



MolQuest

Version 2.4

Graphical User Interface Manual

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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 Sheet](#) 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](#). Tasks can be joined in pipelines with pipes connecting their slots.

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](#)).

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 auxiliary 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 Sheet](#) in the [Toolbox tab](#) shows all available converters.

Output from one task is often used as an input for another task. In the previous version of MolQuest, we used pipes to transfer data from one task to another: every task output could be connected with one or several pipes, and every input could be connected with a single pipe. So tasks could be joined in pipelines. Now for more flexible data processing we introduce next generation of task connection system, which allows use several pipes in an input slot. New pipeline are not just a sequential order of tasks, but allows loops, conditions and processing complex sets of data in desirable order.

Now we have new entity between pipes and task input/output, which is called slot. Slot controls dataflow of pipes. An input slot gets data for a task input from pipes and files, an output slot sends corresponded task output to pipes and files. Data arrangement in an input slot depends on slot settings, received internal signals and pipes contents.

Data item

Data item is a portion of data which can be used by a task input or generated by a task output. If our task were a standalone console application, data item usually would have corresponded to a file, either input or output.

Slot

Slot is a data item manager. Slot can buffer data items, send and receive signals, perform some action on particular events. For a given task, an input slot gets data items for a task input from pipes and files and arrange them in desirable way, an output slot sends corresponded task output data items to pipes and files. Slots are automatically created for all task inputs and outputs.

Pipe

Pipe is a channel between an input and an output slot. A pipe transfers data items and flags from its output slot to its input slot.

Pipeline

Pipeline is a set of tasks, connected by pipes. The [Pipeline tab](#) displays all links between tasks in a pipeline. Predefined pipelines from packages are shown in Pipelines Sheet of [Toolbox Tab](#).

Flag

Flag is a special object which can be send by a pipe from its output slot and requires some actions from its input slot when received. Now there are two types of flags: Complete Queue and Complete Pipe.

Signal Signal (Internal signal) is a message which can be sent by a slot or a task to all slots of the task.

Static data of a slot are data items from explicitly set sources, for example, from a file or a list of files.

Dynamic data of a slot are data items from pipes connected to the slot.

Queue

Queue is a sequence of data items and flags delimited by Complete Queue flags. Queue can contain both static and dynamic data, static data always precede. If a queue contains only static data, a Complete Queue flag is not necessary.

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.

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 tab](#). 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 Tab](#) 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:



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" () status ([Task Status](#)).

Completed tasks have status "Completed" () status ([Task Status](#)).



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

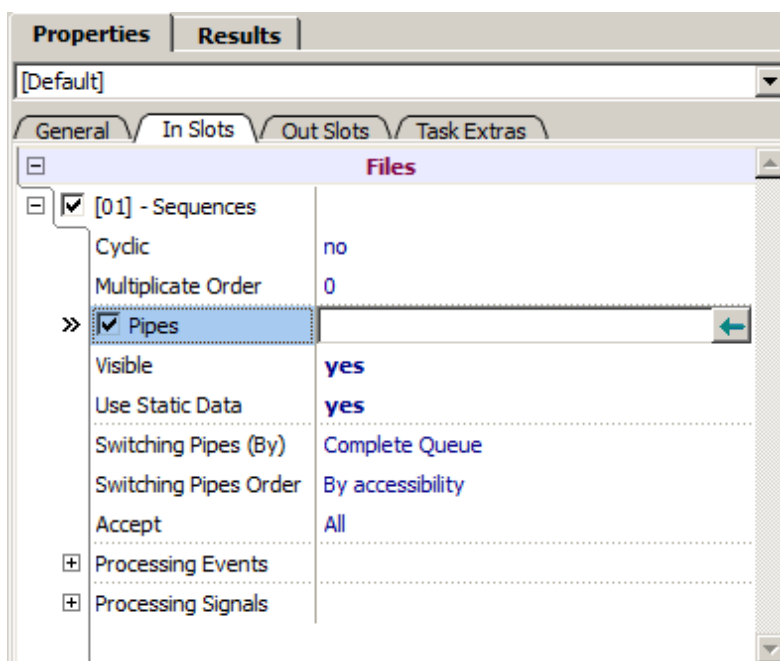
An output of a task can be viewed in [Project tab](#) (column "Results"), [Results Tab](#) or [View/Console Tab](#).

Create pipelines

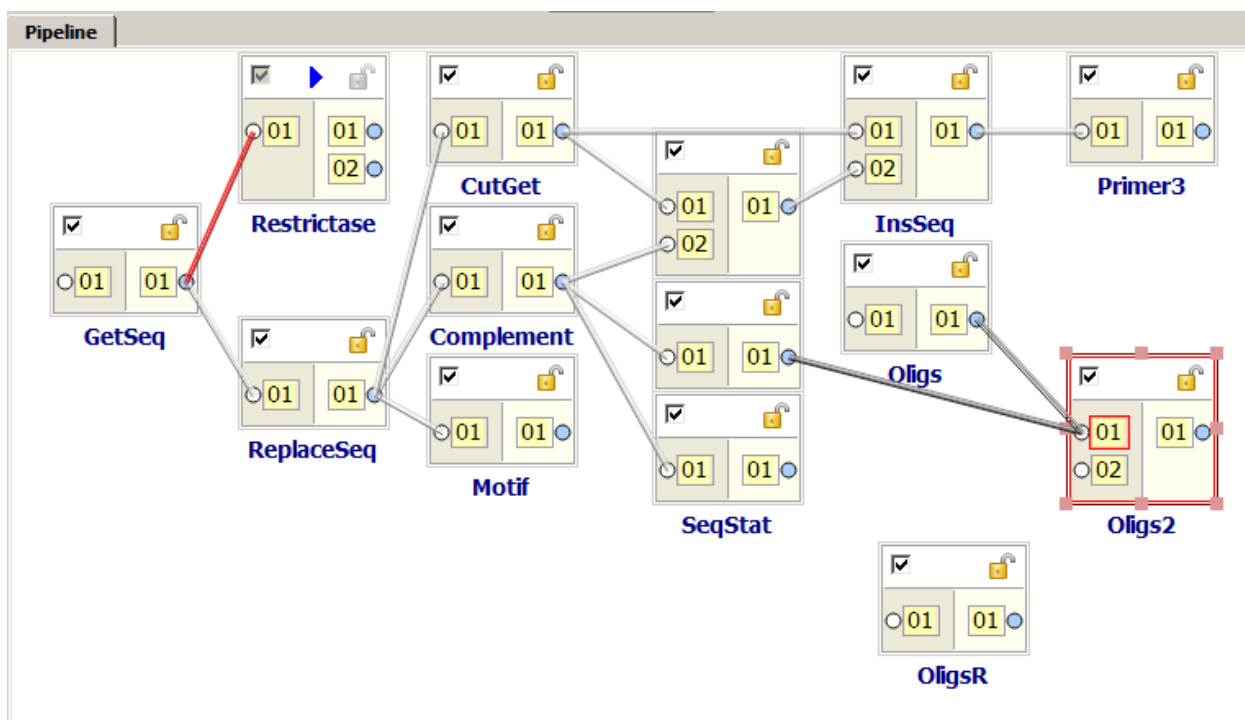
A project may consist of a complex sequence of tasks, where an output of one task is used as an input for another. Such kind of project is called a pipeline.


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 > In Slots page](#), use "Pipe" parameter 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.



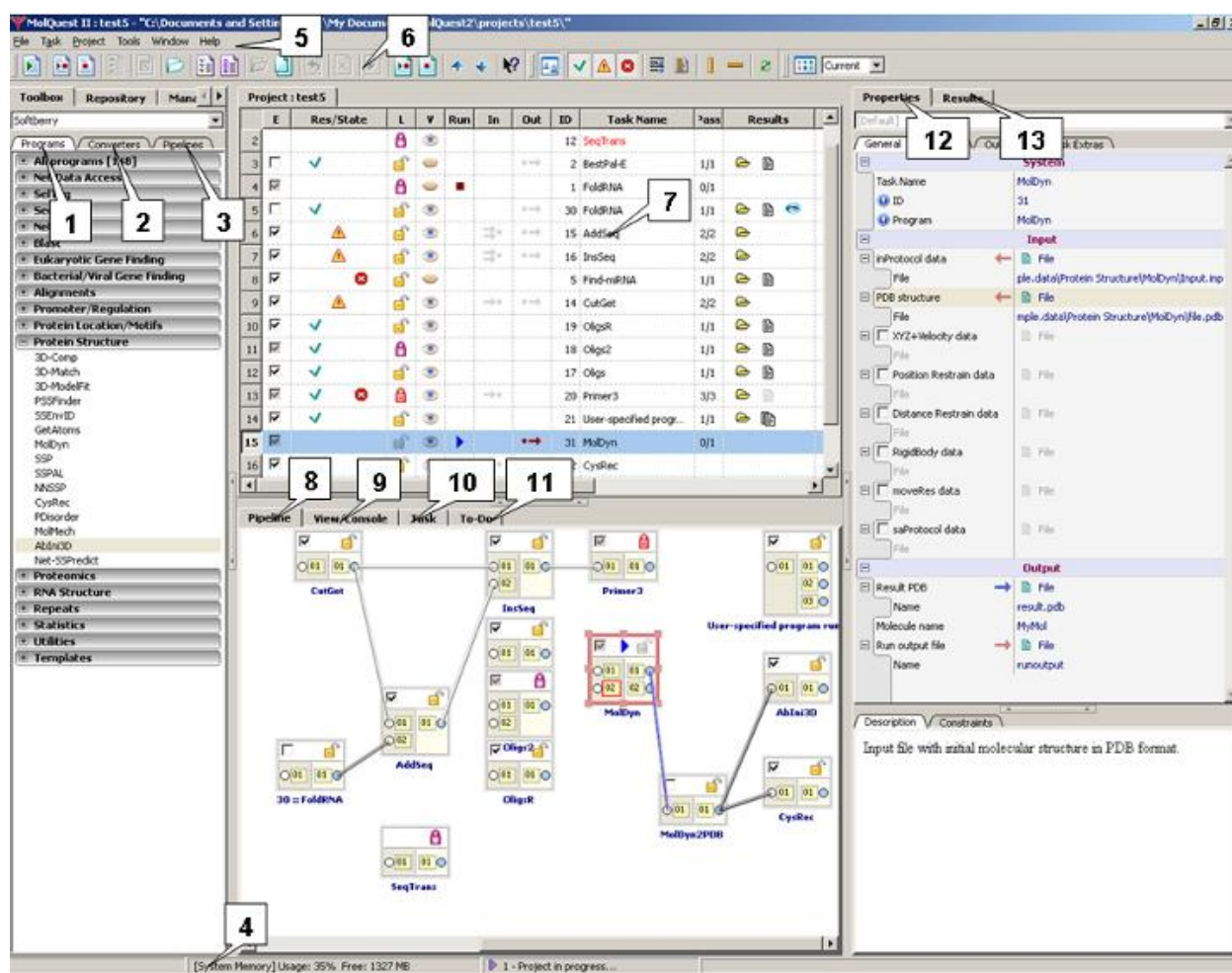
Here, to create a pipeline, connect output and input of corresponding tasks with a mouse: click on an output of a task, and a cursor takes this form: , now move a cursor to an input area of a "downstream" task. Yellow line will follow a cursor there.

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: .

Application window

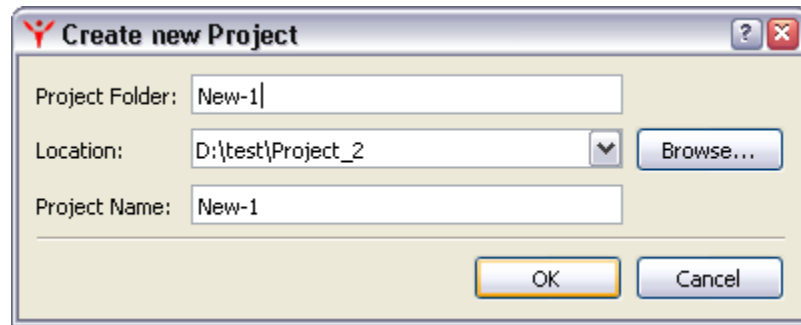


1. [Toolbox Tab](#). 2. [Repository tab](#). 3. [Manager Tab](#). 4. [Status bar](#). 5. [Main menu](#). 6. [Toolbars](#)
7. [Project tab](#). 8. [Pipeline tab](#). 9. [View/Console Tab](#). 10. [Task Tab](#). 11. [To-Do Tab](#).
12. [Properties tab](#). 13. [Results Tab](#).

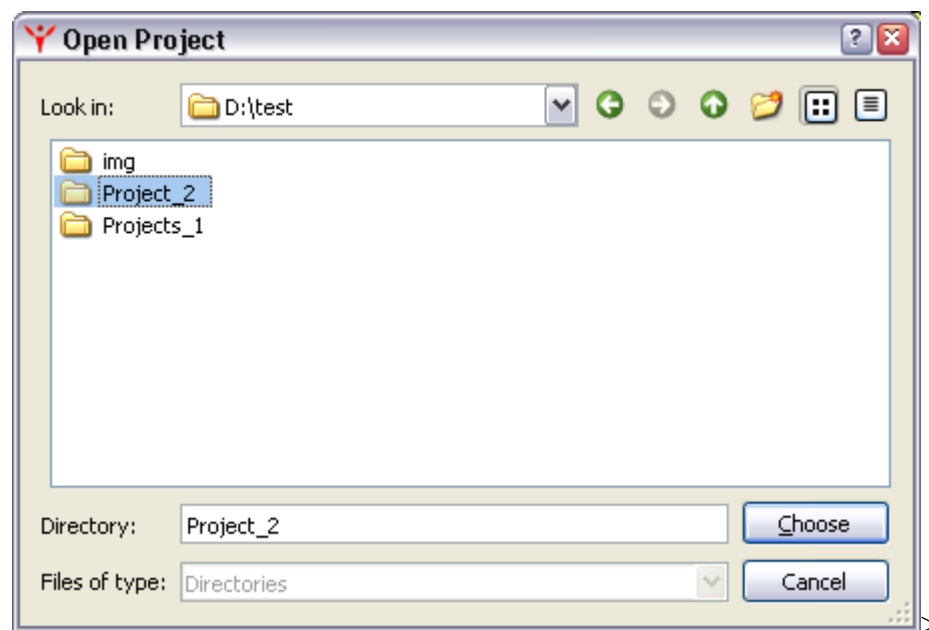
Main Menu

Menu 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.

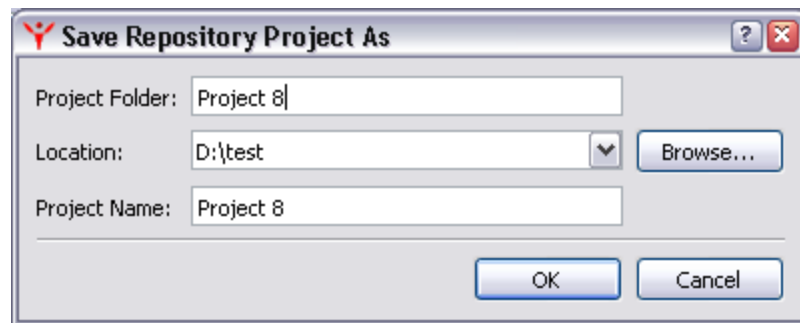


- **Open Project** - Open an existing project. Displays "Open project" dialog. Choose a project folder and press the "Choose" button. The project is now assigned a "current project" status. [Project tab](#) and [Pipeline tab](#) display tasks of current project.

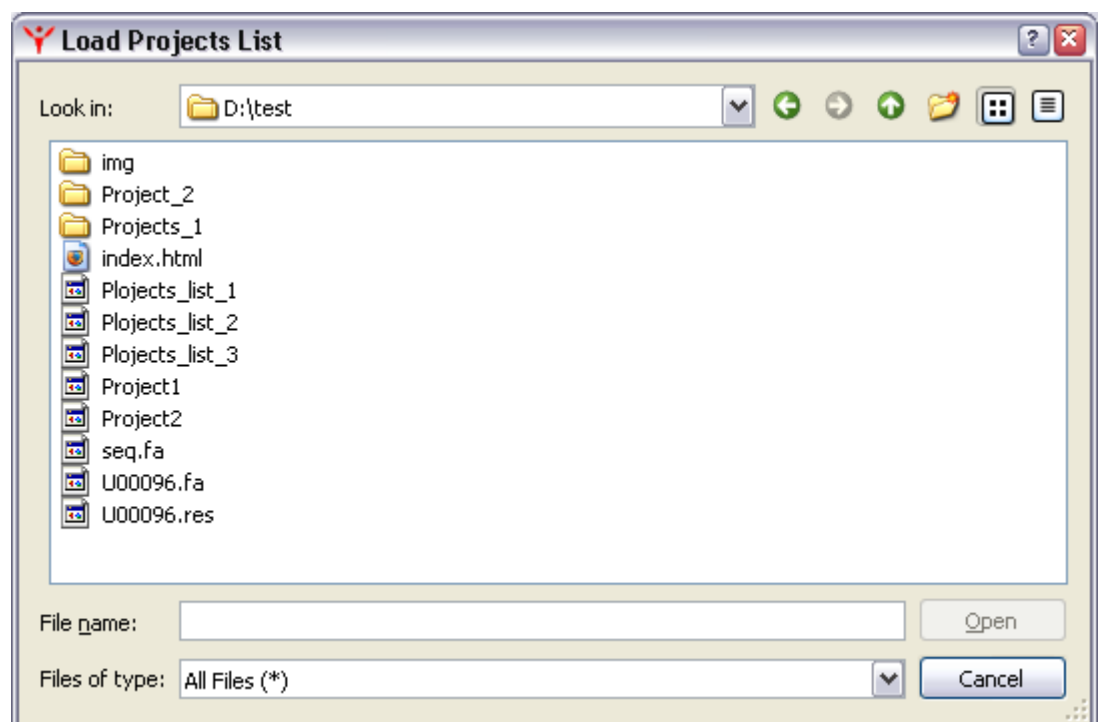


- **Reopen Project** - Reopens current project without saving any changes made during the session.
- **Save All** - Save all projects at their current state.
- **Save Project** - Save current in its current state.
- **Save project as** - This command is used to create a copy of the current project. All 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.

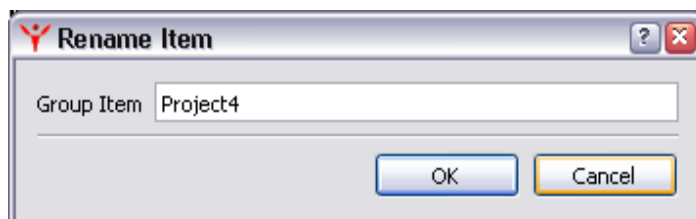
- **Exit without projects saving** - Close All Projects without saving and exit the application.
- **Exit** - Save all projects in their current state and exit the application.

Menu 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 completed. 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**".
- **Lock Task** - set the task lockup status to "locked".
- **Unlock Task** - set the task lockup status to "not locked".
- **Lock Freeze Task** - set the task lockup status to "frozen".
- **Unlock Frozen Task** - remove the frozen status from task.
- **Hide Task** - remove task image from the "Pipeline" tab.
- **View Task** - display task image in the "Pipeline" tab.
- **Move Up** - move a selected task one position up in the 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** - a task and its results.

