***** Facio Ver. 26.2.1 Manual *****

Thank you very much for downloading my program, Facio.

****

****** Citation ******

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The required citation for Facio is the following.

M. Suenaga, *J. Comput. Chem. Jpn.*, Vol. 4, No. 1 pp. 25-32 (2005)

M. Suenaga, *J. Comput. Chem. Jpn.*, Vol. 7, No. 1 pp. 33-53 (2008)

The online version of the journal is available at the web site below.

http://www.sccj.net/publications/JCCJ/v4n1/a11/abst.html

http://www.sccj.net/publications/JCCJ/v7n1/H1920/abst.html

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*** Copyright and Legal Information ***

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*** Pronunciation of "Facio" ***

****

Facio is named after a Latin verb "facio" which means "I make".
Therefore, "c" in Facio is pronounced as "k" as in "car".

****

*** Introduction ***

****

Facio is a 3D-graphics program for molecular modeling and visualization
of quantum chemical calculations, such as molecular orbitals and
normal mode of vibrations. Since Facio internally uses PDB file format,
it can also display a 3D-structure of biological macromolecules,
such as proteins and nucleic acid with emphasizing their secondary or
quaternary structures.

-- Note --
Facio is fully tested on Windows 7
and runs well at least on my PCs.
But it is reported that sometimes Facio does not work properly.
In that case, follow the instructions below to disable or

constrain 3D graphics accleration.

(1) Click on the Start Menu\Settings\Control Panel shortcut.
(2) Double click on the System Icon, in the Control Panel.
(3) Click on the Performance Tab in the System Properties Dialog.
(4) Click on the Graphics button in the Performance tab.
(5) Either slide the acceleration to NONE, or Level 1.
And make sure you have downloaded and installed
the latest driver for your graphics card.

****
*** Installation ***
****

No special installation procedure is required,
for Facio will never touch the registry of Windows OS.
Just extract Facio package by double clicking
the ZIP archive (Facio2621-64.zip, Facio2621-32.zip) and
place the extracted folder at anywhere you like.

But if you perform GAMESS calculation from Facio,
be sure to place GAMESS at the local drive. Not at the remote or network drive.
For more information, see the description of Calculation menu.

****
*** Visualization of Quantum Chemical Calculations ***
****

Reading GAMESS punch file, Facio can visualize normal mode
of vibration by animation and molecular orbital lobes.

After Facio 6.5.1, the corresponding output file is
also loaded for IR intensities which are recorded only in the output file.

Sample data are included in the "NormalMode" folder
and "MolecularOrbital" folder in the Facio package.
Refer to the readme files therein.

MO visualization is implemented only for
STO(MNDO, AM1, PM3) and GTO(STO-3G, MINI).
In addition to this, Facio 8.0.1 can visualize
$CUBE/Molecular Orbitals data, which is the new feature
of PC GAMESS 6.4.

****
*** Tutorial for Saddle Point and IRC calculation ***
****

Saddle point and IRC calculation for an internal rotation of
a methyl group in methane are shown as an example.
Structual data and GAMESS input/output data are
included in the "SaddleIRC" folder.

Refer to the readme file "SaddleIRC.txt" therein.

```
*****************************
***  About Molecular Modeling ***
*****************************
```

In Facio, molecular model is assembled
by replacing a hydrogen with CH3, CH2, CH or Phenyl.
Besides fundamental functions required for molecular modeling,
Facio featues the following functions.

(1) Geometry Optimization with PC GAMESS, WinGamess, MOPAC and TINKER(MM3)

      * Setting GAMESS input option, you can execute geometry optimization
         on the displayed molecule.
      * The optimized geometry is applied to the molecule on the screen,
         immediately after the termination of calculation.

(2) Rendezvous and Docking of Two Molecule

      * Two molecular files (in PDB format) can be successively loaded.
      * And the relative position of the latter molecule can be adjusted.
      * Any two bonds of each two molecule can be aligned.
      * Two hydrogen atoms are deleted and then a bond is formed.
      * One of the two groups attached to the bond
         can be moved along the bond.

      The above process is illustrated by GIF animation on my home page.
      Please visit   http://www1.bbiq.jp/zzzfelis/Facio.html

```
     ############################################################
```
      The second feature makes it possible to construct a model of
      a large molecule from several small subunits which are
      optimized respectively prior to being connected.
```
     ############################################################
```


```
************************************************************
*** Brief Description of Menu and Slide in the Main Form ***
************************************************************
```

    Descriptions are sometimes omitted for self-explanatory menu items.

```
===== (1) Three Slides in the Main Form =======================
```

      Left side slide   : Zoom
      Bottom side slide : Rotation about Y axis
      Right side slixe   : Rotation about X axis

      Drag with Shift key down : Rotation about Z axis

      Drag with Alt key down : Translation in XY plane
                                       Sensitivity is controlled with a parameter TransSens
                                         in Facio.ini file.

      where X and Y axis run through the center of the monitor
      horizontally and vertically in the plane, respectively
      and Z axis is perpendicular to the monitor plane.

