# MacBeads v.1.01 - Users' Manual

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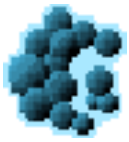




## Contents

# Introduction

This manual describes briefly the use of MacBeads 1.01. Please read it before pitching in - there are some things which might otherwise cause you some problems.

MacBeads is a program which enables the user to build 3D spatial models composed of spherical beads. When a satisfactory model has been built, then a text file output can be requested which gives the size, 3D coordinates and number of all the beads selected. Relevant details of the total model (name, mass, partial specific volume) can also be stored in the same file in a 'tailpiece' Alternatively, a model can be input from a suitably formatted text file produced from crystallographic co-ordinates by a program such as AtoB (Olwyn Byron). MacBEADS models can also be plotted and manipulated in 3D space (APPENDIX)

**Basic Philosophy of MacBeads**

MacBeads has two primary uses:

(i) given some sort of preliminary, low resolution model of a macromolecular structure, MacBeads enables that structure to be mapped out in space as an assembly of spherical beads. The low resolution model might, for example, derive from EM or LAXS data. Programs such as HYDRO (Garcia de la Torre) can evaluate hydrodynamic parameters (frictional coefficient, diffusion & sedimentation coefficients, intrinsic viscosity) from such bead models. They require that the details of the size and (x,y,z) locations of each bead be specified in a suitably formatted text file. MacBeads produces text files containing this data for the model which has been built by the user.

(ii) given an existing bead model, for example derived from crystallographic coordinates, MacBeads provides a convenient way of 'bending it around' – i.e. making adjustments to relative orientations of major domains, to probe the effect of so doing on hydrodynamic parameters. An example of this can be seen in the work on the flexibility of the myosin head in Bayliss et al (1999).

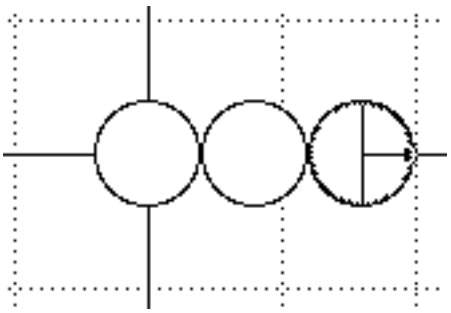
The present Manual concentrates on the first of these uses, as the principles of the use of the program are identical in either case. A familiarity with the normal use of menus etc and with simple graphics operations (e.g. dragging and marqueeing) within the Mac OS is assumed.

# How models are built

## The definition of a bead

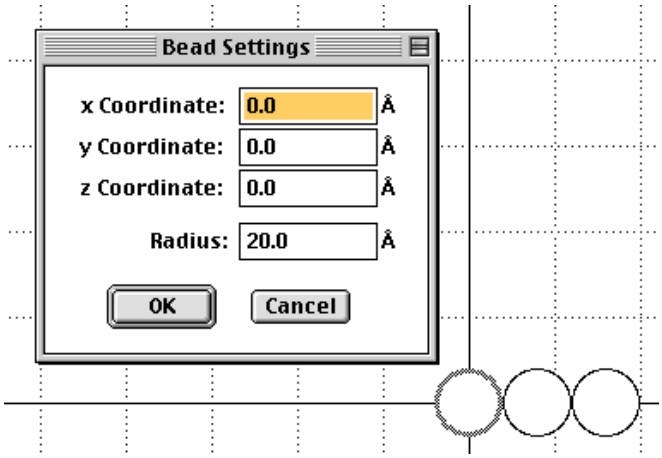
A bead is a single spherical entity of defined radius with its center located at defined (x,y,z) coordinates. Generally the user of MacBeads will have specified the radius such that the molecular mass is defined via an experimentally known or computed partial specific volume (vbar). This is done either from first principles or by making use of a general hydrodynamic utility suite (e.g. **BIOMOLS** from the NCMH). Clearly if n beads are to be used to model a particle (e.g. a protein domain) then the sum of the mass of the n beads should be equal to the known mass of the particle.

Beads are created located and duplicated as needed via the **Bead** Menu (p. 5). Any individual bead is selected by 'clicking' on it, when a 'handle' appears within the bead:



The bead on the right hand end of this row of 3 is the one selected. You can select more than one bead either by 'shift clicking' on the desired beads, *or* by marqueeing the same. You can then **deselect** any given selected bead by 'shift clicking' it. Note: a newly created bead is always in 'selected' mode.

You can OPEN any bead by double-clicking on same (or by selecting it and using **the OPEN BEAD** function, p. 5). The bead is 'greyed' and a dialog box appears:



You can then modify the bead details as required. **Note:** you **must** exit from this dialog box by clicking on either **OK** or **Cancel** or **Close Dialog Boxes** – **not** by clicking back onto any other window ! {if you accidentally do that – re-open the bead and exit properly . . . }

You may also **modify the size property** (radius) of an individually selected bead by simply getting hold of its handle and enlarging or reducing it by dragging.

