BioStation
BioStationViewer Open Ver.1 Rev.23

Users Manual

2020/2

Contents

1. Introduction

List of key BioStation Viewer features:

1) Visualize molecular structures of Protein and DNA
2) Visualize isosurface of electron density, electrostatic potential and molecular orbitals.
3) Visualize isosurface of the electron density, added colors by the value of electrostatic potential.
4) Edit molecular structures
5) Visualize the interaction energy between fragments
6) Visualize Electron Field Vector
7) Animate molecular trajectory

Fig1.1 shows an example of isosurface of electron density, added colors by the value of electrostatic potential

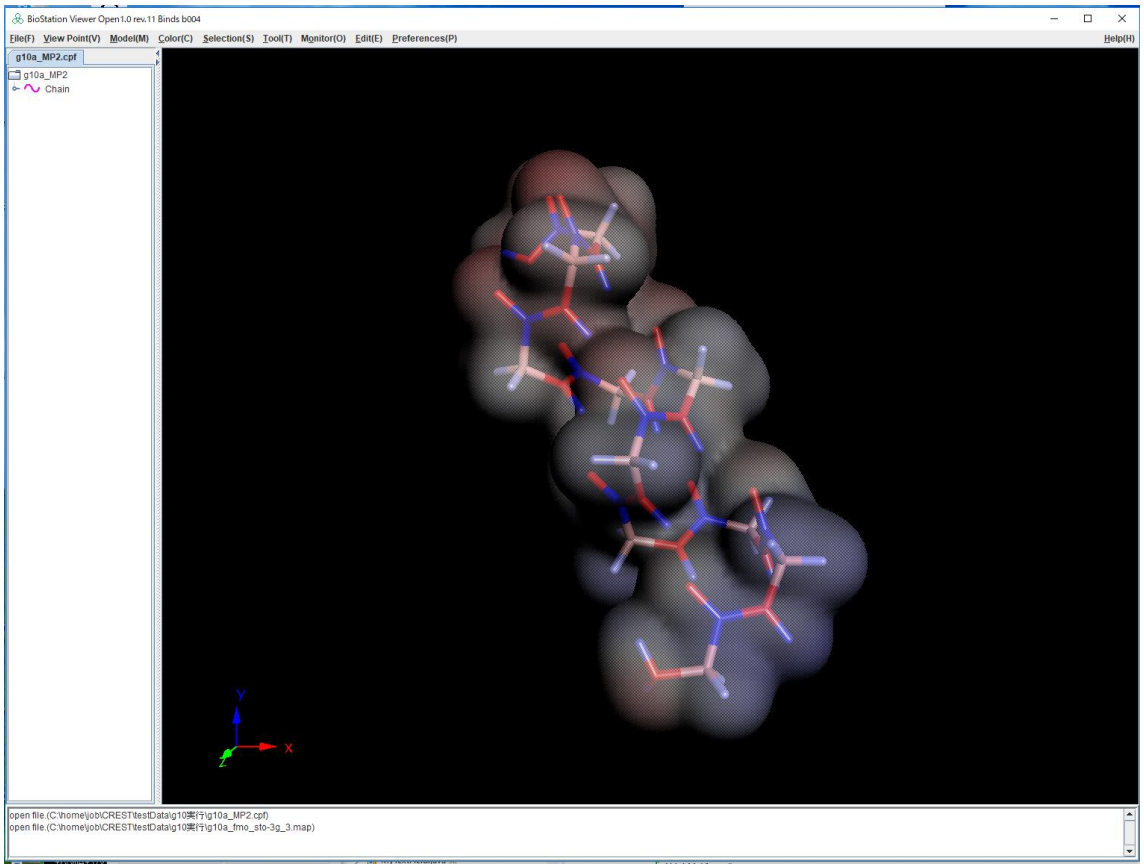


Fig1.1 Isosurface of Electron Density, Added Colors by the Value of Electrostatic Potential

2. How to use BioStation Viewer

2.1. Getting Start BioStation Viewer

Double click on the icon 

of the desktop to start Viewer. Fig2.1 shows the main window. Molecular structures are shown on the hierarchical window on the left side of the window and on the viewing-window by a 3-dimensional image (3D) on the right. You can choose display option from the menu bar. The hierarchical window shows a tree-view of the molecule, the layer of molecule by chains, residues and atoms. By selecting an icon in hierarchical item, the appropriate atom in 3D view-window is highlighted. By selecting the displayed structure in 3D view-window, the appropriate items in hierarchical window are highlighted. The message appears at the bottom of the window.

Fig2.1 Main Window

2.2. Explanation of Menu

Fig2.2 Menu at main window

2.2.1. File

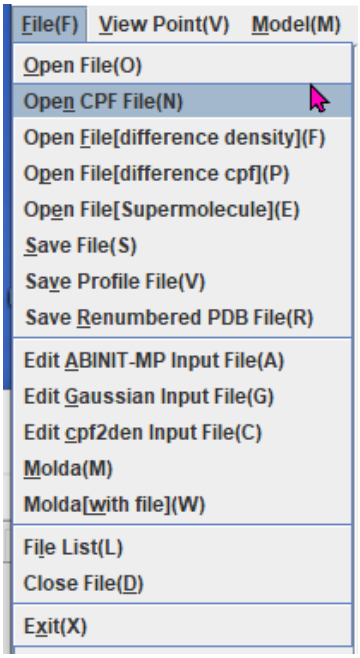


Fig2.3 File menu

- **Open** Load PDB file(*.pdb,*.ent)、ABINIT-MP Check Point File(*.cpf)、ABINIT-MP Grid File(*.den,*esp,*.map,*.mo)、MOL2 file(*.mol2)、MDL file(*.mol, *.mdl) and Gaussian Cube file(*.cube,*.cub), XYZfile(*.xyz), Trajectory file (*.trj,*.tr2,*.trj2,*tj2), Pno file(*.pno), Display profile (*.prof). Please refer to the specification of each file from the following URL.
  - ABINIT-MP : http://www.fsis.iis.u-tokyo.ac.jp/result/software
  - PDB File: http://www.rcsb.org/
  - MOL2File: http://chemyang.ccnu.edu.cn/ccb/server/AIMMS/mol2.pdf
    MDL File:
  - Gaussian Cube File: http://www.gaussian.com の G98 Manual Pages
  - XYZ File:Describe number of atom at first line, comment line, and atom symbol, x,y,z coordinate in one line. As extension, in BioStation Viewer, the vector values of x, y and z is specified behind coordinates, and the vector

display for every atom is possible. Refer to the Arrow of Preference specification for change of the display attribute of a vector.

- Mopac input/output file: Dewar, M.J.S., Thiel, W., J. Am. Chem. Soc., 1977, 99, 4899, 3907
- Trajectory File : refer 2.4.1
- Pno file : http://www.fsis.iis.u-tokyo.ac.jp/result/software
- Display profile : you can reproduce the display state by saving in the file and reading the file. The corresponding functions are shown bellow.
  - ✓ Include 1 of CPF or PDF. The other structure files are not supported
  - ✓ View Point
  - ✓ Model
  - ✓ Color
  - ✓ Atom,Residue (Model,Color,Label)
  - ✓ Tool(Display * in Distance, Set Rotation Center)
  - ✓ Monitor(Distance, Angle, Dihedral Angle, Interaction Energy, IFIE 1:1,N:1
  - ✓ Preference

1) Molecular Structure file

When **PDB** file、**ABINIT-MP Check Point File**、**MOL2** file, **MDL** file, **XYZ** file, **Gaussian output** file and **Mopac input/output** file are loaded, the molecular structures are displayed. When number of atom lower than 300, display slyle is Stick, more than 300 is CA (Line).

2) ABINIT-MP Grid File, Gaussian Cube File

The extension of **ABINIT-MP Grid File** means as follows :

i) **den** : electron density
ii) **esp** : electrostatic potential
iii) **map** : map file of electrostatic potential on the isosurface of the electron density.
iv) **mo** : molecular orbitals
v) **efv** : electron field vector

When **ABINIT-MP Grid File** loaded, specify the isosurface value that you want to visualize.

In the case of a **Gaussian Cube file**, select the file type from electron density, electrostatic potential, and a molecular orbital, and specify covering a value of

the boundary on a periodic display, and performs the display specification of each. **Periodical grid value** is selected “On” for add one a cell at edge of boundary, set “Off” that not add a cell. A dialog box shown in Fig2.4.

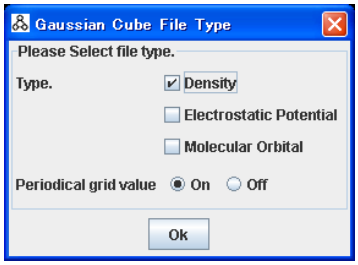


Fig2.4　Gaussian Cube File

3) Specify electron density display option

A dialog box for the electron density and electrostatic potential is shown in Fig2.5. Specify the value of the isosurface value, the color, the transparency, bounding box and section. There are the two methods of coloring. One is to specify a single color and the minimum value and maximum are specified, a color is specified in the range. The Color Preference Dialog Box is shown in Fig2.6.

There are two types specify of isosurface value a value or sigma. σ is calculated by following equation. If the value is more than 1, it is treated as 1.

$$\sigma[\rho] = \left[\frac{\sum_{i=1}^{N}\{\rho(x_i, y_i, z_i) - \bar{\rho}\}^2}{N}\right]^{1/2}$$

Clicking on the “Set” button , display section specify dialog. Refer to Section 2.3 to set section option.

This sigma function is currently suspended.

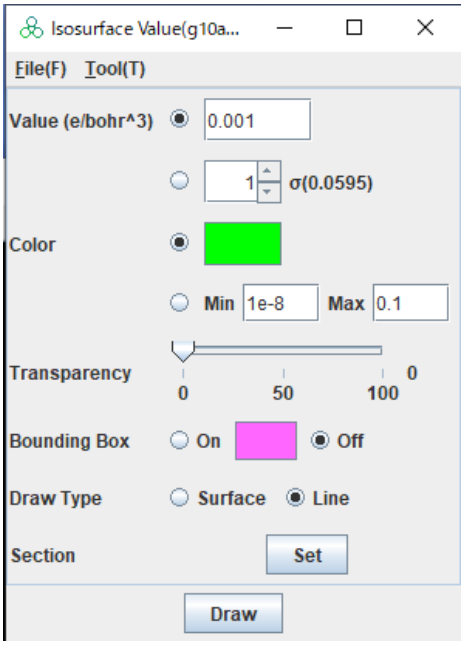


Fig2.5 Isosurface Value Dialog Box

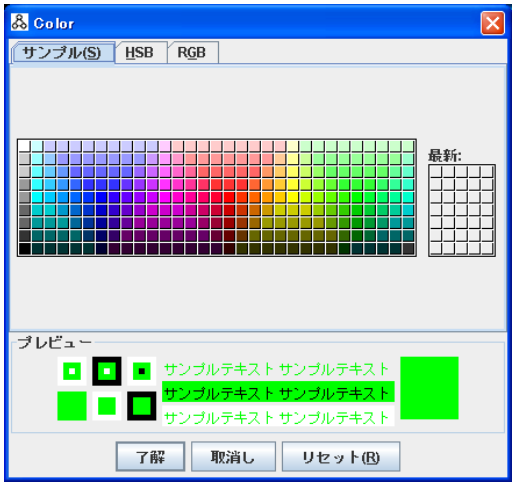


Fig2.6 Color Preference Dialog Box

4) Specify map file and electrostatic potential

In the case of a map file, specify the ranges of both the value of the isosurface value and that of electrostatic potential. This dialog box is shown in Fig2.7. As the value of the default is changed from high to low, the visualize color is changed from red to white to blue. When you set **Min Max(red, blue)** using the button for specifying the range of the value, the display color is changed from blue to white to red.

In the case of electrostatic potential, specify the value of the isosurface value.

The isosurface value is displayed by the two specified values(±).

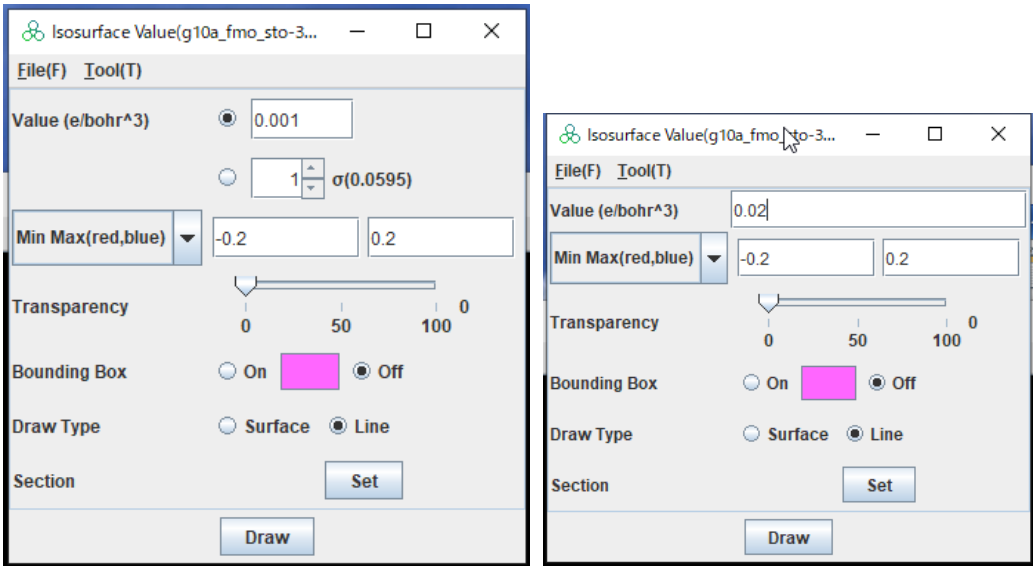


Fig2.7 Map file and Electrostatic Potential Dialog Box

5) Specify display option of Molecular Orbital

In the case of the molecular orbital, the orbital energy graph is displayed. The graph window is shown in **Figure 2.5.** When you move the mouse on each level, the orbital number and the energy value are displayed under the graph. When you click on each level, the orbital number is selected in the **Mo No.** Here the orbital number can be input directly. When you click on the **Draw** button, visualize the isosurface of the specified value (±).

By clicking on "+" and"−" buttons, the graph is scalable. The line width each level can be specified with **Line Width**. Colors of the isosurface value can be specified in the optional colors dialog box. In addition, **Color(-,+)** can be changed into **Color(+,-)**, and the colors will be reversed whenever they are selected.

In **Gaussian Cube** file, without the energy value, the graph is displayed starting from **1**, in the case of the descriptions of multiple orbitals.

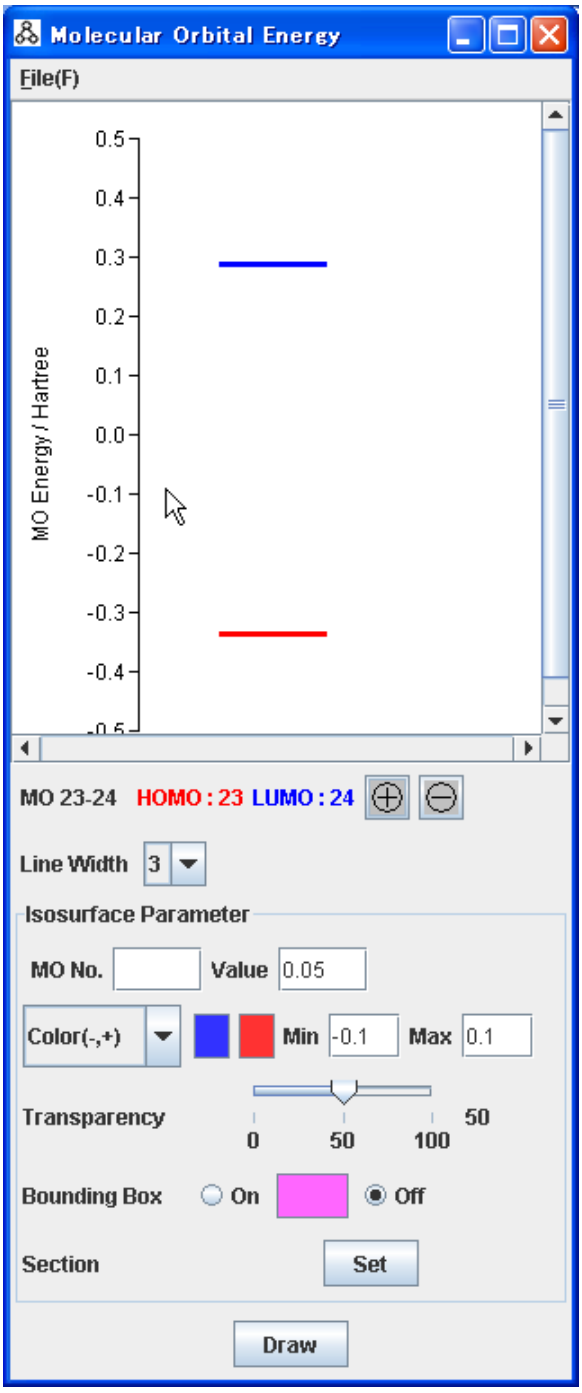


Fig2.8 Graph window of Isosurface of Molecular Orbital .

6) Specify display option of electron field vector

When a electron field vector file loaded, a dialog box(Fig2.9) pops up and displays an electron field vector by the defaults option. An electric field vector is displayed on the basis of the point on isosurface. Display option is explained below.

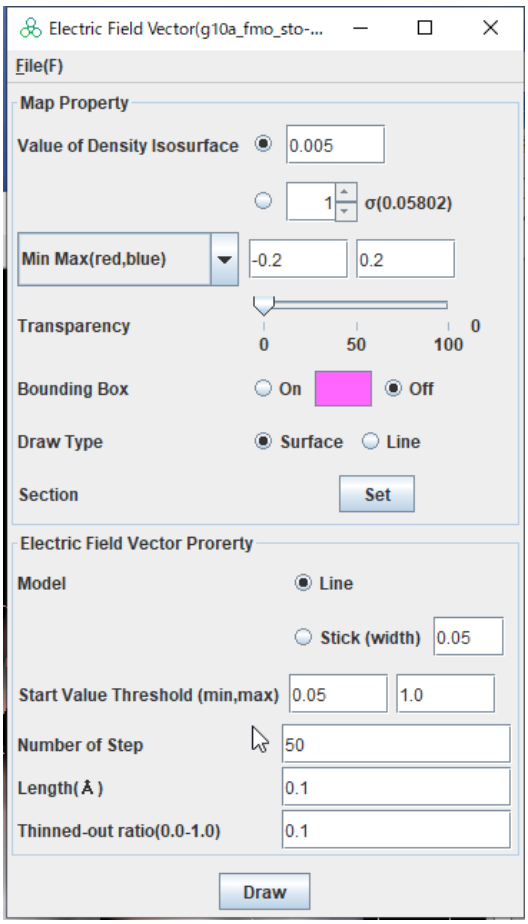


Fig2.9 Electron Field Vector Dialog Box

- Map Property
  - ➢ Value of Density Isosurface

    Specify the value of density Isosurface
  - ➢ Min Max(blue,red)/ (red,blue)

    Specify the range of electrostatic value. As the value of the default is changed from high to low, the visualize color is changed from red to white to blue. When you set **Min Max(red, blue)** using the button for specifying the range of the value, the display color is changed from blue to white to red.
  - ➢ Transparency

    Specify the Transparency
  - ➢ Bounding Box

    Specify to display a bounding box.
  - ➢ Section

Clicking on the **Set** button, display the dialog box for a section view. Refer to Section 2.3 to set the section options.

- Electric Field Vector Property
  - Model
    Specify the model (Line/Stick). When the stick model is selected, specify the radius of stick.
  - Start Value Threshold(min,max)
    Specify the start point range of electrostatic value on the isosurface
  - Number of Step
    Specify the number of step. It repeatedly calculates the specified number of times, and a vector is displayed.
  - Length(Å)
    Specify the length of one step.
  - Thinned-out ratio (0.0-1.0)
    Specify the thinned-out ratio of start point. (value range : 0-1)
- Draw
  Display electron field vector.

7) Trajectory file

Animate the molecular structure in time series. Refer to Section 2.4 for details.

8) Pno(Pair Natural Orbital) file

Display isosurfaces of Pair Natural Orbital. Specify display option for each pair orbital. Display each relaxation energy, occupation number of Hole orbital and Particle orbital. You can specify display on/off each item. The vector is a arrow from Hole grid region to Particle grid region. All pairs can be selected/unselected by "Select All/Unselect All" Button. When a "Apply" button is clicked, it's displayed by the specified style. A dialog box shown in Fig2.10,Fig2.11.

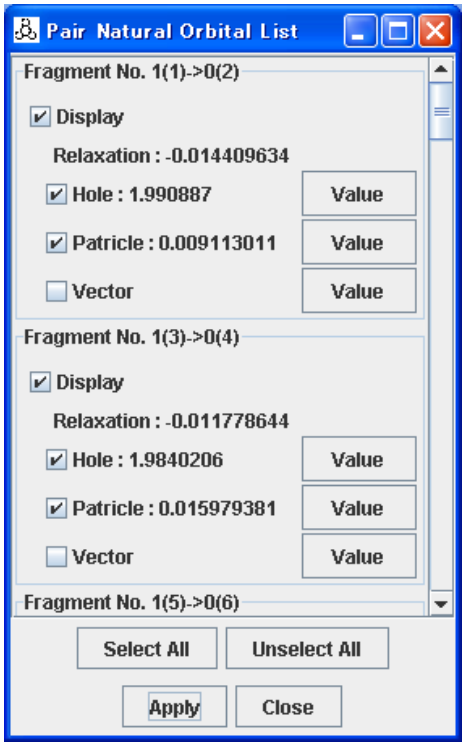


Fig2.10 Pno(Pair Natural Orbital) Dialog Box

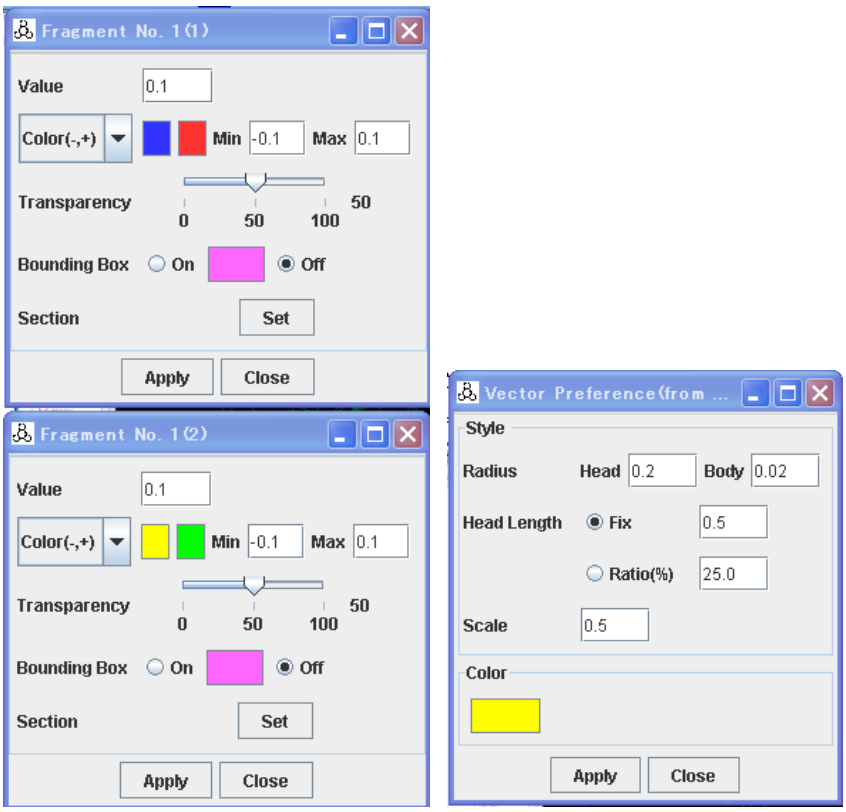


Fig2.11 Hole, Particle,Vector Dialog Box

♦ **Open CPF**

You can specify fragments that are subject to display at open dialog. Only the specified fragments are displayed. Non-display specified fragments are not displayed unless you re-read them. There are four modes.

1) None : It is displayed without any specification.
2) Ignore Fragments : Specify fragment numbers that are not subject to display
3) Fragments in Distance : Display a fragment within the distance from the specifier fragment.
4) Ignore Fragments by dimer value(CPF R23) : Do not display fragments that are not have dimer value.

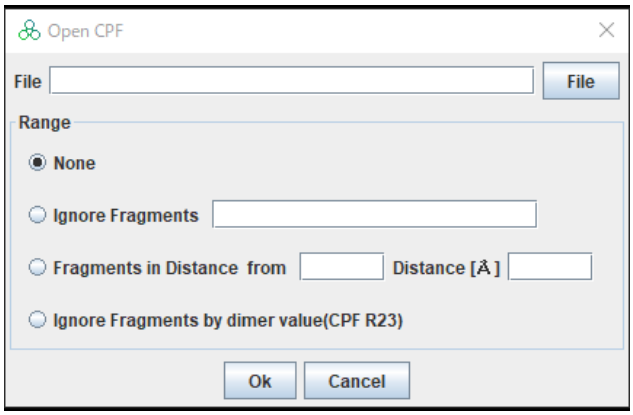


Fig2.12 Open CPF Dialog Box

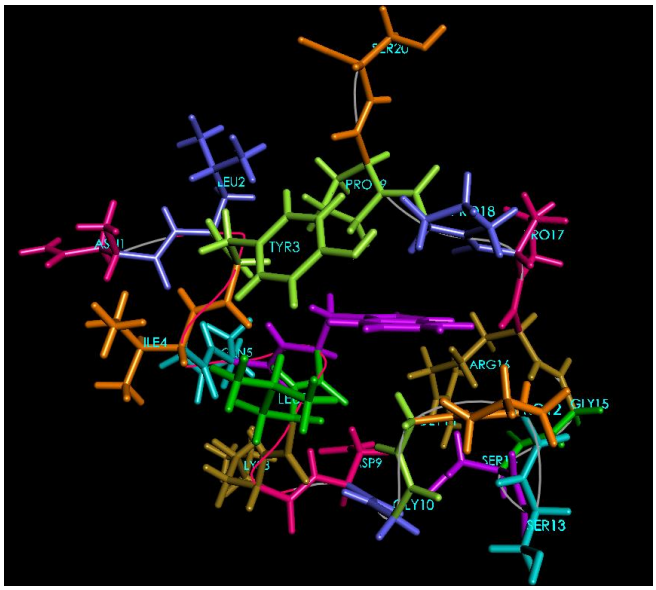


Fig2.13 Exanple of None.

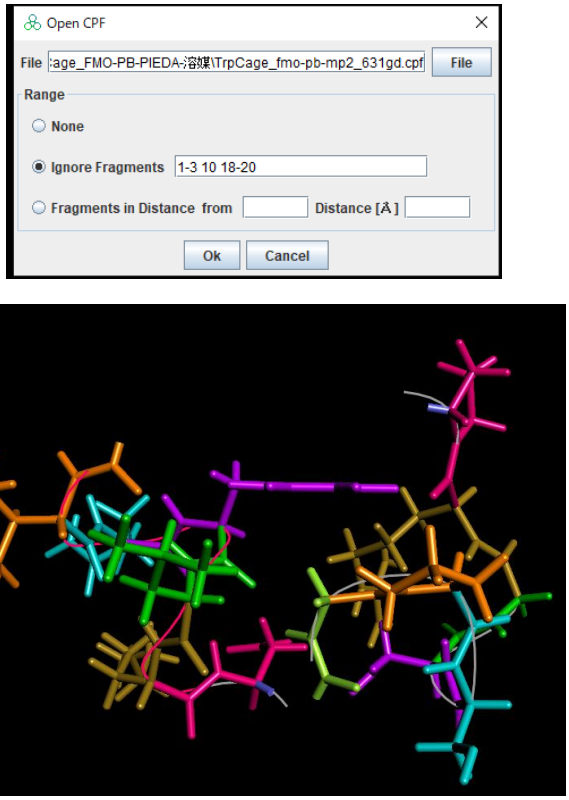


Fig2.14 Example of Ignore Fragments

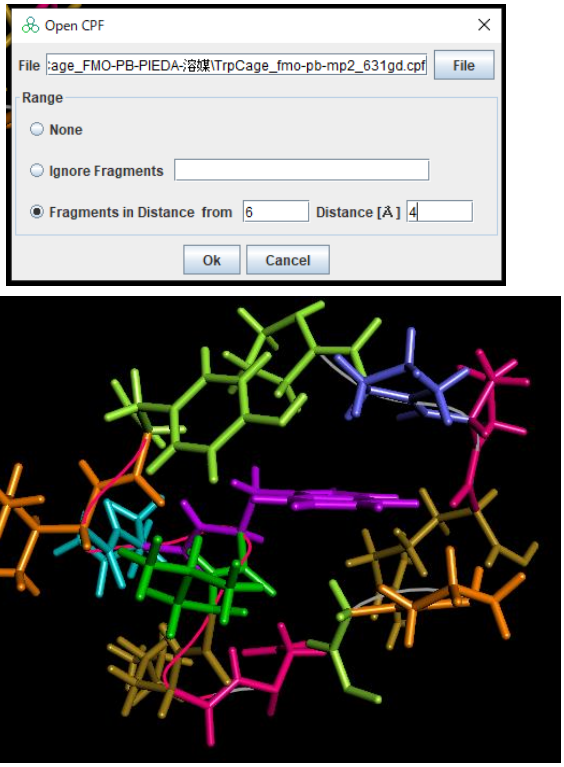


Fig2.15 Example of Fragments in Distance

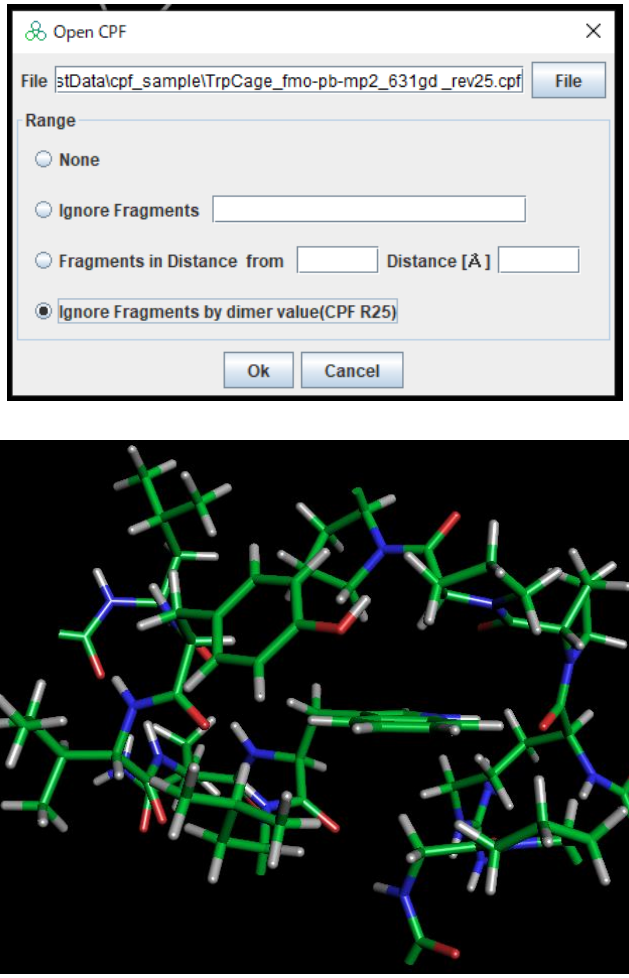


Fig2.16 Example of Ignore Fragments by dimer value(CPF R25)

♦ **Open File[difference density]**

Some Grid files are loaded and the isosurface of difference is displayed. If you specified different grid size data file, error occurred. The maximum number of files is 7. The dialog box is shown in .Fig2.17.

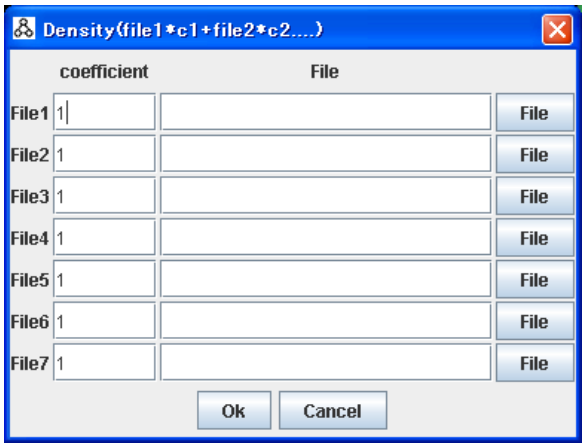


Fig2.17 Difference files Dialog Box

♦ **Open File[difference cpf]**

Some Check Point files are loaded and calculate charge and IFIE. The dialog box is shown in Fig2.18.

Adjust Atom Range : Specify a part of atoms in file that are calculated.

Format : Start atom No. – End Atom No. Corresponding atomic number in this file.

Ex. File2 "10-20 5" atom No.10-20 in file1 correspond to atom No.5-15 in file2. If no specify atom No., all atoms correspond. If selected "**Coddinate**", Display atom No. in this line file.

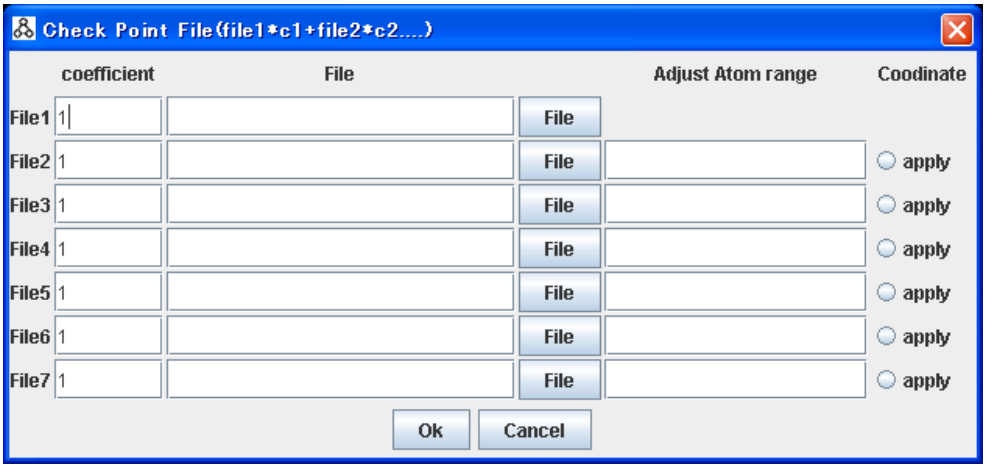


Fig2.18 Check Point Files Dialog Box

♦ **OpenFile[Supermolecule]**

Specify complex, protein and ligand CPF file. The dialog box is shown in Fig2.19. The fragment number of the protein in a complex is specified like this "1-100". Clicking on the Ok button, read files and display the IFIE value which applied electronic relaxation by ligand binding at 3D List and MAP.

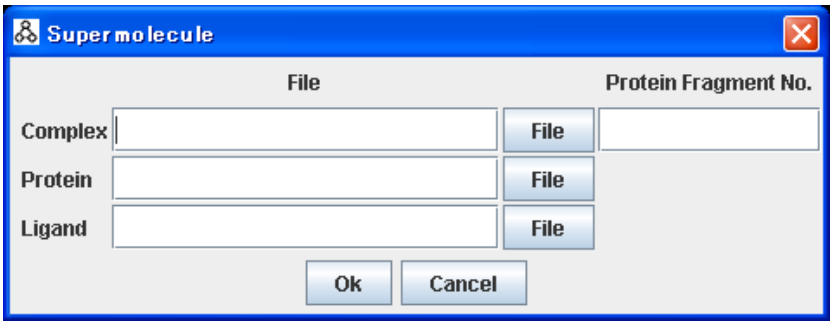


Fig2.19 Supermolecule Dialog Box

♦ **Save File**

You can output each file by selecting the extensions.

1) *pdb, ent* Save molecular structures by PDB file format.

Atomic numbers in the saved files are renumbered.

2) *gjf* Output the input file of Gaussian. Here is an example of file. In the case of a display of ABINIT-MP Check Point File, charged molecules and spin multiplicities are calculated as follows.

Charged molecules = the sum of charged molecules (the sum of nuclear numbers) – the sum of electron numbers of fragments.

Spin multiplicity = If the first letter of an electronic state is S, show 1, if it is D, show 2, and if it is T, show 3.

```
%chk=test.chk
#HF/6-31G(d,p) POPT=(MaxCycle=100) SCF=TIGHT


 0 1
  N  0 x001 y001 z001
  C  0 x002 y002 z002
  C  0 x003 y003 z003
.............
  H  0 x071 y071 z071
  O  0 x072 y072 z072
  H  0 x073 y073 z073
 Variables :
 x001=  0.162000
```

```
 y001= -0.202000
 z001=  0.000000
 x002=  1.612000
.....
 z072= -5.671000
 x073= -4.846000
 y073= 12.697000
 z073= -6.024000
 Constants :
```

3) *jpg* Output the JPEG file.

4) *png* Output the PNG file.

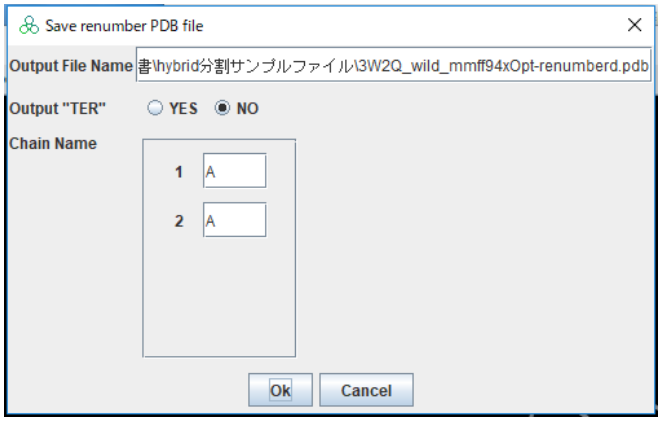
5) *tif* Outpur the Tiff file.

6) *xyz* Output XYZ file. It describes number of atom at first line, and atom symbol, x,y,z coordinate in one line.

7) *prof* Output display profile file.

♦ **Save Renumbered PDB**

Save PDB File which renumbered atom number. File name is xxx-renumbered.pdb. Specify output "TER"(end of chain) and chain names.



♦ Edit **ABINIT-MP File**

Popup the edit window of **ABINIT-MP** input file. Here, you can set the parameters, load and save files. How to edit parameters is explained in **Section2.8**.

♦ Edit **Gaussian Input File**

Popup the simple edit window of **Gaussian** input file. Here, you can set the parameters, load and save files.

♦ Edit **cpf2den Input File**

Popup the simple edit window of **cpf2den** input file(Fig2.20). Here, you can set the parameters, load and save files. If loaded Check point file, set the file name

and the value applied to maximum and the minimum value ±2A is displayed at the column of Domain computing lattice point. Refer to the "ABINIT-MP user's manual" for the details of cpf2den.

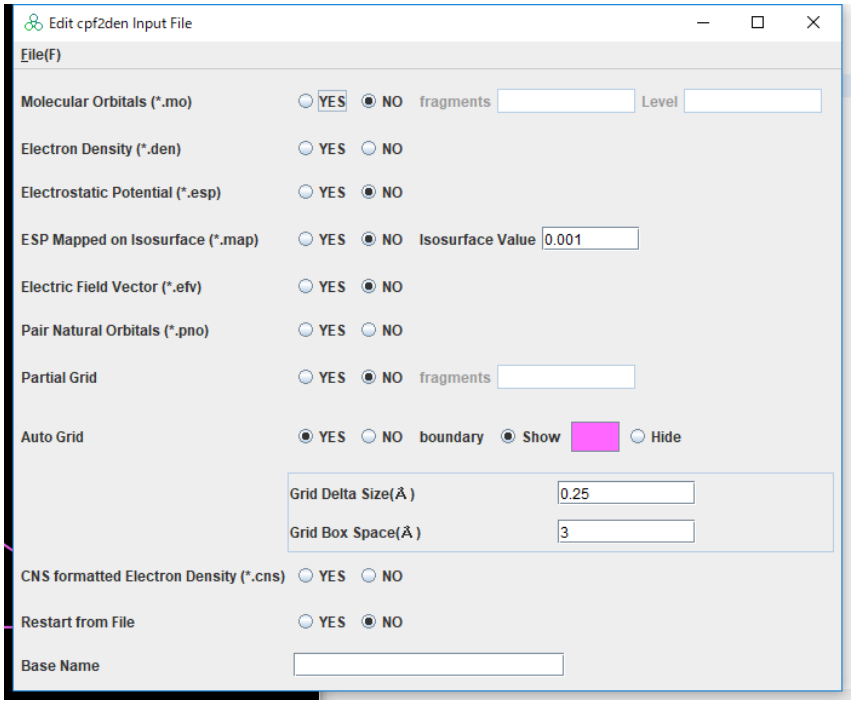


Fig2.20 cpf2den input file edit window

- Mo File(*.mo)
  Specify YES/NO to output the Molecular Orbital grid file.
  Reagion : Specify the fragment number. Ex :'1,2,8-12'
  Level : Specify the level of MO. There are some methods shown below.
  ·Around HOMO-LUMO : Ex ' Homo-5:Lumo+5'
  ·All Orbital:'All'
  ·All occupied Orbital :'Occ'
  ·All un occupied Orbital:'Virtual'
  ·Orbital number : Ex '1-10'
- Electron Density File(*.den)
  Specify YES/NO to output the Electron density grid file.
- Electrostatic Potential File(+.esp)
  Specify YES/NO to output the Electrostatic potential grid file.
- Map File(*.map)
  Specify YES/NO to output the map file.
- Electric Field Vector File(*.efv)

Specify YES/NO to output the Electric Field Vector File.

- Pair Natural Orbitals(*.pno)

  Specify YES/NO to output the Pair Natural Orbitals file.

- Partial Grid

  Specify YES/NO to output the Partial Grid file. NO : calculate all molecular.

  Reagion : Specify the fragment number. Ex. :'1,2,8-12'

- Auto Grid

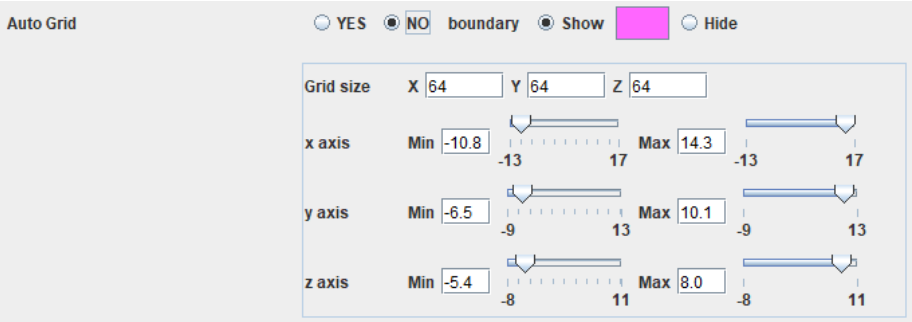
  YES/No : Calculate grid size based on Grid Delta Size and Grid Box Space

  Boundary how/Hide : Specify display boundary.

  Grid Delta Size : Specify a grid size. (Unit is Å)

  Grid Box Space : Calculate grid size from molecular size and Grid Box Space is shortest distance from box to the molecule of edge. (Unit is Å)

  NO : Specify number of x, y and z grid, and coordinate of start and end point. Dialog is shown bellow.



- CNS formatted Electron Dnty(*.cns)

  Specify YES/NO to output the CNS file.

- Restart from file

  Specify YES/NO to output the restart file.

- Base Name

  Specify base name for output grid file. if do not specify it, use input file name as base name.

- **Molda**

  Execute Molda. Please refer to the manual of Molda for the useage of Molda.

- **Molda(with file)**

  Execute Molda with loaded structure file.

- **File List**

When multiple files are loaded, select the file, which you want to display. **File list** dialog box is shown in Fig2.21. In the case of **ABINIT-MP Grid File,** by clicking on **Value** button, the dialog boxes as Fig2.5, Fig2.7, Fig2.8 and Fig2.9 are displayed, the display option can be modified.

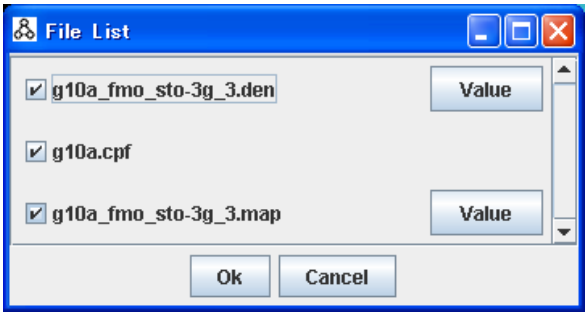


Fig2.21 File List

- **Close File List**

  You choose the check box and click on **Ok** in order to delete the display file on the Viewer. This dialog box is shown in Fig2.22.

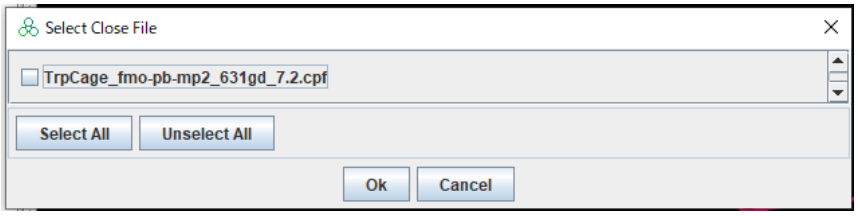


Fig2.22 Select Delete Display File

- **Exit**

  Exit this application.

2.2.2. Viewpoint

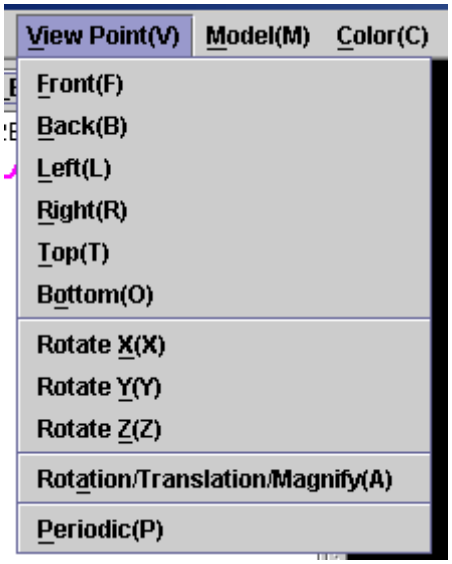


Fig2.23 Viewpoint menu

Move a viewpoint to the set-position. Fig2.24 shows a coordinate system.

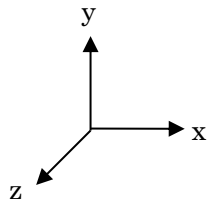


Fig2.24 Coordinate system

- **Front** : See the front side(from plus direction on the **z**-axis)
- **Back** : See the back side(from minus direction on the **z**-axis)
- **Left** : See the left side(from minus direction on the **x**-axis)
- **Right** : See the right side (from plus direction on the **x**-axis)
- **Top** : See the topside (from plus direction on the **y**-axis)
- **Bottom** : See the downside (from minus direction on the **y**-axis)
- **Rotate X** : Rotate around the **X** axis
- **Rotate Y** : Rotate around the **Y** axis
- **Rotate Z** : Rotate around the **Z** axis
- **Rotation/Translation/Magnify** :

Move the viewpoint position. The Dialog is shown in Fig2.25 and display specification is explained below.

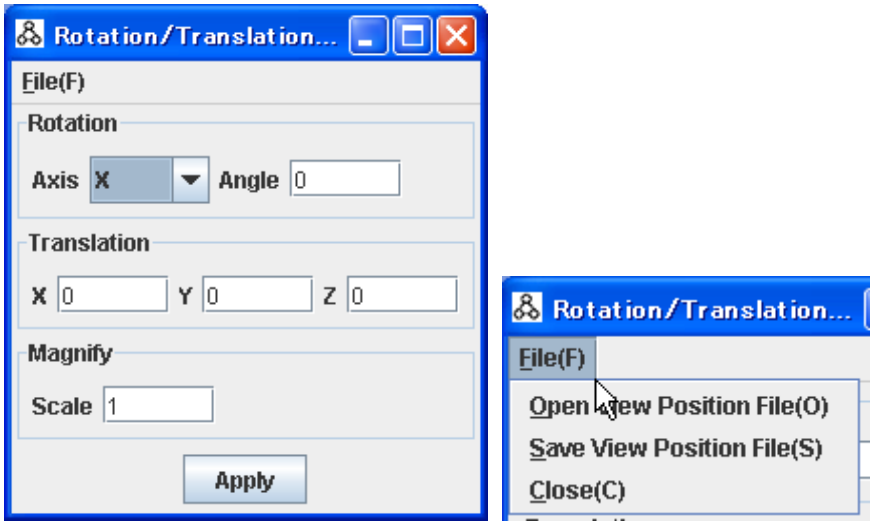


Fig2.25 Rotation/Translation/Magnify Dialog Box and file menu

- File : Load and save a viewpoint position. The file extension is *.pos.
  - Open ViewPosition File : Load file.
  - Save ViewPosition File : Save file.
- Rotation
  - Axis : Specify axis.
  - Angle : Specify angle.
- Translation
  - X,Y,Z : Specify rach distance of x,y and z directions.
- Magnify
  - Scale : Specify ratio.

♦ Periodic : Function of periodic display. Only the number specified in X, Y and Z directions displays the same thing. The dialog box is shown in Fig2.26 and the display specification is explained below.

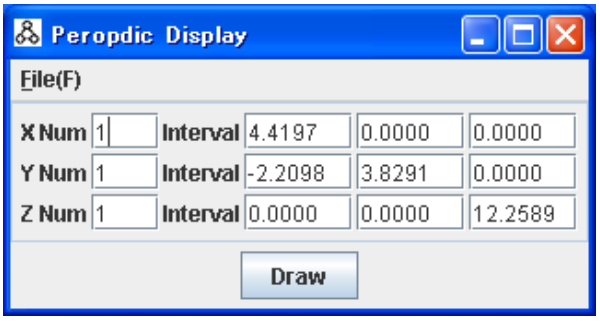


Fig2.26 Dialog Box of periodic display（example of Gaussian Cube file）

- File
  - Reset

    Reset display.
  - Close

    Close dialog.
- X ,Y, Z

  Specify the number of each direction and interval. In case of Gaussian Cube File you specify three values.
- Draw

  Display periodically.

2.2.3. Model

Model menu consists two parts (Atom/Structure).

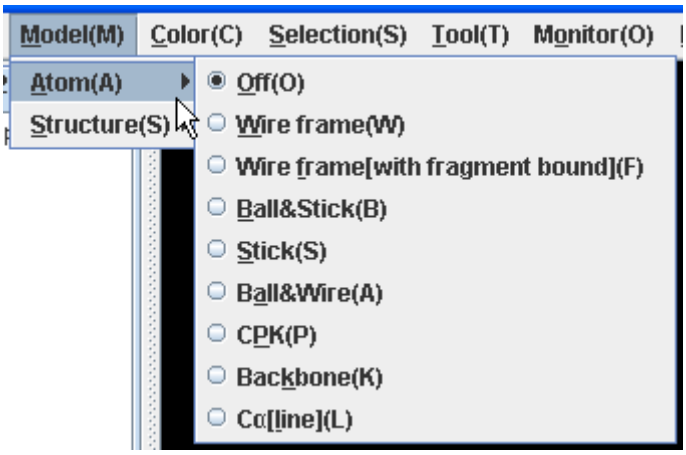


Fig2.27 Model(Atom) menu

Atom menu

- **Off :** Disable to display
- **Wire frame :** Molecule appears as a wire frame model.
- **Wire frame(with fragment bound)** : Molecule appears as a wire frame model, with a ball on **Cα** atom to show the fragment bound
- **Ball & Stick :** Molecule appears as a ball & stick model
- **Stick :** Molecule appears as a stick model
- **Ball & Wire:** Molecule appears as a ball & wire model
- **CPK :** Molecule appears as a space filling model
- **Backbone** : Backbone appears as a tube model
- **Cα [line] :** Display **Cα** atom with a line by a **spline** interpolation

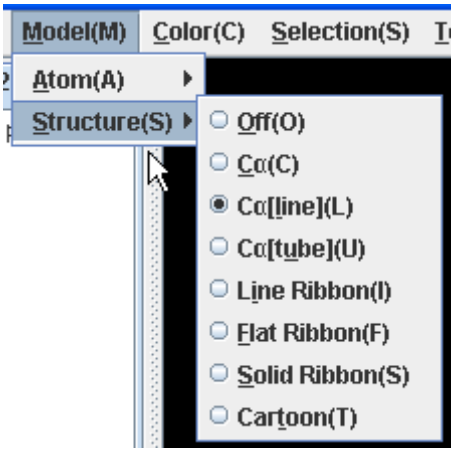


Fig2.28 Model(Structure) menu

Structrue menu

- **Off :** Disable to display
- **Cα** : Display **Cα** atom with a straight line
- **Cα [line]** : Display **Cα** atom with a line by a **spline** interpolation
- **Cα [tube]** : Display **Cα** atom in the tube model by a **spline** interpolation.
- **Line Ribbon :** Display Ribbon(Line)
- **Flat Ribbon :** Display Ribbon(Flat)
- **Solid Ribbon :** Display Ribbon(Solid)
- **Cartoon Ribbon :** Display Cartoon

Example of ERE_EST.cpf is shown in Fig2.29-Fig2.35.

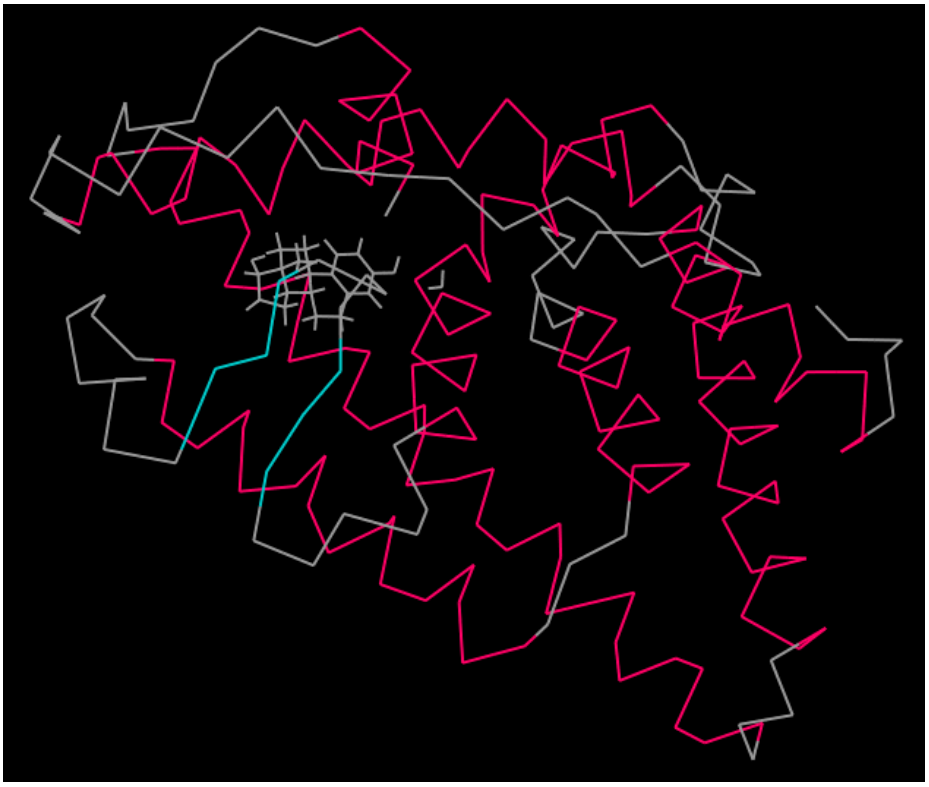


Fig2.29 C α

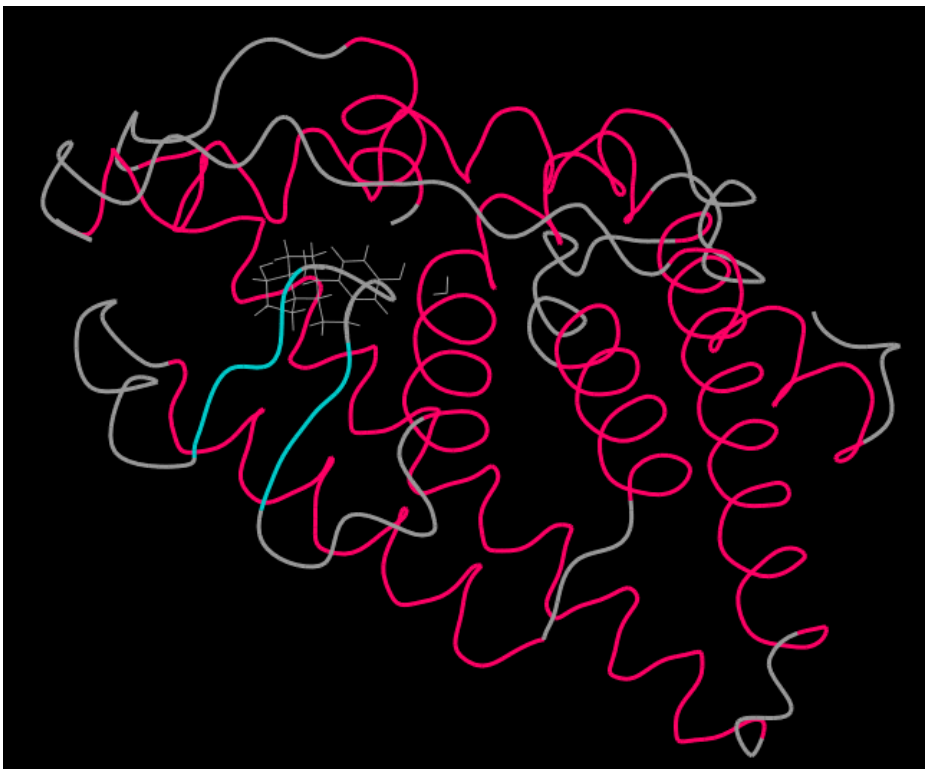


Fig2.30 C α Line

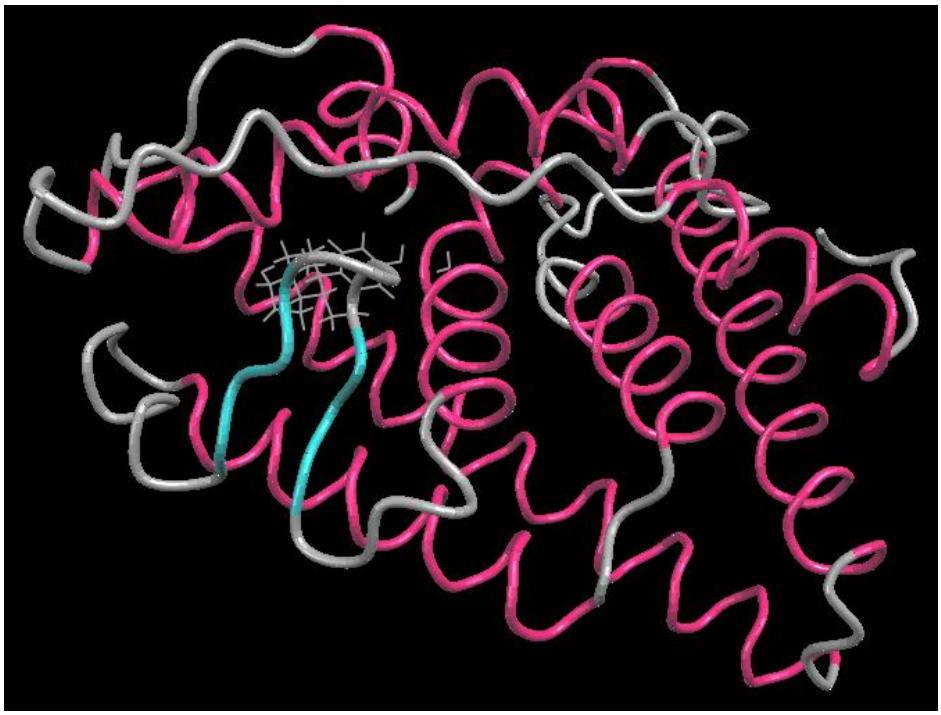


Fig2.31 C α Tube

Fig2.32 Line Ribbon

Fig2.33 Flat Ribbon

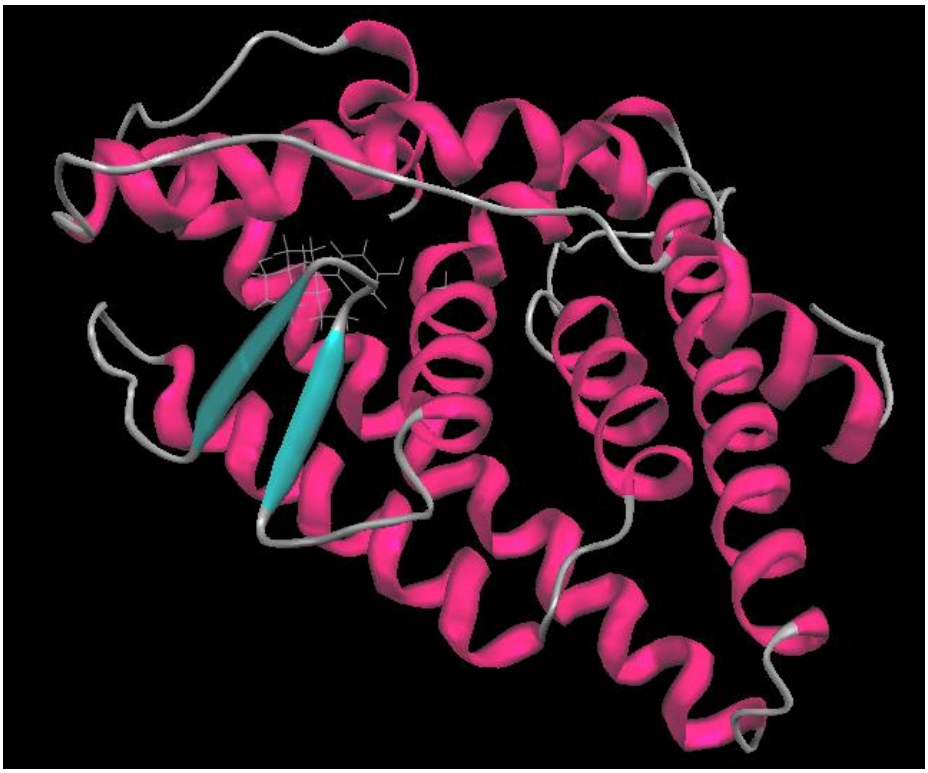


Fig2.34 Solid Ribbon

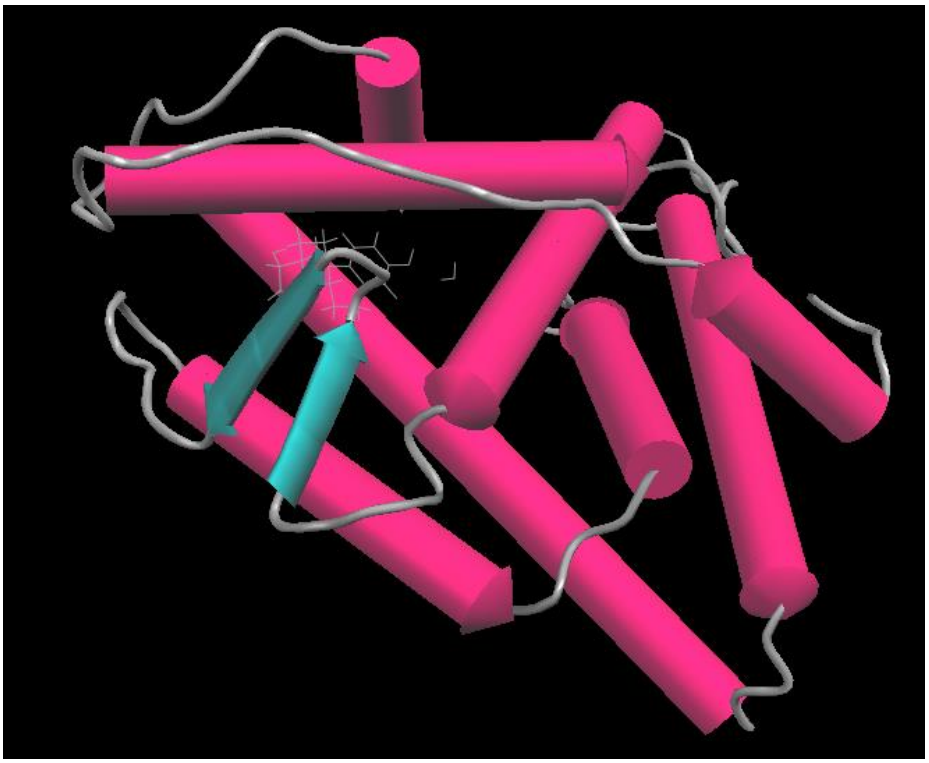
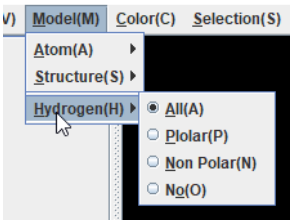


Fig2.35 Cartoon

1) display type of hidrogen



- **All** display all.
- **Polar** display hydrogens that connected N.
- **Non Polar** display hydrogens that connected except N.
- **No** No display.

2.2.4. Color

Color menu consists two parts(Atom/Structure). Atom and Structure menu has the same item. The default value is Atom:Atom, Structure:Structure

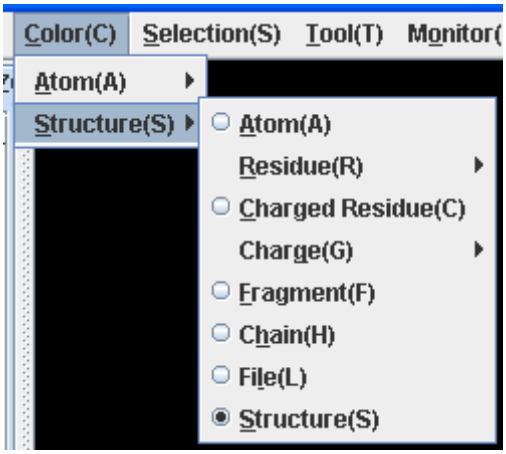


Fig2.36 Color menu

- **Atom** Set colors by atoms
- **Residue**
  - **Name** Set colors by the residue name, in case of DNA by four kind of colors ATGC
  - **Hydrophilic/Hydrophobic** Set colors by Hydrophilic( )/Hydrophobic( )
  - **Hydrophilic/Hydrophobic/Surface** Set colors by Hydrophilic ( ) /Hydrophobic( )/Surface( ). With the exception of the molecule surface, Hydrophilic/Hydrophobic are colored.
  - **Function** Set colors by functions

Function	Color	Peptide
Acid		Asp,Glu
Basic		Arg,Lys,His
Neutral		Ser,Thr,Asn,Gln
Aliphatic		Gly,Ala,,Val,Ile,,Leu,,Met
Aromatic		Phe,Tyr,Trp
Thiol-containing		Cys
Imono		Pro

  - **Select Residue** Set colors by selected residues, and other residues are white.
- **Charged Residue** Set colors by the value of charged residues.
  (+: 0 : −:)
- **Charge** Set colors by the value of charged molecules.If Check point file is ersion.2 , you can choose value HF/MP2. The displayed color is changed from red to white to blue, according to the changing values of electric charges. When the

electric charge is not specified, set colors by atoms.

- **Atom** Displayed color by atom charge.
- **B Factor** Displayed color by temperature factor. Specify min/max value.

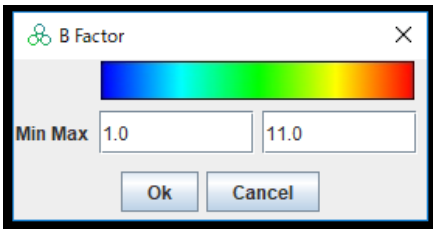


Fig2.37 B Factor Dialog Box

- **Fragment** Displayed color by fragment charge.
- **Residue** Displayed color by residue charge.

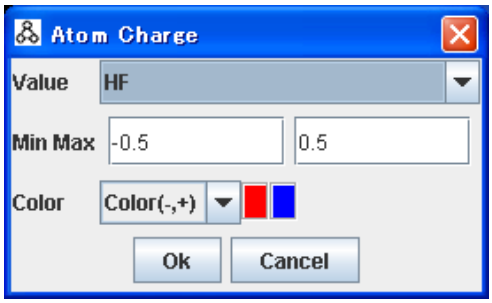


Fig2.38 Charge Dialog Box

- **Fragment** Set colors by fragments from the eight colors cyclically as follows.

- **Chain** Set colors to each chain from the eight colors cyclically as follows.

- **File** Set colors to each file from the eight colors cyclically as well.

- **Structure** Displayed color by 2nd Structure(α Helix, β sheet,others).

2.2.5. Selection

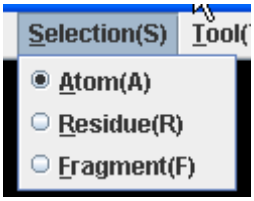


Fig2.39 Selection menu

Click on the display to choose atoms or residues as subjects.

- **Atom** Choose atoms as subjects.
- **Residue** Choose residues as subjects.
- **Fragment** Choose fragments as subjects.

2.2.6. Tool

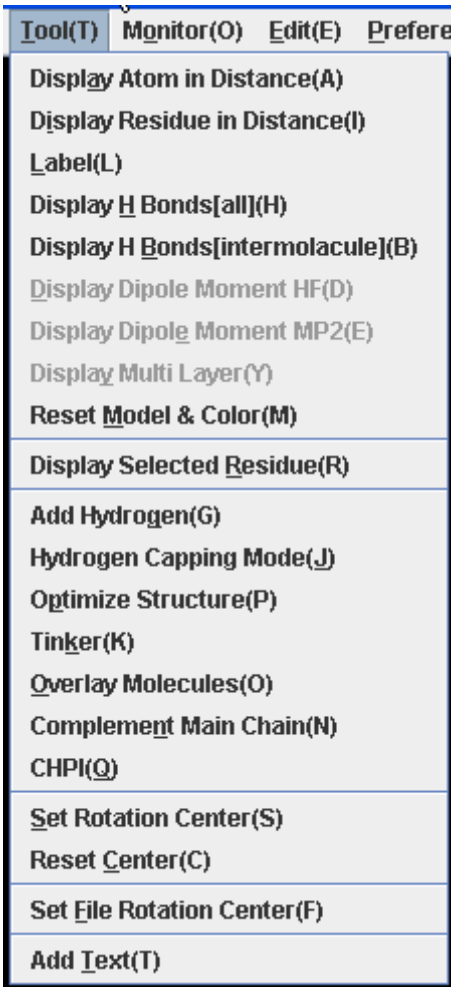


Fig2.40 Tool menu

- **Display Atom in Distance** You can display atoms within the distance from selected a atom or a residue. Before this menu is selected, click on atoms as subjects and specify the distance in the dialog box (Fig2.41). In the **From selected** option, choose between **Atom** and **Residue**. In the **Display List** option, specify the display list of atoms, **On** or **Off.** An example of the display list is shown in Fig2.42. The contents of the atom list can be saved in text format from the **[File] – [Save].** In the **Distance** option, specify the distance.

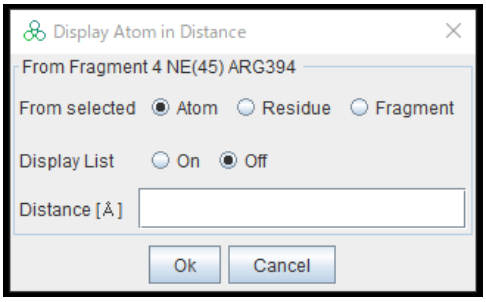


Fig2.41 Display Atoms in Distance dialog box.

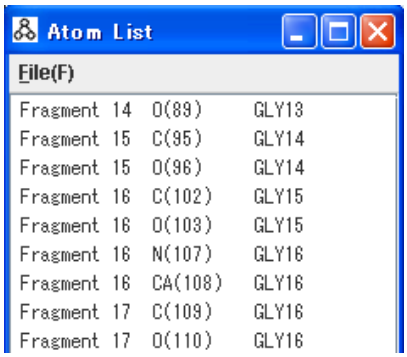


Fig2.42 Atom Lists on Distance Display

♦ **Display Residue in Distance** Display residues within the distance from selected a atoms, a residue or a fragment. The residue can be displayed when any of the comprising atoms is within the distance. Before this menu is selected, click on atoms as subjects and specify the distance in the dialog box (Fig2.43). In the **From selected** option, choose **Atom, Residue or Fragmnet.** In the **Display List** option, specify the display list of atoms, **On** or **Off.** The contents of the atom list can be saved in text format from the **[File] – [Save].** In the **Distance** option, specify the distance.

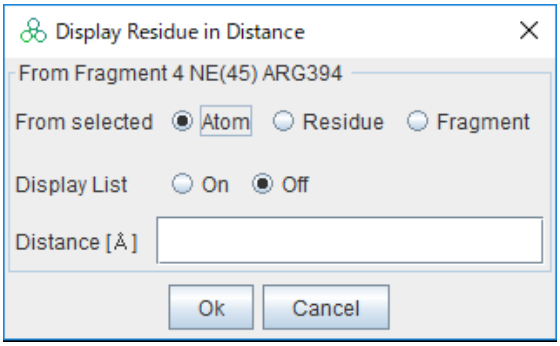


Fig2.43 Display Residues in Distance Dialog Box

♦ **Display Fragment in Distance** Display fragments within the distance from selected a atoms, a residue or a fragment. The residue can be displayed when any of the comprising atoms is within the distance. Before this menu is selected, click on atoms as subjects and specify the distance in the dialog box (Fig2.44 Display Fragment in Distance Dialog Box). In the **From selected** option, choose **Atom, Residue or Fragmnet.** In the **Display List** option, specify the display list of atoms, **On** or **Off.** The contents of the atom list can be saved in text format from the **[File] – [Save].** In the **Distance** option, specify the distance.Specify the display label for the whole residues,fragment and atoms.

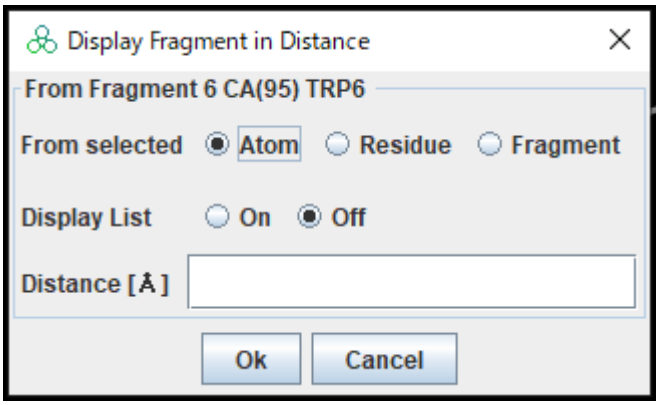


Fig2.44 Display Fragment in Distance Dialog Box

♦ **Label** Specify the display label for the whole residues,fragment and atoms. This dialog box is shown in Fig2.45.

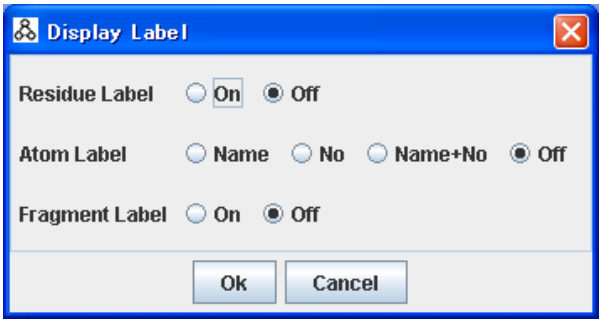


Fig2.45 Display Label Dialog Box

♦ **Display H Bonds [all]** Display all Hydrogen bonds. When they are selected over again, they are deleted.

♦ **Display H Bonds [intermolecular]** Display Hydrogen bonds between molecules. When they are selected over again, they are deleted.

♦ **Display Dipole moment HF** The value of Dipole moment of HF of each

fragmentation is displayed by the arrow. The display option can specified The Preference dialog(Section 2.2.9). The display disappears when selecting it again.

- **Display Dipole moment MP2** The value of Dipole moment of MP2 of each fragmentation is displayed by the arrow. The display option can specified The Preference dialog(Section 2.2.9). The display disappears when selecting it again.
- **Multi Layer** It is available for CPF version 3 or more. Display style : High Layer:Stick. Middle Layer:Wire frame, Low Layer: Cα Line.
- **Reset Model & Color** Reset the display model and colors to the initial condition. Clear the assignment of each residue and atom.
- **Display Selected Residue** Display a dialog box to select residues which you want to display. This dialog box is shown in Fig2.46. When you click on the **Select All** button, all the residues are selected. When you click on the **Unselect All** button, all the residues are unchecked.