=====(2) File Menu ==

Load New PDB File
  For molecular modeling, you have to load a molecule in PDB format.

Load New Structure (other than PDB)
--------- Cartesian Coordinate File
--------- Free Formatted / WebLab XYZ File
--------- MDL Molfile
--------- Tripos Mol2 File
--------- CIF File
-------- Facio Cartesian Coordinate File
--------- Multi File (in Drag-and-Drop Mode)

Load New Gamess
--------- Output for Optimized Geometry

  For open file, Facio sets the initial directory
  to the directory where GAMESS executable exists.
  Set properly the location of GAMESS
  with Preference Menu >> External Programs

--------- Punch for Normal Mode Vibration
--------- Punch for $VEC/Molecular Orbitals
-------- Punch for $CUBE (ElDens and ElPot)
-------- Punch for $CUBE (Molecular Orbitals)
--------- Extract Optimized Geometries from PC GAMESS Relaxed PES Scan

  To visualize energy profile of PES and the corresponding structures,
  use Tools Menu >> PES Scan Data Viewer

--------- WinGamess Output for Bulk Model in SIMOMM Calc.
--------- IRC Data
--------- Input for Cartesian Coordinate
--------- $HESS group (Hessian Matrix) from GAMESS Punch
--------- $VEC group (MO coefficients) from GAMESS Punch

Load New Tinker xyz

Load New Gaussian Output for Optimized/Intermediate Geometry

Load and Append Another Molecule
--------- by Drag and Drop (for all readable format)
--------- with Open Dialog (for PDB only)

  Rendezvous and docking of two molecules.
  To adjust the relative position of the second molecule,
  a relevant control panel automatically appears
  See also the description of
  Utilities >> Adjust Position and Tilting Angles.

Save

  Save the current molecular structure as HETATM/CONECT format PDB
  Disabled when protein or nucleic acid or non-PDB file is loaded,
  because ATOM records of these molecule are deleted.

Save As
--------- (HETATM/CONECT) Format PDB

       Even for protein and nucleic acid, the structure is saved
       as HETATM/CONECT format.

--------- Cartesian Coordinate 2
--------- WebLab XYZ
-------- Facio Cartesian Coordinate
--------- GAMESS Input

       Save GAMESS Input file containing input option and coordinates.
       This command is enabled only when the GAMESS Input Option
       Panel is open.
--------- User Defined Substituent

Quit

===== (3) Edit Menu ==

  ****
  *   When modifying the model, first select the mode   *
  *   in the Edit Menu and then click atom(s).   *
  ****

Undo

       Undo the following eight operations.

Delete Atom,	Make Bond,
Delete Bond,	Add Hydrogen,
Replace H with CH3,	Replace H with C(sp2)H2,
Replace H with C(sp)H,	Replace H with Phenyl

Atom
--------- Move Atom

       Select this mode and click atom sphere,
       then operation panel appears.

       Coordinate axis
       X axis (yellow)
       Y axis (cyan)
       Z axis (green)

--------- Delete Atom

       Select this mode and click atom sphere,
       then the clicked atom is deleted.
       Attached hydrogen(s) are also deleted.

--------- Change Atom

       Select this mode and click atom sphere,
       then operation panel appears.

--------- Add Hydrogen

Select this mode and click atom sphere,
then a hydrogen atom is added.

Bond
--------- Make Bond

In this mode, a bond will be made between
two successively clicked atoms.

--------- Delete Bond

In this mode, a bond will be deleted between
two successively clicked atoms.

*** No effect for clicking bond itself. ***

In the following three mode, group of atoms are
moved according to the change of bond length,
angle or rotated around the bond.

For example, in the Move Group Along Bond mode,
if you click bonded two atoms, group of atoms
attached directly or indirectly to the secondly clicked
atom are moved with the change of bond length.

Group
--------- Move Group Along Bond
--------- Move Group with Angle Change
--------- Rotate Group around Bond

In the following four mode, if you click a hydrogen atom,
it is replaced with CH3, CH2, CH, Phenyl, Glycosyl, OH,
Formyl or NH2, respectively.

Replace H with
--------- CH3
--------- C(sp2)H2
--------- C(sp)H
--------- Phenyl

--------- Glycosyl

New panel will appear for selection of glycosyl group.

