User Guide - Quickstart

post-R676 (Nov. 2014)

Introduction

Caution about evolving program versions

This part of the user guide is based on an initial user manual from November 2014 for the SweetUnityMol version of our software. It is currently being adapted and updated to match the current development builds of the 0.9.5 series. In the meantime, several descriptions and screen captures may still pertain to previous versions of the software and may be inaccurate for the current builds. Please be aware of this limitation.

Warning

Screenshots and examples in this document may differ from the current UnityMol version

Todo:

Complete user and developer guide(s) with data from internship reports.

Installing the software

The software described below has been initially developed based on revision 676 of UnityMol and version4.5.2f1 of Unity3D. All source code was implemented using C# and Cg languages built into Unity 3D and is available along with executables for Mac, Windows and Linux platforms on the sourceforge project website. Current UnityMol versions run within version 5.3.2f1 of Unity3D.

https://sourceforge.net/projects/unitymol/files/

Further documentation, input files, and series of illustrations can be found at

http://glycopedia.eu/IMG/pdf/unitymol-user-manual.pdf

and in the online UnityMol doxygen documentation available from:

http://www.baaden.ibpc.fr/umol/Doc/manual/html/pages.html

Windows version (date: 2014 10 02)

- 32 bits
  - umol-win32-20141002_Data
  - Run_SweetUmol_32.bat
  - umol-win32-20141002.exe
- 64 bits
  - umol-win64-20141002_Data
  - Run_SweetUmol_64.bat
  - umol-win64-20141002.exe

Note

This part and the following need to be updated to version 0.9.5

Mac version (date: 2014 10 02)

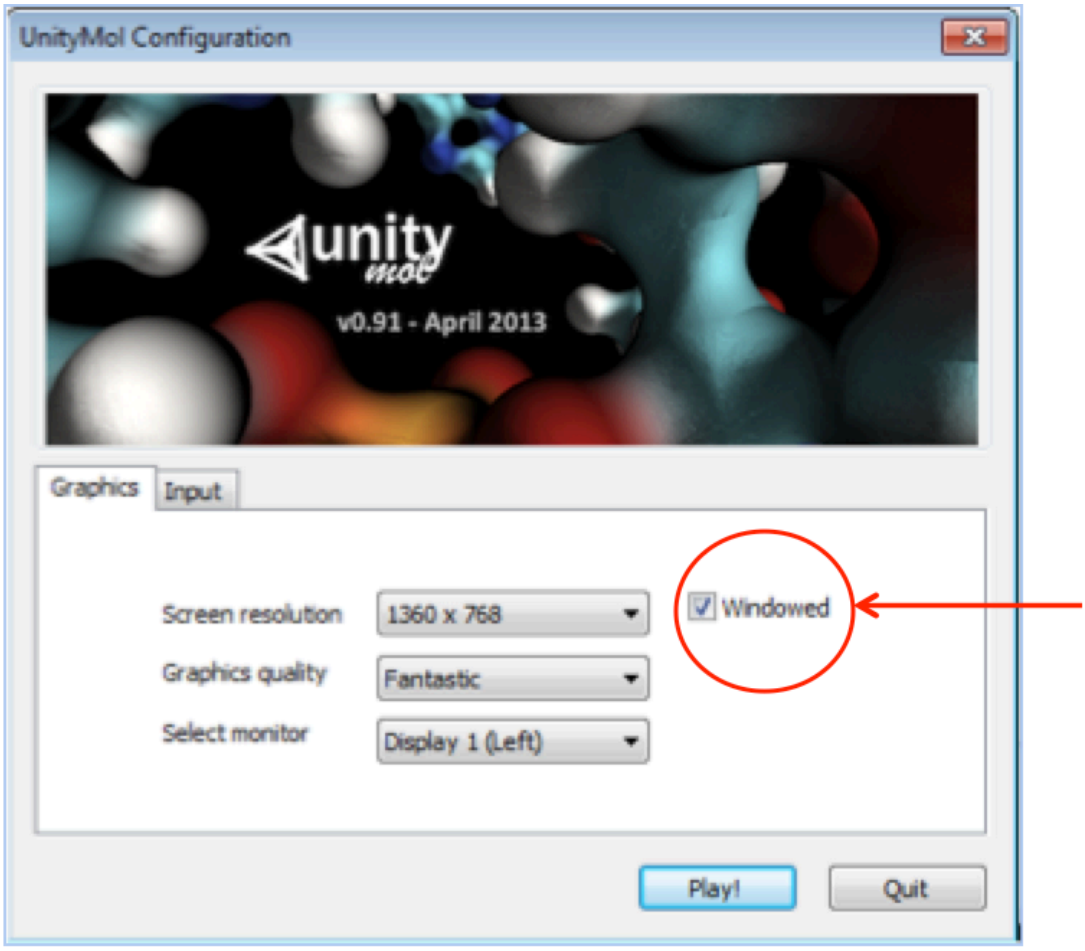
- umol-macosx-universal-20141002.app

SugarRibbons
Special Effect
Miscellaneous

Linux version (data: 2014 10 02)

- umol-linux-20141002_Data
- umol-linux-20141002.x86
- umol-linux-20141002.x86_64

Running the 32 and 64 bits Windows version



Warning

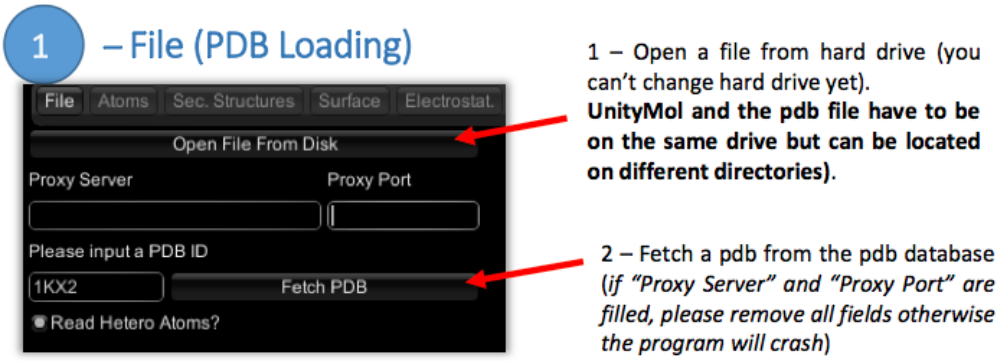
If you encounter issues running UnityMol, try to **NOT USE THE FULL SCREEN MODE** (check `Windowed` in the "UnityMol Configuration" menu (this menu is the menu where you set the resolution and click on `Play!`).

UnityMol's main menu bar

The menu bar sits on the top and groups several submenus together that are described hereafter.

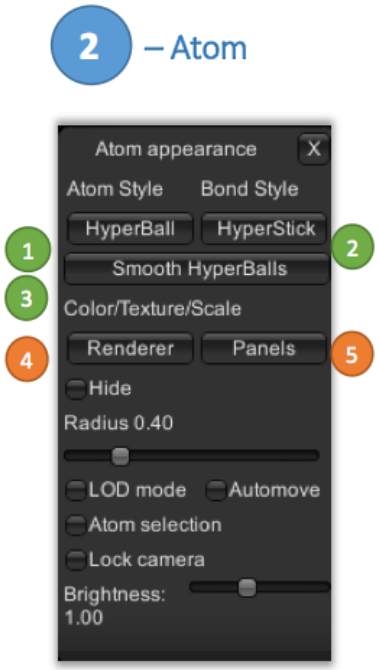
Some of these options offering advanced visualization and manipulations (haptic arm) are being implemented and are not functional at this time: November 2014.

1 - File menu (PDB Loading)



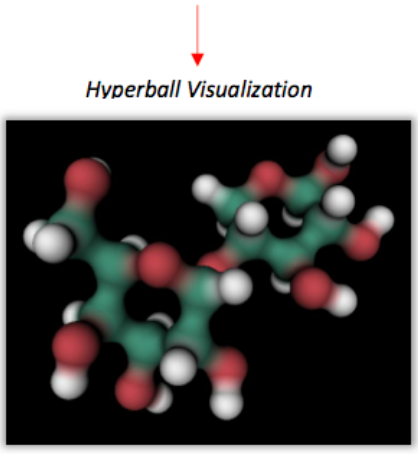
By default the visualization of UnityMol is the Particle mode. This mode uses the particle system of Unity3D to display the molecule. This may not be the most appropriate visualization. Changing to SmoothHyperballs mode offers a better visualization (this setting is the default in more recent builds of UnityMol).

2 - Atom Menu



Different types of representations are available, by **Atom** (1) or by **Bond** (2).

The preselected visualization is called **Hyperballs** (3) (the most interesting one).



The `Renderer` (4) and `Panels` (5) menus are made to change the **color** and the **texture** of either the entire molecule, or a selection.

`Hide`: Hide the molecule (This option is activated when some visualization option (like secondary structures) is activated. Uncheck this box to display both the secondary structure and the molecule.

`Radius`: Change the radius of atom spheres.

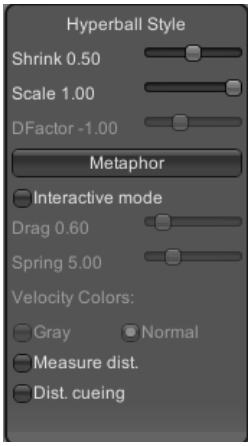
`LOD mode` : when in the Hyperballs mode and this option is checked (and upon changing the orientation of the camera) the molecule will be displayed in the *particle* mode prior recreating the Hyperball representation. This is to be used for large macromolecular systems for which the Hyperballs representation reduces frame rate too much. FPS: Frame Per Second.

Automove (or `SPACE` key): the camera will turn around the molecule.

Lock Camera: The camera will not be able to move when this option is checked.

Brightness : adjust the brightness of Hyperballs. This is useful for some dark textures, or when using texture grayscale plus added colors.

A – HyperBall Style menu.

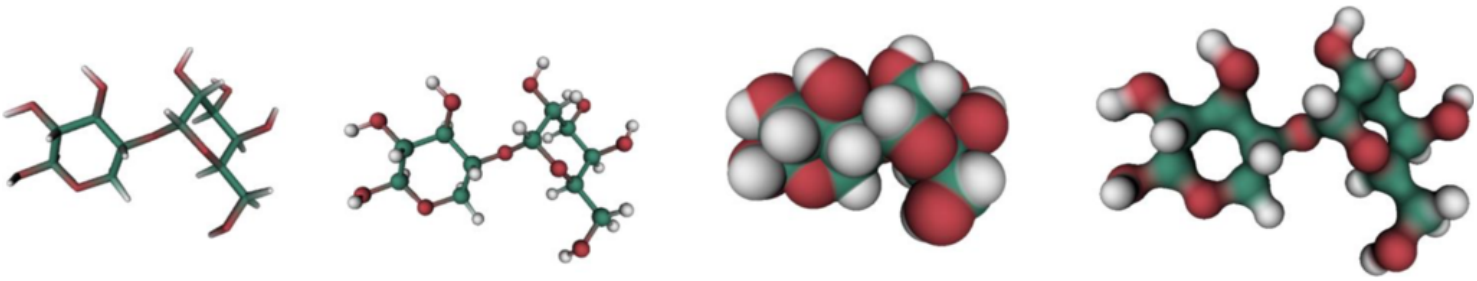


Shrink : to adjust the shape of the bond.

Scale : to adjust the scale of the bond.

DFactor : only for Biological Networks.

Metaphor : pre-configured style (CPK, Licorice, VdW, Smooth Hyperballs)



Above: example rendering of Ball & Sticks, Licorice, VdW, Smooth Hyperballs metaphors

Interactive mode : use spring forces to make an interactive molecule (an atom can be dragged and it will go back to its original position).

