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| **Fragalysis front-end** |
| Functional and non-functional requirements |

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|  |
| Version 0.5 |

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# The current state of the application

## Definitions

**Application** is React UI (front-end) of Fragalysis

**Project** is a collection of snapshots. Project is owned by single user.

**Session** is the ability to save the state of a page, load it, and save over it. These are owned by a single user

**Snapshot** is a capture of state that can be accessed by any user, but cannot be saved over

**Protein** is a 3D structure that can be loaded into the central protein viewer

**Target** is a collection of proteins of the same structure. The target (name) is usually the name or label given to the protein

**Features** can be any piece of data: selected compounds, 3D coordinates of compounds, details of calculations, notes etc.

**Fragment** is small organic molecules which is small in size and low in molecular weight

**Fragment hit** is molecule of low molecular weight that has been validated to bind to a target protein

**Job** is…

**Site** Site is a region of the protein that is complementary to a specific molecule or ion.

User can select or unselect some of them or all of them.

**PanDDA** Pan-Dataset Density Analysis - Multi-dataset crystallographic analysis for the identification of ligand binding and structural events

## General

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| 1. **User menu** | |
| As a user I want to select any part of system from menu list. | |
| Details | * Home – home page (view, that is displayed after successful login) * Projects – Project List * Management – see in Req. 2 * Contributors – List of organizations that support or cooperate with Fragalysis * Login/Logout – user can log in or log out |
| Screen |  |
| #TC | [[EXT] Oxford-1](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-1), [[EXT] Oxford-2](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-2) |

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| 1. **User menu - management** | |
| As a user I want to manage Proposal and target list. | |
| Details | * User can set wanted targets. * User can set if they will be private or public. |
| Screen |  |
| #TC | [[EXT] Oxford-91](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-91) |

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| 1. **Work without login** | |
| As a user I want to work with system without login. | |
| Details | * As a logged-out user I can select target and create one snapshot from it. * It is not possible to create project from snapshot from logged out user, only share. |
| Screen |  |
| # TC | [[EXT] Oxford-1](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-1) |
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| 1. **Login** | |
| As a user I have to enter my login and password to enter the application. | |
| Details | * Load login page. * Enter username, password. * Having login and password from other organizations from the list, user can login with them – clicking appropriate button. * Logged in user can save and edit own projects in the project list. * Not logged in user can work with application, but can’t save own project, can’t see other projects, only work with own snapshots |
| Screen |  |
| #TC | [[EXT] Oxford-2](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-2) |

## First thing first

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| 1. **Target list** | |
| As a user I want to select target at main screen to start new project. | |
| Details | * Target is a collection of proteins all of the same structure. * Targets are loaded to system, user can’t create one. * Every user (logged in or not) can select all targets. |
| Screen |  |
| #TC | [[EXT] Oxford-52](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-52) |

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| 1. **Target list- filtering** | |
| As a user I want to filter and sort Target list. | |
| Details | * Target list table contains filtering and sorting actions. * User can change width of column. * User can search/ filter target. |
| Screen |  |
| #TC | [[EXT] Oxford-132](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-132) |

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| 1. **Open SGC summary** | |
| As a user I want to see SGC summary of selected target. | |
| Details | * Clicking the Open SGC summary link for required target, description of the target in details is displayed. * It is like online library, where user can read information about selected target in detail. * This library is external source, it is not part of application. |
| Screen |  |
| #TC | [[EXT] Oxford-3](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-3) |

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| 1. **Project list** | |
| As a user I want to see list of projects and select required project. | |
| Details | * When user is logged in, he can see and select own projects. * When user is logged out, there is no project to display. * Choose “Projects” option in menu to display all projects. * User can create new project clicking the Plus button. |
| Screen |  |
| # TC | [[EXT] Oxford-46](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-46) |

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| 1. **Creating new project** | |
| As a user I want to create new project. | |
| Details | * User can create new project clicking the Plus button  in the header of the Project list. * It is possible to create project from target or from own snapshot. * To create a project, it is needed to select target/snapshot and enter required data, then confirm by Create button. |
| Screen |  |
| #TC | [[EXT] Oxford-50](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-50) |

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| 1. **Project list - paging** | |
| As a user I want to set the number of displayed projects at the home page. | |
| Details | * At the bottom part of displayed list there is dropdown selection. * User can select the number of displayed projects. * When there is more project than this number, user can see more projects by clicking on the right arrow button. |
| Screen |  |
| #TC | [[EXT] Oxford-46](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-46) |

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| 1. **Project list – searching for project** | |
| As a user I want to search for a particular project. | |
| Details | * In the head section searching field is displayed. * User can enter project name – a particular project is displayed. |
| Screen |  |
| #TC | [[EXT] Oxford-46](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-46) |

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| 1. **Project list – delete project** | |
| As a user I want to delete selected project. | |
| Details | * User can delete required project – by clicking Trash button next to the project. |
| Screen |  |
| #TC | [[EXT] Oxford-46](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-46) |

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| 1. **Project list – open selected project** | |
| As a user I want to open existing project. | |
| Details | * Each listed (own) project it is possible to open – by click on the project name. |
| Screen |  |
| #TC | [[EXT] Oxford-92](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-92) |

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| 1. **Project list – open selected target** | |
| As a user I want to open target from project list. | |
| Details | * Each target displayed next to the existing project it is possible to open  – by click on the target name. |
| Screen |  |
| #TC | [[EXT] Oxford-47](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-47) |