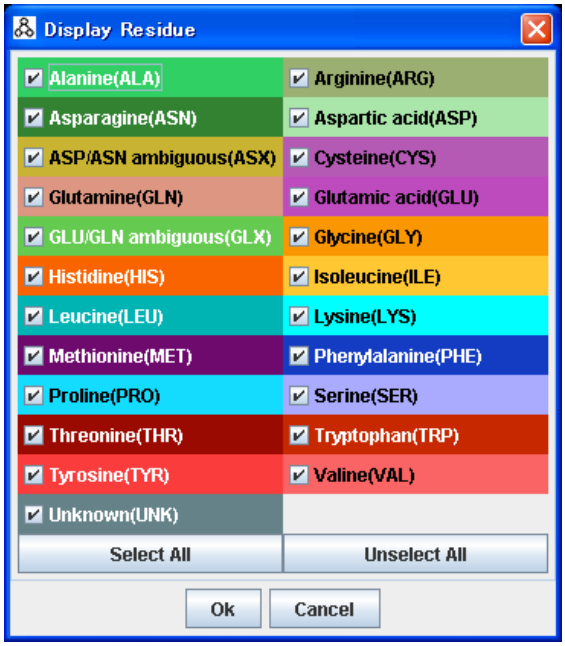


Fig2.46 Display Residue Dialog Box

- **Add Hydrogen** You can add Hydrogen to molecules in the **PDB** format. Set **Options, Input File and Output File** in the dialog box (Fig2.47) The **PDB** file name is set in the **Input File** and the other **PDB** file name added **_addH** is set in the **Input File** as the initial display. After the execution, a dialog box is displayed, that ask if you want to switch the displayed file to the result file. Here, clicking on the Ok button lets the display switch. Refer to Section **7.5**to set Reduce**,** Section **7.6** to set babel, Section **7.7** to set bond Builder.

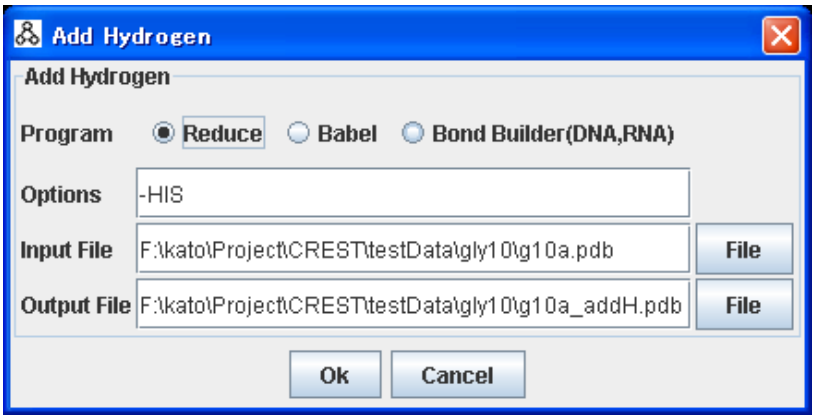


Fig2.47 Adding Hydrogen Dialog Box

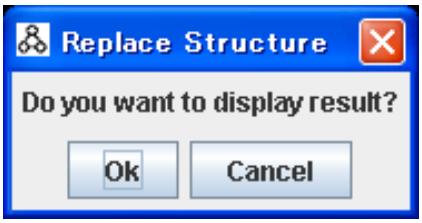


Fig2.48 Confirm to replace Dialog Box

♦ **Hydrogen Capping Mode**

Specify hydrogen capping mode.

Terminal: specify N,C edge process.

Histidine : select hydrogen type at HIS.

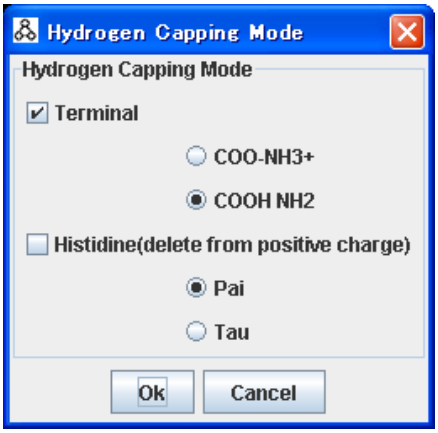


Fig2.49 Hydrogen Capping Mode Dialog Box

♦ **Optimize Structure**

Hydrogen Option file : Specify option file for add hydrogen.

Optimize Option file : Specify option file for optimize. Option detail are

described at Section 5.

Input File : Specify the input file.

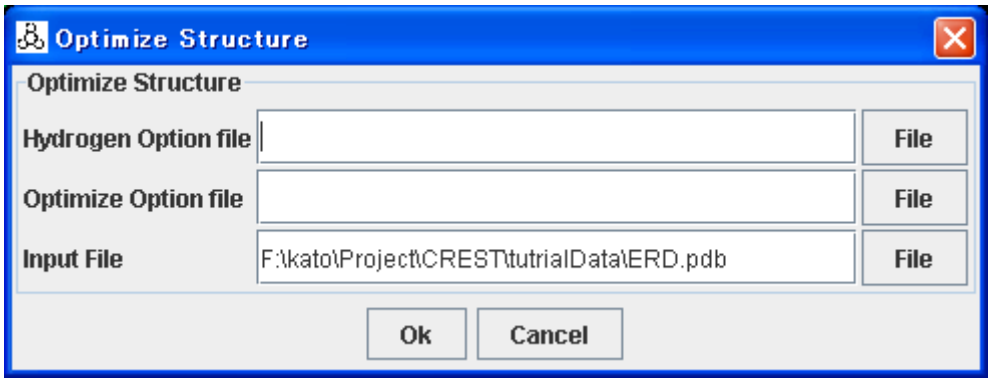


Fig2.50 Optimize Structure Dialog Box

♦ **TINKER**

Exectute Tinker program and display result.

Program : Select a program. If you select Other, please input program name at text field.

Options : Specify options for selected program.

Input File : Specify the input file.

Key File : Specify the key file.

After the execution, a dialog box is displayed, that ask if you want to switch the displayed file to the result file. Here, clicking on the Ok button lets the display switch. The Result file name is ABC_*program name*.pdb if input file name is ABC.pdb.

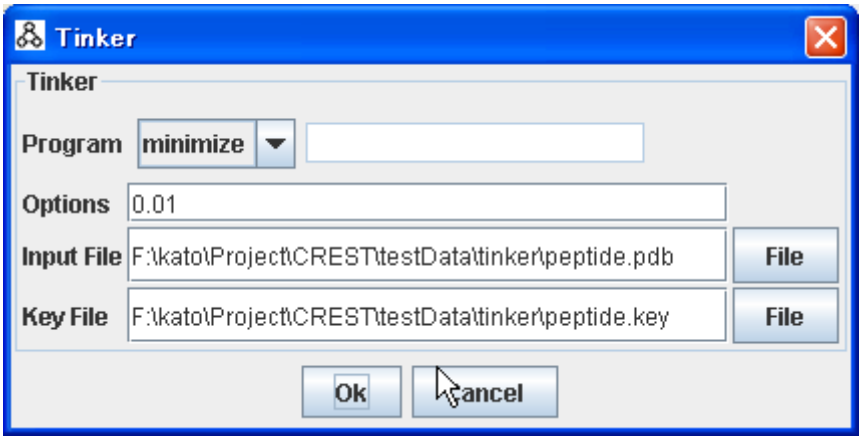


Fig2.51 Tinker Dialog Box

♦ **Overlay Molecule** This option allows you to overlay molecules. Fig2.52 shows a dialog box for overlaying molecules.

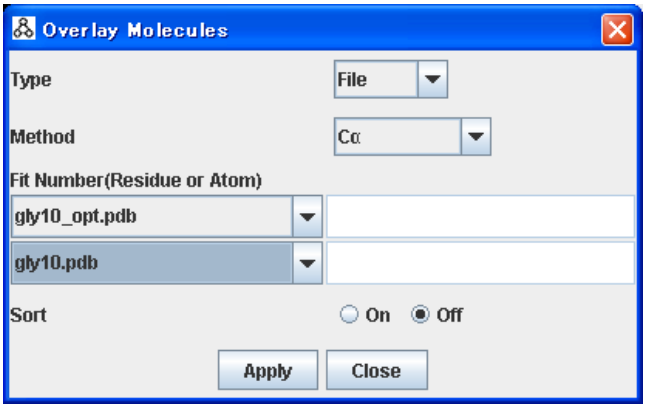


Fig2.52 Overlaying Molecules Dialog Box

Specify **Type, Method**, and **Fit Number** (**Residue** or **Atom**).

1) **Type**

Select a type as a subject to overlay from **File, Residue** and **Atom.**

2) **Method**

Select a method from **Cα, Heavy Atoms** and **All Atoms.** By selecting this menu in the case of **File** or **Residue** in the **Type**, specify the atoms as subjects.

3) **Fit Number (Residue or Atom)**

You can specify files as subjects and set the numbers of atoms or residues of the files. The numbers can be selected by clicking on the residues and the atoms as subjects from a molecule structure display or **Tree** figure. You can also type to input them. If a number is a serial number, connect the serial numbers with a hyphen, **"- "**. If it isn't, type them separated by commas, **" , ".**

Example 1 In the case of residues from **1** to **5,** type**" 1-5 "**

Example 2 In the case of residues, **1,2,5,** type **"1,2,5".**

As the number which you select once can be deleted, use **Back Space** or **Delete** in order to cancel it.

If the number of atoms that you type is higher or lower, the lower number is selected. By clicking on the **Ok** button, an overlaid branch structure is displayed. Here, the center of the movement each atomic group is that of the gravity of all the atoms which are used to overlay. **RMSD** of the selected atoms is shown a message area

4) **Sort**

Specify sort for typed in atom numbers.

♦ **Complement Main Chain**

Complement main chain. Specify main chain No. that is complemented at **Start**

Residue NO. If you do not specify main chain No., viewer complement automatically for lock main chain. You can select residue No. by clicking residue object on Tree. **Complement PDB File** is used to complement. The result file are stored at start folder as xxx_complement.pdb (xxx is original file name)

Fig2.53 Complement main chain Dialog Box

- **CHPI** Execute CHPI program. Please refer section .
- **Set Rotation Center** This allows you to set a rotation center for mouse operation. The display can be rotated around an axis of selected atoms.
- **Reset Center** Reset rotation center for mouse operation.
- **Set File Rotation Center** Set the center of gravity in each file for keyboard operation.
- **Add Text** Display 3D text on 3D window. The Dialog is shown in Fig2.54. Load and save file which specified parameter at File menu.

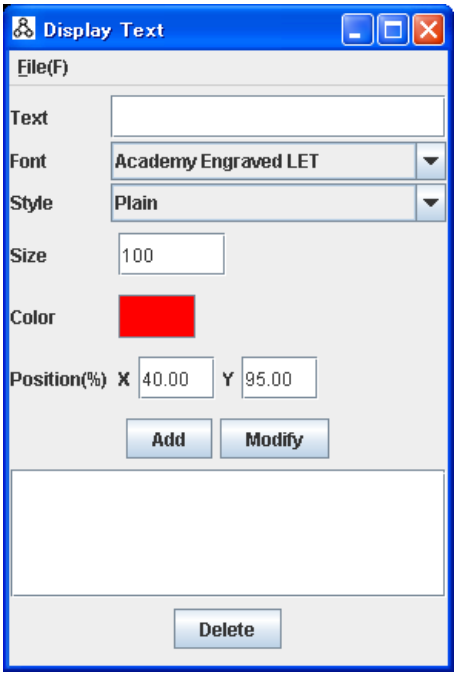


Fig2.54 3D Text dialog

- **Text** Specify text.
- **Font** Specify font.
- **Style** Specify Plane, Bold, Italic, Bold Italic
- **Color** Specify color.
- **Position(%)** Specify position. After display text you can adjust the poison by mouse. Although the position of a mouse is at the lower left of a text, it may shift a little.
- **Add** Display text. Added to the list under a button. Modification and deletion is possible by choose list.
- **Modify** Modify display property. Click to the text list, display property of this text.
- **Delete** Delete text.

2.2.7. Monitor

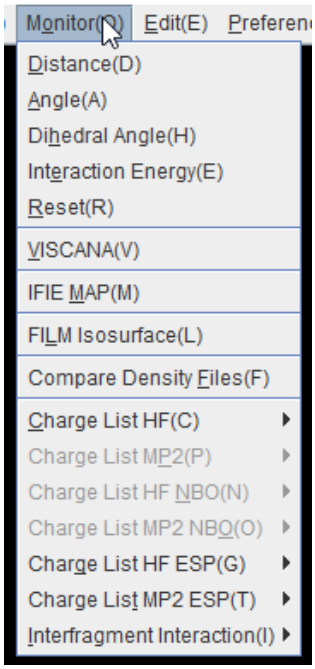


Fig2.55 Monitor menu

- **Distance** Display a distance between atoms. After selecting a menu, clicking on two atoms lets the distance display. In this mode, a color of the menu is green. By clicking on the same atoms, they disappear on the screen.
- **Angle** Display angles between atoms. After selecting a menu, clicking on three atoms lets the angles display. In this mode, a color of the menu is green. By clicking on the same atoms, they disappear on the screen.
- **Dihedral Angle** Display a dihedral angle among atoms. After selecting a menu, clicking on four atoms lets the dihedral angle display. In this mode, a color of the menu is green. By clicking on the same atoms, they disappear on the screen.
- **Interaction Energy** Display the values of the interaction energy between selected fragments. After selecting a menu, clicking on two atoms lets the value of the interaction energy between the fragments display. In this mode, a color of the menu is green.
- **Reset** This option allows you to reset an specified monitor.
- **VISCANA** Amari et al. have proposed the visualized cluster analysis of protein-ligand interaction (VISCANA) for virtual ligand screening based on the FMO method, by using the dissimilarity between the interaction energy

patterns of two ligands and by representing each data point with a color that quantitatively and qualitatively reflects the interaction energy. Details are described in Section2.5 .

- **IFIE MAP**

  Two-dimensional visual representation of IEIE matrix . Details are described in Section 2.6 .

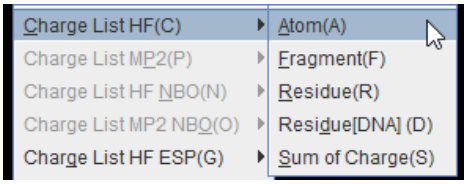
- **FILM Isosurface** Ishikawa et al. have developed a method named ”fragment interaction analysis based on local MP2 (FILM)” by combining the FMO method and local MP2 (LMP2). This function display isosurface by result of FILE. Details are described in Section2.7 .

- **Charge List(HF,MP2,HF NBO,MP2 NBO,HF ESP, MP2 ESP)**

  Display charge value of HF,MP2,HF NBO,MP2 NBO,HF ESP, MP2 ESP.

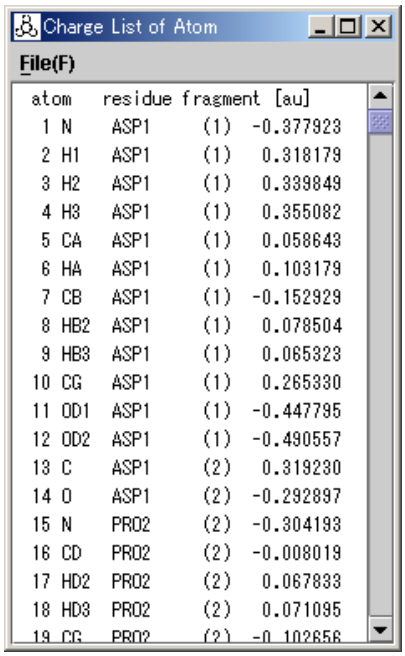
  It’s also possible to output a list from **File menu** to a text file.

  MP2 is available after CPF Version 2, NBO is available after CPF Version 3.

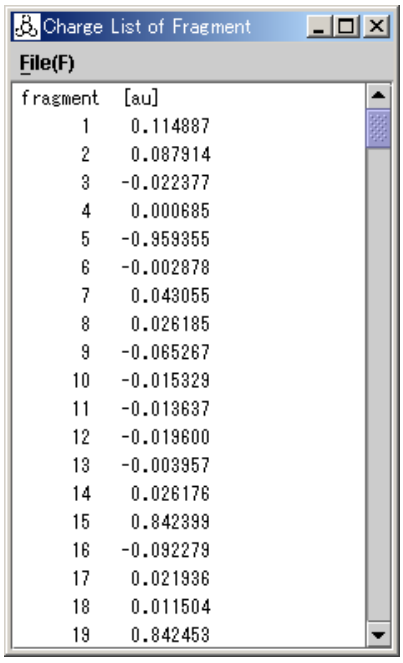


  - **Atom** Display charge list of atoms.
  - **Fragment** Display charge list of fragments.
  - **Residue** Display charge list of residues.
  - **Residue (DNA)** Display charge list of residues. The sum total of the portion with the as other portion of DNA as a base is displayed.

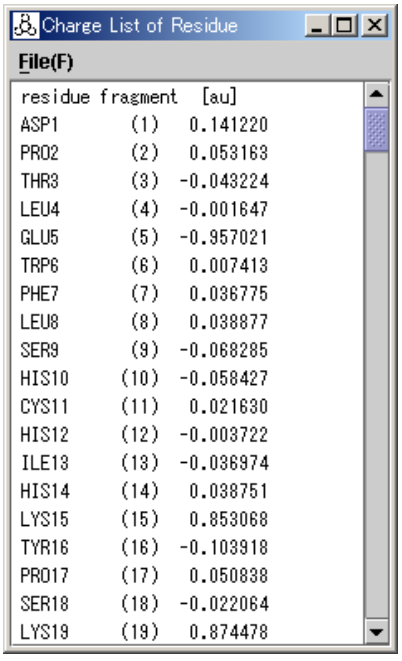
  Example is shown in Fig2.56. It is also possible to output the list to the file.



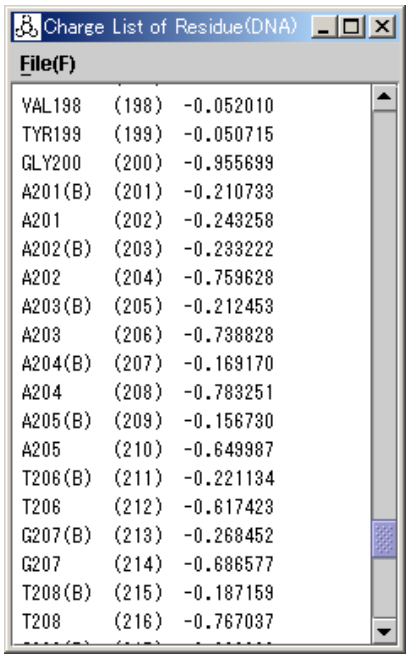
(1) Atom



(2) Fragment



(3) Residue



(4) Residue(DNA)

Fig2.56 Example of charge list.

- **Sum of Charge** The total of the charge of the fragments, residues and atoms within the specified range are displayed. Fig2.57 shows the range specify window.

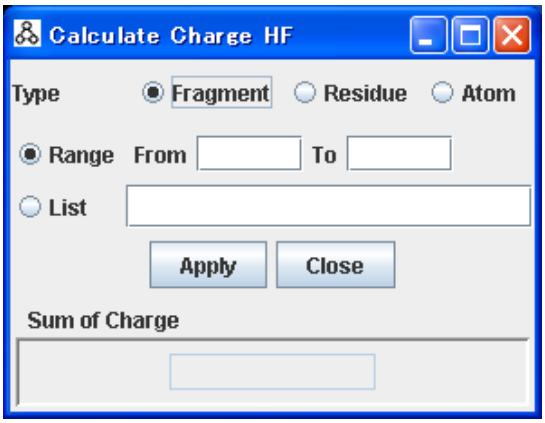


Fig2.57 The range specify window.

- **Interfragment Interaction**
  - 1:1

    You can set colors by the value of the interaction energy between fragments. Select a reference fragment before selecting this menu. Set colors by the energy value from the reference fragment. Selecting this menu lets a dialog (Fig2.58) display to specify the value type, the range of values and the threshold values to set colors. The selection item of Value changes by Version of CPF. Please refer to section 2.6 for details. This is shown by kcal/ mol. Minimum and maximum values of whole files mean the defaults.

    Many Body Calculation (Value:main+side chain)

    This option is available after CPF Version3. If checked it and the fragment is divided by fragmentation with a main chain and an another side chain, the IFIE value is colored one residue from the value which add value of main and side one.

    Color

    Once you modify them, the interaction energy added colors within the range remains displayed until you select this menu next time. When the minimum and the maximum are modified, put **0** to each value in order to set back to the default values. When the threshold value is specified, the fragment under the threshold value of an absolute value can not be displayed. This makes it possible to constrain the display on small fragments of the interaction.

    In the case of the selection of this menu, when you click on molecular

structures, they are added colors by fragments you click.

When the fragments are not selected before opening this menu, molecular structures are added colors by fragments you select next.

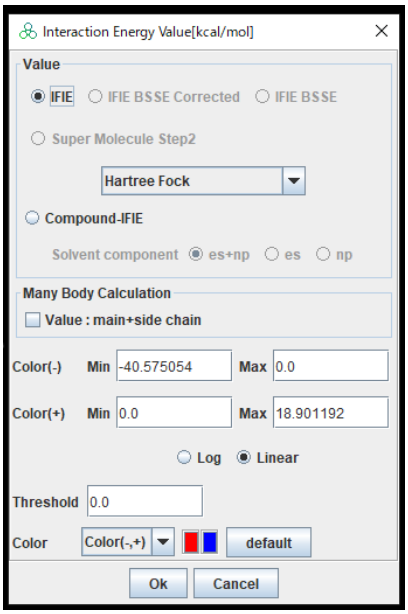


Fig2.58 1:1 Interaction Energy between Fragments Dialog Box

- **1:1 [lock]**

  Set colors by the value of interaction energy between fragments. Unlike the description above, when molecular structures are clicked, the reference fragment is not modified, and the atom's information which you click on is displayed in the message area. Use this in order to get the atom's information which you want to focus attention on, leaving the display on the screen. In the case of this mode, residues and atoms can not be selected and the display attribute can not be modified.

- **N:1**

  Select reference fragments before selecting this menu. Set colors by the energy value from the reference fragments. Selecting this menu lets a dialog (Fig2.59) display to specify the base fragments, the range of values and the threshold values to set colors. User can select multi-fragments on 3D window by pushing the shift key, and also select them on the hierarchical window and the keyboard input.

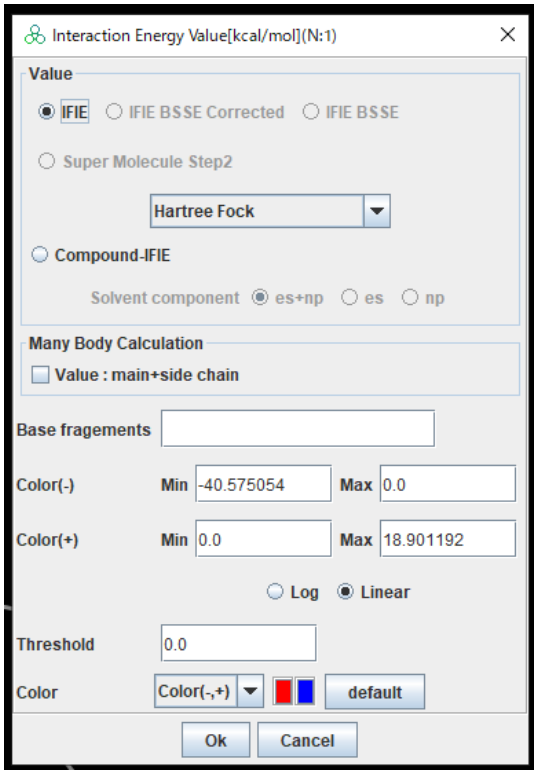


Fig2.59 N:1 Interaction Energy between Fragments Dialog Box

- **N:N**

By selecting reference fragments and object fragments, calculate the interfragment interaction energy between both fragments. Display the value on the message area. A dialog box for N:N interfragment interaction is shown Fig2.60. Before selecting fragments , mark the check box on the left side of input field.

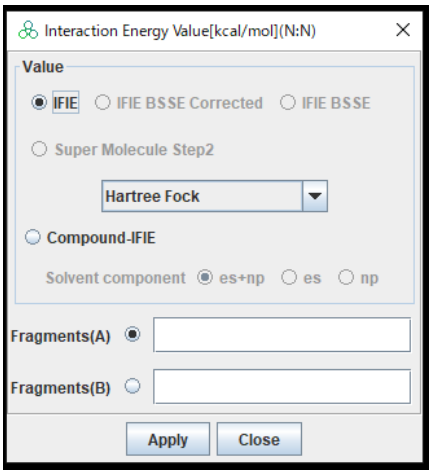


Fig2.60 N:N Interaction Energy between Fragments Dialog Box

- **List**

  List the values of the interaction energy between a selected fragment and each fragment. This list can be saved in the file. Select **[File]**-**[Save]** under the menu bar and specify a file name so as to save the file. If the fragment is a side chain, "_s" is added to the residue name. An example of the display is shown in Fig2.61.

  If **PIEDA** selected, total, ES, EX, CT+mix, DI, Solvent are displayed.

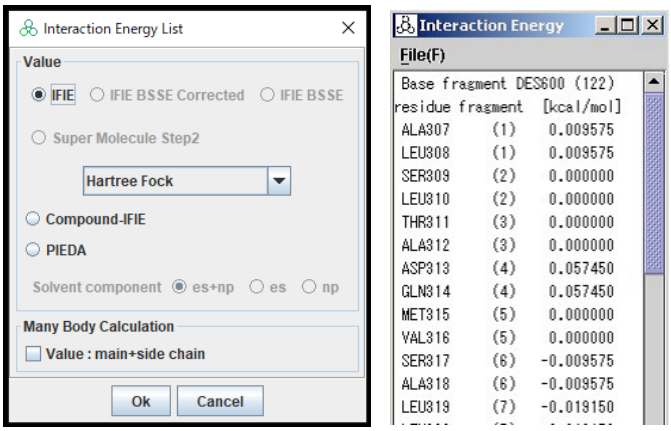


Fig2.61 List of Interaction Energy between Fragments

- **3 Body List** Display value of 3 body and fragment#. If you click a list, correspond fragment is highlighted. Display options are energy lebel, maximum value and minimum. An example is shown in Fig2.62.

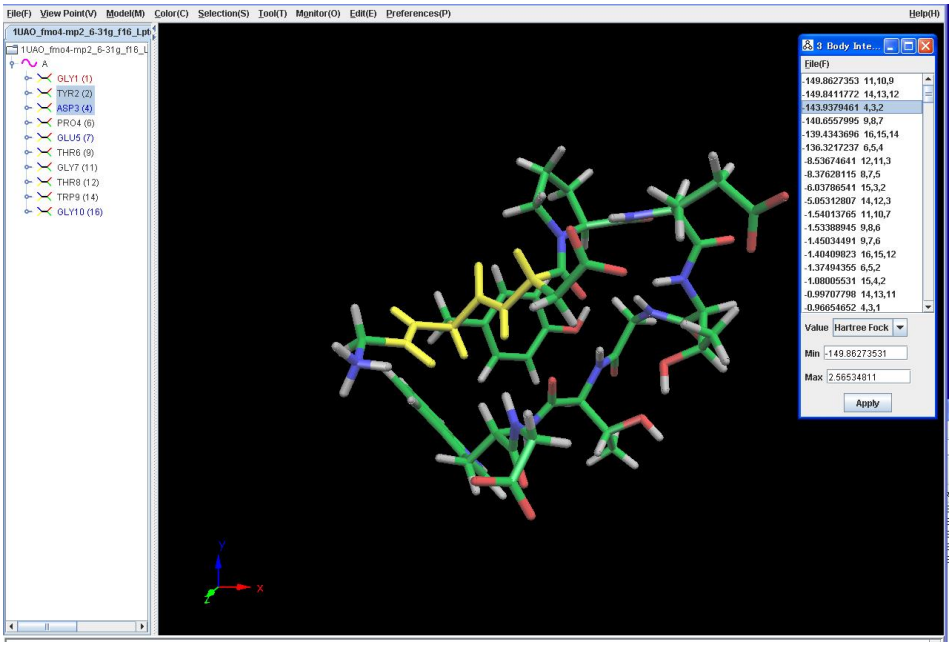


Fig2.62 Example of 3 body value list.

- **4 Body List** Display value of 4 body and fragment#. If you click a list, correspond fragment is highlighted. Display options are energy lebel, maximum value and minimum. An example is shown in Fig2.63.

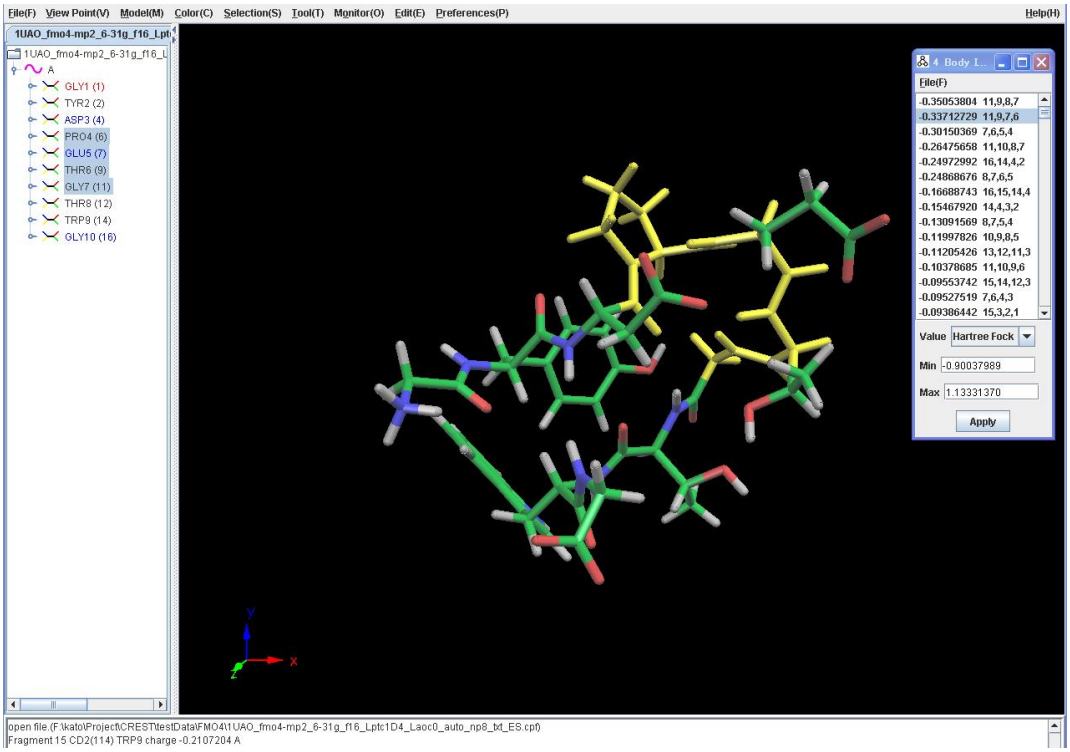


Fig2.63 Example of 4 body value list.

This is example of **Fragment Value:main+side chain** parameter. The molecule is Tripcage. This fragments generated separately main chain and side chain. In Fig2.64 SER20 is colored by each value, then In Fig2.65 colored by a residue.

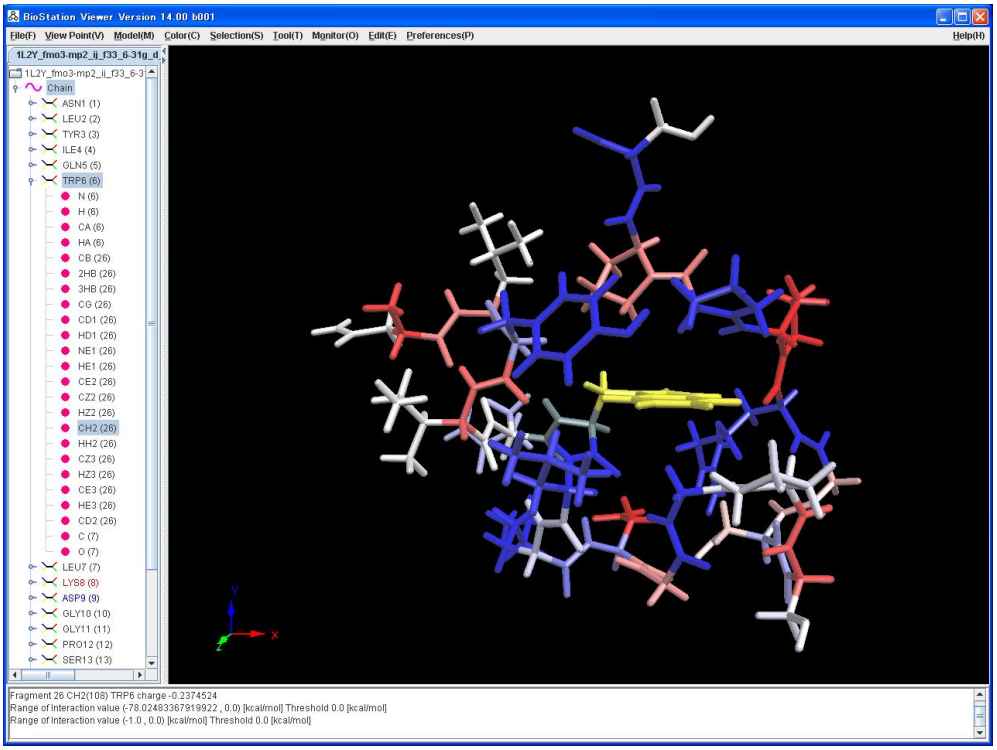


Fig2.64 Example IFIE : Colored by fragment

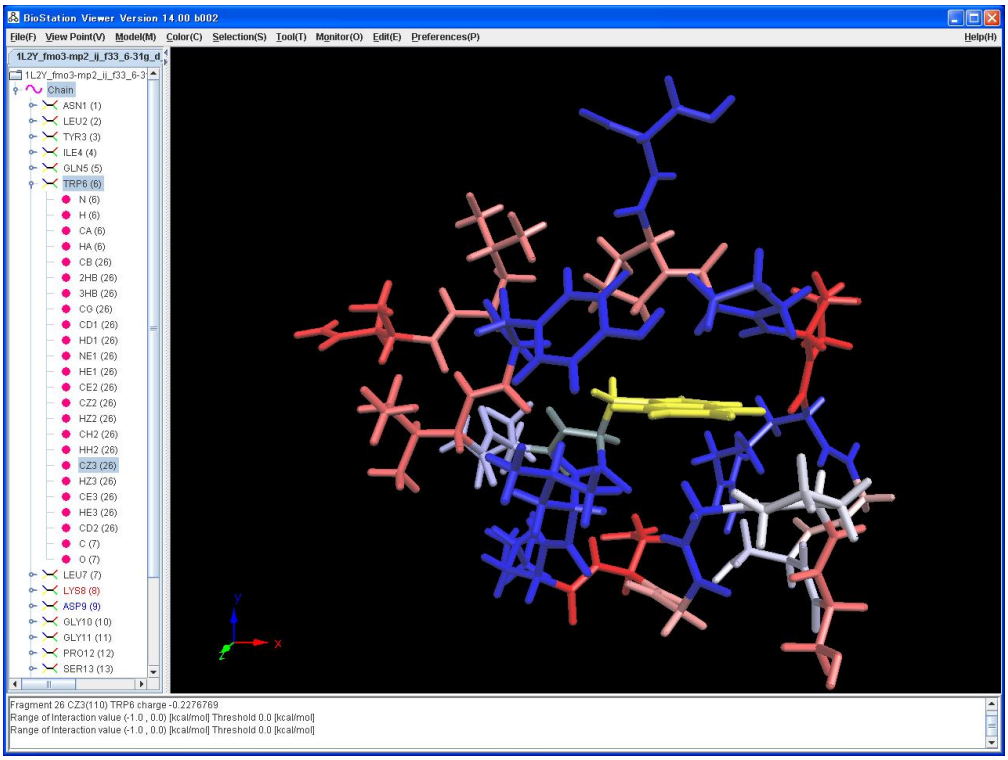


Fig2.65 Example IFIE : Colored by residue

2.2.8. Edit

- **Cut (selected)** This option allows you to cut the selected objects.
- **Cut(unselected)** This option allows you to cut the unselected objects.
- **Undo** This option allows you to undo and cut the objects.
- **Redo** This option allows you to redo the previous action.

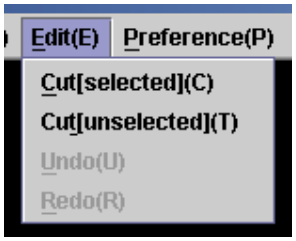


Fig2.66 Edit menu

2.2.9. Preferences

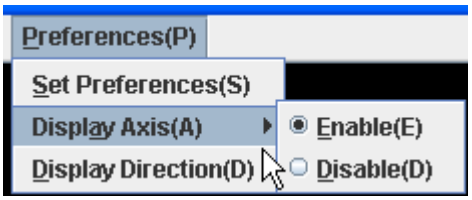


Fig2.67 Preference menu

- **Set Preferences** Popup a preference dialog box, which is shown in Fig2.68. A specification item is changed with a tab. The value on the right side of the input field shows the suggested range. If you increase the resolution to make the nice visualization, but you'll need lots of time and a large memory to display. When done, click on the **Apply** button.

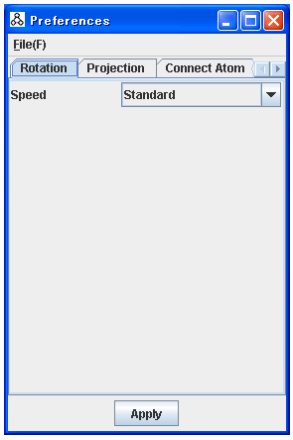


Fig2.68 Preference Dialog Box

1) **File**

This option allows you to load and save files by selecting **[Open]-[Save]** under the file menu. When you execute BioStationViewer, load the file named **.bioViewer** from the current directory to the home directory in order. If there is a file, the setting is reflected.

The value of a default is set with **Set Default Value**.

2) **Rotation**

① **Speed** Specify the rotation speed when **Rotation** in **the** ViewPoint is selected.

3) **Projection**

Specify **Perspective** or **Parallel** for the projection. If user choose **Parallel**, user do not magnify/shrink on mouse operation. User do magnify/shrink on **Rotation/Translation/Magnify** at the **Viewpoint** menu

4) **Connect Aom**

Select judgment standard for connecting bond from Van der Waals or covalent. Scale factor effect on judgment standard.

5) **Resolution**

① **Line Width** : Specify a line width of a wire frame model.
② **Cα Line With** : Specify a line width of a **Cα [Line]** model.
③ **Ball** : Specify a resolution of a ball and stick model.
④ **Stick** : Specify a resolution of a stick model.
⑤ **CPK** : Specify a resolution of a space –filling model.
⑥ **Tube** : Specify a resolution of a **Cα [tube]** model.
⑦ **Ribbon Width** : Specify a width of Ribbon.
⑧ **Ribbon Height** : Specify a height of Ribbon(Solid)
⑨ **Ribbon Line Width** : Specify a width of line Ribbon(Line)
⑩ **Cartoon α Head Height** : Specify a height of cone of Cartoon(α Helix)
⑪ **Cartoon α Radius** : Specify a radius of Cartoon(α Helix)
⑫ **Cartoon width** : Specify a width of Cartoon(other)
⑬ **Cartoon β Height** : Specify a height of Cartoon(β sheet)

6) **Radius**

① **Ball** : Specify a size of a ball in the ball and stick model.
② **Bond** : Specify a line width of a bond in the ball and stick model.
③ **Stick**: Specify a line width in the stick model.
④ **Tube** : Specify a line width of Tube in the **Cα [tube]** model.

7) Color

① **Background** : Select background colors in the display.

② **Atom** : Set colors to each atoms. This dialog box is shown in Fig2.69.

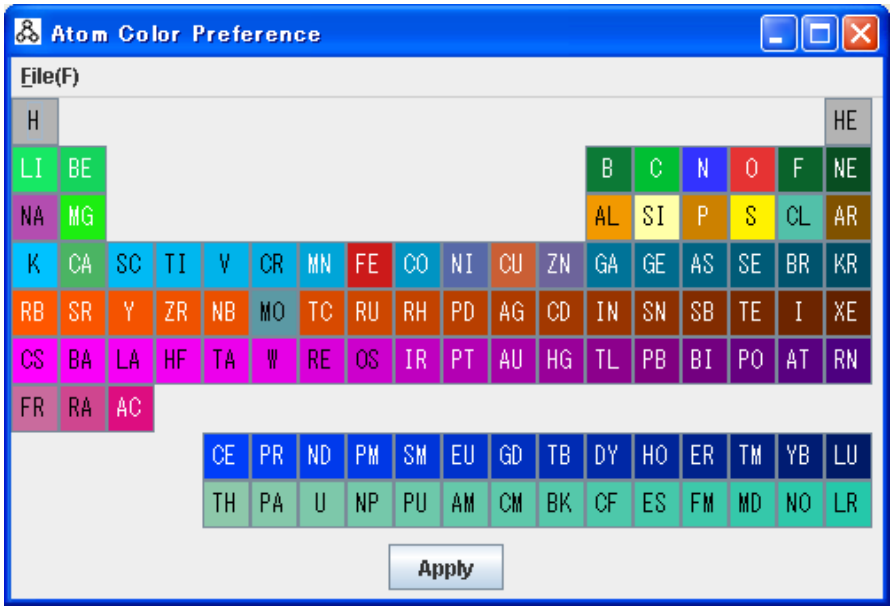


Fig2.69 Atom Colors Preference

③ **Residue** : Set displayed colors to each residue. This dialog box is shown in Fig2.70.

Fig2.70 Display Colors of Residues Preference

④ **Fragment** ： Select displayed colors of fragments. This dialog box is shown in Fig2.71. Set colors to fragments, chains and files from the eight colors cyclically.

Fig2.71 Display Colors of Fragments Preference

⑤ **Chain** ： Set displayed colors of chains.

⑥ **File** ： Set displayed colors of files.

⑦ **DNA**： Set displayed colors of **ATGC** of **DNA**.

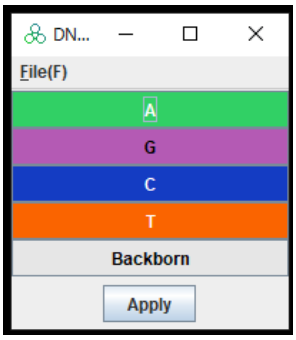


Fig2.72 Display Colors of the DNA

⑧ **Isosurface** ： Set colors of the isosurface value. This dialog box is shown in Fig2.72.

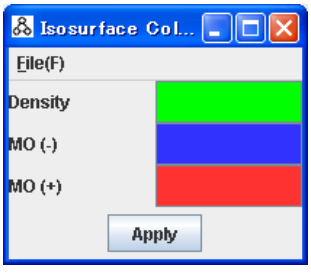


Fig2.73 Display Colors of the Isosurface Value

⑨ **2nd Structure** : Second Structure.

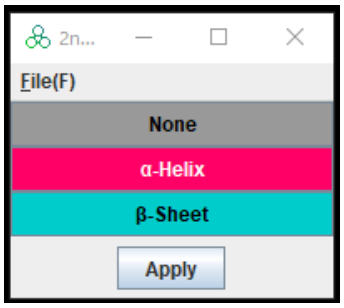


Fig2.74 Display Colors of the 2nd Structure

⑩ **Selected** : Set color of selected item.

⑪ **IFIE** : IFIE value

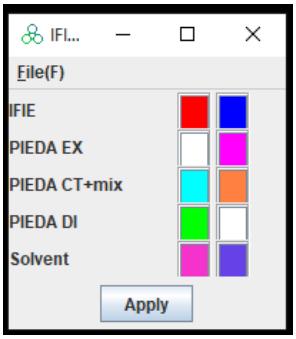


Fig2.75 Display Colors of the IFIE Value

8) Arrow : Specify the vector property. The dialog box is shown in Fig2.76.
Arrow(Trajectory) : Specify arrow preference for trajectory.
Arrow(Dipole moment HF) : Specify arrow preference for Dipole moment(HF)
Arrow(Dipole moment MP2) : Specify arrow preference for Dipole moment(MP2)

① Display The On/Off of a display of an arrow is specified.

② Style Specify style of arrow.

1. Radius Specify the body and head width.
2. Head Length Specify the head length fix or ratio.
3. Scale Specify scale of arrow. The length of 1 of a display is 1Å.

③ Color Specify color.

1. Value Specify min,max value. The display color is changed from blue to read.
2. One color Display the color which is specified

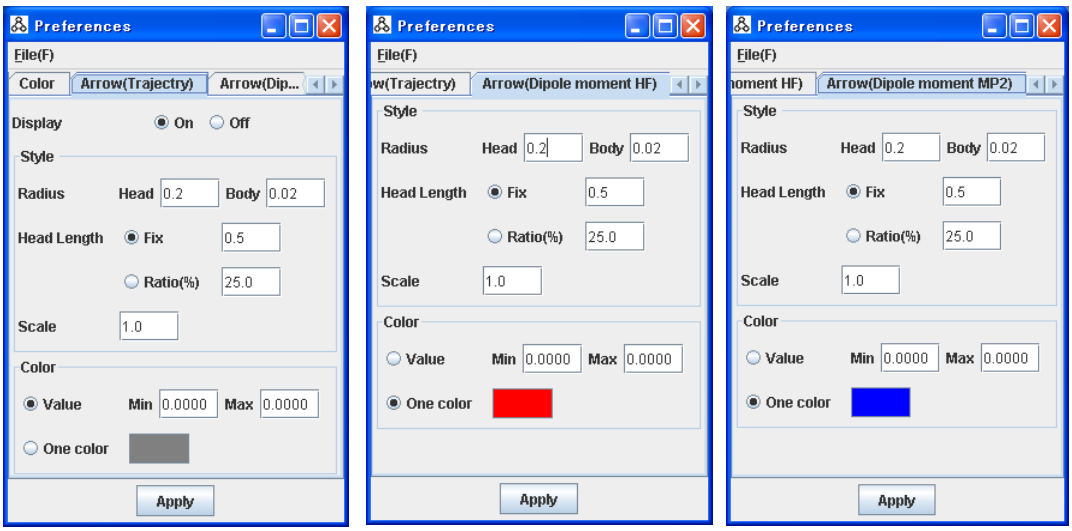


Fig2.76 Arrow Dialog Box

9) Number of decimal

Number of decimal for angle, distance, and IFIE value on 3D.

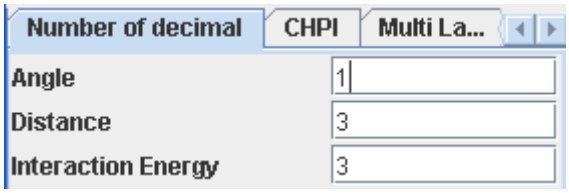


Fig2.77 Number of decimal Dialog Box

10) CHPI

Specify CHPI result preference. The dialog box is shown in Fig2.78.

① Model Select Model (Line Solid/Line Dash/Stick)

② Color Specify color.

③ Line Width Specify line width

④ Stick Radius Specify Stick radius

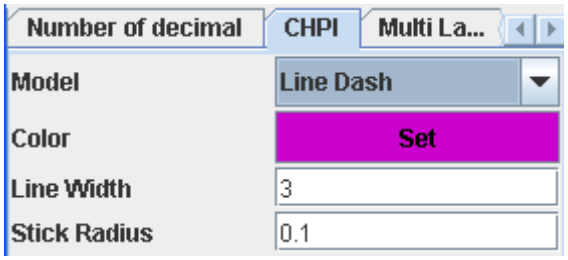


Fig2.78 CHPI Dialog Box

11) Multi Layer

Specify the color of each layer. The dialog box is shown in Fig2.79.

① High Layer Color　Specify the color of High Layer

② Middle Layer Color　Specify the color of Middle Layer

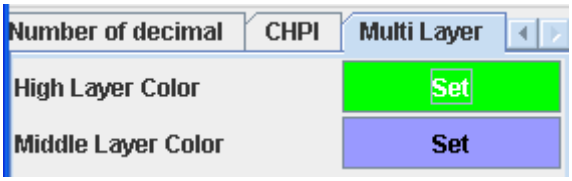


Fig2.79 Multi Layer Dialog Box

12) Font size

Fig2.80 Font size Dialog Box

- **Display Axis** Specify the presence of a coordinate axis in the lower-left side of the screen.
- **Display Direction**　Specify the presence of the direction to each file by typing.

2.2.10. Help

- **View Help(Japanese/English)**　　Open a **Pdf file** to display a manual.

2.3. Section

Section specification is performed on GUI by the specification of the central point, the specification of a rotation angle, or the normal vector of a section plane. Fringe and isoline are available. It is colored with the value of the file to input. The color scale range can be manually set to a specific minimum and maximum value. Multi-section is available. The diagram of section is shown in Fig2.81, and The Section dialog is shown in Fig2.82.

- No.

  The number of the specified section is shown. By clicking **Add** button, add section. The specified section display as white transparency plane in 3d window. By clicking **Delete** button, delete the section.

- Specify Section Plane
  - Center

  Specify the center points(X,Y,Z) of section by using the slider or the keyboard input.
  - Angle

  Specify the angle of section by using the slider or the normal vector of section. A purple axis is the center of an angle and an orange axis the is center of B angle. C rotates centering of the normal vector of section.

  When specifying the normal vector(x,y,z), move the section by hitting Return key.
  - Set Plane

  Select a standard plane(xy, yz or xz).

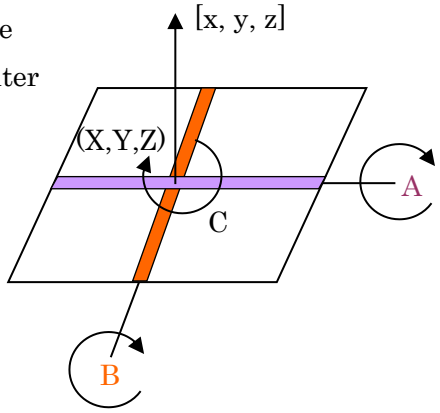


Fig2.81 The diagram of section

- Section Property
  - Display

  Specify enable/disable to display the section.
  - Value

  Select value from the electrostatic potential or the electron density.
  - Color Range

  Specify the color range of value.
  - Type

  Select type from fringe or isoline.

➢ Transparency

Specify transparency.

➢ Number of Lines

Specify the number of Lines . In the case of molecular orbital 1e-8 is zero value.

➢ Draw

Draw the section.

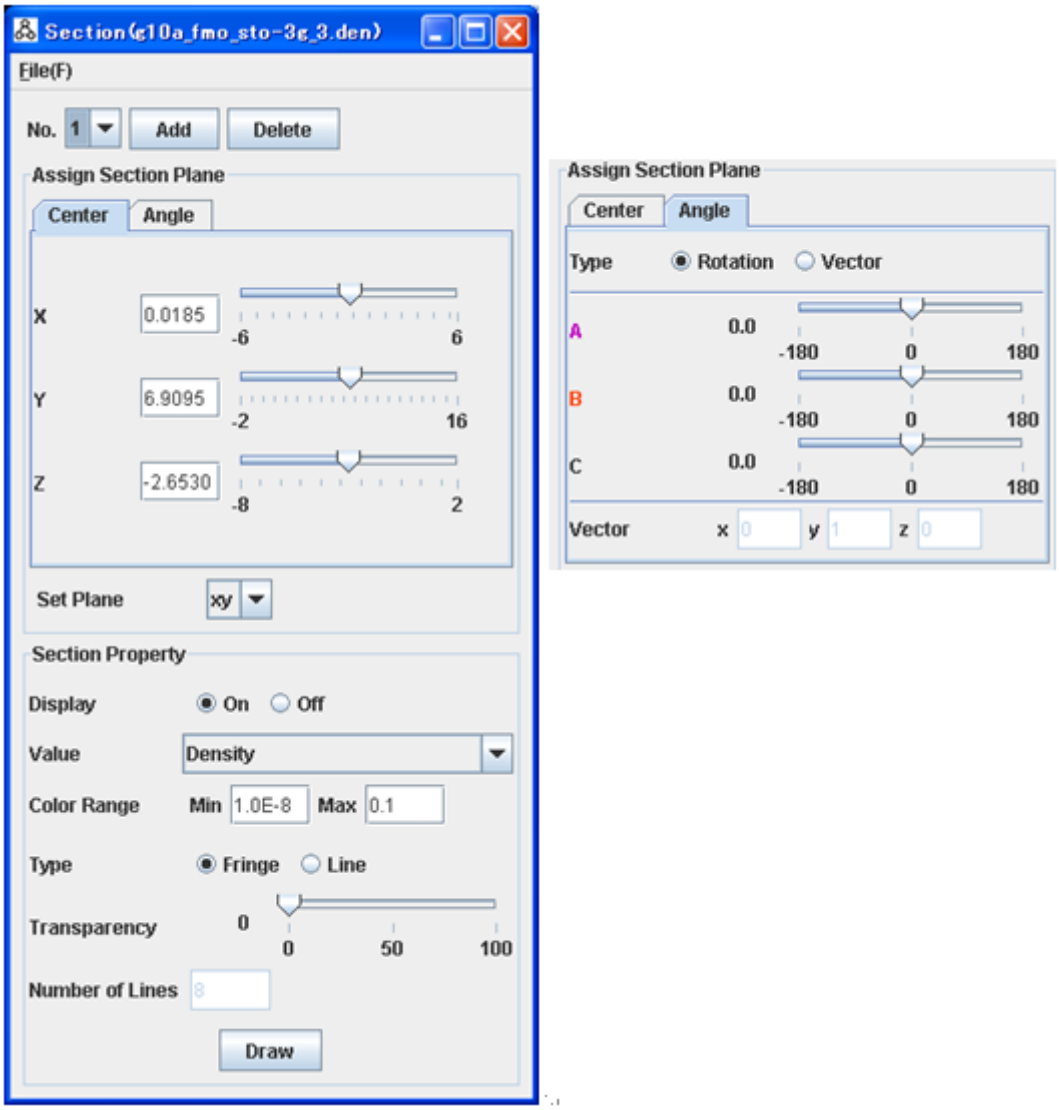


Fig2.82 The Section Dialog box

2.4. Trajectory

2.4.1. File format

The file format are two types.

1) A file extension is trj. The file includes the value of the energy of each step. Type the number of atoms at the first line, an energy value at the next line and the coordinate of atom. Without energy value, type 0 at the energy line. # is a comment until the end of the line.

   Add Fragment No. at end of line for recognition of fragment. There may not be the description by you if there is no necessity of the fragmentation. Before load file select Color -> Fragment, molecular structure is colored by fragment number.

Example of file.

```
1000     # number of atom
# step 0
9.87654  # energy
O 1.23345678 1.23345678 1.23345678
H 1.23345678 1.23345678 1.23345678
N 1.23345678 1.23345678 1.23345678
C 1.23345678 1.23345678 1.23345678
.....
# step 1
9.87654  # energy
O 1.23345678 1.23345678 1.23345678
H 1.23345678 1.23345678 1.23345678
N 1.23345678 1.23345678 1.23345678
C 1.23345678 1.23345678 1.23345678
.....
```

Example of file with fragment number

```
1000     # number of atom
# step 0
9.87654  # energy
O 1.23345678 1.23345678 1.23345678 1
H 1.23345678 1.23345678 1.23345678 1
N 1.23345678 1.23345678 1.23345678 1
C 1.23345678 1.23345678 1.23345678 2
.....
# step 1
9.87654  # energy
O 1.23345678 1.23345678 1.23345678 1
H 1.23345678 1.23345678 1.23345678 1
N 1.23345678 1.23345678 1.23345678 2
C 1.23345678 1.23345678 1.23345678 2
.....
```

2) New trajectory file format. File extensions are trj2, tj2,tr2. It is extensional format of XYZ. The number of atoms, a comment, atomic coordinates, and the vector value are described for every step. A comment is expressed in the group of a tag and a value and displays graph with this value. When a tag is “Label”, it becomes the text of 3d viewer. "=" is described between a tag and a value. There may be "," between items. Refer to the Arrow of Preference specification for change of the display attribute of a vector.

Example of file.

```
8
label="MD step 1" Ekin(Ha)=0.0000000000 Epot(Ha)=-31.6395526318
Etot(Ha)=-31.6395526318 Fmax(Ha/bohr)=0.1505408174
Si 0.8686973703168 0.5700826492704 0.67866982056 -0.090561 0.076468 -0.082145
Si 4.6421015726304 4.7235419510976 4.75068874392 0.026857 0.018088 0.002683
Si 0.67866982056 3.4204958956224 3.5019362740896 -0.022970 0.000783 -0.024173
Si 4.75068874392 2.03600946168 2.03600946168 0.032733 -0.001620 -0.002599
Si 3.4204958956224 0.7872569918496 3.3933491028 -0.012222 -0.029104 -0.017059
Si 1.764541533456 4.886422708032 2.03600946168 0.101043 -0.077951 0.079853
Si 3.5019362740896 3.3933491028 0.7058166133824 -0.050445 -0.000565 0.003814
Si 2.03600946168 2.0088626688576 4.6421015726304 0.015567 0.013899 0.039625
8
label="MD step 2" Ekin(Ha)=0.0000001274 Epot(Ha)=-31.6395536508
Etot(Ha)=-31.6395535234 Fmax(Ha/bohr)=0.1505348131
Si 0.868696441081553 0.570083434040259 0.678668977580644 -0.090558 0.076465 -0.082141
Si 4.64210184833175 4.72354213683881 4.75068877143722 0.026857 0.018087 0.002683
Si 0.678669585076125 3.42049590356006 3.50193602590547 -0.022970 0.000783 -0.024173
Si 4.75068907994755 2.0360094452755 2.03600943522114 0.032732 -0.001620 -0.002599
Si 3.42049577020739 0.787256693393632 3.39334892764233 -0.012222 -0.029103 -0.017058
Si 1.76454257011423 4.88642190844518 2.03601028084638 0.101040 -0.077948 0.079849
Si 3.50193575655425 3.39334909697905 0.705816652541516 -0.050443 -0.000565 0.003814
Si 2.03600962149153 2.00886281120628 4.64210197903853 0.015567 0.013899 0.039623
 …. .
```

2.4.2. Control animation

Load a trajectory file from **File** menu at the main window. Display processing is performed at the time of file reading. In proportion to the number of steps, the number of atoms, and the display style of molecular structures, it takes processing time. After processing pop up a trajectory control dialog box(). If the file includes energy, an energy graph appears on the panel.

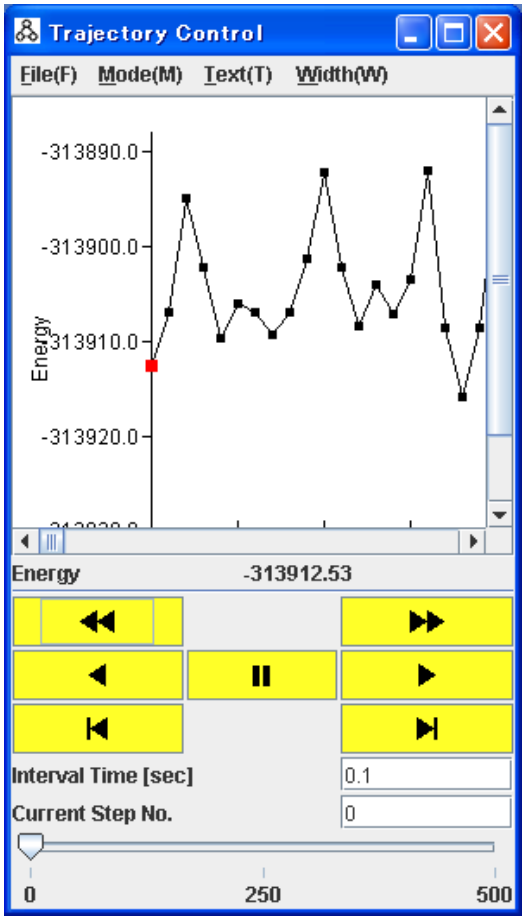


Fig2.83 Trajectory Control Dialog box

1) menu

- File
  - ♦ Create image files

    Output a JPEG file to create an animation file at the specified directory. The file name is imageXXX.jpg. Sequential numbers go into XXX. Specify Output Folder and Screen Size, and by clicking **Create** button, display each step and output files. However, keep in mind that it may drop out some frames with the performance of CPU and a graphic card.

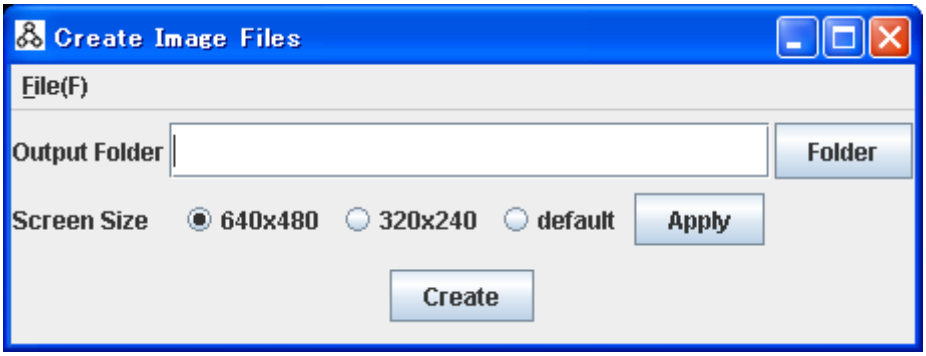


Fig2.84 Create Image Dialog box

♦ Create Video File

Create video file as output file name. You can choose two Video Format, MSVIDEO and Quick Time. MSVIDEO needs a large disk but easy to use with Power Point. Quick Time file is small file size and needs Quick Time player to play video.

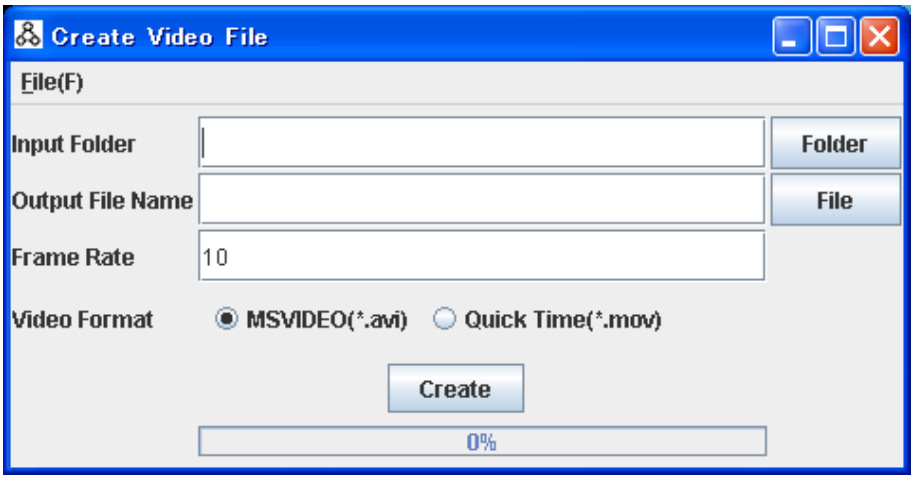


Fig2.85 Create Video Dialog box

♦ Save Graph Image File

The graph currently displayed can be saved as JPEG, PNG, or a Postscript file. Form is judged by the extension of the file name specified on the file selection dialog.

♦ Close

Close this dialog.

- Mode
  - ♦ Cyclic

    Play cyclic.

- Text

  Specify 3D text property. Font, Style, Size, Color and Position. The dialog box is shown in Fig2.86.

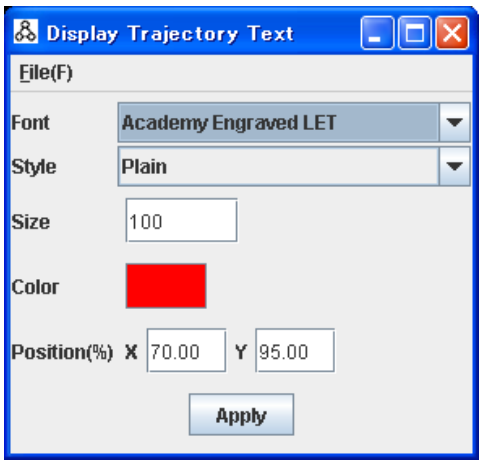


Fig2.86 Text Dialog box

- Width
  - ♦ Ajust

    The size of a graph horizontal axis is united with the size of a display window, and the whole is displayed.

2) Control Panel

- ◀◀ top

  skip to the top frame.
- ◀ reverse

  reverse play
- ⏮ back

  back 1 frame
- ⏸ stop

  stop
- ▶▶ tail

  skip to the last frame

- play

  play
- forward

  forward 1 step
- Interval Time [sec]

  Interval Time. Too small value is not available.
- Current Step No.

  Display a current step number. If user input a step number and hit Return key, display that frame. The step number starts from 0.

2.5. VISCANA

The visualized cluster analysis of protein-ligand interaction (VISCANA) for virtual ligand screening based on the FMO method, by using the dissimilarity between the interaction energy patterns of two ligands and by representing each data point with a color that quantitatively and qualitatively reflects the interaction energy.

When you select **[Monitor]-[VISCANA]**, popup an window of VISCANA(Fig2.87). Main View consists three parts. At the left side, show the dendrogram that described result of cluster analysis. At the middle part, show the ligand name and add color by binding energy. When you take the mouse cursor on the item, show the binding energy of this ligand. At the right side, show interaction energy between ligand and each fragment of protein.

When you take the mouse cursor on the item, show the interaction energy and fragment number. It is working with 3D View. Select a fragment by push left button of mouse cursor on the fragment, and clicked "**3D Model View" button**, display molecular structure on 3D View with highlighted that fragment. It is easily understood where there is a position of the fragment that you are selected.(Fig2.88)

There are two tabs "Data" and "Analysis" the lower part of window. Specify display properties at "Data" tab, display result of Cluster Analysis at "Analysis" tab.

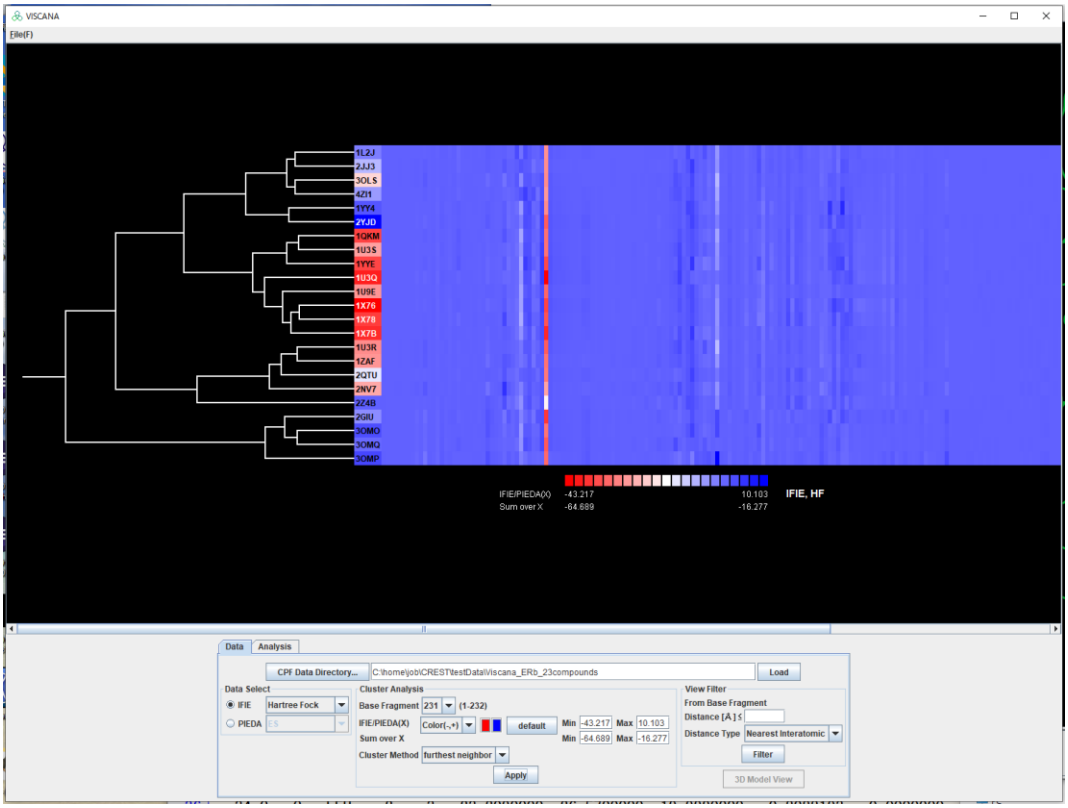
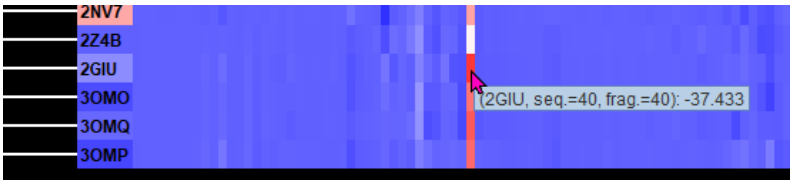


Fig2.87 VISCANA window



Select 2GIUcell, and click “3D Model View” button

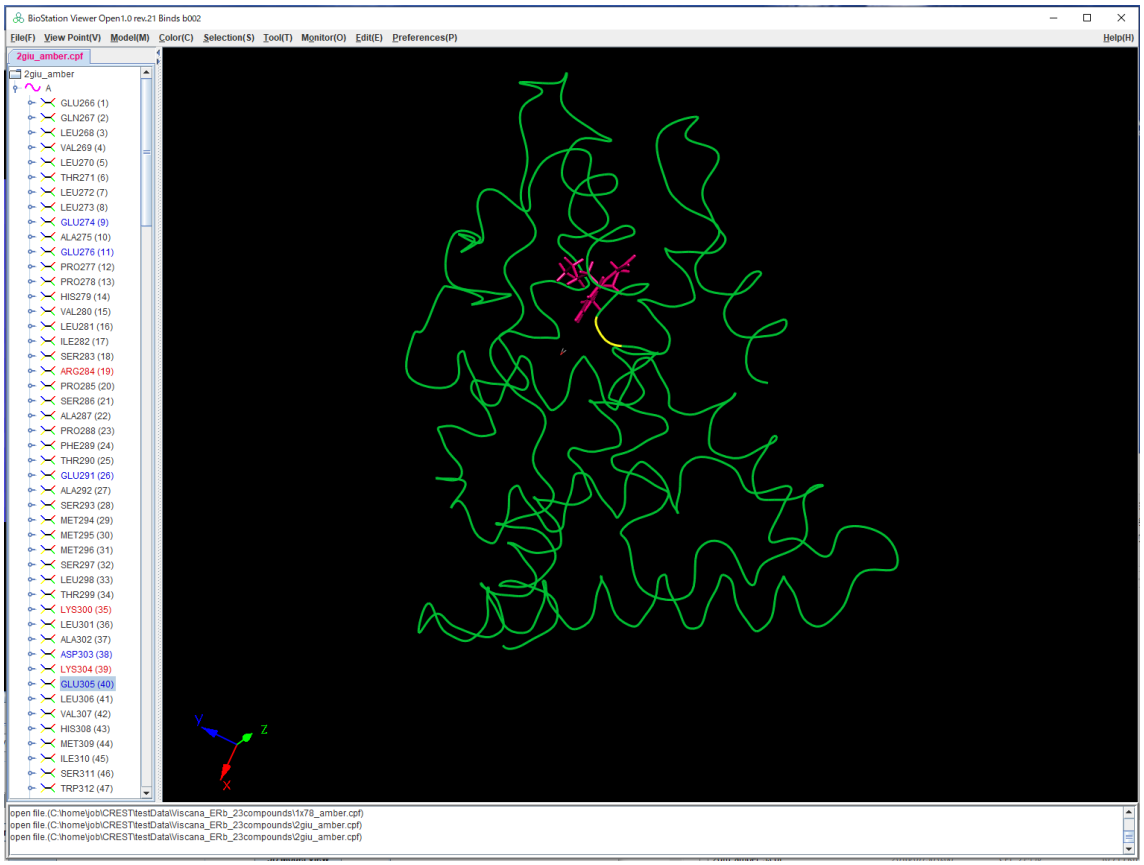


Fig2.88 High light No.40 fragmnet.

2.5.1. Menu

- File menu
  - ♦ Load CSV File

    Load CSV file and visualized. File format : 1 line shows 1 file.

    file name, value#1, value#2 …. value#N

    It continues number of files.
  - ♦ Save image

    Save image file(PNG/Tiff)
  - ♦ Save CSV file(Raw data)

output IFIE raw data as CSV.

```
"1ERE H2O EST600","0.06704805904155364","0.004935882592690177","-0.004161305550951511","-0.003949102
"1L2J ETC600","0.09012984097353183","-0.01233636905089952","-0.06828176585258916","-0.01509068469749
"2I0G I0G1","0.017258612366276793","-0.001573896166519262","0.018046159180812538","0.007235390599817
"1QKM GEN600","0.06880561851721723","-0.021663096427801065","0.014909053323208354","0.00948922598036
"1U3Q 272501","0.03297848604415776","-0.022831991052953526","-0.029928279720479622","-0.030791792451
```

Fig2.89 Example file of Save CSV file(Raw data).

- Save CSV file (Raw data with cluster#)
  output IFIE raw data with cluster# as CSV.

```
"Cluster","Title","GLU266(1)","GLN267(2)","LEU268(3)","VAL269(4)","LEU270(5)","THR271 …
"1","1L2J","0.004422543410328217","-0.0017177658883156255","-0.00244106788886711","-0 …
"1","2JJ3","-0.002946797889308072 6","0.009508218805422075","0.00513503716501873","0.0 …
"1","3OLS","-0.02434854664898012","0.016759303412982263","1.7115636728703976E-4","0.0 …
"1","4ZI1","-0.010549071987043135","0.008117687830235809","-0.0062418528978014365","0 …
"1","1YY4","-0.01569034659769386","-0.0017285672220168635","-0.01229054767463822","-0 …
"1","2YJD","0.0018548246443970129","-0.016161552906851284","-0.01687829554430209","-0 …
"2","1QKM","-0.01033311647188384","0.016623245552182198","-0.009609946864657104","-0. …
"2","1U3S","-0.029734298965195194","-0.002225780044682324","-0.018211634043836966","- …
"2","1YYE","-0.03943274790071882","-0.0013379475567489862","-0.021705138933612034","- …
"2","1U3Q","-0.03647428649128415","0.0033225355291506276","-0.02517848760180641","-0. …
"2","1U9E","-0.01673011857928941","-0.0054608482751064","-0.010434834490297362","-0.0 …
"2","1X76","-0.0112376005272381","-0.0026311323599657044","-0.021413976384792477","-0 …
"2","1X78","0.007286158637725748","0.010399236518424004","-0.010982639651047066","-0. …
"2","1X7B","-0.028911706773214974","0.002566304348874837","-0.011377972521586344","7. …
"3","1U3R","-0.029407480076770298","0.007906074039055966","-0.0059105008986080065","0 …
"3","1ZAF","-0.027610782271949574","0.009124418895225972","2.941601269412786E-4","0.0 …
"3","2QTU","0.023051065276376903","0.011827122478280216","-0.0036844993592239916","-0 …
"3","2NV7","-0.04559103159408551","0.010739662931882776","-0.0036646668886533007","0. …
"4","2Z4B","0.023356488600256853","0.008737203490454704","-0.0036989772343076766","-0 …
"5","2GIU","0.04086011557956226","-0.008129799374728464","-0.018197902871179394","-0. …
"5","3OMO","0.008137744909618 05","-0.010438287048600614","-0.01630014342663344","-0.0 …
"5","3OMQ","-0.01761319577053655","-0.013049710614723153","-0.021847352050826885","-0 …
"5","3OMP","0.05095229222206399","-0.0370117163984105","-0.022769159768358804","-0.03 …
```

Fig2.90 Example file of Save CSV file(Raw data with cluster#).