Menu Project

- **Rename Project** - rename selected project. Displays "Rename Project" dialog.



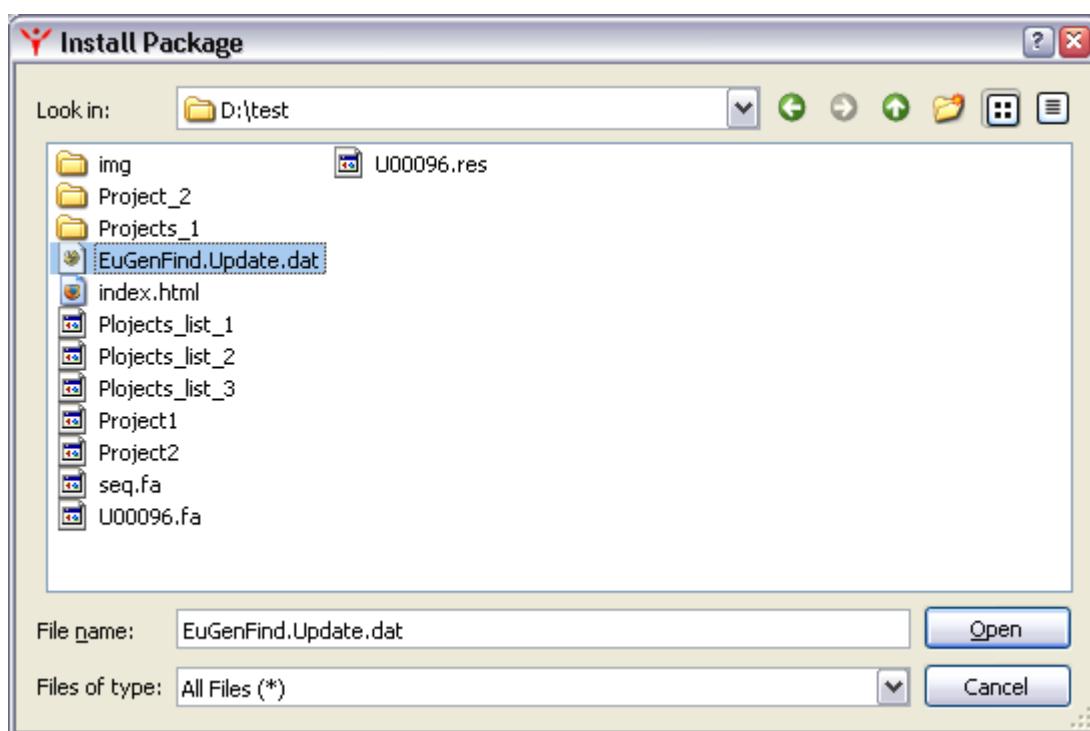
- **Run Project** - run a project. Only enabled tasks will run.
- **Stop Project** - stop execution of a project immediately after a task pass in progress is completed.
- **Abort Project** - immediately abort execution of a project, not waiting until currently running pass is finished.
- **Enable All 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".
- **Lock All Tasks** - lock all tasks of the project (does not affect the frozen tasks).
- **Unlock All Tasks** - unlock all tasks of the project (does not affect the frozen tasks).
- **Invert Locked** - invert the tasks lockage.
- **Special Lock :**
 - **Lock All Completed** - lock all completed tasks.
 - **Lock All Not Completed** - lock all non-completed tasks.
 - **Lock All Hidden** - lock all hidden tasks.
 - **Lock All Visible** - lock all visible tasks .
 - **Lock All Enabled** - lock all enabled tasks.
 - **Lock All Disabled** - lock all tasks without “enabled” status.
- **Special Unlock:**
 - **Unlock All Completed** - unlock all completed tasks.
 - **Unlock All Not Completed** - unlock all non-completed tasks .
 - **Unlock All Hidden** - unlock all hidden tasks .
 - **Unlock All Visible** - unlock all visible tasks.
 - **Unlock All Enabled** - unlock all enabled tasks.
 - **Unlock All Disabled** - unlock all tasks without “enabled” status.
- **Hide All Tasks** - remove flowcharts of all tasks of the projects from the “Pipeline” tab.
- **View All Task** - display all tasks of the project in the “Pipeline” tab.
- **Invert Visible** - invert visibility of the project tasks.
- **Special Hide:**
 - **Hide All Completed** - hide all completed tasks.
 - **Hide All Not Completed** - hide all non-completed tasks.
 - **Hide All Locked** - hide all locked tasks .
 - **Hide All Unlocked** - hide all non-locked tasks.
 - **Hide All Enabled** - hide all enabled tasks.
 - **Hide All Disabled** - hide all tasks without “enabled” status.
- **Special View:**
 - **View All Completed** - display flowcharts of all completed tasks of the project in the “Pipeline” tab.
 - **View All Not Completed** - display flowcharts of all non-completed tasks of the project in the “Pipeline” tab.
 - **View All Locked-** - display flowcharts of all locked tasks of the project in the “Pipeline” tab.
 - **View All Unlocked** - display flowcharts of all non-locked tasks of the project in the “Pipeline” tab.
 - **View All Enabled** - display flowcharts of all tasks with “Enabled” status.
 - **View All Disabled** - display flowcharts of all tasks without “Enabled” status.
- **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.

Menu 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.



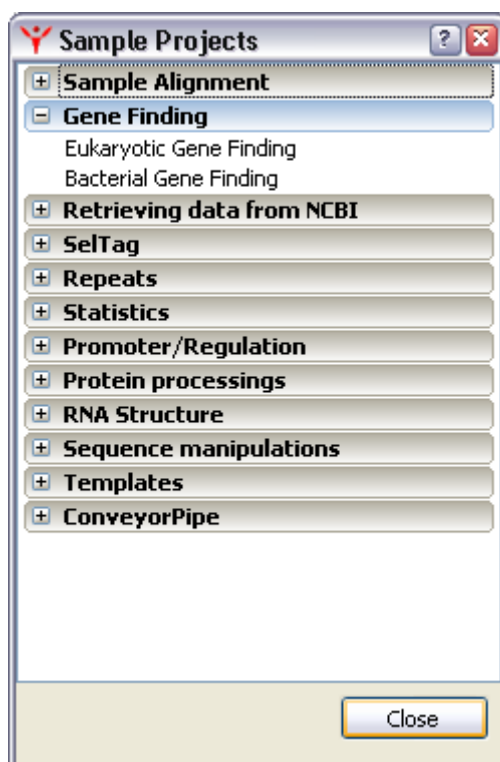
- **Install License** - install a new license.
- **Viewers** - run selected viewer.

Menu Window

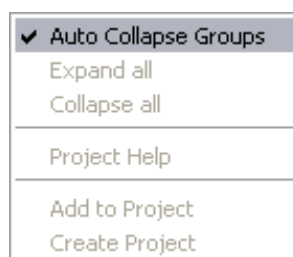
- **Style** - sets interface window.
- **Toolbars** - chooses toolbars to display (see [Toolbars](#)).
- **Screen Shot** - choosing this menu option makes a shot of MolQuest screen, and a dialog for saving a screenshot is displayed. A shot is saved in png format.

Menu 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.

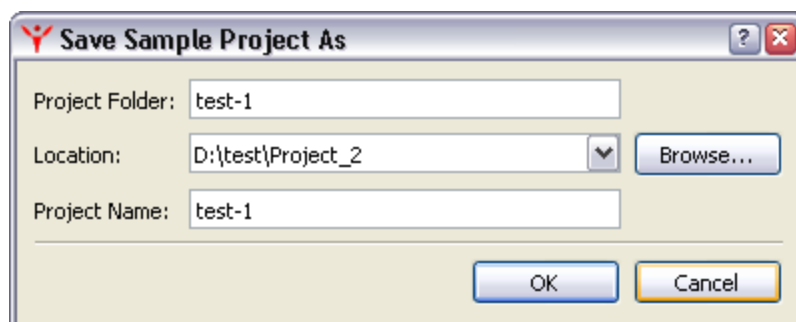


Mouse right click calls out the contextual dialog menu:



- **Auto Collapse All** - 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.

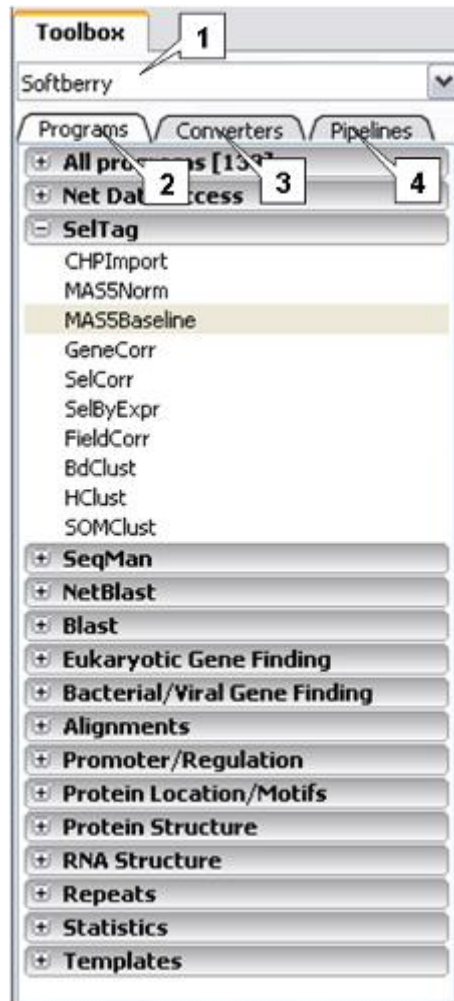
- **Program (Converter, Project) Help** - open help for selected program (converter, pipeline).
- **Add to Project** - добавляет все задачи из sample проекта в текущий проект (если он есть).
- **Create Project** - create a project based on sample project. Displays "Save Sample Project As" dialog. See [Save Project As](#).



Mouse double-click adds all tasks of the sample project to the current one (if it exists).

- **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.

Toolbox tab



1. List of distribution companies. 2. List of programs. 3. List of converters. 4. List of pipelines.

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.

Contextual menu of the **Toolbox Tab** contains the following commands:

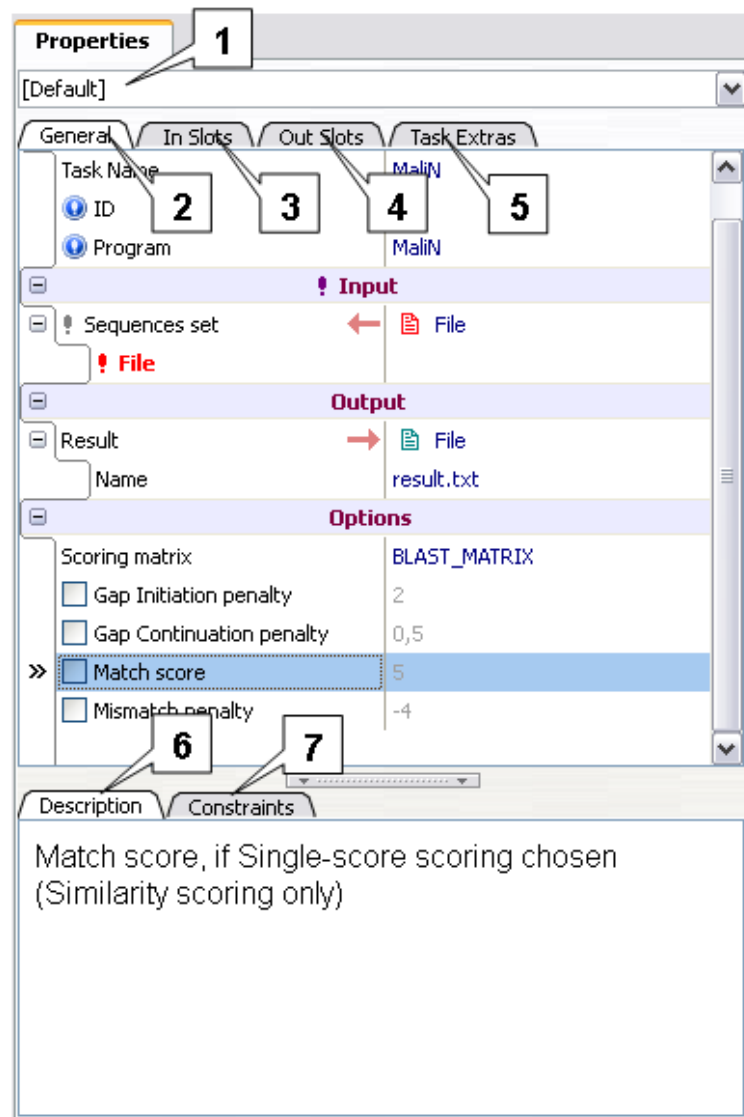


- **Auto Collapse All** - if checked, selecting one program group collapses all other program groups.
- **Collapse All** - collapse all program groups.
- **Expand All** - expand all program groups. If "Auto Collapse" mode is checked, this option is inactive.
- **Program (Converter, Project) Help** -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

Properties tab

The **Properties** tab is purposed for setting up task parameters. The Properties tab contains:

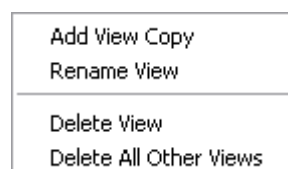
- [View List](#)
- [Property Editor - General page](#)
- [Description page](#)
- [Constrains page](#)
- [Task Extras page](#)
- [Slots setup pages](#)



1. View List. 2. "General" page. 3. "In Slots" page. 4. "Out Slots" page. 4. "Task Extras" page. 6. "Description" page. 7. "Constrains" page.

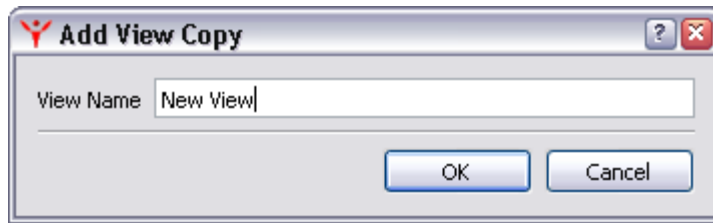
View List.

View List contains a list of predefined task's Views (see [View](#)). The contextual menu of View List is as follows:

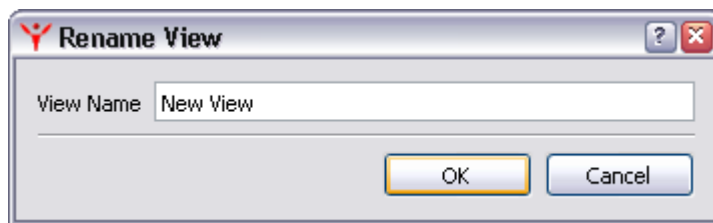


The contextual list menu contains the following commands:

- **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 View.
- **Delete All Other Views** - Deletes all Views except selected one.

Property Editor - General page.

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 (on General page):

- **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.
- **Preprocessing** - includes settings for preliminary processing of input data.

Property Icons and Property Activity

Below is a window of Property Editor General page.

Properties	
[Default]	
General In Slots Out Slots Task Extras	
System	
Task Name	SeqMatch-N
ID	3
Program	SeqMatch-N
Input	
Target sequence	File
File	a\Alignments\SeqMatch-N\seq1.fa
Format	Fasta
Query sequence(s)	File List
File List	
Format	Fasta
Output	
Result	File
Name	result.txt
Format	Output alignment
Graphic data	File
Name	result.bin
Preprocessing	
Target	
Remove	
Cut Sequence	
Query	
Options	
Precision	Rough alignment (fast)
Score method	No scoring the alignment
Threshold	0
Target chain(s)	In direct chain only
Fine adjustment	no
Multiply variants :: Alternate va	10
Alternate variants :: Number	10
Number	10
All	yes
Non-overlapped variants ::	10
Number	10
All	yes

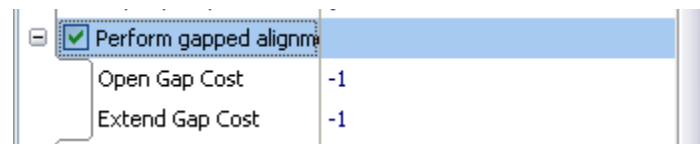
Left column contains name of each property, right column - its value. Some of properties can have the following information icons next to their names:

	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.
	<p>This property is "Read only", and its value can't be changed. Unlike system property, value of read only property affects task results.</p> <ul style="list-style-type: none"> 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:

[-] <input checked="" type="checkbox"/> Multiply variants :: Alternate variants :: Number	10
[-] <input checked="" type="radio"/> Alternate variants :: Number	10
<input checked="" type="radio"/> Number	10
<input type="radio"/> All	yes
[-] <input type="radio"/> Non-overlapped variants :: Number	10
<input type="radio"/> Number	10
<input type="radio"/> All	yes
[-] <input type="radio"/> Different variants :: Number	10
<input type="radio"/> Number	10
<input type="radio"/> All	yes

If "Multiply variants....." property is set to read only, all nested properties except selected become disabled, and selected properties become read only.

[-] <input checked="" type="checkbox"/> Multiply variants :: Alternate variants :: Number	10
[-] <input checked="" type="radio"/> Alternate variants :: Number	10
<input checked="" type="radio"/> Number	10
<input type="radio"/> All	yes
[-] <input type="radio"/> Non-overlapped variants :: Number	10
<input type="radio"/> Number	10
<input type="radio"/> All	yes
[-] <input type="radio"/> Different variants :: Number	10
<input type="radio"/> Number	10
<input type="radio"/> All	yes

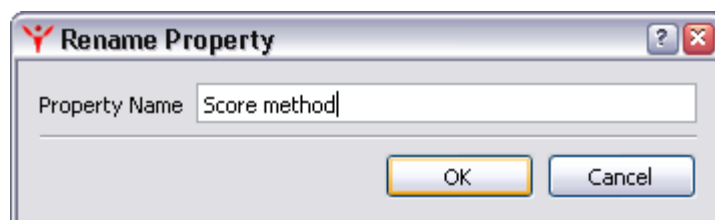
Contextual menu of Property Editor

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.

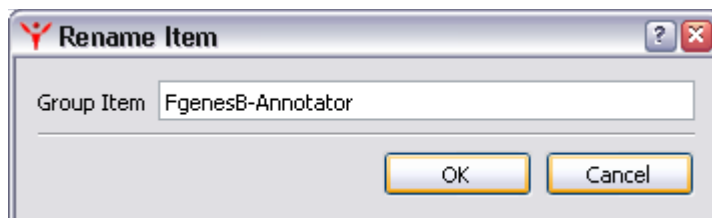
Collapse All
Expand All
Top Position
Copy Value
Paste Value
Copy Parameter
Open folder
Open with text editor
Open with viewer
Property - Rename
Property - Move Up
Property - Move Down
Property - Permanently Active
Property - Permanently Hide
Property - Permanently ReadOnly
List Item - Rename
List Item - Permanently Active
List Item - Permanently Hide
List Item - Permanently ReadOnly
SubNodes - Permanently Hide

- **Open with viewer** - 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.

