

----- Ver.13.1.2 ----- October 3, 2009 Bug fix version of 13.1.1 To Vista user (see ReadMe)  
----- Ver.13.1.1 ----- September 24, 2009 Updated to be compatible with Gaussian 09 outputs

----- Ver.12.2.1 ----- September 12, 2009  
Algorithm of FMO fragmentation has been revised for very special cases, such as solid surface.

----- Ver.12.1.3 ----- August 22, 2009

(1) New feature of PDB utilities

To add hydrogen atoms in ATOM record format to nucleic acid PDB.

To convert bad name field of ATOM record of nucleic acid to proper one.

(2) The default behavior of hydrogen bond detection

It is determined by SkipHBondDetection parameter of [AppControl] section in the Facio.ini.

SkipHBondDetection=1 (Skip hydrogen bond detection)

SkipHBondDetection=0 (Execute hydrogen bond detection for every new structure)

(3) New amino residues are available for Polypeptide Builder

Orn (Ornithine), Aib (Methylananine), Pca (Pyroglutamic Acid)

Hid (Histidine with hydrogen on the delta nitrogen)

Hie (Histidine with hydrogen on the epsilon nitrogen)

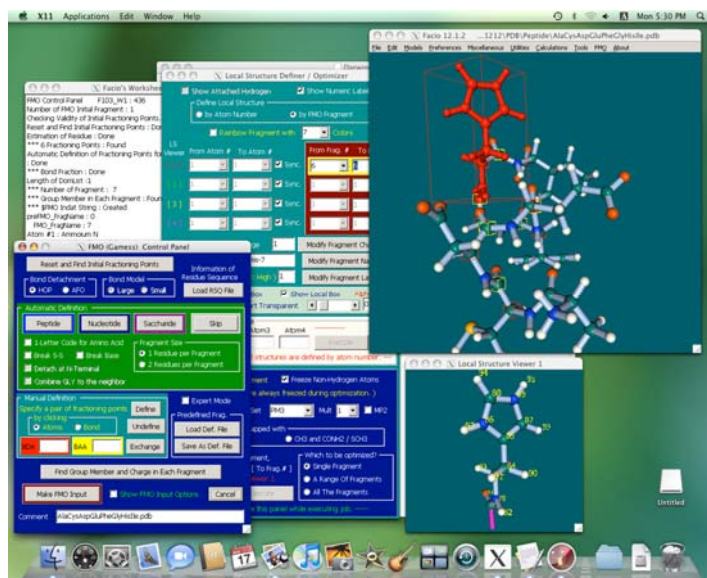
cf. His (Positively charged Histidine with hydrogens on both the nitrogens)

(4) Facio on Macintosh

It was confirmed that Facio can work on Intel Mac with a help of Darwine, which allows Mac OS X to execute Windows native softwares. See the screenshot below.

Darwine <http://www.kronenberg.org/darwine/>

Please notice that Darwine requires X11, the X window system. But it is usually not installed by default. So, please make sure to install X11 from your Mac OS X install CD.



On Darwine environment, two problems are known up to now.

(a) Slide boxes in the main window are invisible.

But the slide boxes can work well. So, there is practically no problem.

(b) Drag & drop operation does not work.

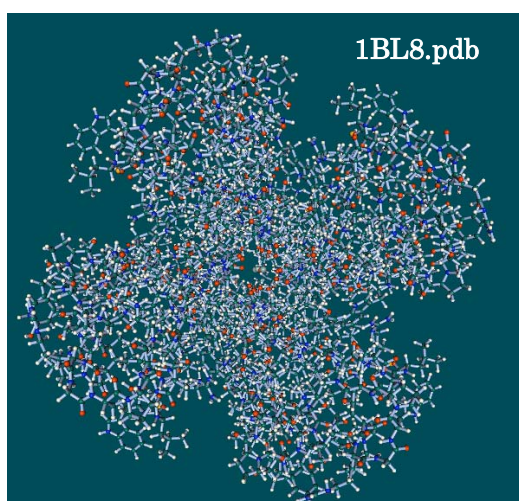
This may be a problem of Darwine.

