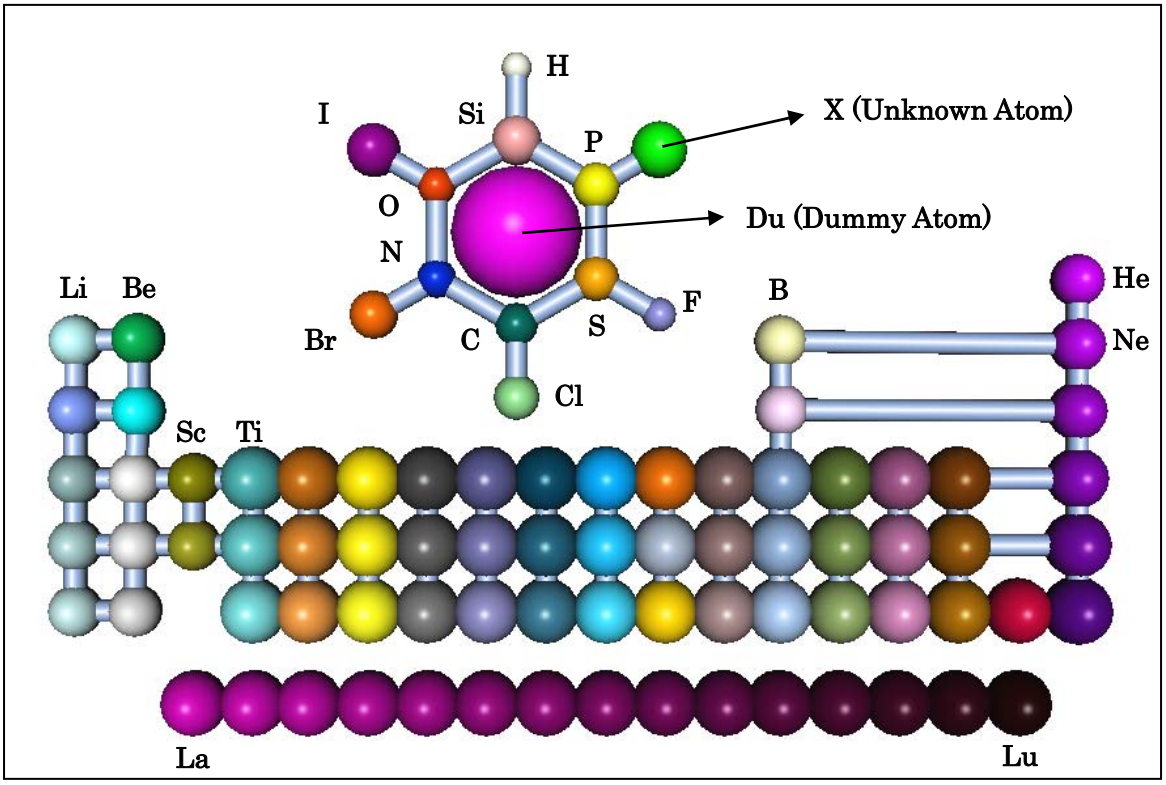
----- Ver.11.8.8 ----- March 27, 2009 Bug fix version of 11.8.7

----- Ver.11.8.7 ----- March 25, 2009

(1) Facio now supports AFO (Adaptive Frozen Orbital) method, which is a newly developed FMO fragmentation scheme and implemented in Gamess from version of Jan. 12, 2009.

Reference for AFO
Dmitri G. Fedorov, Jan H. Jensen, Ramesh C. Deka, and Kazuo Kitaura
***J. Phys. Chem. A* 2008, *112*, 11808-11816**

(2) Up to Facio 11.8.6, atom colors and diameters of H, C, N, O, F, P, S, Si, Br, I were defined in Facio.ini. From 11.8.7, all the atom colors and diameters of Ball-and-Stick type molecular model are defined in AtomProp.ini. If you want to customize these atom properties, please use All_Elements_Colors.pdb, which is a virtual molecule as shown below and included in Facio's distributing archive as sample molecule.



(3) For naming of FMO fragments, the information of residue name and number in protein PDB can be preserved in newly defined RSQ (residue sequence) file. See also Miscellaneous Menu >> Highlight PDB Residue Sequence for creation of RSQ file.

(4) Zoom in and out can be automatically performed according to the size of a molecule loaded.
(5) New function for FMO : You can load two Gamess/FMO outputs and create difference file of fragment-fragment interactions.

(6) When effective core potential type basis functions, such as SBKJC and HW are used, sequential number of MO is different from the one based on usual type of basis functions. Now Facio can respond to this change and show correct sequential number of MO.

(7) You can load Gamess input file to retrieve the structure in Cartesian coordinate.

----- Ver.11.8.6 ----- December 13, 2008

(1) A new chemical file format, FCC (Facio Cartesian Coordinate) has been created in order to store Cartesian coordinates of GAMESS or Gaussian calculation without any truncation of the values and complete connectivity of the compound.

The following example of FCC is created based on a H2O calculated with Gaussian.

```
Facio Cartesian Coordinate :  C:¥G03W¥Facio¥H2O.out
3
  O       1       0.0000000000      0.1146870000      0.0000000000      2       3
  H       2       0.7540650000     -0.4587490000      0.0000000000      1
  H       3      -0.7540650000     -0.4587490000      0.0000000000      1
```

The 1st line should contain string "Facio Cartesian Coordinate". You can write a comment after the colon of the 1st line. The 2nd line contains the number of atoms. After the 3rd line, each contains a kind of the atom, serial number, Cartesian coordinates and connectivity in the following format.

A3, I7, 3(F17.10), n(I7) (where n is the number of bonds and varies from 0 to 8)

Cartesian coordinates can be saved as a number which has 10 digits after the decimal point. This feature is useful for recording Cartesian coordinates of GAMESS or Gaussian outputs. The connectivity data is also useful for complete reconstruction of the structure. Thus, FCC (Facio Cartesian Coordinate) is suitable chemical file format of computational chemistry.

