

***** Facio's Release History *****

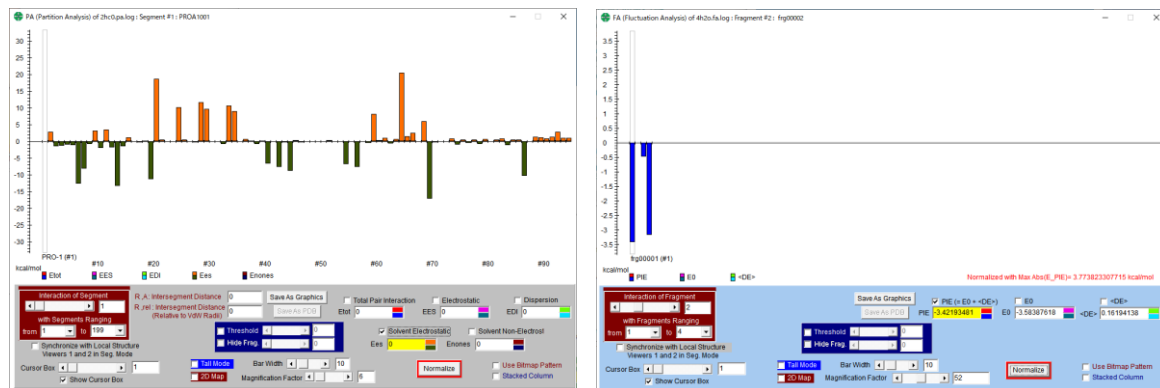
----- Ver.27.4.1 Bug fix and modification of Edit Tool Box

----- Ver.27.2.1 and 27.3.1 ----- May 24 and June 4, 2025 Bug fix

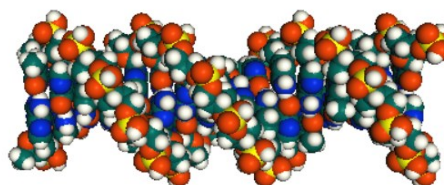
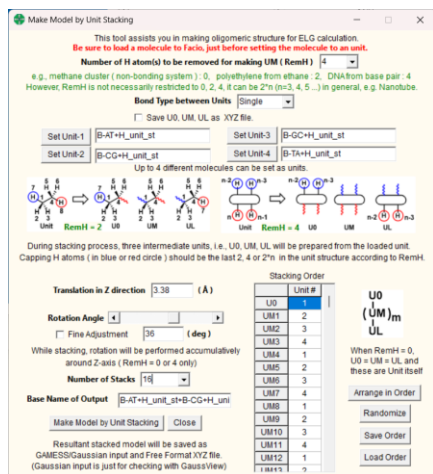
----- Ver.27.1.1 ----- April 3, 2025

(1) Visualizations of Three-body FMO properties, RC (remainder correlation, DFT) and Basis Set Correction (HF-3C) was implemented in FMO PIEDA panel.

(2) FMO PA (Partition Analysis) panel and FA (Fluctuation Analysis) panel are developed. These panels automatically pop up according to the contents of FMO calculation.

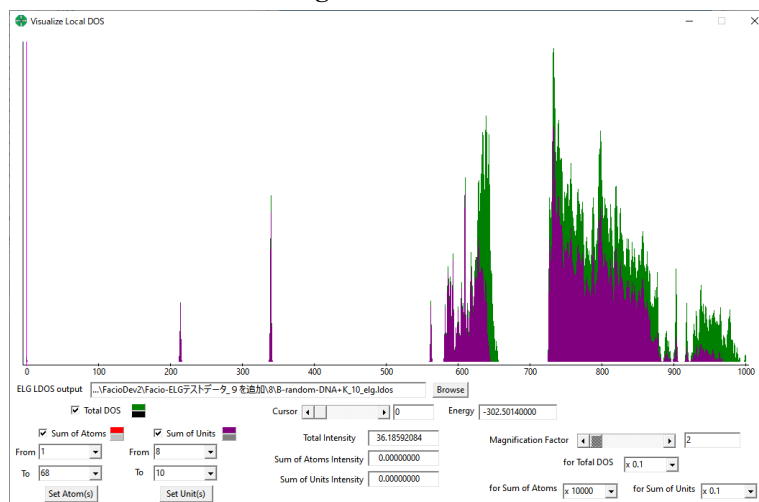


(3) Molecular modelling from unit structures and preparation of input file for Elongation method



In this example, using four base pair (AT, TA, CG and GC) as unit structures, and specifying number of stacks, DNA model and input file for Elongation method calculation.

(4) Visualization of Local DOS from Elongation calculation.



----- Ver.26.1.1 ----- January 22, 2025

FMO 5.5 (Gamess) Control Panel

Reset and Find Initial Fracturing Points

Bond Detachment: ☐ HOP ☐ AFO ☐ Bond Model: ☐ Large ☐ Small

Information or Residue Sequence Load RSG File

Residue Sequence File:

Manual Definition of Initial Fracturing Points

Add IFP: Cell IFP: Define Domain:

Enabled only when invalid IFP found or in expert mode.

Automatic Definition

☐ Conventional Peptide ☐ Conventional Nucleotide ☐ Break Nucleobase ☒ Detach at N-Terminus ☐ Combine S-LV to the neighbor ☐ Break S-L

Fragment Size (*)

1	3	5
2	4	6

(*) residue(s) per fragment

Manual Definition

Specify a pair of fracturing points by clicking: ☐ Atoms ☐ Bond

BDA BAA Exchange

Define Define

Load Def. File Save As Def. File

Find Group Member and Charge in Each Fragment

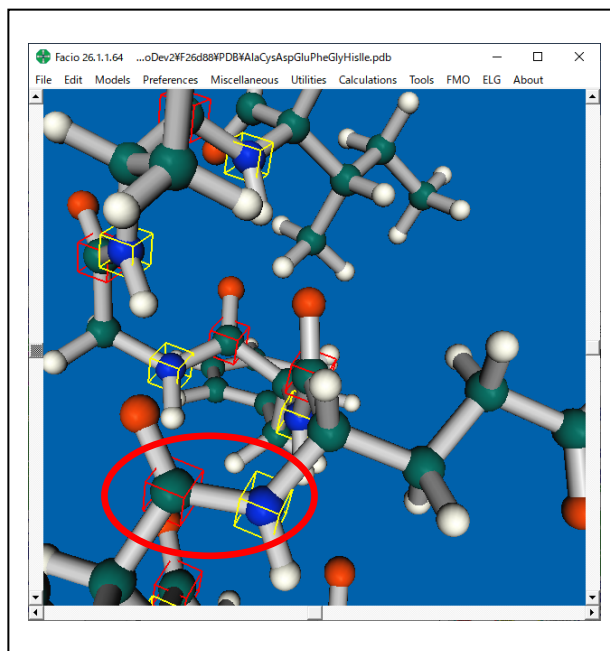
Make FMO Input ☒ Show FMO Input Options Cancel

Manual Definition of Non-Bonded Fracturing Points

These FPs are not used for bond fracturing. Used only for SFMOBND data.

Define Define

For Expert Users Only Load NBF File Save As NBF File



So far, X-axis (yellow), Y-axis (sky blue), Z-axis (lime green). Now the color of Y-axis has changed to red and the negative part of all axes are drawn in white.

Elongation Method Input

Reset and Initialize

Peptide Nucleotide Saccharide Oligo

☐ Conventional Peptide
☐ 1-Letter Code for Amino Acid
☐ Break Nucleobase
☒ Detach at N-Terminus
☐ Combine OLV to the neighbor
☐ Break S-S

Unit Size (*)
 1 2 3 4 5 6
 (*) residue(s) per unit

☐ Allow Confirmed FP

Define Underline Exchange

Load Def File Save As Def File

Find Unit Member Reassign Group Numbers

CONTROL

SCFCONV 1.00-8 SCFYPE RHF
 MULT 1 RUNTYPE ENERGY
 DETYPE NONE MAXVAL 100
 STATOPT
 OPTOL 10-4 NSTEP 100

SCFCONV 1.00-8 SYSTEM MEMORY 100000000

BASIS
 OBASE RC13 NGALUS 6
 NDFUNC 1 NFFUNC 0
 NDFUNC 0 DIFFSP 0 DIFFS

Unit member can be checked with Local Structure Viewers at FMO menu

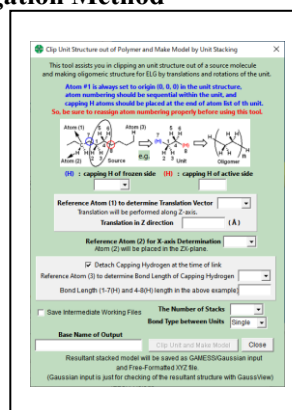
SEL0
 NMLONG 3
 NMLBS 1

SELGRP
 NBLUNT 3

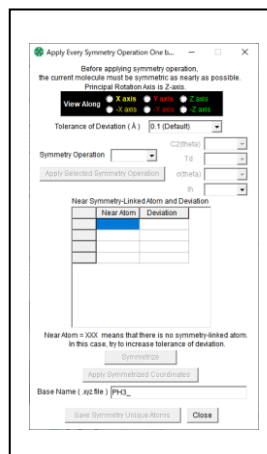
☐ Z-Matrix

Comment
 ELG.PH3.pdb

Make OLV Input Cancel



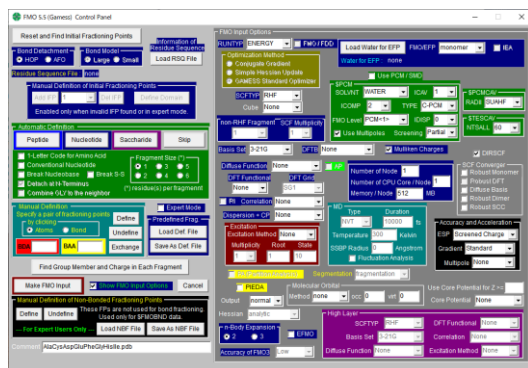
(5) Z-Matrix Editor

[illegible]

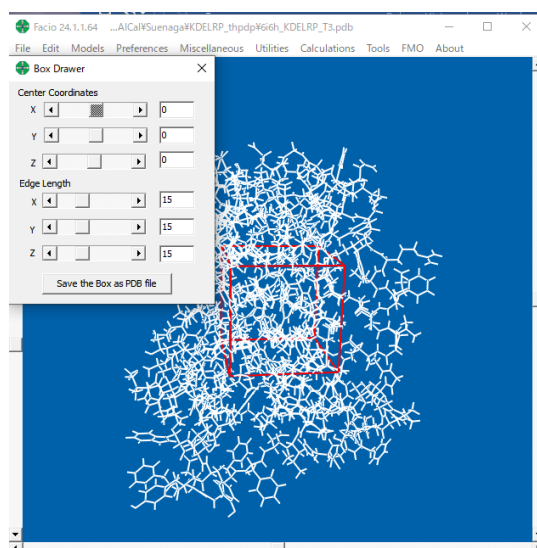
----- Ver.25.1.1 ----- April 25, 2023 Bug fix and some modifications.
 ----- Ver.24.1.3 ----- October 1, 2022 Execution of Gamess and MOPAC as Facio's child process was fully checked and revised. Implementation of invert IFREEZ at Gamess input panel.

----- Ver.24.1.2 ----- September 13, 2022
 Default of FMO/ESP was changed to "Standard"

----- Ver.24.1.1 ----- September 5, 2022



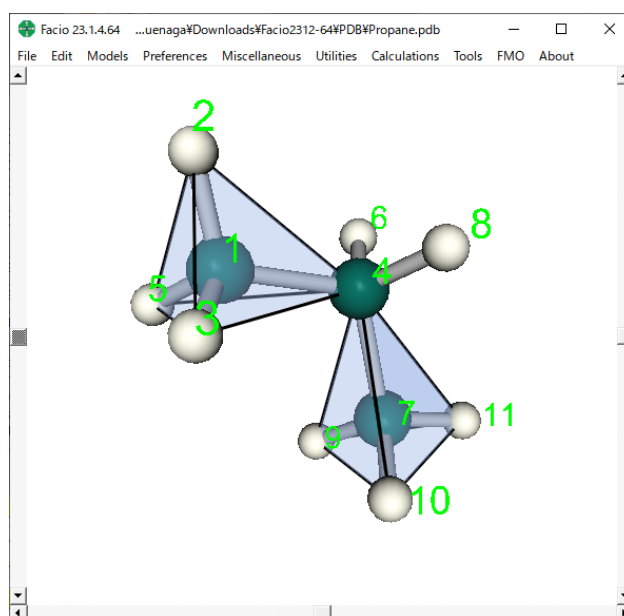
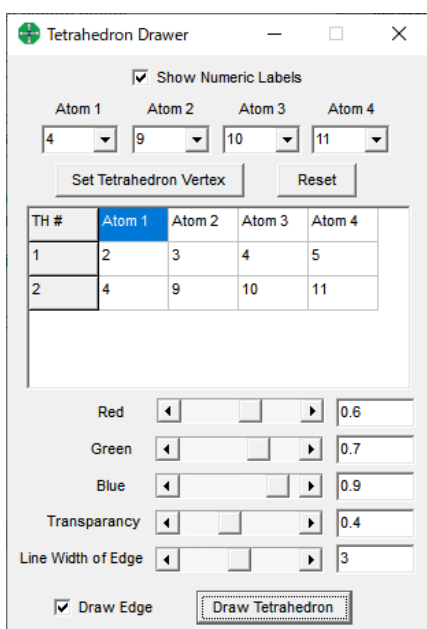
GUI for FMO 5.5



Box Drawer

----- Ver.23.1.5 ----- July 14, 2021 bug fixed
 ----- Ver.23.1.4 ----- July 1, 2021

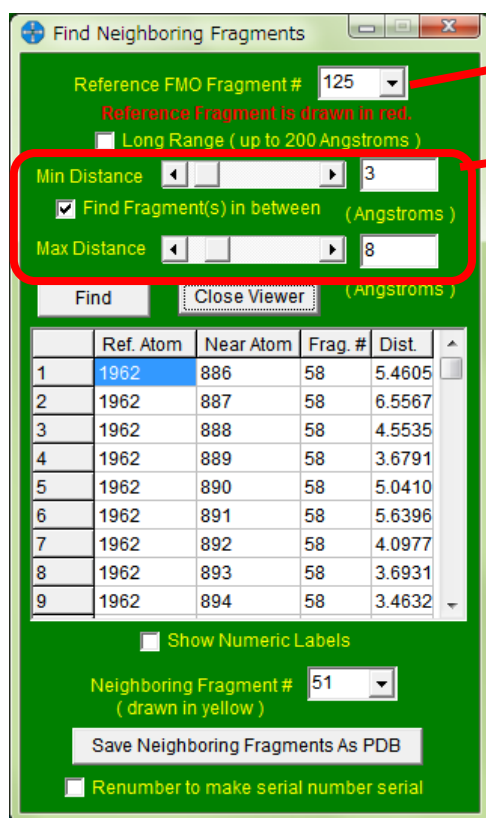
Tetrahedron Drawer has been implemented. See at Tools menu. This utility can draw translucent tetrahedron with vertices at specified atoms, as shown below.



----- Ver.23.1.3 ----- October 16, 2020 bug fixed
 ----- Ver.23.1.2 ----- October 12, 2020 Revision of GUI for FMO 5.4 for 32bit version and bug fix
 ----- Ver.23.1.1 ----- October 5, 2020 Revision of GUI for FMO 5.4 and bug fix
 ----- Ver.22.1.1 ----- December 25, 2018 Revision of GUI for FMO 5.3 and bug fix
 ----- Ver.21.2.1 ----- October 19, 2018 bug fixed
 ----- Ver.21.1.1 ----- April 24, 2018 64bit version released and bug fixed
 ----- Ver.20.1.3 ----- September 12, 2017 bug fixed
 ----- Ver.20.1.2 ----- August 17, 2017 bug fixed
 ----- Ver.20.1.1 ----- August 12, 2017 Revision of GUI for FMO

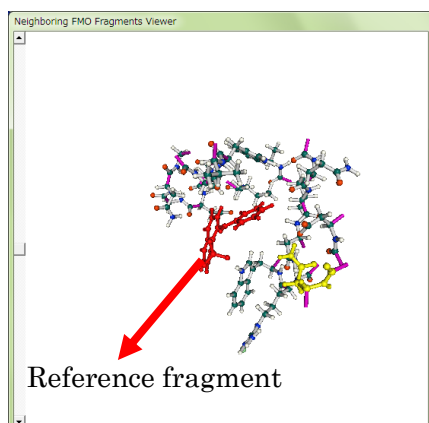
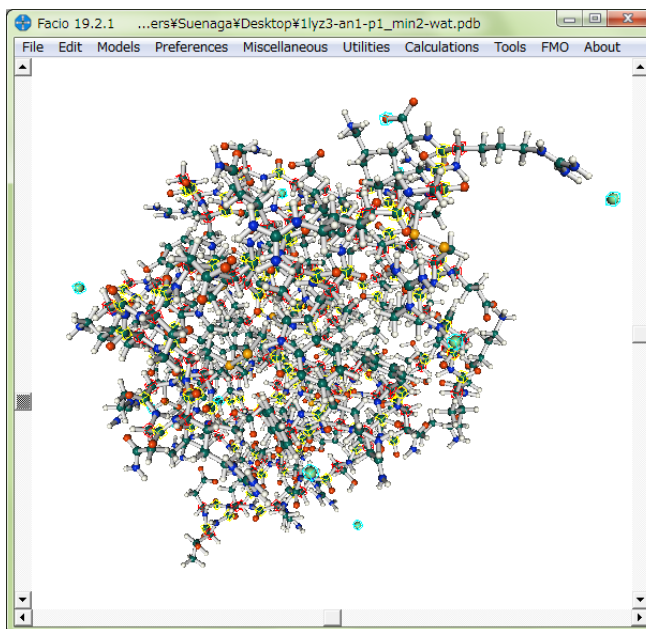
----- Ver.19.2.1 ----- July 23, 2016

Revision of the function “Find Neighboring Fragments” in FMO menu.

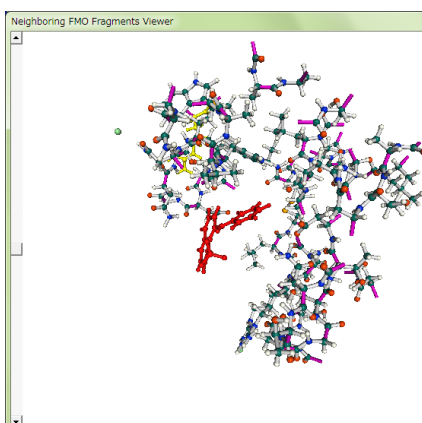


Reference fragment

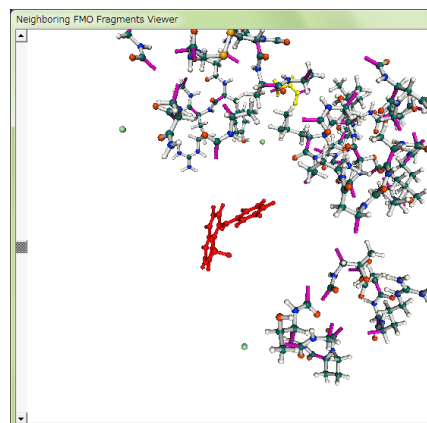
Range that defines “neighboring fragments”



within 5-10 Angstroms



within 10-15 Angstroms



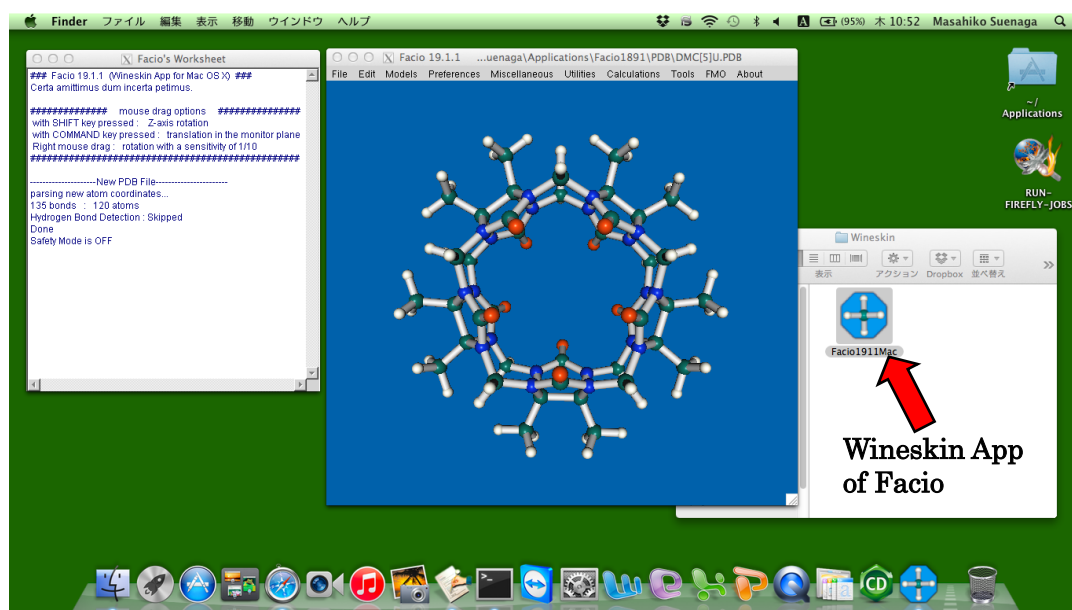
within 15-20 Angstroms

---- Ver.19.1.7 ---- May 25, 2016 Minor bug fix for MOPAC2016 ver.16
 ---- Ver.19.1.6 ---- February 17, 2016 Bug fix for Summarize Energy/Grad/Geometry Change
 ---- Ver.19.1.5 ---- February 3, 2016 Bug fix for Summarize Energy/Grad/Geometry Change
 ---- Ver.19.1.4 ---- July 18, 2015 Minor bug fix for NMR Shielding Tensor reading
 ---- Ver.19.1.3 ---- April 23, 2015 For two different output formats of MOPAC 6.06
 ---- Ver.19.1.2 ---- April 9, 2015 Minor bug fix for MOPAC2012 ver.15
 ---- Ver.19.1.1 ---- April 4, 2015

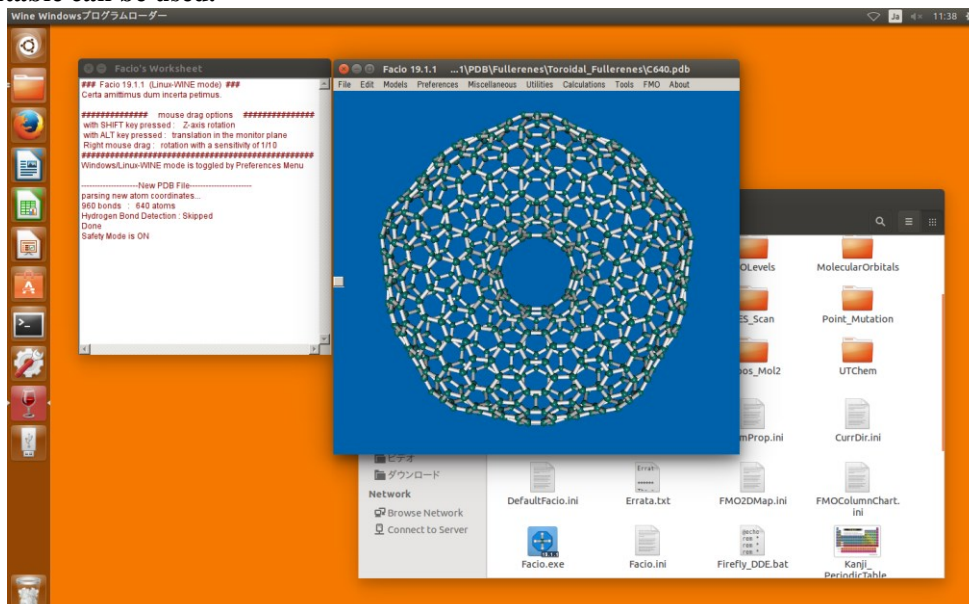
The behavior of Facio on Mac OS X or Ubuntu Linux, especially in executing external programs (such as, Tinker, MSMS, MOPAC, Firefly and Gamess) as Facio's child process, has been fully examined and revised.