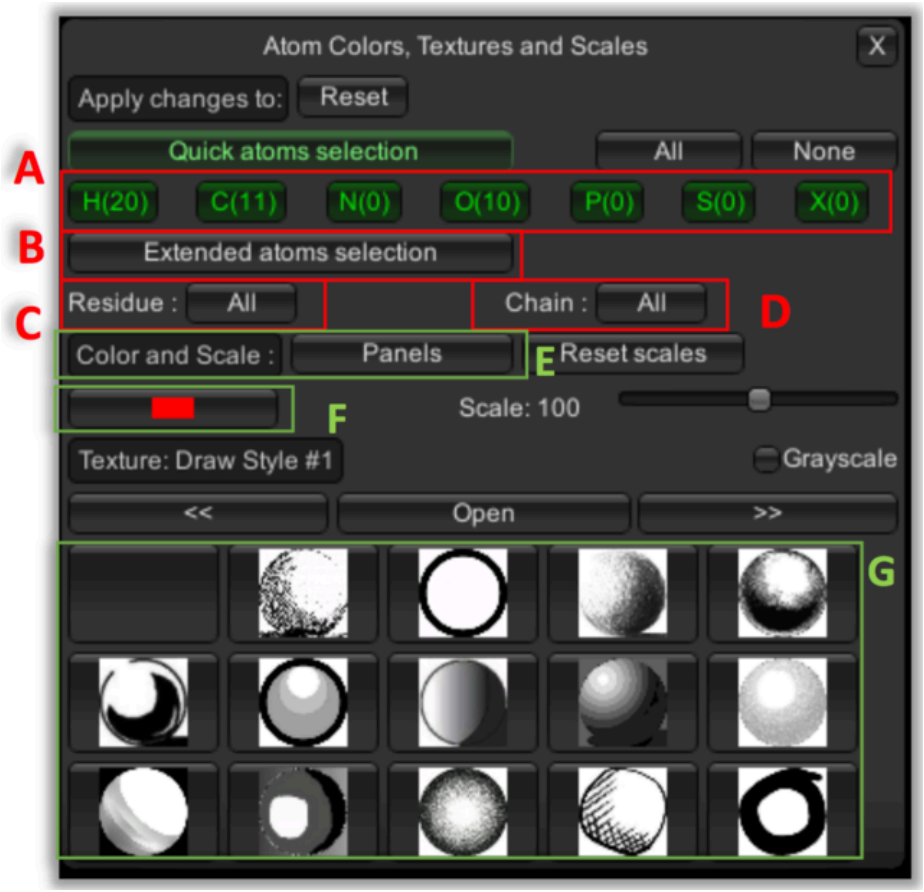
Drag/Spring : spring parameters for interactive mode.

Velocity Colors : colors each atom in interactive mode from white (slow) to black (very fast) based on the velocity of each particle.

Measure dist : activate and click on 2 atoms to display their distance.

Dist. Cueing : adjust the light according to the distance of the camera.

B - Render Menu (4)



The whole molecule is selected by default. The selection can be changed by:

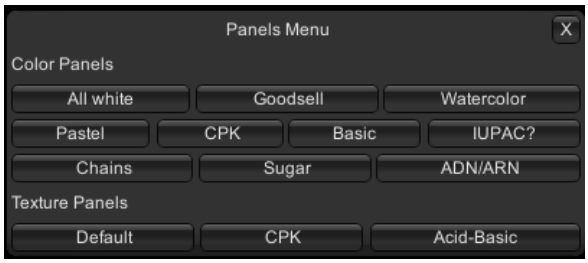
- Atom Type (A)
- Atom name (B)
- Residue name (C)
- By chain (D)

The selection can be combined.

Pre-configured coloration is on the **Panels** menu (E). Another color can be selected by clicking on the Color Button (F).

A texture can be selected and applied to the selection (G). Several textures are available on other pages (you can switch pages by clicking << and >>).

C – Panels Menu (3)



This menu contains pre-configured colors. You can switch by clicking on the buttons.

Color Panels:

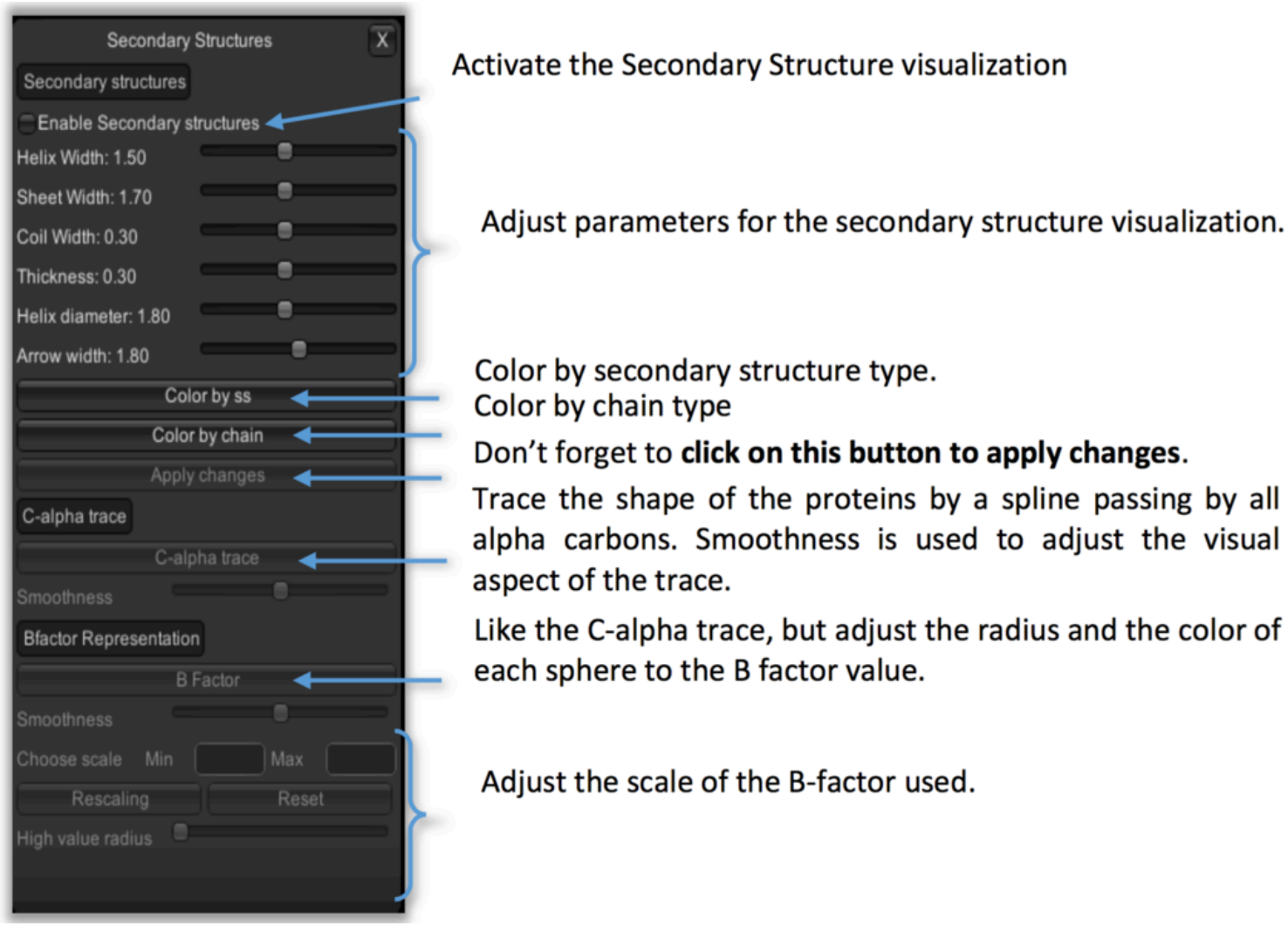
- **All white:** make the molecule all white.
- **Goodsell:** make the color softer.
- **WaterColor:** color carbons in blue.
- **Pastel:** default colors.
- **CPK** : color with the CPK color code.
- **Basic** : color carbon in green.
- **IUPAC** : color with the IUPAC color code.

- **Chains** : color by chain
- **Sugar** : color by sugar Type (the molecule must contain sugar).
- **ADN/ARN** : coloration for DNA and RNA.

Texture Panels:

- **Default** : default texture
- **CPK** : CPK coloration with adapted texture.
- **Acid-Basic** : coloration and texture according to the acid-basic status of amino acids.

3 – Secondary Structures



4 – Surface

T : Density threshold used to generate the iso-surface

Generate : generate the surface.

BFactor : adjust the shape of the surface according to the B-factor value.

Volumetric : show the volumetric space of the protein with a particle system.

Toggle surface : hide surface representation (when you change a parameter, you have to hide the surface and press the *Generate* button again).

HetAtoms / Sugars : show surface for HetAtoms or/and Sugars molecules.

Upon selecting the *Generate* button, the following window will appear.

Color : change the color of the surface (external face).

Inside color : change the inside color.

Use atom color : Color the surface according to the type of atom under each portion of it.

Use chain color : use the color of the chains.

Hydrophobic scale : Color the surface according to different hydrophobic scale of residues.

Use properties color : Color the surface according to the properties of amino acids (basic, acids etc...)

Use BFactor color: Color the surface according to the B-factor value of the surface atoms.

Texture : apply a texture on the surface.

Static cut : cut the surface (you can control the cutting by a pad that will appear in the upper right corner).

Mobile cut : cut the surface and the cut will remain the same upon changing the orientation of the camera.

Brightness : adjust the brightness of the surface

Color weight : adjust the color concentration on the surface.

5 – Electrostat.

To use this menu, the following files have to be in the same folder: the `PDB file` and (with the same name) a file with extension `.dx` and `.apf` generated with softwares such as APBS (a wide-spread software for evaluating the electrostatic properties of biomolecular systems).

Transparency : Add transparency to the mesh generated upon loading the negative and positive electrostatic visualization.

T : Threshold value used to generate the electrostatic isosurface.

Load Neg/Pos : load electrostatic visualization.

Toggle Neg/Pos : show or hide the electrostatic visualization.

Volumetric Fields : volume rendering of the electrostatic fields.

Field Lines : show the Field Lines visualization (examine the local intensity of electric fields).

6 – Display

This menu is made to take screenshots, change the background and add special effects.

Screenshot (or `P` key) : take a screenshot (prefer the `P` key or you will get all menus included with the screen capture).

ScreenShot Sequence : doesn't work yet.

Background : add a picture in the background (switch between yes/no)

White/Gray/Black : quick selection of background color

Background Color : choose your background color with a color panel.

Effects : add special effect.

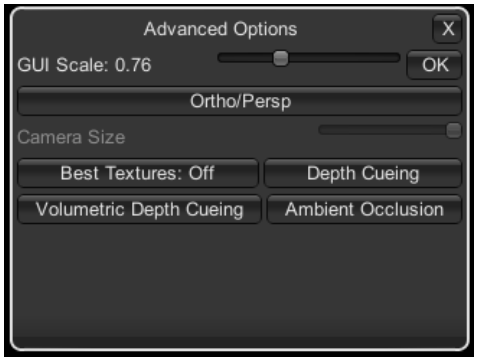
Infos : show/hide FPS info and Atom/Bond number.

List of all visual effects:

- **SSAO** : Screen Space Ambient Occlusion. Works on spheres, cubes, surfaces and secondary structures
- **DOF** : focus on a point and make fuzzy all atoms far away from this point. This effect requires selecting (by clicking) an atom. It works better for large molecules.
- **EDGE** : the edge of every atom is black.
- **CREASE** : add a thick contour to the molecule.
- **SEPIA** : use a SEPIA coloration.
- **GRAYS** : make the molecule black and white.
- **GLOW** : make all atoms shiny.
- **BLUR** : add a blur effect upon moving the camera.
- **NOISE** : add noise on the screen
- **BLUR2** : constant blur.
- **VORTEX** : twist the molecule around the center.
- **TWIRL** : similar to VORTEX

7 – Advanced

This menu offers advanced options (only some are fully implemented and functional).



GUI Scale : change the size of the GUI (buggy).