- Save CSV file (filtered data)
  Output IFIE data from Base Fragment in specified distance. Specify output file name(ex. IFIE_filtered.csv), then output index information file(ex. IFIE_filtered_fragment_number.csv) . Example shows in Fig2.91.

```
"1ERE H2O EST600","0.06704805904155364","0.004935882592690177","-0.004161305550951511","-0.003949102
"1L2J ETC600","0.09012984097353183","-0.01233636905089952","-0.06828176585258916","-0.01509068469749
```

```
"2I0G I0G1","0.017258612366276793","-0.001573896166519262","0.018046159180812538","0.007235390599817
"1QKM GEN600","0.06880561851721723","-0.021663096427801065","0.014909053323208354","0.00948922598036
"1U3Q 272501","0.03297848604415776","-0.022831991052953526","-0.029928279720479622","-0.030791792451
```

a) output file

```
"1ERE H2O EST600","1;19;19","1;20;20","1;21;21","1;33;33","1;34;34","1;35;35","1;36;36","1;37;37","1
"1L2J ETC600","2;19;17","2;20;18","2;21;19","2;33;30","2;34;31","2;35;32","2;36;33","2;37;34","2;38;
2I0G I0G1","5;19;17","5;20;18","5;21;19","5;33;30","5;34;31","5;35;32","5;36;33","5;37;34","5;38;35"
"1QKM GEN600","3;19;17","3;20;18","3;21;19","3;33;30","3;34;31","3;35;32","3;36;33","3;37;34","3;38;
"1U3Q 272501","4;19;17","4;20;18","4;21;19","4;33;30","4;34;31","4;35;32","4;36;33","4;37;34","4;38;
```

b) index information

Fig2.91 Example file of Save CSV file(filtered data).

- Close

  Close this window.

2.5.2. Data tab

1) CPF Data Directory

Specify data directory that stored data files. The result files are check point files that applied to different ligands for the same protein and must be same fragment number. Click "**Load**" button then load files. After load files, "**3D Model View**", "**Apply**" button and "**Ligand Fragment No.**" is available.

2) Data Select

Specify energy type for clustering. IFIE Energy or PIEDA value.

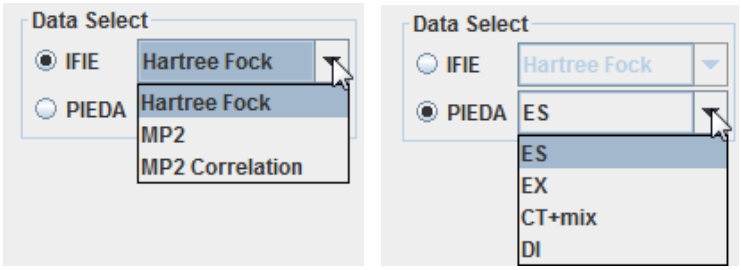


Fig2.92 Data Select Panel.

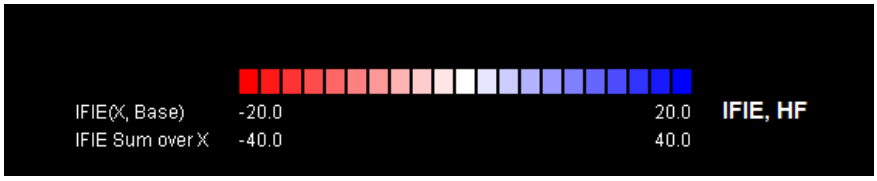


Fig2.93 Example of Legend.

3) Cluster Analysis

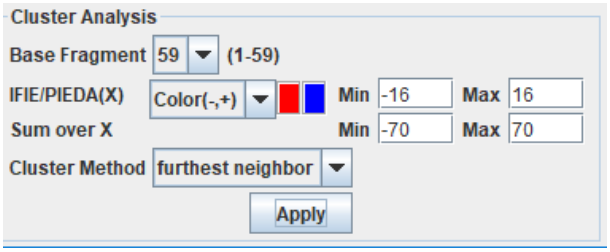


Fig2.94 Cluster Analysis Panel.

- Base Fragment
  It is base fragment number that for cluster analysis.
- IFIE/PIEDA(X)
  Specify color and range of Interaction Energy. The default min/max value set from loaded file.
- Sum over X
  Specify range of Binding Energy. The default min/max value set from loaded file.
- Cluster Method
  Select method for cluster analysis. There are bellow methods.
  - furthest neighbor
  - nearest neighbor
  - group average
  - centroid
  - median
  - Ward
  - flexible
- Apply
  Click "Apply" button, then redisplay by specified parameter.

4) View Filter

- Distance
  Specify distance from Base Fragment.
- Distance Type
  Specify distance method.
  Neaest Interatomic : nearest distance between atoms.
  Center of mass : distance from center of the fragment.

- Filter

  Click “Filter” button, then redisplay by specified parameter.

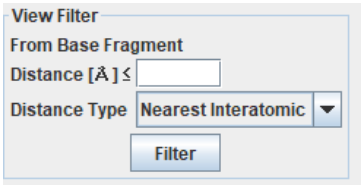


Fig2.95　View Filer Panel.

5)　3D Model View

” **3D Model View**” button function：At first visualized data and select a fragment on the right side, then click ” **3D Model View**” button, display molecular structure on 3D View with highlighted fragment. Show the example (エラー! 参照元が見つかりません。) .

2.5.3.　Analysis tab

Display yellow dash line on dendrogram at mouse position, when select “On” at “cluster No” parameter. Then display cluster# root of dendrogram. When you’d like to display the cluster # in the desired position, hold the mouse cursor in that position and it goes out of the top or the bottom of dendrogram.

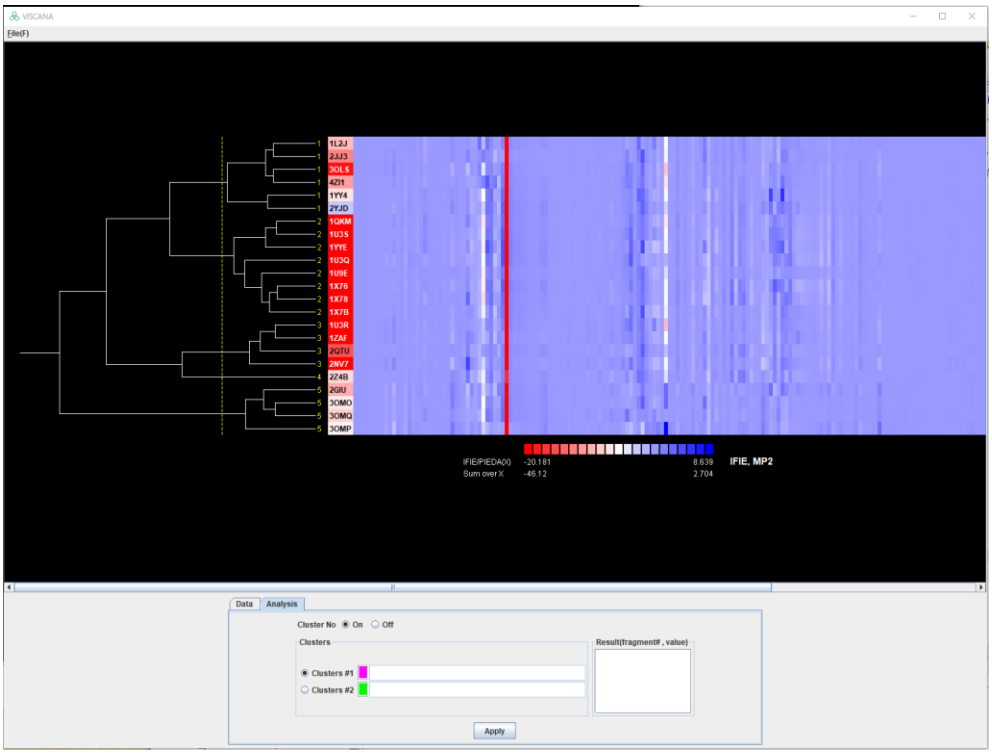


Fig2.96　Anaysis tab.

When a horizontal line of a dendrogram is clicked, the selected cluster number is shown as "*", and ligand name set on the text area at checked box #1 or #2. Color of ligand name #1 set mazenda and #2 set green. If you click other than a horizontal line, the selection will be canceled.

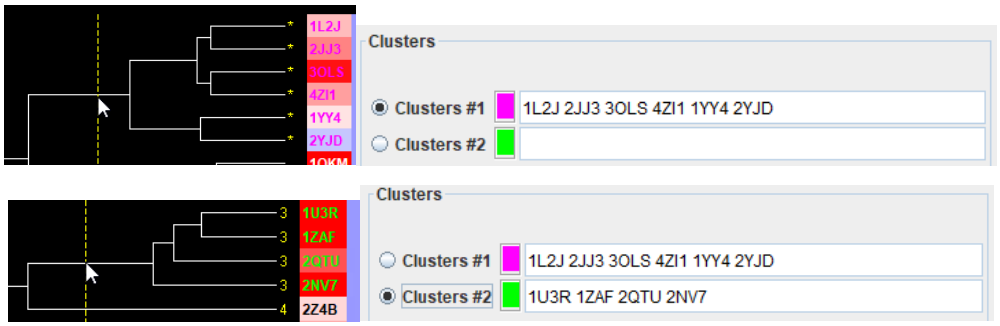


Fig2.97　Select cluster.

Click “Apply” button then calculate the difference of average in values. Display fragment number and value in order absolute value on the Result list panel.　If clicked list value, the applicable fragments are displayed in a yellow frame.

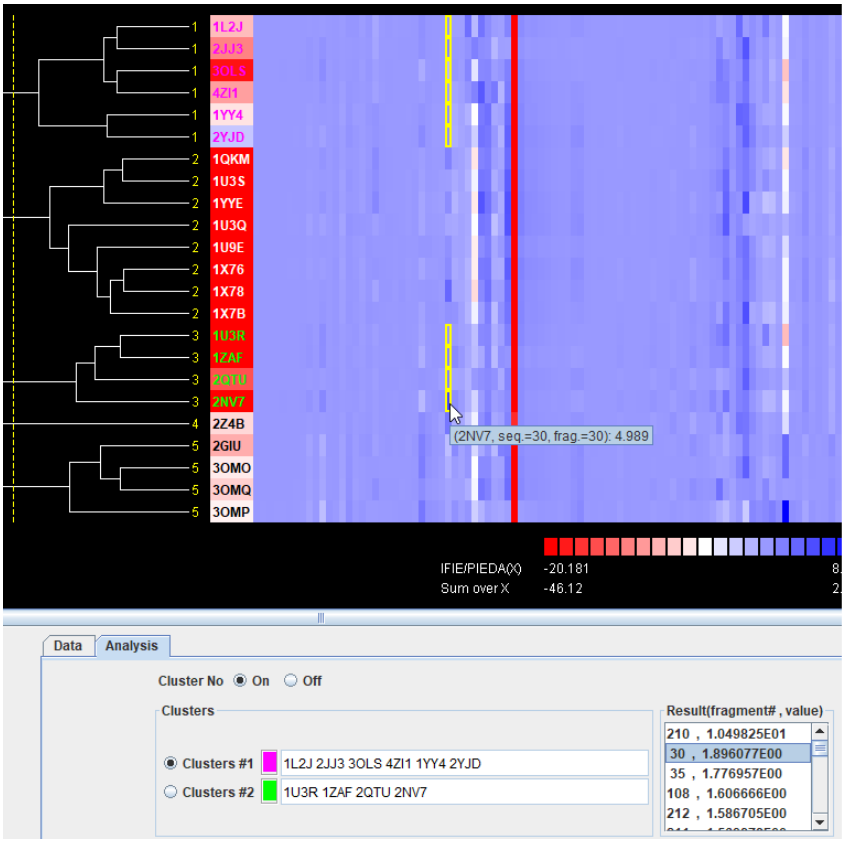


Fig2.98　Example of cluster analysis.

2.6. IFIE MAP

The IFIEs illustrate the information about the interaction energies between the fragments consisting of amino acids, nucleotides and other molecules. The whole IFIEs are represented as a matrix form called an IFIE matrix and visualized as MAP. The Map add color by IFIE value, and Second Structure is shown at upper and left part. By clicking on "+" "−" buttons, the graph is scalable. When you take the mouse cursor on the item, show the interaction energy and fragment number. By clicking the item, display highlighted that fragments on 3D View.

Select **File->Open** File menu and load check point file. Select **Monitor->IFIE MAP** menu then IFIE window is displayed. Example is shown in Fig2.99

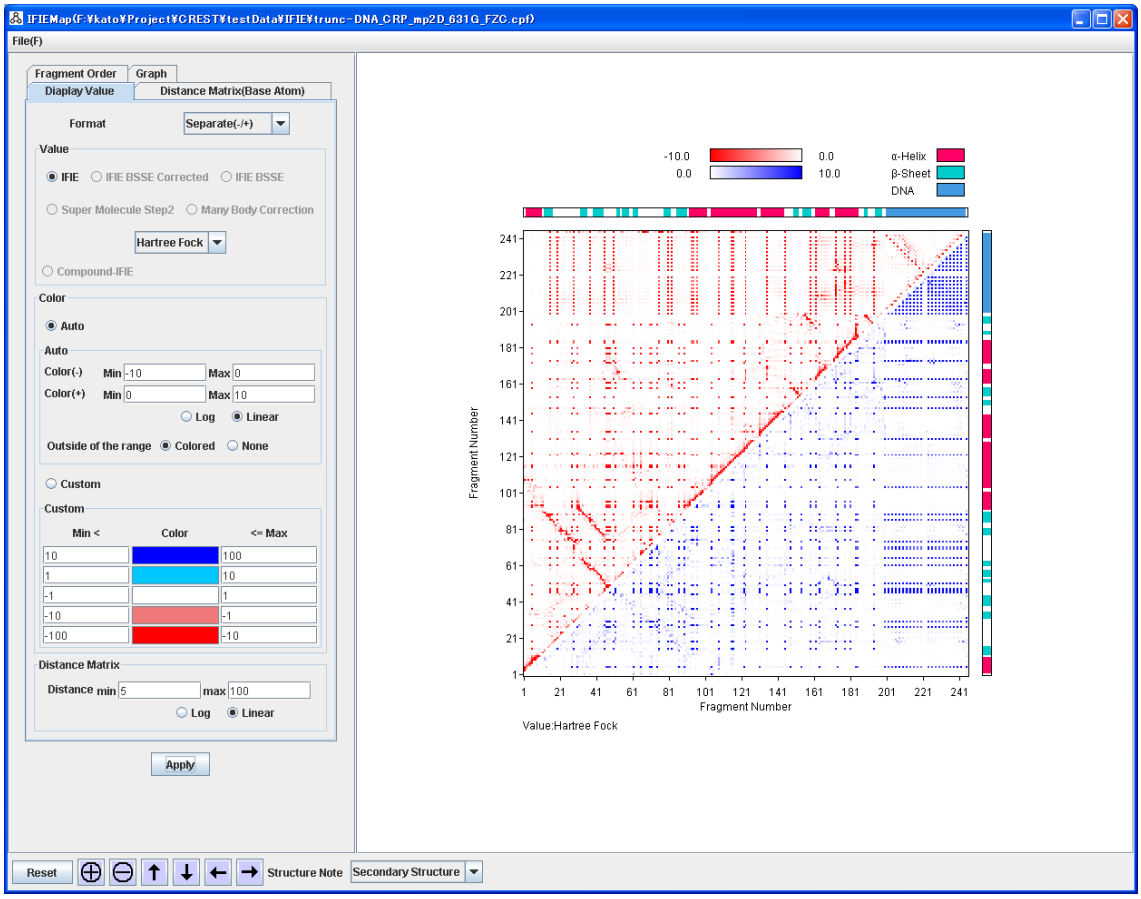


Fig2.99 IFIE MAP Window

1) Instruction of menu

- File menu
  - ♦ Save image

    Save image file(PNG/Tiff/Jpeg).
  - ♦ Save text

Save text file(index, value).

♦ Close

Close this window.

2) Visualize Parameters

A specification item is changed with a tab. When "**Apply**" button is clicked after parameter specifies , the MAP is changed.

- Display Value

The color parameter panel is shown in Fig2.100.

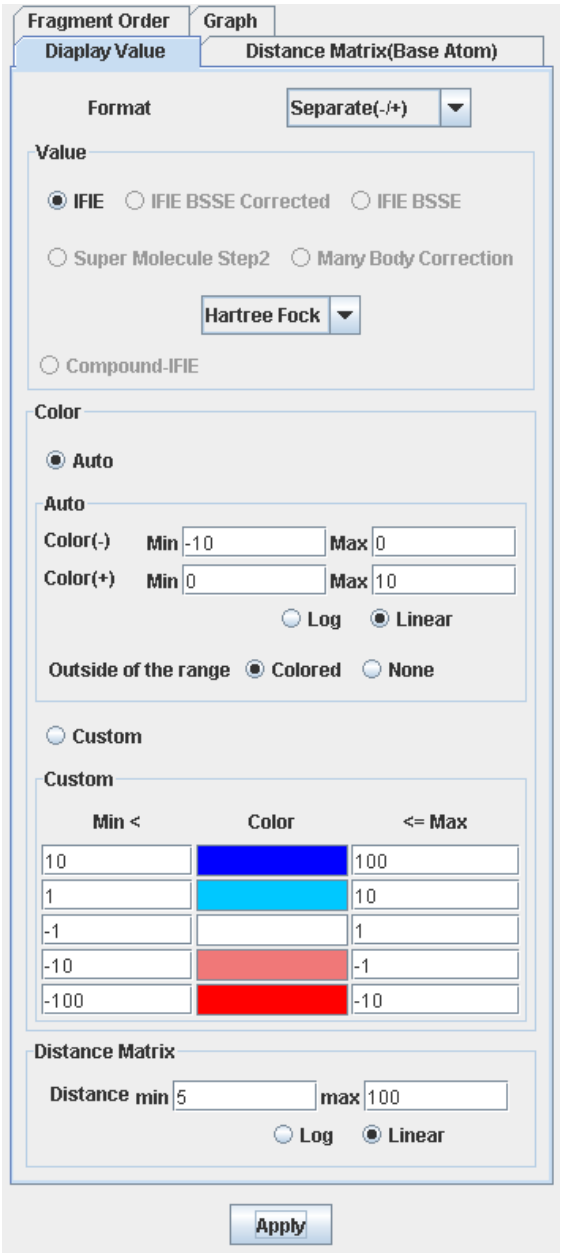


Fig2.100 IFIE MAP Display Value panel

♦ Format

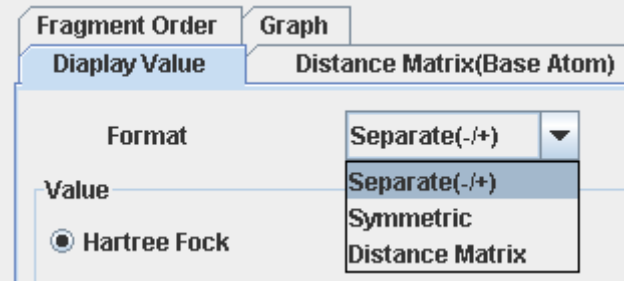


Fig2.101 Format panel

➢ Separate(-/+)

The negative values are displayed on left side and the positive values are displayed on right side. The example is shown in Fig2.99.

➢ Symmetric

The negative/positive values are displayed on both side. The example is shown in Fig2.102.

➢ Distance Matrix

The Symmetric is displayed on left side, the distance between fragments is displayed on right side. The atom that becomes base of distance is specified next panel. The example is shown in Fig2.103.

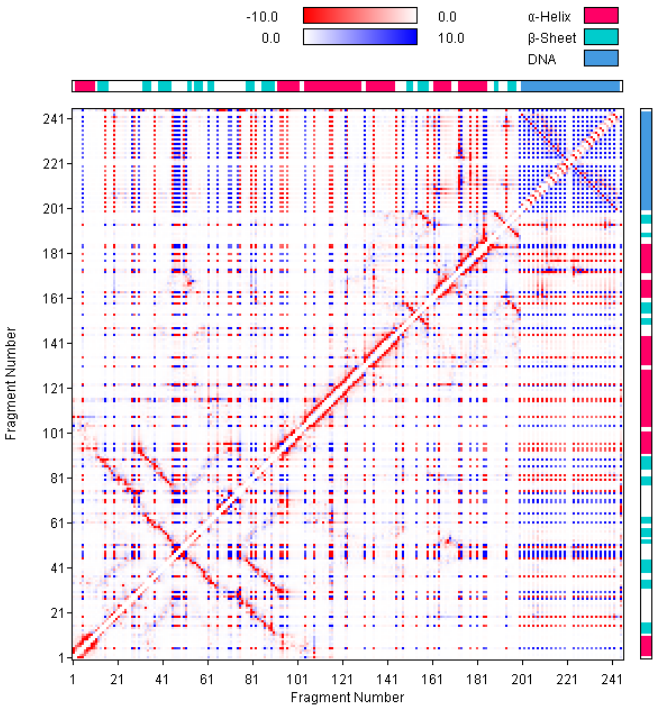


Fig2.102 Example of Symmetric

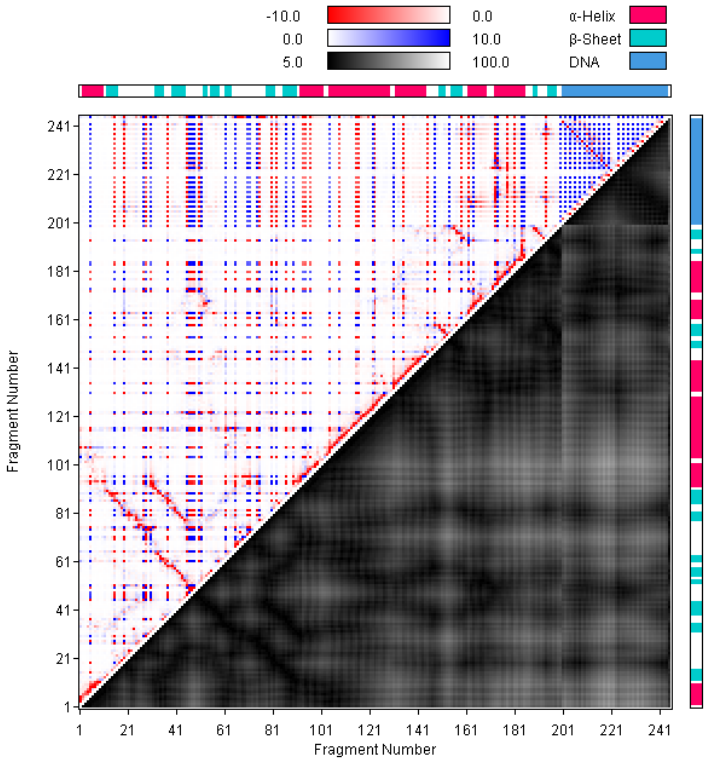
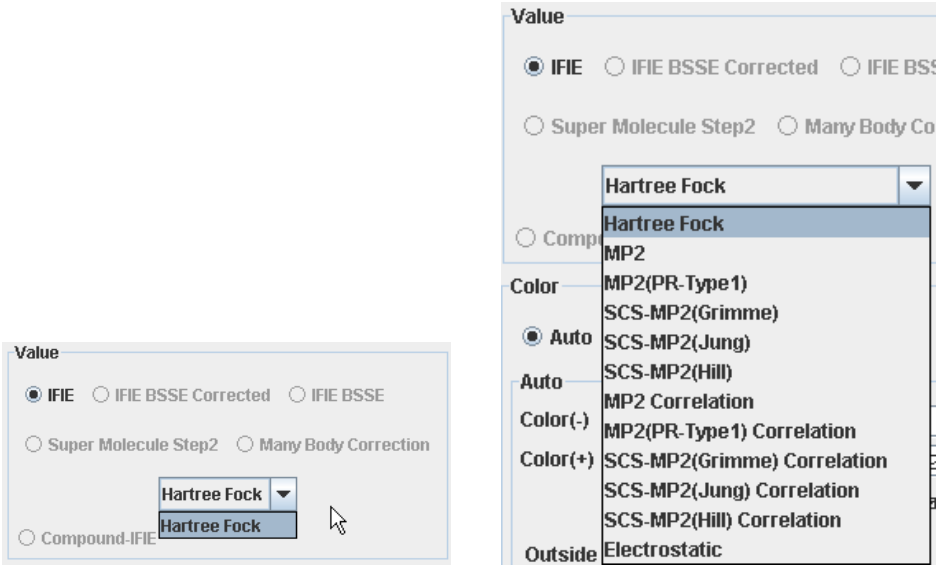


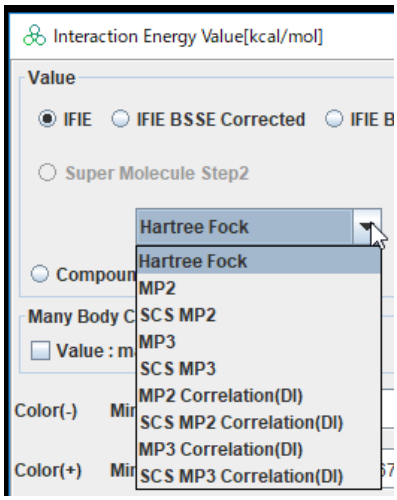
Fig2.103　Example of Distance Matrix

- Value

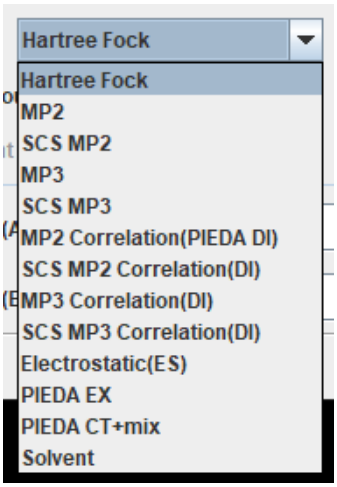
  Select the kind of energy. This menu item changes by the version of CPF. The each menu item is shown in Fig2.104.



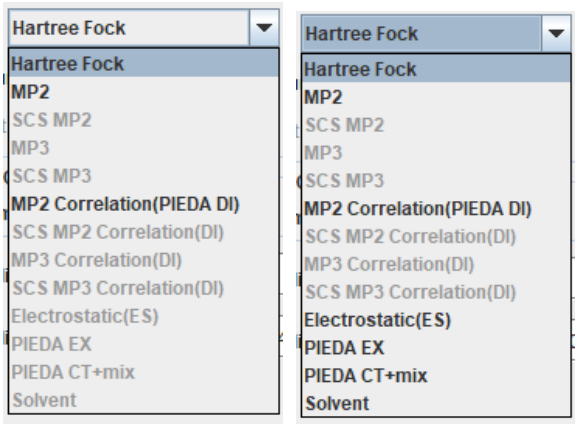
a)　Version1　　b) Version2



c) Version3,4.-4.2, 7.0



d) Version 4,201, 7.0-4.0, Open1.0 rev10



e) Open1.0 rev21 では、記述されていないエネルギーはグレーアウトされる

Fig2.104　　IFIE MAP Value panel each version

In case of the result of super molecule, **Super Molecule Step2** button is available, select this button and the step2 result is displayed as MAP.

In case of the result of many body, **Many Body Correction** button is available, select this button and the many body correction value is displayed as MAP.

If CPF version is 3, you can choose compound-IFIE. This dialog is shown in Fig2.105. Calculate value from some results. Specify coefficient and Value for each file.

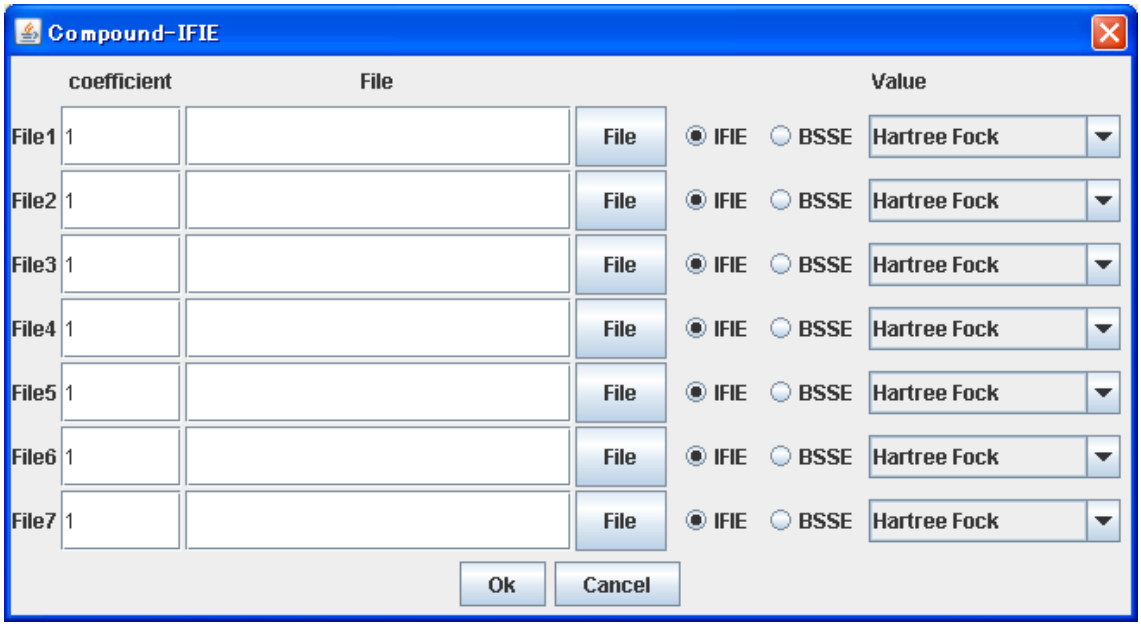


Fig2.105 Compound IFIE Dialog box

- Color
  - ✧ Auto

    Add color by range of value(**min,max**) each of **Color(-)** and **Color(+)**. Log and linear can be specified for the type of scale. If 0 is specified as Log value, it is changed to 1e-10.

    If you select "**Colored**" as **Outside the range,** the beyond the limits of minimum/maxmum value is displayed by the color of the maximum value and minimum value. If you selects "**None**", do not add color.
  - ✧ Custom

    The value within specified range (min<max) is displayed by the specified color. It becomes white outside the range. When "**Color**" button is clicked popup the color dialog. The example is shown in Fig2.106.

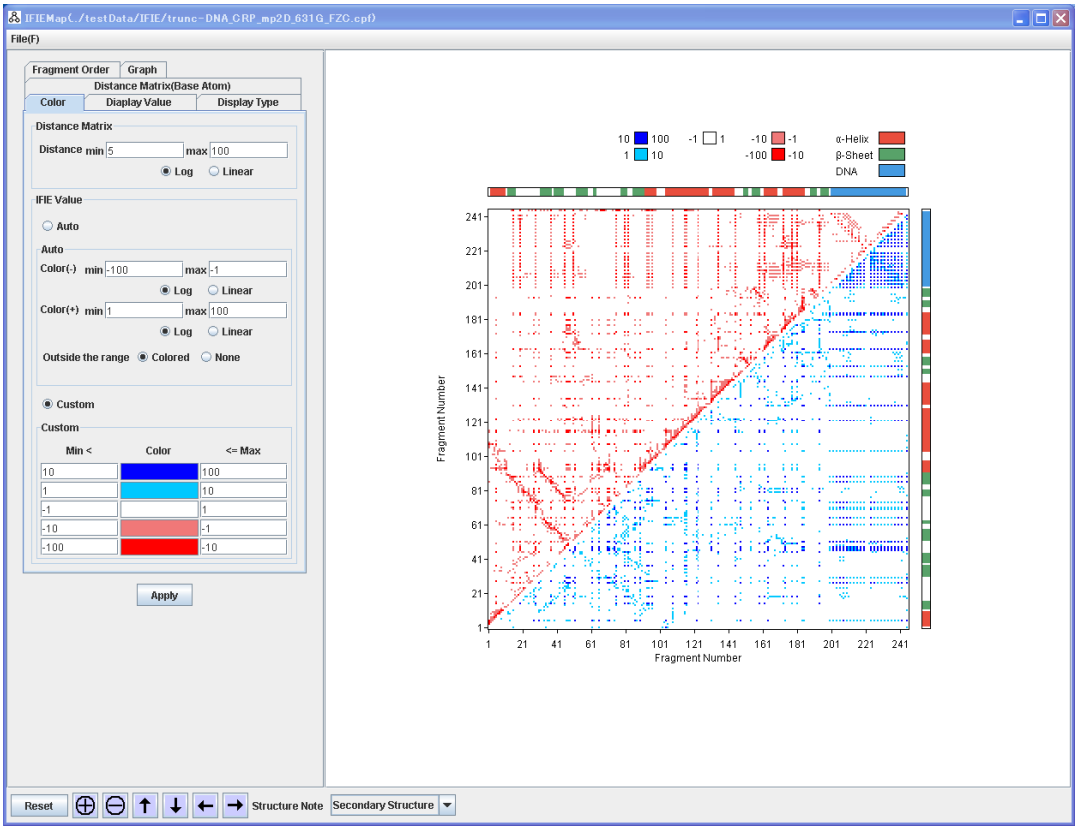


Fig2.106　Example of custom color

♦ Distance Matrix

Add color by range of value(**min,max**). Log and linear can be specified for the type of scale. If 0 is specified as Log value, it is changed to 1e-10.

- Distance Matrix(Base atom)

Specify the atom that becomes base of distance incase of peptide, DNA and others.

1) Center of Mass

2) The shortest interatomic

3) custom

Please specify atom type name in the check point file. In the case of DNA(1fragment is 1DNA) , select as the base atom either of backbone or base. In the case of others(fragments is not peptide and DNA), specify the base atom in text field. This format is “fragment No. : atom name”. If there are some parameters, input parameters that are separated by the space character. Example “222:C3’ 244:P”

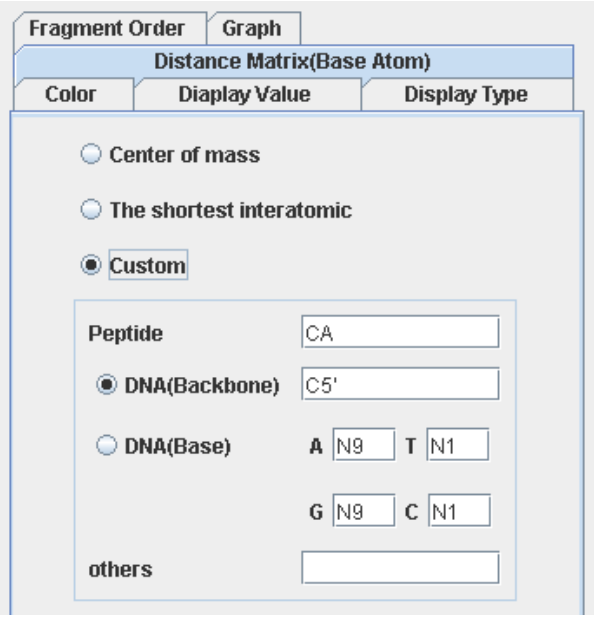


Fig2.107　Distance Matrix 表示例

- Fragment Order

  Specify the order of displaying the fragmentation on MAP.

  All: specify the order for all fragments.

  Chain : specify the order for each chain.

  If mark the check box , it is displayed. It is displayed in input order and the format is possible to specify it as follows.

  1) Start fragment No. — End fragment No. : increment

     Specify the start fragment No. , end fragment No. and increment. example 200-220:2

  2) Residue name

     It is specified three character such as GLY, ASP.

     (This format is only available in All)

  ♦ Clear fragments

  Clear input parameters.

  ♦ Set Default

  Set default values.

  ✧ Add fragments in range

  It is a miscellaneous function to specify the fragmentation number at All and Chain. Click the fragment in 3D view, that fragment No. is displayed at **No.** field. Two or more fragments can be specified. Specify the distance from fragment at front of Å then by clicking the "Add" button, the

fragment No.s that in range are added at parameter fields.

There are two methods in calculation of distance. "**Center of mass**" is center of mass of fragments, "**The shortest interatomic**" is The shortest interatomic distance.

✧ Sort by base/backbone(DNA)

The displayed order sort by base/backbone.

✧ Sort by Main/Side Chain

In case of multi layer calculation, it will be displayed in the oerder of main/side chains.

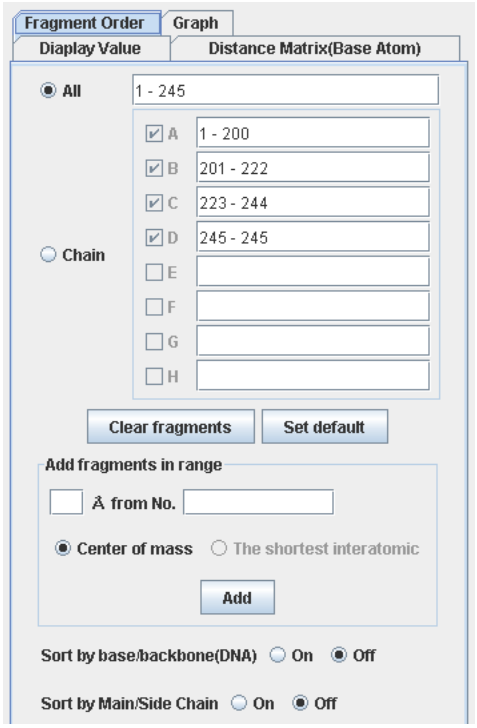


Fig2.108 IFIE MAP Fragment Order panel

- Graph

Display the graph that have a horizontal axis as fragment No. and a vertical axis as IFIE value. The fragments No. is specified for the field. If two or more fragments are specified display sum of these values. Label display at upper of graph. The range of value is specified as a vertical axis. By Clicking the "**Draw Graph**" button, display the graph. The example is shown in Fig2.110.

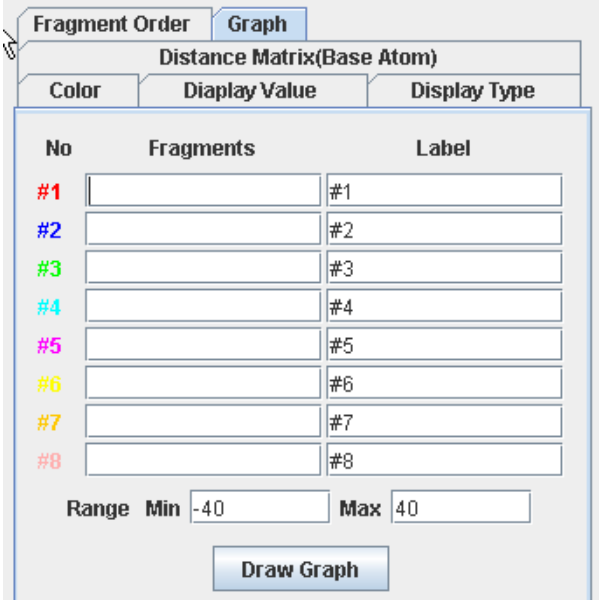


Fig2.109 IFIE MAP Graph panel

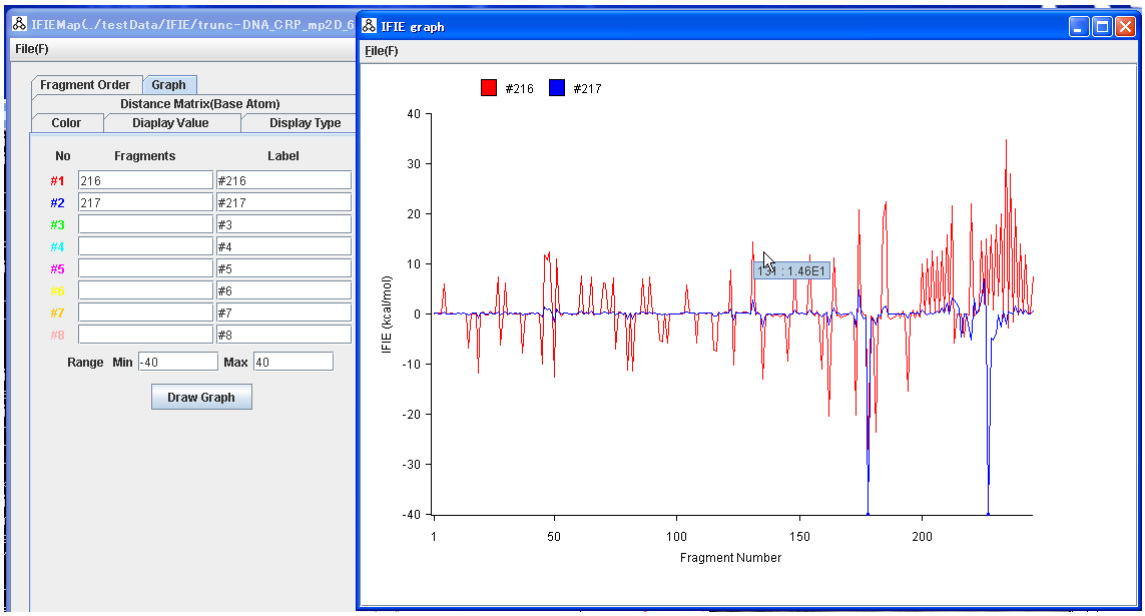


Fig2.110 Example of graph

When you take the mouse cursor on the graph, show the fragment No. and value.

Show the File menu in bellow.

- Load CSV file
  Load CSV file that saved by "**Save CSV file**".
- Save CSV file

Save the file that format is CSV.

- Save Image

  Save the image file(png,jpg,tiff).

3) instructions

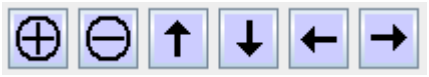
- Apply

  Display the MAP with parameters.

- Reset

  Reset the MAP.

- Enlargement, Shrink and Translate



- Structure Note

  Display second structure or chain at upper/right of MAP.

- Enlargement by mouse

  The rubber band is appear by push the left button on mouse. When release the button, enlarge display area.

- Display value

  When you take the mouse cursor on the graph, show the fragment No. and value.

- Highright fragment in 3D view

  By clicking the right button of mouse on item, display highlighted that fragments on 3D View.

2.7. FILM Isosurface

Load FILM result file, specify the orbital and display isosurface. At first load the check point file then select **Monitor→Film isosurface.** Popup FILM window.

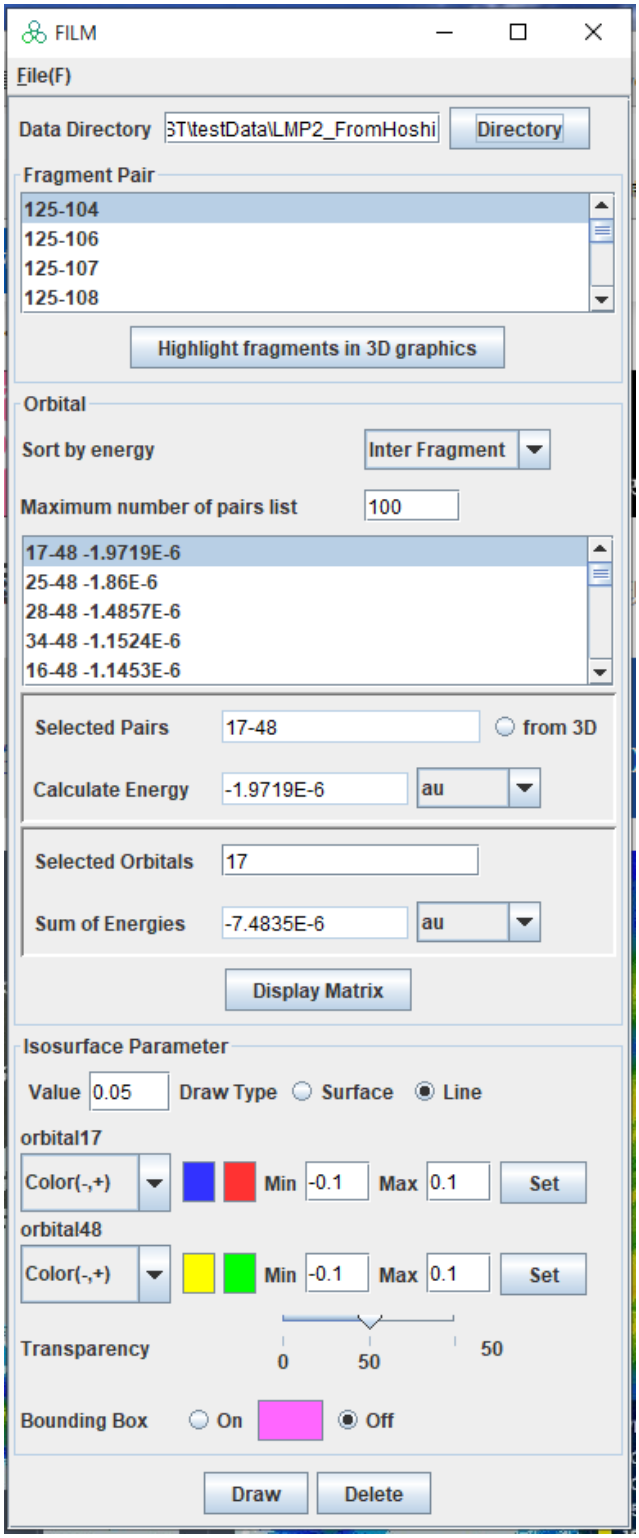


Fig2.111 FILM Window

1) Menu

- File menu
  - ♦ Close

    Close the window.

2) Parameters

- Data Directory

  Specify the folder that is stored result files. The convention of result filename is xxx_n_m.lmp2.(xxx:any、n.m fragment No.)。After specify the folder, load result files and display **Fragment Pair.**
- Fragment Pair

  Display fragment pair. Select a fragment pair, display that orbital at **Orbital**. By clicking **"Highlight fragments in 3D graphics"** button then display the highlighted fragment in 3D View.
- Orbital

  Select item(Inter Fragment/Inner Fragment/All/None) of **Sort by energy.**

  Inter Fragment：list item are sorted by the energy between inter fragment.

  Inner Fragment：list item are sorted by the energy between inner fragment.

  All：list item are sorted by the energy of all pair.

  None：Select the each orbital.

  Display orbital number at **Selected pairs** and sum of energy between selected orbitals at **Calculate Energy.** Two or more orbitals can be specified. **Selected orbitals** is possible to edit. After edit this field, enter the return key then display that energy.

  Maximum number of pairs list：Specify maximum number of orbital pairs in list. It is available by pressing enter key.

  If **from 3D marked,** when click the atom in 3D view, display related orbitals at **Selected pairs.**

  Selected orbitals：The starting track number of the selected orbital is set. It's editable, if you press the Return key, S**um of Energies** will be calculated.

  Sum of Energies：Display value which the total sum of the combination of the selected orbitals. Integrated target is Inter,Inner or All which is selected option of **Sort by energy.**

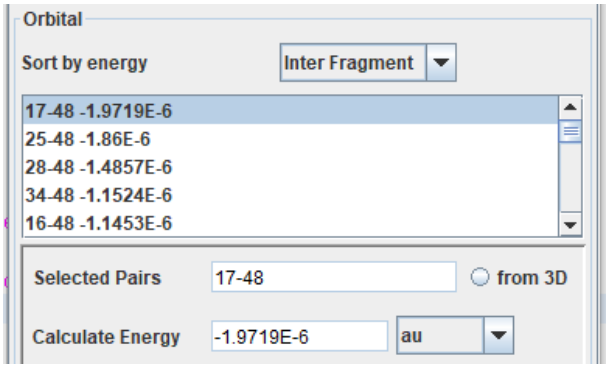


Fig2.112　Example of Inter Fragment list

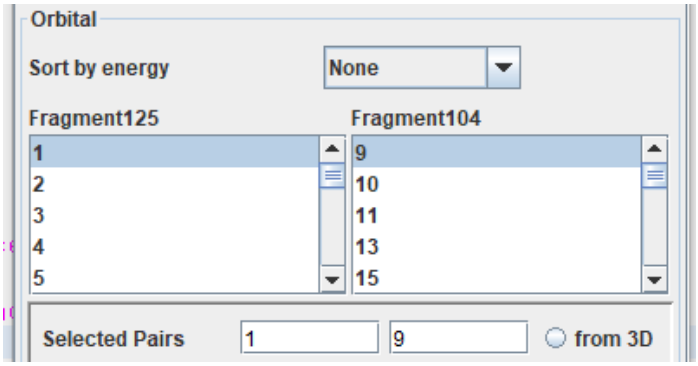


Fig2.113　Example of None

- Display Matrix

  Display energy matrix between orbitals on the other window. Display energy that included fragment by fragment order. The displayed color is changed from red to white. Change min/max value and by Clicking "**Apply**" button, redisplay matrix. When you take the mouse cursor on the matrix, show the orbital index and energy. By Clicking item on matrix, set orbital index at "**Selected orbitals**". Click item with push control key, add orbital index. Ezample is showed in Fig2.126.

  There are three display types, "Inner Frament","Inter Fragment" and "All".

  Save image file(PNG,Tiff,JPG) by selecting **File→Save Image** menu.

- Isosurface Parameter

  The color of each fragment can be specified. phase

  If draw two or more orbitals that have different phase so upset isosurface color, the color in each orbital can be specified according to the following instructions. By clicking "Set" button, set parameters on selected orbital. Draw a isosurface, if

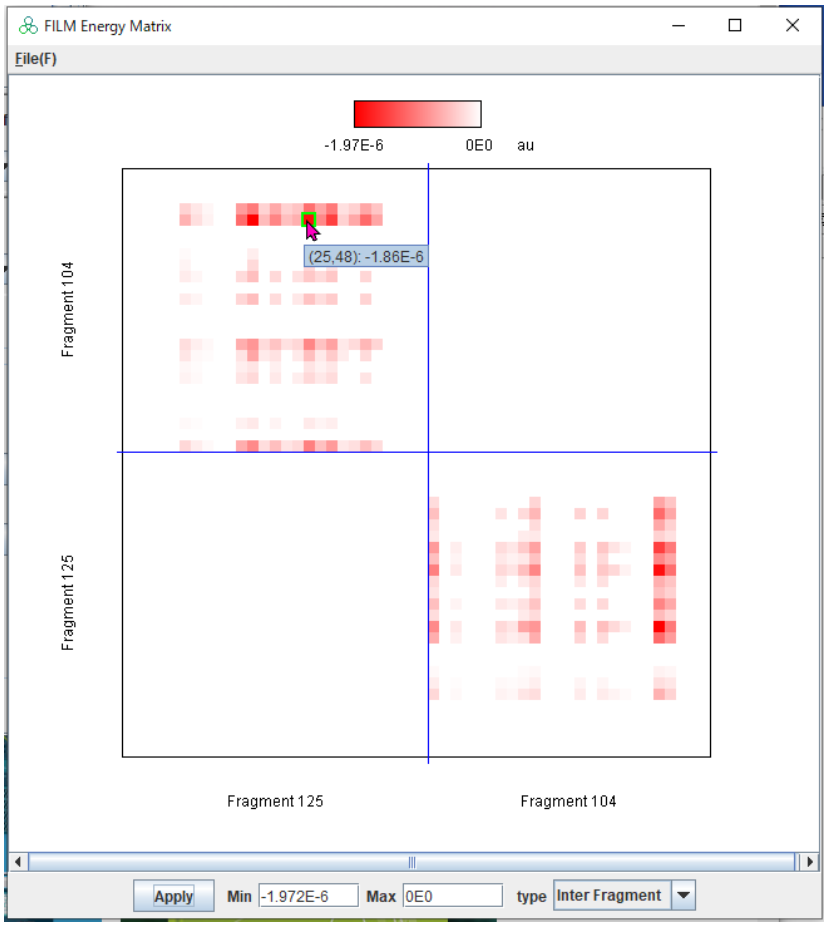
upset isosurface color, select **Color(+,-)** button and click **Set** button. This setting of each orbital is done, all orbital draw at the same time.

- Draw

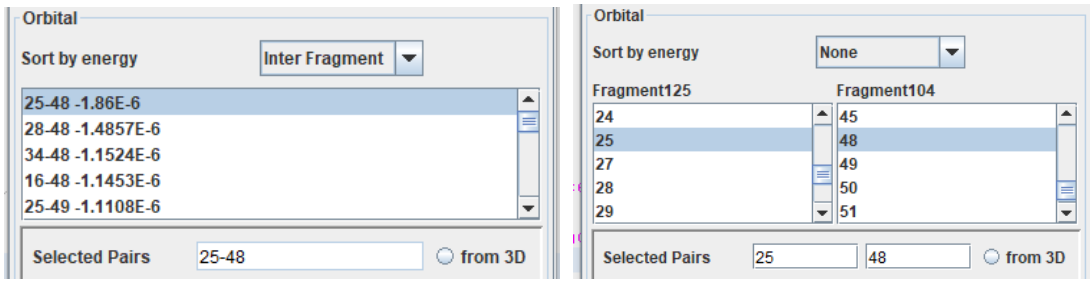
  Draw isosurfaces that are selected.

- Delete

  Delete isosurface.



a) click at (25,48)



b) selected orbital pair on the list

Fig2.114 Example of Matrix

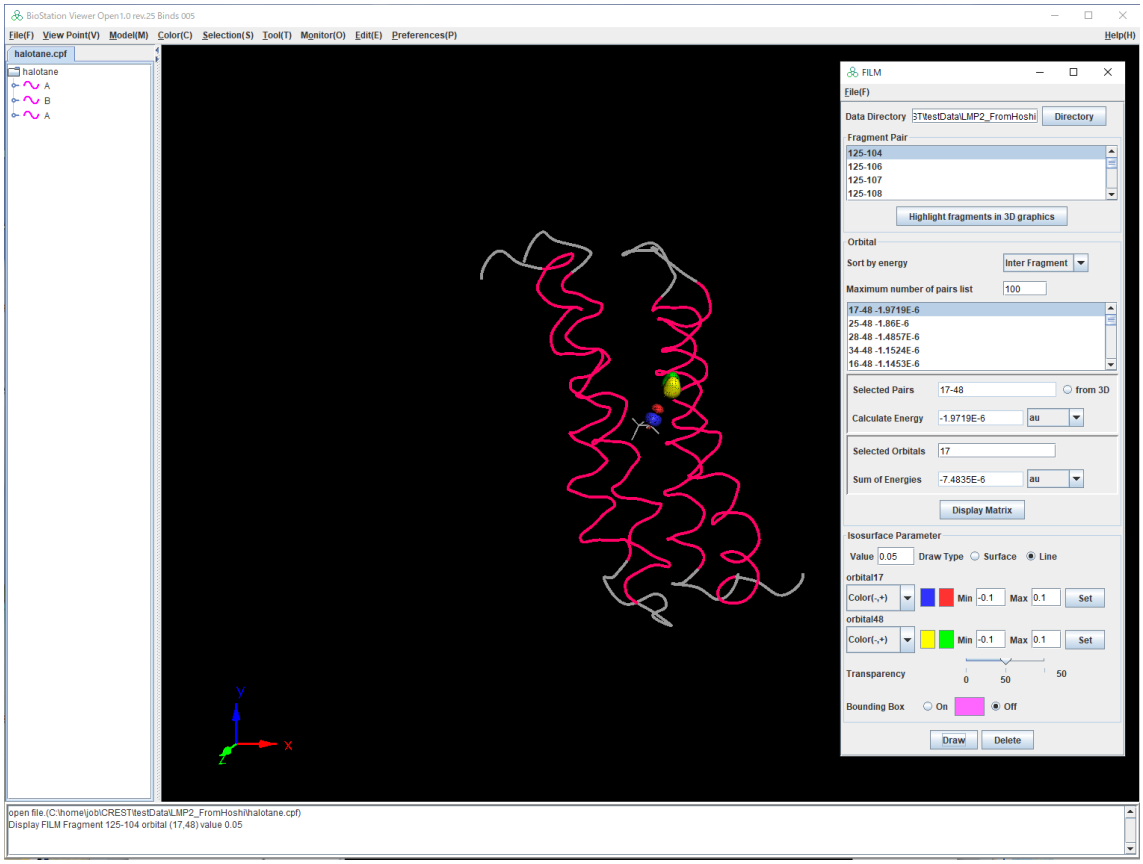


Fig2.115 Example of FILM isosurface

2.8. Editing ABINIT-MP Input File

When you select **[File]-[Edit ABINIT-MP Input File]**, popup an edit window of **ABINIT-MP** input file. This input file version is ABINIT-MP Open 1.0 rev.10. Input fields in **Optimize** and **FMO Calculation** are displayed by choosing **On.** CNTRL,FMOCNTRL,SCF and BASIS are mandatory parameters, Please set other items if necessary. Please refer "ABINIT-MP manual" about detail of parameters. This edit display is shown in the Fig2.116.

This window consist tabs. Please input parameters that you need at each tab. Default file name is set to "**Read Geometory File**" at the Control tab, but you have to change the path for the calculate server when you execute by this file on it.

Please refer to ABINIT-MP program manual for details of each item. I explain the File menu, Fragment editing function (FMOCNTRL) and Fragment Pair (FRAGPAIR).

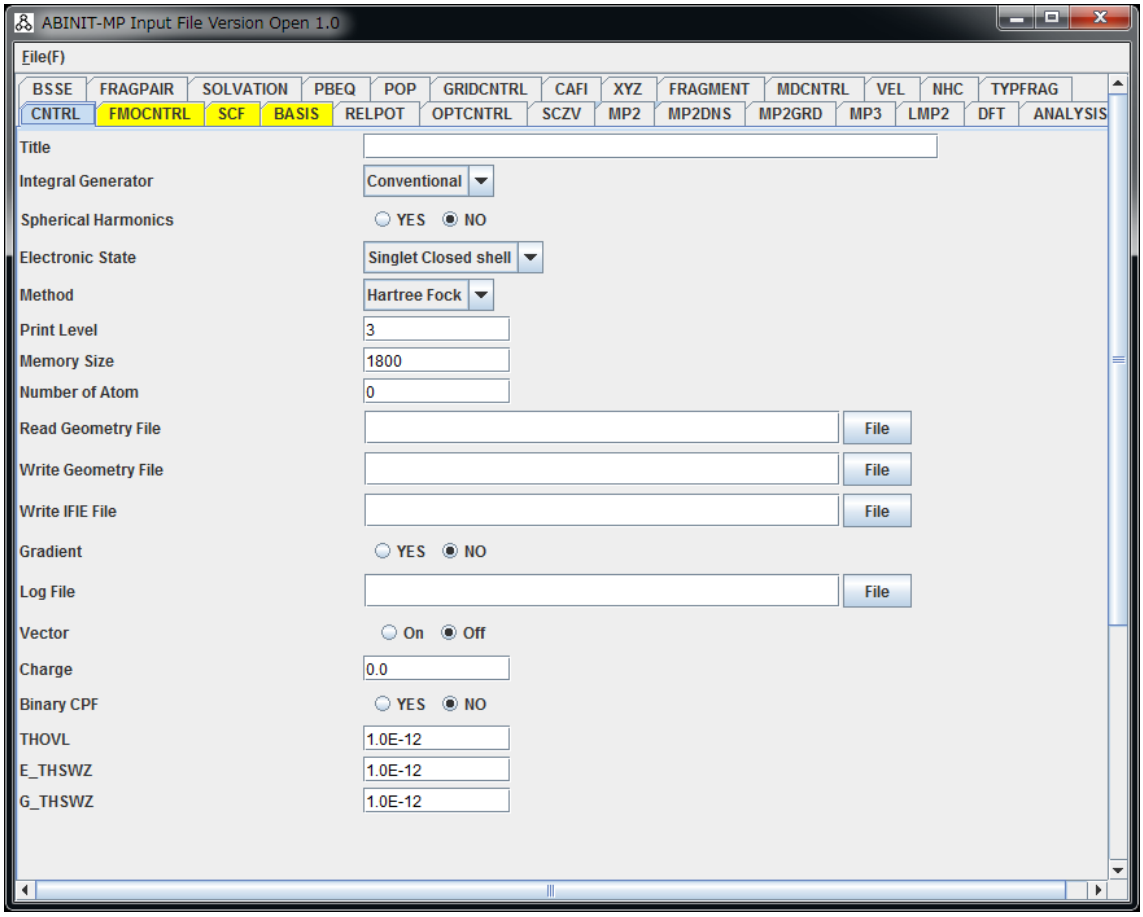


Fig2.116 ABINIT-MP Input file edit window

2.8.1. File Menu

Show the File menu in bellow

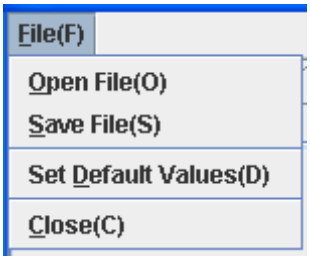


Fig 2.117 File menu at ABINIT-MP Input file edit window

1) Open File
   Open input file.
2) Save File
   Save input file
3) Set Default Value
   Set Default Values
4) Close
   Close this dialog.

2.8.2. Edit fragment (FMOCNTRL)

FMOCNTRL tab is for fragmentation parameters. **Auto Fragmentation** is division parameter of fragments, it has 3 mode(**On/Off/Hybrid**), explain them following.

1) **On** : generate fragments by automatic method. Some parameter needs.
2) **Off** : at first generate fragments by automatic method, then divide the fragments manually. All the information about fragments is described in AJF.
3) **Hybrid** : at first generate fragments by automatic method, then divide the fragments manually. Only the modified information about fragments is described in AJF. It's convenient if you check only the part of manually fragments.

Selected **"On"** is shown in Fig 2.118, selected **"off"** or **"hybrid"** is shown in Fig 2.119. By Clicking **"Set Fragmentation"** button, then pop up the fragment edit window(Fig 2.120).

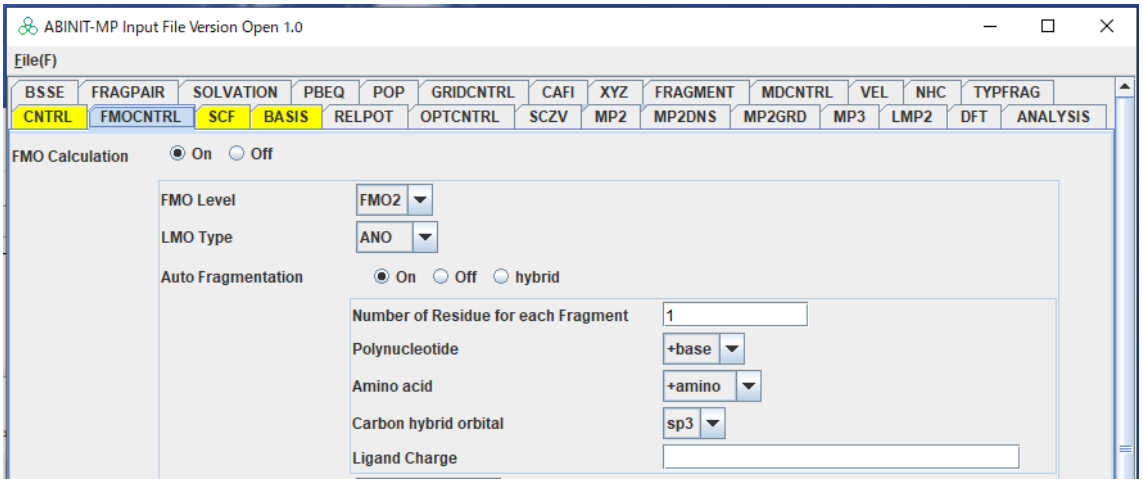


Fig 2.118 Auto Fragmentation is “On”

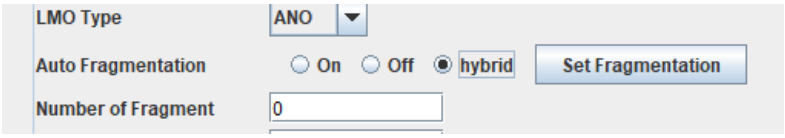


Fig 2.119 Auto Fragmentation is Off or hybrid

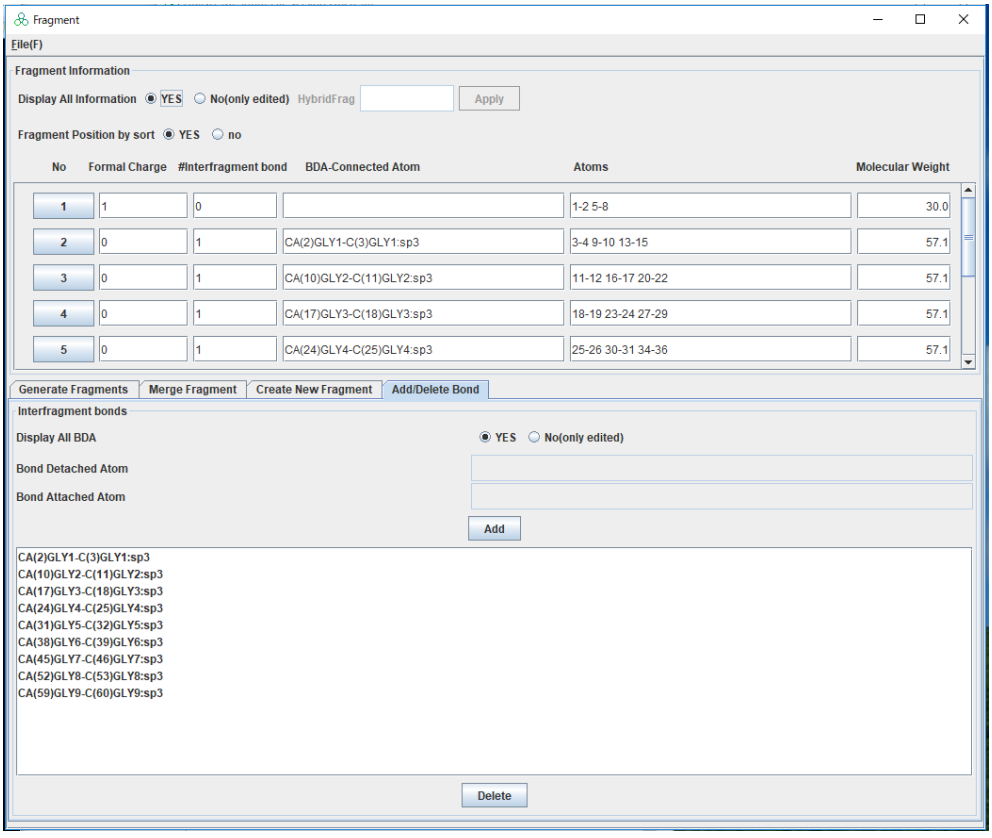


Fig 2.120 Fragment edit window

The edit window displays information of fragment at the upper part and consists of four tabs for editing at the bottom, explain them following.

a) Fragment information

The following information is shown as fragment information.

- Fragment number : It is button. By clicking it, high light atoms in 3D display.
- Formal charge : editable.
- Number of interfragment bond
- BDA connected atom
- The atom no. of fragment
- Molecular Weight

"Display All Information" Specify the way of display information

Yes : Display all information.

No : Display only edited fragments and specified fragmnets at **HybridFrag**. If you click "**Apply**" button after specified fragmnets at **HybridFrag**, it will change to the display of specified fragments only. The edited fragment displays "*" on the left. The number that specify as **HyblidFrag** is decided one when divided automatically.

"Fragment Position by sort" Specify how to insert edited fragments in case of hybrid.

Yes : The insertion location is determined by the atomic numbers other hydrogen contained in the fragment

No : Add it at the end of automatically generated fragment.

b) Edit fragments

It has four tabs, Generate Fragments, Merge Fragment, Create New Fragment and Add/Delete Bond.

By clicking the atom on 3D view or Tree view, then set the atom No. or fragment No. on input field. The atom# add the input field automatically so you have to clear before click the atom if you don't add one.

(1) Generate Fragments

If you want to auto fragmentation for protein, select **"Auto"** tab. If you want to manually fragmentation for protein/demdrimer, select **"Manual"** tab. If you want to auto fragmentation for crystalline molecules, select **"Crystal"** tab.

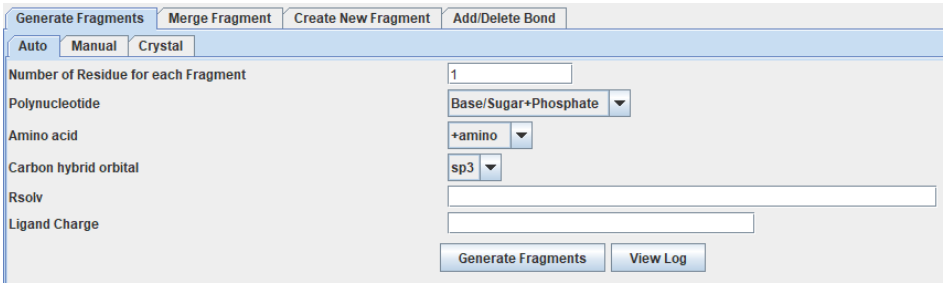
1) Auto fragmentation for protein

After specify the parameters, by clicking **"Generate Fragment"** button**,** execute auto

fragmentation and display result on 3D view. By clicking "**View Log"** button**,** display log file. If there is a charge at the connecting part between fragments, display the ellipse ball and small boll. The small boll is a bond detached atom. The Formal Charge and #Interfragment calculate automatically then set input field at Add/Delete Bond tab.

Example is shown in Fig2.121.

Parameters



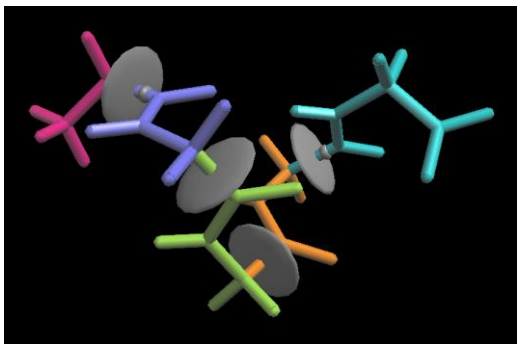


Fig2.121 Result of auto fragmentation for Gly5 (add color by fragment)

Number of Residue for each Fragment Number of fragment per 1 residue.

Polynucleotide When a DNA is divided, this option specifies whether to divide nucleotide into small fragments.

+base : Do not divide a nucleotide into small fragments.

/base : Divide a nucleotide into base and backbone fragments.

/suger : Divide a nucleotide into base, sugar and phosphate group frament.

Aminoacid When a protein is divided, this option specifies whether to divide an amino acid into small fragments.

+amino: Do not divide an amino acid into small fragments.

/amino: Divide an amino acid into main chain and side chain fragment.

Carbone hybrid orbital How to divide carbon chain.

sp3: sp3 : divide at –C–C-connect

sp2: sp2 : divide at –C=C-connect

Rsolv This keyword specifies the distance threshold values used to determine if the ions are merged into the surrounding fragments. In the following example, the Ca and Zn ions are merged into their surrounding fragment, which exists within 2.8 and 2.4 Angstrom from the ions, respectively.

Ex) Rsolv='Ca=2.8,Zn=2.4'

Na, Mg, K, Ca, Mn, Fe, Co, Ni, Cu, Zn, Br atoms can be specified in the keyword.

Ligand Charge charge per fragment.

2) Manual fragmentation

Fragment at the same atom name of start atom while search for the direction is Start→Next. Click the start atom and next atom in 3D view, so the atom is set at input field of **"Start Atom"**,**"Next Atom"**. **"BDA"** specifies the direction for BDA. "Interval" specifies whether to set the fragment point at intervals when the same atom name as Start is found. If you have some fragment direction, click "**Add**" button and specify parameters. By clicking "**Delete**" button, delete current parameters. The example of parameters is shown in Fig2.122, the example of result is shown in Fig2.123. In case of Si12H26, cannot check connect atoms by default preference. So Please parameter of Scale set 1.3 at Preferences→Set Preference→ Connect Atom.

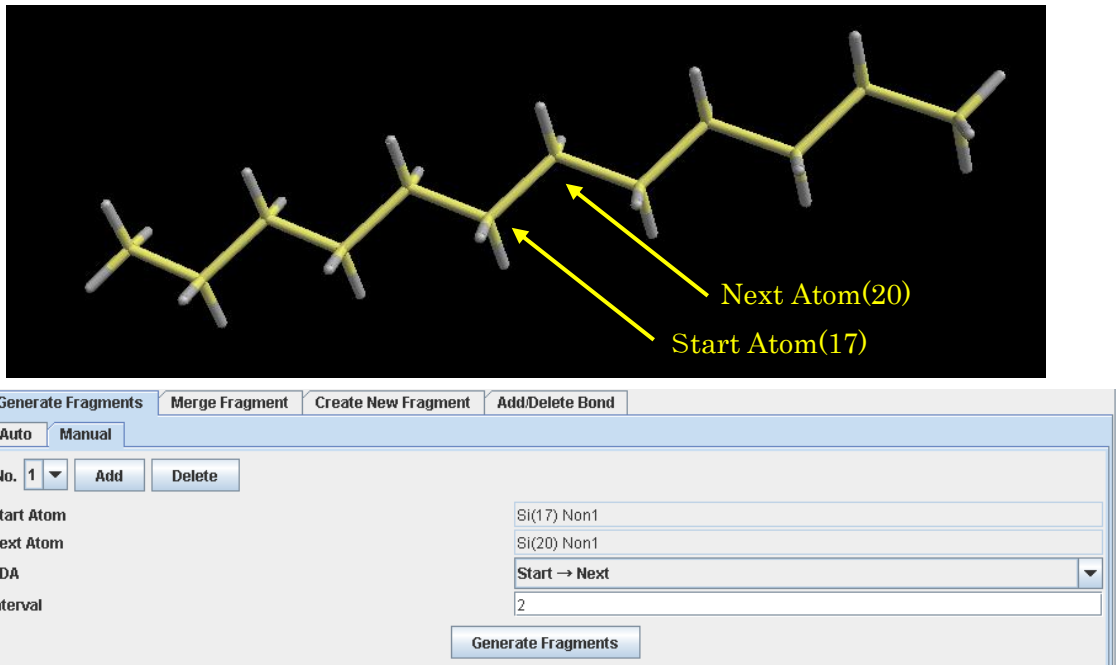


Fig2.122 Example of dendrimer parameters

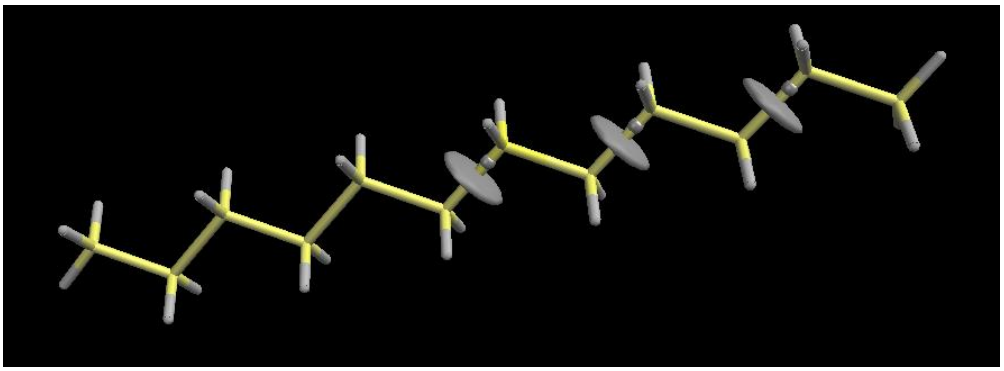


Fig2.123 Result of auto fragmentation for Si12

3) Auto fragmentation for Crystal

Click button **"Generate Fragment"** to execute the automatic fragmentation after specifying the following parameters.

Crystal (residue name) If the given system is composed of a crystal and other molecules, the residue name of the crystal need to be specified in the text input field. The residue name is used to separate the crystal. The residue name appears in the PDB file.

Minimun atoms to marge This specifies the number of atoms for minimum fragment. In the fragmentation specified the **Detail Fragmentation** (see below), the generated fragment, whose number of atoms is less than the number specified in this field, automatically merged into the surrounding fragment.

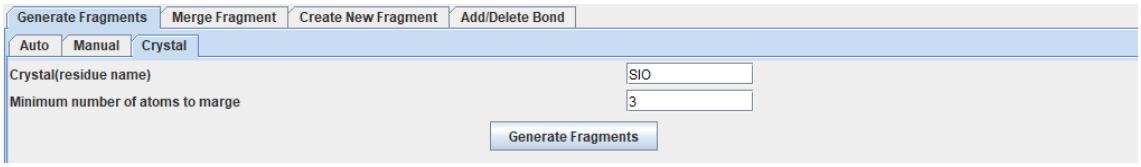


Fig2.124 Example of parameter for crystal.

Fig2.125 shows a screenshot during the automatic fragmentation for the complex of SiO2 cluster model and absorbed peptide.