For Tinker, MSMS, MOPAC2012, please use Windows executable even if on Mac OS X or Linux environment. For Firefly or Gamess (US), see below.

Wineskin App version of Facio is now available for Mac OS X.

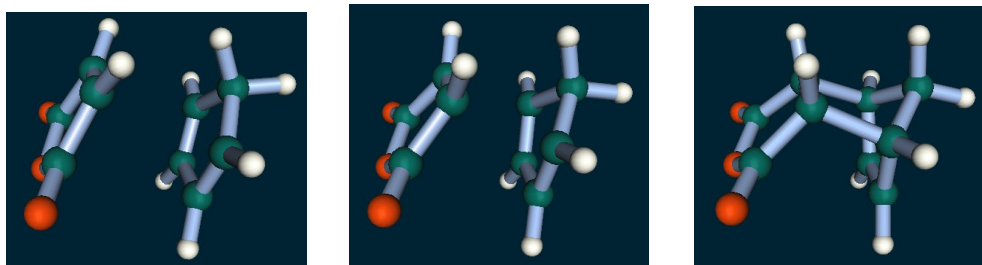
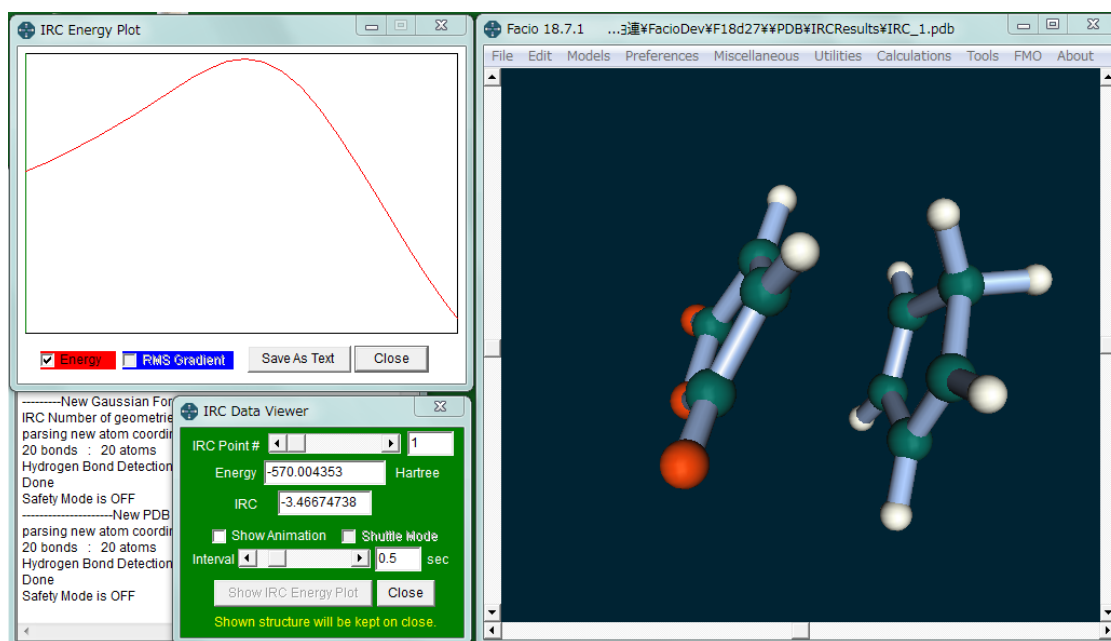


If you want to use Facio on Ubuntu Linux, be sure to install wine by typing “sudo apt-get install wine” and set Facio to Linux-WINE mode. On Ubuntu Linux, both Windows and Linux version of Firefly can be used with Facio as in Windows environment. For Gamess (US), only Linux executable can be used.



- Ver.18.8.2 ----- October 24, 2014 Bug about reading MOPAC2012 Ver.14 calculations of 1 atom and 2 atoms molecule was fixed.
- Ver.18.8.1 ----- August 14, 2014 Bug in the routine which finds bonds to isolated hydrogen atom was fixed. This bug has influenced possibly to FMO fragmentation since ver. 16.1.1.
- Ver.18.7.4 ----- July 26, 2014 Bug about Gamess's current directory fixed
- Ver.18.7.3 ----- July 1, 2014
 \$DATA record of FMO input file was incomplete in Facio 18.6.1 to 18.7.2. Bug fixed.
- Ver.18.7.2 ----- June 28, 2014
 Minor modification to the function of recording Gaussian's current directory
- Ver.18.7.1 ----- June 16, 2014

- (1) IRC Viewer has been fully revised. Each structure at respective IRC point is saved as PDB in the PDB\IRCResults in Facio's root folder. With this change, bonds are properly displayed at each IRC point as shown below.

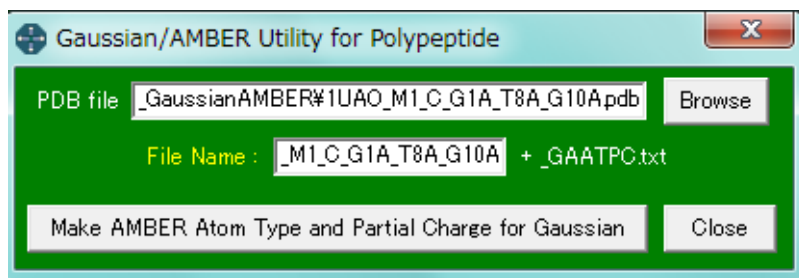


Transition State

- (2) Output format of MOPAC2012 Ver.14 and Ver.13 are slightly different in the part of Cartesian Coordinate. Facio is now compatible with both version.
- (3) %NProc in Gaussian Link 0 has been changed to %NProcShared.
- (4) Current directory for the respective PDB, Gamess, Gaussian and Gaussian formatted check files are now saved in CurrDir.ini in the Facio's root folder. This function will be useful when you change folder to save or read these files.

----- Ver.18.6.2 ----- April 12, 2014
Bug related to the execution of Tinker/newton.exe was fixed.

----- Ver.18.6.1 ----- April 5, 2014
Function to generate atom type and partial charge data for Gaussian/AMBER calculation from protein PDB file has been implemented.



Gaussian/AMBER Utility in Tools Menu

-N3-0.1414
-CT-0.0962
-C-0.6163
-O--0.5722
-CT--0.0597
-H-0.1997
-H-0.1997
-H-0.1997
-HP-0.0889
-HC-0.0300
...
...

Atom Type and Partial Charge

Amber Opt

*** GaussianAMBER ***

-2	1			
N1		-6.778000	-1.424000	4.200000
C2		-6.878000	-0.708000	2.896000
C3		-5.557000	-0.840000	2.138000
O4		-4.640000	-1.504000	2.579000
C5		-7.165000	0.737000	3.141000
H6		-5.778000	-1.527000	4.462000
H7		-7.214000	-2.365000	4.112000
H8		-7.273000	-0.879000	4.933000
H9		-7.677000	-1.140000	2.309000
H10		-7.347000	1.267000	2.189000
...				
...				

Delete serial
number

Amber Opt

*** GaussianAMBER ***

-2	1			
N		-6.778000	-1.424000	4.200000
C		-6.878000	-0.708000	2.896000
C		-5.557000	-0.840000	2.138000
O		-4.640000	-1.504000	2.579000
C		-7.165000	0.737000	3.141000
H		-5.778000	-1.527000	4.462000
H		-7.214000	-2.365000	4.112000
H		-7.273000	-0.879000	4.933000
H		-7.677000	-1.140000	2.309000
H		-7.347000	1.267000	2.189000
...				
...				

Paste atom type
and partial charge

Gaussian/AMBER
calculation

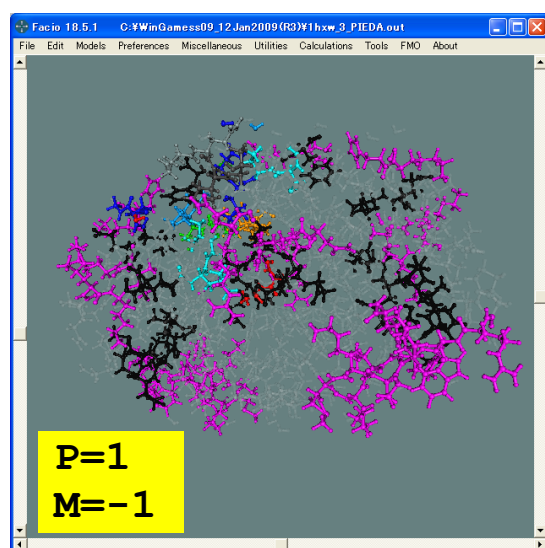
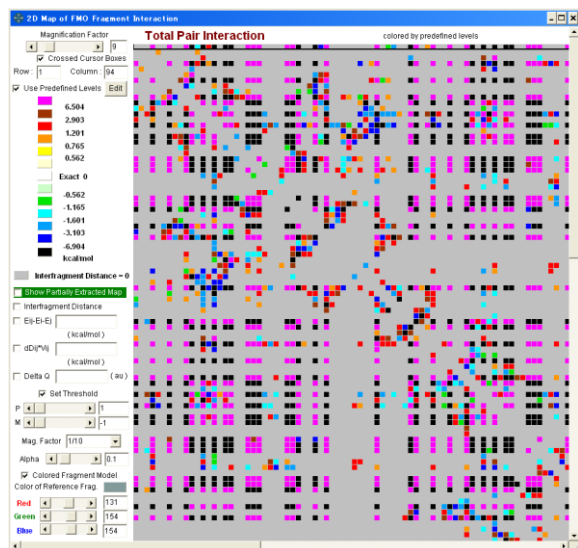
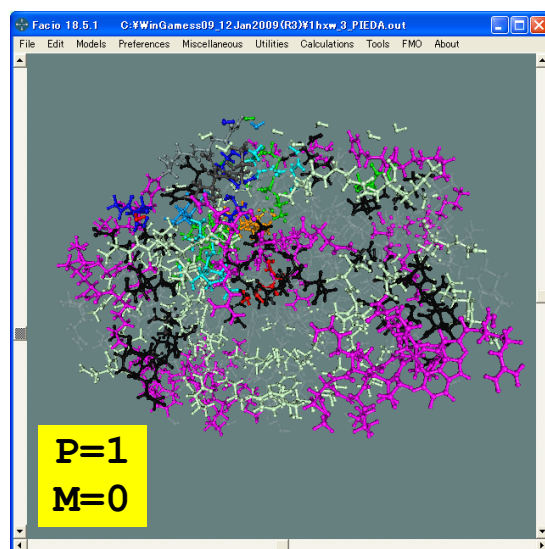
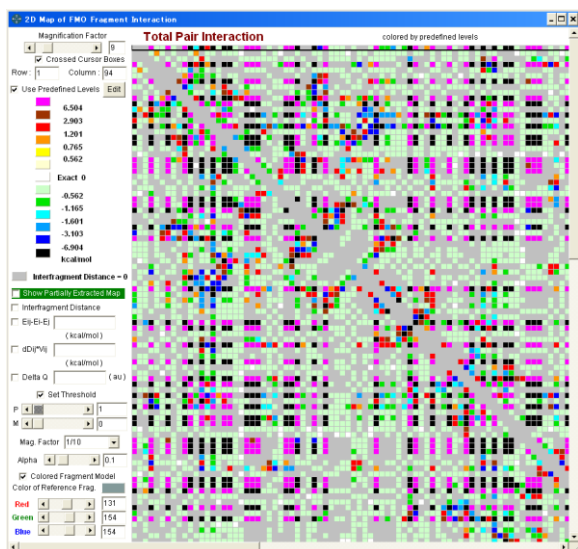
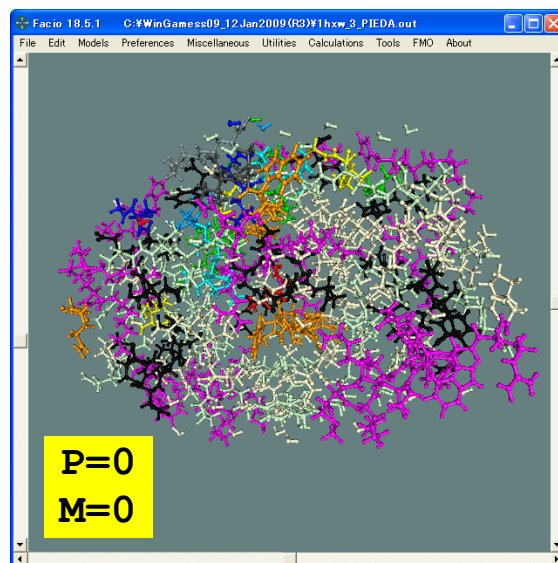
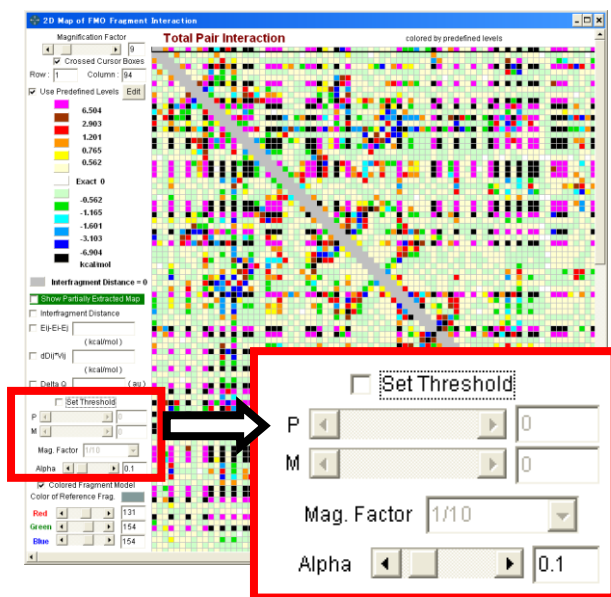
Amber Opt

*** GaussianAMBER ***

-2	1			
N	N3-0.1414	-6.778000	-1.424000	4.200000
C	CT-0.0962	-6.878000	-0.708000	2.896000
C	C-0.6163	-5.557000	-0.840000	2.138000
O	O--0.5722	-4.640000	-1.504000	2.579000
C	CT--0.0597	-7.165000	0.737000	3.141000
H	H-0.1997	-5.778000	-1.527000	4.462000
H	H-0.1997	-7.214000	-2.365000	4.112000
H	H-0.1997	-7.273000	-0.879000	4.933000
H	HP-0.0889	-7.677000	-1.140000	2.309000
H	HC-0.0300	-7.347000	1.267000	2.189000
...				
...				

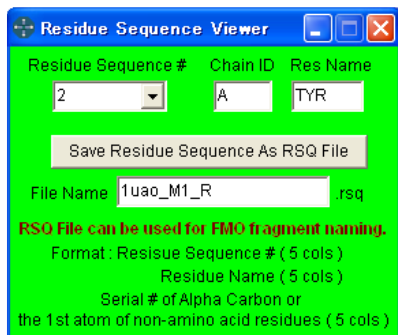
----- Ver.18.5.2 ----- February 1, 2014 Minor bug fixes version
 ----- Ver.18.5.1 ----- December 14, 2013

Fragments which have lower interaction energies than specified threshold can be displayed as white translucent models. The translucency can be adjusted by alpha value (default=0.1).



- (1) Residue name and number in PDB can be utilized for FMO fragment name. This function is useful especially when residue number starts from other than 1.

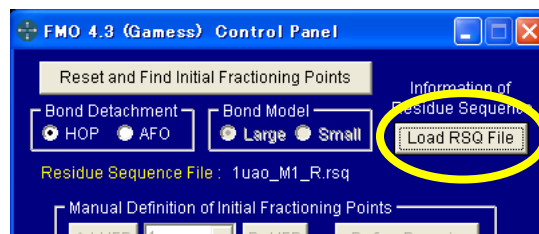
FMO Menu > PDB Utilities >
Residue Sequence Viewer



Residue name, number and the atom number of alpha carbon are saved as RSQ file.

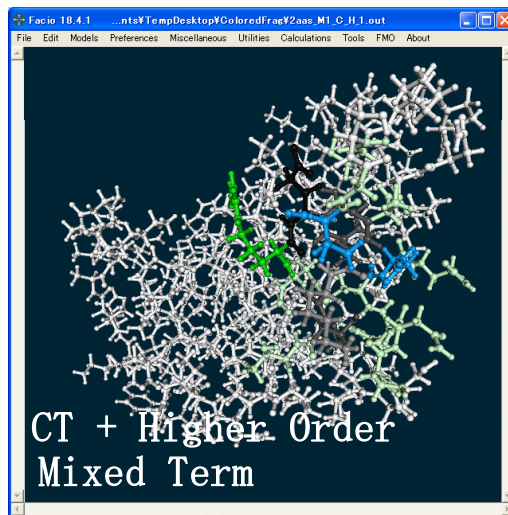
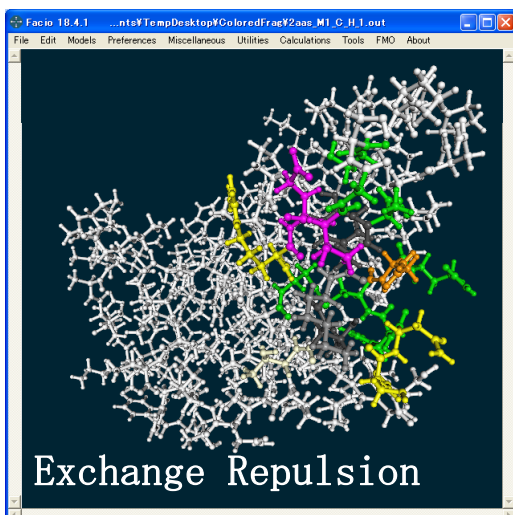
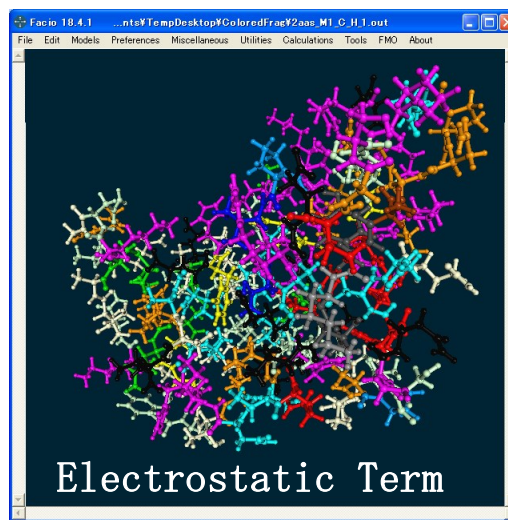
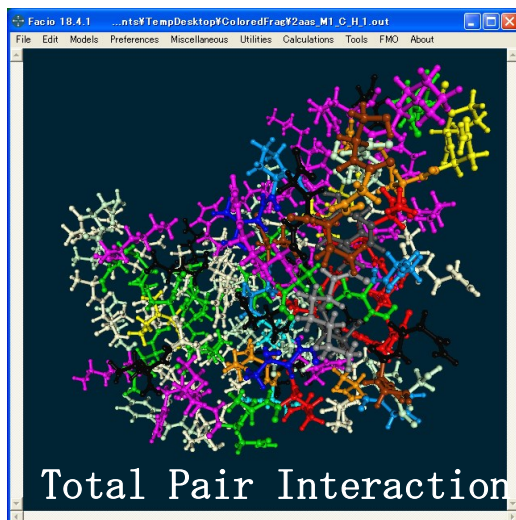
32	GLY	2
33	ALA	15
34	GLU	25
35	LEU	40
36	LEU	59
37	SER	78
38	GLN	89
39	GLN	106
40	TRP	123

RSQ file



Load RSQ file, before making FMO fragment.

- (2) FMO Fragment can be colored according to the interaction energies. To enable this function, see FMO 2D Map of Fragment Interaction panel.



