MolQuest

Version 2.3

Graphical User Interface Manual

CONTENTS

Introduction

MOLQUEST is the most comprehensive, easy-to-use desktop application sequence analysis and molecular biology data management available in the market today. The package includes versatile family of genefinders, FGENESH/H+, with parameters for wide variety of genomes, as

well as pipelines for fully automatic annotation of eukaryotic (FGENESH++) and bacterial (FGENESB) genomes, which proved to be the most accurate genefinding tools overall (see here).

The package has a user-friendly interface for sequence editing, primer design, internet database searches, gene prediction, promoter identification, regulatory elements mapping, patterns discovery protein analysis, multiple sequence alignment, phylogenetic tree reconstruction, and a wide variety of other functions.

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Fundamental Definitions

Program

MolQuest integrates various programs for molecular biology data processing. Programs are distributed by their developers in packages. Packages are installed by the main menu command Tools -> Install Package. All available programs are displayed in Programs List of the Toolbox Tab.)

Task

In MolQuest, a task is a command to run a program using certain values of its parameters (properties). Same program with two different sets of values of its parameters is considered to represent two different tasks. Current status of a task (being processed, finished, ready) is displayed in Project Tab.

Project

Project is the key element and executable unit of MolQuest workflow, consisting of an ordered set of tasks, defined by user. For each new project, MolQuest creates a separate folder. That folder contains subfolders corresponding to each of a project's task, where those tasks' outputs are written and can be accessed by user. A list of a project's tasks is shown in Project Tab and Pipeline tab. While executing a project, only tasks with status Enabled are executed (see Task Status).

Pipeline

An output of a task can be as an input for another task, which creates a sequential order of tasks, called pipeline. The Pipeline Tab displays all links between tasks in a pipeline. Predefined pipelines from packages are shown in Pipelines List of Toolbox Tab

View

Quite often, users run the same program with varied values of program's parameters (properties). Each set Program + Properties can be specified as a separate task: for instance, program P with

several different sets of parameters can be defined as several separate tasks, T1, T2 etc. In many cases, however, an alternative approach, which uses MolQuest's concept called View, is more convenient. View is a set of parameters values within a task, so that instead of separate tasks as above we get a set of separate views, V1, V2 etc. Each task has at least one view, Current View, which is used when task is executed. Each of existing views within a task can be set as Current View, which is done when user wants to run a task with a different set of values of program's parameters.

User can not only set parameters to different values, but also hide non-essential parameters from being shown Properties Tab. For instance, user can take view V1 and hide all non-essential parameters, creating view V2 – identical in all respects except visual representation of parameter values. This is useful in case of multi-parameter tasks, when only few parameters are varied, while the majority remain the same and are hidden from view in order not to distract user.

Converter

In most cases of pipeline-like queues of tasks, an output of one task, supposed to be used as an input of another task, has format that is incompatible with «downstream» task. To convert an output to format suitable for another program, special auxilliary programs, called converters, are used. In many cases, MolQuest can automatically add an appropriate converter to a pipeline. As most programs, converters are distributed in packages. The Converters List in the Toolbox Tab shows all available converters.

Getting Started

As we now know, in order to execute even a single task, user has to create and run a project. Here we discuss how to work with projects, specifically:

1. Create/open a project.
2. Add tasks to the project.
3. Define task properties.
4. Enable tasks.
5. Run the project.
6. View results

The user also may create pipelines

Create/open a project

To open an existent project, choose File->Open Project in the main menu. Then choose the project's folder.

To create a new project, use File->New Project in the main menu. In the "Create new Project" dialog, enter folder name for a new project. It will also be assigned as a name of a project itself. If you want to change the location of the project folder, press Browse button. If the project folder already exists in the current location or contains invalid symbols, the "OK" button in the "Create new Project" dialog will be inactive. The project name is shown on top of the Project Panel. You

can change the name, it does not have to match the folder name or be unique. Press the "OK" button to confirm. A new project with the specified name has now been created.

Add tasks to the project.

Choose a program group in Toolbox and double click to a program to append it to a list in Project Tab. Generally, the task is not yet ready and cannot be enabled unless its mandatory parameters (also called properties) are assigned values – for instance, FGENESH cannot run unless genefinding matrix (human, monocot plants etc.) is specified. Project tasks are also displayed in Pipeline tab.

Define task properties

The properties (parameter values) of a task can be edited in Property Editor of Properties tab. Before a task can be executed, you must set values to all necessary parameters. If a mandatory parameter is not set or its value is wrong, MolQuest highlights it with red color and "!" mark, like this:

! File List

Enable a task

Since only enabled tasks are executed during the project, a task scheduled for execution should be enabled first. To enable a task, do one of the following:

- Use the **Task->Enable Task** command on the Main Menu
- In the list of project tasks, tick the check box ☑ in the "Status" field.
- Press the ⊟ button. This enables all tasks within a project that are in "Ready" status.

Only tasks that are in "Ready" status can be enabled (see Task Status).

Run a project

When a project is run, its tasks are executed one by one in the same order as they appear in the list of project tasks, from top to bottom (Project Tab). A user can, at any time, change an order in which tasks are executed. To change an order, use **Task->Move Up** and **Task->Move Down** commands of the Main Menu or ⬆ and ⬇ buttons.

To run a project, do one of the following:

- use the **Run->Run Project** command on the Main Menu
- Press the ▶ button on the Toolbar.

If you want to execute only one task of a project, select the task at the Project Tab or the Pipeline tab.and click ▶ If you run a single task rather than a project, that task can have not only status "Enabled", but also "Ready".

When a task is being run, its status is "In Progress" (see Task Status).

Completed tasks have status "Completed" (see Task Status).

If an error occurred during the execution of a task, the task gets either "Completed with Warnings!" ⚠ or "Completed with ERROR!" ⊗ status (see Task Status).

Interrupting execution of a project or a task

To interrupt execution of a project, do one of the following:

- Press the ▶■ button or use **Run->Stop Project** command in the Main Menu. This stops the execution of a project immediately after completion of any task pass that is currently running.
- Press the ■ button or use **Run->Abort Project** command in the Main Menu. This aborts a task currently running and stops the execution of a project immediately.

To interrupt the execution of a task, do one of the following:

- Press the ▶■ or use **Task->Stop Task** command in the Main Menu. Stops the execution of a task immediately after completion of a pass that is in progress.
- Press the ■ button or use the **Task->Abort Task** command on the Main menu. Aborts a task immediately.

If you interrupt a task, a project continues running, the next task in a queue being executed, unless you run a single task by pressing a ▶¹ button (see above).

Viewing results

Executed task assumes one of three states:

"Completed" – Normal completion, output was created

"Completed with Warnings" – Output was created, but may be wrong: user should check warnings.

"Completed with Errors" – Output may be missing. Even if it exists, it is wrong.

An output of a task can be viewed in Project Tab (column "Results"), Results Tab or View/Console Tab.

Create pipelines

A project may consist of a complex sequence of tasks, where an output of one task is used as an input for another. Such kind of project is called a pipeline.

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There are two ways of making an output of one task an input of another task: You can use either Property Editor or Pipeline tab.

In Property Editor, choose "Pipe" type for required input source. The button appears which, when pressed, displays "Select Task Output" dialog listing outputs of all project's tasks that can potentially be used as inputs.
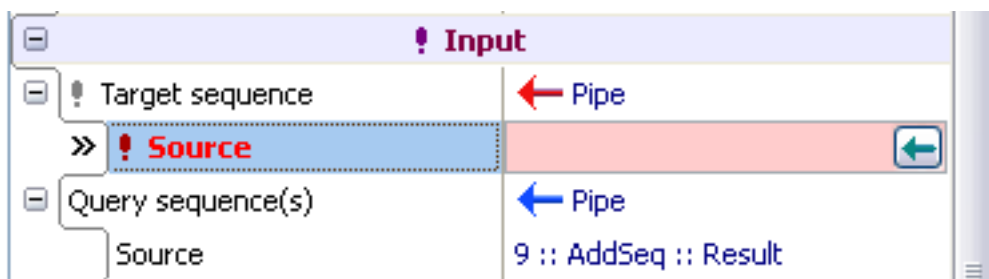
Alternatively, you can use Pipeline tab, which displays MolQuest projects as block diagrams in user-editable form. Here, to create a pipeline, connect output and input of corresponding tasks with a mouse: click on an output of a task, and a cursor takes this form:
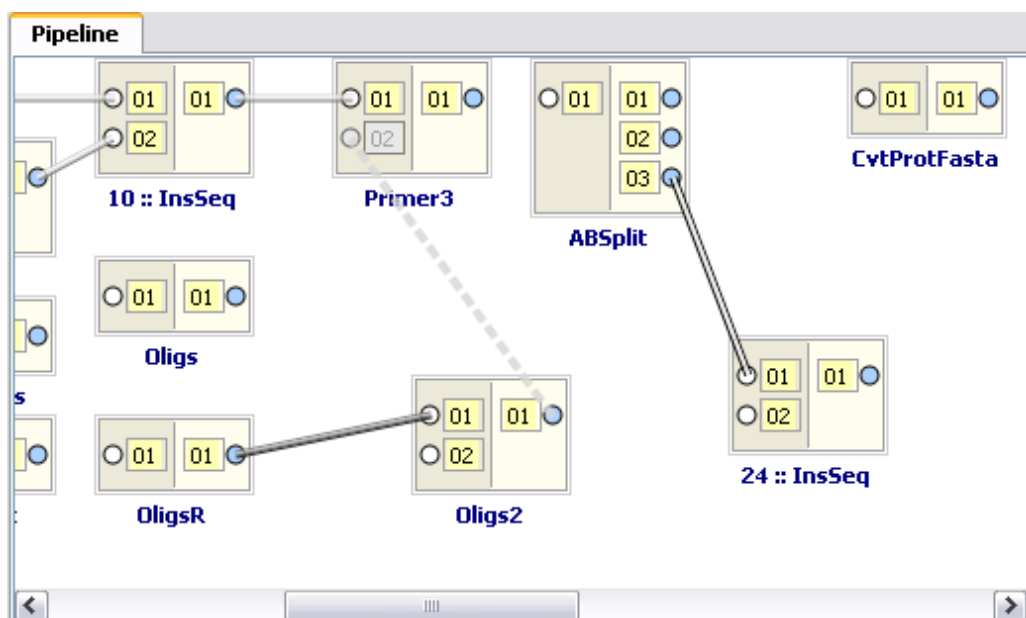
, now move a cursor to an input area of a "downstream" task. Yellow line will follow a cursor there. If two tasks cannot be linked in a pipeline, a cursor transforms into this icon: .

If, however, link is possible, it will look like this: . Click on an input area, and two tasks are linked into pipeline relationship. Similarly, you can start with an input field of a downstream task and move to output field of an upstream task. In such case, cursor will assume this look: .
If output and input formats of tasks are compatible, a pipeline link between them looks as a solid gray line: . If formats are incompatible, but a correspondent converter is registered with MolQuest, a link looks like a dotted gray line: . Finally, if formats are incompatible and there is no converter available, it looks as a black line: .

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Interface

Application window
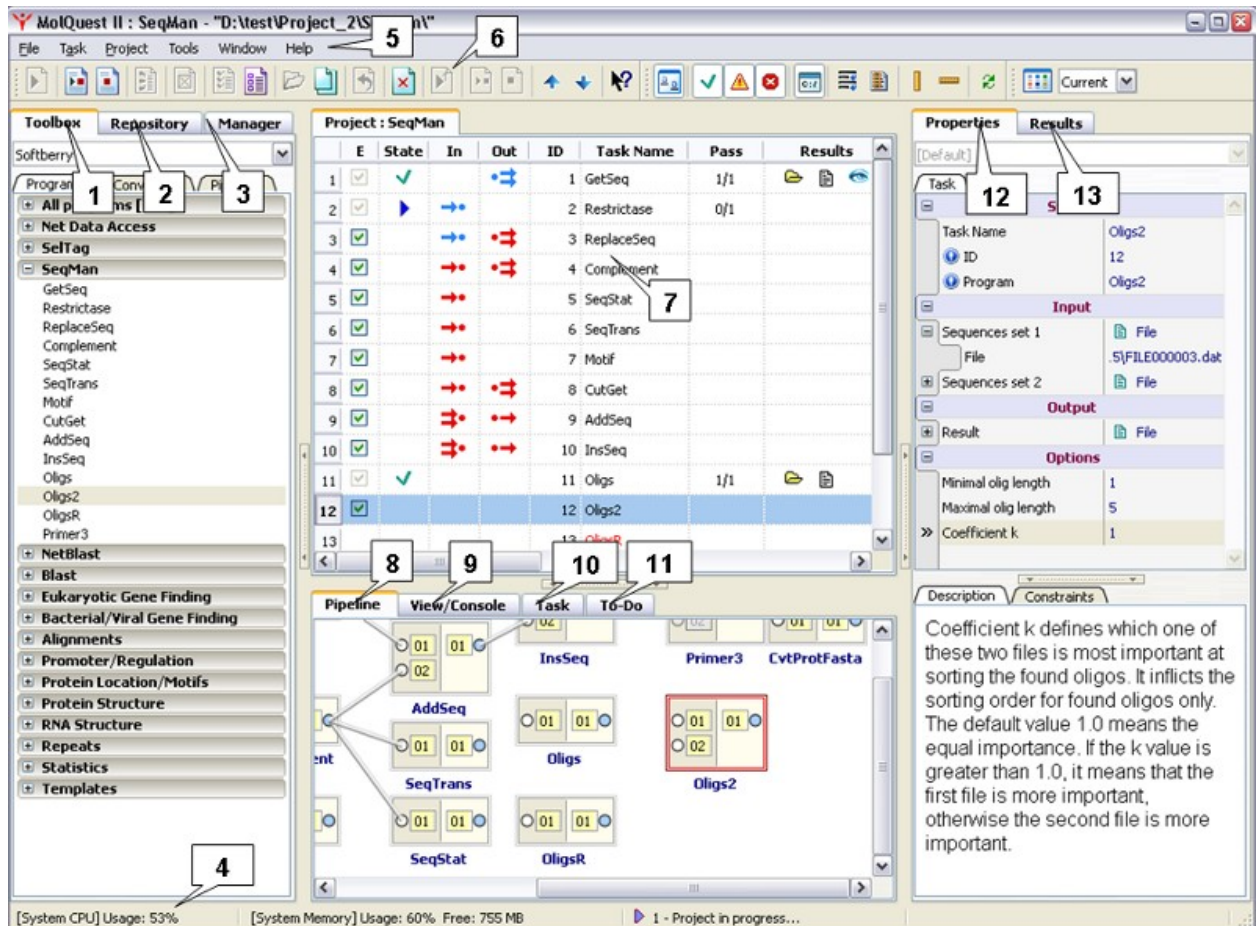
1. Toolbox tab. **2.** Repository tab. **3.** Manager tab. **4.** Status bar. **5.** Main menu. **6.** Toolbar. **7.** Project tab. **8.** Pipeline tab. **9.** View/Console tab. **10.** Task tab. **11.** To-Do tab. **12.** Properties tab. **13.** Results tab.