Orto/Persp : doesn't work fully yet.

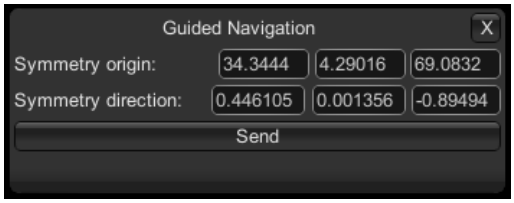
Best Textures : switch between a moderate and large selection of lit sphere textures.

Depth Cueing : doesn't work yet.

Volumectric Depth Cueing: Doesn't work yet.

Ambient Occlusion : darkens the densest parts of the molecule to improve depth perception.

8 – Guided Navigation



This menu is used to enable a "guided navigation" feature, but for now it works only with the pdb `3EI0` (GLIC ion channel) as part of work in progress. See the following paper by Trellet in IEEE VR 2015 for more detail.

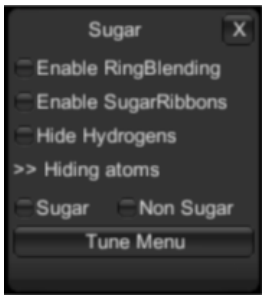
Symmetry origin : X,Y,Z coordinates of the center of symmetry.

Symmetry direction : vector of the symmetry direction.

Send : activate the guided navigation mode.

9 – Sugar

This menu is made to deal with the specific features of sugar visualization (the atomic coordinate file can be generated (pdb format) by several molecular builders, but the *POLYS 2.0* software is the most appropriate). The visualization mode called `Ring Blending` works with all molecules.



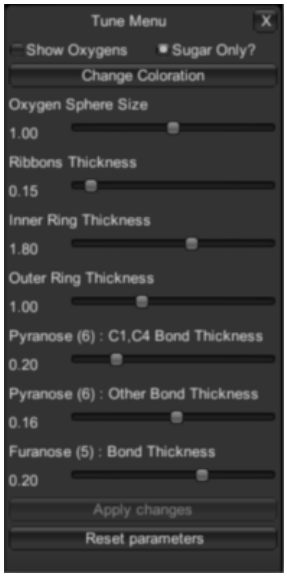
Enable Ring Blending : enable the filling of all rings (aromatic, sugar, or other rings) with a semi-transparent color.

Enable SugarRibbons : enable the **SugarRibbons** visualization (to transform a sugar into a "schematic" representation like secondary structures, but adapted for sugars).

Hide Hydrogens : hide hydrogens atoms. Sugar: hide sugar atoms.

Non Sugar : hide non sugar atoms.

Tune submenu



Show Oxygens : to display the intracyclic oxygen atom as a sphere.

Sugar Only : apply the sugar **Ribbons** visualization only on “sugar residues” (will detect the 3 letter sugar codes in the PDB file. List of recognized 3 letters code is given below).

Change Coloration : open the Color Tune Menu to change color of: sphere, rings and outer ring.

Oxygen Sphere size : To adjust the size of the radius of the sphere.

Ribbons Thickness : to adjust the thickness of the ribbon.

Inner Ring Thickness : to adjust the thickness of the ring.

Outer Ring Thickness : to adjust the thickness of the ring.

Pyranose : to adjust the thickness of the glycosidic bond (for pyranose).

Pyranose : to adjust the thickness of other bonds (for pyranose).

Furanose : to adjust the thickness of bonds for Furanose.

Note

Do not forget to **click on *Apply changes*** to apply the selected new parameters.

Color Tune submenu

For Oxygen Sphere, Outer Rings and Bond:

- **Sugar** : use the sugar color to color Oxygen/Outer Rings or Bonds.
- **Chain** : use the chain color to color Oxygen/Outer Rings or Bonds
- **Custom color** : open a color picker windows to choose a custom color for Oxygen/Outer Rings or Bonds.
- The color can be made darker or lighter with the Light Color Factor slider.

Note

Apply Changes button **not needed** for this feature.

10 – VRPN

This menu is used to connect a **haptic arm**, but a **VRPN** server needs to be installed on the computer. Work in progress.

11 – MDDriver

This menu is meant to visualize a real-time molecular simulation. Work in progress.

12 – Reset

Reset the view.

Key Bindings

Todo:

Verify the key bindings and check against `Edit` > `Project Settings` > `Input`

General

Key to press	Action to carry out
LEFT Arrow – `A`	Move LEFT
RIGHT Arrow – `D`	Move RIGHT
DOWN arrow - `S`	Move DOWN
UP arrow – `W`	Move UP
`Q`	Rotation DOWN
`E`	Rotation UP
`Z`	Rotation LEFT
`X`	Rotation Right
`N`	ZOOM +
`B`	ZOOM –
`P`	Screenshot (only on local pdb; doesn't work yet on fetched PDB)
`BACKSPACE`	Hide GUI
`SPACE`	Automove (rotation right)
`R`	Reset to center
`C`	Center to one or several atoms (select an atom/group with the selection mode first).

Guided Navigation (only for 3EI0)

These controls are only available when `Guided Navigation` mode is activated. The actual version is specific to pentameric channels (especially the PDB file 3EI0).

Constrained navigation

Key to press	Action to carry out
`U`	Enable/Disable automatic Constrained Navigation UP (panoramic mode)
`J`	Enable/Disable automatic Constrained Navigation DOWN (panoramic mode)
UP ARROW - `W`	Constrained Navigation Up
DOWN ARROW - `S`	Constrained Navigation Down
RIGHT ARROW - `D`	move RIGHT
LEFT ARROW - `A`	move LEFT

Spreading

This mode doesn't work for particles and cubes. Second step is only available by fetching PDB 3EI0.

Key to press	Action to carry out
`Numpad +` or `B`	Spreading chains
`Numpad —` or `V`	Narrowing chains
`Numpad \*` or `T`	Reset chains
`L`	Enable/Disable spreading near the structure (active by default)

Panoramic mode

Key to press	Action to carry out
`I`	Enable/Disable panoramic mode
LEFT ARROW - `A`	turn LEFT
RIGHT ARROW - `D`	turn RIGHT
DOWN ARROW - `S`	move DOWN
UP ARROW - `W`	move UP

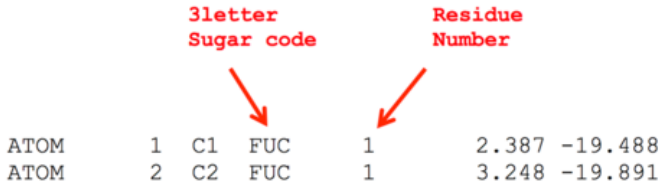
Monomer jump mode

Key to press	Action to carry out
M	Enable/Disable monomer jump mode
LEFT ARROW - `A`	Next monomer on left
RIGHT ARROW - `D`	Next monomer on right

Appendix

Description of the PDB coordinate input file

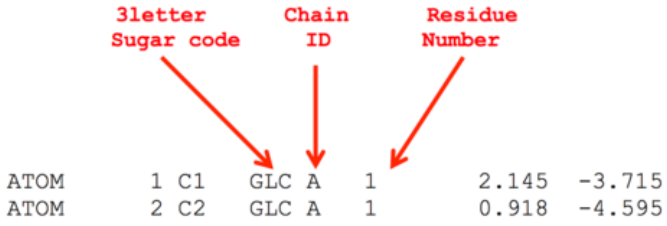
Input File generated by SWEET




```
 1 ATOM      1  C1  FUC     1       2.387 -19.488 -11.522  0.00  0.00  C1
 2 ATOM      2  C2  FUC     1       3.248 -19.891 -12.734  0.00  0.00  C2
 3 ATOM      3  C3  FUC     1       4.696 -19.417 -12.550  0.00  0.00  C3
 4 ATOM      4  C4  FUC     1       5.229 -19.916 -11.196  0.00  0.00  C4
 5 ATOM      5  C5  FUC     1       4.278 -19.476 -10.072  0.00  0.00  C5
 6 ATOM      6  C6  FUC     1       4.703 -19.967  -8.682  0.00  0.00  C6
 7 ATOM      7  OR  FUC     1       2.950 -19.963 -10.295  0.00  0.00 O7
 8 ATOM      8  OW  FUC     1       2.124 -18.089 -11.437  0.00  0.00 O8
 9 ATOM      9  O2H FUC     1       2.615 -19.391 -13.909  0.00  0.00 OH2
10 ATOM     10  O3H FUC     1       5.479 -19.850 -13.659  0.00  0.00 OH3
11 ATOM     11  O4H FUC     1       5.336 -21.339 -11.160  0.00  0.00 OH4
12 ATOM     12  H5  FUC     1       4.272 -18.370 -10.039  0.00  0.00 H5
13 ATOM     13  H1  FUC     1       1.402 -19.965 -11.595  0.00  0.00 H1
14 ATOM     14  H2  FUC     1       3.255 -20.998 -12.784  0.00  0.00 H2
15 ----------------------------------------------------------------------
16 ATOM     23  C1  GAL     2       1.456 -16.523  -9.755  0.00  0.00  C1
17 ATOM     24  C2  GAL     2       1.018 -17.688 -10.638  0.00  0.00  C2
18 ATOM     25  C3  GAL     2      -0.154 -17.316 -11.531  0.00  0.00  C3
19 ATOM     26  C4  GAL     2      -1.262 -16.689 -10.717  0.00  0.00  C4
20 ATOM     27  C5  GAL     2      -0.709 -15.522  -9.900  0.00  0.00  C5
21 ATOM     28  C6  GAL     2      -1.722 -14.822  -9.021  0.00  0.00  C6
22 ----------------------------------------------------------------------
23 ATOM     44  C1  XYL     3       2.801 -16.388  -6.544  0.00  0.00  C1
24 ATOM     45  C2  XYL     3       3.027 -16.035  -8.001  0.00  0.00  C2
25 ATOM     46  C3  XYL     3       4.524 -16.021  -8.286  0.00  0.00  C3
26 ATOM     47  C4  XYL     3       5.231 -15.028  -7.349  0.00  0.00  C4
27 ATOM     48  C5  XYL     3       4.854 -15.404  -5.899  0.00  0.00  C5
28 ----------------------------------------------------------------------
29 ATOM     74  H1  GLC     4       6.312 -20.297  -3.897  0.00  0.00 H1
30 ATOM     75  H2  GLC     4       4.081 -21.295  -1.991  0.00  0.00 H2
31 ATOM     76  H3  GLC     4       4.709 -22.175  -4.882  0.00  0.00 H3
```