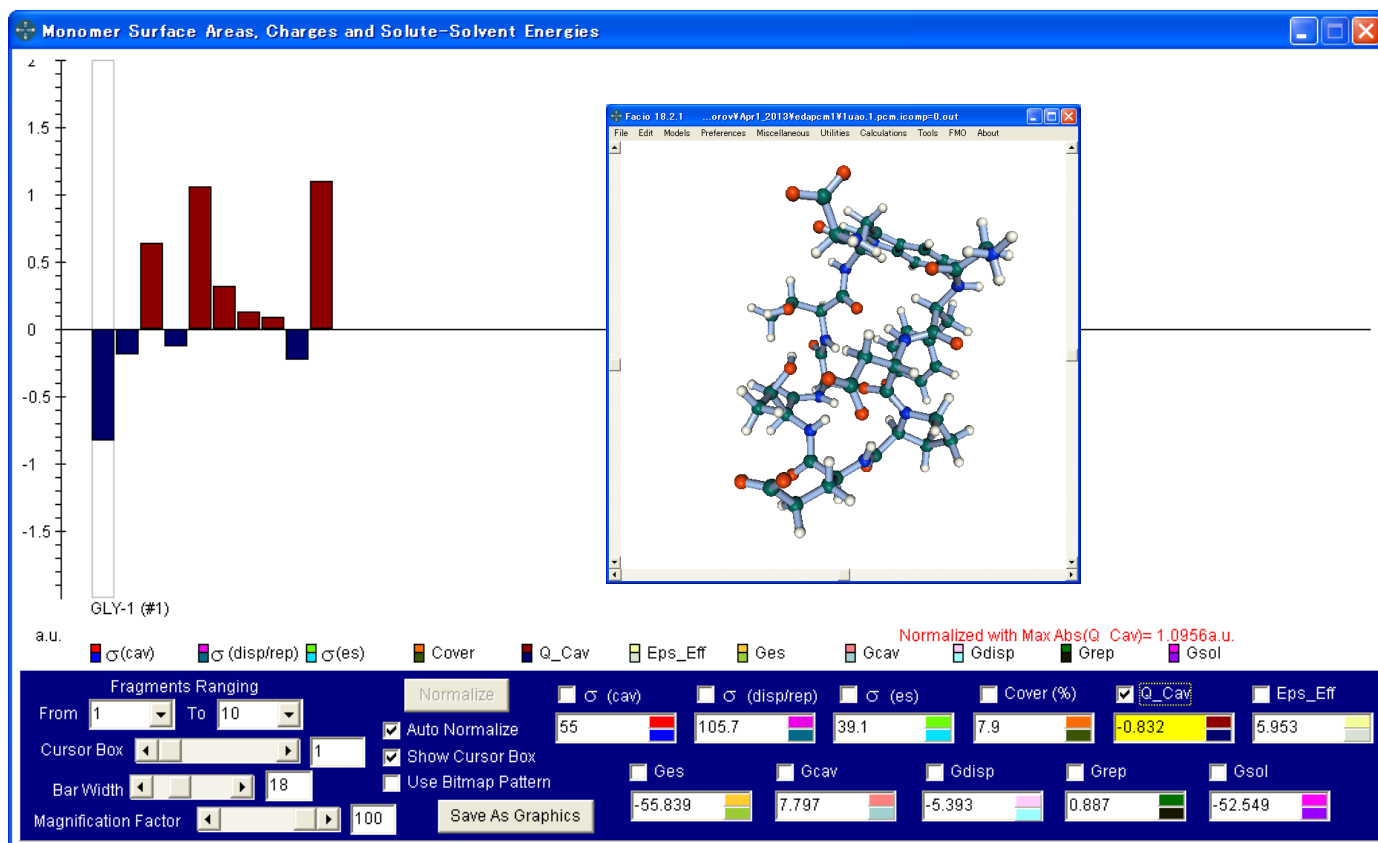
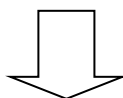
----- Ver.18.3.1 ----- August 31, 2013 Bug fix

----- Ver.18.2.1 ----- August 17, 2013

(1) Visualization of fragment properties and pair interaction energies in solution, computed with FMO/PCM.

Monomer surface areas (in Å²), charges (a.u.) and solute-solvent energies (kcal/mol).

I		surf_cav	disp/rep	surf_es	cover,%	q_cav	eps_eff	Ges	Gcav	Gdisp	Grep	Gsol
1	(GLY-1)	55.0	105.7	39.1	7.9	-0.8320	5.953	-55.839	7.797	-5.393	0.887	-52.549
2	(TYR-2)	139.9	107.5	56.6	11.4	-0.1865	0.000	-7.014	18.871	-7.198	1.038	5.697
3	(ASP-3)	78.5	56.3	36.3	7.3	0.6364	2.750	-44.025	10.512	-3.198	0.516	-36.195
4	(PRO-4)	82.5	84.7	34.1	6.9	-0.1293	0.000	-0.670	11.404	-5.161	0.761	6.336
5	(GLU-5)	107.6	159.1	74.4	15.0	1.0617	-16.207	-71.093	14.511	-9.263	1.424	-64.421
6	(THR-6)	76.1	72.0	38.5	7.8	0.3186	0.000	-7.465	10.432	-4.005	0.590	-0.448
7	(GLY-7)	44.3	41.2	22.4	4.5	0.1317	0.000	-4.375	5.997	-2.166	0.369	-0.174
8	(THR-8)	87.0	95.8	41.6	8.4	0.0877	0.000	-6.946	11.989	-5.640	0.837	0.240
9	(TRP-9)	161.9	206.9	85.6	17.3	-0.2301	0.000	-6.334	21.831	-13.948	1.924	3.473
10	(GLY-10)	95.2	124.5	66.9	13.5	1.0956	-10.459	-85.693	12.682	-7.004	1.154	-78.860



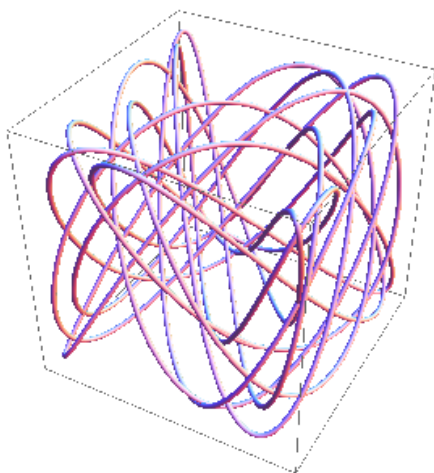
Ref. *J. Phys. Chem. A* 2012, 116, 704-719. D. G. Fedorov and K. Kitaura
 "Energy Decomposition Analysis in Solution Based on the Fragment Molecular Orbital Method"

(1) Quaternion Rotation

Rotations of molecular model in 3D by mouse movement was completely revised and quaternion rotation has been implemented. With this revision, all the problems related to 3D rotation has been fixed.

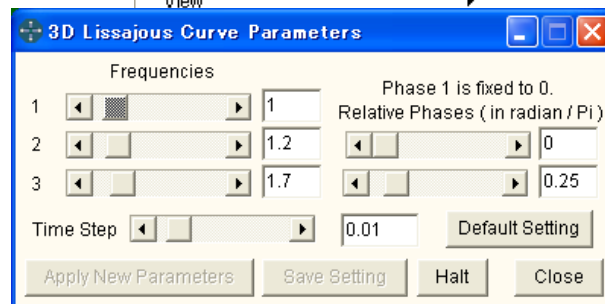
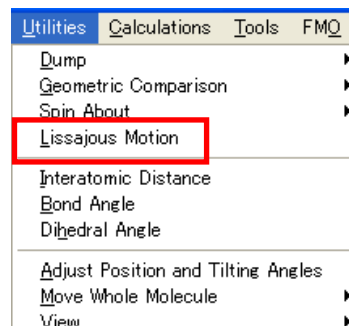
(2) Lissajous Motion

Having implemented quaternion rotation, very complex rotation, such as Lissajous motion is now possible. This feature is useful for demonstration of molecular models.



3D Trajectory of Lissajous motion simulated by Mathematica

Utilities Menu

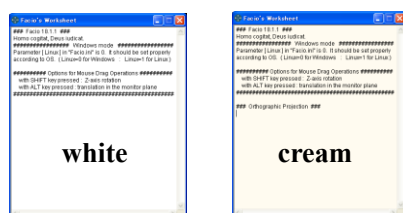


Controller of 3D Lissajous Curve Parameters

(3) Orthographic Projection

Orthographic projection was also completely revised and mouse click operation, such as atom selection, is now possible as in perspective projection.

The background color of Facio's Worksheet changes according to the projection type.



Perspective

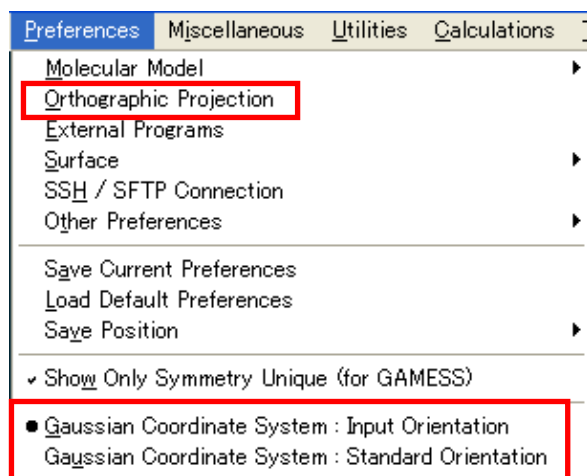
Orthographic

(4) Input Orientation and Standard Orientation

There are two coordinate systems in Gaussian, i.e. input orientation and standard orientation. When you see structural change during geometry optimization process, input orientation is suitable. If you use standard orientation for this purpose, you will see sudden structural change. (cf. NoSymm keyword will prevents such molecular reorientation.)

On the other hand, when you see dipole moment, standard orientation is required. If you use input orientation instead, incorrect vector will be displayed.

Preferences Menu



----- Ver.17.1.2 ----- May 29, 2013 Bug fix
 ----- Ver.17.1.1 ----- May 3, 2013 New GUI for FMO 4.3

FMO 4.3 (Gamess) Control Panel

Reset and Find Initial Fractioning Points

Bond Detachment: ☒ HOP ☐ AFO Bond Model: ☒ Large ☐ Small Information of Residue Sequence: Load RSQ File

Residue Sequence File: none

Manual Definition of Initial Fractioning Points

Add IFP: 1 Del IFP: Define Domain: Enabled only when invalid IFP found or in expert mode.

Automatic Definition

Peptide Nucleotide Saccharide Skip

☐ 1-Letter Code for Amino Acid ☐ Break S-S ☐ Break Base ☐ Detach at N-Terminal ☐ Combine GLY to the neighbor

Fragment Size: ☒ 1 Residue per Fragment ☐ 2 Residues per Fragment

Manual Definition

Specify a pair of fractioning points by clicking: ☒ Atoms ☐ Bond Define: Undefine: Exchange: BDA: BAA: Predefined Frag.: Load Def. File: Save As Def. File: Expert Mode: ☐

Find Group Member and Charge in Each Fragment

Make FMO Input: ☒ Show FMO Input Options: Cancel

Manual Definition of Non-Bonded Fractioning Points

Define: Undefine: These FPs are not used for bond fractioning. Used only for \$FMOBND data.

--- For Expert Users Only --- Load NBF File: Save As NBF File: Comment: 1UAO_M1m.pdb

FMO Input Options

RUNTYP: ENERGY Load Water for EFP: FMO/EFP monomer IEA: ☐

Water for EFP: none Use PCM: ☐

Optimization Method: ☐ Conjugate Gradient ☐ Simple Hessian Update ☒ GAMESS Standard Optimizer

Wave Function: RHF

non-RHF Fragment: 1 SCF Multiplicity: 1

Basis Set: 3-21G Diffuse Function: None DFT Functional: None DFT Grid: SG1

☐ RI Correlation: None Dispersion: None

Excitation: Excitation Method: None Multiplicity: 1 Root: 1 State: 10

n-Body Expansion: ☒ 2 ☐ 3 EFMO: ☐

Accuracy of FMO3: Low

MD: Type: NVE Duration: 10000 fs Temperature: 300 Kelvin SSBP Radius: 0 Angstrom

SCF Converger: ☐ Robust Monomer ☐ Robust DFT ☐ Diffuse Basis ☐ Robust Dimer ☐ Robust SCC

Accuracy and Acceleration: ESP: Standard Gradient: Standard Multipole: None

High Layer: Wave Function: RHF Basis Set: 3-21G Diffuse Function: None DFT Functional: None Correlation: None Excitation Method: None

\$PCM: SOLVNT: WATER ICAV: 1 ICOMP: 2 TYPE: C-PCM Use Multipoles: ☒ IDISP: 1 FMO/PCM Level: PCM(1(2))

\$PCMCAY: RADII: SUAHF \$TESCAV: NTSALL: 60

For backward compatibility, GUI for FMO 4.1 or before is still available. See FMO menu bar.

FMO 4.1 (Gamess) Control Panel

Reset and Find Initial Fractioning Points

Bond Detachment: ☒ HOP ☐ AFO Bond Model: ☒ Large ☐ Small Information of Residue Sequence: Load RSQ File

Manual Definition of Initial Fractioning Points

Add IFP: 1 Del IFP: Define Domain: Enabled only when invalid IFP found or in expert mode.

Automatic Definition

Peptide Nucleotide Saccharide Skip

☐ 1-Letter Code for Amino Acid ☐ Break S-S ☐ Break Base ☐ Detach at N-Terminal ☐ Combine GLY to the neighbor

Fragment Size: ☒ 1 Residue per Fragment ☐ 2 Residues per Fragment

Manual Definition

Specify a pair of fractioning points by clicking: ☒ Atoms ☐ Bond Define: Undefine: Exchange: BDA: BAA: Predefined Frag.: Load Def. File: Save As Def. File: Expert Mode: ☐

Find Group Member and Charge in Each Fragment

Make FMO Input: ☒ Show FMO Input Options: Cancel

Manual Definition of Non-Bonded Fractioning Points

Define: Undefine: These FPs are not used for bond fractioning. Used only for \$FMOBND data.

--- For Expert Users Only --- Load NBF File: Save As NBF File: Comment: 1UAO_M1m.pdb

FMO Input Options

RUNTYP: ENERGY Use PCM: ☐ Load Water for EFP: IEA: ☐

Optimization Method: ☐ Conjugate Gradient ☐ Simple Hessian Update ☒ GAMESS Standard Optimizer

Wave Function Type: RHF

Basis Set: 3-21G Add Diffuse Functions on Carboxylate: ☒ Dispersion: none

DFT Functional: B3LYP DFT Grid: Lebedev

☒ Mulliken Charges ☒ PIEDA n-Body Expansion: ☒ 2 ☐ 3 Accuracy of FMO3: Low

SCF Converger: ☐ Robust Monomer ☐ Robust Dimer ☐ Robust DFT ☐ Robust SCC ☐ Diffuse Basis

High Layer: Wave Function Type: RHF Basis Set: 3-21G DFT Functional: B3LYP

\$PCM: SOLVNT: WATER ICAV: 1 ICOMP: 2 IEF: C-PCM Use Multipoles: ☒ IDISP: 1 FMO/PCM Level: PCM(1(2))

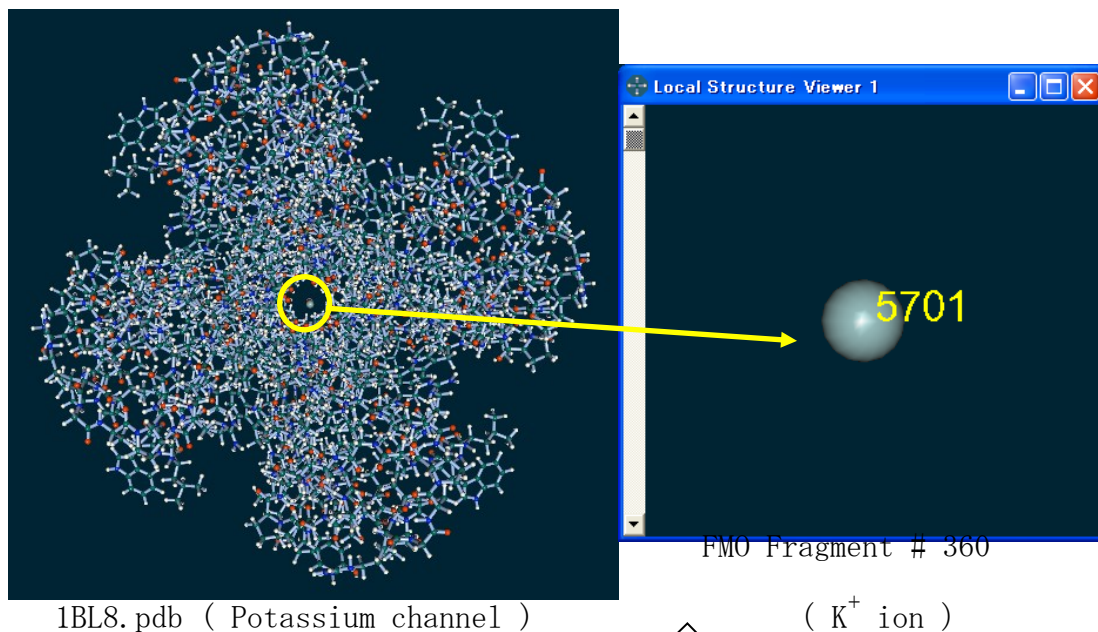
\$PCMCAY: RADII: SUAHF \$TESCAV: NTSALL: 60

Number of Node: 1 Number of CPU Core per Node: 1 Memory per Node: 64 MB

Residue Sequence File: none Water for EFP: none

----- Ver.16.3.1 ----- Aug 4, 2012 Bug fixes and some modifications
 ----- Ver.16.2.1 ----- May 26, 2012 Bug fixes and some modifications
 ----- Ver.16.1.1 ----- March 30, 2012

(1) New function to find neighboring FMO fragments within specified distance and save them as PDB.



Find Neighboring Fragments

Reference FMO Fragment # 360

Min Distance 4 (Angstroms)

Find

Close Viewer

☐ Show Numeric Labels
Reference Fragment is drawn in red

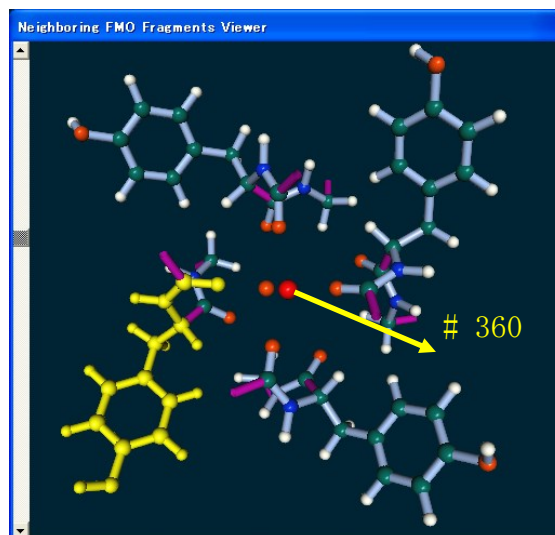
	Ref. Atom	Near Atom	Frag. #	Dist.
1	5701	790	50	3.1346
2	5701	796	51	3.6585
3	5701	797	51	3.0811
4	5701	820	51	3.4881
5	5701	2215	140	3.1195
6	5701	2221	141	3.6411
7	5701	2222	141	3.0659
8	5701	2245	141	3.4662
9	5701	3640	230	3.1492

Neighboring Fragment(s) # 50 (Drawn in yellow)

Save Neighboring Fragments As PDB

☒ Renumber to make serial number serial

Finding neighboring FMO fragments within 4 Angstroms of # 360.



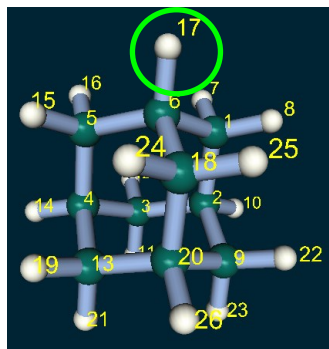
Neighboring fragments :
 # 50, 51, 140, 141, 230, 231, 320, 320, 321 and 363

Save as PDB

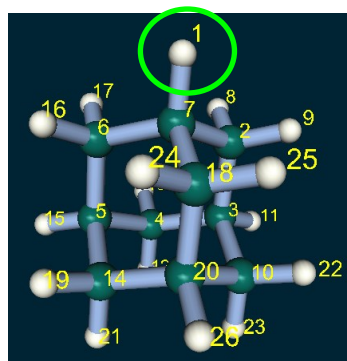
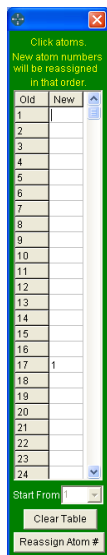
----- Ver.15.1.2 ----- January 22, 2012 Compatible with GAMESS VERSION = 11 AUG 2011 (R1)

----- Ver.15.1.1 ----- July 18, 2011

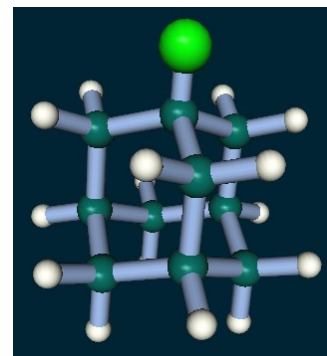
(1) User defined substituent



Example to make
1-adamantyl from
adamantane



Change atom #17 to #1 with
Utilities menu >> Reassign
Atom Numbers.

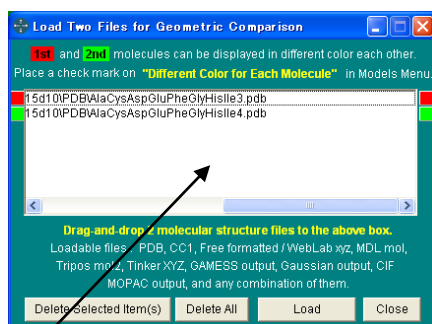


Save as User Defined
Substituent from File menu

How to use : Place check mark on User Defined Substituent of "Replace H with" in Edit menu.
Then click the hydrogen to be substituted. Substituent list will appear. Select substituent you want.

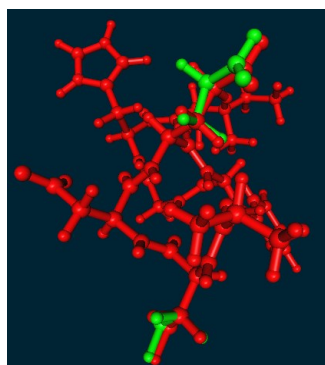
(2) RMS fit

Geometry Comparison >>
Load Two Molecules for Geometry Comparison
in the Utilities menu



Drag & drop two structures to be compared.

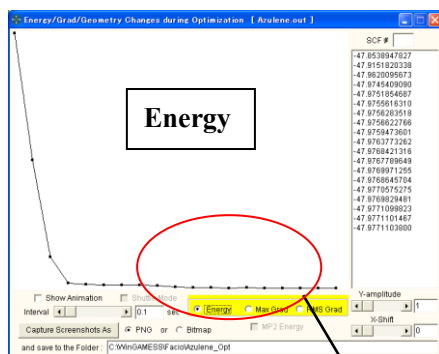
Geometry Comparison >> RMS Fit by Quaternion
in the Utilities menu



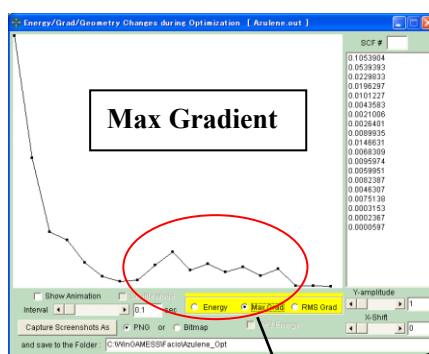
Different Colors for
Two Molecules in
the Models menu.

