Software Requirements

**R package**

**DAS-COMBAT**

**Document approval and release**

The signatures in the table below ensure that all items in this Software Specifications are accepted by PAMGENE Den Bosch, Netherlands. PAMGENE is responsible for the review and approval of this Software Specifications.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **-** | **Name** | **Function** | **Signature** | **Date** |
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**Version history**

|  |  |  |  |
| --- | --- | --- | --- |
| **Version** | **Author** | **Date** | **Description** |
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**INDEX Page**

[1. Introduction 4](#_Toc27132433)

[2. Scope 4](#_Toc27132434)

[2.1. Out of Scope 5](#_Toc27132435)

[3. Definitions 5](#_Toc27132436)

[4. Software requirements Analysis 6](#_Toc27132437)

[4.1. System requirements 6](#_Toc27132438)

[4.2. Software requirements content 6](#_Toc27132439)

[4.3. Risk Control Measures in Software Requirements [Class B, C] 11](#_Toc27132440)

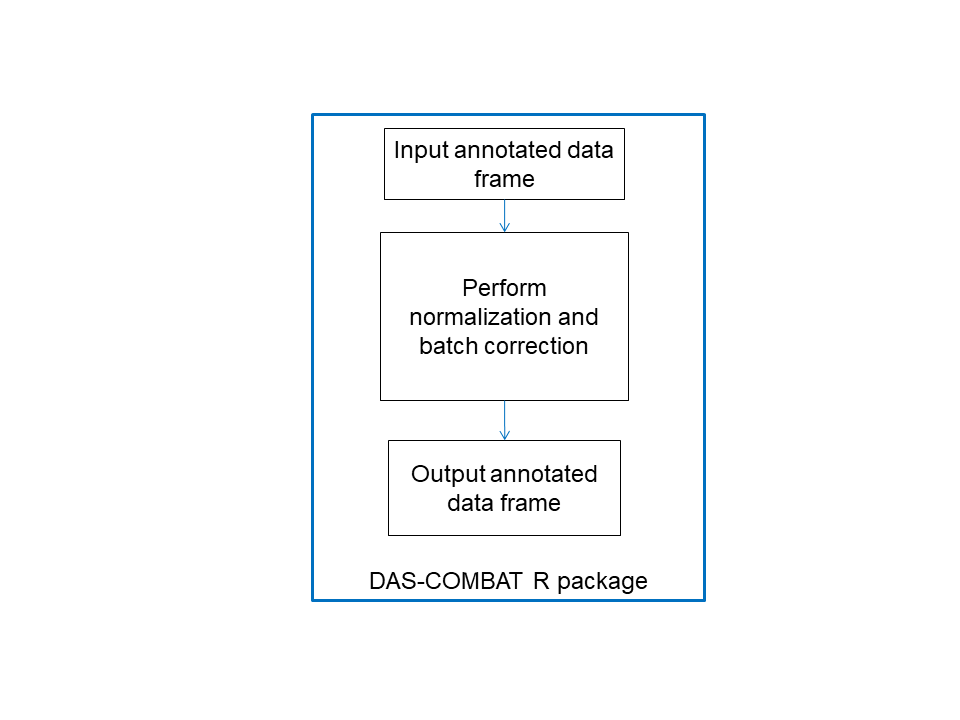
[5. Appendix 11](#_Toc27132441)

# Introduction

This document defines the software capabilities that must be present for the user to perform the functionalities provided by the software product (SP, i.e. DAS-COMBAT).

# Scope

This software requirement is for the DAS-COMBAT R Package. It is an R Package used in the DAS-NORMALIZE and performs batch correction. The input of the R Package is a pre-processedkinase activity profile measured on DAS and REF using any PAMCHIP. The input is received via the R PACKAGE ENVIRONMENT. The output of the DAS-COMBAT is a corrected version of the input data.



A schematic overview of the R Package architecture is shown above. The DAS-COMBAT R Package performs the following process:

* Receives kinase activity measurement profiles as an annotated data frame
* Calculates the batch correction
* Returns the corrected values as a data frame

## Out of Scope

The R Package DAS-COMBAT will be used with the DAS-NORMALIZE a module of the DAS-PLATFORM. The DAS-PLATFORM is used for image analysis and pre-processing of the measurement data. This legacy software is out of scope for these requirements.