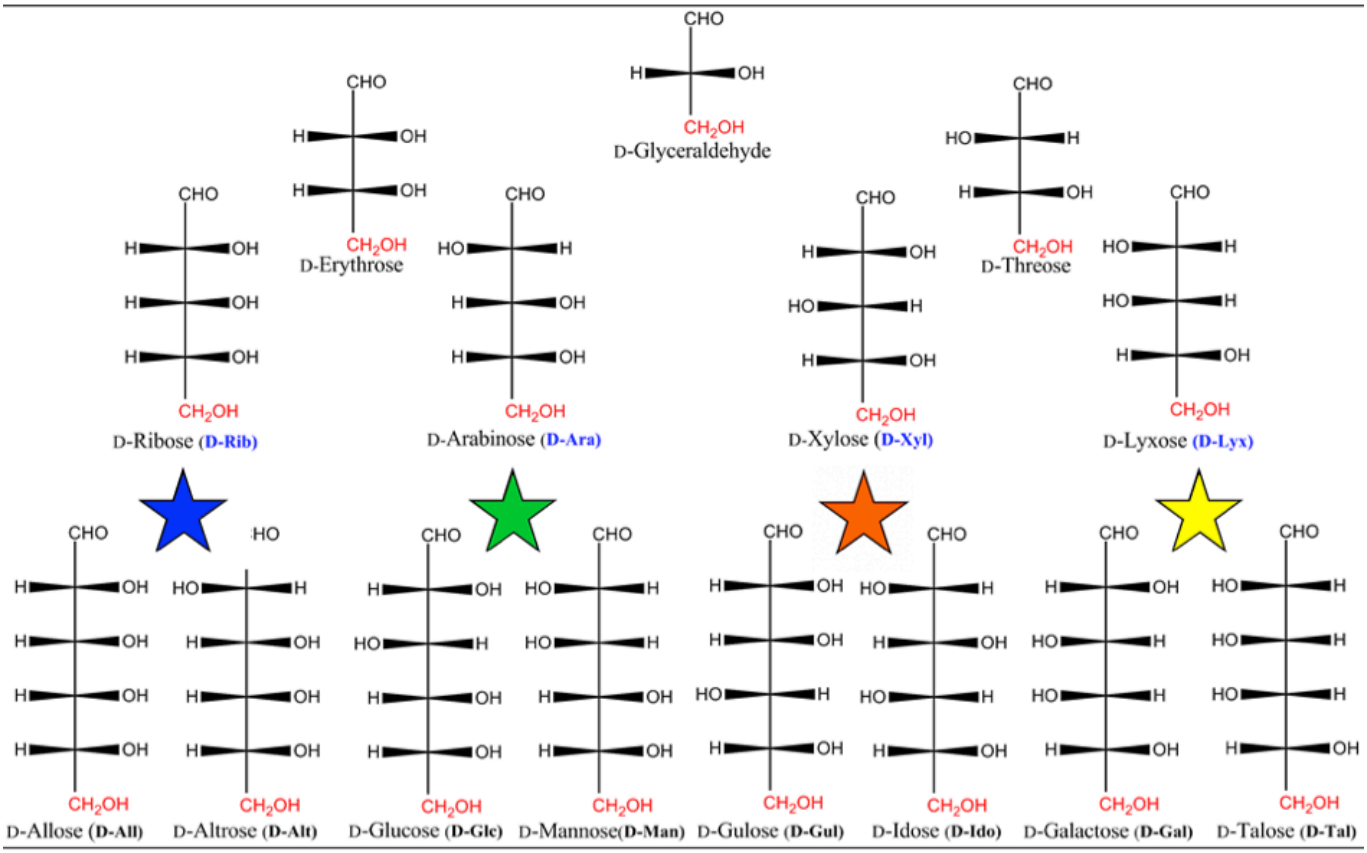
```
ATOM      77  H4  GLC     4       2.240 -20.654  -3.830  0.00  0.00 H4
ATOM      78  H5  GLC     4       4.504 -19.584  -5.636  0.00  0.00 H5
ATOM      79  H6  GLC     4       1.833 -18.619  -5.118  0.00  0.00 H6
ATOM      80  H24 GLC     4       2.931 -17.520  -4.272  0.00  0.00 H24
----------------------------------------------------------------------
ATOM      81  C1  GLC     5       1.057 -21.319  -5.860  0.00  0.00  C1
ATOM      82  C2  GLC     5       0.609 -21.564  -7.318  0.00  0.00  C2
----------------------------------------------------------------------
ATOM     199  C1  GAL    11       5.825 -12.737   3.053  0.00  0.00  C1
ATOM     200  C2  GAL    11       4.966 -12.753   1.793  0.00  0.00  C2
ATOM     201  C3  GAL    11       3.486 -12.876   2.114  0.00  0.00  C3
ATOM     202  C4  GAL    11       3.243 -14.031   3.058  0.00  0.00  C4
ATOM     203  C5  GAL    11       4.137 -13.890   4.291  0.00  0.00  C5
ATOM     204  C6  GAL    11       4.003 -15.003   5.307  0.00  0.00  C6
----------------------------------------------------------------------
ATOM     255  H5  XYL    13      19.537 -11.651  -0.139  0.00  0.00 H5
ATOM     256  H1  XYL    13      16.585 -11.560  -2.329  0.00  0.00 H1
ATOM     257  H2  XYL    13      18.338 -12.051  -3.974  0.00  0.00 H2
ATOM     258  H3  XYL    13      19.481 -13.841  -1.798  0.00  0.00 H3
ATOM     259  H4  XYL    13      20.596 -11.287  -3.032  0.00  0.00 H4
TER
```

Input File generated by POLYS (Starch Double Helical Structure)




```
ATOM      1 C1   GLC A   1       2.145  -3.715   3.129  1.00  0.00
ATOM      2 C2   GLC A   1       0.918  -4.595   2.908  1.00  0.00
ATOM      3 C3   GLC A   1      -0.334  -3.978   3.523  1.00  0.00
ATOM      4 C4   GLC A   1      -0.058  -3.703   4.999  1.00  0.00
ATOM      5 C5   GLC A   1       1.189  -2.828   5.142  1.00  0.00
ATOM      6 C6   GLC A   1       1.589  -2.597   6.600  1.00  0.00
ATOM      7 O1   GLC A   1       1.983  -2.496   2.397  1.00  0.00
ATOM      8 O2   GLC A   1       0.715  -4.752   1.496  1.00  0.00
---------------------------------------------------------------------
ATOM    214 C1   GLC B  11      -3.715   2.145   1.564  1.00  0.00
ATOM    215 C2   GLC B  11      -3.093   3.520   1.344  1.00  0.00
ATOM    216 C3   GLC B  11      -1.699   3.613   1.959  1.00  0.00
ATOM    217 C4   GLC B  11      -1.801   3.236   3.434  1.00  0.00
ATOM    218 C5   GLC B  11      -2.444   1.855   3.577  1.00  0.00
ATOM    219 C6   GLC B  11      -2.675   1.455   5.035  1.00  0.00
ATOM    220 O1   GLC B  11      -2.965   1.171   0.832  1.00  0.00
ATOM    221 O2   GLC B  11      -2.995   3.758  -0.068  1.00  0.00
ATOM    222 O3   GLC B  11      -1.264   4.978   1.894  1.00  0.00
```

Sugar ring color code for monosaccharides



White (Generic)	Blue	Green	Yellow	Orange	Pink	Purple	Light Blue	Brown	Red
Hexose	Glc	Man	Gal	Gul	Alt	All	Tal	Ido	
HexNAc	GlcNAc	ManNAc	GalNAc	GulNAc	AltNAc	AllNAc	TalNAc	IdoNAc	
Hexosamine	GlcN	ManN	GalN	GulN	AltN	AllN	TalN	IdoN	
Hexuronate	GlcA	ManA	GalA	GulA	AltA	AllA	TalA	IdoA	
Deoxyhexose	Qui	Rha			6dAlt		6dTal		Fuc
DeoxyhexNAc	QuiNAc	RhaNAc							FucNAc
Di-deoxyhexose	Oli	Tyv		Abe	Par	Dig	Col		
Pentose		Ara	Lyx	Xyl	Rib				
Nonulosonate		Kdn				Neu5Ac	Neu5Gc	Neu	
Unknown	Bac	LDManHep	Kdo	Dha	DDManHep	MurNAc	MurNGc	Mur	
Assigned	Api	Fru	Tag	Sor	Psi				

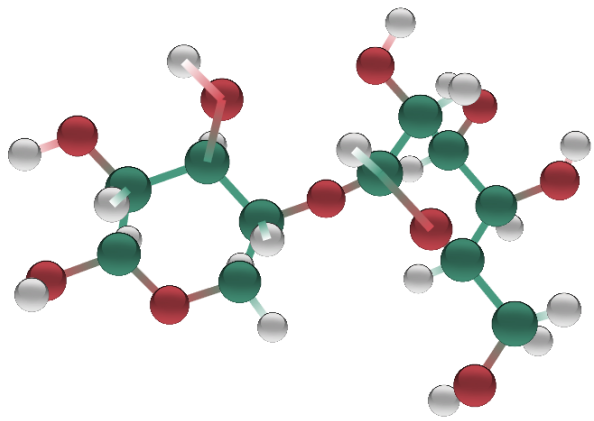
Color code for monosaccharides table

3 letter code	Colour	3 letter code	Colour
6DAL	Pink	**LDM**	Green
6DTA	Light Blue	**LYX**	Yellow
ABE	Orange	**M5A**	Purple
ALL	Purple	**M5C**	Light Blue
ALT	Pink	**MAN**	Green
API	Blue	**MUR**	Bown
ARA	Green	**N5G**	Light Blue
BAC	Blue	**NEU**	Brown
COL	Light Blue	**OLI**	Blue
DDM	Pink	**PAR**	Pink
DHA	Orage	**PSI**	Pink
DIG	Purple	**QUI**	Blue
FRU	Green	**RHA**	Green
FUC	Red	**RIB**	Pink
GAL	Yellow	**SIA**	Purple
GLC	Blue	**SOR**	Orange
GUL	Orange	**TAL**	Light Blue
IDO	Brown	**TYV**	Green
KDN	Green	**XYL**	Orange
KDO	Yellow	-	-
-	-	-	-
3 letter code	**Colour**	**3 letter code**	**Colour**
BLU	Blue	**PUR**	Purple
GRE	Green	**LBL**	Light Blue
YEL	Yellow	**BRO**	Brown
ORA	Orange	**RED**	Red
PIN	Pink	**GRE**	Grey

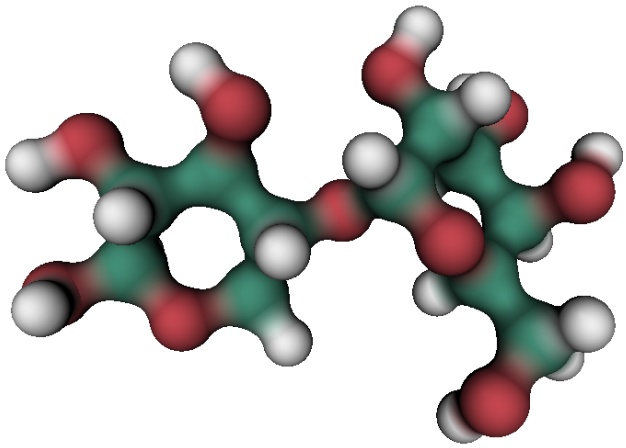
Examples

This section features screenshots of various representations available in UnityMol.