(2) Definition of FMO fractioning points (BDA and BAA) is now performed by clicking bond which you want fraction. Which of the two atoms is set to be BDA (Bond Detached Atom) is determined automatically.

(3) FMO input file is now concurrently loaded to retrieve Cartesian coordinates of the compound during loading FMO output which contains no geometrical data. Since all the information about FMO fragment, such as INDAT(1), FRAGNAM(1), $FMOBND (if any), are also obtained, you can see whole the fragments with Local Structure Viewer without re-fragmentation with Facio.

(4) New ini keys, AddPause2Bat and UseFacioDriveLetter are introduced to [AppControl] section of Facio.ini.
AddPause2Bat determines whether add or not "pause" commant to the batch file which invoke Tinker-MM3 calculation. If you want to insert pause after MM3 calculation finished, please set AddPause2Bat=1 (default value is 0).

UseFacioDriveLetter determines whether use of not the drive letter of Facio as the drive letter for GamessBase or TinkerBase. For example, When GamessBase=C:¥PCGAMESS, the drive letter of PC GAMESS is C:.But if you set UseFacioDriveLetter=1, the drive letter varies according to the drive letter where Facio resides. Thus if Facio is installed at F: drive, GamessBase is set to be F:¥PCGAMESS, even if it C:¥PCGAMESS in Facio.ini.
This feature is especially useful, when drive letter can vary due to the login environment.

(5) A new "Monitor Energy Conv." button in the Gamess Input Option panel is cerated. With this button, you can monitor energy/geometry change during the optimization process.

(6) When Tinker-Amber, Charm, Oplsaal input file is created, the batch file to invoke the calculation and key file is now also created.

----- Ver.11.8.5 ----- November 8, 2008

(1) While the number of grid point per 1 angstrom to draw MO lobe using coefficients of MO was fixed to 10 up to Ver. 11.8.4, now the value is customizable. In addition to this change, default values of the two parameters in $VEC/Molecular Orbital Viewer (surface thickness and isosurface value) was revised.

(2) FMO fractioning points can be specified with clicking bond which has two atoms to be set to. Which atom is to be BDA (Bond Detached Atom) is determined automatically by judging the kind and configuration of the atoms.

(3) 3D rotation via mouse move was revised.

(4) Mouse drag with holding down ALT key can translate molecular model in the monitor plane. Sensitivity to the mouse drag is controlled with the parameter TransSens in Facio.ini file.

(5) Periodic Table of the Elements was revised.

(6) The format of Normal Coordinate Analysis are completely different between MOPAC Ver.7.101 and MOPAC Ver. 8.211, as shown below. Now Facio supports this new format.

(MOPAC Ver.7.101)

NORMAL COORDINATE ANALYSIS

Root No.	1	2	3	4	5	6	7	8
	1 E2u	1 E2u	1 B1g	1 E2g	1 E2g	1 A2u	1 E1g	1 E1g
	341.2	341.2	582.1	589.4	589.4	768.9	899.2	899.2
1	0.0000	0.0000	0.0000	-0.0039	0.0714	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000	-0.0804	0.0655	0.0000	0.0000	0.0000
3	-0.0442	-0.0581	-0.0415	0.0000	0.0000	0.0129	-0.0326	-0.0019
4	0.0000	0.0000	0.0000	-0.0159	0.0698	0.0000	0.0000	0.0000
5	0.0000	0.0000	0.0000	-0.0593	-0.0855	0.0000	0.0000	0.0000

(MOPAC Ver.8.211)

MASS-WEIGHTED COORDINATE ANALYSIS (NORMAL COORDINATES)

Root No.	1	2	3	4	5	6	7	8
	1 E2u	1 E2u	1 E2g	1 E2g	1 B1g	1 A2u	1 B2u	1 E1g
	367.0	367.0	591.5	591.5	598.7	800.0	916.0	922.6
1	0.0001	-0.0003	0.3155	0.0079	0.0002	0.0001	-0.1976	0.0001
2	-0.0003	0.0005	0.2970	0.3506	-0.0004	-0.0001	-0.3423	0.0001
3	-0.2190	0.4121	-0.0002	-0.0004	-0.3130	-0.1136	0.0005	-0.0315
4	0.0002	0.0003	0.3091	0.0638	-0.0002	0.0001	-0.1977	-0.0001
5	-0.0003	-0.0005	-0.3687	0.2742	0.0004	-0.0001	0.3423	0.0001

----- Ver.11.8.4 ----- October 4, 2008

(1) You can drag-and-drop Gamess/FMO output on the main display of Facio to read the file.

(2) When you load Gaussian output of a calculation with key words, Opt Freq, the initial structure was shown instead of the optimized structure. This bug has been fixed.

(3) Upper limit of the parameter MAXIT of WinGamess is 200. But the value 300 is shown in the option panel. This has been fixed. Please note that MAXIT=300 is acceptable for PC GAMESS.

(4) When you make an input of QST2 or QST3 calculation of Gaussian, comment lines of Product and Initial_TS are same as Reactant. This has been fixed.

(5) When you open IRC Data Viewer, CPU usage become nearly 100%. And when IRC Data Viewer is opened, in some case, atom cannot be selected by mouse click. These have been fixed. The same bugs found at Trajectory Viewer have also been fixed.

(6) The EIGENVECTORS format of MOPAC Ver.7.101 and that of MOPAC Ver.8.211 are completely different, as shown below. Now Facio supports this new format.