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| 1. **Download structures** | |
| As a user I want to download created project. | |
| Details | * Open the Project you want to download. * Click on Download structures button. * User can set files to download and other options for downloaded. zip file. * User can see size of file in lower part of the window. * Click on Download button - .zip file is downloaded to user´s PC. * User can Copy JSON for API call by relevant button. * Click on Show examples button and system navigates you to GitHub thread with curl and python examples. |
| Screen |  |
| #TC | [[EXT] Oxford-32](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-32) |

## Left hand side (LHS)

### Tag Details

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| 1. **Tag Details – new tag** | |
| As a user I want to create a new tag. | |
| Details | * User can create a new tag for categories: sites, series, discussion and other. * Tag categories are provided by the system's drop-down menu. * Each category offers a predefined colour. It can be changed using the colour palette. |
| Screen |  |
| #TC | [[EXT] Oxford-106](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-106) |

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| 1. **Tag list/grid view** | |
| As a user I want to change view of Tag details. | |
| Details | * User can change view of tag details by using switch button. * ***List:*** view with all detail information about tag (tag name, category, Creator, Date) * ***Grid:*** view with tag icons (Tag name) |
| Screen |  |
| #TC | [[EXT] Oxford-117](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-117) |

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| 1. **Tag assignment** | |
| As a user I want to assign compound to required tag. | |
| Details | * User can assign tag to required compound in the Hit navigator section. * ***Mass assignment***- Check the required compound with checkboxes in Hit navigator section and open the window for assign tags (pencil button - Edit tags). The assigned tags are completely coloured. * ***Individual assignment***- click on edit pencil next to the tags on molecule. Pop up window with all tags is displayed. Click on tags you want to assign or un assign. * List of Assigned tags are displayed when hovering on tags under molecule name (Id). |
| Screen |  |
| #TC | [[EXT] Oxford-107](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-107) |

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| 1. **Union or Intersection view** | |
| As a user, I want to see all compound that is labelled with any of the active tags- Union.  As a user, I want to see only compounds, that are labelled with all of the active tags- Intersection. | |
| Details | * User can manage the view with toggle button. * User can see selected compounds in Hit navigator. |
| Screen |  |
| #TC | [[EXT] Oxford-112](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-112) |

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| 1. **Show untagged hits** | |
| As a user, I want to see compounds that have no tags assigned to them | |
| Details | * User can see compounds without tags assigned by clicking on Show untagged hits button. * User can see selected compounds in Hit navigator. |
| Screen |  |
| #TC | [[EXT] Oxford-118](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-118) |

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| 1. **Show all hits** | |
| As a user, I want to see all compounds. | |
| Details | * The user can see all compounds that have a tag assigned to them or do not have a tag assigned to them. |
| Screen |  |
| #TC | [[EXT] Oxford-119](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-119) |

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| 1. **Select/unselect all tags** | |
| As user I want to Select all tag/Unselect all tags at one step. | |
| Details | * All Tags in Tag details is checked. * All Tags in Hit list Filter is dark colour. * The user can see all compounds assigned to all tags in Hit navigator. |
| Screen |  |
| #TC | [[EXT] Oxford-120](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-120) |

### Hit navigator

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| 1. **Hit navigator – list of molecules** | |
| As a user I want to see all molecules of selected target with required tags. | |
| Details | * Each tag contains several molecules. * These molecules are displayed based on selected tag in hit list filter. * Next to each molecule name is displayed list of assigned tags. |
| Screen |  |
| #TC | [[EXT] Oxford-113](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-113) |

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| 1. **Hit navigator – molecule description** | |
| As a user I want to see information about each molecule. | |
| Details | * Numbers in front of molecule represent appropriate ordinal number. * From each molecule I can select what I want to display in NGL viewer:  A – all (ligand – L, sidechains – P and interactions – C are displayed) L – ligand (3D molecule) – it is a place, where molecule connects to protein   P - sidechains C – interactions S – surface D – electron density  V – vectors - vector is a group of compounds, colour of the vector depends on compounds quantity (vector in the viewer has not the same colour as other parts)   * After selection of any part of the molecule, random colour is assigned to molecule – every part of the molecule has this colour in NGL view (except vectors) * **Atom quality:** quality of compound observation * **Image**: image of molecule * **Properties:** Names of properties are displayed at the top part of the Hit navigator.   MW – Molecular weight IogP - IogP TPSA – Topological polar surface area HA -Heavy atom count Hacc - H-bond acceptors  Hdon-bond donors Rots Rotatable bounds  Rings - rings Velec -valence electrons |
| Screen |  |
| #TC | [[EXT] Oxford-14](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-14), [[EXT] Oxford-15](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-15), [[EXT] Oxford-64](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-64), |

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| 1. **´Centre on´ button for each ligand** | |
| As a user I want to have a button that centres on the ligand when I click on it. | |
| Details | * Every ligand has centre on button for each ligand * This button is active only when the ligand is turned on * When the user clicks on the button the ligand is centred. |
| Screen |  |
|  | [[EXT] Oxford-69](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-69) |

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| 1. **Large 2D in tooltip when hovering over small 2D image** | |
| As a user I want to see larger image in tooltip. | |
| Details | * tooltip that shows the image 3x larger when user hovers the mouse over the 2D image. |
| Screen |  |
| #TC | [[EXT] Oxford-114](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-114) |