Menus of application window

Main window has the following pull-down menus:

- File
- Task
- Project
- Tools
- Window
- Help

File

- **New Project**: Create a new project. In "Create New Project" dialog, enter folder name for a new project. It will also be assigned as a name of a project itself. If you want to change the location of the project folder, press Browse button. If the project folder already exists

in the current location or contains invalid symbols, the "OK" button in "Create new Project" dialog will be inactive. The project name is shown on top of the Project Panel. You can change the name, it does not have to match folder name or be unique. Press the "OK" button to confirm. A new project with the specified name has now been created.
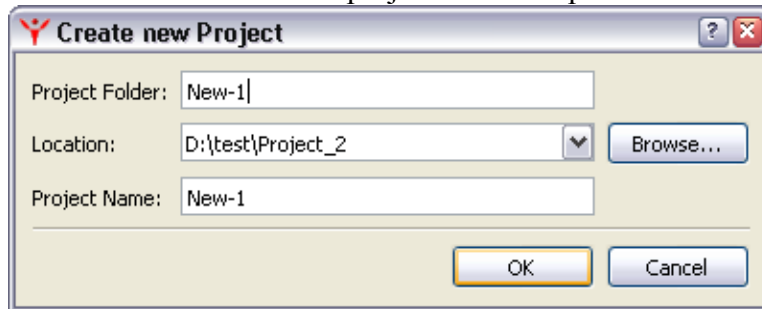

- Open Project - Open an existing project. Displays "Open project" dialog. Choose a project folder and press the "Choose" button. The project is now assigned a "current project" status. Project Tab and Pipeline Tab display tasks of current project.
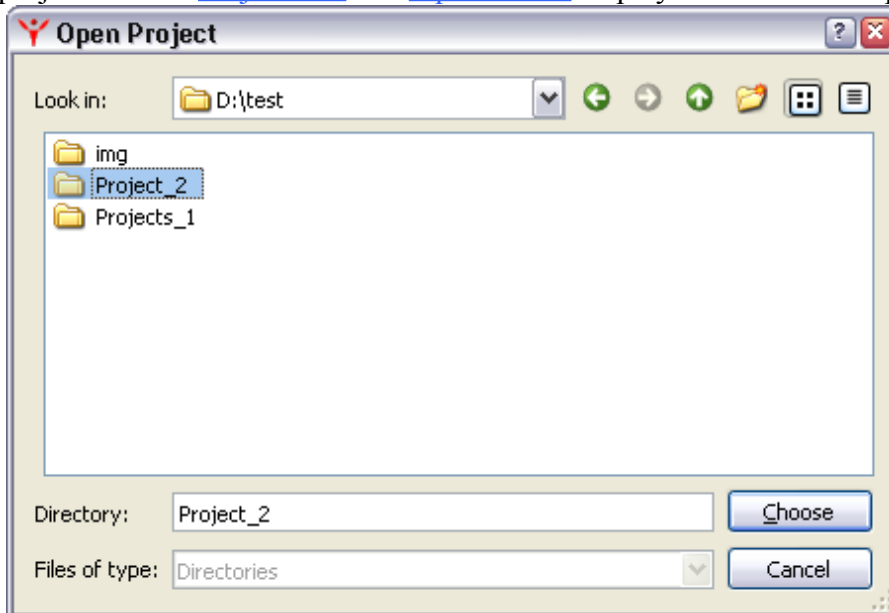
- Reopen Project - Reopens current project without saving any changes made during the session.
- **Save All** - Save all projects in their current state.
- **Save Project** - Save current in its current state.
- **Save project as** - This command is used to create a copy of the current project. All tasks and their properties are copied, while outputs/results are not. Completed tasks change their status to "ready", states of other tasks are unaffected. A dialog "Save project As" is displayed. Type a unique name of a project copy. If name already exists or contains invalid symbols, the "OK" button in the "Create Project" dialog will be inactive. Valid symbols are same as for Windows filenames. Press the "OK" button to confirm. The copied project is now the current project.
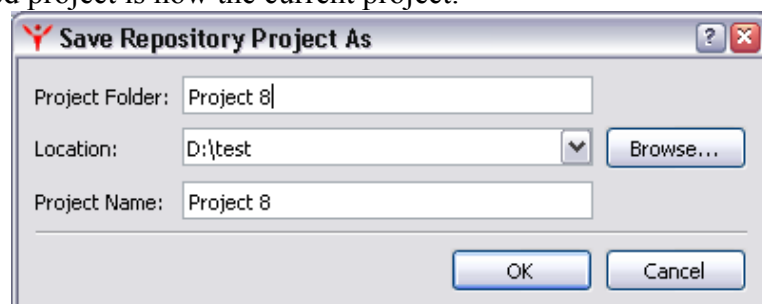
- Close Project - Close current project. The project is saved at its current stage of progress and then closed.
- **Close All Projects** - Close all projects. The projects are saved at its current stage of progress and then closed.
- **Load Projects List** – Load projects from previously saved projects list. These projects are appended to a list of open projects (see below).
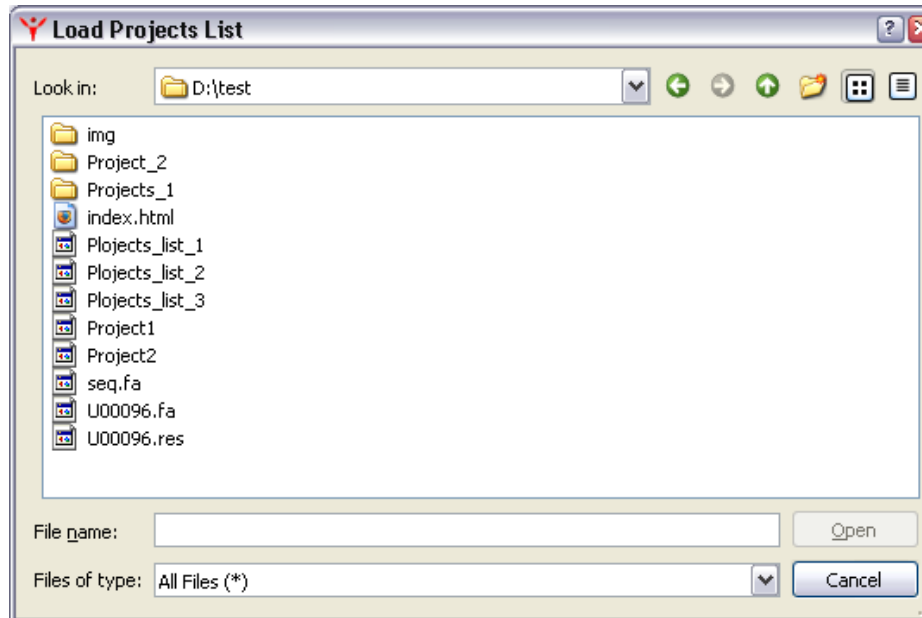

- **Save Projects List** – Save a list of open projects. This list is also shown in Manager Tab.
- **Close Project without saving** - Close current project without saving. Any unsaved changes will be lost.
- **Close All Projects without saving** - Close All Projects without saving.
- **Exit without projects saving** - Close All Projects without saving and exit the application.
- **Exit** - Save all projects in their current state and exit the application.

Task

- **Run Task** – run Selected Task. Task status must be Ready or Enabled
- **Stop Task** – stop execution of selected running task. If a task has several passes, it stops after current pass is copleted. This command does not stop the execution of a project. Other enabled tasks, if any, will be executed.
- **Abort Task** – immediately abort a task. This command does not stop the execution of a project. Other enabled tasks, if any, will be executed.
- **Enable Task** – enable a task. Only enabled task are run when a project is executed.
- **Disable Task** – change task status from Enabled to Ready.
- **Move Up** – move selected task one position up in a list of project tasks.
- **Move Down** – move a task one position down.
- **Copy Task** – create a copy of selected task and its properties. Results/output are not copied.
- **Open Task Folder** – open a folder with task output files.
- **Delete Results** –delete results of selected task and resets its status to Ready.
- **Delete Task** – delete a task and its results.

Project

- **Rename Project** - rename selected project. Displays "Rename Project" dialog.
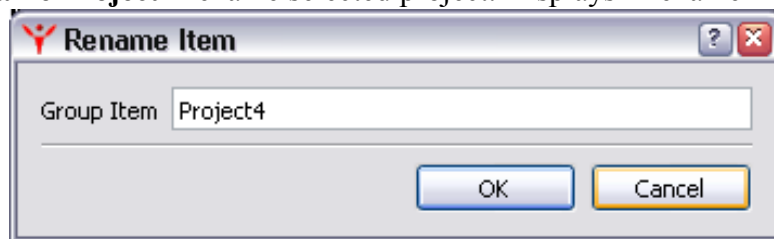
- Run Project - run a project. Only enabled tasks will run.
- **Stop Project** - stop execution of a project immediately after a task pass in progress is completed.
- **Abort Project** – immediately abort execution of a project, not waiting until currently running pass is finished.
- **Enable All Ready Tasks** - enable all tasks in current project. Only enabled tasks are run when a project is executed.
- **Disable All Enabled Tasks** – change status of all enabled tasks to Ready.
- **Delete All Results** - delete results of all tasks within a project that have been completed.
- **Clear Project** - delete all tasks from current project.
- **Delete Project** - delete current project.

Tools

- **Start With Selected Profile** – If enabled, the last selected profile (see Profile Manager dialog) is loaded when MolQuest is started. If disabled, MolQuest loads at start up the same configuration in had when exited.
- **Profile Manager** - displays Profile Manager dialog for changing existing profile settings or creating new ones.
- **Options** - Displays Options dialog, which is used to control various MolQuest settings.
- **Panels Settings** - displays Panels dialog.
- **Property Editor Options** – displays Property Editor Options dialog .
- **Install Package** - Displays "Install Package" dialog, used to install new programs and converters within MolQuest. Requires administrator privileges.
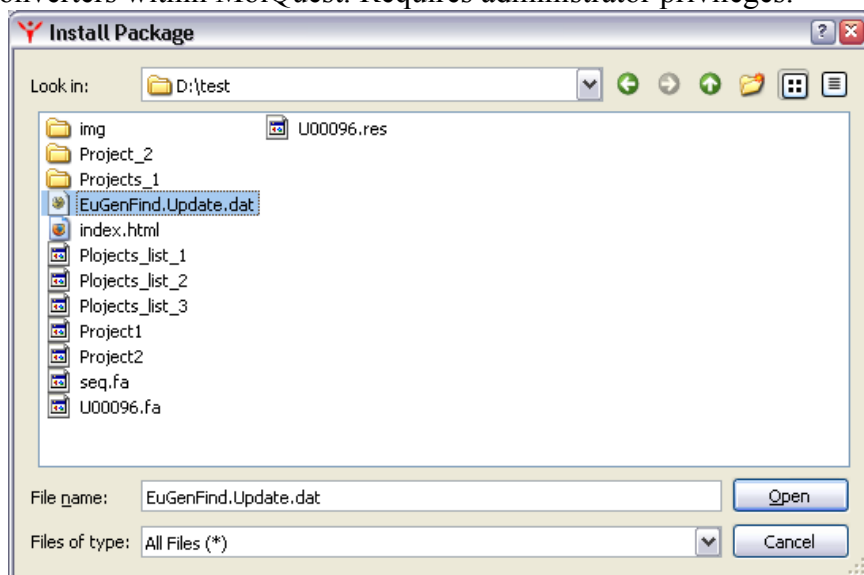
- Install License – install a new license.

Window

- **Style** – sets interface window.

- **Toolbars** – chooses toolbars to display (see Toolbars).
- **Screen Shot** – choosing this menu option makes a shot of MolQuest screen, and a dialog for saving a screenshot is displayed. A shot is saved in png format.

Help

- **MolQuest Help** – displays MolQuest help.
- **MolQuest License Agreement** - displays MolQuest license agreement.
- **Tutorials** – submenu with a list of flash tutorials.
- **"Company" Main Help** - displays main help for selected company (currently only Softberry).
- **"Company" Help Files** – submenu with all help files for selected company.
- **"Company" Sample Data** – open a folder with sample data for selected company.
- **"Company" Sample Projects** - displays "Sample Projects" dialog with list of premade sample projects for selected company.
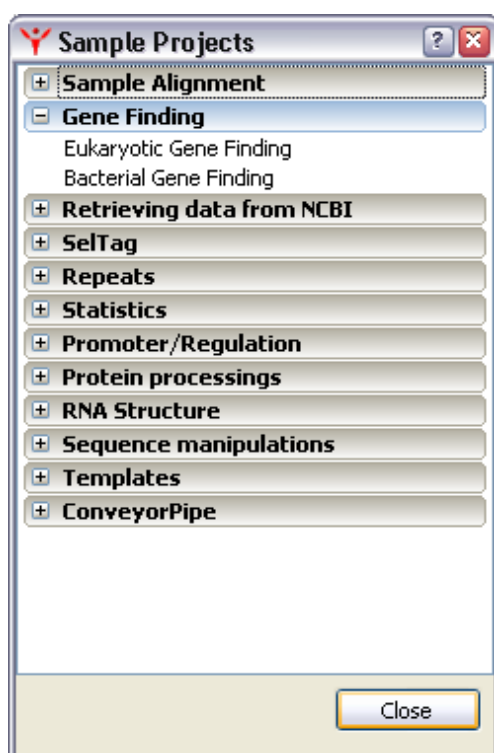
Choose program group and double click a program to create a project based on sample project. After choosing a project, "Save Sample Project As" dialog is displayed. See Save Project As.
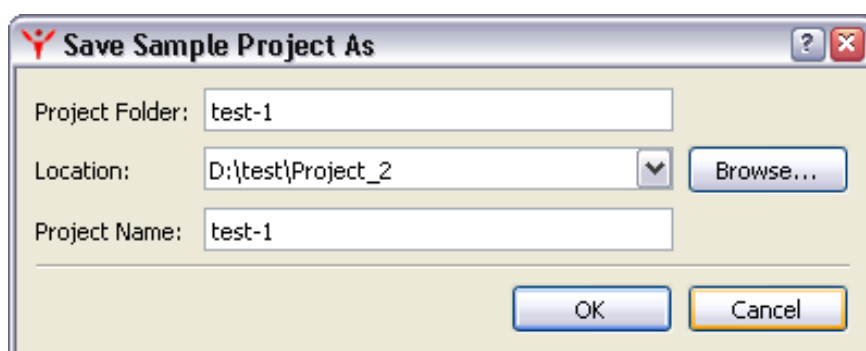
- Softberry Home Page - opens Softberry home page.
- **MolQuest Home Page** - opens MolQuest home page.
- **MolQuest Updates** - opens MolQuest Updates page.
- **MolQuest Technical Support Page** - opens MolQuest Technical Support page.
- **MolQuest Technical Support Mail** - send an e-mail to MolQuest Technical Support.
- **About** - displays "About" dialog.

Toolbars

MolQuest has three toolbars: Project, View/Console, Configuration.

Project toolbar

Project Toolbar contains buttons for work with projects and tasks, which have the following functions:

	Same as: Project->Run Project in Main Menu
	Same as: Project->Stop Project in Main Menu
	Same as: Project->Abort Project in Main Menu
	Deletes all Tasks from Project
	Same as: Project->Delete All Results in Main Menu
	Same as: Project->Enable All Ready Tasks in Main Menu
	Same as: Project->Disable All Enabled Tasks in Main Menu
	Same as: Task->Open Task Folder in Main Menu
	Same as: Task->Copy Task in Main Menu
	Same as: Task->Delete Results in Main Menu
	Same as: Task->Delete Task in Main Menu
	Same as: Task->Run Task in Main Menu
	Same as: Task->Abort Task in Main Menu
	Same as: Task->Move Up in Main Menu
	Same as: Task->Move Down in Main Menu
	Evokes help cursor. Point it to a window object and click to get help.