(MOPAC Ver.7.101)

Root No.			7	8	9	10	11	12	13	14
			1 b2u	1 b1u	2 e1u	2 e1u	1 a2u	2 e2g	2 e2g	1 e1g
			-15.732	-15.068	-14.200	-14.195	-13.161	-11.940	-11.936	-9.639
S	C	1	-0.2149	0.0001	-0.0704	-0.0023	0.0000	0.0112	-0.0005	0.0000
Px	C	1	0.0000	-0.4079	0.0040	-0.1309	0.0000	0.0191	0.3594	0.0000
Py	C	1	-0.2241	-0.0001	0.4662	0.0148	0.0000	0.3397	-0.0182	0.0000

(MOPAC Ver.8.211)

Root No.			7	8	9	10	11	12	13	14
			1 b2u	1 b1u	2 e1u	2 e1u	1 a2u	2 e2g	2 e2g	1 e1g
			-15.730	-15.067	-14.197	-14.196	-13.160	-11.941	-11.933	-9.638
S	C	1	-0.2146	-0.0002	-0.0014	-0.0702	0.0002	0.0002	-0.0110	-0.0004
Px	C	1	0.0000	0.4090	-0.1275	0.0019	-0.0013	0.3595	0.0059	0.0011
Py	C	1	-0.2233	0.0004	0.0085	0.4667	0.0007	0.0055	-0.3402	-0.0017
Pz	C	1	0.0008	0.0009	-0.0002	-0.0015	0.4083	0.0014	0.0004	-0.5319

----- Ver.11.8.2 and Ver.11.8.3 ----- August 19, 27, 2008

These are minor bug fix versions of Ver. 11.8.1 and Ver.11.8.2, respectively.

----- Ver.11.8.1 ----- July 25, 2008

(1) New function to show all the intermediate geometries sequentially with the corresponding energies when GAMESS or Gaussian optimization output file is loaded. Even if the calculation is not finished, the output can be loaded. If MP2 energy is available, MP2 energy is also displayed.

The retrieved intermediate geometries are stored as Opt_1.pdb, Opt_2.pdb, Opt_3.pdb…in Facio's base folder¥PDB¥OptResults, which is automatically created.

(2) Geometric information lists (bond length, bond angle and dihedral angle) are generated for plural files. Loadable file formats are PDB, CC1, Free formatted / WebLab xyz, MDL mol, Tripos mol2, TINKER XYZ, GAMESS output and Gaussian output.

To use the function, select Utilities Menu >> Load File(s) and Dump Geometric Informations

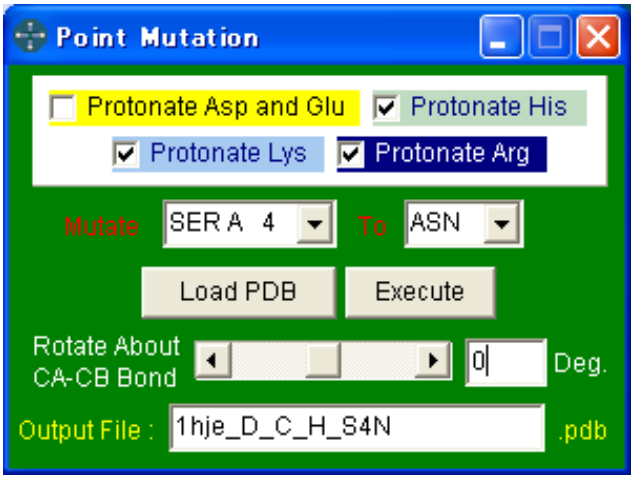
(3) Point mutation of protein

Load PDB file of protein in ATOM record and change the side chain of the specified amino residue to that of the new amino residue and save as PDB file in ATOM record. Atom numbers are automatically renumbered. If there are CONECT record for S-S bond of Cys-Cys, CONECT record are also revised accordingly. In case the new amino residue is Glu, Asp, His, Lys or Arg, there is an option to decide whether protonation is performed or not. When the side chain of the new amino residue collide with the already existing chains, adjust "Rotation angle about CA-CB bond". (CA : alpha carbon, CB : beta carbon)

When one of the Cys of Cys-Cys is replaced, hydrogen atom is added to the remaining Cys and the corresponding CONECT record is deleted. When Pro is substituted with other residue, hydrogen atom is added to the nitrogen. For N-term residue, two hydrogen atoms are added. When the new residue is Pro, hydrogen on N is deleted and five-membered ring is prepared. Please note that the formed ring structure is usually distorted. But you can modify the ring structure by changing the rotation angle about CA-CB.

Suffix which shows point mutation is automatically added to the output file. For example, when Ser 4 is mutated to Asn, "_S4N" is added as suffix, which is consist of old residue and new residue in one-letter notation.

Examples are included in the folder Point_Mutation.



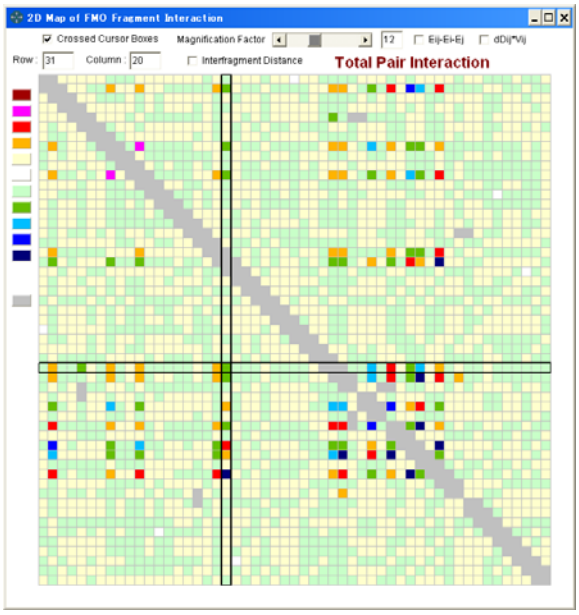
(4) 2D map representation of two-body FMO properties was revised.

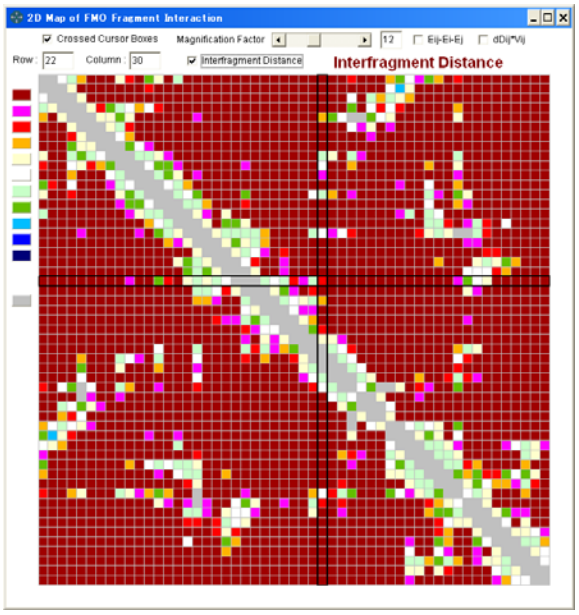
(5) Up to 16 colors available for Rainbow Fragment representation

(6) Automatic generation of input file for Tinker-OPLSAAL calculation.