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| 1. **Hit navigator - manage all molecules at once** | |
| As a user I want to manage all displayed molecules at once. | |
| Details | * There are buttons for select all hits - above displayed molecules. * All molecules in Hit navigator has marked checkbox. * L, P, C buttons and number of selected molecules are displayed above molecules. * Clicking given button, selected part of each molecule is selected and displayed in NGL viewer. * Clicking give button again, selected part of each molecule is unselected. * L, P, C buttons are medium colour when some of selected molecules (not all) has displayed this part in NGL viewer. * When the L button is unselected, the V button is at the same time unselected too (without pushing it). * Clicking “Centre on” button , the ligand is in the centre of view. * By clicking Unselect all hits, all checkboxes are unchecked. * All bulk actions are disabled and no longer displayed above molecules. * All bulk actions done in previous step are still active. |
| Screen | C:\Users\simona.dachova\Pictures\Screenpresso\2023-09-25_09h26_41.png |
| #TC | [[EXT] Oxford-63](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-63), [[EXT] Oxford-115](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-115), [[EXT] Oxford-69](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-69), [[EXT] Oxford-109](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-109), [[EXT] Oxford-116](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-116) |

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| 1. **Hit navigator - Warning** | |
| As a user I want to check atom quality. | |
| Details | * Molecules are marked with orange warning triangle. * Atom quality is displayed by default. * Clicking on triangle turn off the atom quality representation in NGL viewer. |
| Screen |  |
| #TC | [[EXT] Oxford-121](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-121) |

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| 1. **Hit navigator - search** | |
| As a user I want to search for compound. | |
| Details | * In the Hit navigator user can enter searching term. * A list of matching molecules is displayed. * In list of molecules are displayed not only matching molecules, but also molecules with any checked button (displayed in NGL viewer). |
| Screen |  |
| #TC | [[EXT] Oxford-122](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-122) |

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| 1. **Copy smiles** | |
| As a user I am able to copy smiles of compound. | |
| Details | * Functions is for each hit (LHS) and compound (RHS) which will be shown on when user enters the picture with structure area. After clicking the icon, the SMILES (smiles attribute on the molecule) will be copied to user’s clipboard. |
| Screen |  |
| #TC | [[EXT] Oxford-111](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-111) |

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| 1. **Hit navigator- Buttons “Next 30”, “Next 100 “and “Load all”** | |
| **As a user I want to have 3 buttons to load the list of compounds.** | |
| Details | | * As a user I have available three buttons at the bottom of both LHS and RHS lists, that provide: * load next 30 * load next 100 * load full list (with warning modal if the list is >300) * Left next to "load buttons" is displayed how many compounds are available in the list | |
| Screen | |  | |
| #TC | | [[EXT] Oxford-89](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-89) | |

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| 1. **Hit navigator - filter** | |
| As a user I want to filter and sort molecules by required criteria. | |
| Details | * In the Hit navigator user can click Sort/filter button to set filter parameters. * In the filter selection it is possible to set what will be displayed and sort molecules by their properties. * Filter setting are applied to Hit navigator – molecules are filtered and sorted based on these criteria, settings are visible in Hit navigator right after any change without confirmation * User can order properties to set sorting criteria. User can choose the type of sorting for each property (ascending/descending). * **Priority:** clicking the arrow up/down for particular property order  of properties is changed * **Order**: user can set whether order should be ascending or descending for each property * **Property**: name of each property * **Min/max**: user can set the interval for each property – only these molecules that fulfil criteria are displayed |
| Screen |  |
| #TC | [[EXT] Oxford-16](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-16) |

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| 1. **Hit navigator filter – clear filter** | |
| As a user I want to clear filter settings. | |
| Details | * Clicking Clear button, default settings of filter are set. |
| Screen |  |
| #TC | [[EXT] Oxford-16](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-16) |

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| 1. **Hit navigator edit tag** | |
| As a user I want to edit tags for all marked molecules at once. | |
| Details | * Mark all compounds whose tags you want to edit. * Clicking pencil button on Hit navigator panel. * Click on each tag you want add or remove. |
| Screen | C:\Users\simona.dachova\Pictures\Screenpresso\2023-09-25_09h29_37.png |
| #TC | [[EXT] Oxford-107](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-107) |

## Project

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| 1. **New project** | |
| As a user I want to create new project. | |
| Details | * Click on New project button in appropriate target. * Mandatory information is filled in with generated data. * New project is created in Project table. |
| Screen |  |
| #TC | [[EXT] Oxford-50](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-50) |

## Snapshot

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| 1. **Save snapshot** | |
| As a user I want to save created snapshot. | |
| Details | * User can save snapshot clicking the Save button. * Snapshot must be part of existing project. * Every saved snapshot has relation to previous one. * Snapshot can be in the same branch as a predecessor or in the new one (start of the branch) |
| Screen |  |
| #TC | [[EXT] Oxford-93](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-93) |

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| 1. **Anonymous snapshot** | |
| As a user I want to work with anonymous snapshot. | |
| Details | * Anonymous snapshot is snapshot created by logged out user. * This snapshot is possible to share to another user (logged in or not). * It is possible to work with this snapshot, but it is not possible to save changes, create new snapshot from anonymous snapshot or create project from anonymous snapshot. |
| Screen |  |
| #TC | [[EXT] Oxford-55,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-55) [[EXT] Oxford-56](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-56), [[EXT] Oxford-94](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-94) |