**The three coordinate planes**

MacBeads display 3 windows which give the view of the assembly of beads which you have created in the 3 coordinate planes (YZ, ZX, XY). You will be asked to specify the (z,y,z) coordinates of each bead which you create. You can select which view you require *either* by use of the **View** Menu (p. 6) *or* by simply clicking on the required window.

**How beads are moved in space**

You do not need to make a decision as to where a newly created bead should be finally located at the time of its creation. You can, for example, create all beads at some reference position, and then *either* **drag** them to the position desired, *or* use the **translate** function available from the **Transform** Menu (p. 6). **Dragging** works fine of course with any given selection of beads – or with your whole model, selected by marqueeing everything.

**Working with built or part-built models**

The ability to select either the whole or a part of a model (by marqueeing or by shift-clicking) means that it is easy to manipulate the orientation of whatever is selected, whilst leaving any unselected regions unchanged. Moreover, the four very useful functions contained in the **Transform** Menu (p. 6) mean that one can opt to work on your model (or a part of it) in **any plane** – not just the 3 principal planes – by simply rotating it in any desired way until the plane to be worked on coincides with a principal plane.

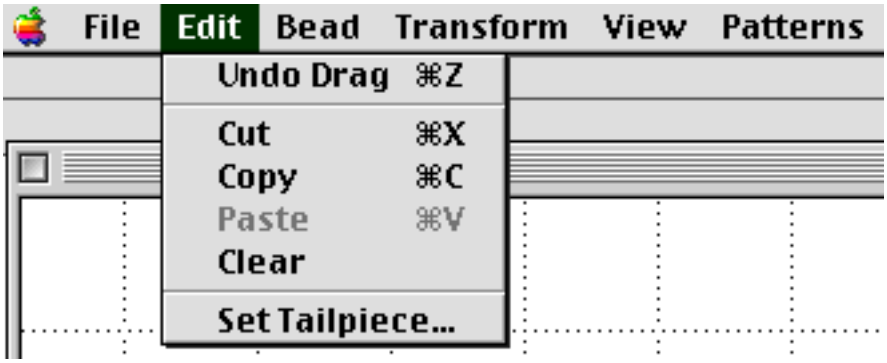
## The use of the Menus in MacBeads

The functionality provided by the various Menu functions are a central, powerful feature of MacBeads. These are described below, in order (L to R) as they appear in the Menu Bar:

**File**

These are standard Apple File Menu functions – but note the **Save as Text** command which enables you to save the output details of your model

**Edit**




This again resembles the standard Apple Menu – except that there is now a **Set Tailpiece** option. You us this to enter the name etc of your model, and the details entered will appear in your final output file.

**Bead**


This Menu enables you to create beads. **New Bead** creates a new bead, with a dialog box enabling you to specify size and location. **Old Bead** creates a new bead identical to the last one created. **Open Bead** is a (little used) alternative to double-clicking. You must have selected a bead (by single clicking) before use of this command.

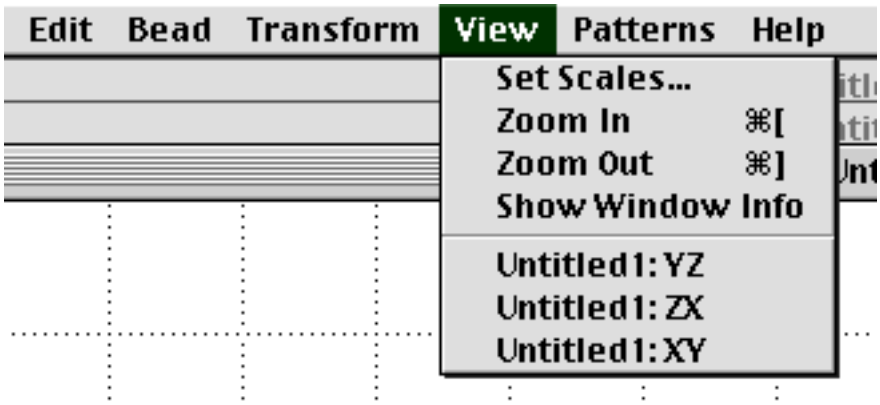
The **Close All Dialogs** command is here (well, it had to go somewhere).

All these commands have keyboard equivalents.

**Transform**


These four commands, with the relevant dialog boxes, provide a comprehensive set of tools for manipulation of models. They do exactly what their names say they do.

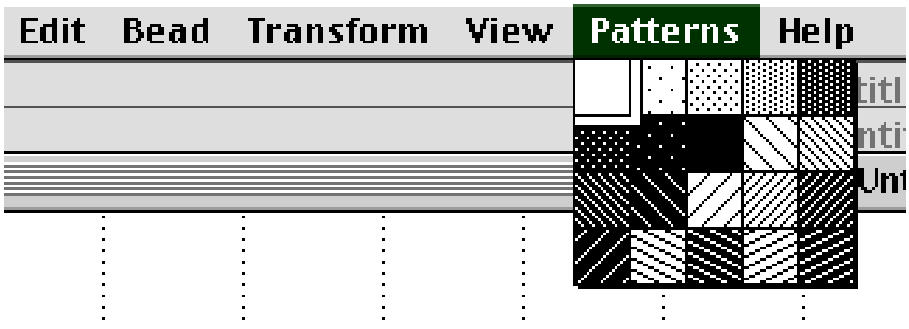
**View**




The **Set Scales** option allows you to set the relationship between the bead dimensions (in Å) and the scale within the document, as printed at 100%. The **Zoom** options are self-defining (and have keyboard alternatives). The **Show Window Info** command is so useful to remind you as to which axis goes in which direction that it is generally advantageous to keep it 'switched on' all the time (standard convention – it's 'on' when it's ticked).