----- Ver.11.7.1 ----- June 12, 2008

(1) 2D map representation of two-body FMO properties





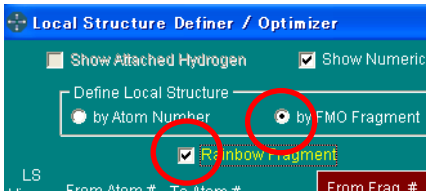
Two-body FMO properties of non-PIEDA calculation can also be displayed.

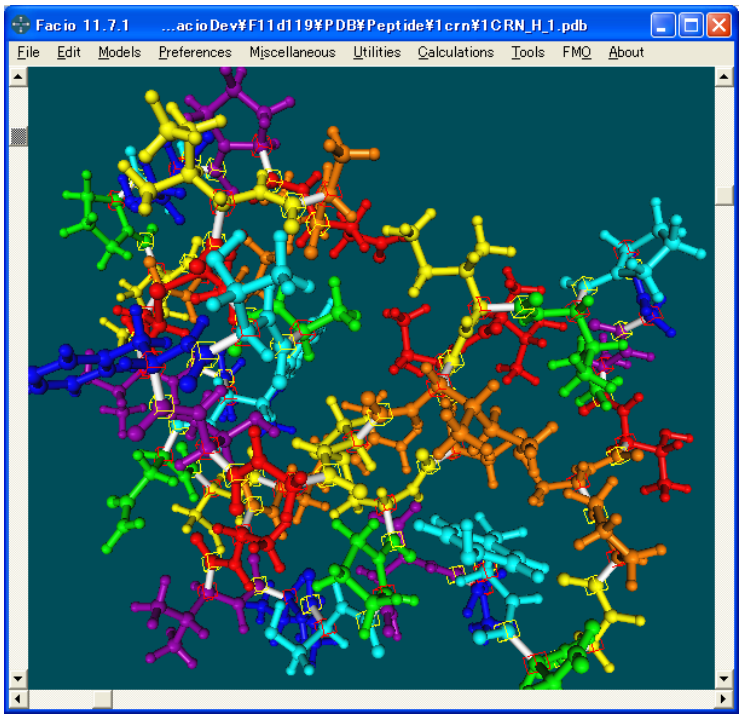
(2) Rainbow Fragment representation

In this representation, each FMO fragments are drawn using rainbow colors (red, orange, yellow, green, cyan, blue and purple) which are cyclically applied.

How to display Rainbow Fragment

1. Make FMO fragment.
2. Open Local Structure Viewer.
3. Define local structure "by FMO Fragment".
4. Check "Rainbow Fragment".





(3) Automatic generation of input file for Tinker-Charmm calculation.

(4) When missing hydrogen atoms are completed in ATOM record, the already existing CONECT records (if any) are preserved. The numbering in CONECT record is automatically renumbered.

----- Ver.11.6.1 ----- May 10, 2008

(1) PDB Utilities (See FMO menu items.)

(A) Utility to delete alternate locations in ATOM record of PDB

```
         1         2         3         4
1234567890123456789012345678901234567890123456789012345 (Columns)

ATOM     18  CD1ATYR A 327      16.886  14.518  -8.371
ATOM     19  CD1BTYR A 327      14.840  15.316  -5.413
ATOM     20  CD2ATYR A 327      15.466  14.119  -6.496
ATOM     21  CD2BTYR A 327      16.667  14.101  -6.351
```

Alternate Location Indicator

```
ATOM     18  CD1ATYR A 327      16.886  14.518  -8.371
ATOM     20  CD2ATYR A 327      15.466  14.119  -6.496
```

(B) Utility to convert format of Atom Name Field in ATOM record of PDB

```
ATOM     24  HB2 TYR A   2      -5.189  -0.788  -1.616
ATOM     25  HB3 TYR A   2      -4.918   0.937  -1.380
...
ATOM    104 HG21 THR A   8       0.813  -5.501  -2.562
ATOM    105 HG22 THR A   8       2.533  -5.563  -2.176
ATOM    106 HG23 THR A   8       1.885  -4.210  -3.104
```

```
ATOM     24 1HB  TYR A   2      -5.189  -0.788  -1.616
ATOM     25 2HB  TYR A   2      -4.918   0.937  -1.380
...
ATOM    104 1HG2 THR A   8       0.813  -5.501  -2.562
ATOM    105 2HG2 THR A   8       2.533  -5.563  -2.176
ATOM    106 3HG2 THR A   8       1.885  -4.210  -3.104
```