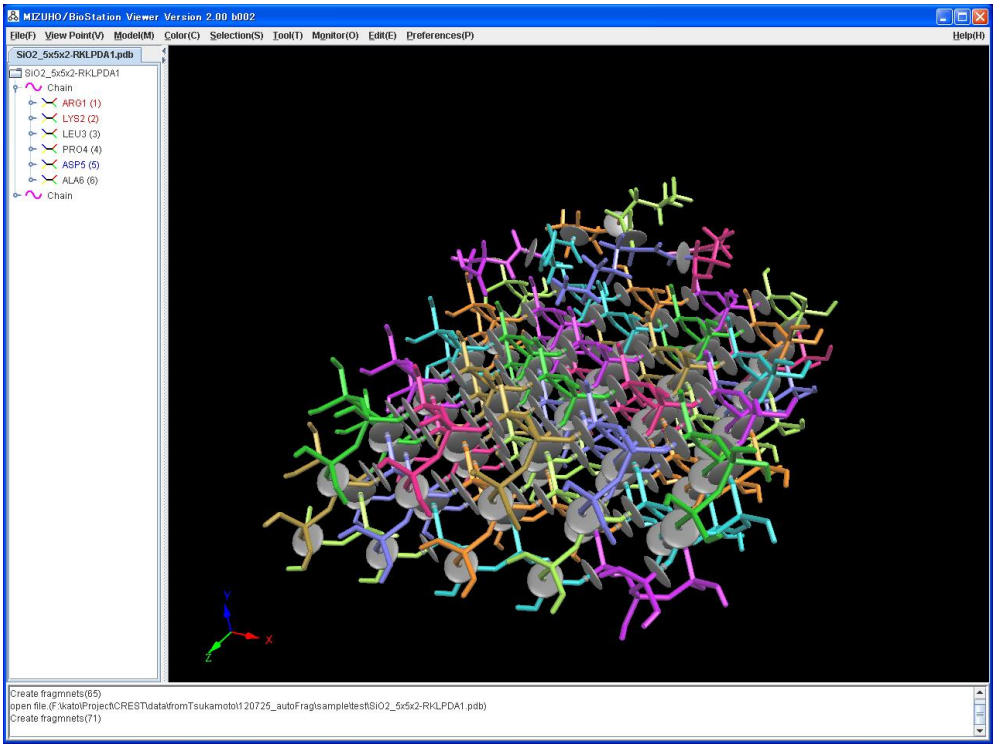
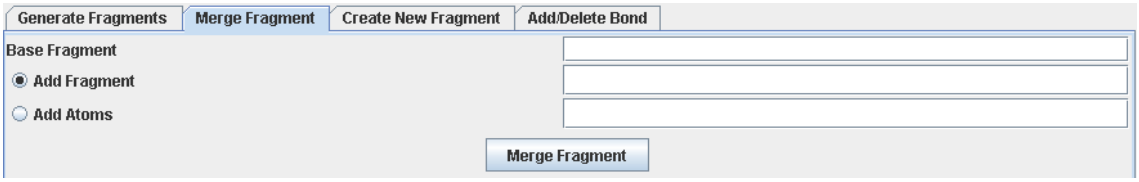


Fig2.125 Specifying parameters on GUI and the result of automatic fragmentation for the complex of SiO2 and peptide.

(2) Marge Fragment

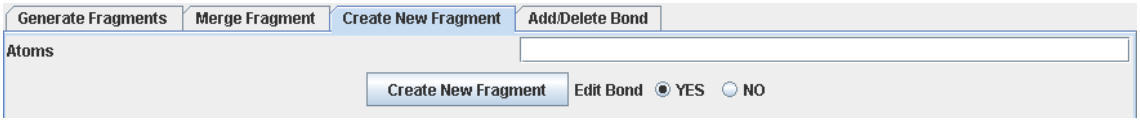
Marge two fragments or atoms for selected fragment. When the input field of **Base Fragment** is cleared, set the fragment# or atom# of the atom is clicked by 3D view or the Tree view. The number is set in the field that is selected by radio button.



(3) New Fragment

Create new fragment with the specified atoms. If you select **"YES"** at **"Edit Bond"**, move to Add/Delete Bond tab by clicking **"Create New Fragment"** button.

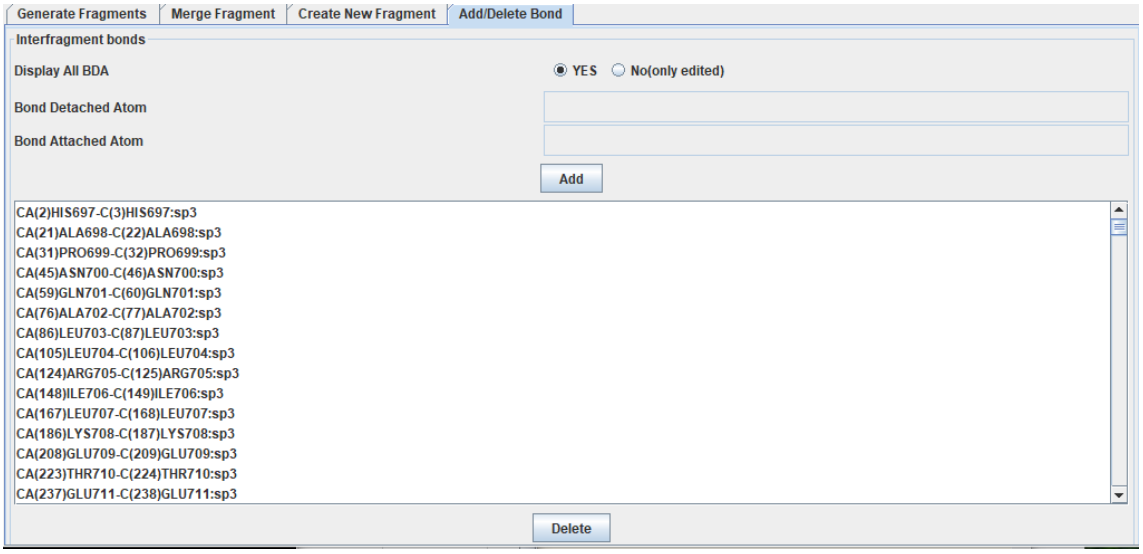
Please set to YES, and specify BDA when connected fragmentation already made. In case that create new fragmentation of Ligand, set to No at "Edit Bond", please set BDA after making all fragmentations.



(4) Add/Delete Bond

Specify bond between fragments. If there is a BDA between fragments, click two atoms and click “Add” button then add a bond. The formal charge allocates from **“Bond Detached Atom”** to **“Connected Atom”** .

By clicking BDA node in 3D view or select in list, and click “Delete” button then delete the bond. Please edit Formal Charge if it is necessary.



Remark!!

- If it have a connecting between fragments and not specify a bond, the error occurred when save a parameter file. The message dialog is shown in Fig2.126.

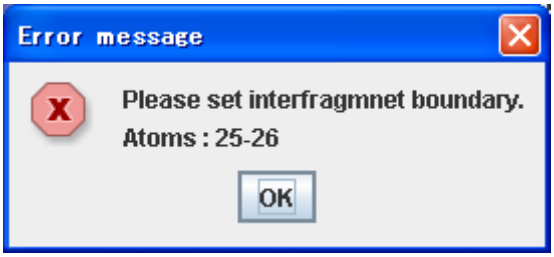


Fig2.126 The error dialog about bond.

- When close fragment window, disappear bond nodes in 3D view.

2.8.3. Fragment pair(FRAGPAIR)

Specify Fragmentation Pair used to calculate BSSE. This panel is shown in Fig2.127.

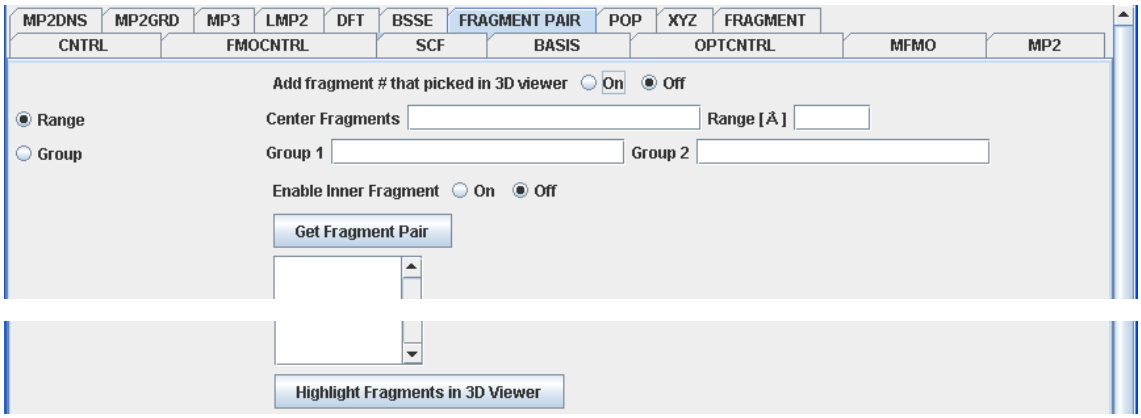


Fig2.127 Fragment Pair panel

1) Add fragment # that picked in3D viewer
   Please select **On** when you display the fragmentation number to the text area with the cursor when the fragmentation is clicked by 3D viewer.
2) Range
   The fragmentation pair in specified range.
3) Group
   The Pair between fragmentations specified for Group1 and Group2. If you choose **On** at **Enable Inner Fragment,** generate pairs in same group fragmentation.
4) Get Fragment Pair
   Display Fragmentation Pairs that was specified for the above.
5) Fragment Pair List
   Display Fragmentation Pairs. You can edit it.
6) Highlight Fragments in 3D Viewer
   The fragmentations in 3d viewer is shown highlighted.

2.9. Basic Action

2.9.1. Enlargement, Shrink, Rotation and Translate

A displayed figure can be enlarged, reduced, rotated and moved. Operations of each action are shown in **Table 2.1**.

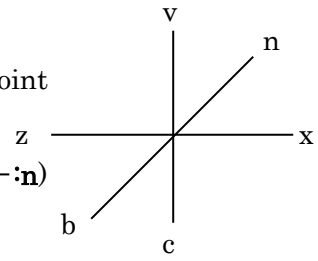
Table 2.1 Operations of Enlargement, Shrink, Rotation and Translate (two buttons with windows)

Action	Operation
Enlargement	Hold down the **Alt** key while clicking the left mouse button , move the mouse pointer down.
Shrink	Hold down the **Alt** key while clicking the left mouse button, move the mouse pointer up.
Rotation	Hold down the left mouse button, and move the mouse pointer in the direction you want to rotate.
Translate	Hold down the right mouse button, and move the mouse pointer in the direction you want to move.

2.9.2. Coordinate Rotation and Translation of Molecule Structure

The coordinate rotation and translation of molecule structures each file can be input by typing. This operation modifies the coordinates of molecule structures in the files as subjects, and is available for the editing of molecule structures.

The mark which shows the translation direction are displayed at the midpoint of rotation like an example on the right. Key binds are



Translation **x** direction (−:**z**+:**x**), **y** direction(−:**c**+:**v**), **z** direction(−:**b**+:**n**)

Rotation **x** axis (−:**a**+:**s**), **y** axis (−:**d**+:**f**), **z** axis(−:**g**+:**h**).

The coordinate of the atom is modified when it is rotated and translated.

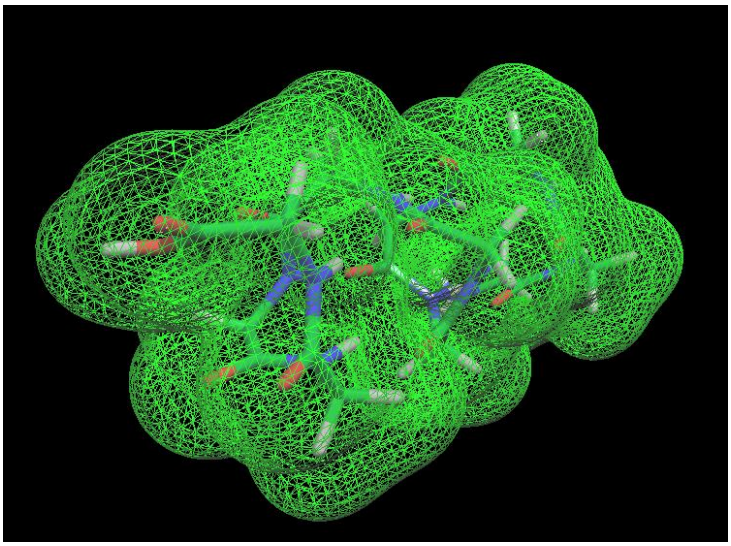
As for the translation, you can move the coordinate of the atom by **0.1Å** each time you press the key. To translate it by **0.5Å**, hold down the **Shift** key, and to translate it by **1.0Å**, hold down the **Ctrl** key. As for the rotation, you can rotate it through **1°** each time you press the key. To rotate it through **5°**, hold down the **Shift** key, and to move it through**45°**, hold down the **Ctrl** key.

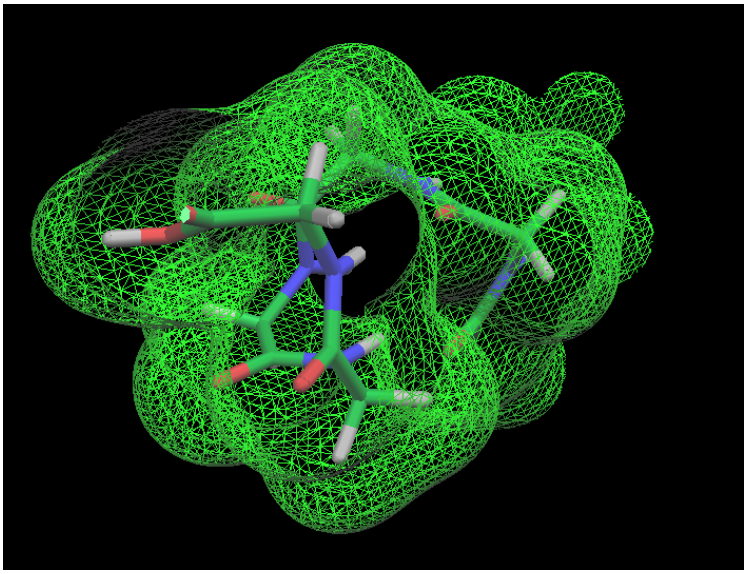
When you input files, the center of the rotation is that of the gravity of the whole atoms. The coordinate of the particular atom can be the center of rotation. To make the position of an atom the center of rotation, click on the atom and select **[Set File Rotation Center]** under **[Tool]** menu.

Without selecting, the center of rotation is set to that of the gravity of each atom by selecting **[Set File Rotation Center]** under **[Tool]** menu.

2.9.3. Control of visualization area

You can control visualization area by mouse wheel operation. Example is shown Fig2.128. The operation controls the clip distance before and after the display according to the amount of movement of the mouse wheel. In this way it will not be displayed except the designated range. Just turn the wheel, then clip the front area, turn the wheel with Shift-key pressed, then clip the back area. Clip volume is 0.1 times by pressing with Control-key. With pressed Alt-key, then reset clip area.





upper: standard, lower : clip front and back

Fig2.128 Example of control clip area.

2.10. How to Select Structures as Subjects

When you click on molecular structures on viewing-window, the atom's information is shown in a message area. And the structures as subjects are added colors in yellow and highlighted in hierarchical window. Click on an atom or a residue and click on another one while holding down the Shift key to select the intervening ones. Click on an atom or a residue while holding down the Ctrl key to add it. This example of a display is shown in Fig2.129.

By clicking on names of a residue and an atom in hierarchical window, they can be selected. They are displayed in yellow on 3D view-window. Click on an atom or a residue and click on another one while holding down the Shift key to select the intervening ones. Click on an atom or a residue while holding down the Ctrl key to add it.

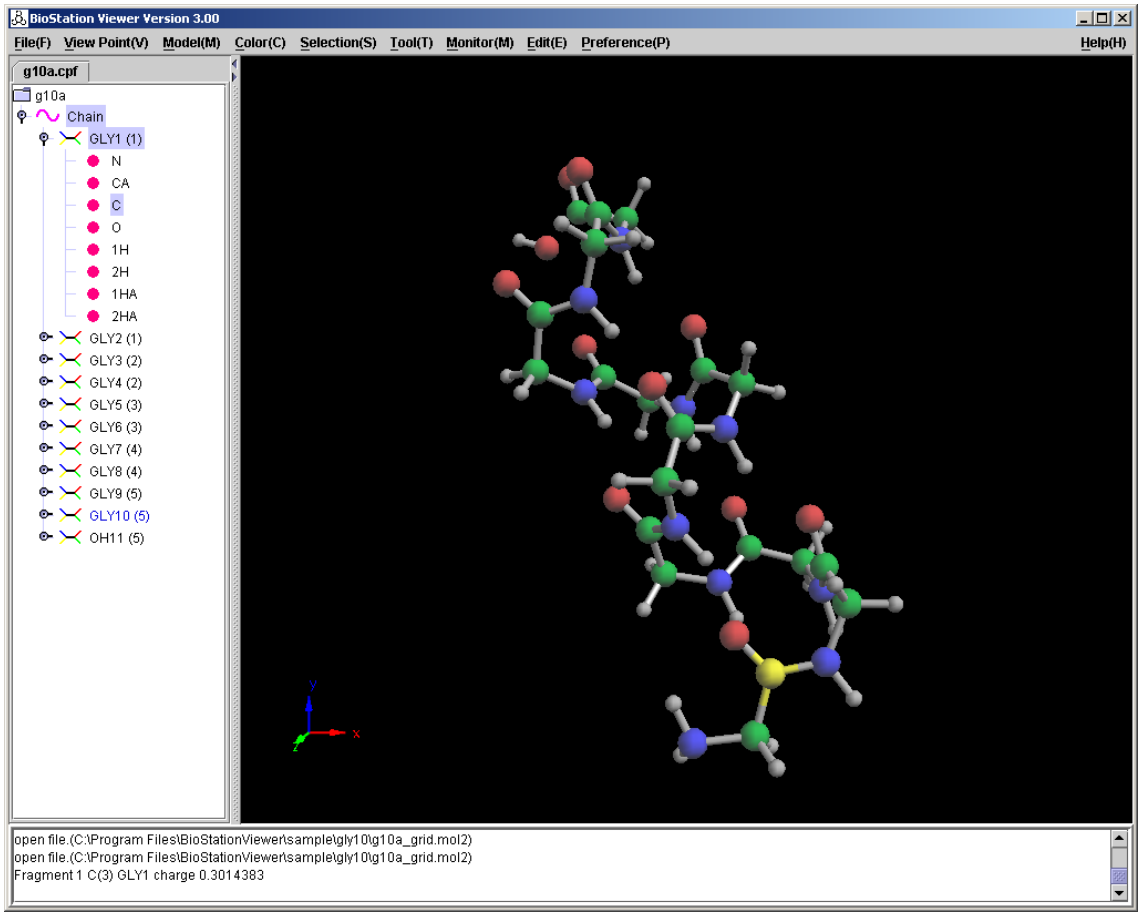


Fig2.129 Example of Selected Atoms

2.11. Setting Preference Categories

In the case that you click on atoms or residues with the right button on the mouse, the pop-up dialog box appears to specify each category: Display, Model, Color and Label. Atoms dialog box is shown in Fig2.130 and Residues dialog box in Fig2.131. By clicking on the atom or residue in hierarchical window with the left button on the mouse and clicking on it with the right button on the mouse, the dialog box is displayed as well. This assignment apply to the Atom and Structure.

Display : Specify the display, on or off

Model : In the case of residues, select the display model from **None, Wire Frame, Eire Frame with Fragment Bond, Ball & Stick, Stick, Ball & Wire** and **CPK**. When you select **None**, the residue is displayed in the model specified in the menu bar.

Label: Specify a label. In the case of atoms, the names and numbers can be selected. In the case of residues, the names and the names with numbers can be selected

Color: Select the display color from **None, Atom, Residue, Charged Residue, Atom Charge, Fragment, Interaction Energy, Interaction Energy[lock], Chain, File** and **Other**. When you select **None**, the residue is displayed in the color selected in the menu bar. In the case of **Other**, setting colors are displayed beside the button. By clicking on it, a color preference dialog box is displayed.

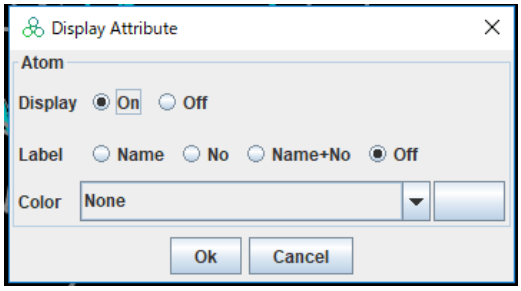


Fig2.130 Display Atom Dialog Box

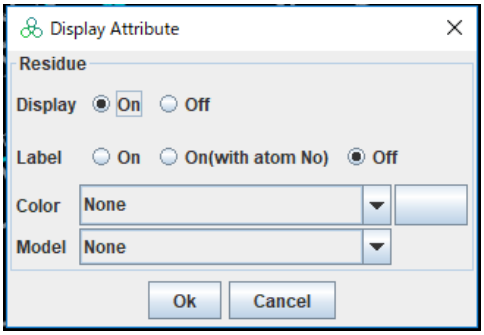


Fig2.131 Display Residues Dialog Box

2.12. Setting the Bounding box

The bounding box can be displayed using **MOL2** file. Type **"grid. file"** above **@<TRIPOS>ATOM** and type the top of the coordinate with the proper atom. Specify the line which you want to display with **@<TRIPOS>BOND**, in the index, then. An example of the display is shown as follows.

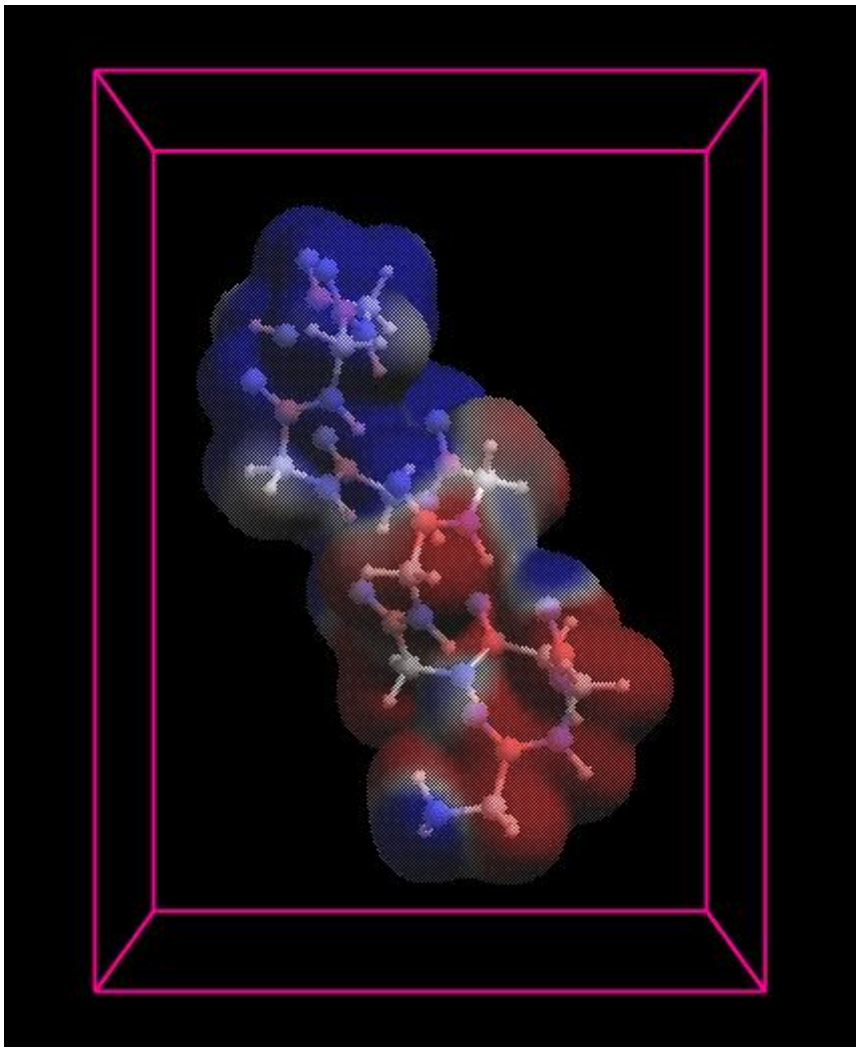


Fig2.132 Domain of Analysis Display

```
@<TRIPOS>MOLECULE
test data
    8   12    0
    0    0    0    0


grid file
@<TRIPOS>ATOM
      1 N     -8.0000   -4.0000   -9.0000 N.4     1  GLY         0.0000
      2 N      8.0000   -4.0000   -9.0000 N.4     1  GLY         0.0000
      3 N     -8.0000   -4.0000    4.0000 N.4     1  GLY         0.0000
      4 N      8.0000   -4.0000    4.0000 N.4     1  GLY         0.0000
      5 N     -8.0000   18.0000   -9.0000 N.4     1  GLY         0.0000
      6 N      8.0000   18.0000   -9.0000 N.4     1  GLY         0.0000
      7 N     -8.0000   18.0000    4.0000 N.4     1  GLY         0.0000
      8 N      8.0000   18.0000    4.0000 N.4     1  GLY         0.0000
@<TRIPOS>BOND
      1       1       2 1
      2       2       4 1
      3       3       4 1
      4       3       1 1
      5       5       6 1
      6       6       8 1
      7       7       8 1
      8       7       5 1
      9       1       5 1
     10       2       6 1
     11       3       7 1
     12       4       8 1
```

Fig2.133 Example of files for the Bounding box(g10a_grid.mol2)

2.13. Molda

This section describes Creation DNA/RNA, Mutation DNA/RNA, and Adding Nucleotide DNA/RNA. Refer to Molda Users Guide about other Molda.

2.13.1. Creation DNA

(1) Molda Menu

Input DNA/RNA, Mutation DNA/RNA and Add Nucleotide DNA/RNA are added to **Model** menu.

Fig2.134 Molda Menu

(2) Input DNA sequence

Select **[Molda]-[Input]-[DNA]** menu. The menu is shown in Fig2.135. Create DNA dialog box is displayed and shown in Fig2.136. For instance, input AAGGCCTT to the text area of the dialog box as **Input sequence** and click **OK**. The text area has to input DNA-bases: A, G, C and T. The result is displayed on Molda viewer and shown in Fig2.137. The other chain will be created automatically.

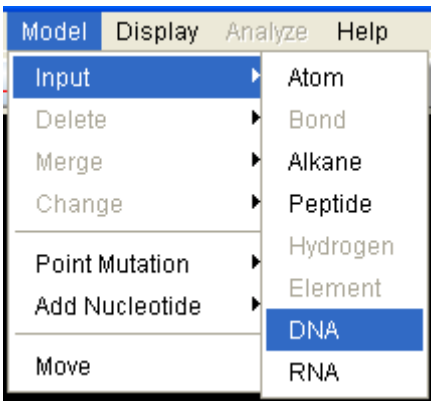


Fig2.135 Input DNA menu

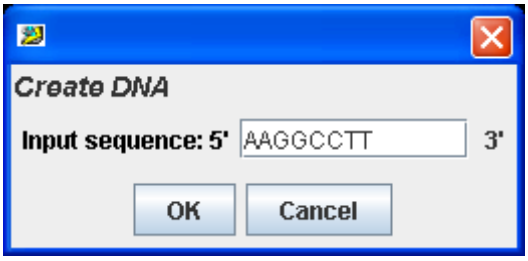


Fig2.136 Create DNA dialog box

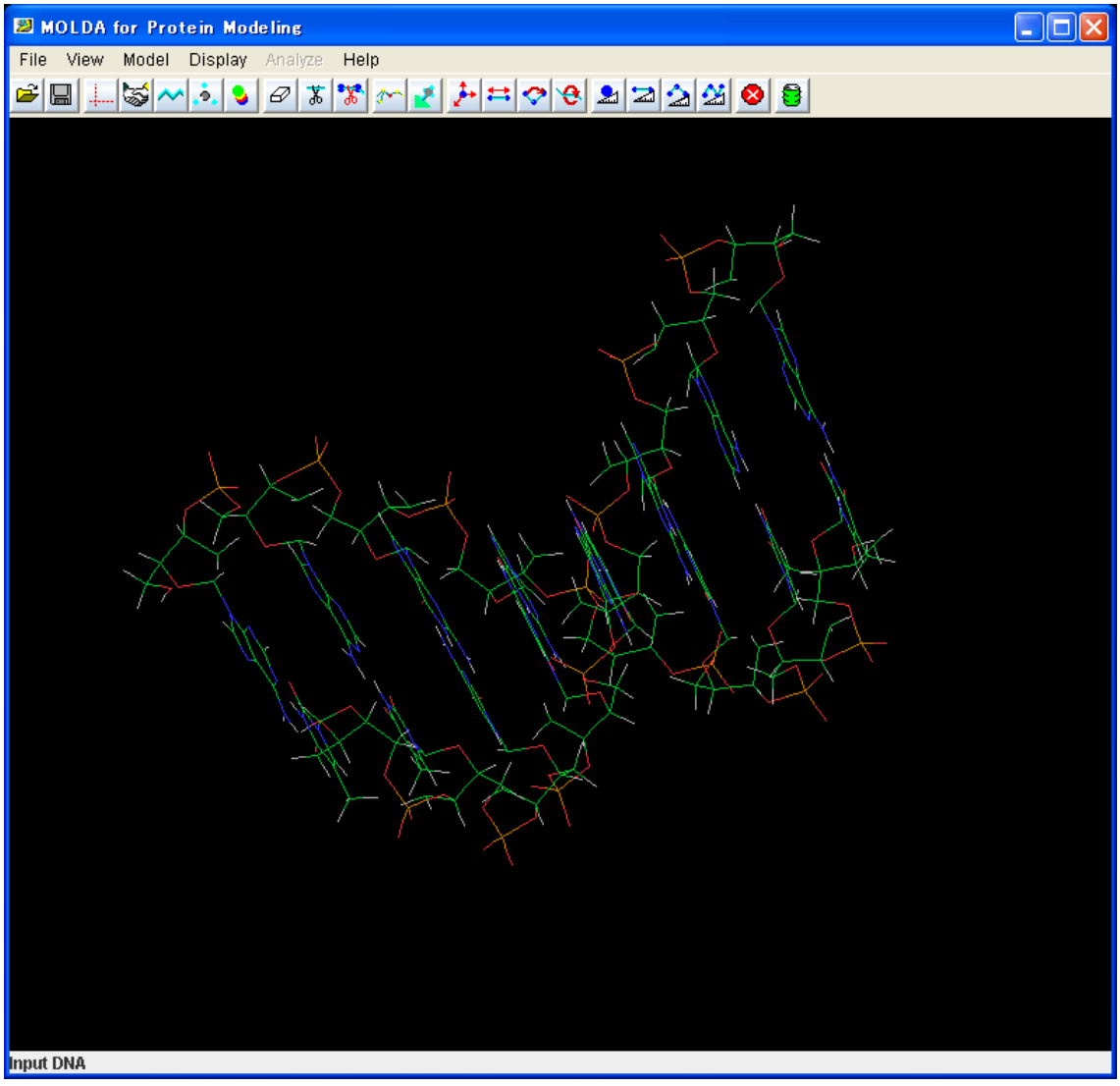


Fig2.137 Result of create DNA

(3) To Viewer

If you want to display the DNA on BioStation main window then select **[Display]-[To Viewer]** menu. The DNA is displayed on BioStation main window. Result of display is shown in Fig2.138.

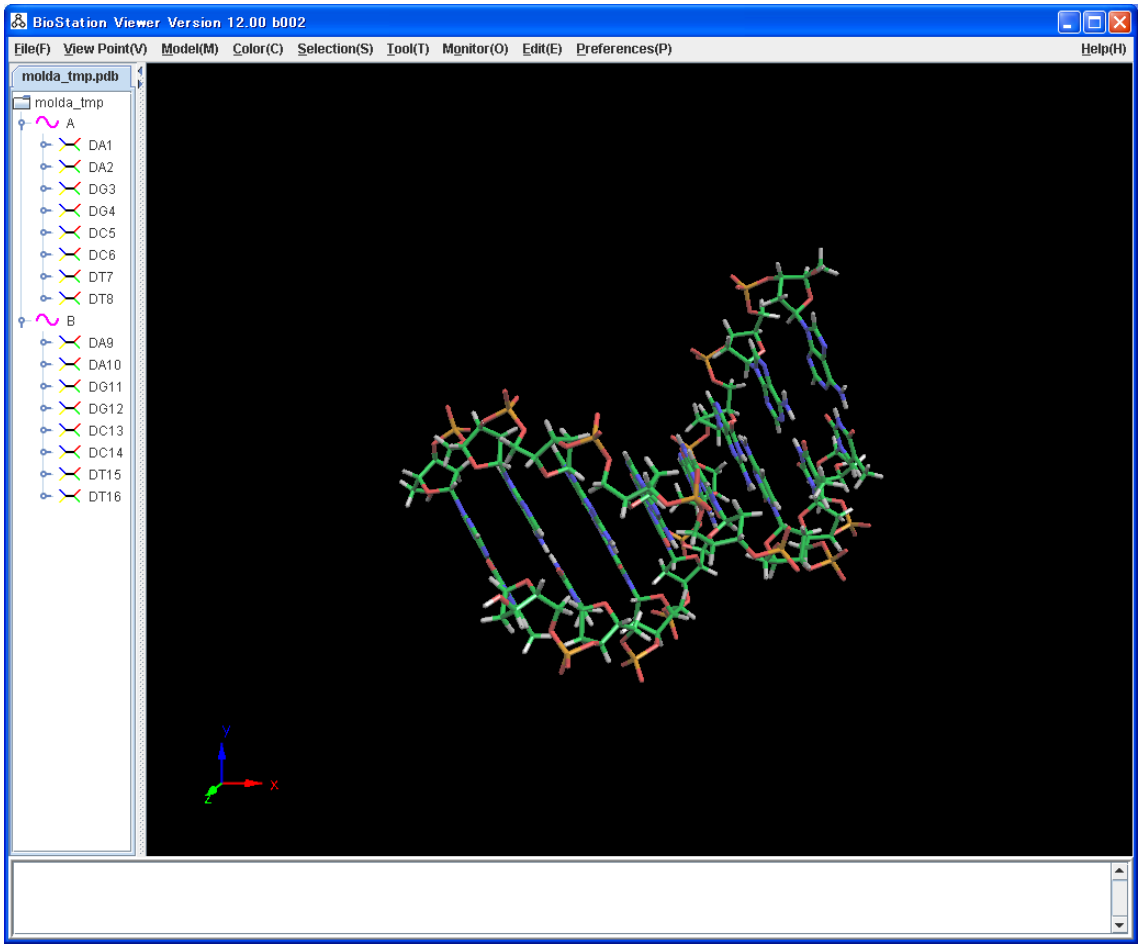


Fig2.138 Result of display DNA on BioStation viewer

2.13.2. Creation RNA

(1) Input RNA sequence

Select **[Molda]-[Input]-[RNA]** menu. The menu is shown in Fig2.139. Create DNA dialog box is displayed and shown in Fig2.140. For instance, input AAGGCCUU to the text area of the dialog box as **Input sequence** and click **OK**. The text area has to input RNA-bases: A, G, C and U. The result is displayed on Molda viewer and shown in Fig2.141.

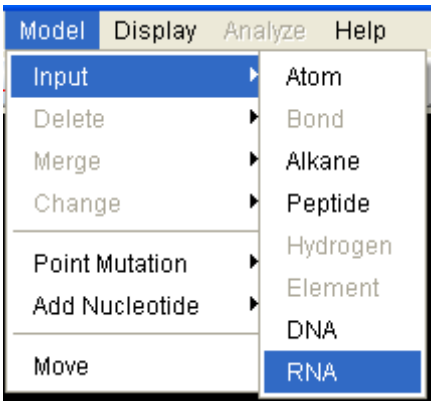


Fig2.139 Input RNA menu

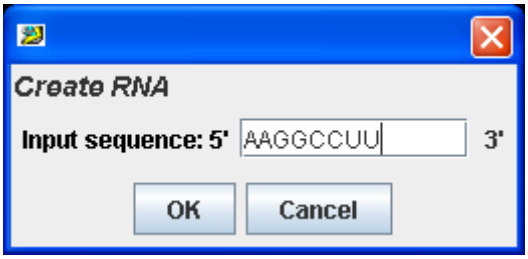


Fig2.140 Create RNA dialog box

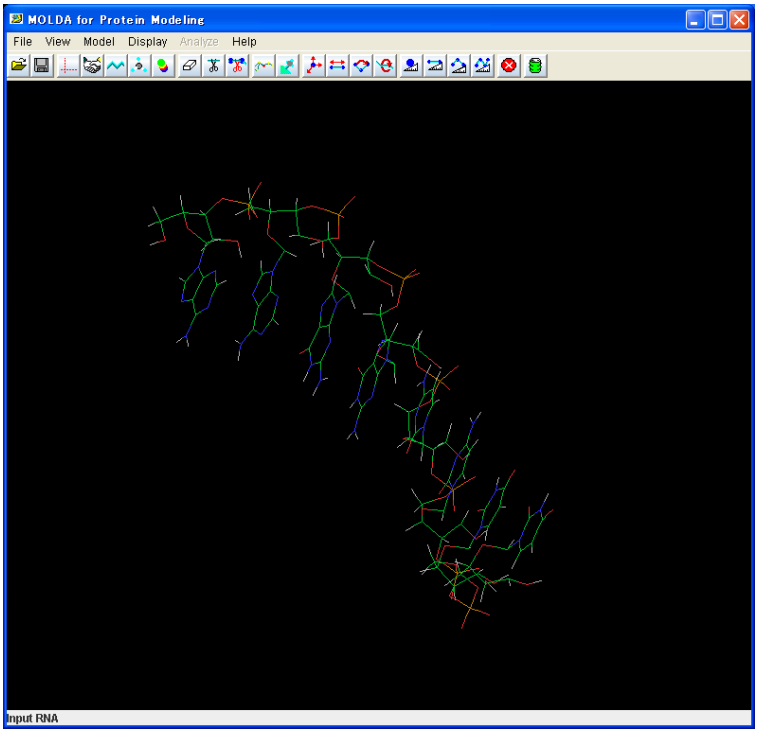


Fig2.141 Result of create RNA

(2) To Viewer

If you want to display the RNA on BioStation main window then select **[Display]-[To Viewer]** menu. The RNA is displayed on BioStation main window. Result of display is shown in Fig2.142.

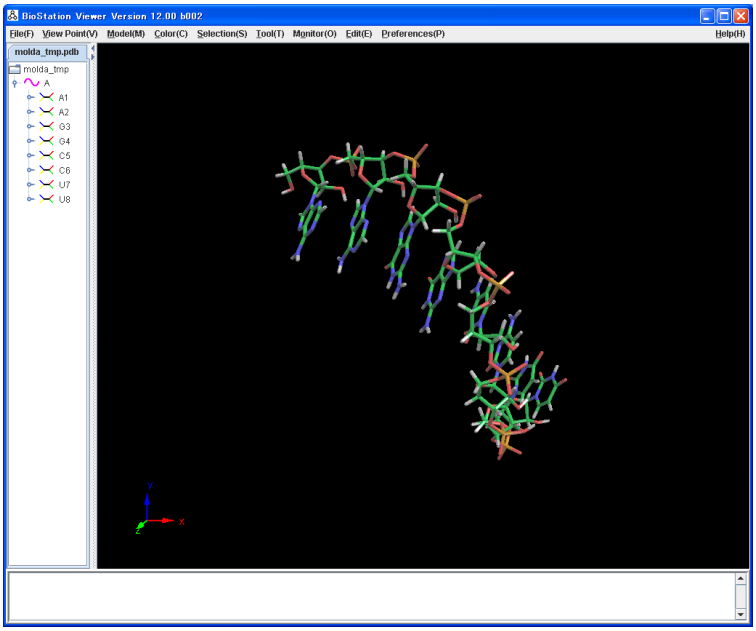


Fig2.142 Result of display RNA on BioStation viewer

2.13.3. Mutation DNA

(1) Display DNA on BioStation

Open pdb file of DNA on BioStation Viewer.

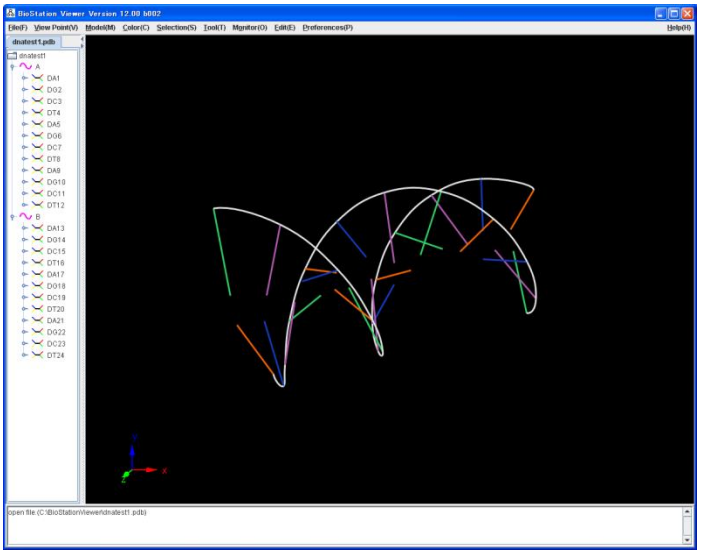


Fig2.143 Result of display pdb file of DNA on BioStation viewer

(2) Display on Molda

Display the DNA on Molda. Select **[File]-[Molda [with file]]** menu of BioStation Viewer. The DNA is displayed on Molda. It is shown in Fig2.144.

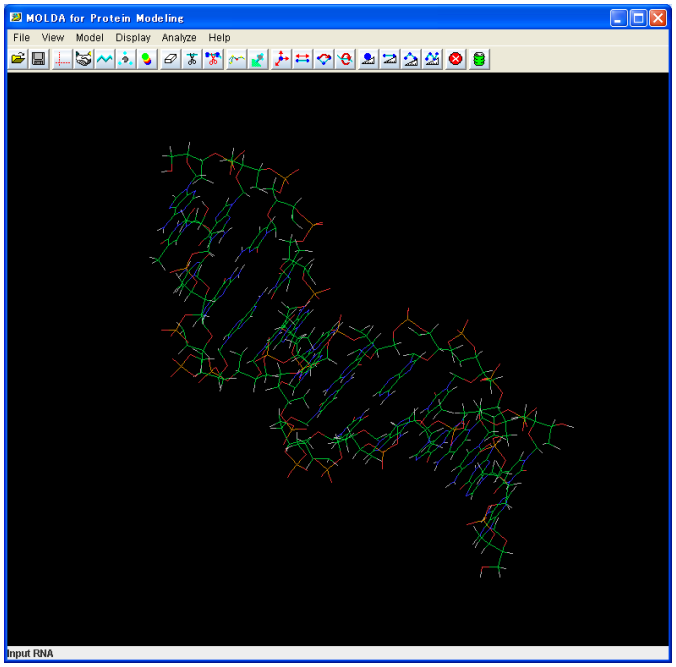


Fig2.144 Result of display DNA on Molda

(3) Select nucleotide

Select **[View]-[Sequence Viewer]** menu and Sequence Viewer is displayed. Select a mutated nucleotide and click **OK** on Sequence Viewer. The selected nucleotide changes the color to cyan on Molda. For instance, select DC3 and click **OK** on Sequence Viewer. It is shown in Fig2.145 and Molda is shown in Fig2.146.

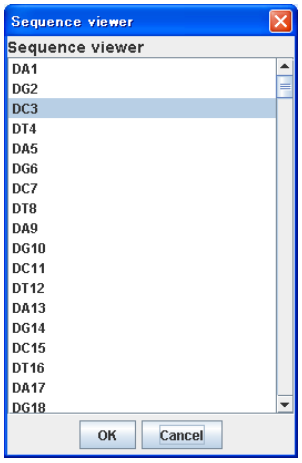


Fig2.145 Selected DC3 on Sequence Viewer

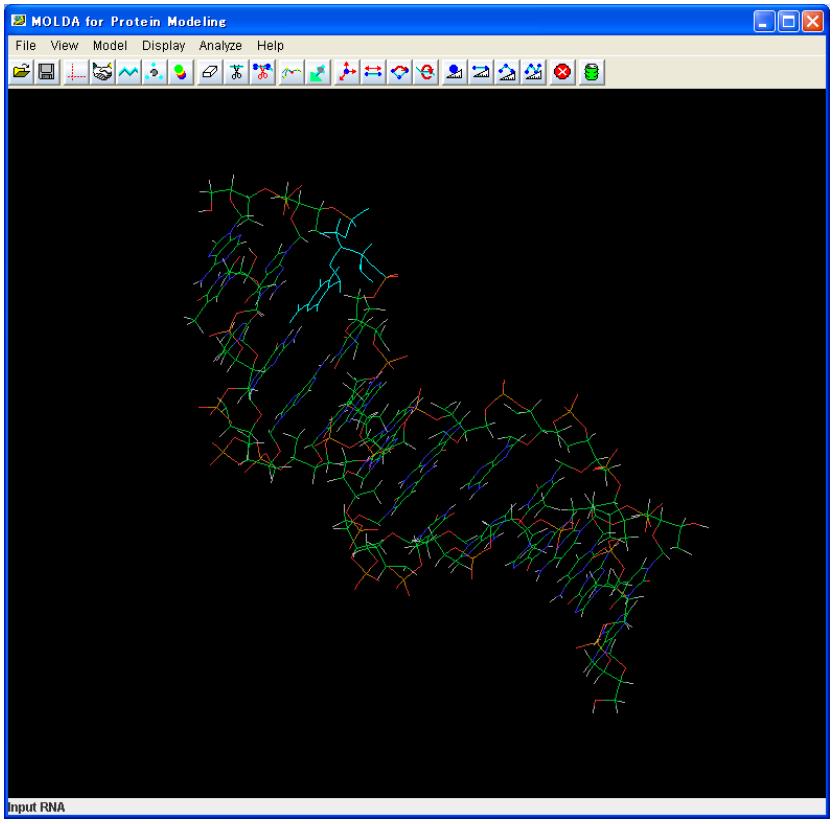


Fig2.146 Selected DC3 on Molda

(4) Mutate DNA

Select **[Molda]-[Point Mutation]-[DNA]** menu. The menu is shown in Fig2.147. Mutation DNA dialog box is displayed and shown in Fig2.148. If selected DC3 in (3) mutate into DT then select **DT** from the combo box of the dialog box and click **OK**. The combo box has DNA-bases: DA, DG, DC and DT. The result is displayed on Molda viewer and shown in Fig2.149.

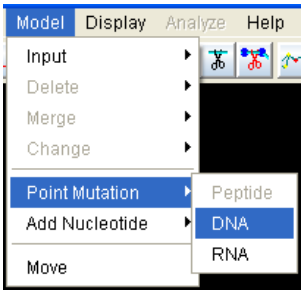


Fig2.147 Point Mutation DNA menu

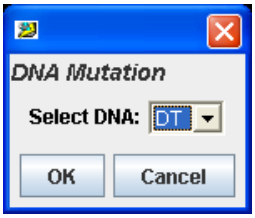


Fig2.148 Point Mutation DNA dialog box

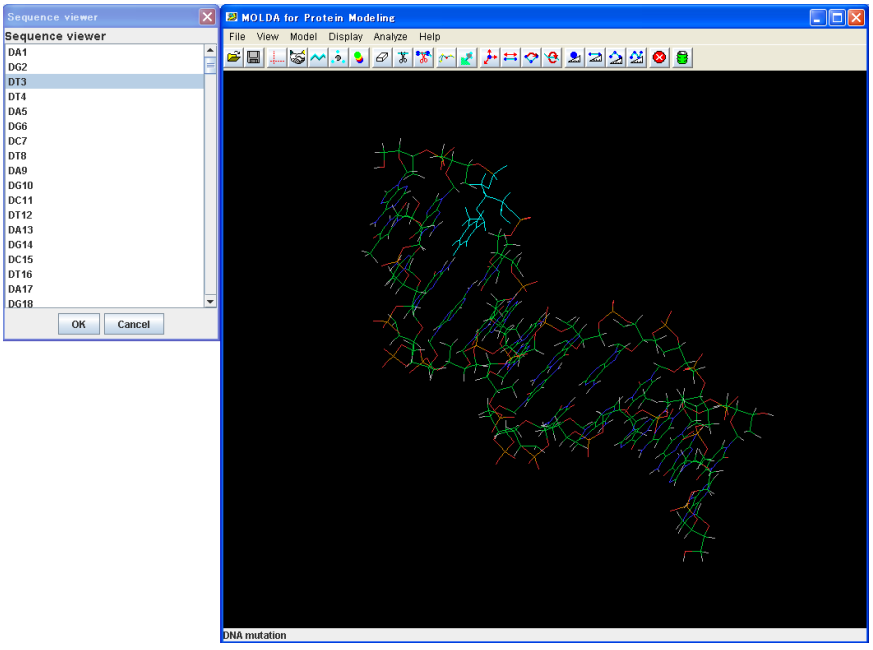


Fig2.149 Result of Mutation DNA

(5) To Viewer

If you want to display the DNA on BioStation main window then select **[Display]-[To Viewer]** menu. The DNA is displayed on BioStation main window. Result of display is shown in Fig2.150.

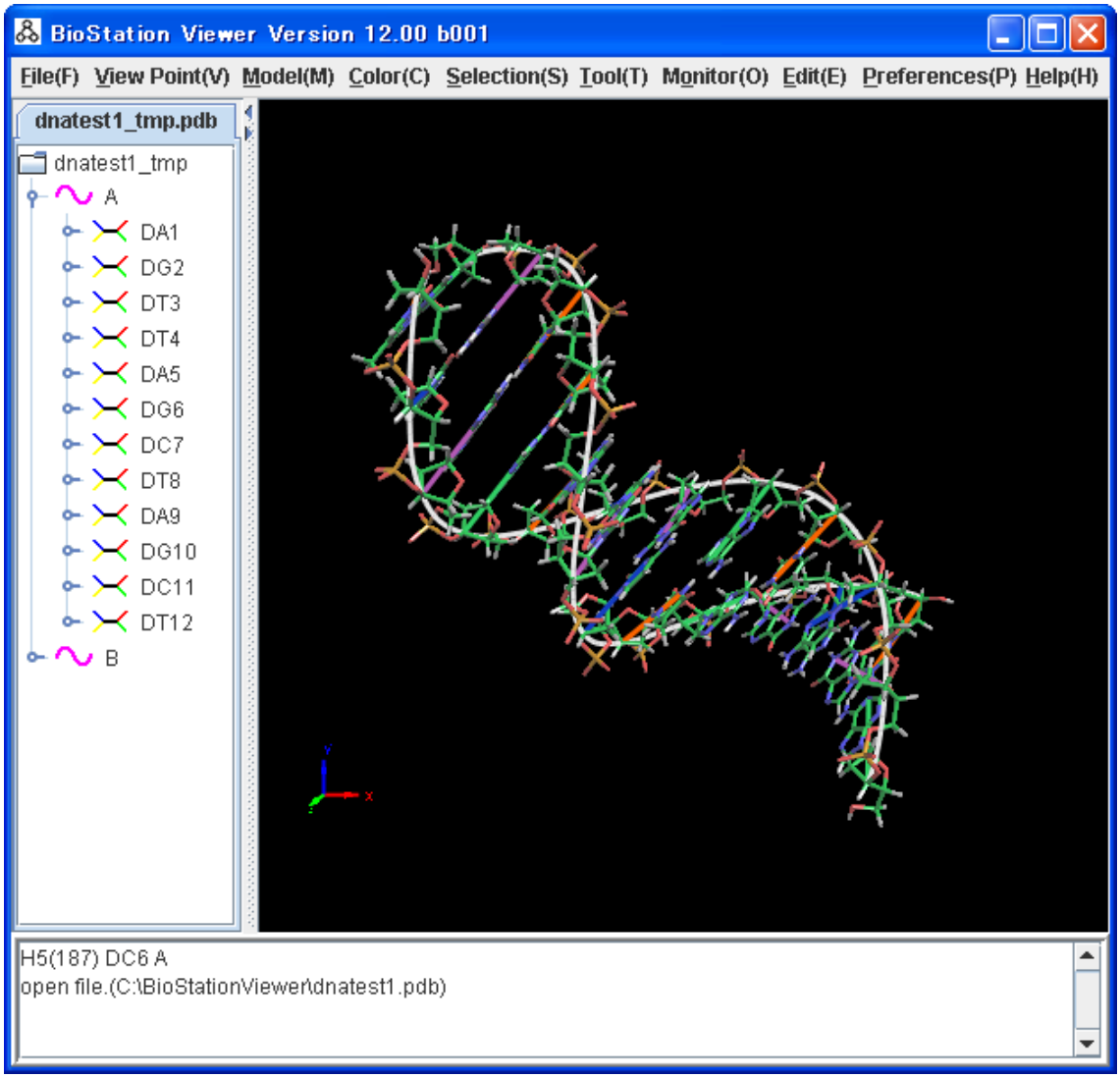


Fig2.150 Result of display DNA on BioStation viewer

2.13.4. Mutation RNA

(1) Display RNA on BioStation

Open pdb file of RNA on BioStation Viewer.

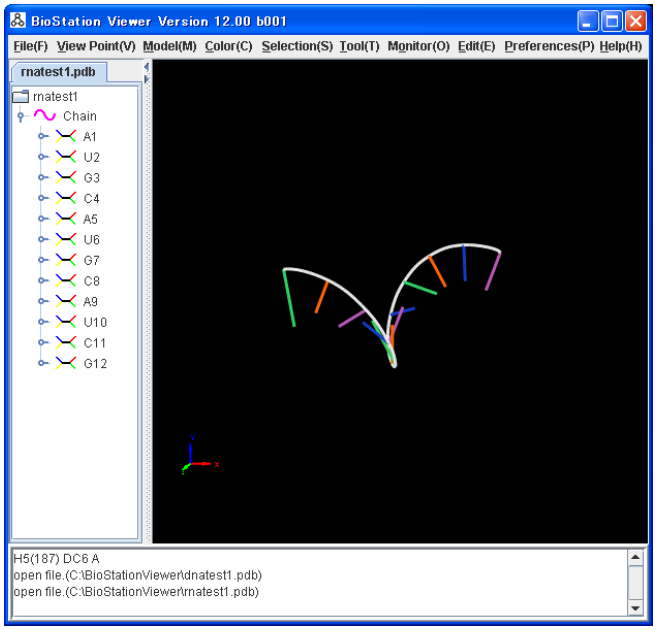


Fig2.151 Result of display pdb file of RNA on BioStation viewer

(2) Display Molda

Display the RNA on Molda. Select **[File]-[Molda [with file]]** menu of BioStation Viewer. The RNA is displayed on Molda. It is shown in Fig2.152.

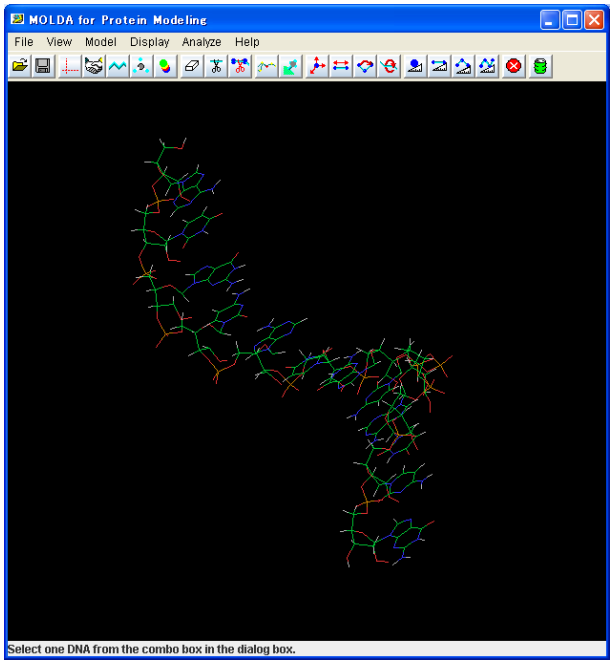


Fig2.152 Result of display RNA on Molda

(3) Select nucleotide

Select **[View]-[Sequence Viewer]** menu and Sequence Viewer is displayed. Select a mutated nucleotide and click **OK** on Sequence Viewer. The selected nucleotide changes the color to cyan on Molda. For instance, select U2 and click **OK** on Sequence Viewer. It is shown in Fig2.153 and Molda is shown in Fig2.154.

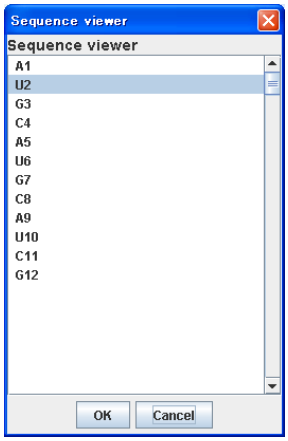


Fig2.153 Selected U2 on Sequence Viewer

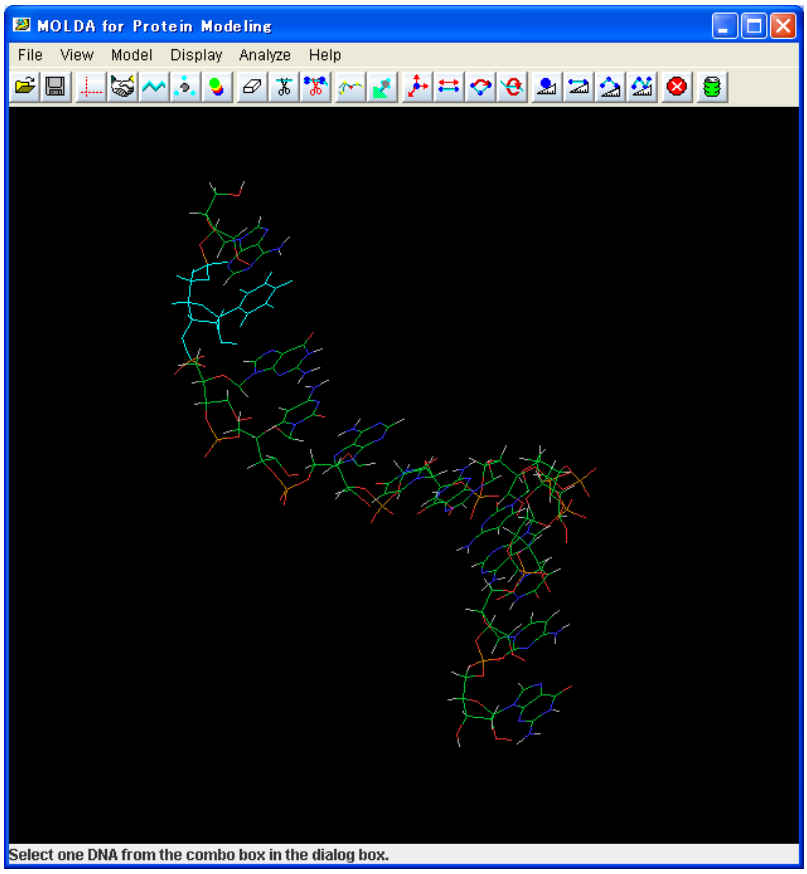


Fig2.154 Selected U2 on Molda

(4) Mutate RNA

Select **[Molda]-[Point Mutation]-[RNA]** menu. The menu is shown in Fig2.155. Mutation RNA dialog box is displayed and shown in Fig2.156. If selected U2 at (3) mutate into A then select **A** from the combo box of the dialog box and click **OK**. The combo box has RNA-bases: A, G, C and U. The result is displayed on Molda viewer and shown in Fig2.157.

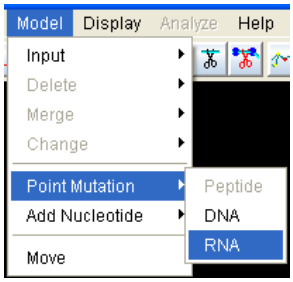


Fig2.155 Point Mutation RNA menu

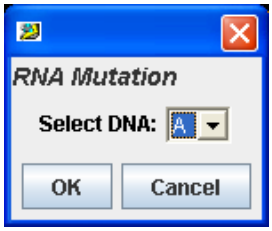


Fig2.156 Point Mutation RNA dialog box

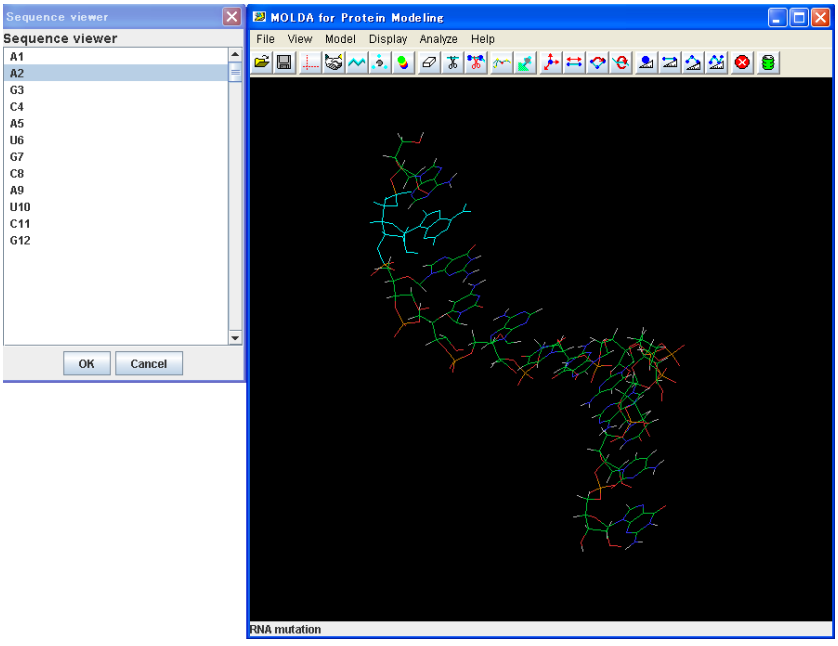


Fig2.157 Result of Mutation RNA

(5) To Viewer

If you want to display the DNA on BioStation main window then select **[Display]-[To Viewer]** menu. The RNA is displayed on BioStation main window. Result of display is shown in Fig2.158.

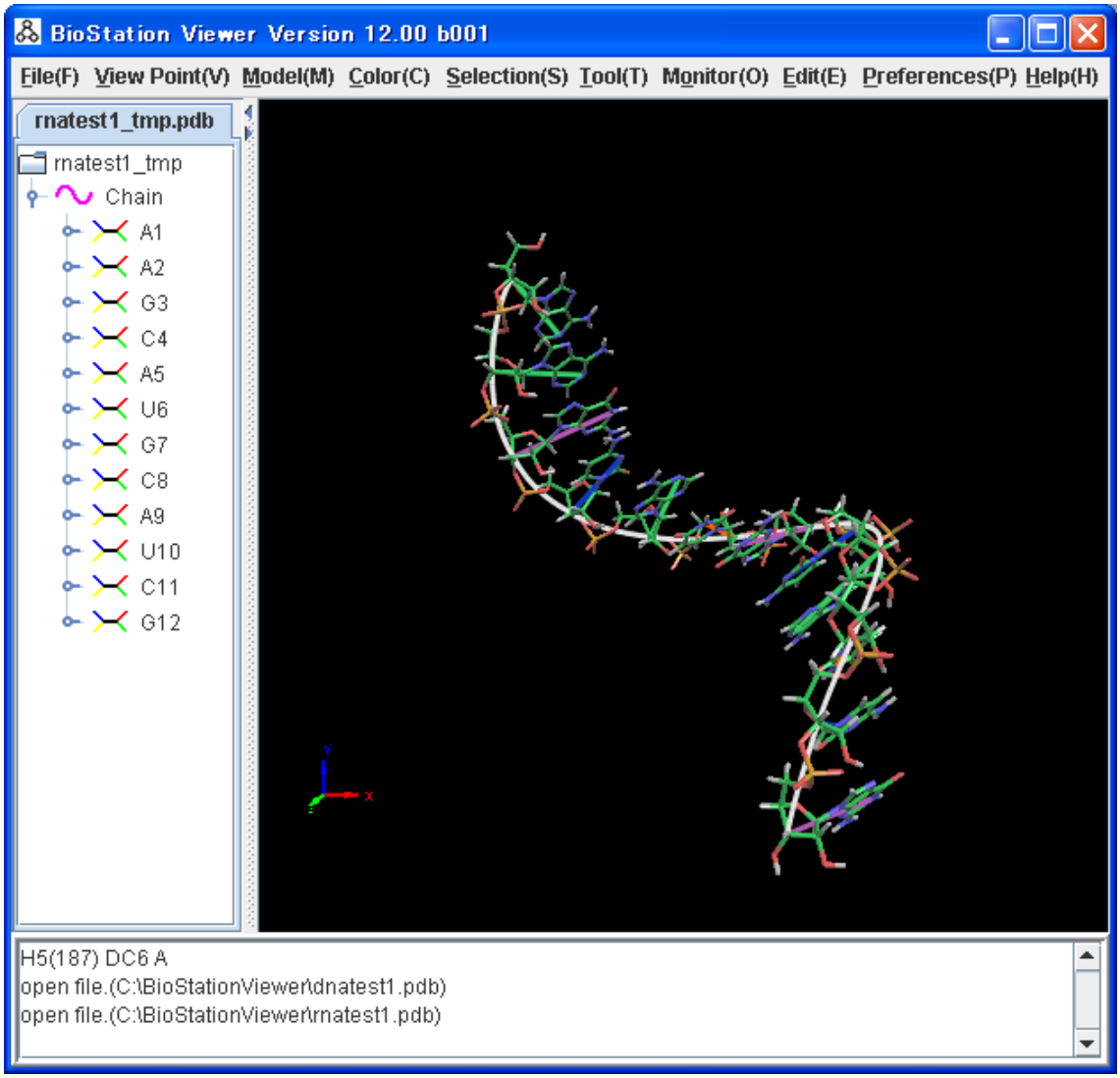


Fig2.158 Result of display RNA on BioStation viewer

2.13.5. Adding Nucleotides of DNA

In the **Adding Nucleotides of DNA** you can choose position from **5'Terminal**, **3'Terminal** and **Middle**. This section describes each positions.

2.13.5.1 Position : 5'Terminal

If you want to Adding Nucleotides in 5'-end direction then select **5'Terminal**.

(1) Display DNA on BioStation

Open pdb file of DNA on BioStation Viewer. The following display properties are setting for describing: **[Model]-[Atom (A)]** sets Off, **[Model]-[Structure(S)]** sets **C α [line]**, and **[Tool]-[Label]**'s **Residue Label** sets on.

For instance, if a base pair of B chain's DC9 is missing then add DG in 5'-end direction as next to DA1 on A chain.

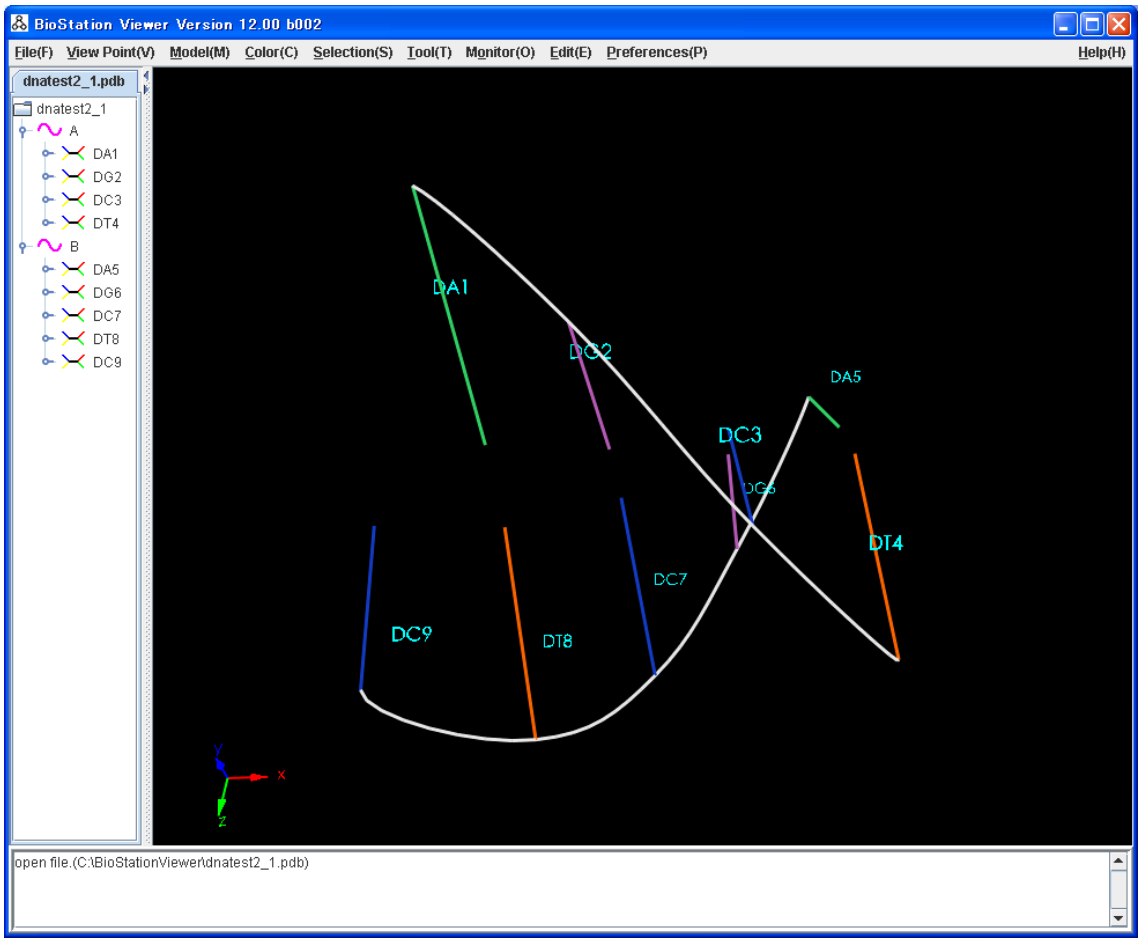


Fig2.159 Result of display pdb file of DNA on BioStation viewer

(2) Display Molda

Display the DNA on Molda. Select **[File]-[Molda [with file]]** menu of BioStation Viewer. The DNA is displayed on Molda. It is shown in Fig2.160.

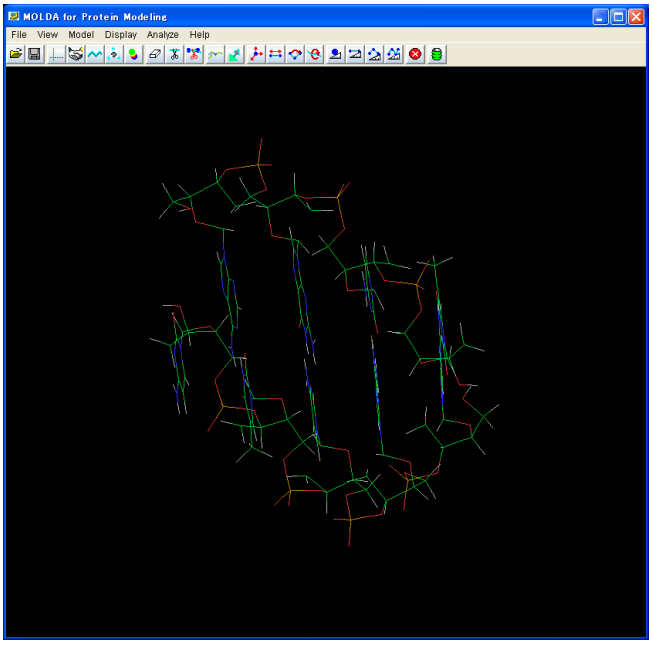


Fig2.160 Result of display DNA on Molda

(3) Select starting DNA-base for Add

Select **[View]-[Sequence Viewer]** menu and Sequence Viewer is displayed. Select a stating nucleotide and click **OK** on Sequence Viewer. The selected nucleotide changes the color to cyan on Molda. For instance, select DA1 and click **OK** on Sequence Viewer. It is shown in Fig2.161 and Molda is shown in Fig2.162.

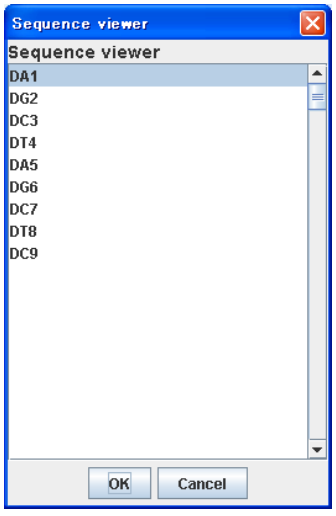


Fig2.161 Selected DA1 on Sequence Viewer

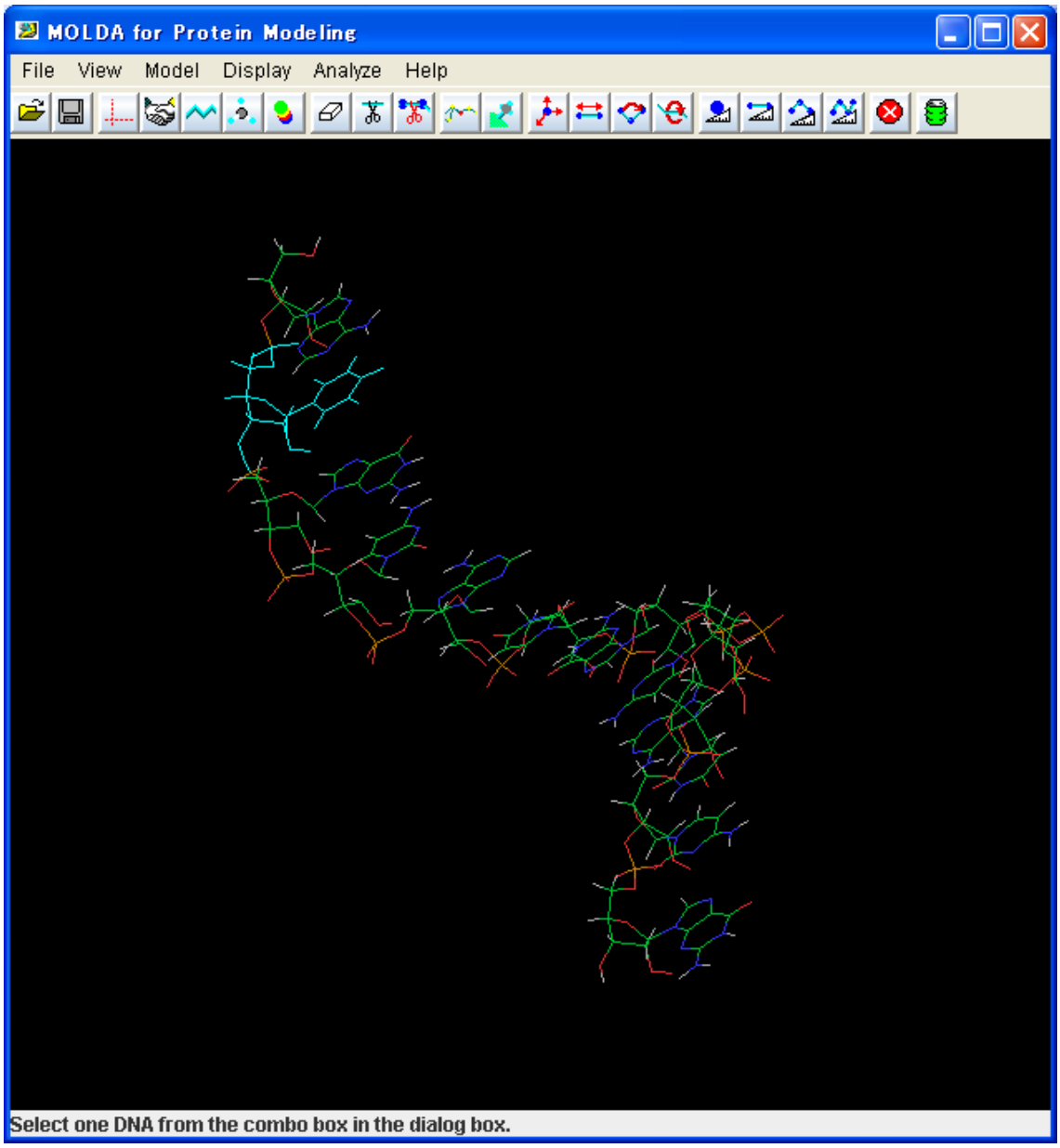


Fig2.162 Selected DA1 on Molda

(4) Adding Nucleotide

Select **[Molda]-[Add Nucleotide]-[DNA]** menu. The menu is shown in Fig2.163. DNA Adding Nucleotide dialog box is displayed and shown in Fig2.164. If DG adds next to DA1 in 5'-end direction then choose **5'Terminal** from **Position**, input G to the text area as **Sequence** and click **OK**. Sequence has to input DNA-bases: A, G, C and T. The result is displayed on Molda viewer and shown in Fig2.165.

