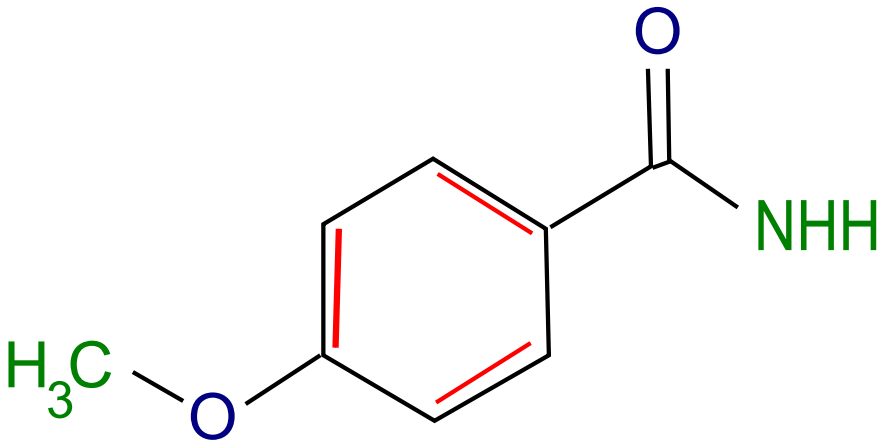
Requirements Document for UM-BBD/PPS



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Contents

Part I

Glossary

Administrator
The administrator in this document is the server administrator, a computer scientist which maintains the server system.

API
API (Application programming interface) builds the bridge between the core system and the extensions. The API is provided by the core system and offers the possibility to the extensions to interact with the elements of the system (e.g. database, input and output devices). The more extended the API is the more can other developers augment the functionality of the system.

Compound
A chemical substance consisting of two or more different chemical elements.

Compound database
A structured collection of chemical substances that consist of two or more different chemical elements. A database containing information about compounds, elements and other objects that participate in the degradation process. It also contains references to articles and publications about the entries in the database.

Core system
See system.

Database (db)
A database is a structured collection of data. Simplifying it is a digital table where each row is an entry in the database.

Degredation tree
A graph that has compounds as its edges and rules as its vertices and shows a decomposition of compounds according to the stated rules

EULA
End-user license agreement is the contract between the licensor and purchaser, establishing the purchaser's right to use the software.

Extension
Extension is a piece of software written by developers that can but must not belong to the main development team. It extends or changes the functionality of the system but is in general not needed for the core system to work. Extensions can easily be added (installed) and removed from the system. Some extensions may need other extensions for working properly. The communication between the extension and the system is realized by the API.

Icon
Icon is a small image or symbol serving as quick and intuitive representation of a software tool, function or system status.

Interface
Interface - An Interface provides the possibility for other programs to communicate and send requests to the software offering the interface.

Mass spectrometry
Mass spectrometry is an analytical technique that measures the mass-to-charge ratio of charged particles.

Module
See extension.

Mol2
A data format for storing and exchanging 3D molecule models.

NMR
NMR spectroscopy is a research technique that exploits the magnetic properties of certain atomic nuclei to determine physical or chemical properties of atoms or the molecules in which they are contained.

Opentox
Opentox is a open framework which may be used as an enabling platform for the creation of predictive toxicology application.

Package
A package is a collection of different compounds and rules. Packages are used to structure the data.

Query
Query is a request for information retrieval with database and information systems. Queries can be both user-oriented and internal system behaviour. A user can place a query to the system (e.g. search for a compound or a degredation path) and the system can itself place a query to its database.

Rule database
A structured collection of transformation rules that are applied to compounds of the degradation process . A database containing degradation rules. It contains both the information needed for the degradation prediction system and information about the chemical reactions these rules model.

SDF
A chemical-data file format (structure data format).

SMILES
A specification in form of a line notation for describing the structure of chemical molecules using short ASCII strings.

System
System describes all elements or components of this application or software including its database, input and output devices and all installed

extensions. The core system is the center of the system. It provides the basis (API) for all extensions and is in charge of the main functionalities. Core system and extensions form up the system.