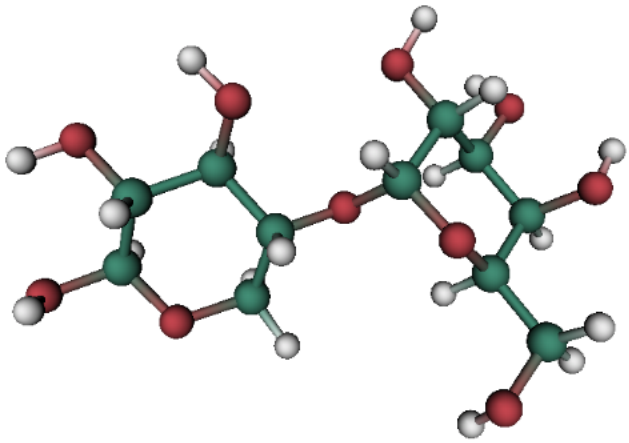
Particles mode



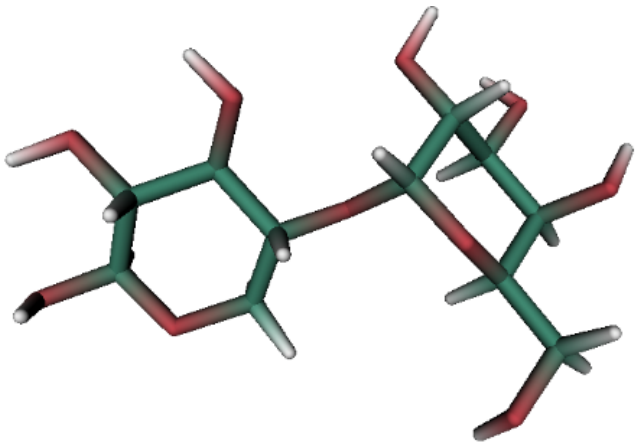
Smooth HyperBalls mode



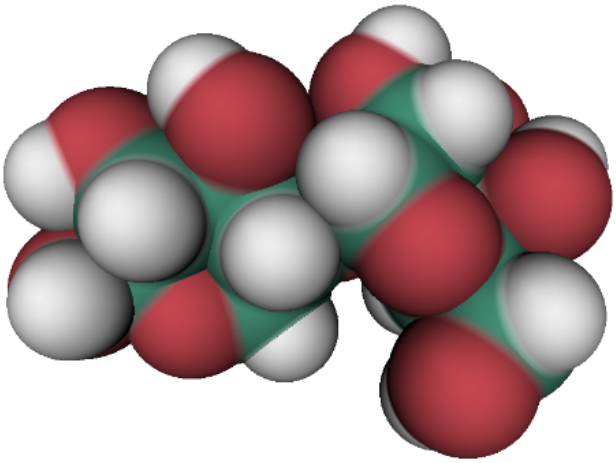
Default Smooth HyperBalls mode



CPK mode

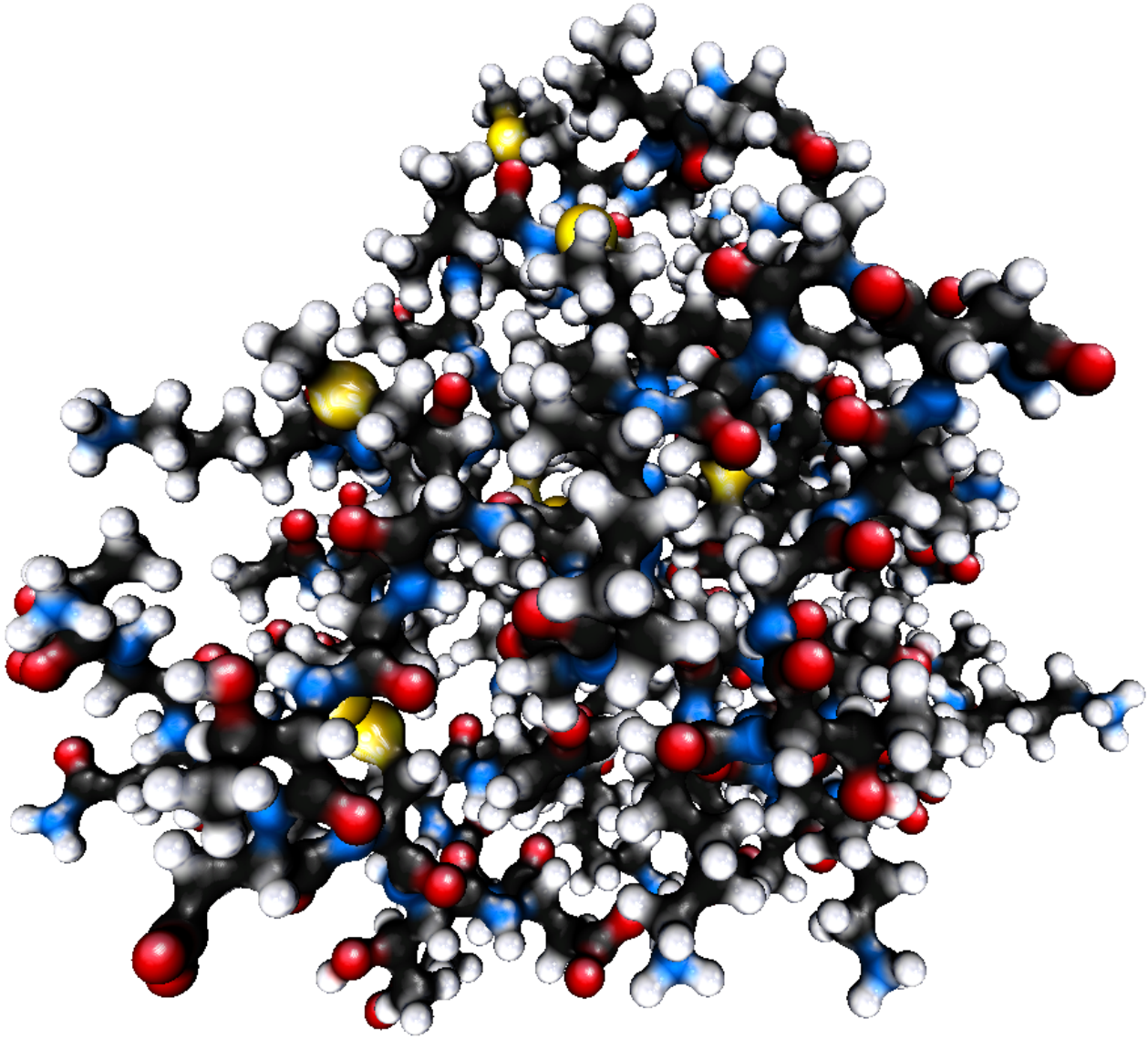


Licorice

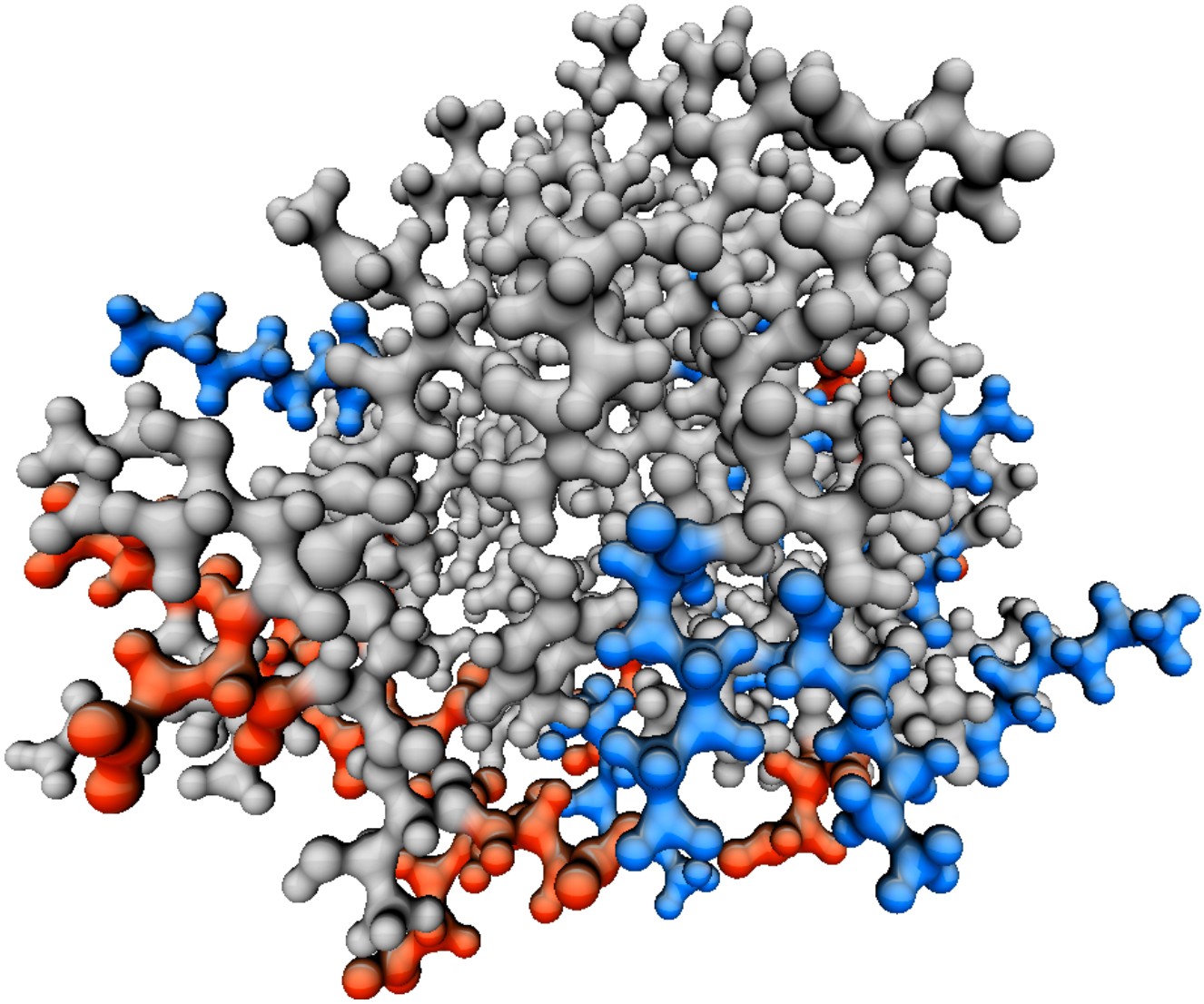


VDW

Texture sets

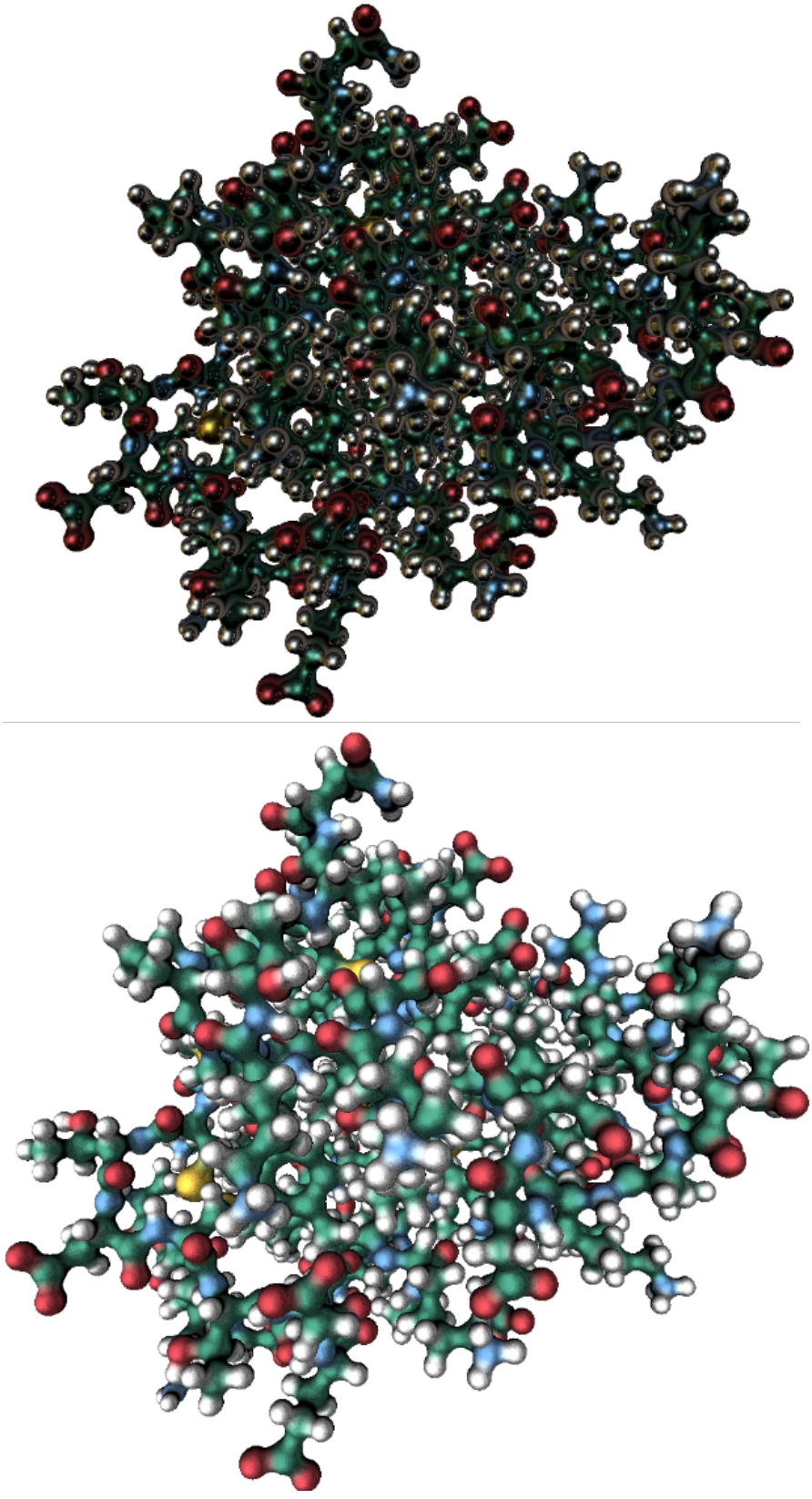


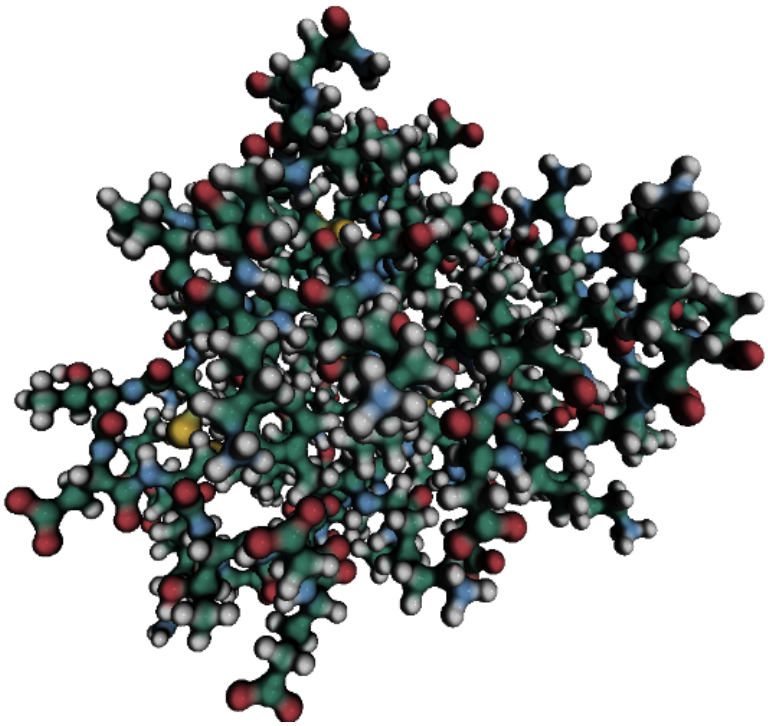
CPK



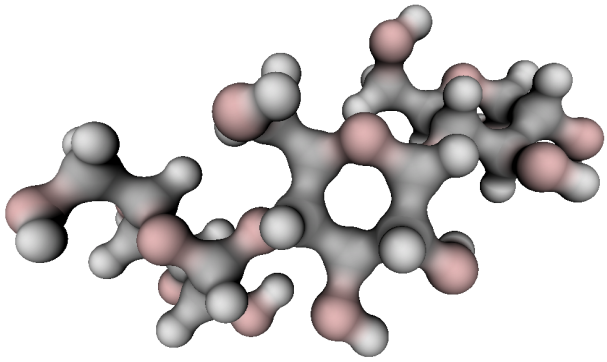
Acid-Basic

Other examples (Renderer Menu)