# Definitions

SP Software Product, (i.e. DAS-COMBAT)

|  |  |
| --- | --- |
| SOUP | Software of unknown provenance |
|  |  |

# Software requirements Analysis

## System requirements

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
| 002 | DAS-COMBAT receives pre-processed kinase activity profile. The data can be represented as an annotated data frame with columns representing arrays and rows representing the (named) peptides. The elements of the matrix are the measurement values that represent the phosphorylation signal. See requirement 21 for detail on the input format. | C |
| 003A1 | The results for DAS-COMBAT are batch corrected of the input data table but with correct values. | C |
| 004 | Because the pre-processing performed on the kinase activity profile (see 001) is done using Exposure Time Integration the range of the measurement values on input will be between -200 and 100000 for each value. | C |
| 005 | Exceptions raised by the DAS-COMBAT will be transmitted to the DAS-COMBAT via the R PACKAGE ENVIRONMENT. | C |
| 006 | The kinase activity profiles are measured using any PamChip | C |

***[Define and document software system requirements from the system level requirement]***

## Software requirements content

### Functional and capability requirements

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
| 011A | SP calculates a batch model, i.e. fits a model | C |
| 011B | SP calculates a batch correction i.e. applies a model | C |
| 014A1 | Table 1 is called “**Y data table”** and defined in req21A1 | C |
| 014A2 | Table 2 is called “**aFITmodel data**  **table”** and defined in req21A2 |  |
| 015 | The applicable calculations are performed every time the R Package is executed. | C |
| 017A1 | The corrected table is the same format as the input database (see req 021A) | C |
| 018A11 | The batch model is defined for: No reference, mean.only = FALSE  Y is the input data  dascombat::fit(Y, mean.only=FALSE, REF=FALSE)  *what is returned batch mean and batch scale, all the data Y* |  |
| 018A12 | The batch model is defined for: No reference, mean = TRUE  dascombat::fit(Y, mean.only=TRUE, REF=FALSE)  *what is returned batch mean based on all the data Y* |  |
| 018A13 | The batch model is defined for: ref.batch, mean.only = FALSE  dascombat::fit(Y, mean.only=FALSE, REF=TRUE)  *what is returned batch mean and batch scale, all the REF data of Y is used to adjust by REF* |  |
| 018A14 | The batch model is defined for: ref.batch, mean.only = TRUE  dascombat::fit(Y, mean.only=TRUE, REF=TRUE)  *returned batch mean based on all the REF data in Y, adjusted by REF* |  |
| 018A16 | The batch correction is defined for: No reference, mean.only = FALSE  dascombat::apply(Y, mean.only=FALSE, REF=FALSE, MODEL= aFITtable)  *returned corrected Y* |  |
| 018A17 | The batch correction is defined for: No reference, mean = TRUE  dascombat::apply(Y, mean.only=TRUE, REF=FALSE, MODEL= aFITtable)  *returned corrected Y* |  |
| 018A18 | The batch correction is defined for: ref.batch, mean.only = FALSE  dascombat::apply(Y, mean.only=FALSE, REF=TRUE, MODEL= aFITtable)  *returned corrected Y* |  |
| 018A19 | The batch correction is defined for: ref.batch, mean.only = TRUE  dascombat::apply(Y, mean.only=TRUE, REF=TRUE, MODEL= aFITtable)  *returned corrected Y* |  |

[Describe the functional and capability requirements that the system need to fulfill]

* *Performance (e.g. purpose of software, timing requirements)*
* *Physical characteristics (e.g. code language, platform, operating system),*
* *Computing environment (e.g. hardware, memory size, processing unit, time zone, network infrastructure) under which the software needs to perform*
* *Need for compatibility with upgrades or multiple SOUP or other device versions*

