

## ***Homology Modeling Professional for HyperChem Release Notes***

This document lists additional information about *Homology Modeling Professional for HyperChem*.

### **Current Revision**

Revision H1 (Version 8.1.5)

### **Current Versions of Module Programs**

The module programs interface to *HyperChem* using its *Chemist's Developer Kit* (TclPro). These control *HyperChem* as well as its back-end computational programs.

File Name	Full Name	Version	Application
controller.tbc	ControlCenter.tbc	2.40	TclPro1.2
correction.tbc	GeometryCorrection.tbc	2.10	TclPro1.2
estimatewater.tbc	EstimationHydrogenAtomsWater.tbc	3.11	TclPro1.2
homologymodel.tbc	HomologyModelingPro.tbc	3.50	TclPro1.2
interface.tbc	InterfaceSelection.tbc	2.20	TclPro1.2
peripheral.tbc	PeripheralModelingPro.tbc	3.51	TclPro1.2
proteinsuperpose.tbc	ProteinSuperposition.tbc	2.25	TclPro1.2
ramachan.tbc	RamachandranPlot.tbc	2.13	TclPro1.2
restraint.tbc	Restraints.tbc	2.23	TclPro1.2
rotamermodeling.tbc	SideChainRotamerModelingPro.tbc	4.24	TclPro1.2
trajectory.tbc	TrajectoryAnalyzer.tbc	2.17	TclPro1.2
align.exe	AlignSequence.exe	1.01	Win32
sse.exe	SecondaryStructureExtraction.exe	1.21	Win32
ssa.exe	SecondaryStructurePrediction.exe	1.00	Win32
ffcontrol.exe		1.00	Win32
mfhcinter.exe		1.01	Win32
mfupdate.exe		1.05	Win32
mftapi.dll		1.03	Win32
rotamer.rdb	SideChainRotamerDatabase.rdb	1.00	
database2k24.prm		1.00	

### **Sample Files**

Test  
Tutorial\_1  
1hxx.ent

hRhodopsin.seq  
hRhodopsin.sec (sample): secondary structure prediction data format

1hzx\_1.sec (sample): secondary structure prediction data format  
1hzx\_2.sec (sample): secondary structure prediction data format

Tutorial\_2  
1brp.ent  
1brq.hin

Tutorial\_3  
1a28.ent  
hAndrogen.seq  
hAndrogen.sec (sample): secondary structure prediction data format  
1a28\_1.sec (sample): secondary structure prediction data format  
1a28\_3.sec (sample): secondary structure prediction data format

Small\_1  
norbornenylcation.hin

Small\_2  
hapto6.hin

Protein  
2lbd.ent

---

## Changes

Revision H (Package Version 8.x): Current Version  
Revision G (Package Version 7.x): New License Version  
Revision F (Package Version 6.x): Improved Versions for Windows 8.1, 8, 7 and Vista  
Revision E (Package Version 5.x): Renewal Version  
Revision D (Package Version 4.x): C++ Dynamic Link Library Based Version  
Revision C (Package Version 3.x): *HyperChem*8.03 Compatible Version  
Revision B (Package Version 2.x): *HyperChem*7.52 OpenGL Support Version  
Revision A (Package Version 1.x): First Available Version

### Revision H1

In the Revision H1, function of ONIOM Interface is largely improved for the latest Gaussian, and the file conversion function is available for performing the fragment molecular orbital programs and is compatible to the CHARMM-based NAMD molecular dynamics calculations.

Default force field was changed to AMBER99 from AMBER94. Manually changed atomic charges are retained through all module programs.

Control Center ver. 2.40:

Changes in version 2.40

1. Minor change in loading PDB for nucleotides.

Changes in version 2.39

1. Minor change in loading PDB.

Changes in version 2.38

1. Improved the MOL2 conversion.

Changes in version 2.35

1. Improved the Conversion PDB to CHARMM-based NAMD PDB command for Metals.

Changes in version 2.34

1. Added the Conversion PDB to CHARMM-based NAMD PDB command to the Utilities menu for obtaining the NAMD compatible PDB.

Changes in version 2.33:

1. Added the counterion command to neutralize the system.

Changes in version 2.32

1. Added the Export function which converts the opened molecular system in PDB or HIN format to one in Tripos MOL2, AutoDock PDBQT, and MDL SDF formats using Babel program.
2. Added the Conversion of CHARMM-based NAMD PDB command to the Utilities menu for obtaining the formal PDB format file from the modified PDB file by VMD (NAMD).
3. Added the Prepare PDB File for FMO (Fragment Molecular Orbital) command to the Utilities menu for obtaining the BioStationViewer (ABINIT-MP) and Fu and Facio (GAMESS) readable PDB file from the formal PDB format file.
4. Default force field was changed to AMBER99 from AMBER94.
5. Modified a function getting HyperChem version information.
6. Improved the PDB format corresponding to molecular system which contains from 100,000 atoms to 999,999 atoms.

Geometry Correction ver. 2.10:

Changes in version 2.10

1. Corresponded to manual atomic charges which are modified by user.
2. Modified a function getting HyperChem version information.

Estimation of Hydrogen Atoms in Water ver. 3.11:

1. Modified a function getting HyperChem version information.

Homology Modeling Professional ver. 3.50:

Changes in version 3.50

1. Improved treatment of temporary files.

Changes in version 3.49

1. Improved the S-S bond generation function under automatic residue numbering condition.

Changes in version 3.47

1. Improved the S-S bond generation function under automatic residue numbering condition.

Changes in version 3.46

1. Modified the Loop Generation function with the automatic residue number.

Changes in version 3.43

1. Changed to the residue number based on the target sequence length in the Loop Generation function.

Changes in version 3.42

1. Corresponded to manual atomic charges which are modified by user.
2. Default force field was changed to AMBER99 from AMBER94.
3. Modified a function getting HyperChem version information.
4. Improved the proline structure in the case of non-insertion sequence modeling mode.