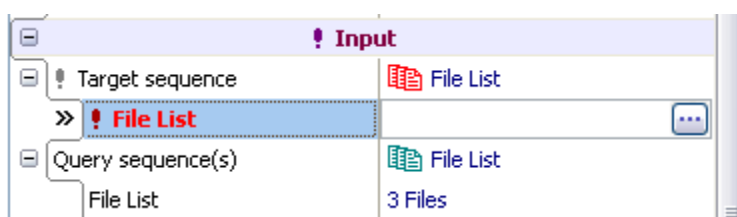
Values of properties


Depending on property type, values can be:

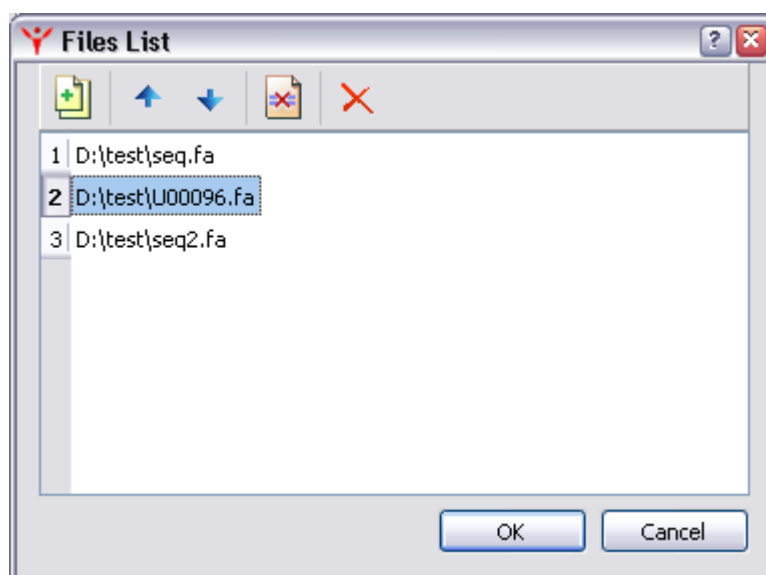
- selected from a list
- typed in manually
- files selected using standard Select File dialog, which appears when the corresponding button in property value column is pressed. Full path is required for input files, for output files - filename only. Path to a file can be typed in or selected in Select 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.

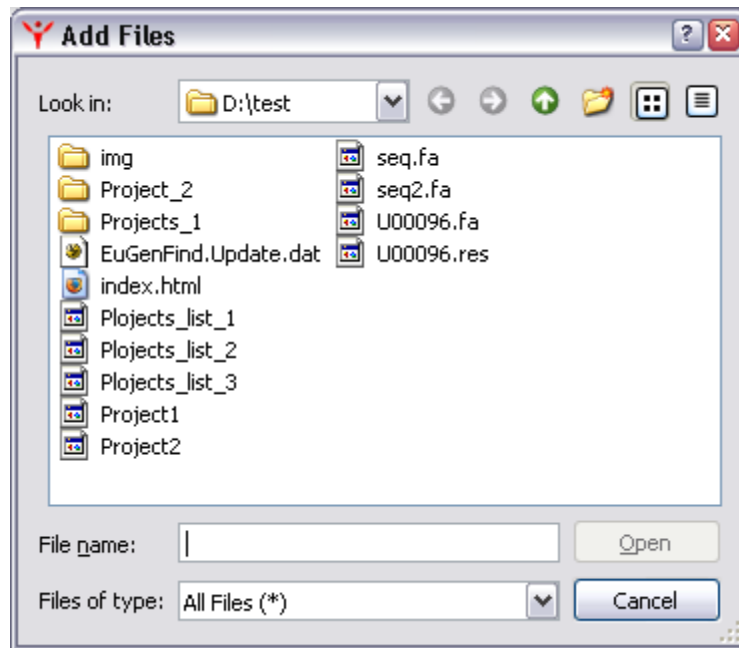
For properties that define input data source, there are three possible value variants: **File**, **Files list** and **Pipe**:

- **File** - data are located in  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 that file list is empty, while  means that it is not.









In **File List** dialog (see picture below), pressing  button opens standard **Add File** window, which is used to add files to a list.




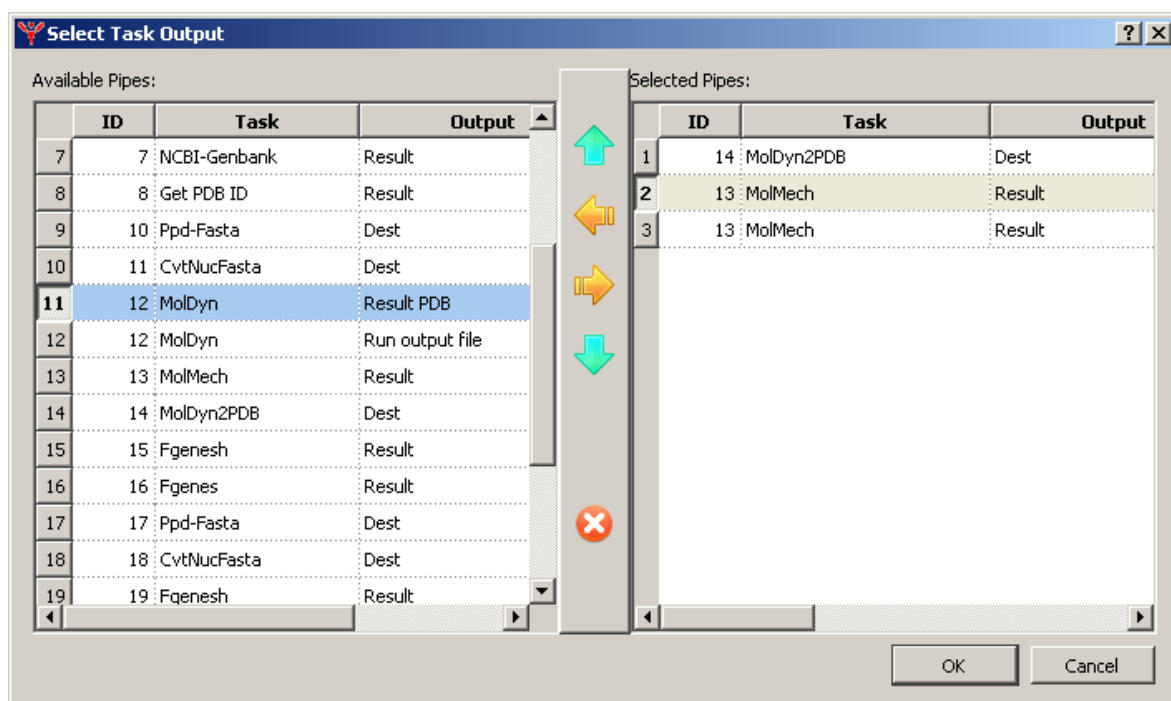
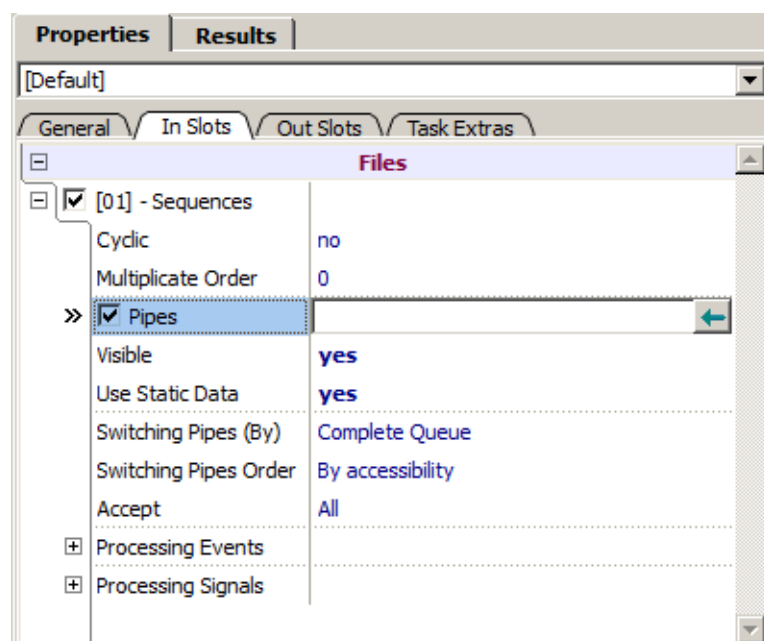


Order of files in a list can be changed by using  and  buttons.

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

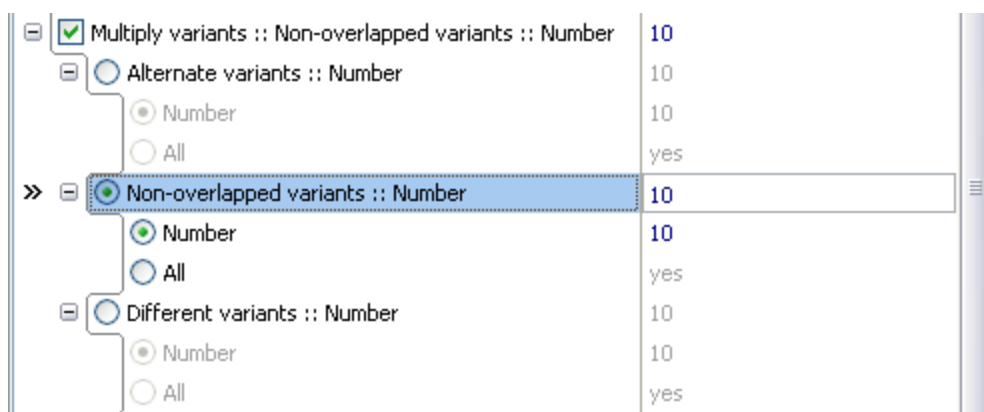
- **Pipe** - input data are taken directly from output of another task in the same project. Correct link to pipe data source is indicated by icon , while undefined or wrong link - by icon . Similarly,  icon means that destination for output data is correct, and the  - that link is not defined or incorrect.

To choose the link for input data, use  button (Placed on [In Slots page](#)), which displays "[Select Task Output](#)" dialog with list of outputs of task within current project. Moving outputs between "Available pipes" and "Selected pipes" lists is performing by mouse double-click.

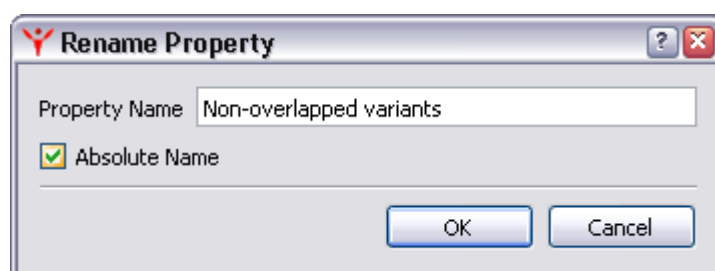


Some properties are mutually exclusive, i.e. if value of Property 1 is set, value of Property 2 cannot be set. Such properties are grouped into a radio node. In such cases, a separator ":" is placed after a name of a node (parent property), separating it from a name of selected nested property. User can change this default style with alternative ones in Rename Property dialog below.

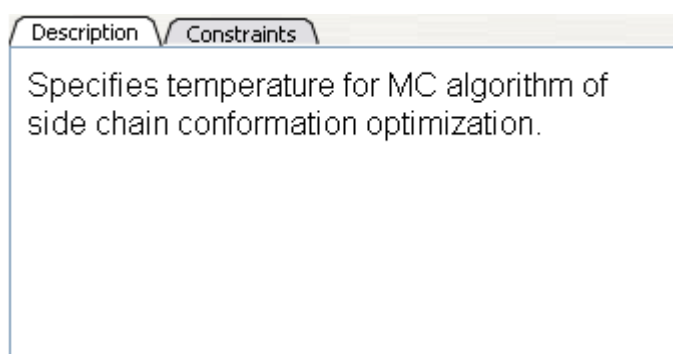
For example, label "Multiply variants::Non-Overlapped variants::Number" means that parent property "Multiply variants" has nested property "Non-Overlapped variants" selected as its value, and this property "Non-Overlapped" has its own nested property, "Number" as its value:



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.

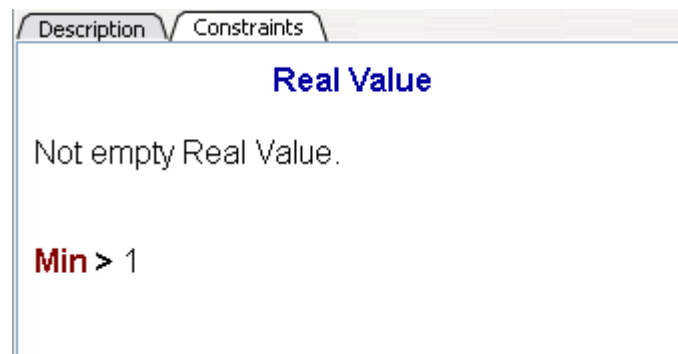


Description page



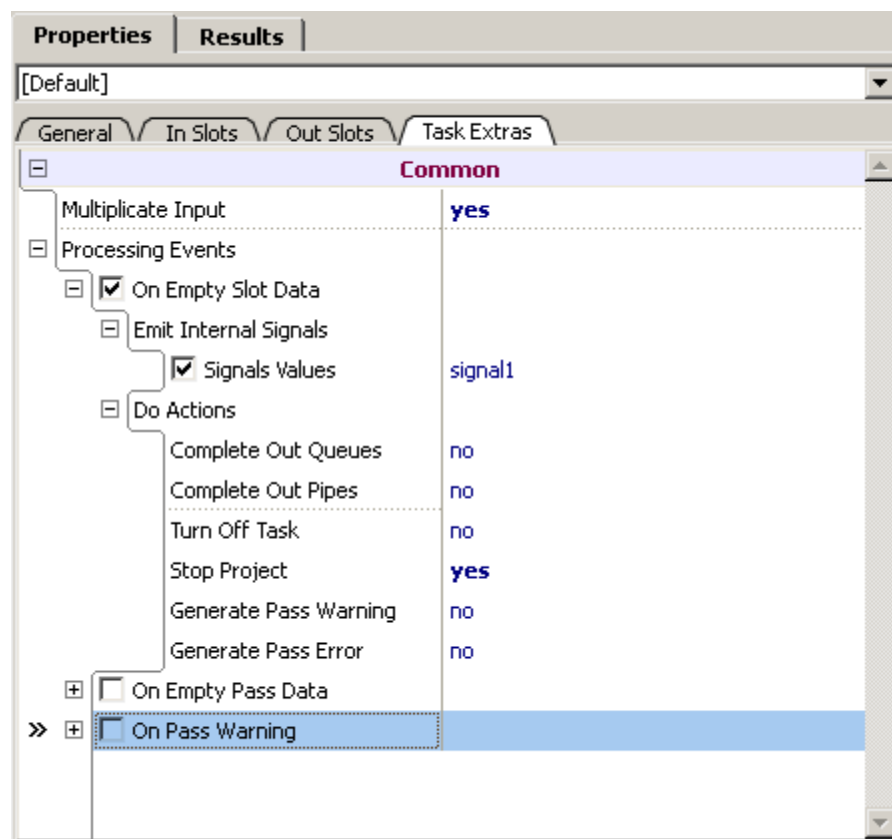
Description page contains brief descriptions of some selected properties or their values.

Constrains page



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

Task Extras Page

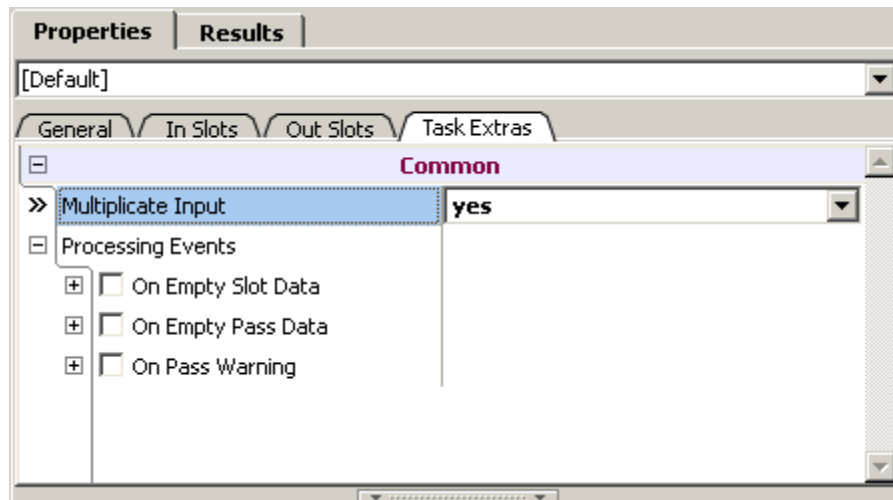


Additional task run settings.

In the "Task Extras" page the following parameters can be specified:

- [Multiply Input](#)
- [Processing Events](#)

Multiply input



Multiply Input - the way to combine input data. The current option makes sense for the programs with two or more data inputs and can be enabled ("Yes", set by default) or disabled ("No").

Yes - on putting multiple data (list of files or pipeline multiple output data) to a program entries, all possible combinations of input data are to be checked. For example, to the first entry the list of 3 files and to the second one - the list of 4 files are set, then 12 different results will be at the end:

- 1 variant - the first file from list one and the first file from list two;
- 2 variant - the first file from list one and the second file from list two;
- 3 variant - the first file from list one and the third file from list two;
- 4 variant - the first file from list one and the fourth file from list two;
- 5 variant - the second file from list one and the first file from list two;
-
- 12 variant - the third file from list one and the fourth file from list two;

Priority of slots can be specified in the "In Slots" tab.

No - consecutive combinations are to be used only. The number of results is determined by the the smallest data input. For example, to the first entry the list of 3

files and to the second one - the list of 4 files are set, then 3 different results will be at the end:

1 variant - the first file from list one and the first file from list two;

2 variant - the second file from list one and the second file from list two;

3 variant - the third file from list one and the third file from list two;

See more at Input Slots>Multiply Order

Processing Events – processing of task run events

Reactions on the following events can be specified:

- **On Empty Slot Data** — This event occurs on empty data received by, at least, one output slot at the current pass. For the file data it means no file or empty one.
- **On Empty Pass Data** — This event occurs on empty data received by all output slots at the current pass.
- **On Pass Warning** — This event occurs on completion of the current pass with warning. On pass warning — warning is received during the current pass.
- **Note.** This event does not occur on explicit warning generation by the "Generate Pass warning" operation (see "Actions" section).

For these events the followings are possible:

- [Emit internal signals](#) — To generate internal signals (see "Emit internal signals" section). ;
- [Do Actions](#) — To perform the chosen actions. The possible types of action – actions for the input slots and service ones.