(5) Batch job control feature for Gaussian on remote server has been completely revised. In the new version, user has to specify batch job script file by setting parameter BatchJobScript in Facio.ini. Script file name should be relative to the Facio root folder. For example, if you want to use xxx.jcf in JCF folder at Facio root folder, please set the parameter as follows.  
BatchJobScript=JCF\xxx.jcf

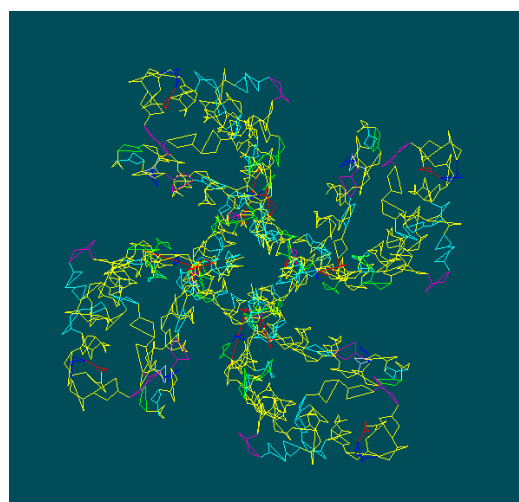
----- Ver.12.1.2 ----- July 13, 2009 Bug fix version of 12.1.1

----- Ver.12.1.1 ----- June 27, 2009

- (1) Pull-down menu items have been fully revised and organized properly into submenus.
- (2) For Tinker 5 user, set Tinker5 parameter of [AppControl] section in the Facio.ini file to 1. For Tinker 4.2 user, set the parameter to 0. Default setting : Tinker5=1
- (3) A new coarse-grained model ( Trapezoidal Quad representation ) of protein  
Each amino residue consists of four points ( C and O of amide carbonyl, alpha C, and N of amide), which is called as Trapezoidal Quad. Type of amino acid is represented by color. Although you can use different color for different amino residue, use of four or five colors (for example, hydrophobic, aromatic, basic, and acidic) are recommended.  
For TQ representation, no missing hydrogen atom should be present. If there are missing hydrogen atoms, please complete them.

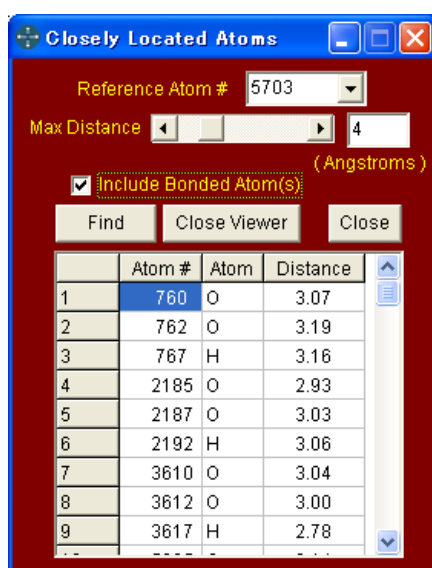


Ball & Stick model



Trapezoidal Quad model

- (4) New function to find closely located atoms around a specified atom and to show them.



The screenshot shows a dialog box titled "Closely Located Atoms" with a red background. It features a "Reference Atom #" dropdown menu set to "5703", a "Max Distance" slider set to "4" (Angstroms), and a checked "Include Bonded Atom(s)" option. Below these are "Find", "Close Viewer", and "Close" buttons. A table lists the results of the search:

	Atom #	Atom	Distance
1	760	O	3.07
2	762	O	3.19
3	767	H	3.16
4	2185	O	2.93
5	2187	O	3.03
6	2192	H	3.06
7	3610	O	3.04
8	3612	O	3.00
9	3617	H	2.78
...	...	...	...



This example shows closely located atoms within a radius of 4 Angstroms around a potassium atom of 1BL8.pdb

- (5) Visualization of MOs calculated with MOPAC2009/PM6, which has parameters for 70 elements( from H to Ba, La and Lu, and from Hf to Bi).  
Transition metal complex models constructed from scratch only with Facio and MOPAC/PM6 are included in the folder named "MetalComplexes\_by\_PM6".