Bugs fixed in version 3.45

1. Fixed minor bugs.

Interface Selection ver. 2.20:

Changes in version 2.20

1. Added the Select Backbone command to the Selection menu for selecting the peptide and nucleotide backbone.
2. Corresponded to manual atomic charges which are modified by user.
3. Default force field was changed to AMBER99 from AMBER94.
4. Modified a function getting HyperChem version information.

Bugs fixed in version 2.20

1. Fixed minor bugs.

Peripheral Modeling Professional ver. 3.51:

Changes in version 3.51

1. Modified the Cap Group function.

Changes in version 3.49

1. O3' hydroxylation can be selected at using the 5'- and 3'-capping command.

Changes in version 3.48

1. Improved the ONIOM Interface and Gaussian Interface. See below.
2. Corresponded to manual atomic charges which are modified by user.
3. Default force field was changed to AMBER99 from AMBER94.
4. Modified a function getting HyperChem version information.
5. Added a function that generates automatically atom names for the added hydrogens of small molecules.
6. Added a function that rewrites the HIN file corresponding to PDB file.

Protein Superpose ver. 2.25:

Changes in version 2.25

1. Corresponded to manual atomic charges which are modified by user.
2. Default force field was changed to AMBER99 from AMBER94.
3. Modified a function getting HyperChem version information.

Ramachandran Plot ver. 2.13:

1. Modified a function getting HyperChem version information.

Restraints ver. 2.23:

Changes in version 2.23

1. Corresponded to manual atomic charges which are modified by user.
2. Default force field was changed to AMBER99 from AMBER94.
3. Modified a function getting HyperChem version information.

Side Chain Rotamer Modeling Professional ver. 4.24:

Changes in version 4.24

1. Improved the Load Alignment function.

Changes in version 4.23

1. Corresponded to manual atomic charges which are modified by user.
2. Default force field was changed to AMBER99 from AMBER94.
3. Modified a function getting HyperChem version information.

Bugs fixed in version 4.23

1. Fixed minor bugs.

Trajectory Analyzer ver. 2.17:

1. Modified a function getting HyperChem version information.

Gaussian Interface for HyperChem ver. 2.09:

Changes in version 2.08

1. Supported Gaussian16W
2. Improved some functions.

ONIOM Interface for Receptor ver. 2.31

Changes in version 2.30

1. The ONIOM method was further improved for a multiple molecular system.
2. Supported Gaussian16W
3. Added some Gaussian functions.
4. Added the Setup menu to menu bar for improving Amber (low layer) functions.

5. Added the Option menu to menu bar for treating and rendering the molecular system in the HyperChem workspace.
  6. Improved the MM link atoms for nucleotide.
- Bugs fixed in version 2.30
1. Fixed minor bugs.

## **Revision G1**

In the Revision G1, the license method was changed.

Control Center ver. 2.13:

Changes in version 2.13

1. The license method was changed.
2. Blast Interface was compatible to the latest Blast programs.

Geometry Correction ver. 2.08:

Changes in version 2.08

1. The license method was changed.

Estimation of Hydrogen Atoms in Water ver. 3.10:

Changes in version 3.10

1. The license method was changed.

Homology Modeling Professional ver. 3.21:

Changes in version 3.21

1. The license method was changed.
2. Improved the Secondary Structure Alignment Method.

Interface Selection ver. 2.15:

Changes in version 2.15

1. The license method was changed.

Peripheral Modeling Professional ver. 3.29:

Changes in version 3.29

1. The license method was changed.
2. The ONIOM method was improved for a multiple molecular system.

Protein Superpose ver. 2.11:

Changes in version 2.11

1. The license method was changed.

Ramachandran Plot ver. 2.12:

Changes in version 2.12

1. The license method was changed.

Restraints ver. 2.12:

Changes in version 2.12

1. The license method was changed.

Side Chain Rotamer Modeling Professional ver. 4.14:

Changes in version 4.14

1. The license method was changed.

Trajectory Analyzer ver. 2.15:

Changes in version 2.15

1. The license method was changed.
2. Added RMSD trajectories for backbone atoms and all atoms as well as Ca carbons.

Gaussian Interface for HyperChem ver. 2.05:

Bugs fixed in version 2.05

1. Fixed minor bugs.

ONIOM Interface for Receptor ver. 2.10

Changes in version 2.10

1. The ONIOM method was improved for a multiple molecular system.

### **Revision F3**

In the Revision F3, window control was improved for Windows 8.1 and 8.

Control Center ver. 2.12:

Changes in version 2.12

1. Improved window control for Windows8 and 8.1.

Geometry Correction ver. 2.07:

Changes in version 2.07

1. Improved window control for Windows8 and 8.1.

Estimation of Hydrogen Atoms in Water ver. 3.09:

Changes in version 3.09

1. Improved window control for Windows8 and 8.1.

Homology Modeling Professional ver. 3.17:

Changes in version 3.17

1. Improved window control for Windows8 and 8.1.
2. Improved the S-S bond formation function.

Interface Selection ver. 2.13:

Changes in version 2.13

1. Improved window control for Windows8 and 8.1.

Peripheral Modeling Professional ver. 3.13:

Changes in version 3.13

1. Improved window control for Windows8 and 8.1.

Protein Superpose ver. 2.10:

Changes in version 2.10

1. Improved window control for Windows8 and 8.1.

Ramachandran Plot ver. 2.10:

Changes in version 2.10

1. Improved window control for Windows8 and 8.1.

Restraints ver. 2.11:

Changes in version 2.11

1. Improved window control for Windows8 and 8.1.

2. Improved the output format for Trajectory Analyzer module program.

#### Side Chain Rotamer Modeling Professional ver. 4.13:

##### Changes in version 4.13

1. Improved window control for Windows8 and 8.1.

#### Trajectory Analyzer ver. 2.14:

##### Changes in version 2.14

1. Improved window control for Windows8 and 8.1.
2. Improved the extraction function of the trajectory structure.
3. Added RMSD trajectories for Ca carbons.