Slots setup

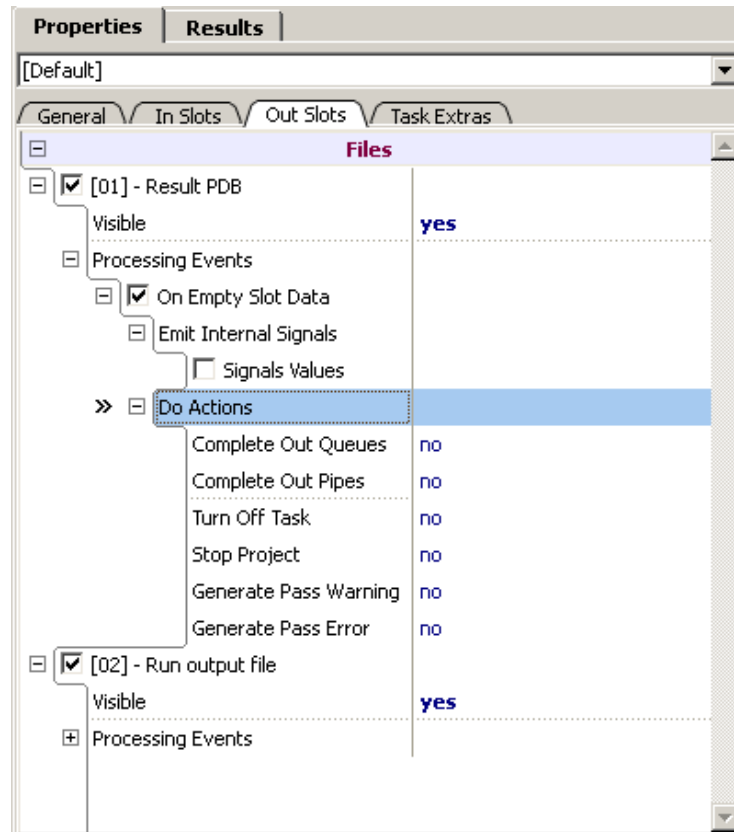
- [Output slots setting up - Out Slots page](#)
- [Input slots setting up - In Slots page](#)

Output Slots setting up

Out Slots page

The page allows to set up the parameters of the task output slots working.

To enable the additional options on the slot working, check in the box next to the slot name.



Visible

If the "no" value is selected, the slot with its links is not displayed on the task image in the "Pipeline" tab. If the "yes" value is selected, the slot with its links is displayed on the task image in the "Pipeline" tab.

Processing Events – processing of the events on output slots

For the output slot the reactions on following events can be specified:

- **On Empty Slot Data** - This event means empty data receiving by the slot. For the file data it means no file or empty one. The possible reactions to this event are:
 - [Emit internal signals](#) — To generate internal signal(s).
 - [Do Actions](#) — To perform the chosen actions. The possible types of action – actions for the output slots and service ones.).

Input slots setting up

In Slots page

The page allows to set up the parameters of the task input slots working:

- Cyclic
- Multiply Order

- Pipes
- Visible
- Use Static Data
- Switching Pipes (By)
- Switching Pipes Order
- Accept
- Processing Events
- Processing Signals

Properties Results

[Default]

General In Slots Out Slots Task Extras

Files

<input checked="" type="checkbox"/> [01] - inProtocol data	
Cyclic	no
Multiply Order	0
<input checked="" type="checkbox"/> Pipes	35 :: NCBI-Protein :: Result
Visible	yes
Use Static Data	yes
Switching Pipes (By)	Complete Queue
Switching Pipes Order	By accessibility
Accept	All
<input type="checkbox"/> Processing Events	
<input checked="" type="checkbox"/> On Complete Queue <input type="checkbox"/> Emit Internal Signals <input type="checkbox"/> Do Actions <input type="checkbox"/> On Complete Pipe	
<input type="checkbox"/> Processing Signals	
<input checked="" type="checkbox"/> On Signals If Signals Match Expression	x
<input type="checkbox"/> Do Actions	
Clear Queue	no
Next Queue	no
Reset Pipe Queue	no
Reset Static Data	no
Complete Queue	no
Complete Pipe	no
Complete Out Queues	no
Complete Out Pipes	no
>> Turn Off Task	no
Stop Project	no
Generate Pass Warning	no
Generate Pass Error	no
<input type="checkbox"/> On Signals	
<input type="checkbox"/> On Signals	
<input checked="" type="checkbox"/> [02] - PDB structure	

Cyclic

Cyclic – to «cycle» the data processing at the slot. All incoming data will be processed repeatedly ad infinitum. This mode is independent on settings of other task slots (slots priority, for example).

Multiply order

Multiply order - sets the priority of slots at multiplicative processing. The mode of multiplicative processing can be enabled in the "Task Extras" page.

If the multiplicative processing is disabled, the priorities have no significance.

Priorities definition.

For all slots, the priorities are specified explicitly and can not be equal. If values specified in the **Multiply order** are equal, the higher priority belongs to a slot that is lower in the list. If values differ, the higher priority belongs to a slot with higher value.

Slot processing order in dependance on priority.

The data at slots with higher priority are being iterated primarily. E.g. if data from the first slot have a lower priority than that from the second one, the processing will be performed in the following way:

1st element of the 1st slot is being processed with all elements of the 2nd slot, 2nd element of the 1st slot with all elements of the 2nd slot, etc.

Main and auxiliary slots.

Besides priority there is the concept of main and auxiliary slots.

On a vector data processing (Multiply Input = "no") all slots are referred to as main.

On multiplicative data processing (Multiply Input = " yes") the main slot is that with the least priority. All other slots are auxiliary.


Data processing on main and auxiliary slots by default is being performed in the following way:






For the main slot. Data in slots are being processed sequentially, i.e. on reaching the end of queue, the automatic switch to the next queue occurs.

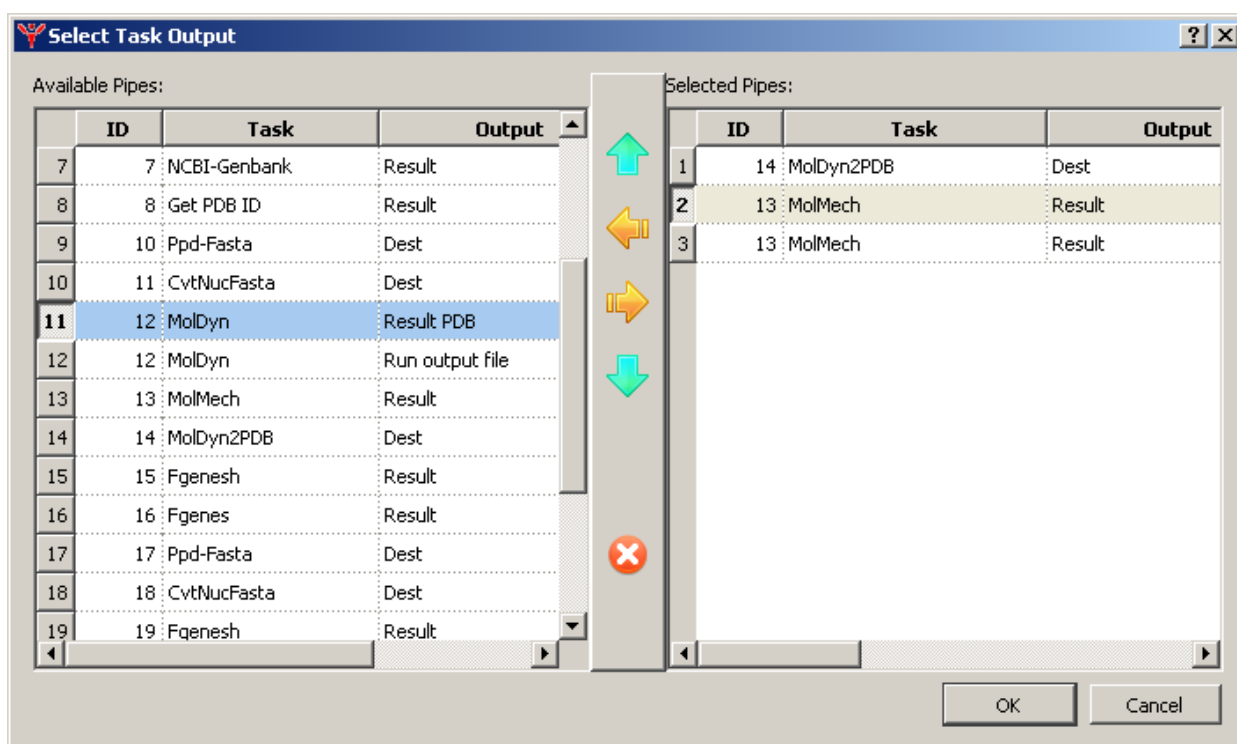
For the auxiliary slot. On reaching the end of queue, the automatic switch to the beginning of the same queue occurs.

The way of slots processing can be changed manually by a number of settings.

Pipes

Pipes — the  button calls out the dialog for the pipes selection "Select Task Output", that allows to specify the project tasks output slots that will be used as input ones for the current slot.

"Select Task Output" dialog contains list of outputs of task within current project. Moving outputs between "Available pipes" and "Selected pipes" lists is performing by mouse double-click or by arrows  and . Order of slots in the list can be changed by arrows  and . Any output slots can be selected, including the one of the own task. The  button clears all data of the "Selected Pipe" list.

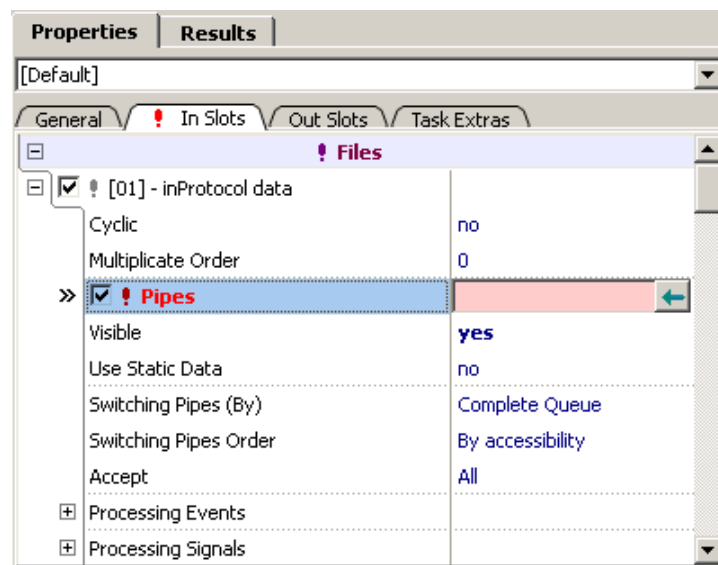


Visible

Visible. If the "no" value is selected, the slot with its links is not displayed on the task image in the "Pipeline" tab. If the "yes" value is selected, the slot with its links is displayed on the task image in the "Pipeline" tab

Use Static Data

Use Static Data — If the "yes" value is selected, then the data corresponding to the slot at the "General" page (so called "Static data") are being included in the list of data to be processed. "No" - the data only from pipes linked to the current slot are being included in the list of data to be processed. If the "yes" value is selected, but no static data are specified at the "General" page, then the error message appears in front of page name. If "no" value is selected, but no pipes (so called "dynamic data") are linked to the slot at the "In Slots" page, then the error message appears in front of page name.



Switching Pipes (By)

Specifies the pipes switching method:

- **Complete Queue** - - switch to another pipe occurs on the "Complete Queue" event (that, for example, occurs at receiving the "Complete Queue" flag by the slot).
- **Complete Pipe** - switch to another pipe occurs on the "Complete Pipe" event (that, for example, occurs at receiving the "Complete Pipe" flag by the slot).
- **Note.** If switching from pipe to pipe takes place, the "Complete Pipe" event is being generated independently on switching method.

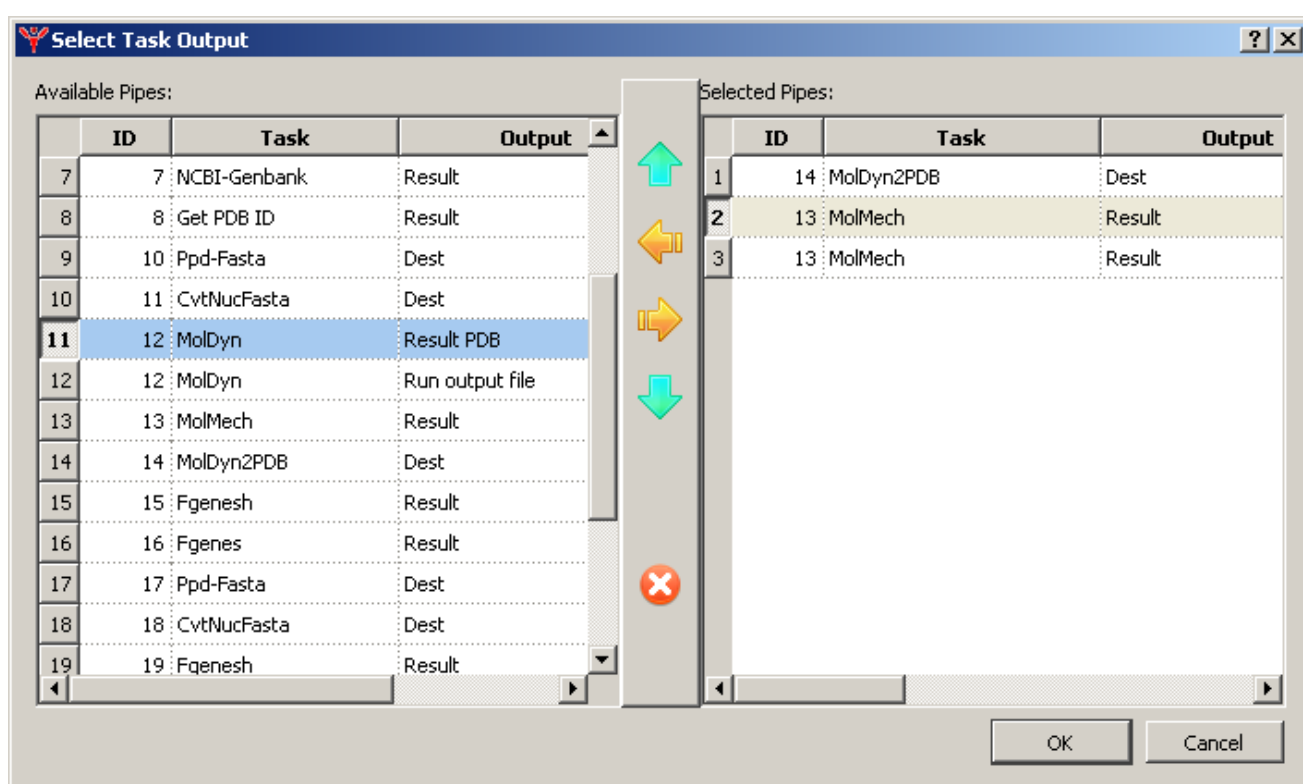
Switching Pipes Order

Species the pipes processing order:

- **By accessibility** - – Pipes are being processed in the order that specified in the "Selected Pipes" list in the ["Select Task Output" dialog](#). On reaching the end of list, the processing continues from its beginning. In the case, when it's necessary to switch a pipe, but there are no unprocessed data on the current

one, the process switches to the next pipe. If there are unprocessed data, switching is completed and processing of these data begins. If there are no data, switching to the next pipe in the list occurs, and so on until the appropriate pipe is found. If no appropriate pipe is found, switching is considered uncompleted. It will be completed when unprocessed data emerged on any pipe of the list. This processing order is used by default.

- **Strict Order** - Pipes are to be processed strictly in the order they are in the "Selected Pipes" list of the ["Select Task Output" dialog](#). Switching occurs to the next pipe by the order. If pipe, to which the switching has been done, contains no unprocessed data, the processing goes to stop until such data emerge. After the end of list is reached, the processing begins from the start of list round.



Accept

Accept — which data slot can accept:

- **All** — all incoming data.
- **Last In Queue** — just the last data item in the line. In the case of static data only are used by slot, the mode does not work, i.e. processing of all static data items will be performed. To perform the processing of the single element is always possible by its direct definition, e.g specifying the single file instead of list of them.

Processing Events

The reaction to the following events can be specified:

- **On Complete Queue** — may occur on:
 - Finding the marker of the queue end
 - Reaching the end of static data list, in the case of dynamic data (data from pipes) absence
 - On explicit event generation at performing of certain actions (see [Do Actions](#) section, actions for input slots).
- **On Complete Pipe** — may occur on:
 - Finding the "On Complete Pipe" marker.
 - On any switch necessity specified at "Switching Pipes (By)"
 - On explicit event generation at performing of certain actions(see "Do Actions" section, actions for input slots).

For these events the following can be done:

- [Emit internal signals](#) — To generate internal signals.
- [Do Actions](#) — To perform selected actions. The allowed action types – actions for input slots, actions for output slots and service actions.

Processing signals

Input slot can process the received signals.

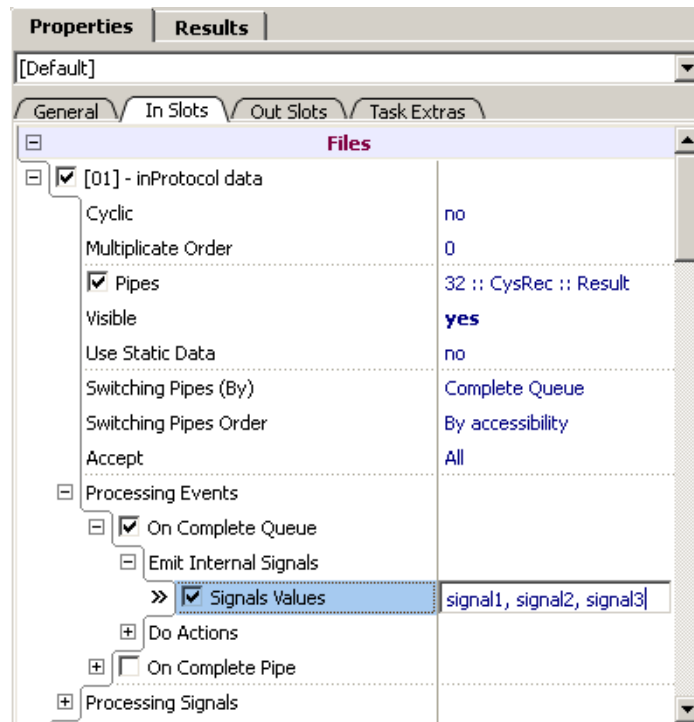
In the node "On Signals" in the line "If Signals Match Expression" the logical expression of signal names can be specified. The following symbols are allowed the logical expression: "&", "|", "!" as well as grouping by brackets "(" ")".

On completion of pass, to the input slots signals from various sources arrive. Processing occurs if the "On Signals" checkbox is checked in. If a signal with a certain name has arrived, it's being assigned with "true" value, if has not arrived - "false". After this, the logical expression is being checked for validity. If it's valid, the actions specified in the "Do Actions" node are being performed.

Emit internal signals

To enable this option, check in the box next to the name "Signals Values" and fill in the field. In the field the one or several signals can be specified. Signals can be separated by symbols " ", ",", or ";". The signal value can be specified in Latin symbols (case sensitive) in both cases, numerical symbols and underlines. Excessive separators are being ignored.

Signals are being sent within the task only. Any signal is being sent to all input task slots.



















Do Actions

Actions can be performed for various events and on signals processing. To make action to be performed, set the "yes" value in front of its name in the list. For some events not all actions are declared, since they are either not related to current event type or their performing has no sense. There are 3 various action variants: for output slots, "service" and for input slots.