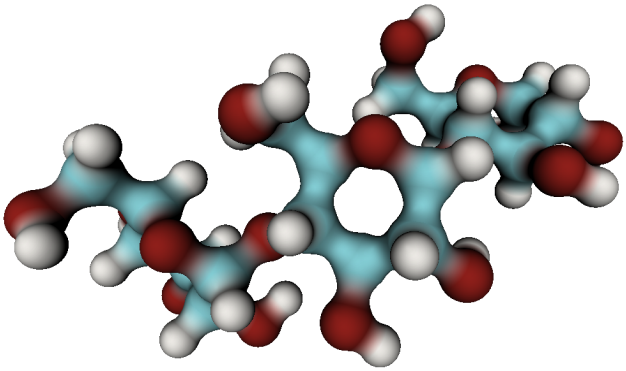




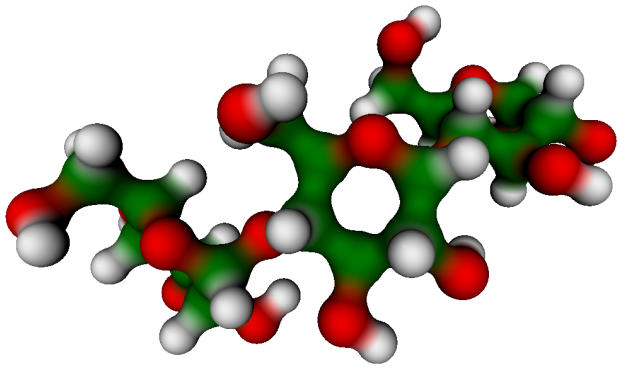
Coloration Mode



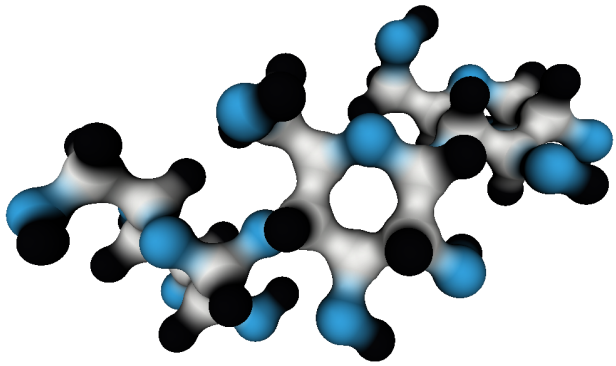
GoodSell



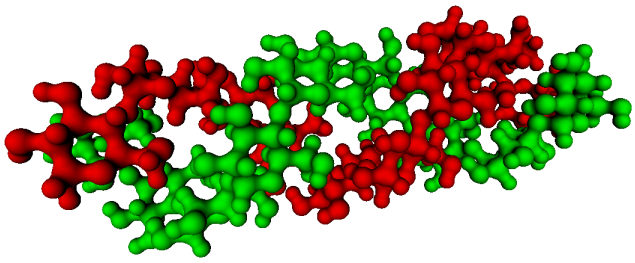
WaterColor



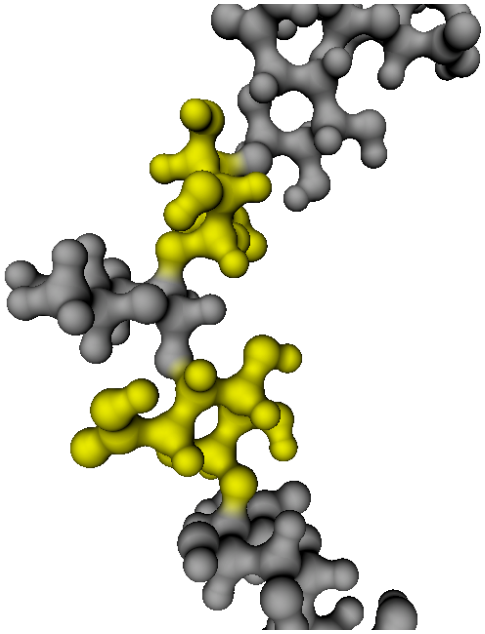
Basic



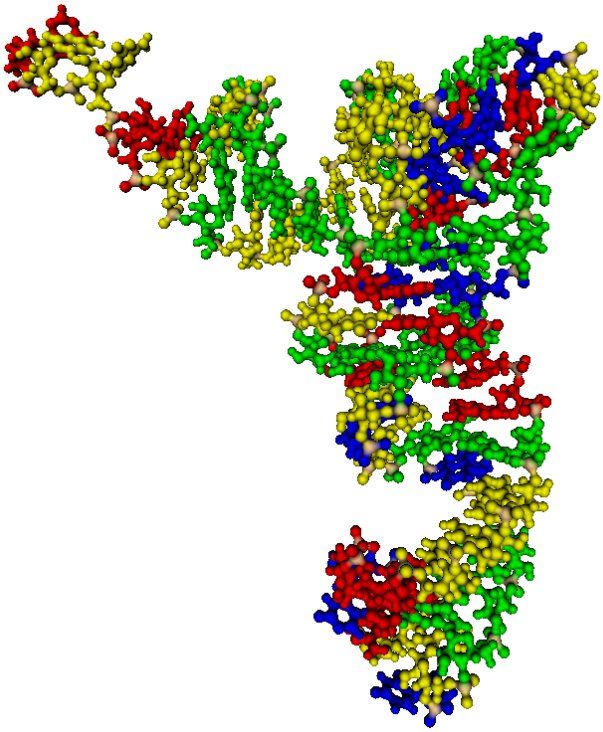
IUPAC



Chain



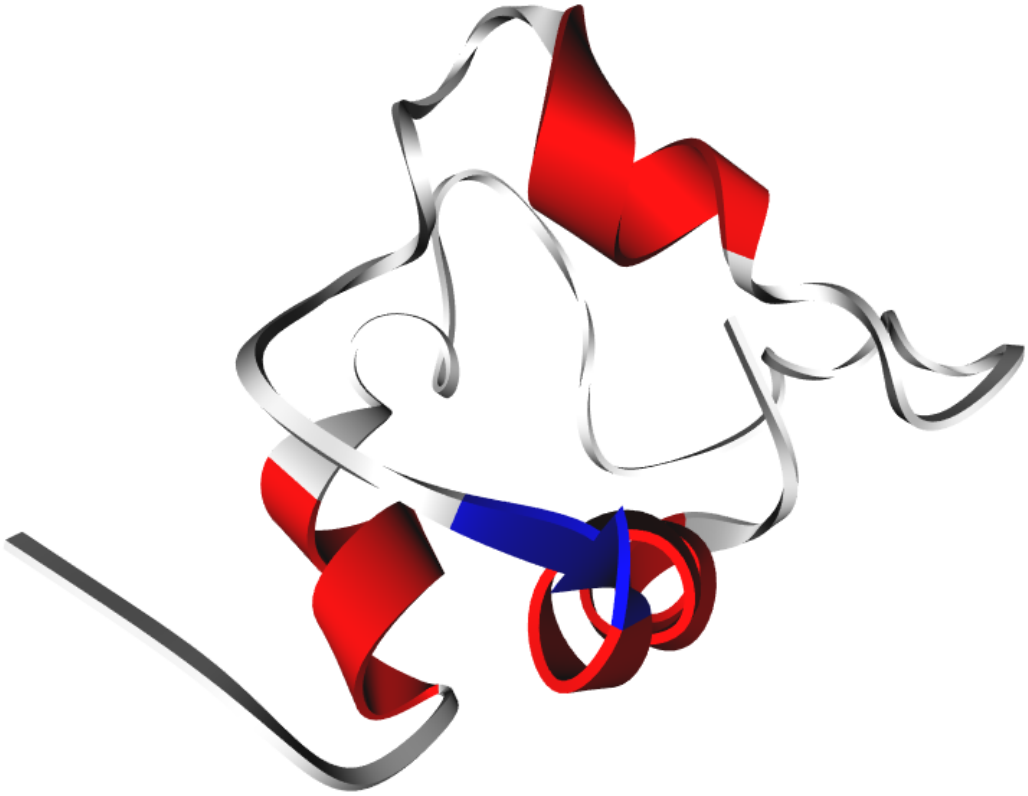
Sugar



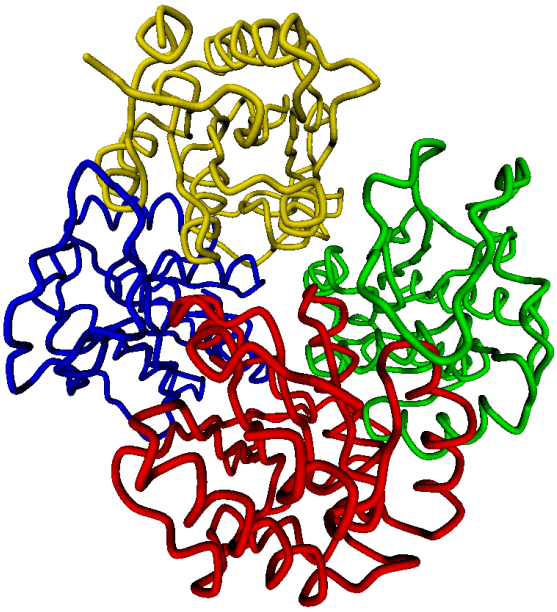