(3) Compatible with new FMO 4.0 features (gradient and optimization with PCM, and empirical dispersion correction)

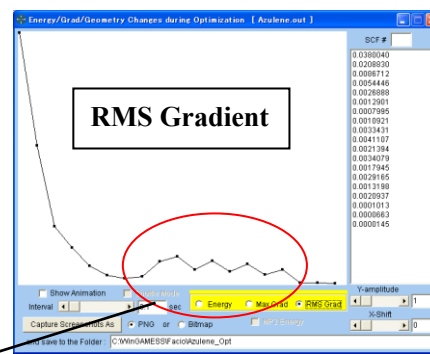
(4) Max and RMS gradient changes during optimization are shown as a graph, such as below.



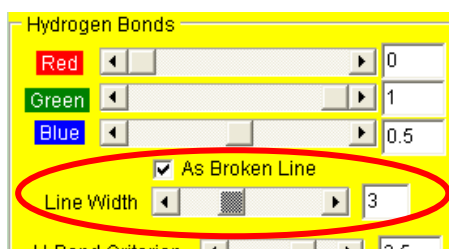
Energy seems to be converged...



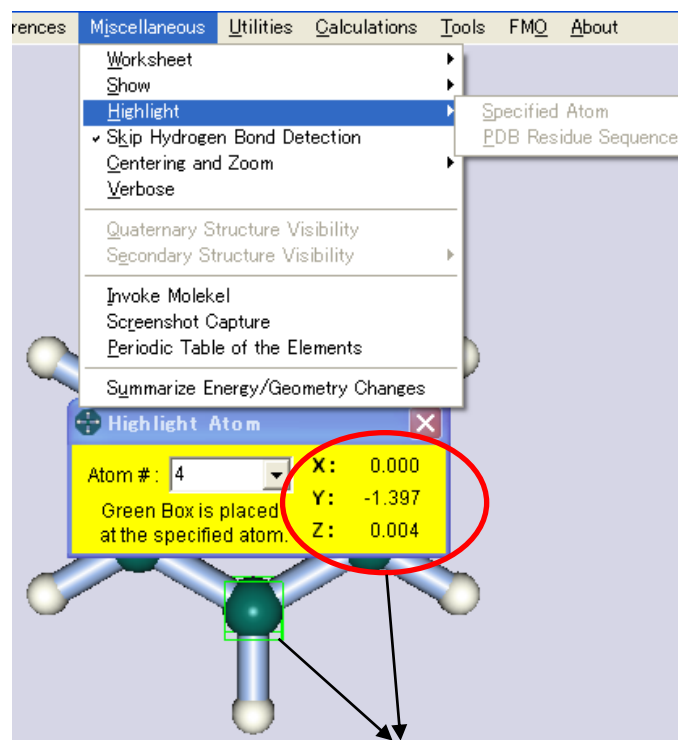
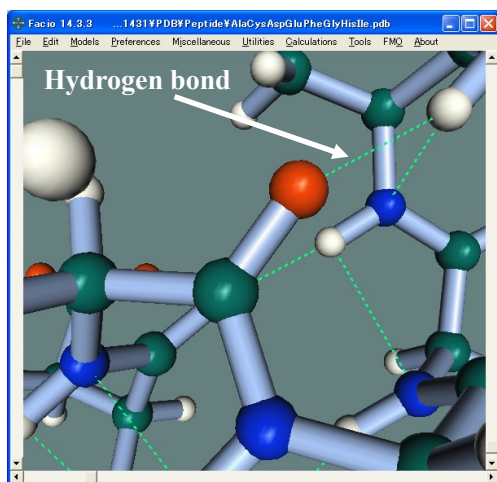
But it's not yet.



----- Ver.14.3.3 ----- March 28, 2011 Bug fixes and new representation of hydrogen bond.



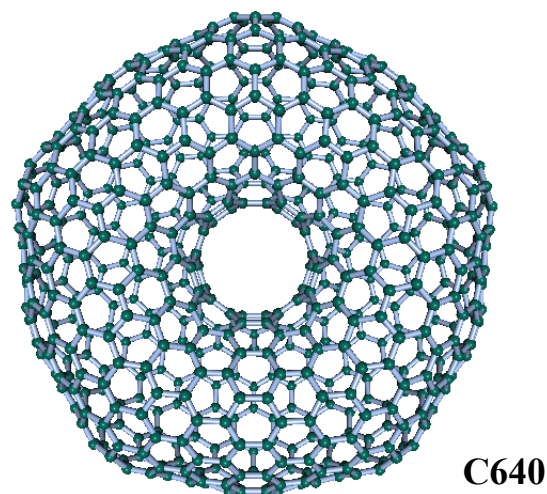
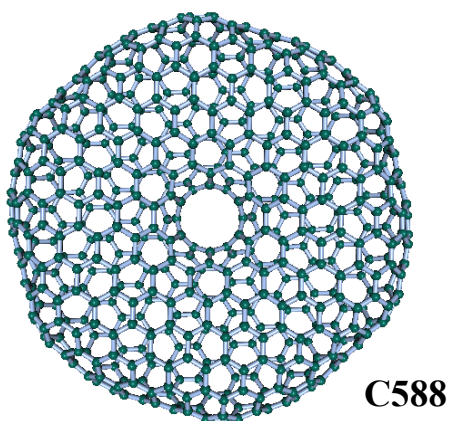
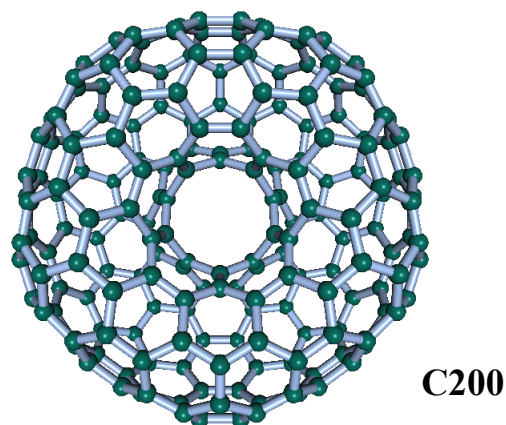
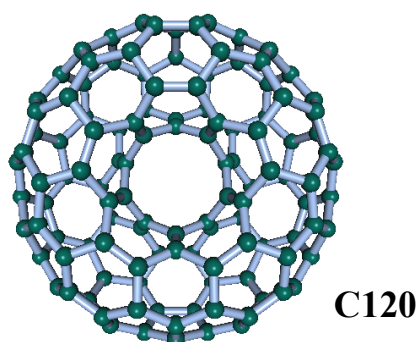
Bond Properties in Preferences menu



Highlighted atom and its coordinate

----- Ver.14.3.2 ----- November 6, 2010 Bug fixes and toroidal fullerene models

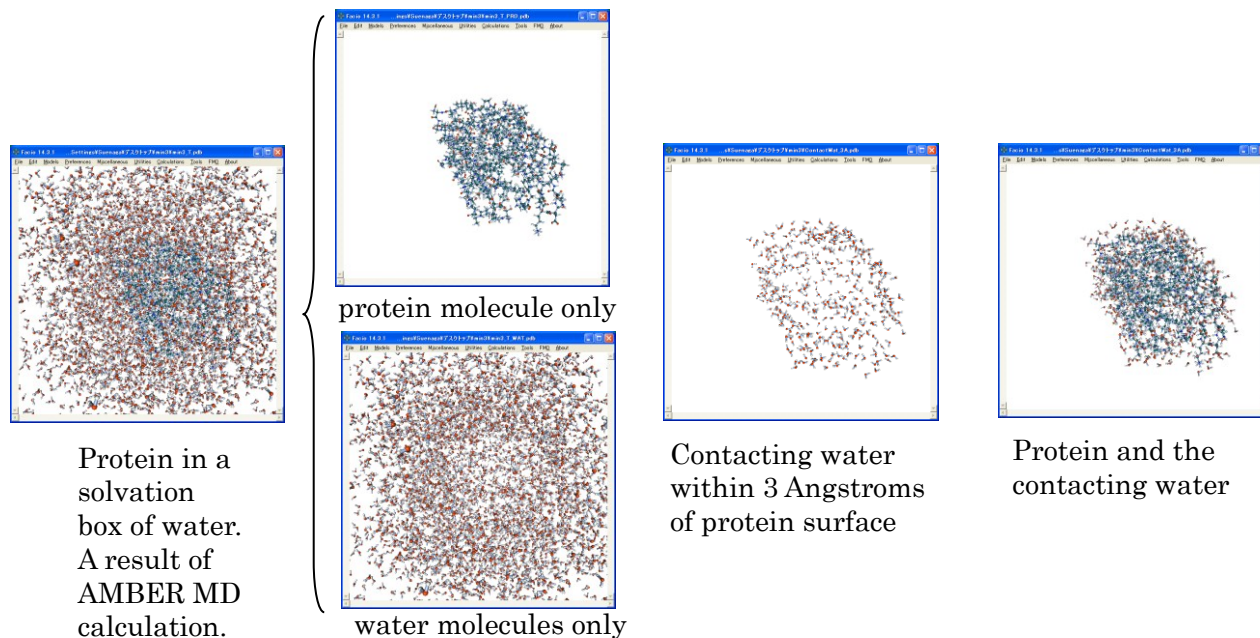
Toroidal Fullerenes



(1) New feature of PDB Utilities

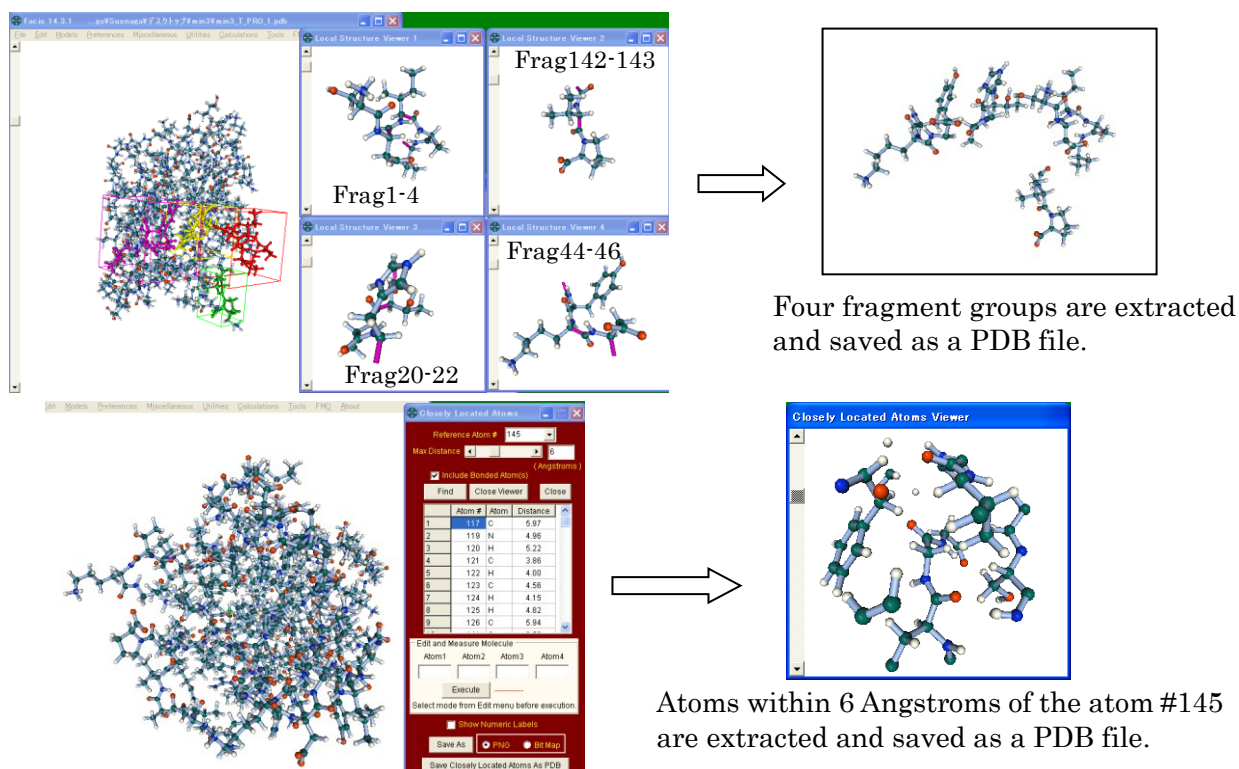
It can find contacting water within a specified distance from solvated molecule.

For example, solvated protein is divided into protein molecule only PDB and water molecules only PDB. Using these two files, Facio will search and find contacting water within a specified distance and save as a PDB file.



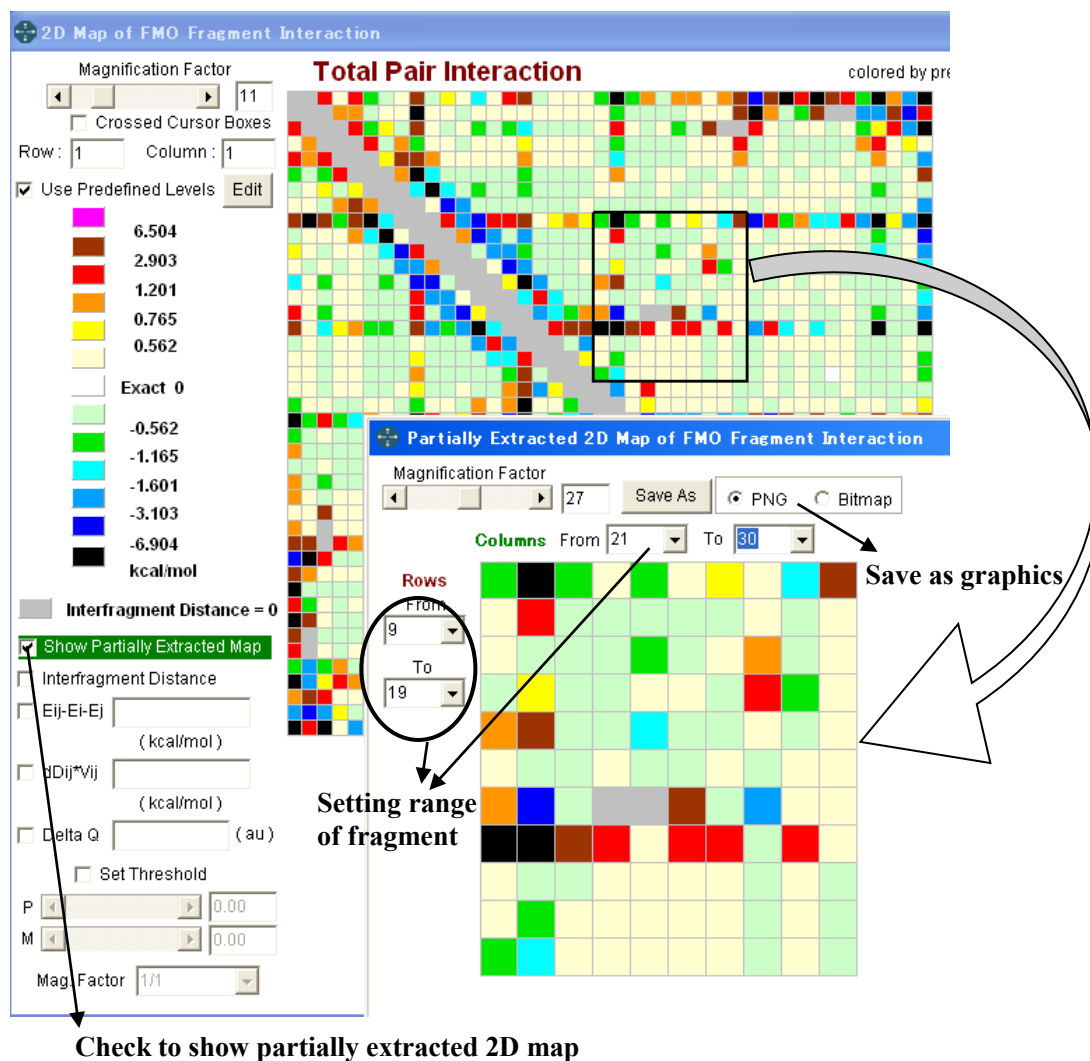
Contacting waters can be used as EFP (Effective Fragment Potential) of Gamess/FMO calculation. For such calculation, input file can be automatically created. Just specify the PDB file of the contacting water by clicking "Load Water for EFP" button in the FMO control panel.

(2) FMO fragments shown in Local Structure Viewer and atoms found in Closely Located Atoms panel can be saved as a PDB file.



----- Ver.14.2.4 -----	March 19, 2010	Bug fixes
----- Ver.14.2.3 -----	March 14, 2010	Bug fixes and some modifications
----- Ver.14.2.2 -----	January 9, 2010	Compatible with Firefly (PC GAMESS) 7.1.G
----- Ver.14.2.1 -----	December 25, 2009	

(1) Any part of FMO's PIEDA 2D map can be extracted and shown in new window as shown below.



(2) Two-body FMO properties can be saved as reloadable file for Facio in Gamess version = 24 MAR 2007 (R6) format. See FMO menu >> Save PIEDA in Gamess Output Format

This feature makes it possible to create FMO difference file from two FMO difference files.

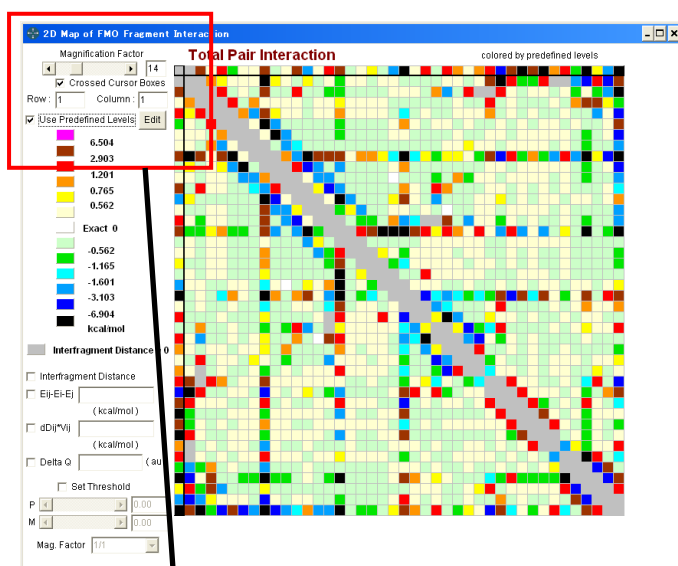
To the name of output file, suffix '_PIEDA_' is added by default. If you want to use other suffix, please edit SavePIEDA_Suffix parameter of [AppControl] section in the Facio.ini file.

(3) Molecular model editor function on Closely Located Atoms Viewer

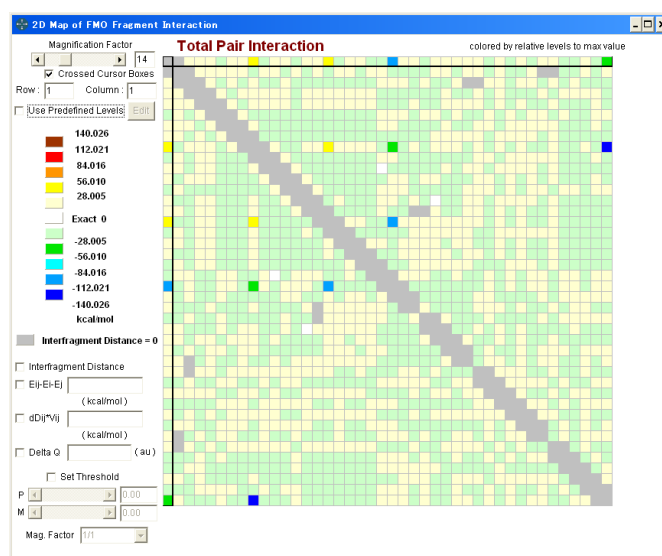
This new feature makes it possible to edit partial molecular model created by Closely Located Atoms Viewer. How to use : select mode from Edit menu and type the relevant atom number in the textbox, Atom1, Atom2, Atom3 and Atom4, then click Execute button.

Closely Located Atoms Viewer can find and show atoms which are within specified distance from specified atom.

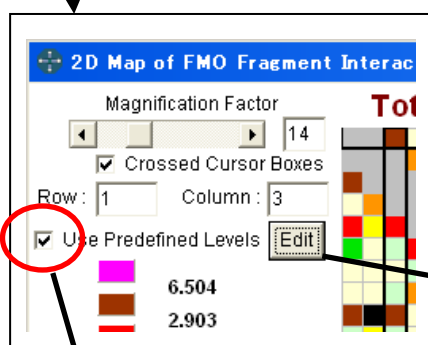
- (1) 2D map representation of two-body FMO properties has been fully revised : energy levels to determine colors of the map can be predefined by user. This new feature makes it possible to visualize small energy difference as shown below.



New representation



Old representation



Checkbox to use predefined energy levels which determine colors of the 2D map. (Default = Checked)

If it is not checked, automatically defined energy levels are used.

Level	Value (kcal/mol)
Level_5	6.504
Level_4	2.903
Level_3	1.201
Level_2	0.765
Level_1	0.562
Level_M1	-0.562
Level_M2	-1.165
Level_M3	-1.601
Level_M4	-3.103
Level_M5	-6.904

Editor to set energy level values.

Levels to be modified are relevant to the currently displayed energies on the 2D map.

Symmetrize button is to symmetrize energy levels with respect to positive or negative values.

All the energy levels are saved in the FMO2Dmap.ini in the Facio's root folder.

----- Ver.13.1.1 ----- September 24, 2009 Updated to be compatible with Gaussian 09 outputs

----- Ver.12.2.1 ----- September 12, 2009

Algorithm of FMO fragmentation has been revised for very special cases, such as solid surface.