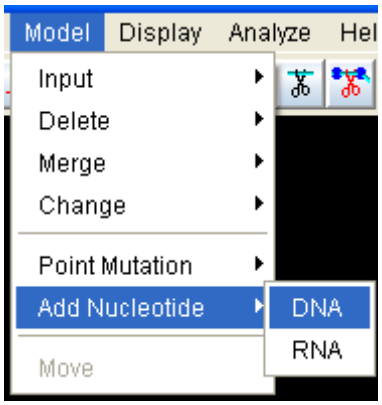


Fig2.163 DNA Add Nucleotide menu

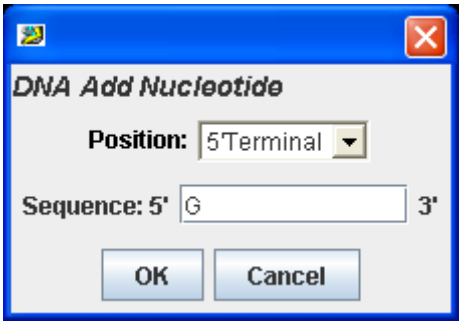


Fig2.164 DNA Add Nucleotide dialog box

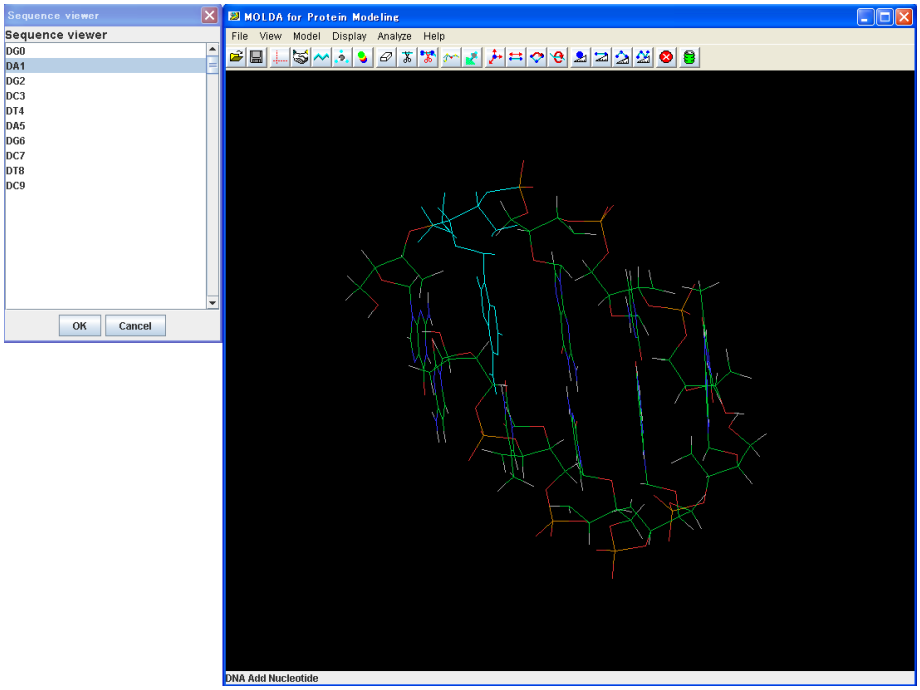


Fig2.165 Result of DNA Adding Nucleotide

Remark

- If selected chain in (3) has only one DNA-base then it doesn't allow you to add any nucleotides to the chain.
- If the **Position** selects **5'Terminal** then selected DNA-base in (3) has to be on 5'-end.

(5) To Viewer

If you want to display the DNA on Molda to BioStation main window then select **[Display]-[To Viewer]** menu. The DNA is displayed on BioStation main window. Result of display is shown in Fig2.166.

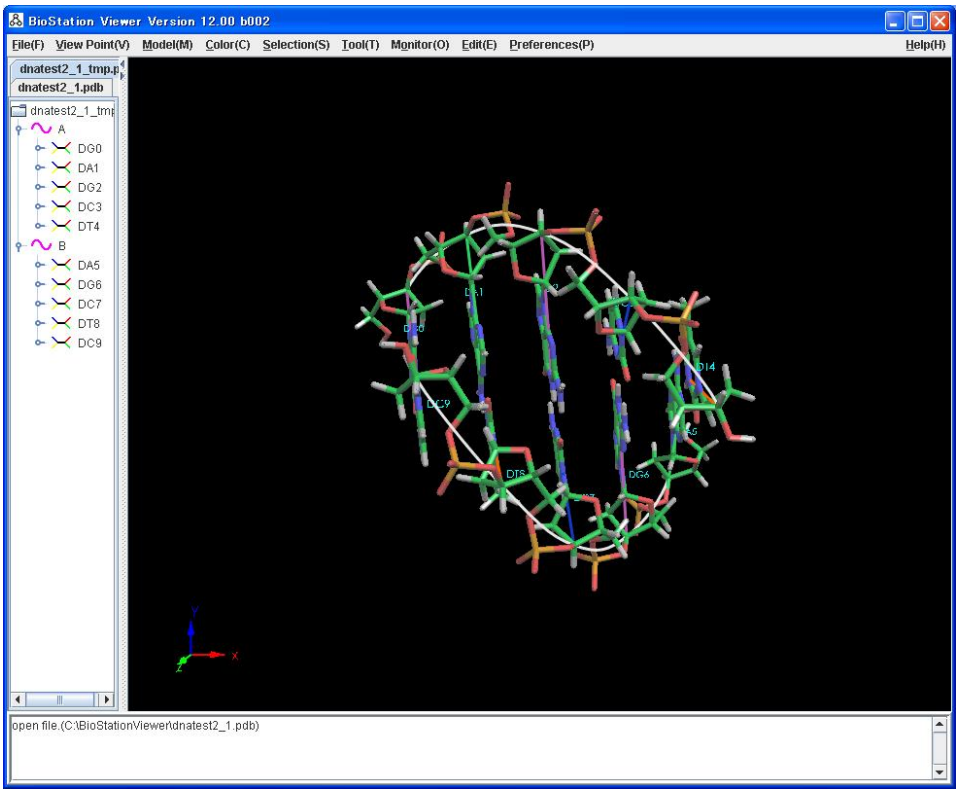


Fig2.166 Result of display DNA on BioStation viewer

2.13.5.2 Position : Middle

If you want to add nucleotides in 3'-end direction and selected DNA-base isn't on 3'-end then select **Middle**.

(1) Display DNA on BioStation

Open pdb file of DNA on BioStation Viewer. The following display properties are setting for describing: **[Model]-[Atom (A)]** sets Off, **[Model]-[Structure(S)]** sets **C α [line]**, and **[Tool]-[Label]**'s **Residue Label** sets on.

For instance, if two base pair of A chain's DG2 and DC3 are missing then add DG and DC in 3'-end direction as next to DA5 on B chain.

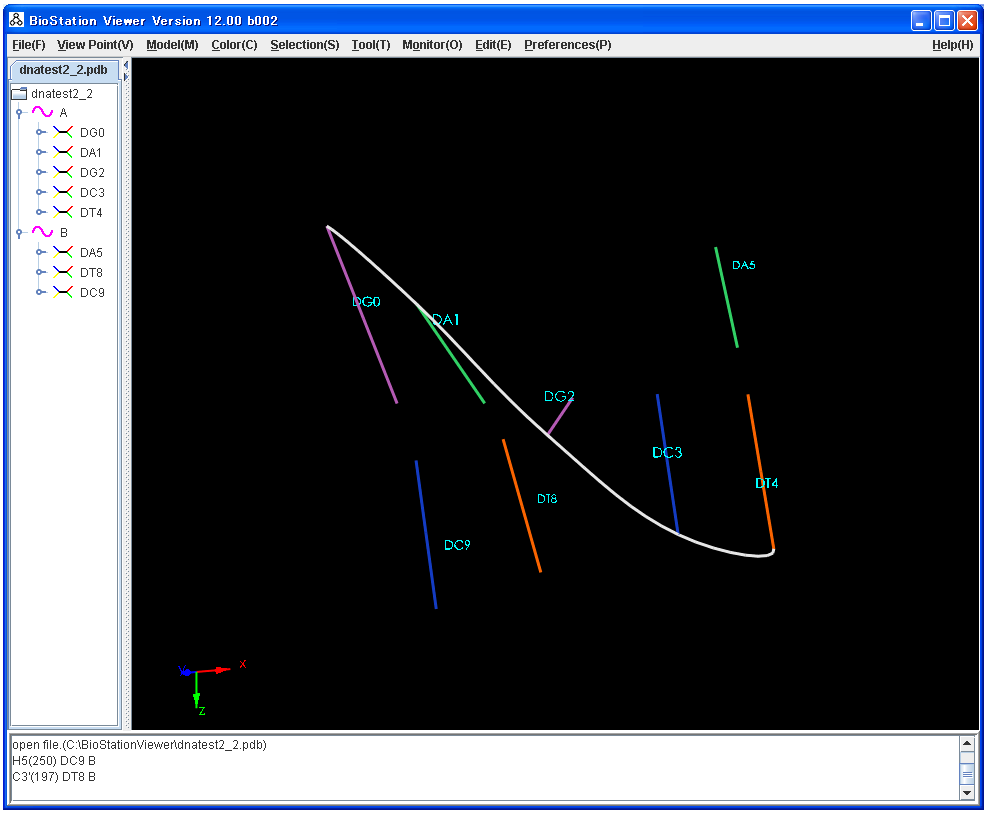


Fig2.167 Result of display pdb file of DNA on BioStation viewer

(2) Display Molda

Display the DNA on Molda. Select **[File]-[Molda [with file]]** menu of BioStation Viewer. The DNA is displayed on Molda. It is shown in Fig2.168.

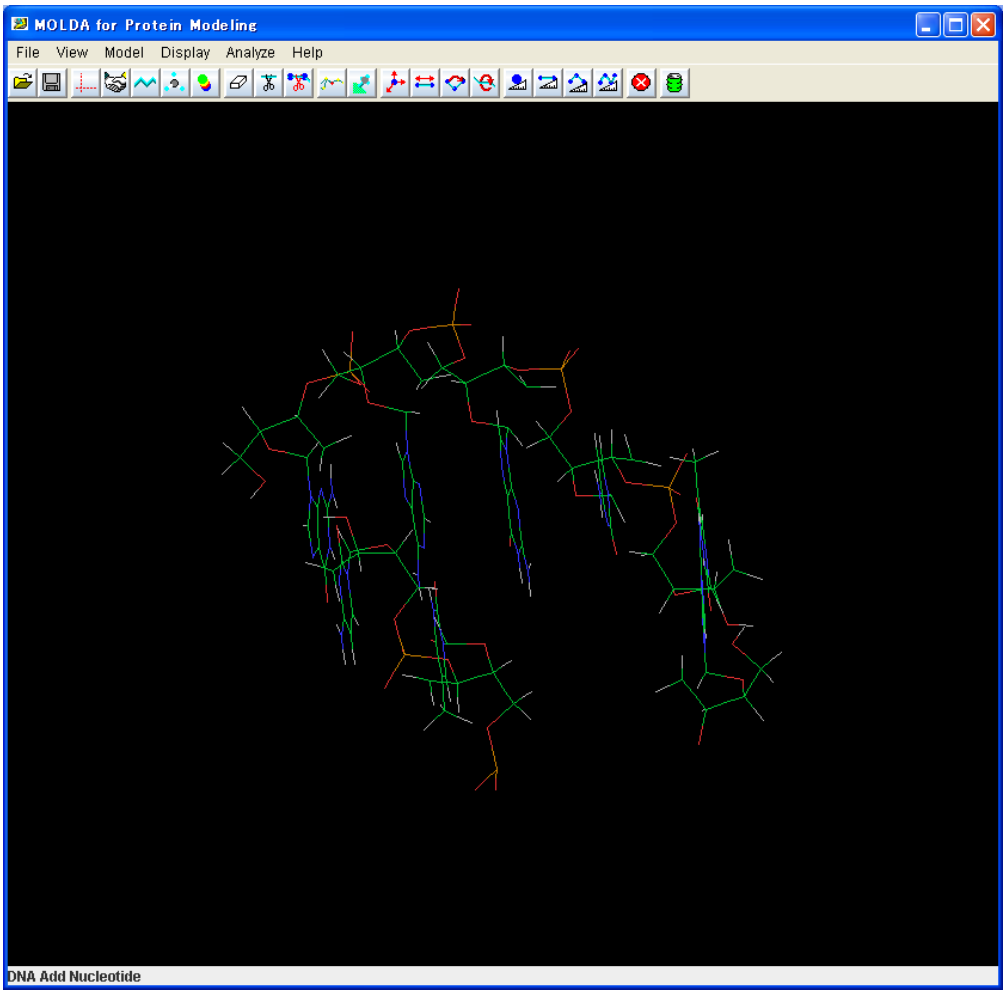


Fig2.168 Result of display DNA on Molda

(3) Select starting DNA-base for Adding

Select **[View]-[Sequence Viewer]** menu and Sequence Viewer is displayed. Select a stating nucleotide and click **OK** on Sequence Viewer. The selected nucleotide changes the color to cyan on Molda. For instance, select DA5 and click **OK** on Sequence Viewer. It is shown in Fig2.169 and Molda is shown in Fig2.170.

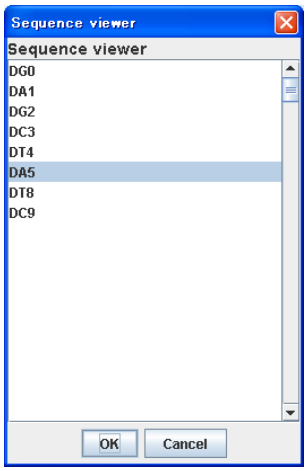


Fig2.169 Selected DA5 on Sequence Viewer

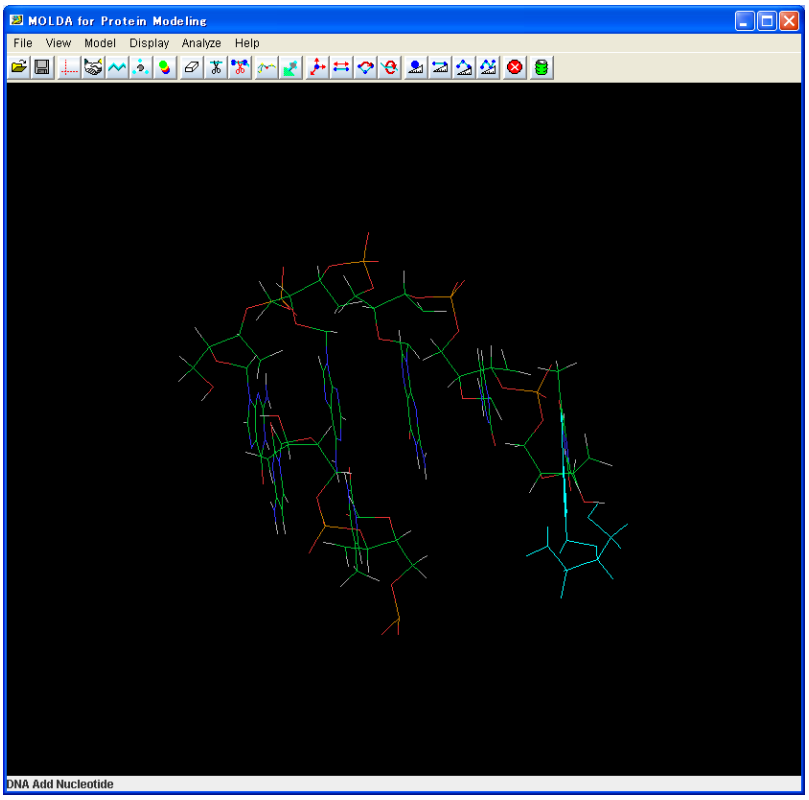


Fig2.170 Selected DA5 on Molda

(4) Add Nucleotide

Select **[Molda]-[Add Nucleotide]-[DNA]** menu. DNA Add Nucleotide dialog box is displayed and shown in Fig2.171. For instance, if DG and DC adds next to DA5 in 3'-end direction then choose **Middle** from **Position,** input GC to the text area as **Sequence** and click **OK**. **Sequence** has to input DNA-bases: A, G, C and T. The result is displayed on Molda viewer and shown in Fig2.172.

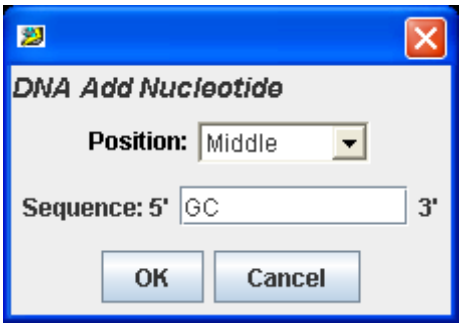


Fig2.171 DNA Add Nucleotide dialog box

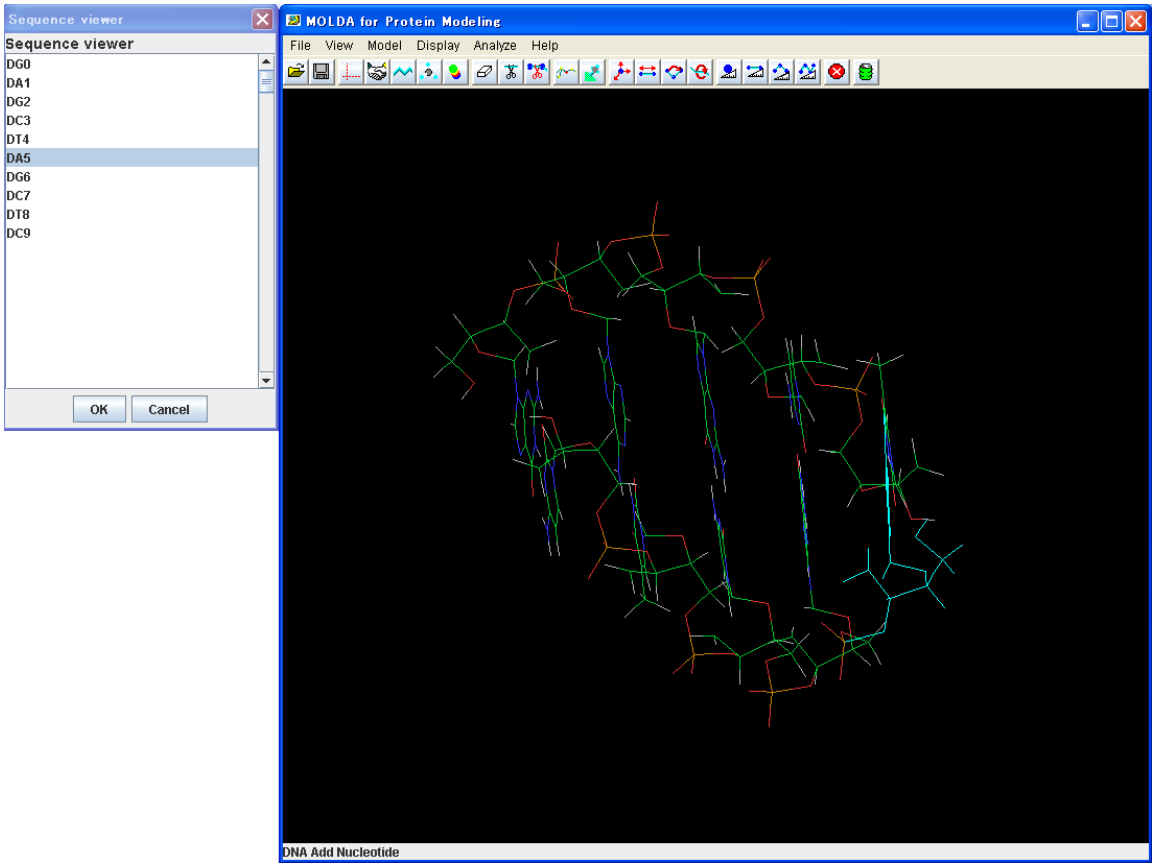


Fig2.172 Result of DNA Adding Nucleotide

Remark

- If selected chain in (3) has only one DNA-base then it doesn't allow you to add any nucleotides to the chain.
- If the **Position** selects **Middle** then selected DNA-base in (3) has to be on 5'-end or middle, not on 3'-end.
- If the **Position** selects **Middle** then add nucleotides equal or less than number of missing nucleotides.

(5) To Viewer

If you want to display the DNA on BioStation main window then select **[Display]-[To Viewer]** menu. The DNA is displayed on BioStation main window. Result of display is shown in Fig2.173.

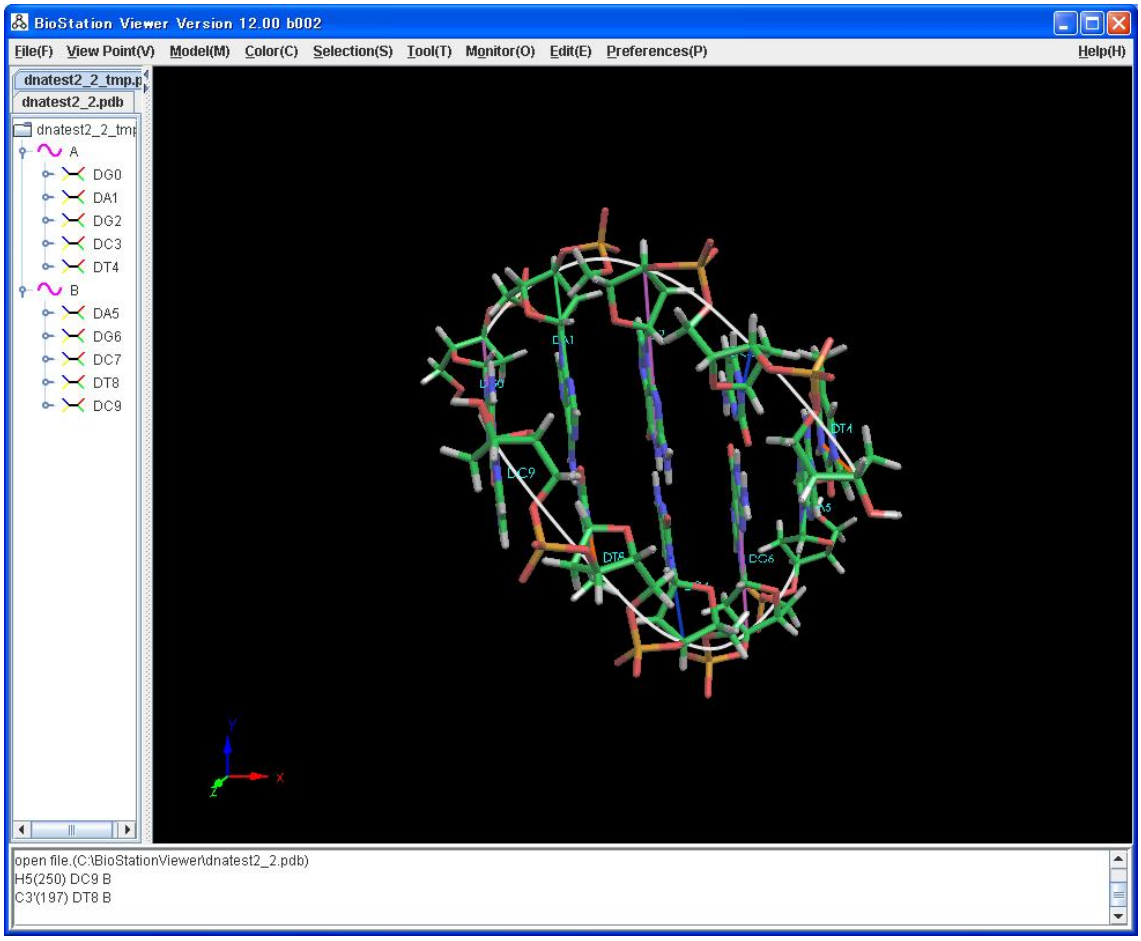


Fig2.173 Result of display DNA on BioStation viewer

2.13.5.3 Position : 3”Terminal

If you want to add nucleotides in 3'-end direction and selected DNA-base is on the 3’-end then select **Middle**.

(1) Display DNA on BioStation

Open pdb file of DNA on BioStation Viewer. The following display properties are setting for describing: **[Model]-[Atom (A)]** sets Off, **[Model]-[Structure(S)]** sets **C α [line]**, and **[Tool]-[Label]**’s **Residue Label** sets on.

For instance, if a base pair of B chain’s DA4 is missing then add DT in 3'-end direction as next to DG3 on A chain.

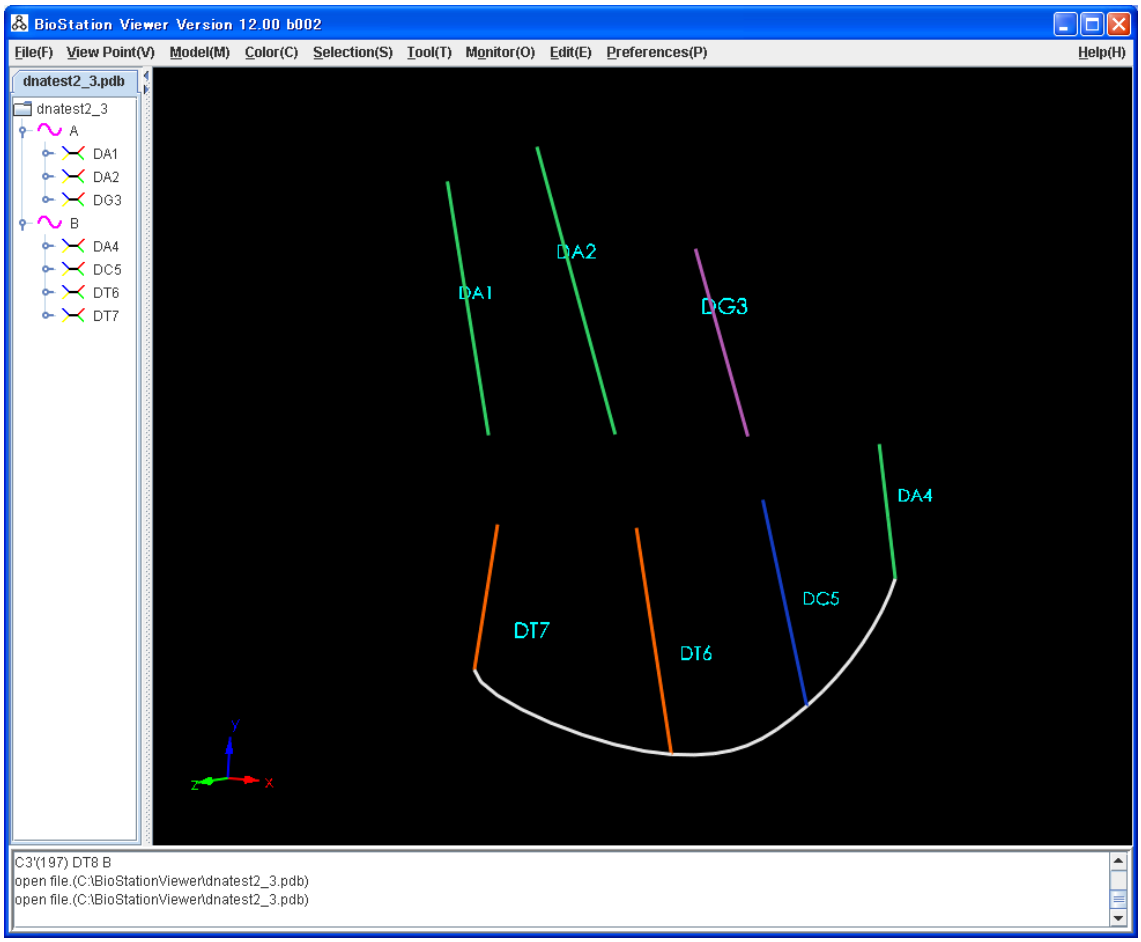


Fig2.174 Result of display pdb file of DNA on BioStation viewer

(2) Display Molda

Display the DNA on Molda. Select **[File]-[Molda [with file]]** menu of BioStation Viewer. The DNA is displayed on Molda. It is shown in Fig2.175.

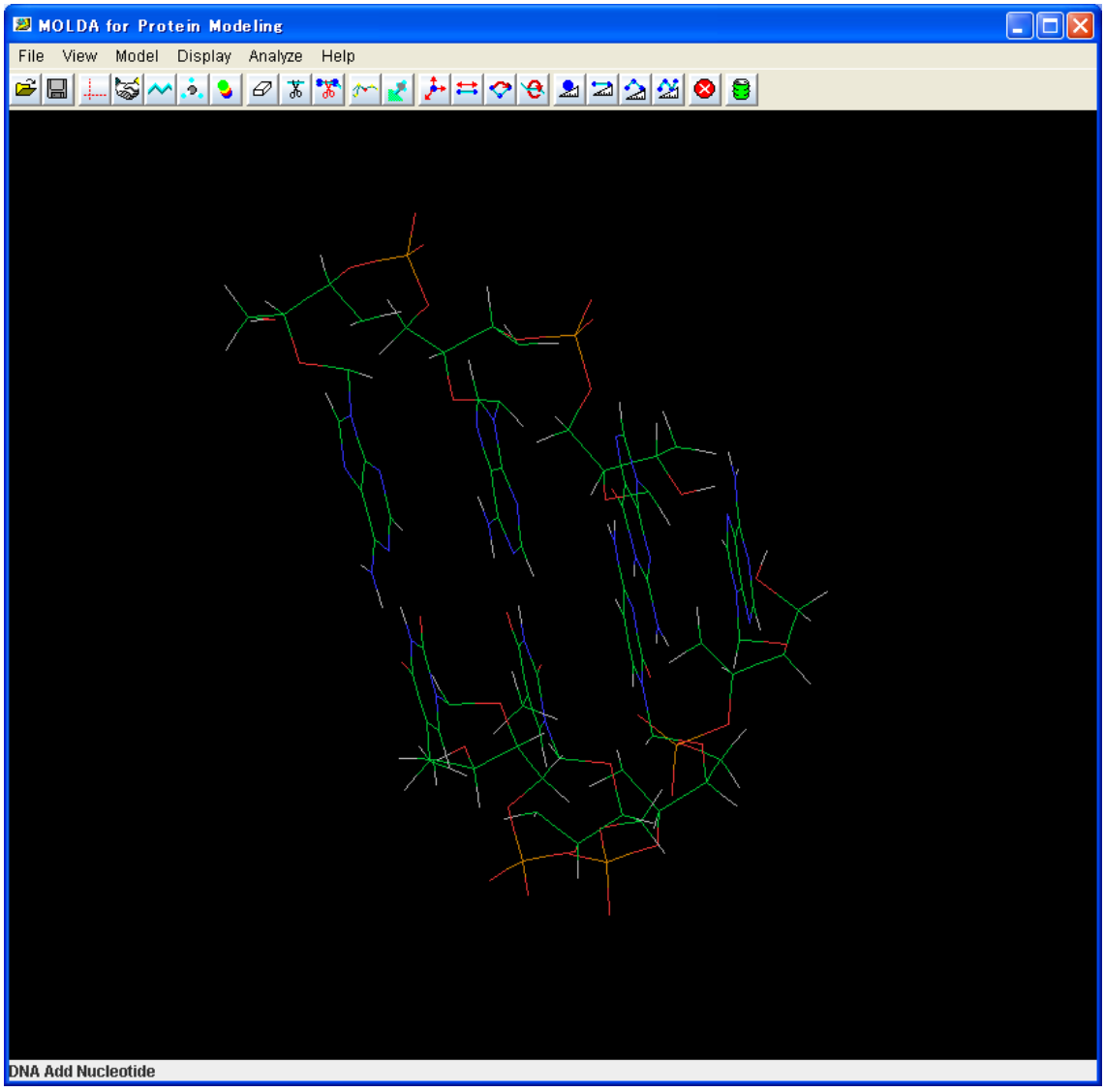


Fig2.175 Result of display DNA on Molda

(3) Select starting DNA-base for Adding

Select **[View]-[Sequence Viewer]** menu and Sequence Viewer is displayed. Select a stating nucleotide and click **OK** on Sequence Viewer. The selected nucleotide changes the color to cyan on Molda. For instance, select DG3 and click **OK** on Sequence Viewer. It is shown in Fig2.176 and Molda is shown in Fig2.170.

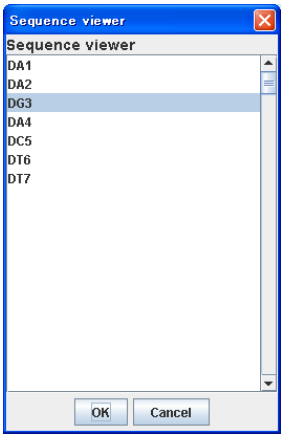


Fig2.176 Selected DG3 on Sequence Viewer

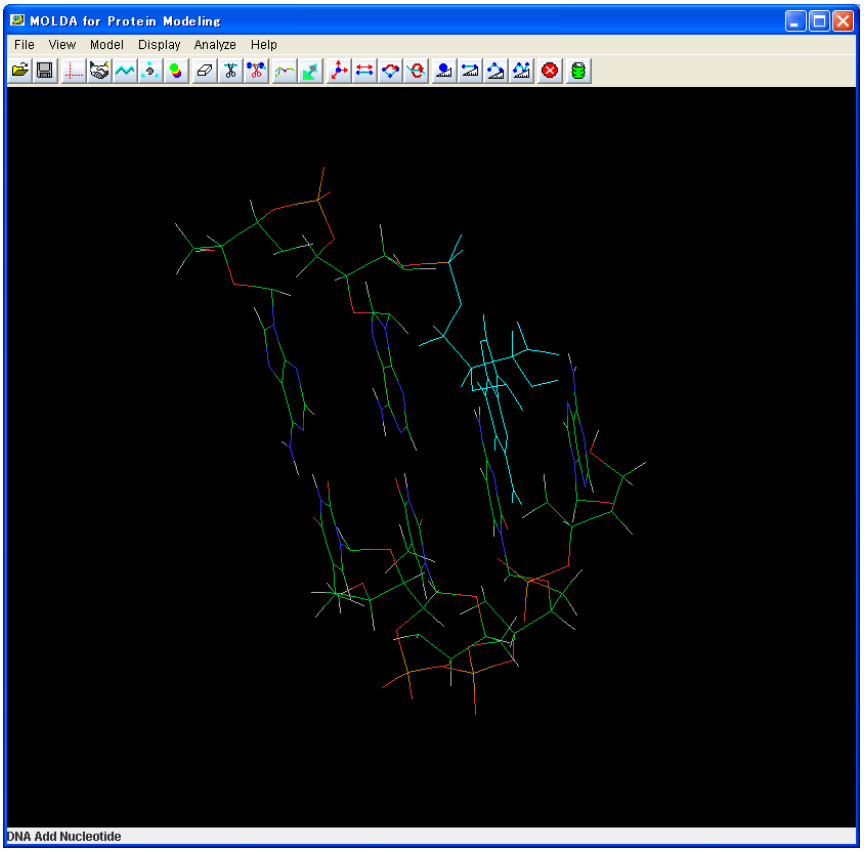


Fig2.177 Selected DG3 on Molda

(4) Add Nucleotide

Select **[Molda]-[Add Nucleotide]-[DNA]** menu. DNA Add Nucleotide dialog box is displayed and shown in Fig2.178. For instance, if DG and DC adds next to DG3 in 3'-end direction then choose **3'Terminal** from **Position,** input T to the text area as **Sequence** and click **OK**. **Sequence** has to input DNA-bases: A, G, C and T. The result is displayed on Molda viewer and shown in Fig2.179.

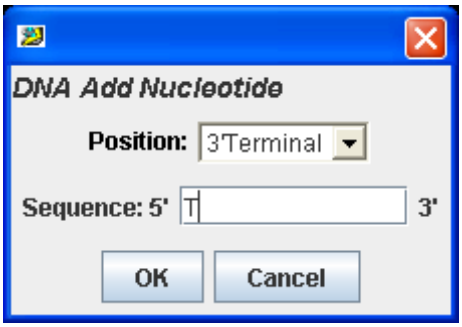


Fig2.178 DNA Add Nucleotide dialog box

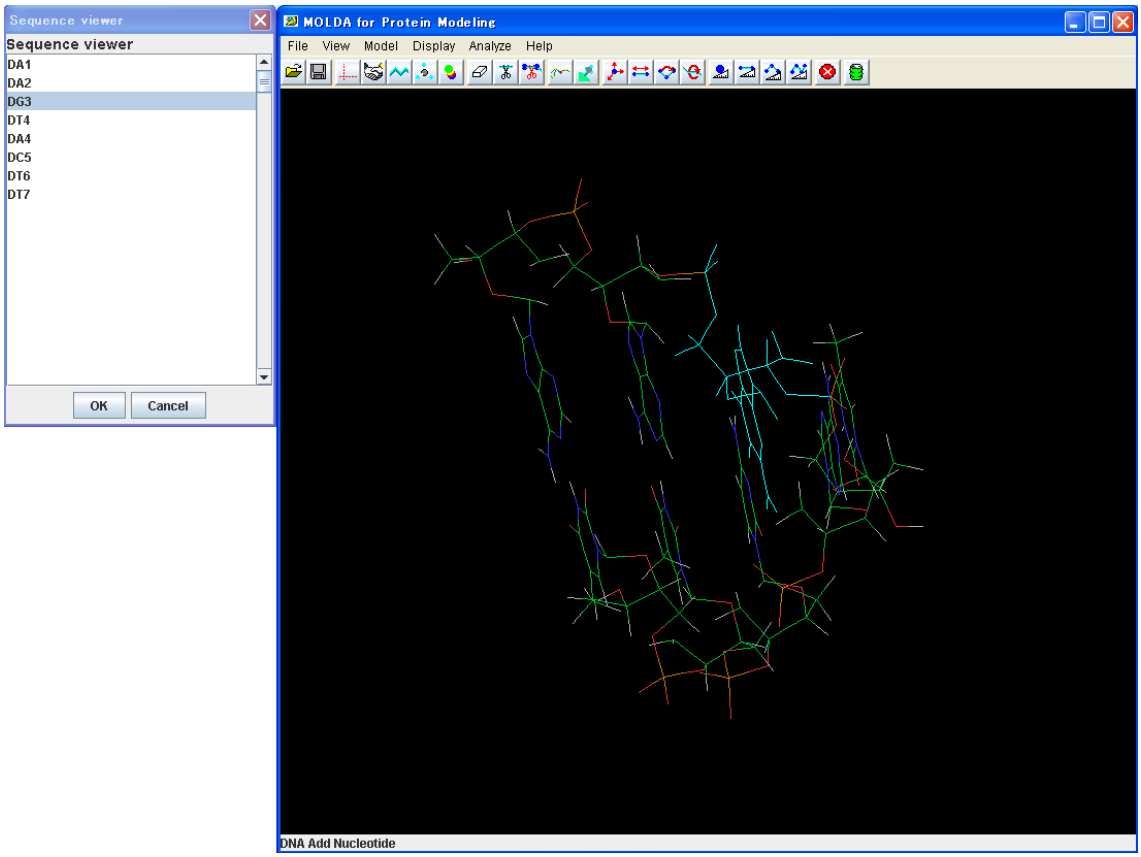


Fig2.179 Result of DNA Adding Nucleotide

Remark

- If selected chain in (3) has only one DNA-base then it does not allow you to add any nucleotides to the chain.
- If the **Position** selects **3'Terminal** then selected DNA-base in (3) has to be on the 3' -end.
- If the **Position** selects **3'Terminal** and the selected nucleotide dose not have previous nucleotide, first add missing nucleotides by **Middle** and then add nucleotides in 3'-end direction on the 3'-end.

(5) To Viewer

If you want to display the DNA on BioStation main window then select **[Display]-[To Viewer]** menu. The DNA is displayed on BioStation main window. Result of display is shown in Fig2.180.

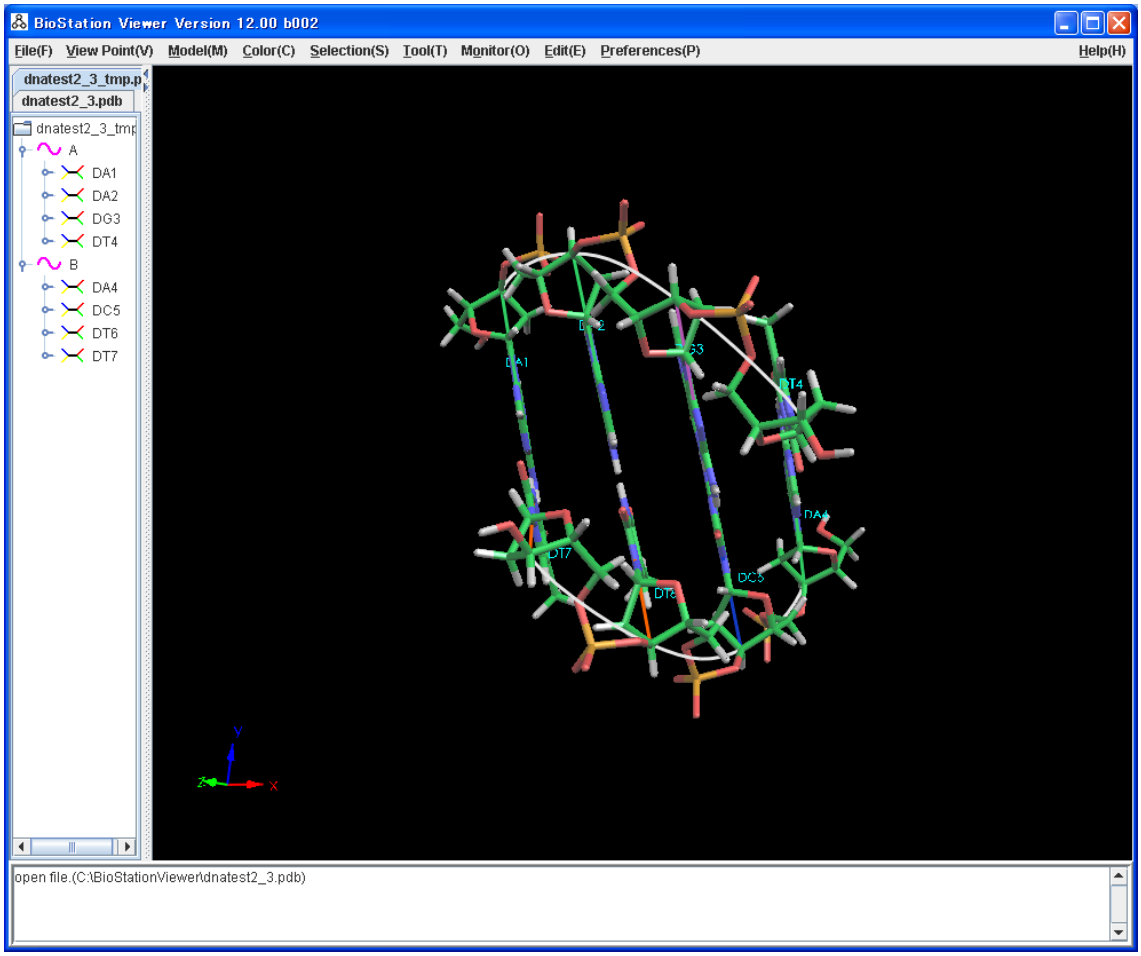


Fig2.180 Result of display DNA on BioStation viewer

2.13.6. Adding Nucleotides of RNA

Adding Nucleotide of RNA's operations are same as DNA's.

This section describes Adding Nucleotide of RNA when the **Position** is chosen **Middle**.

(1) Display RNA on BioStation

Open pdb file of DNA on BioStation Viewer. The following display properties are setting for describing: **[Model]-[Atom (A)]** sets Off, **[Model]-[Structure(S)]** sets **C α [line]**, and **[Tool]-[Label]**'s **Residue Label** sets on.

For instance, if between G3 and C8 nucleotides are missing then add three nucleotides in 3'-end direction as next to G3.

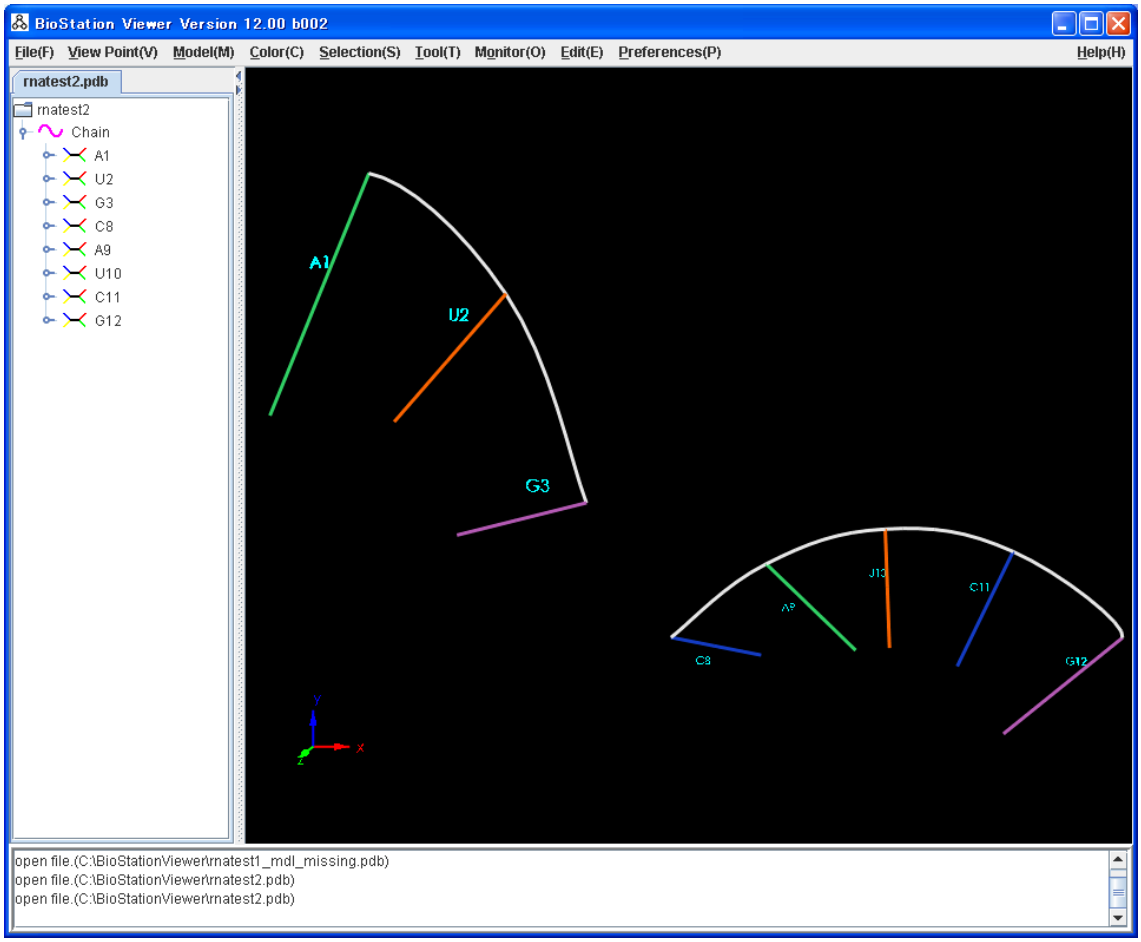


Fig2.181 Result of display pdb file of RNA on BioStation viewer

(2) Display Molda

Display the DNA on Molda. Select **[File]-[Molda [with file]]** menu of BioStation Viewer. The DNA is displayed on Molda. It is shown in Fig2.182.

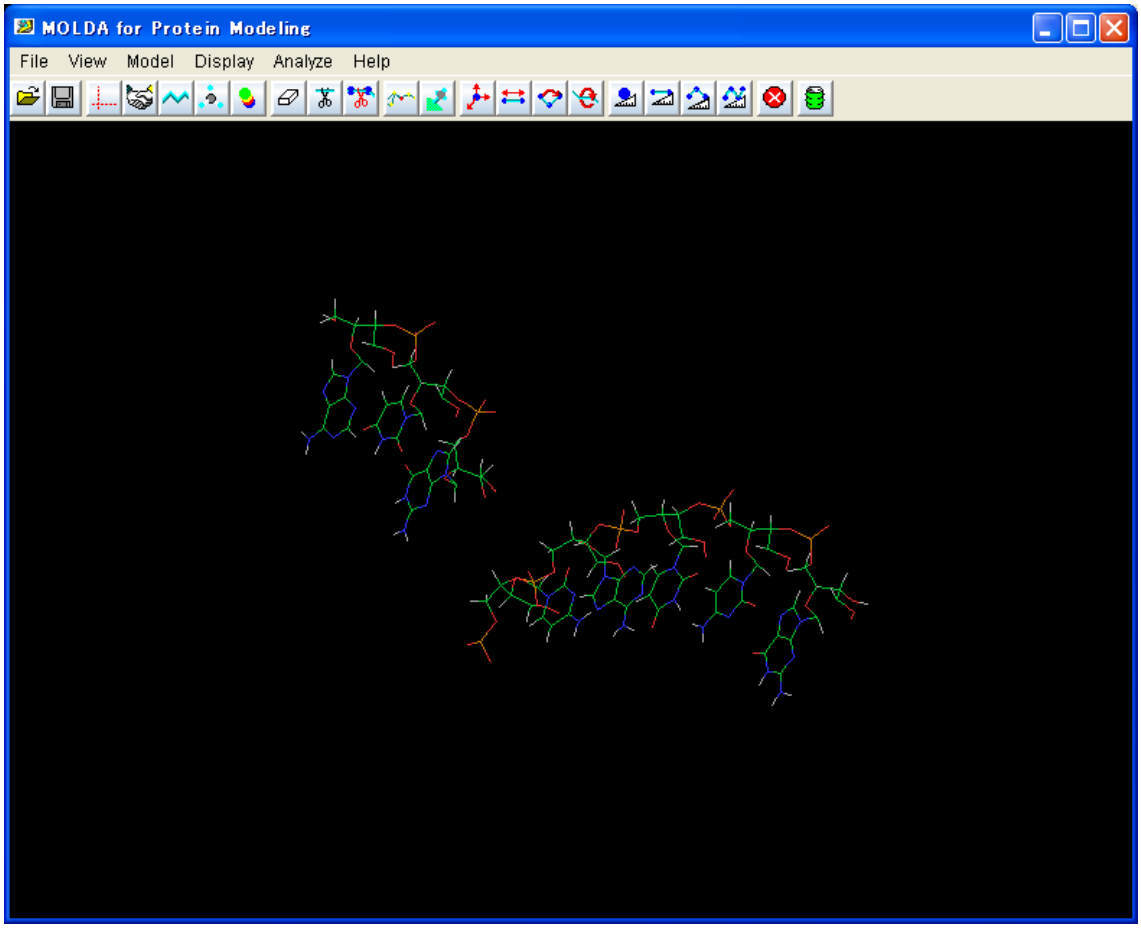


Fig2.182 Result of display RNA on Molda

(3) Select starting RNA-base for Adding

Select **[View]-[Sequence Viewer]** menu and Sequence Viewer is displayed. Select a stating nucleotide and click **OK** on Sequence Viewer. The selected nucleotide changes the color to cyan on Molda. For instance, select G3 and click **OK** on Sequence Viewer. It is shown in Fig2.183 and Molda is shown in Fig2.184.

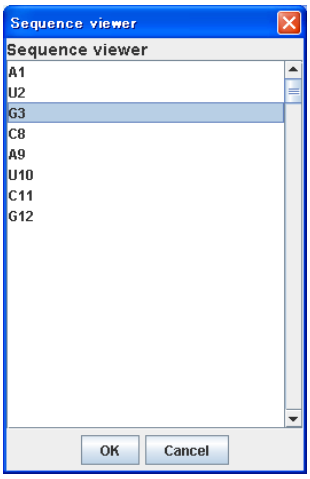


Fig2.183 Selected G3 on Sequence Viewer

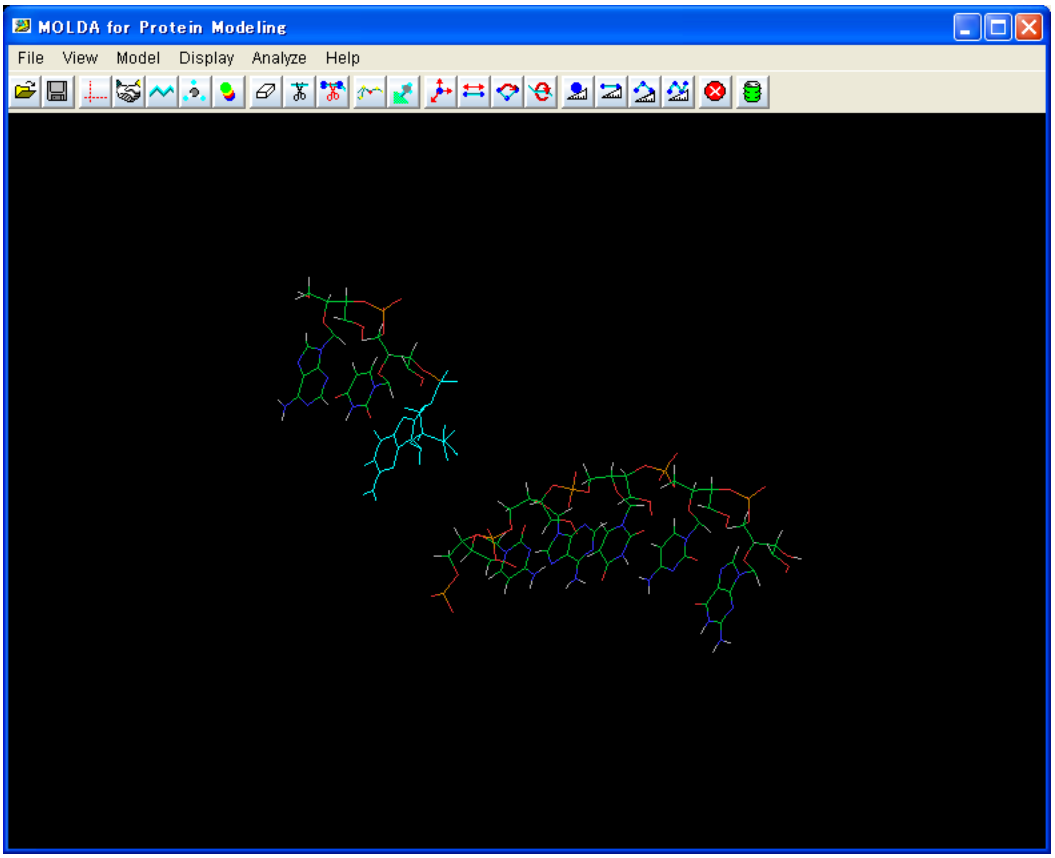


Fig2.184 Selected G3 on Molda

(4) Add Nucleotide

Select **[Molda]-[Add Nucleotide]-[DNA]** menu. The menu is shown in Fig2.185. DNA Add Nucleotide dialog box is displayed and shown in Fig2.186. For instance, if A, G and U add next to G3 in 3'-end direction then choose **Middle** from **Position,** input AGU to the text area as **Sequence** and click **OK**. **Sequence** has to input RNA-bases: A, G, C and U. The result is displayed on Molda viewer and shown in Fig2.187.

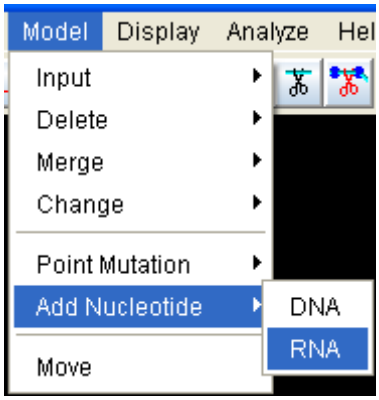


Fig2.185 RNA Add Nucleotide menu

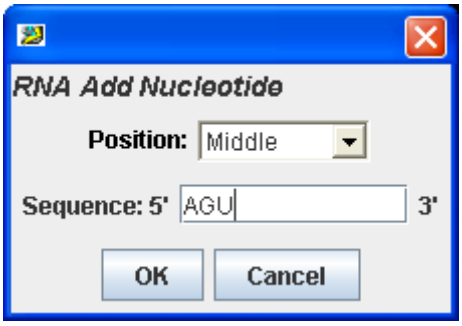


Fig2.186 RNA Add Nucleotide dialog box

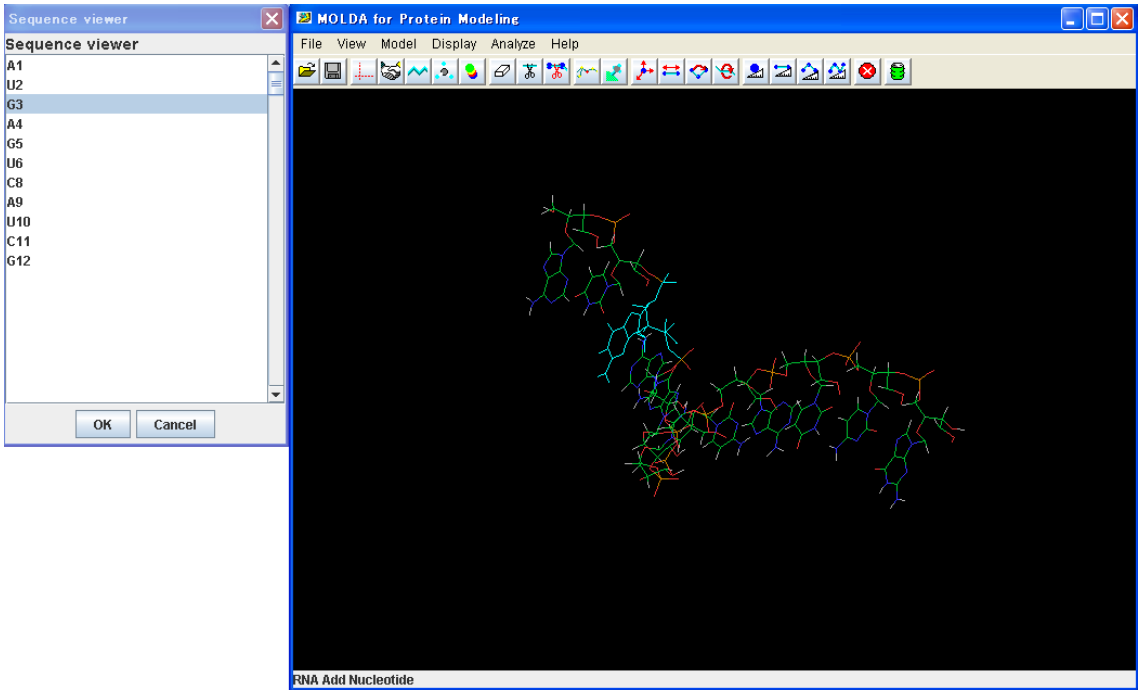


Fig2.187 Result of RNA Adding Nucleotide

Remark

- If selected chain in (3) has only one RNA-base then it dose not allow to add any nucleotides to the chain.
- If the **Position** selects **5'Terminal** then selected RNA-base in (3) has to be on the 5'-end.
- If the **Position** selects **Middle** then selected RNA-base in (3) has to be on the 5'-end or middle, not on the 3'-end.
- If the **Position** selects **Middle** then add nucleotides equal or less than number of missing nucleotides.
- If the **Position** selects **3'Terminal** then selected RNA-base in (3) has to be on the 3'-end.
- If the **Position** selects **3'Terminal** and the selected nucleotide dose not have previous nucleotide, first add missing nucleotides and then add nucleotides in 3'-end direction on the 3'-end.

(5) To Viewer

If you want to display the RNA on BioStation main window then select **[Display]-[To Viewer]** menu. The RNA is displayed on BioStation main window. Result of display is shown in Fig2.188.

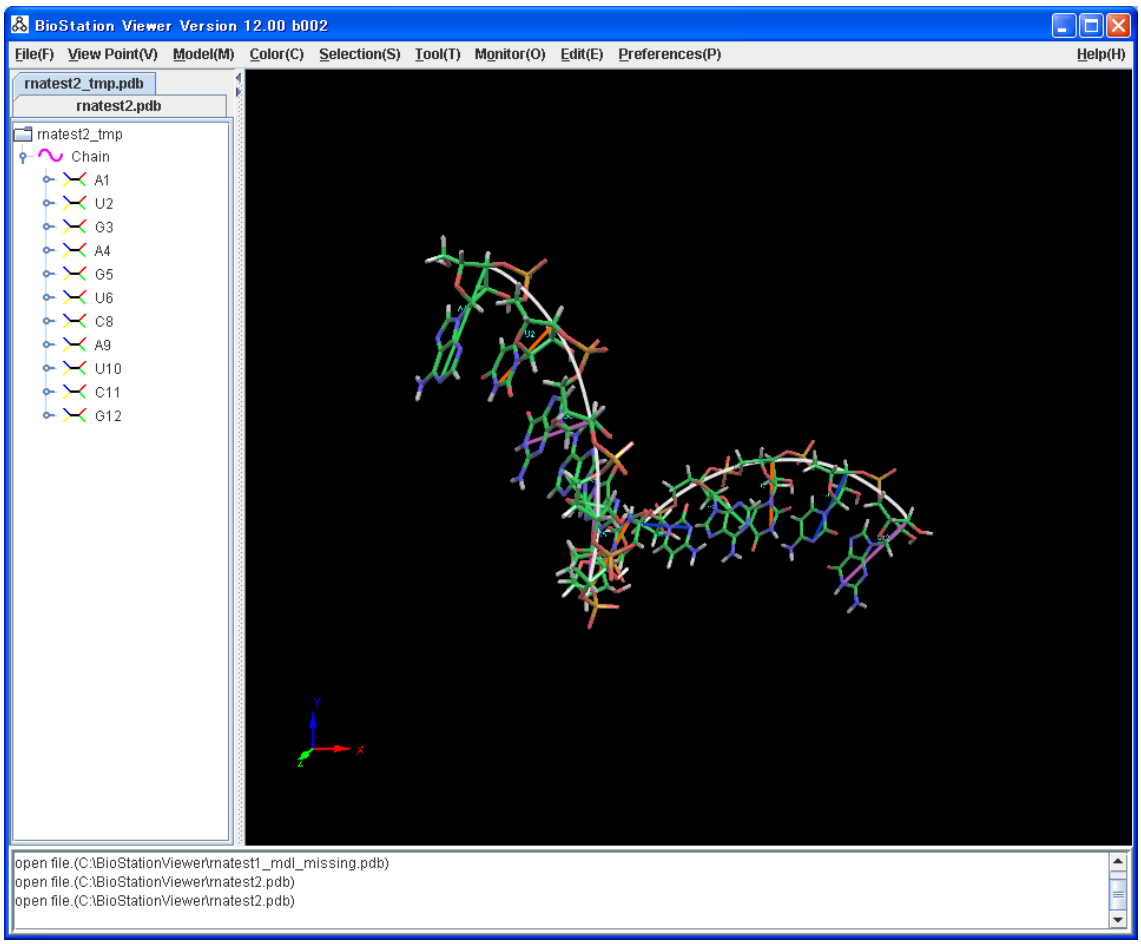


Fig2.188 Result of display RNA on BioStation viewer

3. Examples of How to use

3.1. Displaying the Results of ABINIT-MP Calculations.

Use the sample data which is operating at the Web site of **ABINIT-MP** (http://www.fsis.iis.u-tokyo.ac.jp/en). The sample data are

- the sample data of (Gly) $_{10}$ g10a.zip 803 KB,
  - **g10a.cpf**, **Check point file** of the **FMO-HF/STO-3G** calculation
  - **den.inp**, input data for the calculation of the electron density
  - **g10a_fmo_sto-3g_3.den** , grid data of the electron density
  - **g10a_fmo_sto-3g_3.map** ,electrostatic potential map data on the electron density
  - **g10a_fmo_sto-3g_4.esp** , grid data of electron potential
  - **g10a_fmo_sto-3g_3.mo** , grid data of molecular orbitals
  - **g10a_grid.mol2,** data file of a display example for the domain
  - **g10a_fmo_sto-3g_3.efv**, grid data of electron field vector

3.1.1. Displaying Molecular Structures

Start the **Viewer** and load **g10a.cpf** . An example of this display is shown in Fig3.1. When the **Viewer** is started, molecular structures are displayed in the wire frame model.

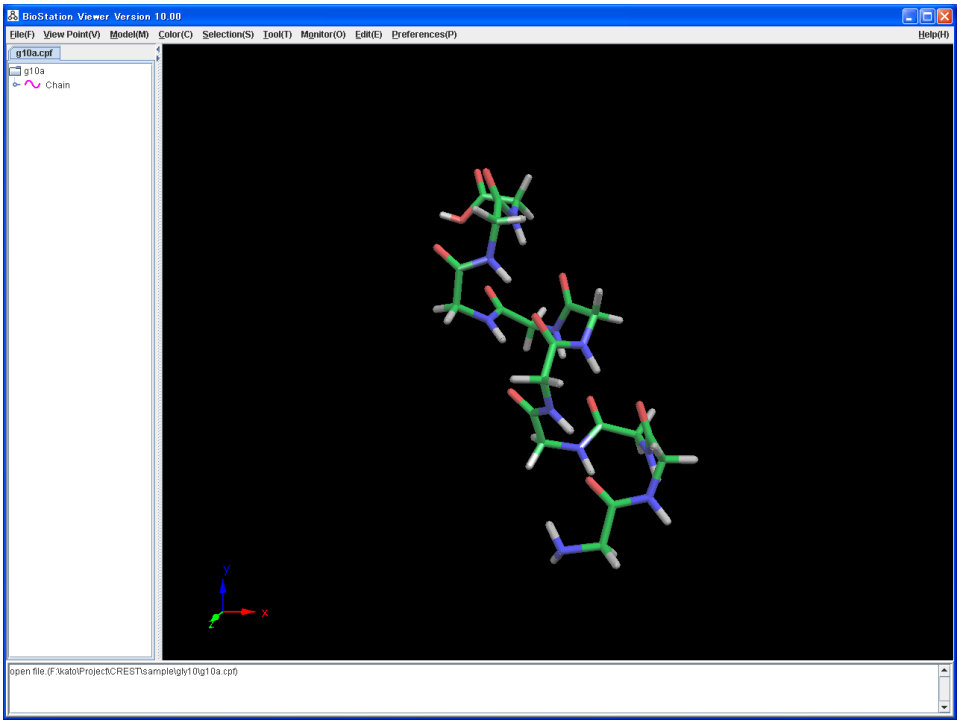


Fig3.1 Example of Display: g10a.cpf

From the **Model** menu, select **Wire frame, Wire frame(with fragment bond)**(specifying **frame** for colors),**Ball & Stick, Ball & Wire, CPK, Backbone, Cα, Ca (line)** and **Cα(tube)** to modify the model. Here are the resulting displays in Fig3.2- Fig3.8

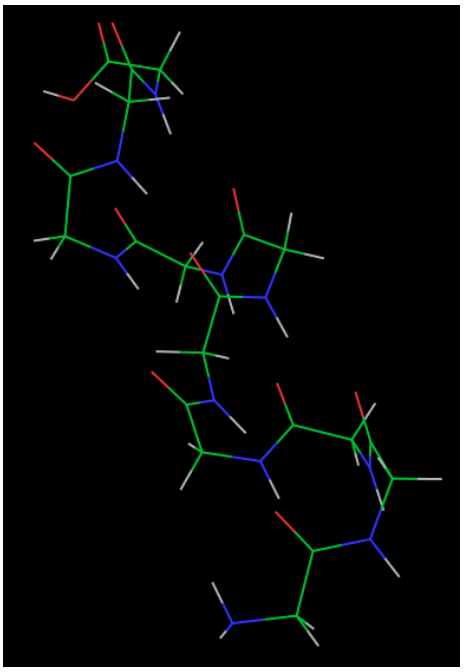


Fig3.2 Wire Frame

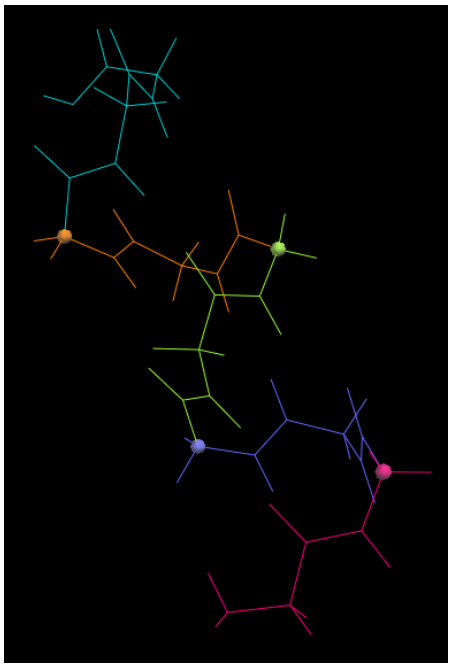


Fig3.3 Wire frame model(with fragment bond)

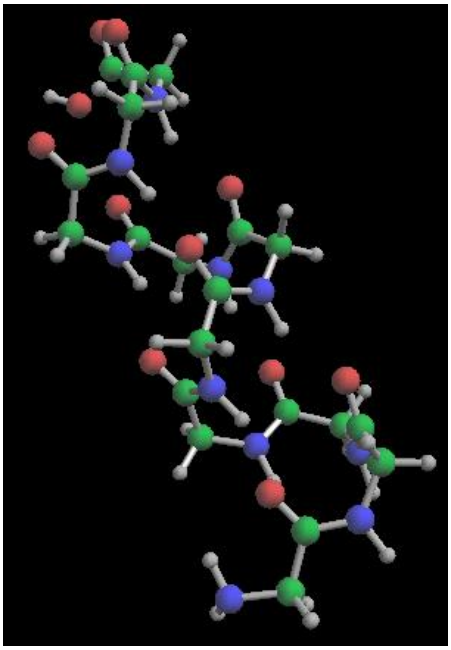


Fig3.4 ball and stick

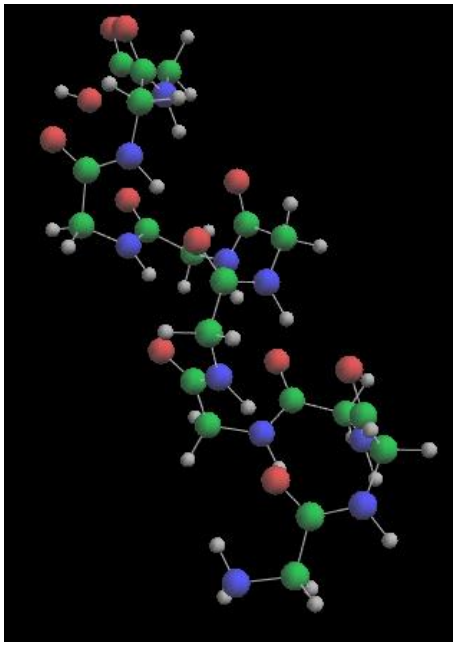


Fig3.5 Ball & Wire model

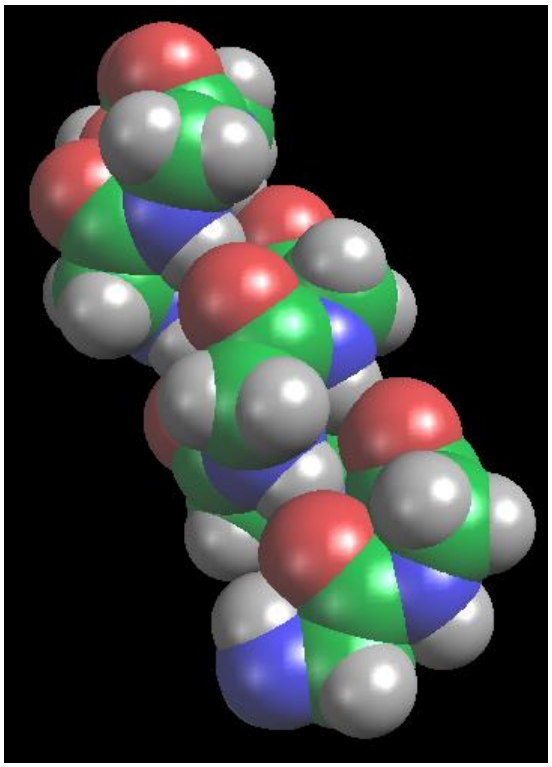


Fig3.6 CPK

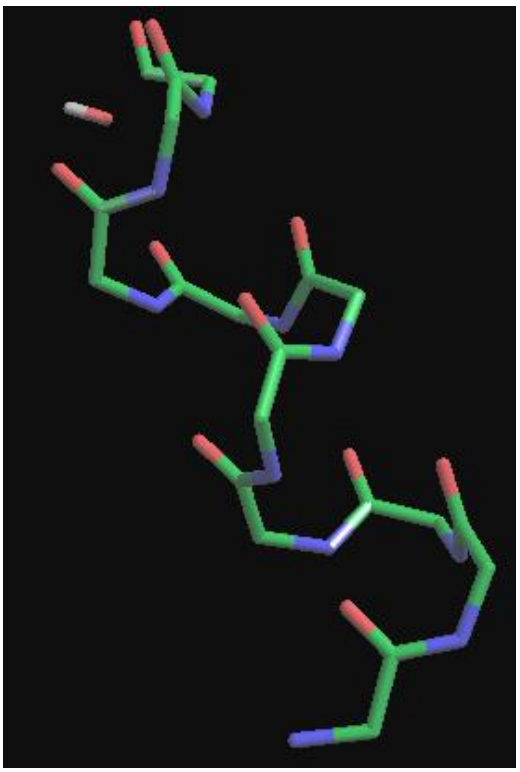


Fig3.7　Backbone model

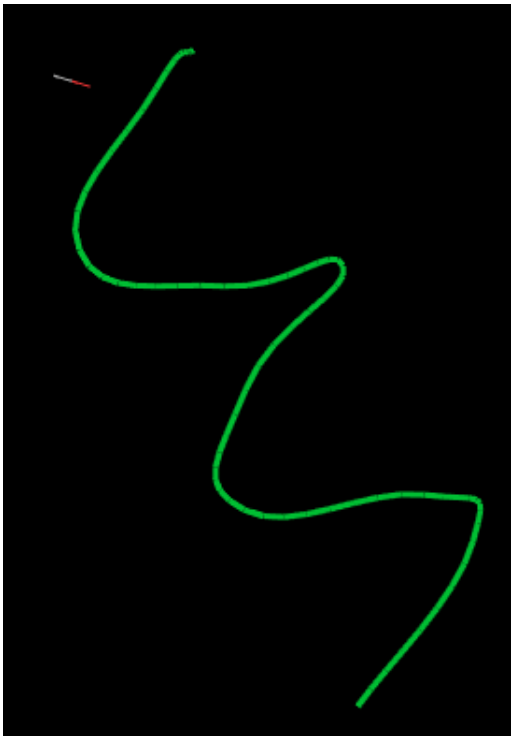


Fig3.8　Cα Line model

3.1.2. Changing Colors

From the **Color** menu, select **Atom, Residue, Charged Residue, Atom Charge, Fragment,** and **Chain** to change the display color. Here are the resulting displays in Fig3.9-Fig3.13.