### **Revision F2**

In the Revision F2, protein secondary structure prediction program was integrated into Homology Modeling module program.

#### Control Center ver. 2.10:

##### Changes in version 2.10

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).

##### Bugs fixed in version 2.10

1. Fixed some minor bugs.

#### Geometry Correction ver. 2.06:

##### Changes in version 2.06

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).

#### Estimation of Hydrogen Atoms in Water ver. 3.08:

##### Changes in version 3.08

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).

##### Bugs fixed in version 3.08

1. Fixed some minor bugs.

#### Homology Modeling Professional ver. 3.15:

##### Changes in version 3.15

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).
2. Added the submenus to the "Show Only Backbone" menu so that you can easily find small molecules and molecules covalently bound to biomacromolecules.
3. Added the "Predict Secondary Structure" commands for the reference and target sequences so that the three-dimensional structure of the insertion sequences can automatically be modeled on the basis of the predicted secondary structure.
4. Improved the S-S bond formation function.

##### Bugs fixed in version 3.15

1. Fixed some minor bugs.

#### Interface Selection ver. 2.12:

##### Changes in version 2.12

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).

Bugs fixed in version 2.12

1. Fixed some minor bugs.

Peripheral Modeling Professional ver. 3.12:

Changes in version 3.12

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).
2. Improved the memory limitation for Gaussian 64bit version.

Bugs fixed in version 3.12

1. Fixed some minor bugs.

Protein Superpose ver. 2.09:

Changes in version 2.09

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).

Ramachandran Plot ver. 2.09:

Changes in version 2.09

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).

Restraints ver. 2.10:

Changes in version 2.10

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).

Bugs fixed in version 2.10

1. Fixed some minor bugs.

Side Chain Rotamer Modeling Professional ver. 4.12:

Changes in version 4.12

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).

Bugs fixed in version 4.12

1. Fixed some minor bugs.

Trajectory Analyzer ver. 2.10:

Changes in version 2.10

1. Use restriction of the specific HyperChem versions (8.0.0 - 8.0.2) was removed in order to recognize the present HyperChem version (8.0.10).

## **Revision F1**

In the Revision F1, Windows 7 and Gaussian09W have been supported.

Control Center ver. 2.09:

Changes in version 2.09

1. Improved for Windows 7 and Vista.
2. Improved the "Update" command.

Geometry Correction ver. 2.05:

Changes in version 2.05

1. Improved for Windows 7 and Vista.

Estimation of Hydrogen Atoms in Water ver. 3.07:

Changes in version 3.07

1. Improved for Windows 7 and Vista.

Homology Modeling Professional ver. 3.12:

Changes in version 3.12

1. Improved for Windows 7 and Vista.
2. Improved the "Save As" command.

Bugs fixed in version 3.12

1. Fixed a bug in which a wrong molecule number is described as the template in the model file.

Interface Selection ver. 2.11:

Changes in version 2.11

1. Improved for Windows 7 and Vista.

Peripheral Modeling Professional ver. 3.09:

Changes in version 3.09

1. Improved for Windows 7 and Vista.
2. Improved the "Zoom In" option.

Protein Superpose ver. 2.08:

Changes in version 2.08

1. Improved for Windows 7 and Vista.

Ramachandran Plot ver. 2.08:

Changes in version 2.08

1. Improved for Windows 7 and Vista.

Restraints ver. 2.08:

Changes in version 2.08

1. Improved for Windows 7 and Vista.
2. Improved a treatment of the Molecular Dynamics option for the later versions of HyperChem 8.03.
3. Improved a window treatment of the "Restraint Matrix" window.

Bugs fixed in version 2.08

1. Fixed a bug that HyperChem hangs up when the file name is changed using the "Save As" command in Windows Vista environment.

Side Chain Rotamer Modeling Professional ver. 4.11:

Changes in version 4.11

1. Improved for Windows 7 and Vista.

Bugs fixed in version 4.11

1. Fixed a bug that HyperChem hangs up when the file name is changed using the "Save As" command in Windows Vista environment.
2. Fixed a bug that a check of modeling does not function on other than the amino acid residues.

Trajectory Analyzer ver. 2.08:

Changes in version 2.08

1. Improved for Windows 7 and Vista.
2. Improved a check function of the "Playback Parameters" options.

Gaussian Interface for HyperChem ver. 2.02:

Changes in version 2.02

1. Improved for Windows 7 and Vista.

2. Improved for Gaussian09.

ONIOM Interface for Receptor ver. 2.01

Changes in version 2.01

1. Improved for Windows 7 and Vista.
2. Improved for Gaussian09.

## **Revision E2**

In the Revision E2, some useful functions have been improved.