--------- OH
--------- Formyl
--------- NH2
--------- User Defined Substituent

Align Four Atoms

This menu item is enabled only if the second molecule is loaded
by "File >> Load and Append Another PDB File" menu item.

In this mode, successively clicked four atoms are
aligned in a line. But be sure the 1st and 2nd atoms belong to the
first molecule and the 3rd and 4th atoms belong to the second
molecule.

```
*********************************************************
    By this command and 'Move Group Along Bond' command,
    two molecules can be easily connected.
*********************************************************
```

Modify
--------- Modify Bond Length

Select this mode and click two atom spheres,
then operation panel appears.

--------- Modify Bond Angle
--------- Modify Dihedral Angle

Enable Safe Mode
Open Edit Tool Box
Z-Matrix Editor

===== (4) Models Menu ==

Select one of these model types.

Ball and Stick model is default for non-peptide or non-nucleic acid.
Plain Wire model is default for peptide or nucleic acid.

"Dot Surface and Stick model" and "Dot Surface and Wire model"
are enabled only when Solvent Excluded Surface is calculated by MSMS.

Wire (colord by ...) models are enabled only for
peptide and nucleic acid.

Ball and Stick
CPK (Space Filling)

Stick
--------- Plain
--------- With Dotted Molecular Surface
--------- With Marbled Molecular Surface

Wire
--------- Plain
--------- Rainbow

Wire's color is changed every (the total number of atoms)/7 atoms.

--------- Colored by Quaternary Structure

In this mode, quaternary structures are distingushed by 10 colors.
9 colors for standard residue chain and
1 color (white) for non-standard resudue chain.

See also Miscellaneous Menu >> Quaternary Structure Visibility

--------- Colored by Secondary Structure

In this model, secondary structures are distingushed by colors.

Alpha Helix ===> red
Beta Sheet   ===> yellow
Beta Turn   ===> green

See also Miscellaneous Menu >> Secondary Structure Visibility

--------- With Dotted Molecular Surface

Trapezoidal Quad for Protein
New representation method for protein, in which each amino residue is represented as
trapezoidal quad (O of amide carbonyl, C of amide carbonyl, alpha carbon, and N of amide).
Different Colors for Two Molecules

===== (5) Preferences Menu ===

Molecular Model
--------- Atom Properties
Adjusts the diameter and color of atom sphere.

--------- Bond Properties
Adjusts the diameter and color of bond cylinder.

--------- Graphics Quality
Adjusts the graphics quality of sphere and cylinder.
No effect for Wire model.

For protein and nucleic acid, graphics quality is
automatically lowered for rendering speed.

--------- Orthographic Projection

External Programs

Set the absolute path to the executable file of the
external programs (TINKER, GAMESS, MSMS and WinGamess).

For TINKER, force field parameter for peptide also must be set.

Menu items(GAMESS and MSMS)
in Calculations Menu are enabled only if the location of the
external programs are properly set.
If the menu "GAMESS" or "MSMS" are not enabled,
please check Preferences >> External Programs.

In this version of Facio, TINKER is used only for peptide building.
So the Calculations Menu >> TINKER ,which is the interface for
molecular mechanics calculation of general organic compound is always
disabled in Ver. 7.0.1.

Default Gamess for file opening can be set.

Surface
--------- Molecular Surface Properties

Adjusts the diameter and color of dot and marble (small sphere)

in Dotted or Marbled Surface model.

--------- Molecular Orbital Properties
        Adjusts the color of molecular orbital lobe
        for positive and negative phase, respectively.

        It also djusts the diameter and color of dot (small sphere)
        for Dot Surface representation of Molecular Orbital.

--------- Isosurface Properties
        Adjusts the color of isovalue surface of electron density
        and electrostatic potentials.

SSH / SFTP Connection Properties (----- disused since Facio 21.1.1 -----)

        Sets server name, user ID, etc. for SSH / SFTP connection.

Other Preferences
--------- Background Color
        Adjusts the background color.

--------- Arrow Properties
--------- Spinning Rate
        Adjusts the spinning rate of model.
        Molecular model is automatically rotated,
        if Utilities >> Spin about X Axis or Utilities >> Spin about Y Axis
        is checked.

--------- Label Properties
        Set the color of sequence atom number label
Linux-WINE Mode

Save Current Properties
        All the preferences are saved in Facio.ini which
        resides at the same folder where Facio executable exists.

        When Facio starts up, it reads the preferences in the Facio.ini.

        Since Facio.ini is simple text file, you can change preferences
        by editing Facio.ini.

Load Default Properties
        DefaultFacio.ini has default preferences for Facio.