DNA/RNA

Secondary Structure Menu

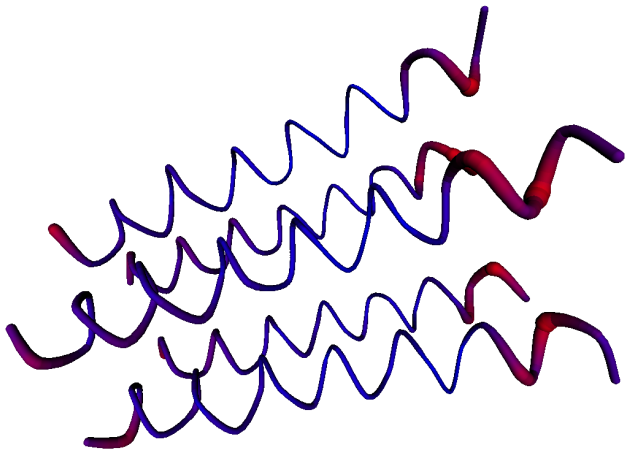
Secondary Structure



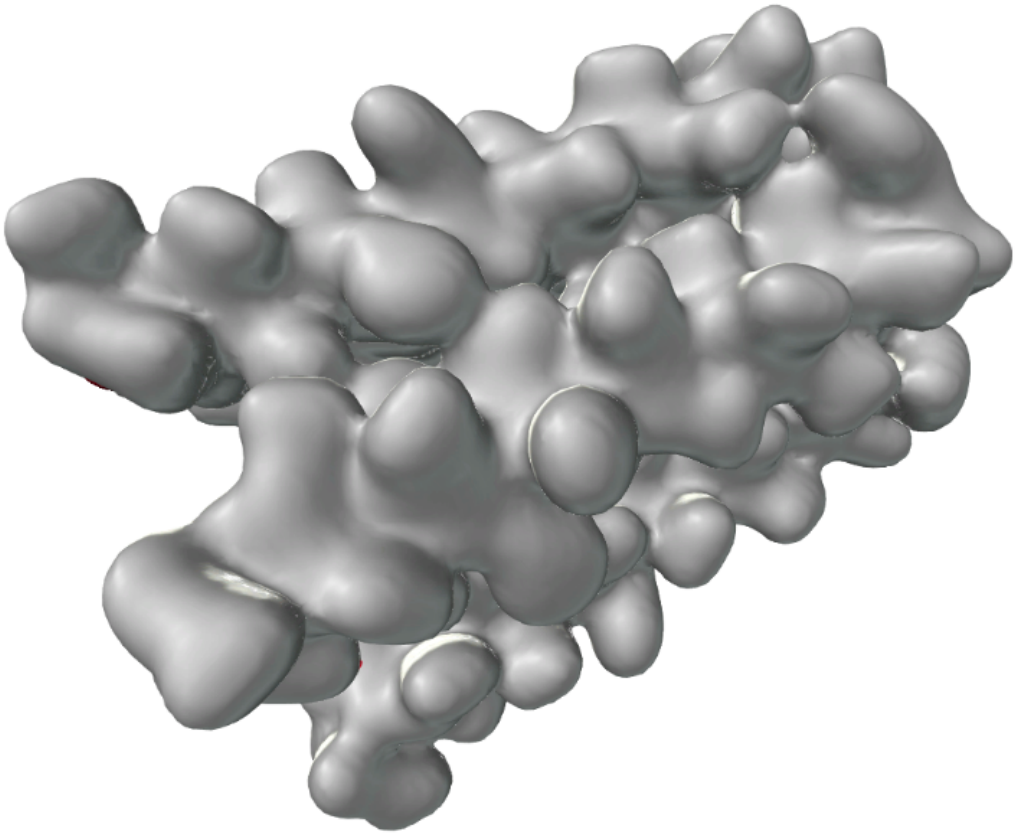
Ca-Trace



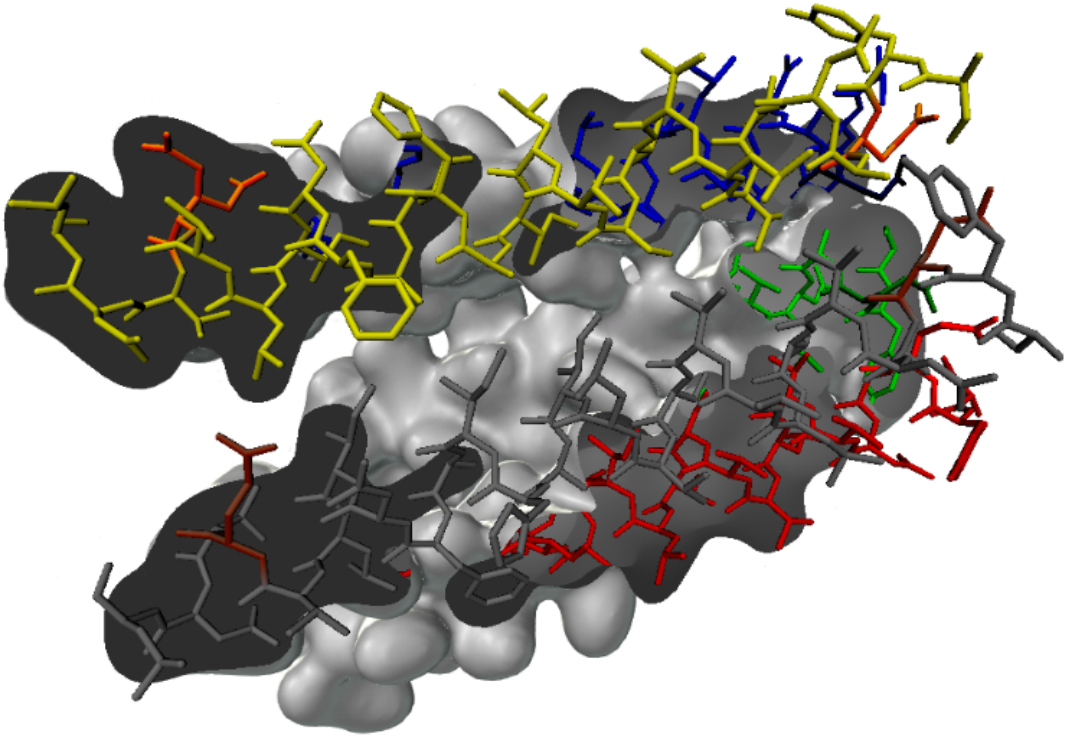
B-factor



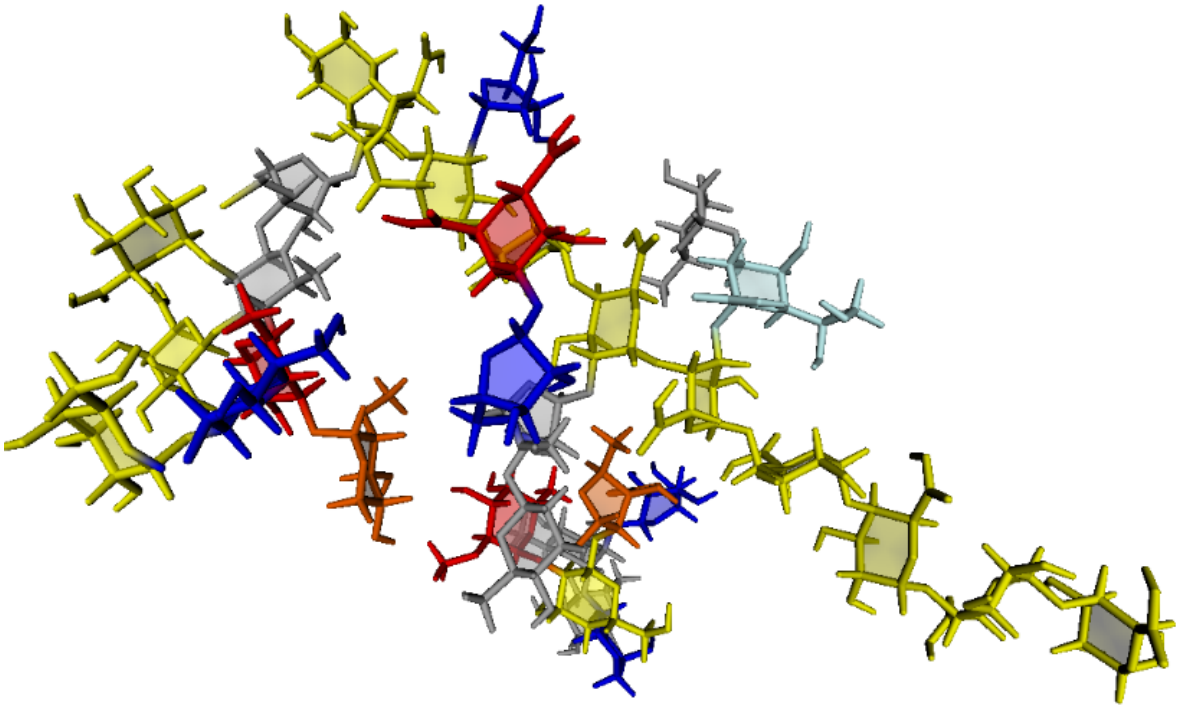
Surface Mode



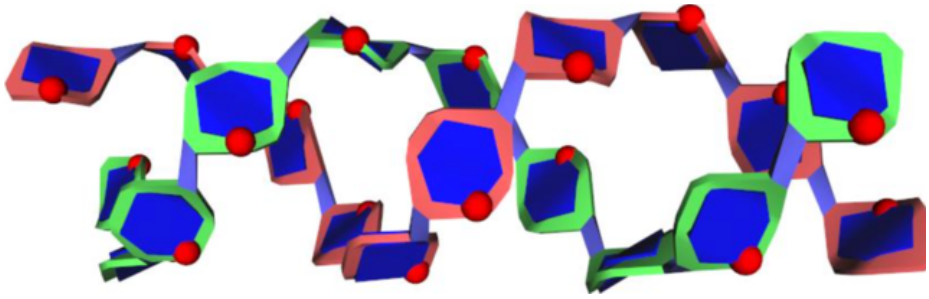
Surface with static/mobile Cut



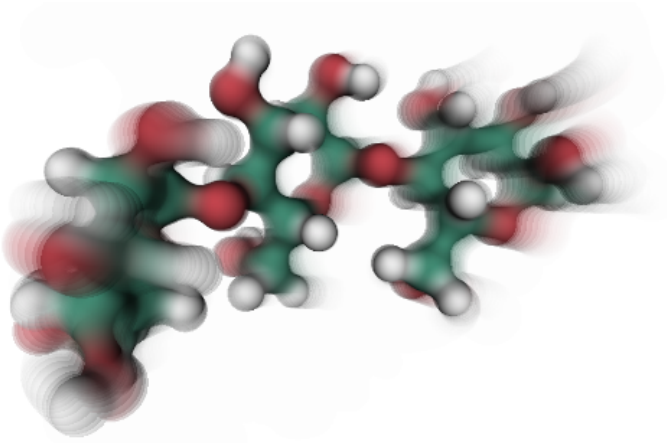
Ring blending (with sugar coloration)