Control Center ver. 2.05:

Changes in version 2.05

1. Altered the updating policy of the Preference.

Geometry Correction ver. 2.01:

Estimation of Hydrogen Atoms in Water ver. 3.03:

Homology Modeling Professional ver. 3.07:

Interface Selection ver. 2.06:

Peripheral Modeling Professional ver. 3.04:

Changes in version 3.04

1. See Gaussian Interface for HyperChem.

Protein Superpose ver. 2.03:

Ramachandran Plot ver. 2.04:

Restraints ver. 2.04:

Side Chain Rotamer Modeling Professional ver. 4.06:

Trajectory Analyzer ver. 2.04:

Changes in version 2.04

1. Added the Status Window for killing the extraction of trajectories.

Gaussian Interface for HyperChem ver. 2.01:

Bugs fixed in version 2.01

1. Fixed a problem that will occur in reflecting an uncorresponding log file of the Gaussian job.

ONIOM Interface for Receptor ver. 2.00

## **Revision E1**

Revision E1 renews user interface of all module programs. All modules carry a window management function.

Control Center ver. 2.04:

Changes in version 2.04

1. Extended the Window Management function.

Changes in version 2.03

1. Added the Forced Termination function to the Close button.  
Changes in version 2.02

1. Added the ClustalW, Blast batch, and Fasta interfaces.
2. Added the Make Folder command to the File menu.

Geometry Correction ver. 2.01:

Changes in version 2.01

1. Extended the Window Management function.

Estimation of Hydrogen Atoms in Water ver. 3.03:

Changes in version 3.03

1. Extended the Window Management function.

Homology Modeling Professional ver. 3.07:

Changes in version 3.07

1. Extended the Window Management function.

Changes in version 3.05

1. Added two test alignment functions using the predicted secondary structures and the amino acid properties with their respective score matrices.

Changes in version 3.04

1. Added the Conditions option for the Insertion Sequence Modeling.
2. Moved the Allow Infrequent Dihedral option to the Conditions option.
3. Added the Window Color option to the Alignment Table window.
4. Changed the command name of the Text Color to the Amino Acid Color.
5. Added the Text Color option to the Alignment Table window.
6. Improved the check function of score matrix format.

Interface Selection ver. 2.06:

Bugs fixed in version 2.06

1. Fixed an initialization problem of the Residue Selection option.

Changes in version 2.05

1. Extended the Window Management function.
2. Added the individual residue selection options.

Changes in version 2.03

1. Added the customization function to the Target Molecules list for making easily the complicated selections.

Peripheral Modeling Professional ver. 3.03:

Changes in version 3.03

1. Extended the Window Management function.

Protein Superpose ver. 2.03:

Changes in version 2.03

1. Extended the Window Management function.

Ramachandran Plot ver. 2.04:

Changes in version 2.04

1. Extended the Window Management function.

Changes in version 2.03

1. Added the "Export Phi-Psi-Omega Values" command.

Restraints ver. 2.04:

Changes in version 2.04

1. Extended the Window Management function.

Bugs fixed in version 2.02

1. Improved the "Parts" menu.
2. Fixed an error that occurs at the change of the molecule number under the opened Restraints windows.

Side Chain Rotamer Modeling Professional ver. 4.06:

Changes in version 4.06

1. Extended the Window Management function.

Bugs fixed in version 4.05

1. Improved a machine-dependent exception treatment for batch calculations.

Trajectory Analyzer ver. 2.03:

Changes in version 2.03

1. Extended the Window Management function.

Gaussian Interface for HyperChem ver. 2.00:

ONIOM Interface for Receptor ver. 2.00

**Revision D1** (Commercial unavailable version)

Part of functions of module programs is replaced to those of dynamic link library.

**Revision C2**

Revision C2 can be used for preparing a nucleic acid molecule system as well as a protein molecule system. Some useful icons such as "Undo" and "Mouse Mode" icons are available from all module programs. Menu bar and toolbar of *HyperChem* are changed to the "Safety Mode" in default.

Control Center ver. 1.25:

Changes in version 1.25

1. Added the Molecular System Information option.
2. Added the interface to the *HyperChem* Renderings option.
3. Added a Keyboard help.

Bugs fixed in version 1.25

1. Fixed the Create Connection function.

Changes in version 1.23

1. Added a function for making connection table of a small molecule.
2. Added an instance management function of *HyperChem*.
3. Added a check function for the "Mode" option of *HyperChem* 8.0.

Bugs fixed in version 1.22

1. Fixed a problem that occurs when the "Save As" command is used using an unavailable file name.

Changes in version 1.21

1. Improved the process management.
2. Supported a nucleic acid molecule system.
3. Changed the General Procedure more logically.
4. Added the mouse mode to the "Utilities" menu.
5. Changed default settings to the "Safety Mode".

Geometry Correction ver. 1.23:

Changes in version 1.23

1. Improved the process management.

#### Estimation of Hydrogen Atoms in Water ver. 2.04:

##### Changes in version 2.04

1. Added a Keyboard help.

##### Bugs fixed in version 2.04

1. Fixed a listbox error that occurs using together with Control or Shift key.

##### Bugs fixed in version 2.03

1. Fixed a file format error that occurs at the end of program if a PDB format is used.

##### Changes in version 2.02

1. Added the "Color Palette" option.

##### Changes in version 2.01

1. Improved the process management.
2. Supported waters in a nucleic acid molecule system.
3. Improved the prediction algorithm.
4. Hydrogen coordinate of water can be estimated in the presence of organic and nucleic acid molecules as well as in the presence of a protein molecule.
5. Added the "Setup" option for preparing calculation conditions.
6. Added the "Mouse Mode Icons" window.
7. Added the "Undo" function for a wrong mouse right-button operation.