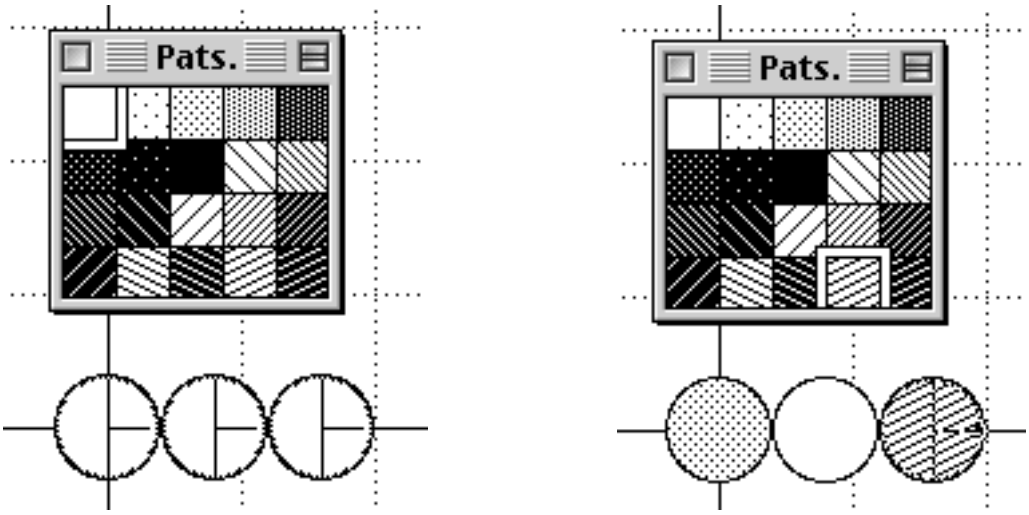
The use of the three commands to view the individual principal planes is useful to avoid 'clicking around' on the screen.

**Patterns**



This Menu enables you to allocate a distinctive pattern to any bead or set of beads. Simply select the beads to which you wish to allocate a pattern, and then select the desired pattern from this Menu.

You can, if you wish, make this palette into a 'floating palette'. Simply 'grab' the palette by one of its patterns (in the example shown above, the top left pattern has been 'grabbed') and drag it to where you would like it to be:




In the examples shown above, all beads have been selected and filled in with pattern white (LEFT) whilst on the RIGHT we seen the result of successively selecting two of the beads and giving them an individual pattern.

This option is useful for identifying individual parts (e.g. those denoting protein domains) within a total structure.

**Help**

This is the standard Apple Balloon Help command – it does not contain any MacBeads specific options.

# Output

Models may be saved using the **File** Menu in the normal manner. The ultimate output for further interpretation is obtained using the **Save as Text** command from the File Menu. This produces a text file which can be opened and if need be edited in any application (MS-WORD, whatever) capable of handling text.

You can also OPEN the text output within EXCEL, specifying that it is **comma delimited** (see the technical notes below). This is obviously useful for sundry further manipulations.

The output (in MS-WORD) looks like this

```
'trial'
  22
   1,   153.2,    21.6,     0.0,    10.0
   2,   174.7,    15.1,     0.0,    12.5
   3,   201.4,    10.4,     0.0,    15.0
   4,   225.6,    15.5,     0.0,    10.0
   5,   146.2,    40.9,     0.0,    10.0
   6,   158.5,    59.7,     0.0,    12.5
   7,   175.9,    80.4,     0.0,    15.0
   8,   197.7,    92.1,     0.0,    10.0
   9,   128.0,    23.6,     0.0,    15.0
  10,    99.8,    13.3,     0.0,    15.0
  11,    43.4,    -7.2,     0.0,    15.0
  12,    71.6,     3.1,     0.0,    15.0
  13,   -69.3,   -48.2,     0.0,    15.0
  14,   -41.2,   -38.0,     0.0,    15.0
  15,   -13.0,   -27.7,     0.0,    15.0
  16,    15.2,   -17.5,     0.0,    15.0
  17,  -238.5,  -109.7,     0.0,    15.0
  18,  -210.3,   -99.5,     0.0,    15.0
  19,   -97.5,   -58.4,     0.0,    15.0
  20,  -125.7,   -68.7,     0.0,    15.0
  21,  -182.1,   -89.2,     0.0,    15.0
  22,  -153.9,   -79.0,     0.0,    15.0
<y/n>
<y/n>
'<name>'
<y/n>
<molecular weight>
<partial specific volume>
1.0e-08
```

The file starts with the name of the model and the number of beads, and then for each beads lists the 3 coordinates followed by the radius. The 'tailpiece' information is appended.