User area
The user area is a view where registered users can see and create their packages, compounds and rules. Also there are the user settings (e.g. for changing ones used packages and extensions).

XML
Extensible markup language is a markup language to encode documents in a format that is both human-readable and machine-readable and easy to process.

Part II

User Requirements

UR001

Statement *A user with at least B. Sc. Chemistry, B. Sc. Biology (or comparable) shall be able to use all the offered functions of the system after a short introduction.*

Priority *A*

UR002

Statement *The graphical interface shall be easy to use.*

Priority *A*

UR003

Statement *Higher resolution shall be possible with respect to rules and compounds. It means that it shall be possibel to zoom in the different compound- and path-graphics.*

Priority *B*

UR004

Statement *A parallel use of the website by a to be specified number of users shall be possible.*

Priority *A*

UR005

Statement *It shall be easy to configure the system: to make one own's server or to use the local version.*

Priority *A*

UR006

Statement *The system shall be accessible not only as a website, but also as a desktop application.*

Priority *A*

UR007

Statement *The system shall be accessible not only via a graphical interface, but also via a terminal.*

Priority *A*

UR008

Statement *It shall be easy to clone and synchronize the system.*

Priority *A*

UR009

Statement *It shall be easy to add new information into the databases - new compounds, as well as new rules.*

Priority *A*

Source *Prof. Kramer*

UR010

Statement *The rules shall be easily interchangeable. Thus, it shall be possible to easily choose the rules/sets of rules that one wants to apply to the biodegradation process.*

Priority *A*

UR011

Statement *Each rule shall include a reference which provides evidence for its correctness, as well as a name of the process that is exemplified by it, e.g. oxidation process.*

Priority *A*

Source *Carsten Prasse*

UR012

Statement *All the information from the old version of the databases shall be adopted by the new databases.*

Priority *A*

UR013

Statement *The structure of the databases shall be improved.*

Priority *A*

UR014

Statement *It shall be possible to submit the information to the biodegradation prediction system in different formats.*

Priority *A*

UR015

Statement *There shall exist not only public, but also private rules that every user can add.*

Priority *A*

UR016

Statement *Extraction of specific paths (in a certain format) from the pathway map shall be possible, so that they can be accessed for futher use, e.g. preparation of a presentation.*

Priority *B*

Source *Carsten Prasse*

UR017

Statement *It shall be possible to add extensible vectors of features for every rule and compound:*

- *List of environmental conditions for each reaction shall be accessible - e.g. the organisms that are involved,the natural environment in which it is taking place - so that specific pathway predictions are enabled that ground on the given environmental conditions.*
- *Additional chemical data shall be implemented for compounds - e.g physico-chemical properties, MS fragmentation, monoisotopic masses - if necessary using the links of the system with other databases.*

Priority *A*

Source *Carsten Prasse*

UR018

Statement *An additional feature should be included to every rule. That is the time that the degradation process takes. This would allow to consider only those biodegradation results in the prediction whose degdaration process is less/equal/more than the given time.*

Priority *B*

Source *Carsten Prasse*

UR019

Statement *Higher specificity of pathway predictions shall be enabled. This shall happen due to taking the relevance of chemical molecules in the neighbourhood into account when applying certain rules on a given molecule within a compound. Thus, more fine-grained rules shall be added to the database that are applied not only to compounds, but also to groups of molecules within those compounds.*

Priority *A*

Source *Carsten Prasse*

UR020

Statement *It shall be easy to add new extensible functions to the already given.*

Priority *A*

UR021

Statement *It shall be possible to link the new UM-BBD with other chemical databases, e.g. ChemSpider, OpenTox.*

Priority *A*

Source *Carsten Prasse, Joerg Wicker*

UR022

Statement *The system shall include a periodical system.*

Priority *A*

Part III

System Requirements

Chapter 1

Non-Functional Requirements

1.1 Product Requirements

1.1.1 Usability Requirements

NFR001

Statement *The application should be usable on every common webbrowser,which includes:*

- *Internet Explorer 9 or greater*
- *Firefox 12 or greater*
- *Chrome 11 or greater*
- *Safari 5 or greater*