#### Homology Modeling Professional ver. 2.45:

##### Changes in version 2.45

1. Added a Keyboard help.
2. Added the "Select None" function to the "Edit" menu for deselecting structural selections.
3. Added the "Residue Selection" option.
4. Added the "Mutate" option.

##### Bugs fixed in version 2.45

1. Fixed a listbox error that occurs using together with Control or Shift key.

##### Changes in version 2.43

1. Added the Distance Selection function for selecting residues located within a desired distance from the individual atoms of a specified residue.

##### Changes in version 2.42

1. Added the "Font", "Font Size", and "Font Style" options to the Alignment Table.

##### Changes in version 2.41

1. Added some useful options for performing an effective sequence alignment to popup menu provided in the Alignment Table window.
  - 1.1 Added the "Reflect Selections" for extracting the binding site to an alignment.
  - 1.2 Added the "Export Extracted Structure" for aligning a pair of sequences using secondary structure information.
  - 1.3 Added the "Import Signals", "Export Signals", "Signal Residue", "Clear Signal", and "Clear All Signals" for aligning a pair of sequences using conserved signal amino acids.
2. Added the "Interface Selection" interface to the Tool menu.
3. Added the "Open Template File" option to the Tool menu.
4. Added the "Import and Export Selections" options for reflecting selection information to an alignment.
5. Added the restraint condition for the assigned secondary structure to the "Restrains" option.
6. Added the "Allow Infrequent Dihedral" option for performing the Insertion Modeling function using rare main chain conformation.
7. Added the "Open Log" option for viewing results outputted by the Insertion Modeling function.
8. Improved the Insertion Modeling function.

##### Changes in version 2.29

1. Added the "Color Palette" option.

##### Changes in version 2.27

1. Improved the process management.
2. Added the partial geometry optimization function for the conventional insertion sequence modeling

method.

3. Added the "Mouse Mode Icons" window.
4. Added the "Undo" function for a wrong mouse right-button operation.
5. Added the "Show Only Backbone" command.
6. Added the mouse-motion selections for selecting part of structure in the "Alignment Table" window.
7. Added the "Load Alignment Table" function for reflecting pairwise alignment sequences prepared by any sequence alignment program such as ClustalW program.
8. Can be customizing text in the "Alignment Table" window using 32 bit color palette.
9. Sequences in the "Alignment Table" window can be shown in some properties such as extracted secondary structure, predicted secondary structure, chemical property, etc.
10. Conserved S-S bond can be modeled automatically.

#### Interface Selection ver. 1.75:

Changes in version 1.75

1. Added a Keyboard help.

Bugs fixed in version 1.75

1. Fixed a listbox error that occurs using together with Control or Shift key.

Changes in version 1.74

1. Added some options to the "Option" menu.

Changes in version 1.71

1. Added the "Color Palette" option.

Changes in version 1.70

1. Improved the process management.
2. Added some options for selecting a part of structure of a nucleic acid.
3. Added the "Mouse Mode Icons" window.
4. Added the "Undo" function for a wrong mouse right-button operation.

#### Peripheral Modeling Professional ver. 2.55:

See also changes in *ONIOM Interface for Receptor* and *Gaussian Interface for HyperChem*.

Changes in version 2.55

1. Added a Keyboard help.

Bugs fixed in version 2.55

1. Fixed a listbox error that occurs using together with Control or Shift key.

Changes in version 2.53

1. Added the "Color Palette" option.

Changes in version 2.52

1. Improved the process management.
2. Added the "Mouse Mode Icons" window.
3. Supported a nucleic acid molecule system.
4. Added a function that prepares conditions of terminal nucleotides of a nucleic acid.
5. Added the "Undo" function for a wrong mouse right-button operation.

Bugs fixed in version 2.52

1. Fixed a series of problems involved in window management and parameter check.

#### Protein Superpose ver. 1.30:

Changes in version 1.30

1. Added a Keyboard help.

Bugs fixed in version 1.30

1. Fixed a listbox error that occurs using together with Control or Shift key.

Changes in version 1.29

1. Added the "Show Only Backbone" options to the "Option" menu.

Bugs fixed in version 1.29

1. Fixed a problem that occurs at program initiation in a particular PDB format.

#### Changes in version 1.28

1. Improved the process management.
2. Added the "Mouse Mode Icons" window.
3. Added the "Undo" function for a wrong mouse right-button operation.

#### Ramachandran Plot ver. 1.29:

##### Changes in version 1.29

1. Added a Keyboard help.

##### Bugs fixed in version 1.29

1. Fixed a listbox error that occurs using together with Control or Shift key.

##### Changes in version 1.28

1. Added the "Show Only Backbone" options to the "Option" menu.

##### Changes in version 1.27

1. Added the "Color Palette" option.

##### Changes in version 1.26

1. Improved the process management.
2. Changed the named selection name for restrained torsions.
3. Added the "Mouse Mode Icons" window.
4. Added the "Undo" function for a wrong mouse right-button operation.

#### Restraints ver. 1.54:

##### Changes in version 1.54

1. Added a Keyboard help.

##### Bugs fixed in version 1.54

1. Fixed a listbox error that occurs using together with Control or Shift key.

##### Changes in version 1.53

1. Added the "Color Palette" option.

##### Changes in version 1.52

1. Improved the process management.
2. Improved affinity with Ramachandran Plot program.
3. Added the "Mouse Mode Icons" window.
4. Supported preparation of restraint conditions for a nucleic acid molecule system.
5. Added the "Undo" function for a wrong mouse right-button operation.