**Getting started**

A simple demonstration file is attached, as well as a copy of the myosin S1 model. Have a go with these, as well as trying to set up a basic model from scratch.

## Some additional technical details

These are some programmer's notes which take some of the issues raised above a little further, and may be helpful to users.

### Output Format

MacBeads creates a text file output suitable for submission to a particular computer package. It should be only a small job to modify these files for other end-software..

The most likely problem is the end-of-line character. The Macintosh convention is to terminate lines with a return character (ASCII 13) and this is the convention followed. Another commonly used convention (used by UNIX and MS-DOS amongst others) is to terminate lines with a linefeed character (ASCII 10). You can use a search-and-replace facility like Word's to exchange things round. You just may need to modify the separator between items on a single line.

### Shift-Clicking:

Shift-clicking an unselected bead selects it without otherwise changing the current selection. Shift-clicking a selected bead deselects it without otherwise changing the current selection. Shift-clicking an open bead has no effect.

### Double-Clicking

Double-clicking an unselected bead clears the current selection and then opens the bead. Double-clicking a selected bead opens the **entire** selection, not just the bead. Double-clicking an already open bead brings the bead's associated dialog to the front.

### Marqueeing

Marqueeing clears the current selection and then selects all beads **completely** enclosed by the marquee rectangle. Open beads are unaffected.

### Shift-Marqueeing

Shift-marqueeing selects all unselected beads completely enclosed by the marquee rectangle and deselects all selected beads completely enclosed by the marquee rectangle. The current selection is otherwise unaffected. Open beads are unaffected.

**Dragging (or Shift-Dragging)**

This moves the **entire** selection around. The movement is constrained to a plane determined by the currently active window.

**File Menu**

Most of the commands in this menu work as you would expect. The only things to note are:

The **Open** command allows you to open both text files and files in the native MacBeads format . Naturally although you can attempt to open any text file, only those that contain the correct information will open successfully. Text files created by MacBeads (via the 'Save As Text' command) will open correctly but this may not be the case for other TRV files.

**Edit Menu**

Again these commands mostly work as you would expect. The exceptions are:

Having cut or copied some beads they can be pasted back into the MacBeads document, into any other MacBeads document or into a document of any other application that can work with the **PICT** format. If you paste into a MacBeads document, you are prompted for the location in three dimensions at which you want the new beads pasted. Only one paste dialog can be open at any time. If you paste into any other document all you get is a two dimensional image of the beads (editable in Appleworks PT etc.), the projection being determined by the active window when the beads were Cut/Copied.

The 'Set Tailpiece' command allows you to enter a string that will be appended to all output text files. The string can include return characters. Clicking on OK in the dialog sets the tailpiece of the active document. Clicking on Set Default sets the tailpiece for all new documents you may subsequently create.

**Bead Menu**

The 'Open Bead' command creates a modeless dialog showing the coordinates and radius of the bead that you open. These values may be edited. If the dialog is closed via 'OK' the bead's settings are changed to the new value. If the dialog is cancelled the bead's settings are unchanged.

MacBeads makes extensive use of modeless dialogs, so a careless user might lose track of open dialogs. The 'Close All Dialogs' is a quick way of cleaning up by effectively cancelling all currently open dialogs.

## Transform Menu

This menu provides commands that apply geometric transformations to the current selection. All dialogs are modeless. Opening a new transformation dialog when one is already open cancels the older one. The transformations are applied to the beads that are selected **when the dialog is confirmed**. Most transformations (Reflect, Rotate and sometimes Resize) take place with reference to some point. This point is always taken to be the centre of the selection. Centre here means the geometric centre of the cuboid that exactly encloses the selection. The centre of mass would be nicer but I do not think the CPU time needed to calculate it would be justified.

Reflect reflects the selection in the xy, yz or zx plane, as specified by the user.

Resize allows the current selection to be transformed in three different ways. Every bead can have its radius changed by a fixed amount. Every bead can have its radius changed by some proportion. A dilatation can be applied to the selection as a whole, effectively expanding or shrinking it.

Rotate rotates the selection by a specified angle about the x, y or z axis.

Translate translates the selection by a specified vector.

## Compatibility

Every file on the Macintosh has a 'signature'. You do not need to worry about the technicalities, you just need to know that for the Finder to work correctly signatures must be unique. Normally before releasing software onto an unsuspecting world one is supposed to register signatures with Apple to ensure their uniqueness. Naturally I haven't done this so there is a (very small) chance that the signatures I have used will already be used by some other file on your hard disc. If this happens the Finder will get confused but program should still function correctly in most respects.

## Reference

R I Bayliss, N Errington, O Byron, A Svensson & A J Rowe (1999) "A conformational spectrum analysis of the morphological states of myosin S1 in the presence of effectors" Progr Colloid Polym Sci **113** 158-163

## Contacts

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# APPENDIX

## The use of pro Fit to display 3D bead models generated by MacBEADS 1.0.1

MacBEADS generates bead models using three principal planes for their construction and visualisation. The powerful **transform** commands enable any translational or rotational operation to be performed on either the whole model or on any selected part of the same. However, it is true that for many purposes it would be advantageous to be able to 'see' the bead models in a simulated 3-dimensional space, with a facility for mouse-driven manipulation of the model - as is routine in programs for display of crystallographic structures.