Save Position
        User-customized position and size of main window, worksheet and Tool Box
        are saved in Facio.ini.

Show Only Symmetry Unique (for GAMESS)
Gaussian Coordinate System : Input Orientation
Gaussian Coordinate System : Standard Orientation
Reset Current Directory of PDB

===== (6) Miscellaneous Menu ==

Worksheet
--------- Show

All the messages from Facio is displayed in Facio's Worksheet.
By default, the worksheet is shown.

--------- Erase

Worksheet can hold only 32 KByte messages.
(This is a limitation of Windows 98 and Me)

Show
--------- Coordinate Axis

X axis : yellow
Y axis : cyan
Z axis : green

--------- Selected Atom Number

If this menu item is checked,
serial number of the clicked atom is shown in Facio's Worksheet.

--------- Numeric Labels
--------- Atom Symbols
--------- _atom_site_label of CIF
--------- Guides
--------- Show Dipole Moment
--------- Hydrogen Bonds

Highlight
--------- Highlight Specified Atom

Specified atom is shown in a yellow box.

--------- Highlight PDB Residue Sequence
(Moved to FMO menu > PDB Utilities > Residue Sequence Viewer from Ver. 18.4.1)

Skip Hydrogen Bond Detection

Centering and Zoom
--------- Auto Centering

If this menu item is checked,
the whole molecule is automatically moved to center
when new substituent is introduced to the model.

--------- Auto Centering OFF for Protein and Nucleic Acid   (Deleted   from Ver. 12.1.2)
--------- Auto Zoom
--------- Zoom Position --> 0

Verbose

If this menu item is checked,
more messages are displayed.

Quaternary Structure Visibility

Control the visibility of quaternary structure.
With nine colors, Facio distingushes quaternary structure.

Enabled only when the model type is

Wire (Colored by Quaternary Structure).

Secondary Structure Visibility

Control the visibility of secondary structure.
With three colors, Facio distingushes secondary
structures (Helix, Sheet, Turn).

Enabled only when the model type is
Wire (Colored by Secondary Structure).

Invoke Molekel

Show Screenshot Capture

Show Periodic Table of the Elements
--------- Ordinary Type
--------- In Kanji (Traditional Chinese Characters)

Summarize Energy/Grad/Geometry Changes

===== (7) Utilities Menu ===

Dump
--------- Connectivity

Saves connectivity data to file

--------- Geometric Information (Bond Length, Angle, Dihedral Angle)
--------- Hydrogen Bonds

Geometric Comparison
--------- Load Two Structures for Geometry Comparison
--------- Geom. Diff. of 1st and 2nd Molecules (by Approximity)

Saves geometrical differences (bond lengths, bond angles and dihedral angles)
of the 1st and 2nd molecules which is loaded with "Load and Append Another PDB File".
Method 1 determines the corresponding atoms by approximity.
Criterion value is "ApproximityCriteria4DumpDiff" in Facio.ini.
So, be sure to superimpose the two molecule as closely as possible before dump.

--------- Geom. Diff. of 1st and 2nd Molecules (by Connectivity)

Almost same as the above. However Method 2 determines the corresponding atoms
by connectivity in PDB file. So, you don't have to superimpose the two molecules.
But they must have an identical connectivity.

--------- RMS Fit by Quaternion Method
--------- Calculate RMSD

Spin About
--------- X Axis

If this menu item is checked, the model is
automatically rotated about X axis.
See also Preferences Menu >> Spinning Rate

--------- **Y Axis**

> **If this menu item is checked, the model is**
> **automatically rotated about Y axis.**

--------- **Z Axis**

Interatomic Distance

> **If this menu item is checked,**
> **interatomic distance is shown for the successively clicked two atoms.**

Bond Angle

> **If this menu item is checked,**
> **bond angle is shown for the successively clicked three atoms.**

Dihedral Angle

> **If this menu item is checked,**
> **dihedral angle is shown for the successively clicked four atoms.**

Adjust Position and Tilting Angle

> **Molecule is translated along the global coordinate and**
> **roteted about the local coordinate of the molecule.**

> **View along X, Y, Z Axis and Orthogonal Projection utilities are**
> **also available in this control panel.**

Move Whole Molecule
--------- **To Center**

> **Moves the average position of all the atom to**
> **the center of monitor**

--------- **by Setting Specified Atom to Center**

> **First click an atom and selct this menu item, then**
> **the clicked atom will be moved to the center of monitor.**

--------- **by Setting Specified Atoms to Axis / Plane**

--------- **by Performing Principal Axes Transformation of Inertia Moment**

> **Calculates tensor of inertia moment and diagonalizes it.**
> **Then performs principal axes transformation so that Ixx < Iyy < Izz.**
> **When principal values are in degenerate, no transformation is performed.**