Priority A

NFR002

Statement *The application should be usable on the following webbrowsers:*

- *Internet Explorer 8*
- *Opera 11 or greater*

Priority B

NFR003

Statement *There should be a downloadable desktop version of the application.*

Priority A

NFR004

Statement *It should be possible to learn all main functionalities of the application for a bachelor of science in biology/chemistry within half an hour*

Priority A

NFR005

Statement *The application should be easy to administrate, which means a person with deeper knowledge in system administration can learn all necessary functions in less then 8 hours*

Priority A

NFR006

Statement *There should be NO app (android or iOS) for this application.*

Priority A

NFR007

Statement *There should be a server application for the system.*

Priority A

1.1.2 Efficiency Requirements

All efficiency and performace requirements describe the core system without extentions.

Performance Requirements

NFR008

Statement *Common operations (which include less then 70 Elements) should be done in less then 30 seconds.*

Priority A

NFR009

Statement *Even complex operations should be done in less then 15 minutes.*

Priority A

Space Requirements

1.1.3 Dependability Requirements

NFR0010

Statement *A single server should not stop working for more then 3 hours at a stretch due to maintance*

Priority A

NFR011

Statement *If a server stops running the application it should refer to other running servers.*

Priority A

NFR012

Statement *The correctness and traceability of the information is only given in the limits of science.*

Priority A

1.1.4 Security Requirements

NFR013

Statement *No encryption required.*

Priority A

NFR014

Statement *The system should be protected against common forms of vandalism.*

Priority A

1.2 Organziational Requirements

1.2.1 Environmental Requirements

NFR015

Statement *There should be interfaces to ohter biochemical databases.*

Priority A

NFR016

Statement *The database should be qualified to be used as scientific sorce (quotability).*

Priority A

NFR017

Statement *Each registered user belongs to one of the following user groups:*

- *normal user*
- *administrator*
- *biochemical expert*

Priority A

1.2.2 Operational Requirements

NFR018

Statement *To obtain a more flexible system the information is structured in packages. A package can contain a set of rules or a set of entries in the compound database. The database consists of all packages installed in the system. A user can - if he or she has the necessary rights - create his or her own packages. A package and its content can be specified to be accessible for the creator, a certain user group or everyone available.*
A user can choose which (for him visible) packages should be applied to his prediction query or compound query.
The syncronisation between servers and the cloning of a server is realised by the exchange of packages.
Packages have a database independent dataformat to provide compability.

Priority A

NFR019

Statement *The calculation of the desktop application should be processed on the server.*

Priority A

1.2.3 Development Requirements

NFR020

Statement *The already existing database should be portable to the new system.*

Priority A

NFR021

Statement *Most of the application's functionality should be realized as extentions to provide a maximum of modifiability. Therefore system offers an API.*

Priority A

1.3 External Requirements

1.3.1 Regulatory Requirements

1.3.2 Ethical Requirements

NFR022

Statement *Develpoment process stands under IEEE standarts of ethical development.*

Priority A

1.3.3 Legislative Requirements

Accounting Requirements

NFR023

Statement *User license corresponding to the legal right (EULA).*

Priority A

NFR024

Statement *Disclaimer in case of wrong information.*

Priority A

Safety / Security Requirements

Chapter 2

Functional Requirements

2.0.4 General API

FR001

Statement *The core system offers an API that is publicly available for external developers (including documentation).*

User requirement *UR020*

Priority *A*

FR002

Statement *The API offers the possibilty to write extensions that influence the user input (e.g. add new input method, validate input).*

User requirement *UR020*

Priority *A*

FR003

Statement *The API offers the possibilty to write extensions that influence the degradation process (e.g. additional environmental conditions, additional rules).*

User requirement *UR020*

Priority *A*

FR004

Statement *The API offers the possibilty to write extensions that influence the output to the user (e.g. graphical representation, links to other systems or databases).*

User requirement *UR020*

Priority *A*

FR005

Statement *The API offers the possibilty to write extensions that influence or add system and database procedures.*

User requirement *UR020*

Priority *A*

FR006

Statement *The API offers the possibilty to write extensions that add different functionality that works on the system's database.*