A simple approach which we have developed is to use the excellent facilities for 3D graphing provided in the recent issues of **pro Fit** (QuantumSoft, Zürich - see p.17) - a widely used and respected curve-fitting and graphing package. Text files (.txt) generated by MacBEADS can be opened within pro Fit, and it is then simple to generate rotatable 3-D models using the **pro Fit** module **Plot 3D DataXY**. The models can be rendered artistically using conventional lighting effects, and individual views can be saved and printed. Movie files, in which the model is rotated around a defined axis, can also be generated.

**MacBEADS 1.0.1** and the **pro Fit** module **Plot 3D DataXY** are thus complementary in their usage. The former is the 'construction kit' with the ability to both generate models *de novo* and to modify existing bead models, including those derived from atomic coordinates. The latter provides a way of checking the models generated, and of presenting the models for publication and presentation purposes.

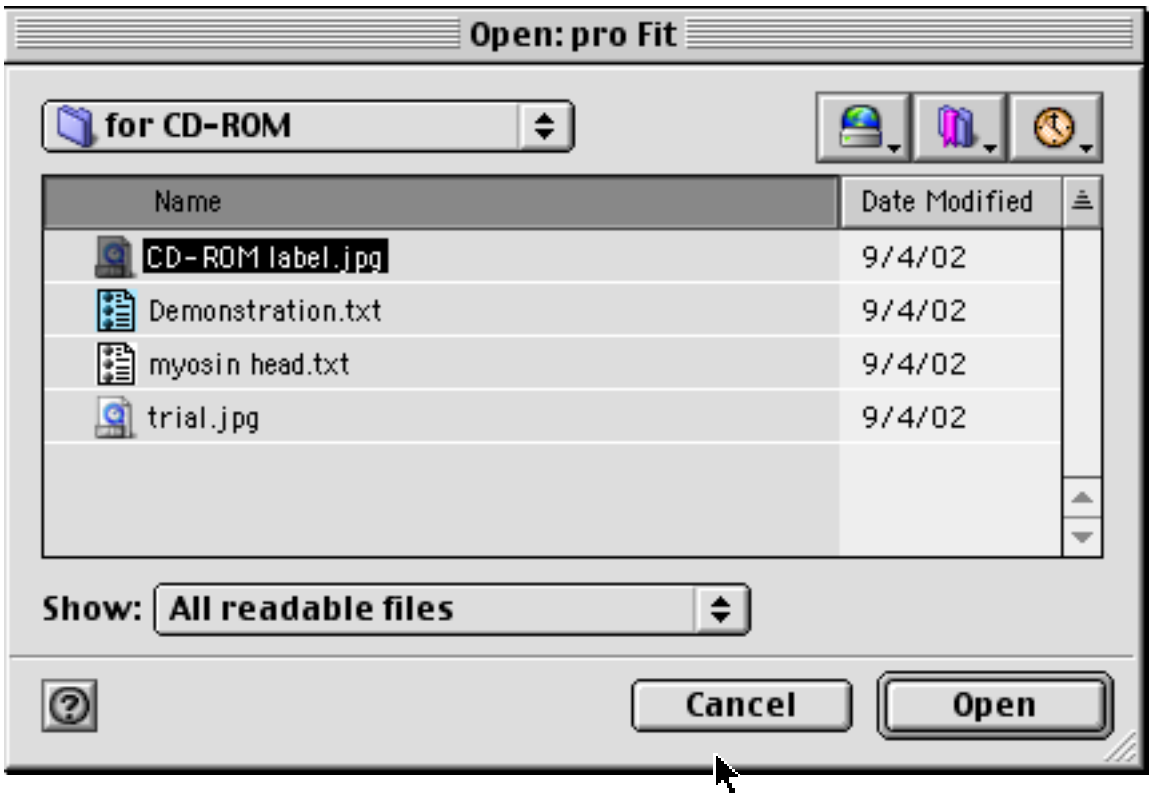
### Hardware and System Requirements for the pro Fit interface

These are more stringent than for MacBEADS. An Apple G3/G4 is needed, running System OS 9.x or OS X (in 'Classic' mode). Pro Fit 5.5 or 5.6 is required, with the appropriate (downloadable) module 3DPlotterGL 1.2 (5.5) or 3DPlotterGL 1.2 (5.6). Note: a download will give you both versions of the module: retain within the **pro Fit Modules** folder only the module version (5.5 or 5.6) which matches your pro Fit software version, as otherwise problems will arise on boot up. Quantum Soft say that only the 5.6 version is fully supported - we have ourselves found that 5.5 works fine, however.

It is sensible to have a reasonable amount of free RAM available when performing 3D operations on large files. Familiarity with the general features of **pro Fit** is assumed.

**How to open a MacBEADS file within pro Fit**

Having launched pro Fit, simply select OPEN from the FILE menu, and select 'all readable files' in the **show** menu in the dialog box:




Only MacBEADS files which have been **saved as text** (.txt files) can be opened. The contents of the MacBEADS .txt file appear in a new pro Fit DATA window.