- **Service actions.** Can be performed for any event and on signals processing.
 - **Turn Off Task** — To remove the "ready to run" status from the task in the "Projects" tab. At this, the task is being turned off until user set it on again.
 - **Stop Project** — To stop the project. At this, the project is being turned off until user set it on again.
 - **Generate Task Warning** — To generate the warning of pass completing. The current pass is being marked with ⚠ status in the "State" column of the "Results" tab (if it was not before).
 - **Generate Task Error** — To generate the error of pass completing. In the "State" column of the "Project" tab, as well as in the "Results" tab, the ❌ status will appear. Data of the pass with error are not to be sent to pipe.
- **Actions for the output slots**
 - **Complete Out Queues** — To add the "Complete Queue" flag, that means the end of queue, to a corresponding element of data stream (relevant to current pass) for every output slot of the current pass. For this pass, in the "Flags" column of the "Results" tab, the "Q" sign will appear.

- **Complete Out Pipes** — Do the same as "Complete Out Queues". Besides it, for every output slot of the current pass the "Complete Pipe" flag, that means the necessity to switch to the next pipe, is being added to a corresponding element of data stream (relevant to current pass). For this pass, in the "Flags" column of the "Results" tab, the "QP" sign will appear.

Properties		Results			
	State	Flags	View	Processing	Start Time
1	✓		 	0.360	2012-06-14 / 16:28:55
2	✓		 	0.359	2012-06-14 / 16:28:58
3	✓		 	0.359	2012-06-14 / 16:29:00
4	✓	Q	 	0.360	2012-06-14 / 16:29:03
5	✓		 	0.360	2012-06-14 / 16:29:05
6	✓		 	0.375	2012-06-14 / 16:29:07
7	✓		 	0.360	2012-06-14 / 16:29:10
8	✓	Q P	 	0.375	2012-06-14 / 16:29:12

- **Actions for the input slots.** These actions control the queues processing at the input slot.
 - **Complete Queue** Completes the queue at the current position. Adds the "Complete Queue" flag to current element. In addition, the completing of this action generates the "On Complete Queue" event.
 - **Complete Pipe** Do the same as "Complete Queue". Besides it control the switching to another pipe in accordance to switch settings (see [here](#)). In addition, the completing of this action generates the "On Complete Pipe" event.
 - **Clear Queue** – Clear the queue (all data in queue are considered to be processed). If it's possible to determine the end of queue by the flag in a pipe, the switching to the next queue occurs. If the end of queue can not be currently detected, the switching to behind the end of data list occurs and at the last element the flag of queue end is being set. The completing of this action generates the "On Complete Queue" event.
 - **Next Queue** – To switch to the next queue. The switching occurs only in the case of next queue existing. If currently there is no flag of the queue end, the system remains at the current queue. If switching to the next queue occurs, the "On Complete Queue" event is being generated.
 - **Reset Pipe Queue** — To set the processing position in the current queue to the beginning of data by pipe.

- **Reset Static Data** — To process static data in the current queue over again.

Order of actions performing for input slots.

Logical order of actions performing is strictly the same as in description. The only exception is part of "Complete Pipe" action – the switching to another pipe. It's being performed just after completion of all other actions. I.e. all actions are being performed for current pipe and just after this, on necessity, the switching to another pipe occurs. The same for switching to another pipe due to other settings ("Switching Pipes By" for example).

Project tab

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

Project : test5													
	E	Res/State	L	V	Run	In	Out	ID	Task Name	Pass	Results	Processing	Last Start Time
1	<input checked="" type="checkbox"/>	✓						11	SeqStat	1/1		00:00:01	2012-08-30 / 14:11:24
2								12	SeqTrans				
3	<input type="checkbox"/>	✓					→	2	BestPal-E	1/1		00:00:01	2012-09-04 / 16:10:33
4	<input checked="" type="checkbox"/>							1	FoldRNA	0/1		00:00:01	2012-09-04 / 15:59:27
5	<input checked="" type="checkbox"/>	✓					→	30	FoldRNA	1/1		00:00:01	2012-09-04 / 16:06:58
6	<input checked="" type="checkbox"/>					→	→	15	AddSeq	1/1		00:00:02	2012-09-04 / 16:13:57
7	<input checked="" type="checkbox"/>					→	→	16	InsSeq	0/1		00:00:01	2012-09-04 / 16:13:58
8	<input checked="" type="checkbox"/>							5	Find-miRNA	1/1		00:00:01	2012-09-04 / 16:00:10
9	<input checked="" type="checkbox"/>					→	→	14	CutGet	1/2		00:00:01	2012-09-04 / 16:09:02
10	<input checked="" type="checkbox"/>	✓						19	OligsR	1/1		00:00:00	2012-08-30 / 14:11:29
11	<input checked="" type="checkbox"/>	✓						18	Oligs2	1/1		00:00:02	2012-08-30 / 14:11:27
12	<input checked="" type="checkbox"/>	✓						17	Oligs	1/1		00:00:00	2012-08-30 / 14:11:27

N - the order number of each task.

E - displays the current [Ready State](#).

Res/State - displays the current [Execution State\(s\)](#) of a task.

V (Visibility) - Displays the current status of task [visibility](#).

L (Locking) - Displays the current status of [task lockup](#).

Run - displays the current [Running 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.

Last Start Time - last 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 or 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.
	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.
	Program Expired. Program Evaluation period is expired.

Visibility Status

The visibility status switches the task display in the “Pipeline” tab.

	View Task. Make task visible in the "Pipeline" tab.
	Hide Task. Make task invisible in the "Pipeline" tab.

Visibility status can be switched by:

- Mouse click over visibility status icon in the "V" column of the "Project" tab.
- Main menu commands:




Task:

- Hide Task
- View Task

Project:

- Hide All Tasks
- View All Tasks
- Invert Visible
- Special Hide
- Special View

Task lockup status

	Task is not locked.
	Regular task lock.
	Task is Frozen.

Lockup status is duplicated at task icon in the "Pipeline" tab.

A task can be both regularly locked and “frozen”.

Regular lockup means the locked task is not to be processed, task parameters can not be edited (excluding addition/removal pipe-links), execution flag can not be set, data can not be removed. Task can be deleted.

"Frozen" lockup does the same, but, in addition, it makes the following commands inactive: Lock All Tasks, Unlock All Tasks, Invert Lock and Special Lock/Unlock.

Lockup statuses can be switched by:

- mouse click over appropriate icon in the "L" column of the "Project" tab.
- mouse click over appropriate icon at task image in the "Pipeline" tab.

- commands of the main menu:



Task:

- Lock Task
- Unlock Task
- Lock Freeze Task
- Unlock Frozen Task

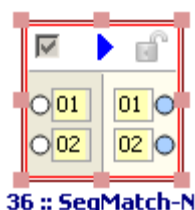
Project:

- Lock All Tasks
- Unlock All Tasks
- Invert Locked
- Special Lock
- Special Unlock









Running State

	In Progress. The task is being run now.
	Aborted. User aborted a task on the first pass. No results to use or to send to a pipeline.

At the task image in the "Pipeline" tab, the information of the "E", "Run" ("Run" status only) and "L" columns is duplicated.



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

This column has the same meaning as the "Input Data" column, but for output data of a task.

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->Stop 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.


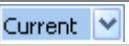
View/Console toolbar

View/Console toolbar has buttons for work with [View/Console Tab](#).

	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.
	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 Tab

Configuration toolbar

	Same as: Tools->Profile Manager in Main Menu.
	Chose profile from a list and make it current.

Results tab

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

For many programs, a list of files can be 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, different combinations of files will be processed. For instance, if Property 1 is specified as a list containing three files, and Property 2 as a list of four files, there will be $4 \times 3 = 12$ passes (if [Multiply Input](#) option is enabled), each one combination of input files. If [Multiply Input](#) is disabled, the number of passes is determined by the smallest data input. For instance, if Property 1 is specified as a list containing three files, and Property 2 as a list of four files, there will be, then 3 passes. Total number of passes for one task cannot exceed 100,000.

Results					
	State	Flags	View	Processing	Start Time
1	✓			1.188	2012-08-24 / 17:40:22
2	✓			1.062	2012-08-24 / 17:40:23
3	✓			1.063	2012-08-24 / 17:40:25
4	✓			0.094	2012-08-24 / 17:44:37
5	✓			0.094	2012-08-24 / 17:44:37
6	✓			0.094	2012-08-24 / 17:44:37
7	✓			0.094	2012-08-24 / 17:44:37
8	✓	Q		0.094	2012-08-24 / 17:44:38
9	✓			0.078	2012-08-24 / 17:44:38
10	✓			0.094	2012-08-24 / 17:44:38
11	✓			0.094	2012-08-24 / 17:44:38
12	✓			0.094	2012-08-24 / 17:44:38
13	✓			0.094	2012-08-24 / 17:44:38
14	✓			0.093	2012-08-24 / 17:44:38
15	✓			0.093	2012-08-24 / 17:44:39
16	✓	Q P D		0.094	2012-08-24 / 17:44:39

Output Files			
Type	View	File	
1	✓	000011\result.txt	
2	✓	000011\result.bin	







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.
- **Flags** - display pass flags (if any). "QP" - means "Complete Pipe" and "Complete Queue" flags. "Q" means "Complete Queue" flag. "QPD" means "Data End" flag – the end of data is found for the current task at the current pipeline configuration. Simultaneously with this marker the End of Queue (Q) and the End of Pipe (P) markers are being set.
- **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:

Output Files		Input Files	
	Type	View	File
1		 	C:\Program Files\Softberry\...
2		 	C:\Program Files\Softberry\...





Type - source of file:

-  - file,
-  - pipeline.




View - preview input files. Icons are the same as those in Results column of [Project tab](#), 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:

Output Files		Input Files	
	Type	View	File
1			2.result.bin
2			2.result.txt

Type - possible output variants:

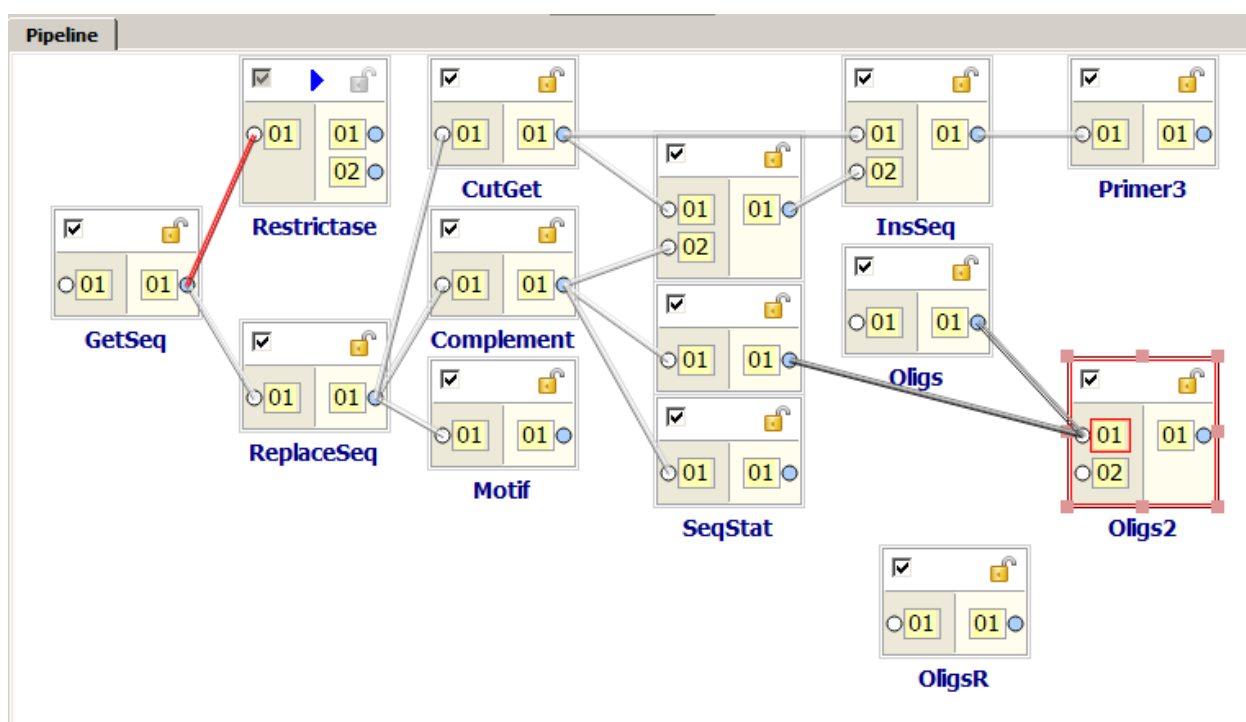
-  - Normal results file;
-  - Warnings log file;
-  - Errors log file.

View - preview results. Icons are the same as those in Results column of [Project tab](#), 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.
- An input slot belongs to a task that is currently running or has been completed.

Slots setup see [here](#).

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).
	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 [Properties 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.

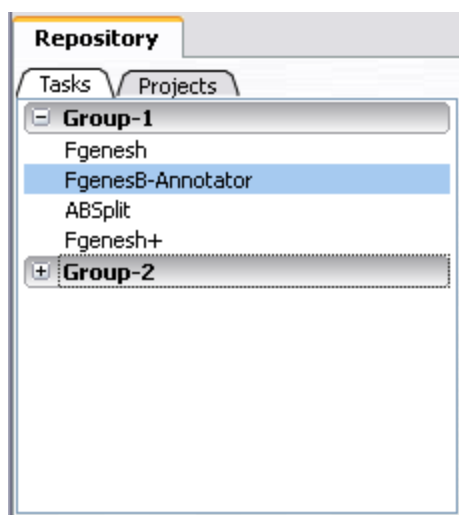
On placing the mouse pointer over the task at hold “Shift” key, in the tab will be displayed only those pipe-links, that belong to current task.

During the task processing, the currently used pipe is highlighted by red in the “Pipeline” tab.

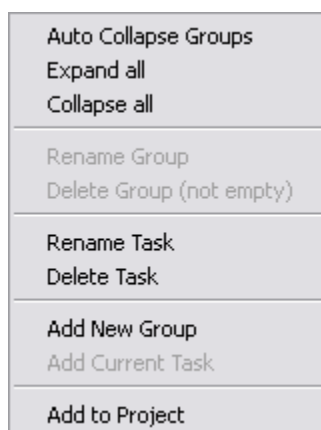
Repository tab

User may want to create libraries of tasks and projects, to be used as templates and building 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.

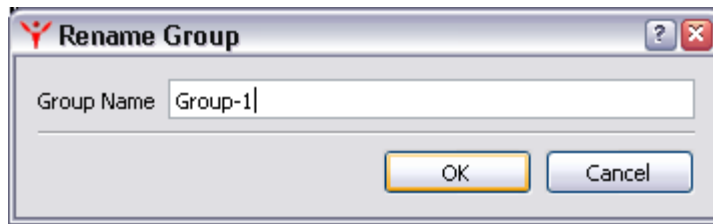
Task page



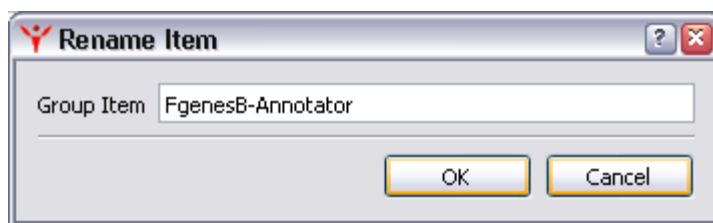
This page contains a list of user-defined groups, each of which can include a number of tasks. Groups can be created, deleted, renamed, or their content can be changed using contextual menu commands.



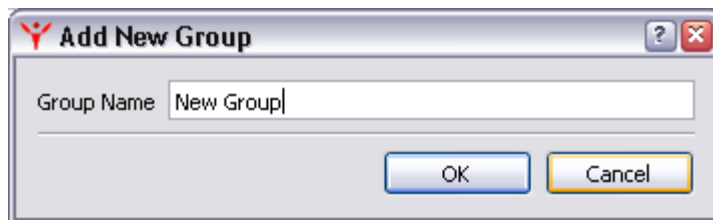
- **Auto Collapse Groups** - if checked, collapses all groups except selected.
- **Collapse All** - collapses all program groups.
- **Expand All** - expands all program groups.
- **Rename Group** - displays "**Rename Group**" dialog.



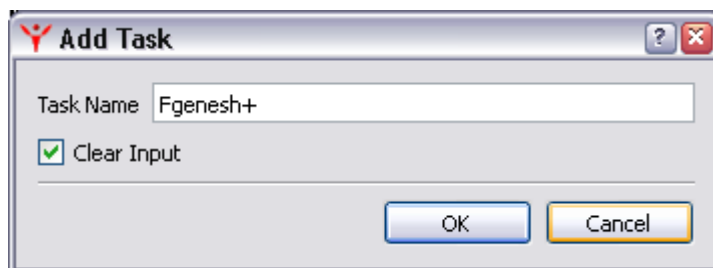
- **Delete Group** - remove selected group from a list. **Warning!** All tasks in that group are deleted as well.
- **Rename Task** - displays "**Rename Item**" dialog, in which selected task can be renamed.



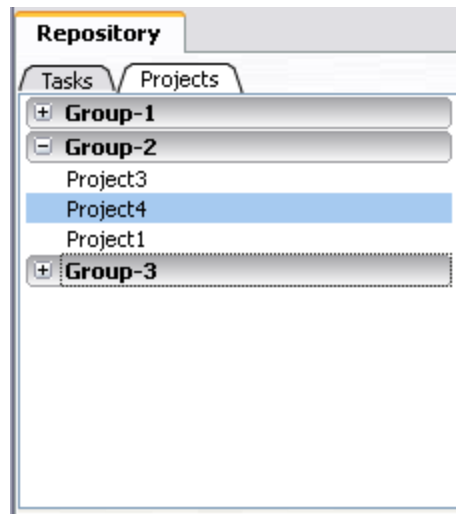
- **Delete Task** - removes selected task from a group.
- **Add New Group** - displays "**Add New Group**" dialog.



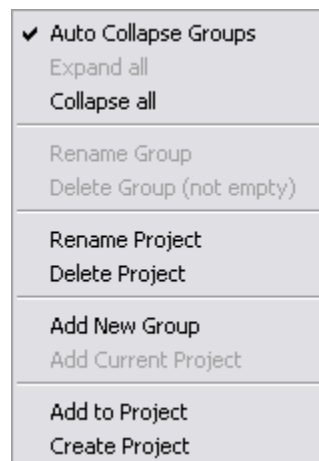
- **Add Current Task** - Displays "**Add Task**" dialog, where selected task from a current project can be added to a group. **Clear Input:** if checked, all input values are erased.