### Software system inputs and outputs

|  |  |  |
| --- | --- | --- |
| **Req.#** | Description | **Class** |
| 020 | The input is retrieved using the API function of the R PACKAGE ENVIRONMENT | C |
| 021A1 | Data is as an annotated data frame represents a peptide measurement. For each row the following columns are included:  "value"  "Barcode"  "Array"  "ID"  An additional column with a batch factor (i.e. RUNID) | C |
| 021A2 | Data is retrieved as an annotated data frame represents a peptide measurement. For each row the following columns are included:  "mean"  "scale"  "mean\_refadjusted"  "scale\_refadjusted"  "Barcode"  "Array"  "ID"  An additional column with a batch factor (i.e. RUNID) |  |
| 022 | Complete arrays only. The DAS-COMBAT checks if there are any missing values. If that is the case the following exception is raised: “missing values are not allowed”. | C |
| 024 | Input matrix columns represent the annotation of the peptide measurement | C |
| 026A1 | Data is returned as an annotated data frame | C |

*[List the inputs and outputs of the system software e.g.:]*

* *Data characteristics (e.g. numerical, alpha numeric, format)*
* *Ranges*
* *Limits*
* *Defaults*

### Interfaces between the software systems and other systems

Not applicable

|  |  |  |
| --- | --- | --- |
| **Req.#** | Description | **Class** |
|  |  |  |
|  |  |  |
|  |  |  |

[Note that if the calculation is done using separate R-packages these should be listed here].

*[List each system interface and identify the functionality of the software to accomplish the system requirement and the interface description to match the system]*

### Software driven alarms, warnings and operator messages

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
| 037 | Any exception returns an informational error message to the DAS-COMBAT via the R PACKAGE ENVIRONMENT. | C |
| 038 | Any exception will result in the execution of the DAS-COMBAT being stopped and the error is non-recoverable. | C |
| 040 | An exception is raised when the input matrix contains any missing values. The informational message is “Missing values are not allowed” | C |
| 041 | An exception is raised when the measurement values are outside of the range defined in req 005. The informational message is:  “Measurement values out of range” | C |
| 42 | Check that the column names of the input data are equal to that defined in req 21A1 and 21A2 |  |
|  |  |  |
|  |  |  |
|  |  |  |

*[Describe all requirements and functionalities that alarm, warning and operator need to fulfill within the system]*

### Security requirements

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
|  | Not applicable the DAS-Platform takes care of security requirements |  |
|  |  |  |

*[Write down the security requirements of the software system e.g.:]*

* *Related to the compromise of sensitive information*
* *Authentication*
* *Authorization*
* *Audit trail*
* *Communication integrity*
* *System security/malware protection*

### User interface requirements implemented by the software

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
|  | Not applicable, the user interface is handled by the DAS-COMBAT | C |

*[List Interface Requirements that need to be implemented by the software, see examples below*:

* *Support for manual operations*
* *Human equipment interactions*
* *Constraints on personnel*
* *Area needing concentrated human attention]*

### Data definition and database requirements

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
| 60 | The Y data table should contain the batch factor values as in aFitModel table |  |

***[****Describe data definition and database requirements below:]*

* *Form*
* *Fit*
* ***Functions***

### Installation and acceptance requirements of the delivered medical device software at the operation and maintenance site

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
| 050 | SP requires passing a test calculation comparing the result to known output. | C |

***[****Specify any installation and acceptance requirements of the delivered software at the operation and maintenance site]*

### Requirements related to methods of operation and maintenance

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
|  | Not applicable, covered by the DAS-COMBAT and DAS laboratory procedures. |  |

*[Identify any applicable requirements related method of operation and maintenance]*

### Requirements related to IT-network aspects

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
|  | Not applicable. DAS-COMBAT is a calculation R Package on single PC. |  |

*[- Network alarms, warnings and operator messages*

* *Network protocols*
* *Handling of unavailability of network services]*

### User Maintenance Requirements

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
|  | Not applicable |  |

*[Identify means for user maintenance requirements]*

### Regulatory Requirements

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
|  | Not applicable for DAS-COMBAT separately. |  |

*[Identify regulatory requirements for the software specifications]*

## Risk Control Measures in Software Requirements [Class B, C]

|  |  |  |
| --- | --- | --- |
| **Req.#** | **Description** | **Class** |
|  |  | C |
|  |  | C |

*[Identify how risk control measures should be implemented.*

*Note: These requirements might not be available at the beginning of the software development and can change as the software is designed and risk control measures are further defined.]*

# Appendix