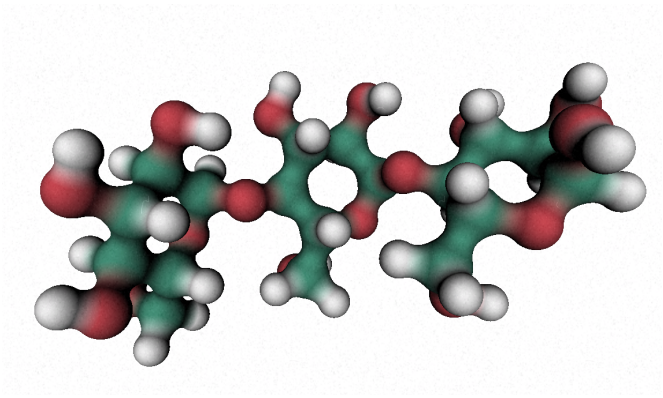
SugarRibbons



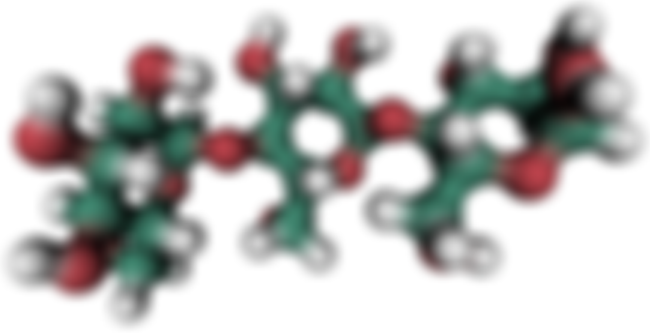
Special Effect



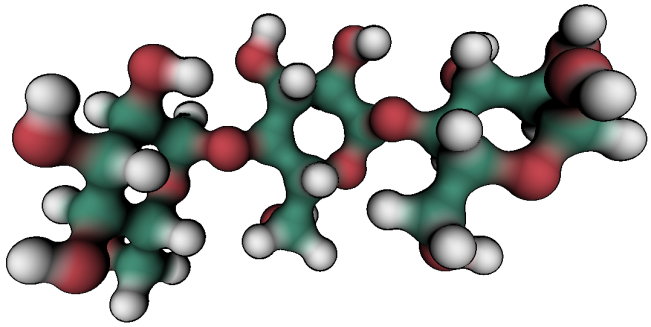
BLUR



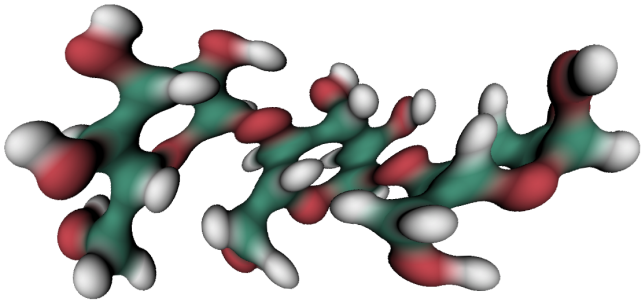
NOISE



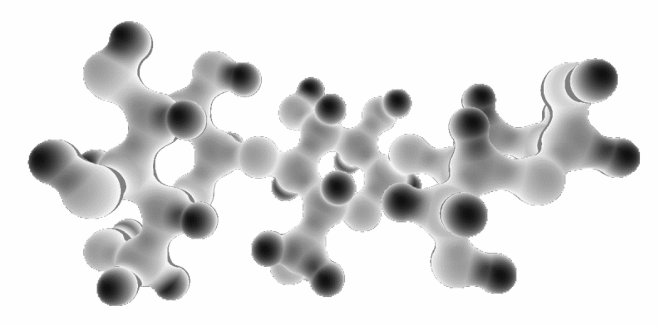
BLUR2



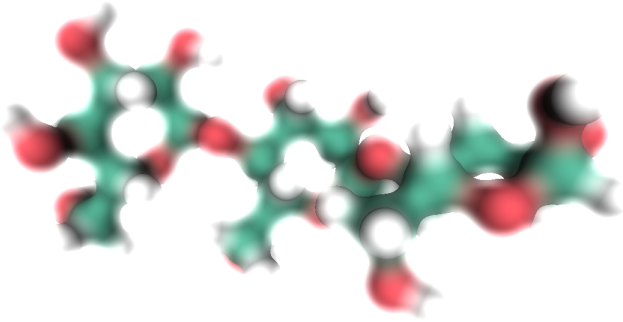
EDGE



VORTEX

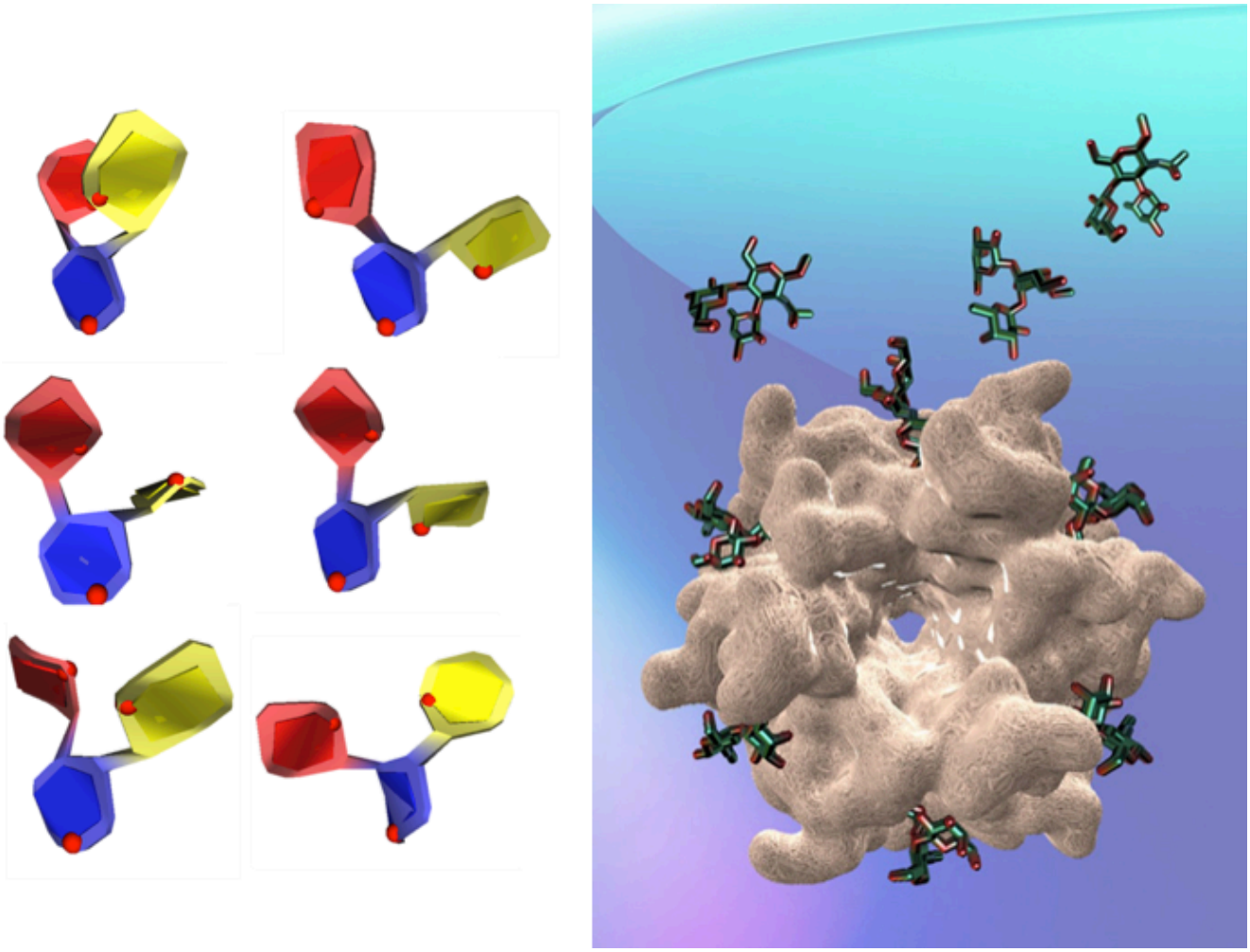


GRAY

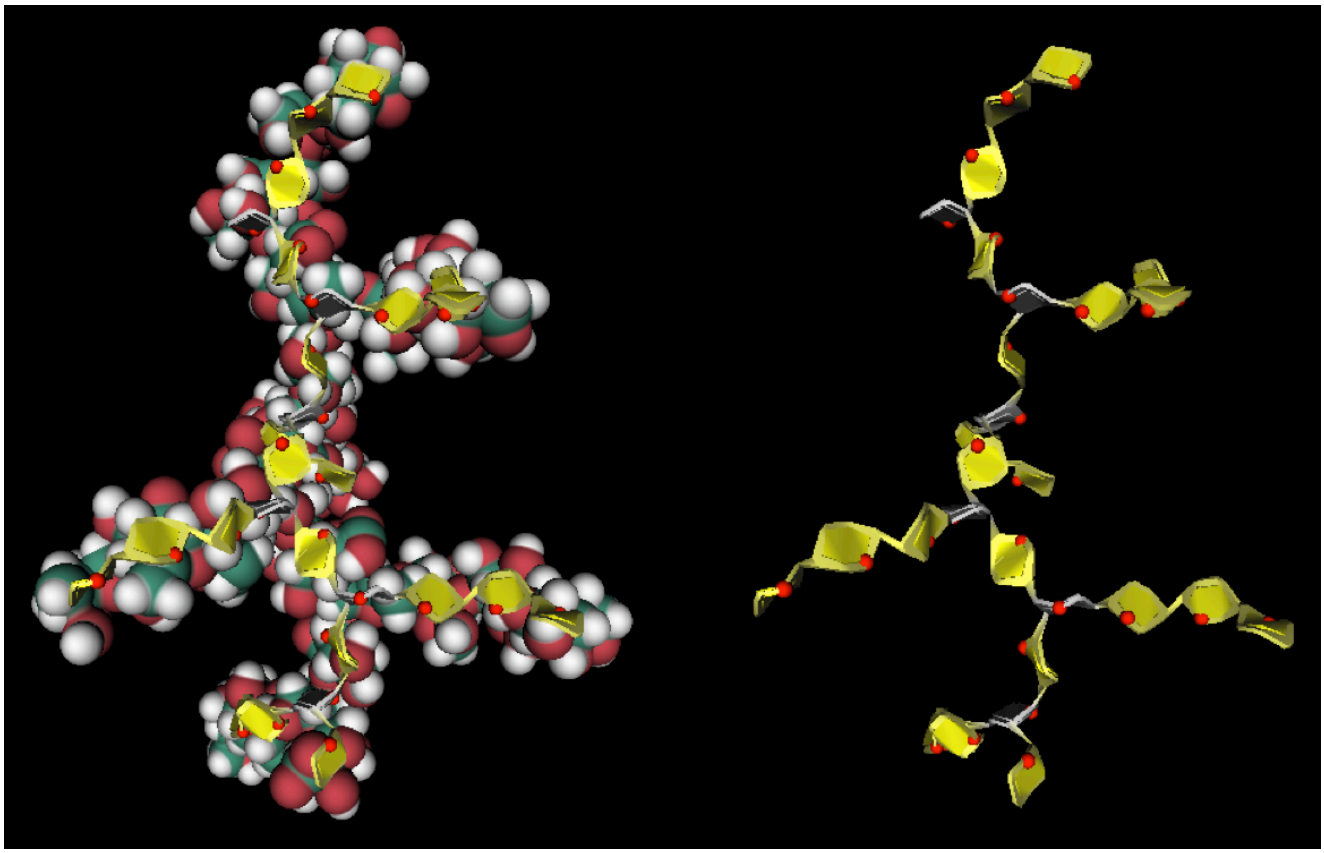


GLOW

Miscellaneous



"Coarse grain" representation of six low energy conformations of LewisX trisaccharide and its interaction with a lectin.



Three modes of graphical representation of a complex plant polysaccharide, making use of some of the options offered by SweetUnityMol.