0.5	57.882
6	T	1.0	100.498
6	T	1.5	138.651
6	T	2.0	147.287
6	T	2.5	154.648
6	T	3.0	122.316
6	T	4.0	132.857
6	T	5.0	126.067
6	T	6.0	140.466
6	T	8.0	115.542
6	T	10.0	102.16
6	T	12.0	113.751
6	T	24.0	101.049
6	T	48.0	92.55
6	T	72.0	69.501
7	R	0.0	0.0
7	R	0.5	19.95
7	R	1.0	128.405
7	R	1.5	136.807
7	R	2.0	113.109
7	R	2.5	153.254
7	R	3.0	123.606
7	R	4.0	142.655
7	R	5.0	112.347
7	R	6.0	139.919
7	R	8.0	105.513
7	R	10.0	134.408
7	R	12.0	123.37
7	R	24.0	110.511
7	R	48.0	90.291
7	R	72.0	58.051
8	R	0.0	0.0
8	R	0.5	136.91
8	R	1.0	126.646
8	R	1.5	118.5
8	R	2.0	134.926
8	R	2.5	113.213
8	R	3.0	130.896
8	R	4.0	138.327
8	R	5.0	22.724
8	R	6.0	53.774
8	R	8.0	55.107
8	R	10.0	102.871
8	R	12.0	134.133
8	R	24.0	108.021
8	R	48.0	98.466

```
|       8 |        R |    72.0 |         74.437 |
|       9 |        T |     0.0 |            0.0 |
|       9 |        T |     0.5 |        113.362 |
|       9 |        T |     1.0 |        128.273 |
|       9 |        T |     1.5 |        125.395 |
|       9 |        T |     2.0 |        146.933 |
|       9 |        T |     2.5 |        140.559 |
|       9 |        T |     3.0 |        167.347 |
|       9 |        T |     4.0 |        157.504 |
|       9 |        T |     5.0 |         141.35 |
|       9 |        T |     6.0 |        140.282 |
|       9 |        T |     8.0 |        105.438 |
|       9 |        T |    10.0 |        164.843 |
|       9 |        T |    12.0 |         135.58 |
|       9 |        T |    24.0 |        117.125 |
|       9 |        T |    48.0 |        109.745 |
|       9 |        T |    72.0 |          93.44 |
|      10 |        R |     0.0 |            0.0 |
|      10 |        R |     0.5 |         13.634 |
|      10 |        R |     1.0 |         62.561 |
|      10 |        R |     1.5 |        112.655 |
|      10 |        R |     2.0 |        125.482 |
|      10 |        R |     2.5 |        116.255 |
|      10 |        R |     3.0 |        112.674 |
|      10 |        R |     4.0 |        116.986 |
|      10 |        R |     5.0 |         119.81 |
|      10 |        R |     6.0 |        107.557 |
|      10 |        R |     8.0 |        120.479 |
|      10 |        R |    10.0 |        124.171 |
|      10 |        R |    12.0 |        106.476 |
|      10 |        R |    24.0 |        116.508 |
|      10 |        R |    48.0 |         45.204 |
|      10 |        R |    72.0 |         42.191 |
'---------'-------------'---------'----------------'
```

8 Appendix 2

See Appendix2.1.pdf, Appendix2.2.pdf.