**Formatting data for use within the 'Plot 3D DataXY' module**

The 'tailpiece' information is contained within the lower rows of columns 1-3, and this prevents the recognition of these columns as pure numerical data. Select all the (X,Y,Z,RADIUS) values, and cut and paste them two (2) columns to the right. Enter the headings (X,Y,Z,RADIUS), as this will facilitate further operations.

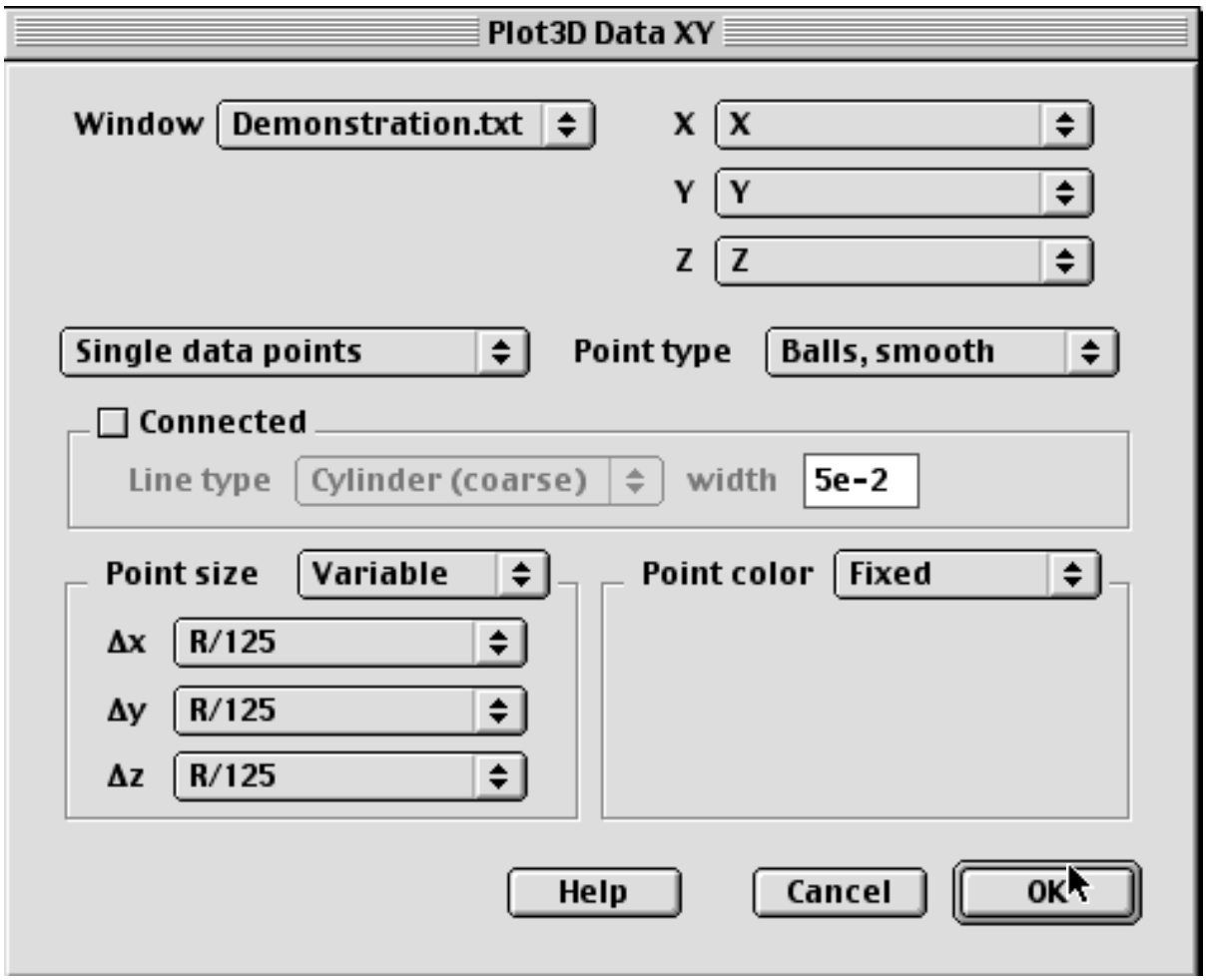
**Bead dimensions**

It is annoying, but although the **'Plot 3D DataXY' module** provides for correct relative sizing of the beads, their absolute size is not in the same units as the principal axes. You need to scale the bead dimensions, and the scaling factor, alas, can vary. Try dividing your bead dimensions (COLUMN RADIUS) by 125 for starters, using the Calculate menu/Transform command to create a new column, which you could label RADIUS/125.