#### Side Chain Rotamer Modeling Professional ver. 3.14:

##### Changes in version 3.14

1. Added a Keyboard help.

##### Bugs fixed in version 3.14

1. Fixed a listbox error that occurs using together with Control or Shift key.

##### Bugs fixed in version 3.13

1. Fixed a problem that occurs when synonym of amino acid name is used.

##### Changes in version 3.12

1. Improved the process management.
2. Improved affinity with Ramachandran Plot program.
3. Added the "Mouse Mode Icons" window.
4. Added the "Undo" function for a wrong mouse right-button operation.

##### Bugs fixed in version 3.12

1. Fixed a problem that the full rotamer batch calculations fail in some cases.

#### Trajectory Analyzer ver. 1.09:

##### Changes in version 1.09

1. Added a Keyboard help.

##### Bugs fixed in version 1.09

1. Fixed a listbox error that occurs using together with Control or Shift key.

Changes in version 1.08

1. Added the "Color Palette" option.

Changes in version 1.07

1. Improved the process management.
2. Added the "Mouse Mode Icons" window.
3. Supported a nucleic acid molecule system.
4. Added the "Undo" function for a wrong mouse right-button operation.

*Gaussian Interface for HyperChem* ver. 1.03:

Changes in version 1.03

1. *Gaussian Interface for HyperChem* no longer needs *Gaussian* executable file.

Bugs fixed in version 1.03

1. Fixed a wrong number of molecule in list provided in the "Add Molecule" option.

*ONIOM Interface for Receptor* ver. 1.05:

Changes in version 1.05

1. Added the Residue Selection Wizard for custom selections.

Bugs fixed in version 1.05

1. Fixed an error that occurs when input file is prepared for 2-layer ONIOM.

Changes in version 1.04

1. *ONIOM Interface for Receptor* no longer needs *Gaussian* executable file.

## Revision C1

Revision C1 supports a new version (8.03 and the earlier versions) of *HyperChem* as well as a new version (3.1 and the earlier versions) of the Protein Data Bank format.

Control Center ver. 1.17:

Changes in version 1.17

1. Added a function which can convert the PDB name system in the version 3.x into the *HyperChem* name system.

Changes in version 1.15

1. Supported *HyperChem*8.03.

Geometry Correction ver. 1.21:

Changes in version 1.21

1. Supported *HyperChem*8.03.

Estimation of Hydrogen Atoms in Water ver. 1.22:

Changes in version 1.22

1. Supported *HyperChem*8.03.

Homology Modeling Professional ver. 2.21:

Changes in version 2.21

1. Supported *HyperChem*8.03.

Interface Selection ver. 1.67:

Changes in version 1.67

1. Supported *HyperChem*8.03.
2. Added the "Calculation" menu for the partial geometry optimization calculations of the selected parts of the structure under the desired force field condition.

Peripheral Modeling Professional ver. 2.13:

Changes in version 2.13

1. Supported *HyperChem*8.03.
2. Supported the intermolecular bond settings between boron, silicon, phosphorus, and sulfur atoms.

Protein Superpose ver. 1.26:

Changes in version 1.26

1. Added check function of the PDB format version.

Changes in version 1.25

1. Supported *HyperChem*8.03.

Ramachandran Plot ver. 1.23:

Changes in version 1.23

1. Supported *HyperChem*8.03.

Restraints ver. 1.20:

Changes in version 1.20

1. Supported *HyperChem*8.03.

Side Chain Rotamer Modeling Professional ver. 3.09:

Changes in version 3.09

1. Supported *HyperChem*8.03.

Trajectory Analyzer ver. 1.04:

Changes in version 1.04

1. Supported *HyperChem*8.03.

*Gaussian Interface for HyperChem* ver. 1.02:

No Changes

*ONIOM Interface for Receptor* ver. 1.03

No Changes

## **Revision B1**

Revision B1 fully supports functions of *HyperChem*7.52 such as the OpenGL rendering function. User interface of the individual module programs is renewed.

Control Center ver. 1.12:

Changes in version 1.12

1. Added the version information to the program.

Changes in version 1.10

1. Supported the *HyperChem* OpenGL function.

Geometry Correction ver. 1.19:

Changes in version 1.19

1. Improved treatment for a hydrogen bond.

Changes in version 1.16

1. Supported the *HyperChem* OpenGL function.
2. Added a function that adds a perpetual tag to the structural file.

Estimation of Hydrogen Atoms in Water ver. 1.21:

Changes in version 1.21

1. Improved treatment for a hydrogen bond.
2. Improved the rendering options.

Changes in version 1.19

1. Improved the user interface.
2. Supported the *HyperChem* OpenGL function.

Homology Modeling Professional ver. 2.20:

Changes in version 2.20

1. Improved the rendering options.
2. Added the structural centralizing function to a reference residue in the "Alignment Table" window.
3. Added some viewing tools to the "View" menu.

Changes in version 2.18

1. Improved the Insertion Sequence Modeling function.
2. Added a structural optimization algorithm, which combined the Steepest Descent and the Polak-Ribiere, to the "Algorithm" option for optimizing structure of an insertion sequence.

Bugs fixed in version 2.17

1. Fixed a problem that an insertion part including an unknown residue was unable to model.

Bugs fixed in version 2.16

1. Fixed a problem that the "Modeling" command did not function in a certain case.

Changes in version 2.14

1. Improved the user interface.
2. Supported the *HyperChem* OpenGL function.
3. Added the insertion modeling function (Professional version).

Interface Selection ver. 1.64:

Changes in version 1.64

1. Improved treatment for a hydrogen bond.
2. Added a function that keeps the structural renderings at the program termination.
3. Improved the rendering options.