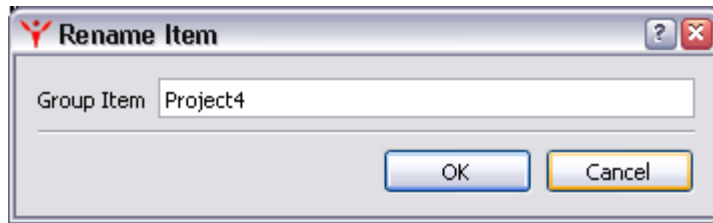
Projects page



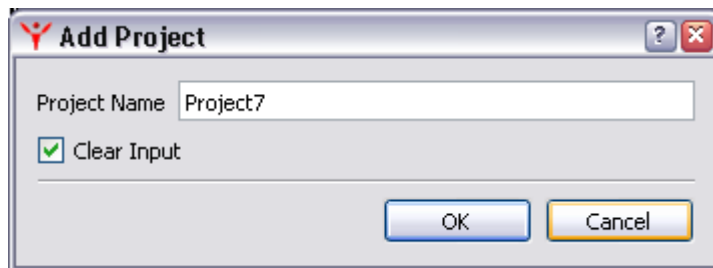
Projects page contains a list projects grouped into user-defined groups. As on tasks page, groups can be created, deleted, renamed, or their content can be changed using contextual menu commands:



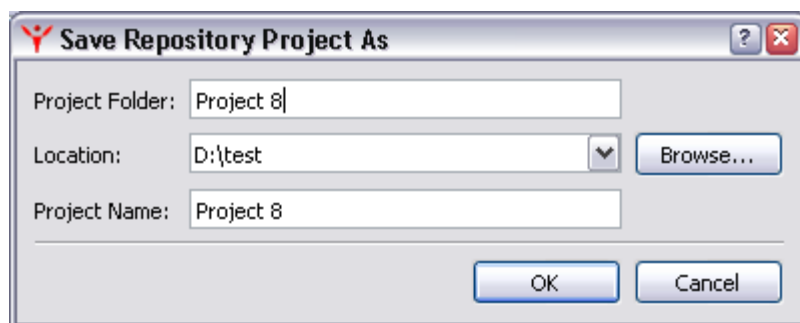
- **Auto Collapse All** - if checked, collapses all groups except selected.
- **Collapse All** - collapses all program groups.
- **Expand All** - expands all program groups. If "Auto Collapse" mode is active, only group is expanded.
- **Rename Group** - "Rename Group" dialog, similar to that of Tasks page.
- **Delete Group** - Deletes selected group and all projects it contains.
- **Rename Project** - displays "Rename Item" dialog for renaming selected project.



- **Delete Project** - removes selected project from a group.
- **Add New Group** - displays "Add New Group" dialog, similar to that of Tasks page.
- **Add Current Project** - Displays "Add 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.



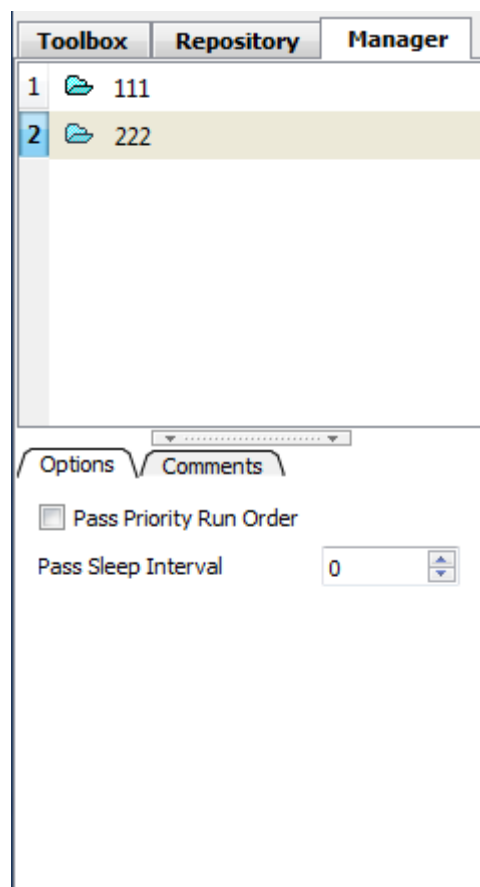
To load a project from repository, click on it. "Save Project As" dialog will be displayed, where you can type project name and title and choose location for it to be saved in.

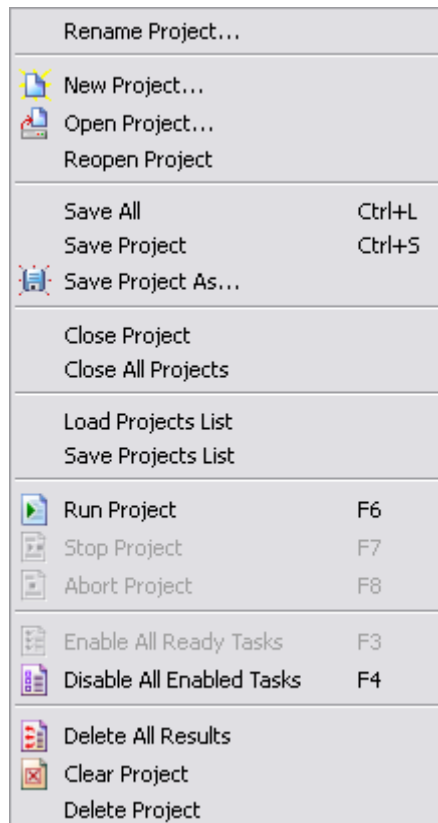


Manager tab Manager tab contains a list of opened projects. Projects can be dragged by a mouse up and down in a list. Click on a project name to switch to that project.

- **Comments page** contains some comments on selected project.

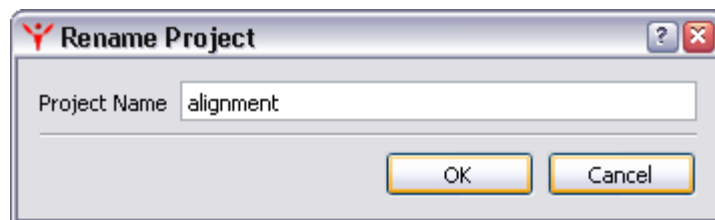
- **Options page** contains options which are applied to passes of the whole project:
 - **Pass Priority Run Order** - when enabled, the project independently on options set in the tabs is being processed in the following way: the first pass of the first task is processed, then the first pass of the second task etc. Once the first pass of the last task is completed, the second pass of the first task is getting processed, then the second pass of the second task and so on.
 - **Pass Sleep Interval** - retardation between the ending of current pass and starting of the next one in milliseconds.



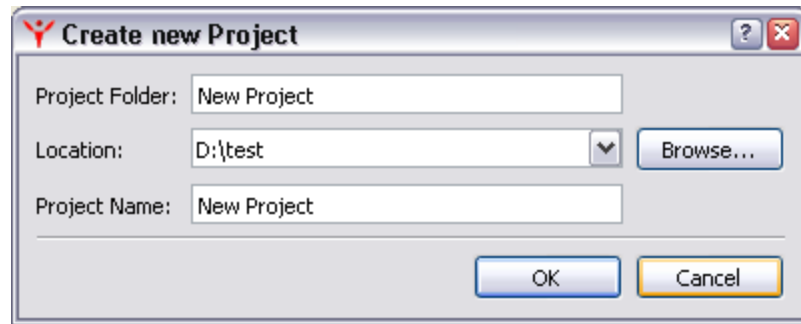


Contextual menu commands of Manager tab:

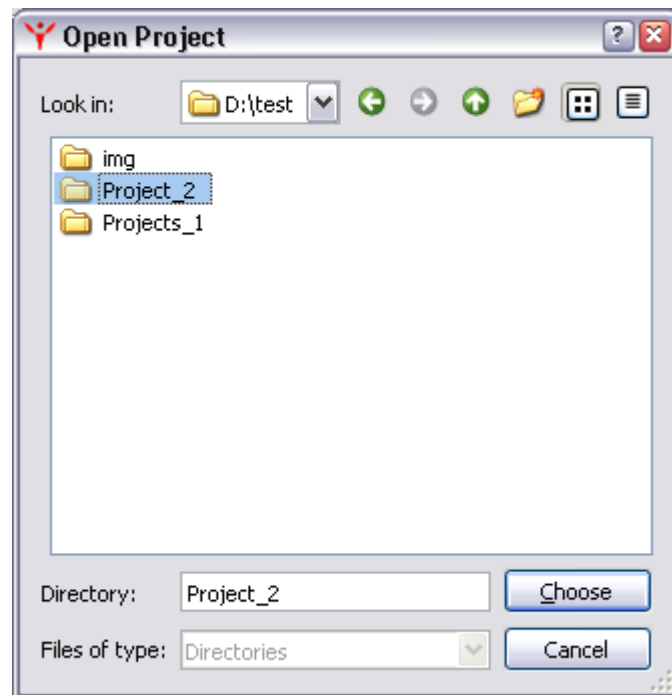
- **Rename Project** - displays "**Rename Project**" dialog.



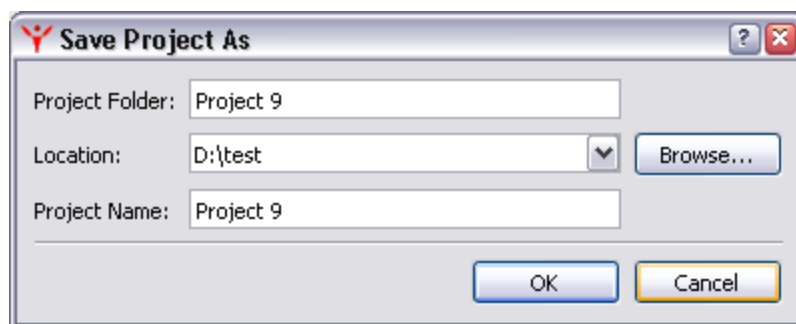
- **New Project** - Displays "**Create new Project**" dialog, where you can enter a folder name for a new project, as well as choose its location. If project folder with the same name already exists in chosen location, or contains invalid symbol (those not allowed in Windows filenames), the "OK" button 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.



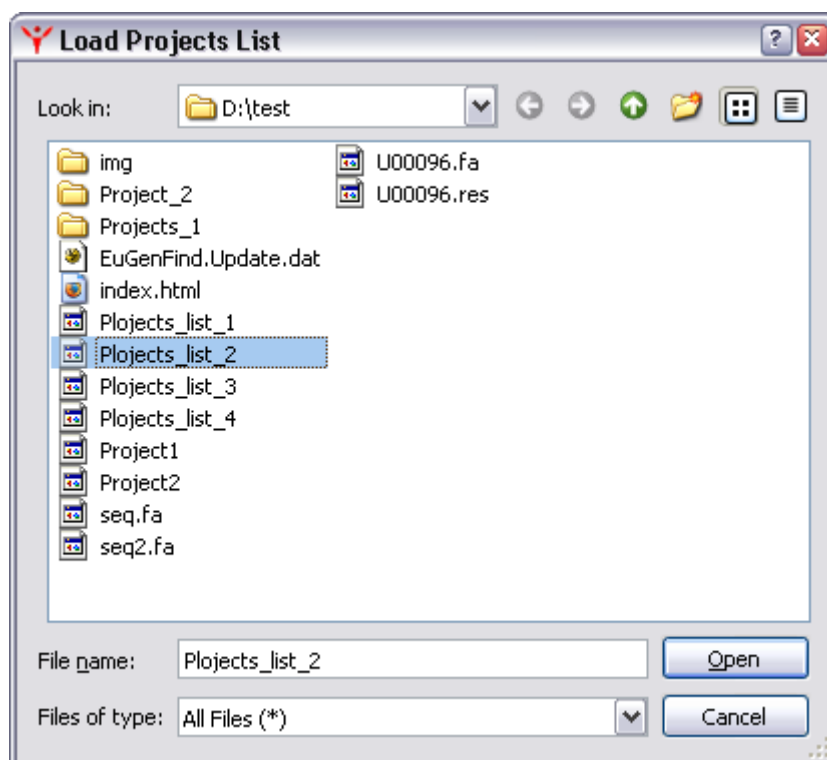
- **Open Project** - displays the "**Open Project**" dialog for opening and existing project. After opening, a project assumes a status of current project.



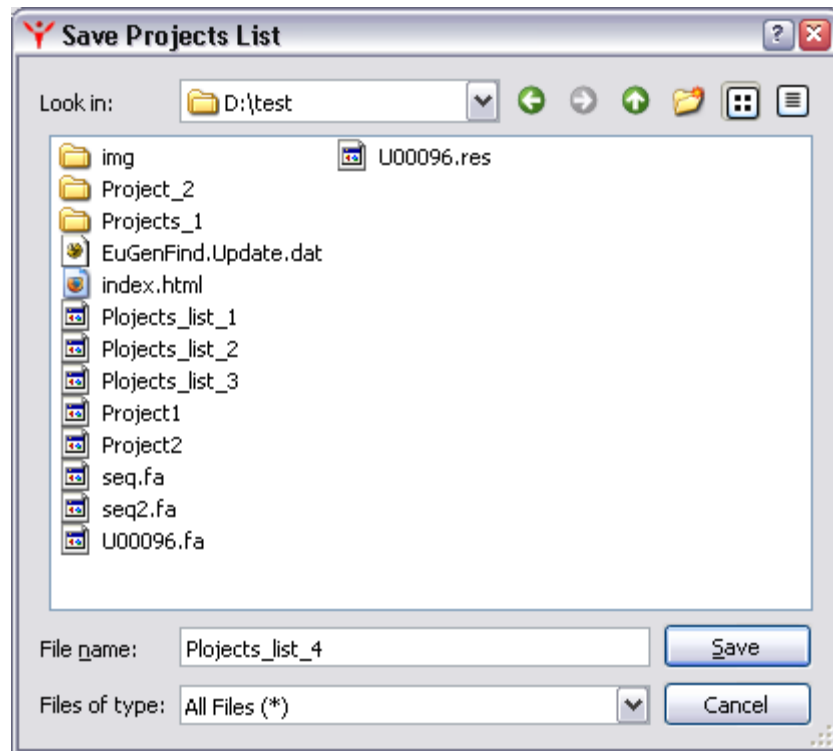
- **Reopen Project** - Reopens current project without saving any changes.
- **Save All** - Saves all projects at their current stage of progress.
- **Save Project** - Saves selected project at its current stage of progress.
- **Save project as** - displays the "**Save Project As**" dialog, used for 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 "Load 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.

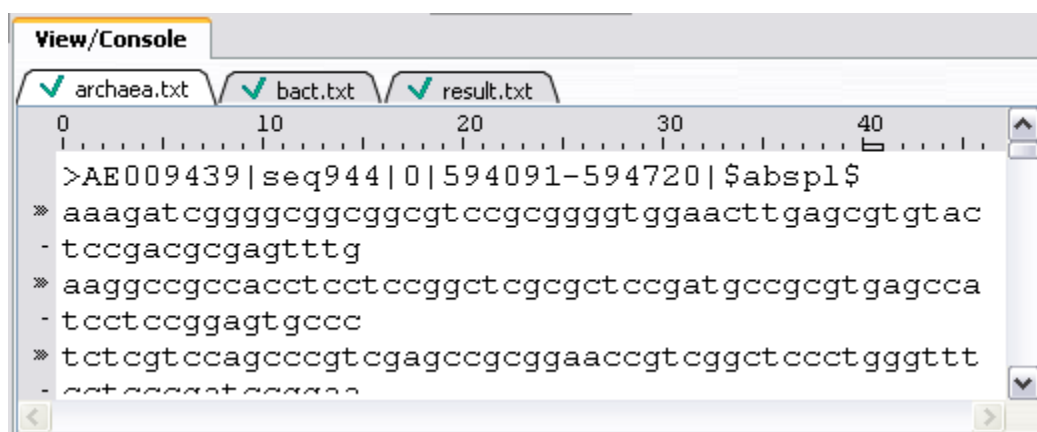


- **Save Projects List** - Save the list of currently opened projects, i.e. those displayed in [Manager Tab](#).



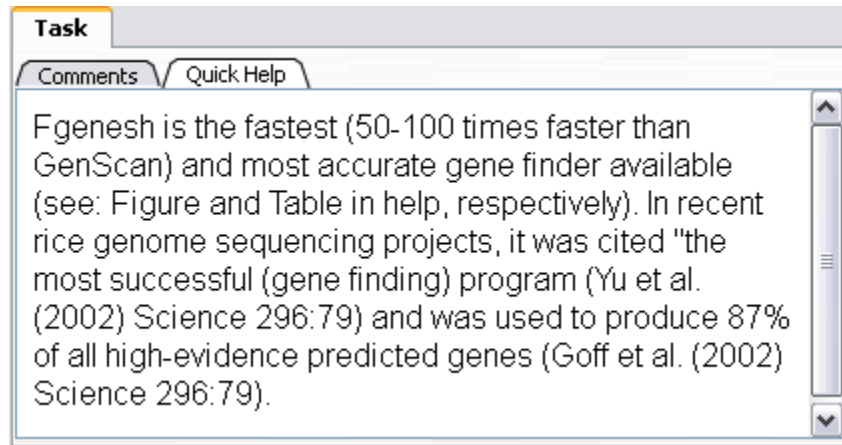
- **Run Project** - runs a project. Only enabled tasks will run.
- **Stop Project** - stops execution of a project upon completion of currently running task.
- **Abort Project** - immediately aborts a project, without waiting for running task or its pass to complete.
- **Enable All Ready Tasks** - enables 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:

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

To-Do tab

To-Do						
	C	!	Category	Caption	Date Add	Date End
1	<input checked="" type="checkbox"/>	0	normal	Item1	2009-12-23 / 22:11:27	2009-12-23 / 22:12:47
2	<input type="checkbox"/>	0	normal	Item2	2009-12-23 / 22:11:37	
3	<input checked="" type="checkbox"/>	2		Item3	2009-12-23 / 22:12:05	2009-12-23 / 22:12:49
4	<input type="checkbox"/>	9		Item3	2009-12-23 / 22:12:38	
*						

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.

The **C** column displays status of item completion,

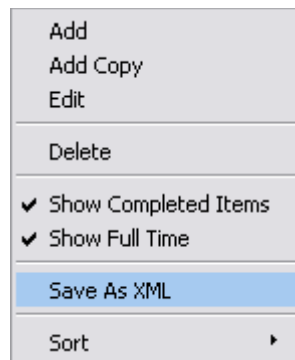
The **!** column indicates item priority;

Category - item category;

Caption - item name;

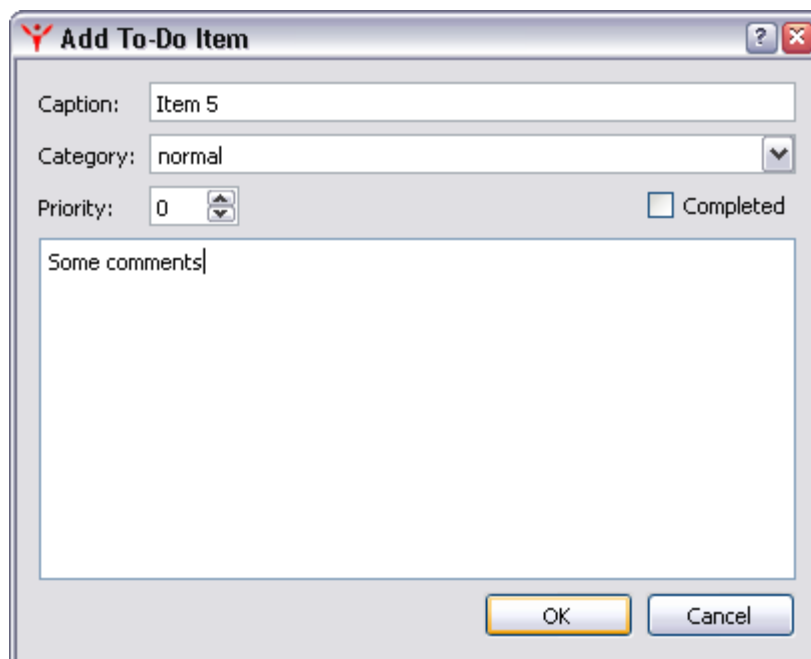
Date Add - and time of item creation;

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 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.