--------- **Reflection in XY Plane**
--------- **Reflection in YZ Plane**
--------- **Reflection in ZX Plane**

Impose Point Group Symmetry
--------- **with Symmetrizer at Tolerance = 0.1 (default)**
--------- **with Symmetrizer at Tolerance = 0.5 (loose)**
--------- **with Symmetrizer at Tolerance = 1.0 (very loose)**
--------- **by Applying Every Symmetry Operation One by One**

View
--------- Along X Axis (yellow)
--------- Along Y Axis (cyan)
--------- Along Z Axis (green)
--------- Open View Point Controller

Forced Move
--------- To XY Plane (sigma-h plane)

      Atoms within ProximityCriteria (default=0.6 angstrom) are
      exactly moved to XY plane. The parameter ProximityCriteria is
      set in the Facio.ini.

--------- To XZ Plane (sigma-v plane)
--------- To Z Axis (principal rotation axis)
--------- To X=Y Plane

Complete
--------- Missing Bonds
--------- Missing Hydrogen Atoms (by HETATM/CONECT Record)

Reassign Atom Numbers
      Shows the utility window. To use this, follow the instructions below.
      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.

Find
--------- TER Record in PDB
--------- Closely Located Atoms
--------- Isolated Atom
--------- Small Interatomic Distance
--------- Find H atom which has two bonds

===== (8) Calculations Menu ==

    These menu items are enabled only if the corresponding executable exists
    at the location specified in Preferences >> External Programs.

    ****
    PC GAMESS cannot be run in the root folder. Therefore, the absolute
    path of GAMESS executable should not be C:\Gamess.exe.
    ****

    Default value of the executable location is

    for GAMESS   c:\Gamess\gms_nt\gamess.exe
    for MSMS   c:\Msms\msms253.exe

    which are described in Facio.ini file.

    These settings can be changed according to user's environment.

Firefly (PC GAMESS)

      Shows a control panel for PC GAMESS calculation.
      In the panel, you can select GAMESS input options
      (Basis Set, Charge, Multiplicity, Run Type , etc.)

and execute GAMESS calculation in two modes described below.

(Mode 1) In this mode, GAMESS calculation is started
using "CreateProcess" Windows API.
Therefore you must not quit Facio until calculation
has finished. However optimized geometry is applied to
the current molecule immediately after the termination of
calculation, when the run type is OPTIMIZE.

(Mode 2) In this mode, GAMESS calculation is started
using "ShellExecute" Windows API.
Since GAMESS process is independently envoked,
you can quit Facio before the termination of calculation.

This mode is highly recommended for time-consuming jobs,
such as ab initio calculation and geometry optimization of
a large molecule.

Before calculation, Facio prepares two files (INPUT and Facio.bat).
Then the Facio.bat is executed.

(1) INPUT   (GAMESS input file)
(2) Facio.bat   (such as below.)

```
cd "c:\Gamess\gms_nt"
del PUNCH.OLD
ren PUNCH PUNCH.OLD
GAMESS.EXE > Facio.out
mkdir Facio
copy INPUT "Facio\ABC.inp"
copy Facio.out "Facio\ABC.out"
copy PUNCH "Facio\ABC.pun"
```

In the above example, the corresponding structural data is ABC.pdb.
After the calculation is over, four files are newly created.

Facio.out   (GAMESS output file)
PUNCH   (GAMESS punch file)
ABC.out   (a copy of Facio.out)
ABC.pun   (a copy of PUNCH)

MSMS   (Molecular Surface)

Shows a control panel for MSMS calculation.
In the panel, you can select MSMS input options
and execute MSMS calculation to computes the reduced surface and
analytical model of the Solvent Excluded Surface (SES).

Before calculation, Facio prepares two files (Facio.xyz and Facio.bat).
Then the Facio.bat is executed.

(1) Facio.xyz   (MSMS input file)
(2) Facio.bat   (such as below.)

```
cd "c:\msms"
"c:\msms\msms253.exe" -if Facio.xyzr -de 16 -prob 1.5 -of Facio
```

Results are saved in Facio.face and Facio.vert.

If calculation is normally terminated, two relevant menu items will
be enabled :   "Dotted Molecular Surface and Stick" and
                      "Marbled Molecular Surface and Wire"

TINKER-MM3   (Molecular Mechanics)

Molecular mechanics calculation with MM3 parameter starts.
After the calculation, optimized geometry will be retrieved and
applied to the current structure automatically.

Molecular mechanics geometry optimization is useful
especially for the modeling of large-membered alicyclic ring system
or higher fullerenes.