Changes in version 1.62

1. Improved the user interface.
2. Supported the *HyperChem* OpenGL function.

Peripheral Modeling ver. 2.11:

Changes in version 2.11

1. Improved treatment for a hydrogen bond.
2. Improved the rendering options.

Changes in version 2.10

1. Improved the memory management for the *ONIOM Interface for HyperChem*.

Bugs fixed in version 2.09

1. A problem that the auto atom type assignment can not reflect to the individual atoms was fixed.

Changes in version 2.07

1. Improved the user interface.
2. Supported the *HyperChem* OpenGL function.
3. Improved the modeling function of the Cap Group function.
4. The previous normal version was integrated into the Professional version.

Protein Superpose ver. 1.24:

Bugs fixed in version 1.24

1. Fixed a problem that secondary structure does not disappear using the "Unmerge" command.

Changes in version 1.23

1. Improved the user interface.
2. Supported the *HyperChem* OpenGL function.

Ramachandran Plot ver. 1.22:

Changes in version 1.22

1. Improved the rendering options.

Changes in version 1.21

1. Improved the user interface.
2. Supported the *HyperChem* OpenGL function.
3. The previous "Restrained" mode was integrated into the "View" mode.

Restraints ver. 1.19:

Changes in version 1.19

1. Improved the rendering options.

Changes in version 1.18

1. Improved the user interface.
2. Supported the *HyperChem* OpenGL function.
3. Improved the restraint condition setting function.
4. Added some calculation options.

Side Chain Rotamer Modeling Professional ver. 3.08:

Changes in version 3.08

1. Improved the status bar of the batch calculations.
2. Improved the rendering options

Bugs fixed in version 3.08

1. Fixed an error that occurs by loading a wrong batch list file.

Bugs fixed in version 3.07

1. Fixed a problem that occurred at reflecting an insufficient alignment.

Changes in version 3.06

1. Improved the "Load Alignment" command.

Changes in version 3.05

1. Improved the user interface.
2. Supported the *HyperChem* OpenGL function.
3. The previous normal version was integrated into the Professional version.
4. The batch calculation became available for all residues (Professional version).

Trajectory Analyzer ver. 1.03:

Changes in version 1.03

1. Improved the rendering options.

Changes in version 1.02

1. Improved the user interface.
2. Supported the *HyperChem* OpenGL function.

*Gaussian Interface for HyperChem* ver. 1.02:

Changes in version 1.02

1. All functions of the *Gaussian Interface for HyperChem* became available for the previous normal version.

*ONIOM Interface for Receptor* ver. 1.03

Changes in version 1.03

1. Supported a protein molecule that binds to an unknown residue.

## Revision A3

Revision A3 is the first release version of the package.

Revision A3 improved reliability through practical uses.

Some module programs are added into the package.

All processes of homology modeling can be performed on the basis of the energy calculations.

*ONIOM Interface for Receptor* is newly added into the package.

Some packages are added to the *Homology Modeling for HyperChem* family.

Control Center ver. 1.08:

An integrated user interface, Control Center version 1.05, was added to the revision A2.

Changes in version 1.08

1. Function which the individual module programs can initiate from the "General Procedure" window was added to the version 1.05.

Geometry Correction ver. 1.12:

Changes in version 1.12

1. Process communication with *HyperChem* was improved as compared with that in version 1.09.

Estimation of Hydrogen Atoms in Water ver. 1.18:

Changes in version 1.18

1. Process communication with *HyperChem* was improved as compared with that in version 1.13.
2. Hydrogen atom treatment was changed to that in the *HyperChem* coordinate system from that in the PDB coordinate system.

Bugs fixed in version 1.18

1. A problem that did not estimate a hydrogen atom coordinate, when the molecule system contains more than 10,000 atoms, was fixed.

Homology Modeling ver. 2.11:

Changes in version 2.11

1. Process communication with *HyperChem* was improved as compared with that in version 2.04.
2. Many score matrices were added to version 2.04.
3. A simple loop generation function was added to version 2.10.
4. Protonation editing function for a histidine residue was added to version 2.10.

Interface Selection ver. 1.59:

Changes in version 1.59

1. Process communication with *HyperChem* was improved as compared with that in version 1.14.

Bugs fixed in version 1.59

1. A problem that occurred by deletion of cysteine and methionine residues was fixed.

Peripheral Modeling Professional ver. 2.05:

Changes in version 1.08

1. Added *ONIOM Interface for Receptor* to the Peripheral Modeling ver. 1.10.
2. Added an RMS fitting function of the structure, which was optimized by *Gaussian*, to the Peripheral Modeling ver. 1.10.
3. Supported "UNDO" function for the modifications of structure, i.e., the structure optimized by the *HyperChem* geometry optimizations, the structure reflected by the *Gaussian* optimizations, and the structure reflected by the *ONIOM optimizations*.
4. Improved the "Intermolecular Bond Setting" function.

Peripheral Modeling ver. 1.10:

A new program, Peripheral Modeling version 1.10, which can model and edit small molecules, metals, polymers, and metal complexes in a protein structure, was added to the revision A2. This program can also automatically prepare the N- and C-terminal conditions in a protein structure. Moreover, this program has an interface function to *Gaussian* program from *HyperChem*, i.e., *Gaussian Interface for HyperChem*, by which a certain *Gaussian* job can be initiated and the *Gaussian* results can be reflected to the corresponding molecule in the *HyperChem*

workspace.

Protein Superposition ver. 1.22:

Changes in version 2.22

1. Process communication with *HyperChem* was improved as compared with that in version 1.10.
2. Supported the loop generation function of the Homology Modeling module program.