Add To-Do Item

Caption:
 Category:
 Priority: ☐ Completed

Some comments

OK Cancel

Edit - edits an item;

Edit To-Do Item

Caption:
 Category:
 Priority: ☒ Completed

Some comments

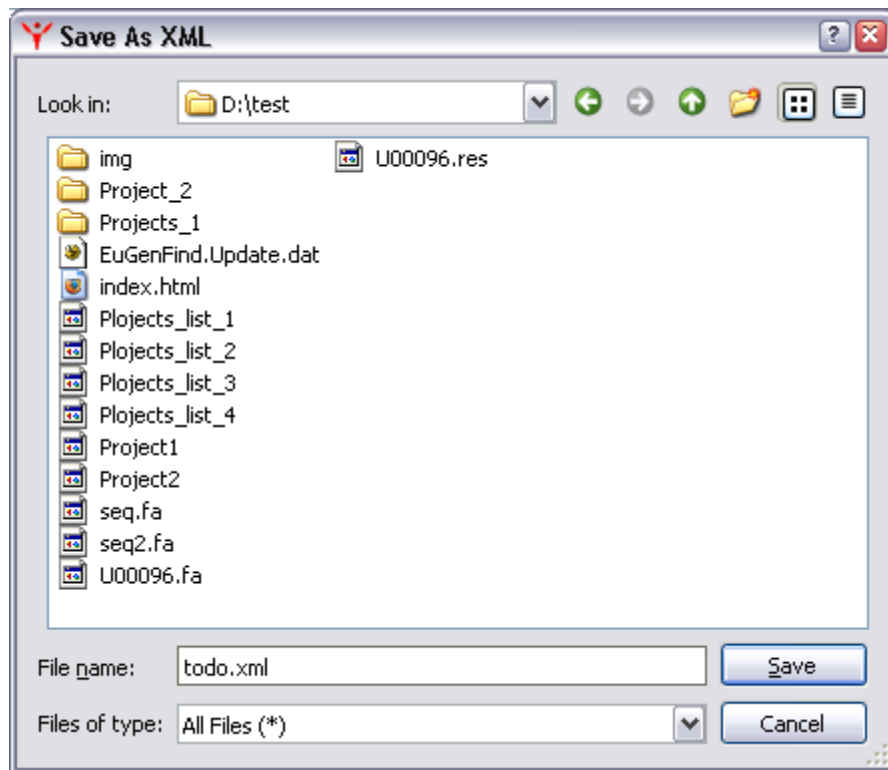
OK Cancel

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;

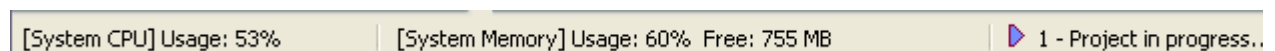


Sort - sorts items by one of the following criteria:

- **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:

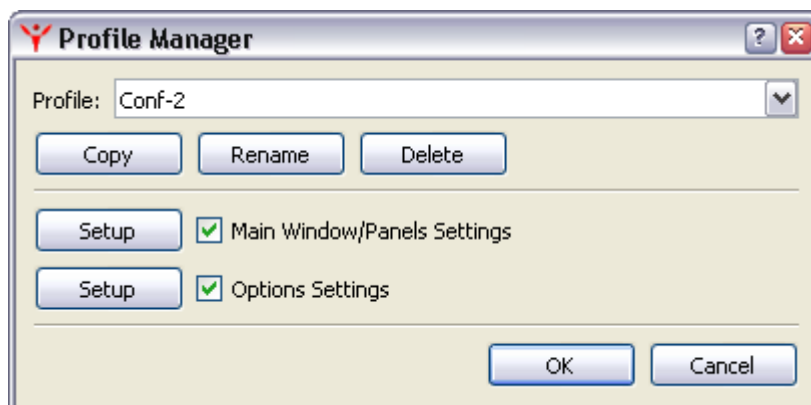
- **CPU Usage:** - CPU percentage usage.
- **Memory Usage:** - percentage of memory used.

- **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

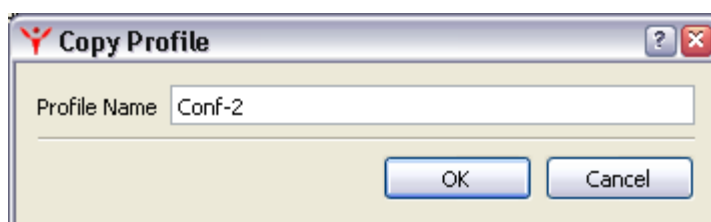


Profiles are designed for fast switching between different MolQuest settings. Profiles can include common application parameters (see [Options](#) dialog) window sizes, tabs location, headers sizes etc.

"**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 "Current".



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 "Current".

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

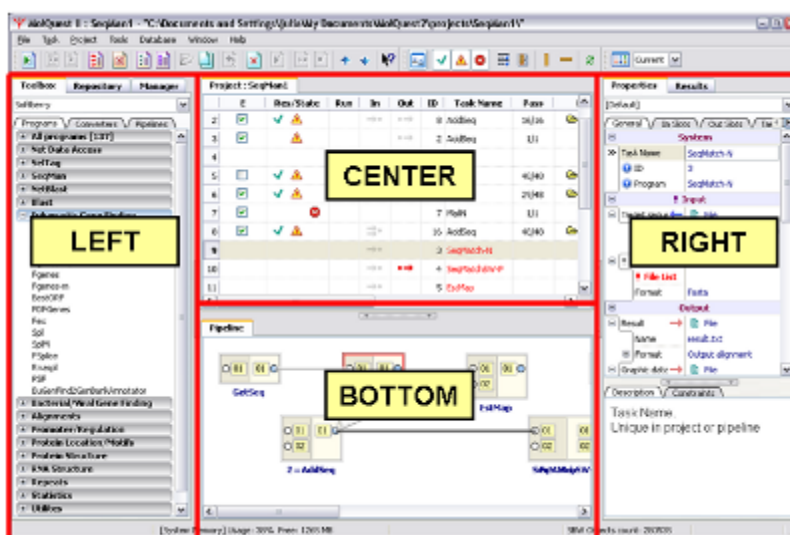
profile, Setup button is enabled. Pressing it saves current settings in current profile, and Setup button becomes disabled again.

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.

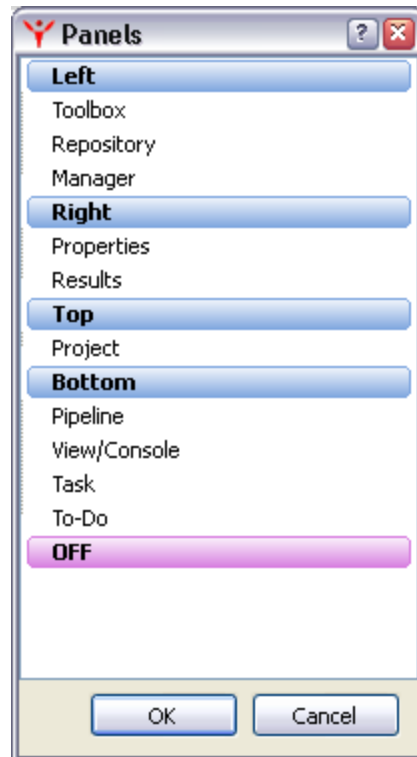
Panels dialog

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.

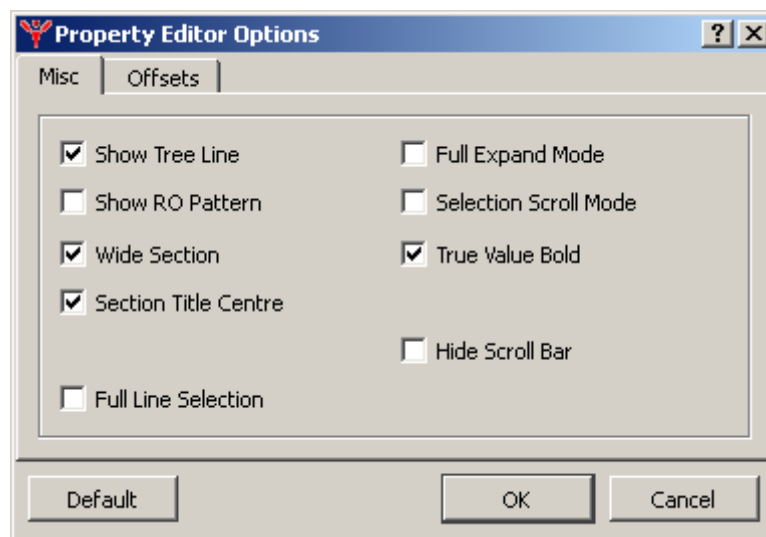
Panels dialog is a convenient tool for rearranging tabs in the main window. Drag a tab name to a zone where you want it to be located. If you want to hide a tab, drag its name to an "OFF" group.



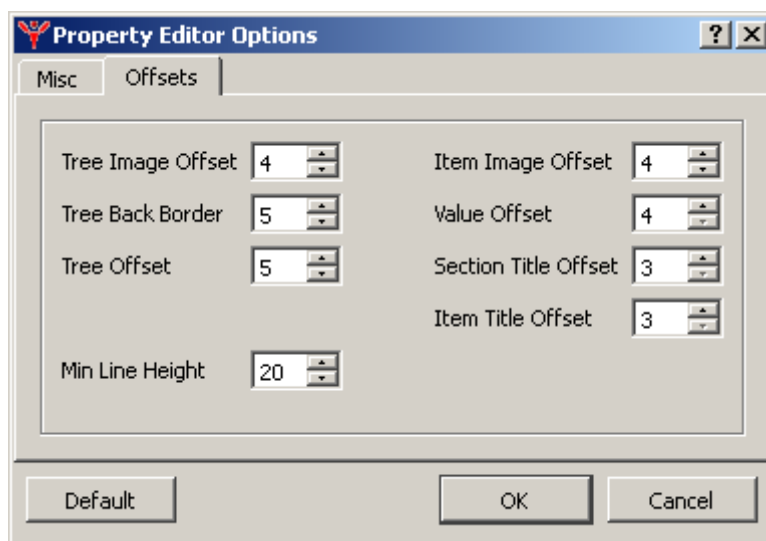
Property Editor Options

This dialog controls some visual and dynamic parameters of **Property Editor** settings, which we don't describe here in details. Pressing Default button resets all options to default. There are two tabs - [Misc](#) and [Offsets](#). You can return to initial options with the **Default** button.

Misc tab



Offsets tab

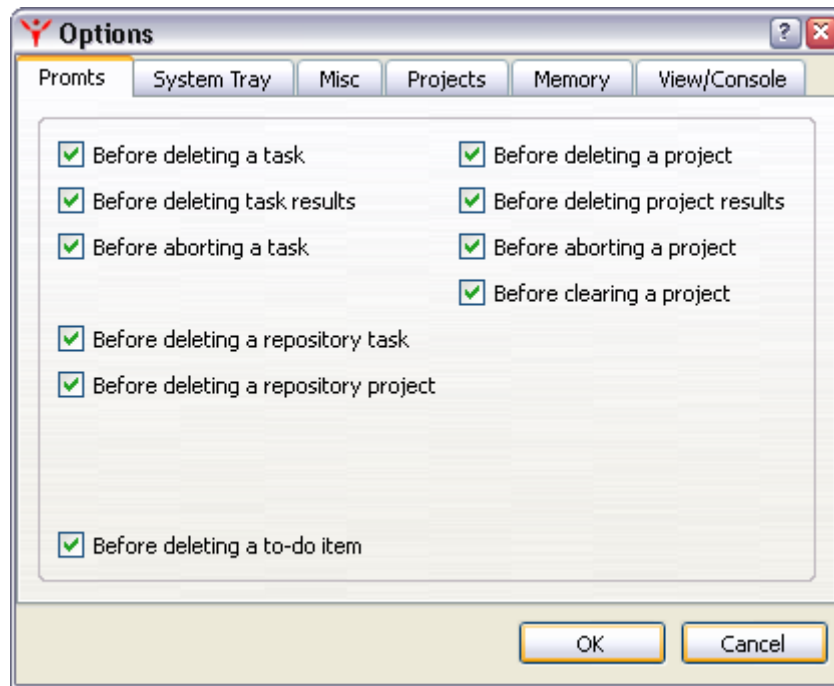


Options

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:

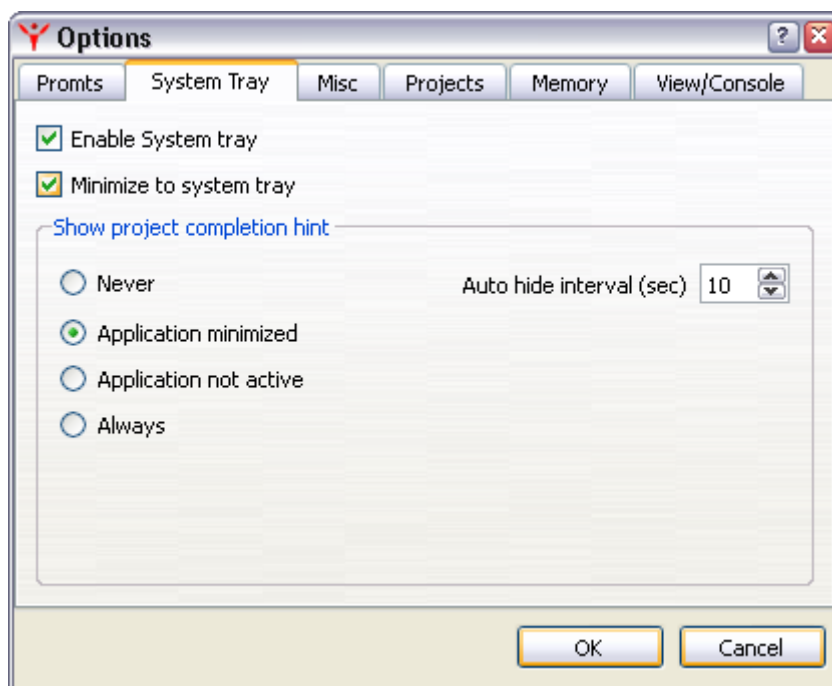
- **Before deleting a task**
- **Before deleting task results**
- **Before aborting a task**

- **Before deleting a repository task**
- **Before deleting a repository project**

- **Before deleting a project**
- **Before deleting project results**
- **Before aborting a project**
- **Before cleaning a project**

- **Before deleting a 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

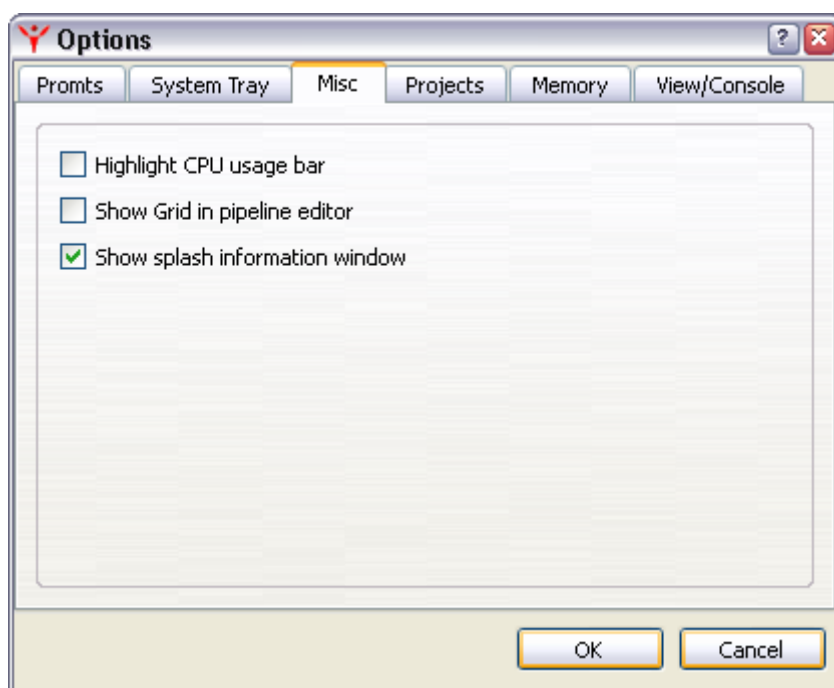
Auto hide interval (sec) - Project completion message disappears after specified time.

Misc tab

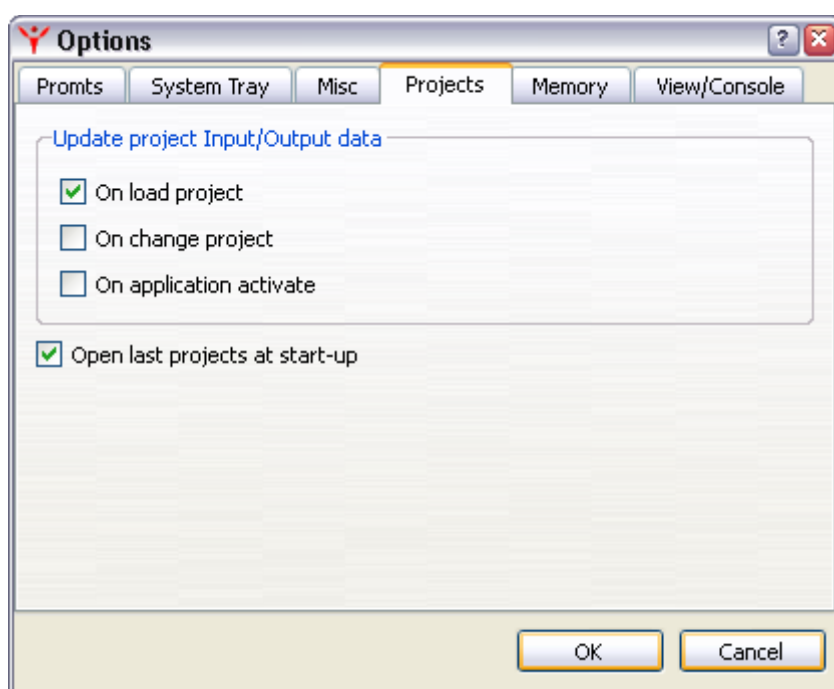
Highlight CPU usage bar - check to display percentage of CPU usage in graphical form and as a number. If unchecked, only a percentage number is displayed.

Show Grid in pipeline editor - check to show gridlines in pipeline editor.

Show splat information window - check to show splash window on a single project open/close.



Projects tab



Contains Project settings.