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

(1) New feature of PDB utilities

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

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

(2) The default behavior of hydrogen bond detection

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

SkipHBondDetection=1 (Skip hydrogen bond detection)

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

(3) New amino residues are available for Polypeptide Builder

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

Hid (Histidine with hydrogen on the delta nitrogen)

Hie (Histidine with hydrogen on the epsilon nitrogen)

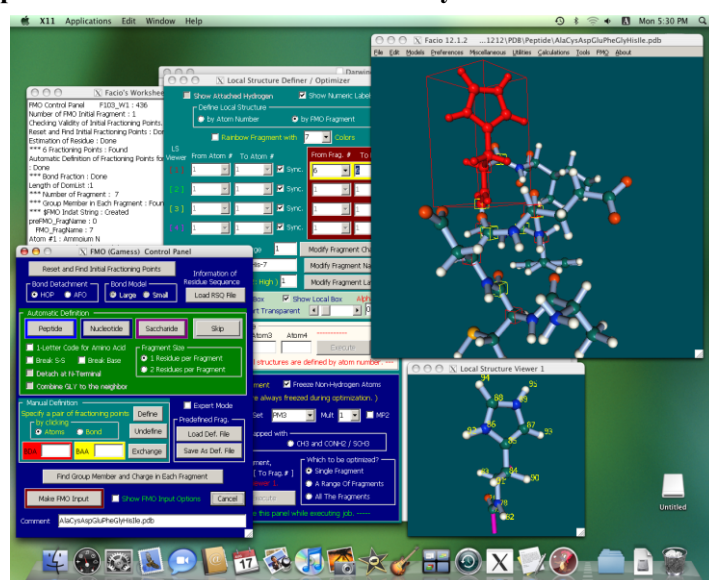
cf. His (Positively charged Histidine with hydrogens on both the nitrogens)

(4) Facio on Macintosh

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

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

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



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

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

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

(b) Drag & drop operation does not work.

This may be a problem of Darwine.

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

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

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

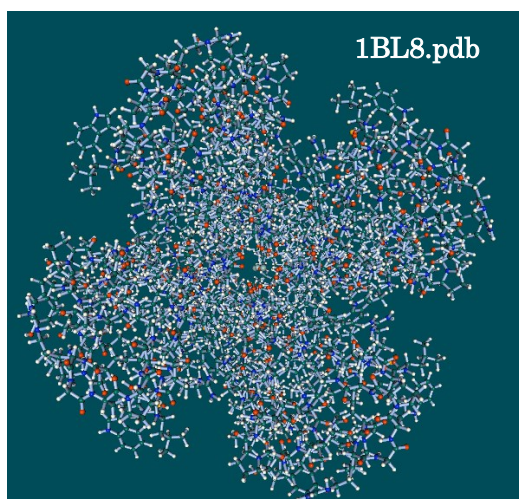
(1) Pull-down menu items have been fully revised and organized properly into submenus.

(2) For Tinker 5 user, set Tinker5 parameter of [AppControl] section in the Facio.ini file to 1. For Tinker 4.2 user, set the parameter to 0. Default setting : Tinker5=1

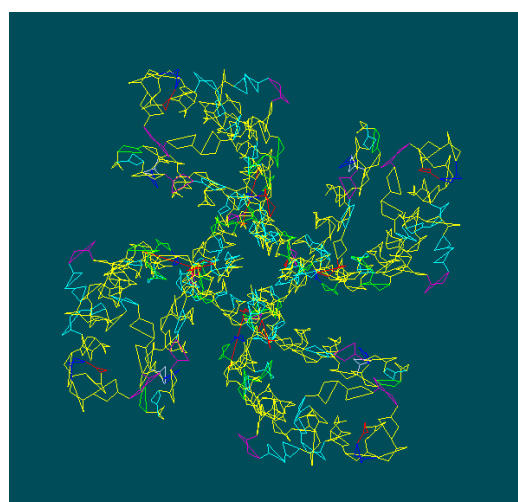
(3) A new coarse-grained model (Trapezoidal Quad representation) of protein

Each amino residue consists of four points (C and O of amide carbonyl, alpha C, and N of amide), which is called as Trapezoidal Quad. Type of amino acid is represented by color. Although you can use different color for different amino residue, use of four or five colors (for example, hydrophobic, aromatic, basic, and acidic) are recommended.

For TQ representation, no missing hydrogen atom should be present. If there are missing hydrogen atoms, please complete them.

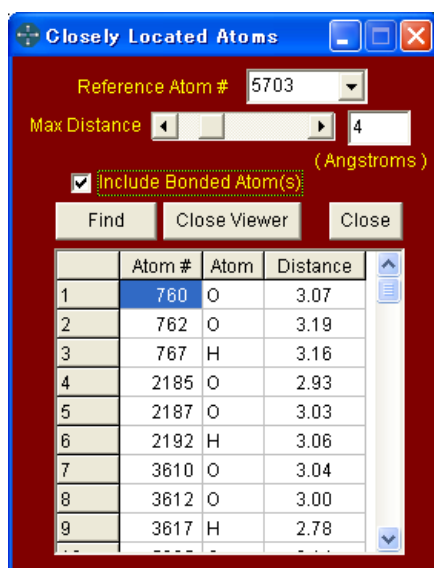


Ball & Stick model



Trapezoidal Quad model

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



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

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



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

(5) Visualization of MOs calculated with MOPAC2009/PM6, which has parameters for 70 elements(from H to Ba, La and Lu, and from Hf to Bi).

Transition metal complex models constructed from scratch only with Facio and MOPAC/PM6 are included in the folder named "MetalComplexes_by_PM6".

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

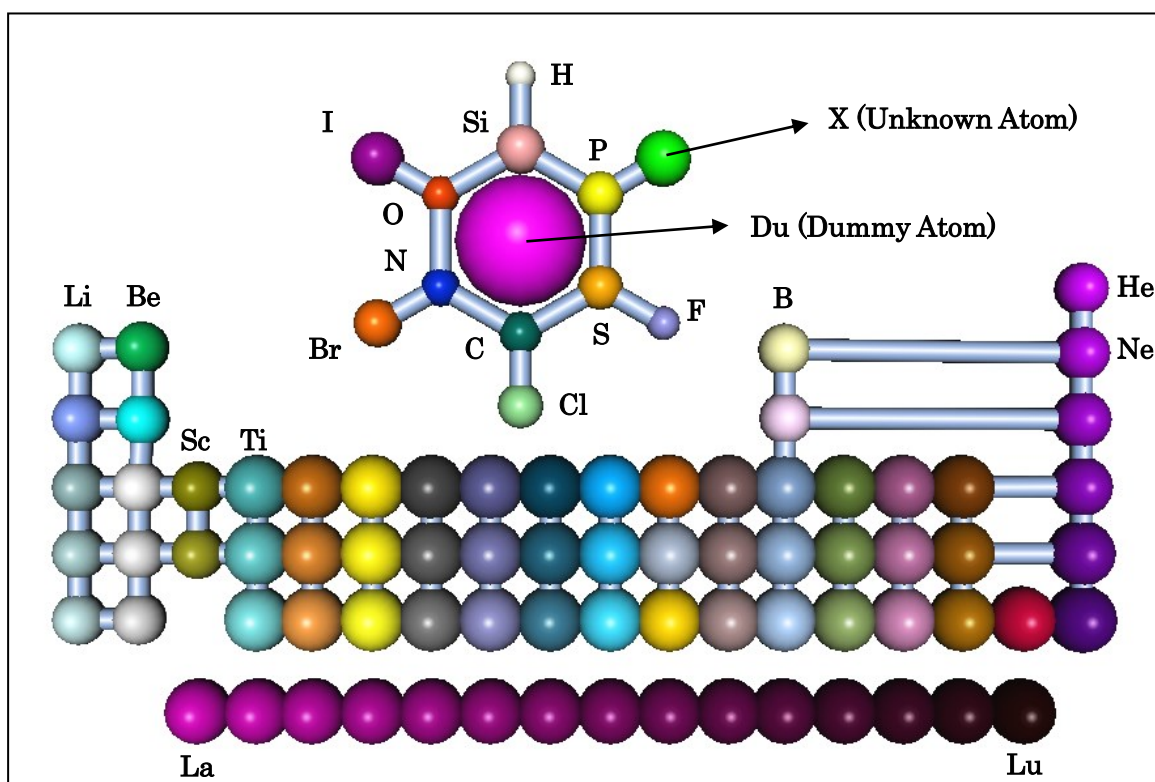
----- Ver.11.8.7 ----- March 25, 2009

- (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.

- (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\YPDB\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

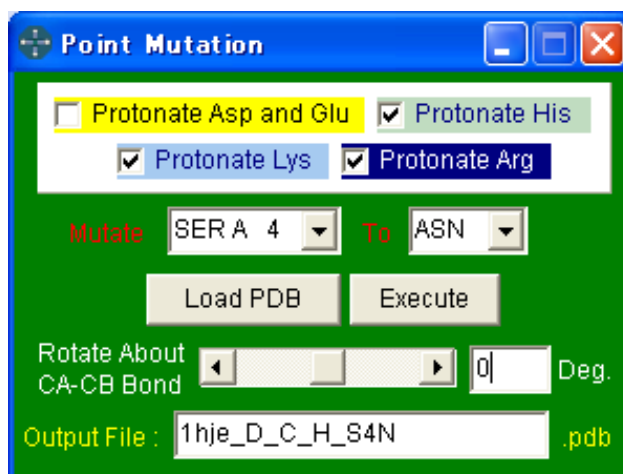
- (3) Point mutation of protein

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.

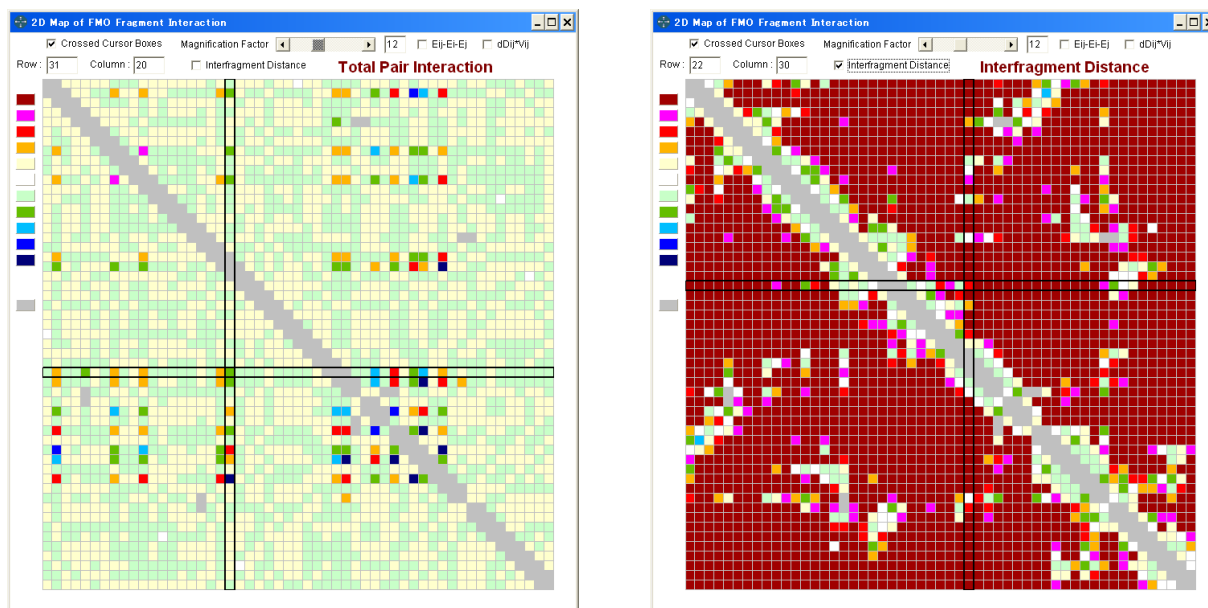


- (4) 2D map representation of two-body FMO properties was revised.

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

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

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



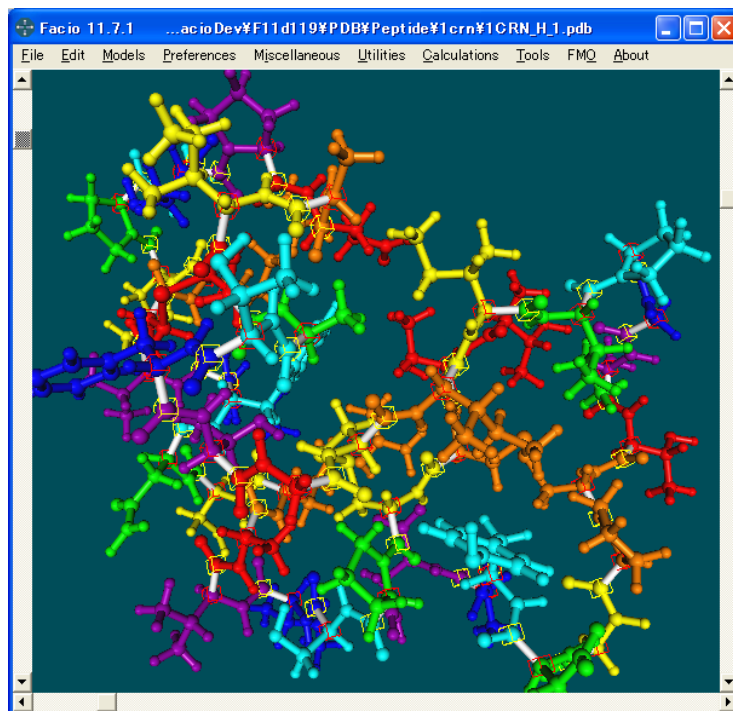
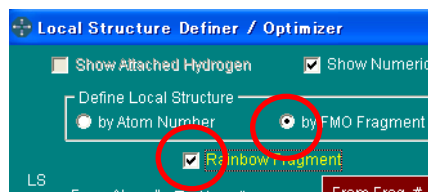
Two-body FMO properties of non-PIEDA calculation can also be displayed.

(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.

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

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

	1	2	3	4	
	123456789012345678901234567890123456789012345	(Columns)			
ATOM	18	CD1	ATYR A 327	16.886	14.518 -8.371
ATOM	19	CD1B	ATYR A 327	14.840	15.316 -5.413
ATOM	20	CD2	ATYR A 327	15.466	14.119 -6.496
ATOM	21	CD2B	ATYR A 327	16.667	14.101 -6.351

Alternate Location Indicator

ATOM	18	CD1	ATYR A 327	16.886	14.518 -8.371
ATOM	20	CD2	ATYR 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

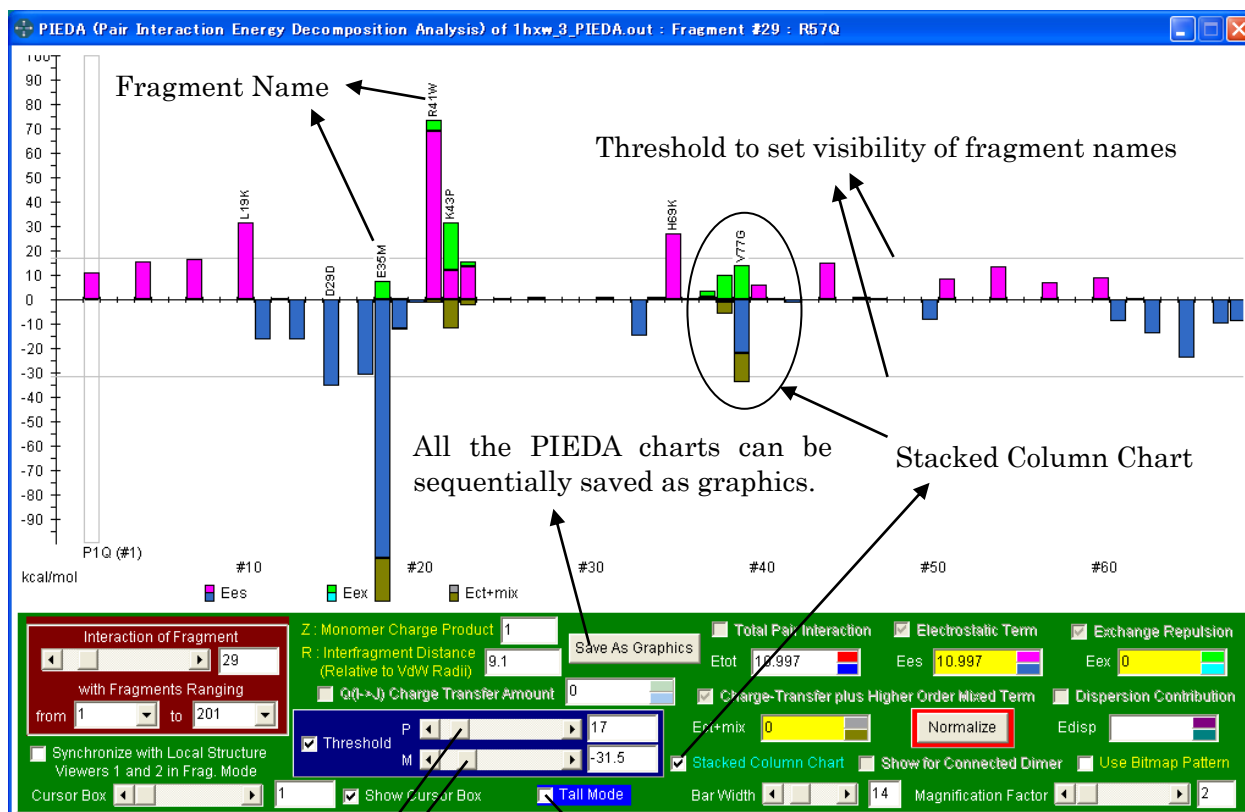
(C) Utility to add hydrogen atoms in ATOM record format to protein PDB

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.

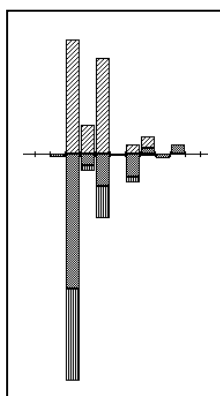
(1) Upgrade of visualization panel for FMO PIEDA



Slidebox for setting threshold

In Tall Mode, the height of the panel is about two times as long as in default mode.

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



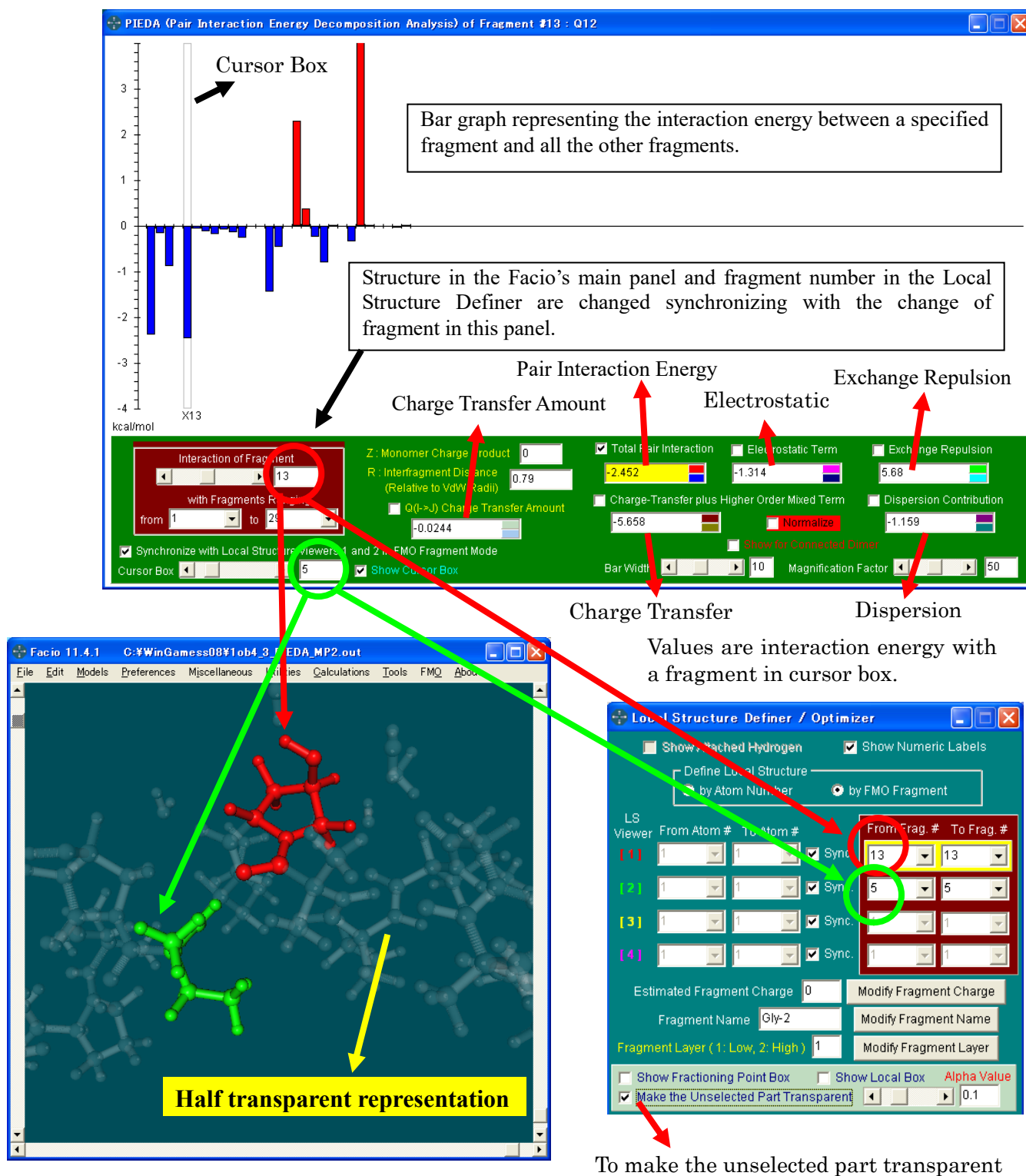
The bitmap files are included in the folder, Brush_BMP.

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 patterns 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.

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



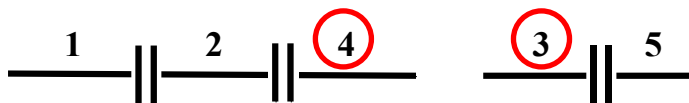
(2) Please notice that input file generated by Facio 11.3.1 for PIEDA calculation has an error.

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

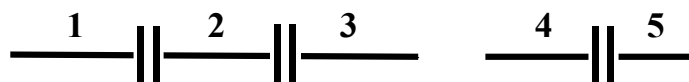
For detail, see the samples and ReadMe.txt in the Tinker-Amber folder.