View/Console toolbar
View/Console toolbar has buttons for work with View/Console tab

	Does the same as «Activate View/Console» in dialog Tools->Options->View/Console in Main Menu
	Same as «Show Results» in dialog Tools->Options->View/Console in Main Menu

⚠	Same as «Show warnings» in dialog Tools->Options->View/Console in Main Menu
⊗	Same as «Show errors» in dialog Tools->Options->View/Console in Main Menu
c:\	Same as «Console Mode» in dialog Tools->Options->View/Console in Main Menu
≡↓	Same as «Wrap by View Width» in dialog Tools->Options->View/Console in Main Menu
🗎	Same as «Column Selection Mode» in dialog Tools->Options->View/Console in Main Menu
▯	Same as «Show Left Ruler» in dialog Tools->Options->View/Console in Main Menu
▭	Same as «Show Top Ruler» in dialog Tools->Options->View/Console in Main Menu
♺	Reopen current file in View/Console

Configuration toolbar

▦	Does the same as: Tools->Profile Manager in Main Menu
Current ⌄	Chose profile from a list and make it current

Toolbox tab

Toolbox tab is used to add a program or a converter to a project. The drop down list at the top of the tab contains the names of companies whose programs are included in MolQuest (currently only Softberry).
The tab contains the following lists:

Programs list. This list contains all included programs of a given company. To add a task to a project, expand appropriate group and double click on a program name.

Converters list. To add a converter to a project, double click on a converter name. Converters are special programs for changing file formats. Unlike regular programs, converters can be added to a project not only by user, but also automatically at pipeline level (see Pipeline Tab)

Pipelines list. Contains a list of pipeline template projects. To create a project from a pipeline template, double click on a pipeline name.
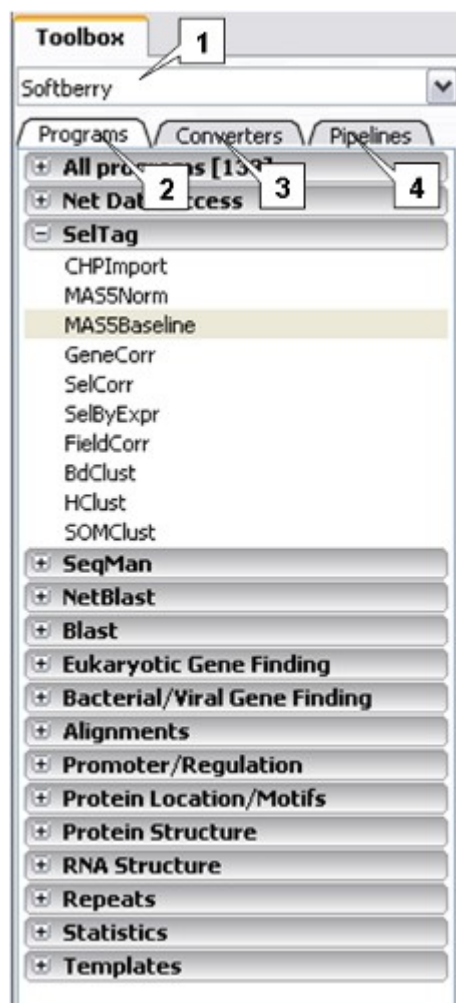
1. List of distribution companies. 2. List of programs. 3. List of converters. 4.List of pipelines.

**Contextual menu** of the "Toolbox" tab contains the following commands:

- Auto Collapse Groups – if checked, selecting one program group collapses all other program groups.
- **Collapse All** - collapse all program groups.
- **Expand All** - expand all program groups. If "Auto Collapse" mode is checked, this option is inactive.
- **Program (Converter, Project) Help** - open help for selected program **(**converter, pipeline**).**

Properties tab

Properties tab is for setting up task properties (parameters). The Properties tab contains:

- View List
- Property Editor
- Description page
- Constrains page
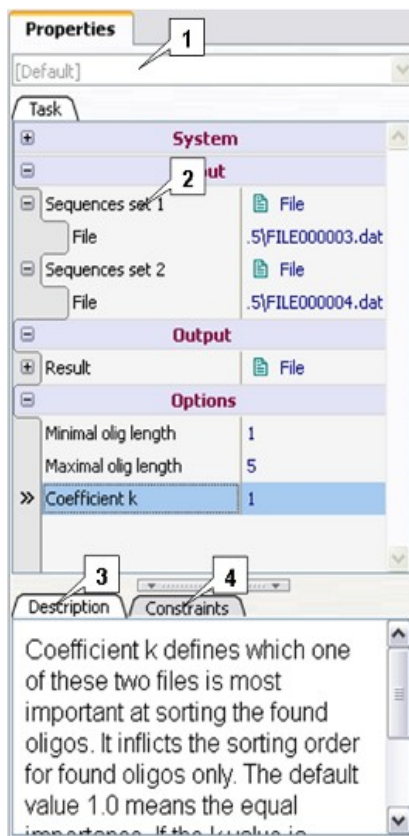
1. View List. **2.** Property Editor. **3.** Description page. **4.** Constrains page.

- **View List**

View List contains a list of predefined task's Views (see View). The contextual menu of View List is as follows:
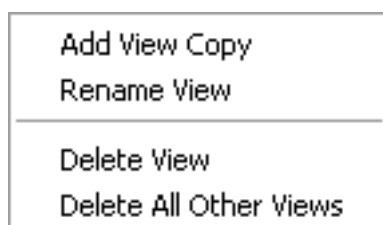
- **Add View Copy –** Create a copy of current view**.** Displays "Add View Copy" dialog, where user enters a name of a new View.
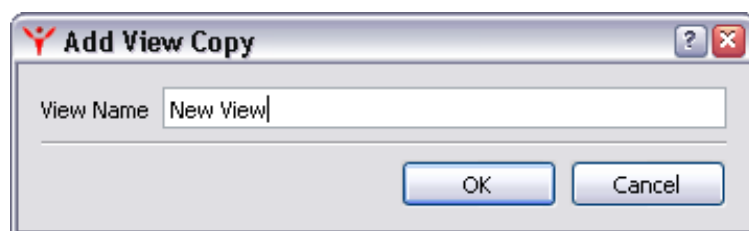
- Rename View. Displays "Rename View" dialog, where user can change a name of a current View.
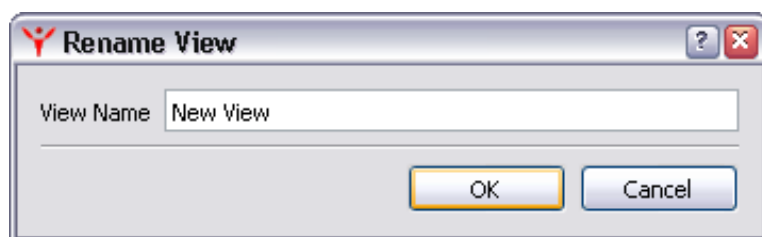
- **Delete View**.
- **Delete All Other Views**. Deletes all Views except selected one.

▪ Property Editor.

Before executing a task, user has to specify all task's properties (parameters), for instance type and location of an input, output options, and program options: for instance, organism-specific matrix or codon table for FGENESH. Some tasks have several dozens of properties with complex dependencies. Any single property can be mandatory or optional. Some properties have default values.

Property Editor handles all task properties in a convenient way. User can specify strings, numbers, files, lists of files, folders and other types of data as property values. Every property has a value, and some values are incompatible with each other. Property Editor checks properties for such incompatibilities or other errors, as well as for omissions. Properties can be nested (see example below).

Properties are grouped in sections, which vary depending on program. The most common sections are following:

- **System** - contains such informational properties as task name, program name and version etc. This section is mandatory, but filled automatically.
- **Input** - includes various input properties, such as a source of input data (pipe, file, list of files etc.), definitions for detailed input (lists of variables or cases in SelTag) etc.
- **Output** - includes various output properties, such as an output filename, its format, etc.
- **Options** - includes various task properties, such as processing modes, restrictions, coefficients etc.

▪ Property Icons and Property Activity

Below is a window of Property Editor.

Left column contains name of each property, right column – its value. Some of properties can have the following information icons next to their names:

ⓘ	This is a system property, not defined by user. One such property is program name.
❗	The value for this property is undefined or wrong.
❗	This node contains one or more nested properties, for which the values are undefined or wrong.
☐	This property is inactive and not used by the task, so its value can't be set.
☑	This property is active and its value must be set.
■	This property is "Read only", and its value can't be changed. Unlike system property, value of read only property affects task results. A property can become "read only" either by user's choice (selection of "Property Permanently ReadOnly" command in contextual menu) or by such combination of values of other properties that allow only single value of this property.
✕	This property is disabled. If parent property is inactive or read only, nested properties are disabled.

Disabled and other inactive properties are shown in grey.
A program can have optional parameters, so some properties may be switched between active

and inactive states by checking/unchecking the box: ☐ / ☑ . Other properties are permanently active. Active properties are used by a task, inactive are not.

Examples of disabled properties are below.
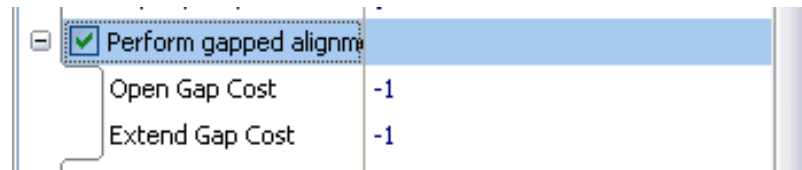
«Perform gapped alignment» property is optional and set active (box is checked), its nested properties are «Open Gap Cost» and «Extend Gap Cost». If «Perform gapped alignment» property is set inactive (box is unchecked), nested properties «Open Gap Cost» and «Extend Gap Cost» are disabled.
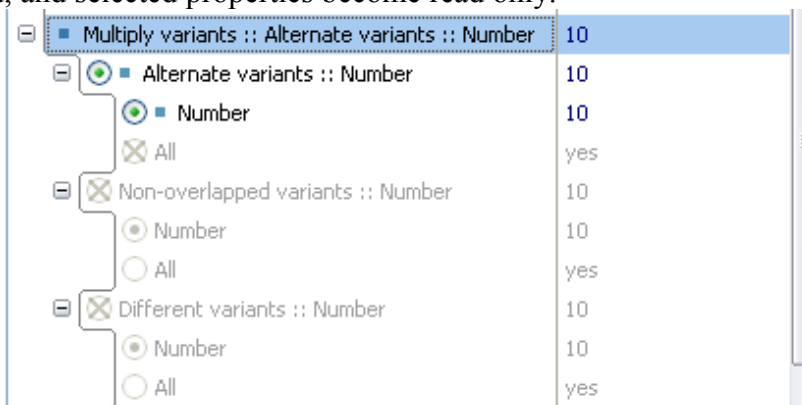

If a property is inactive, all nested properties are inactive as well, so Property Editor disables editing their values.

A property is also disabled if its parent property is read only, for example:
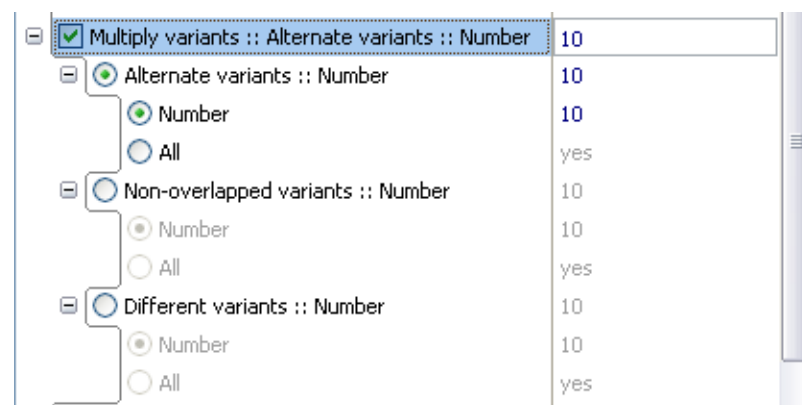
If «Multiply variants……» property is set to read only, all nested properties except selected become disabled, and selected properties become read only.

- **Contextual menu of Property Editor**

Contextual menu of [Property Editor](#) contains the following commands:

- **Collapse All** - collapse all nodes.
- **Expand All** - expand all nodes.
- **Top position** - go to the top of a list.

- **Copy Value** - copy property value to clipboard.
- **Paste Value** - paste property value from clipboard.
- **Copy Property String** - copy property name and value to clipboard.
- **Open folder** - open folder where selected file is located.
- **Open with text editor** - open file using text editor.
- **Open with viewer** - open file using special graphical viewer (must be installed).

- **Property - Rename** - rename a property. Displays "Rename Property" dialog.
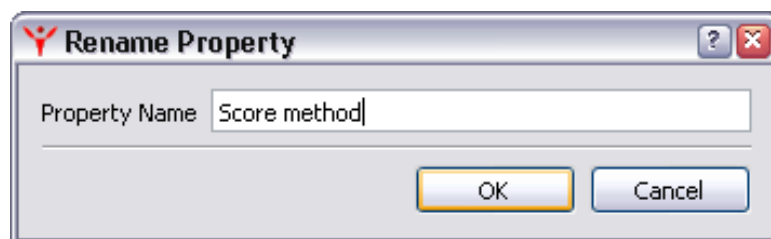
- **Property - Move Up** - moves property up. Property can also be moved within nested group of parent property.
- **Property - Move Down** - moves property down.
- **Property - Permanently Active** – makes an optional property permanently active, i.e. mandatory. This action can't be undone in current View.
- **Property - Permanently Hide** - Hides property, locking its value and activity status at the same time. This action can't be undone in current View.

- **Property - Permanently ReadOnly** – makes property read only. All active nested properties also become read only, while inactive nested properties become disabled. This action can't be undone in current View.
- **List Item - Rename** - Some properties have only a fixed set of acceptable values. For instance, genefinding parameters for FGENESH can only be human, mouse, Drosophila etc. This action renames one of such values chosen from a list, for instance user can change Drosophila to fruit fly. Displays "Rename Item" dialog.
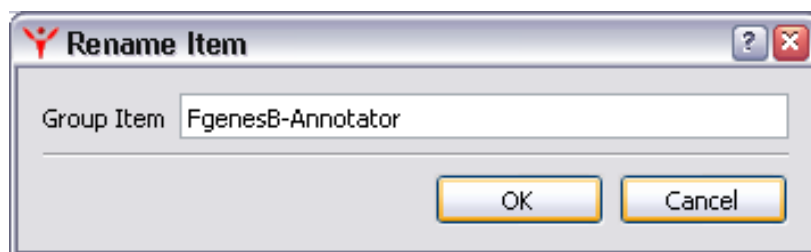
- **List Item - Permanently Active** - make a list item permanently active, i.e. locks property value at this list item. This action can't be undone in current View.
- **List Item - Permanently Hide** - hides a list item permanently, i.e. deletes it from a list of acceptable values. This action can't be undone in current View.
- **List Item - Permanently ReadOnly** - set nested properties of this list item into read only mode, i.e. they become unavailable for editing. This action can't be undone in current View.
- **SubNodes - Permanently Hide** - hide children nodes. This command is available for radiogroups only. This action can't be undone in current View.

Warning! All commands with «Permanently …» in their names can't be undone in the current View. Therefore, before taking such actions, create a copy of current View so that you can restore original View. Otherwise, in order to undo such actions, you'll have to create a new View from scratch.

▪ **Values of properties**

Depending on property type, values can be:

- selected from a list
- typed in manually
- files selected using standard Select File dialog, which appears when the corresponding button in property value column is pressed. Full path is required for input files, for output files - filename only. Path to a file can be typed in or selected in Select File dialog. You can also drag and drop files or paste them from a clipboard. In certain cases, files can be selected from a drop down menu.