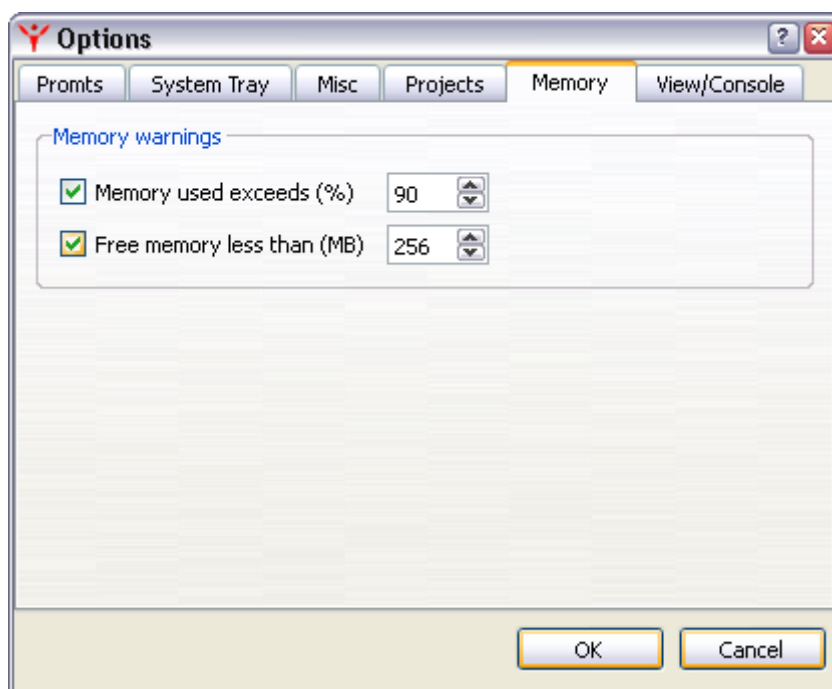
Open last projects at start-up - check to make MolQuest open at startup all projects that were open at the end of last session.

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 Sheet](#) and/or [Input Files Sheet](#).

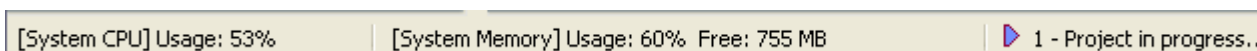
- **On load project** - files are checked when a project is loaded.
- **On change project** - - when projects are switched in [Manager Tab](#).
- **On application activate** - every time MolQuest becomes current application.

Memory tab



Settings of monitoring system memory.

Memory used exceeding - if checked, displays the warning on a [Status bar](#), if percent of memory used exceeds preset percentage threshold.



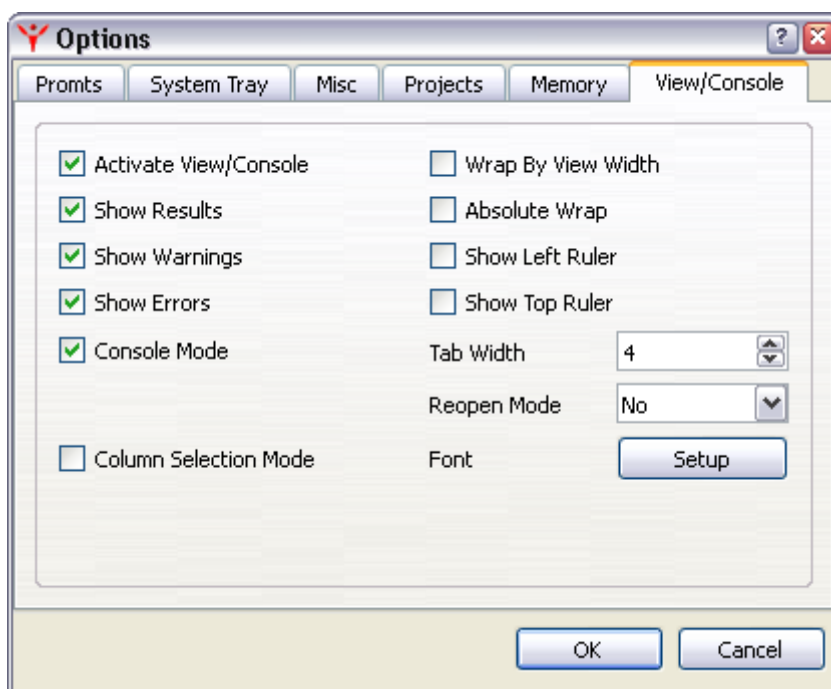
Free memory less than - if checked, displays the warning on a [Status bar](#), if free memory falls below preset threshold in MB.

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 refreshed; Auto - automatically refreshed; Message - when file is changed, asks user whether to refresh.

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;
- [Options](#) - sets up command line options.

Properties Results

01 Input; 01 Output; 05 Option

General In Slots Out Slots Task Extras

System

Task Name Standard Template

ID 19

Program Standard Template

exe

Exe File D:\test\test.exe

Start Detached no

Quote Type GCC, ...

Run exe destination Auto

☒ Debug Log File → File

Name debug.log.txt

! Input

☒ 01.Option

☒ ! 01.Input ← File

! Output

☒ 01.Option

☒ ! 01.Output → File

☒ STDOUT.Option

☒ ! STDOUT.Outp → File

☒ STDERR.Option

☐ STDERR.Output File

! Options

☒ 01.Option

☒ ! 01.Value

☒ ! String

☐ Integer

☐ Real

☐ Char

System section

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

exe section

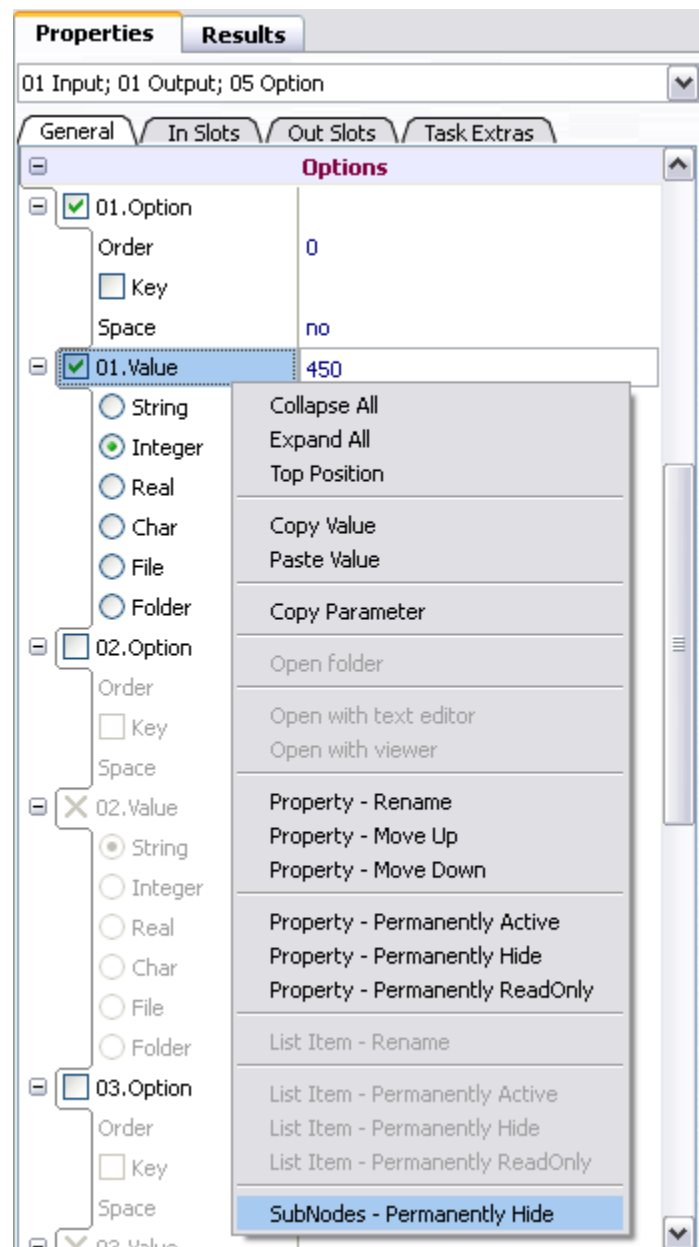
- **Exe File** - path to application executable file.
- **Quote Type** - rules for command line quoting (depends on compiler). It is necessary to specify if properties can contain nonstandard or punctuation characters.
- **Run exe destination** - work directory of application executable file. There are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

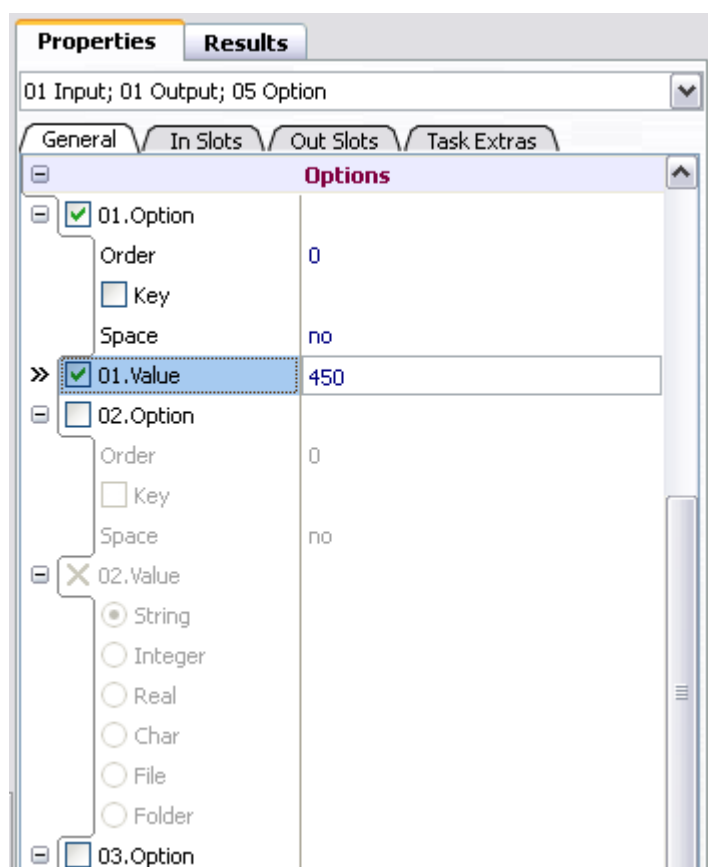
As for MolQuest's own tasks, "Input files" can be single or multiple files and can be specified by user or taken from a pipeline, and output files can be sent to another task via pipeline.

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

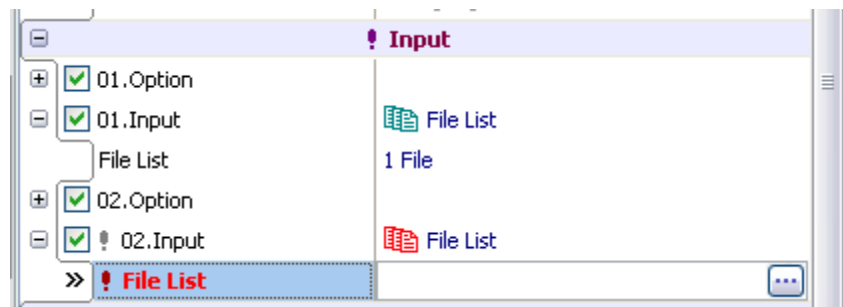
To define program input, two subsections: XX.Option and XX.Input shall be filled.


01 Option - describes the way to specify input file name in command line:

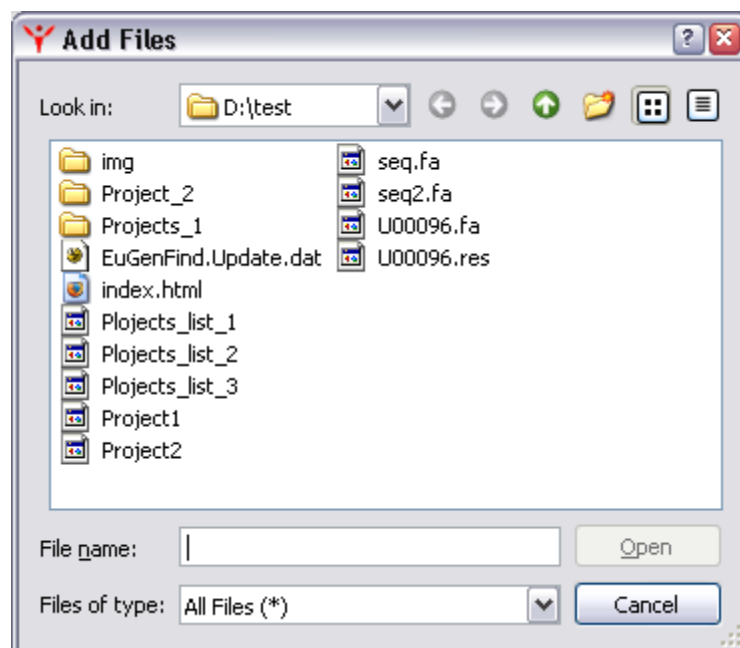
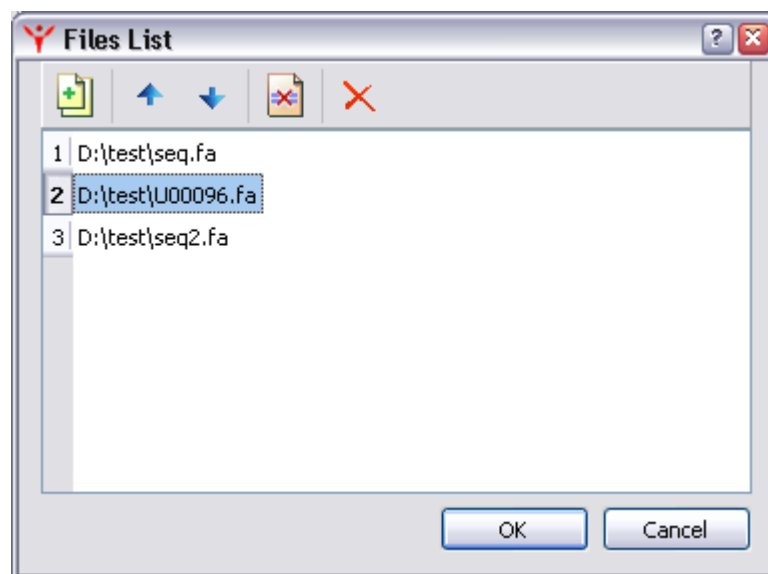
- **Order** - position number of this option in command line. By default, 0.
- **Key** - prefix for current option.
- **Space** - "no" means no space between prefix and value, otherwise - "yes".

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 [Results Tab](#). Icon  indicates that file list is empty, while  means that it is not.








In **File List** dialog (see picture below), pressing  button opens standard Add File window, which is used to add files to a list.

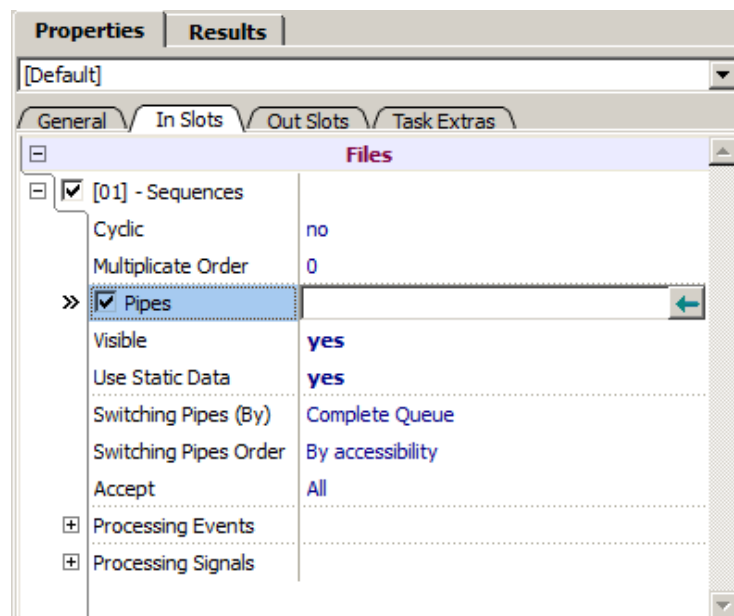


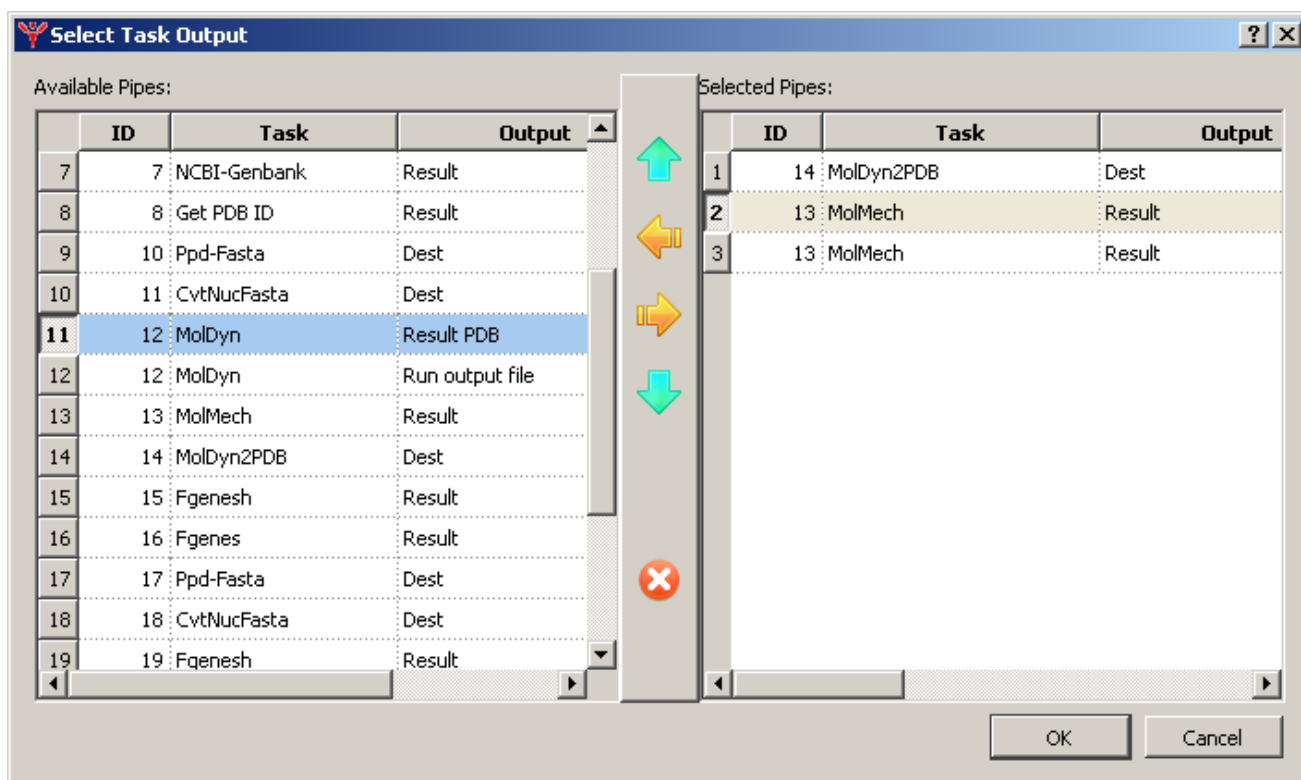
Order of files in a list can be changed by using  and  buttons.

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. Correct 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 the  - that link is not defined or incorrect.

To choose the link for input data, use  button (Placed on [In Slots page](#)), which displays "[Select Task Output](#)" dialog with list of outputs of task within current project. Moving outputs between "Available pipes" and "Selected pipes" lists is performing by mouse double-click.







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  icon means that output means that output data destination is correct, the  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  icon means that output means that output data destination is correct, the  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  icon means that output means that output data destination is correct, the  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.