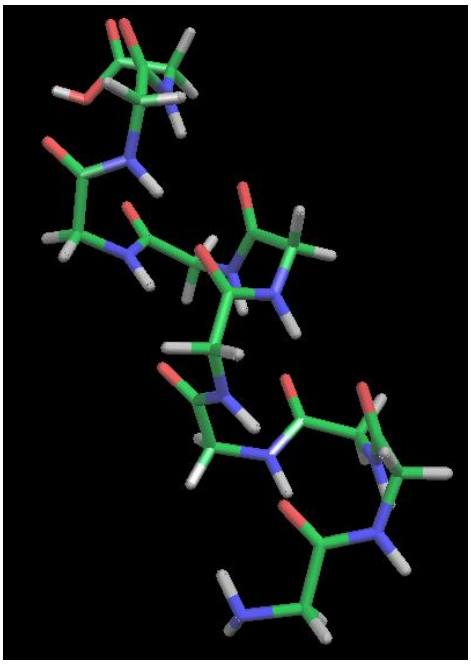


Fig3.9 Adding Colors by Atom Type

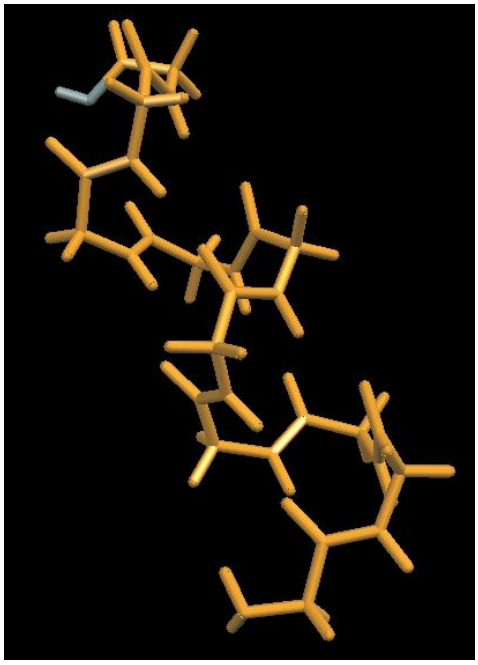


Fig3.10 Adding Colors by Residues

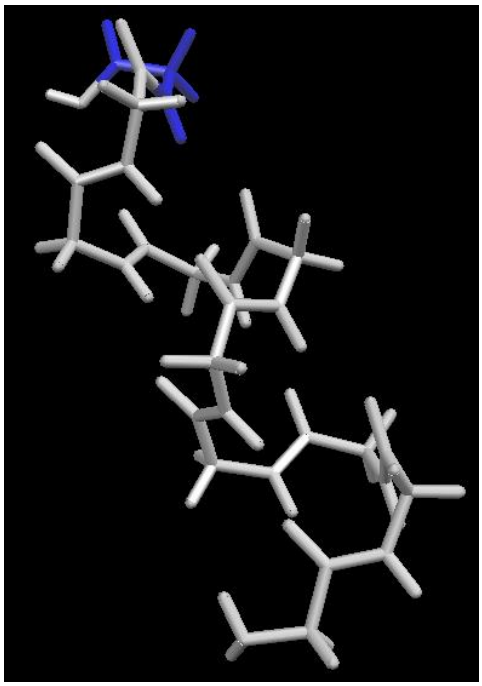


Fig3.11 Adding Colors by residue Charge

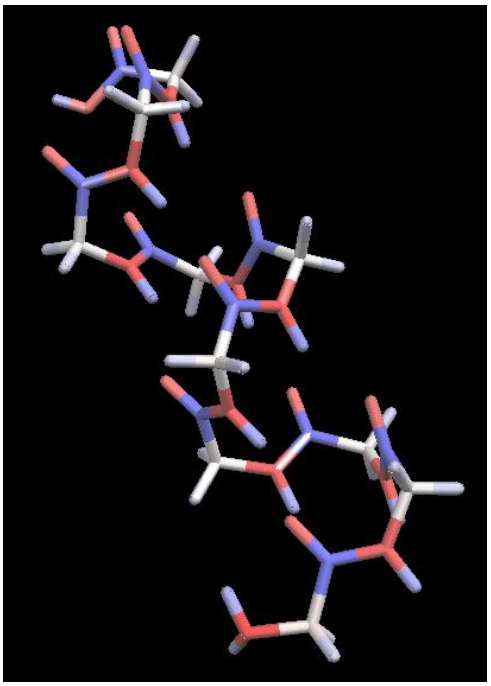
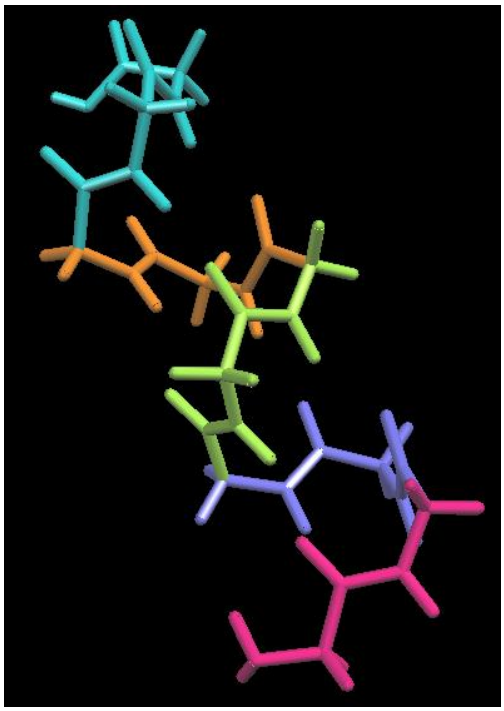


Fig3.12 Adding Colors by Chrges Atoms



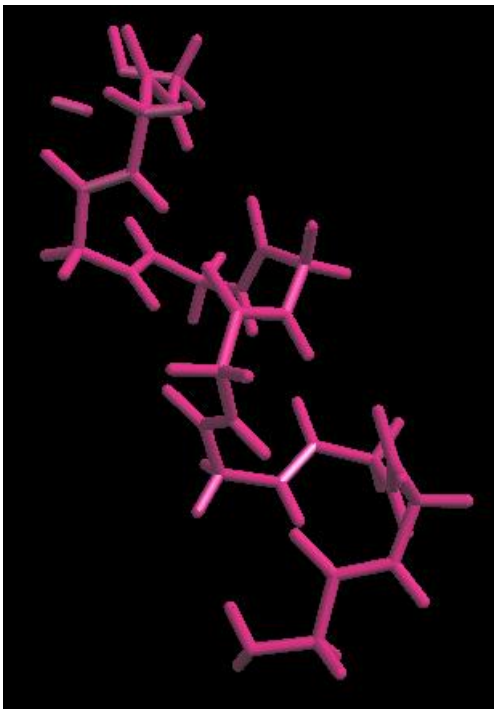


Fig3.13 Adding Colors by fragment　Fig3.14 Adding Colors by Chains (one color with one chain)

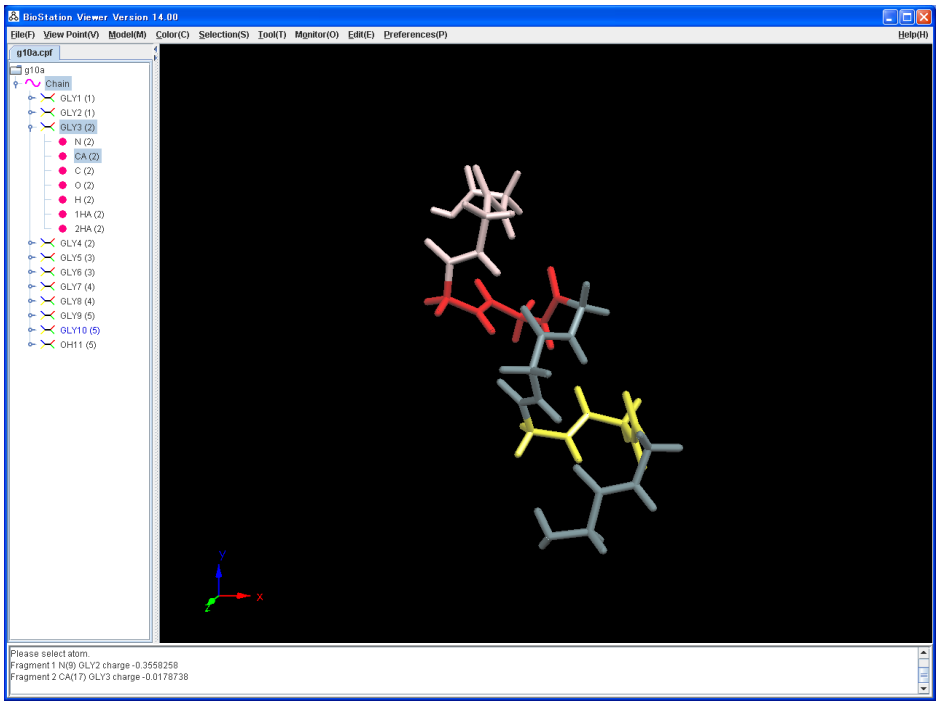
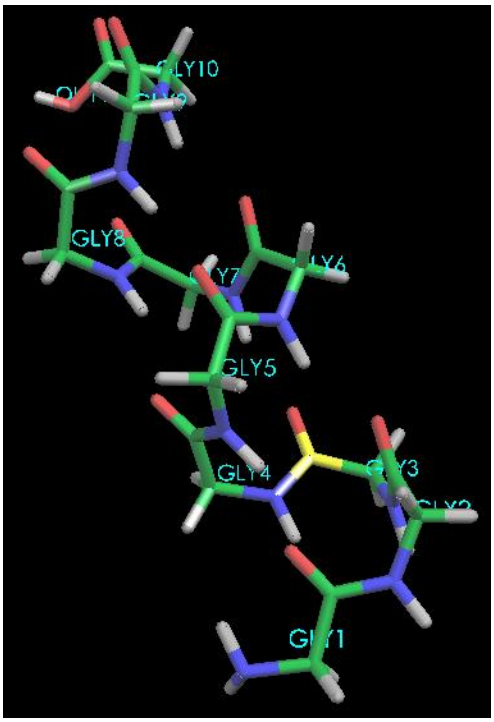


Fig3.15 Adding Colors by the Interaction Energy between Fragments. The Second Fragment in Yellow is Displayed as a Reference.

3.1.3. Adding Labels

When you select **[Tool]-[Label]**, a dialog box to add labels is displayed. Fig3.16 shows an example with labels of residues in, and Fig. 3.19 shows it with those of atoms.



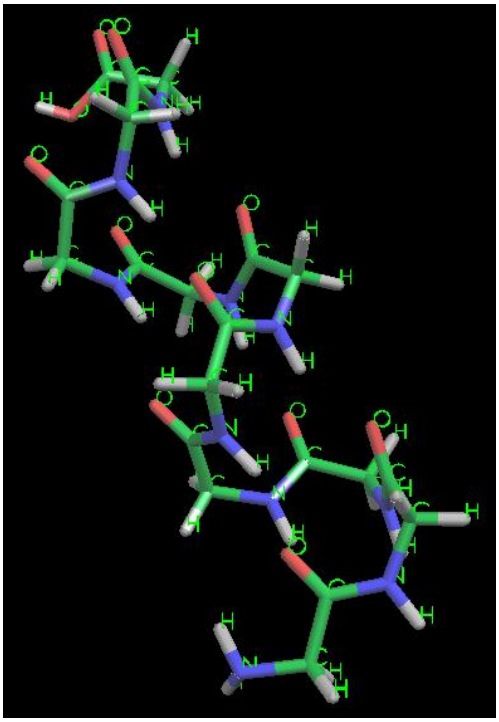


Fig3.16 Residue Lables Fig3.17 Molecules with Labels of Atoms (names of atoms)

3.1.4. Displaying the Isosurface of the Electron Density

Load **g10a_fmo_sto-3g_3.den** with **[File]- [Open].** A dialog box for the isosurface is displayed, which value is generated in the file. Clicking on the **Ok** button lets the isosurface of the electron density display. The example is shown in Fig3.18. Select **[File]–[File List],** and the list of input files is displayed. Here, click on the **Value** button beside **g10a_fmo_sto-3g_3.den.** Since a dialog box for the isosurface value is displayed, change colors. When you click on the button beside **Color**, a color preference dialog box is displayed. Here, select the appropriate color. The example is shown in Fig3.19.

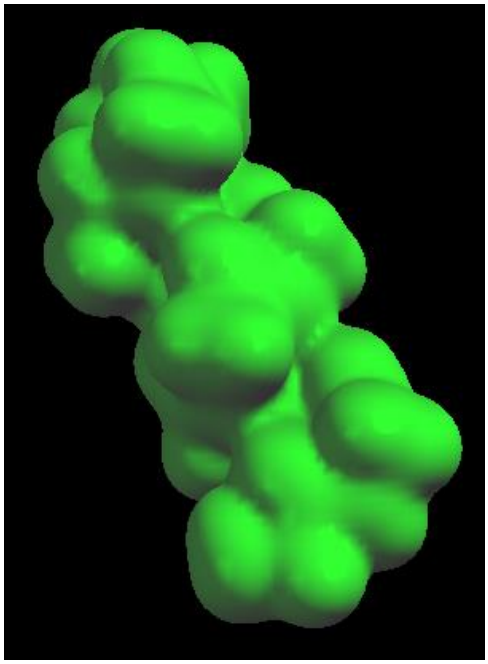


Fig3.18 Isosurface

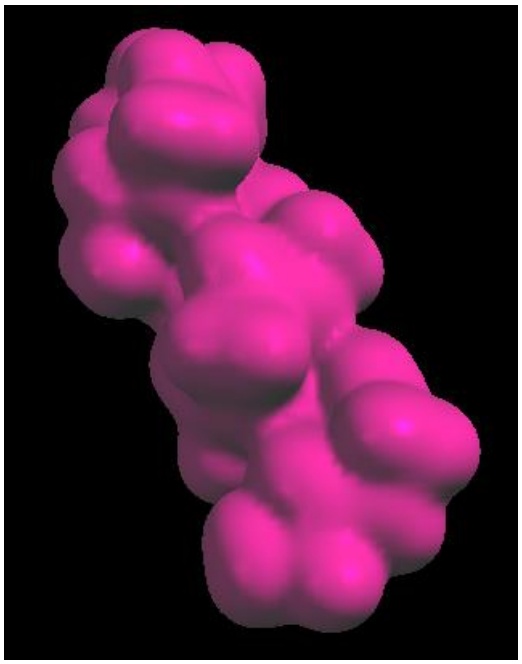


Fig3.19 Isofurface with the Color Changed

When you select [File]–[Delete File List], the list of input files is displayed. Here, select g10a_fmo_sto-3g_3.den and click on the Ok button. The isofurface is deleted.

3.1.5. Adding Colors to the Isosurface of the Electron Density by the Value of Electrostatic Potentia.

Load **g10a_fmo_sto-3g_3.map** with **[File]- [Open]**. An electrostatic potential dialog box appears on the screen. Set **Min Max** to **-0.05 0.05**. Clicking on **Ok** lets the isofurface of the electron density display. This example is shown in Fig3.20**.**

You can change the transparency of the isosurface. Selecting **[File]–[File List]** lets the list of the input file displayed. Here, click on the Value button beside **g10a_fmo_sto-3g_3.map.** Since electrostatic potential dialog box is displayed, set **Transparency** to **50**. Select **[Color]–[Atom]–[Charge]–[Atom]** as well. This example is shown in **Figure 3.23.**

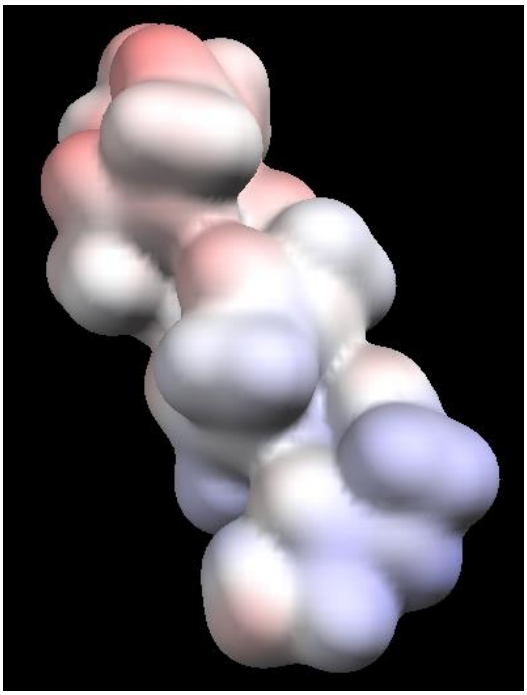


Fig3.20 Adding Colors to the Isosurface of the Electron Density by the Value of Electrostatic Potential

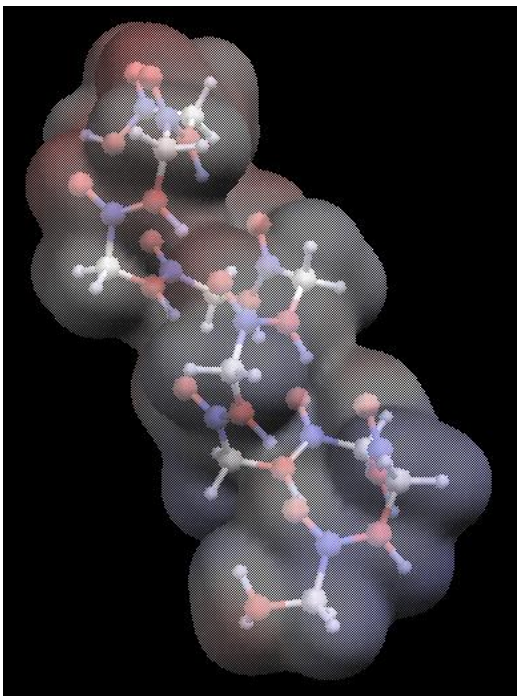


Fig3.21 Changed the Transparency of Isosurface

3.1.6. Isosurface of Electrostatic Potential

Load **g10a_fmo_sto-3g_4.esp** with **[File]-[Open]**. An electrostatic potential dialog box is displayed. When you set **Transparency** to **50** and click on the **Ok** button, the isofurface value of electrostatic potential is displayed. The example of molecule structures with **Stick** is shown in Fig3.22.

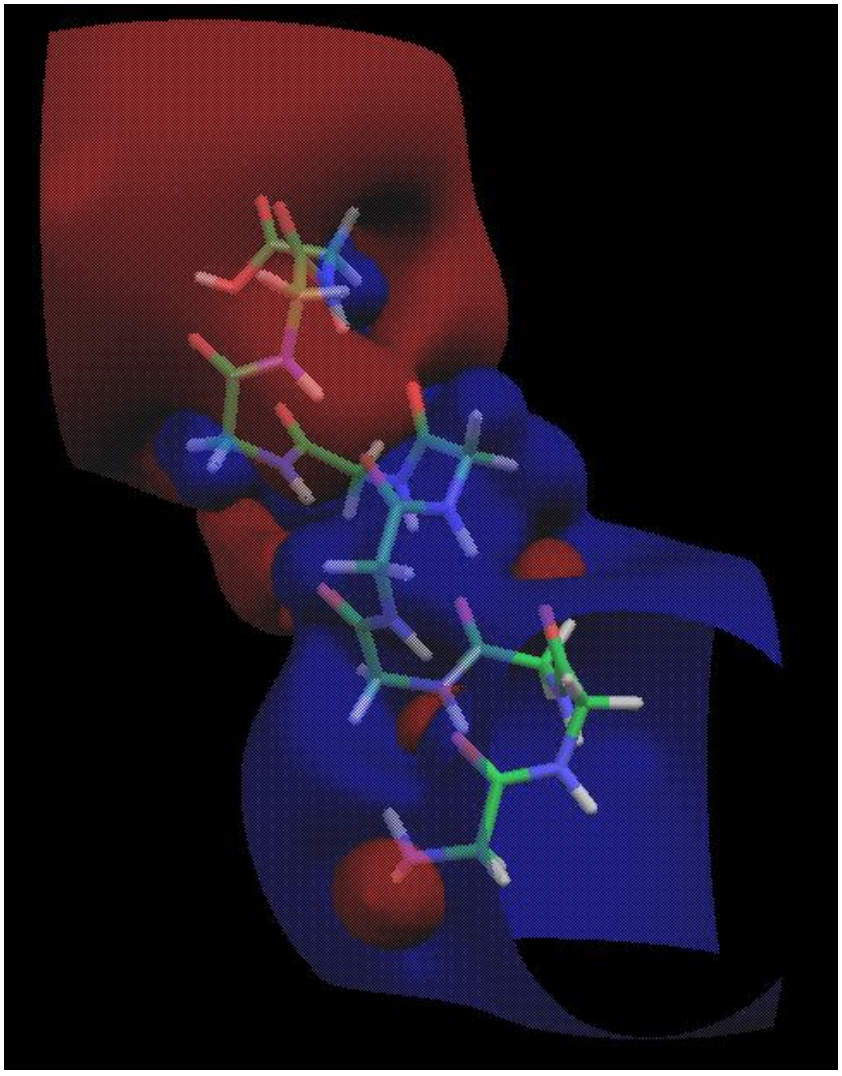


Fig3.22 Isosurface of Electrostatic Potential

3.1.7. Isosurface of Molecular Orbitals

Load **g10a_fmo_sto-3g_3.mo** with **[File]- [Open]**. A molecular orbital dialog box is displayed. Here, when you select an orbital that you want to display from the graphic and click on **draw**, the isosurface of the molecular orbital is displayed. This example shows the isosurface of the first fragment, **LUMO**, which is shown in the Fig3.23.

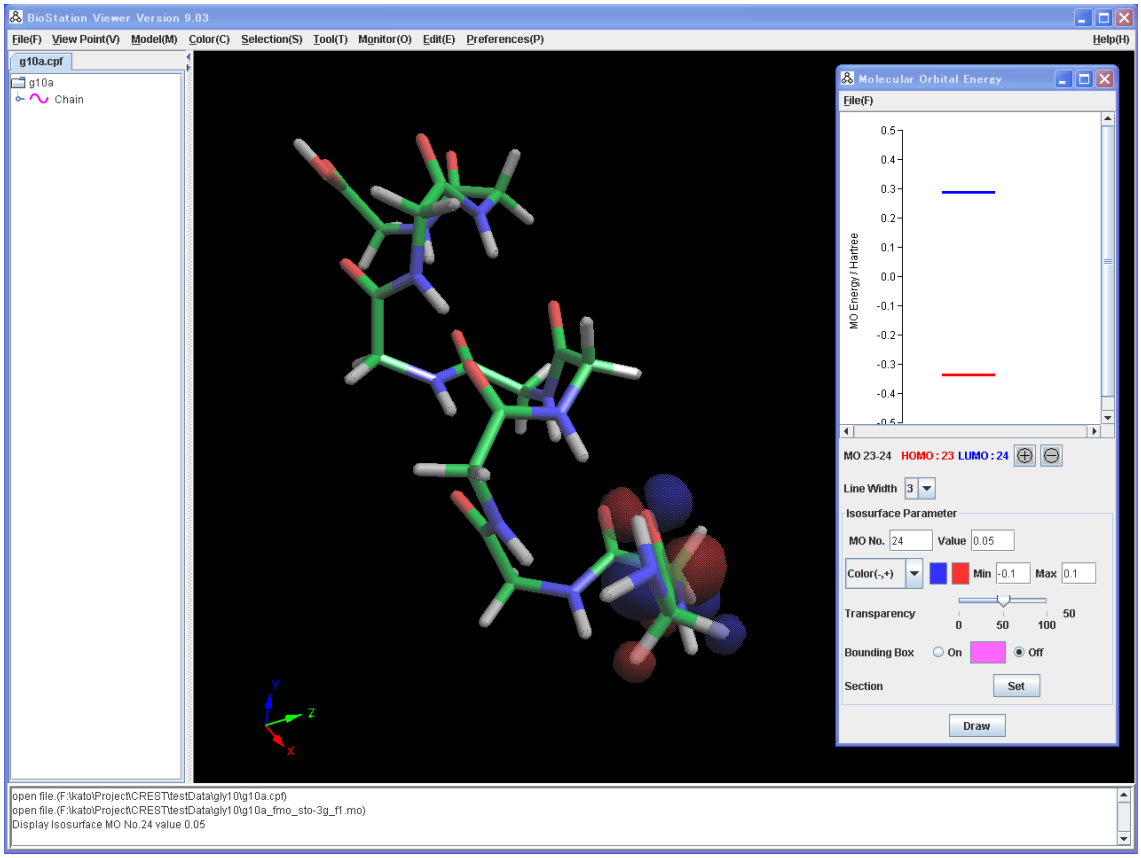


Fig3.23 Isosurface of Molecular Orbitals

3.1.8. Electron field vector

Load **g10a_fmo_sto-3g_4.efv** with **[File]-[Open]**. Display the electron field vector by default options.（Fig3.24）

Next is a example which changes options. Min,Max の値を-0.1,0.1 にします。Set section options to, B set –27 and select **Density** for value.By clicking **Draw** button, the section is displayed(Fig3.26). An option dialog is shown in Fig3.25.

Set the next Model of molecular structure to Ball&Stick, transparency to 50, model of vector to Stick and Number of step to 150. by Clicking **Draw** button, an example of stick vector is displayed(Fig3.28). Since the number of steps was increased, an electric field vector is displayed from lower Glycine(+) to upper Glycine(-).

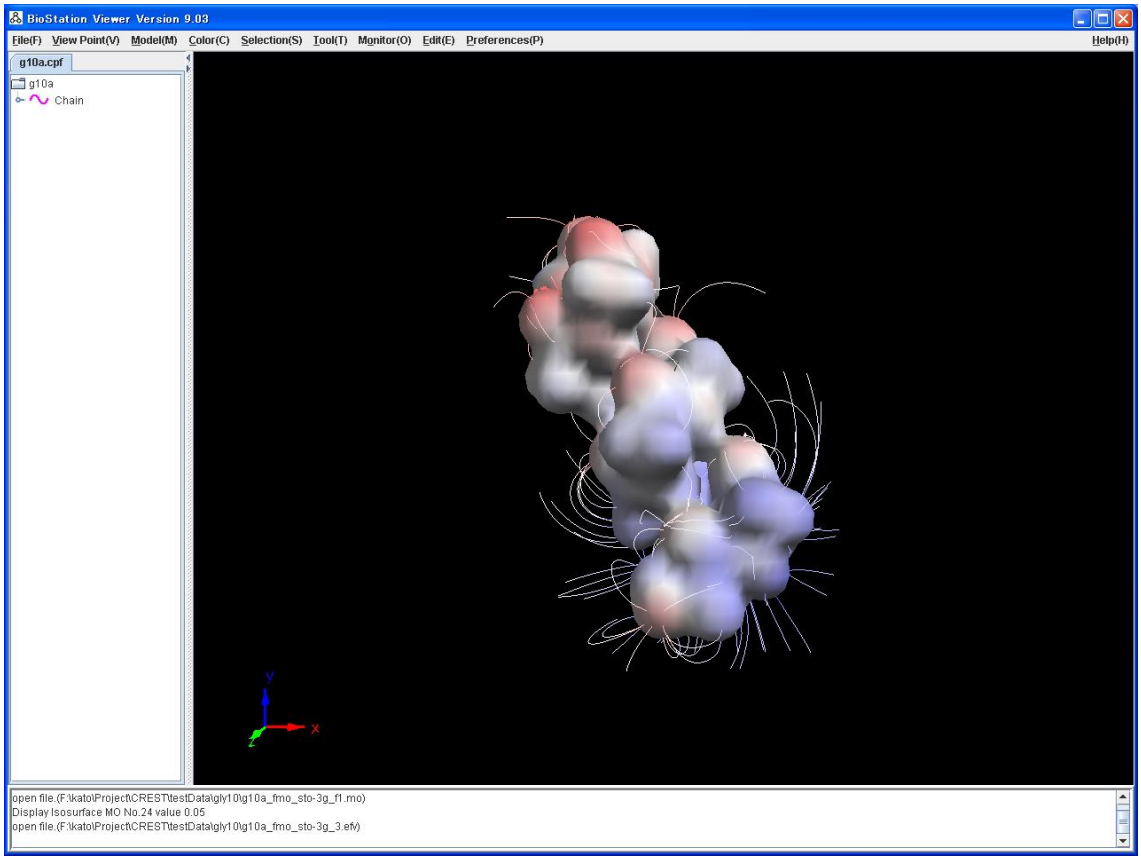


Fig3.24 Example of electron field vector

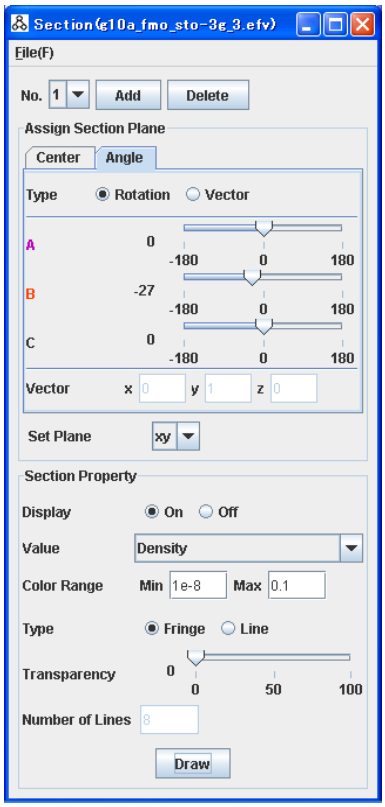


Fig3.25 Section dialog box

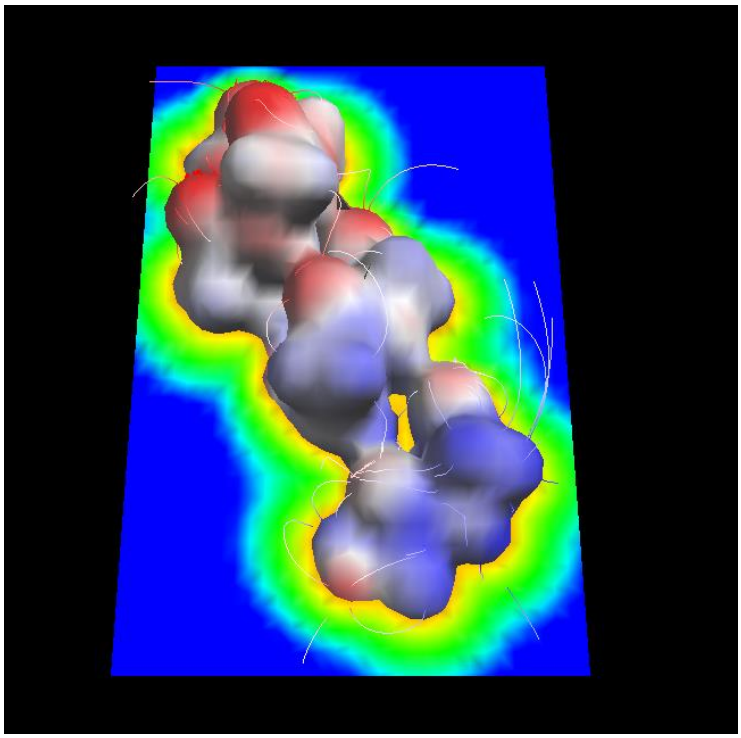


Fig3.26 Example of vector with section

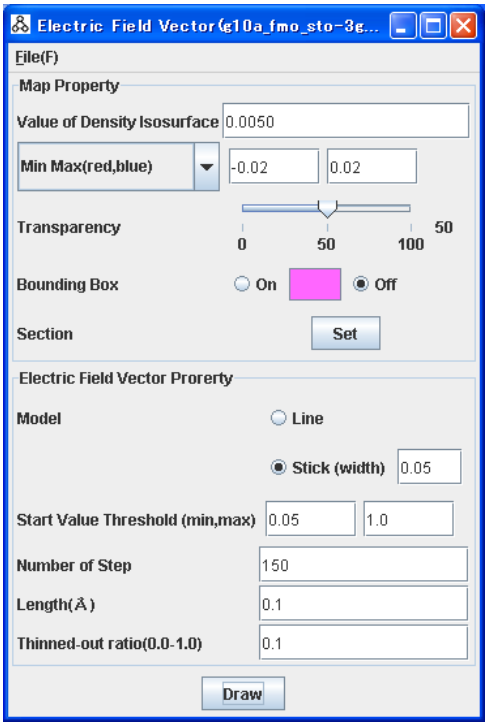


Fig3.27 Electron field vector dialog box

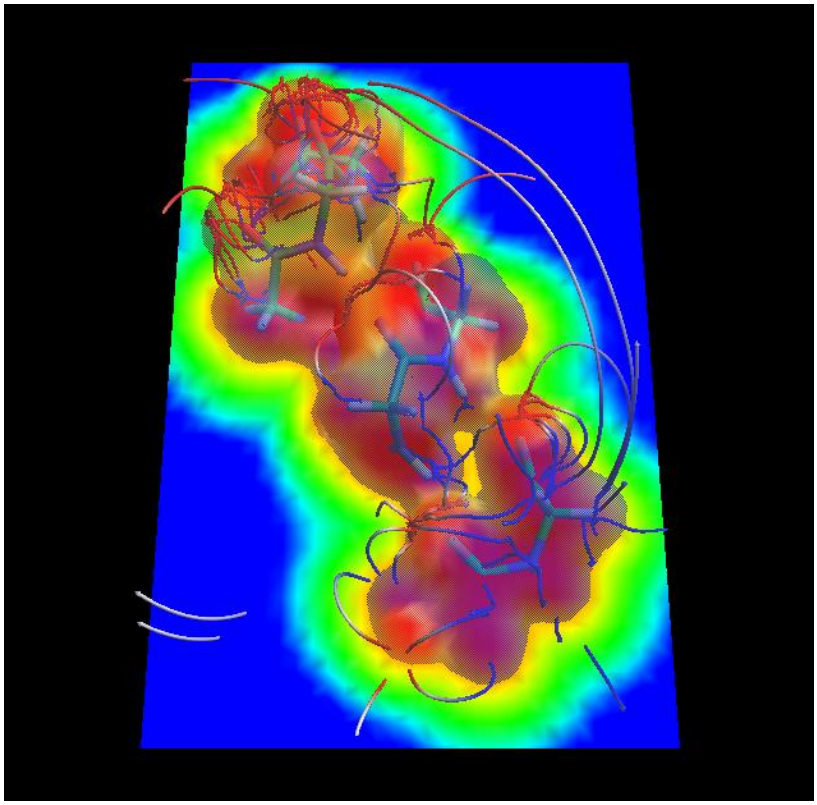


Fig3.28 Example of stick vector

3.2. Example of Structures of Estrogen Receptors – Ligand Complexes

Visualizing structures with using sample data. Use estrogen receptors- ligand complexes as the sample data, located in the folder, sample. Use the **pdb** file, **ERE_EST.pdb** and **ERR_RAL.pdb**, of the bond between an agonist as a ligand, 17 β -estradiaol and a selective agonist, raloxifene.

3.2.1. Peptide Chains in the the Cα Line Model

Start the Viewer and load **ERE_EST.pdb**. Default model is **[Model(Atom)]-[Off], [Model(Structure)]- [C α Line].** This example is shown in Fig3.29.
The another model examples are shown in Fig2.29-Fig2.35.

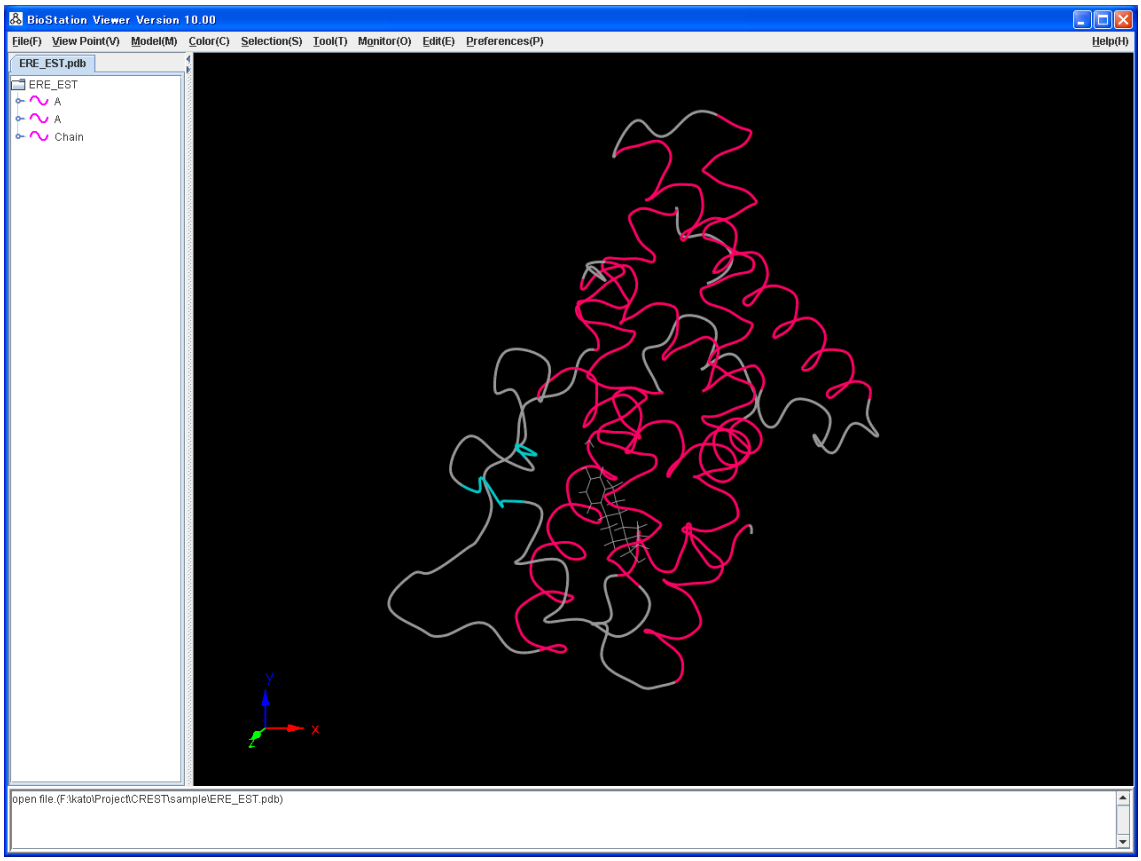


Fig3.29 Molecular Structures

3.2.2. Modifying the model of Cα Line of Peptide and the model of Ligands

Select **[Selection]-[Residue]** and click on the ligand with the left mouse button. Fig3.30 shows an example of the highlighted a ligand which you click.

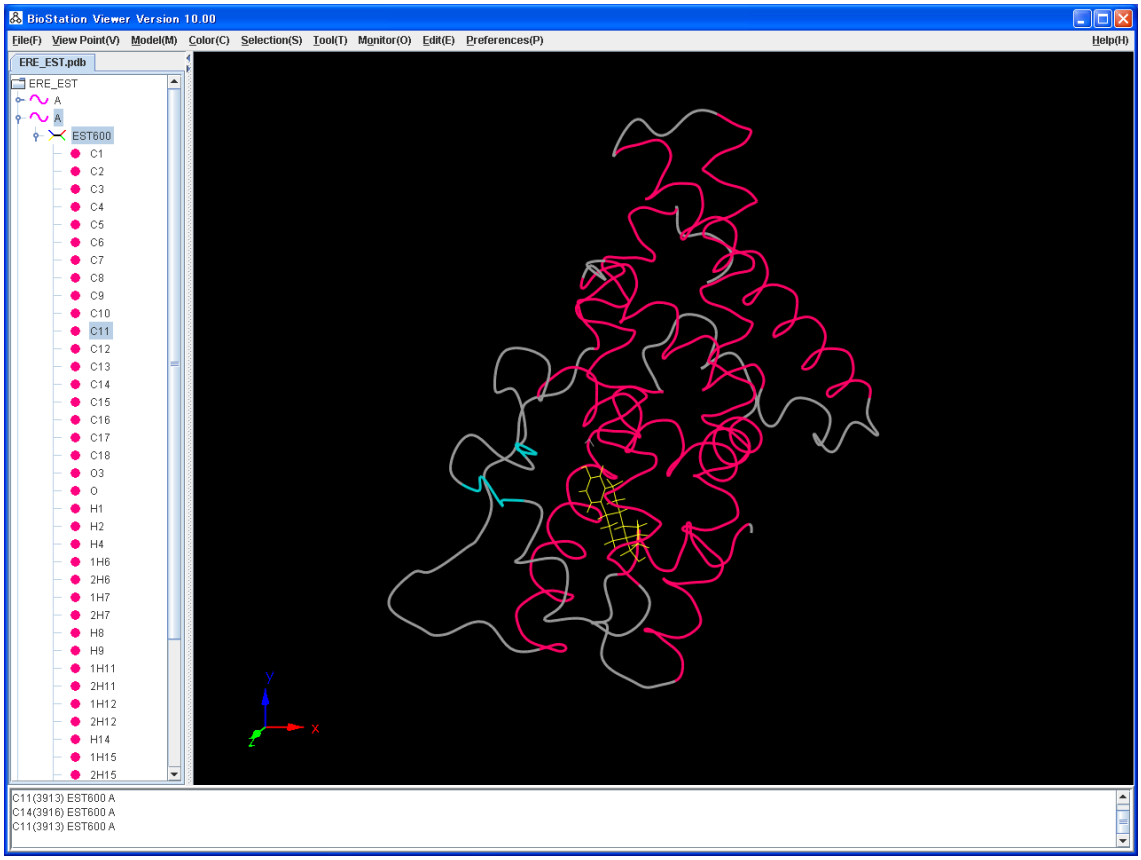


Fig3.30 Highlighted a Ligand

Next, click on the ligand by the right mouse button. Since a dialog box for specifying residues is displayed, select **Atom** in the **Color** and **Ball & Stick** in the **Model** option and click on the **Ok** button. (Fig3.31) This allows you to display a ligand in the **Ball & Stick** model. This example is shown in Fig3.32.

Fig3.31 Displaying Residue Dialog Box

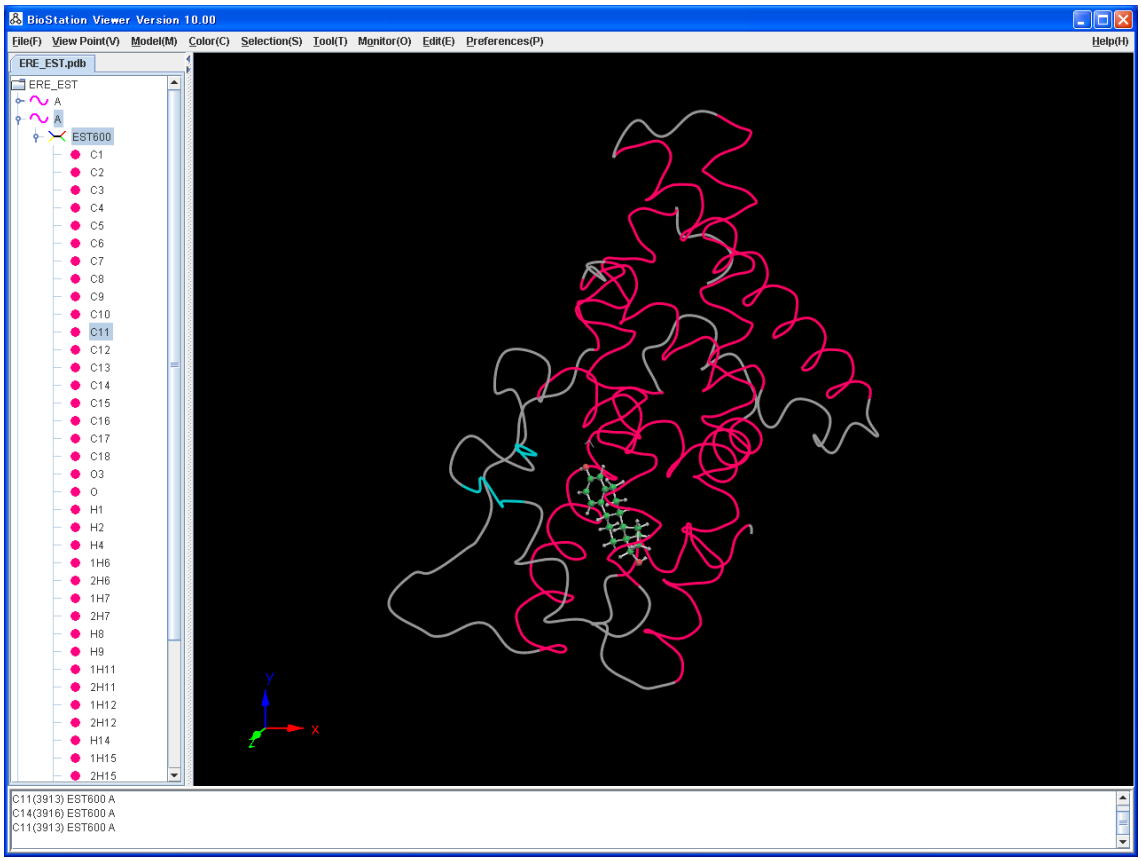


Fig3.32 Ligand in the Ball & Stick Model

Next, click on the ligand with the right mouse button and select **CPK** in the **Model** option of the residue dialog box. Set **other** in the **Color** option and select the appropriate color by clicking on the side button. The ligand is displayed with colors selected in the space-filling model. This example is shown in Fig3.33.

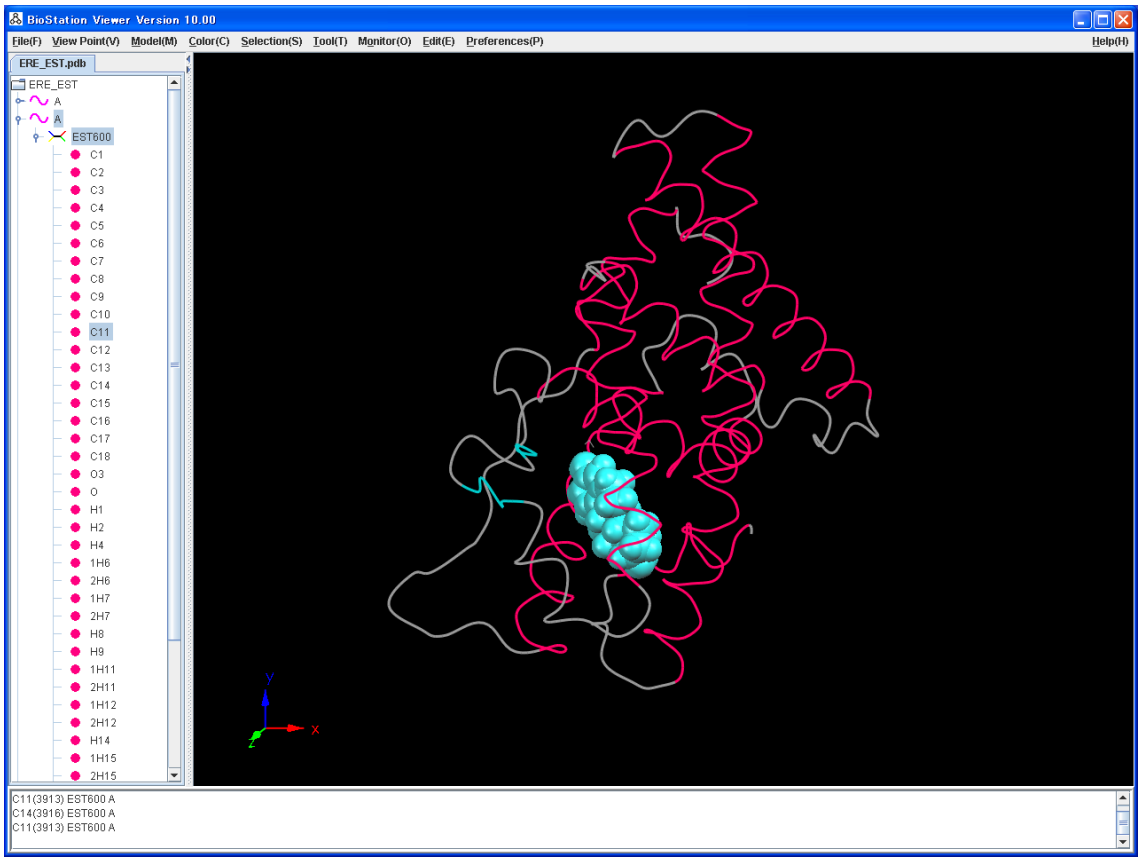


Fig3.33 Ligand in the Space Filling Model

3.2.3. Display Peptide Chains in the Cα Line Model+ Ligands+ Selected Residues

You can display residues around ligands in the **Wire Frame** model. Click on the four residues around ligands (**ASN519～GLU523** in this example) with the left button on the mouse while holding down the **Shift**. Click on the one of them with the right mouse button while holding down the **Shift**. Since the Residue dialog box is displayed, select **Wire Frame** in the **Model** and click on the **Ok** button. This displays the selected residues in the **Wire Frame** model. This example is shown in Fig3.34.

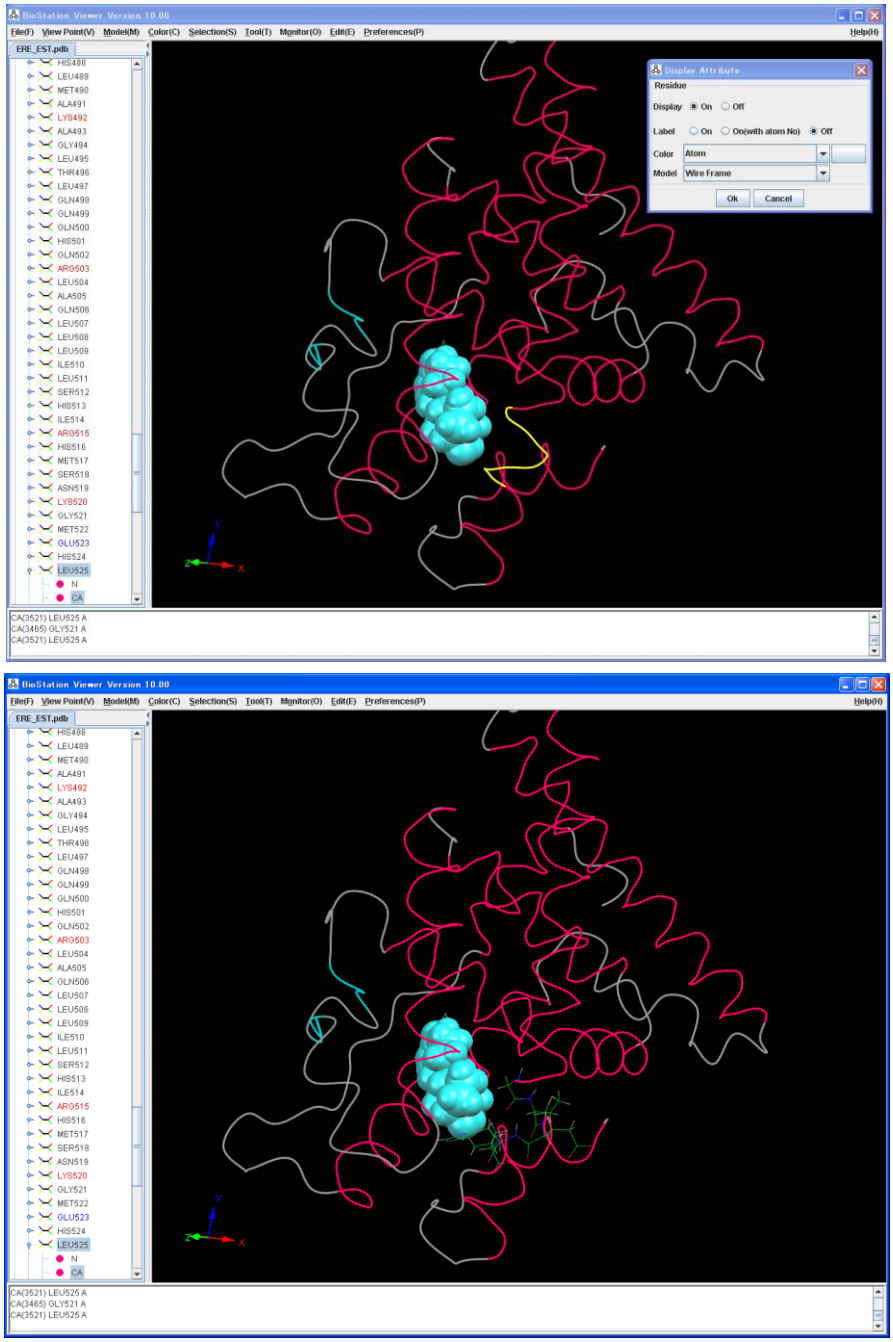


Fig3.34 Selected Residues in the Wire Frame

Next, you can change the display from hierarchical window. Click on residues around ligands. Since the selected residues in hierarchical window are highlighted, click on beside the names of residues and close the current display of the residues. And then, click on this residue again and the residue below five ones (GLY420～PHE425 in this example) while holding down the **Shift**. Here, some residues are selected. Next, click on the selected residues with the right button on the mouse. Since the Residue dialog box is displayed, select **Wire Frame** in the **Model** and click on the **Ok** button. This displays the selected residues in the **Wire Frame** model. This example is shown in Fig3.35.

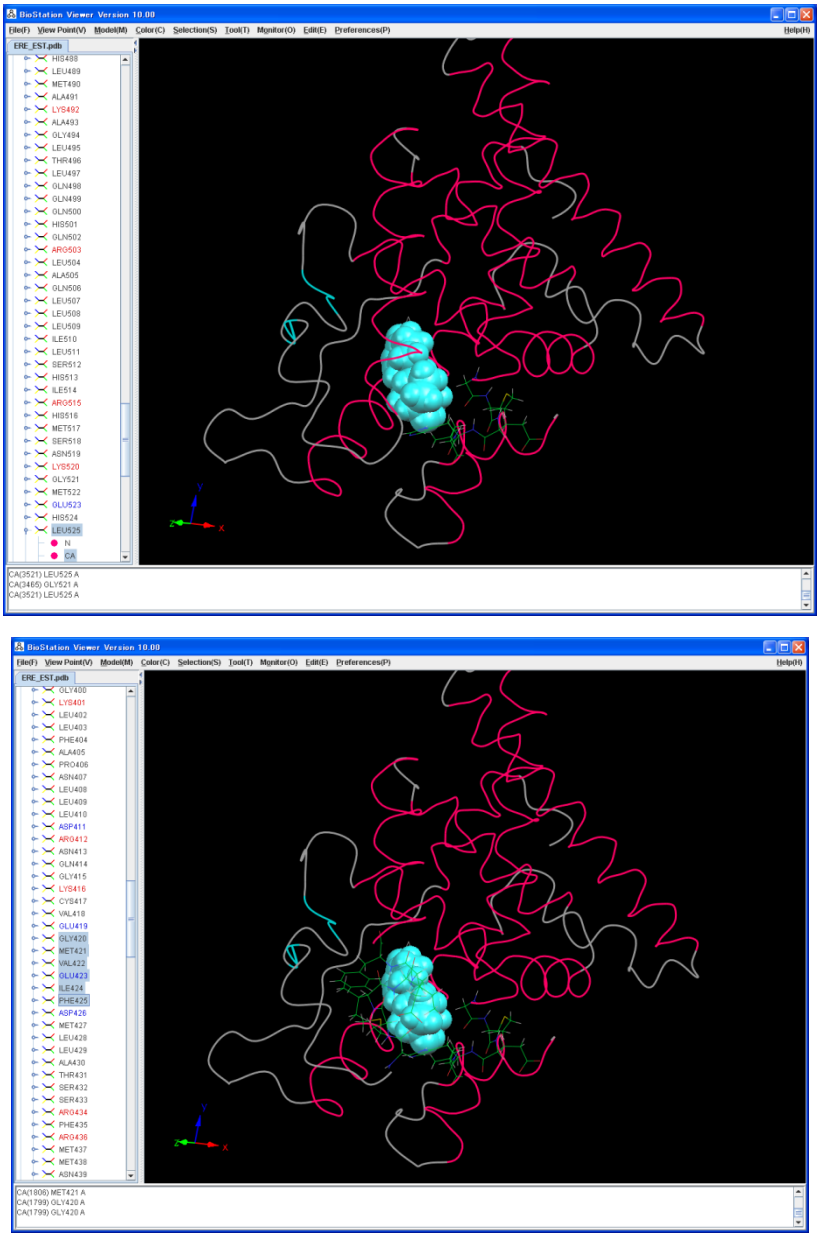


Fig3.35 Residues Selected in Tree figure in the Wire Frame Model

3.2.4. Display Ligands and Charged Residues

You can display the whole residues in the **Wire Frame** model by selecting **[Model(Atom)]-[Wire Frame]** and **[Model(Structure)]-[Off].** Select **[Tool]-[Display Selected Residue]**. Since the residue dialog box appears, click on **Unselect All** and select charged residues (**ASP,GLU,LYS,ARG**). This allows you to display the only charged residues which you select. This example is shown in Fig3.36. The only residue which is selected optionally can be displayed as well.

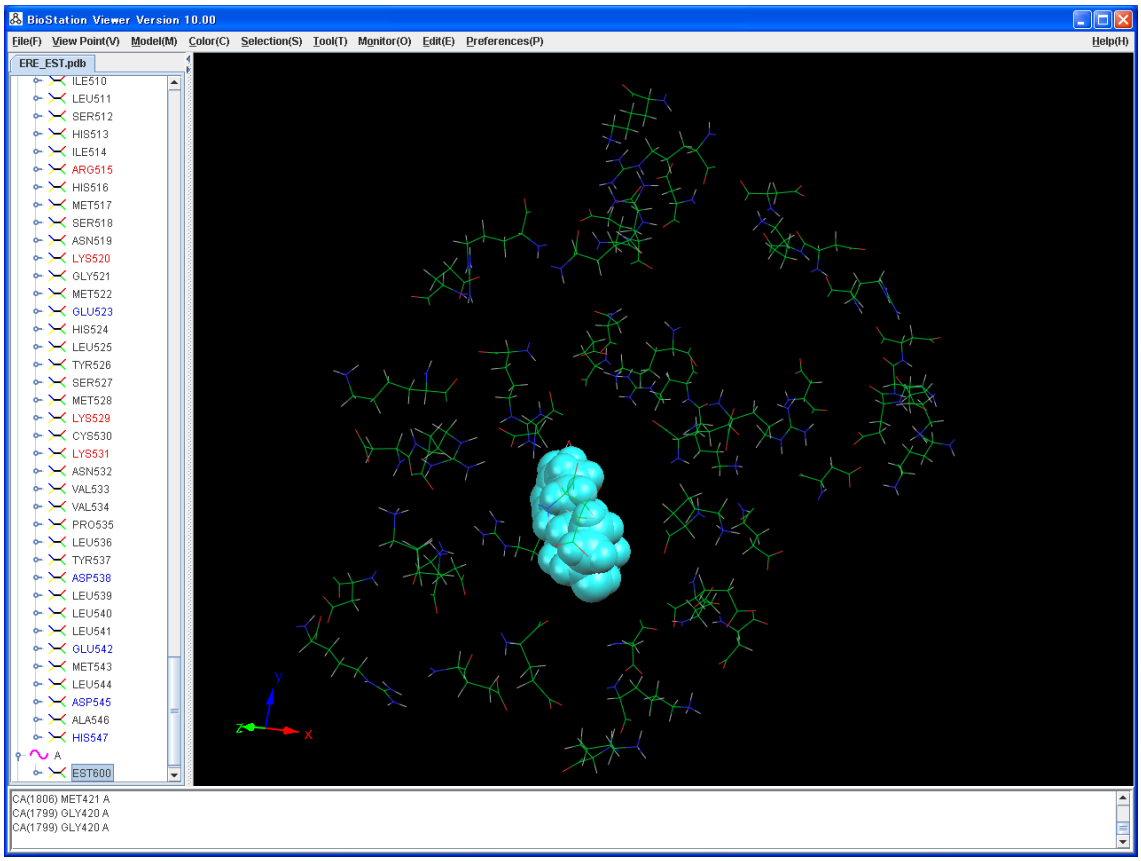


Fig3.36 Charged Amino Acid

When you select [**Color(Atom)**]-[**Charged Residue**], the displayed residues are added colors by the charged values. This example is shown in Fig3.37.

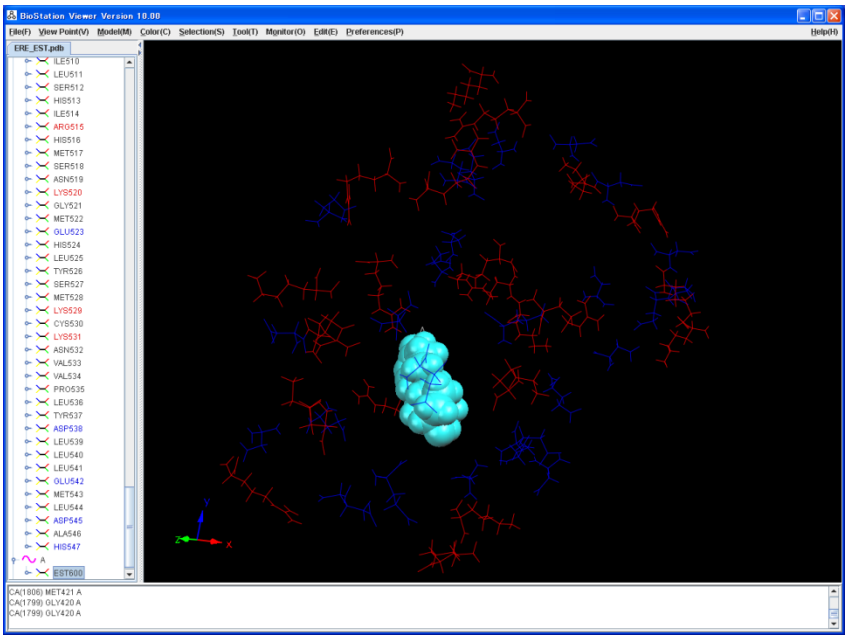


Fig3.37 Residues Added Colors by Charged Amino Acid

Select [**Tool**]-[**Display Selected Residue**]. Since the residue dialog box appears, click on **Select All**. The setting of residues is unspecified, which displays the whole residues. This example is shown in Fig3.38.

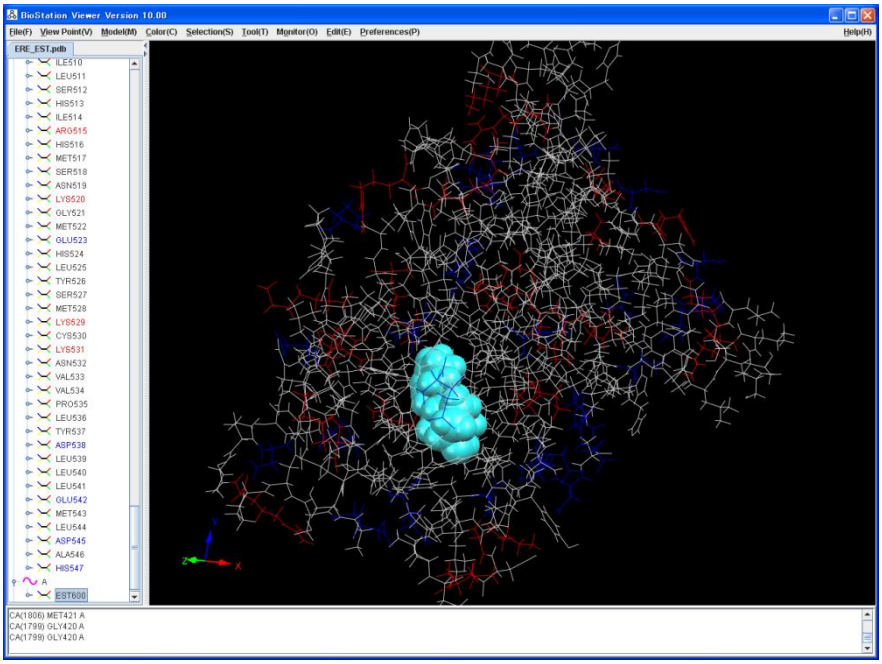


Fig3.38 All the Residues Added Colors by Charged Amino Acid

3.2.5. Display Atoms around Ligand in specified Distance

Click on the ligand and select **[Tool]-[Display Atom in Distance].** Since the dialog box for the assignment of a distance appears, select **Residue** from **From selected** and input **4** in the **Distance**. And then, atoms within **4Å** from the ligand are displayed. This example is shown in Fig3.40. Here, click on the atom around the center of the ligand and select **[Tool]-[Set Rotation Center]**. This makes you move the display easier, since the center of the rotation can be the selected atom.

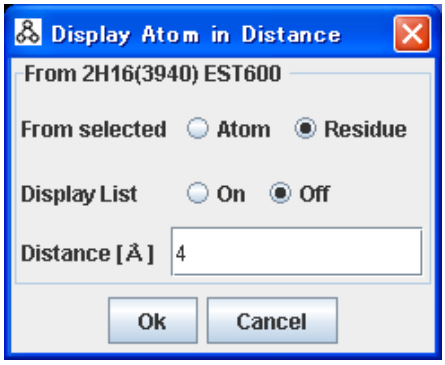


Fig3.39 Atoms in the Distance Dialog Box

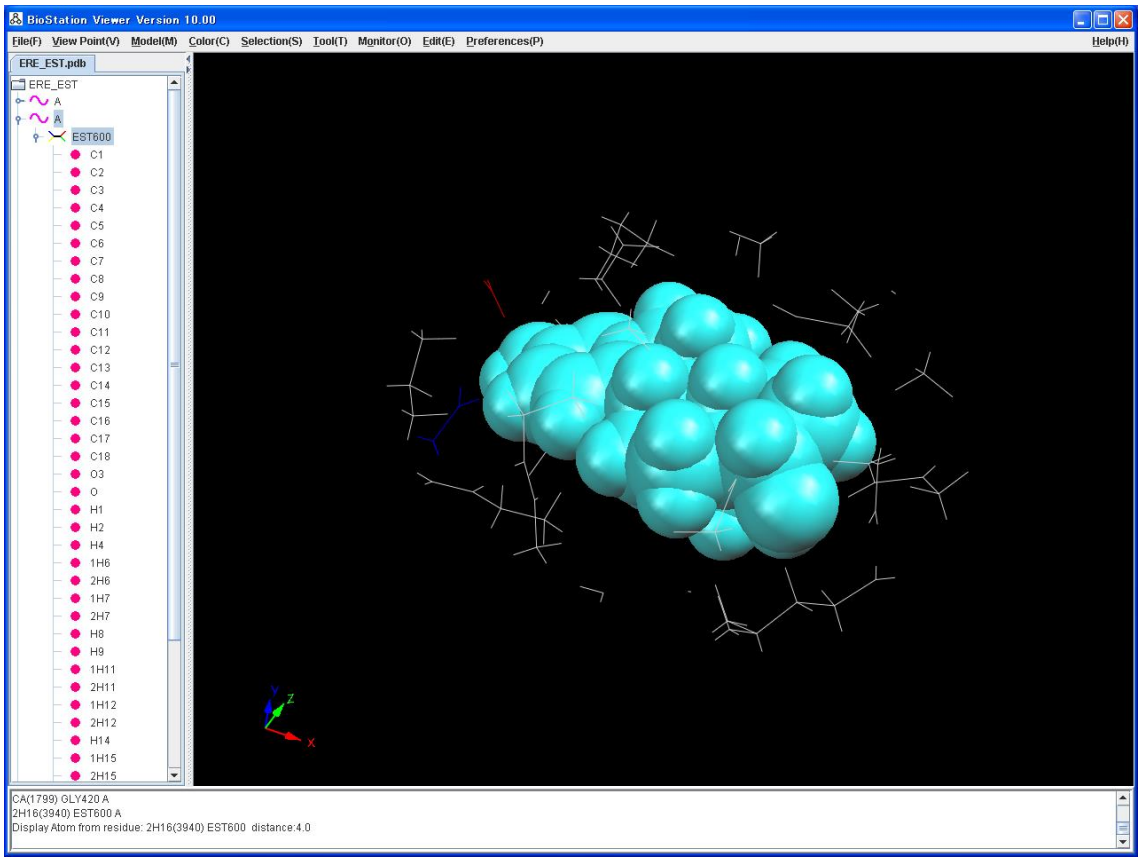


Fig3.40 Atoms within the Distance

Next, you can display the distance between atoms. Select **[Color]-[Atom]** to set colors to the whole atoms. Click on the ligand with the right button on the mouse and set it in the **Ball & Stick** model. Here, select **[Monitor]-[Distance]**. Click on the hydrogen of a side of the ligand. Next, click on the nearby oxygen. This displays the distance between the atoms in the message area. This example is displayed in Fig3.41.

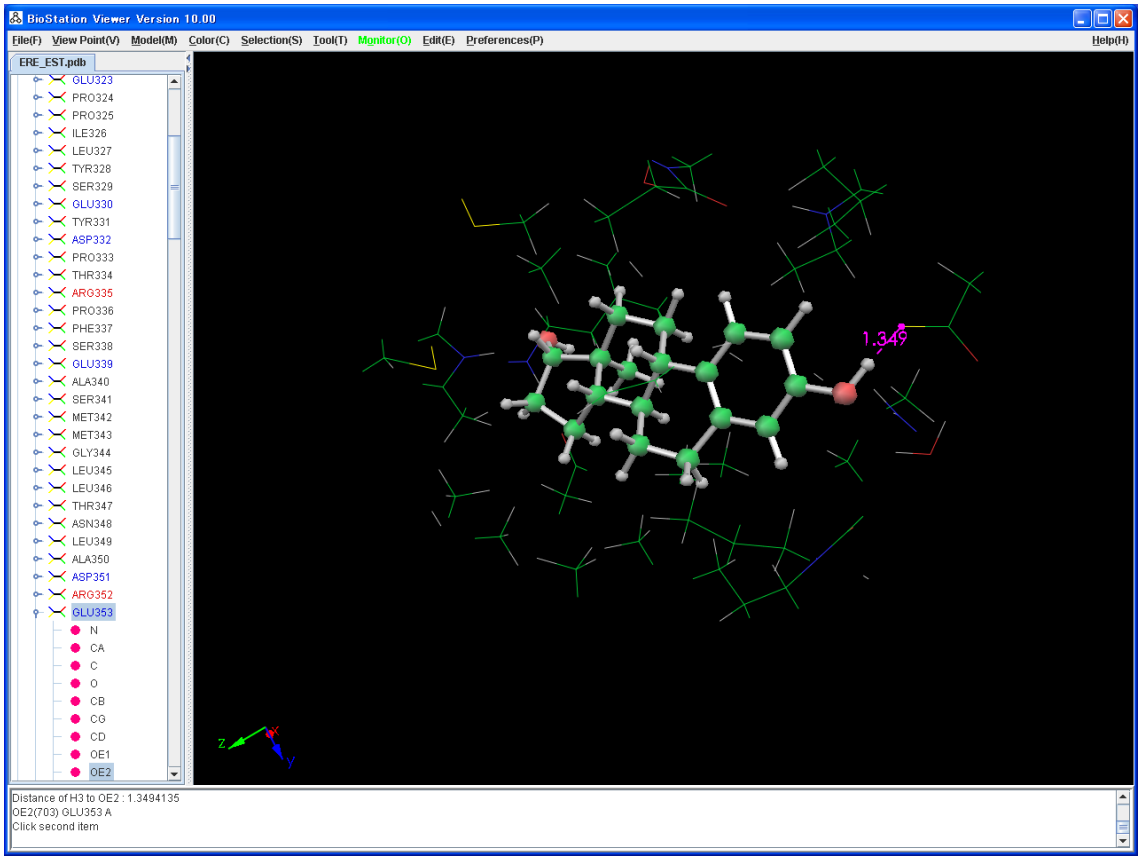


Fig3.41 Distance between the Atoms

3.3. Example of the Display of Interaction Energy between Fragments

Use the result of computations of the estrogen receptor – the ligand complex. With the calculation as 1fragment = 1 residue, the interactions between residues and between residues and ligands can be displayed.

3.3.1. Load File

Start the **Viewer** and load **ERD_EST.cpf**. This display is shown in Fig3.42.

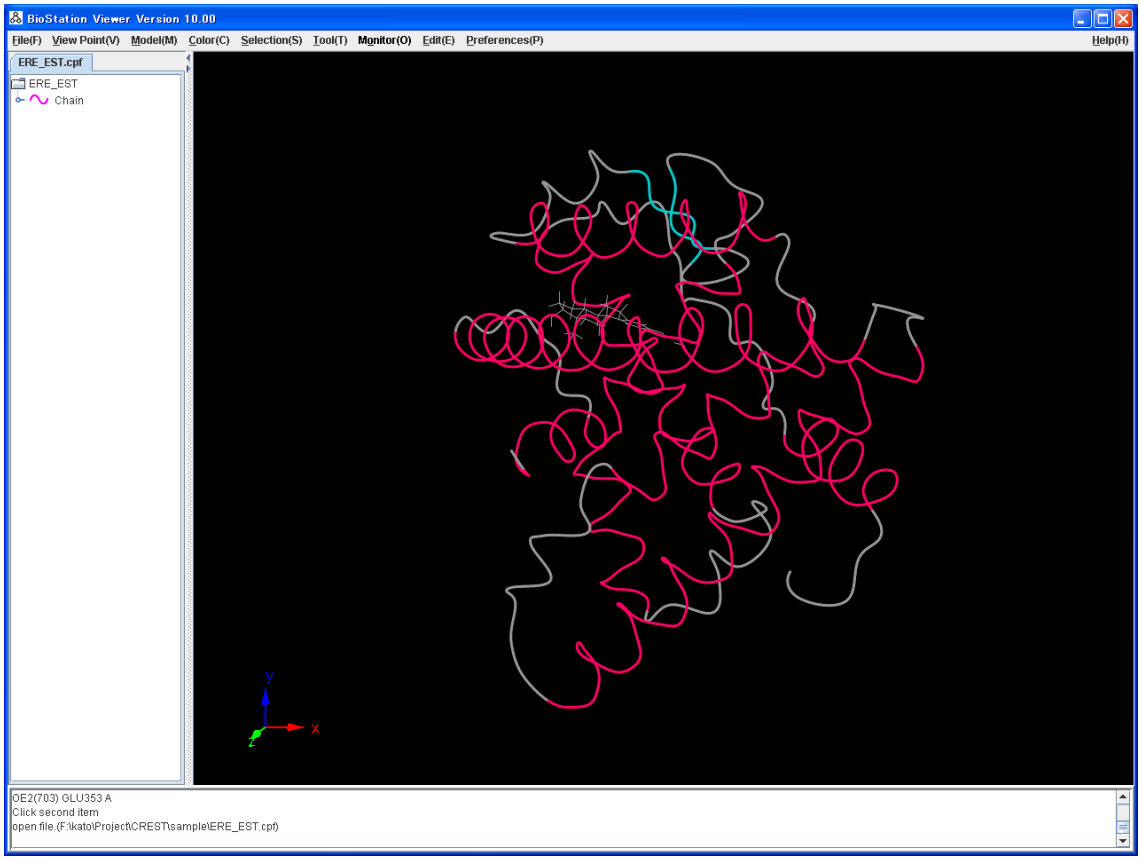


Fig3.42 Molecular Structure from the Input File

3.3.2. Assignment of Interaction Energy between Fragments

Click on a ligand, **EST600**, in hierarchical window with the left mouse button. Select **[Monitor]-[Interfragmnet Interaction]-[1:1]** and popup the dialog box for the values of interaction energy (Fig3.43.). Here, type **min:-10, max:10** and click on the **Ok** button. This allows you to display molecular structures, which are added colors to the interaction energy between each residue from ligands within the range, **-10～10kcal/mol**. An example of the display is shown in Fig3.44.

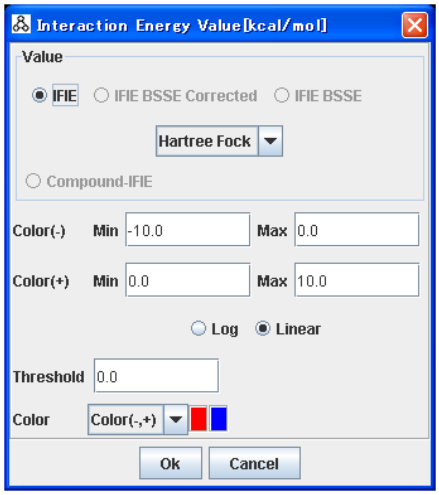


Fig3.43 Interaction Energy between Fragments Dialog Box

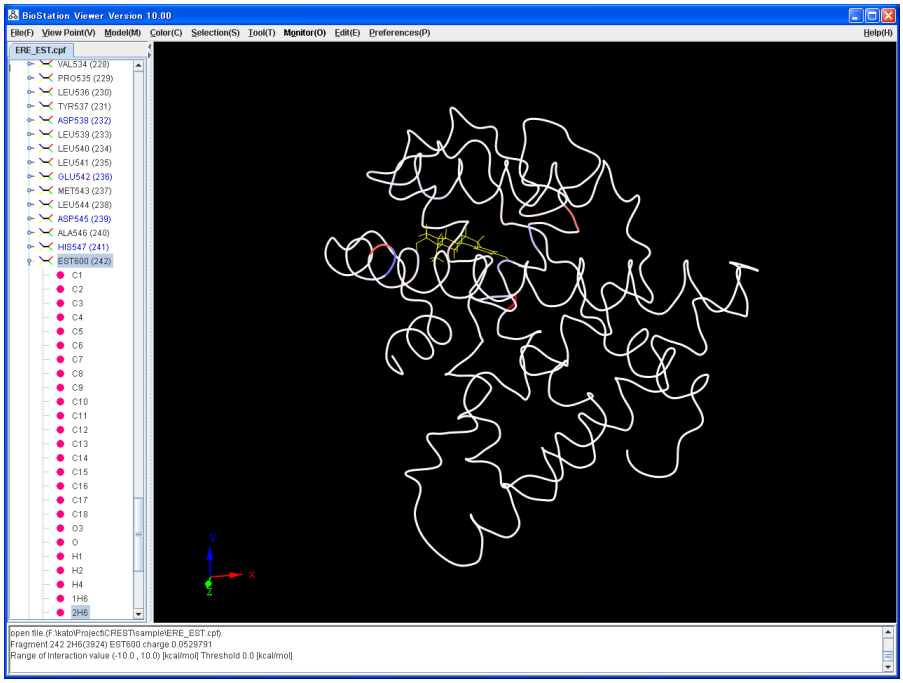


Fig3.44 Interaction Energy between Fragments Display

3.3.3. Assignment of Threshold

To highlight ligands, a display attribute dialog box is displayed by clicking on **EST 600** in hierarchical window with the right mouse button. Here, click on the button in the **Color** to select the proper color and specify **CPK** in the **Model** (Fig3.45) Next, select **[Monitor]-[Interfragment Interaction]-1:1[lock]** and put **2** in the **threshold** at the dialog box for values. This makes it impossible to display residues with absolute values of the interaction energy under **2kcal/mol.** An example of the display is shown in Fig3.46.