For properties that define input data source, there are three possible value variants: **File**, **Files list** and **Pipe**:

- **File** - data are located in a file with user-specified path. Icon indicates that specified file exists, icon - that path or filename are incorrect, i.e. file cannot be located.
- **Files list** – a list consisting of one or more files created in File List dialog (evoked by pressing button) is used as an input. In such case MolQuest runs several passes, one file from a list at a time, in the same order they appear in a dialog window, until all files are processed. Results of each pass are shown in a list in Results tab. Icon indicates
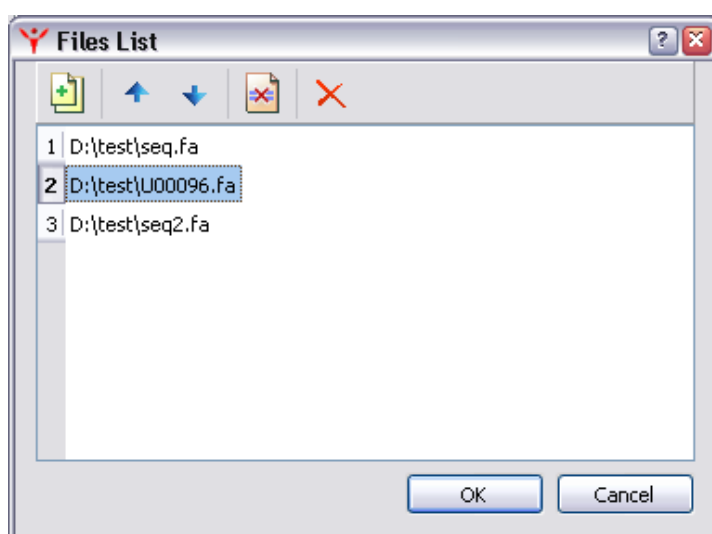
21

that file list is empty, while means that it is not.
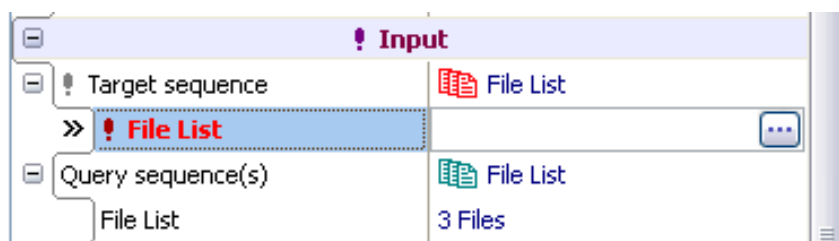
In File List dialog (see picture below), pressing button opens standard Open File window, which is used to add files to a list.

Order of files in a list can be changed by using and buttons.

To remove an individual file from a list, press button, and to remove all files, button.

- **Pipe** – input data are taken directly from output of another task in the same project. Correst link to pipe data source is indicated by icon ,while undefined or wrong link – by icon . Similarly, icon means that destination for output data is correct, and that link is not defined or incorrect.

To choose the link for input data, use button, which displays "Select Task Output" dialog with list of outputs of task within current project.
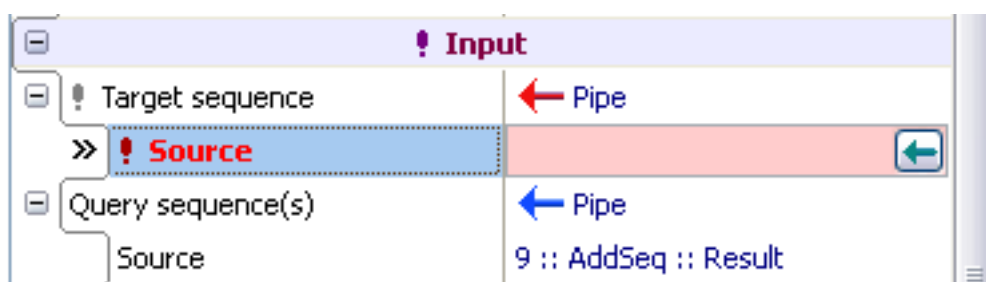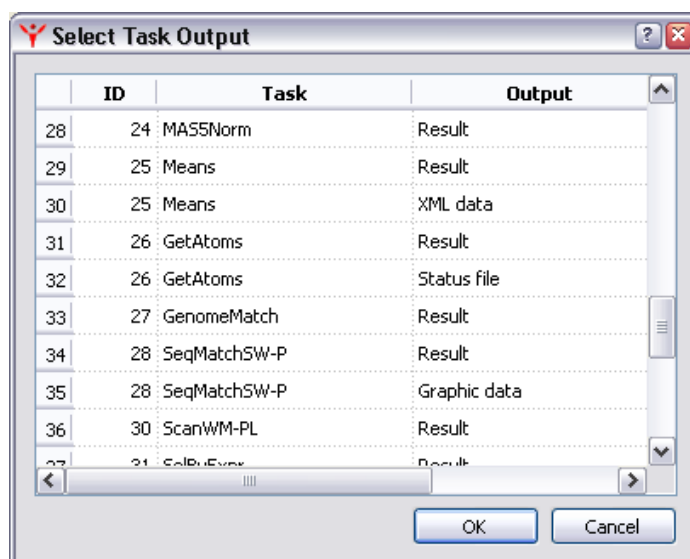
Some properties are mutually exclusive, i.e. if value of Property 1 is set, value of Property 2 cannot be set. Such properties are grouped into a radio node. In such cases, a separator "::" is placed after a name of a node (parent property), separating it from a name of selected nested property. User can change this default style with alternative ones in Rename Property dialog below.

For example, label "Multiply variants::Non-Overlapped variants::Number" means that parent property "Multiply variants" has nested property "Non-Overlapped variants" selected as its value, and this property "Non-Overlapped" has its own nested property, "Number" as its value:
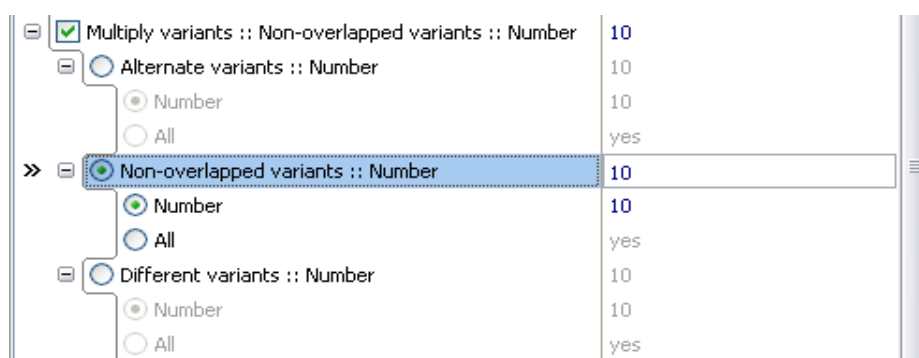
Property Rename command in the contextual menu opens Rename Property dialog. If "Absolute Name" box is checked, name of selected nested property won't be added to node name after a separator.
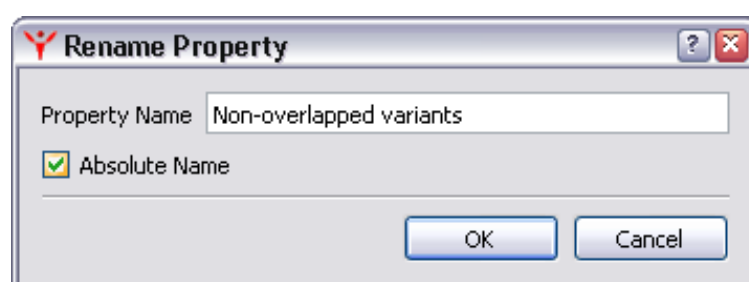
- **Description page**

Description page contains brief descriptions of some selected properties or their values.

Specifies temperature for MC algorithm of side chain conformation optimization.
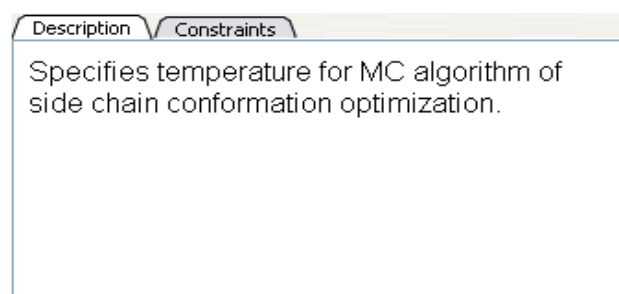
- **Constrains page**

Constrains page contains requirements to values of some properties (value type, minimum and maximum value etc.)
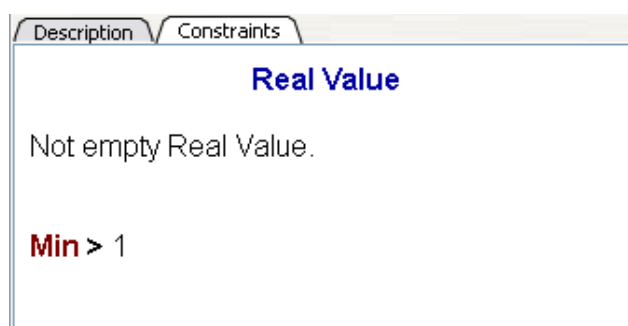
Project tab

Project tab contains a list of tasks in a current project:

The table has the following columns:

N - the order number of each task.
E – displays the current Ready State.
State - displays the current Execution State of a task.
In - displays source of Input Data.
Out - displays destination of Output Data.
ID - displays unique ID of a task. in a project.

Task Name - displays the name of a task.

Pass – displays number of completed passes / total number of passes.

Results column contains shortcuts to task results (output):

- **Results Folder** - opens a folder with output files and log files

- **Results File** - opens "text/plain" file containing task output, if not empty. If this icon is shaded: , MolQuest can't find text viewer for this "text/plain" file.

- **Results Files** – opens nonempty "text/plain" files containing task output. This icon appears instead of the **Results File** ( ) icon if more than output file was generated by a task. Shaded icon indicates that either multiple passes resulted in creation of several sets of output files, which can be viewed in **Results** tab, or MolQuest can't find a viewer for these files

- opens output in a graphical viewer. MolQuest has multiple graphical viewers for many output file formats.

- more than one output file is available for viewing with graphical viewers.

- multiple passes resulted in sets of output files.

Processing – time it took to process task

Start Time – time when task started.

- **Task Status**

Ready State

This is a status of task's readiness for execution:

	Not Ready. Some required properties are not defined and/or some of their values are set incorrectly.
	Ready. All required properties were defined.
✔	**Enabled**. This task will be run during the execution of a project.
✓	**Completed.** The task is completed**.**

Execution State

This is current execution status of a task. Move the mouse cursor over a status icon to display details.

	The task has not been started.
▶	**In Progress**. The task is being run now.
✔	**Completed**. The task was completed without errors or warnings.
⚠	**Completed with Warnings** – Some warnings or errors occurred during task execution, and at least one pass has finished without errors. Put a mouse over the icon to see a diagnostic message. Click the shortcut in Results column to open a

	log file.
	Completed With Error – There are no passes that finished without errors. Every pass of the task were been executed with errors. A task has no meaningful results to use or to send to a pipeline. Put a mouse over the icon to see a diagnostic message. Click the shortcut in Results column to open a log file. See also Results Tab for more information
■	**Aborted**. User aborted a task on the first pass. No results to use or to send to a pipeline.

- **Input Data**

If a task is part of a pipeline, state of input data is displayed here. ➡• icon means that a task uses an output of one pipe as input data, ⇒• means that it uses more than one input pipe. Shaded icons (➡• ⇒•) mean that all input data are ready but are not currently in use by other task, blue symbols (➡• ⇒•) mean that input data are currently being used by running task, red symbols (➡• ⇒•) mean that some data are not ready.

- **Output Data**

Tis column has the same meaning as the «Input Data» column, but for output data of a task.

Results Tab

This tab shows a list of all passes for selected task, with their states.

For many programs, a list of files can the set as an input, in which case each file from a list will be processed by a separate pass of a program. If a task has more than one property set as a list of files, all combinations of files will be processed. For instance, if Property 1 is specified as a a list containing three files, and Property 2 as a list of four files, there will be 4 x 3 = 12 passes, each one combination of input files. Total number of passes for one task cannot exceed 100,000.

The column in Results tab have the following meaning:

- **Pass** – an order number of current pass;
- **State** - pass status:

▶ - in process;

✔ - completed without errors or warnings;

⚠ - completed with warnings;

✖ - completed with errors;

■ - aborted.
- **View** – view results. Icons have the same meaning as those in Results column of Project Tab, but for current pass only.
- **Processing** - pass processing time;
- **Start time** - pass start time.

For a pass selected in Results tab, the following information is displayed:

In the **Input Files** page, input files that were used by current pass:

     Type - source of input:
     ⬜- file,
- ➡•- pipeline.

View – preview input files. Icons are the same as those in Results column of <u>Project Tab,</u> but for current pass only.

File - path of an input file or pipe identifier.

In the **Output Files** page, a list of output files with their status and shortcuts to preview:

Type - possible output variants:

- ✔ - Normal results file;
- ⚠ - Warnings log file;
- ✖ - Errors log file.

View – preview results. Icons are the same as those in Results column of <u>Project Tab,</u> but for current pass only.

File - name of output file.

Pipeline tab

The Pipeline tab is intended for viewing and editing of MolQuest projects as block diagrams. It provides convenient way for creating pipelines, where output data generated by one task is used as input data for another task.

In Pipeline tab, every task or converter in a project is shown as a box, with task name underneath, input slots, representing input data, in left half of a box, and output slots in its right half. Moving mouse pointer over a slot displays a name of property corresponding to that slot. Boxes can be moved and resized, and slots can be moved and rearranged within their box halves. Selecting a task in Pipeline tab also selects it in Project tab, and vice versa. In Property tab you can view and edit properties of a selected task.

If output data of one task is used as input for another task, corresponding output and input slots are linked by a line. An output slot can have several outgoing links; an input slot can have only one incoming link. To link tasks, click on slot, move pointer to a slot of another task, and click there. Clicking on a first of two slots to be linked enters mouse pointer into linking mode. In this mode, a pointer turns yellow when between slots, and is followed by a yellow line, it becomes

green on slots that are permitted to be linked, and red on slots that can't be linked. To exit linking mode, click anywhere outside slots.
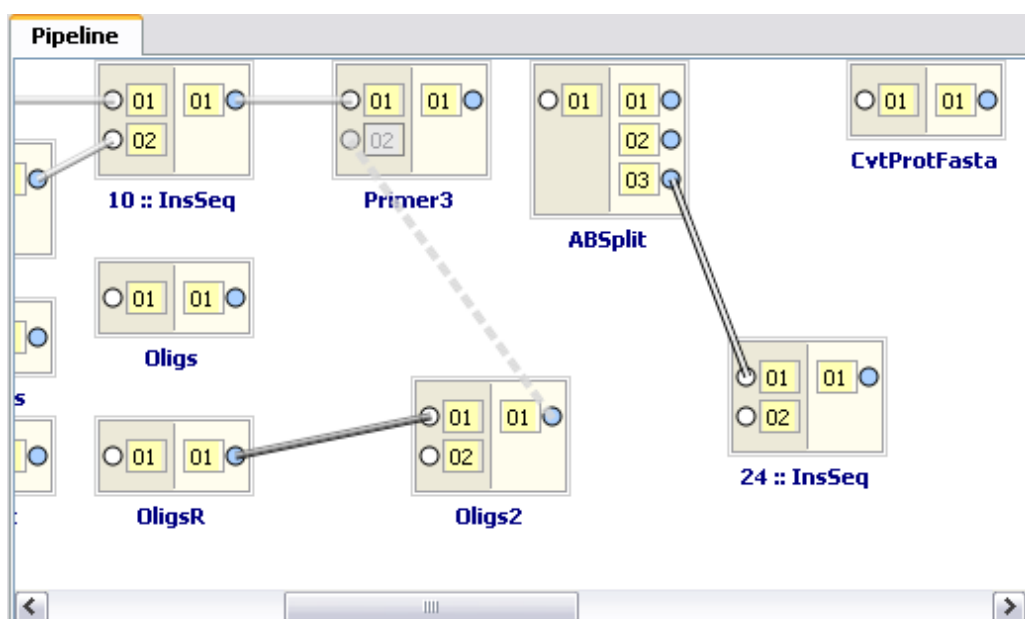
You **cannot** link tasks if:

- You are trying to link input to input or output to output.
- Both ends of a link point to the same task, or links form endless loop.
- An input slot belongs to a task that is currently running or has been completed.
- An input slot is already connected.