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| 1. **Add new snapshot to project** | |
| As a user I want to save created snapshot to existing project. | |
| Details | * User can save snapshot to existing project clicking on the Save button and entering snapshot details * New snapshot is placed to project history tree – placing is based on starting snapshot. * Every saved snapshot has relation to previous one * Snapshot can be in the same branch as a predecessor or in the new one (start of the branch) |
| Screen |  |
| #TC | [[EXT] Oxford-59](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-59), [[EXT] Oxford-58](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-58), [[EXT] Oxford-61](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-61), [[EXT] Oxford-100](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-100), [[EXT] Oxford-95](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-95), [[EXT] Oxford-93](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-93) |

## Project history

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| 1. **Project history overview** | |
| As a user I want to see the history of project. | |
| Details | * Project is collection of snapshots. * When project is created, history of the project is displayed. * Clicking the arrow button , Project history window is displayed/hidden. * Small circles in project history represent snapshots. * The application displays snapshot details on mouse hover * User can click on the circle to display required snapshot in NGL viewer without reloading the page. |
| Screen |  |
| #TC | [[EXT] Oxford-97](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-97), [[EXT] Oxford-60](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-60), [[EXT] Oxford-57](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-57) |

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| 1. **Project history overview – open detail** | |
| As a user I want to see the history of a project in detail. | |
| Details | * User can click on Detail button in Project history – details of project history are displayed in new window. |
| Screen |  |
| #TC | [[EXT] Oxford-57](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-57) |

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| 1. **Project history overview – detail window** | |
| As a user I want to see stored project’s snapshots at the timeline. | |
| Details | * Details of snapshots are displayed in Project history. * Timeline has branch view * Every branch has a name and description |
| Screen |  |
| #TC | [[EXT] Oxford-55,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-55) [[EXT] Oxford-56](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-56) |

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| 1. **Project history overview – share snapshot** | |
| As a user I want to share snapshot form project history. | |
| Details | * Details of snapshots are displayed in Project history. * User can share required snapshot clicking on Share button next to the required snapshot. * User can choose method of sharing – copy link or open in new tab. * Sharing snapshot to logged in project author – whole project including history is shared, possible to edit (save changes, new snapshots) * Sharing snapshot to logged in user, but not the author – only snapshot is displayed, user can make some changes, but it is not possible to save them |
| Screen |  |
| #TC | [[EXT] Oxford-55,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-55) [[EXT] Oxford-56](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-56) |

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| 1. **Restore project from the snapshot – Project history detail** | |
| As a user I want to restore project from the snapshot displayed on the timeline. | |
| Details | * User can choose snapshot in Project history detail. * User can select snapshot clicking Snapshot name or appropriate circle * After snapshot selection, every new created snapshot is connected to selected snapshot * Project will continue from the restored snapshot * The Application will keep snapshot after selected one until new snapshot is created * The Application shall ask before snapshot is open / actual work is saved and closed |
| Screen |  |
| #TC | [[EXT] Oxford-97](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-97) |

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| 1. **Save changes confirmation** | |
| As a user I want to be asked to save changes before select another snapshot. | |
| Details | * When user select snapshot from Project history or Project history detail, pop-up for Save or Cancel changes is displayed. * Changes are saved as new snapshot related with previous opened snapshot. |
| Screen |  |
| #TC | [[EXT] Oxford-98](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-98) |

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| 1. **Read only snapshot** | |
| As a user I want to see snapshot of the other user as a read only snapshot. | |
| Details | * If the user is not owner of the snapshot, he is not able to see history and the detail of the project where the snapshot belongs. User is not able to save snapshot which he doesn't own. |
| Screen |  |
| #TC | [[EXT] Oxford-99](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-99) |

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| 1. **Overwrite current snapshot** | |
| As a user I want to have an option to overwrite current snapshot. | |
| Details | * Sometimes user wants to continuously save his work just not to lose progress which creates clutter on the timeline. * When saving an idea which is a part of the project user can choose whether a new idea shall be created or current idea shall be overwritten. |
| Screen |  |
| #TC | [[EXT] Oxford-65](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-65) |

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| 1. **Project history – restore snapshot** | |
| As a user I want to restore snapshot. | |
| Details | * When snapshot is selected and displayed and user made some changes, it is possible to return these changes to initial state of snapshot – by click on the Restore button. |
| Screen |  |
| #TC | [[EXT] Oxford-101](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-101) |

## NGL viewer

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| 1. **NGL Viewer - protein** | |
| As a user I want to display protein in NGL viewer. | |
| Details | * When no more parts of molecules are displayed, user can see only protein in NGL viewer. |
| Screen |  |
| #TC | [[[EXT] Oxford-102](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-102)](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-102) |

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| 1. **NGL Viewer - ligand** | |
| As a user I want to select ligand of required molecule to display in NGL viewer. | |
| Details | * User can select ligand from required molecule to display. * Select ligand by clicking on L button in LHS (Hit navigator) or RHS (Custom dataset). * It is possible to select more than one ligand. * In the picture below there is a ligand without protein displayed. |
| Screen |  |
| #TC | [[EXT] Oxford-102](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-102) |

