

# MacVector<sup>®</sup> 8.1

for Mac OS X

## System Requirements

MacVector runs on any PowerPC Macintosh and Mac OS compatible system that runs Mac OS 9.0 or later, including Mac OS X up to and including Mac OS X 10.4. We recommend the use of OS X version 10.1 or higher as this solves certain problems with USB hardware copy protection devices. Memory requirements depend on your system software and virtual memory allocation. Under Mac OS 9.0, 9.1 or 9.2, MacVector requires a minimum partition of 5000 KB; the suggested partition is 8000 KB if virtual memory is on. This may have to be increased if you are working with many large sequences. Mac OS X does not require a minimum memory partition to be assigned.

## Changes for MacVector 8.1

### NCBI BLAST

The NCBI BLAST code has been completely rewritten to take advantage of the newer “Qblast” API. This means that all connectivity takes place using standard web-style http communications. In practice, this means that MacVector is now far more firewall friendly – previous versions of MacVector frequently required ports to be opened in the firewall for blast to work correctly – this should no longer be necessary.

There is a new “Internet Server Options...” item in the Options menu. You should normally never have to change these settings unless your system administrator has replicated an NCBI Qblast server on your local network.

### Job Manager

In addition to the Blast code changes, MacVector now has a Job Manager that is accessible from the Windows menu. Blast jobs can now run in the background so that you can continue to work with MacVector while Blast jobs are in progress. You can also submit additional blast jobs without waiting for existing jobs to complete.

You can monitor the status of jobs and stop them at any time from the Job Manager Window. If a job completes while you are working in a different area of MacVector, or in a different application, you will be notified by a bouncing icon in the dock (OS X only).

## **Miscellaneous Changes and Bug Fixes**

Subsequence search map results now account for the length of the subsequence and the strand of the match. This means that you can now assign other graphic types to the results (e.g. hollow arrows or rectangles) and get a much clearer picture of the location of matches on your sequence. The default appearance of subsequence results has been changed to an open arrow.

Edits made in the Sequence Confirmation editor now do not split features. This cleans up the feature list and prevents the accumulation of multiple [split] features.

Deletions at the beginning and ends of sequences in the Sequence Confirmation editor now physically delete the residues, rather than replacing them with gaps.

Using the delete key in the Sequence Confirmation editor now correctly positions the cursor after the deletion is made.

Features passed in to the sequence confirmation editor no longer switch strands when you save the assembly.

You can now undo paste events in the Map window directly from that window (previously, you had to switch to the Editor window).

When pasting restriction fragments into a Map window, the Edit->Paste menu now changes text to read "Flip and Paste" if you hold down the option key. This lets you paste a fragment in the opposite orientation.

When pasting a fragment in the opposite orientation, the clipboard copy of the sequence is no longer left in a reverse-complemented state.

When creating new features, you can click in the feature type list box and press a key to move alphabetically to the first feature starting with that letter. In addition, the dialog remembers the last type of feature you were working with.

Files containing multiple sequences can now be opened as single sequences even if they do not have a valid OS 9 -style file type.

FastA sequence files are now correctly imported as single- or multiple- sequence files with no added characters.

## **Changes for MacVector 8.0.2**

### **Graphical Interactivity Improvements**

You can now click on graphical features in the map views to select that feature or result and the selection is propagated to all open windows belonging to that sequence. For example, clicking on a box representing an open reading frame in the map view will select that box and the region of the open reading frame will become selected in the parental sequence editor. If you have the feature list window open, the feature will be selected there too. Similarly, the feature will also be selected in the floating feature palette and in any other open map windows (e.g. restriction enzyme results) belonging to that sequence.

You can also select features by clicking in the feature list window, by clicking on an item in the floating feature palette, or by selecting a feature in the “range” popup menu at the right hand end of the Editor window toolbar.

Double-clicking on a feature in a map window opens up the feature appearance editor dialog so that you can change the colors, fonts and location of the feature on the map. Double-clicking on a feature in the feature list window now opens up the feature editor where you can change the coordinates, qualifiers and type of the feature.

Clicking on results in the map views is also supported (Restriction Enzymes were supported in 8.0). The selections propagate appropriately to all open windows. However, double-clicking on a result item does not open the feature appearance editor. In addition, ORF results are not selectable in this release. You can hold down the <shift> key to select two or more features and/or results – in this case the region between the start of the first item and the end of the last item will be selected in the editor. As in 8.0, you can paste a restriction enzyme fragment copied from another map view and MacVector will ensure the sticky ends are compatible before inserting the new DNA fragment.

### **Sequence Confirmation**

You can now assemble just a subset of the trace files in a sequence confirmation editor window. Simply select the sequences to be assembled by clicking on their titles (hold down the <shift> key to select more than one sequence) and selecting the calculate button on the toolbar.