User requirement *UR020*

Priority *A*

FR007

Statement *Extensions can be visible to the user as additional elements or just be additional steps during the calculation.*

User requirement *UR020*

Priority *A*

FR008

Statement *An extension has the same access/restrictions to data as the user who is using this extension. Administrative tasks can only be activated by administrative users and have full access to all data.*

User requirement *UR020*

Priority *A*

FR009

Statement *An extension may offer the user the possibility to activate or deactivate it. This activation/deactivation may be possibile in the user area or - if the extension displays itself to the user - as an extra element in the area where this extension is used. The developer of the extension can choose if and where to display this possibility.*

Szenarios *1*

User requirement *UR020*

Priority *A*

FR010

Statement *The system is able to convert from the different compound formats into each other. This is required for the search and for the download from lexicon*

Priority *A*

FR011

Statement *The system API provides the possibility to copy the packages and extensions to another server*

Priority *A*

2.0.5 User input

FR012

Statement *A user can enter a compound using the SMILES format in a string text field.*

Application *Compound search, entering new compounds in database, entering compounds for degradation query*

Szenario *1,2*

User requirement *UR014*

Priority *A*

FR013

Statement *A user can enter a compound by uploading a file in Mol2 format (contains one compound per file)*

Application *Compound search, entering new compounds in database, entering compounds for degradation query*

Szenario *1,2*

User requirement *UR014*

Priority *A*

FR014

Statement *A user can enter one or more compounds by uploading a file in SDF format (can contain one or more compounds per file)*

Application *Compound search, entering new compounds in database, entering compounds for degradation query*

Szenario *1,2*

User requirement *UR014*

Priority *A*

FR015

Statement *The API offers the possibility to write extensions that add input methods for entering compounds.*

Application *Compound search, entering new compounds in database, entering compounds for degradation query*

Szenarios *1,2*

User requirement *UR014*

Priority *A*

FR016

Statement *The user can enter additional information for the degradation prediction (e.g. environmental conditions) along with the compounds.*

Szenarios *1*

User requirement *UR014*

Priority *A*

FR017

Statement *The compound-input form provides the option to add additional data. Additional data consists of a key and a value (e.g. "radiation" & "0.2"). A user may add as much additional data as he wants.*

Priority *A*

FR018

Statement *The System provides an rule-input form. The rules provide information about the degredation process of a certain compound. Rules specify enviromental conditions under which they can be used.*

Priority *A*

FR019

Statement *The rule-input form supports Extensions to deal with additional data or additional conditions.*

Priority *A*

FR020

Statement *The rule-input form provides a method to access additional data if it exists and use them like the enviromental data.*

Priority *A*

2.0.6 Users

FR021

Statement *Users can register on the Server.*

Priority *A*

FR022

Statement *Every registered User has a User Area to create and administrate his own packages.*

Priority *A*

FR023

Statement *Registered users can create their own packages, rules and compounds - compounds via the compound-input-form (FR...).*

Priority *A*

FR024

Statement *Registered users are able to select packages for their use.*

Priority *A*

FR025

Statement *Registered users may choose which on the Server installed extensions are used for their calculations.*

Priority *A*

FR026

Statement *Registered users can publish their packages so that everyone is able to see them and to add them to one's used packages. There is also an option to just publish a package to certain other users.*

Priority *A*

FR027

Statement *Registered users can download every public package.*

Priority *A*

FR028

Statement *Registered users can upload packages to their account.*

Priority *A*

FR029

Statement *Experts are able to set packages as default and change the default packages content. Experts are the non technical system administrators.*

Priority *A*

2.0.7 Server Application

FR030

Statement *The system provides a server application which is easy to set up.*

Priority *A*

FR031

Statement *The server application provides a graphical backend for the administrative settings.*

Priority *A*

FR032

Statement *The backend provides settings to integrate the own Server to the network so that all information gets synchronized or to create an independent system which only can be synchronized manually.*

Priority *A*

FR033

Statement *The server backend provides the possibility to install new extensions.*

Prioriy *B*

FR034

Statement *The server admin shall be able to set installed extensions as default.*