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| 1. **NGL Viewer - sidechains** | |
| As a user I want to select sidechains of required molecule to display in NGL viewer. | |
| Details | * User can select sidechains from required molecule to display. * Select sidechains by clicking on P button in LHS (Hit navigator) or RHS (Custom dataset). * It is possible to select sidechains for more than one molecule. * In the picture below there are sidechains without protein displayed. |
| Screen |  |
| #TC | [[EXT] Oxford-102](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-102) |

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| 1. **NGL Viewer - interactions** | |
| As a user I want to select interactions of required molecule to display in NGL viewer. | |
| Details | * User can select interactions from required molecule to display. * Select interactions by clicking on C button in LHS (Hit navigator) or RHS (Custom dataset). * It is possible to select interactions for more than one molecule. * In the picture below there are interactions without protein displayed. |
| Screen |  |
| #TC | [[EXT] Oxford-102](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-102) |

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| 1. **NGL Viewer - surface** | |
| As a user I want to select surface of required molecule to display in NGL viewer. | |
| Details | * User can select surface from required molecule to display. * Select surface by clicking on S button in LHS (Hit navigator) or RHS (Custom dataset). * It is possible to select more than one surface. * In the picture below there is surface without protein displayed. |
| Screen |  |
| #TC | [[EXT] Oxford-102](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-102) |

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| 1. **NGL Viewer - vector** | |
| As a user I want to select vector of required molecule to display in NGL viewer. | |
| Details | * User can select vector from required molecule to display. * Select vector by clicking on V button in LHS (Hit navigator). * It is possible to select more than one vector at once. * In the picture below there is vector without protein displayed. |
| Screen |  |
| #TC | [[EXT] Oxford-102](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-102) |

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| 1. **NGL Viewer – electron density** | |
| As a user I want to select electron density of required molecule to display in NGL viewer. | |
| Details | * User can select electron density from required molecule to display. * Select electron density by clicking on D button in LHS (Hit navigator). * Density rendering maps selection window is displayed. * User can choose from several options (Render map sigma, Render map diff, Render atom quality). * User can choose multiple options at once. * It is possible to select more than one electron density at once. * User can click on D button again, and electron density will be displayed as continuous surface. * Ligand of required molecule is selected and displayed automatically. * In the picture below there is electron density without protein displayed. |
| Screen |  |
| #TC | [[EXT] Oxford-102](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-102) |
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| 1. **NGL Viewer – all parts together** | |
| As a user I want to display many parts from required molecules. | |
| Details | * User can select required parts from each molecule. * Selected parts are highlighted in the hit navigator and displayed in NGL viewer. * In the picture below there are all parts together displayed. |
| Screen |  |
| #TC | [[EXT] Oxford-102](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-102) |

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| 1. **Managing** **NGL Viewer** | |
| As a user I want to manage view in NGL viewer. | |
| Details | * By clicking on mouse icon under NGL viewer open Mouse controls window.      * It is possible to manage view:  scroll – zoom scene * Scroll-ctrl move near clipping plane scroll-shift – move near clipping plane and far fog scroll-alt – change isolevel of isosurfaces drag-right move scene   drag-middle – zoom scene drag-left – rotate scene  drag-shift-right - zoom scene drag-left+right – zoom scene drag-ctrl-right pan/translate hovered component  Drag-ctrl-left – rotate hovered component clickPick-middle – auto view picked component element  hoverPick – show tooltip for hovered component element i – toggle stage spinning  k – toggle stage rocking p – pause all stage animations r – reset stage auto view |
| Screen |  |
| #TC | [[EXT] Oxford-20](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-20) |

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| 1. **NGL viewer settings** | |
| As a user I want to set parameters of view in NGL viewer. | |
| Details | * By clicking on gear icon under NGL viewer open Settings window. * There are several settings of view:  *clip near* and *clip far* options allow user to set an area of final view clip distance fog near – adds fog effect to front part of view fog far– adds fog effect to back part of view * background colour(on/off > background will be white or black) |
| Screen |  |
| #TC | [[EXT] Oxford-21](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-21) |

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| 1. **Display controls** | |
| As a user I want to set each part of view. | |
| Details | * By clicking on PC icon under NGL viewer open Display controls window. * To each part of view (molecule, vector, etc.) it is possible to set: * Style of view – select from dropdown * If it is visible in view or not – eye button * Optical effects (metalness, diffuse, etc.) – by pen button * Some parts it is possible to delete – trash button * Protein and vector parts it is not possible to delete * Add next elements by plus button |
| Screen |  |
| #TC | [[EXT] Oxford-22](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-22) |

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| 1. **Restore NGL viewer settings** | |
| As a user I want to have button to restore NGL settings. | |
| Details | * Under the NGL view the button 'Restore NGL viewer settings’ is displayed. * After pressing this button, the last known settings for the NGL view are restored***.*** |
| Screen |  |
| #TC | [[EXT] Oxford-75](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-75) |

## Right hand side (RHS)

### Custom dataset

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| 1. **RHS – dataset selection** | |
| As a user I want to select dataset from right hand side. | |
| Details | * Every custom dataset is displayed on separate tab. * The tabs are scrollable to be able to display and navigate any number of custom datasets. * The compound is displayed in the same manner as are displayed molecules in the Hit navigator with specific additions. * Link to dataset is available. |
| Screen |  |
| #TC | [[EXT] Oxford-76](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-76), [[EXT] Oxford-77](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-77), [[EXT] Oxford-81](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-81), [[EXT] Oxford-84](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-84) |