(C) Utility to add hydrogen atoms in ATOM record format to protein PDB

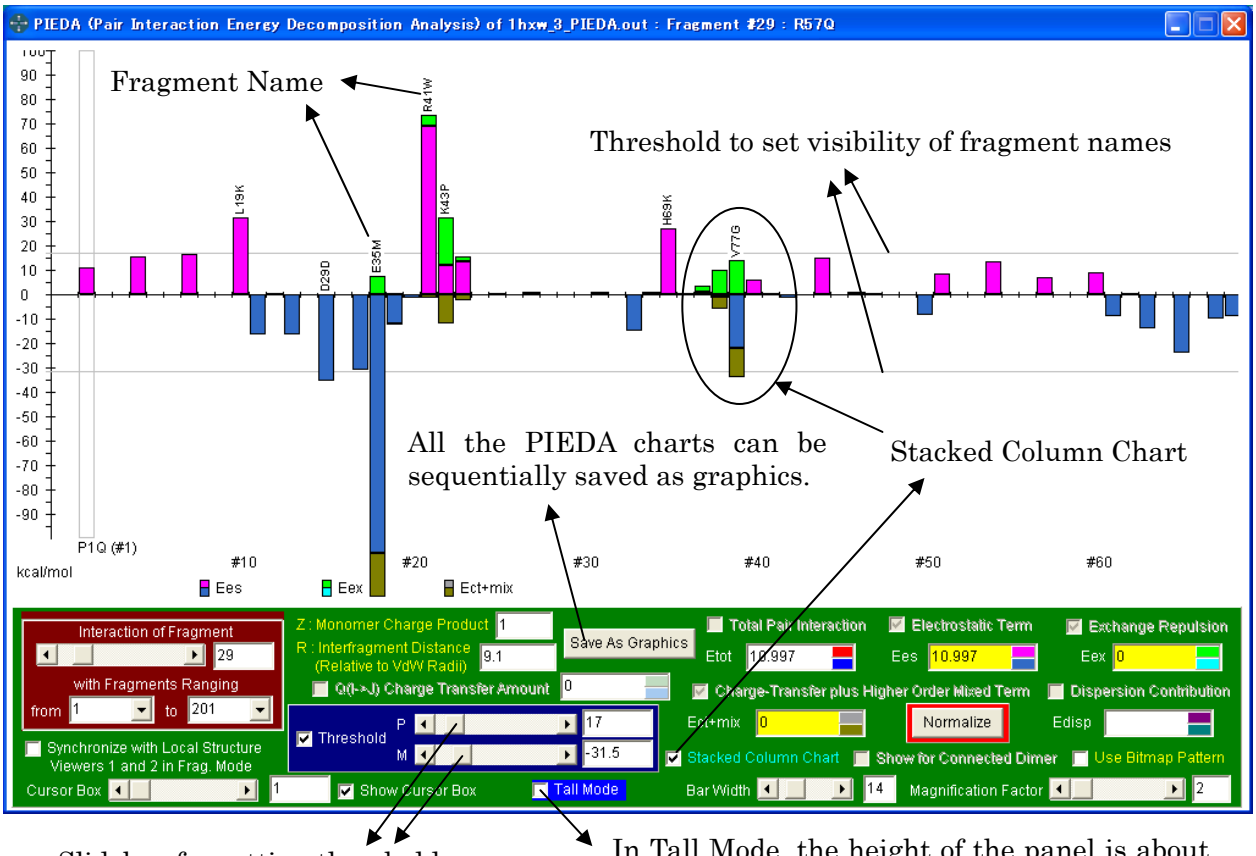
```
ATOM      1  N   PRO A   1       8.316  21.206  21.530
ATOM      2  CA  PRO A   1       7.608  20.729  20.336
ATOM      3  C   PRO A   1       8.487  20.707  19.092
ATOM      4  O   PRO A   1       9.466  21.457  19.005
ATOM      5  CB  PRO A   1       6.460  21.723  20.211
ATOM      6  CG  PRO A   1       7.110  23.002  20.661
ATOM      7  CD  PRO A   1       7.873  22.569  21.889
```

```
ATOM      1  N   PRO A   1       8.316  21.206  21.530
ATOM      2  CA  PRO A   1       7.608  20.729  20.336
ATOM      3  C   PRO A   1       8.487  20.707  19.092
ATOM      4  O   PRO A   1       9.466  21.457  19.005
ATOM      5  CB  PRO A   1       6.460  21.723  20.211
ATOM      6  CG  PRO A   1       7.110  23.002  20.661
ATOM      7  CD  PRO A   1       7.873  22.569  21.889
ATOM      8 1H   PRO A   1       9.407  21.194  21.355
ATOM      9 2H   PRO A   1       8.144  20.515  22.375
ATOM     10  HA  PRO A   1       7.255  19.678  20.535
ATOM     11 1HB  PRO A   1       5.606  21.397  20.832
ATOM     12 2HB  PRO A   1       6.082  21.739  19.173
ATOM     13 1HG  PRO A   1       6.341  23.772  20.853
ATOM     14 2HG  PRO A   1       7.744  23.411  19.853
ATOM     15 1HD  PRO A   1       7.219  22.614  22.778
ATOM     16 2HD  PRO A   1       8.698  23.275  22.092
```

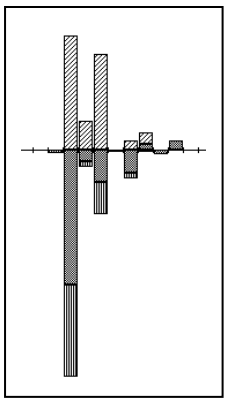
(2) FMO fragmentation is now possible for the systems, where there is no fractioning point, such as a cluster of water or there are isolated atoms, like noble gas system.

----- Ver.11.5.1 ----- April 13, 2008

(1) Upgrade of visualization panel for FMO PIEDA



Columns in the chart can be represented using bitmap patterns as shown below.



The bitmap files are included in the folder, Brush_BMP.