Priority *B*

FR035

Statement *The server admin can choose whether everyone can register or people have to get approved to get registered. The server admin also has an easy to use form to approve registration requests.*

Priority *B*

FR036

Statement *The backend provides the user management where users can be deleted and user roles can be assigned.*

Priority *B*

FR037

Statement *The server admin is able to add and remove packages from the server.*

Priority *B*

FR038

Statement *The server admin can set packages as default, so that they are considered by the default search. Also compound descriptions which are contained in this packages are added to the default lexicon view.*

Priority *B*

FR039

Statement *Servers create an user prefix for users registering on them.*

Priority *A*

2.0.8 Degradation prediction

FR040

Statement *Based on the compounds (one or more) and the additional information the user entered, the system applies rules from the degradation database to these compounds and predicts the resulting degraded compounds.*

Szenarios *1*

Priority *A*

FR041

Statement *The depth of the prediction can be specified by the user.*

Szenarios *1*

Priority *A*

FR042

Statement *The results are presented to the user as a prediction tree.*

Szenarios *1*

Priority *A*

FR043

Statement *The degradation prediction is based on rules. These rules model*

- *the degradation and interaction of functional groups*
- *the influence of parts and functional groups on their neighbours*
- *the influence of environmental conditions*

. Based on the additional information entered by the user the rules are weighted.

Szenarios *1*

User requirement *UR019*

Priority *A*

FR044

Statement *The calculation of the degradation process shall prevent circles in the predicted process.*

Priority *A*

FR045

Statement *The API offers the possibility to write extensions that can add other ways how rules can influence the degradation prediction.*

Szenarios *1*

User requirement *UR019*

Priority *A*

FR046

Statement *The user can choose to apply an extension that influences the degradation predcition on his queries or not. He or she might add specific information for this extension.*

Szenarios *1*

Priority *A*

FR047

Statement *The system shows the user an estimation of the time needed for the degradation process' calculation after the user started the calculation process.*

Szenarios *1*

Priority *A*

2.0.9 Predicted degradation path

FR048

Statement *A user can select one ore more paths presented to him in the degradation prediction tree. If he then clicks on the "next" button and if a path has not reached a final state, the prediction is carried on until the specified depth.*

Szenarios *1*

Priority *A*

FR049

Statement *The API offers the possibility to write extensions that obtain all the information about a user's currently chosen degradation prediction (the full degradation tree or the selected paths) and process this data.*

Application FR, FR

Priority *A*

FR050

Statement *The system can export a whole degradation tree or the selected paths to the PDF file format. The user can download this PDF file.*

Szenarios *1*

User requirement *UR016*

Priority *A*

FR051

Statement *The system can export a whole degradation tree or the selected paths into a printable design and activate the user's printer function if possible.*

Szenarios *1*

User requirement *UR016*

Priority *A*

FR052

Statement *If a predicted compound has an entry in the compound database, a link to the database is offered. This is solved by an extension.*

Szenarios *1*

Priority *A*

FR053

Statement *An extension shall calculatte and present the mass and the mass spectrum of a predicted component.*

Priority *A*

FR054

Statement *An extension offers the possibility to get information about a predicted component or a component in the compound database from the MassBank High Quality Mass Spectral Database.*

User requirement *UR021*

Priority *A*

FR055

Statement *An extension offers the possibility to get information about a predicted component or a component in the compound database from the OpenTox database.*

User requirement *UR021*

Priority *A*

FR056

Statement *An extension offers the possibility to get information about a predicted component or a component in the compound database from the ChemSpider database.*

User requirement *UR021*

Priority *A*

FR057

Statement *If a rule is applied during the degradation prediction the system presents the user the name of the reaction this rule models (e.g. oxidation, cleavage of acetate). The name of the reaction is shown next to the path in the degradation tree.*

Priority *A*

2.0.10 Lexicon View

FR058

Statement *A lexicon view is provided to get detailed information to the rules and the compounds.*

Priority *A*

FR059

Statement *The lexicon detail page of the compounds provides the compound in all supported formats to be downloaded.*

Priority *A*

FR060

Statement *The lexicon provides a search-form. The search-form can either be used by entering strings or by entering a compound via the compound-input*