## Bug Fixes

More cosmetic glitches and refresh problems in the Sequence confirmation editor have been resolved.

Sequences downloaded from Entrez direct to disk no longer have ~100 gaps inserted at the beginning of the sequence.

A bug where the Restriction Enzyme graphical map view would not display unless a second result window was also requested has been resolved.

Result window ordering has been refined yet again.

Font changes and line-length changes from the Format Annotated Display options dialog are now correctly propagated to all open windows.

The MSA consensus sequence visibility now correctly honors the setting in the MSA Preferences Consensus tab.

Copy/Pasting from the Sequence Confirmation consensus sequence to the reference sequence now correctly handles the case where the consensus sequence is blank. If you want to “save” the consensus sequence, double click on it to select the entire sequence, choose Copy from the Edit menu, position the cursor on the first residue of the reference line and choose Paste. This will overwrite the reference wherever there is a valid non-blank consensus residue. You can then choose “Save As...” from the File menu to save the reference sequence as a MacVector format file.

The left margin in annotated sequence text displays has been reduced.

The “reverse Complement” button in the Test PCR Primer Pairs dialog now correctly complements the central residue.

Minimized windows in the OS X dock are now correctly handled by all MacVector windowing routines.

The installer now correctly assigns read/write status to all restriction enzyme files so that they can be used from user accounts other than the administrator. Note that if you use an updater to upgrade to 8.0.2, the permissions of the files will not be changed.

A bug where Entrez sequences could not always be downloaded when multiple users are logged into a single computer has been resolved.

Translations in the annotated sequence display are now correctly in frame when a range is selected.

## **Changes for MacVector 8.0.1**

### **Pairwise Alignment Matrix Window**

The Multiple Sequence Alignment Views dialog now has an Identity/Similarity Matrix display option. Selecting this opens a window containing a matrix of the identity and similarity scores of each pairwise combination of sequences in the alignment. The similarity scores are calculated based on the currently selected color group. The matrix uses tab characters to separate the individual fields, so you can select/copy the entire table and paste into Microsoft Excel for further analysis.

### **Sequence Confirmation Enhancements**

The Sequence Confirmation functionality introduced in MacVector 8.0 has had a few improvements;

- The assembly algorithm has been tuned to handle gaps more effectively.
- Added sequences are now automatically ordered alphabetically.
- Individual sample sequences can now be reordered by selecting the sequence title and dragging into place.
- Spaces are now handled correctly when copy/pasting from the consensus sequence.

### **Miscellaneous Changes**

Additional analysis dialogs have been cleaned up so that they refresh more consistently and have true group boxes.

Result windows now have more consistent ordering. They are now brought to the front when an analysis is repeated but remain as ordered when selections are made.

### **Bug Fixes**

A number of display glitches under OS X 10.4 ("Tiger") have been fixed. In particular, refresh problems in the sequence confirmation window have been resolved.

A "reverse and complement" bug in the sequence confirmation window has been fixed – this would cause the central residue of a sample trace to not be complemented when aligned in the minus strand orientation.

The GenBank file reading code has been revised to address the following issues; (1) All annotations are now correctly imported from GenBank files, (2) The entire LOCUS line is now retained, rather than just the sequence name, (3) MacVector can now determine the sequence type of partially specified GenBank files without prompting.

The color selection popup palettes and pattern selection popup palettes now display correctly when display colors is set to less than millions.

An annoying beep on startup has been eliminated.

Some glitches in the stickiness of the multiple sequence alignment consensus visibility parameter have been resolved. This is now entirely controlled by the setting in the "Consensus" tab of the preferences dialog.

## **Changes for MacVector 8.0**

### **BSML File Support**

MacVector 8.0 can read and write BSML sequence files. This is the XML file format used by DS Gene and a number of other sequence analysis/manipulation programs. Like all XML files, BSML files can be edited with a simple text editor if required. See <http://www.bsml.org/> for details of the file format. Note that MacVector can only read and write single sequence BSML files. Alignment files, and other DS Gene files such as Dot Plot and Entrez result files cannot be read by MacVector. In addition, the DS Gene BSML file format does not support the full range of feature appearance information used by MacVector. Thus, certain custom format appearance information may not be saved into the file.

To load a BSML file, simply ensure you have "show all files"

selected in the file open dialog, and select the file you wish to open. The file type and extension are not important - MacVector will scan any unknown file to see if it is in BSML format, regardless of designated type of extension.

To save a sequence in BSML format, choose "Save As..." from the file menu and choose "BSML Text File" in the "Format:" popup menu. MacVector will add ".bsml" to the file name by default. However, the file is saved in TEXT format that can be read by any standard text editor, including TextEdit and Microsoft Word.