(1) Completely revised algorithm of FMO fragmentation

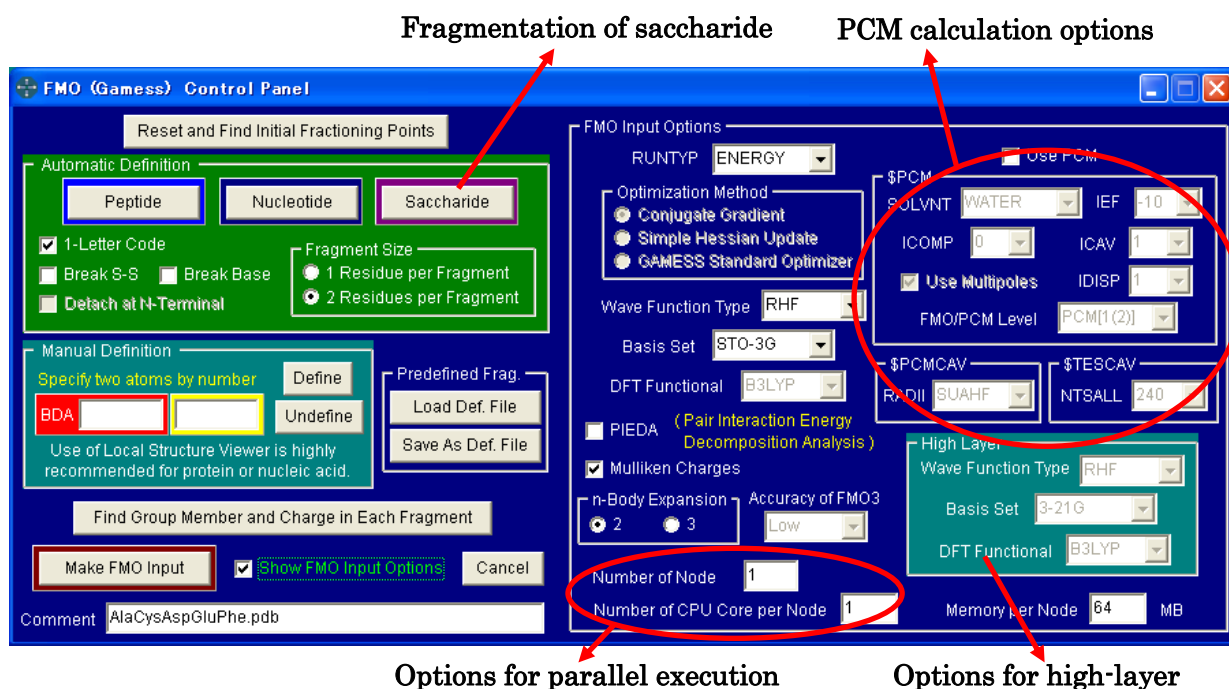
Up to Ver. 11.2.1, when peptide consists of more than two strands, numbering of the fragment is as shown in the scheme, where numbering is not sequential within a single strand.



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



(2) New FMO input option panel



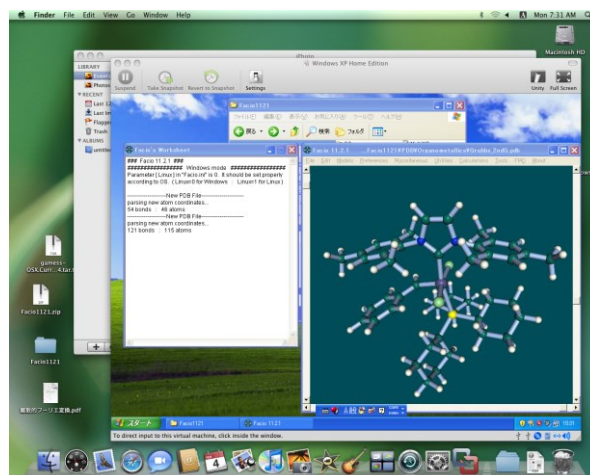
FMO layer is assigned in the Local Structure Viewer control panel.

(3) Facio on Macintosh

It was confirmed that Facio can work on Intel Mac, which uses Intel x86 processors.

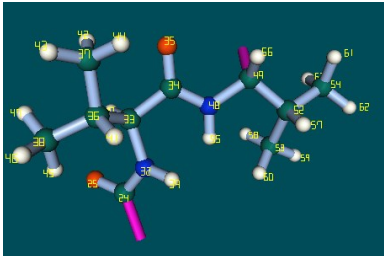
The recommended virtual machine to run Facio is VMWare Fusion. See the screenshot.

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.



(1) Optimization of FMO fragment

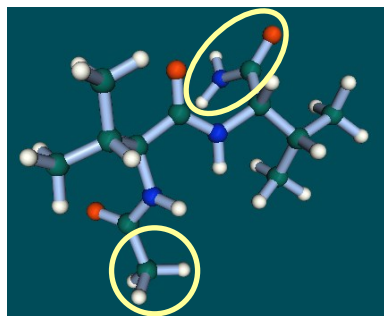
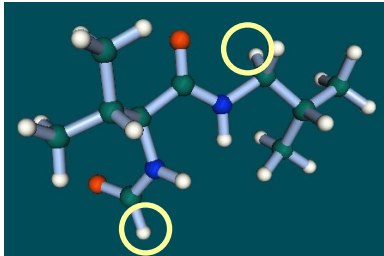
FMO fragment is optimized with semi-empirical MO (PM3) or ab initio MO (STO-3G, 3-21G, 6-31GG). Keeping the position of fractioning atoms, coordinates of hydrogen atoms are optimized. Optimization of non-hydrogen atom is also possible. Dangling atoms in the fragment are capped with hydrogen or appropriate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

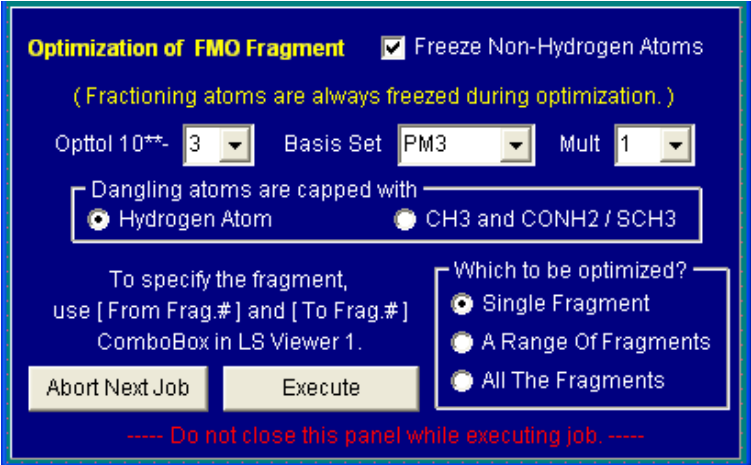


FMO fragment, in which fuchsia bonds are fractioning bond.

Capped with H

Capped with group





Carbonyl and alpha carbon are capped with CH₃ 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 H₂S₂ and the latter ones are from GAMESS Edmiston-Ruedenberg LMO of H₂S.

(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.

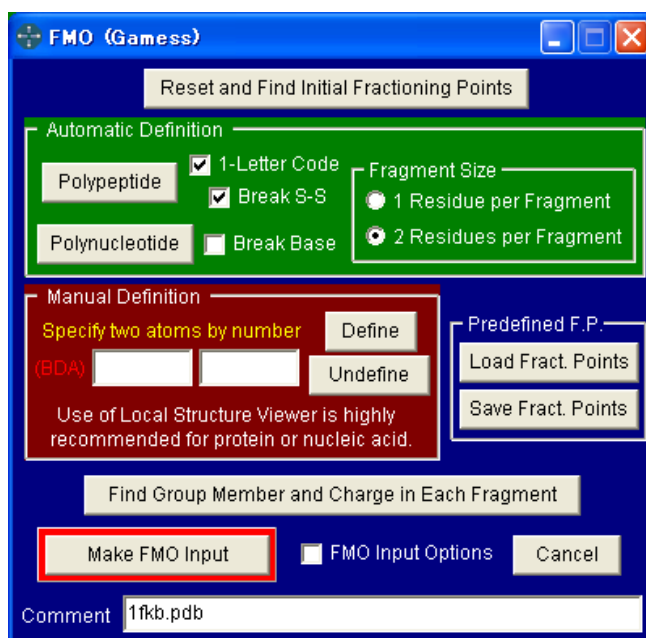
(1) GUI for FMO (Gamess)

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.

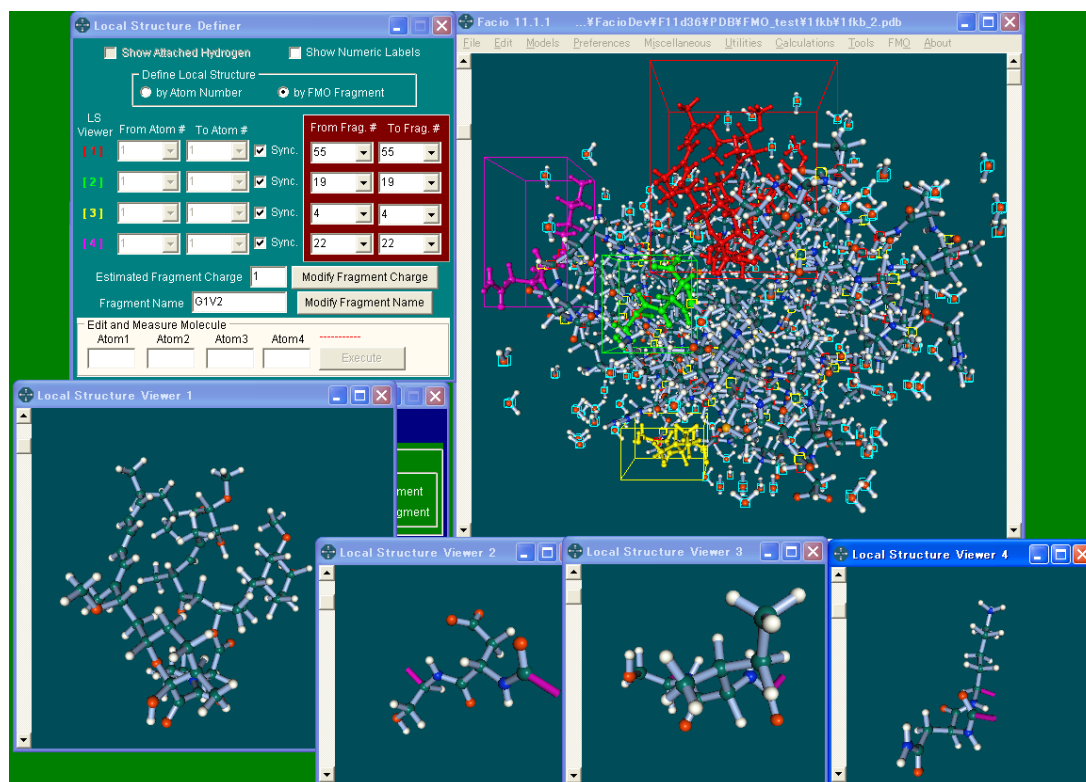
Input file of FMO calculation is automatically generated. For each fragment, charge is estimated and name of fragment is created based on the amino acid residue(s) therein.

INDAT array which contains the information of atom member in each fragment is set without any consideration.



(2) Local Structure Viewer

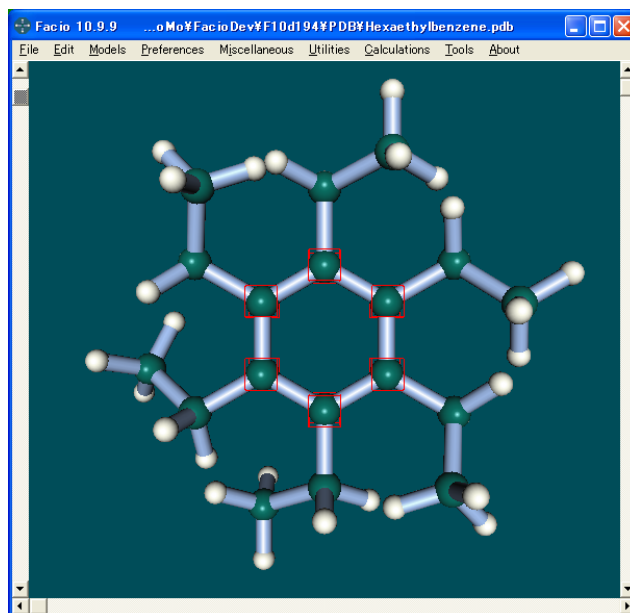
Local structure is specified by a range of atom numbers or FMO fragment numbers. There are four independent windows for the viewers. With this local structure viewer, you can edit large and complex molecules, such as protein, much easily.



1fkb.pdb (Rapamycin - FKBP12 complex)

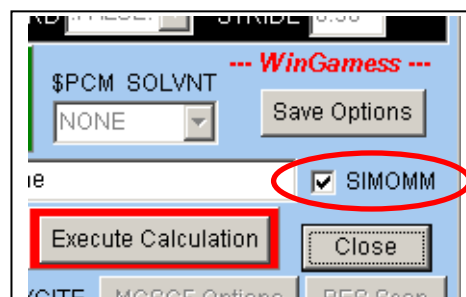
In the above screenshot, FMO fragment #55, #19, #4 and #22 are shown in each viewer. In the whole molecule in the main window, the corresponding local structures are displayed in Red, Lime, Yellow and Fuchsia, respectively.

- (1) Utility for specification of SIMOMM layers in WinGamess/Tinker(MM3) SIMOMM and automatic generation of input file for the calculation.



Select "SIMOMM Layers" in Calculation menu to open the control panel. To assign SIMOMM layers, select layer in the panel and click atom in the main window. Atoms assigned to High Layer are shown in a red box. Atoms which are not in a red box are assigned to Low Layer. (In the example, six carbon atoms of the aromatic ring are set to High Layer.) To define SIMOMM layer, click Apply button.

To execute WinGamess/Tinker(MM3) SIMOMM calculation, select "WinGamess" in Calculation menu, make a checkmark on SIMOMM and execute. Input file which requires \$TINXYZ and \$LINK data is automatically generated.



To load the structure of QM/MM whole molecule, use "Load New WinGamess Output for Bulk Model in SIMOMM Calc. " in the File menu. To load QM part only, load Gamess output as usually.

- (2) New version of batch utilities for drag-and-drop execution of GAMESS are released.

PCG_DDE.bat (for PC GAMESS)
WG_DDE.bat (for WinGamess)

To execute GAMESS calculation, drag-and-drop input file(s) on it.
It accepts up to 9 GAMESS inputs and sequentially executes them.

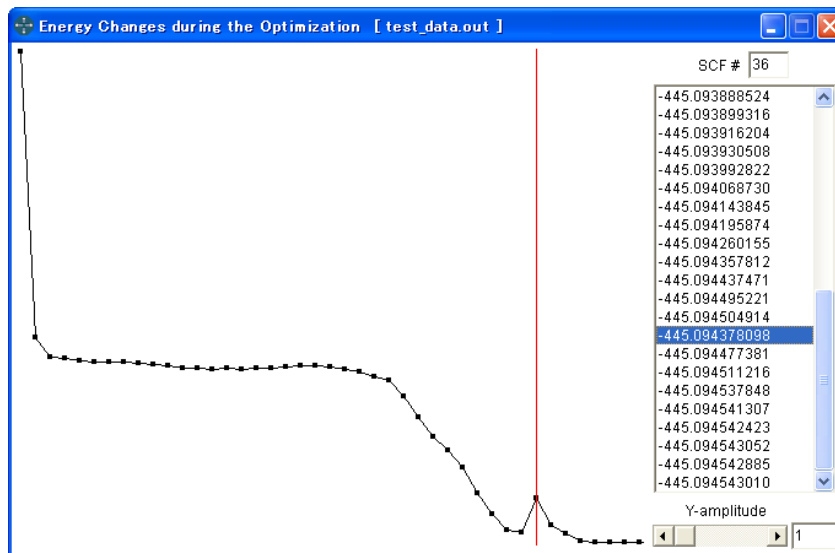
- (3) If you click multi display (see Facio 10.9.7) or multi MO display (see Facio 10.7.1), molecular model or MO lobe in the multi display is now shown in the main window.
- (4) For animation representation of normal mode vibration, movement of atoms is modified so as to be symmetrical to the equilibrium position. According to this change, the parameter "Frames per half cycle" is restricted to odd number.
- (5) Default values of BondCriterion and HX_Max are changed to 2.1 and 1.5, respectively. These parameters determine the existence of bond between atom X and atom Y. In case that both X and Y are non-hydrogens, BondCriterion is used. HX_Max is the parameter when either X or Y is hydrogen.

(1) Energy changes during optimization are shown as a graph, such as below.

With this tool, you can recognize how geometry optimization proceeds and find abnormal behavior in SCF calculation, which causes difficulty of convergence.

Select "Summarize Energy Changes During Optimization" in Miscellaneous menu. This menu item is enabled whenever output file of GAMESS or Gaussian are loaded.

Y-amplitude slide bar set the magnifying factor of the graph.



Click energy value in the box located at the right side, a red vertical line appears.

This vertical line indicate where the energy corresponds to the point in the graph. If you drag a mouse in the energy value list, the red vertical line moves accordingly.

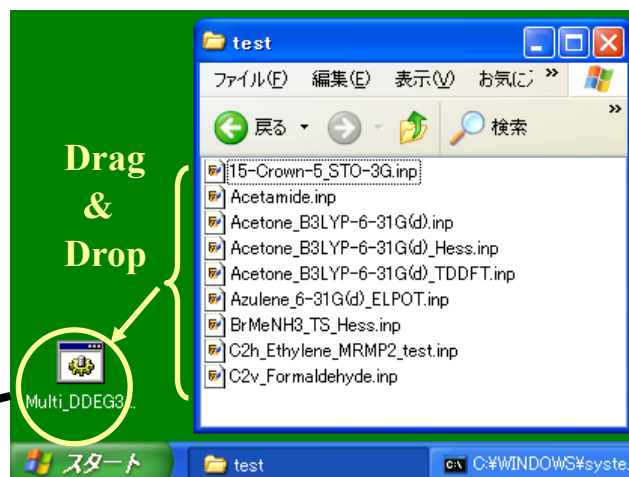
(2) Output file of Gaussian 90 and 94, which is different from Gaussian 98 and 03 can be read at least for optimized geometry. Reading of other type data are not guaranteed, since the author of Facio does not have any output files or checkpoint files of Gaussian 90 and 94 to test.

(3) New version of Drag-and-drop execution utility for PC GAMESS (Multi_DDEG3.bat) are released. To start PC GAMESS calculation, drag-and-drop input file(s) on it. It accepts up to 9 PC GAMESS inputs and sequentially executes them.

After Facio 10.9.9,
PCG_DDE.bat (for PC GAMESS)
and
WG_DDE.bat (for WinGames).

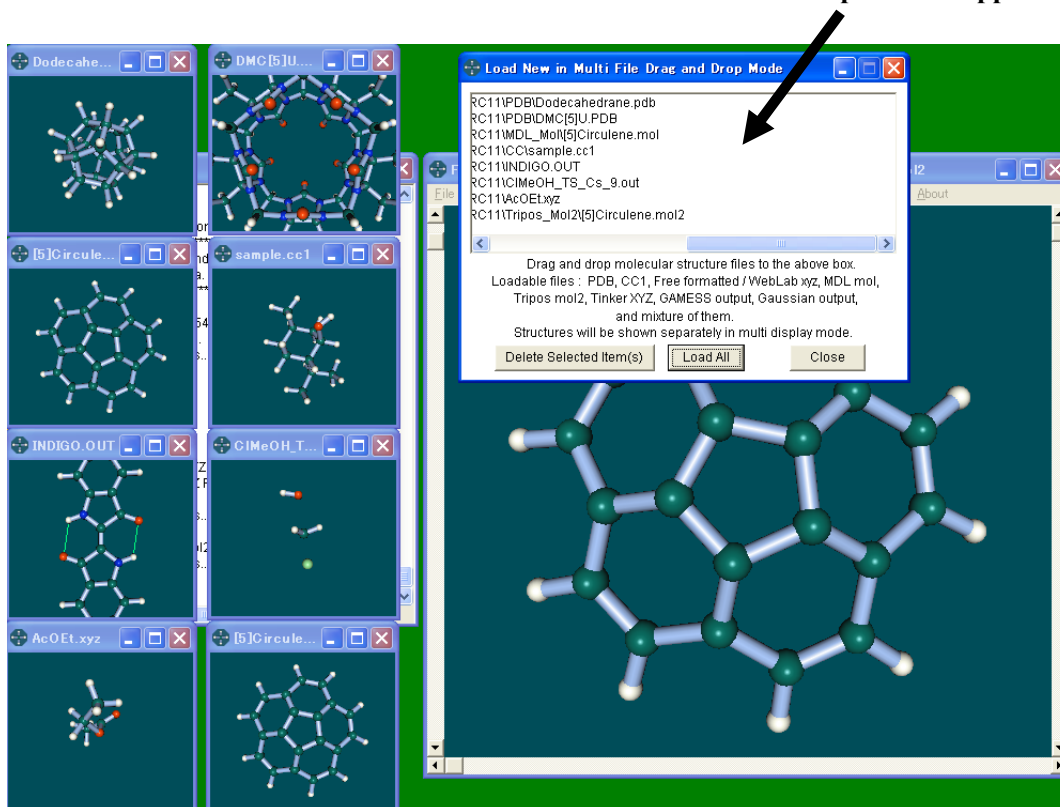


Multi_DDEG3.bat



(1) Multi display as show in the screen shot below has been implemented.

Select "Load New Multi File" in the File menu. "Load New Multi File" panel will appear.



To the list box of this panel, you can drag-and-drop up to 10 PDB, CC1, free formatted or WebLab XYZ, MDL mol, Tripos mol2, TINKER XYZ, GAMESS output and Gaussian output and mixture of them. If you click "Load All" button, then listed molecules will be shown in the multi display. The movement of the molecule in each sub window is synchronized with that of the main window.

Sizes and positions of multi display are automatically saved in MultiDisp.ini file at Facio's root folder, when you close the Load New Multi File panel with Close button.

If there are display problems, please try to set graphics hardware acceleration back. It will fix the problem.

(2) Slight modification of the GUI in GAMESS Input Option panel

- (a) "Clear button" for IFREEZ input field
- (b) SOLVNT parameter of PCM calculation
- (c) Text box for setting base file name of the calculation to be executed.

(3) Graphics format for saving scree shot are now PNG and Bitmap. In the previous version, these were JPEG and Bitmap. You can set the default value with isPNG parameter in Facio.ini.
asPNG=1 (default format is PNG) asPNG=0 (default format is Bitmap)

(4) Initial magnification is set by the parameter EyeZdiff in Facio.ini.

EyeZdiff=0 (default, maximum zoom-in level) (0 <= EyeZdiff <= 400)

(1) Detection and visualization of hydrogen bonds are implemented.

Criteria for detection are as follows.