Completed link assumes various styles and colors depending on compatibility of formats of linked output and input. Light gray solid line means that input and output data formats are compatible without using a converter. Light gray dotted line means that input and output formats are compatible after using a converter that was automatically selected by MolQuest (so-called implicit converter) and included in a project, implicit converters are not shown as separate tasks. If MolQuest cannot automatically select a converter, the line is shown as solid dark gray. If user adds a converter to a project (explicit converter), it must be inserted between two corresponding tasks, and is shown in Pipeline tab as a task. Lines to/from explicit converter are shown in blue. If one or both linked slots are inactive, the link is shown as a dashed line. Pipelines containing formats judged by MolQuest as incompatible, or containing explicit converters, can be run, but user has to be sure that he can get meaningful results.

	Formats for input and output data are compatible.
	Formats are incompatible, but converter is found and added automatically.
	Formats for input and output data do not match and MolQuest cannot automatically find an appropriate converter.
	Formats do not match selected converter (will be shown for explicit converters unknown to MolQuest).
	Output is disabled.
	Input is disabled.

	The format of input file is a subset of a format of output file. For example: Input file format is "Fasta", output file format is "Multifasta".

To delete a link, click on its input. You can't delete input links of running or completed tasks. To delete tasks or converters, use Project tab. To edit task properties, use the Property tab. To add new task or converter, use **Toolbox** tab.

Properties of a completed task cannot be edited. If you want to alter some properties and preserve task results, use Task->Copy Task command in the main menu and edit properties of a task copy.

Repository tab

User may want to create libraries of tasks and projects, to be used as templates and building blocks blocks for creating new tasks/projects. MolQuest has a repository which can be used for such purpose: Projects (Projects page) and tasks (Tasks page) with user-defined properties can be saved in Repository tab.
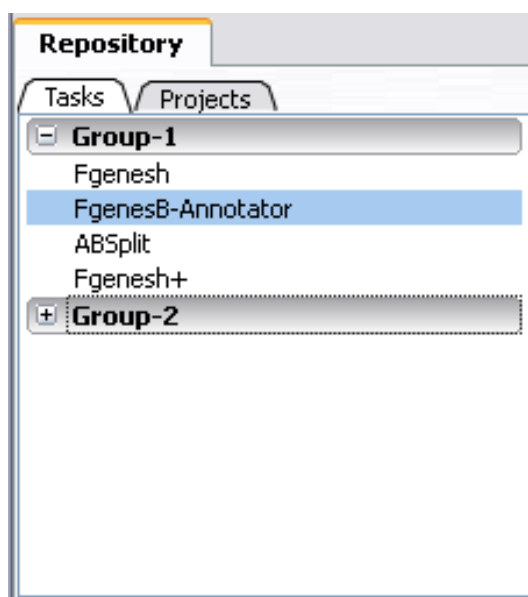
Task page
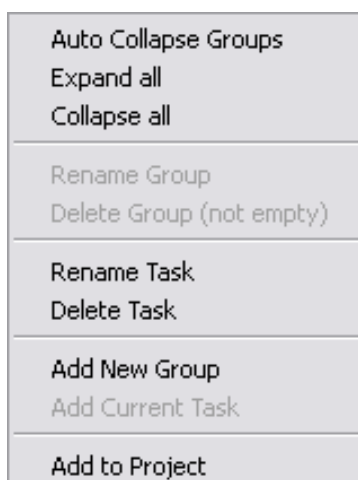
This page contains a list of user-defined groups, each of which can include a number of tasks. Groups can be created, deleted, renamed, or their content can be changed using contextual menu commands:

- **Auto Collapse Groups** – if checked, collapses all groups except selected.
- **Collapse All** - collapses all program groups.
- **Expand All** - expands all program groups.
- **Rename Group** – displays "Rename Group" dialog.
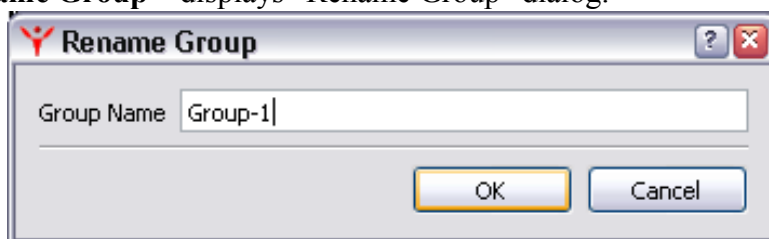
- Delete Group - remove selected group from a list. **Warning!** All tasks in that group are deleted as well.
- **Rename Task** - displays "Rename Item" dialog, in which selected task can be renamed.
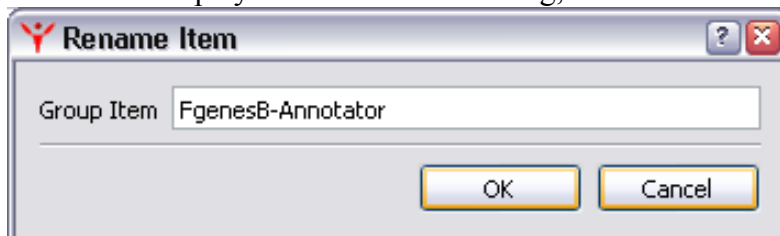
- Delete Task - removes selected task from a group.
- **Add New Group** - displays "Add New Group" dialog.

- Add Current Task - Displays "Add New Task" dialog, where selected task from a current project can be added to a group. **Clear Input:** if checked, all input values are erased.
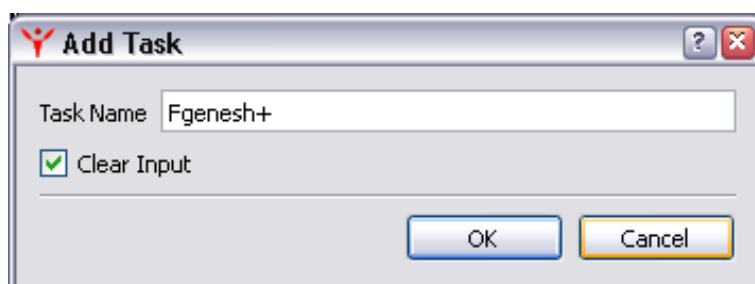
Projects page

Projects page contains a list projects grouped into user-defined groups. As on tasks page, groups can be created, deleted, renamed, or their content can be changed using contextual menu commands:
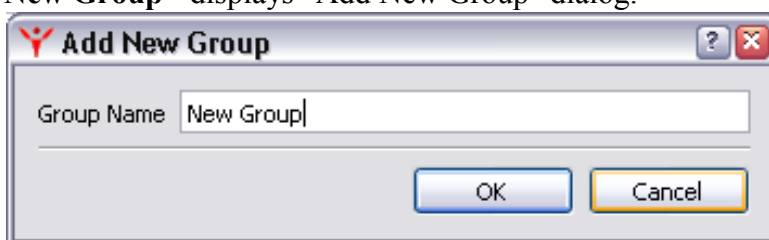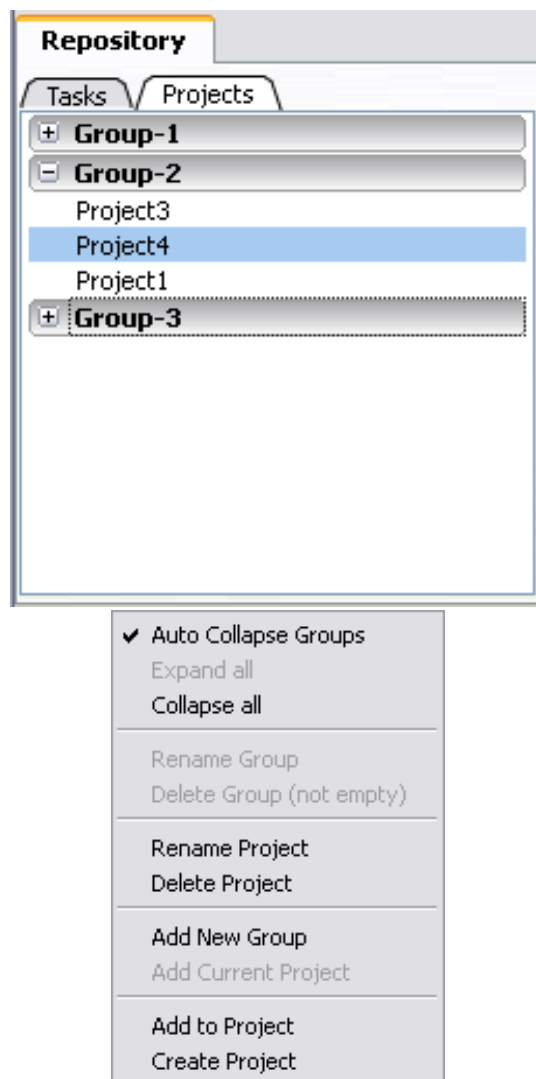
- o **Auto Collapse All** - if checked, collapses all groups except selected.
- o **Collapse All** - collapses all program groups.
- o **Expand All** - expands all program groups. If "Auto Collapse" mode is active, only group is expanded
- o **Rename Group** - displays "Rename Group" dialog, similar to that of Tasks page.
- o **Delete Group** - Deletes selected group and all projects it contains.
- o **Rename Project** - displays "Rename Item" dialog fro renaming selected project.
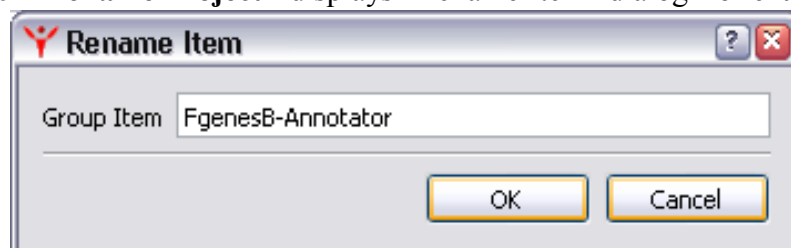
- o **Delete Project** - removes selected project from a group.
- o **Add New Group** - displays "Add New Group" dialog.
- o **Add Current Project** - Displays "Add New Project" dialog for adding current project to a selected group. **Clear Input:** If checked, all input data are deleted, but pipeline links remain in place.
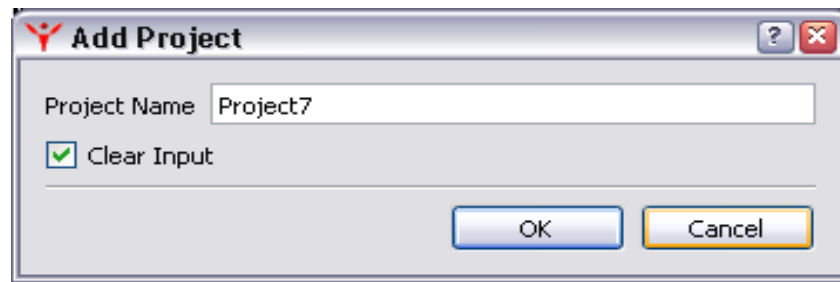
- To load a project from repository, click on it. "Save Project As" dialog will be displayed, where you can type project name and title and choose location for it to be saved in.
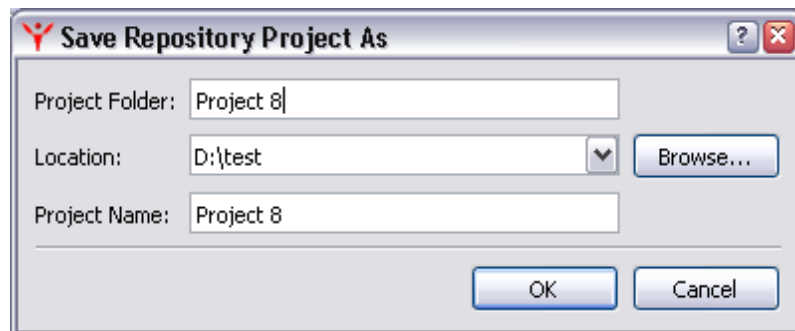
Manager tab
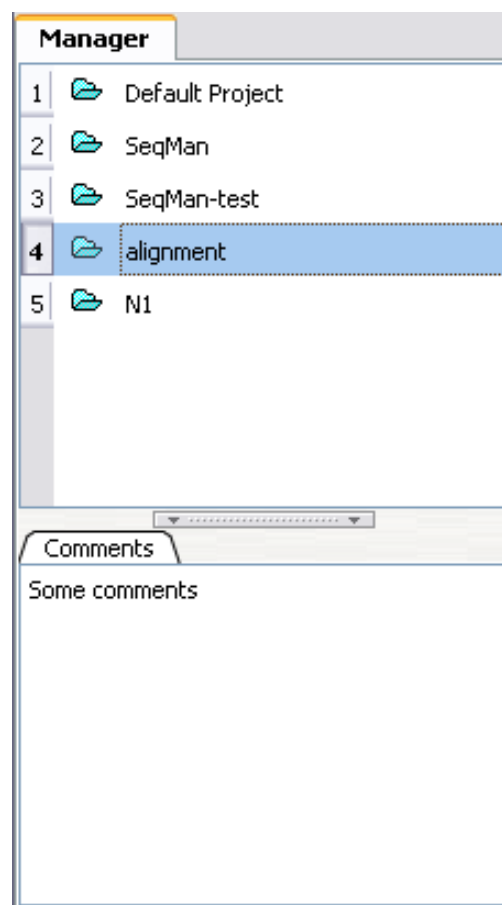
Manager tab contains a list of opened projects. Projects can be dragged by a mouse up and down a list. Click on a project name to switch to that project. **Comments page** contains some comments on selected project.
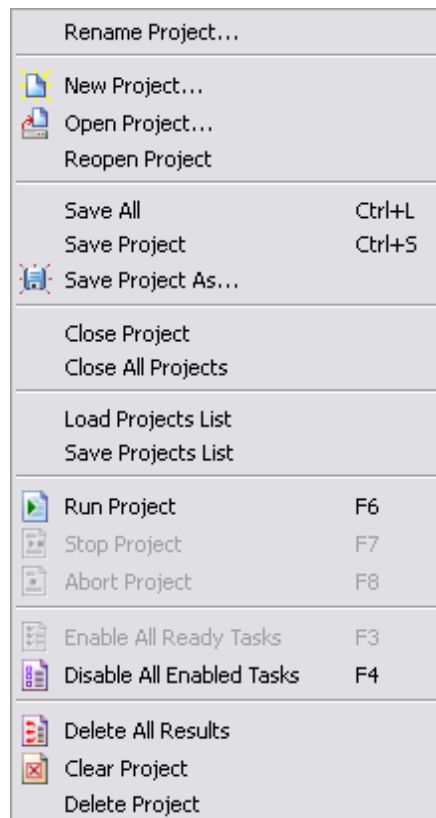
Contextual menu commands of Manager tab:

- **Rename Project** - displays "Rename Project" dialog.
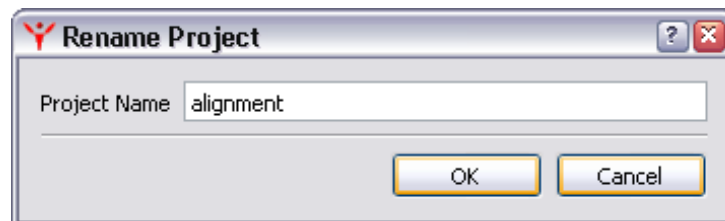
- **New Project** - Displays "Create new Project" dialog, where you can enter a folder name for a new project, as well as choose its location. If project folder with the same name already exists in chosen location, or contains invalid symbol (those not allowed in Windows filenames), the "OK" button is inactivated. Entered folder name is automatically assigned as a title of the project, which is shown on top of Project Panel. You can change a title, it doesn't have to match to the folder name or be unique.
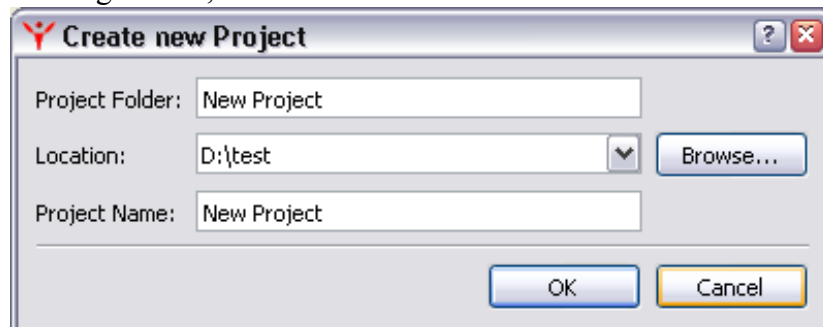
- Open Project - displays the "Open Project" dialog for opening and existing project. After opening, a project assumes a status of current project.
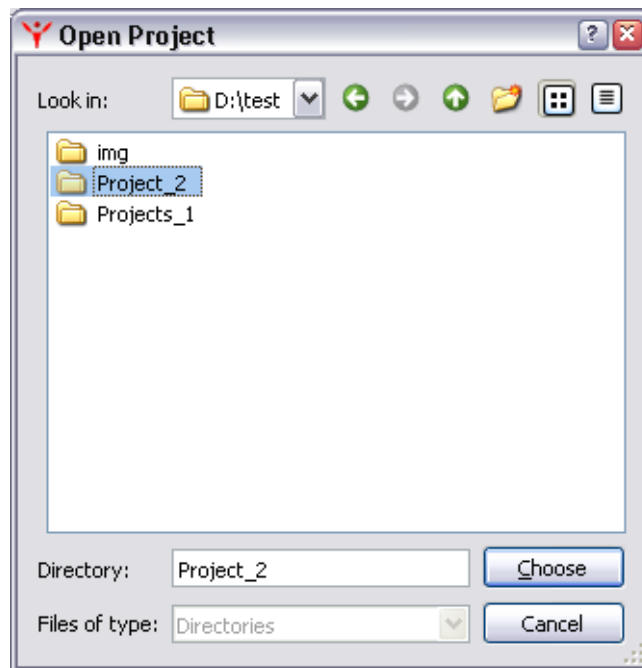
- Reopen Project - Reopens current project without saving any changes.
- **Save All** - Saves all projects at their current stage of progress.
- **Save Project** - Saves selected project at its current stage of progress.
- **Save project as** - displays the "Save Project As" dialog, used for copying all tasks of selected project, as well as their properties, if defined, into a new project. Tasks results are not copied, completed tasks switch their states to Ready, states of other tasks are unaffected. Fields in "Save Project As" dialog are the same as those in "Create New Project":
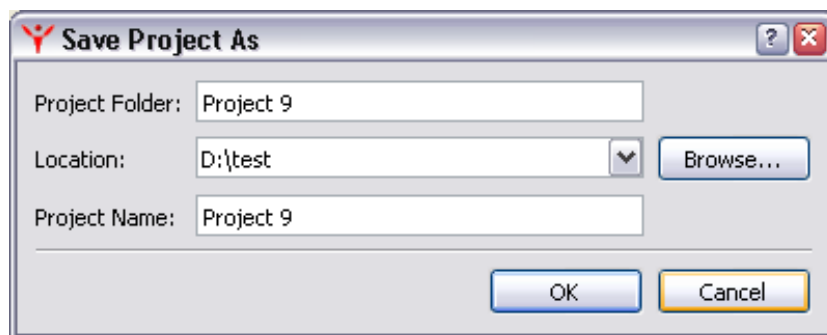
- Close Project - The project is saved at its current stage and closed.
- **Close All Projects** – All opened projects are saved and closed.
- **Load Projects List** – Load projects from previously saved projects list using "Lad Projects List" dialog. If Manager tab currently contains any projects, loaded projects are appended to it. If a project was deleted, it is automatically removed from all lists.
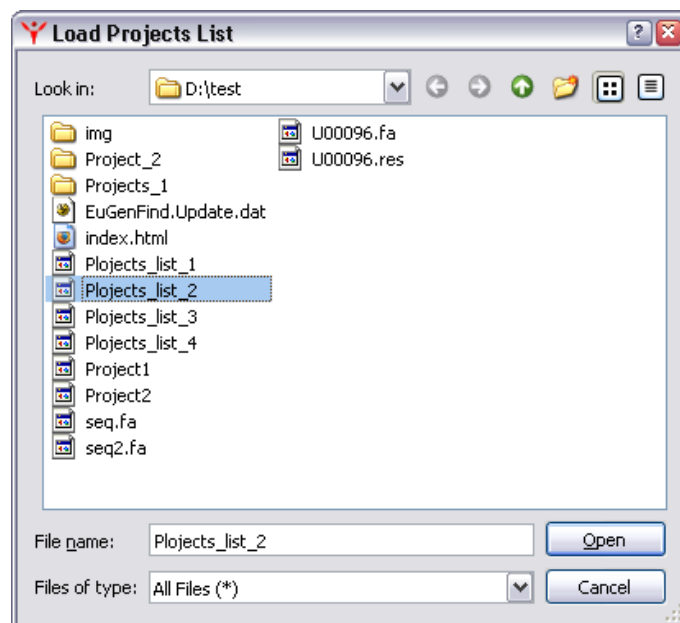
- Save Projects List – Save the list of currently opened projects, i.e. those displayed in Manager Tab.
- **Run Project** - runs a project. Only enabled tasks will run.
- **Stop Project** - stops execution of a project upon completion of currently running task.
- **Abort Project** – immediately aborts a project, without waiting for running task or its pass to complete.
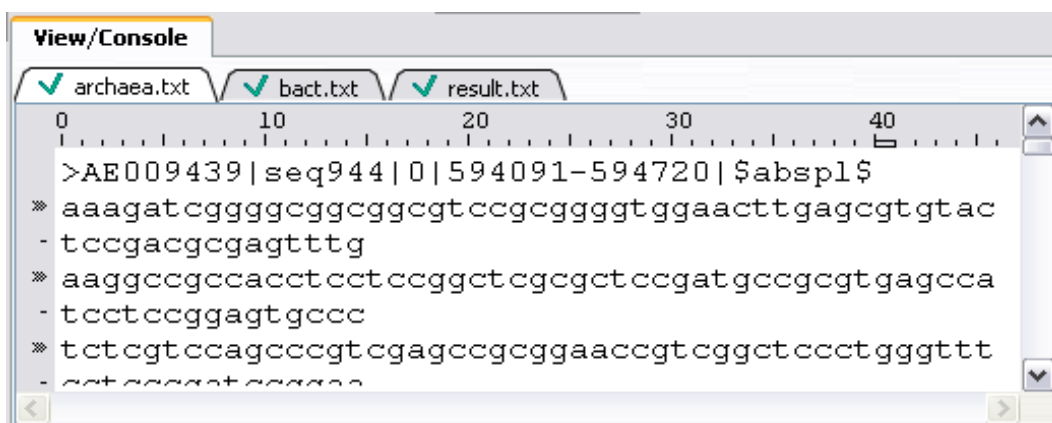- **Enable All Ready Tasks** - enables all Ready tasks in a project.
- **Disable All Enabled Tasks** – Changes status of all Enabled tasks to Ready.
- **Delete All Results** - deletes results of all completed tasks.
- **Clear Project** - Deletes all tasks from a project.
- **Delete Project** - deletes current project.

View/Console tab

View/Console displays output of a pass selected in Results tab (by default – first pass), if such pass resulted in an output. Selecting and copying text in this window is limited to visible lines. Vertical scrolling removes text selection.

Task tab
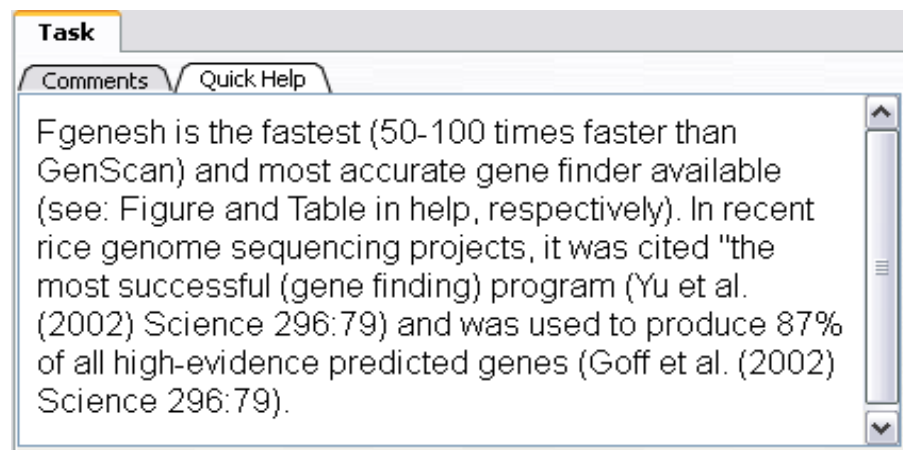
The Task tab contains certain information about selected task and consists of two pages:

- o **Comments** - User comments on a task
- o **Quick help** - Short program help.

To Do tab

To Do tab represents a list of items and serves as a scratchpad or to do list. An item can be added by double-clicking on empty line or from contextual menu. It can be changed by double-clicking on an item or from contextual menu.

C column displays status of item completion,

! column indicates item priority;

Category - item category;

Caption - item name;

Date Add - date and time of item creation;

Date End - date and time of completion.
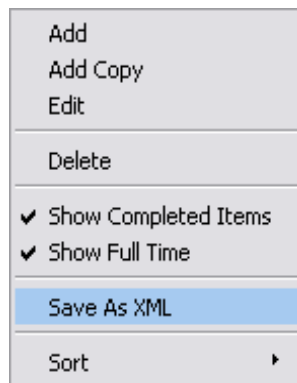
Contextual menu has the following commands:

Add - displays "Add To-Do Item" dialog with fields corresponding to columns mentioned earlier on this page, plus **Task commentary field** which provides commentary on an item.

Add Copy - adds a copy of existing item to a list. Displays "Add To-Do Item" dialog which already has fields pre-filled with properties of copied item.

Edit - edits an item;

Delete - deletes an item;

Show Completed Items - displays/hides completed items;

Show Full Time - if checked, displays time and date, otherwise date only.

Save As XML - saves a list in a file in Unicode XML format.

Sort - sorts items by one of the following criteria:

- **Completed**
- **Priority**
- **Category**
- **Caption**
- **Date Add**
- **Date End**

Items can also be sort by clicking on corresponding column header.

Status Bar
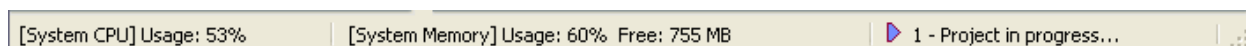
Status Bar displays the following information.

Resource usage:

- **CPU Usage:** - CPU percentage usage.
- **Memory Usage:** - percentage of memory used.
- **Free:** - amount of free available memory.

Project status:

- **Project not specified** - no project is opened.
- ▶ **N - Projects in progress** - the number of projects running.

Profile Manager

Profiles are designed for fast switching between different MolQuest settings. Profiles can include common application parameters (see Options dialog) window sizes, tabs location, headers sizes etc.

"Profile Manager" dialog allows changing profiles or creating new ones. Profile named "Current" contains MolQuest settings currently in use.
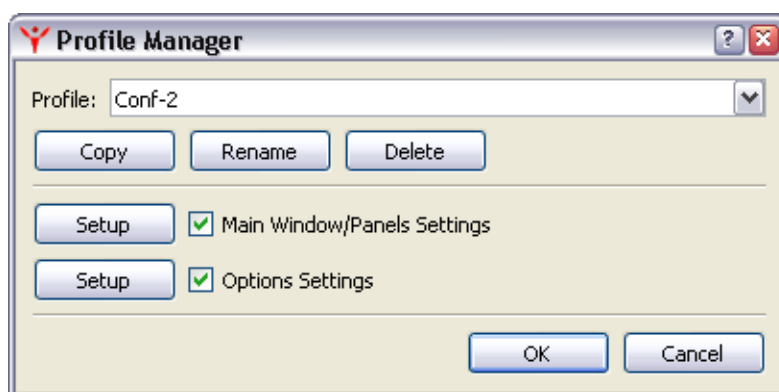
Pressing Copy button creates a copy of selected profile, Rename button renames a profile, and Delete button deletes it.

To create a new profile, select an existing one, create a copy and then edit it. Profile containing current MolQuest window and options setting always exists with name "Curent".
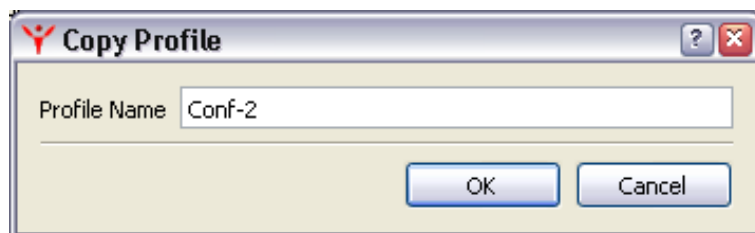
Enter name of new profile and press OK, a new profile will be created.

Main Window/Panels Settings. – determines window sizes, tabs location, headers sizes etc.

If checked, a profile sets window/panel parameters. If unchecked, a profile doesn't set these parameters. If current sizes of windows and panes differ from those of current profile, Setup button is enabled. Pressing it saves current settings in current profile, and Setup button becomes disabled again.

Options Settings – determines common application parameters.

If checked, a profiles common application parameters, if unchecked, a profile doesn't set them. "Setup" button displays Options dialog, where common application parameters can be changed. Checkboxes in Options dialog have three possible states: usual on ☑ and off ☐ and also unchanged ◼, meaning that current setting doesn't change by changing profiles.