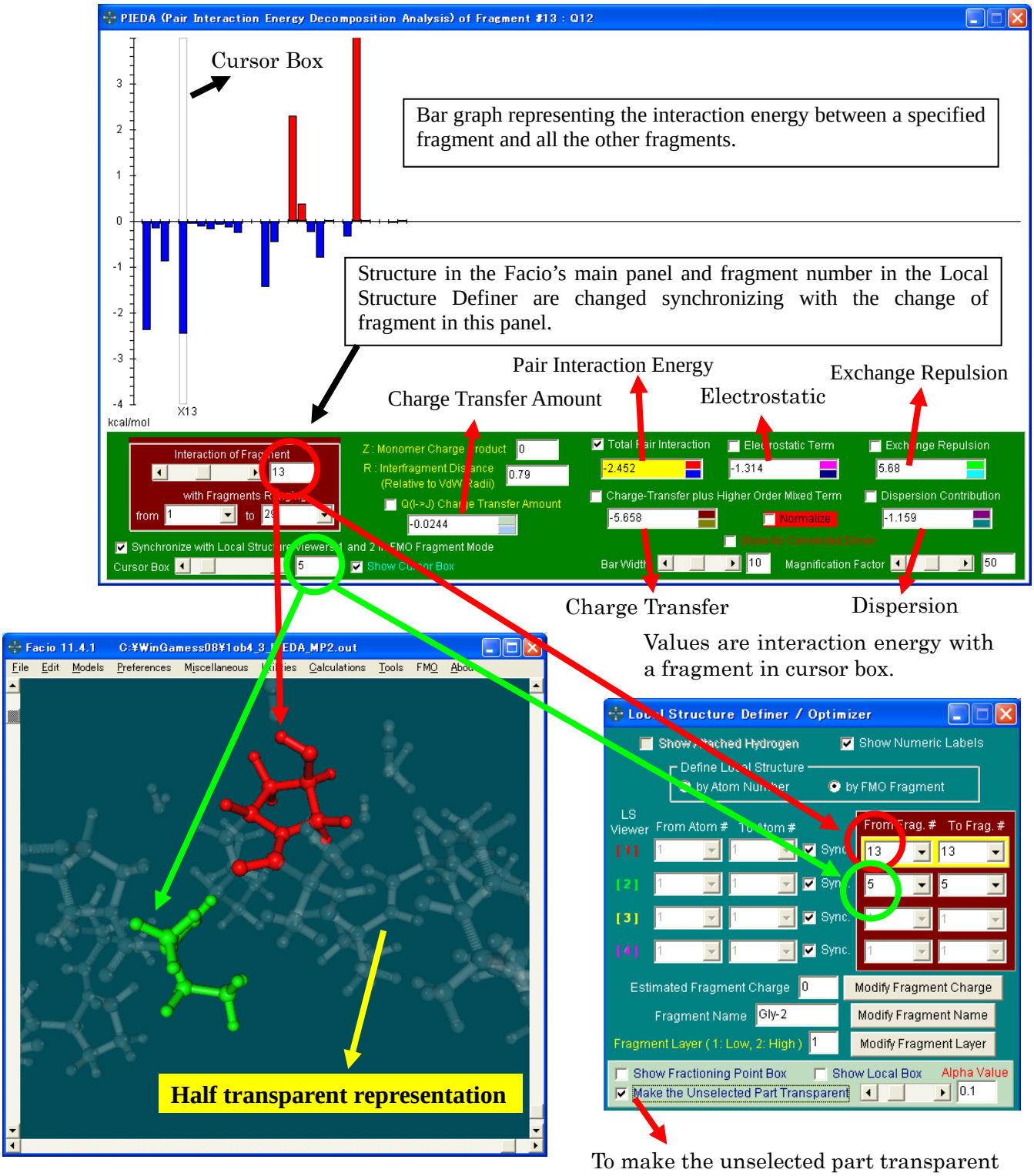
BM-1.bmp Total Pair Interaction
BM-2.bmp Electrostatic Term
BM-3.bmp Exchange Repulsion
BM-4.bmp Charge-Transfer plus Higher Order Mixed Term
BM-5.bmp Dispersion Contribution

These are just 8 x 8 bitmap files. So, you can freely change these bitmap patterns with other patters you like.

(2) FMO fragmentation of (A)-B-(C)-D, where (A) and (C) are BDA (Bond Detached Atom) is now possible. Use "Expert Mode", in the FMO Fragmentation Panel.
(3) Header file for OpenGL has been changed for compatibility with Windows Vista.
(4) CIF file is now loadable.
(5) The way to display a series of structure obtained by IRC with Gaussian was modified.
(6) GUI for setting folder for screenshot capture was changed.
(7) Outline font for showing numeric labels and atomic symbols
(8) The behavior when TER record PDB is saved as HETATM/CONECT format was modified.

----- Ver.11.4.1 ----- March 15, 2008

(1) Visualization panel for FMO PIEDA (Pair Interaction Energy Decomposition Analysis)



(2) Please notice that input file generated by Facio 11.3.1 for PIEDA calculation has an error.

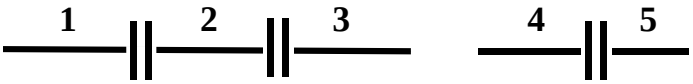
(3) Automatic generation of input file for Tinker-Amber calculation.
For detail, see the samples and ReadMe.txt in the Tinker-Amber folder.

----- Ver.11.3.1 ----- February 10, 2008

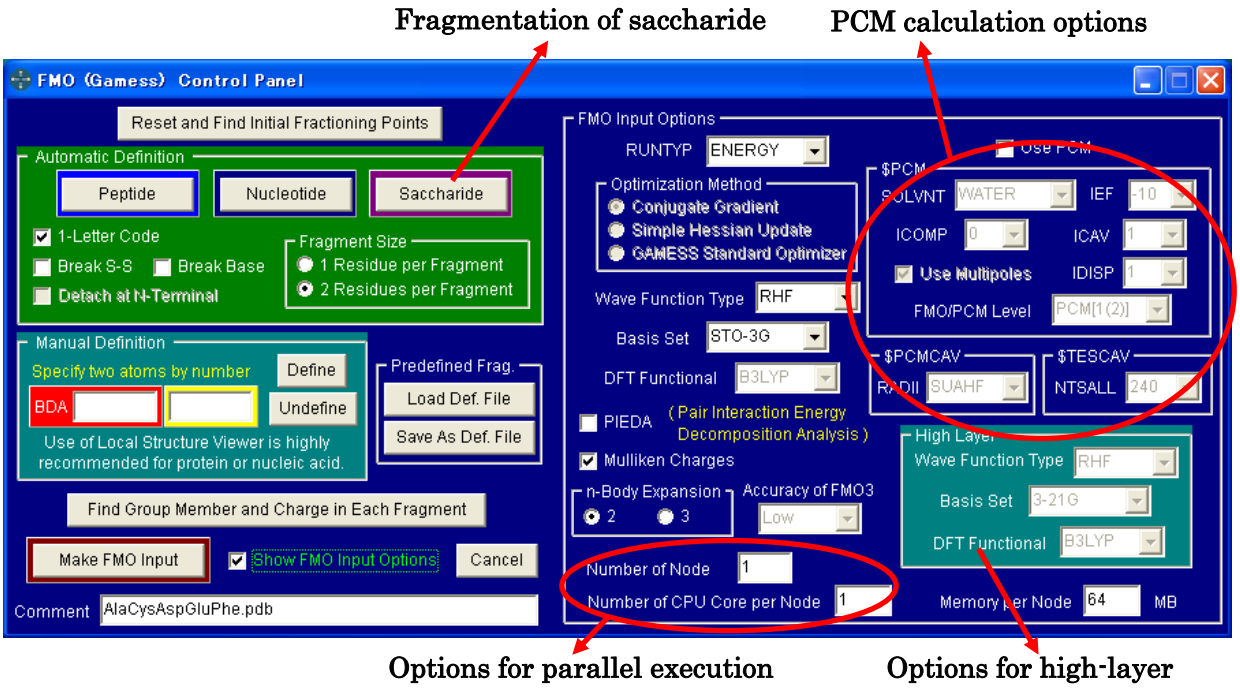
(1) Completely revised algorithm of FMO fragmentation