WinGamess

Shows a control panel for WinGamess calculation.

SIMOMM Layer

Gaussian

Shows a control panel for Gaussian calculation.

Gaussian Utilities

Shows a control panel for Gaussian Utilities

ONIOM Layer

Shows a control panel for Gaussian ONIOM layer specification

UTChem

Shows a GUI for UTChem to make an input file and to execute the job.

MOPAC

Shows a GUI for MOPAC to make an input file and to execute the job.

===== (9) Tools Menu ===

Viewers
--------- Normal Mode Vib. Viewer

Shows a control panel for normal mode of vibration.
This menu item is enabled only if data of mormal mode
of vibration is loaded from GAMESS punch file.

--- How to use the control panel ---

        (1) Specify the number of normal mode.

        (2) Specify the value of Frames per half cycle.
             Default value is 5.

(3) Click "Start/Shift Frame" button.

(4) If "Stop frame by frame" is checked,
animation stops frame by frame.
This is useful when you capture the Facio screen
in order to make a GIF animation.

--- The following button is enabled only when IR intensities are available ---

(5) Open IR Spectrum Window.

IR intensities are recorded in the corresponding output file and
NOT in the punch file loaded. Thus Facio automatically loads
the corresponding output file for IR intensities. In that process,
Facio requires that the output file must reside on the same
folder where the corresponding punch file is.

--------- $VEC/Molecular Orbital Viewer

Shows a control panel for molecular orbital.
This menu item is enabled only if $VEC data (MO coefficients)
is loaded from GAMESS punch file.

****
MO visualization is implemented only for
STO(MNDO, AM1, PM3) and GTO(STO-3G, MINI).
****

--- How to use the control panel ---

(1) Specify the molecular orbital number.
Default is HOMO.

When Facio load $VEC data from punch file,
ABC.pun for example, it also access the corresponding
GAMESS output file, ABC.out to get the number of
occupied orbital and MO energies.
If ABC.out does not exist in the same folder of ABC.pun,
the molecular orbital number is set to 1 and
MO energy is labled as "No Data".

(2) Click "Calculate MO Lobe and show".

(3) Isosurface grid point of molecular orbital is determined
with two parameters :   "Isosurface Value" and
"Surface Thickness" with the following criteria.

Grid points P(x,y,z) which are

for positive region	for negative region
$IV < P(x,y,z) < IV + ST$	$- IV - ST < P(x,y,z) < - IV$

are displayed.

where IV : Isosurface Value;   ST : Surface Thickness

(4) If "Marbled surface representation" is checked,
MO lobes are represented as dot(small sphere) surface.

(5) If "Point Size = 2" is checked,
  MO lobes are drawn with point size 2.
  Use this option, when the MO lobes are difficult to see.

(6) If Mesh surface is checked,
  MO lobes are drawn as mesh surface.

--- The following two buttons are enabled only for ab initio calculations. ---

(7) Calculate Electron Density with coefficients of semiempirical MOs

  The calculated electron density is visualized with
  Tools Menu >> ElDensandElPot item.

(8) Save calculated ElDens to 'CalcElDens.txt'

  The calculated electron density can be saved as a text file
  in the same format of GAMESS' CUBE file.
  The file name is fixed to 'CalcElDens.txt'.
  If you append CalcElDens.txt to the corresponding punch file,
  the punch file can be loaded as CUBE data.

--------- ElDens and ElPot Viewer

Shows a control panel for isovalue surface of electron density
and electrostatic potentials.
This menu item is enabled only if data of electron density or
electrostatic potentials are loaded from GAMESS punch file.

To calculate electron density and/or electrostatic potentials,
GAMESS calculation needs to be excuted with ELDENS and/or
ELPOT checked in the Input Option panel and with basis sets for
ab initio methods. When MNDO, AM1 or PM3 is used, electron density
and electrostatic potentials are never output in punch file.

--- How to use the control panel ---

(1) Specify what to display.
  (Electron Density or Electrostatic Potentials)

(2) Specify the value of isosurface.
  Default value is 0.0001.

(3) Specify the Thickness value.
  Default value is 0.0001. This parameter is simultaneously
  changed with the isosurface value. But it can be adjusted
  between 1/10 and 5 times of the isosurface value.

(4) Click "Calculate Isosurface and Show" button.

(5) If Mesh surface is checked,
  isosurface is drawn as mesh surface.

--------- IRC Data Viewer

Shows a control panel for IRC Data viewer.
This menu item is enabled only if IRC data are loaded

from GAMESS IRC file and Gaussian formatted check file.

--------- CUBE/Molecular Orbital Viewer

Shows a control panel for molecular orbital.
This menu item is enabled only if CUBE/Molecular Orbital
data (Grid data of MO) is loaded from GAMESS punch file or Gaussian cube file.