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| 1. **RHS – shopping cart** | |
| As a user I want to add the compounds to the shopping cart and all selected to see in selected tab. | |
| Details | * On 2D image is action add to shopping cart. |
| Screen |  |
| #TC | [[EXT] Oxford-103](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-103) |

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| 1. **´Centre on´ button for each ligand** | |
| As a user I want to have a button that centres on the ligand when I click on it. | |
| Details | * Every ligand has centre on button for each ligand * This button is active only when the ligand is turned on * When the user clicks on the button the ligand is centred. |
| Screen |  |
| #TC | [[EXT] Oxford-68](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-68) |

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| 1. **Buttons “Next 30”, “Next 100 “and “Load all”** | |
| As a user I want to have 3 buttons to load the list of compounds. | |
| Details | * As a user I have available three buttons at the bottom of both LHS and RHS lists, that provide: * load next 30 * load next 100 * load full list (with warning modal if the list is >300) * Left next to "load buttons" is displayed how many compounds are available in the list |
| Screen |  |
| #TC | [[EXT] Oxford-89](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-89) |

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| 1. **Arrows – buttons to skip to next compound** | |
| As a user I want to skip to next compound by arrow buttons. | |
| Details | * When a user investigates compounds (RHS), he can jump to the next (or previous) one with a single button-click, with all view settings applied. * Clicking the down button is turned off the one above while turning on the one below, transferring everything from the compound above to the one below * All other compounds are turned off, not only the compound that had the arrow * The arrows show up only for highlighted (i.e. displayed) compounds * The pressing the next or previous arrow is treated as a bulk action. |
| Screen |  |
| #TC | [[EXT] Oxford-70](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-70), [[EXT] Oxford-124](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-124), [[EXT] Oxford-125](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-125), |
|  | |
| 1. **Large 2D in tooltip when hovering over small 2D image** | |
| As a user I want to see larger image in tooltip. | |
| Details | * tooltip that shows the image 3x larger when user hovers the mouse over the 2D image. |
| Screen |  |
| #TC | [[EXT] Oxford-114](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-114) |

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| 1. **Copy smiles** | |
| As a user I am able to copy smiles of compound. | |
| Details | * Functions is for each hit (LHS) and compound (RHS) which will be shown on when user enters the picture with structure area. After clicking the icon, the SMILES (smiles attribute on the molecule) will be copied to user’s clipboard. |
| Screen |  |
| #TC | [[EXT] Oxford-111](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-111) |

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| 1. **RHS – Select compound in custom dataset** | |
| As a user I want to select compounds in custom dataset and see all in selected tab. | |
| Details | * On each compound there is colour of each group. * If the colour of group is checked, it means that compound is selected. * User can change name of group by clicking the pen icon next to the group name. * One compound can belong to more than one group. |
| Screen |  |
| #TC | [[EXT] Oxford-126](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-126) |

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| 1. **RHS – modal windows “F”** | |
| As a user I want to display the inspirational fragments for compound. | |
| Details | * There is added F display toggle. This toggle is displayed modal window where all the inspirational fragments are displayed. * F toggle stays on as long as any button inside the modal is turned on (it doesn't depend on type of toggle button, even if modal is closed) * F toggle turns dark blue when something in the modal has been turned on * F toggle turns light blue when everything in the modal has been turned off (light) * F toggle turns dark blue if some molecule turned on the left-hand side, is an inspiration for some molecule on the right-hand side |
| Screen |  |
| #TC | [[EXT] Oxford-78](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-78) |

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| 1. **RHS – modal windows “F” Mass actions** | |
| As a user I want to do mass actions with Inspirations fragments. | |
| Details | * Only with inspirations fragments displayed in NGL viewer can user do mass actions. * Required inspiration fragments can user check by checkbox next to the molecule. * Checked fragments can be managed by mass actions in the upper part of the window. |
| Screen |  |
| #TC | [[EXT] Oxford-87](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-87) |

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| 1. **RHS – modal window “X”** | |
| As a user I want to display the same compound from all datasets with relevant scores. | |
| Details | * There is added X display toggle. This toggle is displayed modal window where same compound from all datasets is displayed with relevant scores. * Backend will provide API function to retrieve scores of the compound from all defined datasets. |
| Screen |  |
| #TC | [[EXT] Oxford-79,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-78) [[EXT] Oxford-88](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-88) |

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| 1. **RHS – Search in custom data sets** | |
| As a user I want to search in custom data set. | |
| Details | * In the custom data sets tabs is a search bar * Also, contents of the given tab should dynamically reflect contents of the search bar i.e., tab is populated only with compounds which name contains the given substring. |
| Screen |  |
| #TC | [[EXT] Oxford-82](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-82) |

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| 1. **RHS - manage all molecules at once** | |
| As a user I want to manage all displayed molecules at once. | |
| Details | * Click on check button on molecules which you want to manage. * There are buttons for manage all molecules (hits) at once - above displayed molecules. * Clicking give button, selected part of each molecule is selected and displayed in NGL viewer. |
| Screen |  |
| #TC | [[EXT] Oxford-86](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-86) |

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| 1. **Inspirations – selecting parts to NGL viewer** | |
| As a user I want to select which parts of inspirations will be displayed in NGL viewer. | |
| Details | * From each inspiration compound user can select what he wants to display in NGL viewer:  A – all (ligand – L, sidechains – P and interactions – C are displayed) L – ligand (3d molecule) – it is a place, where molecule connects to protein   P - sidechains C – interactions S – surface After selection of any part of the molecule, random colour is assigned to compound – every part of the molecule has this colour in viewer, except interactions and surface. |
| Screen |  |
| #TC | [[EXT] Oxford-78,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-78) [[EXT] Oxford-87](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-87) |