## **Sequence Confirmation**

This is a major new analysis module in MacVector 8.0. It is designed to help users assemble one or more sequence files (typically trace chromatograms) against a reference sequence and quickly identify mismatches between the sample files and the reference. There are a number of features that simplify the identification and correction of mismatches;

- A toolbar button switches the display so that all matches to the reference are shown as dots – this significantly clarifies the display so that users can easily identify mismatches.
- A “Find Mismatch” utility lets users quickly look for the next mismatch between alignments and reference.
- Clicking on the reference sequence immediately aligns all of the overlapping trace files so that users can evaluate if a mismatch is due to missed calls in the chromatogram files or due to an actual change in the residues of the sample clone.
- The reference can be saved at any time as a MacVector single sequence file, complete with all original annotations.
- Any MacVector nucleic acid analysis can be performed on the reference sequence without needing to save the alignment. This lets users quickly identify e.g. open reading frames or new restriction enzyme sites resulting from changes in the sequence.

There is an extensive tutorial in the Documentation folder that describes this new functionality in more detail.

## **Click Cloning**

Copy/Pasting restriction enzyme fragments into the Graphics window is now "sticky-end aware". If ends of the copied fragment do not match the ends of the selected site(s) in the target molecule, an alert is displayed to the user. Fragments will be automatically "flipped" if they can only fit in the opposite orientation. You can also force a flip by holding down the <option> key while selecting "Paste" in the edit menu. Note that sticky end information is only copied to the clipboard from selections in the Restriction Enzyme Map Result window. Copying from the standard editor window generates undefined ends that can be pasted into any site.

## **Bug Fixes/Other Enhancements**

Some of the more important noticeable changes in this version are;

In the Map window, if you set the feature display position to "above or below", MacVector now uses strand information to help determine where to place features on the map. Where possible, "plus" strand features are placed above the sequence line (outside for circular graphics) and "minus" strand features are placed below.

The NCBI toolkit has been updated to the latest version. Although no new features have been added, the update should provide more stability, better firewall support and forward compatibility with future changes at the NCBI Internet site.

There have been numerous changes to the Entrez retrieval code to fix bugs where certain annotations were not correctly downloaded from the NCBI server.

Many dialogs have been cleaned up to use true group boxes and to have a clearer layout.

There is a new "Reverse and Complement" button in the PCR Primer "Test" dialog that lets you easily flip the second primer.

The ClustalW result picture window no longer erroneously outlines gaps as valid matches.

MacVector now assigns the LOCUS ID as the default name for sequences downloaded from Entrez.

Analysis result windows now come to the front when an analysis is repeated.

## **Troubleshooting**



## **In General**

Where possible, under OS 9, restart your Macintosh with system extensions off and try repeating your actions. (To turn system extensions off, hold down the Shift key while starting up until you see the message “Extensions Disabled” displayed.) It may not always be possible to do this, particularly if you need to access network services that require certain extensions to operate, but minimizing the number of non-Apple extensions that are loaded in your system can help to isolate conflicts.

This is less of a problem under OS X. We highly recommend that you upgrade to OS X if at all possible. MacVector 8.0 is likely to be the last major version of MacVector that supports OS 9.

## **BLAST and Entrez services**

If BLAST or *Entrez* searches fail, first check that your Internet connection is working properly by testing whether you can access Internet Web sites using your Web browser. If your Web browser does work correctly but BLAST and *Entrez* searches do not work, it is possible that your site has an Internet firewall installed for security, and that this is preventing MacVector's Internet connection from working. Full information on configuring NCBI clients and firewalls is in the file NCBI Firewall Info in the Documentation folder.

If you have previously performed successful BLAST or Entrez searches with MacVector 6.5.3 or higher, and you are therefore sure that there is not a firewall problem, please bear in mind that the success of these services relies on the availability of the NCBI Internet servers. If your network, or the Internet connection your network uses, or the NCBI's Internet connection, or their server machine(s) have any problems, you may be temporarily unable to perform BLAST or Entrez searches. Also, the time of day can affect the speed of your search, depending on how much other data is “on the Internet” at the time. Because of the transient nature of the above problems, you will often find that if you try your search again at a later time - either an hour later or the next morning - it works.

## **Support information**

For assistance with MacVector, please contact your local Accelrys office. From April 1<sup>st</sup> 2005 you will need a current MacVector maintenance contract to be eligible for technical support other than for basic installation problems. New sales of MacVector include 12

months of support that also entitles you to any upgrades to MacVector released during the maintenance period.

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When contacting Customer Support with a technical problem, please be prepared to give your product serial number as well as a detailed description of your problem and any error messages you encounter. Visit the MacVector Web site for details of any available updates, and any relevant information that could not be added to these release notes in time for publication:

<http://www.accelrys.com/products/macvector/index.html>