Panels dialog

There are four zones (panels) in MolQuest main window, each containing various tabs: Left, Right, Center and Bottom:
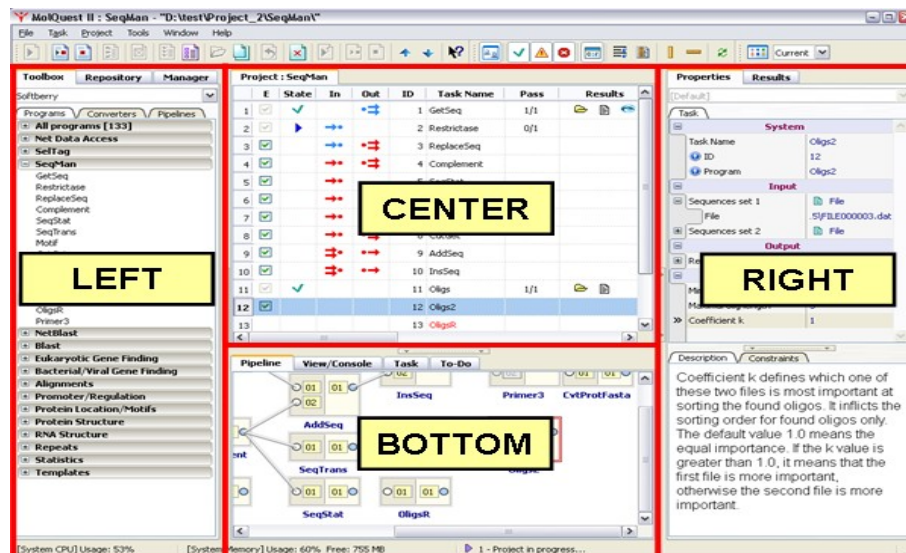
Panel boundaries can be moved by a mouse.

Panels dialog is a convenient tool for rearranging tabs in the main window. Drag a tab name to a zone where you want it to be located. If you want to hide a tab, drag its name to an "OFF" group.
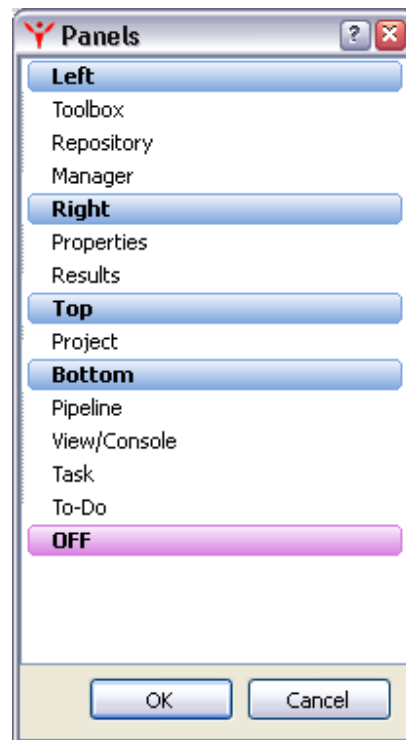
Options dialog

Options dialog is displayed by choosing **Tools>Options** from Main Menu and is used to view or change various MolQuest settings. It has six tabs:

- Prompts
- System tray
- Misc
- Projects
- Memory
- View/Console

Prompts tab

Sets operations for which confirmation prompts will be displayed:
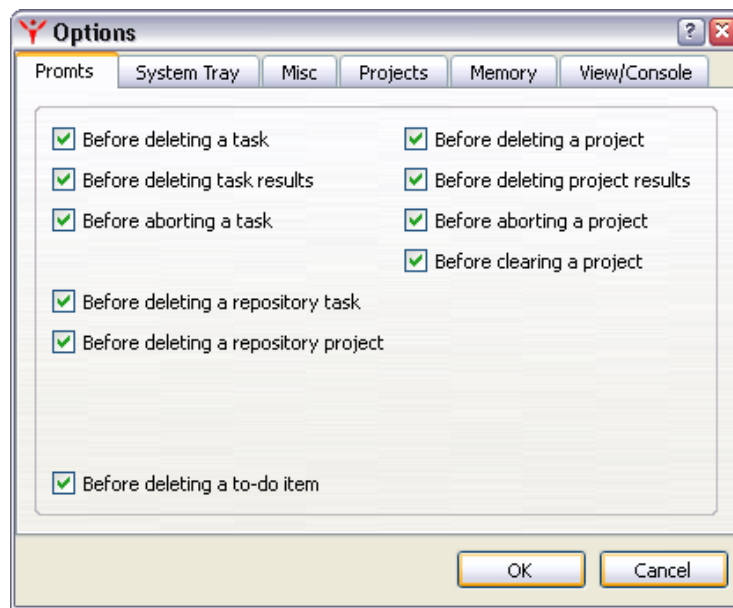
- **Before deleting a task**
- **Before deleting task results**
- **Before aborting a task**
- **Before deleting a repository task**
- **Before deleting a repository project**
- **Before deleting a project**
- **Before deleting project results**
- **Before aborting a project**
- **Before clearing a project**
- **Before deleting to-do item**- displays a confirmation prompt before deleting an item from To-Do list.

System Tray tab
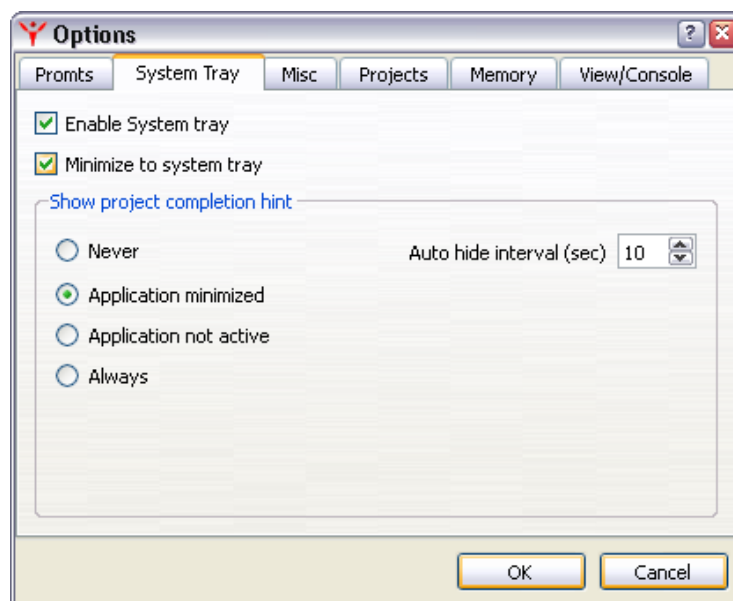
Enable System tray – MolQuest icon is displayed in the system tray.

Minimize to system tray –MolQuest main window is minimized to the system tray. Clicking it restores main window.

Show project complete hint - Once the project is finished, a message "Project complete "Project name"" is displayed in one of the following cases:

- Never
- Application minimized
- Application not active
- Always

Auto hide interval (sec) - Project completion message disappears after specified time.

Misc tab
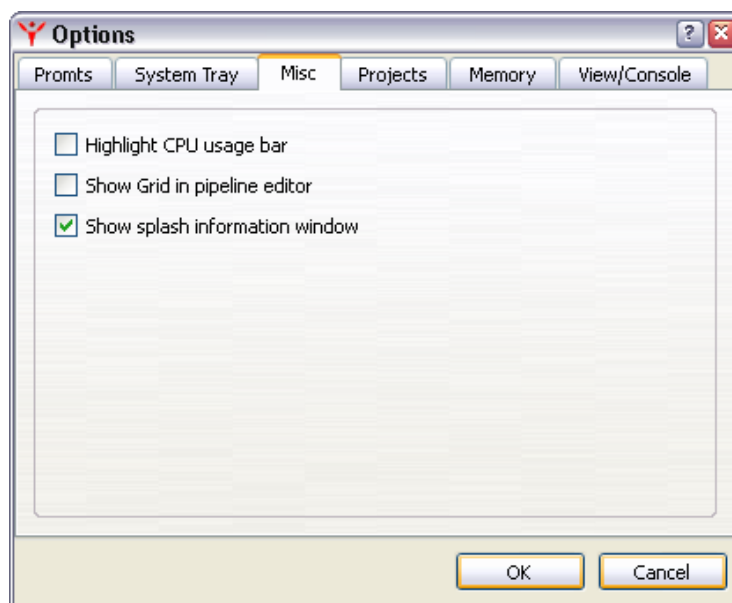
- **Highlight CPU usage bar** - check to display percentage of CPU usage in graphical form and as a number. If unchecked, only a percentage number is displayed.
- **Show Grid in pipeline editor** - check to show gridlines in pipeline editor.
- **Show splash information window** - check to show splash window on a single project open/close.

Projects tab

Contains Project settings.

Open last projects at start-up – check to make MolQuest open at startup all projects that were open at the end of last session.

Update project Input/Output data – Makes MolQuest check that all necessary input/output files are available (exist and are readable). If any of them are unavailable, it is displayed in Results Tab, Output Files Page and/or Input Files Page.
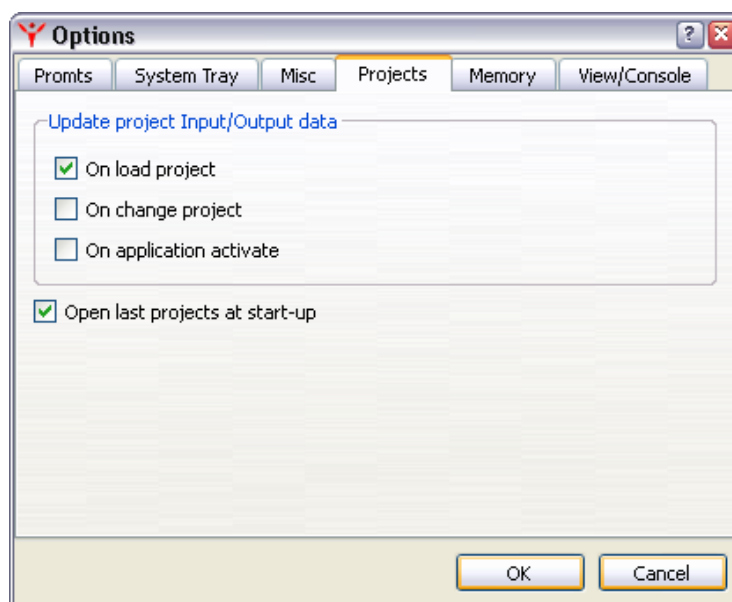
- **On load project** – files are checked when a project is loaded.
- **On change project** – when projects are switched in Manager Tab.
- **On application activate** – every time MolQuest becomes current application.

Memory tab

Settings of monitoring system memory
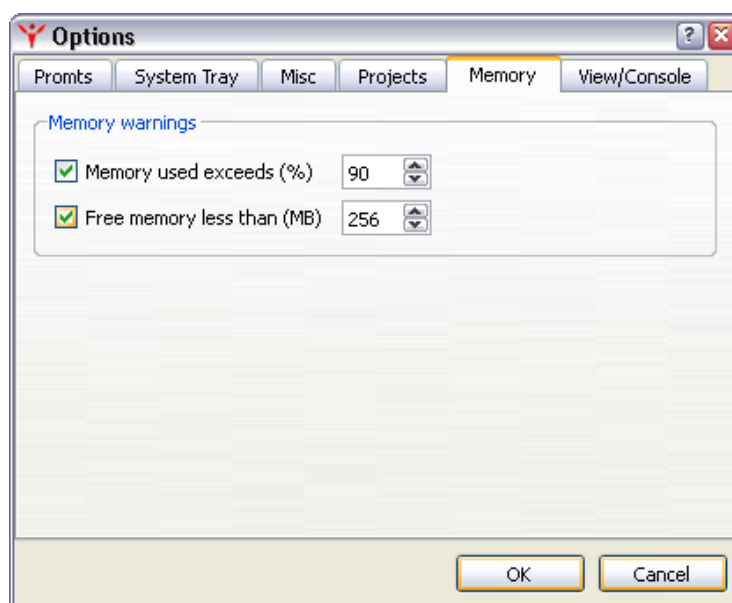
Memory used exceeds – if checked, displays the warning on a status bar (Status Bar), if percent of memory used exceeds preset percentage threshold.

Free memory less than - if checked, displays the warning on a status bar (Status Bar), if free memory falls below preset threshold in MB.

View/Console tab

Contains View/Console tab settings.

- **Activate View/Console** - activate/deactivate View/Console tab.
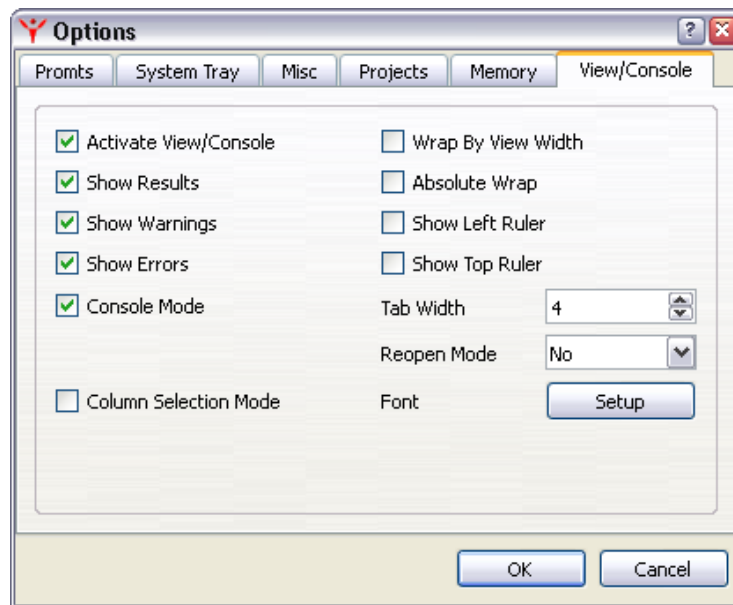- **Show results** - show result files of a chosen task on View/Console tab.
- **Show warnings** - show warning files of a chosen task on View/Console tab.
- **Show errors** – show error of a chosen task on View/Console tab.
- **Console Mode** – If checked, all output data are displayed in real time in a console while a task is running.
- **Column Selection Mode** – switch between column and line selection modes.
- **Wrap by View Width** – wrap lines in View/Console tab window.
- **Show Left Ruler** – Display left-side ruler with line wrap symbols, if exist.
- **Show Top Ruler** – Display top-side ruler on top of window.
- **Absolute Wrap** – Forces wrapping lines larger than 4096 characters. Applicable only to files <1 MB in size, as larger files are always force wrapped.
- **Tab Width** – sets tab width
- **Font** – pressing Setup button opens a font selection dialog. Selected font must be of fixed width, though a dialog shows all fonts.
  Reopen Mode – applicable only if console mode (see above) is off. Sets mode of refreshing displayed output file: No - not refershed; Auto – automatically refreshed; Message – when file is changed, asks user whether to refresh.

Property Editor Options dialog

This dialog controls some visual and dynamic parameters of Property Editor settings, which de don't describe here in details. Pressing Default button resets all options to default.
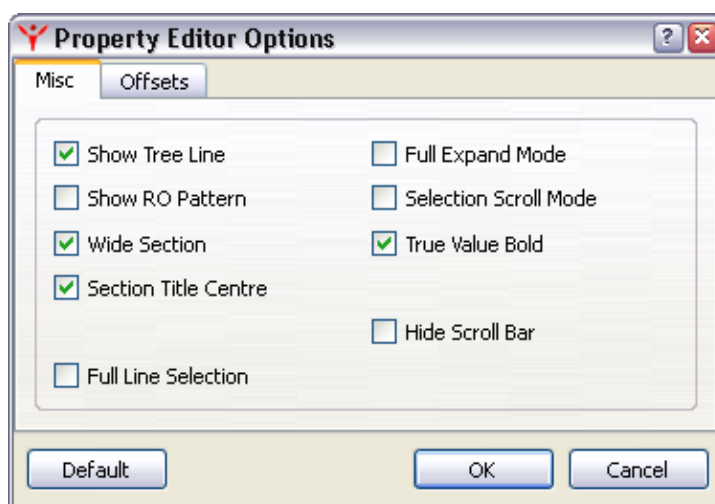
Templates

User can integrate console applications into MolQuest GUI shell on his own. To do this, add "Standard Template" task from Templates group of Programs list of Toolbox tab. In this template, name and path to an executable file, as well as its running options (input and output files, command line options and other necessary information) have to be specified.