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| 1. **RHS - filter and sort** | |
| As a user I want to filter and sort compounds by required criteria. | |
| Details | * User can click Filter button to set filter and sorting parameters. * Filter settings are applied to compounds list (selected dataset) – compounds are filtered based on these criteria, settings are visible in the compounds list right after any change is made - without confirmation * **Is shown:** It is possible to select which properties will be showed in the compounds list - by clicking the given checkboxes – at most 7 properties should be selected. By default, there are selected first 7 properties.  Properties are displayed in the order how they were selected * **Property**: name of each property * **Min/max**: user can set the interval for each property – only these molecules that fulfil criteria are displayed * User can order properties to set sorting criteria. User can choose the type of sorting for each property (ascending/descending/ ignore). |
| Screen |  |
| #TC | [[EXT] Oxford-83](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-83) |

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| 1. **Right hand side - clear filter** | |
| As a user I want to clear all filtering criteria. | |
| Details | * User can click Clear button to clear all filtering criteria. * Then it is possible to set new criteria. |
| Screen |  |
| #TC | [[EXT] Oxford-83](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-83) |

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| 1. **Right hand side – link to dataset** | |
| As a user I want to open dataset link. | |
| Details | * User can click the Link to dataset button. * Dataset page is opened in new tab. |
| Screen |  |
| #TC | [[EXT] Oxford-83](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-84) |

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| 1. **Right hand side – Delete dataset** | |
| As a user I want to delete dataset. | |
| Details | * User can click the Delete dataset button. * Confirmation window is displayed. |
| Screen |  |
| #TC | [[EXT] Oxford-127](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-127) |

### Selected compounds

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| 1. **RHS – adding CSV button and SDF file button** | |
| As a user I want to have an option to download the CSV. | |
| Details | * Download CSV button is added to Selected Compounds tab (RHS). It contains following columns: smiles, data set from where they come from. * Selected vector compounds are added to 'selected compounds' tab & include in selection for download. |
| Screen |  |
| #TC | [[EXT] Oxford-71](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-71) |

### Compounds on vector

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| 1. **Compound on vector to pick – show molecules** | |
| As a user I want to show all molecules from selected vector. | |
| Details | * By clicking single vector in NGL viewer, all molecules of the vector are displayed in *Compounds on vector to pick* window. * Molecule and compound are synonyms in this case * By clicking on vector in NGL viewer, number of possible compounds of selected vector are displayed and number of molecules for whole vector group. * Name of each molecule is displayed in Compounds on vector to pick window. When vector has red colour, it means, that contains only few molecules or no one – if there is no molecule in selected vector, there is nothing to display * When vector is yellow colour it means, that contains medium number of molecules. * When vector is green colour it means, that contains many molecules. |
| Screen |  |
| #TC | [[EXT] Oxford-23](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-23) |

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| 1. **Compound on vector to pick – manage molecules** | |
| As a user I want to manage displayed molecules. | |
| Details | * User can give name for every colour. * Each colour it is possible to highlight (bound) by clicking on it and pressing Enter button * When some colour is highlighted (bounded), user can mark relevant molecules (picture will have selected colour). * When some colour is highlighted and user clicks on molecule with the same colour, colour is removed from molecule (molecule is not picked) * All coloured molecules are picked and their count is displayed in the Summary info. * Clicking on the Select all button, all molecules are picked. * Clicking on the Clear selection button, selection is cancelled. |
| Screen |  |
| #TC | [[EXT] Oxford-24](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-24), [[EXT] Oxford-126](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-126), |

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| 1. **Compound on vector to pick – select molecules to NGL viewer.** | |
| As a user I want to select molecules to show in NGL viewer. | |
| Details | * Shift + click on molecule – molecule is displayed in the NGL viewer. * Shift + click on the same molecule – molecule is removed from NGL viewer. * Picked molecule has a little bit lighter colour in Compounds to pick |
| Screen |  |
| #TC | [[EXT] Oxford-128](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-128) |

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| 1. **Summary info** | |
| As a user I want to see summary info based on selected molecules. | |
| Details | * When molecules in *Compounds on vector to pick* part are selected, summary is displayed * Summary information contains info:   ***Number of picked molecules Number of vectors explored Number series explored  Estimated cost Selected interaction*** |
| Screen |  |

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| #TC | [[EXT] Oxford-35](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-35) |

## Track actions

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| 1. **Track action history of the user** | |
| As a user I want to have history of significant actions tracked. | |
| Details | Tracked are following actions:   1. Loaded target 2. Site turned on 3. Ligand turned on for a molecule 4. Sidechains turned on for a molecule 5. Interactions turned on for a molecule 6. Surface turned on for a molecule 7. Vectors turned on for a molecule 8. Vector selected in NGL view 9. Molecule added to shopping cart 10. Compound from custom dataset is selected 11. Ligand turned on for a compound from custom dataset 12. Sidechains turned on for a compound from custom dataset 13. Interactions turned on for a compound from custom dataset 14. Surface turned on for a compound from custom dataset 15. Ligand turned on for an inspiration of a compound 16. Sidechains turned on for an inspiration of a compound 17. Interactions turned on for an inspiration of a compound 18. Surface turned on for an inspiration of a compound 19. Vectors turned on for an inspiration of a compound 20. Ligand turned on for a cross-reference of a compound 21. Sidechains turned on for a cross-reference of a compound 22. Interactions turned on for a cross-reference of a compound 23. Surface turned on for a cross-reference of a compound 24. Representation is changed of NGL view object 25. Viewer settings are changed 26. Filter settings are set  * Action contains following information: timestamp, object type, object name, action type |
| Screen |  |
| #TC | [[EXT] Oxford-90](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-90) |