$X \cdots H \cdots A$ (Atom X = N, O, F, Cl, Br, I and atom A = N, O, F, Cl, Br, I, S)

(a) $HX_Max < Length(X \cdots A) \leq H_BondCriterion$

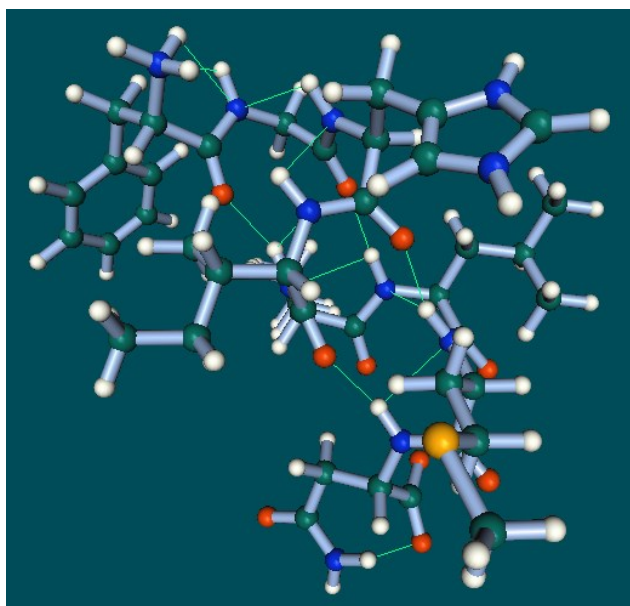
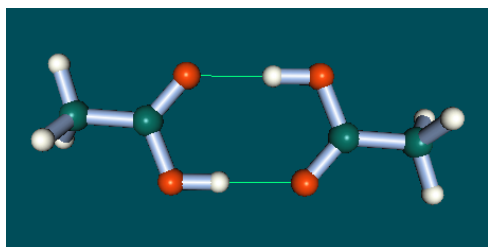
(b) $H_BondAngleCriterion < Angle(X \cdots H \cdots A) \leq 180$ degrees

Default values :

$HX_Max = 1.3$ Angstroms $H_BondCriterion = 2.5$ Angstroms

$H_BondAngleCriterion = 90$ degrees

Detection of hydrogen bonds is automatically performed whenever new molecular structure loaded. If you check "Show Hydrogen Bonds" in the Miscellaneous Menu, hydrogen bonds are displayed as lines. See the screen shot below.



"Dump Hydrogen Bonds" in the Utilities Menu will output hydrogen bonding data (sequential number, hydrogen bond length, and so on) as text file.

(2) Using Bondi's van der Waals radii and the equations below, van der Waals volume can be calculated.

$$V_{vdw} = \sum_{All\ Atoms} V_A$$
$$V_A = \frac{4\pi}{3} R^3 - \sum_{i=Bonded\ Atom} \frac{1}{3} \pi h_i^2 (3R - h_i) \quad \text{where} \quad h_i = R - \frac{R^2 + d_i^2 - R_i^2}{2d_i}$$

(3) XYZ format of WebLab ViewerLite is now a supported molecular structure file.

----- Ver.10.9.5 ----- April 27, 2007

- (1) Simulated IR, Raman and VCD spectra can be saved as text file in three resolutions :
COARSE (5cm⁻¹), MEDIUM (1cm⁻¹) and FINE (0.1cm⁻¹).
COARSE is the resolution of Facio's spectrum window.
- (2) Additional parameter for TINKER/MM3 are newly produced in order to make molecular mechanics calculation of esters, carbonates and carboxylic acids possible. These parameters are not optimized but will be useful for modeling of medium-sized lactone or polycarbonates.

Please append the contents of "Additional_MM3PRM.txt" to mm3.prm.

- (3) Up to the previous version, MOPAC versions of FORCE calculation which Facio can read were MOPAC2000, MOPAC93, MOPAC6, WinMOPAC3.0, 3.5 and 3.9. Each version of MOPAC has a different output format of FORCE calculation. Now Facio supports MOPAC2007, which has another different format.
- (4) Facio visualizes molecular orbitals of MOPAC2007. Since Facio can generate graphics data without using PSI-88, input key word, GRAPH is not required for MO visualization.

After geometry optimization, Facio can automatically load molecular orbital coefficients from output file. So, you can visualize HOMO only with two mouse-clicks!

1. evoke MO viewer -----
2. show MO

For loading MO coefficients, the only supported version of MOPAC is MOPAC2007.

----- Ver.10.9.4 ----- April 12, 2007

- (1) Solvent-excluded surface volume and area calculated by MSMS are shown.
- (2) If you utilize EM64T feature of CPU for PC GAMESS, set EM64T=1 in Facio.ini.

----- Ver.10.9.3 ----- April 7, 2007

- (1) PC GAMESS input options which are useful for MRMP2 calculation are automatically set.
- (2) PC GAMESS input option which enables EM64T feature of CPU is automatically set.
- (3) Bug related to energy levels representation of ROHF calculation has been fixed.

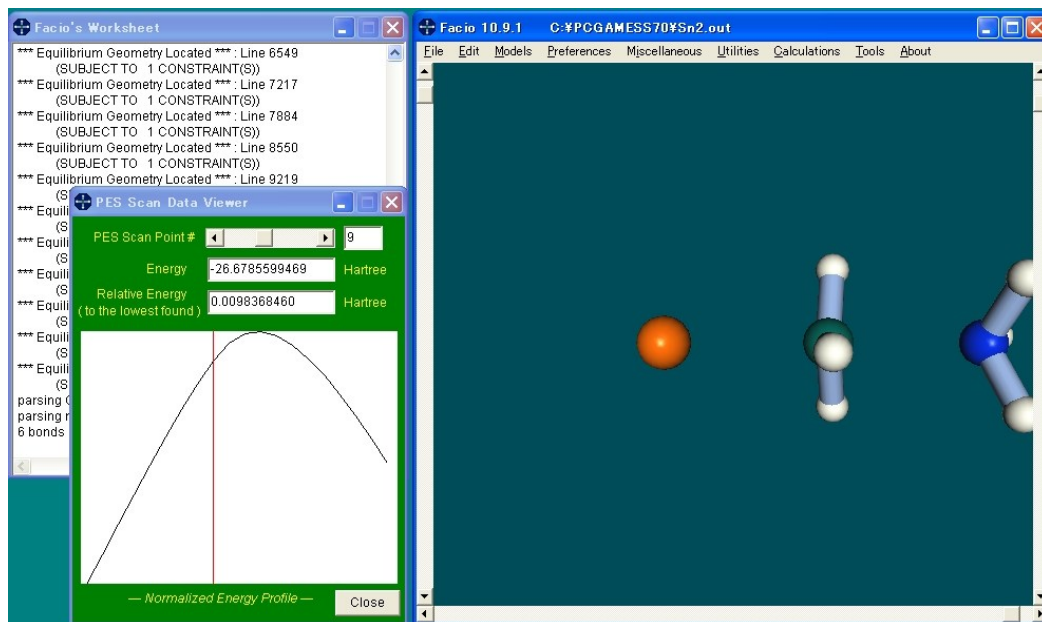
----- Ver.10.9.2 ----- April 1, 2007

- (1) Energy levels of alpha and beta MO in UHF calculation can be separately displayed.
- (2) TDDFT calculation is possible in WinGamess, VERSION = 7 SEP 2006 (R4). GUI for this is implemented.
- (3) Original folder icons are included.



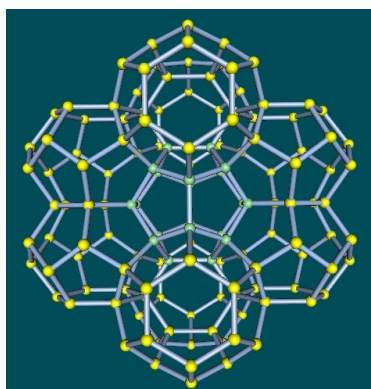
----- Ver.10.9.1 ----- March 14, 2007

- (1) GUI for relaxed PES Scan (Potential Energy Surface Scan) calculation of PC GAMESS is newly implemented. It can permit you to set parameters for two dimensional scan. To visualize energy profile of PES and the corresponding structures, use Tool Menu >> PES Scan Data Viewer.

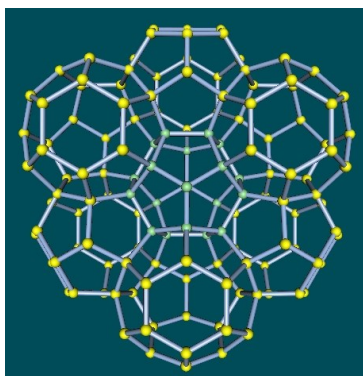


GUI is not available for WinGamess, since it is not able to perform PES Scan along internal coordinate of bond angle and dihedral angle.

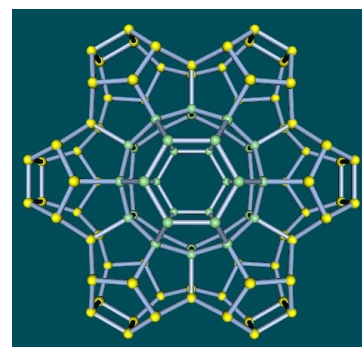
- (2) Models of gas hydrate skeleton are included as sample. They were modeled with Facio from scratch. Corresponding imaginary polyhedranes, which are intermediate of the models, are also included.



Type I



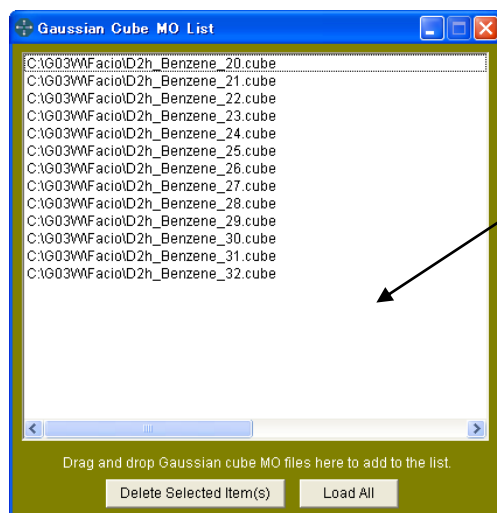
Type II



Type H

----- Ver.10.8.1 ----- February 4, 2007

- (1) New feature of loading more than one Gaussian cube MO is implemented.
 Select "Load Gaussian Cubes for MOs (in Multi File Drag-and-Drop Mode) to open list box window. To this window, drag-and-drop Gaussian cube MO(s). Then click "Load All" button. Then use CUBE/Molecular Orbital Viewer in Tools Menu. This is very convenient feature when you want to view only selected MOs.

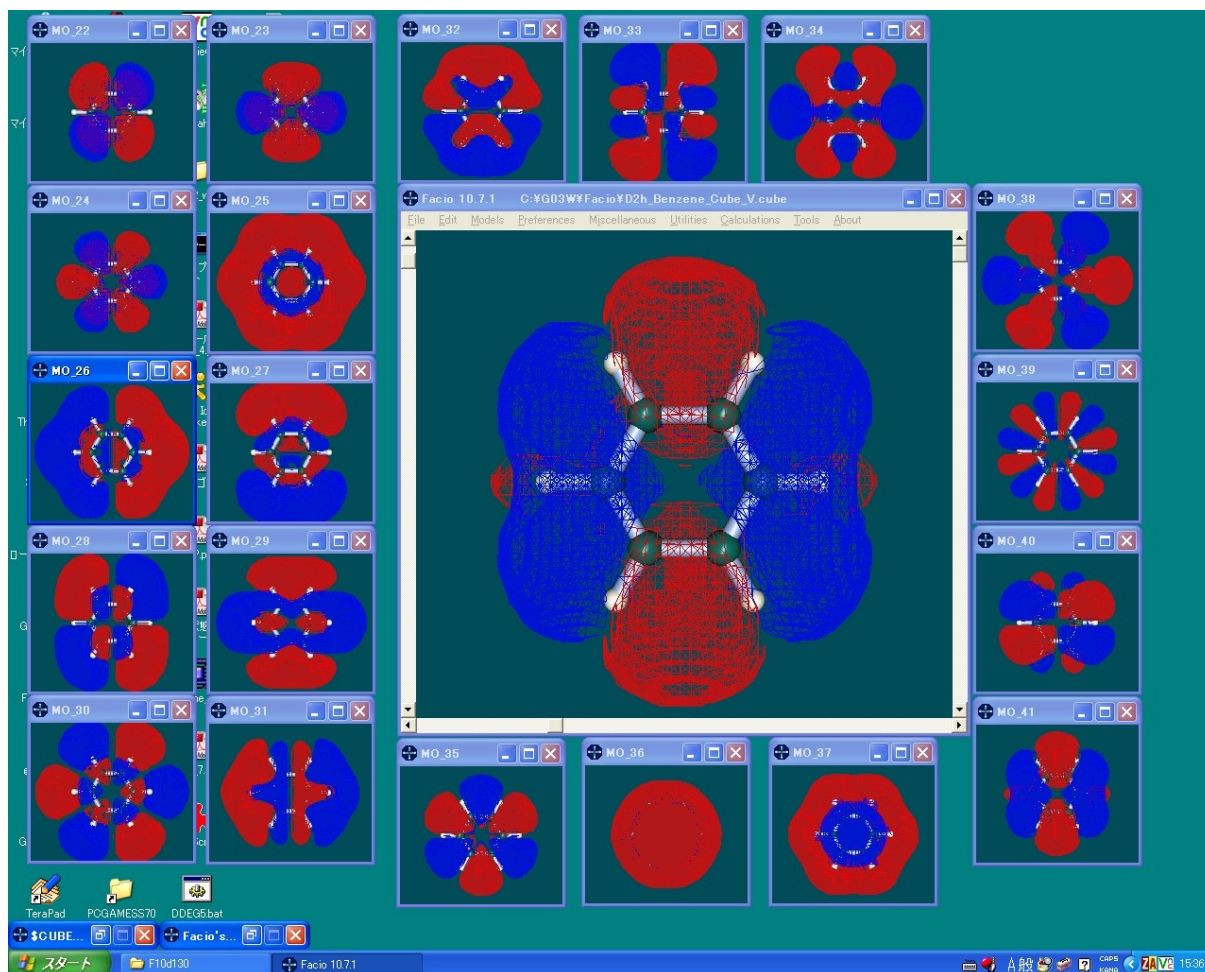


Drag & drop Gaussian cube MO files to the window.

- (2) New feature of generating sequential Gaussian cube MOs is implemented.
 See Gaussian Utilities in Tools menu. Load formatted checkpoint, check "Generate Sequential Cube MOs, and set the range of MO by specifying "From" and "To" parameters. Then click "Execute" button to generate cube MOs. Each cube data is saved as a separated file with MO number attached automatically to the file name.
 (CubeGen radio button is automatically checked, if formatted checkpoint is loaded before.)
- (3) Molecular geometry can now be retrieved from Gaussian formatted checkpoint file.

----- Ver.10.7.1 ----- January 17, 2007

- (1) Up to 20 MOs can be viewed simultaneously. (See the screen shot below) The movement of the molecule in each sub window is synchronized with that of the main window. Each MO can also be automatically saved as bitmap files. The position and size of sub windows are automatically stored in MultiMO.ini at Facio's root folder.



- (2) View point controller is implemented. See Utilities menu. This numerically changes the view point of the molecule. You can also lock the view point.
- (3) Up to ver. 10.6.2, double run of Facio has been intentionally prevented. But now multi run of Facio is allowed. This is very useful for viewing many molecules at the same time.

----- Ver.10.6.2 ----- December 10, 2006

- (1) Drag & drop execution utility for PC GAMESS (DDEG4.bat) is now released.
- (2) Bug related to NMOFZC in \$MCQDPT of GAMESS input option is fixed.
- (3) SYMLOC=.TRUE. and MVOQ=6 are automatically set when LOCAL=BOYS or POP and GROUP is other than C1.

----- Ver.10.6.1 ----- November 23, 2006

(1) Atom number reassigning utility

In order to use this utility, select "Assign Atom Numbers" in Utilities Menu.

Set the "Start From" parameter (default=1), then click atoms of which just you want to change the number and finally click the "Assign Atom #" button. You don't have to click all the atom. The numbers of the atoms which are not clicked are automatically reassigned.

(2) GUI for PC GAMESS can now make an input for MRMP2 calculation.

Input options are automatically included to speed up integral transformation & effective Fock matrix construction steps, which dominates the overall cost of CI and MCSCF calculation.

(3) GUI for changing Arrow properties.

Arrow is used to represent normal mode vibration or dipole moment.

(4) Schematic representation of MO energy levels can now be saved as PostScript file.

(5) GUI for MOPAC.

----- Ver.10.5.1 ----- October 8, 2006

(1) Full revision of OpenGL-graphics rendering routines has dramatically lowered CPU usage.

(2) Drag & Drop operation is supported for loading structure files. Supported file types are PDB, CC1, CC2, free-formatted XYZ, MDL Mol, Tripos Mol2, GAMESS output and Gaussian output.

(3) MDL Molfile and Tripos Mol2 files can now be used as input files.

(4) FORCE calculation data of MOPAC93 and MOPAC2000 can be read to show normal mode vibration as animation. MOPAC6, WinMOPAC3.0, 3.5 and 3.9 were already supported in Facio 9.8.3.

(5) Dipole moment are shown as an arrow.

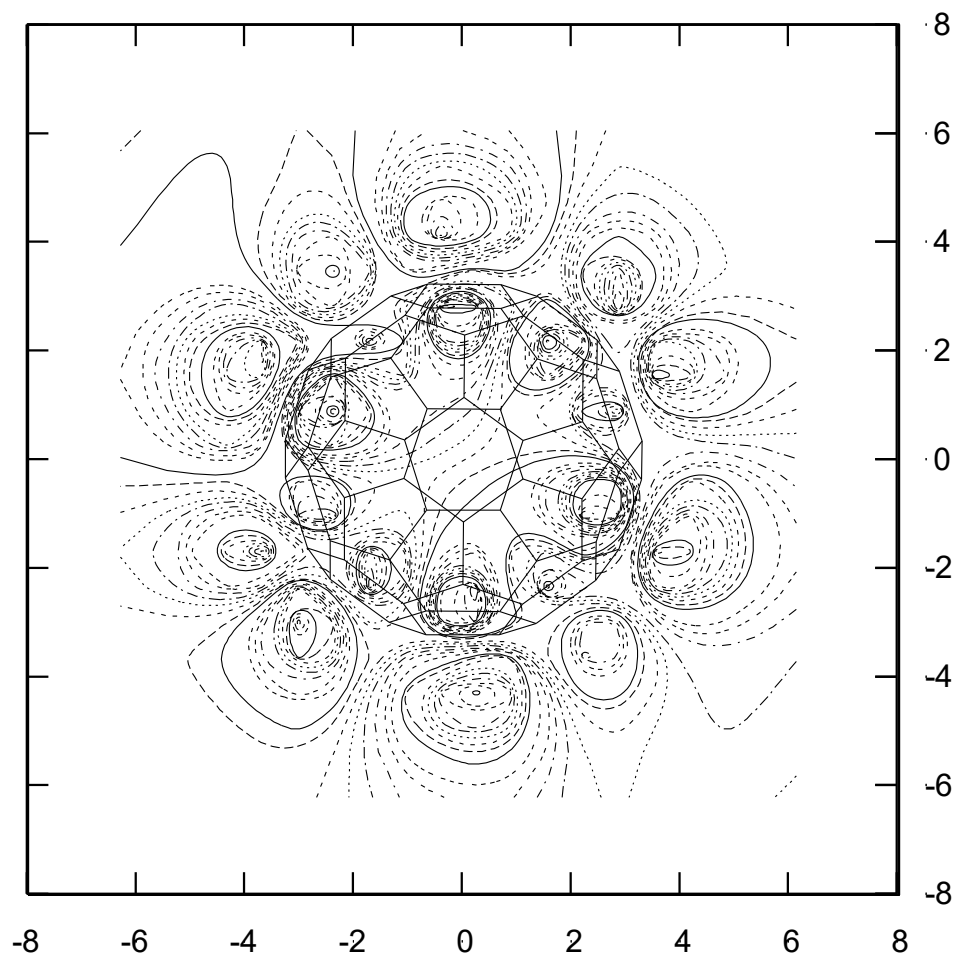
----- Ver.10.4.1 ----- August 21, 2006

(1) Arbitrary cross section of MO can be shown as contour plot with a help of GNUPLOT.

Contour plot shown below is a cross section of C₆₀'s LUMO.

Samples are included in the folder "CubeMO_CrossSection".

To Linux user : Set write permission for the directory where GNUPLOT executable resides.



In order to superimpose wire model of the molecule to the contour plot of the cross section, appropriate software, such as Illustrator is required.

(2) Gaussian input file for Multi-Step Job is supported.

(3) Custom route section for Gaussian can be set up to 30 items and shown as list.

(4) Under symmetry restricted condition, there was a bug in automatic setting of parameter NMCC in \$GUGA group and parameter NELN in \$DET group. The bug has been fixed.

(5) Compression format of Facio's distributing archive has been changed to ZIP for Linux user's convenience.

----- Ver.10.3.1 ----- May 27, 2006

- (1) Schematic representation of MO energy levels is implemented for GAMESS.
- (2) Atom sequence numbers are displayed near each atom as numeric labels.
Try “Miscellaneous Menu >> Show Numeric Labels”.
- (3) Input file formation for TDDFT calculation of PC GAMESS 7.0 are supported.
- (4) Input file for GAMESS calculation can be reviewed and edited before calculation.
The base file name for calculation can be modified before calculation as well.
- (5) Periodic table is included. Try “Miscellaneous Menu >> Show Periodic Table”.

Periodic Table

Group numbering is based on the new IUPAC system.
Atomic weights are based on $^{12}\text{C} = 12$ and conform to the 1993 IUPAC reported values. Number in () indicates the isotope of longest half-life.

Lanthanides: La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu
Actinides: Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr

Illustrated by Masahiko Nozawa
<http://www.3dmg.jp/periodic/>

- (6) New atom colors for X atoms (other than H, C, N, O, F, Si, P, S, Cl, Br, I).
- (7) Guide marker for molecular modelling. Try “Miscellaneous Menu >> Show Guides”.
- (8) Molecular models of Organometallics newly created with Facio are included as samples.

----- Ver.10.2.1 ----- Apr. 16, 2006

- (1) Moment inertia of a molecule is calculate and the principal axes transformation is performed.
- (2) Comparison of two molecule which are the identical molecule but have slightly different geometry is performed and the geometrical differences (bond length, bond angles and dihedral angles) can be saved as a text file.
- (3) Schematic representation of energy level of molecular orbitals are modified.
- (4) H-H coupling constants are extracted from Gaussian output file and saved as a texe file.
- (5) Molecular structure can be extracted from “finished but not converged” or “not finished” Gamess geometry optimization.

----- Ver.10.1.1 ----- Mar. 5, 2006

- (1) Facio is now working on Linux (Fedora Core 4 and Scientific Linux 4.2)
with a help of WINE and Mesa.
WINE: <http://www.winehq.com/> Mesa: <http://www.mesa3d.org/>

- (2) A new GUI for UTChem. UTChem is a software package for ab initio quantum chemistry calculation, developed at Hirao's Laboratory of Tokyo University.
<http://utchem.qcl.t.u-tokyo.ac.jp/>
- (3) PC GAMESS(Ver.7.0), MSMS and Tinker/MM3 on Linux can be executed from Facio on Linux.
- (4) Animated graphics of normal mode vibration can be sequentially stored as JPEG files.