In drop down list at the very top of Properties Tab, maximum allowable number of input files (NN Input), output files (NN Outputs) and command line options (NN Options) has to be specified.. For example, "01 Input; 01 Output; 05 Option" means that application can have no more than one input file, one output file and five command line options. Once a program is added, all unused properties can be hidden.

Template properties include the following sections:

- **System** - contains the information on template and task names, and task ID;
- **exe** - selects executable file of console application;
- **Input** – specifies types of input data;
- **Output** - specifies types of output data;
- **Option** – sets up command line options.

System section

- **Task Name** field contains the current task name. It can be changed.
- **ID** - task identifier.
- **Program** - template name.

exe section

- **Exe File** - path to application executable file.
- **Quote Type** - rules for command line quoting (depends on compiler). It is necessary to specify if properties can contain nonstandard or punctuation characters.
- **Run exe destination** - work directory of application executable file. There are two variants: **Auto** - MolQuest chooses work directory; or Exe path – work directory is set to location of exe file.

Debug Log File - name for MolQuest debug file, which contains the executed command line and other information about the application. Data in that file can be useful for troubleshooting and testing program integration.
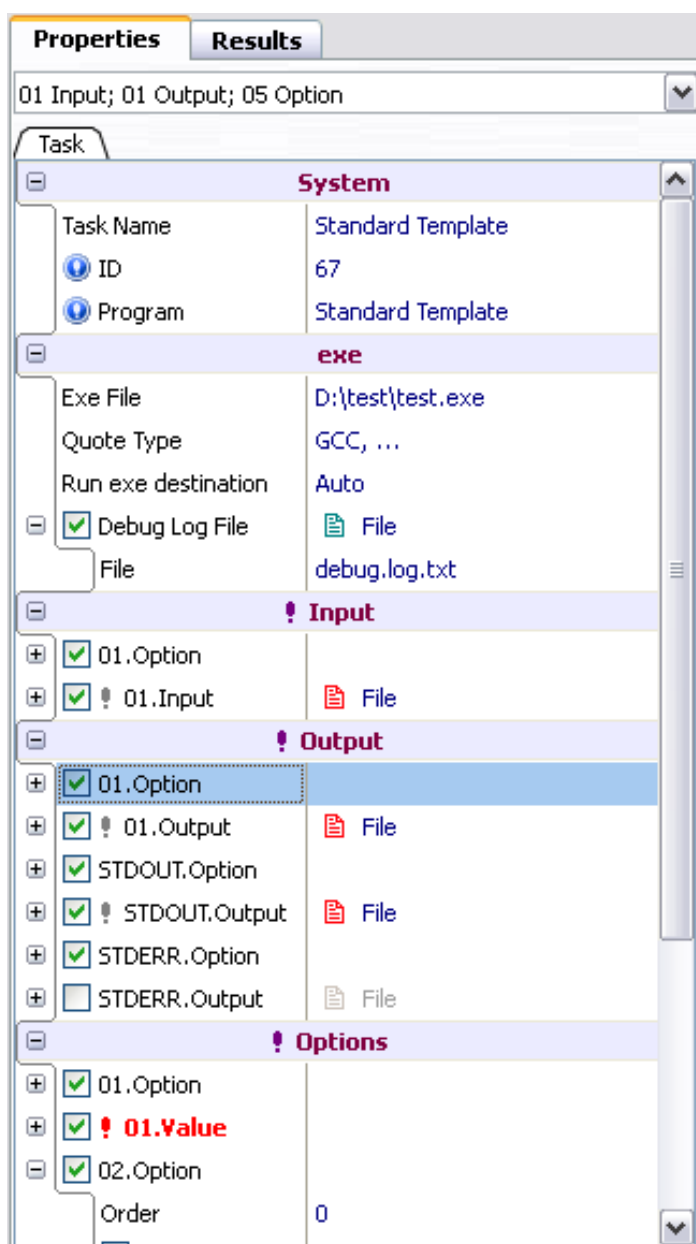

**Common rules for editing the application options:**

As for MolQuest's own tasks, "Input files" can be single or multiple files and can be specified by user or taken from a pipeline, and output files can be sent to another task via pipeline.

To activate a property, the appropriate box should be checked (☑).

To prevent property from being displayed (e.g. a property that doesn't change its value in all conceivable task variants), right-click on it and choose "SubNodes - Permanently Hide" command from contextual menu.
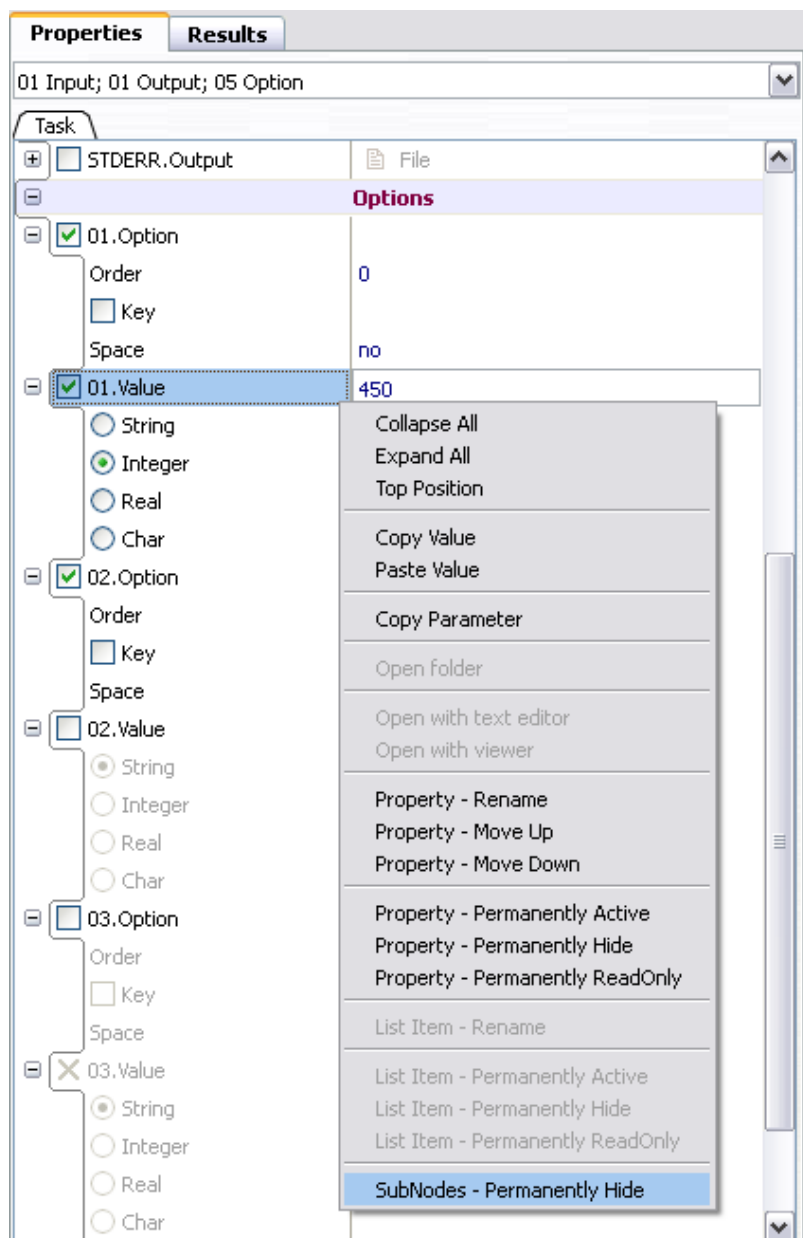
The item becomes invisible, but its value is sent to a command line if that property is active.
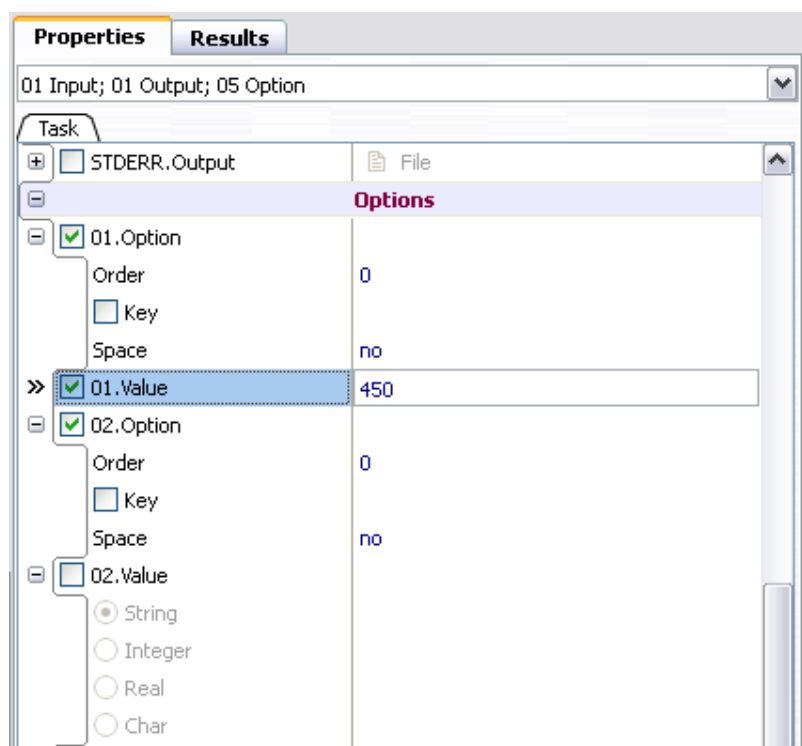
Property name can be changed using "Property Rename" command from contextual menu.
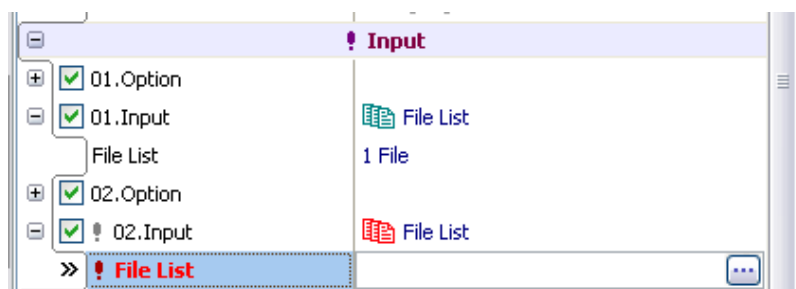
Input section

To define program input, two subsections: XX.Option and XX.Input shall be filled.

> **01.Option** - describes the way to specify input file name in command line:
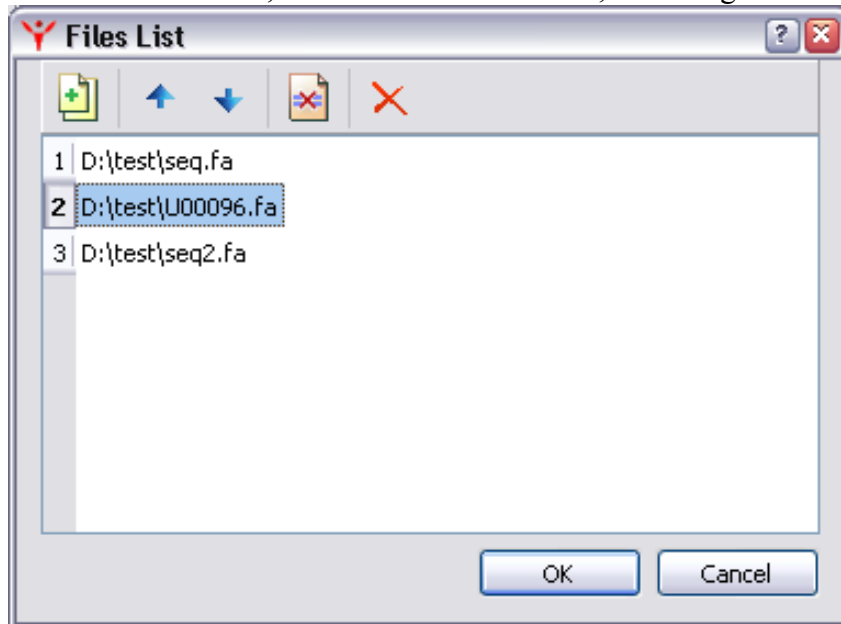>
> - **Order** - position number of this option in command line. By default, 0.
> - **Key** - prefix for current option.
> - **Space** - "no" means no space between prefix and value, otherwise - "yes".
>
> **01.Input**. Choose appropriate type of input data from drop-down list:
>
> - **File** - data will be taken from a file with user-specified path. Icon 📄 means that file exists, 📄 - path to file is wrong or file does not exist.
> - **Files list** – a list consisting of one or more files created in **File List** dialog (evoked by pressing ⋯ button) is used as an input. In such case MolQuest runs several passes, one file from a list at a time, in the same order they appear in a dialog window, until all files are processed. Results of each pass are shown in a list in <u>Results Tab</u>. Icon 📚 indicates that file list is empty, while 📚 means that it is not.

- Button adds files to a list. In a dialog, user can select one or more files and press "Open" button, buttons and move files up and down in a list, button removes selected file from a list, and button clears list, removing all files.

- **Pipe** - data will be taken directly from another task in a project. Icon means that a link to input data source is correct, that a link is not defined or wrong, means that output data destination is correct, and that a link is not defined or wrong.

Output section

To define an output file, two subsections: XX.Option and XX.Output should be filled.

01.Option - describes the way to specify the output file name in a command line:

- **Order** - position number of this option in command line. By default, 0.
- **Key** - prefix for current option.
- **Space** - "no" means no space between prefix and value, otherwise - "yes".
- **Type**- from a drop down menu, select how an output is treated: as data, as warning messages, or as error messages.

01.Output. Choose output type from drop down menu:

- **File** - output file with specified name will be generated in the task-specific folder.

- **Pipe** - output file will be sent to an appropriate pipeline. Icon means that output data destination is correct, that link is not defined or wrong.

STDOUT.Options
- **Type**- select in the drop down menu how the application standard output is treated: as data, as warning messages or as error messages.

STDOUT.Output. Choose type of output data from drop down list:
- **File** - output file with specified name will be generated in the task-specific folder.

- **Pipe** - output file will be sent to an appropriate pipeline. Icon ➡ means that output data destination is correct, ➡ that link is not defined or wrong.

If **STDOUT** subsections are not set, but a program outputs data to standard output, it would generate a warning.

STDERR.Options

    Type- select in the drop down menu how the application standard output is treated: as data, as warning messages or as error messages.

STDERR.Output. Choose type of output data from drop down list:
- **File** - output file with specified name will be generated in the task-specific folder.

- **Pipe** - output file will be sent to an appropriate pipeline. Icon ➡ means that output data destination is correct, ➡ that link is not defined or wrong.

If **STDERR** subsections are not set, but a program outputs data there, it would generate a warning.

Options section

To define an option, two subsections: XX.Option and XX.Value should be filled.

01.Option - describes the way to specify an option in command line:
- **Order** - position number of this option in command line. Default value is 0.
- **Key** - prefix for current option.
- **Space** - "no" means no space between prefix and value, otherwise - "yes".

    01.Value. choose an appropriate type of option data:
- **String**
- **Integer**
- **Real**
- **Char**

Once selection is done, all unused subnodes can be hidden. To do so, use "SubNodes Permanently Hide" command from contextual menu.

Once all properties have been specified, the task can be added to repository (Repository Tab) for further use in various projects.

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