--- How to use the control panel ---

Same as $VEC/Molecular Orbital Viewer.

****
CUBE/Molecular Orbital is a new feature of PC GAMESS 6.4.
****

--------- Gaussian ADMP/BOMD Trajectory Viewer

This menu item is enabled only if Gaussian Trajectory data is available.
Trajectory is loaded with Tools Menu>>Load Gaussian Formatted Check File for Trajectory.

--------- NMR Data Viewer

--------- PES Scan Data Viewer

Builders
--------- Polypeptide Builder

Shows a control panel for Polypeptide Builder.
This menu item is enabled only if TINKER executables and
Force Field parameters exist in the folder which is set
in the External Programs of Preferences Menu.

--- How to use the control panel ---

(1) Make a polypeptide sequence with amino residue buttons.
    For each residue, predefined Phi, Psi and Omega angles are
    applied by specifying secondary stracture type.
    For example, if you select Helix (Alpha Helix) then
    Phi, Psi and Omega are set to -57, -47 and 180, respectively.

(2) Terminate the sequence with "Terminate", "Cyclize",
    "NME" or "NH2" buttons.

(3) Build a polypeptide structure with "Build" button and
    TINKER (protein.exe) creates it.

(4) Then optimize the geometry with "Minimize" or "Optimize"
    button.

(5) For procedure (3) and (4), outputfile (TINKER XYZ format) is
    fixed to "Facio.xyz". But if you would like to save the XYZ
    file, specify the file name in "Save As Textbox".

--------- Polynucleotide Builder

Shows a control panel for Polynucleotide Builder.
This menu item is enabled only if TINKER executables and
Force Field parameters exist in the folder which is set

in the External Programs of Preferences Menu.

--- How to use the control panel ---

(1) Specify helix form : A-, B-, or Z-form.

(2) Make a polynucleotide sequence with amino residue buttons.

(3) Terminate the sequence with "Terminate" button.

(4) Build a polynucleotide structure with "Build" button and TINKER (nucleic.exe) creates it.

(5) Then optimize the geometry with "Minimize" or "Optimize" button.

(6) For procedure (4) and (5), outputfile (TINKER XYZ format) is fixed to "Facio.xyz". But if you would like to save the XYZ file, specify the file name in "Save As Textbox".

Cross Section Controller for CUBE MO
Setting arbitrary cross section of CUBE MO for contour map

Load Gaussian
--------- Cube for MO(s) (in single file mode)
--------- Cubes for MOs (in multi file drag and drop mode)
--------- Output for Normal Mode Vib.
--------- Cube for Density
--------- Cube for Electrostatic Potential
--------- Formatted Checkpoint for IRC
--------- Formatted Checkpoint for Trajectory
--------- Formatted Checkpoint for Geometry

MO Levels Graphical Viewer
--------- Alpha MO
--------- Beta MO

NMR Shielding Tensor
--------- WinGamess
--------- Gaussian

Load UTChem Output for Geometry

Load MOPAC
--------- Output for Normal Mode Vibration
--------- Output for Optimized Geometry and MO

Gaussian/AMBER Utility
--------- Generate atom type and partial charge data for Gaussian/AMBER calculation

TINKER-MM Input File Maker

Load MSMS vertex (*.vert)

Tetrahedron Drawer

Box Drawer

===== (10) FMO Menu ==

FMO (Gamess) Control Panel   GUI for FMO calculation

Local Structure Viewers
--------- #1
--------- #2
--------- #3
--------- #4

#####PDB Utilities
--------- Residue Sequence Viewer
--------- Extract MODEL
--------- Delete Alternate Location (Atom Variant) of PDB
--------- PDB Atom Name Field Converter
--------- Add Hydrogen Atoms to Protein PDB by ATOM Record
--------- Point Mutation
--------- Add Hydrogen Atoms to Nucleic Acid PDB by ATOM Record
--------- Translate to Center (+ Offset)
--------- PDB Atom Name Field Converter (for Xleap/AMBER)
--------- Find Contacting Waters
--------- Find Contacting Waters (in Multi Job Mode)
--------- Make Serial Number Serial
--------- Delete TER Record Serial Number and Renumber

Load GAMESS/FMO Output

Make FMO Output Difference

Save PIEDA in Gamess Output Format

Select FMO Version (4.1, 5.3, 5.4, 5.5)

===== (11) ELG Menu ==

Elongation Method Input

Clip Unit and Make Model by Unit Stacking

****
*** External Programs ****
****

    Facio uses 8 external programs,
    Firefly (PC GAMESS), WinGamess, MSMS, TINKER, MOPAC, UTChem, Gaussian and
    Symmetrizer.
    But no modification has been made to these programs:
    Facio just execute the programs in Windows / Linux environment
    and receive the result.