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| 1. **Bulk actions** | |
| As a user I want to have only one entirety in the action list when the mass button is pressed | |
| Details | * In the action list user can see that mass button was turned on or off as one entirety * User can undo and redo this action in its entirety. * Mass actions:   **LHS:** Turn on or off all L Turn on or off all P Turn on or off all C Turn on or off A for a molecule **RHS** (custom datasets and selected compounds): Turn on or off all L Turn on or off all P Turn on or off all C Turn on or off A for a molecule **Inspirations:** Turn on or off all L Turn on or off all P Turn on or off all C Turn on or off A for a molecule **Cross-references:** Turn on or off all L Turn on or off all P Turn on or off all C Turn on or off A for a molecule |
| Screen |  |
| #TC | [[EXT] Oxford-85,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-85) [[EXT] Oxford-86,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-86) [[EXT] Oxford-87,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-87) [[EXT] Oxford-88,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-88) [[EXT] Oxford-66](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-66) |

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| 1. **Edit auto-caption of action** | |
| As a user I want to have a thumbnail of button to annotate or edit item in the action list. | |
| Details | - User can annotate an item in the action list  - User can edit auto-caption of action  - User has the option to change the icon for each list item: check, clear, warning, favourite, star |
| Screen |  |
| #TC | [[EXT] Oxford-105,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-105) |

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| 1. **Undo/redo actions** | |
| As a user I want to have available to use undo/redo actions. | |
| Details | * Undo/Redo functionality is available for actions. * After pressing combination of ctrl-z (cmd-z on mac) the last action is undone. * After pressing ctrl-y (cmd-y on mac) the last undone action is redone. * Undo/redo icon buttons are added bellow NGL view. * If I hover the mouse over the button, the tooltip with the undo (redo)action is displayed |
| Screen |  |
| #TC | [[EXT] Oxford-85,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-85) [[EXT] Oxford-86,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-86) [[EXT] Oxford-87,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-87) [[EXT] Oxford-88,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-88) |

## Other

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| 1. **Direct links – exact match** | |
| As a user I want to have direct link with option exact match. | |
| Details | * Name of the molecule in the URL must exactly (sort of... on that later) match the name of the molecule (protein\_code) in the data and the toggles are applied only on these exact matches. * Protein\_code has structure targetName-moleculeName and exact match must only match the moleculeName part of the protein\_code. * Max length of the url is 2048 characters. * NGL view zooms in on the first ligand in the URL * Format URL: baseurl/viewer/react/preview/direct/target/**name\_of\_the\_target**/mols/   **part\_of\_the\_mol\_name1/toggle/toggle/.../part\_of\_the\_mol\_name2/**  **toggle/toggle/...** In bold are variable parts of the URL. **name\_of\_the\_target** - is the name of the target **part\_of\_the\_mol\_name1** - it's a part of the molecule name. This doesn't need to be full name because molecule name often contains characters which forbidden in URL. Currently the first match is taken into the account but it can be changed that toggles will be applied to all matches **toggle** - toggle which will be turned on for given molecule - accepted values: L, P, C, S, V URL length is limited to 2048 characters. After the result is rendered all subsequent selections and/or de selections are not reflected in the URL (the main reason is the URL limit which can be exceeded quite easily when using mass selection toggles but there are also other technicalities like reloading when rewriting URL in react router etc).   * All the sites where the molecules in the URL are present should be turned on. |
| Screen |  |
| #TC | [[EXT] Oxford-73,](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-73) |

## Job launcher

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| 1. **Job launcher** | |
| As a user I want to manage jobs. | |
| Details | * Use Job launcher button on Project History panel. * User can choose inputs and protein, fragment molecules, PDF file for protein and number of molecules to generate. * ***Open in squonk***- User can open job in squonk by clicking on appropriate button. * ***Switch to snapshot***- User can leave modal window by clicking on appropriate button. * In custom dataset are displayed molecules with generated names. * Inspirations on custom dataset molecules are molecules on the basis of which they were calculated |
| Screen |  |
| #TC | [[EXT] Oxford-129](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-129) |

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| 1. **Job launcher - manage** | |
| As a user I want to manage done jobs. | |
| Details | * User can click on Job shown as an arrow in Project history. * User can see detail of each Job, Status, Parameters… |
| Screen |  |
| #TC | [[EXT] Oxford-130](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-130) |

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| 1. **Job Table** | |
| As a user I want to have information about all Jobs. | |
| Details | * User can click on Job table button on Project history panel. * User can see detail of each Job, Status, Parameters… |
| Screen |  |
| #TC | [[EXT] Oxford-131](https://testlink.ad.m2ms.sk/linkto.php?tprojectPrefix=%5BEXT%5D+Oxford&item=testcase&id=%5BEXT%5D+Oxford-131) |