Fig3.45 Display Attribute for Ligands Dialog Box

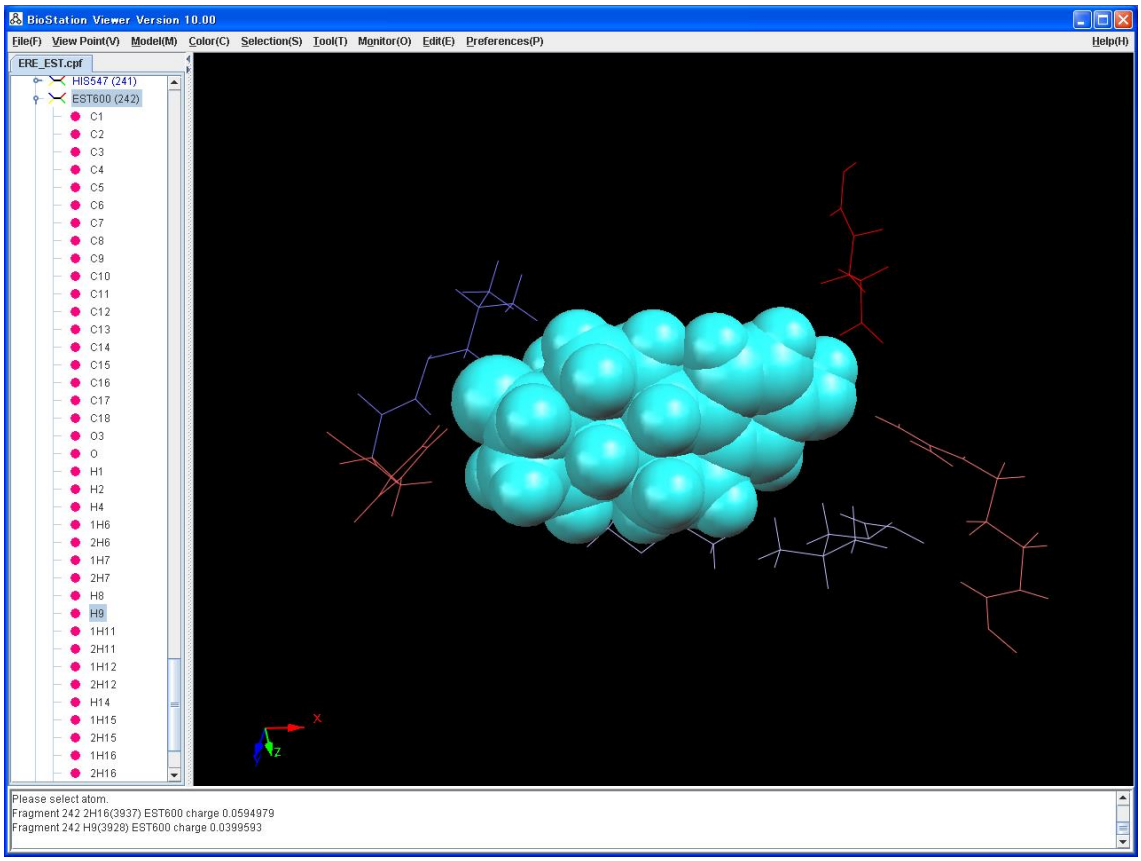


Fig3.46 Interaction Energy between Fragments, Specifyed Threshold Display

3.3.4. Interaction Energy between Selected Fragments

Select **[Model(Atom)]-[Stick]**. Select **[Monitor]-[Interaction Energy].** Menu is displayed in green until this menu is selected again. And by selecting the display, the interaction energy between selected fragments (residues) is displayed. An example of the display by clicking on the ligands and fragments around them is shown in Fig3.47**.** In addition, the interaction energy list between fragments (residues) can be displayed as Fig2.61.

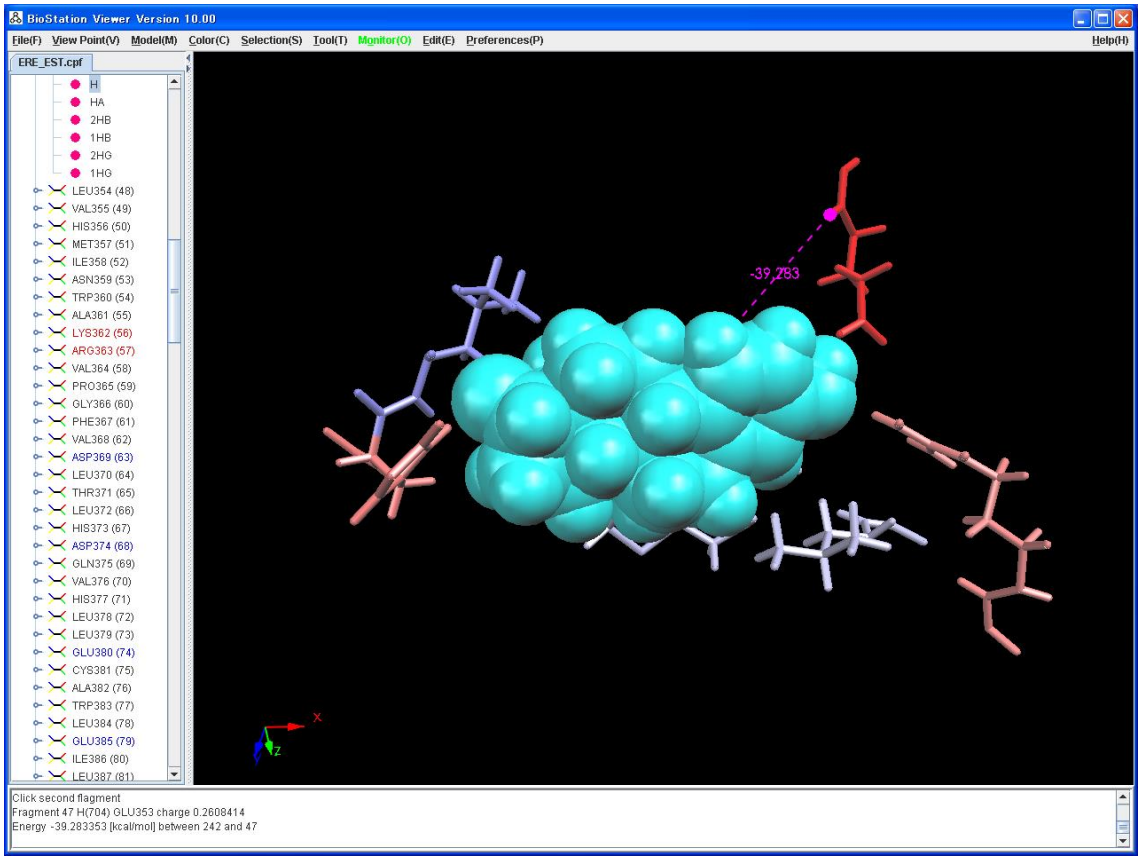


Fig3.47 Interaction Energy between Selected Fragments Display

3.4. How to Overlay

Use data of **ERE_EST.cpf** and **ERR_RAL.cpf** to overlay.

3.4.1. Load File

Start the Viewer and select **[Model(Structure)]-[Cα]**, **[Color(Structure)]-[File]** and load **ERE_EST.cpf , ERR_RAL.cpf**. This allows you to set colors to the molecules each file. An example of the display is shown in Fig3.48.

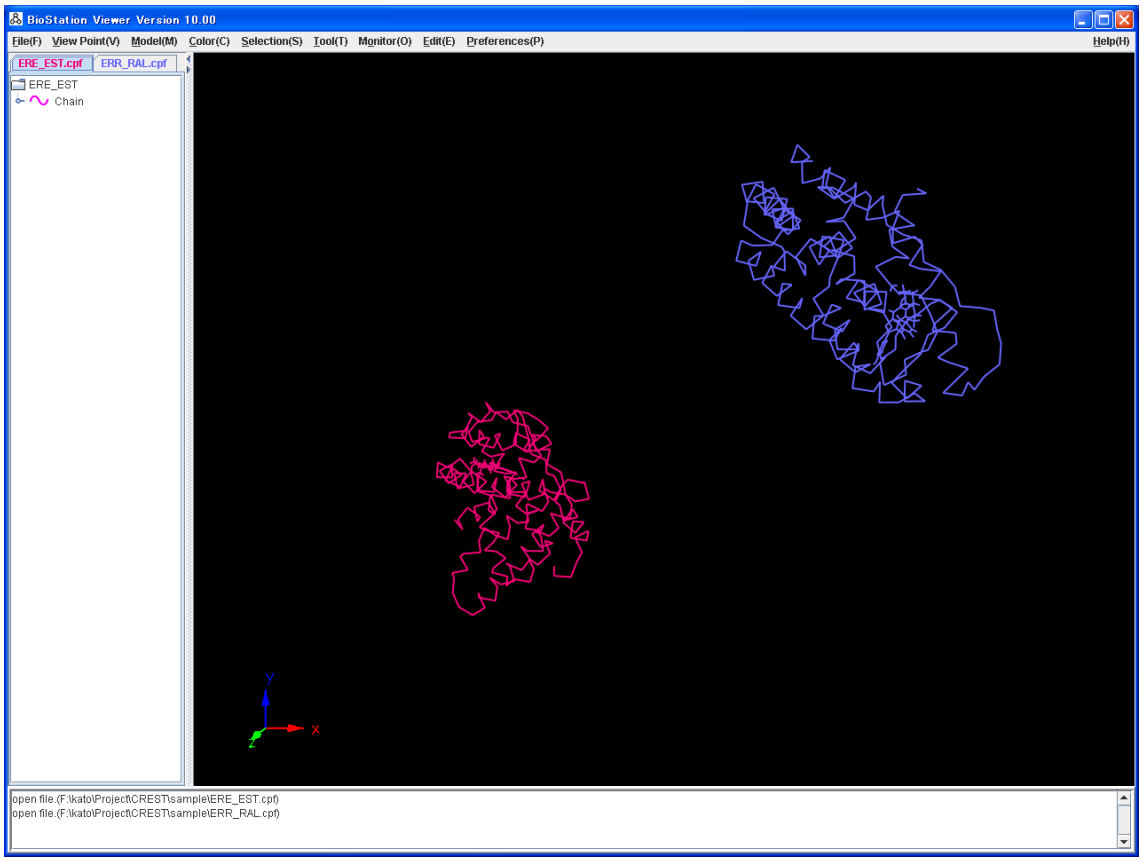


Fig3.48 Two Molecules Load from the Files

3.4.2. Overlay with All the Cα Coordinate

Select **[Tool]-[Overlay Molecules]**. Popup A dialog box for the overlay. As you use the default value, click on the **Ok** button. In the default, overlay the molecules each file with the C α coordinate. An example of a display after the overlay is shown in Fig3.49. Since all over the molecules are overlaid, they are not lined up on the whole.

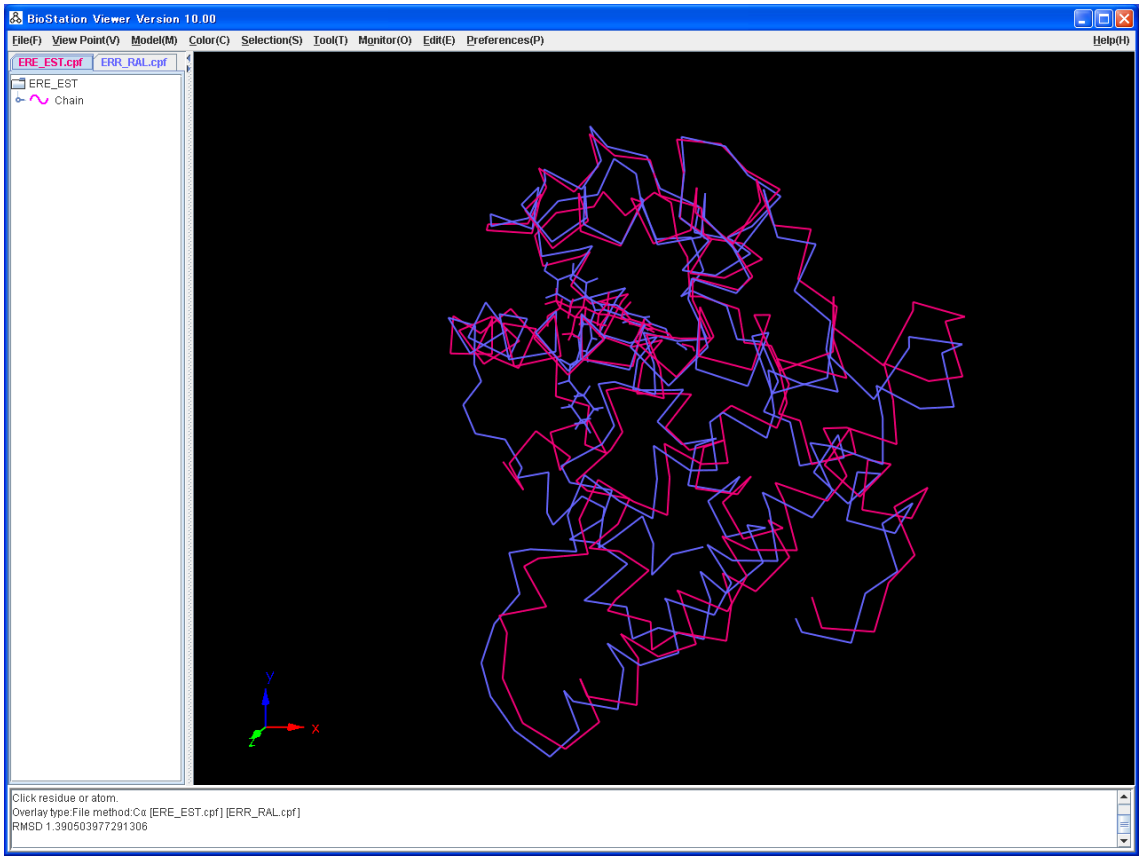


Fig3.49 Molecules Overlaid Each File with the C α Coordinate

3.4.3. Overlay by Atom(Cα within Selected Residues)

Next, you can overlay molecules by selecting 3 atoms**(C α)**. Select **[Tool]-[Overlay Molecules].** Set **Residue** in the **Type**, and **C α** in the **Method**. Click on 3 parts of each residue, which is similar to each other structurally by turns. The residue numbers, which you click are displayed in the input field, where you can modify them by using the key board. In the case that you put the wrong number, it can be deleted by the keyboard. This dialog box is shown in Fig3.50. Here, click on the **Ok** button. Display both ligands (**EST600 and RAL600**) in the **Stick** model. You can see the difference of the position of **Herix 12 in** the end side, **C**, of both agonist (**EST pink**) and antagonist (**RAL purple**).(Fig3.51)

Next, select [Model]-[Cα{tube}]. An example of the display is shown in Fig3.52.

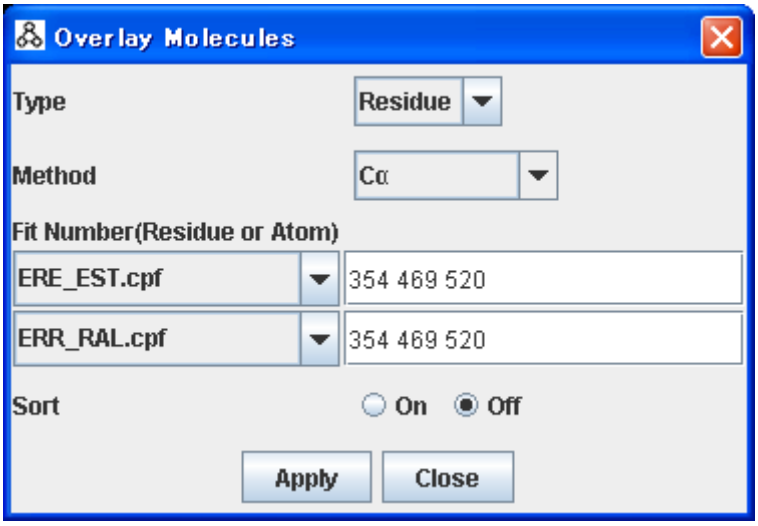


Fig3.50 Overlay Molecules Dialog Box

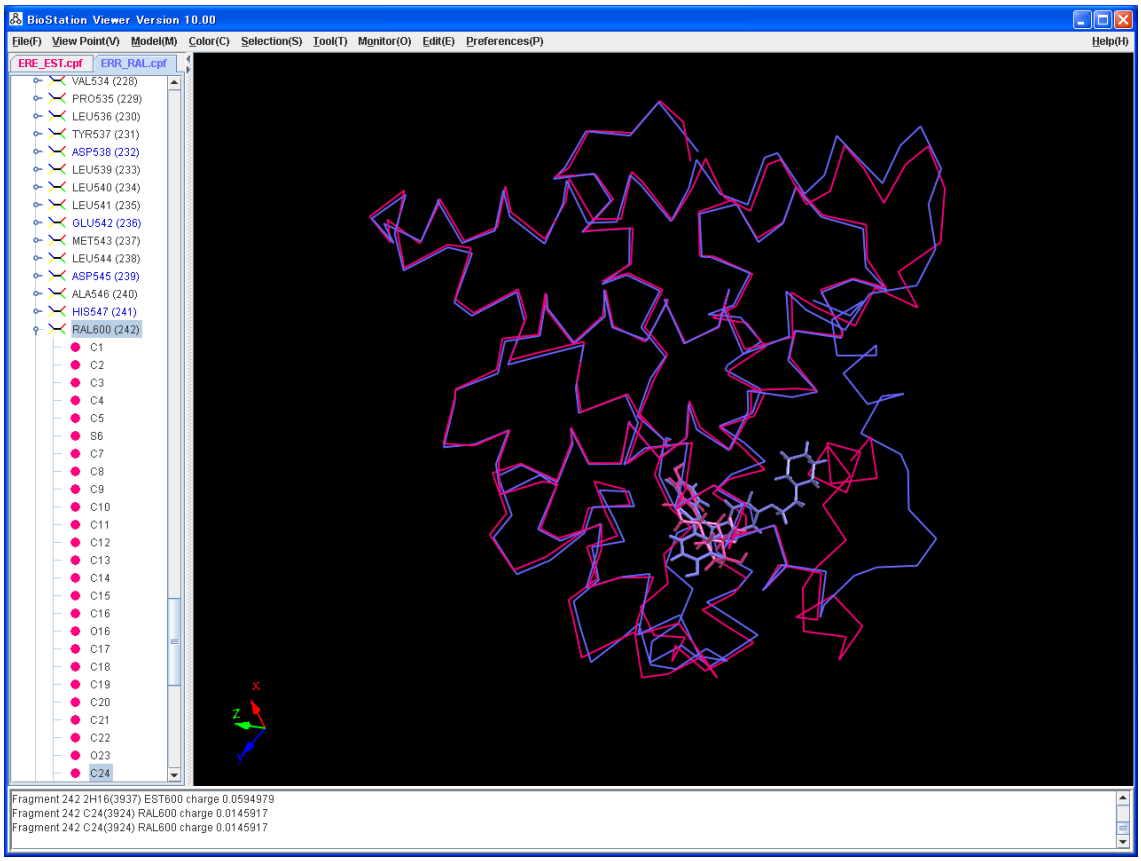


Fig3.51 The Result of Molecules Overlaid by Selected Residues

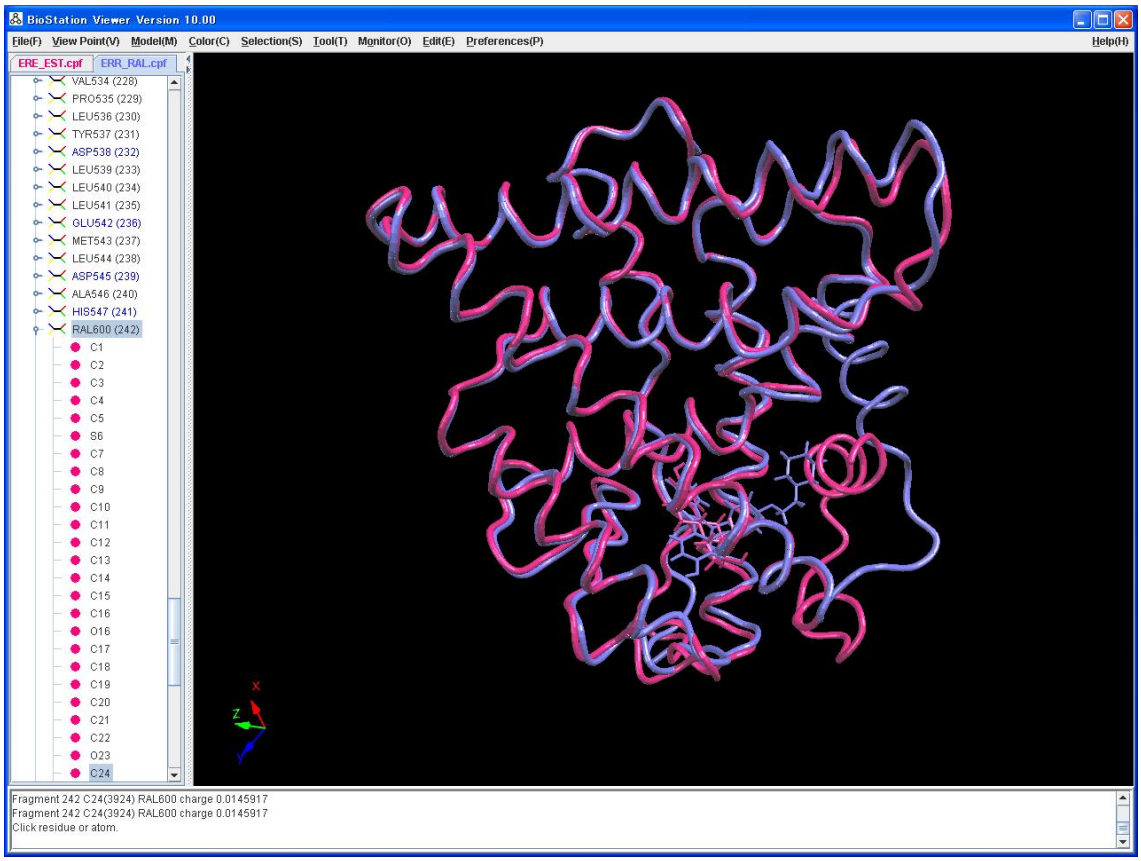


Fig3.52 The Result of Molecules Overlaid by Selected Residues (Cα{tube})

3.5. Example of How to Add Hydrogen

Use a sample file **(ERE_EST_noH.pdb)** with hydrogen removed in advance. In order to add hydrogen, **Reduce** needs to be preconditioned to be installed. Refer to the setting of **Reduce** in **Section 4.5** so as to install.

Load **ERE_EST_noH.pdb** and select **[Tool]-[Add Hydrogen]**. Popup a dialog box to add hydrogen. (Fig3.53). Input file name added **_addH** is displayed in the output file field as a default. In the **Options**, set options which can be used in **Reduce.** By click on the **Ok** button, a display of a command prompt is displayed to appear a log for the execution. Input **exit** to close the window.(Fig3.54)

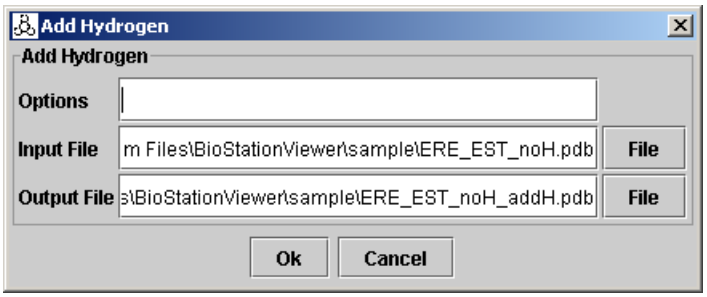


Fig3.53 Add Hydrogen Dialog

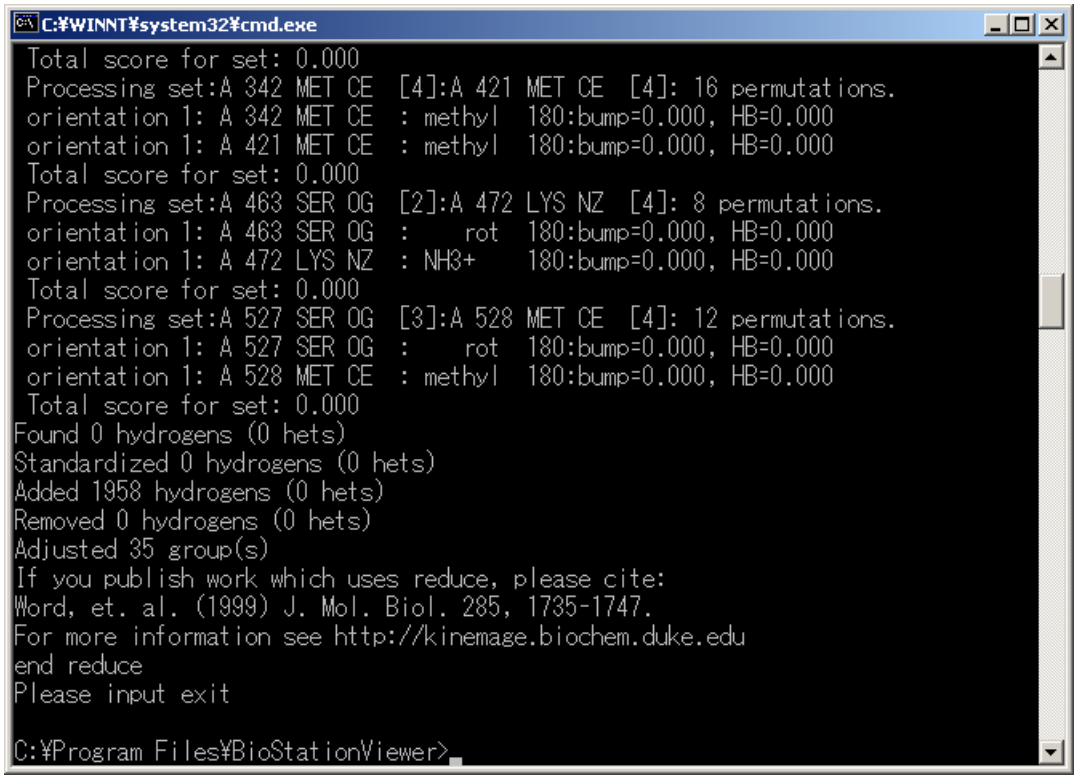


Fig3.54 Command Prompt Window

When you close the command prompt, you could be asked if you want to display the result or not. Here, clicking on the **Ok** button lets the display replace it with added hydrogen.

Fig3.55 Confirmation of Displaying the Result

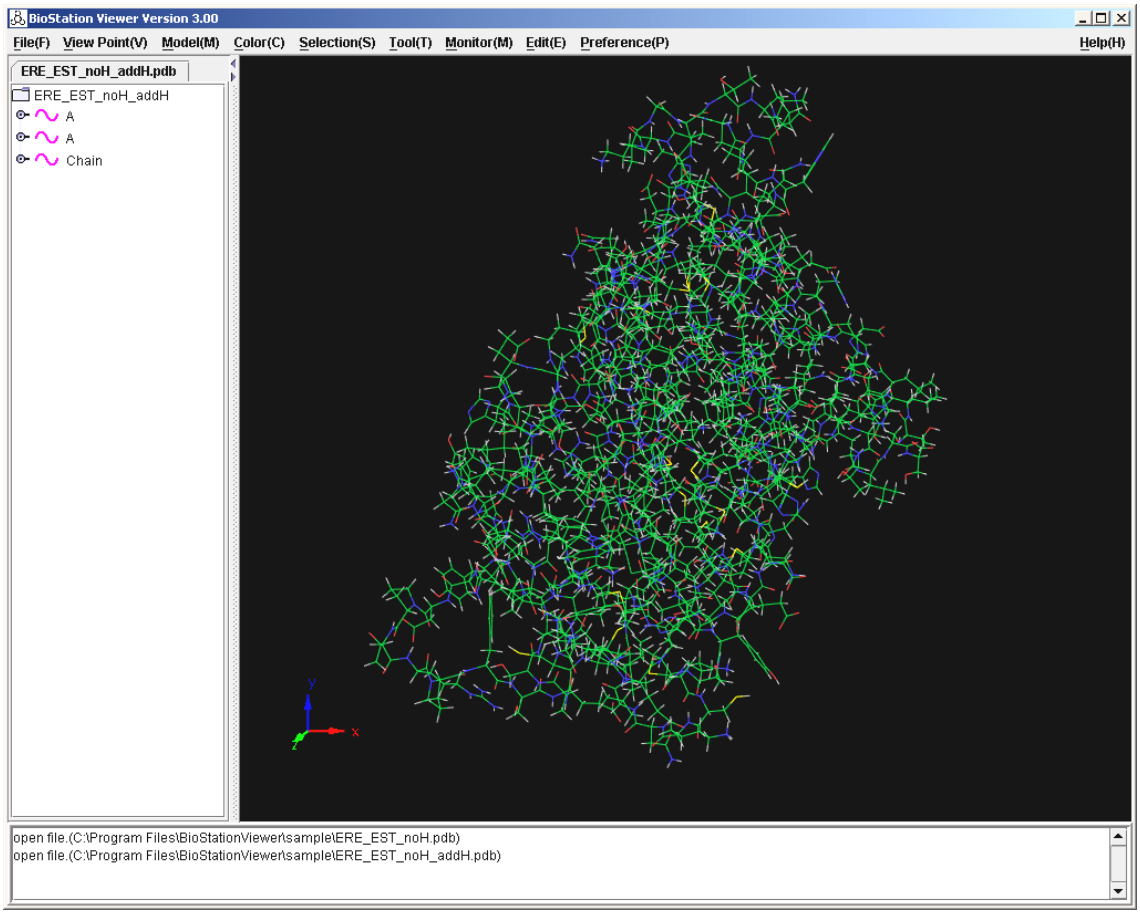


Fig3.56 Molecule Structure Added Hydrogen

3.6. Example of Interfragment interaction energy N:1

Display an example of Interfragment interaction energy N:1 using of the calculation results of DNA and protein. By load a sample file, trunc-DB7_Hopt_moe_DNA.cpf, display molecular structures with the C α [tube] model. By selecting **[Monitor]- [Interfragment Interaction]-[N:1]**, pop up a dialog box. This data consist of protein(fragment number 23-222), lagend (223) and DNA(1-22). In order to show Interaction energy between protein, ligand and DNA, input 23-223 for the Base fragment, and set Min,Max to -100,100, By clicking on **OK** button, protein, ligand and DNA are colored by the value of interaction energy. Red parts are stable relations.

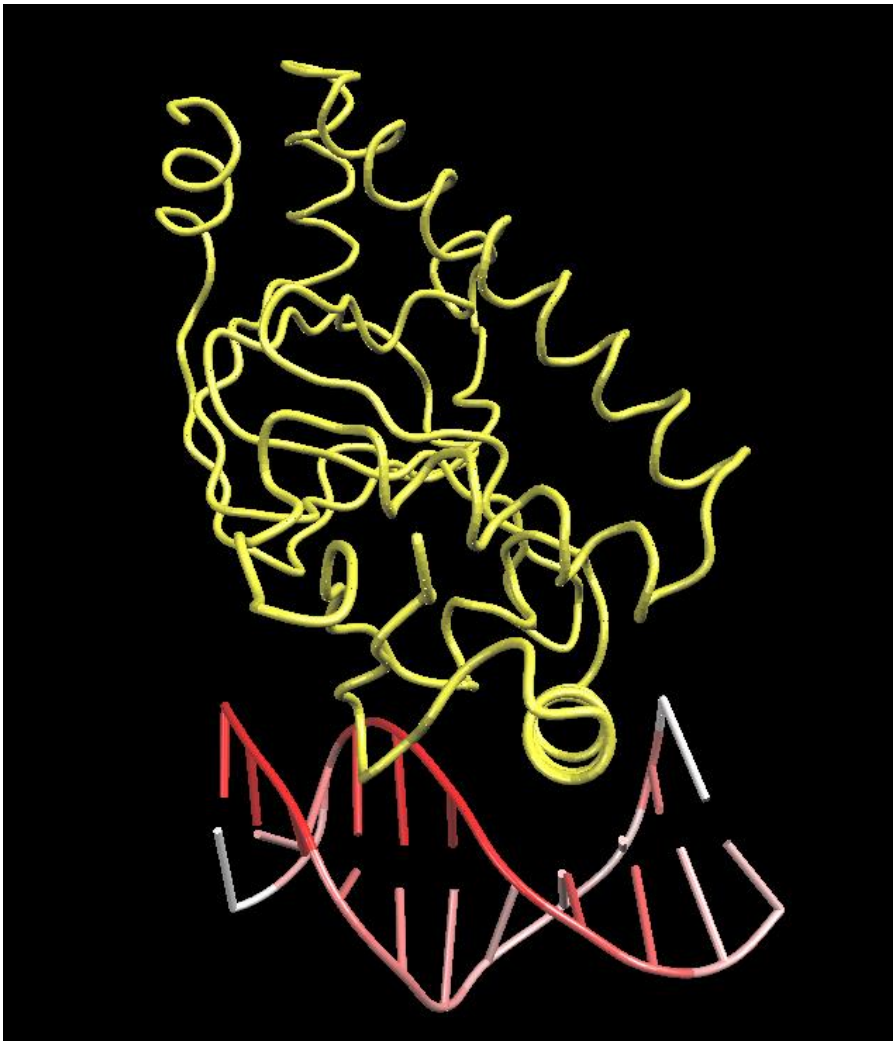


Fig3.57 Example of Interfragment interaction energy N:1

3.7. Example of trajectory

3.7.1. Glyine

By loading a sample file, G05A.trj, molecular structure at first step(Fig3.58) is displayed. Clicking on the ▶ button lets the trajectory of molecular structure display. The Molecular structure at the last step is shown in Fig3.59.

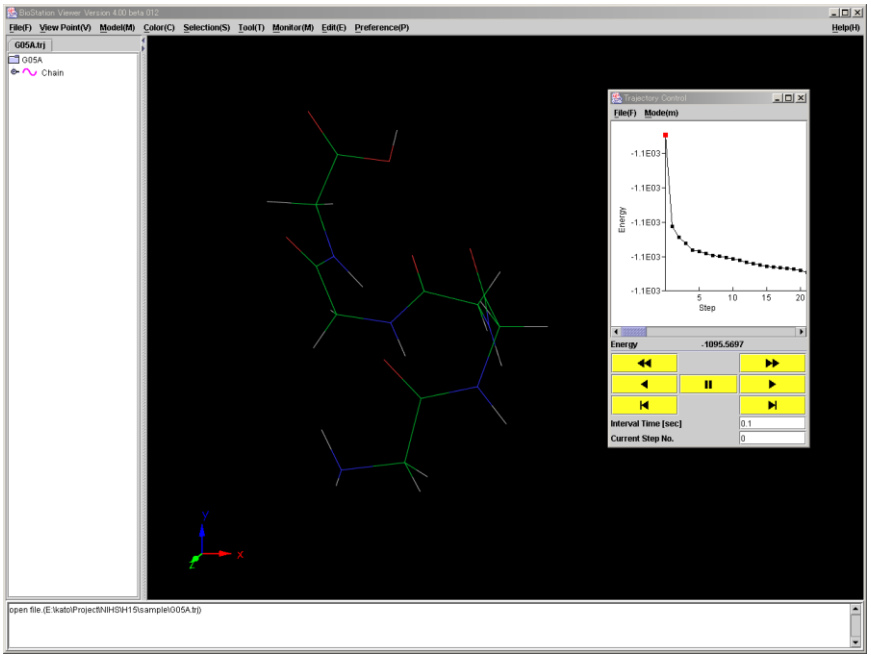


Fig3.58 Molecular structure at the first step

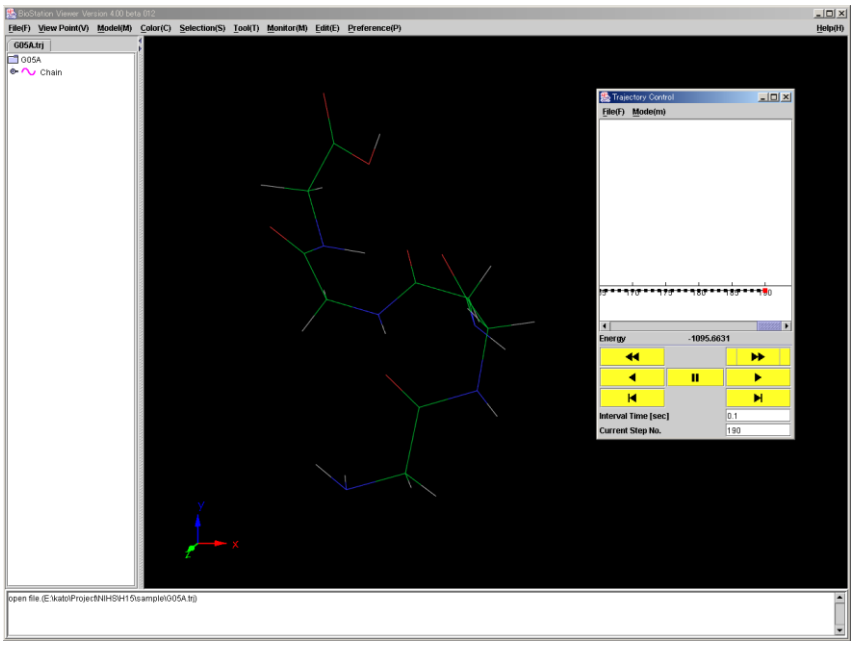


Fig3.59 Molecular structure at the last step

3.7.2. Si8

By loading a sample file, dyna_pot_test.tr2. Nano scale device simulation team of Frontier Simulation Software for Industrial Science provided this result. This is Si8 MD calculation result. It edits every ten steps for this display example. The vector expresses the force in which it is influence on an atom. Please specify **[Model(Atom)]-[Wire Frame]**, **Model(Atom)→Wire Frame、Preference→Set Preferences→Arrow(Trajectory)** arrow scale property is 10 in preference dialog. The first step is shown in Fig3.60. Clicking on the ▶ button lets the trajectory of the vector animation. The last step is shown in Fig3.61.

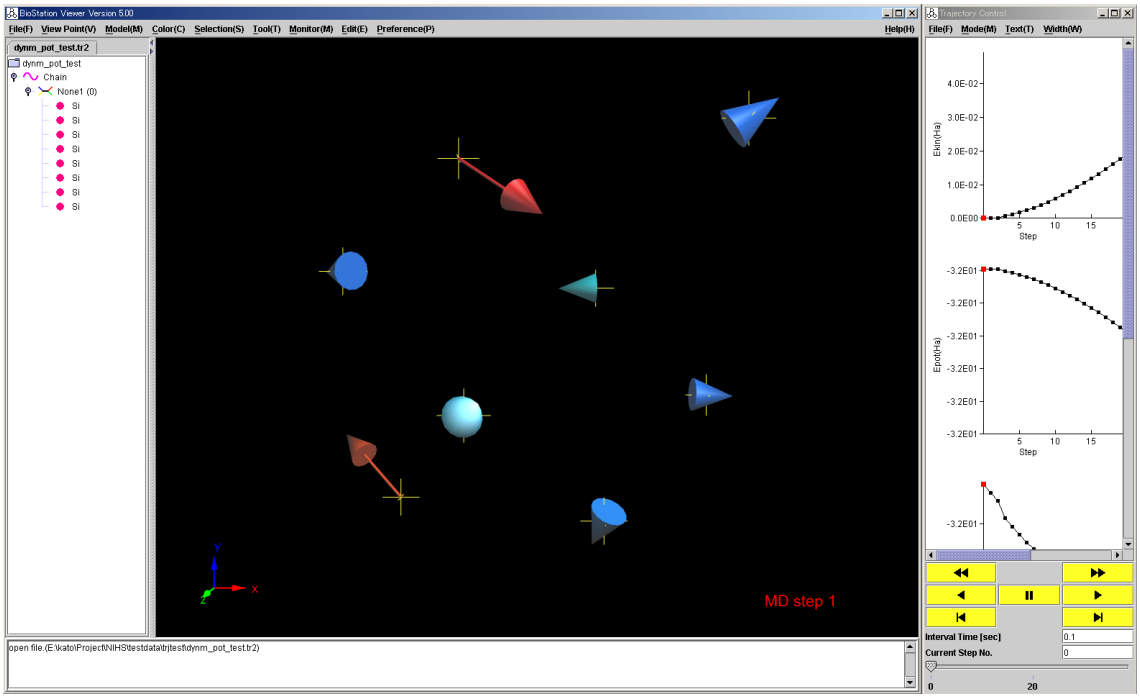


Fig3.60 The first step of vector example.

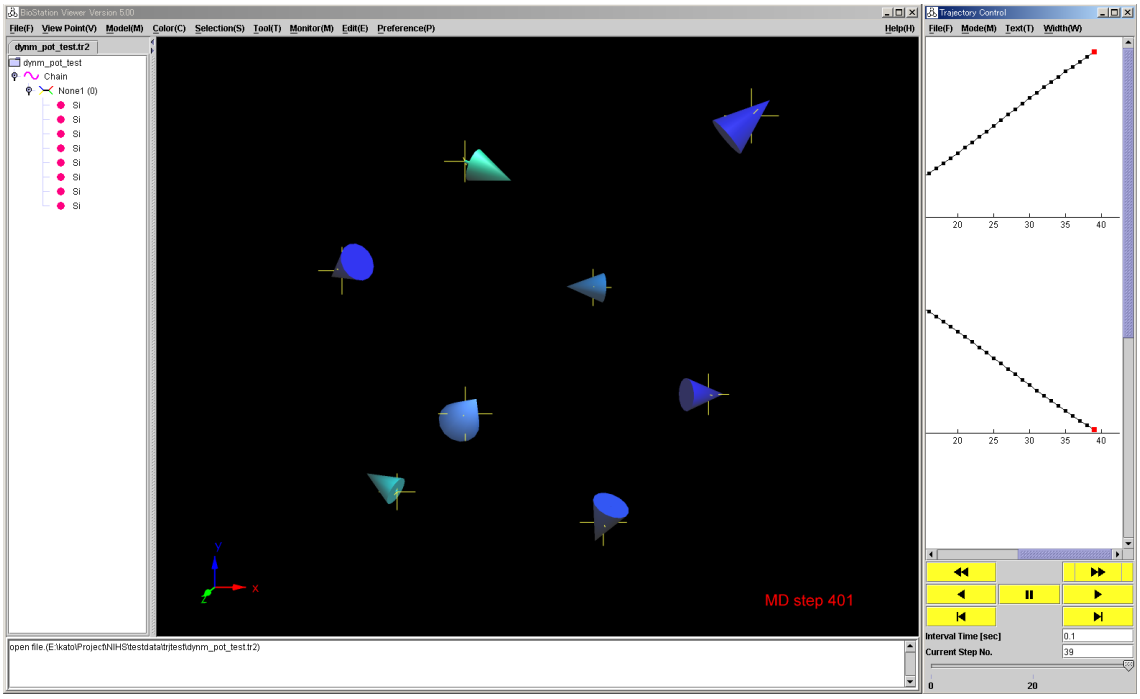


Fig3.61 The last step of vector example.

3.7.3. Create a movie file of trajectory

This section explains ho to make a movie file by using FFmpeg that is free software.

1) Open file

   Open a trajectory file by selecting **`File→Open.`** In this case, when **Trajectory file** is selected with Files of Type, it becomes easy to choose filing because only trajectory file is displayed in the list. After load the file, popup the trajectory window.

2) Specify options

   If you want to add color by fragment, select **Color→fragment** menu on main window. Set resolution options of Ball, Stick, CPK and Tube to 64 by Preference menu(**Preferences→Set Preference→Resolution**), It becomes nice to visualize a molecular model. By selecting **Disable** at Preferences →Display Axis、then the xyz axis at lower/left in window disappear.

3) Create image files

   Specify the folder that is saved image files (**File→Create image files** menu) Format of images is JPEG. Convention of file name is sequential number for six digits.

4) Prepare to create a movie file

   The source code of FFmpeg can be downloaded from http://ffmpeg.org/. The executable file for windows can be downloaded from http://blog.k-tai-douga.com/.

Copy ffmpeg.exe to C:¥Program Files¥ffmpeg, the copied folder is added to the end of PATH like bellow.

;C:¥Program Files¥ffmpeg

It is useful to execute the ffmpeg without specified install folder.

5) Create a movie file

Please type in bellow command at the folder that is stored image files by using command prompt. It is easy to change folder to drag the folder from explorer.

```
ffmpeg -r 75 -i "image%06d.jpg" -vcodec wmv2 -sameq -s 640x480
out_r75_640x480.wmv
```

-r 75 :set frame rate(frame per 1 second) to 75(default value is 25).
-i "image%06d.jpg": Spceify image file name. %06d means sequential number for six digits.
-vcodec wmv2:set Windows Media Video as codec. If you specify mjpeg or mspeg4v2(MS-MPEG4), according to PC you can not play this file on PowerPoint. So you may not specify this option.
-s 640x480: Specify size of screen 640x480. if not specify this option, output size is same size of input. You had better specify this option if input size is bigger. Because it puts a strain in CPU.
-sameq:Image quality of output is same quality as input.
out_r75_640x480.wmv: output file name

```
ffmpeg -h > ffmpeg.txt  : output help
ffmpeg -formats > formats.txt : output format
```

6) Attach a movie file on PowerPoint

Select menu Insert→Video→File.

It is only to link the file, so if you copy the PowerPoint file, you have to copy the movie file with it.

Reference

1) http://opensourceaki.blogspot.com/2007/10/ffmpeg_19.html
2) 原一浩、寺田学、本間雅洋、足立健誌、堀内康弘、堀田直孝、月村潤、尾花衣美、FFmpeg で作る動画共有サイト(毎日コミュニケーションズ、2008)

3.8. Example of crystal

Load the Gaussian Cube file that includes the atomic structure of a Bi super-thin film (four layers), and the electron density in order to visualize an isosurface and a periodic display. Nano scale device simulation team of Frontier Simulation Software for Industrial Science provided this result.

3.8.1. Load a file and visualize the isosurface

Load a sample file(4LBi.cube) and choose **Density** for the file type because this file includes electron density data. Next, set **Ball&Stick** to the mode, isosurface value to 0.009, transparency to 50 and Bonding box to **on**. The dialogs and the result display are shown in Fig3.62～Fig3.64.

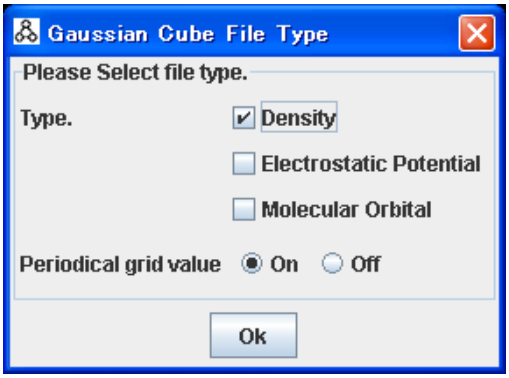


Fig3.62 File type dialog

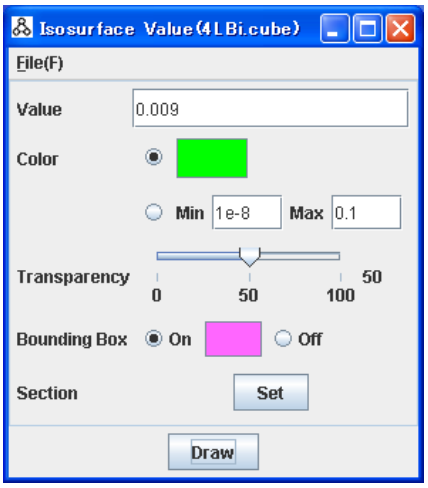


Fig3.63 Isosurface dialog

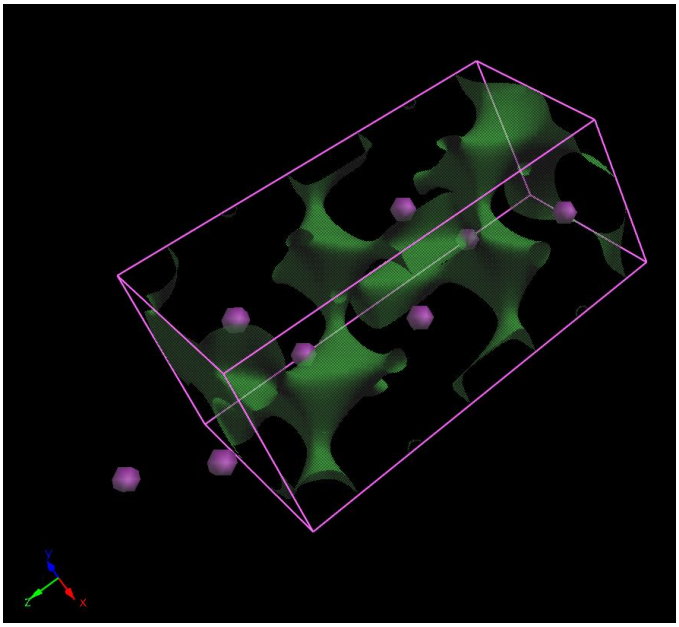


Fig3.64 Example of isosurface of electron density

3.8.2. Periodic display

By selecting **[Viewpoint]-[Periodic]**, popup a dialog box to specify periodic options. The example file is Gaussian Cub, so there are a three input fields for each X,Y and Z Interval. The value from the file is specified by the default. X and Y Nums are to 2, and clicking **Draw** button. Then each direction X and Y is displayed two times. The color of bounding box is to cyan. A display result is shown in Fig3.65

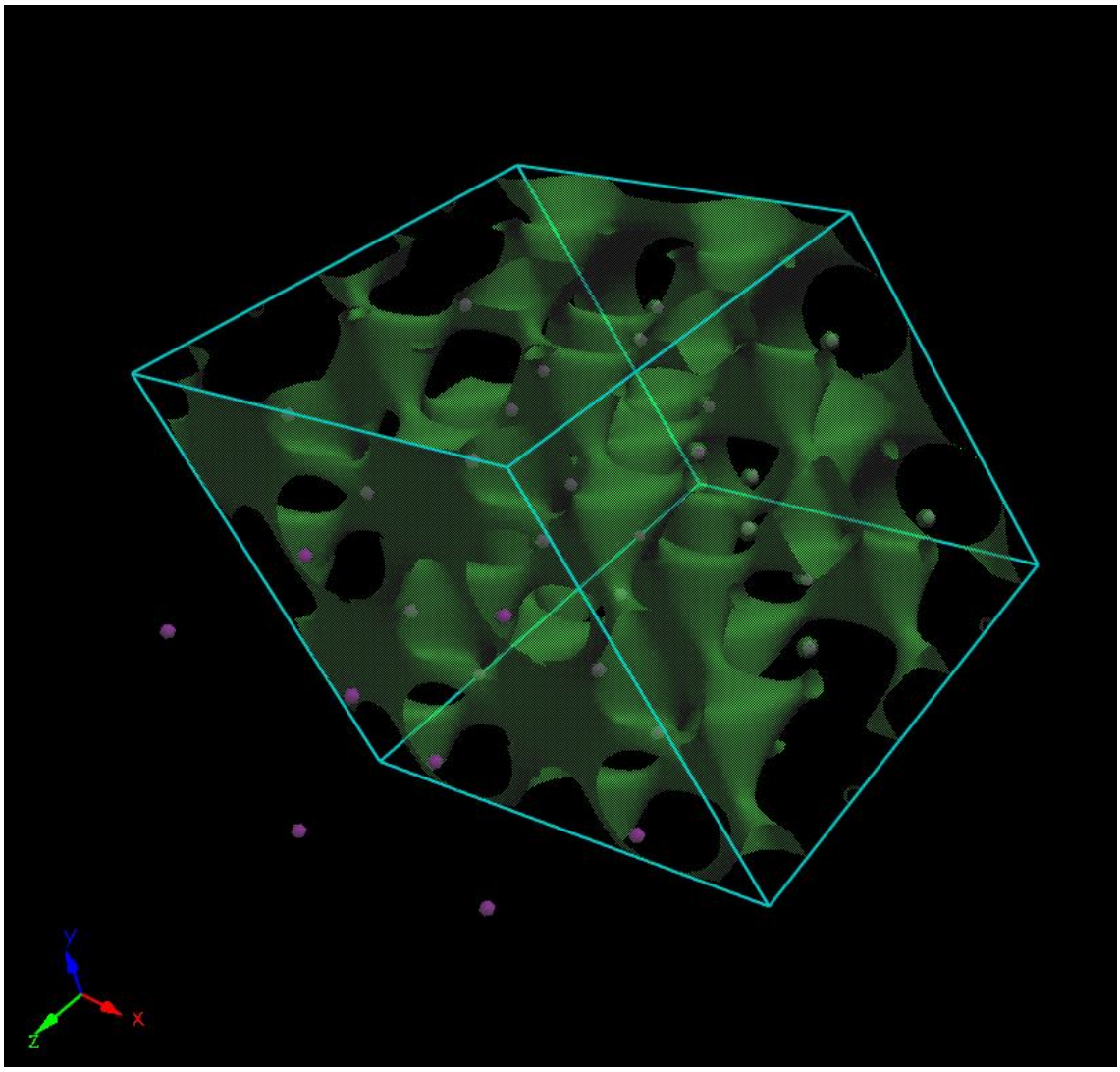


Fig3.65 Example of periodic display

3.8.3. Display a section

By clicking **Set** button on the isosurface dialog box, pop up the section dialog and display a half-transparent section on 3D window. Move a position of **Z** direction a little by slider and set **Color Range Min** to 1.0E-3. By clicking **Draw** Button, a section displayed.

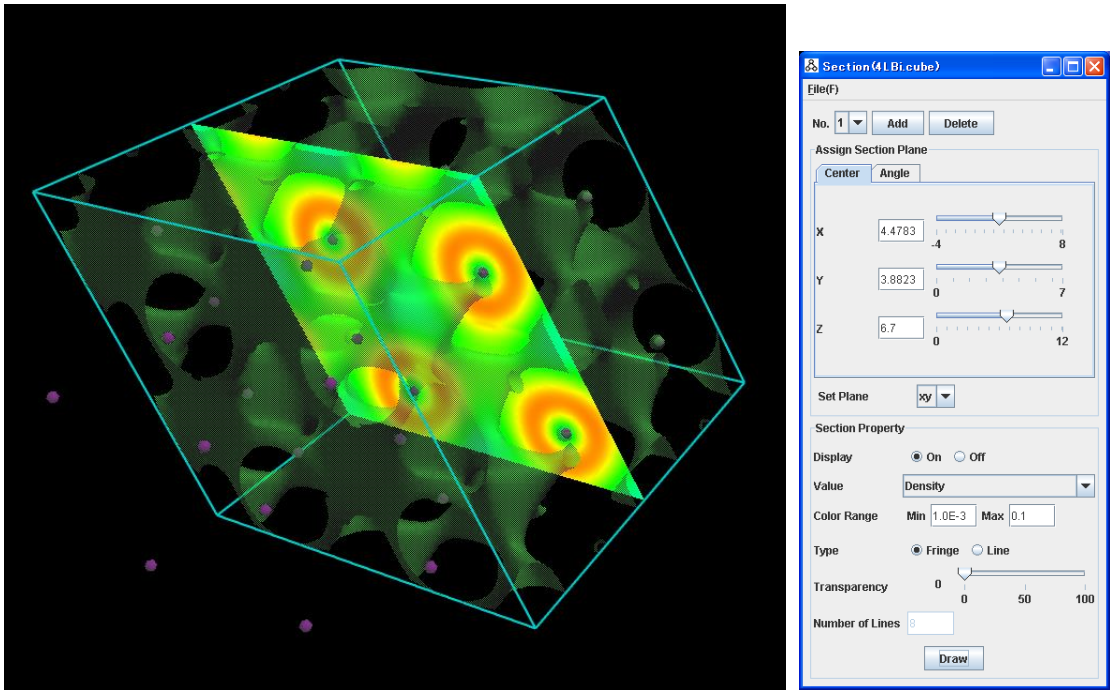


Fig3.66 Section dialog and example of section

Next, set **Type** to **Line**, **Number of lines** to 32. By clicking **Draw** button, isolines are displayed.

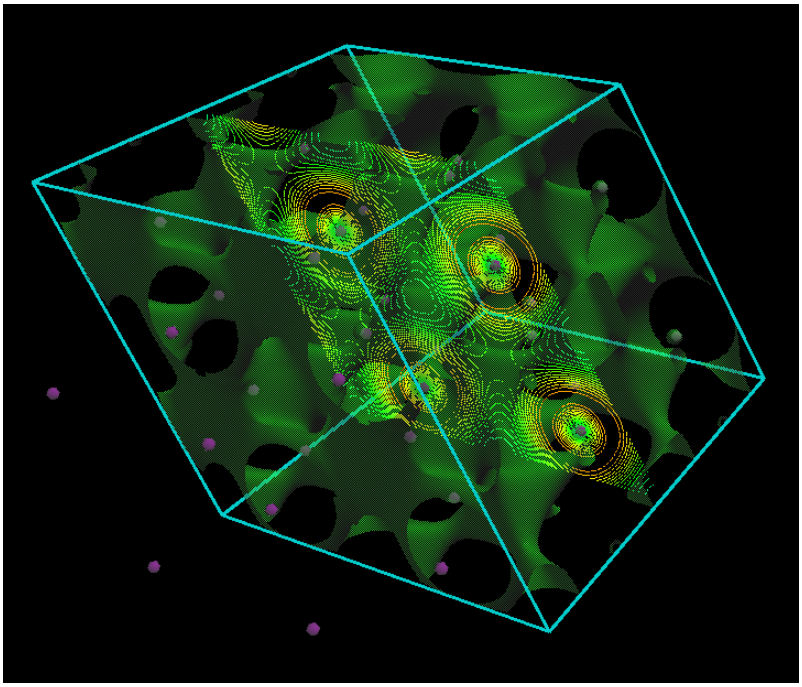


Fig3.67 Example of isolines

Set **Type** to **Fringe**, **Color Min** to 1e-3. Since the way to add colors to the section and the isosurface is same, color of them is the same.

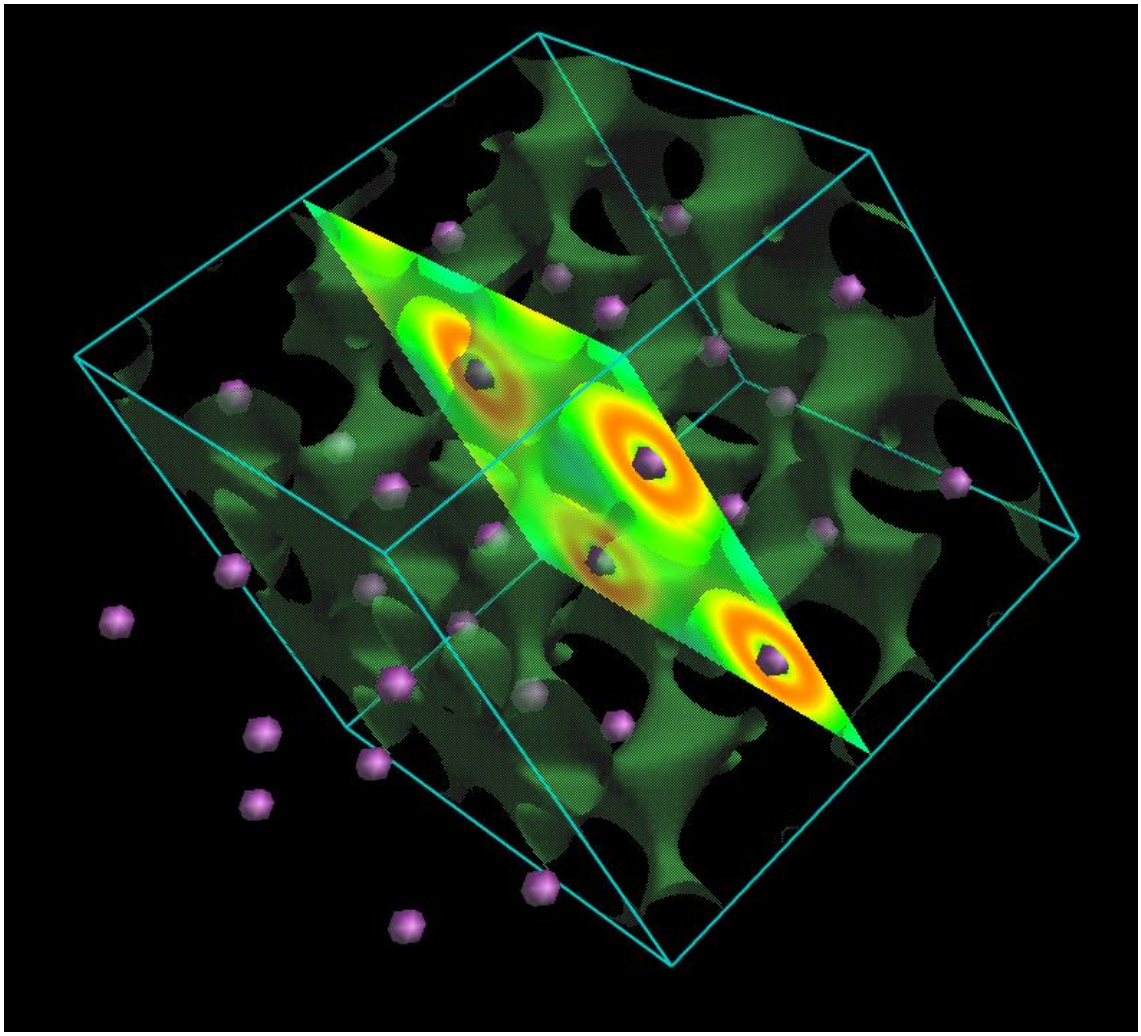


Fig3.68 Example of isosurface colored by minimum and maximum value

3.8.4. Display bond

By selecting **[Preference]-[Set Preference]**, pop up a dialog box to specify preference. Set **Scale** of Connect Atom to 1.1, select **Covalent** , set resolution of balls to 16. By clicking **Apply** button, atom bonds appear and the atom rendering is smooth.

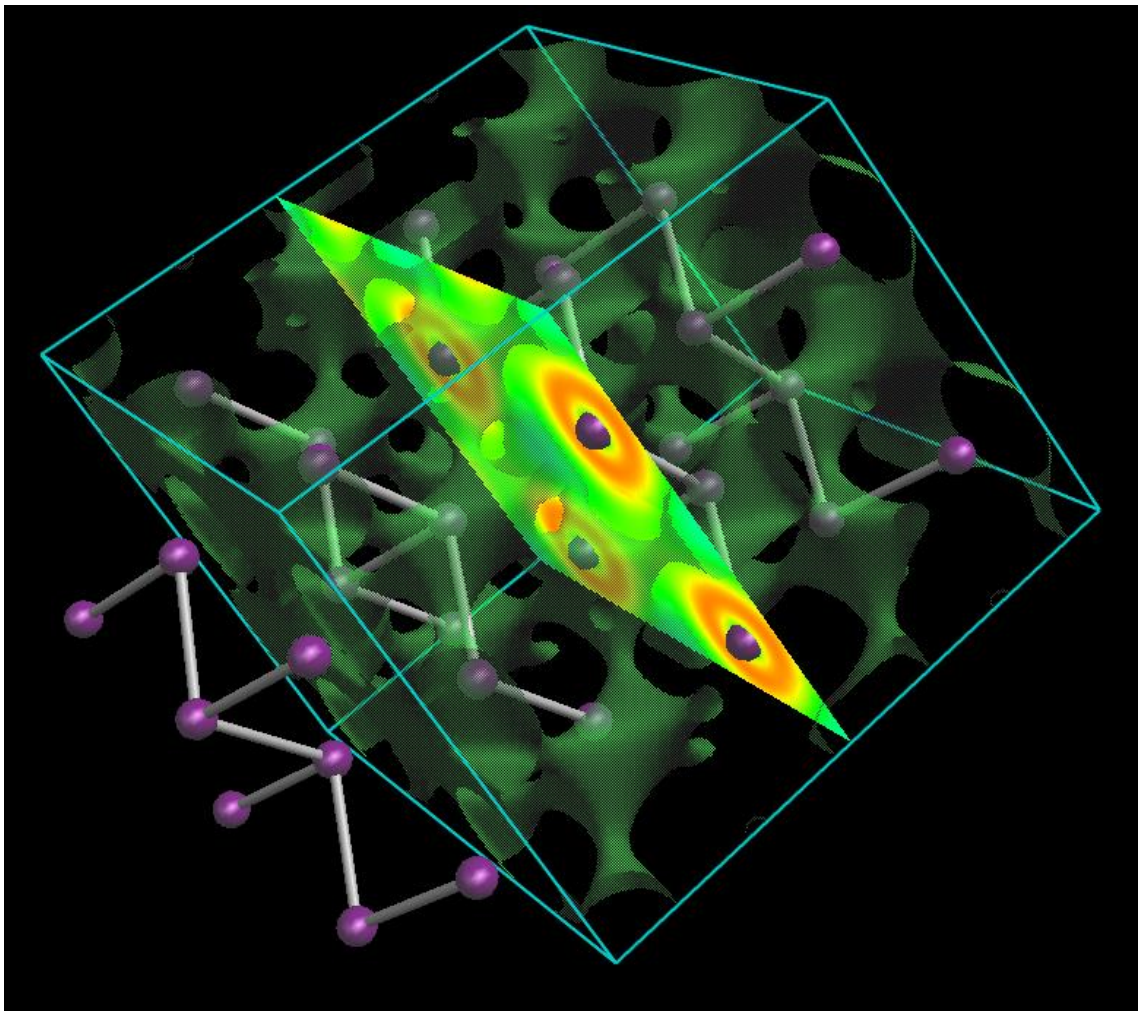


Fig3.69 Change connect scale and ball resolution

3.9. Example of CHPI

CHPI[27] is developed by Dr. Umezawa(Microbial Chemistry Research Center)、Dr. Nishio(CHPI Institute) and Microbial Chemistry Research Foundation. If you write a paper by using this function, please describe to refer No.27. BioStationViewer supports to edit parameters, execute program and display result. Please refer the book "The CH/π Interaction" about detail of CH/π Intereaction.

At first load PDB file, and select **Tool→CHPI** then popup CHPI Dialog.

If you use default parameters, just clicking the "**Execute CHPI Program**" button, to execute the program and display result. Explain parameters as below.

3.9.1. Method for exploring XH/π contacts

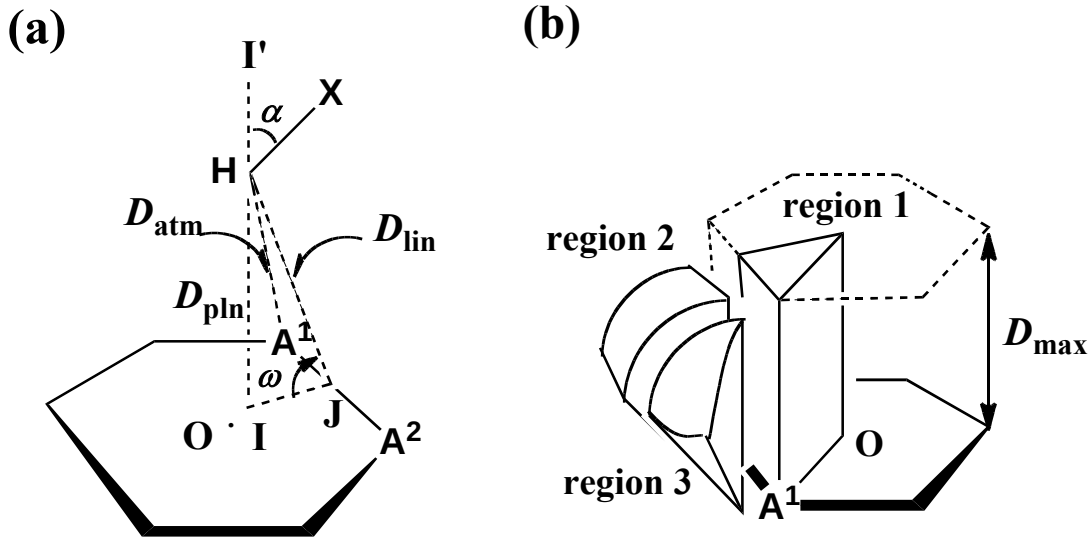


Fig3.70 Method for exploring XH/π contacts

Method for exploring XH/π contacts (the six-membered aromatic ring is shown as an illustrative example). (a) O: centre of the π-plane. A^1 and A^2: nearest and second nearest sp^2-atoms, respectively, to the hydrogen H. ω: dihedral angle defined by A^1OA^2 and HA^1A^2 planes. α: X-H-I' angle. D_{pln}: perpendicular distance between H and the π-plane (H/I). D_{atm}: HA^1 distance. D_{lin}: distance between H and the line A^1-A^2 (H/J). (b) Regions to be searched. Region 1: zone where H is above the ring. Regions 2 and 3: zones where H is out of region 1 but may interact with the π-ring. Unless otherwise noted, the program was run to search for short H/π contacts with the following conditions: D_{max} = 3.05 Å; $D_{pln} < D_{max}$ (region 1); $D_{lin} < D_{max}$ (region 2); $D_{atm} < D_{max}$ (region 3); ω_{max} = 127.5°, $-\omega_{max} < \omega < \omega_{max}$; α < 63°. D_{hpi}: H/π distance (D_{pln} for region 1, D_{lin} for region 2, D_{atm} for region 3).

3.9.2. Edit parameter

The dialog is shown in Fig3.71. Specify input parameters.

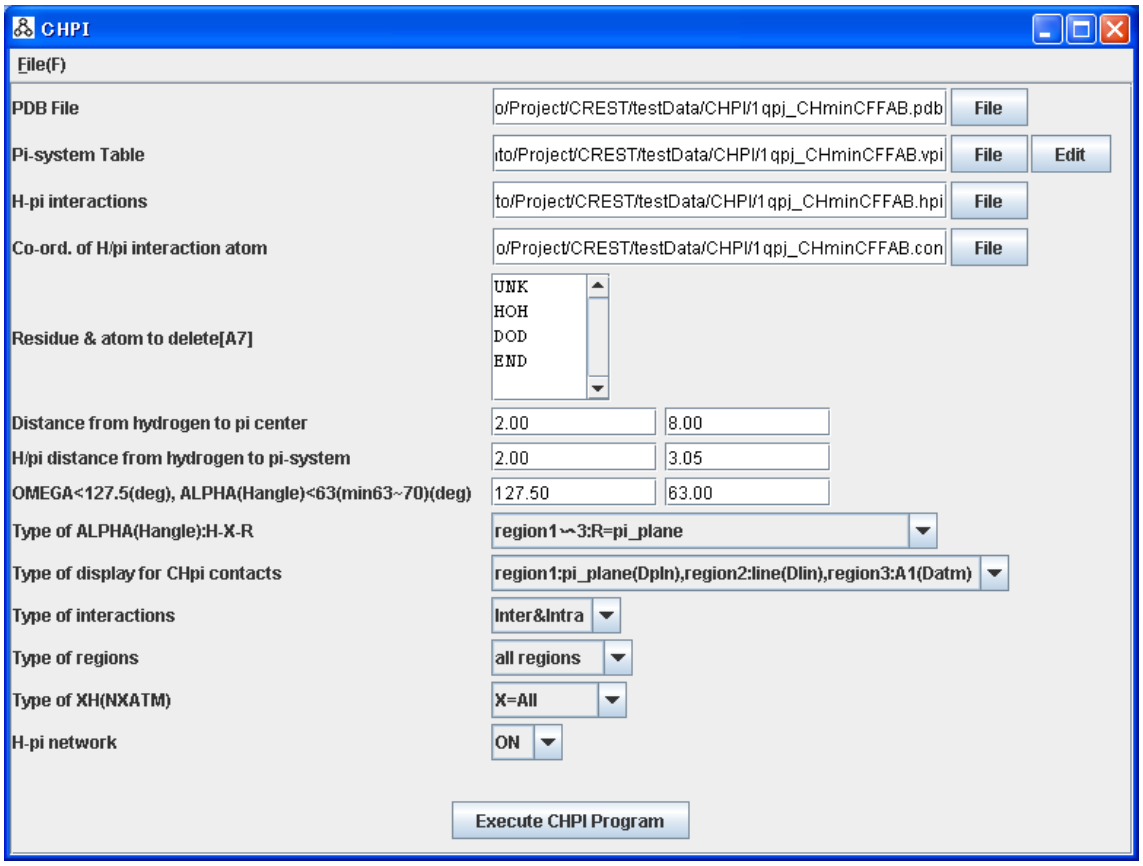


Fig3.71 Input parameter dialog

It explains the behavior of File menu.

1) **Open**

   Open parameter file and those parameters is set in GUI. The file that specified at Pi-system loaded and set PI Information tab.

2) **Save**

   Save parameters.

3) **Set Default Value**

   Set default value. PDB File set displayed file at 3D view. **Pi-system Table** is set as "PDB filename.vpi", and if this file exists load this file as PI Information. If this file dose not exist, default value is set.

4) **Close**

   Close the dialog.

It explains input parameters.

1) **PDB File**

   Specify the PDB file to be analyzed.

2) **Pi-system Table**

   Specify the PI information file. By clicking the **Edit** button, PI Information dialog is popup.

3) **H/pi interactions**

   Specify the output file.

4) **Co-ord. of H/pi interaction atom**

   Specify the coordinate file.

5) **Residue & atom to delete[A7]**

   Specify the atom and residue name that dose not analyzed. Please input "END" at last line.

6) **Distance from hydrogen to pi center**

   Specify the range of distance(D_{cent}) from H and center of the ring(O). Please do not change usually.

7) **H/pi distance from hydrogen to pi-system**

   Specify the range of region1(D_{max})

8) **OMEGA<127.5(deg), ALPHA(Hangle)<63(min63~90)(deg)**

   Specify ω and α. Please do not change usually.

9) **Type of ALPHA(Hangle):H-X-R**

   Specify the H-X-R angle [R=pi_plane, line(A^1-A^2), A^1(closest pi_atom)]. Defilt is a).

   a) region1~3: R=pi_plane All region use H-X-pi_plane (= α)

   b) region1: R=pi_plane,region2:R=line,region3: R=A^1

   c) region1~3:R=A^1 use `H-X-A`^{1} `for all region.`

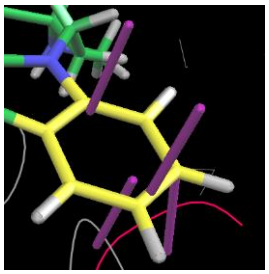
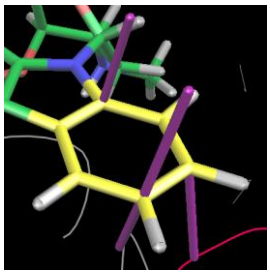
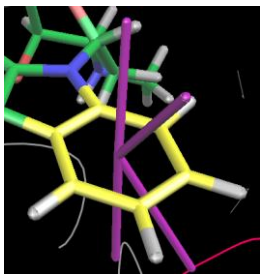
10) **Type of display for CHpi contacts**

   Specify contact coordinate on pi plane

   a) region1: pi_plane (Dpln), region2: line (Dlin), region3: A^1 (Datm)

   b) region1~3: A^1 (Datm)

   c) region1~3: O (Dcent)

a)  b)  c) 

11) **Type of interactions**

Specify type of interactions. The distinction of inter/intra is distinguished in chain ID of the PDB file.

12) **Type of regions**

Specify type of regions.

13) **Type of XH(NXATM)**

Specify the atom.

14) **H-pi network**

Specify output H-pi network on/off

15) **Execute CHPI Program**

Execute CHPI program by clicking this button.

3.9.3. Edit PI Information file

Cliking the button of **Edit** at **Pi-system Table,** the dialog is popuped. It is shown in Fig3.72.