Up to Ver. 11.2.1, when peptide consists of more than two strands, numbering of the fragment is as shown in the scheme, where numbering is not sequential within a single strand.

The new algorithm can generate FMO fragments with sequential numbering as follows.

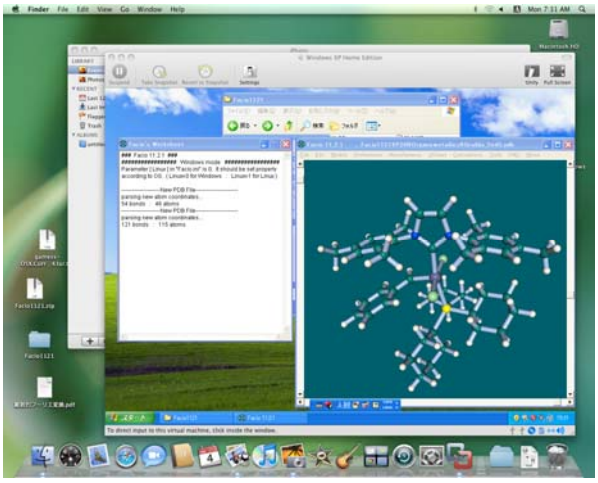


(2) New FMO input option panel



FMO layer is assigned in the Local Structure Viewer control panel.

(3) Facio on Macintosh



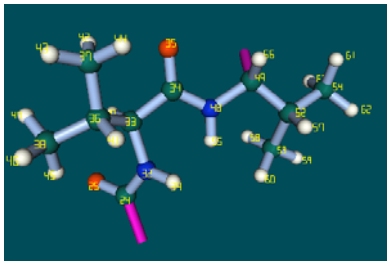
It was confirmed that Facio can work on Intel Mac, which uses Intel x86 processors.
The recommended virtual machine to run Facio is VMWare Fusion. See the screenshot.

Besides VMWare Fusion, you can use CrossOver Mac 6.21. On this environment, there are some problems. (Menu bar and slide boxes in the main window are invisible.) But the pull-down menu is visible and slide boxes can work well. Thus, they are practically no problem.

----- Ver.11.2.1 ----- November 3, 2007

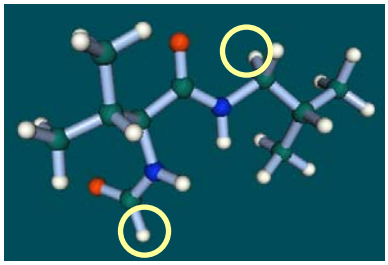
(1) Optimization of FMO fragment

FMO fragment is optimized with semi-empirical MO (PM3) or ab initio MO (STO-3G, 3-21G, 6-31GG). Keeping the position of fractioning atoms, coordinates of hydrogen atoms are optimized. Optimization of non-hydrogen atom is also possible. Dangling atoms in the fragment are capped with hydrogen or appropriate groups. (See below) Optimizations of a range of fragments or all the fragments are performed successively.

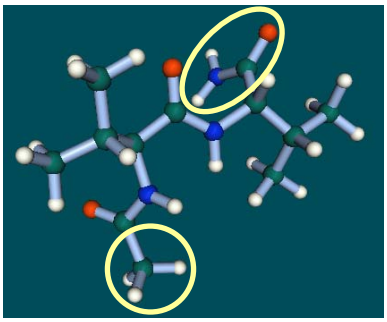


FMO fragment, in which fuchsia bonds are fractioning bond.

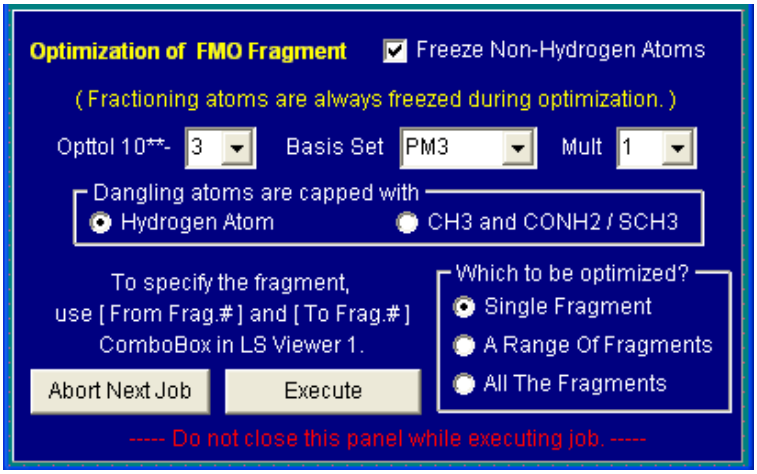
Capped with H



Capped with group



Carbonyl and alpha carbon are capped with CH_3 and CONH2, respectively.



Radio buttons to determine which fragment to be minimized. Use local structure viewer 1 to set fragment number or a range of fragment.