----- Ver.9.9.1 ----- Dec. 25, 2005

- (1) Molecular models of icosahedral higher fullerenes (C80, C180, C240, C320, C500, C540, C720, C960, C980, C1280) are newly assembled from scratch with Facio.
- (2) GIAO isotropic shielding values calculated with Gaussian / WinGamess are read in and chemical shifts relative to the TMS absolute shielding value are shown in table.

----- Ver.9.8.9 ----- Nov. 29, 2005

- (1) It was found again that there are cases where vibrational vectors of Gaussian normal mode calculation are not properly read. This bug has been fixed.

----- Ver.9.8.8 ----- Nov. 28, 2005

- (1) Resolution with which intensity and wave number of IR, Raman and VCD are saved as text file is changed from 5.0 (1/cm) in the previous version to 0.1 (1/cm).
- (2) It was found that there are cases where vibrational vectors of Gaussian normal mode calculation are not properly read. This bug has been fixed.

----- Ver.9.8.7 ----- Nov. 12, 2005

- (1) The way to display a series of structure obtained by IRC calculation with Gaussian is modified.
For example, if the calculation was performed for 13 points on IRC, results are stored in the formatted check file in the order of 7-6-5-4-3-2-1-8-9-10-11-12-13, in which the structure #7 corresponds to the transition state. The older version of Facio displays these structures in the order as stored, i.e. 7-6-5-4-3-2-1-8-9-10-11-12-13. Ver.9.8.7 displays them in the order of 1-2-3-4-5-6-7-8-9-10-11-12-13 so as to show continuous change of the structures.
- (2) In IRC display mode, inter atomic distance, bond angle and dihedral angle are incorrectly measured. This bug has been fixed.
- (3) Trajectory data obtained by ADMP or BOMD MD calculation with Gaussian can be visualized. Energy changes (nuclear kinetic energy, electron kinetic energy, potential energy and total energy) are plotted along the time in trajectory.
- (4) Cartesian coordinate 1 and 2, and "free formatted XYZ" file are newly supported as an input file.
Free formatted XYZ file is a simple XYZ file, in which each line consists of only atom symbol and x, y, z coordinates separated with at least one space. See the sample.xyz in the XYZ folder in Facio folder.

----- Ver.9.8.6 ----- Oct. 2, 2005

- (1) Intensity and wave number of IR, Raman and VCD can be saved as text file.
- (2) You can see atomic number with "Miscellaneous Menu >> Highlight Specified Atom"

----- Ver.9.8.5 ----- Sept. 24, 2005

- (1) In a special case, CUBE MO data is incorrectly determined to be "truncated" with the warning message "CUBE data may be truncated", even if it is not so. This bug has been fixed.

----- Ver.9.8.4 ----- Sept. 17, 2005

- (1) GUI for Gaussian ONIOM Layer specification has been implemented.
- (2) VCD(Vibrational Circular Dichromism) spectrum is simulated.
VCD calculations of *d*-Menthol and *l*-Menthol are included as example data.
- (3) Displacement vectors of normal mode vibration are shown as arrows.
- (4) You can use g03w.exe instead of g03.exe for command line execution of Gaussian.

----- Ver.9.8.3 ----- Aug. 27, 2005

- (1) Completion of missing hydrogens has been implemented.
- (2) Facio can read FORCE calculation data of MOPAC6, WinMOPAC3.0, 3.5, and 3.9 to show normal mode vibration as animation.
- (3) You can capture the screenshot of main window of Facio and save as JPEG file.
Unlike Windows' Alt-PrintScreen function, Facio's screenshot function excludes window frame and menu bar.

----- Ver.9.8.2 ----- Jul. 9, 2005

- (1) For transition structure search using the STQN method, the reactant, product, and initial TS structure can be specified through GUI.
- (2) Facio has failed to read PDB file which has MODEL and CONECT records.
This bug has been fixed.

----- Ver.9.8.1 ----- Jun. 17, 2005

- (1) SSH / SFTP client has been implemented. Through SSH / SFTP connection, Gaussian job can be submitted to batch job system on the remote server and calculation results can be retrieved from the server. Supported batch job systems are LoadLeveler and NQS.

----- Ver.9.7.6 ----- Apr. 18, 2005

- (1) Facio and external programs can be installed in different disk drives each other.
For example, Facio in D: drive and PC Gamess in C: drive.

(2) User-customized position and size of main window and position of Facio's worksheet is saved in Facio.ini. See Edit menu >> Save Position and Size of Main Window

(3) Edit Tool Box :

Selected Edit Menu items are separated from menu and packed in a box which can be placed anywhere in display. Edit Tool Box facilitates molecular modeling.

See Miscellaneous menu >> Show Edit Tool Box

----- Ver.9.7.5 ----- Apr. 9, 2005

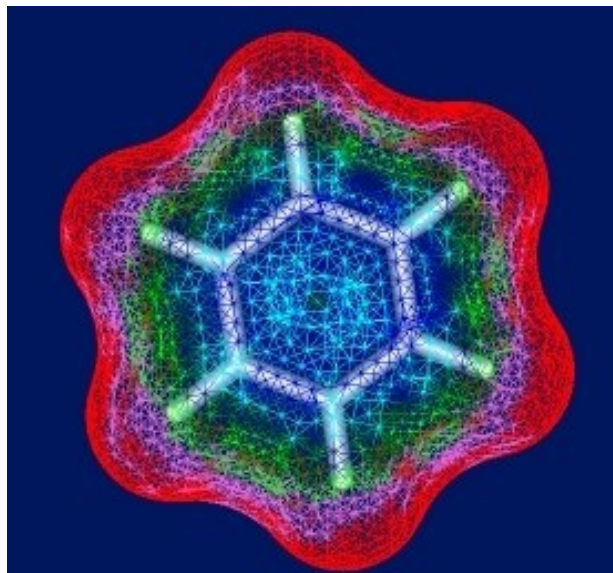
(1) Criteria to determine mesh representation of CUBE MO is now adjustable.
If no mesh representation is shown, please increase Mesh Criteria value.

----- Ver.9.7.4 ----- Mar. 12, 2005

(1) IRC data (in Gaussian formatted check file) is visualized.

----- Ver.9.7.3 ----- Feb. 26, 2005

(1) Electrostatic Potential CUBE data calculated with PC GAMESS or Gaussian 03W is mapped onto Solvent Excluded Surface calculated with MSMS.
The following graphics shows this feature.



Electrostatic potential of Benzene mapped onto solvent excluded surface

(2) With Facio Ver.9.6.1 and Ver9.7.1, PC GAMESS input file for CUBE electrostatic potential and electron density has not been calculated even if user properly sets input options.
This bug has been fixed.

(3) Utility which is useful for modeling of compound with symmetry are added.
With this utility, atoms which are within ApproxityCriteria are exactly moved to Z axis. The parameter ApproxityCriteria is set in the Facio.ini.

----- Ver.9.7.2 ----- Feb. 5, 2005

- (1) Visualization of Gaussian 03W CUBE molecular orbital and normal mode vibration has been implemented. Graphical Viewer of MO level and multiplicity is also built in. GUI for Gaussian 03W Utilities (CubeGen, FormChk, FreqCheck) are also created.
- (2) Molekel is invoked within Facio.
- (3) In the case that PC Gamess or WinGAMESS is placed in the folder whose absolute path contains "space", a required fonder (Facio) has not been properly produced. This bug has been fixed.

----- Ver.9.7.1 ----- Jan. 22, 2005

- (1) GUI for MCSCF calculation has been implemented.
Parameters in \$DRT and \$DET group are automatically set according to the charge and spin multiplicity.
- (2) GUI for Gaussian 03W has been implemented.
With this GUI you can make an input file (Gaussian job file, *.gjf) and start the execution of the job.
Customized route section commands for individual user are stored in Facio.ini as CustomRoute1, CustomRoute2, ... and CustomRoute9.

*** Visualization of Gaussian output, such as molecular orbitals and normal mode of vibration will be implemented in the next version of Facio. ***
- (3) In the case of Gamess option \$CONTRL NOSYM=0 and \$DATA GROUP=(other than C1), Facio failed to read some orbital energies. This bug has been fixed.
- (4) Symmetry of molecular orbital is displayed in the MO Viewer panel.
- (5) In the cases other than GROUP=C1, molecular orbital numbers of HOMO and LUMO have not been properly calculated. This bug has been fixed.
- (6) Utility which is useful for modeling of compound with symmetry are added.
With this utility, atoms which are within ApproxityCriteria are exactly moved to XY plane or YZ plane. The parameter ApproxityCriteria is set in the Facio.ini.
- (7) Winmostar is invoked within Facio. <http://winmostar.com/>
- (8) Examples of compounds with symmetry are included in the SymmetryUnique folder.
- (9) In some cases, preferences has not been properly saved. This bug has been fixed.

----- Ver.9.6.2 ----- Nov. 14, 2004

- (1) In the case of Gamess option \$CONTRL NOSYM=0 RUNTYP=OPTIMIZE and \$DATA GROUP=(other than C1), "COORDINATES OF SYMMETRY UNIQUE ATOMS" are output. But the output format is slightly different between PC GAMESS and WinGamess. And this diffecence causes an input error when WinGamess output is loaded. This bug has been fixed.

- (2) New checkbox is added
in the Menu>>Preferences>>External Programs.

When coordinates of symmetry unique atoms are available,
this checkbox determines whether only symmetry unique atoms are shown or not.
This option is valid only for "Load New Gamess Output".

----- Ver.9.6.1 ----- Nov. 7, 2004

- (1) Interactive pre/post-processor for WinGamess has been implemented.

WinGamess is PC WIN32/GCC VERSION of GAMESS
(VERSION = 19 MAY 2004 (R4))
precompiled under the Cygwin environment by Nuno A.G. Bandeira.

<http://www.msg.ameslab.gov/GAMESS/dist.pc.html>

Facio makes an input file and execute WinGamess job
with runscript.csh and ddickick.exe in the WinGamess package

- (2) When CUBE MO data is loaded from punch file, MO energies are also
loaded from the corresponding output file.
There was no problem about this up to now. But it was found that
MO energies are not properly loaded in special cases,
for example, 6-31G(d)/UHF calculation of ammonia cation radical. This bug has been fixed.

----- Ver.9.5.1 ----- Oct. 24, 2004

- (1) Parameters in TINKER Key file is described as relative path name,
when the absolute path name of TINKER parameter file contains "space",
e.g. "C:\My Document\Tinker\params\amber.prm".

In such a case, the author assumes that the TINKER is
installed as follows.

```
Tinker ----- bin ----- optimize.exe
                |
                --- params --- mm3.prm
                        |
                        -- amber.prm
```

(folder name 'bin' may be other name)

or

```
Tinker ----- optimize.exe
                |
                --- params --- mm3.prm
                        |
                        -- amber.prm
```

In both case, folder name 'params' is fixed.

However, if the absolute path name of TINKER parameter file
DOES NOT contain "space", parameters in TINKER Key file is described
as absolute path name.

- (2) Although alpha and beta orbitals are obtained from UHF calculation, only alpha orbitals have been taken in the previous version of Facio. Now Facio can display both orbitals of UHF calculation. For ICORBS input data of GAMESS, Facio can automatically set negative orbital numbers for beta orbital CUBE data and visualize them.

For example,

HOMO and LUMO of H₂O radical cation is #5 and #6 MO, respectively. If you set GAMESS input option of ICORBS in UHF calculation as follows

HOMO-2 and LUMO+1,

\$ELDEN in the GAMESS input file will be

```
$ELDEN IEDEN=1 ICORBS(1)=3, 4, 5, 6, 7,  
-3, -4, -5, -6, -7 $END
```

where negative numbers are corresponding beta orbitals.

About this new feature, I appreciate the useful suggestion of Prof. emeritus Ernst Schumacher (University of Bern), the author of RUNpcg and Cygam which are the GUI for executing the GAMESS code.

<http://www.chemsoft.ch/qc/RUNpcg.htm>

<http://www.msg.ameslab.gov/GAMESS/dist.pc.html>

- (3) Zoom In/Out operation can be performed with mouse wheel.

----- Ver.9.0.1 ----- Sept. 12, 2004

- (1) Interface to Tinker-MM3 calculation has been implemented. So you can perform geometry optimization with Tinker-MM3.

Atom types which Facio can recognize are ...

1	C	sp ³ Alkane
2	C	sp ² Alkene
3	C	sp ² Carbonyl
4	C	sp Alkyne
5	H	except on N, O, S
6	O	C-O-H, C-O-C, O-O
7	O	C=O Carbonyl
8	N	sp ³
9	N	sp ² (Amide)
11	F	Fluoride
12	Cl	Chloride
13	Br	Bromide
14	I	Iodide
15	S	-S- Sulfide
16	S+	>S+ Sulfonium
17	S	>S=O Sulfoxide
18	S	>SO ₂ Sulfone
19	Si	Silane
21	H	-OH Alcohol
22	C	Cyclopropane
23	H	NH Amine/Imine
25	P	Phosphine

28	H	Amide
37	N	Pyridine
38	C	Cyclopropene
(but bond stretching parameter 38-38 is undefined in MM3)		
39	N+	N sp3 Ammonium
40	N	N sp2 Pyrrole
41	O	O sp2 Furan
42	S	S sp2 Thiophene
44	H	SH Thiol
46	N	Nitro
47	O	Carboxylate
48	H	Ammonium
49	O	Epoxy
56	C	C sp3 Cyclobutane
57	C	C sp2 Cyclobutene
58	C	C=O Cyclobutanone
124	H	C-H Acetylene

----- Ver.8.7.1 ----- Jul. 30, 2004

- (1) Mesh surface representation for MO, total electron density and electrostatic potential has been implemented.

----- Ver.8.5.1 ----- Jul. 5, 2004

- (1) Using RUNTYP=RAMAN option, you can calculate Raman intensities with which Raman spectrum is simulated.

About this new feature, I appreciate the useful suggestion of Prof. emeritus Ernst Schumacher (University of Bern), the author of RUNpcg.

- (2) In order to demonstrate the modeling ability of Facio, highly complex molecular models for natural toxins listed below are included in the folder PDB/Toxins. Not only the final structures but also intermediate structures are included to show how I constructed them.

Brevetoxin-A	Halichondrin-B
Maitotoxin	Neosurugatoxin
Okadaic Acid	Pinnatoxin-A

----- Ver.8.3.1 ----- Jun. 22, 2004

- (1) Polynucleotide model is built from scratch with a help of Tinker 3.9 (nucleic.exe).

Because of bugs in "nucleic.exe" module in Ver.4.1 and 4.2 (before minor revision: Sept. 8, 2004), collision will occur between the complementary base pairs for B-form double helix (base pairs ≥ 4) and Z-form one.

For B-form double helix, the bugs have been fixed in the Ver. 4.2 (minor revision: Sept. 8, 2004)

However, the bugs on Z-form have not yet been fixed.

- (2) It was revealed that external programs cannot be run in the root folder. Thus, Facio checks whether they are installed in the root folder or not before enabling the menu item for them.

----- Ver.8.0.2 ----- May 31, 2004

- (1) The scale of IR spectrum is shifted in some cases other than Japanese Windows system and Lorentzian line shape of IR spectrum is incorrectly calculated. These bugs have been fixed.

About this bug fix, I appreciate the useful comment of Prof. emeritus Ernst Schumacher (University of Bern), the author of RUNpcg, which is a graphical interface for executing the GAMESS code.

<http://www.chemsoft.ch/qc/RUNpcg.htm>
<http://www.msg.ameslab.gov/GAMESS/dist.pc.html>

RUNpcg is a 'Dialect' GUI to be used in conjunction with Gamess.

'Dialect' is a general purpose programming language that includes an integrated development environment with debugging support.

<http://www.downlinux.com/proghtml/104/10441.htm>

- (2) Structure of an origosaccharide sample PDB (Raffinose.pdb) was incorrect at the connection of fructose and glucose. Correct structure has been included in this version.

----- Ver.8.0.1 ----- Apr. 30, 2004

- (1) Visualization of \$CUBE/Molecular Orbitals which is the new feature of PC GAMESS 6.4.
(2) Bugs in deletion of isolated atom are fixed.
(2) Procedure AddHydrogen was modified.

----- Ver.7.5.1 ----- Apr. 5, 2004

- (1) Glycosyl substituents are available for polysaccharide modeling.
(2) OH, Formyl, NH2 substituents are also available.
(3) Point group symmetry can be specified for GAMESS calculation. Related parameters are GROUP and NAXIS. (GROUP=C1, CN only)
(4) Array of Cartesian coordinates to freeze during a geometry optimization will be set with a parameter IFREEZ.
(5) \$STATPT METHOD=CONOPT with a parameter IFOLOW

This can be used for locating transition states.

- (6) When GAMESS calculation terminated abnormally, the reason will be shown.

- (7) \$VEC data (MO coefficients) can be retrieved from GAMESS punch file and pasted to input file with GUESS=MOREAD.
- (8) When molecular geometry is adjusted, the current value is also shown.
- (9) Auto Centering is OFF by default. For proteins or nucleic acids, default is ON.

----- Ver.7.0.1 ----- Mar. 11, 2004

- (1) Polypeptide model is built from scratch with a help of TINKER's protein.exe

See the description of Tools Menu >> Polypeptide Builder.

- (2) Interface to DFT calculation is implemented.
DFT calculation is a new feature of PC GAMESS ver.6.4.
- (3) Molecular geometry can be adjusted more precisely.
For angle adjustment 0.1 degree is the minimum change and for distance 0.001 angstrom, if "Fine adjustment" is checked.

----- Ver.6.5.1 ----- Feb. 9, 2004

- (1) IR spectrum can be simulated with IR intensities data, which is available in normal mode calculation.
How to use : see the description of Tools Menu >> Normal Mode Vib. Viewer.

- (2) Total electron density can be calculated with semiempirical MOs.

GAMESS produces total electron density as CUBE data only when ab initio calculation is performed. But this feature makes it difficult to visualize the electron density of a very large molecule. Thus, the calculation of electron density using coefficients of semiempirical MO is implemented in Facio 6.5.1.

How to use : see the description of Tools Menu >> Molecular Orbital Viewer.

- (3) Bug fix in 'Delete Atom'.

Fatal exception sometimes occurred when solitary atom was deleted.
Solitary atom is an atom which has no bond to other atoms.

----- Ver.6.0.1 ----- Jan. 24, 2004

- (1) \$HESS group (Hessian Matrix) can be retrieved from GAMESS Punch and attached to the GAMESS input file using GAMESS option HESS=READ.
- (2) The number of Imaginary frequency is checked after RUNTYP=HESSIAN calculation.
- (3) IRC data (a series of structures obtained after RUNTYP=IRC calculation) is visualized.
- (4) New GAMESS Input Options:

```
$CONTRL  RUNTYP=SADPOINT
          =IRC
```

\$STATPT HESS METHOD

\$BASIS NDFUNC NFFUNC NPFUNC DIFFSP DIFFS

\$SIRC PACE SADDLE FORWRD NPOINT STRIDE

- (5) If optimized geometry or saddle point is available, coordinates will be written in 15.10F format to the GAMESS input file for the next run. If not, it will be written in 8.3F format as in PDB file.

Availability of the stationary point coordinates is shown in the GAMESS input option panel.

- (6) You can select perspective projection or orthogonal projection. Orthogonal projection is useful especially when you adjust relative position and tilting angle of two separately loaded molecules.

See also Utilities Menu > "Adjust Position and Tilting Angle".

----- Ver.5.0.1 ----- Dec. 24, 2003

- (1) Isovalue surface of electron density and electrostatic potentials are displayed with dot surface representation.

- (2) New GAMESS Input Options:

MESH Specifies desired density of points
 along each side of the cube.
 Values are COARSE, MEDIUM, and FINE.

ELDENS Electron density is calculated.
ELPOT Electrostatic potentials are calculated.

MORB **MORB=0** (Generates Total Electron Density)
 MORB=xxx (Generates Electron Density for MO # xxx)

- (3) In the previous versions, Facio.ini was not read in on Windows XP. This bug was fixed.

----- Ver.4.7.1 ----- Dec. 11, 2003

- (1) OpenGL rendering has been fully revised.

Result : For example, animation of normal mode vibration is displayed much faster than former versions.
Compare Ver.4.6.1 and Ver.4.7.1.

- (2) On Germany or French system, Facio has been freezed.
This problem was fixed.

Some European countries use a comma for a floating point separator instead of a period. In particular, StrToFloat function will cause an exception if the string passed to it has the wrong decimal separator.

- (3) Exception (e.g. access violation) occurred during the execution

of Facio is fully trapped. This feature can be customized by editing the following init record in Facio.ini.

```
[AppControl]
ExceptionMessage=ON
```

where

ON ==> Trap exception

OFF ==> Egnore exception (But Facio may be freezed in case of vital exception)

- (4) Visualization of electron density and electrostatic potential is not yet implemented in Ver.4.7.1.

----- Ver.4.6.1 ----- Nov. 7, 2003

- (1) Facio can be launched as a command line application, which accepts one command line argument (i.e. pdb file) at run time.

How to use :

MS-DOS prompt> Facio.exe xxx.pdb

where the xxx.pdb is a PDB file.

- (2) Graphics rendering interval can be customized in Facio.ini file. Since no GUI is provided for adjusting this parameter, please edit the following init record in Facio.ini.

```
[Timer]
Interval=50
```

This means that graphics are rendered every 50 microseconds.

If your graphics card does not have sufficient power, try to set this parameter higher value, e.g. Interval=100.

If your graphics card have sufficient power, you can set it lower value, e.g. Interval=30. In that case, Facio will more quickly respond to your mouse movement. However, never set it 10 or lower : your machine may be freezed.

This feature is no more necessary for Ver.4.7.1 or higher

- (3) MODEL records in PDB file are recognized.
Only one model is displayed and other models are omitted for clarity.
- (4) Hydrogen atoms of standard residues in PDB file are parsed to produce connectivity record.
- (5) Hydrogen atom can be attached to lone atom.

----- Ver.4.5.1 ----- Oct. 17, 2003

- (1) MO visualization is implemented for basis set MINI.
This means that MOs of all the atoms up to Rn can be visualized. You can see 4f orbitals for lanthanides.

- (2) New GAMESS input options(IREST and GUESS) are supported.**
With input option IREST=-1, GAMESS execution can be easily restarted where it left off.
- (3) Several bugs about parsing Protein PDB files are fixed.**