Priority *A*

FR061

Statement *Is no search result found in the default packages (and the packages the searching user has added to his used packages) the system provides the possibility to search in all public packages.*

Priority *B*

FR062

Statement *If there are more than one search results for a compound (for example there exists one result in the default package, as well as in a private self-created one) the pieces of information are displayed with a hint where the information come from.*

Priority *B*

2.0.11 Alternative interfaces

FR063

Statement *A desktop application for Windows (7 and 8), Linux (Debian 6.0.6, Ubuntu 12.10, Fedora 17 and Gentoo) and Mac (OS X 10.7) is to be provided. It shall be able to do the same things the web application can.*

User requirement *UR006*

Priority *B*

FR064

Statement *The system provides all functionality that is offered through the user interface also as web request and XML response interface.*

Priority *B*

FR065

Statement *The system provides all functionality that is offered throught the graphical user interface also through a shell/terminal interface.*

User requirement *UR007*

Priority *B*

2.0.12 Packages

FR066

Statement *The system can import the entries from the old database (compounds and rules) and transform them to the new package format. It informs about all entries that can not be converted.*

User requirement *UR012*

Priority *A*

FR067

Statement *The user can download all packages that are available to him or her in the user area.*

Priority *A*

FR068

Statement *Packages provide meta information about the author, the date etc.*

Priority *A*

2.0.13 Miscellaneous

FR069

Statement *The system offers a biochemical periodic table supplying information about the effect of the known elements to biochemical procedures in general. The information about the elements is stored in the compound database. The periodic table is a static page that links to the entries in the database.*

User requirement *UR022*

Priority *A*

FR070

Statement *An Extension is provided which enables a "trust"-Button next to Packages. Users can click on it to show others that they trust this package. Other users will informed about the amount and the identity of users trusting this package.*

Priority *C*

FR071

Statement *Compounds and rules include scientifical references which provide evidence for their correctness.*

User requirement *UR011*

Priority *A*

Chapter 3

Scenarios

3.1 Scenario for looking up the degradation tree

INITIAL ASSUMPTION: *The normal user (scientist or student) wants to know the biological degradation of a compound or a composition of compounds.*

NORMAL: *The user visits the website. On the main page he clicks on an easy to notice button that directs him to the input form. He can choose between entering the compounds as SMILES-strings, upload one or more SDF-files - each SDF-file can contain one or more compounds -, upload them as Mol2-files - each containing one compound - or with the help of a graphical drawing tool. The user can also combine these methods of entering compounds. He can unfold two areas. In the first area he can define options that concern representation (e.g. depth and width of the degradation tree, aerobic likelihood of rules). In the second area the user can define the rule packages, environmental conditions or other kinds of information that influences the process of the degradation. After clicking on the calculate-button the information is sent to the server. While the server applies the selected rules and conditions, the user is shown a message that he has to wait for the end of the calculation time. After the calculation is finished, the user is redirected to the page that shows him the given steps of the degradation (in the form of a degradation tree). On the top of the page he finds the same two areas to change the options. He can click the apply button, after he has chosen his favored options. This will restart the process.*

If a compound in the tree has an entry in the compound-database, then it freatures a button that redirects to the entry in this database. The same applies to rules in the tree and the rule-database.

Each compound in the last row of the tree has a "select" icon. After selecting one or more of these compounds, the user can click on the "next" button with which he or she can restart the degradation process starting

with the selected elements. The user can print out or convert the whole path - beginning with the first entered element - to a pdf-file at every time.