**Doing an initial 3D plot**

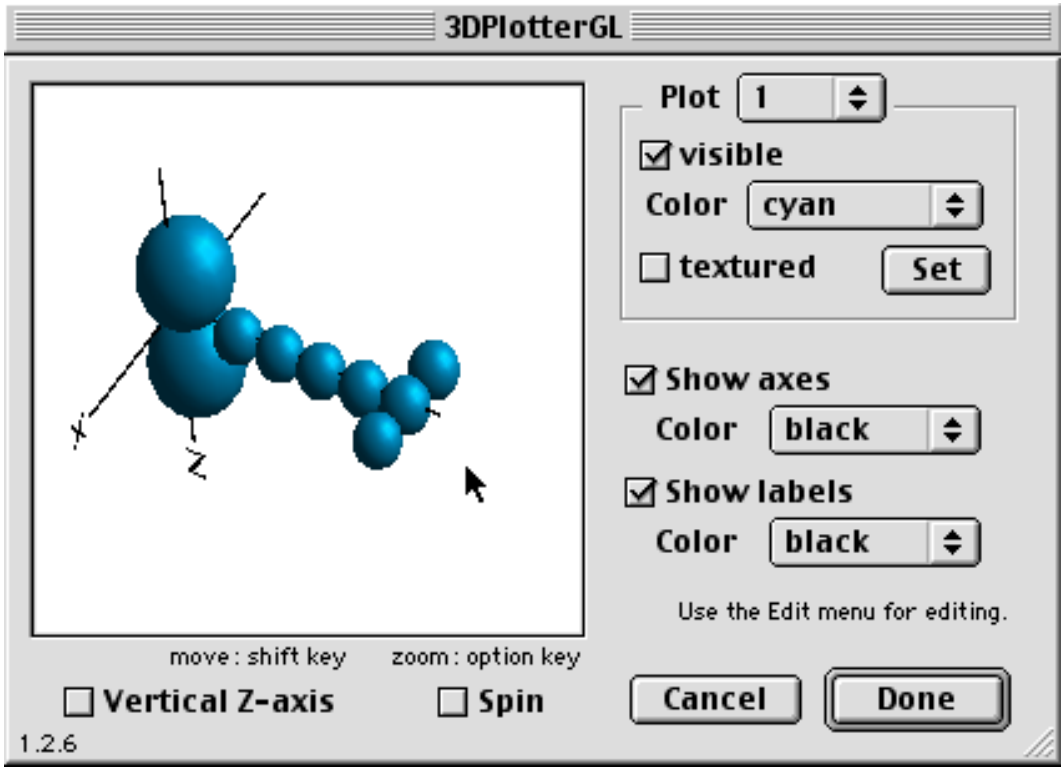
The first time you do it, you will have to use the **LOAD MODULE** command from the **Customize** menu, to select and import the 3DPlotterGL 1.2 (5.x) module. Thereafter it will appear within the **Prog** menu, and is selected and started from there.

Upon starting the module, a dialog box appears on the screen:

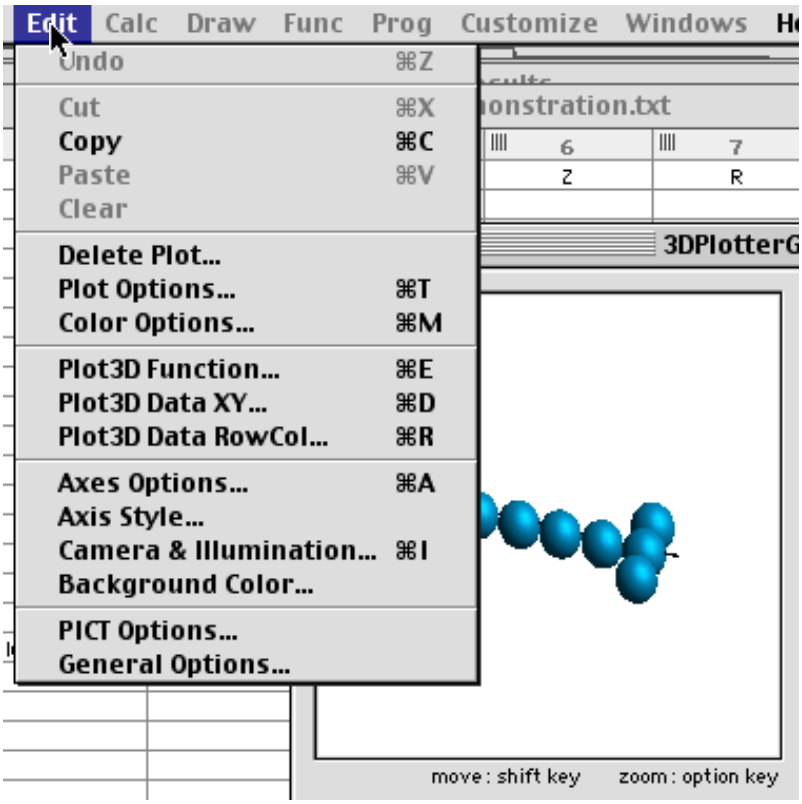



Select your columns for plotting, including R/125 to specify the relative bead dimensions. Other options are recommended to be as shown above. You can try using the variable hue etc options, instead of Fixed Color, but the results are not easy to predict !