    Facio's distribution archive does not contain those programs.
    So please visit their home page to download.

    (1) Firefly (former PC GAMESS) and WinGamess

        Intel x86 (Win32,Linux,OS/2,DOS) VERSION

copyright (c) 1994, 2000 by Alex. A. Granovsky,
Laboratory of Chemical Cybernetics,
Moscow State University, Moscow, Russia.
Some parts of this program include code due to
work of Jim Kress, Peter Burger, and Robert Ponec.

http://classic.chem.msu.su/gran/gamess/index.html   (Firefly home page)

GAMESS is maintained by the members of the Gordon research group
at Iowa State University.

http://www.msg.ameslab.gov/gamess/download.html

--- GAMESS (US) QC package ---
M.W.SCHMIDT, K.K.BALDRIDGE, J.A.BOATZ, S.T.ELBERT,
M.S.GORDON, J.H.JENSEN, S.KOSEKI, N.MATSUNAGA,
K.A.NGUYEN, S.J.SU, T.L.WINDUS,
TOGETHER WITH M.DUPUIS, J.A.MONTGOMERY
J.COMPUT.CHEM.   14, 1347-1363(1993)

FMO method in GAMESS should reference:
D.G. Fedorov, K. Kitaura, J. Chem. Phys. 120, 6832 (2004).

****
The appropriate Firefly (former PC GAMESS) citation is as follows:

... calculations were performed using
the PC GAMESS version [1, 2] of the GAMESS (US) QC package [3]

[1]   A.A. Granovsky, PC GAMESS version 7.0,
      http://classic.chem.msu.su/gran/gamess/index.html

[2]   A. V. Nemukhin, B. L. Grigorenko, A. A. Granovsky
      Molecular modeling by using the PC GAMESS program:
      From diatomic molecules to enzymes
      Moscow University Chemistry Bulletin.
      2004, Vol. 45, No. 2, P. 75.

[3]   M.W.Schmidt, K.K.Baldridge, J.A.Boatz, S.T.Elbert, M.S.Gordon, J.J.Jensen,
      S.Koseki, N.Matsunaga, K.A.Nguyen, S.Su, T.L.Windus, M.Dupuis, J.A.Montgomery,
      J.Comput.Chem. 14, 1347-1363 (1993)
****

(2) MSMS   (Solvent Excluded Surface calculation)

http://mgltools.scripps.edu/downloads#msms

Sanner, M.F., Spehner, J.-C., and Olson, A.J. (1996)
Reduced surface: an efficient way to compute molecular surfaces.
Biopolymers, Vol. 38., (3), 305-320.

(3) TINKER

http://dasher.wustl.edu/tinker/

Selected References for the TINKER Package:

P. Ren and J. W. Ponder, J. Phys. Chem. B, 107, 5933-5947 (2003)
R. V. Pappu, R. K. Hart and J. W. Ponder, J. Phys. Chem. B, 102, 9725-9742 (1998)

M. E. Hodsdon, J. W. Ponder and D. P. Cistola, J. Mol. Biol., 264, 585-602 (1996)

M. J. Dudek and J. W. Ponder, J. Comput. Chem., 16, 791-816 (1995)
C. E. Kundrot, J. W. Ponder and F. M. Richards, J. Comput. Chem., 12, 402-409 (1991)

J. W. Ponder and F. M. Richards, J. Comput. Chem., 8, 1016-1024 (1987)

(4) Gaussian 03W, 09W and 16W
http://www.gaussian.com/

(5) UTChem
   Not available now

(6) MOPAC2016
MOPAC has been re-released under the open-source LGPL license, and users no longer need to sign a license agreement.

http://openmopac.net/Download_MOPAC_Executable_Step2.html

(7) Symmetrizer
"Symmetrizer: Algorithmic Determination of Point Groups in Nearly Symmetric Molecules"
R. J. Largent, W. F. Polik, J.R. Schmidt,
J. Comput. Chem. 2012, 33, 1637-1642. DOI: 10.1002/jcc22995
https://www.chem.hope.edu/~polik/software.htm

   Place symmetrizer.jar at the same folder where Facio.exe is.

****
******   Citation   ******
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The required citation for Facio is the following.

   M. Suenaga, *J. Comput. Chem. Jpn.,* Vol. 4, No. 1 pp. 25-32 (2005)

   M. Suenaga, *J. Comput. Chem. Jpn.*, Vol. 7, No. 1 pp. 33-53 (2008)

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