WHAT CAN GO WRONG:

- *The SMILES-string cannot be converted into a chemical compound: the user will be informed about this problem.*
- *The uploaded Mol2- or SDF-files cannot be converted to chemical compounds: the user will be informed about this problem.*
- *There are too many possible paths (combinatorial explosion): the user will be shown only the most probable. He has the possibility to display the omitted paths upon clicking a button.*
- *A part of the calculation process fails: the system stops the calculation, prints as much of the degradation tree as possible and also prints an error message containing the module which reported failure.*

OTHER ACTIVITIES: *The process has no influence on other processes. Only rules that have been added before the start of the calculation are used during the given calculation.*

SYSTEM STATE ON COMPLETION: *After the user has completed printing or converting the degradation tree, he can click the return-button to be able to repeat the calculation with different components.*

3.2 Scenario for looking up information on a given compound

INITIAL ASSUMPTION: *The normal user (scientist or student) wants to read a description for the given compound from the compounds database.*

NORMAL: *The user clicks on the database-button on the main page. He is redirected to the page, on which he can choose the kind of the database that he wants to search in (rule or compound database). He selects the packages that he wants to use for the search and clicks on the compound database-button. On the page that he is redirected to, he has a search bar on top and a list of the compounds under this bar in alphabetical order. He can either scroll or enter the name of the compound. In the first case he has to click on the name of the compound in the list,in the second case he has to press a search-button. He is redirected to a page containing the information on a given compound.*

WHAT CAN GO WRONG:

- *A certain link does not work: the user is informed about the kind of a mistake that has occured (e.g. no internet connection, technical problems).*

OTHER ACTIVITIES: *The search does not affect other activities.*

SYSTEM STATE ON COMPLETION: *Upon clicking on the return-button the user is redirected to the main page.*

3.3 Scenario for creating custom rules

INITIAL ASSUMPTION: *A registered user wants to create his own rules for his personal usage.*

NORMAL: *The user enters the homepage and loggs in via the login form. He enters the Tap "personal data". There he creates a new Package for his new rule or chooses an already existing Package. After choosing a Package a "create new rule" Button appeares.*
After clicking the "create new rule" Button the Rule creating form appears. After filling the form and saving the new Rule is saved to the Database. The user can continue working.

WHAT CAN GO WRONG:

- *Server not available.*
- *Server crashes while saving to the DB.*
- *Package already exists - ERROR.*
- *User exits page without saving.*

OTHER ACTIVITIES: *nothing dangerous here*

SYSTEM STATE ON COMPLETION: *The user is logged in. His new Rule is added to the Rule Database.*

3.4 Scenario for un-/publishing packages

INITIAL ASSUMPTION: *A registered User wants to publish/unpublish one of his packages.*

NORMAL: *The user enters the homepage and loggs in via the login form. He enters the Tap "personal data". There he sees an overview about all of his packages. On the right side of every package is an icon which symbolizes the current publishing state. On clicking on this icon a popup appears to accept the changes. Afterwards the icon changes to a loading bar and after a short while to the other icon the package is public/private.*

WHAT CAN GO WRONG:

- *An other user using the package is using it in the same moment it gets private*

OTHER ACTIVITIES: *nothing evil happens*

SYSTEM STATE ON COMPLETION: *The User is logged in, the DB entry of the package the publish state changed.*

3.5 Scenario for registration

INITIAL ASSUMPTION: *A user wants to become a registered user.*

NORMAL: *The user enters the homepage and presses the "register"-Button next to the login form. The user gets directed to the register form. There he has to fill in some personal data.*

- *username*
- *email-adress*

The user gets an Email with an activation link to a page where he can choose his password.

WHAT CAN GO WRONG:

- *user already exists.*
- *user with same email address already exists.*
- *the mailed link is not clicked the next days.*

OTHER ACTIVITIES: *nothing evil happens*

SYSTEM STATE ON COMPLETION: *The user is registered and logged in. In the Database a new user is created with a default user role.*

3.6 Scenario for creating custom Compounds

INITIAL ASSUMPTION: *A registered User wants to create a new Compound.*

NORMAL: *The user enters the homepage and loggs in via the login form. He enters the Tap "personal data". There he creates a new Package for his new rule or chooses an already existing Package. After choosing a Package a "create new compound" Button appeares.*
After clicking the "create new compound" Button the user has to upload an mal2 or sdf File or enter an smile string. After that he comes to the Compound details editing form. After saving the Compound is successfully added.

WHAT CAN GO WRONG:

- *Session times out*

OTHER ACTIVITIES: *nothing funny happens*

SYSTEM STATE ON COMPLETION: *The user is logged in the new data is added to the db.*