Likewise, you can go for the smoothest available point type - but bear in mind that this inevitably uses up memory. Now you can hit the OK button, and a 3D graph appears in a new window. After setting all axes to a common scale (this has to be done manually), the resulting image is as shown:




So - how did we fix those axes ? Well, whilst this window (above) is open, and before we eventually touch the **Done** button, a whole range of manipulations can be effected using the **Edit** menu:



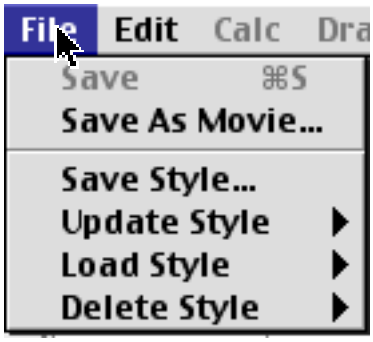
So - its 'Axes Options' that is the command needed to set all axes equal. Sadly, there is no global command for this: you have to inspect the range covered by your data, and then set the range of the three principal axes to be of equal magnitude: e.g. 200 units in all cases, with start point set to encompass the data range.

**Other modifications to the plotting style**

As you can see from the Edit menu, facilities are available to modify your 3D plot in a whole range of ways, as long as the plotting window is open. You can vary the degree of 'polish' on the beads, or their specular reflectivity, among other things. Try them out - or for further details, see the **pro Fit** Manual or Help Screens.

**Saving a 'style'**

Having spent a few moments getting the axes right, and setting other controls (e.g. illumination) to your liking, then you do not want to have to repeat this every time you open your data and plot it. The 'style' of plotting which you have defined is not attached to your document in any way in pro Fit, but you can use the **File** menu to save your settings:




The commands are - hopefully - self-evident in what they do.

**Putting additional plots into the same window**

**Plot 3D DataXY** is recursive - i.e. the module can call itself, as you can see from the **Edit** menu on the previous page. So it is easy, whilst the plotting window is still open (do not press the **Done** button !) to place multiple plots into one 3D window by having your data assorted into sets of (X,Y,Z,RADIUS) columns. Using this facility, different parts of the same model can easily have different colours assigned to them.

**Moving the 3D plot in space**

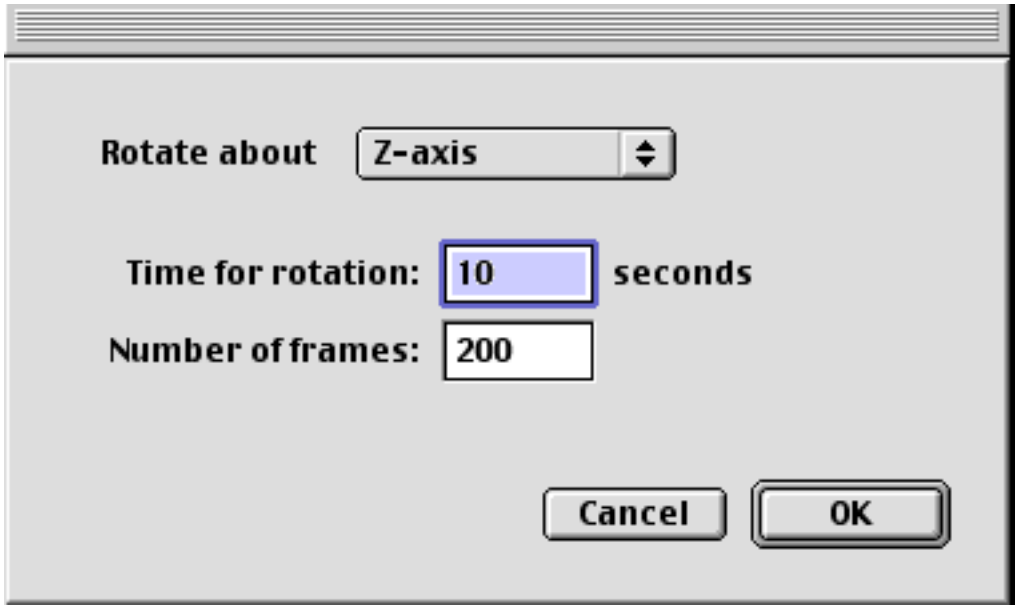
The mouse can be used to rotate, translate or zoom - just follow on-screen commands for the latter two. All you have to do is 'grab' the 3D plot with your mouse !

**Getting a 2D image of your final plot**

After checking the **PICT Options** in the **Edit** menu, hitting the Done button results in a file being generated which is a 2D image of your final plot. **Note**: this image is irrevocably 2D - it cannot be opened as a 3D plot. You have to re-plot (using your saved style) for that.

**Making a movie**

Once you have the 3D plot as you want it to be, it is simple to make a movie in which the image rotates around any specified (principal) axis. The axes remain as you have set them in space - hence you can see the rotation from any angular viewpoint.




The values suggested above give a reasonably smooth movement, without generating too huge a file. The plots always rotates through 360 degrees - it ends up in the starting orientation. The files generated run in standard movie players(Quicktime etc) and import readily into Powerpoint if so required.

**Pro Fit Software**

This is available for on-line purchase from QuantumSoft:

http://www.quansoft.com/