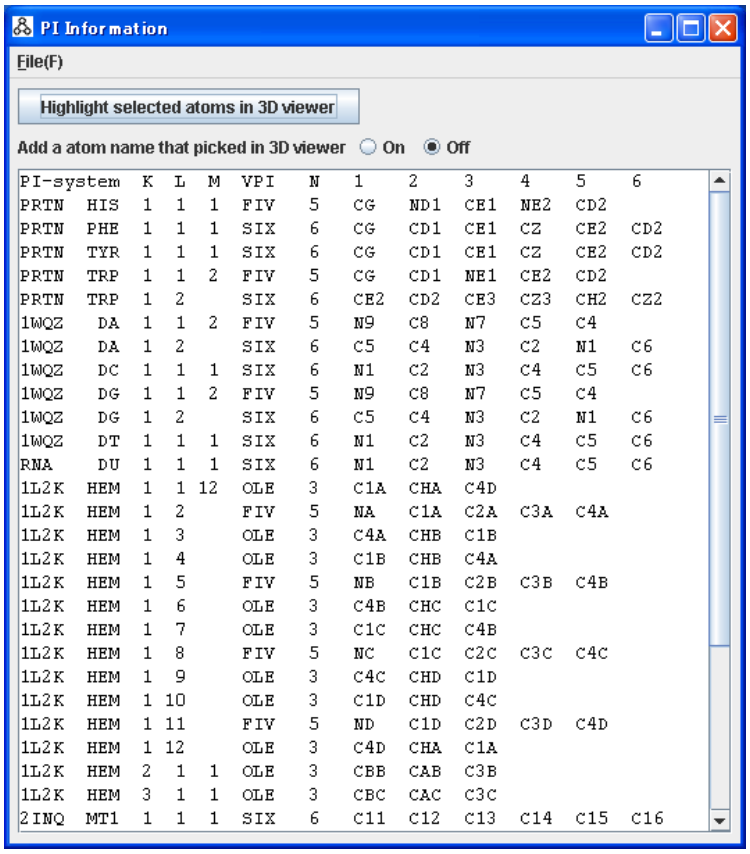


Fig3.72 PI Information panel

The file format

- ID unique name
- Residue name Specify residue name that are in PDB.
- K Specify the component number in residue.
- L Specify the serial number in one component .
- M Specify number of ring element in component at first line only .
- VPI Specify FIV/SIX/OLE
- N Specify number of atom in ring element.
- 1-6 Specify atom name in ring element.

The example of editing PI information is shown.

Clicking the suitable atom(C18) in 3D view and select **Tool→Display Residue in Distance**. Specify 10Å at the dialog. Select **Tool→Set Rotation Center**(Fig3.73). So displayed around C18 and set center of spinning.

Clicking STU at Tree view by right button on mouse, popup the display attribute dialog. Specify **Color**(Atom) and **Model**(Stick). (Fig3.74)

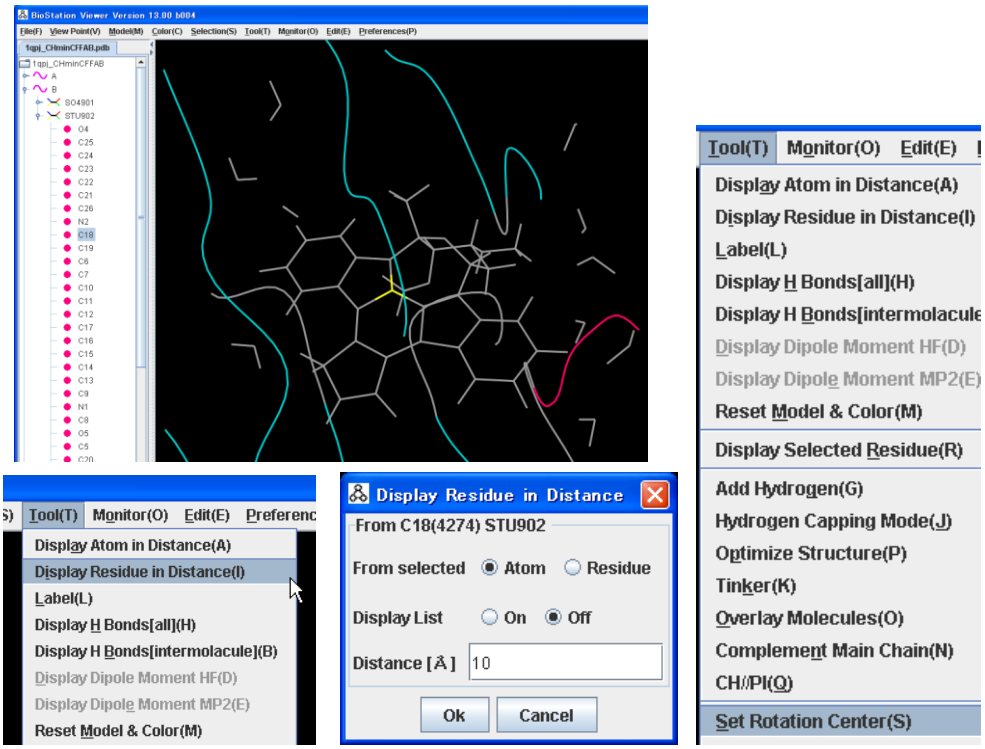


Fig3.73 Select "Display Residue in Distance" and "Set Rotation Center"

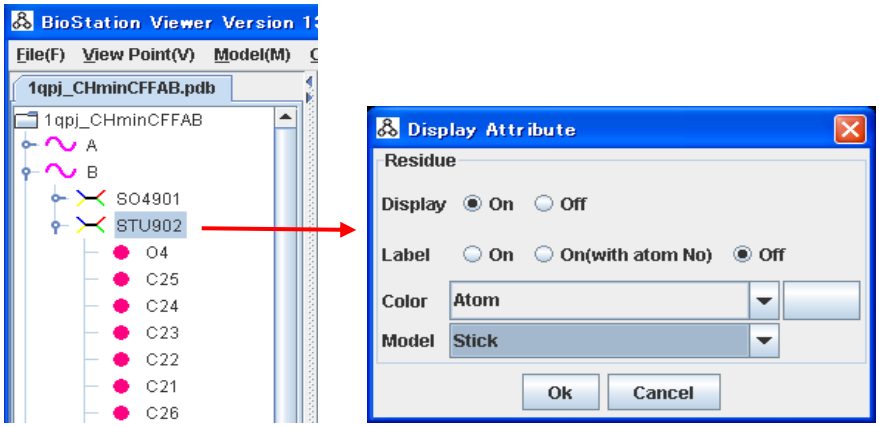
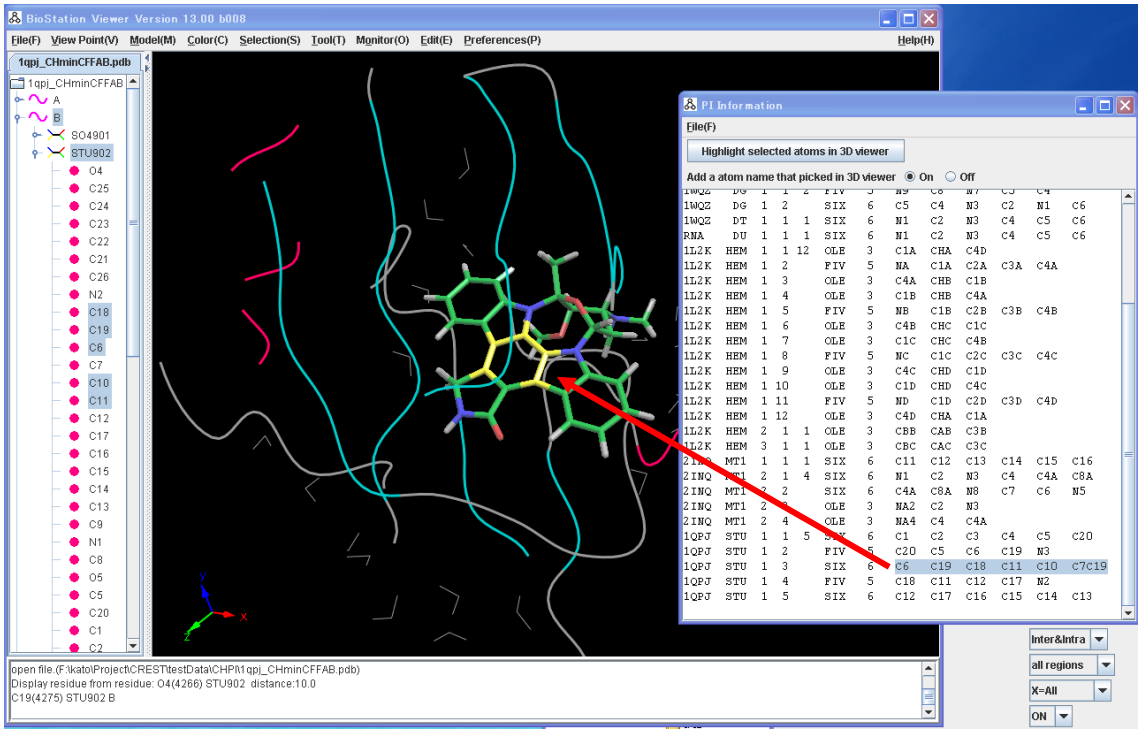


Fig3.74 Set Model and Color of STU by clicking right button of mouse

It explains the behavior of each button.

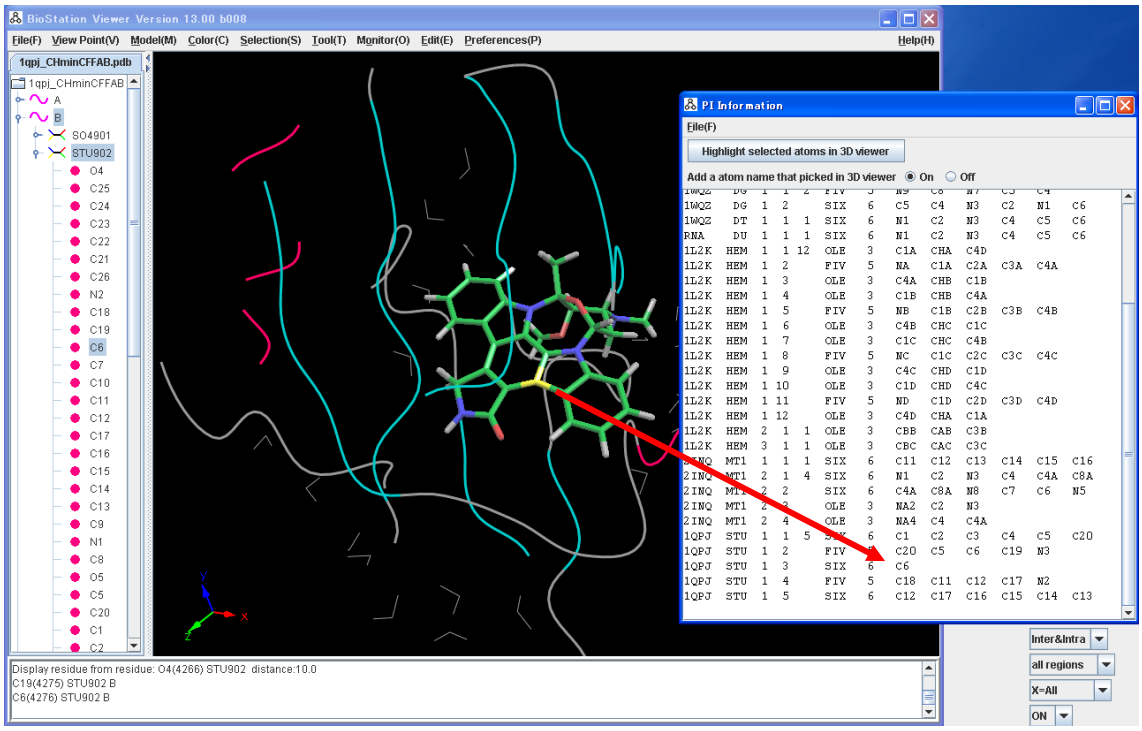
1) **Highlight selected atoms in 3D viewer**

The selected Atoms in 3d viewer is shown highlighted.



2) **Add a atom name that picked in 3D viewer**

If you select “On”, insert atom name at cursor position.



Explain the File Menu.

1) **Open**

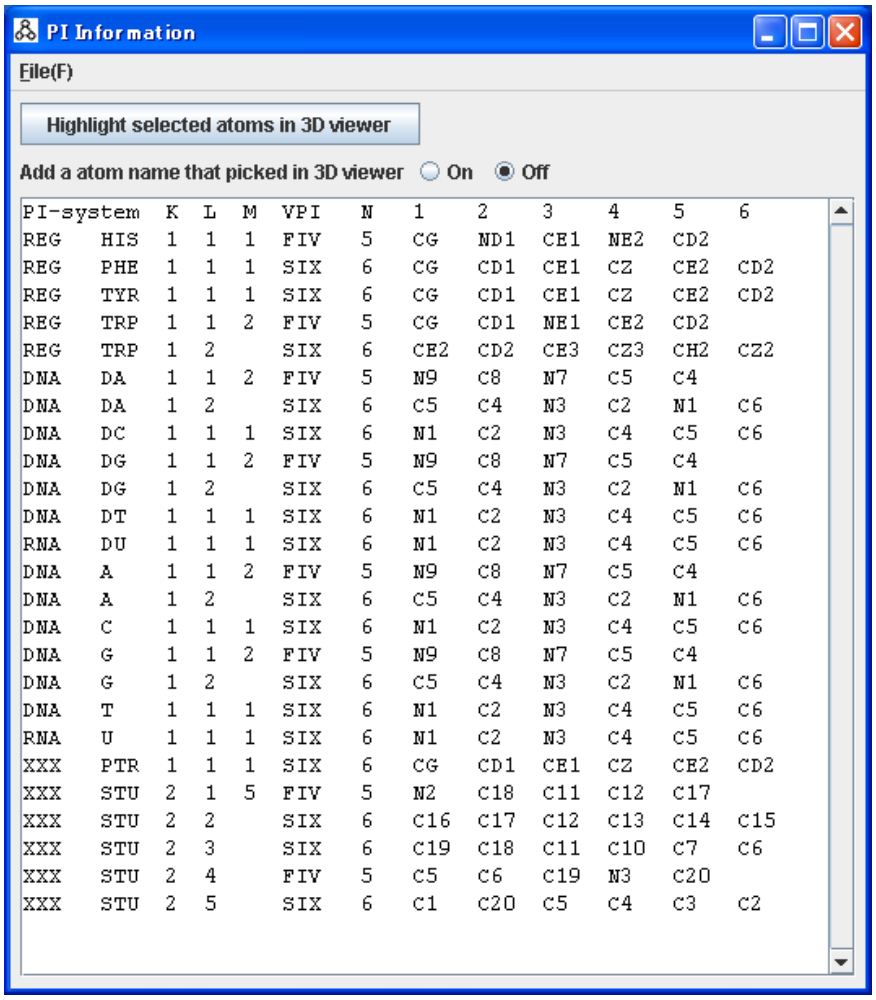
   Open PI Information file and those parameters is set in GUI.

2) **Save**

   Save PI Information.

3) **Set Default Value**

   Set default value. Information on the fixed form on amino acid, DNA, and RNA is set. Besides, it is set recognizing the ring of the part of HEM of the PDB file specified with PDB File at Input Data tab. ID is set as XXX. It is generated one element from some rings. The user can edit it. The example of 1qpj_CHminCFFAB.pdb is shown below.



PI-system	K	L	M	VPI	N	1	2	3	4	5	6
REG HIS	1	1	1	FIV	5	CG	ND1	CE1	NE2	CD2	
REG PHE	1	1	1	SIX	6	CG	CD1	CE1	CZ	CE2	CD2
REG TYR	1	1	1	SIX	6	CG	CD1	CE1	CZ	CE2	CD2
REG TRP	1	1	2	FIV	5	CG	CD1	NE1	CE2	CD2	
REG TRP	1	2		SIX	6	CE2	CD2	CE3	CZ3	CH2	CZ2
DNA DA	1	1	2	FIV	5	N9	C8	N7	C5	C4	
DNA DA	1	2		SIX	6	C5	C4	N3	C2	N1	C6
DNA DC	1	1	1	SIX	6	N1	C2	N3	C4	C5	C6
DNA DG	1	1	2	FIV	5	N9	C8	N7	C5	C4	
DNA DG	1	2		SIX	6	C5	C4	N3	C2	N1	C6
DNA DT	1	1	1	SIX	6	N1	C2	N3	C4	C5	C6
RNA DU	1	1	1	SIX	6	N1	C2	N3	C4	C5	C6
DNA A	1	1	2	FIV	5	N9	C8	N7	C5	C4	
DNA A	1	2		SIX	6	C5	C4	N3	C2	N1	C6
DNA C	1	1	1	SIX	6	N1	C2	N3	C4	C5	C6
DNA G	1	1	2	FIV	5	N9	C8	N7	C5	C4	
DNA G	1	2		SIX	6	C5	C4	N3	C2	N1	C6
DNA T	1	1	1	SIX	6	N1	C2	N3	C4	C5	C6
RNA U	1	1	1	SIX	6	N1	C2	N3	C4	C5	C6
XXX PTR	1	1	1	SIX	6	CG	CD1	CE1	CZ	CE2	CD2
XXX STU	2	1	5	FIV	5	N2	C18	C11	C12	C17	
XXX STU	2	2		SIX	6	C16	C17	C12	C13	C14	C15
XXX STU	2	3		SIX	6	C19	C18	C11	C10	C7	C6
XXX STU	2	4		FIV	5	C5	C6	C19	N3	C20	
XXX STU	2	5		SIX	6	C1	C20	C5	C4	C3	C2

Fig3.75 Default PI information of 1qpj_CHminCFFAB.pdb

4) **Close**

   Close this dialog.

3.9.4. Execute program

Clicking by the "**Execute CHPI Program**" button, then to start to execute CHPI program at Command Prompt. The Execute log is shown in it.

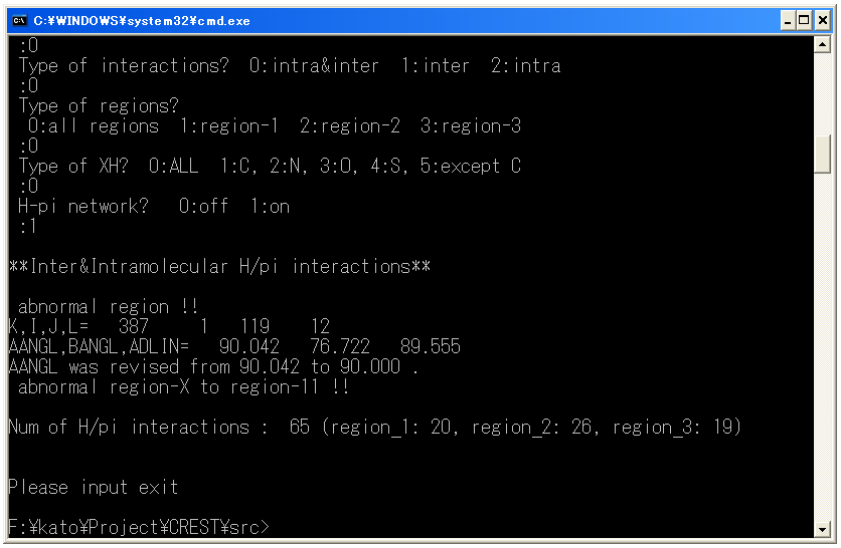


Fig3.76 Command prompt of CHPI execution

When end the program, to close the command prompt. Then result is displayed in 3D view. One interaction is named as CHPIn(n:serial number), By clicking CHPI on 3D view, then display distance of this interaction at message area. The example is shown in Fig3.77, Fig3.78 and Fig3.79.

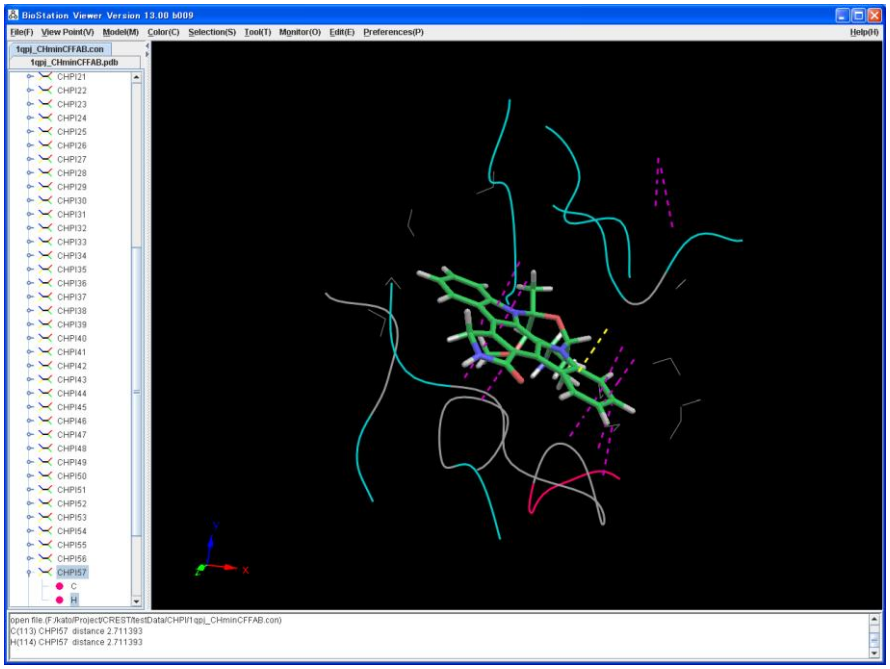


Fig3.77 Result of CHPI(Click CHPI75)

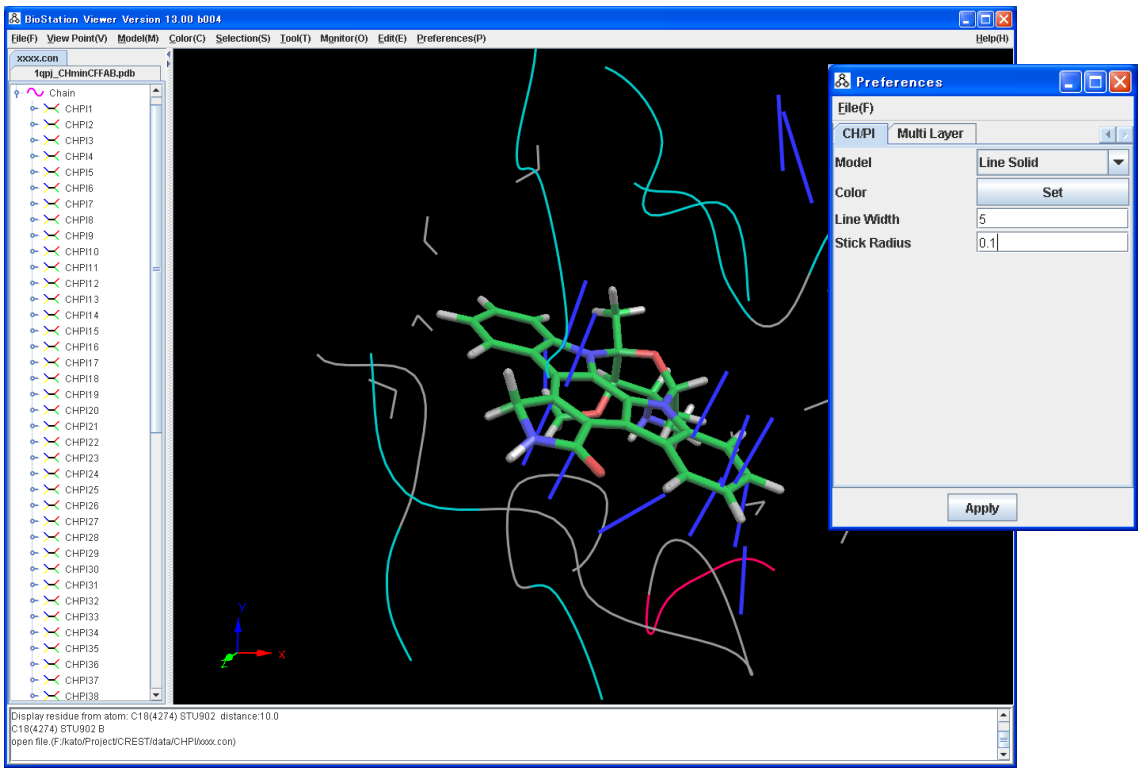


Fig3.78 Change preference (Model : Line Solid, Color : blur)

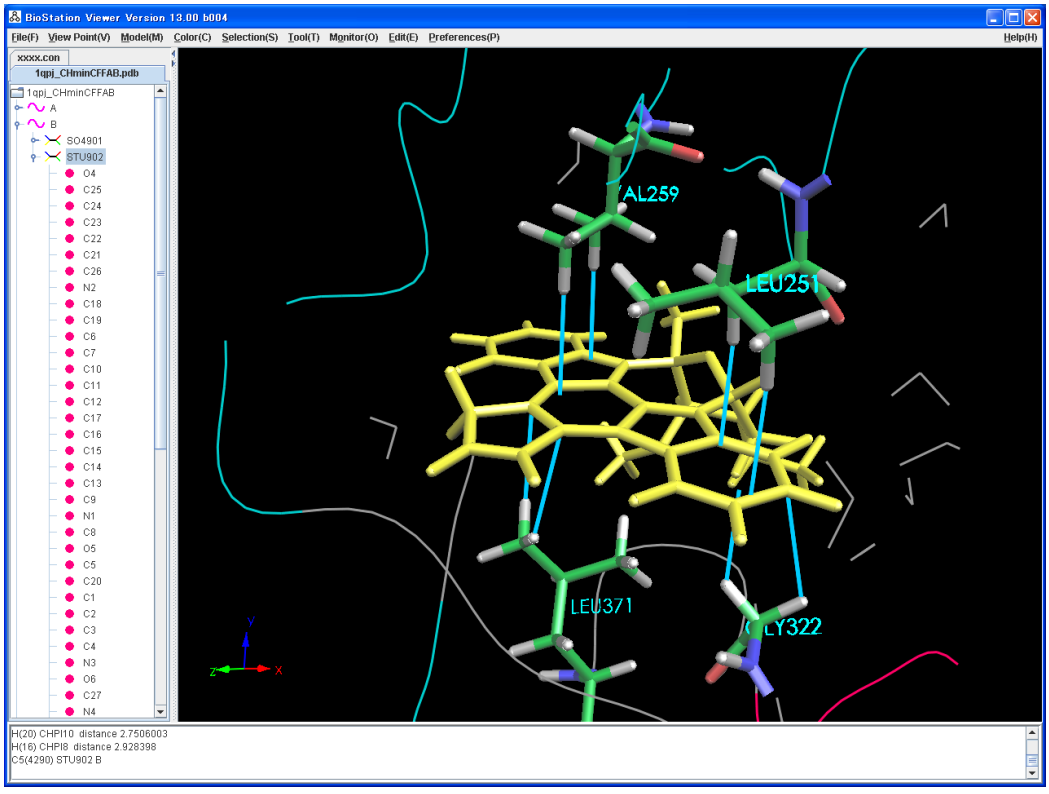


Fig3.79 The residue that is around the ligand displayed by Stick Model.

4 Tutorials

4.1 Intermolecular Interactions in (Gly)10

This section reports a example of (Gly)10 IFIE analysis. The fragmentation is 1 fragment / 1 residue. Calculations were performed at the FMO-HF level with STO-3G.

4.1.1. Modeling

Start the viewer and select File→Molda then popup Molda window. By Selecting Model →input→Peptide, popup Peptide Dialog. Type in "g"(short name of Glycin) ten times and click "OK" button so structure of (gly)10 is displayed on Molda window. The input dialog is shown in Fig4.1.

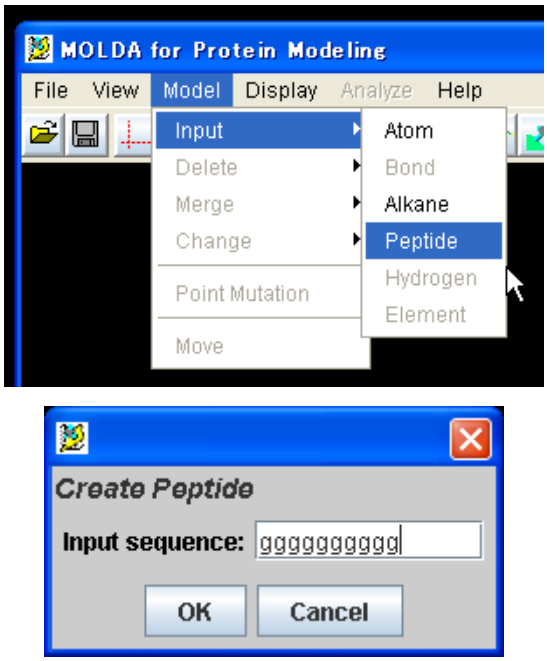
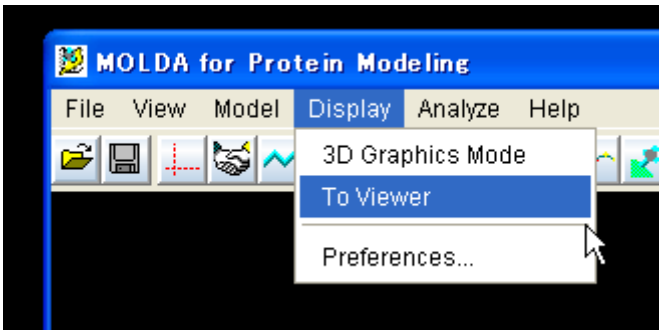


Fig4.1 Peptide dialog

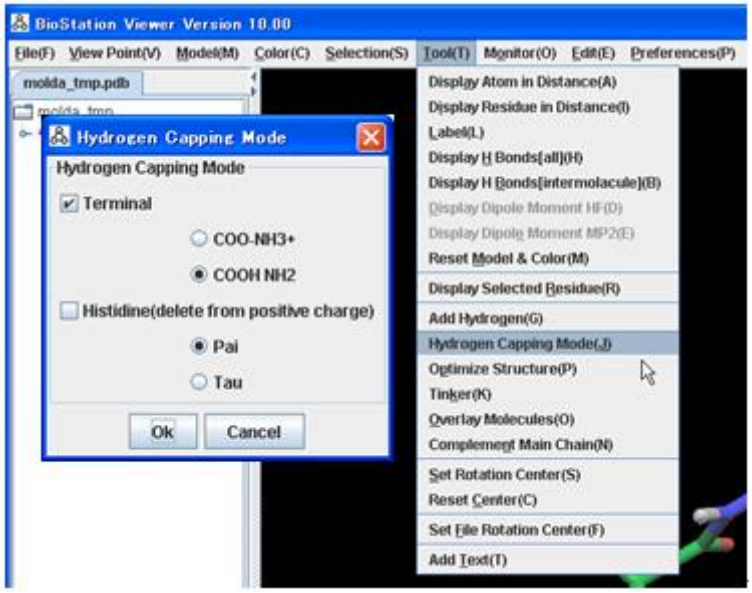
And select menu File→Display→To Viewer to copy this structure to viewer. It is displayed to Viewer by the file name of molda_tmp.pdb.



4.1.2. Structure Optimization

There is this file in a current folder that starts Viewer. Change file name to gly10.pdb, close molda_tmp.pdb on main window by selecting menu File→Close File and load gly10.pdb by selecting menu File→Open.

Select Tool→Hydrogen Capping Mode, mark Terminal and COOH NH2 on dialog as Hydrogen Capping Mode, then click the OK Button.



Specify Hydrogen Capping Mode

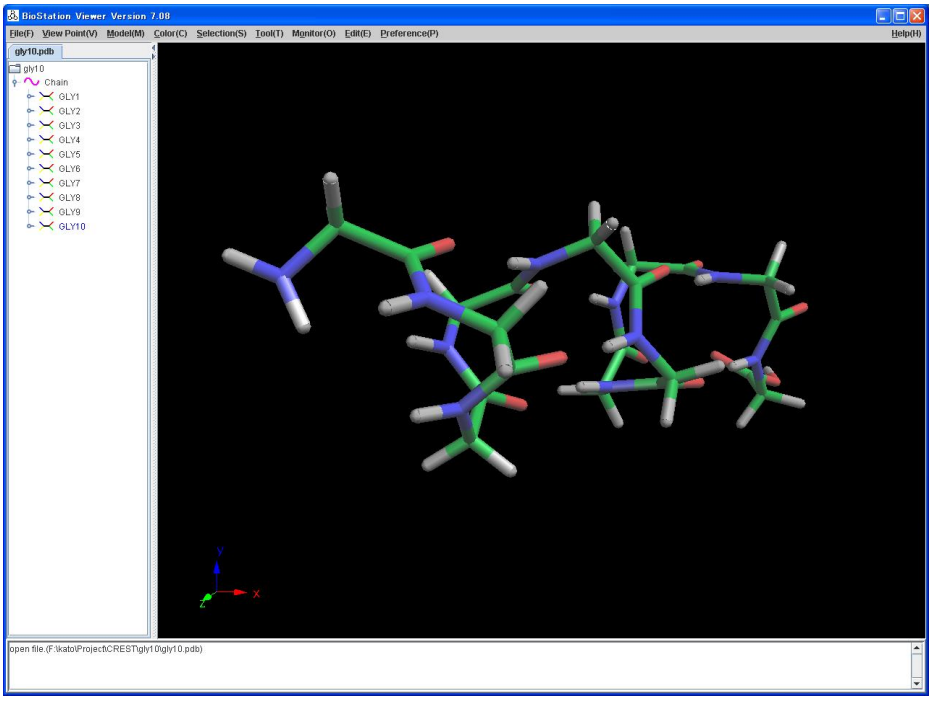


Fig4.2 Structure Gly10 after hydrogen capping

By selecting menu Tool→Optimize structure then popup the structure optimize dialog(Fig4.3). Specify three file names, Hydrogen Options, Optimize Options and input file name.

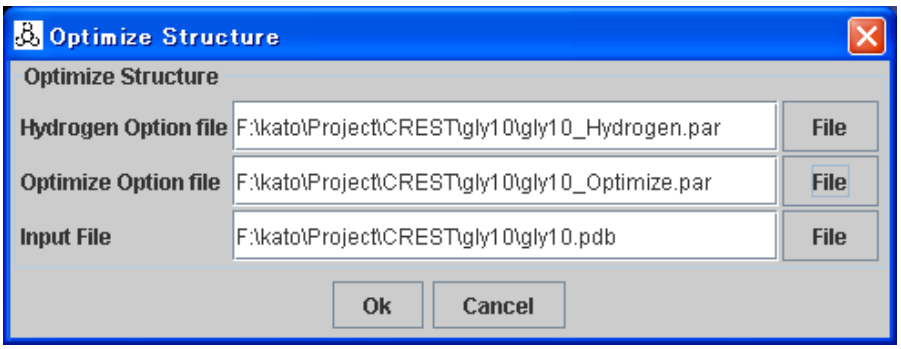


Fig4.3 Structure Optimize dialog

By clicking the OK button, execute structure optimize and display result structure on main window. The result file name is gly10_H_opt.pdb, it is added _H_opt on input file name. The options are shown below. Please refer section 5 about the detail of options. The methodology of optimize is an eXtended Universal Force Field Universal Force Field (XUFF). This is our own program.

gly10_Hydrogen.par

```
-B
-R
```

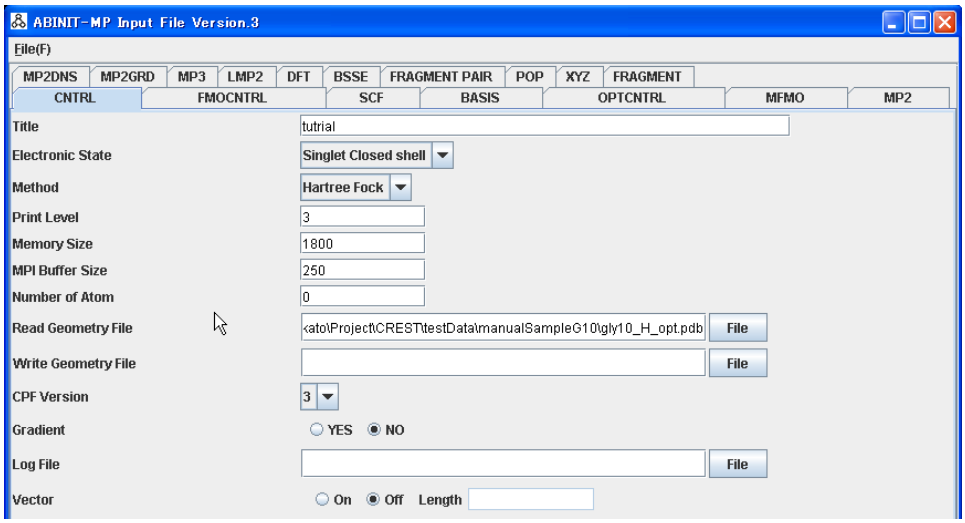
gly_Optimize.par

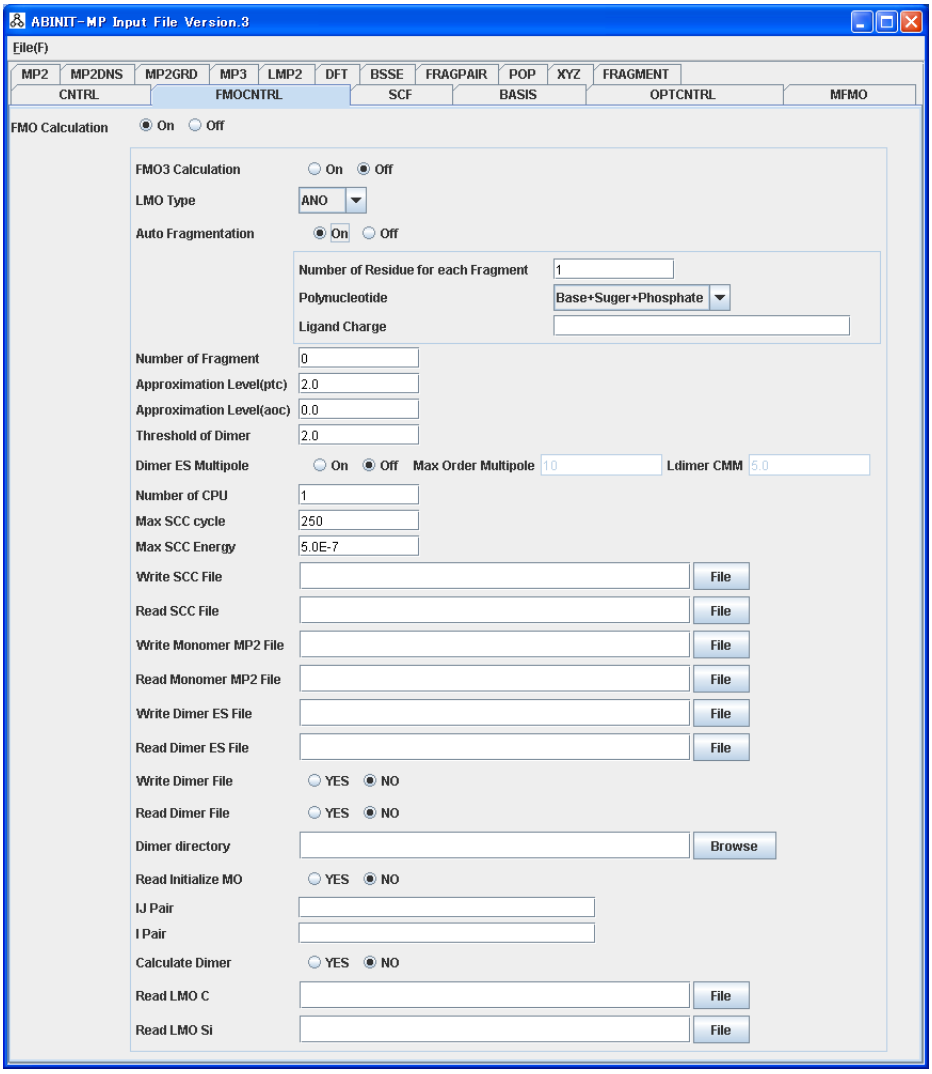
```
-O
-h
OPTIMIZATION 100
SDLOOP 100
MAXLOOP 500
SDGRADIENT 1000.0.
CGGRADIENT 0.1
RGRADIENT 0.1
RENERGY 0.0001
```

4.1.3. Calculation

By Selecting menu **[File]→[Edit ABINIT-MP Input File]** then popup the parameters for input file window. Input parameters, save a input file and execute ABINIT-MP by using this file.

Please modify Read Geometory File and Write Geometory to real file names on execution machine. The parameters are show in below.





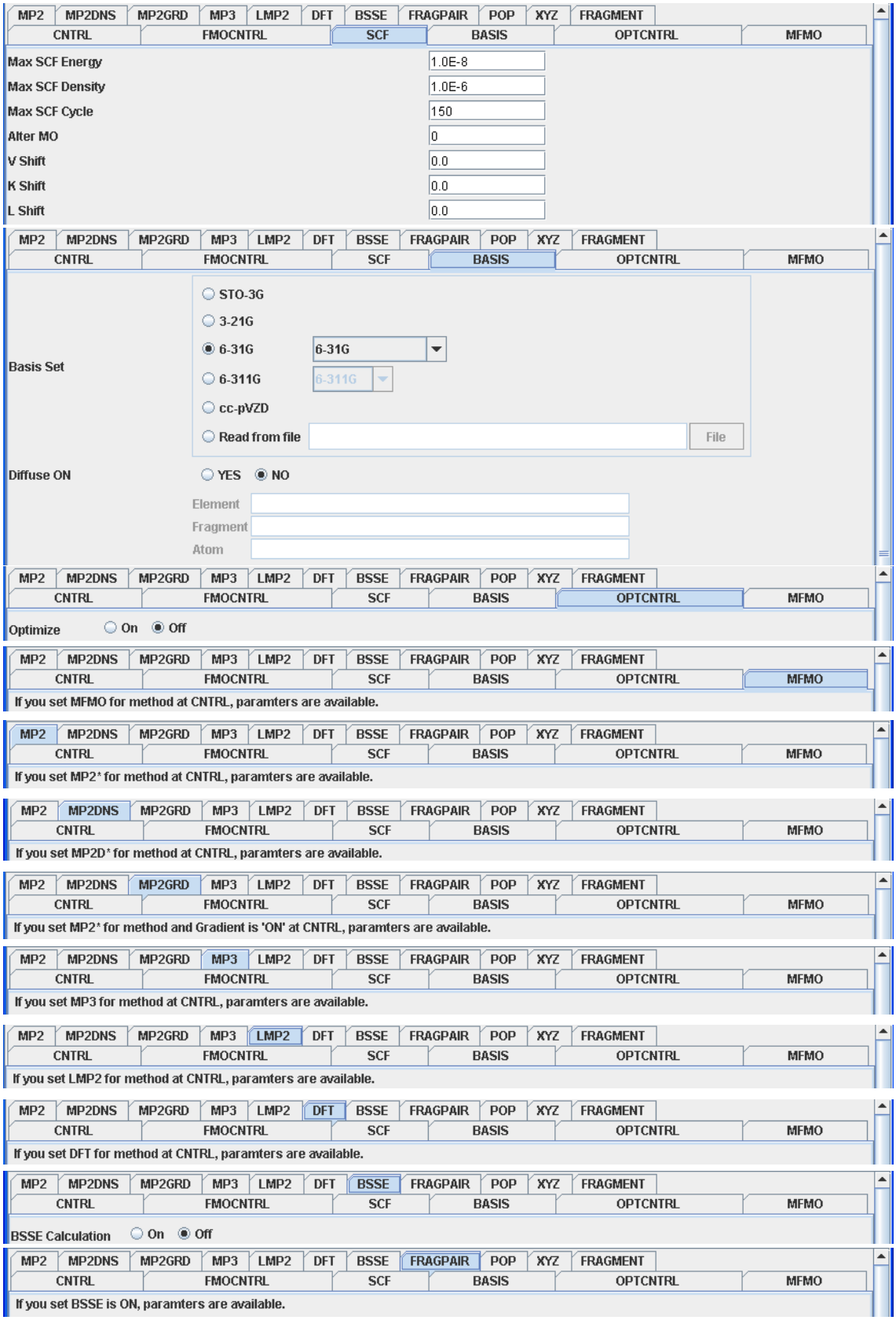

MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
Max SCF Energy 1.0E-8
Max SCF Density 1.0E-6
Max SCF Cycle 150
Alter MO 0
V Shift 0.0
K Shift 0.0
L Shift 0.0
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
Basis Set
STO-3G
3-21G
6-31G 6-31G
6-311G 6-311G
cc-pVZD
Read from file File
Diffuse ON YES NO
Element
Fragment
Atom
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
Optimize On Off
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
If you set MFMO for method at CNTRL, paramters are available.
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
If you set MP2* for method at CNTRL, paramters are available.
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
If you set MP2D* for method at CNTRL, paramters are available.
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
If you set MP2* for method and Gradient is 'ON' at CNTRL, paramters are available.
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
If you set MP3 for method at CNTRL, paramters are available.
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
If you set LMP2 for method at CNTRL, paramters are available.
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
If you set DFT for method at CNTRL, paramters are available.
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
BSSE Calculation On Off
MP2 MP2DNS MP2GRD MP3 LMP2 DFT BSSE FRAGPAIR POP XYZ FRAGMENT
CNTRL FMOCNTRL SCF BASIS OPTCNTRL MFMO
If you set BSSE is ON, paramters are available.

Fig4.4　Parameters

4.1.4.　Result

We show 2 case results.

1) Molecular structure is optimized by XUFF(apply to Hydrogen atoms)
2) No optimized structure. It is just modeling by Molda.

The hydrogen bond appears every 3 fragments in α-Helix, so it shows IFIE is stable reaction between the fragmentations n^{th} and $n+3^{th}$. When you compare with two results, they show more stabilized (approximately 0.4 kcal/mol)) by optimizing for the hydrogen atoms at hydrogen bond.

(1) Result 1：Molecular structure is optimized by XUFF(apply to Hydrogen atoms)

Total energy

```
=========================
   ## FMO TOTAL ENERGY
=========================
      Nuclear repulsion =      5342.1817591836
      Electronic energy =     -7458.3751057039
      Total      energy =     -2116.1933465204
```

IFIE

Table 4.1　IFIE：molecular structure is optimized by XUFF (FMO-HF/STO-3G)

	Gly1	Gly2	Gly3	Gly4	Gly5	Gly6	Gly7	Gly8
Gly1								
Gly2								
Gly3	0.72							
Gly4	**0.46**	1.44						
Gly5	0.81	**−4.66**	1.85					
Gly6	0.61	−2.48	**−4.85**	1.95				
Gly7	0.24	−0.24	−2.40	**−4.73**	1.75			
Gly8	0.14	−0.16	−0.21	−2.39	**−4.72**	1.92		
Gly9	0.11	−0.26	−0.16	−0.22	−2.47	**−4.94**	1.84	
Gly10	0.10	−0.23	−0.41	−0.23	0.00	−2.54	**−7.71**	5.15

(2) Result 2 : No optimized structure

Total energy

```
========================
   ## FMO TOTAL ENERGY
========================
      Nuclear repulsion =      5352.4874175133
      Electronic energy =     -7468.6560823049
      Total      energy =     -2116.1686647916
```

(IFIE)

Table 4.2 IFIE : No optimized structure (MO-HF/STO-3G)

	Gly1	Gly2	Gly3	Gly4	Gly5	Gly6	Gly7	Gly8
Gly1								
Gly2								
Gly3	1.77							
Gly4	**0.77**	1.53						
Gly5	0.54	**−4.27**	1.47					
Gly6	0.55	−2.46	**−4.43**	1.56				
Gly7	0.27	−0.27	−2.41	**−4.34**	1.48			
Gly8	0.15	−0.17	−0.25	−2.41	**−4.29**	1.64		
Gly9	0.08	−0.25	−0.17	−0.26	−2.49	**−4.47**	1.57	
Gly10	0.10	−0.23	−0.40	−0.24	−0.01	−2.55	**−7.30**	5.04

5 Super molecule

This section describes that the formula of supermolecule calculation.

In case of the supermolecule calculation by FMO Method, the Complex Fragmentation simply consist of protein and ligand.(C:Complex P:Protein L:Ligand → C= P∪L). Each energy described to Complex total energy : E^C、Protein total energy : E^P、Ligand Protein total energy : E^L. The Interaction Energy between protein and ligand: Δ E was given by

$$\Delta E = E^C - (E^P + E^L) \qquad \text{(exp 5.1)}$$

Supposing E^C, E^P, E^L were calculated by FMO2, Δ E was given by

$$\begin{aligned}\Delta E &= E^C - (E^P + E^L) \\ &= \sum_{\substack{I \\ I \in C}} E'^C_I + \sum_{\substack{I>J \\ I,J \in C}} \Delta\tilde{E}^C_{IJ} - \left(\sum_{\substack{I \\ I \in P}} E'^P_I + \sum_{\substack{I>J \\ I,J \in P}} \Delta\tilde{E}^P_{IJ} + \sum_{\substack{I \\ I \in L}} E'^L_I + \sum_{\substack{I>J \\ I,J \in L}} \Delta\tilde{E}^L_{IJ} \right)\end{aligned}$$

(exp 5.2)

(E': Monomer energy excluding contribution from environmental electrostatic potential, $\Delta\tilde{E}_{IJ}$: Inter-fragment interaction energy) If E^C is decomposed into the term that inner protein, inner lgand and intermolecule protein-ligand,

$$E^C = \sum_{\substack{I \\ I \in P}} E'^C_I + \sum_{\substack{I>J \\ I,J \in P}} \Delta\tilde{E}^C_{IJ} + \sum_{\substack{I \\ I \in L}} E'^C_I + \sum_{\substack{I>J \\ I,J \in L}} \Delta\tilde{E}^C_{IJ} + \sum_{\substack{I \\ I \in P}} \sum_{\substack{J \\ J \in L}} \Delta\tilde{E}^C_{IJ} \qquad \text{(exp 5.3)}$$

and pack terms of protein and ligand.

$$\begin{aligned}\Delta E'_I &= E'^C_I - E'^P_I \qquad I \in P \\ &= E'^C_I - E'^L_I \qquad I \in L\end{aligned} \qquad \text{(exp 5.4)}$$

$\Delta\Delta\tilde{E}_{IJ}$ is calcutated as bellow,

$$\begin{aligned}\Delta\Delta\tilde{E}_{IJ} &= \Delta\tilde{E}^C_{IJ} - \Delta\tilde{E}^P_{IJ} \qquad I,J \in P \\ &= \Delta\tilde{E}^C_{IJ} - \Delta\tilde{E}^L_{IJ} \qquad I,J \in L\end{aligned} \qquad \text{(exp 5.5)}$$

Δ E is given by

$$\Delta E = \left(\sum_{\substack{I \\ I \in P}} \Delta E'_I + \sum_{\substack{I>J \\ I,J \in P}} \Delta\Delta\tilde{E}_{IJ} \right) + \left(\sum_{\substack{I \\ I \in L}} \Delta E'_I + \sum_{\substack{I>J \\ I,J \in L}} \Delta\Delta\tilde{E}_{IJ} \right) + \sum_{\substack{I \\ I \in P}} \sum_{\substack{J \\ J \in L}} \Delta\tilde{E}^C_{IJ} \qquad \text{(exp 5.6)}$$

The first term is stabilization energy by electronic relaxation of protein that given by binding protein and ligand. The second term is stabilization energy by electronic relaxation of ligand. The third term is IFIE of between protein and ligand.

In Viewer, read each CPFs(complex, protein and ligand), and specified corresponding fragmentation number in that.

Next describes the concrete calculation method which calculates super molecule value from IFIE and momomer value.

1) Step1 calculation of $\Delta E'_I$

Subtract complex from protein and ligand at monomer value.

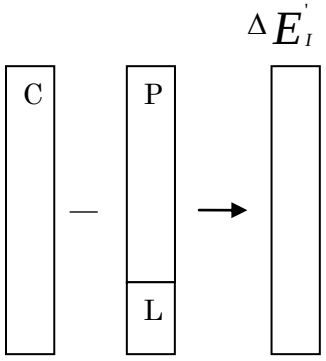


図 5.1 Memory image of $\Delta E'_{IJ}$

2) Step2 calculation of $\Delta\Delta\tilde{E}_{IJ}$

Subtract complex from protein and ligand at IFIE

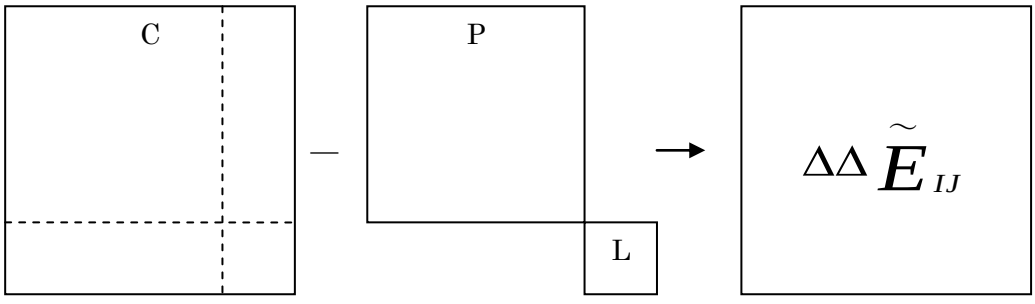


図 5.2 Memory image of $\Delta\Delta\tilde{E}_{IJ}$

3) Step3　calculation of Supermolecule IFIE $\Delta\tilde{E}_{IJ}^{C'}$

Calculate Supermolecule IFIE using Step1 and Step2 results.

Protein　: $\Delta E_I'' = \Delta E_I' + \frac{1}{2}\sum_{\substack{K\neq I \\ K\in P}} \Delta\Delta\tilde{E}_{IK}$　　(exp 5.7)

Logand　: $\Delta E_J'' = \Delta E_J' + \frac{1}{2}\sum_{\substack{K\neq J \\ K\in L}} \Delta\Delta\tilde{E}_{JK}$　　(exp 5.8)

$$\Delta\tilde{E}_{IJ}^{C'} = \Delta\tilde{E}_{IJ}^{C} + \Delta E_I'' / J + \Delta E_J'' / I \qquad \text{(exp 5.9)}$$

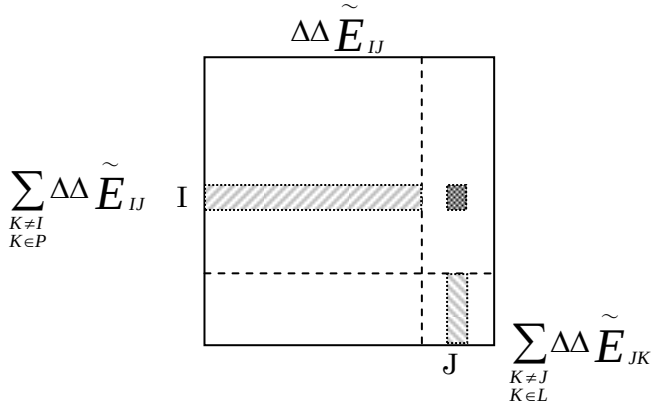


図 5.3　Memory image of $\sum\Delta\Delta\tilde{E}_{IJ}$

Each half of the changed portion of IFIE values by electronic relaxation inner protein is restored to each fragmentation at the second term of (exp 5.7). The ligand is the same at (exp 5.8).

The Protein – ligand IFIE analysis that regards the effect of the electronic relaxation by protien – ligand binding in fragment unit becomes possible by this calculation result.

6 Option of optimize structure

The Structure optimization is executed by calling another program from Viewer. Here, the option that can be specified is shown below. The file that describes this option is prepared, and it specifies it on the screen of the structure optimization.

<table>
<tr><td>Hydrogenation of protein (arbitrariness)</td><td>-B
The calculation of Atom type is specified.
-n
Addition of hydrogen atom (When -B is specified, it is effective).
When you add hydrogen : No filling in
When you do not add hydrogen : -n</td></tr>
<tr><td>Specification of structure optimization (arbitrariness)</td><td>-O
Execution of structure optimization by XUFF force field.
When you do the structure optimization calculation : -O
When you do not do the structure optimization calculation
: No filling in

-X #
The optimization calculation loop interval of the charge recalculation by the MQEq method (when -O is specified, it is effective) is specified by positive integer #.

-h
Optimization of atomic site of hydrogen (when -O is specified, it is effective). It is assumed that ACTIVE shown by the following was specified for all the hydrogen atoms and processes it. It is assumed that INACTIVE shown by the following was specified for all atoms except the hydrogen atom and processes it.

-S
A heavy atomic location of a main chain is fixed. Optimization of side chain structure and atomic site of hydrogen (when -O is specified, it is effective). It is assumed that ACTIVE shown by the following was specified for all atoms except a heavy atom of a main chain and processes it. It is assumed that INACTIVE shown by the following was specified for all heavy atoms of a main chain and processes it.

The method of recognizing a main chain in the PDB form and the MOL2 form is as follows.

Main chain of PDB form :
<table><tr><td>Atom name</td></tr><tr><td>N</td></tr><tr><td>CA</td></tr><tr><td>C</td></tr><tr><td>O</td></tr><tr><td>OXT</td></tr></table></td></tr>
</table>

Main chain of MOL2 form :

Atom name	Atom type
N	N.4 或いは N.am
CA	C.3
C	C.2
O	O.2
OXT	O.3

(The one to fill both)

-T

Processing of N end and C end.

When you dissociate N end and C end : -T
(NH4+, COO-)

When you dissociate neither N end nor C end : No filling in
(NH3, COOH)

-R

Processing ASP, GLU, LYS and ARG.

When you specify the charge state : -R

When you specify the state of the neutral : No filling in

-H #

Processing of imidazole ring of histidine (Default is π type).

π type (d type) : -H d

τ type (e type) : -H e

p type (p type) : -H p

-C # c

All charges of each molecule are specified.

: Number of molecule

c : charge

In default, all charges of each molecule are zero.

The method of distinguishing the molecule in the PDB form and the MOL2 form is as follows.

Distinction of molecule of PDB form : (Uncorrespondence of part)

It confirms it in order of TER, HETATM, a molecular name (residue name), and the residue number. In the following cases, the molecule is changed.

- When TER appears.
- When HETATM appears.
- When a molecular name in HETATM is changed (A molecule that is smaller than about five atoms is excluded. The water molecule is excluded.).
- When changing from HETATM into ATOM.

	・ When the residue number becomes small Distinction of main chain of MOL2 form : Information on following Substract id and Substract name is used and distinguished. Substract id : Given integer of amino-acid residue and each low molecular weight compound. It is counted in ascending order. Substract name : Name of amino-acid residue and compound. Even when Substract id is not changed, this Substract name is changed if a different low molecular weight compound is continuously specified. -k [Tinker_key_file] : The Keyword Control file of the Tinker form is specified (When -O is specified, it is effective.). The default name is tinker.key. Whether each atom is ACTIVE or INACTIVE can be specified. Example) ACTIVE 4 -9 17 23 When atoms 4, 9-17, and 23 are calculated, it is activated. Minus (-) means the start of the range. Two or more ACTIVE can be specified. Two or more INACTIVE can be still specified in the meaning opposite to actively. However, when the same atoms are specified for both ACTIVE and INACTIVE, it becomes ACTIVE. The atom not specified even for any ACTIVE and INACTIVE becomes ACTIVE. -f [xuffopt_parameter_file] [xuffopt_parameter_file] : The file of the parameter of xuffopt original form is specified. Options other than -f, the following total conditions ACTIVE_RESIDUE, INACTIVE_RESIDUE and ACTIVE_SIDECHAIN concerning the amino-acid residue, and conditions SDLOOP, CGLOOP, MAXLOOP, SDGRADIENT, CGGRADIENT, RENERGY and RGRADIENT concerning the convergent calculation of the optimization loop can be specified. The default name is xuffopt.par. Whether each amino-acid residue is ACTIVE_RESIDUE or INACTIVE_RESIDUE can be specified. The specification method is the same as ACTIVE and INACTIVE. Example) ACTIVE_RESIDUE 4 -9 17 23 When residue 4, 9-17, and 23 are calculated, it is activated. Minus (-) means the start of the range. Two or more ACTIV_RESIDUE can be specified. Two or more INACTIVE_RESIDUE can be still specified in the meaning opposite to actively. However, when same residue are specified for both ACTIVE_RESIDUE and INACTIVE_RESIDUE, it becomes ACTIVE_RESIDUE. The residue not specified even for any ACTIVE_RESIDUE and INACTIVE_RESIDUE

	becomes ACTIVE_RESIDUE. ACTIVE_SIDECHAIN can be specified for the side chain of each amino-acid residue (parts except a main chain). The specification method is the same as ACTIVE and ACTIVE_RESIDUE. The settling calculation frequency and the settling judgment condition of the optimization loop can be specified (The following examples are the default values). Example) SDLOOP 100 CGLOOP 400 MAXLOOP 500 SDGRADIENT 1000.0 CGGRADIENT 0.1 RGRADIENT 0.1 RENERGY 0.0001 SDLOOP : Number of maximum Steepest Descent law loops (SD loop) CGLOOP : Number of maximum Conjugate Gradient law loops (CG loop) LOOPMAX : Number of maximum loops SDGRADIENT : Gradient discontinuance value of SD loop CGGRADIENT : Gradient discontinuance value of CG loop RGRADIENT : Tolerance for convergence of Gradient RENERGY : Tolerance for convergence of rest error (kcal/mol) of all energy Gradient is judged by the value of the second power harmony route. The unit is (kcal/mol･Å). The CG loop continues to "Number of maximum SD loops + number of maximum CG loops" when the SD loop is discontinued on the way. Because the BFGC method is not being calculated now, CGLOOP and CGGRADIENT are invalid.

7 Installation

7.1 Distribution

We have a windows installer file.

7.2 System Installation

Double-clicking install file icon then installs it. To execute the viewer by selecting menu that is start→ABINIT-MP Open Consortium→BioStationViewer.

The wroking folder is install folder. You can change it to change property of menu item and add a install path to PATH like bellow.

C:¥Program Files¥ ABINIT-MP Open Consortium ¥BioStationViewer

7.3 System Requirements

System Requirements is shown in **Table 7.1**.

Table 7.1 System Requirements

Item	Business
OS	Windows(2000/XP,7)
CPU	Pentium Ⅱ 400MHz or more
Memory	Recommended memory 2GB or more

7.4 File Acquisition

Obtain **Biostation Viewer files** from a web site of **ABINIT-MP**. The following files needs to run **Biostation Viewer.**

File name	Explanation
BioStationViewerOpen_1.0_rev25.exe	BioStation Installer file
sampleData.zip	Sample files
tutrial.zip	Tutorial data files

7.5 Reduce

You can use **Reduce** in order to add hydrogen. **Reduce** can be downloaded from http://kinemage.biochem.duke.edu/software/software2.html#reduce

, which is a program free of charge.

Download the program and save it to the appropriate place. Set **Path** to the folder, then. Refer to the preceding paragraph so as to set **Path.** Options are shown as follows.

reduce: version 2.15 10/4/01, Copyright 1997-2001, J. Michael Word

arguments: [-flags] filename or -

Adds hydrogens to a PDB format file and writes to standard output.
(note: By default, HIS sidechain NH protons are not added. See -BUILD)

Flags:

-Trim	remove (rather than add) hydrogens
-NOOH	remove hydrogens on OH and SH groups
-OH	add hydrogen on OH and SH groups (default)
-HIS	create NH hydrogen on HIS rings
-FLIPs	allow complete ASN, GLN and HIS side chains to flip (usually used with -HIS)
-NOHETh	do not attempt to add NH proton on Het groups
-ROTNH3	allow lysine NH3 to rotate (default)
-NOROTNH3	do not allow lysine NH3 to rotate
-ROTEXist	allow existing rotatable groups (OH, SH, Met-CH3) to rotate
-ROTEXOH	allow existing OH & SH groups to rotate
-ALLMEthyls	allow all methyl groups to rotate
-ONLYA	only adjust 'A' conformations (default)
-ALLALT	process adjustments for all conformations
-NOROTMET	do not rotate methionine methyl groups
-NOADJust	do not process any rot or flip adjustments
-BUILD	add H, including His sc NH, then rotate and flip groups (except for pre-existing methionine methyl hydrogens) (same as: -OH -ROTEXOH -HIS -FLIP)
-Keep	keep bond lengths as found
-NBonds#	remove dots if cause within n bonds (default=3)
-Model#	which model to process (default=1)
-Nterm#	max number of nterm residue (default=1)
-DENSity#.#	dot density (in dots/A^2) for VDW calculations (default=16)
-RADius#.#	probe radius (in A) for VDW calculations (default=0)
-OCCcuttoff#.#	occupancy cutoff for adjustments (default=0.01)

-H2OBcuttoff#.# B-factor cutoff for water atoms (default=40)
-H2OOCCcuttoff#.# occupancy cutoff for water atoms (default=0.66)
-PENalty#.# fraction of std. bias towards original orientation (default=1)
-HBREGcuttoff#.# over this gap regular HBonds bump (default=0.6)
-HBCHargedcut#.# over this gap charged HBonds bump (default=0.4)
-BADBumpcut#.# at this gap a bump is 'bad' (default=0.4)
-SEGIDmap "seg,c..." specify chainID based on segment identifier field
-Xplor use Xplor conventions for naming polar hydrogens
-NOCon drop connect records
-LIMIT# max num iter. for exhaustive search (default=100000)
-NOTICKs do not display the set orientation ticker during processing
-SHOWSCore display scores for each orientation considered during processing
-FIX "filename" if given, file specifies orientations for adjustable groups
-DB "filename" file to search for het info
(default="/usr/local/reduce_het_dict.txt")
note: can also redirect with unix environment variable: REDUCE_HET_DICT

-Quiet do not write extra info to the console
-REFerence display citation reference
-Help more extensive description of command line arguments

7.6 Babel

Set BABEL_DIR(Environment Parameter)
C:¥Program Files¥ ABINIT-MP Open Consortium ¥BioStationViewer¥babel-lis

7.7 Bond Builder

The use of "bond_builder" which is the hydrogenation program is shown in Table 7.2.

Table 7.2 Explanation of the use of "bond_builder".

Command line	% bond_builder.exe –i [input_file_name] [input_file_type] –o [output_file_name] [output_file_type] –B –n –T –R –H #
Setting of the input file	–i [input_file_name] [input_file_type] [input_file_name] : Input file name (indispensable). [input_file_type] : Type of the input file (arbitrariness). pdb, ent : For the type of PDB mol2 : For the type of mol2 Default file type is decided by the extension of the input file name. File type is PDB in the case of pdb or ent , and mol2 in the case of mol2.
Setting of the output file	–o [output_file_name] [output_file_type] [output_file_name] : Output file name. [output_file_type] : Type of the output file (arbitrariness). pdb, ent : For the type of PDB mol2 : For the type of MOL2 Default file type is decided by the extension of the output file name. File type is PDB in the case of pdb or ent , and mol2 in the case of mol2. When "－o" is not specified, the file name that adds "_builder" to the input file name is output. example) input_builder.mol2 At this time ("-o" is not specified), when "-B" (see below) is specified, the file name that adds "_H" to the input file name is output. example) input_H.pdb
Hydrogenation of protein (arbitrariness)	–B The calculation of Atom type is specified. –n Addition of hydrogen atom (When -B is specified, it is effective). When you add hydrogen : No filling in When you do not add hydrogen : -n
Processing of N terminal and C terminal of the protein (arbitrariness)	–T When you dissociate N terminal and C terminal : -T (NH4+, COO-) When you dissociate neither N terminal nor C terminal : No filling in (NH3, COOH)
Processing of charged residues ASP, GLU, LYS and ARG (arbitrariness)	–R When you specify the charge state : -R When you specify the state of the neutral : No filling in
Processing of imidazole ring of histidine (Default is π type)	–H # π type (d type) : -H d τ type (e type) : -H e p type (p type) : -H p

7.8 TINKER

Download from http://dasher.wustl.edu/tinker/, and add Path (*install folder*/bin). Copy *install folder*/jre/bin/client/jvm.dll to bin.

8 Acknowledgement

We refere the following projects.

- Information-Technology Promotion Agency, Japan(IPA)
  "Research of protein functional prediction system for biotechnology industry"
  "Development of ab initio fragment molecular orbital method program: ABINIT-MP"
- Japan Science and Technology Corporation
  Research and Development for Applying Advanced Computational Science and Technology
  Ab initio Approach to Nanoscale Dynamics of **DNA**

This work was supported the following projects.

- Ministry of Education, Culture, Sports, Science and Technology
  Frontier Simulation for Industrial Science
  " Quantum Molecular Interaction Analysis"
- The Japan Science and Technology Agency
  Core Research for Evolutional Science and Technology(CREST)
  Development of Bio-Simulation Systems Based on the Fragment Molecular Orbital Method
- Ministry of Education, Culture, Sports, Science and Technology
  Revolutionary Simulation Software for 21st Century (RSS21)
- Ministry of Education, Culture, Sports, Science and Technology
  Research and Development of Innovative Simulation Software (RISS)

MOLDA is developed by Dr. Hiroshi Yoshida. Sad to say he was lost in 2005. He was a member of our CREST project, so he gave us a permission to use the MOLDA.

Eigenvalue are required to evaluate in the calculation, with using **JAMA:Java Matrix Package** (http://math.nist.gov/javanumerics/jama/). **JAMA** is operating free of charge.

We are deeply grateful to following people.

Kobe University Dr. Sigenori Tanaka, Dr. Ikuo Kurisaki

Rikkyou University Dr. Yuji Mochizuki

Kagoshima University Dr. Takeshi, Ishikawa

MOLSIS Inc. Dr. Shinji Amari

Hiroshima University Dr. Hiroshi Yoshida

Advance Soft co. Dr. Tetsuji Ogawa, Dr. Masato Kobayashi

Advanced Industrial Science and Technology Dr. Yuto Komeiji, Dr. Kazuo Kitaura

Microbial Chemistory Research Center Dr. Yuji Umezawa

The CHPI Institute Dr. Motihiro Nishio

Hoshi University Dr. Kaori Fukuzawa

National Institute of Health Sciences Dr. Tatsuya Nakano, Dr. Yoshio Okiyama.

RIKEN Dr. Chiduru Watanabe

Mizuho Information & Research Institute, Inc. Kouichuro Kato, Takashi Tsukamoto, Naoki Tanimura

Scorpion Tech LLC. Akifumi Kato

FMODD Consortium

(In random order)

9 References

FMO

1. K. Kitaura, T. Sawai, T. Asada, T. Nakano, M. Uebayasi *Chem Phys Lett* **312**, 319-324 (1999).
2. K. Kitaura, E. Ikeo, T. Asada, T. Nakano, M. Uebayasi *Chem Phys Lett* **313**, 701-706 (1999).
3. T. Nakano, T. Kaminuma, T. Sato, Y. Akiyama, M. Uebayasi, K. Kitaura *Chem Phys Lett* **318**, 614-618 (2000).
4. T. Nakano, T. Kaminuma, T. Sato, K. Fukuzawa, Y. Akiyama, M. Uebayasi and K. Kitaura *Chem. Phys. Lett.*, **351**, 475-480 (2002).
5. edited by D. G. Fedorov and K. Kitaura "The Fragment Molecular Orbital Method: Practical Applications to Large Molecular Systems" Taylor & Francis/ CRC Press, Boca Raton, FL, (2009)

FMO Structure Optimize(Differential)

6. K. Kitaura, S. Sugiki, T. Nakano, Y. Komeiji, M. Uebayasi *Chem Phys Lett* **336**, 163-170 (2001).

FMO-MD

7. Y. Komeiji, T. Nakano, K. Fukuzawa, Y. Ueno, Y. Inadomi, T. Nemoto, M. Uebayasi, D. G. Fedorov and K. Kitaura "Fragment Molecular Orbital Method: Application to Molecular Dynamics Simulation, '*ab initio* FMO-MD'" *Chem. Phys. Lett.*, **372**, 342-347 (2003).
8. Y. Mochizuki, Y. Komeiji, T. Ishikawa, T. Nakano, H. Yamataka "A fully quantum mechanical simulation study on the lowest n–π* state of hydrated formaldehyde" *Chem. Phys. Lett.*, 437, 66-72 (2007).

FMO-MP2

9. Y. Mochizuki, T. Nakano, S. Koikegami, S. Tanimori, Y. Abe, U. Nagashima, K. Kitaura, *Theor. Chem. Acc*. **112**, 442–452 (2004).
10. Y. Mochizuki, S. Koikegami, T. Nakano, S. Amari, K. Kitaura *Chem. Phys. Lett.* **396**, 473-479 (2004).

LMP2

11. T. Ishikawa et. al., submitted.

CIS

12. Y. Mochizuki, S. Koikegami, S. Amari, K. Segawa, K. Kitaura, T. Nakano *Chem Phys Lett.*, **406**, 283–288 (2005).

CIS(D)

13. Y. Mochizuki, S. Koikegami, S. Amari, K. Segawa, K. Kitaura, T. Nakano *Chem Phys Lett.* 2005, **406**, 283–288 (2005).
14. Y. Mochizuki, K. Tanaka, K. Yamashita, T. Ishikawa, T. Nakano, S. Amari, K. Segawa, T. Murase, H. Tokiwa, M. Sakurai *Theor. Chem. Acc*. in press

CAFI

15. Mochizuki, Y. Chem. Phys. Lett. 2005, 410, 165–171.
16. Y. Mochizuki, K. Fukuzawa, A. Kato, S. Tanaka, K. Kitaura and T. Nakano, *Chem. Phys. Lett.*, **410**, 247–253 (2005).

MCP

17. T. Ishikawa, Y. Mochizuki, T. Nakano, S. Amari, H. Mori, H. Honda, T. Fujita, H. Tokiwa, S. Tanaka, Y. Komeiji, K. Fukuzawa, K. Tanaka, E. Miyoshi *Chem. Phys Lett.*, **427**, 159-165 (2006).

物性

18. Y. Mochizuki, T. Ishikawa, K. Tanaka, H. Tokiwa, T. Nakano and S. Tanaka “Dynamic polarizability calculation with fragment molecular orbital scheme” *Chemical Physics Lett*. **418**, 418-422 (2006).

VISCANA

19. S. Amari, M. Aizawa, J. Zhang, K. Fukuzawa, Y. Mochizuki, Y. Iwasawa, K. Nakata, H. Chuman and T. Nakano *J. Chem. Information and Modeling*, **46**, 221-230 (2006).

Estrogen accepter

20. K. Fukuzawa, K. Kitaura, K. Nakata, T. Kaminuma and T. Nakano, *Pure Appl. Chem.*, **75**, 2405-2410 (2003).
21. K. Fukuzawa, K. Kitaura, M. Uebayasi, K. Nakata, T. Kaminuma and T. Nakano *J. Comp. Chem.*, **26**, 1-10 (2005).

22. K. Fukuzawa, Y. Mochizuki, S. Tanaka, K. Kitaura, and T. Nakano *J. Phys. Chem. B*, **110**, 16102-16110 (2006).
23. K. Maeda, A. Schug, H. Watanabe, K. Fukuzawa, Y. Mochizuki, T. Nakano, S. Tanaka "Effects of Point Mutations on the Binding Energies of Estrogen Receptor with Estradiol" *J. Comput. Chem. Jpn.*, **6**, 33-46 (2007).

DNA-Protein(CRP)

24. K. Fukuzawa, Y. Komeiji, Y. Mochizuki, A. Kato, T. Nakano and S. Tanaka *J. Comp. Chem.*, **27**, 948-960 (2006).
25. T. Watanabe, Y. Inadomi, K. Fukuzawa, T. Nakano, S. Tanaka, L. Nilsson, and U. Nagashima "DNA and Estrogen Receptor Interaction Revealed by the Fragment Molecular Orbital Calculation" *J. Phys. Chem B*, submitted.

ナノ

26. T. Ishikawa, Y. Mochizuki, K. Imamura, T. Nakano, H. Mori, H. Tokiwa, K. Tanaka, E. Miyoshi, S. Tanaka "Application of fragment molecular orbital scheme to silicon-containing systems" *Chem. Phys. Lett.* **430**, 361–366 (2006).

CH/π

27. Yuji Umezawa, Motohiro Nishio, "CH/π Interactions as Demonstrated in the Crystal structure of Guanine-nucleotide Binding Proteins, Src homology-2 Domains and Human Growth Hormone in Complex with their Specific Ligands", Bioorganic & Medicinal Chemistry Volume 6, Issue 4, Pages 493-504 (1998,)
28. M. Nishio, M., Hirota, Y. Umezawa, "The CH/π Interaction Evidence, Nature, and Consequences",1998, Wiley-VCH, New York
29. 西尾元宏「新版　有機化学のための分子間力入門」講談社 2008

ABINIT-MP

30. 中野、谷森、加藤、小池上、雨宮、福澤　「フラグメント分子軌道法入門　―ABINIT-MP によるタンパク質の非経験的量子化学計算―　アドバンスソフト 2004
31. 佐藤、中野、望月編「プログラムで実践する生体分子量子化学計算」森北出版 2008
32. Dmitri G. Fedorov edited　"The FRAGMENT MOLECULAR ORBITAL METHOD"　2009 CRC Press

BioStation Viewer

33. 加藤、福澤、望月、甘利、中野　「BioStation Viewer：生体高分子の相互作用も解析と可視化」可視化情報　p2-7 Vol.26 No.101 2006.4
34. Wolfgang Kabsch and Christian Sander ,"Dictionary of Protein Secondary Structure: Pattern Recognition of Hydrogen-Bonded and Geometical Features", Biopolymers, Vol. 22, 2577-2637, 1983.

Appendix

1) ABINIT-MP File Format：another file
2) MOLDA users manual：another file