(2) Hybrid orbitals for sp3 S

They are requisite when fractioning atoms contain sulfur. But in the previous version of Facio, they are missing. Hybrid orbitals of STO-3G and MINI were kindly provided by Prof. Kitaura (Graduate School of Pharmaceutical Sciences, Kyoto University). Hybrid orbitals of 3-21G, 6-31G and 6-31G(d) were built by the author of Facio. The former orbitals are obtained from Gaussian NLMO of H_2S_2 and the latter ones are from GAMESS Edmiston-Ruedenberg LMO of H_2S.

(3) FMO fragment definition file

When you manually set fractioning points for FMO calculation, or when you change fragment charge which is sometimes wrong value and necessary to be fixed, or when you modify fragment name which is automatically set, you would like to save those changes in a text file. This is a FMO fragment definition file. If you load the definition file, you don't have to set fractioning point, fragment charge and fragment name any more. It is especially useful in the case that manual definition of fractioning point is necessary.

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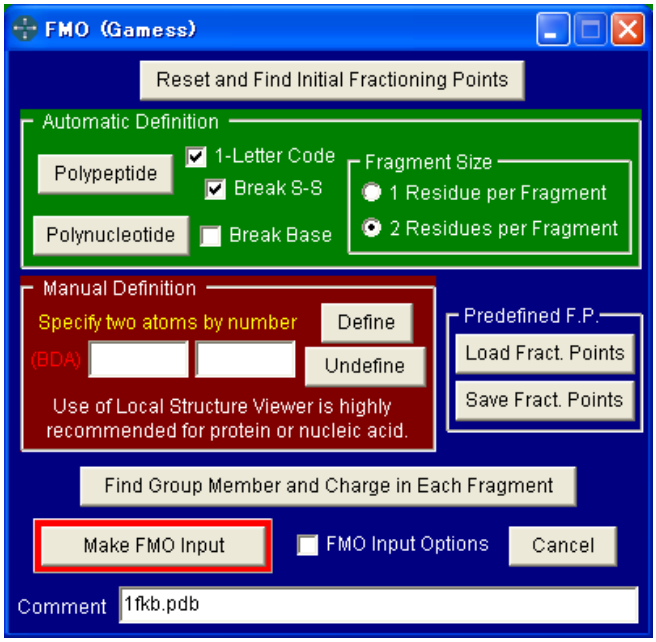
(1) GUI for FMO (Gamess)

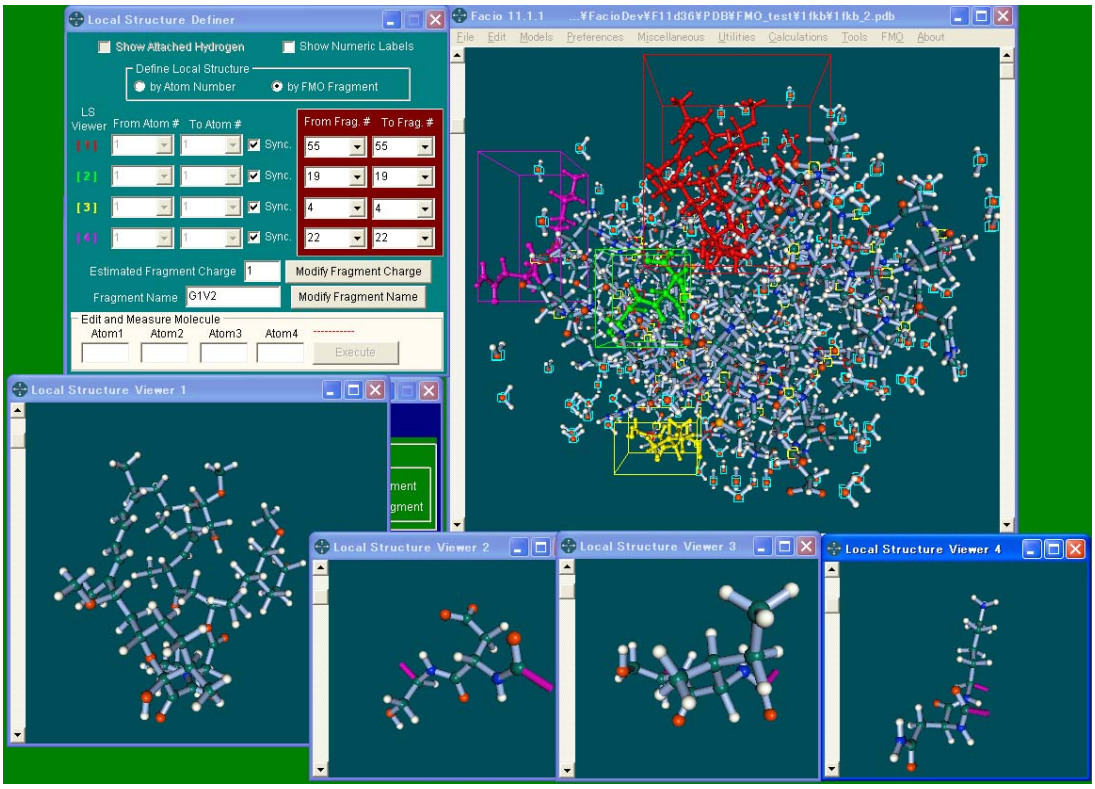
Bond fractioning for polypeptide and polynucleotide is automatically performed.
For non-peptide and non-nucleotide, you can manually define and undefine fractioning point for FMO fragment.

Input file of FMO calculation is automatically generated. For each fragment, charge is estimated and name of fragment is created based on the amino acid residue(s) therein.
INDAT array which contains the information of atom member in each fragment is set without any consideration.



(2) Local Structure Viewer

Local structure is specified by a range of atom numbers or FMO fragment numbers. There are four independent windows for the viewers. With this local structure viewer, you can edit large and complex molecules, such as protein, much easily.



1fkb.pdb (Rapamycin - FKBP12 complex)

In the above screenshot, FMO fragment #55, #19, #4 and #22 are shown in each viewer. In the whole molecule in the main window, the corresponding local structures are displayed in Red, Lime, Yellow and Fuchsia, respectively.