Ramachandran Plot ver. 1.19:

Changes in version 1.19

1. Process communication with *HyperChem* was improved as compared with that in version 1.11.
2. A balloon information of the phi and psi values was added to the "Ramachandran Plot" window.
3. A function locked for any operations under the structural modifications was added to the main window.
4. Supported the protonation editing function of the Homology Modeling module program.

Bugs fixed in version 1.19

1. A problem that a circle of the "Ramachandran Plot" window disappears, when the scroll bar is used, was fixed.

Restraints ver. 1.17:

Changes in version 1.17

1. Process communication with *HyperChem* was improved as compared with that in version 1.12.
2. Response of the "Restraint" window was improved.
3. A function that can simultaneously restrain a set of water molecules was added to the version 1.12.

Bugs fixed in version 1.17

1. A problem that occurred at a deletion part of sequence was fixed.

Side Chain Rotamer Modeling Professional ver. 3.03:

Supported *ONIOM Interface for Receptor*.

Added a batch function to the auto-rotamer search function of the Side Chain Rotamer Modeling ver. 2.35.

Side Chain Rotamer Modeling ver. 2.35:

Changes in version 2.35

1. Process communication with *HyperChem* was improved as compared with that in version 2.12.
2. Database search function was supported for a side-chain rotamer modeling.
3. Auto-rotamer search function was supported for the rotamer database search.
4. Supported the loop generation function of the Homology Modeling module program.
5. Supported the protonation editing function of the Homology Modeling module program.
6. Supported the rotamer database, Rotamer Database version 1.00.

Trajectory Analyzer ver. 1.01:

A new program, Trajectory Analyzer version 1.01, which can serve for analyzing a trajectory for the molecular dynamics calculations, was added to the package.

*Gaussian Interface for HyperChem* ver. 1.01:

*Gaussian Interface for HyperChem* is integrated into the Peripheral Modeling program.

*ONIOM Interface for Receptor* ver. 1.02:

*ONIOM Interface for Receptor* is integrated into the Peripheral Modeling Professional program.

## Revision A2

Revision A2 is a beta version of the package.

Estimation of Hydrogen Atoms in Water ver. 1.13:

#### Changes in version 1.13

1. User interface was renewed.
2. A prediction precision of a second hydrogen position was improved as compared with that in version 1.04.
3. A file manager function was added to the version 1.04.

#### Bugs fixed in version 1.13

1. A problem under the hydrogen bond conditions was fixed.

#### Geometry Correction ver. 1.09:

##### Changes in version 1.09

1. User interface was renewed.

##### Bugs fixed in version 1.09

1. A problem under the hydrogen bond conditions was fixed.

#### Homology Modeling. ver 2.04:

##### Changes in version 2.04

1. User interface was renewed.
2. Added a function that can retain the latest alignment.
3. Added a function that can maintain a customized size of the "Alignment Table" window.
4. Output log file function of an alignment table was added to the version 1.06
5. File management function was added to the version 1.06.
6. Added a function that can display a secondary-structure prediction information on a sequence in the "Alignment Table" window.
7. The secondary structure information became available for all protein molecules in the *HyperChem* workspace.

##### Bugs fixed in version 2.04

1. A problem that occurred at a glycine or a disulfide cysteine residue in a template structure was fixed.
2. An existing window problem was fixed.

#### Interface Selection ver. 1.14:

##### Changes in version 1.14

1. User interface was renewed.
2. Many options for the selection and deletion menus were added to version 1.08.
3. Selection algorithm was improved.

#### Protein Superposition ver. 1.10:

##### Changes in version 1.10

1. User interface was renewed.
2. File management function was added to the version 1.00.
3. A function that can unmerge a merged system was added to the version 1.00.
4. A function that can stack an additional molecule system was added to the version 1.00.

#### Ramachandran Plot ver. 1.11:

##### Changes in version 1.11

1. User interface was renewed.
2. File management function was added to the version 1.05.

##### Bugs fixed in version 1.11

1. Keyboard-binding error in the "Ramachandran Plot" window was fixed.
2. A problem under the hydrogen bond conditions was fixed.

#### Restraints ver. 1.12:

##### Changes in version 1.12

1. User interface was renewed.
2. File management function was added to the version 1.05.

Bugs fixed in version 1.12

1. A problem under the hydrogen bond conditions was fixed.
2. File-read error of a final coordinate file was fixed.

Side Chain Rotamer Modeling ver. 2.12:

Changes in version 2.12

1. User interface was renewed.
2. Auto-rotamer search function using single-point molecular mechanics calculations was added to the version 1.19.
3. A new interface for the auto-rotamer search function was added to the version 1.19.
4. The original rotamer number was fixed to 0.
5. File management function was added to the version 1.19.
6. A function that can load both an alignment table and a modified rotamer data was added to the version 1.19.
7. Interface of the rotamer database modeling was added to the "Torsion Switch" window.
8. Auto-rotamer search function using partial geometry optimizations was added to the version 1.19.
9. A detailed log file became available for the auto-rotamer search function.

Bugs fixed in version 2.12

1. A problem that could not clear a restraint condition used by the program was fixed.
2. An existing window problem was fixed.

AlignSequence ver. 101:

Bugs fixed in version 1.01

1. An unexpected memory dump was fixed.

SecondaryStructureExtraction ver. 1.21:

Changes in version 1.21

1. Removed restrictions of the secondary structure extraction function to the first protein molecule.

## **Revision A1**

Revision A1 is an alpha version of the package.

## **Citation**

The current required citation for *Homology Modeling Professional for HyperChem* is the following.

Motonori Tsuji. Homology Modeling Professional for HyperChem, Revision H1; Saitama, JAPAN, 2018.